



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 08:23 PM JST

PDB ID : 9WXP / pdb_00009wpx
EMDB ID : EMD-66353
Title : cryo-EM structure of a mammalian collagen fibril
Authors : Lou, X.; Cong, Y.; Xu, Y.; Yan, C.
Deposited on : 2025-09-25
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
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) : 2.50

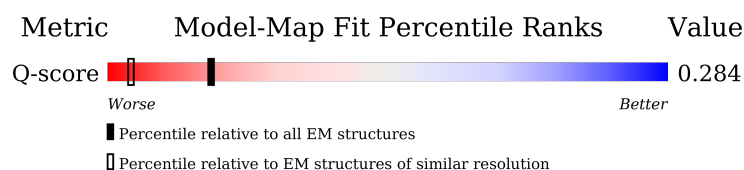
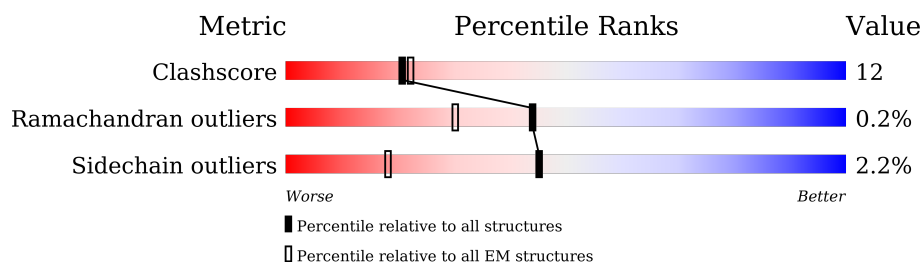
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.



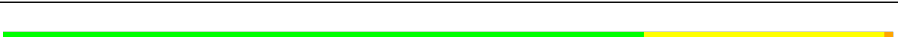
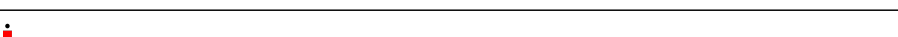
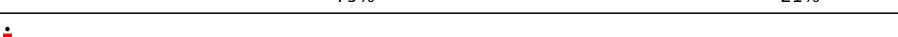
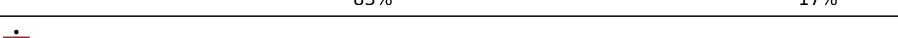
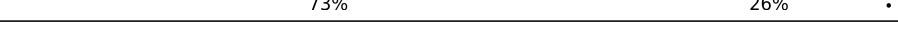
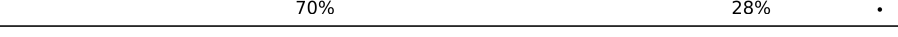
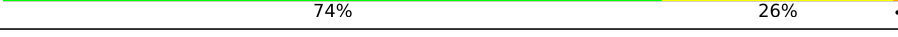
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	AA	246	
1	FA	246	
1	KA	246	
1	PA	246	

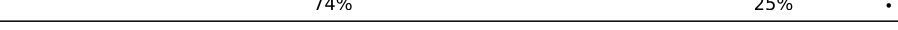
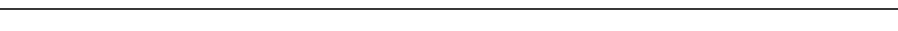
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	BA	233	 76%22%
2	GA	233	 76%22%
2	LA	233	 77%21%
2	QA	233	 76%23%
3	CA	234	 79%20%
3	HA	234	 78%21%
3	MA	234	 78%21%
3	RA	234	 76%22%
4	DA	237	 74%25%
4	IA	237	 73%27%
4	NA	237	 72%27%
4	SA	237	 74%25%
5	EA	77	 83%17%
5	JA	77	 79%21%
5	OA	77	 83%17%
5	TA	77	 82%18%
6	AC	246	 73%26%
6	FC	246	 73%26%
6	KC	246	 70%28%
6	PC	246	 74%26%
7	BC	233	 76%24%
7	GC	233	 78%21%
7	LC	233	 76%23%
7	QC	233	 76%23%
8	CC	235	 84%15%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
8	HC	235		84% 14% .
8	MC	235		83% 16% .
8	RC	235		82% 16% .
9	DC	236		77% 23%
9	IC	236		78% 22%
9	NC	236		77% 23%
9	SC	236		77% 23%
10	EC	76		82% 17% .
10	JC	76		79% 20% .
10	OC	76		80% 18% .
10	TC	76		80% 18% .
11	AB	231		75% 24% .
11	FB	231		74% 26% .
11	KB	231		74% 25% .
11	PB	231		74% 25% .
12	BB	233		76% 23%
12	GB	233		77% 23%
12	LB	233		76% 23% .
12	QB	233		77% 22%
13	CB	234		79% 18% .
13	HB	234		79% 18% .
13	MB	234		79% 18% .
13	RB	234		80% 17% .
14	DB	237		79% 21%
14	IB	237		78% 21%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
14	NB	237	
14	SB	237	
15	EB	76	
15	JB	76	
15	OB	76	
15	TB	76	
16	AD	169	
16	AE	169	
16	AF	169	
16	AG	169	
16	AH	169	
16	AI	169	
16	FD	169	
16	FE	169	
16	FF	169	
16	FG	169	
16	FH	169	
16	FI	169	
16	KD	169	
16	KE	169	
16	KF	169	
16	KG	169	
16	KH	169	
16	KI	169	
16	PD	169	

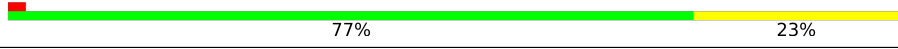
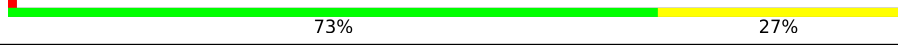
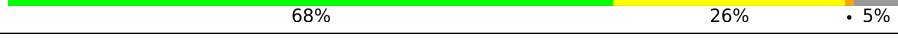
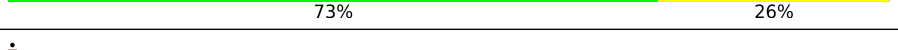
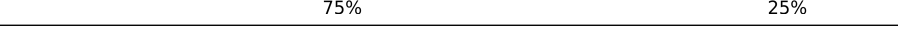
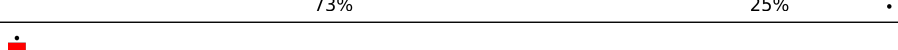
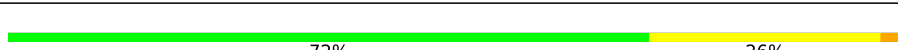
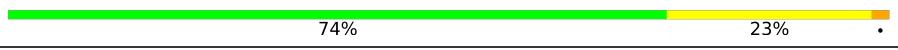
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
16	PE	169	
16	PF	169	
16	PG	169	
16	PH	169	
16	PI	169	
17	BD	248	
17	BE	248	
17	BF	248	
17	BG	248	
17	BH	248	
17	BI	248	
17	GD	248	
17	GE	248	
17	GF	248	
17	GG	248	
17	GH	248	
17	GI	248	
17	LD	248	
17	LE	248	
17	LF	248	
17	LG	248	
17	LH	248	
17	LI	248	
17	QD	248	
17	QE	248	

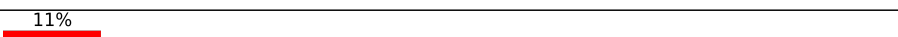
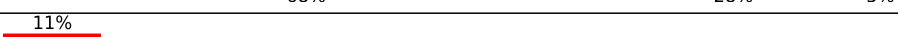
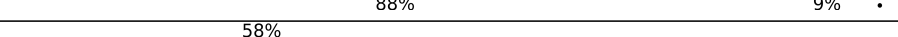
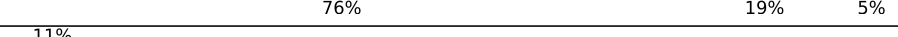
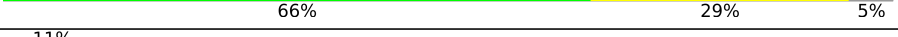
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	QF	248	
17	QG	248	
17	QH	248	
17	QI	248	
18	CD	223	
18	CE	223	
18	CF	223	
18	CG	223	
18	CH	223	
18	CI	223	
18	HD	223	
18	HE	223	
18	HF	223	
18	HG	223	
18	HH	223	
18	HI	223	
18	MD	223	
18	ME	223	
18	MF	223	
18	MG	223	
18	MH	223	
18	MI	223	
18	RD	223	
18	RE	223	
18	RF	223	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	RG	223	
18	RH	223	
18	RI	223	
19	DD	237	
19	DE	237	
19	DF	237	
19	DG	237	
19	DH	237	
19	DI	237	
19	ID	237	
19	IE	237	
19	IF	237	
19	IG	237	
19	IH	237	
19	II	237	
19	ND	237	
19	NE	237	
19	NF	237	
19	NG	237	
19	NH	237	
19	NI	237	
19	SD	237	
19	SE	237	
19	SF	237	
19	SG	237	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
19	SH	237	
19	SI	237	
20	ED	162	
20	EE	162	
20	EF	162	
20	EG	162	
20	EH	162	
20	EI	162	
20	JD	162	
20	JE	162	
20	JF	162	
20	JG	162	
20	JH	162	
20	JI	162	
20	OD	162	
20	OE	162	
20	OF	162	
20	OG	162	
20	OH	162	
20	OI	162	
20	TD	162	
20	TE	162	
20	TF	162	
20	TG	162	
20	TH	162	

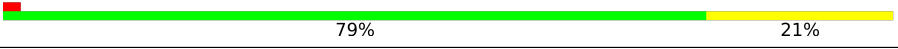
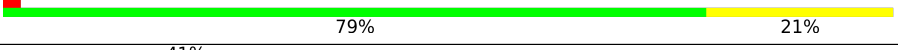
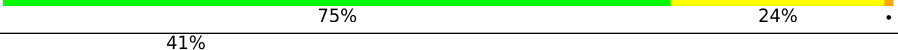
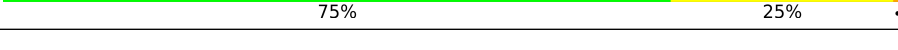
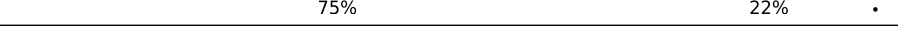
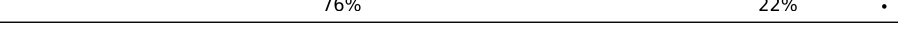
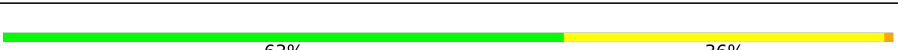
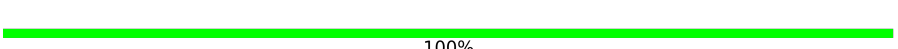
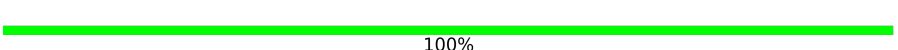
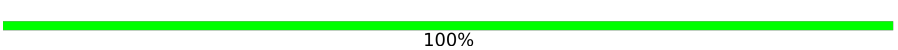
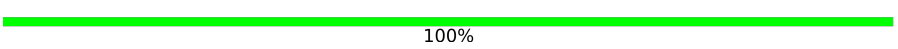
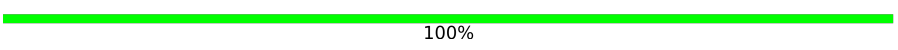
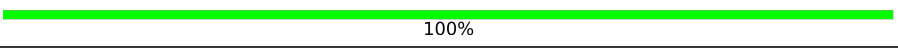
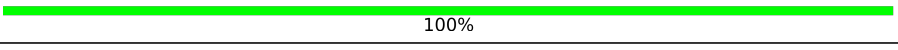
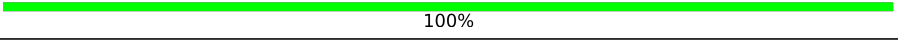
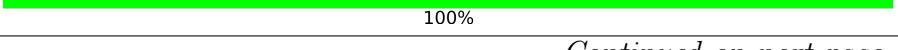
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
20	TI	162	
21	AJ	58	
21	DJ	58	
21	GJ	58	
21	JJ	58	
22	BJ	231	
22	EJ	231	
22	HJ	231	
22	KJ	231	
23	CJ	171	
23	FJ	171	
23	IJ	171	
23	LJ	171	
24	AK	58	
24	DK	58	
24	GK	58	
24	JK	58	
25	BK	232	
25	EK	232	
25	HK	232	
25	KK	232	
26	CK	170	
26	FK	170	
26	IK	170	
26	LK	170	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
27	AL	58	
27	DL	58	
27	GL	58	
27	JL	58	
28	BL	232	
28	EL	232	
28	HL	232	
28	KL	232	
29	CL	170	
29	FL	170	
29	IL	170	
29	LL	170	
30	AM	210	
30	BM	210	
30	CM	210	
30	DM	210	
31	Aa	2	
31	Ab	2	
31	Ac	2	
31	Ad	2	
31	Ae	2	
31	Af	2	
31	Ag	2	
31	Ah	2	
31	Ai	2	

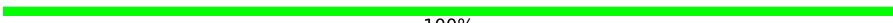
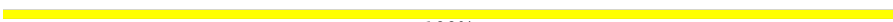
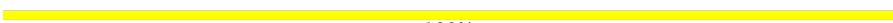
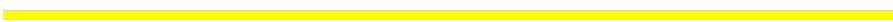
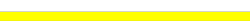
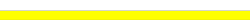
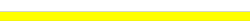
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Aj	2	 100%
31	Ak	2	 100%
31	Al	2	 100%
31	Ba	2	 50% 50%
31	Bb	2	 50% 50%
31	Bc	2	 50% 50%
31	Bd	2	 50% 50%
31	Be	2	 50% 50%
31	Bf	2	 50% 50%
31	Bg	2	 50% 50%
31	Bh	2	 50% 50%
31	Bi	2	 100%
31	Bj	2	 100%
31	Bk	2	 100%
31	Bl	2	 100%
31	Ca	2	 100%
31	Cb	2	 100%
31	Cc	2	 100%
31	Cd	2	 100%
31	Ce	2	 100%
31	Cf	2	 100%
31	Cg	2	 100%
31	Ch	2	 100%
31	Ci	2	 100%
31	Cj	2	 100%

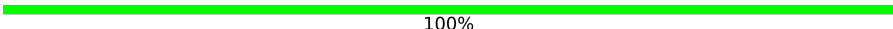
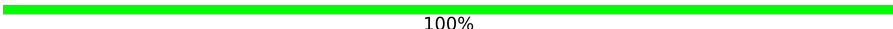
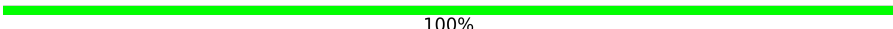
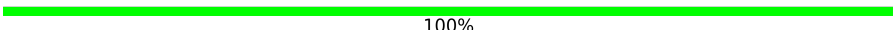
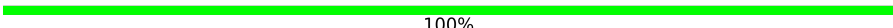
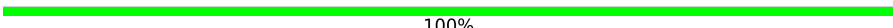
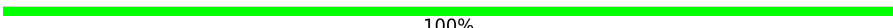
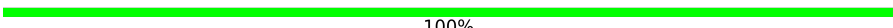
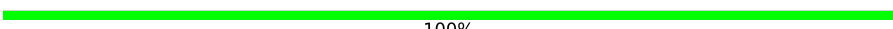
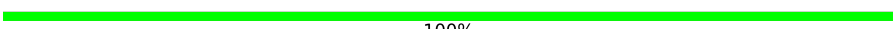
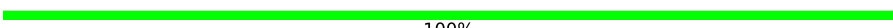
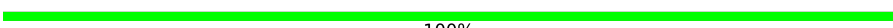
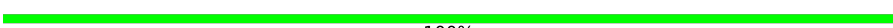
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Ck	2	 100%
31	Cl	2	 100%
31	De	2	 100%
31	Df	2	 100%
31	Dg	2	 100%
31	Dh	2	 100%
31	Di	2	 100%
31	Dj	2	 100%
31	Dk	2	 100%
31	Dl	2	 100%
31	Ea	2	 100%
31	Eb	2	 100%
31	Ec	2	 100%
31	Ed	2	 100%
31	Ee	2	 50%  50%
31	Ef	2	 50%  50%
31	Eg	2	 50%  50%
31	Eh	2	 50%  50%
31	Fi	2	 100%
31	Fj	2	 100%
31	Fk	2	 100%
31	Fl	2	 100%
31	Ga	2	 50%  50%
31	Gb	2	 50%  50%
31	Gc	2	 50%  50%

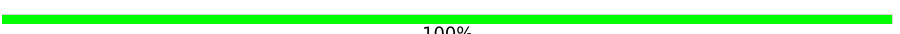
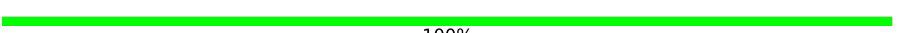
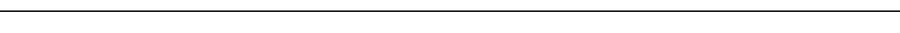
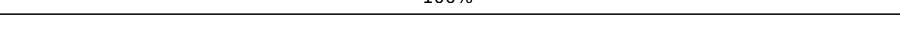
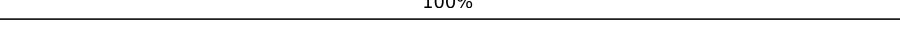
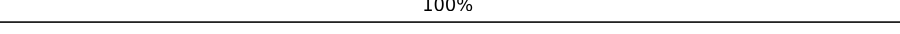
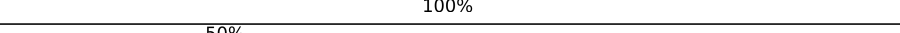
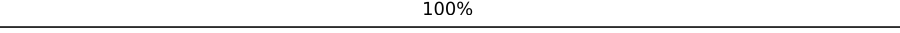
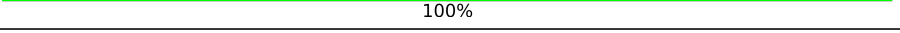
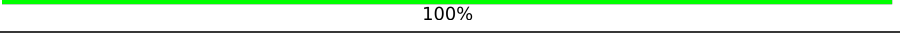
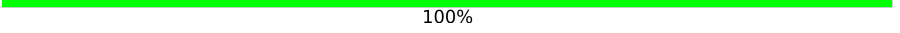
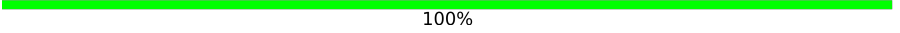
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Gd	2	 50% 50%
31	Ge	2	 100%
31	Gf	2	 100%
31	Gg	2	 100%
31	Gh	2	 100%
31	Gi	2	 100%
31	Gj	2	 100%
31	Gk	2	 100%
31	Gl	2	 100%
31	Ha	2	 50% 50%
31	Hb	2	 50% 50%
31	Hc	2	 50% 50%
31	Hd	2	 50% 50%
31	He	2	 100%
31	Hf	2	 100%
31	Hg	2	 100%
31	Hh	2	 100%
31	Hi	2	 50% 50%
31	Hj	2	 50% 50%
31	Hk	2	 50% 50%
31	Hl	2	 50% 50%
31	Ia	2	 100%
31	Ib	2	 100%
31	Ic	2	 100%
31	Id	2	 100%

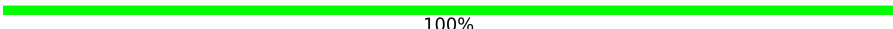
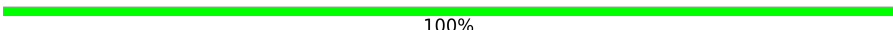
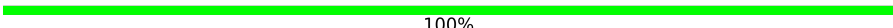
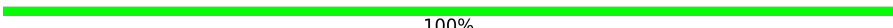
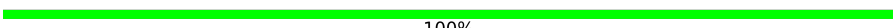
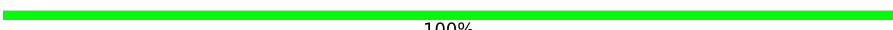
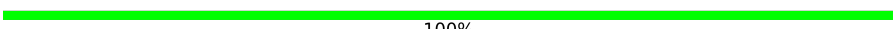
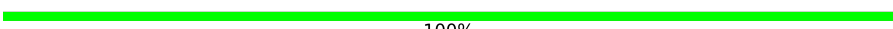
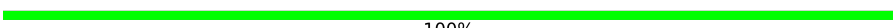
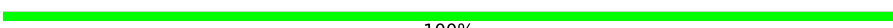
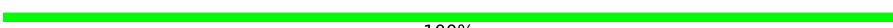
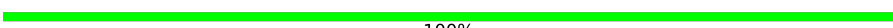
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Ie	2	 50% 50%
31	If	2	 50% 50%
31	Ig	2	 50% 50%
31	Ih	2	 50% 50%
31	Ii	2	 100%
31	Ij	2	 100%
31	Ik	2	 100%
31	Il	2	 100%
31	Ja	2	 100%
31	Jb	2	 100%
31	Jc	2	 100%
31	Jd	2	 100%
31	Je	2	 50% 50%
31	Jf	2	 50% 50%
31	Jg	2	 100%
31	Jh	2	 50% 50%
31	Ji	2	 50% 100%
31	Jj	2	 100%
31	Jk	2	 100%
31	Jl	2	 50% 100%
31	Ka	2	 100%
31	Kb	2	 100%
31	Kc	2	 100%
31	Kd	2	 100%
31	Ke	2	 50% 50%

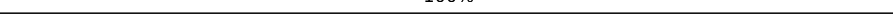
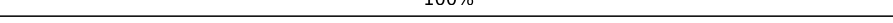
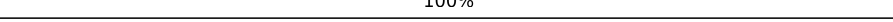
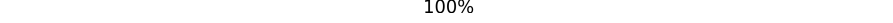
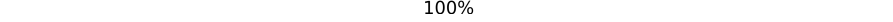
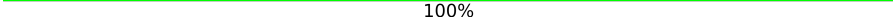
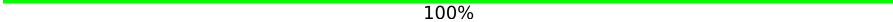
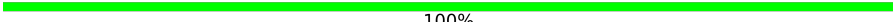
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Kf	2	 50% 50%
31	Kg	2	 50% 50%
31	Kh	2	 50% 50%
31	Ki	2	 100%
31	Kj	2	 100%
31	Kk	2	 100%
31	Kl	2	 100%
31	La	2	 50% 50%
31	Lb	2	 50% 50%
31	Lc	2	 50% 50%
31	Ld	2	 50% 50%
31	Le	2	 100%
31	Lf	2	 100%
31	Lg	2	 100%
31	Lh	2	 100%
31	Li	2	 100%
31	Lj	2	 100%
31	Lk	2	 100%
31	Ll	2	 100%
31	Ma	2	 50% 50%
31	Mb	2	 50% 50%
31	Mc	2	 50% 50%
31	Md	2	 50% 50%
31	Me	2	 100%
31	Mf	2	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Mg	2	 100%
31	Mh	2	 100%
31	Mi	2	 50% 50%
31	Mj	2	 50% 50%
31	Mk	2	 50% 50%
31	Ml	2	 50% 50%
31	Na	2	 100%
31	Nb	2	 100%
31	Nc	2	 50% 50%
31	Nd	2	 100%
31	Ne	2	 100%
31	Nf	2	 100%
31	Ng	2	 100%
31	Nh	2	 100%
31	Ni	2	 100%
31	Nj	2	 100%
31	Nk	2	 100%
31	Nl	2	 100%
31	Oa	2	 100%
31	Ob	2	 100%
31	Oc	2	 100%
31	Od	2	 100%
31	Oe	2	 100%
31	Of	2	 100%
31	Og	2	 100%

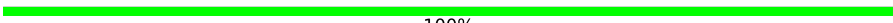
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Oh	2	100%
31	Oi	2	100%
31	Oj	2	100%
31	Ok	2	100%
31	Ol	2	100%
31	Pa	2	100%
31	Pb	2	100%
31	Pc	2	100%
31	Pd	2	100%
31	Pe	2	100%
31	Pf	2	100%
31	Pg	2	100%
31	Ph	2	100%
31	Pi	2	50%
31	Pj	2	50%
31	Pk	2	50%
31	Pl	2	50%
31	Qa	2	100%
31	Qb	2	100%
31	Qc	2	100%
31	Qd	2	100%
31	Qi	2	100%
31	Qj	2	100%
31	Qk	2	100%
31	Ql	2	100%

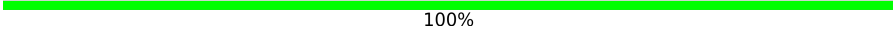
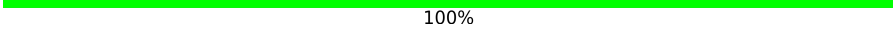
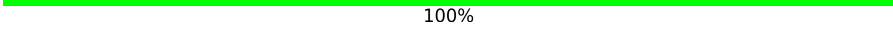
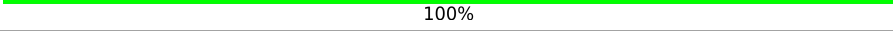
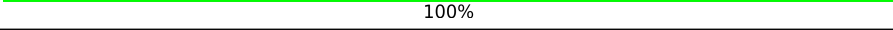
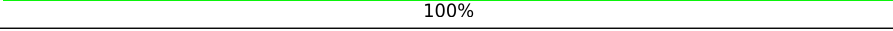
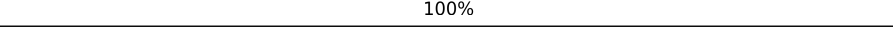
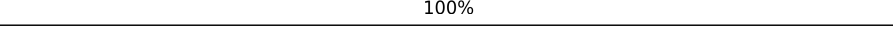
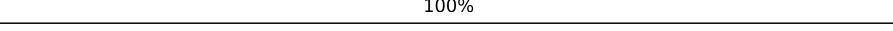
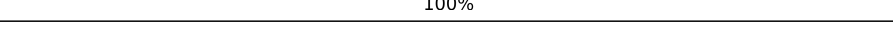
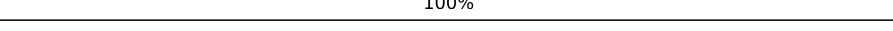
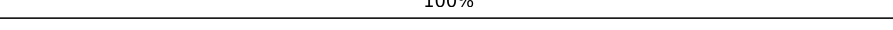
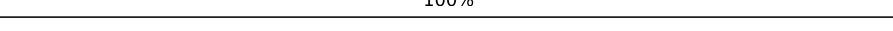
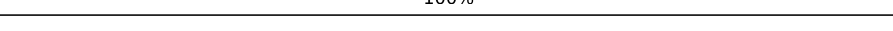
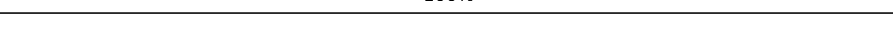
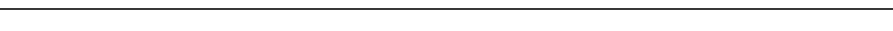
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Ra	2	 100%
31	Rb	2	 100%
31	Rc	2	 100%
31	Rd	2	 100%
31	Re	2	 100%
31	Rf	2	 100%
31	Rg	2	 100%
31	Rh	2	 100%
31	Se	2	 100%
31	Sf	2	 100%
31	Sg	2	 100%
31	Sh	2	 100%
31	Si	2	 50% 50%
31	Sj	2	 50% 50%
31	Sk	2	 50% 50%
31	Sl	2	 50% 50%
31	Ta	2	 50% 50%
31	Tb	2	 50% 50%
31	Tc	2	 50% 50%
31	Td	2	 50% 50%
31	Ti	2	 100%
31	Tj	2	 100%
31	Tk	2	 100%
31	Tl	2	 100%
31	Ua	2	 50% 50%

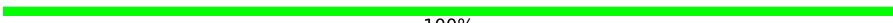
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Ub	2	 50% 50%
31	Uc	2	 50% 50%
31	Ud	2	 50% 50%
31	Ui	2	 100%
31	Uj	2	 100%
31	Uk	2	 100%
31	Ul	2	 100%
31	Va	2	 100%
31	Vb	2	 100%
31	Vc	2	 100%
31	Vd	2	 100%
31	Ve	2	 100%
31	Vf	2	 100%
31	Vg	2	 100%
31	Vh	2	 100%
31	We	2	 100%
31	Wf	2	 100%
31	Wg	2	 100%
31	Wh	2	 100%
31	Xi	2	 100%
31	Xj	2	 100%
31	Xk	2	 100%
31	Xl	2	 100%
31	Ya	2	 100%
31	Yb	2	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	Yc	2	 100%
31	Yd	2	 100%
31	Yi	2	 100%
31	Yj	2	 100%
31	Yk	2	 100%
31	Yl	2	 100%
31	Za	2	 50% 50%
31	Zb	2	 50% 50%
31	Zc	2	 100%
31	Zd	2	 100%
31	Zi	2	 100%
31	Zj	2	 100%
31	Zk	2	 100%
31	Zl	2	 100%
31	aa	2	 100%
31	ab	2	 100%
31	ac	2	 100%
31	ad	2	 100%
31	bi	2	 100%
31	bj	2	 100%
31	bk	2	 100%
31	bl	2	 100%
31	ca	2	 100%
31	cb	2	 100%
31	cc	2	 100%

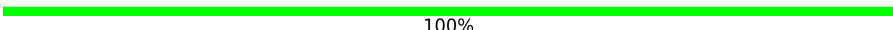
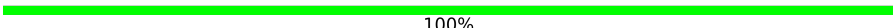
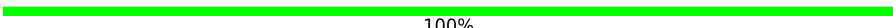
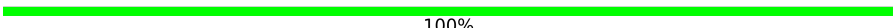
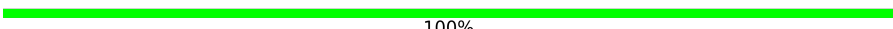
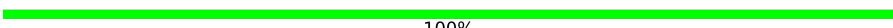
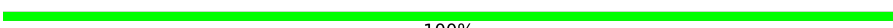
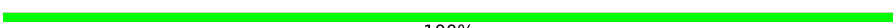
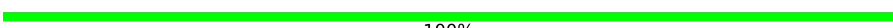
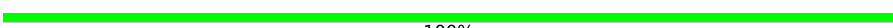
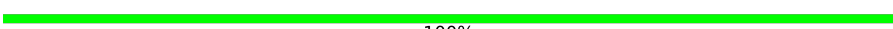
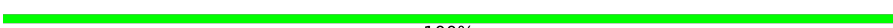
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	cd	2	 100%
31	ci	2	 50% 50%
31	cj	2	 50% 50%
31	ck	2	 50% 50%
31	cl	2	 50% 50%
31	da	2	 100%
31	db	2	 100%
31	dc	2	 100%
31	dd	2	 100%
31	di	2	 100%
31	dj	2	 100%
31	dk	2	 100%
31	dl	2	 100%
31	ea	2	 100%
31	eb	2	 100%
31	ec	2	 100%
31	ed	2	 100%
31	ei	2	 100%
31	ej	2	 100%
31	ek	2	 100%
31	el	2	 100%
31	fa	2	 100%
31	fb	2	 100%
31	fc	2	 100%
31	fd	2	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	gi	2	 50% 50%
31	gj	2	 50% 50%
31	gk	2	 50% 50%
31	gl	2	 50% 50%
31	ha	2	 100%
31	hb	2	 100%
31	hc	2	 100%
31	hd	2	 100%
31	ii	2	 50% 50%
31	ij	2	 100%
31	ik	2	 50% 50%
31	il	2	 100%
31	ja	2	 50% 50%
31	jb	2	 50% 50%
31	jc	2	 50% 50%
31	jd	2	 50% 50%
31	ji	2	 100%
31	jj	2	 100%
31	jk	2	 100%
31	jl	2	 100%
31	ka	2	 100%
31	kb	2	 100%
31	kc	2	 100%
31	kd	2	 100%
31	ki	2	 50% 50%

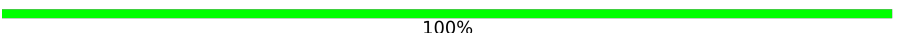
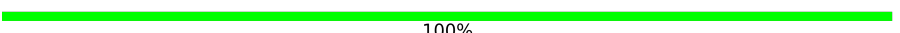
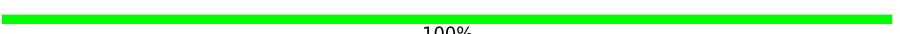
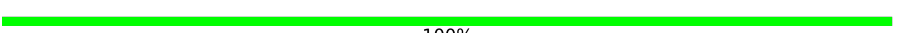
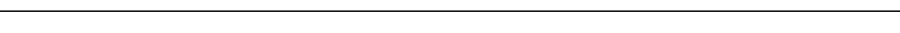
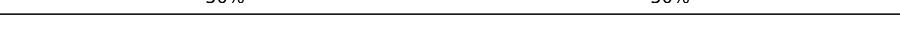
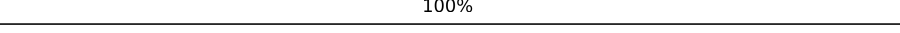
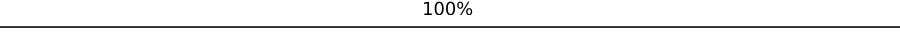
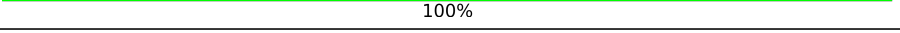
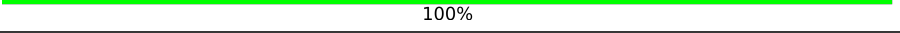
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	kj	2	50%50%
31	kk	2	50%50%
31	kl	2	50%50%
31	la	2	50%50%
31	lb	2	50%50%
31	lc	2	50%50%
31	ld	2	50%50%
31	li	2	50%50%
31	lj	2	50%50%
31	lk	2	50%50%
31	ll	2	50%50%
31	ma	2	100%
31	mb	2	100%
31	mc	2	100%
31	md	2	100%
31	mi	2	100%
31	mj	2	100%
31	mk	2	100%
31	ml	2	100%
31	na	2	50%50%
31	nb	2	50%50%
31	nc	2	50%50%
31	nd	2	50%50%
31	ni	2	50%50%
31	nj	2	50%50%

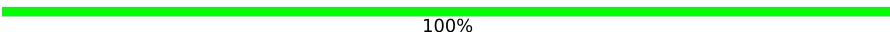
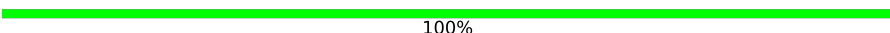
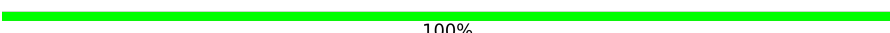
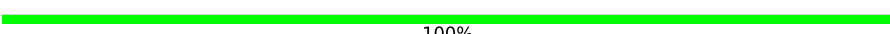
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	nk	2	 50% 50%
31	nl	2	 50% 50%
31	oa	2	 100%
31	ob	2	 100%
31	oc	2	 100%
31	od	2	 100%
31	oi	2	 50% 100%
31	oj	2	 50% 100%
31	ok	2	 50% 100%
31	ol	2	 50% 100%
31	pa	2	 50% 50%
31	pb	2	 50% 50%
31	pc	2	 50% 50%
31	pd	2	 100%
31	pi	2	 50% 50%
31	pj	2	 50% 50%
31	pk	2	 50% 50%
31	pl	2	 50% 50%
31	qa	2	 100%
31	qb	2	 100%
31	qc	2	 100%
31	qd	2	 100%
31	qi	2	 50% 50%
31	qj	2	 50% 50%
31	qk	2	 50% 50%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	ql	2	 50% 50%
31	ra	2	 100%
31	rb	2	 100%
31	rc	2	 100%
31	rd	2	 100%
31	ri	2	 50% 50%
31	rj	2	 100%
31	rk	2	 50% 50%
31	rl	2	 100%
31	sa	2	 100%
31	sb	2	 100%
31	sc	2	 100%
31	sd	2	 100%

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
31	GLC	Aa	2	X	-	-	-
31	GLC	Ab	2	X	-	-	-
31	GLC	Ac	2	X	-	-	-
31	GLC	Ad	2	X	-	-	-
31	GLC	Ae	2	X	-	-	-
31	GLC	Af	2	X	-	-	-
31	GLC	Ag	2	X	-	-	-
31	GLC	Ah	2	X	-	-	-
31	GLC	Ai	2	X	-	-	-
31	GLC	Aj	2	X	-	-	-
31	GLC	Ak	2	X	-	-	-
31	GLC	Al	2	X	-	-	-
31	GLC	Ba	2	X	-	-	-
31	GLC	Bb	2	X	-	-	-
31	GLC	Bc	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	Bd	2	X	-	-	-
31	GLC	Be	2	X	-	-	-
31	GLC	Bf	2	X	-	-	-
31	GLC	Bg	2	X	-	-	-
31	GLC	Bh	2	X	-	-	-
31	GLC	Bi	2	X	-	-	-
31	GLC	Bj	2	X	-	-	-
31	GLC	Bk	2	X	-	-	-
31	GLC	Bl	2	X	-	-	-
31	GLC	Ca	2	X	-	-	-
31	GLC	Cb	2	X	-	-	-
31	GLC	Cc	2	X	-	-	-
31	GLC	Cd	2	X	-	-	-
31	GLC	Ce	2	X	-	-	-
31	GLC	Cf	2	X	-	-	-
31	GLC	Cg	2	X	-	-	-
31	GLC	Ch	2	X	-	-	-
31	GLC	Ci	2	X	-	-	-
31	GLC	Cj	2	X	-	-	-
31	GLC	Ck	2	X	-	-	-
31	GLC	Cl	2	X	-	-	-
31	GLC	De	2	X	-	-	-
31	GLC	Df	2	X	-	-	-
31	GLC	Dg	2	X	-	-	-
31	GLC	Dh	2	X	-	-	-
31	GLC	Di	2	X	-	-	-
31	GLC	Dj	2	X	-	-	-
31	GLC	Dk	2	X	-	-	-
31	GLC	Dl	2	X	-	-	-
31	GLC	Ea	2	X	-	-	-
31	GLC	Eb	2	X	-	-	-
31	GLC	Ec	2	X	-	-	-
31	GLC	Ed	2	X	-	-	-
31	GLC	Ee	2	X	-	-	-
31	GLC	Ef	2	X	-	-	-
31	GLC	Eg	2	X	-	-	-
31	GLC	Eh	2	X	-	-	-
31	GLC	Fi	2	X	-	-	-
31	GLC	Fj	2	X	-	-	-
31	GLC	Fk	2	X	-	-	-
31	GLC	Fl	2	X	-	-	-
31	GLC	Ga	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	Gb	2	X	-	-	-
31	GLC	Gc	2	X	-	-	-
31	GLC	Gd	2	X	-	-	-
31	GLC	Ge	2	X	-	-	-
31	GLC	Gf	2	X	-	-	-
31	GLC	Gg	2	X	-	-	-
31	GLC	Gh	2	X	-	-	-
31	GLC	Gi	2	X	-	-	-
31	GLC	Gj	2	X	-	-	-
31	GLC	Gk	2	X	-	-	-
31	GLC	Gl	2	X	-	-	-
31	GLC	Ha	2	X	-	-	-
31	GLC	Hb	2	X	-	-	-
31	GLC	Hc	2	X	-	-	-
31	GLC	Hd	2	X	-	-	-
31	GLC	He	2	X	-	-	-
31	GLC	Hf	2	X	-	-	-
31	GLC	Hg	2	X	-	-	-
31	GLC	Hh	2	X	-	-	-
31	GLC	Hi	2	X	-	-	-
31	GLC	Hj	2	X	-	-	-
31	GLC	Hk	2	X	-	-	-
31	GLC	Hl	2	X	-	-	-
31	GLC	Ia	2	X	-	-	-
31	GLC	Ib	2	X	-	-	-
31	GLC	Ic	2	X	-	-	-
31	GLC	Id	2	X	-	-	-
31	GLC	Ie	2	X	-	-	-
31	GLC	If	2	X	-	-	-
31	GLC	Ig	2	X	-	-	-
31	GLC	Ih	2	X	-	-	-
31	GLC	Ii	2	X	-	-	-
31	GLC	Ij	2	X	-	-	-
31	GLC	Ik	2	X	-	-	-
31	GLC	Il	2	X	-	-	-
31	GLC	Ja	2	X	-	-	-
31	GLC	Jb	2	X	-	-	-
31	GLC	Jc	2	X	-	-	-
31	GLC	Jd	2	X	-	-	-
31	GLC	Je	2	X	-	-	-
31	GLC	Jf	2	X	-	-	-
31	GLC	Jg	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	Jh	2	X	-	-	-
31	GLC	Ji	2	X	-	-	-
31	GLC	Jj	2	X	-	-	-
31	GLC	Jk	2	X	-	-	-
31	GLC	Jl	2	X	-	-	-
31	GLC	Ka	2	X	-	-	-
31	GLC	Kb	2	X	-	-	-
31	GLC	Kc	2	X	-	-	-
31	GLC	Kd	2	X	-	-	-
31	GLC	Ke	2	X	-	-	-
31	GLC	Kf	2	X	-	-	-
31	GLC	Kg	2	X	-	-	-
31	GLC	Kh	2	X	-	-	-
31	GLC	Ki	2	X	-	-	-
31	GLC	Kj	2	X	-	-	-
31	GLC	Kk	2	X	-	-	-
31	GLC	Kl	2	X	-	-	-
31	GLC	La	2	X	-	-	-
31	GLC	Lb	2	X	-	-	-
31	GLC	Lc	2	X	-	-	-
31	GLC	Ld	2	X	-	-	-
31	GLC	Le	2	X	-	-	-
31	GLC	Lf	2	X	-	-	-
31	GLC	Lg	2	X	-	-	-
31	GLC	Lh	2	X	-	-	-
31	GLC	Li	2	X	-	-	-
31	GLC	Lj	2	X	-	-	-
31	GLC	Lk	2	X	-	-	-
31	GLC	Ll	2	X	-	-	-
31	GLC	Ma	2	X	-	-	-
31	GLC	Mb	2	X	-	-	-
31	GLC	Mc	2	X	-	-	-
31	GLC	Md	2	X	-	-	-
31	GLC	Me	2	X	-	-	-
31	GLC	Mf	2	X	-	-	-
31	GLC	Mg	2	X	-	-	-
31	GLC	Mh	2	X	-	-	-
31	GLC	Mi	2	X	-	-	-
31	GLC	Mj	2	X	-	-	-
31	GLC	Mk	2	X	-	-	-
31	GLC	Ml	2	X	-	-	-
31	GLC	Na	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	Nb	2	X	-	-	-
31	GLC	Nc	2	X	-	-	-
31	GLC	Nd	2	X	-	-	-
31	GLC	Ne	2	X	-	-	-
31	GLC	Nf	2	X	-	-	-
31	GLC	Ng	2	X	-	-	-
31	GLC	Nh	2	X	-	-	-
31	GLC	Ni	2	X	-	-	-
31	GLC	Nj	2	X	-	-	-
31	GLC	Nk	2	X	-	-	-
31	GLC	Nl	2	X	-	-	-
31	GLC	Oa	2	X	-	-	-
31	GLC	Ob	2	X	-	-	-
31	GLC	Oc	2	X	-	-	-
31	GLC	Od	2	X	-	-	-
31	GLC	Oe	2	X	-	-	-
31	GLC	Of	2	X	-	-	-
31	GLC	Og	2	X	-	-	-
31	GLC	Oh	2	X	-	-	-
31	GLC	Oi	2	X	-	-	-
31	GLC	Oj	2	X	-	-	-
31	GLC	Ok	2	X	-	-	-
31	GLC	Ol	2	X	-	-	-
31	GLC	Pa	2	X	-	-	-
31	GLC	Pb	2	X	-	-	-
31	GLC	Pc	2	X	-	-	-
31	GLC	Pd	2	X	-	-	-
31	GLC	Pe	2	X	-	-	-
31	GLC	Pf	2	X	-	-	-
31	GLC	Pg	2	X	-	-	-
31	GLC	Ph	2	X	-	-	-
31	GLC	Pi	2	X	-	-	-
31	GLC	Pj	2	X	-	-	-
31	GLC	Pk	2	X	-	-	-
31	GLC	Pl	2	X	-	-	-
31	GLC	Qa	2	X	-	-	-
31	GLC	Qb	2	X	-	-	-
31	GLC	Qc	2	X	-	-	-
31	GLC	Qd	2	X	-	-	-
31	GLC	Qi	2	X	-	-	-
31	GLC	Qj	2	X	-	-	-
31	GLC	Qk	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	Ql	2	X	-	-	-
31	GLC	Ra	2	X	-	-	-
31	GLC	Rb	2	X	-	-	-
31	GLC	Rc	2	X	-	-	-
31	GLC	Rd	2	X	-	-	-
31	GLC	Re	2	X	-	-	-
31	GLC	Rf	2	X	-	-	-
31	GLC	Rg	2	X	-	-	-
31	GLC	Rh	2	X	-	-	-
31	GLC	Se	2	X	-	-	-
31	GLC	Sf	2	X	-	-	-
31	GLC	Sg	2	X	-	-	-
31	GLC	Sh	2	X	-	-	-
31	GLC	Si	2	X	-	-	-
31	GLC	Sj	2	X	-	-	-
31	GLC	Sk	2	X	-	-	-
31	GLC	Sl	2	X	-	-	-
31	GLC	Ta	2	X	-	-	-
31	GLC	Tb	2	X	-	-	-
31	GLC	Tc	2	X	-	-	-
31	GLC	Td	2	X	-	-	-
31	GLC	Ti	2	X	-	-	-
31	GLC	Tj	2	X	-	-	-
31	GLC	Tk	2	X	-	-	-
31	GLC	Tl	2	X	-	-	-
31	GLC	Ua	2	X	-	-	-
31	GLC	Ub	2	X	-	-	-
31	GLC	Uc	2	X	-	-	-
31	GLC	Ud	2	X	-	-	-
31	GLC	Ui	2	X	-	-	-
31	GLC	Uj	2	X	-	-	-
31	GLC	Uk	2	X	-	-	-
31	GLC	Ul	2	X	-	-	-
31	GLC	Va	2	X	-	-	-
31	GLC	Vb	2	X	-	-	-
31	GLC	Vc	2	X	-	-	-
31	GLC	Vd	2	X	-	-	-
31	GLC	Ve	2	X	-	-	-
31	GLC	Vf	2	X	-	-	-
31	GLC	Vg	2	X	-	-	-
31	GLC	Vh	2	X	-	-	-
31	GLC	We	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	Wf	2	X	-	-	-
31	GLC	Wg	2	X	-	-	-
31	GLC	Wh	2	X	-	-	-
31	GLC	Xi	2	X	-	-	-
31	GLC	Xj	2	X	-	-	-
31	GLC	Xk	2	X	-	-	-
31	GLC	Xl	2	X	-	-	-
31	GLC	Ya	2	X	-	-	-
31	GLC	Yb	2	X	-	-	-
31	GLC	Yc	2	X	-	-	-
31	GLC	Yd	2	X	-	-	-
31	GLC	Yi	2	X	-	-	-
31	GLC	Yj	2	X	-	-	-
31	GLC	Yk	2	X	-	-	-
31	GLC	Yl	2	X	-	-	-
31	GLC	Za	2	X	-	-	-
31	GLC	Zb	2	X	-	-	-
31	GLC	Zc	2	X	-	-	-
31	GLC	Zd	2	X	-	-	-
31	GLC	Zi	2	X	-	-	-
31	GLC	Zj	2	X	-	-	-
31	GLC	Zk	2	X	-	-	-
31	GLC	Zl	2	X	-	-	-
31	GLC	aa	2	X	-	-	-
31	GLC	ab	2	X	-	-	-
31	GLC	ac	2	X	-	-	-
31	GLC	ad	2	X	-	-	-
31	GLC	bi	2	X	-	-	-
31	GLC	bj	2	X	-	-	-
31	GLC	bk	2	X	-	-	-
31	GLC	bl	2	X	-	-	-
31	GLC	ca	2	X	-	-	-
31	GLC	cb	2	X	-	-	-
31	GLC	cc	2	X	-	-	-
31	GLC	cd	2	X	-	-	-
31	GLC	ci	2	X	-	-	-
31	GLC	cj	2	X	-	-	-
31	GLC	ck	2	X	-	-	-
31	GLC	cl	2	X	-	-	-
31	GLC	da	2	X	-	-	-
31	GLC	db	2	X	-	-	-
31	GLC	dc	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	dd	2	X	-	-	-
31	GLC	di	2	X	-	-	-
31	GLC	dj	2	X	-	-	-
31	GLC	dk	2	X	-	-	-
31	GLC	dl	2	X	-	-	-
31	GLC	ea	2	X	-	-	-
31	GLC	eb	2	X	-	-	-
31	GLC	ec	2	X	-	-	-
31	GLC	ed	2	X	-	-	-
31	GLC	ei	2	X	-	-	-
31	GLC	ej	2	X	-	-	-
31	GLC	ek	2	X	-	-	-
31	GLC	el	2	X	-	-	-
31	GLC	fa	2	X	-	-	-
31	GLC	fb	2	X	-	-	-
31	GLC	fc	2	X	-	-	-
31	GLC	fd	2	X	-	-	-
31	GLC	gi	2	X	-	-	-
31	GLC	gj	2	X	-	-	-
31	GLC	gk	2	X	-	-	-
31	GLC	gl	2	X	-	-	-
31	GLC	ha	2	X	-	-	-
31	GLC	hb	2	X	-	-	-
31	GLC	hc	2	X	-	-	-
31	GLC	hd	2	X	-	-	-
31	GLC	ii	2	X	-	-	-
31	GLC	ij	2	X	-	-	-
31	GLC	ik	2	X	-	-	-
31	GLC	il	2	X	-	-	-
31	GLC	ja	2	X	-	-	-
31	GLC	jb	2	X	-	-	-
31	GLC	jc	2	X	-	-	-
31	GLC	jd	2	X	-	-	-
31	GLC	ji	2	X	-	-	-
31	GLC	jj	2	X	-	-	-
31	GLC	jk	2	X	-	-	-
31	GLC	jl	2	X	-	-	-
31	GLC	ka	2	X	-	-	-
31	GLC	kb	2	X	-	-	-
31	GLC	kc	2	X	-	-	-
31	GLC	kd	2	X	-	-	-
31	GLC	ki	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	kj	2	X	-	-	-
31	GLC	kk	2	X	-	-	-
31	GLC	kl	2	X	-	-	-
31	GLC	la	2	X	-	-	-
31	GLC	lb	2	X	-	-	-
31	GLC	lc	2	X	-	-	-
31	GLC	ld	2	X	-	-	-
31	GLC	li	2	X	-	-	-
31	GLC	lj	2	X	-	-	-
31	GLC	lk	2	X	-	-	-
31	GLC	ll	2	X	-	-	-
31	GLC	ma	2	X	-	-	-
31	GLC	mb	2	X	-	-	-
31	GLC	mc	2	X	-	-	-
31	GLC	md	2	X	-	-	-
31	GLC	mi	2	X	-	-	-
31	GLC	mj	2	X	-	-	-
31	GLC	mk	2	X	-	-	-
31	GLC	ml	2	X	-	-	-
31	GLC	na	2	X	-	-	-
31	GLC	nb	2	X	-	-	-
31	GLC	nc	2	X	-	-	-
31	GLC	nd	2	X	-	-	-
31	GLC	ni	2	X	-	-	-
31	GLC	nj	2	X	-	-	-
31	GLC	nk	2	X	-	-	-
31	GLC	nl	2	X	-	-	-
31	GLC	oa	2	X	-	-	-
31	GLC	ob	2	X	-	-	-
31	GLC	oc	2	X	-	-	-
31	GLC	od	2	X	-	-	-
31	GLC	oi	2	X	-	-	-
31	GLC	oj	2	X	-	-	-
31	GLC	ok	2	X	-	-	-
31	GLC	ol	2	X	-	-	-
31	GLC	pa	2	X	-	-	-
31	GLC	pb	2	X	-	-	-
31	GLC	pc	2	X	-	-	-
31	GLC	pd	2	X	-	-	-
31	GLC	pi	2	X	-	-	-
31	GLC	pj	2	X	-	-	-
31	GLC	pk	2	X	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	GLC	pl	2	X	-	-	-
31	GLC	qa	2	X	-	-	-
31	GLC	qb	2	X	-	-	-
31	GLC	qc	2	X	-	-	-
31	GLC	qd	2	X	-	-	-
31	GLC	qi	2	X	-	-	-
31	GLC	qj	2	X	-	-	-
31	GLC	qk	2	X	-	-	-
31	GLC	ql	2	X	-	-	-
31	GLC	ra	2	X	-	-	-
31	GLC	rb	2	X	-	-	-
31	GLC	rc	2	X	-	-	-
31	GLC	rd	2	X	-	-	-
31	GLC	ri	2	X	-	-	-
31	GLC	rj	2	X	-	-	-
31	GLC	rk	2	X	-	-	-
31	GLC	rl	2	X	-	-	-
31	GLC	sa	2	X	-	-	-
31	GLC	sb	2	X	-	-	-
31	GLC	sc	2	X	-	-	-
31	GLC	sd	2	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 279032 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 Collagen alpha-1(V) chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AA	246	Total	C	N	O	S	0	0
			1631	993	316	317	5		
1	FA	246	Total	C	N	O	S	0	0
			1631	993	316	317	5		
1	KA	246	Total	C	N	O	S	0	0
			1631	993	316	317	5		
1	PA	246	Total	C	N	O	S	0	0
			1631	993	316	317	5		

- Molecule 2 is a protein called Fibrillar collagen NC1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	BA	233	Total	C	N	O	S	0	0
			1580	963	309	306	2		
2	GA	233	Total	C	N	O	S	0	0
			1580	963	309	306	2		
2	LA	233	Total	C	N	O	S	0	0
			1580	963	309	306	2		
2	QA	233	Total	C	N	O	S	0	0
			1580	963	309	306	2		

- Molecule 3 is a protein called Fibrillar collagen NC1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	234	Total	C	N	O	S	0	0
			1528	938	280	309	1		
3	HA	234	Total	C	N	O	S	0	0
			1528	938	280	309	1		
3	MA	234	Total	C	N	O	S	0	0
			1528	938	280	309	1		
3	RA	234	Total	C	N	O	S	0	0
			1528	938	280	309	1		

- Molecule 4 is a protein called Fibrillar collagen NC1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	DA	237	Total	C	N	O	S	0	0
			1521	926	275	319	1		
4	IA	237	Total	C	N	O	S	0	0
			1521	926	275	319	1		
4	NA	237	Total	C	N	O	S	0	0
			1521	926	275	319	1		
4	SA	237	Total	C	N	O	S	0	0
			1521	926	275	319	1		

- Molecule 5 is a protein called Fibrillar collagen NC1 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	EA	77	Total	C	N	O	0	0
			493	301	90	102		
5	JA	77	Total	C	N	O	0	0
			493	301	90	102		
5	OA	77	Total	C	N	O	0	0
			493	301	90	102		
5	TA	77	Total	C	N	O	0	0
			493	301	90	102		

- Molecule 6 is a protein called Collagen type XI alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AC	246	Total	C	N	O	S	0	0
			1642	997	320	321	4		
6	FC	246	Total	C	N	O	S	0	0
			1642	997	320	321	4		
6	KC	246	Total	C	N	O	S	0	0
			1642	997	320	321	4		
6	PC	246	Total	C	N	O	S	0	0
			1642	997	320	321	4		

- Molecule 7 is a protein called Collagen type XI alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BC	233	Total	C	N	O	S	0	0
			1568	951	309	307	1		
7	GC	233	Total	C	N	O	S	0	0
			1568	951	309	307	1		
7	LC	233	Total	C	N	O	S	0	0
			1568	951	309	307	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
7	QC	233	Total	C	N	O	S	0	0
			1568	951	309	307	1		

- Molecule 8 is a protein called Collagen type XI alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CC	235	Total	C	N	O	S	0	0
			1522	925	283	312	2		
8	HC	235	Total	C	N	O	S	0	0
			1522	925	283	312	2		
8	MC	235	Total	C	N	O	S	0	0
			1522	925	283	312	2		
8	RC	235	Total	C	N	O	S	0	0
			1522	925	283	312	2		

- Molecule 9 is a protein called Fibrillar collagen NC1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	DC	236	Total	C	N	O	S	0	0
			1504	909	278	316	1		
9	IC	236	Total	C	N	O	S	0	0
			1504	909	278	316	1		
9	NC	236	Total	C	N	O	S	0	0
			1504	909	278	316	1		
9	SC	236	Total	C	N	O	S	0	0
			1504	909	278	316	1		

- Molecule 10 is a protein called Fibrillar collagen NC1 domain-containing protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	EC	76	Total	C	N	O	0	0
			482	293	88	101		
10	JC	76	Total	C	N	O	0	0
			482	293	88	101		
10	OC	76	Total	C	N	O	0	0
			482	293	88	101		
10	TC	76	Total	C	N	O	0	0
			482	293	88	101		

- Molecule 11 is a protein called Chromaffin granule amine transporter isoform X1.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AB	231	Total	C	N	O	S	0	0
			1501	910	290	292	9		
11	FB	231	Total	C	N	O	S	0	0
			1501	910	290	292	9		
11	KB	231	Total	C	N	O	S	0	0
			1501	910	290	292	9		
11	PB	231	Total	C	N	O	S	0	0
			1501	910	290	292	9		

- Molecule 12 is a protein called Collagen type V alpha 2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	BB	233	Total	C	N	O	S	0	0
			1526	926	293	305	2		
12	GB	233	Total	C	N	O	S	0	0
			1526	926	293	305	2		
12	LB	233	Total	C	N	O	S	0	0
			1526	926	293	305	2		
12	QB	233	Total	C	N	O	S	0	0
			1526	926	293	305	2		

- Molecule 13 is a protein called Collagen type V alpha 2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	CB	234	Total	C	N	O	S	0	0
			1504	902	289	311	2		
13	HB	234	Total	C	N	O	S	0	0
			1504	902	289	311	2		
13	MB	234	Total	C	N	O	S	0	0
			1504	902	289	311	2		
13	RB	234	Total	C	N	O	S	0	0
			1504	902	289	311	2		

- Molecule 14 is a protein called Collagen alpha-2(V) chain preproprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	DB	237	Total	C	N	O	S	0	0
			1552	926	316	308	2		
14	IB	237	Total	C	N	O	S	0	0
			1552	926	316	308	2		
14	NB	237	Total	C	N	O	S	0	0
			1552	926	316	308	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	SB	237	Total	C	N	O	S	0	0
			1552	926	316	308	2		

- Molecule 15 is a protein called Collagen alpha-2(V) chain preproprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	EB	76	Total	C	N	O		0	0
			478	300	86	92			
15	JB	76	Total	C	N	O		0	0
			478	300	86	92			
15	OB	76	Total	C	N	O		0	0
			478	300	86	92			
15	TB	76	Total	C	N	O		0	0
			478	300	86	92			

- Molecule 16 is a protein called Collagen type II alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	AD	105	Total	C	N	O	S	0	0
			673	406	136	130	1		
16	AE	105	Total	C	N	O	S	0	0
			673	406	136	130	1		
16	AF	105	Total	C	N	O	S	0	0
			673	406	136	130	1		
16	AG	169	Total	C	N	O	S	0	0
			1078	655	209	209	5		
16	AH	169	Total	C	N	O	S	0	0
			1084	658	212	209	5		
16	AI	169	Total	C	N	O	S	0	0
			1087	660	212	209	6		
16	FD	105	Total	C	N	O	S	0	0
			673	406	136	130	1		
16	FE	105	Total	C	N	O	S	0	0
			673	406	136	130	1		
16	FF	105	Total	C	N	O	S	0	0
			673	406	136	130	1		
16	FG	169	Total	C	N	O	S	0	0
			1078	655	209	209	5		
16	FH	169	Total	C	N	O	S	0	0
			1084	658	212	209	5		
16	FI	169	Total	C	N	O	S	0	0
			1087	660	212	209	6		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
16	KD	105	Total 673	C 406	N 136	O 130	S 1	0	0
16	KE	105	Total 673	C 406	N 136	O 130	S 1	0	0
16	KF	105	Total 673	C 406	N 136	O 130	S 1	0	0
16	KG	169	Total 1078	C 655	N 209	O 209	S 5	0	0
16	KH	169	Total 1084	C 658	N 212	O 209	S 5	0	0
16	KI	169	Total 1087	C 660	N 212	O 209	S 6	0	0
16	PD	105	Total 673	C 406	N 136	O 130	S 1	0	0
16	PE	105	Total 673	C 406	N 136	O 130	S 1	0	0
16	PF	105	Total 673	C 406	N 136	O 130	S 1	0	0
16	PG	169	Total 1078	C 655	N 209	O 209	S 5	0	0
16	PH	169	Total 1084	C 658	N 212	O 209	S 5	0	0
16	PI	169	Total 1087	C 660	N 212	O 209	S 6	0	0

- Molecule 17 is a protein called Collagen type II alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	BD	248	Total 1562	C 948	N 305	O 308	S 1	0	0
17	BE	248	Total 1564	C 948	N 307	O 308	S 1	0	0
17	BF	248	Total 1556	C 945	N 302	O 308	S 1	0	0
17	BG	248	Total 1562	C 948	N 305	O 308	S 1	0	0
17	BH	248	Total 1568	C 951	N 308	O 308	S 1	0	0
17	BI	248	Total 1564	C 949	N 308	O 306	S 1	0	0
17	GD	248	Total 1562	C 948	N 305	O 308	S 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
17	GE	248	Total	C	N	O	S	0	0
			1564	948	307	308	1		
17	GF	248	Total	C	N	O	S	0	0
			1556	945	302	308	1		
17	GG	248	Total	C	N	O	S	0	0
			1562	948	305	308	1		
17	GH	248	Total	C	N	O	S	0	0
			1568	951	308	308	1		
17	GI	248	Total	C	N	O	S	0	0
			1564	949	308	306	1		
17	LD	248	Total	C	N	O	S	0	0
			1562	948	305	308	1		
17	LE	248	Total	C	N	O	S	0	0
			1564	948	307	308	1		
17	LF	248	Total	C	N	O	S	0	0
			1556	945	302	308	1		
17	LG	248	Total	C	N	O	S	0	0
			1562	948	305	308	1		
17	LH	248	Total	C	N	O	S	0	0
			1568	951	308	308	1		
17	LI	248	Total	C	N	O	S	0	0
			1564	949	308	306	1		
17	QD	248	Total	C	N	O	S	0	0
			1562	948	305	308	1		
17	QE	248	Total	C	N	O	S	0	0
			1564	948	307	308	1		
17	QF	248	Total	C	N	O	S	0	0
			1556	945	302	308	1		
17	QG	248	Total	C	N	O	S	0	0
			1562	948	305	308	1		
17	QH	248	Total	C	N	O	S	0	0
			1568	951	308	308	1		
17	QI	248	Total	C	N	O	S	0	0
			1564	949	308	306	1		

- Molecule 18 is a protein called Collagen type II alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CD	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	CE	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
18	CF	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	CG	223	Total	C	N	O	S	0	0
			1406	853	269	283	1		
18	CH	223	Total	C	N	O	S	0	0
			1414	858	270	285	1		
18	CI	223	Total	C	N	O	S	0	0
			1400	850	266	283	1		
18	HD	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	HE	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	HF	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	HG	223	Total	C	N	O	S	0	0
			1406	853	269	283	1		
18	HH	223	Total	C	N	O	S	0	0
			1414	858	270	285	1		
18	HI	223	Total	C	N	O	S	0	0
			1400	850	266	283	1		
18	MD	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	ME	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	MF	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	MG	223	Total	C	N	O	S	0	0
			1406	853	269	283	1		
18	MH	223	Total	C	N	O	S	0	0
			1414	858	270	285	1		
18	MI	223	Total	C	N	O	S	0	0
			1400	850	266	283	1		
18	RD	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	RE	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	RF	212	Total	C	N	O	S	0	0
			1339	811	256	271	1		
18	RG	223	Total	C	N	O	S	0	0
			1406	853	269	283	1		
18	RH	223	Total	C	N	O	S	0	0
			1414	858	270	285	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
18	RI	223	Total	C	N	O	S	0	0
			1400	850	266	283	1		

- Molecule 19 is a protein called Collagen type II alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	DD	231	Total	C	N	O		0	0
			1320	802	243	275			
19	DE	231	Total	C	N	O		0	0
			1312	798	242	272			
19	DF	231	Total	C	N	O		0	0
			1315	799	242	274			
19	DG	226	Total	C	N	O		0	0
			1429	857	277	295			
19	DH	226	Total	C	N	O		0	0
			1423	854	274	295			
19	DI	226	Total	C	N	O		0	0
			1429	857	277	295			
19	ID	231	Total	C	N	O		0	0
			1320	802	243	275			
19	IE	231	Total	C	N	O		0	0
			1312	798	242	272			
19	IF	231	Total	C	N	O		0	0
			1315	799	242	274			
19	IG	226	Total	C	N	O		0	0
			1429	857	277	295			
19	IH	226	Total	C	N	O		0	0
			1423	854	274	295			
19	II	226	Total	C	N	O		0	0
			1429	857	277	295			
19	ND	231	Total	C	N	O		0	0
			1320	802	243	275			
19	NE	231	Total	C	N	O		0	0
			1312	798	242	272			
19	NF	231	Total	C	N	O		0	0
			1315	799	242	274			
19	NG	226	Total	C	N	O		0	0
			1429	857	277	295			
19	NH	226	Total	C	N	O		0	0
			1423	854	274	295			
19	NI	226	Total	C	N	O		0	0
			1429	857	277	295			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	Trace
19	SD	231	Total	C	N	O	0	0
			1320	802	243	275		
19	SE	231	Total	C	N	O	0	0
			1312	798	242	272		
19	SF	231	Total	C	N	O	0	0
			1315	799	242	274		
19	SG	226	Total	C	N	O	0	0
			1429	857	277	295		
19	SH	226	Total	C	N	O	0	0
			1423	854	274	295		
19	SI	226	Total	C	N	O	0	0
			1429	857	277	295		

- Molecule 20 is a protein called Collagen type II alpha 1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	ED	162	Total	C	N	O	S	0	0
			959	583	181	194	1		
20	EE	162	Total	C	N	O	S	0	0
			968	588	184	195	1		
20	EF	162	Total	C	N	O	S	0	0
			955	581	180	193	1		
20	EG	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	EH	156	Total	C	N	O	S	0	0
			964	584	188	190	2		
20	EI	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	JD	162	Total	C	N	O	S	0	0
			959	583	181	194	1		
20	JE	162	Total	C	N	O	S	0	0
			968	588	184	195	1		
20	JF	162	Total	C	N	O	S	0	0
			955	581	180	193	1		
20	JG	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	JH	156	Total	C	N	O	S	0	0
			964	584	188	190	2		
20	JI	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	OD	162	Total	C	N	O	S	0	0
			959	583	181	194	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
20	OE	162	Total	C	N	O	S	0	0
			968	588	184	195	1		
20	OF	162	Total	C	N	O	S	0	0
			955	581	180	193	1		
20	OG	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	OH	156	Total	C	N	O	S	0	0
			964	584	188	190	2		
20	OI	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	TD	162	Total	C	N	O	S	0	0
			959	583	181	194	1		
20	TE	162	Total	C	N	O	S	0	0
			968	588	184	195	1		
20	TF	162	Total	C	N	O	S	0	0
			955	581	180	193	1		
20	TG	156	Total	C	N	O	S	0	0
			960	582	187	189	2		
20	TH	156	Total	C	N	O	S	0	0
			964	584	188	190	2		
20	TI	156	Total	C	N	O	S	0	0
			960	582	187	189	2		

- Molecule 21 is a protein called Collagen type IX alpha 1 chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	AJ	58	Total	C	N	O	0	0
			383	229	74	80		
21	DJ	58	Total	C	N	O	0	0
			383	229	74	80		
21	GJ	58	Total	C	N	O	0	0
			383	229	74	80		
21	JJ	58	Total	C	N	O	0	0
			383	229	74	80		

- Molecule 22 is a protein called Collagen alpha-1(IX) chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	BJ	231	Total	C	N	O	S	0	0
			1516	925	290	299	2		
22	EJ	231	Total	C	N	O	S	0	0
			1516	925	290	299	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
22	HJ	231	Total	C	N	O	S	0	0
			1516	925	290	299	2		
22	KJ	231	Total	C	N	O	S	0	0
			1516	925	290	299	2		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
BJ	?	-	PRO	deletion	UNP A0A8D0XSJ2
EJ	?	-	PRO	deletion	UNP A0A8D0XSJ2
HJ	?	-	PRO	deletion	UNP A0A8D0XSJ2
KJ	?	-	PRO	deletion	UNP A0A8D0XSJ2

- Molecule 23 is a protein called Collagen alpha-1(IX) chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	CJ	171	Total	C	N	O	S	0	0
			1147	708	221	211	7		
23	FJ	171	Total	C	N	O	S	0	0
			1147	708	221	211	7		
23	IJ	171	Total	C	N	O	S	0	0
			1147	708	221	211	7		
23	LJ	171	Total	C	N	O	S	0	0
			1147	708	221	211	7		

- Molecule 24 is a protein called Collagen type IX alpha 2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	AK	58	Total	C	N	O	S	0	0
			372	229	68	72	3		
24	DK	58	Total	C	N	O	S	0	0
			372	229	68	72	3		
24	GK	58	Total	C	N	O	S	0	0
			372	229	68	72	3		
24	JK	58	Total	C	N	O	S	0	0
			372	229	68	72	3		

- Molecule 25 is a protein called Collagen type IX alpha 2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	BK	232	Total	C	N	O	S	0	0
			1527	921	295	308	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
25	EK	232	Total	C	N	O	S	0	0
			1527	921	295	308	3		
25	HK	232	Total	C	N	O	S	0	0
			1527	921	295	308	3		
25	KK	232	Total	C	N	O	S	0	0
			1527	921	295	308	3		

- Molecule 26 is a protein called Collagen type IX alpha 2 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	CK	170	Total	C	N	O	S	0	0
			1156	713	224	212	7		
26	FK	170	Total	C	N	O	S	0	0
			1156	713	224	212	7		
26	IK	170	Total	C	N	O	S	0	0
			1156	713	224	212	7		
26	LK	170	Total	C	N	O	S	0	0
			1156	713	224	212	7		

- Molecule 27 is a protein called Collagen alpha-3(IX) chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	AL	58	Total	C	N	O	0	0
			386	243	74	69		
27	DL	58	Total	C	N	O	0	0
			386	243	74	69		
27	GL	58	Total	C	N	O	0	0
			386	243	74	69		
27	JL	58	Total	C	N	O	0	0
			386	243	74	69		

- Molecule 28 is a protein called Collagen alpha-3(IX) chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	BL	232	Total	C	N	O	S	0	0
			1507	902	296	306	3		
28	EL	232	Total	C	N	O	S	0	0
			1507	902	296	306	3		
28	HL	232	Total	C	N	O	S	0	0
			1507	902	296	306	3		
28	KL	232	Total	C	N	O	S	0	0
			1507	902	296	306	3		

- Molecule 29 is a protein called Collagen alpha-3(IX) chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	CL	170	Total	C	N	O	S	0	0
			1126	686	216	221	3		
29	FL	170	Total	C	N	O	S	0	0
			1126	686	216	221	3		
29	IL	170	Total	C	N	O	S	0	0
			1126	686	216	221	3		
29	LL	170	Total	C	N	O	S	0	0
			1126	686	216	221	3		

- Molecule 30 is a protein called Opticin.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	AM	210	Total	C	N	O	S	0	0
			1663	1060	287	309	7		
30	BM	210	Total	C	N	O	S	0	0
			1663	1060	287	309	7		
30	CM	210	Total	C	N	O	S	0	0
			1663	1060	287	309	7		
30	DM	210	Total	C	N	O	S	0	0
			1663	1060	287	309	7		

- Molecule 31 is an oligosaccharide called alpha-D-glucopyranose-(1-2)-beta-D-galactopyranoside.



Mol	Chain	Residues	Atoms			AltConf	Trace
31	Aa	2	Total	C	O	0	0
			22	12	10		
31	Ba	2	Total	C	O	0	0
			22	12	10		
31	Ca	2	Total	C	O	0	0
			22	12	10		
31	Ea	2	Total	C	O	0	0
			22	12	10		
31	Ga	2	Total	C	O	0	0
			22	12	10		
31	Ha	2	Total	C	O	0	0
			22	12	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Ia	2	Total 22	C 12	O 10	0	0
31	Ja	2	Total 22	C 12	O 10	0	0
31	Ka	2	Total 22	C 12	O 10	0	0
31	La	2	Total 22	C 12	O 10	0	0
31	Ma	2	Total 22	C 12	O 10	0	0
31	Na	2	Total 22	C 12	O 10	0	0
31	Oa	2	Total 22	C 12	O 10	0	0
31	Pa	2	Total 22	C 12	O 10	0	0
31	Qa	2	Total 22	C 12	O 10	0	0
31	Ra	2	Total 22	C 12	O 10	0	0
31	Ta	2	Total 22	C 12	O 10	0	0
31	Ua	2	Total 22	C 12	O 10	0	0
31	Va	2	Total 22	C 12	O 10	0	0
31	Ya	2	Total 22	C 12	O 10	0	0
31	Za	2	Total 22	C 12	O 10	0	0
31	aa	2	Total 22	C 12	O 10	0	0
31	ca	2	Total 22	C 12	O 10	0	0
31	da	2	Total 22	C 12	O 10	0	0
31	ea	2	Total 22	C 12	O 10	0	0
31	fa	2	Total 22	C 12	O 10	0	0
31	ha	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	ja	2	Total 22	C 12	O 10	0	0
31	ka	2	Total 22	C 12	O 10	0	0
31	la	2	Total 22	C 12	O 10	0	0
31	ma	2	Total 22	C 12	O 10	0	0
31	na	2	Total 22	C 12	O 10	0	0
31	oa	2	Total 22	C 12	O 10	0	0
31	pa	2	Total 22	C 12	O 10	0	0
31	qa	2	Total 22	C 12	O 10	0	0
31	ra	2	Total 22	C 12	O 10	0	0
31	sa	2	Total 22	C 12	O 10	0	0
31	Ae	2	Total 22	C 12	O 10	0	0
31	Be	2	Total 22	C 12	O 10	0	0
31	Ce	2	Total 22	C 12	O 10	0	0
31	De	2	Total 22	C 12	O 10	0	0
31	Ee	2	Total 22	C 12	O 10	0	0
31	Ge	2	Total 22	C 12	O 10	0	0
31	He	2	Total 22	C 12	O 10	0	0
31	Ie	2	Total 22	C 12	O 10	0	0
31	Je	2	Total 22	C 12	O 10	0	0
31	Ke	2	Total 22	C 12	O 10	0	0
31	Le	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Me	2	Total 22	C 12	O 10	0	0
31	Ne	2	Total 22	C 12	O 10	0	0
31	Oe	2	Total 22	C 12	O 10	0	0
31	Pe	2	Total 22	C 12	O 10	0	0
31	Re	2	Total 22	C 12	O 10	0	0
31	Se	2	Total 22	C 12	O 10	0	0
31	Ve	2	Total 22	C 12	O 10	0	0
31	We	2	Total 22	C 12	O 10	0	0
31	Ai	2	Total 22	C 12	O 10	0	0
31	Bi	2	Total 22	C 12	O 10	0	0
31	Ci	2	Total 22	C 12	O 10	0	0
31	Di	2	Total 22	C 12	O 10	0	0
31	Fi	2	Total 22	C 12	O 10	0	0
31	Gi	2	Total 22	C 12	O 10	0	0
31	Hi	2	Total 22	C 12	O 10	0	0
31	Ii	2	Total 22	C 12	O 10	0	0
31	Ji	2	Total 22	C 12	O 10	0	0
31	Ki	2	Total 22	C 12	O 10	0	0
31	Li	2	Total 22	C 12	O 10	0	0
31	Mi	2	Total 22	C 12	O 10	0	0
31	Ni	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Oi	2	Total	C	O	0	0
			22	12	10		
31	Pi	2	Total	C	O	0	0
			22	12	10		
31	Qi	2	Total	C	O	0	0
			22	12	10		
31	Si	2	Total	C	O	0	0
			22	12	10		
31	Ti	2	Total	C	O	0	0
			22	12	10		
31	Ui	2	Total	C	O	0	0
			22	12	10		
31	Xi	2	Total	C	O	0	0
			22	12	10		
31	Yi	2	Total	C	O	0	0
			22	12	10		
31	Zi	2	Total	C	O	0	0
			22	12	10		
31	bi	2	Total	C	O	0	0
			22	12	10		
31	ci	2	Total	C	O	0	0
			22	12	10		
31	di	2	Total	C	O	0	0
			22	12	10		
31	ei	2	Total	C	O	0	0
			22	12	10		
31	gi	2	Total	C	O	0	0
			22	12	10		
31	ii	2	Total	C	O	0	0
			22	12	10		
31	ji	2	Total	C	O	0	0
			22	12	10		
31	ki	2	Total	C	O	0	0
			22	12	10		
31	li	2	Total	C	O	0	0
			22	12	10		
31	mi	2	Total	C	O	0	0
			22	12	10		
31	ni	2	Total	C	O	0	0
			22	12	10		
31	oi	2	Total	C	O	0	0
			22	12	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	pi	2	Total 22	C 12	O 10	0	0
31	qi	2	Total 22	C 12	O 10	0	0
31	ri	2	Total 22	C 12	O 10	0	0
31	Ab	2	Total 22	C 12	O 10	0	0
31	Bb	2	Total 22	C 12	O 10	0	0
31	Cb	2	Total 22	C 12	O 10	0	0
31	Eb	2	Total 22	C 12	O 10	0	0
31	Gb	2	Total 22	C 12	O 10	0	0
31	Hb	2	Total 22	C 12	O 10	0	0
31	Ib	2	Total 22	C 12	O 10	0	0
31	Jb	2	Total 22	C 12	O 10	0	0
31	Kb	2	Total 22	C 12	O 10	0	0
31	Lb	2	Total 22	C 12	O 10	0	0
31	Mb	2	Total 22	C 12	O 10	0	0
31	Nb	2	Total 22	C 12	O 10	0	0
31	Ob	2	Total 22	C 12	O 10	0	0
31	Pb	2	Total 22	C 12	O 10	0	0
31	Qb	2	Total 22	C 12	O 10	0	0
31	Rb	2	Total 22	C 12	O 10	0	0
31	Tb	2	Total 22	C 12	O 10	0	0
31	Ub	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Vb	2	Total	C	O	0	0
			22	12	10		
31	Yb	2	Total	C	O	0	0
			22	12	10		
31	Zb	2	Total	C	O	0	0
			22	12	10		
31	ab	2	Total	C	O	0	0
			22	12	10		
31	cb	2	Total	C	O	0	0
			22	12	10		
31	db	2	Total	C	O	0	0
			22	12	10		
31	eb	2	Total	C	O	0	0
			22	12	10		
31	fb	2	Total	C	O	0	0
			22	12	10		
31	hb	2	Total	C	O	0	0
			22	12	10		
31	jb	2	Total	C	O	0	0
			22	12	10		
31	kb	2	Total	C	O	0	0
			22	12	10		
31	lb	2	Total	C	O	0	0
			22	12	10		
31	mb	2	Total	C	O	0	0
			22	12	10		
31	nb	2	Total	C	O	0	0
			22	12	10		
31	ob	2	Total	C	O	0	0
			22	12	10		
31	pb	2	Total	C	O	0	0
			22	12	10		
31	qb	2	Total	C	O	0	0
			22	12	10		
31	rb	2	Total	C	O	0	0
			22	12	10		
31	sb	2	Total	C	O	0	0
			22	12	10		
31	Af	2	Total	C	O	0	0
			22	12	10		
31	Bf	2	Total	C	O	0	0
			22	12	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Cf	2	Total 22	C 12	O 10	0	0
31	Df	2	Total 22	C 12	O 10	0	0
31	Ef	2	Total 22	C 12	O 10	0	0
31	Gf	2	Total 22	C 12	O 10	0	0
31	Hf	2	Total 22	C 12	O 10	0	0
31	If	2	Total 22	C 12	O 10	0	0
31	Jf	2	Total 22	C 12	O 10	0	0
31	Kf	2	Total 22	C 12	O 10	0	0
31	Lf	2	Total 22	C 12	O 10	0	0
31	Mf	2	Total 22	C 12	O 10	0	0
31	Nf	2	Total 22	C 12	O 10	0	0
31	Of	2	Total 22	C 12	O 10	0	0
31	Pf	2	Total 22	C 12	O 10	0	0
31	Rf	2	Total 22	C 12	O 10	0	0
31	Sf	2	Total 22	C 12	O 10	0	0
31	Vf	2	Total 22	C 12	O 10	0	0
31	Wf	2	Total 22	C 12	O 10	0	0
31	Aj	2	Total 22	C 12	O 10	0	0
31	Bj	2	Total 22	C 12	O 10	0	0
31	Cj	2	Total 22	C 12	O 10	0	0
31	Dj	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Fj	2	Total 22	C 12	O 10	0	0
31	Gj	2	Total 22	C 12	O 10	0	0
31	Hj	2	Total 22	C 12	O 10	0	0
31	Ij	2	Total 22	C 12	O 10	0	0
31	Jj	2	Total 22	C 12	O 10	0	0
31	Kj	2	Total 22	C 12	O 10	0	0
31	Lj	2	Total 22	C 12	O 10	0	0
31	Mj	2	Total 22	C 12	O 10	0	0
31	Nj	2	Total 22	C 12	O 10	0	0
31	Oj	2	Total 22	C 12	O 10	0	0
31	Pj	2	Total 22	C 12	O 10	0	0
31	Qj	2	Total 22	C 12	O 10	0	0
31	Sj	2	Total 22	C 12	O 10	0	0
31	Tj	2	Total 22	C 12	O 10	0	0
31	Uj	2	Total 22	C 12	O 10	0	0
31	Xj	2	Total 22	C 12	O 10	0	0
31	Yj	2	Total 22	C 12	O 10	0	0
31	Zj	2	Total 22	C 12	O 10	0	0
31	bj	2	Total 22	C 12	O 10	0	0
31	cj	2	Total 22	C 12	O 10	0	0
31	dj	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	ej	2	Total 22	C 12	O 10	0	0
31	gj	2	Total 22	C 12	O 10	0	0
31	ij	2	Total 22	C 12	O 10	0	0
31	jj	2	Total 22	C 12	O 10	0	0
31	kj	2	Total 22	C 12	O 10	0	0
31	lj	2	Total 22	C 12	O 10	0	0
31	mj	2	Total 22	C 12	O 10	0	0
31	nj	2	Total 22	C 12	O 10	0	0
31	oj	2	Total 22	C 12	O 10	0	0
31	pj	2	Total 22	C 12	O 10	0	0
31	qj	2	Total 22	C 12	O 10	0	0
31	rj	2	Total 22	C 12	O 10	0	0
31	Ac	2	Total 22	C 12	O 10	0	0
31	Bc	2	Total 22	C 12	O 10	0	0
31	Cc	2	Total 22	C 12	O 10	0	0
31	Ec	2	Total 22	C 12	O 10	0	0
31	Gc	2	Total 22	C 12	O 10	0	0
31	Hc	2	Total 22	C 12	O 10	0	0
31	Ic	2	Total 22	C 12	O 10	0	0
31	Jc	2	Total 22	C 12	O 10	0	0
31	Kc	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Lc	2	Total 22	C 12	O 10	0	0
31	Mc	2	Total 22	C 12	O 10	0	0
31	Nc	2	Total 22	C 12	O 10	0	0
31	Oc	2	Total 22	C 12	O 10	0	0
31	Pc	2	Total 22	C 12	O 10	0	0
31	Qc	2	Total 22	C 12	O 10	0	0
31	Rc	2	Total 22	C 12	O 10	0	0
31	Tc	2	Total 22	C 12	O 10	0	0
31	Uc	2	Total 22	C 12	O 10	0	0
31	Vc	2	Total 22	C 12	O 10	0	0
31	Yc	2	Total 22	C 12	O 10	0	0
31	Zc	2	Total 22	C 12	O 10	0	0
31	ac	2	Total 22	C 12	O 10	0	0
31	cc	2	Total 22	C 12	O 10	0	0
31	dc	2	Total 22	C 12	O 10	0	0
31	ec	2	Total 22	C 12	O 10	0	0
31	fc	2	Total 22	C 12	O 10	0	0
31	hc	2	Total 22	C 12	O 10	0	0
31	jc	2	Total 22	C 12	O 10	0	0
31	kc	2	Total 22	C 12	O 10	0	0
31	lc	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	mc	2	Total	C	O	0	0
			22	12	10		
31	nc	2	Total	C	O	0	0
			22	12	10		
31	oc	2	Total	C	O	0	0
			22	12	10		
31	pc	2	Total	C	O	0	0
			22	12	10		
31	qc	2	Total	C	O	0	0
			22	12	10		
31	rc	2	Total	C	O	0	0
			22	12	10		
31	sc	2	Total	C	O	0	0
			22	12	10		
31	Ag	2	Total	C	O	0	0
			22	12	10		
31	Bg	2	Total	C	O	0	0
			22	12	10		
31	Cg	2	Total	C	O	0	0
			22	12	10		
31	Dg	2	Total	C	O	0	0
			22	12	10		
31	Eg	2	Total	C	O	0	0
			22	12	10		
31	Gg	2	Total	C	O	0	0
			22	12	10		
31	Hg	2	Total	C	O	0	0
			22	12	10		
31	Ig	2	Total	C	O	0	0
			22	12	10		
31	Jg	2	Total	C	O	0	0
			22	12	10		
31	Kg	2	Total	C	O	0	0
			22	12	10		
31	Lg	2	Total	C	O	0	0
			22	12	10		
31	Mg	2	Total	C	O	0	0
			22	12	10		
31	Ng	2	Total	C	O	0	0
			22	12	10		
31	Og	2	Total	C	O	0	0
			22	12	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Pg	2	Total 22	C 12	O 10	0	0
31	Rg	2	Total 22	C 12	O 10	0	0
31	Sg	2	Total 22	C 12	O 10	0	0
31	Vg	2	Total 22	C 12	O 10	0	0
31	Wg	2	Total 22	C 12	O 10	0	0
31	Ak	2	Total 22	C 12	O 10	0	0
31	Bk	2	Total 22	C 12	O 10	0	0
31	Ck	2	Total 22	C 12	O 10	0	0
31	Dk	2	Total 22	C 12	O 10	0	0
31	Fk	2	Total 22	C 12	O 10	0	0
31	Gk	2	Total 22	C 12	O 10	0	0
31	Hk	2	Total 22	C 12	O 10	0	0
31	Ik	2	Total 22	C 12	O 10	0	0
31	Jk	2	Total 22	C 12	O 10	0	0
31	Kk	2	Total 22	C 12	O 10	0	0
31	Lk	2	Total 22	C 12	O 10	0	0
31	Mk	2	Total 22	C 12	O 10	0	0
31	Nk	2	Total 22	C 12	O 10	0	0
31	Ok	2	Total 22	C 12	O 10	0	0
31	Pk	2	Total 22	C 12	O 10	0	0
31	Qk	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Sk	2	Total 22	C 12	O 10	0	0
31	Tk	2	Total 22	C 12	O 10	0	0
31	Uk	2	Total 22	C 12	O 10	0	0
31	Xk	2	Total 22	C 12	O 10	0	0
31	Yk	2	Total 22	C 12	O 10	0	0
31	Zk	2	Total 22	C 12	O 10	0	0
31	bk	2	Total 22	C 12	O 10	0	0
31	ck	2	Total 22	C 12	O 10	0	0
31	dk	2	Total 22	C 12	O 10	0	0
31	ek	2	Total 22	C 12	O 10	0	0
31	gk	2	Total 22	C 12	O 10	0	0
31	ik	2	Total 22	C 12	O 10	0	0
31	jk	2	Total 22	C 12	O 10	0	0
31	kk	2	Total 22	C 12	O 10	0	0
31	lk	2	Total 22	C 12	O 10	0	0
31	mk	2	Total 22	C 12	O 10	0	0
31	nk	2	Total 22	C 12	O 10	0	0
31	ok	2	Total 22	C 12	O 10	0	0
31	pk	2	Total 22	C 12	O 10	0	0
31	qk	2	Total 22	C 12	O 10	0	0
31	rk	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Ad	2	Total	C	O	0	0
			22	12	10		
31	Bd	2	Total	C	O	0	0
			22	12	10		
31	Cd	2	Total	C	O	0	0
			22	12	10		
31	Ed	2	Total	C	O	0	0
			22	12	10		
31	Gd	2	Total	C	O	0	0
			22	12	10		
31	Hd	2	Total	C	O	0	0
			22	12	10		
31	Id	2	Total	C	O	0	0
			22	12	10		
31	Jd	2	Total	C	O	0	0
			22	12	10		
31	Kd	2	Total	C	O	0	0
			22	12	10		
31	Ld	2	Total	C	O	0	0
			22	12	10		
31	Md	2	Total	C	O	0	0
			22	12	10		
31	Nd	2	Total	C	O	0	0
			22	12	10		
31	Od	2	Total	C	O	0	0
			22	12	10		
31	Pd	2	Total	C	O	0	0
			22	12	10		
31	Qd	2	Total	C	O	0	0
			22	12	10		
31	Rd	2	Total	C	O	0	0
			22	12	10		
31	Td	2	Total	C	O	0	0
			22	12	10		
31	Ud	2	Total	C	O	0	0
			22	12	10		
31	Vd	2	Total	C	O	0	0
			22	12	10		
31	Yd	2	Total	C	O	0	0
			22	12	10		
31	Zd	2	Total	C	O	0	0
			22	12	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	ad	2	Total	C	O	0	0
			22	12	10		
31	cd	2	Total	C	O	0	0
			22	12	10		
31	dd	2	Total	C	O	0	0
			22	12	10		
31	ed	2	Total	C	O	0	0
			22	12	10		
31	fd	2	Total	C	O	0	0
			22	12	10		
31	hd	2	Total	C	O	0	0
			22	12	10		
31	jd	2	Total	C	O	0	0
			22	12	10		
31	kd	2	Total	C	O	0	0
			22	12	10		
31	ld	2	Total	C	O	0	0
			22	12	10		
31	md	2	Total	C	O	0	0
			22	12	10		
31	nd	2	Total	C	O	0	0
			22	12	10		
31	od	2	Total	C	O	0	0
			22	12	10		
31	pd	2	Total	C	O	0	0
			22	12	10		
31	qd	2	Total	C	O	0	0
			22	12	10		
31	rd	2	Total	C	O	0	0
			22	12	10		
31	sd	2	Total	C	O	0	0
			22	12	10		
31	Ah	2	Total	C	O	0	0
			22	12	10		
31	Bh	2	Total	C	O	0	0
			22	12	10		
31	Ch	2	Total	C	O	0	0
			22	12	10		
31	Dh	2	Total	C	O	0	0
			22	12	10		
31	Eh	2	Total	C	O	0	0
			22	12	10		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	Gh	2	Total 22	C 12	O 10	0	0
31	Hh	2	Total 22	C 12	O 10	0	0
31	Ih	2	Total 22	C 12	O 10	0	0
31	Jh	2	Total 22	C 12	O 10	0	0
31	Kh	2	Total 22	C 12	O 10	0	0
31	Lh	2	Total 22	C 12	O 10	0	0
31	Mh	2	Total 22	C 12	O 10	0	0
31	Nh	2	Total 22	C 12	O 10	0	0
31	Oh	2	Total 22	C 12	O 10	0	0
31	Ph	2	Total 22	C 12	O 10	0	0
31	Rh	2	Total 22	C 12	O 10	0	0
31	Sh	2	Total 22	C 12	O 10	0	0
31	Vh	2	Total 22	C 12	O 10	0	0
31	Wh	2	Total 22	C 12	O 10	0	0
31	Al	2	Total 22	C 12	O 10	0	0
31	Bl	2	Total 22	C 12	O 10	0	0
31	Cl	2	Total 22	C 12	O 10	0	0
31	Dl	2	Total 22	C 12	O 10	0	0
31	Fl	2	Total 22	C 12	O 10	0	0
31	Gl	2	Total 22	C 12	O 10	0	0
31	Hl	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

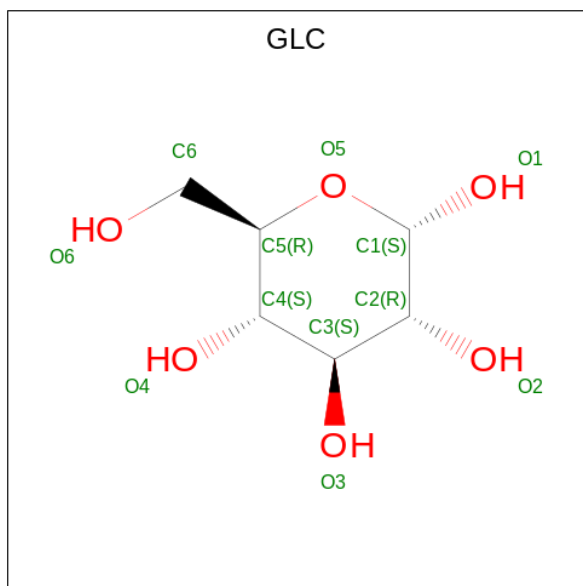
Mol	Chain	Residues	Atoms			AltConf	Trace
31	Il	2	Total 22	C 12	O 10	0	0
31	Jl	2	Total 22	C 12	O 10	0	0
31	Kl	2	Total 22	C 12	O 10	0	0
31	Ll	2	Total 22	C 12	O 10	0	0
31	Ml	2	Total 22	C 12	O 10	0	0
31	Nl	2	Total 22	C 12	O 10	0	0
31	Ol	2	Total 22	C 12	O 10	0	0
31	Pl	2	Total 22	C 12	O 10	0	0
31	Ql	2	Total 22	C 12	O 10	0	0
31	Sl	2	Total 22	C 12	O 10	0	0
31	Tl	2	Total 22	C 12	O 10	0	0
31	Ul	2	Total 22	C 12	O 10	0	0
31	Xl	2	Total 22	C 12	O 10	0	0
31	Yl	2	Total 22	C 12	O 10	0	0
31	Zl	2	Total 22	C 12	O 10	0	0
31	bl	2	Total 22	C 12	O 10	0	0
31	cl	2	Total 22	C 12	O 10	0	0
31	dl	2	Total 22	C 12	O 10	0	0
31	el	2	Total 22	C 12	O 10	0	0
31	gl	2	Total 22	C 12	O 10	0	0
31	il	2	Total 22	C 12	O 10	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			AltConf	Trace
31	jl	2	Total	C	O	0	0
			22	12	10		
31	kl	2	Total	C	O	0	0
			22	12	10		
31	ll	2	Total	C	O	0	0
			22	12	10		
31	ml	2	Total	C	O	0	0
			22	12	10		
31	nl	2	Total	C	O	0	0
			22	12	10		
31	ol	2	Total	C	O	0	0
			22	12	10		
31	pl	2	Total	C	O	0	0
			22	12	10		
31	ql	2	Total	C	O	0	0
			22	12	10		
31	rl	2	Total	C	O	0	0
			22	12	10		

- Molecule 32 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆).



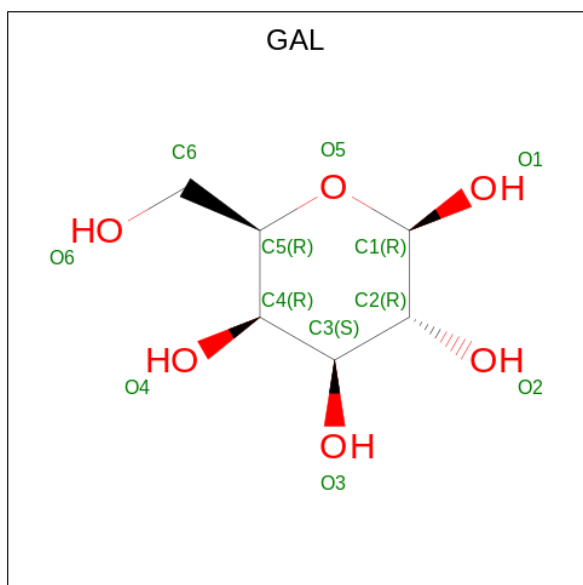
Mol	Chain	Residues	Atoms			AltConf
32	CC	1	Total	C	O	0
			11	6	5	
32	HC	1	Total	C	O	0
			11	6	5	

Continued on next page...

Continued from previous page...

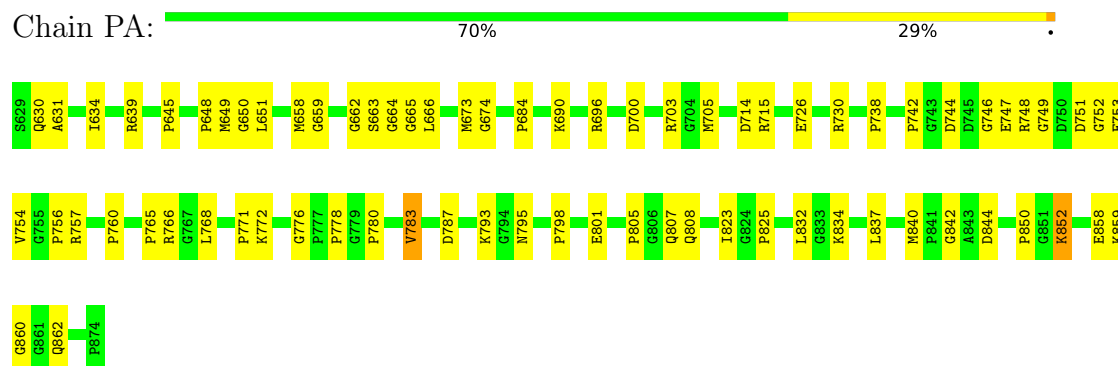
Mol	Chain	Residues	Atoms			AltConf
32	MC	1	Total	C	O	0
			11	6	5	
32	RC	1	Total	C	O	0
			11	6	5	

- Molecule 33 is beta-D-galactopyranose (CCD ID: GAL) (formula: C₆H₁₂O₆).

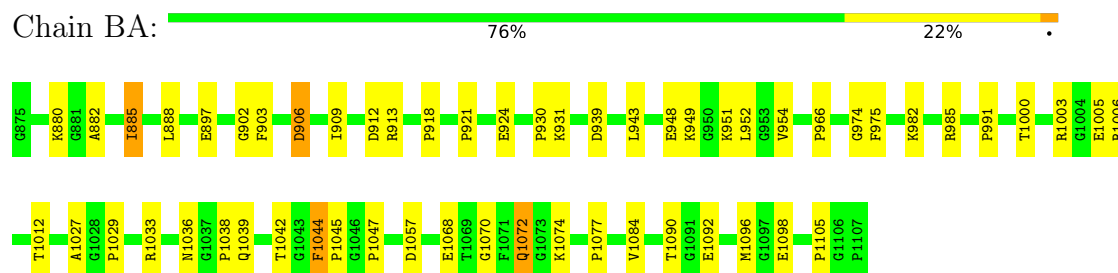


Mol	Chain	Residues	Atoms			AltConf
33	AB	1	Total	C	O	0
			11	6	5	
33	FB	1	Total	C	O	0
			11	6	5	
33	KB	1	Total	C	O	0
			11	6	5	
33	PB	1	Total	C	O	0
			11	6	5	

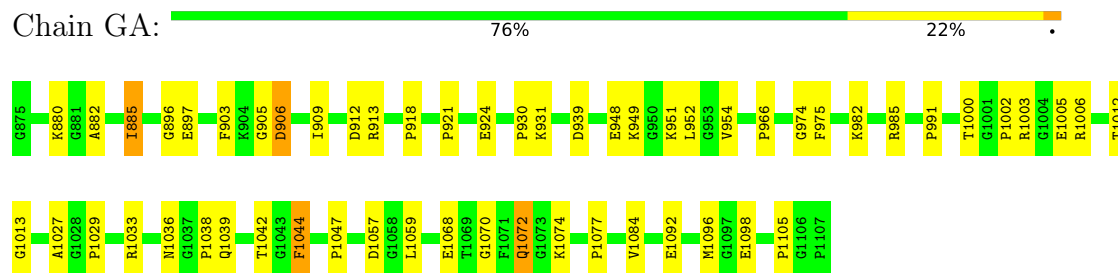
- Molecule 1: Collagen alpha-1(V) chain



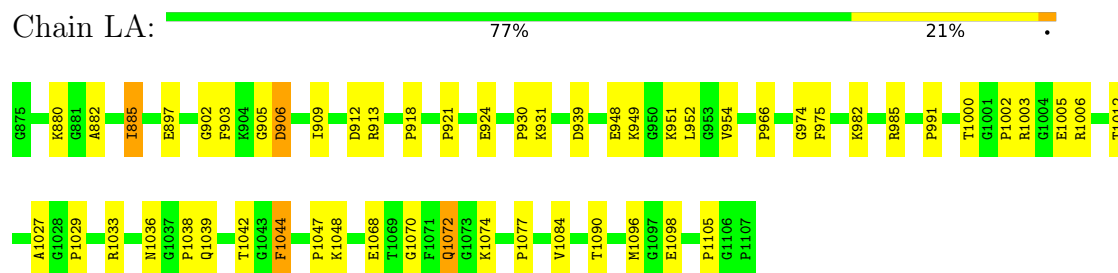
- Molecule 2: Fibrillar collagen NC1 domain-containing protein



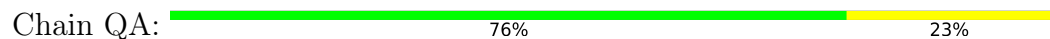
- Molecule 2: Fibrillar collagen NC1 domain-containing protein

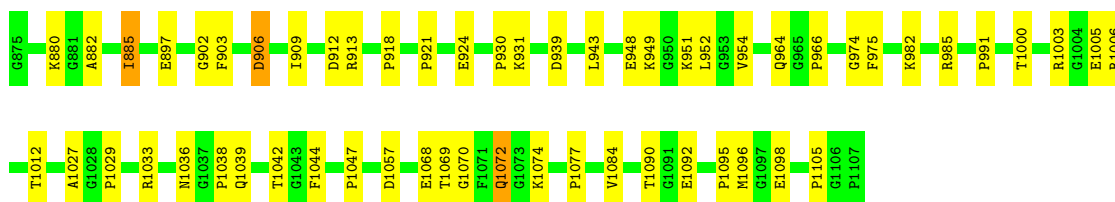


- Molecule 2: Fibrillar collagen NC1 domain-containing protein



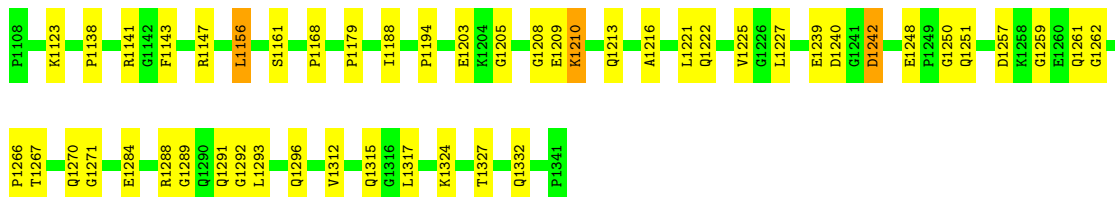
- Molecule 2: Fibrillar collagen NC1 domain-containing protein





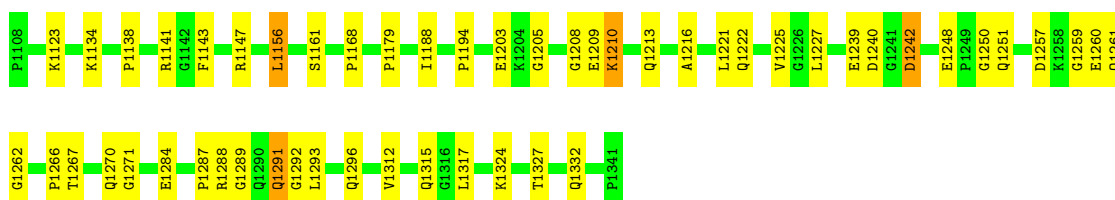
• Molecule 3: Fibrillar collagen NC1 domain-containing protein

Chain CA: 79% 20%



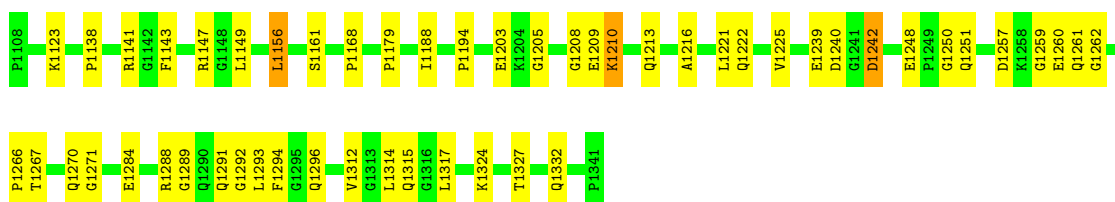
• Molecule 3: Fibrillar collagen NC1 domain-containing protein

Chain HA: 78% 21%



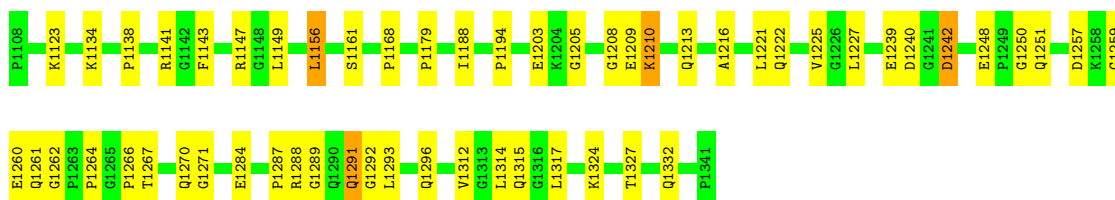
• Molecule 3: Fibrillar collagen NC1 domain-containing protein

Chain MA: 78% 21%



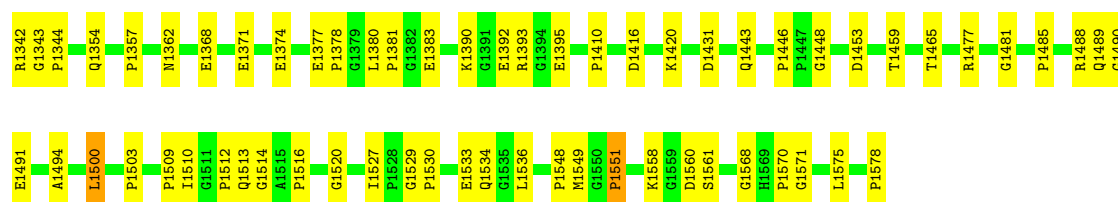
• Molecule 3: Fibrillar collagen NC1 domain-containing protein

Chain RA: 76% 22%



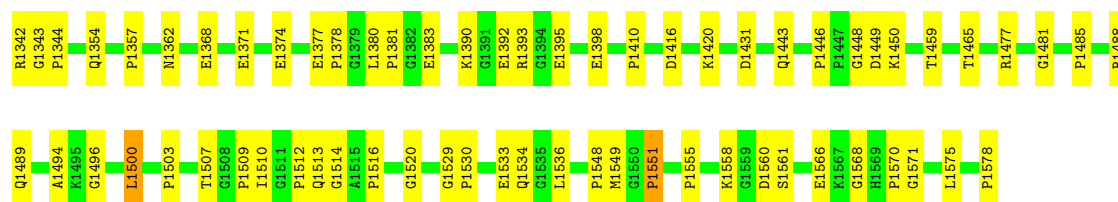
• Molecule 4: Fibrillar collagen NC1 domain-containing protein

Chain DA:  74% 25% .



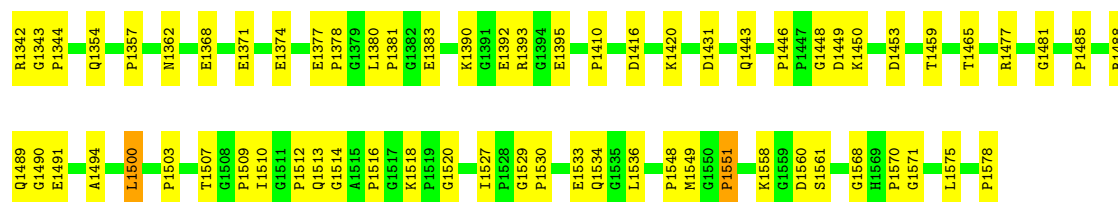
- Molecule 4: Fibrillar collagen NC1 domain-containing protein

Chain IA:  73% 27% .



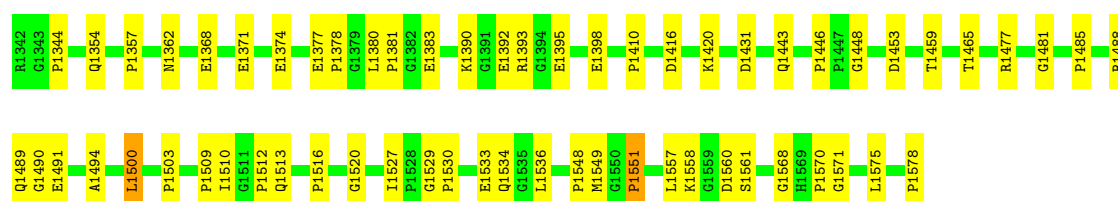
- Molecule 4: Fibrillar collagen NC1 domain-containing protein

Chain NA:  72% 27% .



- Molecule 4: Fibrillar collagen NC1 domain-containing protein

Chain SA:  74% 25% .

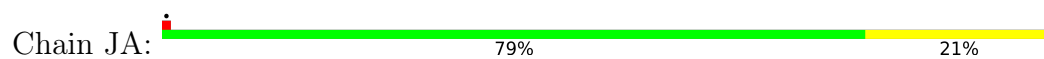


- Molecule 5: Fibrillar collagen NC1 domain-containing protein

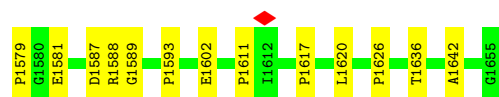
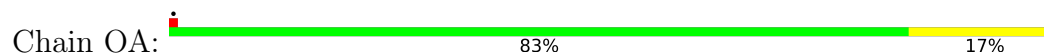
Chain EA:  83% 17% .



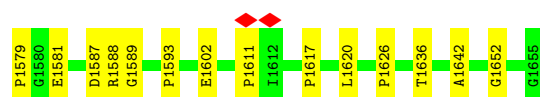
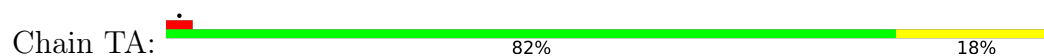
- Molecule 5: Fibrillar collagen NC1 domain-containing protein



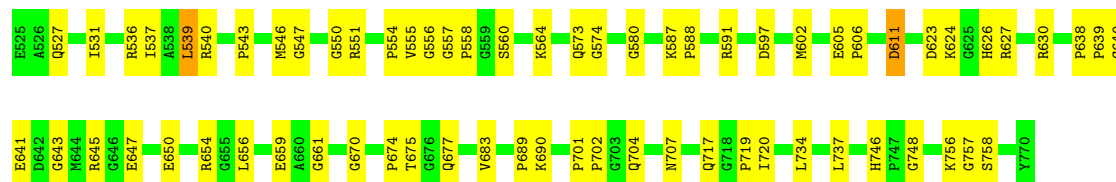
- Molecule 5: Fibrillar collagen NC1 domain-containing protein



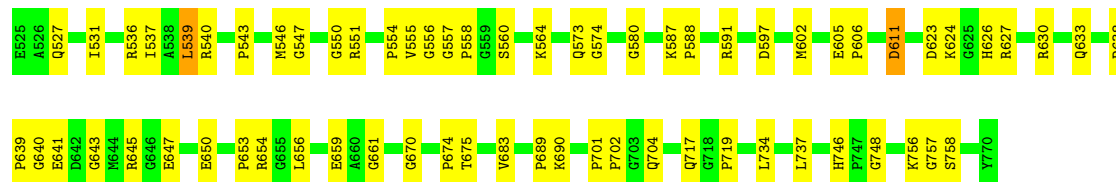
- Molecule 5: Fibrillar collagen NC1 domain-containing protein



- Molecule 6: Collagen type XI alpha 1 chain

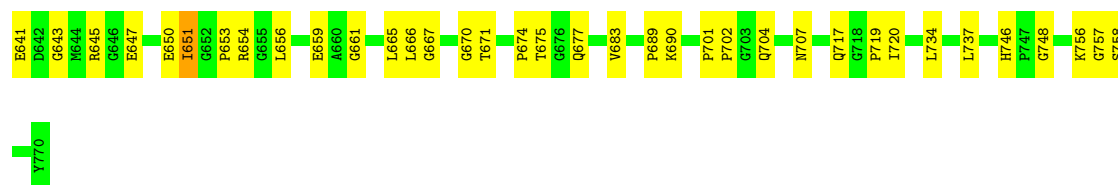


- Molecule 6: Collagen type XI alpha 1 chain



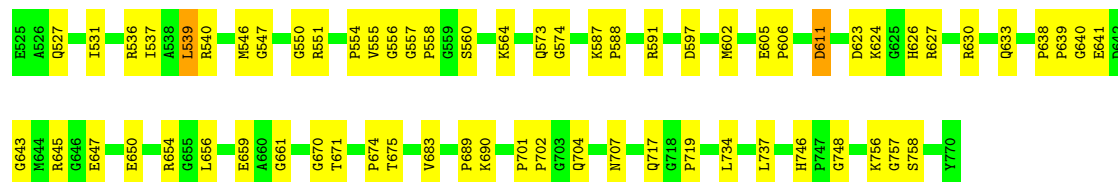
- Molecule 6: Collagen type XI alpha 1 chain





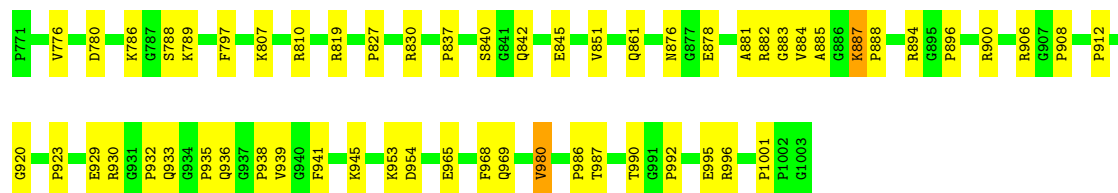
- Molecule 6: Collagen type XI alpha 1 chain

Chain PC: 74% 26%



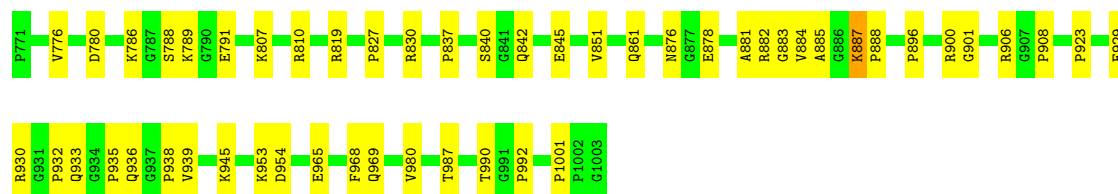
- Molecule 7: Collagen type XI alpha 1 chain

Chain BC: 76% 24%



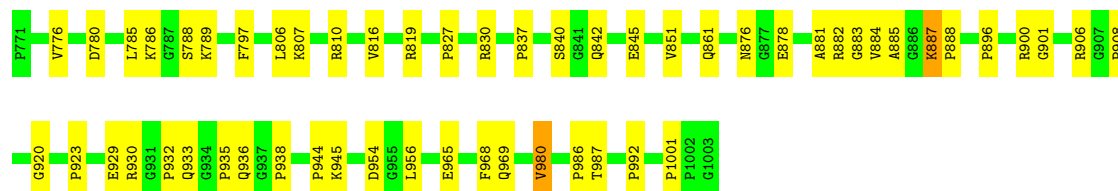
- Molecule 7: Collagen type XI alpha 1 chain

Chain GC: 78% 21%



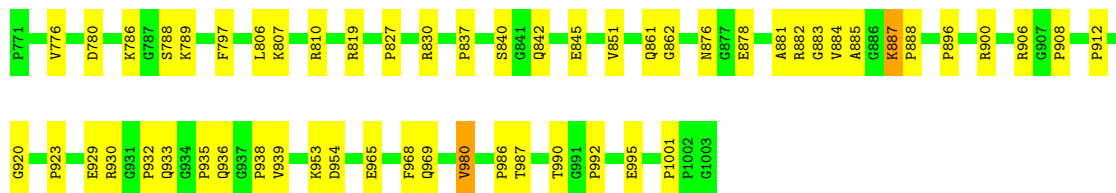
- Molecule 7: Collagen type XI alpha 1 chain

Chain LC: 76% 23%



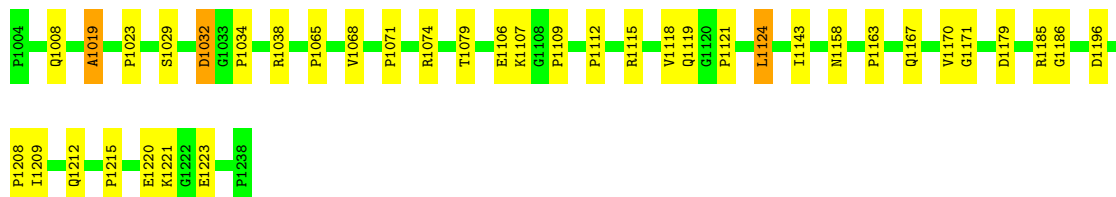
- Molecule 7: Collagen type XI alpha 1 chain

Chain QC:  76% 23%



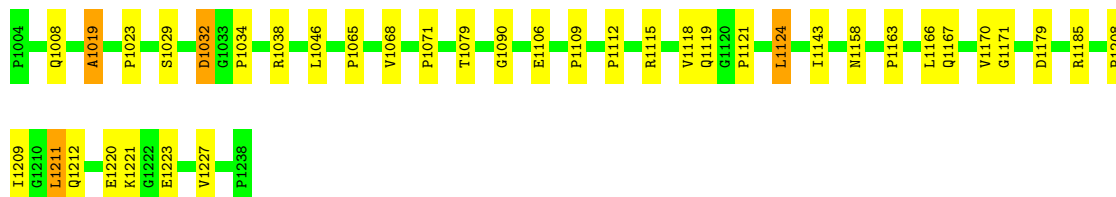
- Molecule 8: Collagen type XI alpha 1 chain

Chain CC:  84% 15%



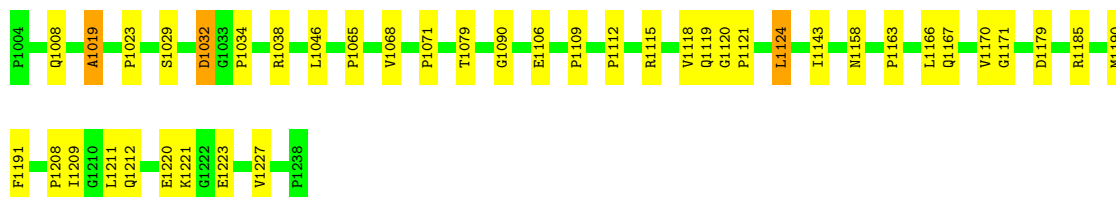
- Molecule 8: Collagen type XI alpha 1 chain

Chain HC:  84% 14%



- Molecule 8: Collagen type XI alpha 1 chain

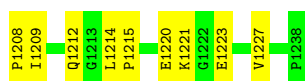
Chain MC:  83% 16%



- Molecule 8: Collagen type XI alpha 1 chain

Chain RC:  82% 16%





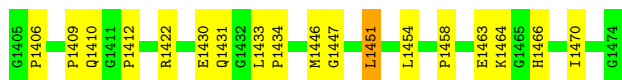
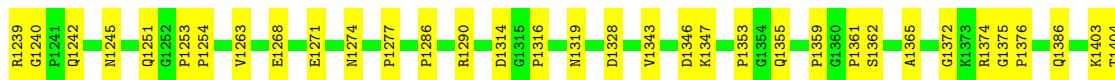
- Molecule 9: Fibrillar collagen NC1 domain-containing protein

Chain DC: 77% 23%



- Molecule 9: Fibrillar collagen NC1 domain-containing protein

Chain IC: 78% 22%



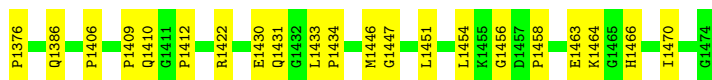
- Molecule 9: Fibrillar collagen NC1 domain-containing protein

Chain NC: 77% 23%



- Molecule 9: Fibrillar collagen NC1 domain-containing protein

Chain SC: 77% 23%



- Molecule 10: Fibrillar collagen NC1 domain-containing protein

Chain EC: 82% 17%



- Molecule 10: Fibrillar collagen NC1 domain-containing protein

Chain JC: 79% 20%



- Molecule 10: Fibrillar collagen NC1 domain-containing protein

Chain OC: 80% 18%



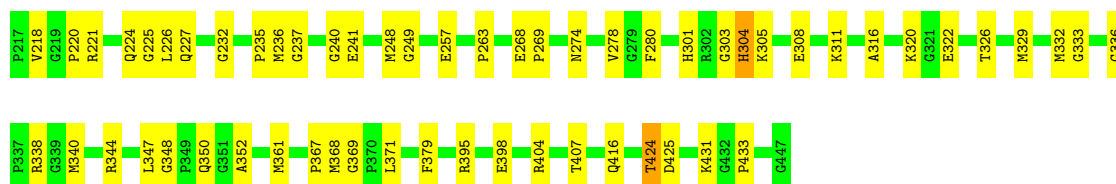
- Molecule 10: Fibrillar collagen NC1 domain-containing protein

Chain TC: 80% 18%



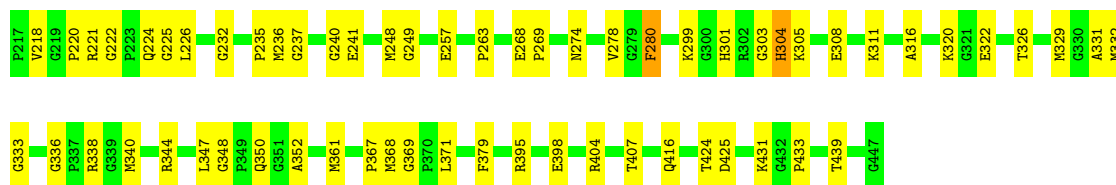
- Molecule 11: Chromaffin granule amine transporter isoform X1

Chain AB: 75% 24%



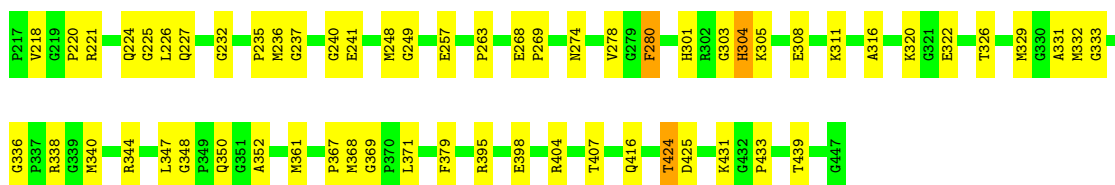
- Molecule 11: Chromaffin granule amine transporter isoform X1

Chain FB: 74% 26%



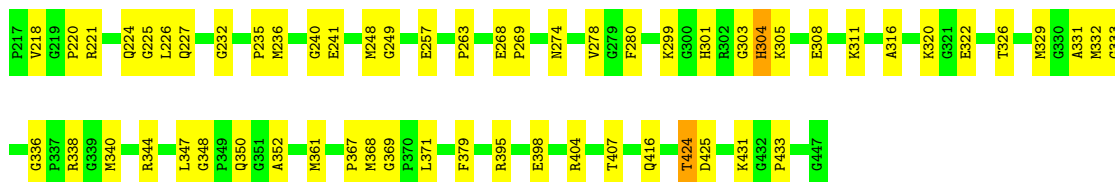
- Molecule 11: Chromaffin granule amine transporter isoform X1

Chain KB: 74% 25%



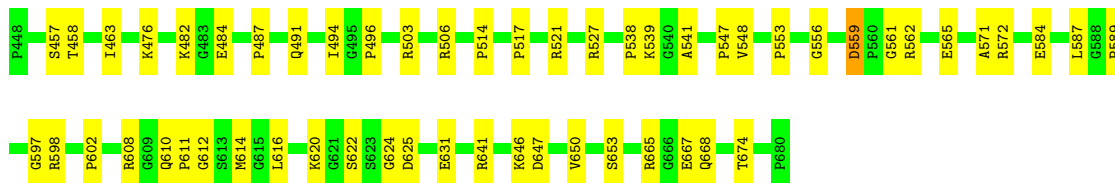
- Molecule 11: Chromaffin granule amine transporter isoform X1

Chain PB: 74% 25%



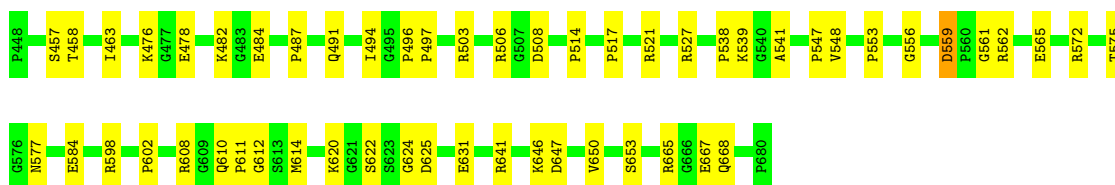
- Molecule 12: Collagen type V alpha 2 chain

Chain BB: 76% 23%



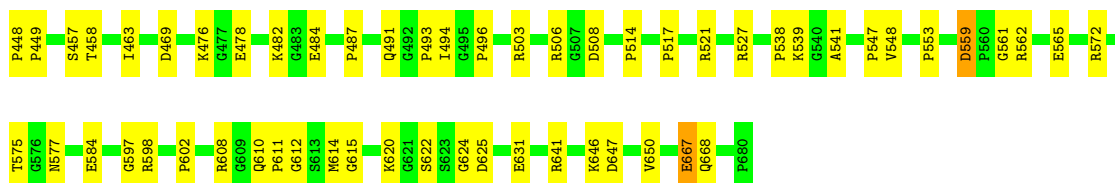
- Molecule 12: Collagen type V alpha 2 chain

Chain GB: 77% 23%



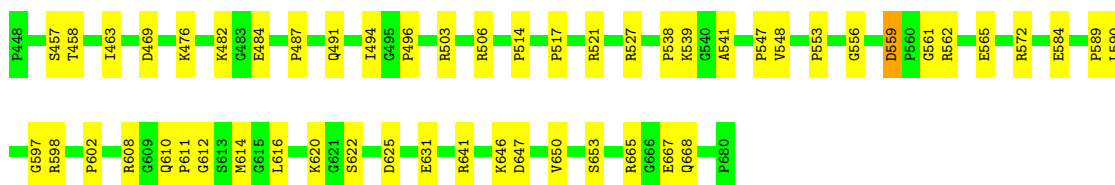
- Molecule 12: Collagen type V alpha 2 chain

Chain LB: 76% 23%



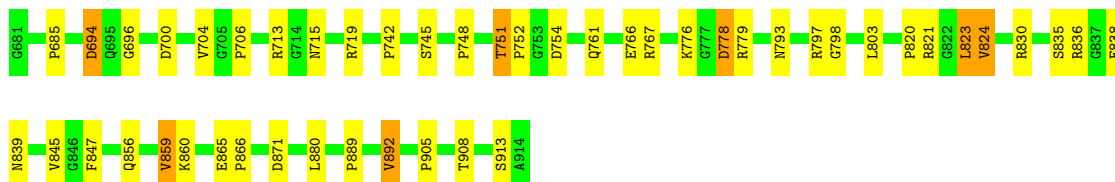
- Molecule 12: Collagen type V alpha 2 chain

Chain QB: 77% 22%



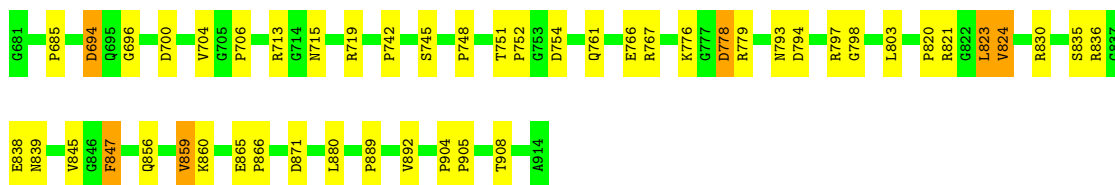
- Molecule 13: Collagen type V alpha 2 chain

Chain CB: 79% 18% .



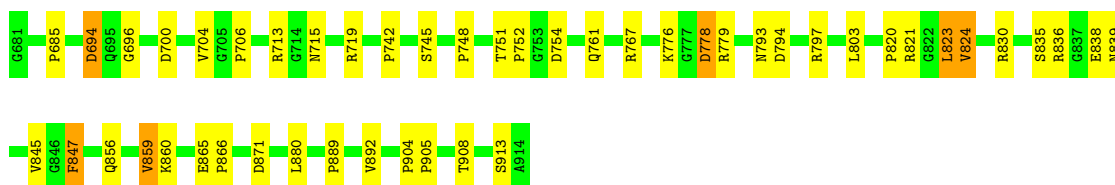
- Molecule 13: Collagen type V alpha 2 chain

Chain HB: 79% 18% .



- Molecule 13: Collagen type V alpha 2 chain

Chain MB: 79% 18% .



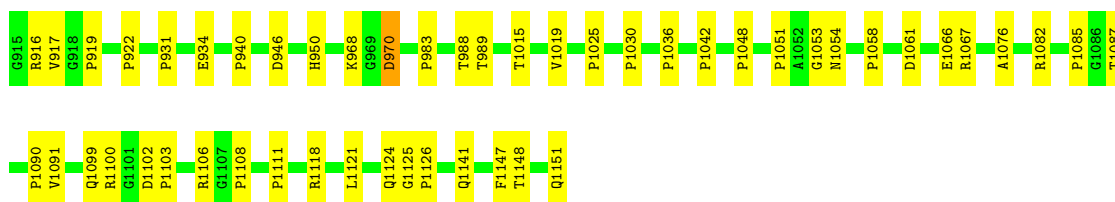
- Molecule 13: Collagen type V alpha 2 chain

Chain RB: 80% 17% .



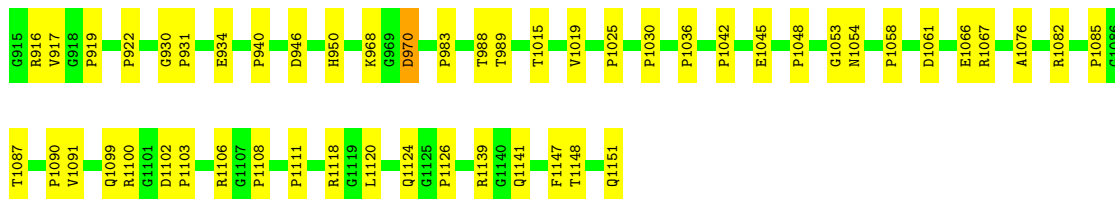
- Molecule 14: Collagen alpha-2(V) chain preproprotein

Chain DB: 79% 21%



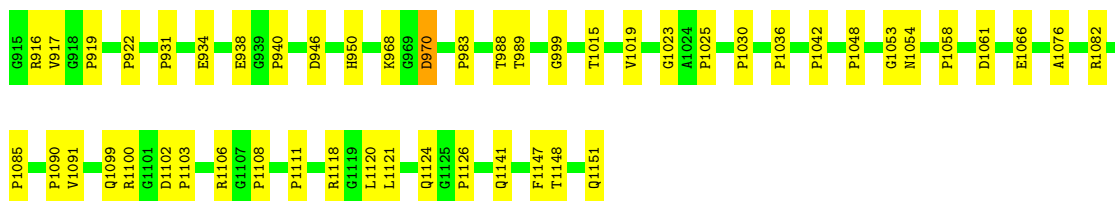
- Molecule 14: Collagen alpha-2(V) chain preproprotein

Chain IB: 78% 21%



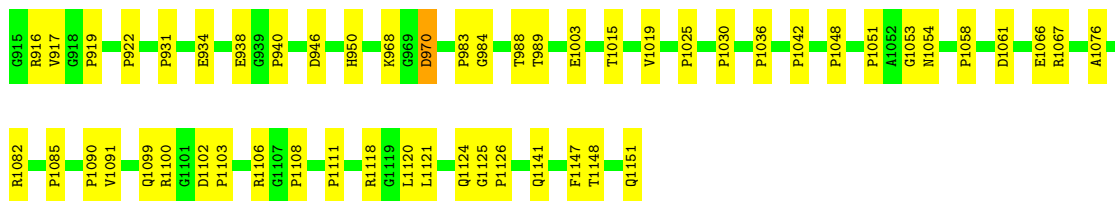
- Molecule 14: Collagen alpha-2(V) chain preproprotein

Chain NB: 79% 21%



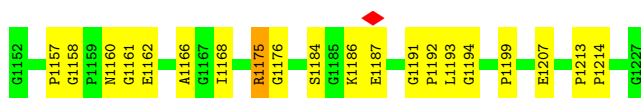
- Molecule 14: Collagen alpha-2(V) chain preproprotein

Chain SB: 78% 22%



- Molecule 15: Collagen alpha-2(V) chain preproprotein

Chain EB: 74% 25%

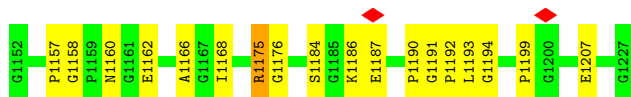
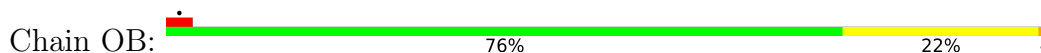


- Molecule 15: Collagen alpha-2(V) chain preproprotein

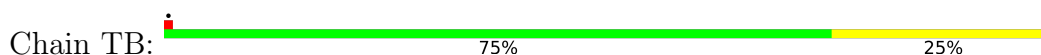
Chain JB: 75% 24%



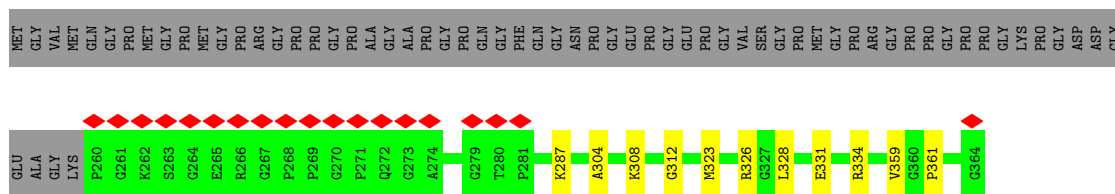
- Molecule 15: Collagen alpha-2(V) chain preproprotein



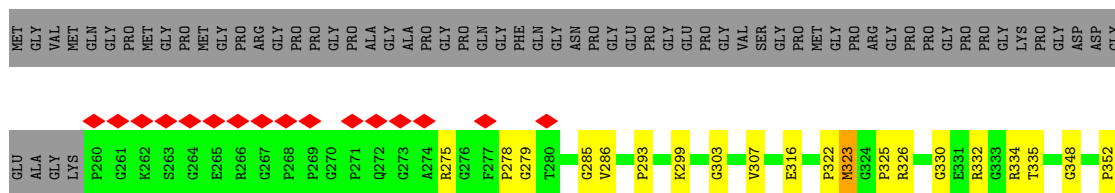
- Molecule 15: Collagen alpha-2(V) chain preproprotein



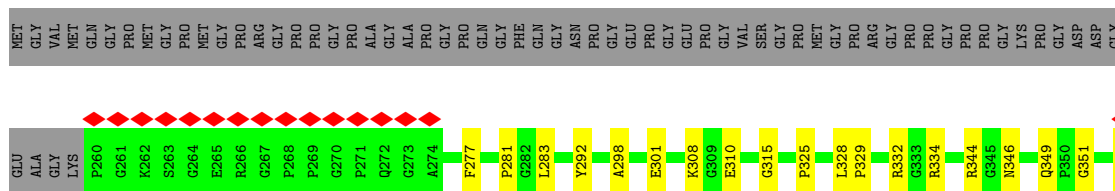
- Molecule 16: Collagen type II alpha 1 chain



- Molecule 16: Collagen type II alpha 1 chain



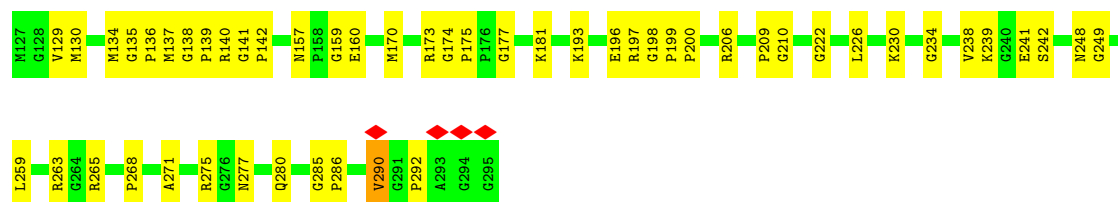
- Molecule 16: Collagen type II alpha 1 chain





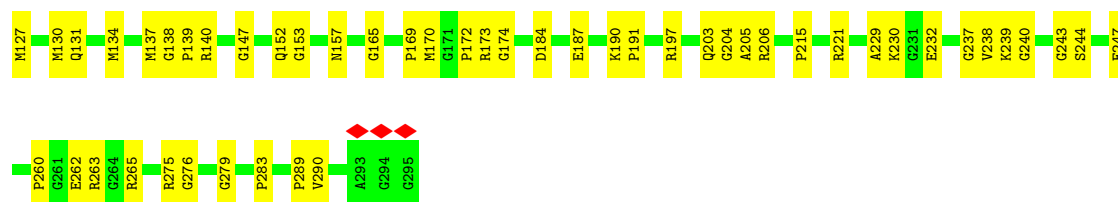
- Molecule 16: Collagen type II alpha 1 chain

Chain AG: 70% 30%



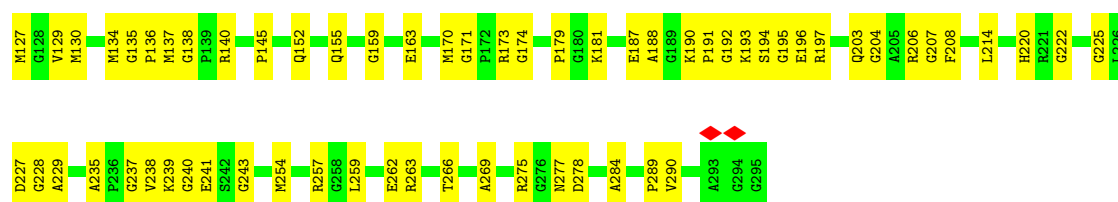
- Molecule 16: Collagen type II alpha 1 chain

Chain AH: 71% 29%



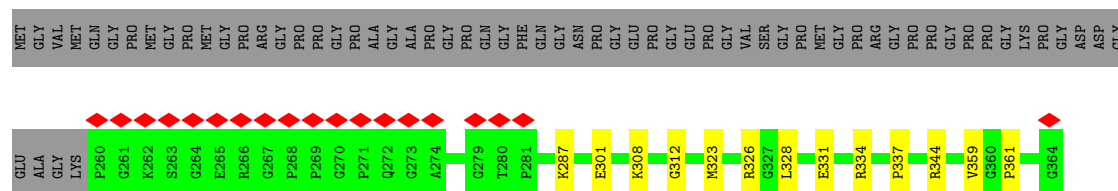
- Molecule 16: Collagen type II alpha 1 chain

Chain AI: 63% 37%



- Molecule 16: Collagen type II alpha 1 chain

Chain FD: 11% 54% 8% 38%

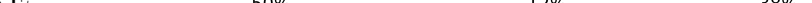


- Molecule 16: Collagen type II alpha 1 chain

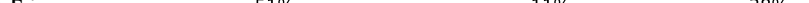
Chain FE: 9% 51% 10% 38%



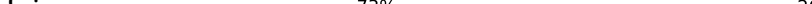


- Chain KE: 

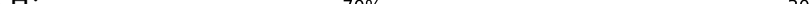


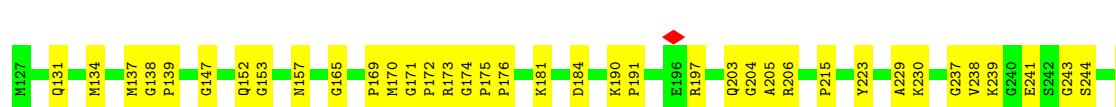
- Chain KF: 



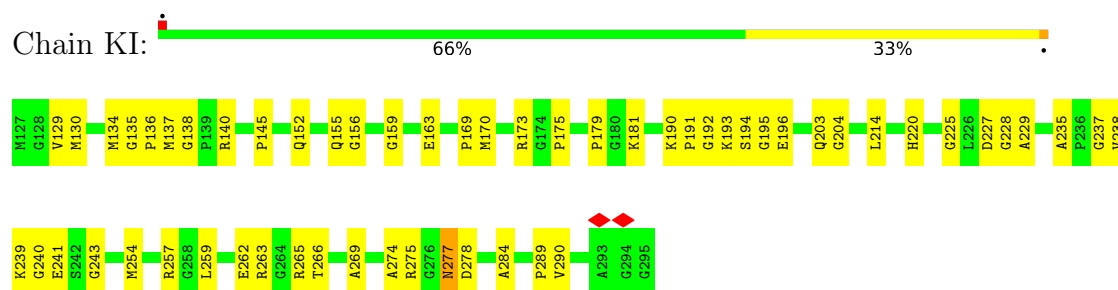
- Chain KG:  73% 26%



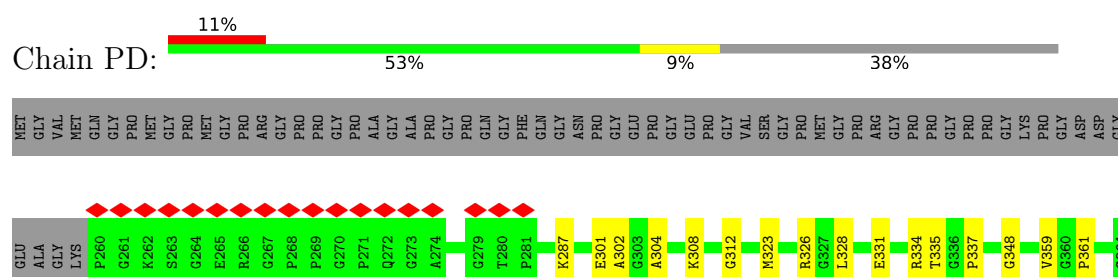
- Chain KH: 



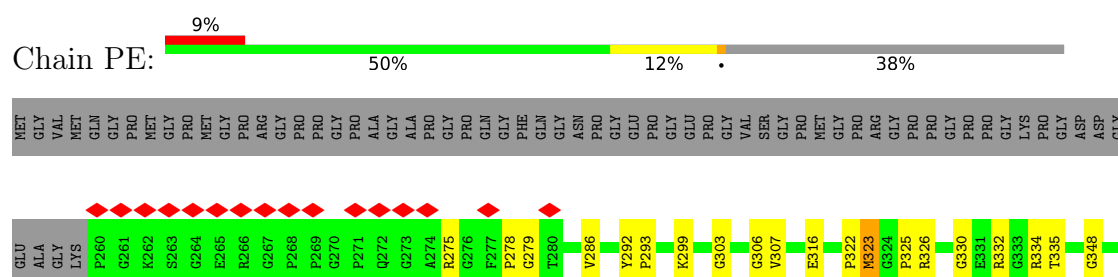
- Molecule 16: Collagen type II alpha 1 chain



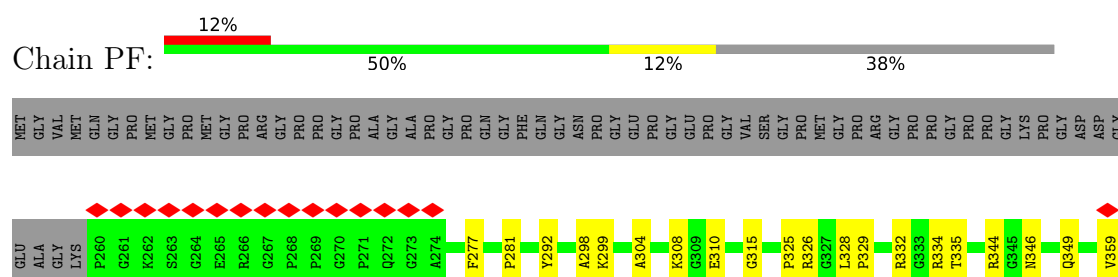
- Molecule 16: Collagen type II alpha 1 chain



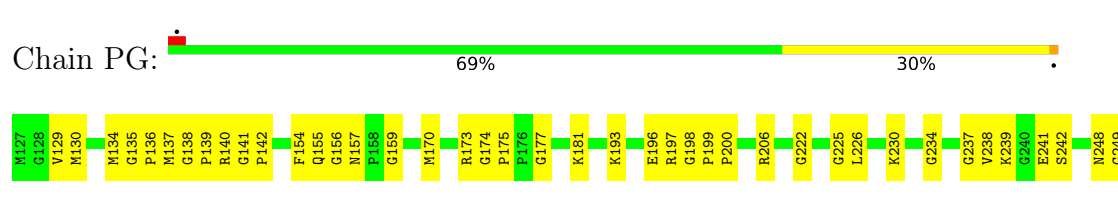
- Molecule 16: Collagen type II alpha 1 chain



- Molecule 16: Collagen type II alpha 1 chain

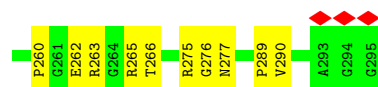
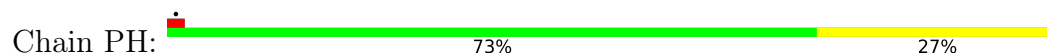


- Molecule 16: Collagen type II alpha 1 chain

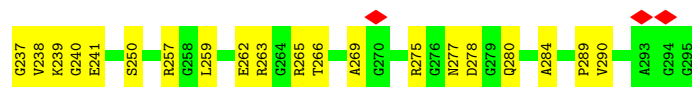
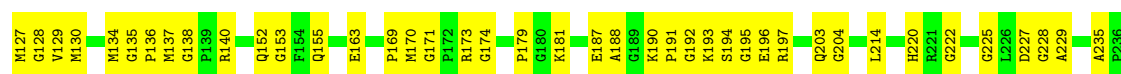




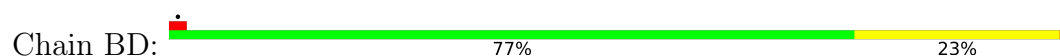
- Molecule 16: Collagen type II alpha 1 chain



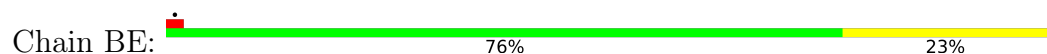
- Molecule 16: Collagen type II alpha 1 chain



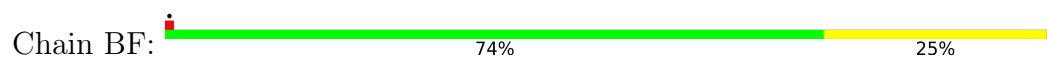
- Molecule 17: Collagen type II alpha 1 chain

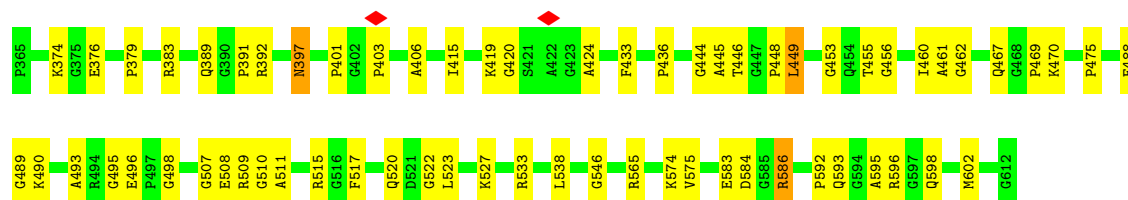


- Molecule 17: Collagen type II alpha 1 chain

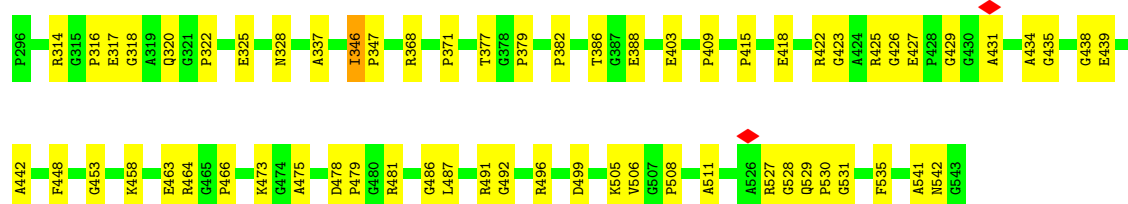
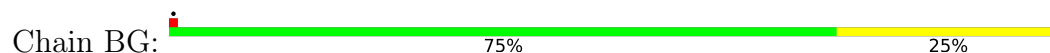


- Molecule 17: Collagen type II alpha 1 chain

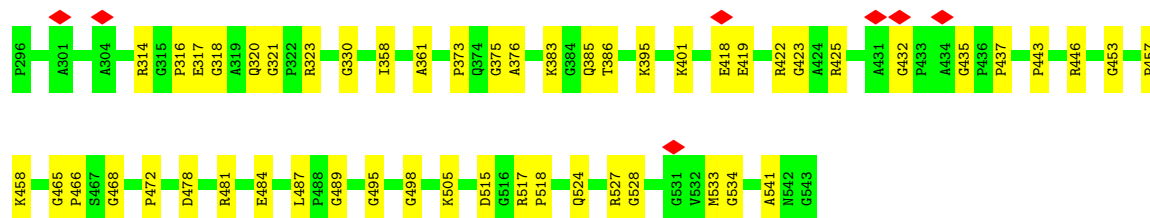
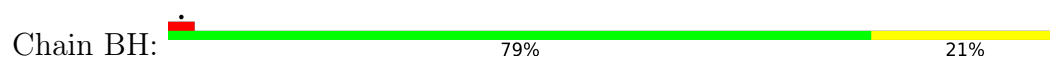




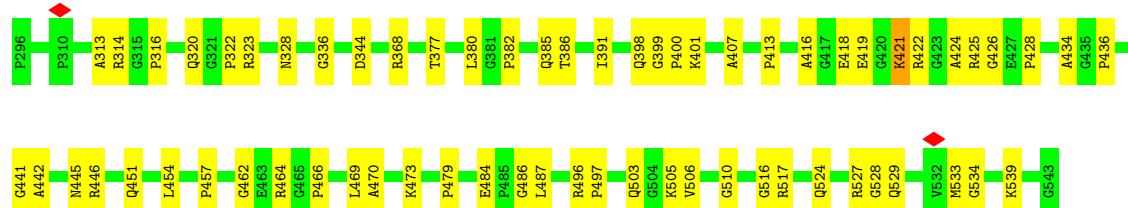
- Molecule 17: Collagen type II alpha 1 chain



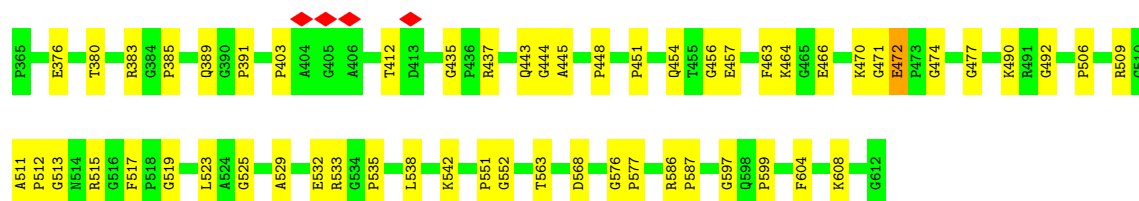
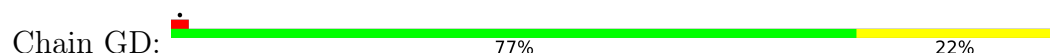
- Molecule 17: Collagen type II alpha 1 chain



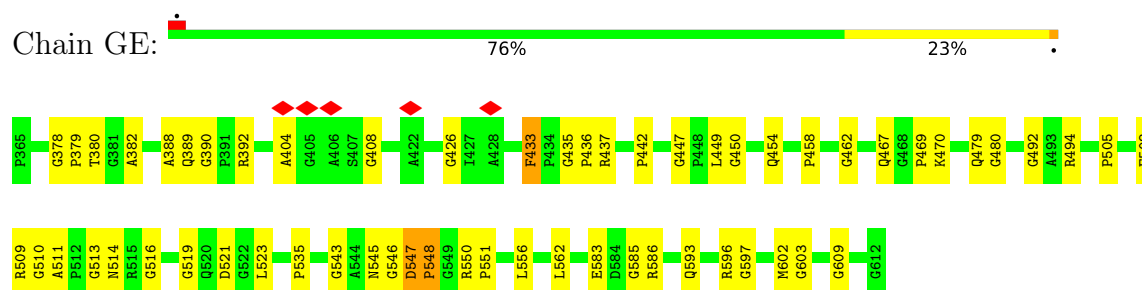
- Molecule 17: Collagen type II alpha 1 chain



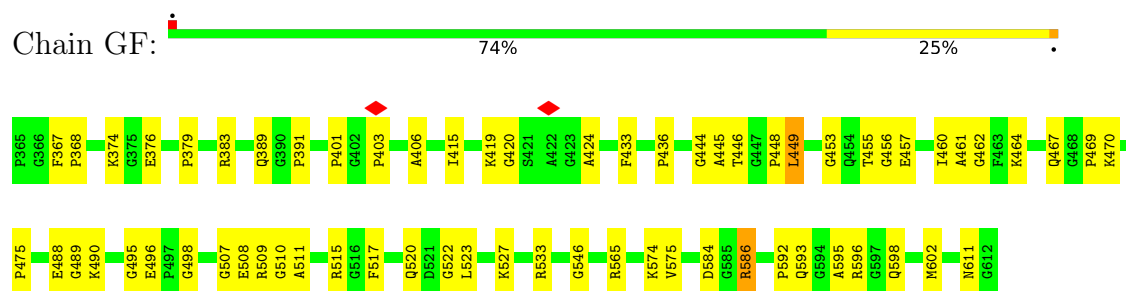
- Molecule 17: Collagen type II alpha 1 chain



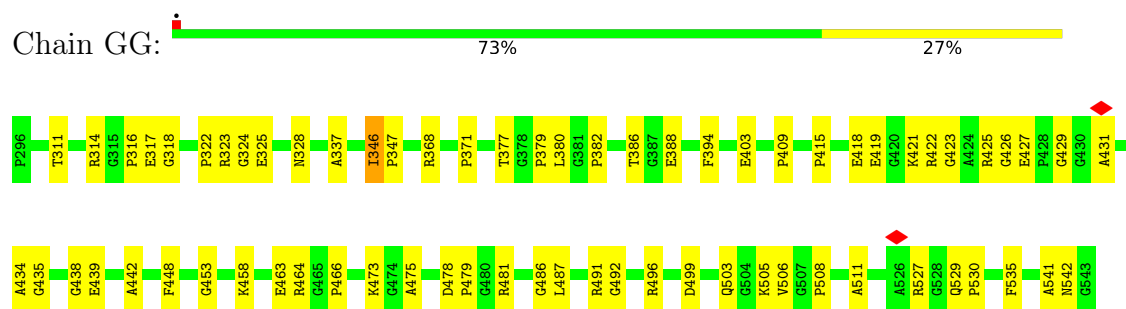
• Molecule 17: Collagen type II alpha 1 chain



• Molecule 17: Collagen type II alpha 1 chain



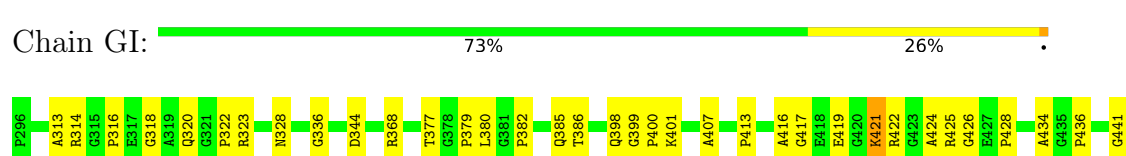
• Molecule 17: Collagen type II alpha 1 chain



• Molecule 17: Collagen type II alpha 1 chain

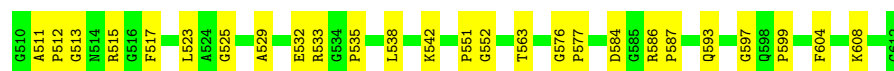
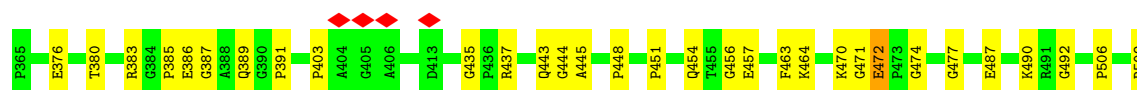
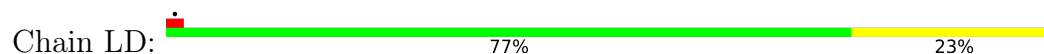


• Molecule 17: Collagen type II alpha 1 chain

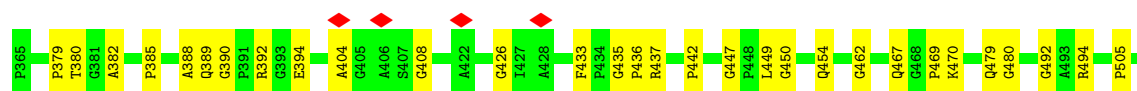
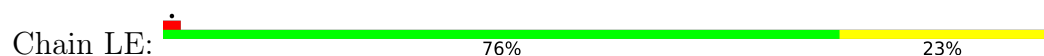




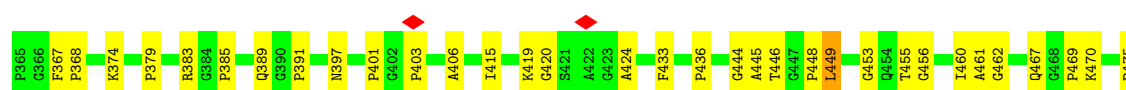
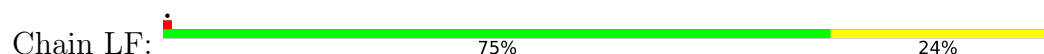
- Molecule 17: Collagen type II alpha 1 chain



- Molecule 17: Collagen type II alpha 1 chain



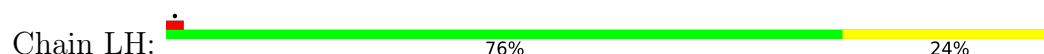
- Molecule 17: Collagen type II alpha 1 chain

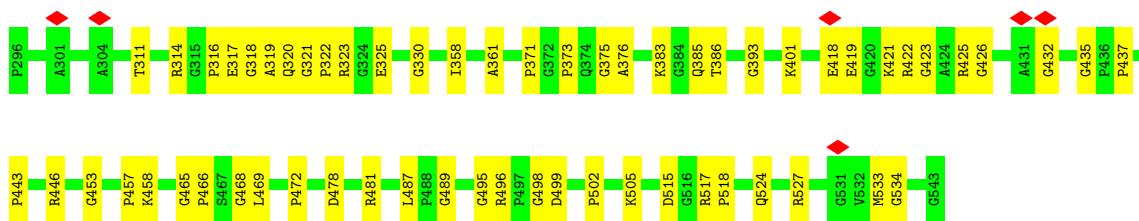


- Molecule 17: Collagen type II alpha 1 chain

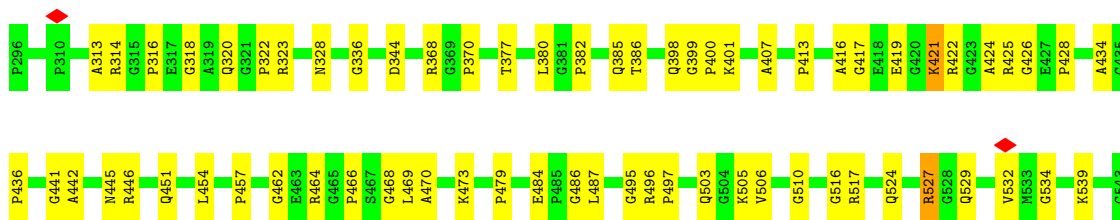


- Molecule 17: Collagen type II alpha 1 chain

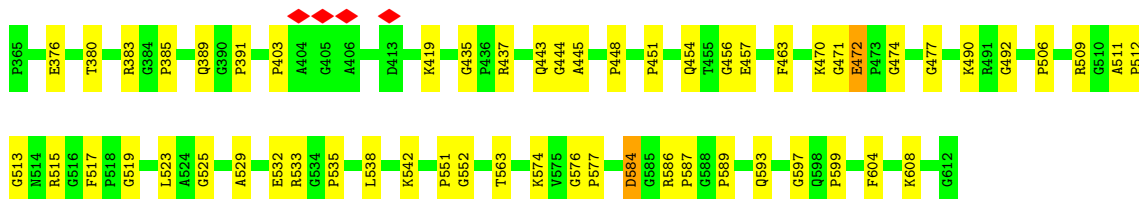
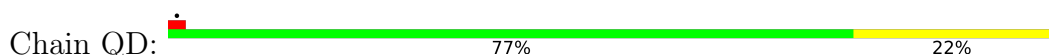




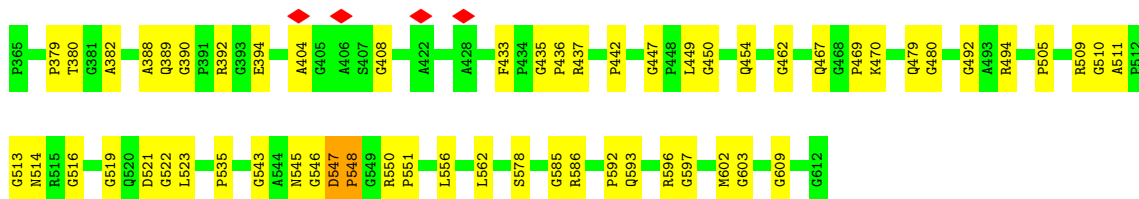
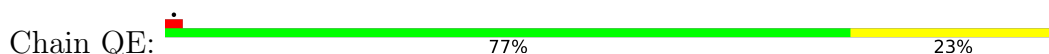
- Molecule 17: Collagen type II alpha 1 chain



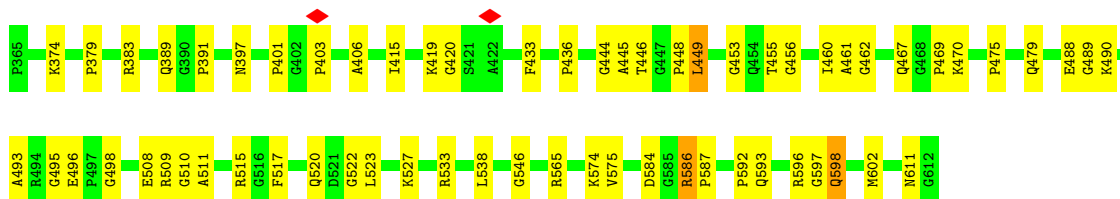
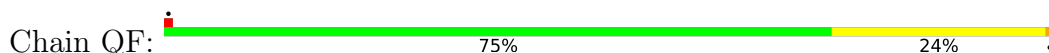
- Molecule 17: Collagen type II alpha 1 chain



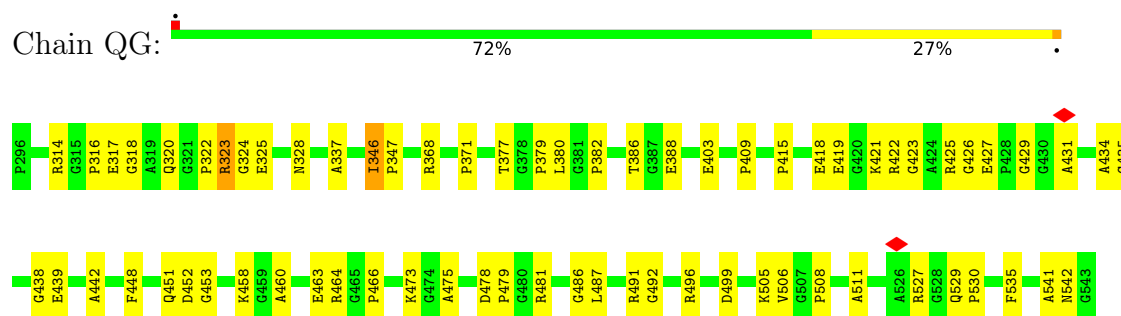
- Molecule 17: Collagen type II alpha 1 chain



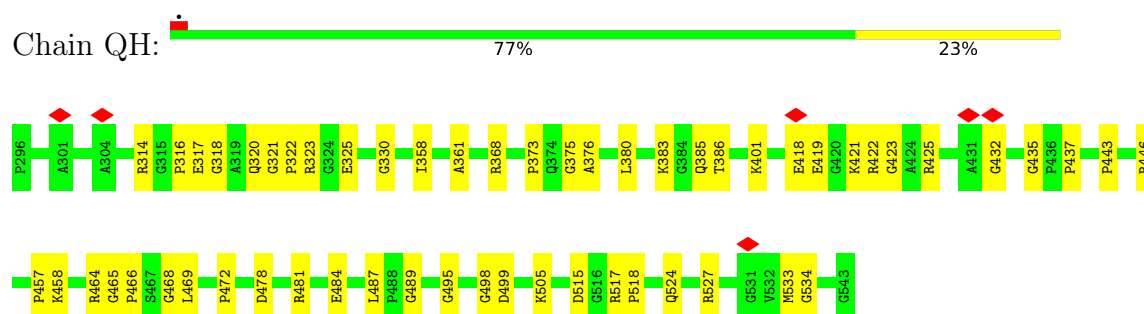
- Molecule 17: Collagen type II alpha 1 chain



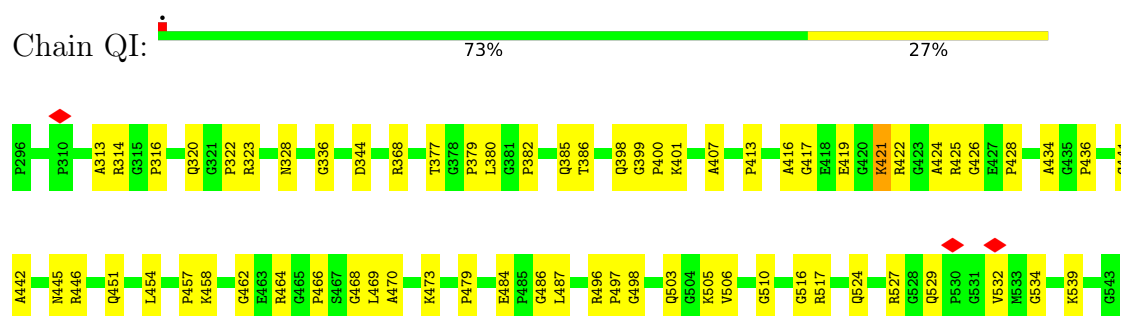
- Molecule 17: Collagen type II alpha 1 chain



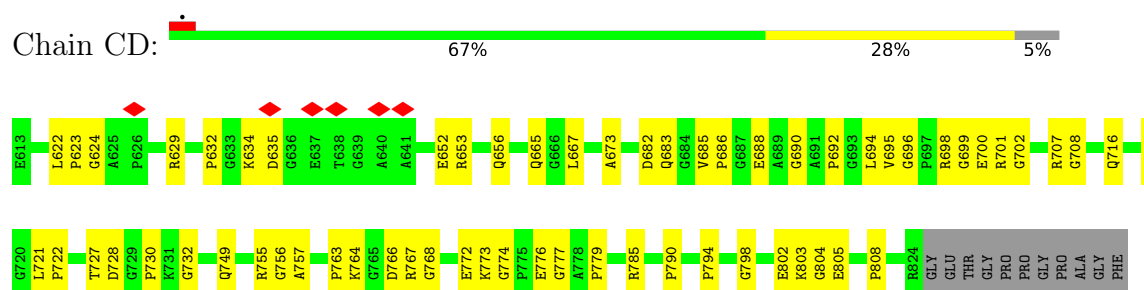
- Molecule 17: Collagen type II alpha 1 chain



- Molecule 17: Collagen type II alpha 1 chain

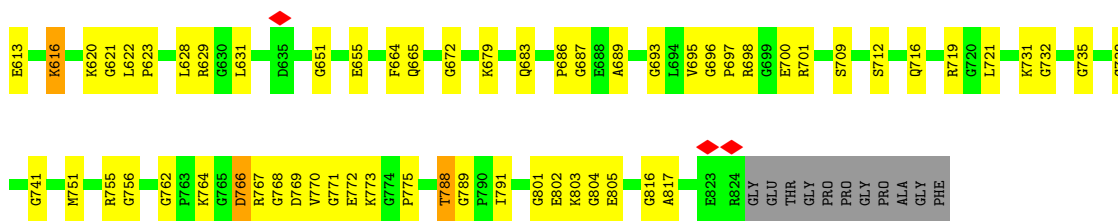


- Molecule 18: Collagen type II alpha 1 chain



- Molecule 18: Collagen type II alpha 1 chain





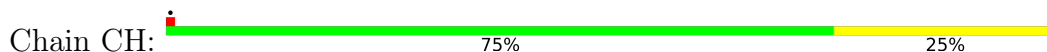
• Molecule 18: Collagen type II alpha 1 chain



• Molecule 18: Collagen type II alpha 1 chain



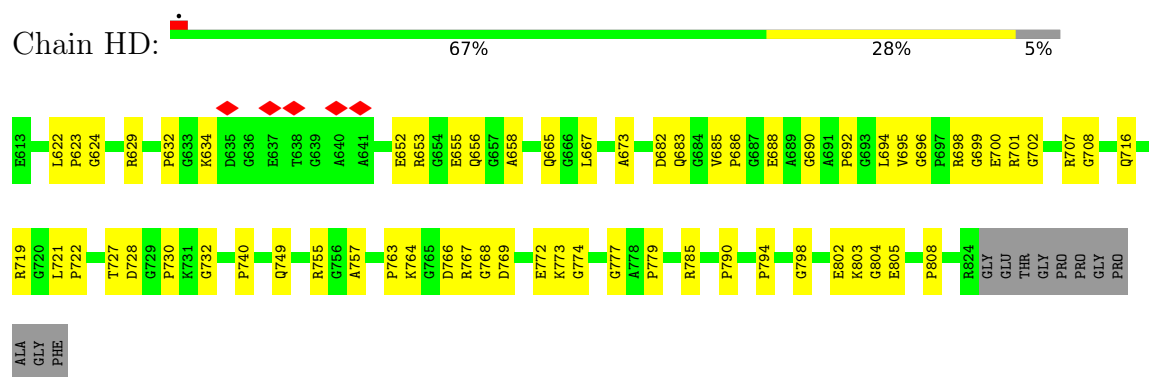
• Molecule 18: Collagen type II alpha 1 chain



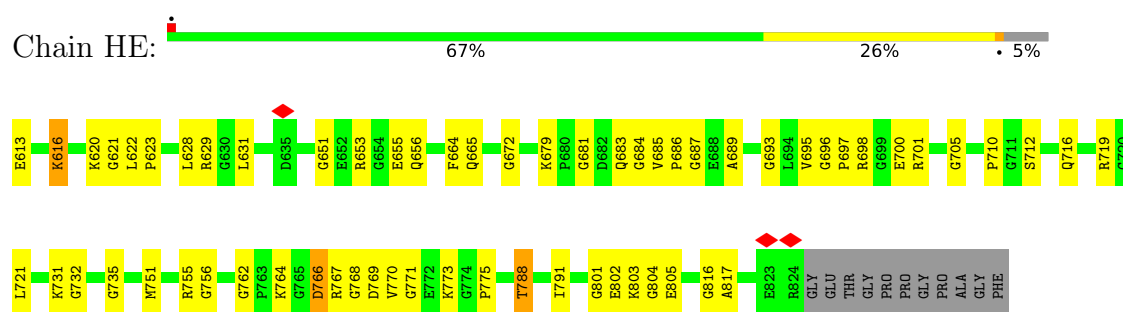
• Molecule 18: Collagen type II alpha 1 chain



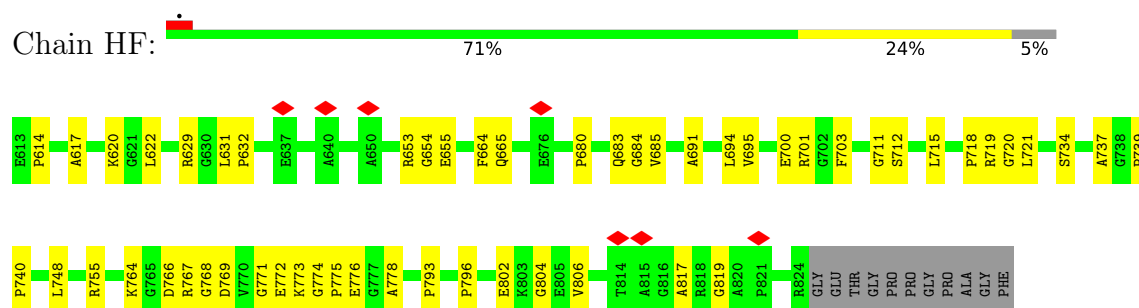
• Molecule 18: Collagen type II alpha 1 chain



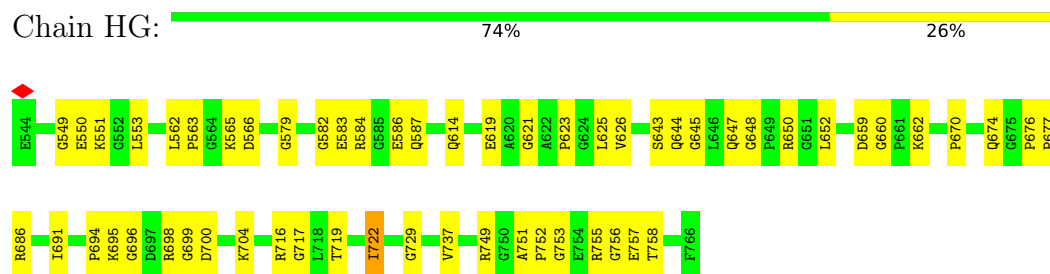
• Molecule 18: Collagen type II alpha 1 chain



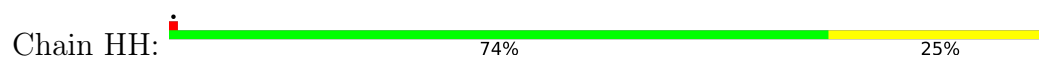
• Molecule 18: Collagen type II alpha 1 chain

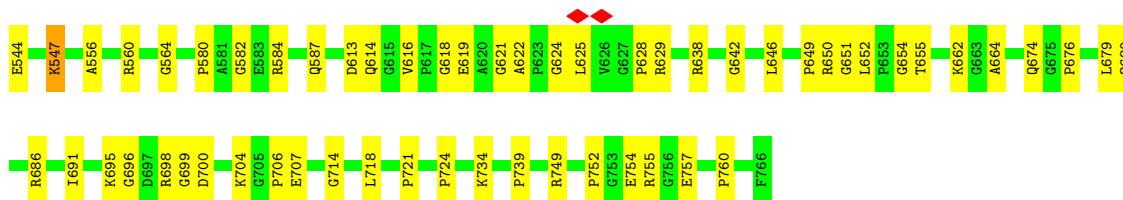


• Molecule 18: Collagen type II alpha 1 chain

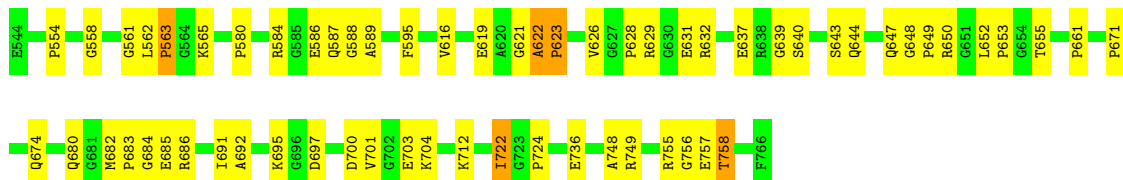


• Molecule 18: Collagen type II alpha 1 chain

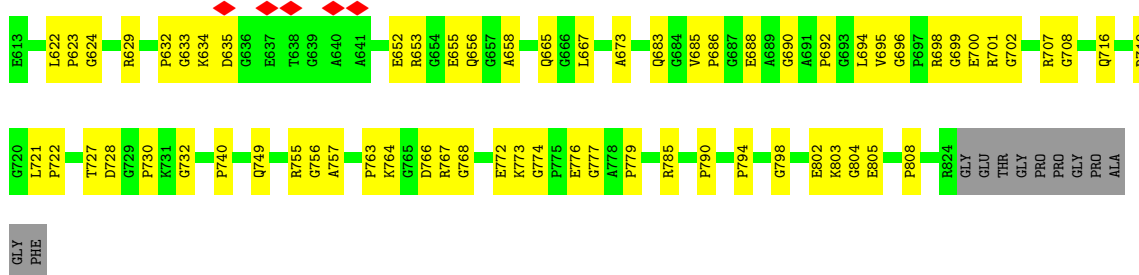




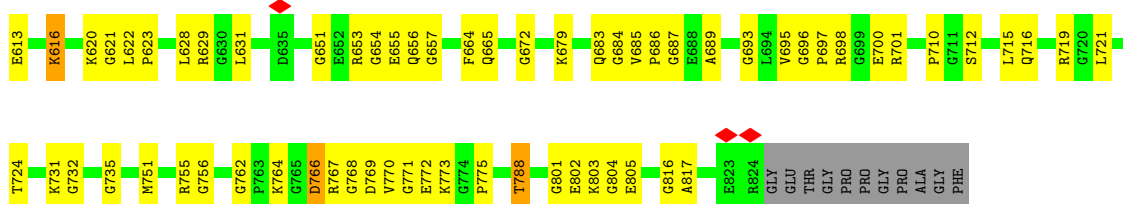
• Molecule 18: Collagen type II alpha 1 chain



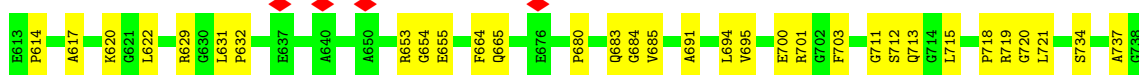
• Molecule 18: Collagen type II alpha 1 chain

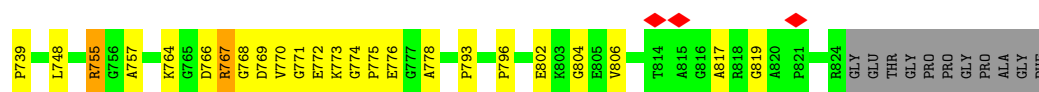


• Molecule 18: Collagen type II alpha 1 chain



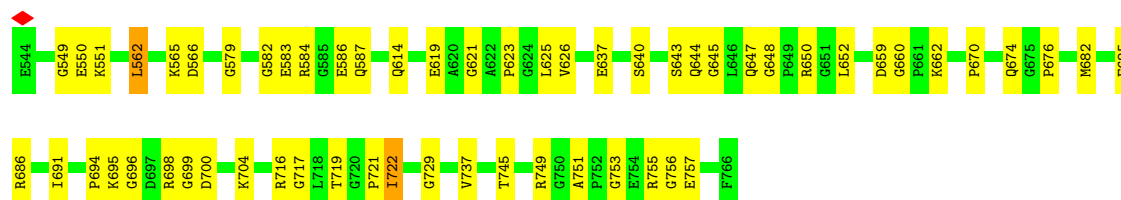
• Molecule 18: Collagen type II alpha 1 chain





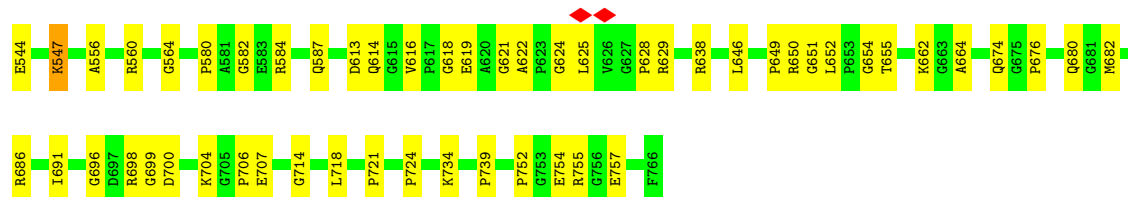
• Molecule 18: Collagen type II alpha 1 chain

Chain MG: 74% 25% .



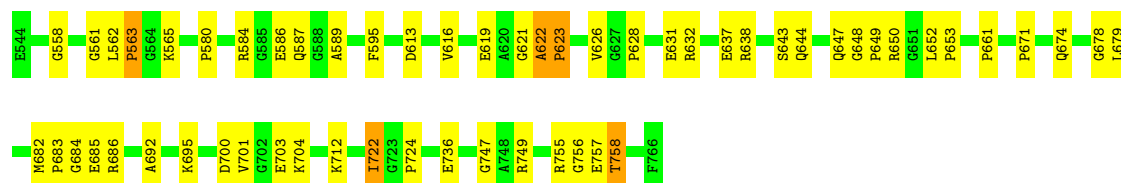
• Molecule 18: Collagen type II alpha 1 chain

Chain MH: 76% 23% .



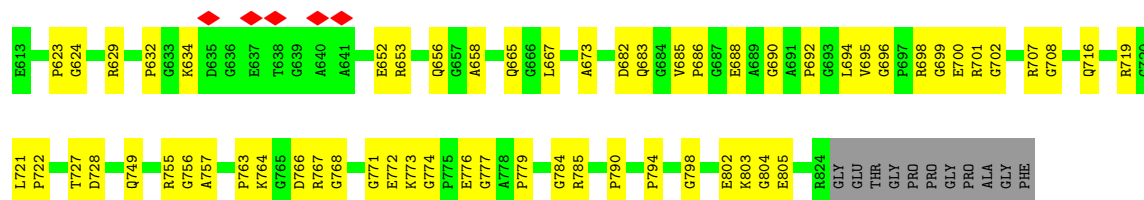
• Molecule 18: Collagen type II alpha 1 chain

Chain MI: 74% 23% .



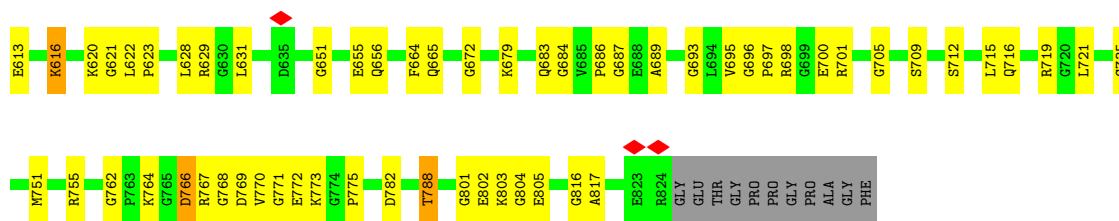
• Molecule 18: Collagen type II alpha 1 chain

Chain RD: 68% 27% 5% .



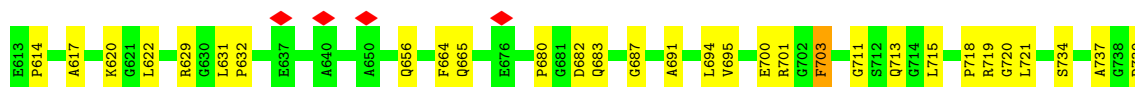
• Molecule 18: Collagen type II alpha 1 chain

Chain RE: 69% 25% 5% .



- Molecule 18: Collagen type II alpha 1 chain

Chain RF: 69% 25% • 5%



- Molecule 18: Collagen type II alpha 1 chain

Chain RG: 73% 26% •



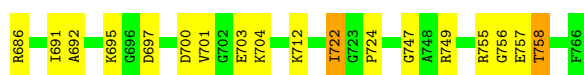
- Molecule 18: Collagen type II alpha 1 chain

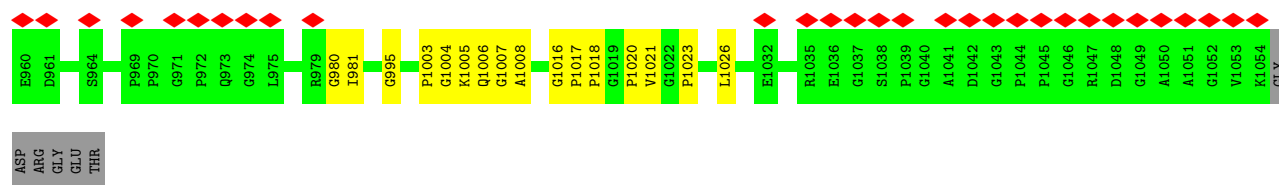
Chain RH: 76% 23% •



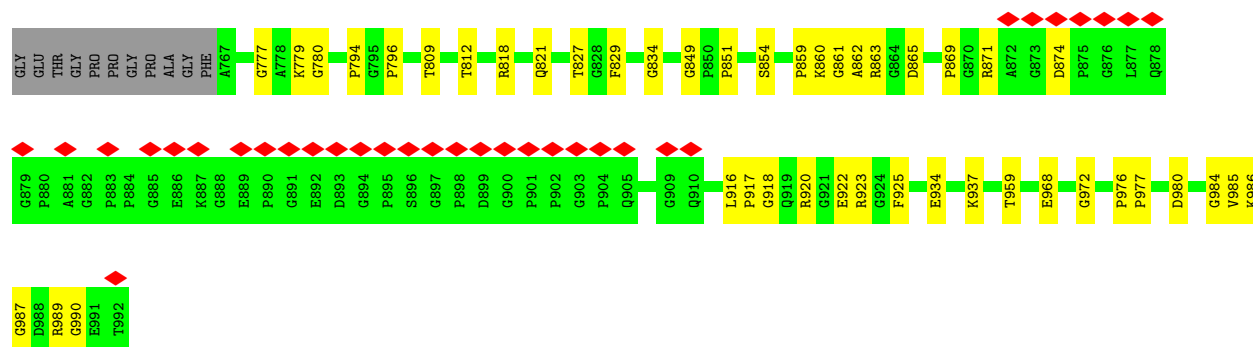
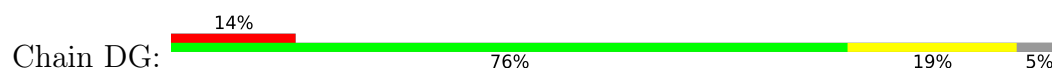
- Molecule 18: Collagen type II alpha 1 chain

Chain RI: 75% 22% •

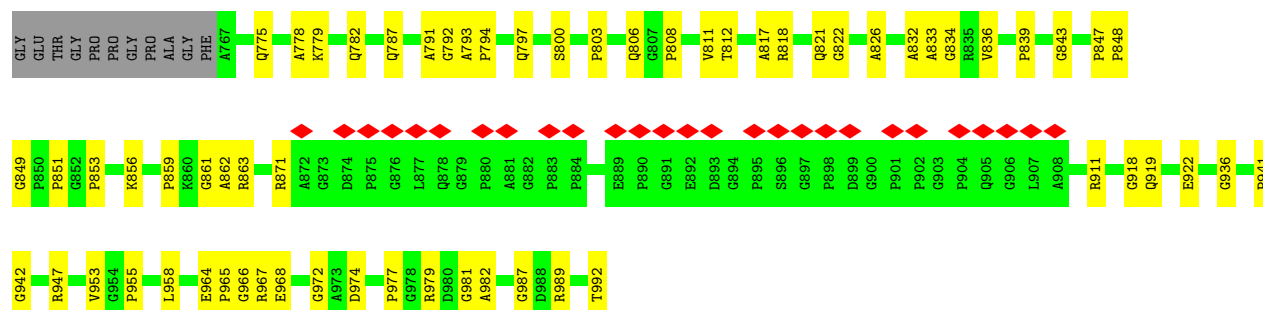




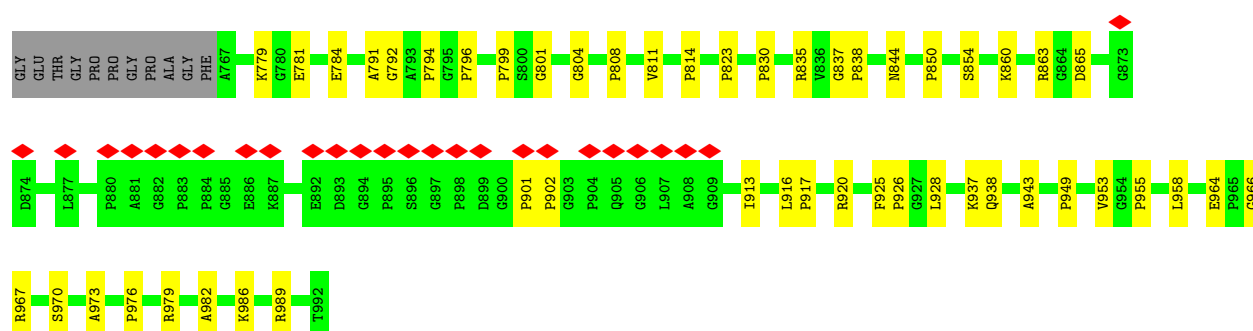
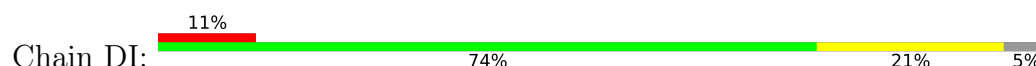
• Molecule 19: Collagen type II alpha 1 chain



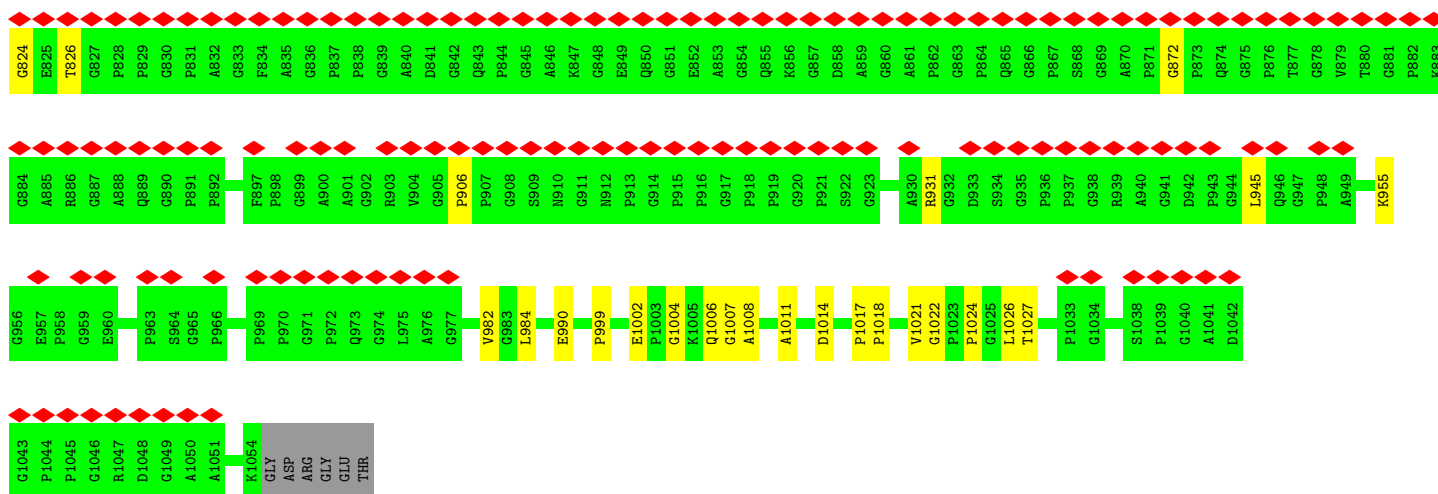
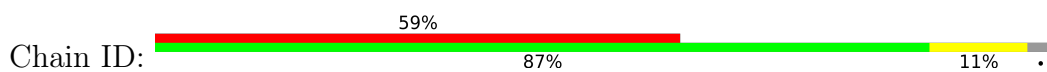
• Molecule 19: Collagen type II alpha 1 chain



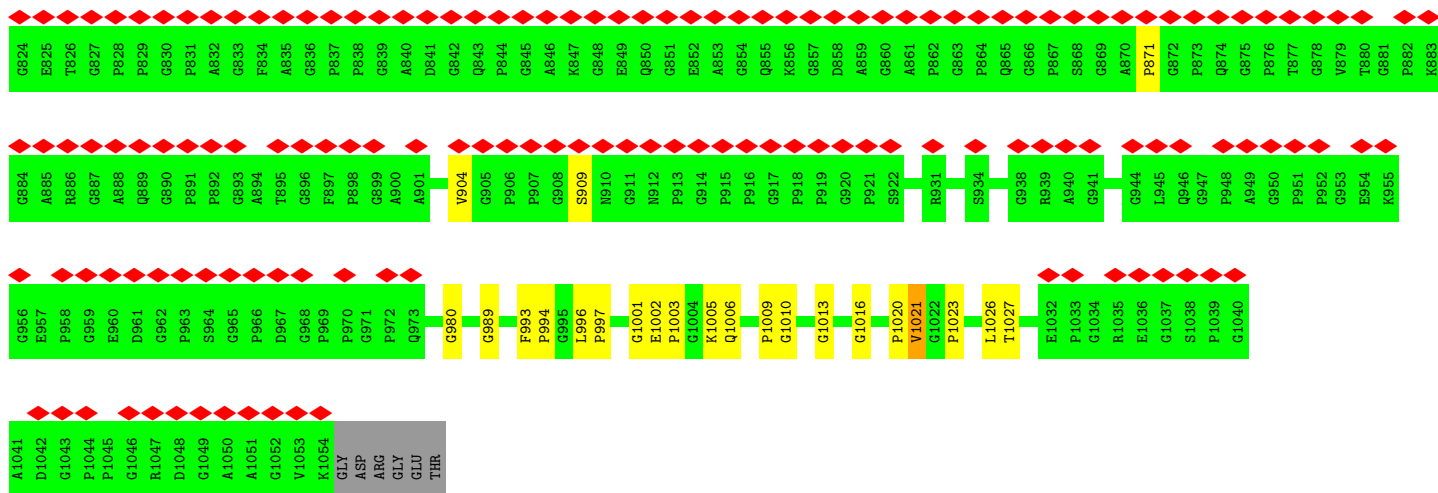
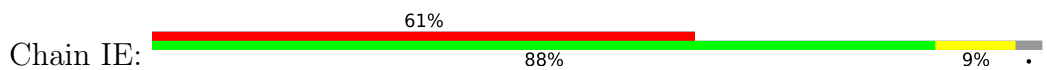
• Molecule 19: Collagen type II alpha 1 chain



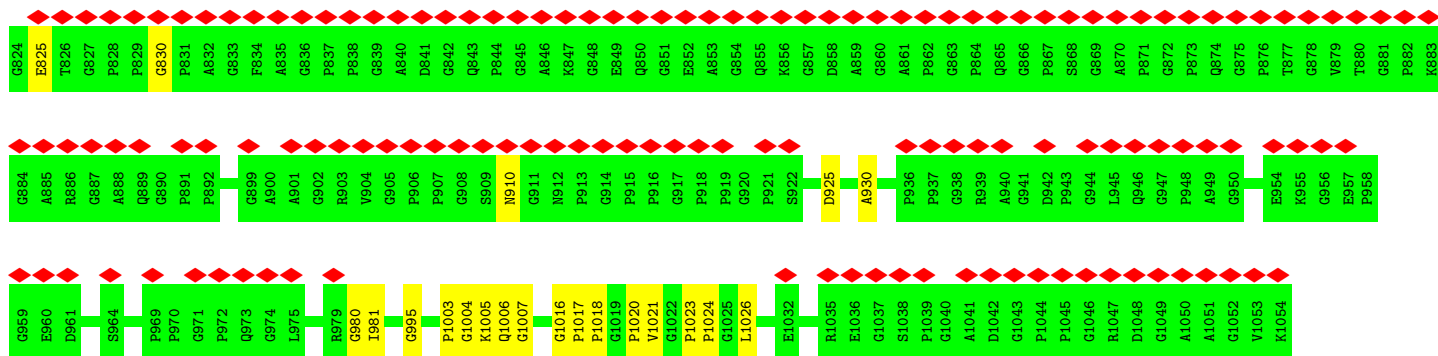
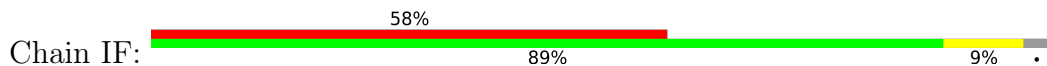
• Molecule 19: Collagen type II alpha 1 chain



• Molecule 19: Collagen type II alpha 1 chain



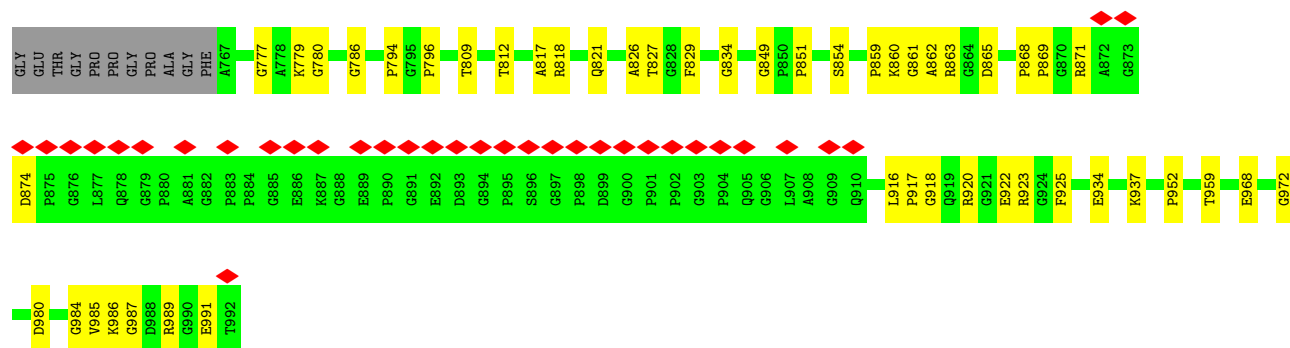
• Molecule 19: Collagen type II alpha 1 chain



GLY
ASP
ARG
GLY
GLU
THR

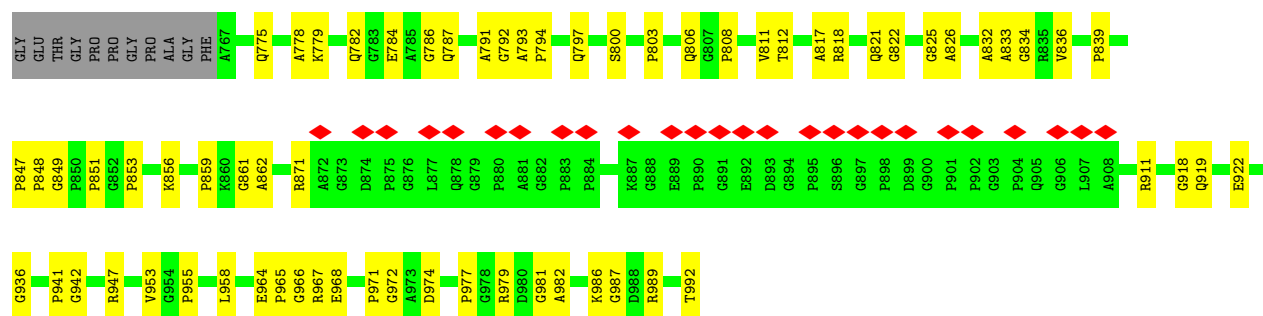
● Molecule 19: Collagen type II alpha 1 chain

Chain IG: 



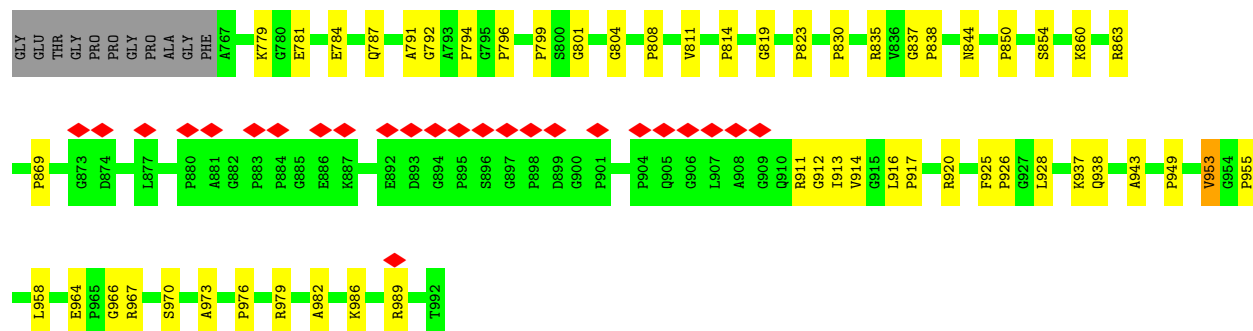
● Molecule 19: Collagen type II alpha 1 chain

Chain IH: 

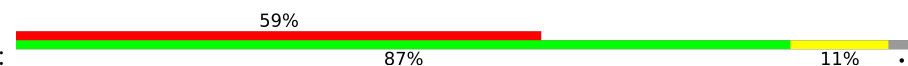


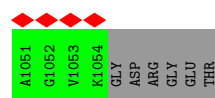
● Molecule 19: Collagen type II alpha 1 chain

Chain II: 

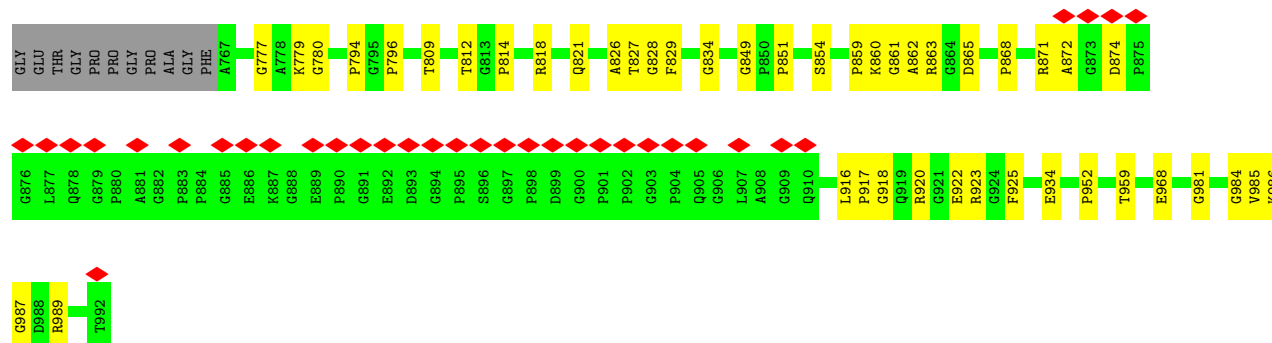
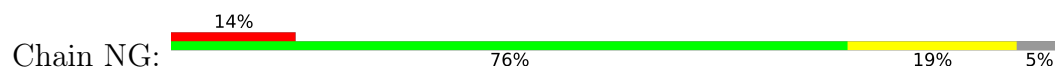


● Molecule 19: Collagen type II alpha 1 chain

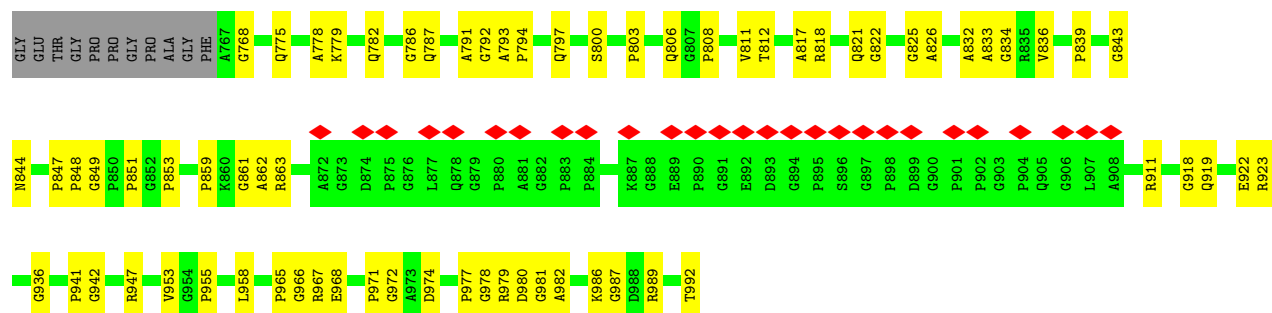
Chain ND: 



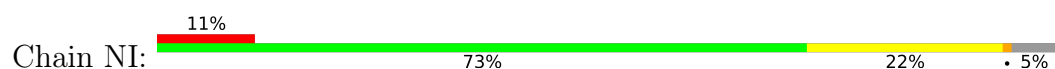
• Molecule 19: Collagen type II alpha 1 chain



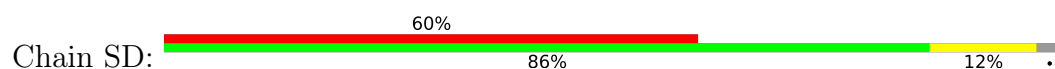
• Molecule 19: Collagen type II alpha 1 chain

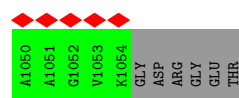


• Molecule 19: Collagen type II alpha 1 chain

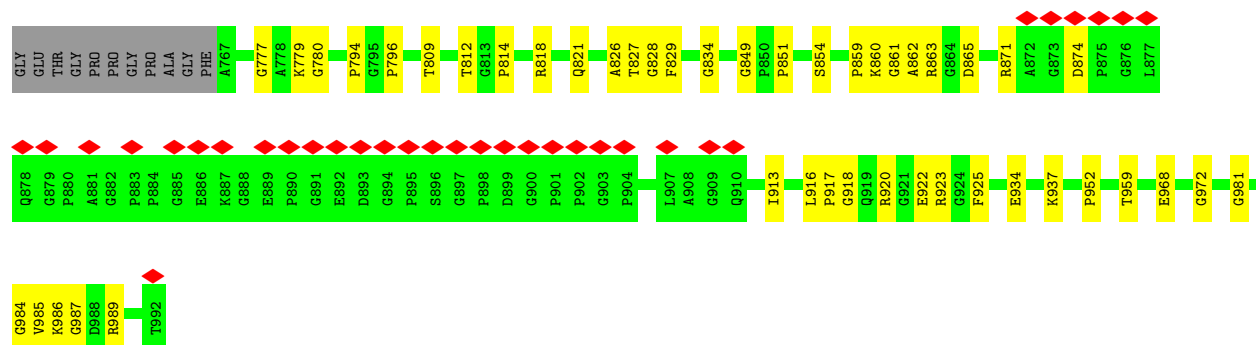
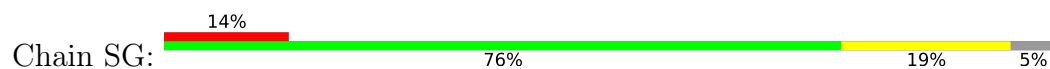


• Molecule 19: Collagen type II alpha 1 chain

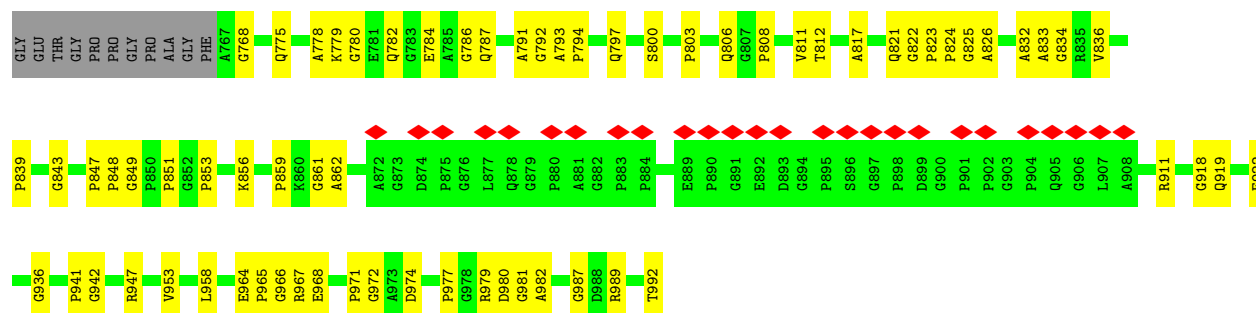




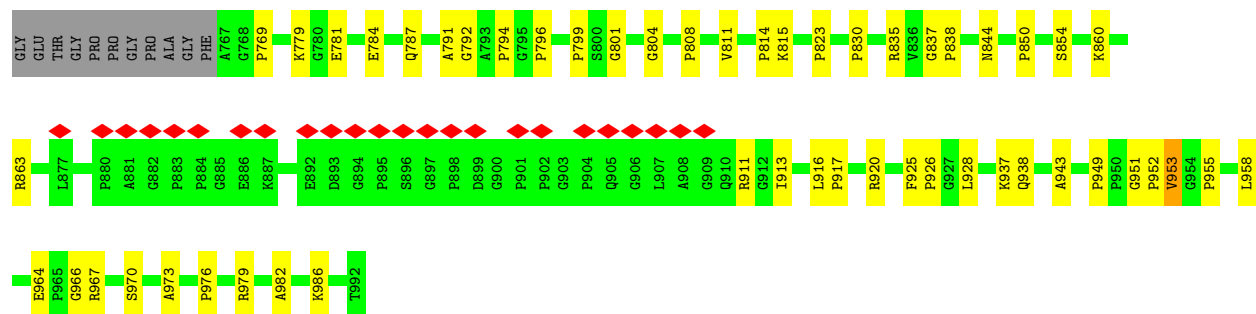
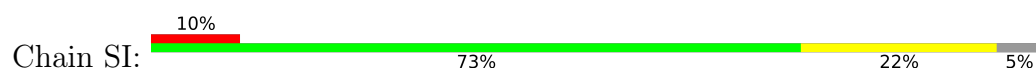
• Molecule 19: Collagen type II alpha 1 chain



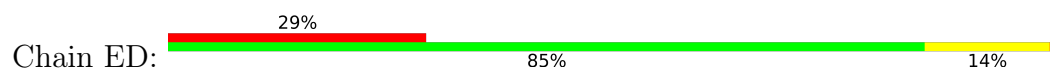
• Molecule 19: Collagen type II alpha 1 chain

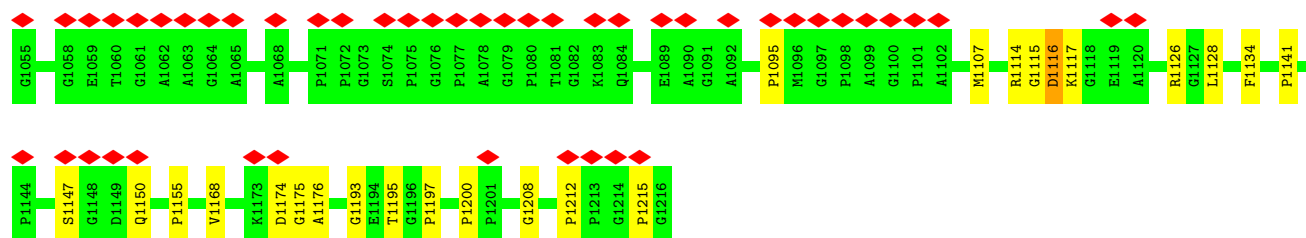


• Molecule 19: Collagen type II alpha 1 chain

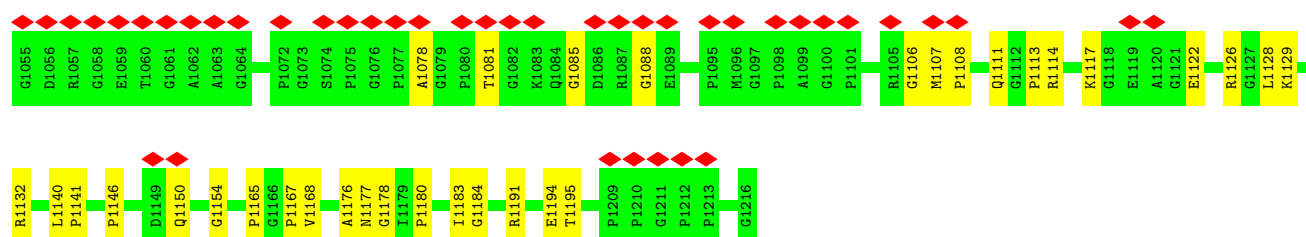
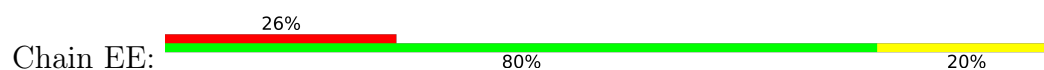


• Molecule 20: Collagen type II alpha 1 chain

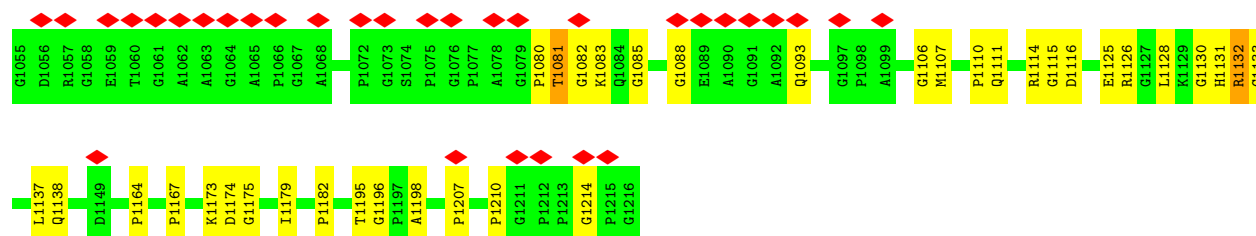
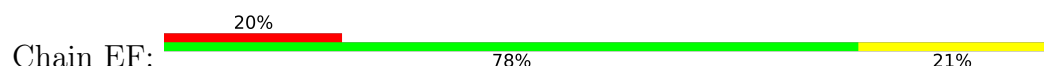




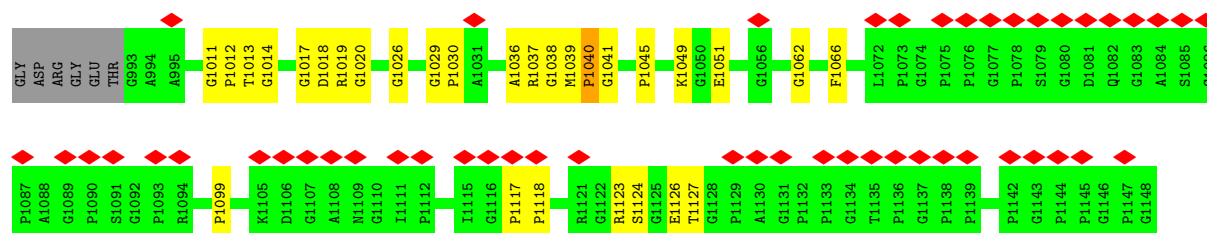
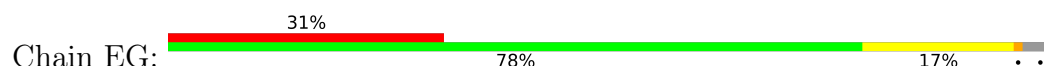
• Molecule 20: Collagen type II alpha 1 chain



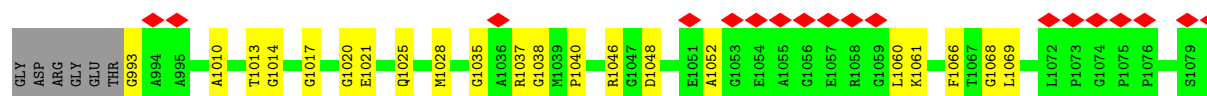
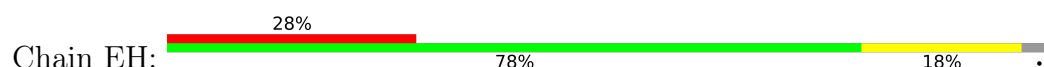
• Molecule 20: Collagen type II alpha 1 chain



• Molecule 20: Collagen type II alpha 1 chain

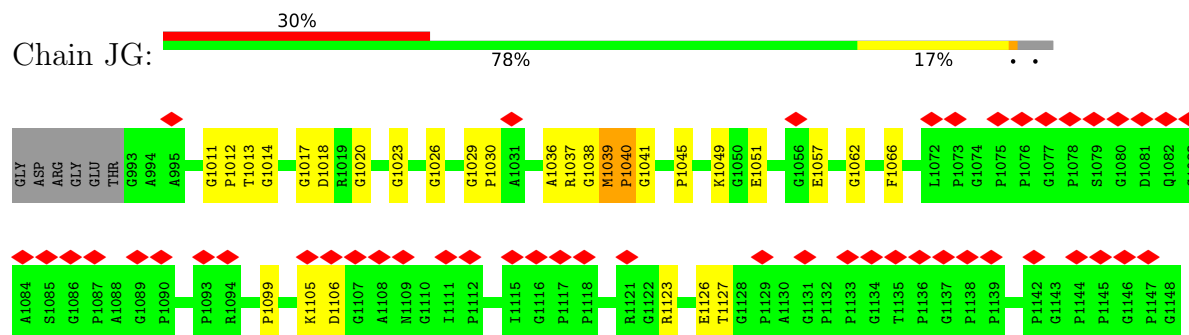


• Molecule 20: Collagen type II alpha 1 chain



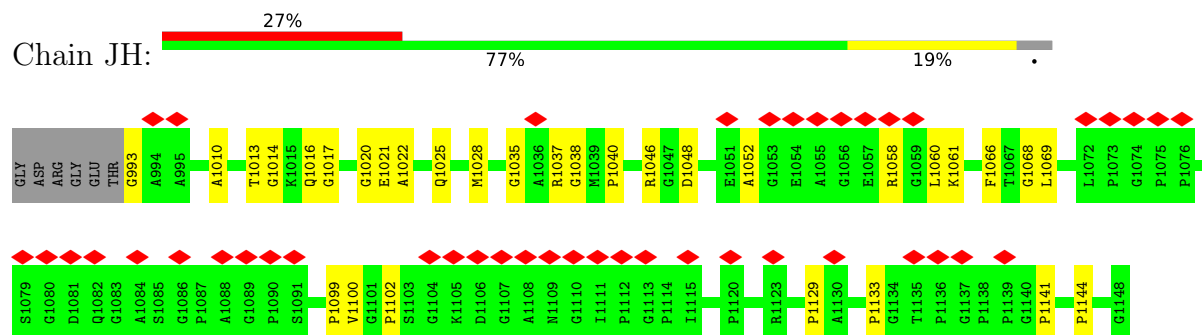
● Molecule 20: Collagen type II alpha 1 chain

Chain JG:



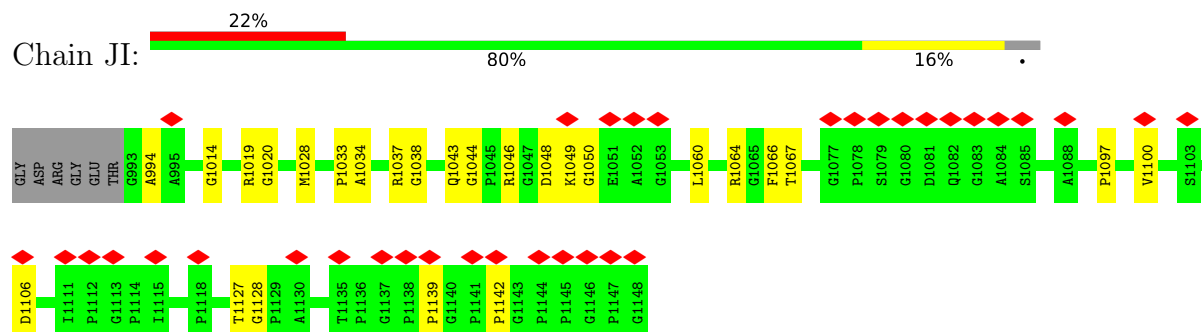
● Molecule 20: Collagen type II alpha 1 chain

Chain JH:



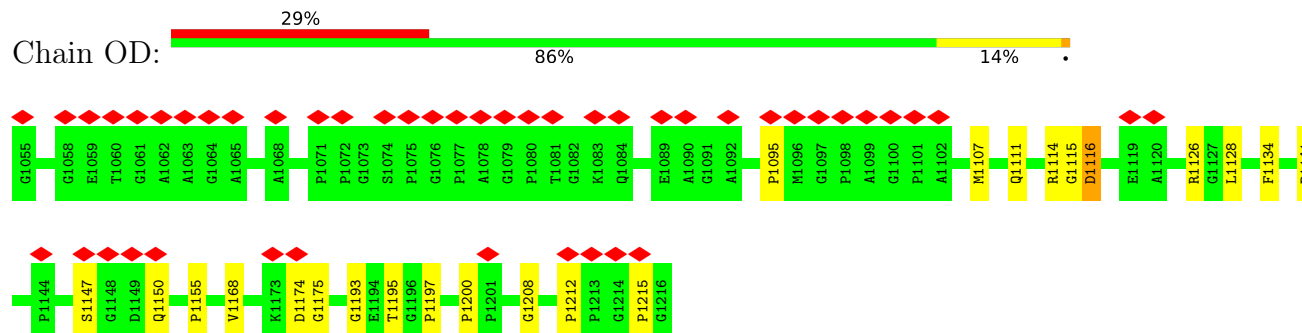
● Molecule 20: Collagen type II alpha 1 chain

Chain JI:



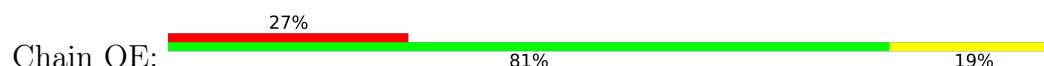
● Molecule 20: Collagen type II alpha 1 chain

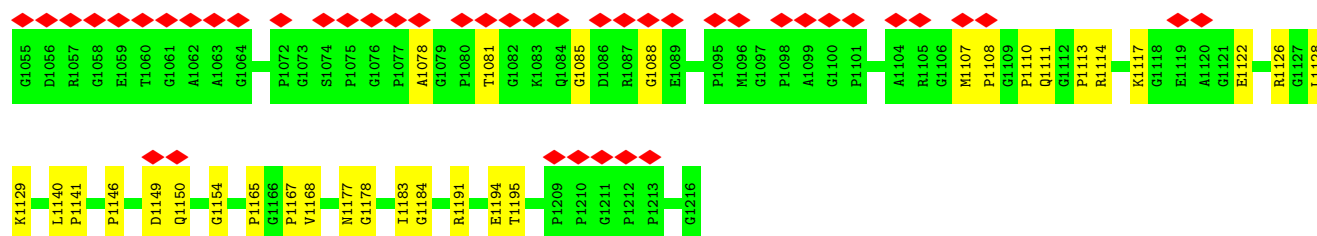
Chain OD:



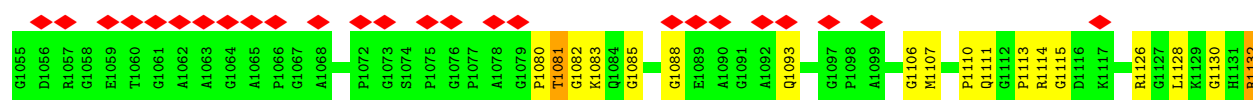
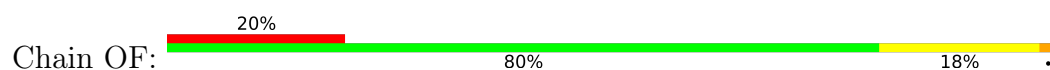
● Molecule 20: Collagen type II alpha 1 chain

Chain OE:

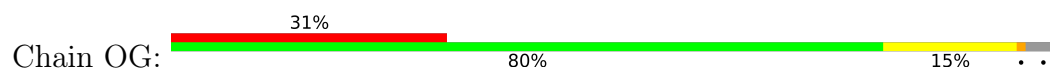




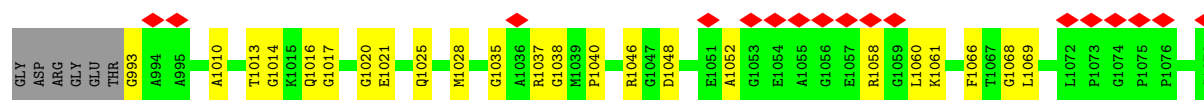
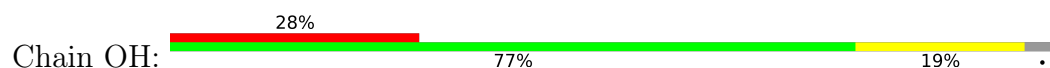
• Molecule 20: Collagen type II alpha 1 chain



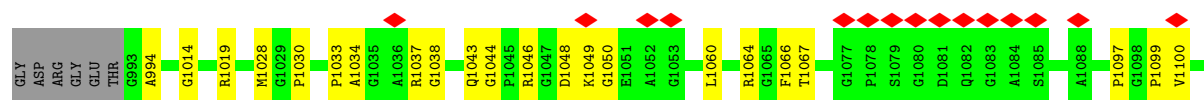
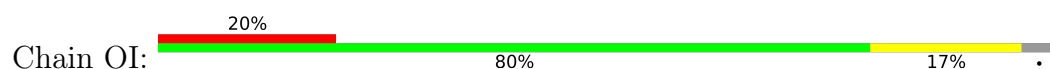
• Molecule 20: Collagen type II alpha 1 chain

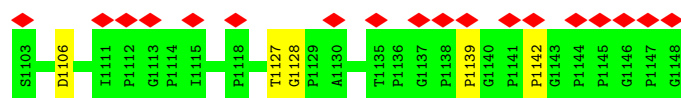


• Molecule 20: Collagen type II alpha 1 chain

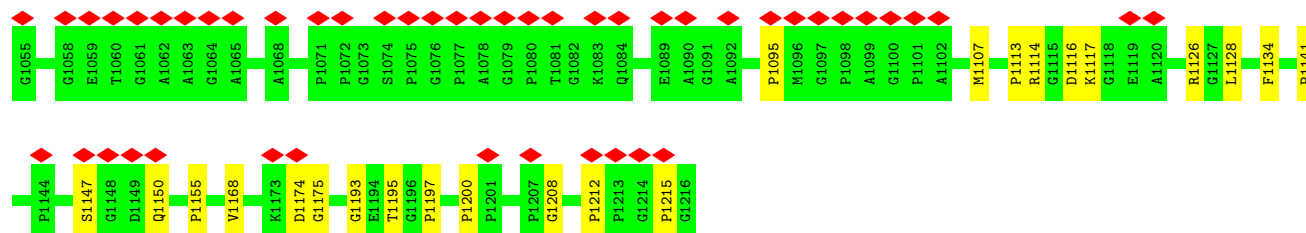
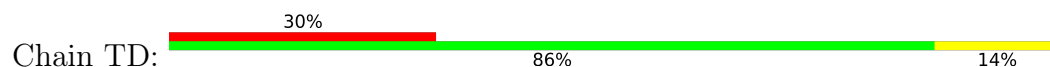


• Molecule 20: Collagen type II alpha 1 chain

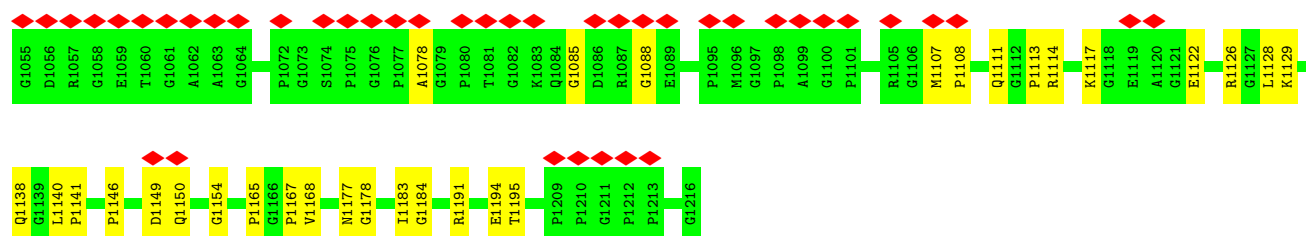
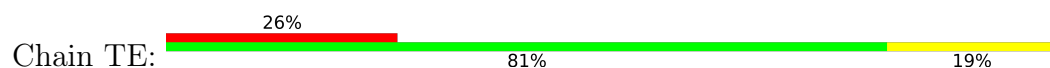




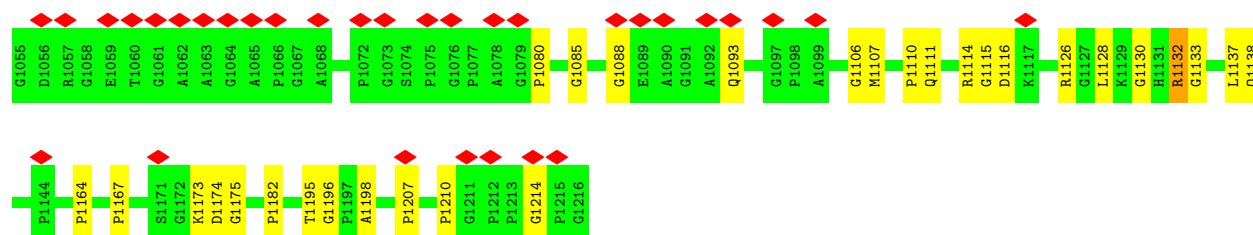
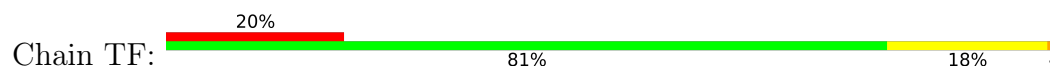
• Molecule 20: Collagen type II alpha 1 chain



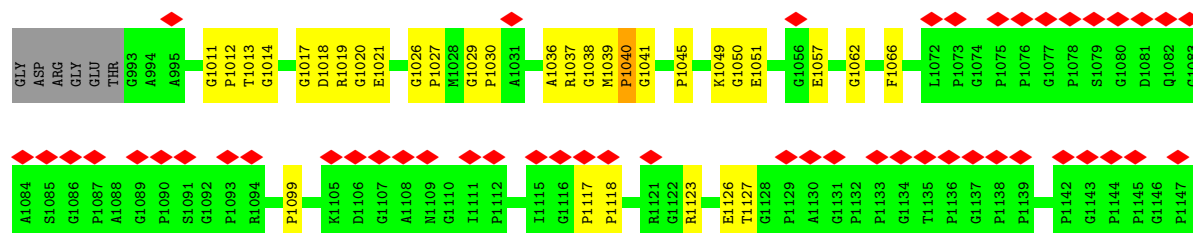
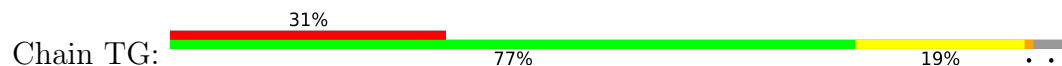
• Molecule 20: Collagen type II alpha 1 chain



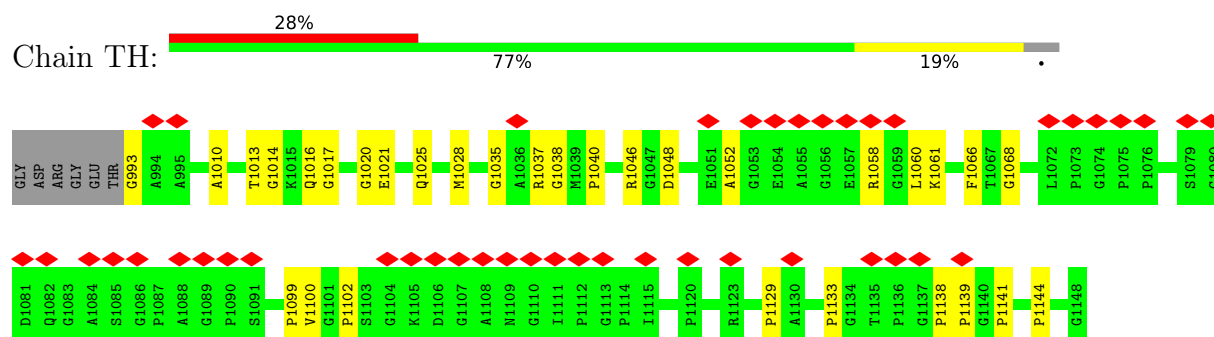
• Molecule 20: Collagen type II alpha 1 chain



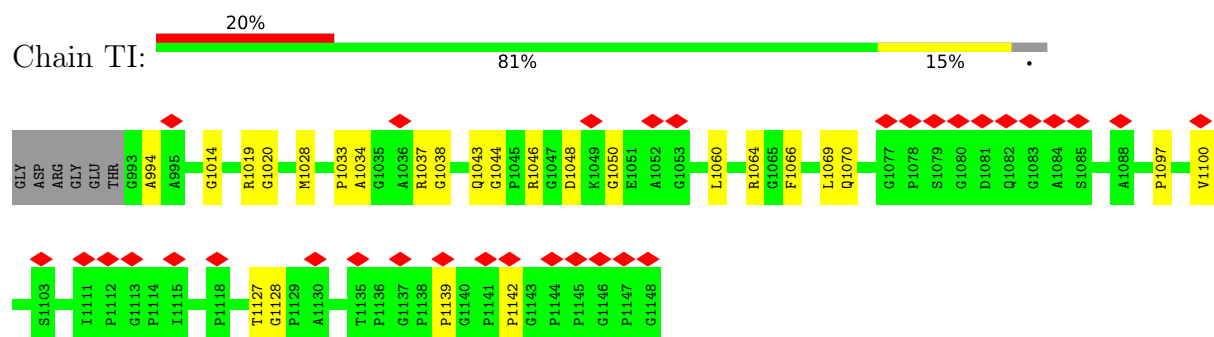
• Molecule 20: Collagen type II alpha 1 chain



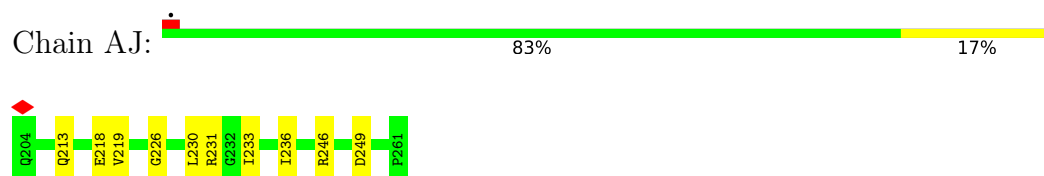
- Molecule 20: Collagen type II alpha 1 chain



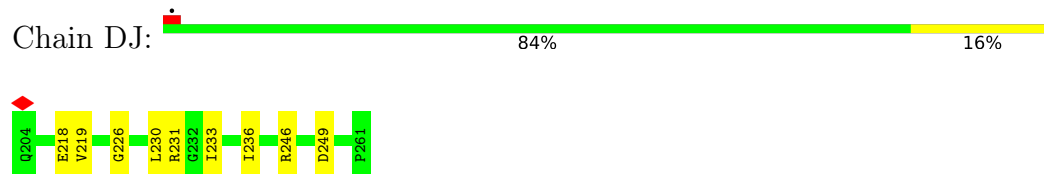
- Molecule 20: Collagen type II alpha 1 chain



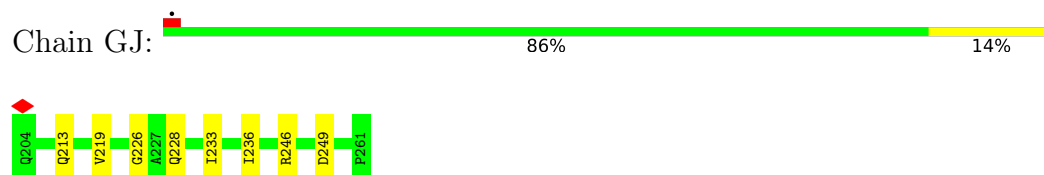
- Molecule 21: Collagen type IX alpha 1 chain



- Molecule 21: Collagen type IX alpha 1 chain

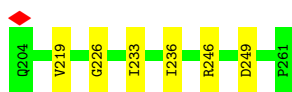


- Molecule 21: Collagen type IX alpha 1 chain

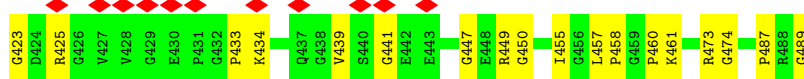
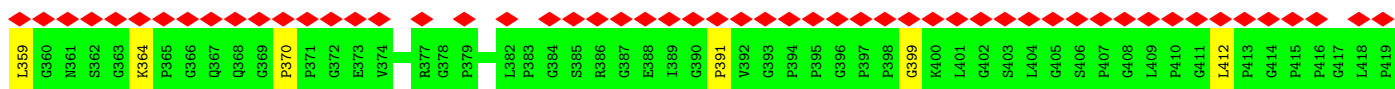
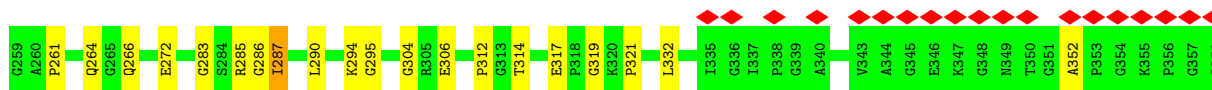
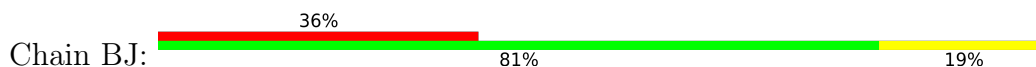


- Molecule 21: Collagen type IX alpha 1 chain

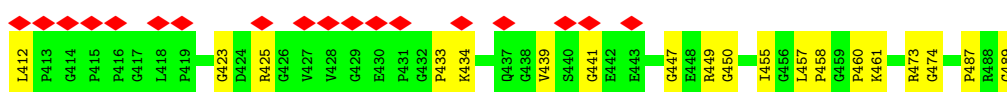
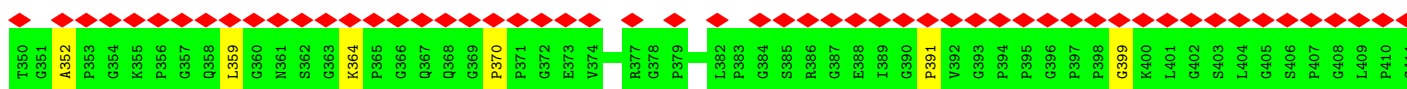
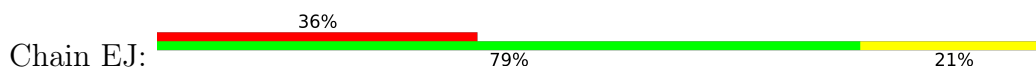




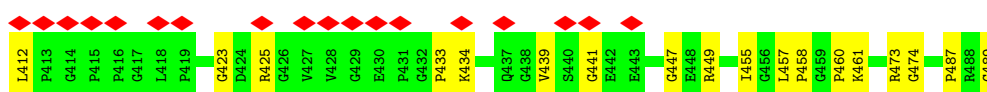
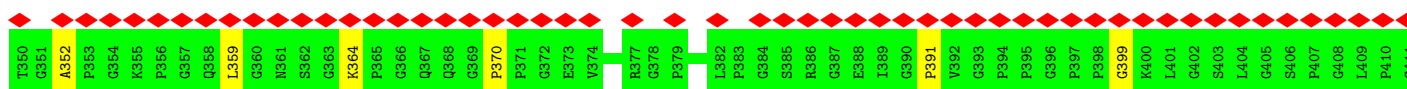
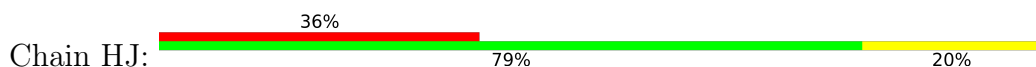
• Molecule 22: Collagen alpha-1(IX) chain



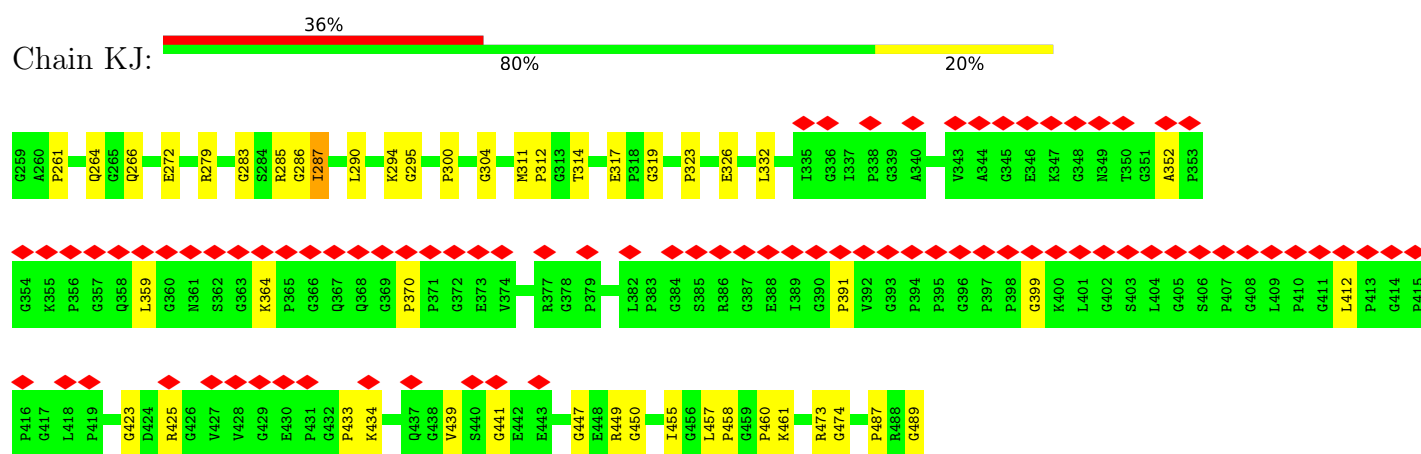
• Molecule 22: Collagen alpha-1(IX) chain



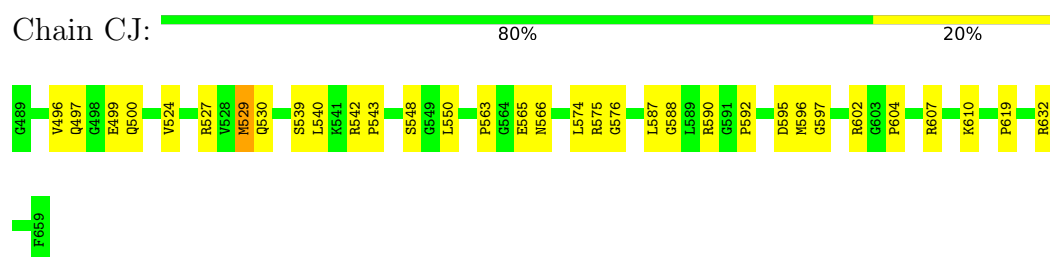
• Molecule 22: Collagen alpha-1(IX) chain



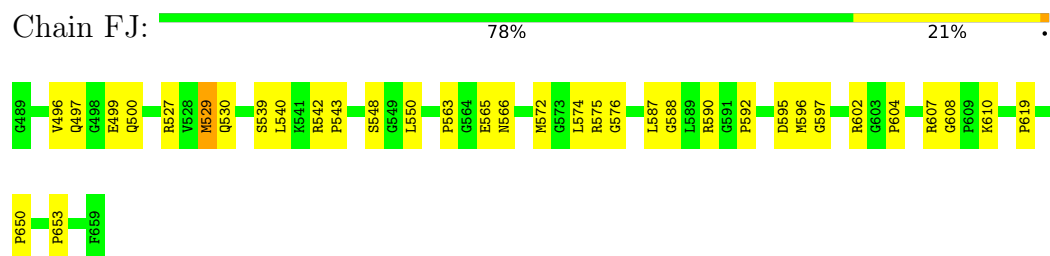
• Molecule 22: Collagen alpha-1(IX) chain



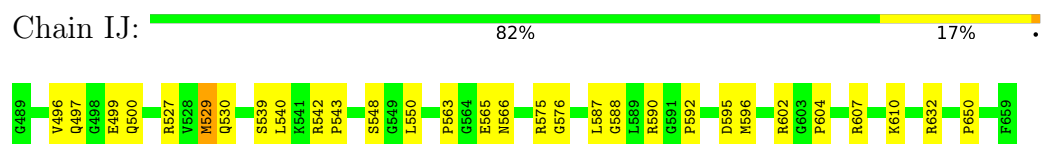
• Molecule 23: Collagen alpha-1(IX) chain



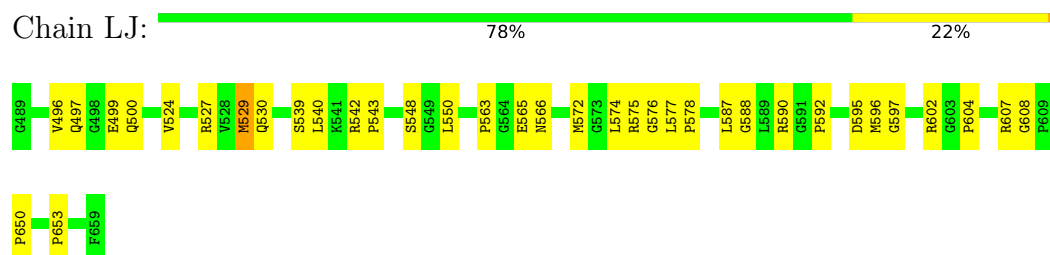
• Molecule 23: Collagen alpha-1(IX) chain



• Molecule 23: Collagen alpha-1(IX) chain

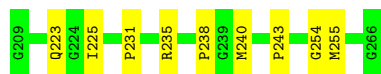


• Molecule 23: Collagen alpha-1(IX) chain



- Molecule 24: Collagen type IX alpha 2 chain

Chain AK:  84% 16%



- Molecule 24: Collagen type IX alpha 2 chain

Chain DK:  84% 14% .



- Molecule 24: Collagen type IX alpha 2 chain

Chain GK:  81% 17% .



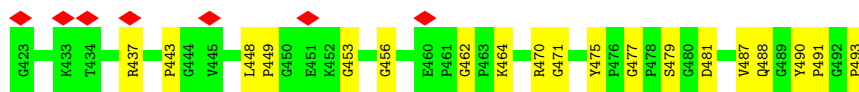
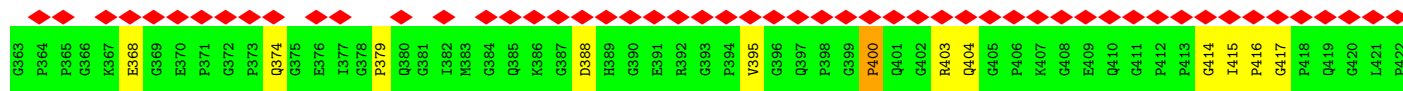
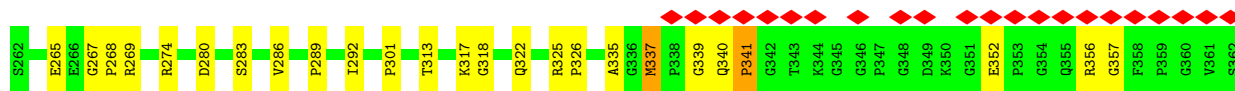
- Molecule 24: Collagen type IX alpha 2 chain

Chain JK:  88% 10% .



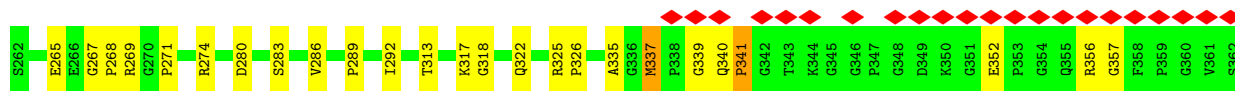
- Molecule 25: Collagen type IX alpha 2 chain

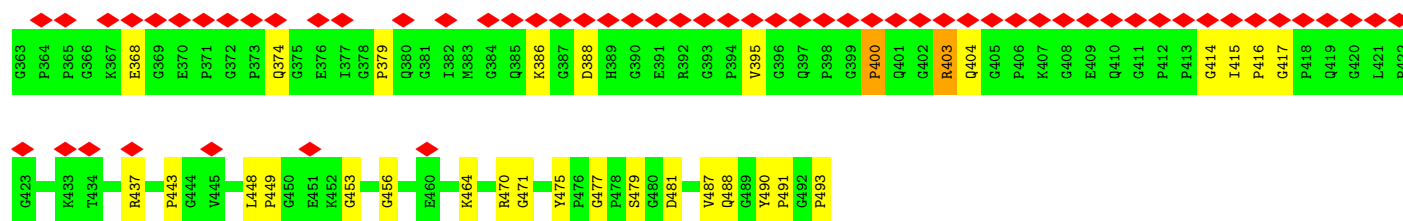
Chain BK:  35% 76% 23% .



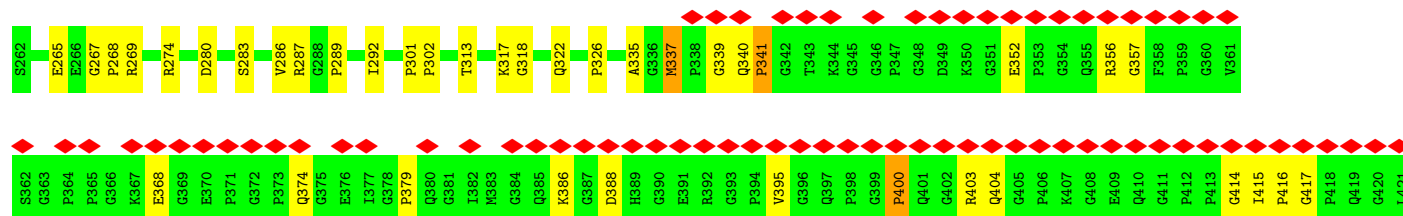
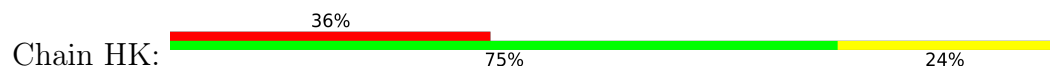
- Molecule 25: Collagen type IX alpha 2 chain

Chain EK:  35% 76% 22% .

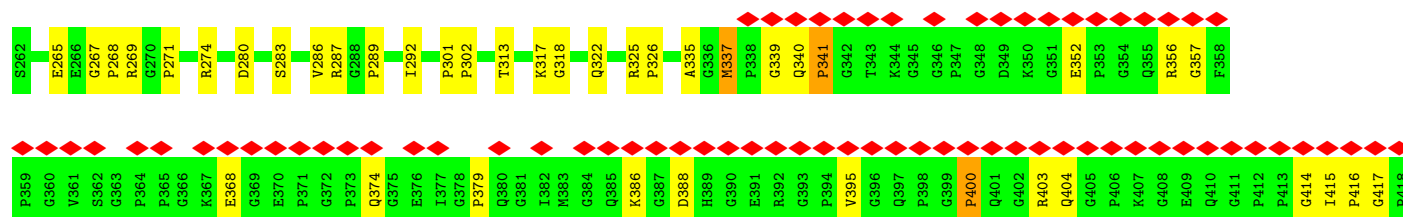
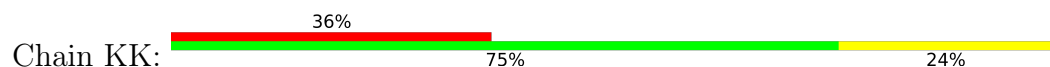




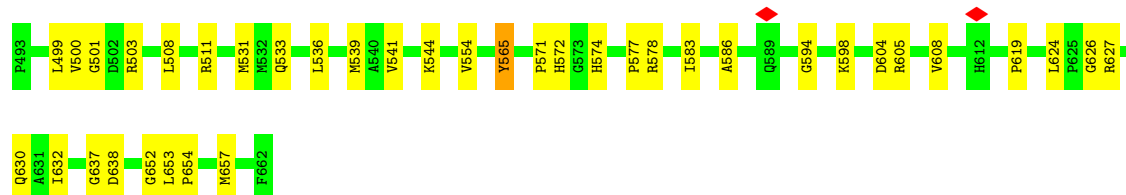
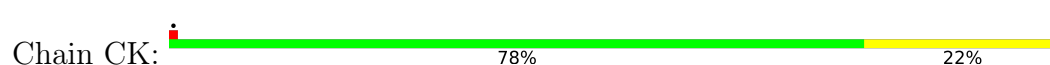
• Molecule 25: Collagen type IX alpha 2 chain



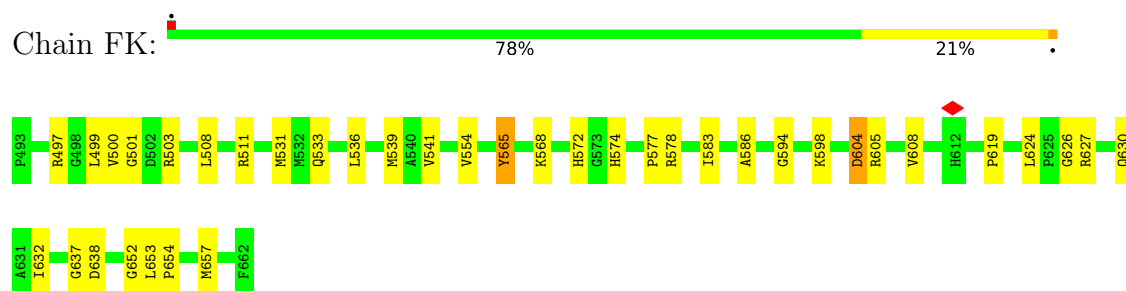
• Molecule 25: Collagen type IX alpha 2 chain



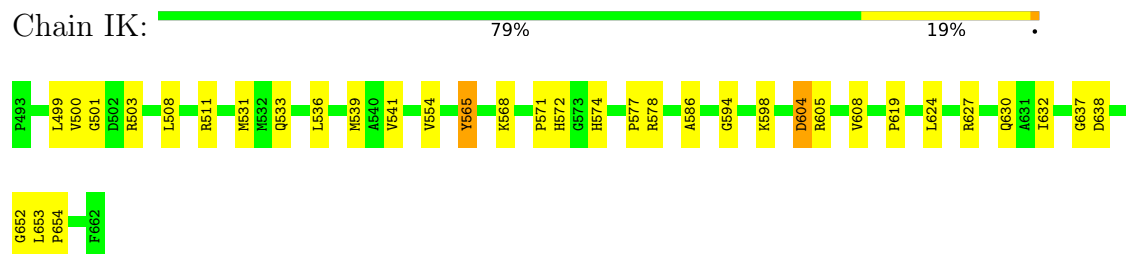
• Molecule 26: Collagen type IX alpha 2 chain



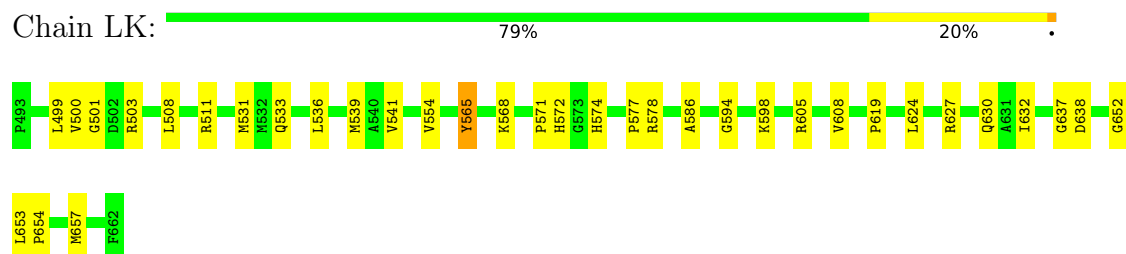
• Molecule 26: Collagen type IX alpha 2 chain



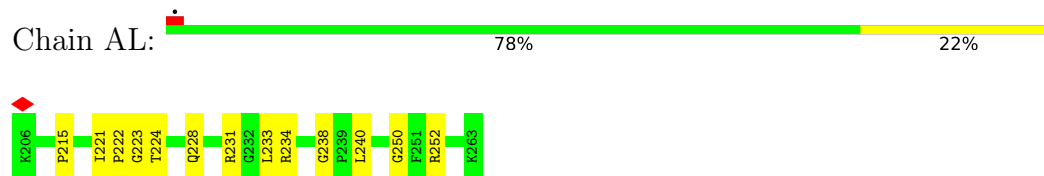
- Molecule 26: Collagen type IX alpha 2 chain



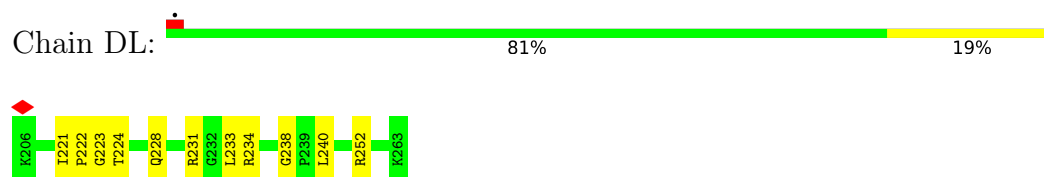
- Molecule 26: Collagen type IX alpha 2 chain



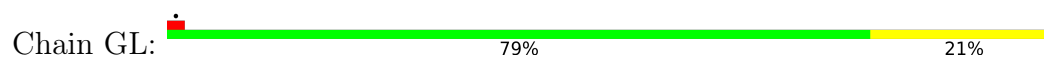
- Molecule 27: Collagen alpha-3(IX) chain



- Molecule 27: Collagen alpha-3(IX) chain

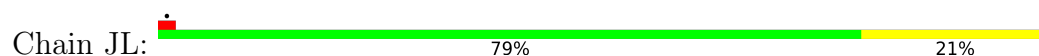


- Molecule 27: Collagen alpha-3(IX) chain

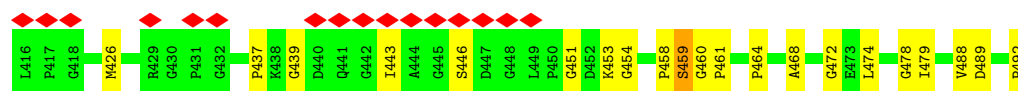
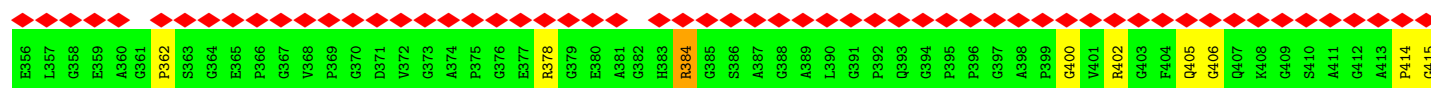
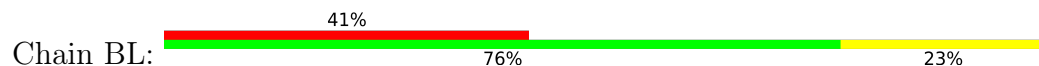




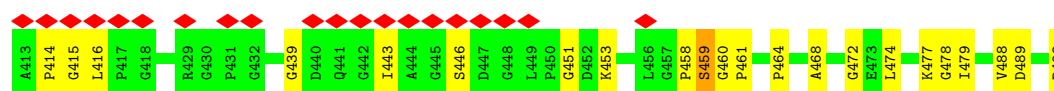
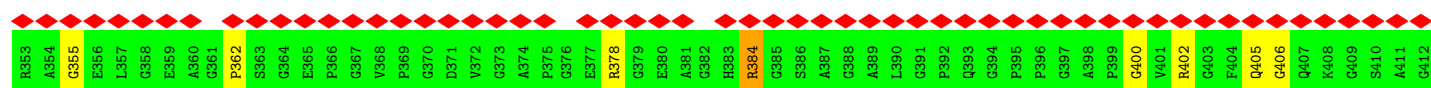
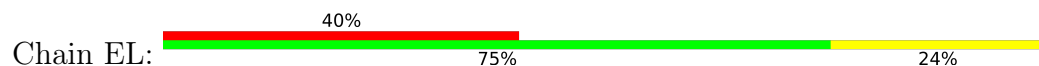
• Molecule 27: Collagen alpha-3(IX) chain



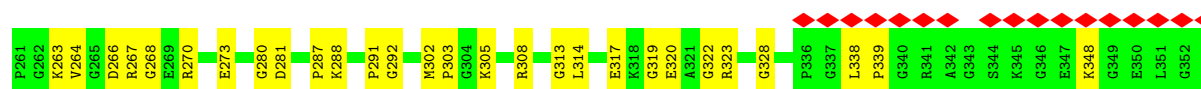
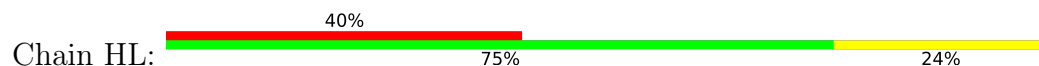
• Molecule 28: Collagen alpha-3(IX) chain

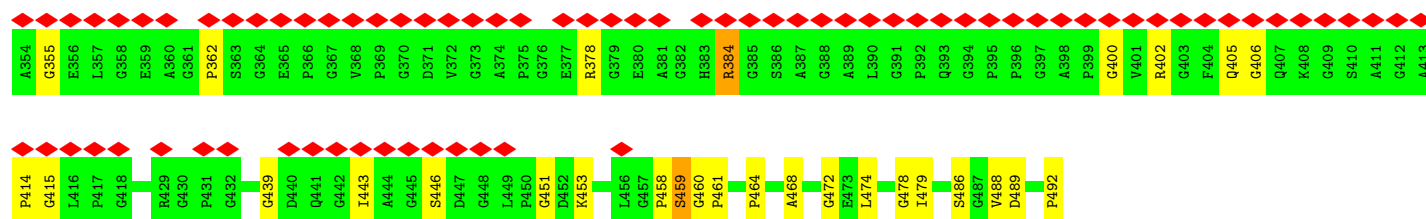


• Molecule 28: Collagen alpha-3(IX) chain

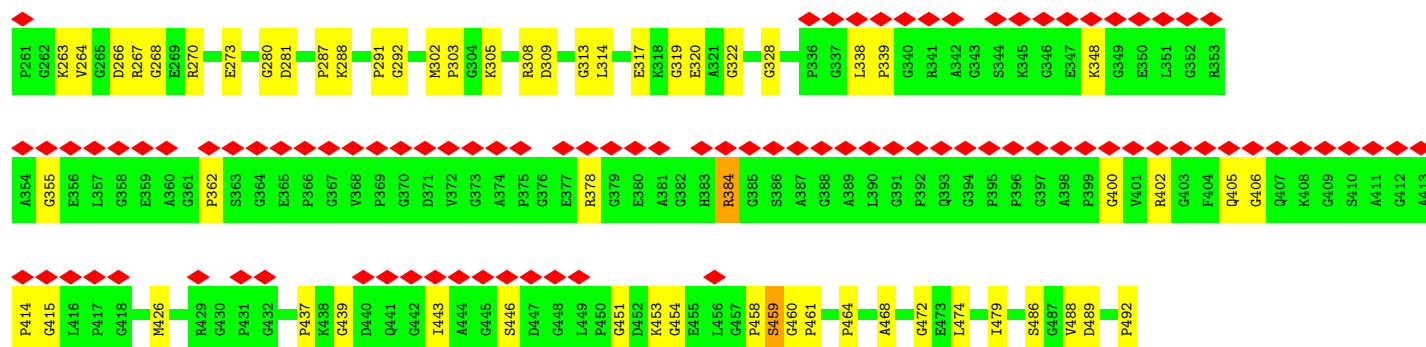
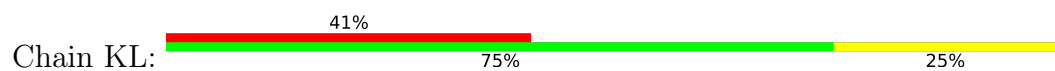


• Molecule 28: Collagen alpha-3(IX) chain

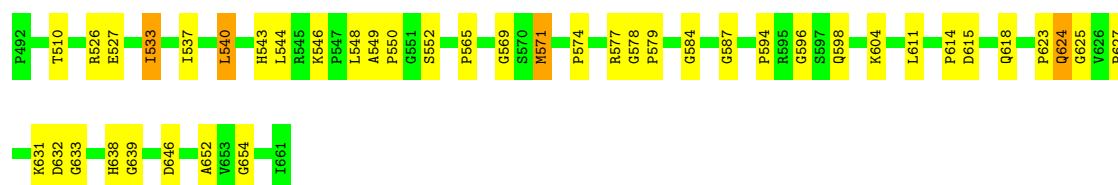
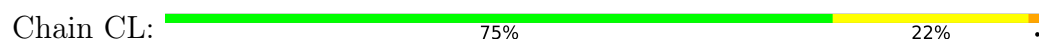




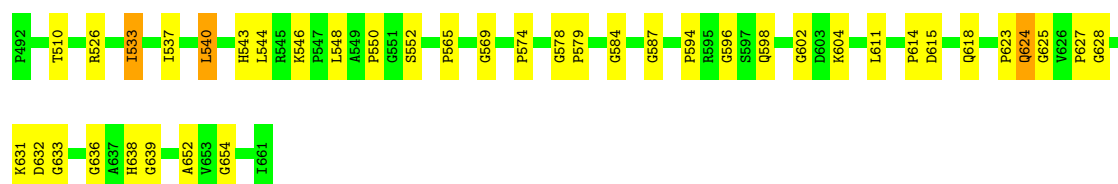
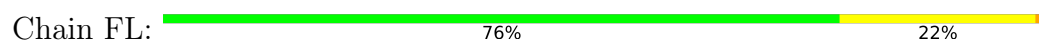
• Molecule 28: Collagen alpha-3(IX) chain



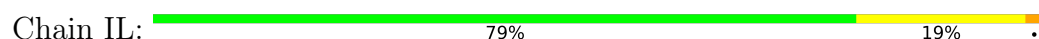
• Molecule 29: Collagen alpha-3(IX) chain



• Molecule 29: Collagen alpha-3(IX) chain



• Molecule 29: Collagen alpha-3(IX) chain





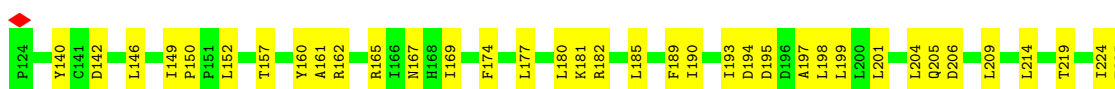
• Molecule 29: Collagen alpha-3(IX) chain

Chain LL: 78% 21%



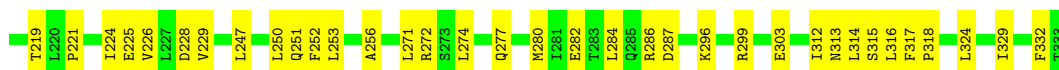
• Molecule 30: Opticin

Chain AM: 68% 32%



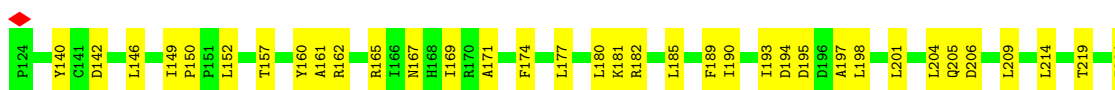
• Molecule 30: Opticin

Chain BM: 65% 34%



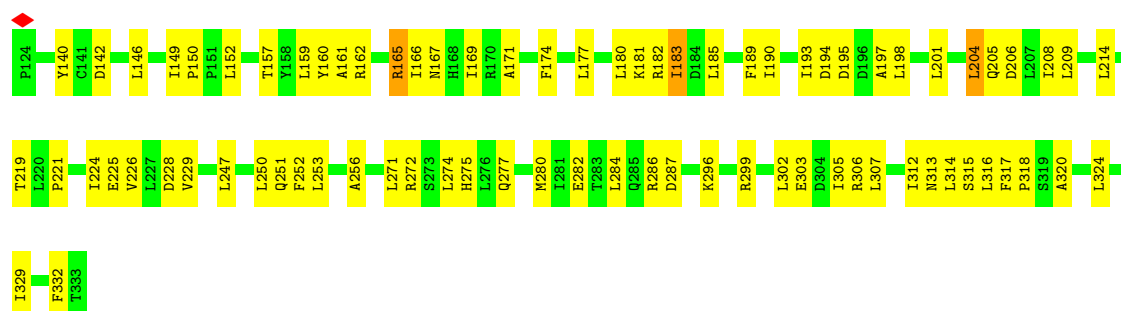
• Molecule 30: Opticin

Chain CM: 67% 33%



• Molecule 30: Opticin

Chain DM: 63% 36%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Aa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ba:  50%

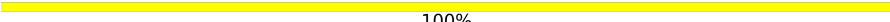


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ca:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ea:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ga:  50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ha:  50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ia:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ja:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ka:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain La:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ma:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Na:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Oa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ra:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ta:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ua:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Va:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ya:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Za:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain aa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ca:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain da:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ea:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain fa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ha:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ja:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ka:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain la:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ma:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain na:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain oa:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain pa:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain qa:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ra:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain sa:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ae:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Be:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ce:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain De:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ee:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ge:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain He:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ie: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Je: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ke: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Le: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Me: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ne: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Oe: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pe:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Re:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Se:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ve:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain We:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ai:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ci:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Di:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Fi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hi:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ii:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ji:  50% 100%

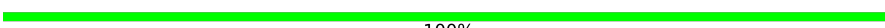


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ki:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Li:  100%

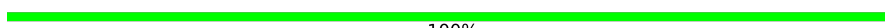


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mi:  50% 50%

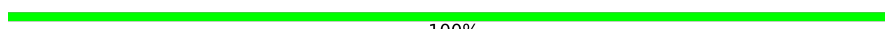


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ni:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Oi:  100%

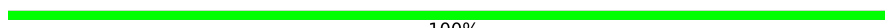


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pi:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qi:  100%

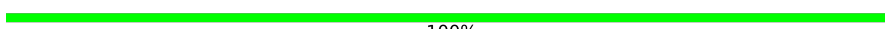


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Si:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ti:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ui:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Xi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Yi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Zi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain bi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ci:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain di:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ei:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain gi:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ii:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ji:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ki:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain li:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain mi:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ni:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



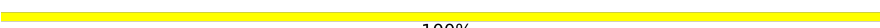
- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Eb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gb:  50% 50%

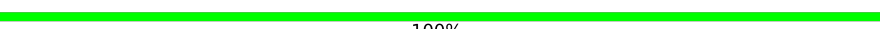


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hb:  50% 50%

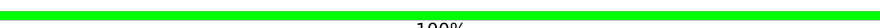


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ib:  100%

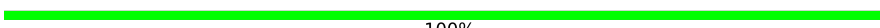


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lb:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mb:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ob:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Rb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Tb:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ub:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Vb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Yb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Zb:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ab:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain cb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain db:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain eb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain fb:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain hb: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain jb: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain kb: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain lb: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain mb: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain nb: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ob: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain pb:  50% 50%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain qb:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain rb:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain sb:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Af:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bf:  50% 50%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Cf:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Df:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ef: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gf: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hf: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain If: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jf: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kf: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lf: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Of:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Rf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Sf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Vf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Wf:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Aj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Cj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Dj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Fj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hj: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ij:  100%

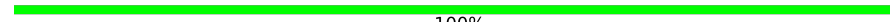


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jj:  100%

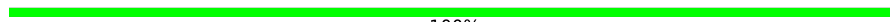


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lj:  100%

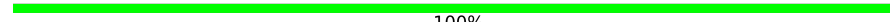


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mj:  50% 50%

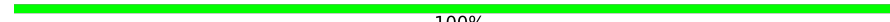


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Oj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pj:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Sj:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Tj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Uj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Xj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Yj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Zj:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain bj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain cj: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain dj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ej: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain gj: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ij: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain jj: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain kj:  50% 50%

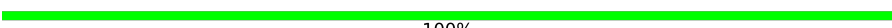


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain lj:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain mj:  100%

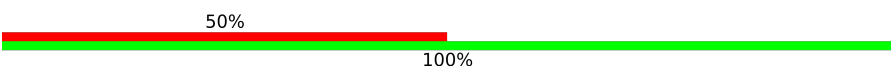


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain nj:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain oj:  50% 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain pj:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain qj:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain rj:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ac:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bc:  50% 50%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Cc:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ec:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gc:  50% 50%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hc:  50% 50%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ic:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lc:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mc:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nc:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Oc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qc:  100%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Rc:  100%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Tc:  50% 50%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Uc:  50% 50%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Vc:  100%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Yc:  100%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Zc:  100%

GLY1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ac:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain cc: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain dc: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ec: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain fc: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain hc: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain jc: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain kc: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain lc:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain mc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain nc:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain oc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain pc:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain qc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain rc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain sc:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ag: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bg: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Cg: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Dg: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Eg: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gg: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hg: 100%

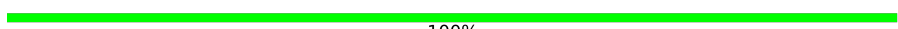


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ig:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jg:  100%

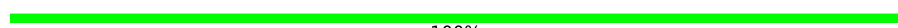


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kg:  50% 50%

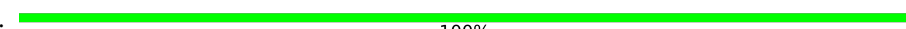


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lg:  100%

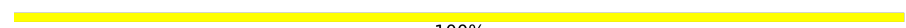


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mg:  100%

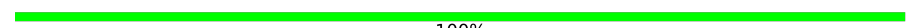


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ng:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Og:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pg:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Rg:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Sg:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Vg:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Wg:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ak:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bk:  100%

GLU1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ck:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Dk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Fk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ik:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ok:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Sk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Tk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Uk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Xk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Yk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Zk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain bk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ck:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain dk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ek:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain gk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ik:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain jk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain kk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain lk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain mk:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain nk:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



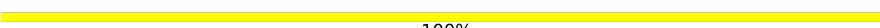
- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ed:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gd:  50% 50%

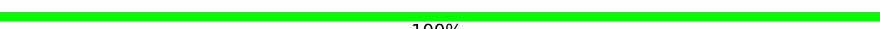


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hd:  50% 50%

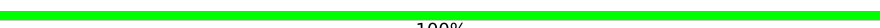


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Id:  100%

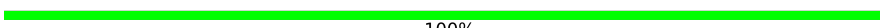


- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ld:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Md:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nd: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Od: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pd: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Qd: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Rd: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Td: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ud: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Vd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Yd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Zd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ad:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain cd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain dd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ed:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain fd:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain hd: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain jd: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain kd: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ld: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain md: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain nd: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain od: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain pd:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain qd:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain rd:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain sd:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ah:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Bh:  50% 50%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ch:  100%

GAL1
GLC2

- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Dh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Eh: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Gh: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Hh: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ih: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jh: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kh: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Lh: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Mh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Oh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ph:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Rh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Sh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Vh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Wh:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain A1:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain B1:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain C1:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain D1:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain E1:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain F1:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain G1:  50%  50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Il:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Jl:  50% 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Kl:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ll:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ml:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Nl:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Ol:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain Pl:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain QI: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain SI: 50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain TI: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain UI: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain XI: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain YI: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ZI: 100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain bl:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain cl:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain dl:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain el:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain gl:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain il:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain jl:  100%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain kl:  50% 50%



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ll:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ml:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain nl:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ol:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain pl:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain ql:



- Molecule 31: alpha-D-glucopyranose-(1-2)-beta-D-galactopyranose

Chain rl:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	600039	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS 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	0.642	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	439.16, 439.16, 1317.48	wwPDB
Map dimensions	400, 400, 1200	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.0979, 1.0979, 1.0979	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, LYZ, GAL

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	AA	0.14	0/1637	0.39	0/2227
1	FA	0.14	0/1637	0.38	0/2227
1	KA	0.14	0/1637	0.38	0/2227
1	PA	0.15	0/1637	0.39	0/2227
2	BA	0.15	0/1518	0.32	0/2046
2	GA	0.15	0/1518	0.32	0/2046
2	LA	0.15	0/1518	0.32	0/2046
2	QA	0.15	0/1518	0.32	0/2046
3	CA	0.17	0/1509	0.35	0/2054
3	HA	0.17	0/1509	0.34	0/2054
3	MA	0.17	0/1509	0.35	0/2054
3	RA	0.17	0/1509	0.35	0/2054
4	DA	0.16	0/1484	0.48	0/2024
4	IA	0.17	0/1484	0.49	0/2024
4	NA	0.17	0/1484	0.48	0/2024
4	SA	0.16	0/1484	0.47	0/2024
5	EA	0.13	0/461	0.41	0/629
5	JA	0.13	0/461	0.41	0/629
5	OA	0.13	0/461	0.41	0/629
5	TA	0.13	0/461	0.43	0/629
6	AC	0.12	0/1644	0.34	1/2230 (0.0%)
6	FC	0.12	0/1644	0.35	1/2230 (0.0%)
6	KC	0.12	0/1644	0.34	1/2230 (0.0%)
6	PC	0.12	0/1644	0.34	1/2230 (0.0%)
7	BC	0.16	0/1501	0.34	0/2019
7	GC	0.15	0/1501	0.33	0/2019
7	LC	0.15	0/1501	0.33	0/2019
7	QC	0.15	0/1501	0.33	0/2019
8	CC	0.16	0/1487	0.35	0/2016
8	HC	0.16	0/1487	0.35	0/2016
8	MC	0.16	0/1487	0.35	0/2016
8	RC	0.16	0/1487	0.35	0/2016

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
9	DC	0.15	0/1460	0.40	0/1985
9	IC	0.14	0/1460	0.38	0/1985
9	NC	0.14	0/1460	0.38	0/1985
9	SC	0.15	0/1460	0.39	0/1985
10	EC	0.13	0/446	0.41	0/607
10	JC	0.12	0/446	0.40	0/607
10	OC	0.12	0/446	0.40	0/607
10	TC	0.13	0/446	0.41	0/607
11	AB	0.12	0/1499	0.36	0/2029
11	FB	0.13	0/1499	0.36	0/2029
11	KB	0.12	0/1499	0.35	0/2029
11	PB	0.12	0/1499	0.35	0/2029
12	BB	0.16	0/1526	0.32	0/2072
12	GB	0.14	0/1526	0.32	0/2072
12	LB	0.15	0/1526	0.31	0/2072
12	QB	0.14	0/1526	0.31	0/2072
13	CB	0.17	0/1478	0.34	0/2007
13	HB	0.17	0/1478	0.34	0/2007
13	MB	0.16	0/1478	0.33	0/2007
13	RB	0.17	0/1478	0.33	0/2007
14	DB	0.13	0/1583	0.35	0/2152
14	IB	0.13	0/1583	0.35	0/2152
14	NB	0.13	0/1583	0.36	0/2152
14	SB	0.13	0/1583	0.35	0/2152
15	EB	0.14	0/504	0.34	0/699
15	JB	0.15	0/504	0.35	0/699
15	OB	0.14	0/504	0.35	0/699
15	TB	0.15	0/504	0.36	0/699
16	AD	0.09	0/696	0.23	0/942
16	AE	0.09	0/696	0.26	0/942
16	AF	0.08	0/696	0.22	0/942
16	AG	0.12	0/1120	0.31	0/1524
16	AH	0.15	0/1126	0.38	0/1531
16	AI	0.14	0/1129	0.47	0/1534
16	FD	0.10	0/696	0.23	0/942
16	FE	0.09	0/696	0.26	0/942
16	FF	0.08	0/696	0.22	0/942
16	FG	0.12	0/1120	0.31	0/1524
16	FH	0.15	0/1126	0.38	0/1531
16	FI	0.15	0/1129	0.45	0/1534
16	KD	0.10	0/696	0.23	0/942
16	KE	0.09	0/696	0.25	0/942
16	KF	0.09	0/696	0.22	0/942

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
16	KG	0.12	0/1120	0.33	0/1524
16	KH	0.14	0/1126	0.35	0/1531
16	KI	0.14	0/1129	0.46	0/1534
16	PD	0.10	0/696	0.23	0/942
16	PE	0.09	0/696	0.26	0/942
16	PF	0.08	0/696	0.21	0/942
16	PG	0.12	0/1120	0.32	0/1524
16	PH	0.15	0/1126	0.38	0/1531
16	PI	0.15	0/1129	0.45	0/1534
17	BD	0.11	0/1619	0.30	0/2202
17	BE	0.12	0/1621	0.33	0/2205
17	BF	0.11	0/1613	0.30	0/2195
17	BG	0.12	0/1619	0.33	1/2202 (0.0%)
17	BH	0.10	0/1624	0.29	0/2206
17	BI	0.11	0/1621	0.32	0/2204
17	GD	0.10	0/1619	0.28	0/2202
17	GE	0.12	0/1621	0.33	0/2205
17	GF	0.11	0/1613	0.33	0/2195
17	GG	0.11	0/1619	0.34	1/2202 (0.0%)
17	GH	0.10	0/1624	0.28	0/2206
17	GI	0.10	0/1621	0.29	0/2204
17	LD	0.13	0/1619	0.29	0/2202
17	LE	0.12	0/1621	0.33	0/2205
17	LF	0.12	0/1613	0.33	0/2195
17	LG	0.11	0/1619	0.32	1/2202 (0.0%)
17	LH	0.10	0/1624	0.29	0/2206
17	LI	0.09	0/1621	0.29	0/2204
17	QD	0.11	0/1619	0.30	0/2202
17	QE	0.12	0/1621	0.33	0/2205
17	QF	0.10	0/1613	0.30	0/2195
17	QG	0.12	0/1619	0.33	1/2202 (0.0%)
17	QH	0.11	0/1624	0.31	0/2206
17	QI	0.10	0/1621	0.29	0/2204
18	CD	0.12	0/1381	0.34	0/1875
18	CE	0.13	0/1381	0.34	0/1875
18	CF	0.13	0/1381	0.36	0/1875
18	CG	0.12	0/1452	0.34	0/1974
18	CH	0.13	0/1460	0.36	0/1983
18	CI	0.16	0/1446	0.46	1/1967 (0.1%)
18	HD	0.13	0/1381	0.35	0/1875
18	HE	0.12	0/1381	0.33	0/1875
18	HF	0.13	0/1381	0.36	0/1875
18	HG	0.12	0/1452	0.35	0/1974

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
18	HH	0.14	0/1460	0.36	0/1983
18	HI	0.17	0/1446	0.46	1/1967 (0.1%)
18	MD	0.12	0/1381	0.34	0/1875
18	ME	0.12	0/1381	0.33	0/1875
18	MF	0.13	0/1381	0.36	0/1875
18	MG	0.12	0/1452	0.34	0/1974
18	MH	0.13	0/1460	0.35	0/1983
18	MI	0.17	0/1446	0.46	1/1967 (0.1%)
18	RD	0.12	0/1381	0.34	0/1875
18	RE	0.12	0/1381	0.33	0/1875
18	RF	0.13	0/1381	0.36	0/1875
18	RG	0.12	0/1452	0.34	0/1974
18	RH	0.12	0/1460	0.34	0/1983
18	RI	0.16	0/1446	0.46	1/1967 (0.1%)
19	DD	0.11	0/1373	0.28	0/1899
19	DE	0.10	0/1365	0.30	0/1889
19	DF	0.09	0/1367	0.25	0/1890
19	DG	0.11	0/1480	0.28	0/2019
19	DH	0.12	0/1474	0.32	0/2012
19	DI	0.12	0/1480	0.35	0/2019
19	ID	0.10	0/1373	0.26	0/1899
19	IE	0.10	0/1365	0.31	0/1889
19	IF	0.08	0/1367	0.25	0/1890
19	IG	0.11	0/1480	0.28	0/2019
19	IH	0.12	0/1474	0.34	0/2012
19	II	0.12	0/1480	0.34	0/2019
19	ND	0.11	0/1373	0.28	0/1899
19	NE	0.10	0/1365	0.29	0/1889
19	NF	0.09	0/1367	0.25	0/1890
19	NG	0.11	0/1480	0.28	0/2019
19	NH	0.12	0/1474	0.31	0/2012
19	NI	0.13	0/1480	0.35	0/2019
19	SD	0.11	0/1373	0.28	0/1899
19	SE	0.10	0/1365	0.29	0/1889
19	SF	0.09	0/1367	0.25	0/1890
19	SG	0.11	0/1480	0.28	0/2019
19	SH	0.12	0/1474	0.32	0/2012
19	SI	0.12	0/1480	0.35	0/2019
20	ED	0.11	0/1000	0.30	0/1378
20	EE	0.11	0/1009	0.32	0/1388
20	EF	0.12	0/996	0.31	0/1373
20	EG	0.13	0/1001	0.33	0/1373
20	EH	0.11	0/1005	0.29	0/1378

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	EI	0.11	0/1001	0.32	0/1373
20	JD	0.13	0/1000	0.34	0/1378
20	JE	0.14	0/1009	0.37	0/1388
20	JF	0.14	0/996	0.35	0/1373
20	JG	0.14	0/1001	0.36	1/1373 (0.1%)
20	JH	0.10	0/1005	0.29	0/1378
20	JI	0.11	0/1001	0.33	0/1373
20	OD	0.11	0/1000	0.31	0/1378
20	OE	0.12	0/1009	0.34	0/1388
20	OF	0.11	0/996	0.31	0/1373
20	OG	0.12	0/1001	0.31	0/1373
20	OH	0.12	0/1005	0.30	0/1378
20	OI	0.12	0/1001	0.33	0/1373
20	TD	0.10	0/1000	0.29	0/1378
20	TE	0.12	0/1009	0.31	0/1388
20	TF	0.12	0/996	0.32	0/1373
20	TG	0.12	0/1001	0.32	0/1373
20	TH	0.11	0/1005	0.30	0/1378
20	TI	0.12	0/1001	0.33	0/1373
21	AJ	0.10	0/390	0.28	0/523
21	DJ	0.10	0/390	0.28	0/523
21	GJ	0.11	0/390	0.30	0/523
21	JJ	0.12	0/390	0.31	0/523
22	BJ	0.12	0/1559	0.36	0/2109
22	EJ	0.12	0/1559	0.36	0/2109
22	HJ	0.12	0/1559	0.36	0/2109
22	KJ	0.13	0/1559	0.37	0/2109
23	CJ	0.15	0/1189	0.36	0/1620
23	FJ	0.14	0/1189	0.35	0/1620
23	IJ	0.14	0/1189	0.33	0/1620
23	LJ	0.14	0/1189	0.33	0/1620
24	AK	0.11	0/383	0.35	0/515
24	DK	0.11	0/383	0.35	0/515
24	GK	0.12	0/383	0.37	0/515
24	JK	0.12	0/383	0.36	0/515
25	BK	0.16	0/1573	0.49	1/2123 (0.0%)
25	EK	0.16	0/1573	0.48	1/2123 (0.0%)
25	HK	0.16	0/1573	0.47	1/2123 (0.0%)
25	KK	0.16	0/1573	0.49	1/2123 (0.0%)
26	CK	0.14	0/1191	0.36	0/1613
26	FK	0.14	0/1191	0.36	0/1613
26	IK	0.14	0/1191	0.34	0/1613
26	LK	0.14	0/1191	0.34	0/1613

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	AL	0.12	0/401	0.32	0/546
27	DL	0.13	0/401	0.32	0/546
27	GL	0.13	0/401	0.33	0/546
27	JL	0.12	0/401	0.29	0/546
28	BL	0.13	0/1542	0.34	0/2070
28	EL	0.13	0/1542	0.33	0/2070
28	HL	0.14	0/1542	0.34	0/2070
28	KL	0.13	0/1542	0.34	0/2070
29	CL	0.17	0/1163	0.38	0/1584
29	FL	0.17	0/1163	0.39	0/1584
29	IL	0.14	0/1163	0.34	0/1584
29	LL	0.14	0/1163	0.35	0/1584
30	AM	0.17	0/1697	0.37	0/2311
30	BM	0.16	0/1697	0.34	0/2311
30	CM	0.17	0/1697	0.37	0/2311
30	DM	0.16	0/1697	0.36	0/2311
All	All	0.13	0/276228	0.34	17/375916 (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
17	BE	0	1
17	GE	0	1
17	LE	0	1
17	QE	0	1
18	CI	0	2
18	HI	0	2
18	MI	0	2
18	RI	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	KK	400	PRO	N-CA-CB	7.30	110.92	103.25
25	BK	400	PRO	N-CA-CB	7.29	110.91	103.25
25	HK	400	PRO	N-CA-CB	7.22	110.83	103.25
25	EK	400	PRO	N-CA-CB	7.21	110.82	103.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	PC	539	LEU	CB-CA-C	-5.83	109.84	116.54

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
17	BE	548	PRO	Peptide
18	CI	562	LEU	Peptide
18	CI	622	ALA	Peptide
17	GE	548	PRO	Peptide
18	HI	562	LEU	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	AA	1631	0	1554	75	0
1	FA	1631	0	1554	78	0
1	KA	1631	0	1554	74	0
1	PA	1631	0	1554	77	0
2	BA	1580	0	1487	67	0
2	GA	1580	0	1487	66	0
2	LA	1580	0	1487	65	0
2	QA	1580	0	1487	67	0
3	CA	1528	0	1438	54	0
3	HA	1528	0	1438	56	0
3	MA	1528	0	1438	58	0
3	RA	1528	0	1438	61	0
4	DA	1521	0	1400	67	0
4	IA	1521	0	1400	67	0
4	NA	1521	0	1400	71	0
4	SA	1521	0	1400	69	0
5	EA	493	0	454	14	0
5	JA	493	0	454	17	0
5	OA	493	0	454	13	0
5	TA	493	0	454	15	0
6	AC	1642	0	1567	69	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	FC	1642	0	1567	69	0
6	KC	1642	0	1567	75	0
6	PC	1642	0	1567	68	0
7	BC	1568	0	1477	68	0
7	GC	1568	0	1477	60	0
7	LC	1568	0	1477	66	0
7	QC	1568	0	1477	66	0
8	CC	1522	0	1417	42	0
8	HC	1522	0	1417	42	0
8	MC	1522	0	1417	47	0
8	RC	1522	0	1417	46	0
9	DC	1504	0	1380	64	0
9	IC	1504	0	1380	63	0
9	NC	1504	0	1380	62	0
9	SC	1504	0	1380	63	0
10	EC	482	0	448	17	0
10	JC	482	0	448	18	0
10	OC	482	0	448	18	0
10	TC	482	0	448	17	0
11	AB	1501	0	1423	61	0
11	FB	1501	0	1423	69	0
11	KB	1501	0	1423	66	0
11	PB	1501	0	1423	64	0
12	BB	1526	0	1441	64	0
12	GB	1526	0	1441	64	0
12	LB	1526	0	1441	66	0
12	QB	1526	0	1441	62	0
13	CB	1504	0	1391	50	0
13	HB	1504	0	1391	51	0
13	MB	1504	0	1391	48	0
13	RB	1504	0	1391	50	0
14	DB	1552	0	1459	57	0
14	IB	1552	0	1459	57	0
14	NB	1552	0	1459	57	0
14	SB	1552	0	1459	60	0
15	EB	478	0	451	17	0
15	JB	478	0	451	17	0
15	OB	478	0	451	17	0
15	TB	478	0	451	18	0
16	AD	673	0	642	12	0
16	AE	673	0	642	25	0
16	AF	673	0	642	21	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	AG	1078	0	1012	65	0
16	AH	1084	0	1023	58	0
16	AI	1087	0	1030	73	0
16	FD	673	0	642	14	0
16	FE	673	0	642	19	0
16	FF	673	0	642	18	0
16	FG	1078	0	1012	64	0
16	FH	1084	0	1023	53	0
16	FI	1087	0	1030	69	0
16	KD	673	0	642	13	0
16	KE	673	0	642	22	0
16	KF	673	0	642	23	0
16	KG	1078	0	1012	54	0
16	KH	1084	0	1023	61	0
16	KI	1087	0	1030	64	0
16	PD	673	0	642	18	0
16	PE	673	0	642	24	0
16	PF	673	0	642	24	0
16	PG	1078	0	1012	67	0
16	PH	1084	0	1023	54	0
16	PI	1087	0	1030	69	0
17	BD	1562	0	1470	73	0
17	BE	1564	0	1470	67	0
17	BF	1556	0	1459	76	0
17	BG	1562	0	1470	68	0
17	BH	1568	0	1480	57	0
17	BI	1564	0	1477	82	0
17	GD	1562	0	1470	69	0
17	GE	1564	0	1470	66	0
17	GF	1556	0	1459	79	0
17	GG	1562	0	1470	77	0
17	GH	1568	0	1480	66	0
17	GI	1564	0	1477	88	0
17	LD	1562	0	1470	71	0
17	LE	1564	0	1470	67	0
17	LF	1556	0	1459	74	0
17	LG	1562	0	1470	78	0
17	LH	1568	0	1480	67	0
17	LI	1564	0	1477	87	0
17	QD	1562	0	1470	69	0
17	QE	1564	0	1470	67	0
17	QF	1556	0	1459	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	QG	1562	0	1470	79	0
17	QH	1568	0	1480	65	0
17	QI	1564	0	1477	86	0
18	CD	1339	0	1270	77	0
18	CE	1339	0	1270	71	0
18	CF	1339	0	1270	68	0
18	CG	1406	0	1326	72	0
18	CH	1414	0	1341	70	0
18	CI	1400	0	1315	67	0
18	HD	1339	0	1270	75	0
18	HE	1339	0	1270	74	0
18	HF	1339	0	1270	63	0
18	HG	1406	0	1326	72	0
18	HH	1414	0	1341	70	0
18	HI	1400	0	1315	66	0
18	MD	1339	0	1270	79	0
18	ME	1339	0	1270	73	0
18	MF	1339	0	1270	60	0
18	MG	1406	0	1326	73	0
18	MH	1414	0	1341	65	0
18	MI	1400	0	1315	63	0
18	RD	1339	0	1270	76	0
18	RE	1339	0	1270	68	0
18	RF	1339	0	1270	61	0
18	RG	1406	0	1326	72	0
18	RH	1414	0	1341	62	0
18	RI	1400	0	1315	62	0
19	DD	1320	0	1131	29	0
19	DE	1312	0	1121	24	0
19	DF	1315	0	1122	25	0
19	DG	1429	0	1328	52	0
19	DH	1423	0	1317	68	0
19	DI	1429	0	1328	54	0
19	ID	1320	0	1131	29	0
19	IE	1312	0	1121	26	0
19	IF	1315	0	1122	24	0
19	IG	1429	0	1328	58	0
19	IH	1423	0	1317	75	0
19	II	1429	0	1328	58	0
19	ND	1320	0	1131	29	0
19	NE	1312	0	1121	25	0
19	NF	1315	0	1122	27	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	NG	1429	0	1328	53	0
19	NH	1423	0	1317	77	0
19	NI	1429	0	1328	60	0
19	SD	1320	0	1131	31	0
19	SE	1312	0	1121	26	0
19	SF	1315	0	1122	25	0
19	SG	1429	0	1328	54	0
19	SH	1423	0	1317	75	0
19	SI	1429	0	1328	58	0
20	ED	959	0	858	30	0
20	EE	968	0	876	37	0
20	EF	955	0	852	36	0
20	EG	960	0	894	29	0
20	EH	964	0	900	32	0
20	EI	960	0	894	25	0
20	JD	959	0	858	33	0
20	JE	968	0	876	40	0
20	JF	955	0	852	36	0
20	JG	960	0	894	28	0
20	JH	964	0	900	34	0
20	JI	960	0	894	23	0
20	OD	959	0	858	27	0
20	OE	968	0	876	38	0
20	OF	955	0	852	32	0
20	OG	960	0	894	27	0
20	OH	964	0	900	34	0
20	OI	960	0	894	24	0
20	TD	959	0	858	28	0
20	TE	968	0	876	35	0
20	TF	955	0	852	29	0
20	TG	960	0	894	31	0
20	TH	964	0	900	32	0
20	TI	960	0	894	21	0
21	AJ	383	0	362	10	0
21	DJ	383	0	362	8	0
21	GJ	383	0	362	7	0
21	JJ	383	0	362	5	0
22	BJ	1516	0	1498	45	0
22	EJ	1516	0	1498	50	0
22	HJ	1516	0	1498	48	0
22	KJ	1516	0	1498	47	0
23	CJ	1147	0	1114	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	FJ	1147	0	1114	46	0
23	IJ	1147	0	1114	36	0
23	LJ	1147	0	1114	44	0
24	AK	372	0	361	10	0
24	DK	372	0	361	11	0
24	GK	372	0	361	15	0
24	JK	372	0	361	10	0
25	BK	1527	0	1451	59	0
25	EK	1527	0	1451	60	0
25	HK	1527	0	1451	61	0
25	KK	1527	0	1451	60	0
26	CK	1156	0	1141	51	0
26	FK	1156	0	1141	49	0
26	IK	1156	0	1141	44	0
26	LK	1156	0	1141	44	0
27	AL	386	0	390	14	0
27	DL	386	0	390	12	0
27	GL	386	0	390	15	0
27	JL	386	0	390	12	0
28	BL	1507	0	1455	59	0
28	EL	1507	0	1455	62	0
28	HL	1507	0	1455	61	0
28	KL	1507	0	1455	62	0
29	CL	1126	0	1071	50	0
29	FL	1126	0	1071	50	0
29	IL	1126	0	1071	42	0
29	LL	1126	0	1071	47	0
30	AM	1663	0	1688	55	0
30	BM	1663	0	1688	60	0
30	CM	1663	0	1688	54	0
30	DM	1663	0	1688	64	0
31	Aa	22	0	19	0	0
31	Ab	22	0	19	0	0
31	Ac	22	0	19	0	0
31	Ad	22	0	19	0	0
31	Ae	22	0	19	0	0
31	Af	22	0	19	0	0
31	Ag	22	0	19	0	0
31	Ah	22	0	19	0	0
31	Ai	22	0	19	0	0
31	Aj	22	0	19	0	0
31	Ak	22	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Al	22	0	19	0	0
31	Ba	22	0	19	1	0
31	Bb	22	0	19	1	0
31	Bc	22	0	19	1	0
31	Bd	22	0	19	1	0
31	Be	22	0	19	1	0
31	Bf	22	0	19	1	0
31	Bg	22	0	19	1	0
31	Bh	22	0	19	1	0
31	Bi	22	0	19	0	0
31	Bj	22	0	19	0	0
31	Bk	22	0	19	0	0
31	Bl	22	0	19	0	0
31	Ca	22	0	19	0	0
31	Cb	22	0	19	0	0
31	Cc	22	0	19	0	0
31	Cd	22	0	19	0	0
31	Ce	22	0	19	0	0
31	Cf	22	0	19	0	0
31	Cg	22	0	19	0	0
31	Ch	22	0	19	0	0
31	Ci	22	0	19	0	0
31	Cj	22	0	19	0	0
31	Ck	22	0	19	0	0
31	Cl	22	0	19	0	0
31	De	22	0	19	0	0
31	Df	22	0	19	0	0
31	Dg	22	0	19	0	0
31	Dh	22	0	19	0	0
31	Di	22	0	19	0	0
31	Dj	22	0	19	0	0
31	Dk	22	0	19	0	0
31	Dl	22	0	19	0	0
31	Ea	22	0	19	1	0
31	Eb	22	0	19	1	0
31	Ec	22	0	19	1	0
31	Ed	22	0	19	1	0
31	Ee	22	0	17	1	0
31	Ef	22	0	17	1	0
31	Eg	22	0	16	1	0
31	Uh	22	0	16	1	0
31	Fi	22	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Fj	22	0	19	0	0
31	Fk	22	0	19	0	0
31	Fl	22	0	19	0	0
31	Ga	22	0	19	1	0
31	Gb	22	0	19	1	0
31	Gc	22	0	19	1	0
31	Gd	22	0	19	1	0
31	Ge	22	0	19	0	0
31	Gf	22	0	19	0	0
31	Gg	22	0	19	0	0
31	Gh	22	0	19	0	0
31	Gi	22	0	19	0	0
31	Gj	22	0	19	0	0
31	Gk	22	0	19	0	0
31	Gl	22	0	19	0	0
31	Ha	22	0	19	1	0
31	Hb	22	0	19	1	0
31	Hc	22	0	19	1	0
31	Hd	22	0	19	1	0
31	He	22	0	19	0	0
31	Hf	22	0	19	0	0
31	Hg	22	0	19	0	0
31	Hh	22	0	19	0	0
31	Hi	22	0	19	2	0
31	Hj	22	0	19	2	0
31	Hk	22	0	19	2	0
31	Hl	22	0	19	2	0
31	Ia	22	0	19	0	0
31	Ib	22	0	19	0	0
31	Ic	22	0	19	0	0
31	Id	22	0	19	0	0
31	Ie	22	0	19	1	0
31	If	22	0	19	1	0
31	Ig	22	0	19	1	0
31	Ih	22	0	19	1	0
31	Ii	22	0	19	0	0
31	Ij	22	0	19	0	0
31	Ik	22	0	19	0	0
31	Il	22	0	19	0	0
31	Ja	22	0	19	0	0
31	Jb	22	0	19	0	0
31	Jc	22	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Jd	22	0	19	0	0
31	Je	22	0	19	1	0
31	Jf	22	0	19	1	0
31	Jg	22	0	19	0	0
31	Jh	22	0	19	1	0
31	Ji	22	0	19	0	0
31	Jj	22	0	19	0	0
31	Jk	22	0	19	0	0
31	Jl	22	0	19	0	0
31	Ka	22	0	19	0	0
31	Kb	22	0	19	0	0
31	Kc	22	0	19	0	0
31	Kd	22	0	19	0	0
31	Ke	22	0	19	1	0
31	Kf	22	0	19	1	0
31	Kg	22	0	19	1	0
31	Kh	22	0	19	1	0
31	Ki	22	0	19	0	0
31	Kj	22	0	19	0	0
31	Kk	22	0	19	0	0
31	Kl	22	0	19	0	0
31	La	22	0	19	1	0
31	Lb	22	0	19	1	0
31	Lc	22	0	19	1	0
31	Ld	22	0	19	1	0
31	Le	22	0	19	0	0
31	Lf	22	0	19	0	0
31	Lg	22	0	19	0	0
31	Lh	22	0	19	0	0
31	Li	22	0	19	0	0
31	Lj	22	0	19	0	0
31	Lk	22	0	19	0	0
31	Ll	22	0	19	0	0
31	Ma	22	0	19	1	0
31	Mb	22	0	19	1	0
31	Mc	22	0	19	1	0
31	Md	22	0	19	1	0
31	Me	22	0	19	0	0
31	Mf	22	0	19	0	0
31	Mg	22	0	19	0	0
31	Mh	22	0	19	0	0
31	Mi	22	0	19	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Mj	22	0	19	1	0
31	Mk	22	0	19	2	0
31	MI	22	0	19	2	0
31	Na	22	0	19	0	0
31	Nb	22	0	19	0	0
31	Nc	22	0	19	1	0
31	Nd	22	0	19	0	0
31	Ne	22	0	19	2	0
31	Nf	22	0	19	2	0
31	Ng	22	0	19	2	0
31	Nh	22	0	19	2	0
31	Ni	22	0	19	0	0
31	Nj	22	0	19	0	0
31	Nk	22	0	19	0	0
31	Nl	22	0	19	0	0
31	Oa	22	0	19	0	0
31	Ob	22	0	19	0	0
31	Oc	22	0	19	0	0
31	Od	22	0	19	0	0
31	Oe	22	0	19	0	0
31	Of	22	0	19	0	0
31	Og	22	0	19	0	0
31	Oh	22	0	19	0	0
31	Oi	22	0	19	0	0
31	Oj	22	0	19	0	0
31	Ok	22	0	19	0	0
31	Ol	22	0	19	0	0
31	Pa	22	0	19	0	0
31	Pb	22	0	19	0	0
31	Pc	22	0	19	0	0
31	Pd	22	0	19	0	0
31	Pe	22	0	19	0	0
31	Pf	22	0	19	0	0
31	Pg	22	0	19	0	0
31	Ph	22	0	19	0	0
31	Pi	22	0	19	2	0
31	Pj	22	0	19	2	0
31	Pk	22	0	19	2	0
31	Pl	22	0	19	2	0
31	Qa	22	0	19	0	0
31	Qb	22	0	19	0	0
31	Qc	22	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Qd	22	0	19	0	0
31	Qi	22	0	19	0	0
31	Qj	22	0	19	0	0
31	Qk	22	0	19	0	0
31	Ql	22	0	19	0	0
31	Ra	22	0	19	0	0
31	Rb	22	0	19	0	0
31	Rc	22	0	19	0	0
31	Rd	22	0	19	0	0
31	Re	22	0	19	0	0
31	Rf	22	0	19	0	0
31	Rg	22	0	19	0	0
31	Rh	22	0	19	0	0
31	Se	22	0	19	0	0
31	Sf	22	0	19	0	0
31	Sg	22	0	19	0	0
31	Sh	22	0	19	0	0
31	Si	22	0	19	2	0
31	Sj	22	0	19	2	0
31	Sk	22	0	19	2	0
31	Sl	22	0	19	2	0
31	Ta	22	0	19	5	0
31	Tb	22	0	19	5	0
31	Tc	22	0	19	5	0
31	Td	22	0	19	5	0
31	Ti	22	0	19	0	0
31	Tj	22	0	19	0	0
31	Tk	22	0	19	0	0
31	Tl	22	0	19	0	0
31	Ua	22	0	19	1	0
31	Ub	22	0	19	1	0
31	Uc	22	0	19	1	0
31	Ud	22	0	19	1	0
31	Ui	22	0	19	0	0
31	Uj	22	0	19	0	0
31	Uk	22	0	19	0	0
31	Ul	22	0	19	0	0
31	Va	22	0	19	0	0
31	Vb	22	0	19	0	0
31	Vc	22	0	19	0	0
31	Vd	22	0	19	0	0
31	Ve	22	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	Vf	22	0	19	0	0
31	Vg	22	0	19	0	0
31	Vh	22	0	19	0	0
31	We	22	0	19	0	0
31	Wf	22	0	19	0	0
31	Wg	22	0	19	0	0
31	Wh	22	0	19	0	0
31	Xi	22	0	19	0	0
31	Xj	22	0	19	0	0
31	Xk	22	0	19	0	0
31	Xl	22	0	19	0	0
31	Ya	22	0	19	0	0
31	Yb	22	0	19	0	0
31	Yc	22	0	19	0	0
31	Yd	22	0	19	0	0
31	Yi	22	0	19	0	0
31	Yj	22	0	19	0	0
31	Yk	22	0	19	0	0
31	Yl	22	0	19	0	0
31	Za	22	0	19	1	0
31	Zb	22	0	19	1	0
31	Zc	22	0	19	0	0
31	Zd	22	0	19	0	0
31	Zi	22	0	19	0	0
31	Zj	22	0	19	0	0
31	Zk	22	0	19	0	0
31	Zl	22	0	19	0	0
31	aa	22	0	19	0	0
31	ab	22	0	19	0	0
31	ac	22	0	19	0	0
31	ad	22	0	19	0	0
31	bi	22	0	19	0	0
31	bj	22	0	19	0	0
31	bk	22	0	19	0	0
31	bl	22	0	19	0	0
31	ca	22	0	19	0	0
31	cb	22	0	19	0	0
31	cc	22	0	19	0	0
31	cd	22	0	19	0	0
31	ci	22	0	19	1	0
31	cj	22	0	19	1	0
31	ck	22	0	19	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	cl	22	0	19	1	0
31	da	22	0	19	0	0
31	db	22	0	19	0	0
31	dc	22	0	19	0	0
31	dd	22	0	19	0	0
31	di	22	0	19	0	0
31	dj	22	0	19	0	0
31	dk	22	0	19	0	0
31	dl	22	0	19	0	0
31	ea	22	0	19	0	0
31	eb	22	0	19	0	0
31	ec	22	0	19	0	0
31	ed	22	0	19	0	0
31	ei	22	0	19	0	0
31	ej	22	0	19	0	0
31	ek	22	0	19	0	0
31	el	22	0	19	0	0
31	fa	22	0	19	0	0
31	fb	22	0	19	0	0
31	fc	22	0	19	0	0
31	fd	22	0	19	0	0
31	gi	22	0	19	1	0
31	gj	22	0	19	1	0
31	gk	22	0	19	1	0
31	gl	22	0	19	1	0
31	ha	22	0	19	0	0
31	hb	22	0	19	0	0
31	hc	22	0	19	0	0
31	hd	22	0	19	0	0
31	ii	22	0	19	1	0
31	ij	22	0	19	0	0
31	ik	22	0	19	1	0
31	il	22	0	19	0	0
31	ja	22	0	19	1	0
31	jb	22	0	19	1	0
31	jc	22	0	19	1	0
31	jd	22	0	19	1	0
31	ji	22	0	19	0	0
31	jj	22	0	19	0	0
31	jk	22	0	19	0	0
31	jl	22	0	19	0	0
31	ka	22	0	19	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	kb	22	0	19	0	0
31	kc	22	0	19	0	0
31	kd	22	0	19	0	0
31	ki	22	0	19	1	0
31	kj	22	0	19	1	0
31	kk	22	0	19	1	0
31	kl	22	0	19	1	0
31	la	22	0	19	2	0
31	lb	22	0	19	2	0
31	lc	22	0	19	2	0
31	ld	22	0	19	2	0
31	li	22	0	19	2	0
31	lj	22	0	19	2	0
31	lk	22	0	19	2	0
31	ll	22	0	19	2	0
31	ma	22	0	19	0	0
31	mb	22	0	19	0	0
31	mc	22	0	19	0	0
31	md	22	0	19	0	0
31	mi	22	0	19	0	0
31	mj	22	0	19	0	0
31	mk	22	0	19	0	0
31	ml	22	0	19	0	0
31	na	22	0	19	1	0
31	nb	22	0	19	1	0
31	nc	22	0	19	1	0
31	nd	22	0	19	1	0
31	ni	22	0	19	1	0
31	nj	22	0	19	1	0
31	nk	22	0	19	1	0
31	nl	22	0	19	1	0
31	oa	22	0	19	0	0
31	ob	22	0	19	0	0
31	oc	22	0	19	0	0
31	od	22	0	19	0	0
31	oi	22	0	19	0	0
31	oj	22	0	19	0	0
31	ok	22	0	19	0	0
31	ol	22	0	19	0	0
31	pa	22	0	19	1	0
31	pb	22	0	19	1	0
31	pc	22	0	19	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	pd	22	0	19	0	0
31	pi	22	0	19	1	0
31	pj	22	0	19	1	0
31	pk	22	0	19	1	0
31	pl	22	0	19	1	0
31	qa	22	0	19	0	0
31	qb	22	0	19	0	0
31	qc	22	0	19	0	0
31	qd	22	0	19	0	0
31	qi	22	0	19	1	0
31	qj	22	0	19	1	0
31	qk	22	0	19	2	0
31	ql	22	0	19	1	0
31	ra	22	0	19	0	0
31	rb	22	0	19	0	0
31	rc	22	0	19	0	0
31	rd	22	0	19	0	0
31	ri	22	0	19	1	0
31	rj	22	0	19	0	0
31	rk	22	0	19	1	0
31	rl	22	0	19	0	0
31	sa	22	0	19	0	0
31	sb	22	0	19	0	0
31	sc	22	0	19	0	0
31	sd	22	0	19	0	0
32	CC	11	0	10	0	0
32	HC	11	0	10	0	0
32	MC	11	0	10	0	0
32	RC	11	0	10	0	0
33	AB	11	0	9	0	0
33	FB	11	0	9	0	0
33	KB	11	0	9	0	0
33	PB	11	0	9	0	0
All	All	279032	0	261326	6468	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 12.

The worst 5 of 6468 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)
29:CL:624:GLN:NE2	29:CL:625:GLY:O	1.95	0.99
29:FL:624:GLN:NE2	29:FL:625:GLY:O	1.95	0.98
17:LG:346:ILE:HD12	17:LG:347:PRO:HD2	1.48	0.96
17:BG:346:ILE:HD12	17:BG:347:PRO:HD2	1.47	0.96
17:QG:346:ILE:HD12	17:QG:347:PRO:HD2	1.48	0.95

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	AA	239/246 (97%)	236 (99%)	2 (1%)	1 (0%)	30	62
1	FA	239/246 (97%)	236 (99%)	2 (1%)	1 (0%)	30	62
1	KA	239/246 (97%)	236 (99%)	2 (1%)	1 (0%)	30	62
1	PA	239/246 (97%)	236 (99%)	2 (1%)	1 (0%)	30	62
2	BA	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
2	GA	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
2	LA	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
2	QA	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
3	CA	225/234 (96%)	223 (99%)	2 (1%)	0	100	100
3	HA	225/234 (96%)	223 (99%)	2 (1%)	0	100	100
3	MA	225/234 (96%)	224 (100%)	1 (0%)	0	100	100
3	RA	225/234 (96%)	223 (99%)	2 (1%)	0	100	100
4	DA	226/237 (95%)	218 (96%)	7 (3%)	1 (0%)	30	62
4	IA	226/237 (95%)	218 (96%)	7 (3%)	1 (0%)	30	62
4	NA	226/237 (95%)	217 (96%)	8 (4%)	1 (0%)	30	62
4	SA	226/237 (95%)	218 (96%)	7 (3%)	1 (0%)	30	62

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	EA	70/77 (91%)	70 (100%)	0	0	100	100
5	JA	70/77 (91%)	70 (100%)	0	0	100	100
5	OA	70/77 (91%)	70 (100%)	0	0	100	100
5	TA	70/77 (91%)	70 (100%)	0	0	100	100
6	AC	239/246 (97%)	230 (96%)	8 (3%)	1 (0%)	30	62
6	FC	239/246 (97%)	230 (96%)	8 (3%)	1 (0%)	30	62
6	KC	239/246 (97%)	230 (96%)	8 (3%)	1 (0%)	30	62
6	PC	239/246 (97%)	231 (97%)	7 (3%)	1 (0%)	30	62
7	BC	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
7	GC	220/233 (94%)	217 (99%)	3 (1%)	0	100	100
7	LC	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
7	QC	220/233 (94%)	216 (98%)	4 (2%)	0	100	100
8	CC	225/235 (96%)	219 (97%)	5 (2%)	1 (0%)	30	62
8	HC	225/235 (96%)	219 (97%)	5 (2%)	1 (0%)	30	62
8	MC	225/235 (96%)	219 (97%)	5 (2%)	1 (0%)	30	62
8	RC	225/235 (96%)	219 (97%)	5 (2%)	1 (0%)	30	62
9	DC	225/236 (95%)	222 (99%)	3 (1%)	0	100	100
9	IC	225/236 (95%)	222 (99%)	3 (1%)	0	100	100
9	NC	225/236 (95%)	223 (99%)	2 (1%)	0	100	100
9	SC	225/236 (95%)	222 (99%)	3 (1%)	0	100	100
10	EC	69/76 (91%)	69 (100%)	0	0	100	100
10	JC	69/76 (91%)	69 (100%)	0	0	100	100
10	OC	69/76 (91%)	69 (100%)	0	0	100	100
10	TC	69/76 (91%)	69 (100%)	0	0	100	100
11	AB	224/231 (97%)	221 (99%)	3 (1%)	0	100	100
11	FB	224/231 (97%)	221 (99%)	3 (1%)	0	100	100
11	KB	224/231 (97%)	221 (99%)	3 (1%)	0	100	100
11	PB	224/231 (97%)	221 (99%)	3 (1%)	0	100	100
12	BB	226/233 (97%)	223 (99%)	3 (1%)	0	100	100
12	GB	226/233 (97%)	222 (98%)	4 (2%)	0	100	100
12	LB	226/233 (97%)	222 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	QB	226/233 (97%)	223 (99%)	3 (1%)	0	100	100
13	CB	225/234 (96%)	217 (96%)	8 (4%)	0	100	100
13	HB	225/234 (96%)	217 (96%)	8 (4%)	0	100	100
13	MB	225/234 (96%)	217 (96%)	8 (4%)	0	100	100
13	RB	225/234 (96%)	217 (96%)	8 (4%)	0	100	100
14	DB	233/237 (98%)	232 (100%)	1 (0%)	0	100	100
14	IB	233/237 (98%)	232 (100%)	1 (0%)	0	100	100
14	NB	233/237 (98%)	232 (100%)	1 (0%)	0	100	100
14	SB	233/237 (98%)	232 (100%)	1 (0%)	0	100	100
15	EB	74/76 (97%)	74 (100%)	0	0	100	100
15	JB	74/76 (97%)	74 (100%)	0	0	100	100
15	OB	74/76 (97%)	74 (100%)	0	0	100	100
15	TB	74/76 (97%)	74 (100%)	0	0	100	100
16	AD	103/169 (61%)	103 (100%)	0	0	100	100
16	AE	103/169 (61%)	103 (100%)	0	0	100	100
16	AF	103/169 (61%)	103 (100%)	0	0	100	100
16	AG	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
16	AH	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
16	AI	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
16	FD	103/169 (61%)	103 (100%)	0	0	100	100
16	FE	103/169 (61%)	103 (100%)	0	0	100	100
16	FF	103/169 (61%)	103 (100%)	0	0	100	100
16	FG	167/169 (99%)	167 (100%)	0	0	100	100
16	FH	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
16	FI	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
16	KD	103/169 (61%)	103 (100%)	0	0	100	100
16	KE	103/169 (61%)	103 (100%)	0	0	100	100
16	KF	103/169 (61%)	103 (100%)	0	0	100	100
16	KG	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
16	KH	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
16	KI	167/169 (99%)	165 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	PD	103/169 (61%)	103 (100%)	0	0	100	100
16	PE	103/169 (61%)	103 (100%)	0	0	100	100
16	PF	103/169 (61%)	103 (100%)	0	0	100	100
16	PG	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
16	PH	167/169 (99%)	164 (98%)	3 (2%)	0	100	100
16	PI	167/169 (99%)	166 (99%)	1 (1%)	0	100	100
17	BD	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	BE	246/248 (99%)	241 (98%)	5 (2%)	0	100	100
17	BF	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	BG	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	BH	244/248 (98%)	238 (98%)	6 (2%)	0	100	100
17	BI	246/248 (99%)	245 (100%)	0	1 (0%)	30	62
17	GD	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	GE	246/248 (99%)	241 (98%)	5 (2%)	0	100	100
17	GF	246/248 (99%)	243 (99%)	3 (1%)	0	100	100
17	GG	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	GH	244/248 (98%)	239 (98%)	5 (2%)	0	100	100
17	GI	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	LD	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	LE	246/248 (99%)	241 (98%)	5 (2%)	0	100	100
17	LF	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	LG	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	LH	244/248 (98%)	239 (98%)	5 (2%)	0	100	100
17	LI	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	QD	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	QE	246/248 (99%)	241 (98%)	5 (2%)	0	100	100
17	QF	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	QG	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
17	QH	244/248 (98%)	240 (98%)	4 (2%)	0	100	100
17	QI	246/248 (99%)	244 (99%)	2 (1%)	0	100	100
18	CD	210/223 (94%)	201 (96%)	9 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	CE	210/223 (94%)	202 (96%)	8 (4%)	0	100	100
18	CF	210/223 (94%)	204 (97%)	4 (2%)	2 (1%)	12	45
18	CG	221/223 (99%)	219 (99%)	2 (1%)	0	100	100
18	CH	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
18	CI	221/223 (99%)	214 (97%)	5 (2%)	2 (1%)	14	47
18	HD	210/223 (94%)	201 (96%)	9 (4%)	0	100	100
18	HE	210/223 (94%)	202 (96%)	8 (4%)	0	100	100
18	HF	210/223 (94%)	203 (97%)	6 (3%)	1 (0%)	24	59
18	HG	221/223 (99%)	219 (99%)	2 (1%)	0	100	100
18	HH	221/223 (99%)	214 (97%)	7 (3%)	0	100	100
18	HI	221/223 (99%)	214 (97%)	5 (2%)	2 (1%)	14	47
18	MD	210/223 (94%)	201 (96%)	9 (4%)	0	100	100
18	ME	210/223 (94%)	202 (96%)	8 (4%)	0	100	100
18	MF	210/223 (94%)	204 (97%)	4 (2%)	2 (1%)	12	45
18	MG	221/223 (99%)	219 (99%)	2 (1%)	0	100	100
18	MH	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
18	MI	221/223 (99%)	214 (97%)	5 (2%)	2 (1%)	14	47
18	RD	210/223 (94%)	200 (95%)	10 (5%)	0	100	100
18	RE	210/223 (94%)	202 (96%)	8 (4%)	0	100	100
18	RF	210/223 (94%)	204 (97%)	4 (2%)	2 (1%)	12	45
18	RG	221/223 (99%)	219 (99%)	2 (1%)	0	100	100
18	RH	221/223 (99%)	213 (96%)	8 (4%)	0	100	100
18	RI	221/223 (99%)	214 (97%)	5 (2%)	2 (1%)	14	47
19	DD	229/237 (97%)	225 (98%)	4 (2%)	0	100	100
19	DE	229/237 (97%)	226 (99%)	3 (1%)	0	100	100
19	DF	227/237 (96%)	227 (100%)	0	0	100	100
19	DG	224/237 (94%)	222 (99%)	2 (1%)	0	100	100
19	DH	224/237 (94%)	217 (97%)	7 (3%)	0	100	100
19	DI	224/237 (94%)	219 (98%)	3 (1%)	2 (1%)	14	47
19	ID	229/237 (97%)	224 (98%)	5 (2%)	0	100	100
19	IE	229/237 (97%)	226 (99%)	3 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	IF	227/237 (96%)	227 (100%)	0	0	100	100
19	IG	224/237 (94%)	222 (99%)	2 (1%)	0	100	100
19	IH	224/237 (94%)	216 (96%)	8 (4%)	0	100	100
19	II	224/237 (94%)	219 (98%)	3 (1%)	2 (1%)	14	47
19	ND	229/237 (97%)	225 (98%)	4 (2%)	0	100	100
19	NE	229/237 (97%)	225 (98%)	4 (2%)	0	100	100
19	NF	227/237 (96%)	227 (100%)	0	0	100	100
19	NG	224/237 (94%)	222 (99%)	2 (1%)	0	100	100
19	NH	224/237 (94%)	217 (97%)	7 (3%)	0	100	100
19	NI	224/237 (94%)	218 (97%)	4 (2%)	2 (1%)	14	47
19	SD	229/237 (97%)	225 (98%)	4 (2%)	0	100	100
19	SE	229/237 (97%)	225 (98%)	4 (2%)	0	100	100
19	SF	227/237 (96%)	227 (100%)	0	0	100	100
19	SG	224/237 (94%)	222 (99%)	2 (1%)	0	100	100
19	SH	224/237 (94%)	217 (97%)	7 (3%)	0	100	100
19	SI	224/237 (94%)	218 (97%)	4 (2%)	2 (1%)	14	47
20	ED	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
20	EE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
20	EF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
20	EG	154/162 (95%)	149 (97%)	4 (3%)	1 (1%)	21	56
20	EH	154/162 (95%)	149 (97%)	5 (3%)	0	100	100
20	EI	154/162 (95%)	148 (96%)	6 (4%)	0	100	100
20	JD	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
20	JE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
20	JF	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
20	JG	154/162 (95%)	150 (97%)	3 (2%)	1 (1%)	21	56
20	JH	154/162 (95%)	149 (97%)	5 (3%)	0	100	100
20	JI	154/162 (95%)	148 (96%)	6 (4%)	0	100	100
20	OD	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
20	OE	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
20	OF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	OG	154/162 (95%)	151 (98%)	2 (1%)	1 (1%)	21	56
20	OH	154/162 (95%)	150 (97%)	4 (3%)	0	100	100
20	OI	154/162 (95%)	150 (97%)	4 (3%)	0	100	100
20	TD	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
20	TE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
20	TF	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
20	TG	154/162 (95%)	150 (97%)	3 (2%)	1 (1%)	21	56
20	TH	154/162 (95%)	150 (97%)	4 (3%)	0	100	100
20	TI	154/162 (95%)	148 (96%)	6 (4%)	0	100	100
21	AJ	56/58 (97%)	56 (100%)	0	0	100	100
21	DJ	56/58 (97%)	56 (100%)	0	0	100	100
21	GJ	56/58 (97%)	56 (100%)	0	0	100	100
21	JJ	56/58 (97%)	56 (100%)	0	0	100	100
22	BJ	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	62
22	EJ	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	62
22	HJ	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	62
22	KJ	229/231 (99%)	223 (97%)	5 (2%)	1 (0%)	30	62
23	CJ	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
23	FJ	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
23	IJ	169/171 (99%)	165 (98%)	4 (2%)	0	100	100
23	LJ	169/171 (99%)	166 (98%)	3 (2%)	0	100	100
24	AK	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
24	DK	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
24	GK	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
24	JK	56/58 (97%)	52 (93%)	4 (7%)	0	100	100
25	BK	230/232 (99%)	210 (91%)	16 (7%)	4 (2%)	7	35
25	EK	230/232 (99%)	210 (91%)	16 (7%)	4 (2%)	7	35
25	HK	230/232 (99%)	211 (92%)	15 (6%)	4 (2%)	7	35
25	KK	230/232 (99%)	211 (92%)	15 (6%)	4 (2%)	7	35
26	CK	168/170 (99%)	160 (95%)	8 (5%)	0	100	100
26	FK	168/170 (99%)	161 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	IK	168/170 (99%)	160 (95%)	8 (5%)	0	100	100
26	LK	168/170 (99%)	161 (96%)	7 (4%)	0	100	100
27	AL	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	DL	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	GL	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
27	JL	56/58 (97%)	55 (98%)	1 (2%)	0	100	100
28	BL	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
28	EL	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
28	HL	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
28	KL	230/232 (99%)	216 (94%)	14 (6%)	0	100	100
29	CL	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
29	FL	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
29	IL	168/170 (99%)	165 (98%)	3 (2%)	0	100	100
29	LL	168/170 (99%)	164 (98%)	4 (2%)	0	100	100
30	AM	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
30	BM	208/210 (99%)	197 (95%)	11 (5%)	0	100	100
30	CM	208/210 (99%)	198 (95%)	10 (5%)	0	100	100
30	DM	208/210 (99%)	196 (94%)	12 (6%)	0	100	100
All	All	41544/43552 (95%)	40624 (98%)	856 (2%)	64 (0%)	44	73

5 of 64 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	DA	1551	PRO
17	BI	418	GLU
18	CI	563	PRO
18	CI	623	PRO
19	DI	811	VAL

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	AA	150/150 (100%)	147 (98%)	3 (2%)	48	72
1	FA	150/150 (100%)	146 (97%)	4 (3%)	39	68
1	KA	150/150 (100%)	147 (98%)	3 (2%)	48	72
1	PA	150/150 (100%)	147 (98%)	3 (2%)	48	72
2	BA	138/138 (100%)	133 (96%)	5 (4%)	31	63
2	GA	138/138 (100%)	133 (96%)	5 (4%)	31	63
2	LA	138/138 (100%)	133 (96%)	5 (4%)	31	63
2	QA	138/138 (100%)	133 (96%)	5 (4%)	31	63
3	CA	137/137 (100%)	133 (97%)	4 (3%)	37	67
3	HA	137/137 (100%)	132 (96%)	5 (4%)	31	63
3	MA	137/137 (100%)	133 (97%)	4 (3%)	37	67
3	RA	137/137 (100%)	131 (96%)	6 (4%)	25	59
4	DA	135/135 (100%)	133 (98%)	2 (2%)	57	76
4	IA	135/135 (100%)	134 (99%)	1 (1%)	76	83
4	NA	135/135 (100%)	133 (98%)	2 (2%)	57	76
4	SA	135/135 (100%)	133 (98%)	2 (2%)	57	76
5	EA	44/44 (100%)	43 (98%)	1 (2%)	44	70
5	JA	44/44 (100%)	43 (98%)	1 (2%)	44	70
5	OA	44/44 (100%)	43 (98%)	1 (2%)	44	70
5	TA	44/44 (100%)	43 (98%)	1 (2%)	44	70
6	AC	150/150 (100%)	148 (99%)	2 (1%)	61	78
6	FC	150/150 (100%)	148 (99%)	2 (1%)	61	78
6	KC	150/150 (100%)	147 (98%)	3 (2%)	48	72
6	PC	150/150 (100%)	148 (99%)	2 (1%)	61	78
7	BC	135/135 (100%)	130 (96%)	5 (4%)	30	63
7	GC	135/135 (100%)	131 (97%)	4 (3%)	36	66
7	LC	135/135 (100%)	131 (97%)	4 (3%)	36	66
7	QC	135/135 (100%)	130 (96%)	5 (4%)	30	63
8	CC	131/131 (100%)	128 (98%)	3 (2%)	44	70
8	HC	131/131 (100%)	127 (97%)	4 (3%)	35	66
8	MC	131/131 (100%)	127 (97%)	4 (3%)	35	66

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	RC	131/131 (100%)	127 (97%)	4 (3%)	35	66
9	DC	127/127 (100%)	123 (97%)	4 (3%)	35	66
9	IC	127/127 (100%)	123 (97%)	4 (3%)	35	66
9	NC	127/127 (100%)	123 (97%)	4 (3%)	35	66
9	SC	127/127 (100%)	121 (95%)	6 (5%)	23	57
10	EC	41/41 (100%)	40 (98%)	1 (2%)	43	70
10	JC	41/41 (100%)	40 (98%)	1 (2%)	43	70
10	OC	41/41 (100%)	40 (98%)	1 (2%)	43	70
10	TC	41/41 (100%)	40 (98%)	1 (2%)	43	70
11	AB	133/133 (100%)	129 (97%)	4 (3%)	36	66
11	FB	133/133 (100%)	129 (97%)	4 (3%)	36	66
11	KB	133/133 (100%)	128 (96%)	5 (4%)	29	62
11	PB	133/133 (100%)	129 (97%)	4 (3%)	36	66
12	BB	141/141 (100%)	138 (98%)	3 (2%)	47	71
12	GB	141/141 (100%)	138 (98%)	3 (2%)	47	71
12	LB	141/141 (100%)	137 (97%)	4 (3%)	38	68
12	QB	141/141 (100%)	137 (97%)	4 (3%)	38	68
13	CB	132/132 (100%)	117 (89%)	15 (11%)	5	24
13	HB	132/132 (100%)	117 (89%)	15 (11%)	5	24
13	MB	132/132 (100%)	116 (88%)	16 (12%)	5	22
13	RB	132/132 (100%)	118 (89%)	14 (11%)	6	27
14	DB	142/142 (100%)	138 (97%)	4 (3%)	38	68
14	IB	142/142 (100%)	138 (97%)	4 (3%)	38	68
14	NB	142/142 (100%)	139 (98%)	3 (2%)	47	71
14	SB	142/142 (100%)	139 (98%)	3 (2%)	47	71
15	EB	48/48 (100%)	47 (98%)	1 (2%)	47	71
15	JB	48/48 (100%)	47 (98%)	1 (2%)	47	71
15	OB	48/48 (100%)	47 (98%)	1 (2%)	47	71
15	TB	48/48 (100%)	48 (100%)	0	100	100
16	AD	59/99 (60%)	59 (100%)	0	100	100
16	AE	59/99 (60%)	58 (98%)	1 (2%)	53	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	AF	59/99 (60%)	59 (100%)	0	100	100
16	AG	97/99 (98%)	96 (99%)	1 (1%)	68	80
16	AH	98/99 (99%)	97 (99%)	1 (1%)	68	80
16	AI	99/99 (100%)	96 (97%)	3 (3%)	36	66
16	FD	59/99 (60%)	59 (100%)	0	100	100
16	FE	59/99 (60%)	57 (97%)	2 (3%)	32	64
16	FF	59/99 (60%)	59 (100%)	0	100	100
16	FG	97/99 (98%)	96 (99%)	1 (1%)	68	80
16	FH	98/99 (99%)	97 (99%)	1 (1%)	68	80
16	FI	99/99 (100%)	95 (96%)	4 (4%)	28	61
16	KD	59/99 (60%)	59 (100%)	0	100	100
16	KE	59/99 (60%)	57 (97%)	2 (3%)	32	64
16	KF	59/99 (60%)	59 (100%)	0	100	100
16	KG	97/99 (98%)	96 (99%)	1 (1%)	68	80
16	KH	98/99 (99%)	97 (99%)	1 (1%)	68	80
16	KI	99/99 (100%)	95 (96%)	4 (4%)	28	61
16	PD	59/99 (60%)	59 (100%)	0	100	100
16	PE	59/99 (60%)	57 (97%)	2 (3%)	32	64
16	PF	59/99 (60%)	59 (100%)	0	100	100
16	PG	97/99 (98%)	96 (99%)	1 (1%)	68	80
16	PH	98/99 (99%)	97 (99%)	1 (1%)	68	80
16	PI	99/99 (100%)	95 (96%)	4 (4%)	28	61
17	BD	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	BE	132/134 (98%)	127 (96%)	5 (4%)	29	62
17	BF	131/134 (98%)	127 (97%)	4 (3%)	35	66
17	BG	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	BH	133/134 (99%)	132 (99%)	1 (1%)	73	82
17	BI	132/134 (98%)	131 (99%)	1 (1%)	73	82
17	GD	132/134 (98%)	130 (98%)	2 (2%)	57	76
17	GE	132/134 (98%)	128 (97%)	4 (3%)	36	66
17	GF	131/134 (98%)	128 (98%)	3 (2%)	44	70

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	GG	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	GH	133/134 (99%)	131 (98%)	2 (2%)	57	76
17	GI	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	LD	132/134 (98%)	130 (98%)	2 (2%)	57	76
17	LE	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	LF	131/134 (98%)	128 (98%)	3 (2%)	44	70
17	LG	132/134 (98%)	128 (97%)	4 (3%)	36	66
17	LH	133/134 (99%)	132 (99%)	1 (1%)	73	82
17	LI	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	QD	132/134 (98%)	130 (98%)	2 (2%)	57	76
17	QE	132/134 (98%)	129 (98%)	3 (2%)	44	70
17	QF	131/134 (98%)	126 (96%)	5 (4%)	29	62
17	QG	132/134 (98%)	128 (97%)	4 (3%)	36	66
17	QH	133/134 (99%)	132 (99%)	1 (1%)	73	82
17	QI	132/134 (98%)	130 (98%)	2 (2%)	57	76
18	CD	115/123 (94%)	115 (100%)	0	100	100
18	CE	115/123 (94%)	111 (96%)	4 (4%)	32	64
18	CF	115/123 (94%)	113 (98%)	2 (2%)	53	75
18	CG	120/123 (98%)	119 (99%)	1 (1%)	73	82
18	CH	122/123 (99%)	118 (97%)	4 (3%)	33	65
18	CI	119/123 (97%)	116 (98%)	3 (2%)	42	69
18	HD	115/123 (94%)	115 (100%)	0	100	100
18	HE	115/123 (94%)	110 (96%)	5 (4%)	26	59
18	HF	115/123 (94%)	114 (99%)	1 (1%)	70	81
18	HG	120/123 (98%)	119 (99%)	1 (1%)	73	82
18	HH	122/123 (99%)	116 (95%)	6 (5%)	22	55
18	HI	119/123 (97%)	115 (97%)	4 (3%)	32	64
18	MD	115/123 (94%)	115 (100%)	0	100	100
18	ME	115/123 (94%)	109 (95%)	6 (5%)	21	54
18	MF	115/123 (94%)	112 (97%)	3 (3%)	40	69
18	MG	120/123 (98%)	118 (98%)	2 (2%)	53	75

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	MH	122/123 (99%)	118 (97%)	4 (3%)	33	65
18	MI	119/123 (97%)	116 (98%)	3 (2%)	42	69
18	RD	115/123 (94%)	115 (100%)	0	100	100
18	RE	115/123 (94%)	111 (96%)	4 (4%)	32	64
18	RF	115/123 (94%)	113 (98%)	2 (2%)	53	75
18	RG	120/123 (98%)	117 (98%)	3 (2%)	42	69
18	RH	122/123 (99%)	116 (95%)	6 (5%)	22	55
18	RI	119/123 (97%)	116 (98%)	3 (2%)	42	69
19	DD	101/136 (74%)	101 (100%)	0	100	100
19	DE	99/136 (73%)	98 (99%)	1 (1%)	68	80
19	DF	100/136 (74%)	100 (100%)	0	100	100
19	DG	129/136 (95%)	129 (100%)	0	100	100
19	DH	128/136 (94%)	128 (100%)	0	100	100
19	DI	129/136 (95%)	127 (98%)	2 (2%)	55	75
19	ID	101/136 (74%)	101 (100%)	0	100	100
19	IE	99/136 (73%)	97 (98%)	2 (2%)	48	72
19	IF	100/136 (74%)	100 (100%)	0	100	100
19	IG	129/136 (95%)	129 (100%)	0	100	100
19	IH	128/136 (94%)	128 (100%)	0	100	100
19	II	129/136 (95%)	127 (98%)	2 (2%)	55	75
19	ND	101/136 (74%)	101 (100%)	0	100	100
19	NE	99/136 (73%)	97 (98%)	2 (2%)	48	72
19	NF	100/136 (74%)	99 (99%)	1 (1%)	68	80
19	NG	129/136 (95%)	129 (100%)	0	100	100
19	NH	128/136 (94%)	127 (99%)	1 (1%)	73	82
19	NI	129/136 (95%)	127 (98%)	2 (2%)	55	75
19	SD	101/136 (74%)	100 (99%)	1 (1%)	68	80
19	SE	99/136 (73%)	98 (99%)	1 (1%)	68	80
19	SF	100/136 (74%)	99 (99%)	1 (1%)	68	80
19	SG	129/136 (95%)	129 (100%)	0	100	100
19	SH	128/136 (94%)	128 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	SI	129/136 (95%)	127 (98%)	2 (2%)	55	75
20	ED	79/91 (87%)	78 (99%)	1 (1%)	61	78
20	EE	81/91 (89%)	81 (100%)	0	100	100
20	EF	78/91 (86%)	76 (97%)	2 (3%)	40	69
20	EG	84/91 (92%)	83 (99%)	1 (1%)	63	79
20	EH	85/91 (93%)	85 (100%)	0	100	100
20	EI	84/91 (92%)	83 (99%)	1 (1%)	63	79
20	JD	79/91 (87%)	78 (99%)	1 (1%)	61	78
20	JE	81/91 (89%)	81 (100%)	0	100	100
20	JF	78/91 (86%)	76 (97%)	2 (3%)	40	69
20	JG	84/91 (92%)	83 (99%)	1 (1%)	63	79
20	JH	85/91 (93%)	85 (100%)	0	100	100
20	JI	84/91 (92%)	83 (99%)	1 (1%)	63	79
20	OD	79/91 (87%)	78 (99%)	1 (1%)	61	78
20	OE	81/91 (89%)	81 (100%)	0	100	100
20	OF	78/91 (86%)	75 (96%)	3 (4%)	29	62
20	OG	84/91 (92%)	84 (100%)	0	100	100
20	OH	85/91 (93%)	85 (100%)	0	100	100
20	OI	84/91 (92%)	83 (99%)	1 (1%)	63	79
20	TD	79/91 (87%)	79 (100%)	0	100	100
20	TE	81/91 (89%)	81 (100%)	0	100	100
20	TF	78/91 (86%)	77 (99%)	1 (1%)	61	78
20	TG	84/91 (92%)	83 (99%)	1 (1%)	63	79
20	TH	85/91 (93%)	85 (100%)	0	100	100
20	TI	84/91 (92%)	83 (99%)	1 (1%)	63	79
21	AJ	33/33 (100%)	33 (100%)	0	100	100
21	DJ	33/33 (100%)	33 (100%)	0	100	100
21	GJ	33/33 (100%)	33 (100%)	0	100	100
21	JJ	33/33 (100%)	33 (100%)	0	100	100
22	BJ	146/146 (100%)	145 (99%)	1 (1%)	76	83
22	EJ	146/146 (100%)	145 (99%)	1 (1%)	76	83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	HJ	146/146 (100%)	145 (99%)	1 (1%)	76	83
22	KJ	146/146 (100%)	145 (99%)	1 (1%)	76	83
23	CJ	110/113 (97%)	107 (97%)	3 (3%)	39	68
23	FJ	110/113 (97%)	107 (97%)	3 (3%)	39	68
23	IJ	110/113 (97%)	107 (97%)	3 (3%)	39	68
23	LJ	110/113 (97%)	107 (97%)	3 (3%)	39	68
24	AK	34/34 (100%)	33 (97%)	1 (3%)	37	67
24	DK	34/34 (100%)	32 (94%)	2 (6%)	18	50
24	GK	34/34 (100%)	33 (97%)	1 (3%)	37	67
24	JK	34/34 (100%)	33 (97%)	1 (3%)	37	67
25	BK	143/145 (99%)	140 (98%)	3 (2%)	47	71
25	EK	143/145 (99%)	139 (97%)	4 (3%)	38	68
25	HK	143/145 (99%)	140 (98%)	3 (2%)	47	71
25	KK	143/145 (99%)	140 (98%)	3 (2%)	47	71
26	CK	110/112 (98%)	109 (99%)	1 (1%)	70	81
26	FK	110/112 (98%)	108 (98%)	2 (2%)	51	74
26	IK	110/112 (98%)	108 (98%)	2 (2%)	51	74
26	LK	110/112 (98%)	109 (99%)	1 (1%)	70	81
27	AL	38/38 (100%)	38 (100%)	0	100	100
27	DL	38/38 (100%)	38 (100%)	0	100	100
27	GL	38/38 (100%)	38 (100%)	0	100	100
27	JL	38/38 (100%)	38 (100%)	0	100	100
28	BL	136/136 (100%)	132 (97%)	4 (3%)	37	67
28	EL	136/136 (100%)	132 (97%)	4 (3%)	37	67
28	HL	136/136 (100%)	131 (96%)	5 (4%)	30	63
28	KL	136/136 (100%)	131 (96%)	5 (4%)	30	63
29	CL	108/111 (97%)	104 (96%)	4 (4%)	30	63
29	FL	108/111 (97%)	105 (97%)	3 (3%)	38	68
29	IL	108/111 (97%)	104 (96%)	4 (4%)	30	63
29	LL	108/111 (97%)	104 (96%)	4 (4%)	30	63
30	AM	191/191 (100%)	191 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
30	BM	191/191 (100%)	188 (98%)	3 (2%)	55	75
30	CM	191/191 (100%)	189 (99%)	2 (1%)	68	80
30	DM	191/191 (100%)	187 (98%)	4 (2%)	47	71
All	All	23916/25364 (94%)	23399 (98%)	517 (2%)	45	71

5 of 517 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	SE	1021	VAL
17	QH	358	ILE
19	SD	922	SER
19	IE	1021	VAL
18	HE	685	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 112 such sidechains are listed below:

Mol	Chain	Res	Type
29	FL	624	GLN
28	KL	405	GLN
18	ME	665	GLN
22	KJ	466	ASN
18	RE	713	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

376 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
11	LYZ	AB	386	11	7,9,10	0.51	0	4,10,12	0.56	0
7	LYZ	QC	792	7	7,9,10	0.51	0	4,10,12	0.59	0
7	LYZ	GC	915	7	7,9,10	0.51	0	4,10,12	0.55	0
5	LYZ	EA	1585	5	7,9,10	0.51	0	4,10,12	0.54	0
3	LYZ	CA	1159	3	7,9,10	0.50	0	4,10,12	0.53	0
12	LYZ	QB	539	12	7,9,10	0.50	0	4,10,12	0.50	0
8	LYZ	RC	1152	8	7,9,10	0.51	0	4,10,12	0.59	0
6	LYZ	AC	609	6	7,9,10	0.50	0	4,10,12	0.55	0
9	LYZ	NC	1464	9	7,9,10	0.51	0	4,10,12	0.57	0
7	LYZ	QC	801	7	7,9,10	0.52	0	4,10,12	0.61	0
7	LYZ	QC	777	7	7,9,10	0.50	0	4,10,12	0.54	0
3	LYZ	CA	1123	3	7,9,10	0.52	0	4,10,12	0.74	0
8	LYZ	CC	1221	8	7,9,10	0.49	0	4,10,12	0.48	0
3	LYZ	CA	1258	3	7,9,10	0.51	0	4,10,12	0.46	0
1	LYZ	KA	712	1	7,9,10	0.51	0	4,10,12	0.49	0
4	LYZ	SA	1567	4	7,9,10	0.50	0	4,10,12	0.56	0
9	LYZ	NC	1389	9	7,9,10	0.51	0	4,10,12	0.59	0
7	LYZ	QC	846	7	7,9,10	0.50	0	4,10,12	0.44	0
3	LYZ	MA	1159	3	7,9,10	0.50	0	4,10,12	0.53	0
9	LYZ	IC	1464	9	7,9,10	0.51	0	4,10,12	0.57	0
2	LYZ	BA	895	2	7,9,10	0.51	0	4,10,12	0.62	0
4	LYZ	IA	1558	4	7,9,10	0.52	0	4,10,12	0.59	0
10	LYZ	OC	1527	10	7,9,10	0.52	0	4,10,12	0.58	0
9	LYZ	SC	1287	9	7,9,10	0.51	0	4,10,12	0.54	0
7	LYZ	BC	807	7	7,9,10	0.51	0	4,10,12	0.61	0
5	LYZ	TA	1630	5	7,9,10	0.51	0	4,10,12	0.64	0
2	LYZ	BA	910	2	7,9,10	0.51	0	4,10,12	0.58	0
8	LYZ	HC	1152	8	7,9,10	0.51	0	4,10,12	0.59	0
4	LYZ	NA	1420	4	7,9,10	0.50	0	4,10,12	0.58	0
7	LYZ	BC	786	7	7,9,10	0.51	0	4,10,12	0.56	0
9	LYZ	DC	1266	9	7,9,10	0.51	0	4,10,12	0.60	0
1	LYZ	FA	712	1	7,9,10	0.51	0	4,10,12	0.49	0
1	LYZ	FA	727	1	7,9,10	0.50	0	4,10,12	0.51	0
5	LYZ	EA	1627	5	7,9,10	0.51	0	4,10,12	0.56	0
10	LYZ	EC	1524	10	7,9,10	0.52	0	4,10,12	0.60	0
2	LYZ	GA	904	2	7,9,10	0.50	0	4,10,12	0.58	0
12	LYZ	GB	476	12	7,9,10	0.52	0	4,10,12	0.65	0
2	LYZ	LA	949	2	7,9,10	0.50	0	4,10,12	0.47	0
6	LYZ	AC	624	6	7,9,10	0.50	0	4,10,12	0.56	0
2	LYZ	QA	895	2	7,9,10	0.51	0	4,10,12	0.62	0
8	LYZ	HC	1149	8	7,9,10	0.52	0	4,10,12	0.61	0
13	LYZ	MB	815	13	7,9,10	0.51	0	4,10,12	0.56	0
9	LYZ	DC	1317	9	7,9,10	0.48	0	4,10,12	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	LYZ	AB	320	11	7,9,10	0.51	0	4,10,12	0.53	0
4	LYZ	IA	1390	4	7,9,10	0.51	0	4,10,12	0.47	0
1	LYZ	AA	667	1	7,9,10	0.51	0	4,10,12	0.57	0
14	LYZ	NB	1130	14	7,9,10	0.52	0	4,10,12	0.55	0
2	LYZ	BA	904	2	7,9,10	0.50	0	4,10,12	0.58	0
13	LYZ	HB	731	13	7,9,10	0.51	0	4,10,12	0.52	0
4	LYZ	NA	1390	4	7,9,10	0.51	0	4,10,12	0.47	0
5	LYZ	JA	1627	5	7,9,10	0.51	0	4,10,12	0.56	0
8	LYZ	HC	1155	8	7,9,10	0.51	0	4,10,12	0.62	0
7	LYZ	BC	777	7	7,9,10	0.50	0	4,10,12	0.54	0
5	LYZ	TA	1585	5	7,9,10	0.51	0	4,10,12	0.54	0
9	LYZ	SC	1392	9	7,9,10	0.51	0	4,10,12	0.59	0
14	LYZ	NB	1142	14	7,9,10	0.51	0	4,10,12	0.48	0
11	LYZ	AB	311	11	7,9,10	0.51	0	4,10,12	0.56	0
7	LYZ	GC	777	7	7,9,10	0.50	0	4,10,12	0.54	0
2	LYZ	LA	892	2	7,9,10	0.51	0	4,10,12	0.64	0
9	LYZ	SC	1293	9	7,9,10	0.51	0	4,10,12	0.67	0
12	LYZ	GB	539	12	7,9,10	0.50	0	4,10,12	0.50	0
7	LYZ	GC	789	7	7,9,10	0.50	0	4,10,12	0.51	0
7	LYZ	QC	789	7	7,9,10	0.50	0	4,10,12	0.52	0
7	LYZ	GC	786	7	7,9,10	0.51	0	4,10,12	0.55	0
3	LYZ	MA	1255	3	7,9,10	0.52	0	4,10,12	0.59	0
8	LYZ	RC	1194	8	7,9,10	0.51	0	4,10,12	0.49	0
3	LYZ	MA	1252	3	7,9,10	0.50	0	4,10,12	0.51	0
4	LYZ	IA	1420	4	7,9,10	0.50	0	4,10,12	0.58	0
11	LYZ	FB	320	11	7,9,10	0.51	0	4,10,12	0.52	0
6	LYZ	FC	690	6	7,9,10	0.51	0	4,10,12	0.62	0
10	LYZ	JC	1524	10	7,9,10	0.52	0	4,10,12	0.60	0
10	LYZ	JC	1482	10	7,9,10	0.50	0	4,10,12	0.46	0
12	LYZ	LB	620	12	7,9,10	0.51	0	4,10,12	0.60	0
8	LYZ	HC	1221	8	7,9,10	0.50	0	4,10,12	0.47	0
3	LYZ	HA	1204	3	7,9,10	0.49	0	4,10,12	0.57	0
12	LYZ	BB	539	12	7,9,10	0.50	0	4,10,12	0.50	0
7	LYZ	QC	786	7	7,9,10	0.51	0	4,10,12	0.56	0
6	LYZ	PC	756	6	7,9,10	0.51	0	4,10,12	0.50	0
2	LYZ	GA	889	2	7,9,10	0.50	0	4,10,12	0.49	0
5	LYZ	OA	1585	5	7,9,10	0.51	0	4,10,12	0.53	0
5	LYZ	JA	1639	5	7,9,10	0.52	0	4,10,12	0.55	0
5	LYZ	JA	1630	5	7,9,10	0.51	0	4,10,12	0.64	0
1	LYZ	PA	793	1	7,9,10	0.51	0	4,10,12	0.56	0
3	LYZ	RA	1123	3	7,9,10	0.52	0	4,10,12	0.72	0
8	LYZ	RC	1056	8	7,9,10	0.50	0	4,10,12	0.61	0
9	LYZ	DC	1287	9	7,9,10	0.51	0	4,10,12	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	LYZ	FB	386	11	7,9,10	0.51	0	4,10,12	0.56	0
2	LYZ	QA	889	2	7,9,10	0.50	0	4,10,12	0.50	0
4	LYZ	SA	1369	4	7,9,10	0.52	0	4,10,12	0.53	0
2	LYZ	LA	967	2	7,9,10	0.50	0	4,10,12	0.54	0
10	LYZ	EC	1527	10	7,9,10	0.52	0	4,10,12	0.59	0
9	LYZ	SC	1266	9	7,9,10	0.51	0	4,10,12	0.60	0
9	LYZ	IC	1455	9	7,9,10	0.50	0	4,10,12	0.55	0
9	LYZ	NC	1287	9	7,9,10	0.51	0	4,10,12	0.54	0
2	LYZ	LA	889	2	7,9,10	0.50	0	4,10,12	0.50	0
12	LYZ	QB	476	12	7,9,10	0.52	0	4,10,12	0.65	0
13	LYZ	HB	815	13	7,9,10	0.51	0	4,10,12	0.55	0
9	LYZ	SC	1461	9	7,9,10	0.51	0	4,10,12	0.57	0
9	LYZ	NC	1461	9	7,9,10	0.51	0	4,10,12	0.56	0
7	LYZ	LC	846	7	7,9,10	0.49	0	4,10,12	0.44	0
11	LYZ	PB	311	11	7,9,10	0.51	0	4,10,12	0.57	0
4	LYZ	DA	1390	4	7,9,10	0.51	0	4,10,12	0.47	0
1	LYZ	AA	712	1	7,9,10	0.51	0	4,10,12	0.49	0
9	LYZ	IC	1461	9	7,9,10	0.51	0	4,10,12	0.57	0
11	LYZ	PB	305	11	7,9,10	0.50	0	4,10,12	0.62	0
8	LYZ	HC	1056	8	7,9,10	0.50	0	4,10,12	0.61	0
5	LYZ	OA	1627	5	7,9,10	0.51	0	4,10,12	0.56	0
10	LYZ	JC	1536	10	7,9,10	0.52	0	4,10,12	0.57	0
7	LYZ	QC	828	7	7,9,10	0.50	0	4,10,12	0.54	0
2	LYZ	GA	967	2	7,9,10	0.50	0	4,10,12	0.54	0
8	LYZ	MC	1020	8	7,9,10	0.48	0	4,10,12	0.62	0
4	LYZ	SA	1492	4	7,9,10	0.51	0	4,10,12	0.55	0
7	LYZ	GC	801	7	7,9,10	0.52	0	4,10,12	0.61	0
5	LYZ	TA	1627	5	7,9,10	0.50	0	4,10,12	0.55	0
9	LYZ	SC	1455	9	7,9,10	0.51	0	4,10,12	0.55	0
2	LYZ	QA	931	2	7,9,10	0.51	0	4,10,12	0.54	0
2	LYZ	QA	892	2	7,9,10	0.51	0	4,10,12	0.63	0
8	LYZ	CC	1152	8	7,9,10	0.51	0	4,10,12	0.59	0
4	LYZ	NA	1495	4	7,9,10	0.52	0	4,10,12	0.55	0
7	LYZ	QC	915	7	7,9,10	0.51	0	4,10,12	0.55	0
2	LYZ	QA	967	2	7,9,10	0.50	0	4,10,12	0.54	0
7	LYZ	GC	792	7	7,9,10	0.51	0	4,10,12	0.59	0
7	LYZ	QC	879	7	7,9,10	0.49	0	4,10,12	0.48	0
8	LYZ	CC	1056	8	7,9,10	0.50	0	4,10,12	0.61	0
8	LYZ	CC	1194	8	7,9,10	0.51	0	4,10,12	0.49	0
1	LYZ	PA	727	1	7,9,10	0.50	0	4,10,12	0.52	0
10	LYZ	JC	1527	10	7,9,10	0.52	0	4,10,12	0.58	0
3	LYZ	RA	1258	3	7,9,10	0.51	0	4,10,12	0.46	0
2	LYZ	GA	880	2	7,9,10	0.50	0	4,10,12	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	LYZ	GA	982	2	7,9,10	0.52	0	4,10,12	0.52	0
8	LYZ	HC	1020	8	7,9,10	0.48	0	4,10,12	0.63	0
8	LYZ	CC	1149	8	7,9,10	0.52	0	4,10,12	0.61	0
11	LYZ	FB	305	11	7,9,10	0.50	0	4,10,12	0.61	0
12	LYZ	BB	482	12	7,9,10	0.51	0	4,10,12	0.50	0
3	LYZ	HA	1252	3	7,9,10	0.50	0	4,10,12	0.51	0
12	LYZ	GB	482	12	7,9,10	0.51	0	4,10,12	0.50	0
13	LYZ	MB	776	13	7,9,10	0.52	0	4,10,12	0.53	0
2	LYZ	QA	982	2	7,9,10	0.52	0	4,10,12	0.52	0
6	LYZ	PC	609	6	7,9,10	0.50	0	4,10,12	0.55	0
7	LYZ	LC	807	7	7,9,10	0.51	0	4,10,12	0.61	0
13	LYZ	RB	785	13	7,9,10	0.50	0	4,10,12	0.54	0
11	LYZ	PB	386	11	7,9,10	0.51	0	4,10,12	0.56	0
7	LYZ	GC	828	7	7,9,10	0.50	0	4,10,12	0.54	0
8	LYZ	CC	1155	8	7,9,10	0.51	0	4,10,12	0.61	0
3	LYZ	RA	1324	3	7,9,10	0.49	0	4,10,12	0.53	0
4	LYZ	DA	1396	4	7,9,10	0.50	0	4,10,12	0.47	0
2	LYZ	LA	895	2	7,9,10	0.51	0	4,10,12	0.62	0
1	LYZ	FA	667	1	7,9,10	0.51	0	4,10,12	0.57	0
13	LYZ	CB	869	13	7,9,10	0.51	0	4,10,12	0.53	0
7	LYZ	GC	846	7	7,9,10	0.49	0	4,10,12	0.43	0
13	LYZ	RB	815	13	7,9,10	0.51	0	4,10,12	0.56	0
11	LYZ	KB	386	11	7,9,10	0.51	0	4,10,12	0.55	0
2	LYZ	LA	880	2	7,9,10	0.50	0	4,10,12	0.60	0
1	LYZ	KA	667	1	7,9,10	0.51	0	4,10,12	0.57	0
11	LYZ	PB	299	11	7,9,10	0.51	0	4,10,12	0.56	0
2	LYZ	QA	1018	2	7,9,10	0.51	0	4,10,12	0.51	0
13	LYZ	CB	896	13	7,9,10	0.51	0	4,10,12	0.61	0
1	LYZ	FA	793	1	7,9,10	0.51	0	4,10,12	0.56	0
5	LYZ	EA	1630	5	7,9,10	0.51	0	4,10,12	0.64	0
9	LYZ	DC	1392	9	7,9,10	0.52	0	4,10,12	0.60	0
4	LYZ	IA	1495	4	7,9,10	0.52	0	4,10,12	0.55	0
14	LYZ	DB	1130	14	7,9,10	0.51	0	4,10,12	0.56	0
5	LYZ	EA	1600	5	7,9,10	0.52	0	4,10,12	0.51	0
3	LYZ	RA	1204	3	7,9,10	0.50	0	4,10,12	0.57	0
9	LYZ	DC	1461	9	7,9,10	0.51	0	4,10,12	0.56	0
5	LYZ	TA	1639	5	7,9,10	0.52	0	4,10,12	0.56	0
7	LYZ	BC	828	7	7,9,10	0.50	0	4,10,12	0.54	0
3	LYZ	HA	1258	3	7,9,10	0.51	0	4,10,12	0.46	0
5	LYZ	OA	1630	5	7,9,10	0.51	0	4,10,12	0.64	0
10	LYZ	OC	1497	10	7,9,10	0.52	0	4,10,12	0.63	0
7	LYZ	BC	801	7	7,9,10	0.52	0	4,10,12	0.61	0
13	LYZ	MB	731	13	7,9,10	0.51	0	4,10,12	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	LYZ	KC	756	6	7,9,10	0.51	0	4,10,12	0.51	0
12	LYZ	LB	539	12	7,9,10	0.50	0	4,10,12	0.50	0
4	LYZ	SA	1564	4	7,9,10	0.52	0	4,10,12	0.56	0
11	LYZ	PB	320	11	7,9,10	0.51	0	4,10,12	0.52	0
9	LYZ	DC	1389	9	7,9,10	0.51	0	4,10,12	0.58	0
3	LYZ	CA	1255	3	7,9,10	0.52	0	4,10,12	0.58	0
7	LYZ	LC	789	7	7,9,10	0.50	0	4,10,12	0.51	0
3	LYZ	CA	1252	3	7,9,10	0.50	0	4,10,12	0.51	0
7	LYZ	LC	777	7	7,9,10	0.50	0	4,10,12	0.67	0
14	LYZ	IB	1130	14	7,9,10	0.51	0	4,10,12	0.56	0
8	LYZ	MC	1194	8	7,9,10	0.51	0	4,10,12	0.49	0
5	LYZ	JA	1585	5	7,9,10	0.51	0	4,10,12	0.53	0
8	LYZ	MC	1149	8	7,9,10	0.52	0	4,10,12	0.61	0
4	LYZ	IA	1396	4	7,9,10	0.50	0	4,10,12	0.47	0
8	LYZ	MC	1101	8	7,9,10	0.51	0	4,10,12	0.47	0
3	LYZ	HA	1159	3	7,9,10	0.50	0	4,10,12	0.53	0
7	LYZ	QC	807	7	7,9,10	0.51	0	4,10,12	0.61	0
4	LYZ	DA	1420	4	7,9,10	0.50	0	4,10,12	0.58	0
7	LYZ	LC	786	7	7,9,10	0.51	0	4,10,12	0.55	0
9	LYZ	DC	1455	9	7,9,10	0.50	0	4,10,12	0.55	0
7	LYZ	BC	789	7	7,9,10	0.50	0	4,10,12	0.52	0
13	LYZ	CB	731	13	7,9,10	0.51	0	4,10,12	0.53	0
7	LYZ	LC	915	7	7,9,10	0.51	0	4,10,12	0.55	0
7	LYZ	GC	807	7	7,9,10	0.51	0	4,10,12	0.61	0
6	LYZ	FC	564	6	7,9,10	0.50	0	4,10,12	0.56	0
9	LYZ	NC	1293	9	7,9,10	0.51	0	4,10,12	0.65	0
1	LYZ	PA	859	1	7,9,10	0.52	0	4,10,12	0.70	0
3	LYZ	HA	1123	3	7,9,10	0.53	0	4,10,12	0.76	0
7	LYZ	GC	864	7	7,9,10	0.49	0	4,10,12	0.53	0
12	LYZ	BB	554	12	7,9,10	0.52	0	4,10,12	0.63	0
14	LYZ	SB	1130	14	7,9,10	0.51	0	4,10,12	0.55	0
9	LYZ	NC	1455	9	7,9,10	0.51	0	4,10,12	0.55	0
12	LYZ	GB	554	12	7,9,10	0.52	0	4,10,12	0.64	0
13	LYZ	MB	743	13	7,9,10	0.50	0	4,10,12	0.56	0
2	LYZ	QA	904	2	7,9,10	0.50	0	4,10,12	0.58	0
1	LYZ	KA	793	1	7,9,10	0.51	0	4,10,12	0.55	0
4	LYZ	DA	1558	4	7,9,10	0.52	0	4,10,12	0.59	0
7	LYZ	LC	792	7	7,9,10	0.51	0	4,10,12	0.59	0
8	LYZ	RC	1101	8	7,9,10	0.51	0	4,10,12	0.47	0
9	LYZ	IC	1392	9	7,9,10	0.51	0	4,10,12	0.58	0
10	LYZ	OC	1524	10	7,9,10	0.52	0	4,10,12	0.60	0
8	LYZ	RC	1149	8	7,9,10	0.52	0	4,10,12	0.61	0
10	LYZ	TC	1524	10	7,9,10	0.52	0	4,10,12	0.60	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	LYZ	LC	864	7	7,9,10	0.49	0	4,10,12	0.54	0
5	LYZ	JA	1600	5	7,9,10	0.52	0	4,10,12	0.51	0
11	LYZ	AB	305	11	7,9,10	0.50	0	4,10,12	0.62	0
10	LYZ	TC	1482	10	7,9,10	0.49	0	4,10,12	0.47	0
13	LYZ	HB	776	13	7,9,10	0.52	0	4,10,12	0.53	0
13	LYZ	CB	743	13	7,9,10	0.50	0	4,10,12	0.56	0
9	LYZ	SC	1464	9	7,9,10	0.51	0	4,10,12	0.57	0
14	LYZ	DB	1142	14	7,9,10	0.51	0	4,10,12	0.48	0
10	LYZ	EC	1536	10	7,9,10	0.52	0	4,10,12	0.57	0
2	LYZ	BA	889	2	7,9,10	0.50	0	4,10,12	0.51	0
8	LYZ	HC	1101	8	7,9,10	0.51	0	4,10,12	0.47	0
2	LYZ	LA	1018	2	7,9,10	0.51	0	4,10,12	0.54	0
8	LYZ	RC	1155	8	7,9,10	0.51	0	4,10,12	0.61	0
11	LYZ	KB	320	11	7,9,10	0.51	0	4,10,12	0.53	0
8	LYZ	MC	1152	8	7,9,10	0.51	0	4,10,12	0.59	0
2	LYZ	GA	931	2	7,9,10	0.51	0	4,10,12	0.54	0
5	LYZ	TA	1600	5	7,9,10	0.52	0	4,10,12	0.51	0
7	LYZ	QC	864	7	7,9,10	0.49	0	4,10,12	0.53	0
9	LYZ	SC	1317	9	7,9,10	0.48	0	4,10,12	0.53	0
4	LYZ	NA	1567	4	7,9,10	0.50	0	4,10,12	0.56	0
12	LYZ	LB	482	12	7,9,10	0.51	0	4,10,12	0.51	0
3	LYZ	HA	1255	3	7,9,10	0.52	0	4,10,12	0.59	0
1	LYZ	KA	727	1	7,9,10	0.50	0	4,10,12	0.47	0
6	LYZ	KC	564	6	7,9,10	0.50	0	4,10,12	0.56	0
7	LYZ	BC	846	7	7,9,10	0.49	0	4,10,12	0.44	0
6	LYZ	PC	624	6	7,9,10	0.50	0	4,10,12	0.56	0
1	LYZ	AA	727	1	7,9,10	0.50	0	4,10,12	0.52	0
7	LYZ	GC	879	7	7,9,10	0.49	0	4,10,12	0.48	0
12	LYZ	QB	620	12	7,9,10	0.51	0	4,10,12	0.60	0
13	LYZ	RB	743	13	7,9,10	0.50	0	4,10,12	0.55	0
4	LYZ	SA	1420	4	7,9,10	0.50	0	4,10,12	0.59	0
2	LYZ	BA	931	2	7,9,10	0.51	0	4,10,12	0.54	0
2	LYZ	BA	892	2	7,9,10	0.51	0	4,10,12	0.63	0
11	LYZ	KB	299	11	7,9,10	0.50	0	4,10,12	0.52	0
3	LYZ	MA	1258	3	7,9,10	0.51	0	4,10,12	0.46	0
10	LYZ	EC	1497	10	7,9,10	0.52	0	4,10,12	0.62	0
4	LYZ	SA	1558	4	7,9,10	0.52	0	4,10,12	0.61	0
13	LYZ	HB	869	13	7,9,10	0.51	0	4,10,12	0.54	0
13	LYZ	HB	785	13	7,9,10	0.51	0	4,10,12	0.54	0
2	LYZ	BA	880	2	7,9,10	0.50	0	4,10,12	0.61	0
3	LYZ	CA	1204	3	7,9,10	0.49	0	4,10,12	0.57	0
2	LYZ	GA	895	2	7,9,10	0.51	0	4,10,12	0.62	0
12	LYZ	QB	482	12	7,9,10	0.51	0	4,10,12	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LYZ	CB	785	13	7,9,10	0.50	0	4,10,12	0.54	0
2	LYZ	LA	931	2	7,9,10	0.51	0	4,10,12	0.54	0
6	LYZ	FC	756	6	7,9,10	0.51	0	4,10,12	0.50	0
4	LYZ	DA	1495	4	7,9,10	0.52	0	4,10,12	0.55	0
1	LYZ	AA	793	1	7,9,10	0.51	0	4,10,12	0.56	0
14	LYZ	SB	1142	14	7,9,10	0.51	0	4,10,12	0.48	0
6	LYZ	FC	624	6	7,9,10	0.50	0	4,10,12	0.56	0
2	LYZ	GA	910	2	7,9,10	0.51	0	4,10,12	0.58	0
3	LYZ	CA	1324	3	7,9,10	0.49	0	4,10,12	0.54	0
13	LYZ	CB	815	13	7,9,10	0.50	0	4,10,12	0.55	0
4	LYZ	DA	1567	4	7,9,10	0.51	0	4,10,12	0.55	0
2	LYZ	BA	982	2	7,9,10	0.52	0	4,10,12	0.52	0
13	LYZ	MB	785	13	7,9,10	0.51	0	4,10,12	0.54	0
10	LYZ	EC	1482	10	7,9,10	0.49	0	4,10,12	0.46	0
13	LYZ	CB	776	13	7,9,10	0.52	0	4,10,12	0.54	0
2	LYZ	LA	904	2	7,9,10	0.50	0	4,10,12	0.58	0
6	LYZ	KC	690	6	7,9,10	0.51	0	4,10,12	0.62	0
9	LYZ	IC	1266	9	7,9,10	0.51	0	4,10,12	0.61	0
1	LYZ	KA	859	1	7,9,10	0.52	0	4,10,12	0.70	0
10	LYZ	TC	1536	10	7,9,10	0.52	0	4,10,12	0.57	0
9	LYZ	IC	1293	9	7,9,10	0.51	0	4,10,12	0.68	0
2	LYZ	QA	910	2	7,9,10	0.51	0	4,10,12	0.58	0
2	LYZ	GA	1018	2	7,9,10	0.51	0	4,10,12	0.54	0
8	LYZ	HC	1194	8	7,9,10	0.51	0	4,10,12	0.49	0
4	LYZ	IA	1564	4	7,9,10	0.52	0	4,10,12	0.56	0
2	LYZ	GA	892	2	7,9,10	0.51	0	4,10,12	0.63	0
8	LYZ	MC	1221	8	7,9,10	0.50	0	4,10,12	0.45	0
13	LYZ	MB	896	13	7,9,10	0.51	0	4,10,12	0.61	0
10	LYZ	TC	1527	10	7,9,10	0.52	0	4,10,12	0.59	0
4	LYZ	IA	1567	4	7,9,10	0.51	0	4,10,12	0.56	0
1	LYZ	FA	859	1	7,9,10	0.51	0	4,10,12	0.71	0
7	LYZ	BC	864	7	7,9,10	0.49	0	4,10,12	0.54	0
2	LYZ	BA	949	2	7,9,10	0.50	0	4,10,12	0.48	0
8	LYZ	CC	1020	8	7,9,10	0.48	0	4,10,12	0.62	0
4	LYZ	DA	1369	4	7,9,10	0.52	0	4,10,12	0.53	0
9	LYZ	NC	1317	9	7,9,10	0.48	0	4,10,12	0.53	0
12	LYZ	LB	476	12	7,9,10	0.52	0	4,10,12	0.65	0
9	LYZ	NC	1392	9	7,9,10	0.51	0	4,10,12	0.60	0
10	LYZ	JC	1497	10	7,9,10	0.52	0	4,10,12	0.62	0
9	LYZ	IC	1389	9	7,9,10	0.52	0	4,10,12	0.63	0
9	LYZ	DC	1464	9	7,9,10	0.51	0	4,10,12	0.57	0
3	LYZ	HA	1324	3	7,9,10	0.49	0	4,10,12	0.53	0
3	LYZ	RA	1159	3	7,9,10	0.50	0	4,10,12	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	LYZ	BB	476	12	7,9,10	0.52	0	4,10,12	0.63	0
11	LYZ	FB	311	11	7,9,10	0.51	0	4,10,12	0.56	0
2	LYZ	LA	910	2	7,9,10	0.51	0	4,10,12	0.58	0
13	LYZ	HB	896	13	7,9,10	0.51	0	4,10,12	0.60	0
11	LYZ	AB	299	11	7,9,10	0.51	0	4,10,12	0.55	0
6	LYZ	PC	564	6	7,9,10	0.51	0	4,10,12	0.55	0
11	LYZ	KB	305	11	7,9,10	0.50	0	4,10,12	0.61	0
4	LYZ	IA	1369	4	7,9,10	0.52	0	4,10,12	0.53	0
13	LYZ	MB	869	13	7,9,10	0.51	0	4,10,12	0.53	0
7	LYZ	LC	879	7	7,9,10	0.49	0	4,10,12	0.47	0
6	LYZ	AC	756	6	7,9,10	0.51	0	4,10,12	0.51	0
4	LYZ	DA	1492	4	7,9,10	0.51	0	4,10,12	0.55	0
2	LYZ	QA	880	2	7,9,10	0.50	0	4,10,12	0.60	0
3	LYZ	MA	1204	3	7,9,10	0.50	0	4,10,12	0.57	0
3	LYZ	RA	1255	3	7,9,10	0.52	0	4,10,12	0.59	0
10	LYZ	TC	1497	10	7,9,10	0.52	0	4,10,12	0.62	0
8	LYZ	RC	1020	8	7,9,10	0.48	0	4,10,12	0.62	0
6	LYZ	KC	624	6	7,9,10	0.50	0	4,10,12	0.56	0
11	LYZ	FB	299	11	7,9,10	0.51	0	4,10,12	0.56	0
8	LYZ	CC	1101	8	7,9,10	0.51	0	4,10,12	0.47	0
4	LYZ	NA	1492	4	7,9,10	0.51	0	4,10,12	0.55	0
14	LYZ	IB	1142	14	7,9,10	0.51	0	4,10,12	0.48	0
7	LYZ	BC	879	7	7,9,10	0.49	0	4,10,12	0.48	0
4	LYZ	NA	1369	4	7,9,10	0.52	0	4,10,12	0.53	0
2	LYZ	BA	967	2	7,9,10	0.50	0	4,10,12	0.54	0
3	LYZ	RA	1252	3	7,9,10	0.50	0	4,10,12	0.51	0
8	LYZ	MC	1155	8	7,9,10	0.51	0	4,10,12	0.62	0
2	LYZ	BA	1018	2	7,9,10	0.51	0	4,10,12	0.54	0
4	LYZ	IA	1492	4	7,9,10	0.51	0	4,10,12	0.55	0
9	LYZ	DC	1293	9	7,9,10	0.51	0	4,10,12	0.65	0
12	LYZ	LB	554	12	7,9,10	0.52	0	4,10,12	0.64	0
12	LYZ	QB	554	12	7,9,10	0.52	0	4,10,12	0.64	0
13	LYZ	HB	743	13	7,9,10	0.50	0	4,10,12	0.56	0
7	LYZ	BC	792	7	7,9,10	0.51	0	4,10,12	0.59	0
4	LYZ	NA	1396	4	7,9,10	0.50	0	4,10,12	0.47	0
8	LYZ	MC	1056	8	7,9,10	0.50	0	4,10,12	0.61	0
5	LYZ	OA	1600	5	7,9,10	0.52	0	4,10,12	0.51	0
6	LYZ	PC	690	6	7,9,10	0.51	0	4,10,12	0.62	0
11	LYZ	KB	311	11	7,9,10	0.51	0	4,10,12	0.57	0
1	LYZ	AA	859	1	7,9,10	0.52	0	4,10,12	0.70	0
3	LYZ	MA	1123	3	7,9,10	0.52	0	4,10,12	0.71	0
7	LYZ	BC	915	7	7,9,10	0.51	0	4,10,12	0.55	0
6	LYZ	KC	609	6	7,9,10	0.50	0	4,10,12	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	LYZ	RB	776	13	7,9,10	0.52	0	4,10,12	0.53	0
12	LYZ	BB	620	12	7,9,10	0.51	0	4,10,12	0.60	0
13	LYZ	RB	731	13	7,9,10	0.51	0	4,10,12	0.53	0
12	LYZ	GB	620	12	7,9,10	0.52	0	4,10,12	0.60	0
7	LYZ	LC	801	7	7,9,10	0.51	0	4,10,12	0.61	0
6	LYZ	FC	609	6	7,9,10	0.50	0	4,10,12	0.55	0
1	LYZ	PA	712	1	7,9,10	0.51	0	4,10,12	0.49	0
10	LYZ	OC	1482	10	7,9,10	0.49	0	4,10,12	0.47	0
13	LYZ	RB	896	13	7,9,10	0.51	0	4,10,12	0.61	0
8	LYZ	RC	1221	8	7,9,10	0.50	0	4,10,12	0.47	0
2	LYZ	GA	949	2	7,9,10	0.50	0	4,10,12	0.47	0
6	LYZ	AC	690	6	7,9,10	0.51	0	4,10,12	0.62	0
9	LYZ	NC	1266	9	7,9,10	0.51	0	4,10,12	0.61	0
4	LYZ	SA	1495	4	7,9,10	0.52	0	4,10,12	0.55	0
7	LYZ	LC	828	7	7,9,10	0.50	0	4,10,12	0.54	0
5	LYZ	OA	1639	5	7,9,10	0.52	0	4,10,12	0.56	0
4	LYZ	NA	1564	4	7,9,10	0.52	0	4,10,12	0.56	0
9	LYZ	IC	1287	9	7,9,10	0.51	0	4,10,12	0.54	0
10	LYZ	OC	1536	10	7,9,10	0.52	0	4,10,12	0.57	0
6	LYZ	AC	564	6	7,9,10	0.50	0	4,10,12	0.55	0
4	LYZ	NA	1558	4	7,9,10	0.52	0	4,10,12	0.61	0
2	LYZ	QA	949	2	7,9,10	0.50	0	4,10,12	0.47	0
2	LYZ	LA	982	2	7,9,10	0.52	0	4,10,12	0.52	0
1	LYZ	PA	667	1	7,9,10	0.51	0	4,10,12	0.55	0
9	LYZ	SC	1389	9	7,9,10	0.51	0	4,10,12	0.58	0
4	LYZ	SA	1390	4	7,9,10	0.51	0	4,10,12	0.47	0
13	LYZ	RB	869	13	7,9,10	0.51	0	4,10,12	0.55	0
9	LYZ	IC	1317	9	7,9,10	0.48	0	4,10,12	0.53	0
4	LYZ	DA	1564	4	7,9,10	0.52	0	4,10,12	0.56	0
5	LYZ	EA	1639	5	7,9,10	0.52	0	4,10,12	0.56	0
4	LYZ	SA	1396	4	7,9,10	0.50	0	4,10,12	0.47	0
3	LYZ	MA	1324	3	7,9,10	0.49	0	4,10,12	0.53	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
11	LYZ	AB	386	11	-	1/8/9/11	-
7	LYZ	QC	792	7	-	0/8/9/11	-
7	LYZ	GC	915	7	-	0/8/9/11	-
5	LYZ	EA	1585	5	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LYZ	CA	1159	3	-	0/8/9/11	-
12	LYZ	QB	539	12	-	0/8/9/11	-
8	LYZ	RC	1152	8	-	0/8/9/11	-
6	LYZ	AC	609	6	-	0/8/9/11	-
9	LYZ	NC	1464	9	-	0/8/9/11	-
7	LYZ	QC	801	7	-	0/8/9/11	-
7	LYZ	QC	777	7	-	0/8/9/11	-
3	LYZ	CA	1123	3	-	0/8/9/11	-
8	LYZ	CC	1221	8	-	0/8/9/11	-
3	LYZ	CA	1258	3	-	0/8/9/11	-
1	LYZ	KA	712	1	-	0/8/9/11	-
4	LYZ	SA	1567	4	-	0/8/9/11	-
9	LYZ	NC	1389	9	-	0/8/9/11	-
7	LYZ	QC	846	7	-	0/8/9/11	-
3	LYZ	MA	1159	3	-	0/8/9/11	-
9	LYZ	IC	1464	9	-	0/8/9/11	-
2	LYZ	BA	895	2	-	0/8/9/11	-
4	LYZ	IA	1558	4	-	0/8/9/11	-
10	LYZ	OC	1527	10	-	0/8/9/11	-
9	LYZ	SC	1287	9	-	0/8/9/11	-
7	LYZ	BC	807	7	-	0/8/9/11	-
5	LYZ	TA	1630	5	-	0/8/9/11	-
2	LYZ	BA	910	2	-	0/8/9/11	-
8	LYZ	HC	1152	8	-	0/8/9/11	-
4	LYZ	NA	1420	4	-	0/8/9/11	-
7	LYZ	BC	786	7	-	0/8/9/11	-
9	LYZ	DC	1266	9	-	0/8/9/11	-
1	LYZ	FA	712	1	-	0/8/9/11	-
1	LYZ	FA	727	1	-	0/8/9/11	-
5	LYZ	EA	1627	5	-	0/8/9/11	-
10	LYZ	EC	1524	10	-	0/8/9/11	-
2	LYZ	GA	904	2	-	0/8/9/11	-
12	LYZ	GB	476	12	-	0/8/9/11	-
2	LYZ	LA	949	2	-	0/8/9/11	-
6	LYZ	AC	624	6	-	0/8/9/11	-
2	LYZ	QA	895	2	-	0/8/9/11	-
8	LYZ	HC	1149	8	-	0/8/9/11	-
13	LYZ	MB	815	13	-	0/8/9/11	-
9	LYZ	DC	1317	9	-	0/8/9/11	-
11	LYZ	AB	320	11	-	0/8/9/11	-
4	LYZ	IA	1390	4	-	0/8/9/11	-
1	LYZ	AA	667	1	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	LYZ	NB	1130	14	-	0/8/9/11	-
2	LYZ	BA	904	2	-	0/8/9/11	-
13	LYZ	HB	731	13	-	1/8/9/11	-
4	LYZ	NA	1390	4	-	0/8/9/11	-
5	LYZ	JA	1627	5	-	0/8/9/11	-
8	LYZ	HC	1155	8	-	0/8/9/11	-
7	LYZ	BC	777	7	-	0/8/9/11	-
5	LYZ	TA	1585	5	-	0/8/9/11	-
9	LYZ	SC	1392	9	-	0/8/9/11	-
14	LYZ	NB	1142	14	-	0/8/9/11	-
11	LYZ	AB	311	11	-	0/8/9/11	-
7	LYZ	GC	777	7	-	0/8/9/11	-
2	LYZ	LA	892	2	-	0/8/9/11	-
9	LYZ	SC	1293	9	-	1/8/9/11	-
12	LYZ	GB	539	12	-	0/8/9/11	-
7	LYZ	GC	789	7	-	0/8/9/11	-
7	LYZ	QC	789	7	-	0/8/9/11	-
7	LYZ	GC	786	7	-	0/8/9/11	-
3	LYZ	MA	1255	3	-	0/8/9/11	-
8	LYZ	RC	1194	8	-	0/8/9/11	-
3	LYZ	MA	1252	3	-	0/8/9/11	-
4	LYZ	IA	1420	4	-	0/8/9/11	-
11	LYZ	FB	320	11	-	0/8/9/11	-
6	LYZ	FC	690	6	-	0/8/9/11	-
10	LYZ	JC	1524	10	-	0/8/9/11	-
10	LYZ	JC	1482	10	-	0/8/9/11	-
12	LYZ	LB	620	12	-	1/8/9/11	-
8	LYZ	HC	1221	8	-	0/8/9/11	-
3	LYZ	HA	1204	3	-	0/8/9/11	-
12	LYZ	BB	539	12	-	0/8/9/11	-
7	LYZ	QC	786	7	-	0/8/9/11	-
6	LYZ	PC	756	6	-	0/8/9/11	-
2	LYZ	GA	889	2	-	0/8/9/11	-
5	LYZ	OA	1585	5	-	1/8/9/11	-
5	LYZ	JA	1639	5	-	0/8/9/11	-
5	LYZ	JA	1630	5	-	0/8/9/11	-
1	LYZ	PA	793	1	-	0/8/9/11	-
3	LYZ	RA	1123	3	-	0/8/9/11	-
8	LYZ	RC	1056	8	-	0/8/9/11	-
9	LYZ	DC	1287	9	-	0/8/9/11	-
11	LYZ	FB	386	11	-	1/8/9/11	-
2	LYZ	QA	889	2	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	LYZ	SA	1369	4	-	0/8/9/11	-
2	LYZ	LA	967	2	-	0/8/9/11	-
10	LYZ	EC	1527	10	-	0/8/9/11	-
9	LYZ	SC	1266	9	-	0/8/9/11	-
9	LYZ	IC	1455	9	-	0/8/9/11	-
9	LYZ	NC	1287	9	-	0/8/9/11	-
2	LYZ	LA	889	2	-	0/8/9/11	-
12	LYZ	QB	476	12	-	0/8/9/11	-
13	LYZ	HB	815	13	-	0/8/9/11	-
9	LYZ	SC	1461	9	-	1/8/9/11	-
9	LYZ	NC	1461	9	-	1/8/9/11	-
7	LYZ	LC	846	7	-	0/8/9/11	-
11	LYZ	PB	311	11	-	0/8/9/11	-
4	LYZ	DA	1390	4	-	0/8/9/11	-
1	LYZ	AA	712	1	-	0/8/9/11	-
9	LYZ	IC	1461	9	-	1/8/9/11	-
11	LYZ	PB	305	11	-	0/8/9/11	-
8	LYZ	HC	1056	8	-	0/8/9/11	-
5	LYZ	OA	1627	5	-	0/8/9/11	-
10	LYZ	JC	1536	10	-	0/8/9/11	-
7	LYZ	QC	828	7	-	0/8/9/11	-
2	LYZ	GA	967	2	-	0/8/9/11	-
8	LYZ	MC	1020	8	-	0/8/9/11	-
4	LYZ	SA	1492	4	-	0/8/9/11	-
7	LYZ	GC	801	7	-	0/8/9/11	-
5	LYZ	TA	1627	5	-	0/8/9/11	-
9	LYZ	SC	1455	9	-	0/8/9/11	-
2	LYZ	QA	931	2	-	0/8/9/11	-
2	LYZ	QA	892	2	-	0/8/9/11	-
8	LYZ	CC	1152	8	-	0/8/9/11	-
4	LYZ	NA	1495	4	-	1/8/9/11	-
7	LYZ	QC	915	7	-	0/8/9/11	-
2	LYZ	QA	967	2	-	0/8/9/11	-
7	LYZ	GC	792	7	-	0/8/9/11	-
7	LYZ	QC	879	7	-	0/8/9/11	-
8	LYZ	CC	1056	8	-	0/8/9/11	-
8	LYZ	CC	1194	8	-	0/8/9/11	-
1	LYZ	PA	727	1	-	0/8/9/11	-
10	LYZ	JC	1527	10	-	0/8/9/11	-
3	LYZ	RA	1258	3	-	0/8/9/11	-
2	LYZ	GA	880	2	-	0/8/9/11	-
2	LYZ	GA	982	2	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	LYZ	HC	1020	8	-	0/8/9/11	-
8	LYZ	CC	1149	8	-	0/8/9/11	-
11	LYZ	FB	305	11	-	0/8/9/11	-
12	LYZ	BB	482	12	-	0/8/9/11	-
3	LYZ	HA	1252	3	-	0/8/9/11	-
12	LYZ	GB	482	12	-	0/8/9/11	-
13	LYZ	MB	776	13	-	0/8/9/11	-
2	LYZ	QA	982	2	-	0/8/9/11	-
6	LYZ	PC	609	6	-	0/8/9/11	-
7	LYZ	LC	807	7	-	0/8/9/11	-
13	LYZ	RB	785	13	-	0/8/9/11	-
11	LYZ	PB	386	11	-	1/8/9/11	-
7	LYZ	GC	828	7	-	0/8/9/11	-
8	LYZ	CC	1155	8	-	0/8/9/11	-
3	LYZ	RA	1324	3	-	0/8/9/11	-
4	LYZ	DA	1396	4	-	0/8/9/11	-
2	LYZ	LA	895	2	-	0/8/9/11	-
1	LYZ	FA	667	1	-	0/8/9/11	-
13	LYZ	CB	869	13	-	0/8/9/11	-
7	LYZ	GC	846	7	-	0/8/9/11	-
13	LYZ	RB	815	13	-	0/8/9/11	-
11	LYZ	KB	386	11	-	1/8/9/11	-
2	LYZ	LA	880	2	-	0/8/9/11	-
1	LYZ	KA	667	1	-	0/8/9/11	-
11	LYZ	PB	299	11	-	0/8/9/11	-
2	LYZ	QA	1018	2	-	0/8/9/11	-
13	LYZ	CB	896	13	-	0/8/9/11	-
1	LYZ	FA	793	1	-	0/8/9/11	-
5	LYZ	EA	1630	5	-	0/8/9/11	-
9	LYZ	DC	1392	9	-	0/8/9/11	-
4	LYZ	IA	1495	4	-	1/8/9/11	-
14	LYZ	DB	1130	14	-	0/8/9/11	-
5	LYZ	EA	1600	5	-	0/8/9/11	-
3	LYZ	RA	1204	3	-	0/8/9/11	-
9	LYZ	DC	1461	9	-	1/8/9/11	-
5	LYZ	TA	1639	5	-	0/8/9/11	-
7	LYZ	BC	828	7	-	0/8/9/11	-
3	LYZ	HA	1258	3	-	0/8/9/11	-
5	LYZ	OA	1630	5	-	0/8/9/11	-
10	LYZ	OC	1497	10	-	1/8/9/11	-
7	LYZ	BC	801	7	-	0/8/9/11	-
13	LYZ	MB	731	13	-	1/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	LYZ	KC	756	6	-	0/8/9/11	-
12	LYZ	LB	539	12	-	0/8/9/11	-
4	LYZ	SA	1564	4	-	0/8/9/11	-
11	LYZ	PB	320	11	-	0/8/9/11	-
9	LYZ	DC	1389	9	-	0/8/9/11	-
3	LYZ	CA	1255	3	-	0/8/9/11	-
7	LYZ	LC	789	7	-	0/8/9/11	-
3	LYZ	CA	1252	3	-	0/8/9/11	-
7	LYZ	LC	777	7	-	0/8/9/11	-
14	LYZ	IB	1130	14	-	0/8/9/11	-
8	LYZ	MC	1194	8	-	0/8/9/11	-
5	LYZ	JA	1585	5	-	1/8/9/11	-
8	LYZ	MC	1149	8	-	0/8/9/11	-
4	LYZ	IA	1396	4	-	0/8/9/11	-
8	LYZ	MC	1101	8	-	0/8/9/11	-
3	LYZ	HA	1159	3	-	0/8/9/11	-
7	LYZ	QC	807	7	-	0/8/9/11	-
4	LYZ	DA	1420	4	-	0/8/9/11	-
7	LYZ	LC	786	7	-	0/8/9/11	-
9	LYZ	DC	1455	9	-	0/8/9/11	-
7	LYZ	BC	789	7	-	0/8/9/11	-
13	LYZ	CB	731	13	-	1/8/9/11	-
7	LYZ	LC	915	7	-	0/8/9/11	-
7	LYZ	GC	807	7	-	0/8/9/11	-
6	LYZ	FC	564	6	-	1/8/9/11	-
9	LYZ	NC	1293	9	-	0/8/9/11	-
1	LYZ	PA	859	1	-	0/8/9/11	-
3	LYZ	HA	1123	3	-	0/8/9/11	-
7	LYZ	GC	864	7	-	0/8/9/11	-
12	LYZ	BB	554	12	-	0/8/9/11	-
14	LYZ	SB	1130	14	-	0/8/9/11	-
9	LYZ	NC	1455	9	-	0/8/9/11	-
12	LYZ	GB	554	12	-	0/8/9/11	-
13	LYZ	MB	743	13	-	0/8/9/11	-
2	LYZ	QA	904	2	-	0/8/9/11	-
1	LYZ	KA	793	1	-	0/8/9/11	-
4	LYZ	DA	1558	4	-	0/8/9/11	-
7	LYZ	LC	792	7	-	0/8/9/11	-
8	LYZ	RC	1101	8	-	0/8/9/11	-
9	LYZ	IC	1392	9	-	0/8/9/11	-
10	LYZ	OC	1524	10	-	0/8/9/11	-
8	LYZ	RC	1149	8	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	LYZ	TC	1524	10	-	0/8/9/11	-
7	LYZ	LC	864	7	-	0/8/9/11	-
5	LYZ	JA	1600	5	-	0/8/9/11	-
11	LYZ	AB	305	11	-	0/8/9/11	-
10	LYZ	TC	1482	10	-	0/8/9/11	-
13	LYZ	HB	776	13	-	0/8/9/11	-
13	LYZ	CB	743	13	-	0/8/9/11	-
9	LYZ	SC	1464	9	-	0/8/9/11	-
14	LYZ	DB	1142	14	-	0/8/9/11	-
10	LYZ	EC	1536	10	-	0/8/9/11	-
2	LYZ	BA	889	2	-	0/8/9/11	-
8	LYZ	HC	1101	8	-	0/8/9/11	-
2	LYZ	LA	1018	2	-	0/8/9/11	-
8	LYZ	RC	1155	8	-	0/8/9/11	-
11	LYZ	KB	320	11	-	0/8/9/11	-
8	LYZ	MC	1152	8	-	0/8/9/11	-
2	LYZ	GA	931	2	-	0/8/9/11	-
5	LYZ	TA	1600	5	-	0/8/9/11	-
7	LYZ	QC	864	7	-	0/8/9/11	-
9	LYZ	SC	1317	9	-	0/8/9/11	-
4	LYZ	NA	1567	4	-	0/8/9/11	-
12	LYZ	LB	482	12	-	0/8/9/11	-
3	LYZ	HA	1255	3	-	0/8/9/11	-
1	LYZ	KA	727	1	-	0/8/9/11	-
6	LYZ	KC	564	6	-	1/8/9/11	-
7	LYZ	BC	846	7	-	1/8/9/11	-
6	LYZ	PC	624	6	-	0/8/9/11	-
1	LYZ	AA	727	1	-	0/8/9/11	-
7	LYZ	GC	879	7	-	0/8/9/11	-
12	LYZ	QB	620	12	-	1/8/9/11	-
13	LYZ	RB	743	13	-	0/8/9/11	-
4	LYZ	SA	1420	4	-	0/8/9/11	-
2	LYZ	BA	931	2	-	0/8/9/11	-
2	LYZ	BA	892	2	-	0/8/9/11	-
11	LYZ	KB	299	11	-	0/8/9/11	-
3	LYZ	MA	1258	3	-	0/8/9/11	-
10	LYZ	EC	1497	10	-	0/8/9/11	-
4	LYZ	SA	1558	4	-	0/8/9/11	-
13	LYZ	HB	869	13	-	0/8/9/11	-
13	LYZ	HB	785	13	-	0/8/9/11	-
2	LYZ	BA	880	2	-	0/8/9/11	-
3	LYZ	CA	1204	3	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYZ	GA	895	2	-	0/8/9/11	-
12	LYZ	QB	482	12	-	0/8/9/11	-
13	LYZ	CB	785	13	-	0/8/9/11	-
2	LYZ	LA	931	2	-	0/8/9/11	-
6	LYZ	FC	756	6	-	0/8/9/11	-
4	LYZ	DA	1495	4	-	1/8/9/11	-
1	LYZ	AA	793	1	-	0/8/9/11	-
14	LYZ	SB	1142	14	-	0/8/9/11	-
6	LYZ	FC	624	6	-	0/8/9/11	-
2	LYZ	GA	910	2	-	0/8/9/11	-
3	LYZ	CA	1324	3	-	0/8/9/11	-
13	LYZ	CB	815	13	-	0/8/9/11	-
4	LYZ	DA	1567	4	-	0/8/9/11	-
2	LYZ	BA	982	2	-	0/8/9/11	-
13	LYZ	MB	785	13	-	0/8/9/11	-
10	LYZ	EC	1482	10	-	0/8/9/11	-
13	LYZ	CB	776	13	-	0/8/9/11	-
2	LYZ	LA	904	2	-	0/8/9/11	-
6	LYZ	KC	690	6	-	0/8/9/11	-
9	LYZ	IC	1266	9	-	0/8/9/11	-
1	LYZ	KA	859	1	-	0/8/9/11	-
10	LYZ	TC	1536	10	-	0/8/9/11	-
9	LYZ	IC	1293	9	-	1/8/9/11	-
2	LYZ	QA	910	2	-	0/8/9/11	-
2	LYZ	GA	1018	2	-	0/8/9/11	-
8	LYZ	HC	1194	8	-	0/8/9/11	-
4	LYZ	IA	1564	4	-	0/8/9/11	-
2	LYZ	GA	892	2	-	0/8/9/11	-
8	LYZ	MC	1221	8	-	0/8/9/11	-
13	LYZ	MB	896	13	-	0/8/9/11	-
10	LYZ	TC	1527	10	-	0/8/9/11	-
4	LYZ	IA	1567	4	-	0/8/9/11	-
1	LYZ	FA	859	1	-	0/8/9/11	-
7	LYZ	BC	864	7	-	0/8/9/11	-
2	LYZ	BA	949	2	-	0/8/9/11	-
8	LYZ	CC	1020	8	-	0/8/9/11	-
4	LYZ	DA	1369	4	-	0/8/9/11	-
9	LYZ	NC	1317	9	-	0/8/9/11	-
12	LYZ	LB	476	12	-	0/8/9/11	-
9	LYZ	NC	1392	9	-	0/8/9/11	-
10	LYZ	JC	1497	10	-	1/8/9/11	-
9	LYZ	IC	1389	9	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	LYZ	DC	1464	9	-	0/8/9/11	-
3	LYZ	HA	1324	3	-	0/8/9/11	-
3	LYZ	RA	1159	3	-	0/8/9/11	-
12	LYZ	BB	476	12	-	0/8/9/11	-
11	LYZ	FB	311	11	-	0/8/9/11	-
2	LYZ	LA	910	2	-	0/8/9/11	-
13	LYZ	HB	896	13	-	0/8/9/11	-
11	LYZ	AB	299	11	-	0/8/9/11	-
6	LYZ	PC	564	6	-	1/8/9/11	-
11	LYZ	KB	305	11	-	0/8/9/11	-
4	LYZ	IA	1369	4	-	0/8/9/11	-
13	LYZ	MB	869	13	-	0/8/9/11	-
7	LYZ	LC	879	7	-	0/8/9/11	-
6	LYZ	AC	756	6	-	0/8/9/11	-
4	LYZ	DA	1492	4	-	0/8/9/11	-
2	LYZ	QA	880	2	-	0/8/9/11	-
3	LYZ	MA	1204	3	-	0/8/9/11	-
3	LYZ	RA	1255	3	-	0/8/9/11	-
10	LYZ	TC	1497	10	-	1/8/9/11	-
8	LYZ	RC	1020	8	-	0/8/9/11	-
6	LYZ	KC	624	6	-	0/8/9/11	-
11	LYZ	FB	299	11	-	0/8/9/11	-
8	LYZ	CC	1101	8	-	0/8/9/11	-
4	LYZ	NA	1492	4	-	0/8/9/11	-
14	LYZ	IB	1142	14	-	0/8/9/11	-
7	LYZ	BC	879	7	-	0/8/9/11	-
4	LYZ	NA	1369	4	-	0/8/9/11	-
2	LYZ	BA	967	2	-	0/8/9/11	-
3	LYZ	RA	1252	3	-	0/8/9/11	-
8	LYZ	MC	1155	8	-	0/8/9/11	-
2	LYZ	BA	1018	2	-	0/8/9/11	-
4	LYZ	IA	1492	4	-	0/8/9/11	-
9	LYZ	DC	1293	9	-	0/8/9/11	-
12	LYZ	LB	554	12	-	0/8/9/11	-
12	LYZ	QB	554	12	-	0/8/9/11	-
13	LYZ	HB	743	13	-	0/8/9/11	-
7	LYZ	BC	792	7	-	0/8/9/11	-
4	LYZ	NA	1396	4	-	0/8/9/11	-
8	LYZ	MC	1056	8	-	0/8/9/11	-
5	LYZ	OA	1600	5	-	0/8/9/11	-
6	LYZ	PC	690	6	-	0/8/9/11	-
11	LYZ	KB	311	11	-	0/8/9/11	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LYZ	AA	859	1	-	0/8/9/11	-
3	LYZ	MA	1123	3	-	0/8/9/11	-
7	LYZ	BC	915	7	-	0/8/9/11	-
6	LYZ	KC	609	6	-	0/8/9/11	-
13	LYZ	RB	776	13	-	0/8/9/11	-
12	LYZ	BB	620	12	-	1/8/9/11	-
13	LYZ	RB	731	13	-	1/8/9/11	-
12	LYZ	GB	620	12	-	1/8/9/11	-
7	LYZ	LC	801	7	-	0/8/9/11	-
6	LYZ	FC	609	6	-	0/8/9/11	-
1	LYZ	PA	712	1	-	0/8/9/11	-
10	LYZ	OC	1482	10	-	0/8/9/11	-
13	LYZ	RB	896	13	-	0/8/9/11	-
8	LYZ	RC	1221	8	-	0/8/9/11	-
2	LYZ	GA	949	2	-	0/8/9/11	-
6	LYZ	AC	690	6	-	0/8/9/11	-
9	LYZ	NC	1266	9	-	0/8/9/11	-
4	LYZ	SA	1495	4	-	1/8/9/11	-
7	LYZ	LC	828	7	-	0/8/9/11	-
5	LYZ	OA	1639	5	-	0/8/9/11	-
4	LYZ	NA	1564	4	-	0/8/9/11	-
9	LYZ	IC	1287	9	-	0/8/9/11	-
10	LYZ	OC	1536	10	-	0/8/9/11	-
6	LYZ	AC	564	6	-	1/8/9/11	-
4	LYZ	NA	1558	4	-	0/8/9/11	-
2	LYZ	QA	949	2	-	0/8/9/11	-
2	LYZ	LA	982	2	-	0/8/9/11	-
1	LYZ	PA	667	1	-	0/8/9/11	-
9	LYZ	SC	1389	9	-	0/8/9/11	-
4	LYZ	SA	1390	4	-	0/8/9/11	-
13	LYZ	RB	869	13	-	0/8/9/11	-
9	LYZ	IC	1317	9	-	0/8/9/11	-
4	LYZ	DA	1564	4	-	0/8/9/11	-
5	LYZ	EA	1639	5	-	0/8/9/11	-
4	LYZ	SA	1396	4	-	0/8/9/11	-
3	LYZ	MA	1324	3	-	0/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	DA	1495	LYZ	O-C-CA-CB
6	AC	564	LYZ	O-C-CA-CB
7	BC	846	LYZ	O-C-CA-CB
9	DC	1461	LYZ	O-C-CA-CB
11	AB	386	LYZ	O-C-CA-CB

There are no ring outliers.

119 monomers are involved in 135 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	QB	539	LYZ	1	0
9	NC	1464	LYZ	2	0
3	CA	1123	LYZ	2	0
8	CC	1221	LYZ	1	0
9	NC	1389	LYZ	1	0
9	IC	1464	LYZ	2	0
4	IA	1558	LYZ	1	0
7	BC	807	LYZ	1	0
4	NA	1420	LYZ	1	0
7	BC	786	LYZ	1	0
12	GB	476	LYZ	1	0
2	LA	949	LYZ	1	0
6	AC	624	LYZ	1	0
11	AB	320	LYZ	1	0
4	IA	1390	LYZ	1	0
4	NA	1390	LYZ	1	0
11	AB	311	LYZ	1	0
12	GB	539	LYZ	1	0
7	GC	789	LYZ	1	0
7	QC	789	LYZ	1	0
7	GC	786	LYZ	1	0
4	IA	1420	LYZ	1	0
11	FB	320	LYZ	1	0
6	FC	690	LYZ	1	0
12	LB	620	LYZ	1	0
8	HC	1221	LYZ	1	0
12	BB	539	LYZ	1	0
7	QC	786	LYZ	1	0
6	PC	756	LYZ	1	0
1	PA	793	LYZ	1	0
3	RA	1123	LYZ	2	0
12	QB	476	LYZ	1	0
11	PB	311	LYZ	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	DA	1390	LYZ	1	0
11	PB	305	LYZ	1	0
2	QA	931	LYZ	1	0
2	GA	880	LYZ	1	0
2	GA	982	LYZ	1	0
11	FB	305	LYZ	1	0
12	BB	482	LYZ	1	0
12	GB	482	LYZ	1	0
13	MB	776	LYZ	2	0
2	QA	982	LYZ	1	0
7	LC	807	LYZ	1	0
3	RA	1324	LYZ	1	0
2	LA	880	LYZ	1	0
11	PB	299	LYZ	1	0
1	FA	793	LYZ	1	0
6	KC	756	LYZ	1	0
12	LB	539	LYZ	1	0
11	PB	320	LYZ	1	0
9	DC	1389	LYZ	2	0
7	LC	789	LYZ	1	0
5	JA	1585	LYZ	1	0
7	QC	807	LYZ	1	0
4	DA	1420	LYZ	1	0
7	LC	786	LYZ	1	0
7	BC	789	LYZ	1	0
7	GC	807	LYZ	1	0
6	FC	564	LYZ	1	0
1	PA	859	LYZ	1	0
3	HA	1123	LYZ	2	0
1	KA	793	LYZ	1	0
4	DA	1558	LYZ	1	0
11	AB	305	LYZ	1	0
10	TC	1482	LYZ	1	0
13	HB	776	LYZ	2	0
9	SC	1464	LYZ	2	0
11	KB	320	LYZ	1	0
2	GA	931	LYZ	1	0
12	LB	482	LYZ	1	0
6	KC	564	LYZ	1	0
6	PC	624	LYZ	1	0
12	QB	620	LYZ	1	0
4	SA	1420	LYZ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BA	931	LYZ	1	0
4	SA	1558	LYZ	1	0
2	BA	880	LYZ	1	0
12	QB	482	LYZ	1	0
2	LA	931	LYZ	1	0
6	FC	756	LYZ	1	0
1	AA	793	LYZ	1	0
6	FC	624	LYZ	1	0
3	CA	1324	LYZ	1	0
2	BA	982	LYZ	1	0
13	CB	776	LYZ	2	0
6	KC	690	LYZ	1	0
1	KA	859	LYZ	1	0
8	MC	1221	LYZ	1	0
1	FA	859	LYZ	1	0
2	BA	949	LYZ	1	0
12	LB	476	LYZ	1	0
9	DC	1464	LYZ	2	0
3	HA	1324	LYZ	1	0
12	BB	476	LYZ	1	0
11	FB	311	LYZ	2	0
6	PC	564	LYZ	1	0
11	KB	305	LYZ	1	0
6	AC	756	LYZ	1	0
2	QA	880	LYZ	1	0
6	KC	624	LYZ	1	0
11	FB	299	LYZ	1	0
6	PC	690	LYZ	1	0
11	KB	311	LYZ	2	0
1	AA	859	LYZ	1	0
3	MA	1123	LYZ	2	0
13	RB	776	LYZ	2	0
12	BB	620	LYZ	1	0
12	GB	620	LYZ	1	0
10	OC	1482	LYZ	1	0
8	RC	1221	LYZ	1	0
2	GA	949	LYZ	1	0
6	AC	690	LYZ	1	0
6	AC	564	LYZ	1	0
4	NA	1558	LYZ	1	0
2	QA	949	LYZ	1	0
2	LA	982	LYZ	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	SA	1390	LYZ	1	0
3	MA	1324	LYZ	1	0

5.5 Carbohydrates

744 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	$\# Z > 2$
31	GAL	Aa	1	31	11,11,12	0.19	0	15,15,17	0.57	0
31	GLC	Aa	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Ab	1	31	11,11,12	0.19	0	15,15,17	0.57	0
31	GLC	Ab	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Ac	1	31	11,11,12	0.18	0	15,15,17	0.57	0
31	GLC	Ac	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Ad	1	31	11,11,12	0.18	0	15,15,17	0.57	0
31	GLC	Ad	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Ae	1	31	11,11,12	0.19	0	15,15,17	0.58	0
31	GLC	Ae	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Af	1	31	11,11,12	0.19	0	15,15,17	0.58	0
31	GLC	Af	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Ag	1	31	11,11,12	0.20	0	15,15,17	0.59	0
31	GLC	Ag	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Ah	1	31	11,11,12	0.19	0	15,15,17	0.58	0
31	GLC	Ah	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Ai	1	31	11,11,12	0.26	0	15,15,17	0.62	0
31	GLC	Ai	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Aj	1	31	11,11,12	0.26	0	15,15,17	0.62	0
31	GLC	Aj	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Ak	1	31	11,11,12	0.26	0	15,15,17	0.62	0
31	GLC	Ak	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Al	1	31	11,11,12	0.26	0	15,15,17	0.62	0
31	GLC	Al	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Ba	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Ba	2	31	11,11,12	0.26	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	Bb	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Bb	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Bc	1	31	11,11,12	0.27	0	15,15,17	0.65	0
31	GLC	Bc	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Bd	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Bd	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Be	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Be	2	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GAL	Bf	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Bf	2	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GAL	Bg	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Bg	2	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GAL	Bh	1	31	11,11,12	0.19	0	15,15,17	0.56	0
31	GLC	Bh	2	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GAL	Bi	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Bi	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Bj	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Bj	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Bk	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Bk	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Bl	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Bl	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Ca	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	Ca	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Cb	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	Cb	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Cc	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	Cc	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Cd	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	Cd	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Ce	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Ce	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Cf	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Cf	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Cg	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Cg	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Ch	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Ch	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Ci	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Ci	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Cj	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	Cj	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Ck	1	31	11,11,12	0.20	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	Ck	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Cl	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Cl	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	De	1	31	11,11,12	0.19	0	15,15,17	0.52	0
31	GLC	De	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Df	1	31	11,11,12	0.19	0	15,15,17	0.52	0
31	GLC	Df	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Dg	1	31	11,11,12	0.19	0	15,15,17	0.52	0
31	GLC	Dg	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Dh	1	31	11,11,12	0.19	0	15,15,17	0.52	0
31	GLC	Dh	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Di	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Di	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Dj	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Dj	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Dk	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Dk	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Dl	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Dl	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Ea	1	31	11,11,12	0.33	0	15,15,17	0.79	1 (6%)
31	GLC	Ea	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Eb	1	31	11,11,12	0.33	0	15,15,17	0.79	1 (6%)
31	GLC	Eb	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Ec	1	31	11,11,12	0.33	0	15,15,17	0.79	1 (6%)
31	GLC	Ec	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Ed	1	31	11,11,12	0.33	0	15,15,17	0.79	1 (6%)
31	GLC	Ed	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Ee	1	31	11,11,12	0.27	0	15,15,17	0.87	0
31	GLC	Ee	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	Ef	1	31	11,11,12	0.26	0	15,15,17	0.87	0
31	GLC	Ef	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	Eg	1	31	11,11,12	0.27	0	15,15,17	0.86	0
31	GLC	Eg	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	Eh	1	31	11,11,12	0.26	0	15,15,17	0.86	0
31	GLC	Eh	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Fi	1	31	11,11,12	0.34	0	15,15,17	0.79	0
31	GLC	Fi	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Fj	1	31	11,11,12	0.35	0	15,15,17	0.80	0
31	GLC	Fj	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Fk	1	31	11,11,12	0.35	0	15,15,17	0.81	0
31	GLC	Fk	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Fl	1	31	11,11,12	0.34	0	15,15,17	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	F1	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Ga	1	31	11,11,12	0.18	0	15,15,17	0.59	0
31	GLC	Ga	2	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GAL	Gb	1	31	11,11,12	0.18	0	15,15,17	0.59	0
31	GLC	Gb	2	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GAL	Gc	1	31	11,11,12	0.18	0	15,15,17	0.60	0
31	GLC	Gc	2	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GAL	Gd	1	31	11,11,12	0.18	0	15,15,17	0.59	0
31	GLC	Gd	2	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GAL	Ge	1	31	11,11,12	0.19	0	15,15,17	0.60	0
31	GLC	Ge	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	Gf	1	31	11,11,12	0.19	0	15,15,17	0.60	0
31	GLC	Gf	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	Gg	1	31	11,11,12	0.20	0	15,15,17	0.60	0
31	GLC	Gg	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	Gh	1	31	11,11,12	0.19	0	15,15,17	0.60	0
31	GLC	Gh	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	Gi	1	31	11,11,12	0.26	0	15,15,17	0.72	0
31	GLC	Gi	2	31	11,11,12	0.30	0	15,15,17	0.57	0
31	GAL	Gj	1	31	11,11,12	0.26	0	15,15,17	0.72	0
31	GLC	Gj	2	31	11,11,12	0.30	0	15,15,17	0.57	0
31	GAL	Gk	1	31	11,11,12	0.24	0	15,15,17	0.71	0
31	GLC	Gk	2	31	11,11,12	0.32	0	15,15,17	0.58	0
31	GAL	Gl	1	31	11,11,12	0.26	0	15,15,17	0.73	0
31	GLC	Gl	2	31	11,11,12	0.30	0	15,15,17	0.57	0
31	GAL	Ha	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Ha	2	31	11,11,12	0.29	0	15,15,17	0.56	0
31	GAL	Hb	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Hb	2	31	11,11,12	0.29	0	15,15,17	0.56	0
31	GAL	Hc	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Hc	2	31	11,11,12	0.29	0	15,15,17	0.56	0
31	GAL	Hd	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Hd	2	31	11,11,12	0.29	0	15,15,17	0.56	0
31	GAL	He	1	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GLC	He	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Hf	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Hf	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Hg	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Hg	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Hh	1	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GLC	Hh	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Hi	1	31	11,11,12	0.24	0	15,15,17	0.62	0
31	GLC	Hi	2	31	11,11,12	0.29	0	15,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	Hj	1	31	11,11,12	0.24	0	15,15,17	0.62	0
31	GLC	Hj	2	31	11,11,12	0.28	0	15,15,17	0.57	0
31	GAL	Hk	1	31	11,11,12	0.24	0	15,15,17	0.62	0
31	GLC	Hk	2	31	11,11,12	0.28	0	15,15,17	0.57	0
31	GAL	Hl	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	Hl	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Ia	1	31	11,11,12	0.20	0	15,15,17	0.57	0
31	GLC	Ia	2	31	11,11,12	0.23	0	15,15,17	0.60	0
31	GAL	Ib	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Ib	2	31	11,11,12	0.23	0	15,15,17	0.60	0
31	GAL	Ic	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	Ic	2	31	11,11,12	0.23	0	15,15,17	0.60	0
31	GAL	Id	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Id	2	31	11,11,12	0.23	0	15,15,17	0.60	0
31	GAL	Ie	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	Ie	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	If	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	If	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Ig	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	Ig	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Ih	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	Ih	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Ii	1	31	11,11,12	0.22	0	15,15,17	0.58	0
31	GLC	Ii	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Ij	1	31	11,11,12	0.22	0	15,15,17	0.58	0
31	GLC	Ij	2	31	11,11,12	0.23	0	15,15,17	0.54	0
31	GAL	Ik	1	31	11,11,12	0.21	0	15,15,17	0.57	0
31	GLC	Ik	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	Il	1	31	11,11,12	0.21	0	15,15,17	0.58	0
31	GLC	Il	2	31	11,11,12	0.24	0	15,15,17	0.55	0
31	GAL	Ja	1	31	11,11,12	0.18	0	15,15,17	0.53	0
31	GLC	Ja	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Jb	1	31	11,11,12	0.18	0	15,15,17	0.53	0
31	GLC	Jb	2	31	11,11,12	0.26	0	15,15,17	0.59	0
31	GAL	Jc	1	31	11,11,12	0.18	0	15,15,17	0.53	0
31	GLC	Jc	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Jd	1	31	11,11,12	0.18	0	15,15,17	0.53	0
31	GLC	Jd	2	31	11,11,12	0.26	0	15,15,17	0.60	0
31	GAL	Je	1	31	11,11,12	0.17	0	15,15,17	0.57	0
31	GLC	Je	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Jf	1	31	11,11,12	0.17	0	15,15,17	0.57	0
31	GLC	Jf	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Jg	1	31	11,11,12	0.18	0	15,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	Jg	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Jh	1	31	11,11,12	0.18	0	15,15,17	0.57	0
31	GLC	Jh	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Ji	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Ji	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Jj	1	31	11,11,12	0.19	0	15,15,17	0.55	0
31	GLC	Jj	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Jk	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Jk	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Jl	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Jl	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Ka	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Ka	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Kb	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Kb	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Kc	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Kc	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Kd	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Kd	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Ke	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	Ke	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Kf	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	Kf	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Kg	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Kg	2	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GAL	Kh	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Kh	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	Ki	1	31	11,11,12	0.17	0	15,15,17	0.52	0
31	GLC	Ki	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Kj	1	31	11,11,12	0.17	0	15,15,17	0.52	0
31	GLC	Kj	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Kk	1	31	11,11,12	0.17	0	15,15,17	0.52	0
31	GLC	Kk	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Kl	1	31	11,11,12	0.17	0	15,15,17	0.52	0
31	GLC	Kl	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	La	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	La	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Lb	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	Lb	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Lc	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	Lc	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Ld	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	Ld	2	31	11,11,12	0.26	0	15,15,17	0.55	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	Le	1	31	11,11,12	0.25	0	15,15,17	0.64	0
31	GLC	Le	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Lf	1	31	11,11,12	0.24	0	15,15,17	0.64	0
31	GLC	Lf	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Lg	1	31	11,11,12	0.24	0	15,15,17	0.64	0
31	GLC	Lg	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Lh	1	31	11,11,12	0.24	0	15,15,17	0.65	0
31	GLC	Lh	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Li	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	Li	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Lj	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	Lj	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Lk	1	31	11,11,12	0.21	0	15,15,17	0.54	0
31	GLC	Lk	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Ll	1	31	11,11,12	0.21	0	15,15,17	0.54	0
31	GLC	Ll	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	Ma	1	31	11,11,12	0.28	0	15,15,17	0.66	0
31	GLC	Ma	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Mb	1	31	11,11,12	0.28	0	15,15,17	0.67	0
31	GLC	Mb	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Mc	1	31	11,11,12	0.28	0	15,15,17	0.67	0
31	GLC	Mc	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Md	1	31	11,11,12	0.28	0	15,15,17	0.66	0
31	GLC	Md	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Me	1	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GLC	Me	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Mf	1	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GLC	Mf	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Mg	1	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GLC	Mg	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Mh	1	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GLC	Mh	2	31	11,11,12	0.29	0	15,15,17	0.57	0
31	GAL	Mi	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Mi	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Mj	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Mj	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Mk	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Mk	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Ml	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	Ml	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Na	1	31	11,11,12	0.28	0	15,15,17	0.66	0
31	GLC	Na	2	31	11,11,12	0.26	0	15,15,17	0.52	0
31	GAL	Nb	1	31	11,11,12	0.28	0	15,15,17	0.66	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	Nb	2	31	11,11,12	0.25	0	15,15,17	0.52	0
31	GAL	Nc	1	31	11,11,12	0.28	0	15,15,17	0.66	0
31	GLC	Nc	2	31	11,11,12	0.26	0	15,15,17	0.52	0
31	GAL	Nd	1	31	11,11,12	0.28	0	15,15,17	0.66	0
31	GLC	Nd	2	31	11,11,12	0.26	0	15,15,17	0.52	0
31	GAL	Ne	1	31	11,11,12	0.16	0	15,15,17	0.83	1 (6%)
31	GLC	Ne	2	31	11,11,12	0.21	0	15,15,17	0.67	0
31	GAL	Nf	1	31	11,11,12	0.16	0	15,15,17	0.83	1 (6%)
31	GLC	Nf	2	31	11,11,12	0.22	0	15,15,17	0.67	0
31	GAL	Ng	1	31	11,11,12	0.16	0	15,15,17	0.83	1 (6%)
31	GLC	Ng	2	31	11,11,12	0.21	0	15,15,17	0.67	0
31	GAL	Nh	1	31	11,11,12	0.16	0	15,15,17	0.83	1 (6%)
31	GLC	Nh	2	31	11,11,12	0.21	0	15,15,17	0.67	0
31	GAL	Ni	1	31	11,11,12	0.30	0	15,15,17	0.76	0
31	GLC	Ni	2	31	11,11,12	0.30	0	15,15,17	0.51	0
31	GAL	Nj	1	31	11,11,12	0.30	0	15,15,17	0.76	0
31	GLC	Nj	2	31	11,11,12	0.30	0	15,15,17	0.51	0
31	GAL	Nk	1	31	11,11,12	0.30	0	15,15,17	0.76	0
31	GLC	Nk	2	31	11,11,12	0.30	0	15,15,17	0.51	0
31	GAL	Nl	1	31	11,11,12	0.30	0	15,15,17	0.76	0
31	GLC	Nl	2	31	11,11,12	0.30	0	15,15,17	0.51	0
31	GAL	Oa	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Oa	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Ob	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Ob	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Oc	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Oc	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Od	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Od	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Oe	1	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GLC	Oe	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Of	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	Of	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Og	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	Og	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Oh	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	Oh	2	31	11,11,12	0.25	0	15,15,17	0.53	0
31	GAL	Oi	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	Oi	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Oj	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	Oj	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Ok	1	31	11,11,12	0.23	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	Ok	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Ol	1	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GLC	Ol	2	31	11,11,12	0.28	0	15,15,17	0.55	0
31	GAL	Pa	1	31	11,11,12	0.25	0	15,15,17	0.64	0
31	GLC	Pa	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Pb	1	31	11,11,12	0.25	0	15,15,17	0.64	0
31	GLC	Pb	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Pc	1	31	11,11,12	0.25	0	15,15,17	0.64	0
31	GLC	Pc	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Pd	1	31	11,11,12	0.25	0	15,15,17	0.64	0
31	GLC	Pd	2	31	11,11,12	0.27	0	15,15,17	0.52	0
31	GAL	Pe	1	31	11,11,12	0.25	0	15,15,17	0.63	0
31	GLC	Pe	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Pf	1	31	11,11,12	0.26	0	15,15,17	0.63	0
31	GLC	Pf	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Pg	1	31	11,11,12	0.26	0	15,15,17	0.63	0
31	GLC	Pg	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Ph	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	Ph	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Pi	1	31	11,11,12	0.22	0	15,15,17	0.57	0
31	GLC	Pi	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Pj	1	31	11,11,12	0.22	0	15,15,17	0.57	0
31	GLC	Pj	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Pk	1	31	11,11,12	0.22	0	15,15,17	0.57	0
31	GLC	Pk	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Pl	1	31	11,11,12	0.22	0	15,15,17	0.57	0
31	GLC	Pl	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Qa	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	Qa	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Qb	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	Qb	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Qc	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	Qc	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Qd	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	Qd	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	Qi	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Qi	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Qj	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Qj	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	Qk	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Qk	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Ql	1	31	11,11,12	0.19	0	15,15,17	0.54	0
31	GLC	Ql	2	31	11,11,12	0.27	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	Ra	1	31	11,11,12	0.17	0	15,15,17	0.55	0
31	GLC	Ra	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	Rb	1	31	11,11,12	0.18	0	15,15,17	0.55	0
31	GLC	Rb	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	Rc	1	31	11,11,12	0.18	0	15,15,17	0.54	0
31	GLC	Rc	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	Rd	1	31	11,11,12	0.18	0	15,15,17	0.54	0
31	GLC	Rd	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	Re	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Re	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	Rf	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Rf	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	Rg	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Rg	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	Rh	1	31	11,11,12	0.28	0	15,15,17	0.65	0
31	GLC	Rh	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	Se	1	31	11,11,12	0.25	0	15,15,17	0.66	0
31	GLC	Se	2	31	11,11,12	0.32	0	15,15,17	0.52	0
31	GAL	Sf	1	31	11,11,12	0.24	0	15,15,17	0.66	0
31	GLC	Sf	2	31	11,11,12	0.32	0	15,15,17	0.52	0
31	GAL	Sg	1	31	11,11,12	0.24	0	15,15,17	0.66	0
31	GLC	Sg	2	31	11,11,12	0.32	0	15,15,17	0.52	0
31	GAL	Sh	1	31	11,11,12	0.24	0	15,15,17	0.66	0
31	GLC	Sh	2	31	11,11,12	0.32	0	15,15,17	0.52	0
31	GAL	Si	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Si	2	31	11,11,12	0.28	0	15,15,17	0.49	0
31	GAL	Sj	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Sj	2	31	11,11,12	0.28	0	15,15,17	0.49	0
31	GAL	Sk	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Sk	2	31	11,11,12	0.28	0	15,15,17	0.49	0
31	GAL	Sl	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Sl	2	31	11,11,12	0.28	0	15,15,17	0.49	0
31	GAL	Ta	1	31	11,11,12	0.30	0	15,15,17	0.97	1 (6%)
31	GLC	Ta	2	31	11,11,12	0.23	0	15,15,17	0.57	0
31	GAL	Tb	1	31	11,11,12	0.30	0	15,15,17	0.98	1 (6%)
31	GLC	Tb	2	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GAL	Tc	1	31	11,11,12	0.30	0	15,15,17	0.96	1 (6%)
31	GLC	Tc	2	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GAL	Td	1	31	11,11,12	0.29	0	15,15,17	0.95	1 (6%)
31	GLC	Td	2	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GAL	Ti	1	31	11,11,12	0.27	0	15,15,17	0.70	0
31	GLC	Ti	2	31	11,11,12	0.30	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	Tj	1	31	11,11,12	0.27	0	15,15,17	0.71	0
31	GLC	Tj	2	31	11,11,12	0.29	0	15,15,17	0.55	0
31	GAL	Tk	1	31	11,11,12	0.27	0	15,15,17	0.70	0
31	GLC	Tk	2	31	11,11,12	0.30	0	15,15,17	0.54	0
31	GAL	Tl	1	31	11,11,12	0.27	0	15,15,17	0.70	0
31	GLC	Tl	2	31	11,11,12	0.29	0	15,15,17	0.54	0
31	GAL	Ua	1	31	11,11,12	0.26	0	15,15,17	0.70	0
31	GLC	Ua	2	31	11,11,12	0.34	0	15,15,17	0.54	0
31	GAL	Ub	1	31	11,11,12	0.27	0	15,15,17	0.70	0
31	GLC	Ub	2	31	11,11,12	0.34	0	15,15,17	0.54	0
31	GAL	Uc	1	31	11,11,12	0.27	0	15,15,17	0.70	0
31	GLC	Uc	2	31	11,11,12	0.34	0	15,15,17	0.54	0
31	GAL	Ud	1	31	11,11,12	0.27	0	15,15,17	0.70	0
31	GLC	Ud	2	31	11,11,12	0.34	0	15,15,17	0.54	0
31	GAL	Ui	1	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GLC	Ui	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	Uj	1	31	11,11,12	0.24	0	15,15,17	0.60	0
31	GLC	Uj	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	Uk	1	31	11,11,12	0.25	0	15,15,17	0.60	0
31	GLC	Uk	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Ul	1	31	11,11,12	0.24	0	15,15,17	0.60	0
31	GLC	Ul	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	Va	1	31	11,11,12	0.18	0	15,15,17	0.56	0
31	GLC	Va	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	Vb	1	31	11,11,12	0.18	0	15,15,17	0.56	0
31	GLC	Vb	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	Vc	1	31	11,11,12	0.18	0	15,15,17	0.56	0
31	GLC	Vc	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Vd	1	31	11,11,12	0.18	0	15,15,17	0.56	0
31	GLC	Vd	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	Ve	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	Ve	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Vf	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Vf	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Vg	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Vg	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	Vh	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	Vh	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	We	1	31	11,11,12	0.26	0	15,15,17	0.61	0
31	GLC	We	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Wf	1	31	11,11,12	0.26	0	15,15,17	0.62	0
31	GLC	Wf	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Wg	1	31	11,11,12	0.26	0	15,15,17	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	Wg	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Wh	1	31	11,11,12	0.26	0	15,15,17	0.62	0
31	GLC	Wh	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Xi	1	31	11,11,12	0.21	0	15,15,17	0.55	0
31	GLC	Xi	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Xj	1	31	11,11,12	0.21	0	15,15,17	0.55	0
31	GLC	Xj	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Xk	1	31	11,11,12	0.21	0	15,15,17	0.55	0
31	GLC	Xk	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Xl	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	Xl	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	Ya	1	31	11,11,12	0.30	0	15,15,17	0.73	0
31	GLC	Ya	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Yb	1	31	11,11,12	0.30	0	15,15,17	0.73	0
31	GLC	Yb	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Yc	1	31	11,11,12	0.30	0	15,15,17	0.72	0
31	GLC	Yc	2	31	11,11,12	0.25	0	15,15,17	0.55	0
31	GAL	Yd	1	31	11,11,12	0.30	0	15,15,17	0.72	0
31	GLC	Yd	2	31	11,11,12	0.24	0	15,15,17	0.55	0
31	GAL	Yi	1	31	11,11,12	0.21	0	15,15,17	0.57	0
31	GLC	Yi	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Yj	1	31	11,11,12	0.22	0	15,15,17	0.57	0
31	GLC	Yj	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Yk	1	31	11,11,12	0.22	0	15,15,17	0.57	0
31	GLC	Yk	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Yl	1	31	11,11,12	0.21	0	15,15,17	0.57	0
31	GLC	Yl	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Za	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	Za	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Zb	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	Zb	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Zc	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	Zc	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Zd	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	Zd	2	31	11,11,12	0.26	0	15,15,17	0.53	0
31	GAL	Zi	1	31	11,11,12	0.25	0	15,15,17	0.62	0
31	GLC	Zi	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Zj	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Zj	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	Zk	1	31	11,11,12	0.25	0	15,15,17	0.61	0
31	GLC	Zk	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	Zl	1	31	11,11,12	0.25	0	15,15,17	0.62	0
31	GLC	Zl	2	31	11,11,12	0.26	0	15,15,17	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	aa	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	aa	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	ab	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	ab	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	ac	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	ac	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	ad	1	31	11,11,12	0.21	0	15,15,17	0.60	0
31	GLC	ad	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	bi	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	bi	2	31	11,11,12	0.27	0	15,15,17	0.54	0
31	GAL	bj	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	bj	2	31	11,11,12	0.27	0	15,15,17	0.54	0
31	GAL	bk	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	bk	2	31	11,11,12	0.27	0	15,15,17	0.54	0
31	GAL	bl	1	31	11,11,12	0.22	0	15,15,17	0.61	0
31	GLC	bl	2	31	11,11,12	0.27	0	15,15,17	0.54	0
31	GAL	ca	1	31	11,11,12	0.30	0	15,15,17	0.76	0
31	GLC	ca	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	cb	1	31	11,11,12	0.31	0	15,15,17	0.77	0
31	GLC	cb	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	cc	1	31	11,11,12	0.31	0	15,15,17	0.77	0
31	GLC	cc	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	cd	1	31	11,11,12	0.30	0	15,15,17	0.76	0
31	GLC	cd	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	ci	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	ci	2	31	11,11,12	0.28	0	15,15,17	0.54	0
31	GAL	cj	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	cj	2	31	11,11,12	0.28	0	15,15,17	0.54	0
31	GAL	ck	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	ck	2	31	11,11,12	0.28	0	15,15,17	0.54	0
31	GAL	cl	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	cl	2	31	11,11,12	0.28	0	15,15,17	0.54	0
31	GAL	da	1	31	11,11,12	0.30	0	15,15,17	0.77	0
31	GLC	da	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	db	1	31	11,11,12	0.30	0	15,15,17	0.77	0
31	GLC	db	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	dc	1	31	11,11,12	0.30	0	15,15,17	0.77	0
31	GLC	dc	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	dd	1	31	11,11,12	0.30	0	15,15,17	0.77	0
31	GLC	dd	2	31	11,11,12	0.25	0	15,15,17	0.54	0
31	GAL	di	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	di	2	31	11,11,12	0.27	0	15,15,17	0.55	0
31	GAL	dj	1	31	11,11,12	0.26	0	15,15,17	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	dj	2	31	11,11,12	0.27	0	15,15,17	0.55	0
31	GAL	dk	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	dk	2	31	11,11,12	0.27	0	15,15,17	0.55	0
31	GAL	dl	1	31	11,11,12	0.26	0	15,15,17	0.64	0
31	GLC	dl	2	31	11,11,12	0.27	0	15,15,17	0.55	0
31	GAL	ea	1	31	11,11,12	0.22	0	15,15,17	0.59	0
31	GLC	ea	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	eb	1	31	11,11,12	0.22	0	15,15,17	0.59	0
31	GLC	eb	2	31	11,11,12	0.28	0	15,15,17	0.56	0
31	GAL	ec	1	31	11,11,12	0.22	0	15,15,17	0.59	0
31	GLC	ec	2	31	11,11,12	0.28	0	15,15,17	0.57	0
31	GAL	ed	1	31	11,11,12	0.22	0	15,15,17	0.59	0
31	GLC	ed	2	31	11,11,12	0.28	0	15,15,17	0.57	0
31	GAL	ei	1	31	11,11,12	0.27	0	15,15,17	0.67	0
31	GLC	ei	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	ej	1	31	11,11,12	0.28	0	15,15,17	0.70	0
31	GLC	ej	2	31	11,11,12	0.27	0	15,15,17	0.57	0
31	GAL	ek	1	31	11,11,12	0.27	0	15,15,17	0.66	0
31	GLC	ek	2	31	11,11,12	0.27	0	15,15,17	0.56	0
31	GAL	el	1	31	11,11,12	0.28	0	15,15,17	0.70	0
31	GLC	el	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	fa	1	31	11,11,12	0.25	0	15,15,17	0.68	0
31	GLC	fa	2	31	11,11,12	0.28	0	15,15,17	0.58	0
31	GAL	fb	1	31	11,11,12	0.25	0	15,15,17	0.68	0
31	GLC	fb	2	31	11,11,12	0.28	0	15,15,17	0.58	0
31	GAL	fc	1	31	11,11,12	0.25	0	15,15,17	0.69	0
31	GLC	fc	2	31	11,11,12	0.28	0	15,15,17	0.58	0
31	GAL	fd	1	31	11,11,12	0.25	0	15,15,17	0.69	0
31	GLC	fd	2	31	11,11,12	0.28	0	15,15,17	0.58	0
31	GAL	gi	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	gi	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	gj	1	31	11,11,12	0.24	0	15,15,17	0.61	0
31	GLC	gj	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	gk	1	31	11,11,12	0.23	0	15,15,17	0.61	0
31	GLC	gk	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	gl	1	31	11,11,12	0.23	0	15,15,17	0.61	0
31	GLC	gl	2	31	11,11,12	0.23	0	15,15,17	0.53	0
31	GAL	ha	1	31	11,11,12	0.27	0	15,15,17	0.64	0
31	GLC	ha	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	hb	1	31	11,11,12	0.27	0	15,15,17	0.64	0
31	GLC	hb	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	hc	1	31	11,11,12	0.27	0	15,15,17	0.64	0
31	GLC	hc	2	31	11,11,12	0.24	0	15,15,17	0.54	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	hd	1	31	11,11,12	0.27	0	15,15,17	0.64	0
31	GLC	hd	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	ii	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	ii	2	31	11,11,12	0.24	0	15,15,17	0.55	0
31	GAL	ij	1	31	11,11,12	0.24	0	15,15,17	0.58	0
31	GLC	ij	2	31	11,11,12	0.24	0	15,15,17	0.55	0
31	GAL	ik	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	ik	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	il	1	31	11,11,12	0.24	0	15,15,17	0.59	0
31	GLC	il	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	ja	1	31	11,11,12	0.19	0	15,15,17	0.53	0
31	GLC	ja	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	jb	1	31	11,11,12	0.19	0	15,15,17	0.53	0
31	GLC	jb	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	jc	1	31	11,11,12	0.19	0	15,15,17	0.53	0
31	GLC	jc	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	jd	1	31	11,11,12	0.19	0	15,15,17	0.53	0
31	GLC	jd	2	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GAL	ji	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	ji	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	jj	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	jj	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	jk	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	jk	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	jl	1	31	11,11,12	0.22	0	15,15,17	0.56	0
31	GLC	jl	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	ka	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	ka	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	kb	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	kb	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	kc	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	kc	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	kd	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	kd	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	ki	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	ki	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	kj	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	kj	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	kk	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	kk	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	kl	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	kl	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	la	1	31	11,11,12	0.21	0	15,15,17	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	la	2	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GAL	lb	1	31	11,11,12	0.21	0	15,15,17	0.58	0
31	GLC	lb	2	31	11,11,12	0.24	0	15,15,17	0.57	0
31	GAL	lc	1	31	11,11,12	0.18	0	15,15,17	0.59	0
31	GLC	lc	2	31	11,11,12	0.24	0	15,15,17	0.58	0
31	GAL	ld	1	31	11,11,12	0.19	0	15,15,17	0.59	0
31	GLC	ld	2	31	11,11,12	0.24	0	15,15,17	0.58	0
31	GAL	li	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	li	2	31	11,11,12	0.27	0	15,15,17	0.59	0
31	GAL	lj	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	lj	2	31	11,11,12	0.27	0	15,15,17	0.59	0
31	GAL	lk	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	lk	2	31	11,11,12	0.27	0	15,15,17	0.59	0
31	GAL	ll	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	ll	2	31	11,11,12	0.27	0	15,15,17	0.59	0
31	GAL	ma	1	31	11,11,12	0.23	0	15,15,17	0.57	0
31	GLC	ma	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	mb	1	31	11,11,12	0.23	0	15,15,17	0.57	0
31	GLC	mb	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	mc	1	31	11,11,12	0.23	0	15,15,17	0.57	0
31	GLC	mc	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	md	1	31	11,11,12	0.23	0	15,15,17	0.57	0
31	GLC	md	2	31	11,11,12	0.26	0	15,15,17	0.57	0
31	GAL	mi	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	mi	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	mj	1	31	11,11,12	0.22	0	15,15,17	0.60	0
31	GLC	mj	2	31	11,11,12	0.24	0	15,15,17	0.56	0
31	GAL	mk	1	31	11,11,12	0.22	0	15,15,17	0.59	0
31	GLC	mk	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	ml	1	31	11,11,12	0.21	0	15,15,17	0.59	0
31	GLC	ml	2	31	11,11,12	0.25	0	15,15,17	0.56	0
31	GAL	na	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	na	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	nb	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	nb	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	nc	1	31	11,11,12	0.24	0	15,15,17	0.58	0
31	GLC	nc	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	nd	1	31	11,11,12	0.24	0	15,15,17	0.58	0
31	GLC	nd	2	31	11,11,12	0.26	0	15,15,17	0.58	0
31	GAL	ni	1	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GLC	ni	2	31	11,11,12	0.27	0	15,15,17	0.53	0
31	GAL	nj	1	31	11,11,12	0.24	0	15,15,17	0.60	0
31	GLC	nj	2	31	11,11,12	0.27	0	15,15,17	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GAL	nk	1	31	11,11,12	0.23	0	15,15,17	0.60	0
31	GLC	nk	2	31	11,11,12	0.27	0	15,15,17	0.53	0
31	GAL	nl	1	31	11,11,12	0.23	0	15,15,17	0.60	0
31	GLC	nl	2	31	11,11,12	0.27	0	15,15,17	0.53	0
31	GAL	oa	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	oa	2	31	11,11,12	0.29	0	15,15,17	0.58	0
31	GAL	ob	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	ob	2	31	11,11,12	0.29	0	15,15,17	0.58	0
31	GAL	oc	1	31	11,11,12	0.20	0	15,15,17	0.55	0
31	GLC	oc	2	31	11,11,12	0.29	0	15,15,17	0.58	0
31	GAL	od	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	od	2	31	11,11,12	0.29	0	15,15,17	0.58	0
31	GAL	oi	1	31	11,11,12	0.21	0	15,15,17	0.57	0
31	GLC	oi	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	oj	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	oj	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	ok	1	31	11,11,12	0.20	0	15,15,17	0.56	0
31	GLC	ok	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	ol	1	31	11,11,12	0.21	0	15,15,17	0.56	0
31	GLC	ol	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	pa	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	pa	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	pb	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	pb	2	31	11,11,12	0.27	0	15,15,17	0.57	0
31	GAL	pc	1	31	11,11,12	0.23	0	15,15,17	0.56	0
31	GLC	pc	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	pd	1	31	11,11,12	0.24	0	15,15,17	0.58	0
31	GLC	pd	2	31	11,11,12	0.26	0	15,15,17	0.56	0
31	GAL	pi	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	pi	2	31	11,11,12	0.27	0	15,15,17	0.57	0
31	GAL	pj	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	pj	2	31	11,11,12	0.27	0	15,15,17	0.57	0
31	GAL	pk	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	pk	2	31	11,11,12	0.27	0	15,15,17	0.57	0
31	GAL	pl	1	31	11,11,12	0.20	0	15,15,17	0.54	0
31	GLC	pl	2	31	11,11,12	0.27	0	15,15,17	0.57	0
31	GAL	qa	1	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GLC	qa	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	qb	1	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GLC	qb	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	qc	1	31	11,11,12	0.23	0	15,15,17	0.59	0
31	GLC	qc	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	qd	1	31	11,11,12	0.23	0	15,15,17	0.59	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	GLC	qd	2	31	11,11,12	0.25	0	15,15,17	0.57	0
31	GAL	qi	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	qi	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	qj	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	qj	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	qk	1	31	11,11,12	0.23	0	15,15,17	0.58	0
31	GLC	qk	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	ql	1	31	11,11,12	0.22	0	15,15,17	0.58	0
31	GLC	ql	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	ra	1	31	11,11,12	0.28	0	15,15,17	0.68	0
31	GLC	ra	2	31	11,11,12	0.26	0	15,15,17	0.55	0
31	GAL	rb	1	31	11,11,12	0.28	0	15,15,17	0.69	0
31	GLC	rb	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	rc	1	31	11,11,12	0.28	0	15,15,17	0.68	0
31	GLC	rc	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	rd	1	31	11,11,12	0.28	0	15,15,17	0.68	0
31	GLC	rd	2	31	11,11,12	0.26	0	15,15,17	0.54	0
31	GAL	ri	1	31	11,11,12	0.25	0	15,15,17	0.58	0
31	GLC	ri	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	rj	1	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GLC	rj	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	rk	1	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GLC	rk	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	rl	1	31	11,11,12	0.25	0	15,15,17	0.59	0
31	GLC	rl	2	31	11,11,12	0.24	0	15,15,17	0.54	0
31	GAL	sa	1	31	11,11,12	0.20	0	15,15,17	0.52	0
31	GLC	sa	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	sb	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	sb	2	31	11,11,12	0.27	0	15,15,17	0.59	0
31	GAL	sc	1	31	11,11,12	0.20	0	15,15,17	0.53	0
31	GLC	sc	2	31	11,11,12	0.27	0	15,15,17	0.58	0
31	GAL	sd	1	31	11,11,12	0.20	0	15,15,17	0.52	0
31	GLC	sd	2	31	11,11,12	0.27	0	15,15,17	0.59	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
31	GAL	Aa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Aa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ab	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Ab	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ac	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ac	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ad	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ad	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ae	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ae	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Af	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Af	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ag	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ag	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ah	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ah	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ai	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ai	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Aj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Aj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ak	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ak	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Al	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Al	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ba	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ba	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Be	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Be	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bk	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Bk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Bl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Bl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ca	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ca	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ce	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ce	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ch	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ch	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ci	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ci	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ck	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ck	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Cl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Cl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	De	1	31	-	0/2/19/22	0/1/1/1
31	GLC	De	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Df	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Df	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Dg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Dg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Dh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Dh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Di	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Di	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Dj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Dj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Dk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Dk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Dl	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Dl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ea	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ea	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Eb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Eb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ec	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ec	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ed	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ed	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ee	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ee	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ef	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ef	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Eg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Eg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Eh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Eh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Fi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Fi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Fj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Fj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Fk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Fk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Fl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Fl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ga	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ga	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ge	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ge	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gi	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Gi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Gl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Gl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ha	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ha	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	He	1	31	-	0/2/19/22	0/1/1/1
31	GLC	He	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Hi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Hi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ia	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ia	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ib	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ib	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ic	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ic	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Id	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Id	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ie	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ie	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	If	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	If	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ig	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ig	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ih	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ih	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ii	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ii	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ij	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ij	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ik	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ik	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Il	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Il	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ja	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ja	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Je	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Je	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ji	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ji	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Jl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Jl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ka	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ka	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kc	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Kc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ke	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ke	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ki	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ki	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Kl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Kl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	La	1	31	-	0/2/19/22	0/1/1/1
31	GLC	La	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Lb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Lc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ld	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ld	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Le	1	31	-	1/2/19/22	0/1/1/1
31	GLC	Le	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lf	1	31	-	1/2/19/22	0/1/1/1
31	GLC	Lf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lg	1	31	-	1/2/19/22	0/1/1/1
31	GLC	Lg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lh	1	31	-	1/2/19/22	0/1/1/1
31	GLC	Lh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Li	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Li	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Lj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Lk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Lk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ll	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Ll	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ma	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ma	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Md	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Md	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Me	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Me	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Mk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Mk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ml	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ml	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Na	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Na	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ne	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ne	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ng	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ng	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ni	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Ni	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Nl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Nl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Oa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Oa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ob	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ob	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Oc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Oc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Od	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Od	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Oe	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Oe	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Of	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Of	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Og	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Og	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Oh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Oh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Oi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Oi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Oj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Oj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ok	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ok	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ol	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ol	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pe	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pe	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pf	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Pf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ph	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ph	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Pl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Pl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Qk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Qk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ql	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ql	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ra	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ra	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Rb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Rb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Rc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Rc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Rd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Rd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Re	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Re	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Rf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Rf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Rg	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Rg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Rh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Rh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Se	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Se	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Sf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Sf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Sg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Sg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Sh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Sh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Si	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Si	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Sj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Sj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Sk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Sk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Sl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Sl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ta	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ta	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Tb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Tb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Tc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Tc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Td	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Td	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ti	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ti	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Tj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Tj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Tk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Tk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Tl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Tl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ua	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ua	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ub	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ub	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Uc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Uc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ud	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Ud	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ui	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ui	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Uj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Uj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Uk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Uk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ul	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ul	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Va	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Va	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Vb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Vb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Vc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Vc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Vd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Vd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ve	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Ve	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Vf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Vf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Vg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Vg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Vh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Vh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	We	1	31	-	0/2/19/22	0/1/1/1
31	GLC	We	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Wf	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Wf	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Wg	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Wg	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Wh	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Wh	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Xi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Xi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Xj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Xj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Xk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Xk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Xl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Xl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Ya	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	Ya	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Yl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Yl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Za	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Za	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	Zl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	Zl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	aa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	aa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ab	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ab	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ac	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ac	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ad	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ad	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	bi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	bi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	bj	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	bj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	bk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	bk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	bl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	bl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ca	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ca	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	cb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	cb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	cc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	cc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	cd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	cd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ci	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ci	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	cj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	cj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ck	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ck	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	cl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	cl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	da	1	31	-	0/2/19/22	0/1/1/1
31	GLC	da	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	db	1	31	-	0/2/19/22	0/1/1/1
31	GLC	db	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	dc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	dc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	dd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	dd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	di	1	31	-	0/2/19/22	0/1/1/1
31	GLC	di	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	dj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	dj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	dk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	dk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	dl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	dl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ea	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ea	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	eb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	eb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ec	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	ec	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ed	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ed	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ei	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ei	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ej	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ej	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ek	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ek	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	el	1	31	-	0/2/19/22	0/1/1/1
31	GLC	el	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	fa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	fa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	fb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	fb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	fc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	fc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	fd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	fd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	gi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	gi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	gj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	gj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	gk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	gk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	gl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	gl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ha	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ha	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	hb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	hb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	hc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	hc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	hd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	hd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ii	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ii	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ij	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ij	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ik	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ik	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	il	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	il	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ja	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ja	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	jb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	jb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	jc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	jc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	jd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	jd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ji	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ji	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	jj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	jj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	jk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	jk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	jl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	jl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ka	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ka	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	kb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	kb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	kc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	kc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	kd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	kd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ki	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ki	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	kj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	kj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	kk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	kk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	kl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	kl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	la	1	31	-	0/2/19/22	0/1/1/1
31	GLC	la	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	lb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	lb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	lc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	lc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ld	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ld	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	li	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	li	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	lj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	lj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	lk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	lk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ll	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ll	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ma	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ma	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	mb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	mb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	mc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	mc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	md	1	31	-	0/2/19/22	0/1/1/1
31	GLC	md	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	mi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	mi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	mj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	mj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	mk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	mk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ml	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ml	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	na	1	31	-	0/2/19/22	0/1/1/1
31	GLC	na	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	nb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	nb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	nc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	nc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	nd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	nd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ni	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ni	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	nj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	nj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	nk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	nk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	nl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	nl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	oa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	oa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ob	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	ob	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	oc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	oc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	od	1	31	-	0/2/19/22	0/1/1/1
31	GLC	od	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	oi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	oi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	oj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	oj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ok	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ok	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ol	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ol	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	pl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	pl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	qa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	qb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	qc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	qd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qi	1	31	-	0/2/19/22	0/1/1/1
31	GLC	qi	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	qj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	qk	1	31	-	0/2/19/22	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	GLC	qk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ql	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ql	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ra	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ra	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	rb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	rb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	rc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	rc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	rd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	rd	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	ri	1	31	-	0/2/19/22	0/1/1/1
31	GLC	ri	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	rj	1	31	-	0/2/19/22	0/1/1/1
31	GLC	rj	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	rk	1	31	-	0/2/19/22	0/1/1/1
31	GLC	rk	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	rl	1	31	-	0/2/19/22	0/1/1/1
31	GLC	rl	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	sa	1	31	-	0/2/19/22	0/1/1/1
31	GLC	sa	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	sb	1	31	-	0/2/19/22	0/1/1/1
31	GLC	sb	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	sc	1	31	-	0/2/19/22	0/1/1/1
31	GLC	sc	2	31	1/1/4/5	0/2/19/22	0/1/1/1
31	GAL	sd	1	31	-	0/2/19/22	0/1/1/1
31	GLC	sd	2	31	1/1/4/5	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	Tb	1	GAL	O2-C2-C3	2.30	114.75	110.14
31	Nh	1	GAL	O2-C2-C3	2.28	114.70	110.14
31	Ta	1	GAL	O2-C2-C3	2.28	114.70	110.14
31	Ng	1	GAL	O2-C2-C3	2.27	114.69	110.14
31	Nf	1	GAL	O2-C2-C3	2.25	114.64	110.14

5 of 372 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	Aa	2	GLC	C1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atom
31	Ba	2	GLC	C1
31	Ca	2	GLC	C1
31	Ea	2	GLC	C1
31	Ga	2	GLC	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	Le	1	GAL	O5-C5-C6-O6
31	Lf	1	GAL	O5-C5-C6-O6
31	Lg	1	GAL	O5-C5-C6-O6
31	Lh	1	GAL	O5-C5-C6-O6

There are no ring outliers.

125 monomers are involved in 153 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Nh	2	GLC	2	0
31	li	2	GLC	2	0
31	Pj	2	GLC	2	0
31	cl	2	GLC	1	0
31	ii	2	GLC	1	0
31	Ta	1	GAL	2	0
31	Ml	2	GLC	2	0
31	Nc	2	GLC	1	0
31	pj	2	GLC	1	0
31	na	2	GLC	1	0
31	pi	2	GLC	1	0
31	Hk	2	GLC	2	0
31	Ud	2	GLC	1	0
31	Uc	2	GLC	1	0
31	nk	2	GLC	1	0
31	Nf	2	GLC	2	0
31	lk	2	GLC	2	0
31	Bh	2	GLC	1	0
31	gk	2	GLC	1	0
31	ql	2	GLC	1	0
31	Ed	2	GLC	1	0
31	Tc	2	GLC	3	0
31	Zb	2	GLC	1	0
31	Pl	2	GLC	2	0
31	Ef	2	GLC	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Gb	1	GAL	1	0
31	Eg	2	GLC	1	0
31	Mj	2	GLC	1	0
31	Ig	2	GLC	1	0
31	Mk	2	GLC	2	0
31	Bg	2	GLC	1	0
31	Tb	1	GAL	2	0
31	Jf	2	GLC	1	0
31	Hc	2	GLC	1	0
31	Bf	2	GLC	1	0
31	Mi	2	GLC	2	0
31	cj	2	GLC	1	0
31	Lb	2	GLC	1	0
31	Ne	2	GLC	2	0
31	Td	1	GAL	2	0
31	ja	2	GLC	1	0
31	ci	2	GLC	1	0
31	Ua	2	GLC	1	0
31	Ec	2	GLC	1	0
31	Ke	2	GLC	1	0
31	Ng	2	GLC	2	0
31	pb	2	GLC	1	0
31	Ld	2	GLC	1	0
31	Pk	2	GLC	2	0
31	Ie	2	GLC	1	0
31	Ma	2	GLC	1	0
31	gi	2	GLC	1	0
31	La	2	GLC	1	0
31	Ga	1	GAL	1	0
31	jb	2	GLC	1	0
31	ll	2	GLC	2	0
31	Eh	2	GLC	1	0
31	kk	2	GLC	1	0
31	Lc	2	GLC	1	0
31	ld	2	GLC	2	0
31	lj	2	GLC	2	0
31	Kf	2	GLC	1	0
31	Ea	2	GLC	1	0
31	pa	2	GLC	1	0
31	Za	2	GLC	1	0
31	pl	2	GLC	1	0
31	kj	2	GLC	1	0

Continued on next page...

Continued from previous page...

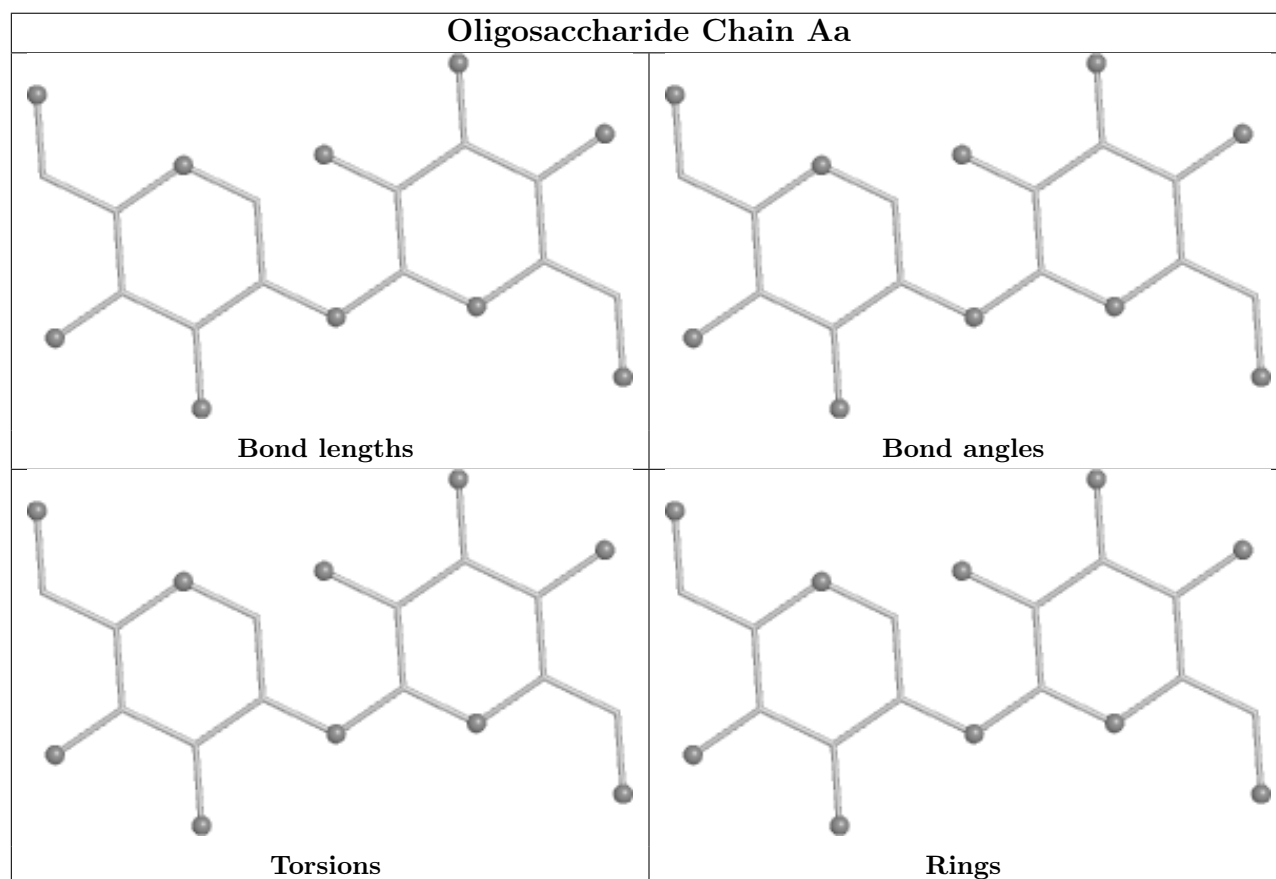
Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	qk	2	GLC	2	0
31	Kh	2	GLC	1	0
31	pc	2	GLC	1	0
31	Pi	2	GLC	2	0
31	lb	2	GLC	2	0
31	Tb	2	GLC	3	0
31	jc	2	GLC	1	0
31	Si	2	GLC	2	0
31	Be	2	GLC	1	0
31	nd	2	GLC	1	0
31	jd	2	GLC	1	0
31	la	2	GLC	2	0
31	ki	2	GLC	1	0
31	Mb	2	GLC	1	0
31	gj	2	GLC	1	0
31	Je	2	GLC	1	0
31	Sk	2	GLC	2	0
31	Hd	2	GLC	1	0
31	Ih	2	GLC	1	0
31	Md	2	GLC	1	0
31	nc	2	GLC	1	0
31	Ta	2	GLC	3	0
31	Sj	2	GLC	2	0
31	qi	2	GLC	1	0
31	Hb	2	GLC	1	0
31	nl	2	GLC	1	0
31	Mc	2	GLC	1	0
31	Ba	2	GLC	1	0
31	Gc	1	GAL	1	0
31	Bb	2	GLC	1	0
31	nj	2	GLC	1	0
31	Ub	2	GLC	1	0
31	Eb	2	GLC	1	0
31	Kg	2	GLC	1	0
31	Bd	2	GLC	1	0
31	kl	2	GLC	1	0
31	ik	2	GLC	1	0
31	Hi	2	GLC	2	0
31	Jh	2	GLC	1	0
31	rk	2	GLC	1	0
31	Ha	2	GLC	1	0
31	ri	2	GLC	1	0

Continued on next page...

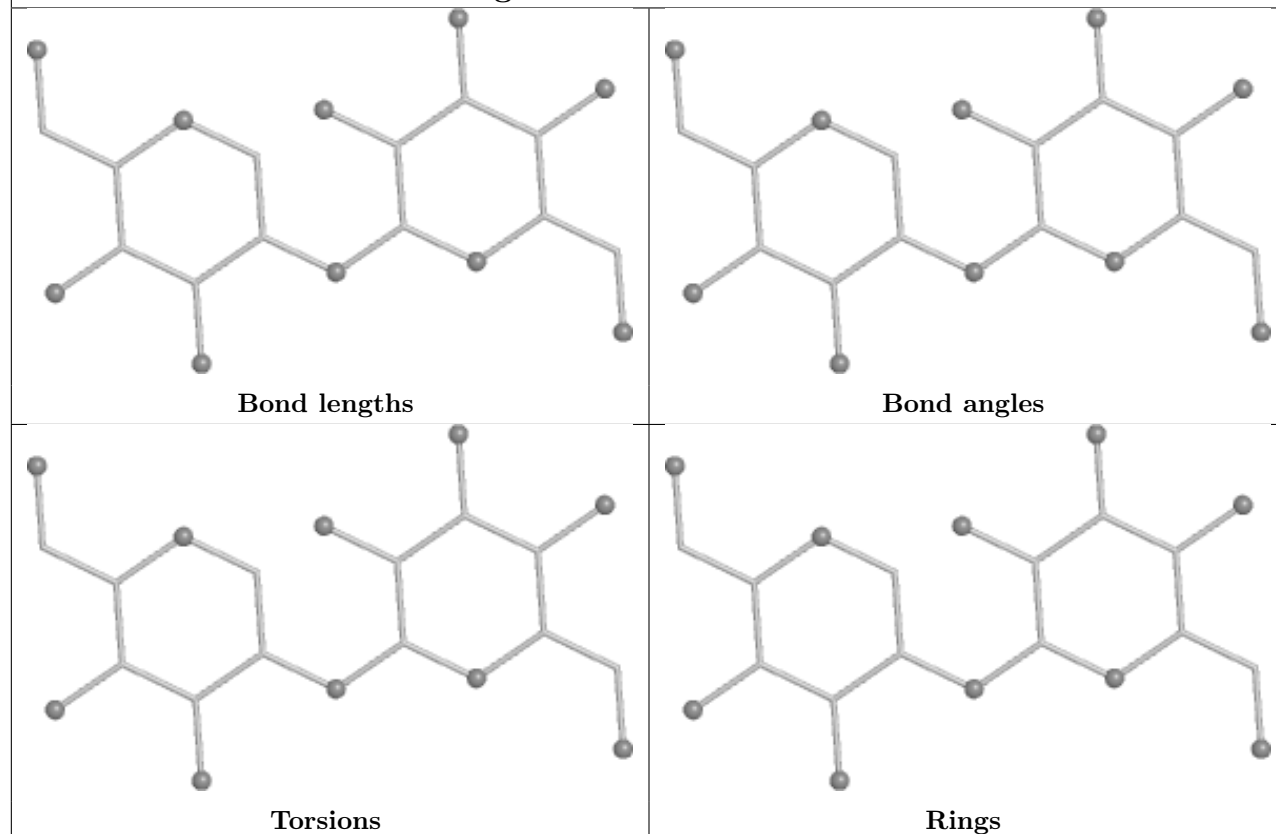
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	lc	2	GLC	2	0
31	Hl	2	GLC	2	0
31	Gd	1	GAL	1	0
31	nb	2	GLC	1	0
31	pk	2	GLC	1	0
31	If	2	GLC	1	0
31	Bc	2	GLC	1	0
31	ni	2	GLC	1	0
31	Td	2	GLC	3	0
31	Tc	1	GAL	2	0
31	Hj	2	GLC	2	0
31	Ee	2	GLC	1	0
31	Sl	2	GLC	2	0
31	qj	2	GLC	1	0
31	ck	2	GLC	1	0
31	gl	2	GLC	1	0

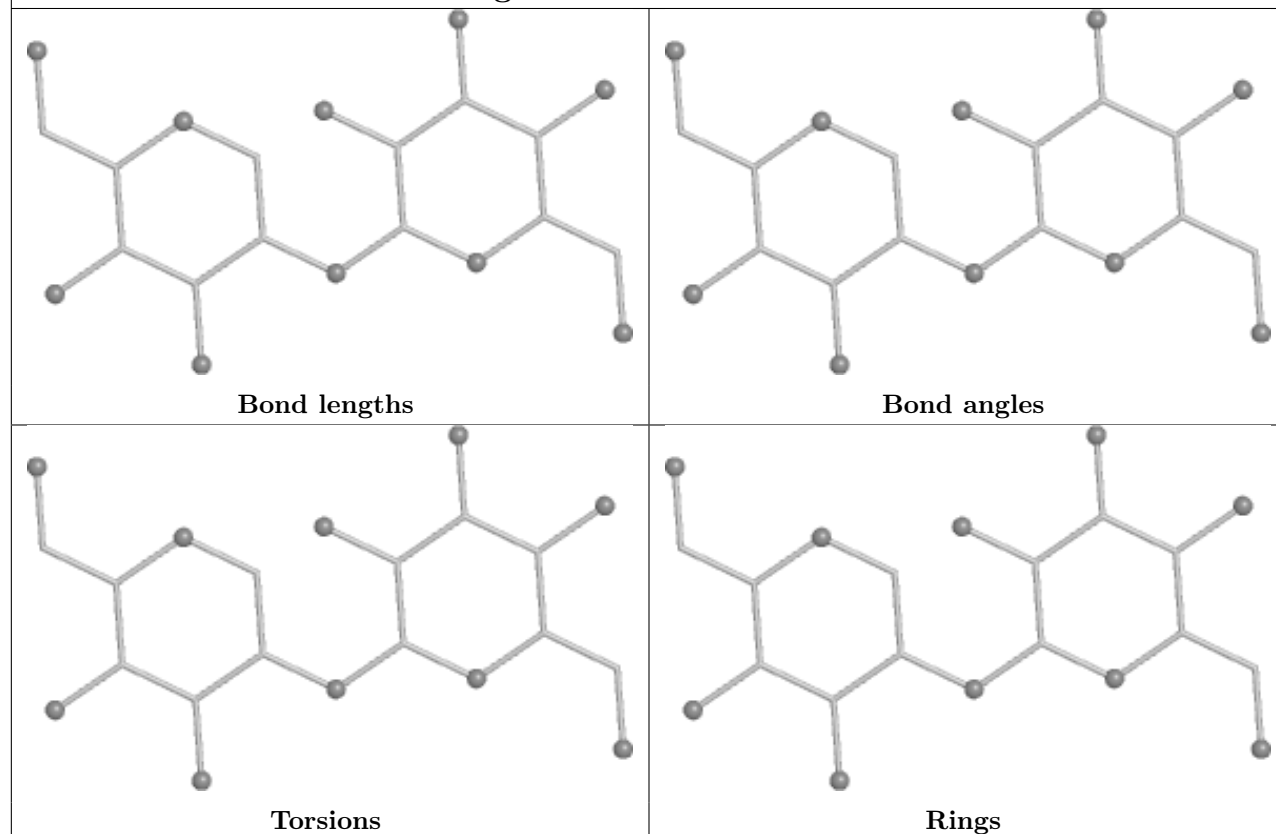
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

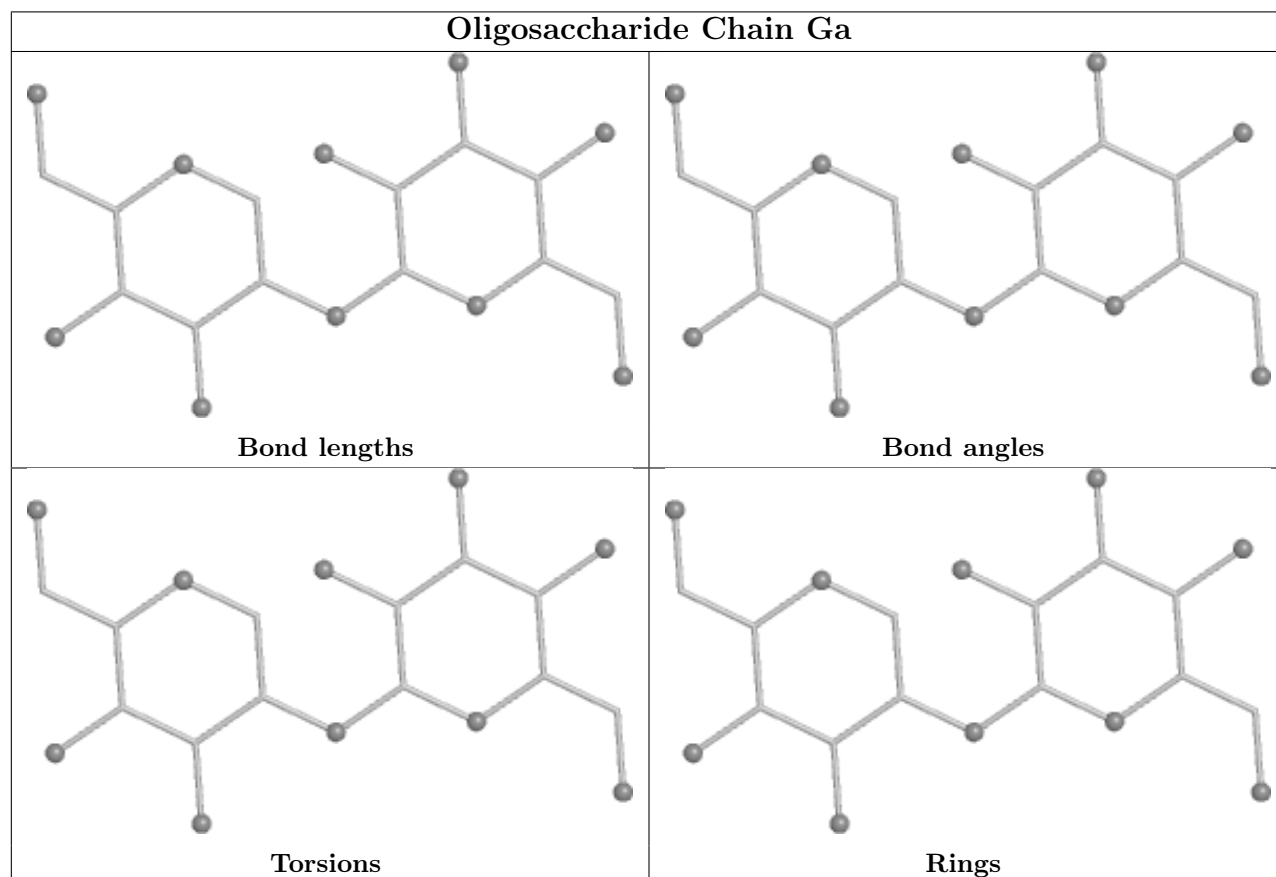
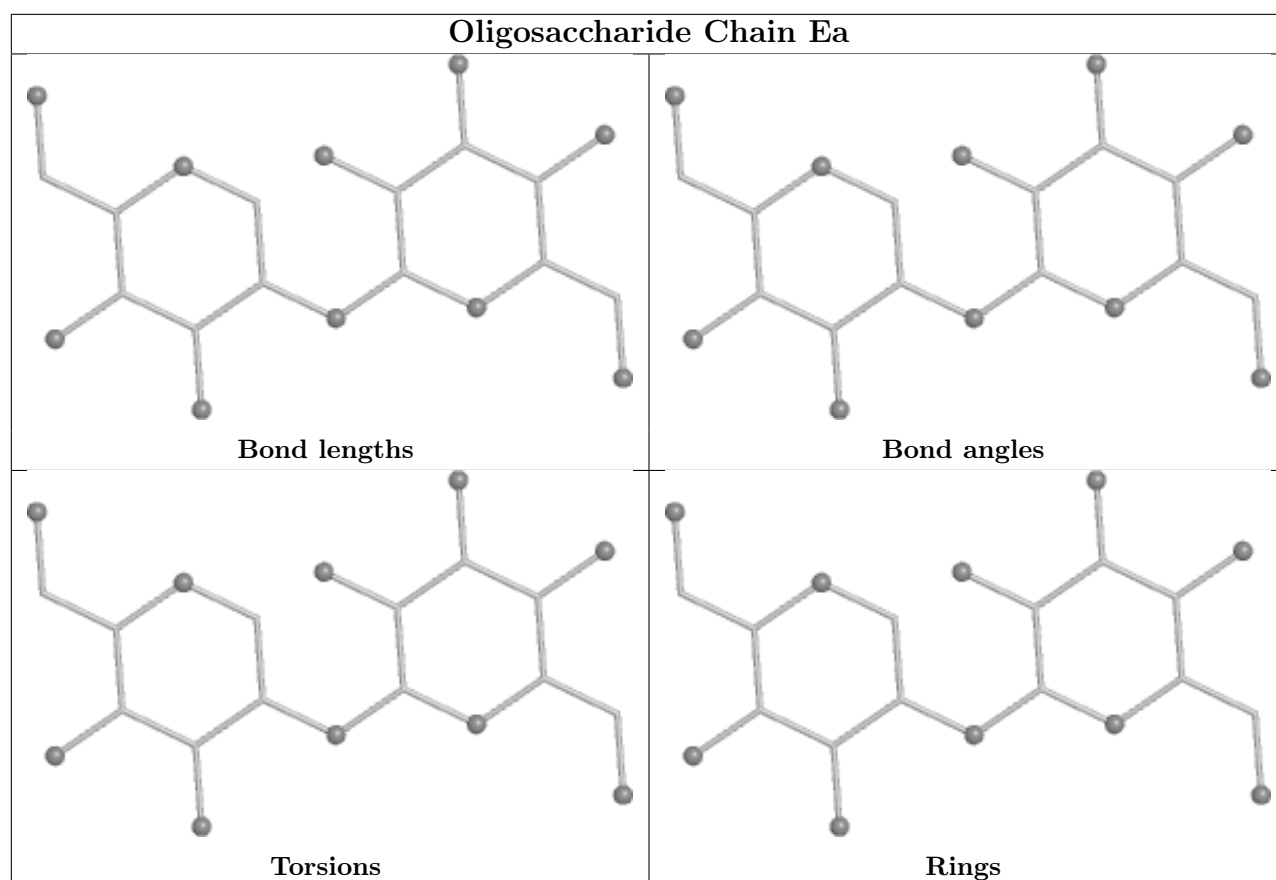


Oligosaccharide Chain Ba

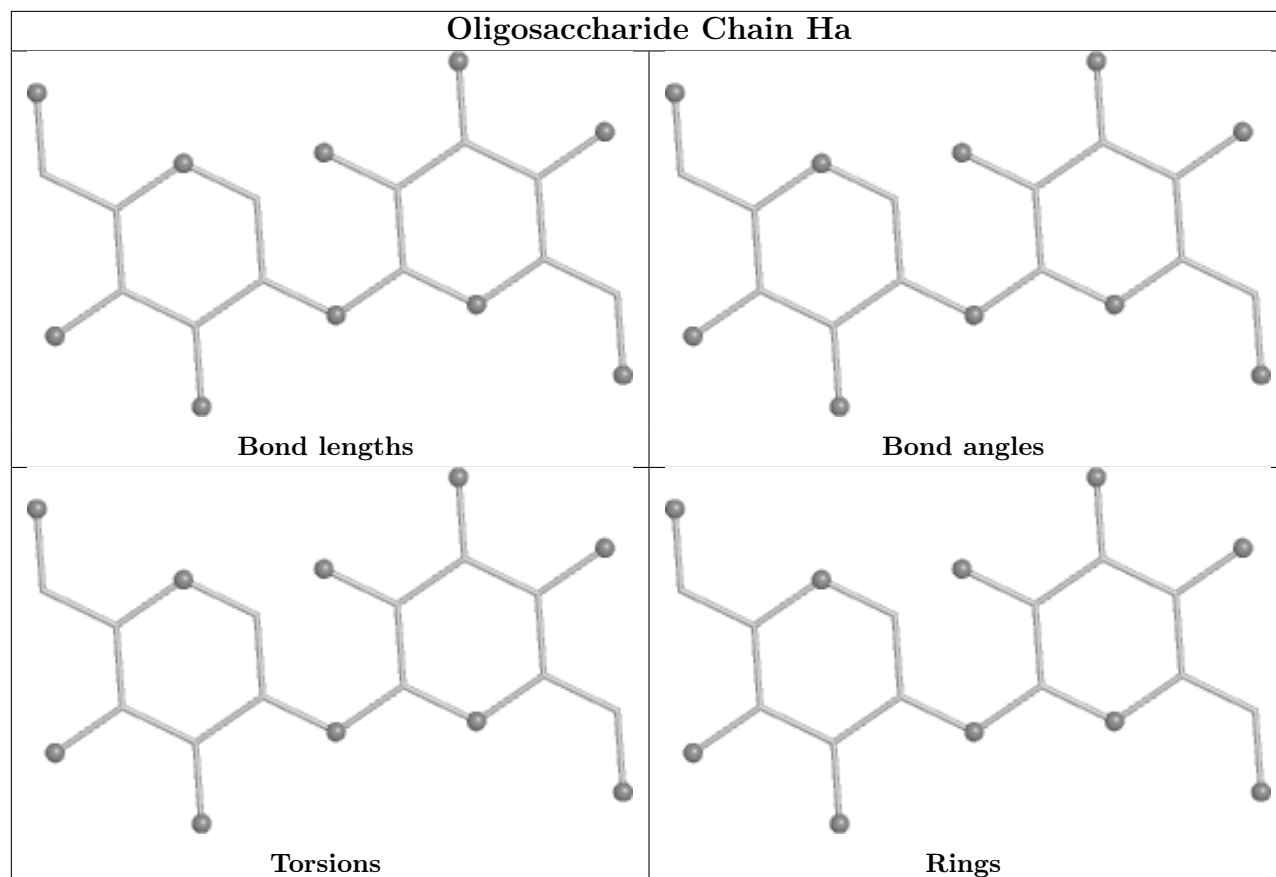


Oligosaccharide Chain Ca

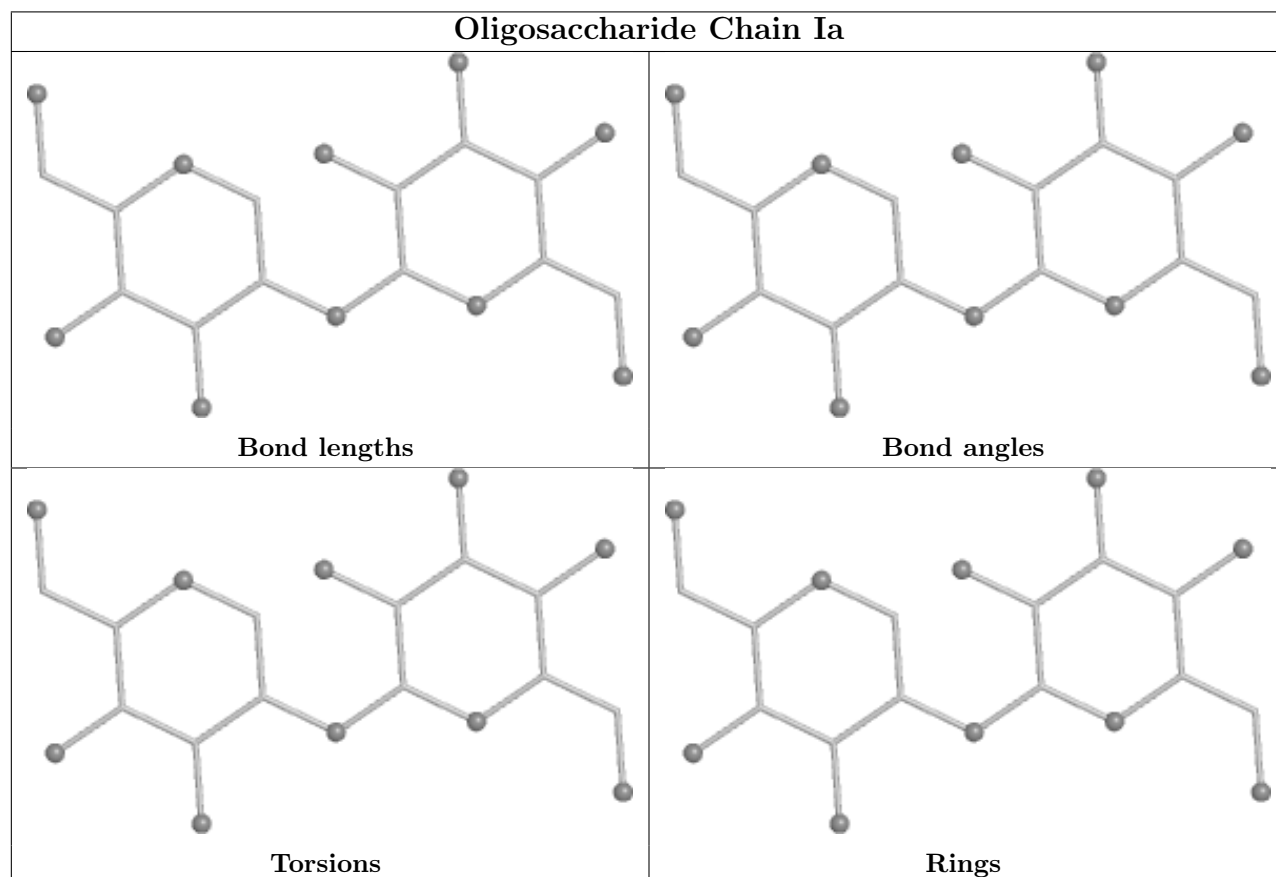


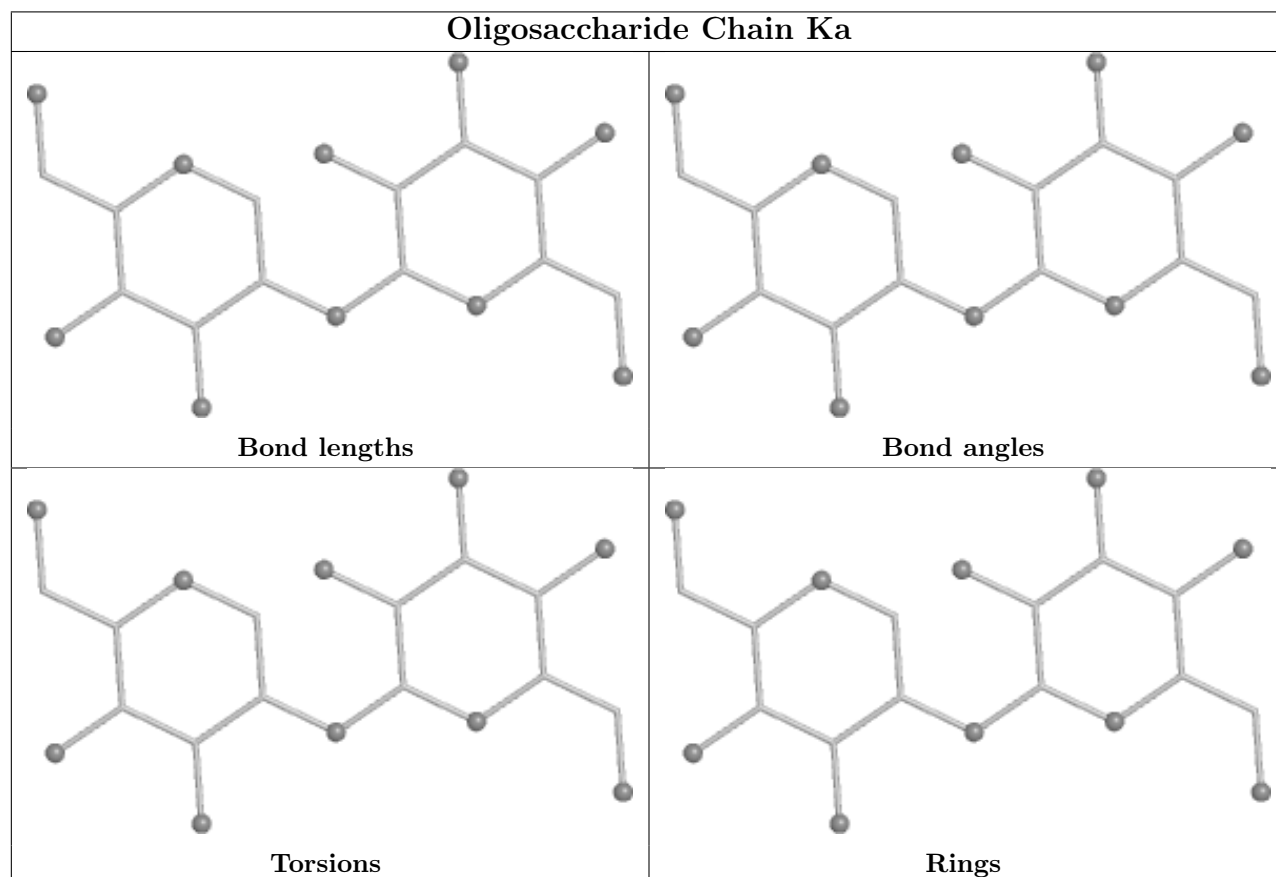
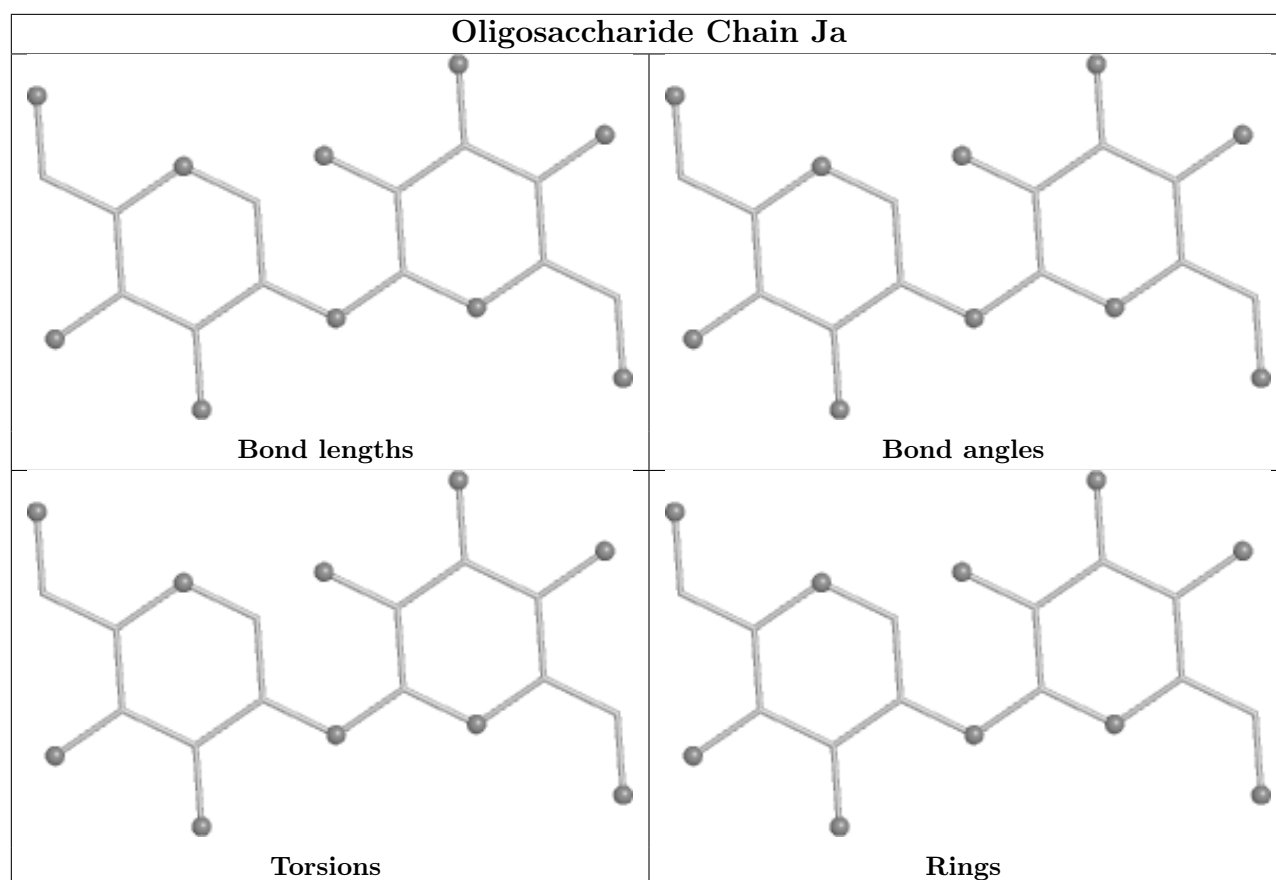


Oligosaccharide Chain Ha

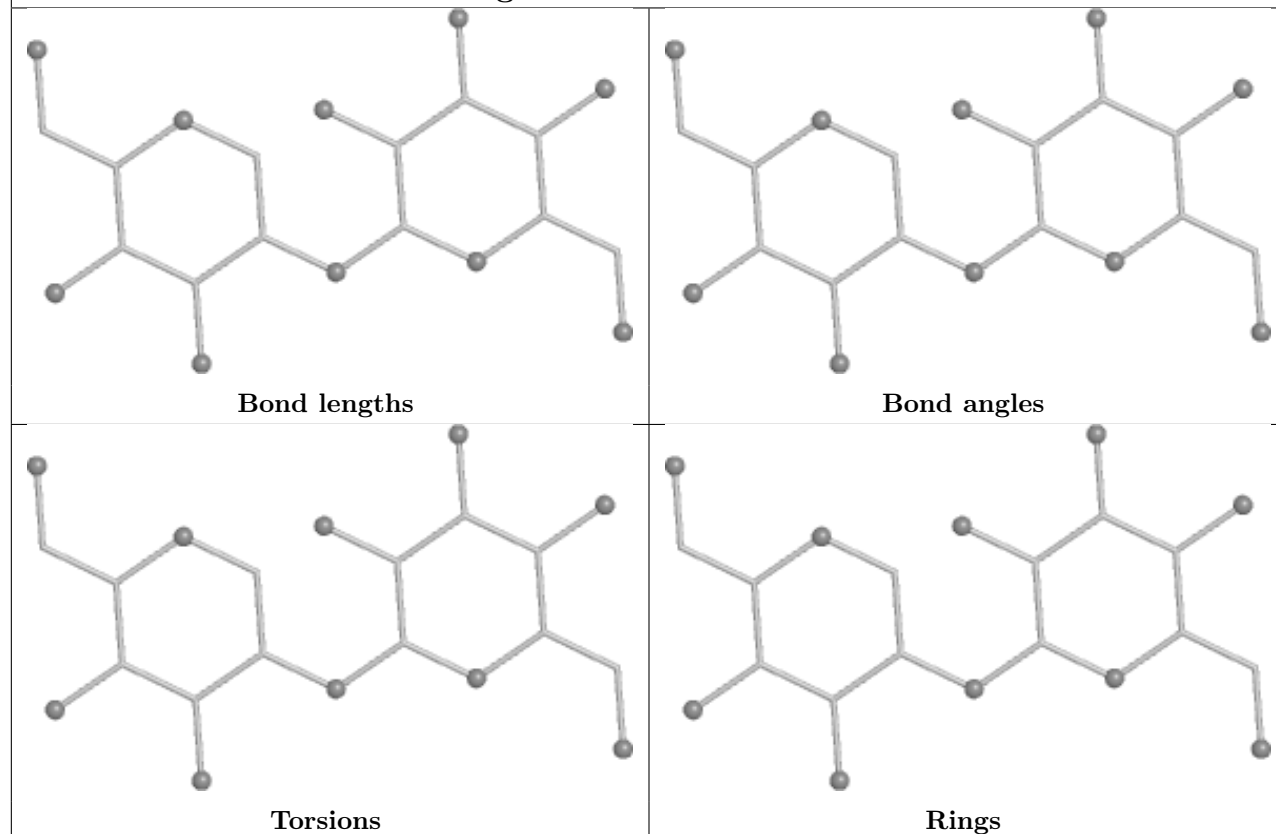


Oligosaccharide Chain Ia

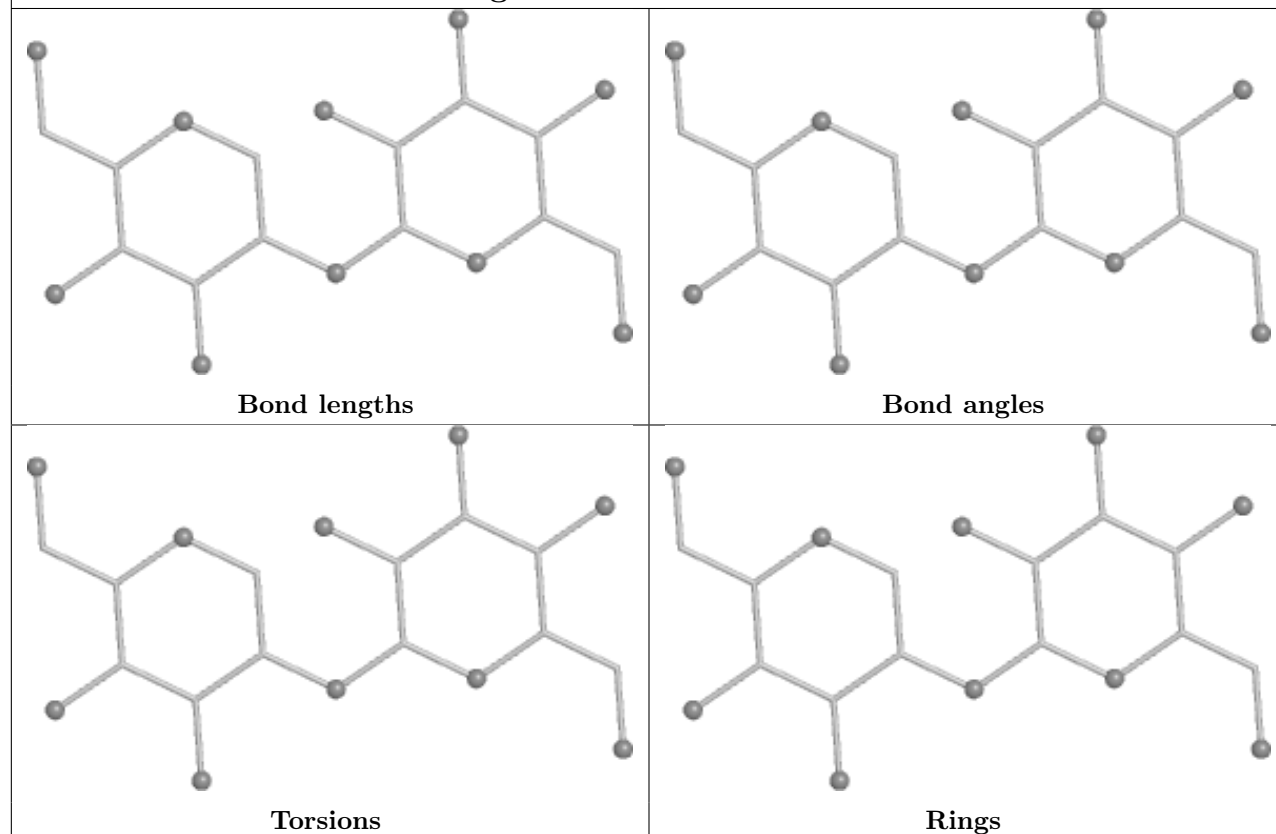




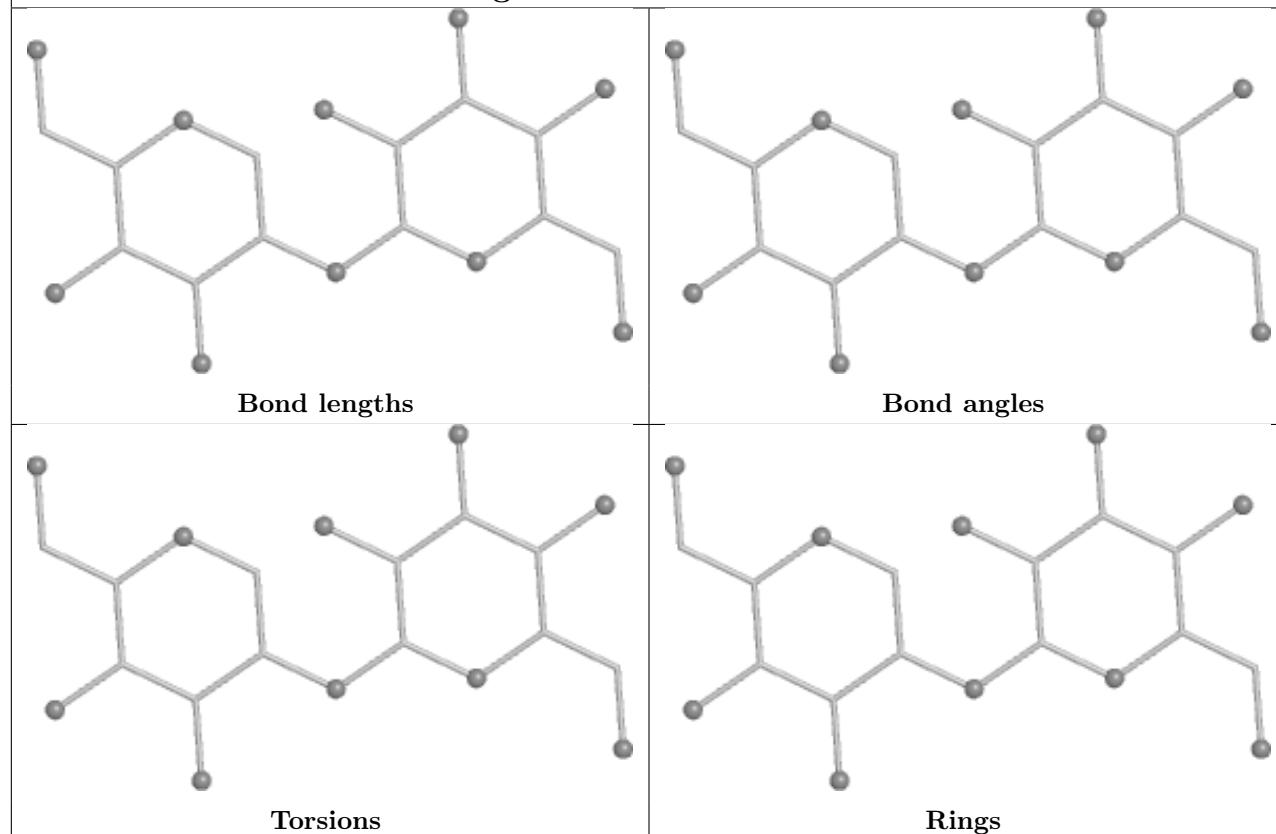
Oligosaccharide Chain La



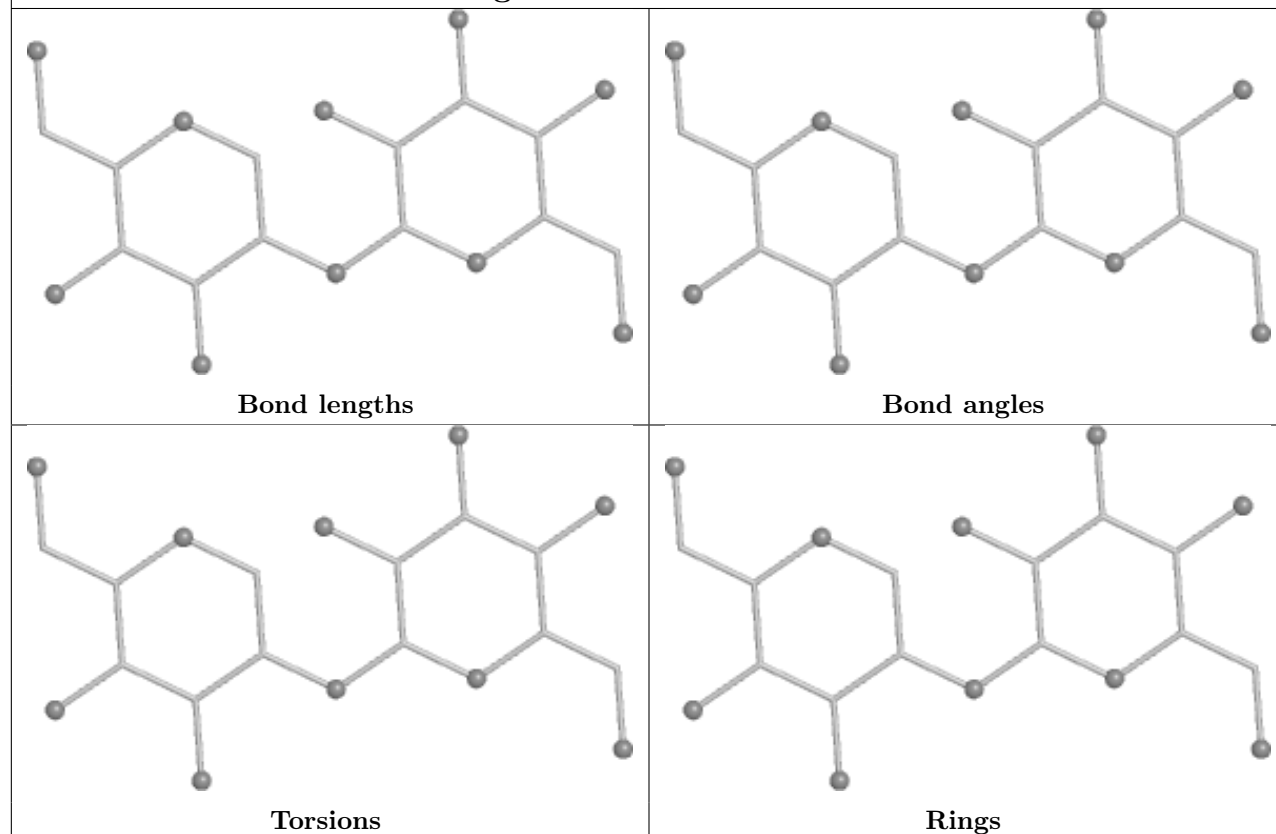
Oligosaccharide Chain Ma

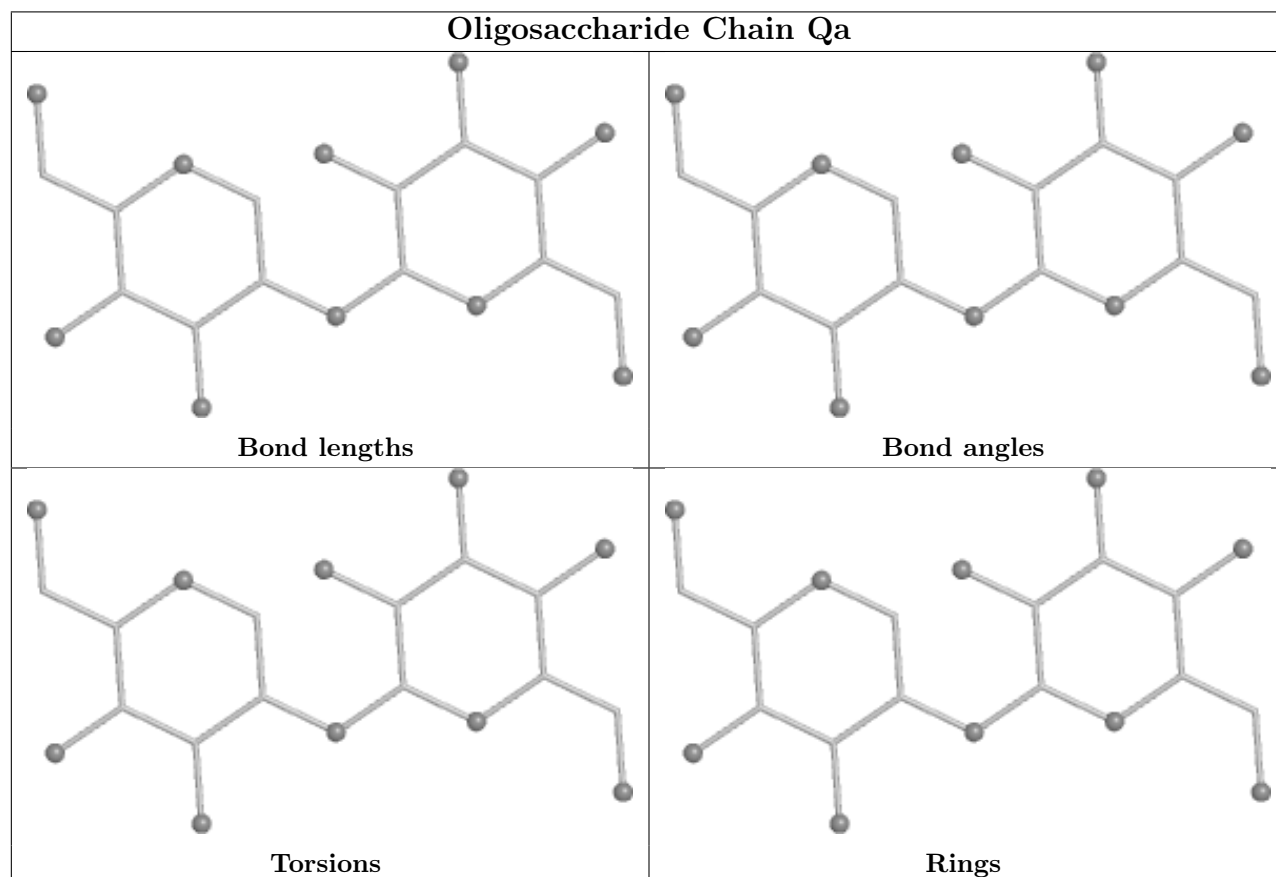
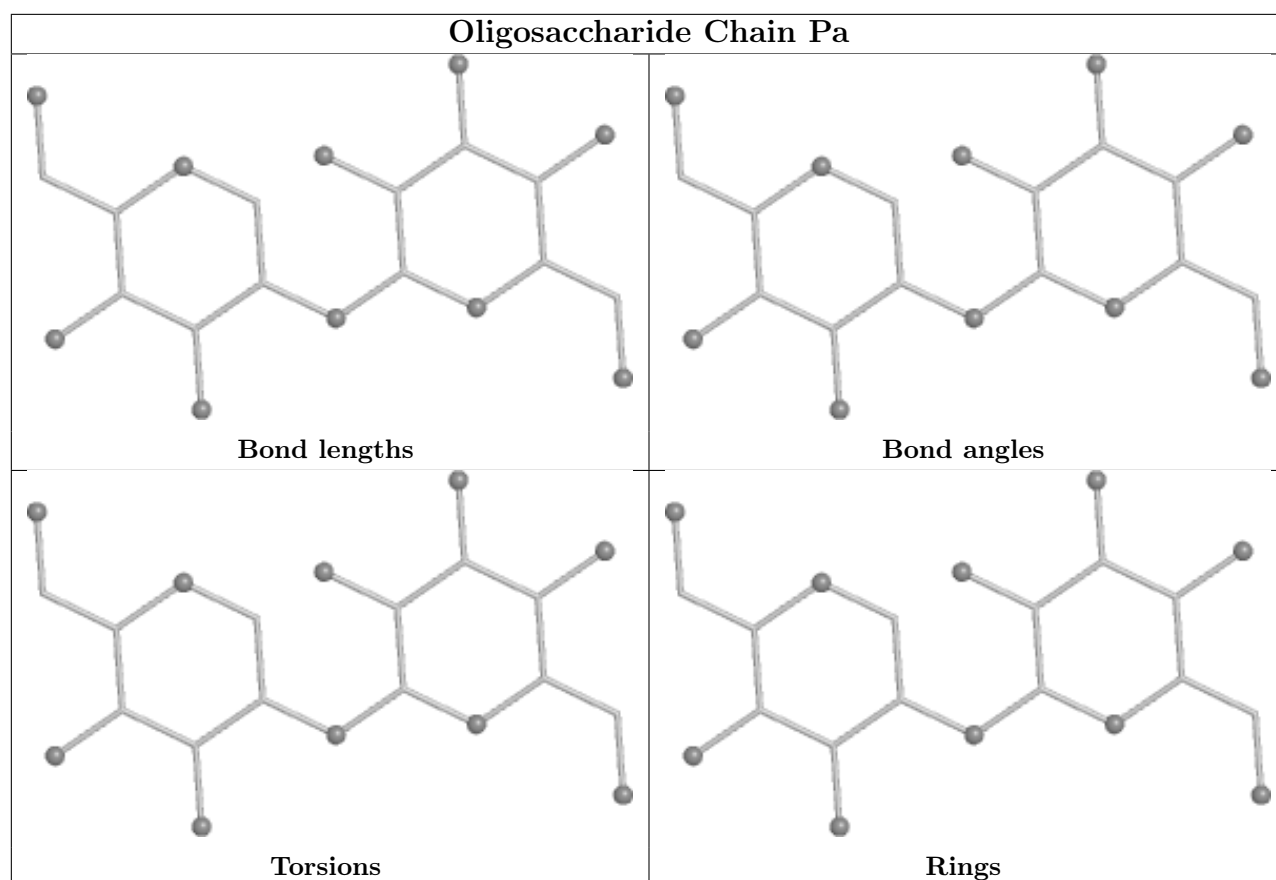


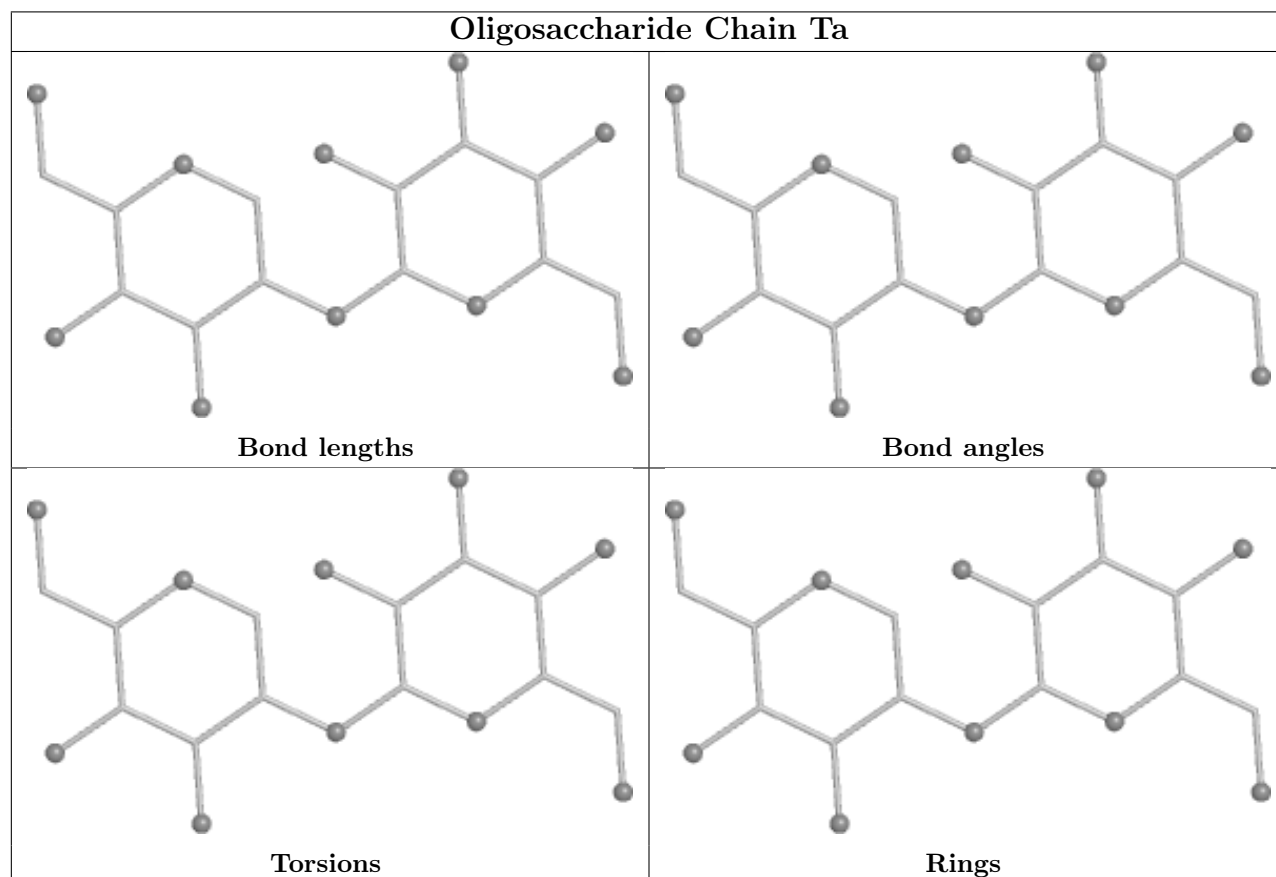
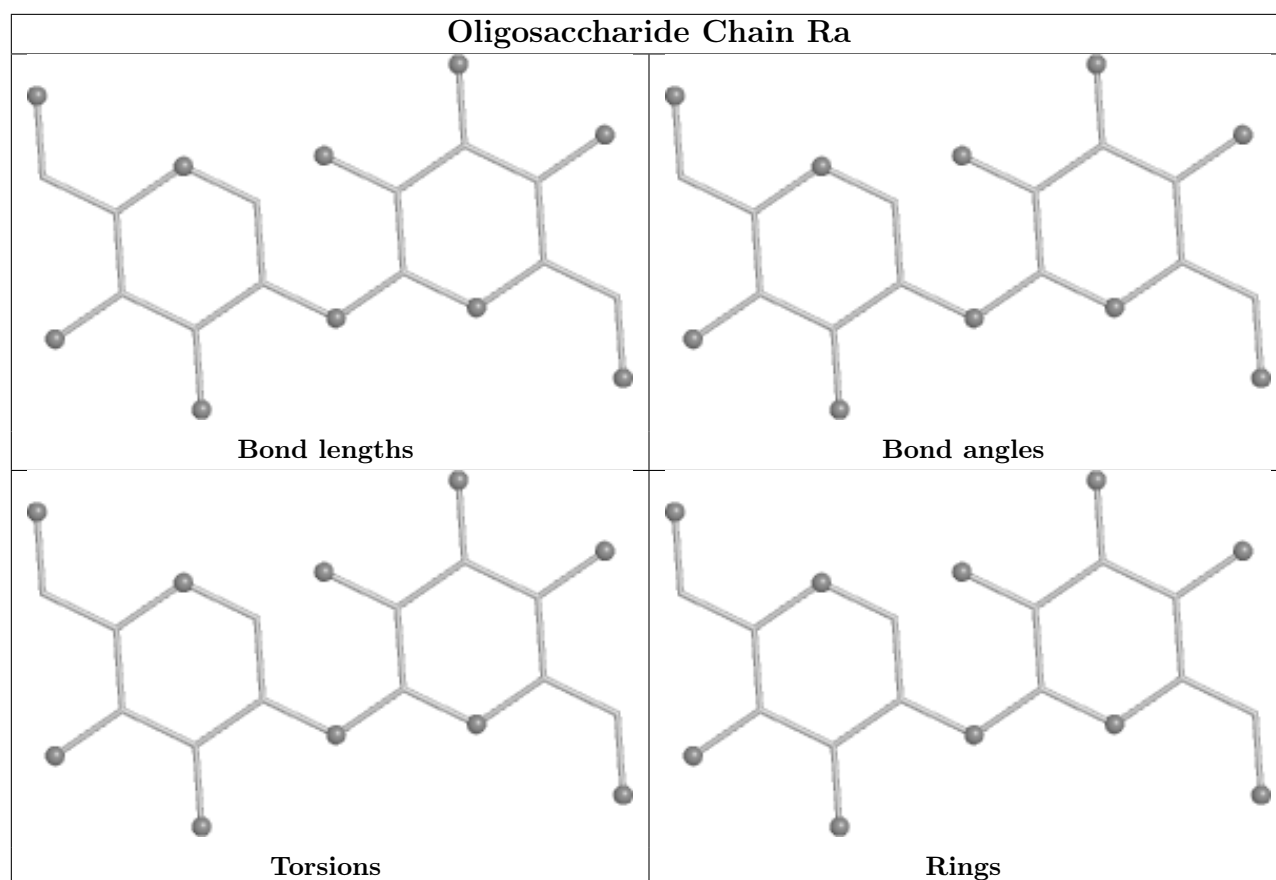
Oligosaccharide Chain Na



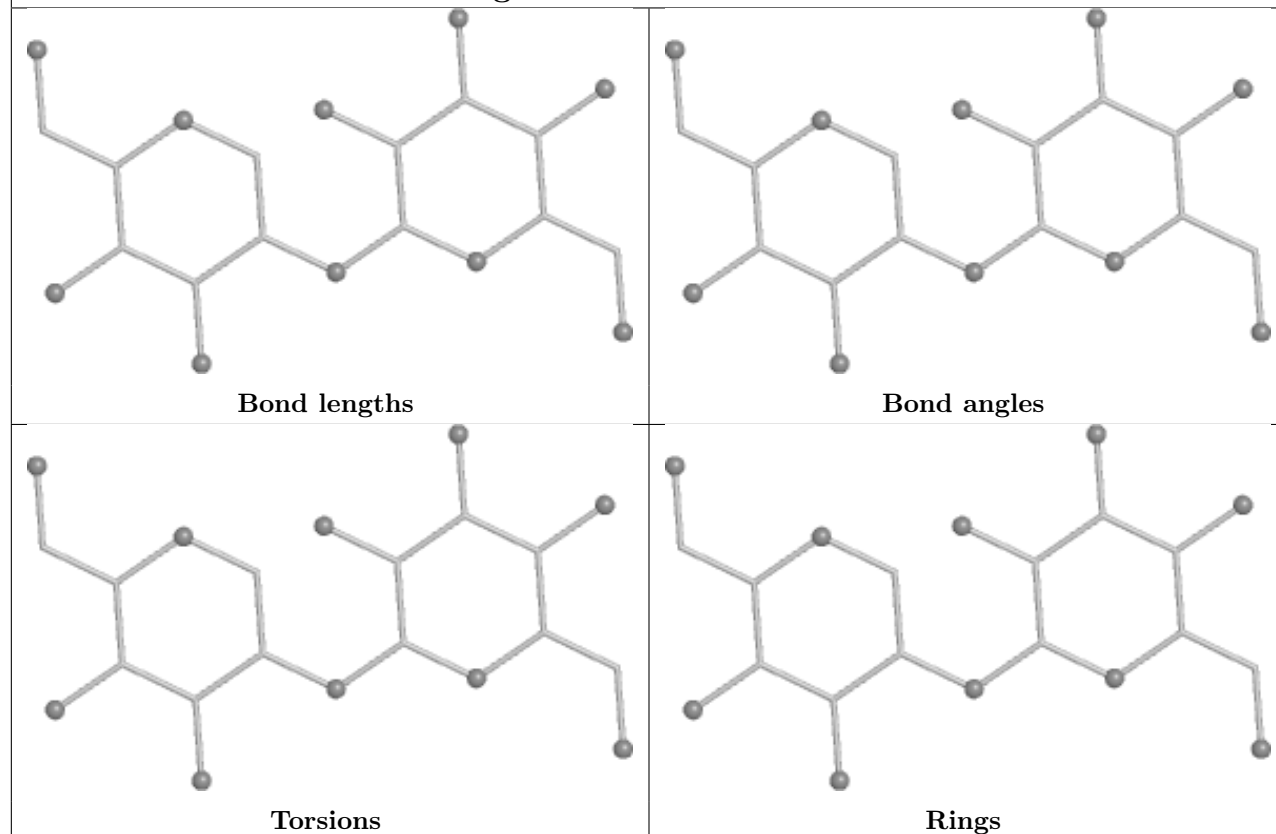
Oligosaccharide Chain Oa



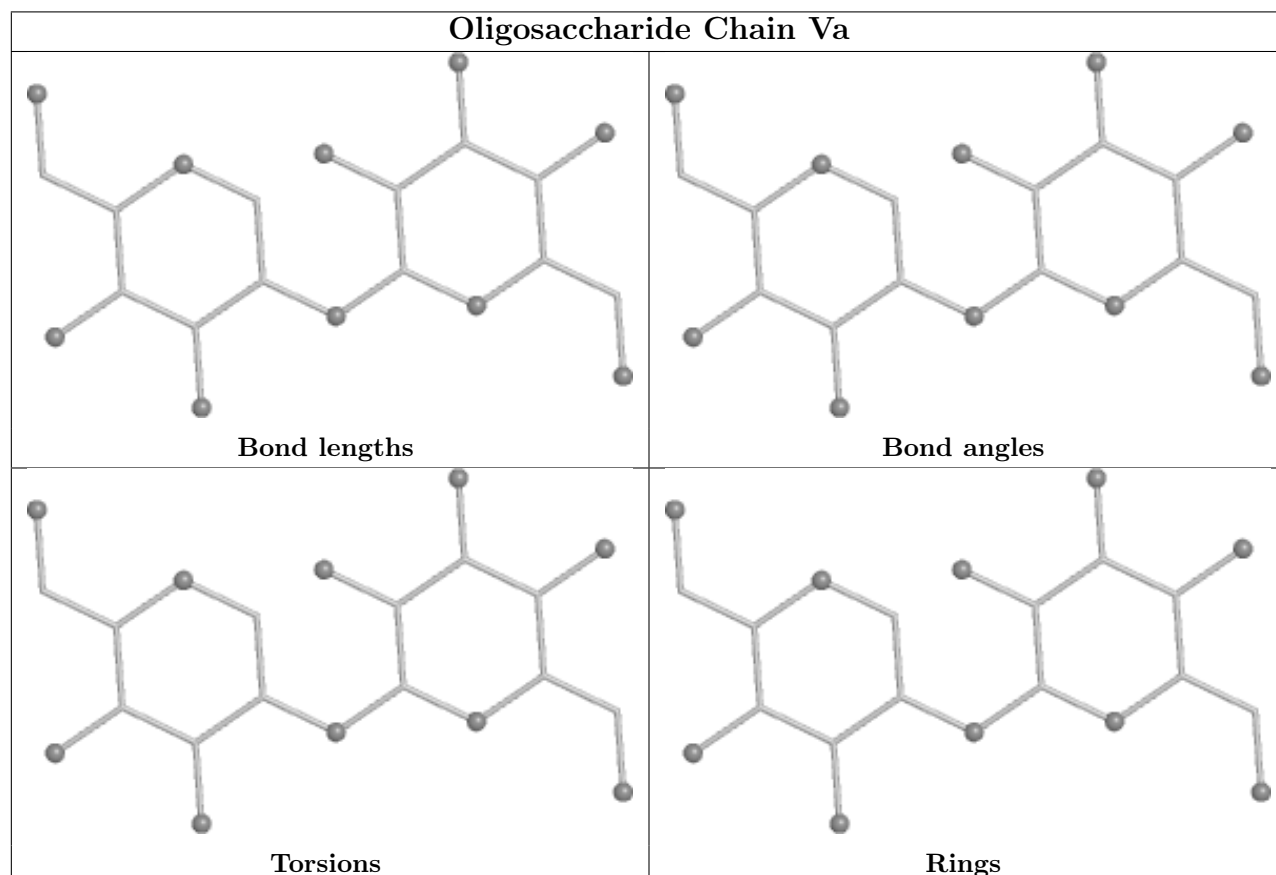




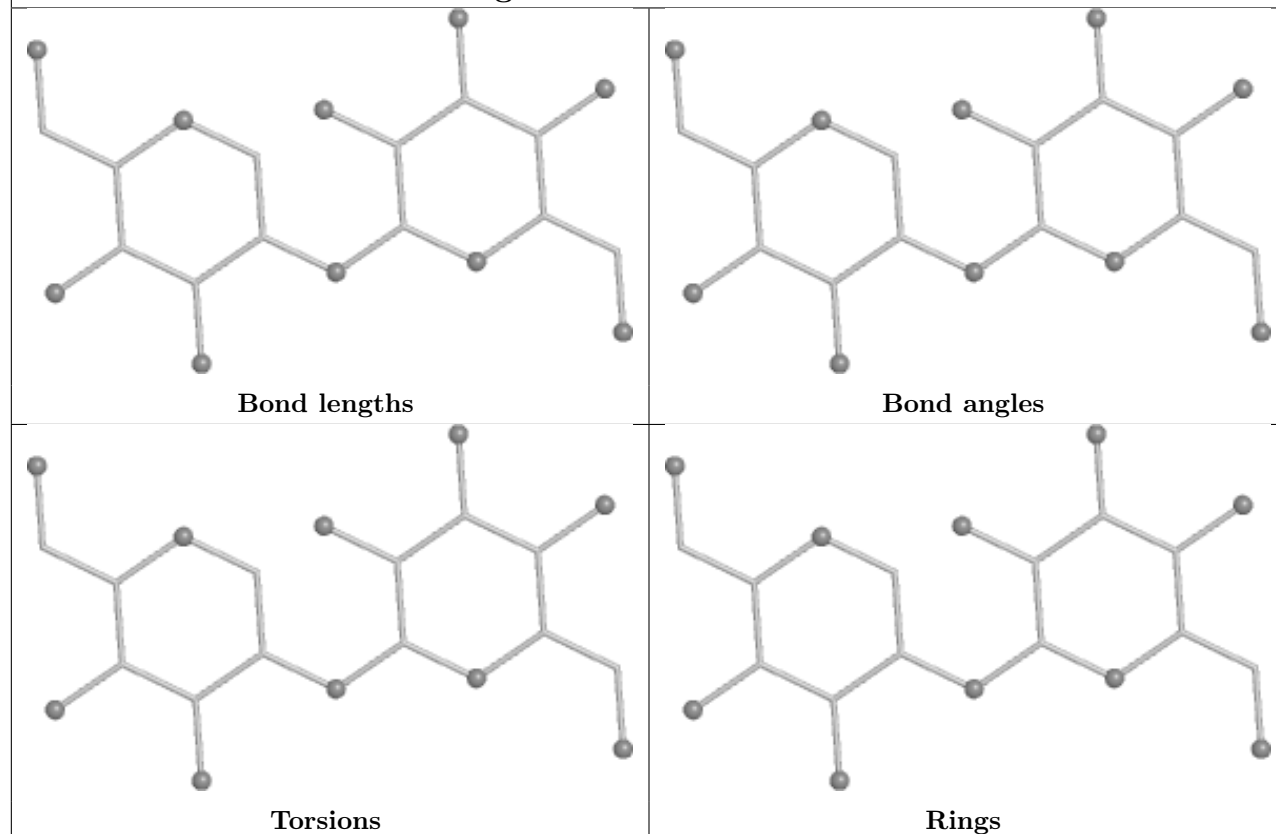
Oligosaccharide Chain Ua



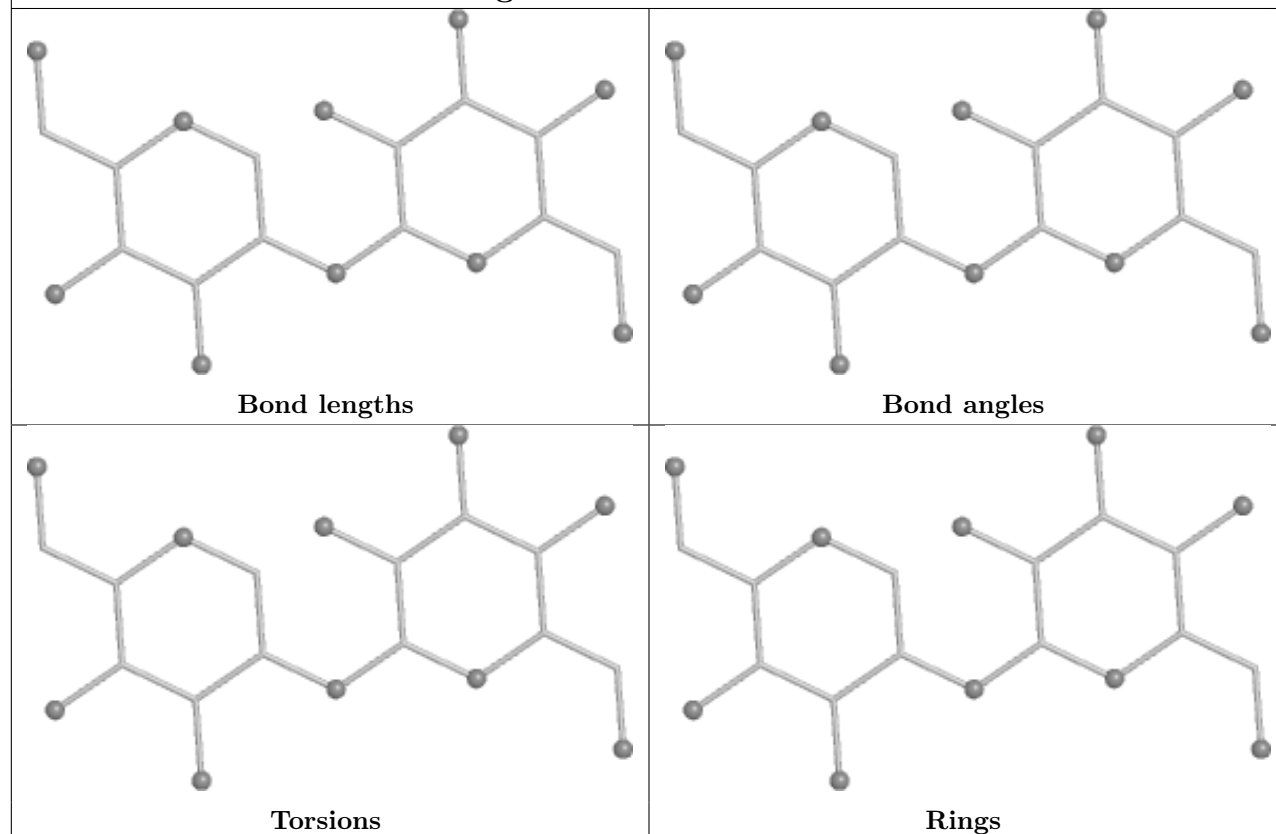
Oligosaccharide Chain Va

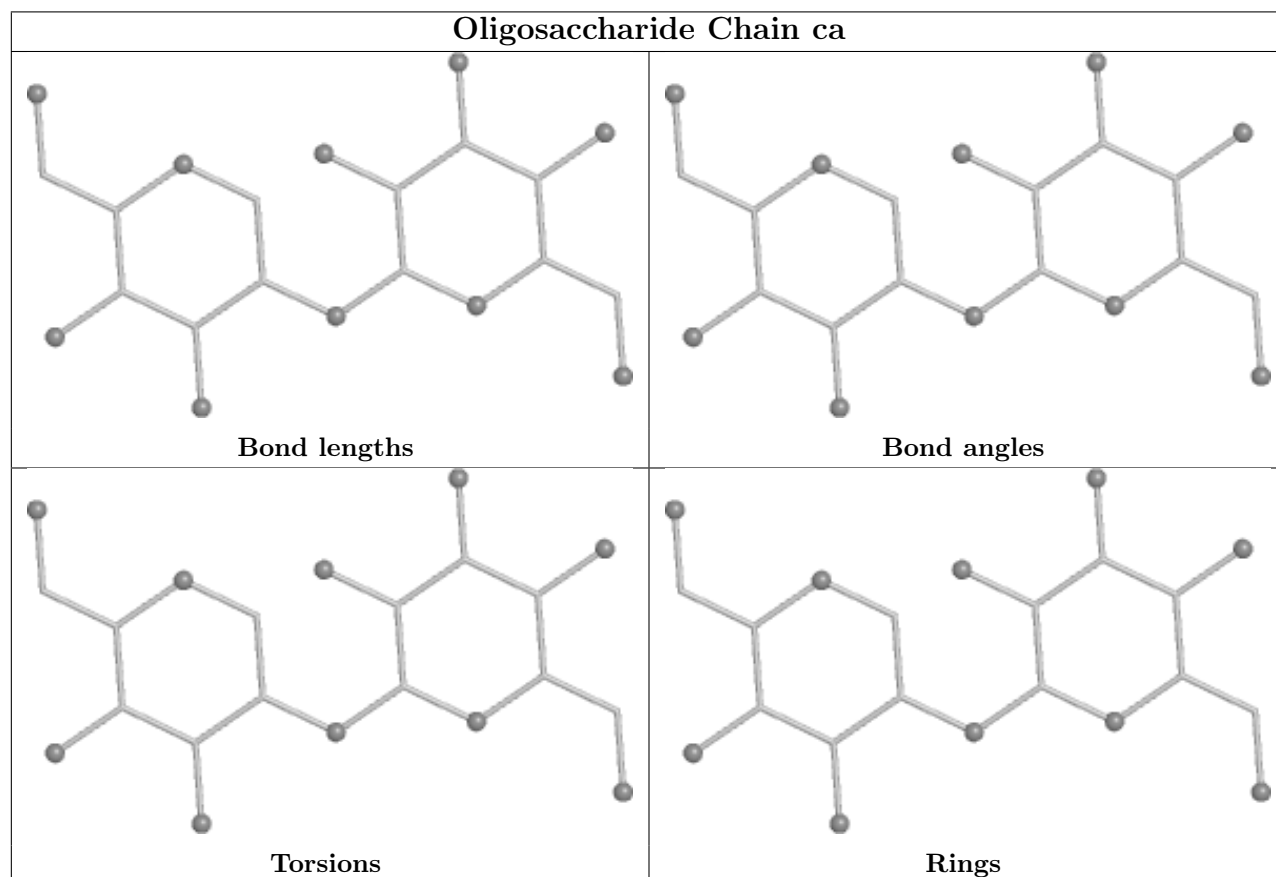
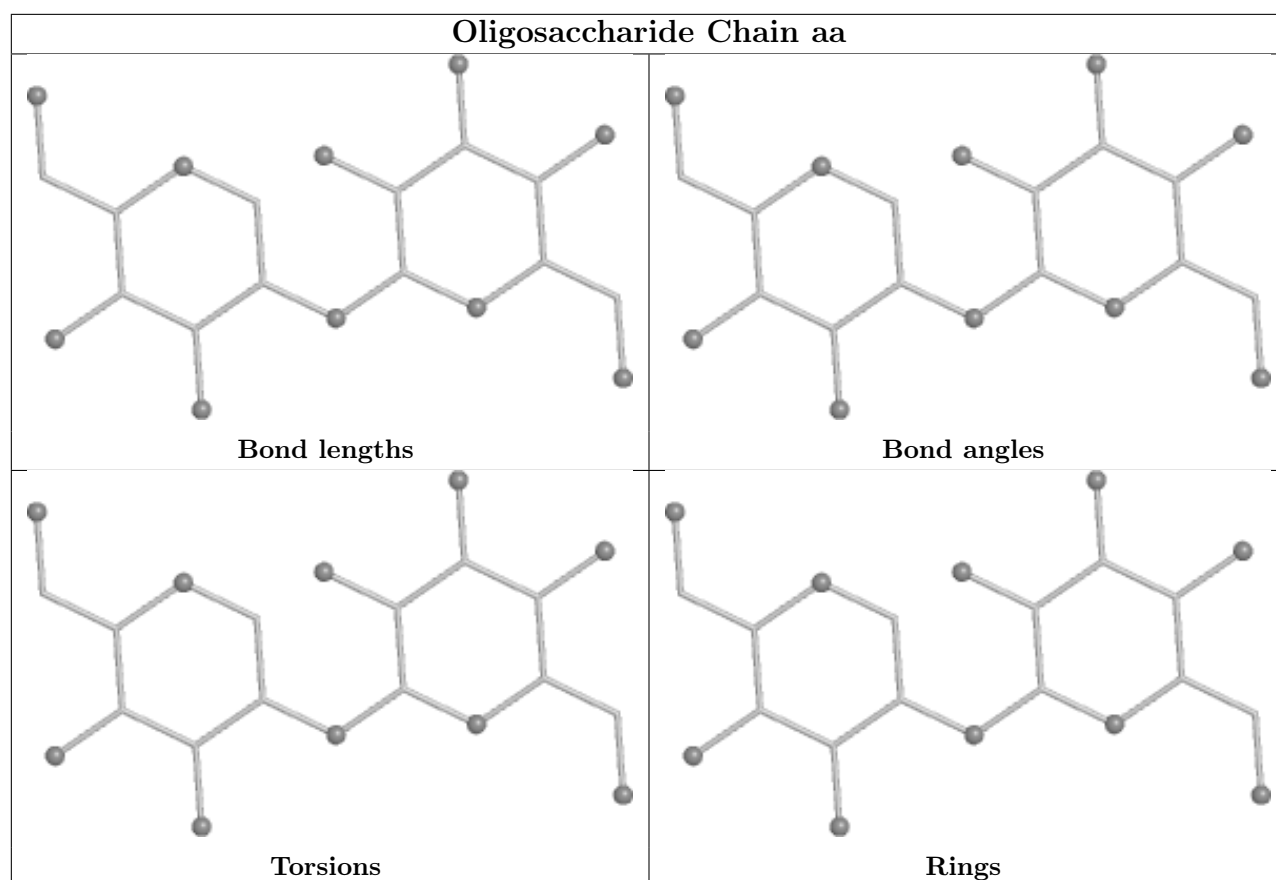


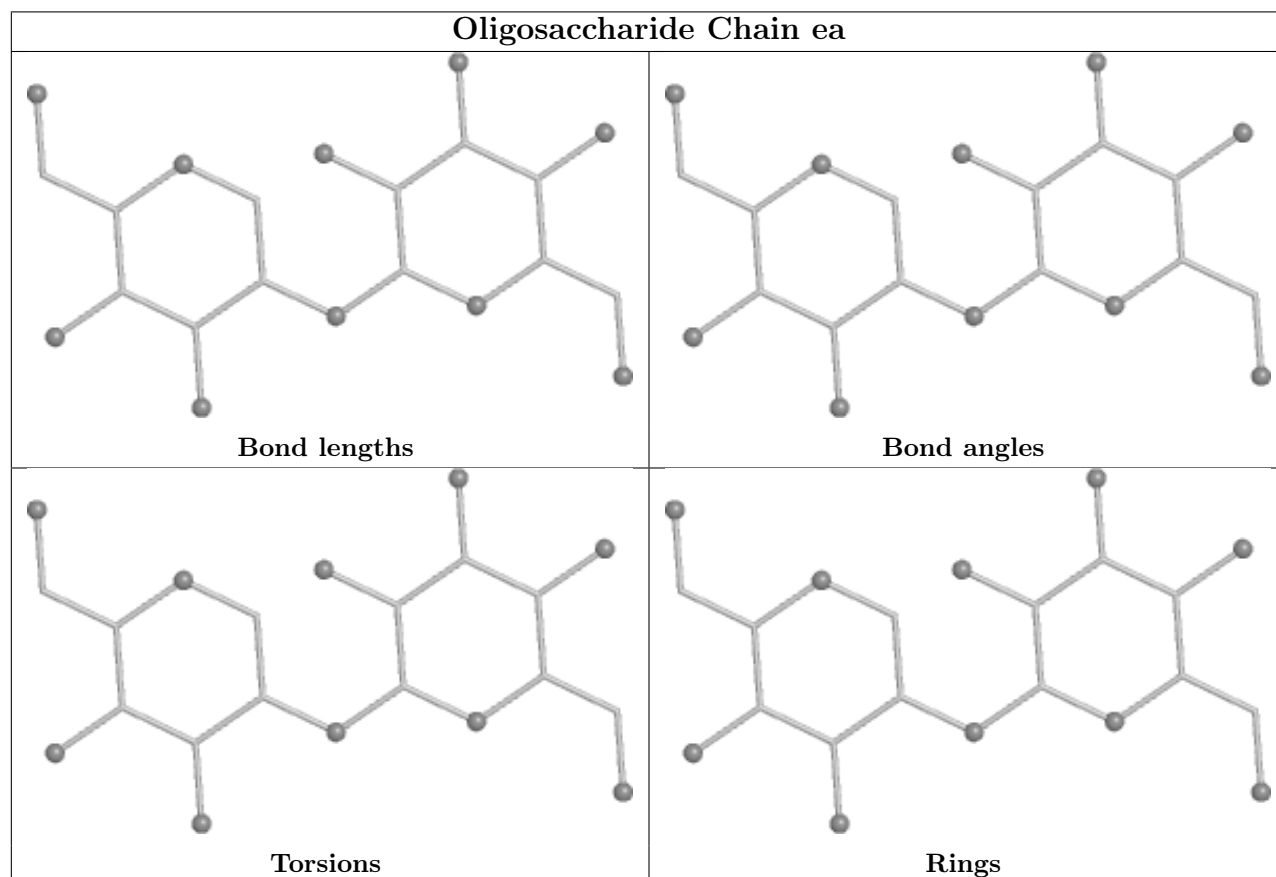
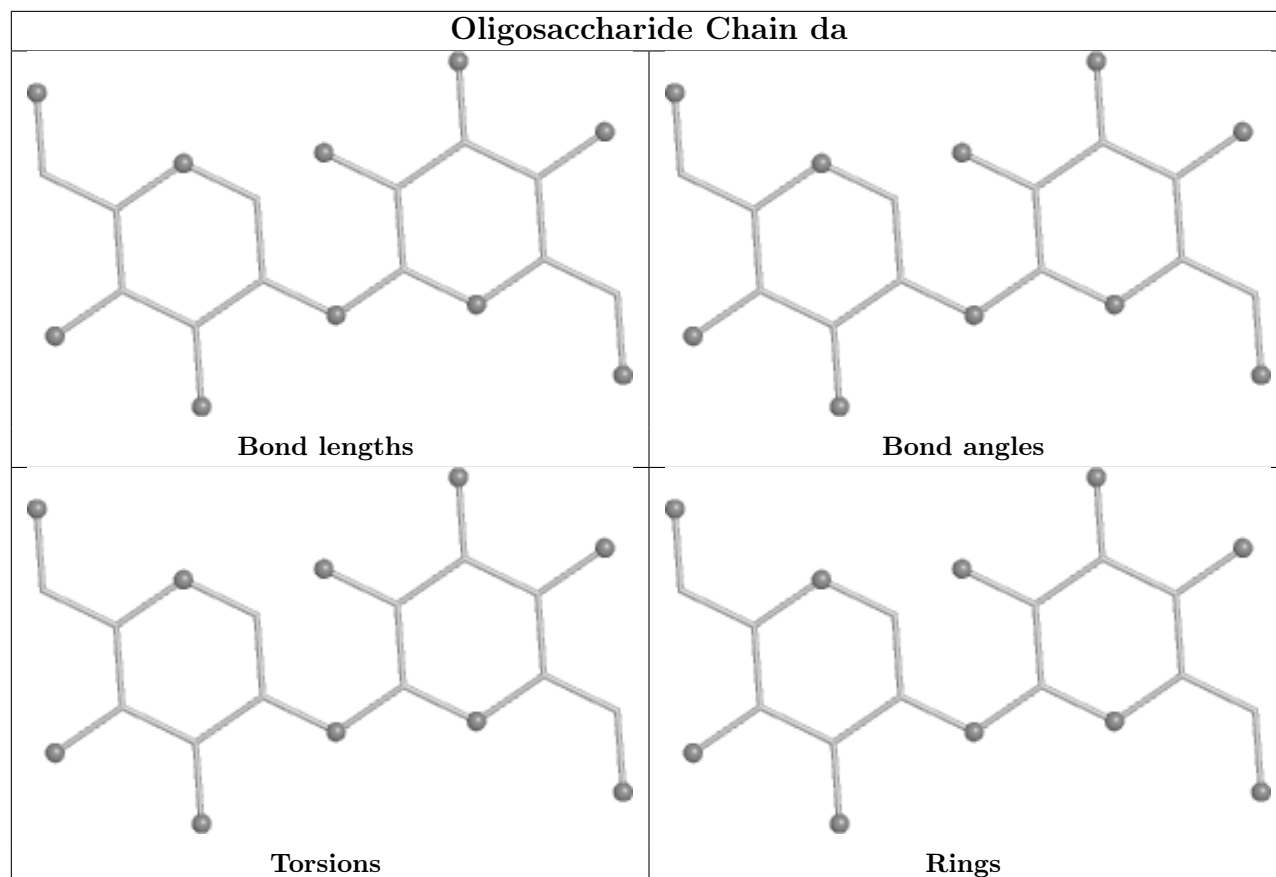
Oligosaccharide Chain Ya

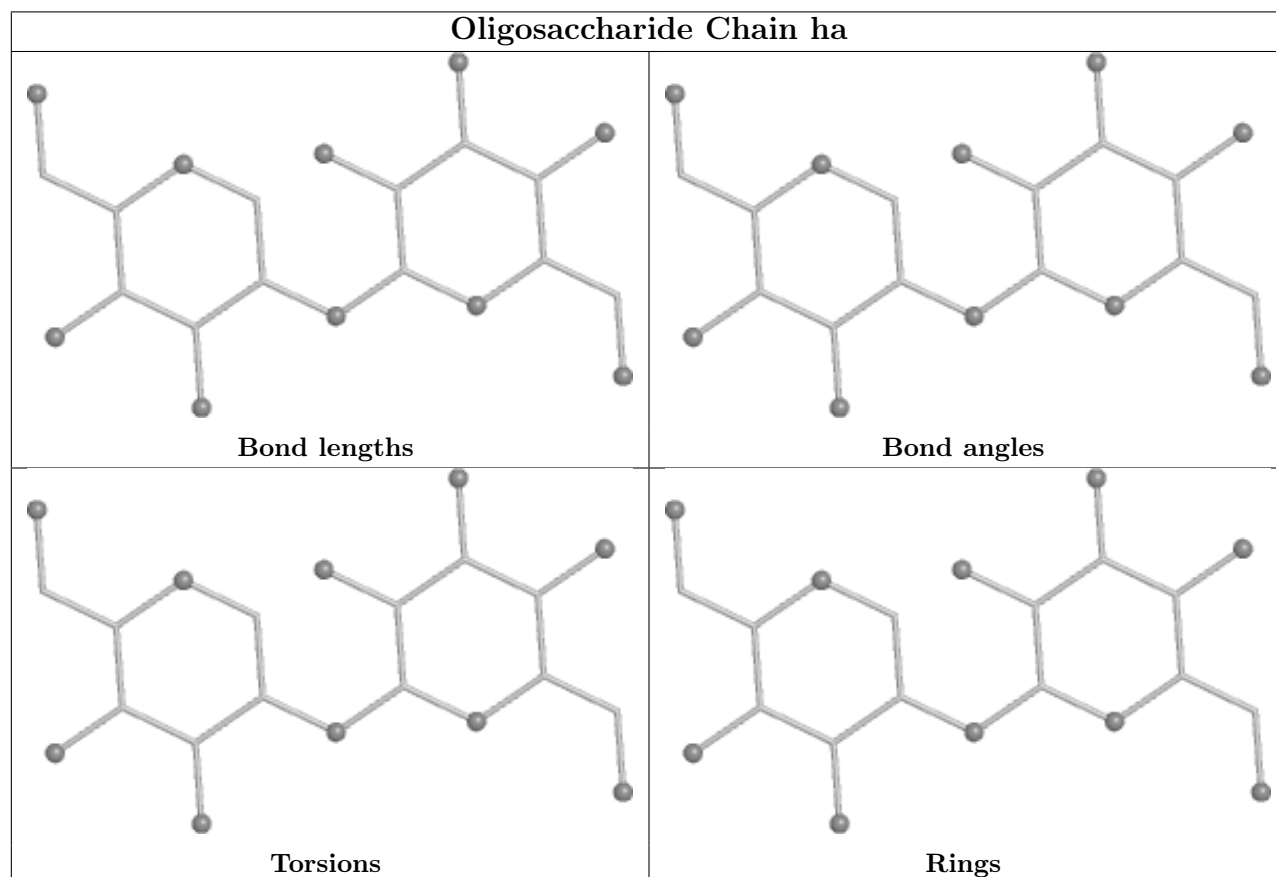
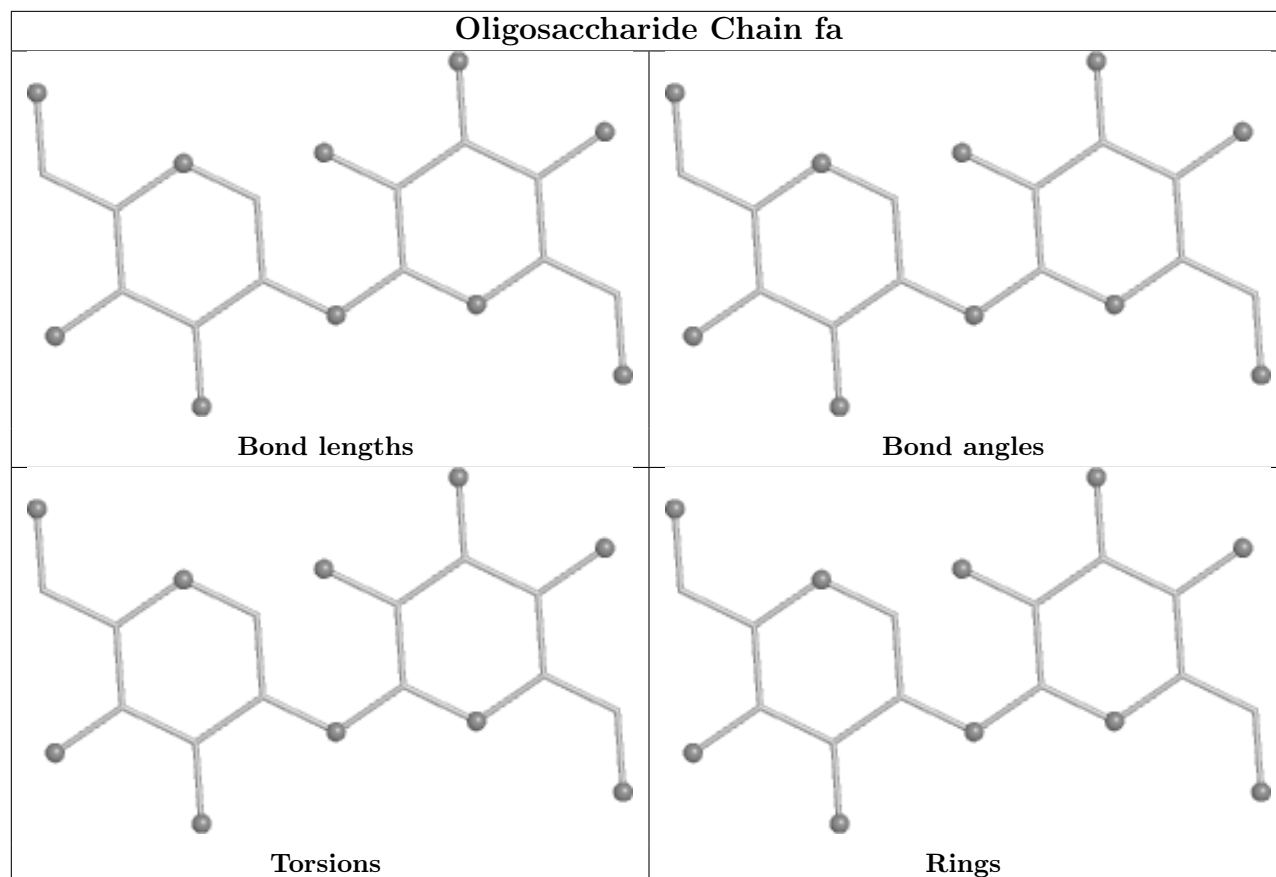


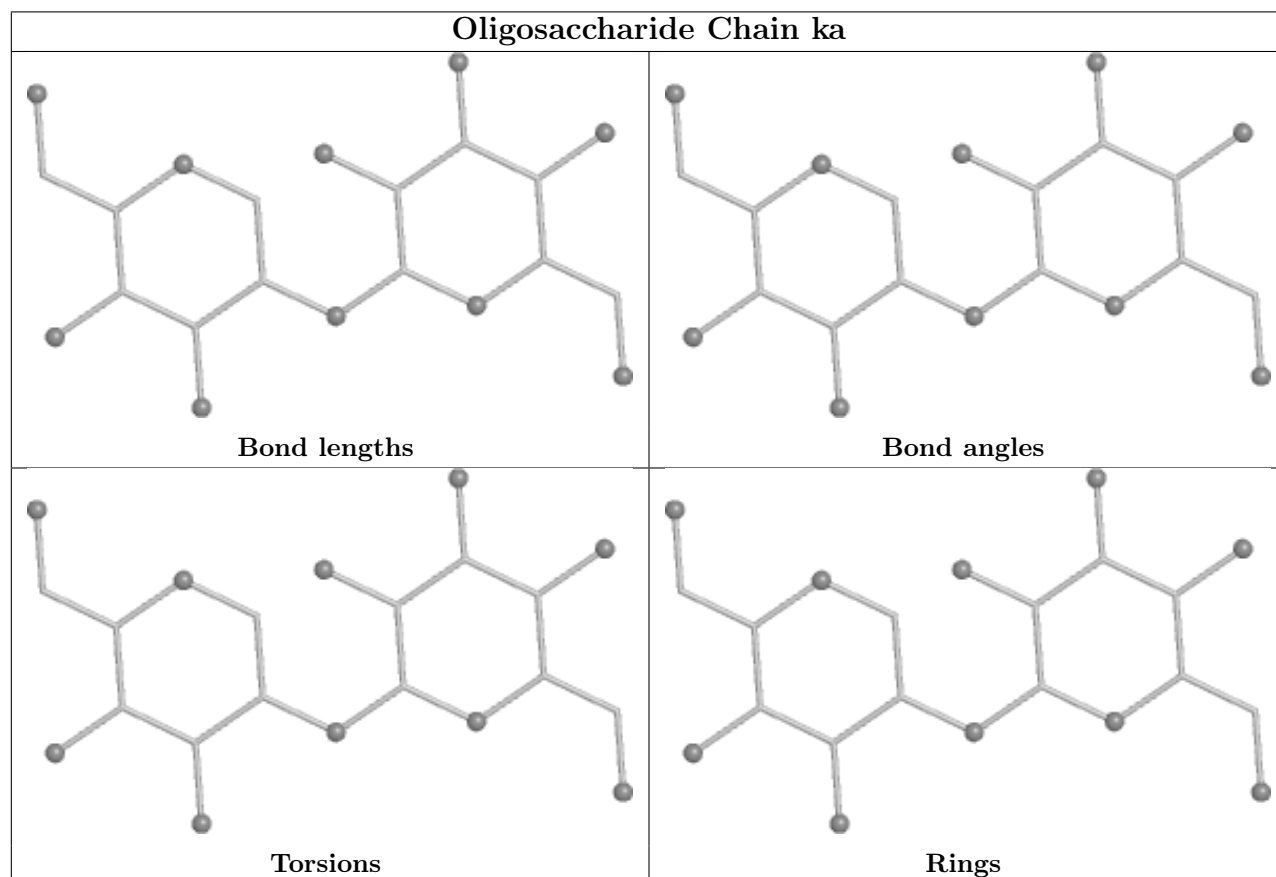
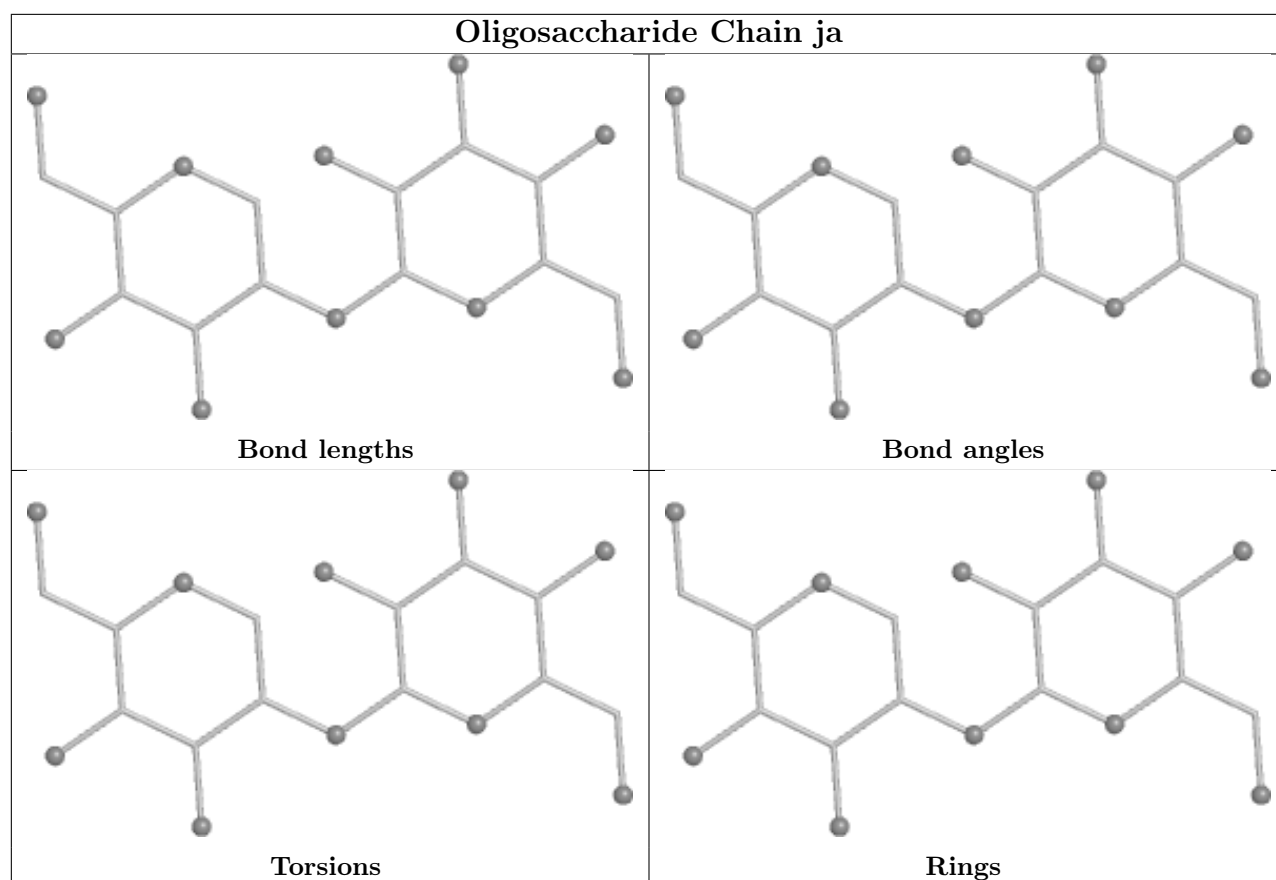
Oligosaccharide Chain Za

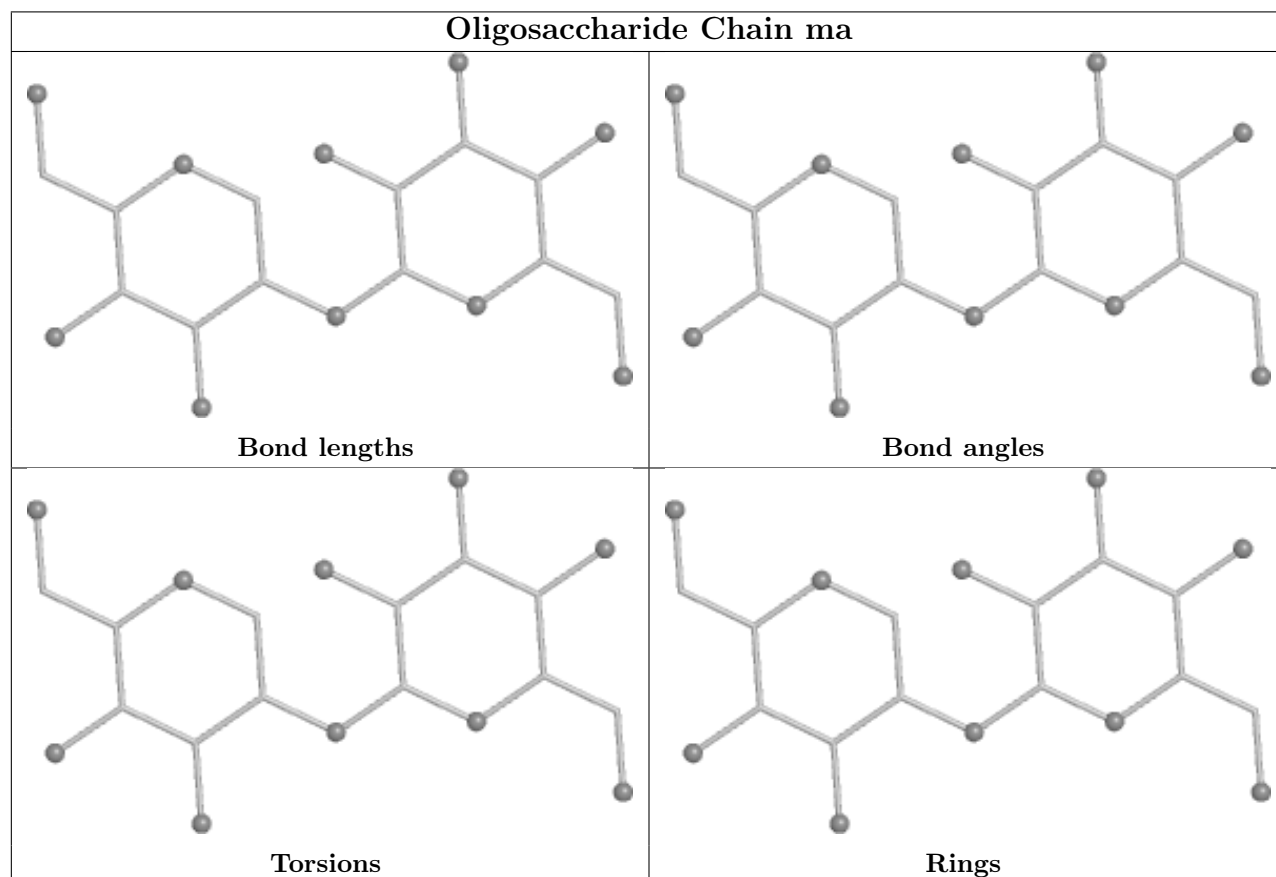
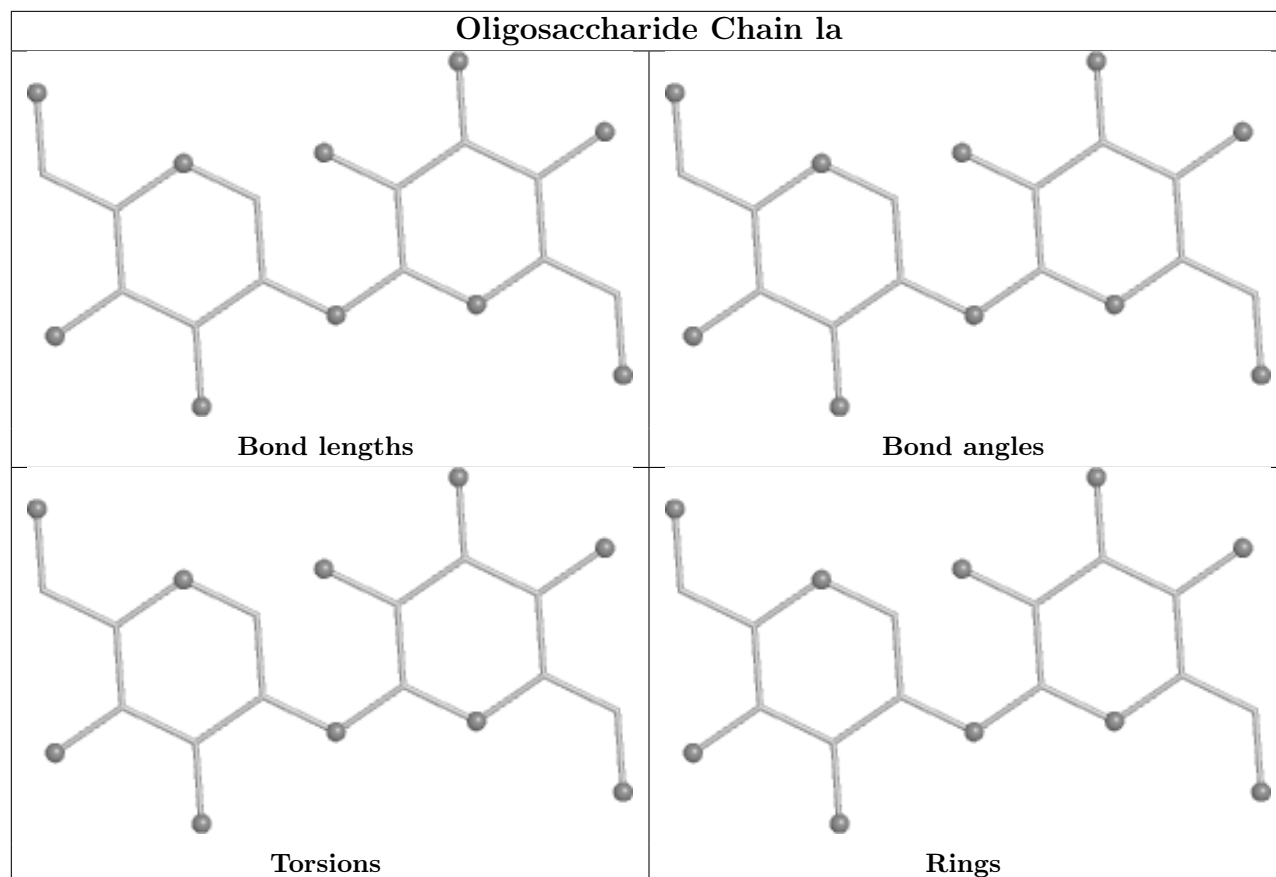


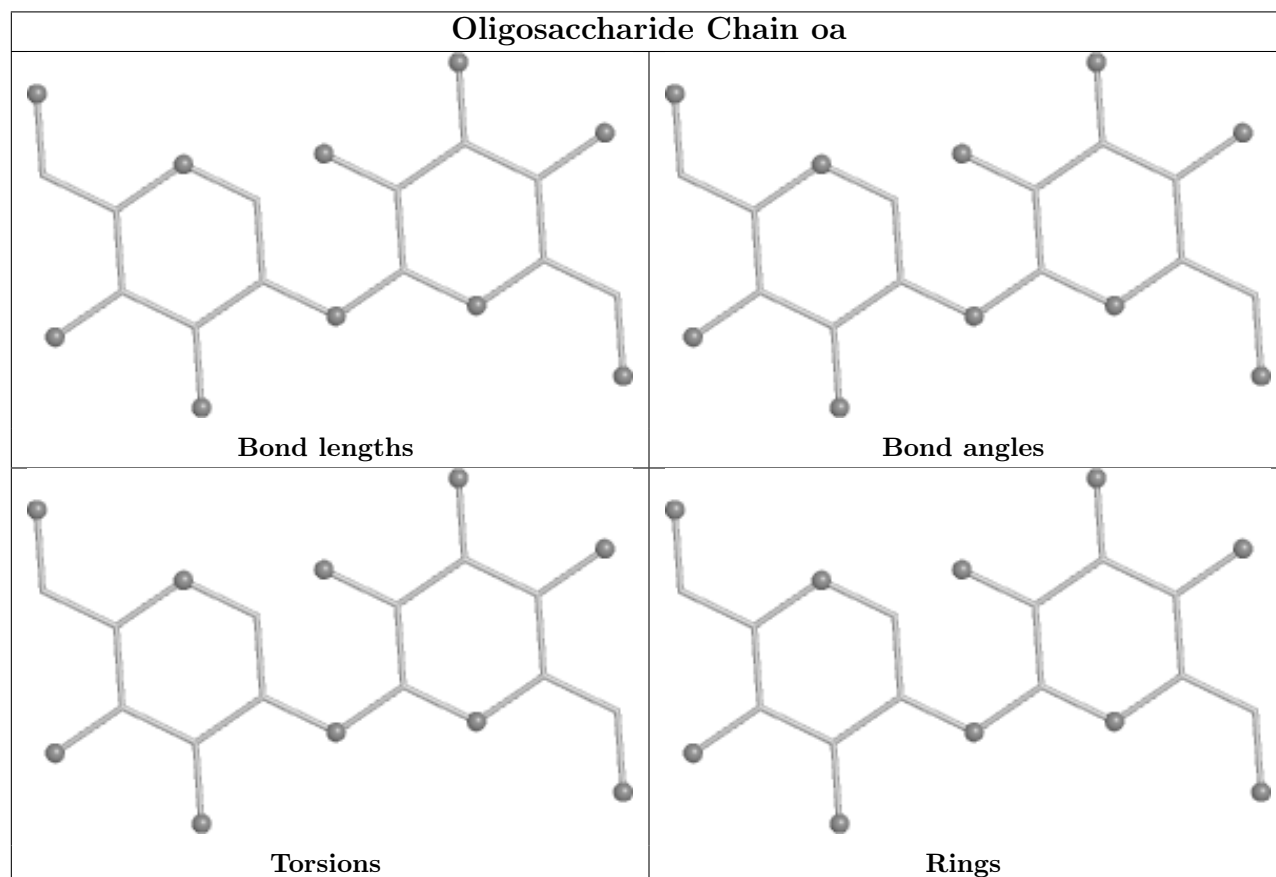
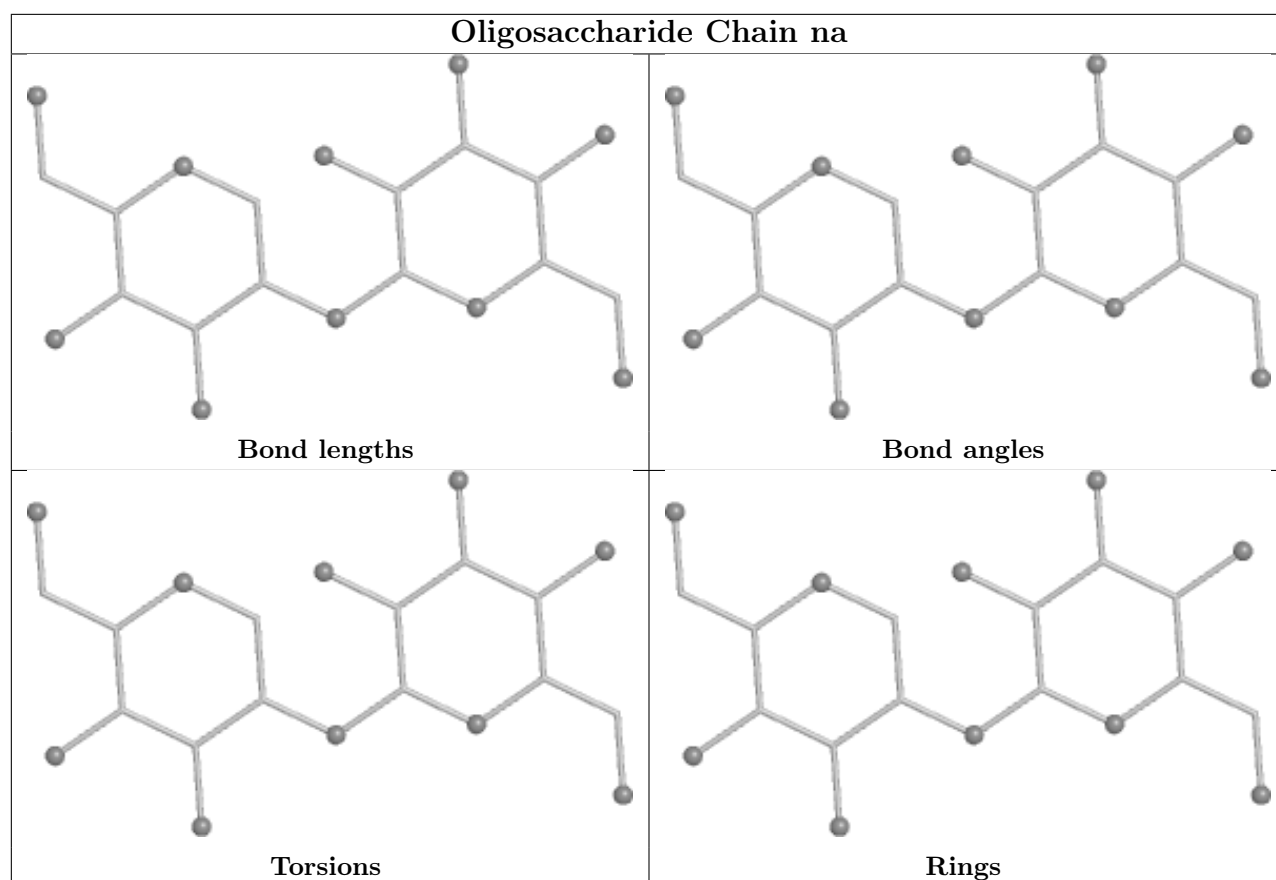


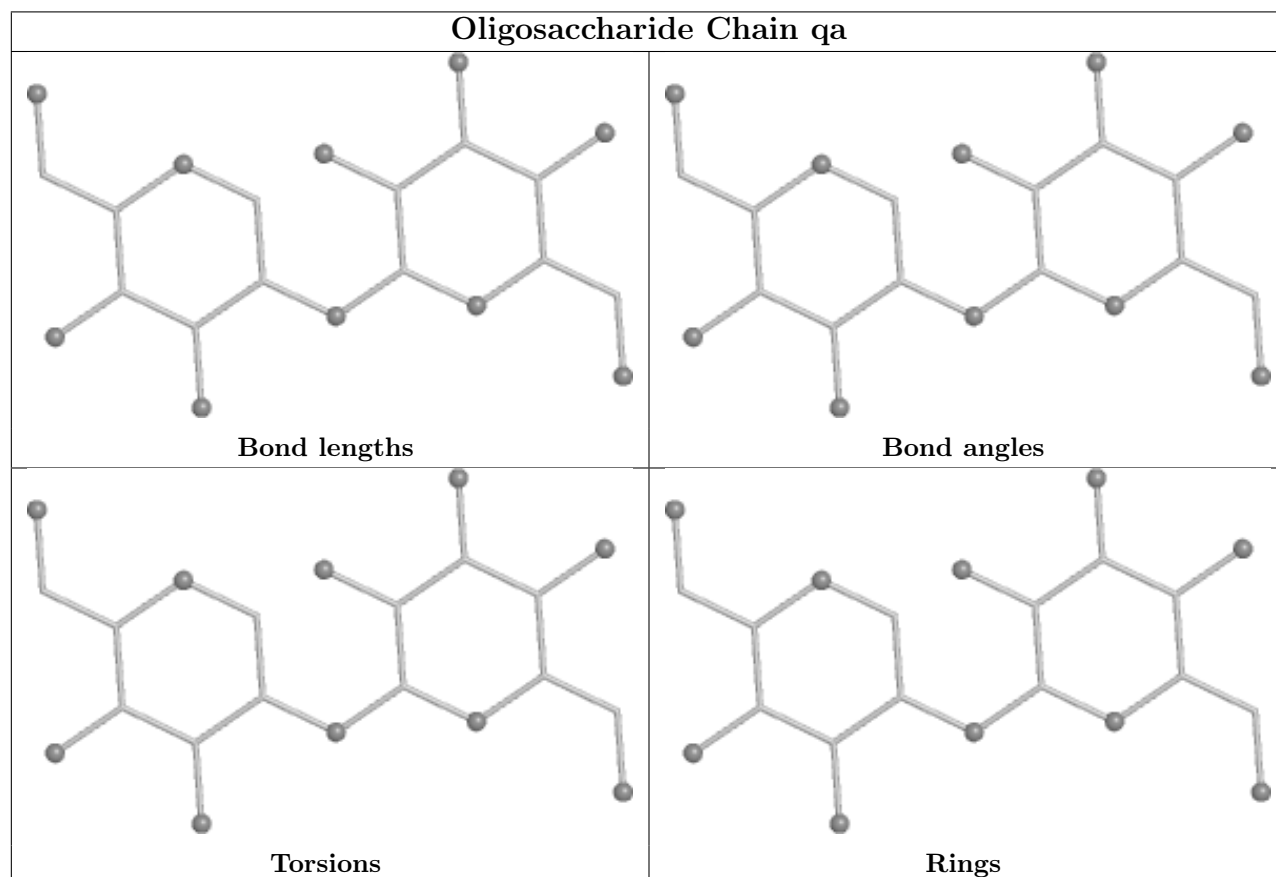
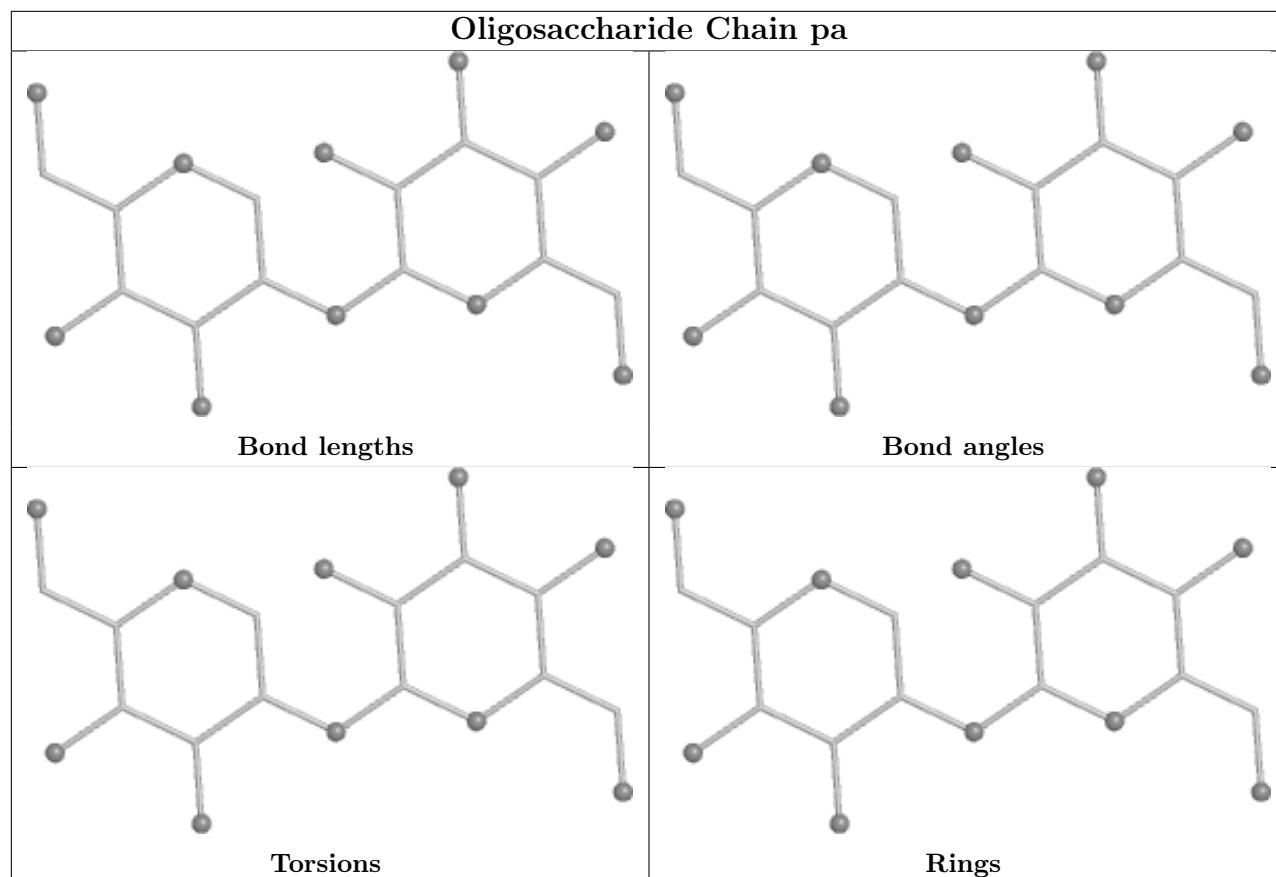


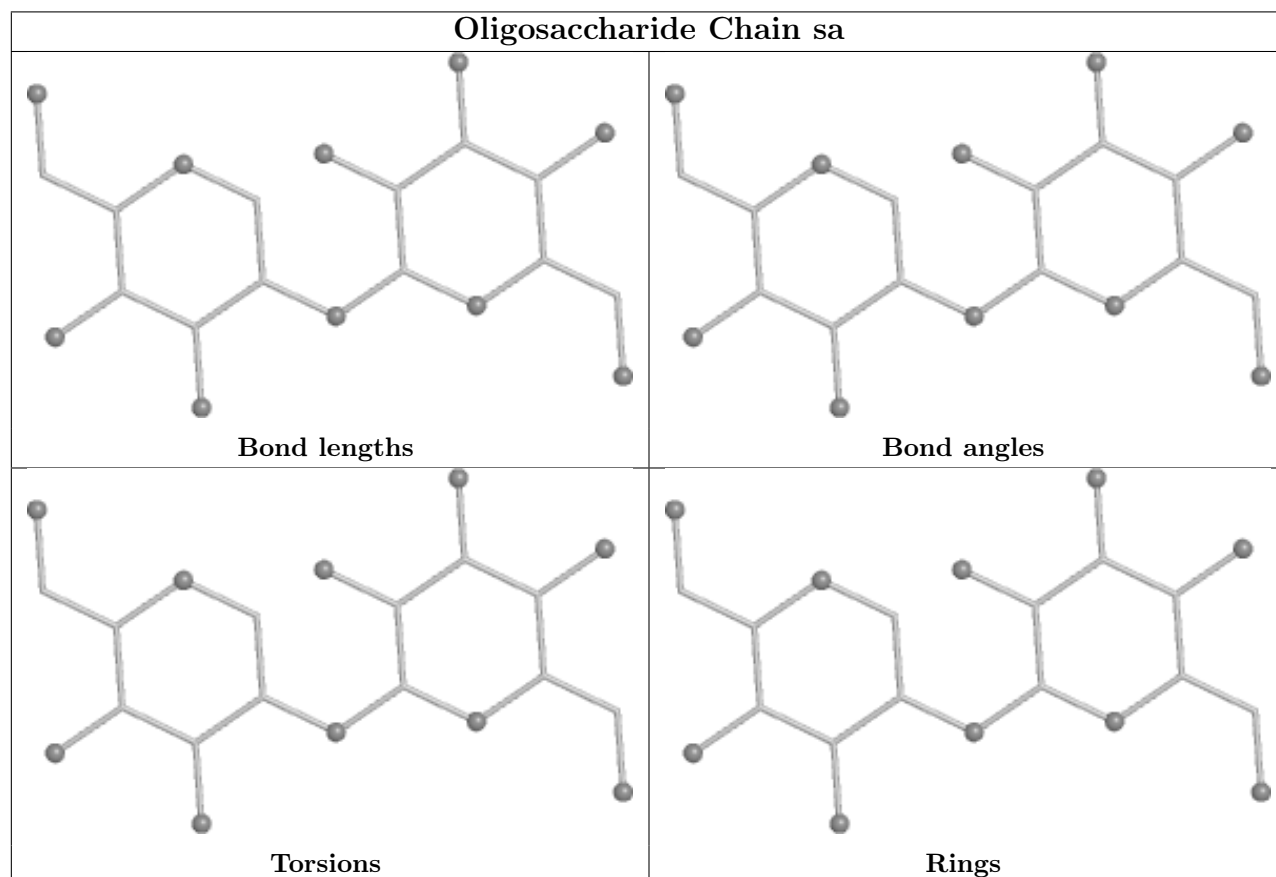
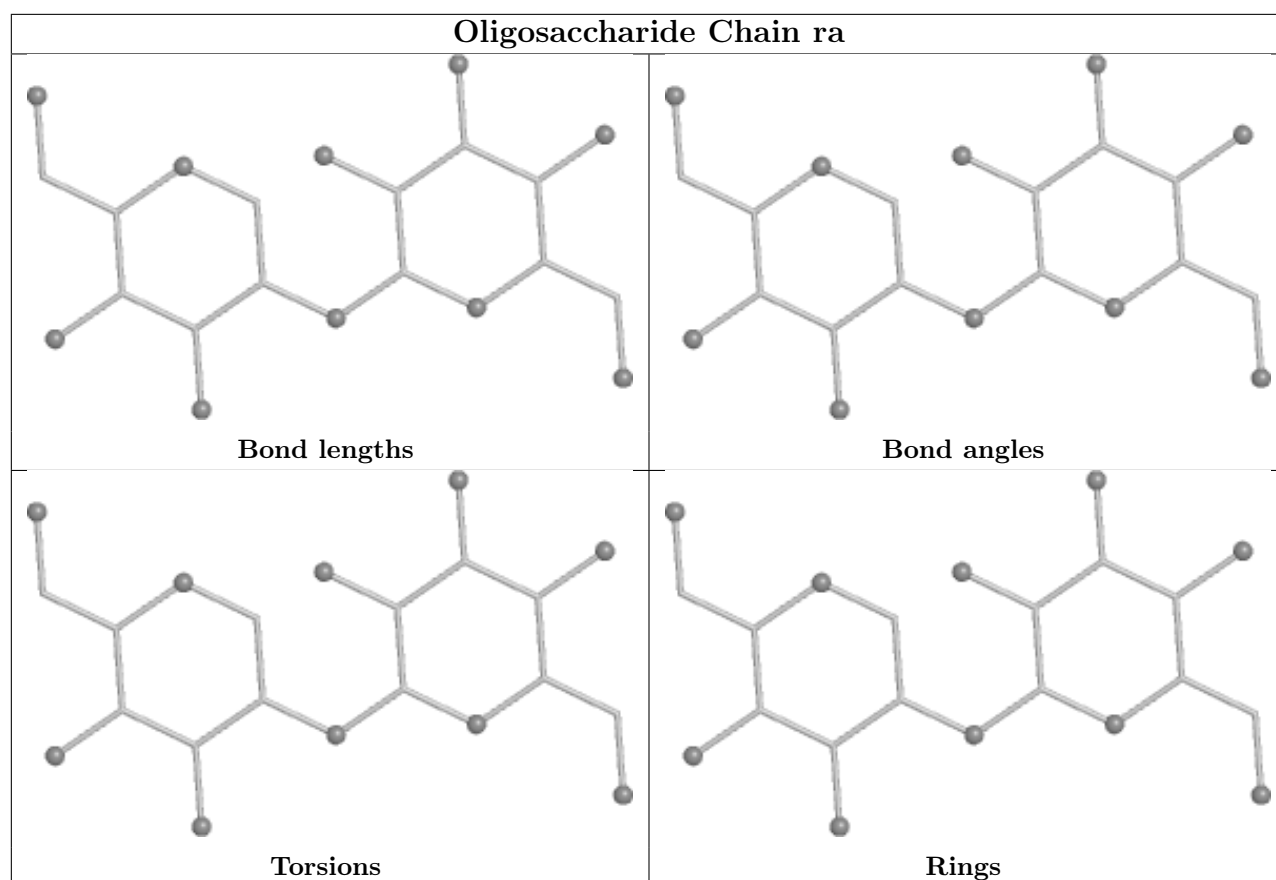


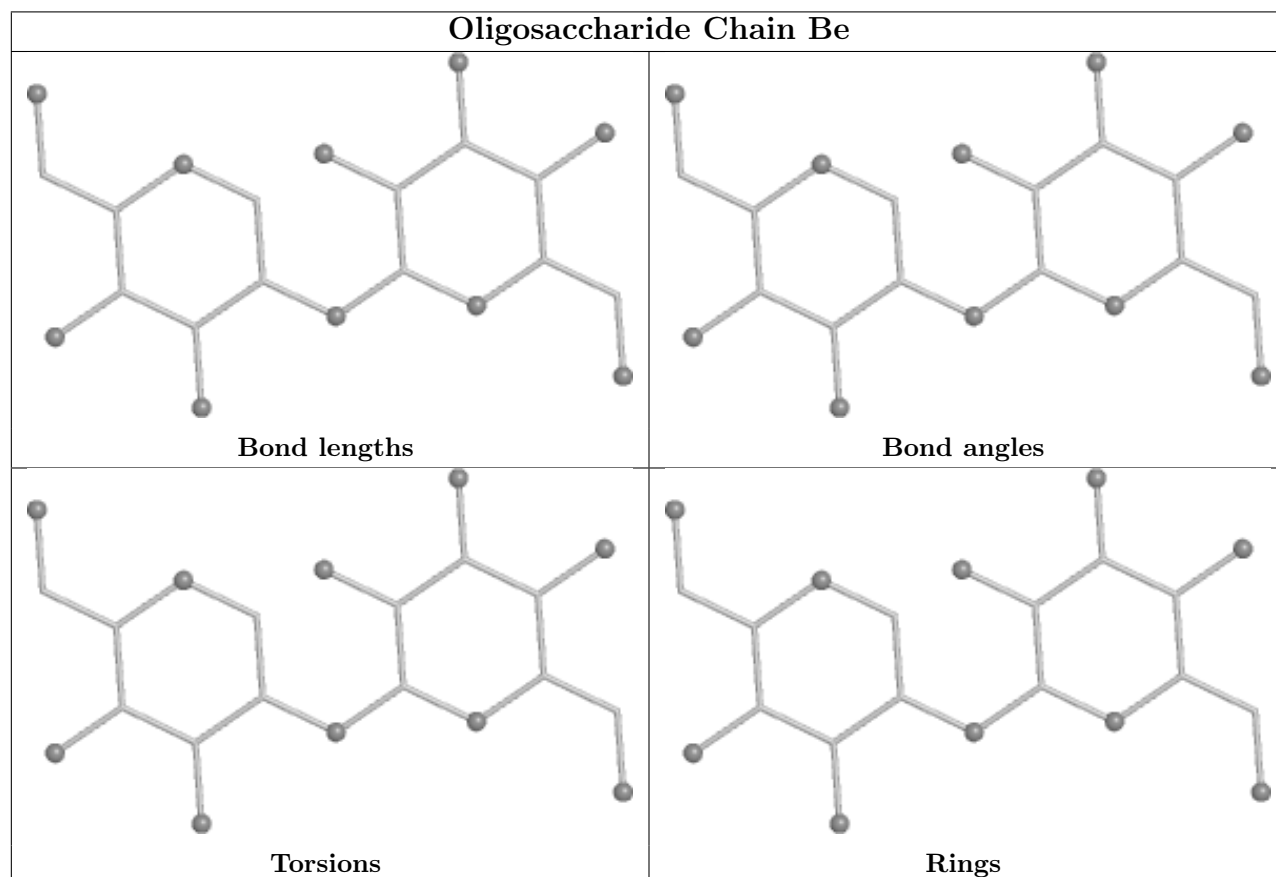
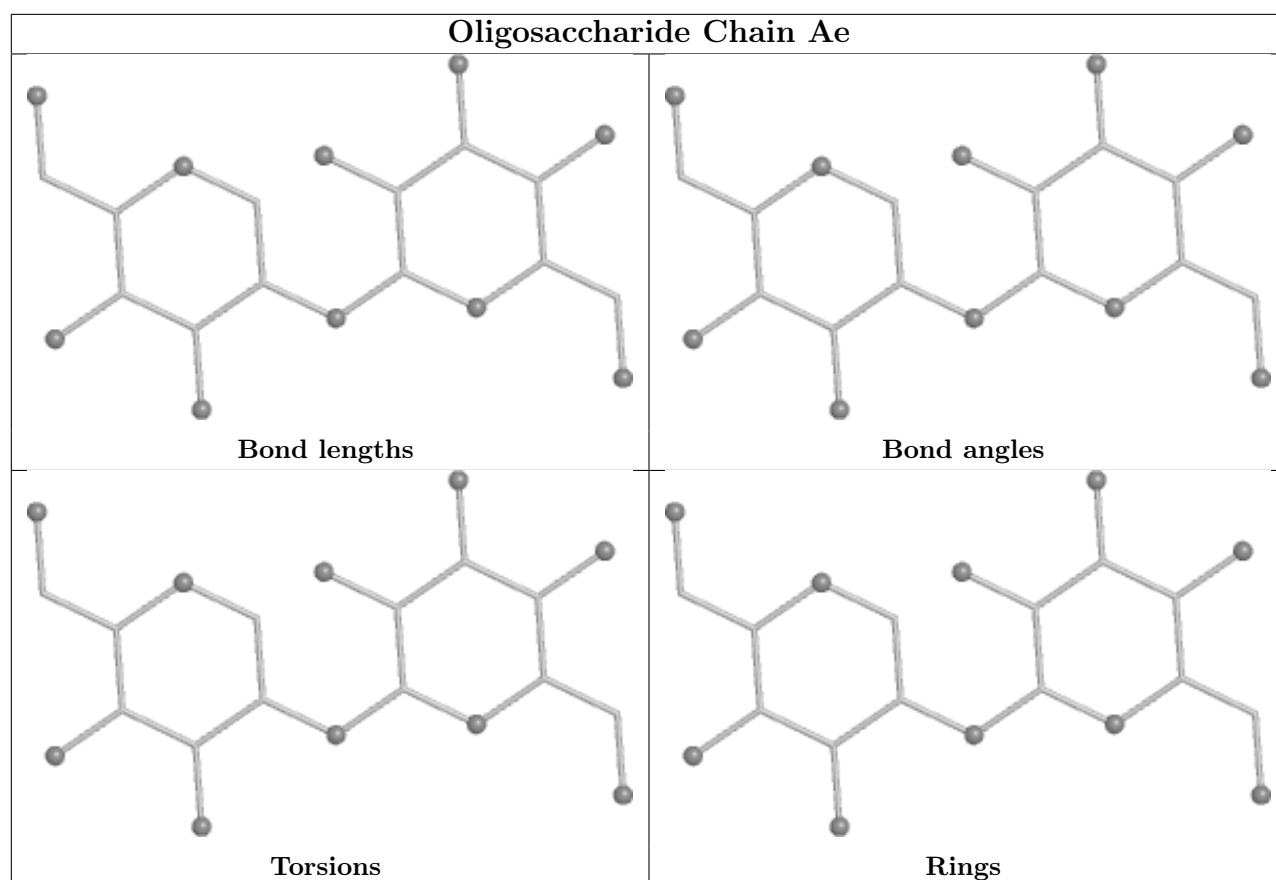


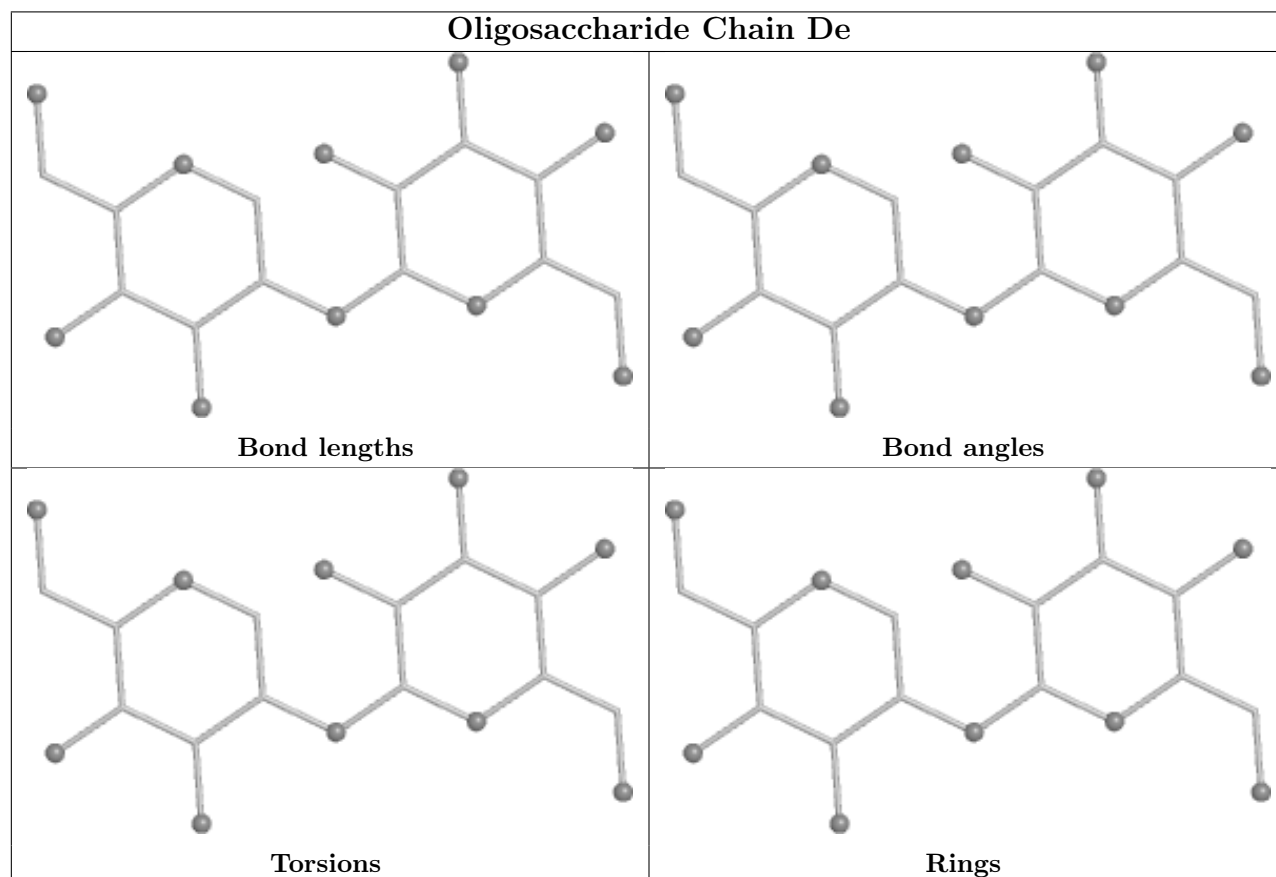
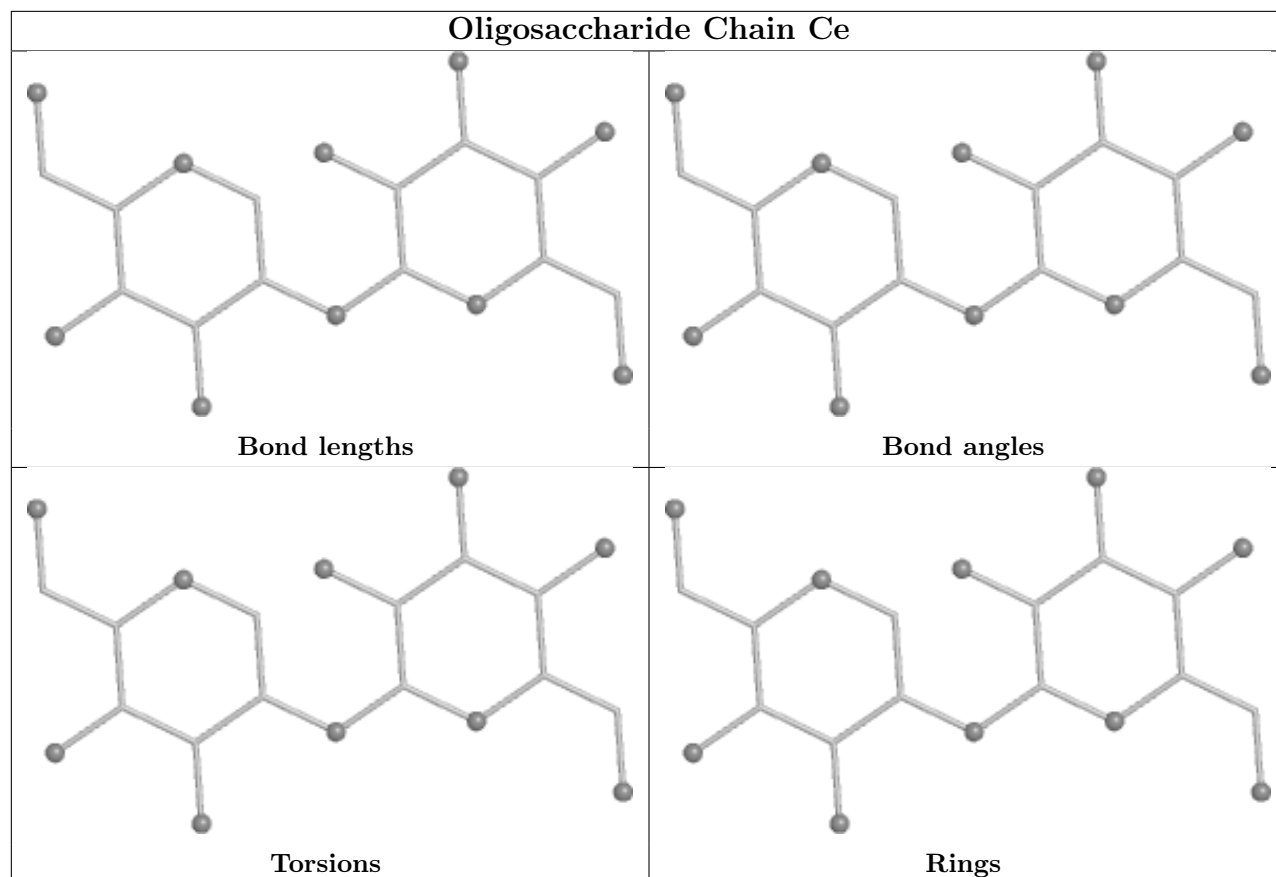


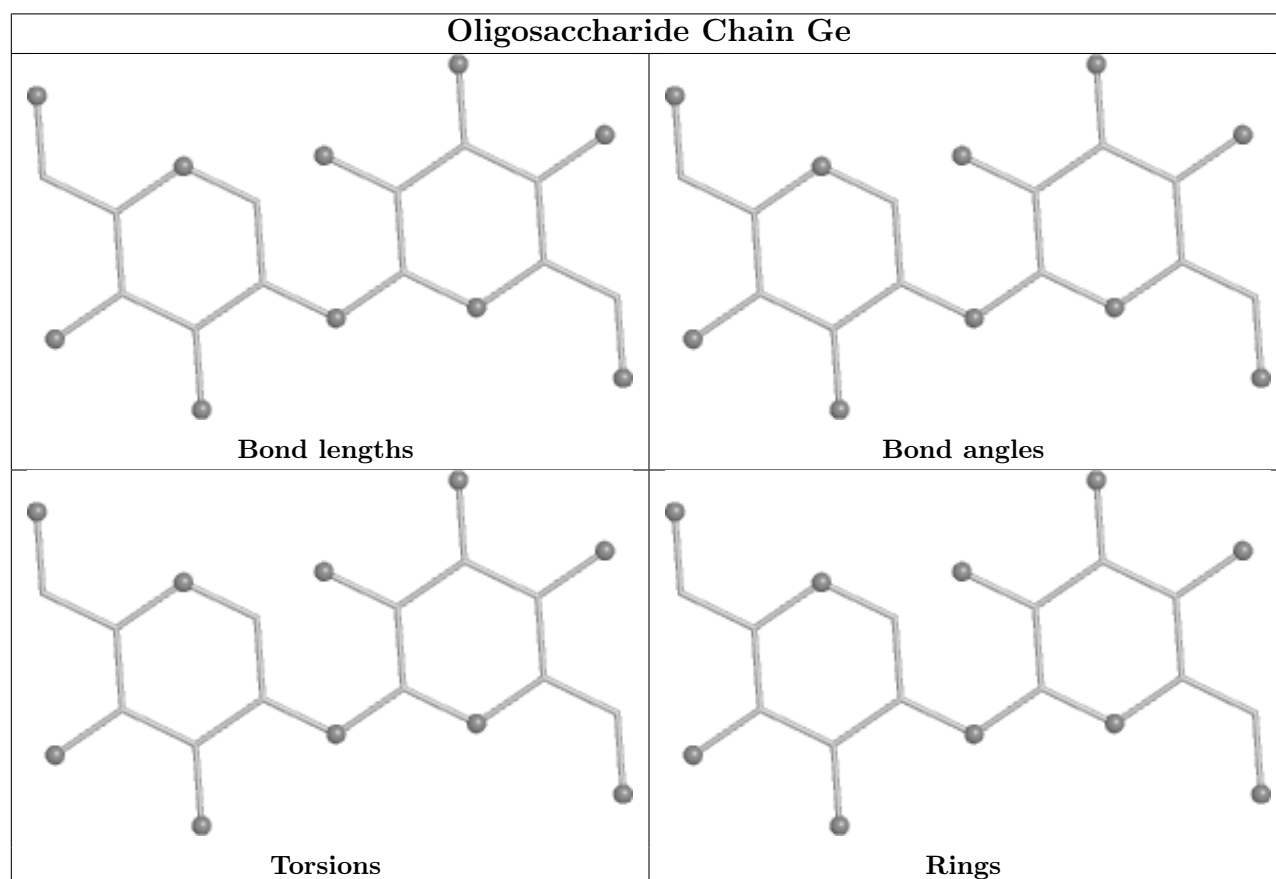
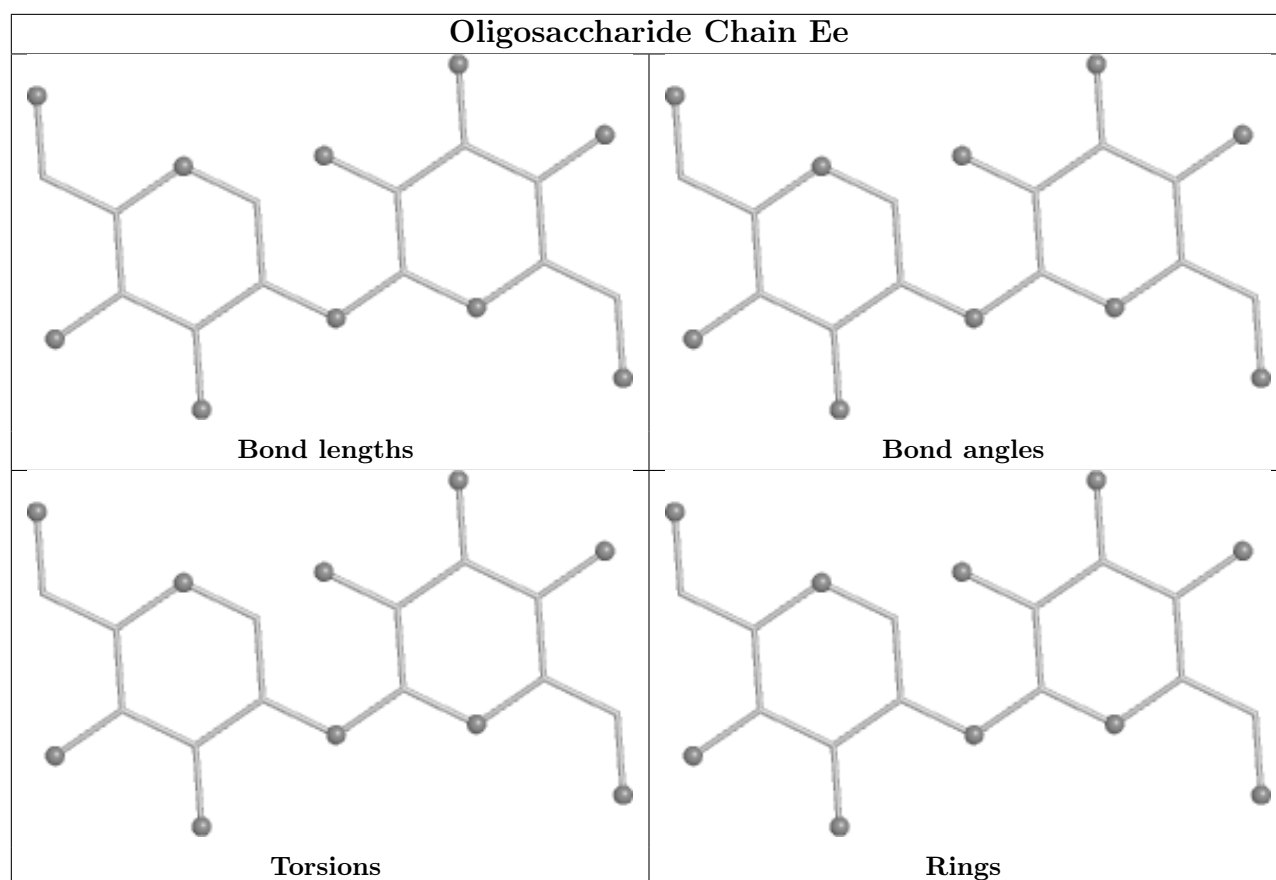




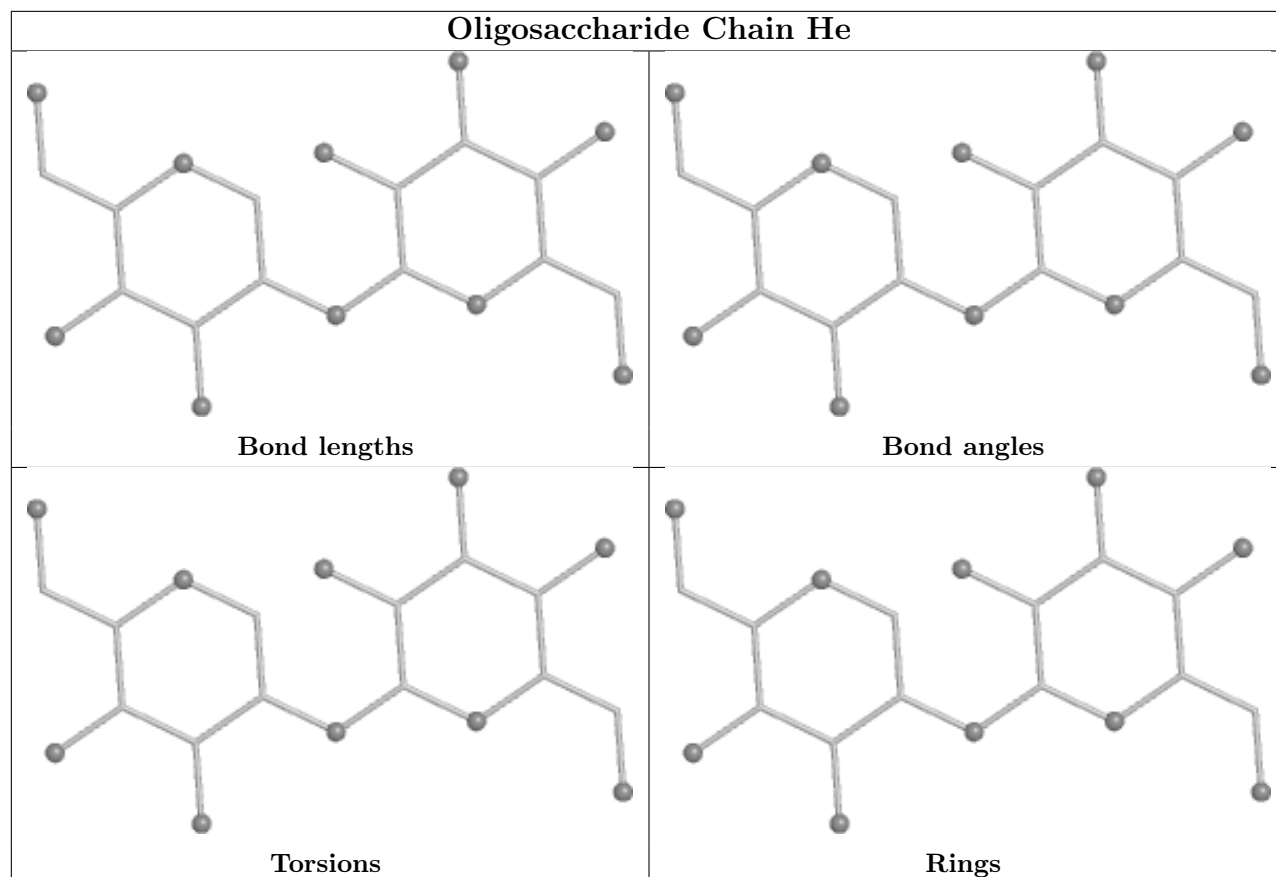




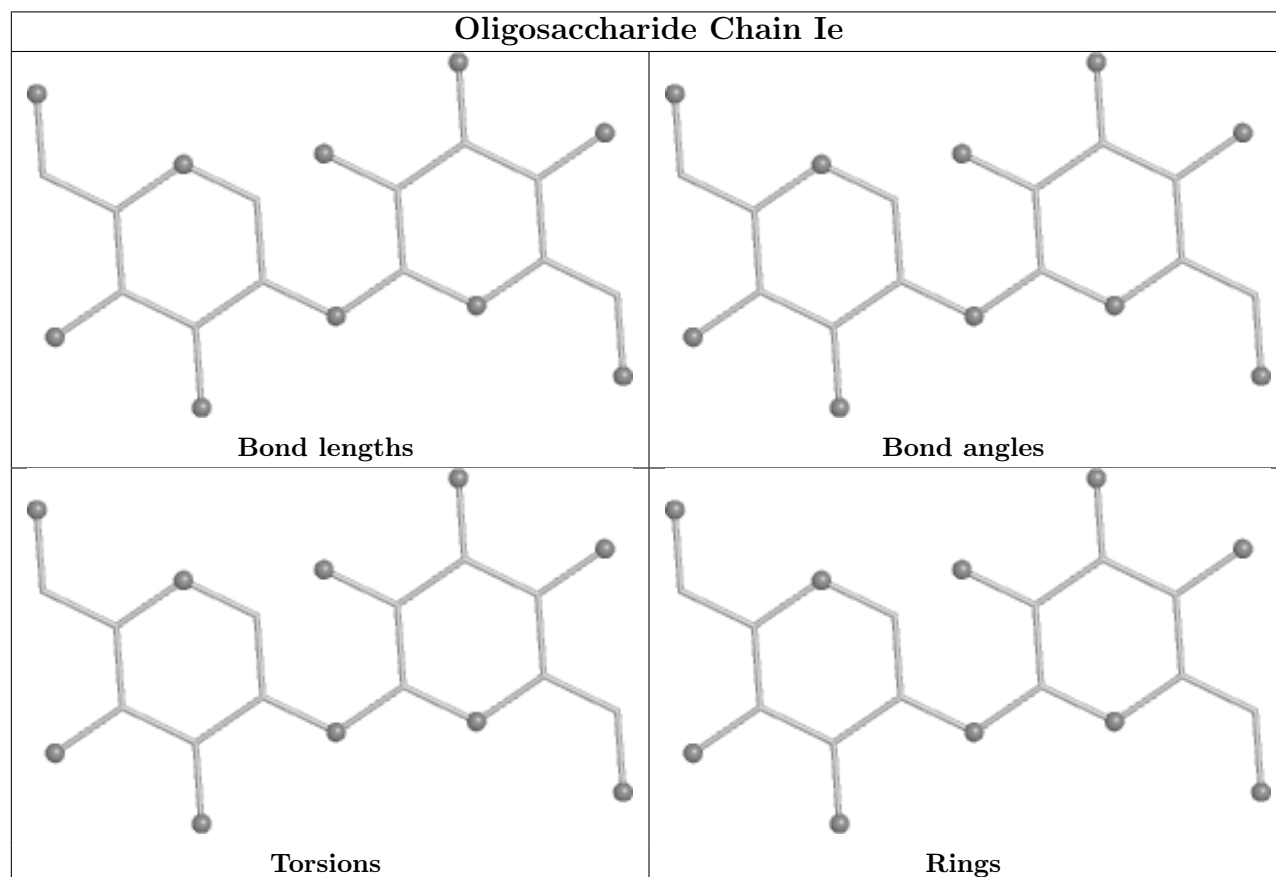


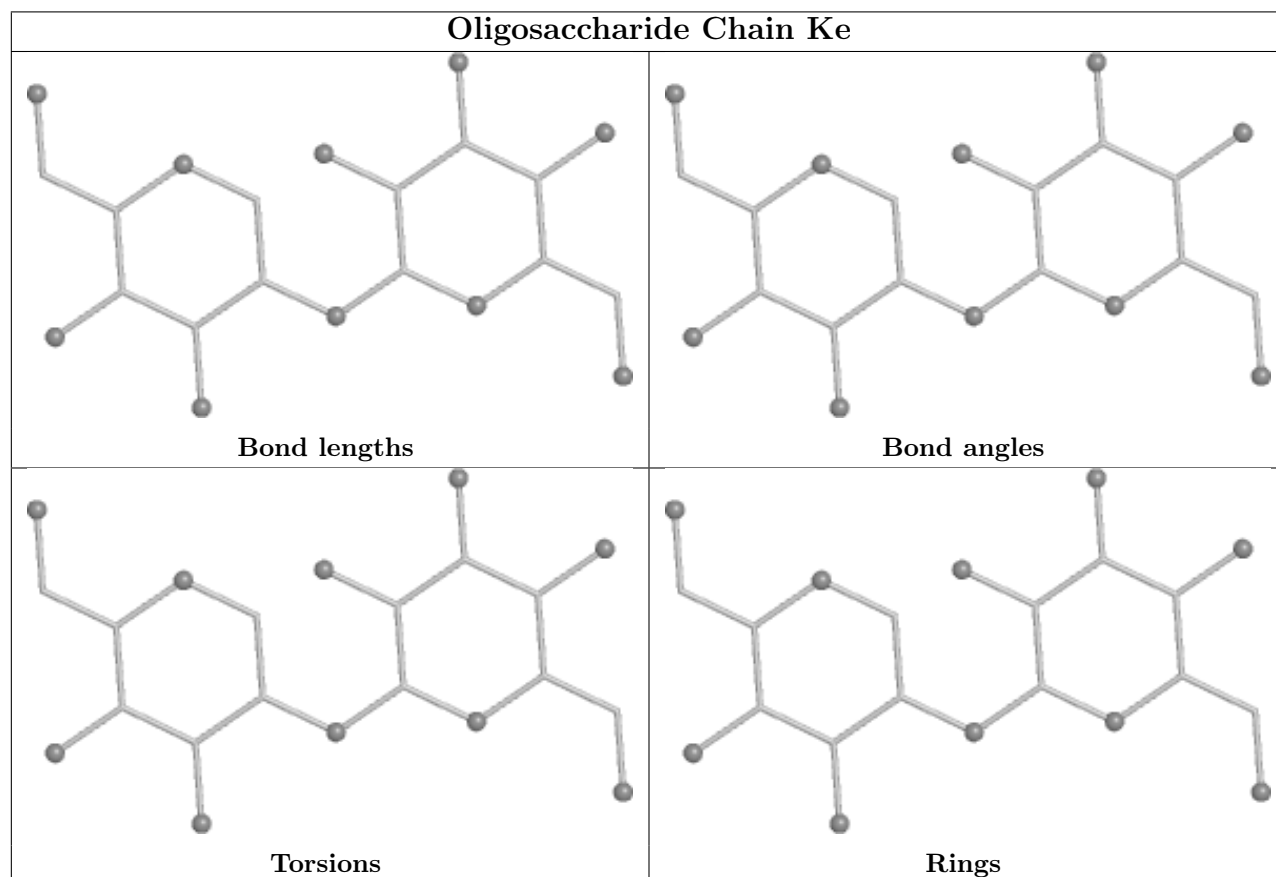
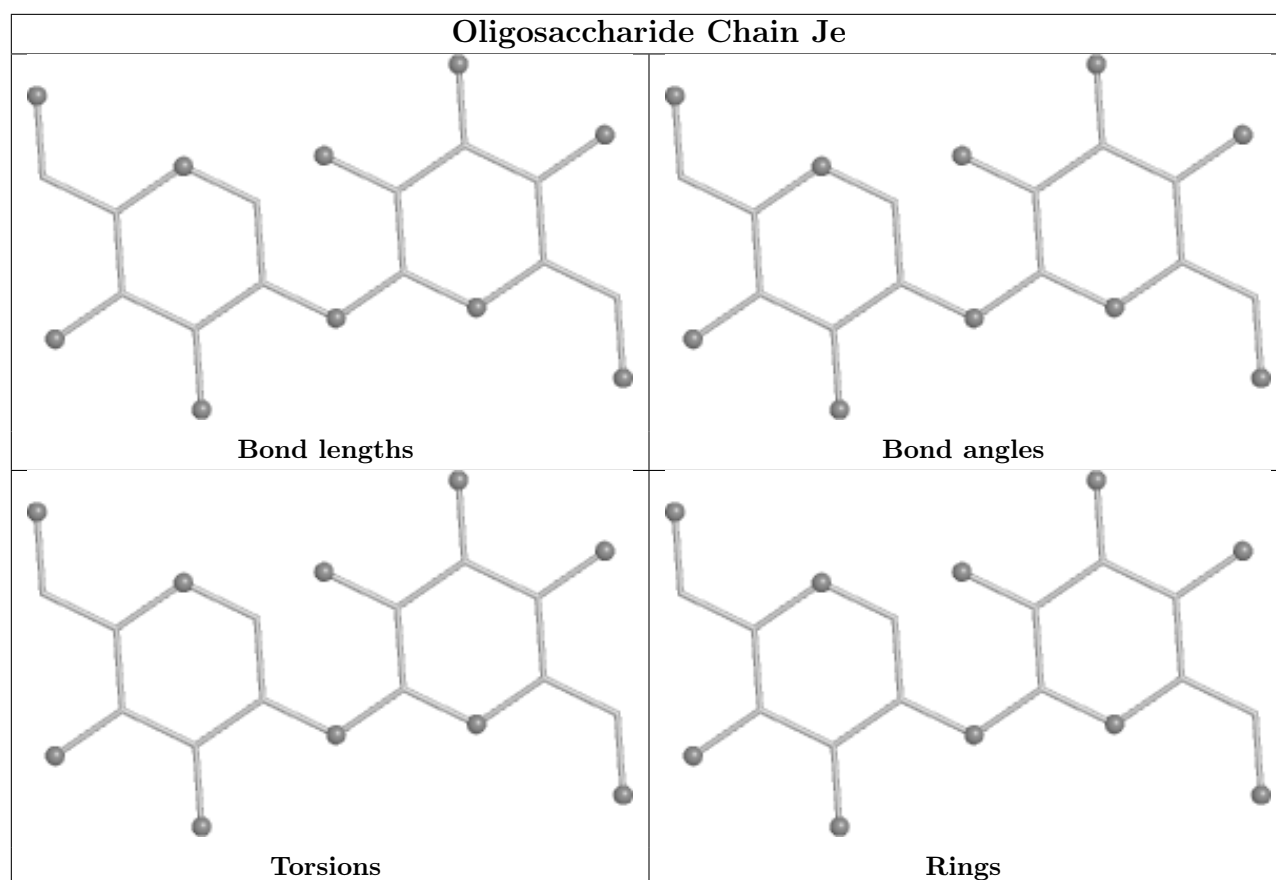


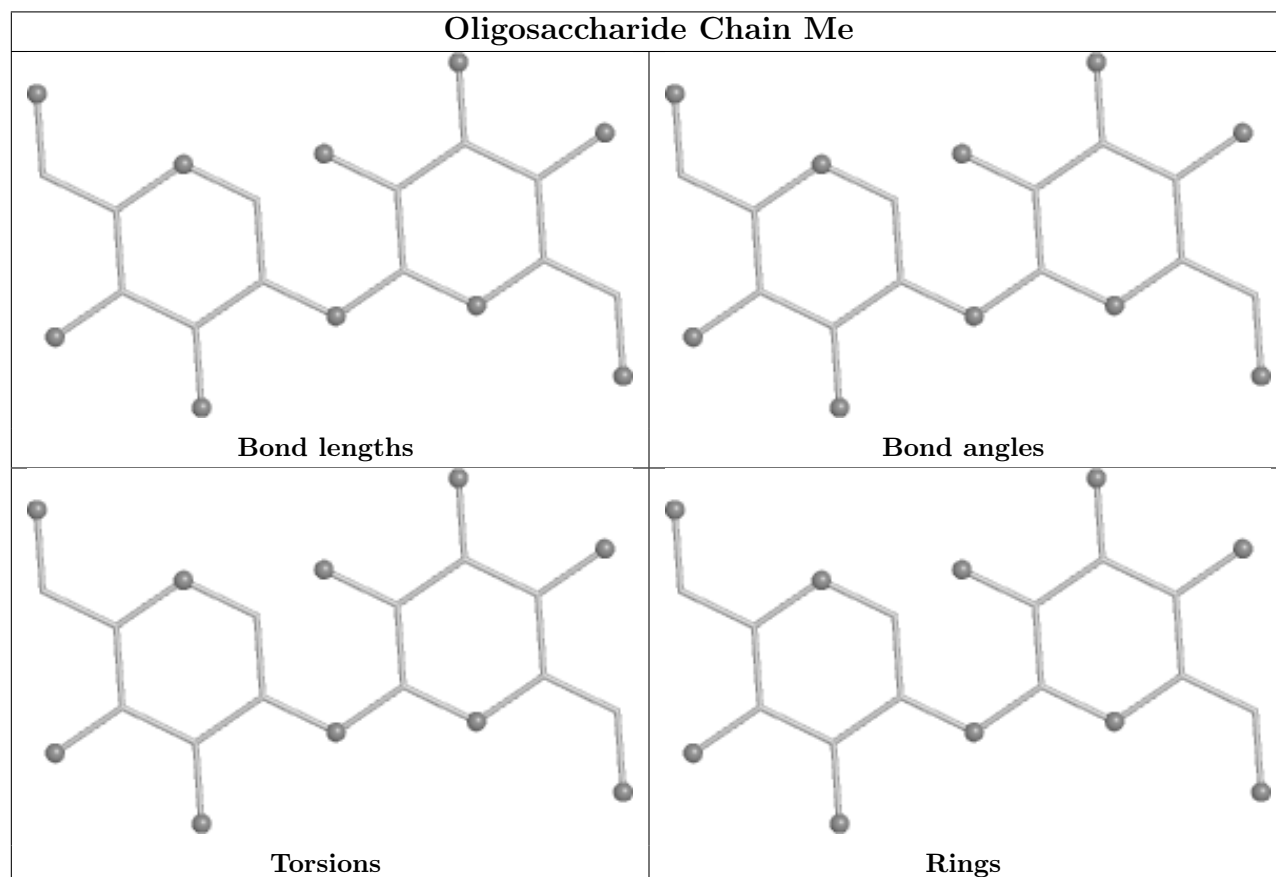
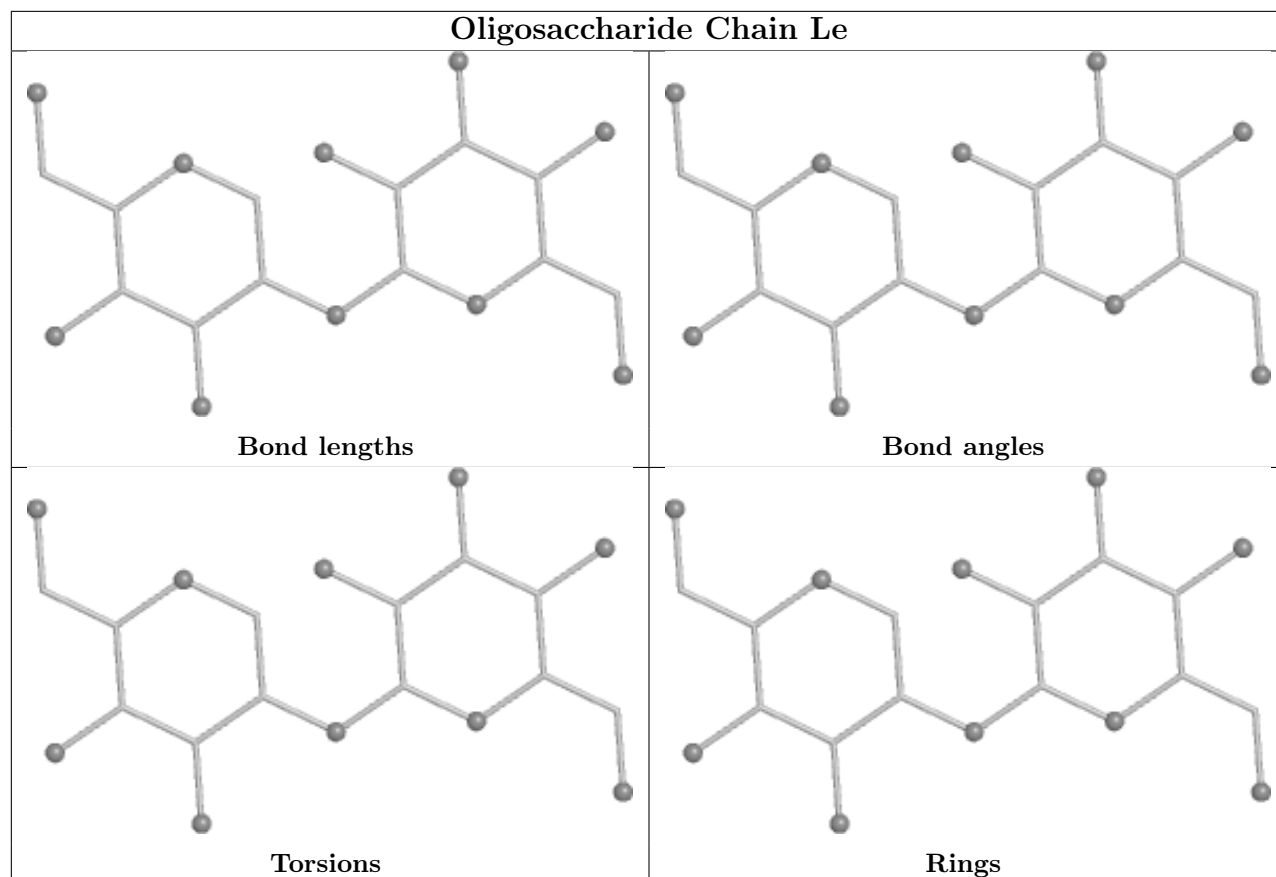
Oligosaccharide Chain He

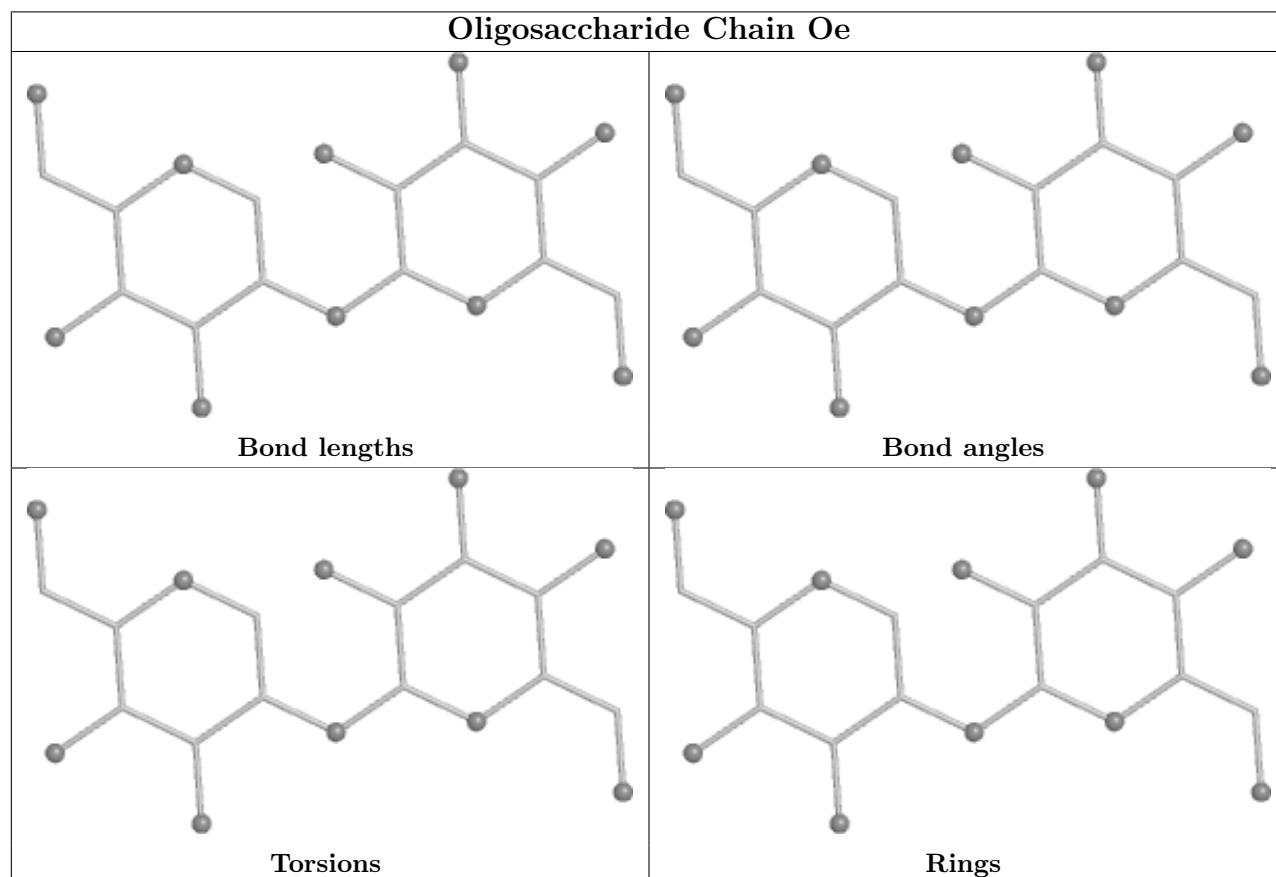
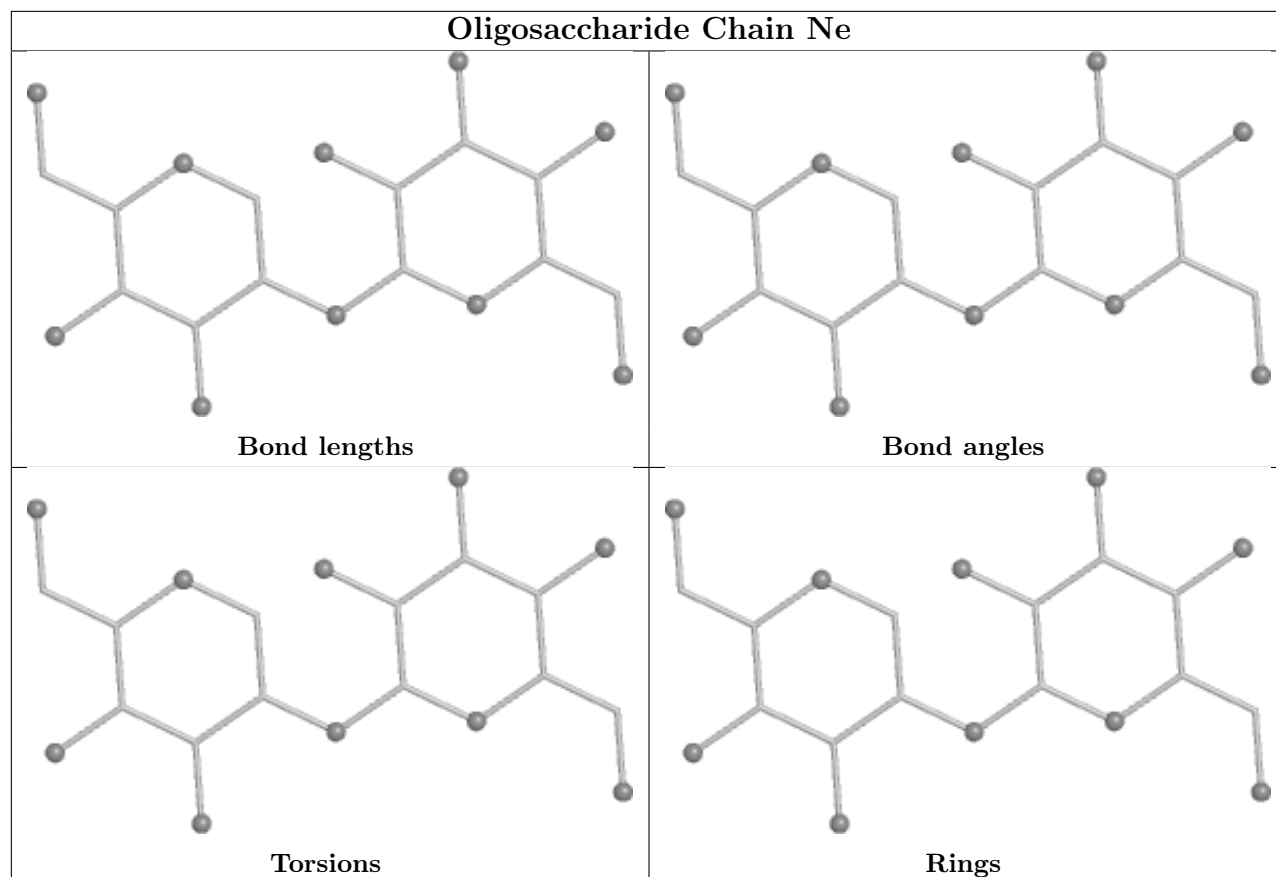


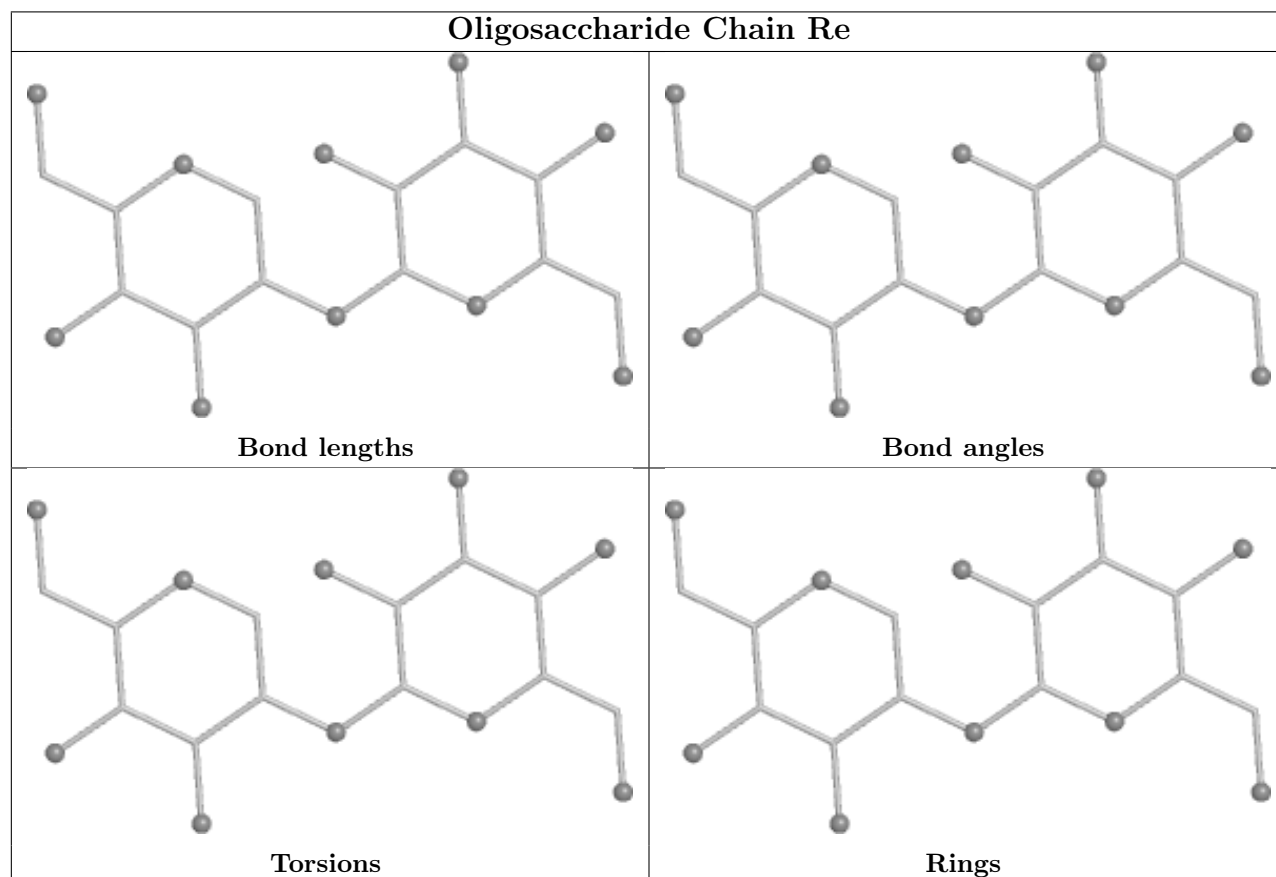
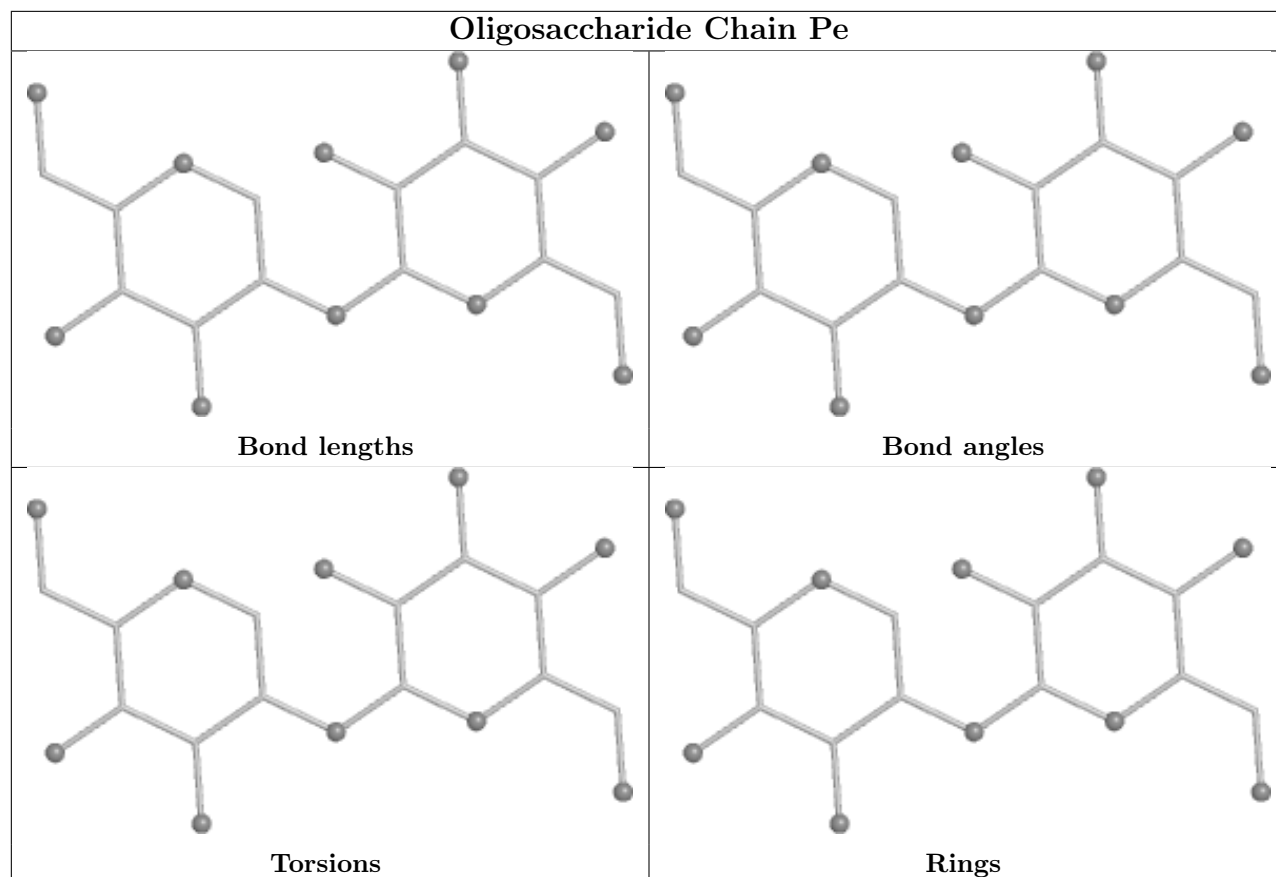
Oligosaccharide Chain Ie

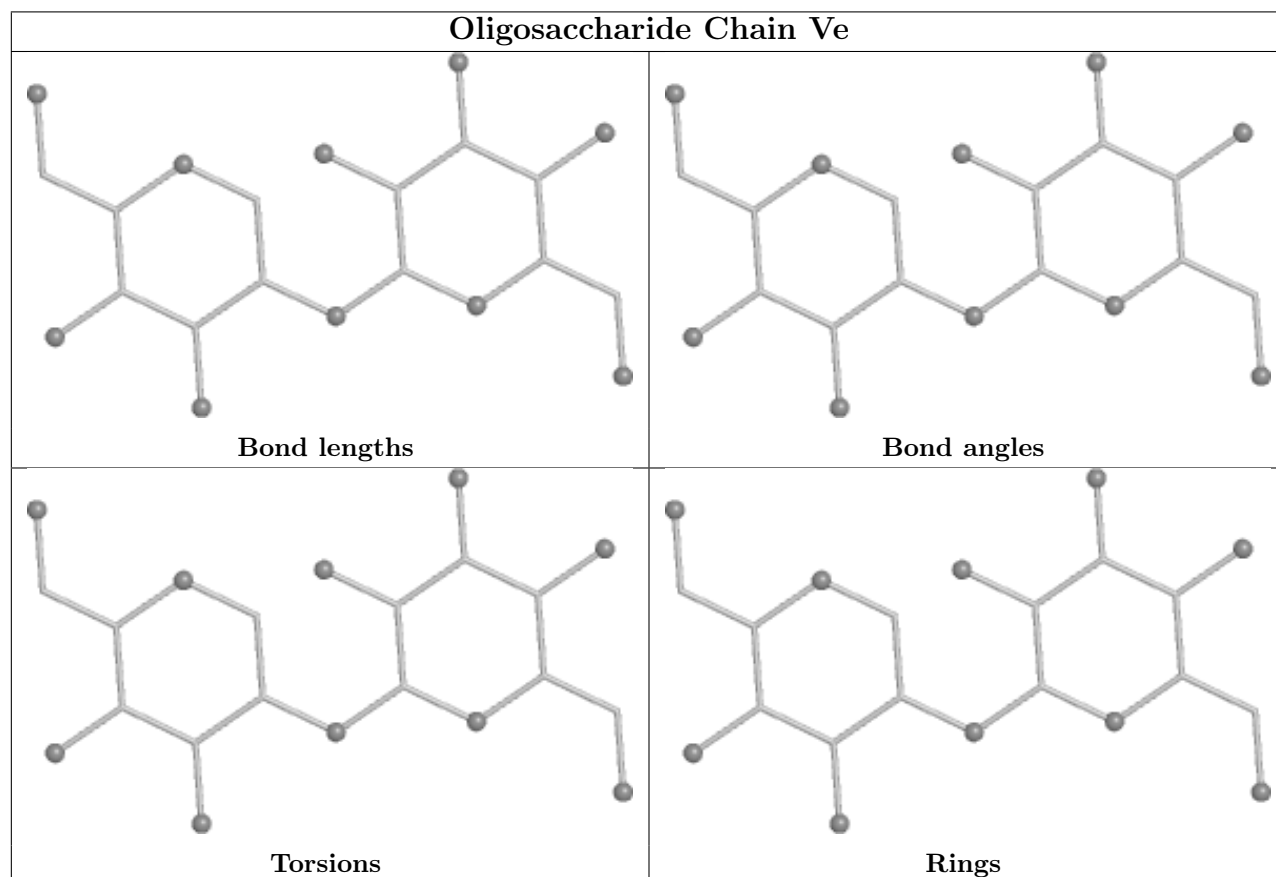
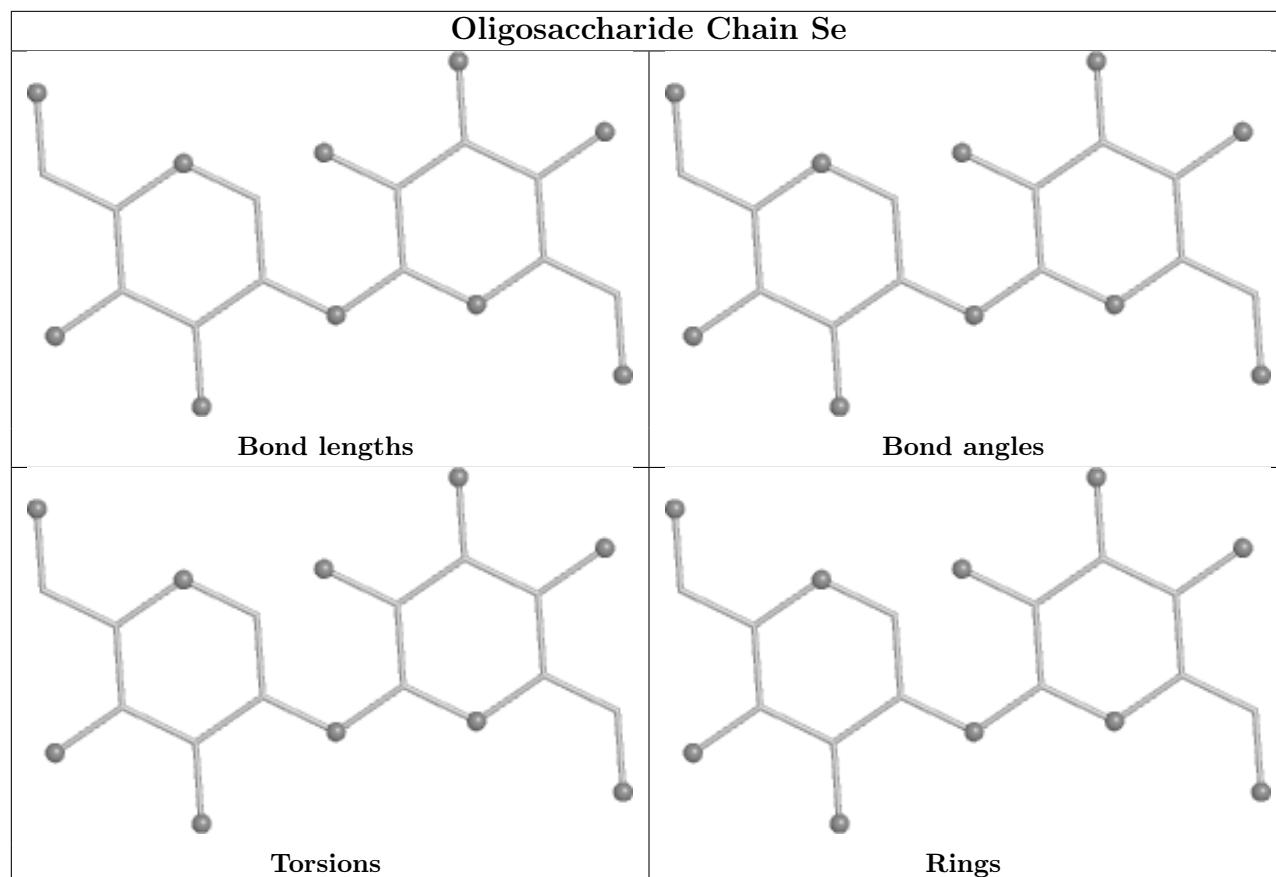




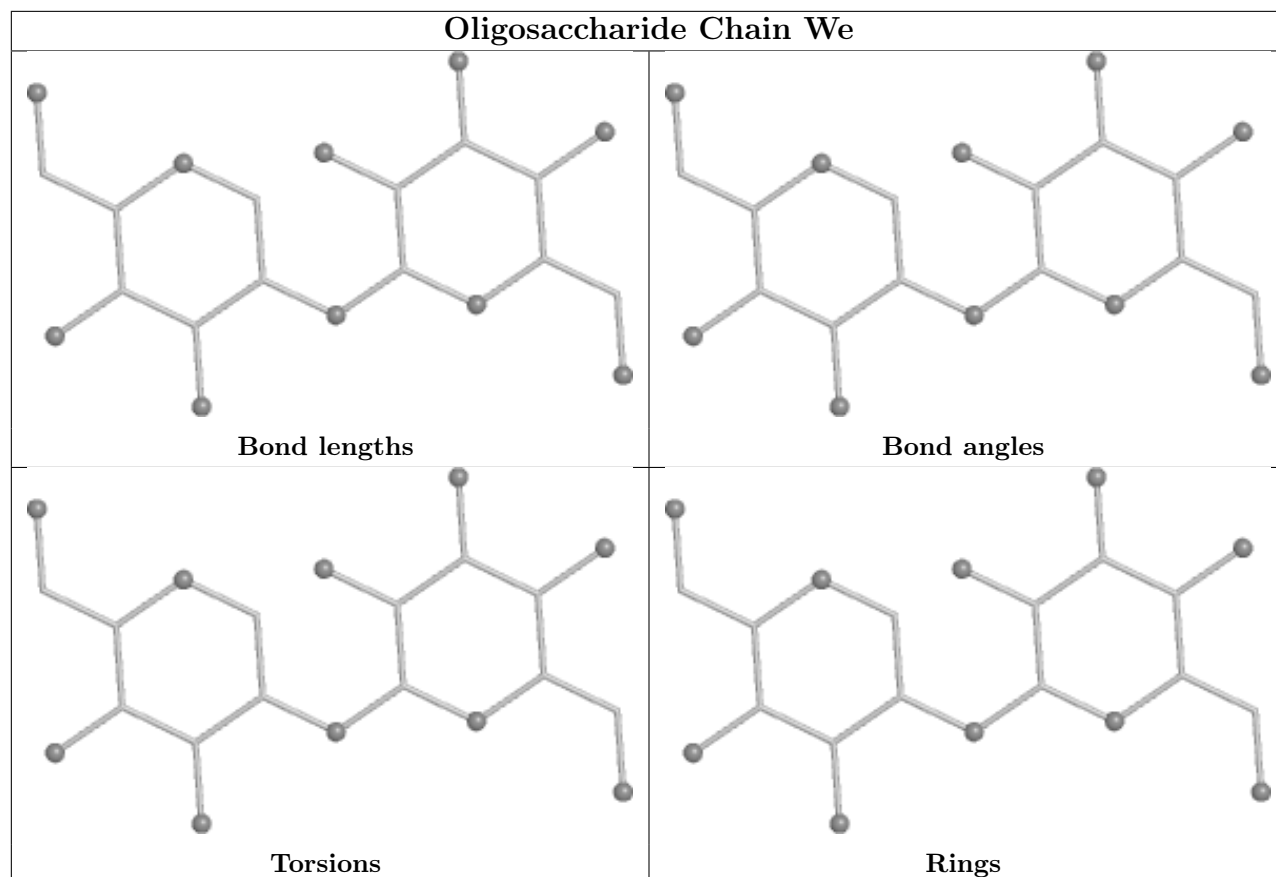




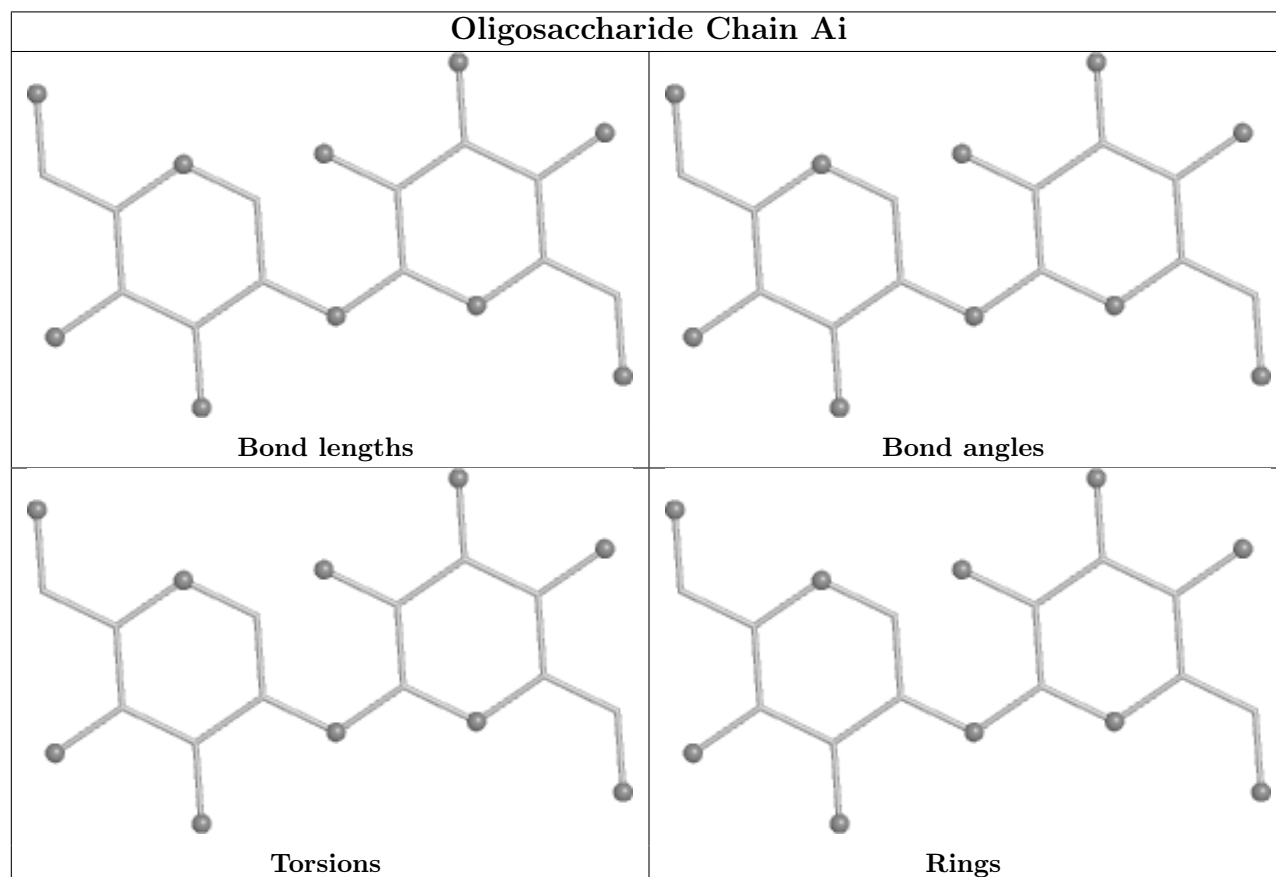


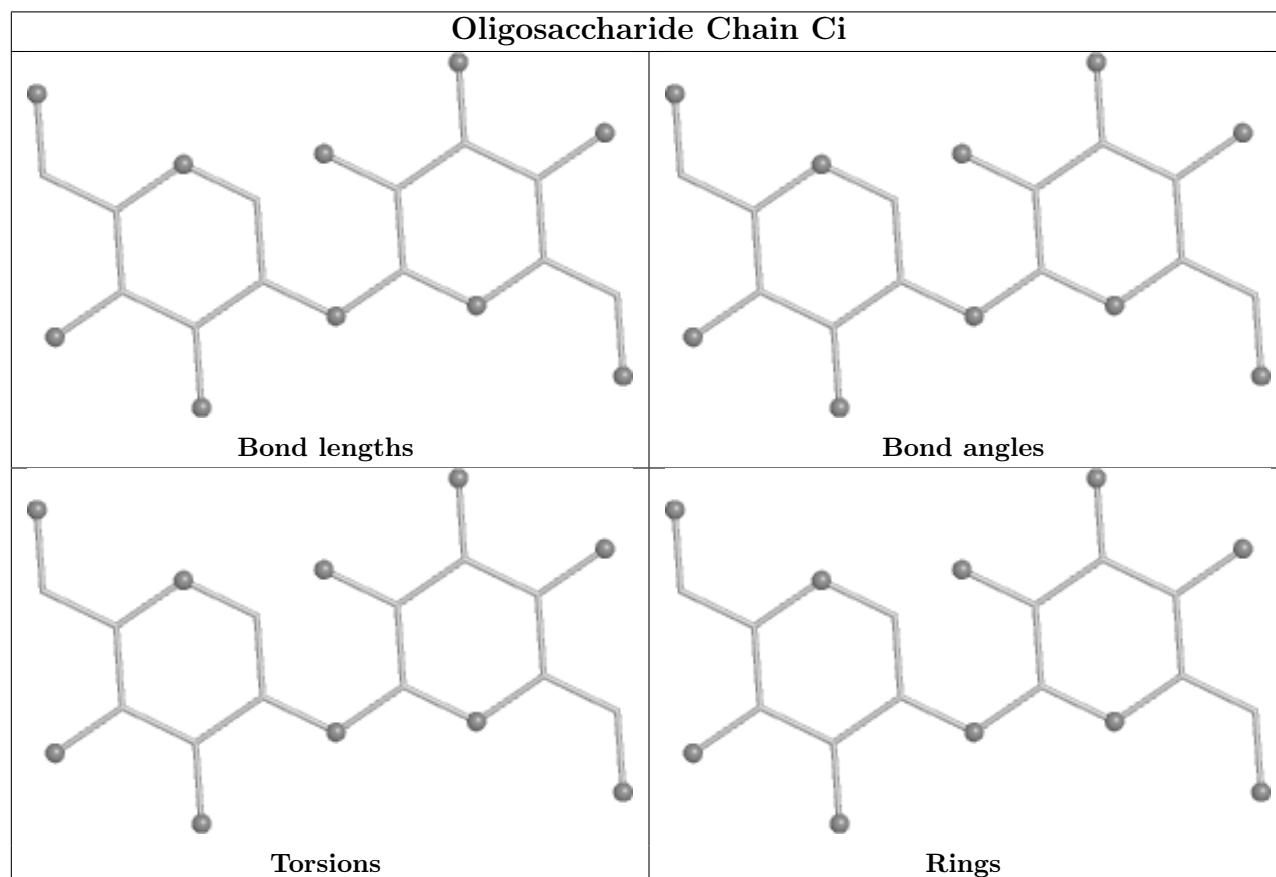
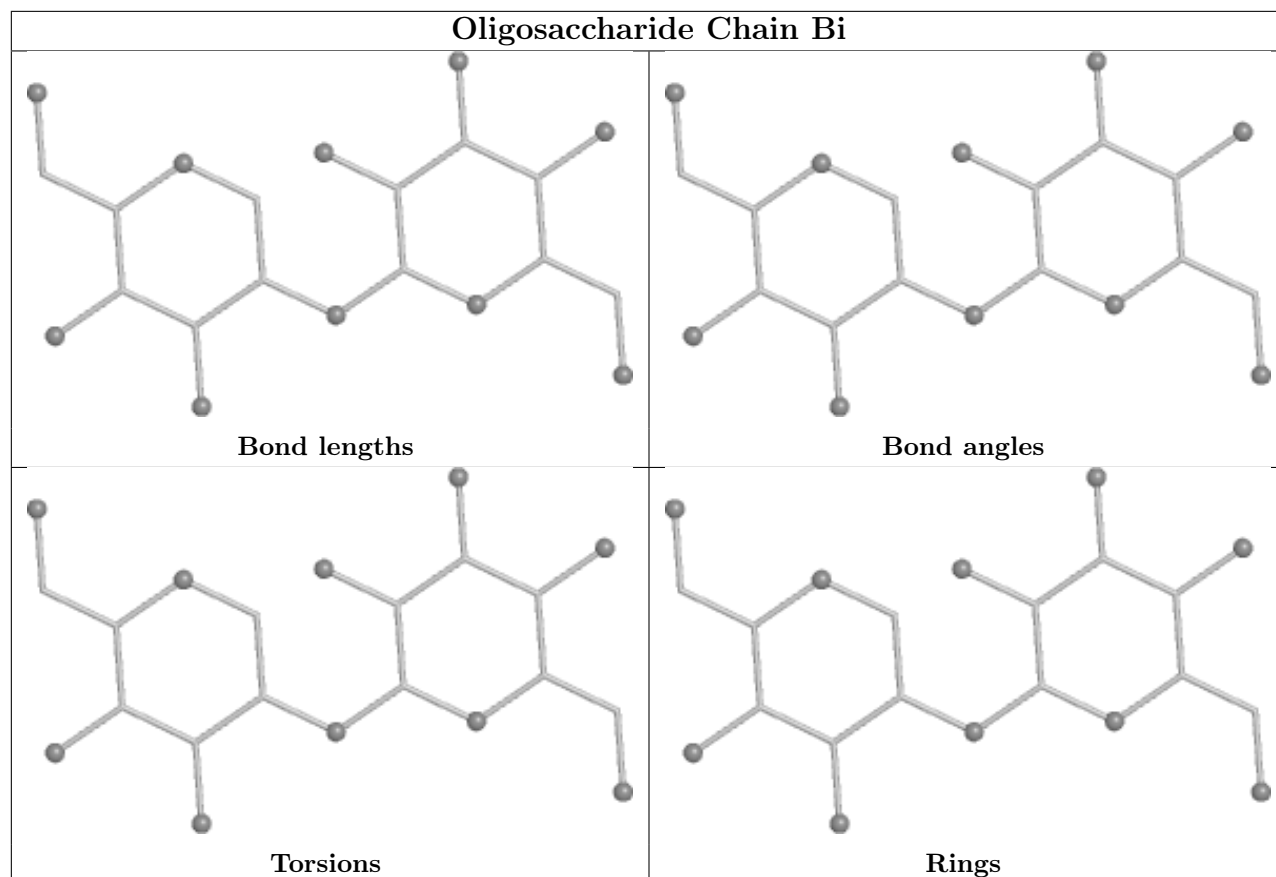


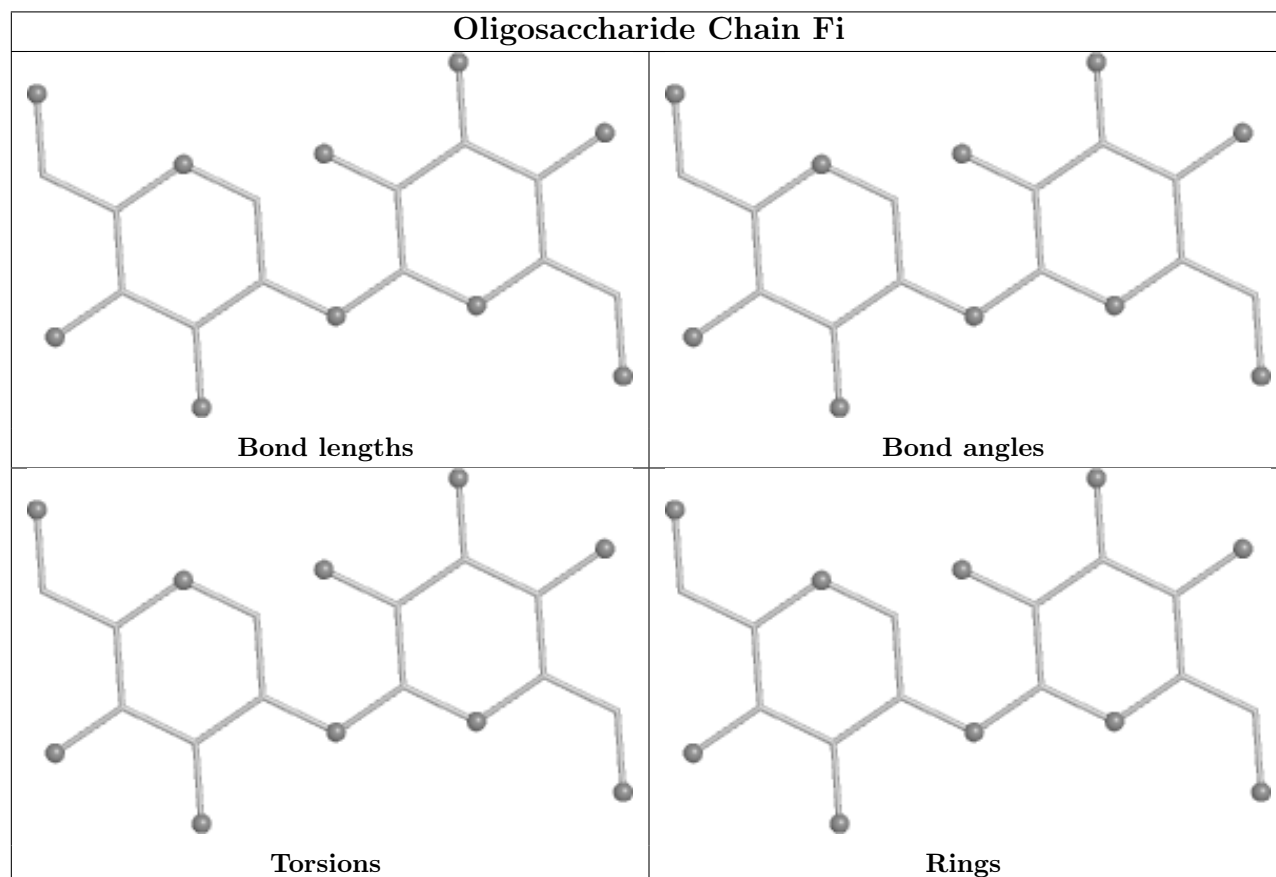
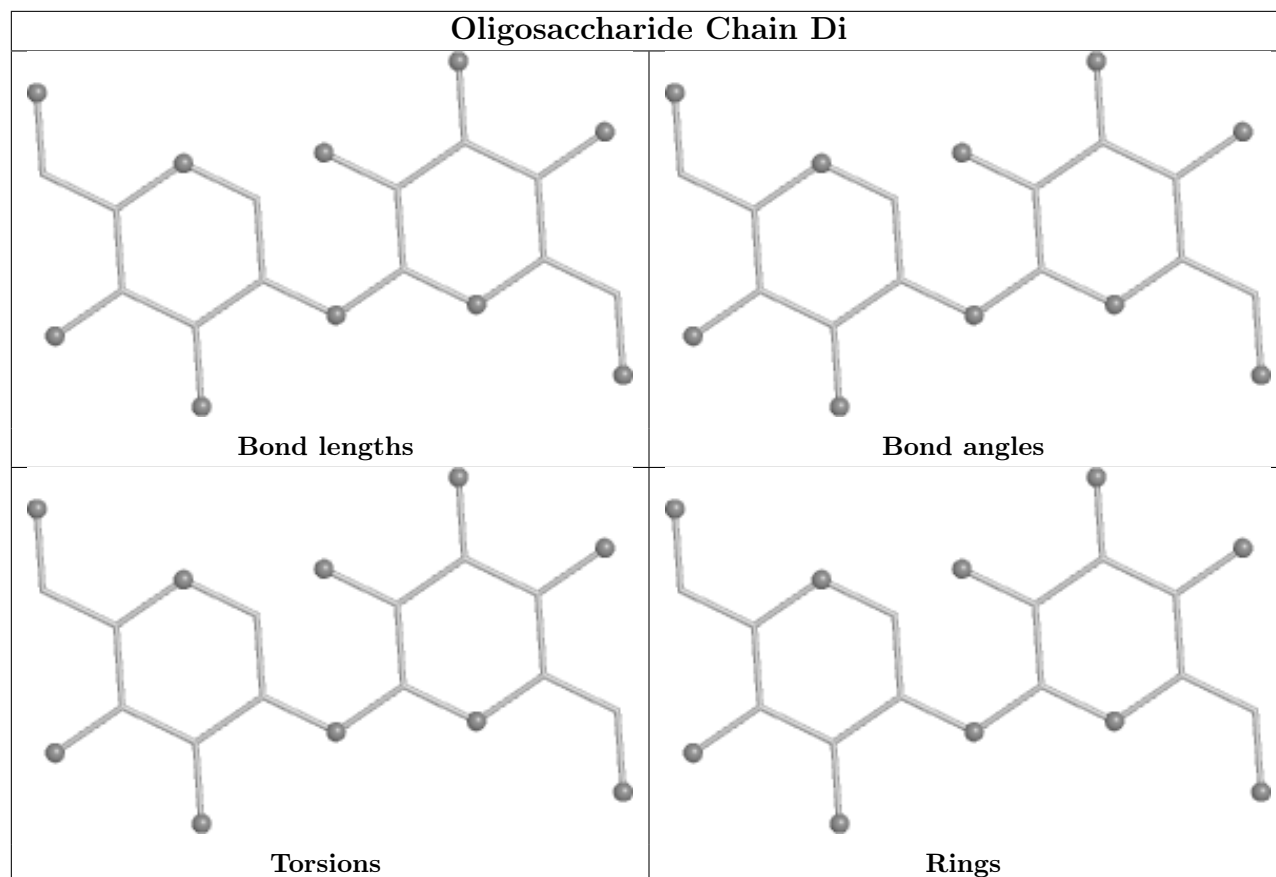
Oligosaccharide Chain We



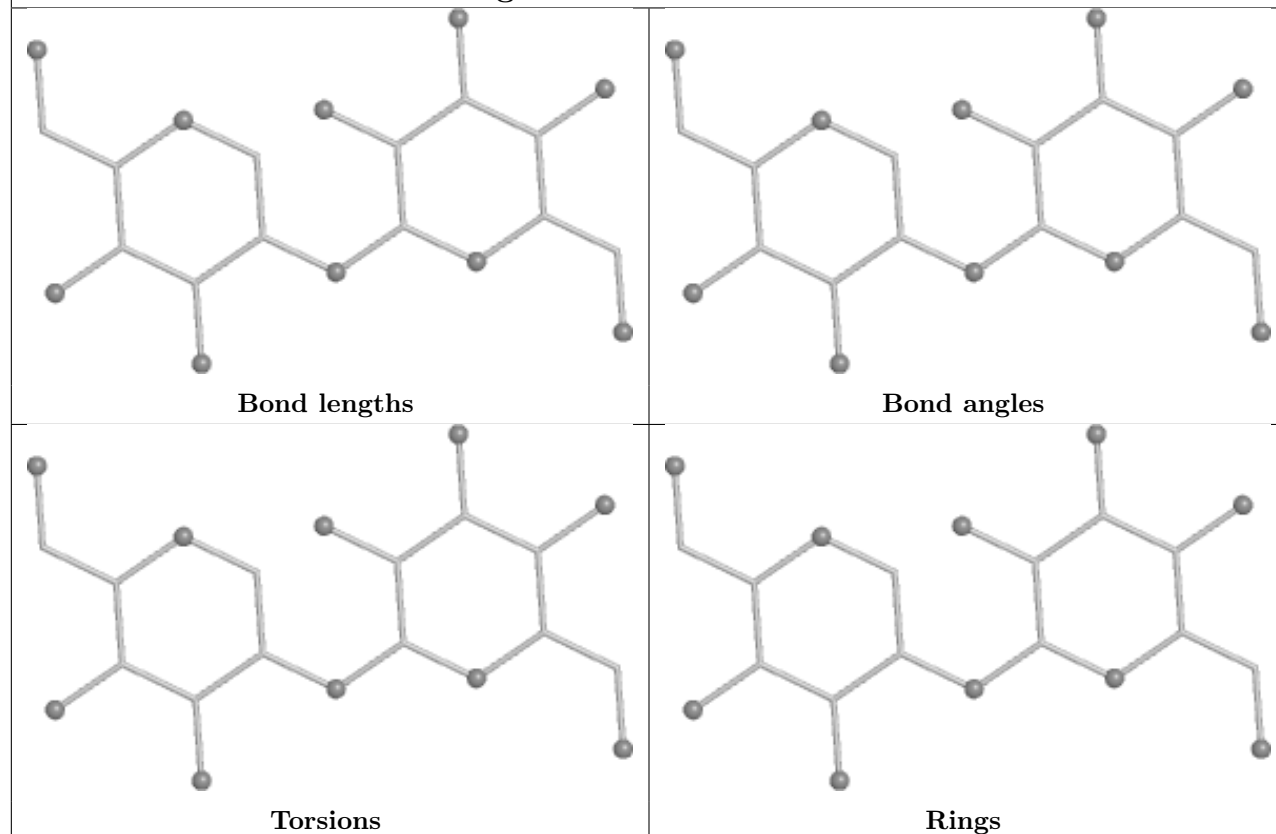
Oligosaccharide Chain Ai



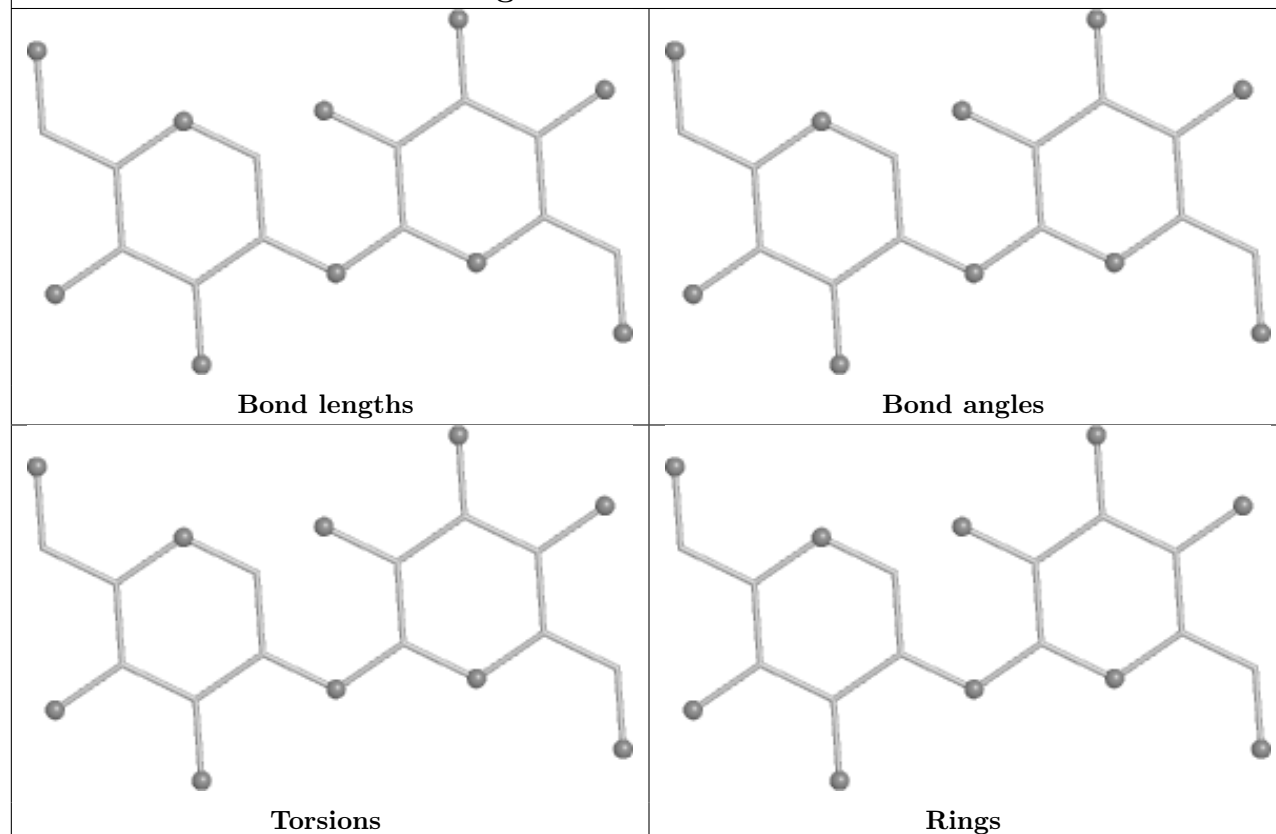


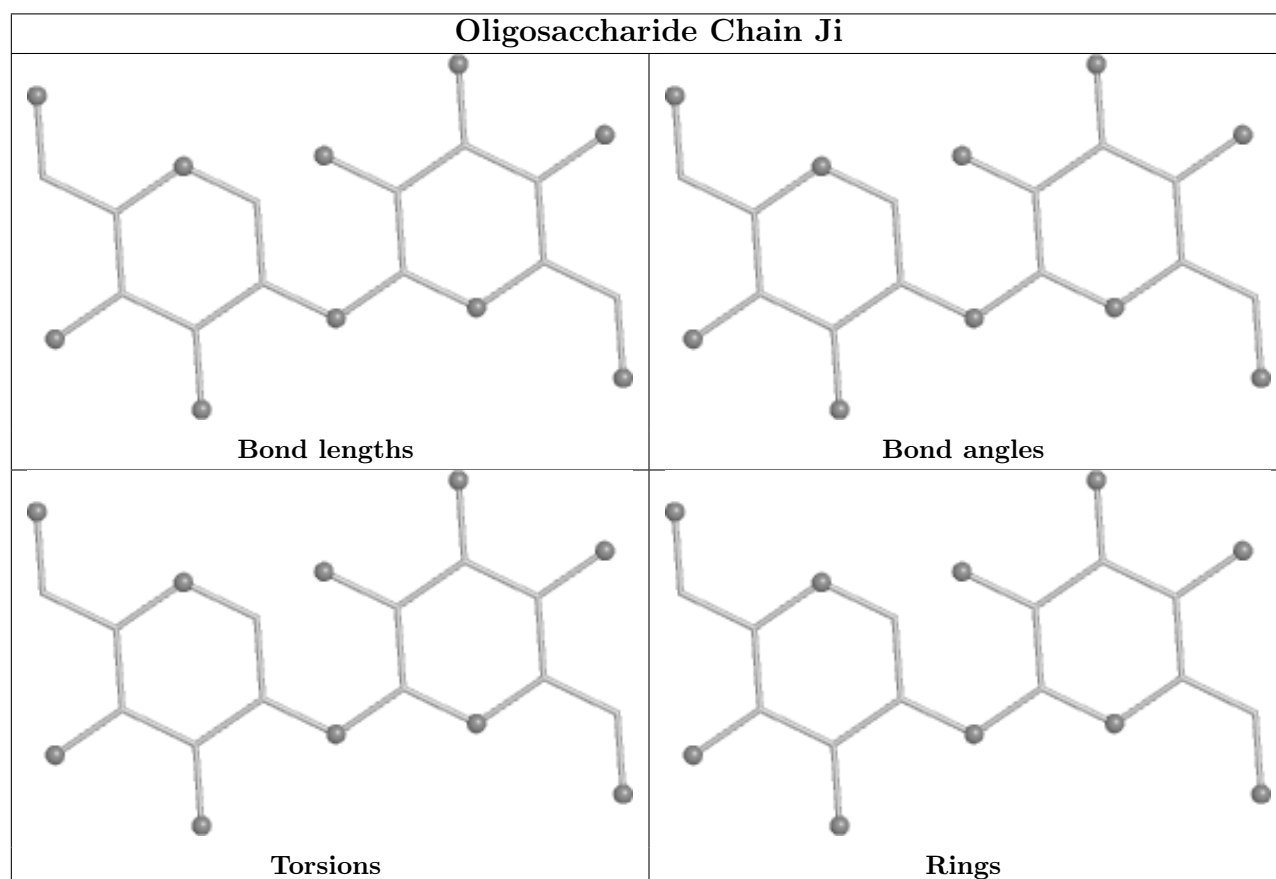
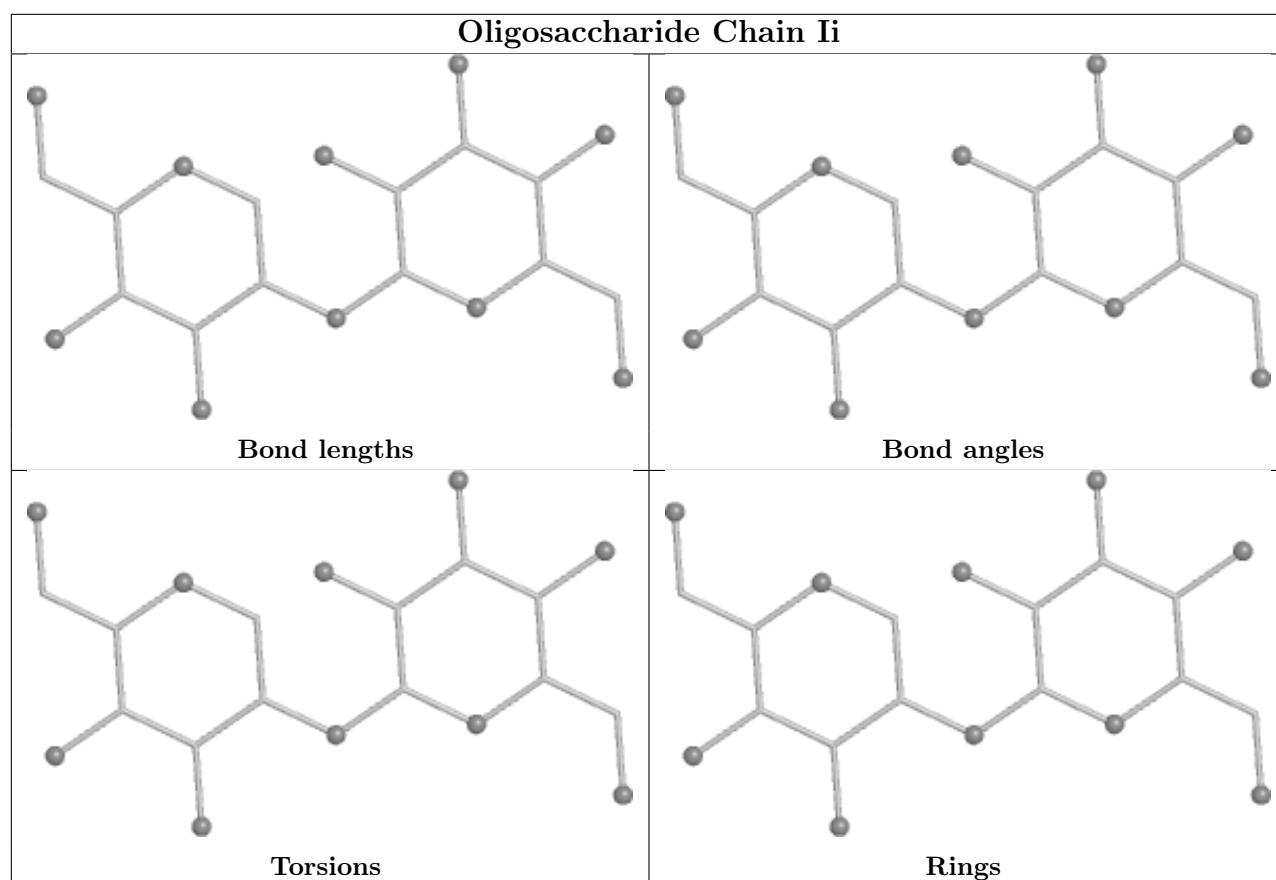


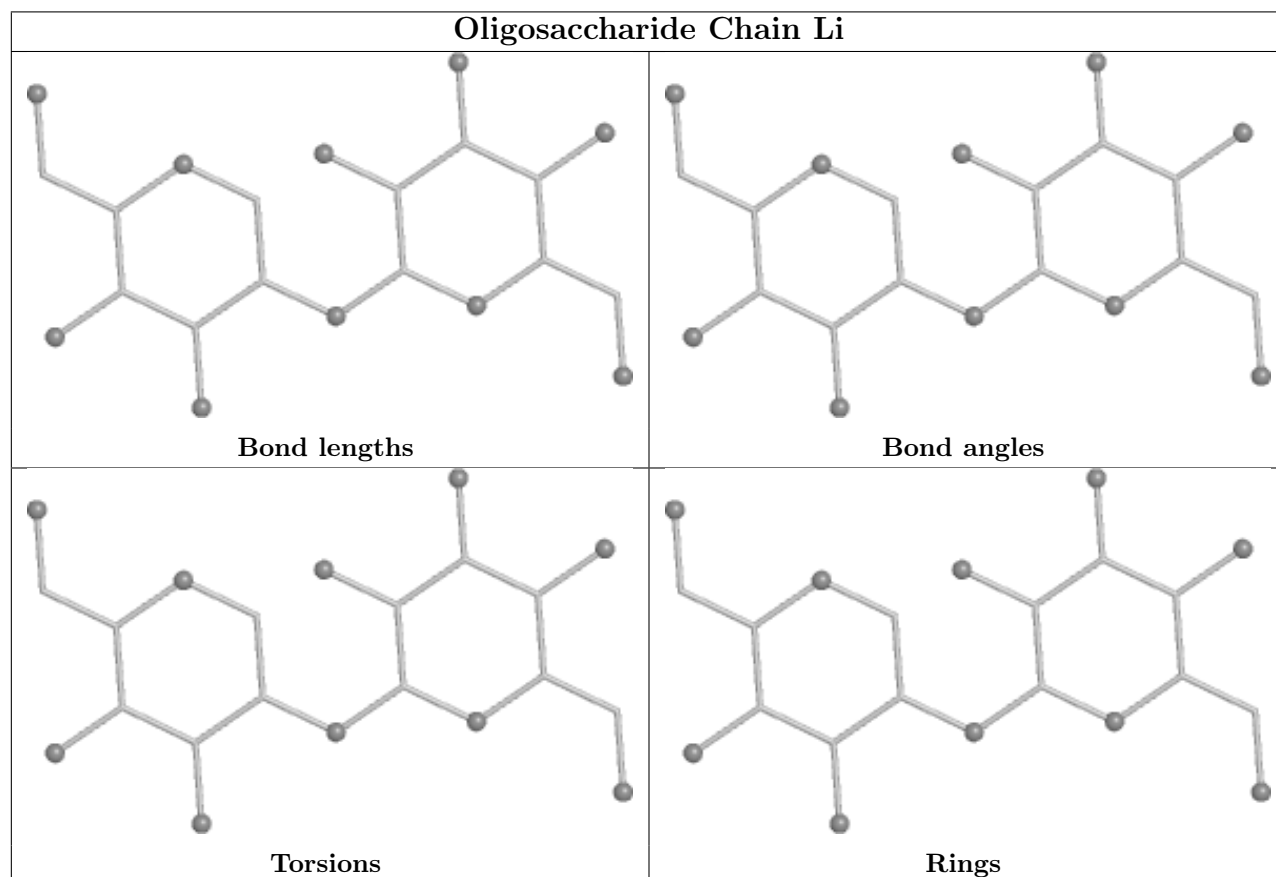
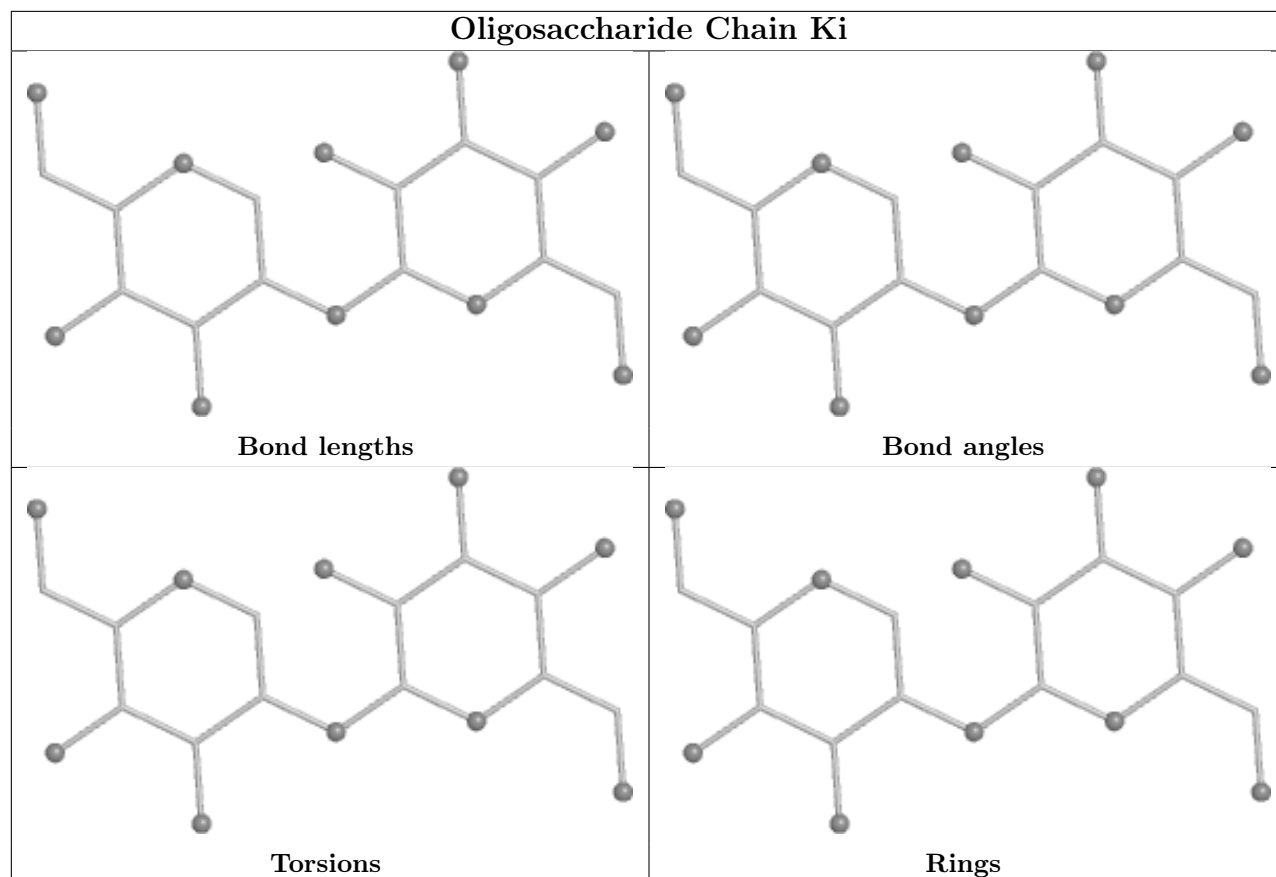
Oligosaccharide Chain Gi

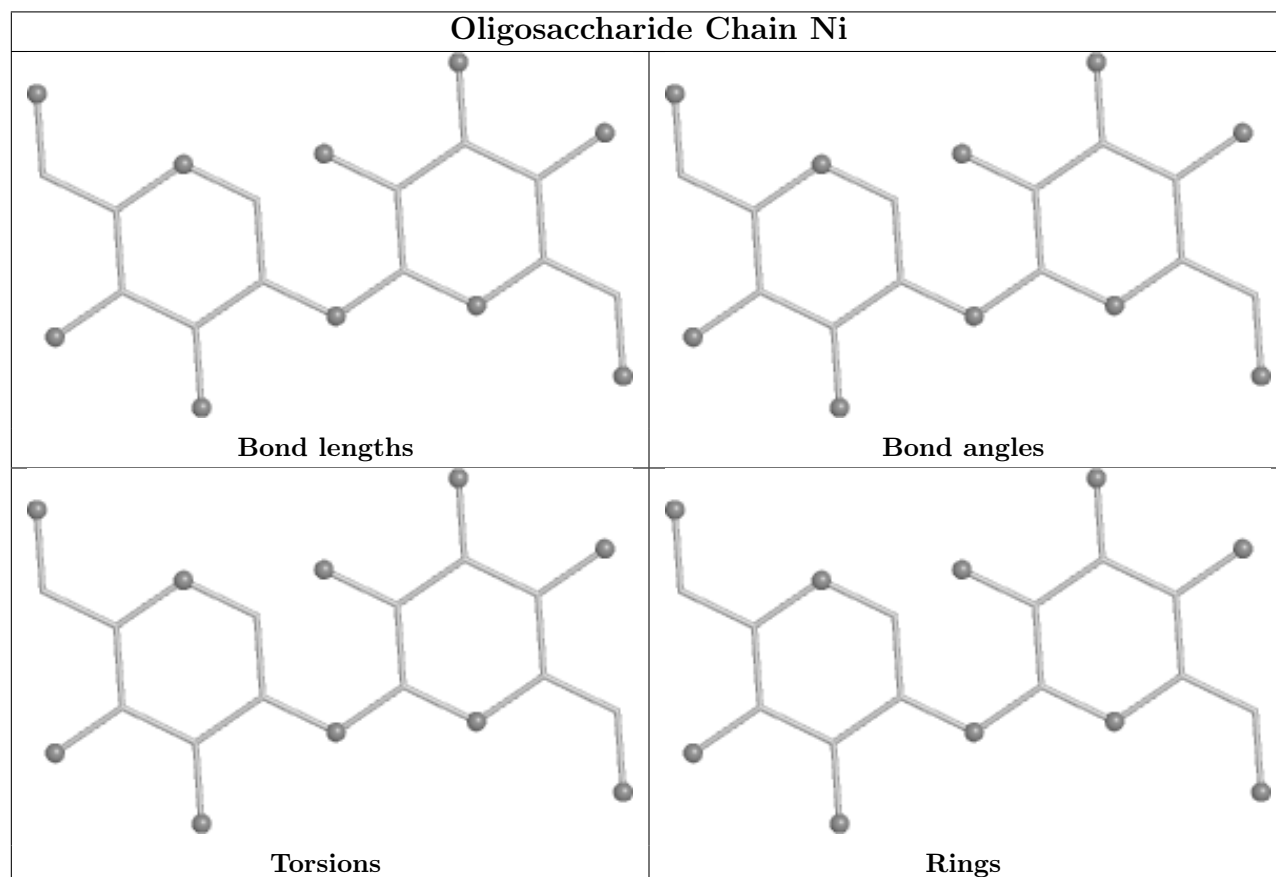
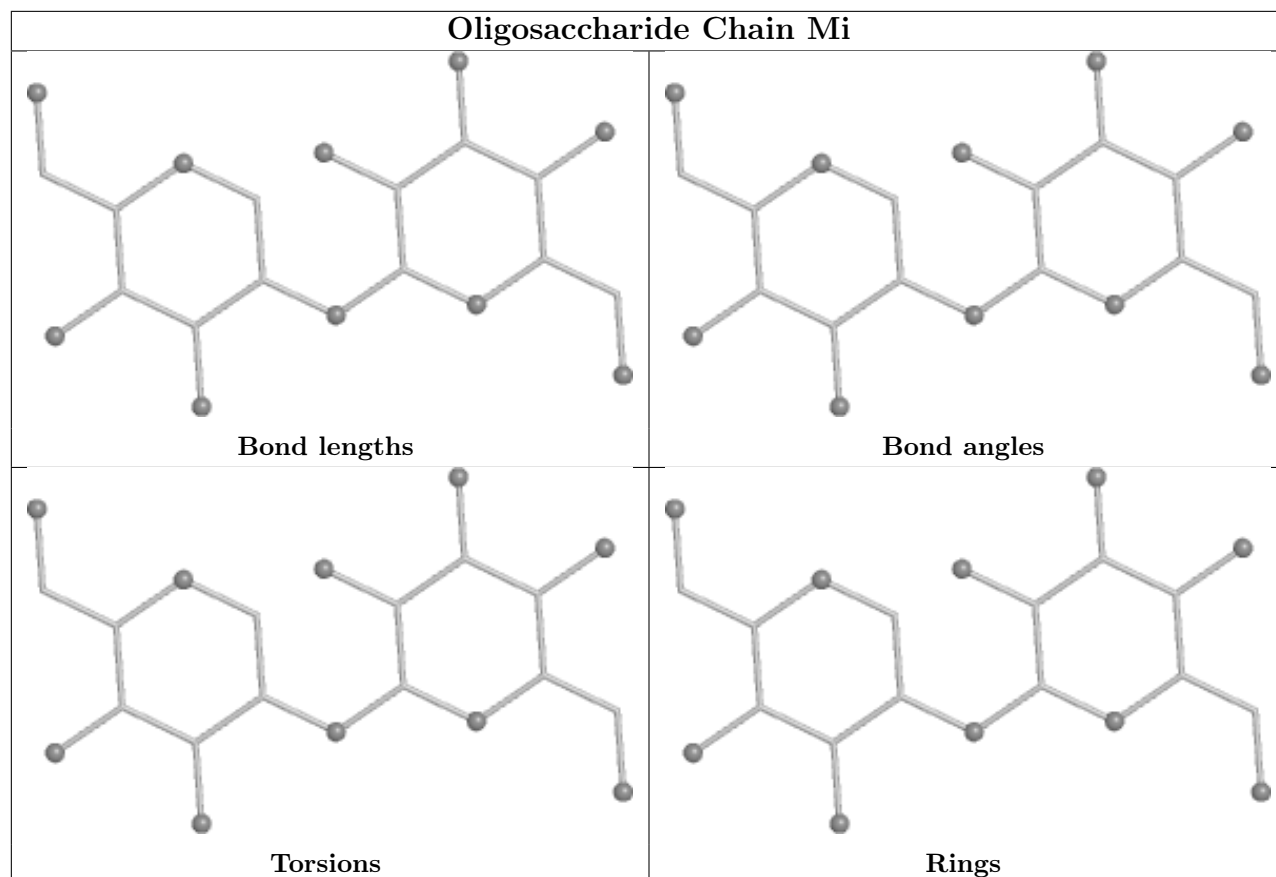


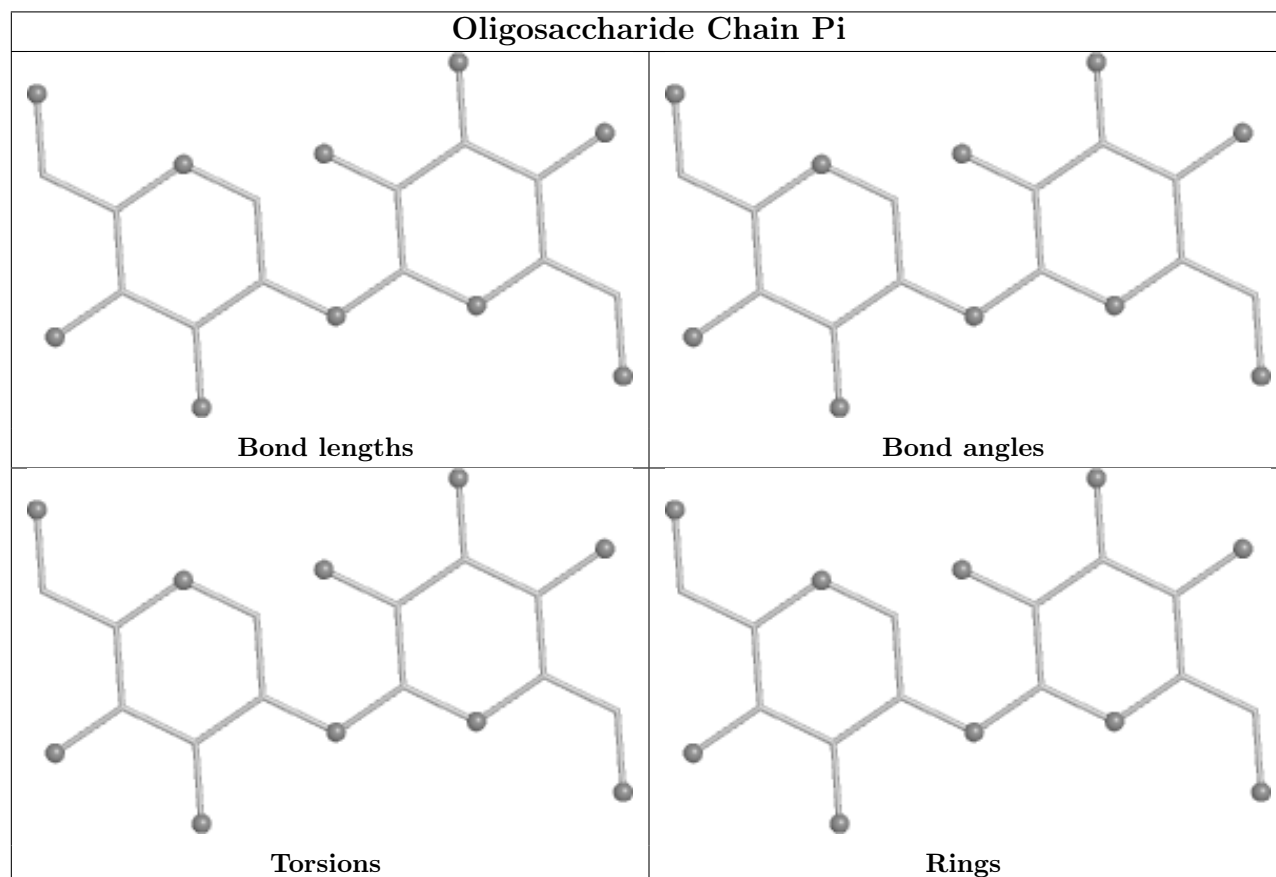
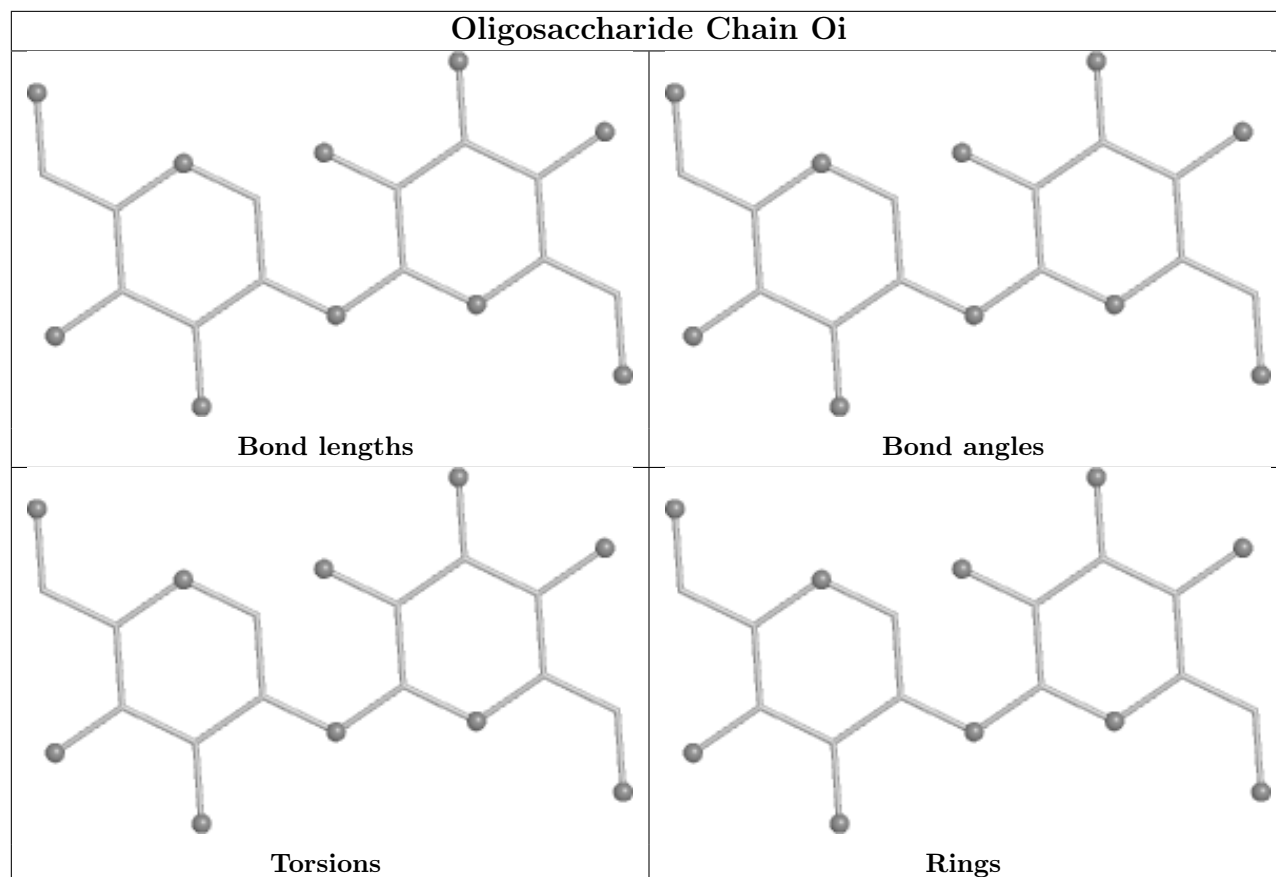
Oligosaccharide Chain Hi

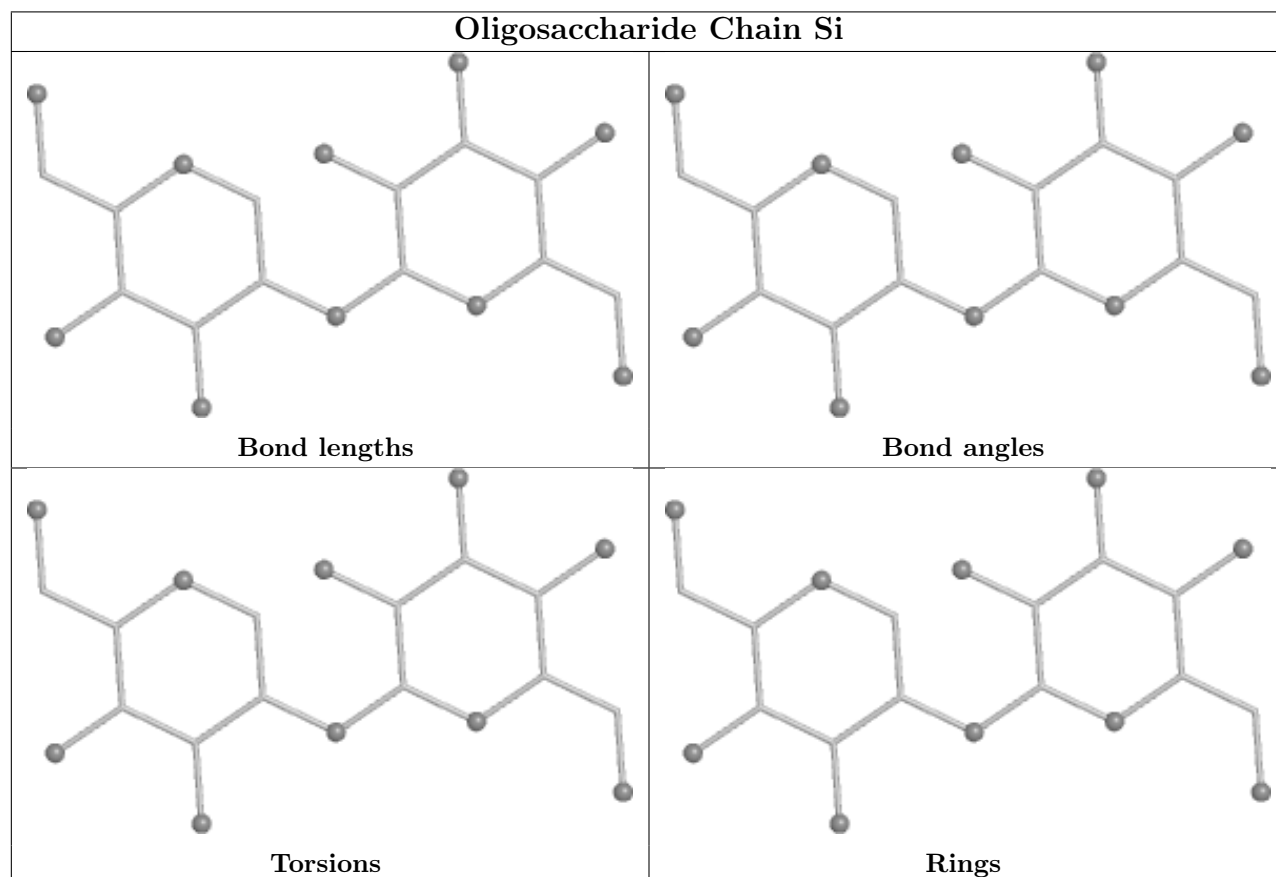
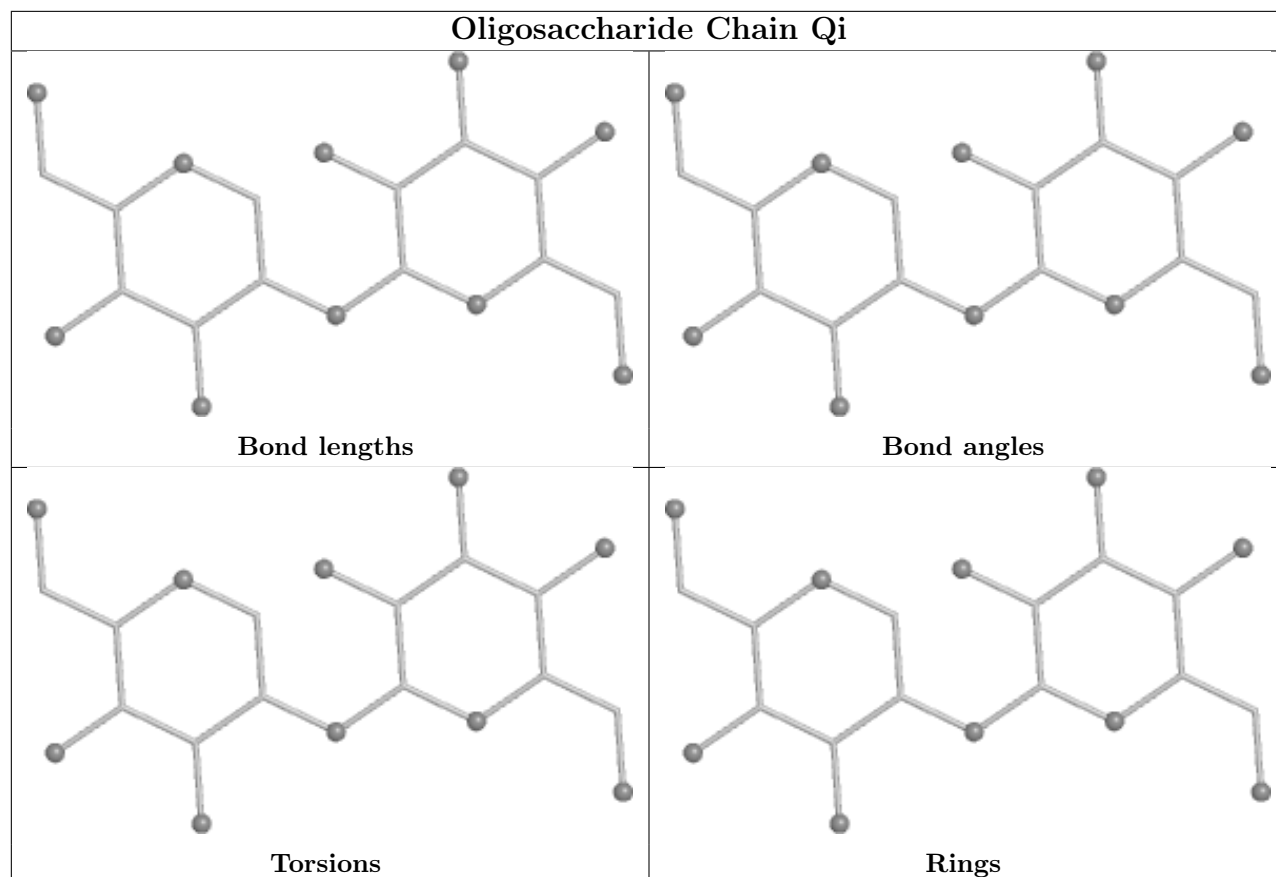


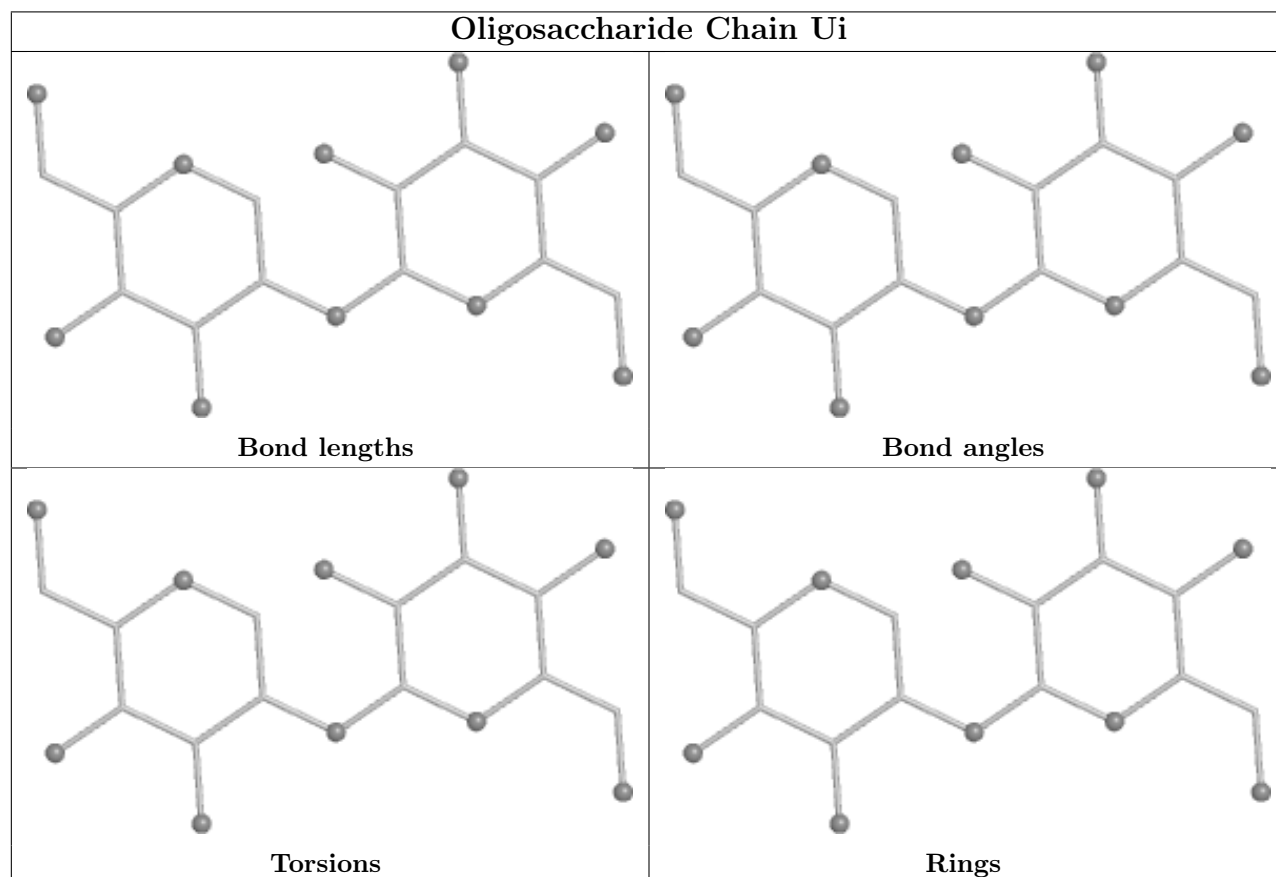
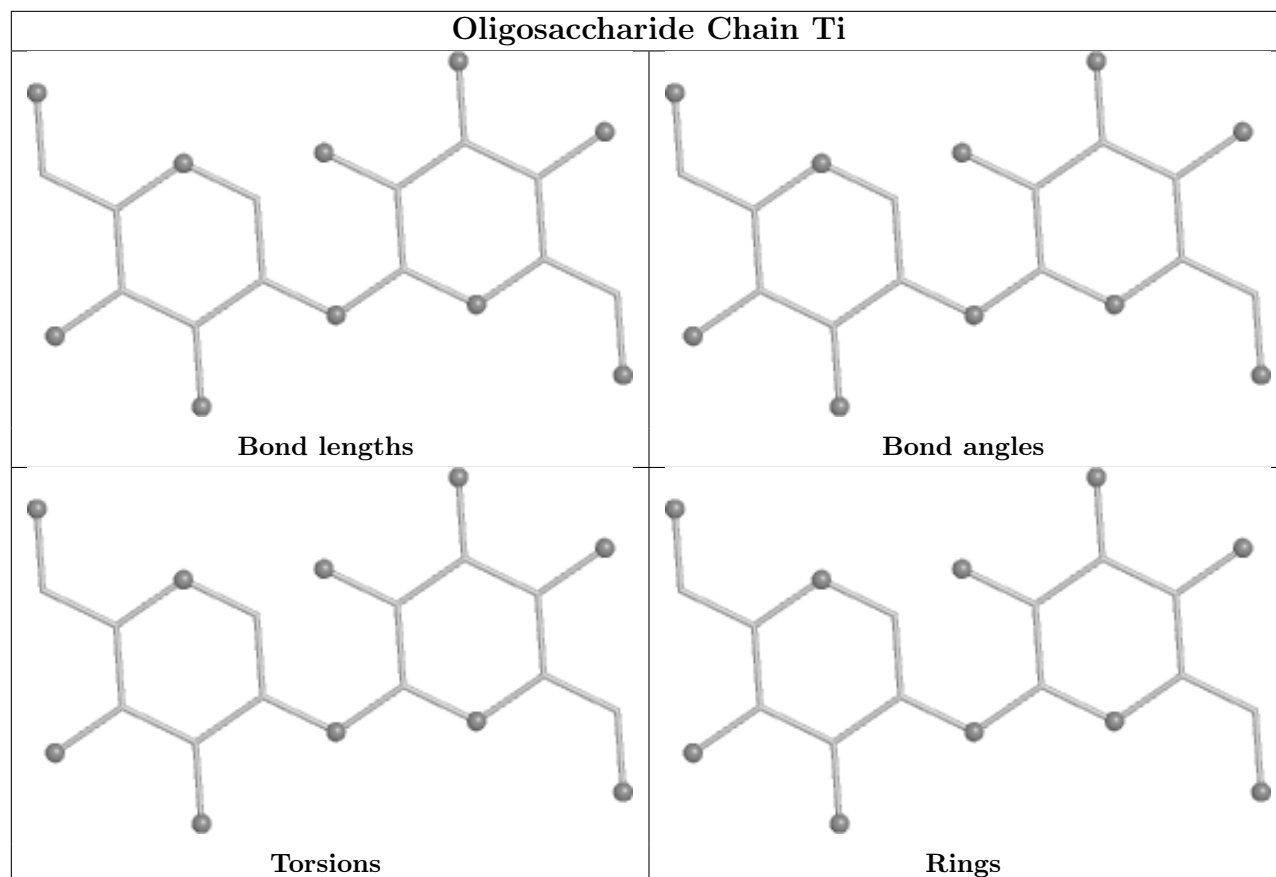




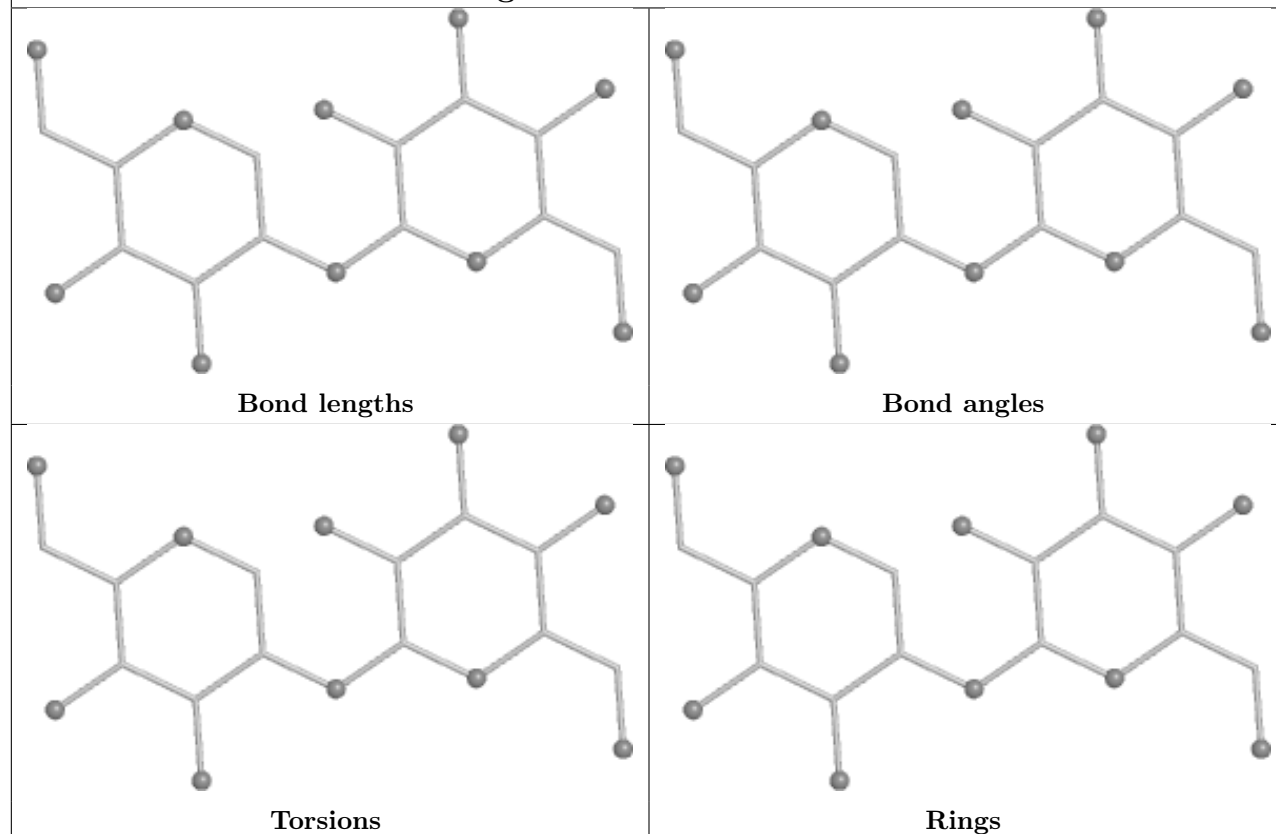




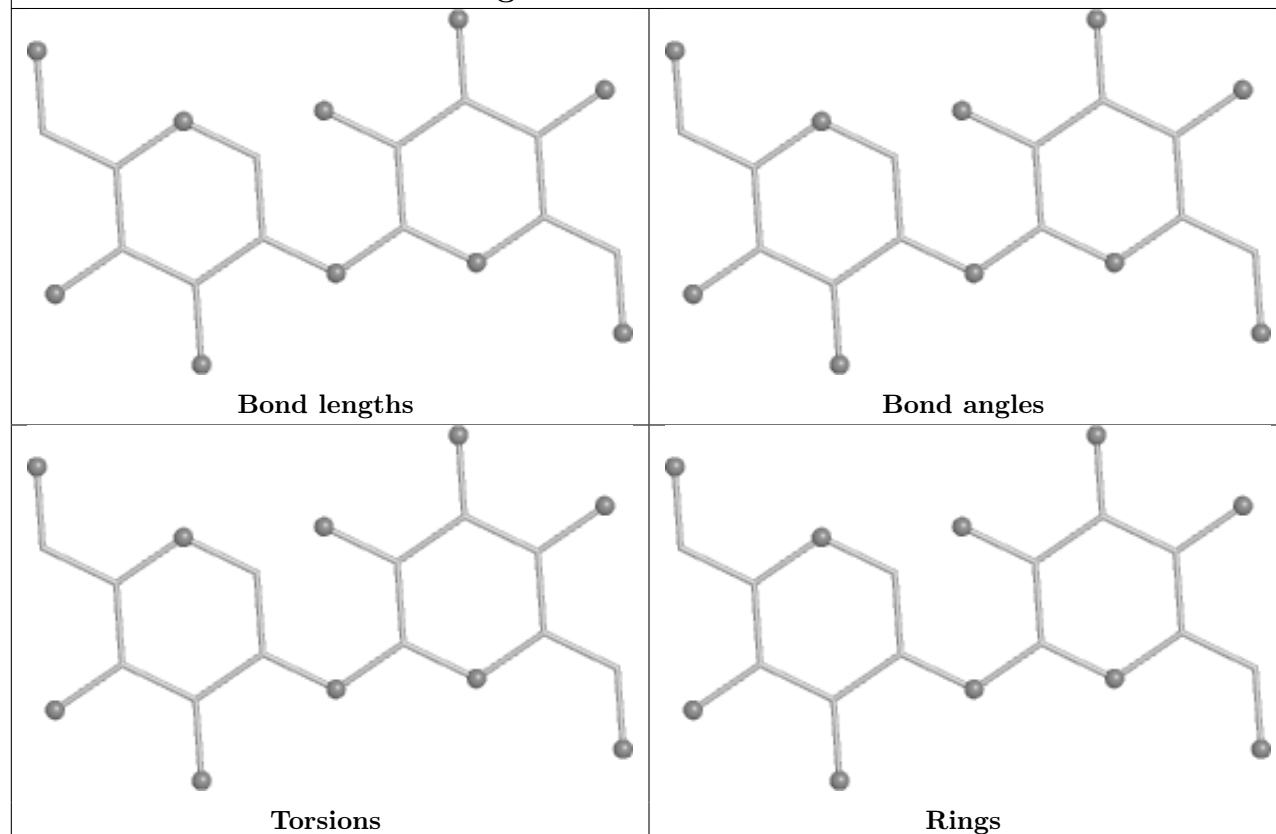


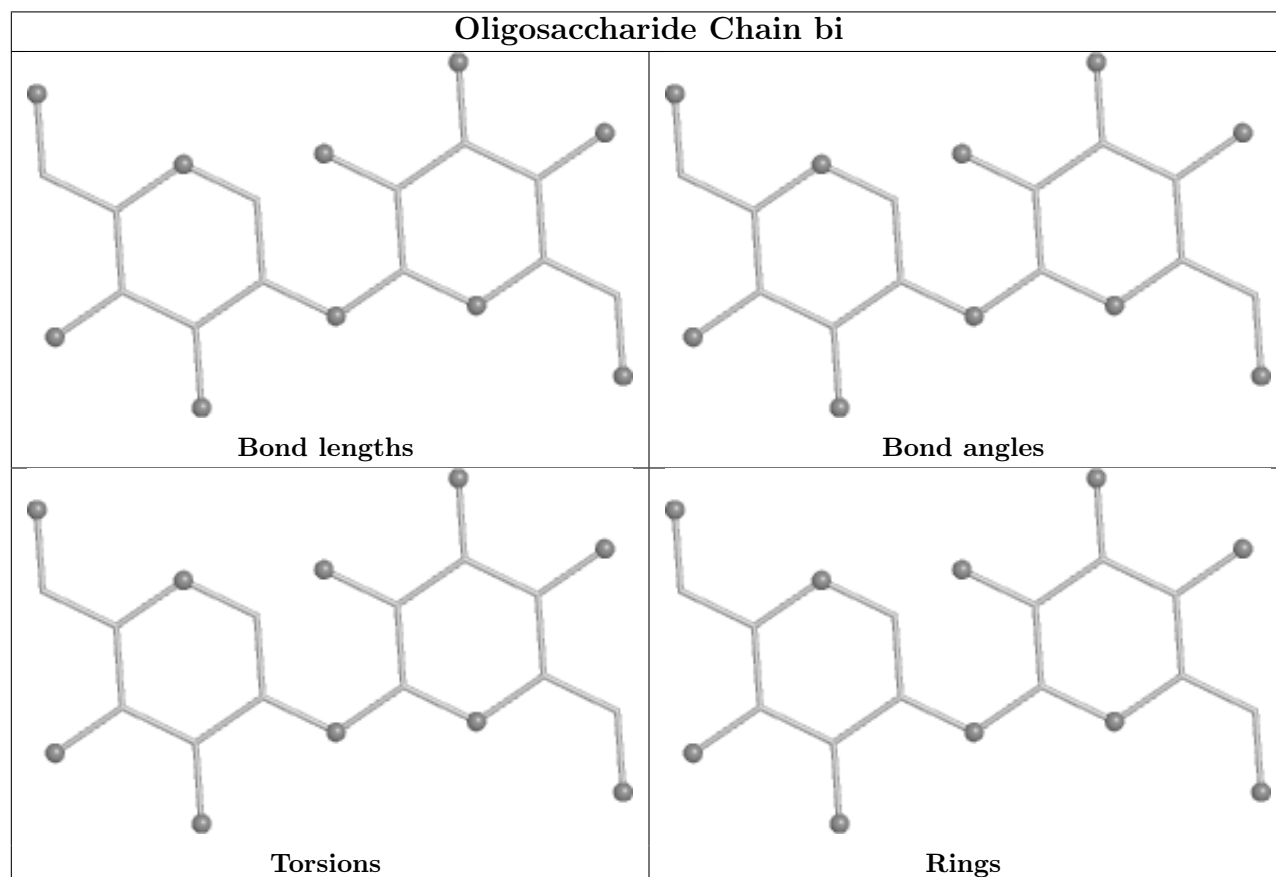
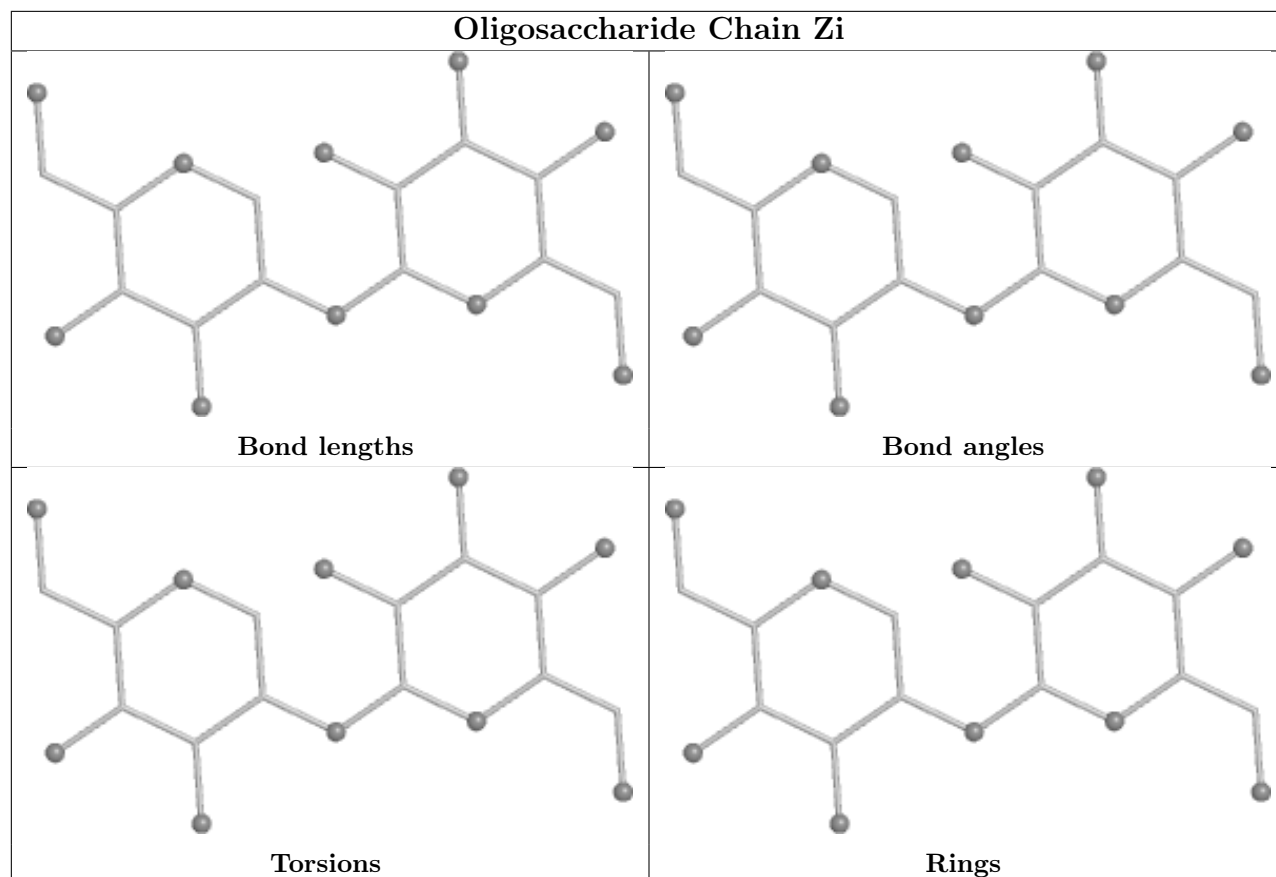


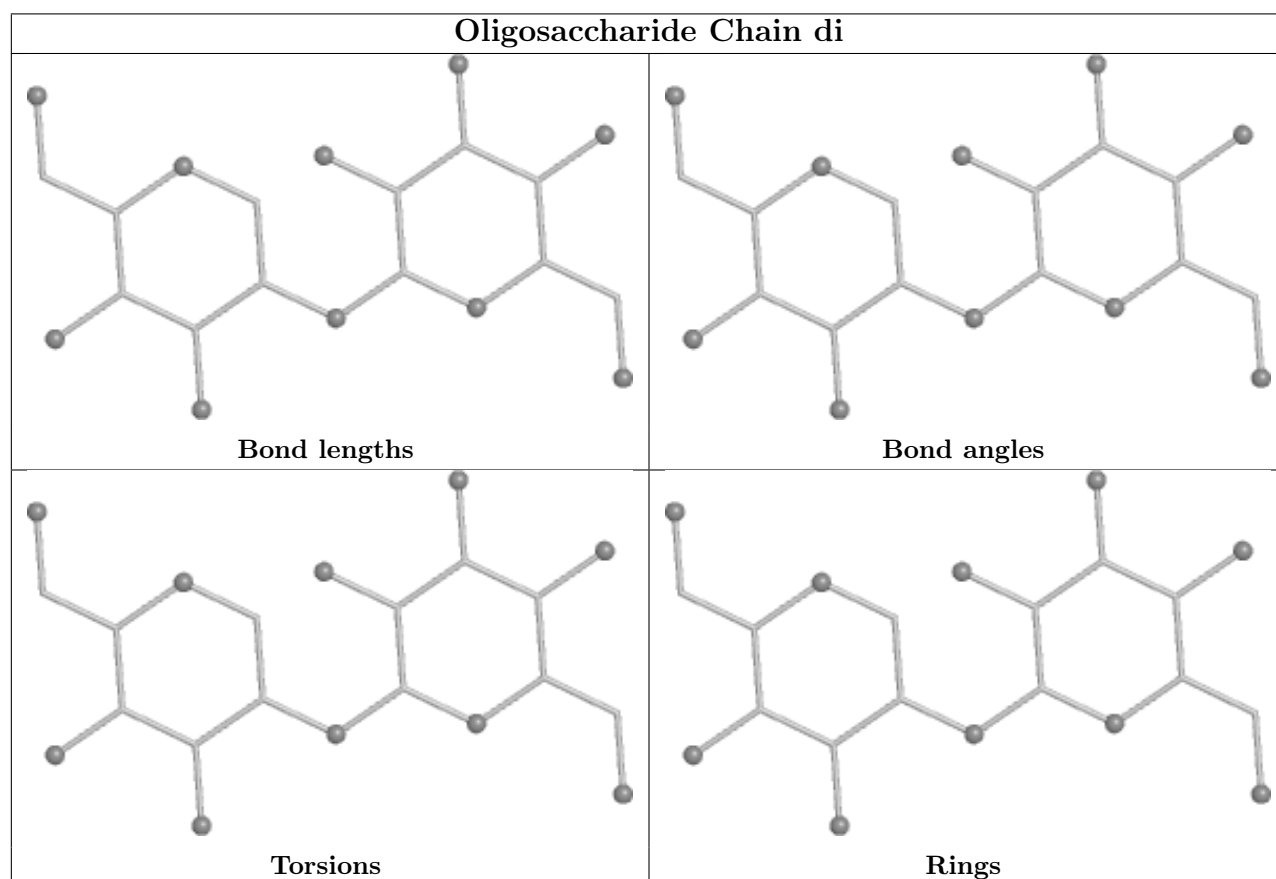
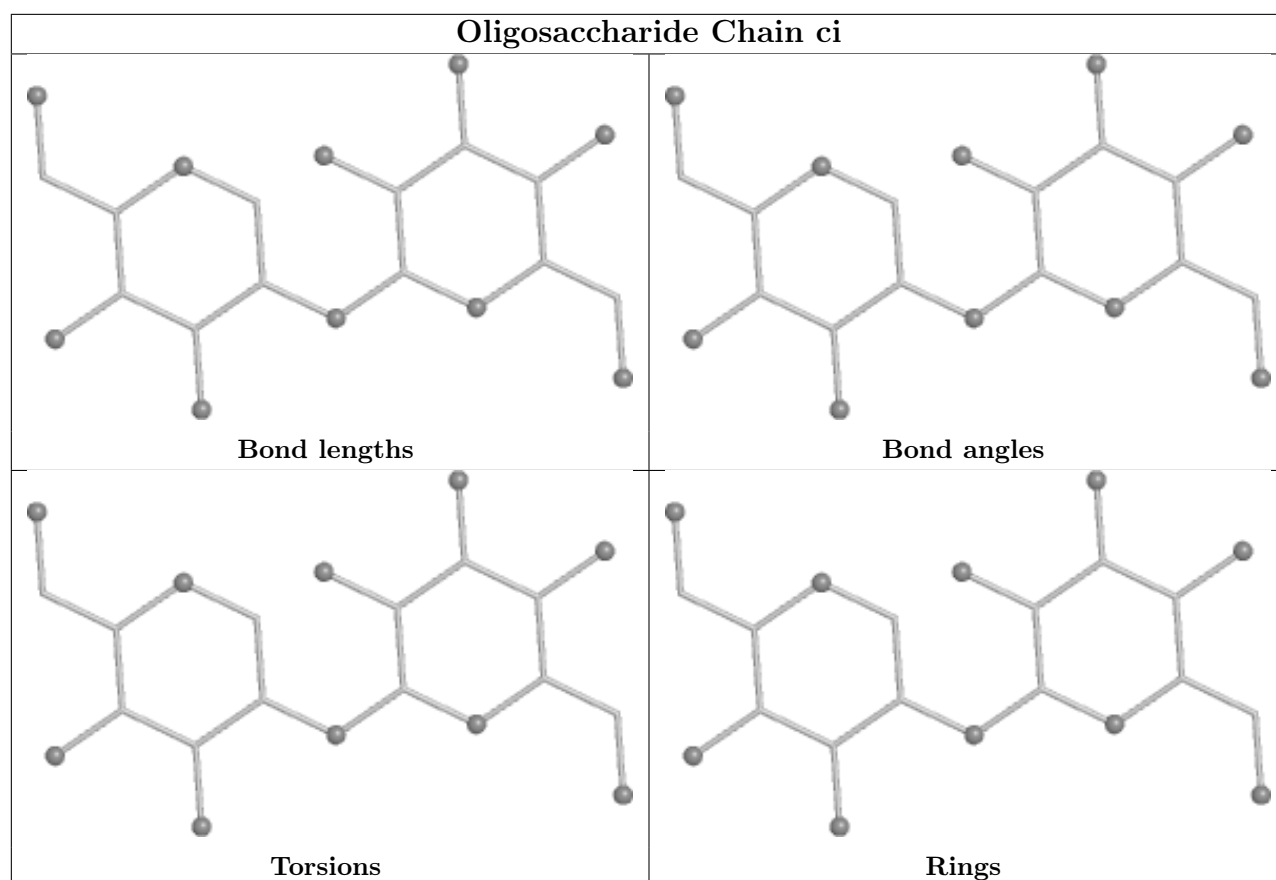
Oligosaccharide Chain Xi

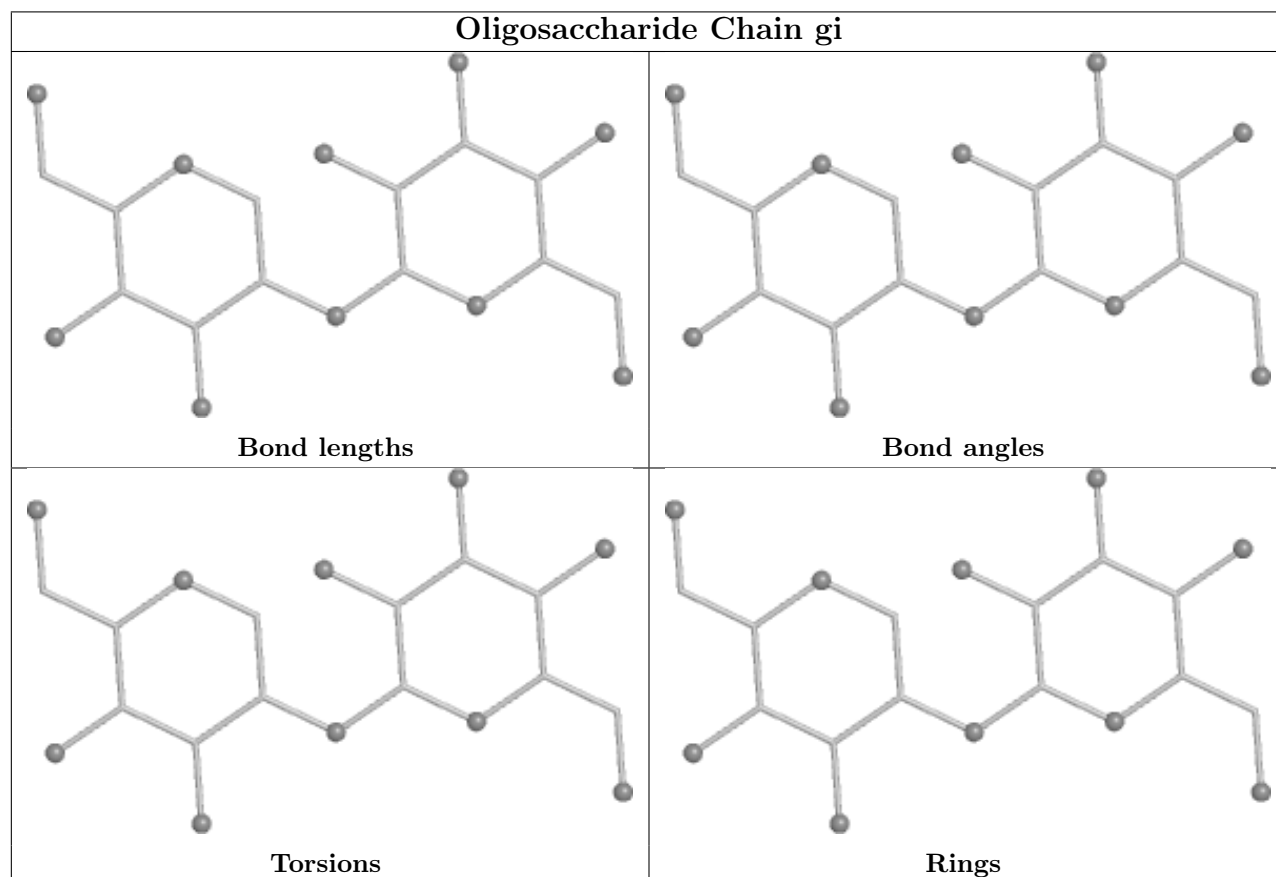
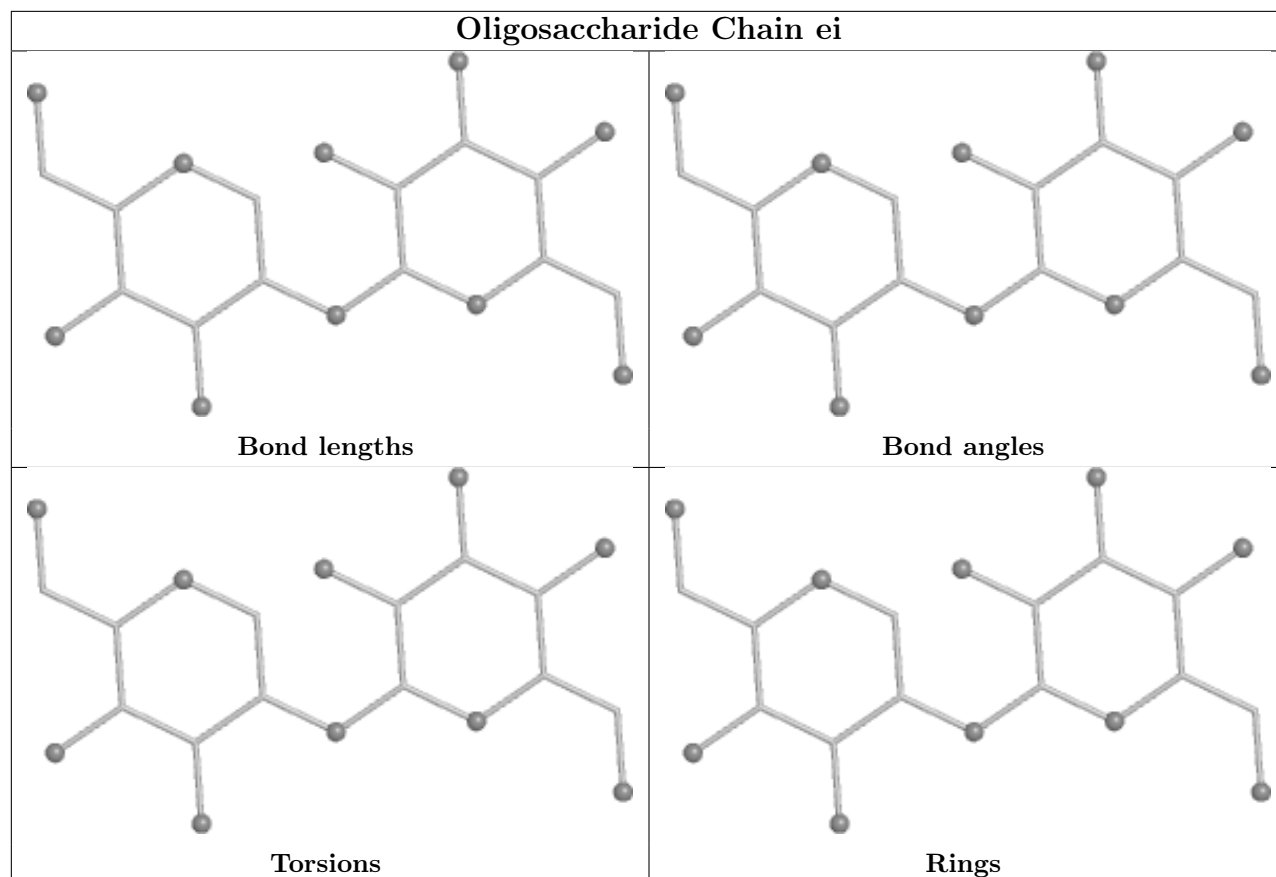


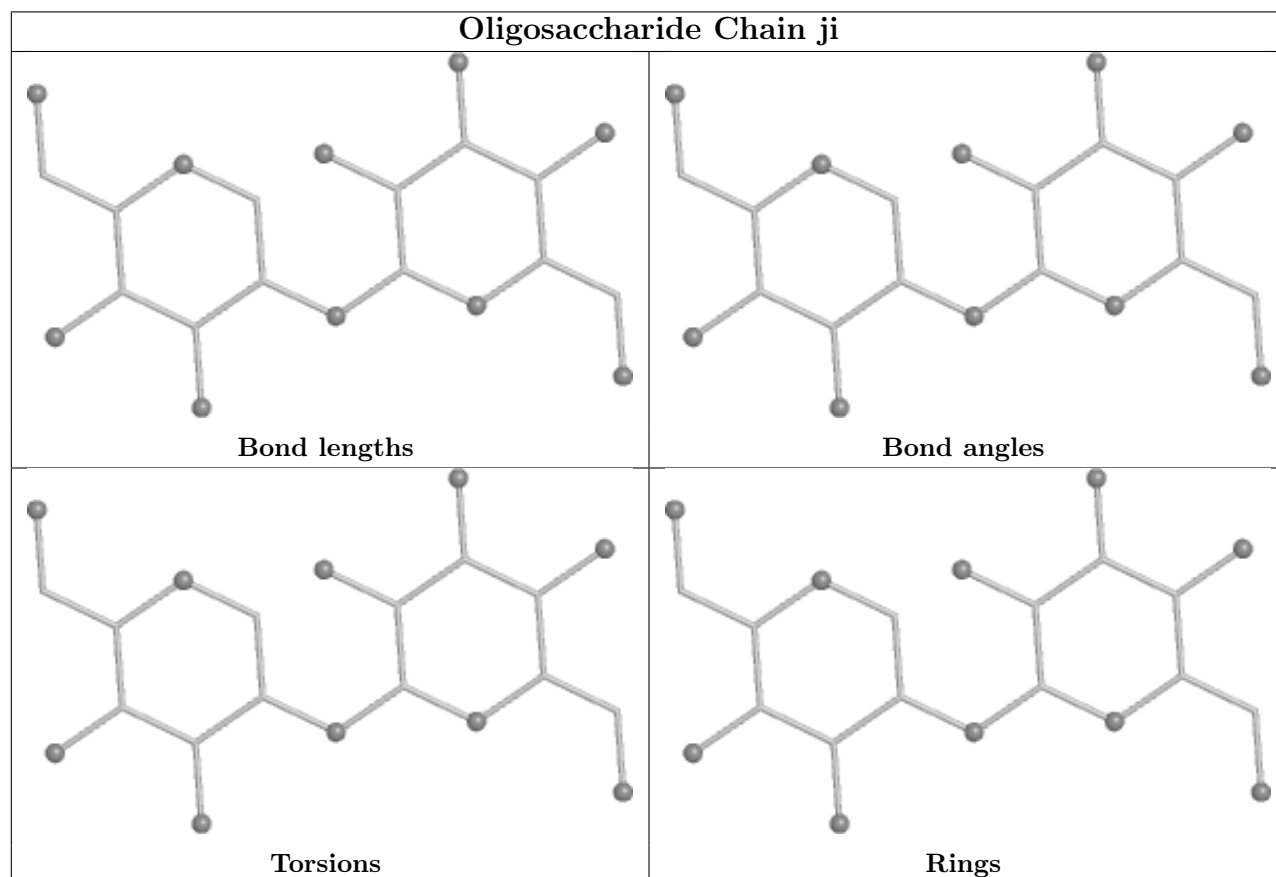
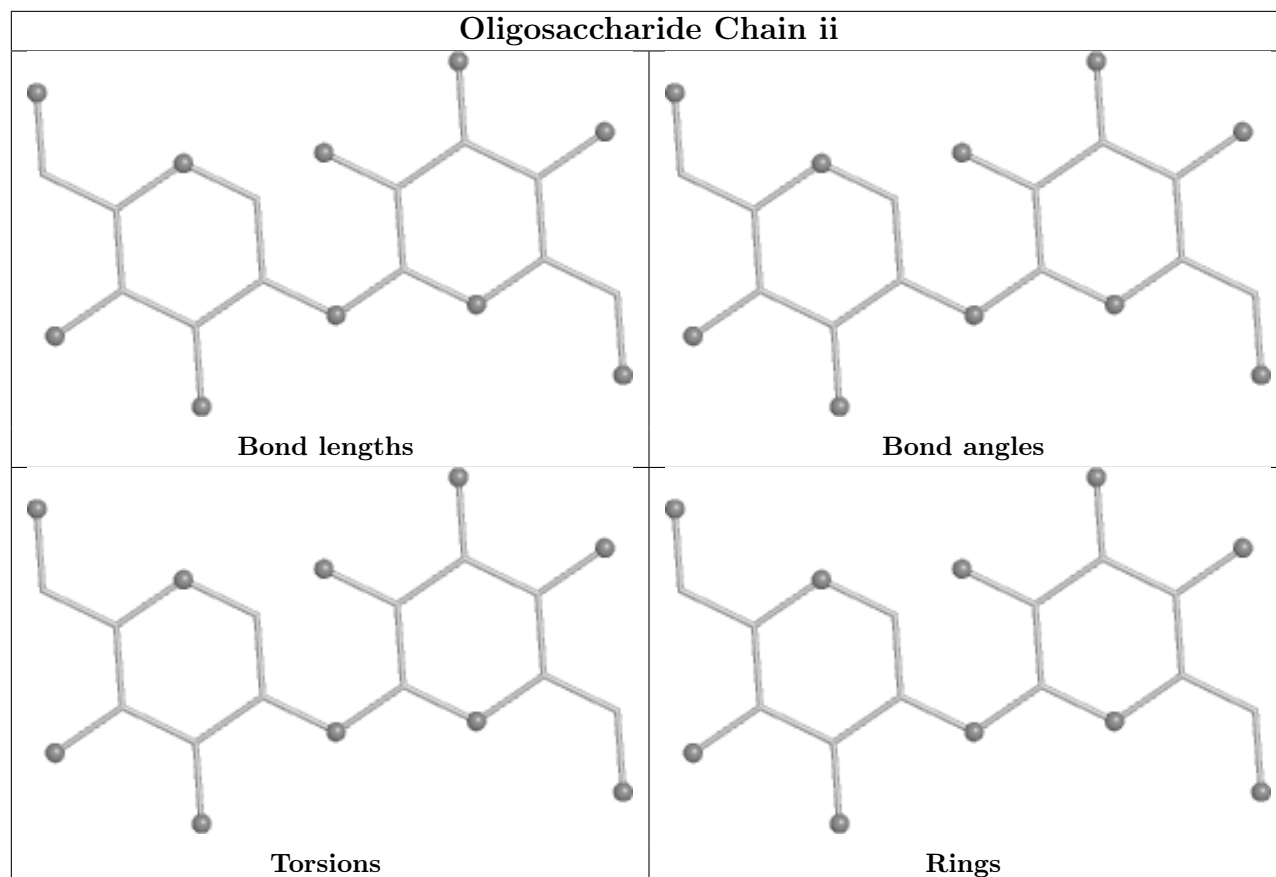
Oligosaccharide Chain Yi

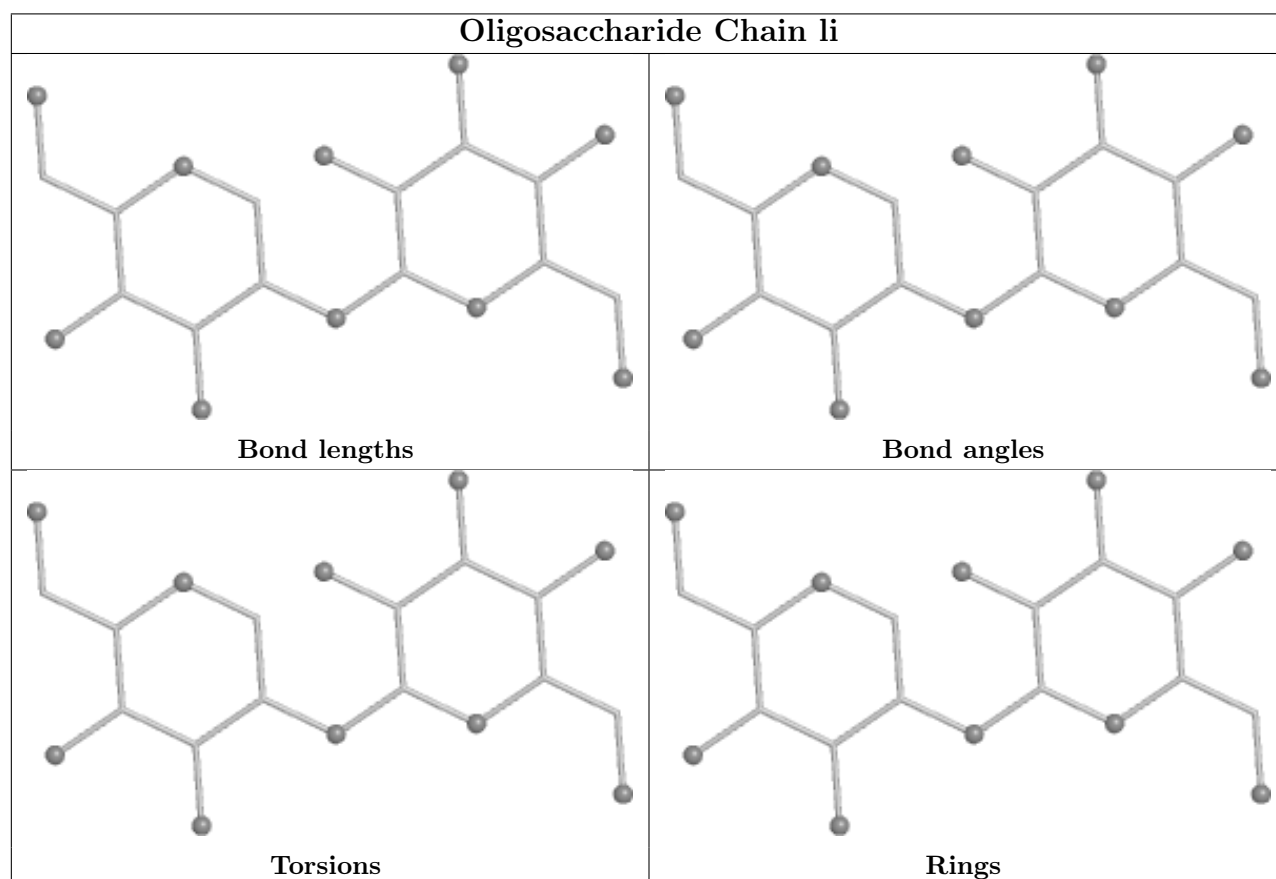
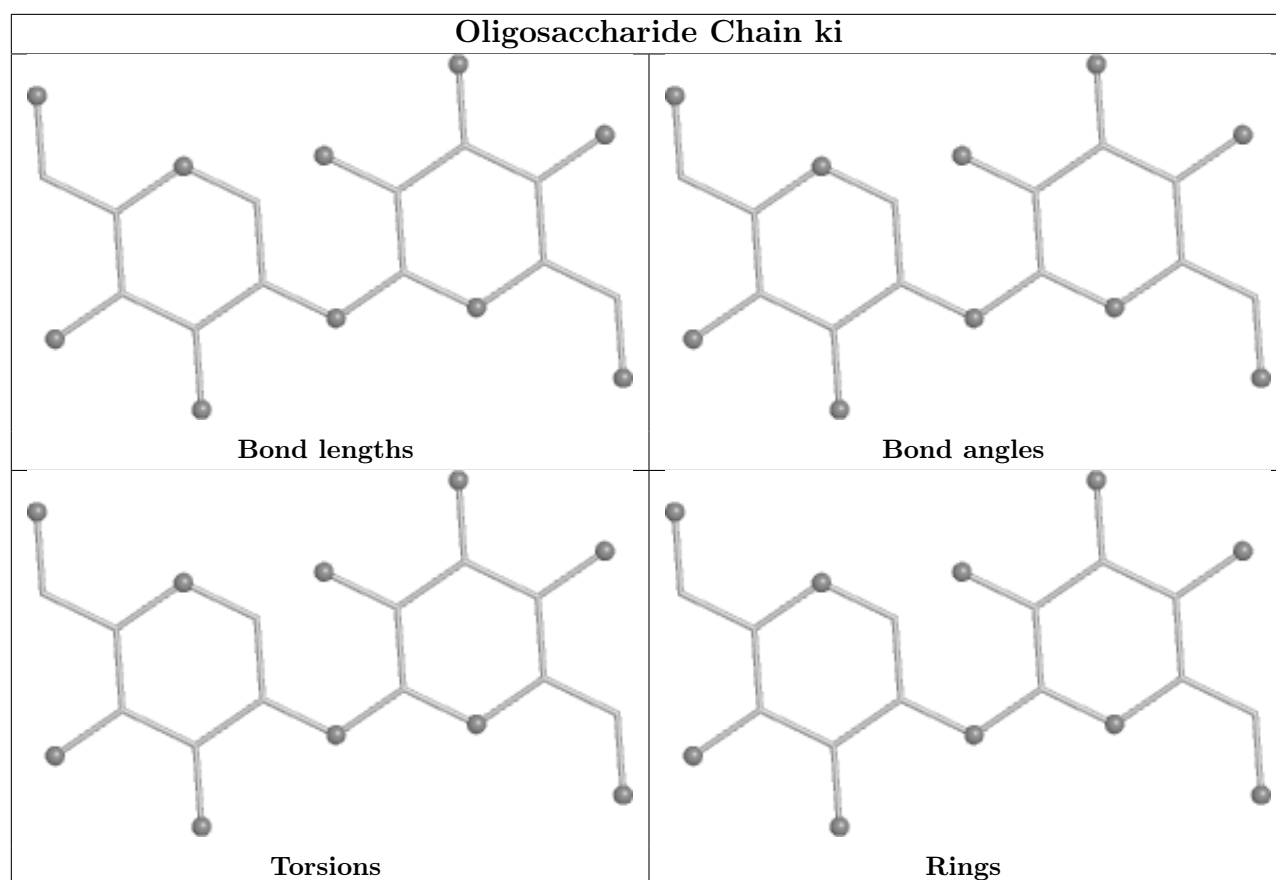


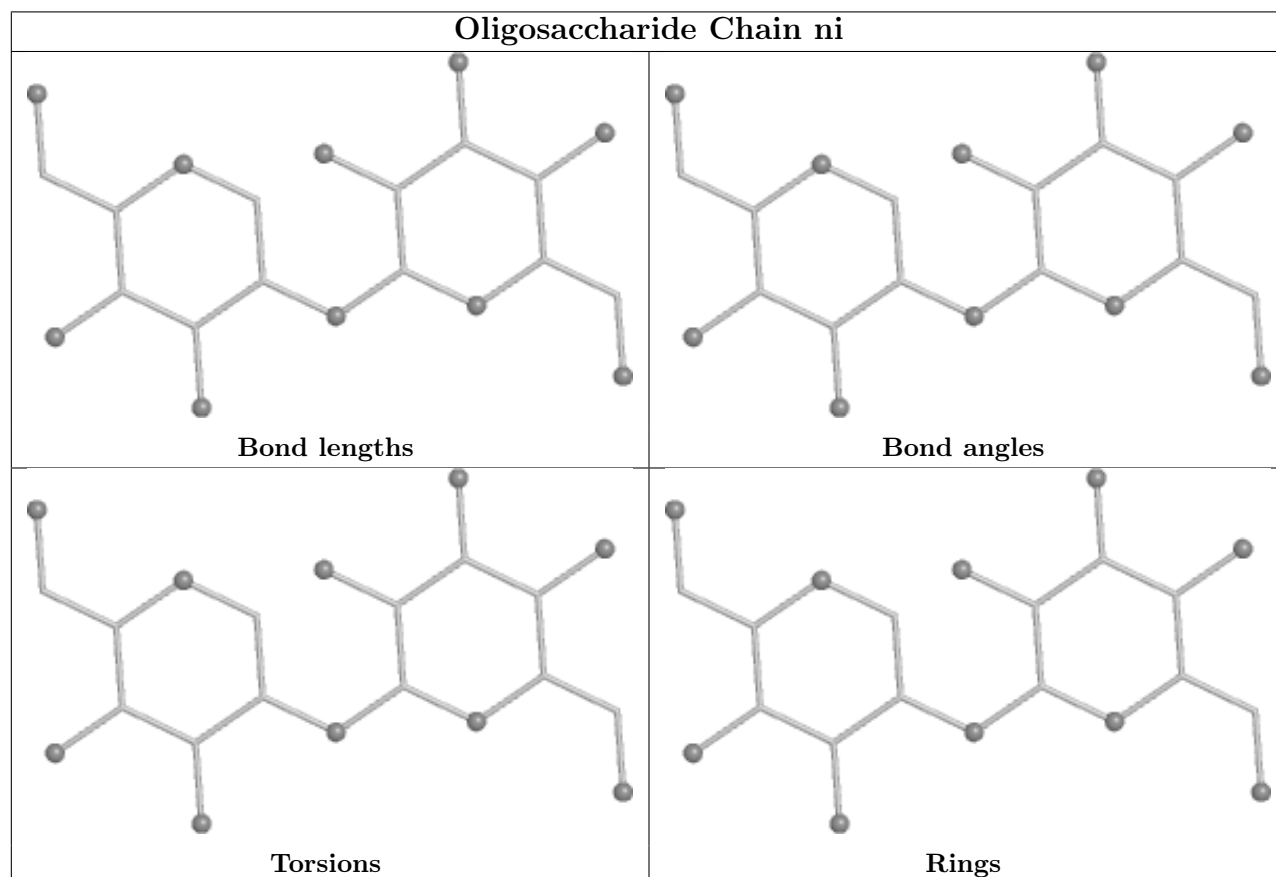
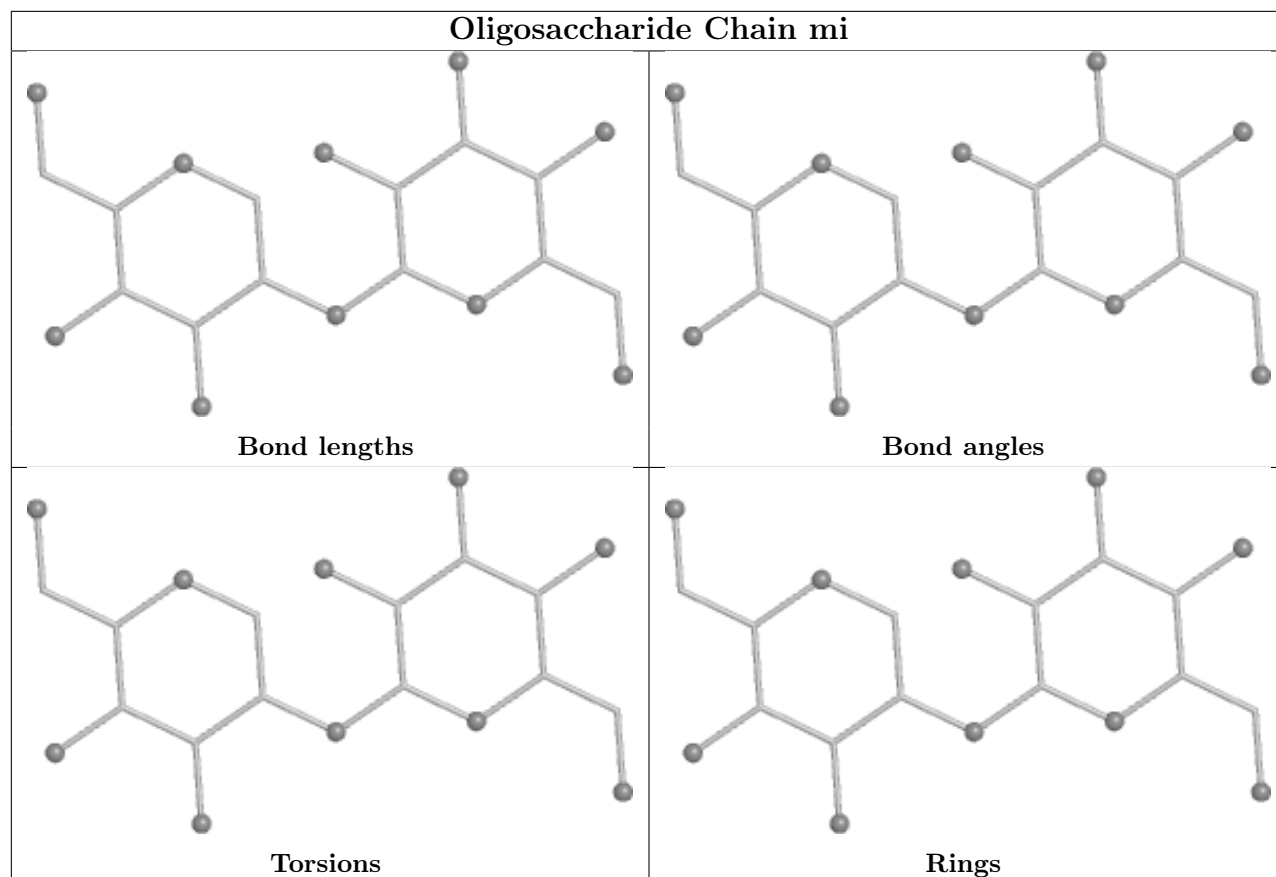


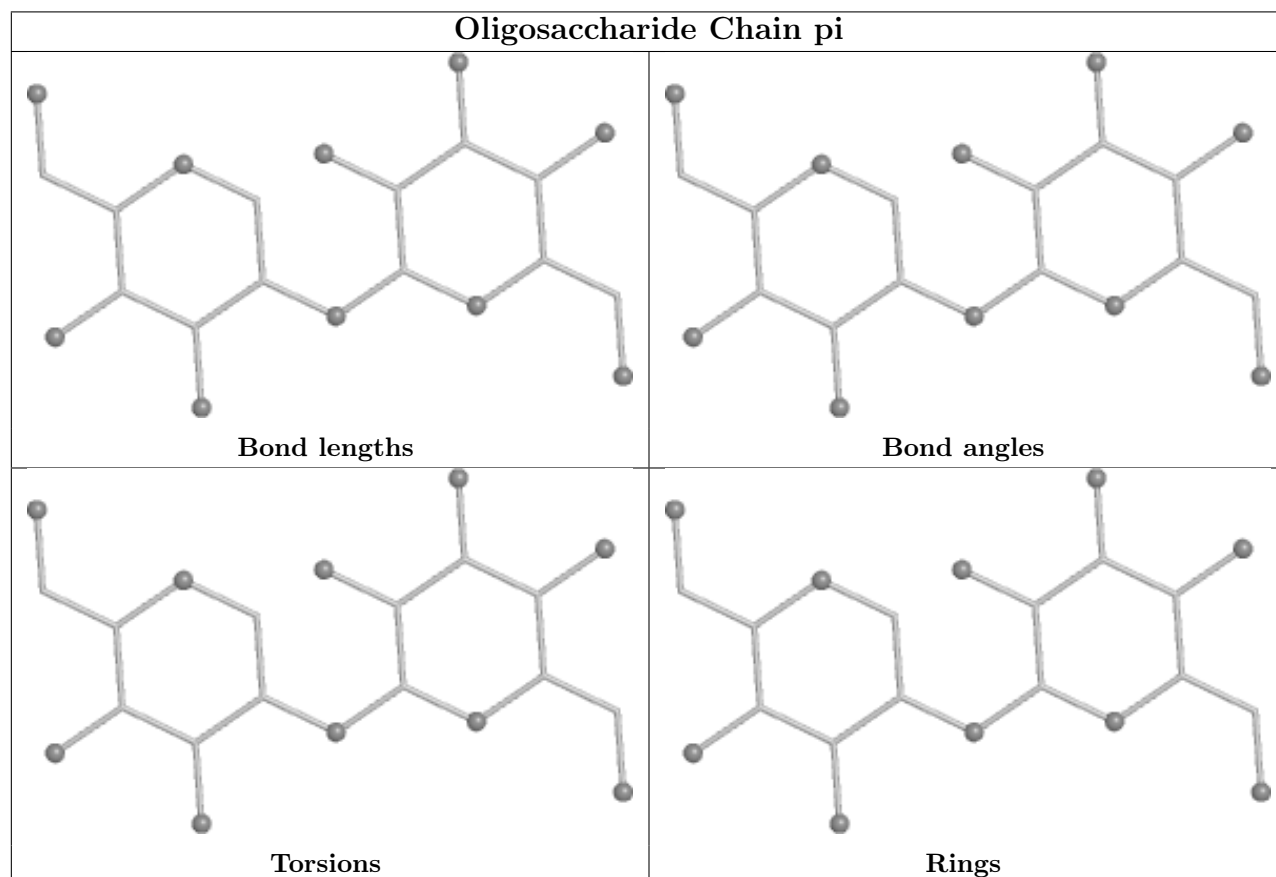
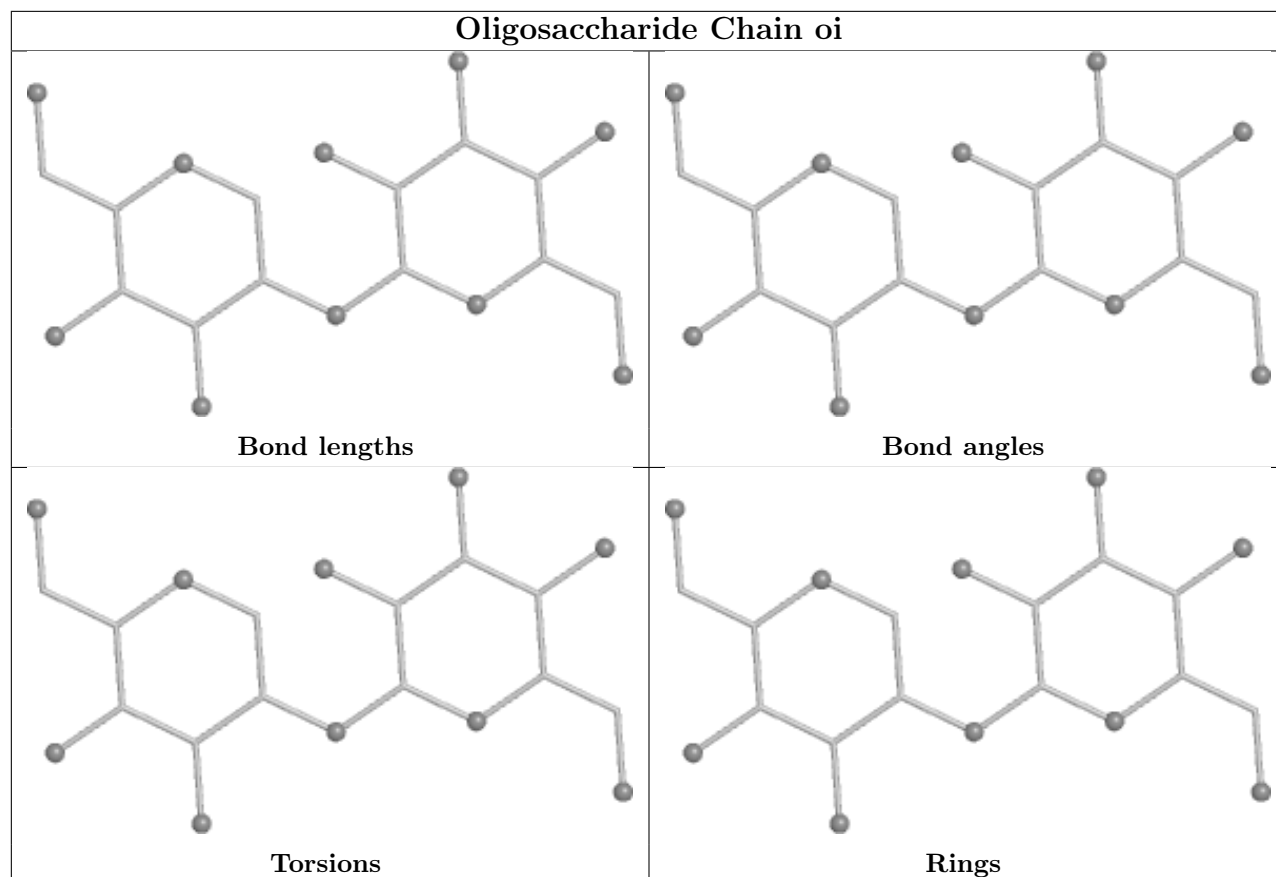


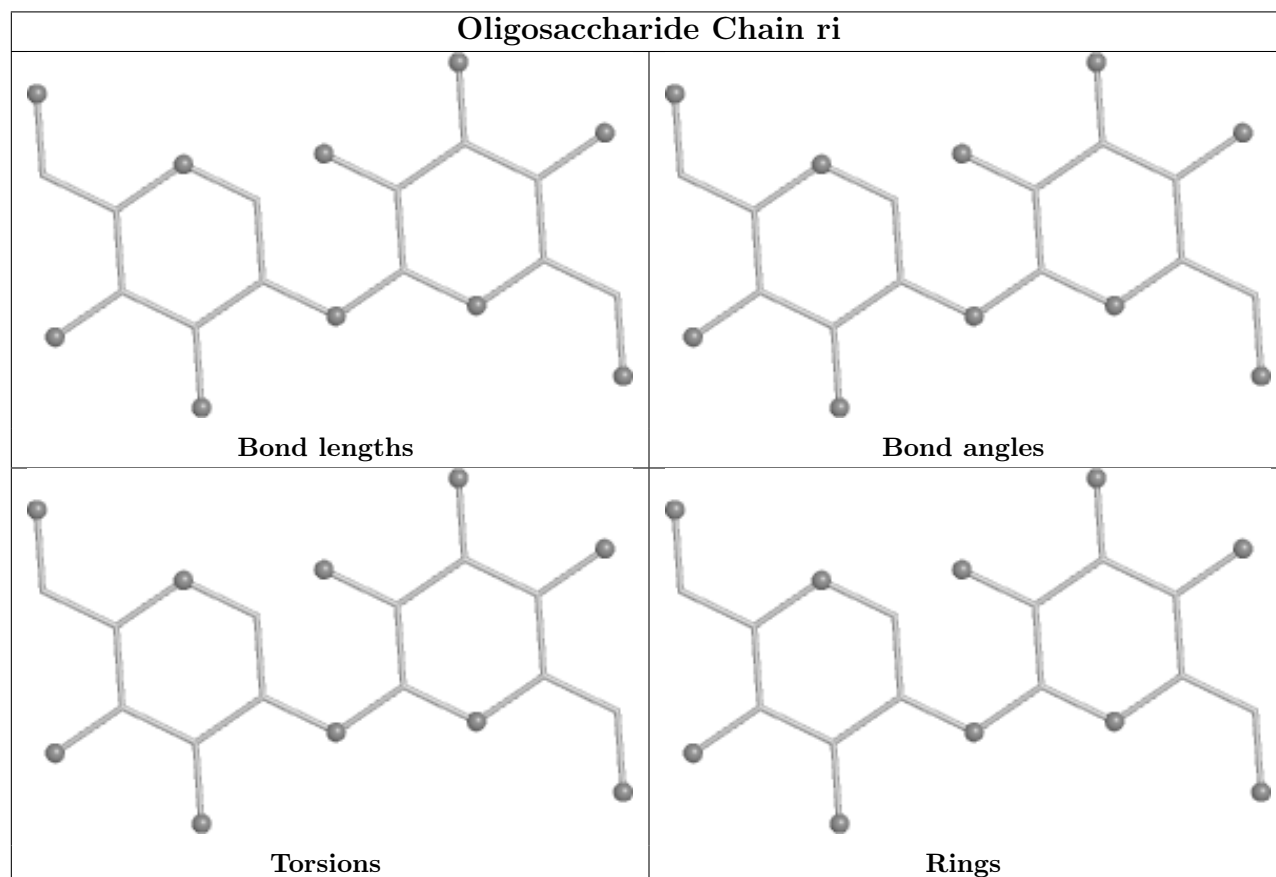
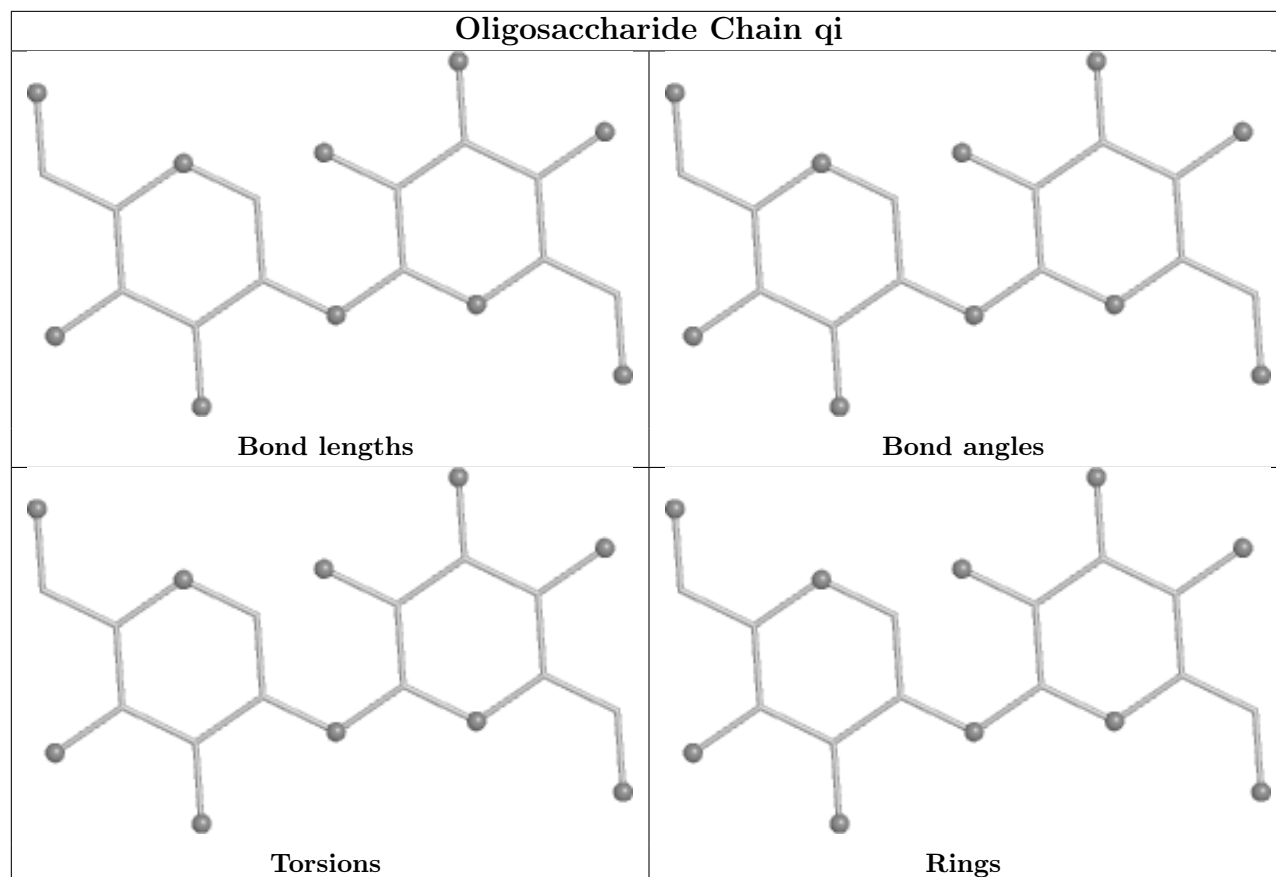




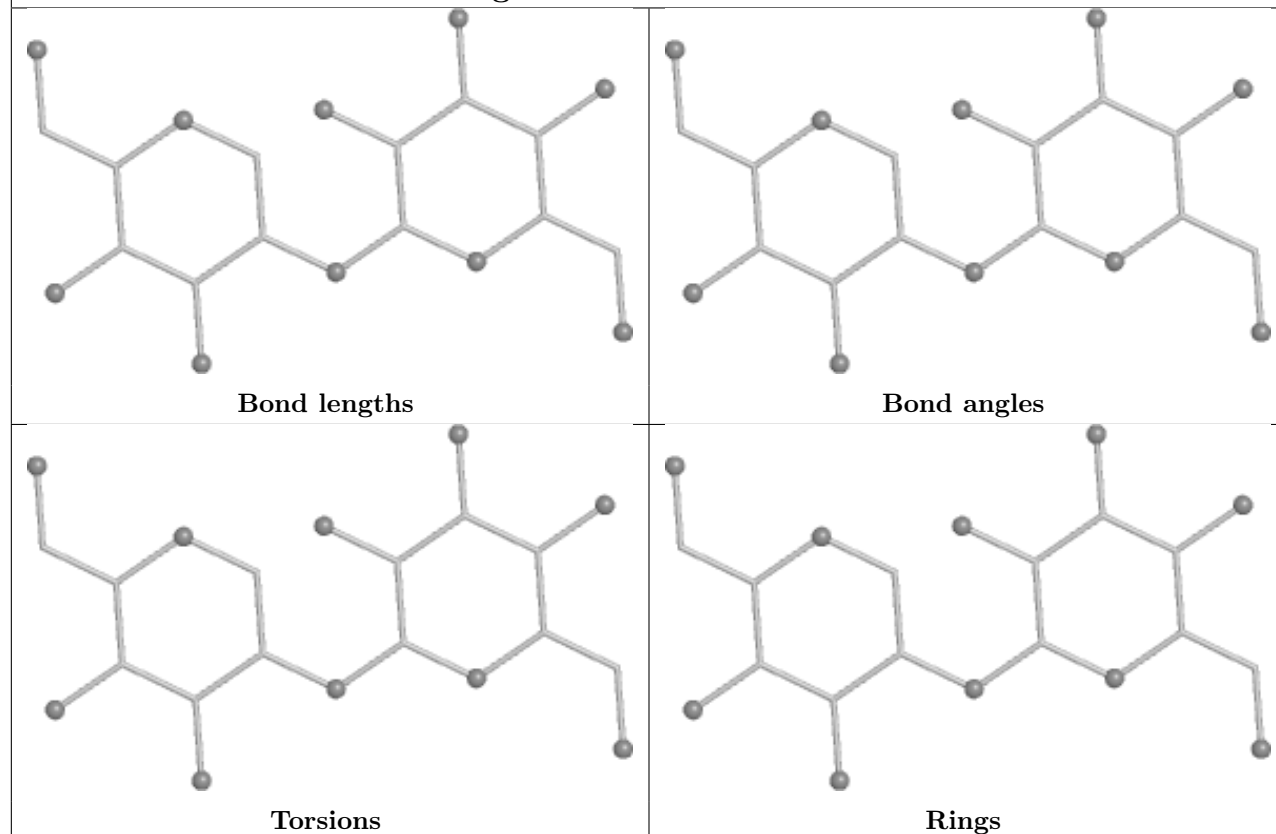




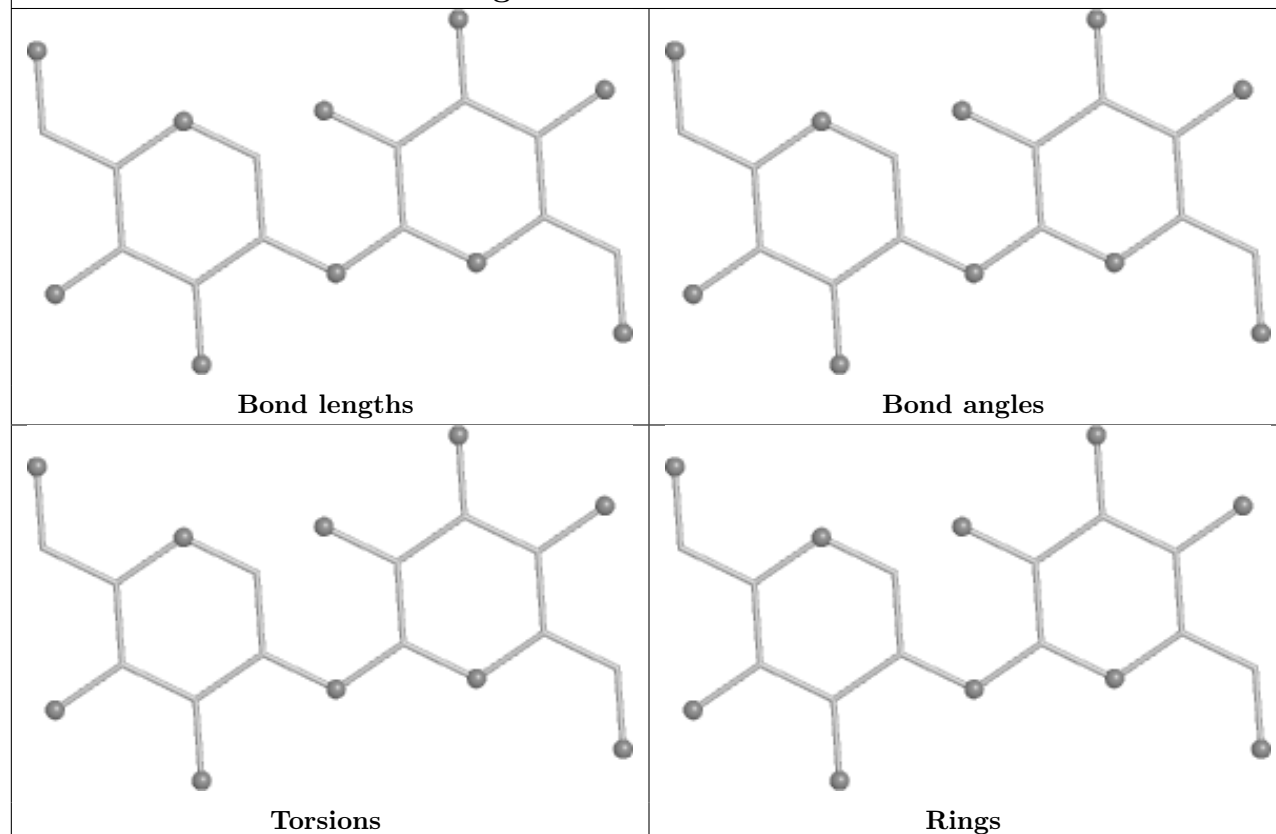




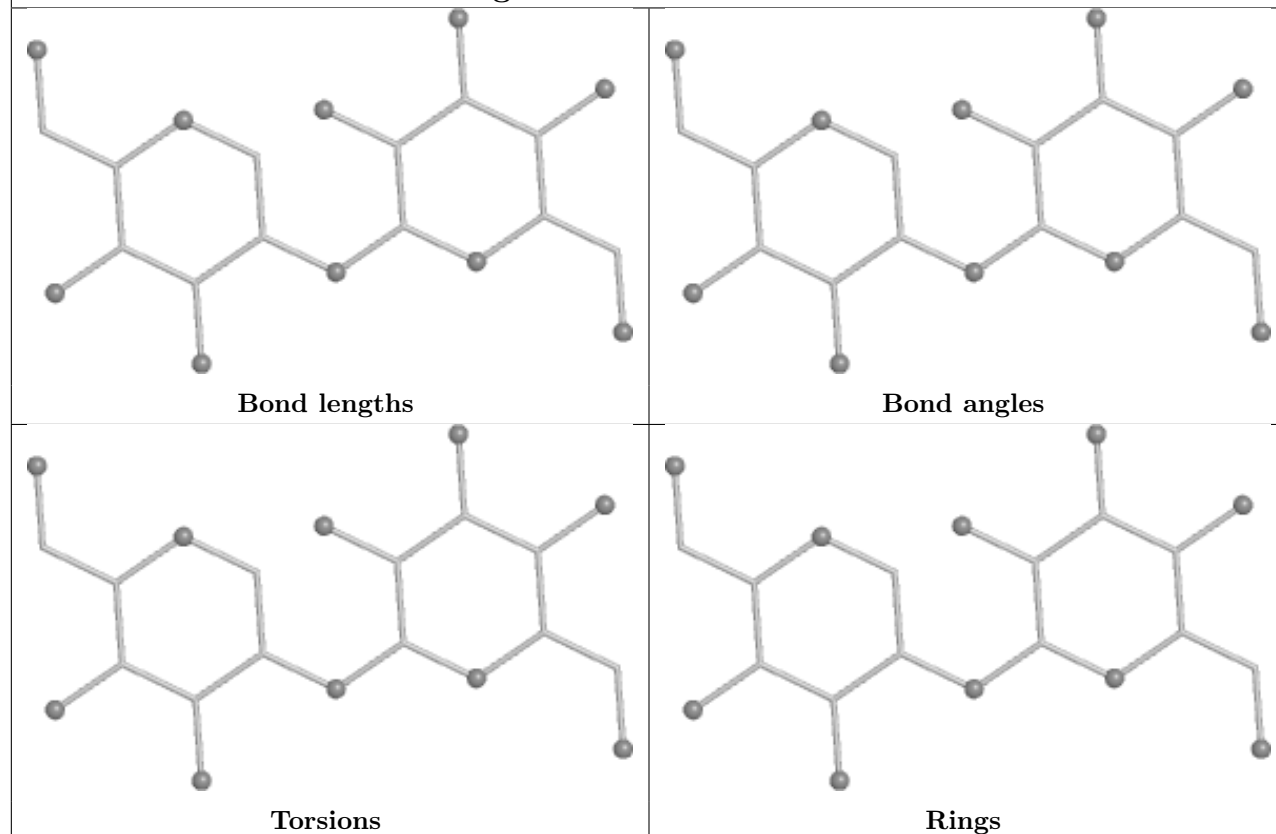
Oligosaccharide Chain Ab



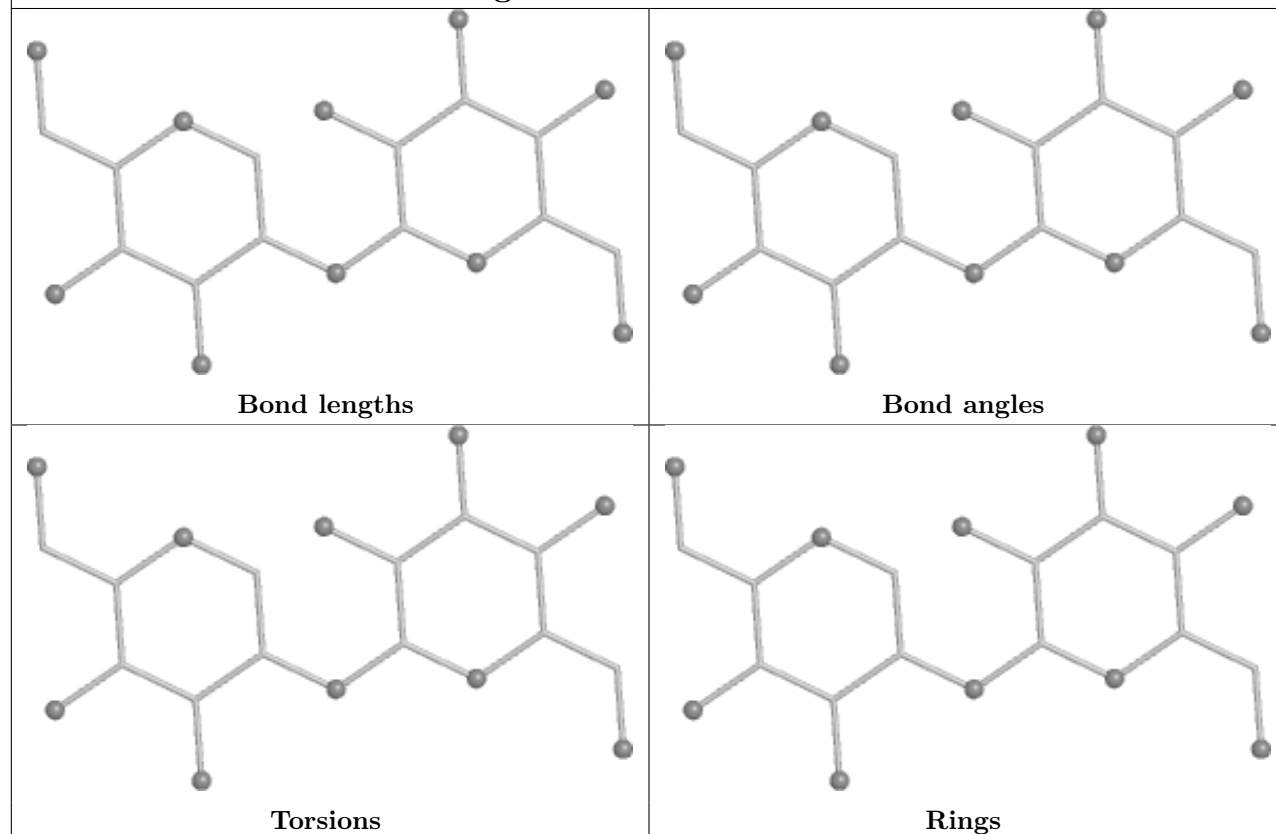
Oligosaccharide Chain Bb



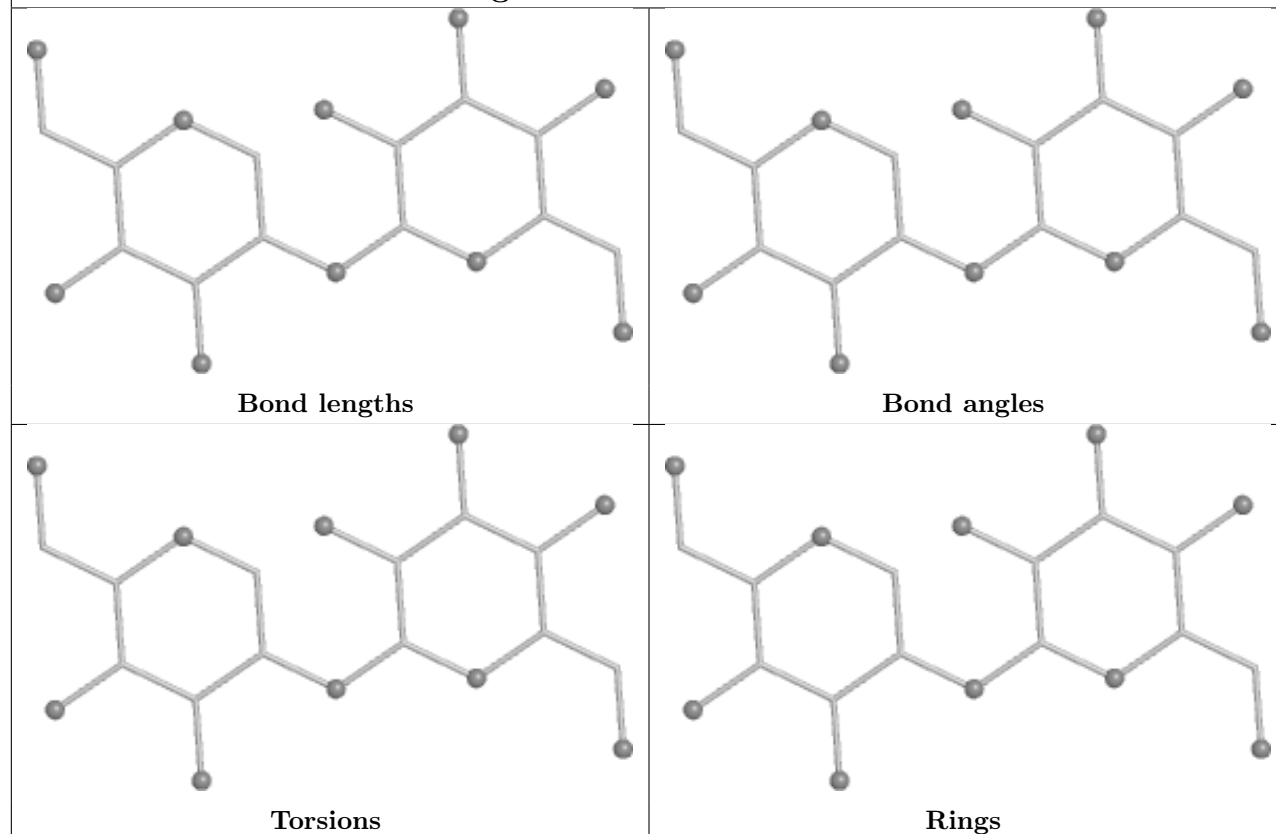
Oligosaccharide Chain Cb



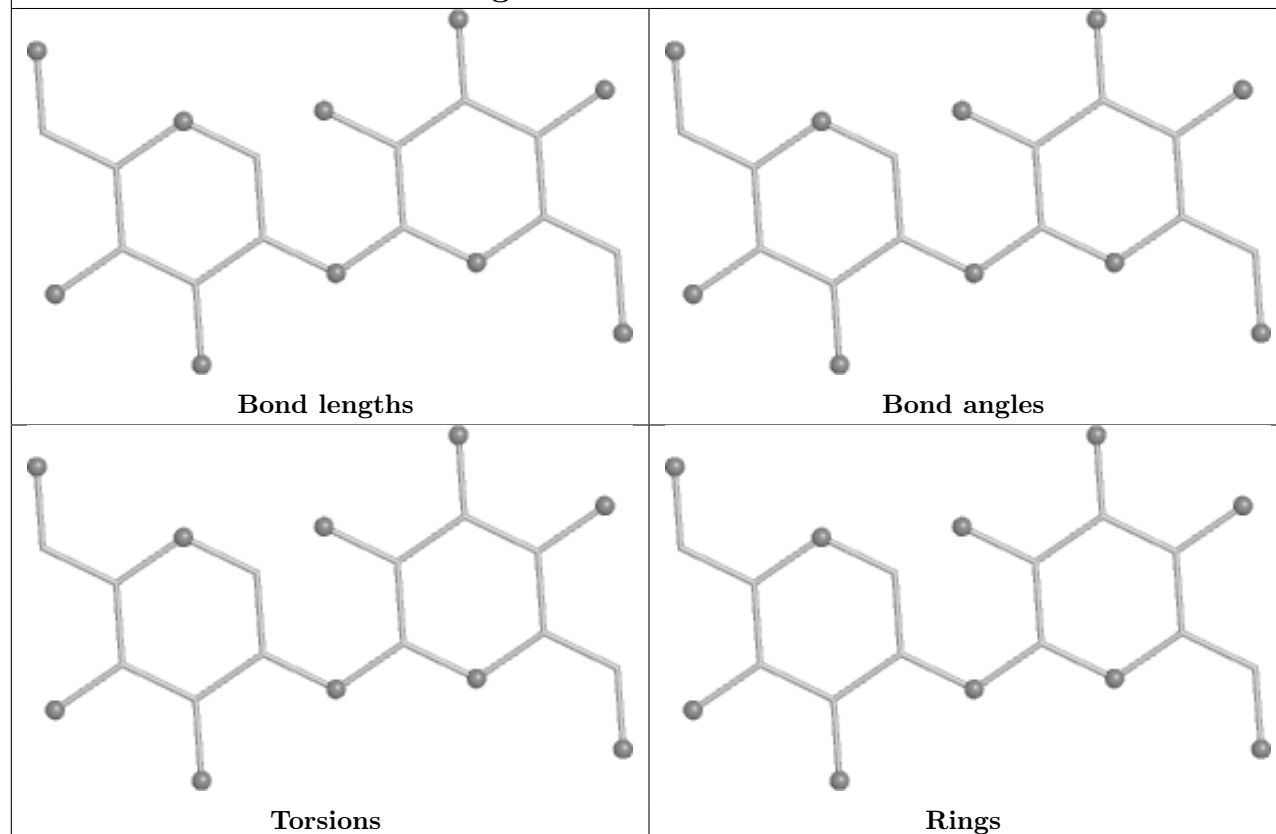
Oligosaccharide Chain Eb

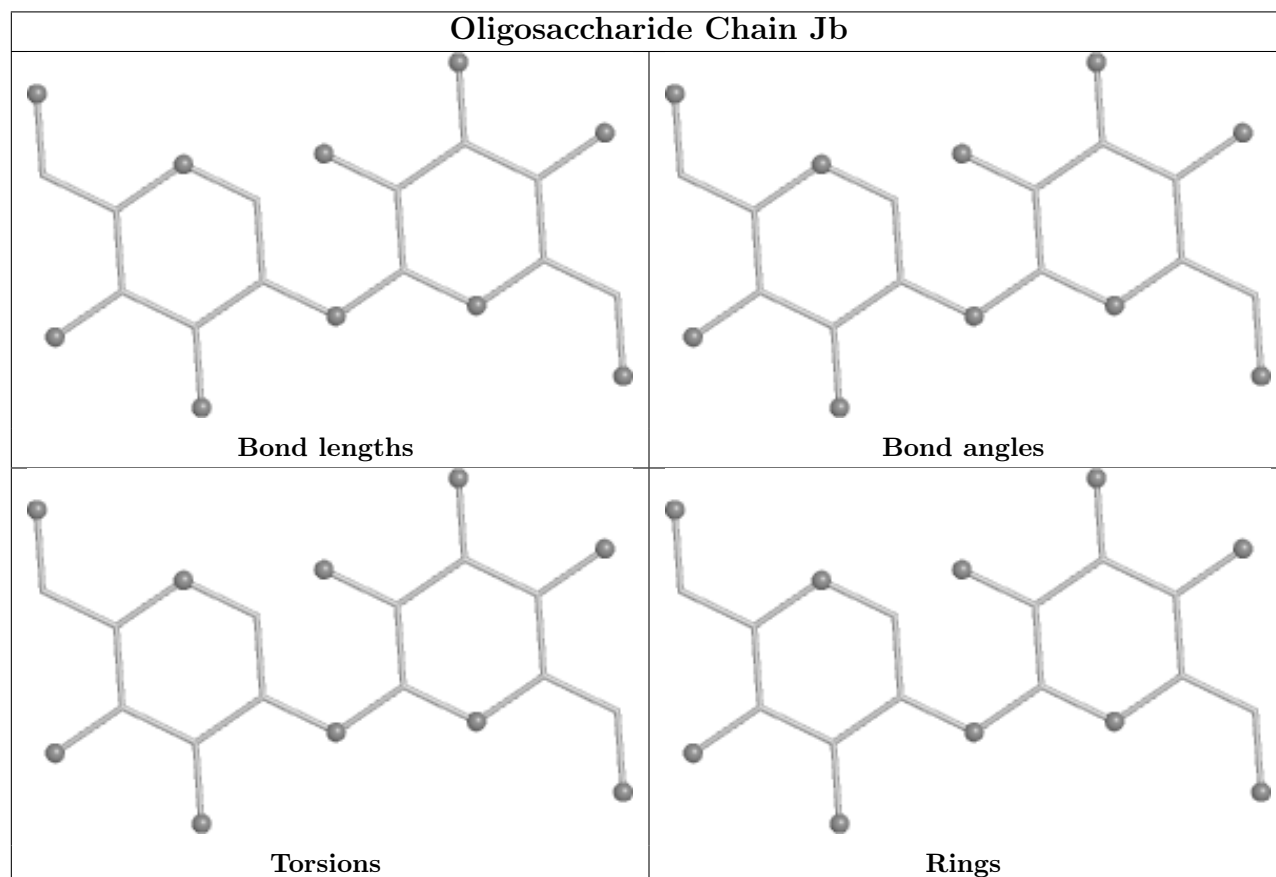
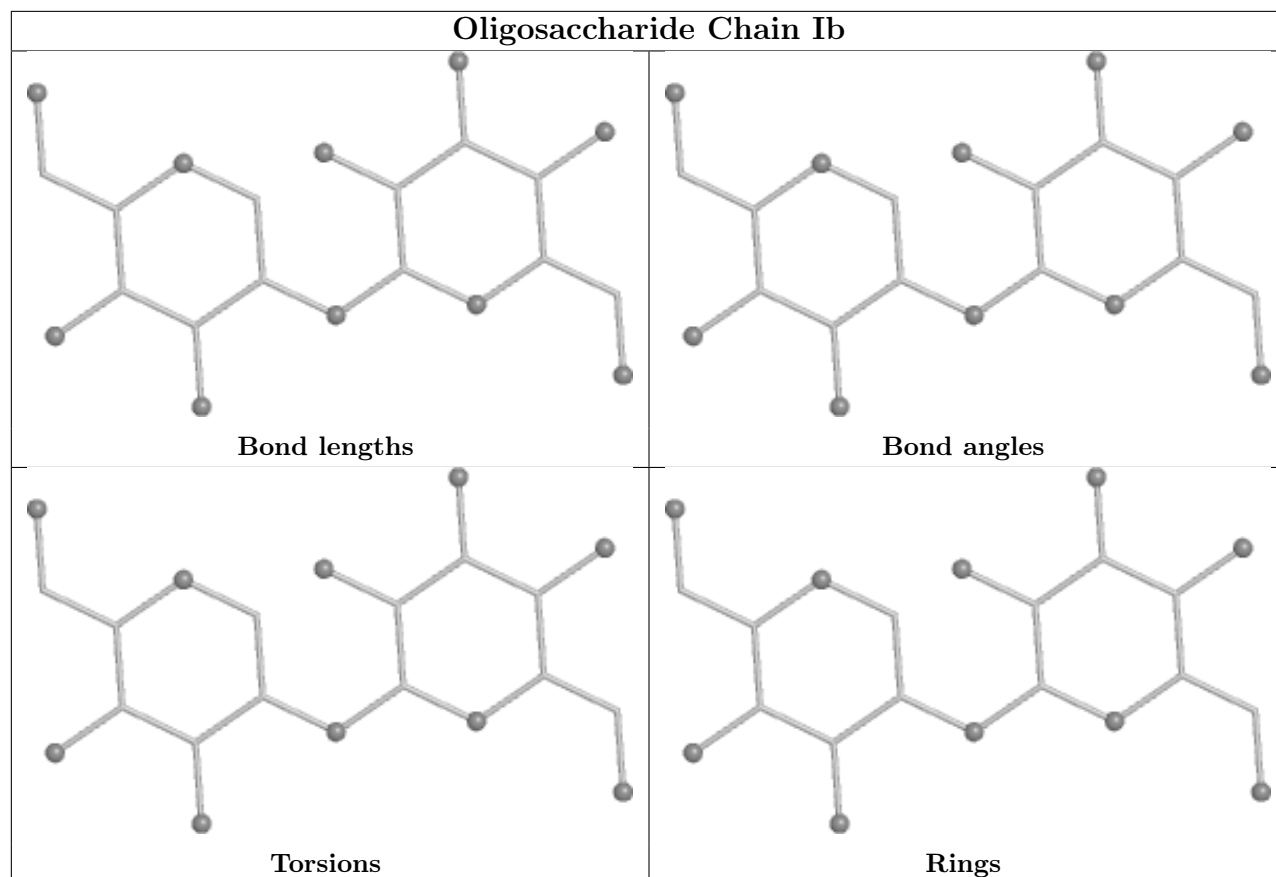


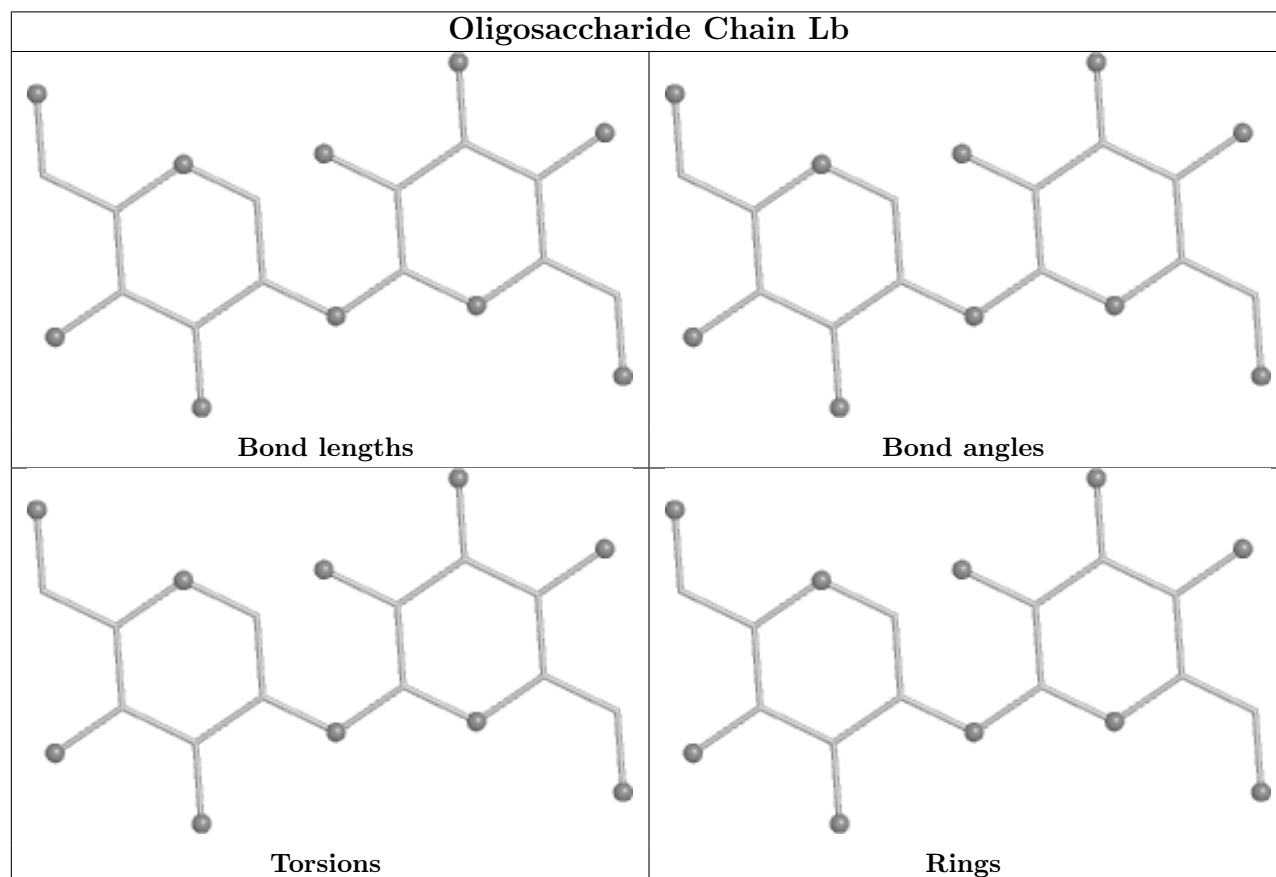
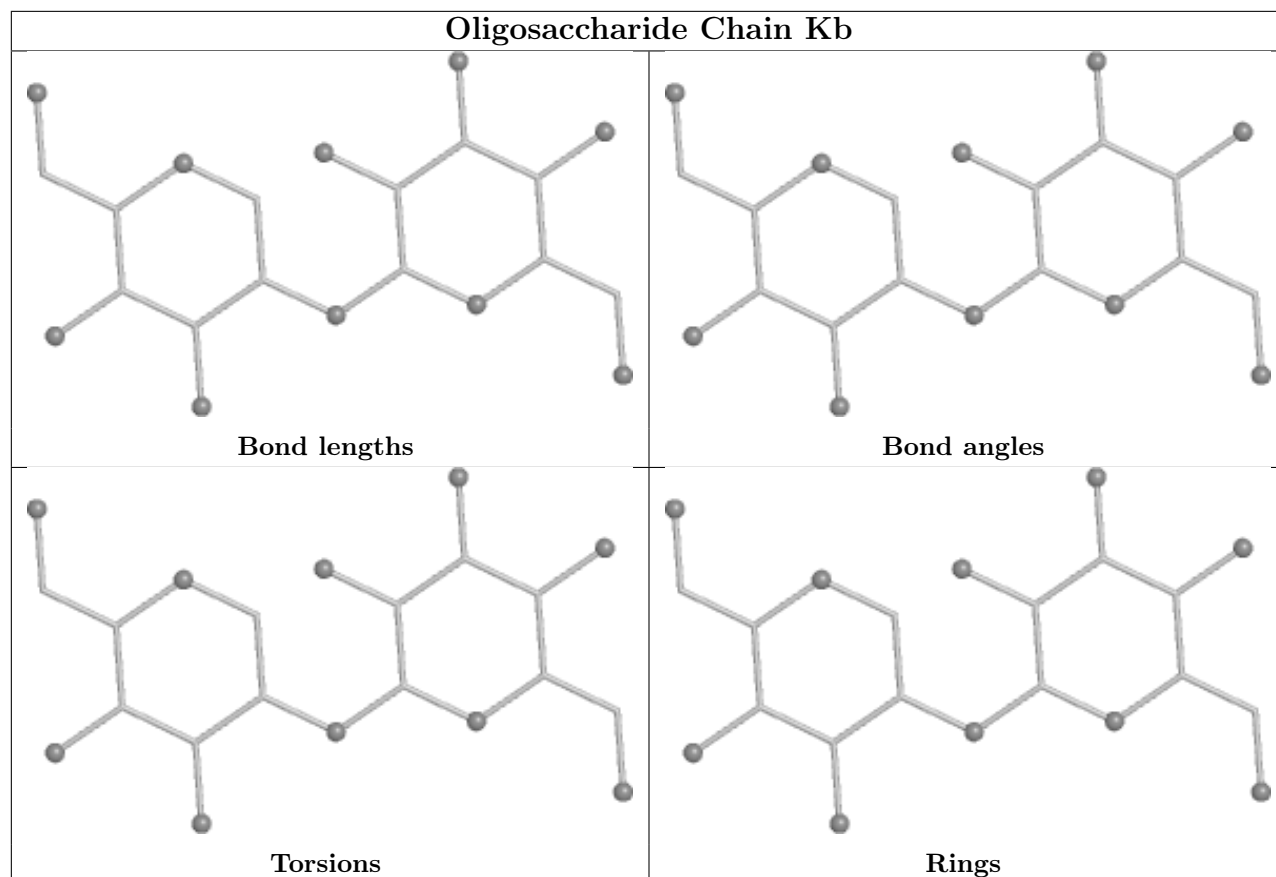
Oligosaccharide Chain Gb

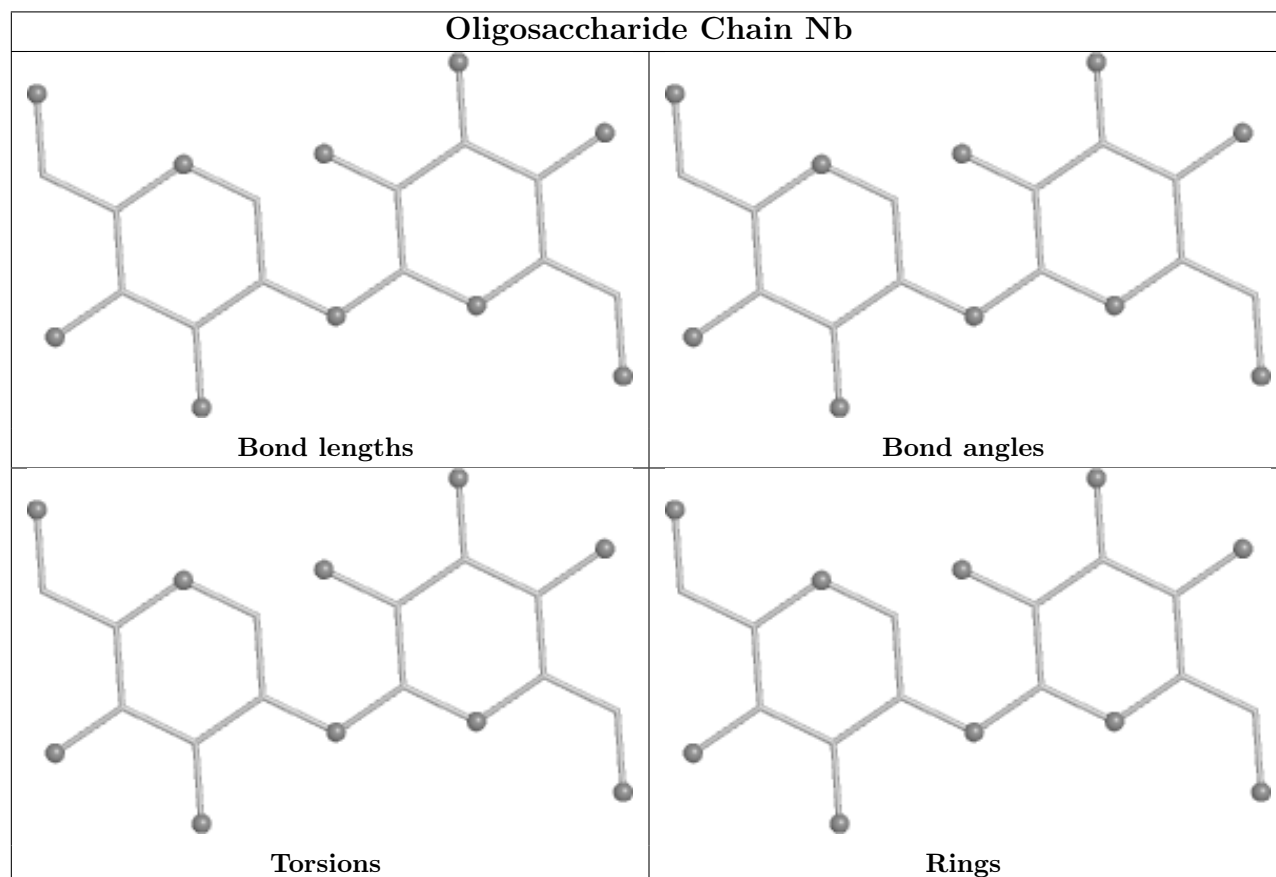
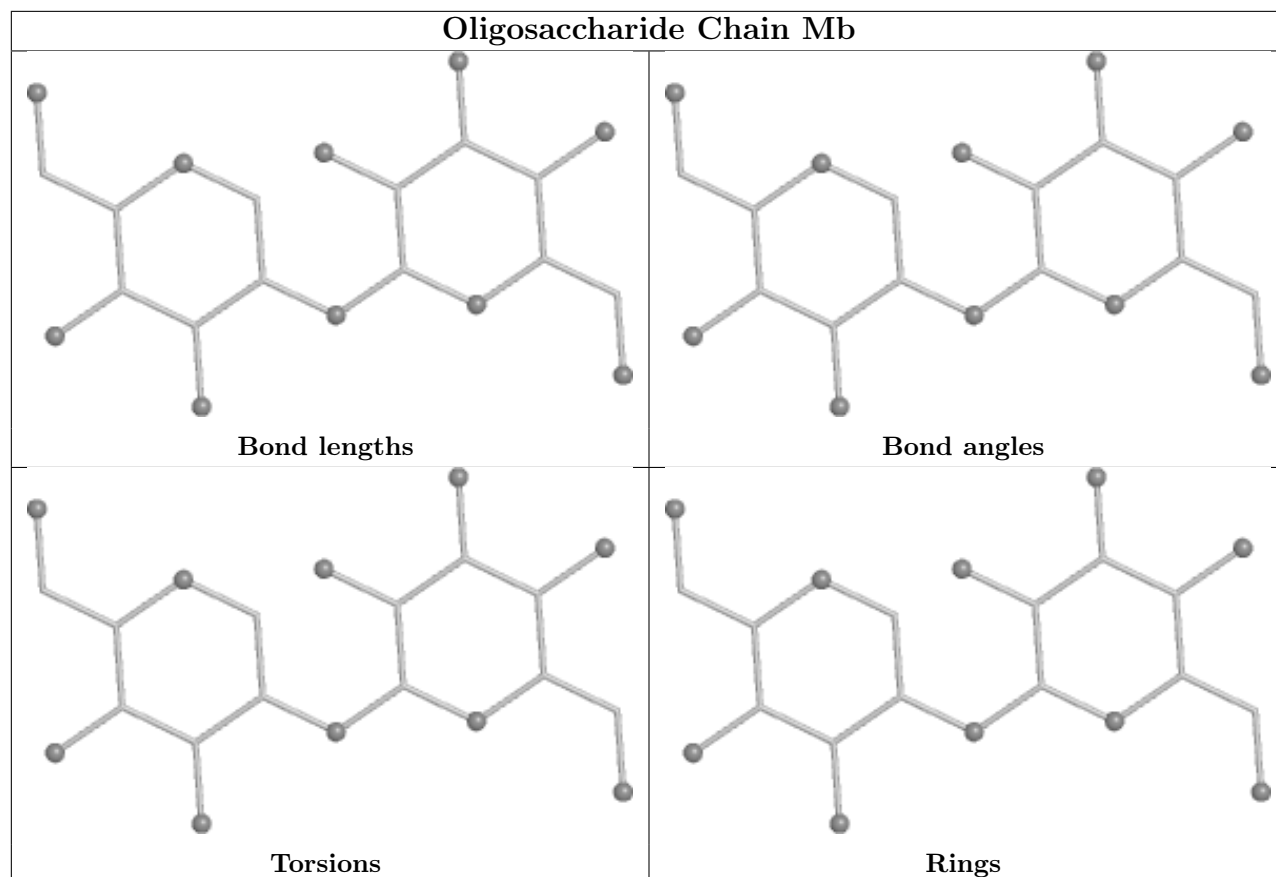


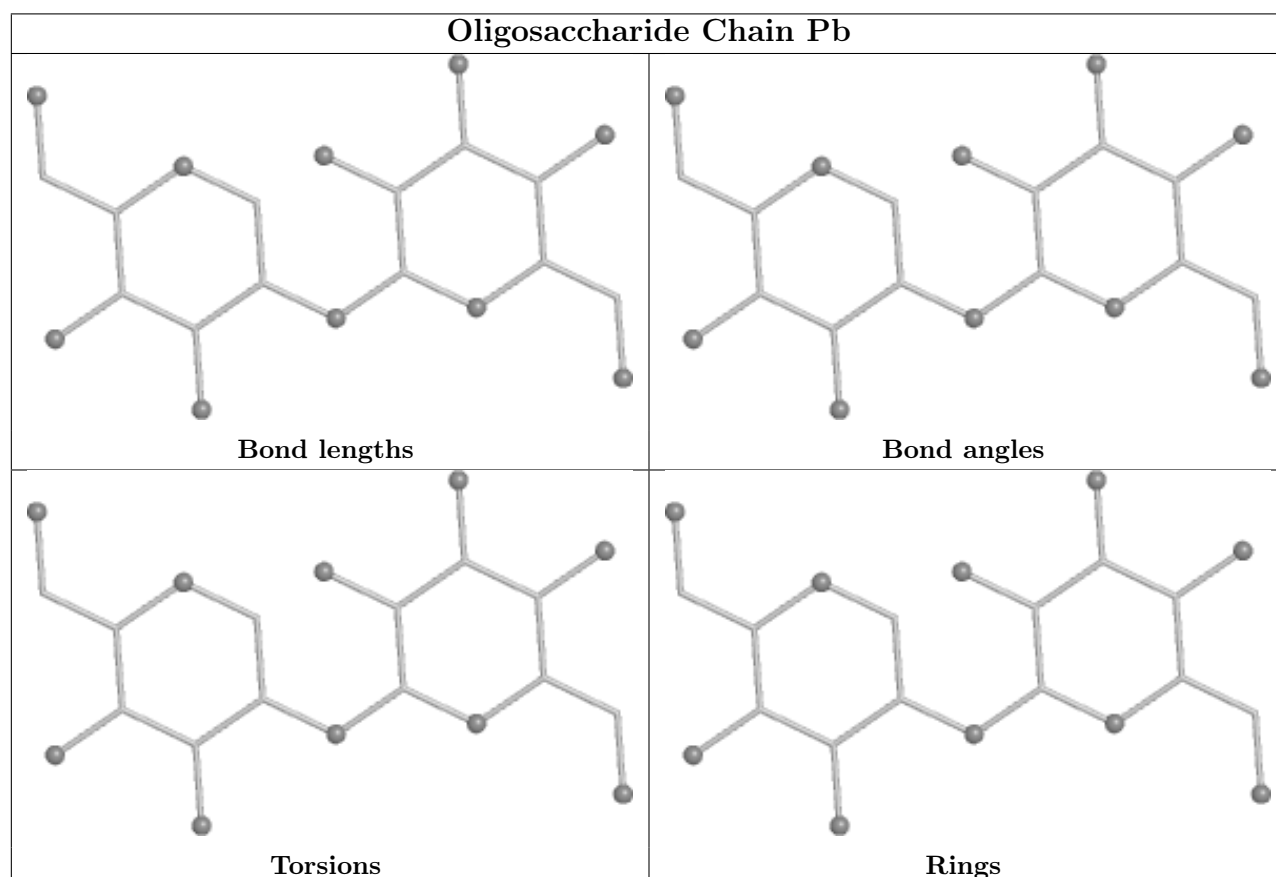
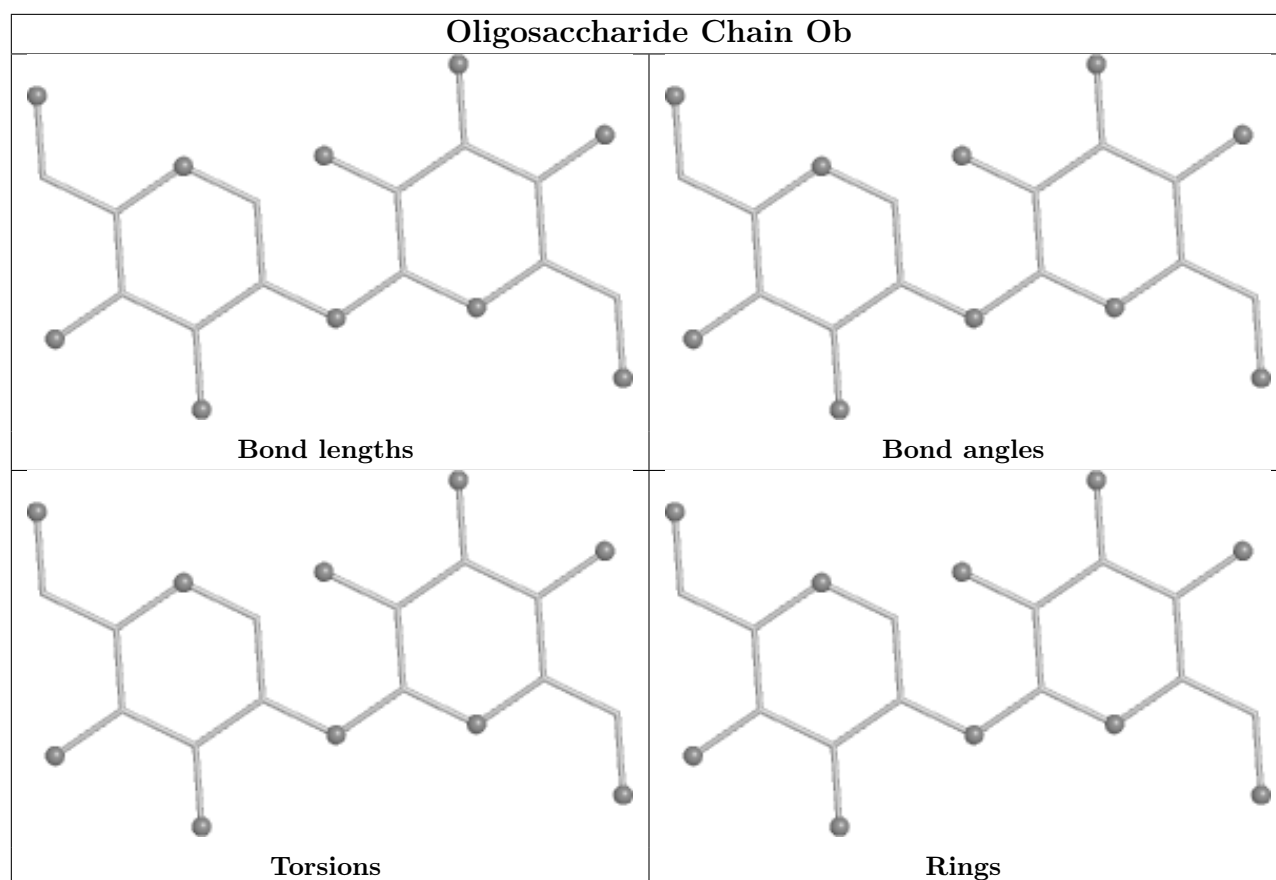
Oligosaccharide Chain Hb



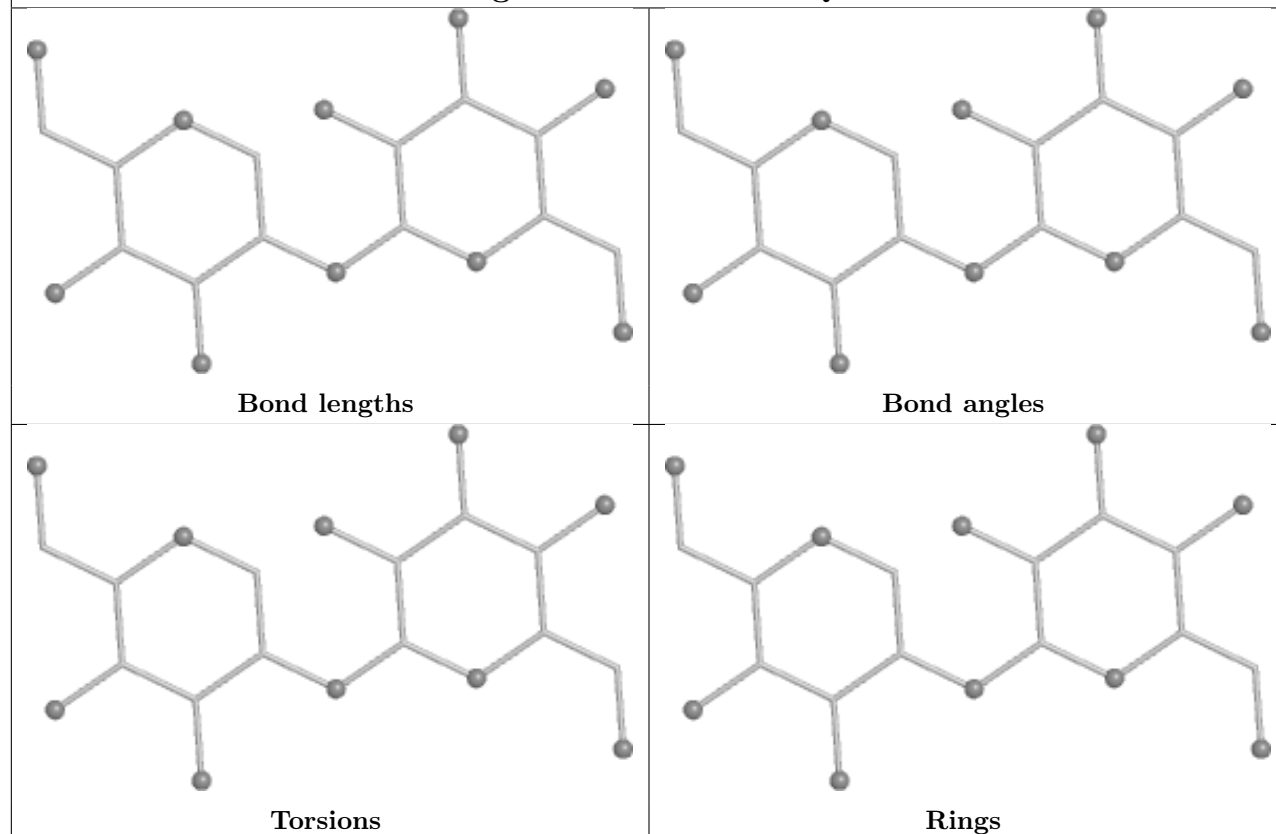




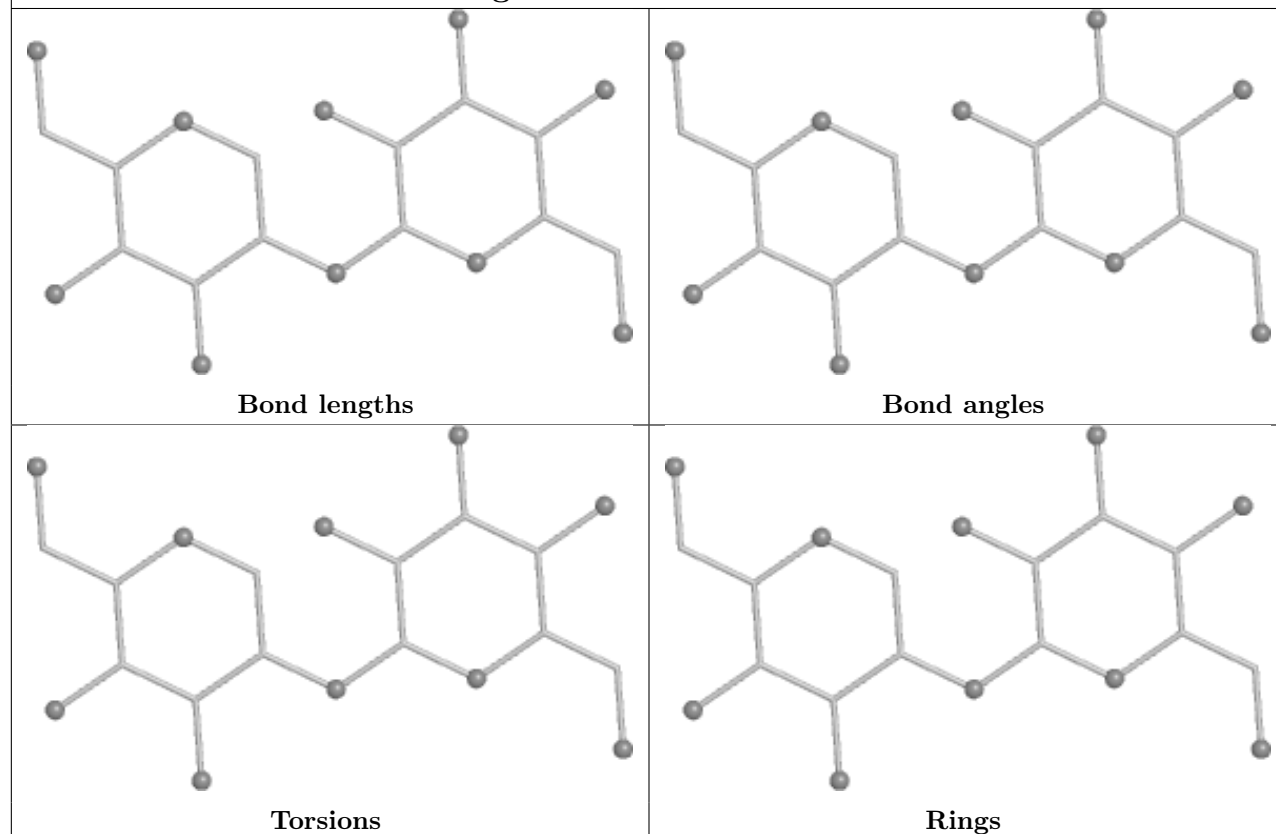




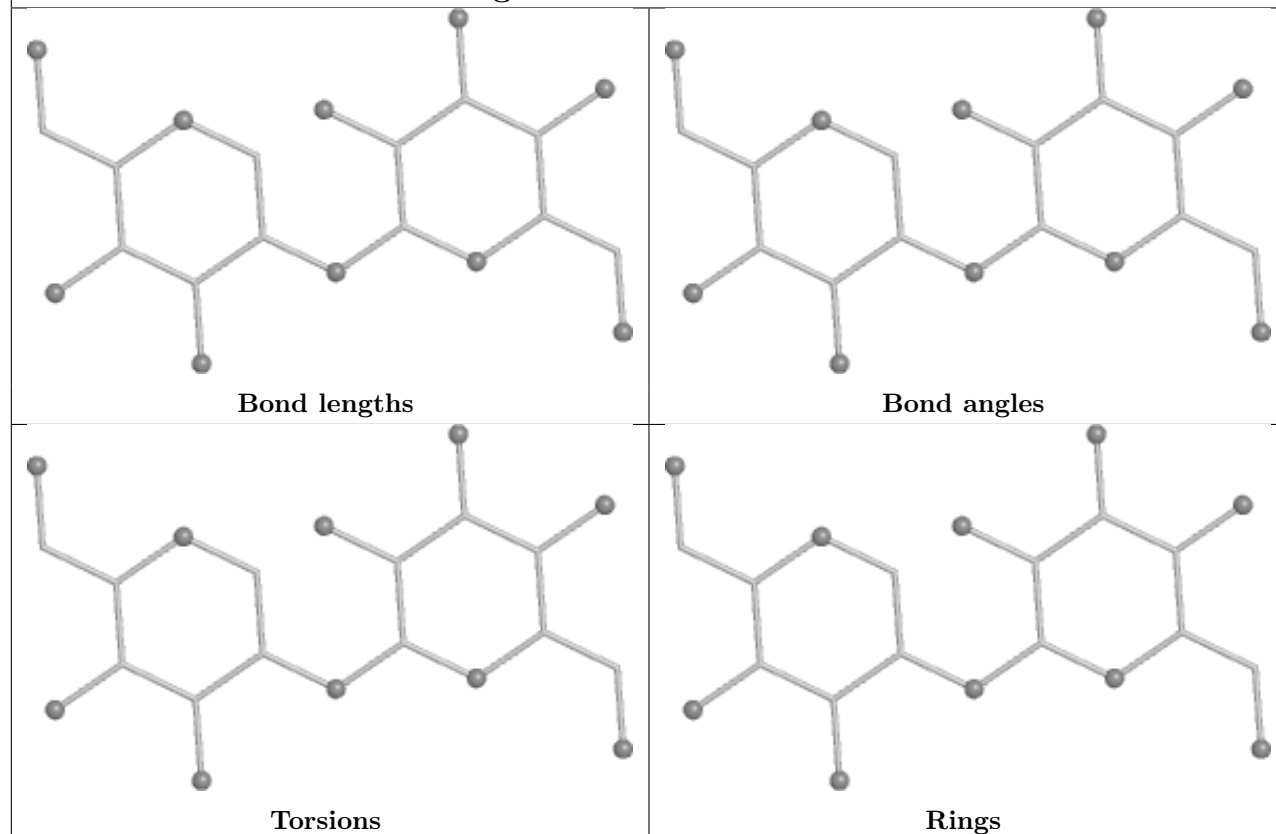
Oligosaccharide Chain Qb



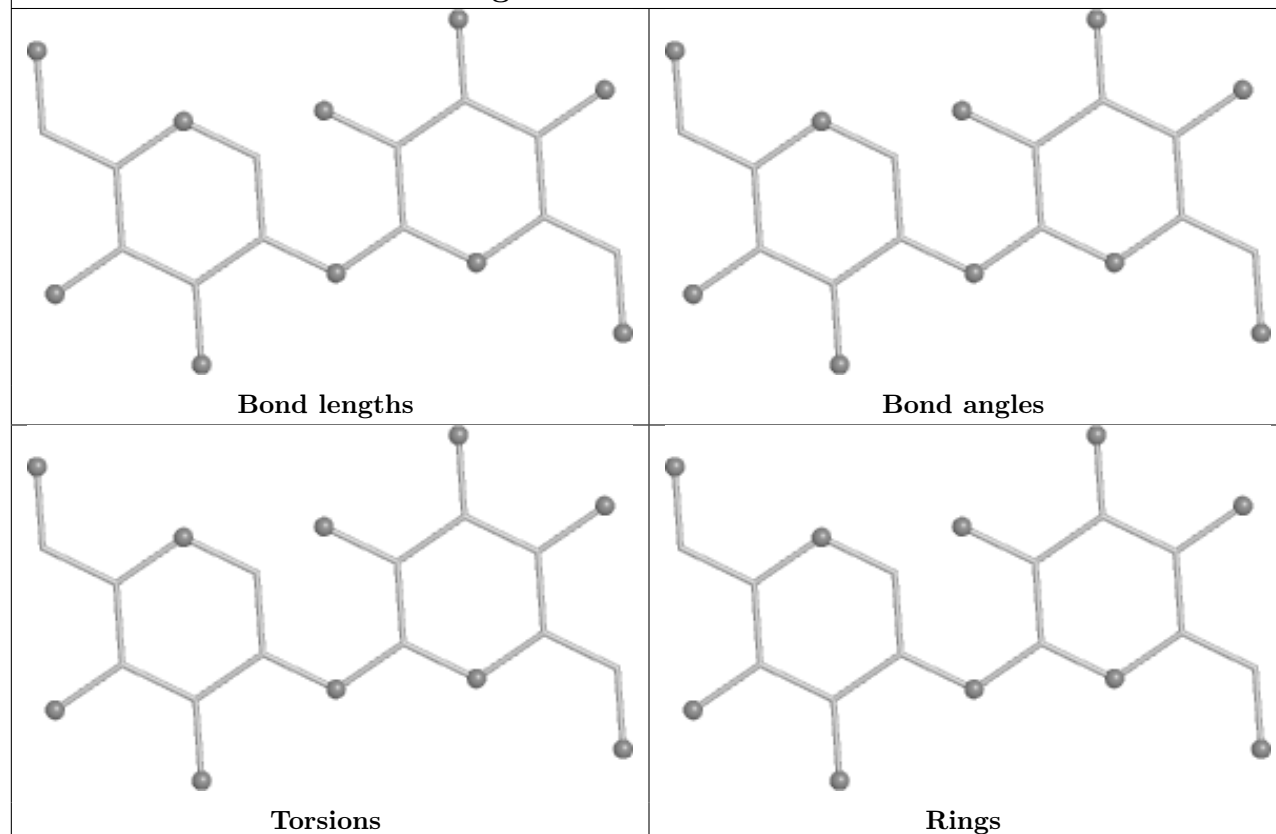
Oligosaccharide Chain Rb



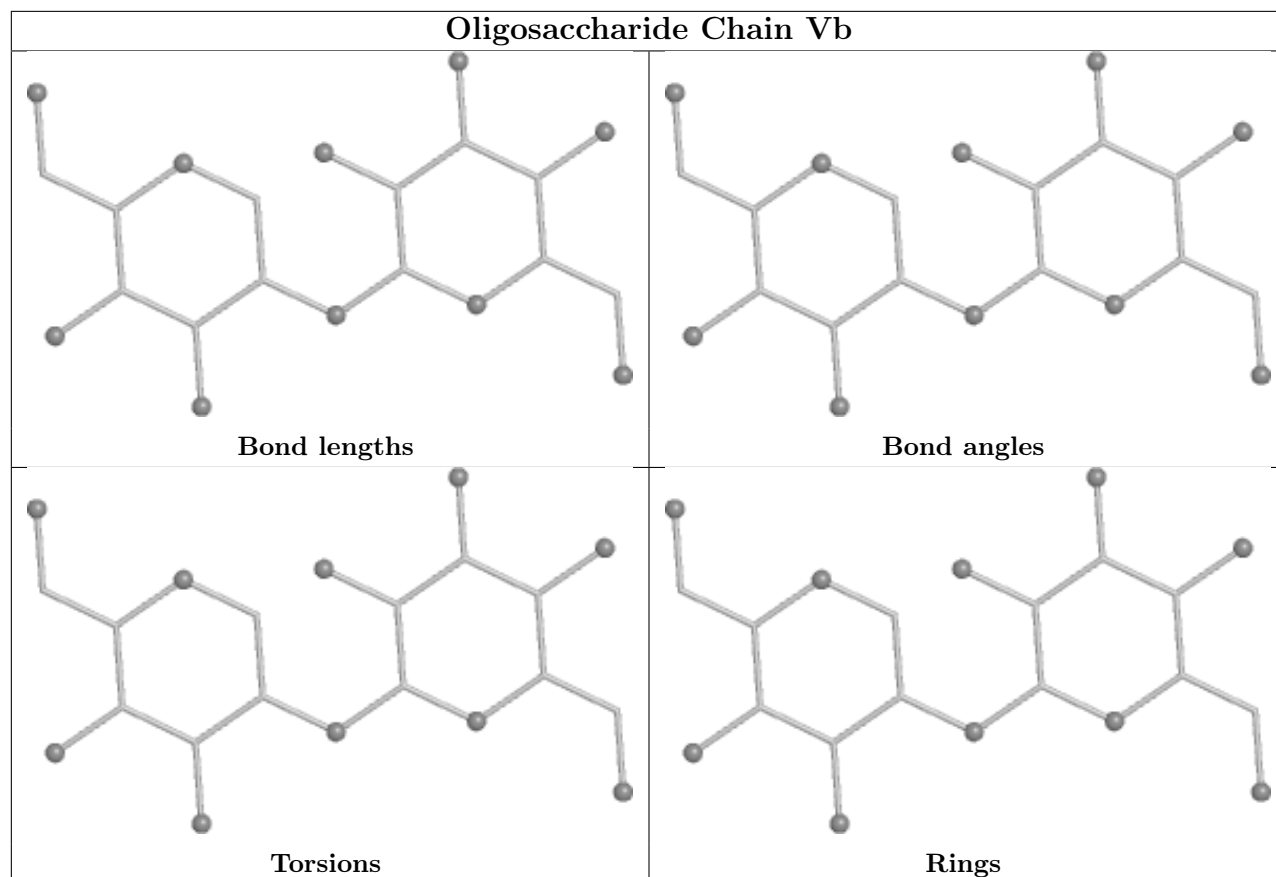
Oligosaccharide Chain Tb



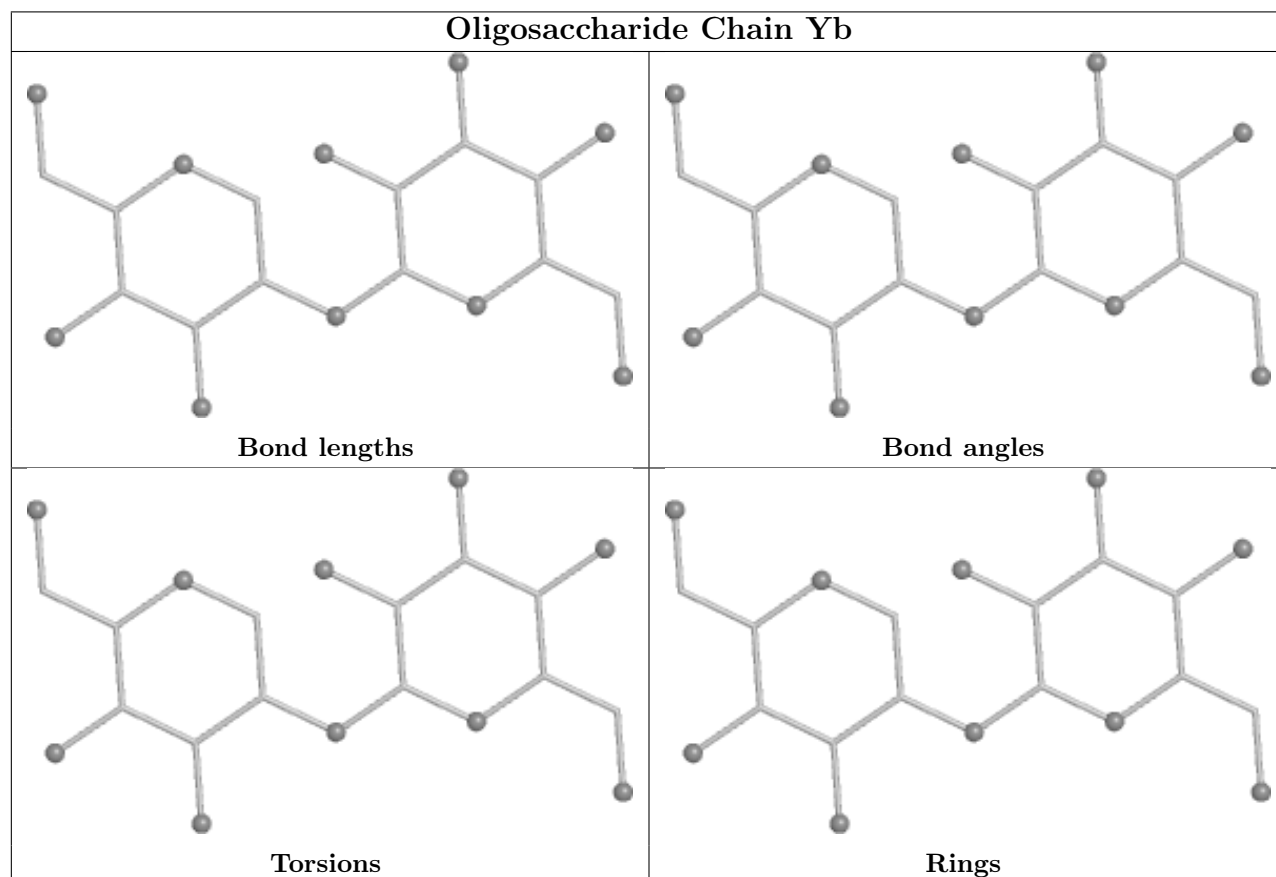
Oligosaccharide Chain Ub

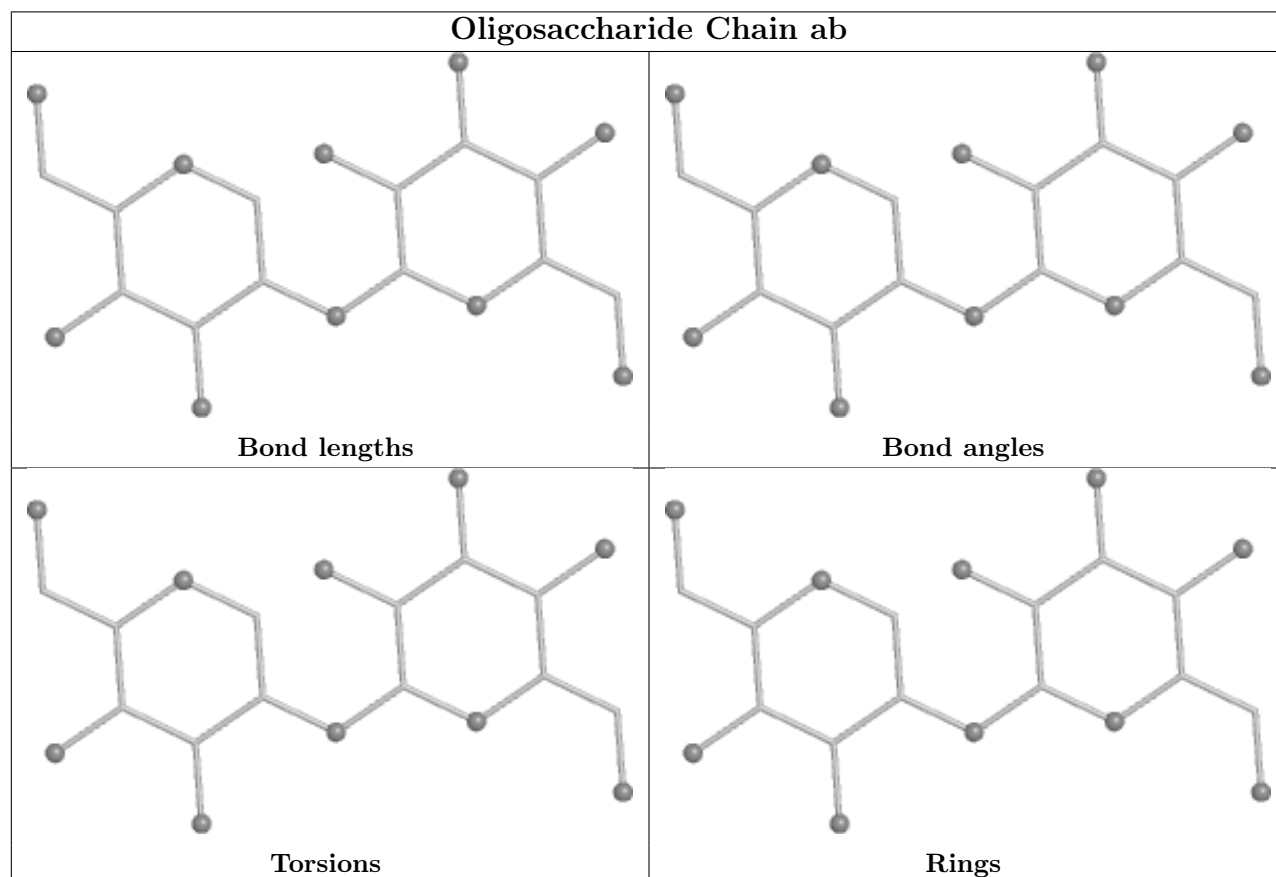
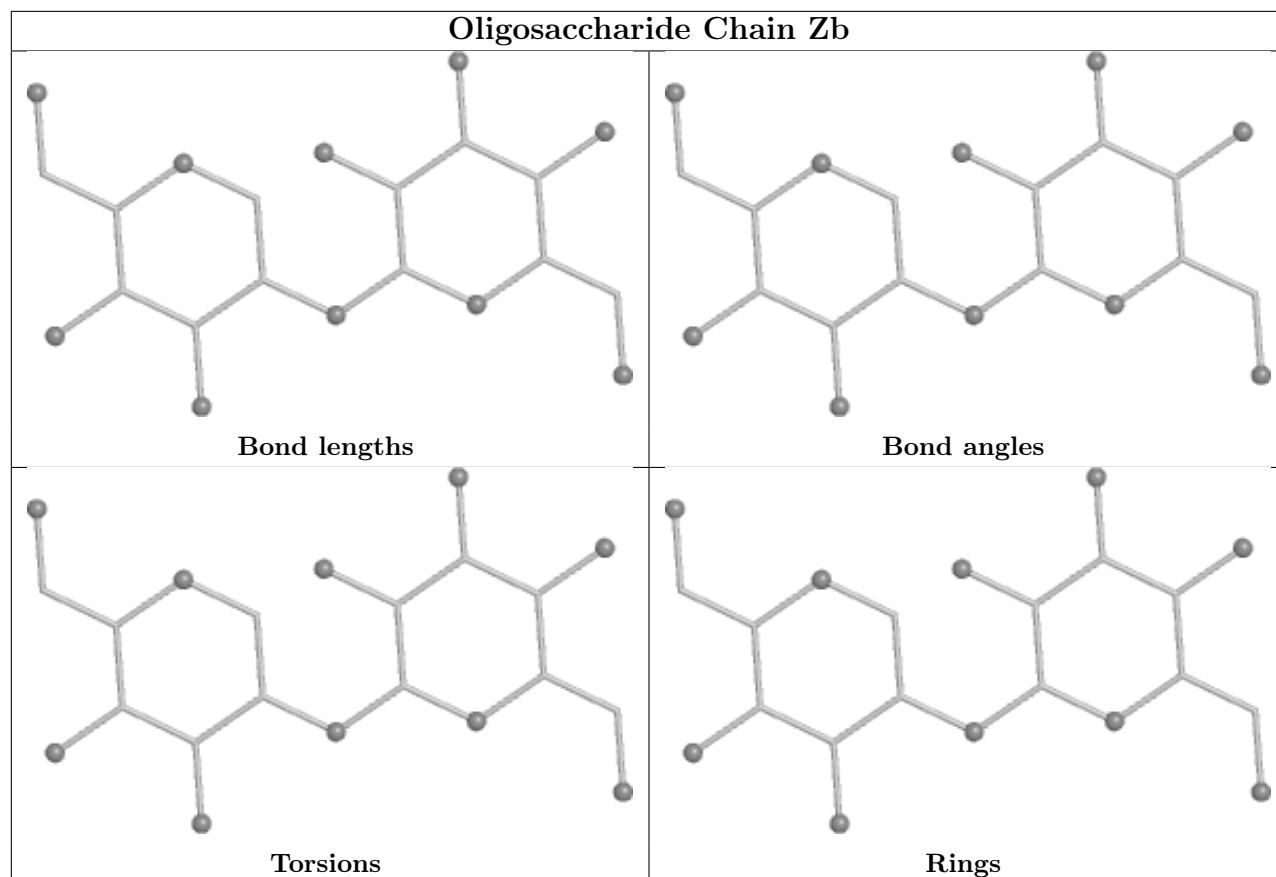


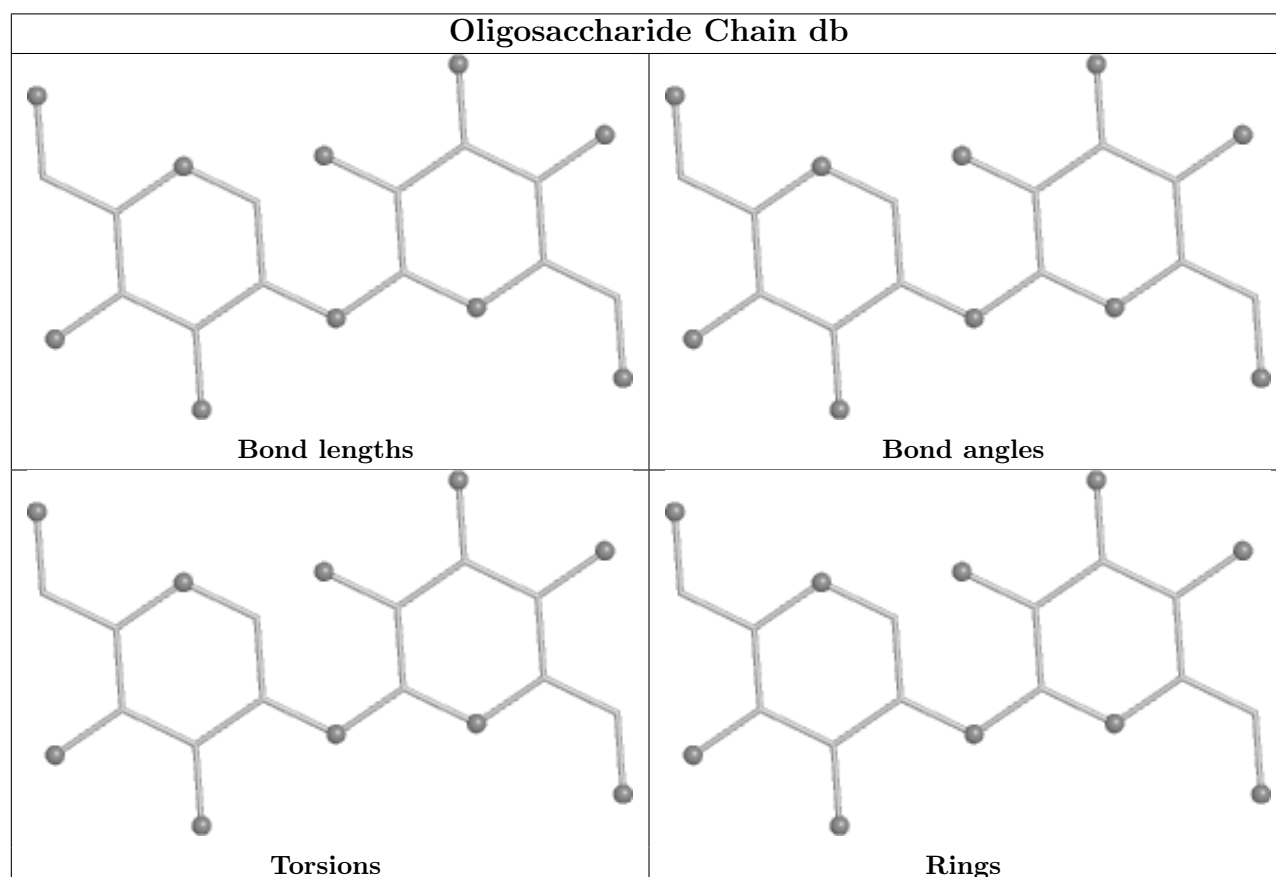
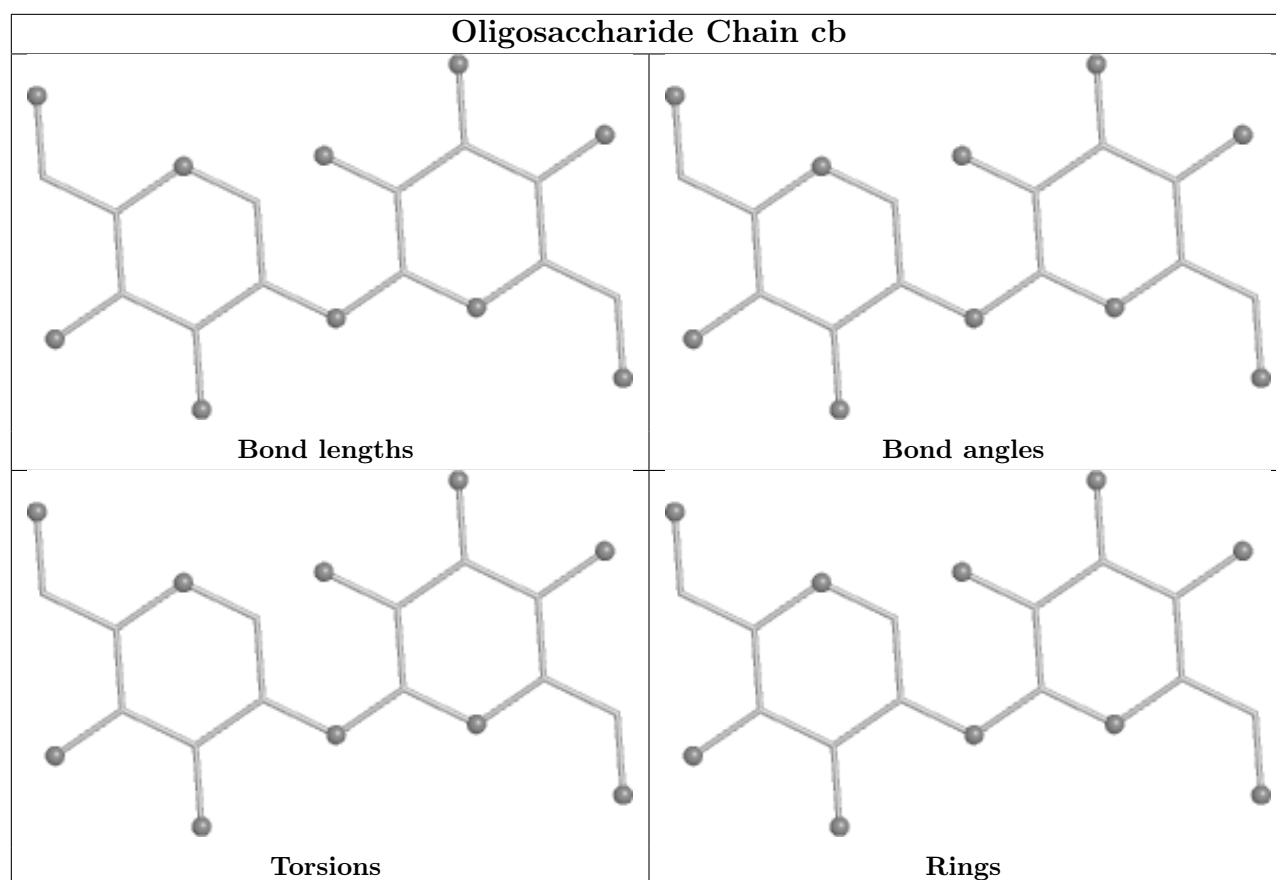
Oligosaccharide Chain Yb

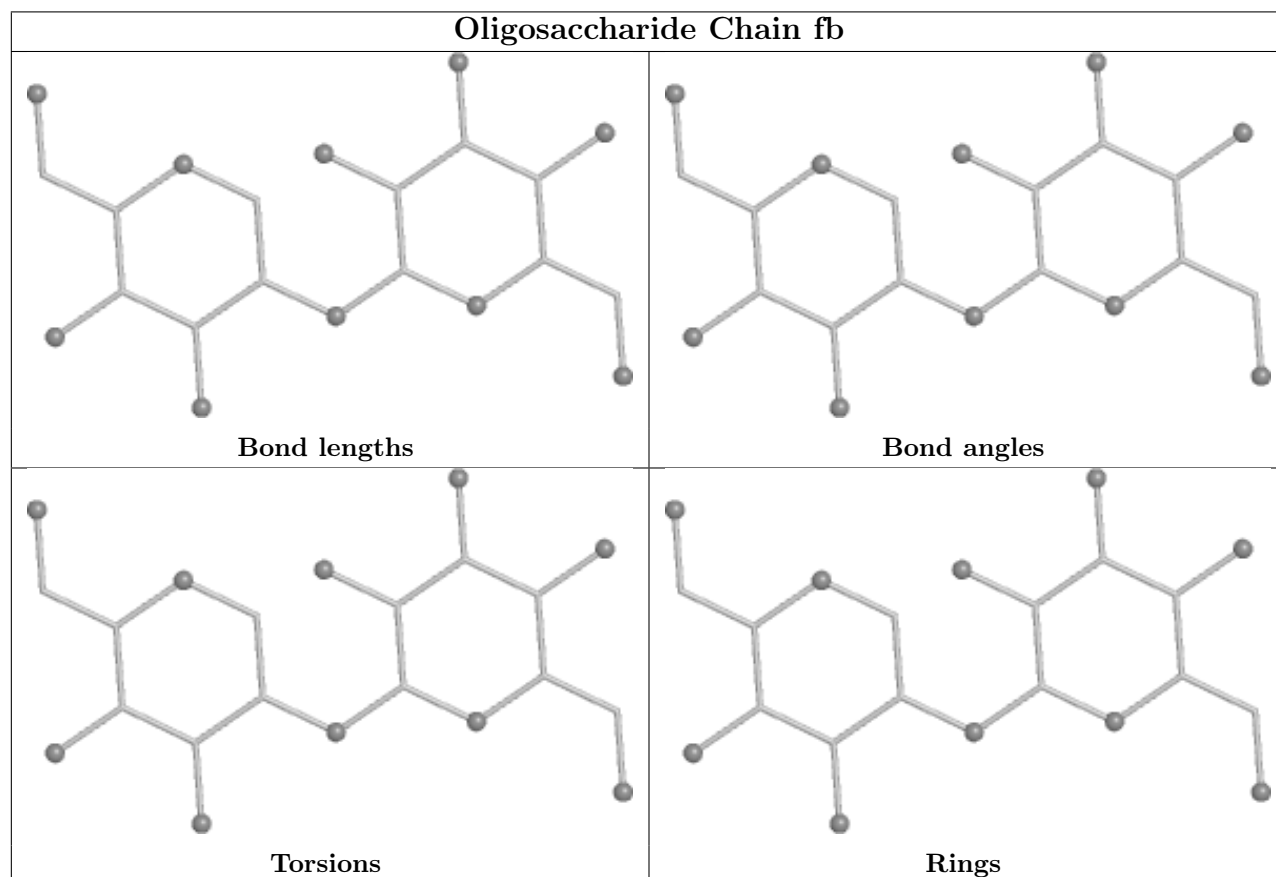
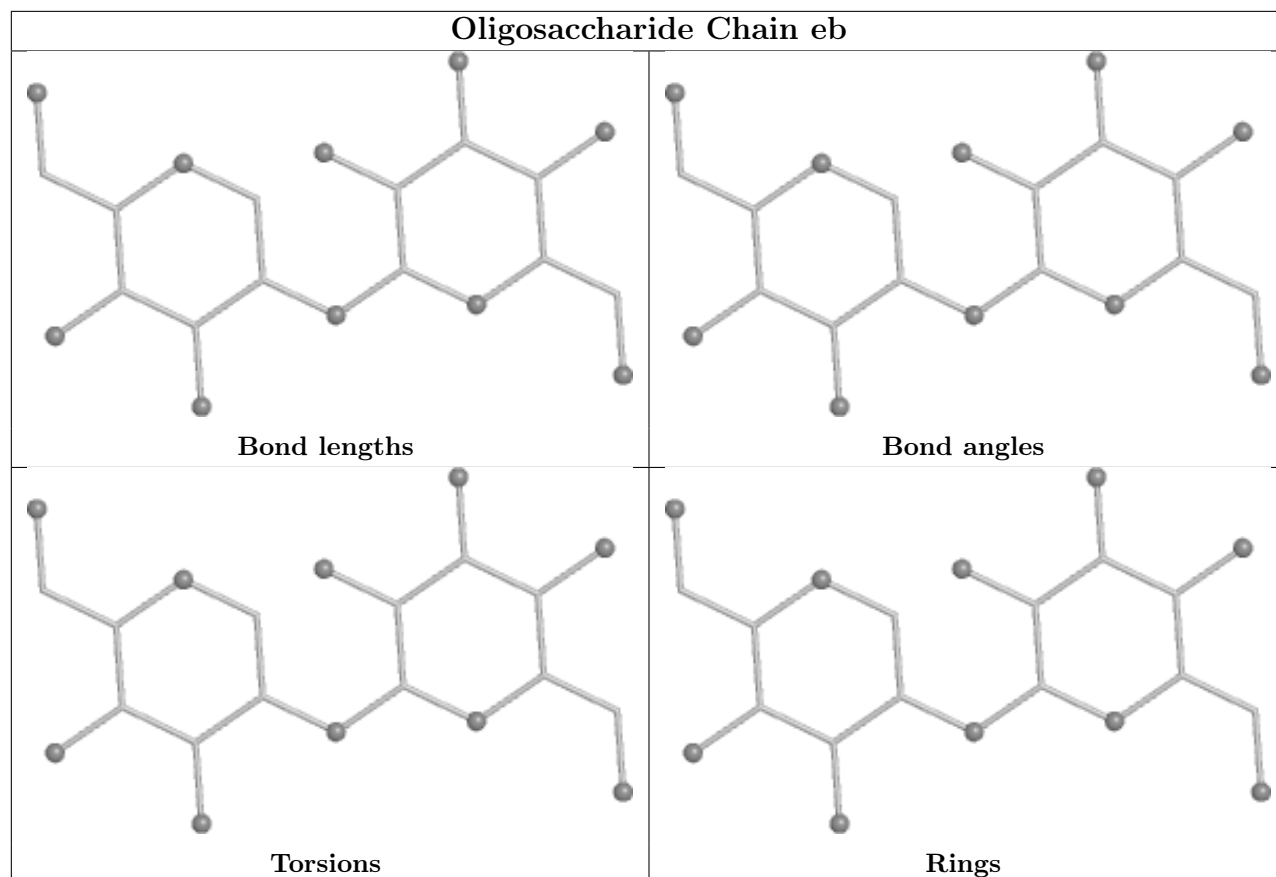


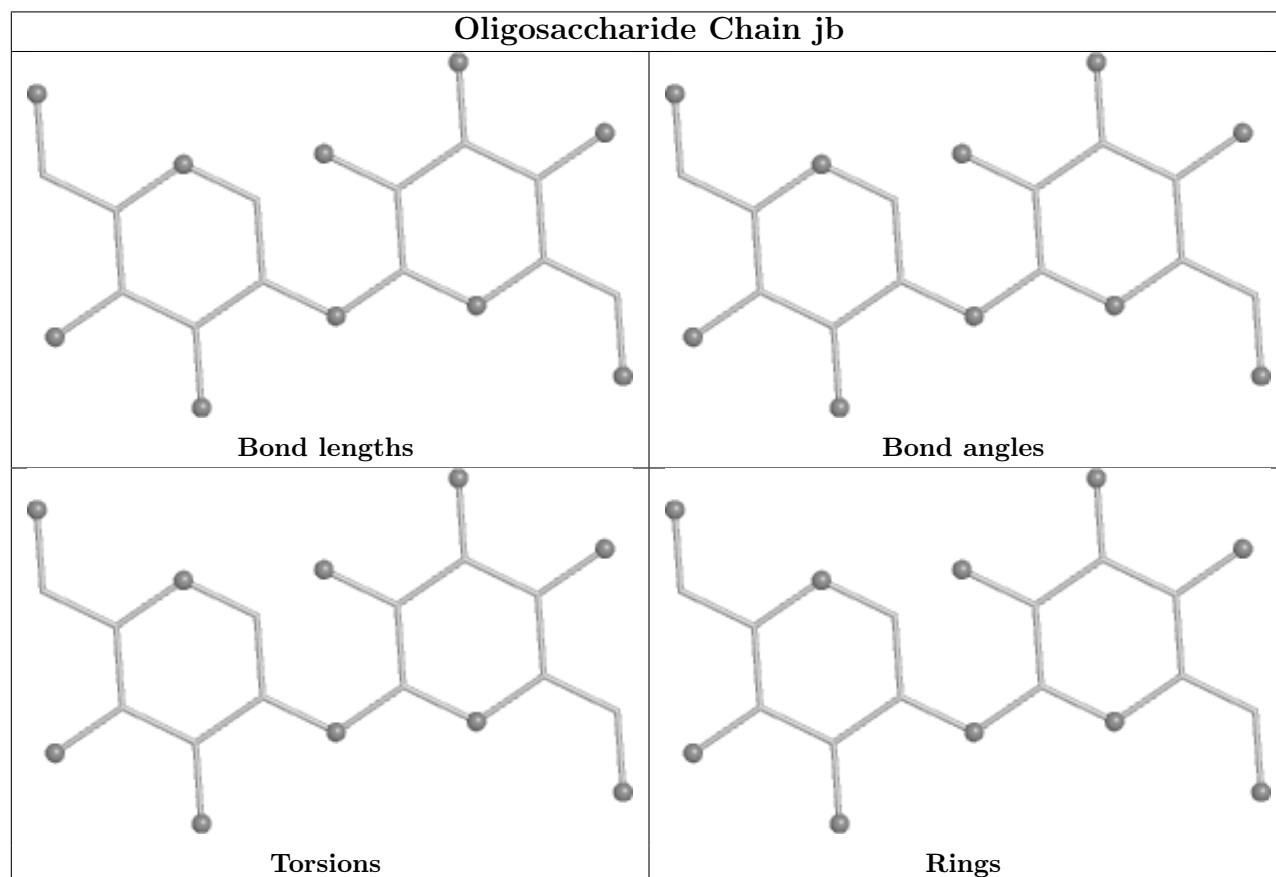
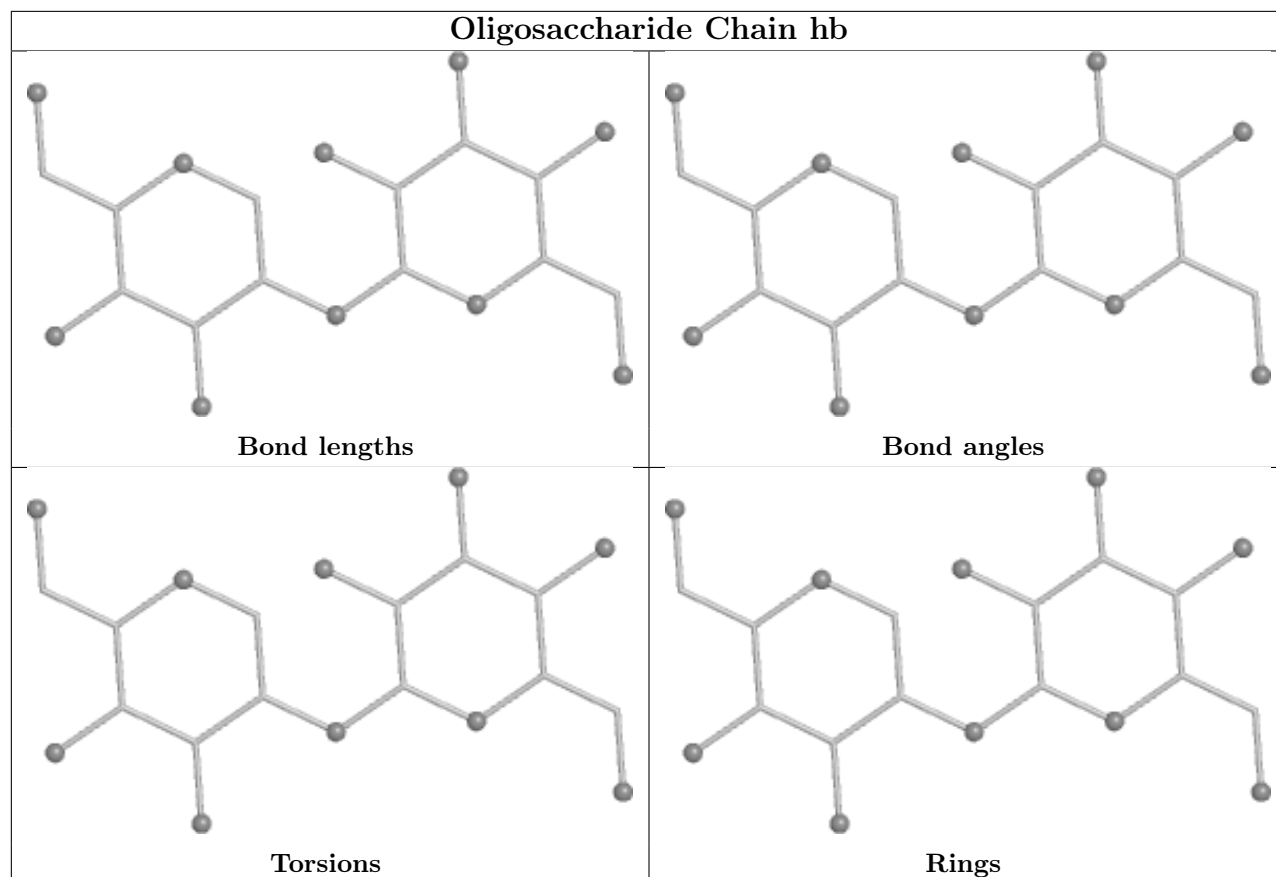
Oligosaccharide Chain Yb

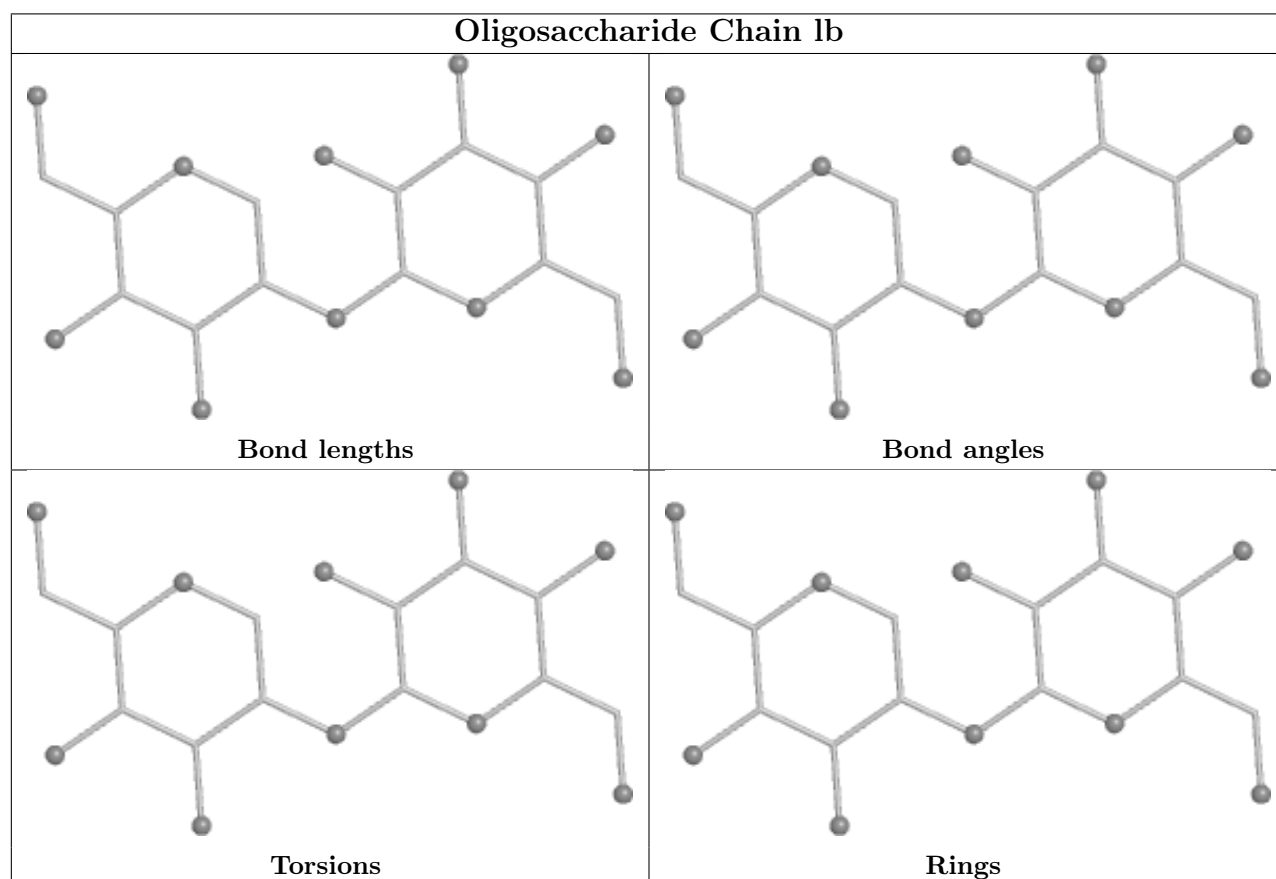
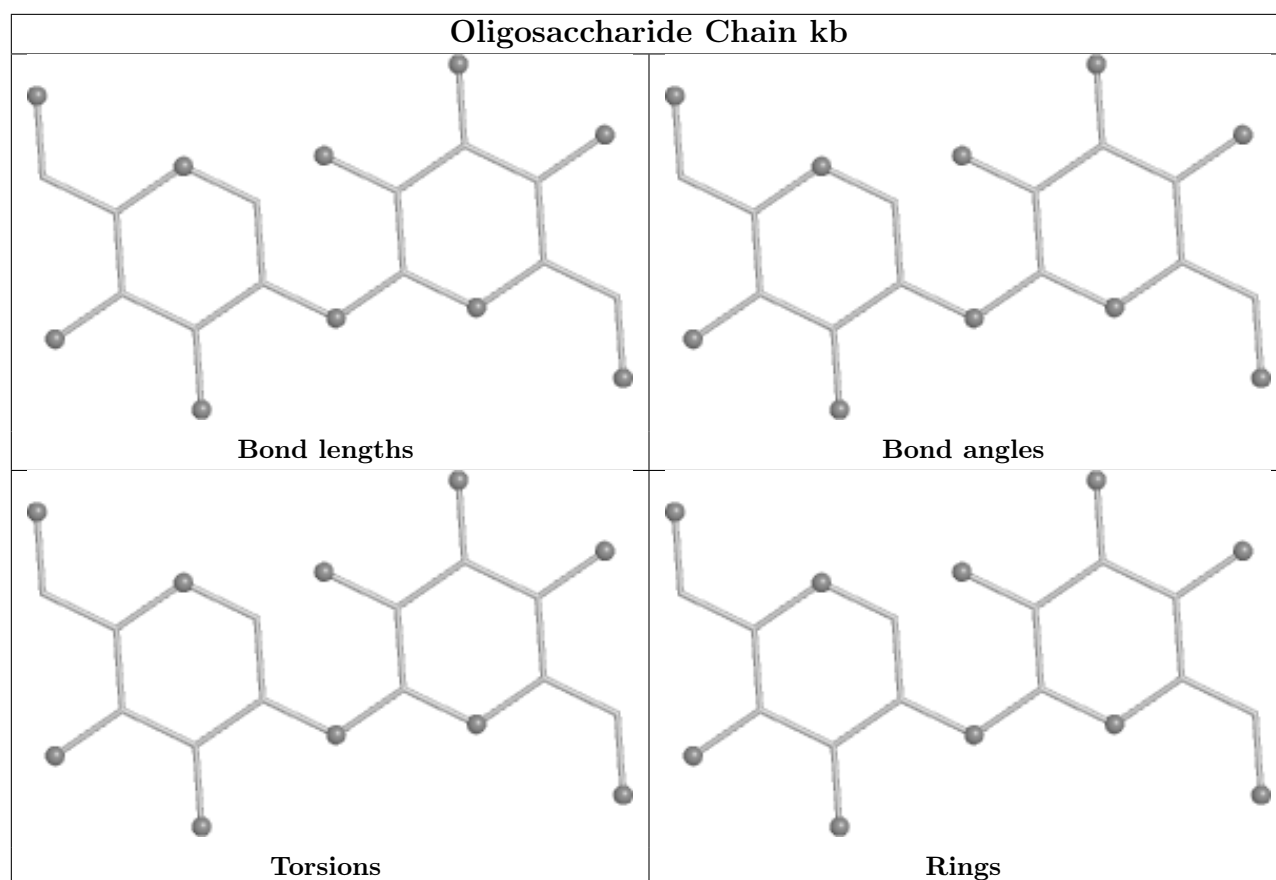


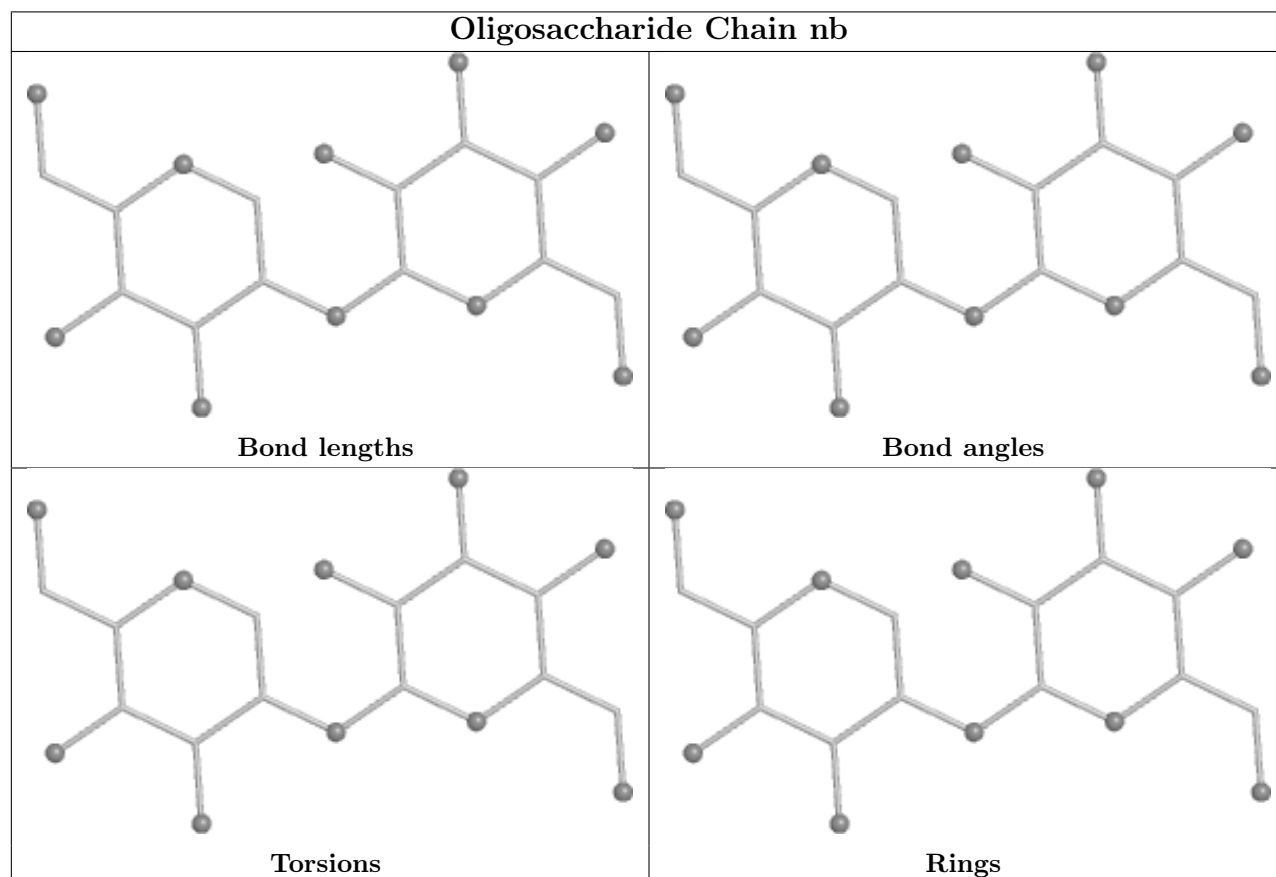
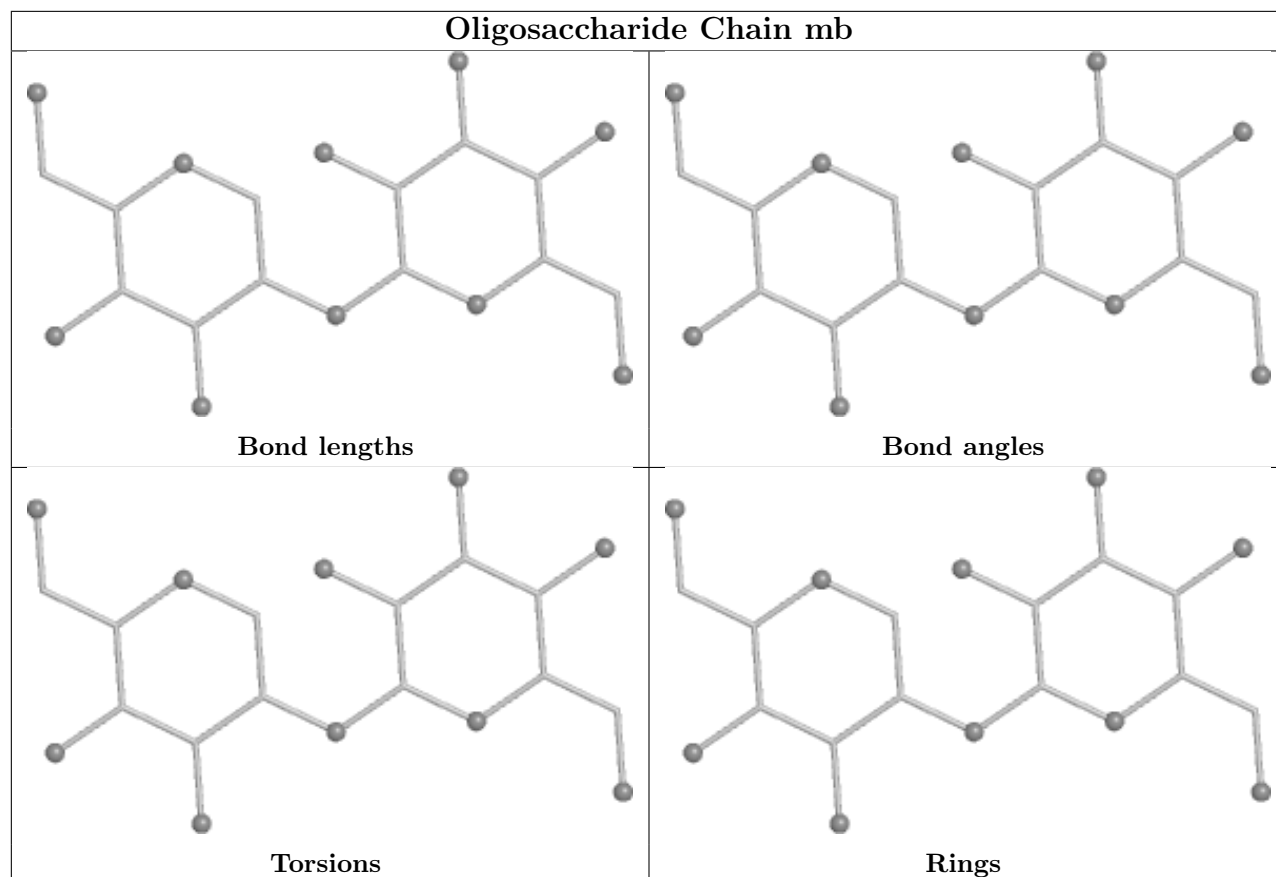


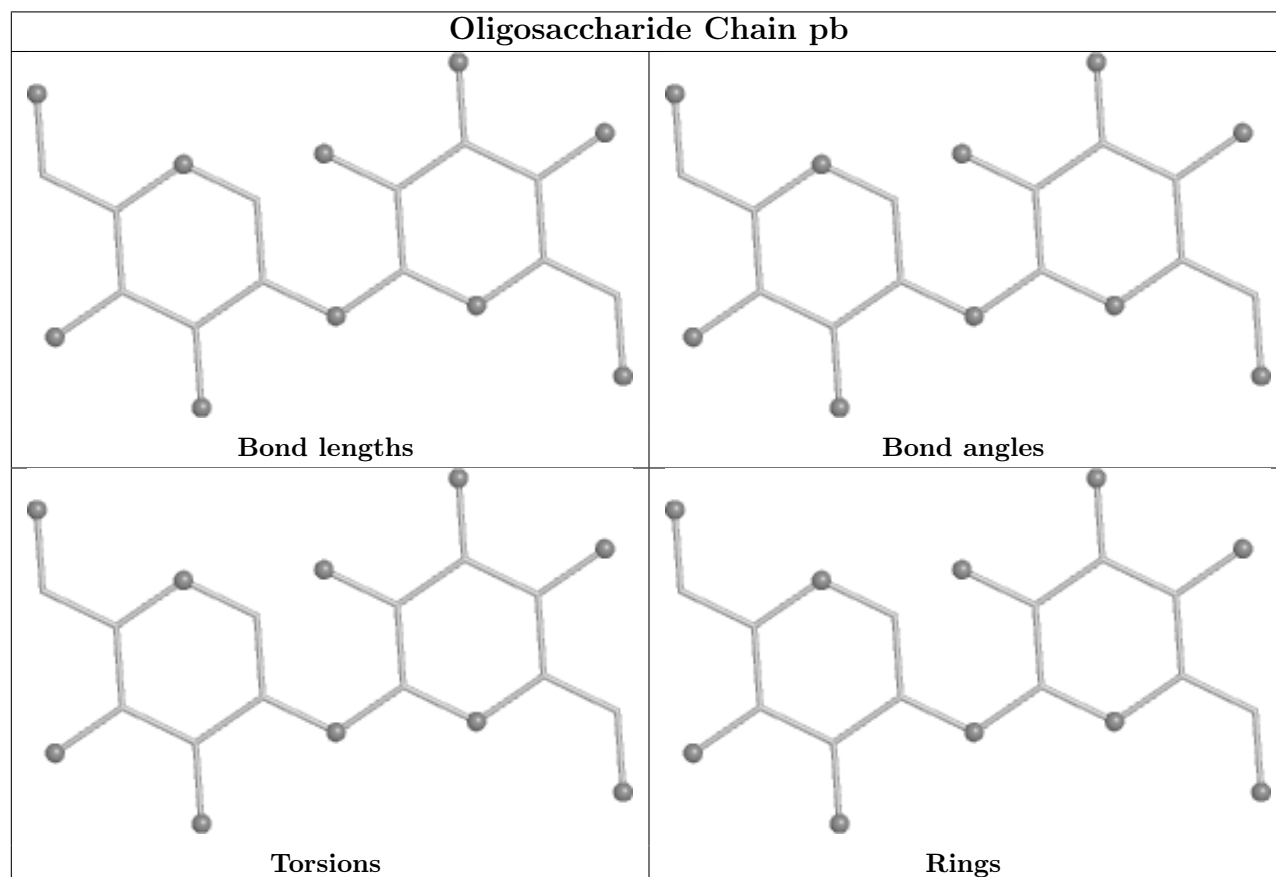
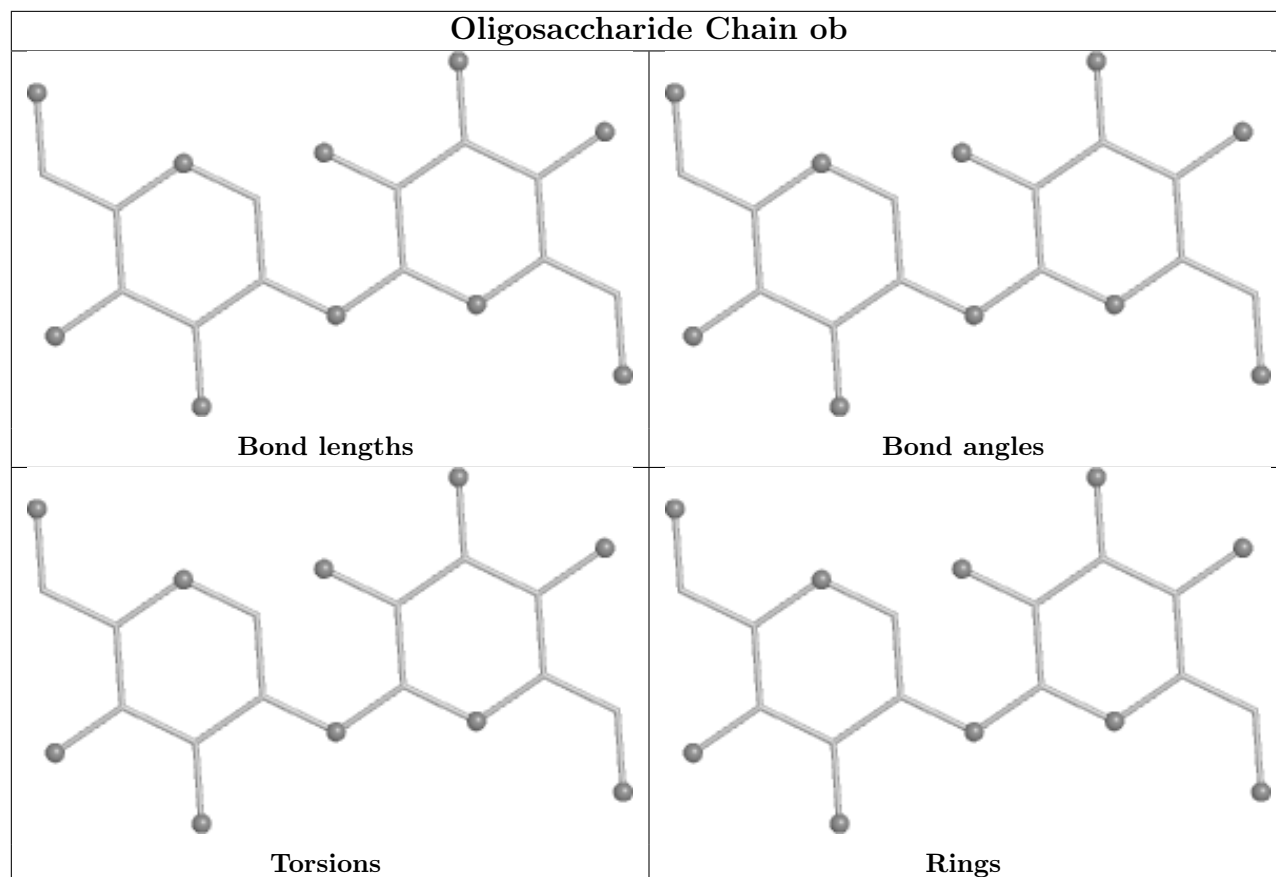


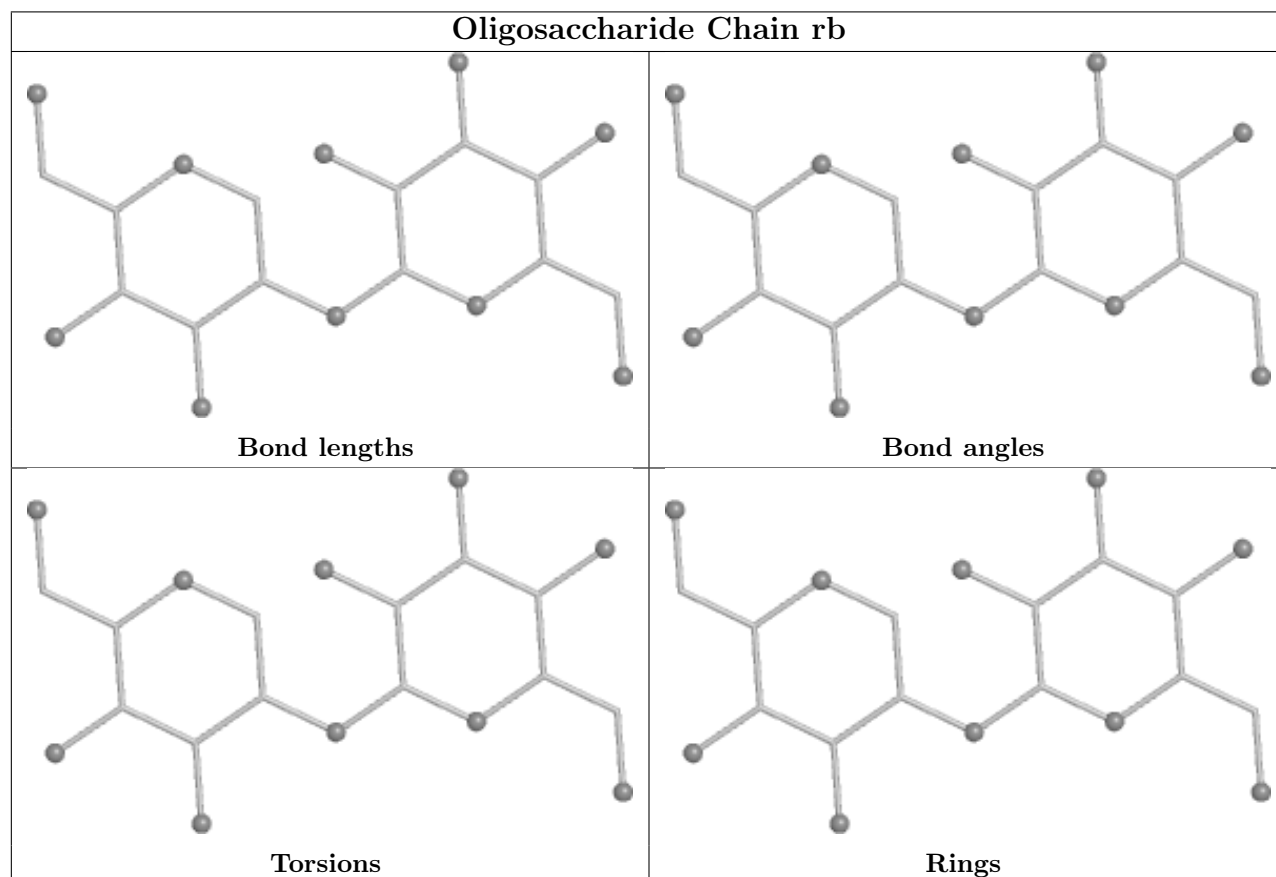
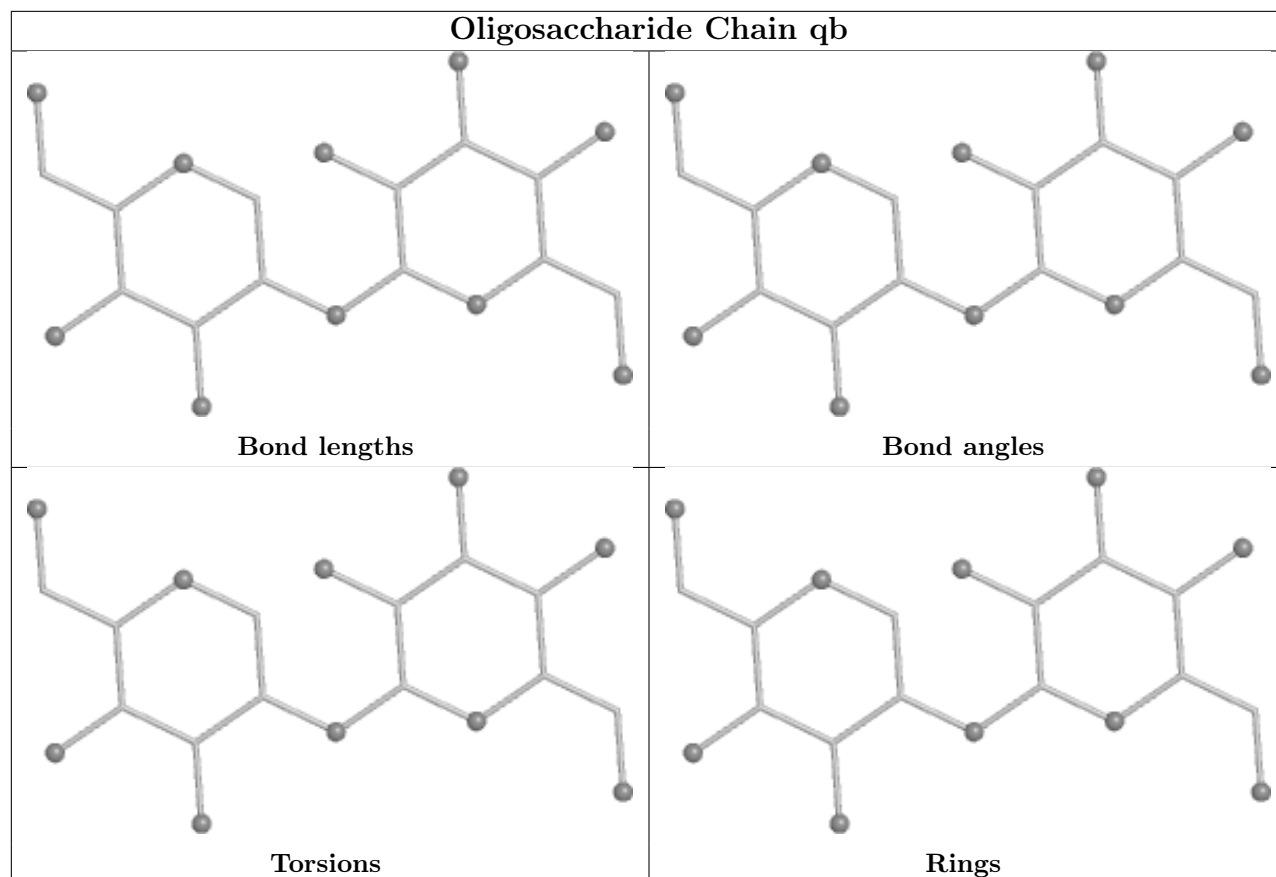


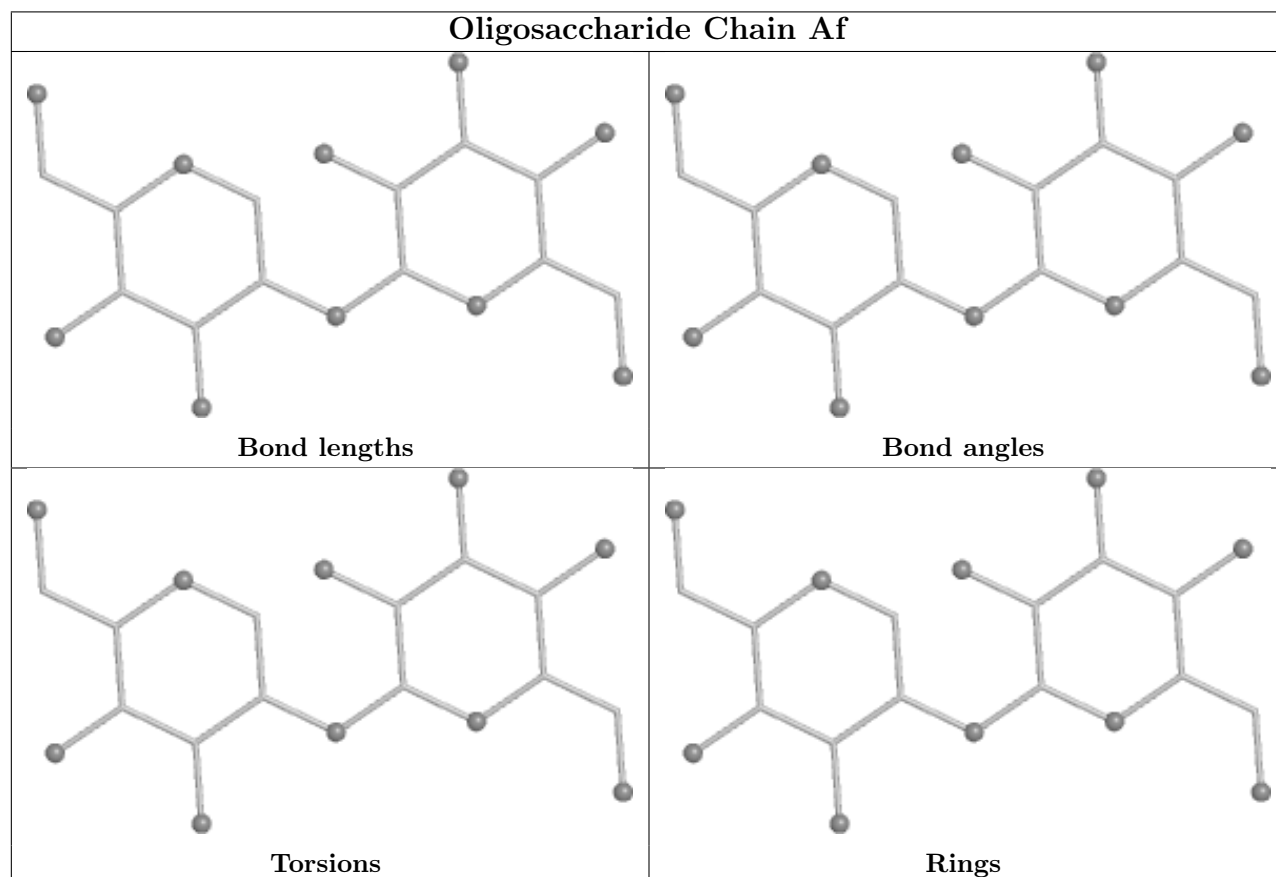
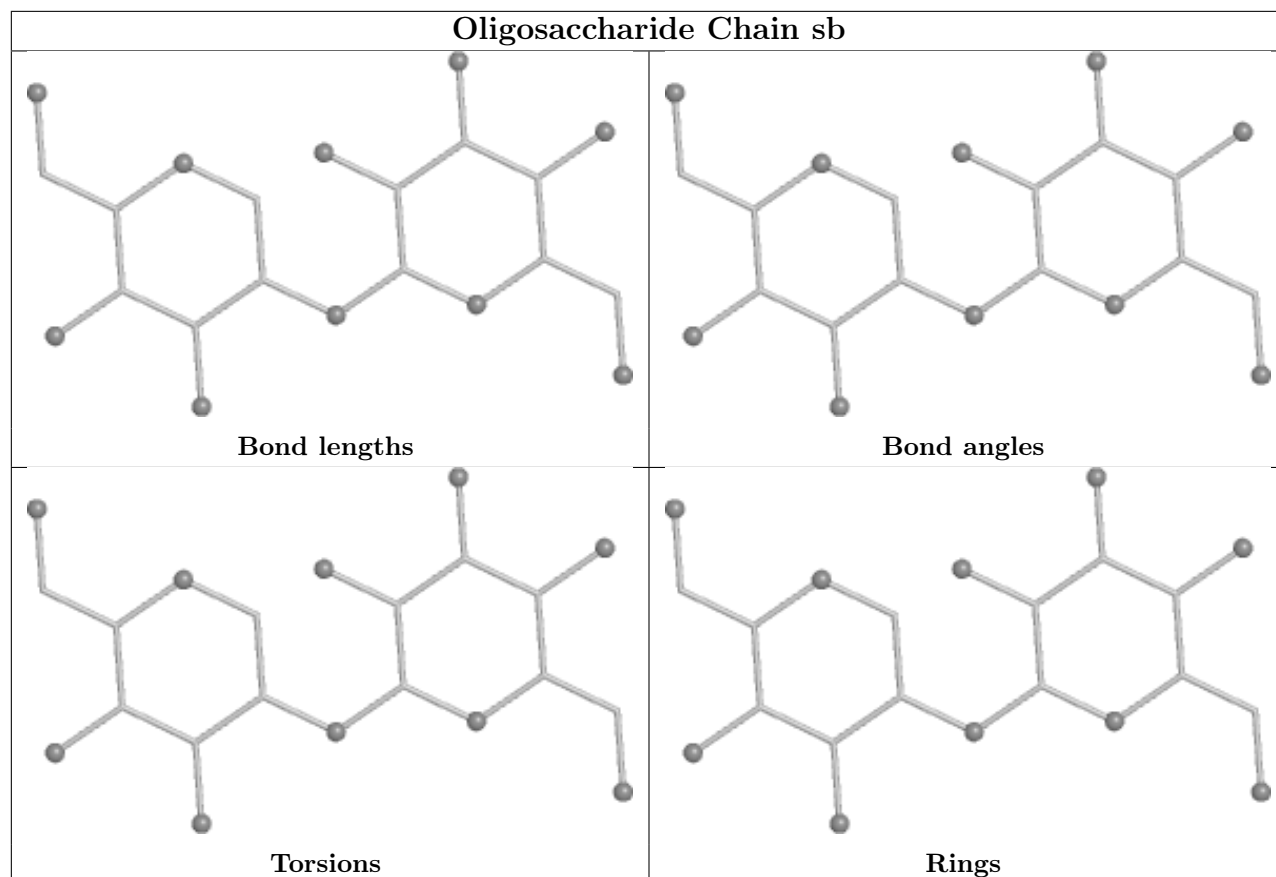


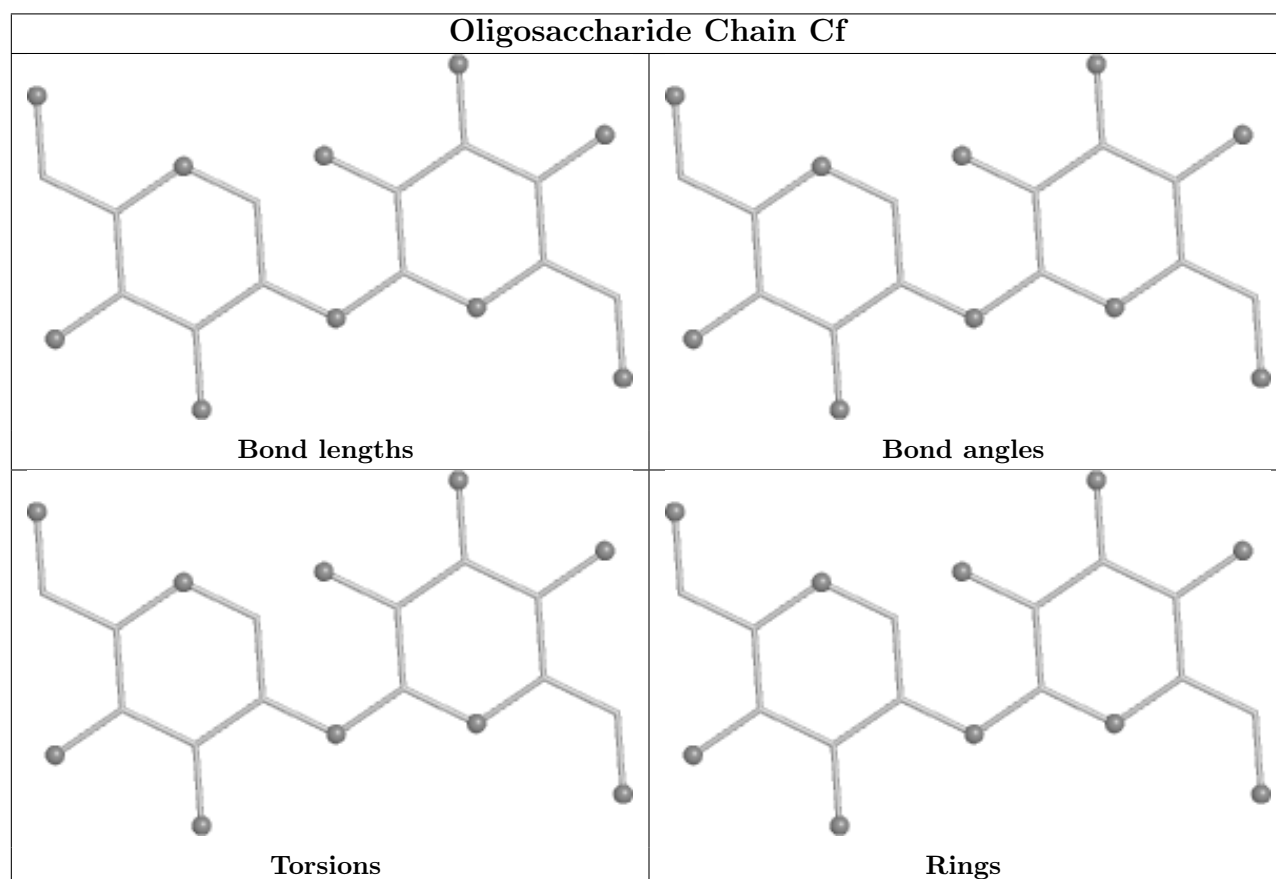
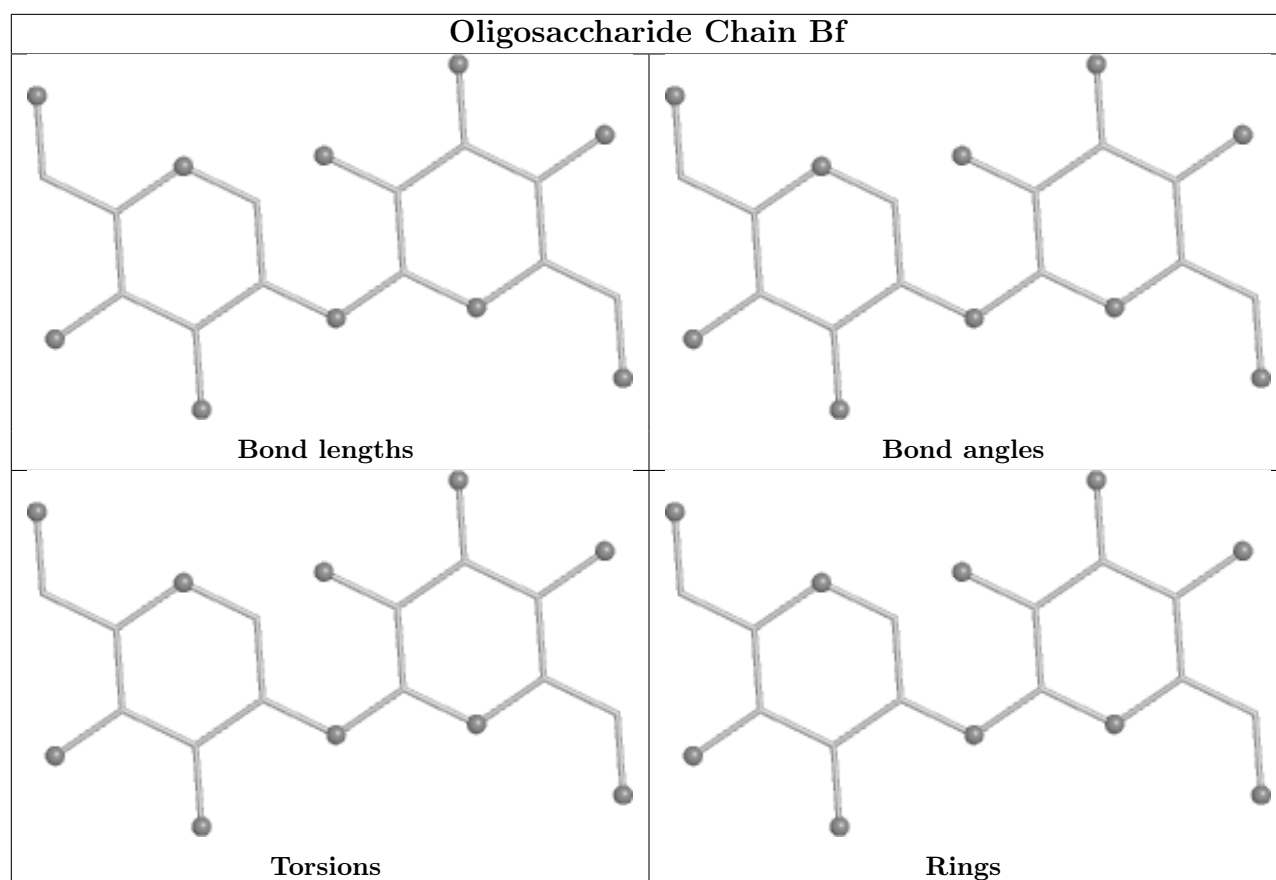


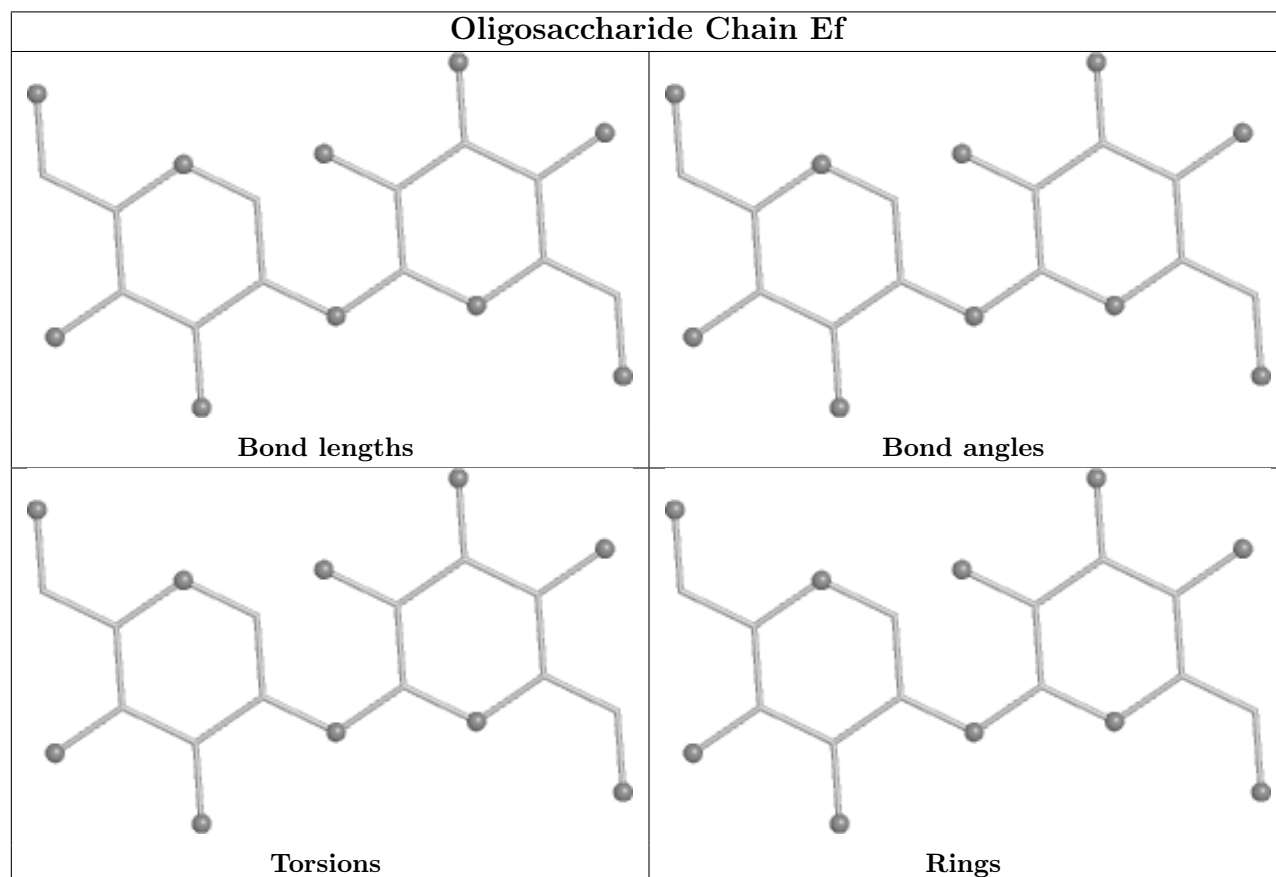
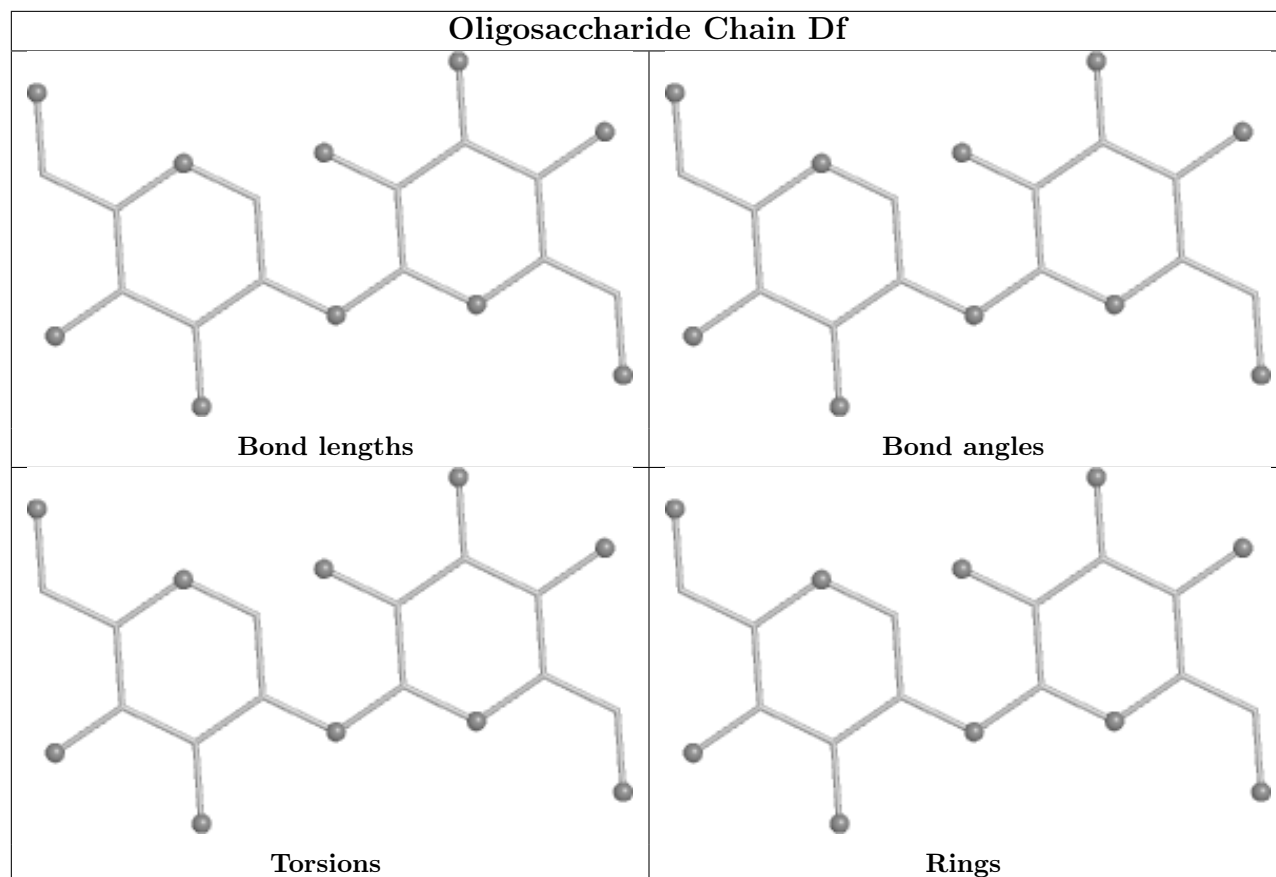




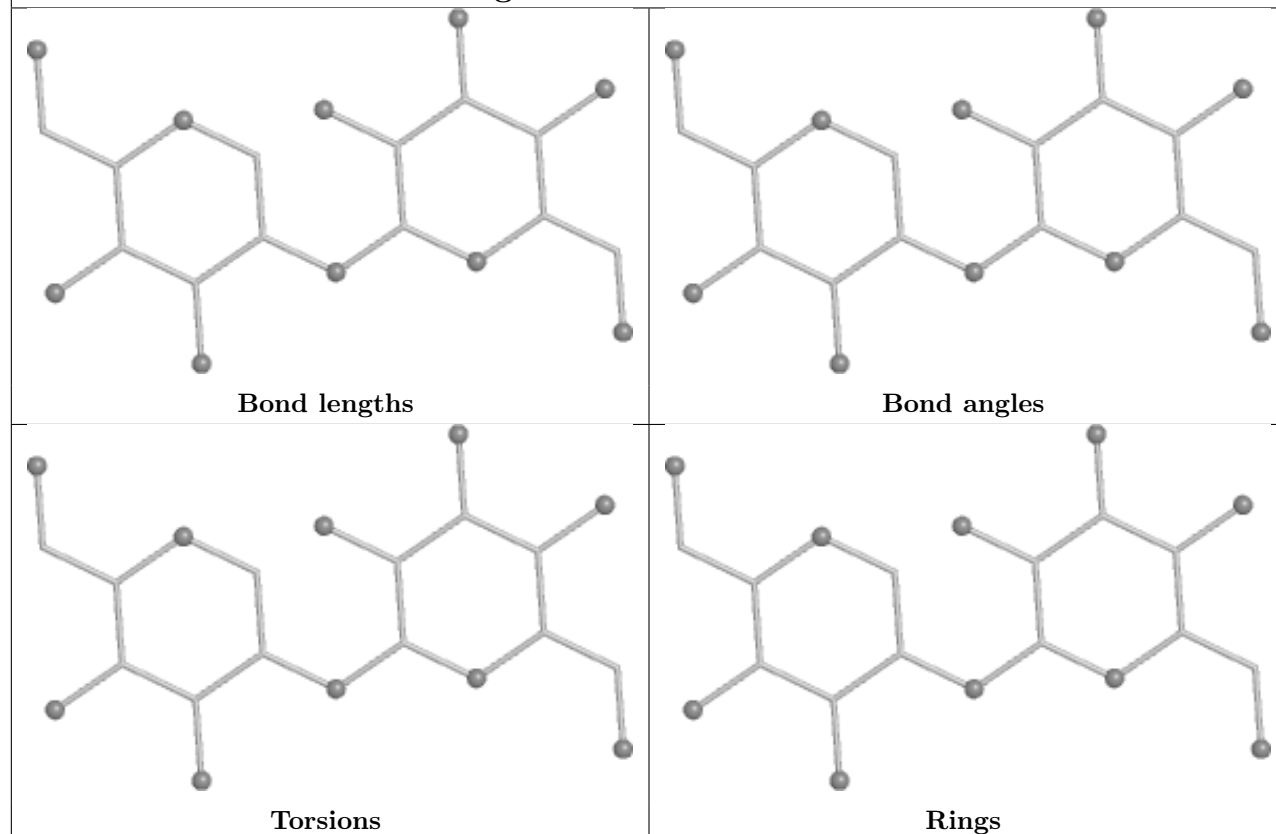




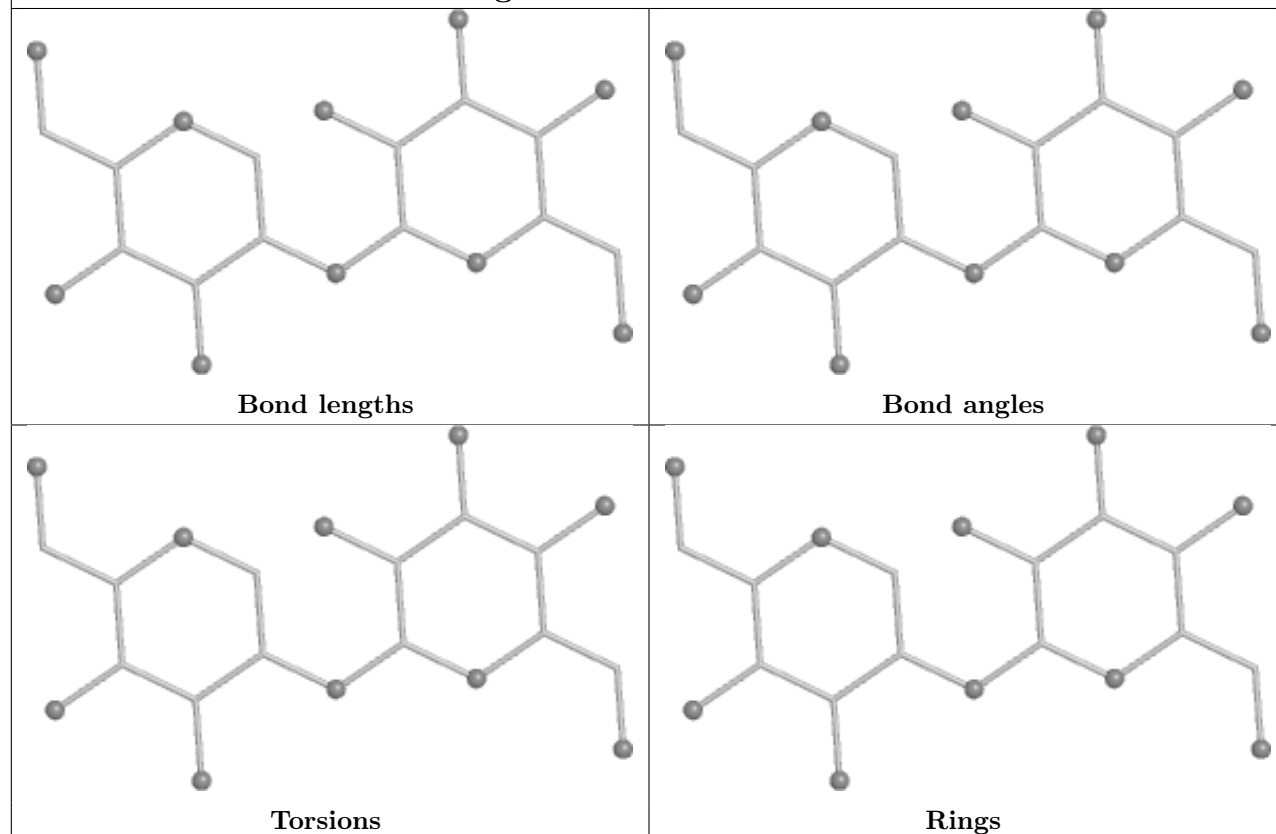


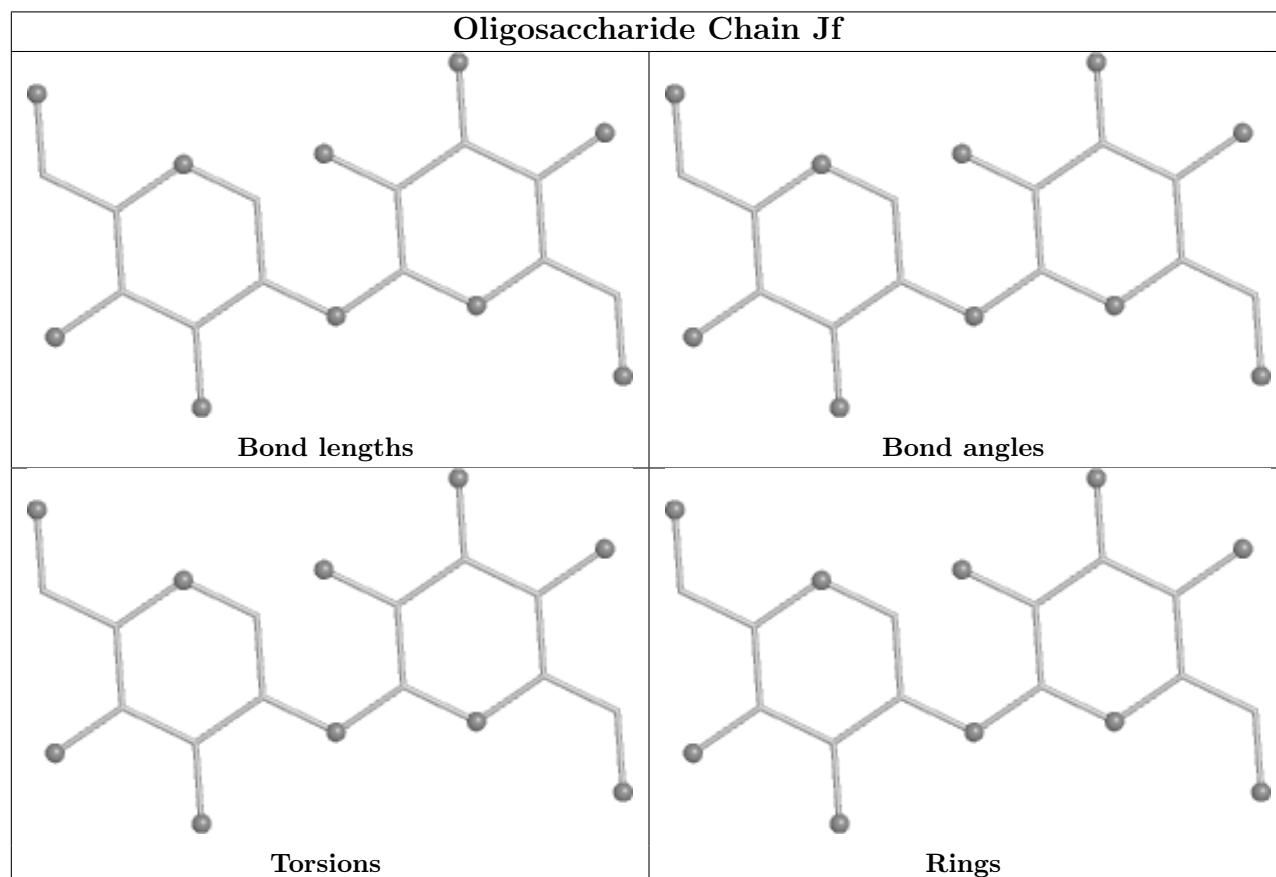
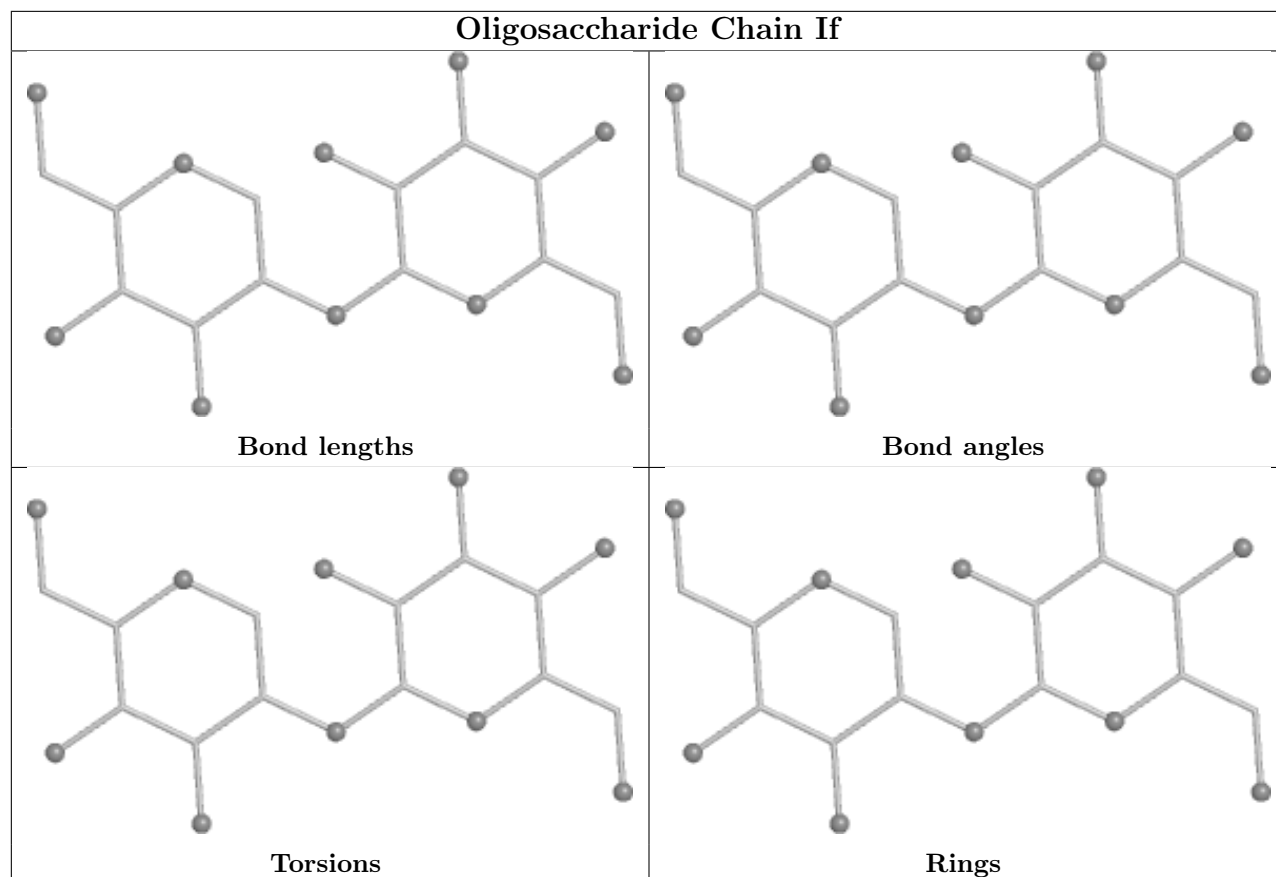


Oligosaccharide Chain Gf

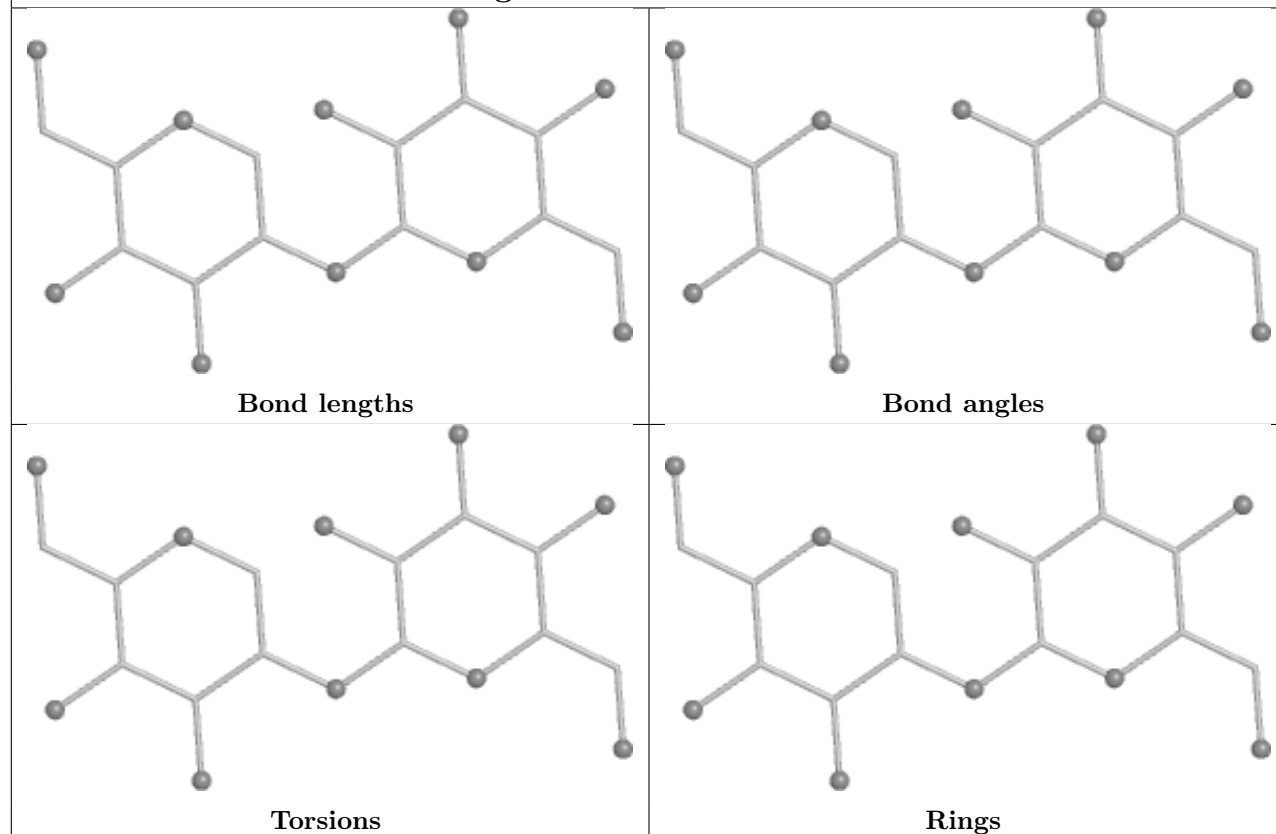


Oligosaccharide Chain Hf

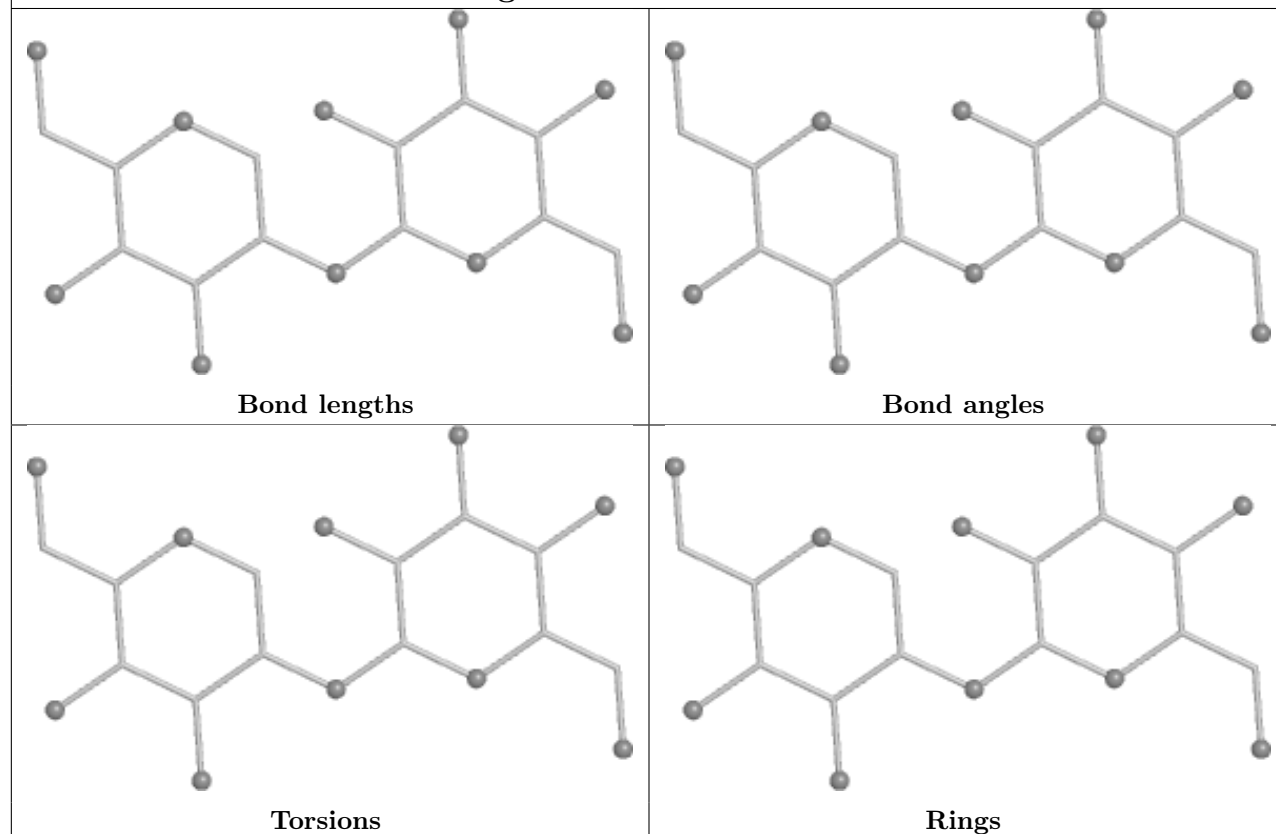


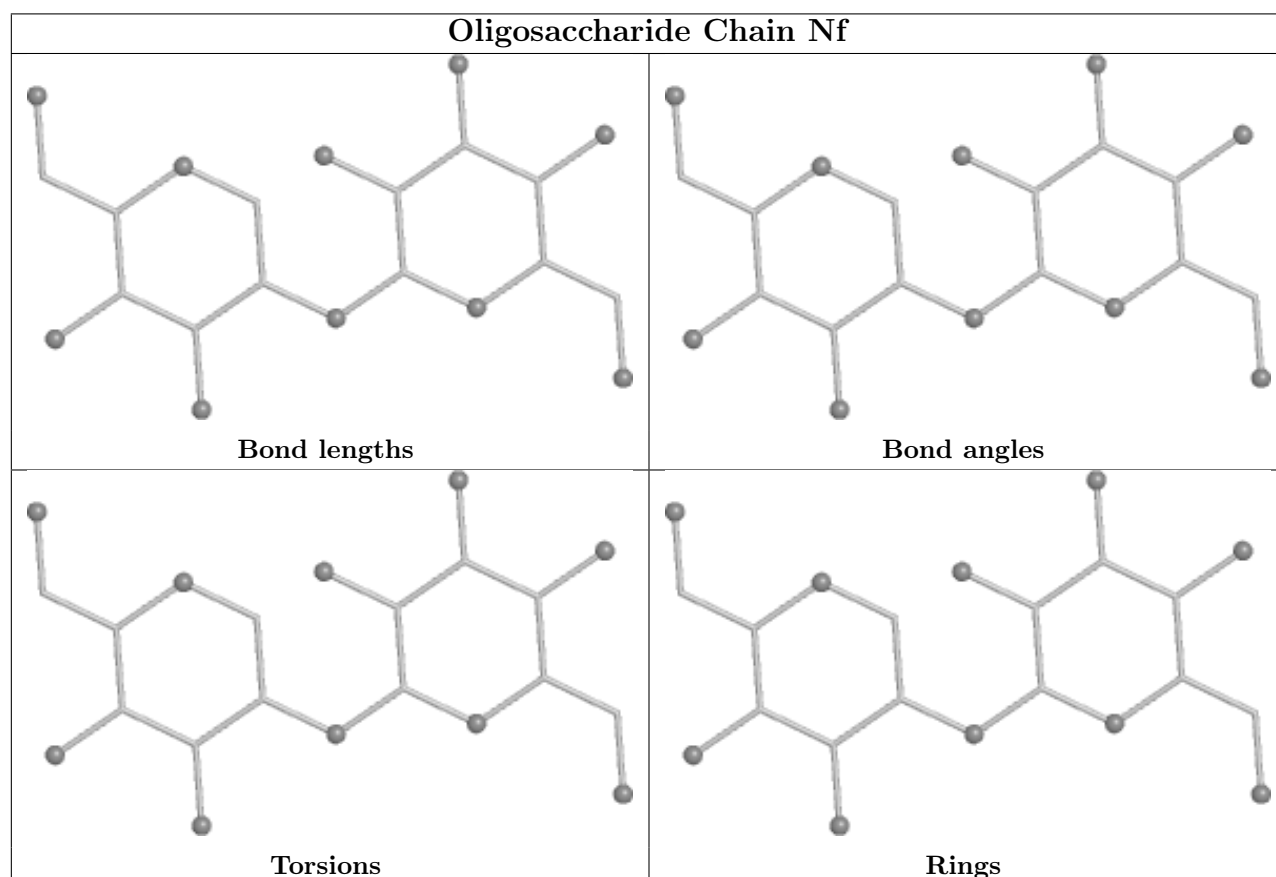
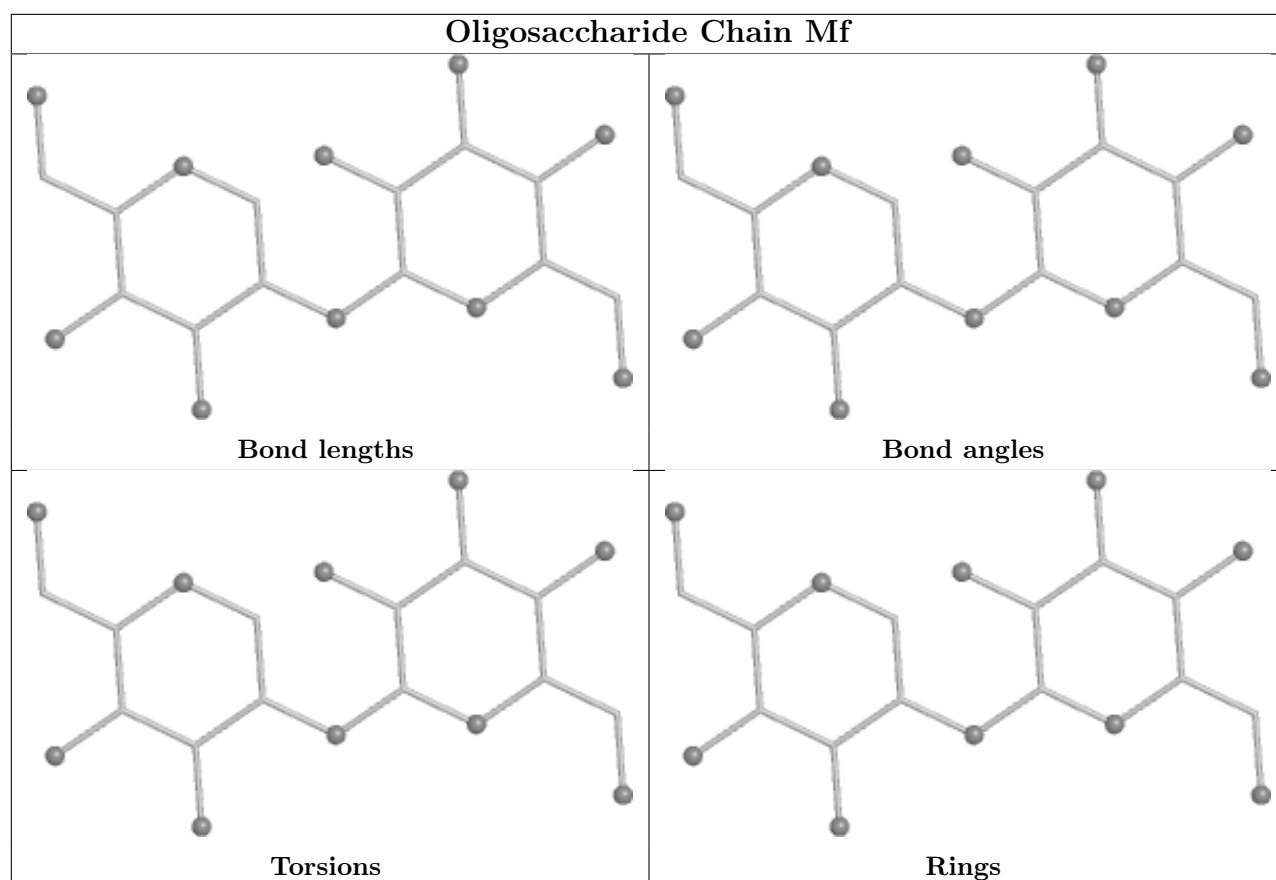


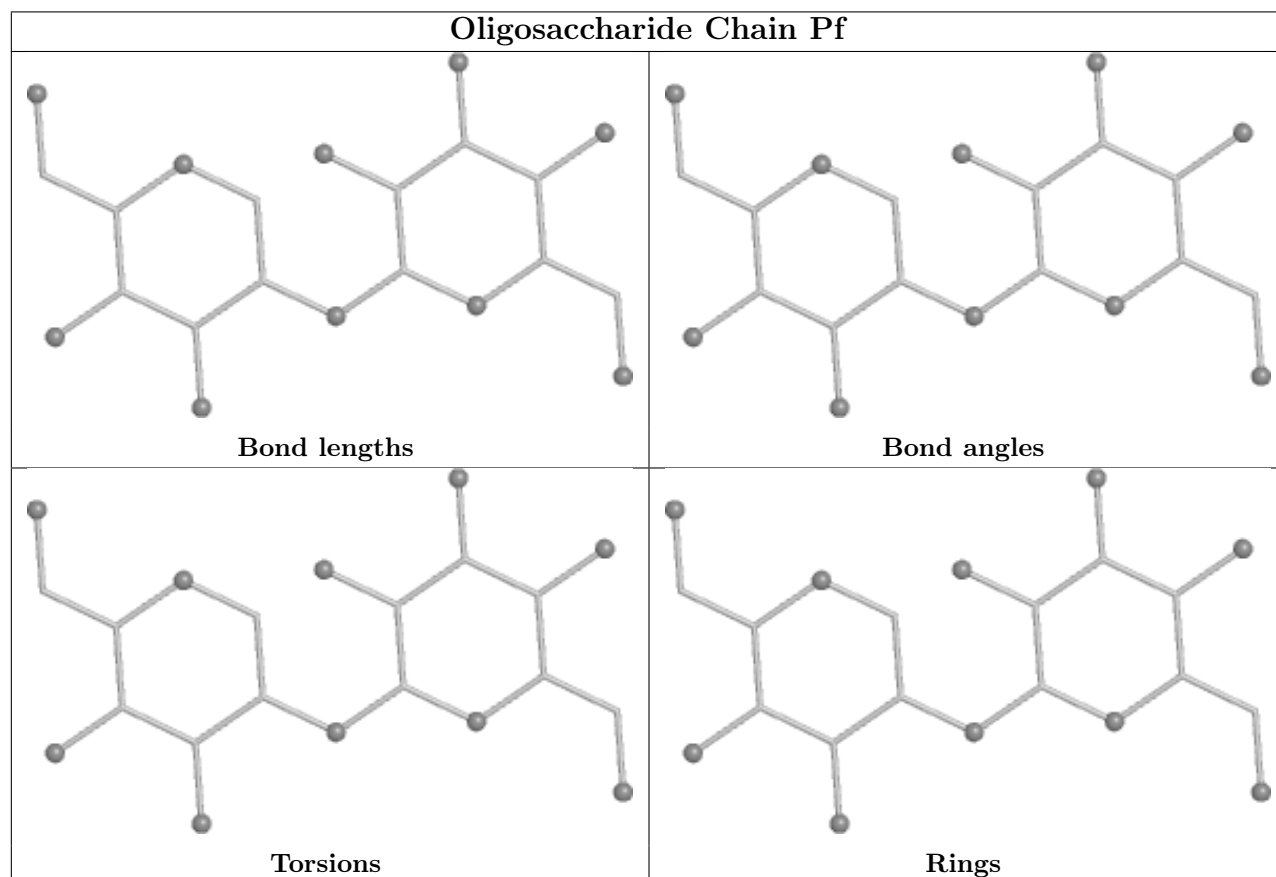
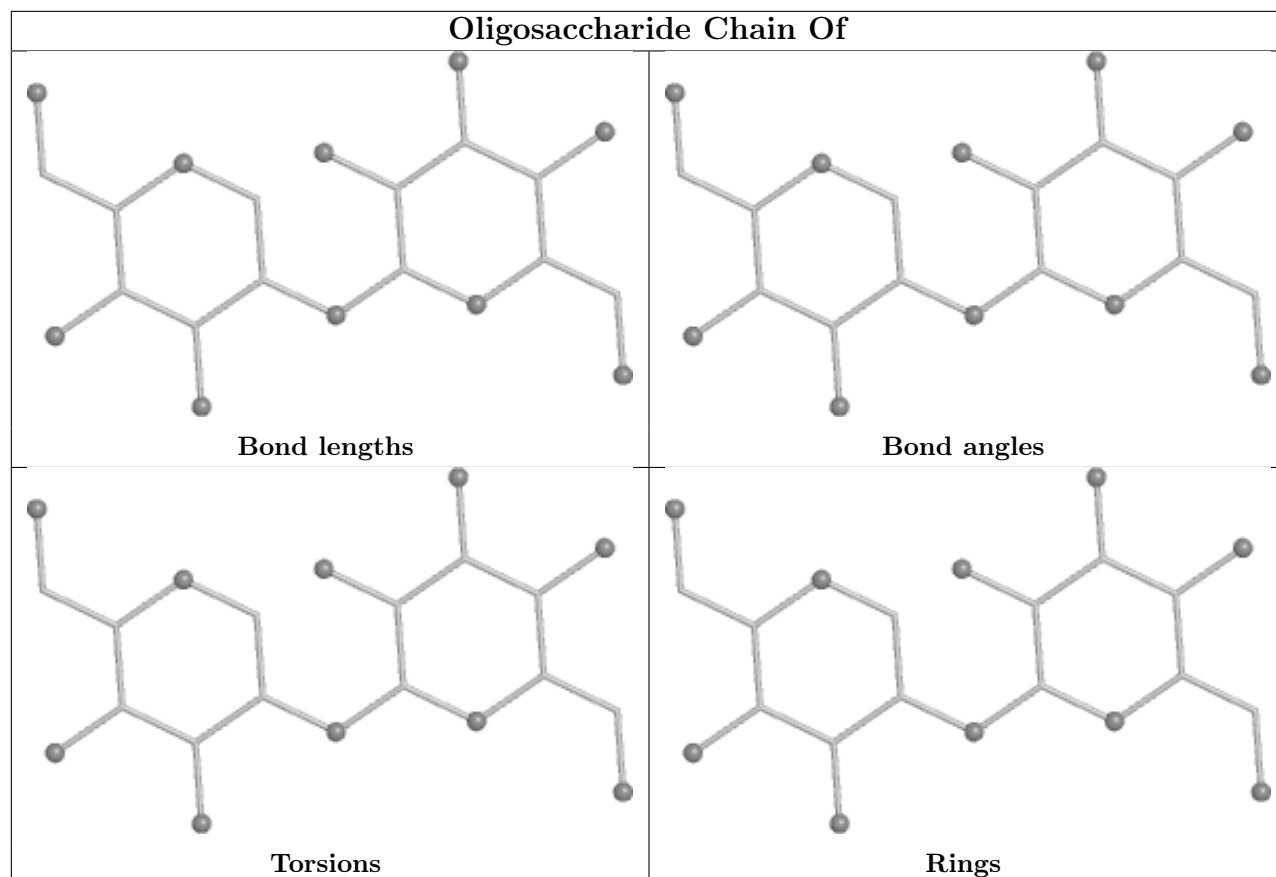
Oligosaccharide Chain Kf

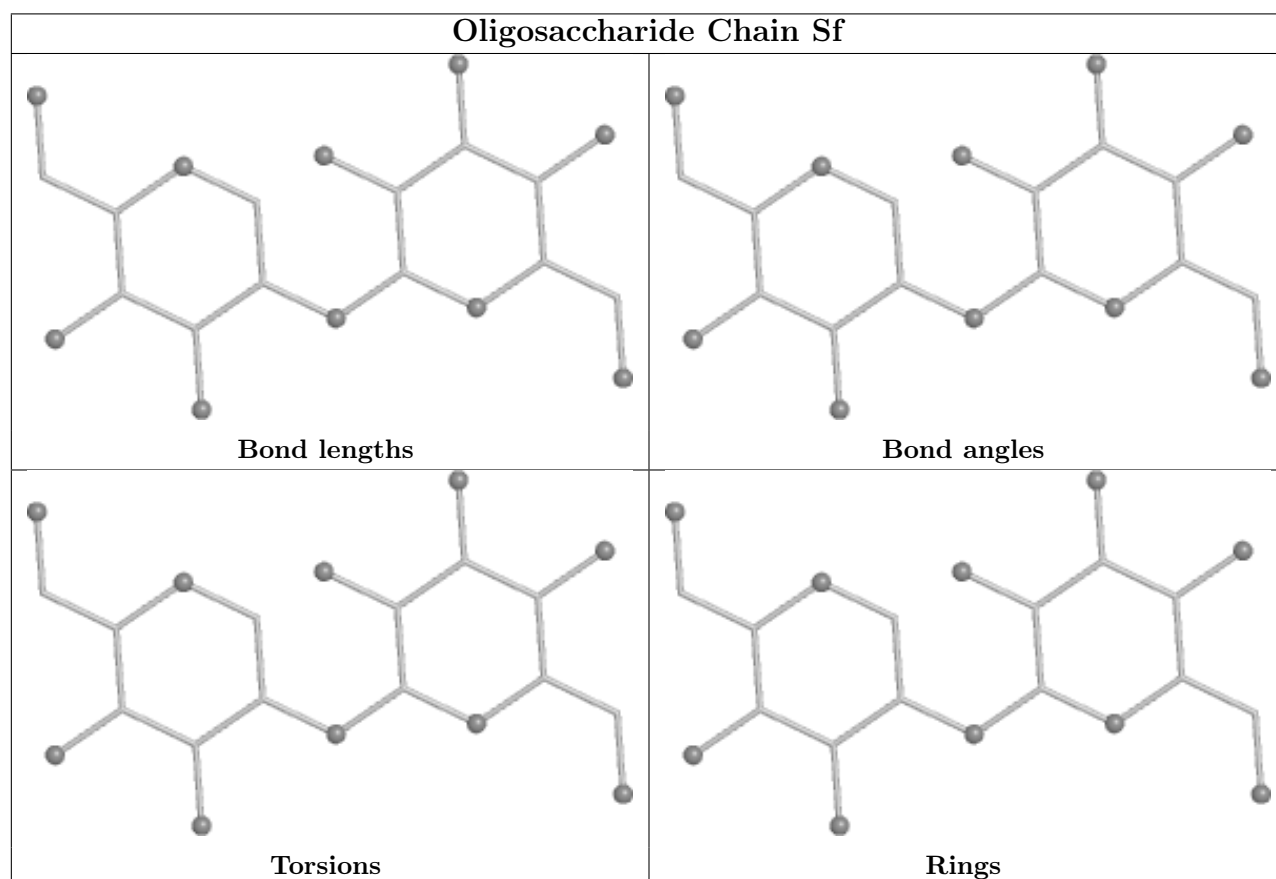
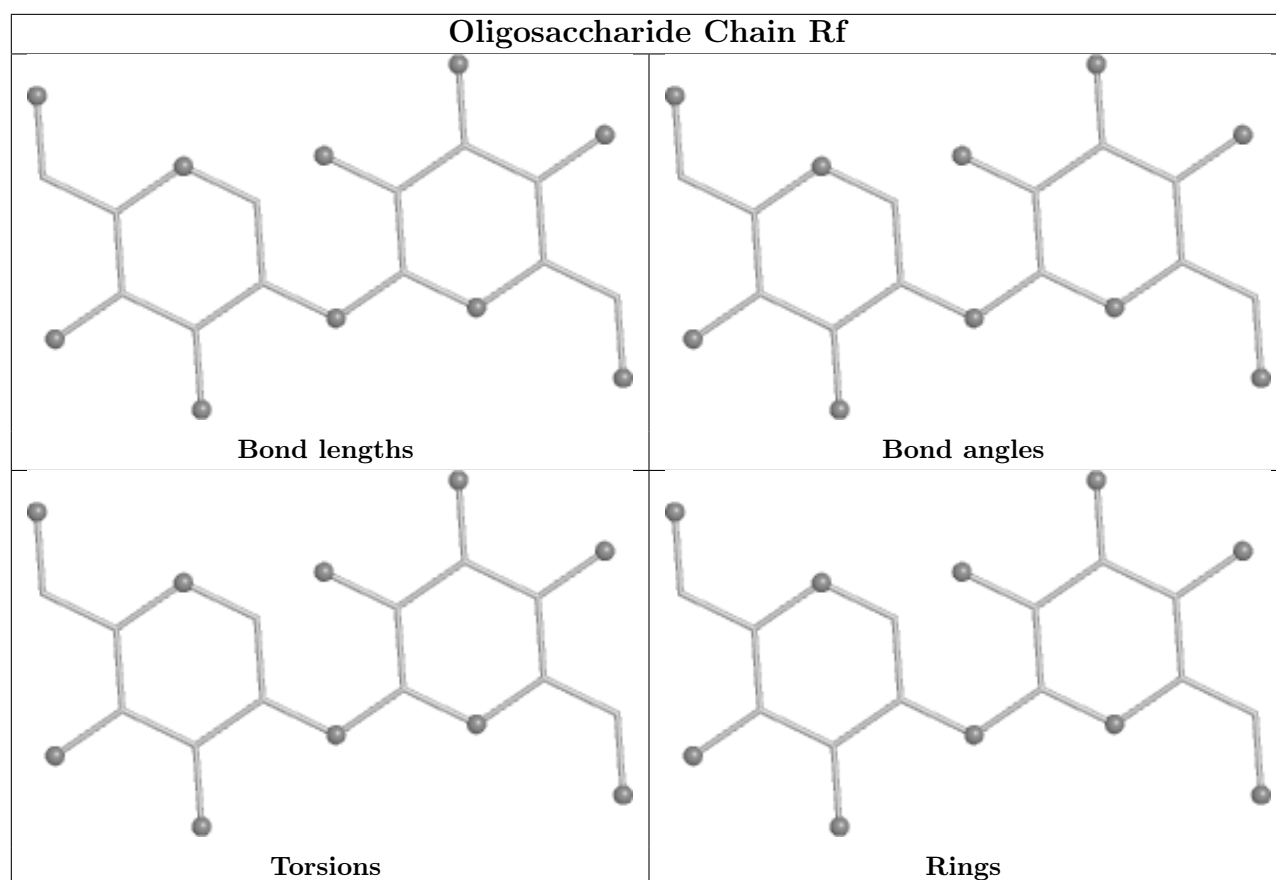


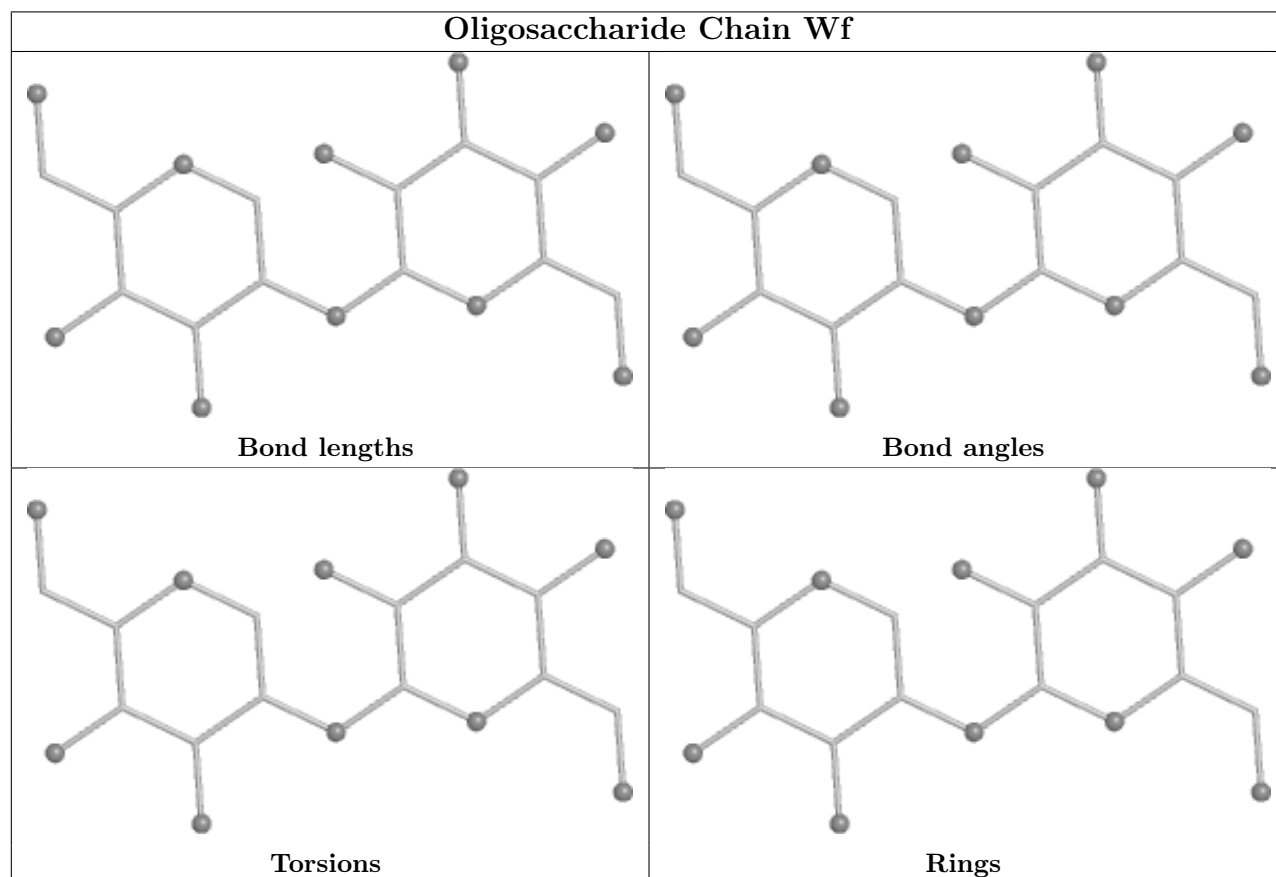
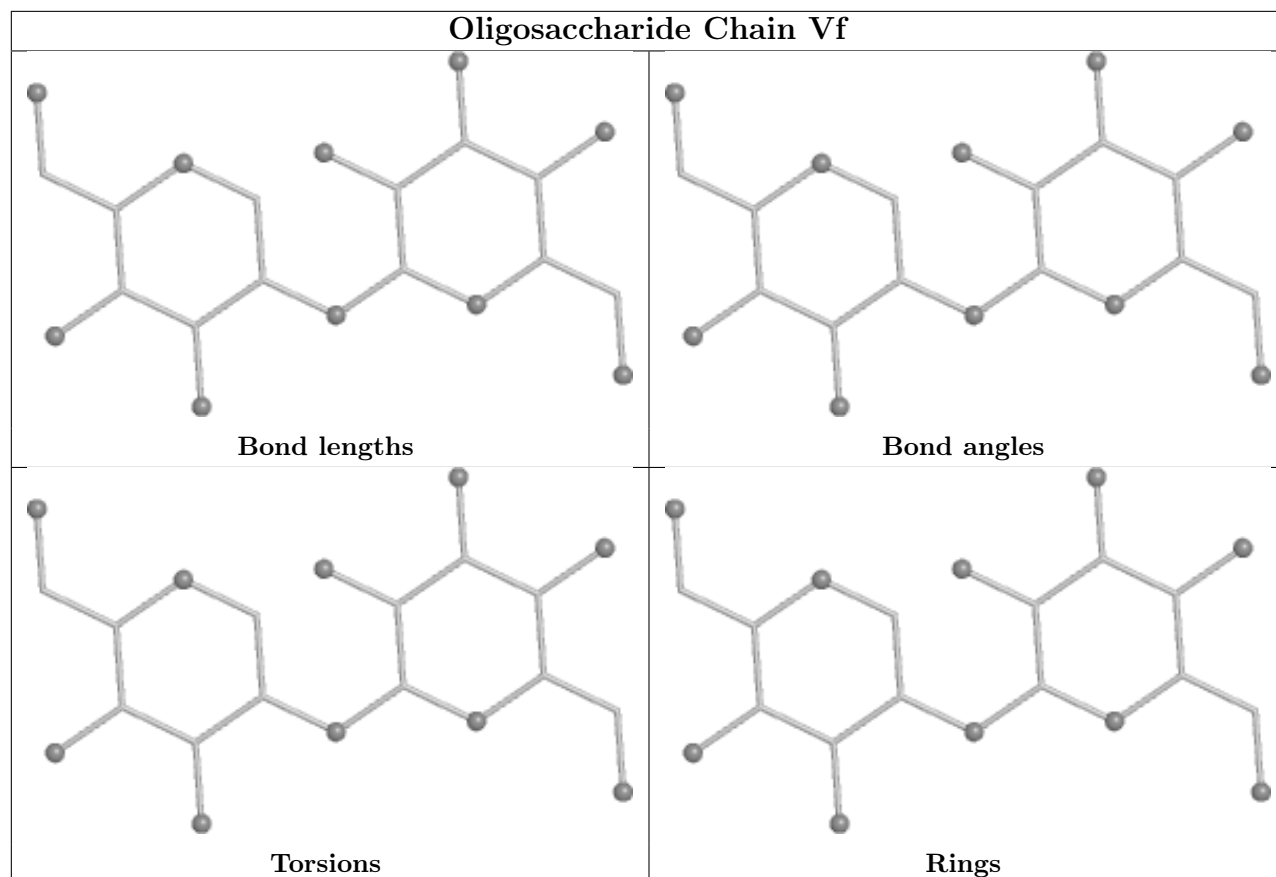
Oligosaccharide Chain Lf

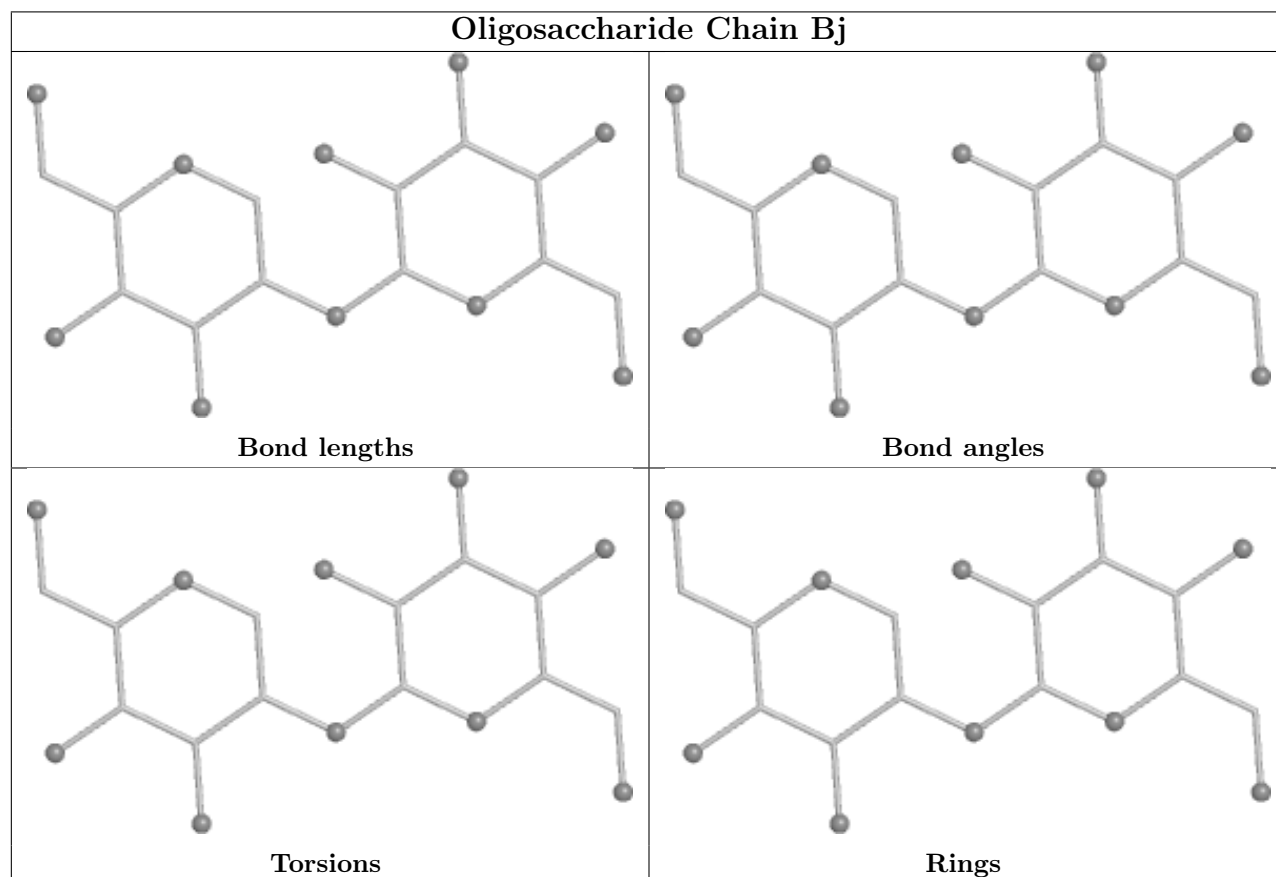
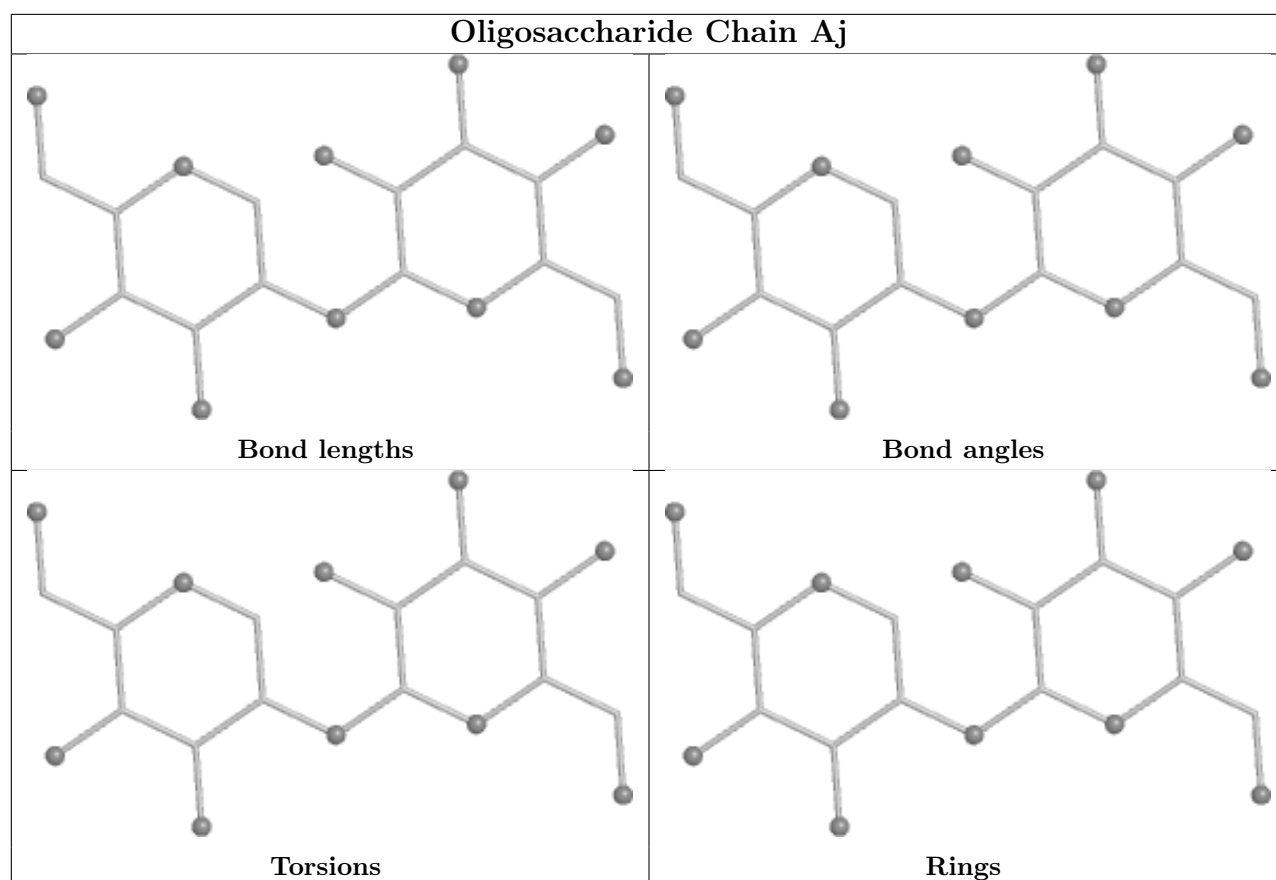


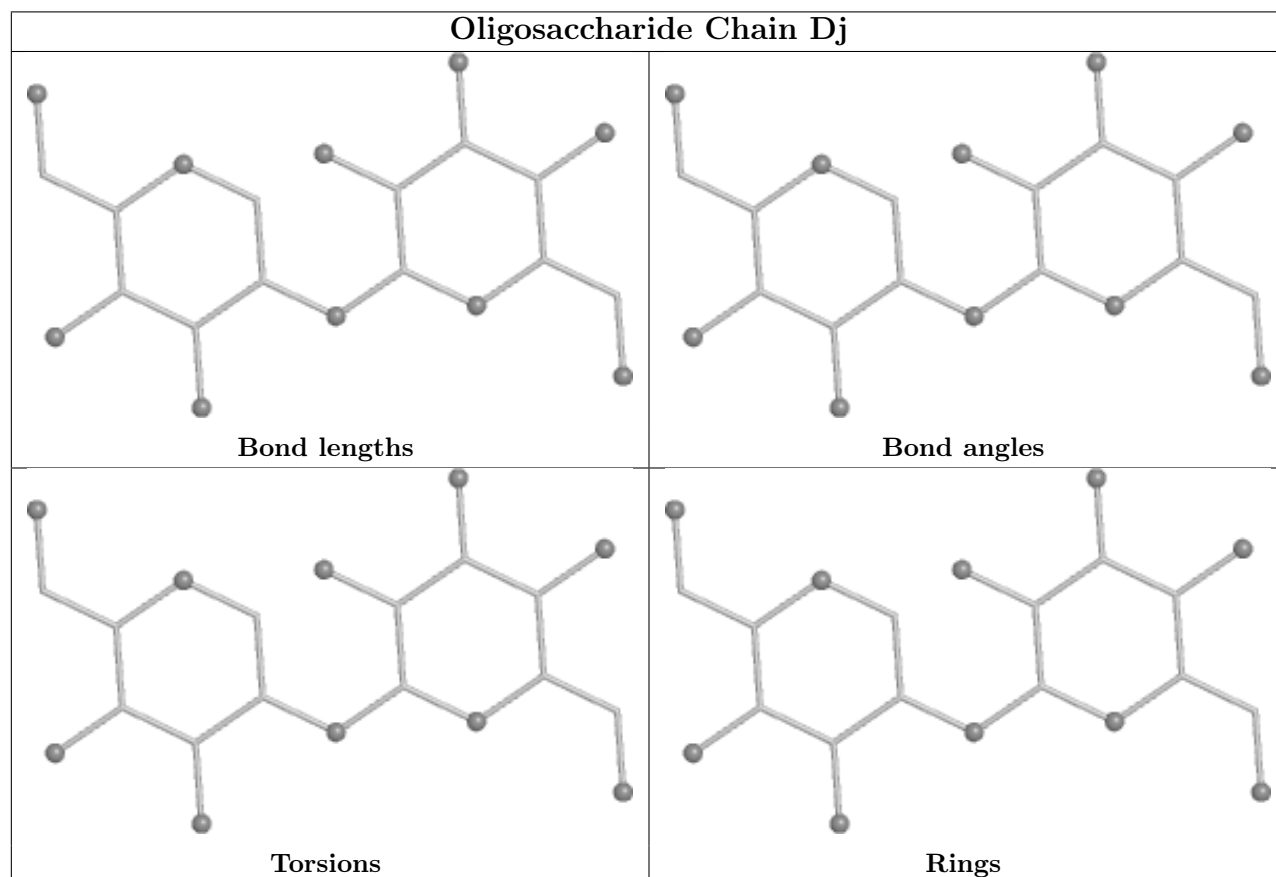
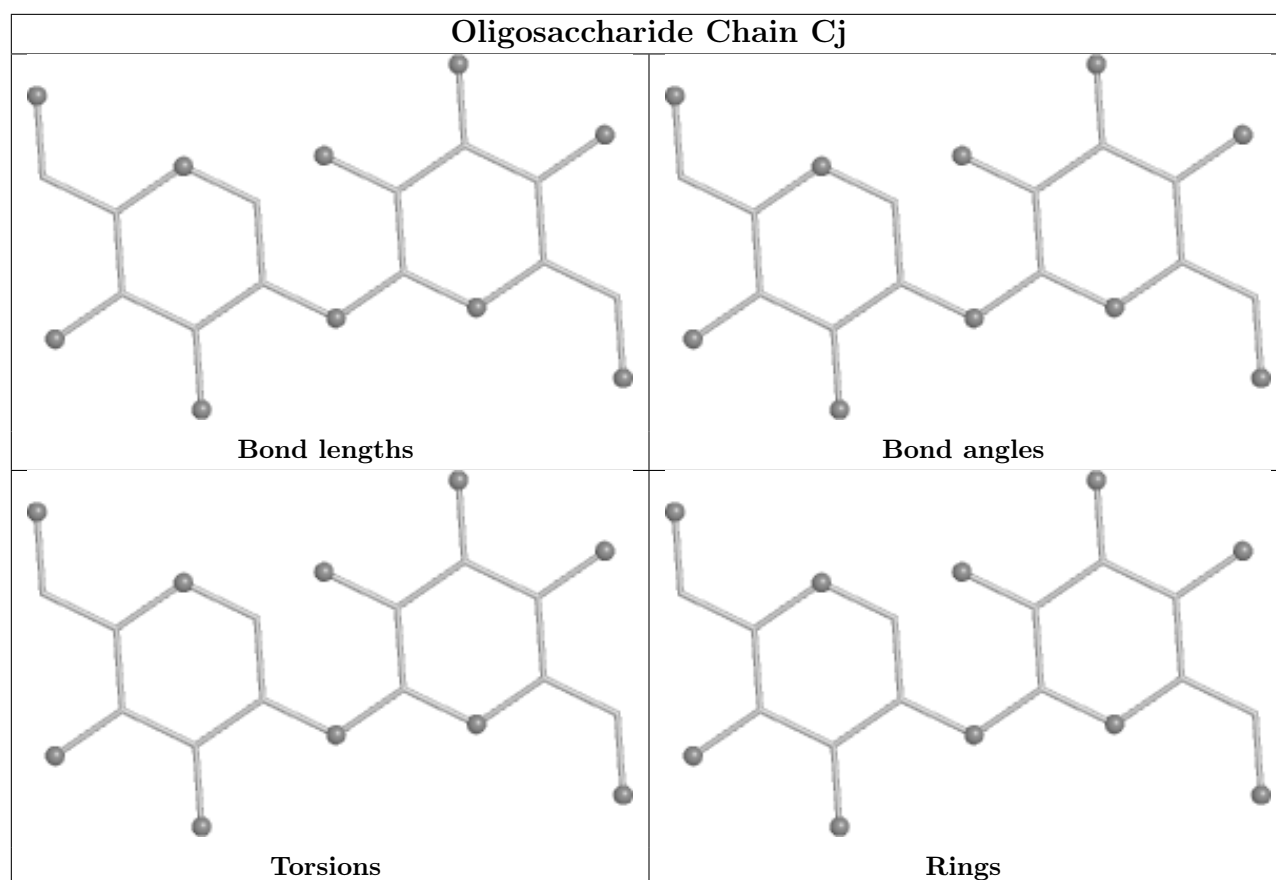


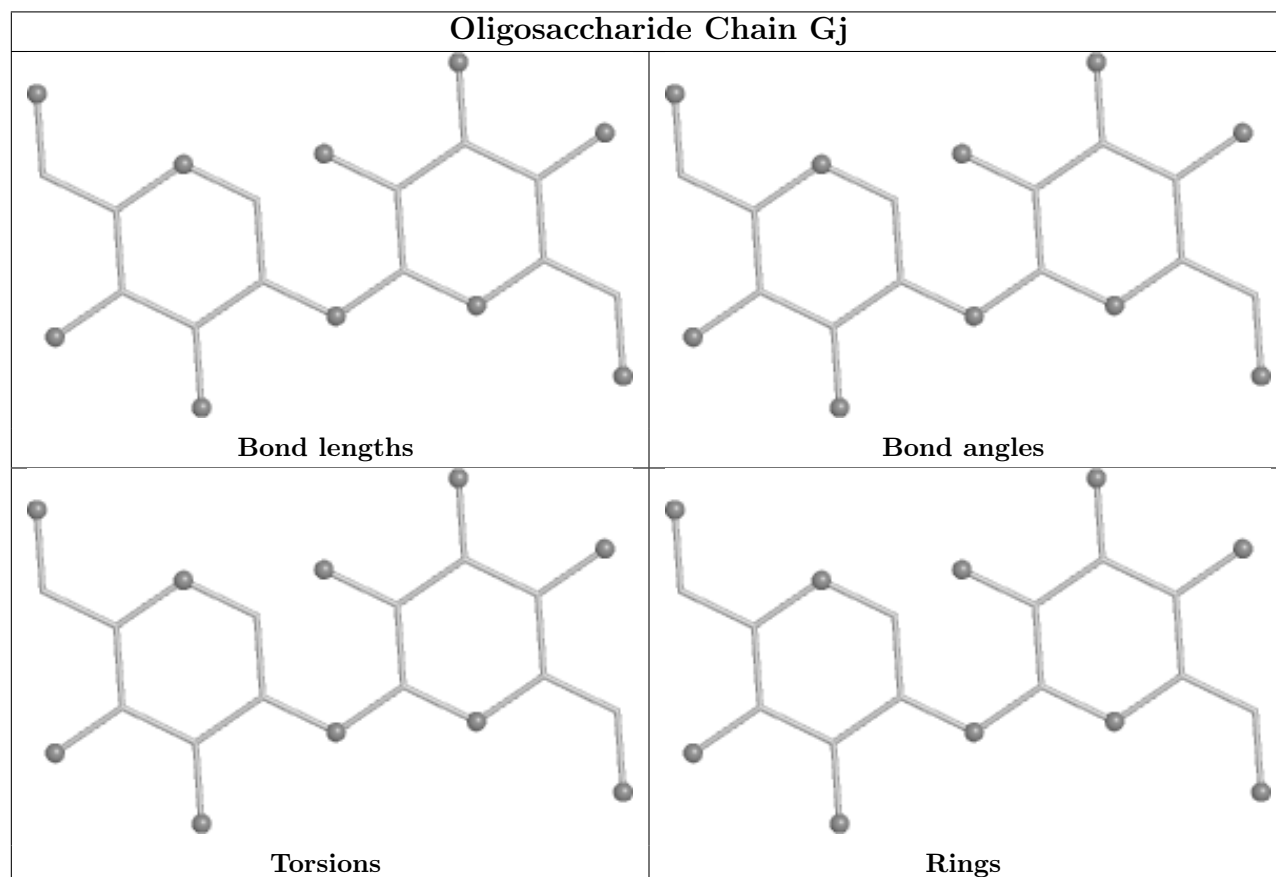
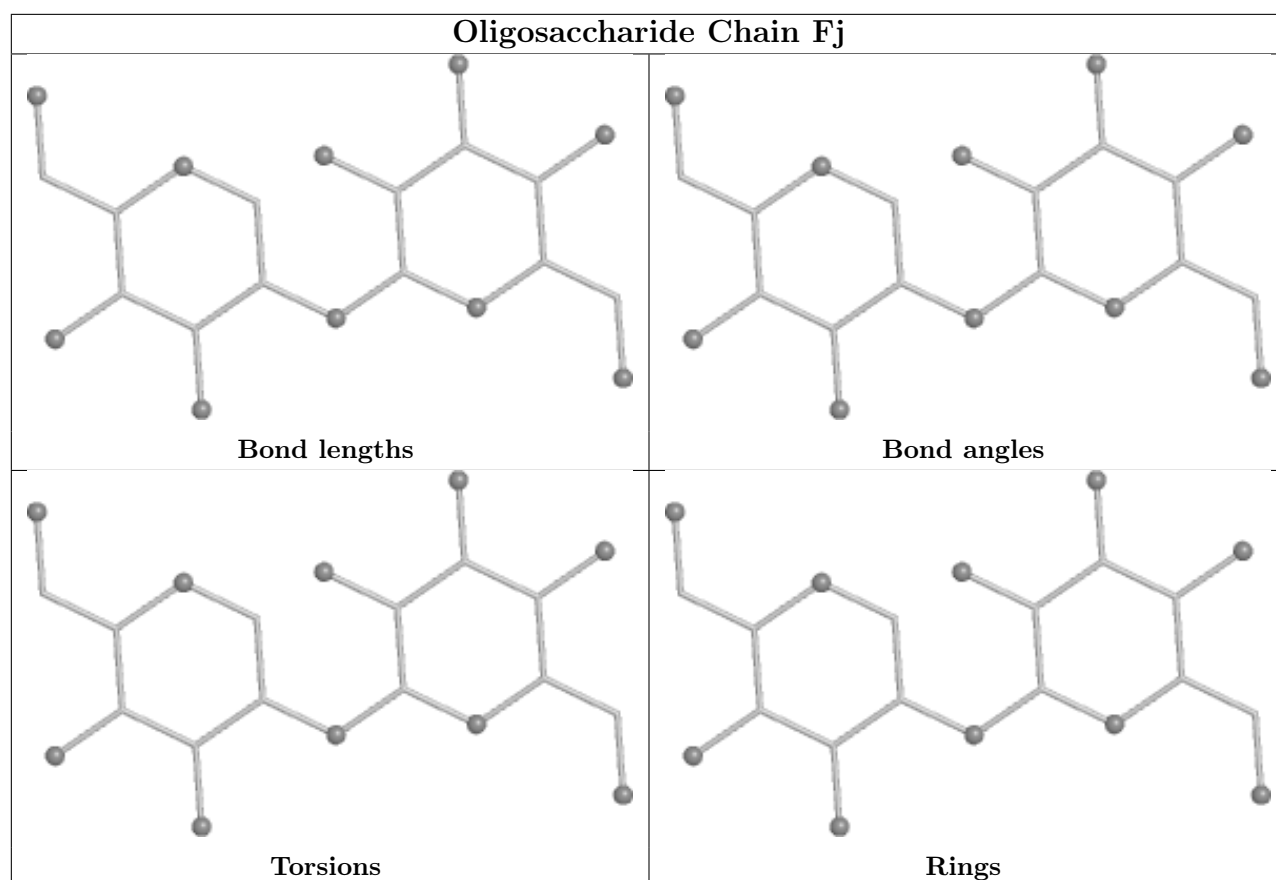




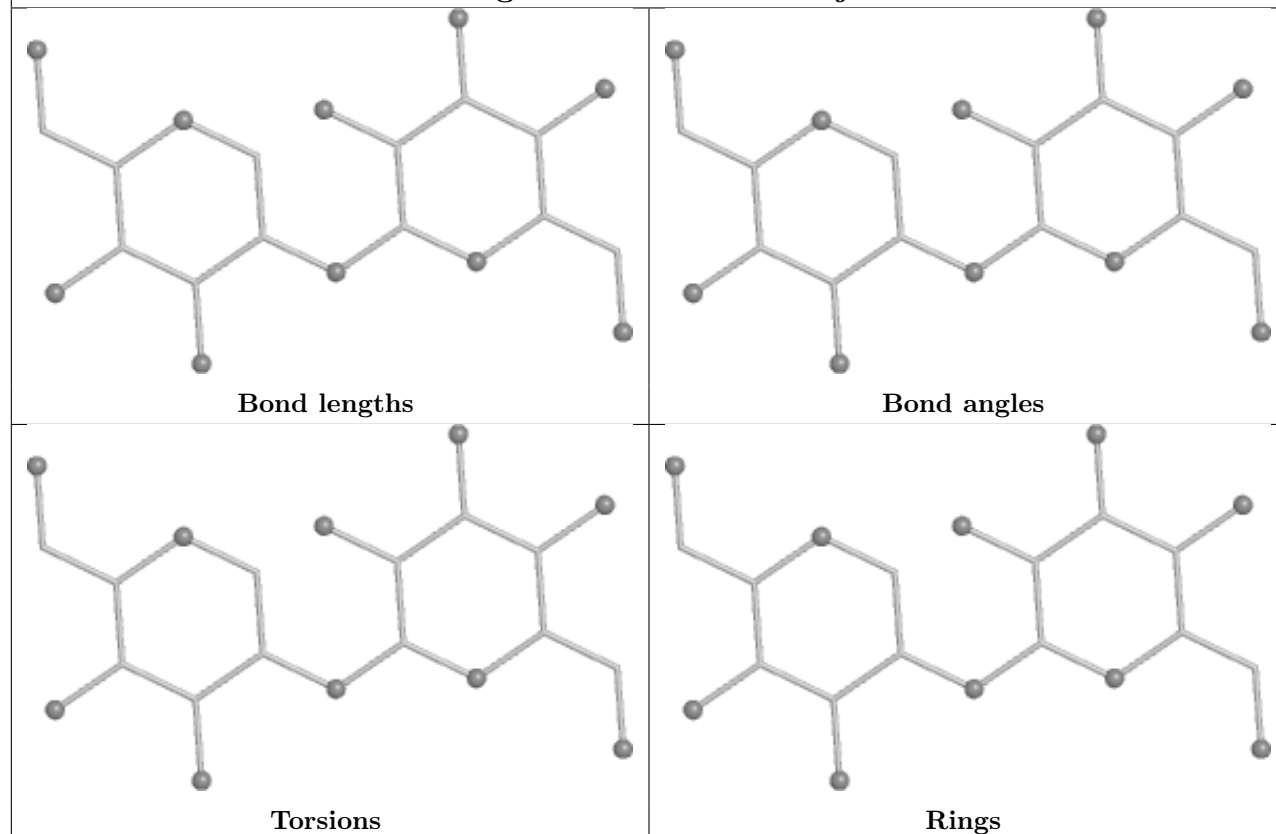




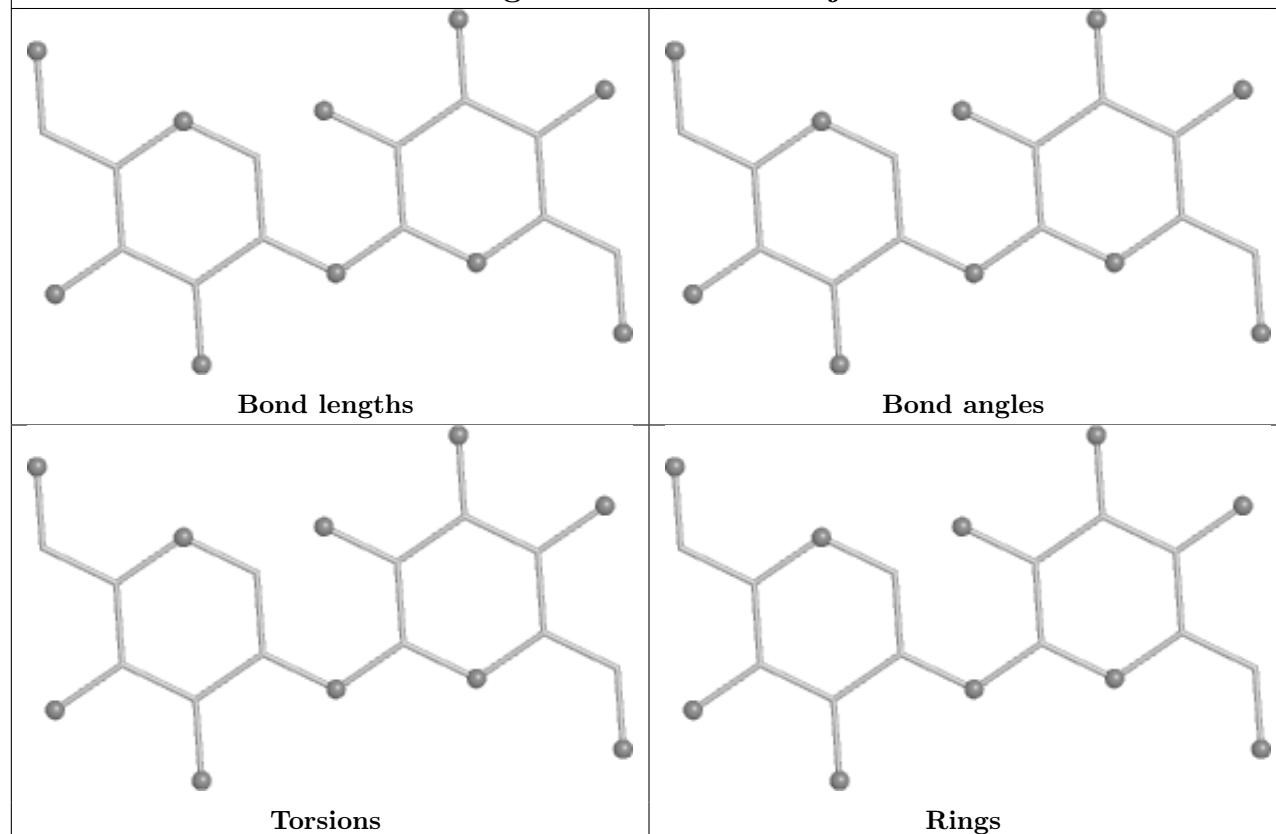


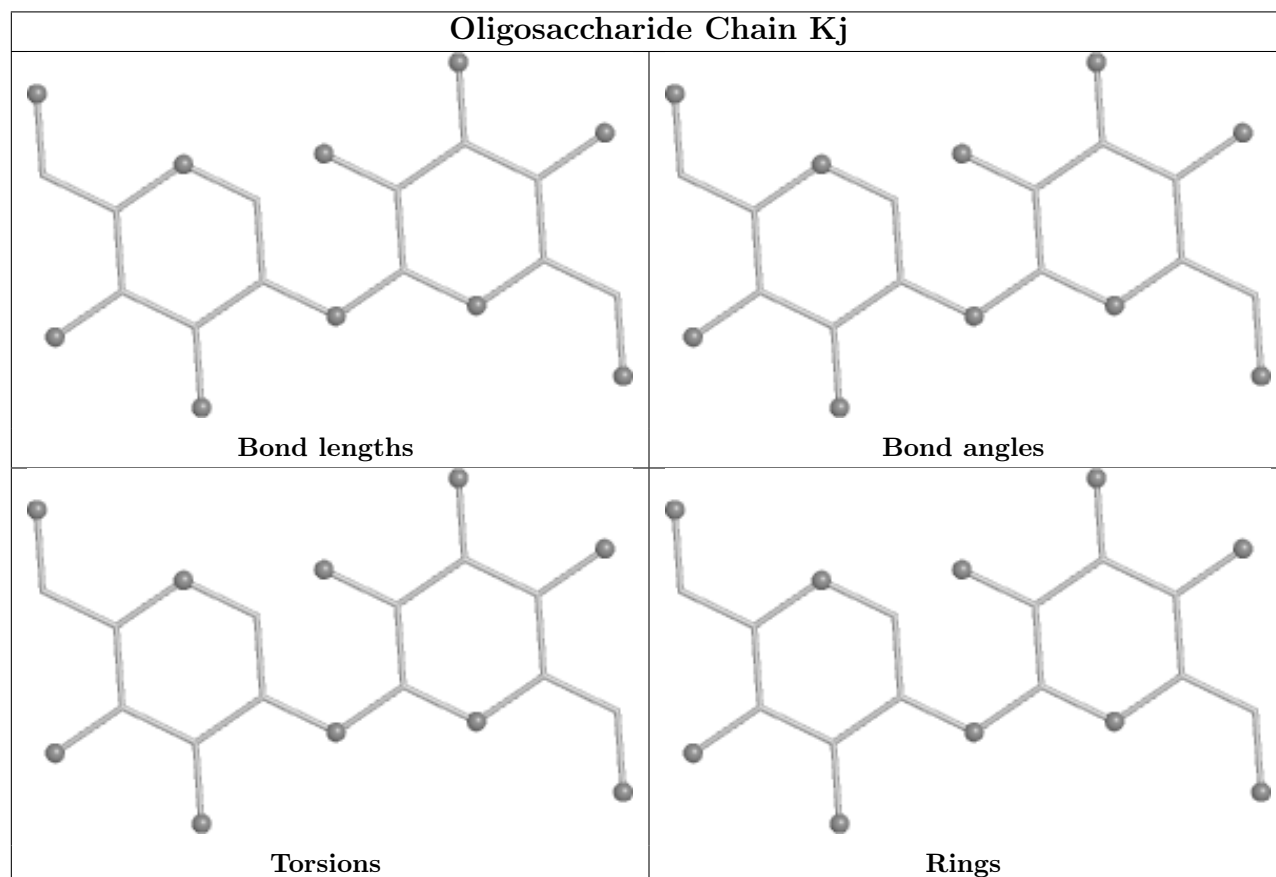
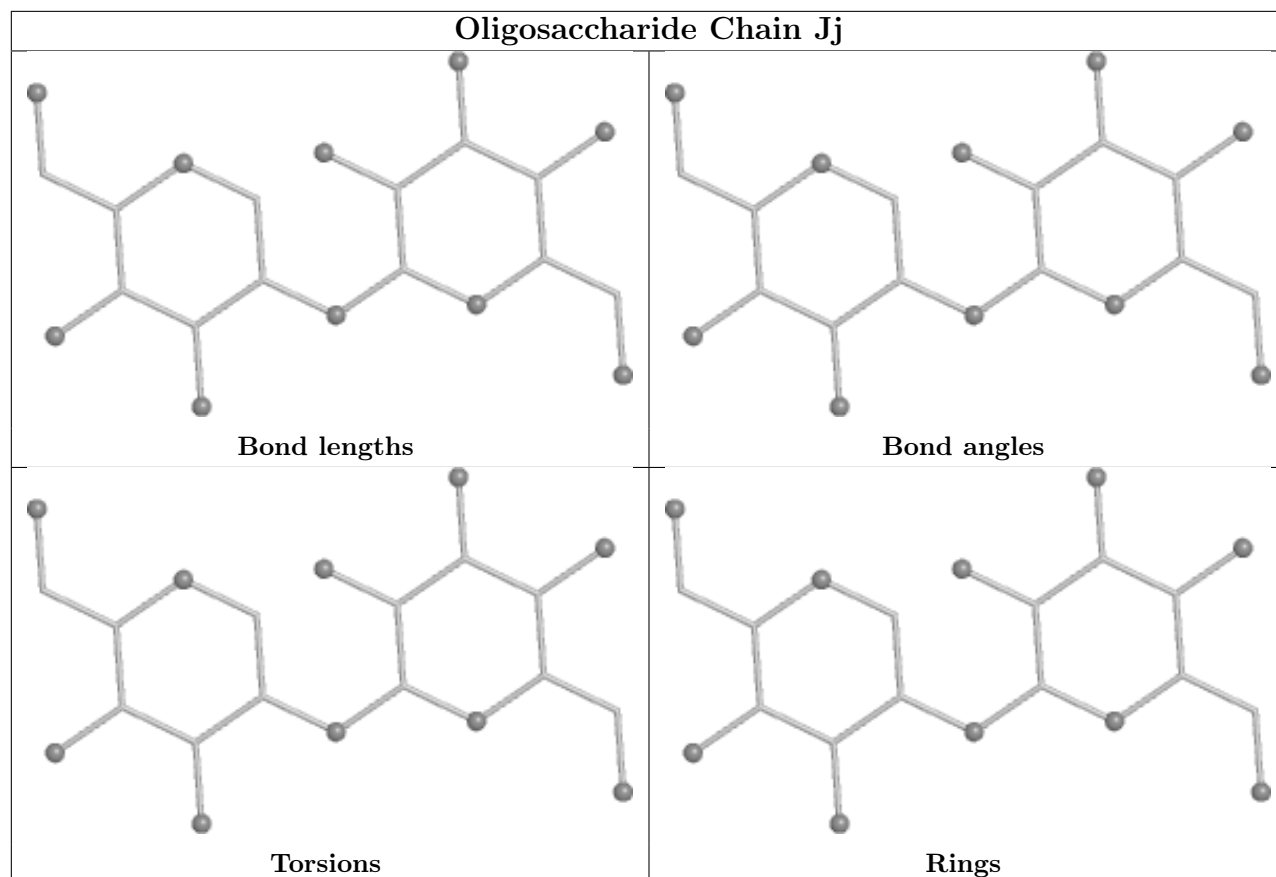


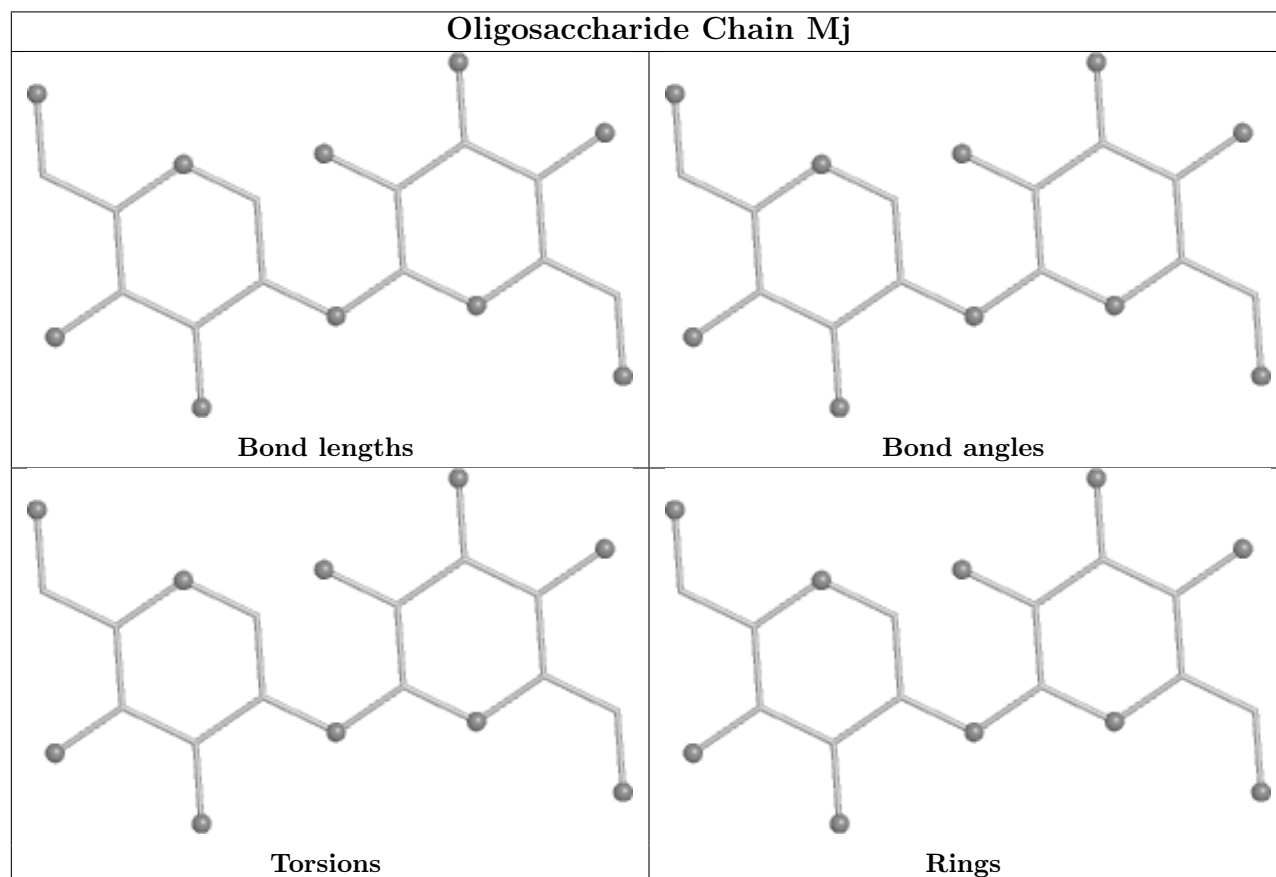
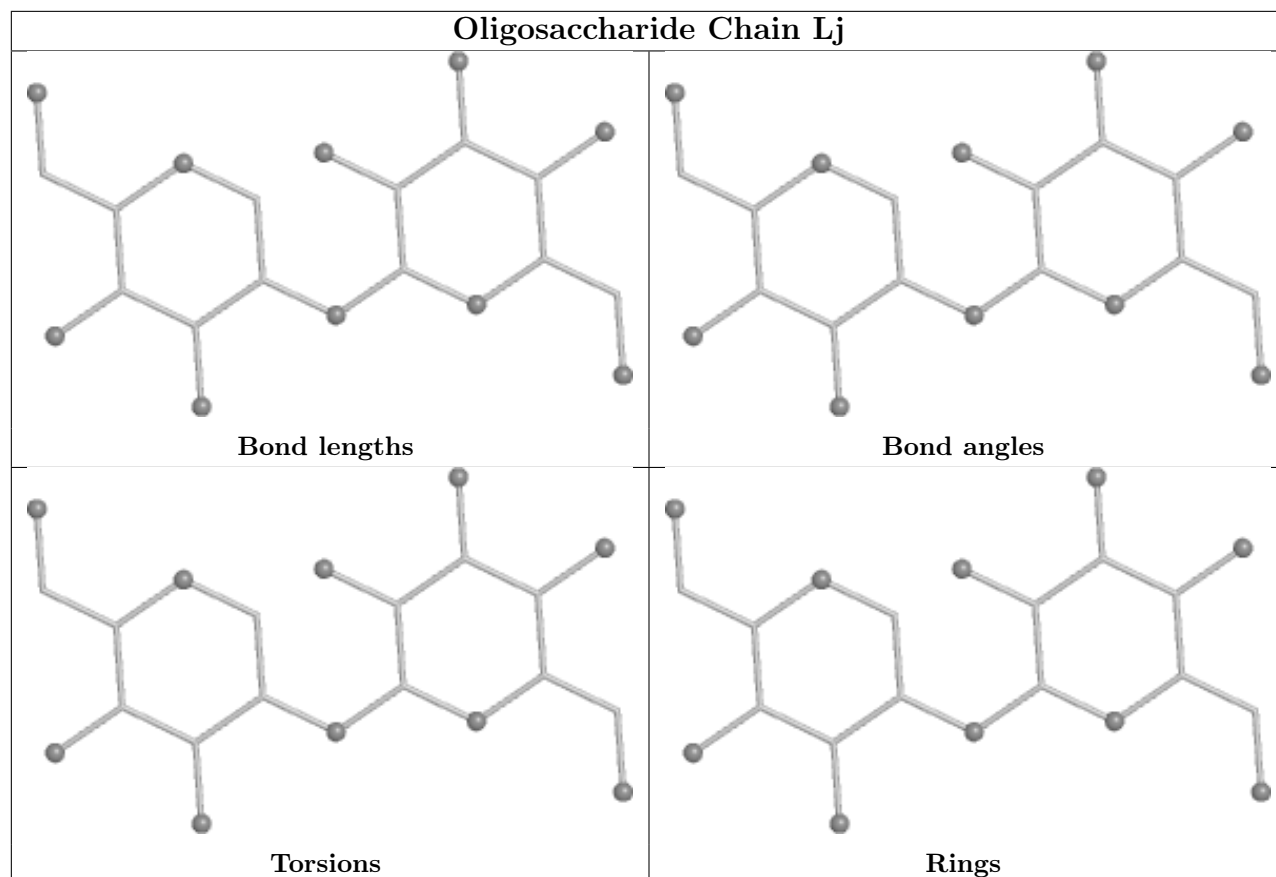
Oligosaccharide Chain Hj

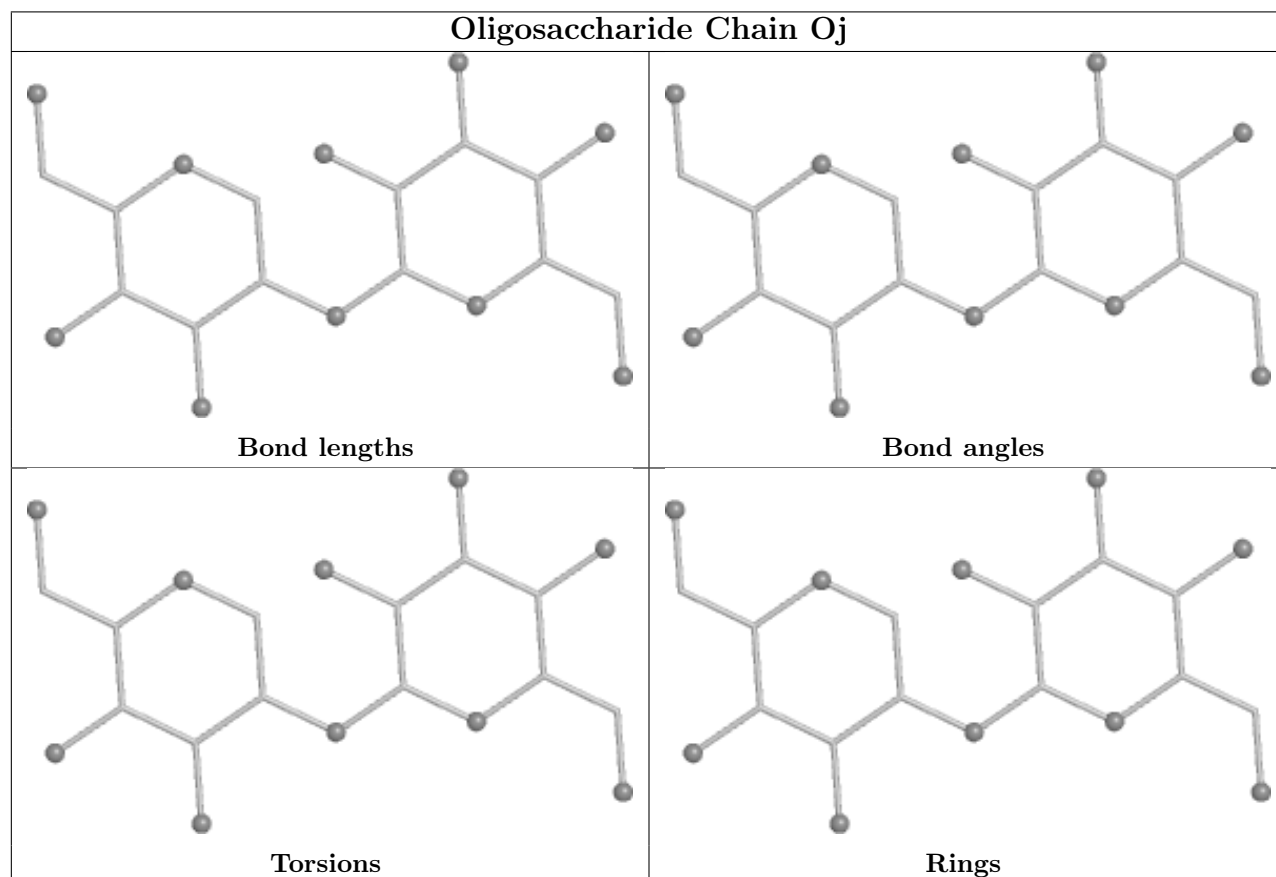
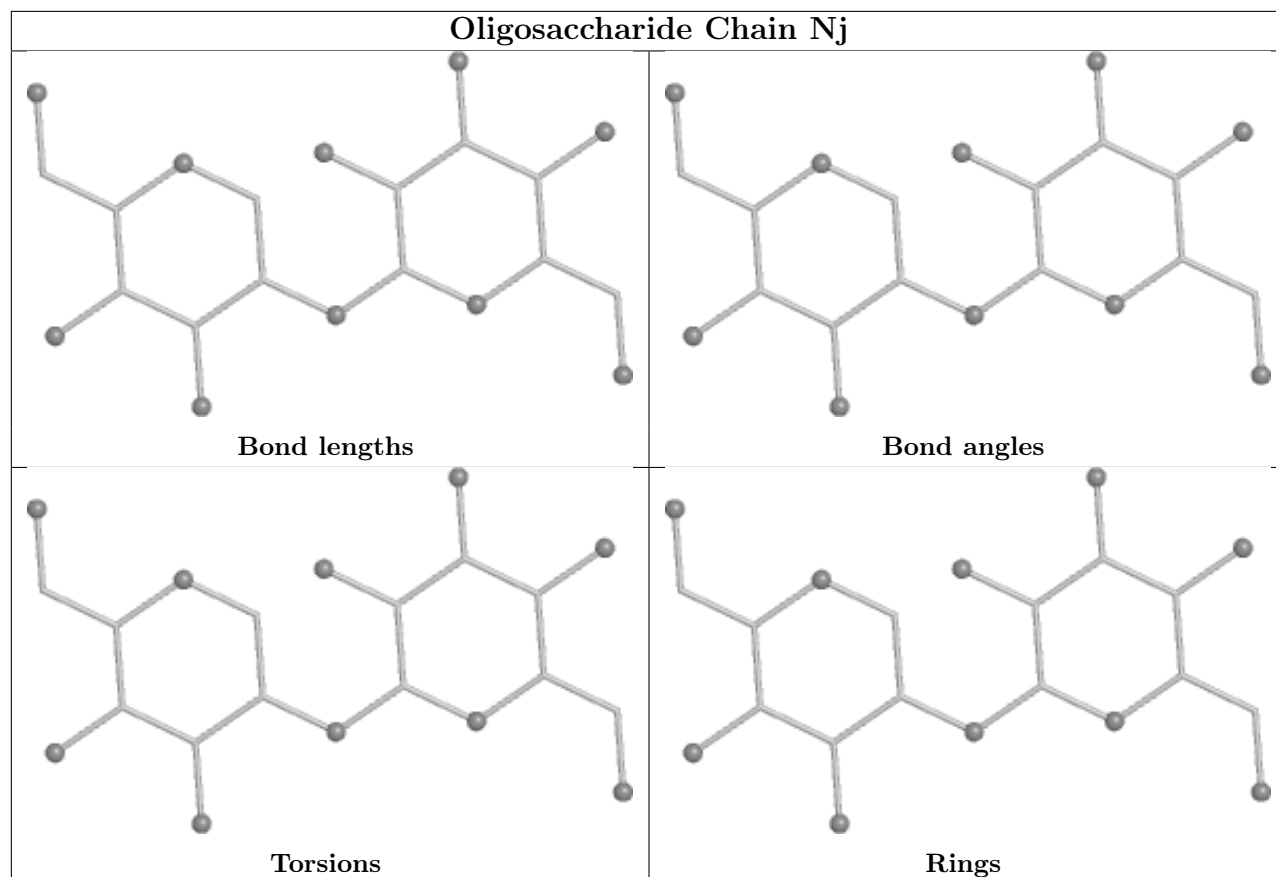


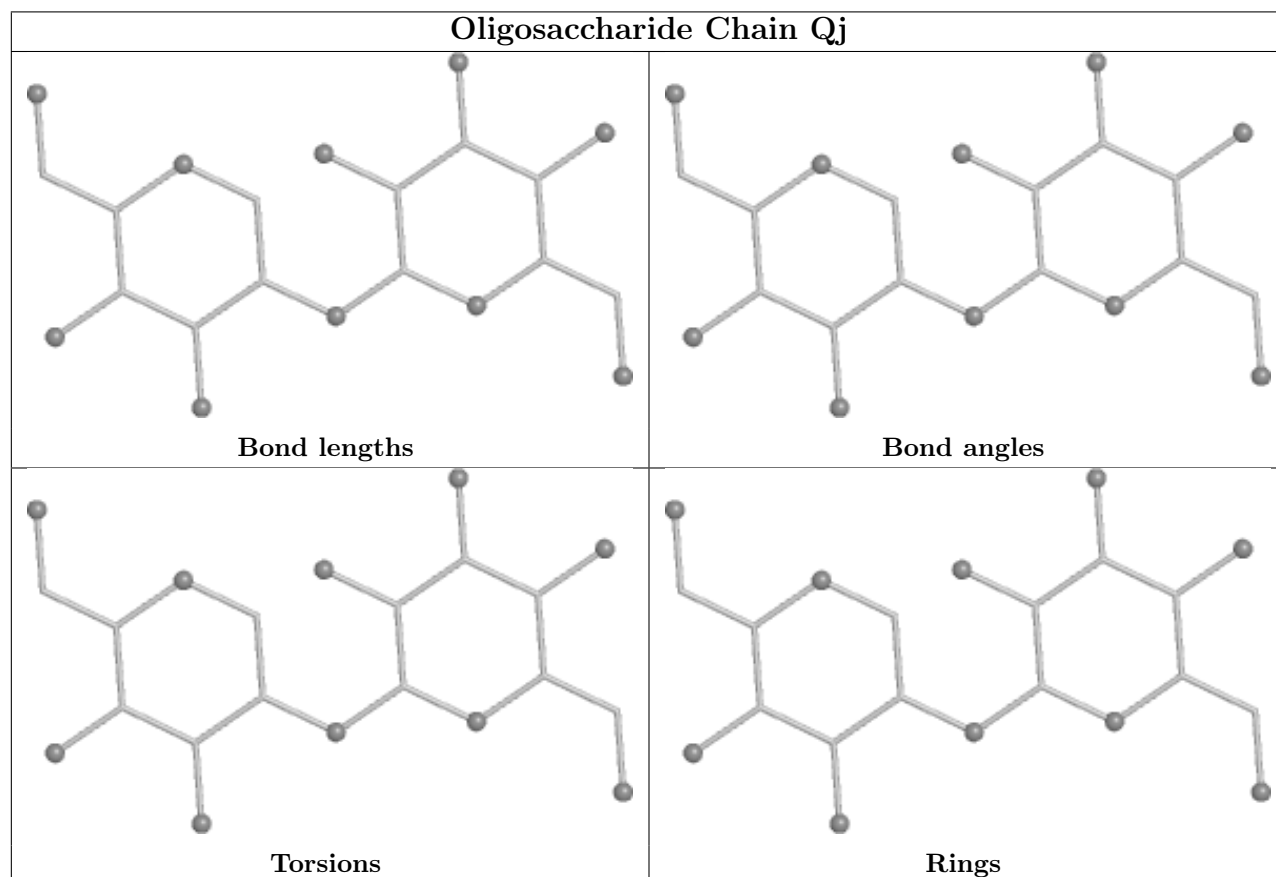
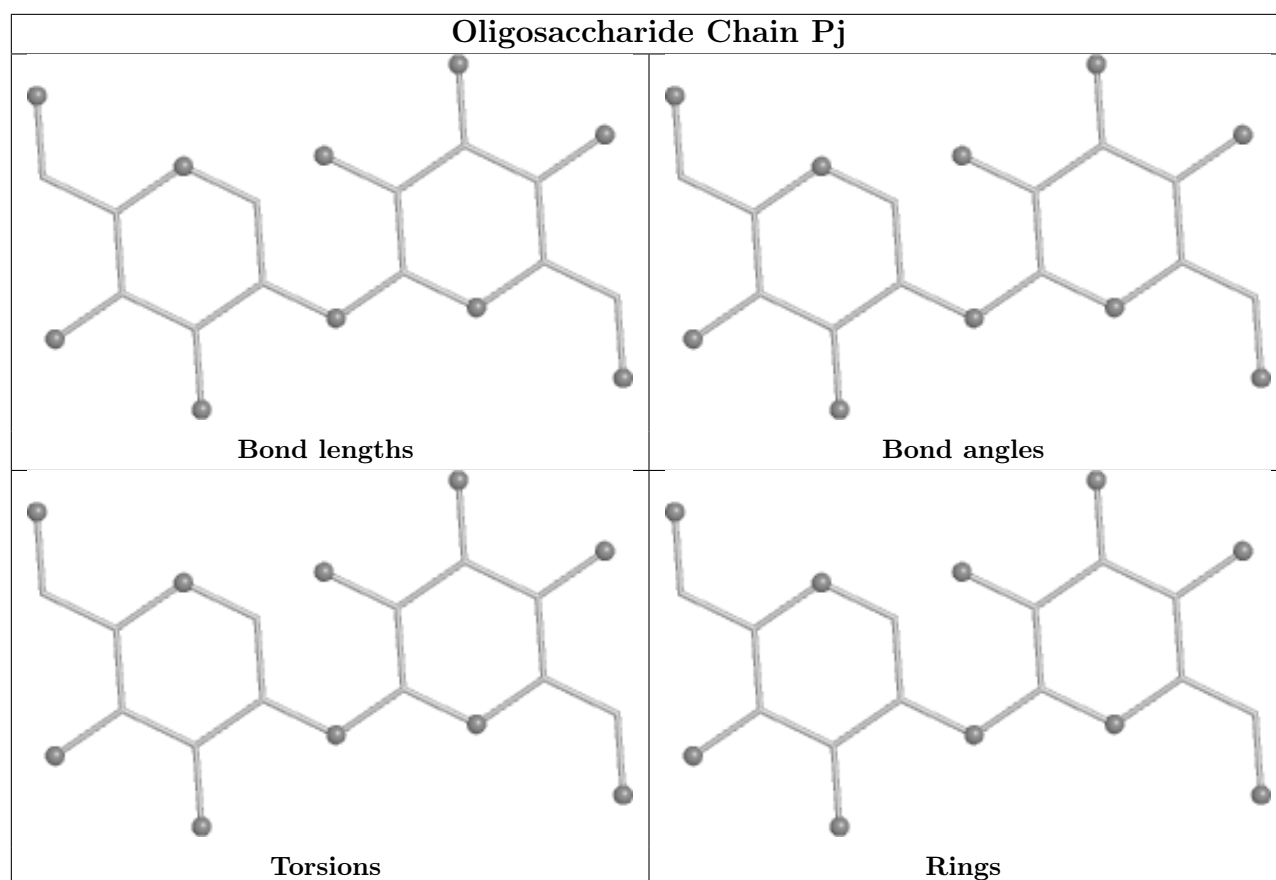
Oligosaccharide Chain Ij

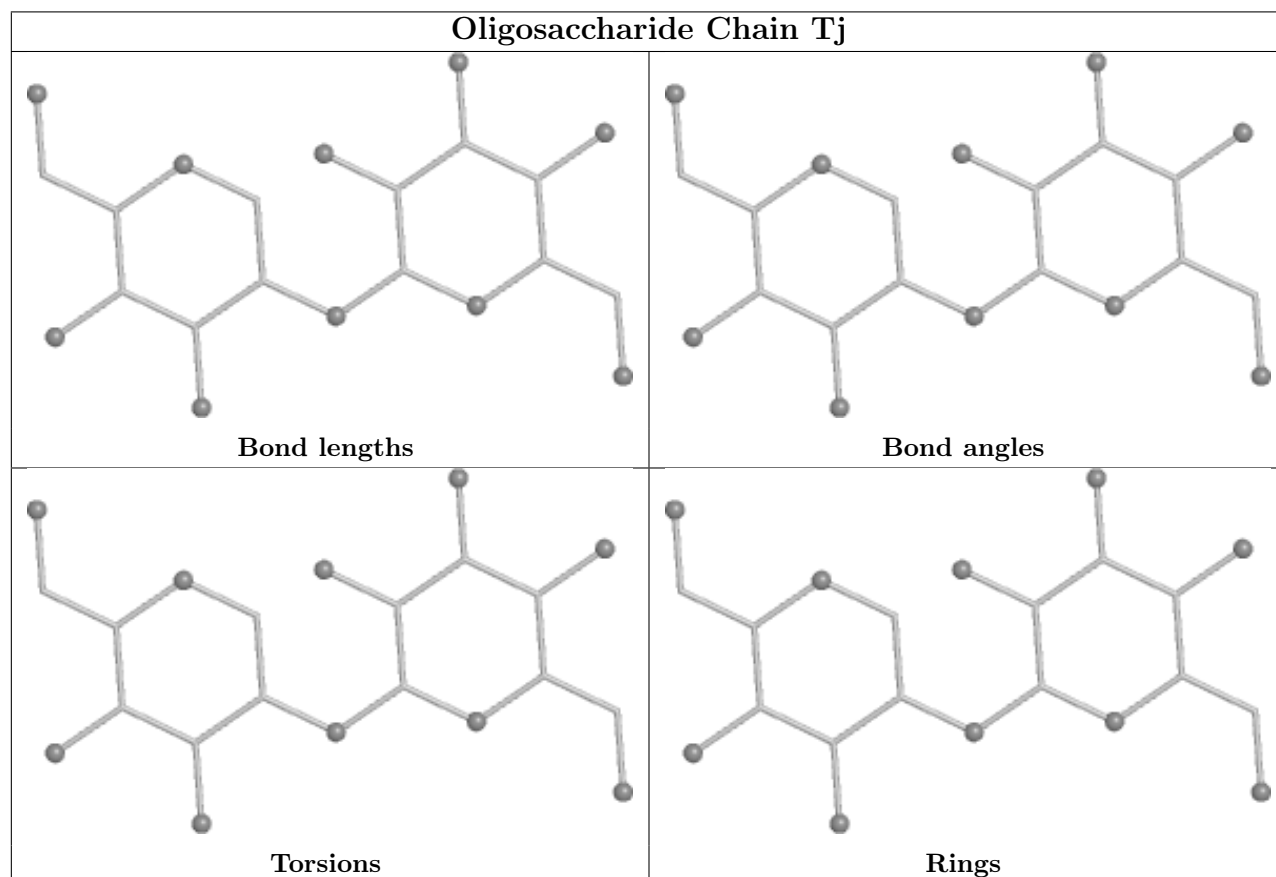
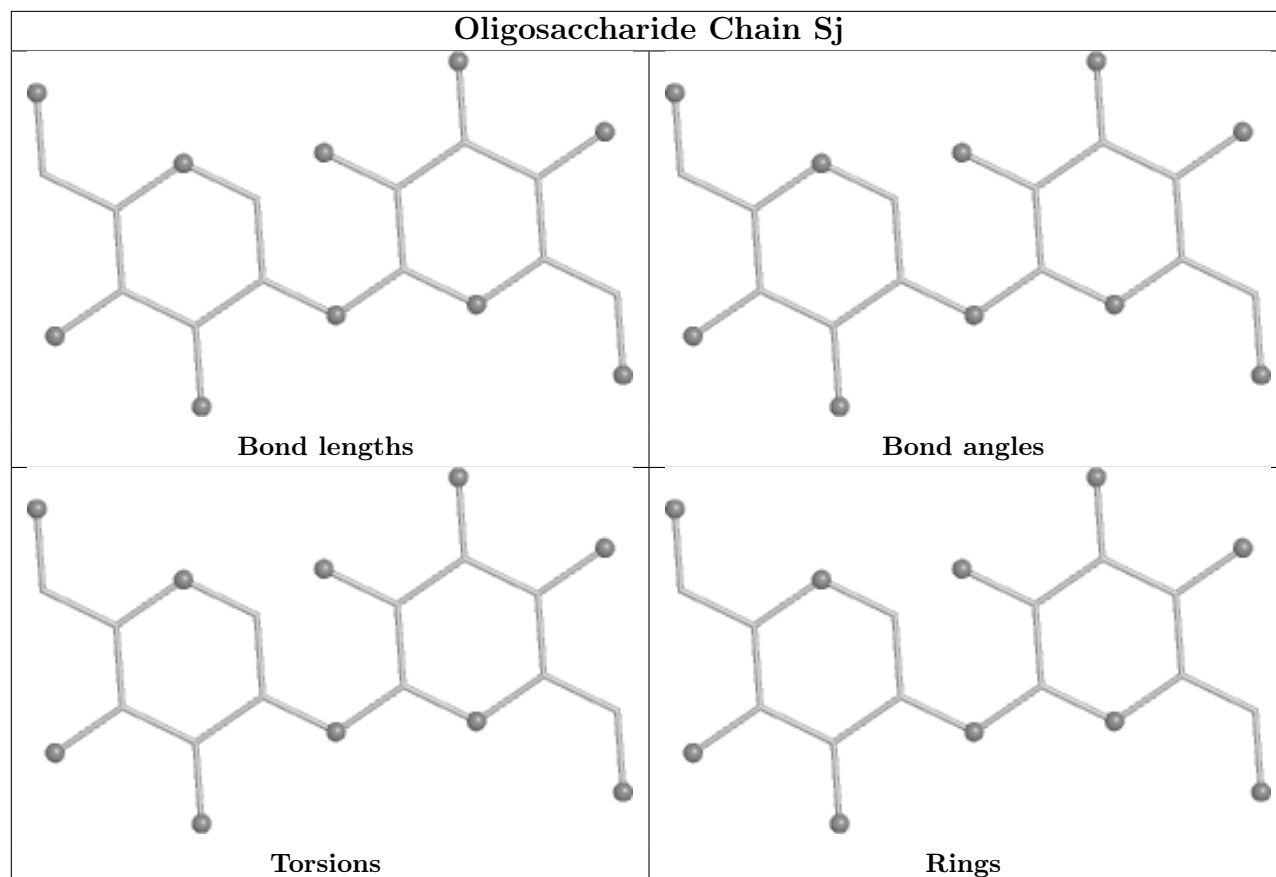


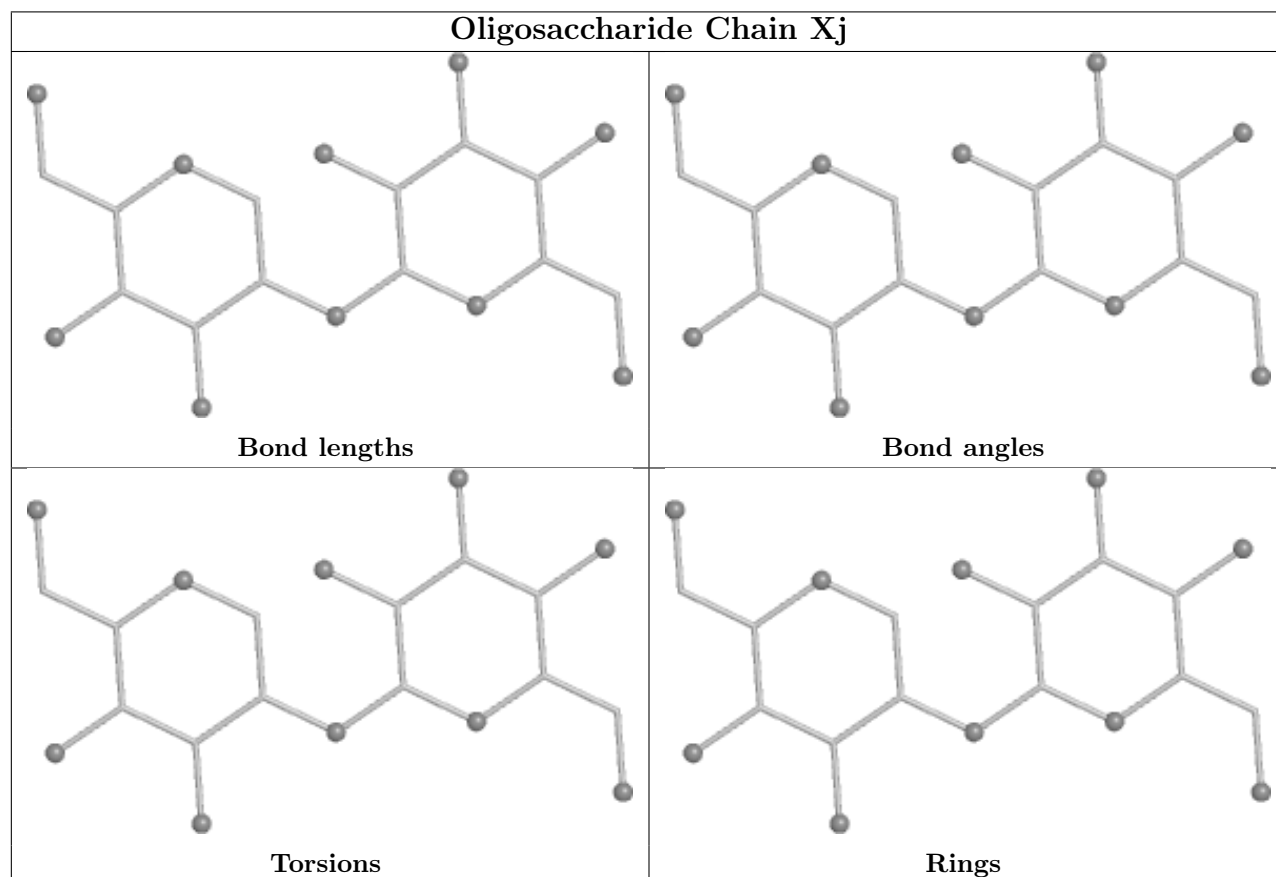
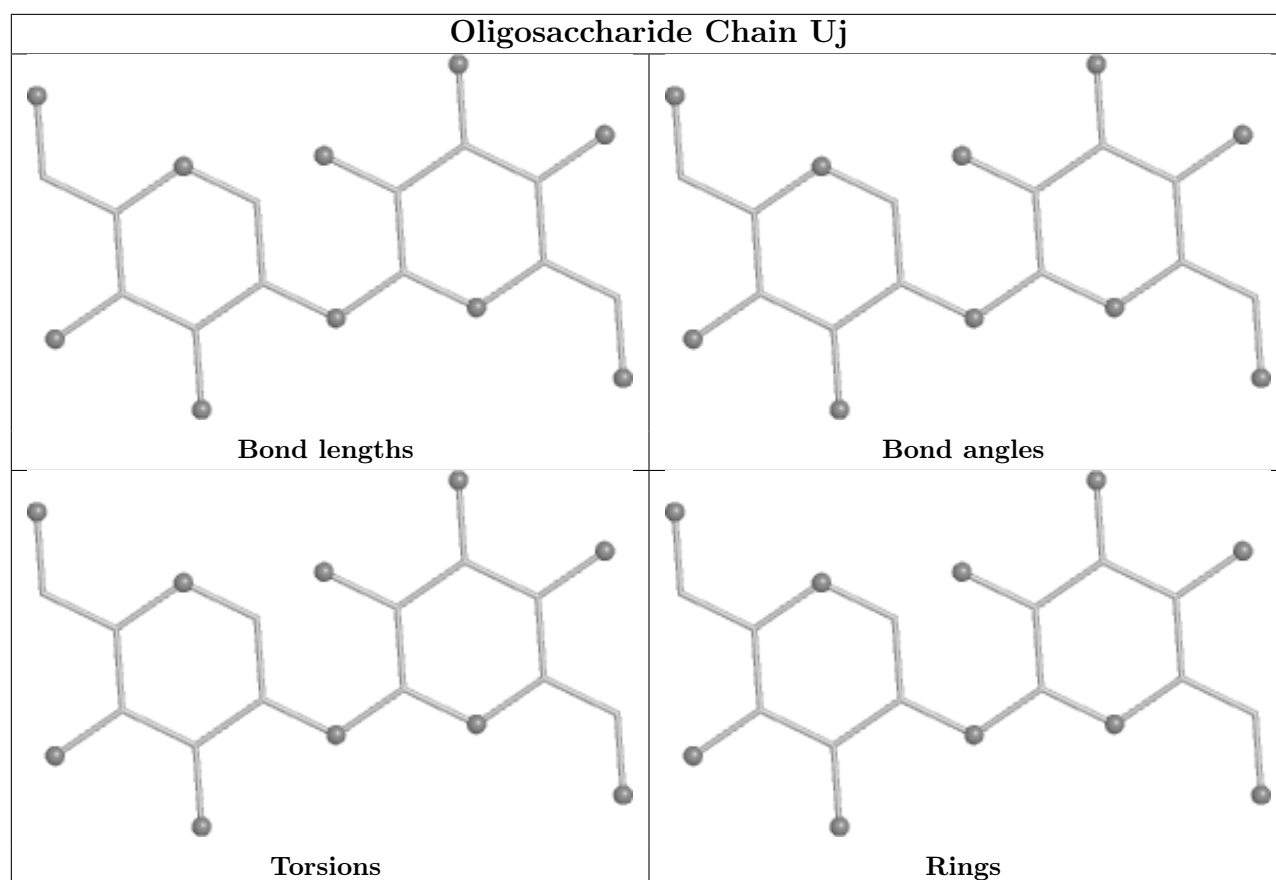


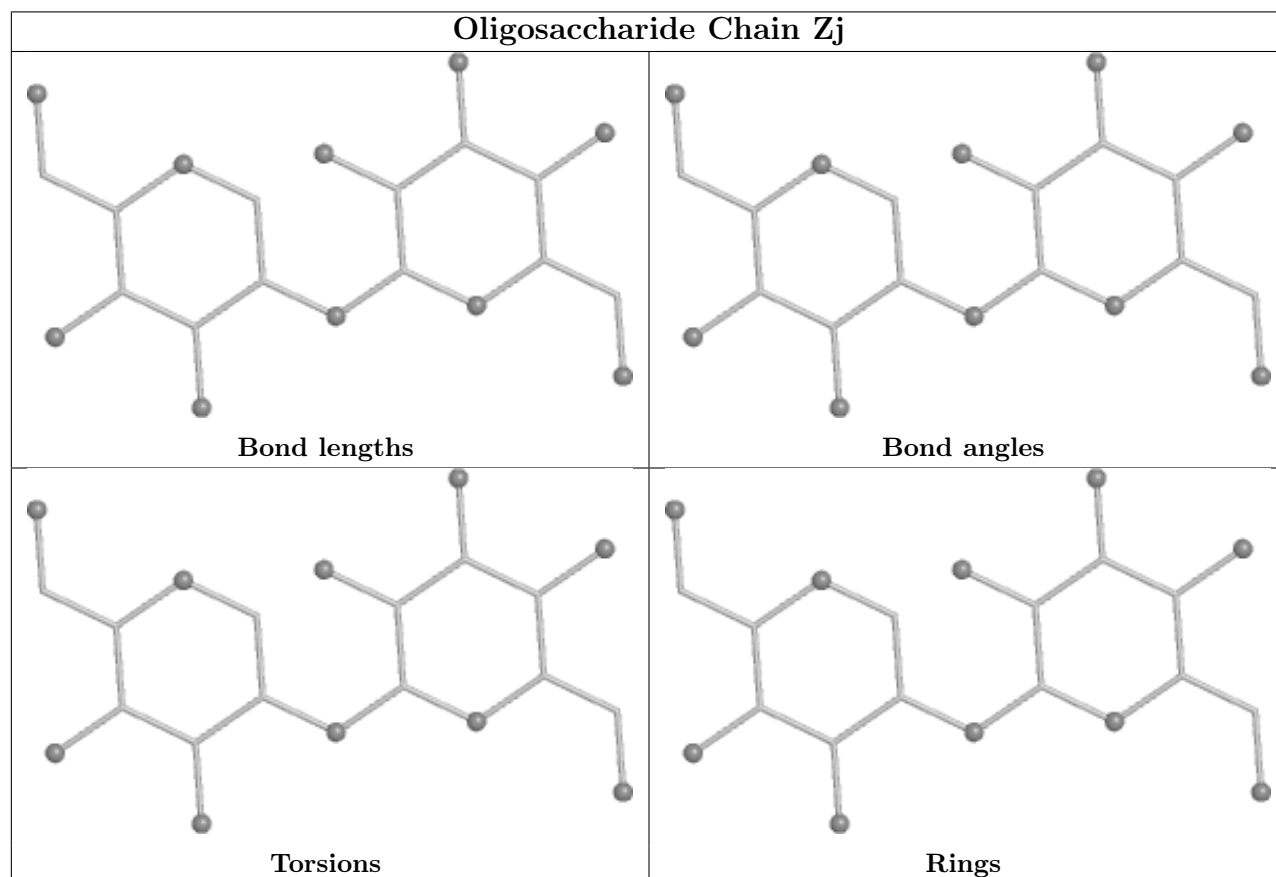
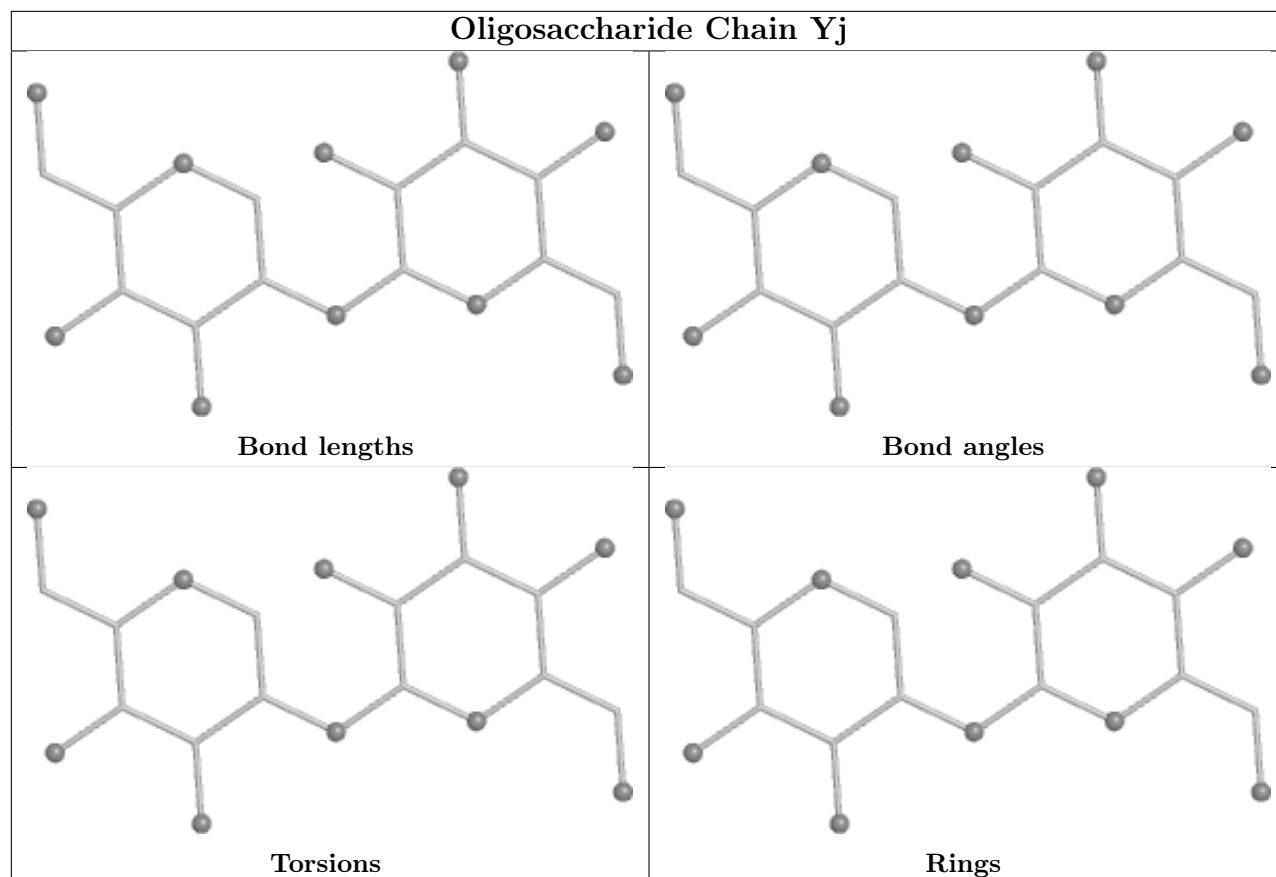


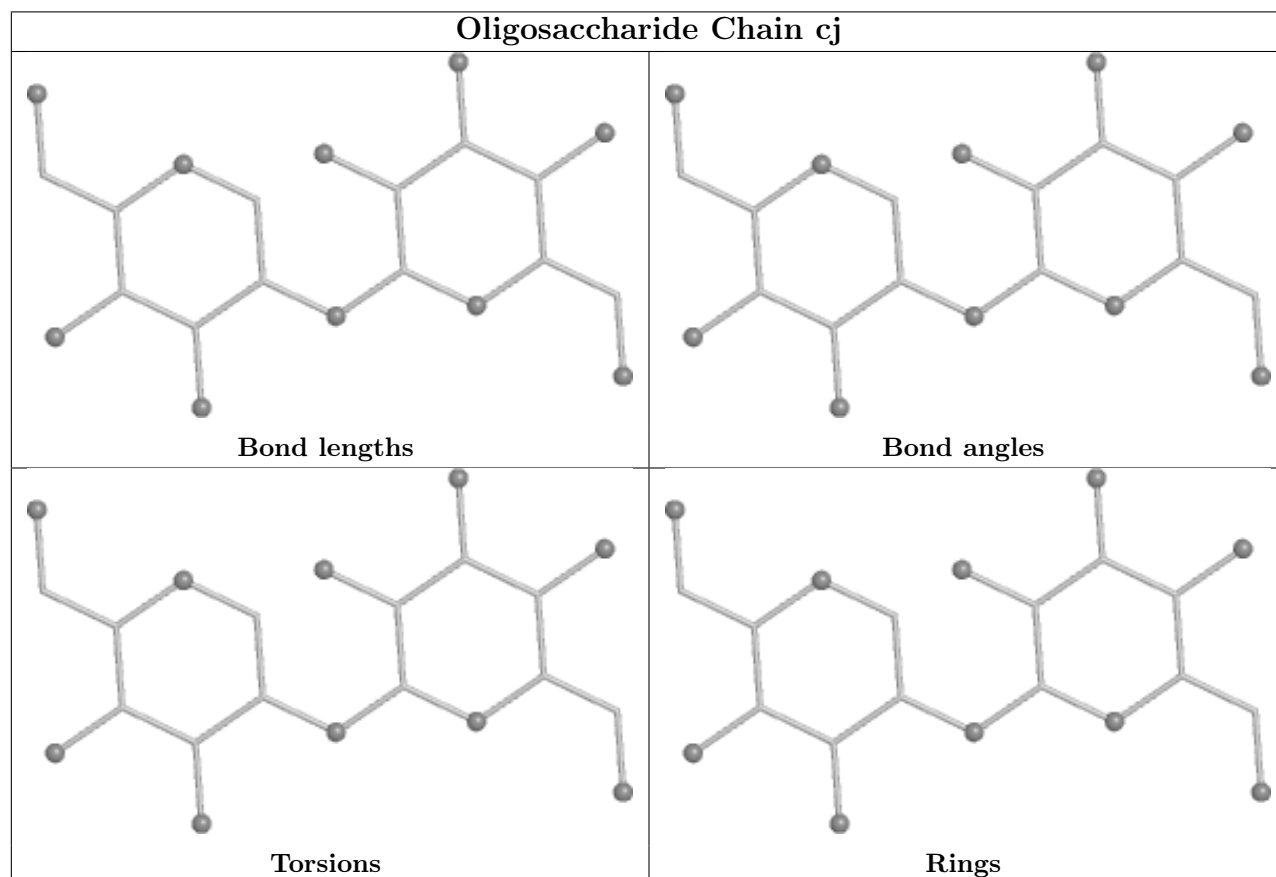
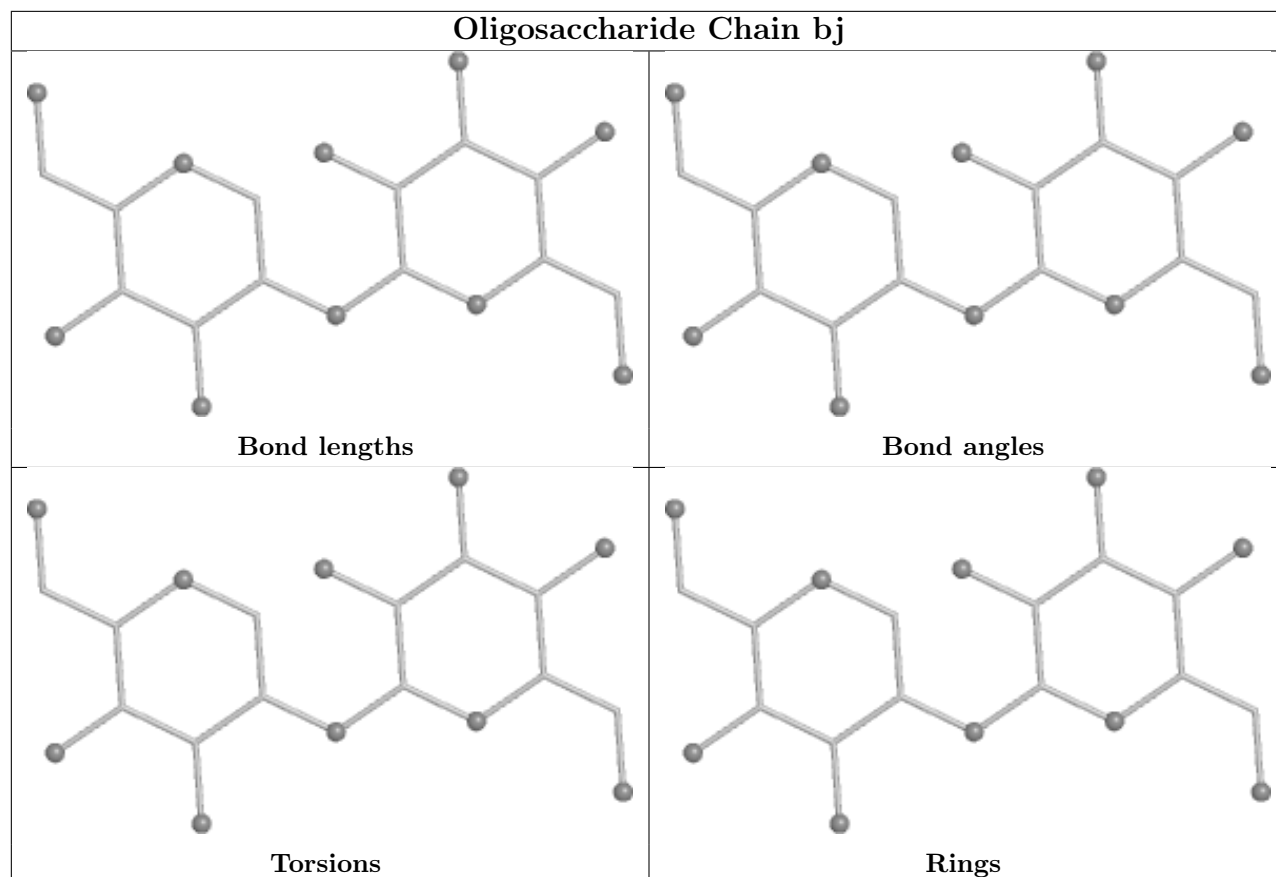


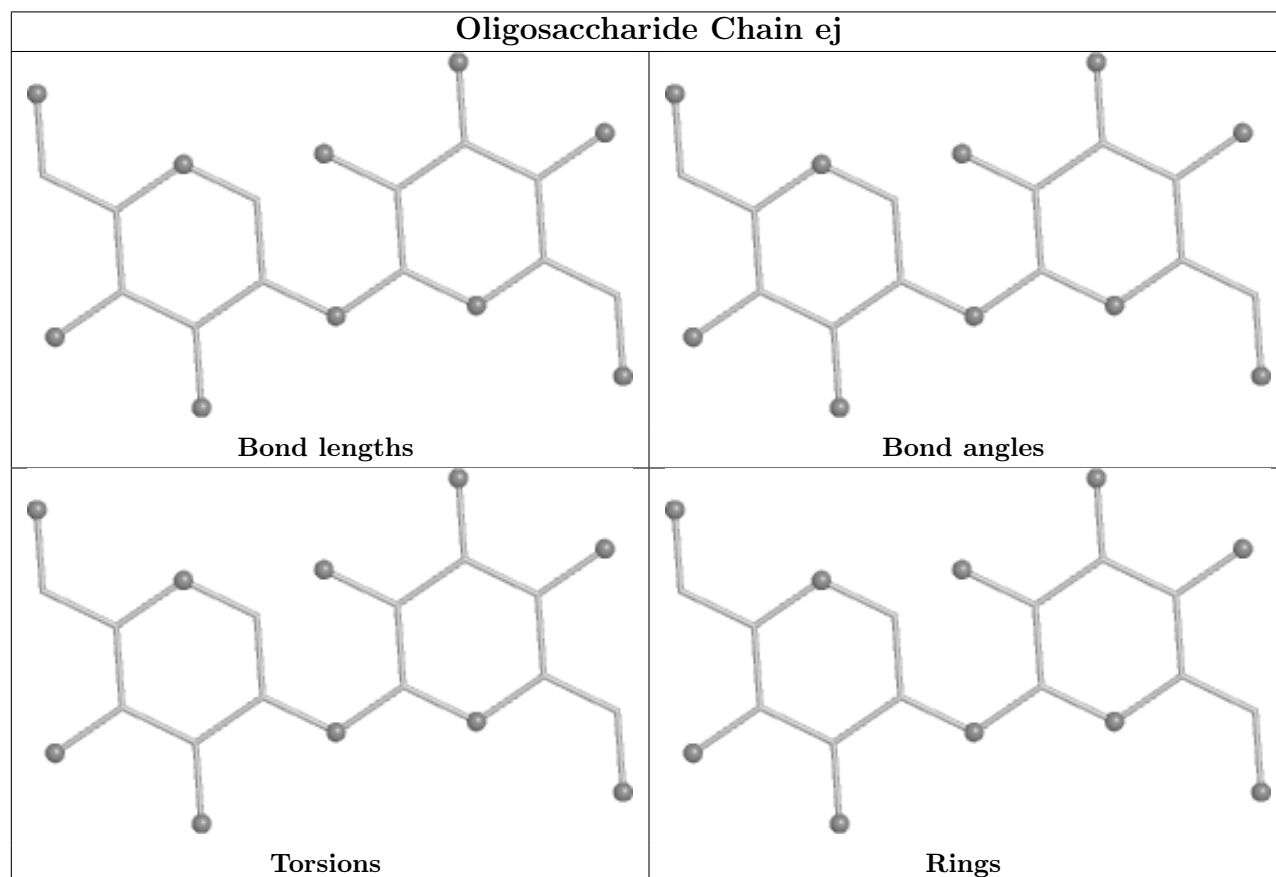
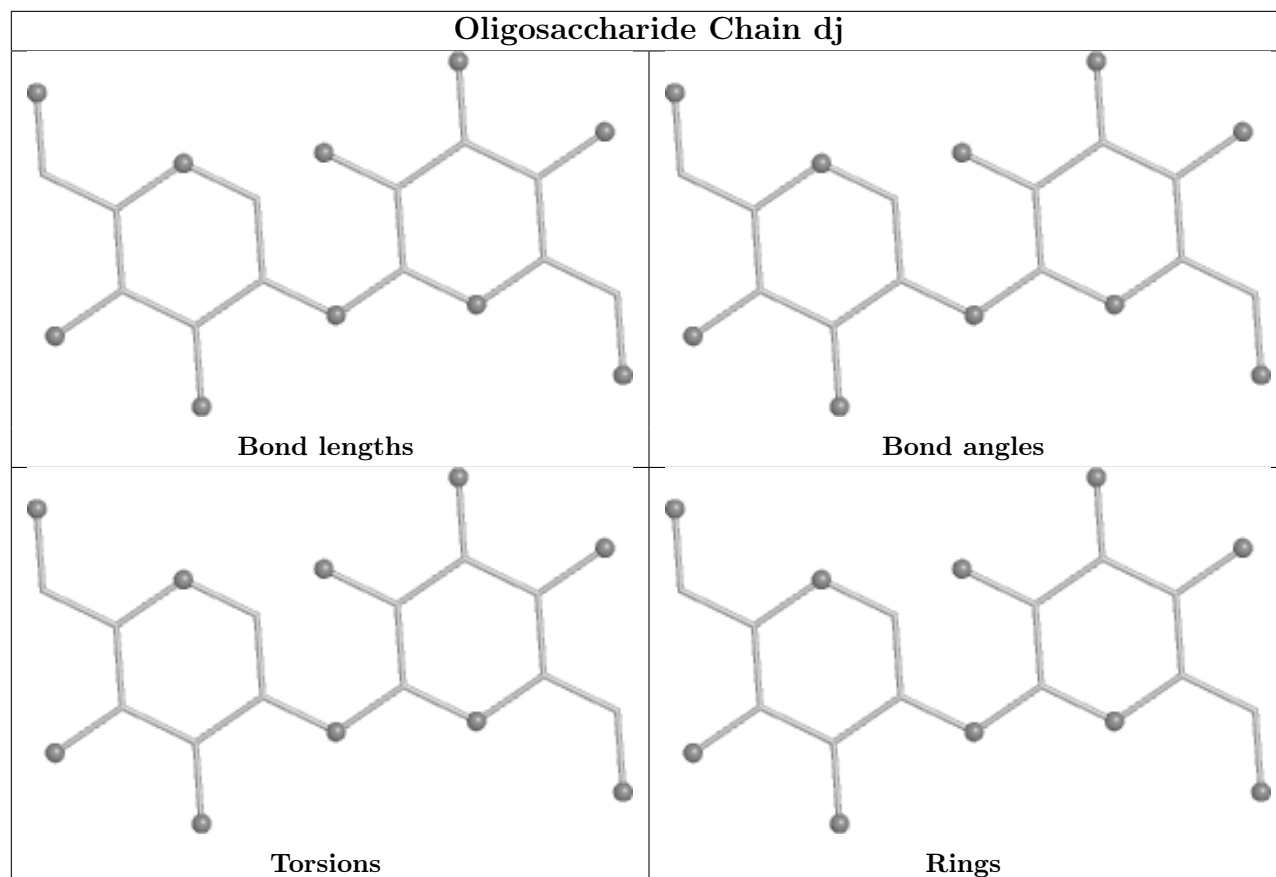


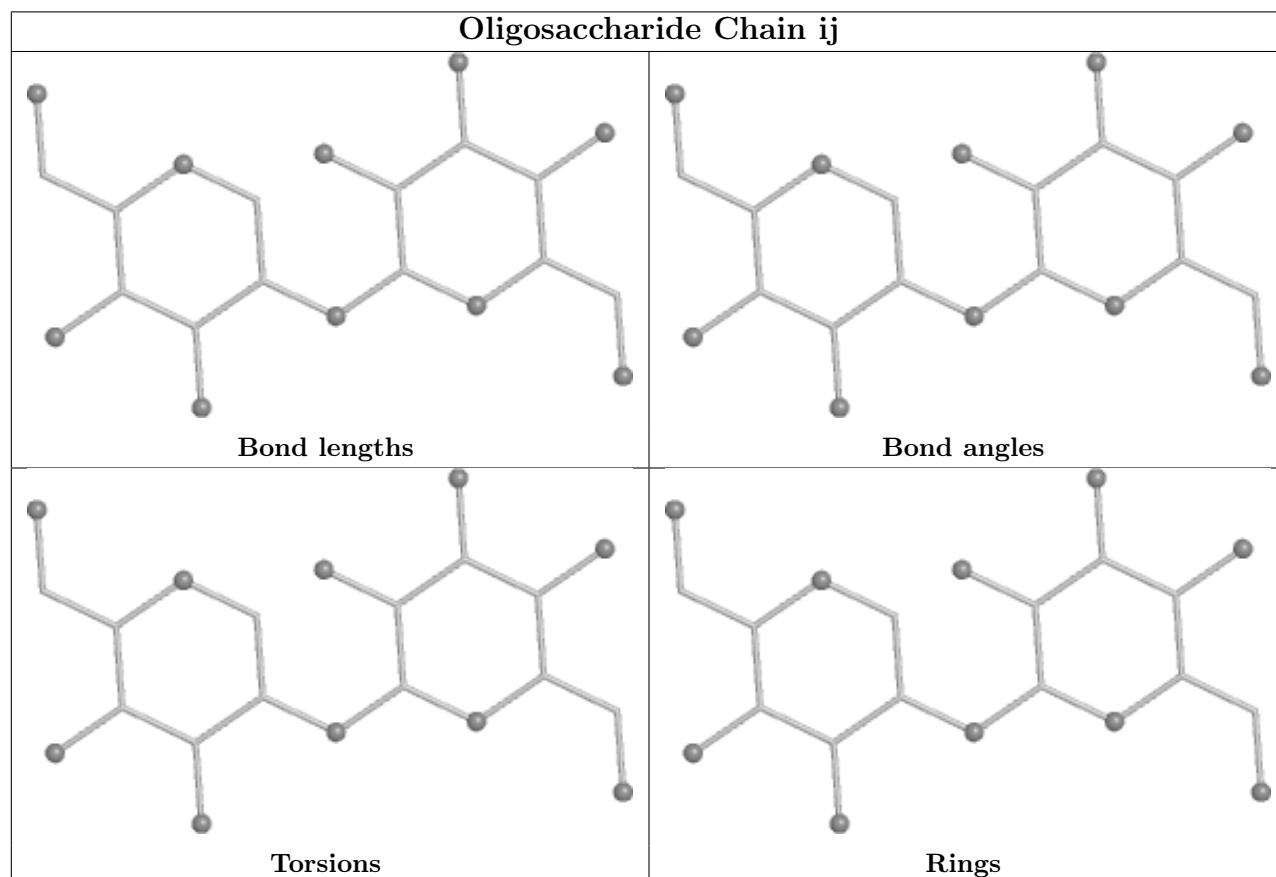
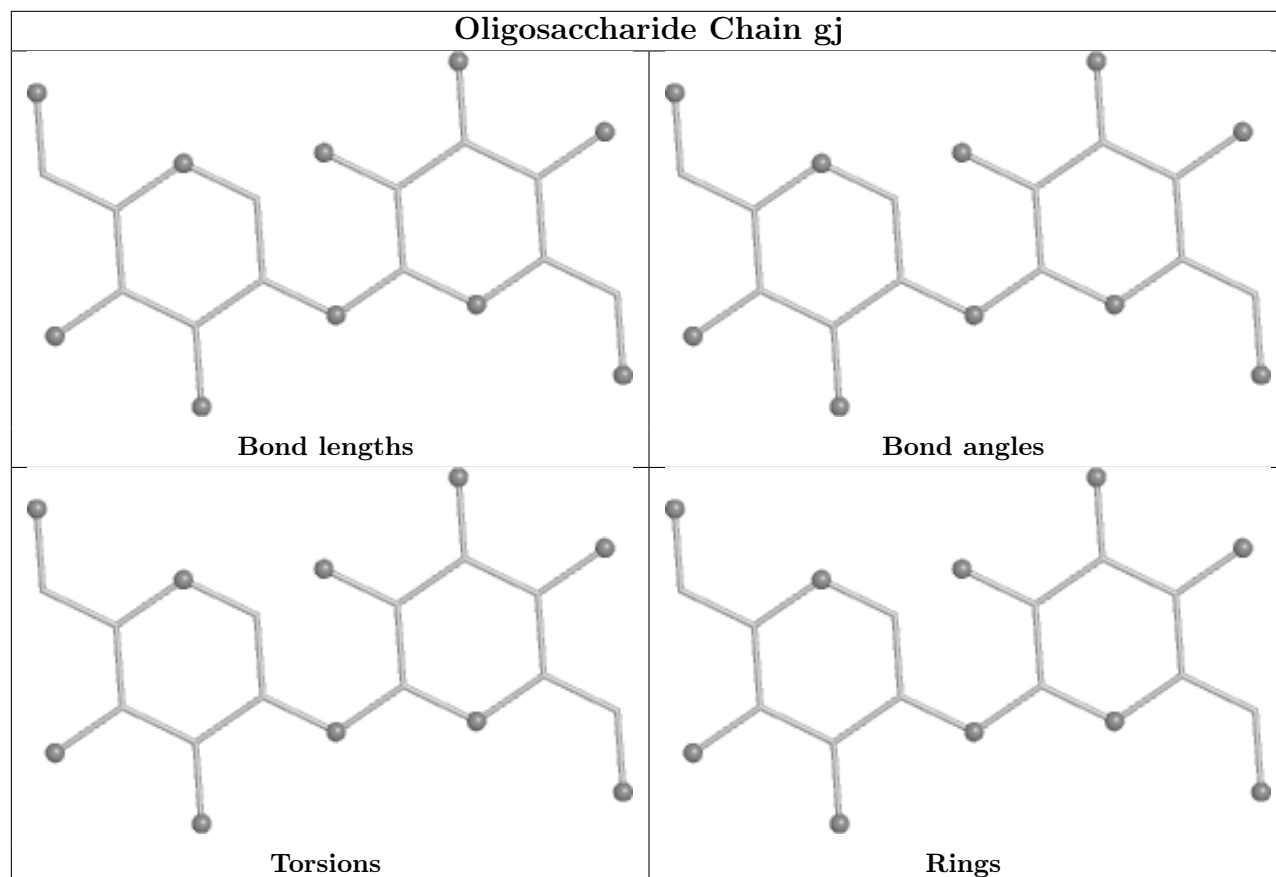


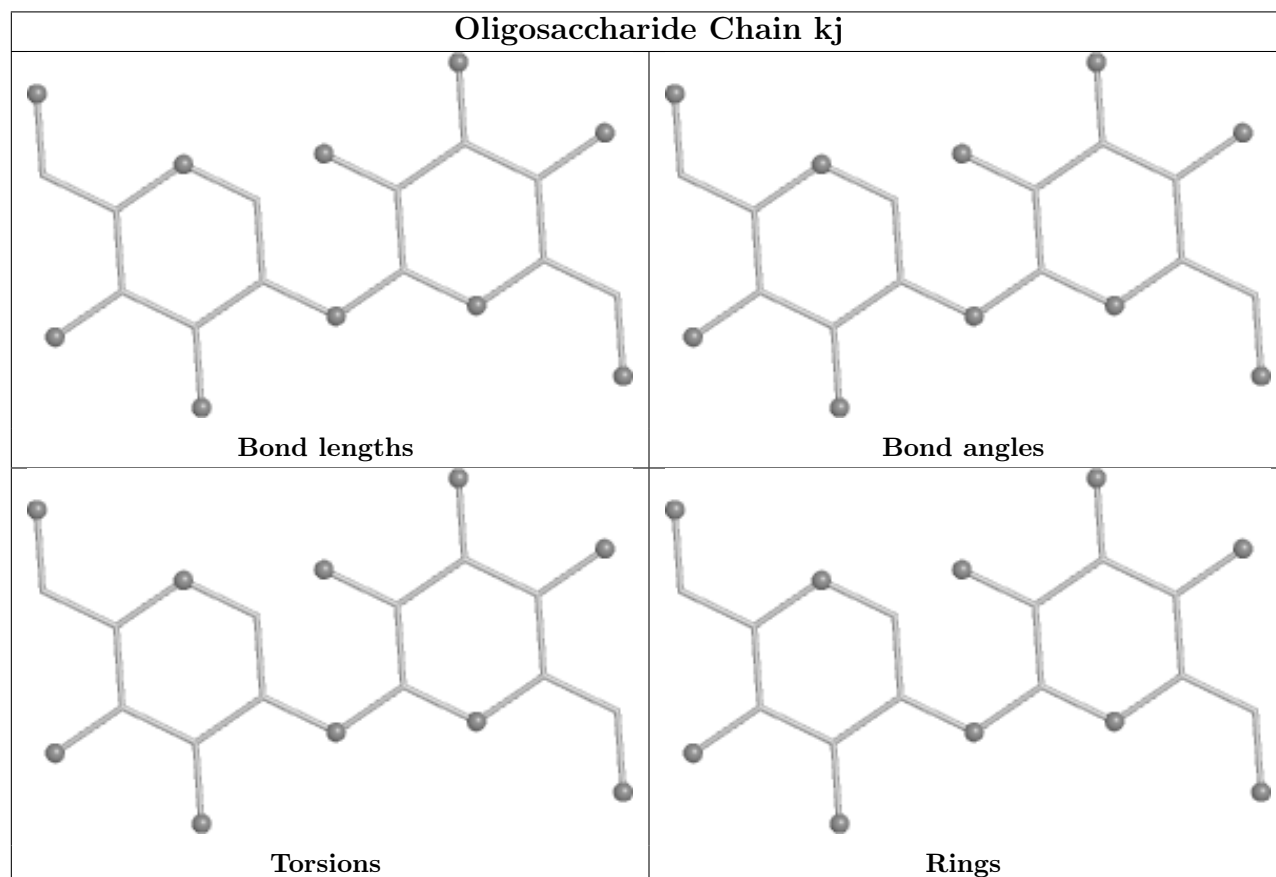
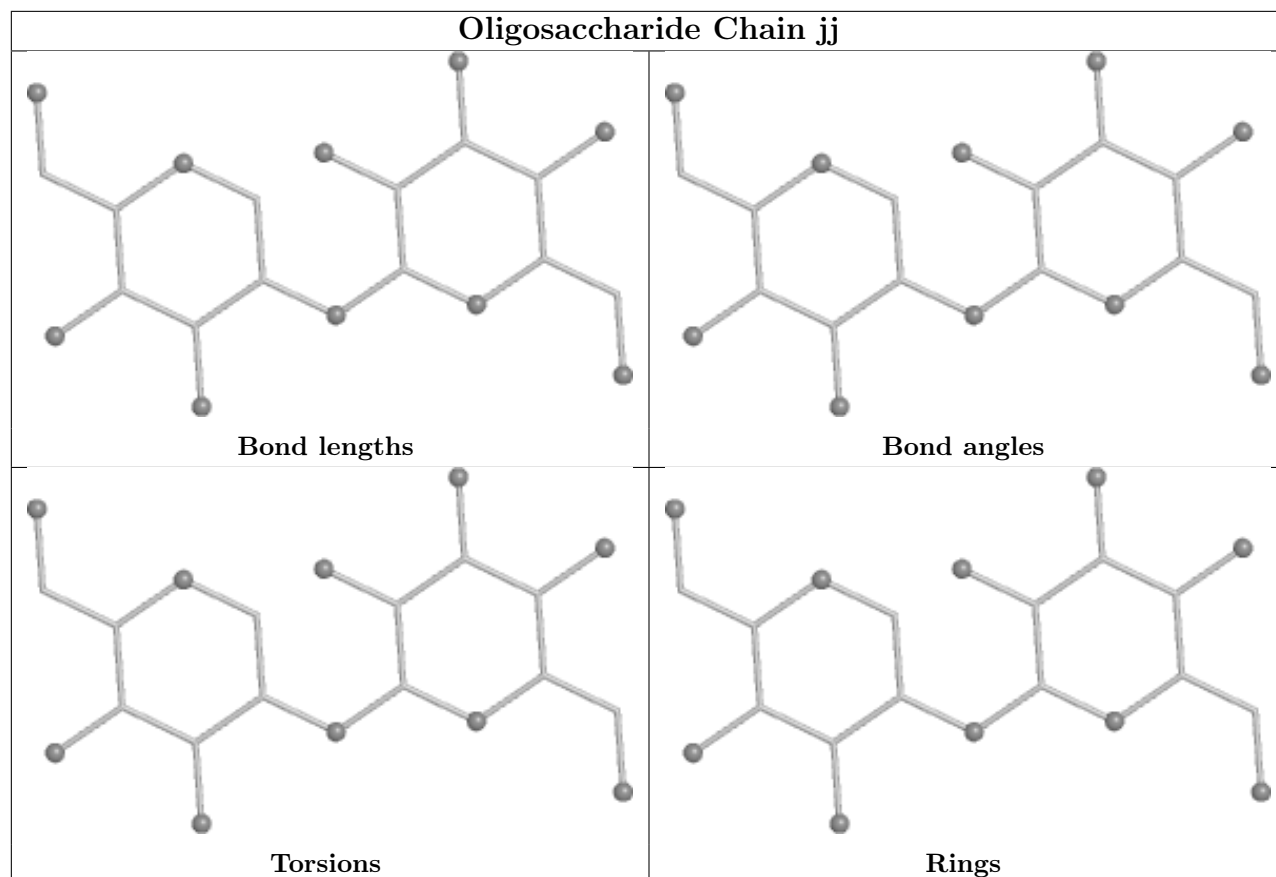


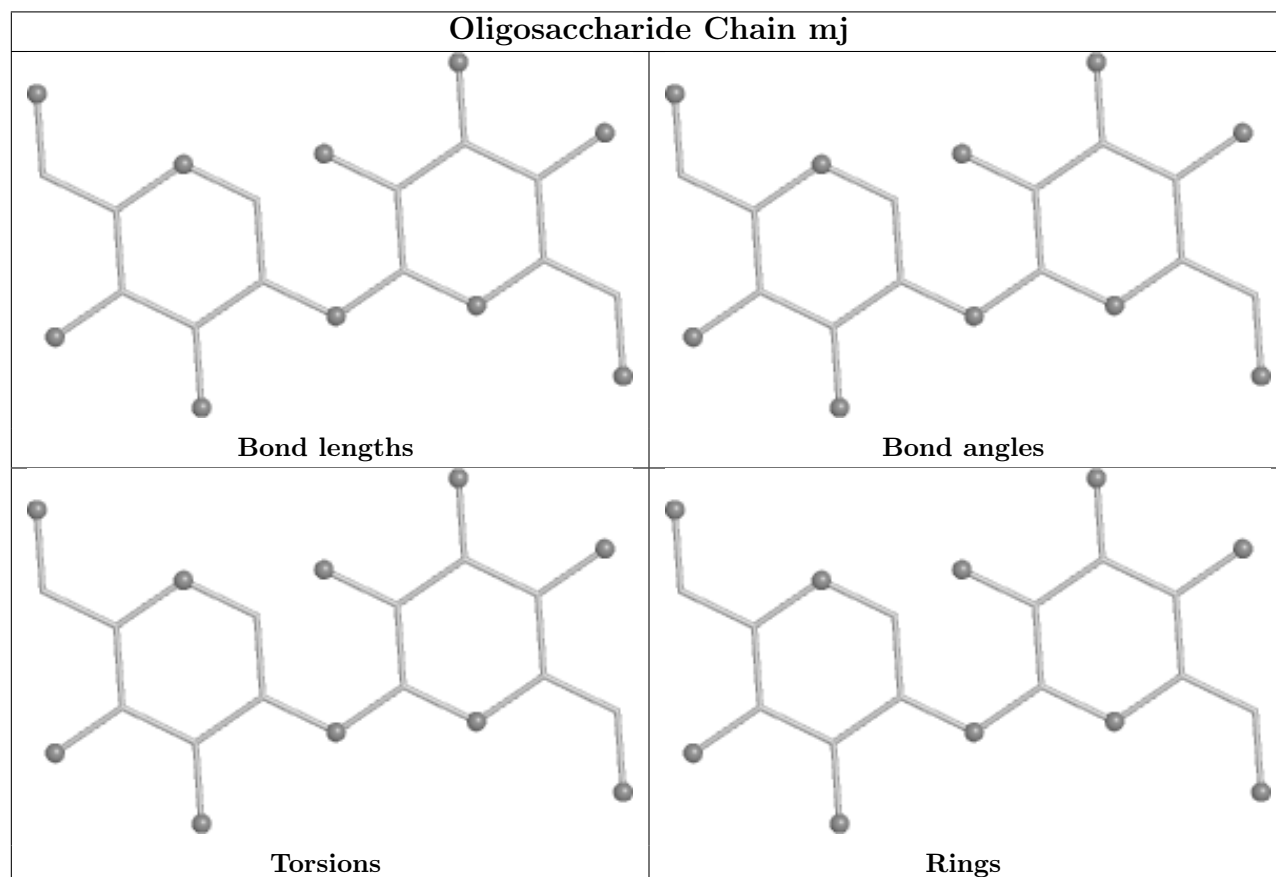
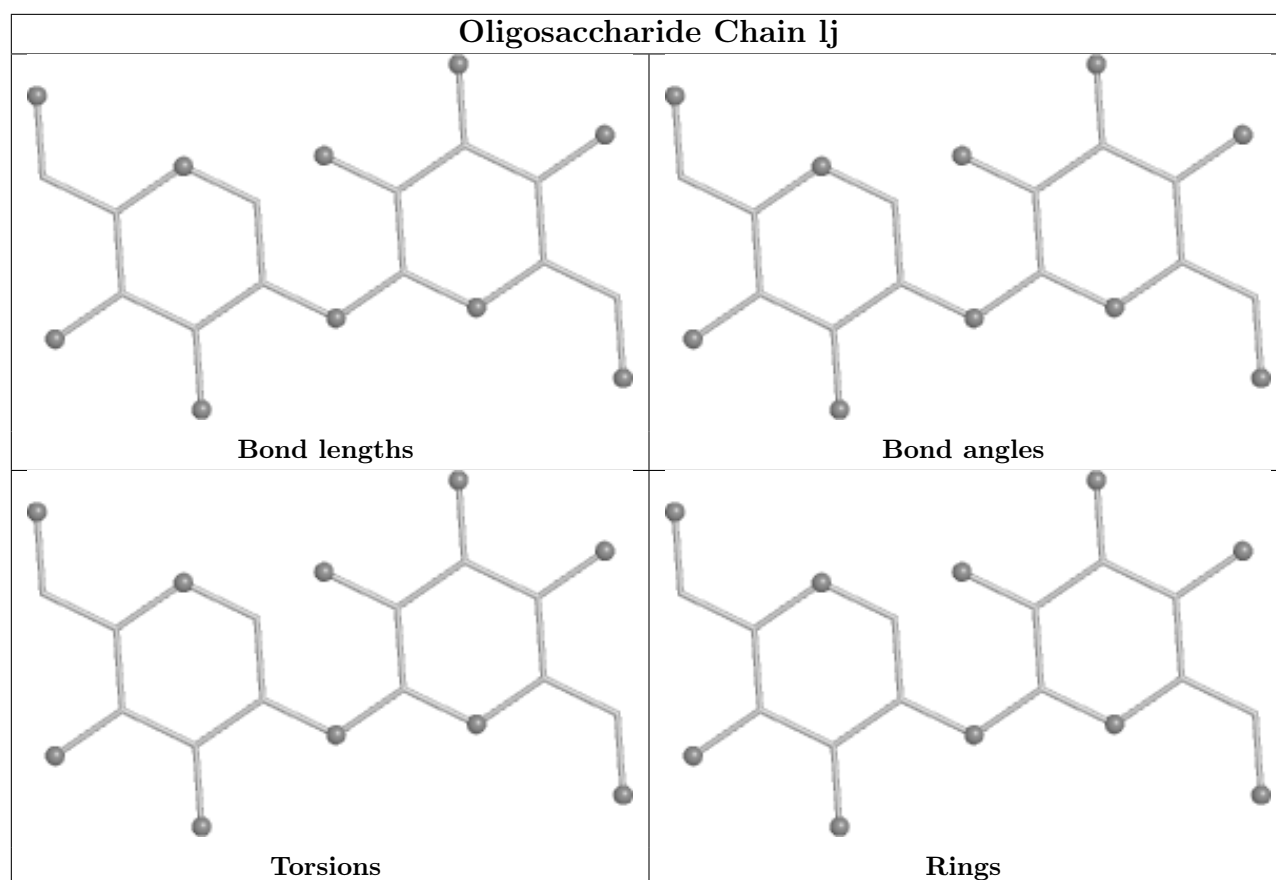


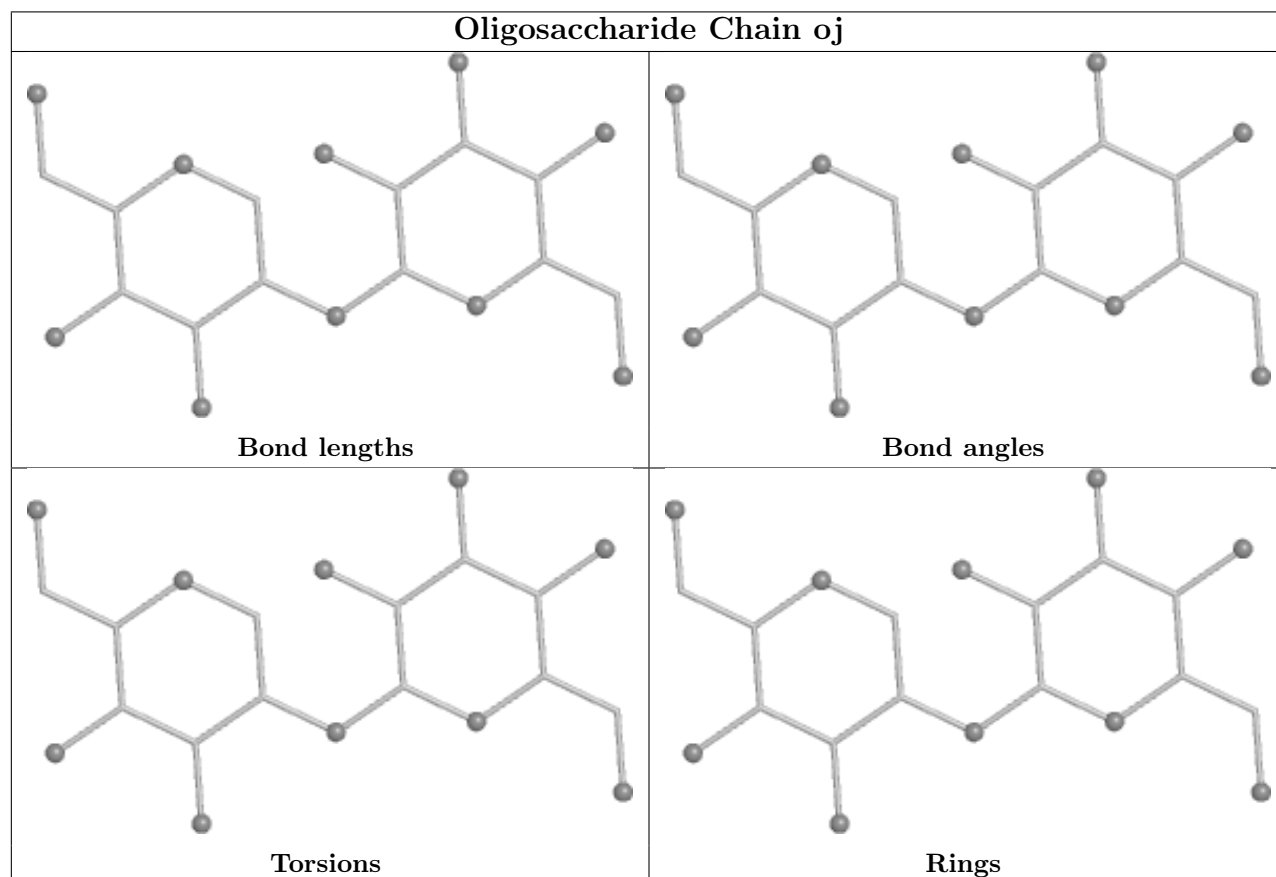
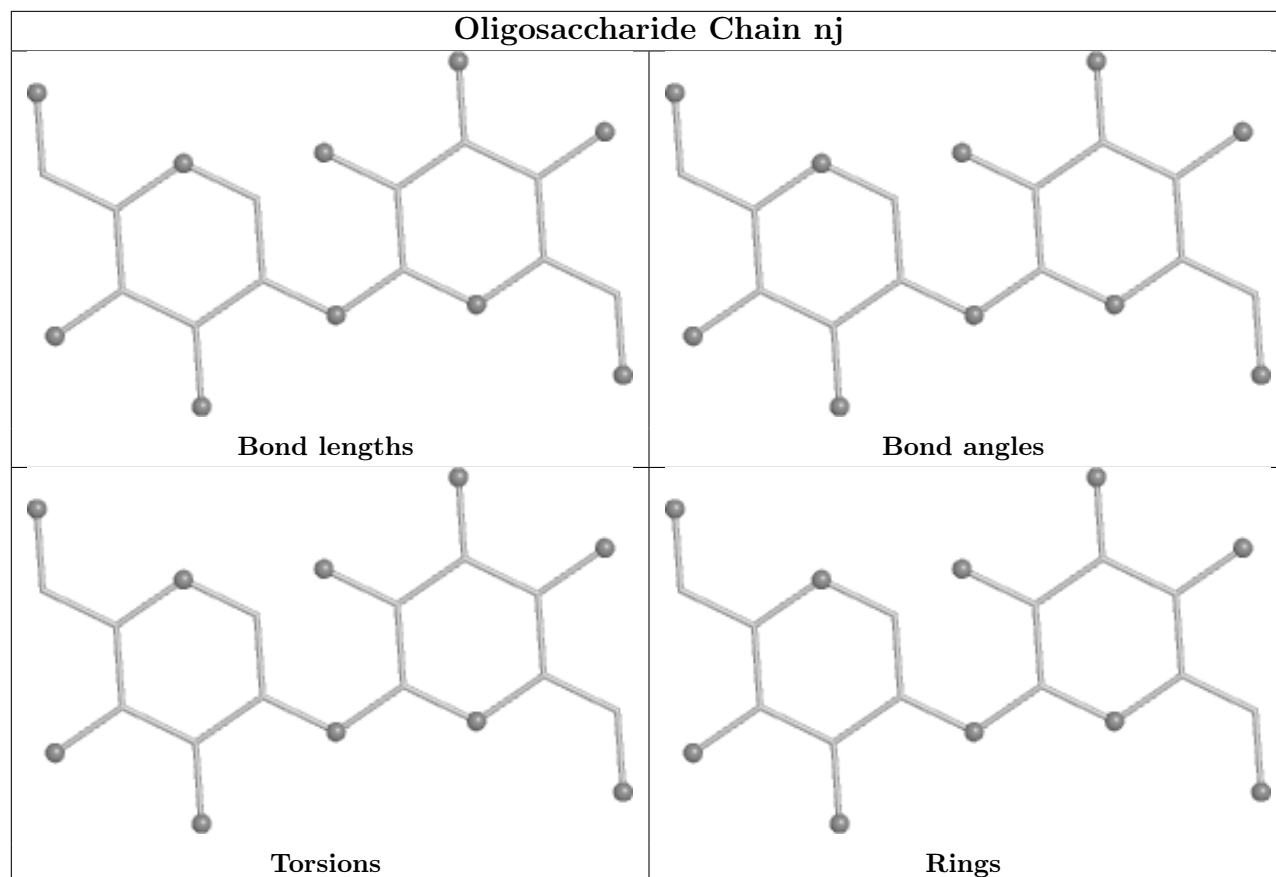


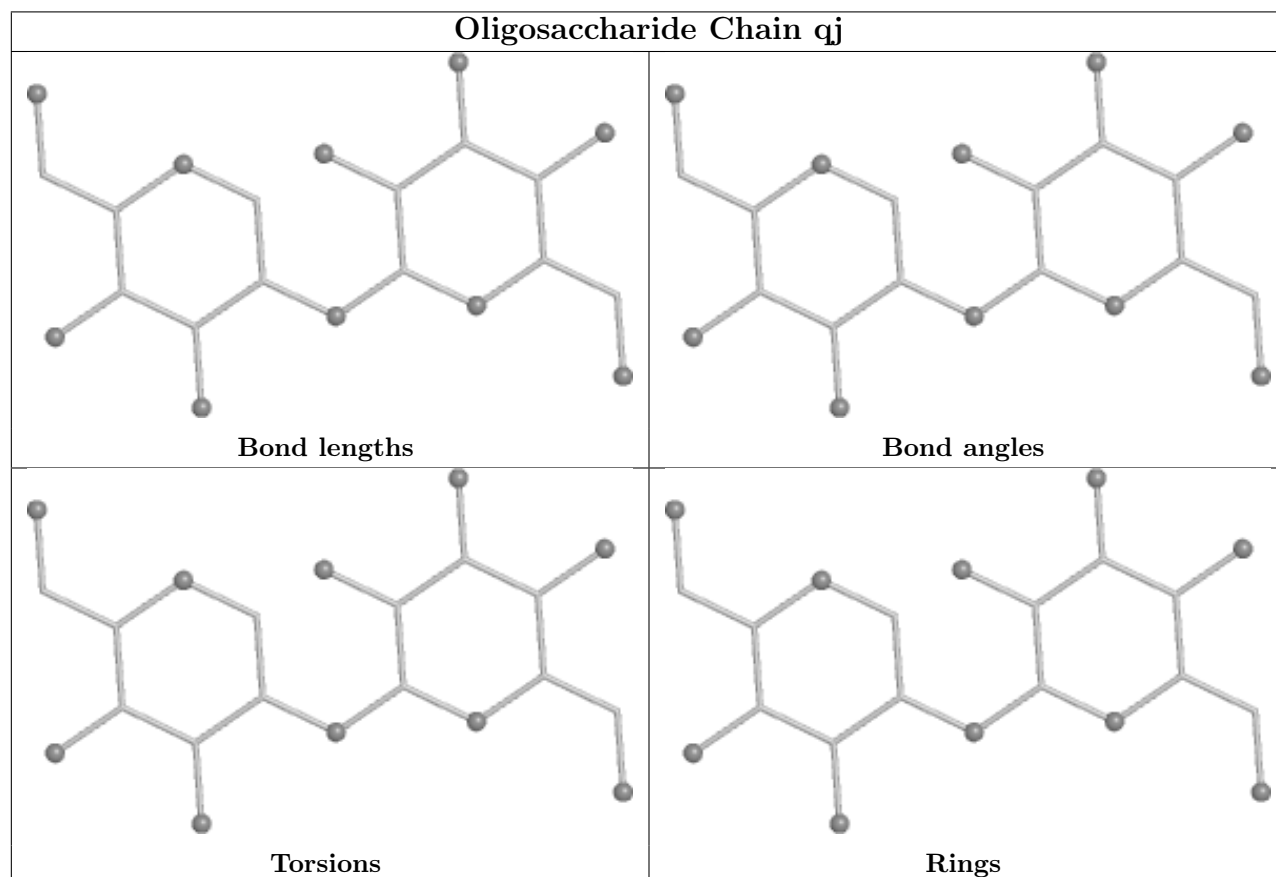
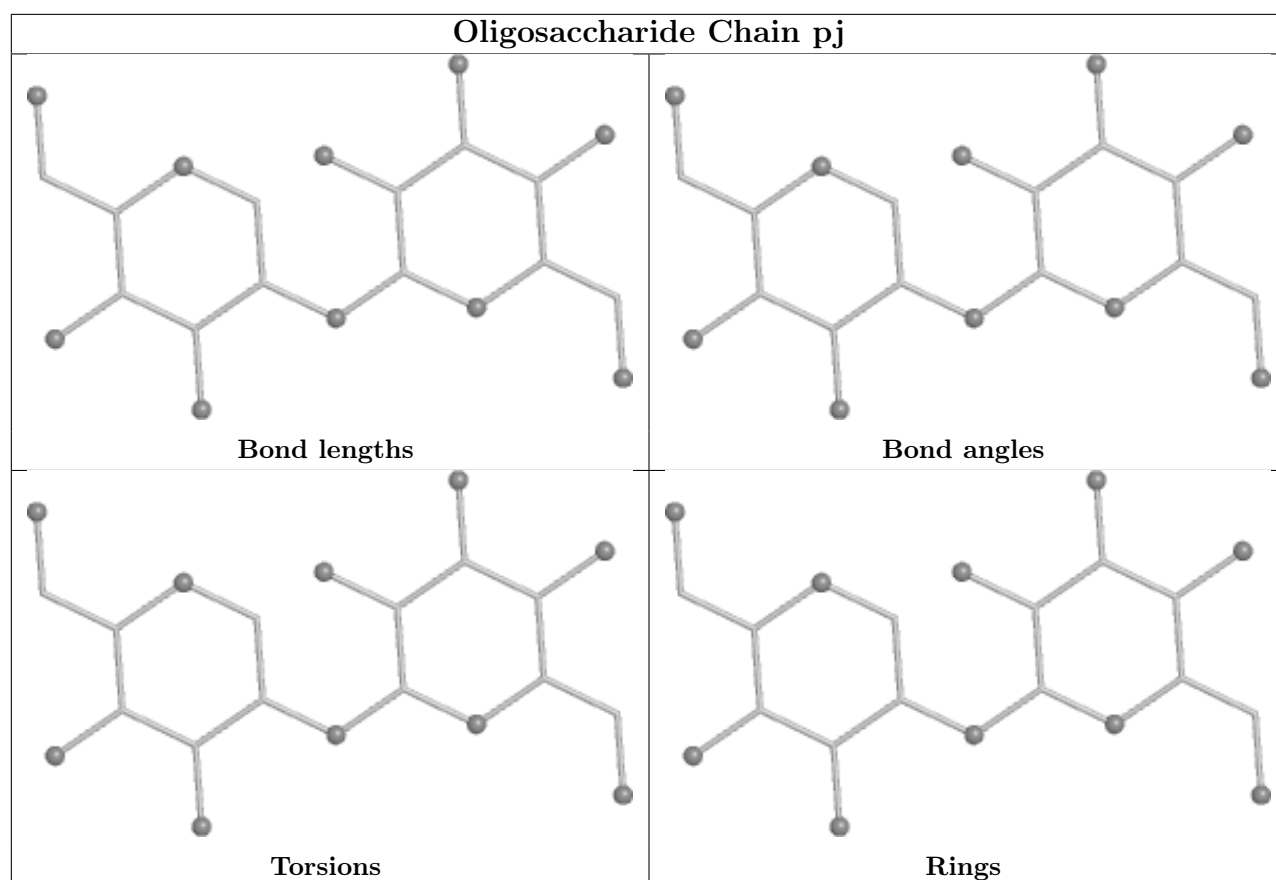


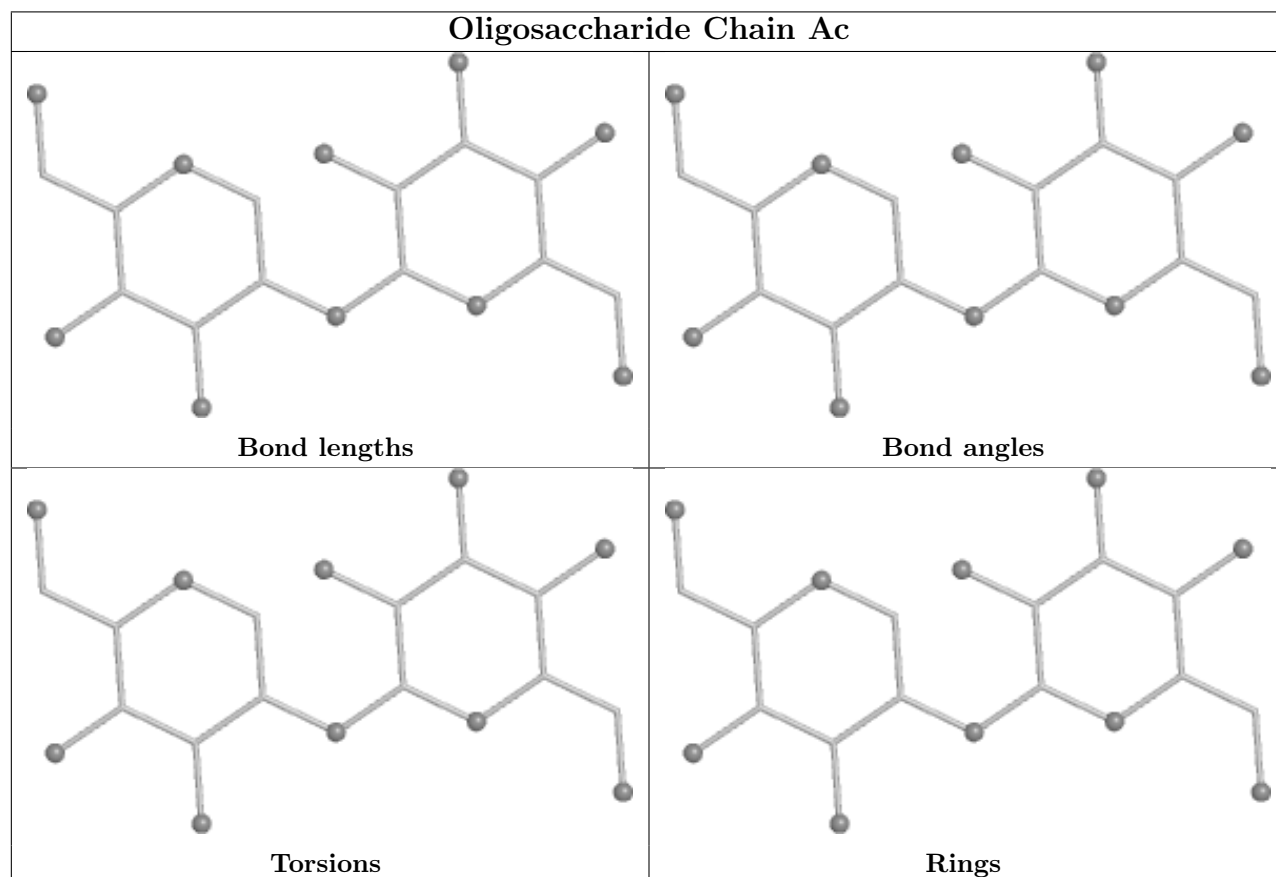
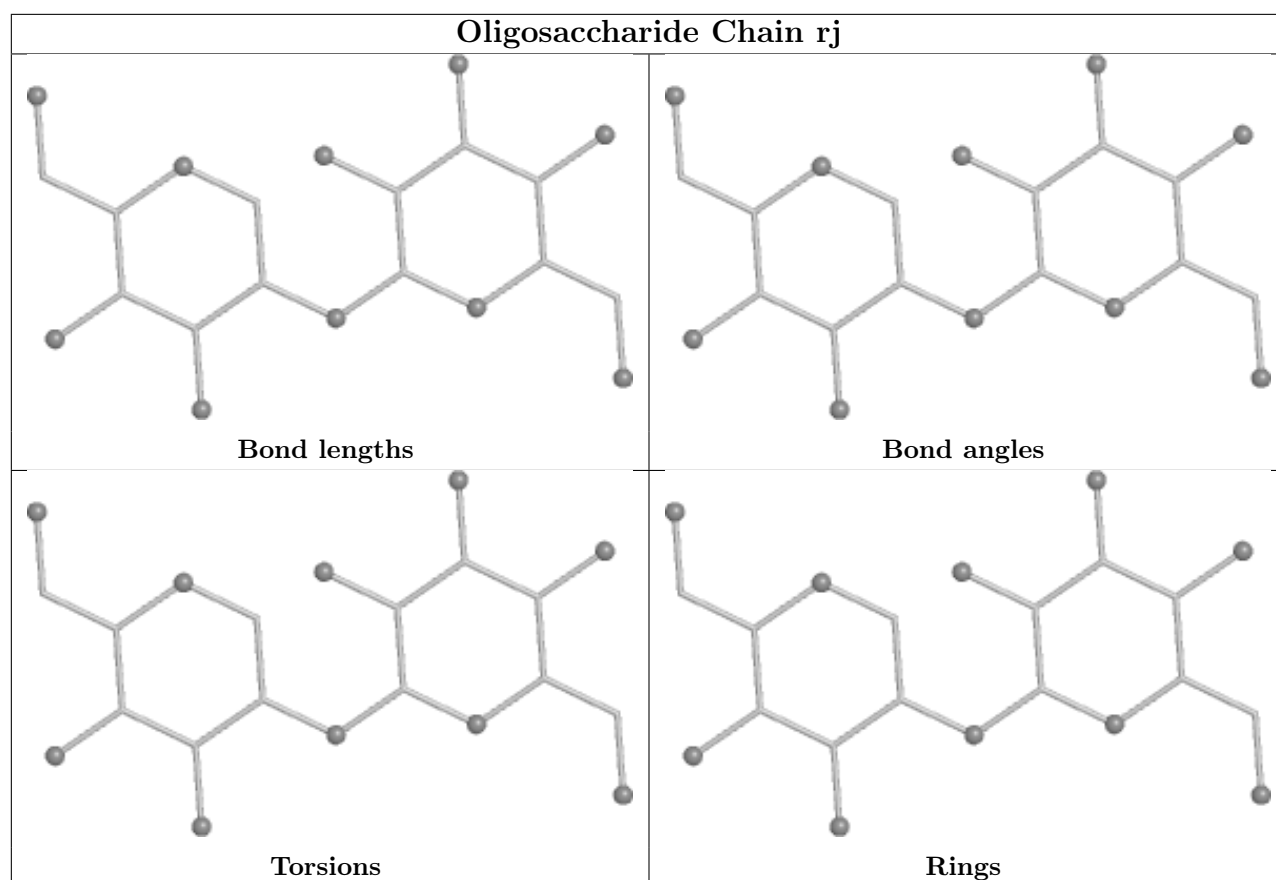


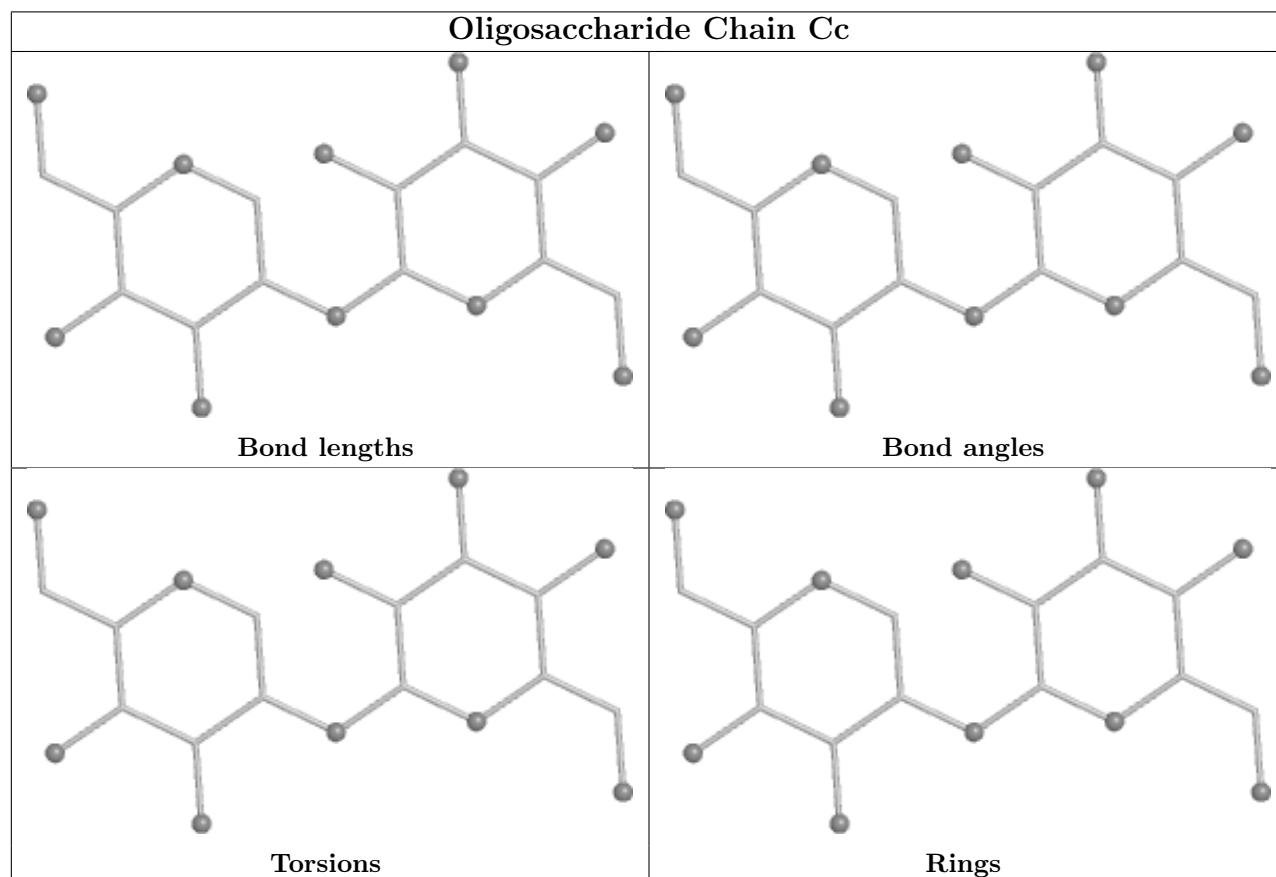
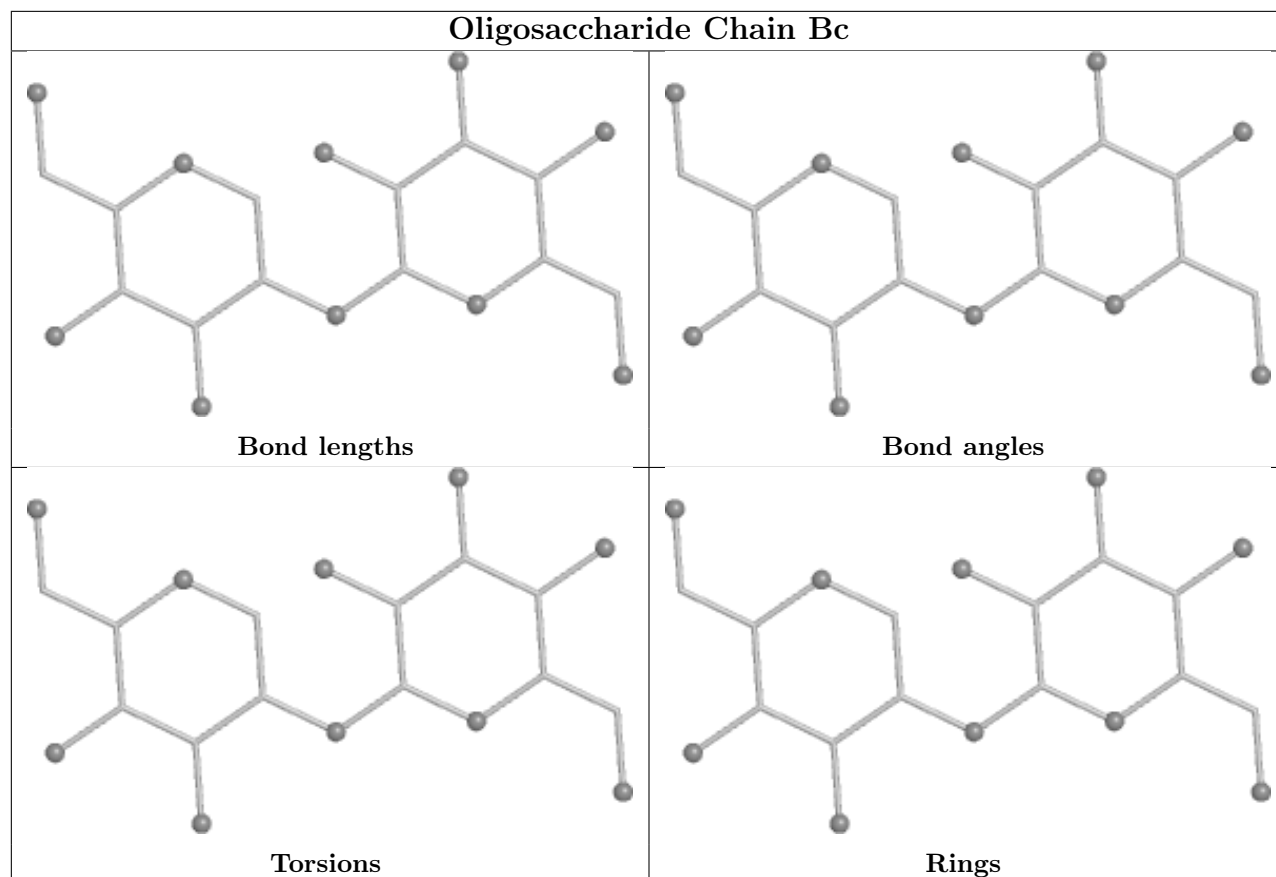


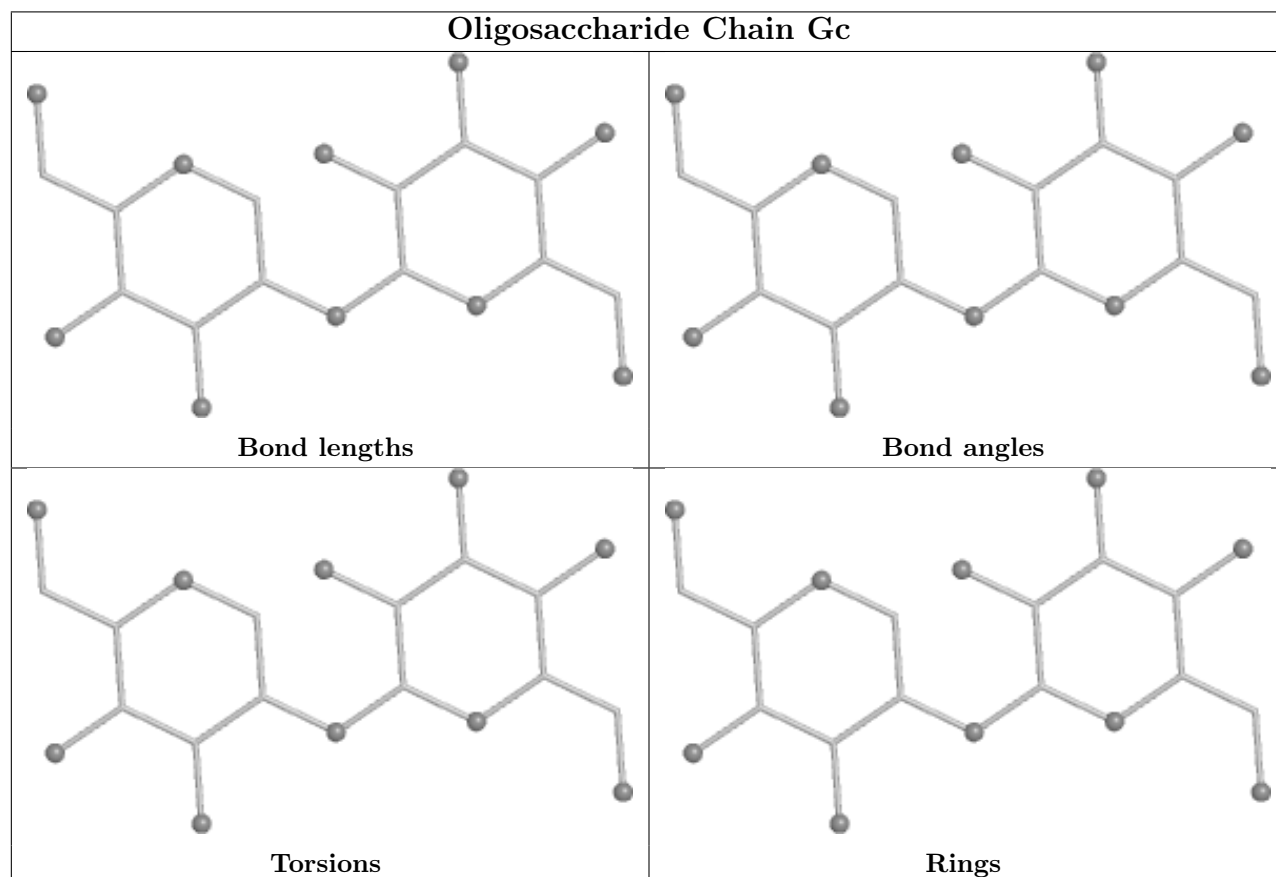
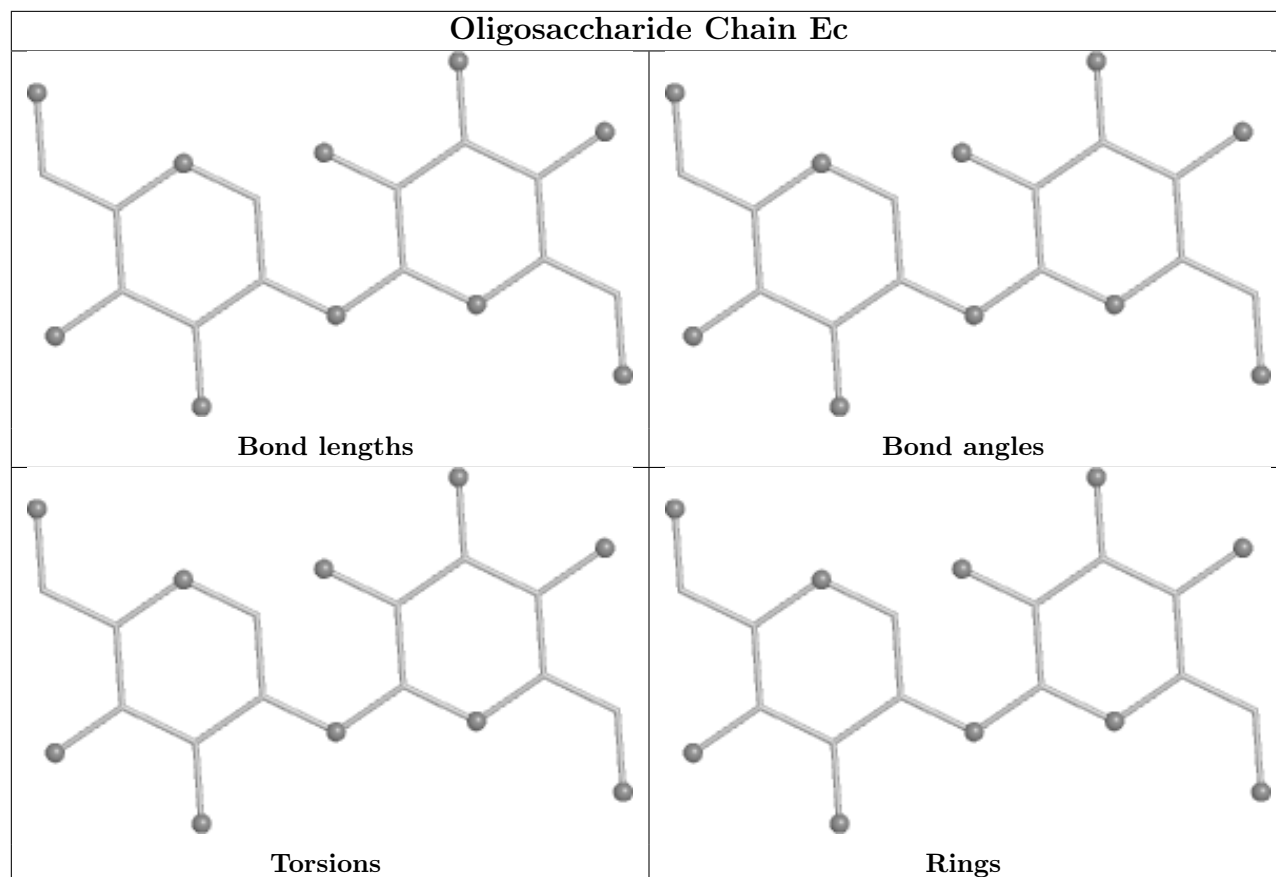




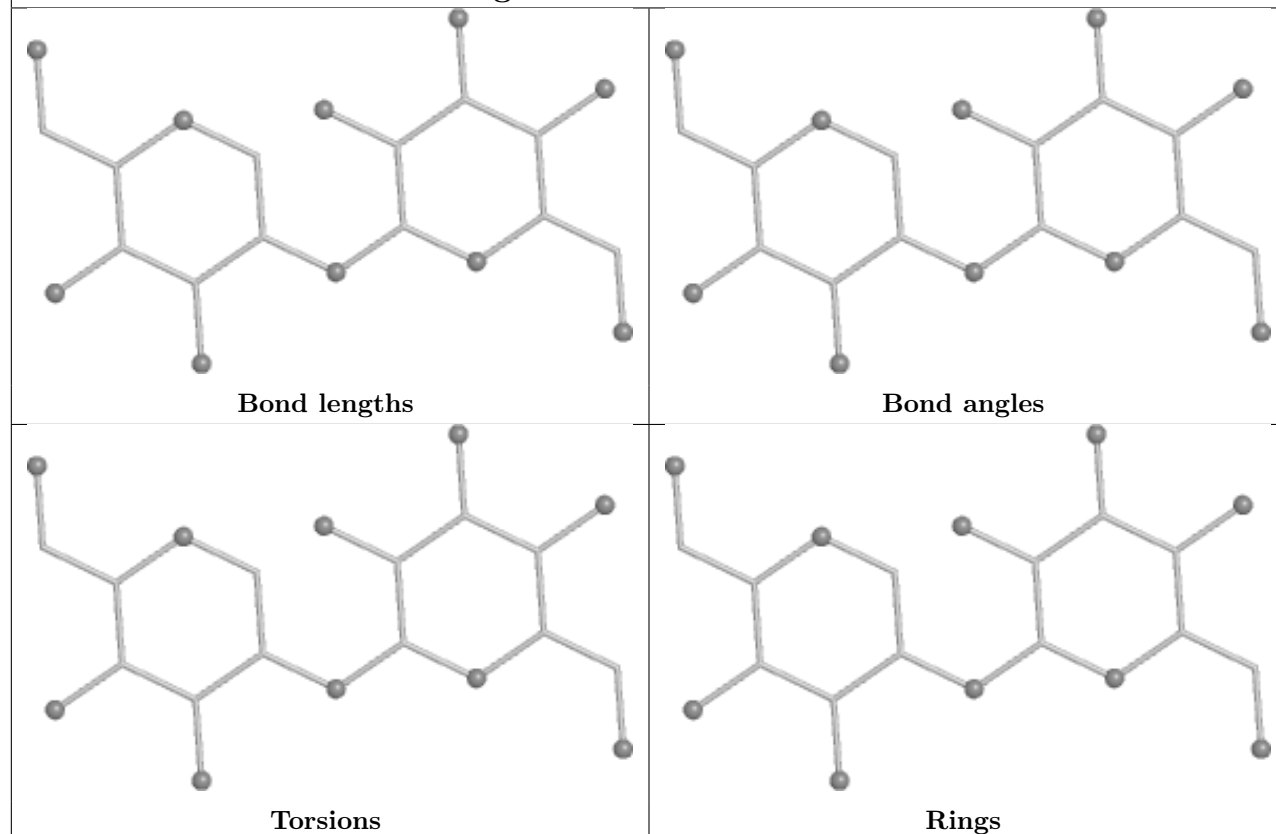




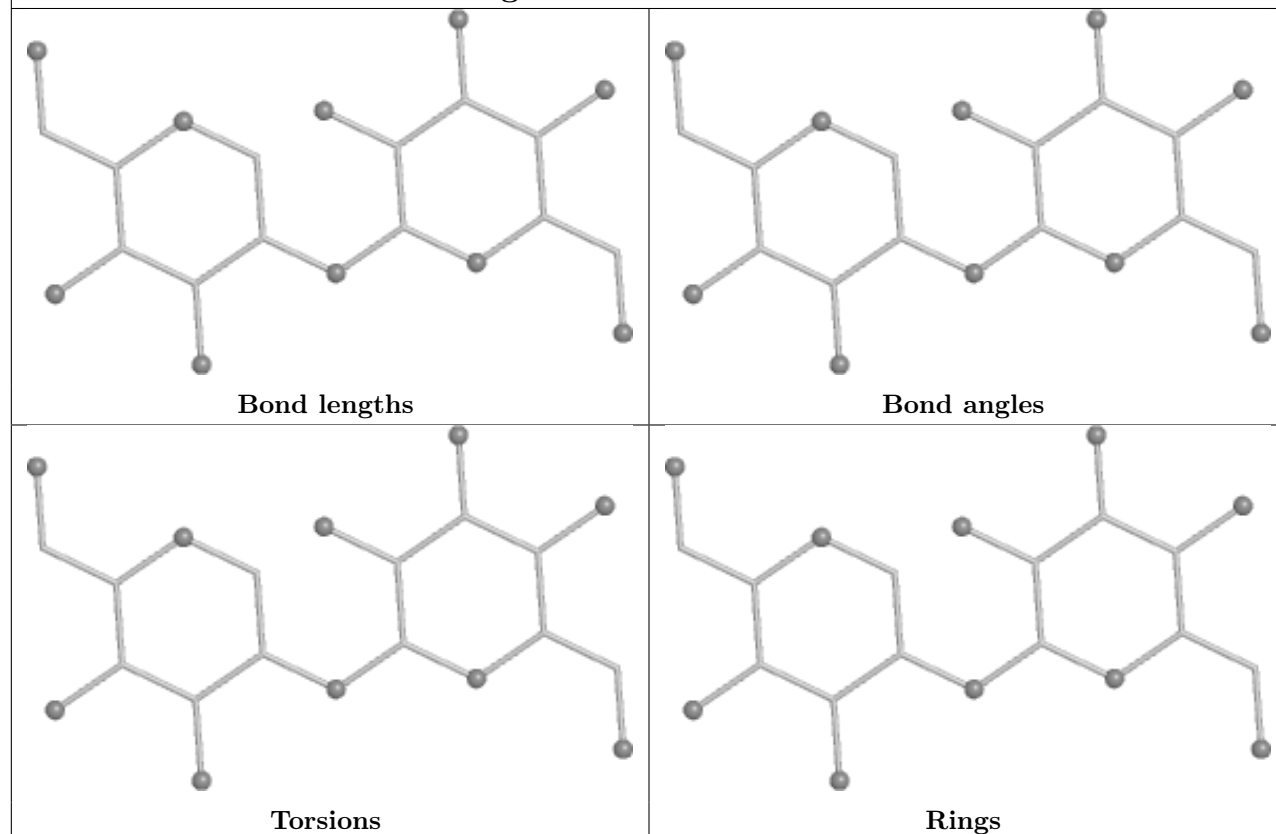


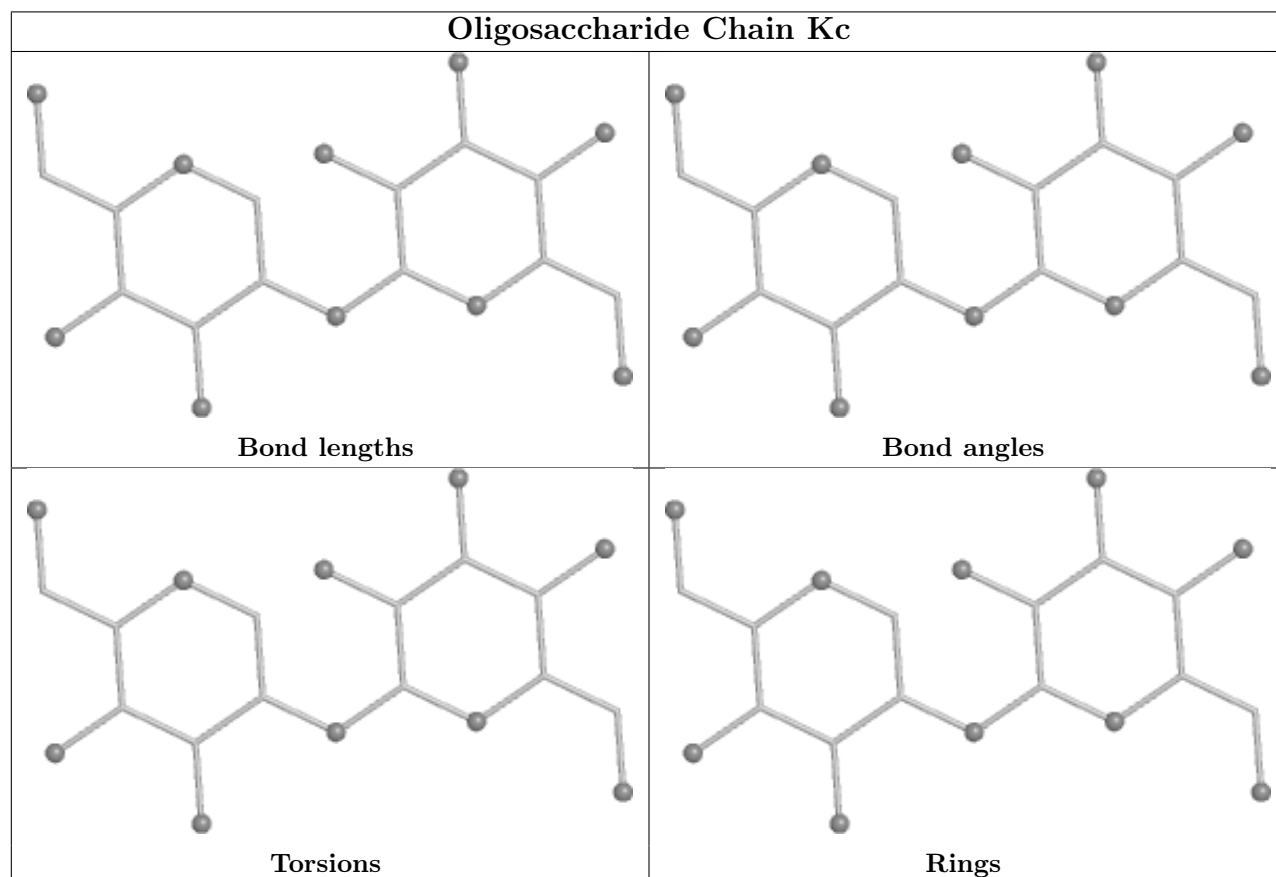
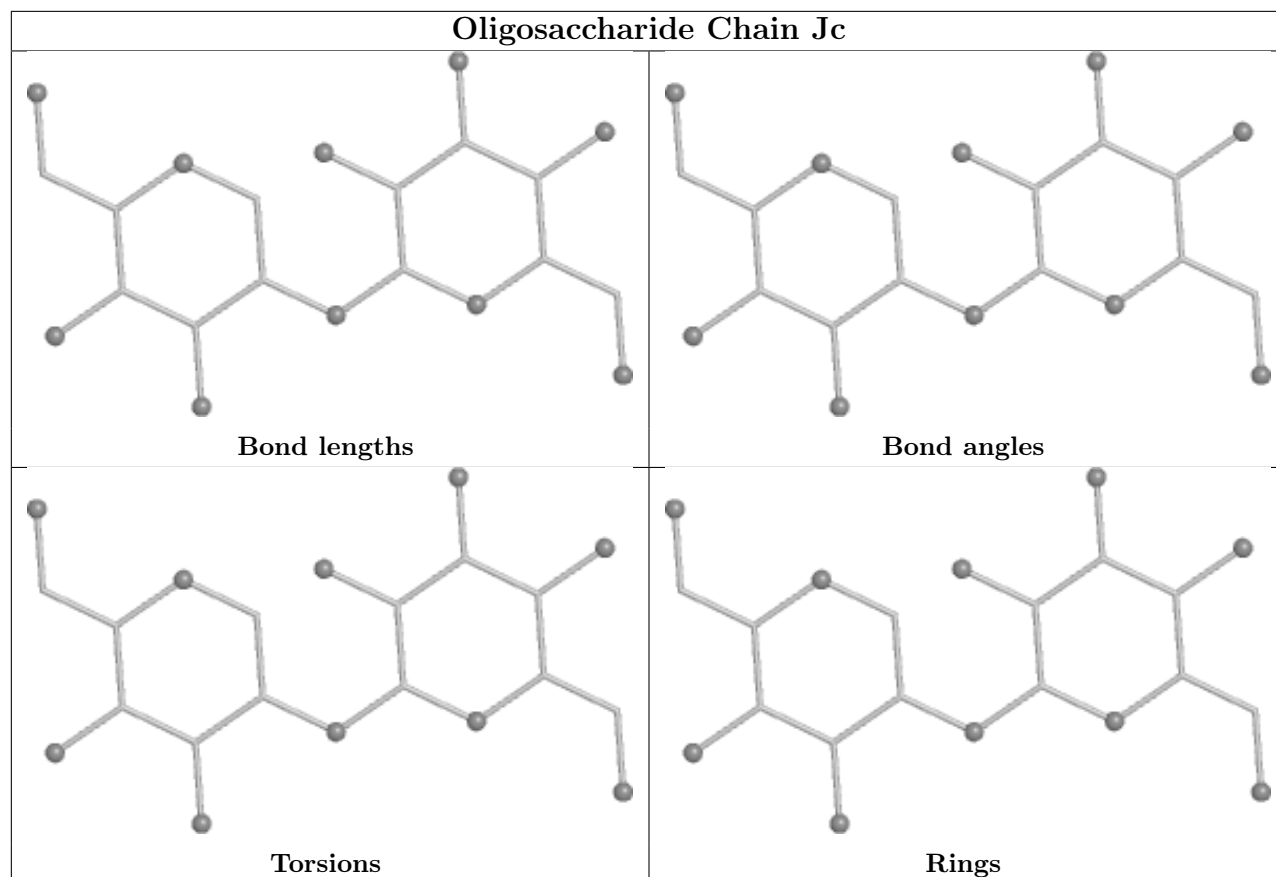


Oligosaccharide Chain Hc

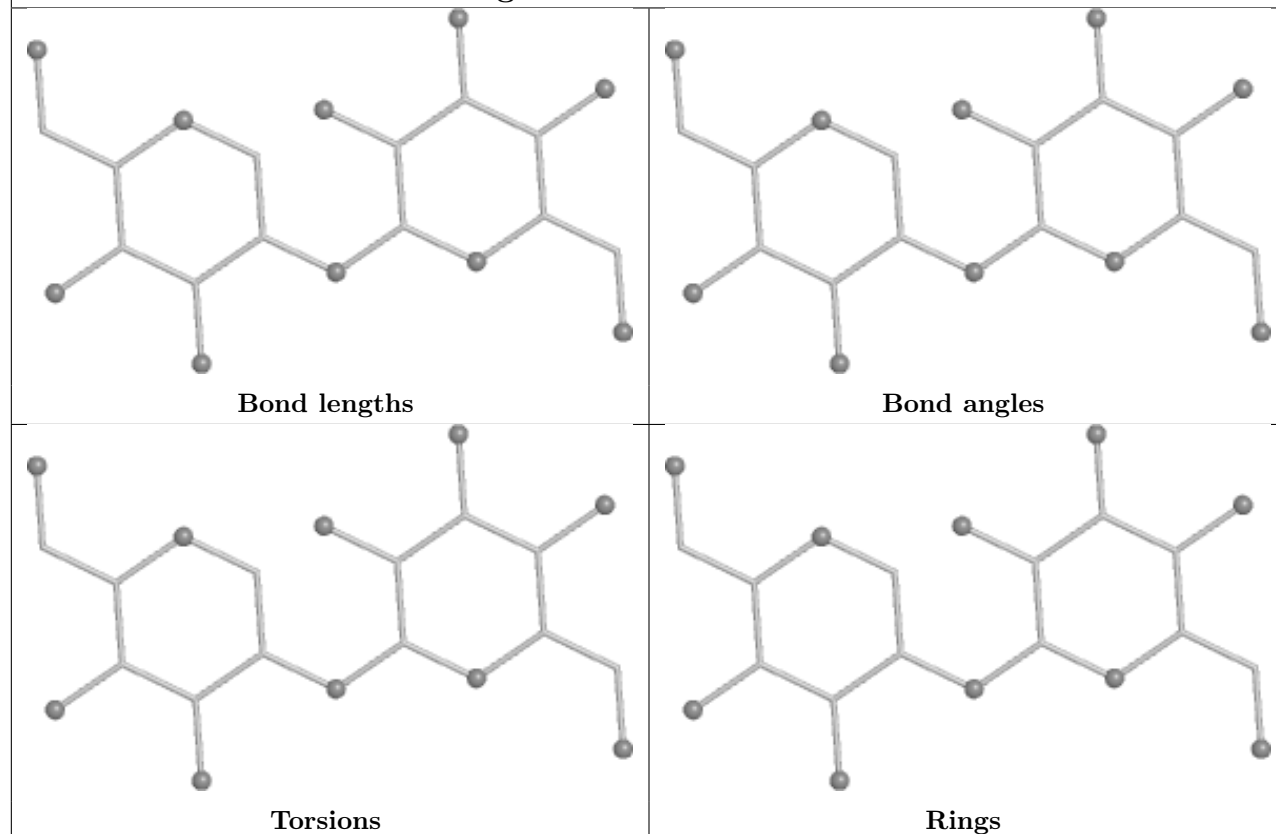


Oligosaccharide Chain Ic

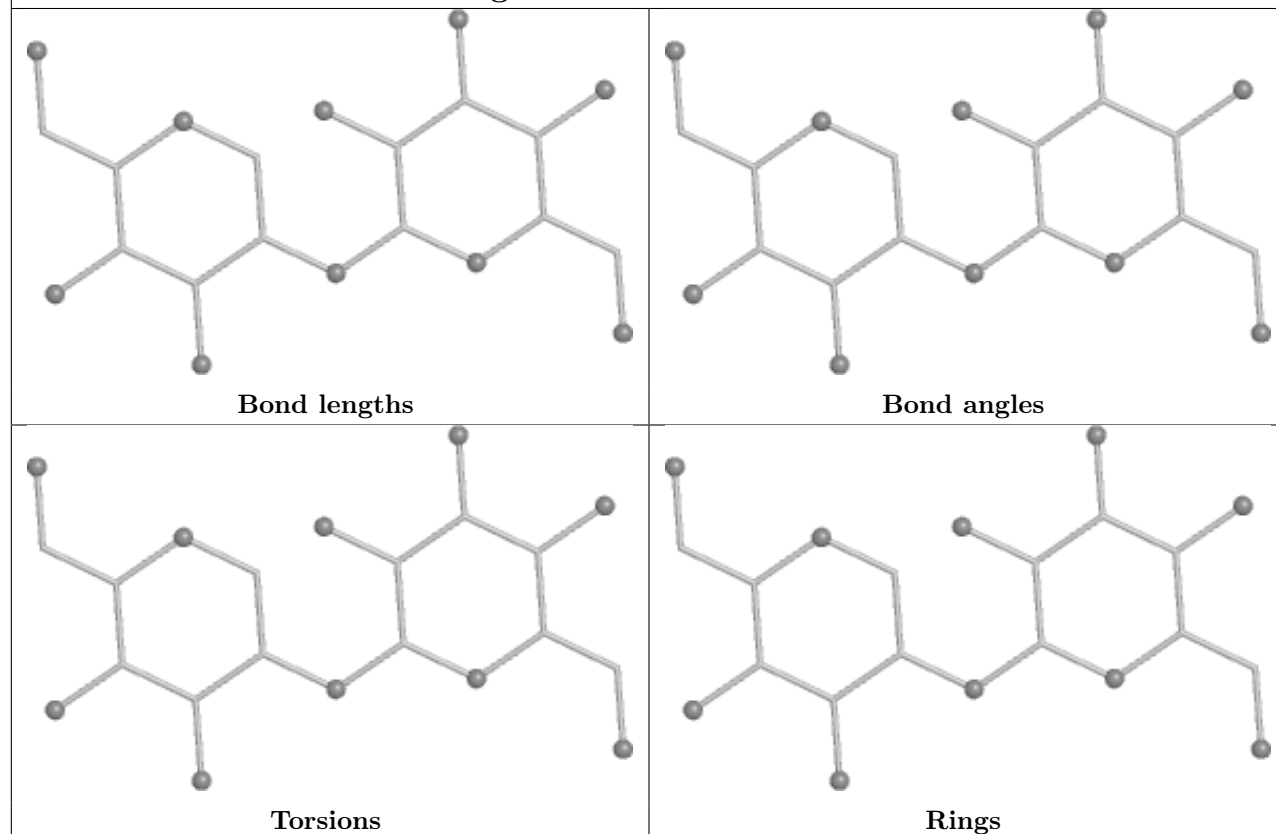




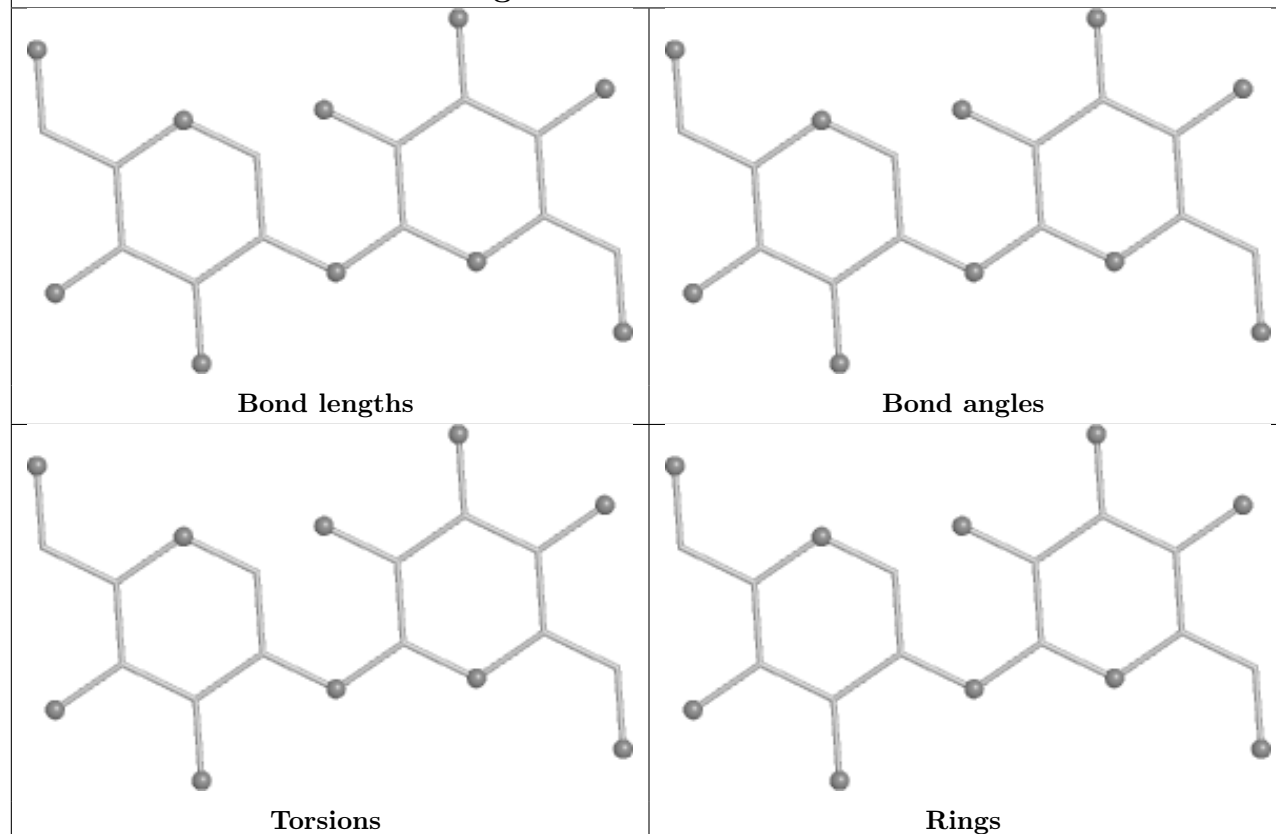
Oligosaccharide Chain Lc



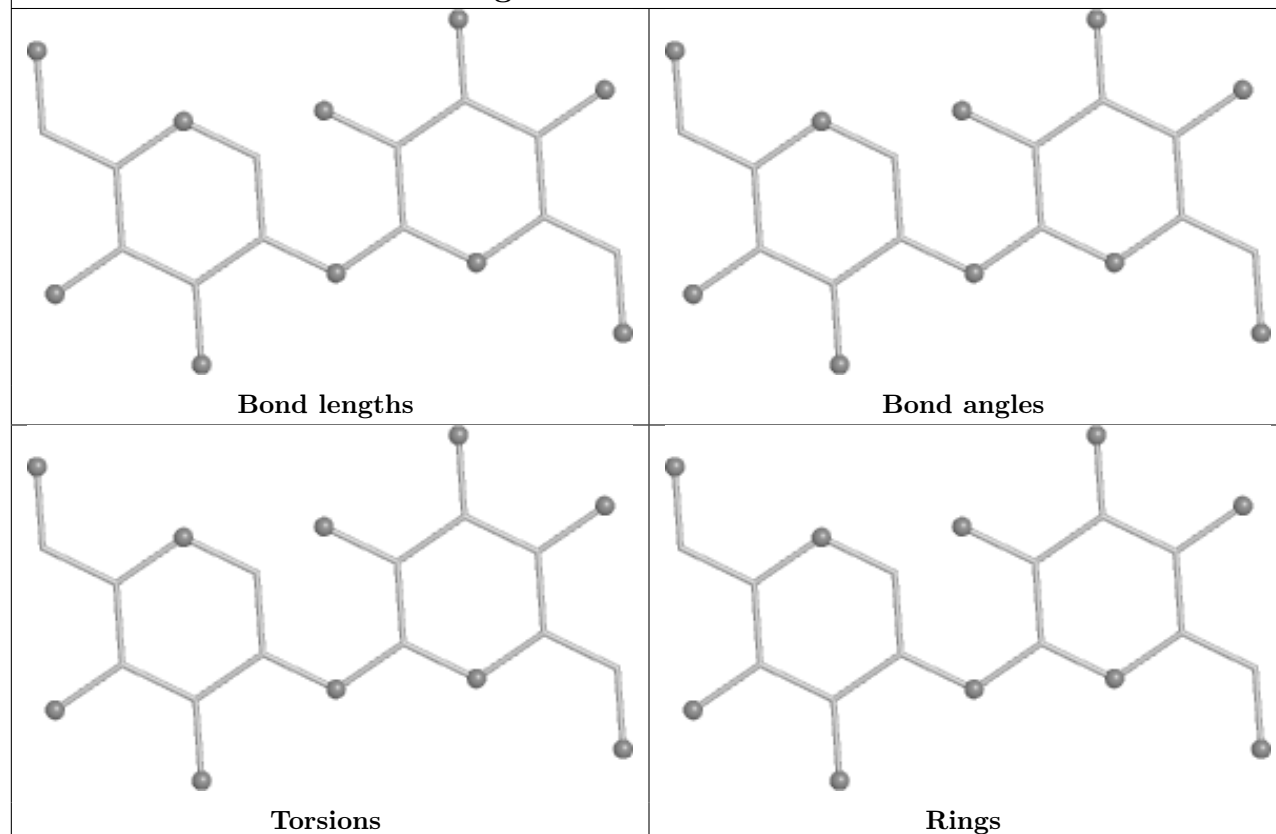
Oligosaccharide Chain Mc



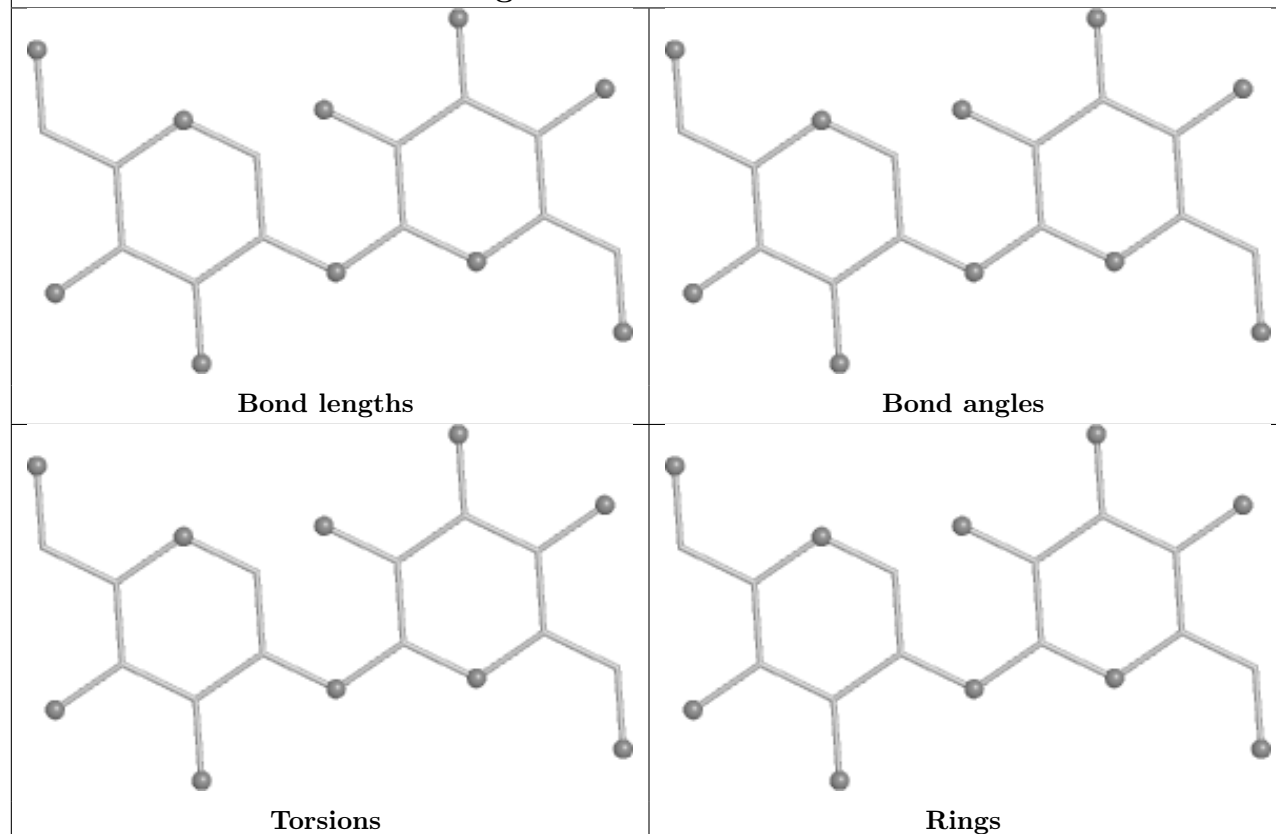
Oligosaccharide Chain Nc



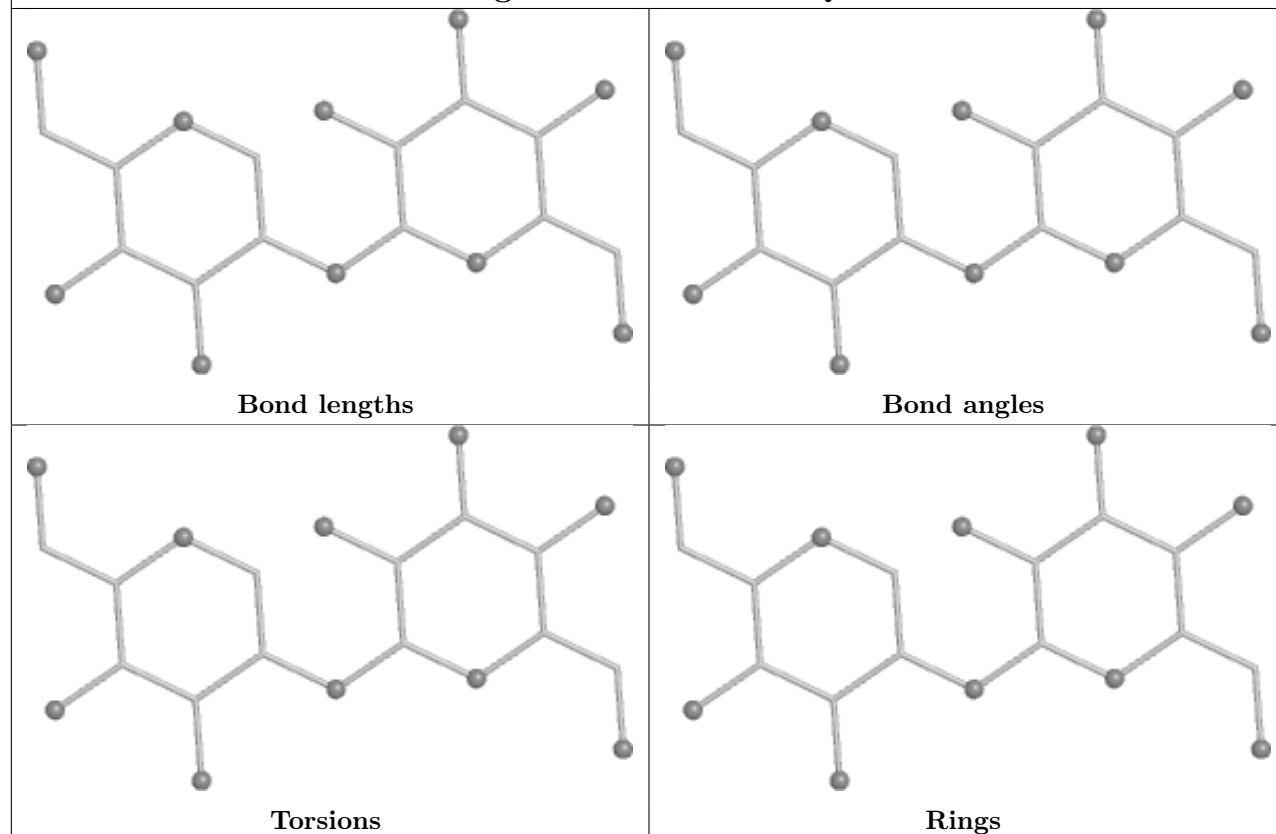
Oligosaccharide Chain Oc

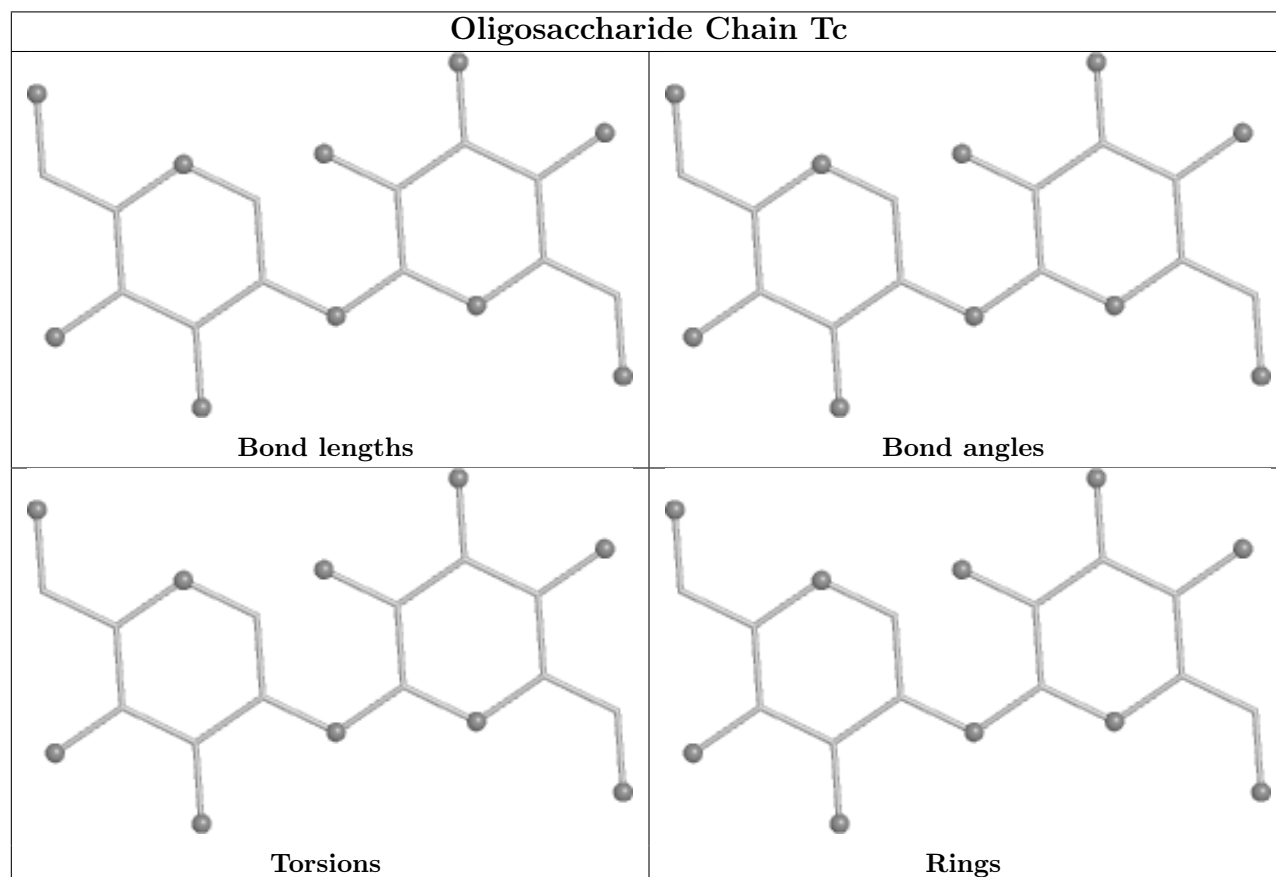
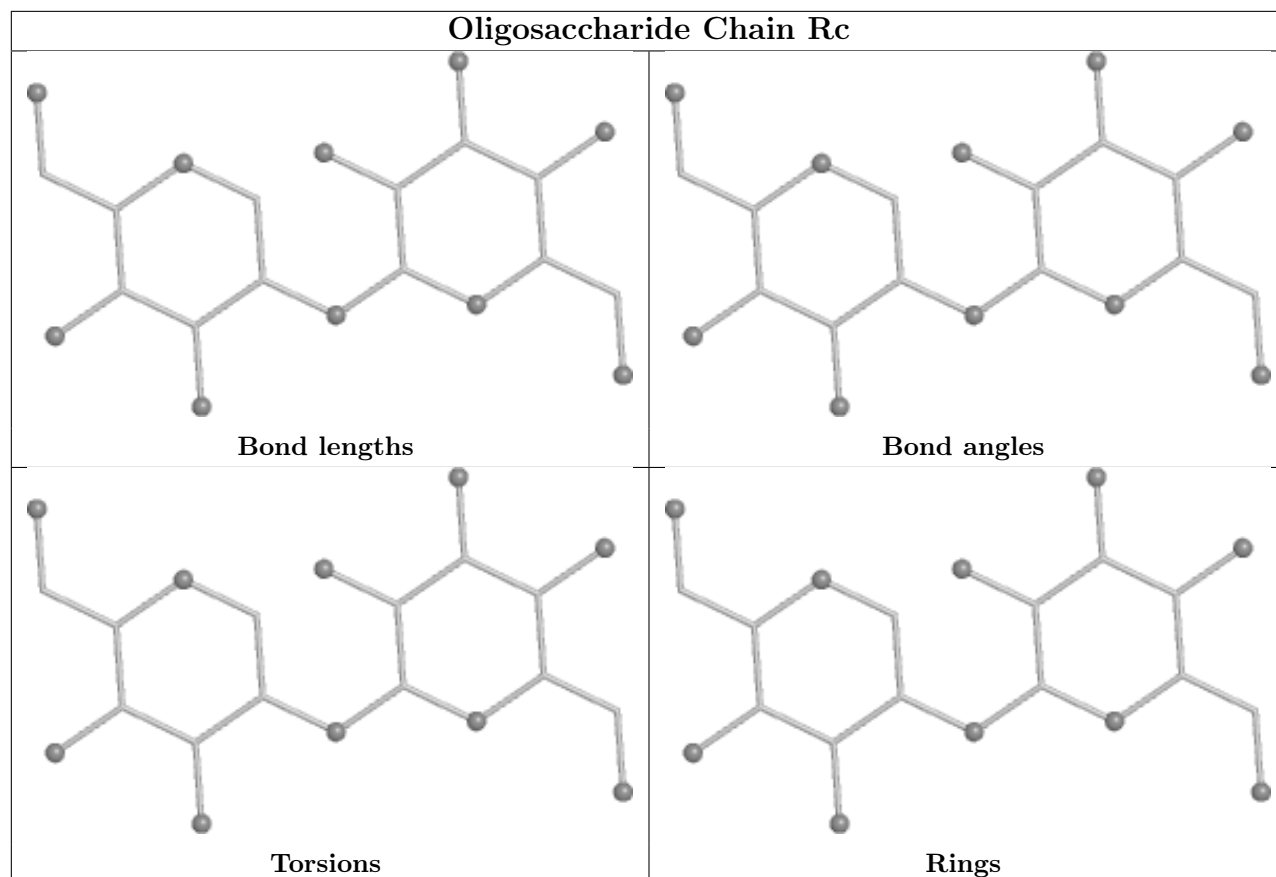


Oligosaccharide Chain Pc

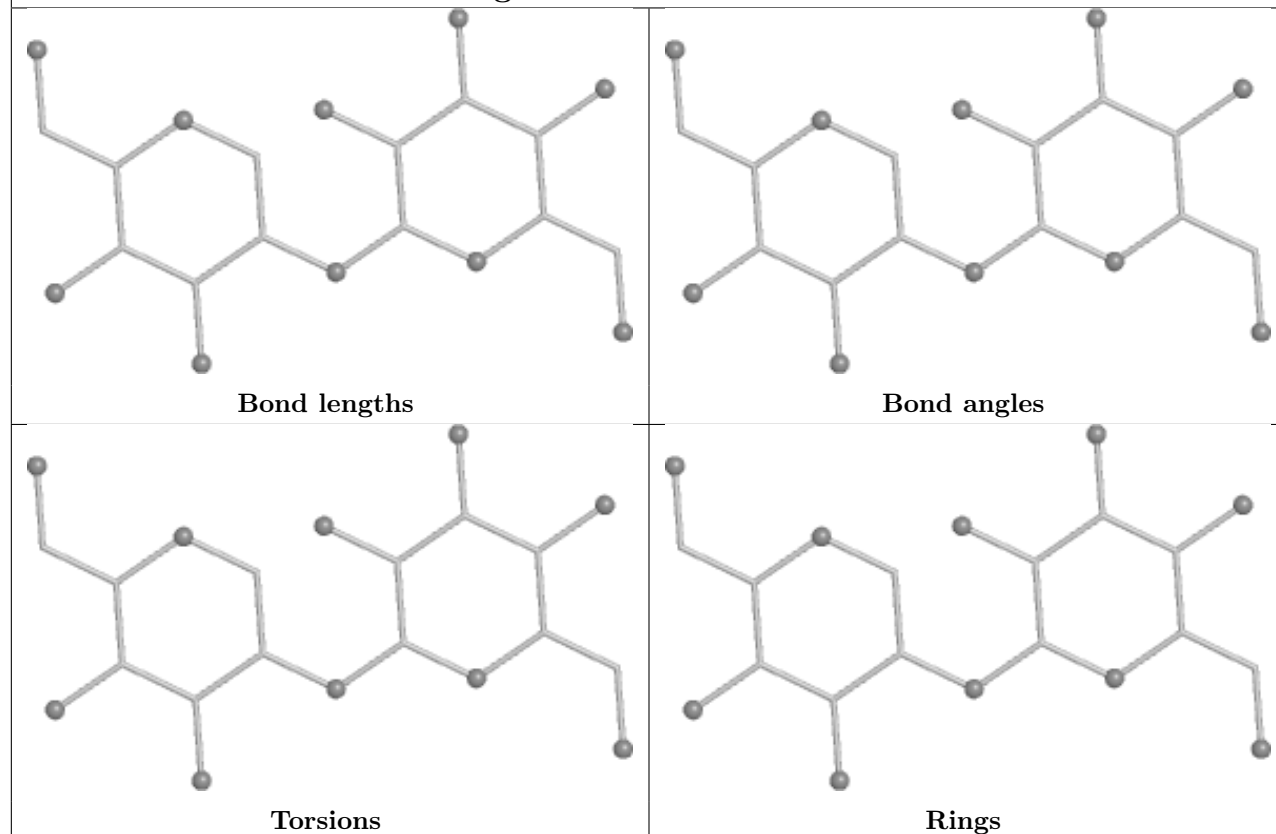


Oligosaccharide Chain Qc

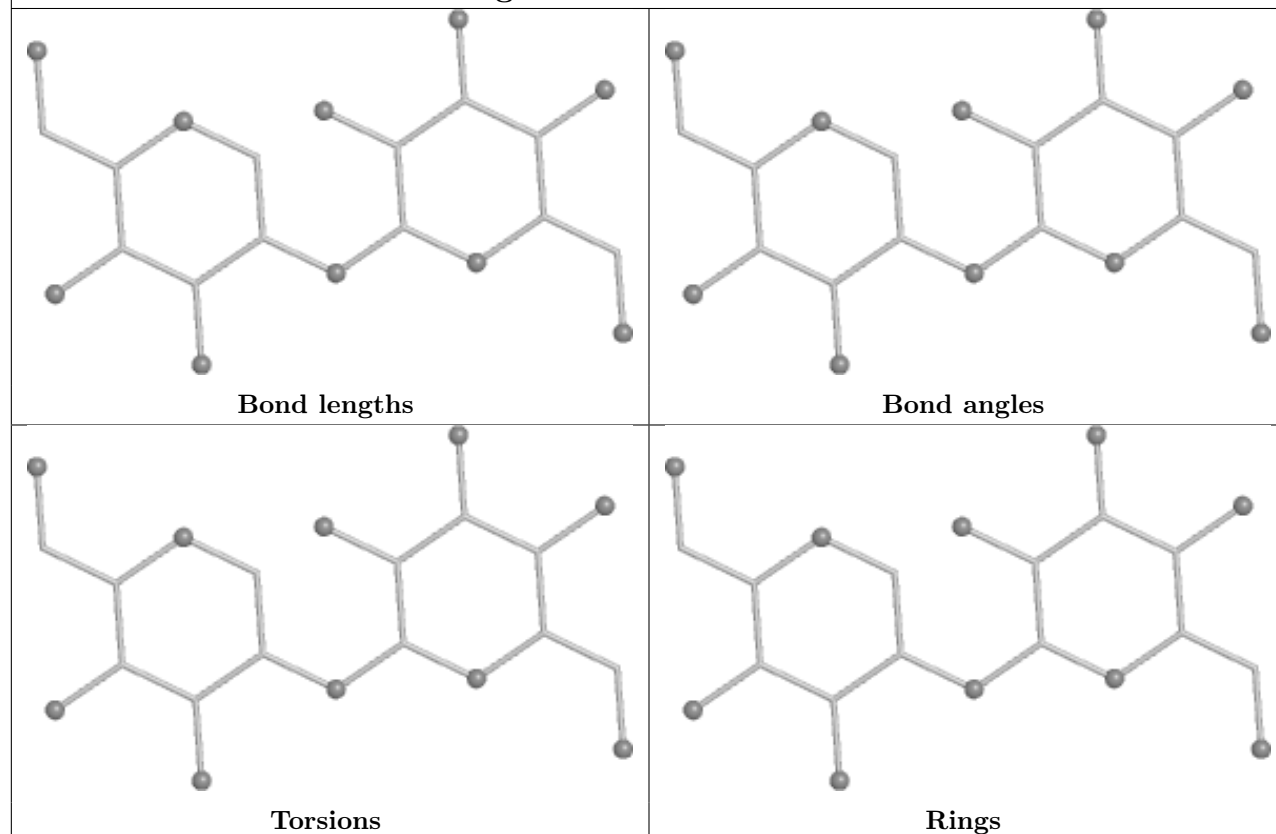




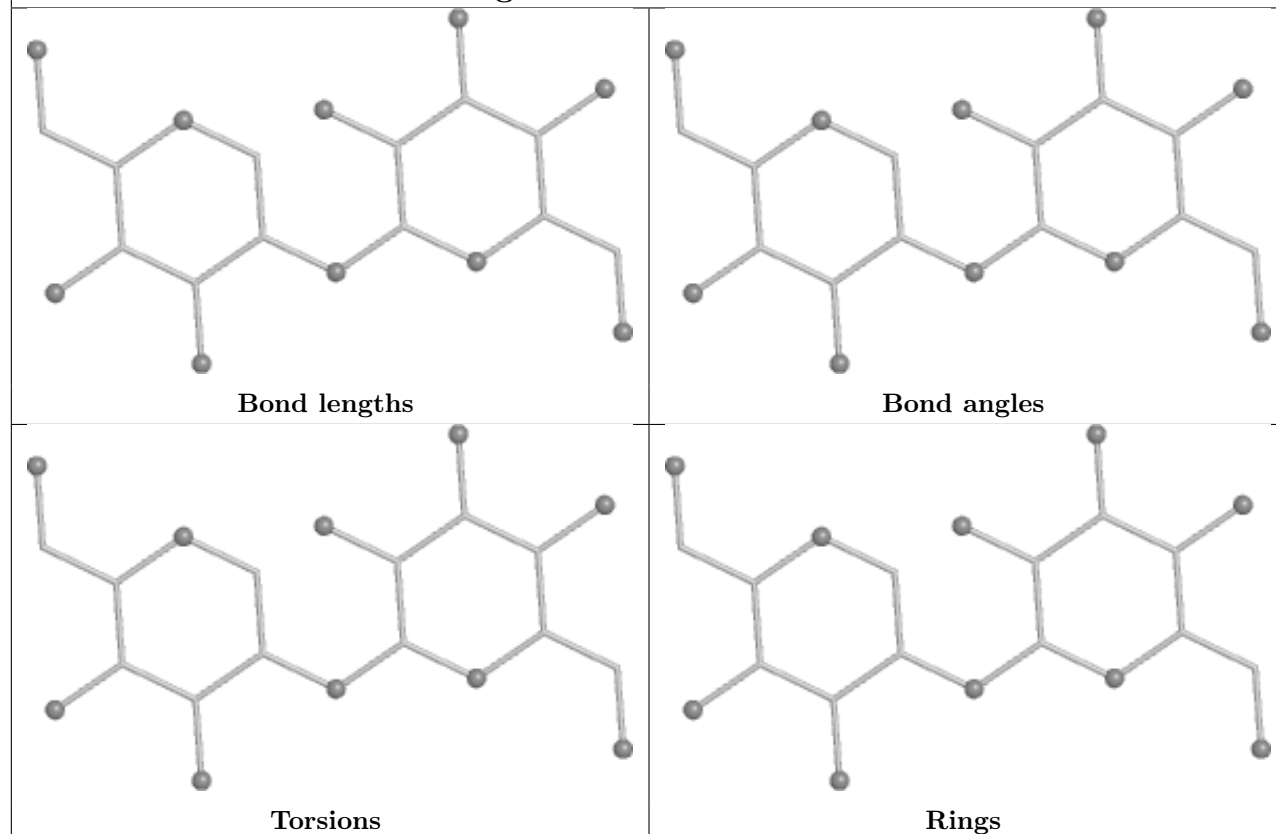
Oligosaccharide Chain Uc



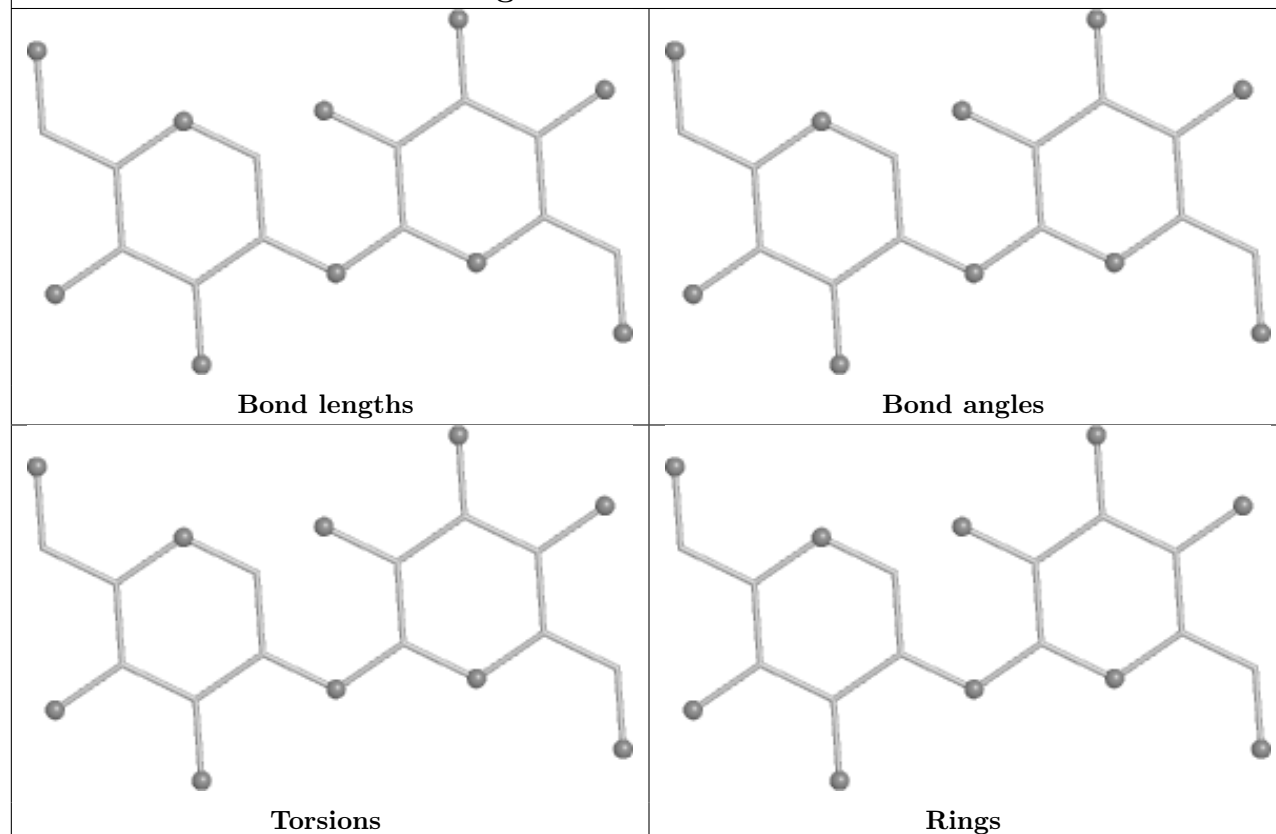
Oligosaccharide Chain Vc

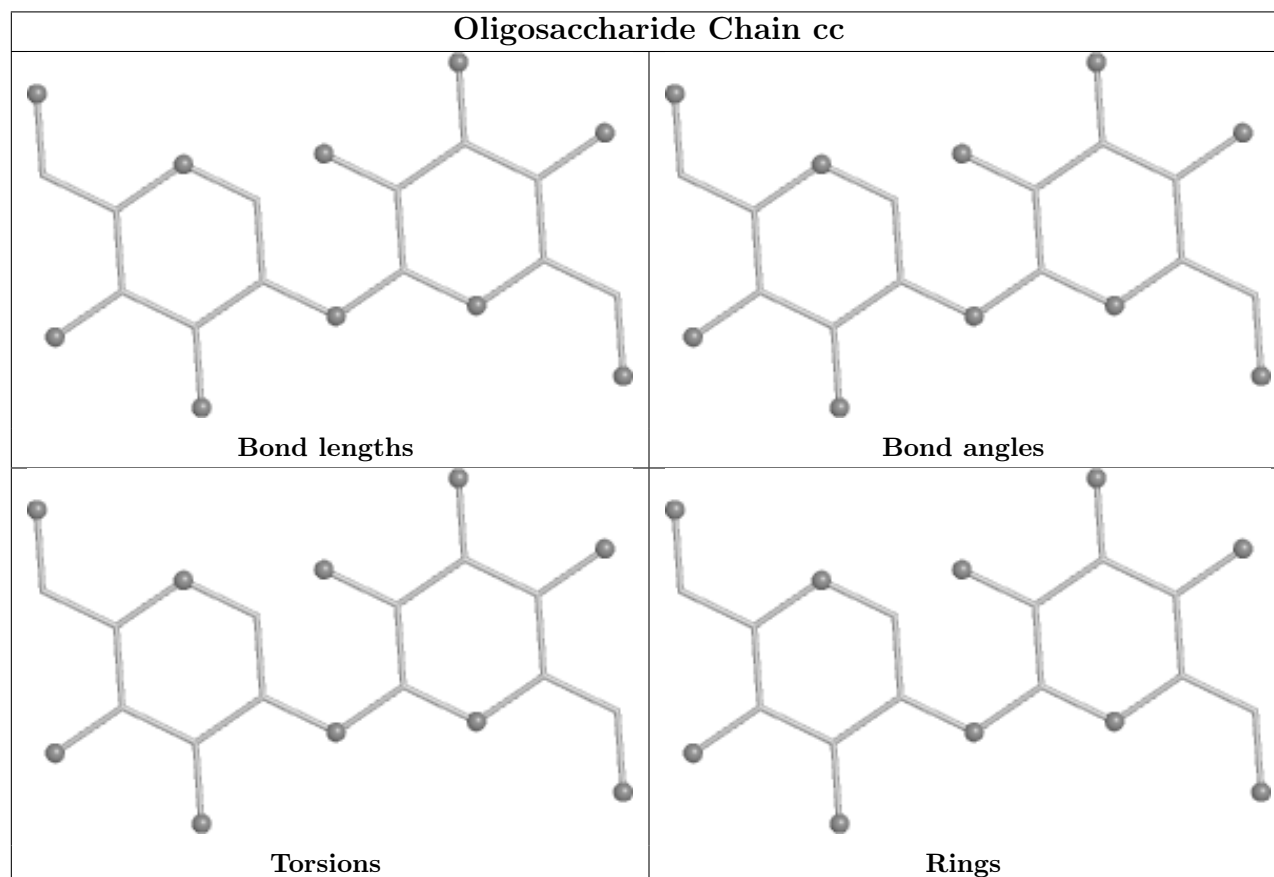
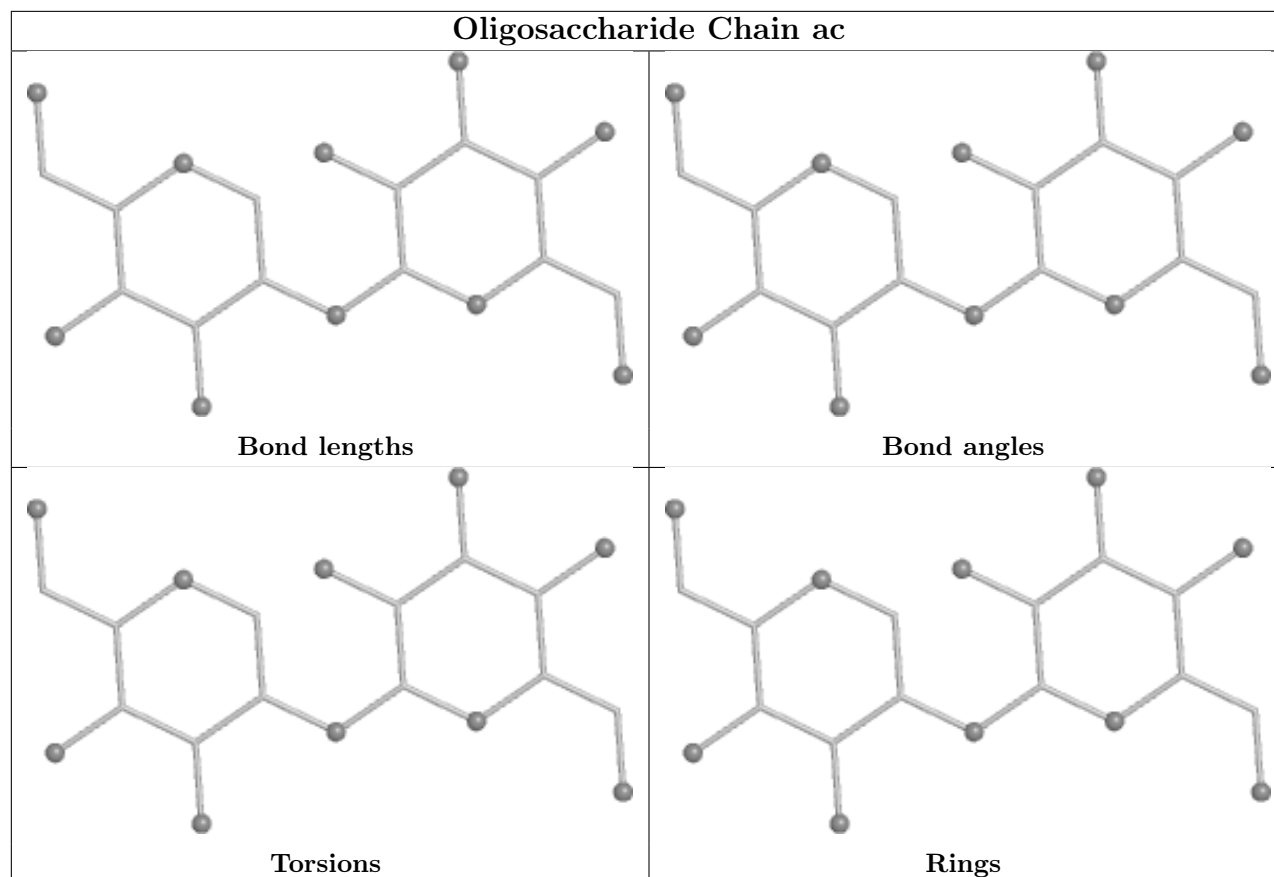


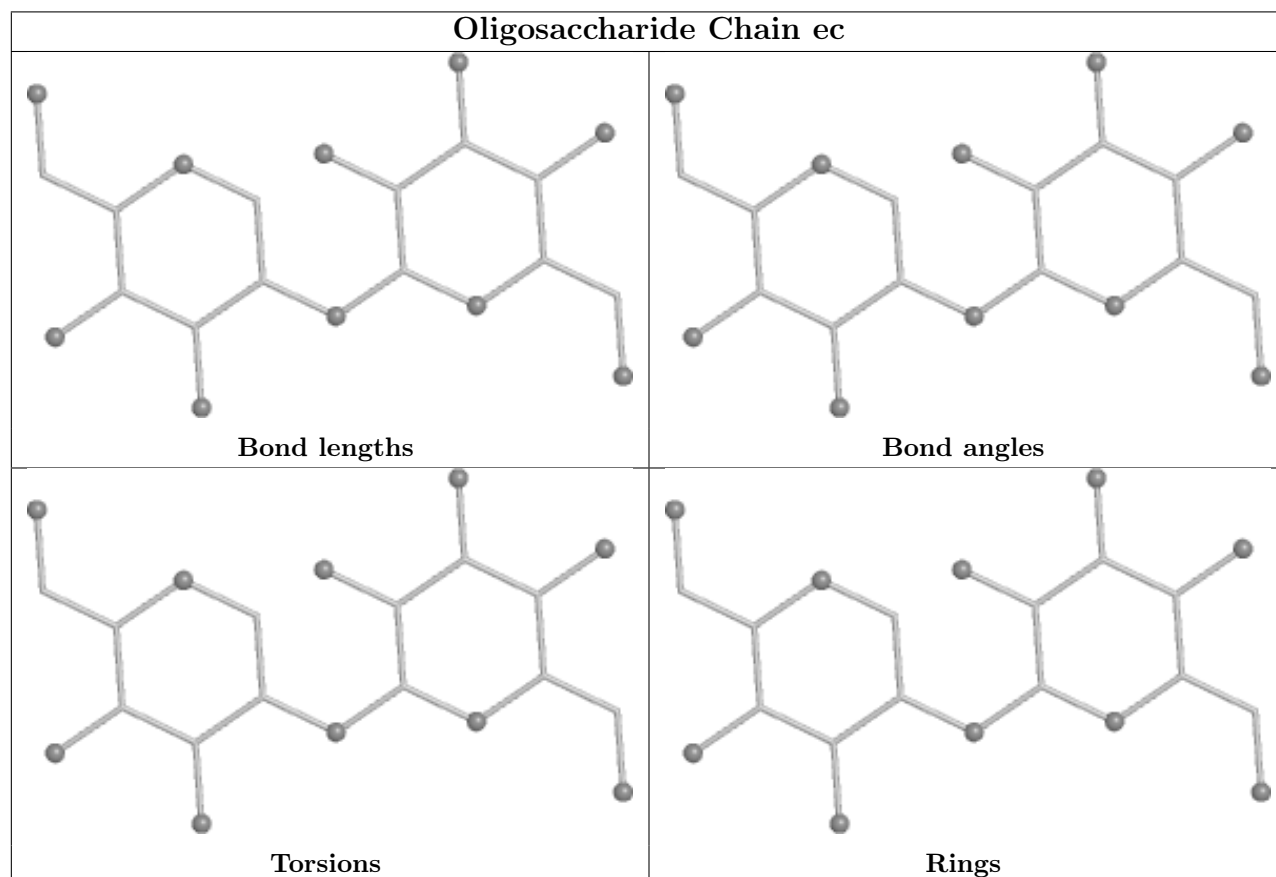
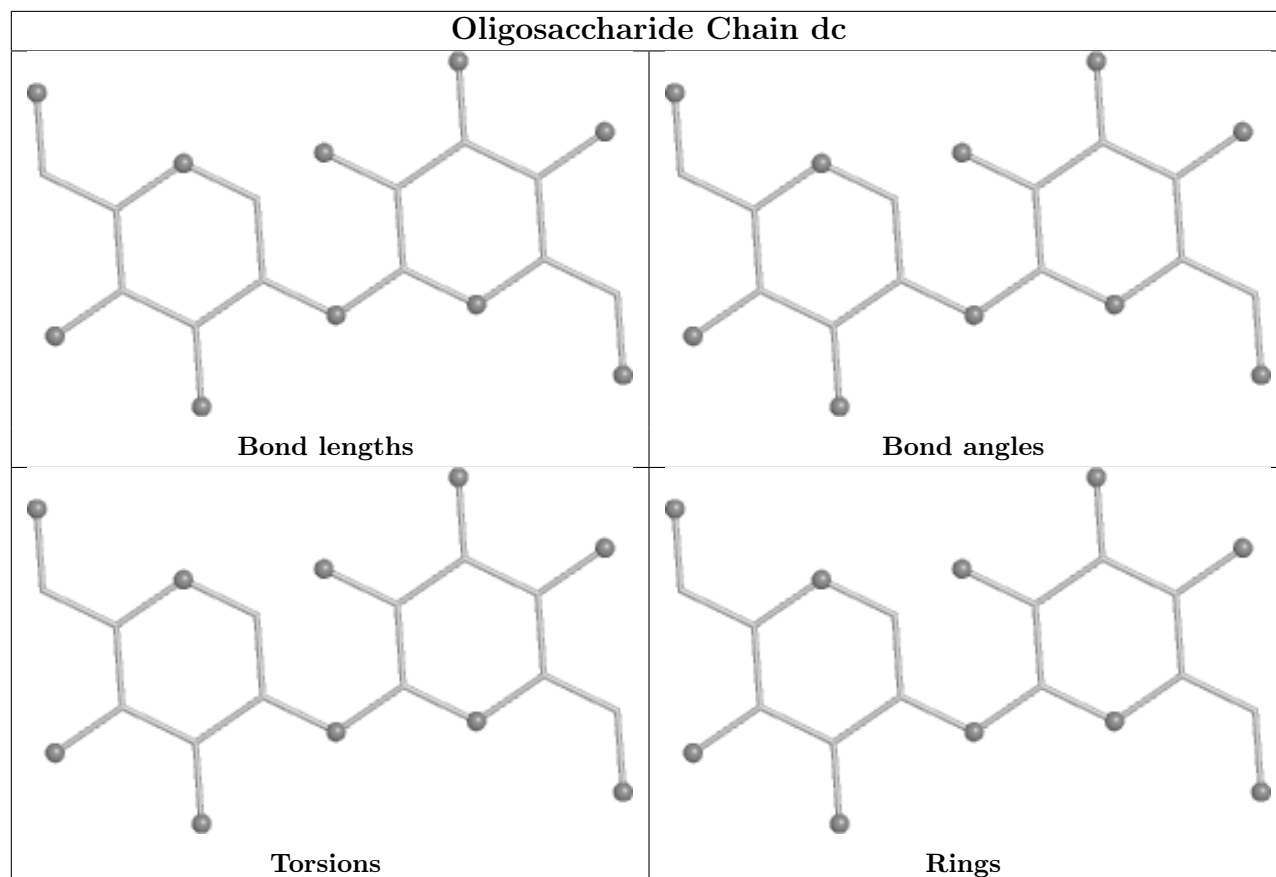
Oligosaccharide Chain Yc

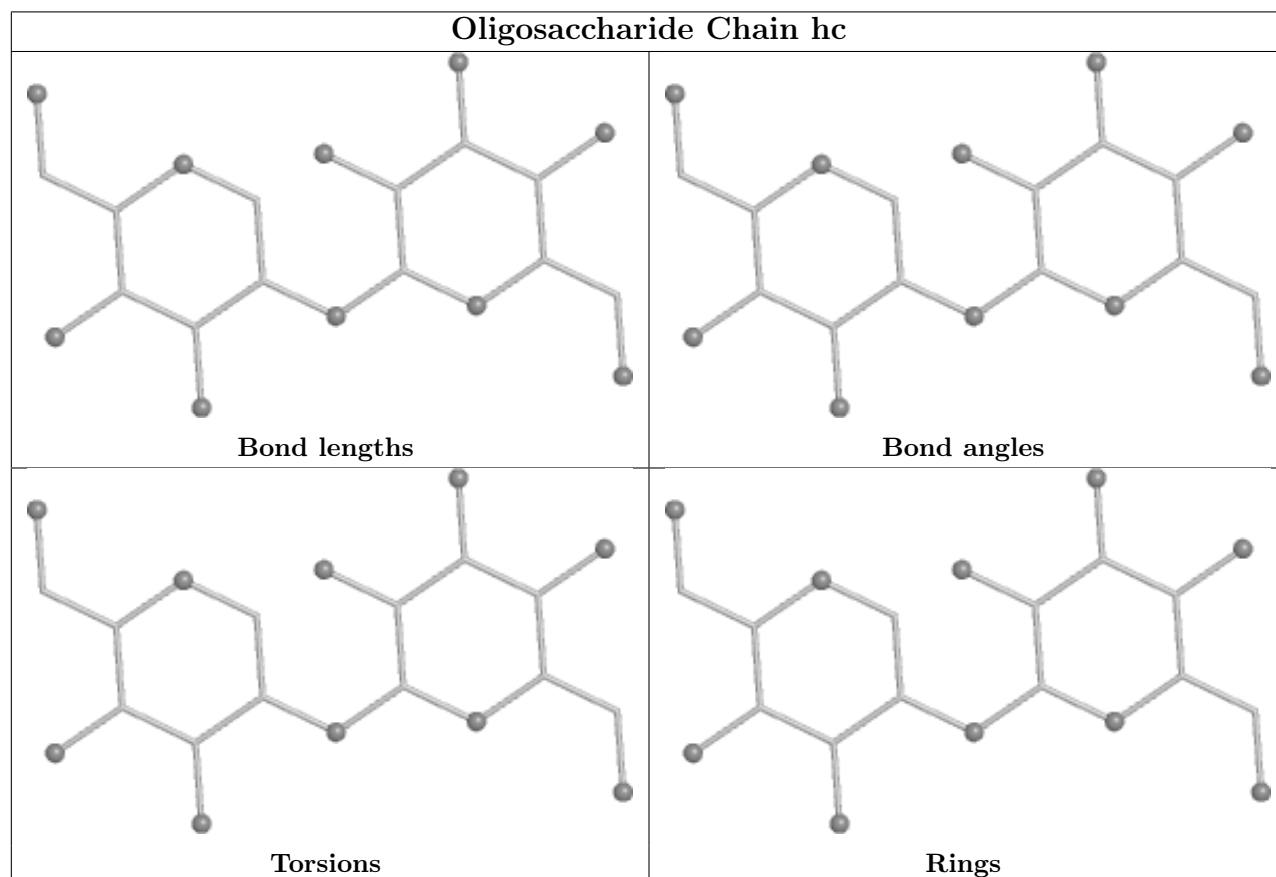
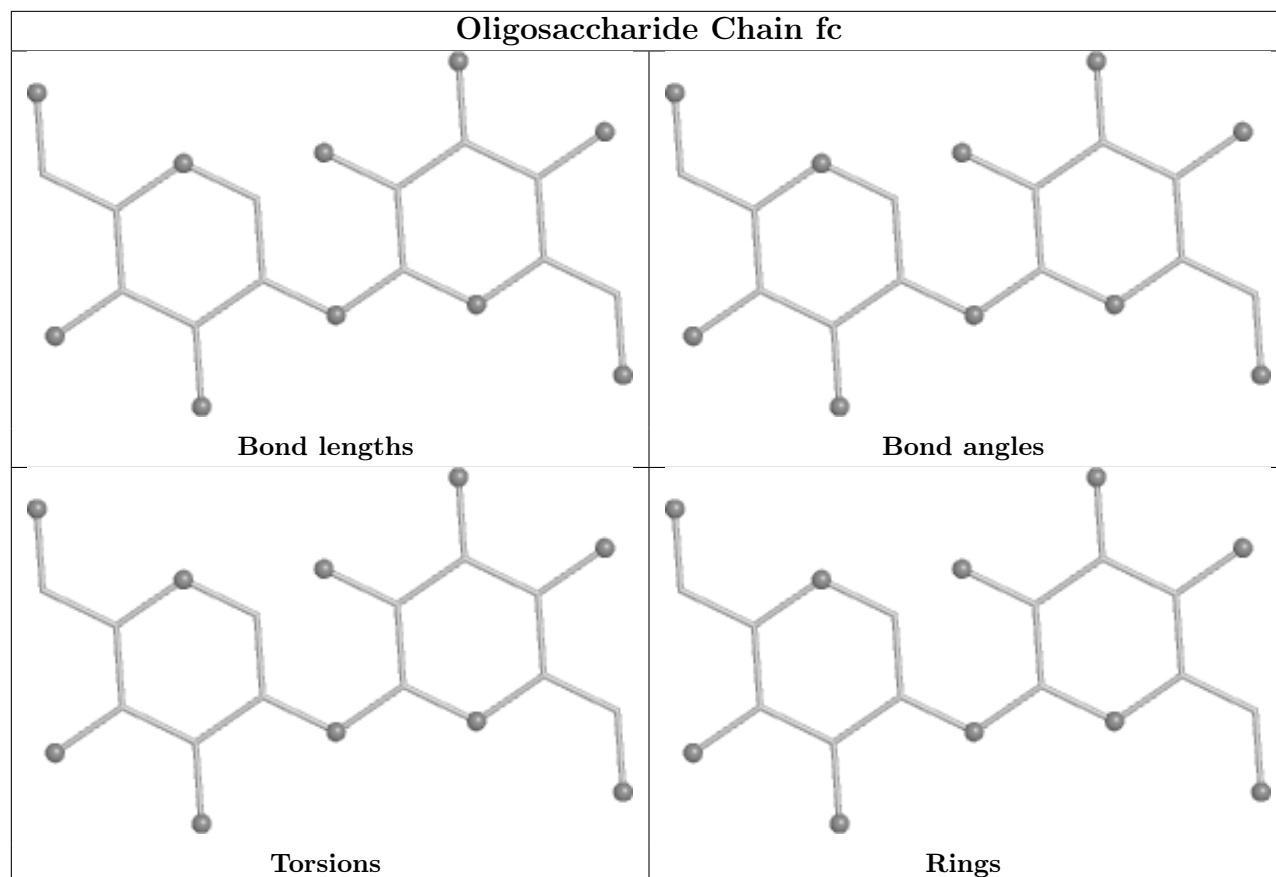


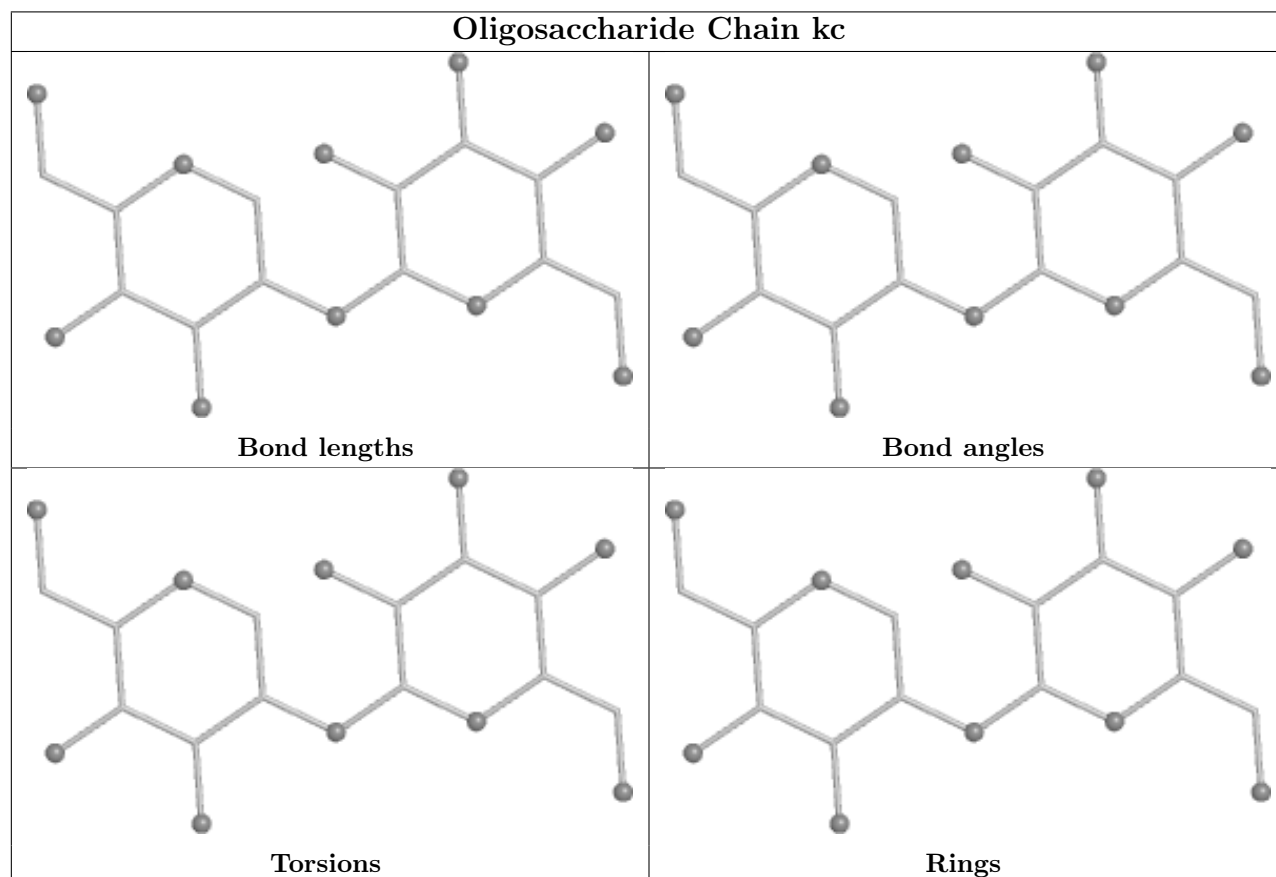
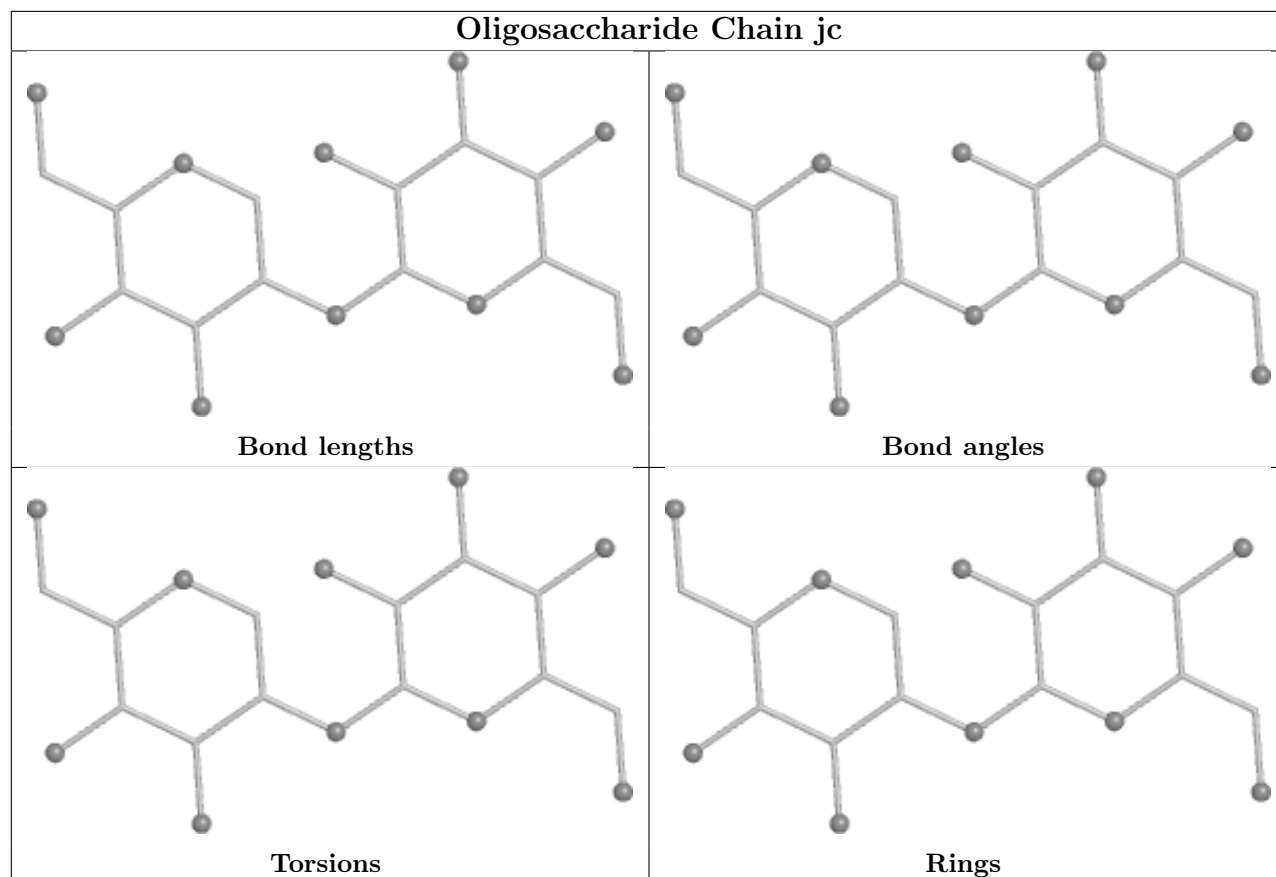
Oligosaccharide Chain Zc

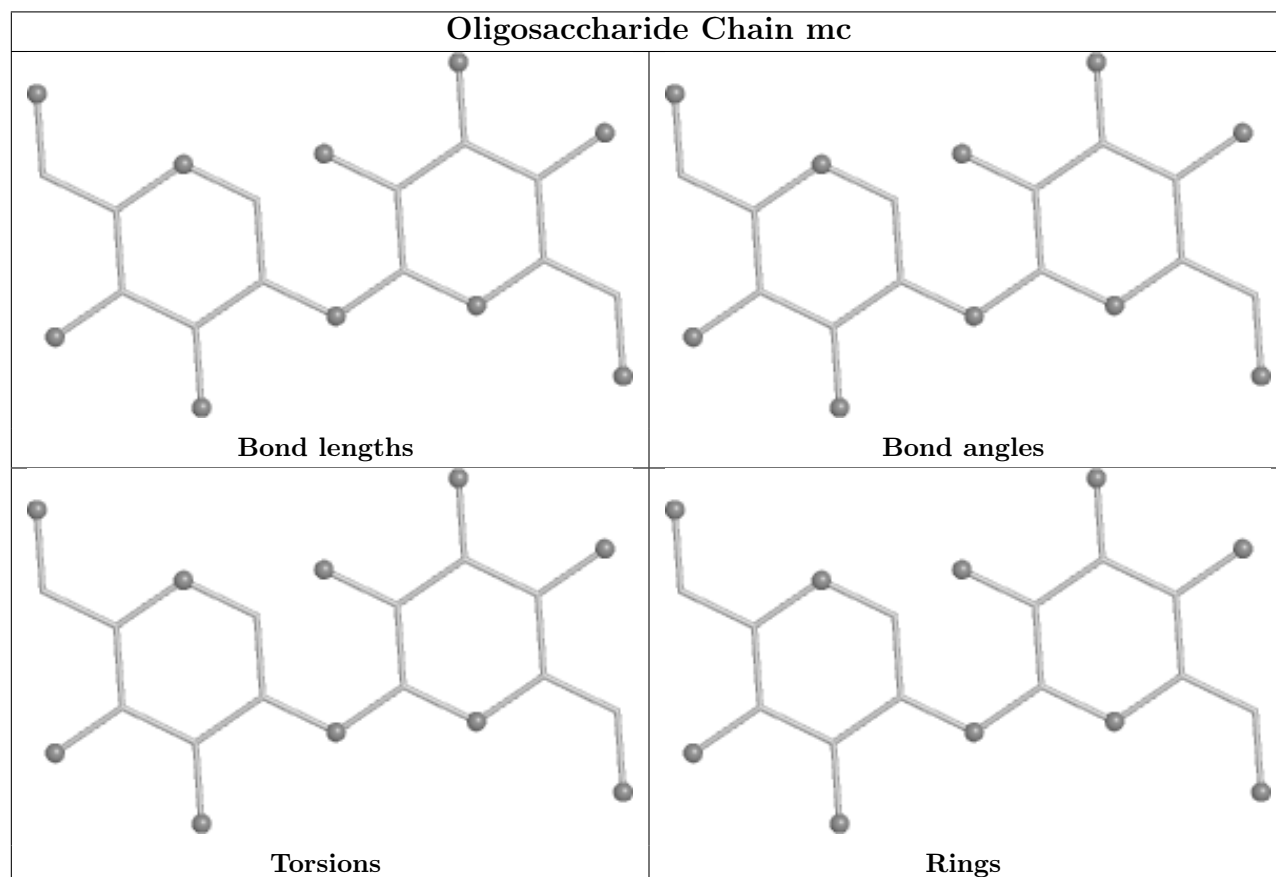
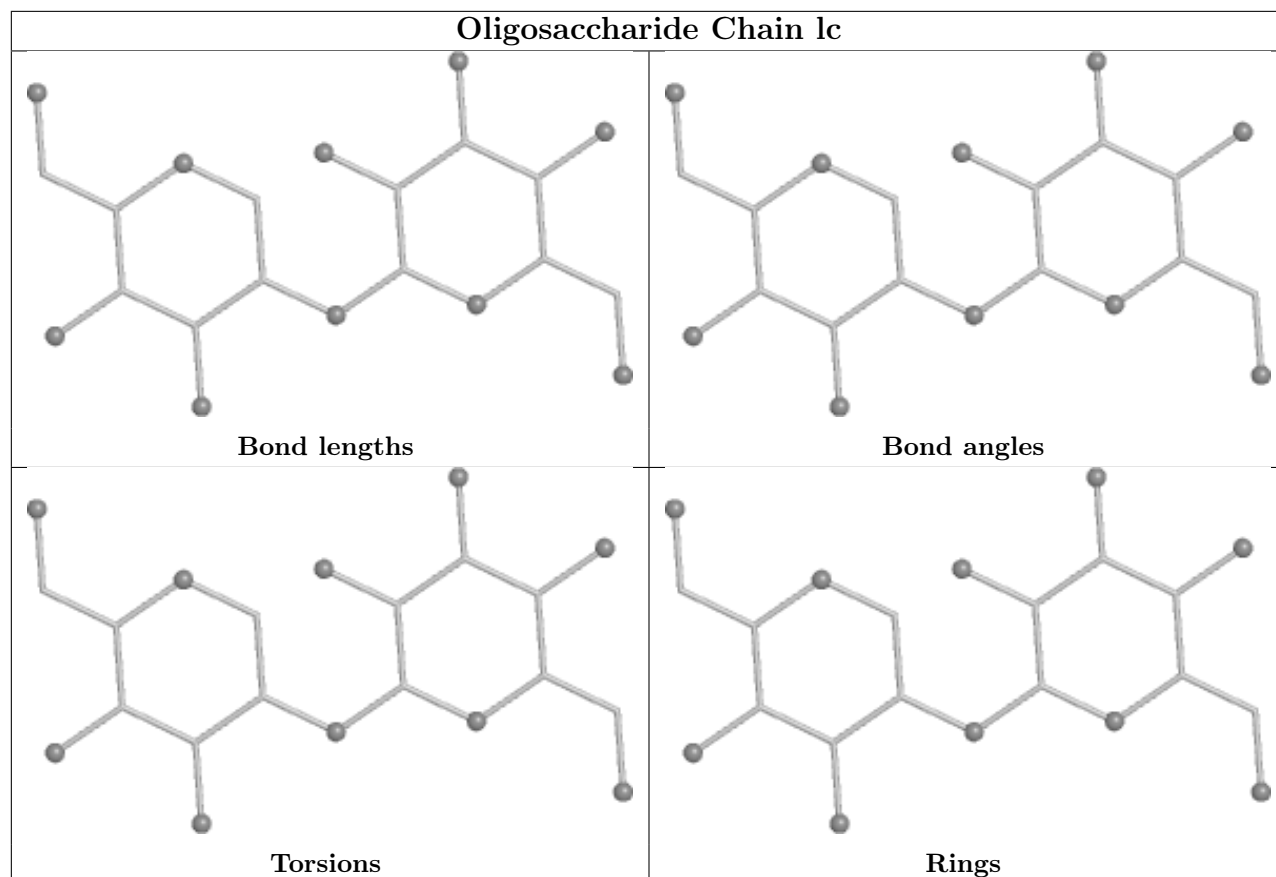


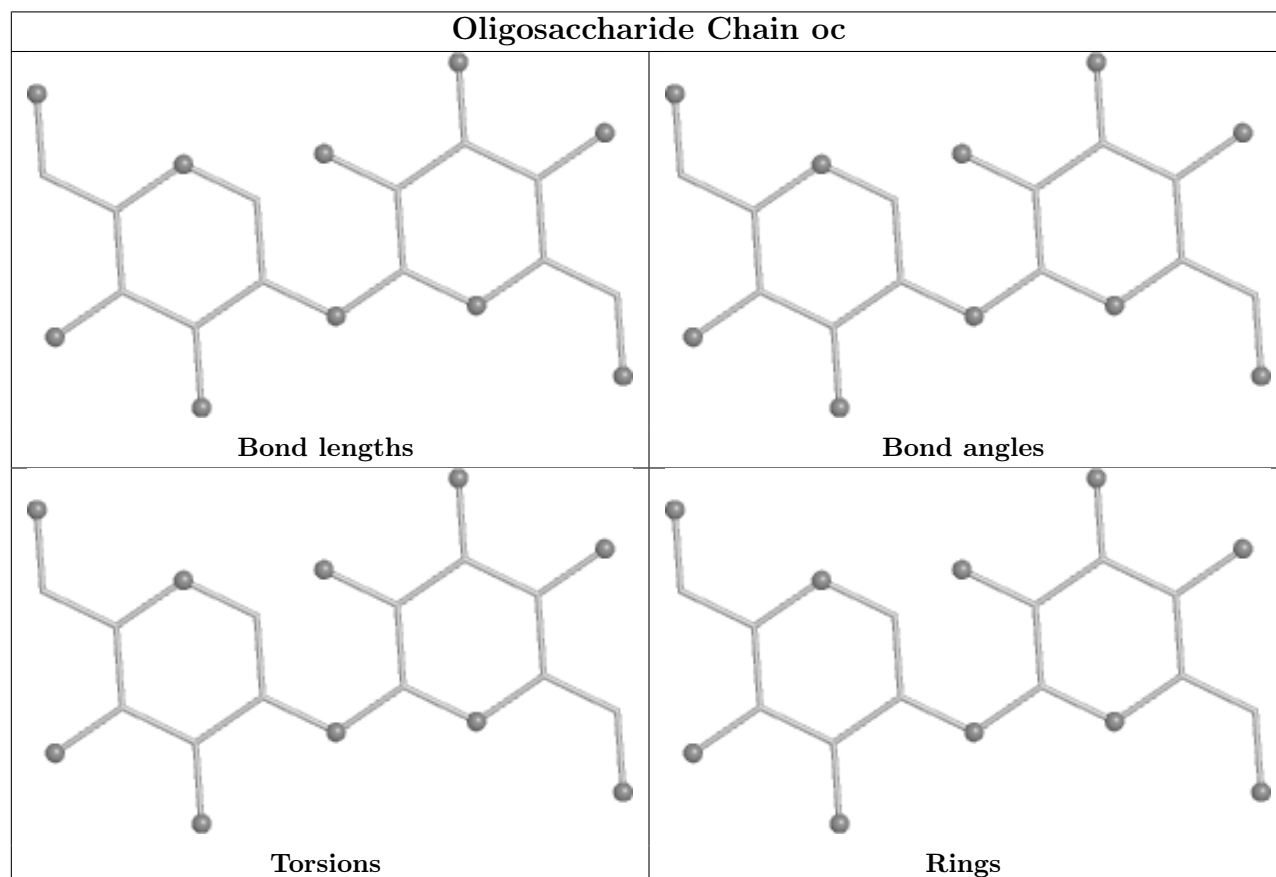
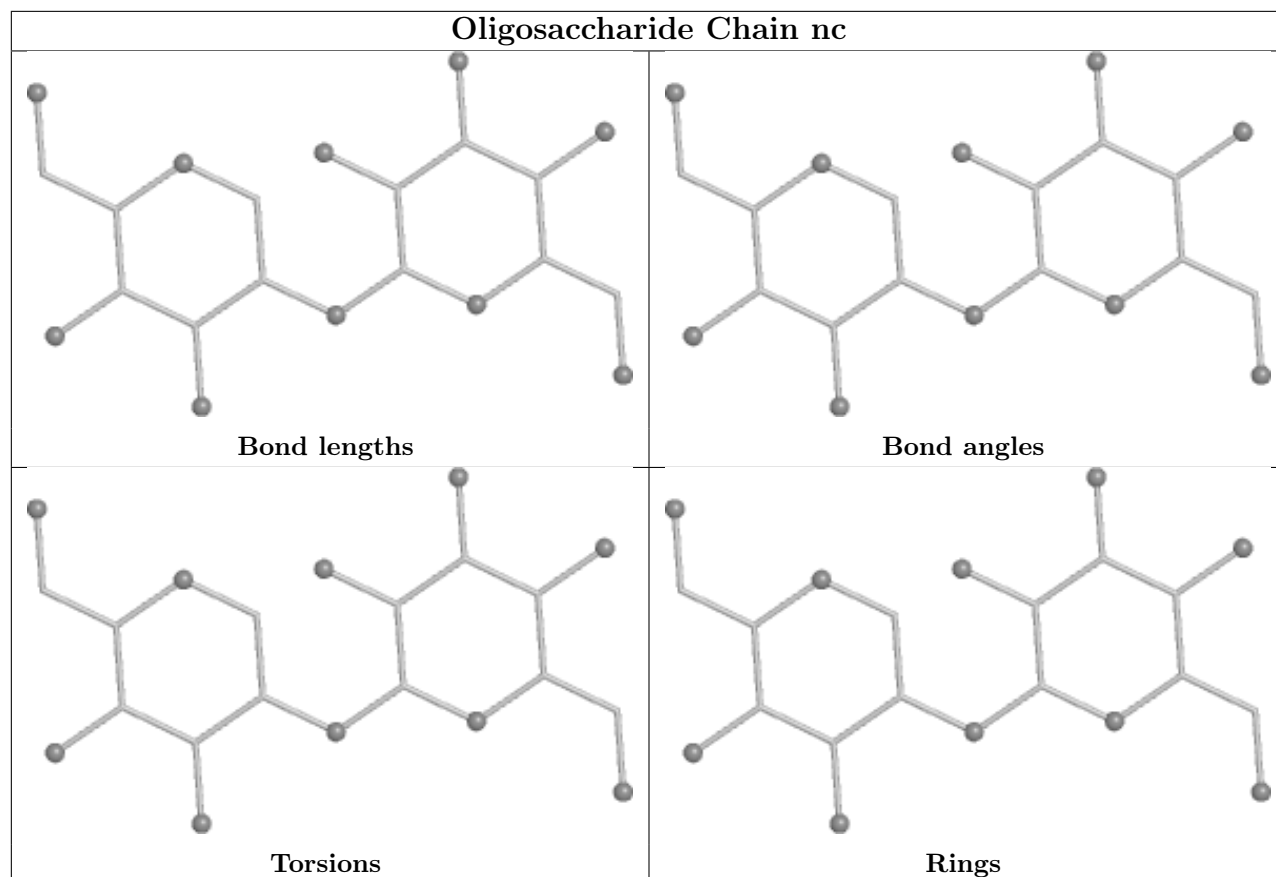


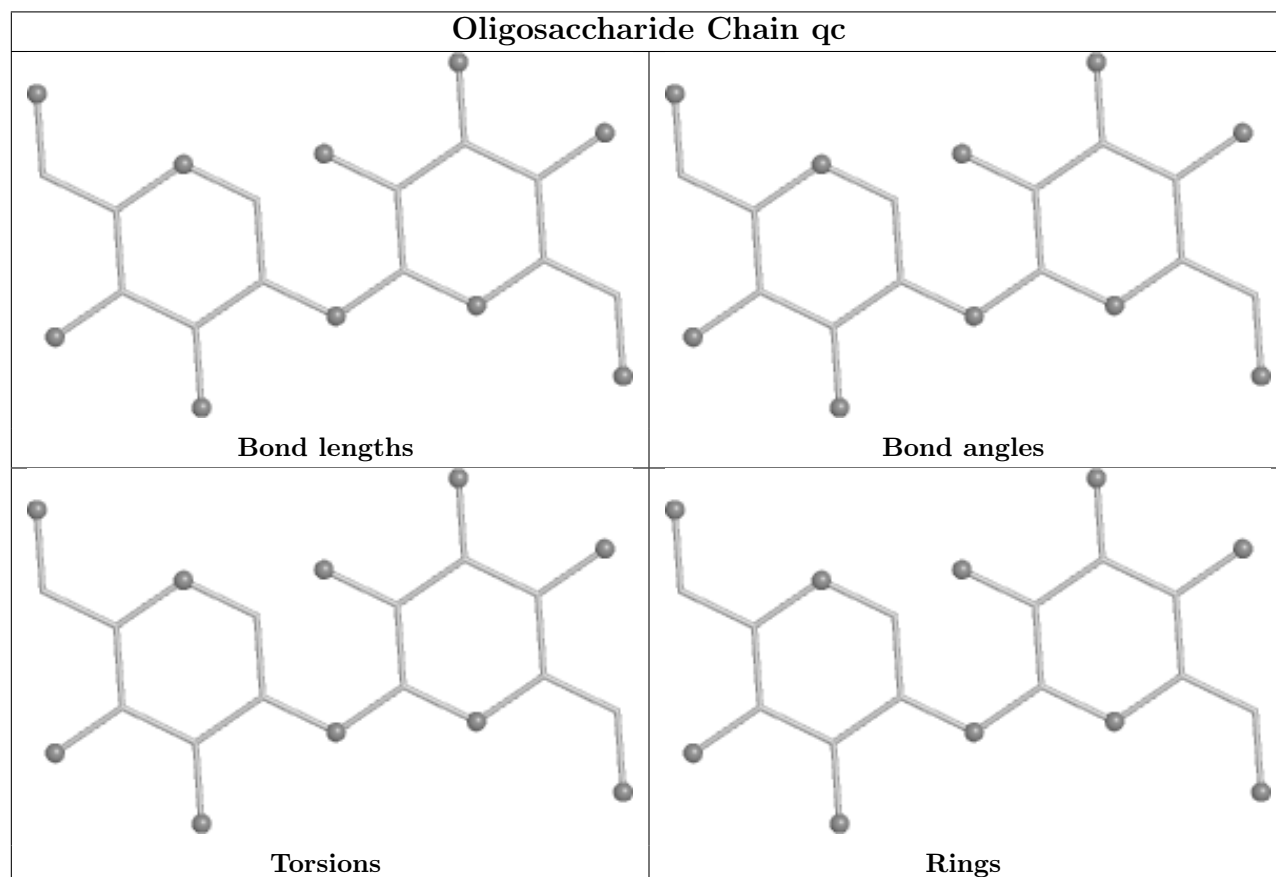
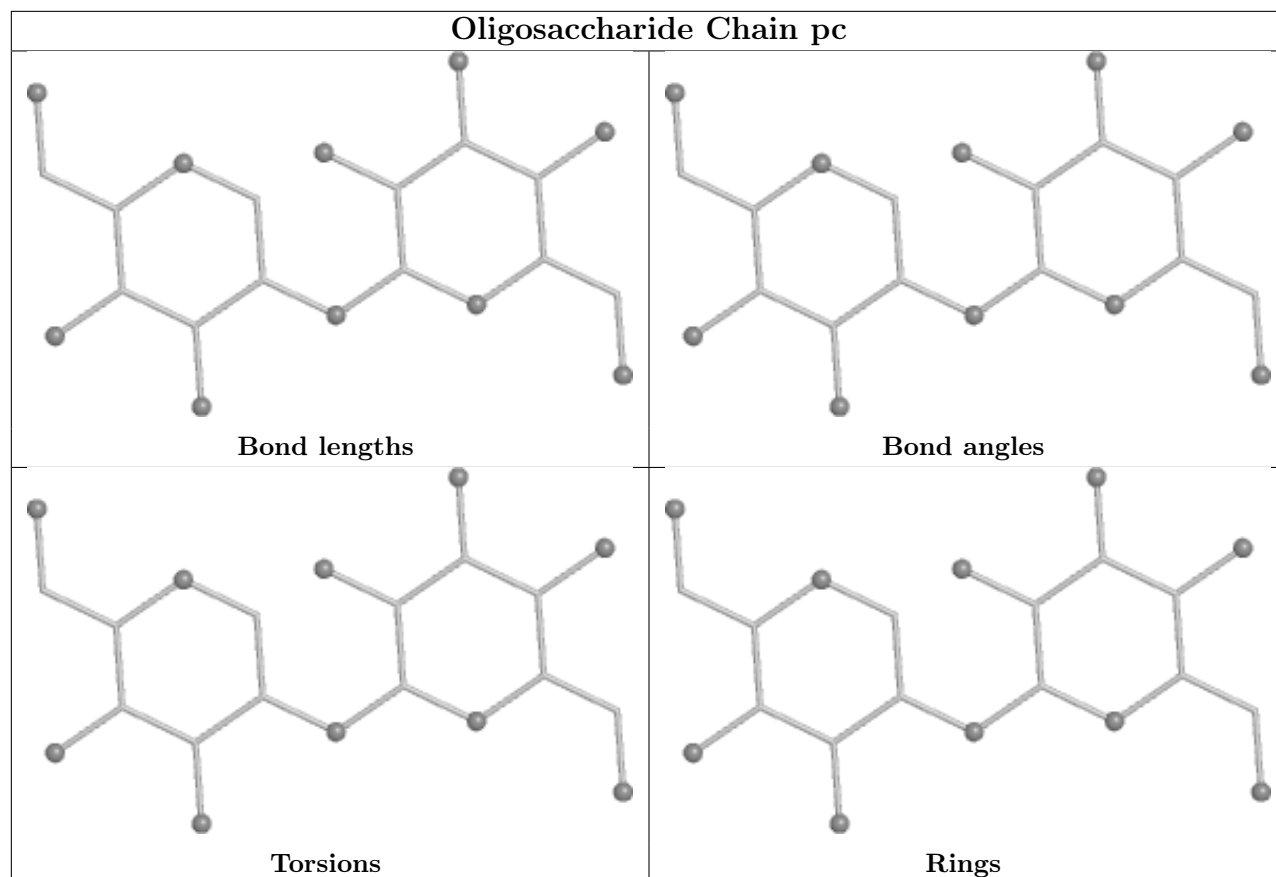


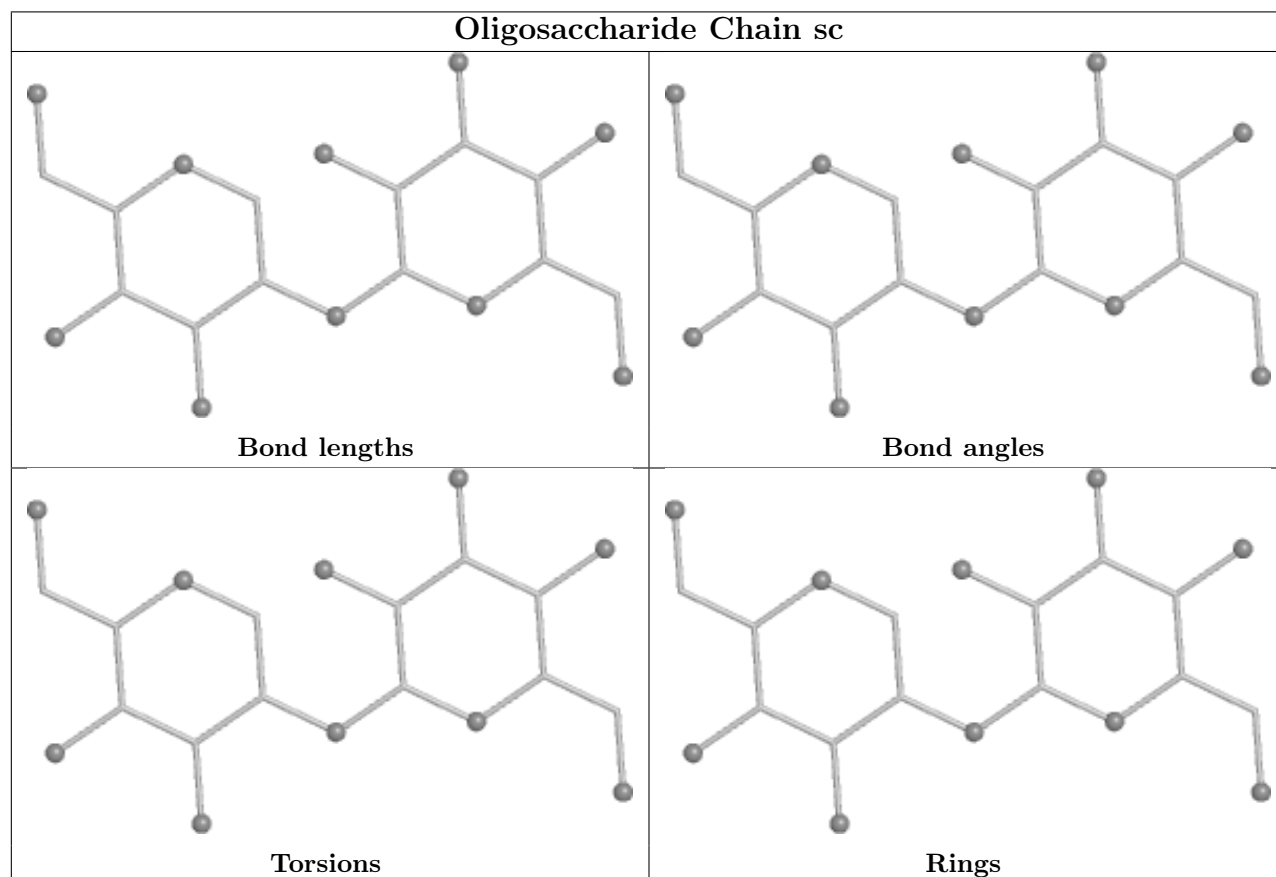
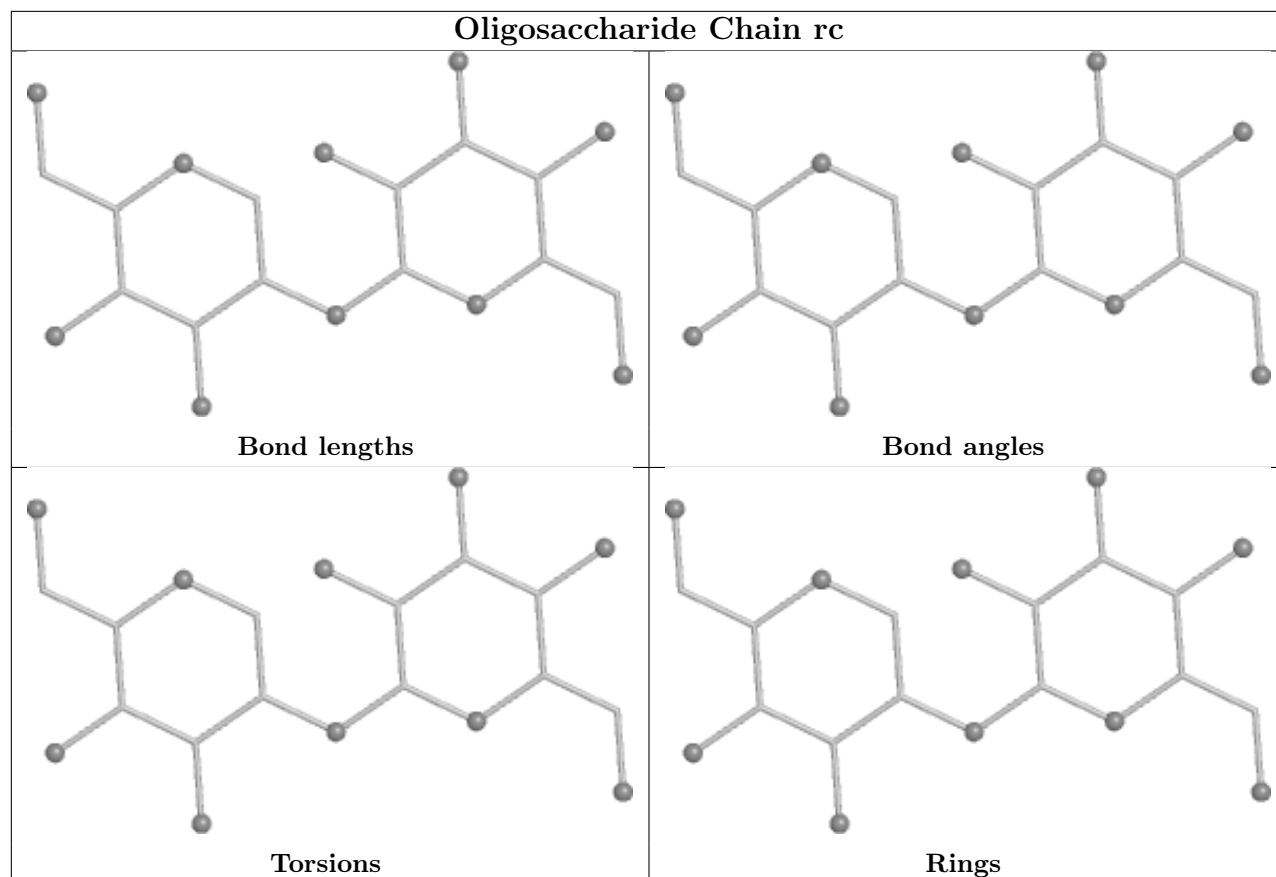


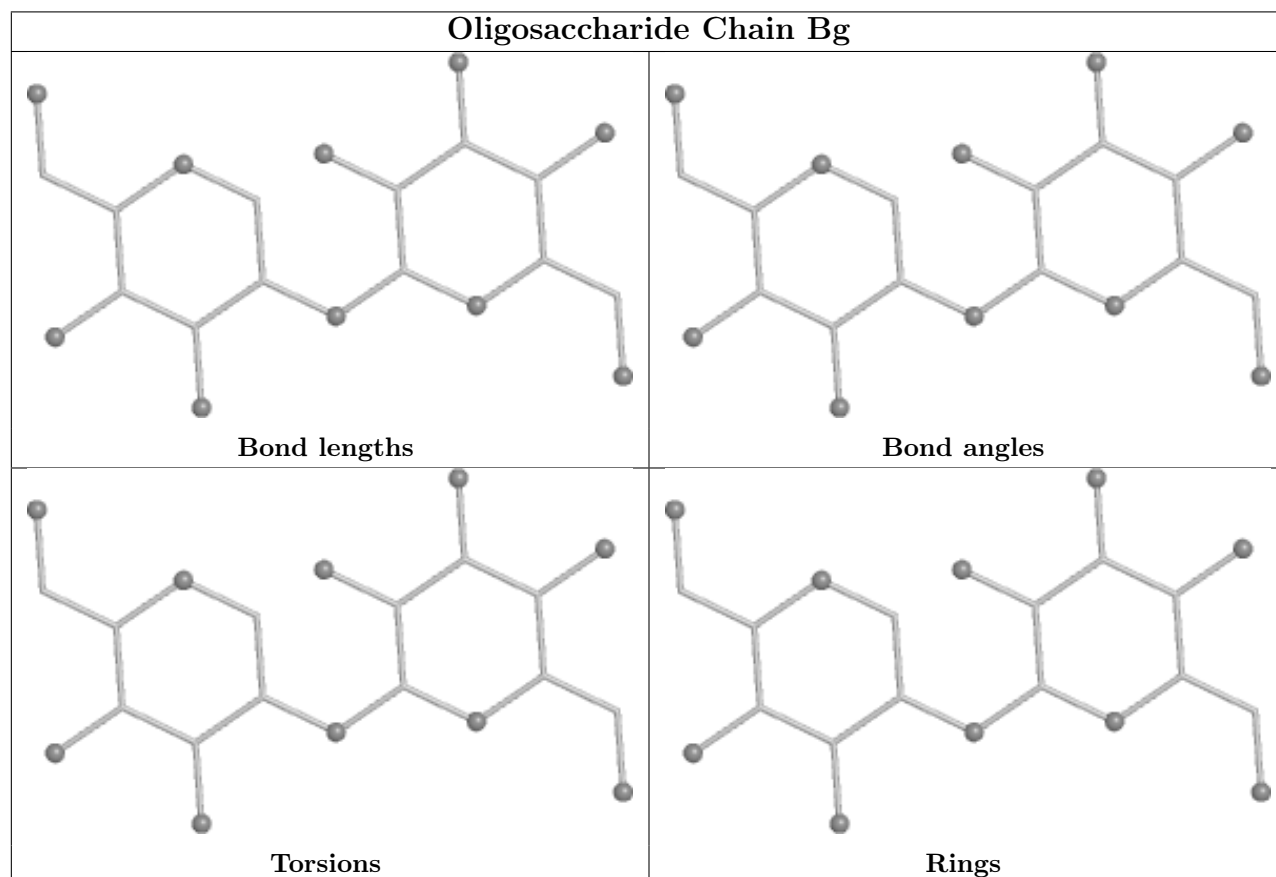
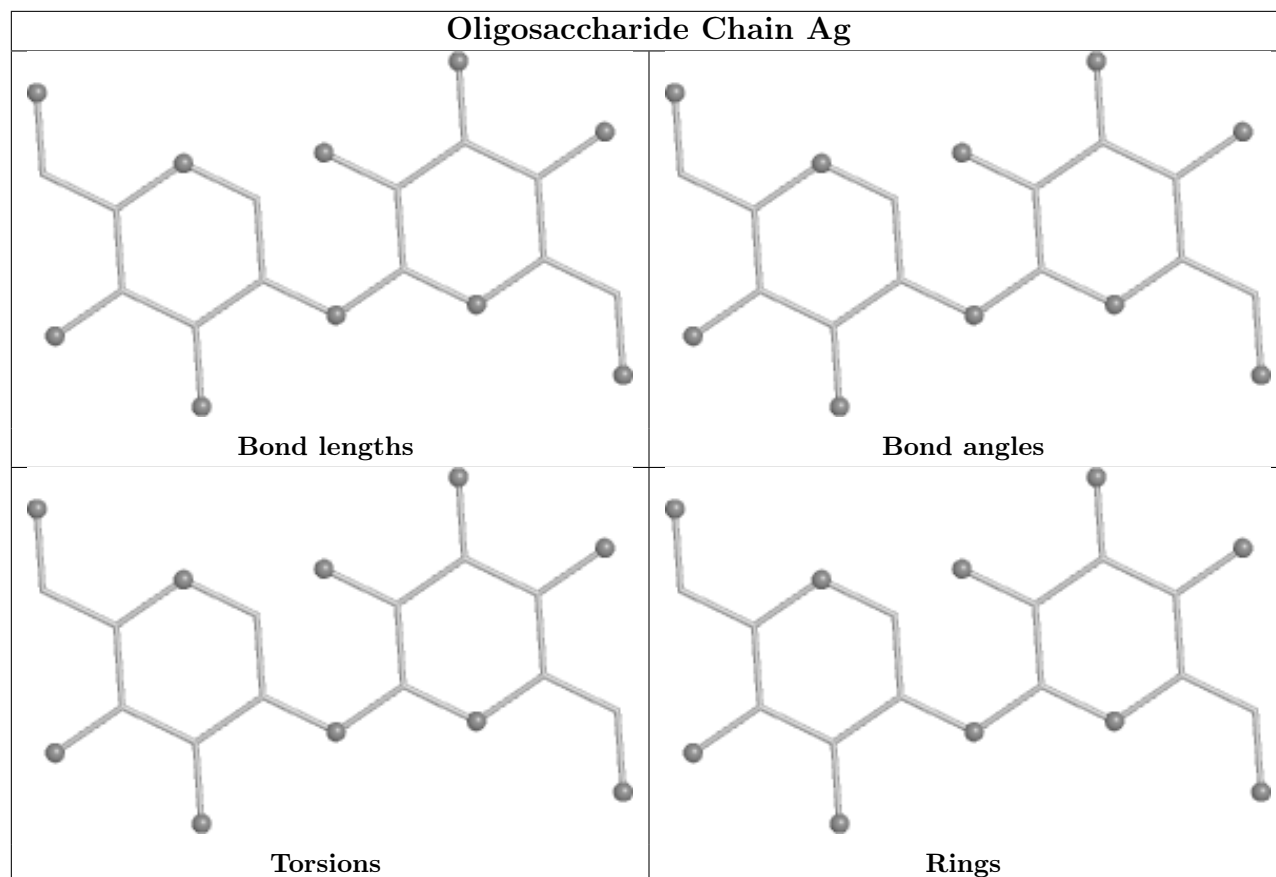


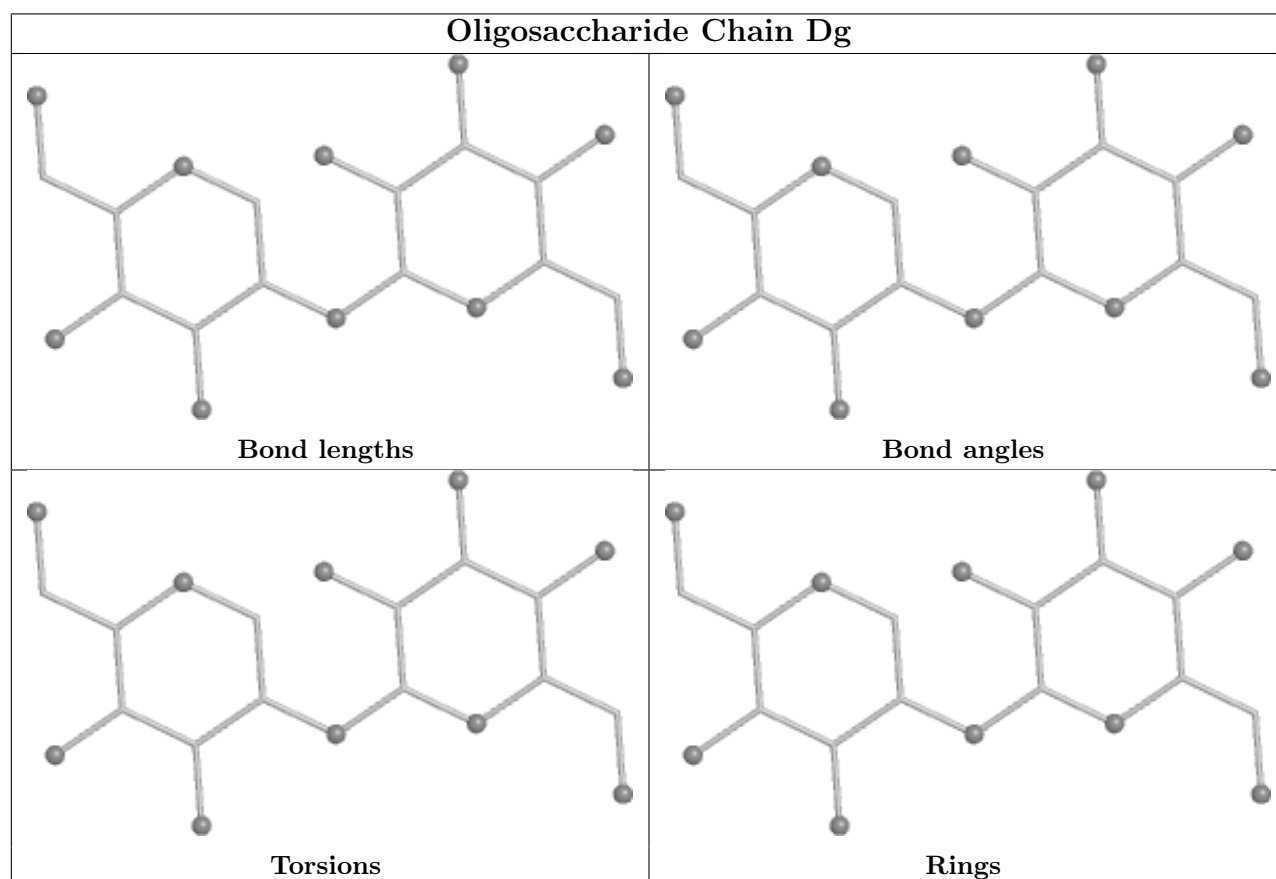
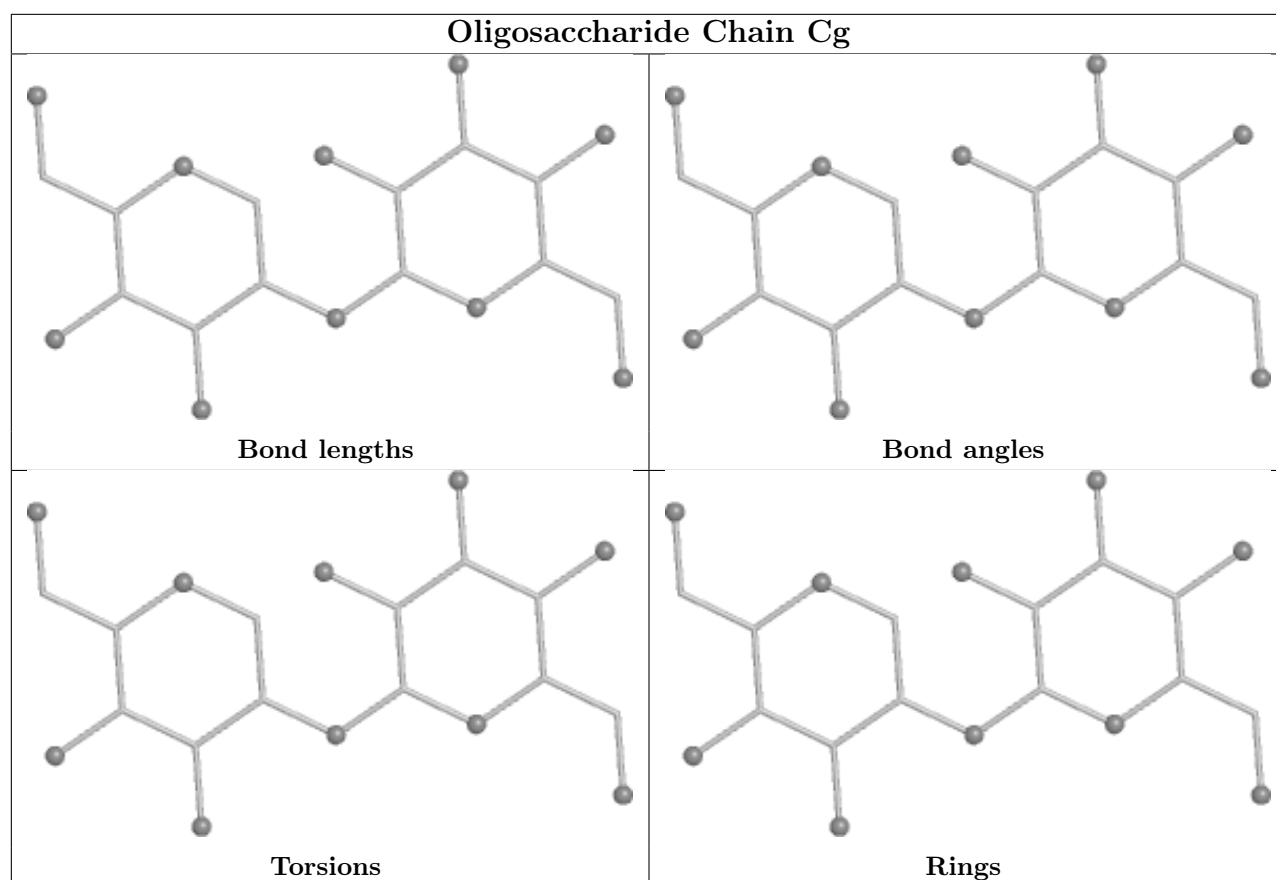


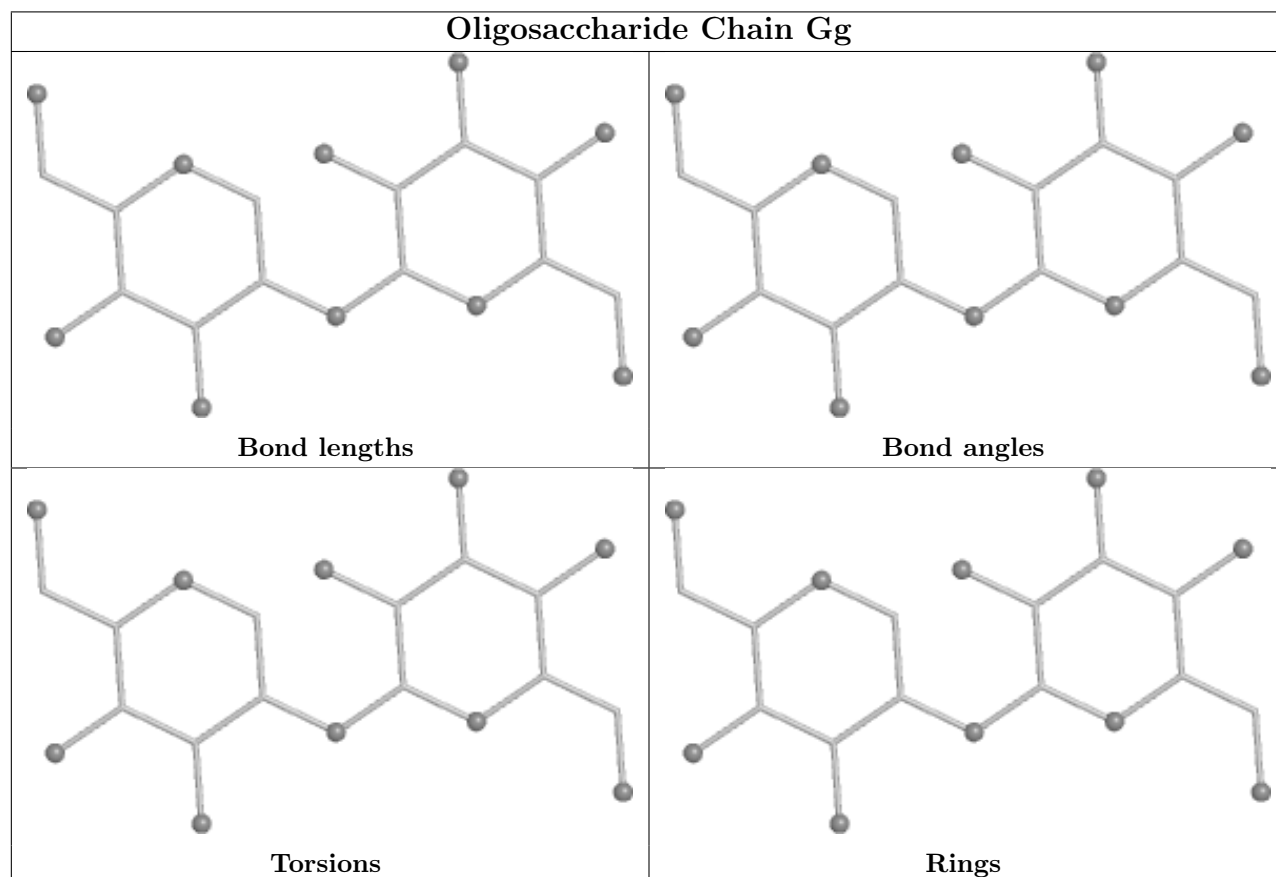
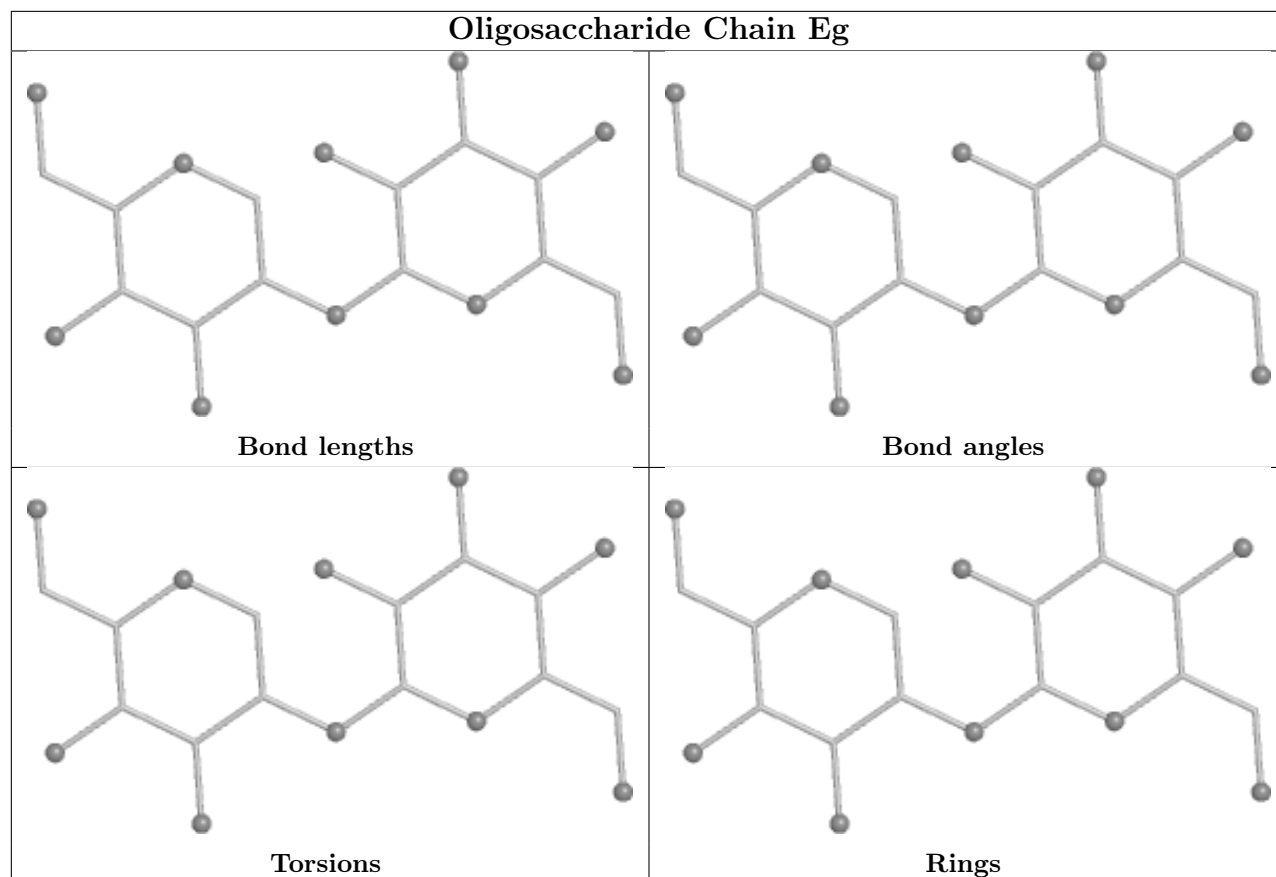


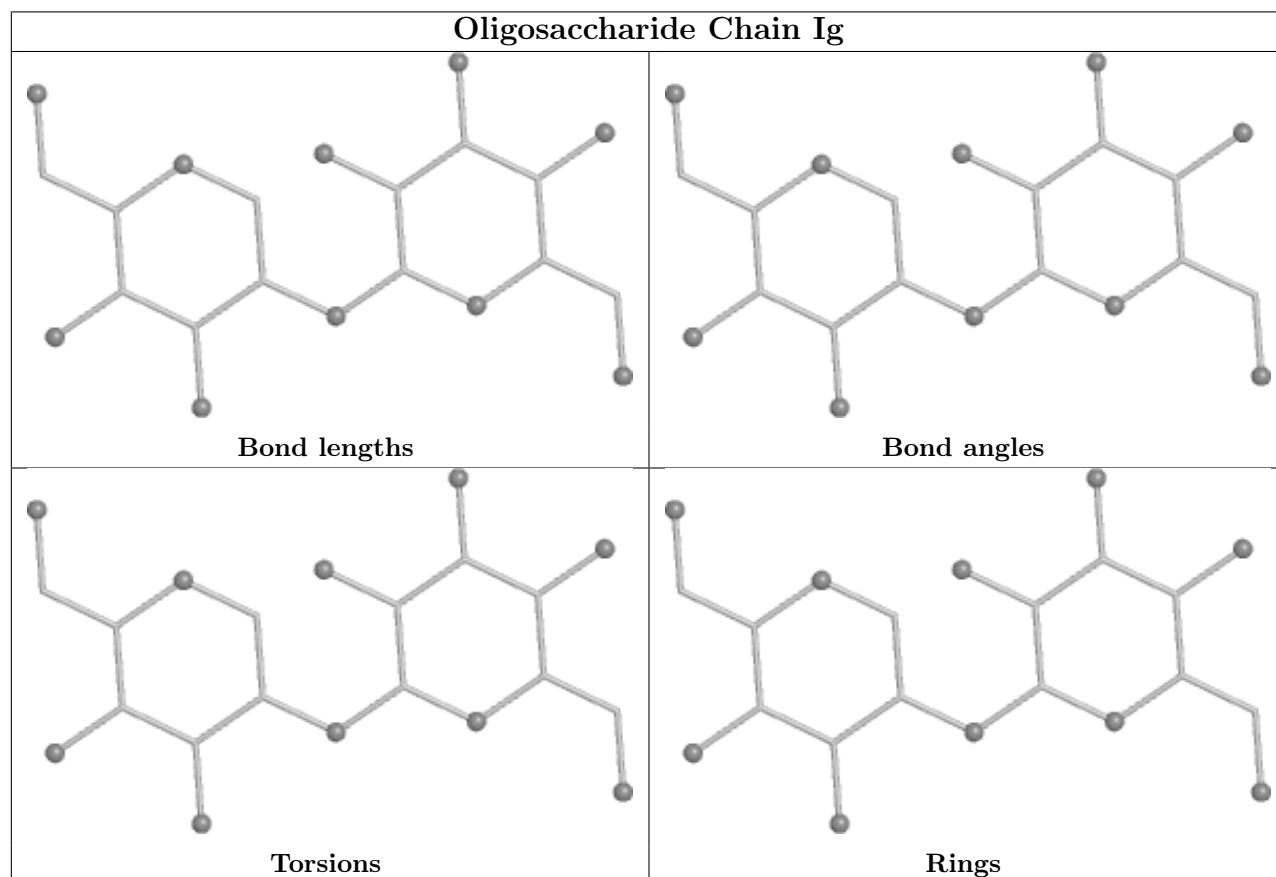
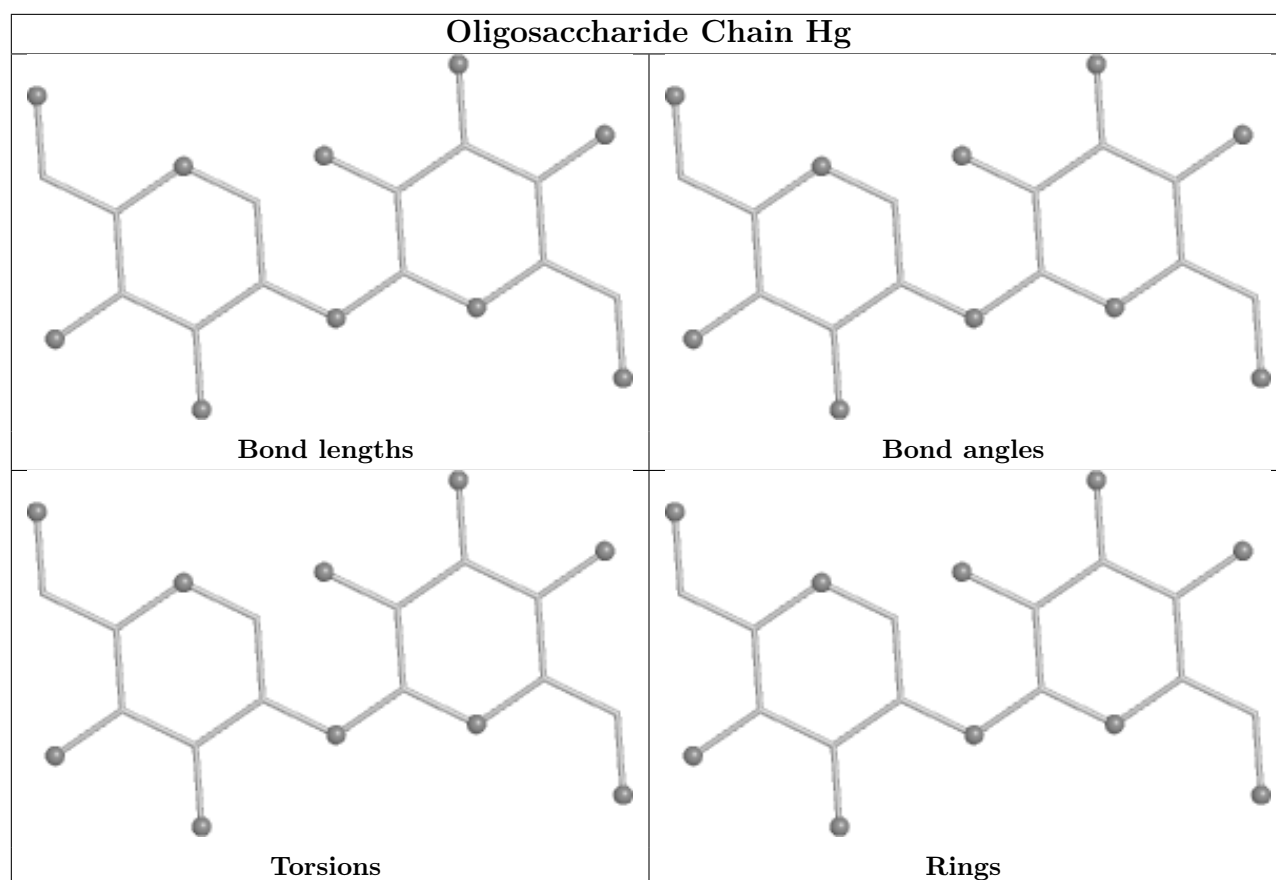




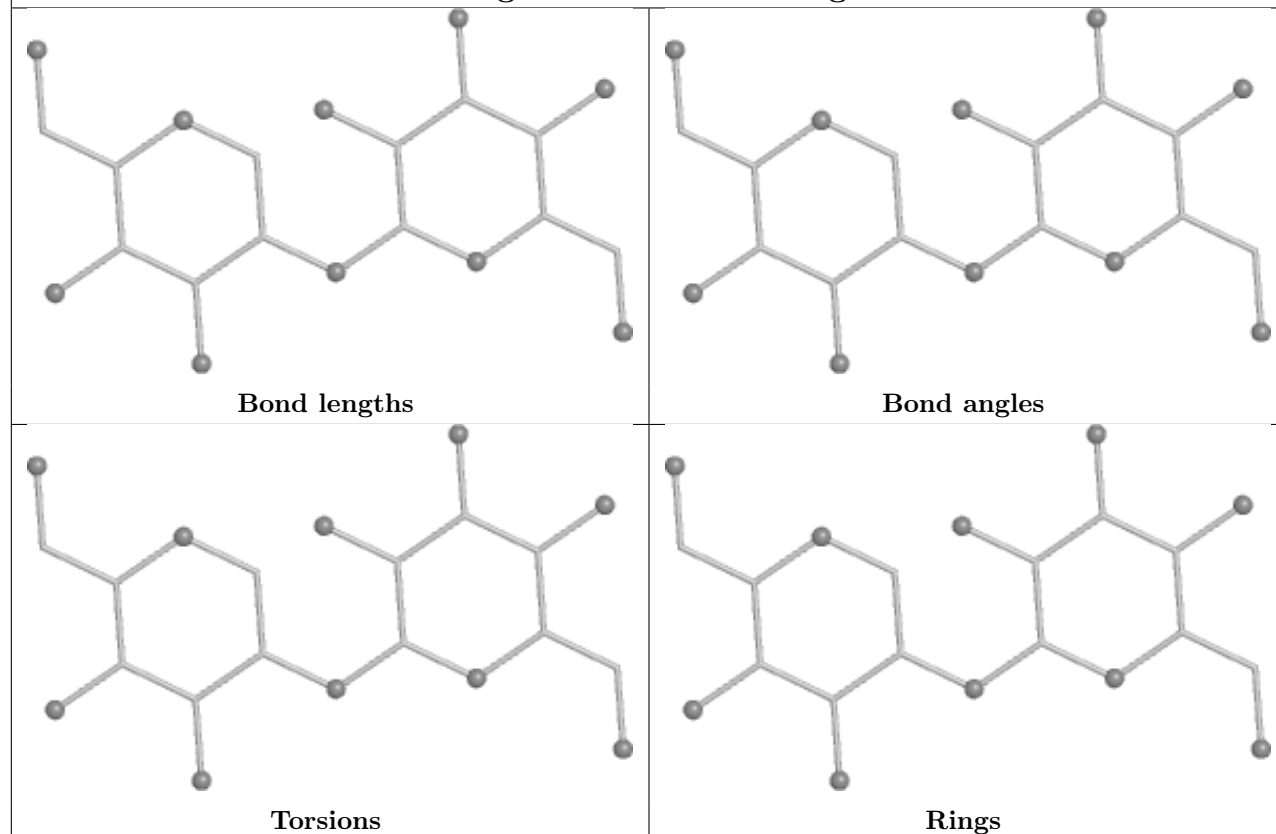




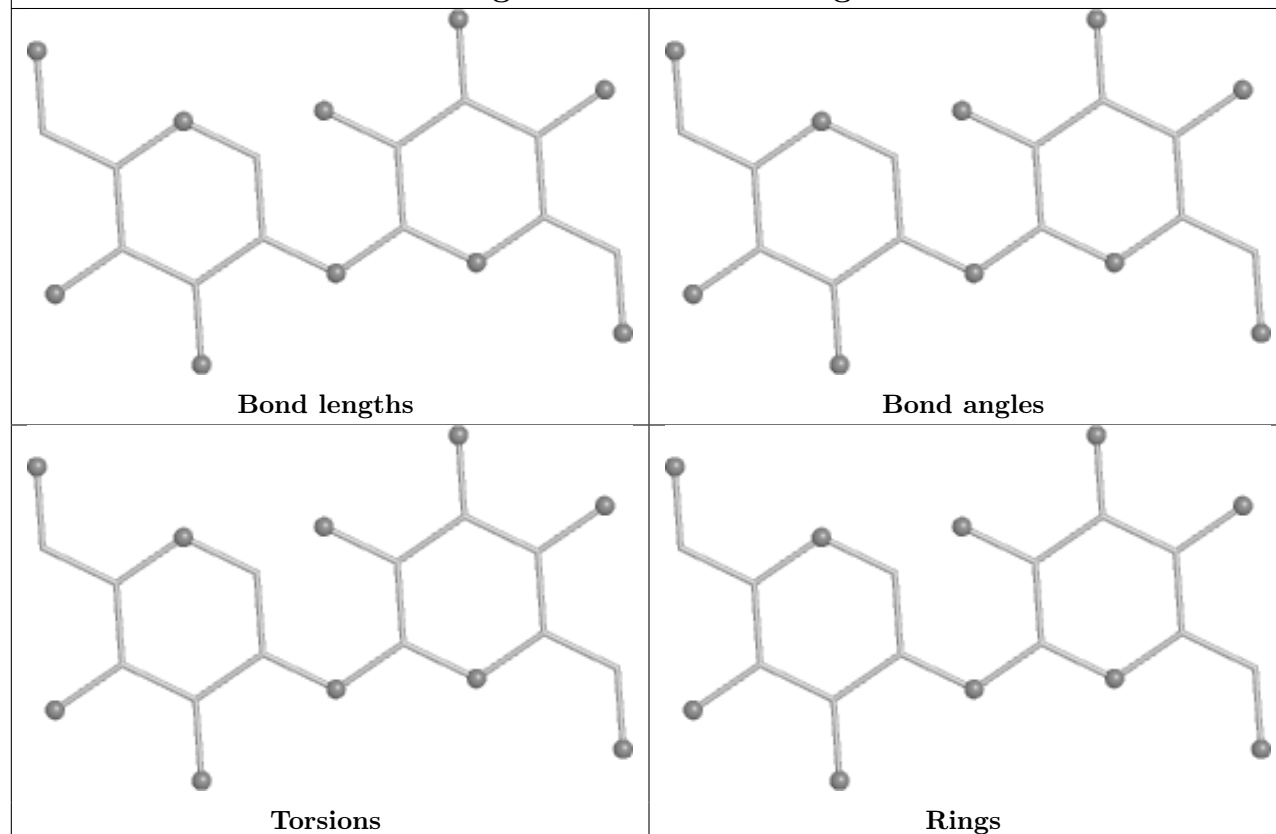


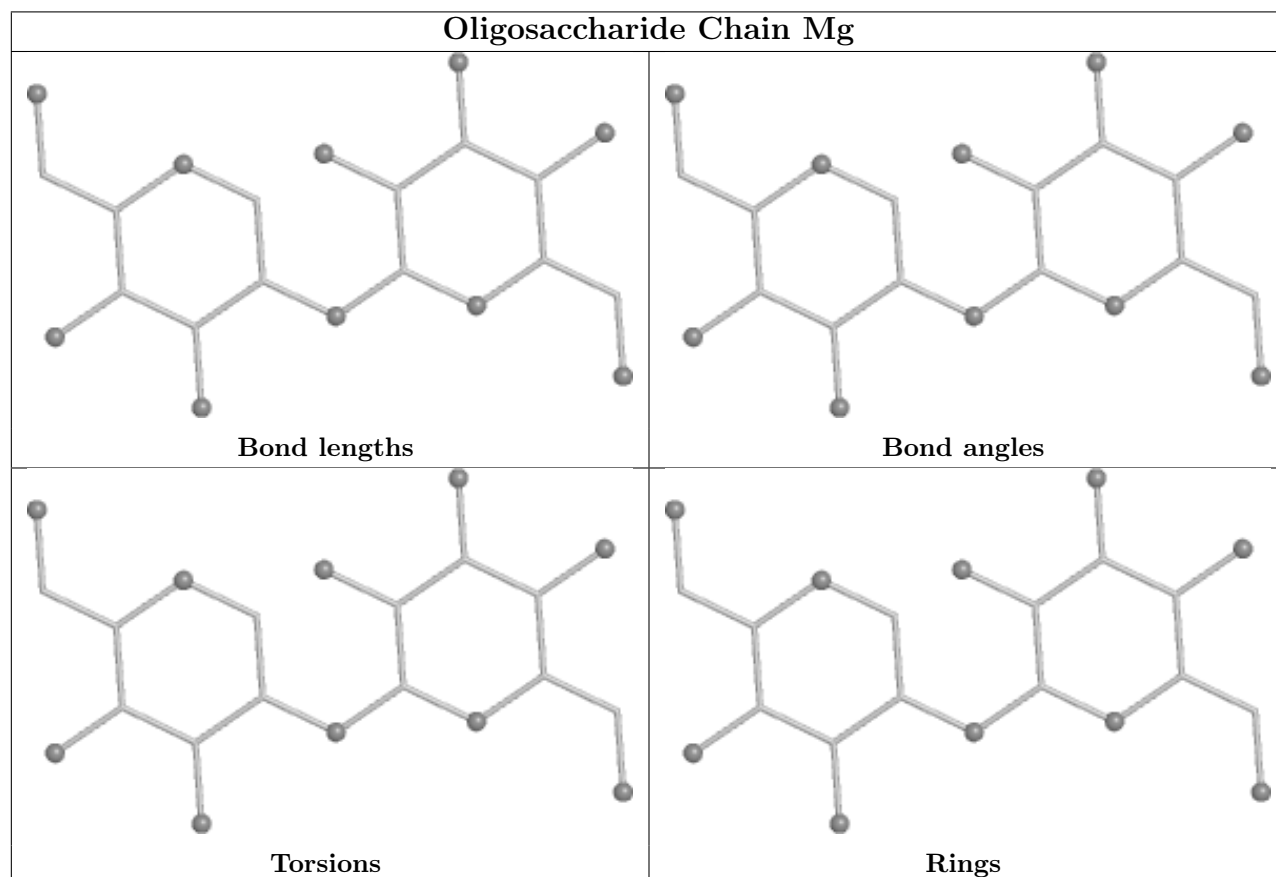
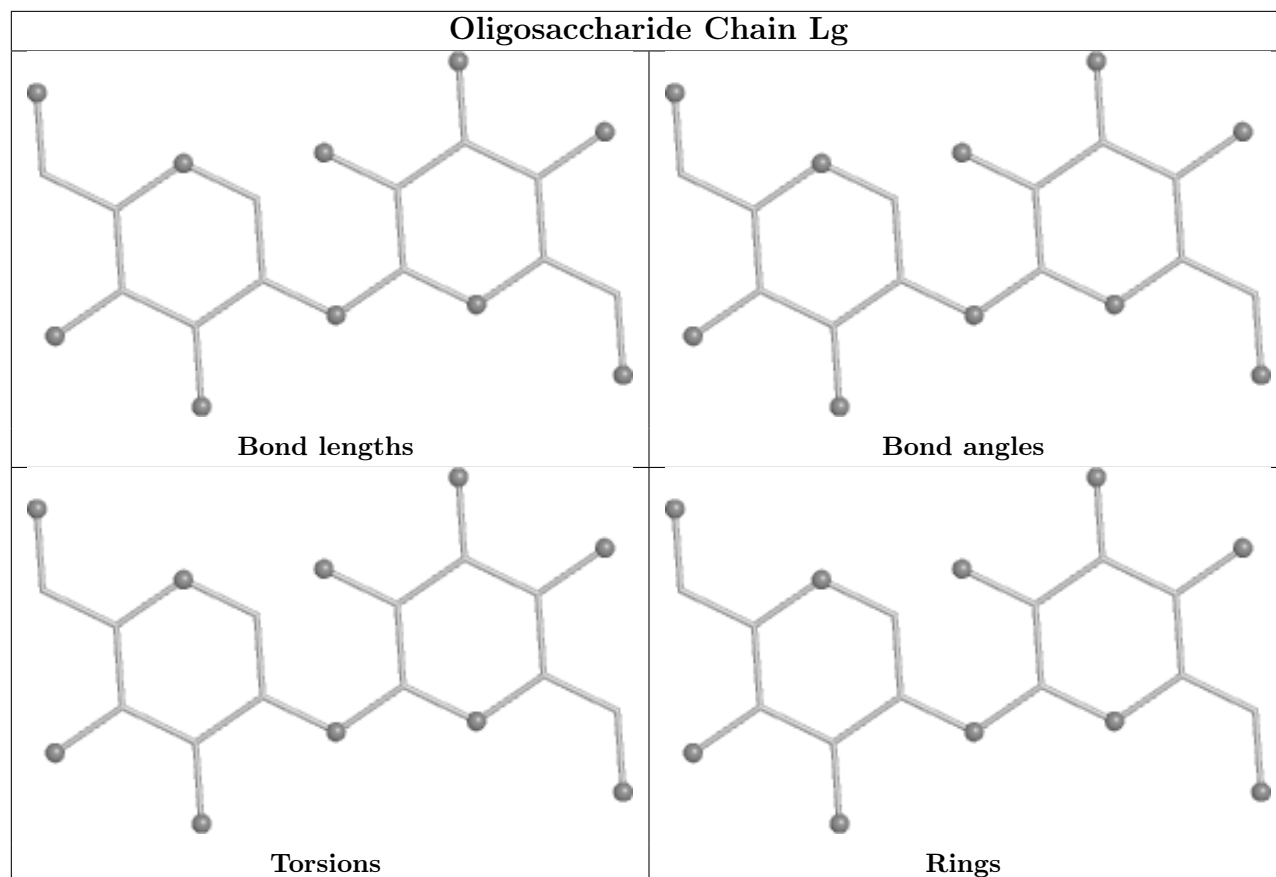


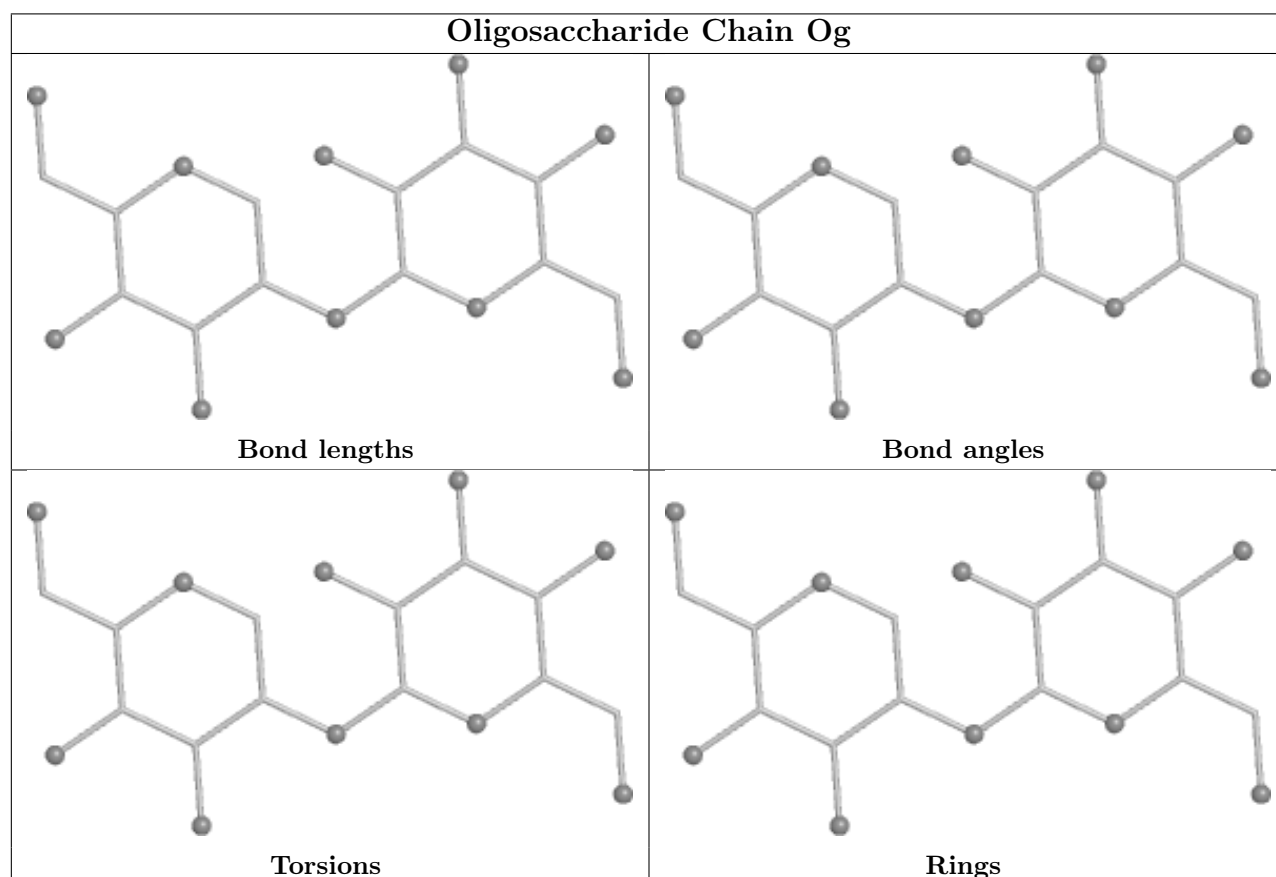
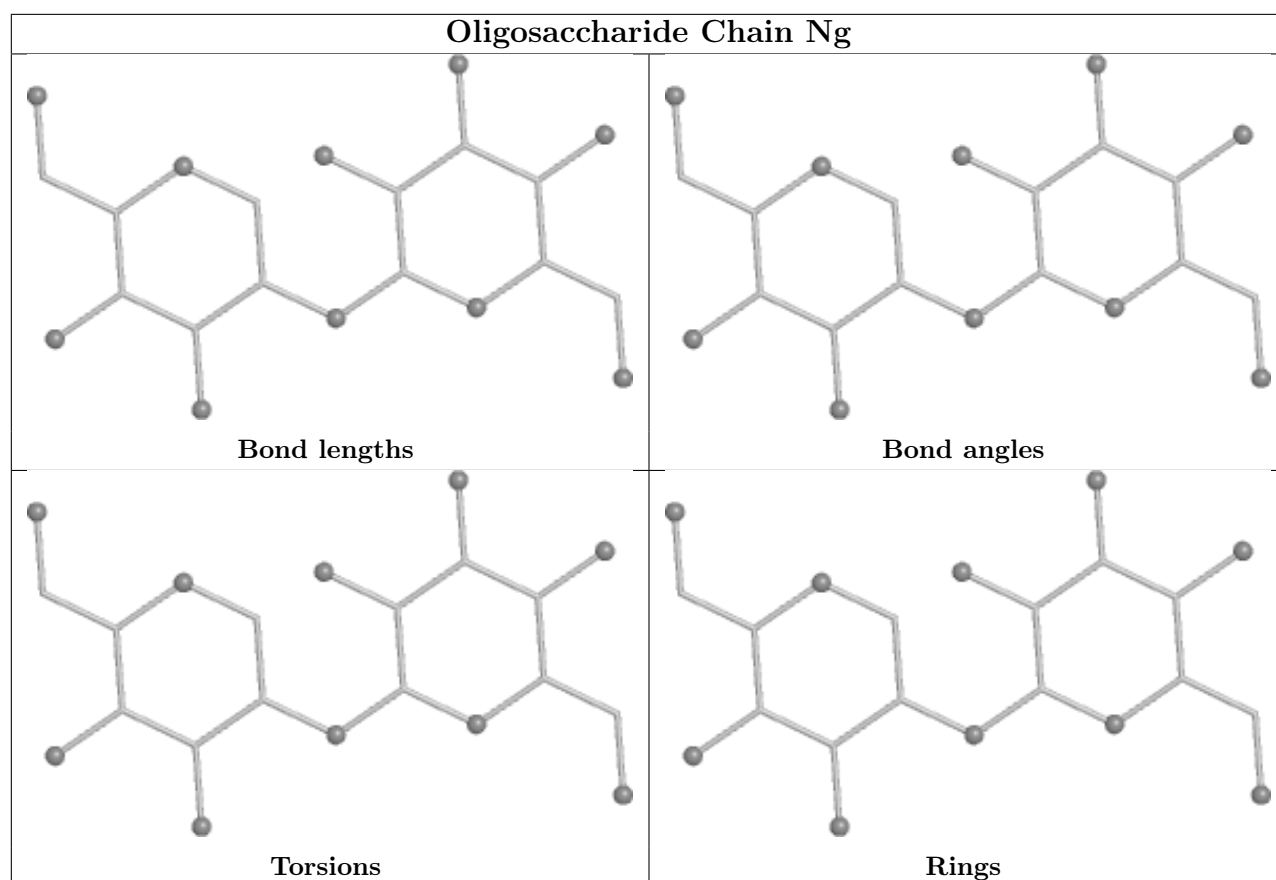
Oligosaccharide Chain Jg

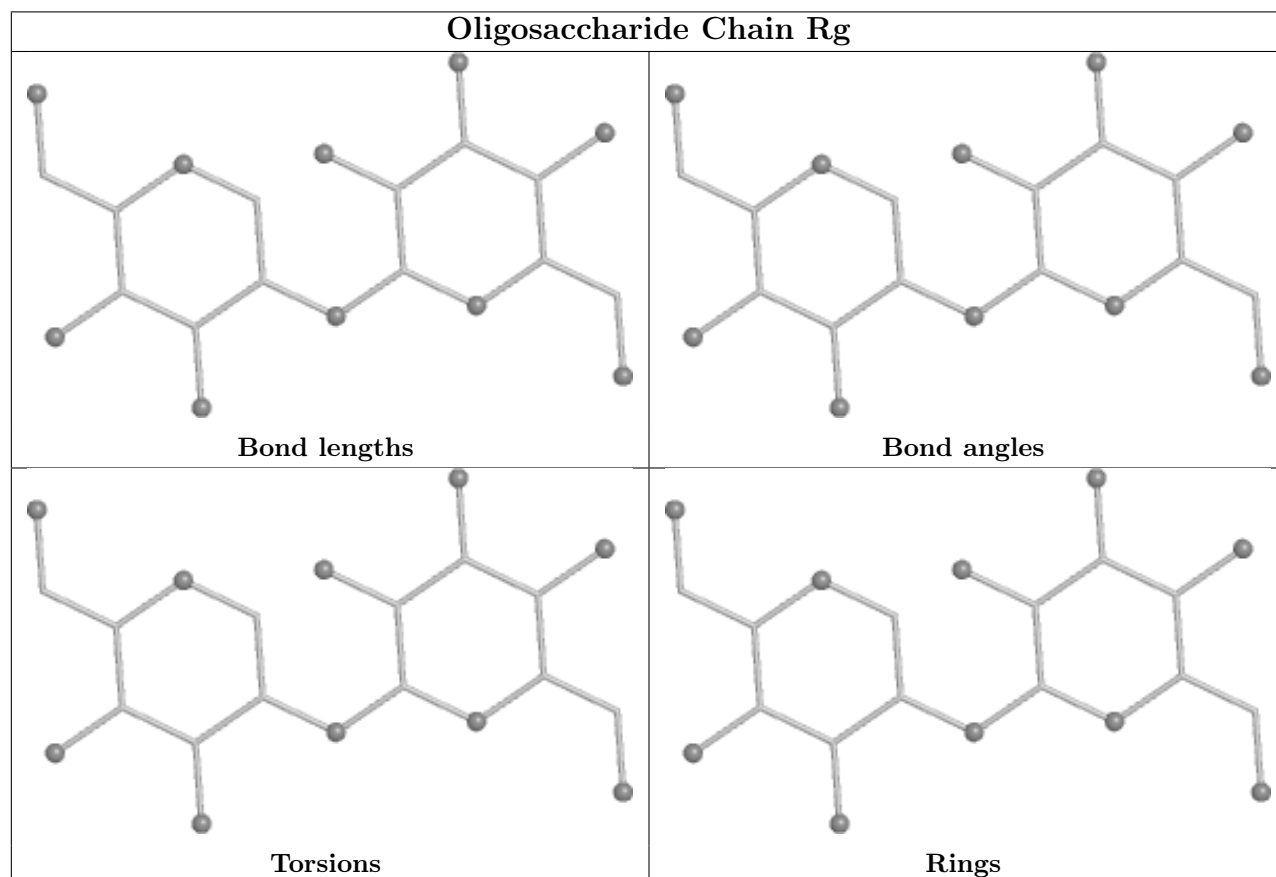
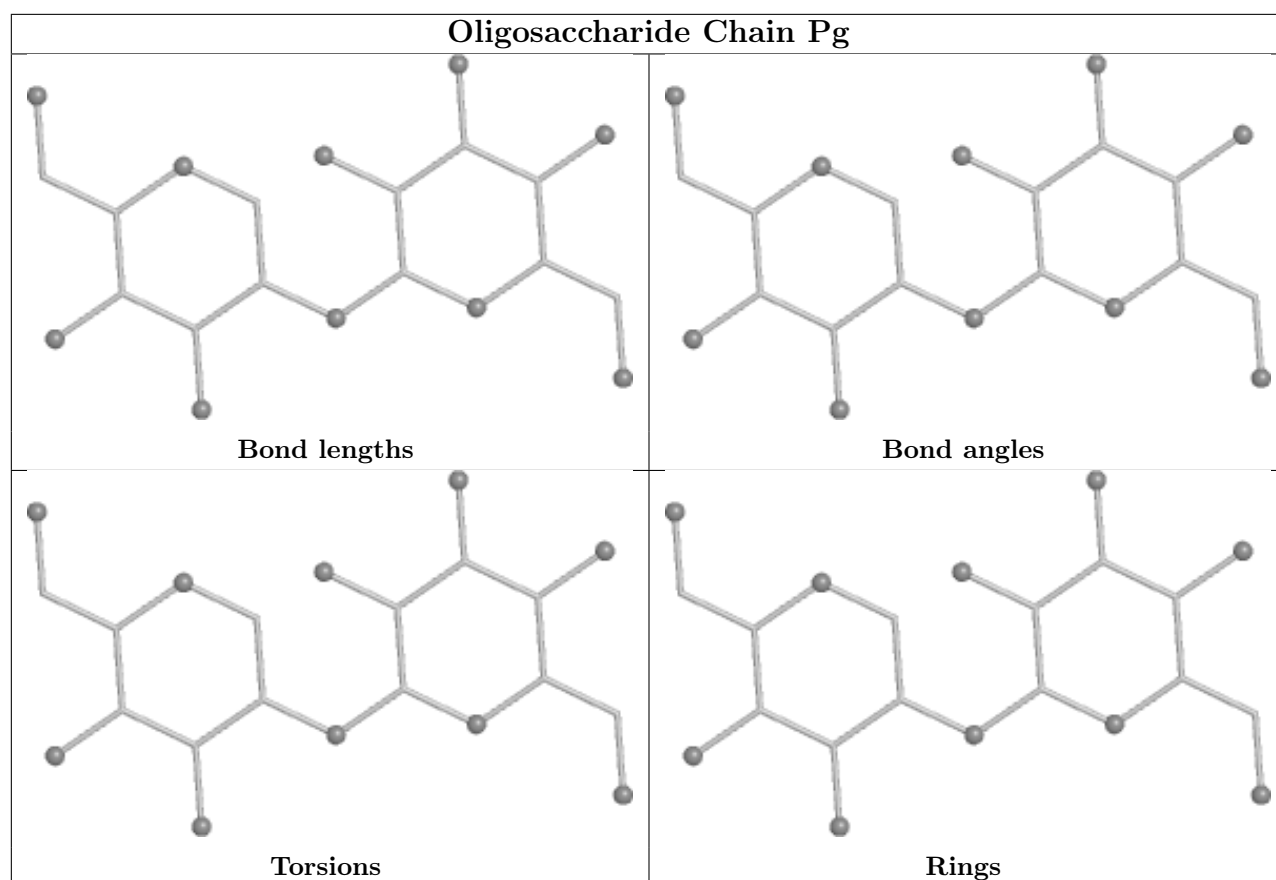


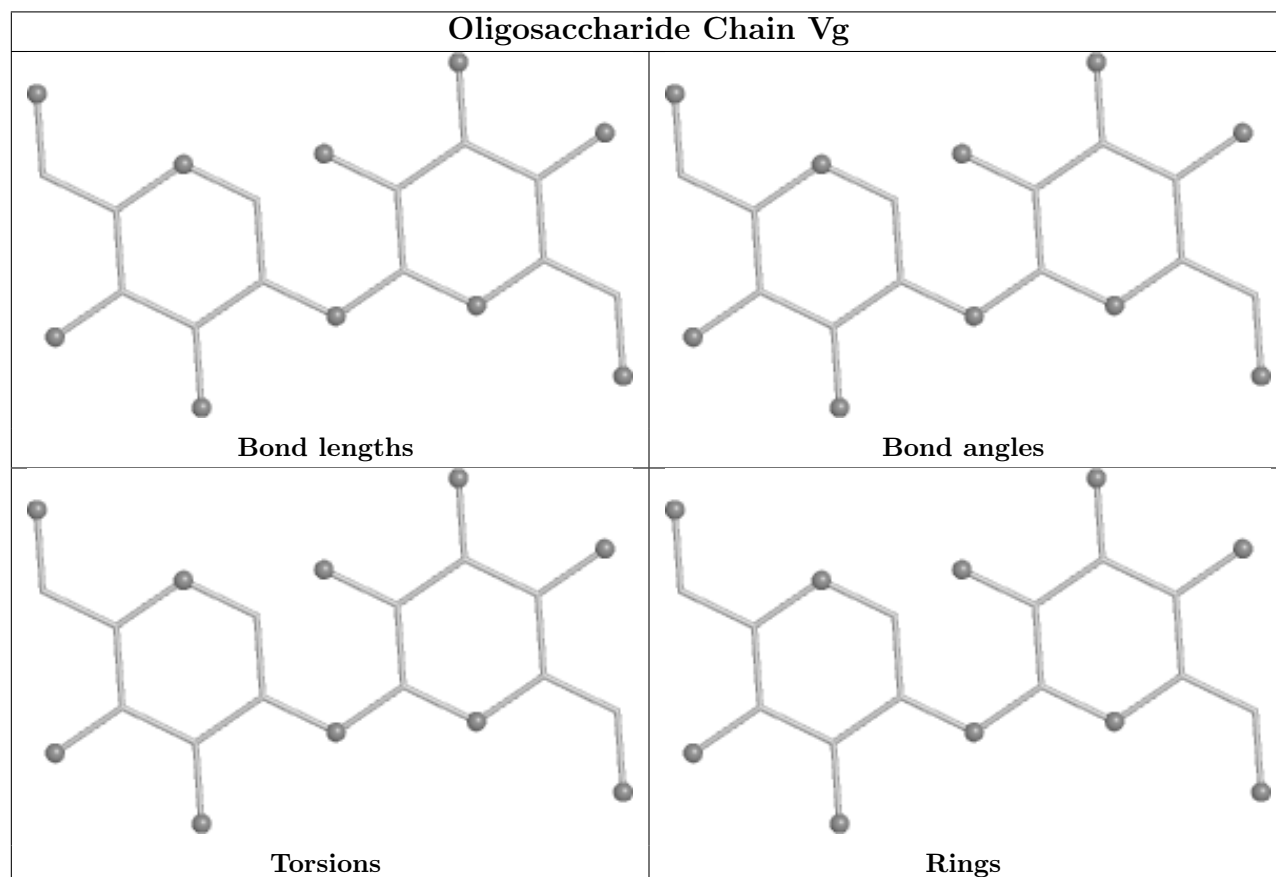
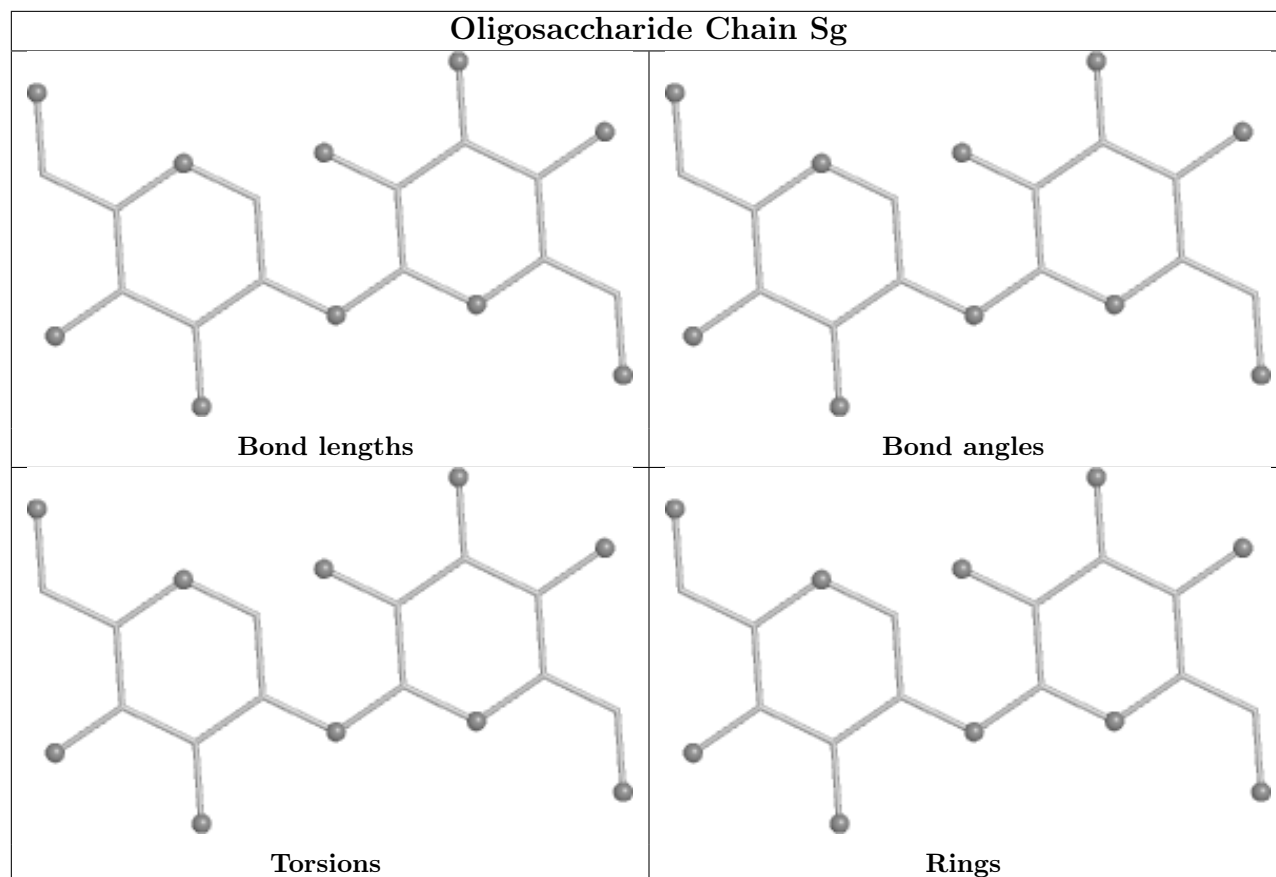
Oligosaccharide Chain Kg

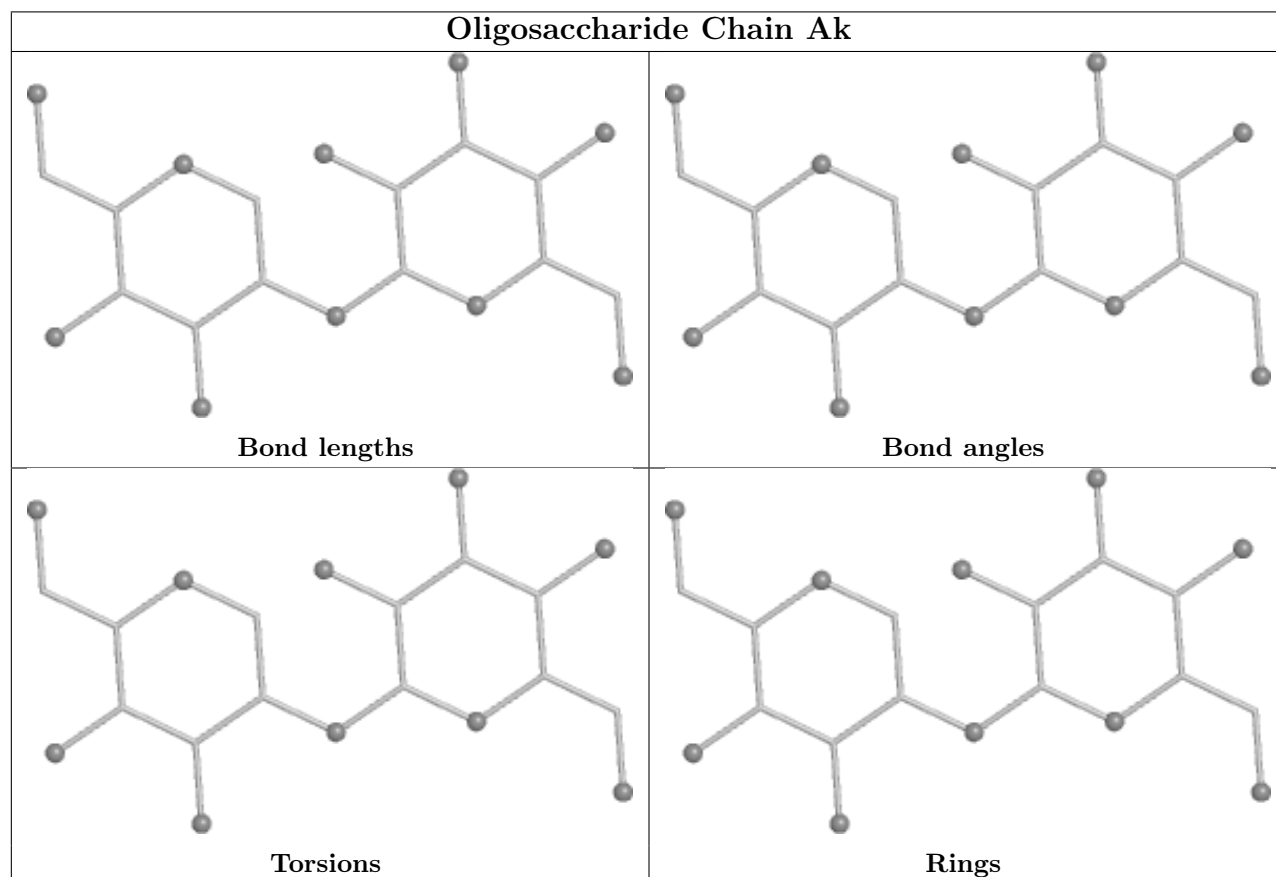
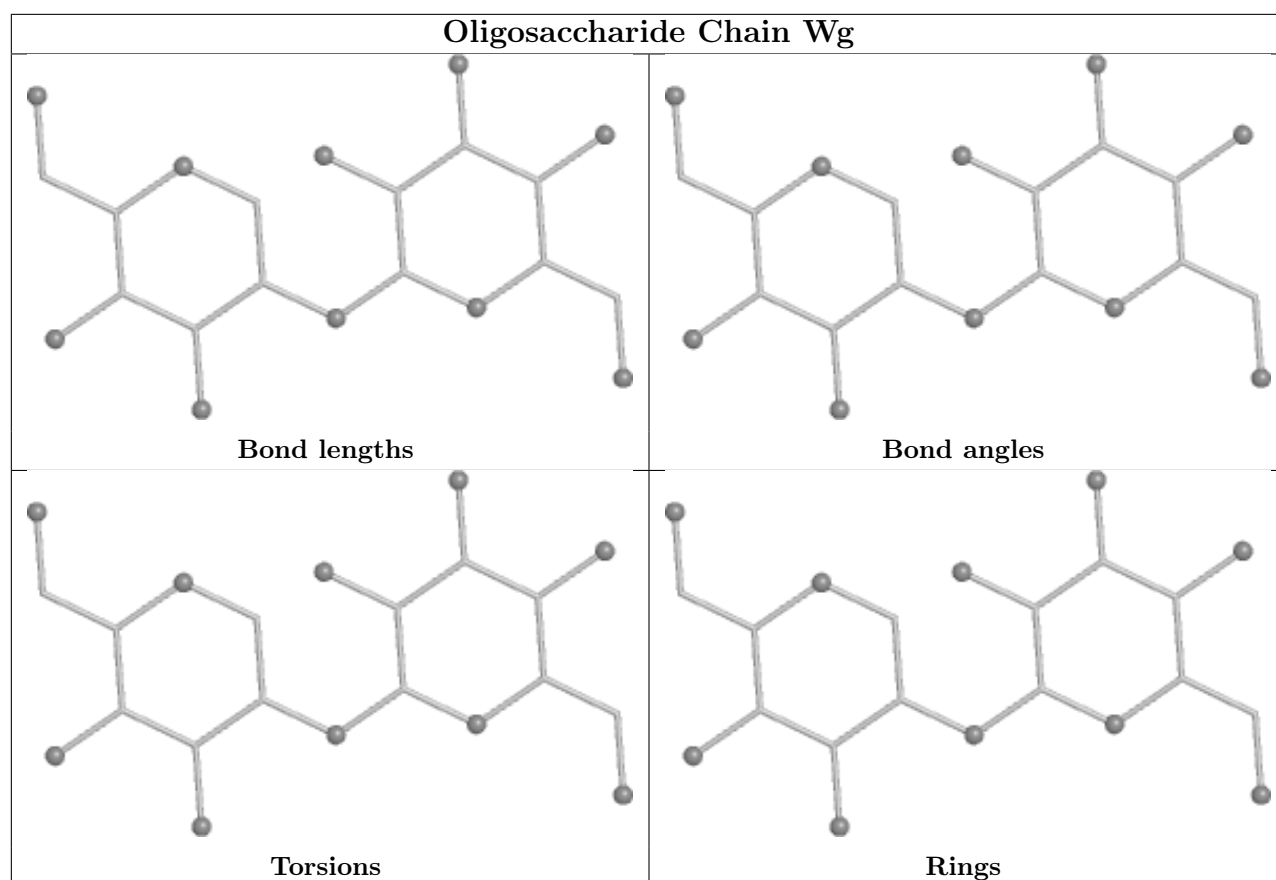


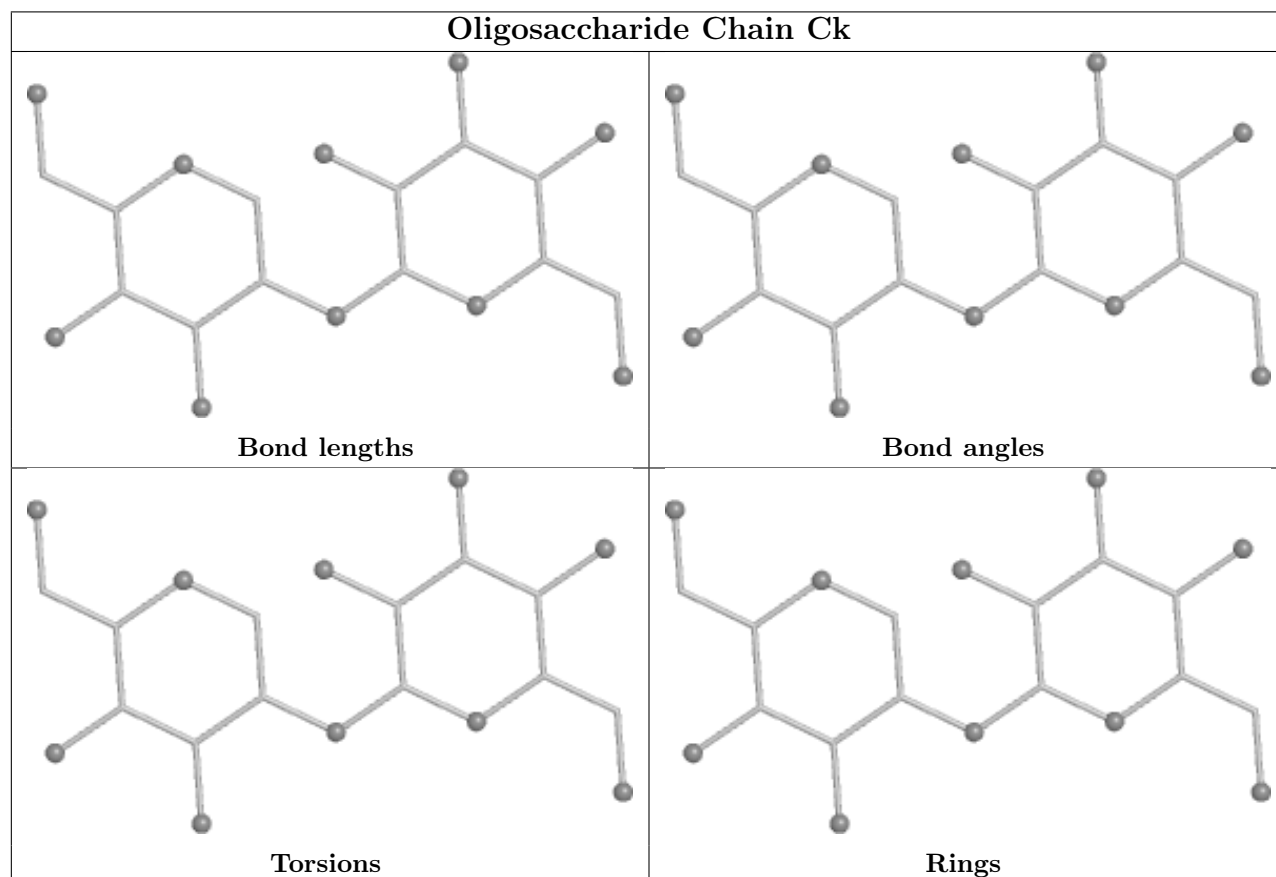
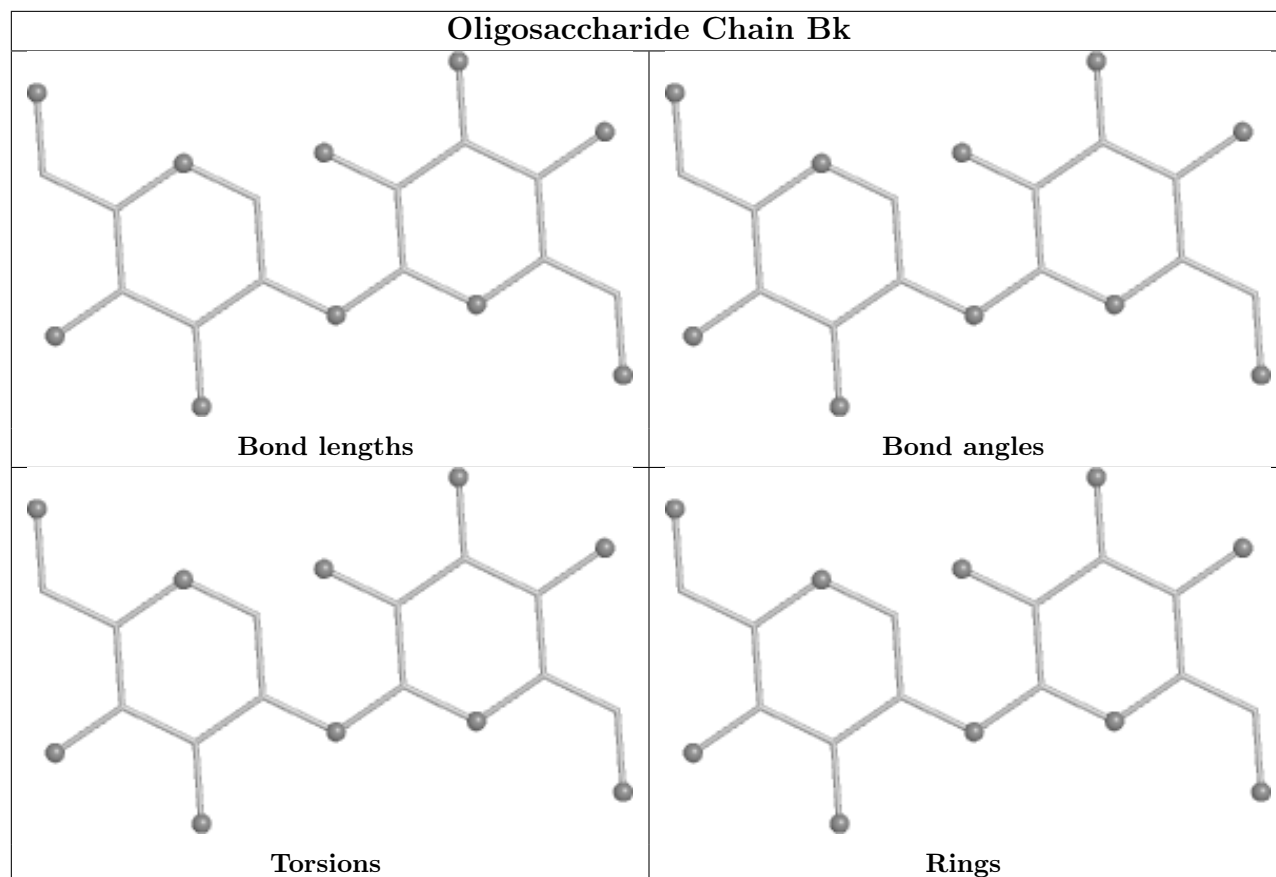




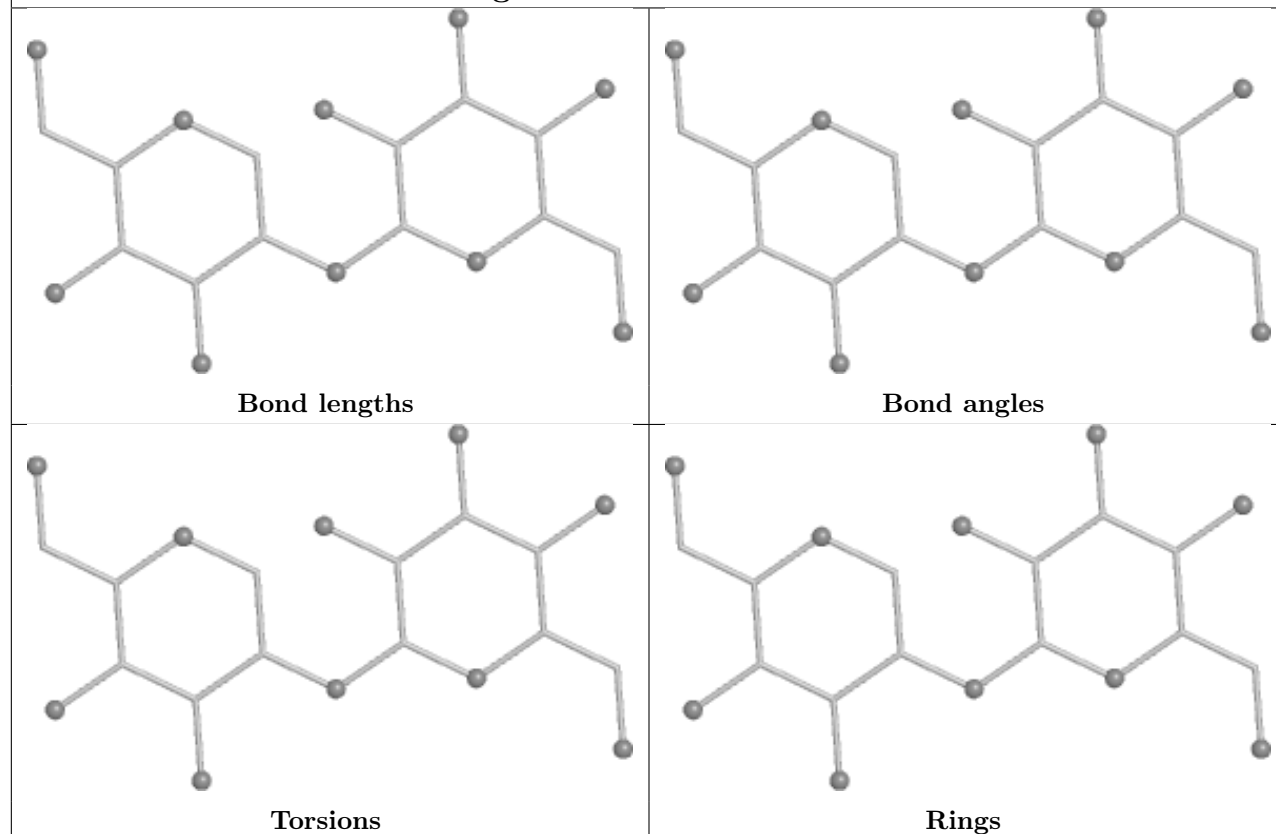




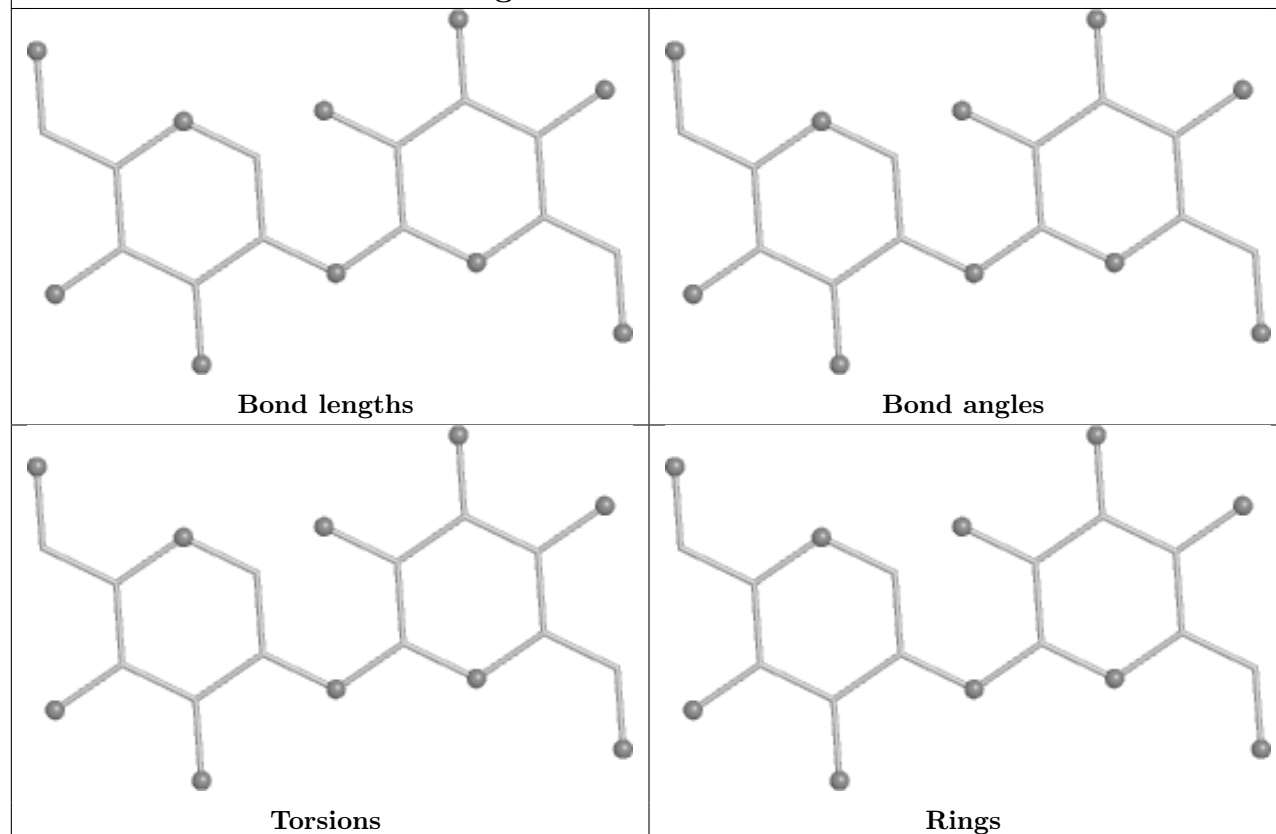




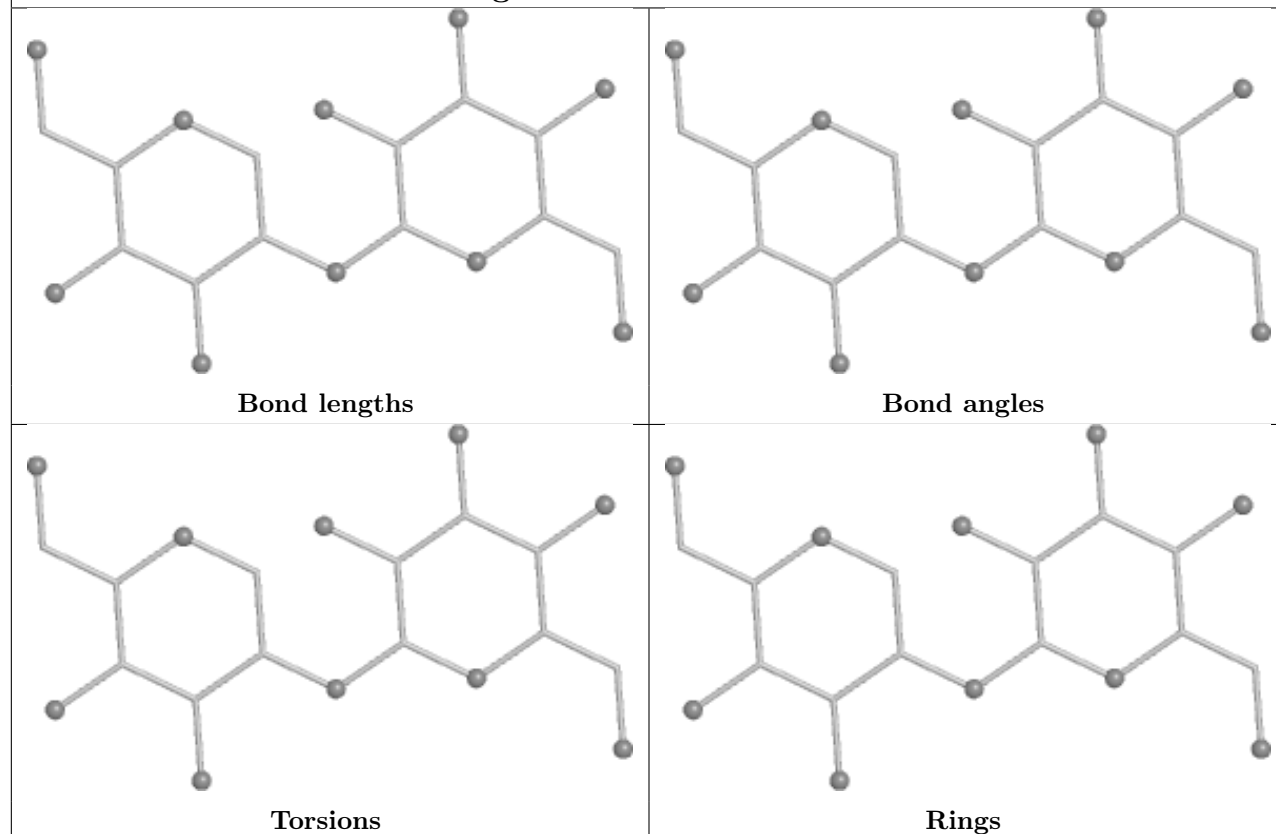
Oligosaccharide Chain Dk



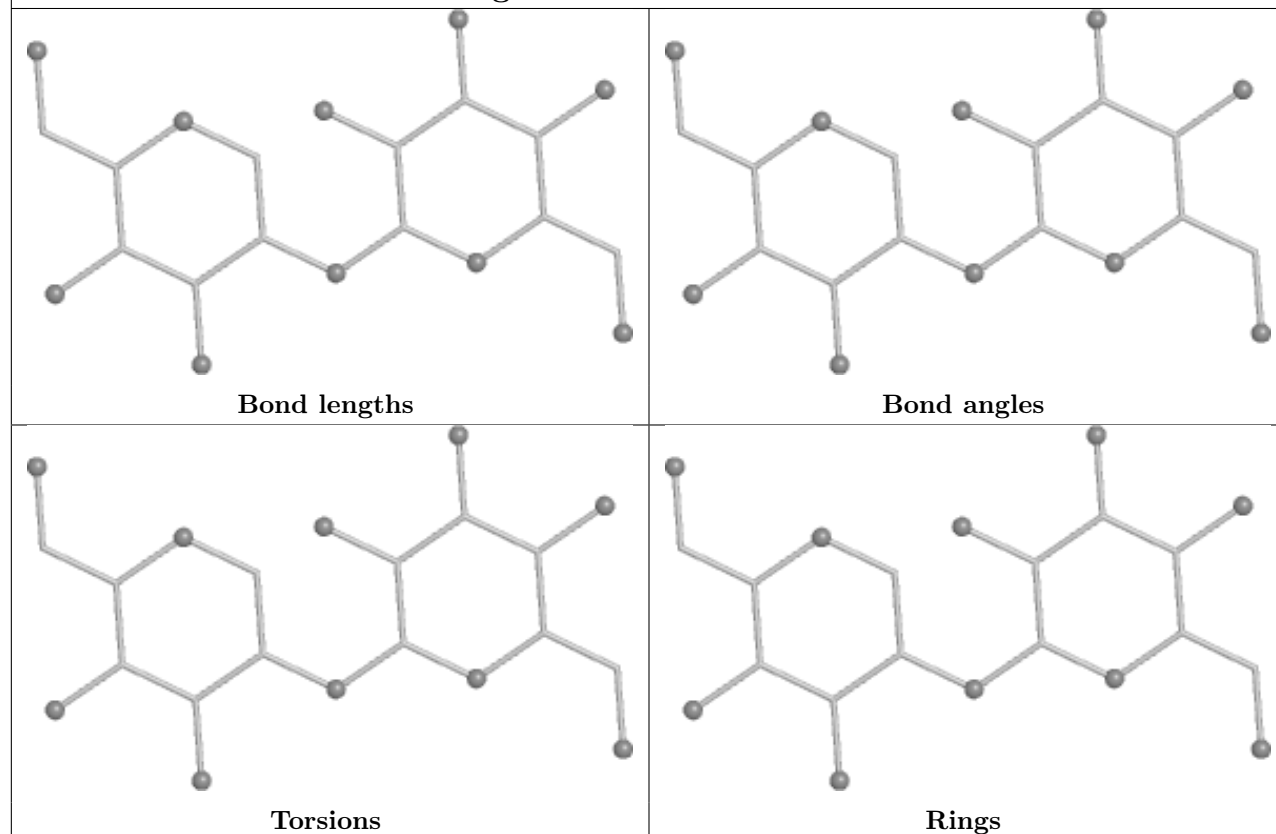
Oligosaccharide Chain Fk

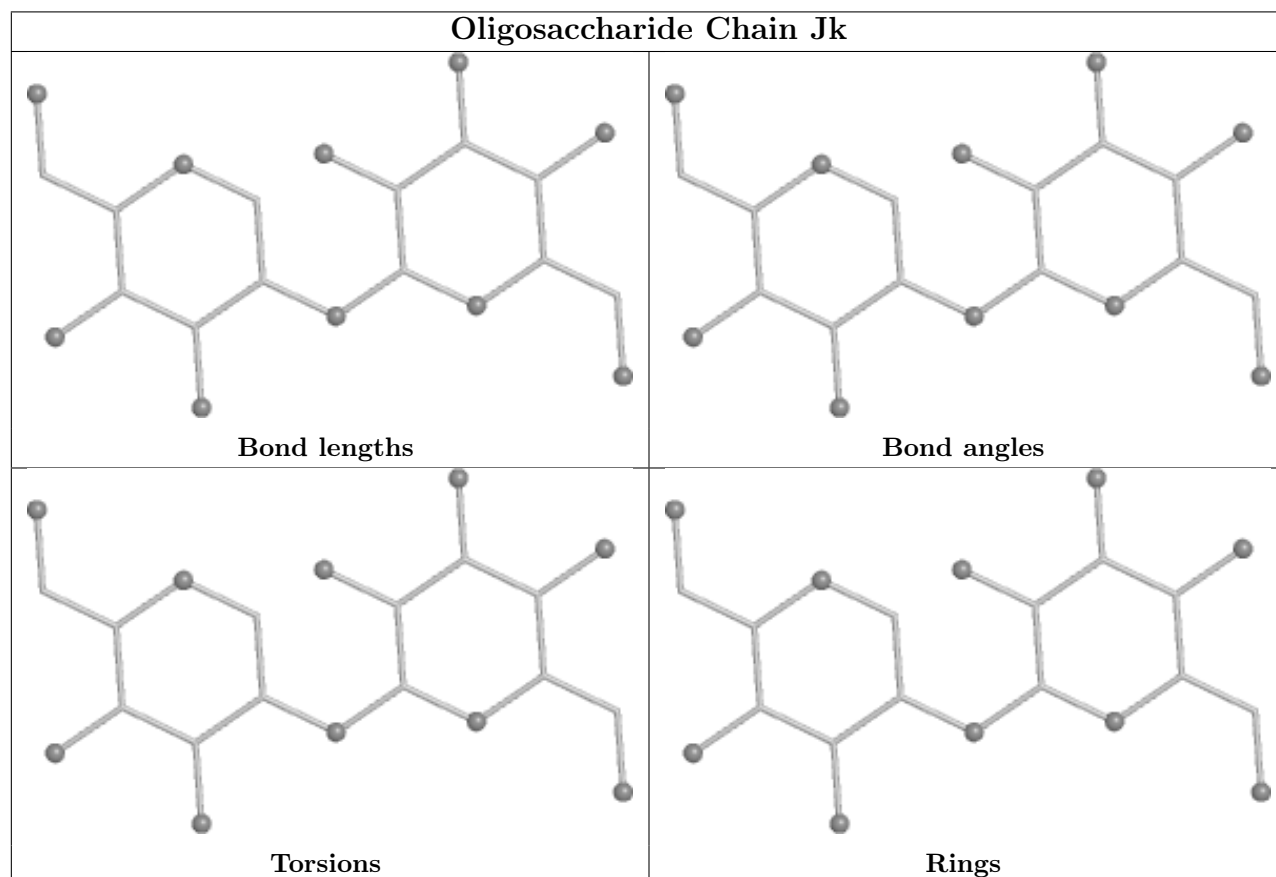
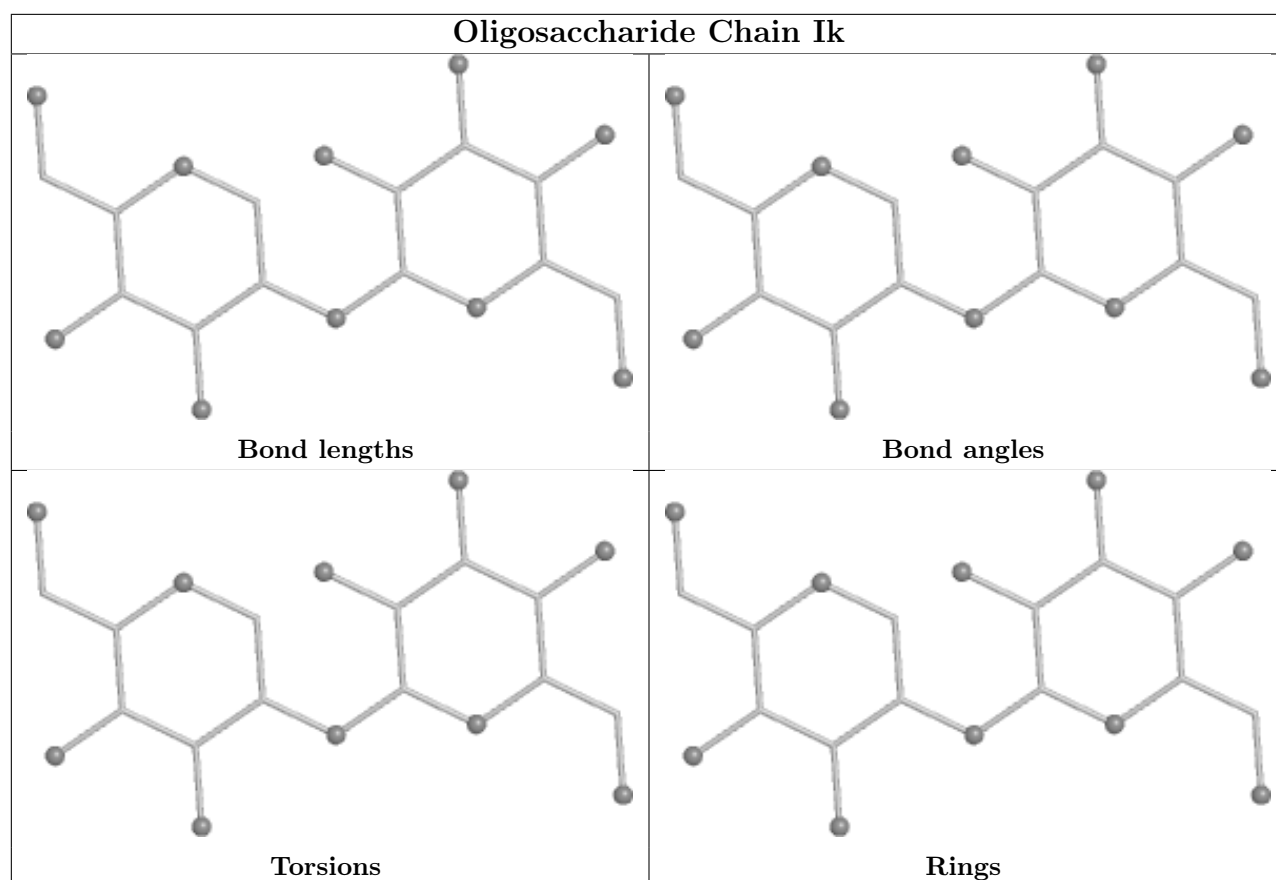


Oligosaccharide Chain Gk

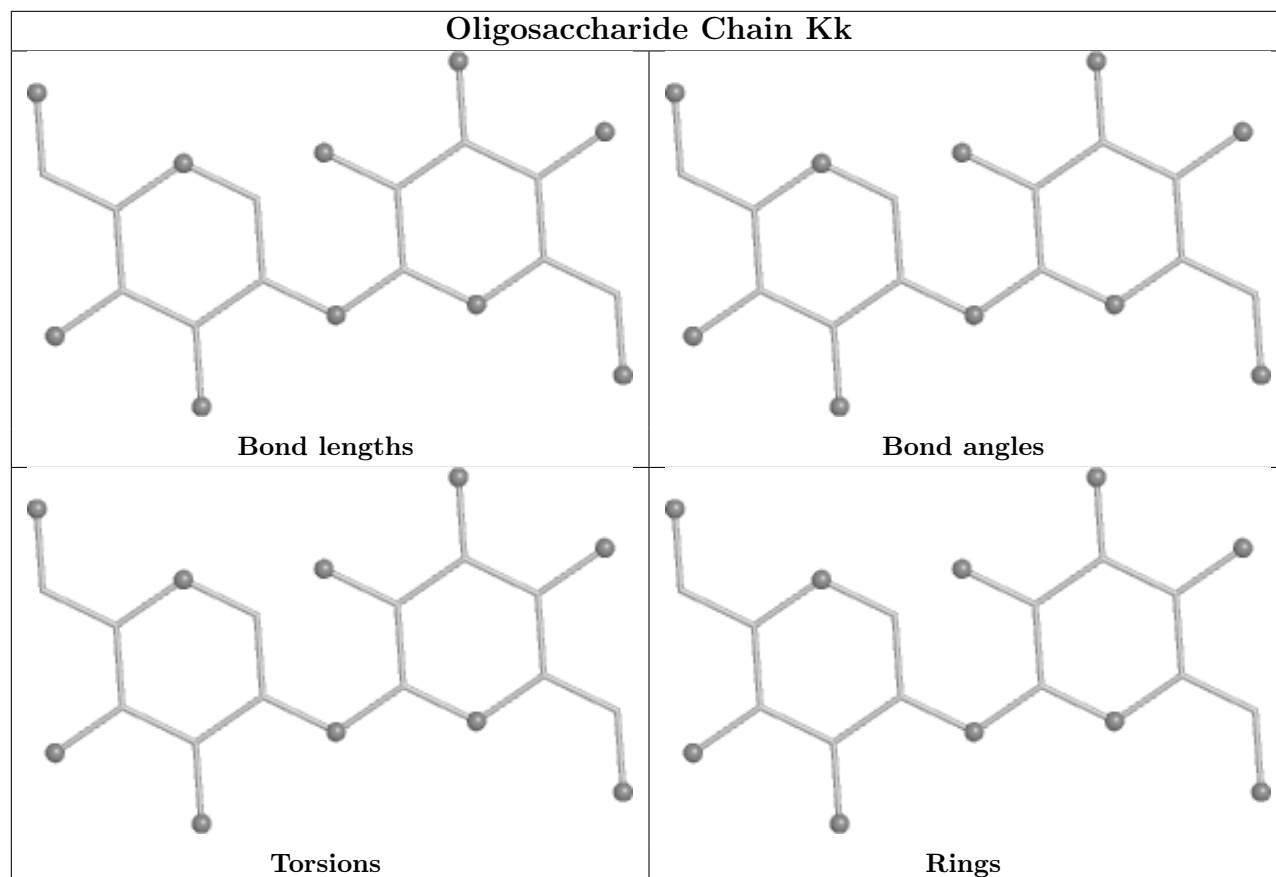


Oligosaccharide Chain Hk

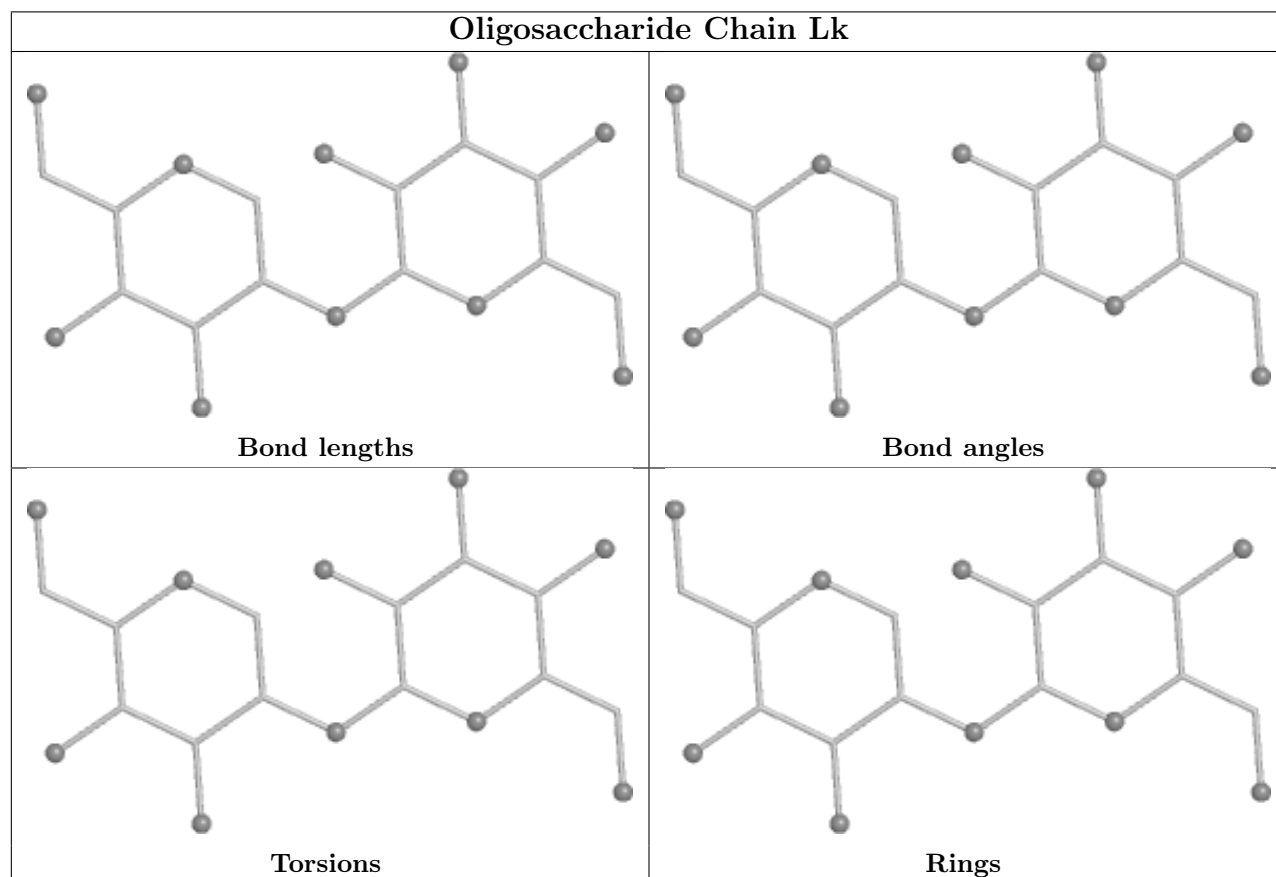




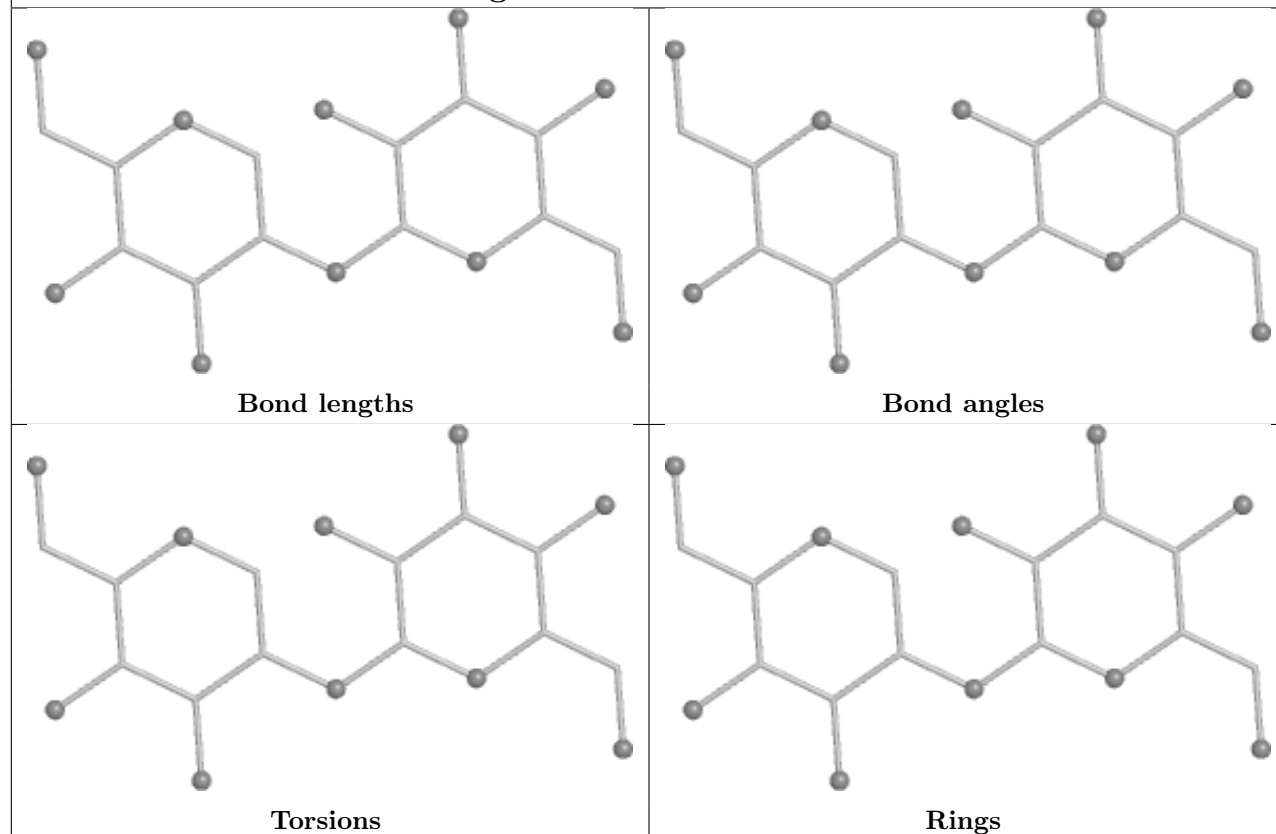
Oligosaccharide Chain Kk



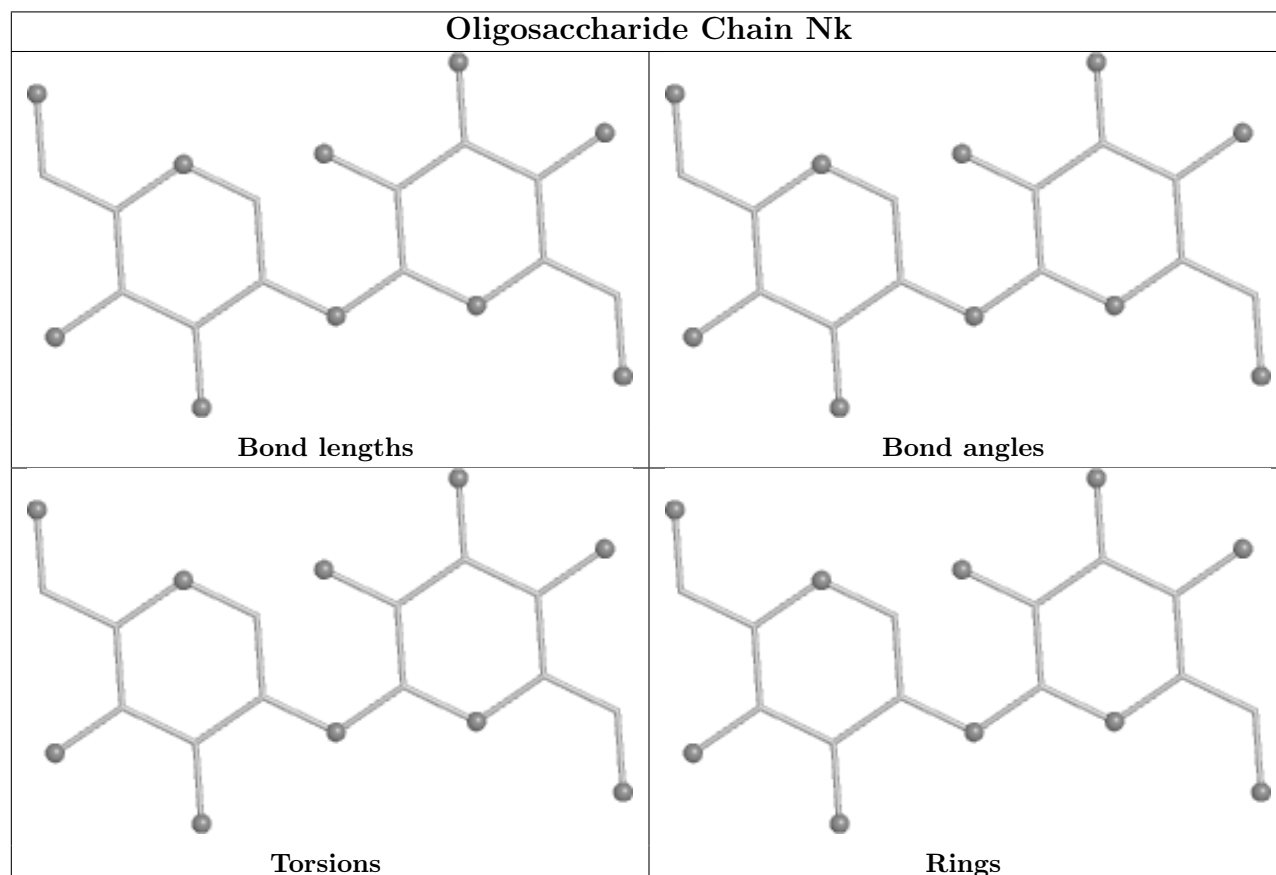
Oligosaccharide Chain Lk



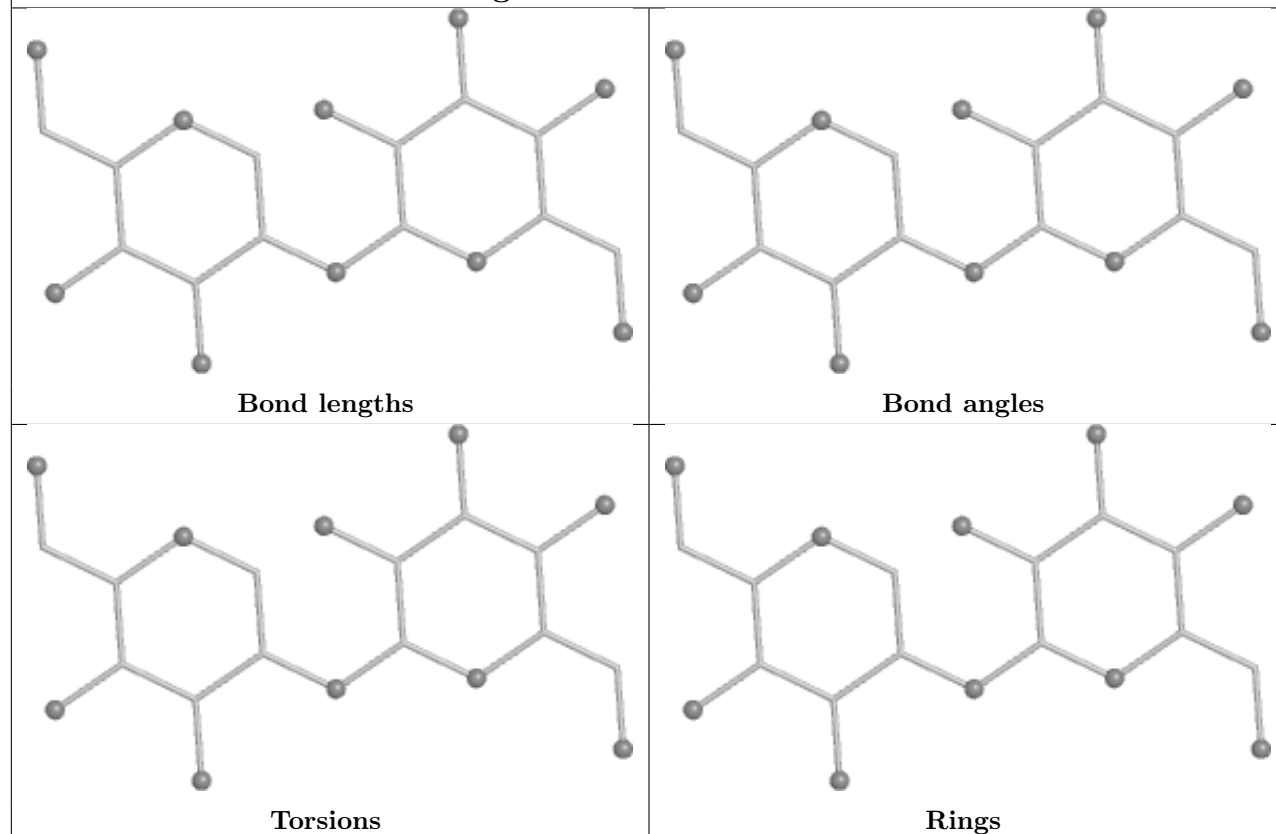
Oligosaccharide Chain Mk



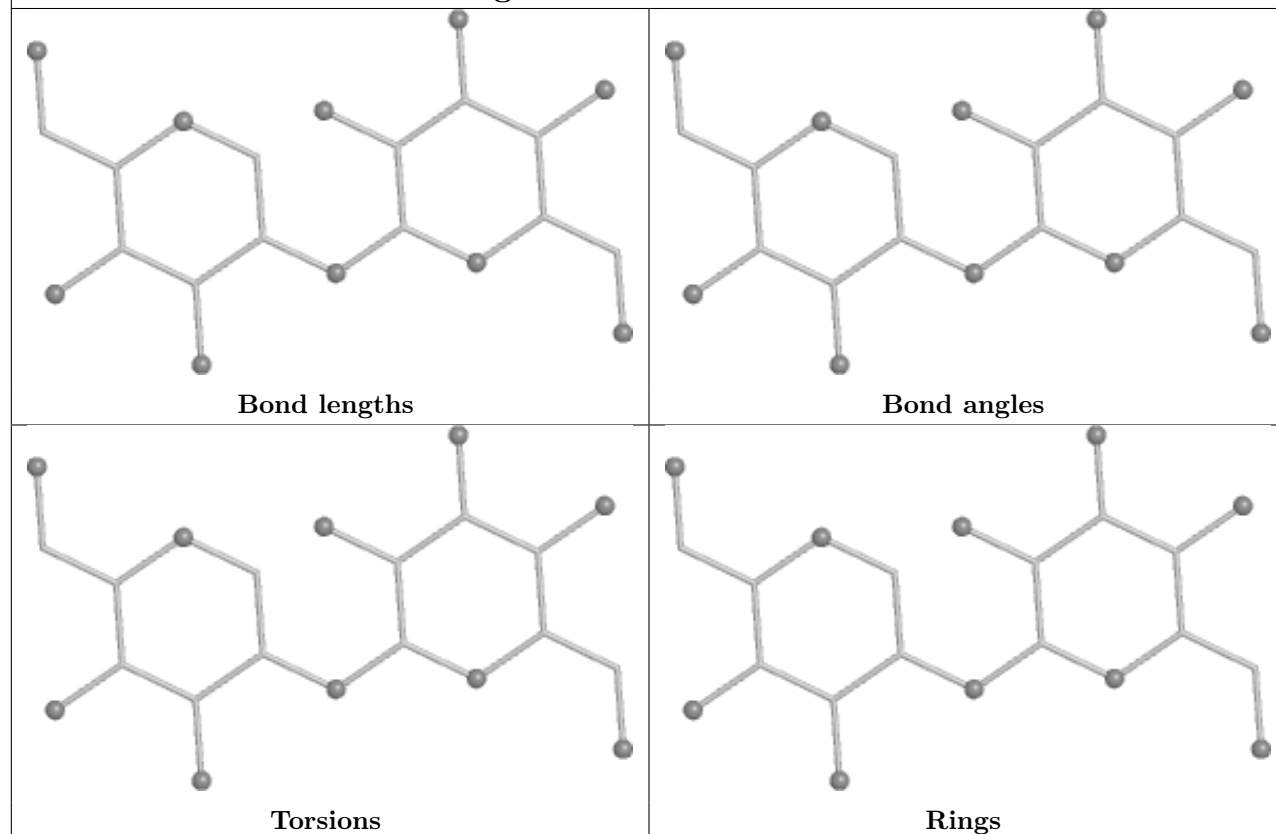
Oligosaccharide Chain Nk



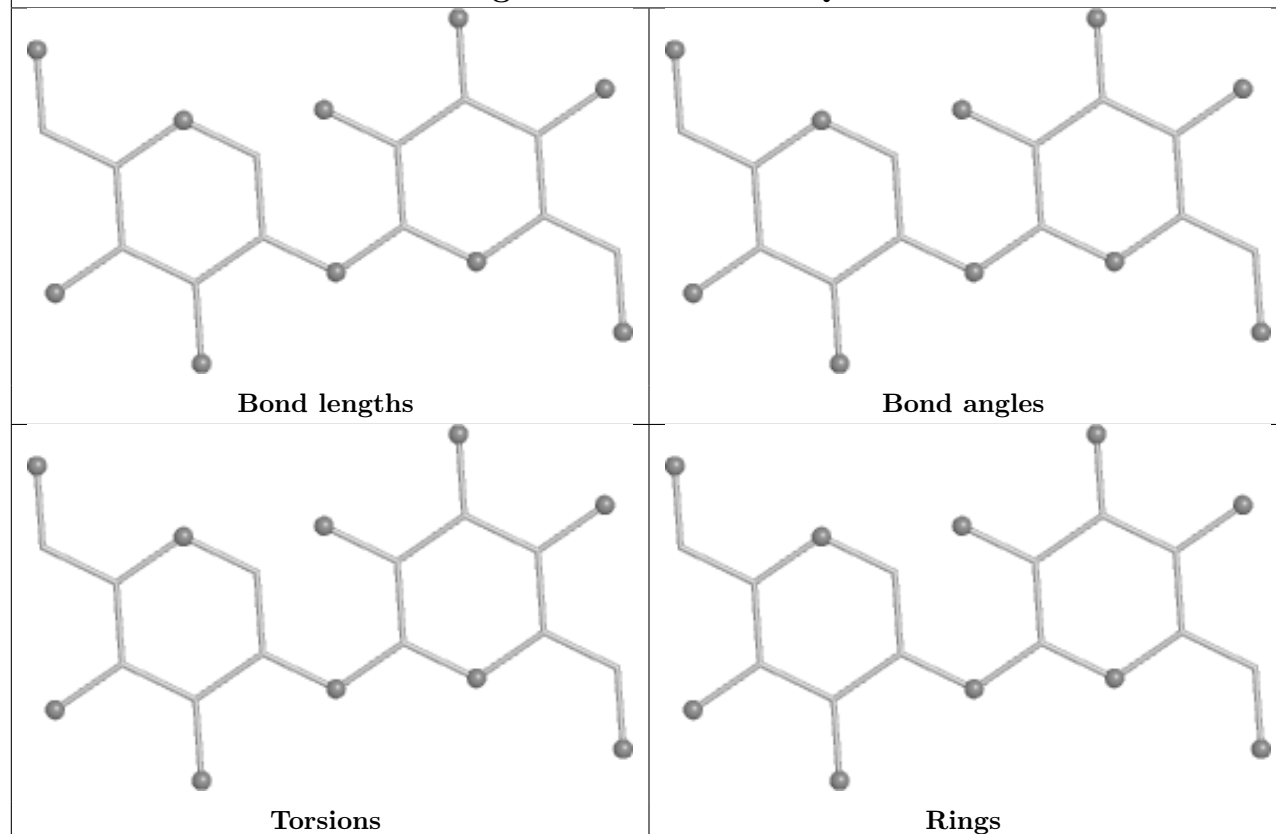
Oligosaccharide Chain Ok



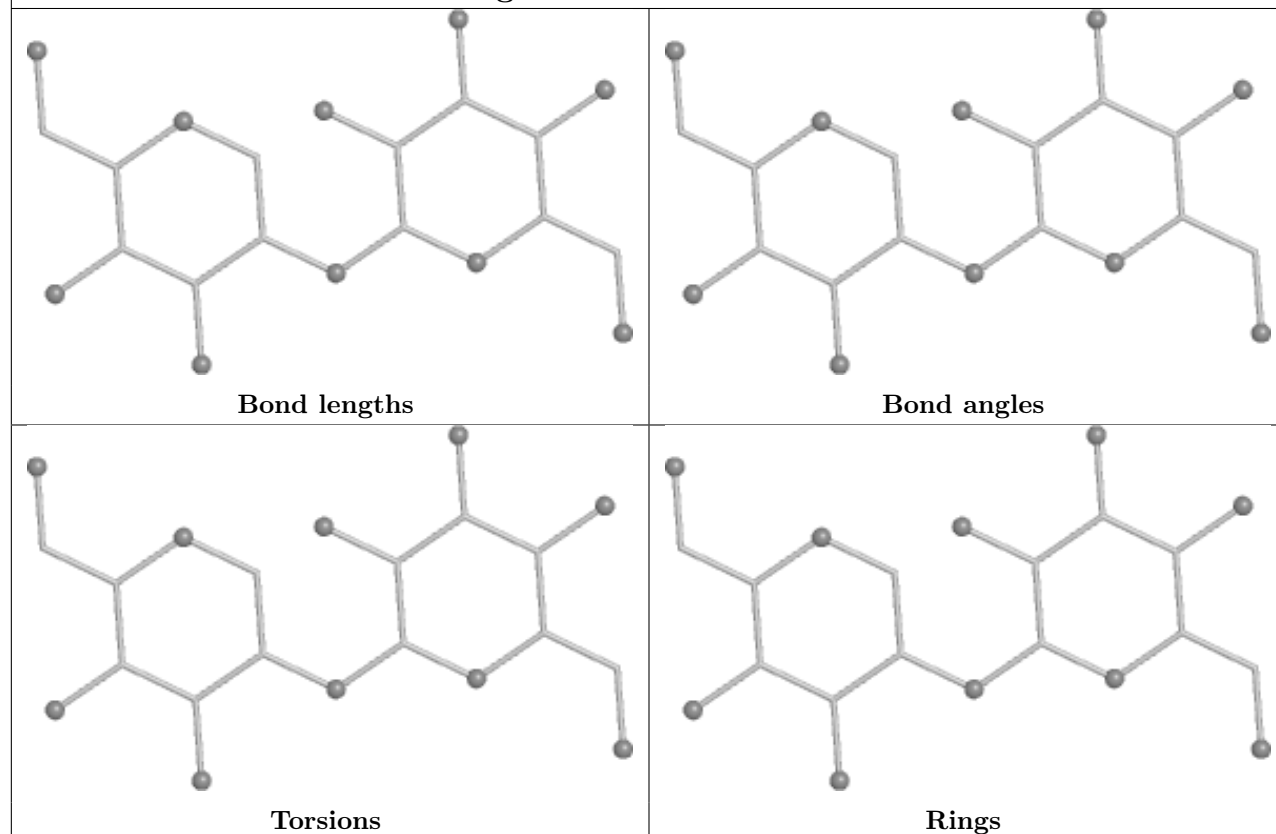
Oligosaccharide Chain Pk

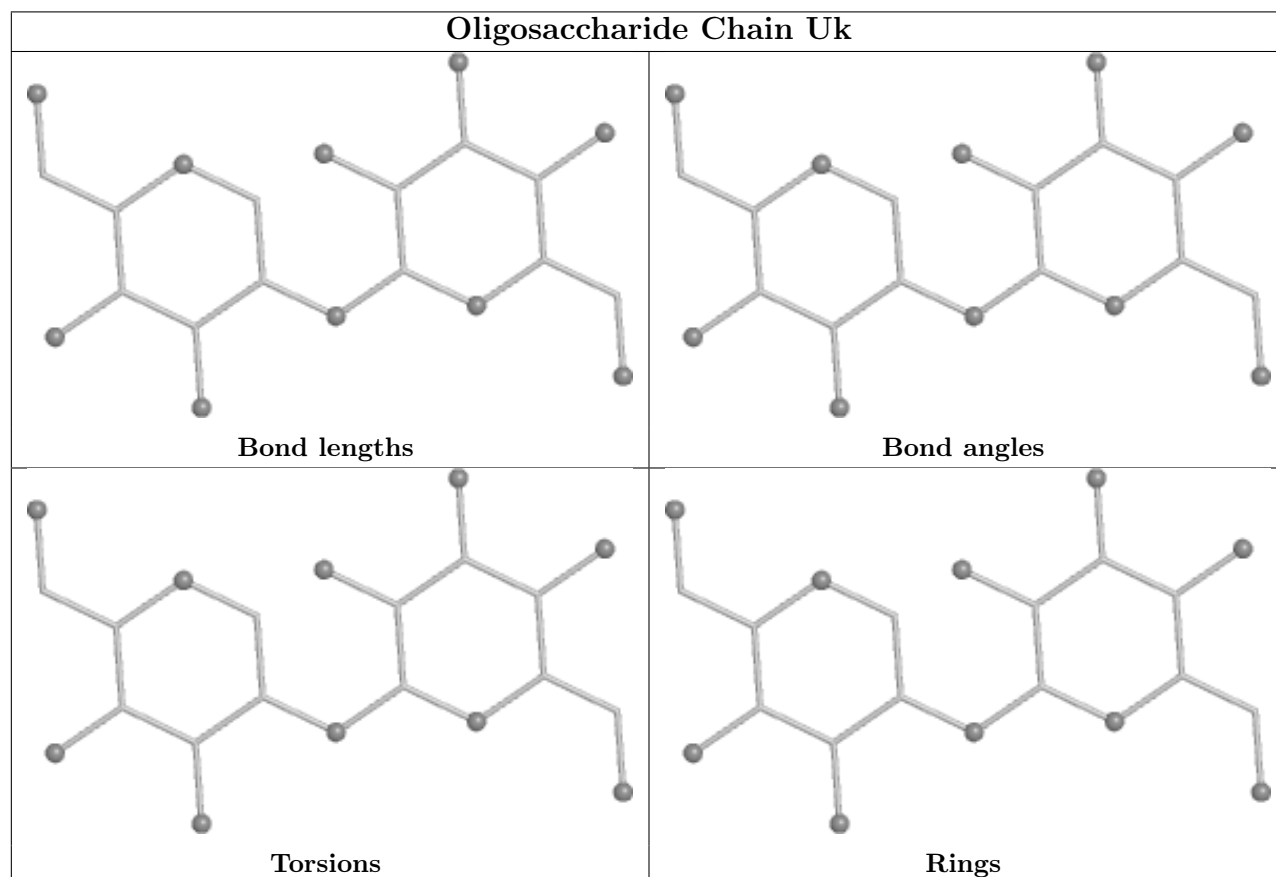
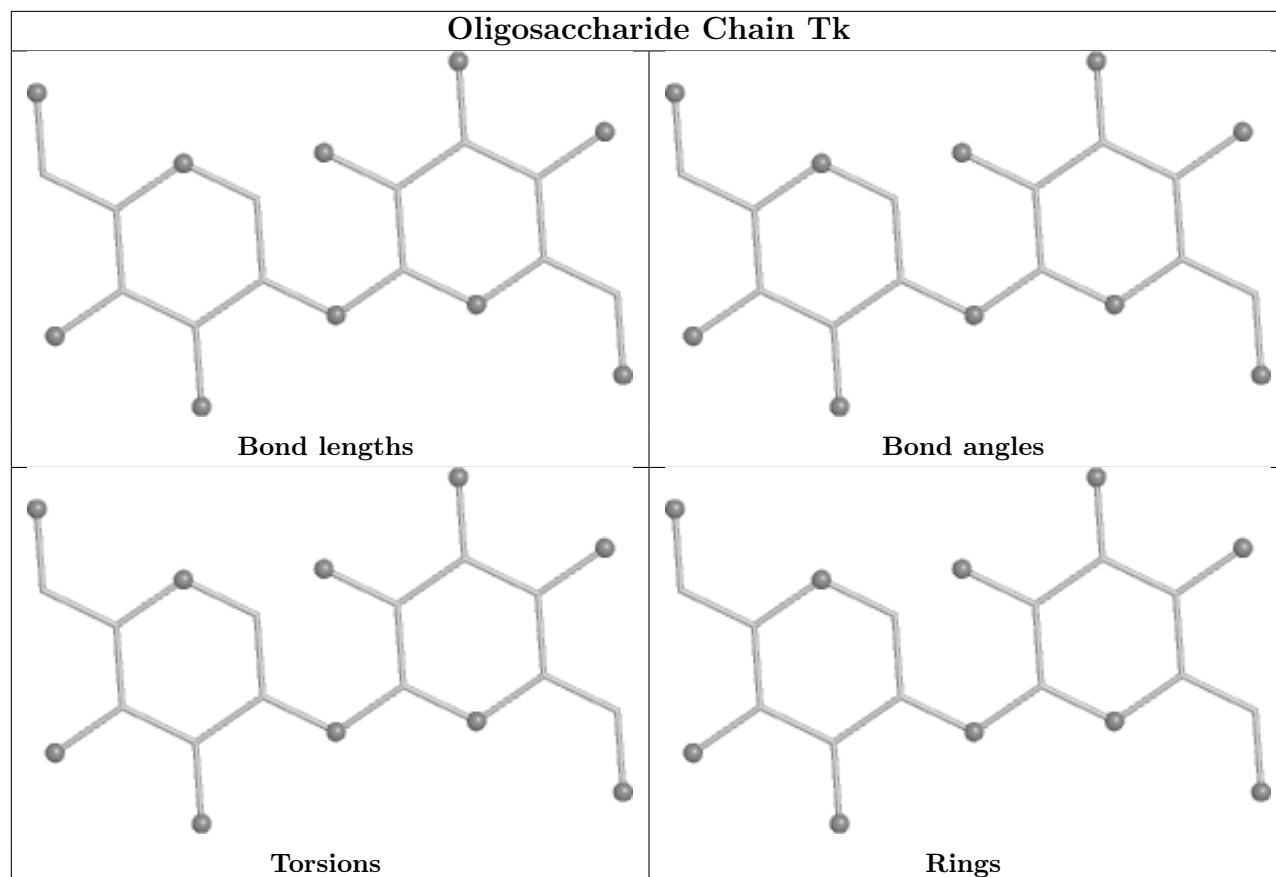


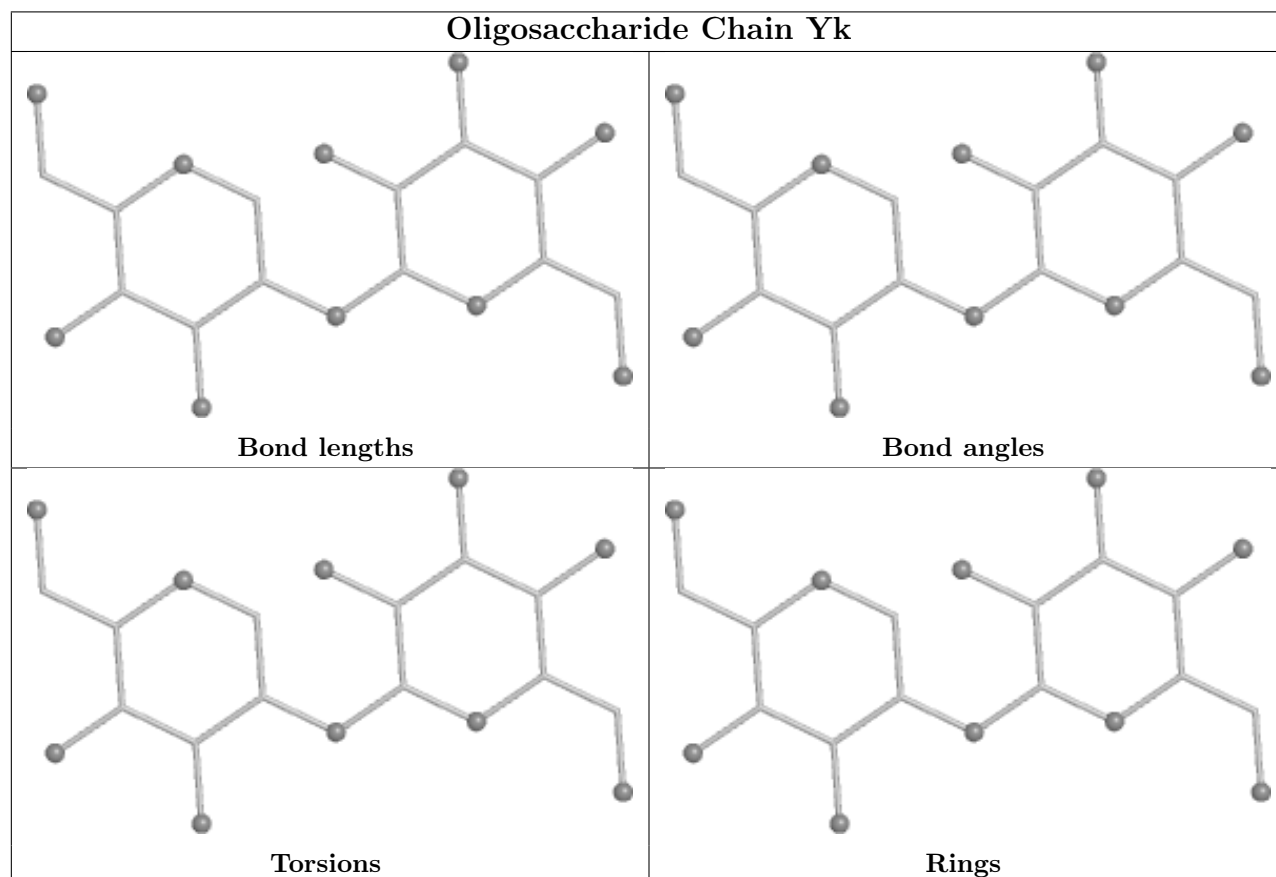
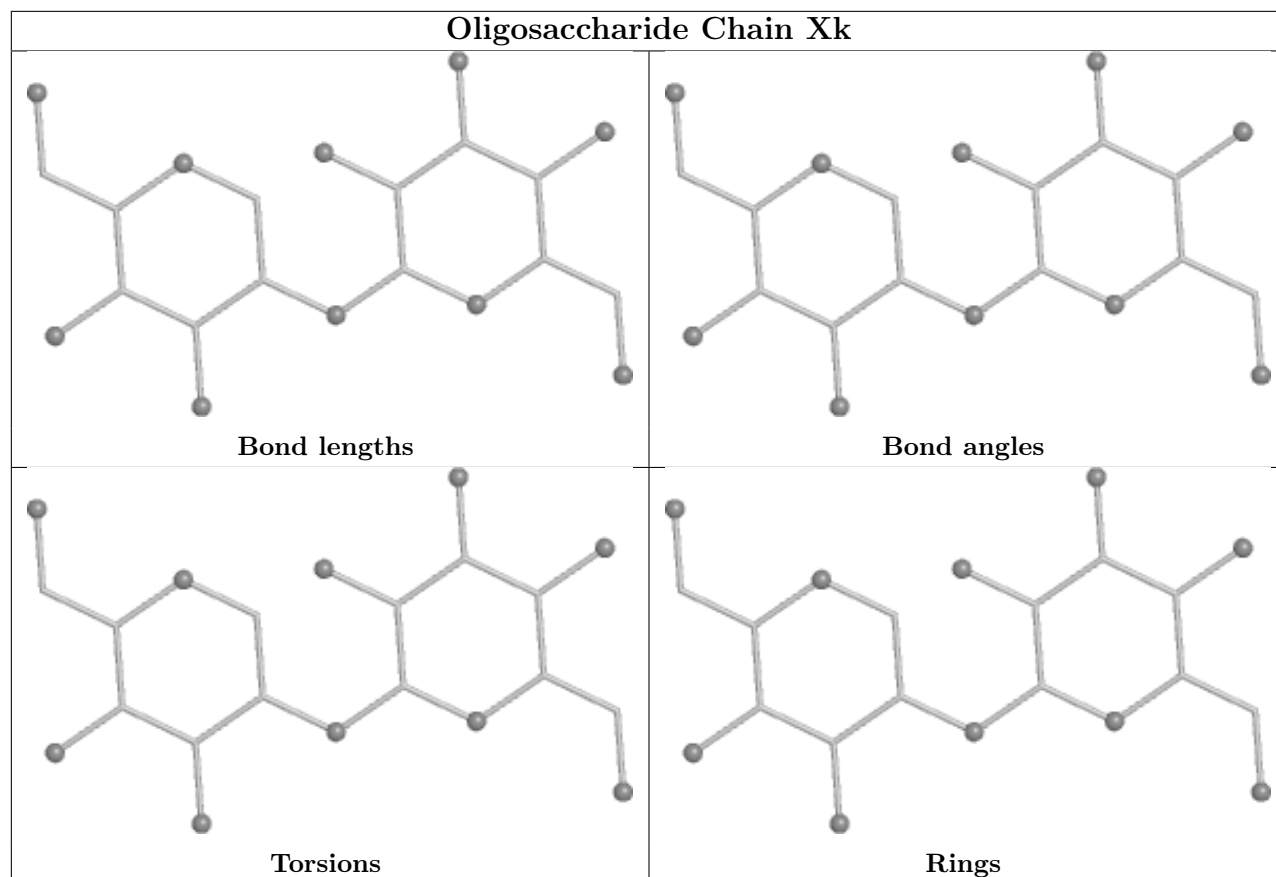
Oligosaccharide Chain Qk

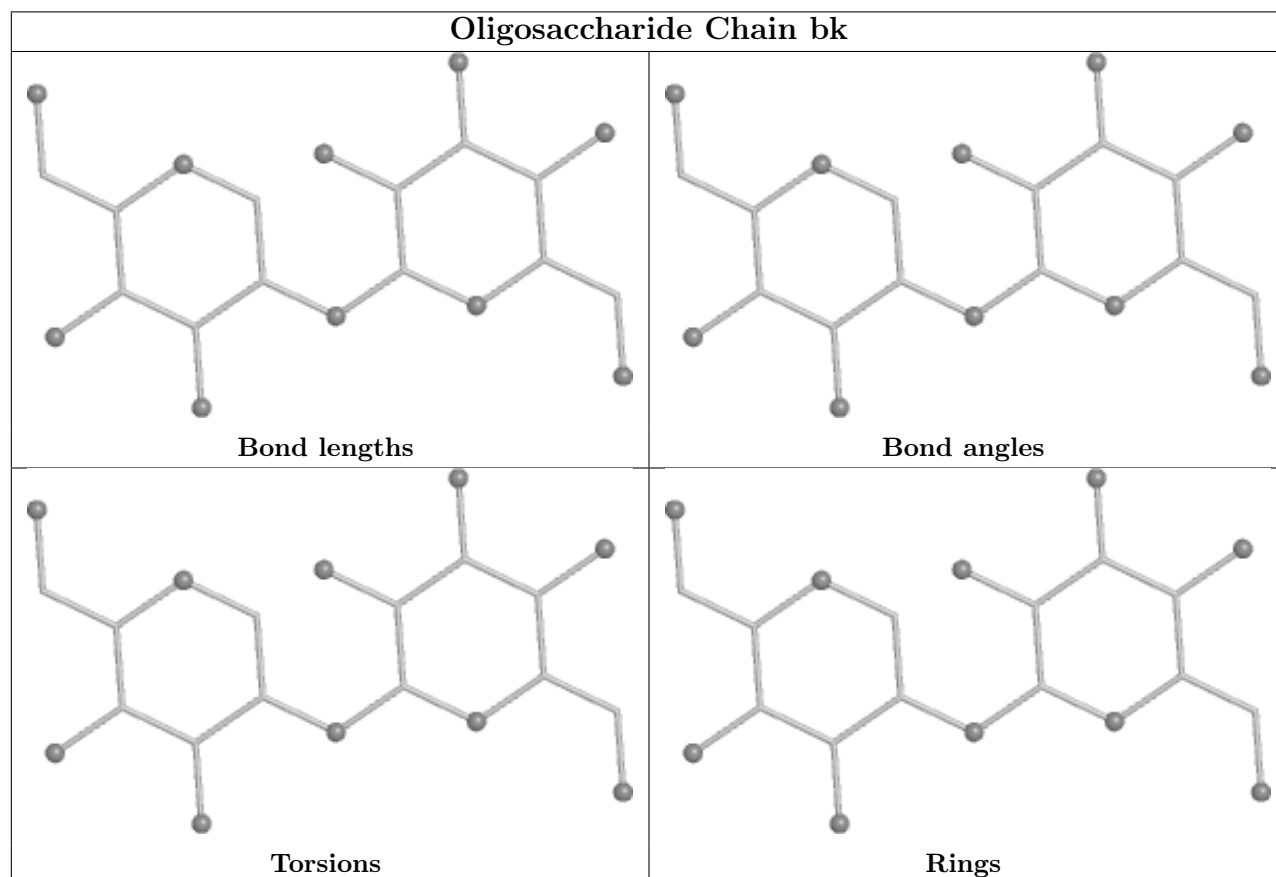
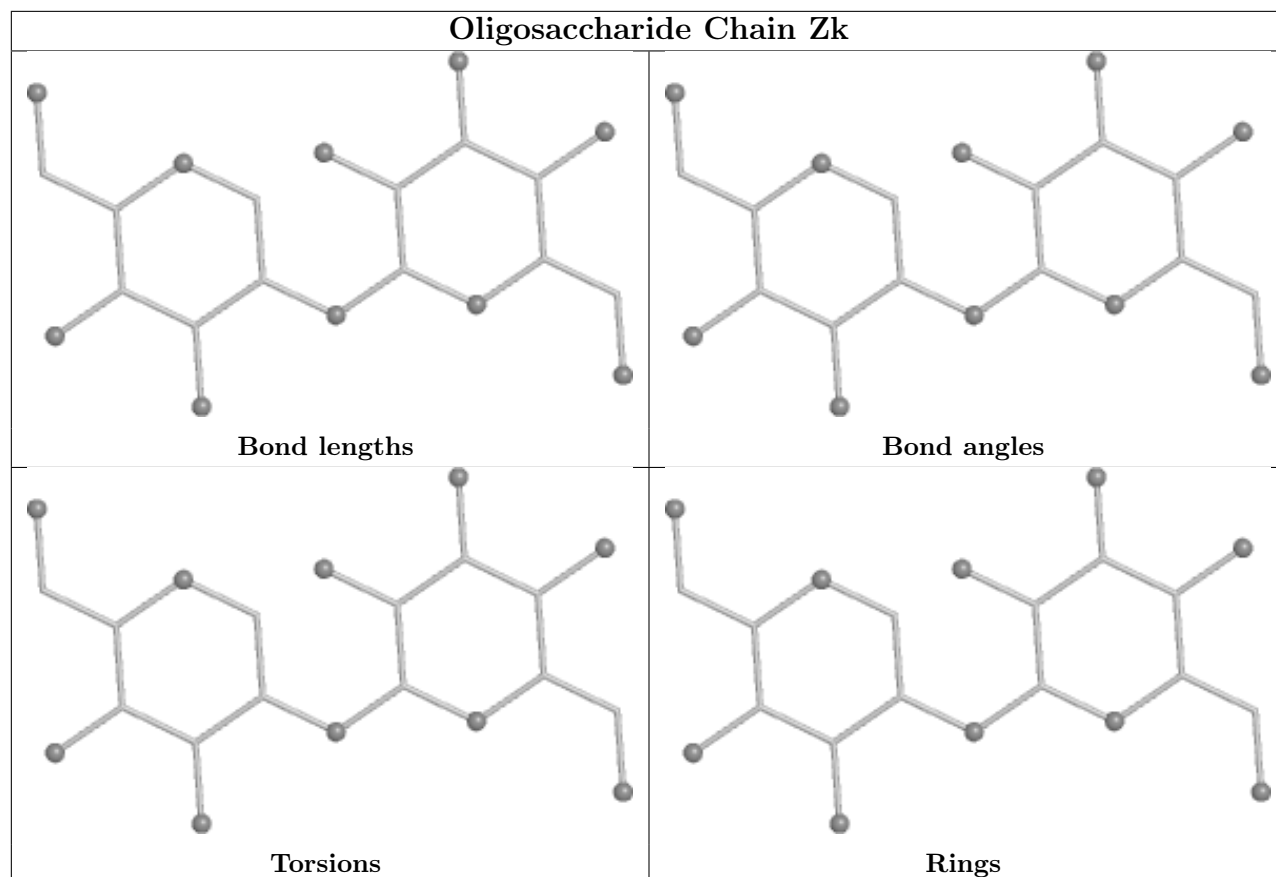


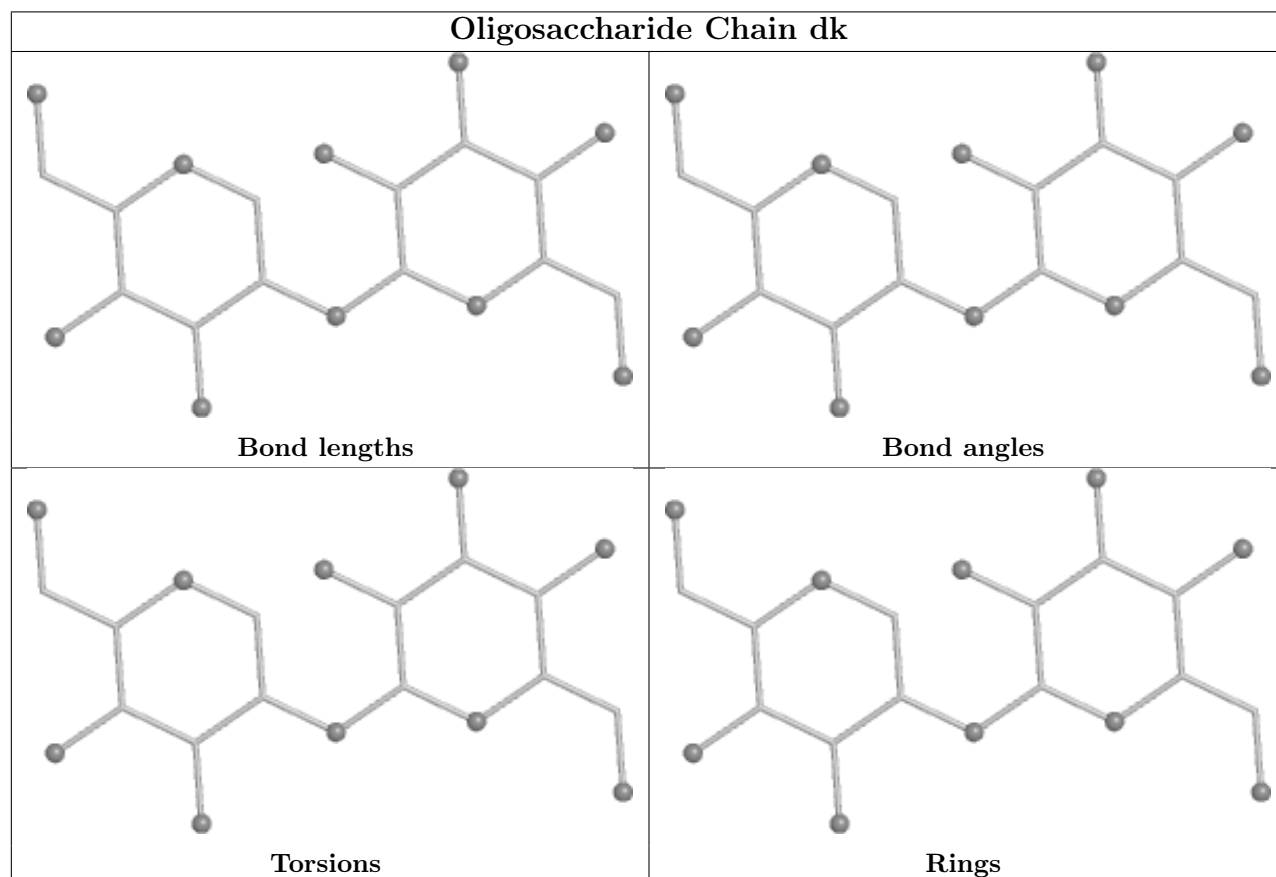
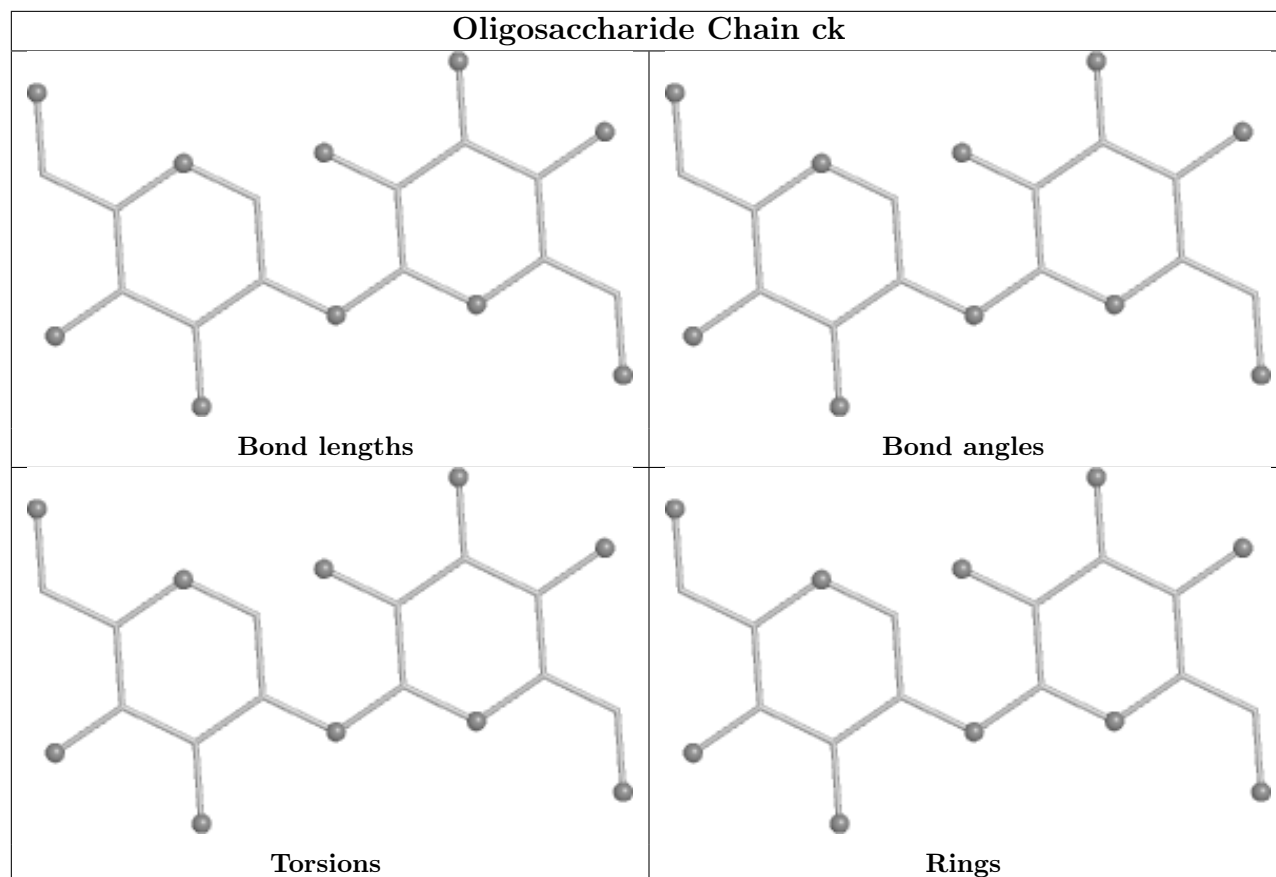
Oligosaccharide Chain Sk

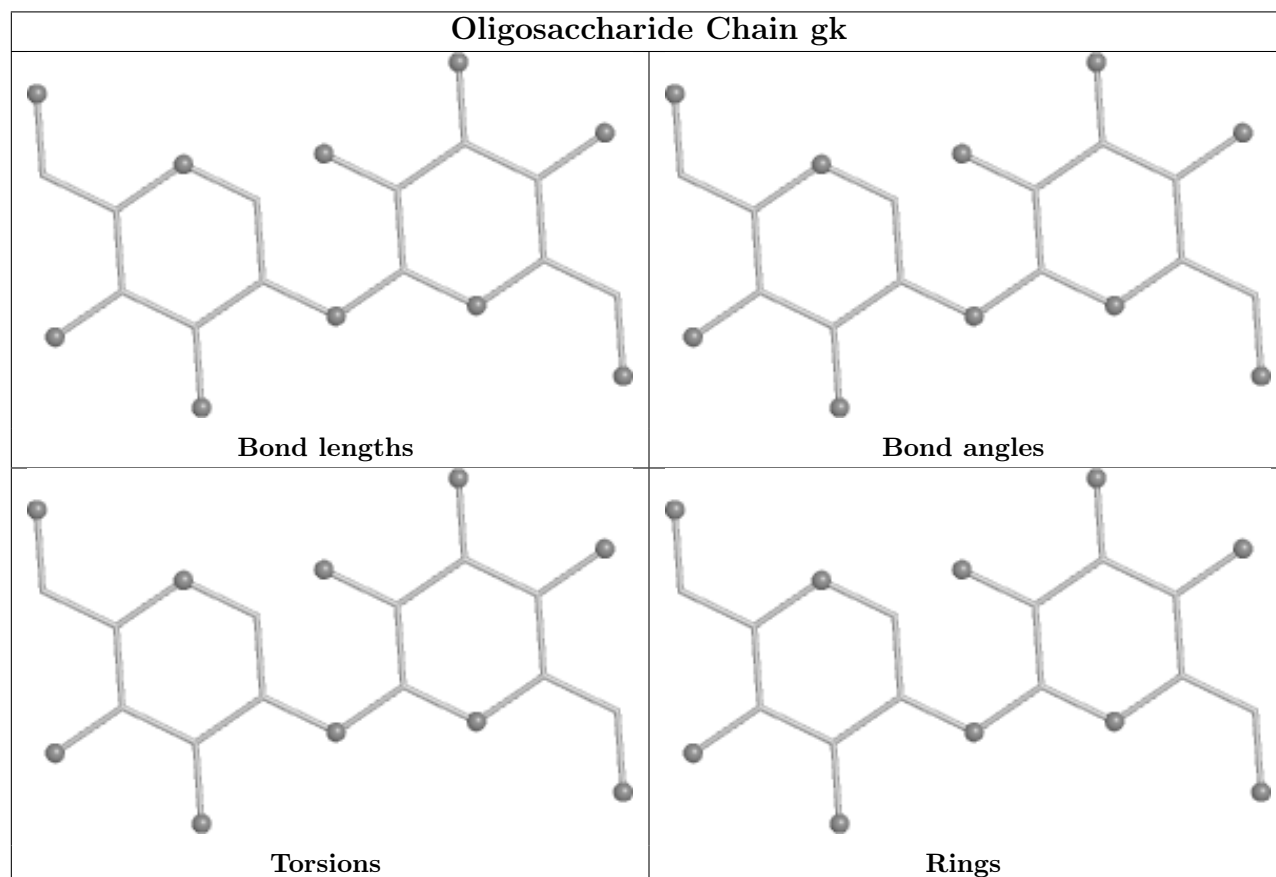
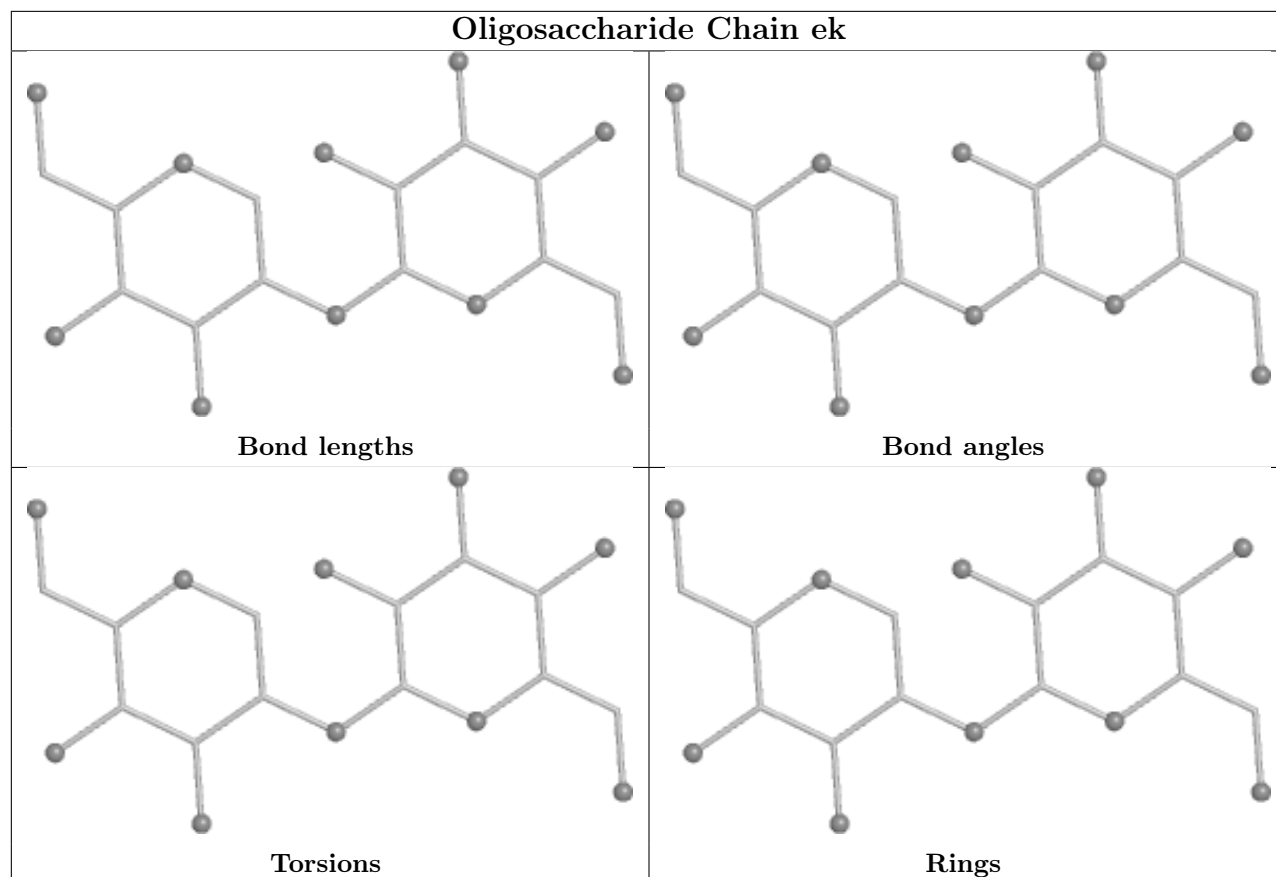


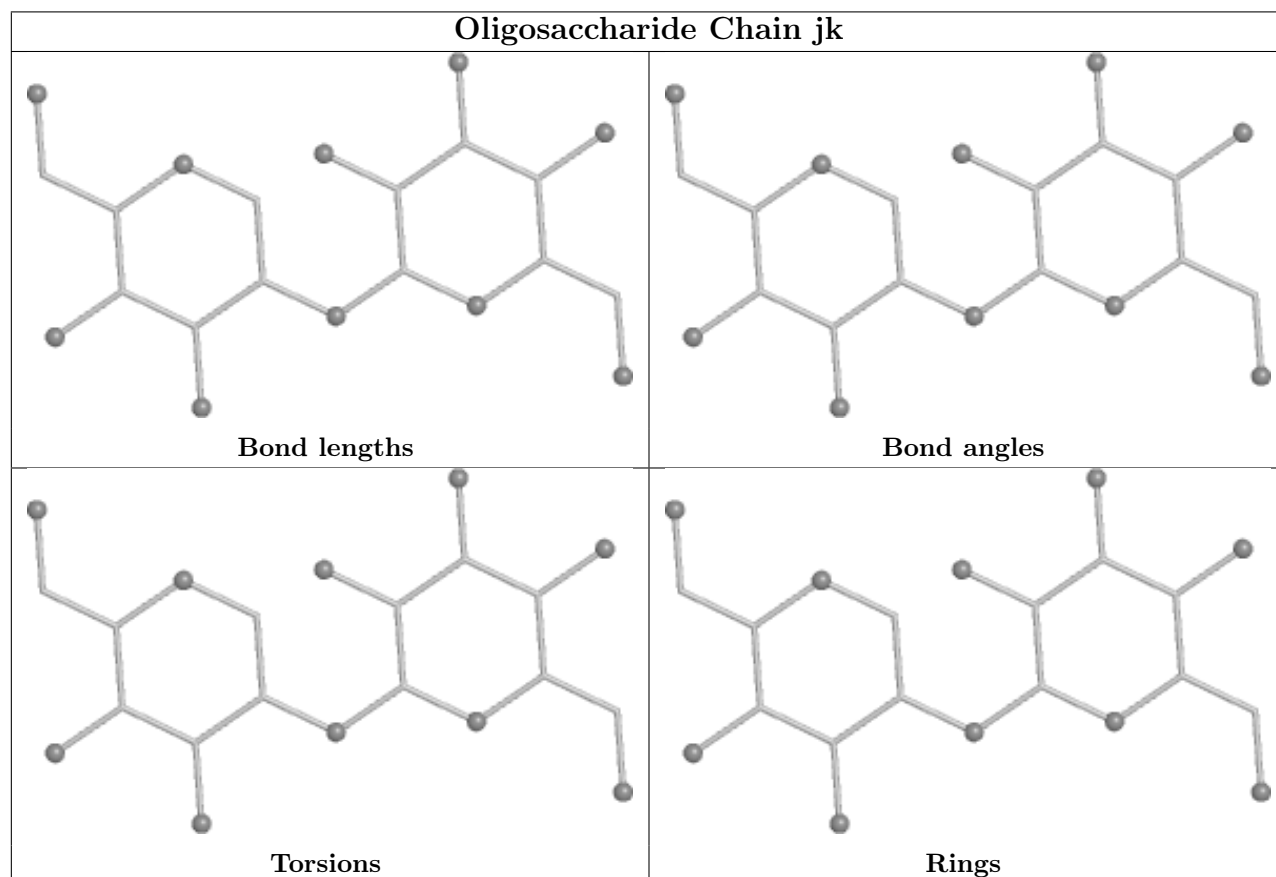
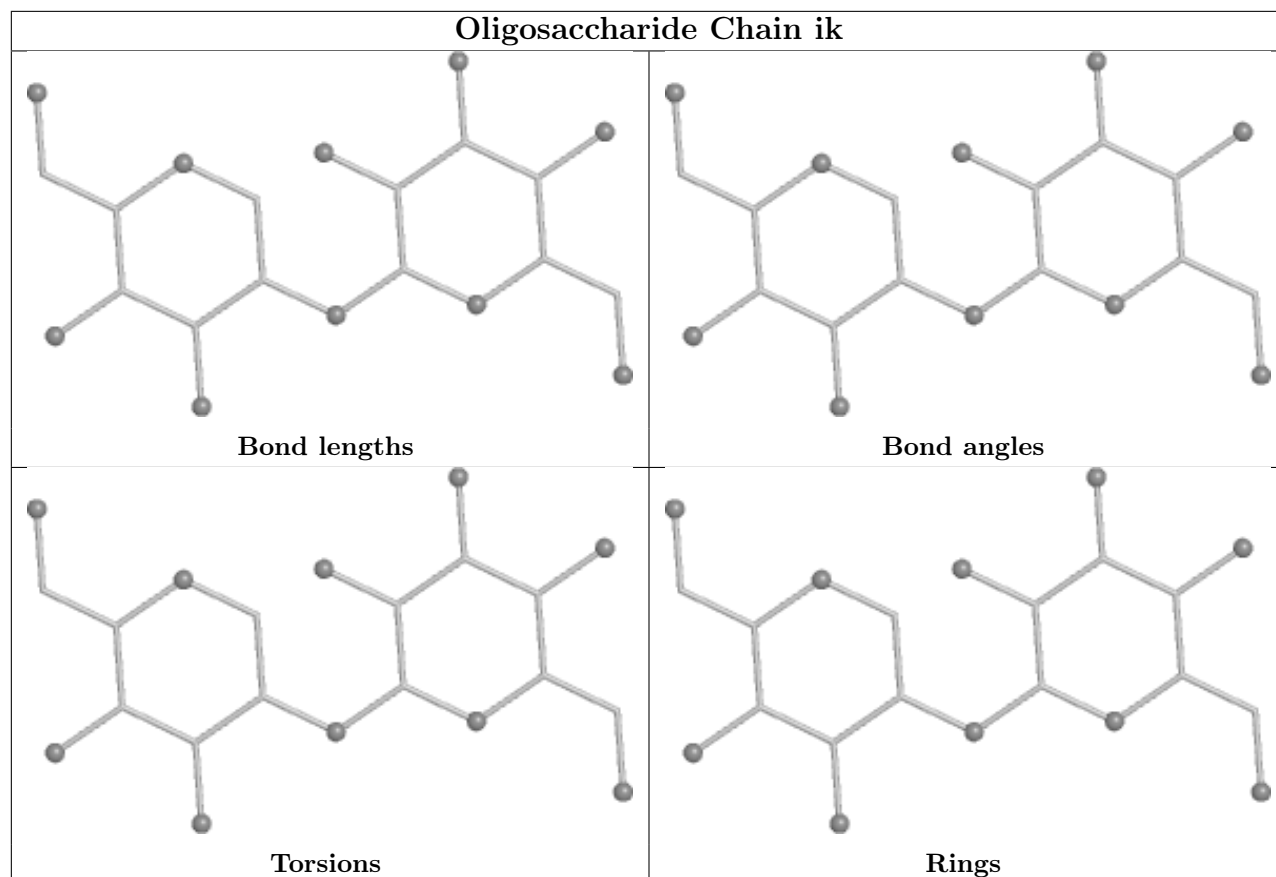


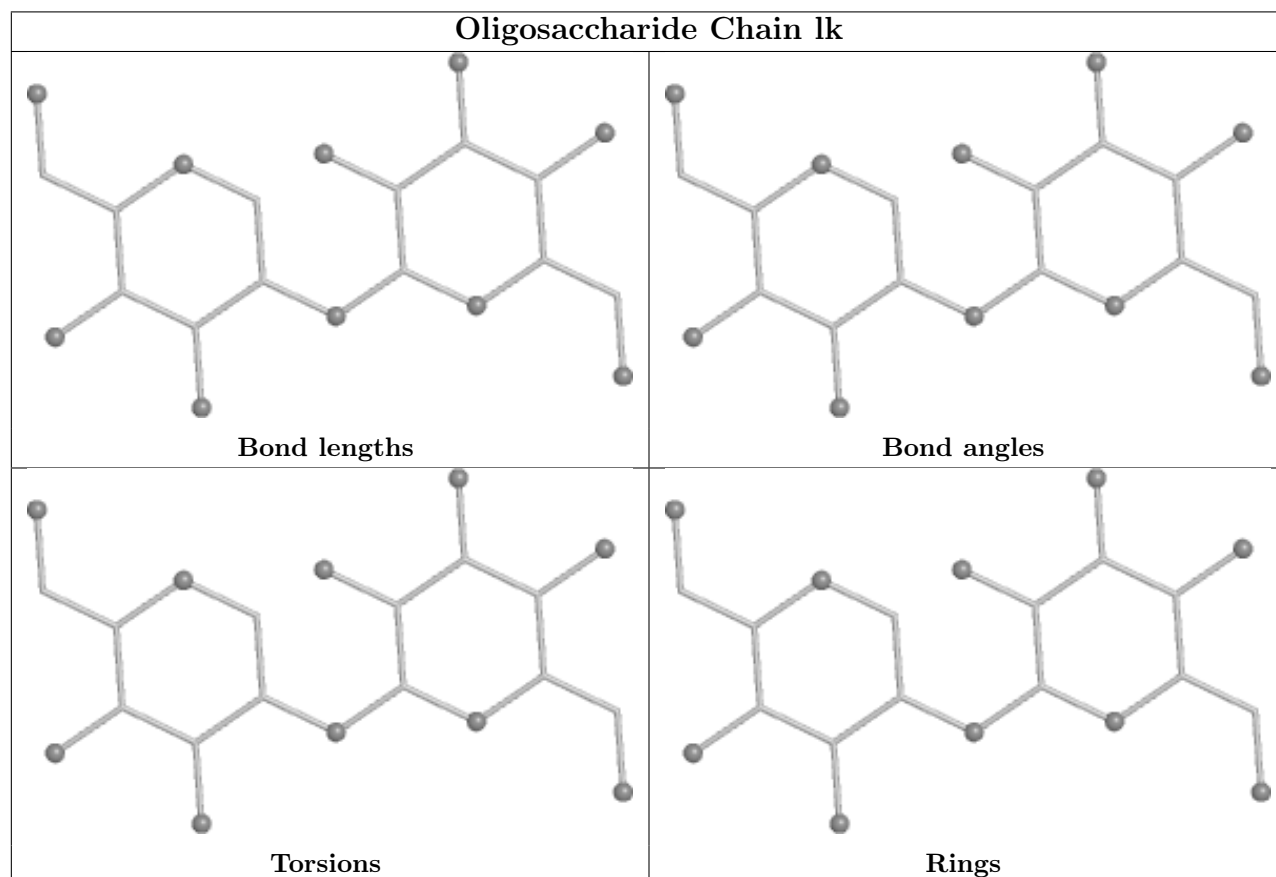
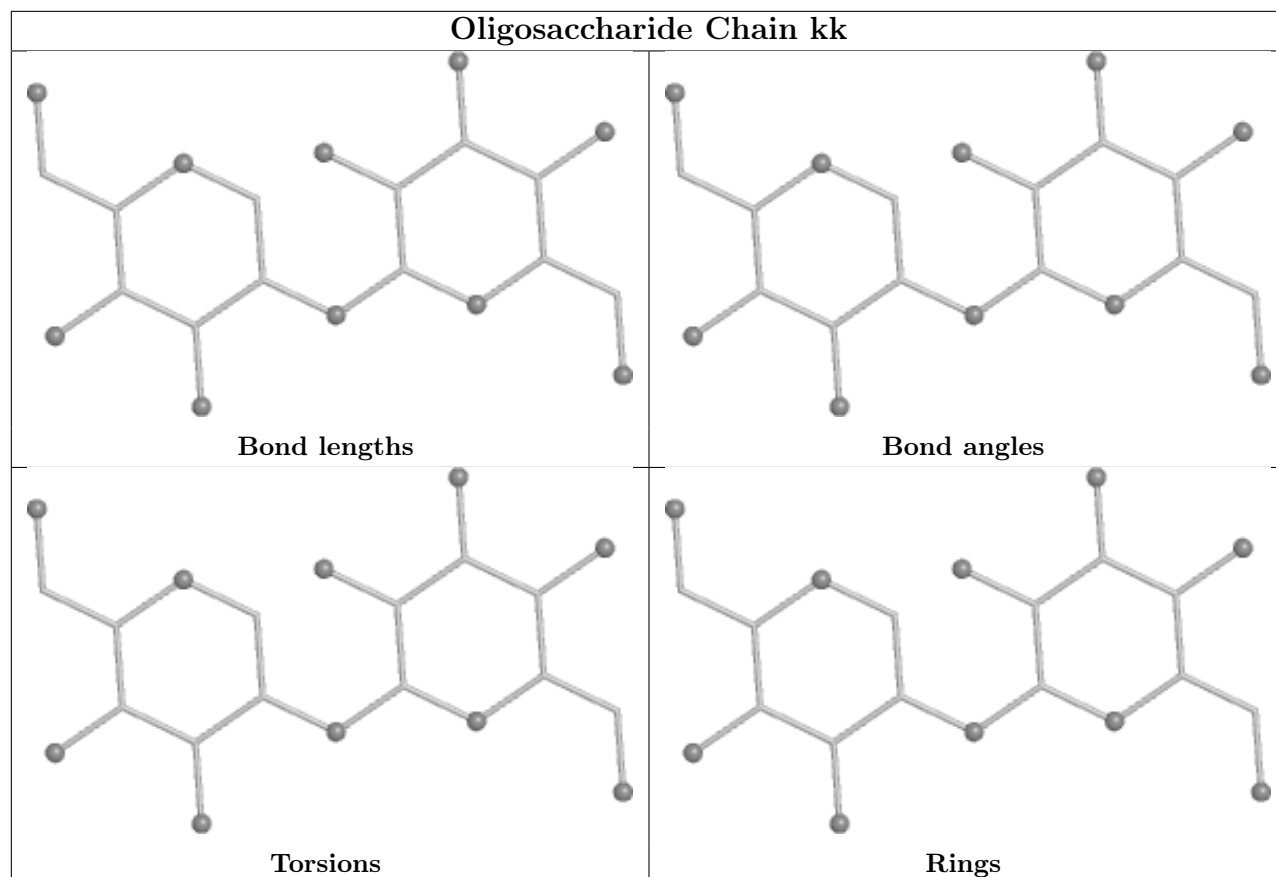


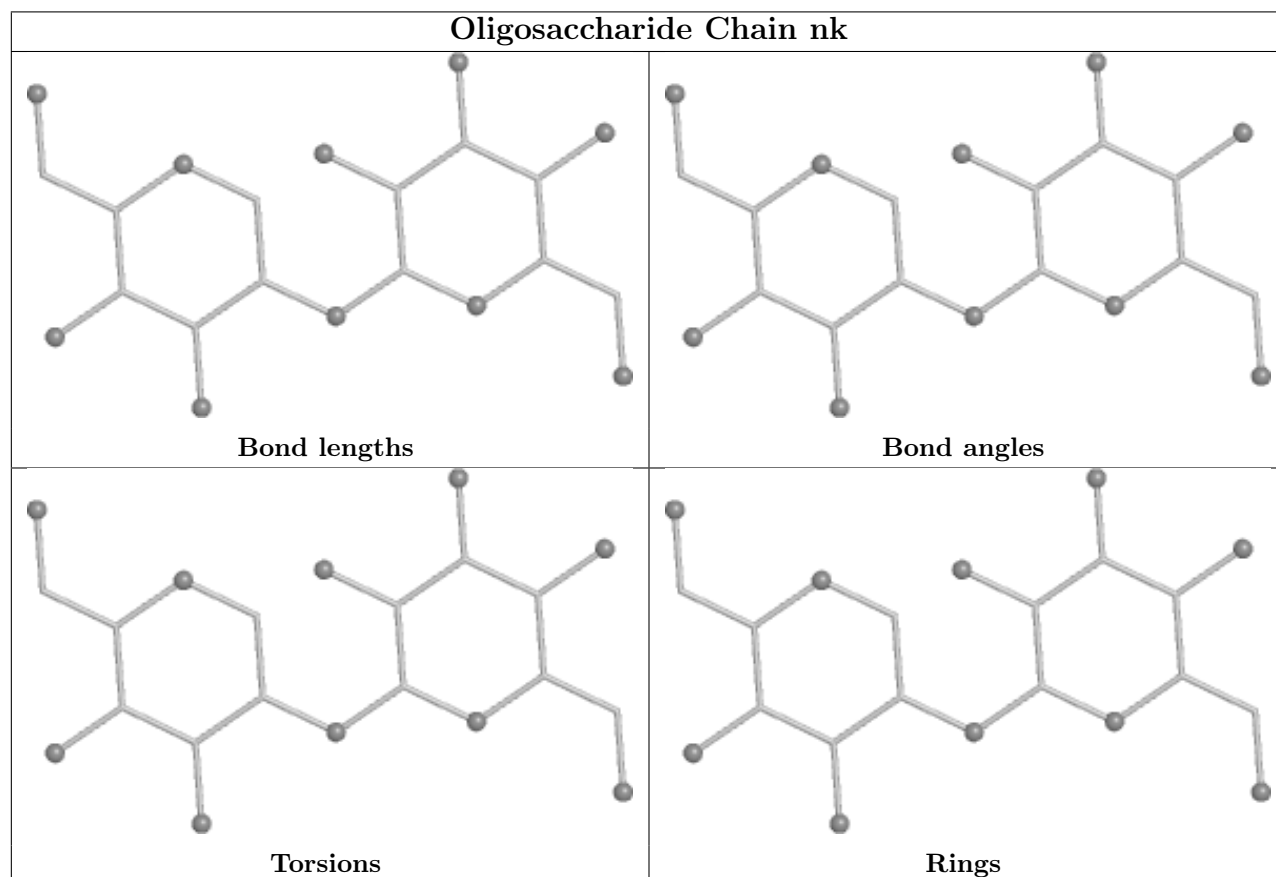
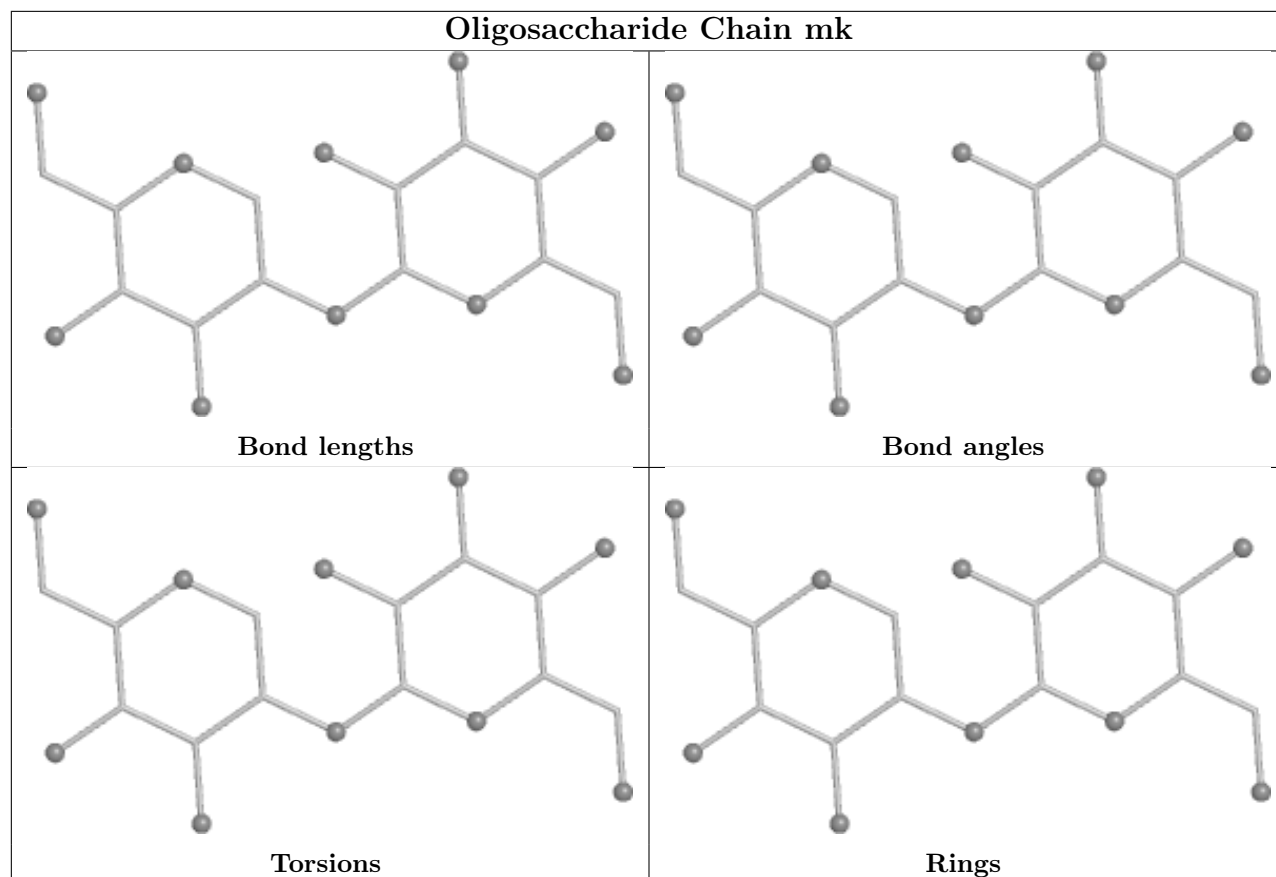


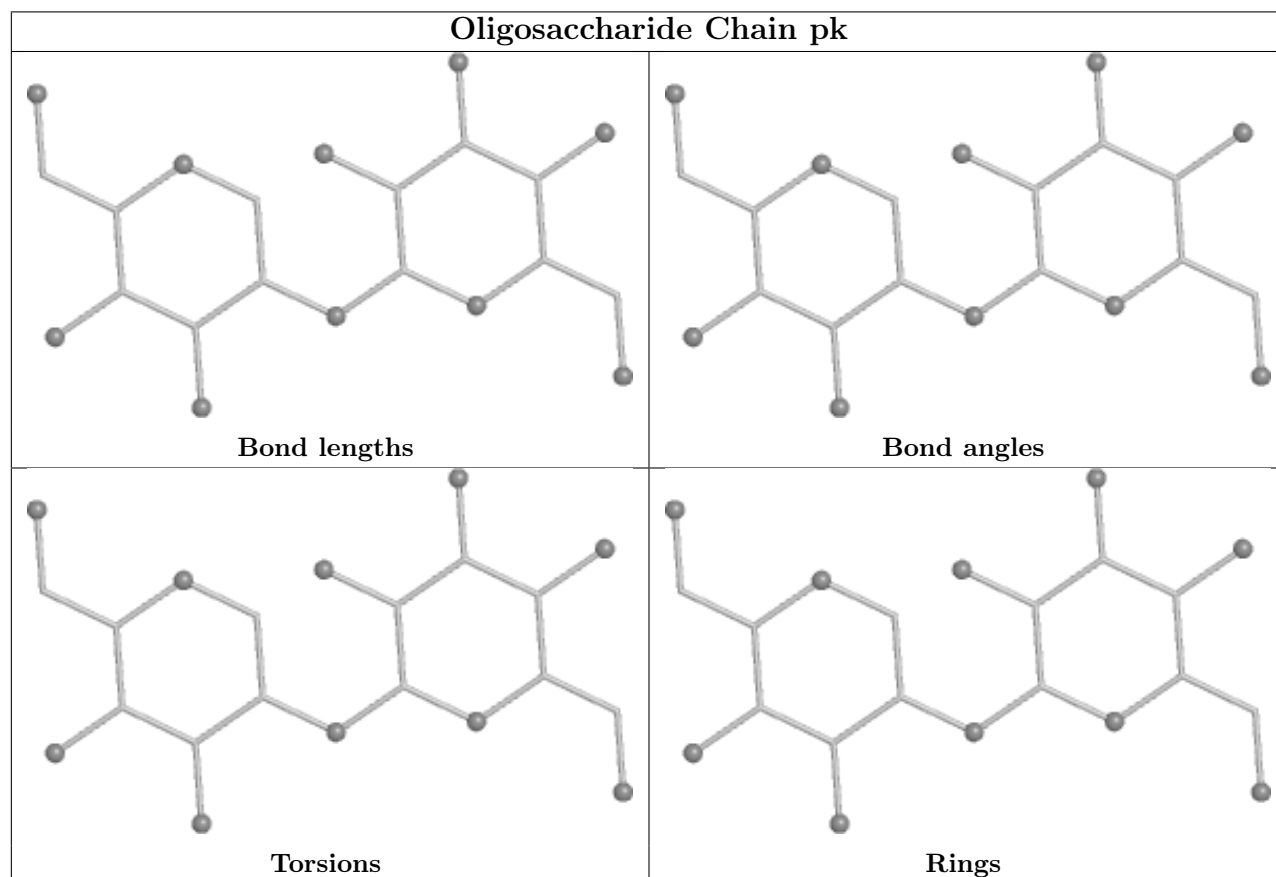
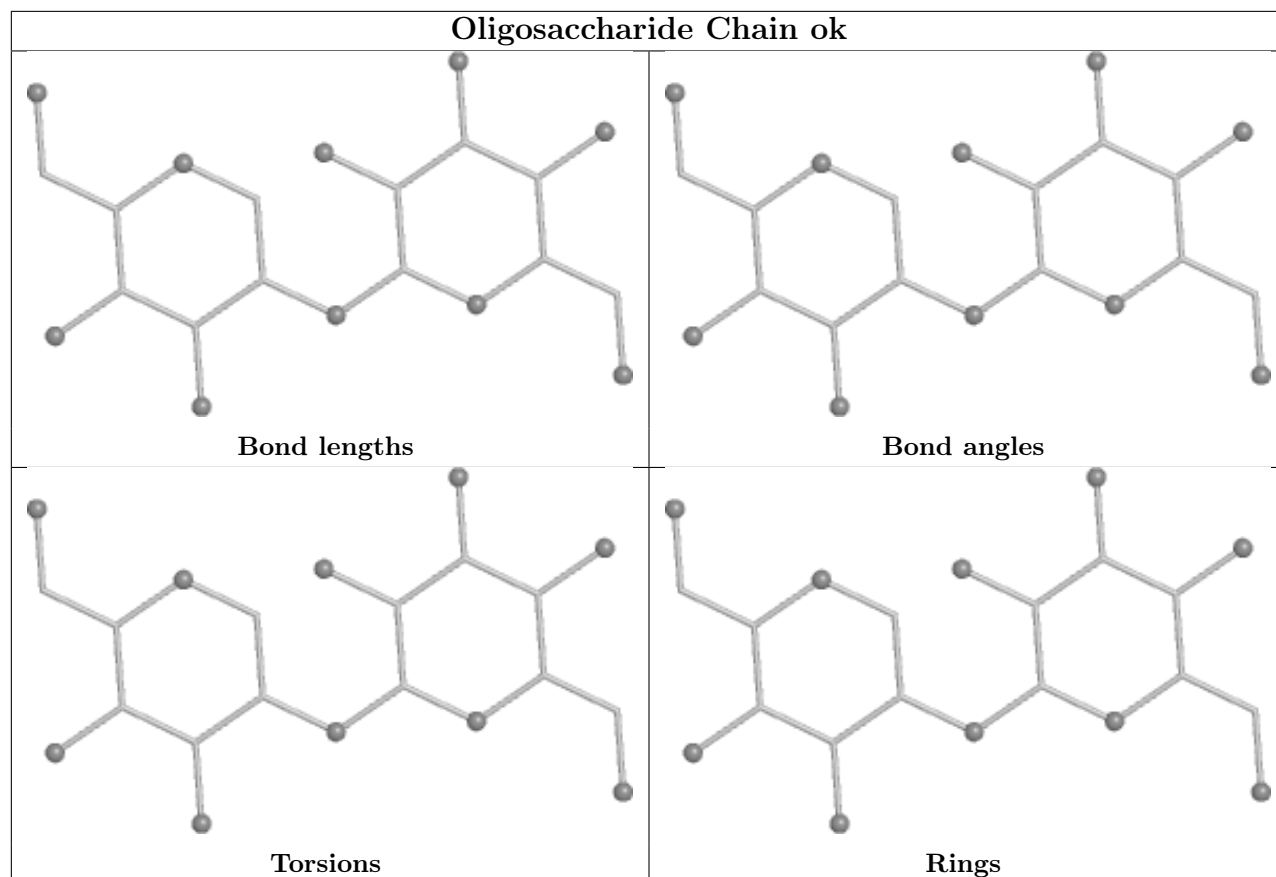


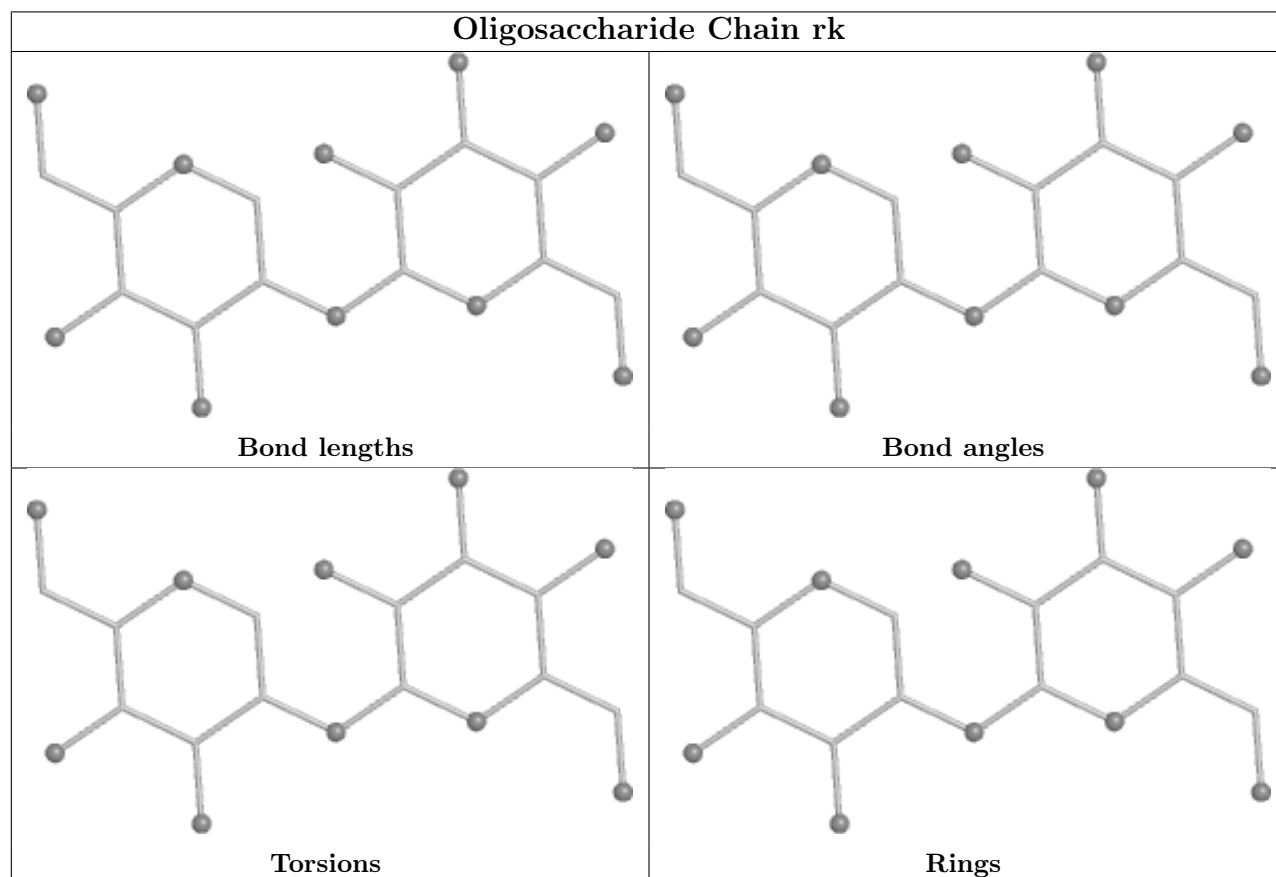
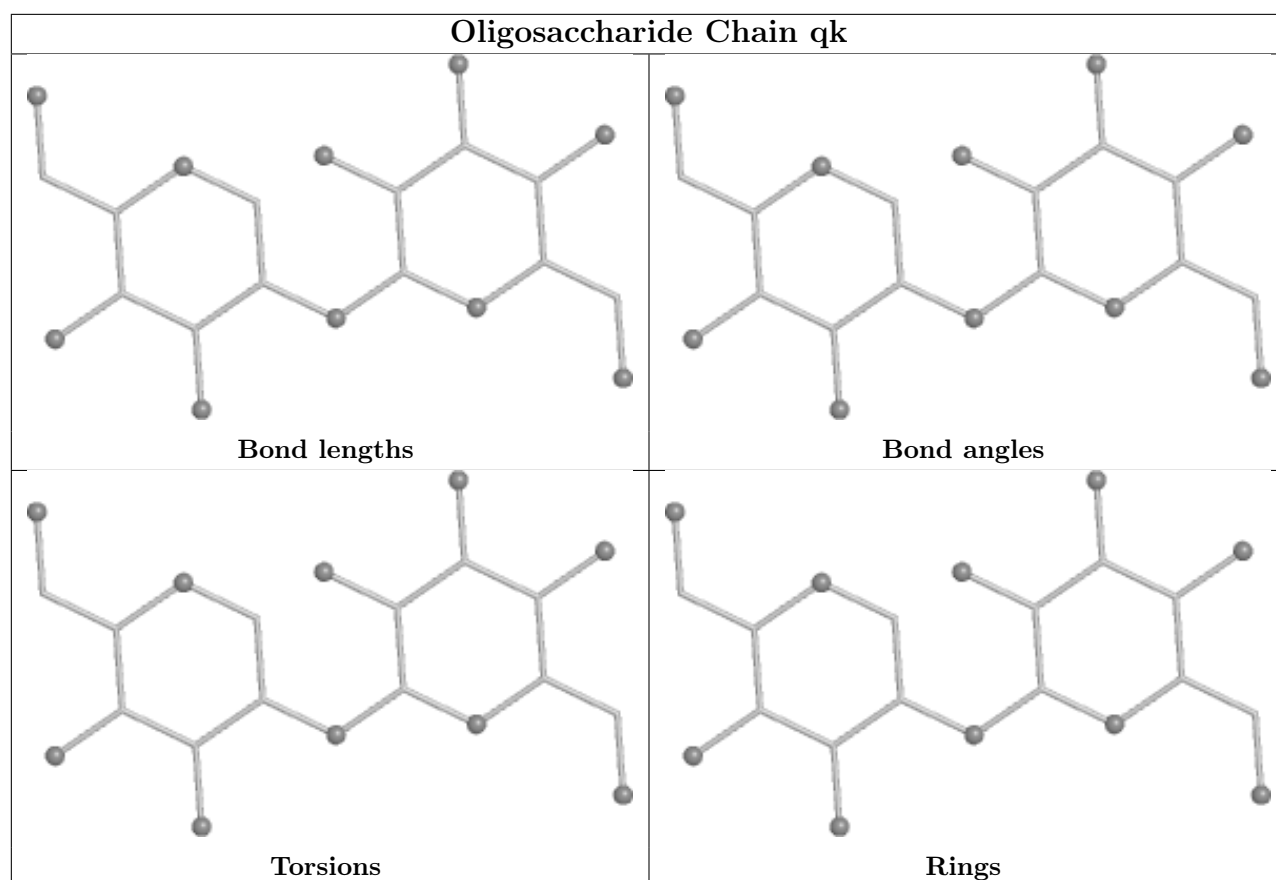


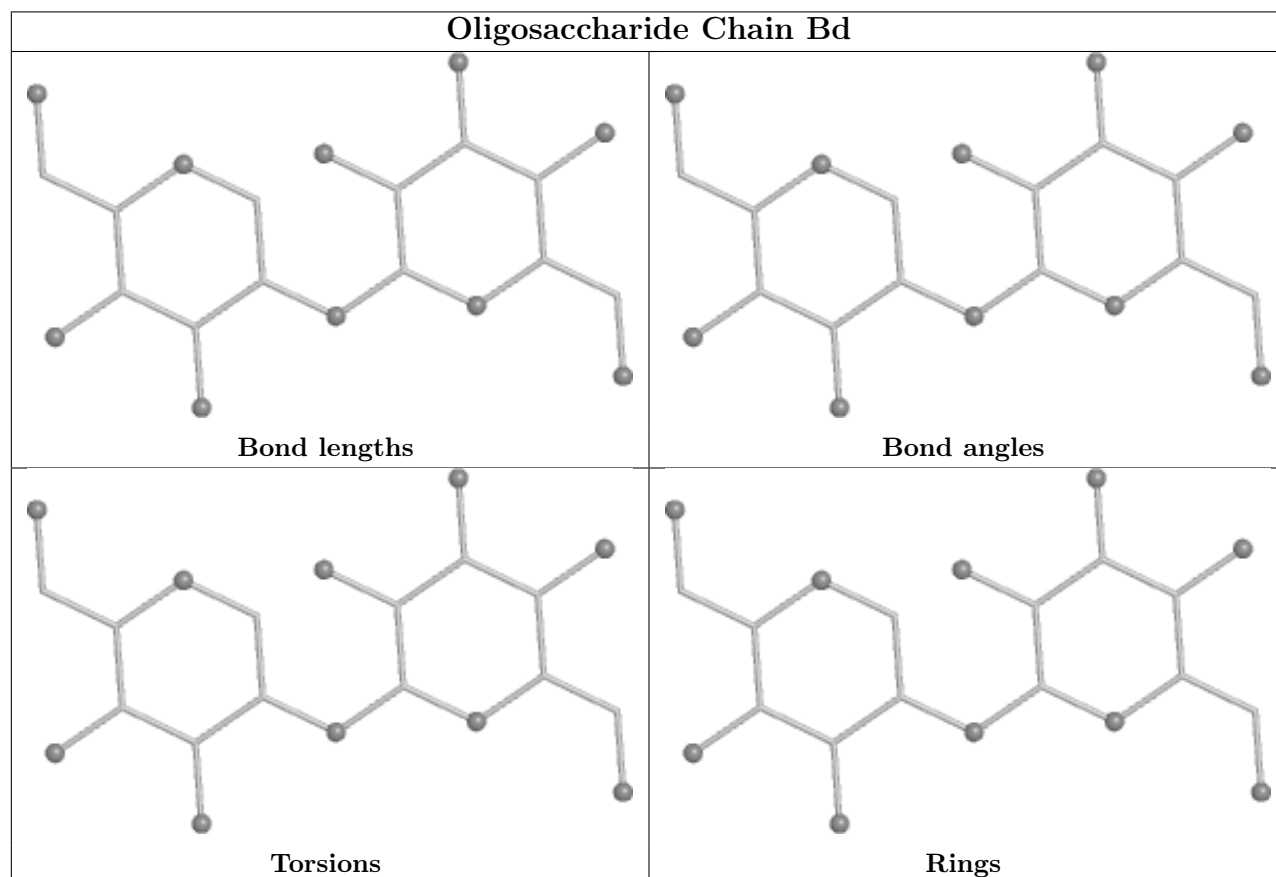
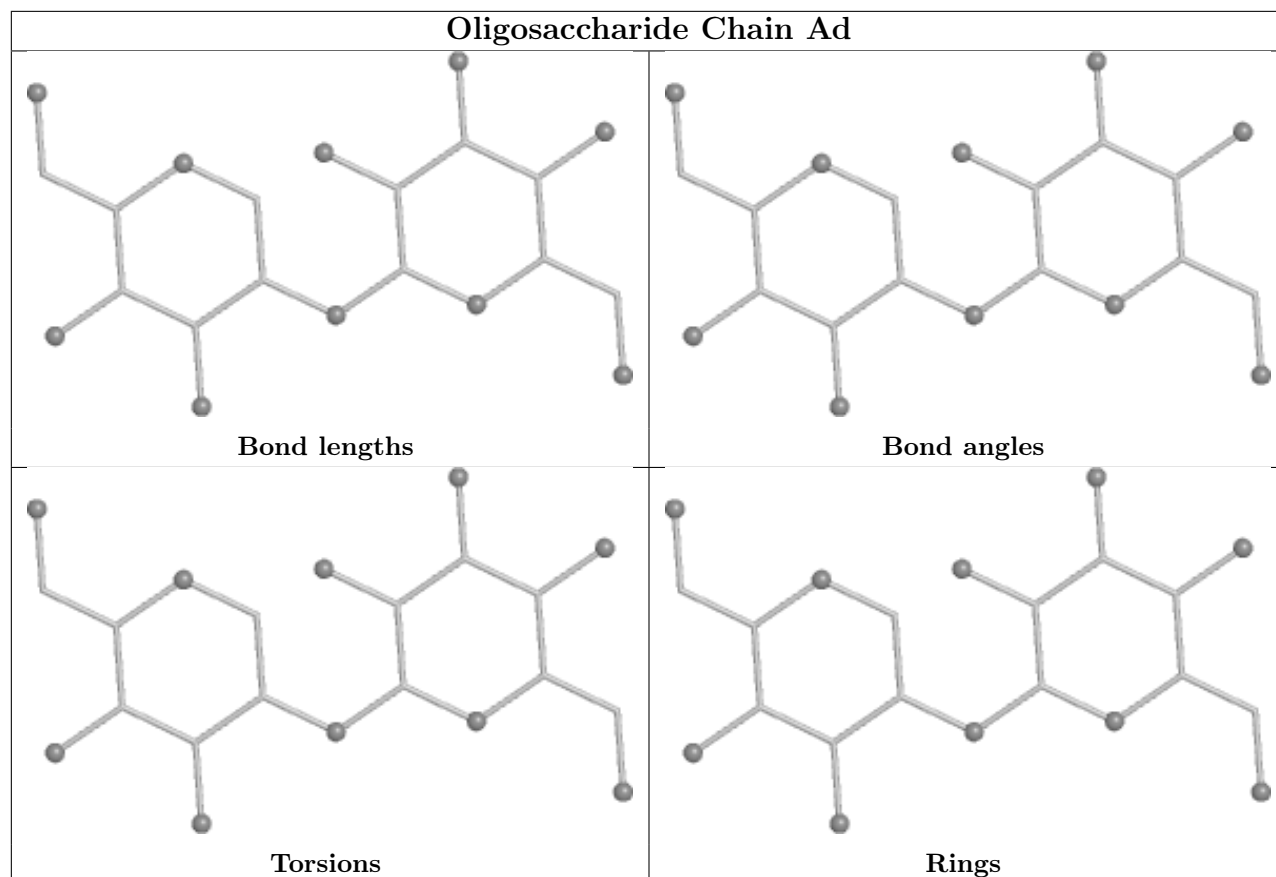


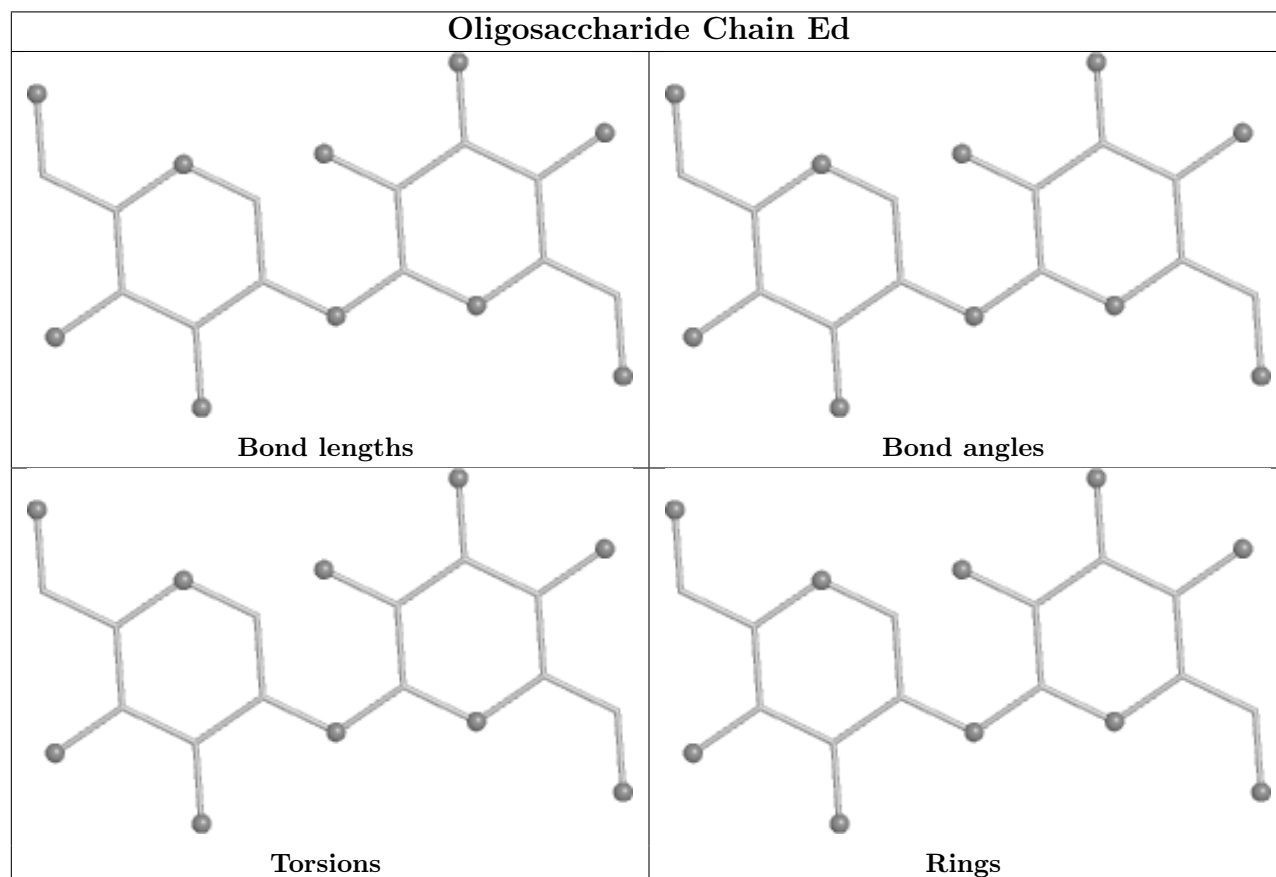
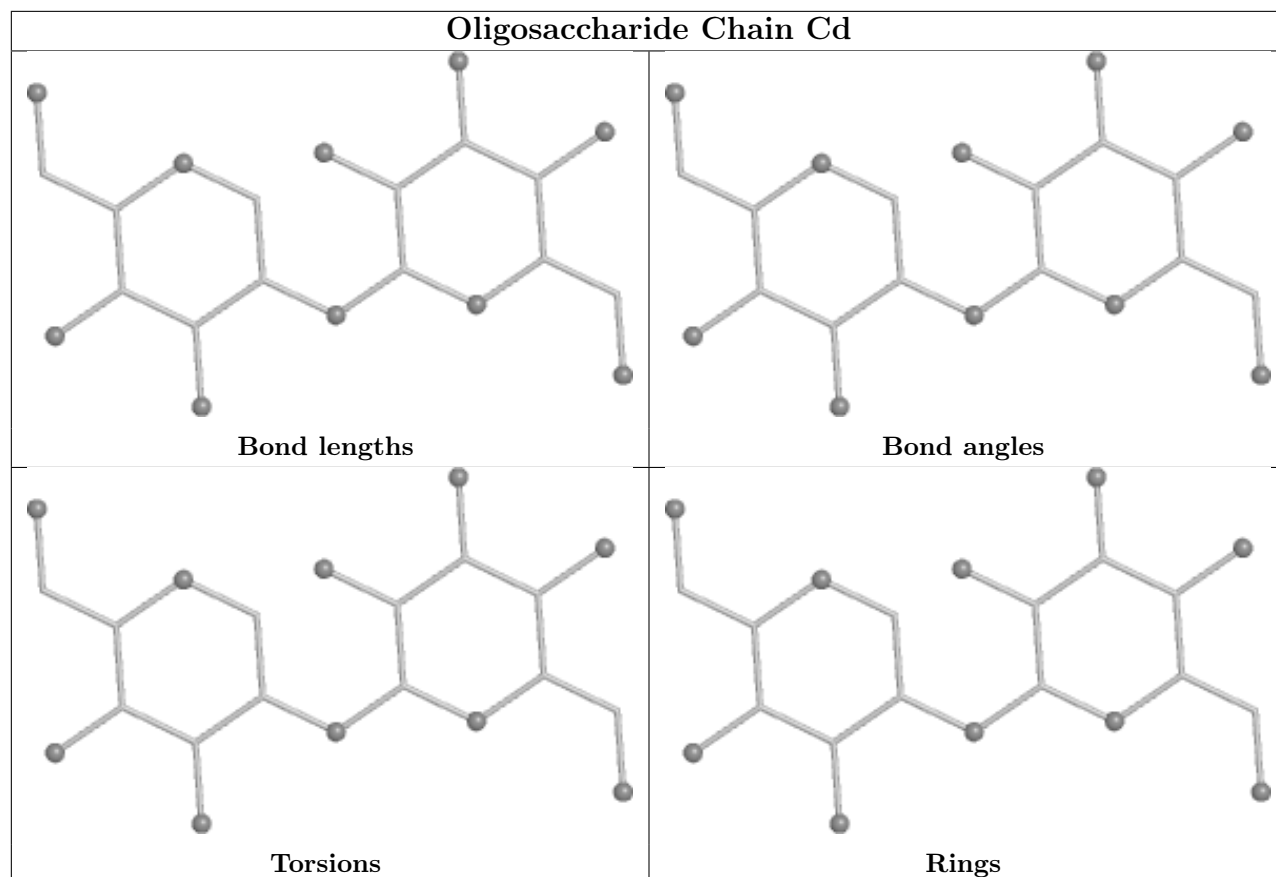




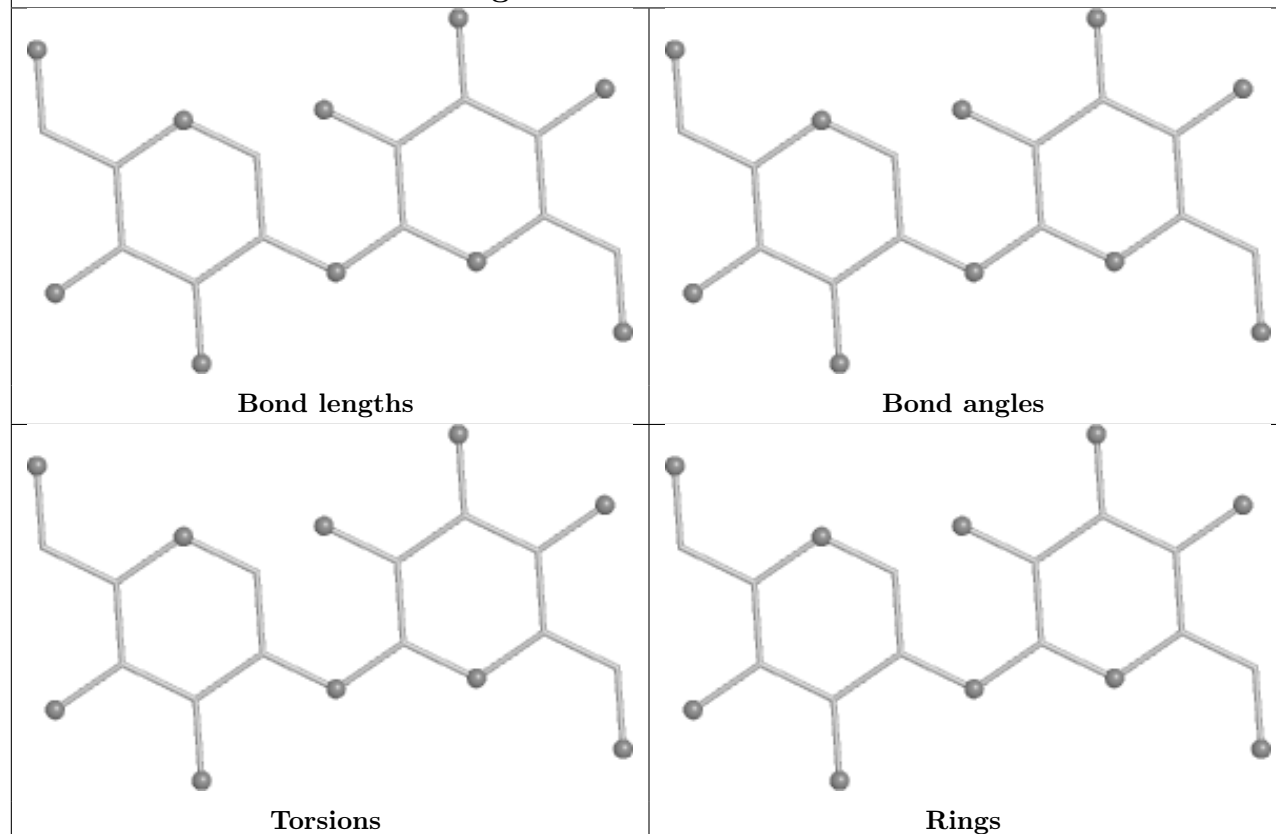




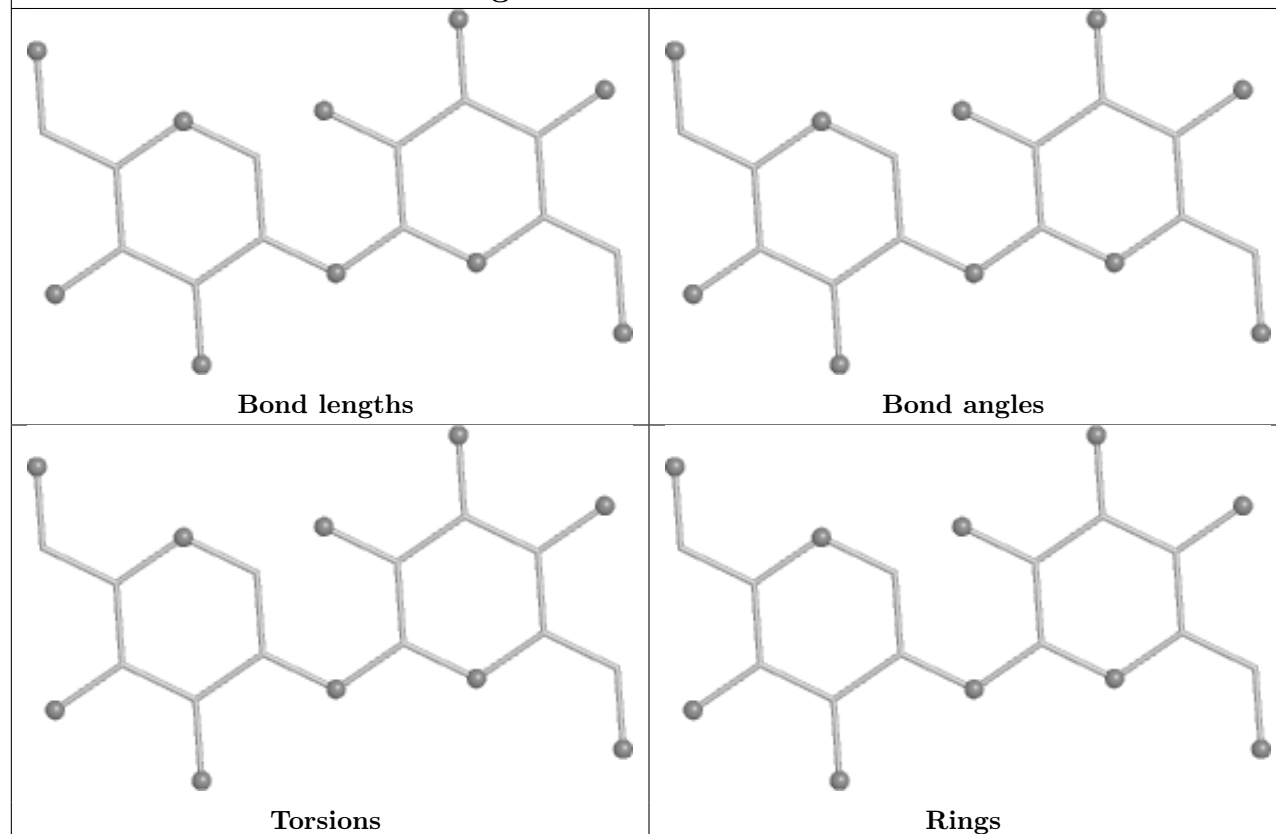


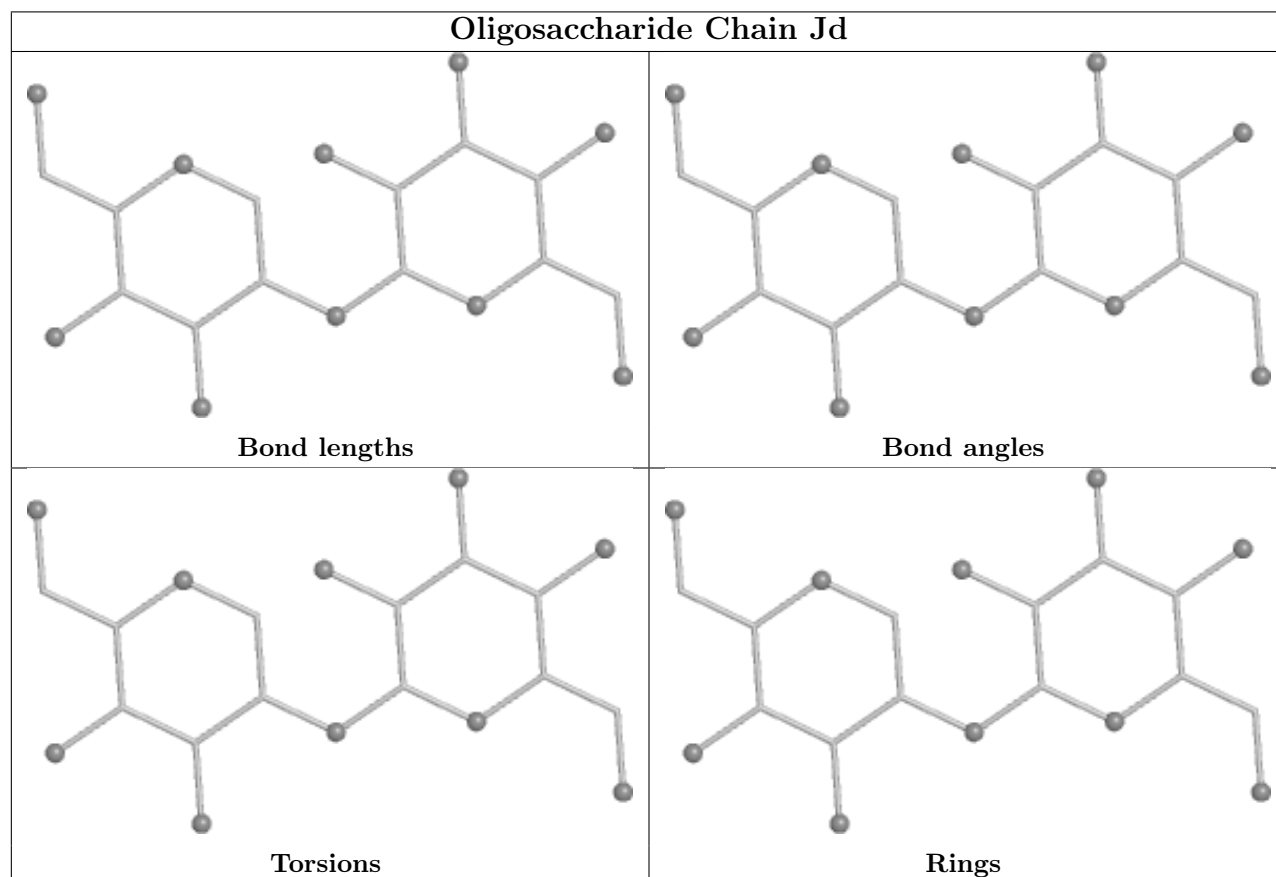
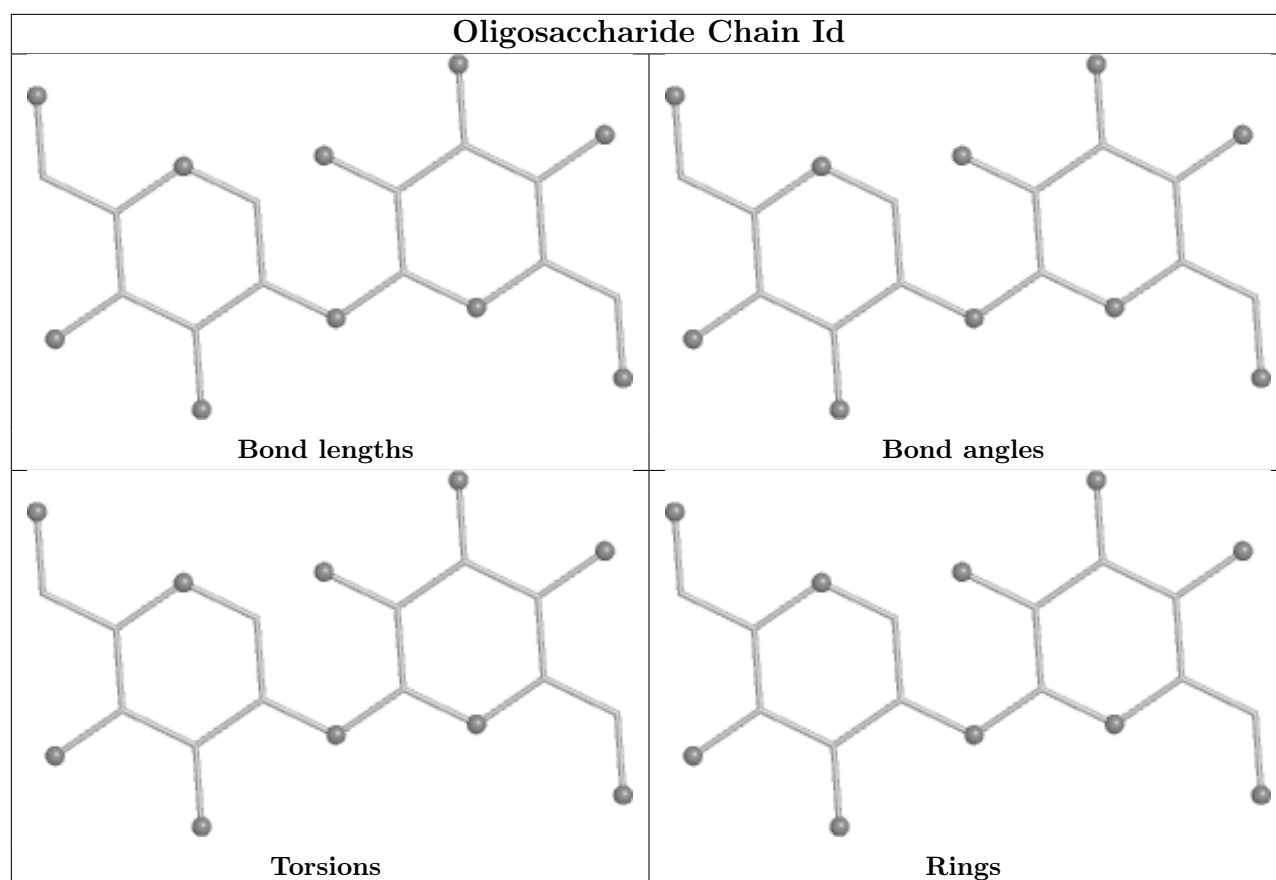


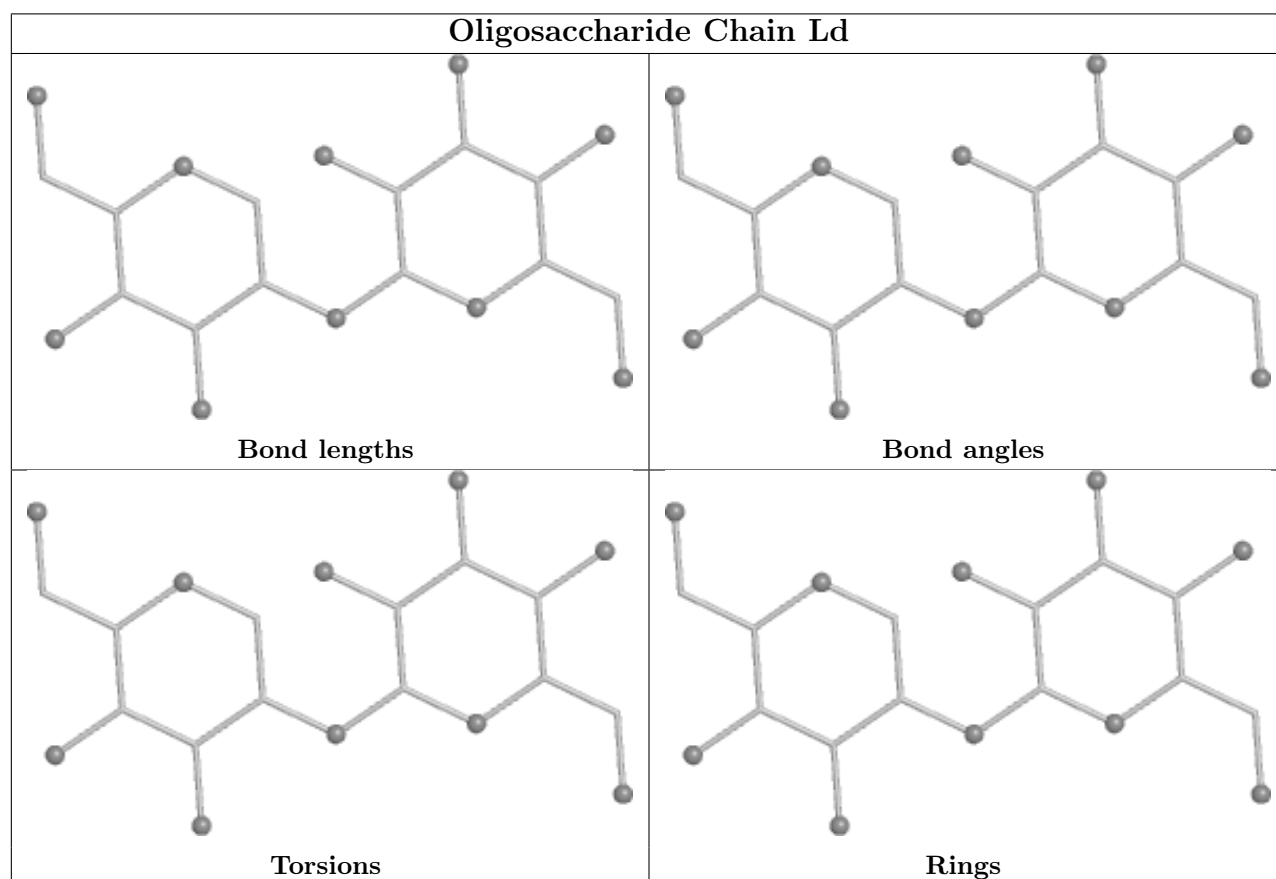
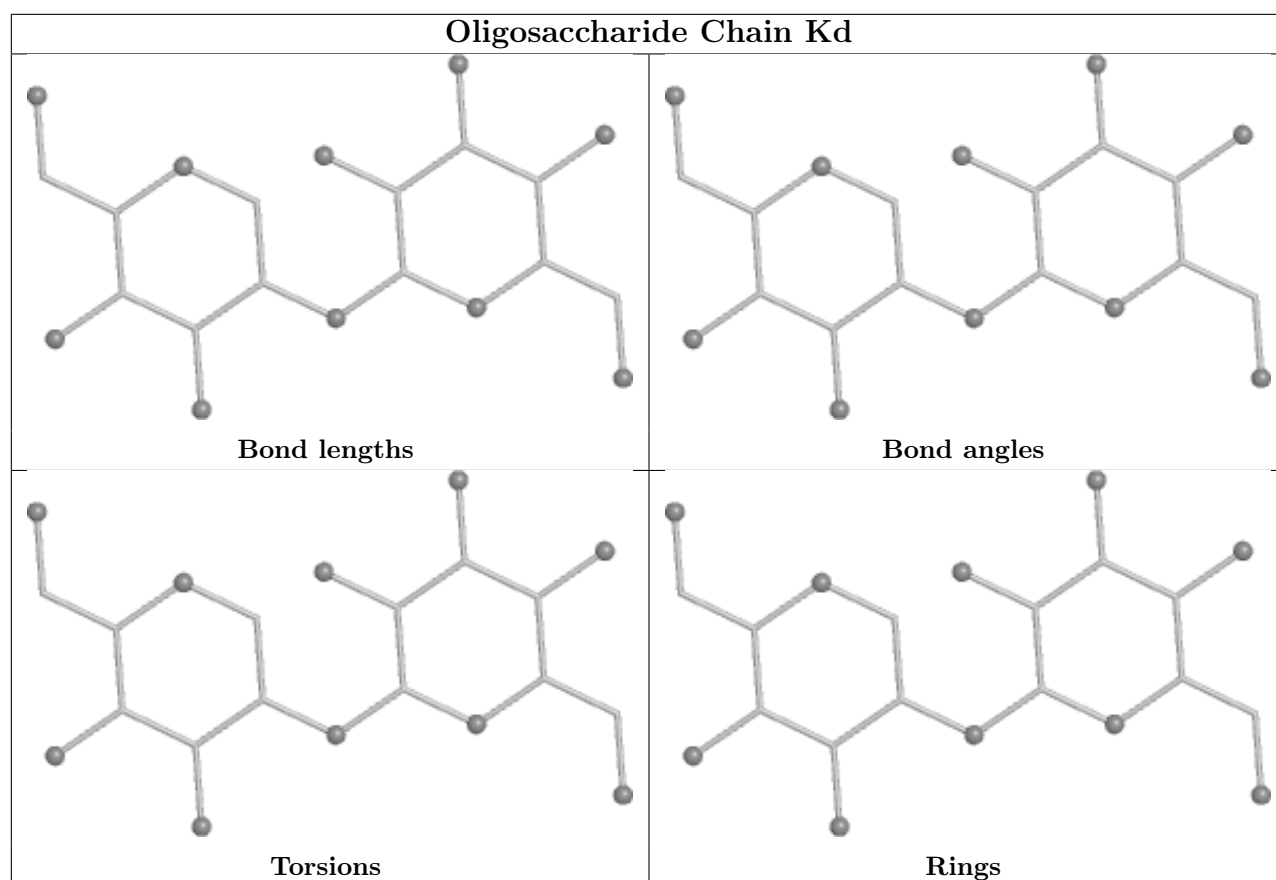
Oligosaccharide Chain Gd



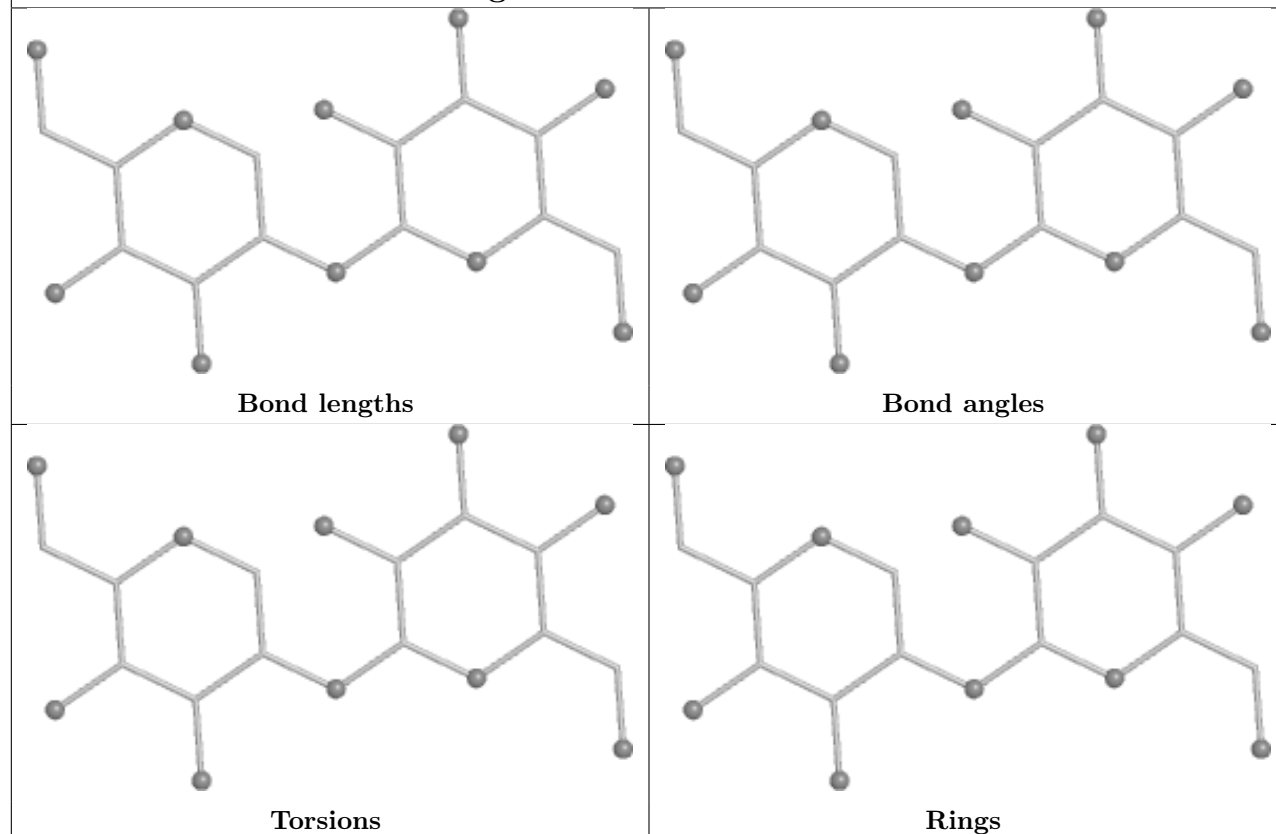
Oligosaccharide Chain Hd



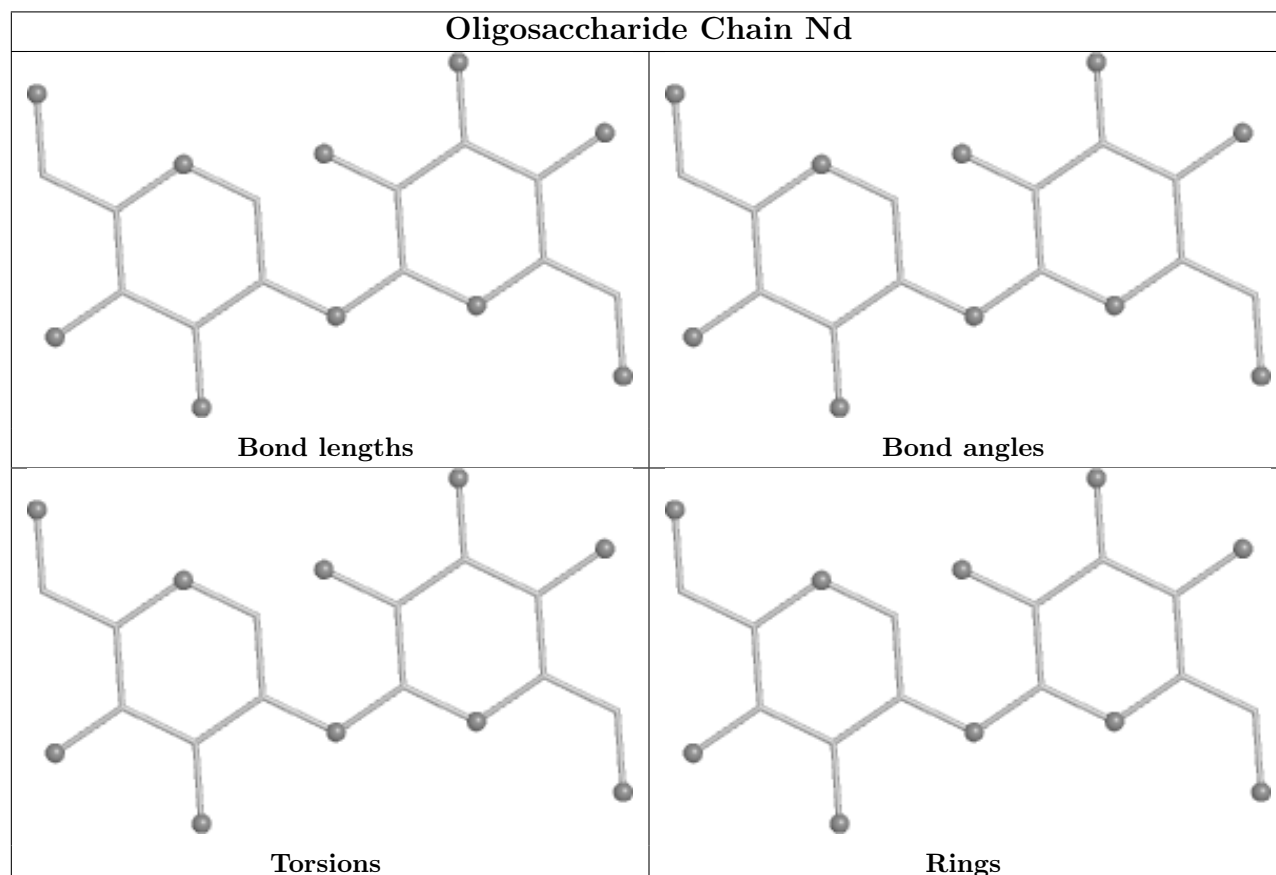


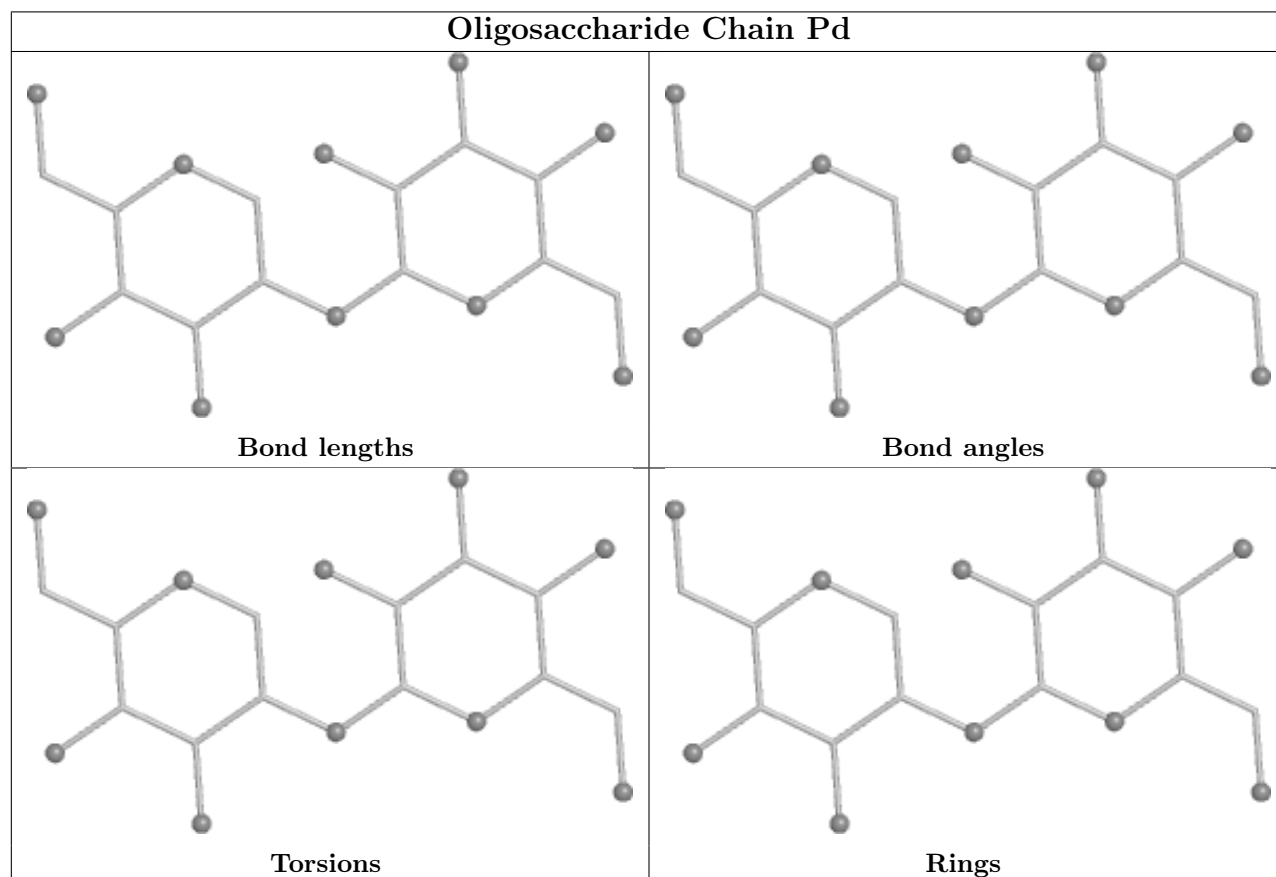
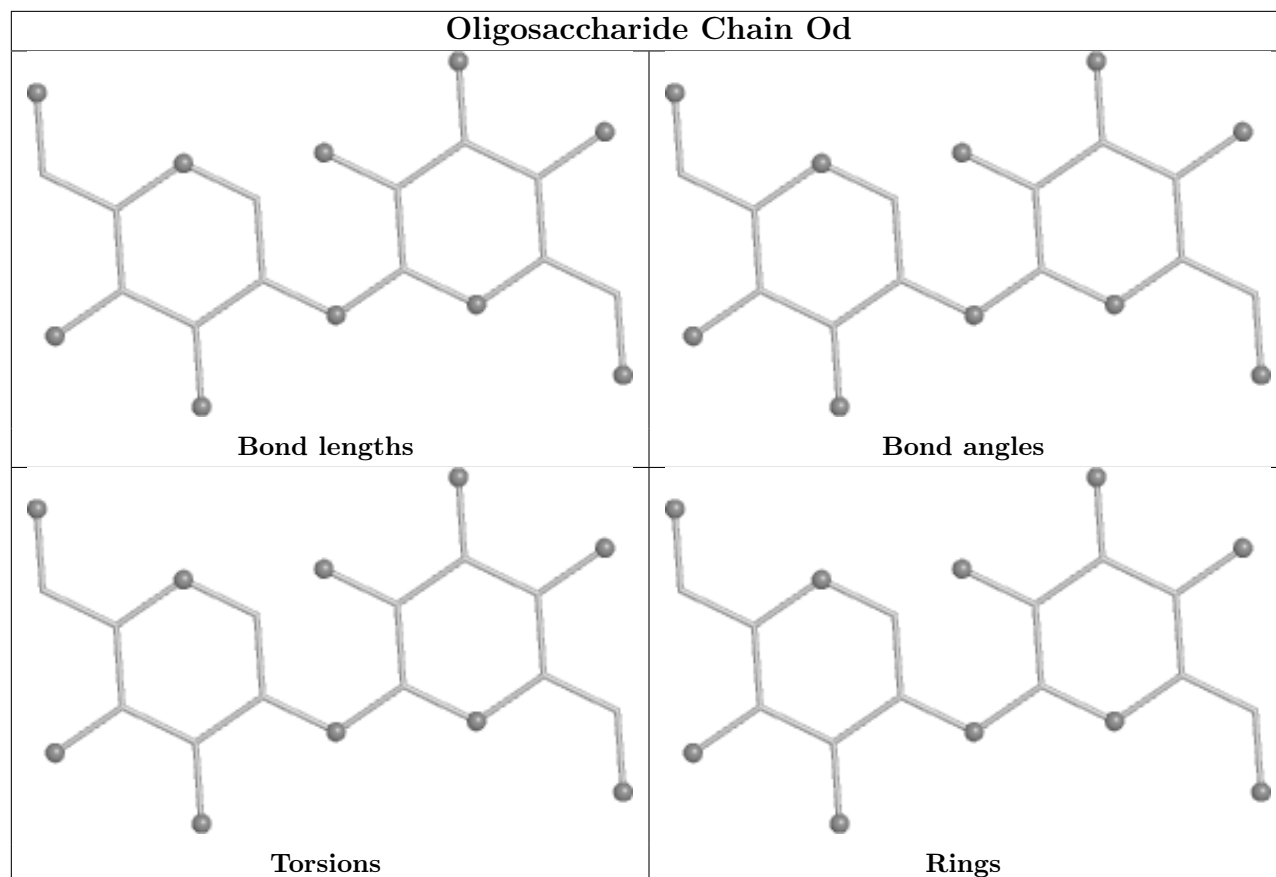


Oligosaccharide Chain Md

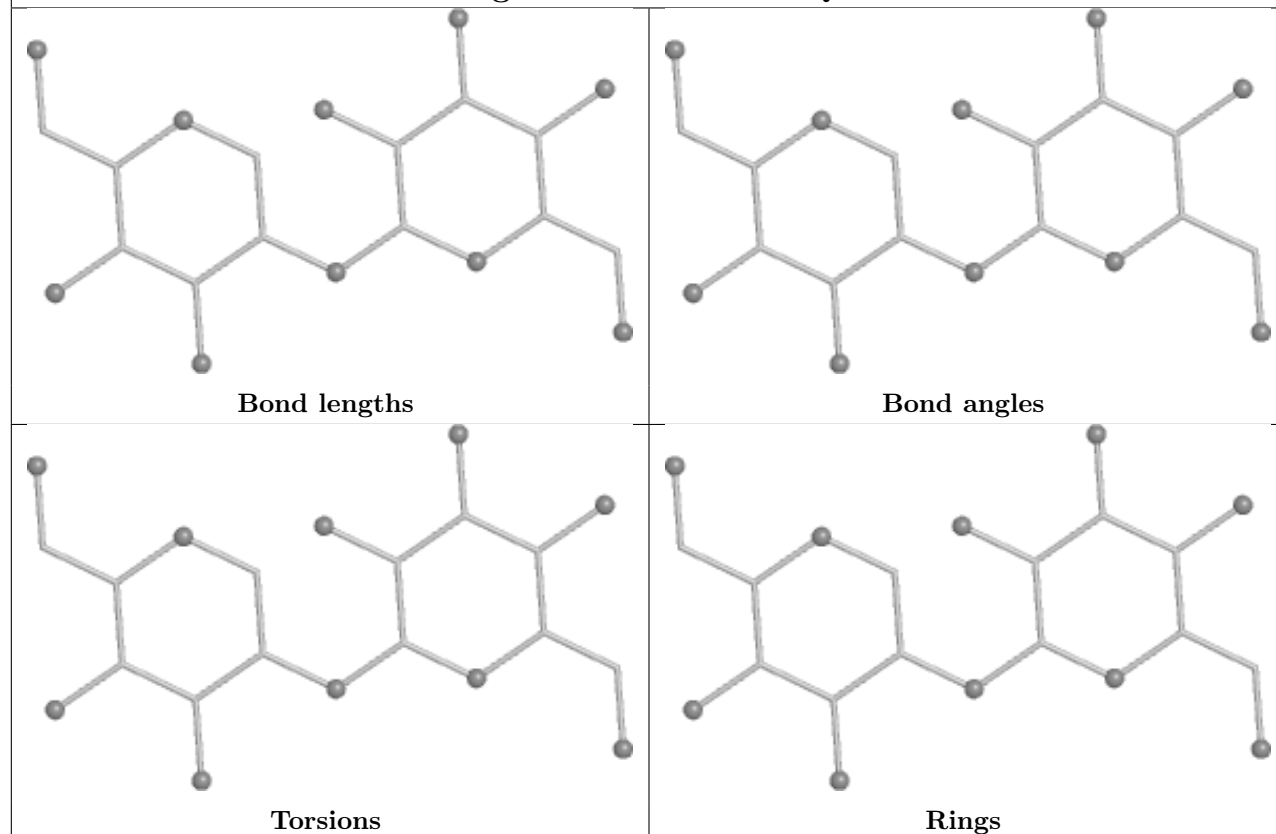


Oligosaccharide Chain Nd

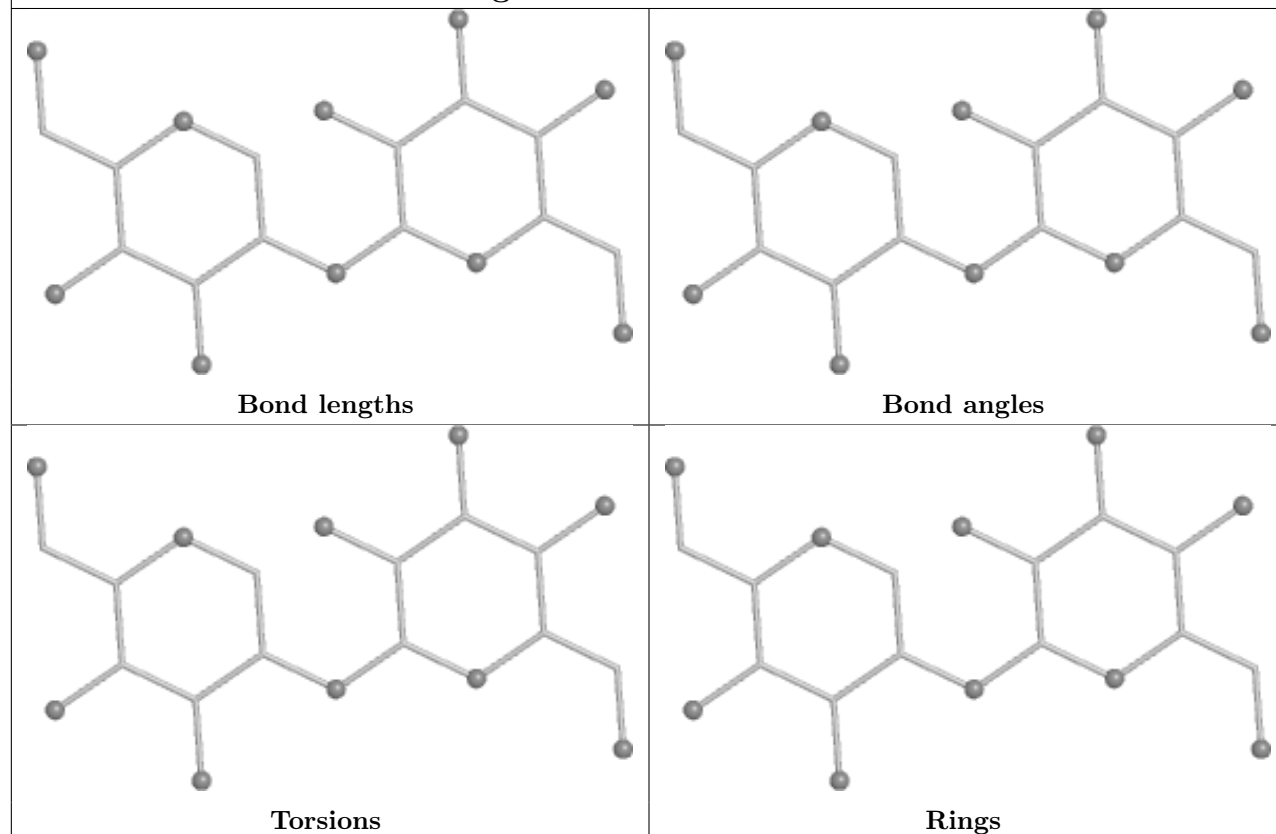




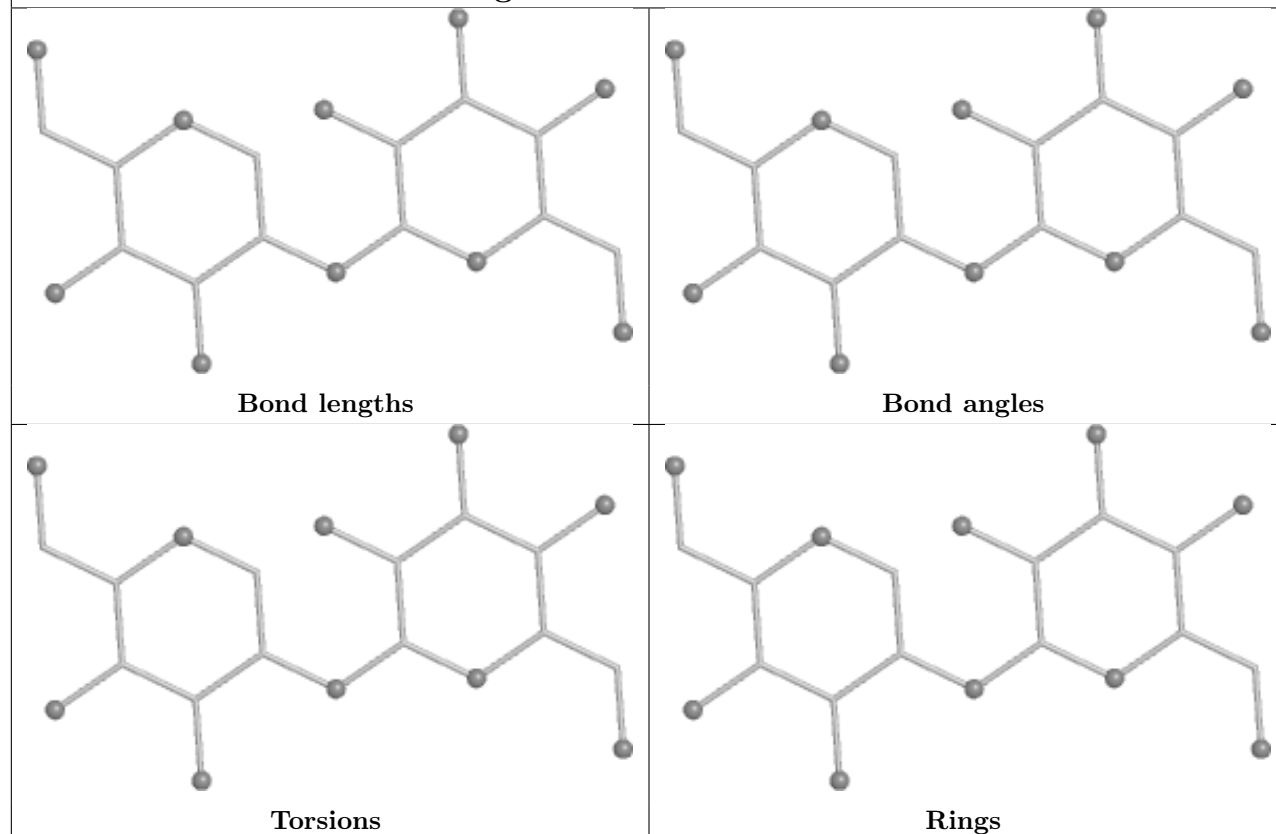
Oligosaccharide Chain Qd



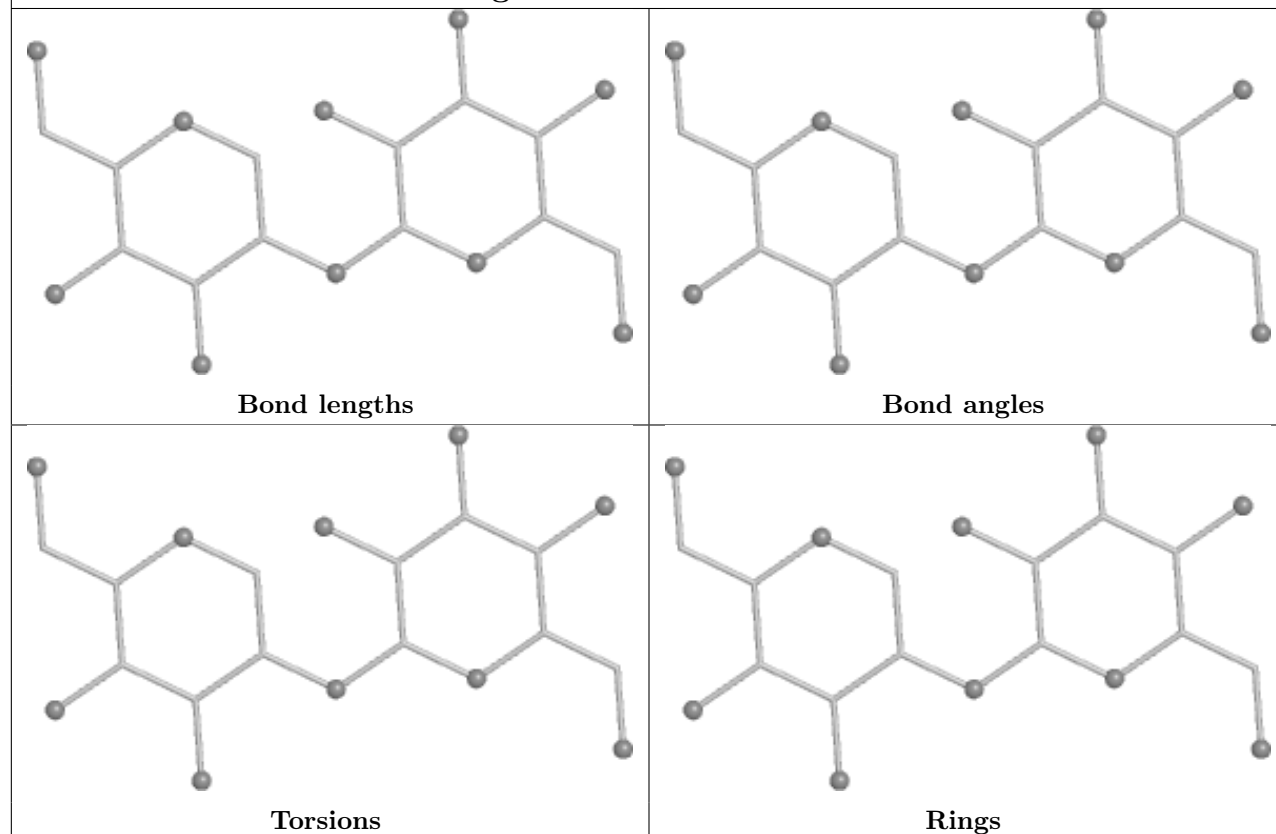
Oligosaccharide Chain Rd

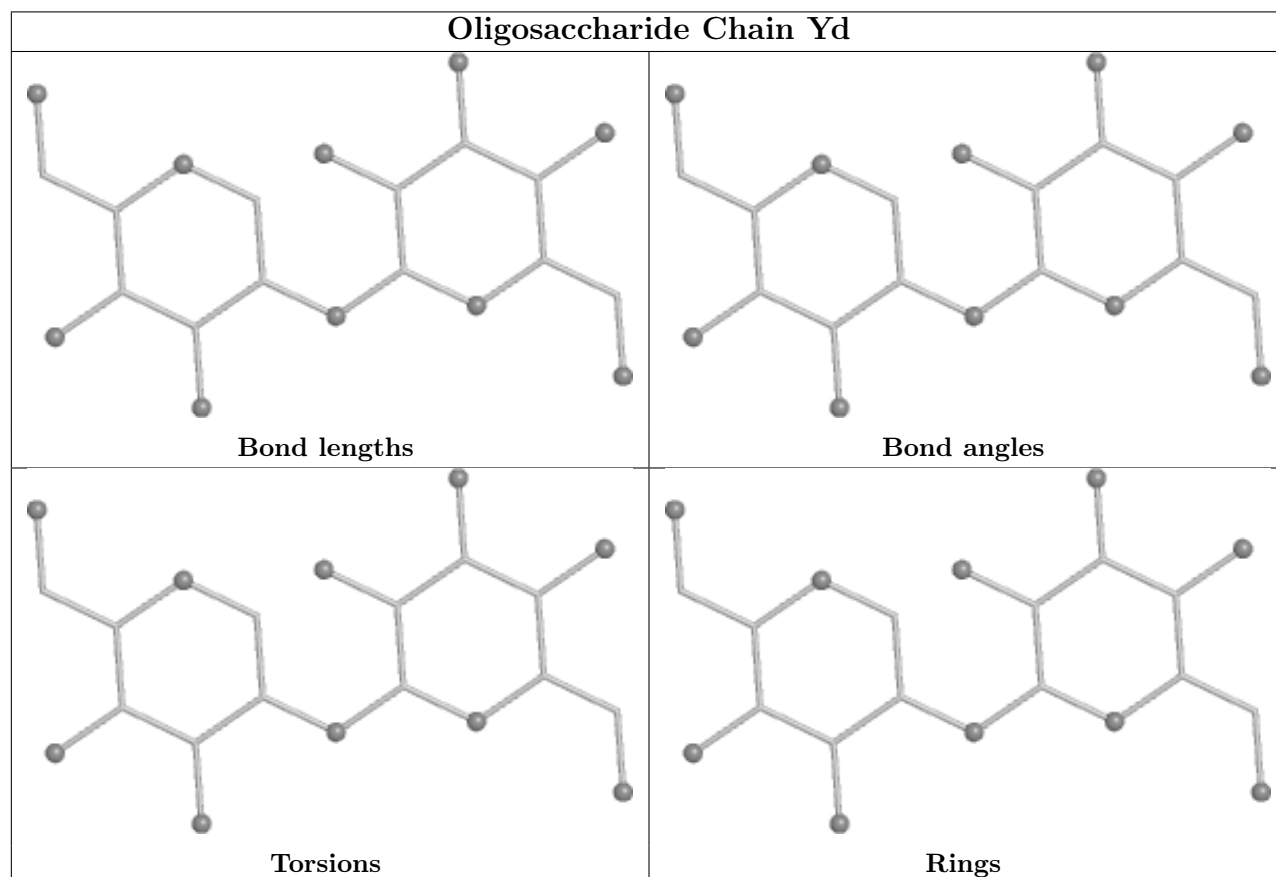
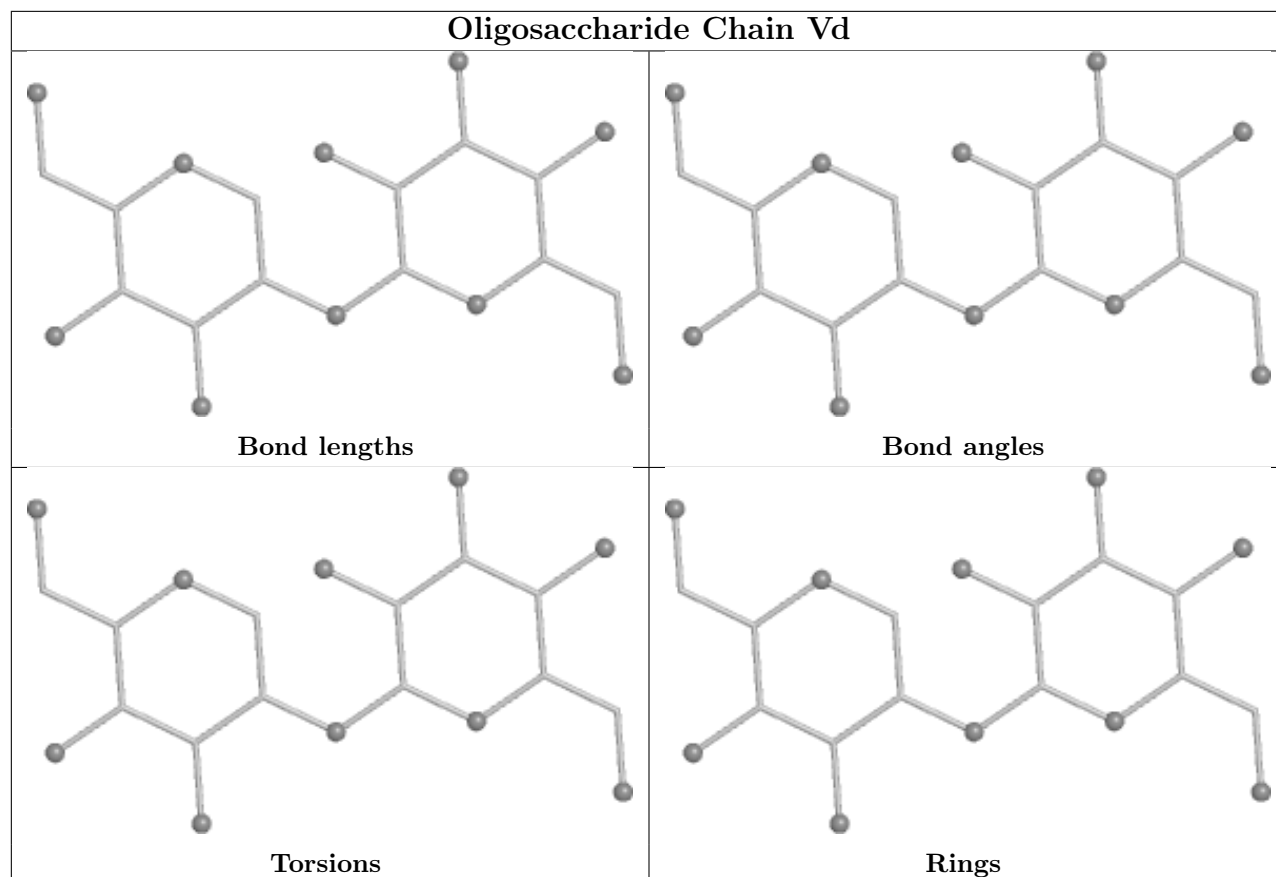


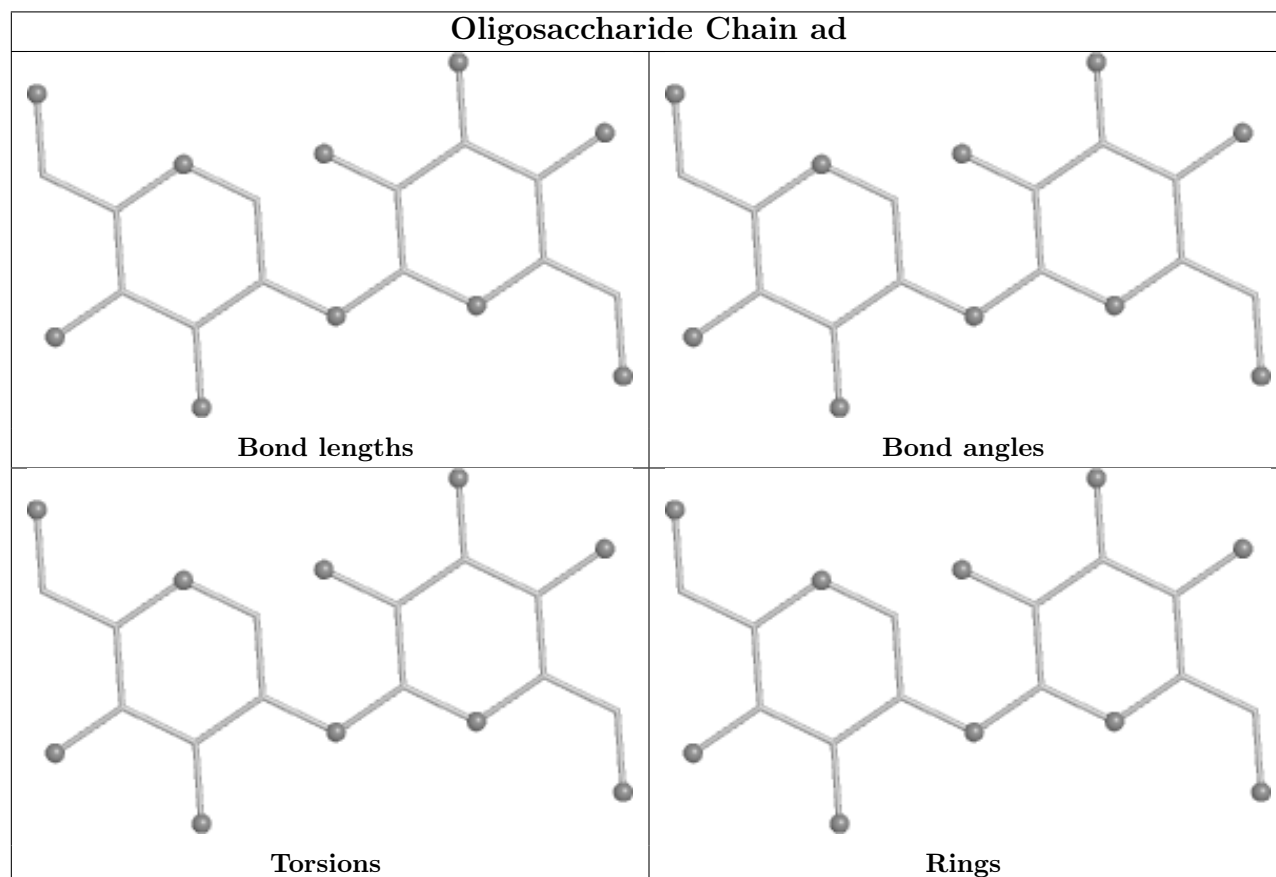
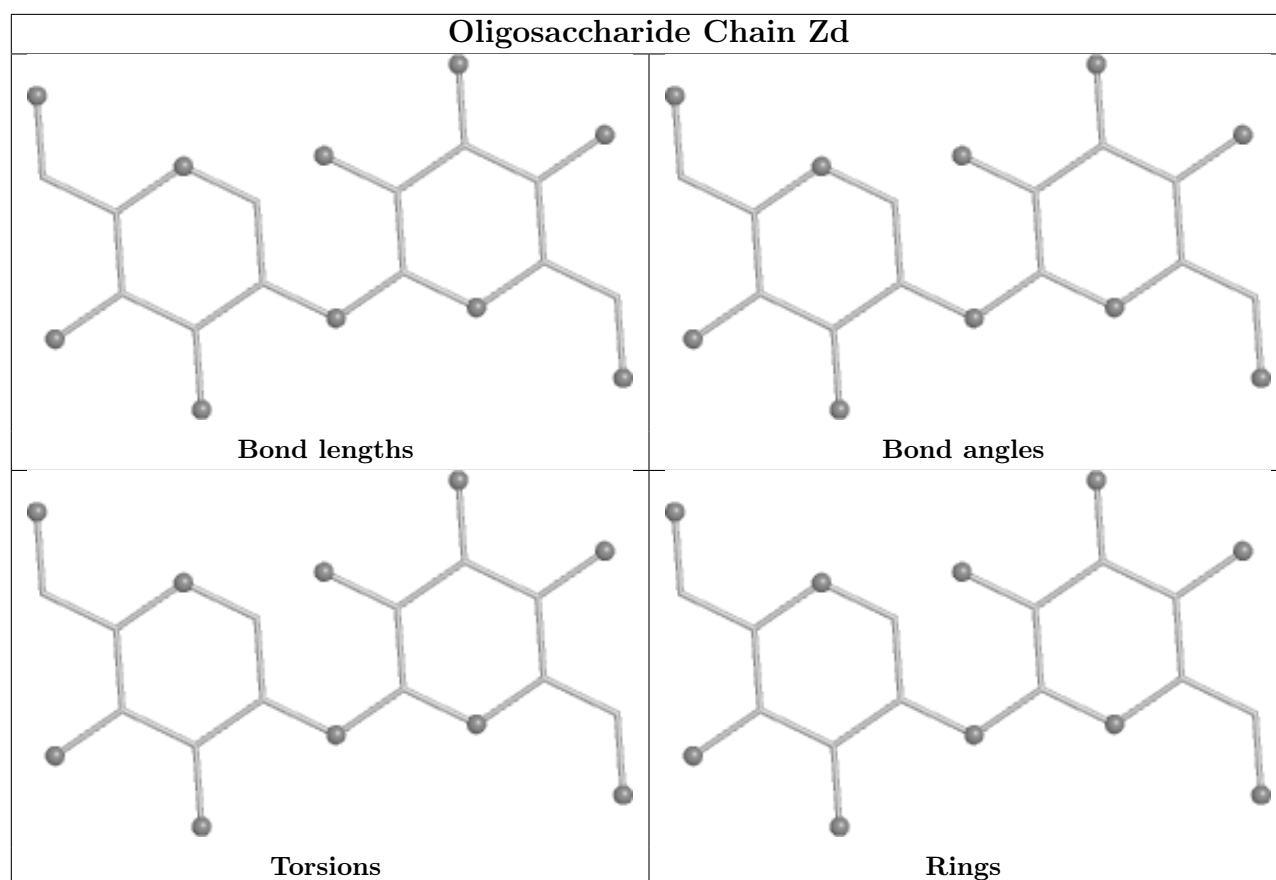
Oligosaccharide Chain Td

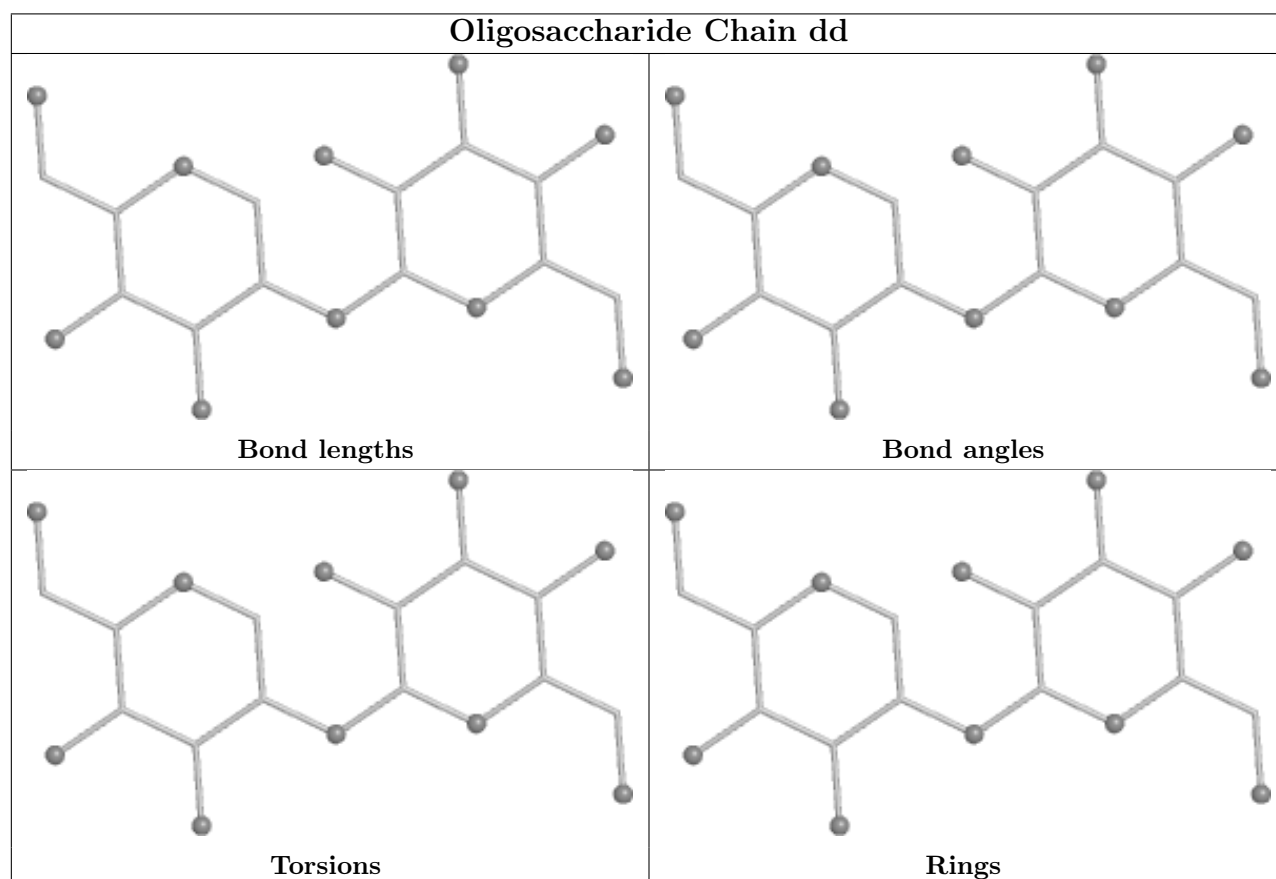
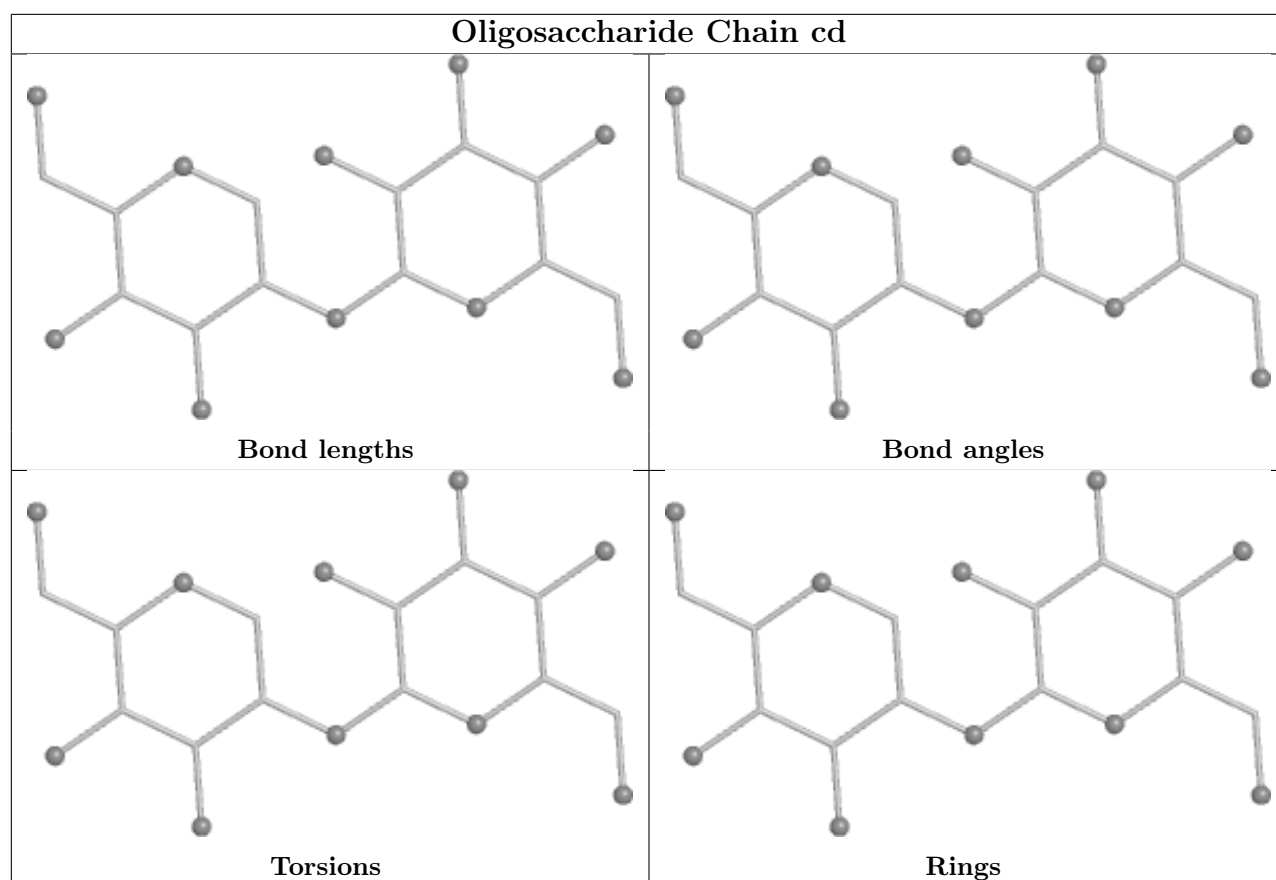


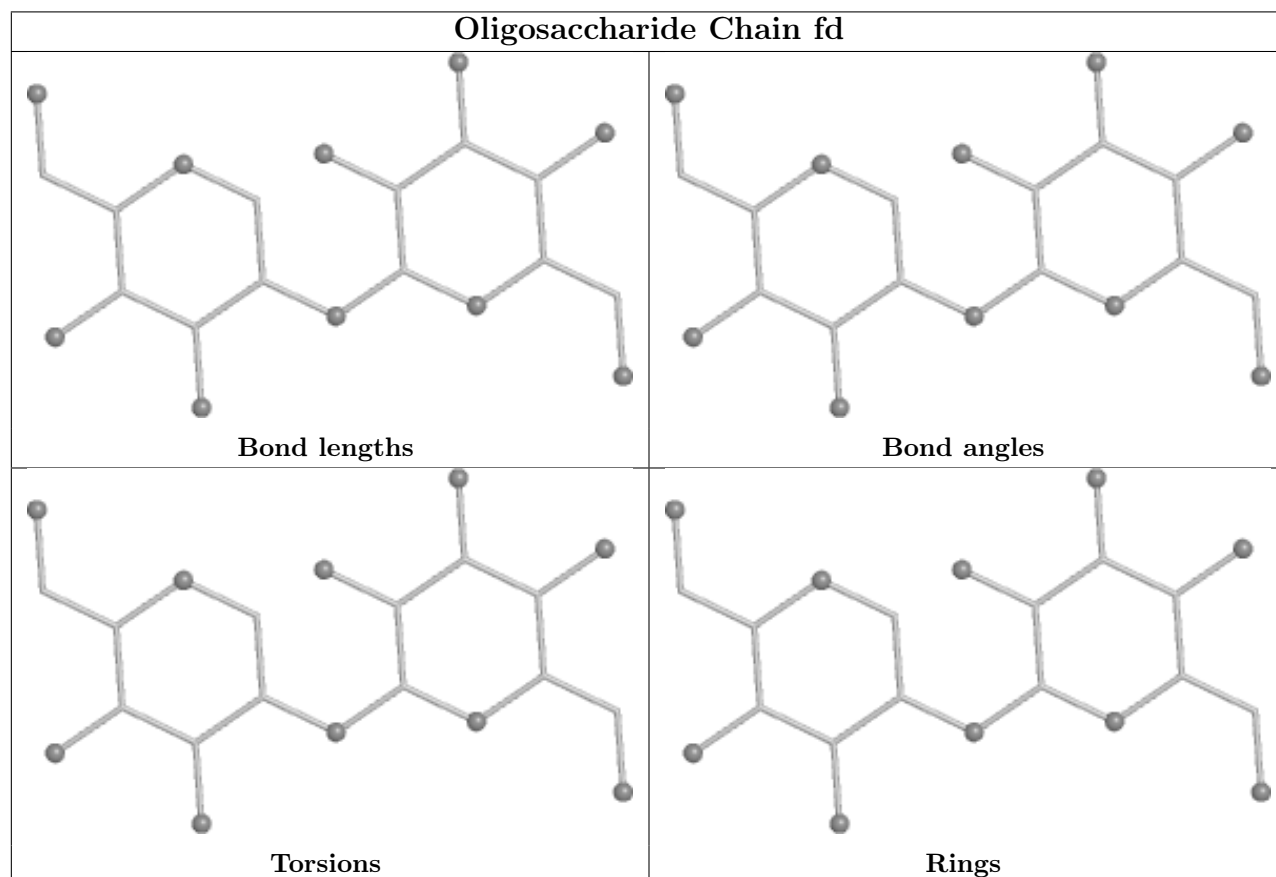
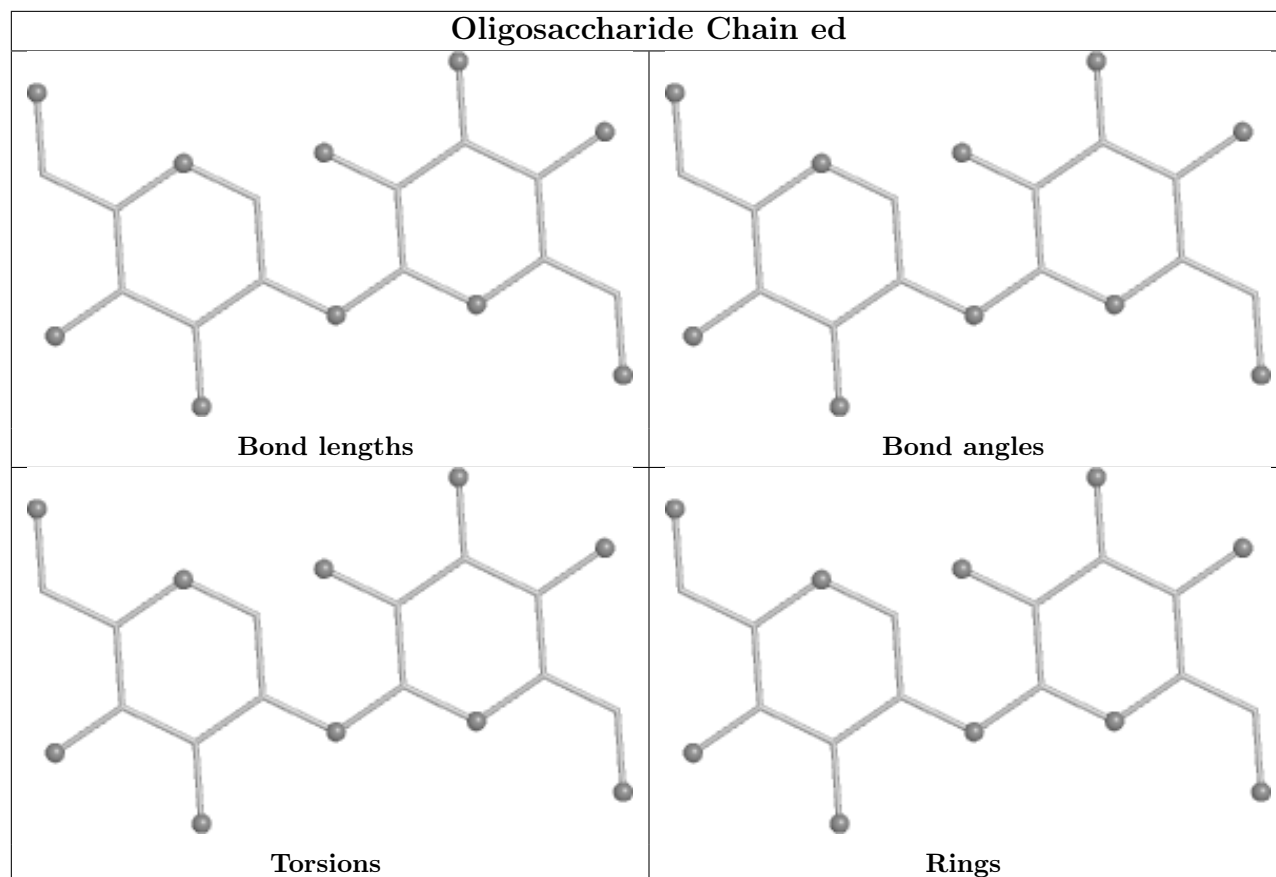
Oligosaccharide Chain Ud

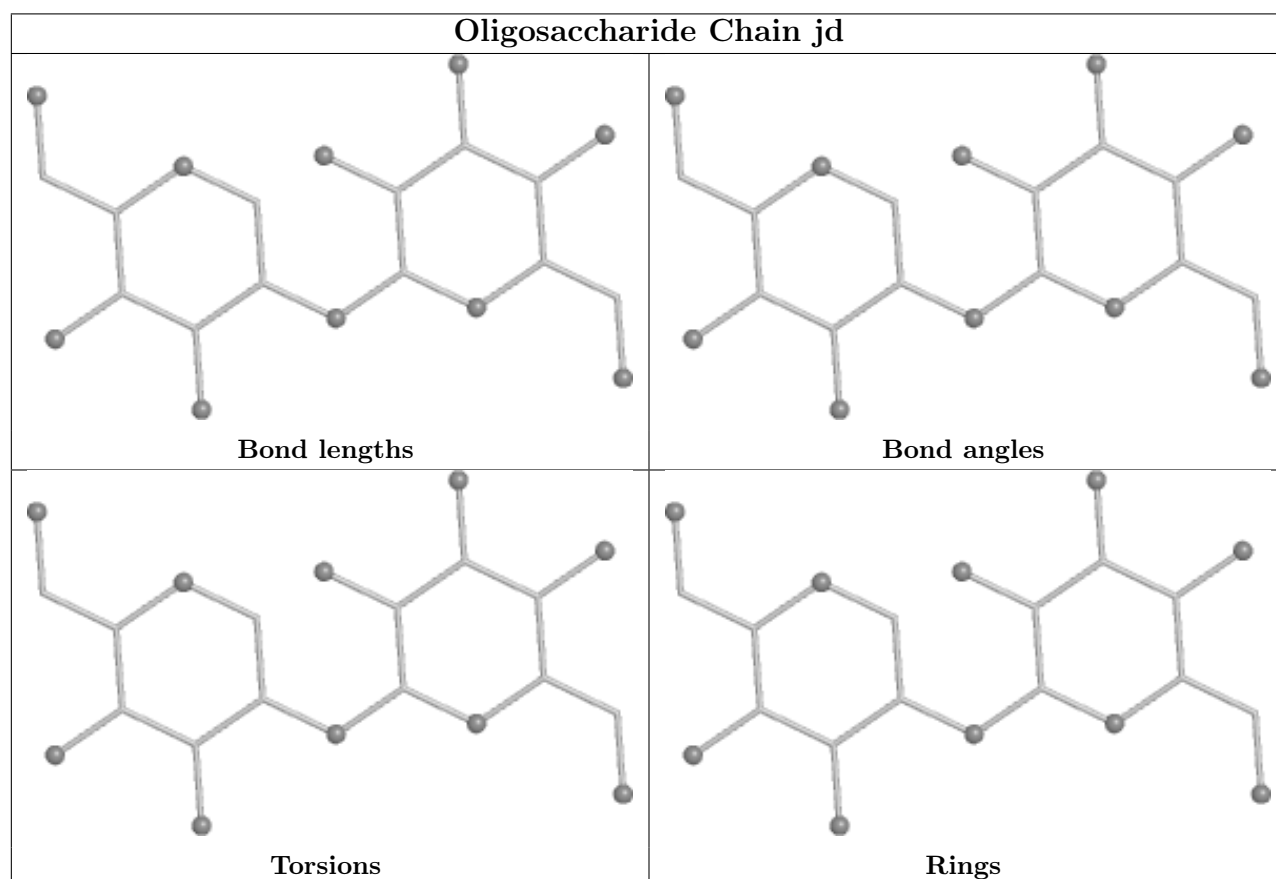
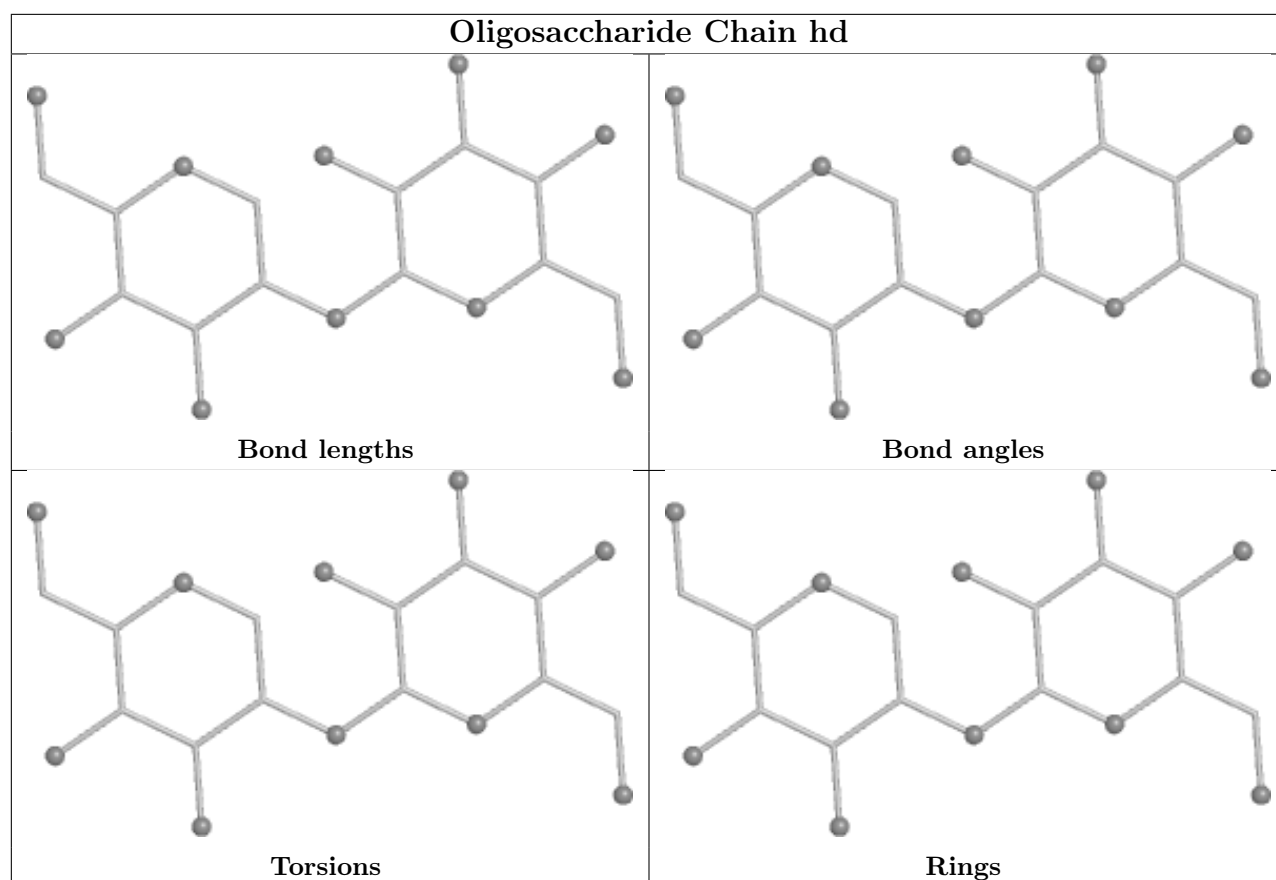


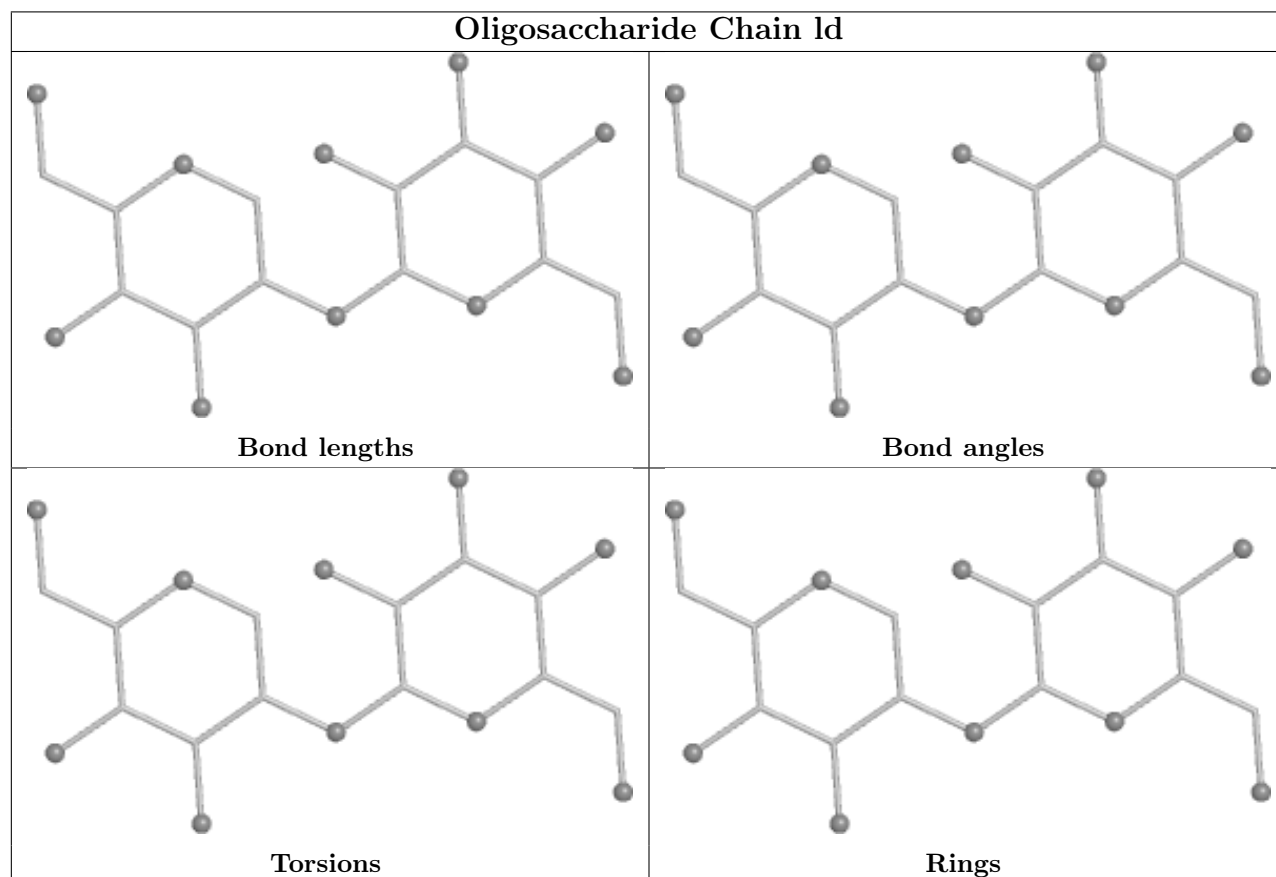
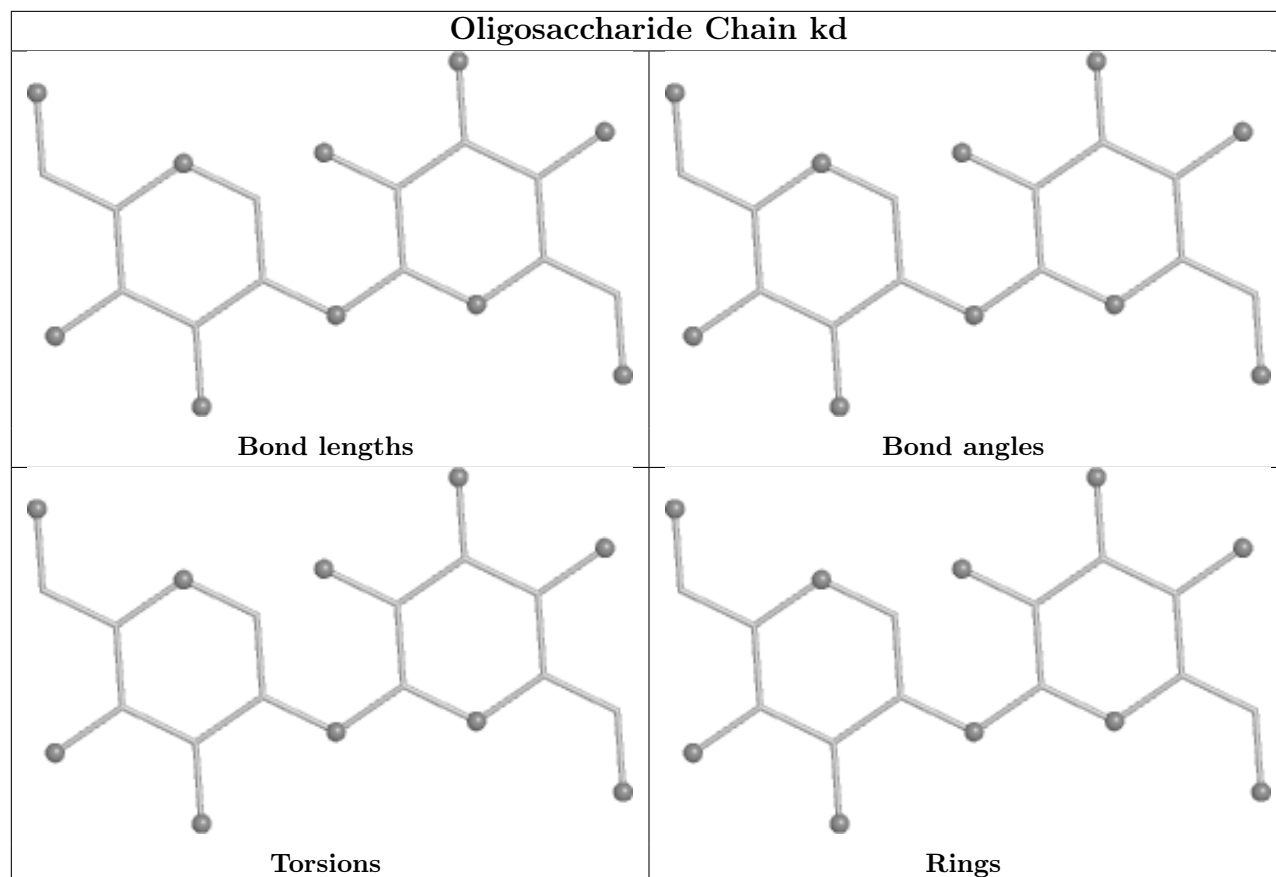


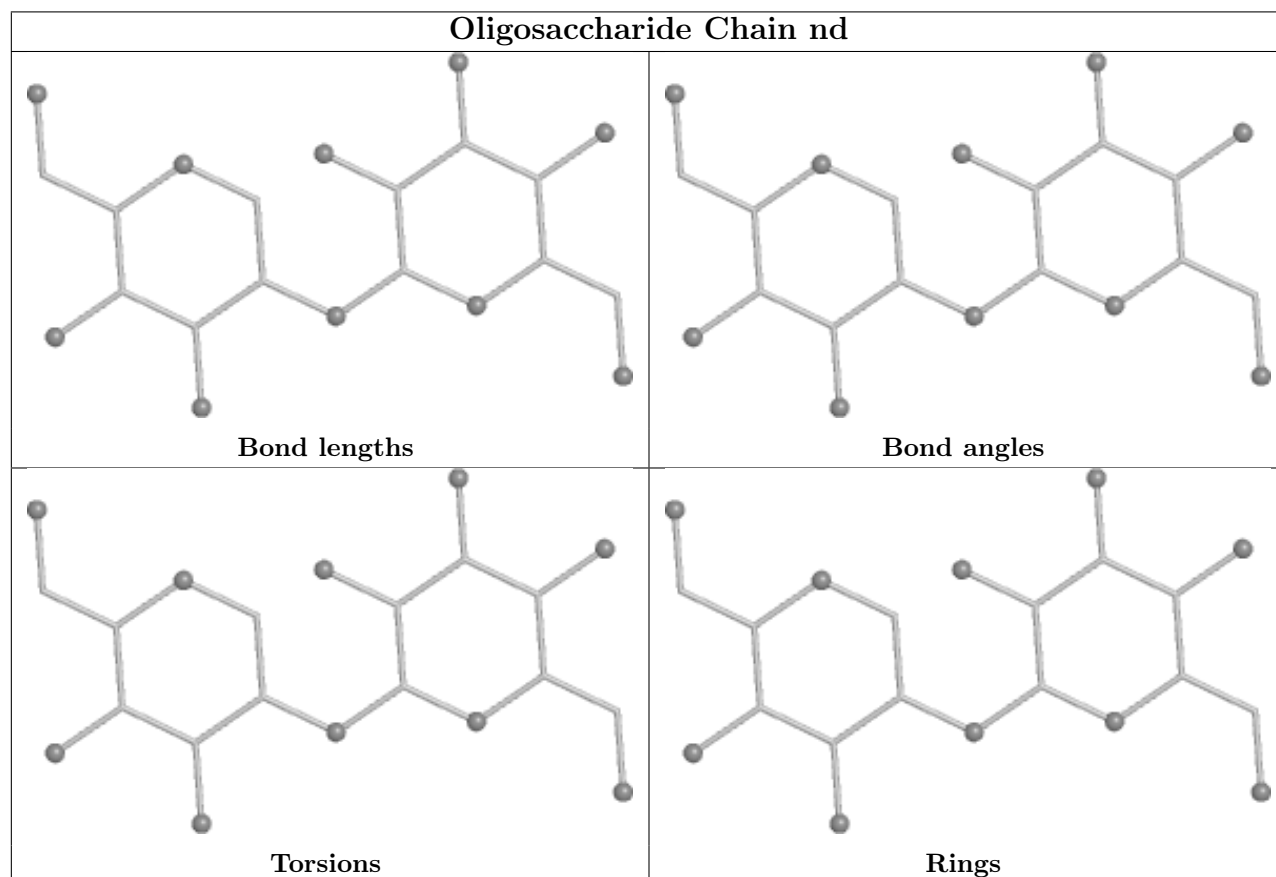
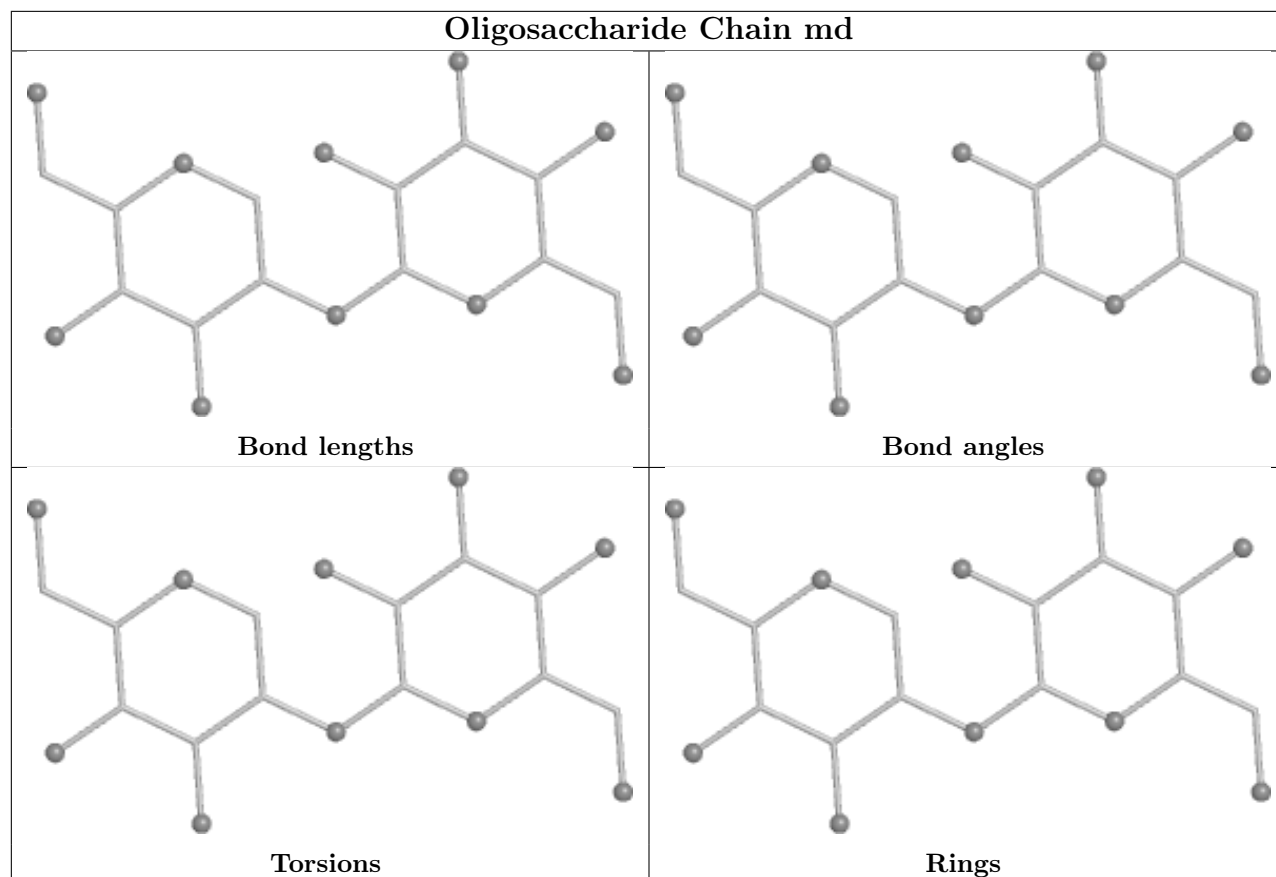


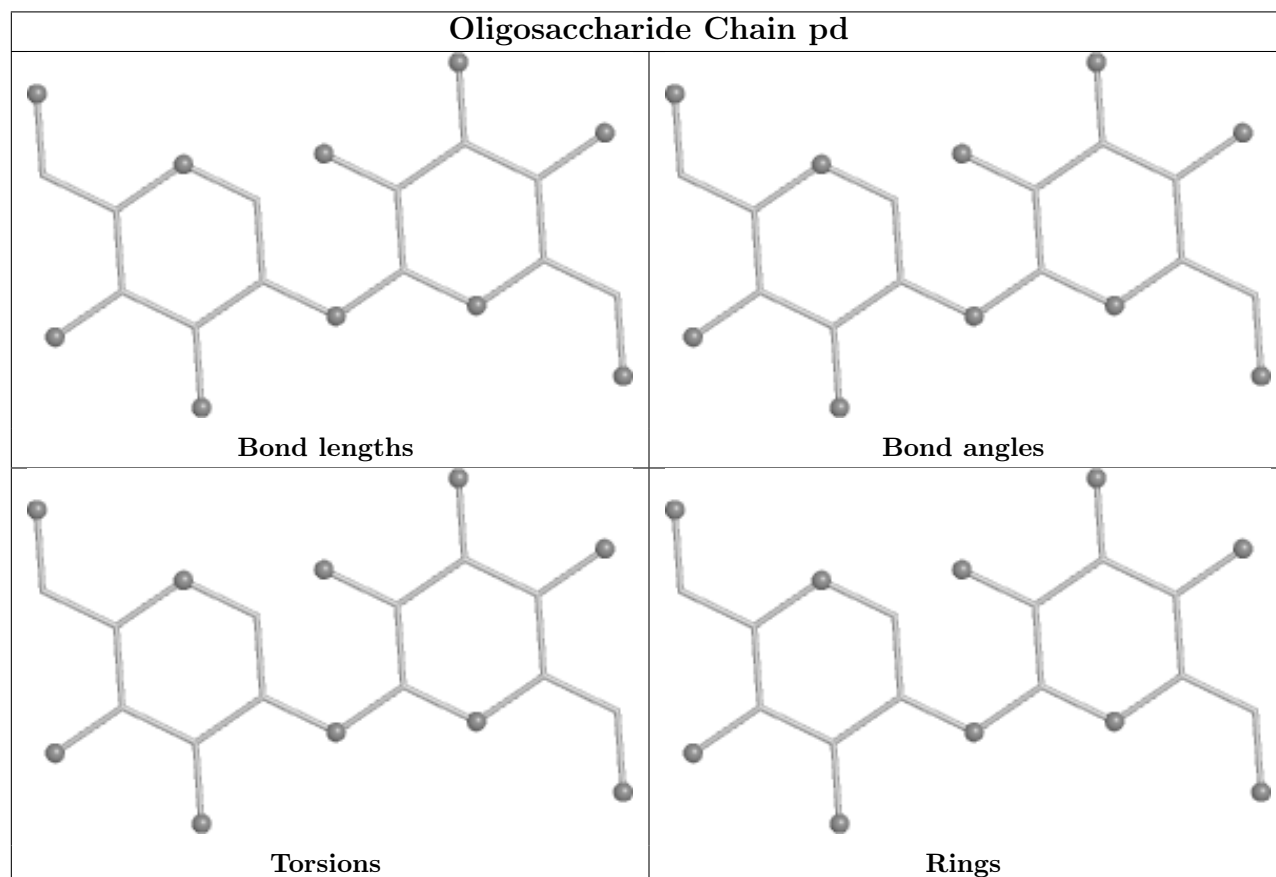
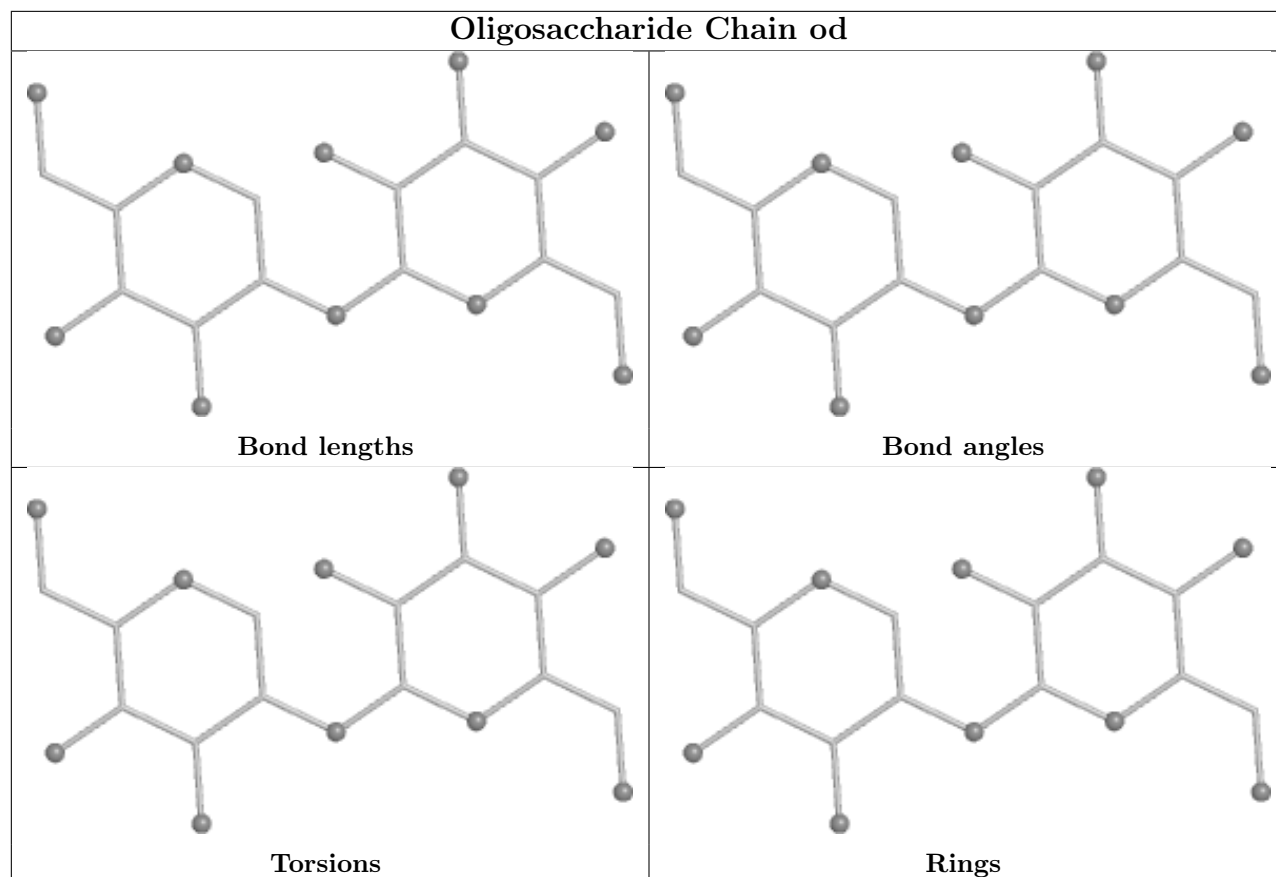


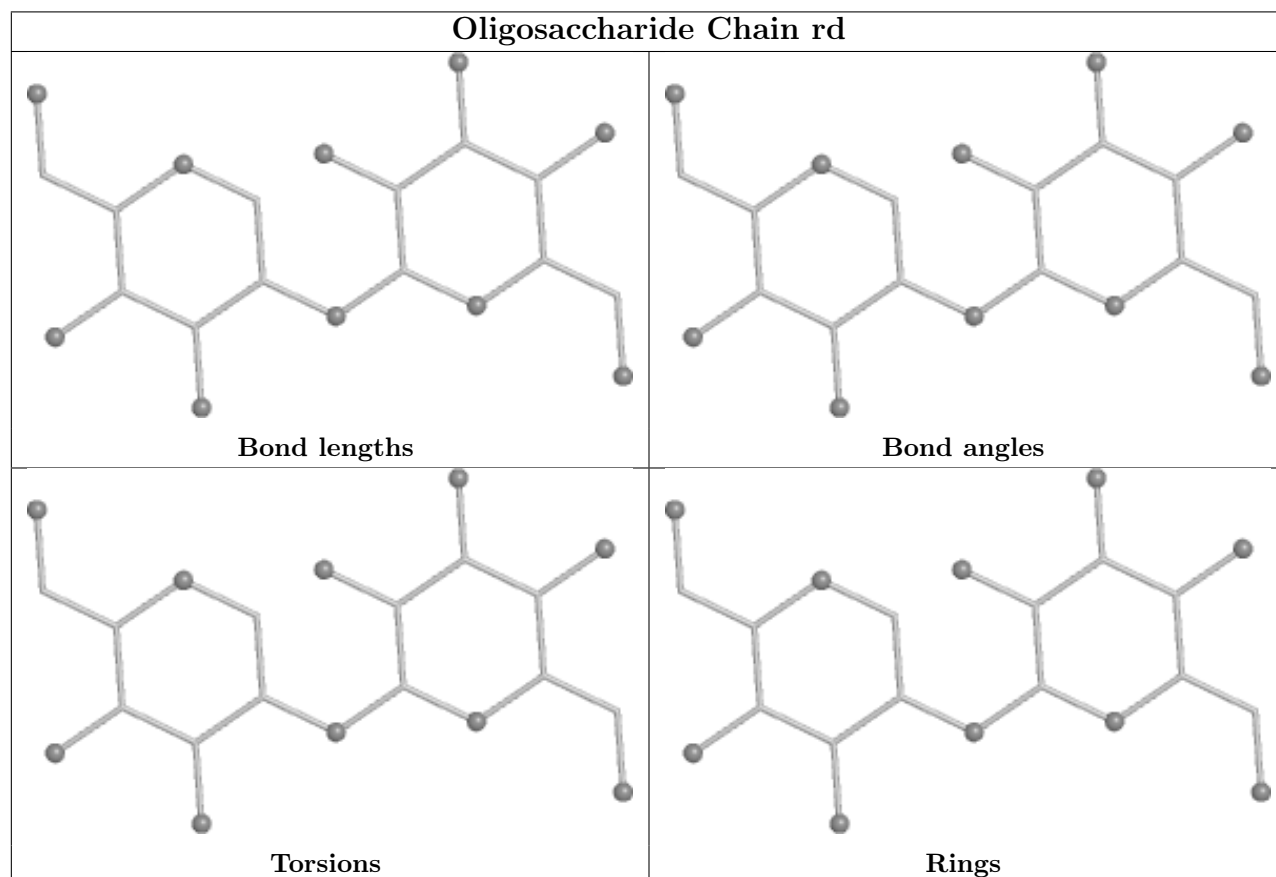
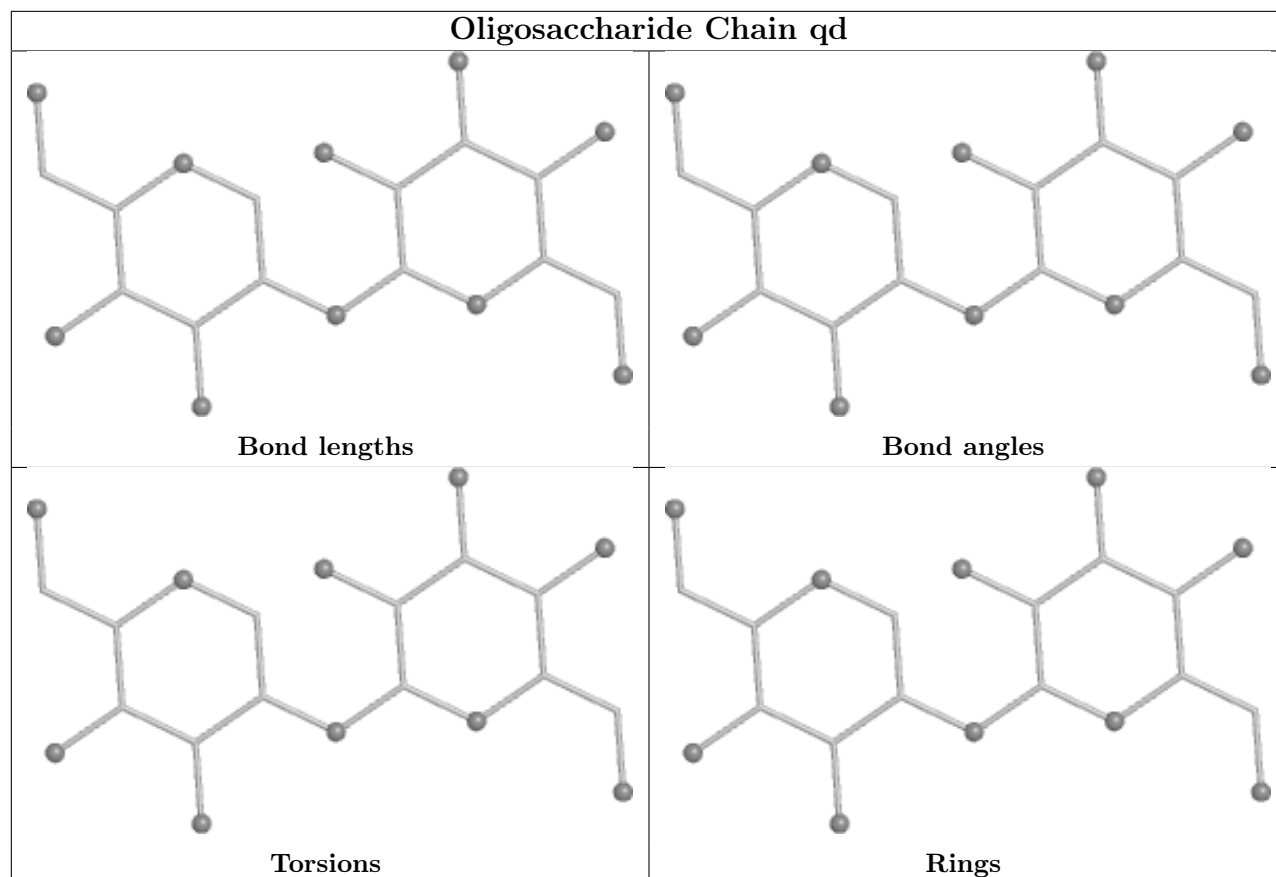


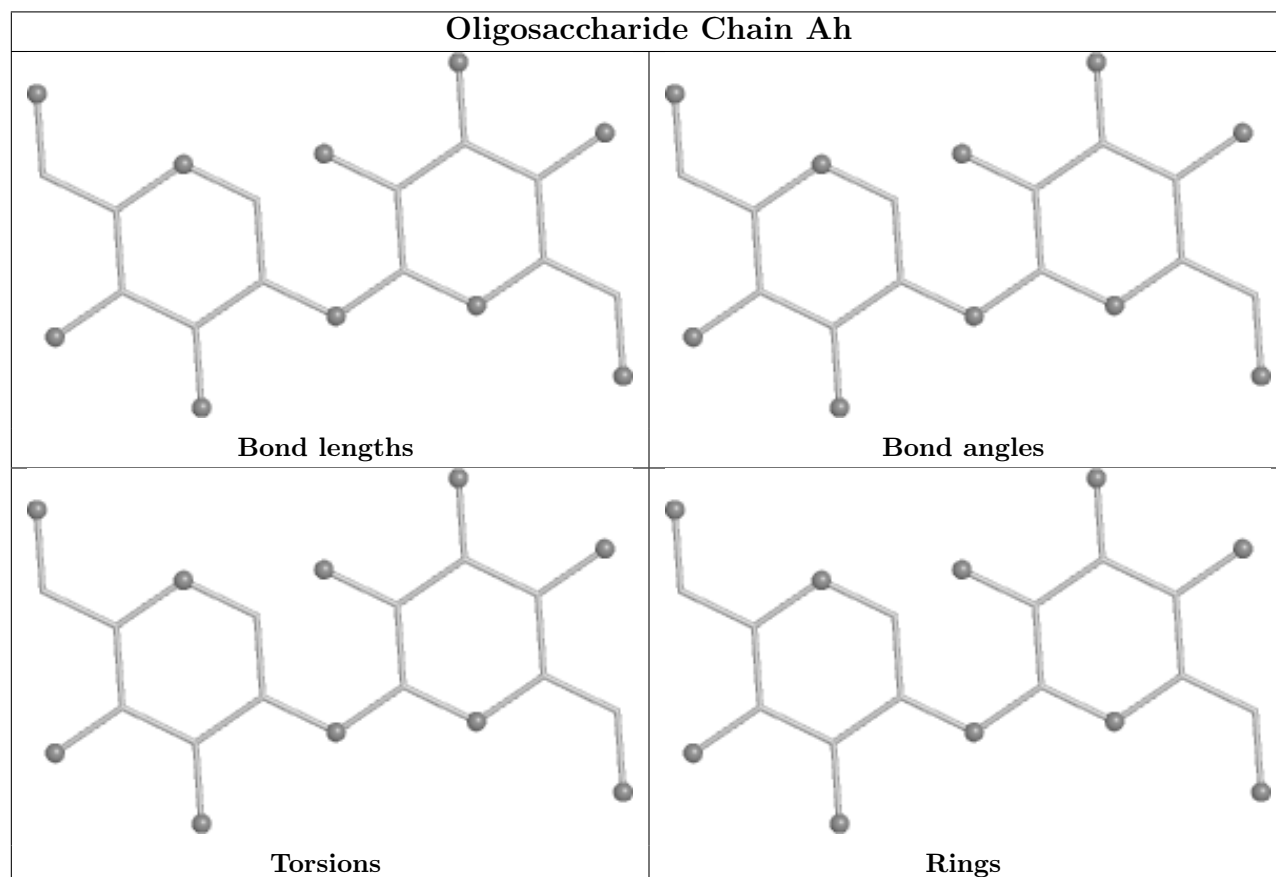
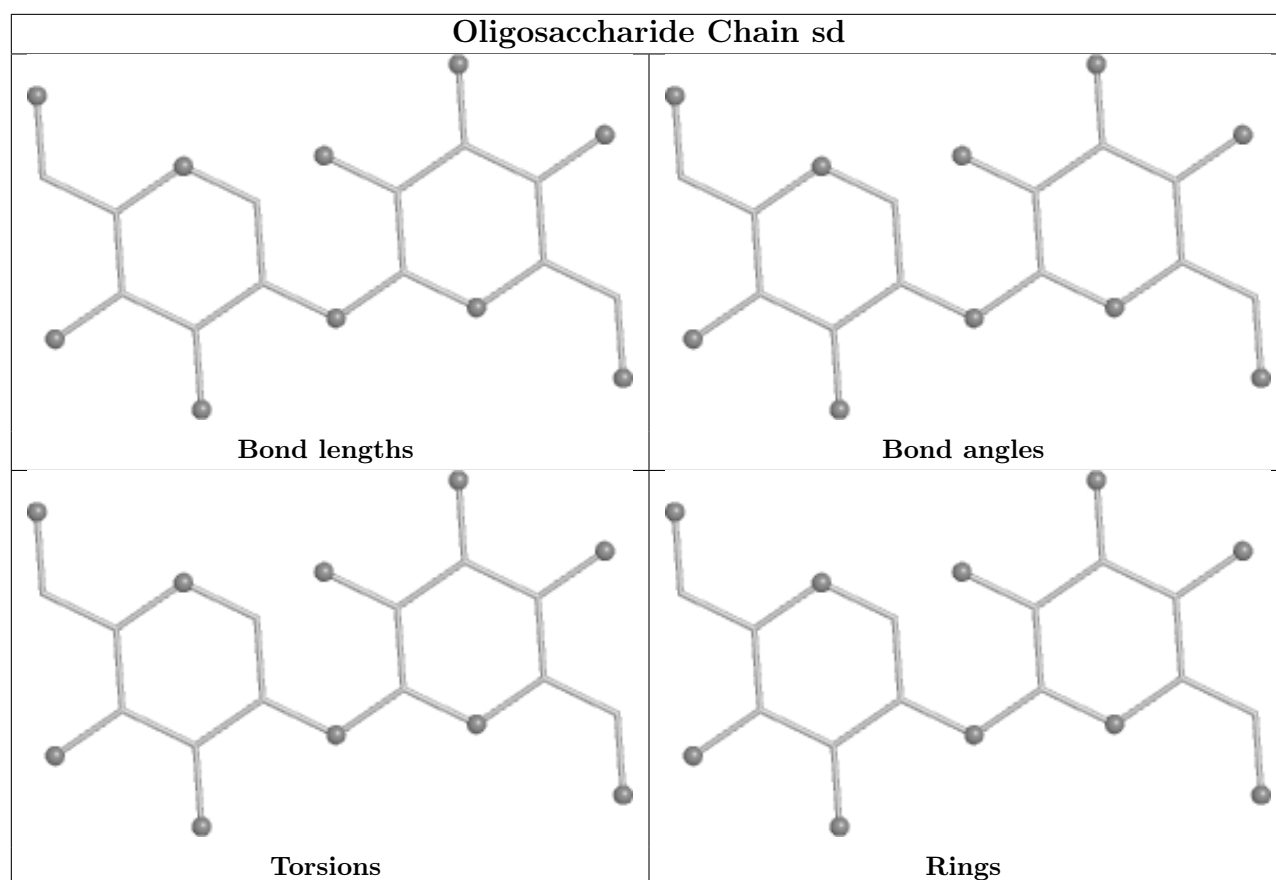




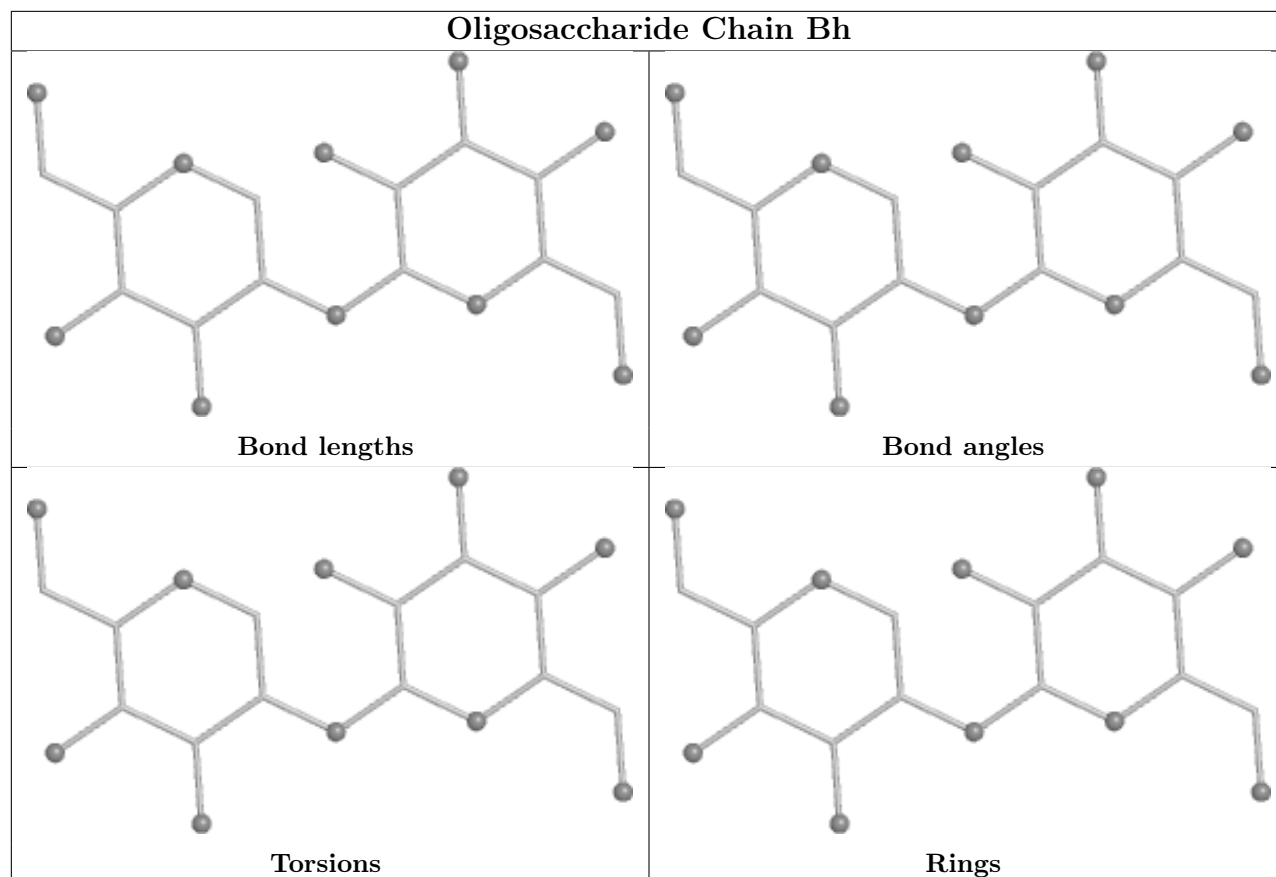




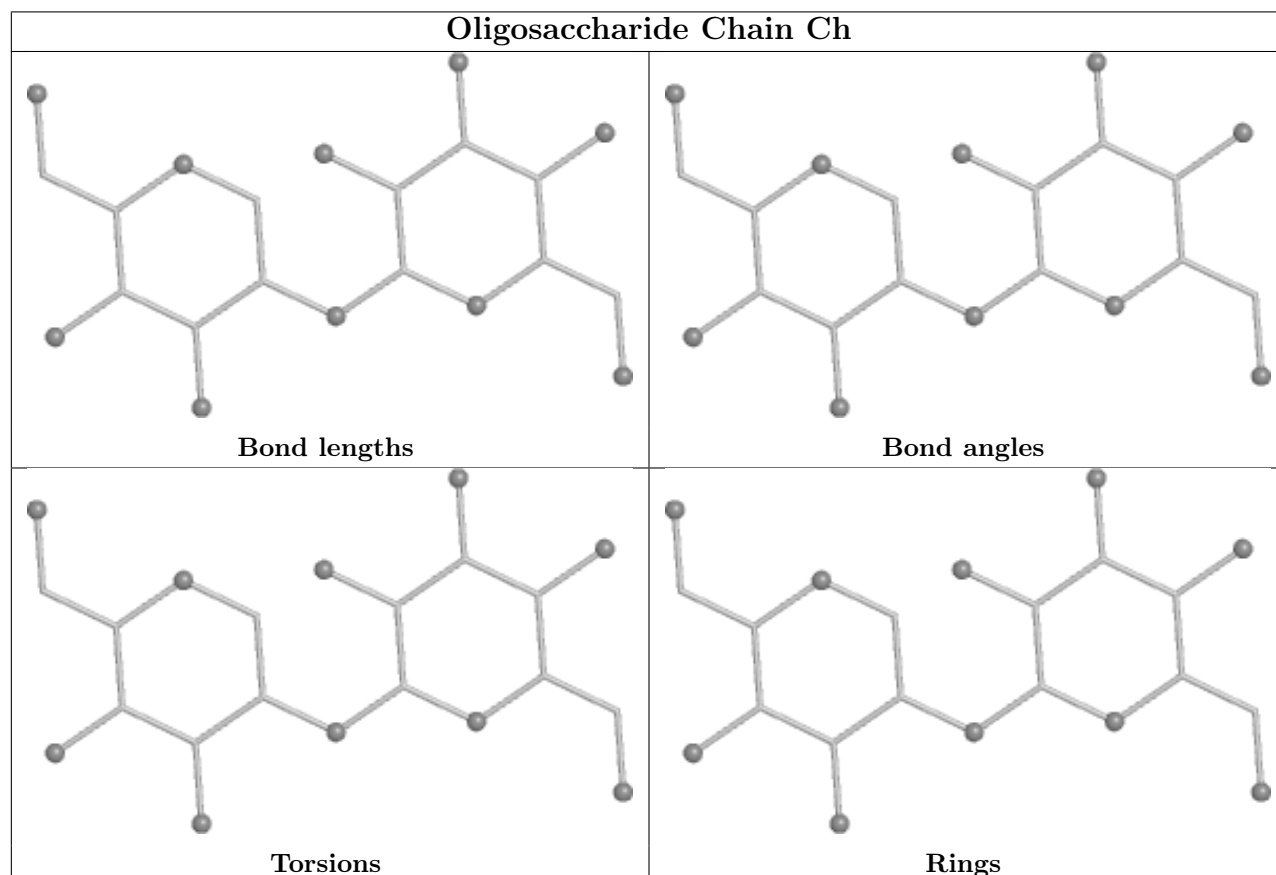


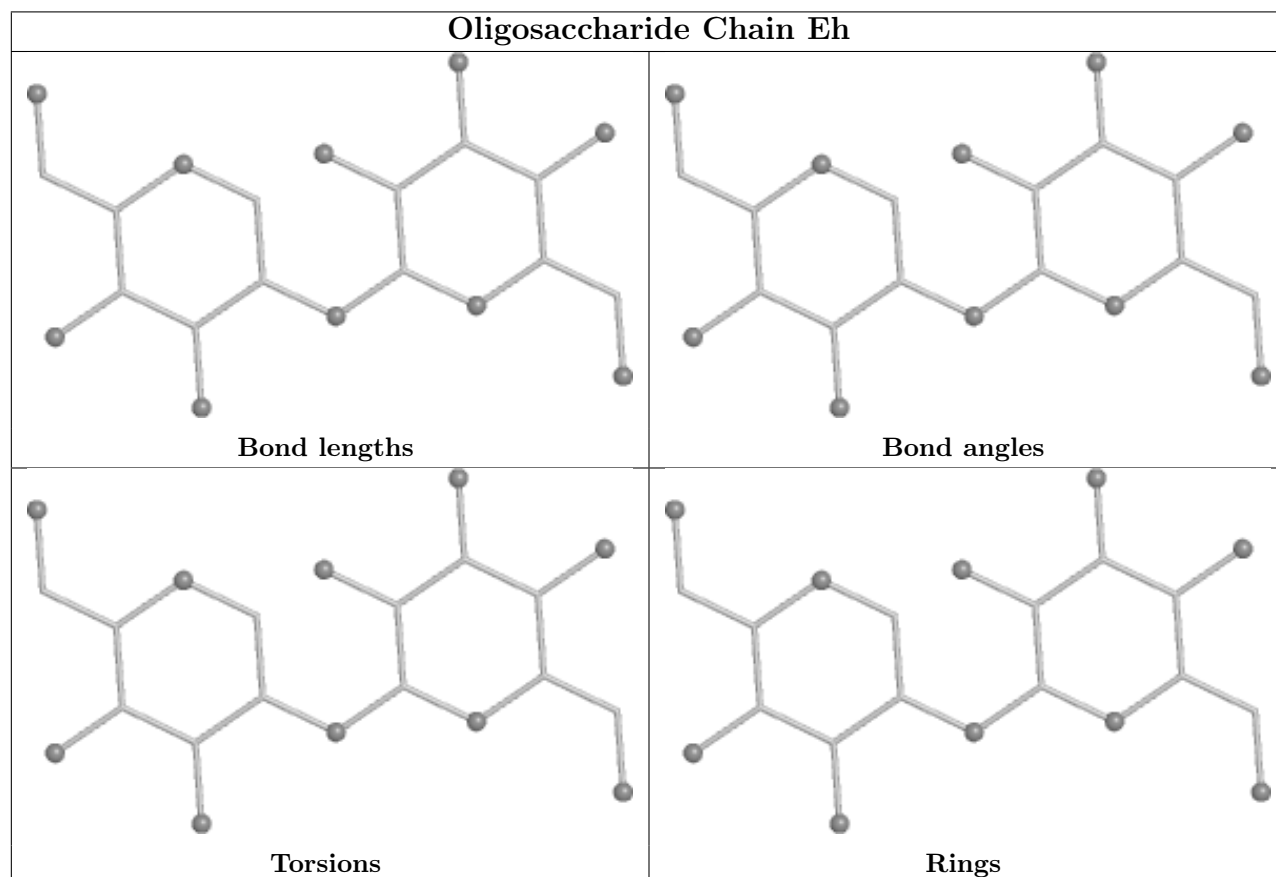
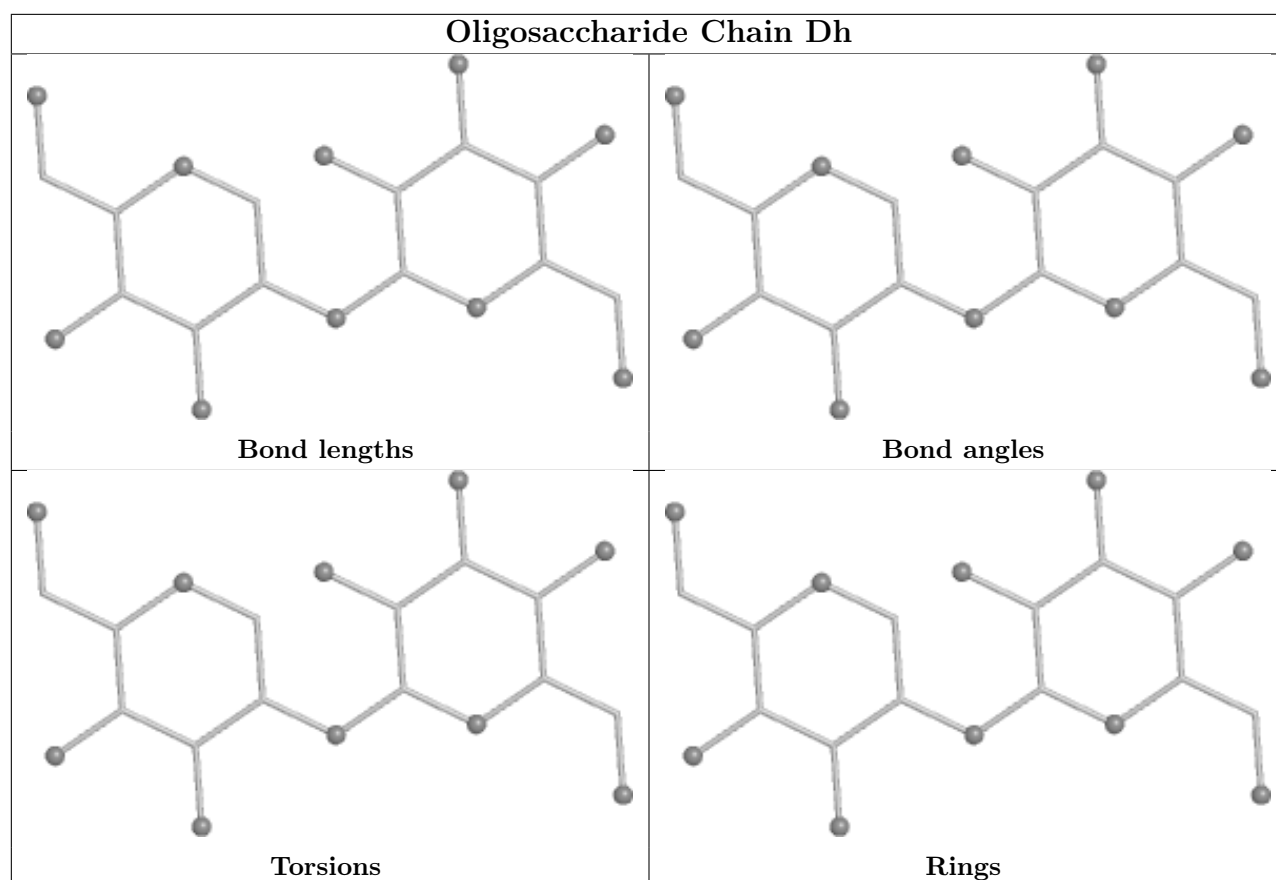


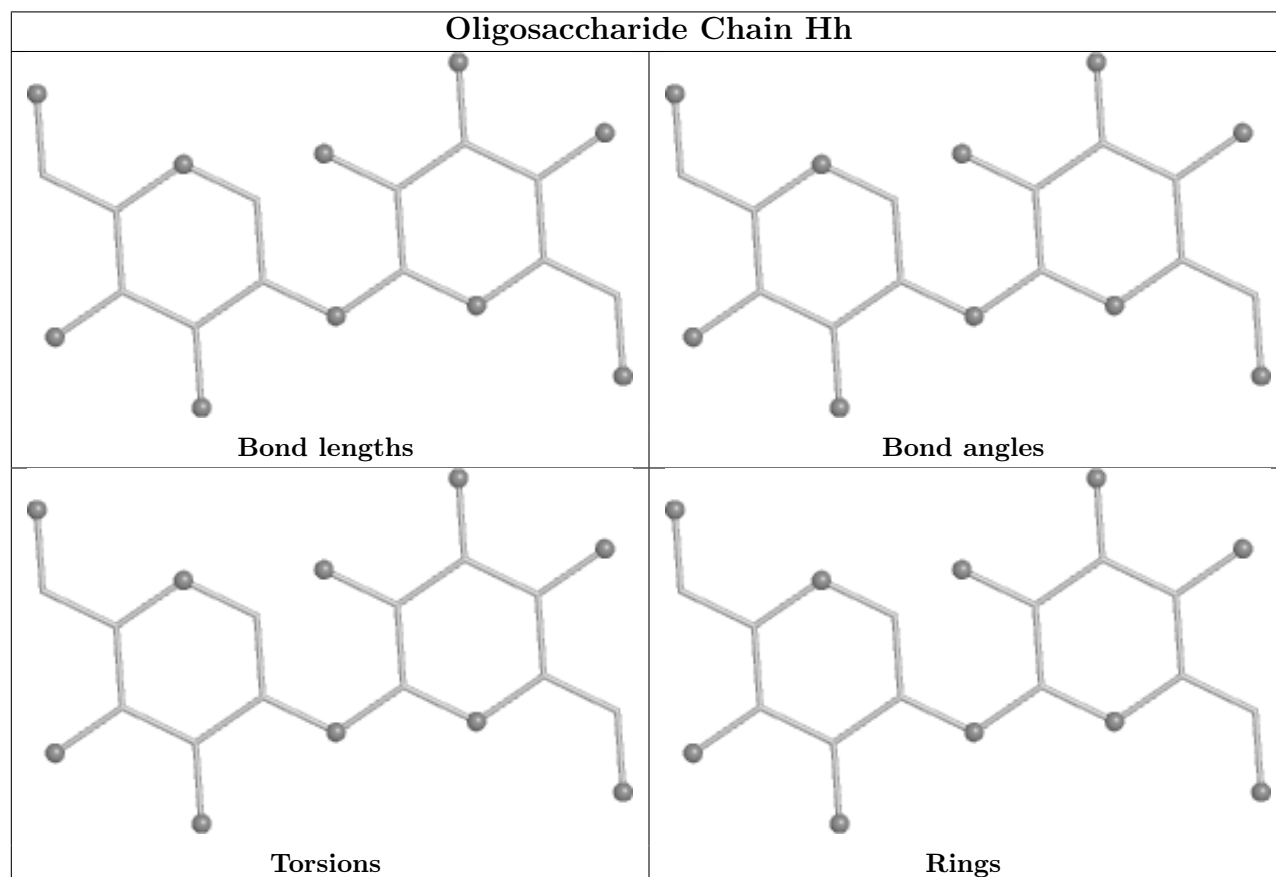
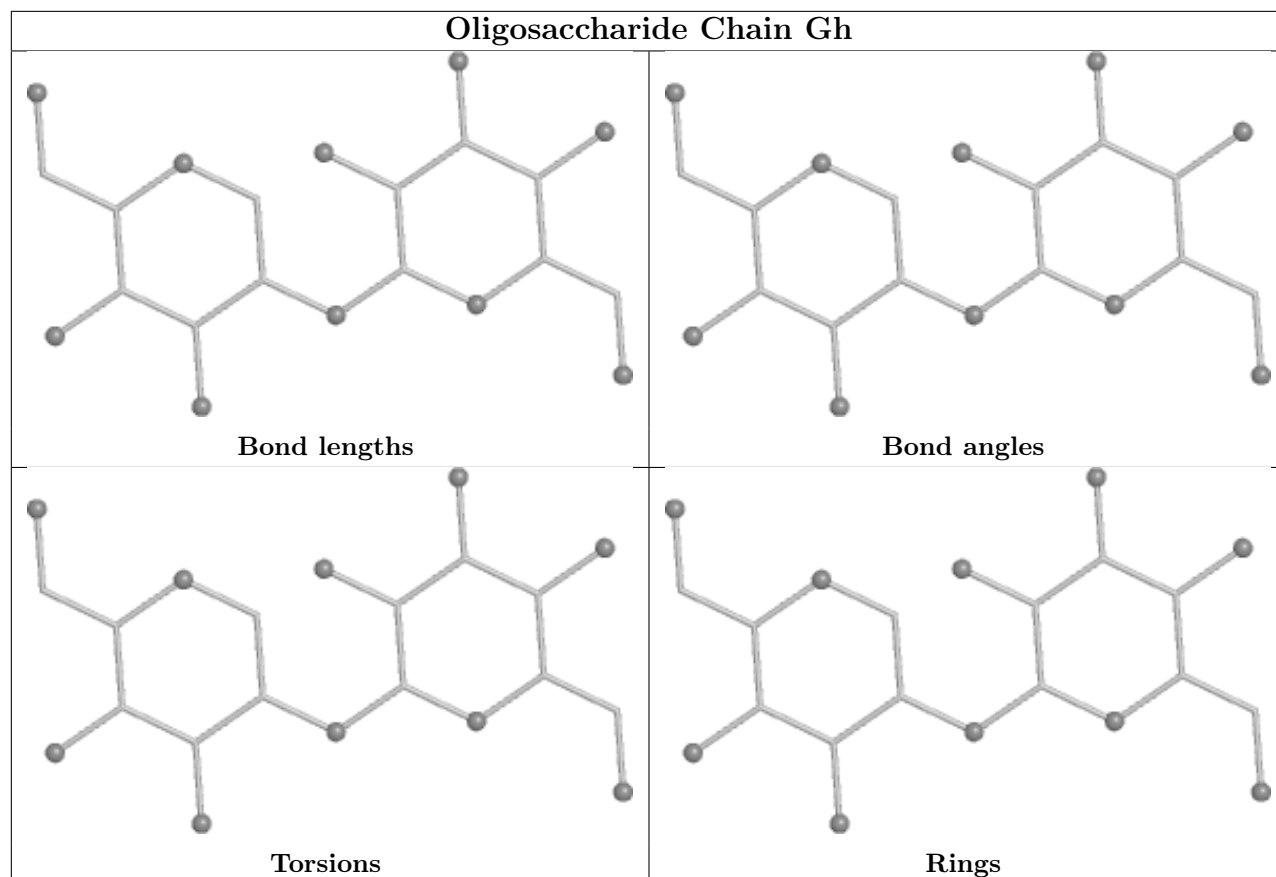
Oligosaccharide Chain Bh

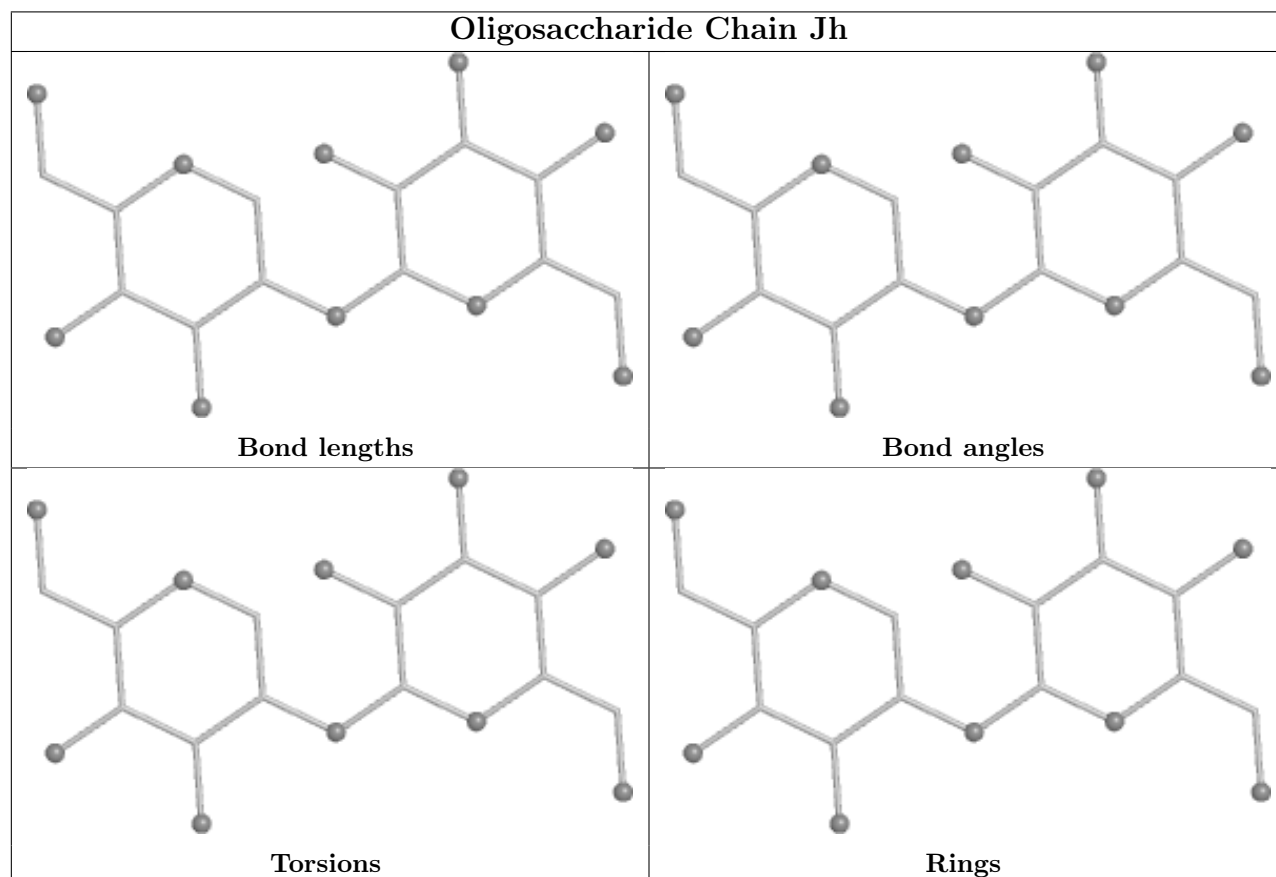
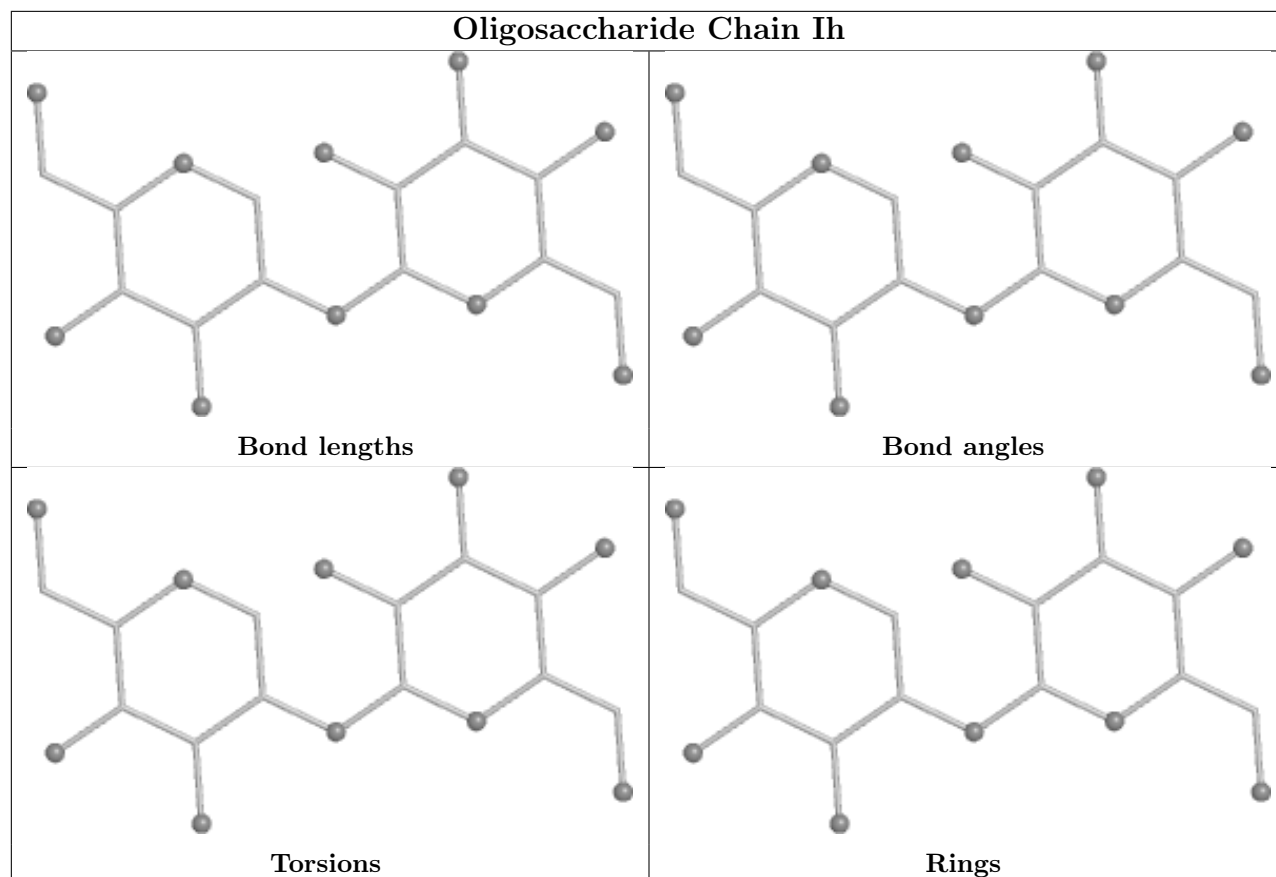


Oligosaccharide Chain Ch

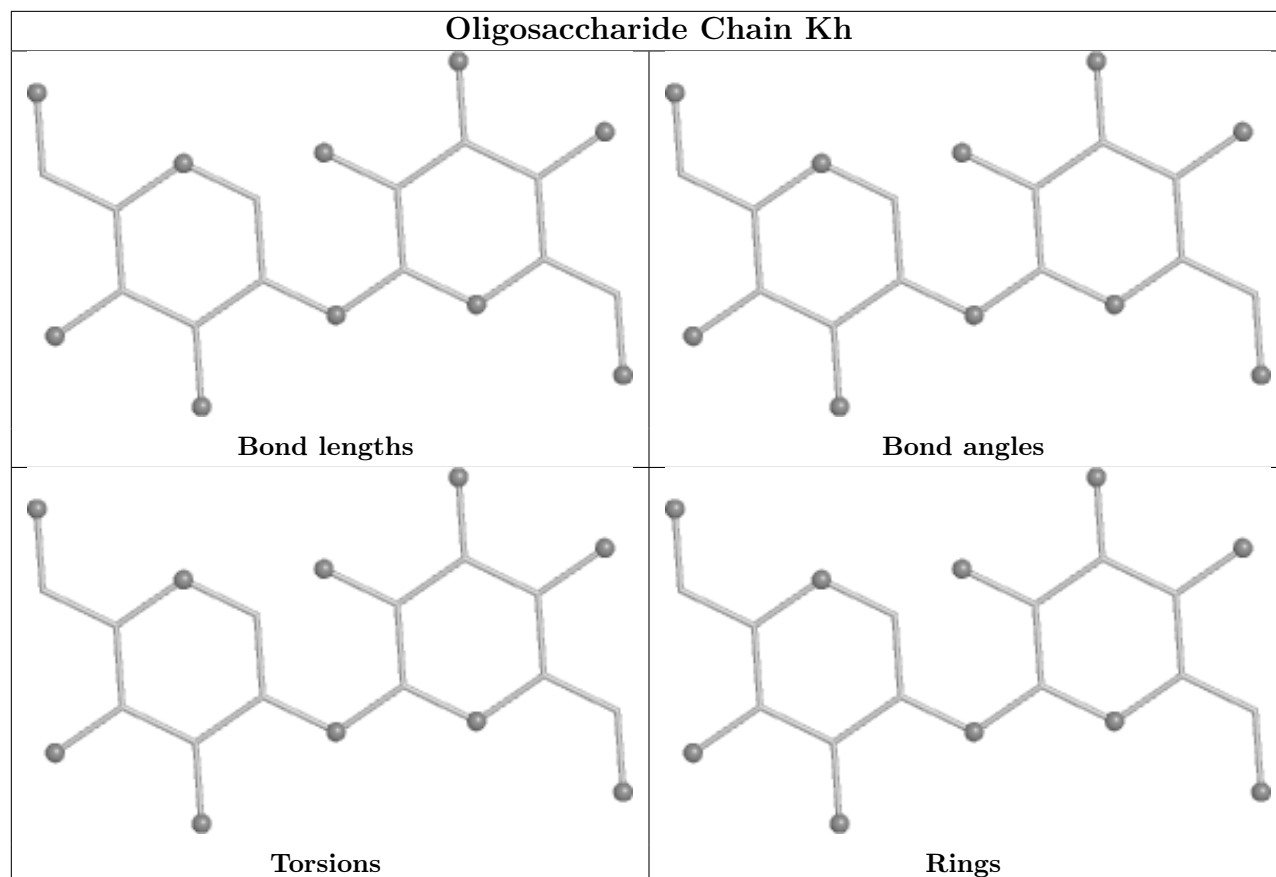




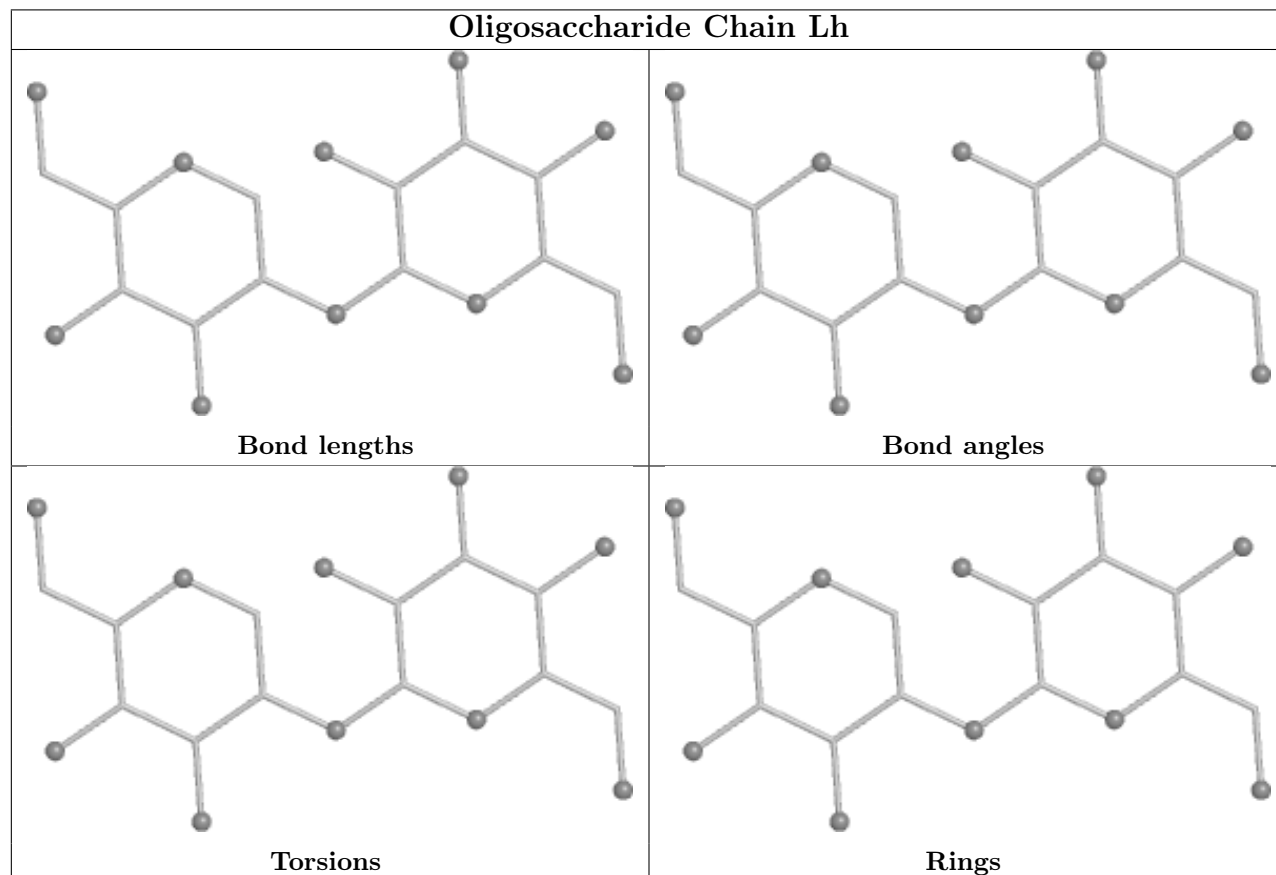


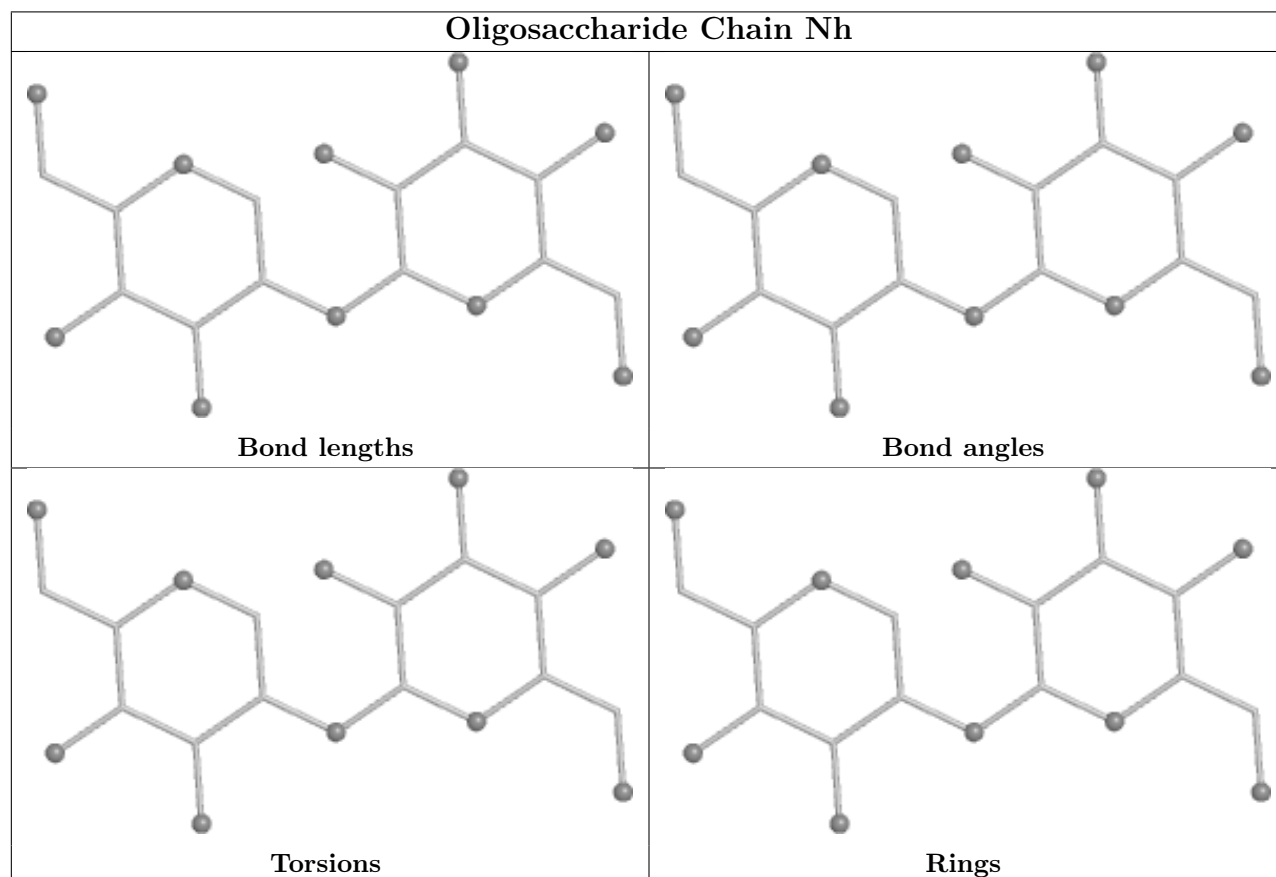
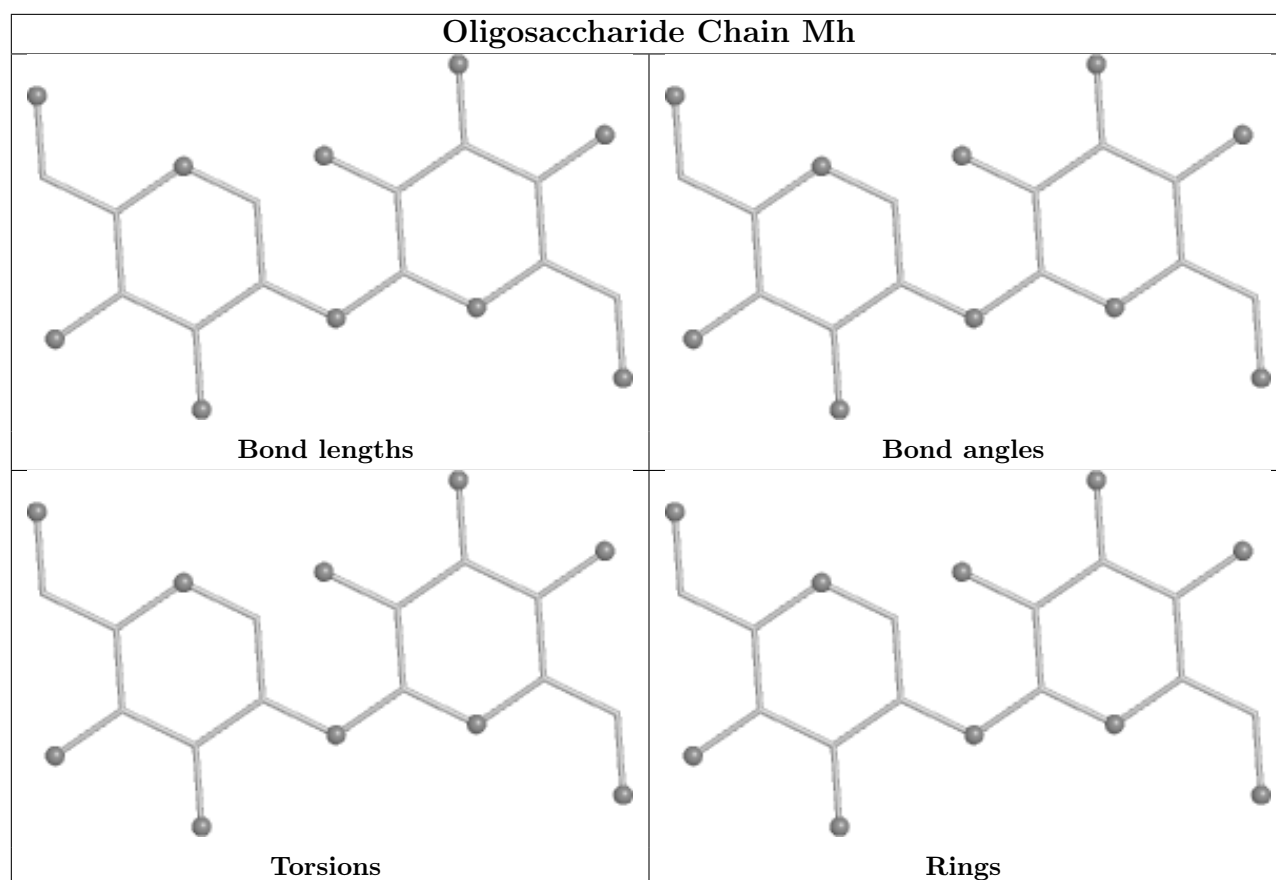


Oligosaccharide Chain Kh

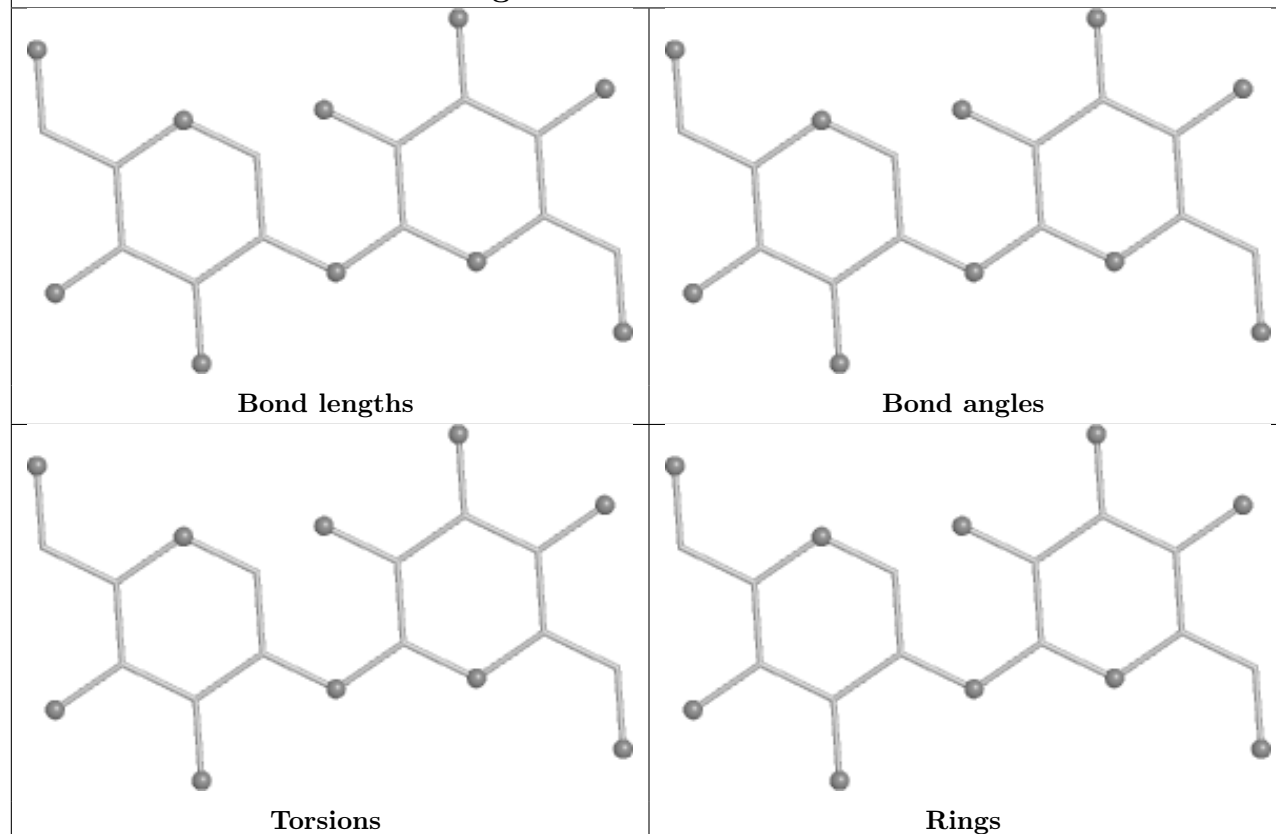


Oligosaccharide Chain Lh

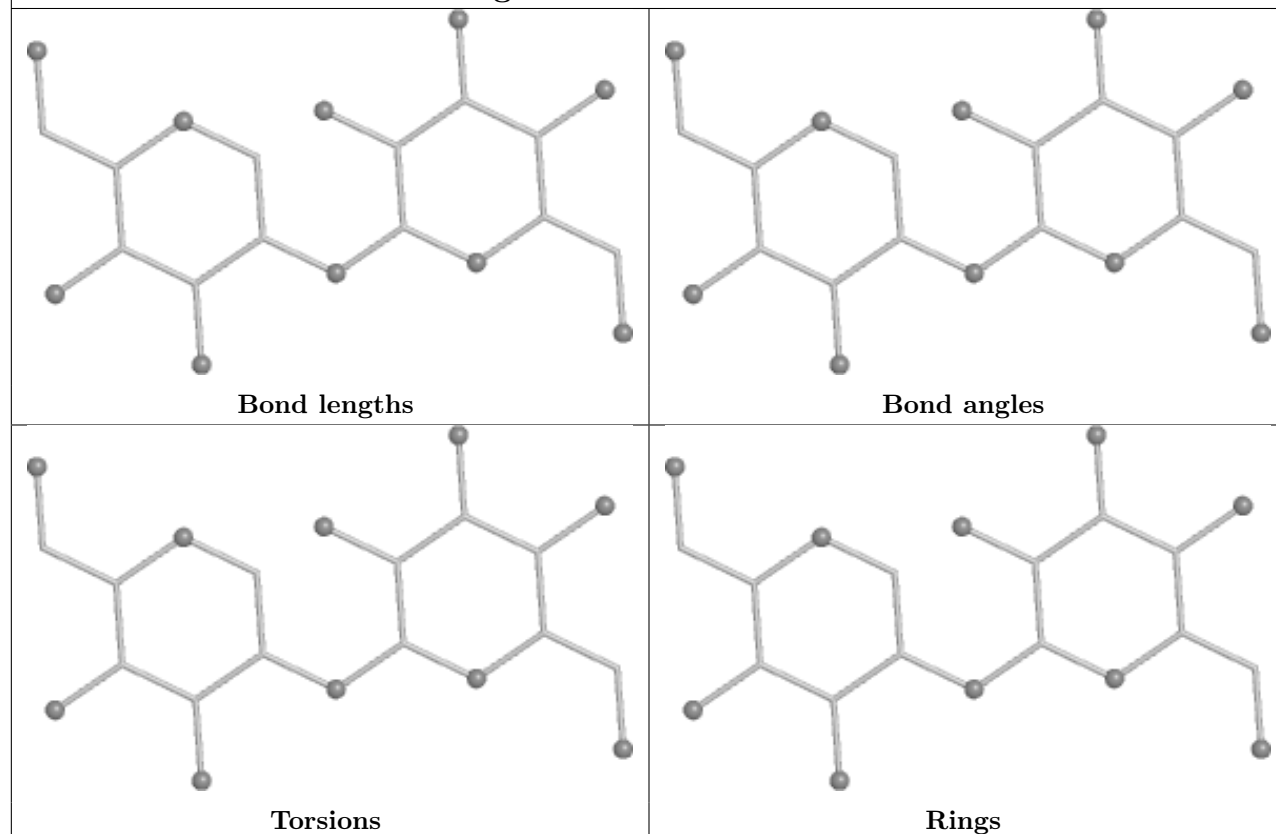




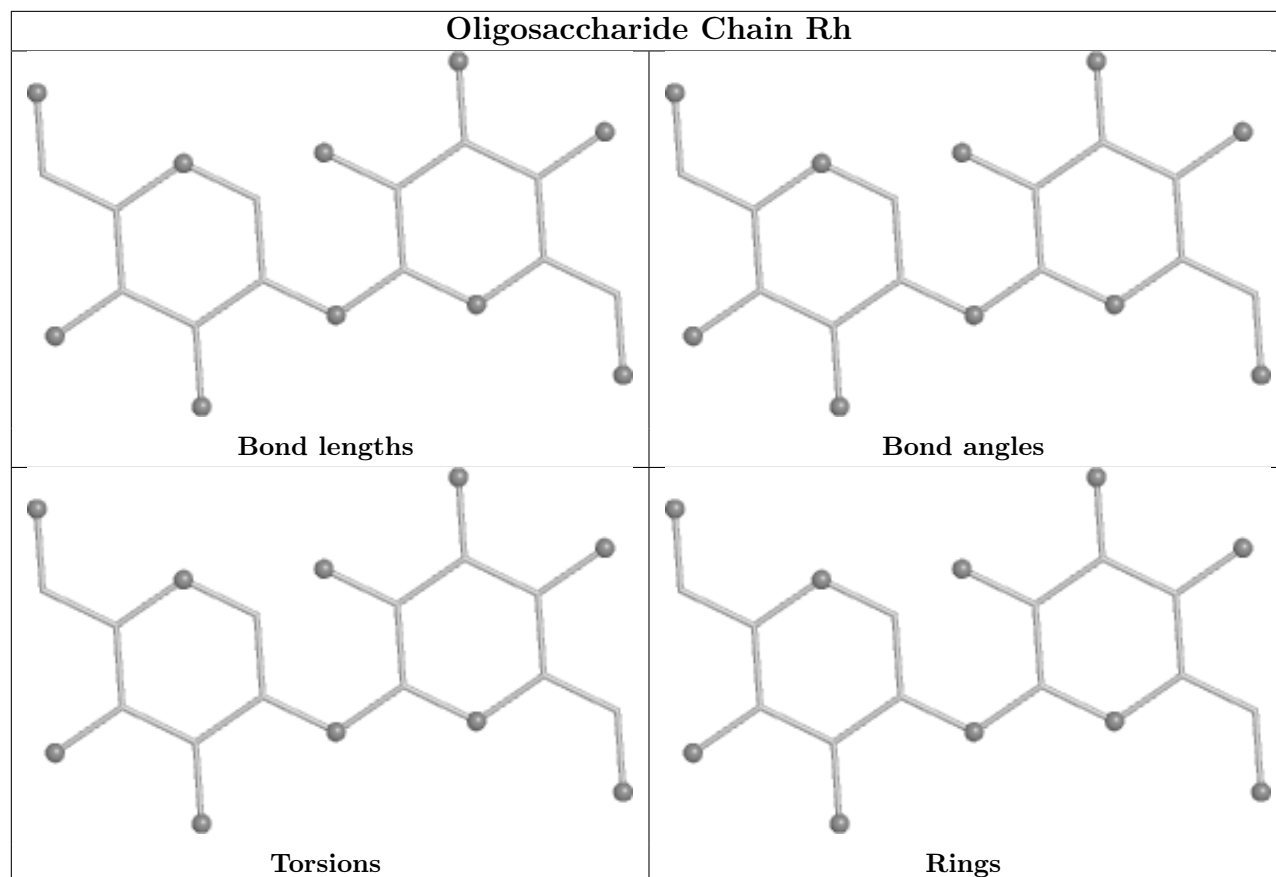
Oligosaccharide Chain Oh



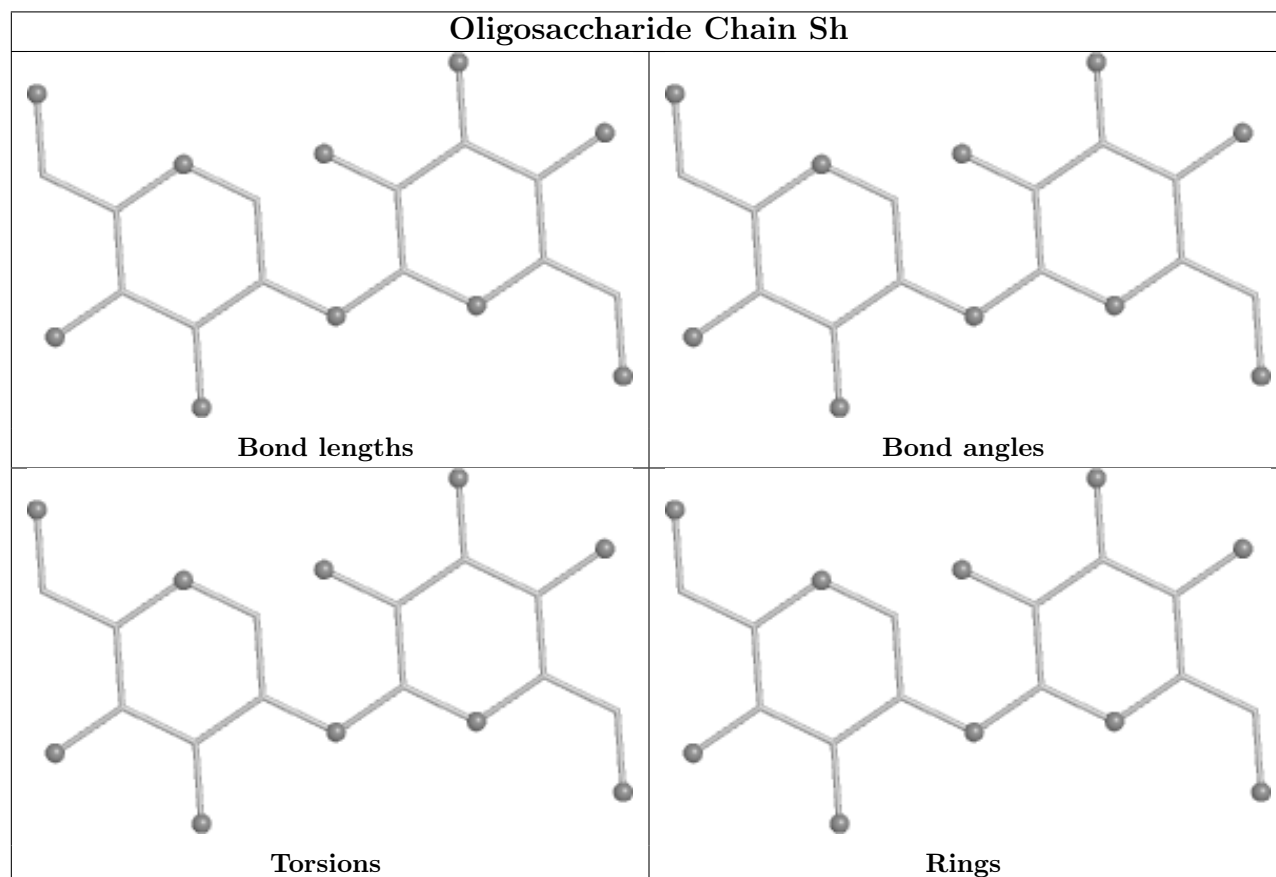
Oligosaccharide Chain Ph

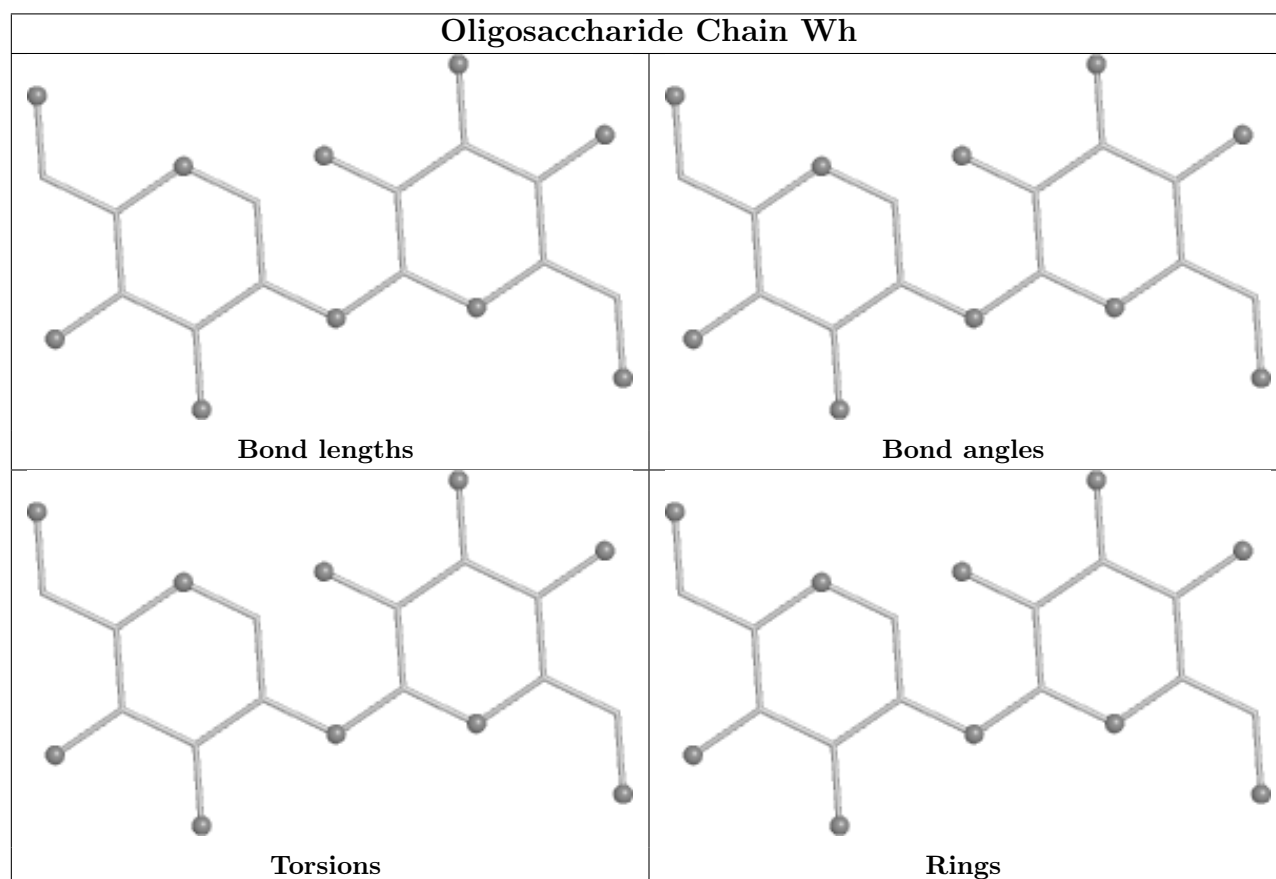
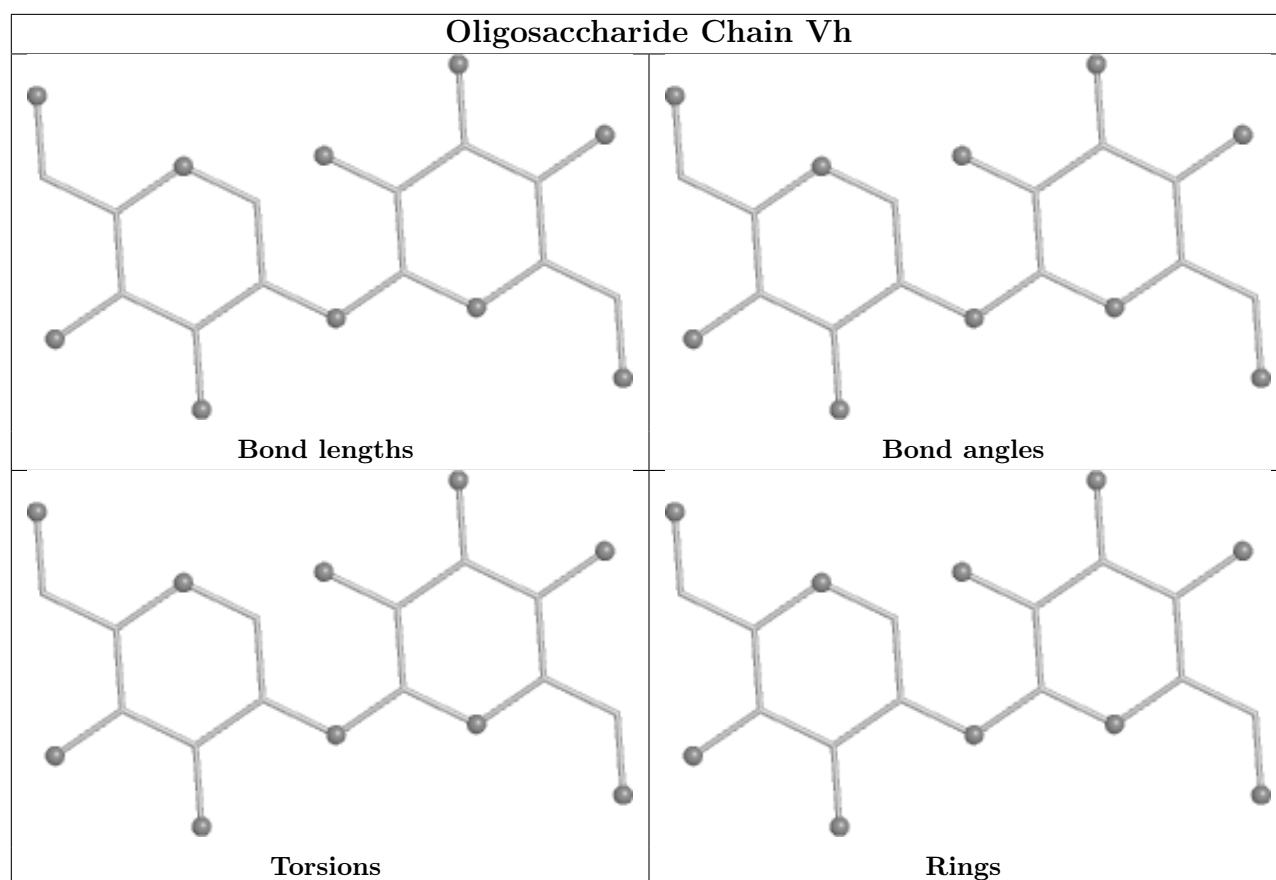


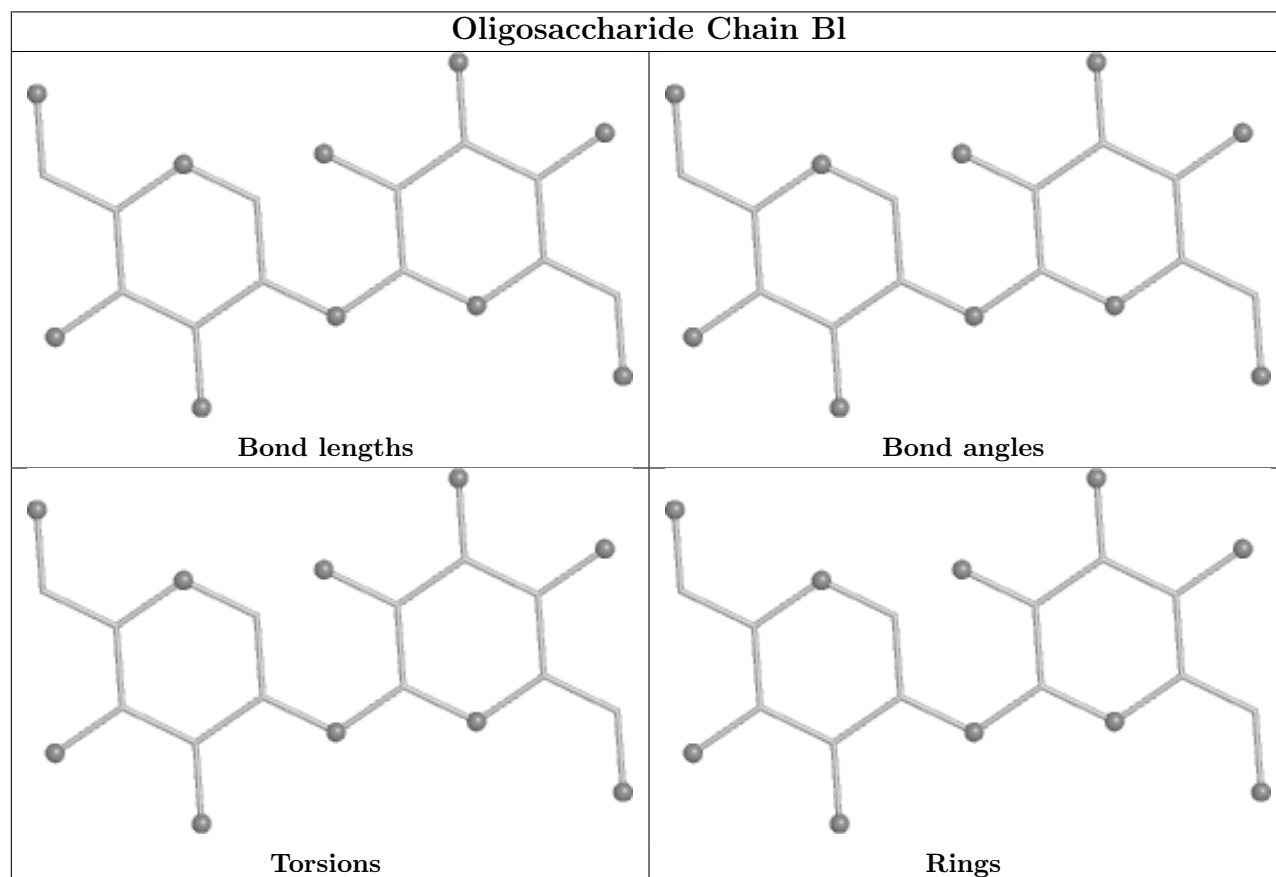
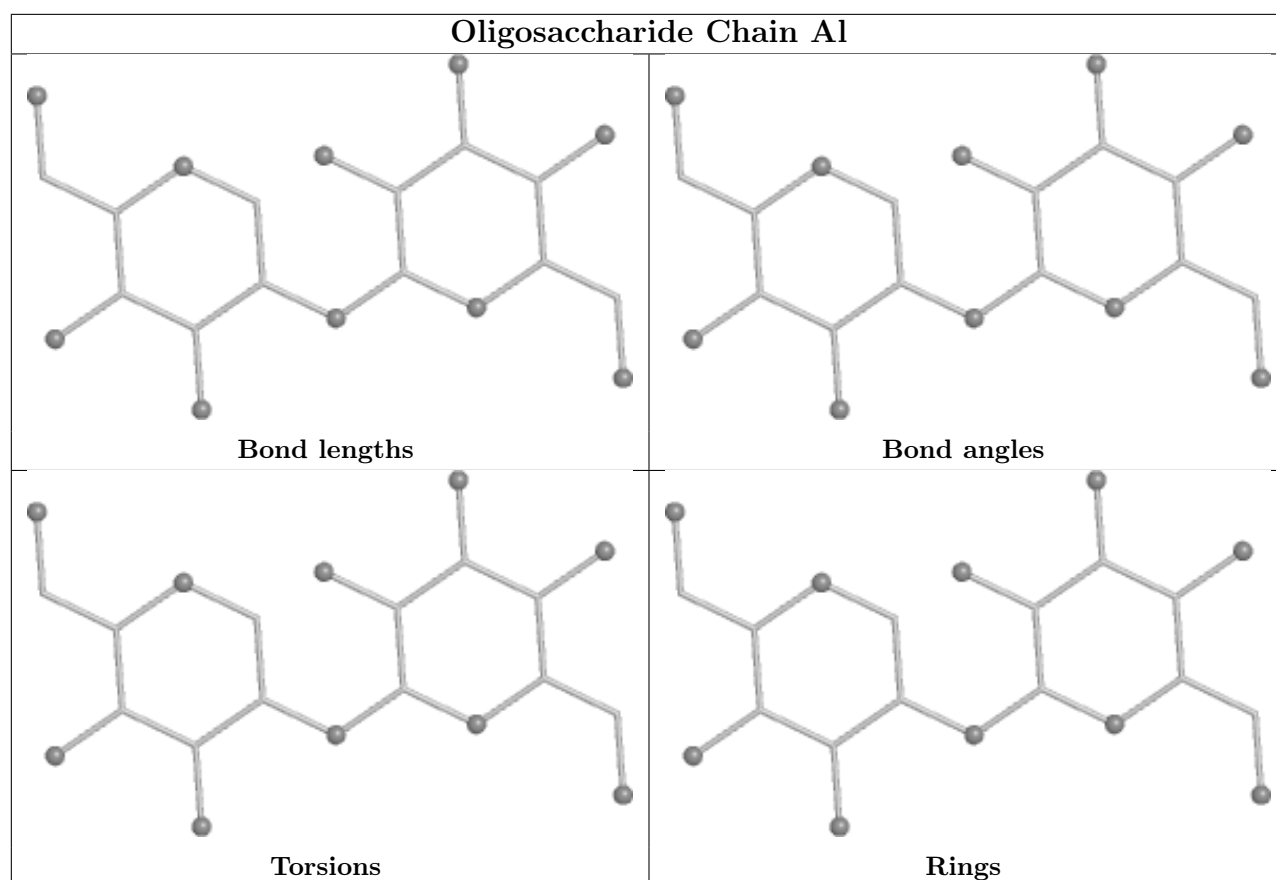
Oligosaccharide Chain Rh



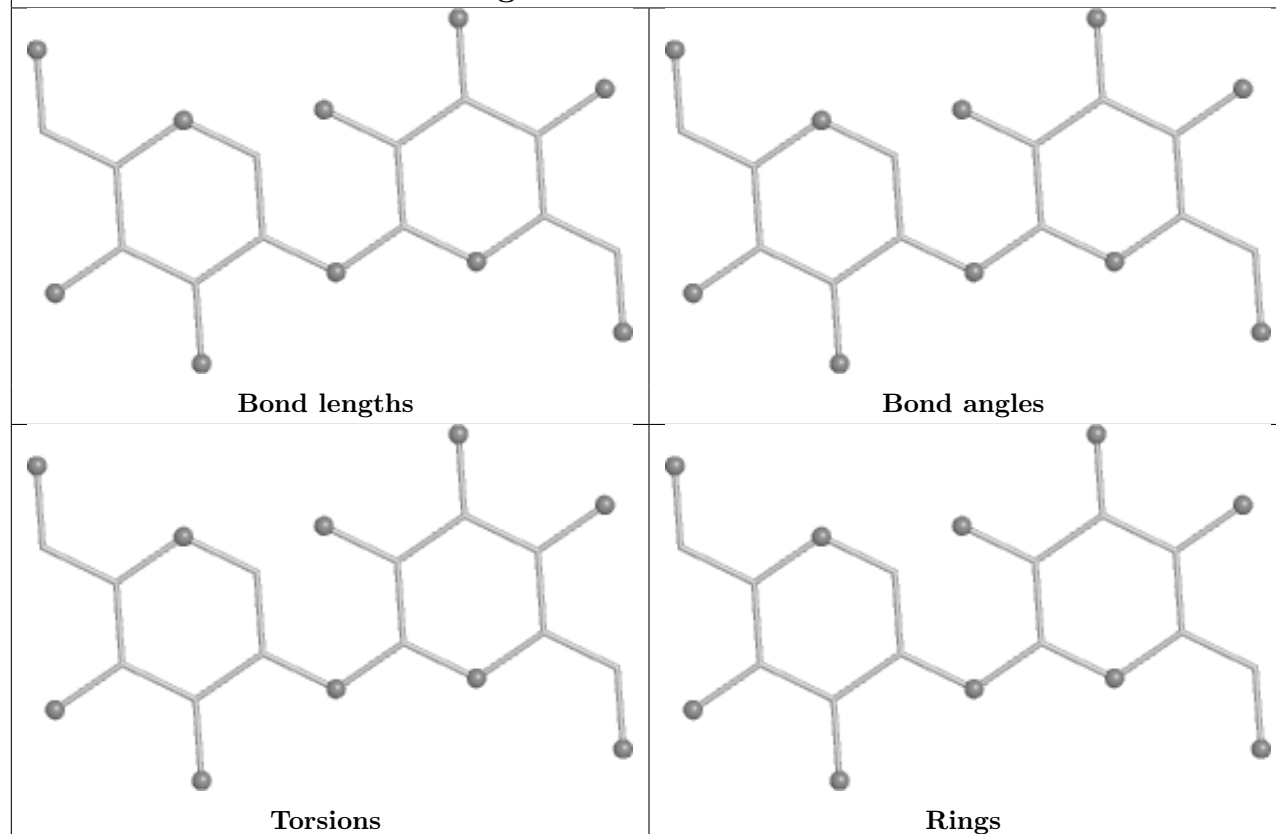
Oligosaccharide Chain Sh



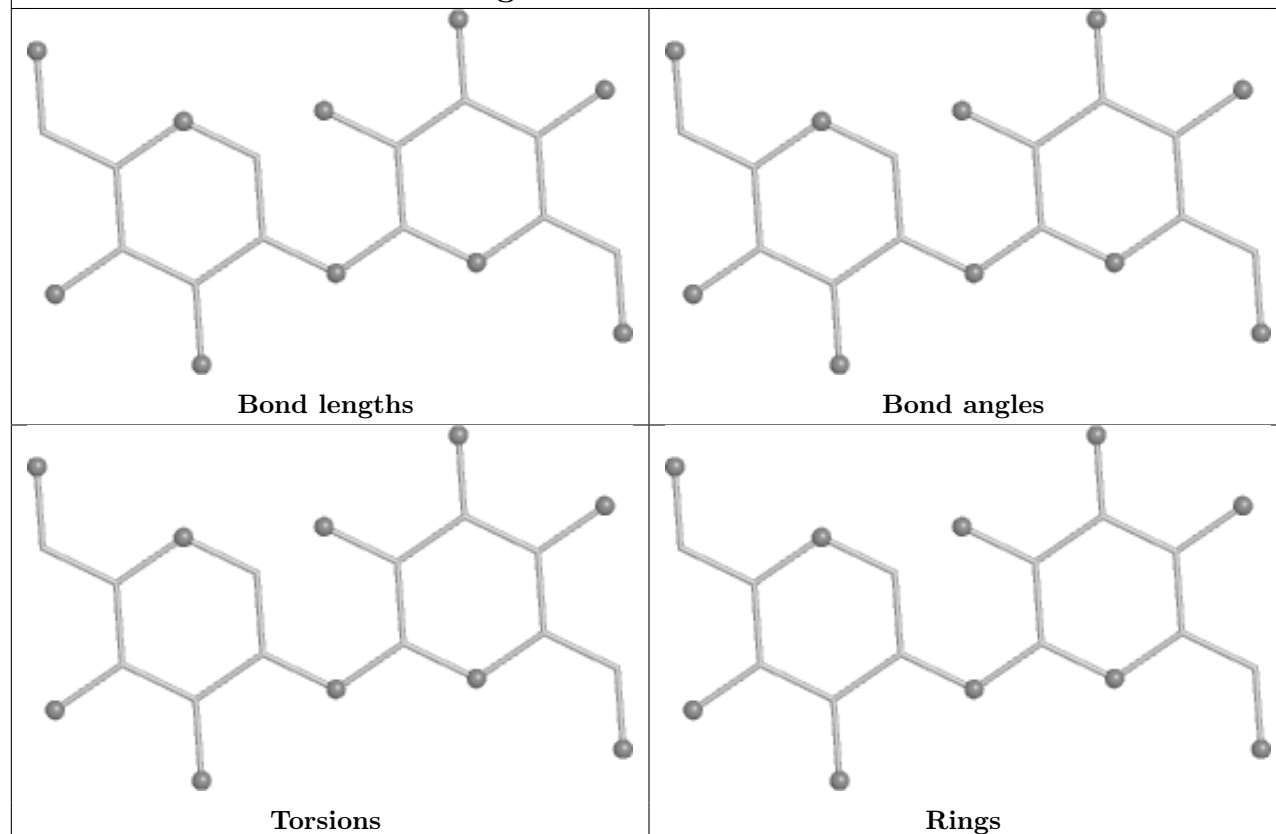


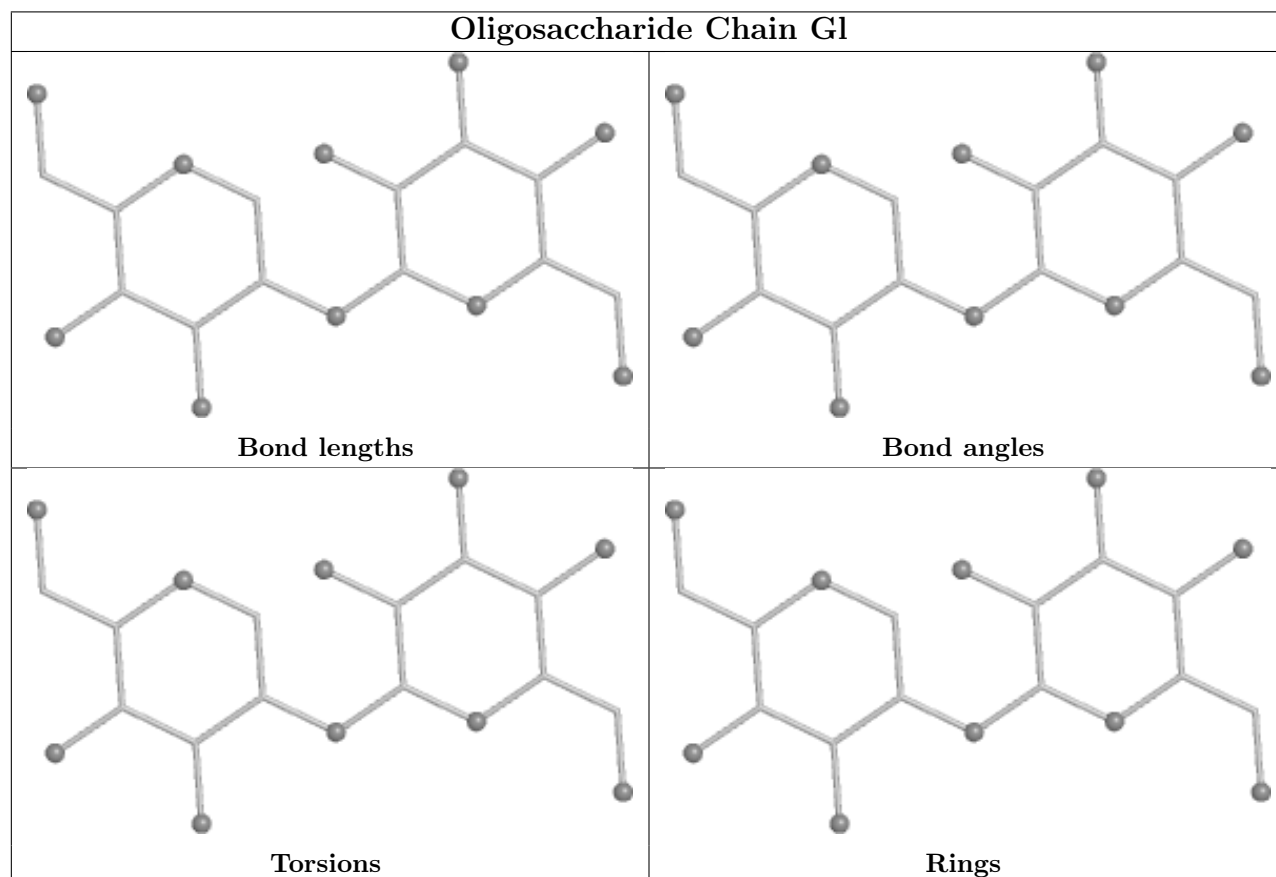
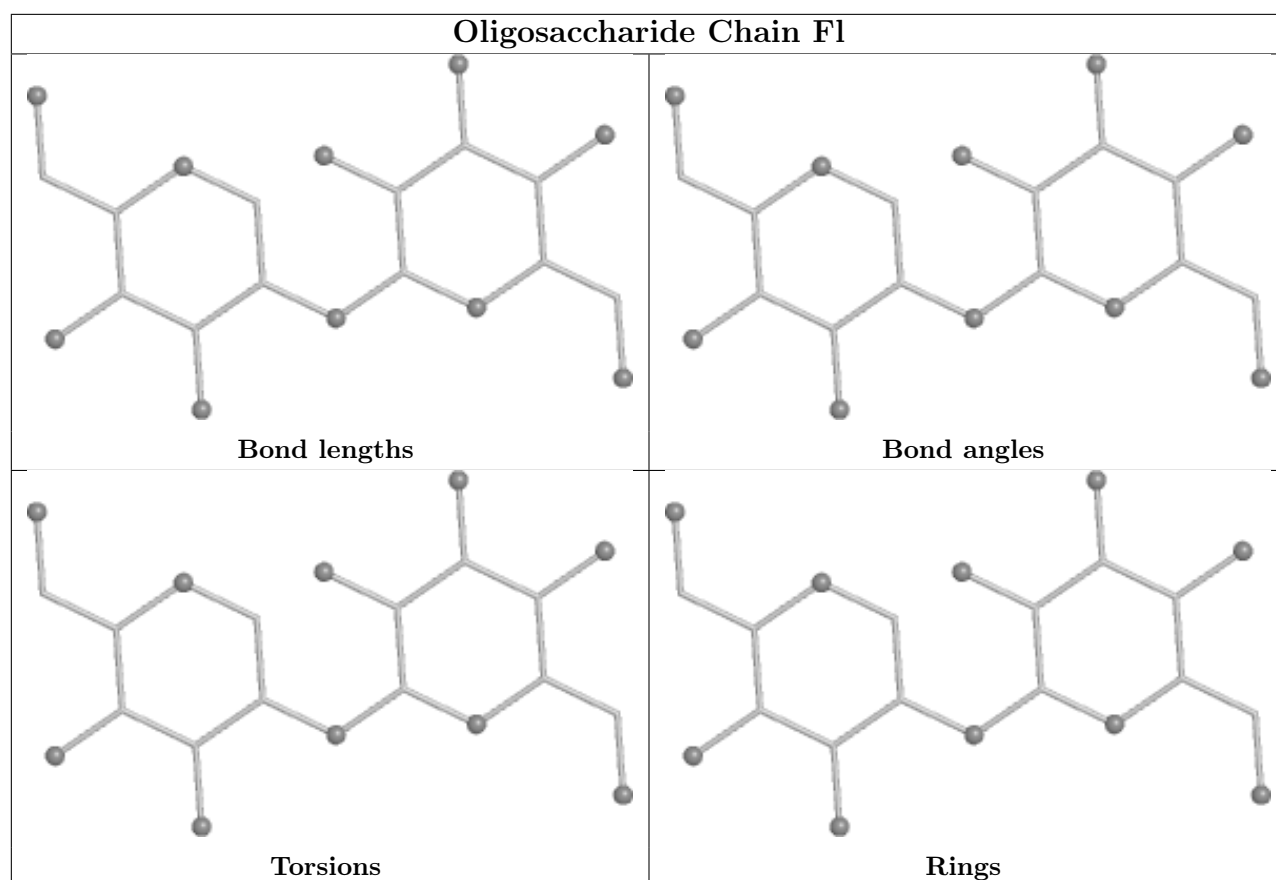


Oligosaccharide Chain Cl

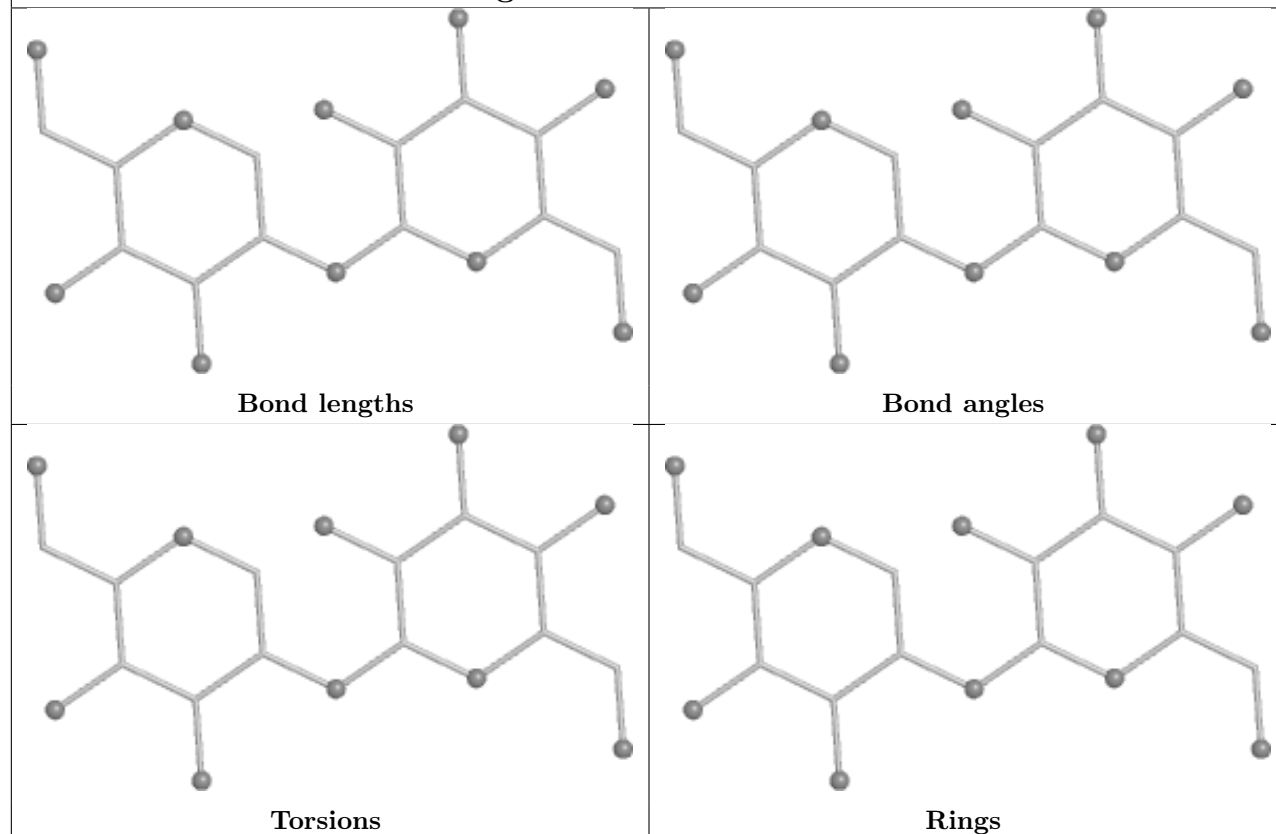


Oligosaccharide Chain D1

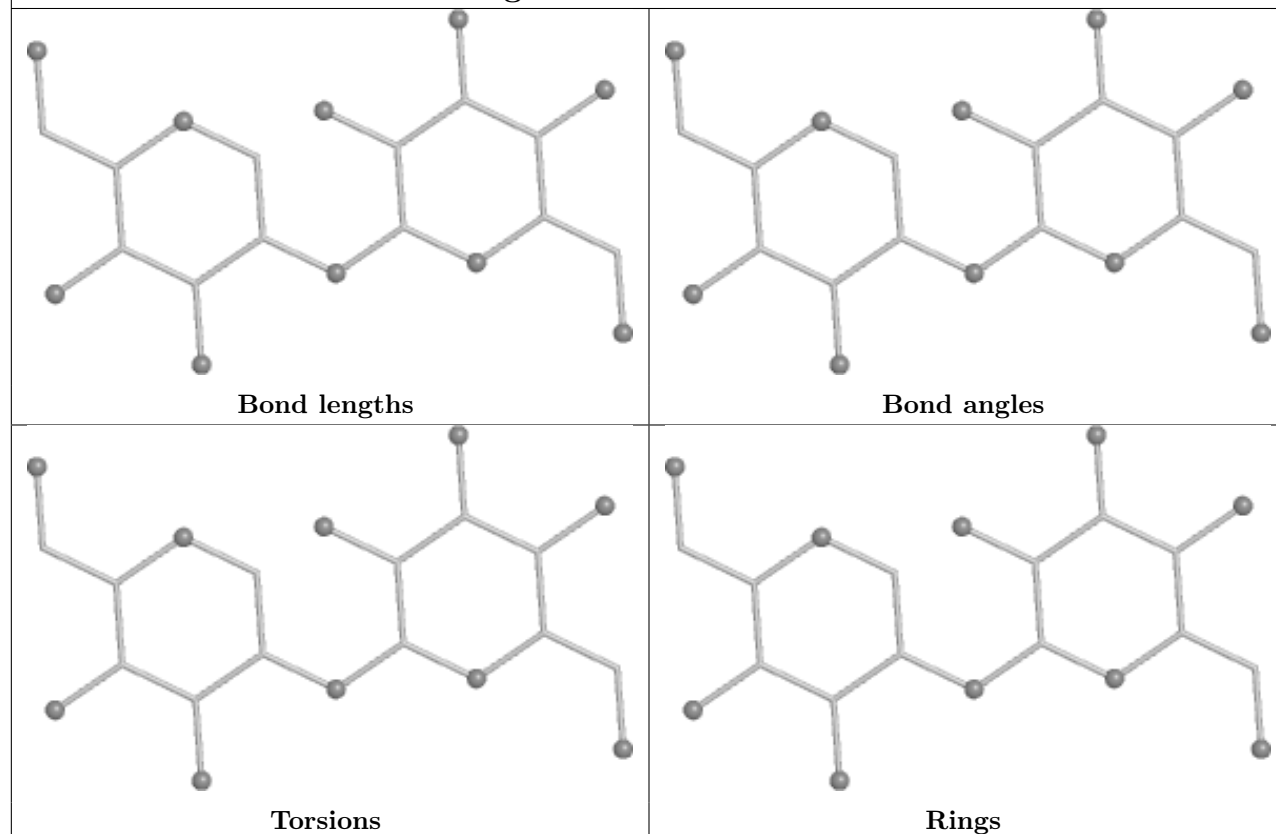




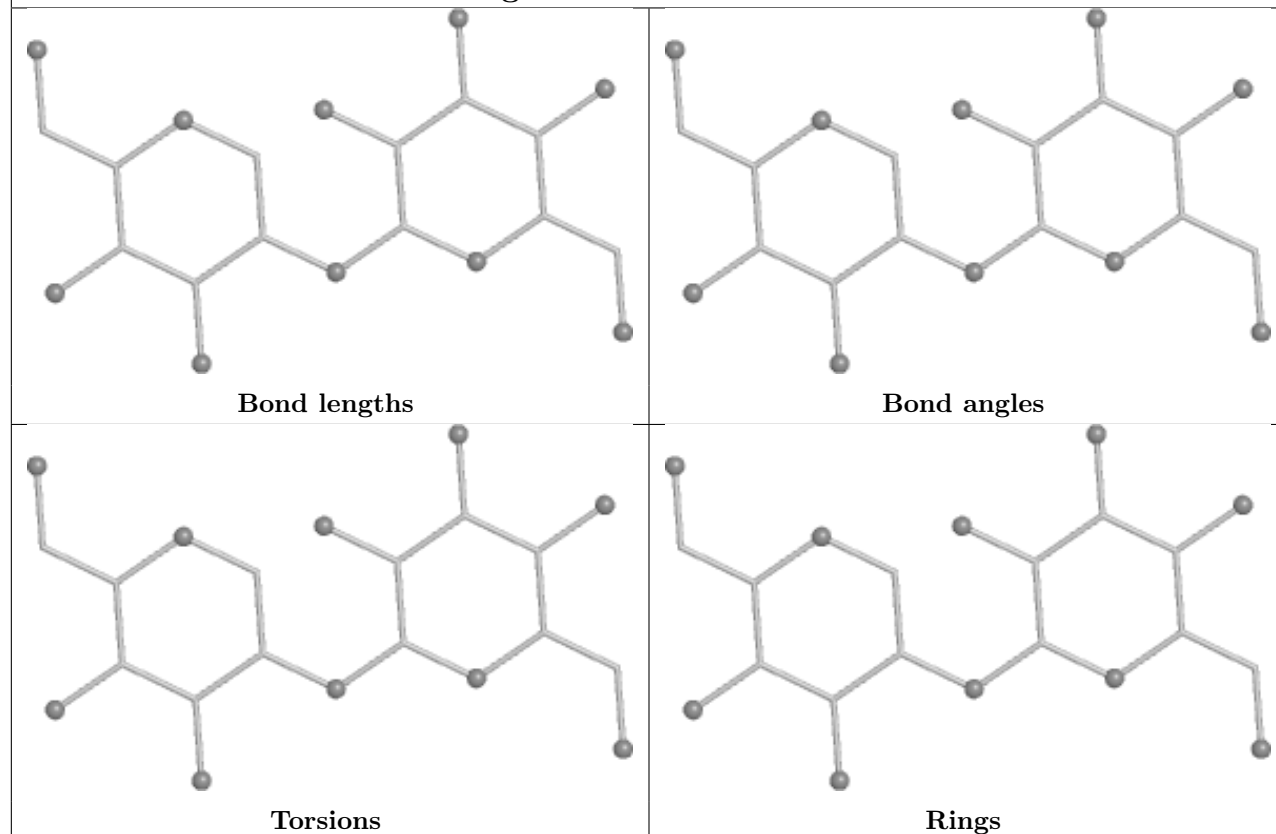
Oligosaccharide Chain H1



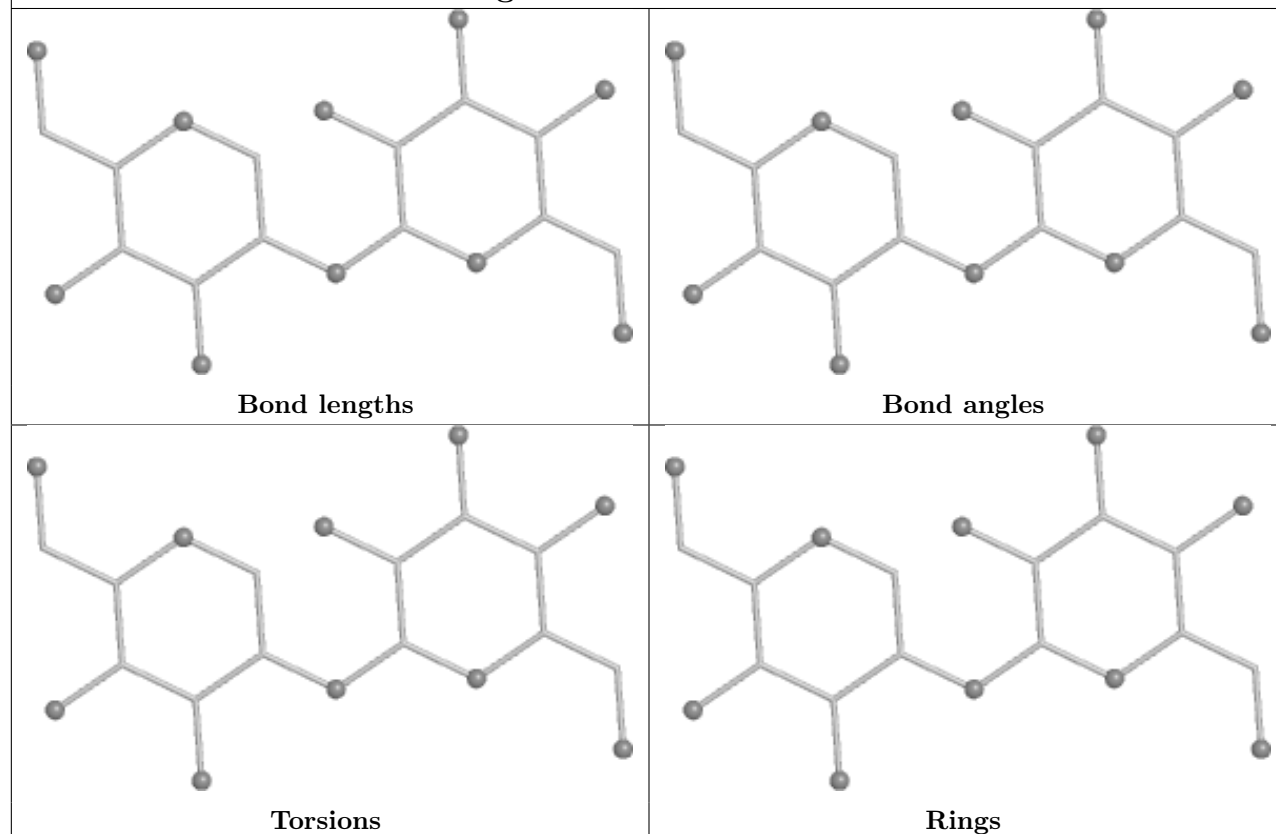
Oligosaccharide Chain H2

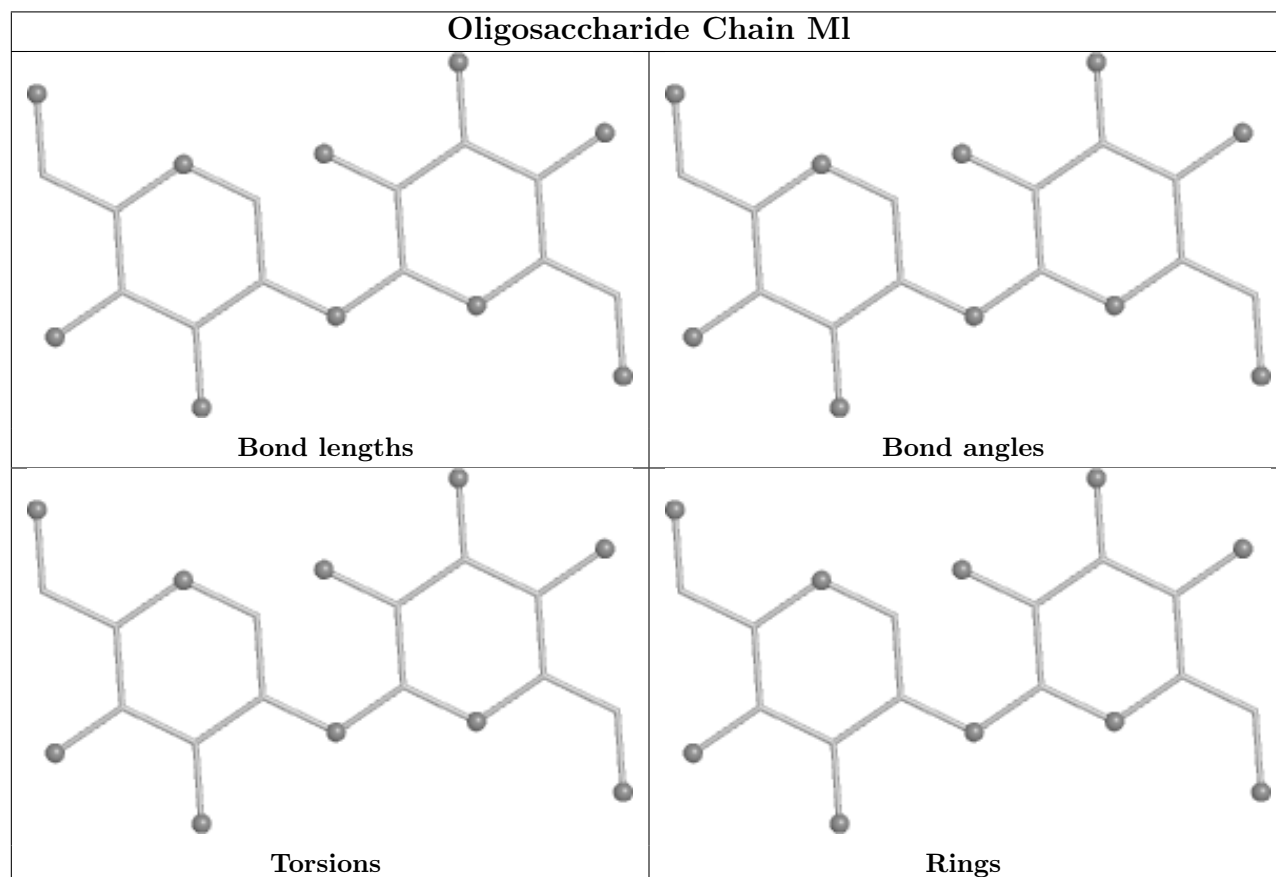
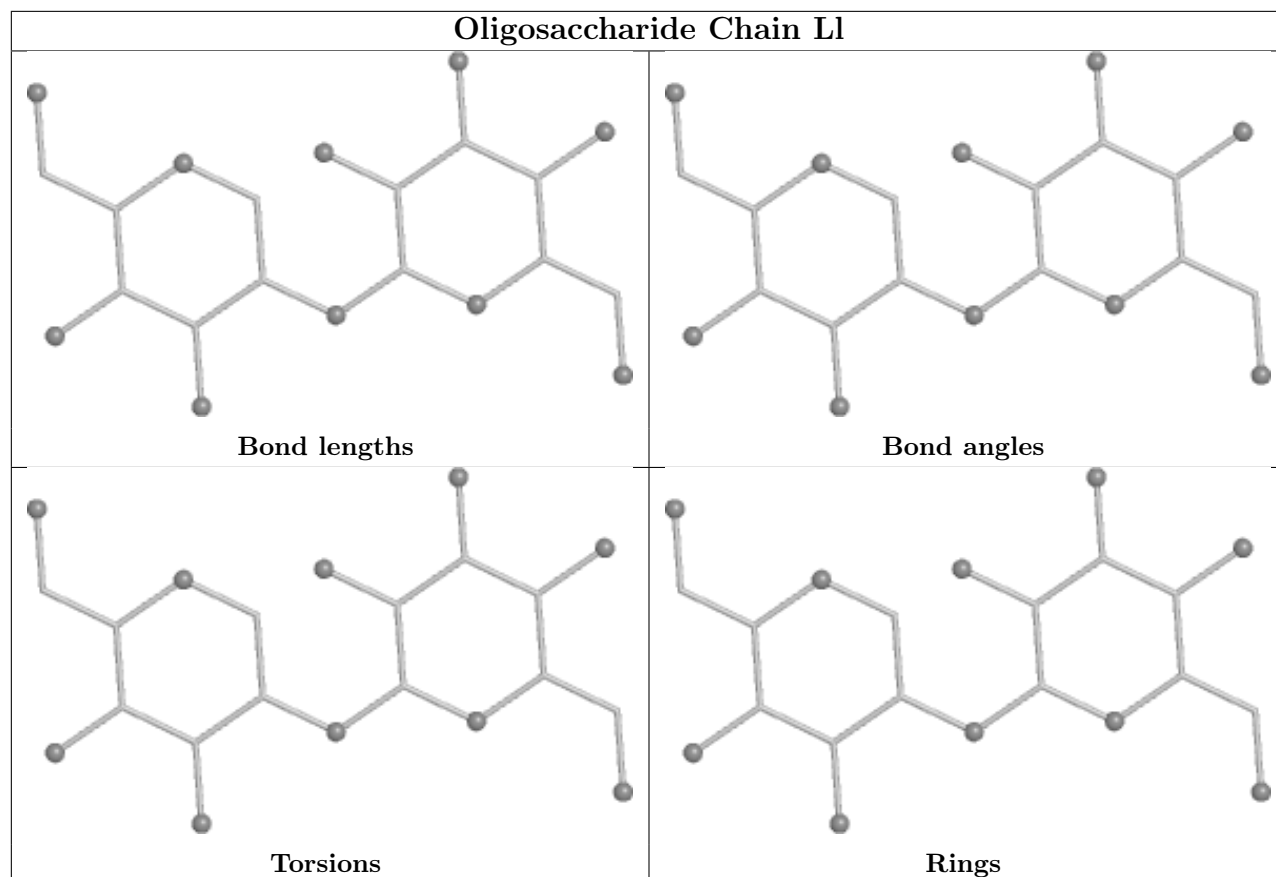


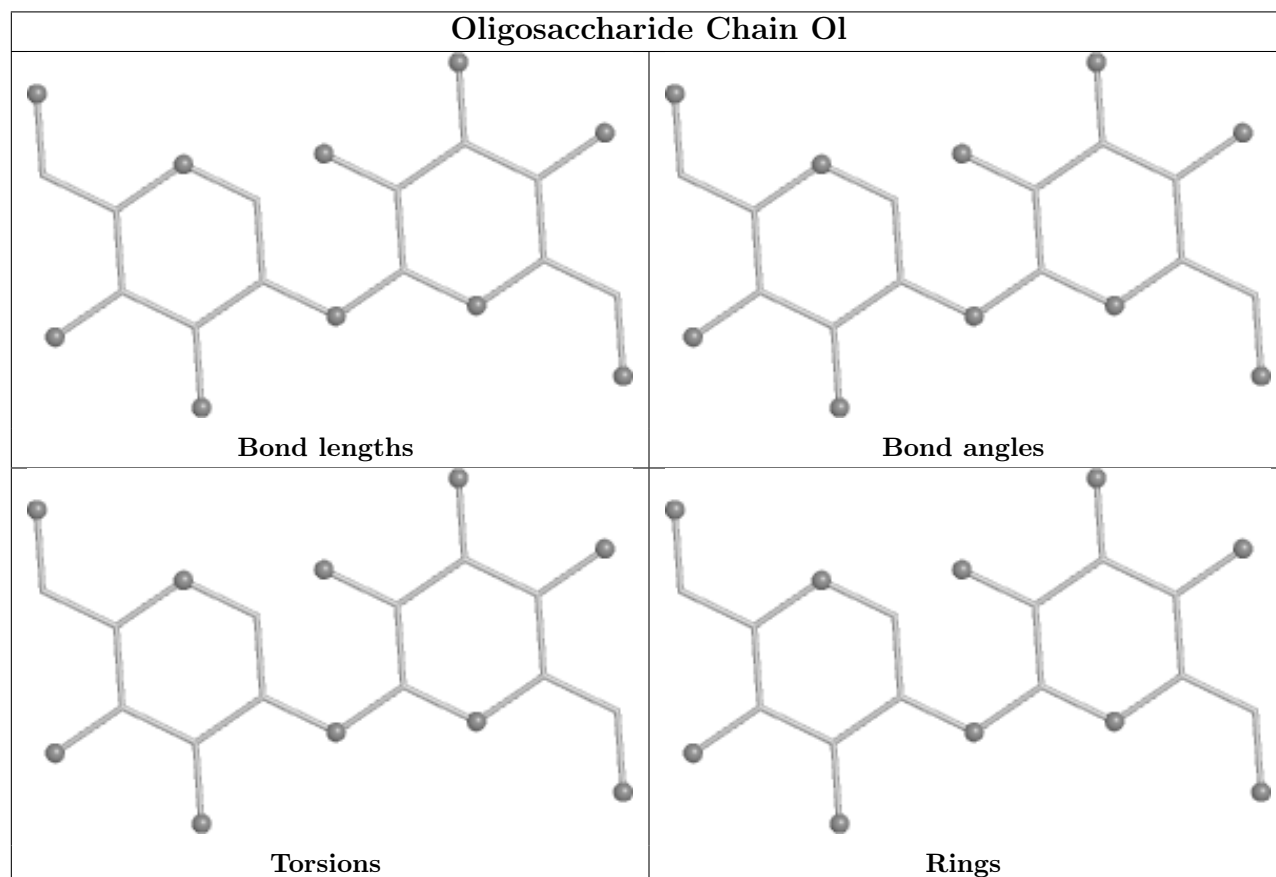
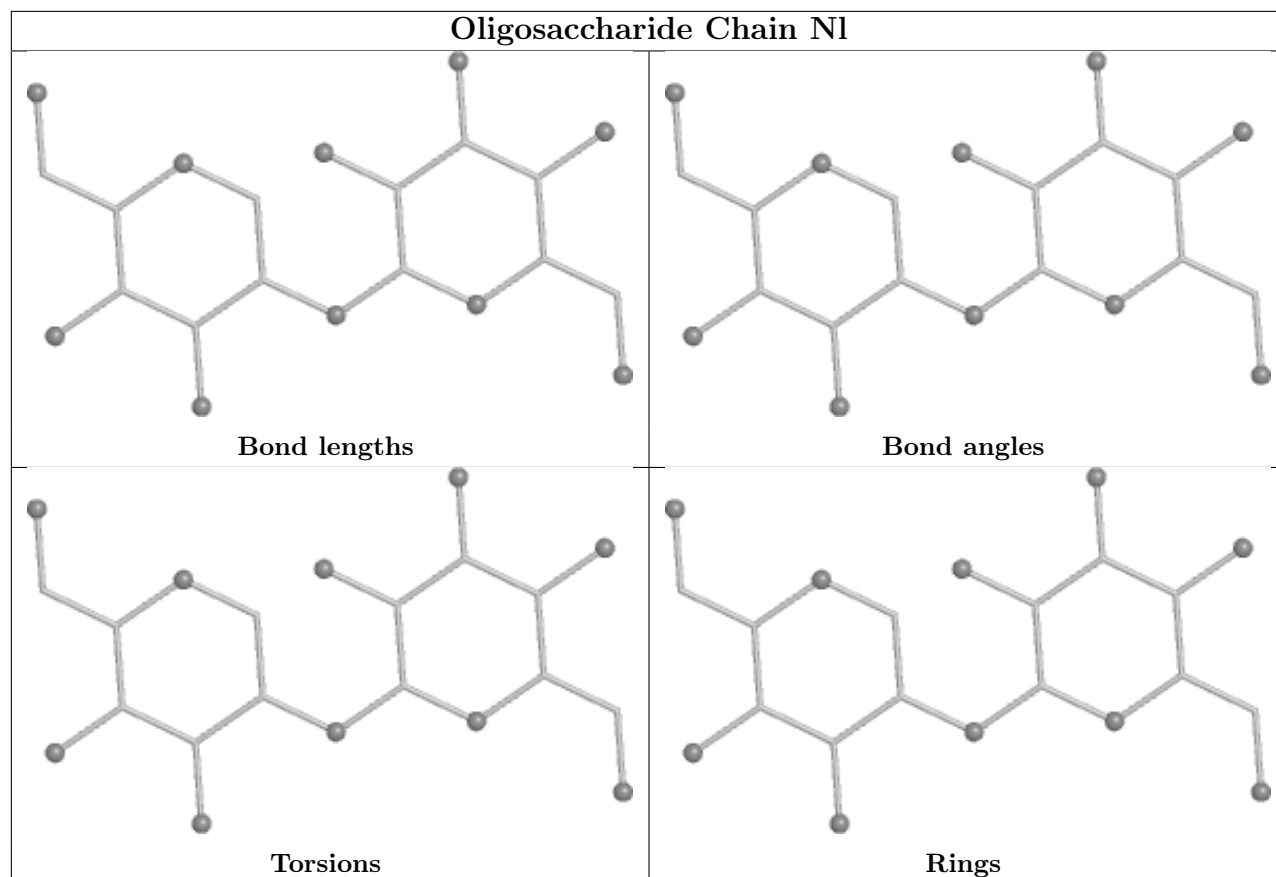
Oligosaccharide Chain JI

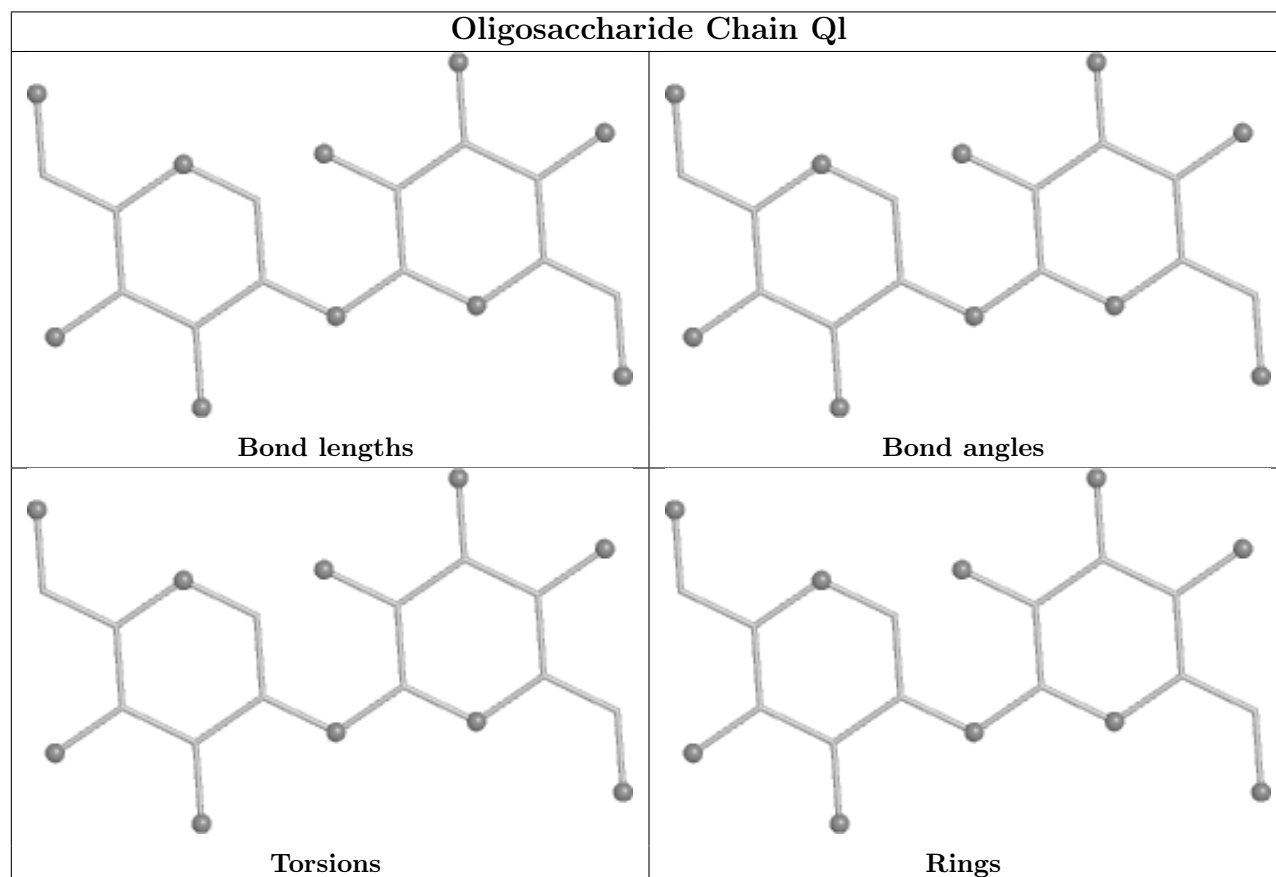
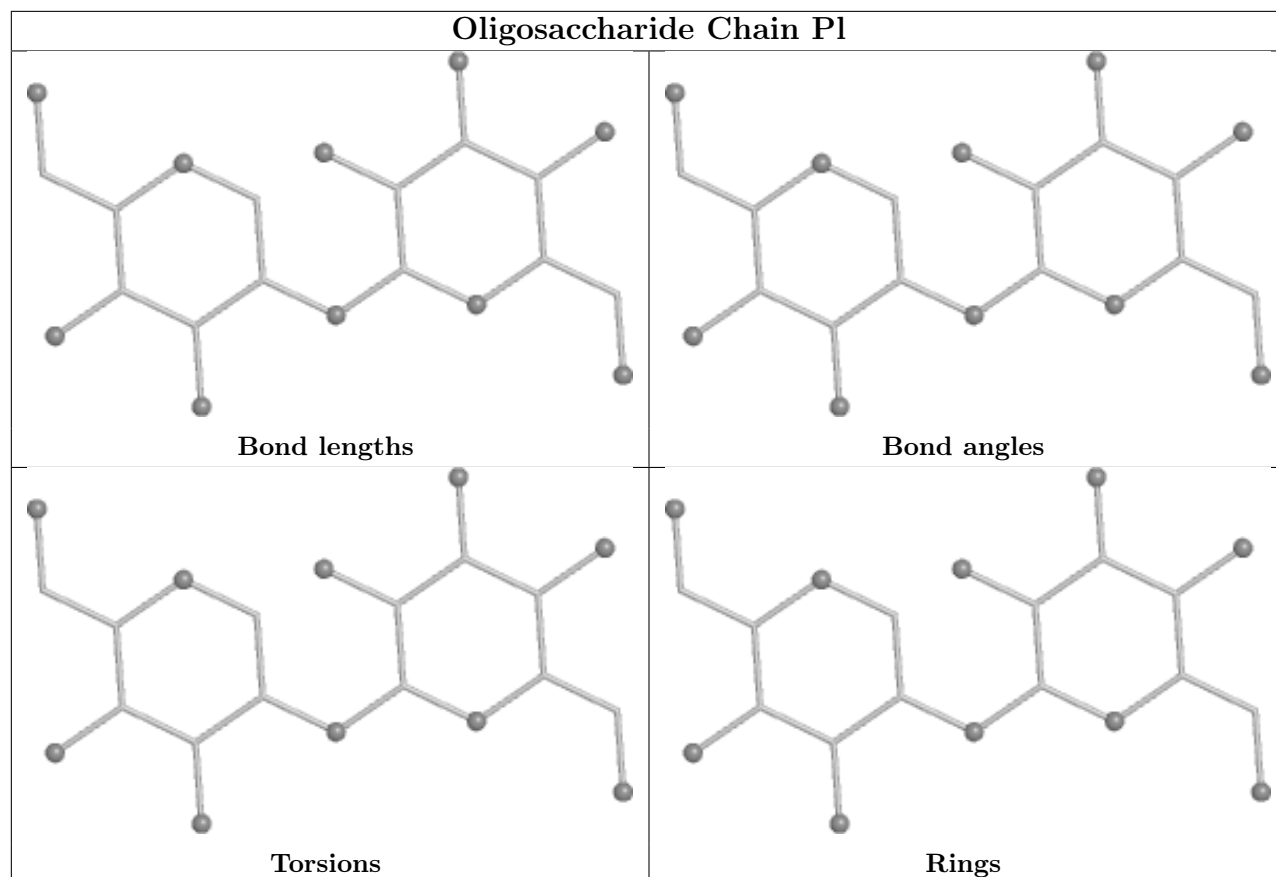


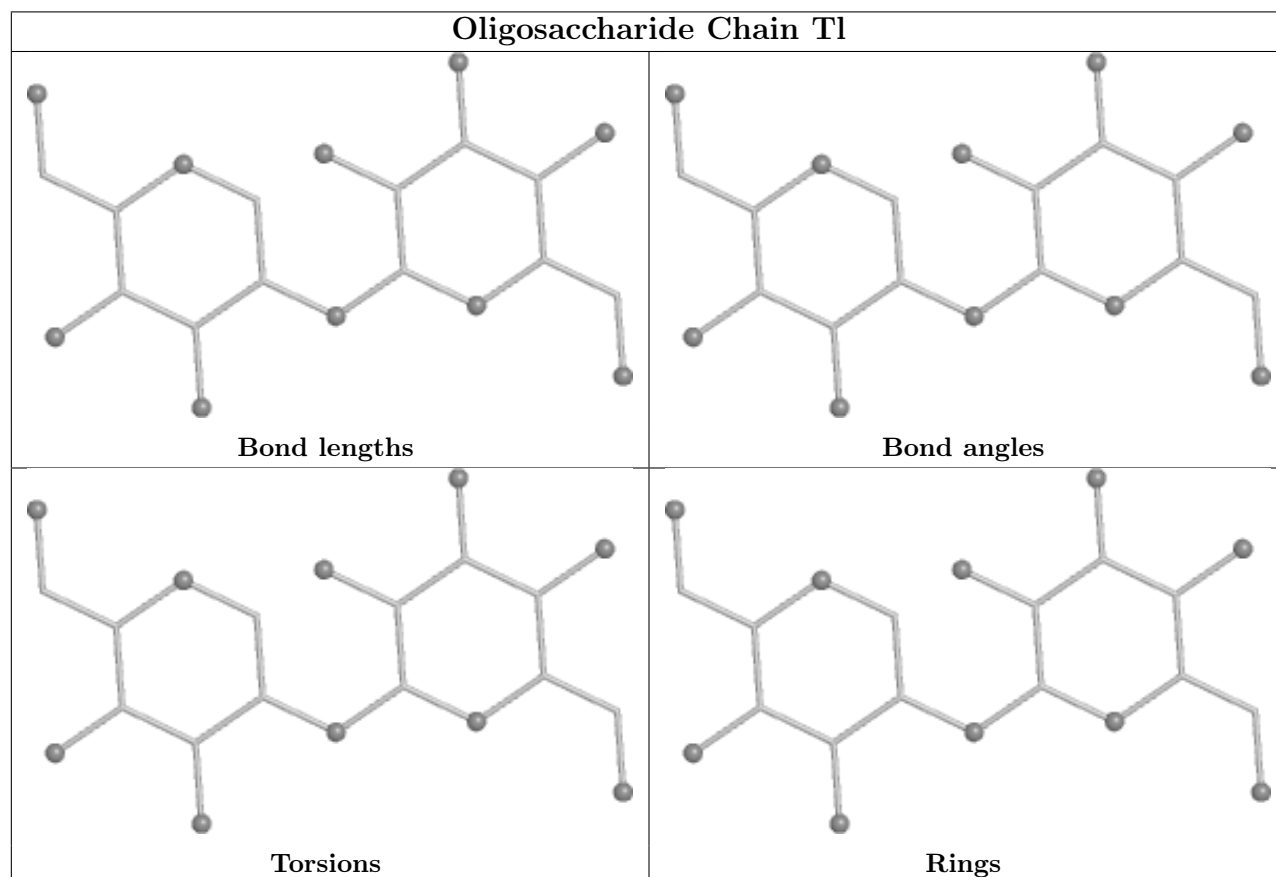
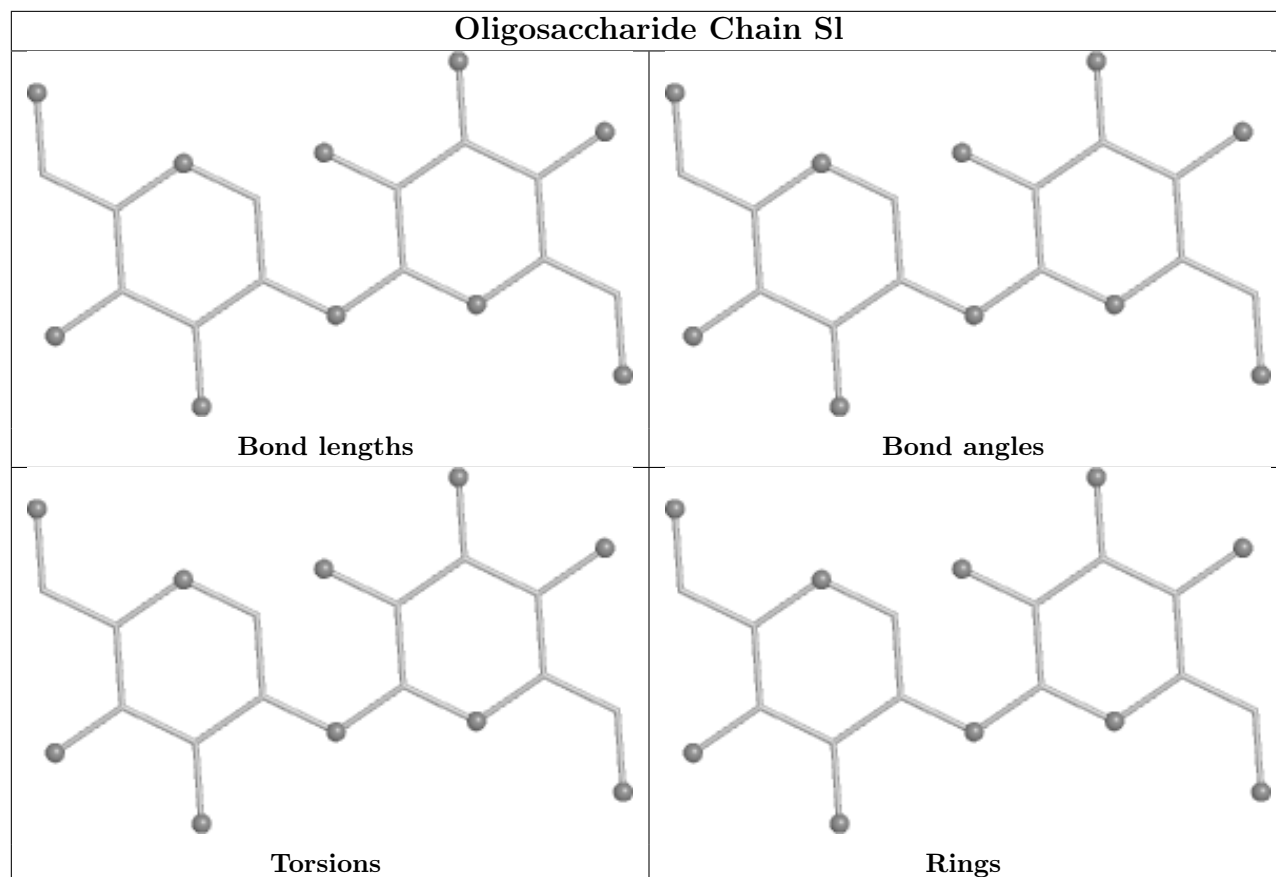
Oligosaccharide Chain KI

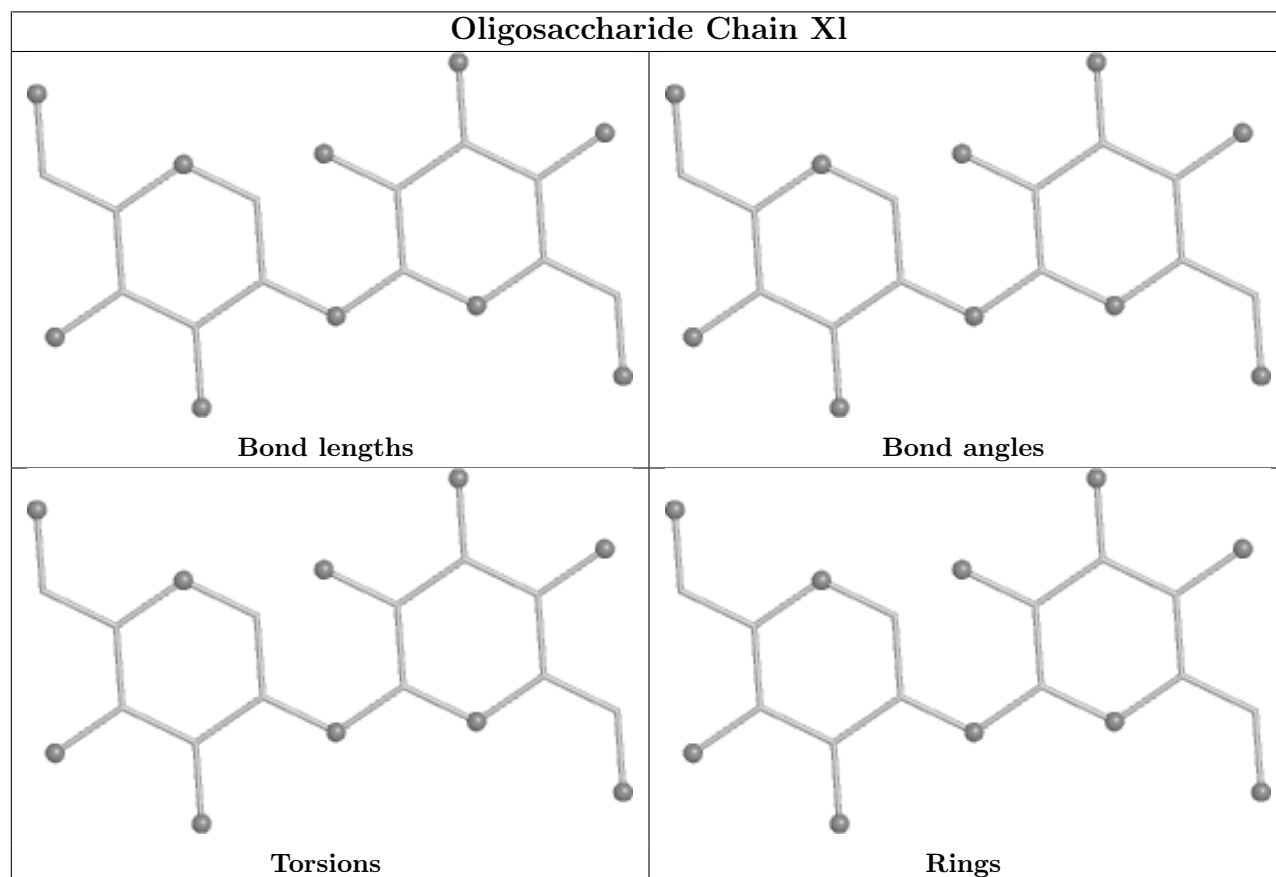
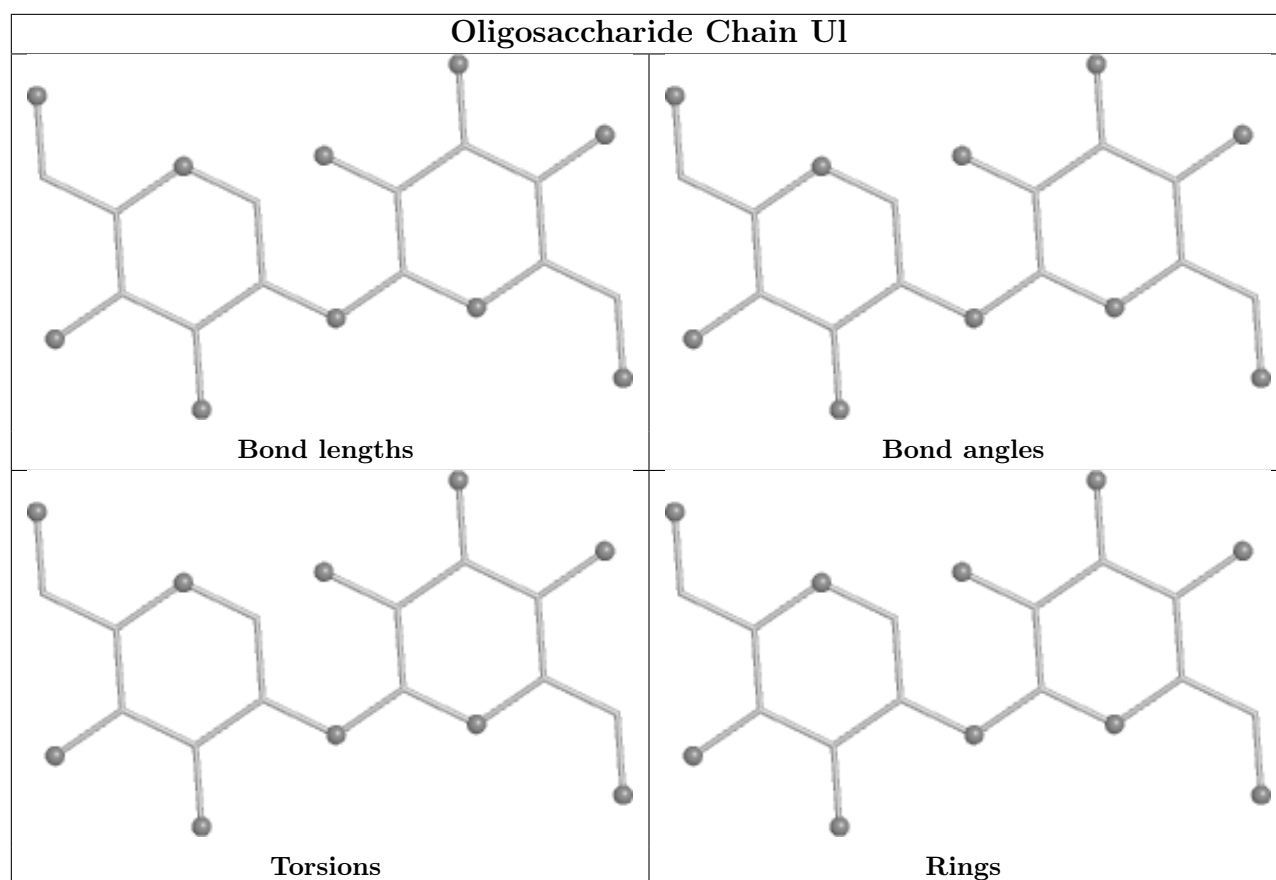




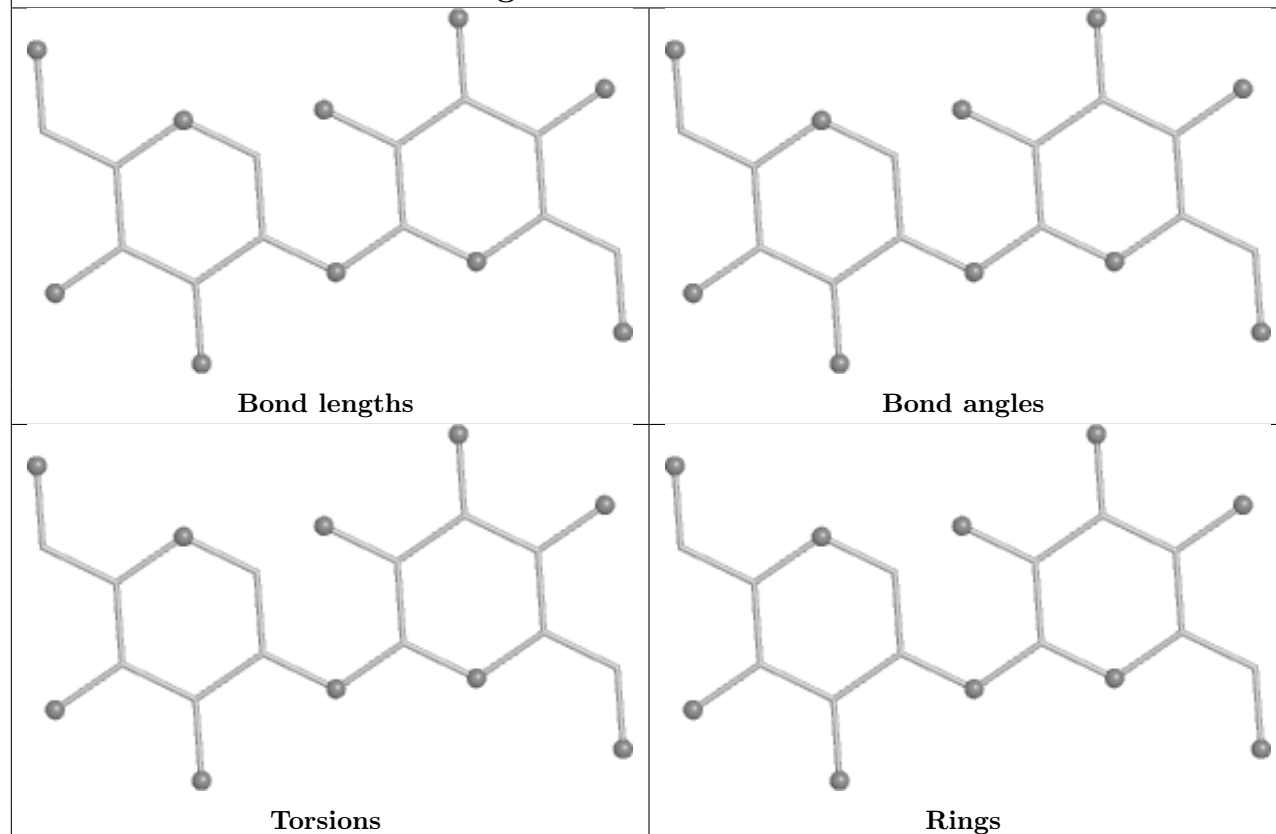




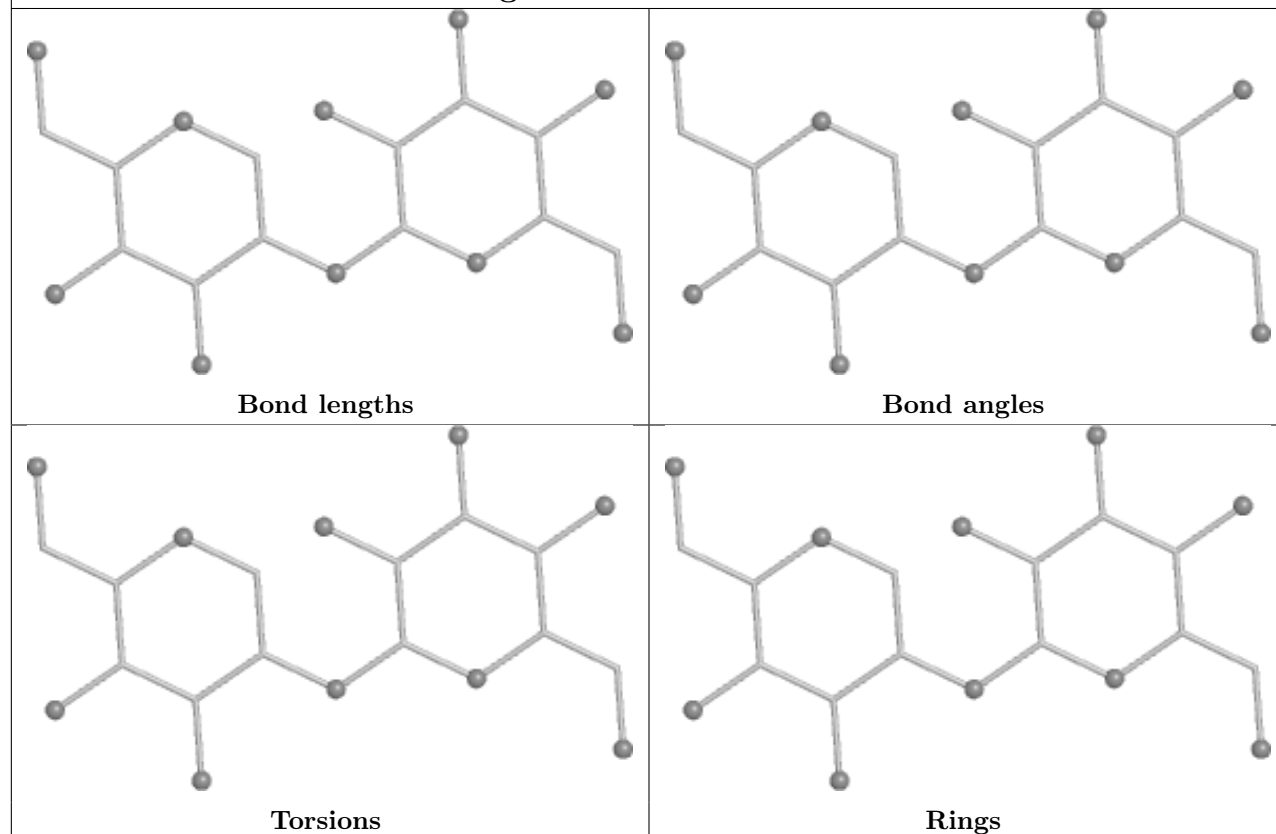


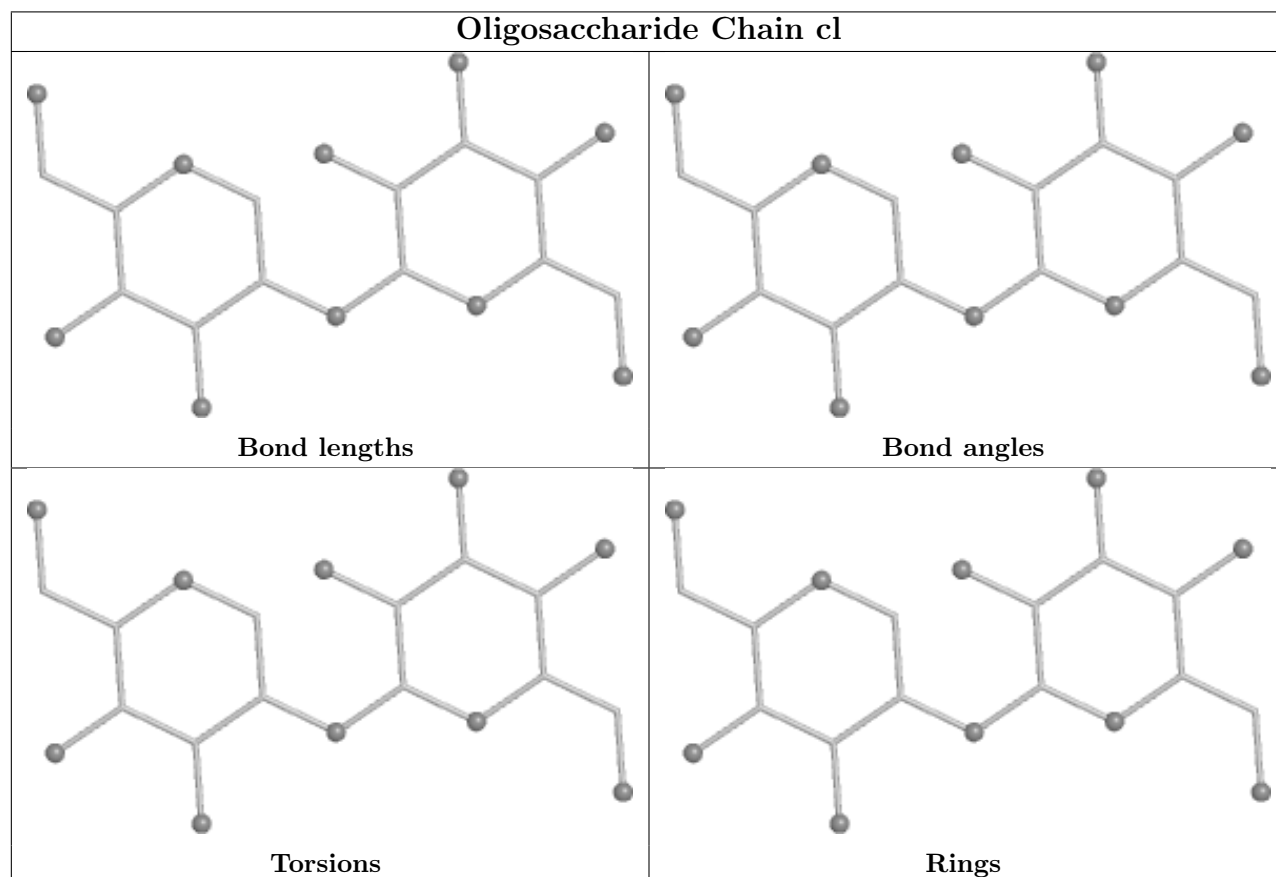
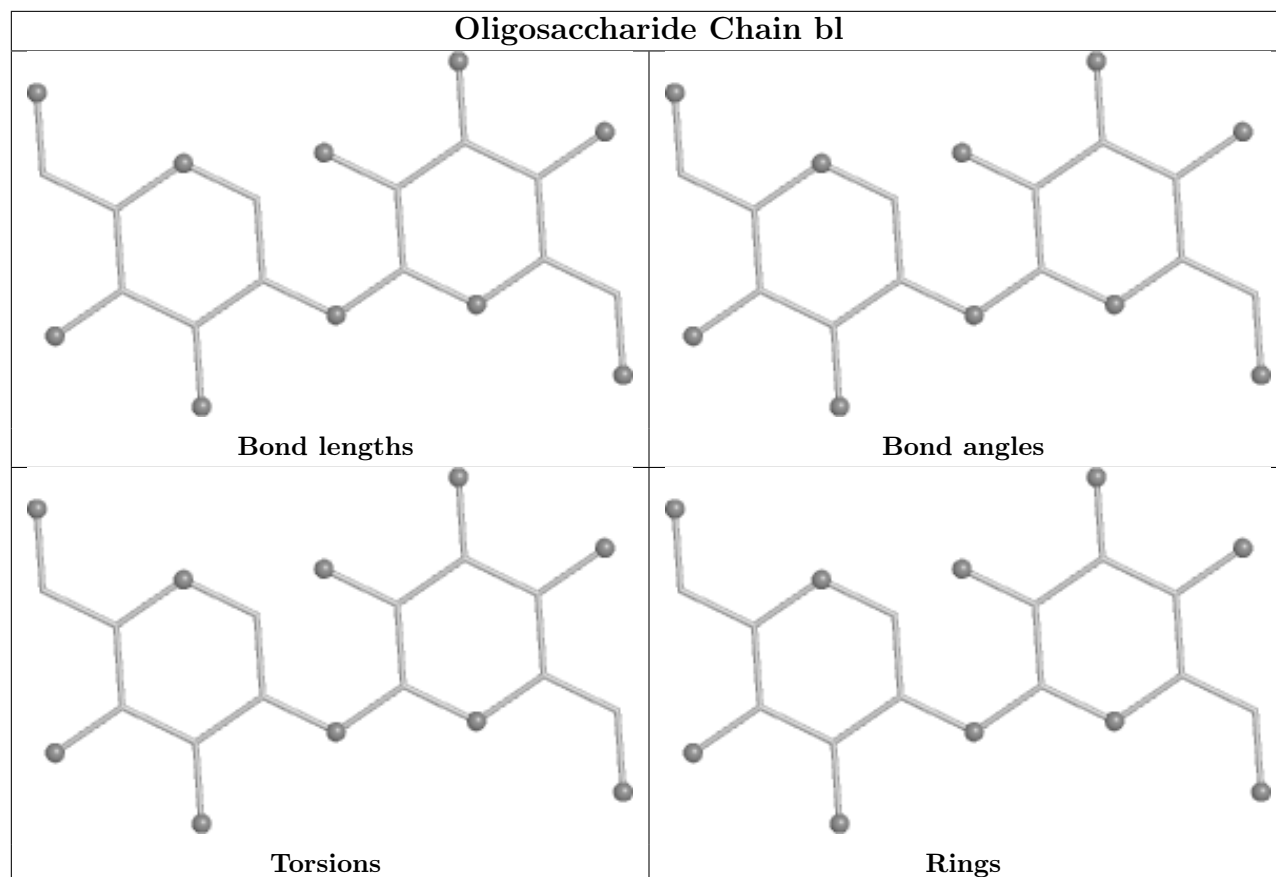


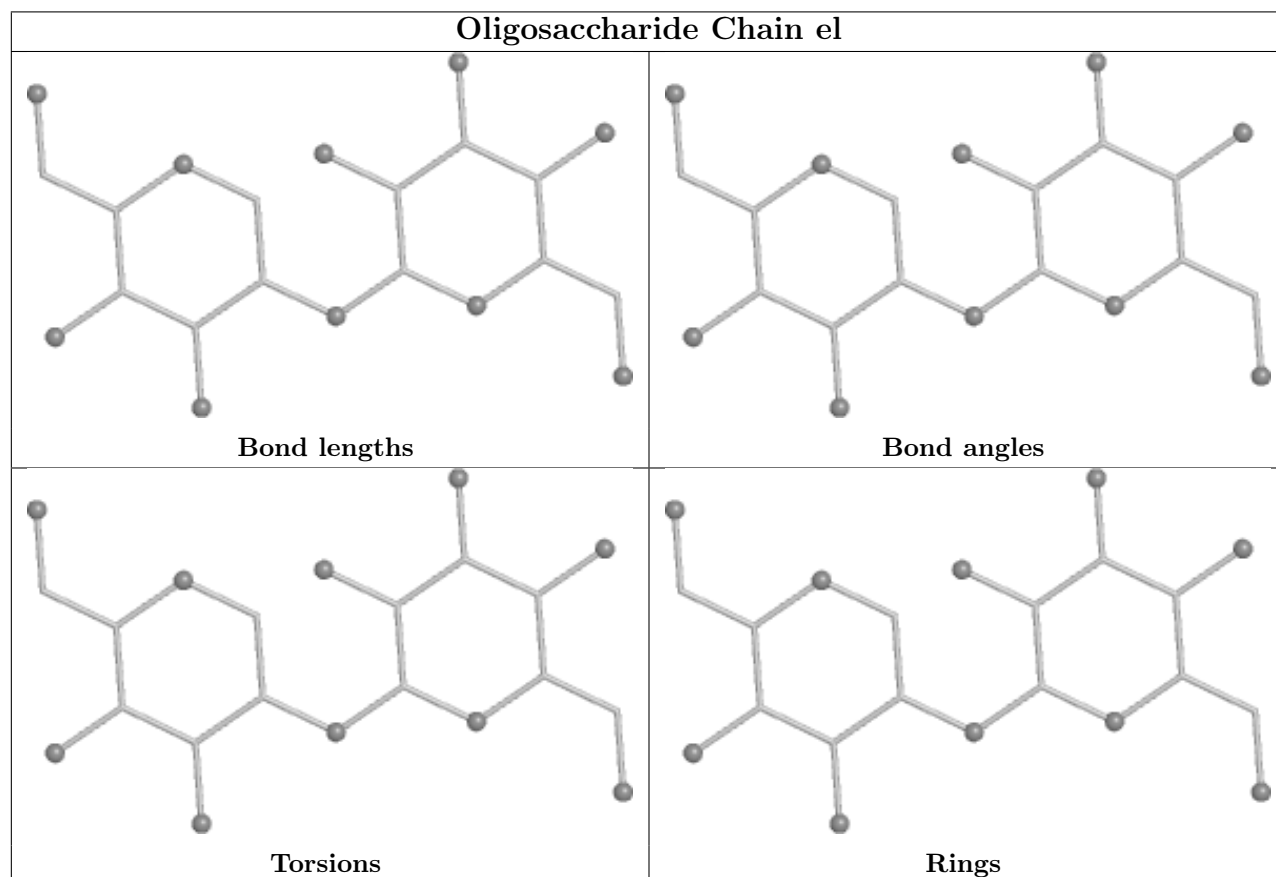
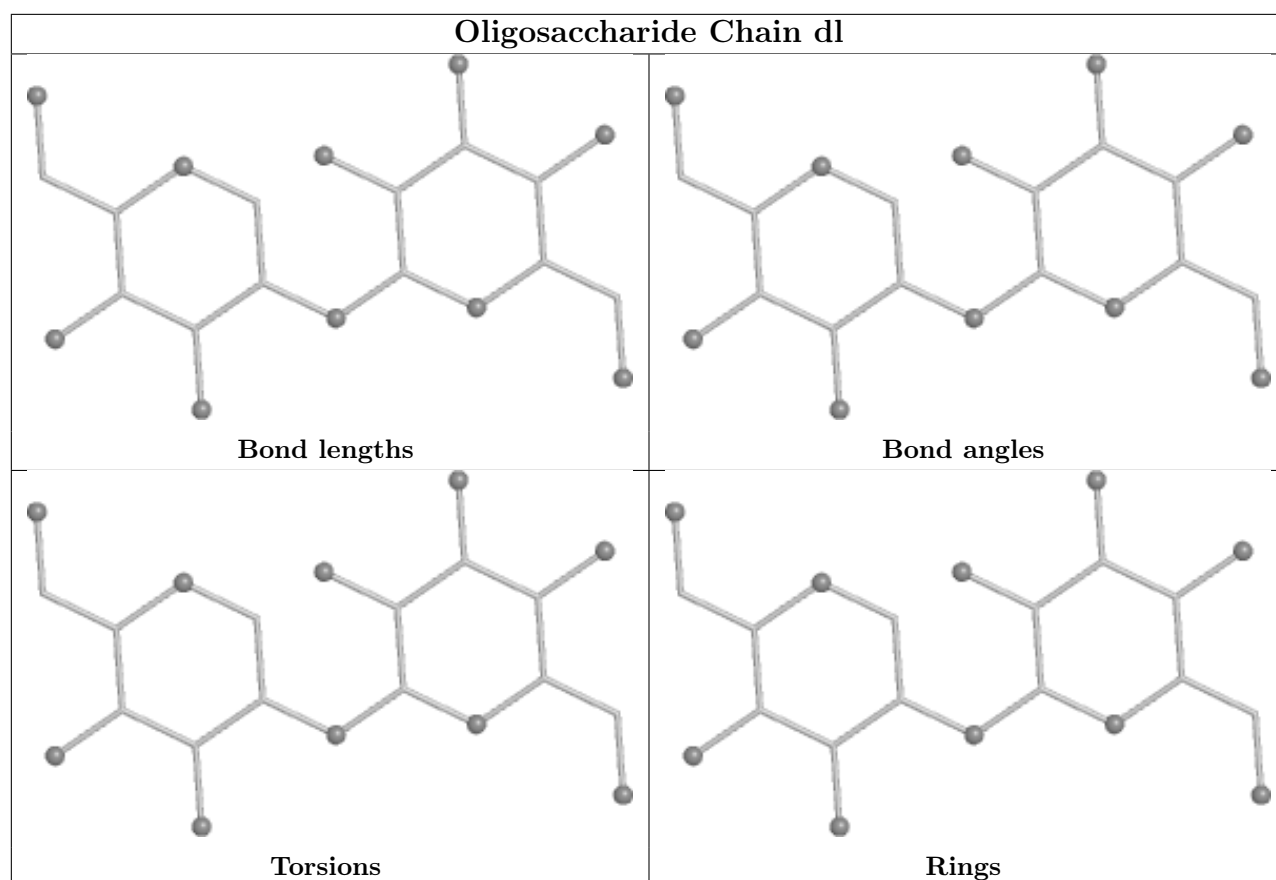
Oligosaccharide Chain Y1

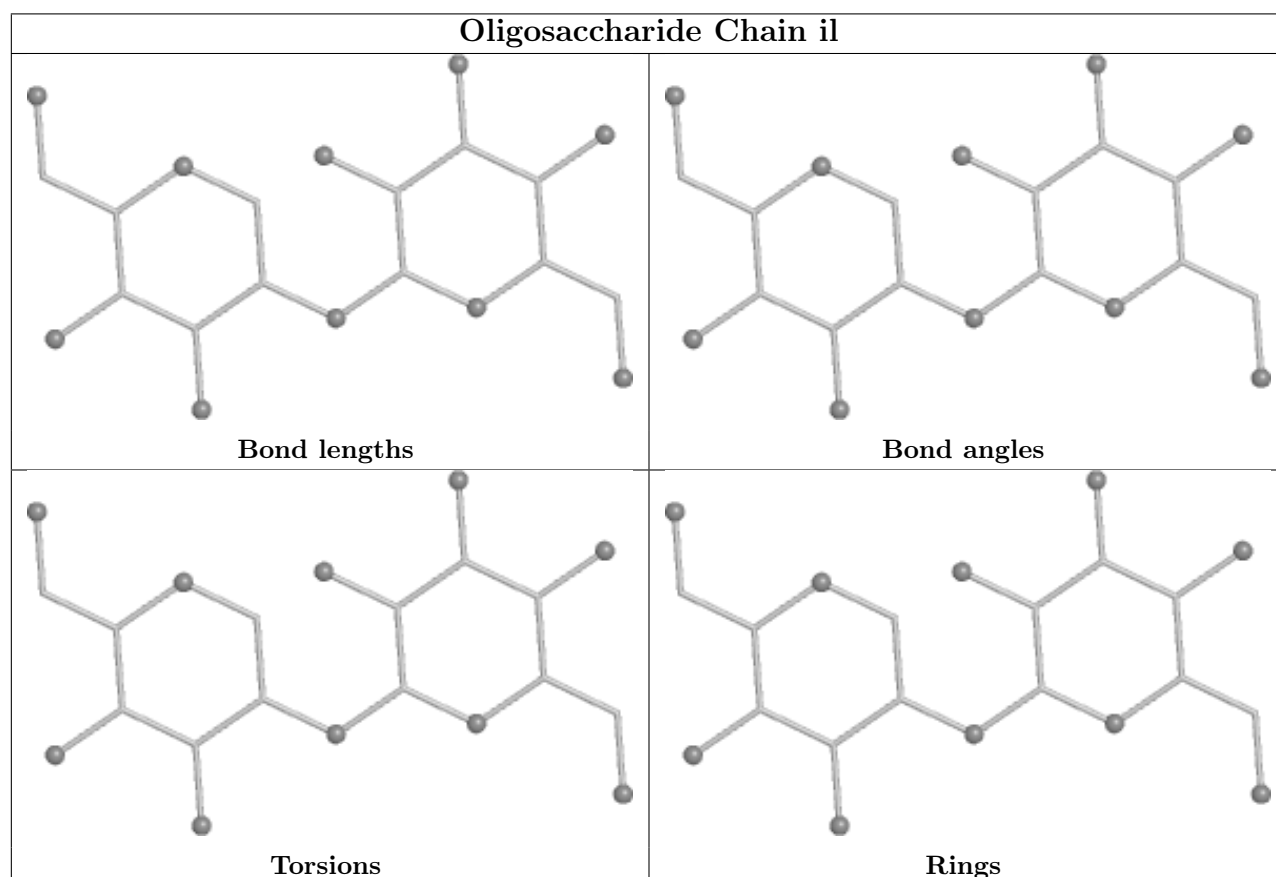
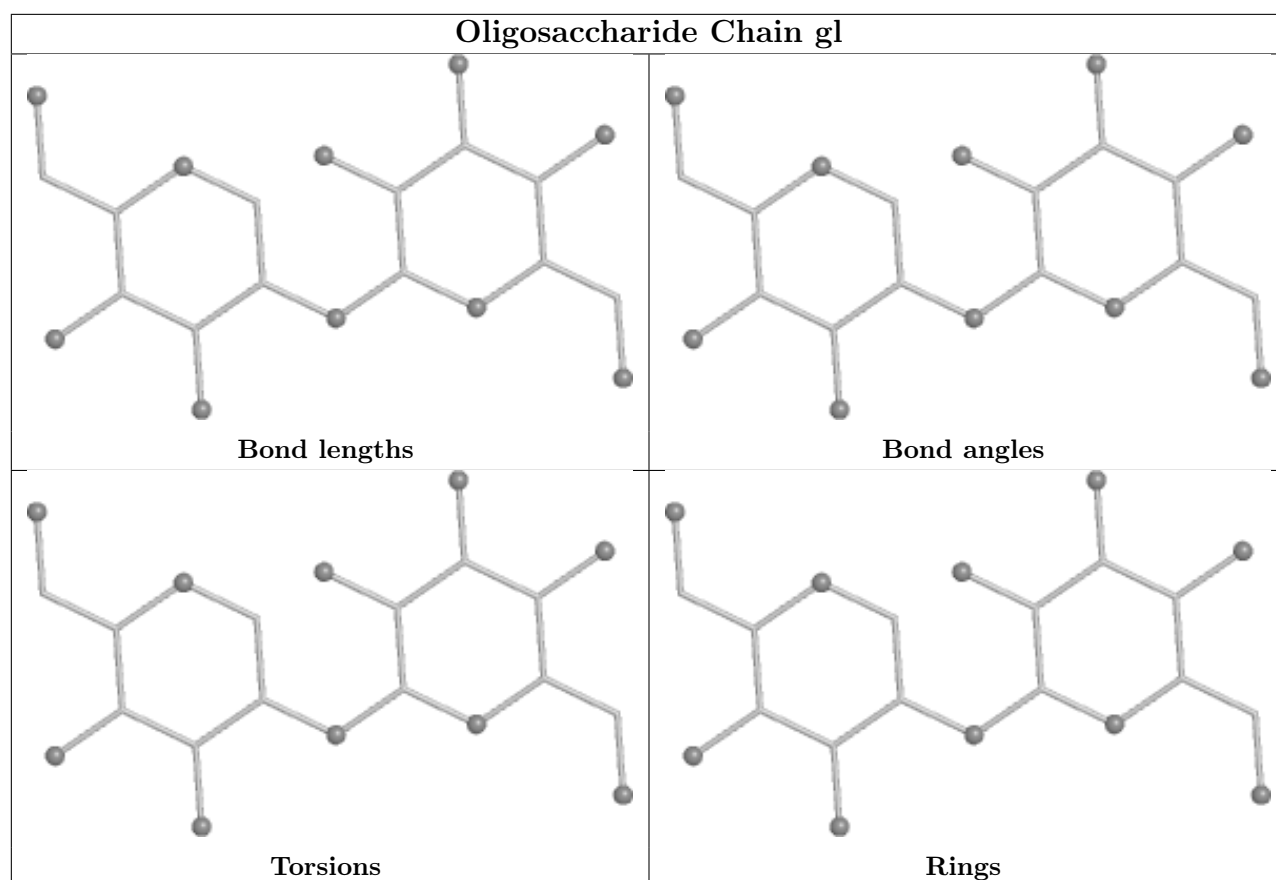


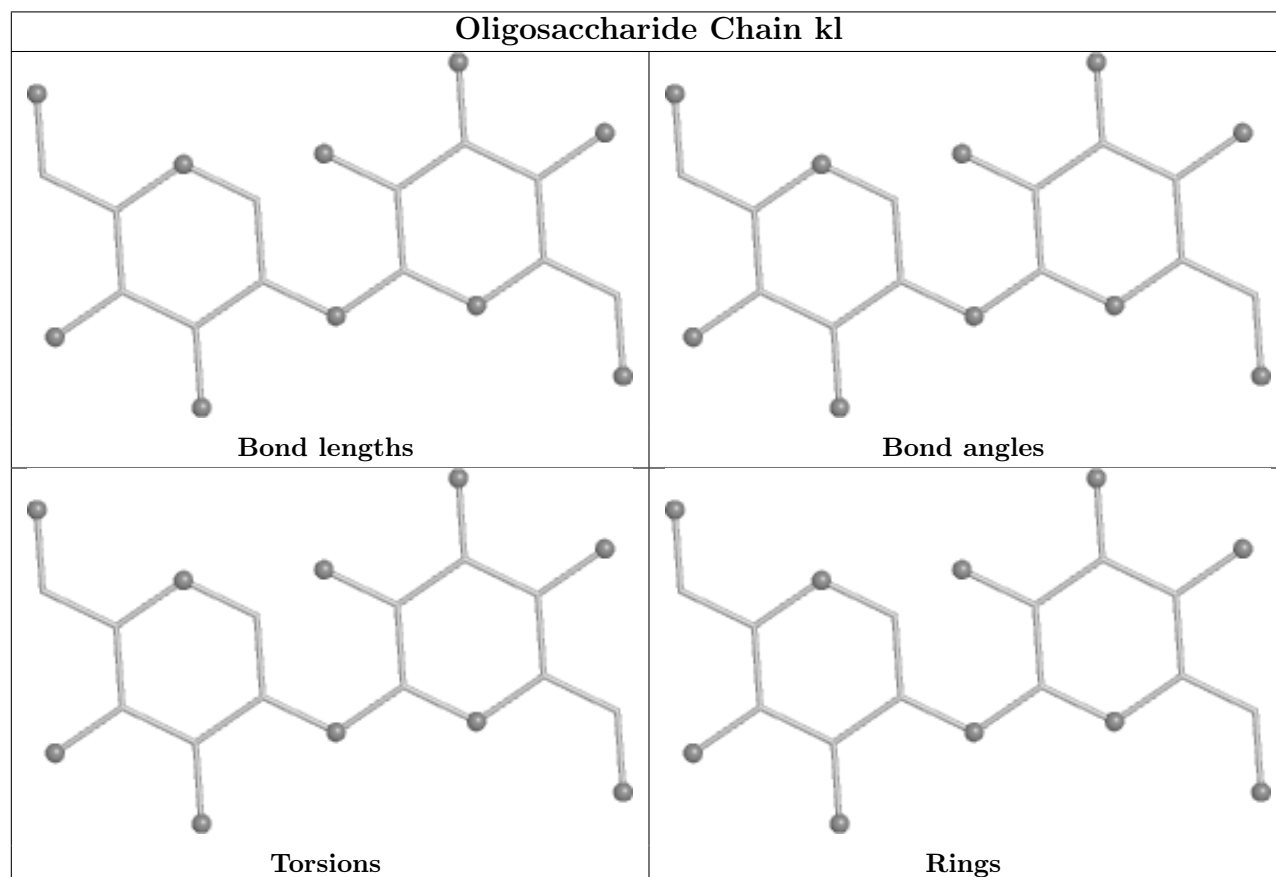
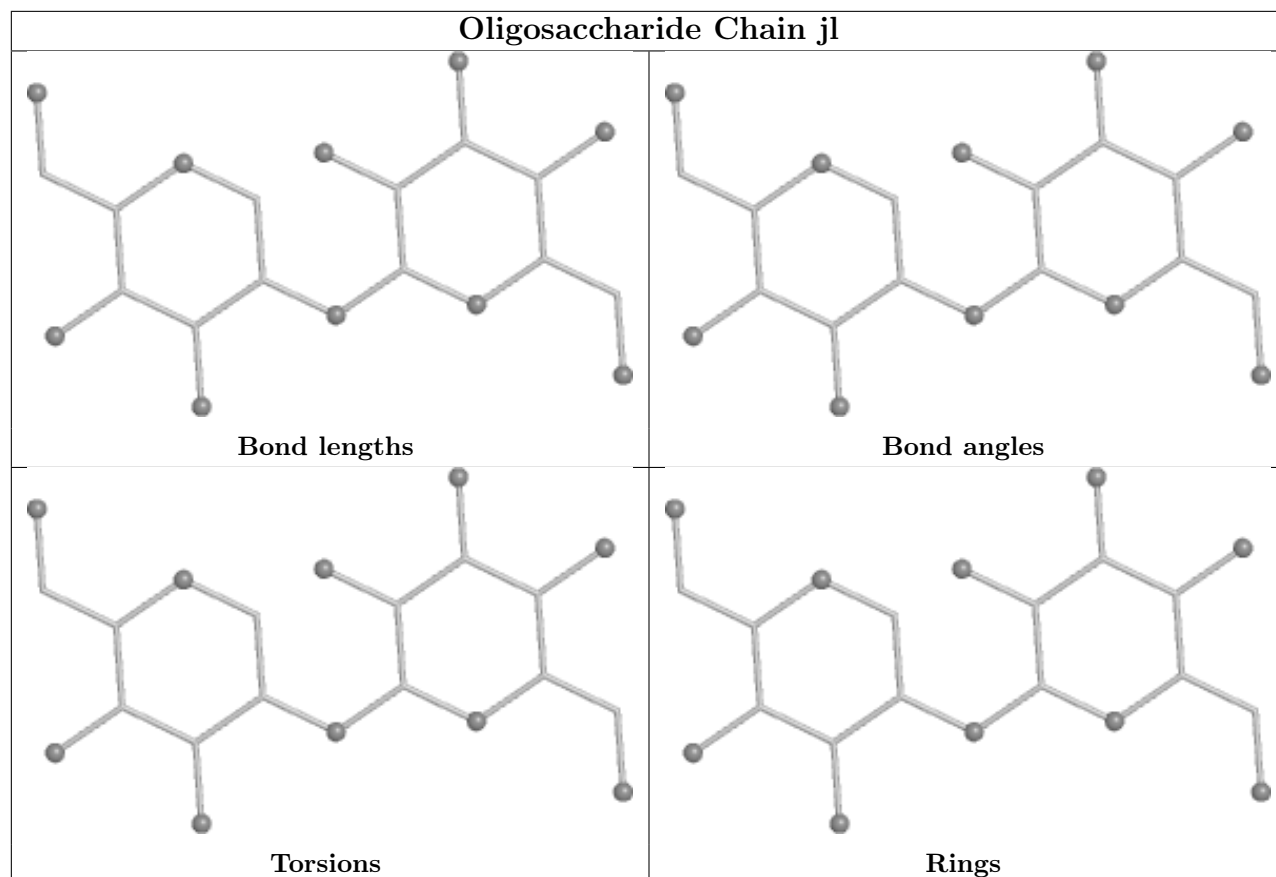
Oligosaccharide Chain Z1

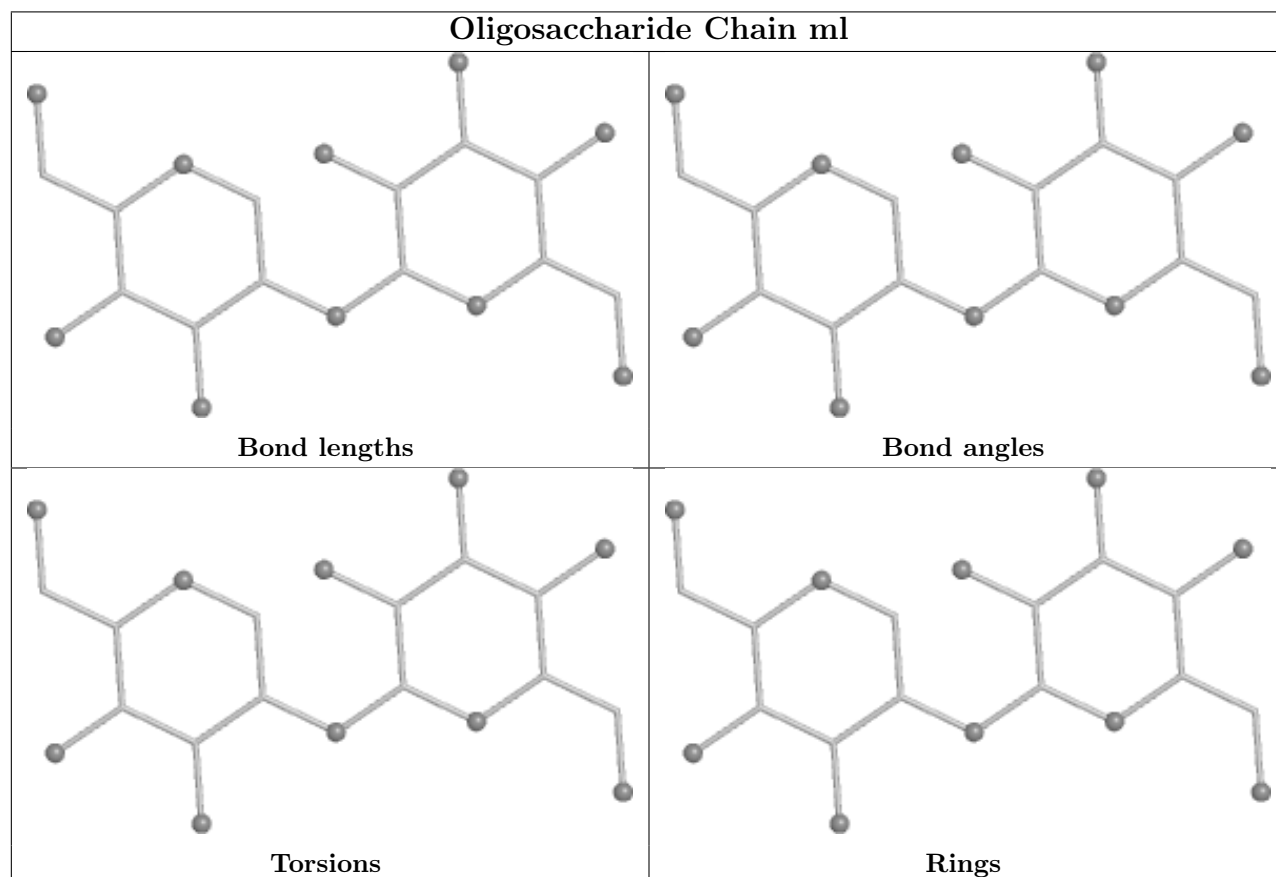
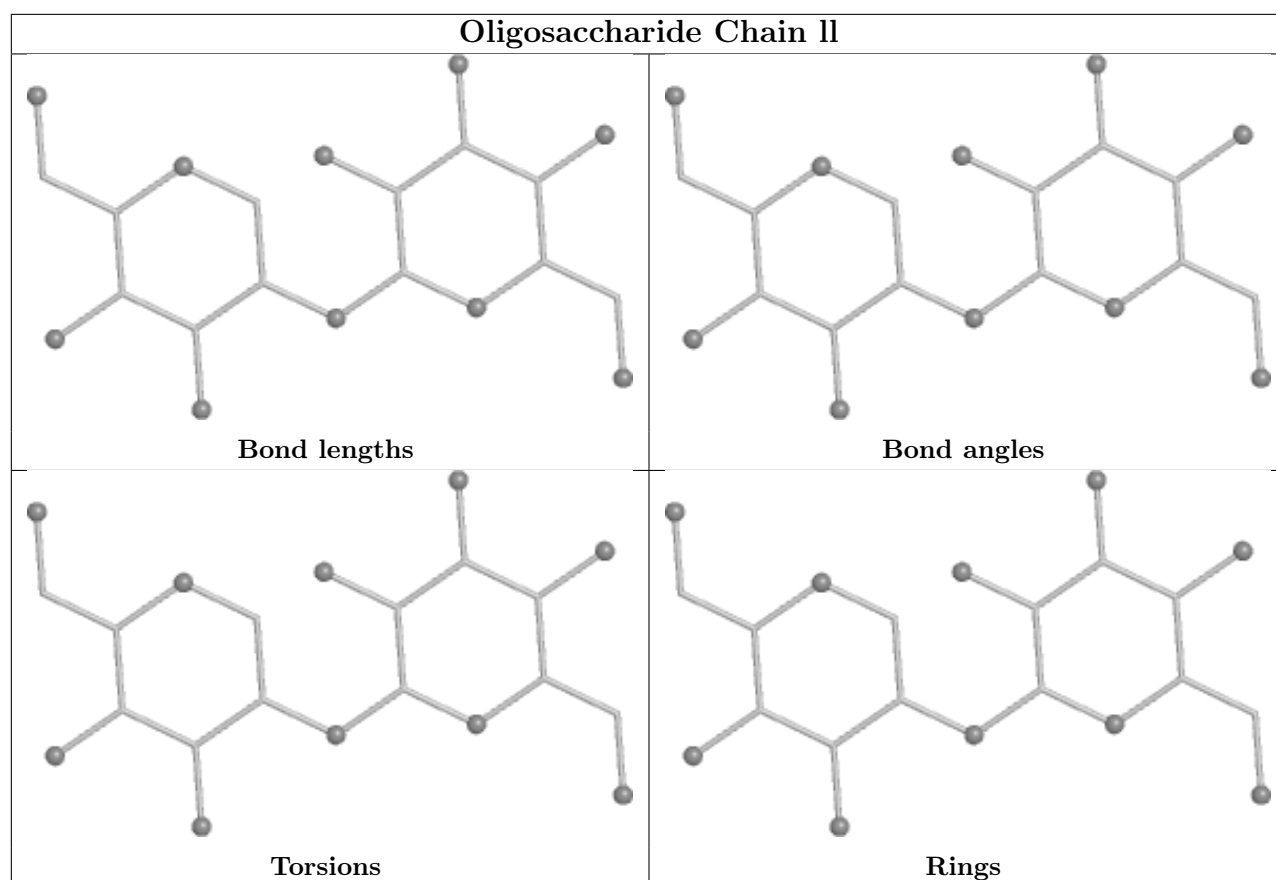


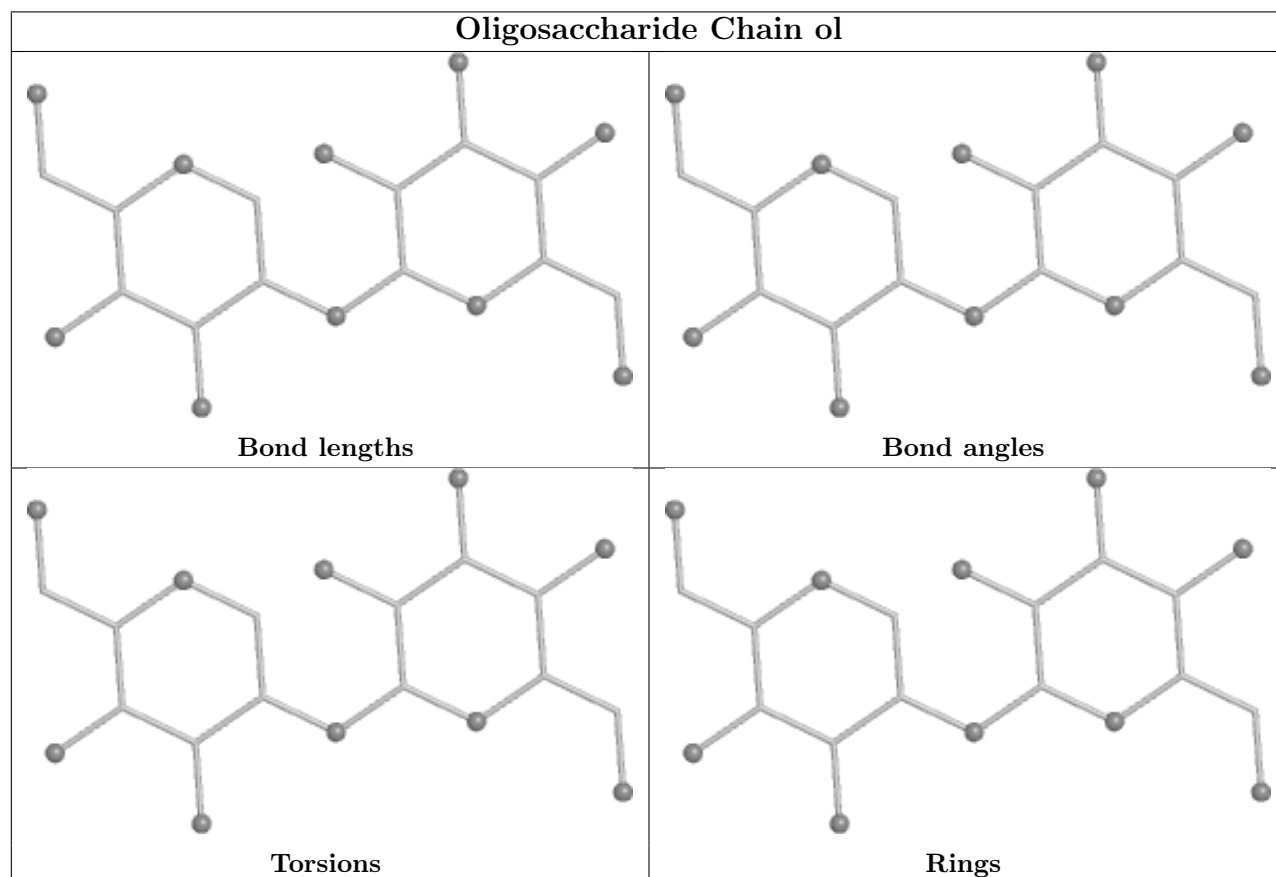
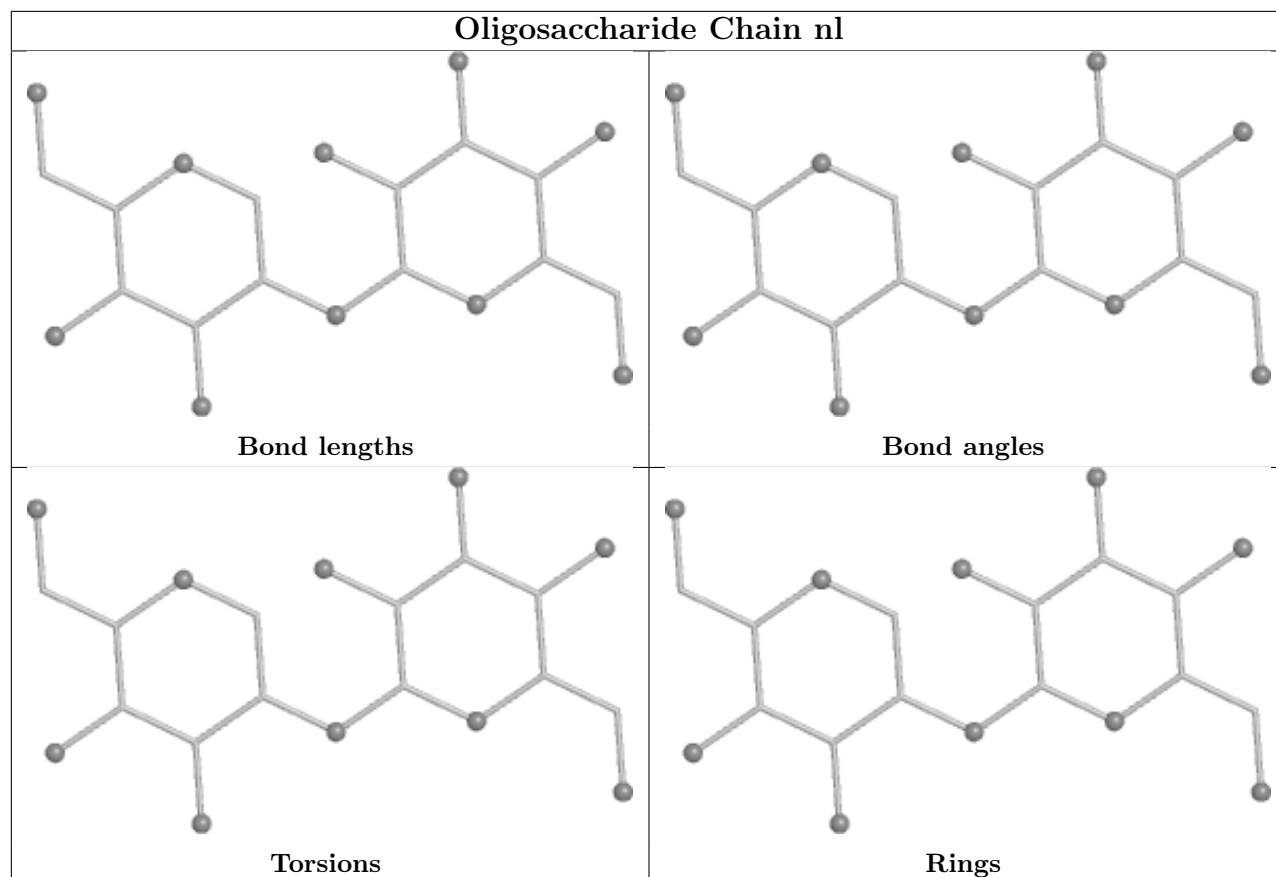


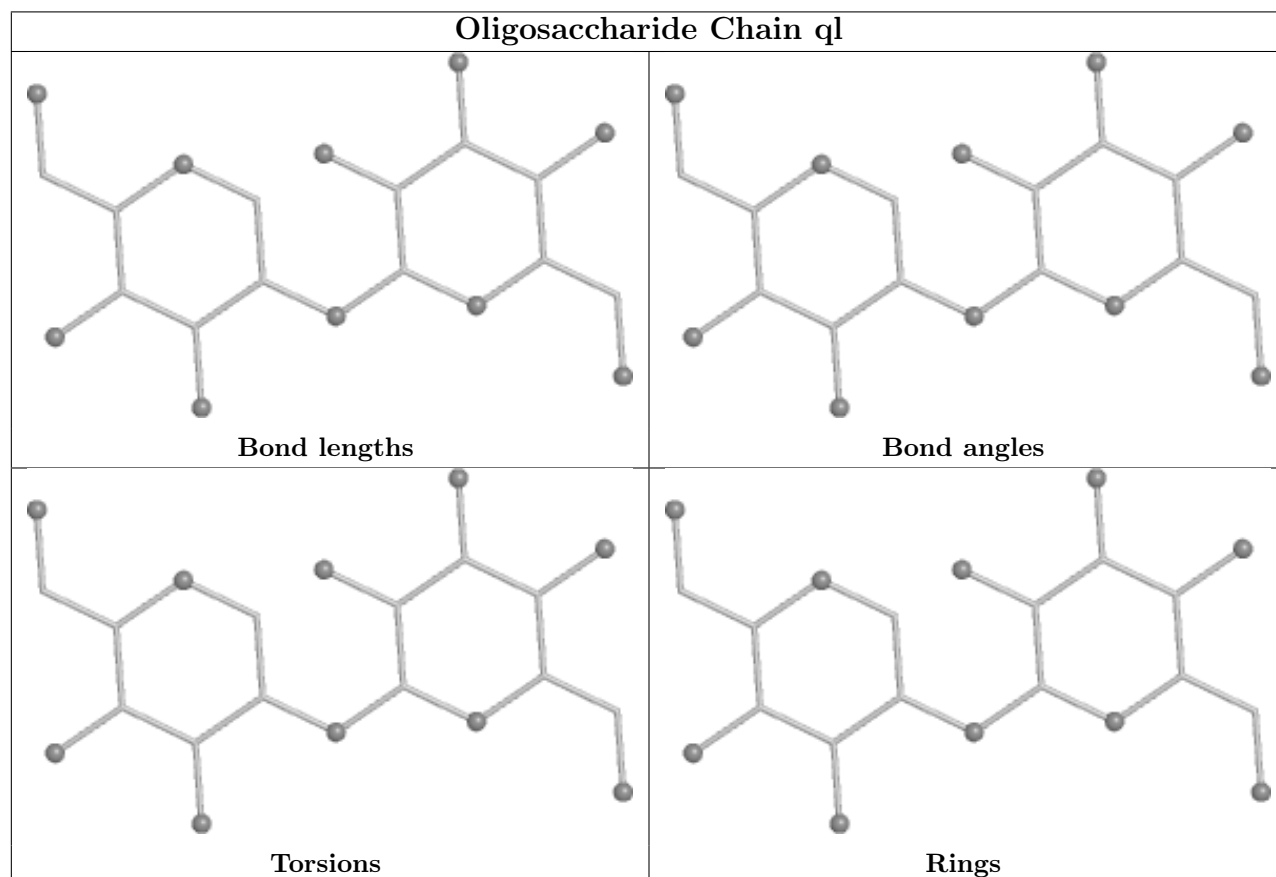
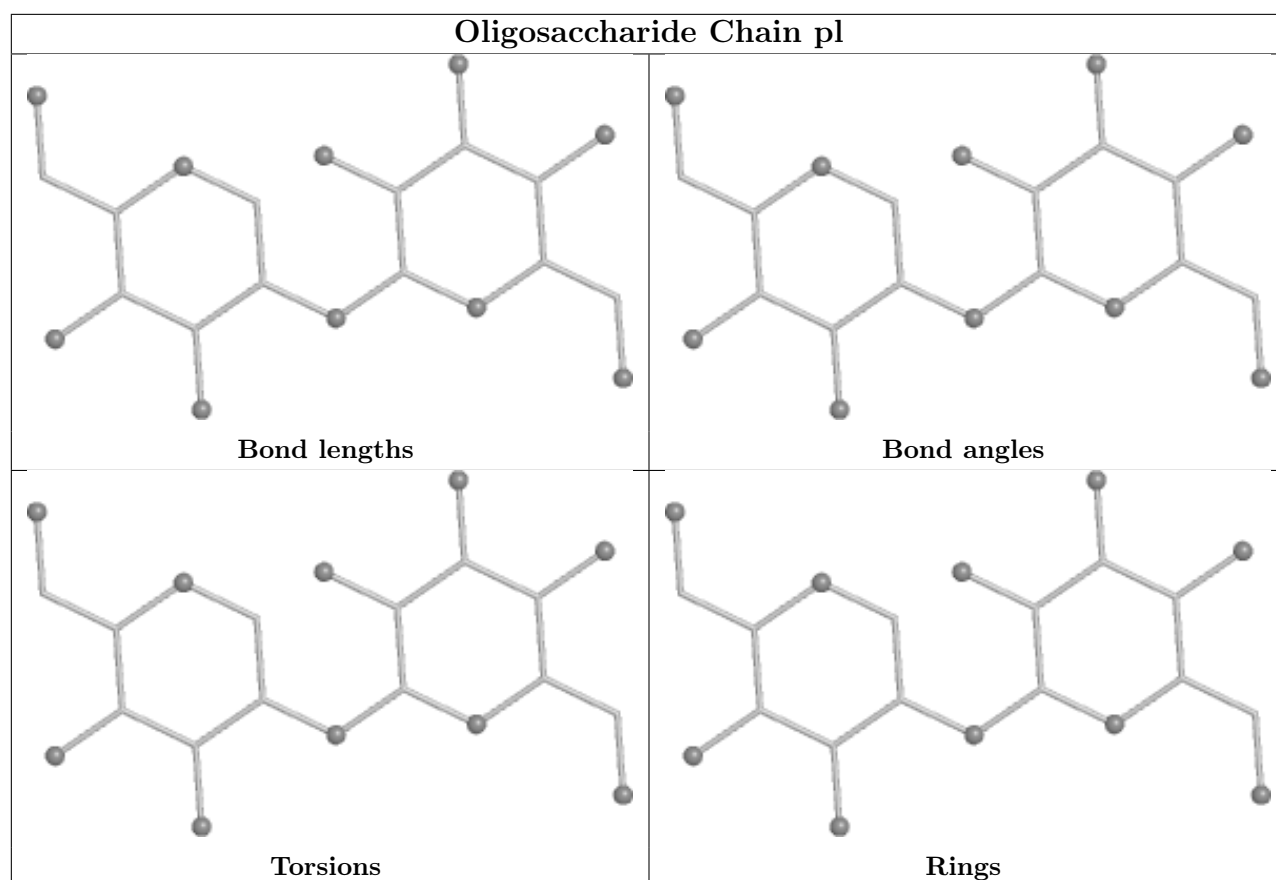


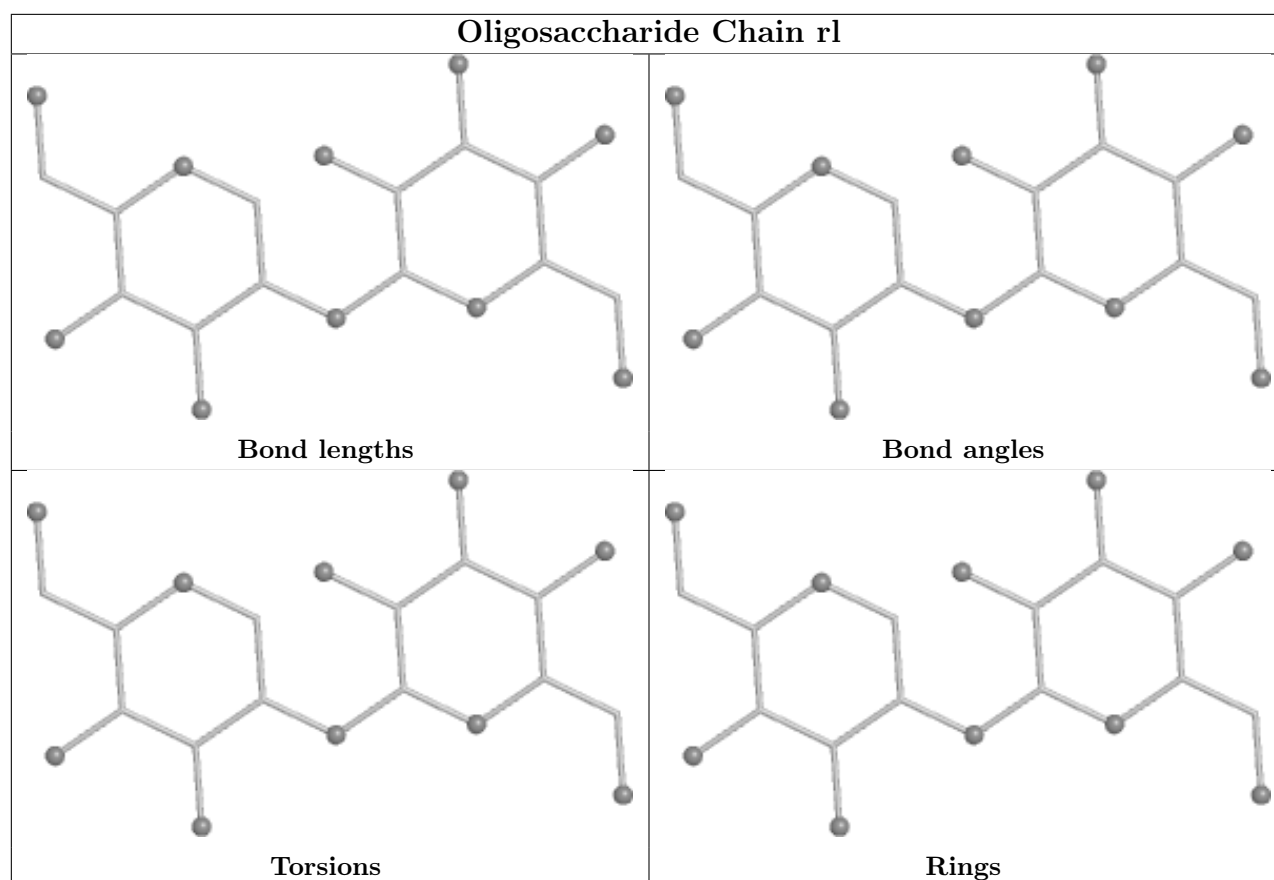












5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
32	GLC	CC	1301	-	11,11,12	0.25	0	15,15,17	0.63	0
32	GLC	RC	1301	-	11,11,12	0.25	0	15,15,17	0.63	0
33	GAL	FB	501	-	11,11,12	0.19	0	15,15,17	0.64	0
33	GAL	KB	501	-	11,11,12	0.19	0	15,15,17	0.64	0
32	GLC	HC	1301	-	11,11,12	0.24	0	15,15,17	0.63	0
33	GAL	AB	501	-	11,11,12	0.19	0	15,15,17	0.65	0
33	GAL	PB	501	-	11,11,12	0.19	0	15,15,17	0.64	0
32	GLC	MC	1301	-	11,11,12	0.25	0	15,15,17	0.63	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
32	GLC	CC	1301	-	-	0/2/19/22	0/1/1/1
32	GLC	RC	1301	-	-	0/2/19/22	0/1/1/1
33	GAL	FB	501	-	-	0/2/19/22	0/1/1/1
33	GAL	KB	501	-	-	0/2/19/22	0/1/1/1
32	GLC	HC	1301	-	-	0/2/19/22	0/1/1/1
33	GAL	AB	501	-	-	0/2/19/22	0/1/1/1
33	GAL	PB	501	-	-	0/2/19/22	0/1/1/1
32	GLC	MC	1301	-	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
19	IF	1
19	NF	1
19	DF	1
19	SF	1
17	BH	1
17	GH	1
17	LH	1
17	QH	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	IF	834:PHE	C	835:ALA	N	3.80
1	NF	834:PHE	C	835:ALA	N	3.78
1	DF	834:PHE	C	835:ALA	N	3.76
1	SF	834:PHE	C	835:ALA	N	3.75
1	BH	438:GLY	C	439:GLU	N	3.06

6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-66353. These allow visual inspection of the internal detail of the map and identification of artifacts.

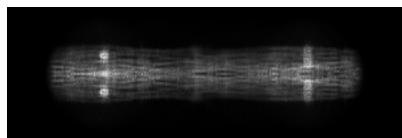
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections ⓘ

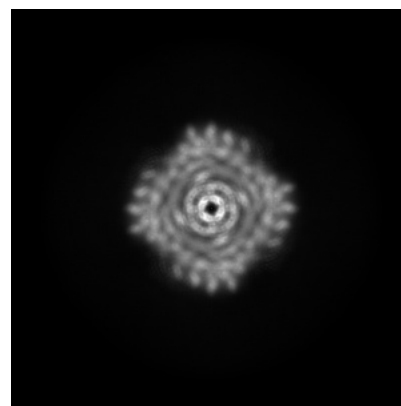
6.1.1 Primary map



X



Y



Z

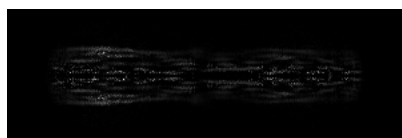
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

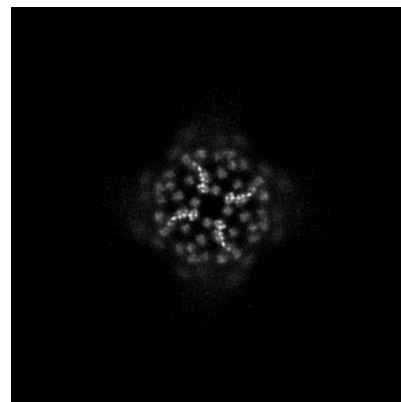
6.2.1 Primary map



X Index:
200



Y Index: 200

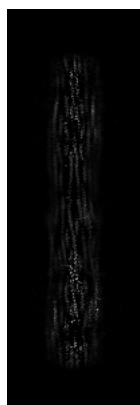


Z Index: 600

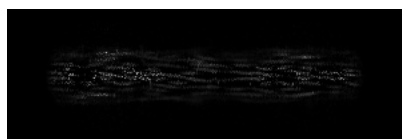
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

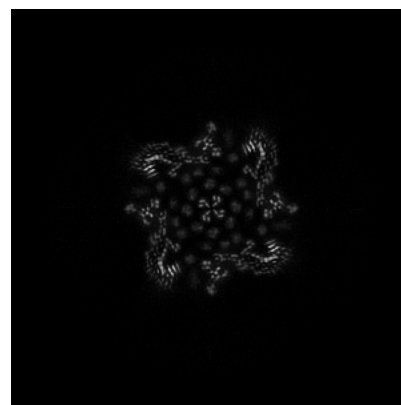
6.3.1 Primary map



X Index:
192



Y Index: 208

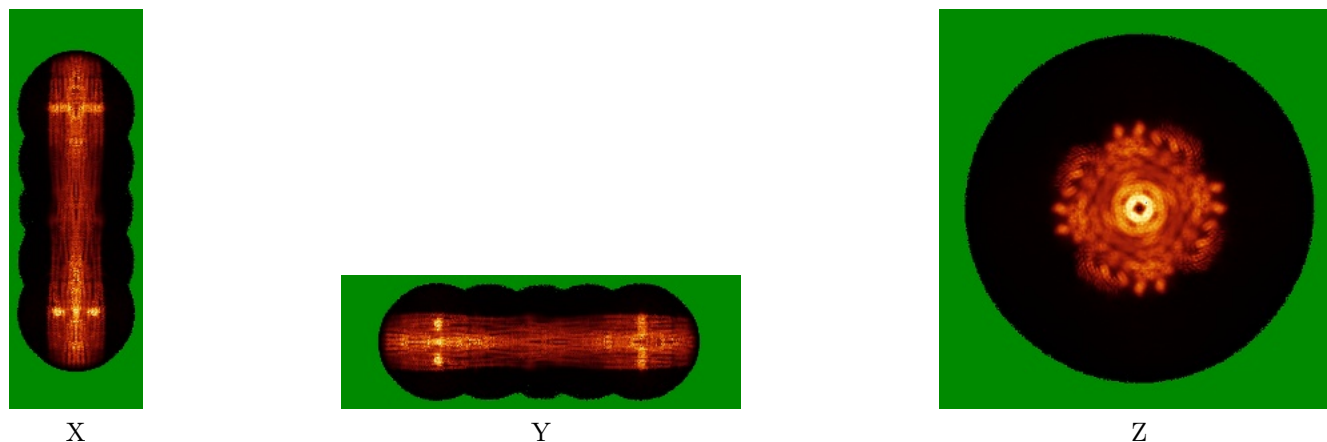


Z Index: 293

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

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

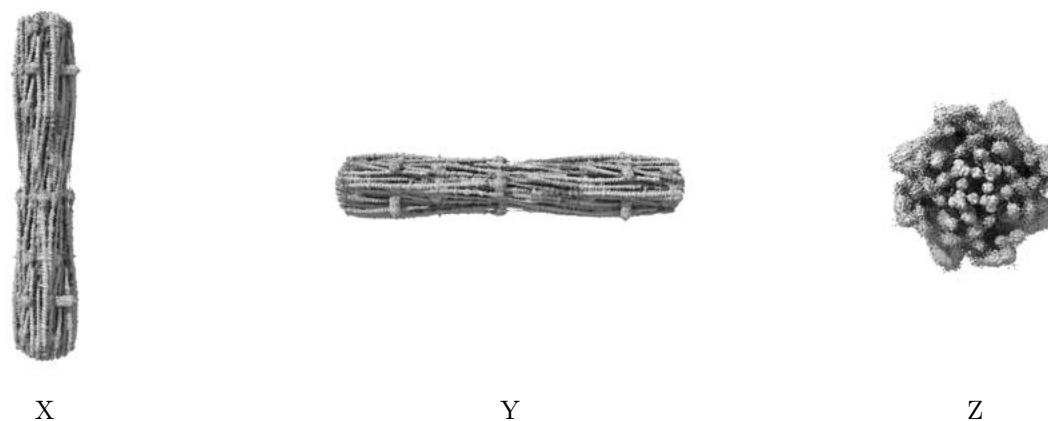
6.4.1 Primary map



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 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

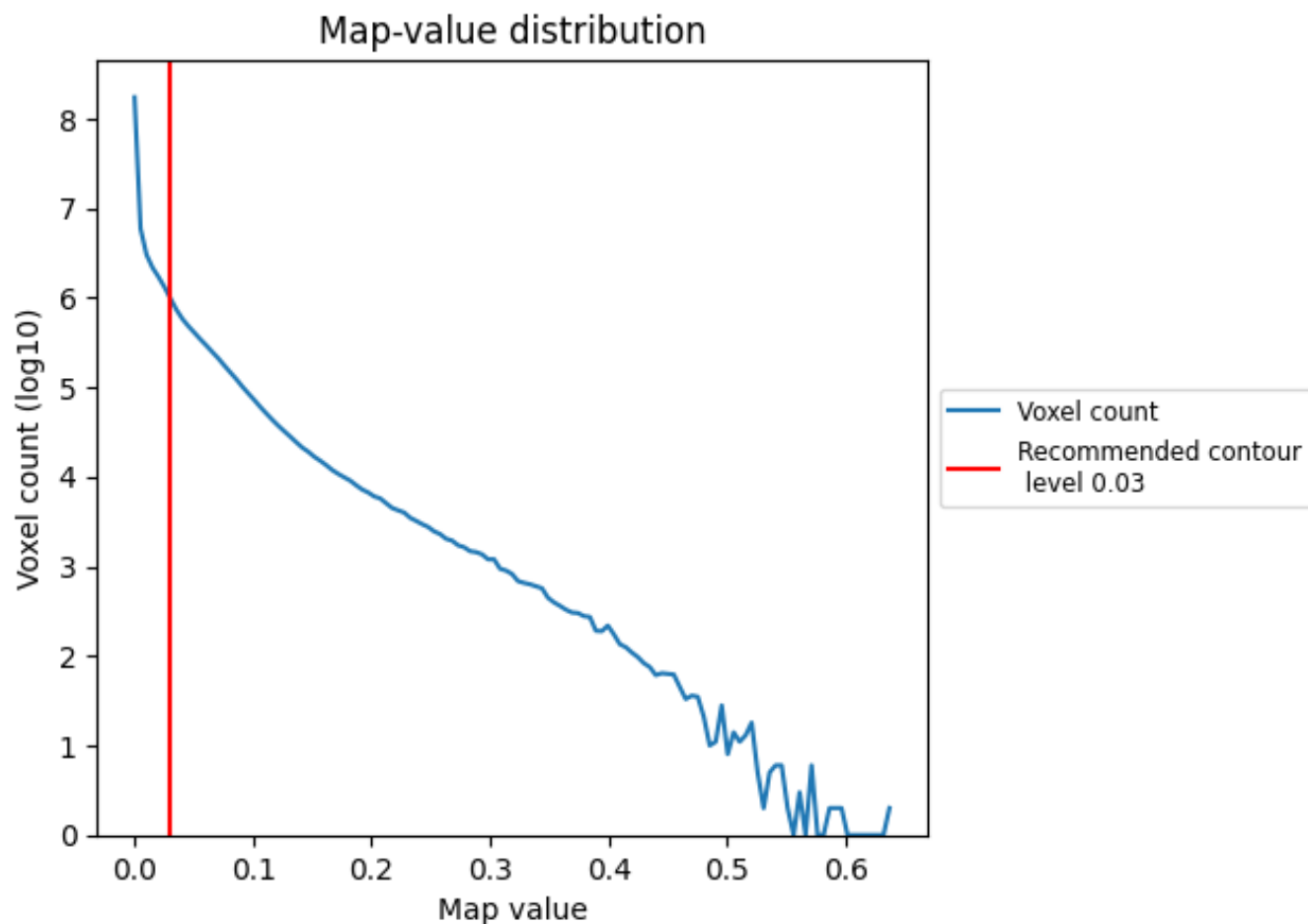
6.6 Mask visualisation

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

7 Map analysis [i](#)

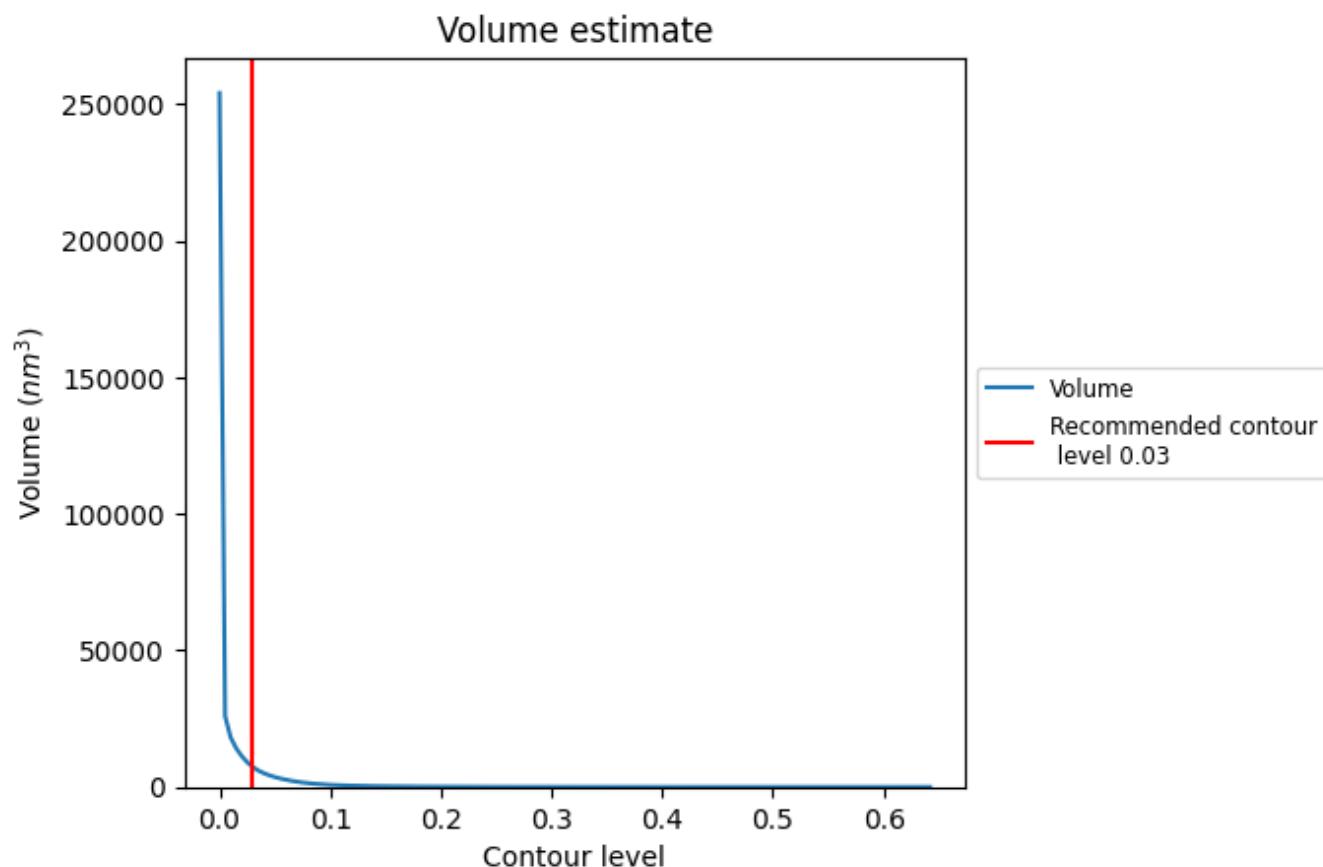
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

7.2 Volume estimate [i](#)



The volume at the recommended contour level is 7317 nm³; this corresponds to an approximate mass of 6610 kDa.

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

7.3 Rotationally averaged power spectrum [i](#)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

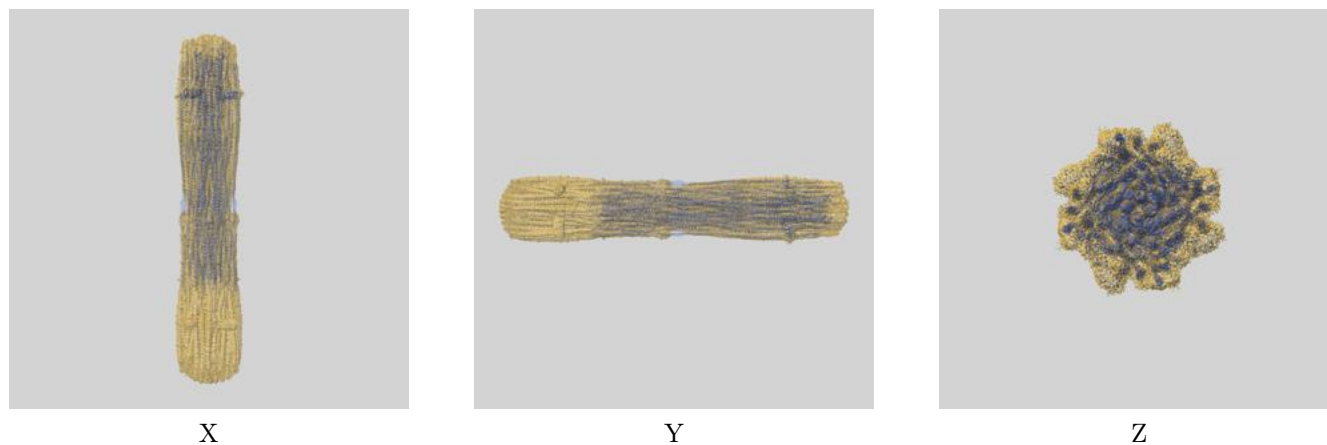
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

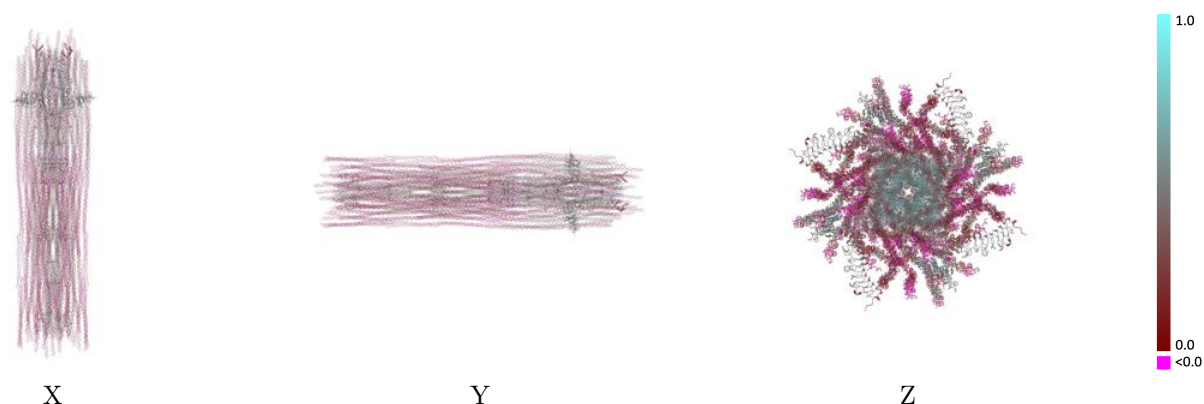
This section contains information regarding the fit between EMDB map EMD-66353 and PDB model 9WXP. Per-residue inclusion information can be found in section [3](#) on page [69](#).

9.1 Map-model overlay [i](#)



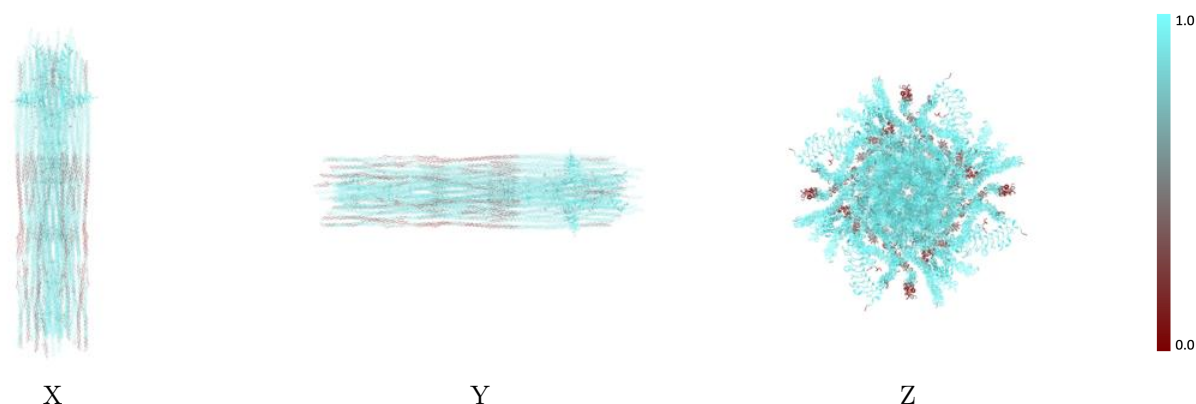
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



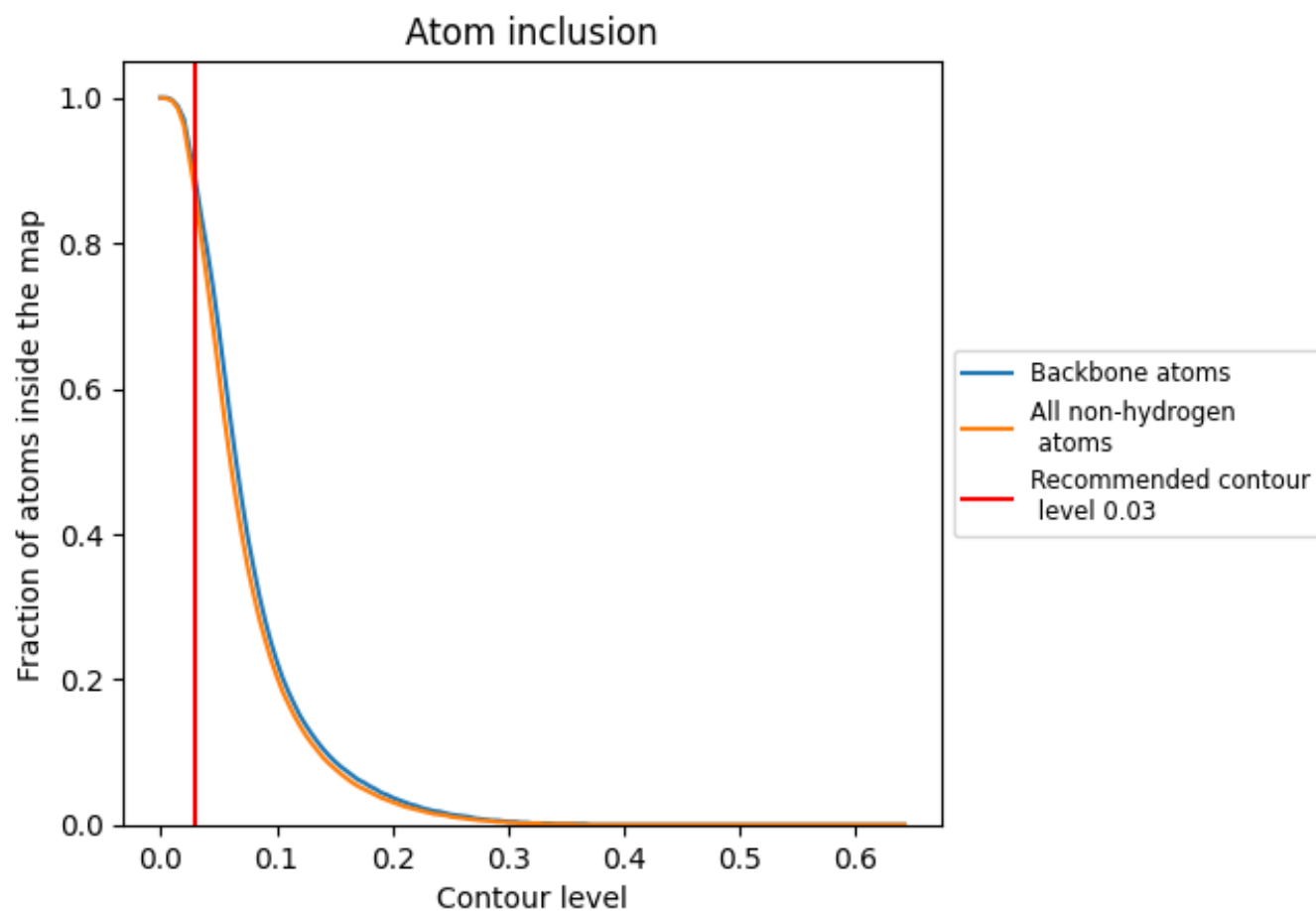
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion ⓘ



At the recommended contour level, 89% of all backbone atoms, 87% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8680	 0.2840
AA	 0.9900	 0.3920
AB	 0.9910	 0.3850
AC	 0.9800	 0.3920
AD	 0.7990	 0.2070
AE	 0.8150	 0.2180
AF	 0.7870	 0.2030
AG	 0.9540	 0.2410
AH	 0.9580	 0.2150
AI	 0.9660	 0.2340
AJ	 0.9710	 0.1730
AK	 0.9920	 0.1610
AL	 0.9710	 0.1730
AM	 0.9900	 0.4270
Aa	 1.0000	 0.4170
Ab	 1.0000	 0.4080
Ac	 1.0000	 0.4060
Ad	 1.0000	 0.4120
Ae	 0.9550	 0.4670
Af	 0.9550	 0.4820
Ag	 0.9550	 0.4900
Ah	 0.9550	 0.4780
Ai	 0.9550	 0.3800
Aj	 0.9090	 0.3800
Ak	 0.9090	 0.3630
Al	 0.9090	 0.3670
BA	 0.9900	 0.4870
BB	 0.9860	 0.4870
BC	 0.9910	 0.4900
BD	 0.9550	 0.2880
BE	 0.9390	 0.2700
BF	 0.9600	 0.2830
BG	 0.9620	 0.2330
BH	 0.9350	 0.2330
BI	 0.9450	 0.2320



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
BJ	 0.6010	 0.1460
BK	 0.5980	 0.1520
BL	 0.5860	 0.1530
BM	 0.9900	 0.4240
Ba	 1.0000	 0.5480
Bb	 1.0000	 0.5530
Bc	 1.0000	 0.5480
Bd	 1.0000	 0.5480
Be	 0.7730	 0.2680
Bf	 0.8180	 0.2820
Bg	 0.8180	 0.2820
Bh	 0.8180	 0.2640
Bi	 0.8640	 0.4500
Bj	 0.8640	 0.4580
Bk	 0.8640	 0.4500
Bl	 0.8640	 0.4580
CA	 0.9860	 0.4990
CB	 0.9900	 0.5020
CC	 0.9900	 0.4900
CD	 0.9140	 0.1750
CE	 0.9250	 0.1830
CF	 0.9000	 0.1770
CG	 0.9710	 0.3150
CH	 0.9480	 0.2950
CI	 0.9730	 0.3210
CJ	 0.9670	 0.3050
CK	 0.9650	 0.3010
CL	 0.9870	 0.3180
CM	 0.9910	 0.4240
Ca	 0.8180	 0.4590
Cb	 0.8180	 0.4570
Cc	 0.8180	 0.4530
Cd	 0.8180	 0.4520
Ce	 0.8640	 0.3540
Cf	 0.8640	 0.3600
Cg	 0.8640	 0.3470
Ch	 0.8640	 0.3600
Ci	 0.9550	 0.3770
Cj	 0.9550	 0.3960
Ck	 0.9550	 0.3820
Cl	 1.0000	 0.3410
DA	 0.9800	 0.3930

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DB	 0.9840	 0.3940
DC	 0.9810	 0.3970
DD	 0.3660	 0.1080
DE	 0.3590	 0.0980
DF	 0.3870	 0.1130
DG	 0.8300	 0.2060
DH	 0.8430	 0.2000
DI	 0.8310	 0.1960
DJ	 0.9740	 0.1780
DK	 0.9920	 0.1650
DL	 0.9710	 0.1740
DM	 0.9890	 0.4240
De	 0.7270	 0.3340
Df	 0.7270	 0.3420
Dg	 0.7270	 0.3430
Dh	 0.7270	 0.3430
Di	 0.9550	 0.3910
Dj	 0.9550	 0.3830
Dk	 0.9550	 0.3830
DI	 0.9550	 0.3730
EA	 0.9440	 0.2730
EB	 0.9220	 0.2820
EC	 0.9640	 0.3080
ED	 0.6380	 0.1160
EE	 0.6800	 0.1190
EF	 0.7060	 0.1380
EG	 0.6300	 0.1340
EH	 0.6460	 0.1380
EI	 0.6670	 0.1610
EJ	 0.6010	 0.1480
EK	 0.5970	 0.1520
EL	 0.5880	 0.1580
Ea	 0.8180	 0.3240
Eb	 0.8640	 0.3380
Ec	 0.8640	 0.3440
Ed	 0.8180	 0.3270
Ee	 0.9090	 0.4290
Ef	 0.9090	 0.4280
Eg	 0.9090	 0.4150
Eh	 0.9090	 0.4060
FA	 0.9880	 0.3920
FB	 0.9910	 0.3850

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
FC	 0.9830	 0.3910
FD	 0.8040	 0.2080
FE	 0.8160	 0.2280
FF	 0.7920	 0.2060
FG	 0.9560	 0.2380
FH	 0.9520	 0.2110
FI	 0.9660	 0.2310
FJ	 0.9690	 0.3030
FK	 0.9650	 0.3030
FL	 0.9870	 0.3180
Fi	 0.9550	 0.4800
Fj	 0.9550	 0.4930
Fk	 0.9550	 0.4900
Fl	 0.9550	 0.4730
GA	 0.9880	 0.4870
GB	 0.9870	 0.4890
GC	 0.9930	 0.4920
GD	 0.9550	 0.2860
GE	 0.9400	 0.2720
GF	 0.9630	 0.2830
GG	 0.9630	 0.2350
GH	 0.9390	 0.2330
GI	 0.9460	 0.2360
GJ	 0.9740	 0.1750
GK	 0.9920	 0.1620
GL	 0.9680	 0.1700
Ga	 1.0000	 0.4430
Gb	 0.9550	 0.4410
Gc	 0.9550	 0.4360
Gd	 1.0000	 0.4340
Ge	 0.9090	 0.4440
Gf	 0.9090	 0.4510
Gg	 0.9090	 0.4330
Gh	 0.9090	 0.4440
Gi	 0.9090	 0.4790
Gj	 0.9090	 0.4710
Gk	 0.9090	 0.4590
Gl	 0.9090	 0.4600
HA	 0.9870	 0.4980
HB	 0.9900	 0.5010
HC	 0.9910	 0.4890
HD	 0.9160	 0.1740

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
HE	 0.9270	 0.1820
HF	 0.9000	 0.1790
HG	 0.9680	 0.3150
HH	 0.9470	 0.2970
HI	 0.9700	 0.3210
HJ	 0.6030	 0.1500
HK	 0.5980	 0.1530
HL	 0.5900	 0.1550
Ha	 0.9090	 0.5100
Hb	 0.9090	 0.4940
Hc	 0.9550	 0.5100
Hd	 0.9550	 0.5110
He	 0.8640	 0.3910
Hf	 0.8640	 0.4140
Hg	 0.8640	 0.4270
Hh	 0.8640	 0.4180
Hi	 0.9550	 0.4710
Hj	 0.9550	 0.4650
Hk	 0.9550	 0.4760
Il	 0.9550	 0.4800
IA	 0.9800	 0.3930
IB	 0.9850	 0.3950
IC	 0.9810	 0.3960
ID	 0.3660	 0.1100
IE	 0.3590	 0.0980
IF	 0.3920	 0.1130
IG	 0.8290	 0.2070
IH	 0.8460	 0.1960
II	 0.8350	 0.1940
IJ	 0.9710	 0.3070
IK	 0.9670	 0.3020
IL	 0.9870	 0.3210
Ia	 1.0000	 0.5460
Ib	 1.0000	 0.5590
Ic	 1.0000	 0.5480
Id	 1.0000	 0.5580
Ie	 0.9550	 0.4810
If	 0.9550	 0.4800
Ig	 0.9550	 0.4810
Ih	 0.9550	 0.4730
Ii	 1.0000	 0.5010
Ij	 1.0000	 0.4930

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ik	 1.0000	 0.4910
Il	 1.0000	 0.4940
JA	 0.9550	 0.2750
JB	 0.9130	 0.2770
JC	 0.9640	 0.3060
JD	 0.6330	 0.1160
JE	 0.6770	 0.1200
JF	 0.7010	 0.1360
JG	 0.6320	 0.1330
JH	 0.6470	 0.1370
JI	 0.6700	 0.1590
JJ	 0.9710	 0.1710
JK	 0.9890	 0.1590
JL	 0.9660	 0.1690
Ja	 0.9550	 0.4830
Jb	 0.9550	 0.4870
Jc	 0.9550	 0.4990
Jd	 0.9550	 0.4950
Je	 0.7730	 0.3670
Jf	 0.7730	 0.3630
Jg	 0.7270	 0.3560
Jh	 0.7730	 0.3520
Ji	 0.5000	 0.2310
Jj	 0.5450	 0.2600
Jk	 0.5450	 0.2320
Jl	 0.5450	 0.2190
KA	 0.9890	 0.3930
KB	 0.9910	 0.3860
KC	 0.9810	 0.3880
KD	 0.8020	 0.2120
KE	 0.8210	 0.2330
KF	 0.7920	 0.2080
KG	 0.9550	 0.2370
KH	 0.9520	 0.2180
KI	 0.9620	 0.2290
KJ	 0.6010	 0.1500
KK	 0.5970	 0.1510
KL	 0.5860	 0.1540
Ka	 0.5910	 0.2550
Kb	 0.5910	 0.2700
Kc	 0.6360	 0.2490
Kd	 0.6360	 0.2610

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ke	 0.8180	 0.3270
Kf	 0.8640	 0.3180
Kg	 0.8180	 0.3360
Kh	 0.8180	 0.3290
Ki	 0.9090	 0.4180
Kj	 0.9090	 0.4070
Kk	 0.8640	 0.4190
Kl	 0.9090	 0.4210
LA	 0.9890	 0.4870
LB	 0.9850	 0.4880
LC	 0.9900	 0.4920
LD	 0.9550	 0.2870
LE	 0.9390	 0.2720
LF	 0.9620	 0.2850
LG	 0.9610	 0.2330
LH	 0.9390	 0.2330
LI	 0.9440	 0.2330
LJ	 0.9670	 0.3070
LK	 0.9640	 0.3020
LL	 0.9880	 0.3210
La	 0.9550	 0.5050
Lb	 0.9550	 0.5150
Lc	 0.9550	 0.5020
Ld	 0.9550	 0.4850
Le	 0.9550	 0.5440
Lf	 1.0000	 0.5490
Lg	 1.0000	 0.5370
Lh	 1.0000	 0.5170
Li	 0.7270	 0.2790
Lj	 0.7270	 0.3000
Lk	 0.6820	 0.2760
Ll	 0.6360	 0.2630
MA	 0.9870	 0.4980
MB	 0.9910	 0.5000
MC	 0.9910	 0.4890
MD	 0.9200	 0.1770
ME	 0.9290	 0.1810
MF	 0.9000	 0.1800
MG	 0.9700	 0.3150
MH	 0.9450	 0.2970
MI	 0.9710	 0.3210
Ma	 0.8180	 0.3410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Mb	 0.8180	 0.3470
Mc	 0.8180	 0.3440
Md	 0.8180	 0.3450
Me	 0.9090	 0.5140
Mf	 0.9090	 0.5100
Mg	 0.9090	 0.4900
Mh	 0.9090	 0.5010
Mi	 0.9550	 0.4690
Mj	 0.9550	 0.4830
Mk	 0.9550	 0.4920
MI	 0.9550	 0.4810
NA	 0.9800	 0.3920
NB	 0.9840	 0.3950
NC	 0.9810	 0.3970
ND	 0.3670	 0.1100
NE	 0.3600	 0.0980
NF	 0.3910	 0.1120
NG	 0.8280	 0.2060
NH	 0.8440	 0.1960
NI	 0.8310	 0.1960
Na	 0.9090	 0.4660
Nb	 0.9090	 0.4550
Nc	 0.9090	 0.4720
Nd	 0.9090	 0.4570
Ne	 0.7730	 0.2850
Nf	 0.7270	 0.2860
Ng	 0.7730	 0.2900
Nh	 0.7730	 0.3020
Ni	 1.0000	 0.5610
Nj	 0.9550	 0.5680
Nk	 1.0000	 0.5610
Nl	 1.0000	 0.5530
OA	 0.9490	 0.2720
OB	 0.9200	 0.2770
OC	 0.9640	 0.3070
OD	 0.6370	 0.1150
OE	 0.6710	 0.1210
OF	 0.7140	 0.1330
OG	 0.6240	 0.1370
OH	 0.6480	 0.1350
OI	 0.6720	 0.1580
Oa	 0.9550	 0.5110

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Ob	 0.9550	 0.5240
Oc	 0.9550	 0.5260
Od	 0.9550	 0.5110
Oe	 0.8640	 0.5060
Of	 0.9090	 0.5030
Og	 0.9090	 0.5070
Oh	 0.8640	 0.4900
Oi	 0.9090	 0.4520
Oj	 0.9090	 0.4570
Ok	 0.9090	 0.4360
Ol	 0.9090	 0.4410
PA	 0.9900	 0.3930
PB	 0.9910	 0.3860
PC	 0.9780	 0.3890
PD	 0.7990	 0.2130
PE	 0.8150	 0.2230
PF	 0.7890	 0.2050
PG	 0.9510	 0.2340
PH	 0.9560	 0.2180
PI	 0.9640	 0.2310
Pa	 1.0000	 0.5500
Pb	 1.0000	 0.5540
Pc	 1.0000	 0.5480
Pd	 1.0000	 0.5540
Pe	 0.8640	 0.4710
Pf	 0.8640	 0.4680
Pg	 0.8640	 0.4570
Ph	 0.8640	 0.4660
Pi	 0.9090	 0.4340
Pj	 0.9090	 0.4390
Pk	 0.9090	 0.4370
Pl	 0.9090	 0.4340
QA	 0.9900	 0.4870
QB	 0.9870	 0.4870
QC	 0.9900	 0.4900
QD	 0.9540	 0.2880
QE	 0.9400	 0.2690
QF	 0.9620	 0.2850
QG	 0.9600	 0.2320
QH	 0.9380	 0.2320
QI	 0.9410	 0.2310
Qa	 0.9090	 0.3780

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Qb	 0.9090	 0.3700
Qc	 0.8640	 0.3630
Qd	 0.8640	 0.3730
Qi	 0.9090	 0.3760
Qj	 0.9550	 0.3840
Qk	 0.9550	 0.3750
Ql	 0.9090	 0.3830
RA	 0.9870	 0.4970
RB	 0.9910	 0.5020
RC	 0.9910	 0.4900
RD	 0.9180	 0.1750
RE	 0.9280	 0.1830
RF	 0.8950	 0.1790
RG	 0.9710	 0.3160
RH	 0.9450	 0.2970
RI	 0.9720	 0.3210
Ra	 0.9090	 0.4430
Rb	 0.9090	 0.4560
Rc	 0.9090	 0.4610
Rd	 0.9090	 0.4550
Re	 0.9090	 0.4500
Rf	 0.9090	 0.4420
Rg	 0.9090	 0.4560
Rh	 0.9090	 0.4550
SA	 0.9810	 0.3920
SB	 0.9840	 0.3940
SC	 0.9800	 0.3970
SD	 0.3640	 0.1090
SE	 0.3580	 0.0970
SF	 0.3850	 0.1130
SG	 0.8310	 0.2060
SH	 0.8450	 0.1950
SI	 0.8320	 0.1970
Se	 1.0000	 0.5350
Sf	 1.0000	 0.5390
Sg	 1.0000	 0.5440
Sh	 1.0000	 0.5390
Si	 1.0000	 0.5500
Sj	 1.0000	 0.5430
Sk	 1.0000	 0.5270
Sl	 1.0000	 0.5370
TA	 0.9440	 0.2700

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
TB	 0.9180	 0.2800
TC	 0.9640	 0.3080
TD	 0.6340	 0.1140
TE	 0.6770	 0.1180
TF	 0.7090	 0.1370
TG	 0.6250	 0.1330
TH	 0.6470	 0.1380
TI	 0.6730	 0.1570
Ta	 0.8640	 0.3330
Tb	 0.8640	 0.3360
Tc	 0.8640	 0.3450
Td	 0.9090	 0.3490
Ti	 1.0000	 0.5570
Tj	 1.0000	 0.5580
Tk	 1.0000	 0.5570
Tl	 1.0000	 0.5720
Ua	 1.0000	 0.5510
Ub	 0.9550	 0.5640
Uc	 1.0000	 0.5650
Ud	 1.0000	 0.5430
Ui	 1.0000	 0.5030
Uj	 1.0000	 0.5090
Uk	 1.0000	 0.4980
Ul	 1.0000	 0.4950
Va	 0.8180	 0.4340
Vb	 0.8180	 0.4390
Vc	 0.8180	 0.4110
Vd	 0.8180	 0.4260
Ve	 0.6360	 0.2430
Vf	 0.6360	 0.2380
Vg	 0.5910	 0.2300
Vh	 0.5910	 0.2230
We	 0.8180	 0.4860
Wf	 0.8180	 0.4930
Wg	 0.8180	 0.4790
Wh	 0.9090	 0.4850
Xi	 0.8180	 0.4060
Xj	 0.8640	 0.3950
Xk	 0.8640	 0.4120
Xl	 0.8180	 0.4080
Ya	 0.9550	 0.4480
Yb	 0.9550	 0.4440

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
Yc	 0.9550	 0.4290
Yd	 0.9550	 0.4230
Yi	 0.8640	 0.4440
Yj	 0.8640	 0.4480
Yk	 0.9090	 0.4450
Yl	 0.8640	 0.4360
Za	 0.8640	 0.4580
Zb	 0.9090	 0.4440
Zc	 0.8640	 0.4400
Zd	 0.8640	 0.4500
Zi	 0.9550	 0.4420
Zj	 0.9550	 0.4370
Zk	 0.9550	 0.4360
Zl	 0.9550	 0.4270
aa	 0.9090	 0.4240
ab	 0.9090	 0.4090
ac	 0.9090	 0.4210
ad	 0.9090	 0.4260
bi	 1.0000	 0.4770
bj	 1.0000	 0.4540
bk	 1.0000	 0.4660
bl	 1.0000	 0.4800
ca	 0.9550	 0.5140
cb	 0.9550	 0.4960
cc	 1.0000	 0.5280
cd	 0.9550	 0.5240
ci	 0.8180	 0.4710
cj	 0.8180	 0.4780
ck	 0.8180	 0.4710
cl	 0.8180	 0.4710
da	 0.9090	 0.5070
db	 0.9090	 0.5060
dc	 0.9090	 0.5150
dd	 0.9090	 0.5020
di	 0.9550	 0.4900
dj	 1.0000	 0.4910
dk	 1.0000	 0.5030
dl	 1.0000	 0.4960
ea	 0.9090	 0.4260
eb	 0.8640	 0.4310
ec	 0.8640	 0.4270
ed	 0.8640	 0.4050

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ei	 0.9550	 0.4750
ej	 1.0000	 0.5040
ek	 1.0000	 0.5000
el	 1.0000	 0.4840
fa	 0.9550	 0.5170
fb	 0.9090	 0.5360
fc	 0.9090	 0.5300
fd	 0.9550	 0.5250
gi	 1.0000	 0.5050
gj	 1.0000	 0.5100
gk	 1.0000	 0.5160
gl	 1.0000	 0.5150
ha	 1.0000	 0.4970
hb	 1.0000	 0.5190
hc	 1.0000	 0.5300
hd	 1.0000	 0.5180
ii	 0.8180	 0.4030
ij	 0.8180	 0.3990
ik	 0.8180	 0.3900
il	 0.8180	 0.3910
ja	 0.9550	 0.4550
jb	 0.9550	 0.4660
jc	 0.9550	 0.4590
jd	 0.9550	 0.4590
ji	 0.7730	 0.3130
jj	 0.7270	 0.2880
jk	 0.7730	 0.3070
jl	 0.7730	 0.3040
ka	 0.8640	 0.4090
kb	 0.8640	 0.4220
kc	 0.9090	 0.4160
kd	 0.9090	 0.4100
ki	 0.5450	 0.0490
kj	 0.5450	 0.0360
kk	 0.5450	 0.0460
kl	 0.5450	 0.0540
la	 0.7730	 0.2280
lb	 0.8180	 0.2440
lc	 0.7730	 0.2420
ld	 0.7730	 0.2370
li	 0.8640	 0.2520
lj	 0.8640	 0.2410

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
lk	 0.8640	 0.2400
ll	 0.8640	 0.2540
ma	 0.8640	 0.3370
mb	 0.8640	 0.3560
mc	 0.8640	 0.3300
md	 0.8640	 0.3400
mi	 1.0000	 0.1630
mj	 1.0000	 0.1570
mk	 1.0000	 0.1600
ml	 1.0000	 0.1540
na	 0.9550	 0.2350
nb	 0.9550	 0.2350
nc	 0.9550	 0.2130
nd	 0.9550	 0.2180
ni	 0.9550	 0.5380
nj	 0.9550	 0.5370
nk	 0.9550	 0.5260
nl	 0.9550	 0.5200
oa	 0.9090	 0.3630
ob	 0.8640	 0.3860
oc	 0.9090	 0.3920
od	 0.9090	 0.3700
oi	 0.4550	 0.1950
oj	 0.5000	 0.1990
ok	 0.5000	 0.2030
ol	 0.4550	 0.1770
pa	 0.6820	 0.1310
pb	 0.6820	 0.1160
pc	 0.6820	 0.1250
pd	 0.6820	 0.1250
pi	 0.8180	 0.3270
pj	 0.8180	 0.3420
pk	 0.8180	 0.3310
pl	 0.8180	 0.3190
qa	 0.8640	 0.3290
qb	 0.8640	 0.3390
qc	 0.8640	 0.3180
qd	 0.8640	 0.3400
qi	 0.7730	 0.3190
qj	 0.7730	 0.3000
qk	 0.7270	 0.2940
ql	 0.7730	 0.2940

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
ra	 0.9090	 0.2880
rb	 0.9090	 0.2840
rc	 0.9090	 0.3010
rd	 0.9090	 0.2950
ri	 0.8180	 0.2480
rj	 0.7730	 0.2200
rk	 0.6820	 0.2310
rl	 0.8180	 0.2630
sa	 0.5910	 0.3190
sb	 0.6360	 0.3230
sc	 0.6360	 0.3110
sd	 0.5910	 0.3230