



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 07:54 PM UTC

PDB ID : 9B4H / pdb_00009b4h
EMDB ID : EMD-43892
Title : Chlamydomonas reinhardtii mastigoneme filament
Authors : Dai, J.; Ma, M.; Zhang, R.; Brown, A.
Deposited on : 2024-03-20
Resolution : 3.10 Å(reported)
Based on initial model : .

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

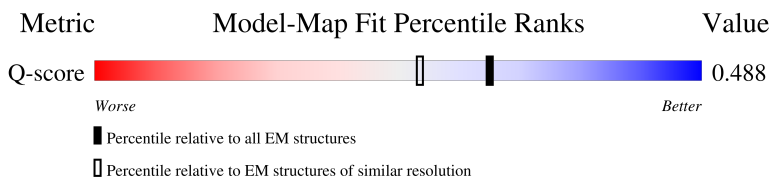
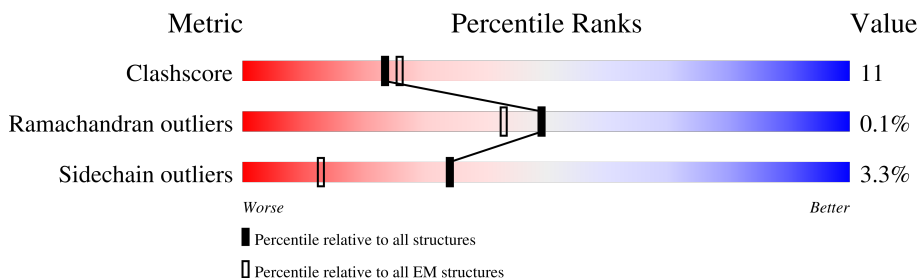
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



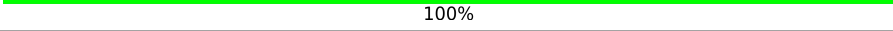
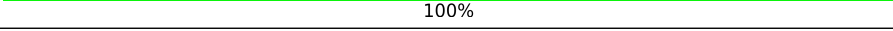
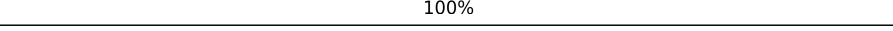
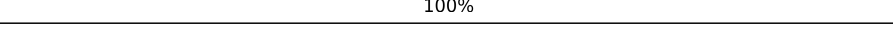
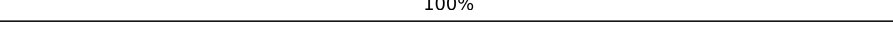
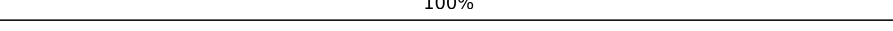
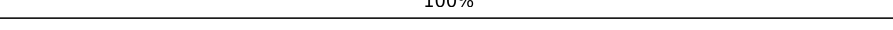
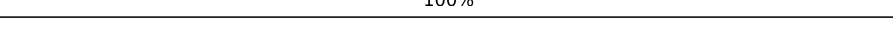
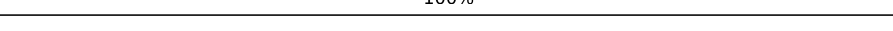
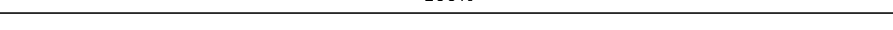
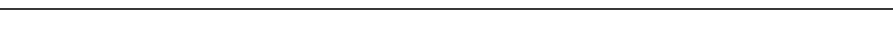
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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

Mol	Chain	Length	Quality of chain
1	A	1987	
1	B	1987	
2	X	8572	
3	A1	2	

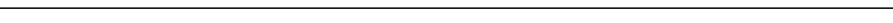
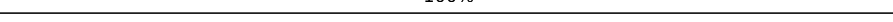
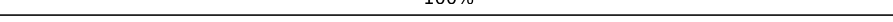
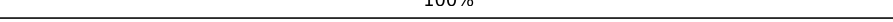
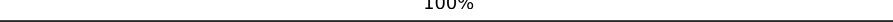
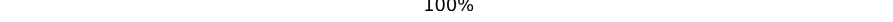
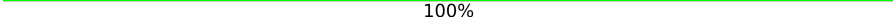
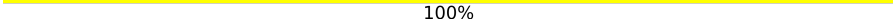
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Mol	Chain	Length	Quality of chain
3	A2	2	 50% 50%
3	A3	2	 50% 50%
3	a1	2	 50% 50%
3	a2	2	 50% 50%
3	a3	2	 50% 50%
4	A4	2	 100%
4	A5	2	 50% 50%
4	A7	2	 100%
4	B0	2	 50% 50%
4	B1	2	 100%
4	B3	2	 50% 50%
4	B4	2	 100%
4	B5	2	 100%
4	B7	2	 100%
4	B9	2	 100%
4	C0	2	 100%
4	C1	2	 100%
4	C2	2	 100%
4	C3	2	 100%
4	C4	2	 100%
4	C5	2	 100%
4	C6	2	 100%
4	C7	2	 100%
4	C8	2	 100%
4	C9	2	 100%

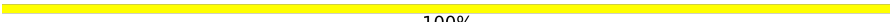
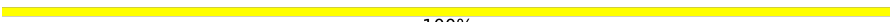
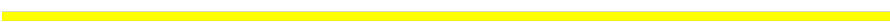
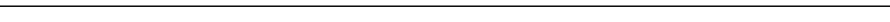
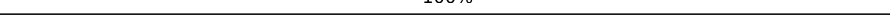
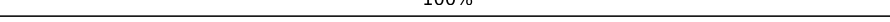
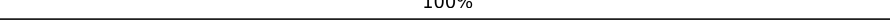
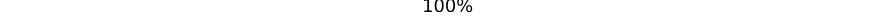
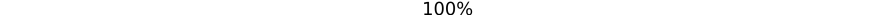
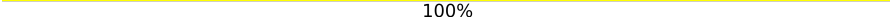
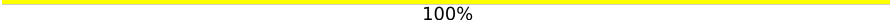
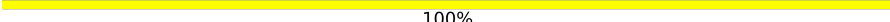
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Mol	Chain	Length	Quality of chain
4	D0	2	 100%
4	D1	2	 50% 50%
4	D2	2	 100%
4	D3	2	 100%
4	D4	2	 100%
4	D5	2	 100%
4	D6	2	 100%
4	D7	2	 100%
4	D8	2	 100%
4	D9	2	 50% 50%
4	E0	2	 100%
4	E1	2	 100%
4	E2	2	 100%
4	E3	2	 100%
4	E4	2	 50% 50%
4	E5	2	 100%
4	E7	2	 100%
4	E8	2	 100%
4	F0	2	 100%
4	F2	2	 100%
4	F3	2	 100%
4	F5	2	 50% 50%
4	F8	2	 100%
4	a5	2	 100%
4	a7	2	 50% 50%

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Mol	Chain	Length	Quality of chain
4	b0	2	 100%
4	b1	2	 100%
4	b3	2	 100%
4	b4	2	 100%
4	b5	2	 100%
4	b7	2	 100%
4	b9	2	 100%
4	c0	2	 100%
4	c1	2	 100%
4	c2	2	 100%
4	c3	2	 100%
4	c4	2	 100%
4	c5	2	 100%
4	c6	2	 100%
4	c7	2	 100%
4	c8	2	 100%
4	c9	2	 100%
4	d0	2	 50% 50%
4	d1	2	 100%
4	d2	2	 100%
4	d3	2	 100%
4	d4	2	 100%
4	d5	2	 100%
4	d6	2	 100%
4	d7	2	 100%

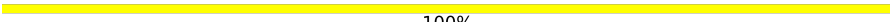
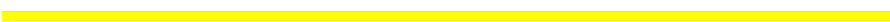
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Mol	Chain	Length	Quality of chain
4	d8	2	100%
4	d9	2	50% 50%
4	e0	2	100%
4	e1	2	100%
4	e2	2	100%
4	e3	2	50% 50%
4	e4	2	50% 50%
4	e5	2	100%
4	e6	2	50% 50%
4	e7	2	50% 50%
4	e8	2	100%
4	f0	2	50% 50%
4	f2	2	50% 50%
4	f3	2	100%
4	f5	2	100%
4	f8	2	100%
5	A6	4	100%
5	A9	4	100%
5	B6	4	100%
5	F6	4	100%
5	F7	4	100%
5	a6	4	100%
5	a9	4	25% 75%
5	b6	4	100%
5	f6	4	100%

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Mol	Chain	Length	Quality of chain
5	f7	4	 100%
6	E6	8	 100%
7	a4	2	 100%
8	e9	6	 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
1	HYP	A	1912	-	-	X	-
1	HYP	A	1927	-	-	X	-
1	HYP	B	1905	-	-	X	-
1	HYP	B	1914	-	-	X	-
10	GLA	B	2060	-	-	X	-
4	FUB	e6	1	-	-	X	-
7	34V	a4	1	X	-	-	-
9	A1AIO	A	2004	X	-	-	-
9	A1AIO	A	2006	X	-	-	-
9	A1AIO	A	2009	X	-	-	-
9	A1AIO	A	2011	X	-	-	-
9	A1AIO	A	2012	X	-	-	-
9	A1AIO	A	2014	X	-	-	-
9	A1AIO	A	2016	X	-	-	-
9	A1AIO	A	2018	X	-	-	-
9	A1AIO	A	2025	X	-	-	-
9	A1AIO	A	2035	X	-	-	-
9	A1AIO	A	2037	X	-	-	-
9	A1AIO	A	2038	X	-	-	-
9	A1AIO	A	2040	X	-	-	-
9	A1AIO	A	2052	X	-	-	-
9	A1AIO	B	2004	X	-	-	-
9	A1AIO	B	2006	X	-	-	-
9	A1AIO	B	2009	X	-	-	-
9	A1AIO	B	2011	X	-	-	-
9	A1AIO	B	2012	X	-	-	-
9	A1AIO	B	2014	X	-	-	-
9	A1AIO	B	2016	X	-	-	-
9	A1AIO	B	2030	X	-	-	-
9	A1AIO	B	2031	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	A1AIO	B	2032	X	-	-	-
9	A1AIO	B	2033	X	-	-	-
9	A1AIO	B	2034	X	-	-	-
9	A1AIO	B	2046	X	-	-	-
9	A1AIO	B	2047	X	-	-	-
9	A1AIO	B	2053	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 32328 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 Tyrosine-protein kinase ephrin type A/B receptor-like domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1908	Total	C	N	O	S	0	0
			13867	8726	2262	2798	81		
1	B	1908	Total	C	N	O	S	0	0
			13867	8726	2262	2798	81		

- Molecule 2 is a protein called C-type lectin domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	X	109	Total	C	N	O	S	0	0
			834	509	116	208	1		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	A1	2	Total	C	N	O	0	0
			28	16	2	10		
3	A2	2	Total	C	N	O	0	0
			28	16	2	10		
3	A3	2	Total	C	N	O	0	0
			28	16	2	10		
3	a1	2	Total	C	N	O	0	0
			28	16	2	10		
3	a2	2	Total	C	N	O	0	0
			28	16	2	10		
3	a3	2	Total	C	N	O	0	0
			28	16	2	10		

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

Mol	Chain	Residues	Atoms			AltConf	Trace
4	A4	2	Total	C	O	0	0
			18	10	8		
4	A5	2	Total	C	O	0	0
			18	10	8		
4	A7	2	Total	C	O	0	0
			18	10	8		
4	B0	2	Total	C	O	0	0
			18	10	8		
4	B1	2	Total	C	O	0	0
			18	10	8		
4	B3	2	Total	C	O	0	0
			18	10	8		
4	B4	2	Total	C	O	0	0
			18	10	8		
4	B5	2	Total	C	O	0	0
			18	10	8		
4	B7	2	Total	C	O	0	0
			18	10	8		
4	B9	2	Total	C	O	0	0
			18	10	8		
4	C0	2	Total	C	O	0	0
			18	10	8		
4	C1	2	Total	C	O	0	0
			18	10	8		
4	C2	2	Total	C	O	0	0
			18	10	8		
4	C3	2	Total	C	O	0	0
			18	10	8		
4	C4	2	Total	C	O	0	0
			18	10	8		
4	C5	2	Total	C	O	0	0
			18	10	8		
4	C6	2	Total	C	O	0	0
			18	10	8		
4	C7	2	Total	C	O	0	0
			18	10	8		
4	C8	2	Total	C	O	0	0
			18	10	8		
4	C9	2	Total	C	O	0	0
			18	10	8		
4	D0	2	Total	C	O	0	0
			18	10	8		
4	D1	2	Total	C	O	0	0
			18	10	8		

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Mol	Chain	Residues	Atoms			AltConf	Trace
4	D2	2	Total	C	O	0	0
			18	10	8		
4	D3	2	Total	C	O	0	0
			18	10	8		
4	D4	2	Total	C	O	0	0
			18	10	8		
4	D5	2	Total	C	O	0	0
			18	10	8		
4	D6	2	Total	C	O	0	0
			18	10	8		
4	D7	2	Total	C	O	0	0
			18	10	8		
4	D8	2	Total	C	O	0	0
			18	10	8		
4	D9	2	Total	C	O	0	0
			18	10	8		
4	E0	2	Total	C	O	0	0
			18	10	8		
4	E1	2	Total	C	O	0	0
			18	10	8		
4	E2	2	Total	C	O	0	0
			18	10	8		
4	E4	2	Total	C	O	0	0
			18	10	8		
4	E5	2	Total	C	O	0	0
			18	10	8		
4	E8	2	Total	C	O	0	0
			18	10	8		
4	F0	2	Total	C	O	0	0
			18	10	8		
4	F3	2	Total	C	O	0	0
			18	10	8		
4	F8	2	Total	C	O	0	0
			18	10	8		
4	a5	2	Total	C	O	0	0
			18	10	8		
4	a7	2	Total	C	O	0	0
			18	10	8		
4	b0	2	Total	C	O	0	0
			18	10	8		
4	b1	2	Total	C	O	0	0
			18	10	8		

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Mol	Chain	Residues	Atoms			AltConf	Trace
4	b3	2	Total	C	O	0	0
			18	10	8		
4	b4	2	Total	C	O	0	0
			18	10	8		
4	b5	2	Total	C	O	0	0
			18	10	8		
4	b7	2	Total	C	O	0	0
			18	10	8		
4	b9	2	Total	C	O	0	0
			18	10	8		
4	c0	2	Total	C	O	0	0
			18	10	8		
4	c1	2	Total	C	O	0	0
			18	10	8		
4	c2	2	Total	C	O	0	0
			18	10	8		
4	c3	2	Total	C	O	0	0
			18	10	8		
4	c4	2	Total	C	O	0	0
			18	10	8		
4	c5	2	Total	C	O	0	0
			18	10	8		
4	c6	2	Total	C	O	0	0
			18	10	8		
4	c7	2	Total	C	O	0	0
			18	10	8		
4	c8	2	Total	C	O	0	0
			18	10	8		
4	c9	2	Total	C	O	0	0
			18	10	8		
4	d1	2	Total	C	O	0	0
			18	10	8		
4	d2	2	Total	C	O	0	0
			18	10	8		
4	d3	2	Total	C	O	0	0
			18	10	8		
4	d4	2	Total	C	O	0	0
			18	10	8		
4	d5	2	Total	C	O	0	0
			18	10	8		
4	e0	2	Total	C	O	0	0
			18	10	8		

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Mol	Chain	Residues	Atoms			AltConf	Trace
4	e1	2	Total	C	O	0	0
			18	10	8		
4	e2	2	Total	C	O	0	0
			18	10	8		
4	e4	2	Total	C	O	0	0
			18	10	8		
4	e5	2	Total	C	O	0	0
			18	10	8		
4	e8	2	Total	C	O	0	0
			18	10	8		
4	f0	2	Total	C	O	0	0
			18	10	8		
4	f3	2	Total	C	O	0	0
			18	10	8		
4	f5	2	Total	C	O	0	0
			18	10	8		
4	f8	2	Total	C	O	0	0
			18	10	8		
4	E3	2	Total	C	O	0	0
			18	10	8		
4	f2	2	Total	C	O	0	0
			18	10	8		
4	e7	2	Total	C	O	0	0
			18	10	8		
4	e6	2	Total	C	O	0	0
			18	10	8		
4	e3	2	Total	C	O	0	0
			18	10	8		
4	d9	2	Total	C	O	0	0
			18	10	8		
4	d7	2	Total	C	O	0	0
			18	10	8		
4	d8	2	Total	C	O	0	0
			18	10	8		
4	d6	2	Total	C	O	0	0
			18	10	8		
4	d0	2	Total	C	O	0	0
			18	10	8		
4	F5	2	Total	C	O	0	0
			18	10	8		
4	F2	2	Total	C	O	0	0
			18	10	8		

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Mol	Chain	Residues	Atoms			AltConf	Trace
4	E7	2	Total	C	O	0	0
			18	10	8		

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

Mol	Chain	Residues	Atoms			AltConf	Trace
5	A6	4	Total	C	O	0	0
			36	20	16		
5	A9	4	Total	C	O	0	0
			36	20	16		
5	B6	4	Total	C	O	0	0
			36	20	16		
5	F6	4	Total	C	O	0	0
			36	20	16		
5	F7	4	Total	C	O	0	0
			36	20	16		
5	a6	4	Total	C	O	0	0
			36	20	16		
5	a9	4	Total	C	O	0	0
			36	20	16		
5	b6	4	Total	C	O	0	0
			36	20	16		
5	f6	4	Total	C	O	0	0
			36	20	16		
5	f7	4	Total	C	O	0	0
			36	20	16		

- Molecule 6 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
6	E6	8	Total	C	O	0	0
			72	40	32		

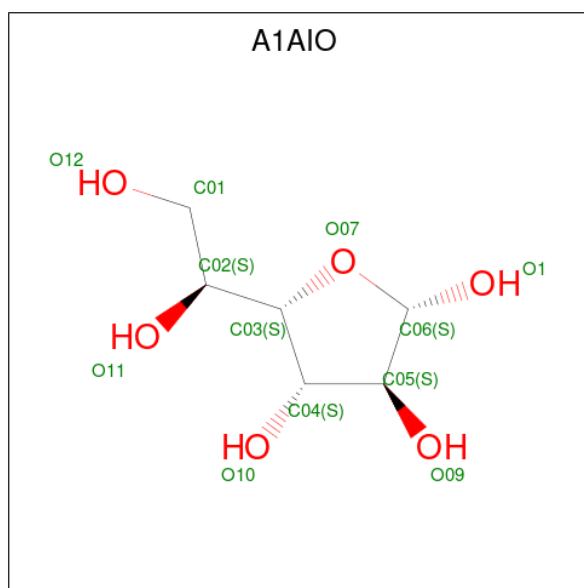
- Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
7	a4	2	Total	C	O	0	0
			18	10	8		

- Molecule 8 is an oligosaccharide called beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose.

Mol	Chain	Residues	Atoms			AltConf	Trace
8	e9	6	Total	C	O	0	0
			54	30	24		

- Molecule 9 is beta-L-glucufuranose (CCD ID: A1AIO) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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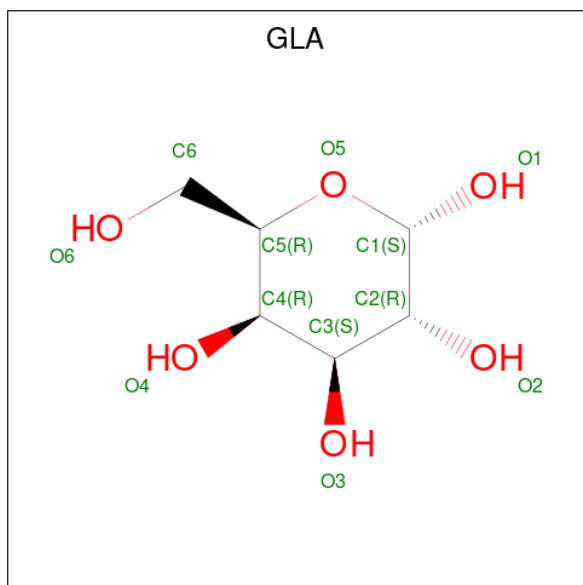
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1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

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

- Molecule 10 is alpha-D-galactopyranose (CCD ID: GLA) (formula: $C_6H_{12}O_6$) (labeled as "Ligand of Interest" by depositor).

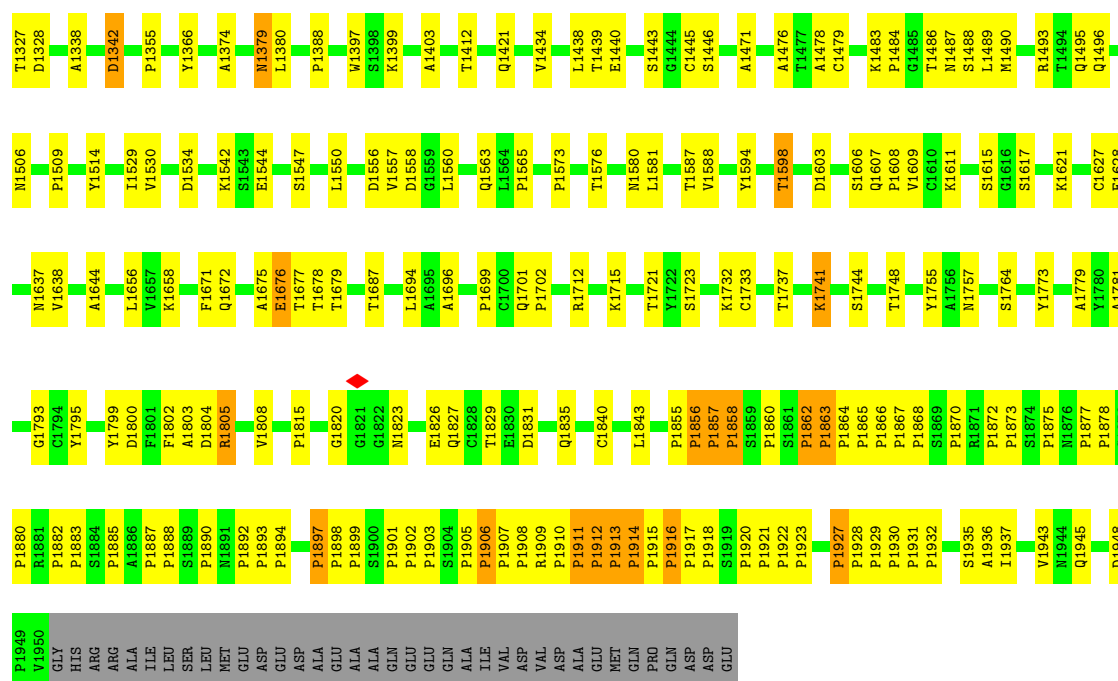


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0
10	A	1	11	6	5	0

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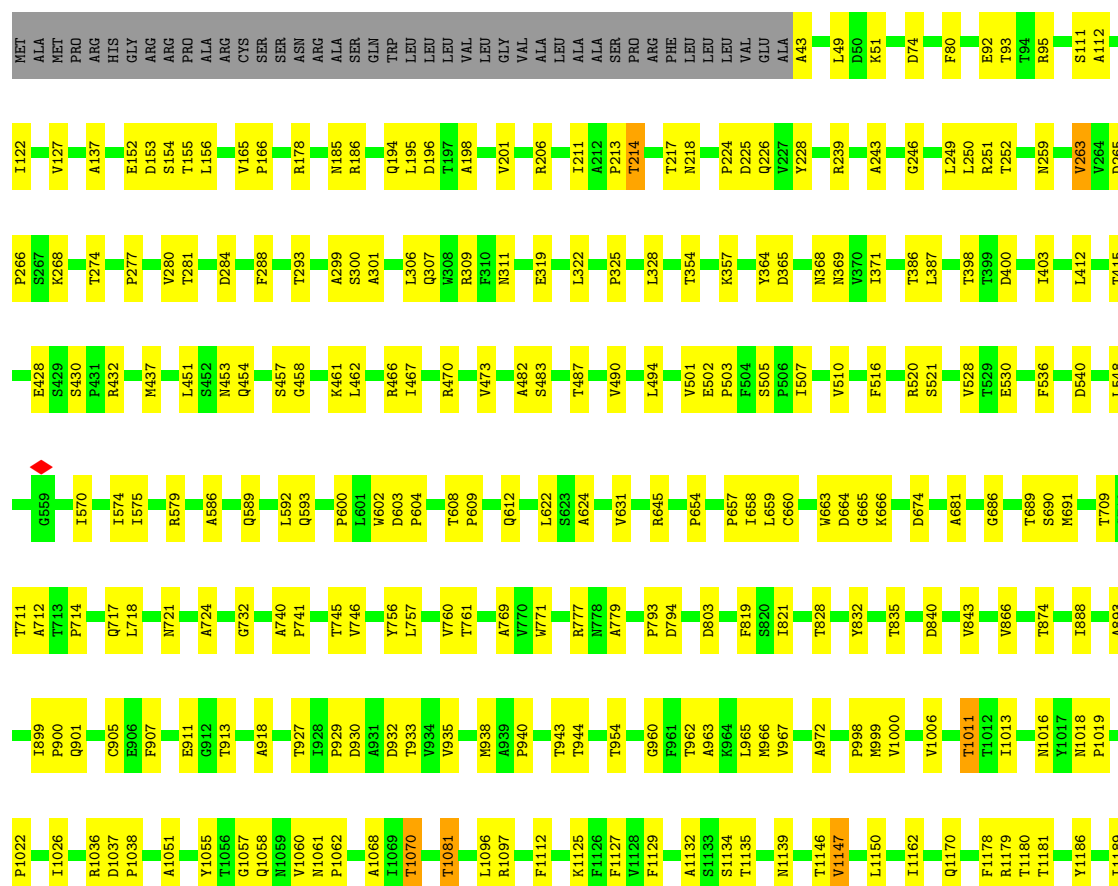
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Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			11	6	5	
10	A	1	Total	C	O	0
			11	6	5	
10	A	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10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



- Molecule 1: Tyrosine-protein kinase ephrin type A/B receptor-like domain-containing protein

Chain B: 72% 22%















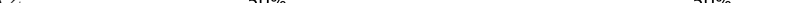
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- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A1:

NAG1
NAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain A2:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



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



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





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

Chain B0:  50% 50%



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

Chain B1:  100%



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

Chain B3:  50% 50%



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

Chain B4:  100%



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

Chain B5:  100%



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

Chain B7:  100%



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

Chain B9:  100%



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

Chain C0:  100%

FUB1
FUB2

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

Chain C1:  100%

FUB1
FUB2

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

Chain C2:  100%

FUB1
FUB2

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

Chain C3:  100%

FUB1
FUB2

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

Chain C4:  100%

FUB1
FUB2

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

Chain C5:  100%

FUB1
FUB2

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

Chain C6:  100%

FUB1
FUB2

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

Chain C7:  100%



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

Chain C8:  100%



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

Chain C9:  100%



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

Chain D0:  100%



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

Chain D1:  50% 50%



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

Chain D2:  100%



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

Chain D3:  100%



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

Chain D4:  100%



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

Chain D5:  100%



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

Chain D6:  100%



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

Chain D7:  100%



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

Chain D8:  100%



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

Chain D9:  50% 50%



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

Chain E0:  100%



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

Chain E1:  100%



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

Chain E2:  100%

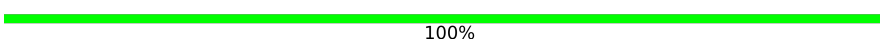


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E4:  50% 50%

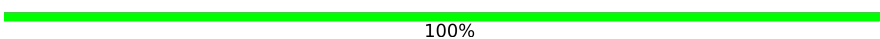


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E5:  100%

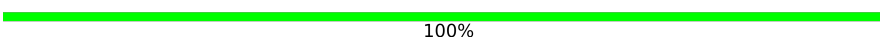


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E8:  100%

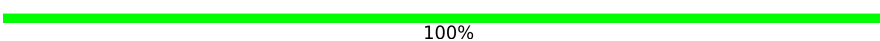


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F0:  100%



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

Chain F3:  100%

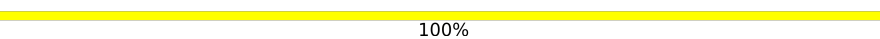


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F8:  100%



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

Chain a5:  100%



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

Chain a7:  50% 50%

FUB1
FUB2

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

Chain b0:  100%

FUB1
FUB2

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

Chain b1:  100%

FUB1
FUB2

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

Chain b3:  100%

FUB1
FUB2

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

Chain b4:  100%

FUB1
FUB2

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

Chain b5:  100%

FUB1
FUB2

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

Chain b7:  100%

FUB1
FUB2

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

Chain b9:  100%

FUB1
FUB2

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

Chain c0:  100%FUB1
FUB2

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

Chain c1:  100%FUB1
FUB2

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

Chain c2:  100%FUB1
FUB2

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

Chain c3:  100%FUB1
FUB2

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

Chain c4:  100%FUB1
FUB2

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

Chain c5:  100%FUB1
FUB2

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

Chain c6:  100%FUB1
FUB2

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

Chain c7:  100%

FUB1
FUB2

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

Chain c8:  100%

FUB1
FUB2

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

Chain c9:  100%

FUB1
FUB2

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

Chain d1:  100%

FUB1
FUB2

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

Chain d2:  100%

FUB1
FUB2

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

Chain d3:  100%

FUB1
FUB2

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

Chain d4:  100%

FUB1
FUB2

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

Chain d5:  100%

FUB1
FUB2

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

Chain e0:  100%FUB1
FUB2

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

Chain e1:  100%FUB1
FUB2

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

Chain e2:  100%FUB1
FUB2

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

Chain e4:  50% 50%FUB1
FUB2

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

Chain e5:  100%FUB1
FUB2

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

Chain e8:  100%FUB1
FUB2

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

Chain f0:  50% 50%FUB1
FUB2

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

Chain f3:  100%

FUB1
FUB2

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

Chain f5:  100%

FUB1
FUB2

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

Chain f8:  100%

FUB1
FUB2

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

Chain E3:  100%

FUB1
FUB2

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

Chain f2:  50% 50%

FUB1
FUB2

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

Chain e7:  50% 50%

FUB1
FUB2

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

Chain e6:  50% 50%

FUB1
FUB2

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

Chain e3:  50% 50%

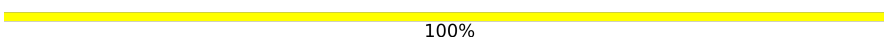


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d9:  50% 50%

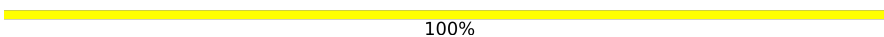


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d7:  100%

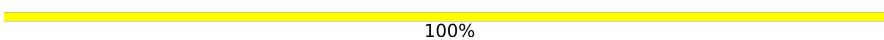


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d8:  100%



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

Chain d6:  100%



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

Chain d0:  50% 50%



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

Chain F5:  50% 50%



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

Chain F2:  100%



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

Chain E7:  100%

FUB1
FUB2

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A6:  100%

FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain A9:  100%

FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain B6:  100%

FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F6:  100%

FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain F7:  100%

FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain a6:  100%

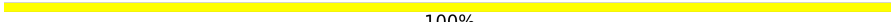
FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain a9:  25% 75%

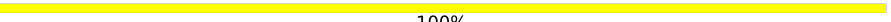
FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain b6:  100%

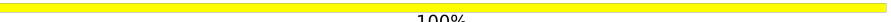
FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f6:  100%

FUB1
FUB2
FUB3
FUB4

- Molecule 5: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain f7:  100%

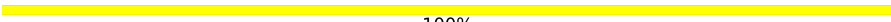
FUB1
FUB2
FUB3
FUB4

- Molecule 6: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain E6:  100%

FUB1
FUB2
FUB3
FUB4
FUB5
FUB6
FUB7
FUB8

- Molecule 7: beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose

Chain a4:  100%

34V1
FUB2

- Molecule 8: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose-(5-5)-beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain e9: 100%

FUB1
FUB2
FUB3
FUB4
FUB5
FUB6

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	687452	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	39	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	2.771	Depositor
Minimum map value	0.000	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.5	Depositor
Map size (Å)	711.68, 711.68, 711.68	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.39, 1.39, 1.39	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 34V, GLA, A1AIO, NAG, FUB, HYP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.11	0/13729	0.25	0/18855
1	B	0.13	0/13729	0.29	0/18855
2	X	0.10	0/157	0.24	0/190
All	All	0.12	0/27615	0.27	0/37900

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1850	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	13867	0	13361	258	0
1	B	13867	0	13371	277	0
2	X	834	0	737	12	0
3	A1	28	0	25	0	0
3	A2	28	0	25	0	0
3	A3	28	0	25	0	0
3	a1	28	0	25	0	0
3	a2	28	0	25	0	0
3	a3	28	0	25	1	0
4	A4	18	0	0	0	0
4	A5	18	0	0	1	0
4	A7	18	0	0	0	0
4	B0	18	0	0	0	0
4	B1	18	0	0	0	0
4	B3	18	0	0	1	0
4	B4	18	0	0	0	0
4	B5	18	0	0	0	0
4	B7	18	0	0	0	0
4	B9	18	0	0	0	0
4	C0	18	0	0	0	0
4	C1	18	0	0	0	0
4	C2	18	0	0	1	0
4	C3	18	0	0	0	0
4	C4	18	0	0	0	0
4	C5	18	0	0	0	0
4	C6	18	0	0	0	0
4	C7	18	0	0	0	0
4	C8	18	0	0	1	0
4	C9	18	0	0	0	0
4	D0	18	0	0	0	0
4	D1	18	0	0	0	0
4	D2	18	0	0	0	0
4	D3	18	0	0	0	0
4	D4	18	0	0	0	0
4	D5	18	0	0	0	0
4	D6	18	0	0	0	0
4	D7	18	0	0	0	0
4	D8	18	0	0	0	0
4	D9	18	0	0	1	0
4	E0	18	0	0	0	0
4	E1	18	0	0	0	0
4	E2	18	0	0	0	0
4	E3	18	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E4	18	0	0	8	0
4	E5	18	0	0	0	0
4	E7	18	0	0	0	0
4	E8	18	0	0	0	0
4	F0	18	0	0	0	0
4	F2	18	0	0	0	0
4	F3	18	0	0	0	0
4	F5	18	0	0	4	0
4	F8	18	0	0	0	0
4	a5	18	0	0	1	0
4	a7	18	0	0	1	0
4	b0	18	0	0	0	0
4	b1	18	0	0	0	0
4	b3	18	0	0	0	0
4	b4	18	0	0	0	0
4	b5	18	0	0	0	0
4	b7	18	0	0	0	0
4	b9	18	0	0	0	0
4	c0	18	0	0	0	0
4	c1	18	0	0	0	0
4	c2	18	0	0	0	0
4	c3	18	0	0	0	0
4	c4	18	0	0	0	0
4	c5	18	0	0	0	0
4	c6	18	0	0	0	0
4	c7	18	0	0	1	0
4	c8	18	0	0	0	0
4	c9	18	0	0	0	0
4	d0	18	0	0	3	0
4	d1	18	0	0	0	0
4	d2	18	0	0	0	0
4	d3	18	0	0	0	0
4	d4	18	0	0	0	0
4	d5	18	0	0	0	0
4	d6	18	0	0	0	0
4	d7	18	0	0	0	0
4	d8	18	0	0	5	0
4	d9	18	0	0	1	0
4	e0	18	0	0	0	0
4	e1	18	0	0	4	0
4	e2	18	0	0	0	0
4	e3	18	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	e4	18	0	0	3	0
4	e5	18	0	0	0	0
4	e6	18	0	0	10	0
4	e7	18	0	0	5	0
4	e8	18	0	0	0	0
4	f0	18	0	0	7	0
4	f2	18	0	0	5	0
4	f3	18	0	0	0	0
4	f5	18	0	0	0	0
4	f8	18	0	0	0	0
5	A6	36	0	0	0	0
5	A9	36	0	0	0	0
5	B6	36	0	0	0	0
5	F6	36	0	0	0	0
5	F7	36	0	0	0	0
5	a6	36	0	0	0	0
5	a9	36	0	0	0	0
5	b6	36	0	0	0	0
5	f6	36	0	0	0	0
5	f7	36	0	0	0	0
6	E6	72	0	0	0	0
7	a4	18	0	7	0	0
8	e9	54	0	0	0	0
9	A	627	0	0	55	0
9	B	627	0	0	57	0
10	A	143	0	130	3	0
10	B	143	0	129	8	0
All	All	32328	0	27885	661	0

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

The worst 5 of 661 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)
1:A:1927:HYP:OD1	4:F5:1:FUB:C1	1.69	1.40
1:B:1893:HYP:OD1	4:d0:1:FUB:C1	1.79	1.28
1:B:944:THR:OG1	4:d9:2:FUB:O5	1.61	1.16
4:e6:2:FUB:C4	4:e3:1:FUB:O5	1.94	1.14
1:A:1927:HYP:CG	4:F5:1:FUB:C1	2.35	1.04

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1849/1987 (93%)	1792 (97%)	57 (3%)	0	100	100
1	B	1849/1987 (93%)	1783 (96%)	65 (4%)	1 (0%)	48	78
2	X	21/8572 (0%)	18 (86%)	1 (5%)	2 (10%)	0	3
All	All	3719/12546 (30%)	3593 (97%)	123 (3%)	3 (0%)	49	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1854	SER
2	X	1627	SER
2	X	1560	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1451/1514 (96%)	1404 (97%)	47 (3%)	34	64
1	B	1451/1514 (96%)	1405 (97%)	46 (3%)	34	64
2	X	17/6717 (0%)	14 (82%)	3 (18%)	2	9
All	All	2919/9745 (30%)	2823 (97%)	96 (3%)	34	63

5 of 96 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	430	SER
1	B	1277	LEU
1	B	528	VAL
1	B	1070	THR
1	B	1459	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	642	ASN
1	B	1661	GLN
1	B	1853	GLN
1	B	333	ASN
1	B	369	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

197 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	HYP	B	1910	1	7,8,9	0.48	0	5,10,12	2.32	2 (40%)
1	HYP	B	1903	1	7,8,9	0.50	0	5,10,12	1.97	1 (20%)
2	HYP	X	1520	2	7,8,9	0.51	0	5,10,12	1.97	2 (40%)
2	HYP	X	1529	2	7,8,9	0.50	0	5,10,12	2.11	2 (40%)
1	HYP	B	1914	1	7,8,9	0.60	0	5,10,12	2.50	2 (40%)
2	HYP	X	1594	2	7,8,9	0.59	0	5,10,12	1.55	1 (20%)
2	HYP	X	1597	2	7,8,9	0.50	0	5,10,12	2.20	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1855	1	7,8,9	0.68	0	5,10,12	2.36	3 (60%)
2	HYP	X	1453	2	7,8,9	0.52	0	5,10,12	1.84	2 (40%)
1	HYP	B	1887	1	7,8,9	0.53	0	5,10,12	2.05	2 (40%)
2	HYP	X	1611	2	7,8,9	0.51	0	5,10,12	2.05	1 (20%)
2	HYP	X	1461	2	7,8,9	0.50	0	5,10,12	2.04	2 (40%)
2	HYP	X	1550	2	7,8,9	0.48	0	5,10,12	2.10	2 (40%)
1	HYP	B	1902	1	7,8,9	0.53	0	5,10,12	2.13	3 (60%)
1	HYP	A	1923	1	7,8,9	0.58	0	5,10,12	2.12	1 (20%)
1	HYP	B	1885	1	7,8,9	0.60	0	5,10,12	2.46	2 (40%)
2	HYP	X	1546	2	7,8,9	0.52	0	5,10,12	2.06	1 (20%)
1	HYP	A	1907	1	7,8,9	0.53	0	5,10,12	1.97	2 (40%)
1	HYP	A	1927	1	7,8,9	0.52	0	5,10,12	2.11	1 (20%)
1	HYP	B	1856	1	7,8,9	0.54	0	5,10,12	2.13	2 (40%)
2	HYP	X	1522	2	7,8,9	0.52	0	5,10,12	1.90	2 (40%)
1	HYP	A	1899	1	7,8,9	0.54	0	5,10,12	1.72	1 (20%)
1	HYP	A	1901	1	7,8,9	0.54	0	5,10,12	2.02	2 (40%)
2	HYP	X	1552	2	7,8,9	0.50	0	5,10,12	2.07	2 (40%)
1	HYP	B	1863	1	7,8,9	0.54	0	5,10,12	2.15	1 (20%)
2	HYP	X	1524	2	7,8,9	0.50	0	5,10,12	2.10	3 (60%)
1	HYP	B	1912	1	7,8,9	0.56	0	5,10,12	2.15	2 (40%)
1	HYP	B	1928	1	7,8,9	0.66	0	5,10,12	1.71	2 (40%)
2	HYP	X	1593	2	7,8,9	0.50	0	5,10,12	2.06	1 (20%)
1	HYP	A	1911	1	7,8,9	0.52	0	5,10,12	1.96	3 (60%)
1	HYP	A	1855	1	7,8,9	0.53	0	5,10,12	1.99	1 (20%)
1	HYP	B	1883	1	7,8,9	0.54	0	5,10,12	1.85	1 (20%)
2	HYP	X	1481	2	7,8,9	0.51	0	5,10,12	2.03	1 (20%)
2	HYP	X	1598	2	7,8,9	0.52	0	5,10,12	2.09	2 (40%)
2	HYP	X	1586	2	7,8,9	0.50	0	5,10,12	2.02	2 (40%)
1	HYP	A	1870	1	7,8,9	0.54	0	5,10,12	1.91	1 (20%)
2	HYP	X	1595	2	7,8,9	0.55	0	5,10,12	1.71	1 (20%)
2	HYP	X	1454	2	7,8,9	0.54	0	5,10,12	1.49	1 (20%)
2	HYP	X	1456	2	7,8,9	0.50	0	5,10,12	2.05	2 (40%)
2	HYP	X	1464	2	7,8,9	0.51	0	5,10,12	1.98	1 (20%)
2	HYP	X	1484	2	7,8,9	0.51	0	5,10,12	2.08	3 (60%)
1	HYP	A	1880	1	7,8,9	0.53	0	5,10,12	1.90	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1893	1	7,8,9	0.55	0	5,10,12	1.96	2 (40%)
1	HYP	A	1913	1	7,8,9	0.52	0	5,10,12	1.96	1 (20%)
1	HYP	B	1916	1	7,8,9	0.55	0	5,10,12	2.00	2 (40%)
1	HYP	A	1860	1	7,8,9	0.51	0	5,10,12	1.95	1 (20%)
2	HYP	X	1548	2	7,8,9	0.51	0	5,10,12	2.17	1 (20%)
1	HYP	A	1883	1	7,8,9	0.55	0	5,10,12	1.80	1 (20%)
1	HYP	A	1932	1	7,8,9	0.56	0	5,10,12	1.91	2 (40%)
1	HYP	B	1918	1	7,8,9	0.59	0	5,10,12	1.76	1 (20%)
2	HYP	X	1455	2	7,8,9	0.51	0	5,10,12	2.02	1 (20%)
1	HYP	B	1932	1	7,8,9	0.53	0	5,10,12	2.20	2 (40%)
1	HYP	A	1865	1	7,8,9	0.59	0	5,10,12	2.03	3 (60%)
1	HYP	B	1907	1	7,8,9	0.55	0	5,10,12	2.04	2 (40%)
1	HYP	A	1862	1	7,8,9	0.51	0	5,10,12	1.98	2 (40%)
2	HYP	X	1480	2	7,8,9	0.52	0	5,10,12	2.04	1 (20%)
2	HYP	X	1462	2	7,8,9	0.53	0	5,10,12	1.87	1 (20%)
1	HYP	A	1894	1	7,8,9	0.59	0	5,10,12	2.36	2 (40%)
1	HYP	B	1921	1	7,8,9	0.63	0	5,10,12	1.65	2 (40%)
1	HYP	B	1923	1	7,8,9	0.54	0	5,10,12	1.89	1 (20%)
1	HYP	B	1878	1	7,8,9	0.53	0	5,10,12	1.77	2 (40%)
1	HYP	A	1887	1	7,8,9	0.53	0	5,10,12	2.17	3 (60%)
2	HYP	X	1527	2	7,8,9	0.50	0	5,10,12	2.02	1 (20%)
1	HYP	A	1916	1	7,8,9	0.55	0	5,10,12	1.83	2 (40%)
1	HYP	B	1920	1	7,8,9	0.52	0	5,10,12	2.04	2 (40%)
2	HYP	X	1553	2	7,8,9	0.51	0	5,10,12	2.05	2 (40%)
2	HYP	X	1487	2	7,8,9	0.51	0	5,10,12	2.02	2 (40%)
1	HYP	B	1868	1	7,8,9	0.54	0	5,10,12	2.22	1 (20%)
2	HYP	X	1489	2	7,8,9	0.51	0	5,10,12	1.95	2 (40%)
1	HYP	B	1913	1	7,8,9	0.55	0	5,10,12	1.93	1 (20%)
1	HYP	A	1897	1	7,8,9	0.54	0	5,10,12	2.15	3 (60%)
1	HYP	A	1892	1	7,8,9	0.57	0	5,10,12	1.58	2 (40%)
2	HYP	X	1615	2	7,8,9	0.51	0	5,10,12	2.09	1 (20%)
1	HYP	A	1931	1	7,8,9	0.57	0	5,10,12	1.99	2 (40%)
2	HYP	X	1490	2	7,8,9	0.52	0	5,10,12	2.01	1 (20%)
1	HYP	B	1915	1	7,8,9	0.52	0	5,10,12	1.87	2 (40%)
1	HYP	A	1888	1	7,8,9	0.50	0	5,10,12	2.01	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1901	1	7,8,9	0.55	0	5,10,12	1.80	2 (40%)
1	HYP	A	1921	1	7,8,9	0.65	0	5,10,12	1.53	0
2	HYP	X	1469	2	7,8,9	0.55	0	5,10,12	1.74	2 (40%)
2	HYP	X	1499	2	7,8,9	0.53	0	5,10,12	2.00	2 (40%)
1	HYP	B	1858	1	7,8,9	0.71	0	5,10,12	1.53	1 (20%)
1	HYP	B	1890	1	7,8,9	0.55	0	5,10,12	1.28	0
2	HYP	X	1619	2	7,8,9	0.50	0	5,10,12	2.07	2 (40%)
1	HYP	B	1877	1	7,8,9	0.62	0	5,10,12	2.34	2 (40%)
2	HYP	X	1626	2	7,8,9	0.58	0	5,10,12	1.72	1 (20%)
2	HYP	X	1457	2	7,8,9	0.50	0	5,10,12	2.10	3 (60%)
1	HYP	A	1885	1	7,8,9	0.56	0	5,10,12	2.59	2 (40%)
2	HYP	X	1556	2	7,8,9	0.52	0	5,10,12	2.00	1 (20%)
1	HYP	A	1929	1	7,8,9	0.55	0	5,10,12	2.05	3 (60%)
1	HYP	A	1882	1	7,8,9	0.54	0	5,10,12	2.07	3 (60%)
2	HYP	X	1459	2	7,8,9	0.50	0	5,10,12	2.06	2 (40%)
1	HYP	B	1927	1	7,8,9	0.55	0	5,10,12	2.03	1 (20%)
2	HYP	X	1485	2	7,8,9	0.51	0	5,10,12	2.01	2 (40%)
1	HYP	A	1868	1	7,8,9	0.57	0	5,10,12	2.01	1 (20%)
1	HYP	A	1873	1	7,8,9	0.51	0	5,10,12	1.90	1 (20%)
1	HYP	A	1920	1	7,8,9	0.53	0	5,10,12	2.28	2 (40%)
2	HYP	X	1465	2	7,8,9	0.53	0	5,10,12	1.90	2 (40%)
1	HYP	B	1911	1	7,8,9	0.51	0	5,10,12	2.10	2 (40%)
2	HYP	X	1612	2	7,8,9	0.50	0	5,10,12	2.09	1 (20%)
2	HYP	X	1601	2	7,8,9	0.49	0	5,10,12	2.12	1 (20%)
2	HYP	X	1587	2	7,8,9	0.53	0	5,10,12	2.07	2 (40%)
2	HYP	X	1614	2	7,8,9	0.51	0	5,10,12	2.04	2 (40%)
1	HYP	B	1922	1	7,8,9	0.53	0	5,10,12	2.12	3 (60%)
1	HYP	A	1867	1	7,8,9	0.52	0	5,10,12	2.06	3 (60%)
1	HYP	B	1894	1	7,8,9	0.54	0	5,10,12	1.99	1 (20%)
2	HYP	X	1482	2	7,8,9	0.52	0	5,10,12	2.08	2 (40%)
2	HYP	X	1613	2	7,8,9	0.52	0	5,10,12	2.09	2 (40%)
1	HYP	B	1906	1	7,8,9	0.49	0	5,10,12	2.06	2 (40%)
1	HYP	B	1872	1	7,8,9	0.52	0	5,10,12	2.09	3 (60%)
2	HYP	X	1463	2	7,8,9	0.49	0	5,10,12	2.05	2 (40%)
1	HYP	A	1863	1	7,8,9	0.56	0	5,10,12	2.44	2 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	B	1917	1	7,8,9	0.58	0	5,10,12	1.77	2 (40%)
1	HYP	A	1866	1	7,8,9	0.57	0	5,10,12	1.79	1 (20%)
1	HYP	A	1912	1	7,8,9	0.56	0	5,10,12	2.50	1 (20%)
2	HYP	X	1617	2	7,8,9	0.50	0	5,10,12	2.04	2 (40%)
1	HYP	A	1928	1	7,8,9	0.55	0	5,10,12	2.08	2 (40%)
1	HYP	A	1898	1	7,8,9	0.52	0	5,10,12	2.04	2 (40%)
1	HYP	B	1899	1	7,8,9	0.51	0	5,10,12	1.85	1 (20%)
2	HYP	X	1596	2	7,8,9	0.49	0	5,10,12	2.02	1 (20%)
1	HYP	A	1905	1	7,8,9	0.53	0	5,10,12	1.78	2 (40%)
1	HYP	A	1930	1	7,8,9	0.53	0	5,10,12	1.76	1 (20%)
1	HYP	A	1857	1	7,8,9	0.54	0	5,10,12	1.80	2 (40%)
1	HYP	B	1888	1	7,8,9	0.49	0	5,10,12	2.09	2 (40%)
2	HYP	X	1562	2	7,8,9	0.51	0	5,10,12	1.93	1 (20%)
2	HYP	X	1458	2	7,8,9	0.50	0	5,10,12	2.03	1 (20%)
1	HYP	A	1910	1	7,8,9	0.48	0	5,10,12	2.03	1 (20%)
1	HYP	A	1903	1	7,8,9	0.52	0	5,10,12	2.00	1 (20%)
1	HYP	A	1908	1	7,8,9	0.51	0	5,10,12	1.97	1 (20%)
2	HYP	X	1468	2	7,8,9	0.50	0	5,10,12	2.10	2 (40%)
1	HYP	B	1908	1	7,8,9	0.53	0	5,10,12	2.04	1 (20%)
2	HYP	X	1486	2	7,8,9	0.54	0	5,10,12	1.80	2 (40%)
1	HYP	A	1914	1	7,8,9	0.57	0	5,10,12	2.48	2 (40%)
2	HYP	X	1488	2	7,8,9	0.50	0	5,10,12	2.06	2 (40%)
2	HYP	X	1532	2	7,8,9	0.56	0	5,10,12	1.94	2 (40%)
2	HYP	X	1547	2	7,8,9	0.49	0	5,10,12	2.06	1 (20%)
1	HYP	A	1917	1	7,8,9	0.55	0	5,10,12	2.00	3 (60%)
2	HYP	X	1602	2	7,8,9	0.53	0	5,10,12	1.88	1 (20%)
2	HYP	X	1460	2	7,8,9	0.52	0	5,10,12	2.01	2 (40%)
1	HYP	B	1870	1	7,8,9	0.54	0	5,10,12	1.95	1 (20%)
2	HYP	X	1493	2	7,8,9	0.52	0	5,10,12	2.05	1 (20%)
2	HYP	X	1554	2	7,8,9	0.50	0	5,10,12	2.05	3 (60%)
2	HYP	X	1523	2	7,8,9	0.50	0	5,10,12	2.01	1 (20%)
2	HYP	X	1525	2	7,8,9	0.49	0	5,10,12	2.09	2 (40%)
1	HYP	A	1902	1	7,8,9	0.52	0	5,10,12	2.00	2 (40%)
1	HYP	B	1929	1	7,8,9	0.54	0	5,10,12	1.98	2 (40%)
1	HYP	A	1872	1	7,8,9	0.55	0	5,10,12	1.51	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	A	1875	1	7,8,9	0.52	0	5,10,12	2.00	2 (40%)
1	HYP	B	1880	1	7,8,9	0.52	0	5,10,12	1.72	1 (20%)
2	HYP	X	1549	2	7,8,9	0.49	0	5,10,12	2.08	1 (20%)
1	HYP	B	1865	1	7,8,9	0.67	0	5,10,12	1.60	1 (20%)
1	HYP	B	1862	1	7,8,9	0.55	0	5,10,12	1.97	1 (20%)
1	HYP	B	1875	1	7,8,9	0.52	0	5,10,12	1.83	1 (20%)
1	HYP	A	1878	1	7,8,9	0.52	0	5,10,12	2.13	2 (40%)
1	HYP	B	1860	1	7,8,9	0.57	0	5,10,12	2.39	1 (20%)
2	HYP	X	1496	2	7,8,9	0.54	0	5,10,12	1.79	1 (20%)
2	HYP	X	1528	2	7,8,9	0.51	0	5,10,12	1.99	1 (20%)
1	HYP	A	1906	1	7,8,9	0.50	0	5,10,12	1.93	2 (40%)
1	HYP	A	1922	1	7,8,9	0.55	0	5,10,12	2.15	2 (40%)
2	HYP	X	1592	2	7,8,9	0.47	0	5,10,12	2.06	2 (40%)
2	HYP	X	1623	2	7,8,9	0.52	0	5,10,12	1.96	1 (20%)
1	HYP	B	1898	1	7,8,9	0.51	0	5,10,12	2.05	3 (60%)
2	HYP	X	1618	2	7,8,9	0.50	0	5,10,12	2.10	3 (60%)
2	HYP	X	1589	2	7,8,9	0.50	0	5,10,12	2.05	1 (20%)
1	HYP	B	1882	1	7,8,9	0.53	0	5,10,12	1.96	2 (40%)
1	HYP	B	1892	1	7,8,9	0.58	0	5,10,12	1.44	1 (20%)
2	HYP	X	1551	2	7,8,9	0.51	0	5,10,12	2.15	1 (20%)
1	HYP	B	1873	1	7,8,9	0.53	0	5,10,12	1.49	0
1	HYP	A	1864	1	7,8,9	0.59	0	5,10,12	2.47	2 (40%)
1	HYP	B	1930	1	7,8,9	0.53	0	5,10,12	2.03	2 (40%)
1	HYP	B	1864	1	7,8,9	0.55	0	5,10,12	2.30	3 (60%)
2	HYP	X	1610	2	7,8,9	0.51	0	5,10,12	2.03	1 (20%)
1	HYP	A	1893	1	7,8,9	0.55	0	5,10,12	1.96	2 (40%)
2	HYP	X	1590	2	7,8,9	0.50	0	5,10,12	2.16	3 (60%)
1	HYP	A	1856	1	7,8,9	0.56	0	5,10,12	2.07	3 (60%)
2	HYP	X	1530	2	7,8,9	0.49	0	5,10,12	2.11	2 (40%)
2	HYP	X	1616	2	7,8,9	0.50	0	5,10,12	2.02	2 (40%)
1	HYP	B	1866	1	7,8,9	0.55	0	5,10,12	2.15	2 (40%)
2	HYP	X	1555	2	7,8,9	0.49	0	5,10,12	2.13	3 (60%)
1	HYP	A	1858	1	7,8,9	0.58	0	5,10,12	1.69	1 (20%)
1	HYP	B	1897	1	7,8,9	0.54	0	5,10,12	1.94	2 (40%)
1	HYP	A	1915	1	7,8,9	0.54	0	5,10,12	1.96	3 (60%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	HYP	A	1918	1	7,8,9	0.53	0	5,10,12	2.18	1 (20%)
2	HYP	X	1483	2	7,8,9	0.51	0	5,10,12	2.08	2 (40%)
1	HYP	B	1867	1	7,8,9	0.55	0	5,10,12	2.13	3 (60%)
2	HYP	X	1521	2	7,8,9	0.52	0	5,10,12	2.10	2 (40%)
2	HYP	X	1591	2	7,8,9	0.51	0	5,10,12	1.98	1 (20%)
1	HYP	B	1905	1	7,8,9	0.53	0	5,10,12	1.67	2 (40%)
1	HYP	B	1931	1	7,8,9	0.54	0	5,10,12	2.00	2 (40%)
2	HYP	X	1531	2	7,8,9	0.49	0	5,10,12	2.14	2 (40%)
2	HYP	X	1620	2	7,8,9	0.51	0	5,10,12	1.97	1 (20%)
1	HYP	A	1890	1	7,8,9	0.53	0	5,10,12	1.89	1 (20%)
1	HYP	A	1877	1	7,8,9	0.57	0	5,10,12	2.21	3 (60%)
1	HYP	B	1857	1	7,8,9	0.53	0	5,10,12	1.77	1 (20%)
2	HYP	X	1588	2	7,8,9	0.51	0	5,10,12	2.03	1 (20%)
2	HYP	X	1559	2	7,8,9	0.53	0	5,10,12	1.93	1 (20%)
2	HYP	X	1526	2	7,8,9	0.49	0	5,10,12	2.18	2 (40%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1903	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1520	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1529	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1914	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1594	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1597	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1855	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1453	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1887	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1611	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1461	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1550	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1546	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	A	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1927	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1522	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1899	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1901	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1552	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1863	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1524	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1912	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1928	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1593	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1911	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1855	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1883	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1481	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1598	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1586	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1595	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1454	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1456	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1464	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1484	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1880	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1893	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1860	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1548	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1883	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1918	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1455	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1932	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1907	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1862	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1480	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1462	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1894	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1921	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	HYP	B	1923	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1887	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1527	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1916	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1920	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1553	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1487	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1868	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1489	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1913	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1892	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1615	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1490	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1888	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1901	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1921	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1469	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1499	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1890	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1619	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1877	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1626	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1457	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1885	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1556	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1882	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1459	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1927	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1485	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1868	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1920	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1465	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1911	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1612	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1601	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	X	1587	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1614	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1922	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1867	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1894	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1482	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1613	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1872	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1463	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1863	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1917	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1866	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1912	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1617	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1928	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1898	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1899	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1596	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1857	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1888	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1562	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1458	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1910	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1903	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1468	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1908	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1486	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1914	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1488	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1532	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1547	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1917	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1602	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1460	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1870	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1493	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1554	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1523	2	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	X	1525	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1902	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1929	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1872	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1880	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1549	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1865	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1862	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1875	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1878	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1860	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1496	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1528	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1906	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1922	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1592	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1623	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1898	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1618	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1589	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1882	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1892	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1551	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1873	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1864	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1930	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1864	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1610	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1893	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1590	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1856	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1530	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1616	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1866	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1555	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1858	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1897	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1915	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1918	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1483	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1867	1	-	0/0/11/13	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HYP	X	1521	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1591	2	-	0/0/11/13	0/1/1/1
1	HYP	B	1905	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1931	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1531	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1620	2	-	0/0/11/13	0/1/1/1
1	HYP	A	1890	1	-	0/0/11/13	0/1/1/1
1	HYP	A	1877	1	-	0/0/11/13	0/1/1/1
1	HYP	B	1857	1	-	0/0/11/13	0/1/1/1
2	HYP	X	1588	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1559	2	-	0/0/11/13	0/1/1/1
2	HYP	X	1526	2	-	0/0/11/13	0/1/1/1

There are no bond length outliers.

The worst 5 of 335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1912	HYP	CB-CG-CD	-4.70	97.92	103.16
1	B	1914	HYP	CB-CG-CD	-4.57	98.07	103.16
1	B	1860	HYP	CB-CG-CD	-4.50	98.14	103.16
1	A	1914	HYP	CB-CG-CD	-4.39	98.27	103.16
1	A	1885	HYP	CB-CG-CD	-4.22	98.46	103.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

51 monomers are involved in 62 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	1520	HYP	2	0
1	B	1914	HYP	7	0
2	X	1594	HYP	2	0
1	B	1855	HYP	1	0
2	X	1453	HYP	1	0
1	B	1885	HYP	1	0
1	A	1927	HYP	4	0
1	B	1856	HYP	1	0
1	B	1863	HYP	2	0
1	B	1912	HYP	2	0
1	B	1928	HYP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	X	1593	HYP	1	0
1	A	1911	HYP	1	0
1	B	1883	HYP	1	0
2	X	1595	HYP	1	0
2	X	1454	HYP	2	0
1	B	1893	HYP	3	0
1	A	1913	HYP	1	0
1	B	1916	HYP	1	0
2	X	1455	HYP	1	0
1	A	1862	HYP	1	0
1	B	1921	HYP	3	0
1	B	1878	HYP	1	0
1	A	1916	HYP	1	0
2	X	1487	HYP	1	0
1	B	1913	HYP	1	0
1	A	1897	HYP	1	0
1	A	1921	HYP	1	0
1	B	1890	HYP	1	0
2	X	1626	HYP	1	0
1	B	1927	HYP	1	0
2	X	1601	HYP	2	0
1	B	1894	HYP	1	0
1	A	1863	HYP	1	0
1	A	1912	HYP	4	0
1	A	1857	HYP	1	0
1	A	1914	HYP	1	0
2	X	1488	HYP	1	0
2	X	1602	HYP	1	0
1	B	1865	HYP	1	0
1	B	1862	HYP	1	0
2	X	1496	HYP	1	0
1	A	1906	HYP	1	0
1	B	1898	HYP	1	0
1	B	1864	HYP	2	0
1	A	1856	HYP	1	0
1	B	1866	HYP	1	0
1	A	1858	HYP	1	0
1	B	1897	HYP	1	0
2	X	1521	HYP	1	0
1	B	1905	HYP	4	0

5.5 Carbohydrates ⓘ

240 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A1	1	3,1	14,14,15	0.76	0	17,19,21	1.03	1 (5%)
3	NAG	A1	2	3	14,14,15	0.71	0	17,19,21	0.86	1 (5%)
3	NAG	A2	1	3,1	14,14,15	0.71	0	17,19,21	1.27	2 (11%)
3	NAG	A2	2	3	14,14,15	0.72	0	17,19,21	0.81	0
3	NAG	A3	1	3,1	14,14,15	0.81	0	17,19,21	0.98	1 (5%)
3	NAG	A3	2	3	14,14,15	0.75	0	17,19,21	0.91	0
4	FUB	A4	1	4	9,9,10	1.06	0	11,12,14	0.77	0
4	FUB	A4	2	4,9	9,9,10	1.01	0	11,12,14	0.82	0
4	FUB	A5	1	4	9,9,10	1.02	0	11,12,14	0.86	0
4	FUB	A5	2	4,9	9,9,10	1.01	0	11,12,14	0.81	0
5	FUB	A6	1	5	9,9,10	1.04	0	11,12,14	0.86	0
5	FUB	A6	2	9,5	9,9,10	1.06	0	11,12,14	0.82	0
5	FUB	A6	3	5	9,9,10	1.03	0	11,12,14	0.89	0
5	FUB	A6	4	9,5	9,9,10	1.03	0	11,12,14	0.85	0
4	FUB	A7	1	4	9,9,10	1.05	0	11,12,14	0.92	0
4	FUB	A7	2	4,9	9,9,10	1.09	0	11,12,14	0.91	0
5	FUB	A9	1	5	9,9,10	1.04	0	11,12,14	0.81	0
5	FUB	A9	2	9,5	9,9,10	1.05	0	11,12,14	0.82	0
5	FUB	A9	3	5	9,9,10	1.02	0	11,12,14	0.90	0
5	FUB	A9	4	9,5	9,9,10	1.03	0	11,12,14	0.80	0
4	FUB	B0	1	4	9,9,10	1.08	1 (11%)	11,12,14	0.96	1 (9%)
4	FUB	B0	2	4,9	9,9,10	1.00	0	11,12,14	0.84	0
4	FUB	B1	1	4	9,9,10	1.04	0	11,12,14	0.87	0
4	FUB	B1	2	4,9	9,9,10	1.03	0	11,12,14	0.79	0
4	FUB	B3	1	4	9,9,10	1.00	0	11,12,14	0.93	0
4	FUB	B3	2	4,9	9,9,10	1.06	0	11,12,14	0.90	0
4	FUB	B4	1	4	9,9,10	1.01	0	11,12,14	0.79	0
4	FUB	B4	2	4,9	9,9,10	1.02	0	11,12,14	0.89	0
4	FUB	B5	1	4	9,9,10	1.03	0	11,12,14	0.80	0
4	FUB	B5	2	4,9	9,9,10	1.03	0	11,12,14	0.82	0
5	FUB	B6	1	5	9,9,10	1.03	0	11,12,14	0.81	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUB	B6	2	9,5	9,9,10	1.02	0	11,12,14	0.81	0
5	FUB	B6	3	5	9,9,10	1.01	0	11,12,14	0.87	0
5	FUB	B6	4	9,5	9,9,10	1.03	0	11,12,14	0.87	0
4	FUB	B7	1	4	9,9,10	1.03	0	11,12,14	0.79	0
4	FUB	B7	2	4,9	9,9,10	1.03	0	11,12,14	0.87	0
4	FUB	B9	1	4	9,9,10	1.03	0	11,12,14	0.83	0
4	FUB	B9	2	4,9	9,9,10	1.02	0	11,12,14	0.86	0
4	FUB	C0	1	4	9,9,10	1.01	0	11,12,14	0.99	0
4	FUB	C0	2	4,9	9,9,10	1.02	0	11,12,14	0.81	0
4	FUB	C1	1	4	9,9,10	1.01	0	11,12,14	0.83	0
4	FUB	C1	2	4,9	9,9,10	1.00	0	11,12,14	0.88	0
4	FUB	C2	1	4	9,9,10	1.02	0	11,12,14	0.82	0
4	FUB	C2	2	4,9	9,9,10	1.01	0	11,12,14	0.87	0
4	FUB	C3	1	4	9,9,10	1.01	0	11,12,14	0.87	0
4	FUB	C3	2	4,9	9,9,10	1.02	0	11,12,14	0.90	0
4	FUB	C4	1	4	9,9,10	1.03	0	11,12,14	0.81	0
4	FUB	C4	2	4,9	9,9,10	1.00	0	11,12,14	0.88	0
4	FUB	C5	1	4	9,9,10	1.03	0	11,12,14	0.88	0
4	FUB	C5	2	4,9	9,9,10	1.03	0	11,12,14	0.90	0
4	FUB	C6	1	4	9,9,10	1.02	0	11,12,14	0.83	0
4	FUB	C6	2	4,9	9,9,10	1.00	0	11,12,14	0.87	0
4	FUB	C7	1	4	9,9,10	1.01	0	11,12,14	0.83	0
4	FUB	C7	2	4,9	9,9,10	1.01	0	11,12,14	0.91	0
4	FUB	C8	1	4	9,9,10	1.02	0	11,12,14	0.88	0
4	FUB	C8	2	4,9	9,9,10	1.00	0	11,12,14	0.87	0
4	FUB	C9	1	4	9,9,10	1.02	0	11,12,14	0.88	0
4	FUB	C9	2	4,9	9,9,10	1.02	0	11,12,14	0.86	0
4	FUB	D0	1	4	9,9,10	1.03	0	11,12,14	0.90	0
4	FUB	D0	2	4,9	9,9,10	1.02	0	11,12,14	0.89	0
4	FUB	D1	1	4	9,9,10	1.03	0	11,12,14	1.13	1 (9%)
4	FUB	D1	2	4,9	9,9,10	1.02	0	11,12,14	0.86	0
4	FUB	D2	1	4	9,9,10	1.05	0	11,12,14	0.95	0
4	FUB	D2	2	4,9	9,9,10	1.03	0	11,12,14	0.81	0
4	FUB	D3	1	4	9,9,10	1.02	0	11,12,14	0.79	0
4	FUB	D3	2	4,9	9,9,10	1.02	0	11,12,14	0.91	0
4	FUB	D4	1	4	9,9,10	1.04	0	11,12,14	0.78	0
4	FUB	D4	2	4,9	9,9,10	1.03	0	11,12,14	0.87	0
4	FUB	D5	1	4	9,9,10	1.05	0	11,12,14	0.91	0
4	FUB	D5	2	4,9	9,9,10	1.04	0	11,12,14	0.88	0
4	FUB	D6	1	4	9,9,10	1.03	0	11,12,14	0.80	0
4	FUB	D6	2	4,9	9,9,10	1.06	0	11,12,14	1.01	0
4	FUB	D7	1	4	9,9,10	1.05	0	11,12,14	0.96	0
4	FUB	D7	2	4,9	9,9,10	1.05	0	11,12,14	0.87	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	D8	1	4	9,9,10	1.03	0	11,12,14	0.79	0
4	FUB	D8	2	4,9	9,9,10	1.02	0	11,12,14	0.86	0
4	FUB	D9	1	4	9,9,10	1.05	0	11,12,14	0.92	0
4	FUB	D9	2	4,9	9,9,10	1.05	0	11,12,14	0.83	0
4	FUB	E0	1	4	9,9,10	1.04	0	11,12,14	0.83	0
4	FUB	E0	2	4,9	9,9,10	1.03	0	11,12,14	0.79	0
4	FUB	E1	1	4	9,9,10	1.03	0	11,12,14	0.85	0
4	FUB	E1	2	4,9	9,9,10	1.04	0	11,12,14	0.94	0
4	FUB	E2	1	4	9,9,10	1.01	0	11,12,14	0.87	0
4	FUB	E2	2	4,9	9,9,10	1.04	0	11,12,14	0.85	0
4	FUB	E3	1	4	9,9,10	1.05	0	11,12,14	0.87	0
4	FUB	E3	2	4,9	9,9,10	1.02	0	11,12,14	0.89	0
4	FUB	E4	1	4	9,9,10	1.00	0	11,12,14	1.07	1 (9%)
4	FUB	E4	2	4,9	9,9,10	1.05	0	11,12,14	1.10	0
4	FUB	E5	1	4	9,9,10	1.03	0	11,12,14	0.80	0
4	FUB	E5	2	4,9	9,9,10	1.02	0	11,12,14	0.85	0
6	FUB	E6	1	6	9,9,10	1.05	0	11,12,14	0.85	0
6	FUB	E6	2	9,6	9,9,10	1.02	0	11,12,14	0.80	0
6	FUB	E6	3	6	9,9,10	1.02	0	11,12,14	0.87	0
6	FUB	E6	4	9,6	9,9,10	1.04	0	11,12,14	0.83	0
6	FUB	E6	5	6	9,9,10	1.01	0	11,12,14	0.88	0
6	FUB	E6	6	9,6	9,9,10	1.04	0	11,12,14	0.79	0
6	FUB	E6	7	6	9,9,10	1.02	0	11,12,14	0.74	0
6	FUB	E6	8	9,6	9,9,10	1.03	0	11,12,14	0.84	0
4	FUB	E7	1	4	9,9,10	1.05	0	11,12,14	0.78	0
4	FUB	E7	2	4,9	9,9,10	1.05	0	11,12,14	0.87	0
4	FUB	E8	1	4	9,9,10	1.02	0	11,12,14	0.81	0
4	FUB	E8	2	4,9	9,9,10	1.01	0	11,12,14	0.86	0
4	FUB	F0	1	4	9,9,10	1.02	0	11,12,14	0.89	0
4	FUB	F0	2	4,9	9,9,10	1.03	0	11,12,14	0.84	0
4	FUB	F2	1	4	9,9,10	1.03	0	11,12,14	0.78	0
4	FUB	F2	2	4,9	9,9,10	1.06	0	11,12,14	0.87	0
4	FUB	F3	1	4	9,9,10	1.05	0	11,12,14	0.85	0
4	FUB	F3	2	4,9	9,9,10	1.04	0	11,12,14	0.87	0
4	FUB	F5	1	4	9,9,10	1.05	0	11,12,14	0.78	0
4	FUB	F5	2	4,9	9,9,10	1.06	0	11,12,14	0.87	0
5	FUB	F6	1	5	9,9,10	1.05	0	11,12,14	0.77	0
5	FUB	F6	2	9,5	9,9,10	1.05	0	11,12,14	0.85	0
5	FUB	F6	3	5	9,9,10	1.04	0	11,12,14	0.83	0
5	FUB	F6	4	9,5	9,9,10	1.05	0	11,12,14	0.86	0
5	FUB	F7	1	5	9,9,10	1.03	0	11,12,14	0.79	0
5	FUB	F7	2	9,5	9,9,10	1.05	0	11,12,14	0.82	0
5	FUB	F7	3	5	9,9,10	1.01	0	11,12,14	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUB	F7	4	9,5	9,9,10	1.02	0	11,12,14	0.81	0
4	FUB	F8	1	4	9,9,10	1.05	0	11,12,14	0.78	0
4	FUB	F8	2	4,9	9,9,10	1.06	0	11,12,14	0.87	0
3	NAG	a1	1	3,1	14,14,15	0.72	0	17,19,21	0.85	1 (5%)
3	NAG	a1	2	3	14,14,15	0.72	0	17,19,21	0.80	0
3	NAG	a2	1	3,1	14,14,15	0.71	0	17,19,21	1.21	1 (5%)
3	NAG	a2	2	3	14,14,15	0.73	0	17,19,21	0.82	0
3	NAG	a3	1	3,1	14,14,15	0.76	0	17,19,21	1.54	2 (11%)
3	NAG	a3	2	3	14,14,15	0.72	0	17,19,21	1.26	2 (11%)
7	34V	a4	1	7	9,9,10	1.24	0	11,12,15	1.48	1 (9%)
7	FUB	a4	2	9,7	9,9,10	1.31	1 (11%)	11,12,14	1.21	2 (18%)
4	FUB	a5	1	4	9,9,10	1.06	0	11,12,14	0.93	0
4	FUB	a5	2	4,9	9,9,10	1.32	1 (11%)	11,12,14	1.09	1 (9%)
5	FUB	a6	1	5	9,9,10	1.09	1 (11%)	11,12,14	1.03	0
5	FUB	a6	2	9,5	9,9,10	1.29	0	11,12,14	1.21	1 (9%)
5	FUB	a6	3	5	9,9,10	1.17	1 (11%)	11,12,14	1.18	1 (9%)
5	FUB	a6	4	9,5	9,9,10	1.21	1 (11%)	11,12,14	1.09	1 (9%)
4	FUB	a7	1	4	9,9,10	1.11	0	11,12,14	1.05	1 (9%)
4	FUB	a7	2	4,9	9,9,10	1.34	0	11,12,14	0.99	1 (9%)
5	FUB	a9	1	5	9,9,10	1.30	1 (11%)	11,12,14	1.04	1 (9%)
5	FUB	a9	2	9,5	9,9,10	1.29	1 (11%)	11,12,14	0.96	0
5	FUB	a9	3	5	9,9,10	1.08	0	11,12,14	1.03	0
5	FUB	a9	4	9,5	9,9,10	1.29	0	11,12,14	1.04	1 (9%)
4	FUB	b0	1	4	9,9,10	1.43	2 (22%)	11,12,14	1.25	2 (18%)
4	FUB	b0	2	4,9	9,9,10	1.32	1 (11%)	11,12,14	1.02	1 (9%)
4	FUB	b1	1	4	9,9,10	1.39	2 (22%)	11,12,14	1.24	2 (18%)
4	FUB	b1	2	4,9	9,9,10	1.26	0	11,12,14	1.03	1 (9%)
4	FUB	b3	1	4	9,9,10	1.05	0	11,12,14	1.04	1 (9%)
4	FUB	b3	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	1.34	2 (18%)
4	FUB	b4	1	4	9,9,10	1.34	1 (11%)	11,12,14	1.01	1 (9%)
4	FUB	b4	2	4,9	9,9,10	1.40	1 (11%)	11,12,14	1.11	1 (9%)
4	FUB	b5	1	4	9,9,10	1.13	0	11,12,14	1.37	2 (18%)
4	FUB	b5	2	4,9	9,9,10	1.21	0	11,12,14	1.12	1 (9%)
5	FUB	b6	1	5	9,9,10	1.33	1 (11%)	11,12,14	1.07	1 (9%)
5	FUB	b6	2	9,5	9,9,10	1.35	1 (11%)	11,12,14	1.11	1 (9%)
5	FUB	b6	3	5	9,9,10	1.28	0	11,12,14	1.10	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	FUB	b6	4	9,5	9,9,10	1.32	0	11,12,14	1.09	1 (9%)
4	FUB	b7	1	4	9,9,10	1.21	0	11,12,14	1.04	1 (9%)
4	FUB	b7	2	4,9	9,9,10	1.35	1 (11%)	11,12,14	1.05	1 (9%)
4	FUB	b9	1	4	9,9,10	1.24	0	11,12,14	1.00	1 (9%)
4	FUB	b9	2	4,9	9,9,10	1.25	0	11,12,14	0.98	1 (9%)
4	FUB	c0	1	4	9,9,10	1.30	1 (11%)	11,12,14	1.19	2 (18%)
4	FUB	c0	2	4,9	9,9,10	1.23	1 (11%)	11,12,14	1.16	2 (18%)
4	FUB	c1	1	4	9,9,10	1.35	2 (22%)	11,12,14	1.03	1 (9%)
4	FUB	c1	2	4,9	9,9,10	1.20	0	11,12,14	1.06	1 (9%)
4	FUB	c2	1	4	9,9,10	1.32	1 (11%)	11,12,14	1.03	1 (9%)
4	FUB	c2	2	4,9	9,9,10	1.22	0	11,12,14	1.03	1 (9%)
4	FUB	c3	1	4	9,9,10	1.29	1 (11%)	11,12,14	1.20	2 (18%)
4	FUB	c3	2	4,9	9,9,10	1.40	2 (22%)	11,12,14	0.98	1 (9%)
4	FUB	c4	1	4	9,9,10	1.29	0	11,12,14	1.03	1 (9%)
4	FUB	c4	2	4,9	9,9,10	1.34	2 (22%)	11,12,14	1.11	1 (9%)
4	FUB	c5	1	4	9,9,10	1.16	0	11,12,14	1.06	1 (9%)
4	FUB	c5	2	4,9	9,9,10	1.24	0	11,12,14	0.95	1 (9%)
4	FUB	c6	1	4	9,9,10	1.37	2 (22%)	11,12,14	1.12	1 (9%)
4	FUB	c6	2	4,9	9,9,10	1.25	0	11,12,14	1.00	1 (9%)
4	FUB	c7	1	4	9,9,10	1.40	2 (22%)	11,12,14	1.26	2 (18%)
4	FUB	c7	2	4,9	9,9,10	1.25	0	11,12,14	1.14	1 (9%)
4	FUB	c8	1	4	9,9,10	1.12	0	11,12,14	1.01	1 (9%)
4	FUB	c8	2	4,9	9,9,10	1.40	2 (22%)	11,12,14	1.08	1 (9%)
4	FUB	c9	1	4	9,9,10	1.15	1 (11%)	11,12,14	1.34	3 (27%)
4	FUB	c9	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	1.30	2 (18%)
4	FUB	d0	1	4	9,9,10	1.14	0	11,12,14	1.01	1 (9%)
4	FUB	d0	2	4,9	9,9,10	1.40	2 (22%)	11,12,14	1.07	1 (9%)
4	FUB	d1	1	4	9,9,10	1.07	1 (11%)	11,12,14	0.84	0
4	FUB	d1	2	4,9	9,9,10	1.07	0	11,12,14	1.52	4 (36%)
4	FUB	d2	1	4	9,9,10	1.07	0	11,12,14	1.14	1 (9%)
4	FUB	d2	2	4,9	9,9,10	1.26	0	11,12,14	1.03	1 (9%)
4	FUB	d3	1	4	9,9,10	1.24	0	11,12,14	1.00	1 (9%)
4	FUB	d3	2	4,9	9,9,10	1.30	0	11,12,14	1.04	1 (9%)
4	FUB	d4	1	4	9,9,10	1.14	0	11,12,14	0.99	1 (9%)
4	FUB	d4	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	0.99	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	d5	1	4	9,9,10	1.20	0	11,12,14	1.08	1 (9%)
4	FUB	d5	2	4,9	9,9,10	1.39	2 (22%)	11,12,14	1.14	1 (9%)
4	FUB	d6	1	4	9,9,10	1.15	0	11,12,14	0.99	1 (9%)
4	FUB	d6	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	0.99	1 (9%)
4	FUB	d7	1	4	9,9,10	1.43	2 (22%)	11,12,14	1.20	1 (9%)
4	FUB	d7	2	4,9	9,9,10	1.29	1 (11%)	11,12,14	1.00	1 (9%)
4	FUB	d8	1	4	9,9,10	1.07	0	11,12,14	1.07	0
4	FUB	d8	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	1.01	1 (9%)
4	FUB	d9	1	4	9,9,10	1.24	0	11,12,14	0.97	1 (9%)
4	FUB	d9	2	4,9	9,9,10	1.40	1 (11%)	11,12,14	1.02	1 (9%)
4	FUB	e0	1	4	9,9,10	1.24	0	11,12,14	1.03	1 (9%)
4	FUB	e0	2	4,9	9,9,10	1.29	1 (11%)	11,12,14	1.25	2 (18%)
4	FUB	e1	1	4	9,9,10	1.09	0	11,12,14	1.08	1 (9%)
4	FUB	e1	2	4,9	9,9,10	1.36	1 (11%)	11,12,14	1.06	1 (9%)
4	FUB	e2	1	4	9,9,10	1.21	0	11,12,14	1.08	1 (9%)
4	FUB	e2	2	4,9	9,9,10	1.31	1 (11%)	11,12,14	0.99	1 (9%)
4	FUB	e3	1	4	9,9,10	1.08	0	11,12,14	1.07	0
4	FUB	e3	2	4,9	9,9,10	1.35	1 (11%)	11,12,14	1.01	1 (9%)
4	FUB	e4	1	4	9,9,10	1.12	1 (11%)	11,12,14	1.21	1 (9%)
4	FUB	e4	2	4,9	9,9,10	1.36	2 (22%)	11,12,14	1.19	2 (18%)
4	FUB	e5	1	4	9,9,10	1.43	2 (22%)	11,12,14	1.20	1 (9%)
4	FUB	e5	2	4,9	9,9,10	1.28	1 (11%)	11,12,14	1.00	1 (9%)
4	FUB	e6	1	4	9,9,10	1.08	0	11,12,14	1.07	0
4	FUB	e6	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	1.00	1 (9%)
4	FUB	e7	1	4	9,9,10	1.08	0	11,12,14	1.07	0
4	FUB	e7	2	4,9	9,9,10	1.33	1 (11%)	11,12,14	1.00	1 (9%)
4	FUB	e8	1	4	9,9,10	1.24	0	11,12,14	0.97	1 (9%)
4	FUB	e8	2	4,9	9,9,10	1.39	1 (11%)	11,12,14	1.02	1 (9%)
8	FUB	e9	1	8	9,9,10	1.19	0	11,12,14	1.07	1 (9%)
8	FUB	e9	2	9,8	9,9,10	1.22	0	11,12,14	1.51	2 (18%)
8	FUB	e9	3	8	9,9,10	1.12	0	11,12,14	1.13	1 (9%)
8	FUB	e9	4	9,8	9,9,10	1.20	0	11,12,14	1.41	1 (9%)
8	FUB	e9	5	8	9,9,10	1.22	0	11,12,14	1.08	1 (9%)
8	FUB	e9	6	9,8	9,9,10	1.28	0	11,12,14	1.20	2 (18%)
4	FUB	f0	1	4	9,9,10	1.08	0	11,12,14	1.07	0
4	FUB	f0	2	4,9	9,9,10	1.34	1 (11%)	11,12,14	1.01	1 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FUB	f2	1	4	9,9,10	1.07	0	11,12,14	1.07	0
4	FUB	f2	2	4,9	9,9,10	1.33	1 (11%)	11,12,14	1.00	1 (9%)
4	FUB	f3	1	4	9,9,10	1.15	0	11,12,14	1.02	1 (9%)
4	FUB	f3	2	4,9	9,9,10	1.42	1 (11%)	11,12,14	1.06	1 (9%)
4	FUB	f5	1	4	9,9,10	1.28	0	11,12,14	1.05	1 (9%)
4	FUB	f5	2	4,9	9,9,10	1.23	1 (11%)	11,12,14	1.35	2 (18%)
5	FUB	f6	1	5	9,9,10	1.14	0	11,12,14	1.06	1 (9%)
5	FUB	f6	2	9,5	9,9,10	1.30	0	11,12,14	1.06	1 (9%)
5	FUB	f6	3	5	9,9,10	1.20	0	11,12,14	1.07	1 (9%)
5	FUB	f6	4	9,5	9,9,10	1.28	1 (11%)	11,12,14	1.41	2 (18%)
5	FUB	f7	1	5	9,9,10	1.33	2 (22%)	11,12,14	1.04	1 (9%)
5	FUB	f7	2	9,5	9,9,10	1.26	0	11,12,14	1.24	1 (9%)
5	FUB	f7	3	5	9,9,10	1.32	2 (22%)	11,12,14	1.04	1 (9%)
5	FUB	f7	4	9,5	9,9,10	1.23	0	11,12,14	1.23	1 (9%)
4	FUB	f8	1	4	9,9,10	1.20	0	11,12,14	1.07	1 (9%)
4	FUB	f8	2	4,9	9,9,10	1.36	2 (22%)	11,12,14	1.26	2 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A1	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	A1	2	3	-	1/6/23/26	0/1/1/1
3	NAG	A2	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	A2	2	3	-	0/6/23/26	0/1/1/1
3	NAG	A3	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	A3	2	3	-	0/6/23/26	0/1/1/1
4	FUB	A4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	A5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A5	2	4,9	-	0/2/15/18	0/1/1/1
5	FUB	A6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	A6	2	9,5	-	0/2/15/18	0/1/1/1
5	FUB	A6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	A6	4	9,5	-	0/2/15/18	0/1/1/1
4	FUB	A7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	A7	2	4,9	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUB	A9	1	5	-	0/2/15/18	0/1/1/1
5	FUB	A9	2	9,5	-	0/2/15/18	0/1/1/1
5	FUB	A9	3	5	-	0/2/15/18	0/1/1/1
5	FUB	A9	4	9,5	-	0/2/15/18	0/1/1/1
4	FUB	B0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	B1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B1	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	B3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B3	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	B4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	B5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B5	2	4,9	-	0/2/15/18	0/1/1/1
5	FUB	B6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	B6	2	9,5	-	0/2/15/18	0/1/1/1
5	FUB	B6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	B6	4	9,5	-	0/2/15/18	0/1/1/1
4	FUB	B7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B7	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	B9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	B9	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C1	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C2	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C3	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C5	2	4,9	-	1/2/15/18	0/1/1/1
4	FUB	C6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C6	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C7	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	C8	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	C9	1	4	-	2/2/15/18	0/1/1/1
4	FUB	C9	2	4,9	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	D0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D1	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D2	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D3	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	D4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D5	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D6	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	D7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D7	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	D8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D8	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	D9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	D9	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	E0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E1	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E1	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E2	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E3	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	E4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E5	2	4,9	-	0/2/15/18	0/1/1/1
6	FUB	E6	1	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	2	9,6	-	0/2/15/18	0/1/1/1
6	FUB	E6	3	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	4	9,6	-	2/2/15/18	0/1/1/1
6	FUB	E6	5	6	-	2/2/15/18	0/1/1/1
6	FUB	E6	6	9,6	-	0/2/15/18	0/1/1/1
6	FUB	E6	7	6	-	0/2/15/18	0/1/1/1
6	FUB	E6	8	9,6	-	2/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	E7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E7	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	E8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	E8	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	F0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	F2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F2	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	F3	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F3	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	F5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F5	2	4,9	-	0/2/15/18	0/1/1/1
5	FUB	F6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	F6	2	9,5	-	2/2/15/18	0/1/1/1
5	FUB	F6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	F6	4	9,5	-	0/2/15/18	0/1/1/1
5	FUB	F7	1	5	-	0/2/15/18	0/1/1/1
5	FUB	F7	2	9,5	-	2/2/15/18	0/1/1/1
5	FUB	F7	3	5	-	0/2/15/18	0/1/1/1
5	FUB	F7	4	9,5	-	0/2/15/18	0/1/1/1
4	FUB	F8	1	4	-	0/2/15/18	0/1/1/1
4	FUB	F8	2	4,9	-	0/2/15/18	0/1/1/1
3	NAG	a1	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	a1	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a2	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a2	2	3	-	0/6/23/26	0/1/1/1
3	NAG	a3	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	a3	2	3	-	0/6/23/26	0/1/1/1
7	34V	a4	1	7	1/1/3/3	0/2/15/19	0/1/1/1
7	FUB	a4	2	9,7	-	0/2/15/18	0/1/1/1
4	FUB	a5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	a5	2	4,9	-	1/2/15/18	0/1/1/1
5	FUB	a6	1	5	-	1/2/15/18	0/1/1/1
5	FUB	a6	2	9,5	-	2/2/15/18	0/1/1/1
5	FUB	a6	3	5	-	0/2/15/18	0/1/1/1
5	FUB	a6	4	9,5	-	0/2/15/18	0/1/1/1
4	FUB	a7	1	4	-	0/2/15/18	0/1/1/1
4	FUB	a7	2	4,9	-	2/2/15/18	0/1/1/1
5	FUB	a9	1	5	-	0/2/15/18	0/1/1/1
5	FUB	a9	2	9,5	-	2/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUB	a9	3	5	-	2/2/15/18	0/1/1/1
5	FUB	a9	4	9,5	-	2/2/15/18	0/1/1/1
4	FUB	b0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	b1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	b1	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	b3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	b3	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	b4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	b4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	b5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b5	2	4,9	-	0/2/15/18	0/1/1/1
5	FUB	b6	1	5	-	2/2/15/18	0/1/1/1
5	FUB	b6	2	9,5	-	2/2/15/18	0/1/1/1
5	FUB	b6	3	5	-	2/2/15/18	0/1/1/1
5	FUB	b6	4	9,5	-	2/2/15/18	0/1/1/1
4	FUB	b7	1	4	-	1/2/15/18	0/1/1/1
4	FUB	b7	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	b9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	b9	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	c0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c0	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	c1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c1	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	c2	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c2	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	c3	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c3	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	c4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	c5	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c5	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	c6	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c6	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	c7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c7	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	c8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	c8	2	4,9	-	0/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	c9	1	4	-	0/2/15/18	0/1/1/1
4	FUB	c9	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	d1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d1	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	d2	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	d3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	d3	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d4	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d4	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d5	1	4	-	1/2/15/18	0/1/1/1
4	FUB	d5	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d6	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d6	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d7	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d8	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	d9	1	4	-	2/2/15/18	0/1/1/1
4	FUB	d9	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	e0	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e0	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	e1	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e1	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	e2	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e2	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	e3	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e3	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	e4	1	4	-	0/2/15/18	0/1/1/1
4	FUB	e4	2	4,9	-	0/2/15/18	0/1/1/1
4	FUB	e5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e5	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	e6	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e6	2	4,9	-	2/2/15/18	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FUB	e7	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e7	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	e8	1	4	-	2/2/15/18	0/1/1/1
4	FUB	e8	2	4,9	-	0/2/15/18	0/1/1/1
8	FUB	e9	1	8	-	1/2/15/18	0/1/1/1
8	FUB	e9	2	9,8	-	1/2/15/18	0/1/1/1
8	FUB	e9	3	8	-	2/2/15/18	0/1/1/1
8	FUB	e9	4	9,8	-	2/2/15/18	0/1/1/1
8	FUB	e9	5	8	-	2/2/15/18	0/1/1/1
8	FUB	e9	6	9,8	-	2/2/15/18	0/1/1/1
4	FUB	f0	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f0	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	f2	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f2	2	4,9	-	2/2/15/18	0/1/1/1
4	FUB	f3	1	4	-	1/2/15/18	0/1/1/1
4	FUB	f3	2	4,9	-	1/2/15/18	0/1/1/1
4	FUB	f5	1	4	-	2/2/15/18	0/1/1/1
4	FUB	f5	2	4,9	-	0/2/15/18	0/1/1/1
5	FUB	f6	1	5	-	0/2/15/18	0/1/1/1
5	FUB	f6	2	9,5	-	1/2/15/18	0/1/1/1
5	FUB	f6	3	5	-	2/2/15/18	0/1/1/1
5	FUB	f6	4	9,5	-	2/2/15/18	0/1/1/1
5	FUB	f7	1	5	-	0/2/15/18	0/1/1/1
5	FUB	f7	2	9,5	-	2/2/15/18	0/1/1/1
5	FUB	f7	3	5	-	0/2/15/18	0/1/1/1
5	FUB	f7	4	9,5	-	2/2/15/18	0/1/1/1
4	FUB	f8	1	4	-	1/2/15/18	0/1/1/1
4	FUB	f8	2	4,9	-	0/2/15/18	0/1/1/1

The worst 5 of 73 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c7	1	FUB	O4-C1	-2.57	1.38	1.43
4	e4	2	FUB	O4-C1	-2.53	1.38	1.43
4	b1	1	FUB	O4-C1	-2.51	1.38	1.43
4	b0	1	FUB	O4-C1	-2.47	1.38	1.43
5	a6	3	FUB	O4-C1	-2.46	1.38	1.43

The worst 5 of 139 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a3	1	NAG	O5-C1-C2	-4.49	104.35	111.29
7	a4	1	34V	O5-C2-C1	3.97	116.58	109.36
8	e9	2	FUB	O4-C4-C3	-3.96	100.98	104.63
8	e9	4	FUB	O4-C4-C3	-3.72	101.20	104.63
3	a3	2	NAG	C1-O5-C5	3.56	116.96	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	a4	1	34V	C3

5 of 170 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	b4	1	FUB	O4-C4-C5-O5
4	b4	1	FUB	C3-C4-C5-O5
4	c3	1	FUB	C3-C4-C5-O5
4	c7	1	FUB	O4-C4-C5-O5
4	c7	1	FUB	C3-C4-C5-O5

There are no ring outliers.

31 monomers are involved in 54 short contacts:

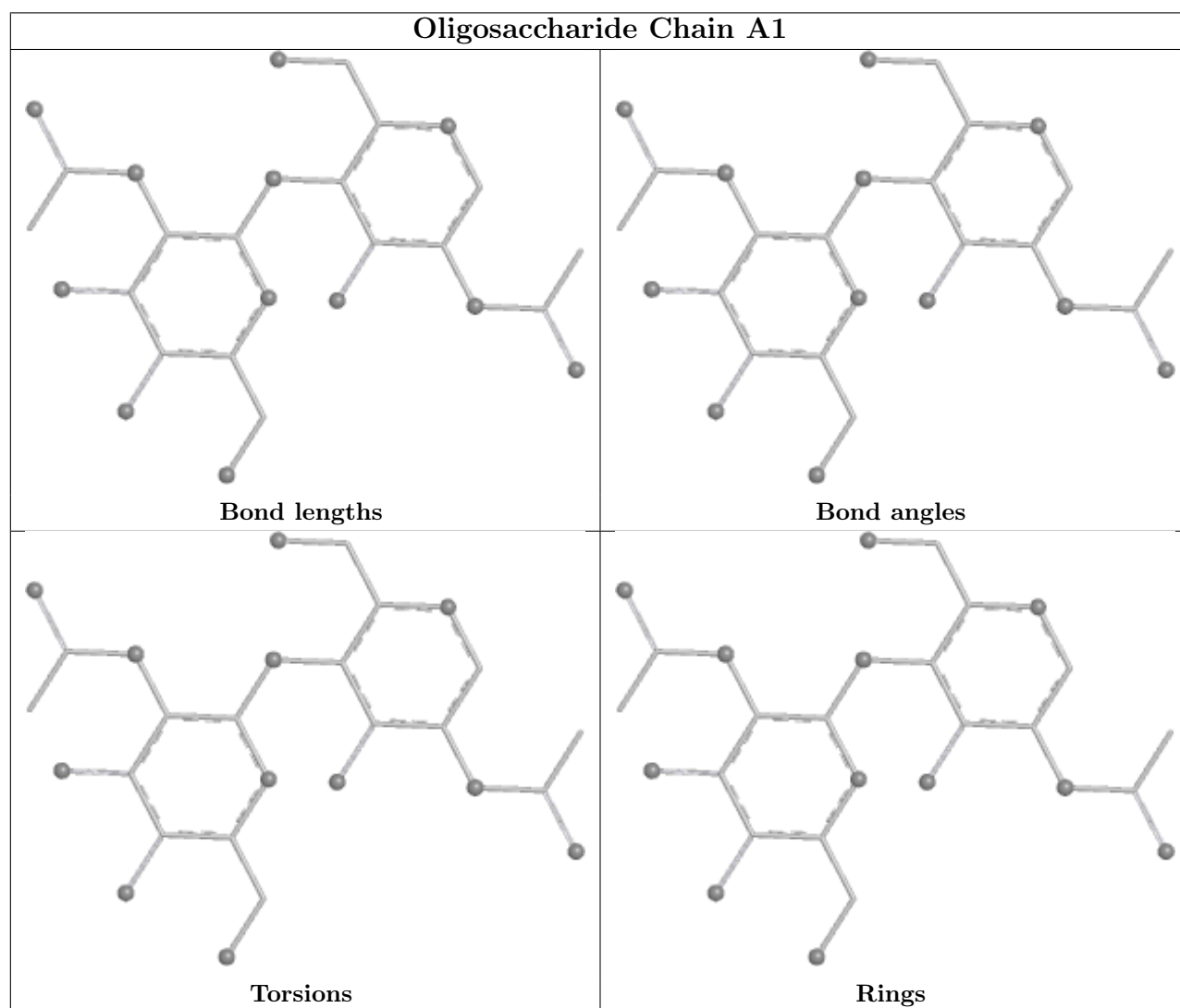
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	e4	1	FUB	3	0
4	f2	1	FUB	2	0
3	a3	1	NAG	1	0
4	a5	1	FUB	1	0
4	e7	2	FUB	1	0
4	d0	1	FUB	3	0
4	C2	2	FUB	1	0
4	D9	2	FUB	1	0
4	B3	1	FUB	1	0
4	f0	1	FUB	3	0
4	f0	2	FUB	4	0
4	C8	2	FUB	1	0
4	c7	2	FUB	1	0
4	e1	1	FUB	2	0
4	a7	2	FUB	1	0
4	f2	2	FUB	3	0
4	C8	1	FUB	1	0
4	c7	1	FUB	1	0
4	e3	2	FUB	2	0

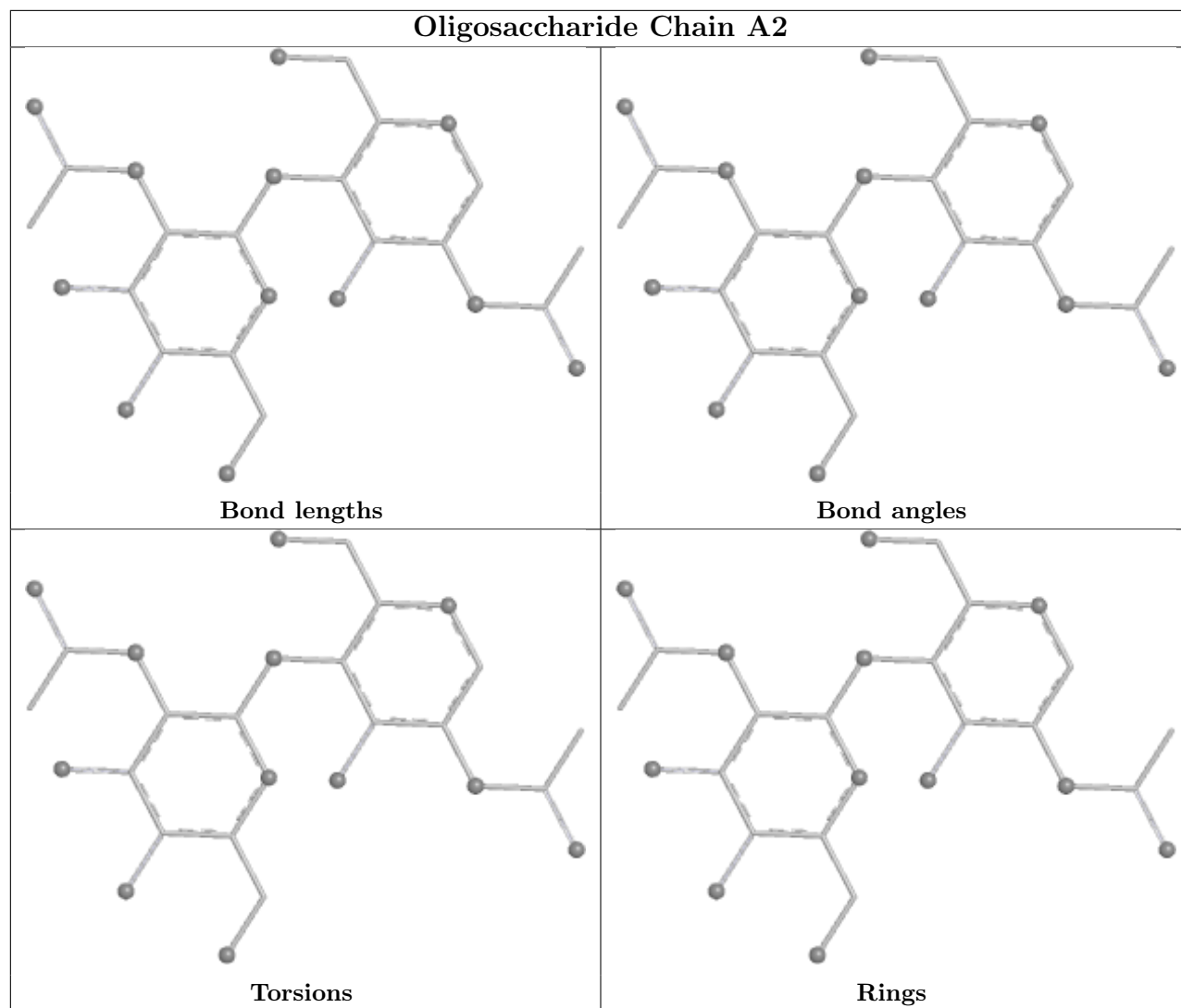
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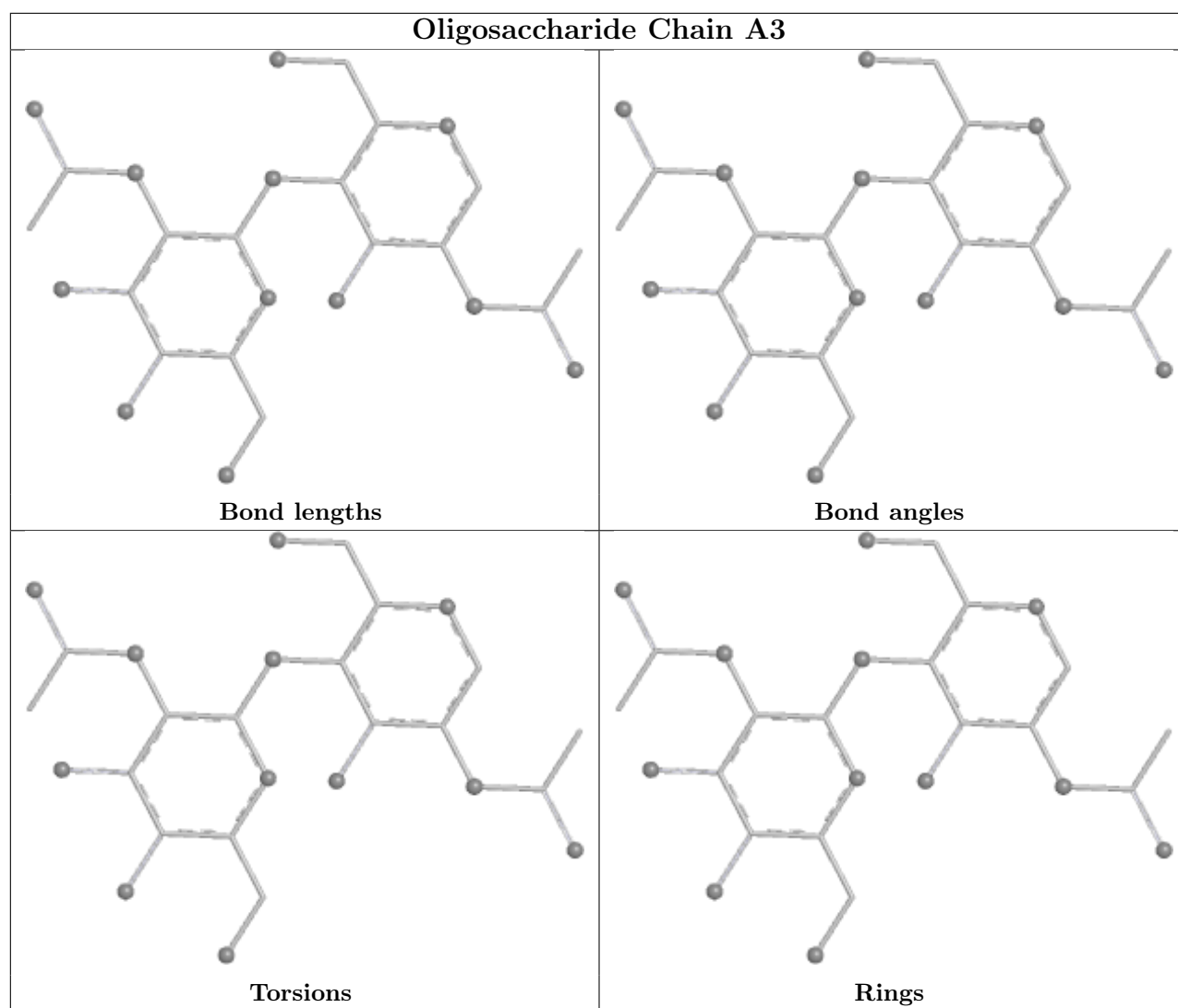
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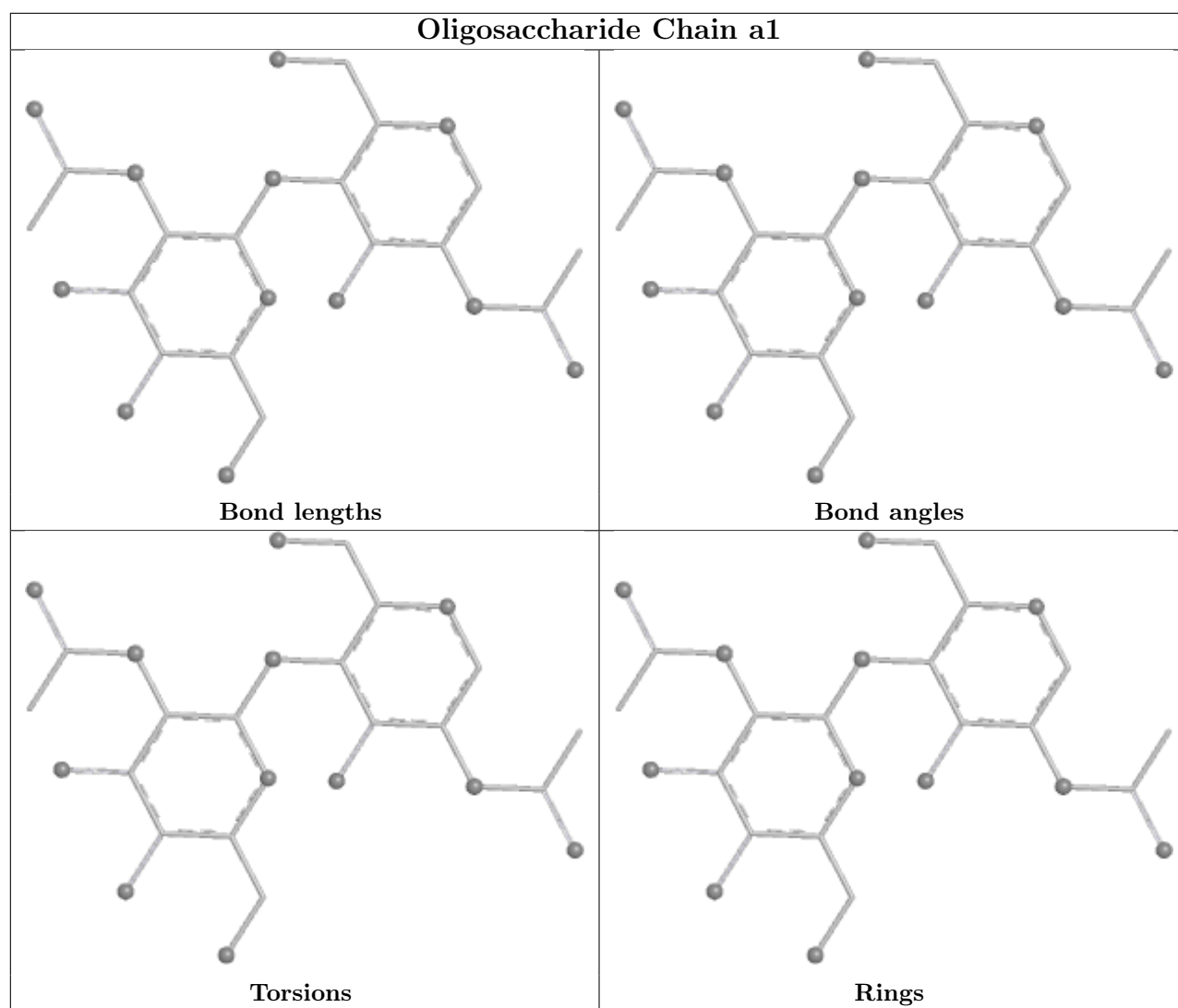
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E4	1	FUB	3	0
4	e3	1	FUB	4	0
4	e7	1	FUB	4	0
4	E4	2	FUB	5	0
4	e6	1	FUB	6	0
4	A5	1	FUB	1	0
4	F5	1	FUB	4	0
4	e6	2	FUB	4	0
4	e1	2	FUB	2	0
4	C2	1	FUB	1	0
4	d9	2	FUB	1	0
4	d8	1	FUB	5	0

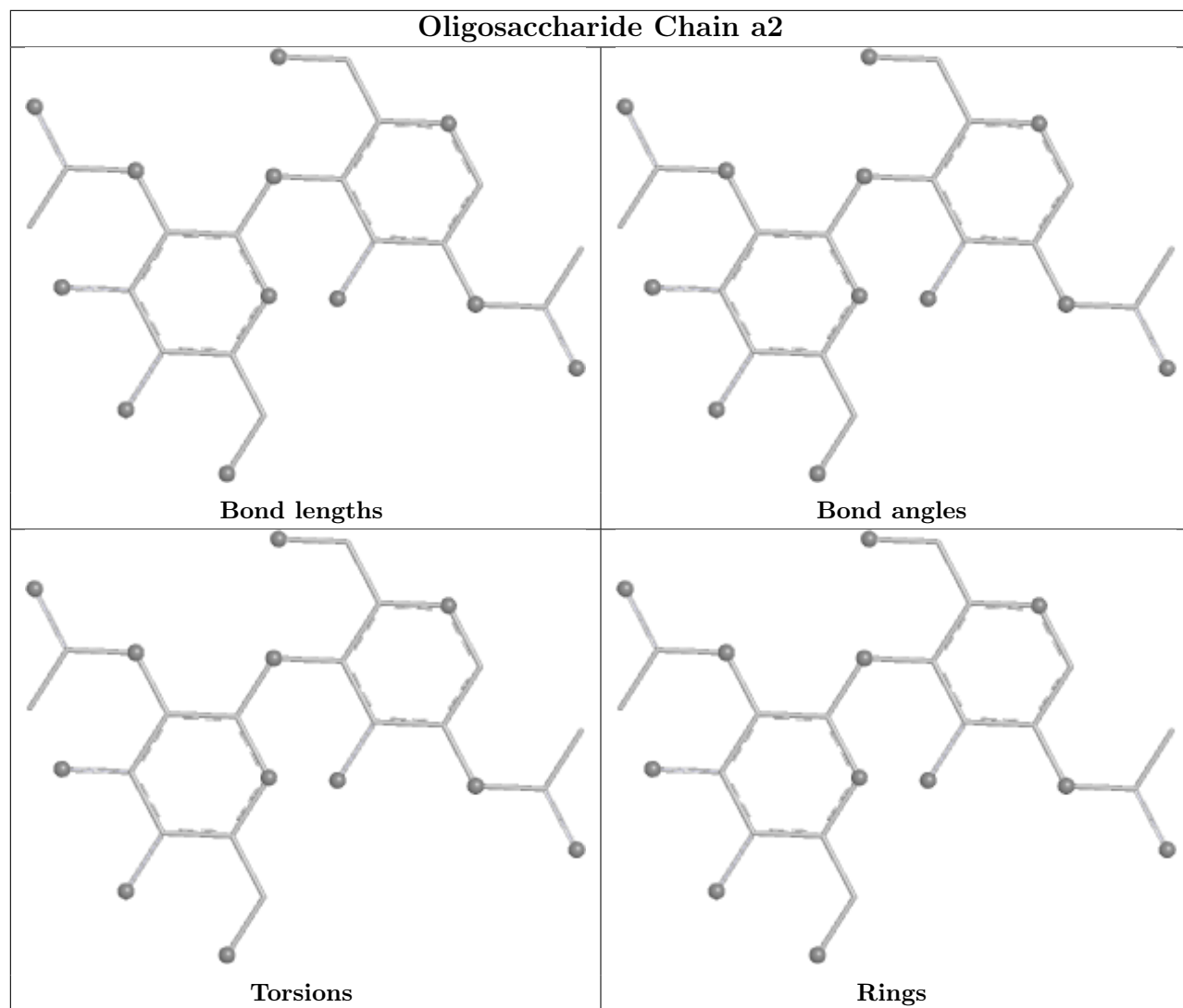
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

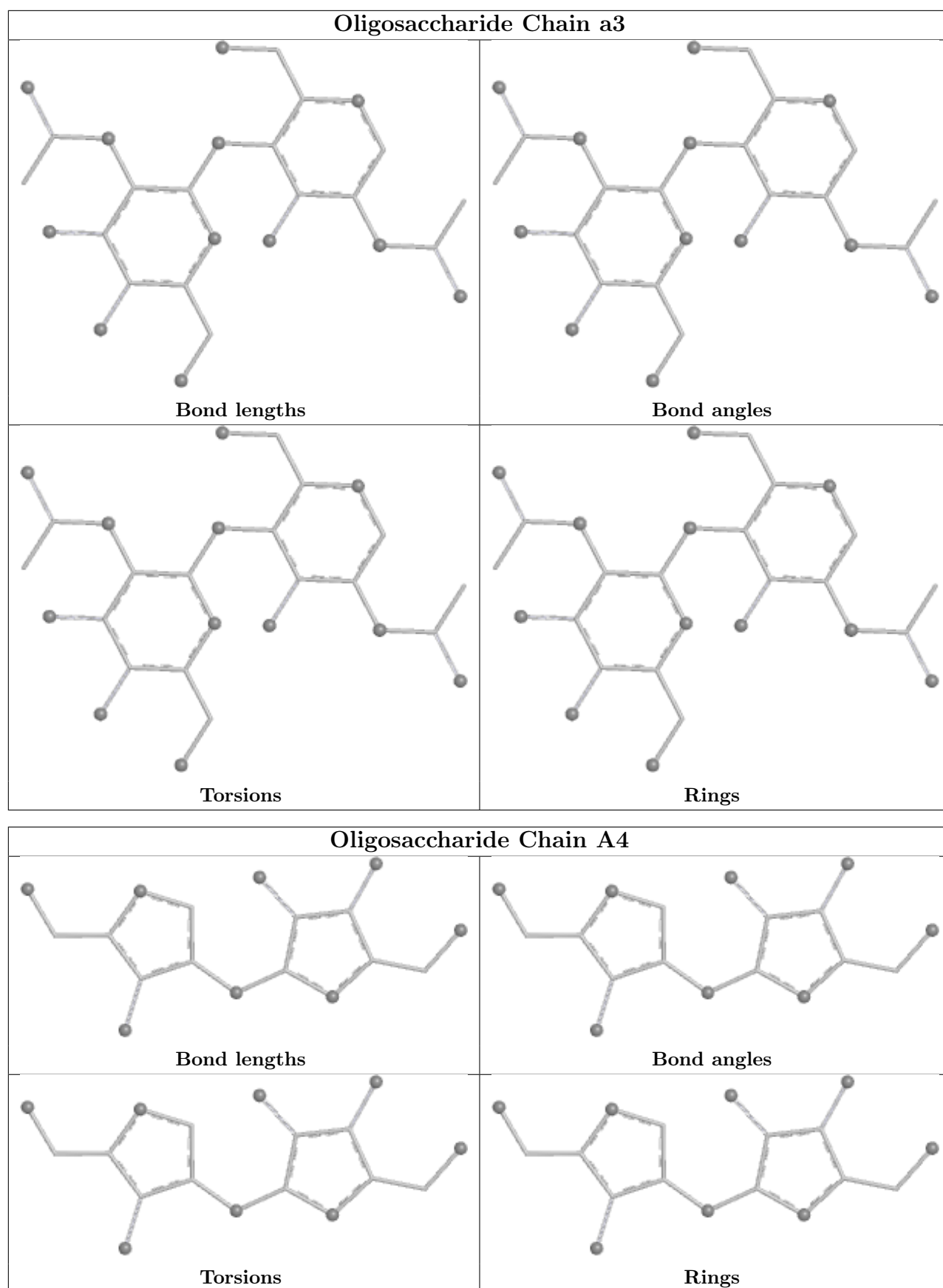


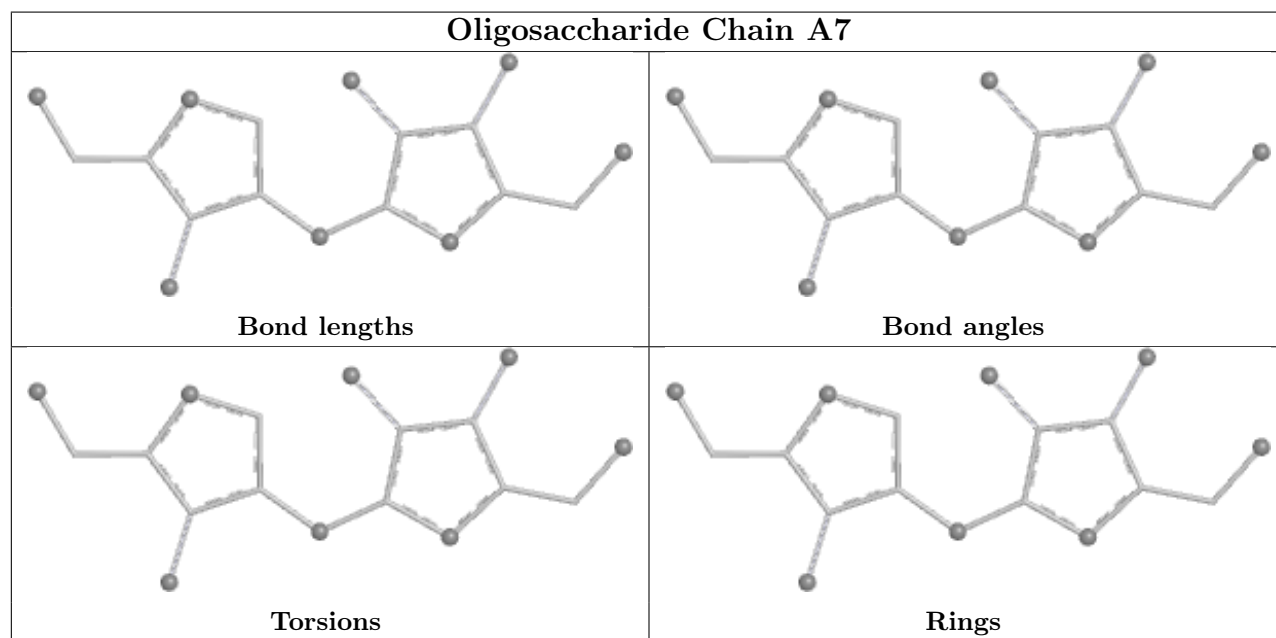
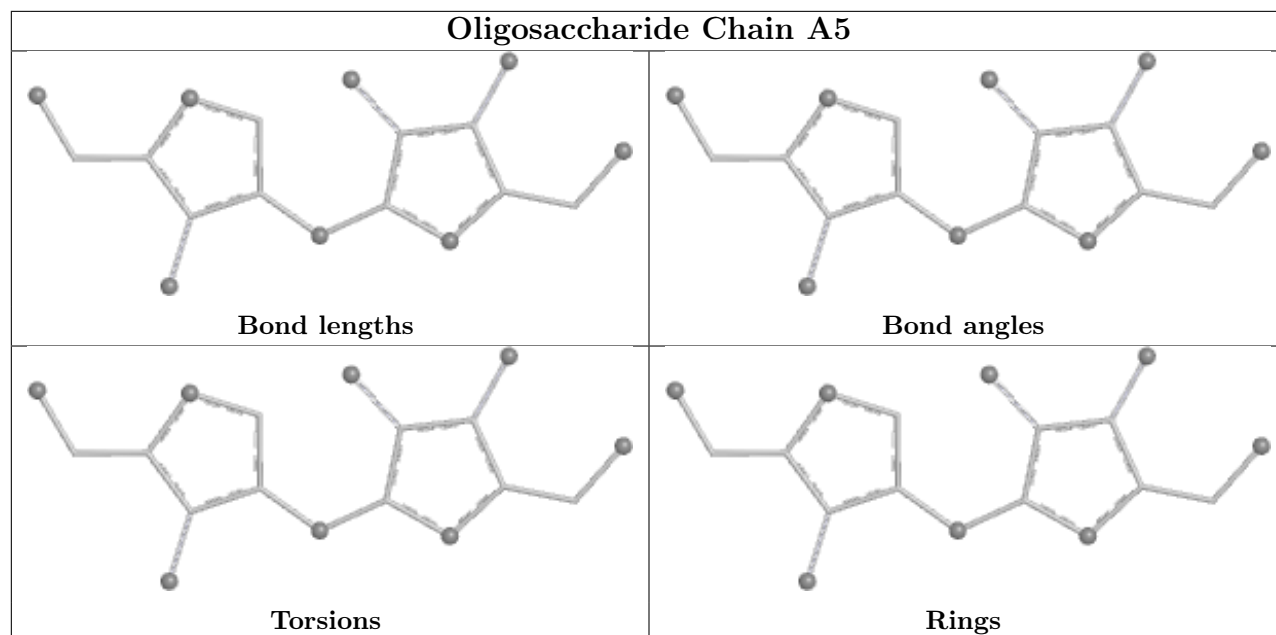


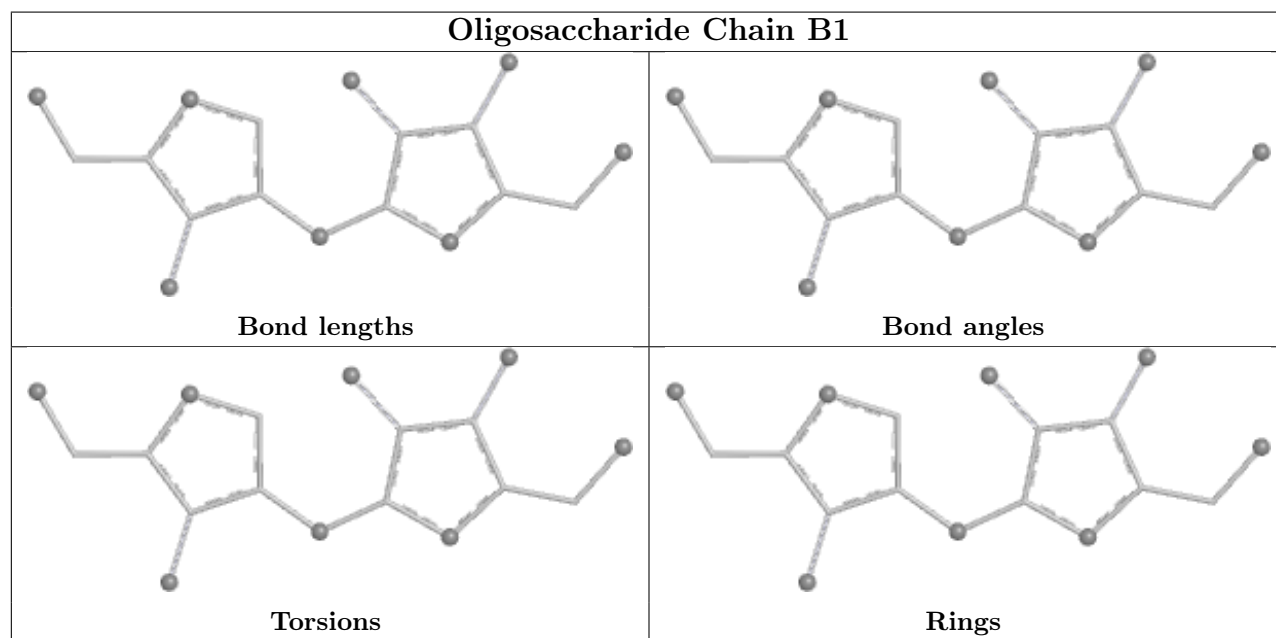
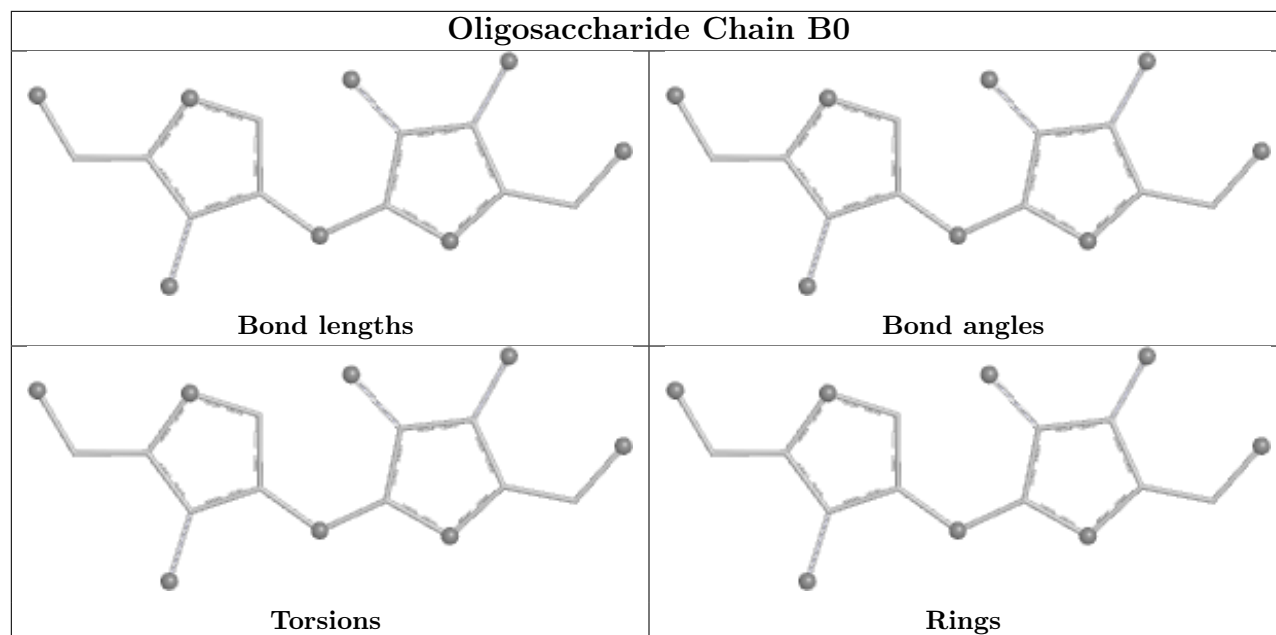


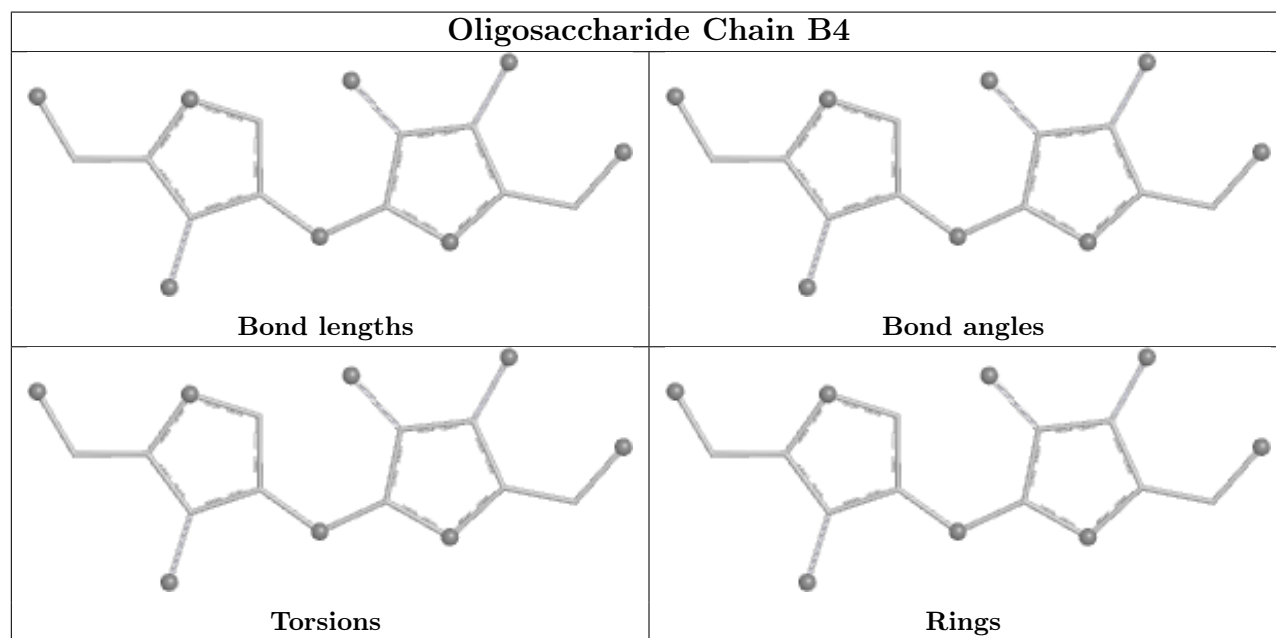
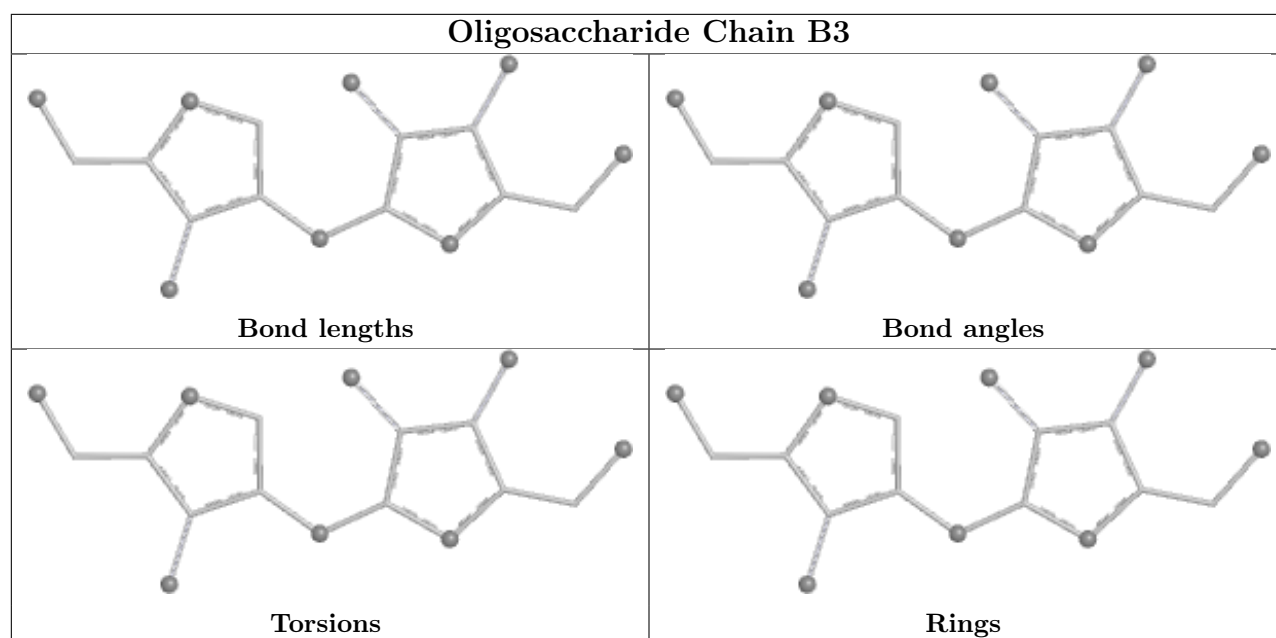


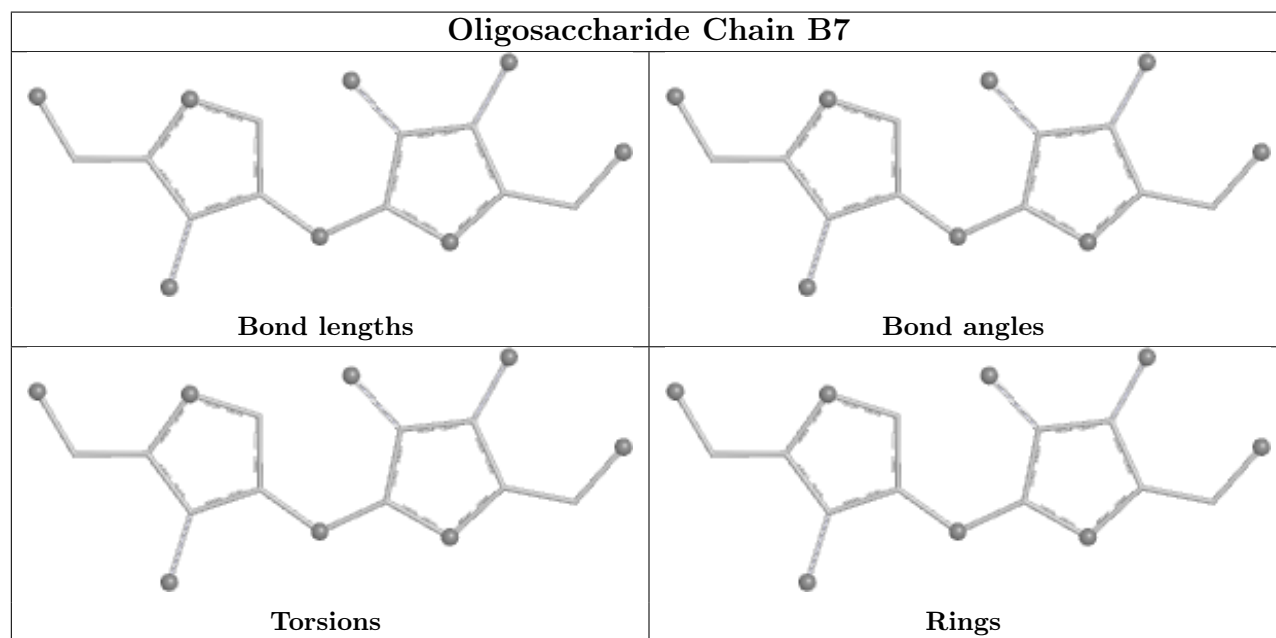
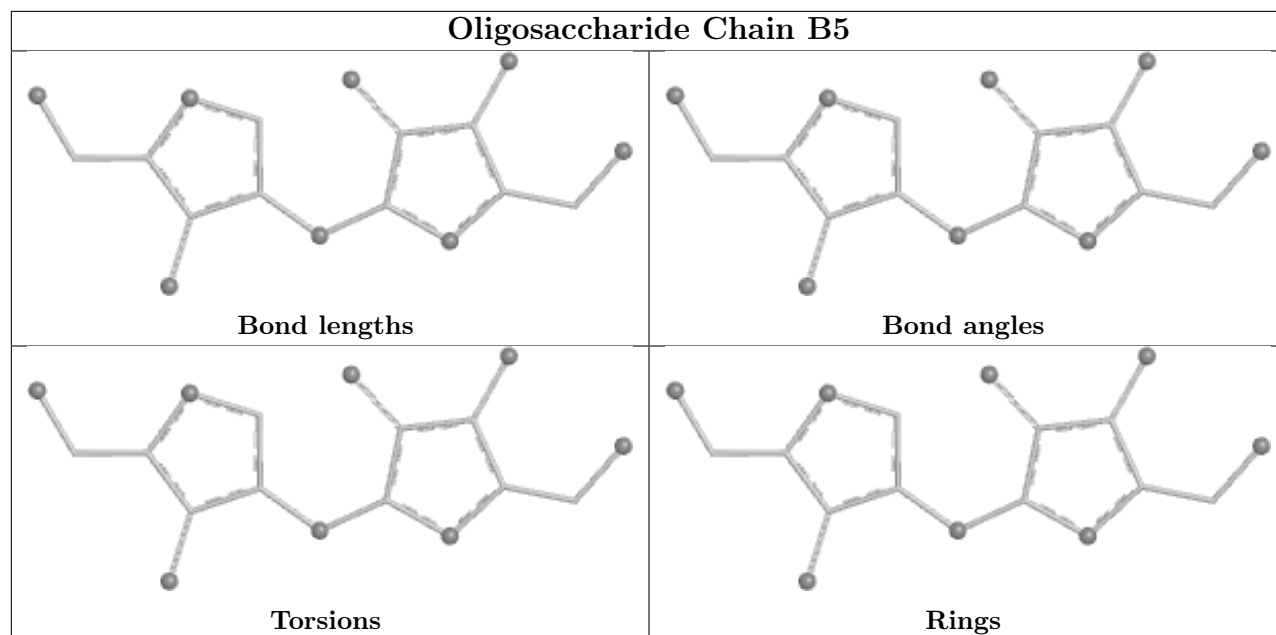


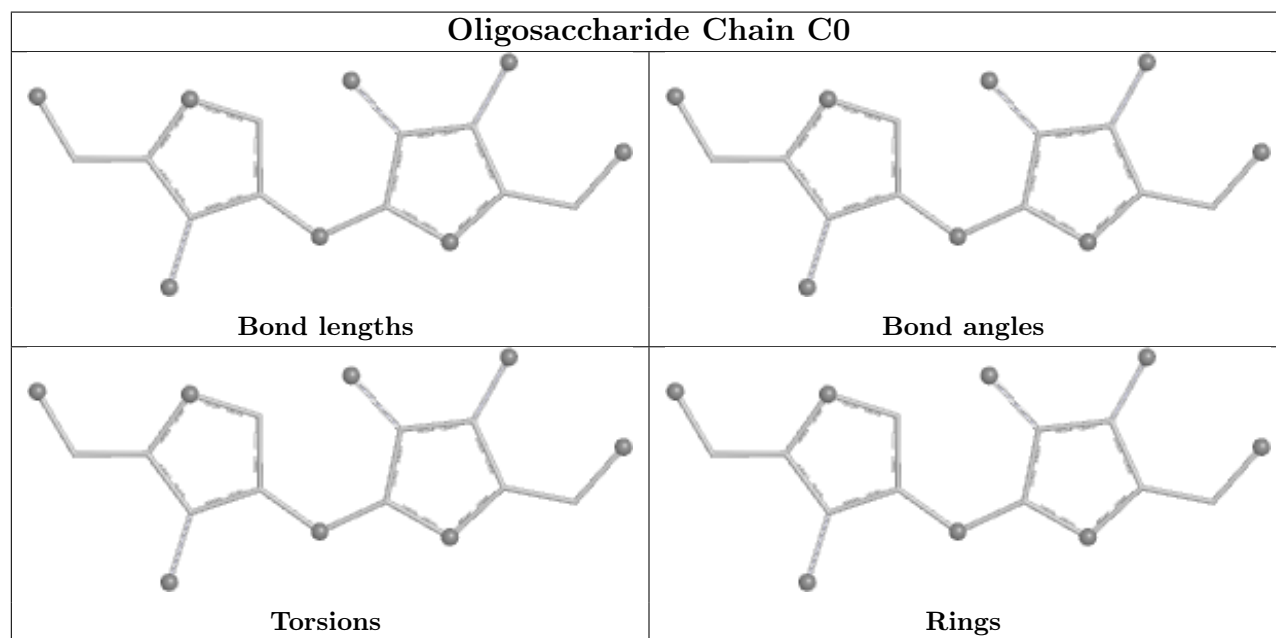
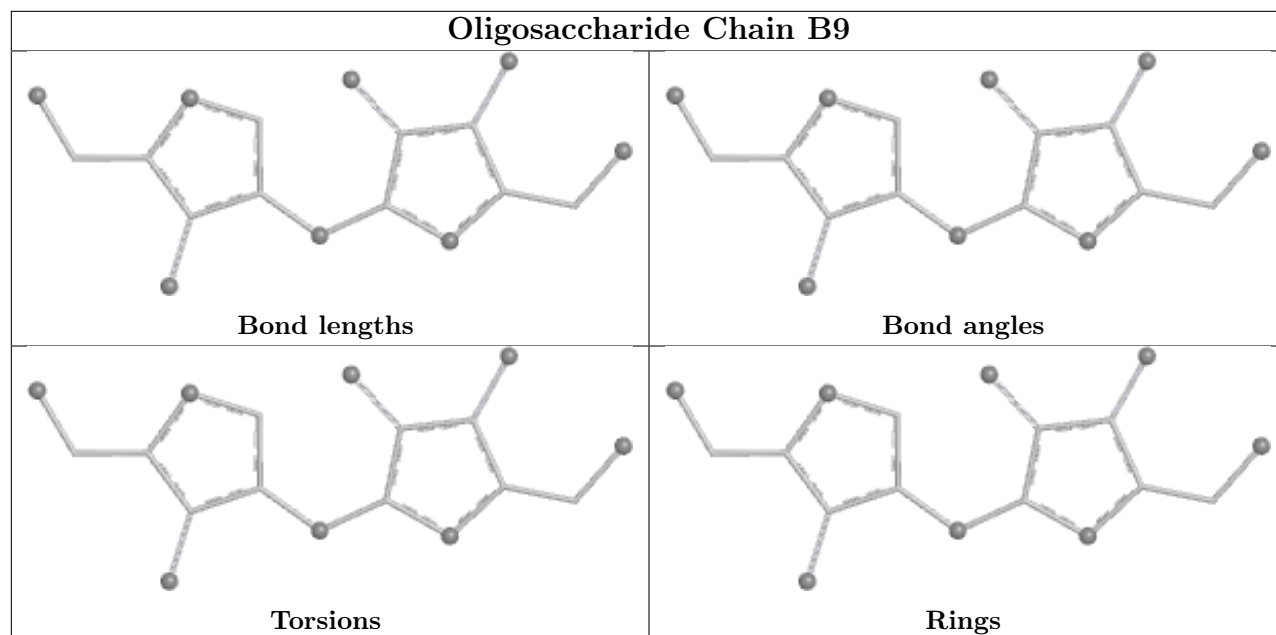


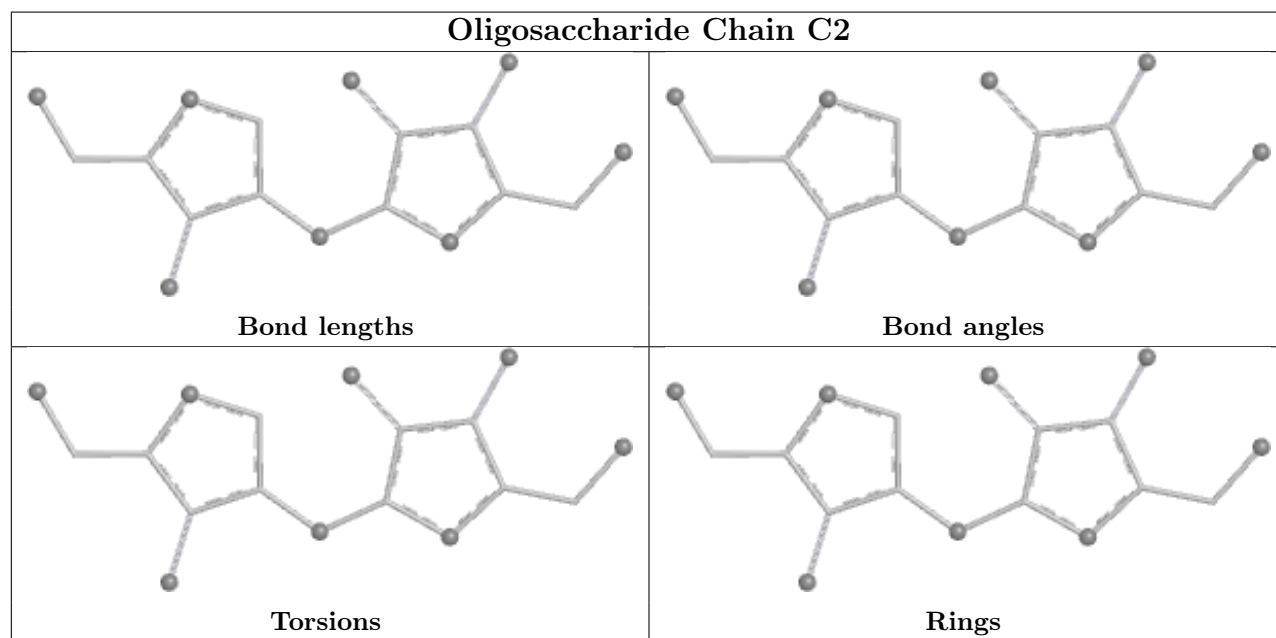
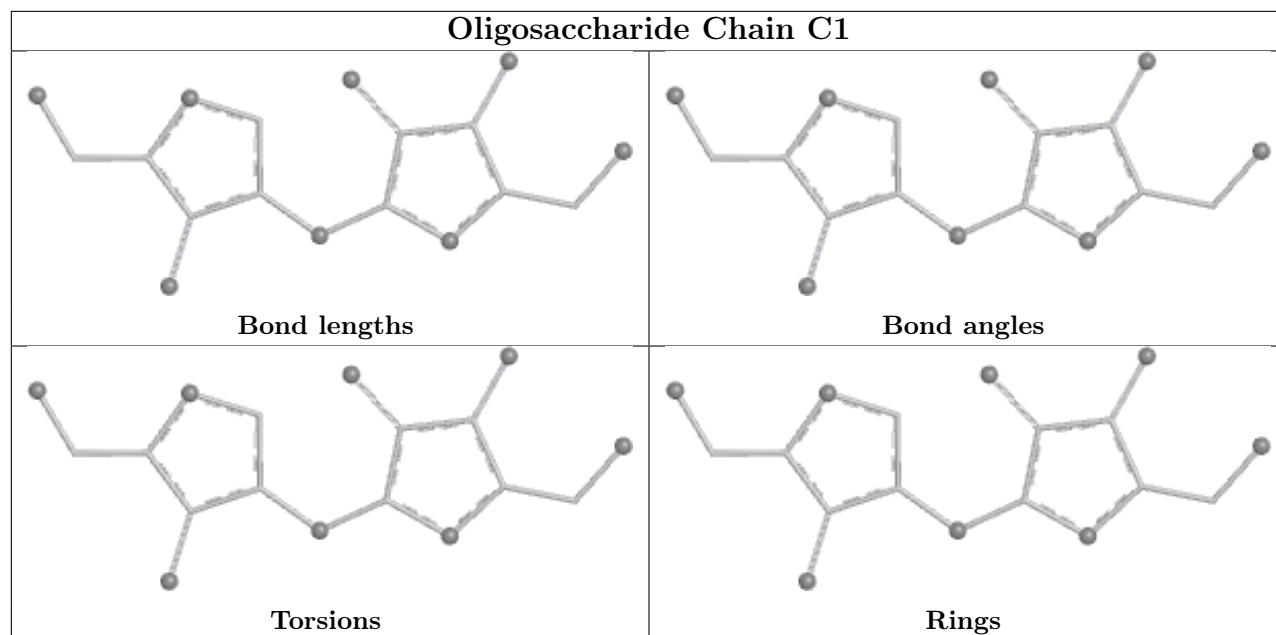


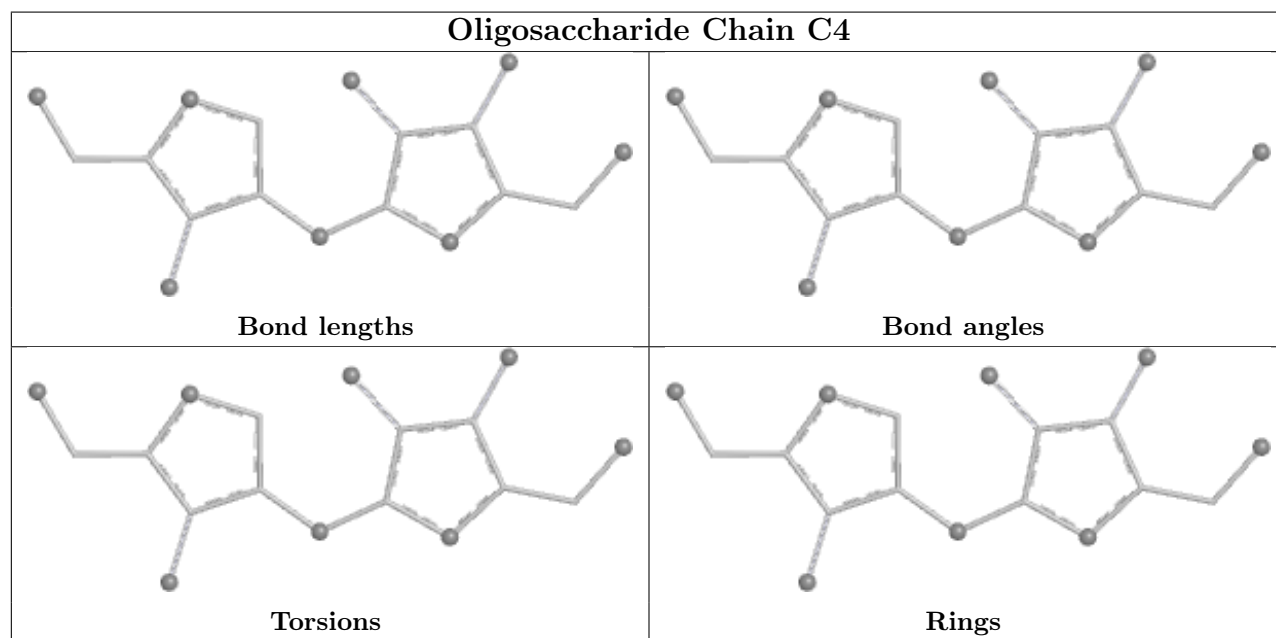
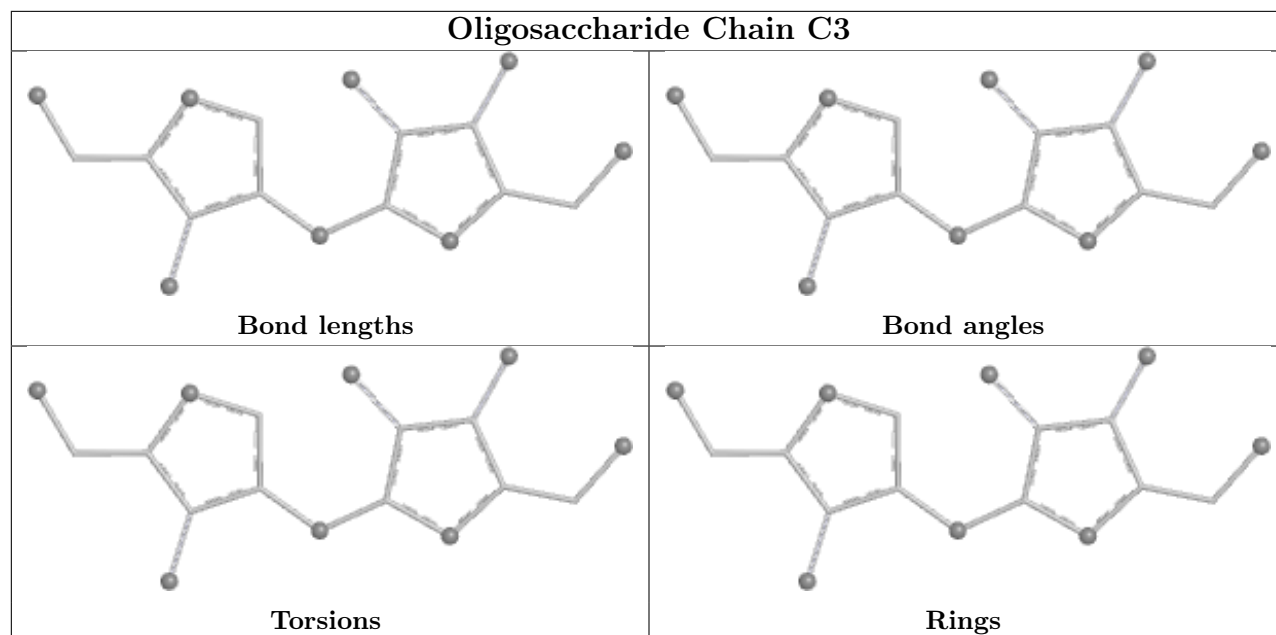


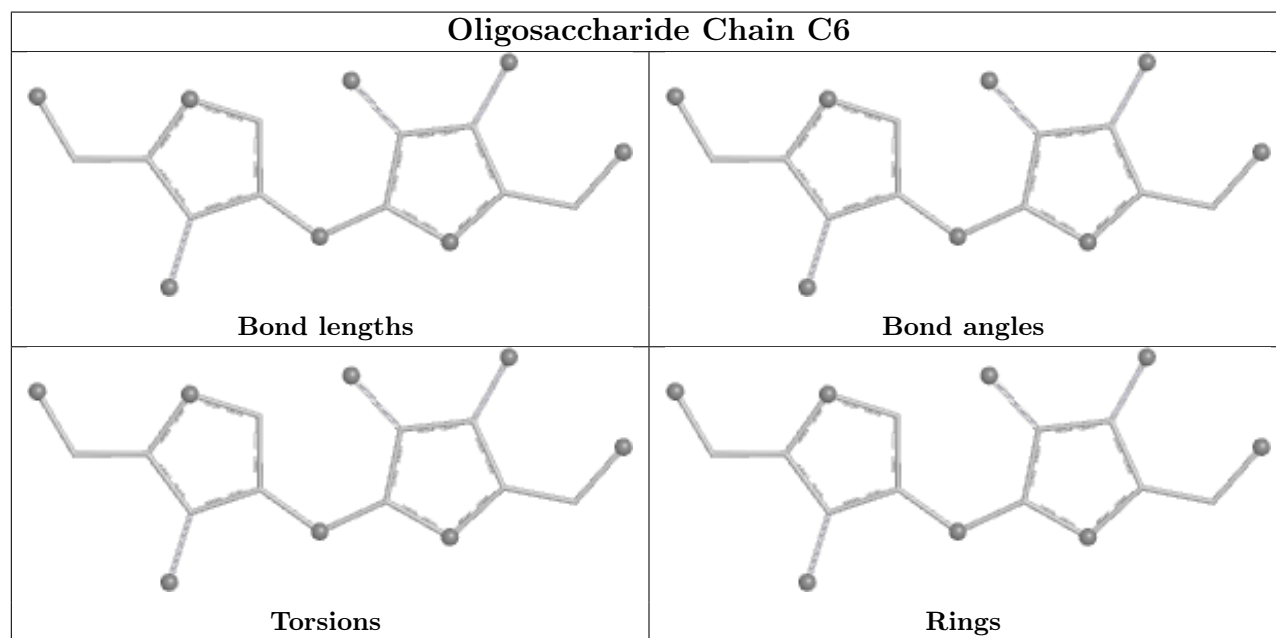
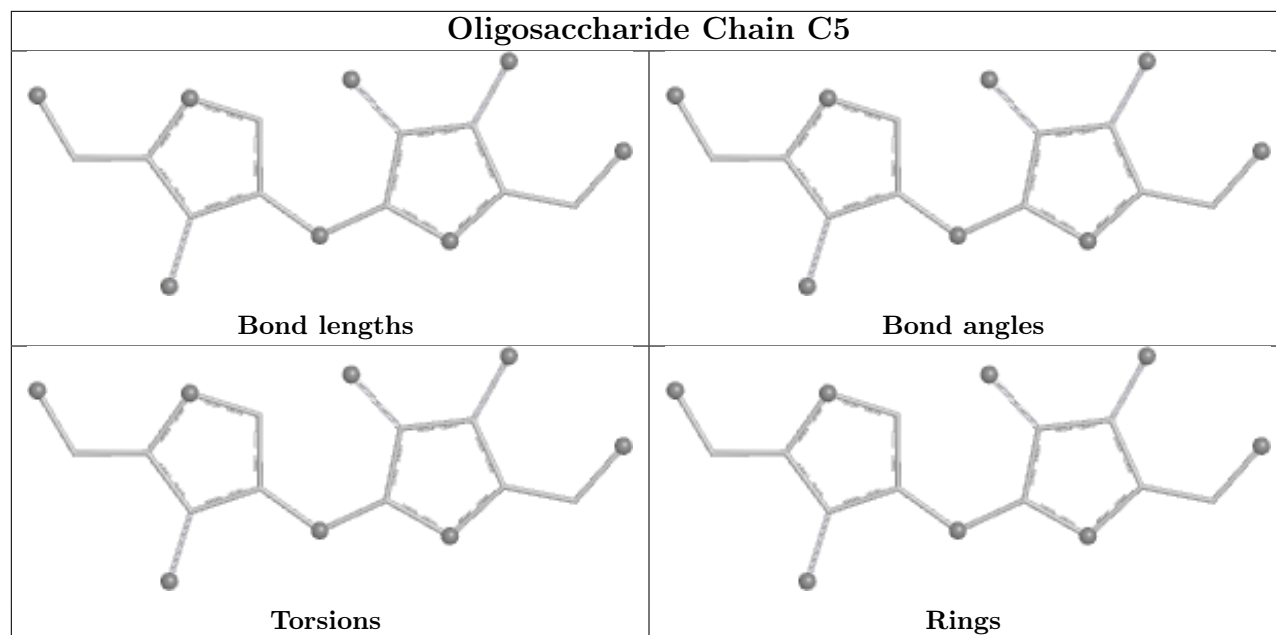


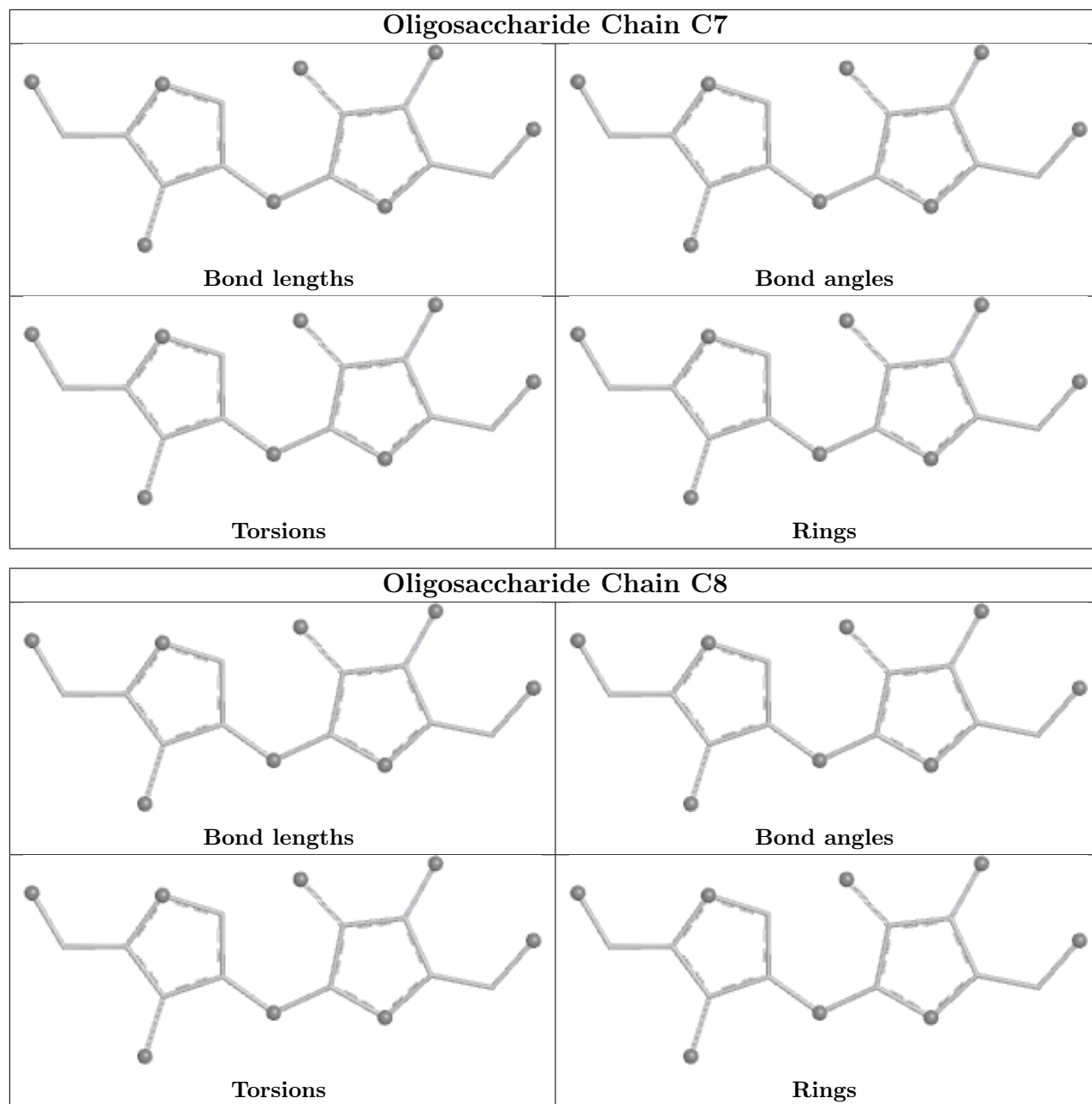


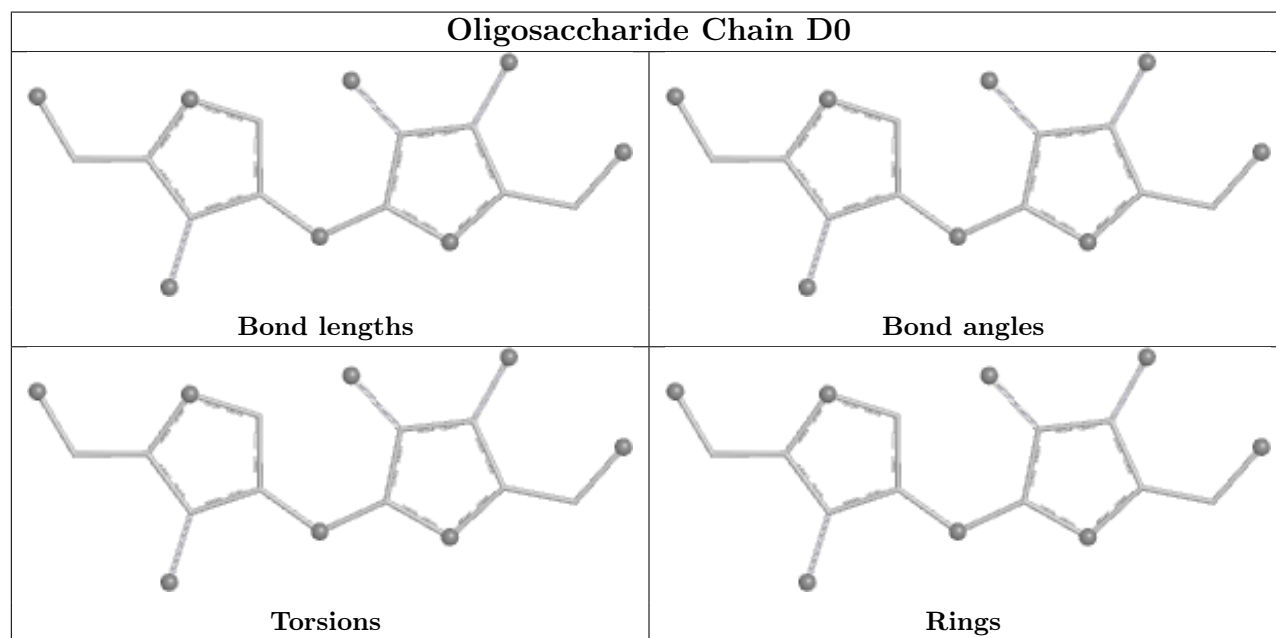
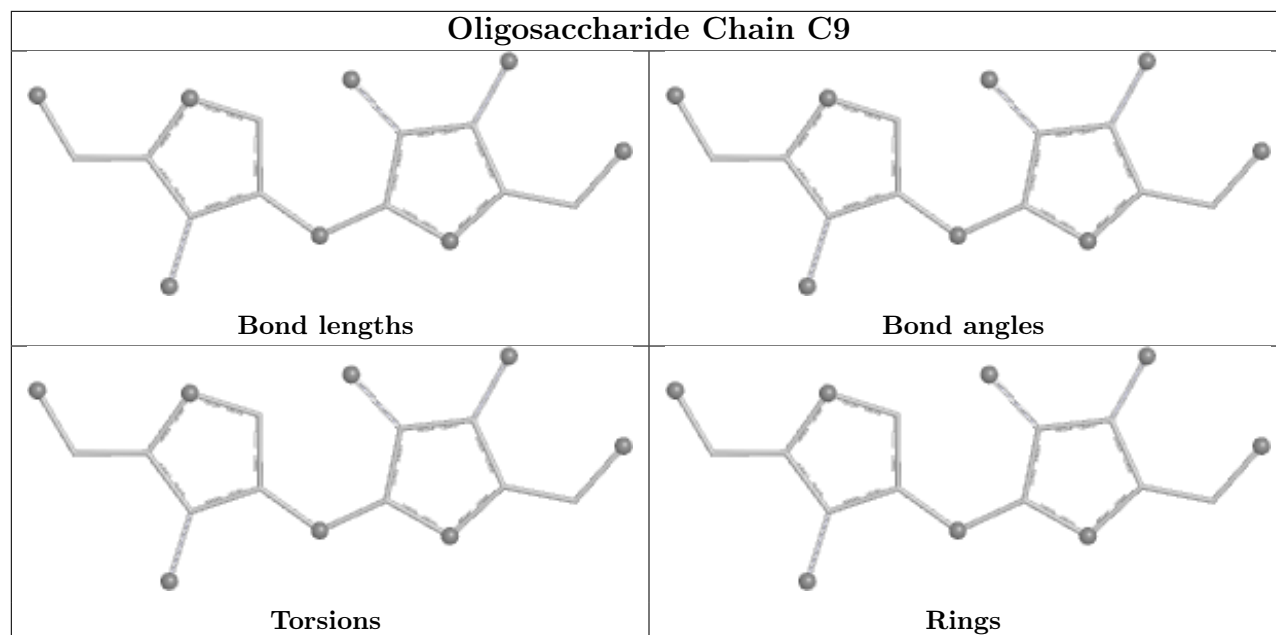


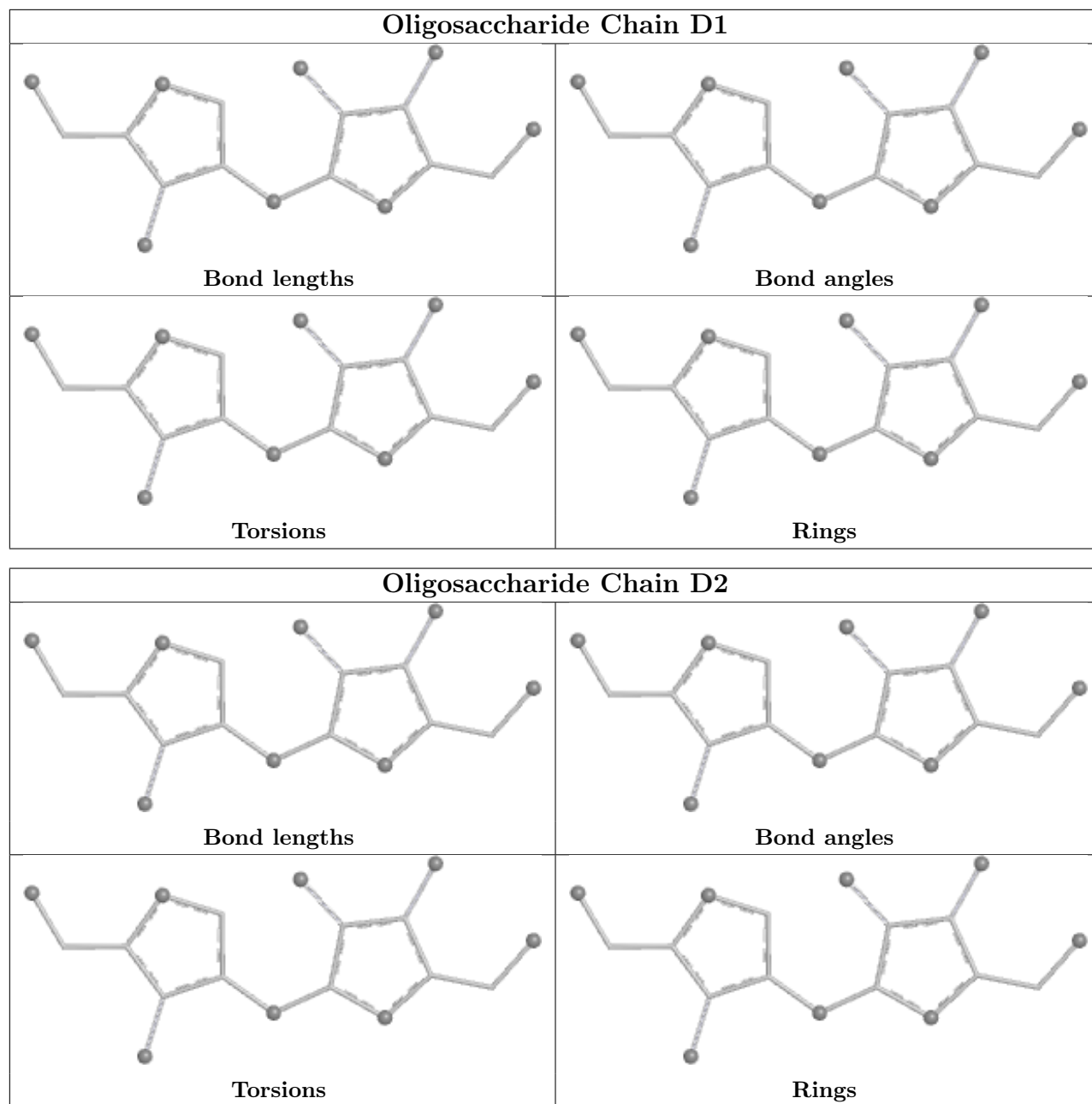


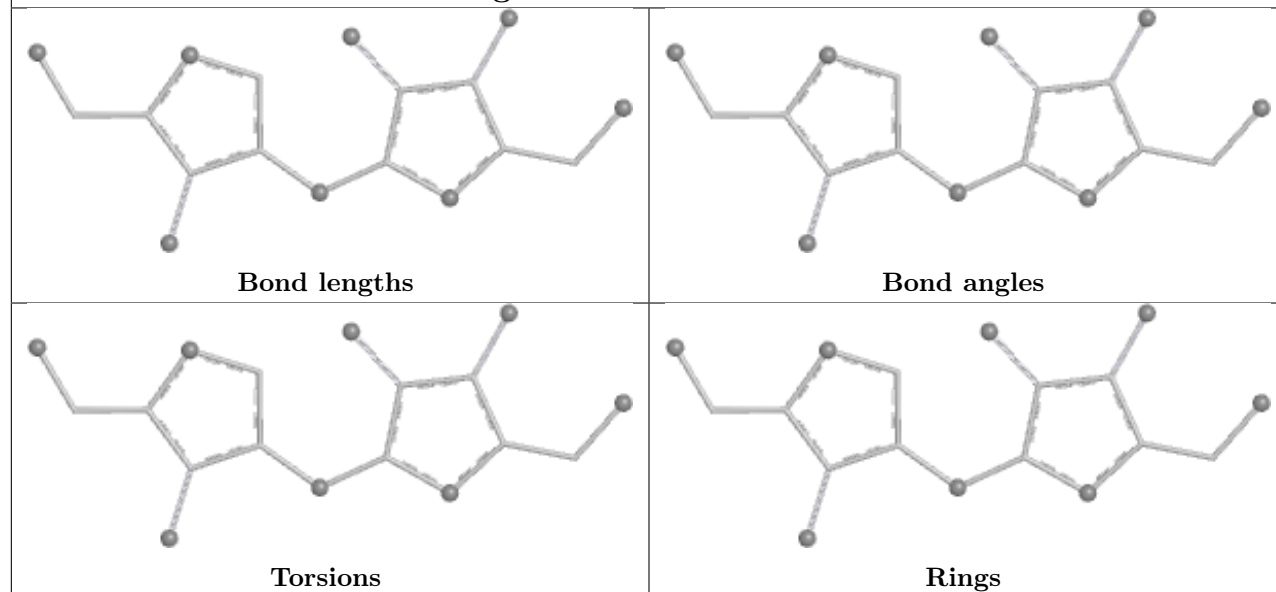
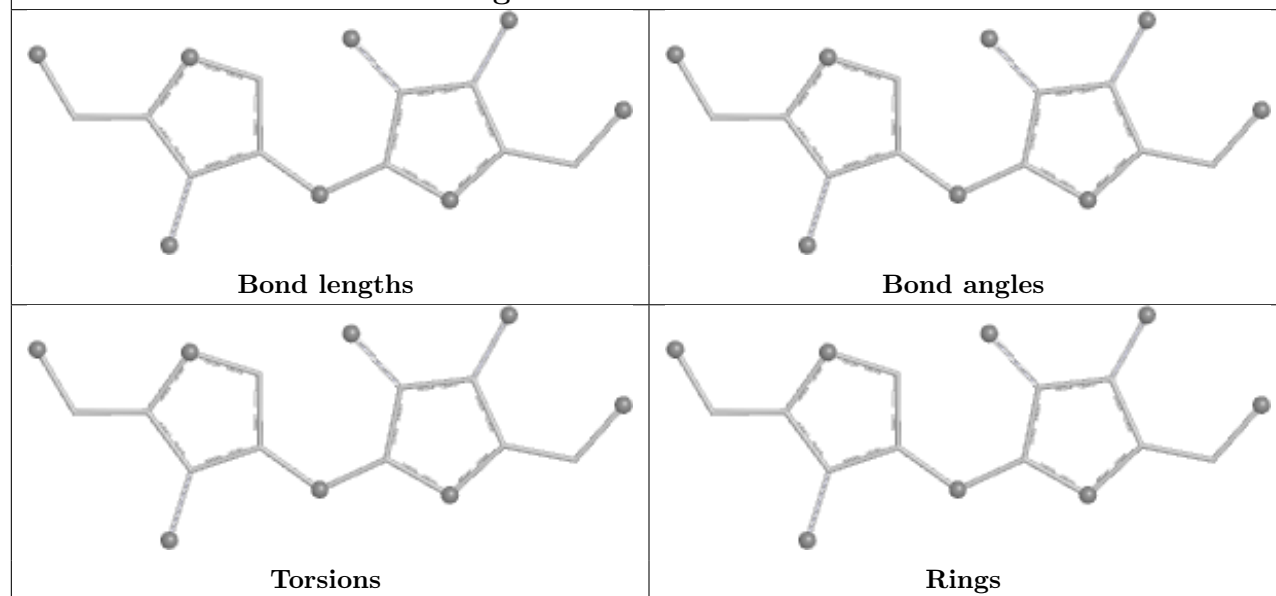


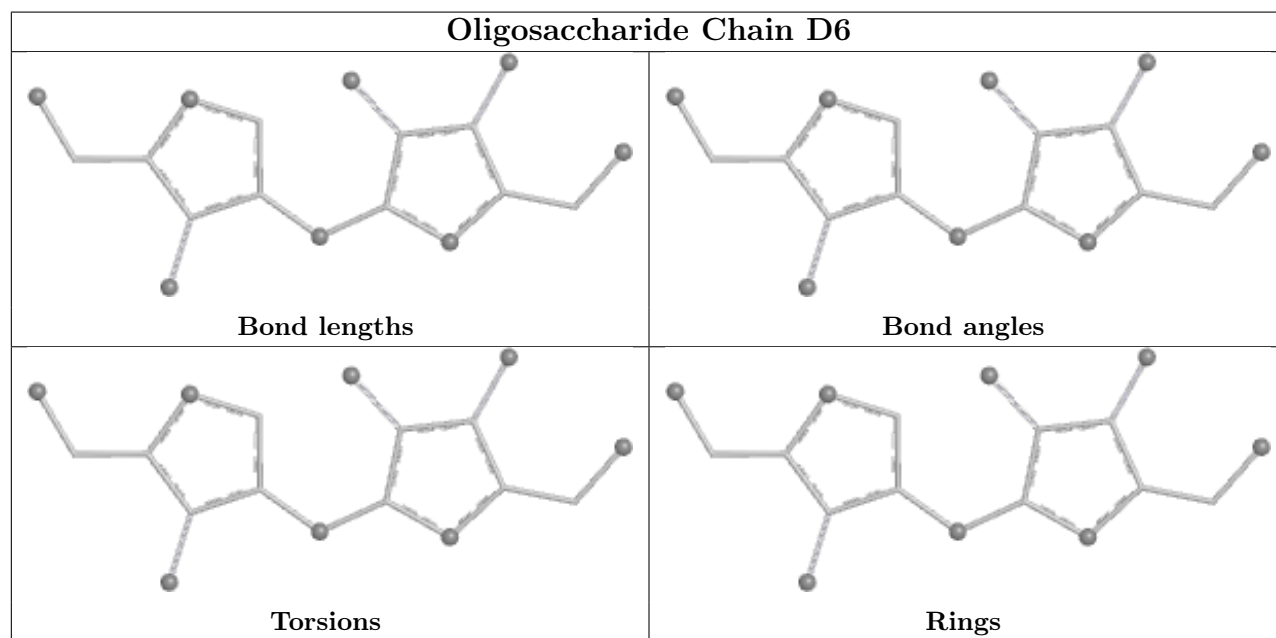
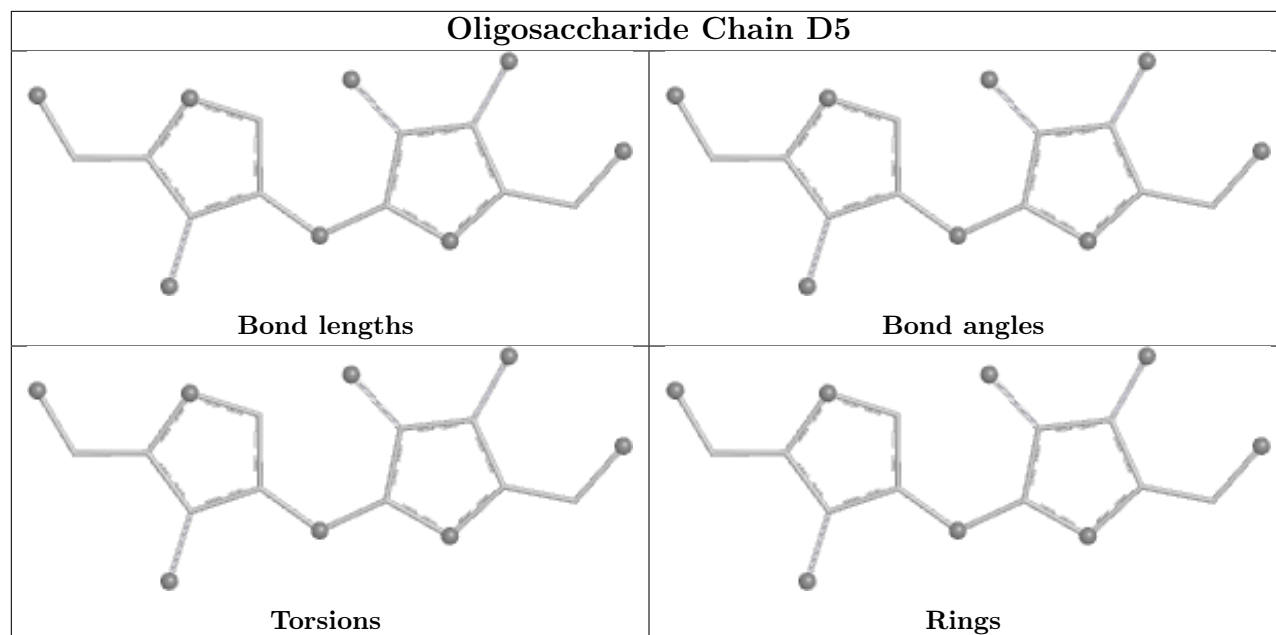




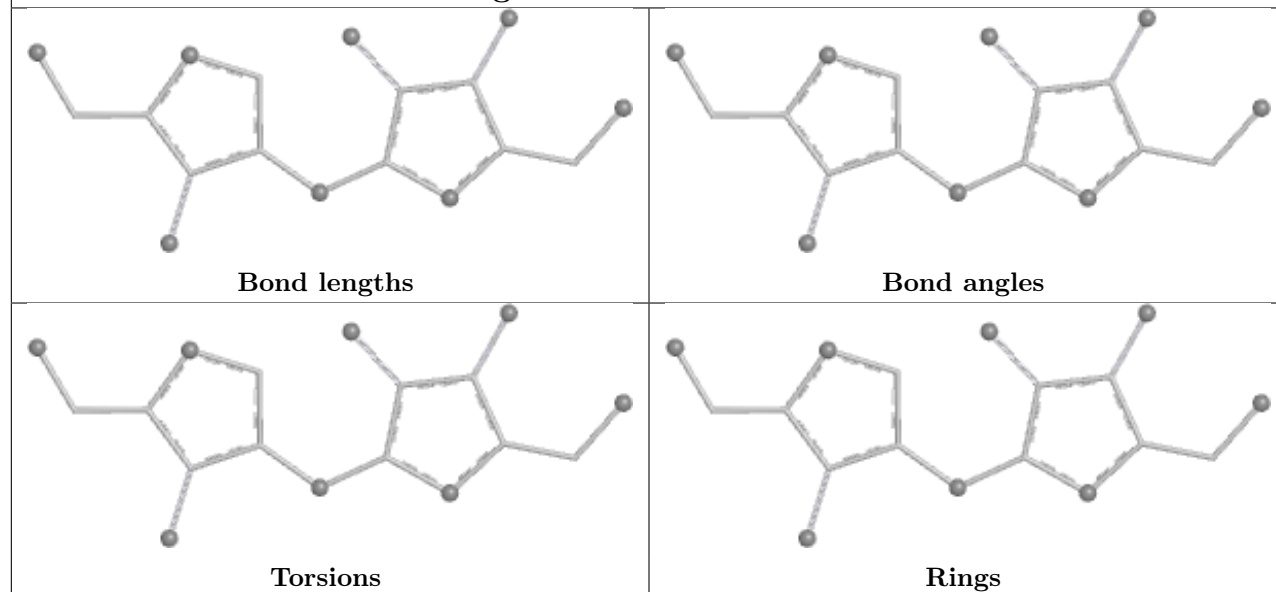




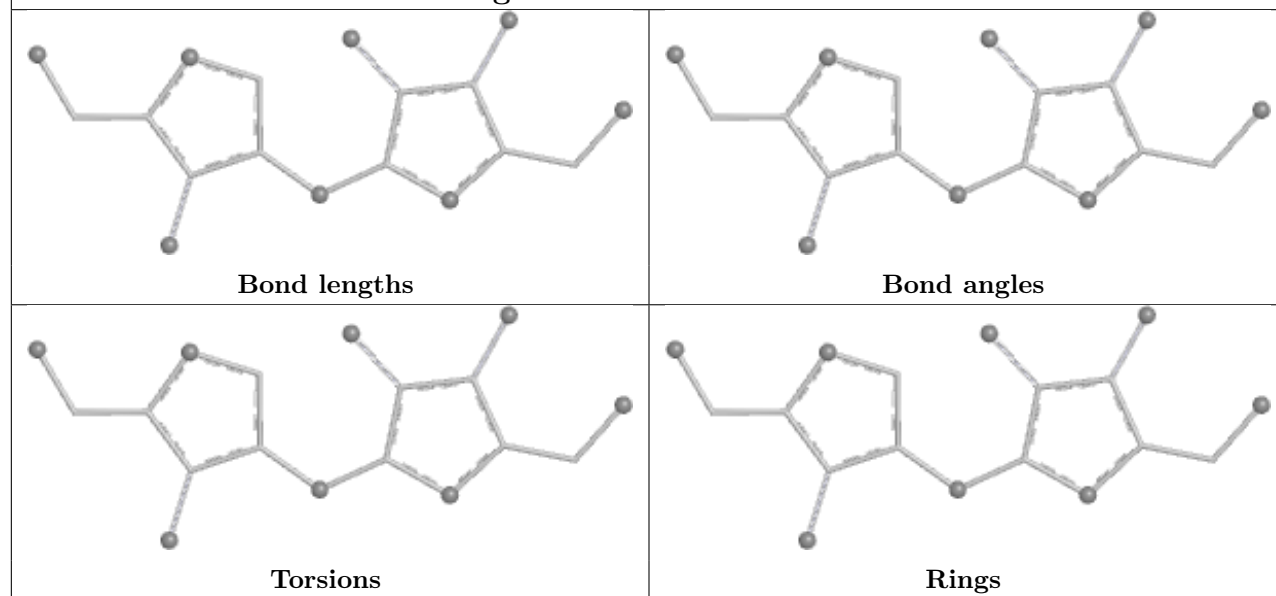
Oligosaccharide Chain D3**Oligosaccharide Chain D4**

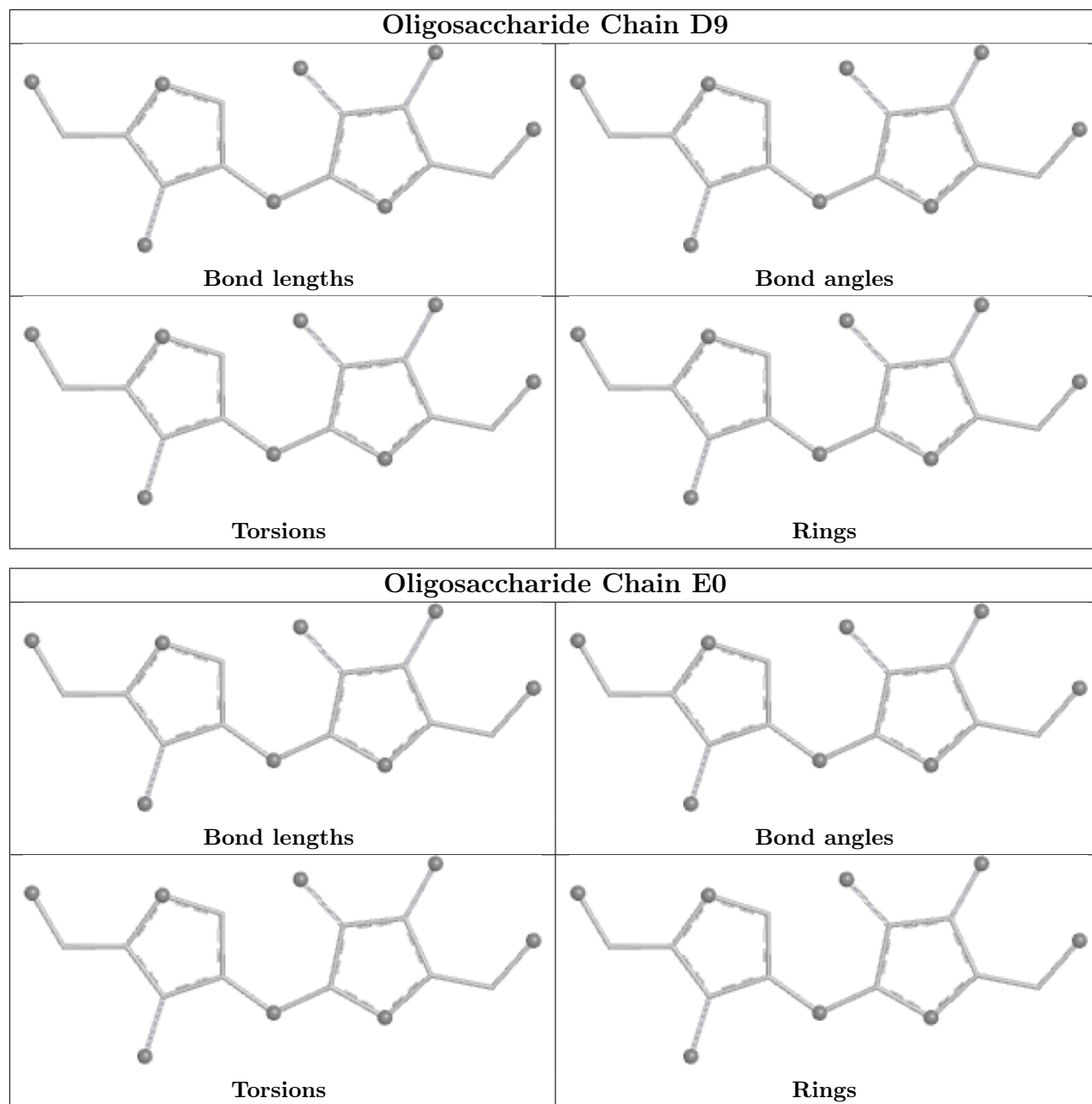


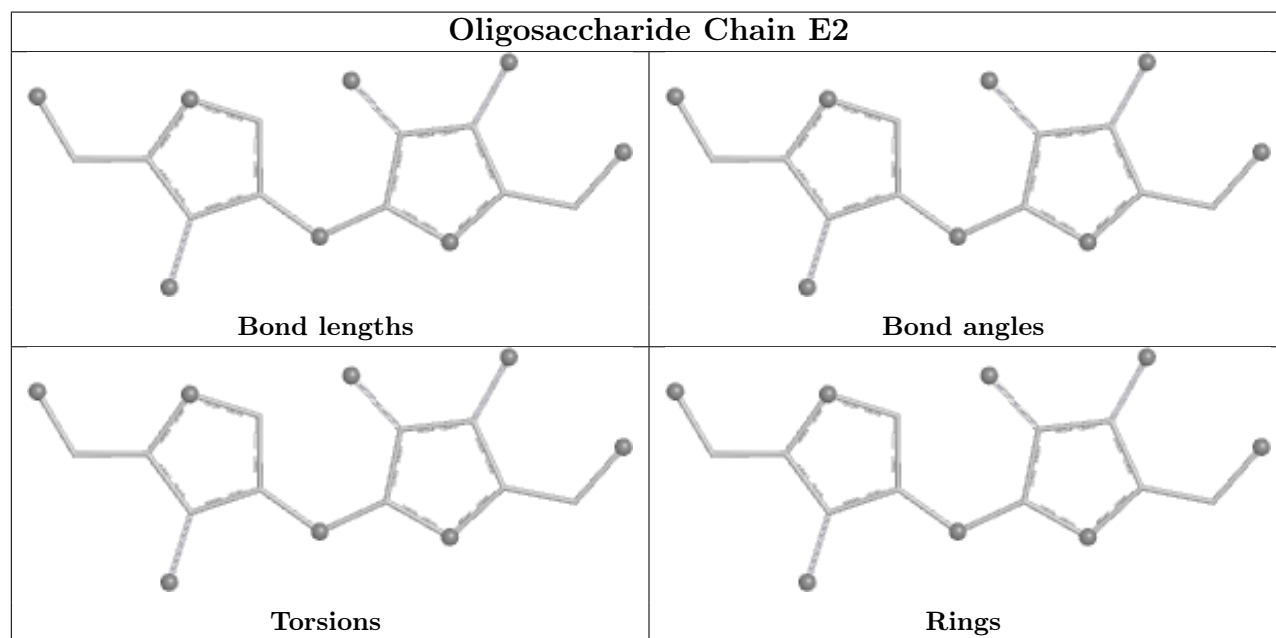
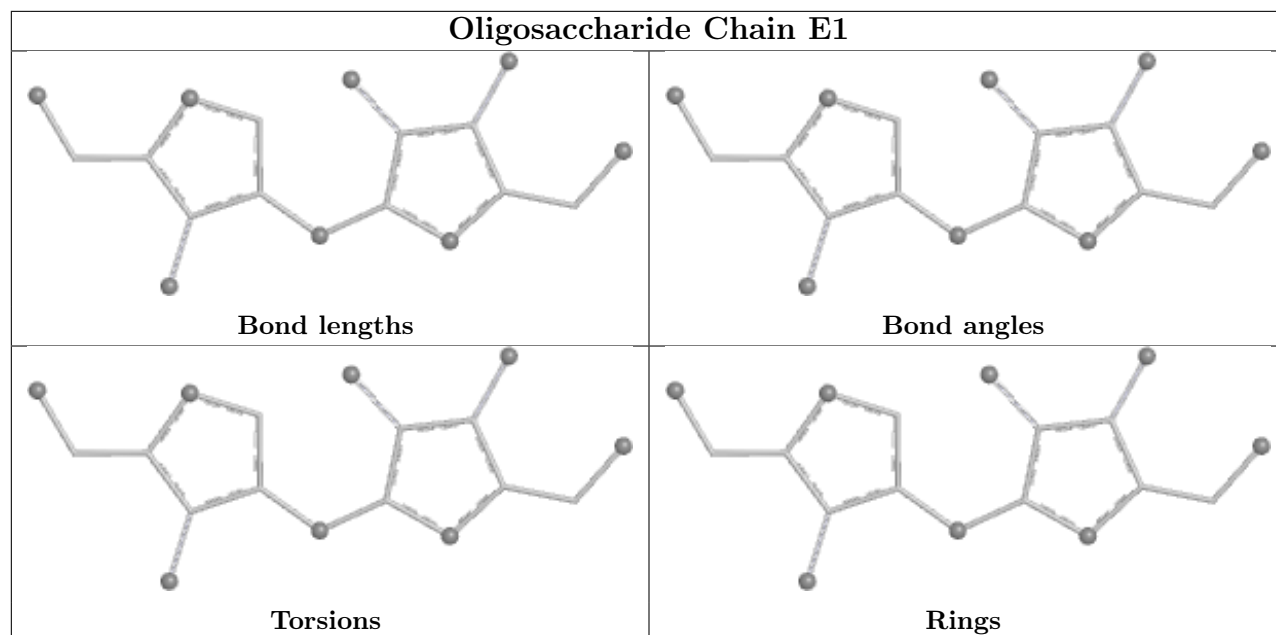
Oligosaccharide Chain D7

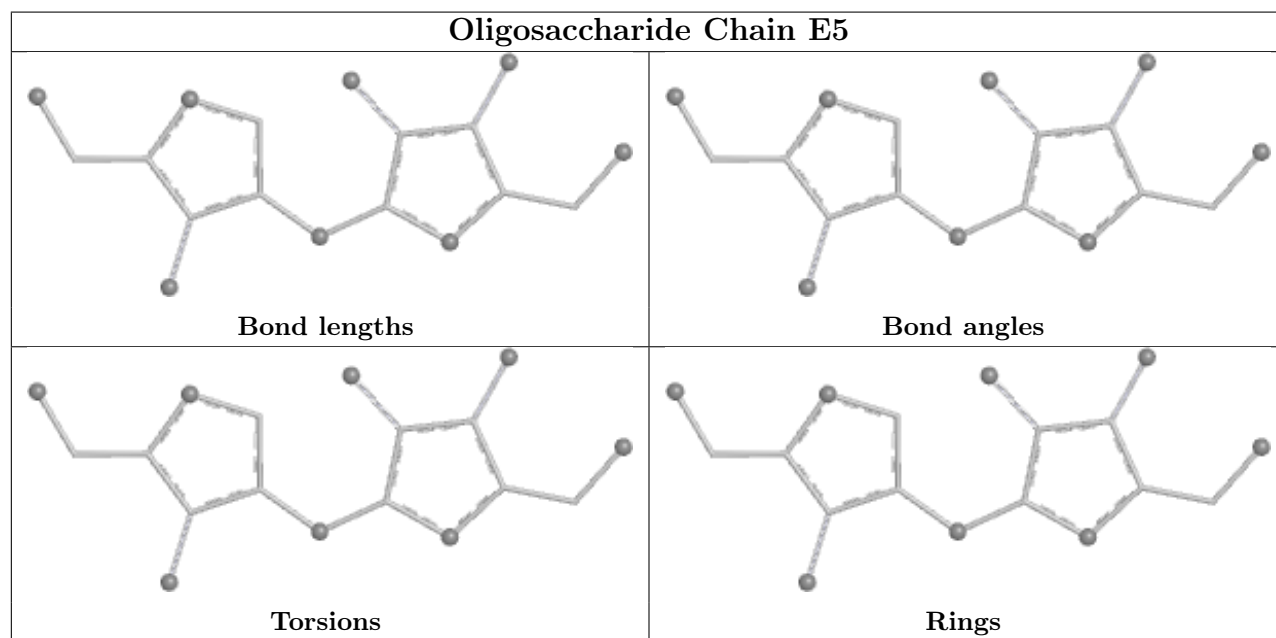
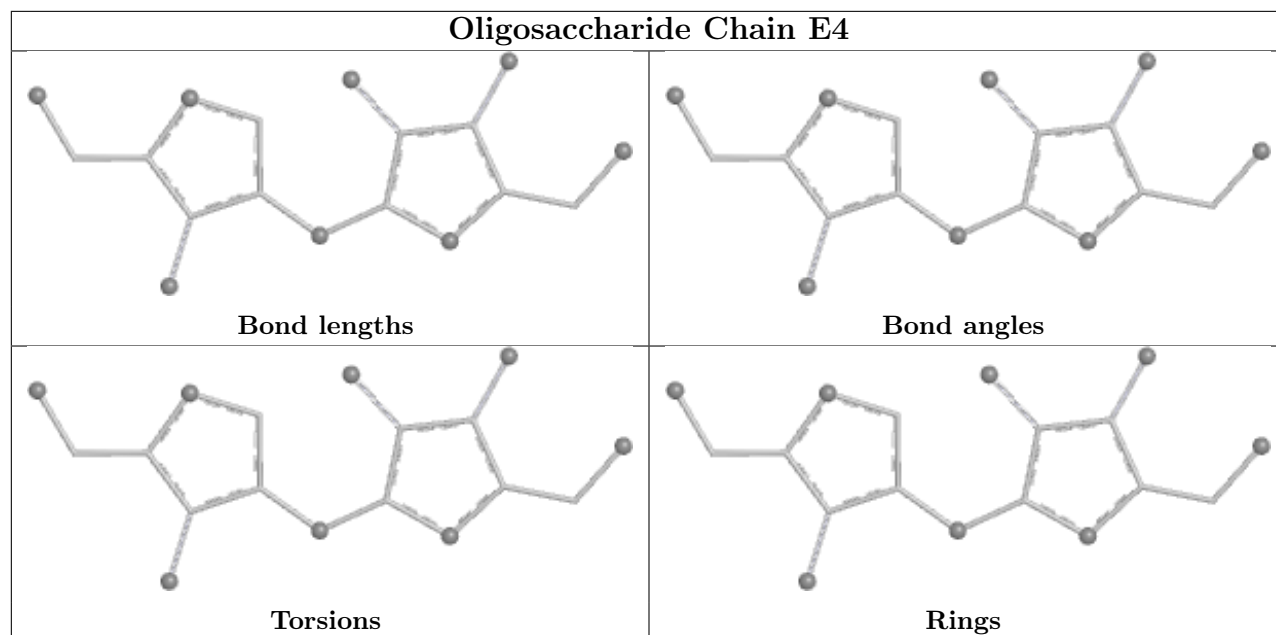


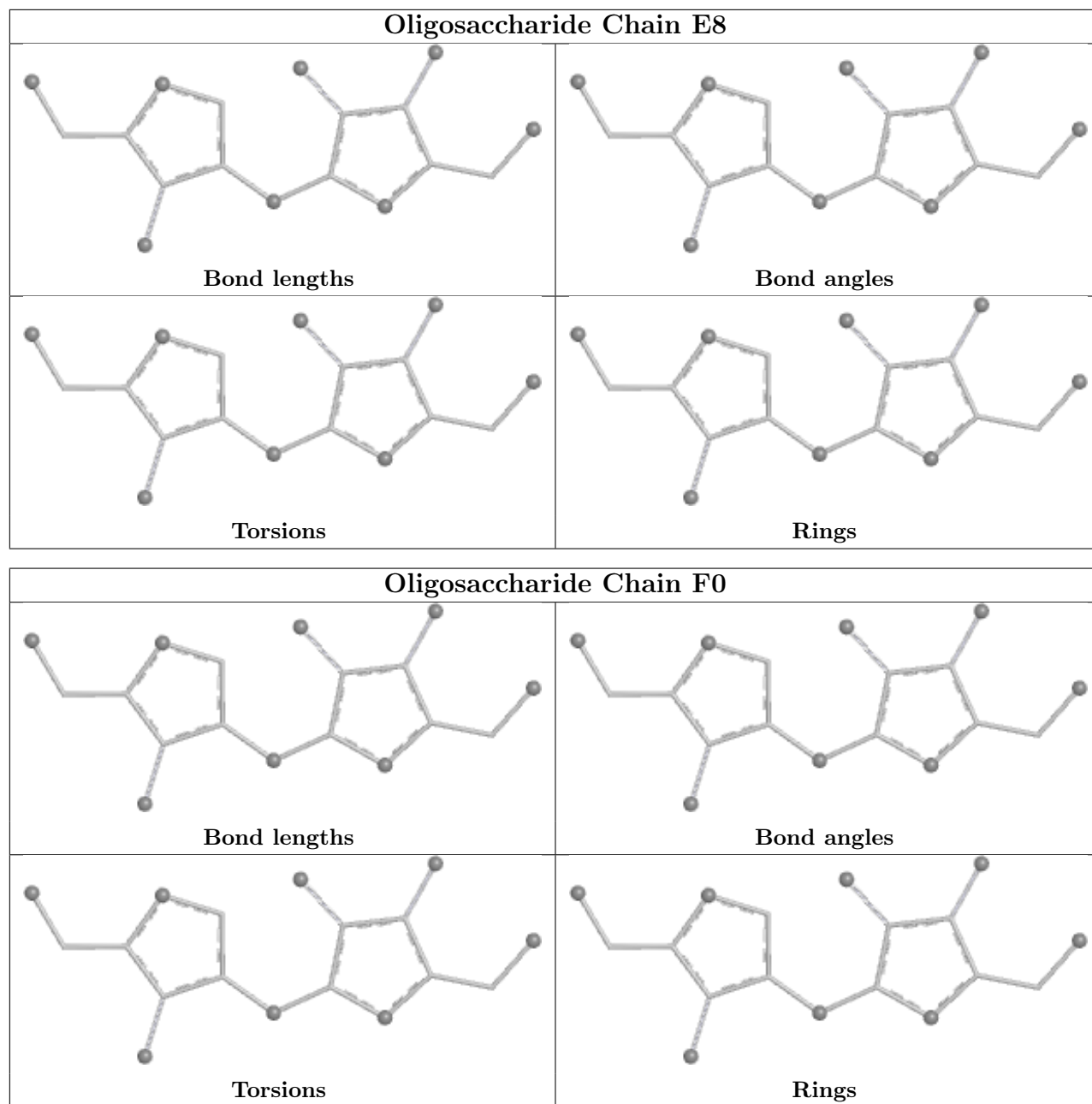
Oligosaccharide Chain D8

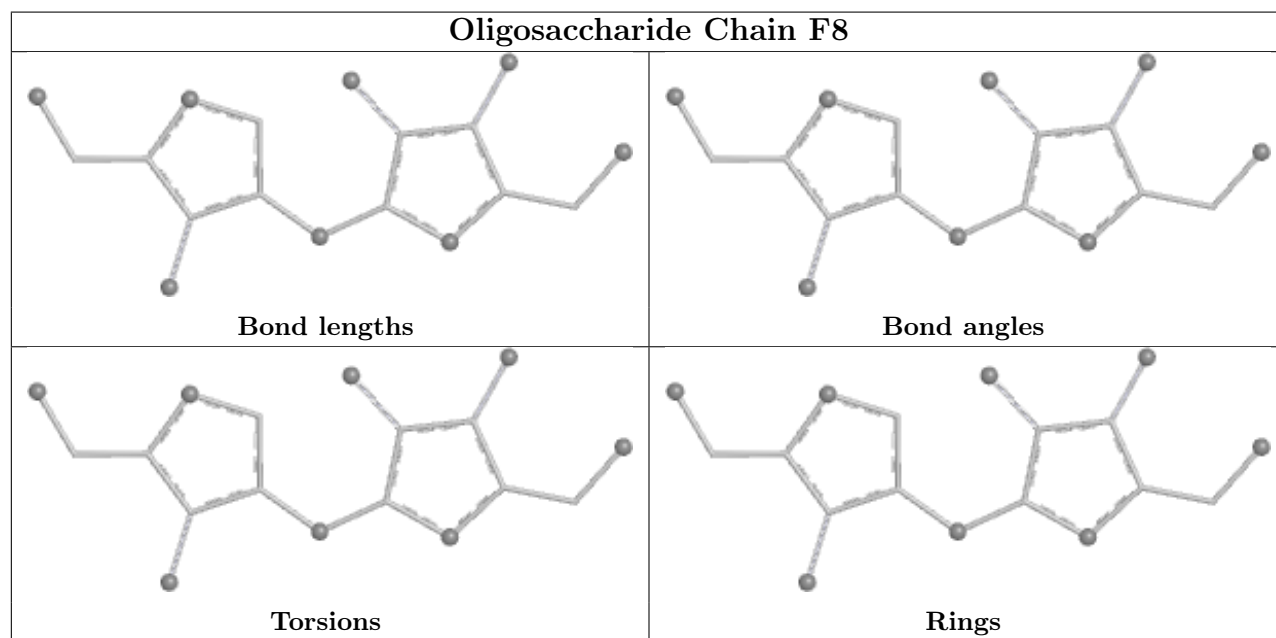
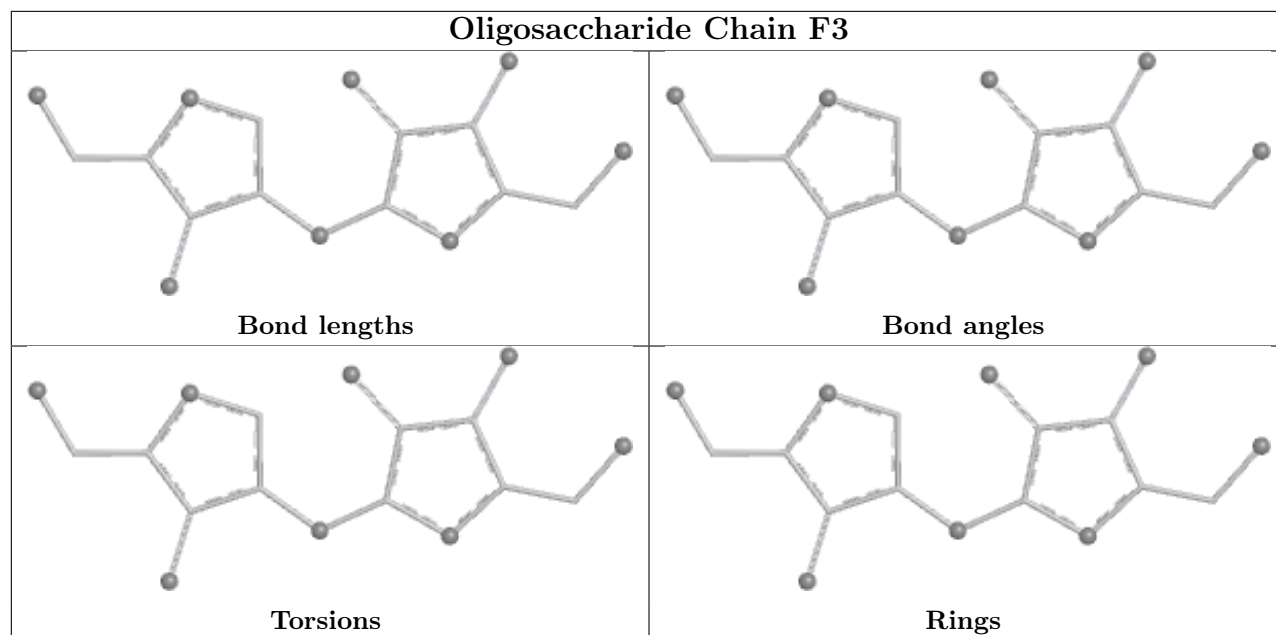


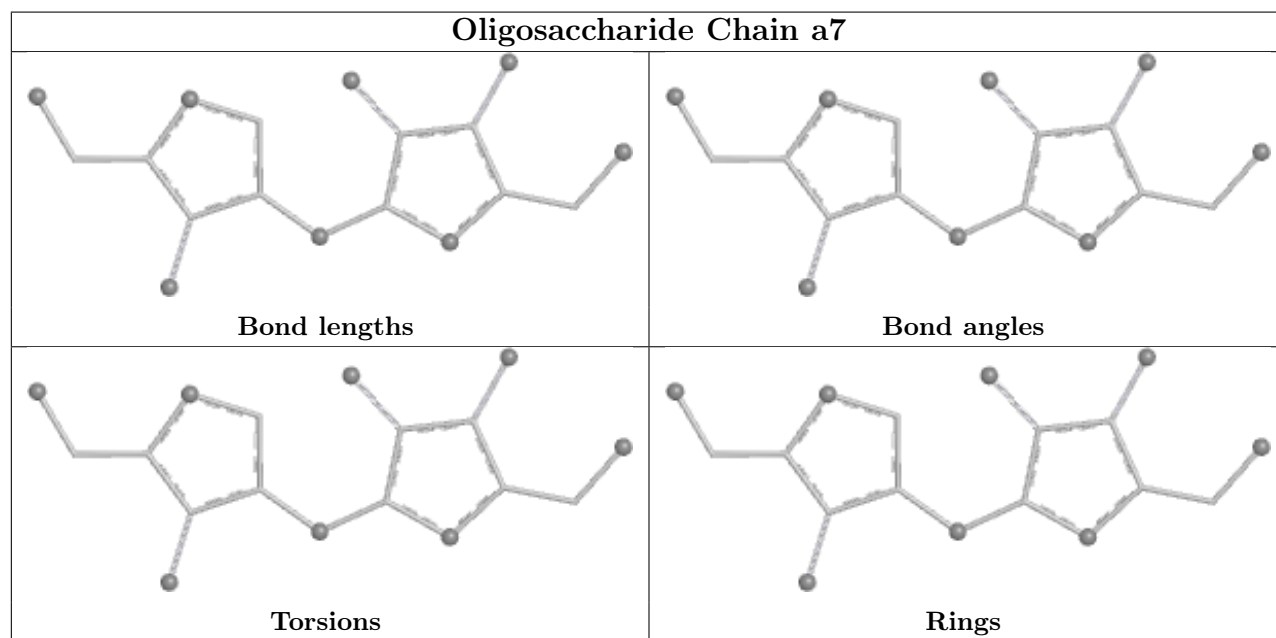
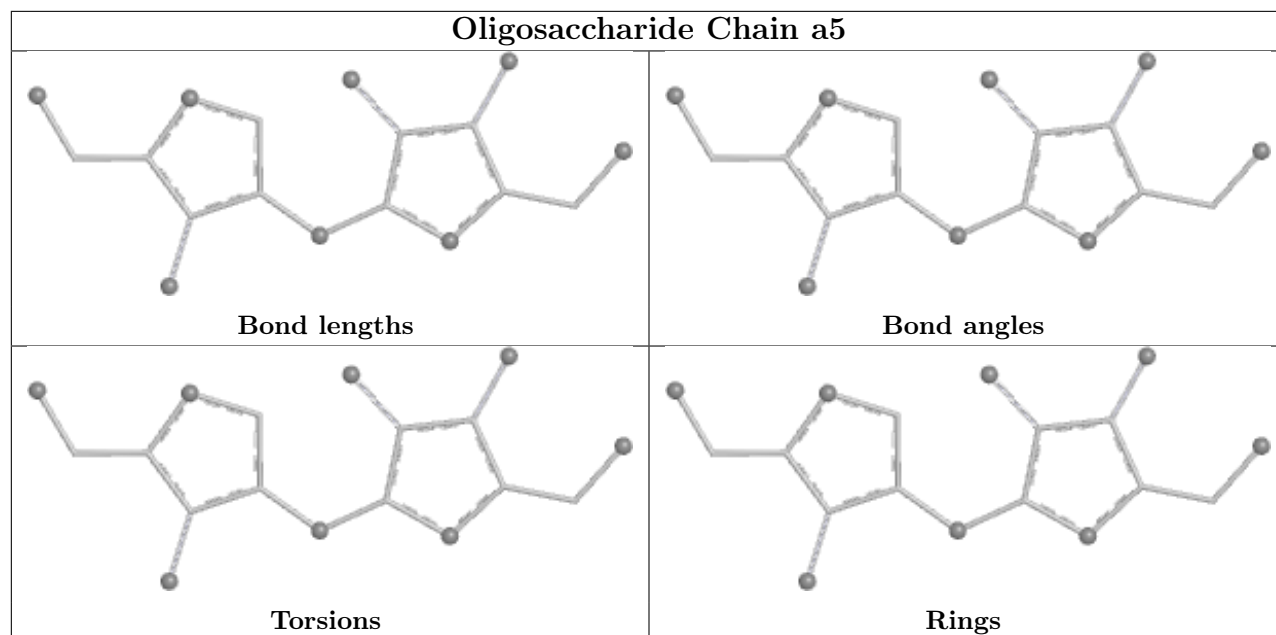


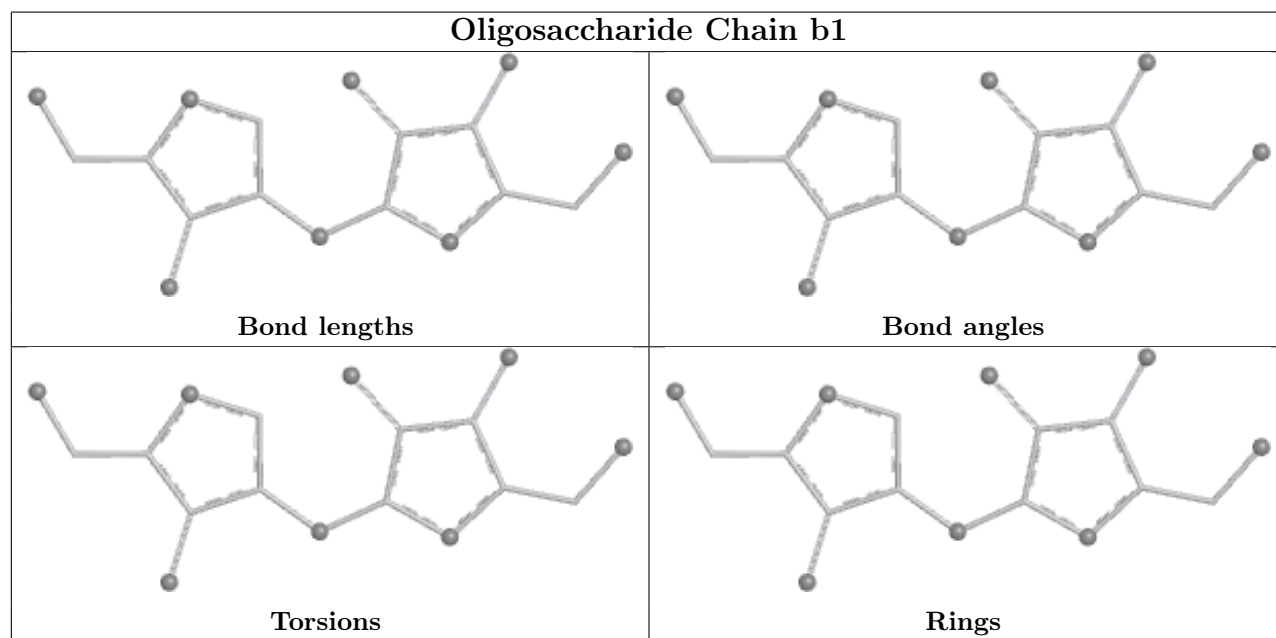
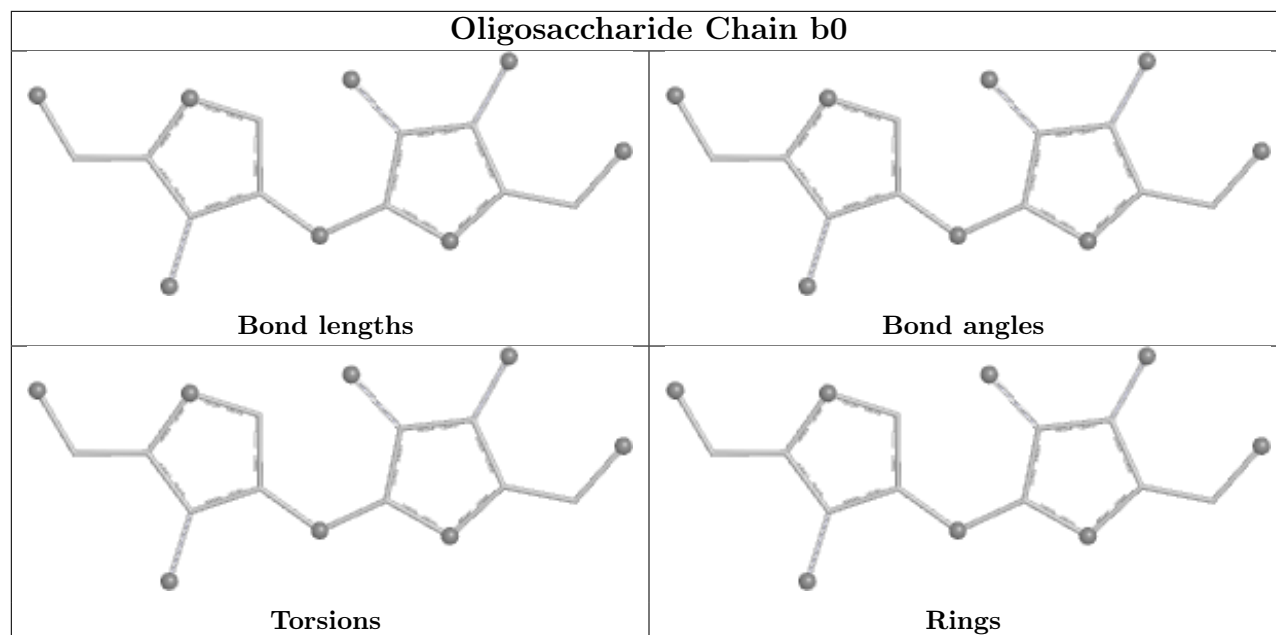


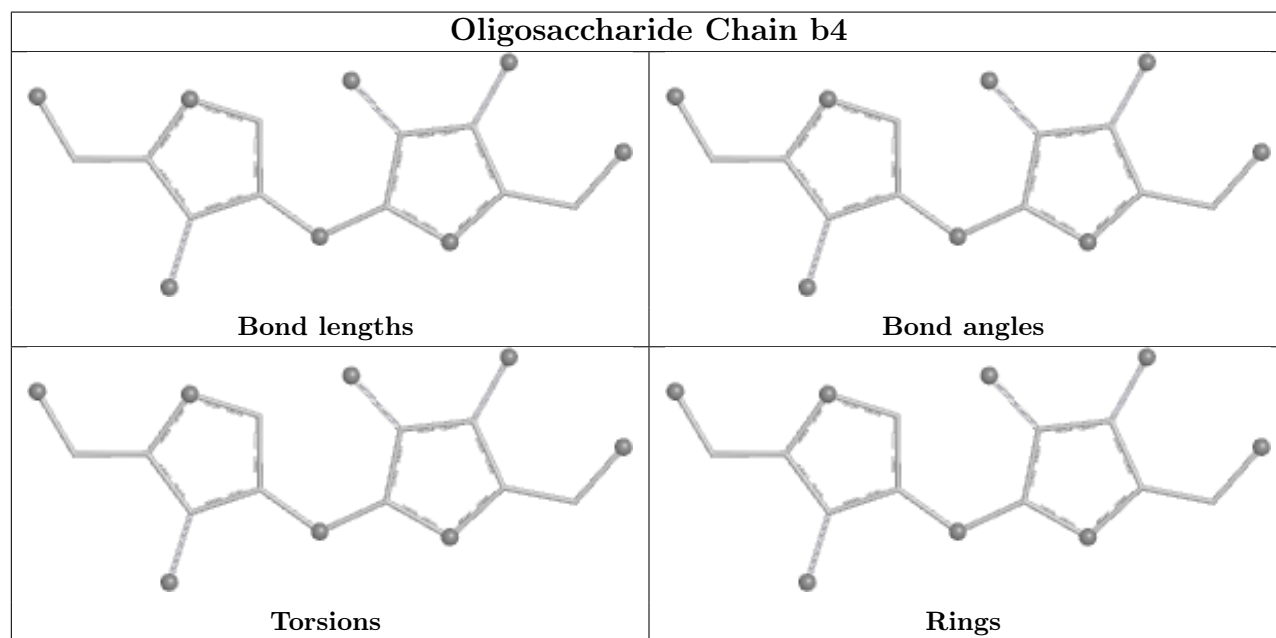
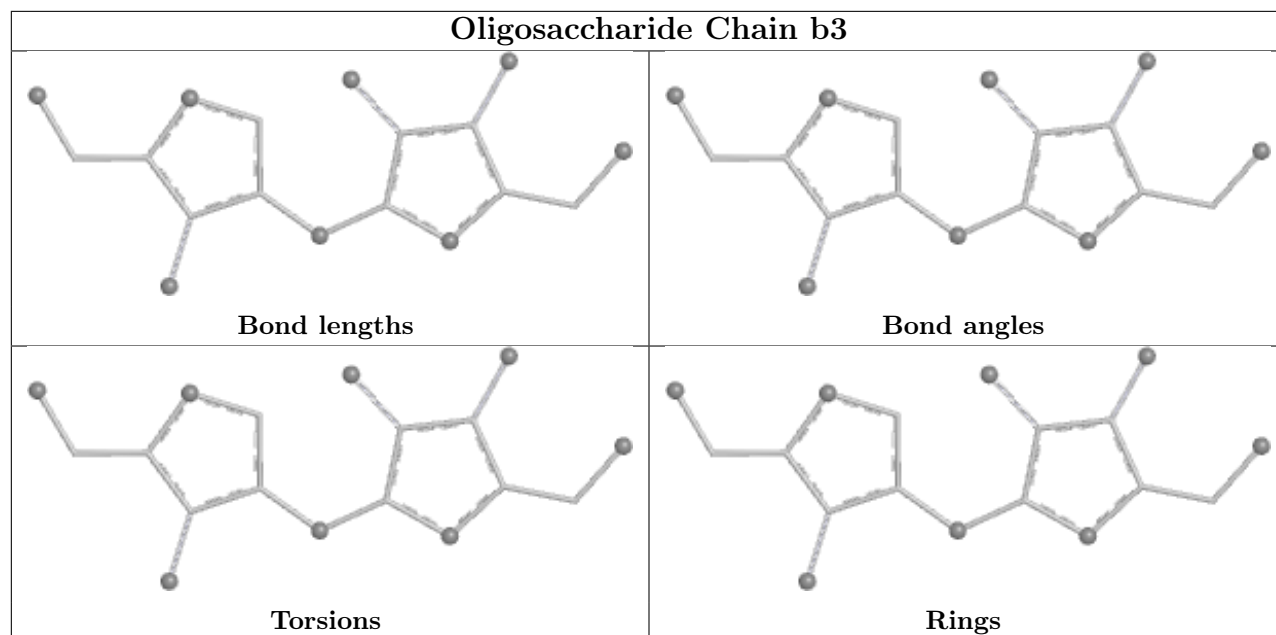


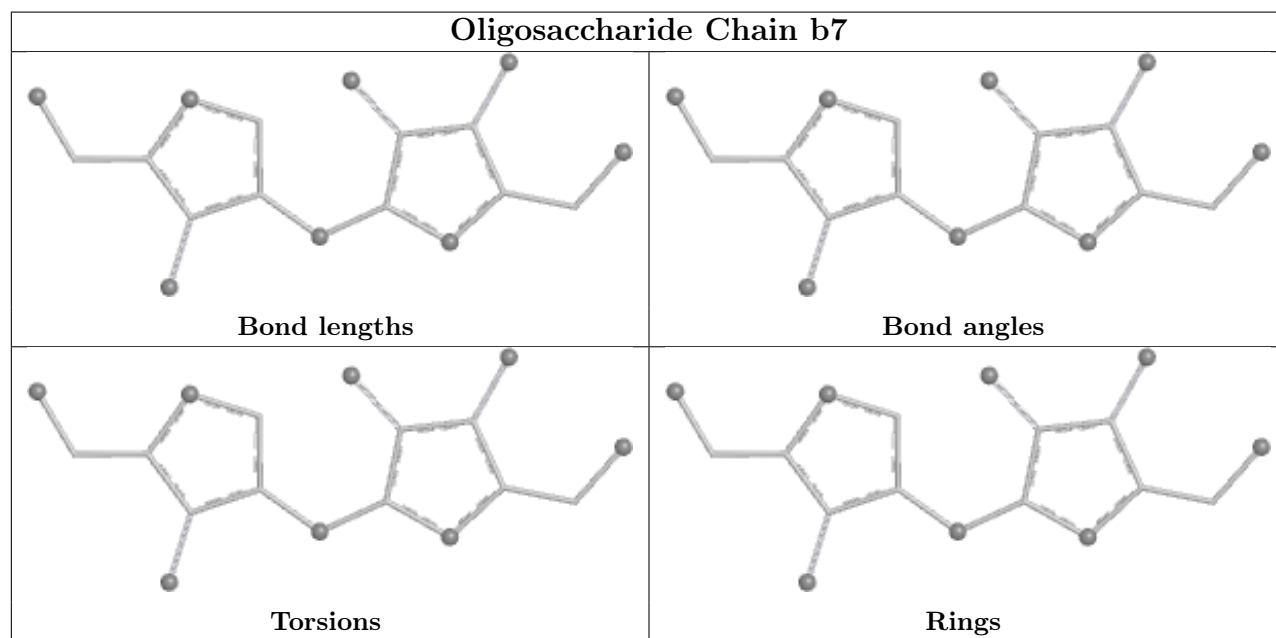
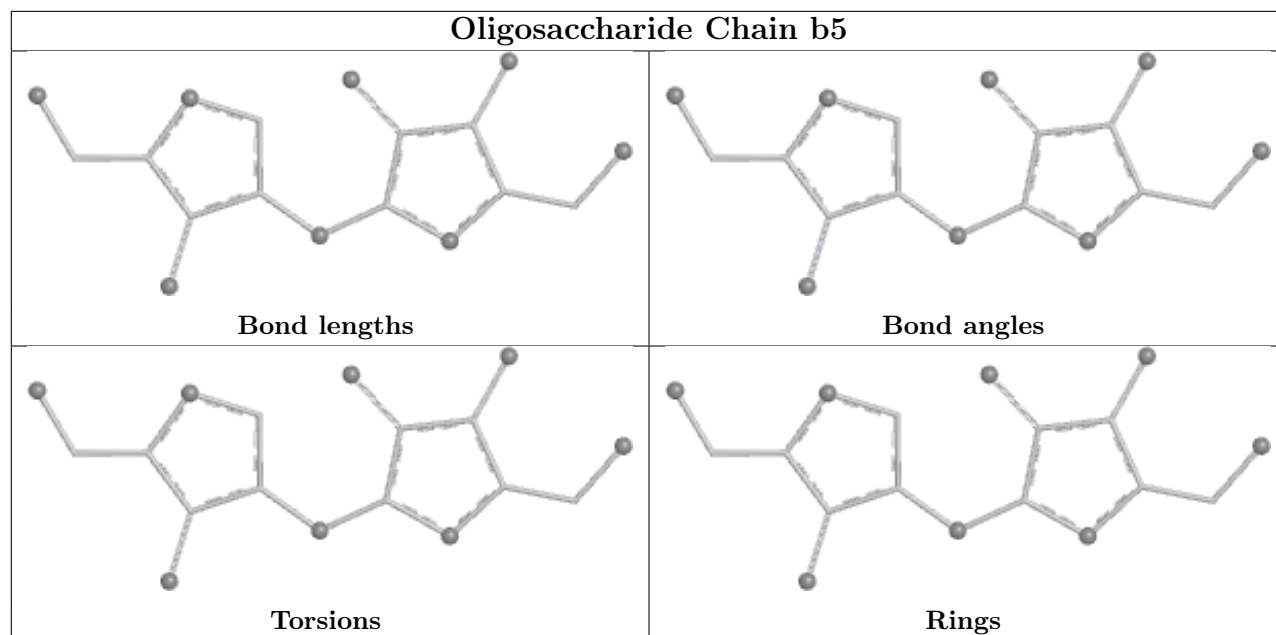


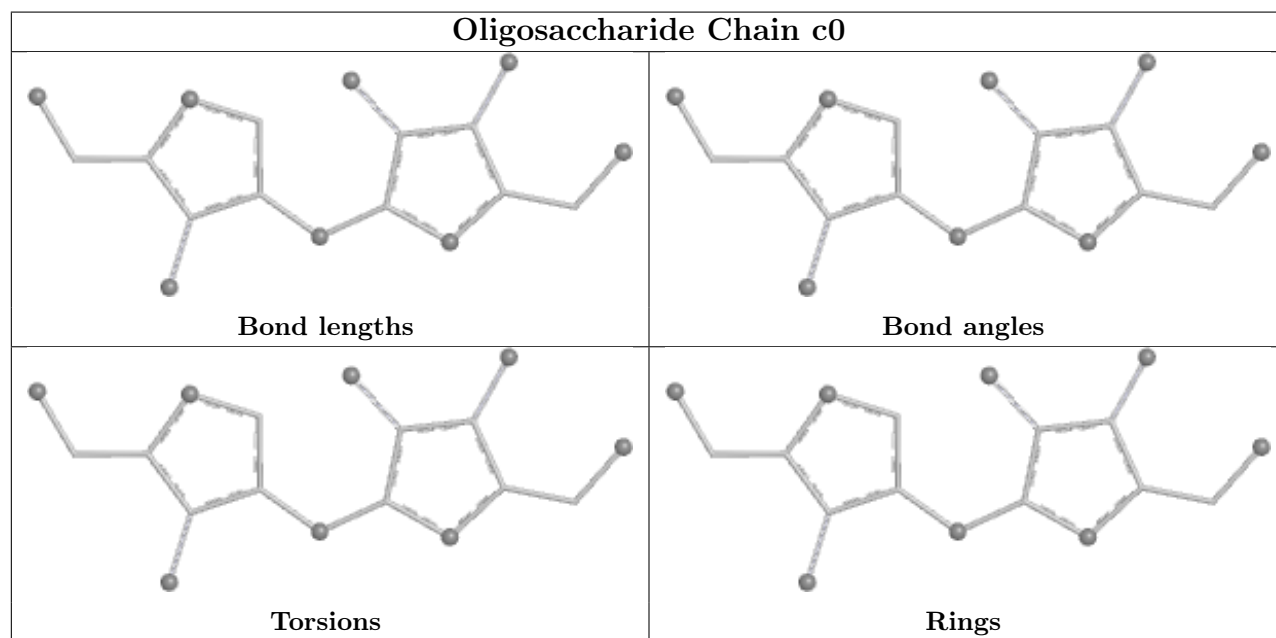
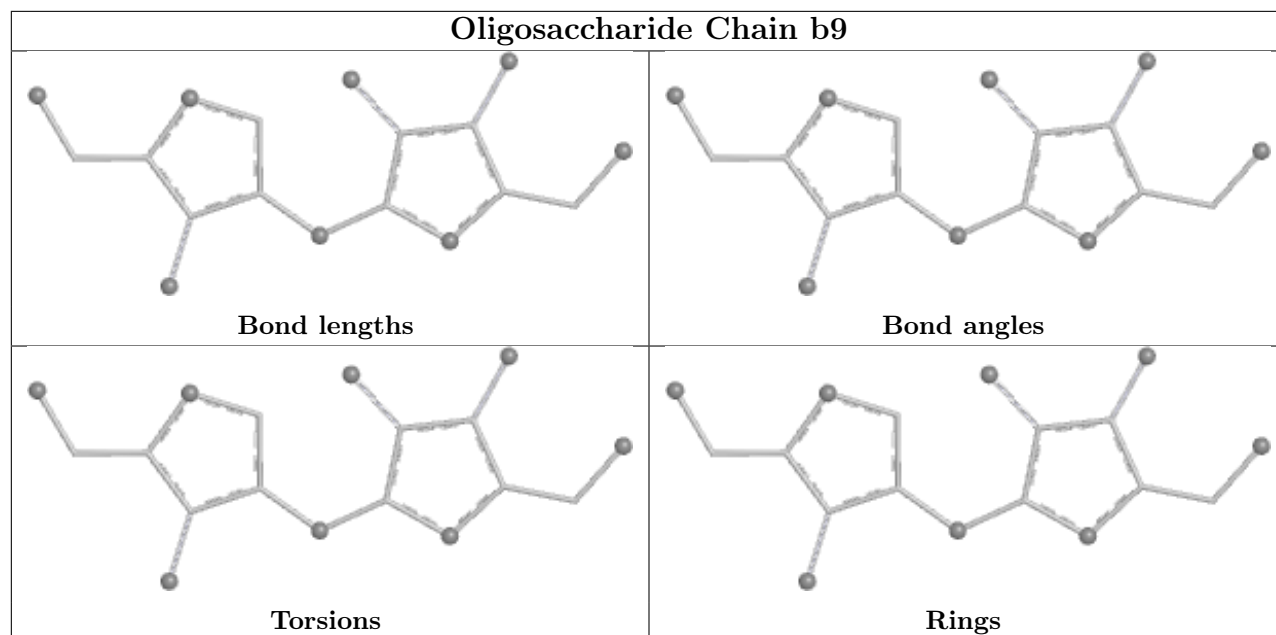


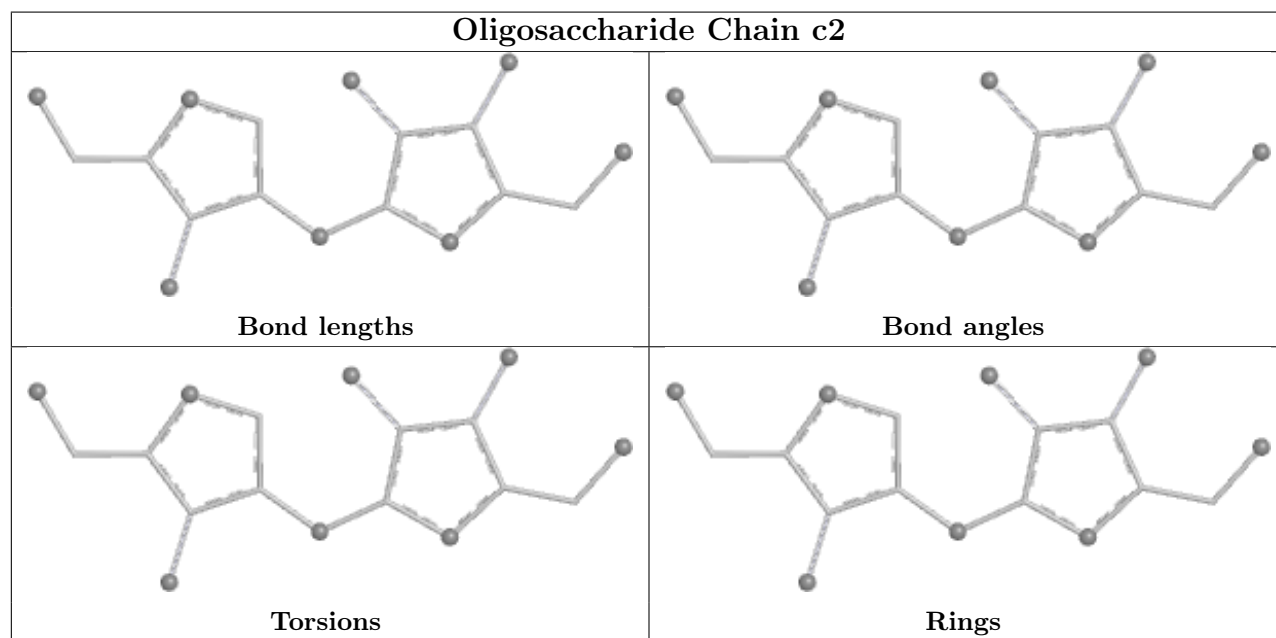
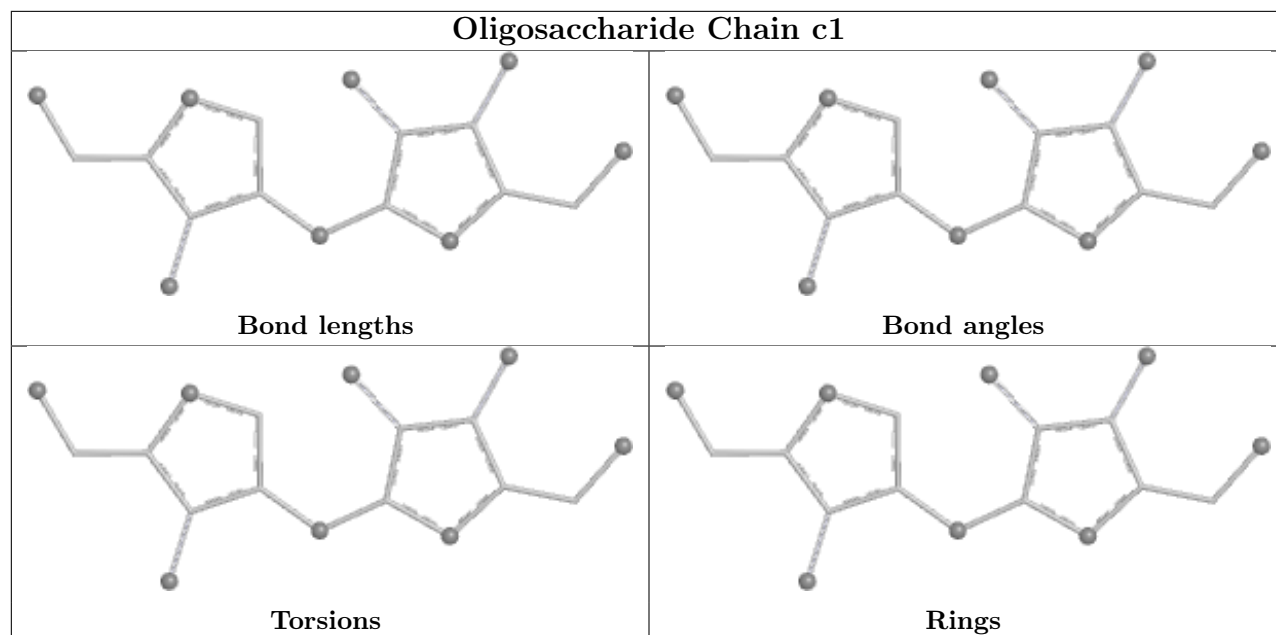


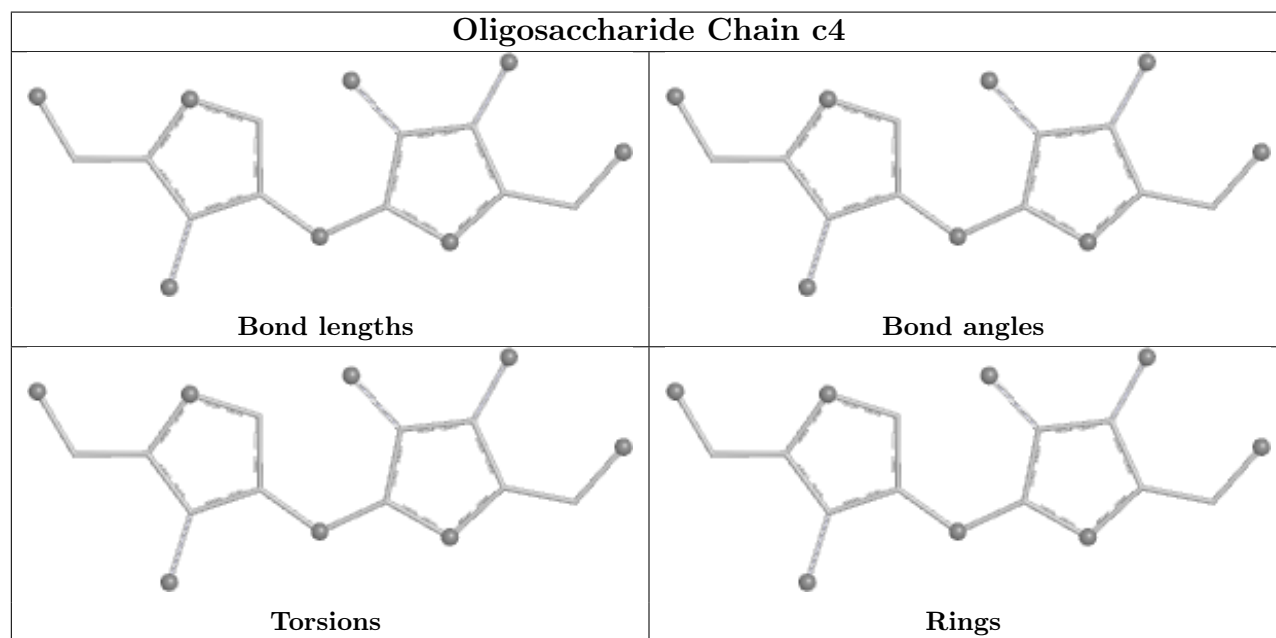
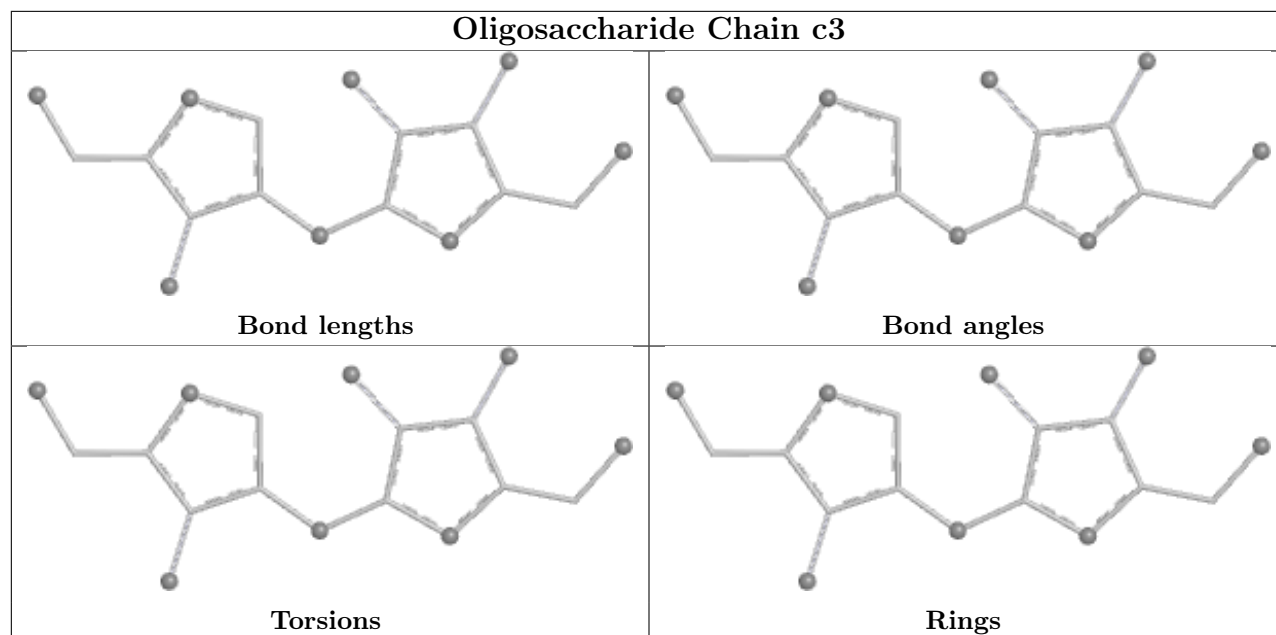


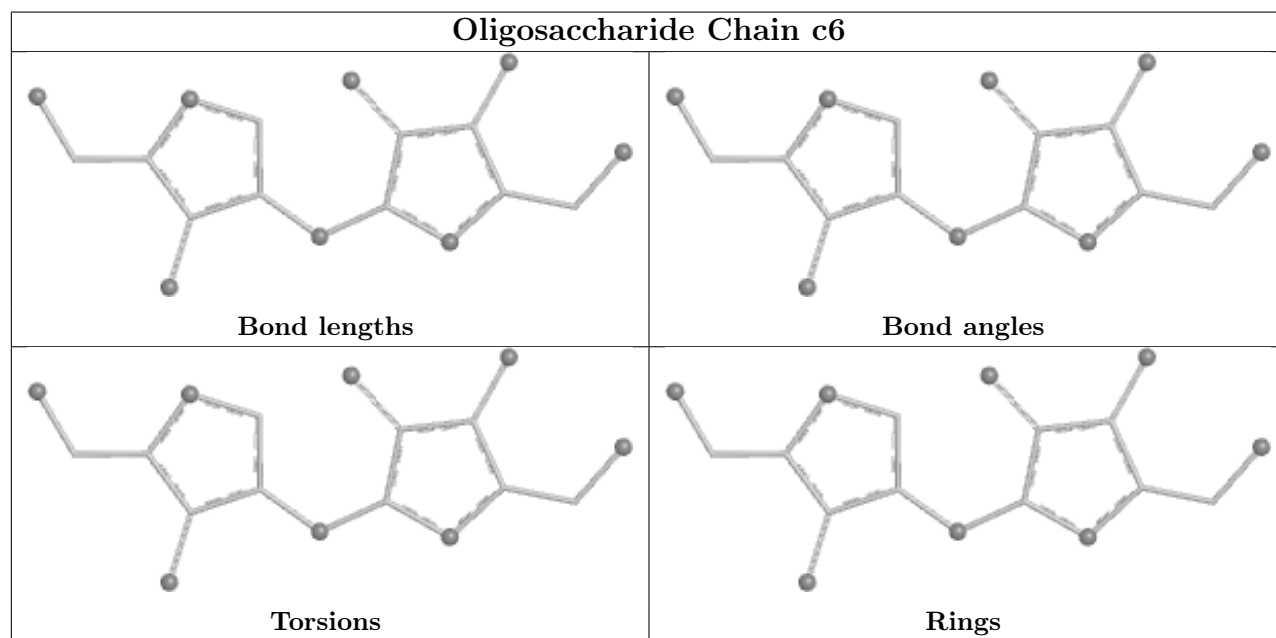
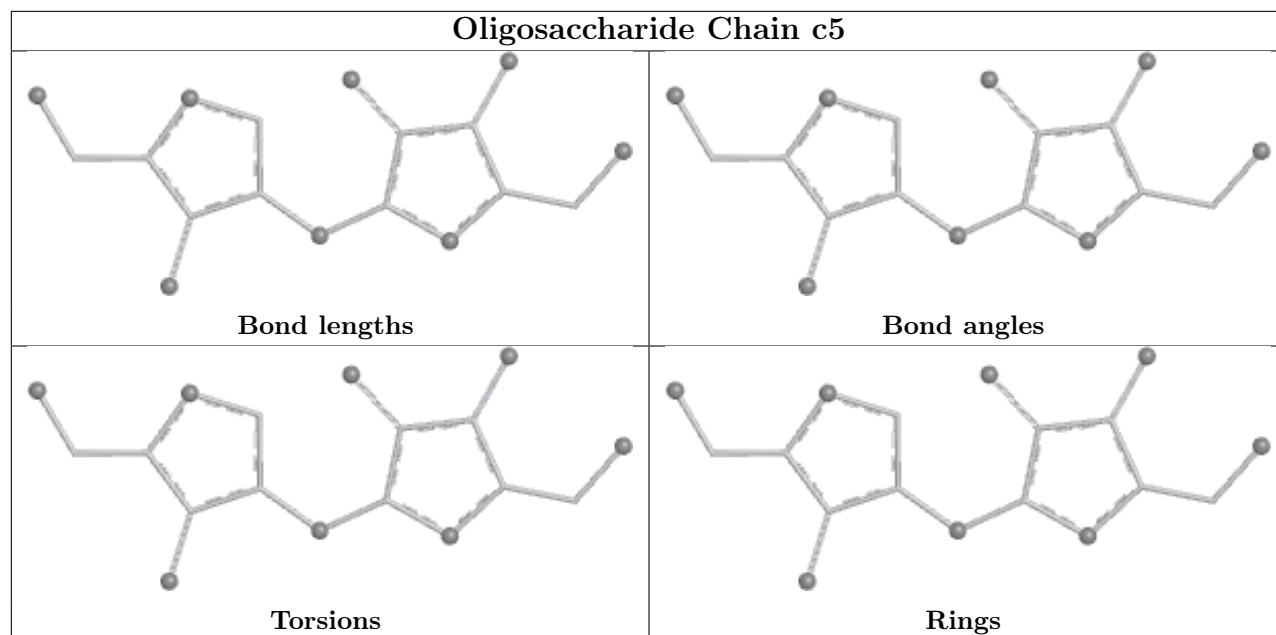


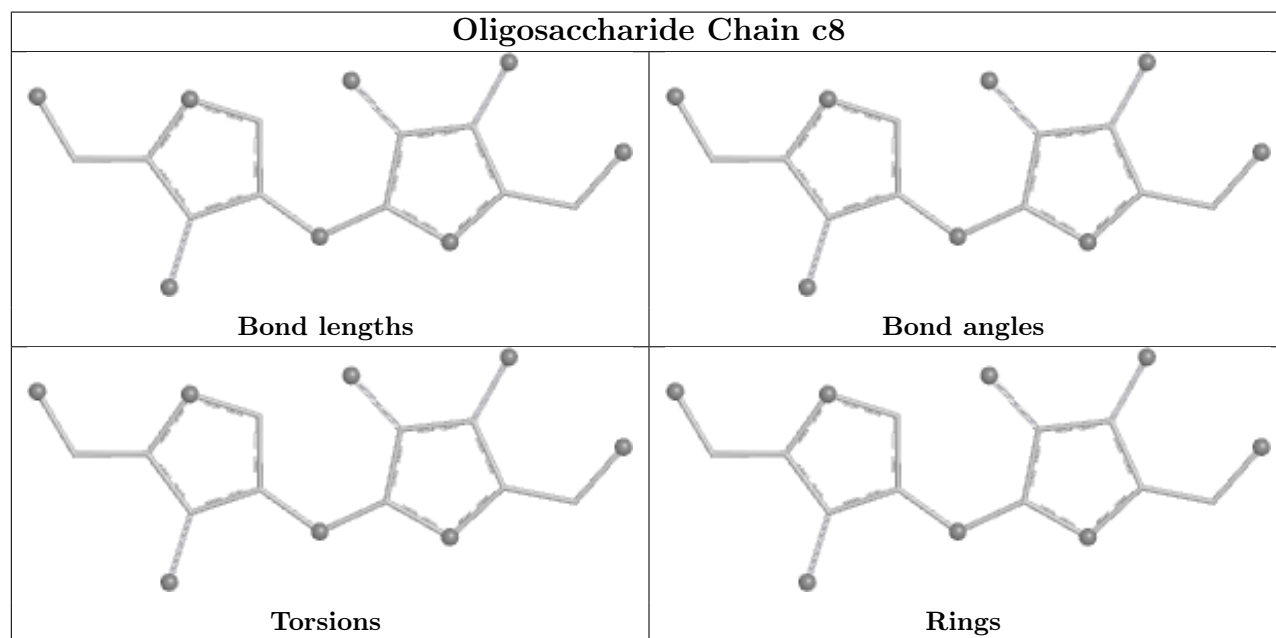
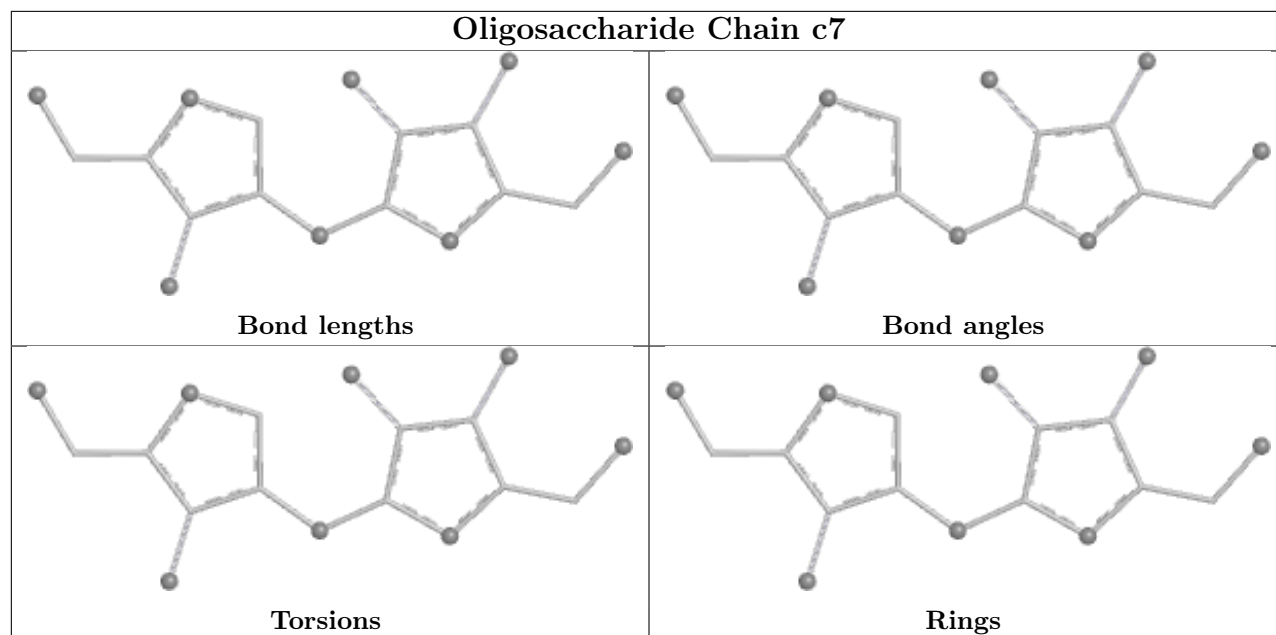


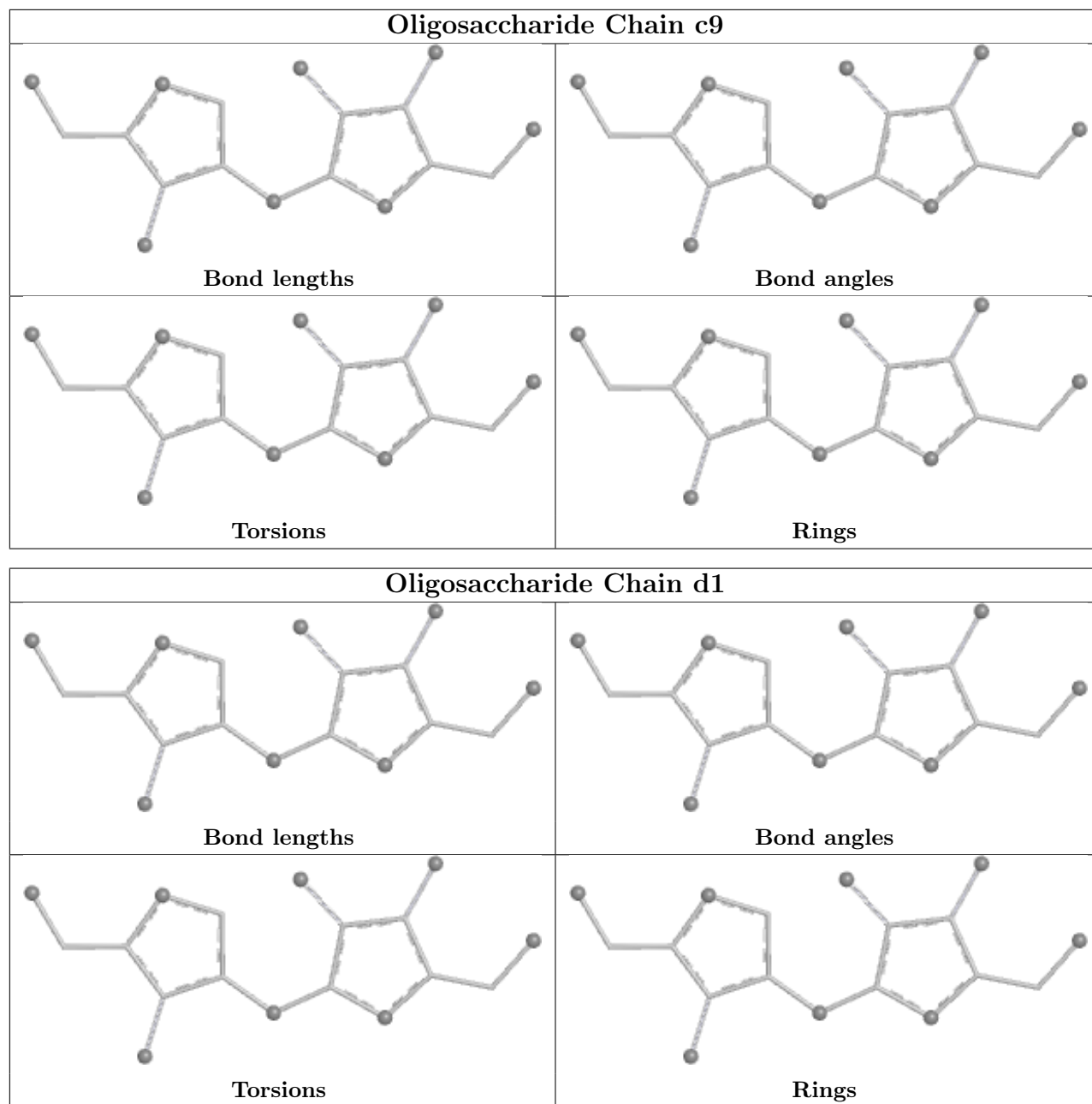


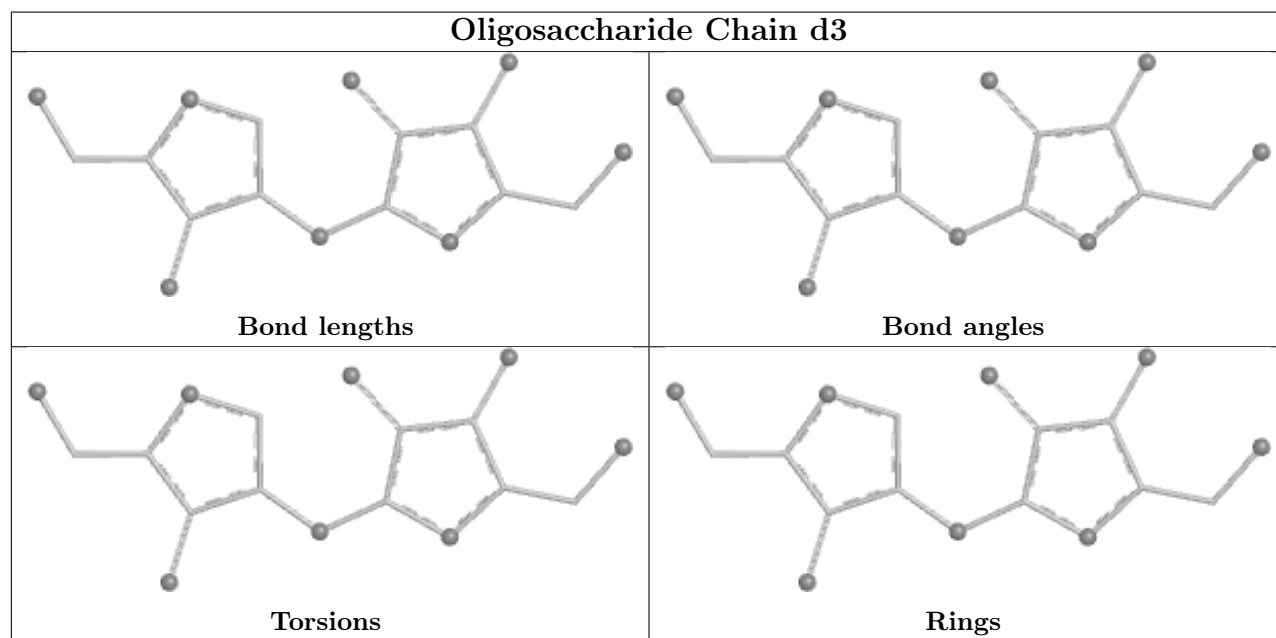
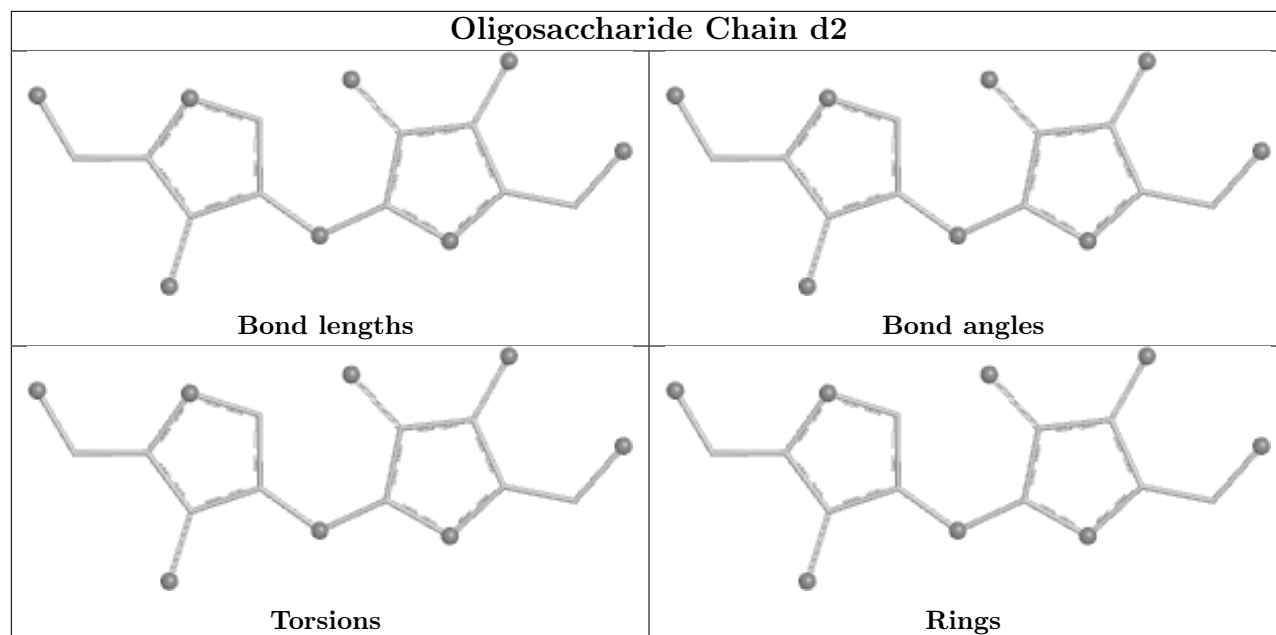


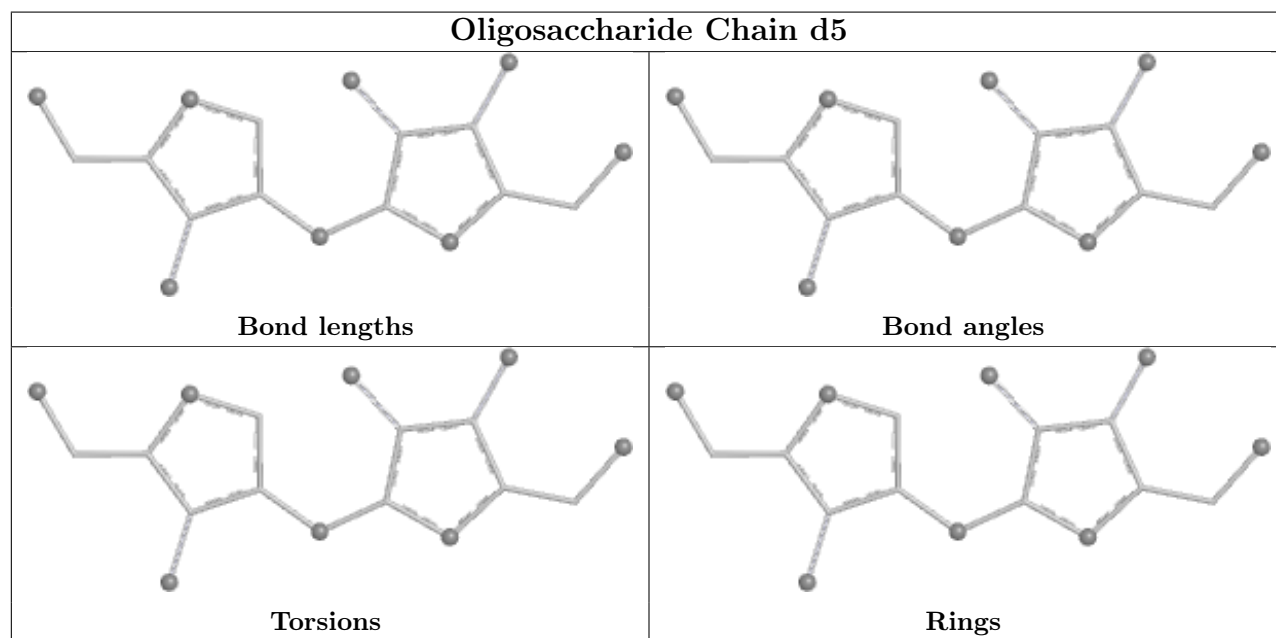
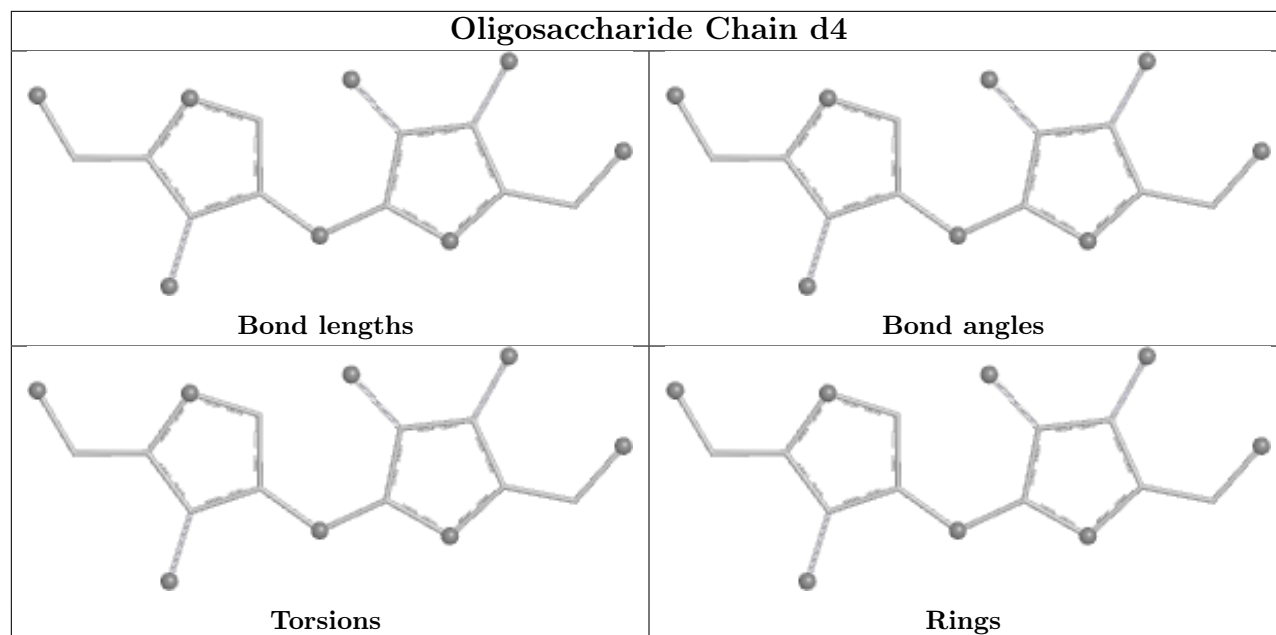


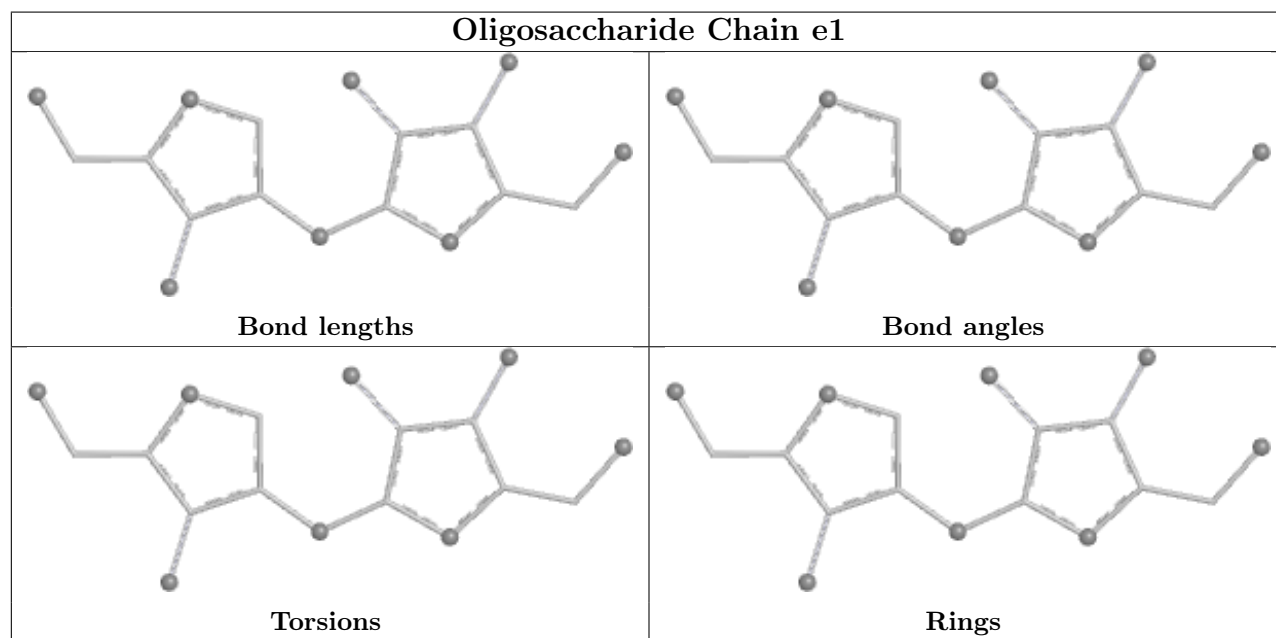
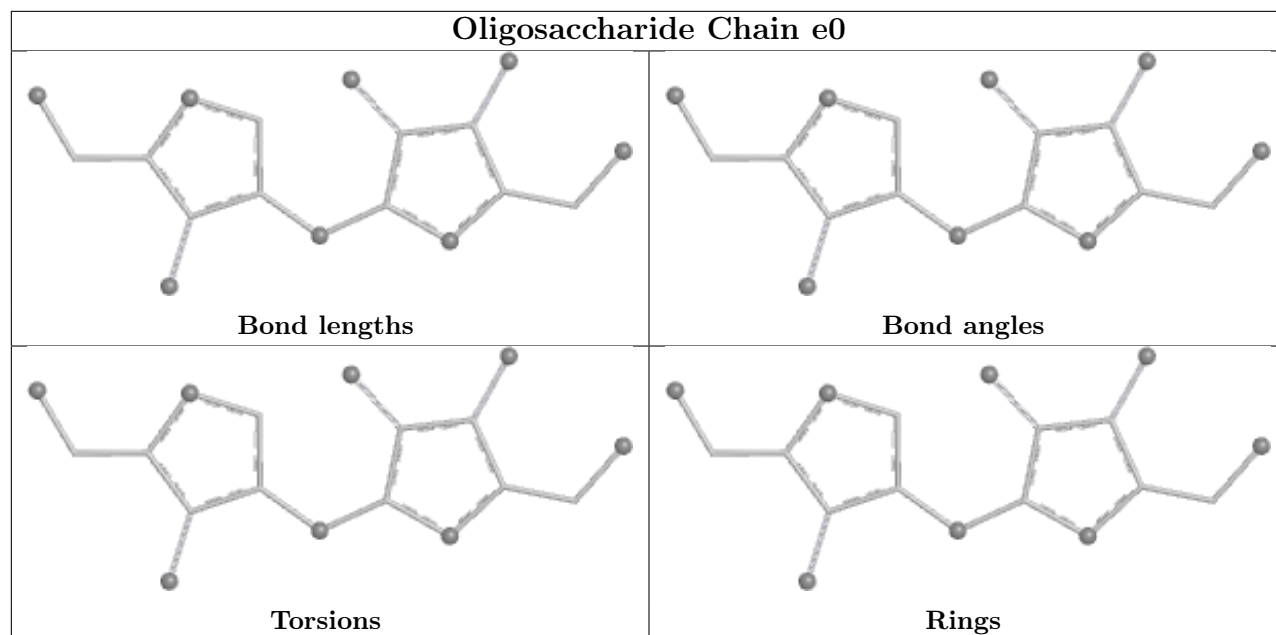


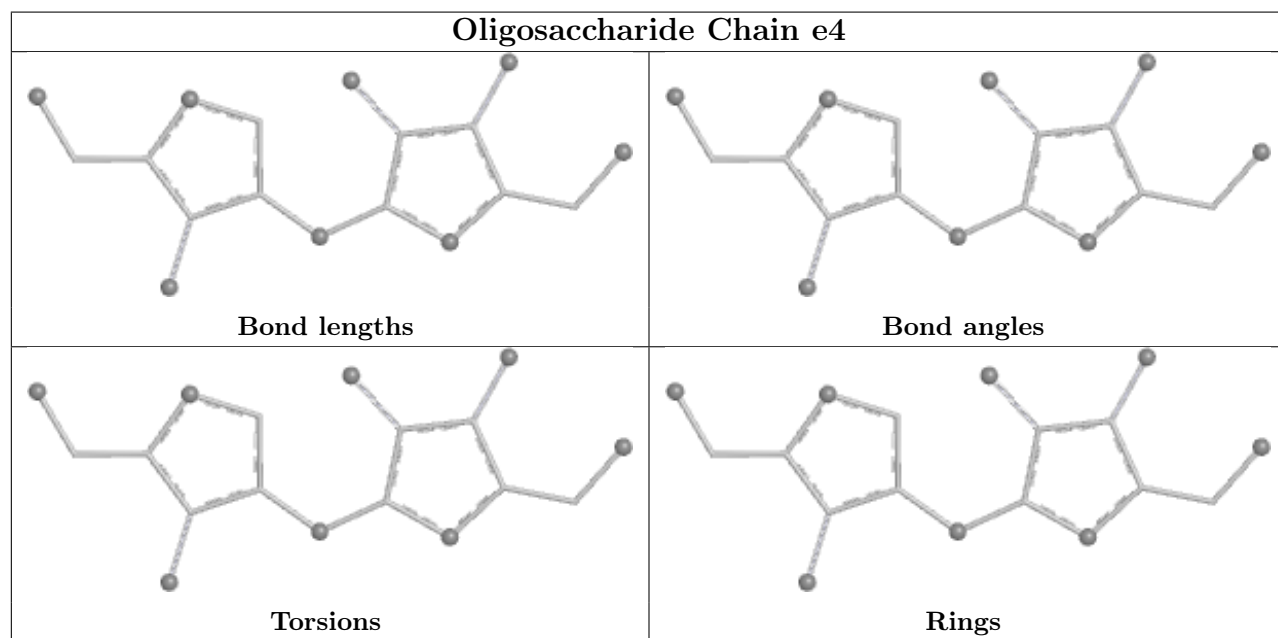
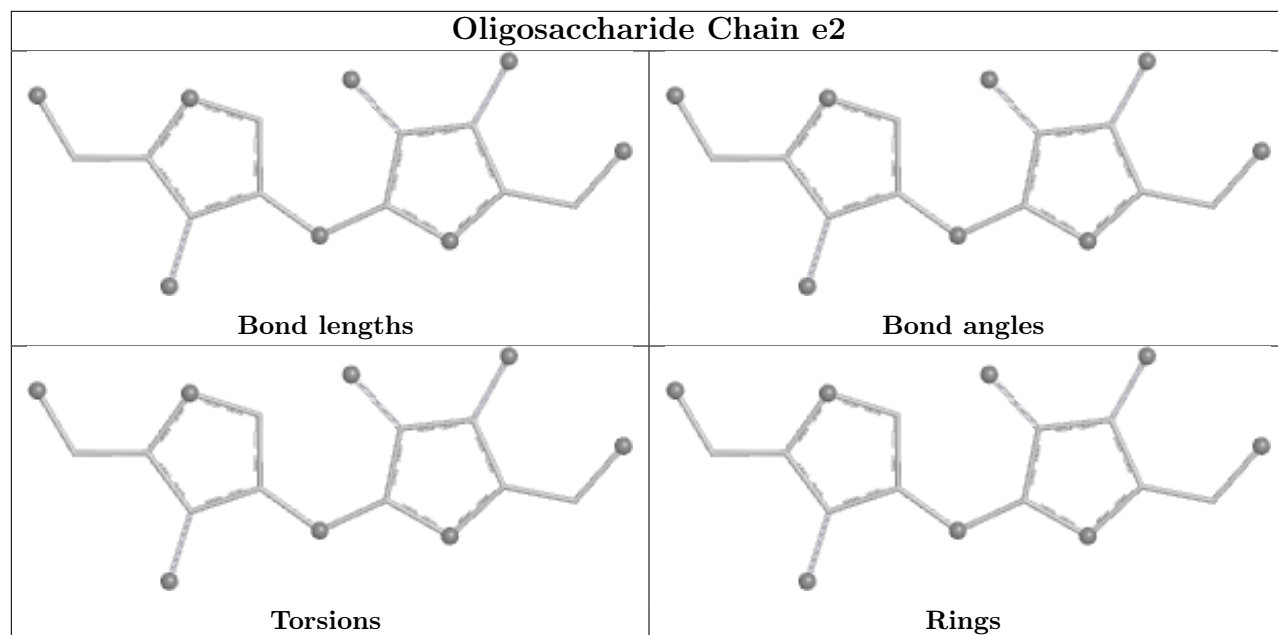


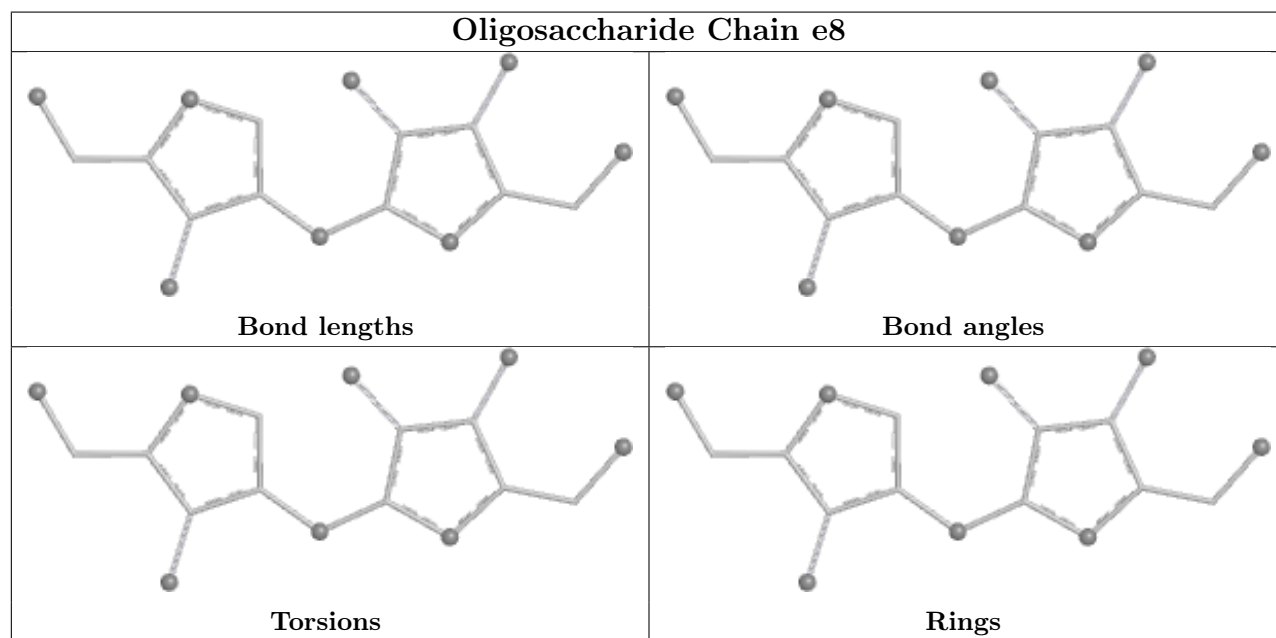
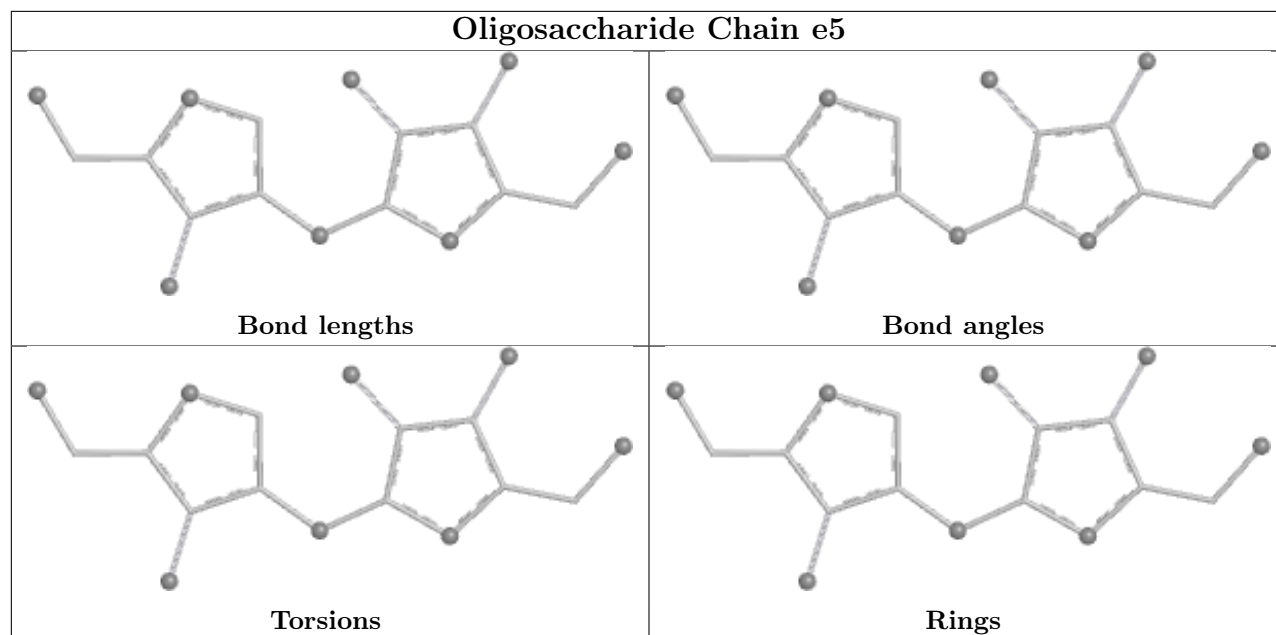


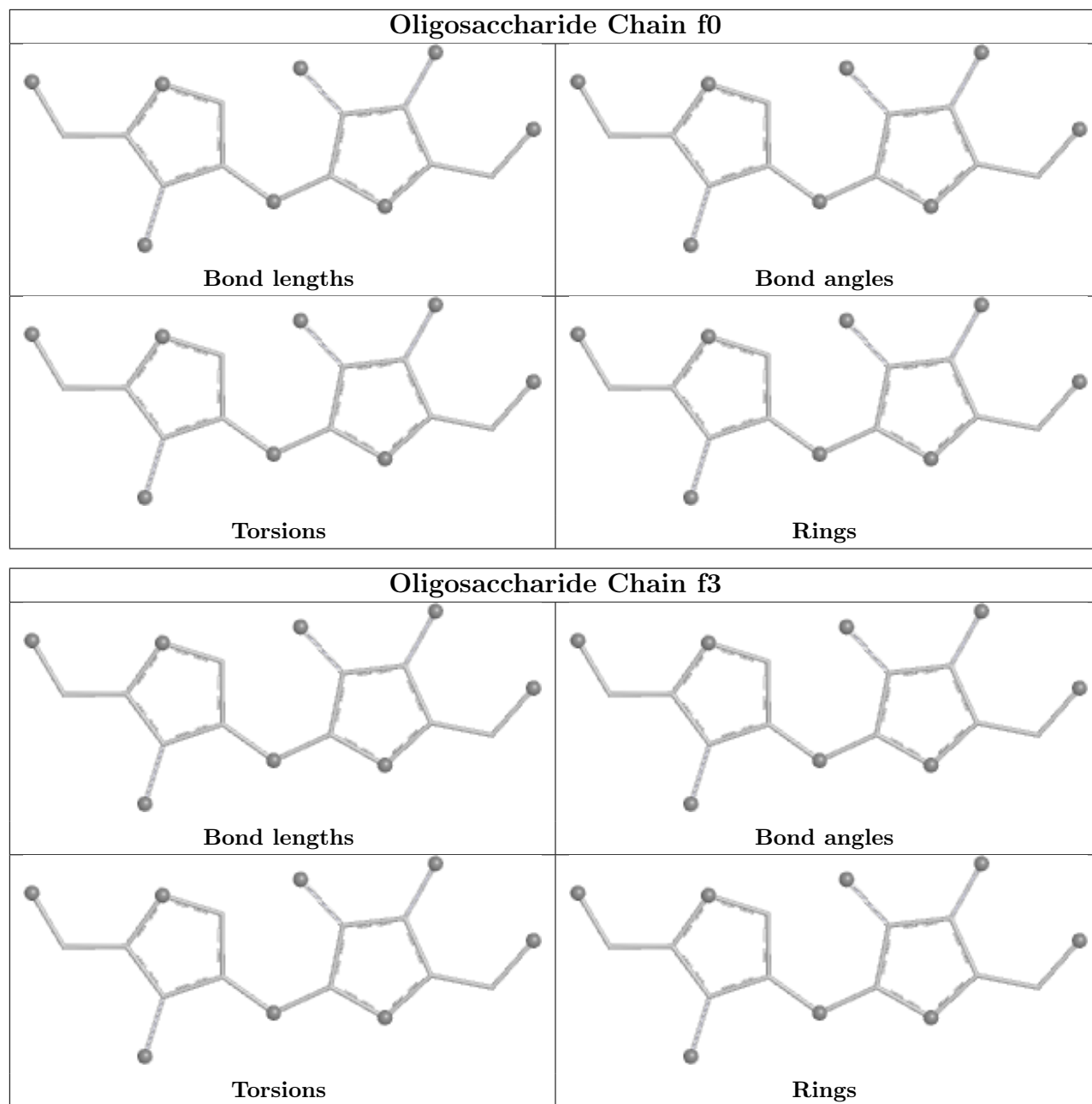


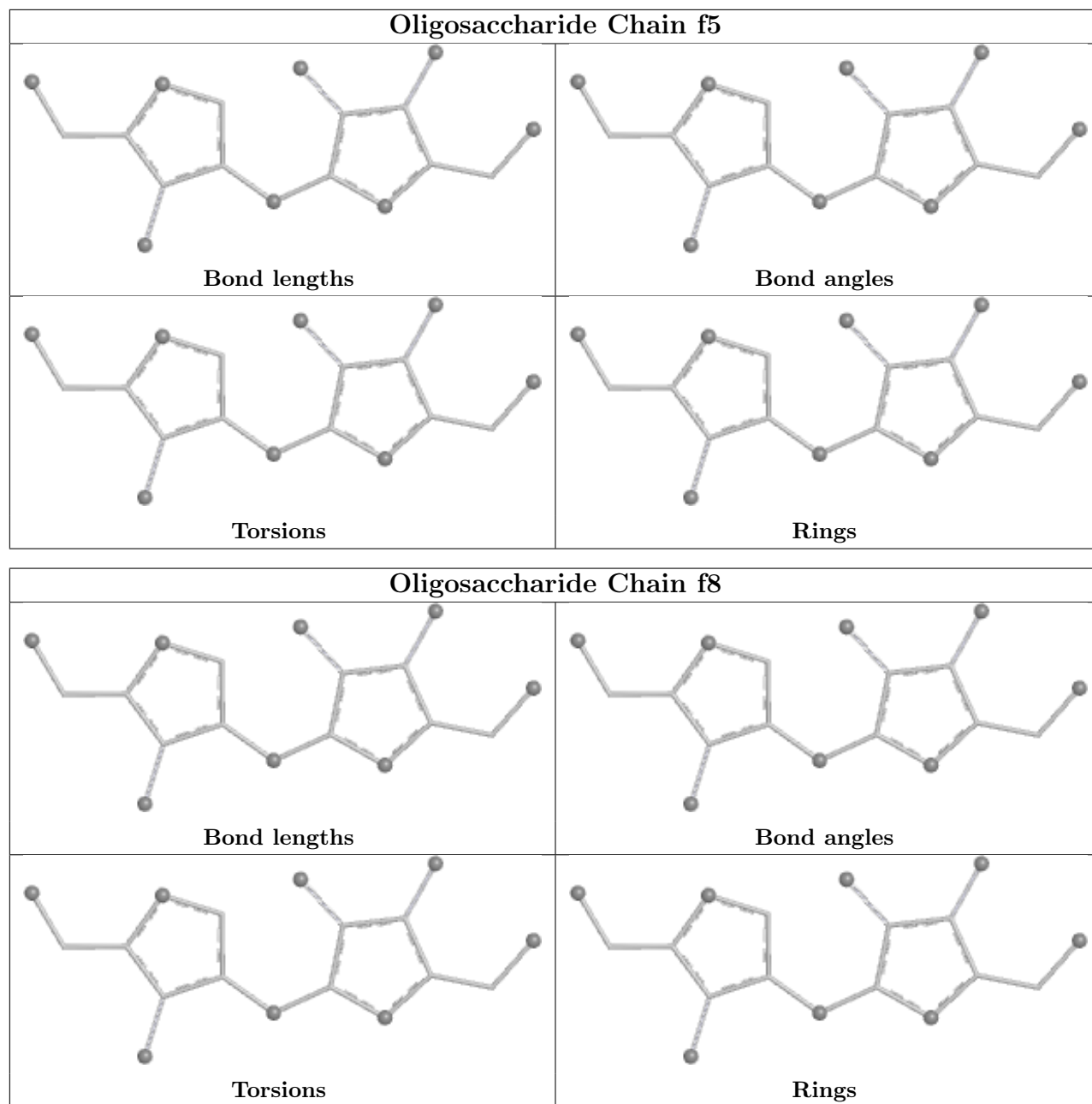


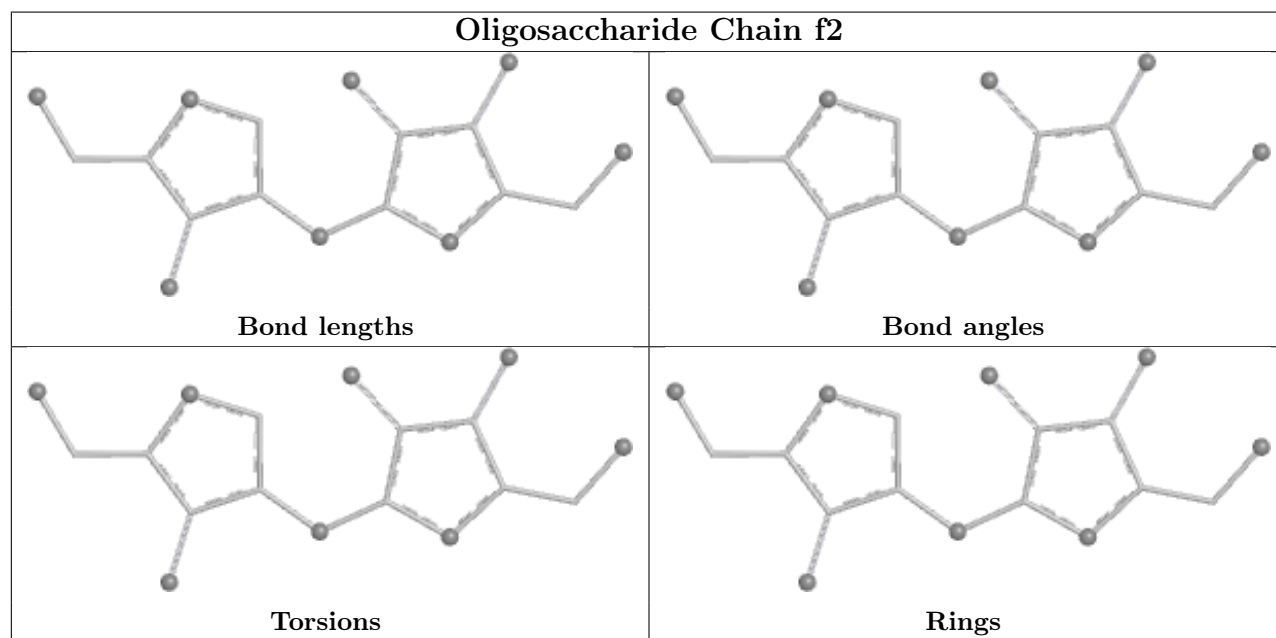
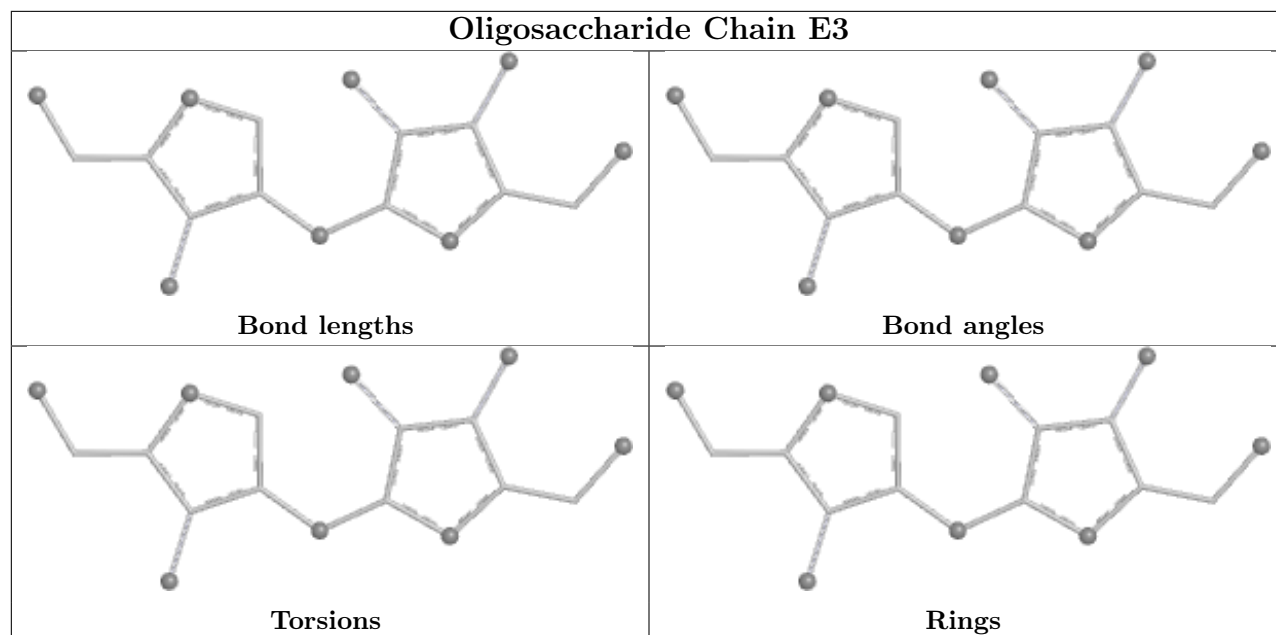


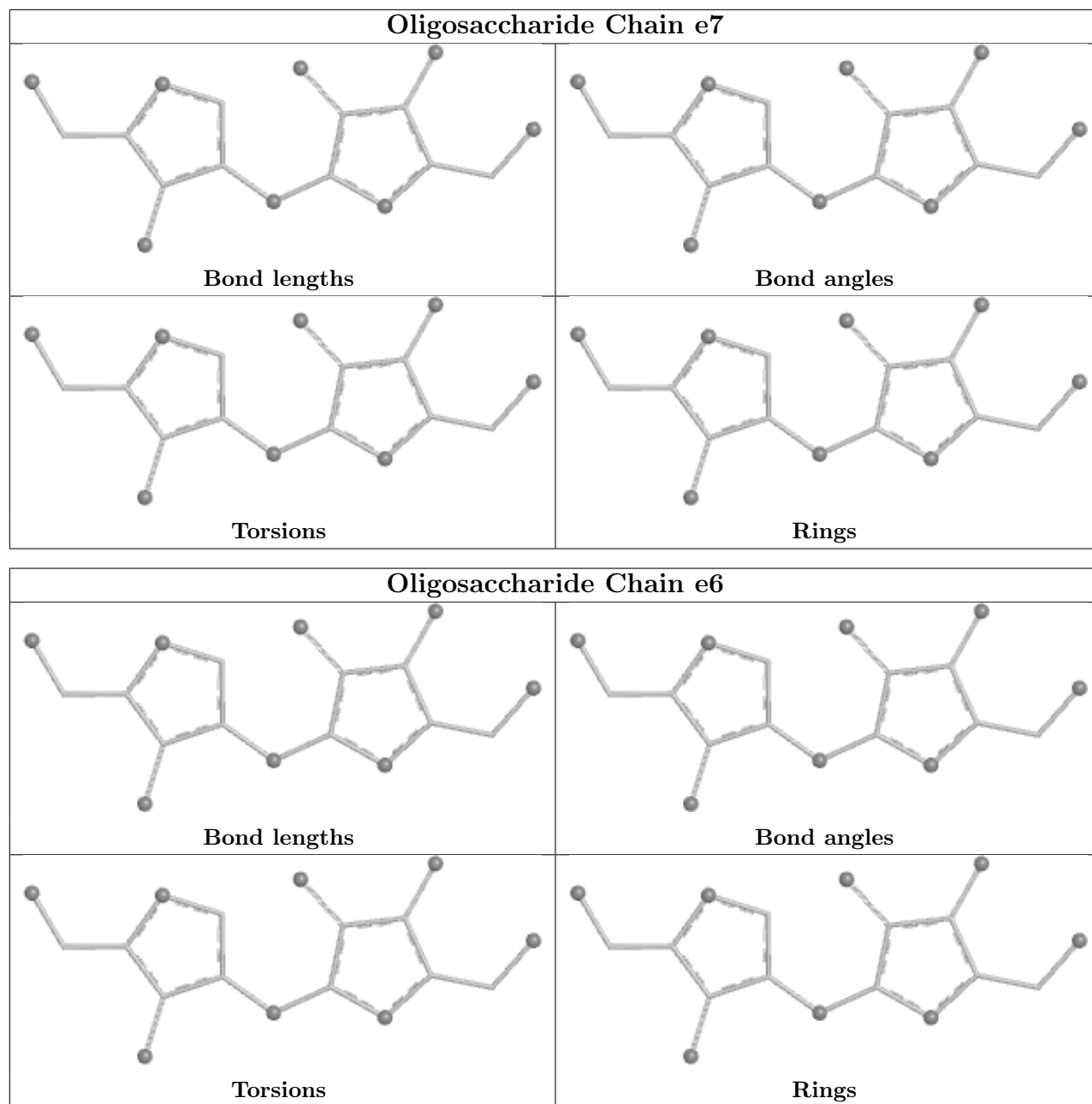




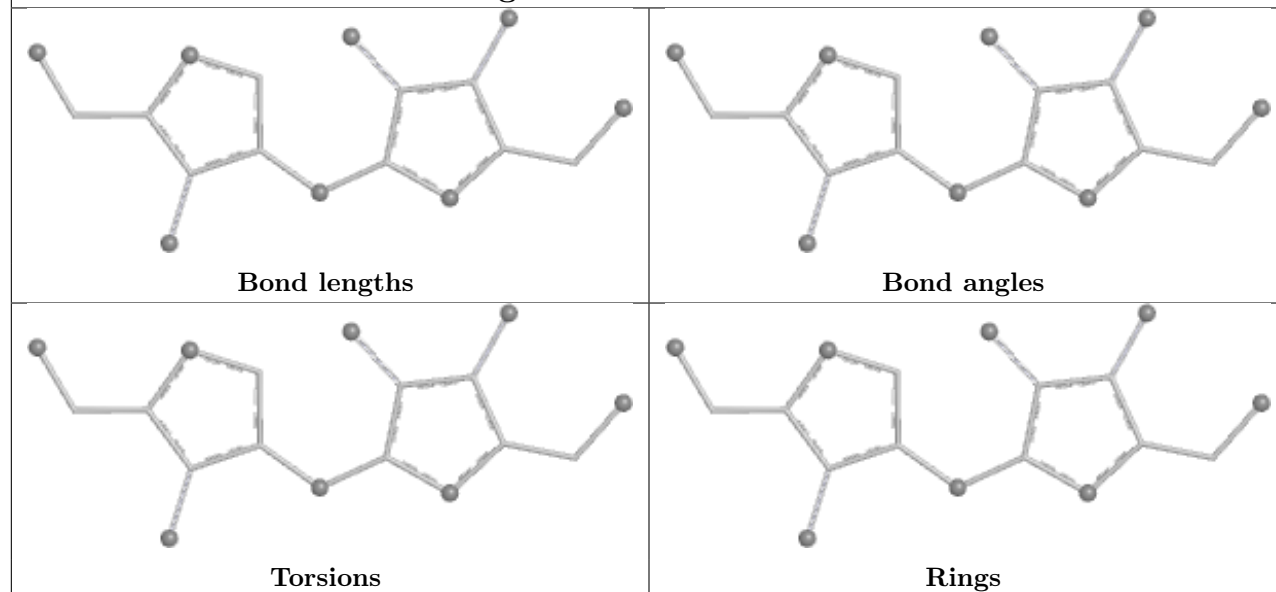




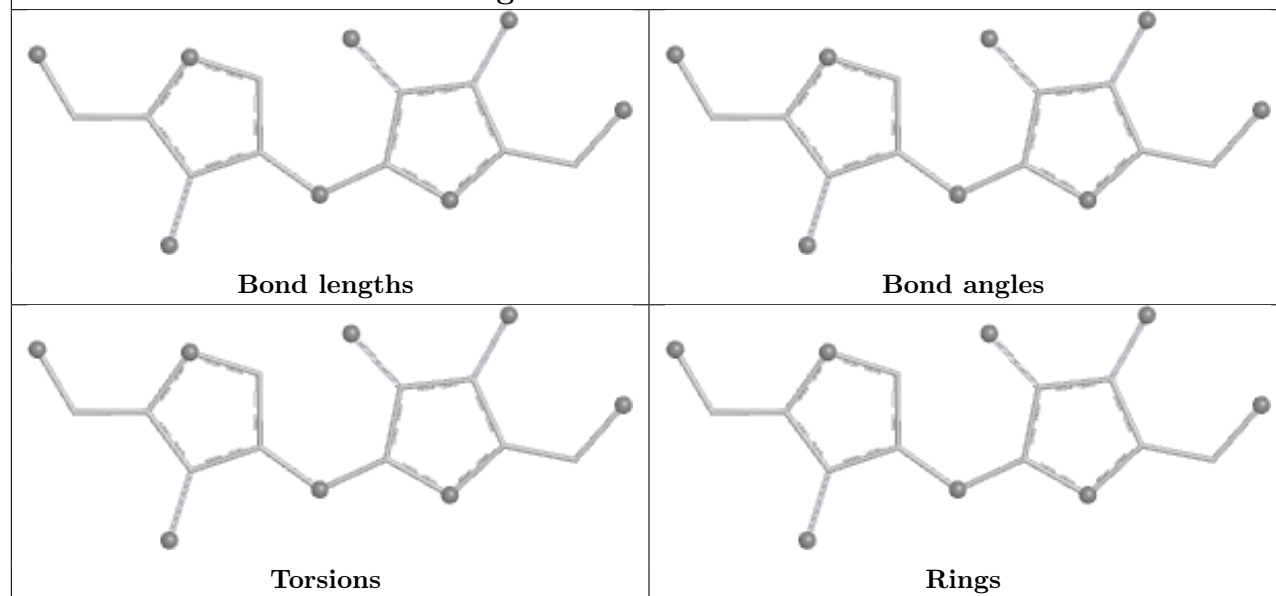


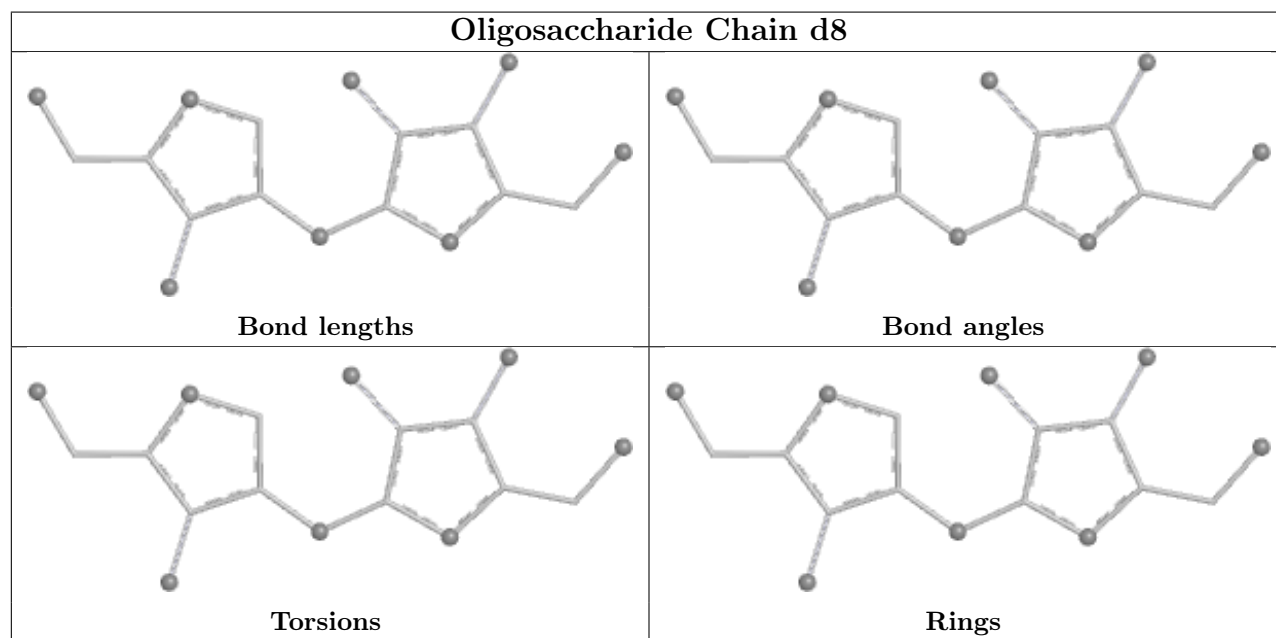
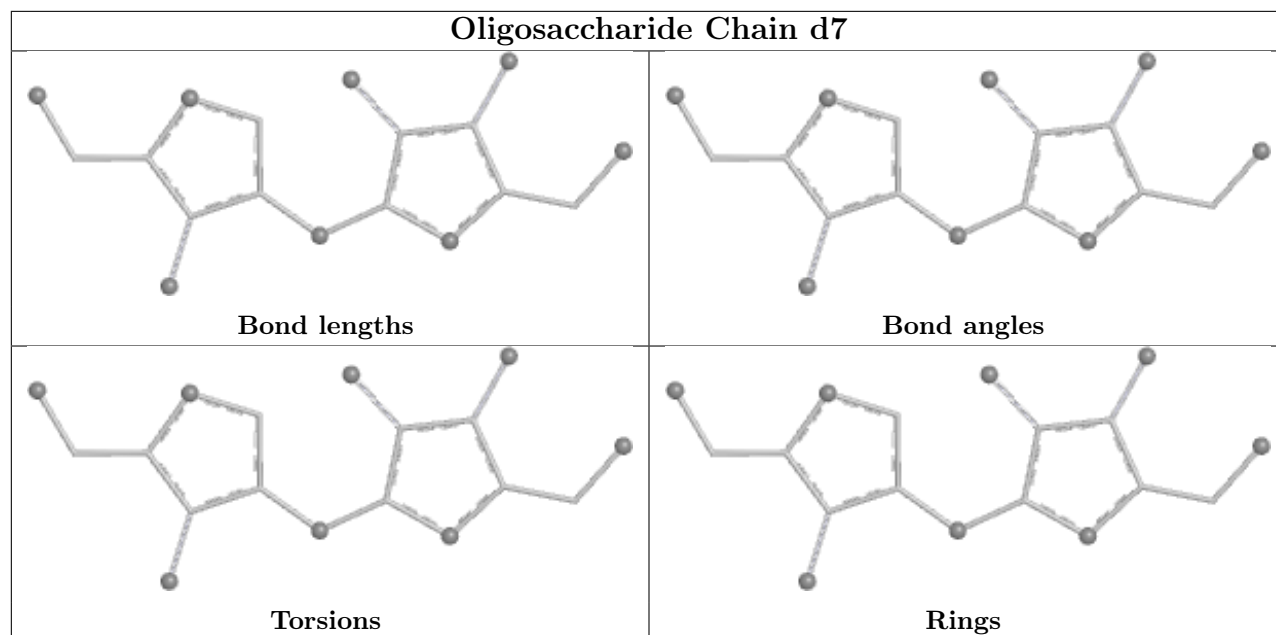


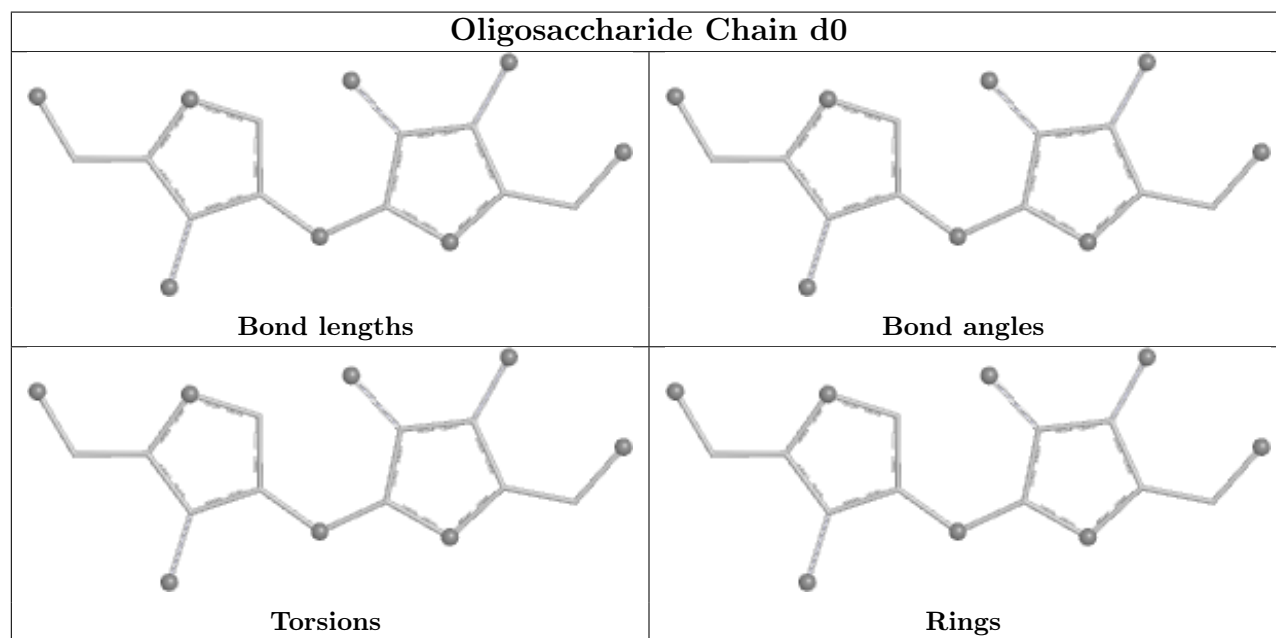
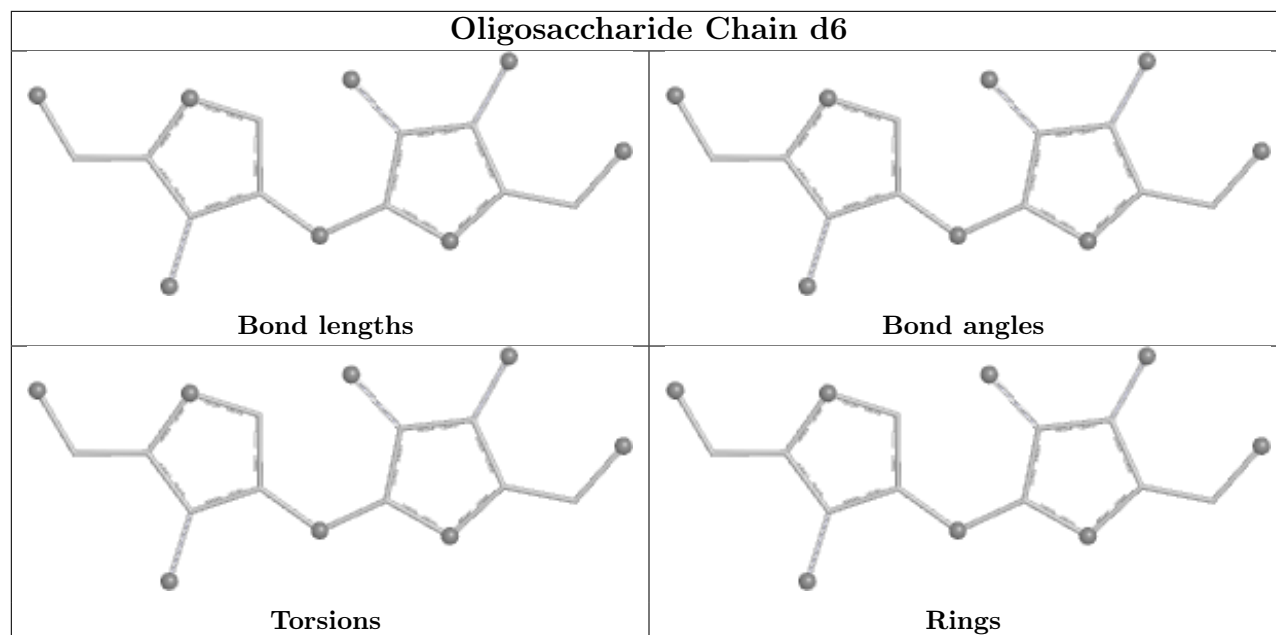
Oligosaccharide Chain e3

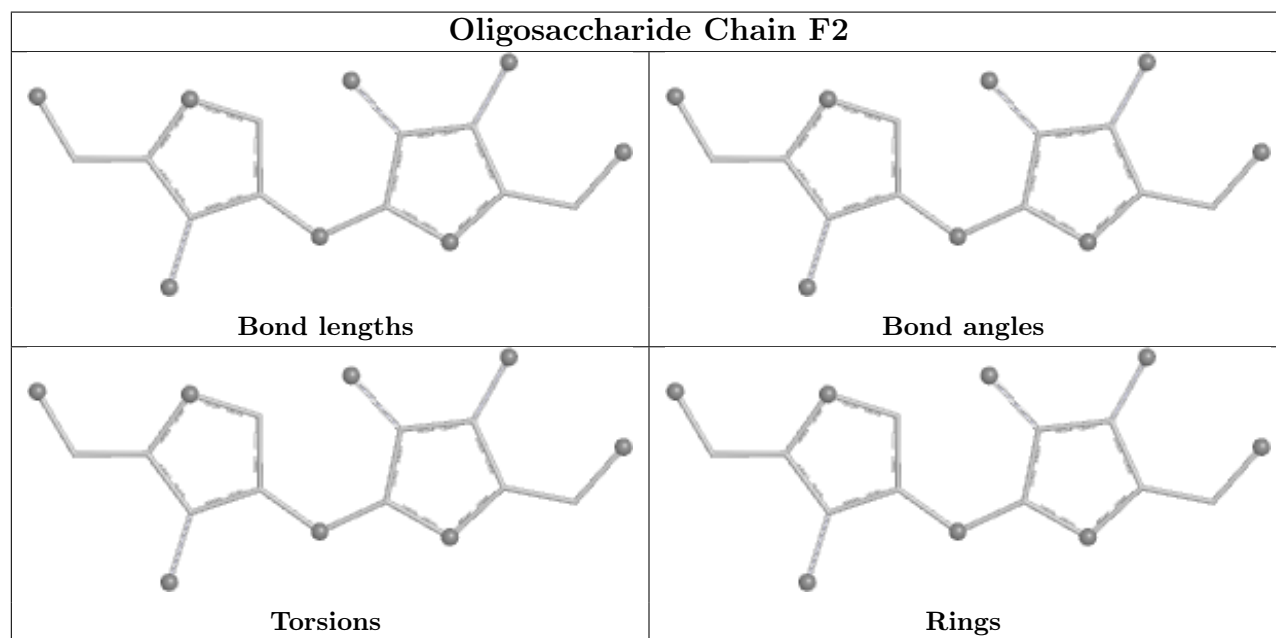
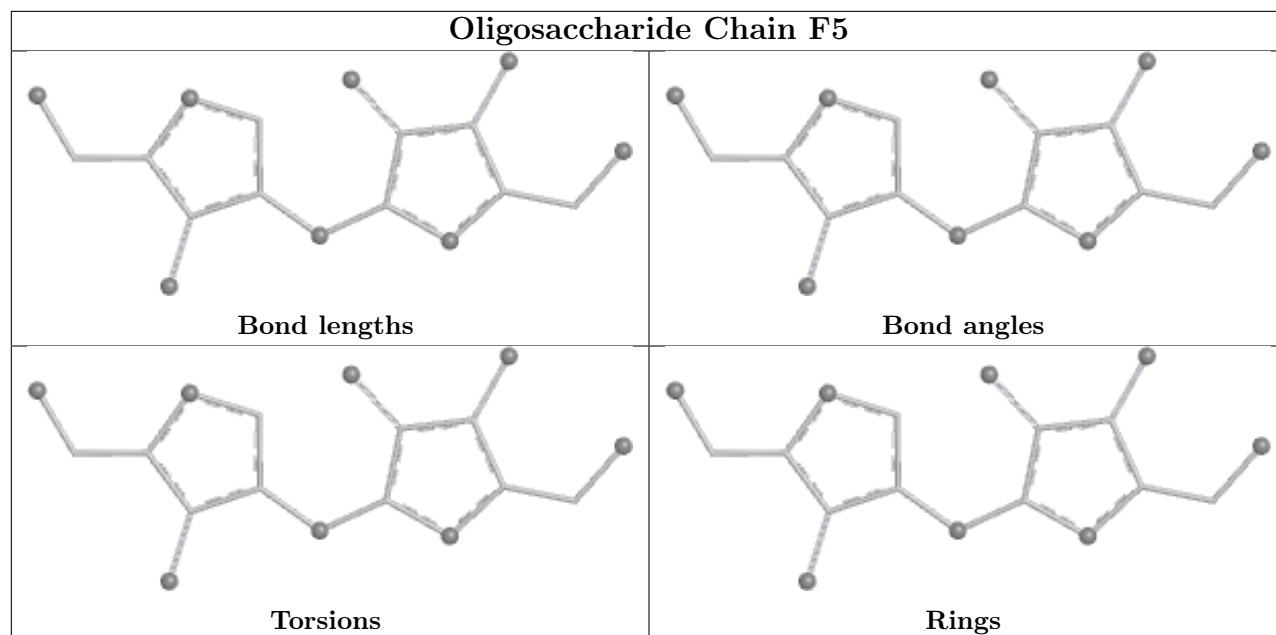


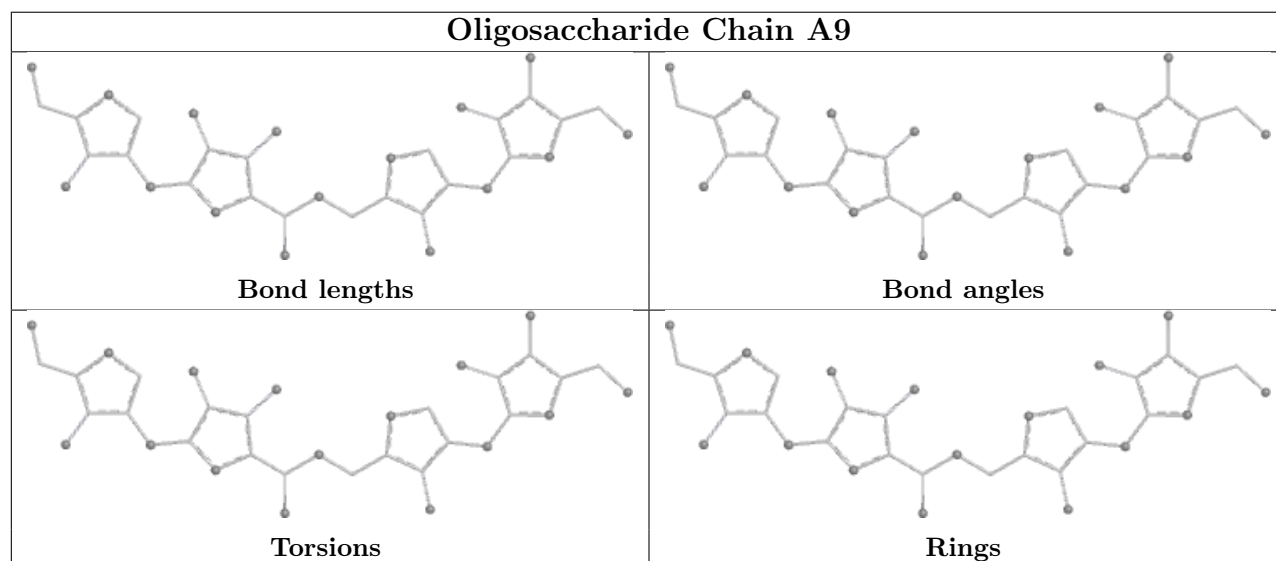
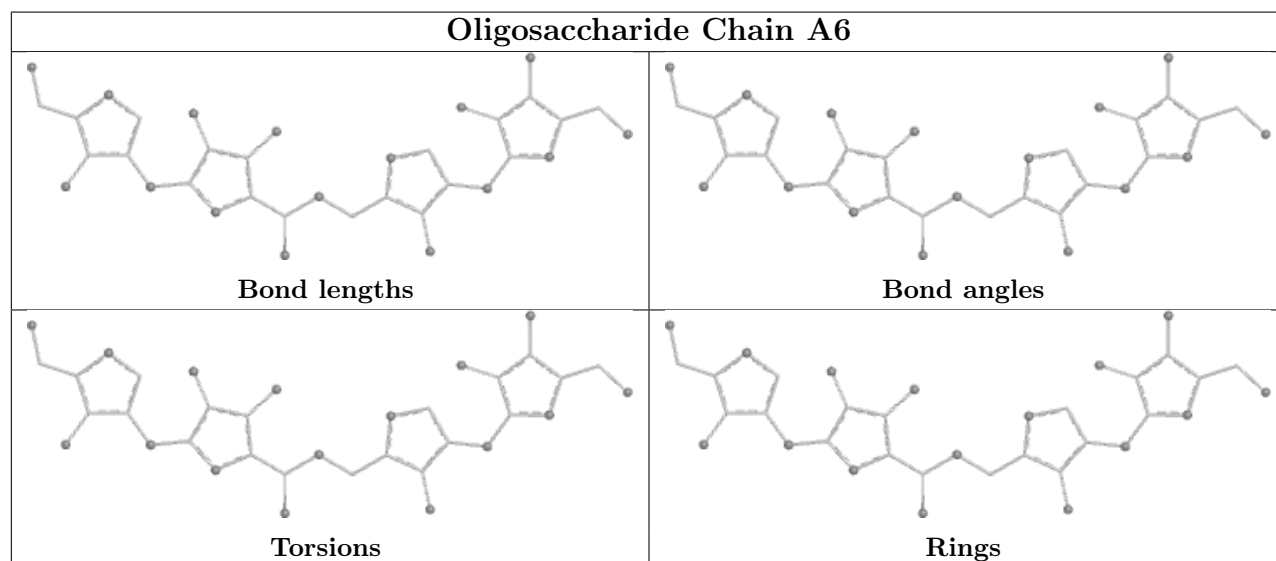
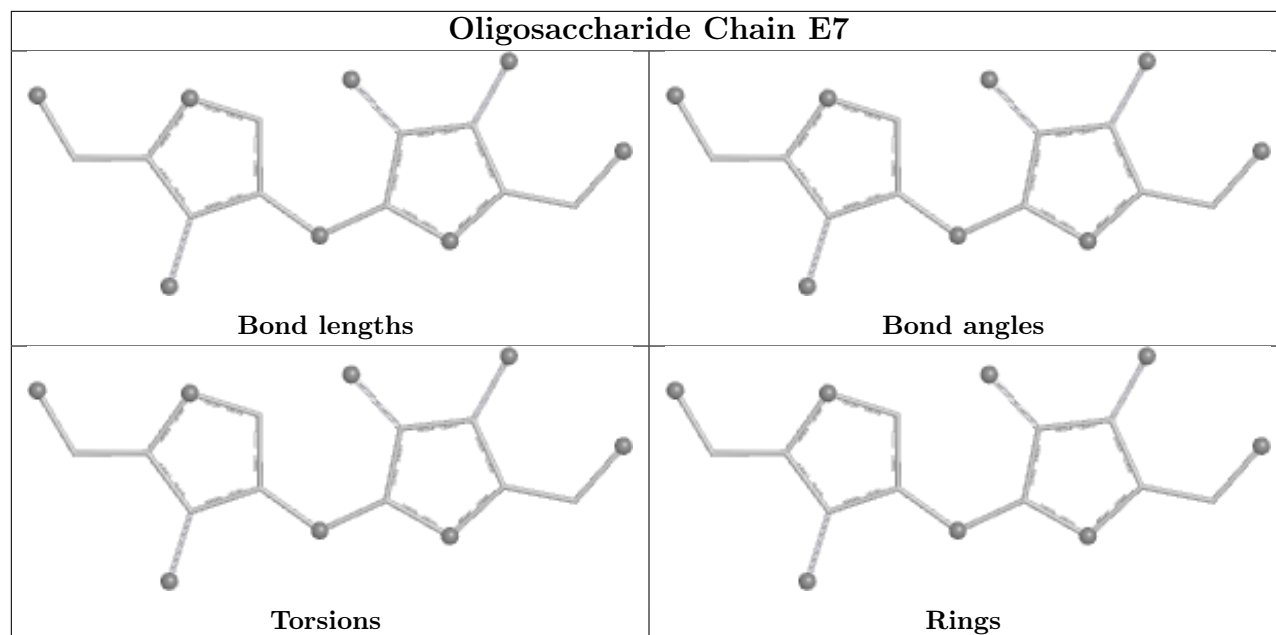
Oligosaccharide Chain d9

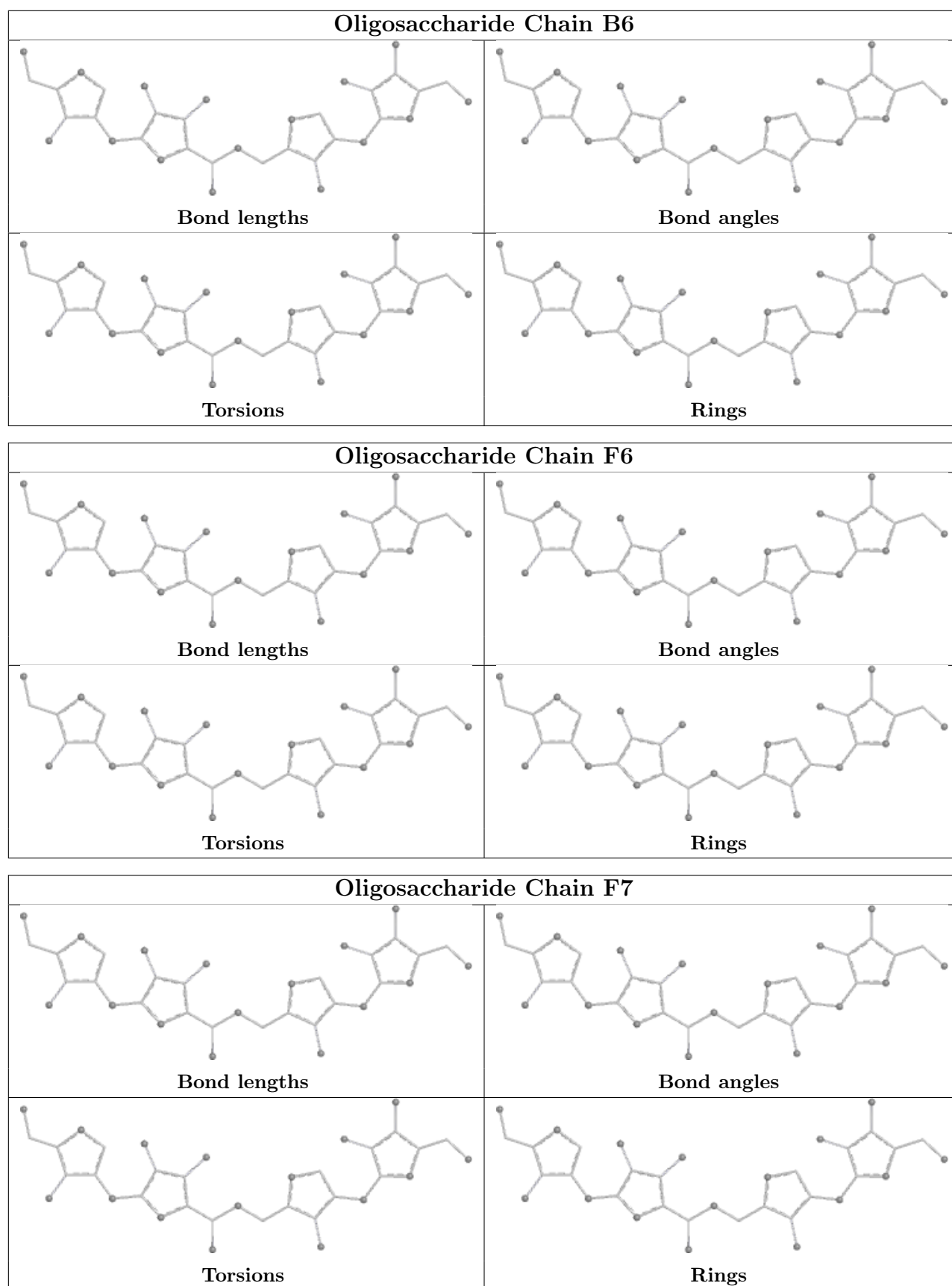


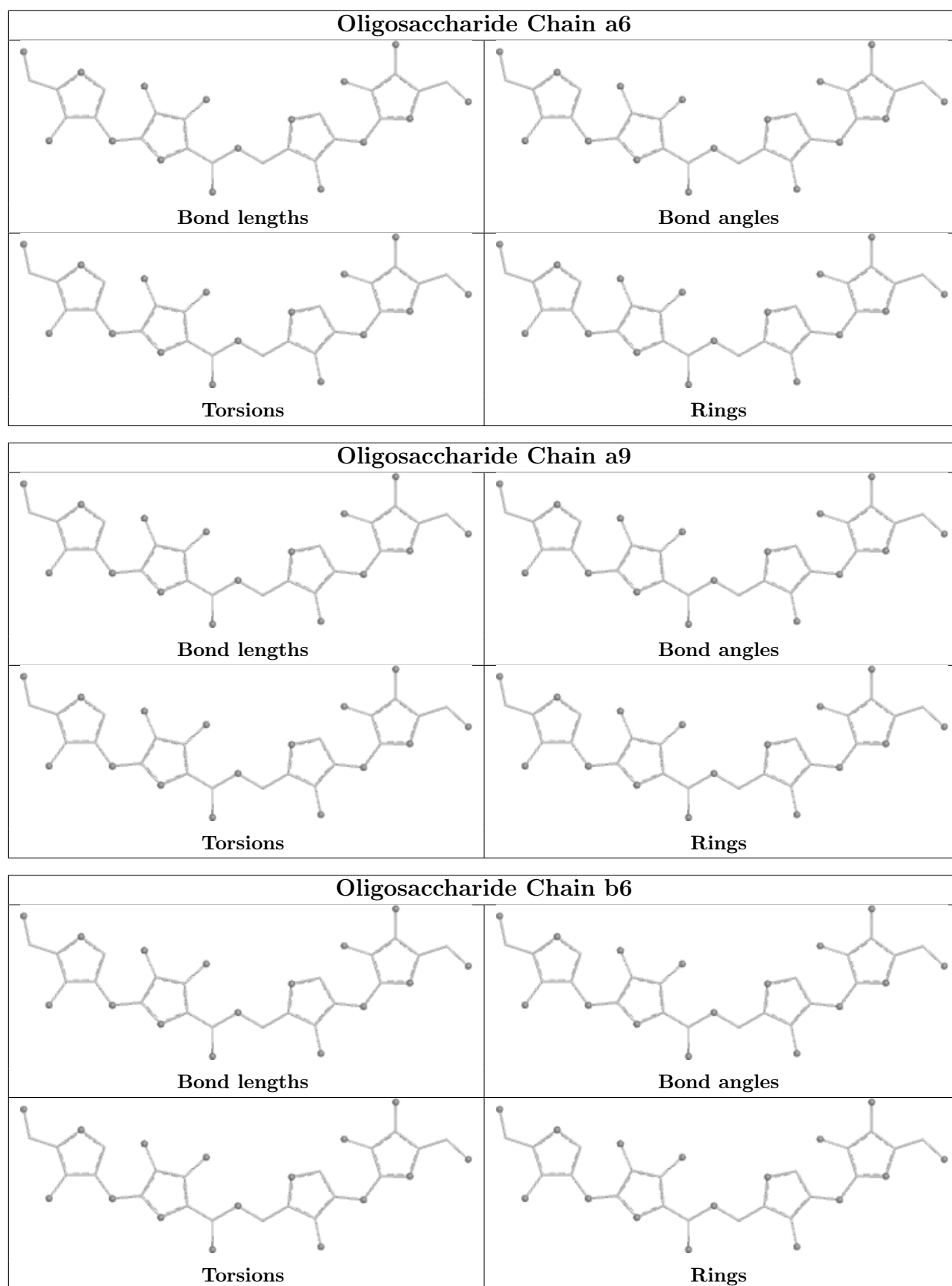


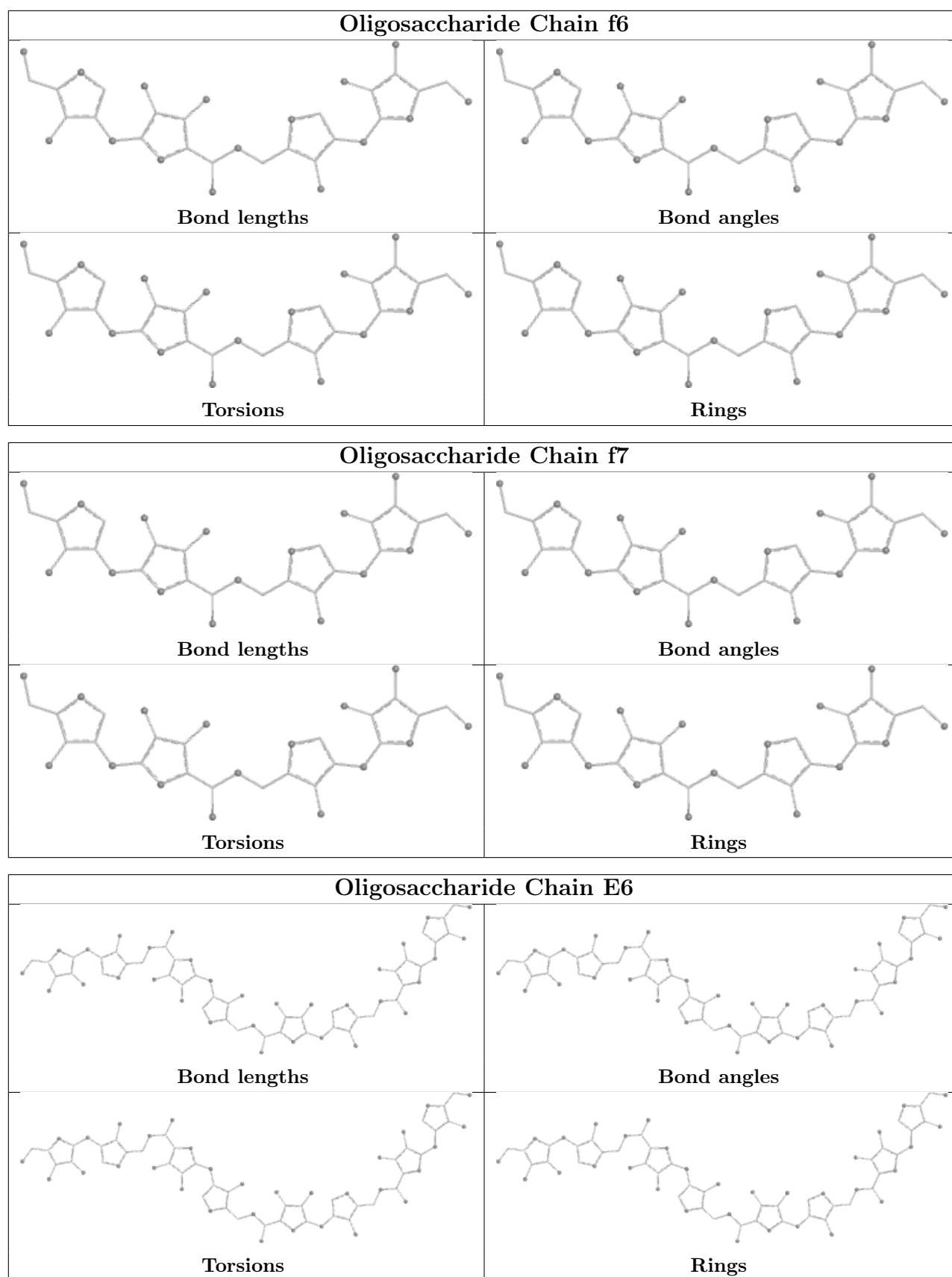


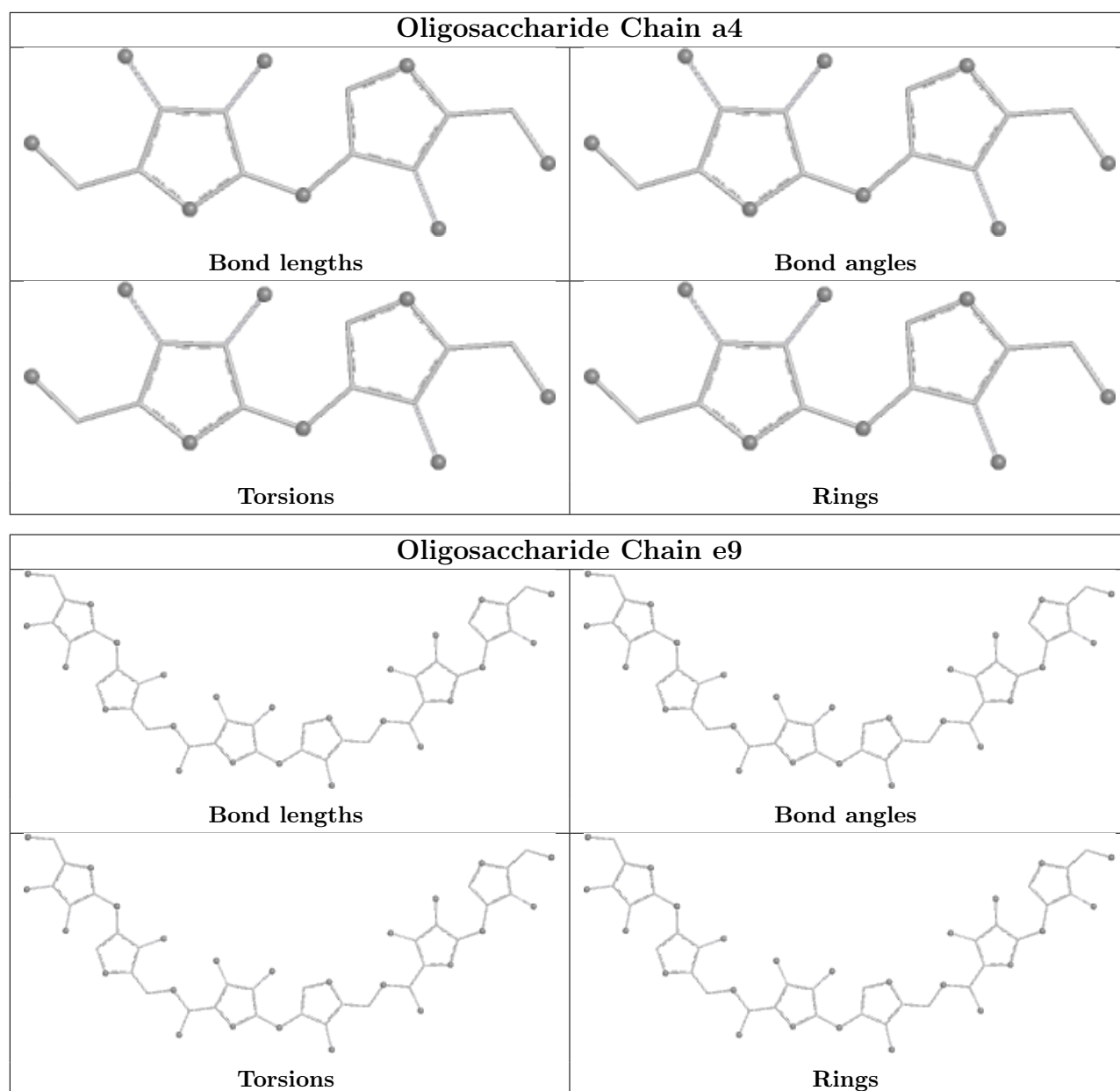












5.6 Ligand geometry [i](#)

140 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
9	A1AIO	A	2010	4	11,11,12	5.59	6 (54%)	13,15,17	1.41	2 (15%)
9	A1AIO	B	2005	5	11,11,12	5.57	6 (54%)	13,15,17	1.27	2 (15%)
10	GLA	B	2069	1	11,11,12	1.68	3 (27%)	15,15,17	0.84	0
9	A1AIO	B	2031	4	11,11,12	5.54	6 (54%)	13,15,17	1.51	2 (15%)
9	A1AIO	A	2011	5	11,11,12	5.57	6 (54%)	13,15,17	1.53	2 (15%)
9	A1AIO	A	2019	4	11,11,12	5.60	6 (54%)	13,15,17	1.37	2 (15%)
9	A1AIO	B	2037	4	11,11,12	5.58	6 (54%)	13,15,17	1.56	2 (15%)
9	A1AIO	A	2031	4	11,11,12	5.59	6 (54%)	13,15,17	1.46	2 (15%)
9	A1AIO	A	2054	6	11,11,12	5.62	6 (54%)	13,15,17	1.41	2 (15%)
9	A1AIO	A	2040	4	11,11,12	5.55	6 (54%)	13,15,17	1.55	2 (15%)
9	A1AIO	B	2025	4	11,11,12	5.60	6 (54%)	13,15,17	1.48	2 (15%)
9	A1AIO	B	2011	5	11,11,12	5.54	6 (54%)	13,15,17	1.59	2 (15%)
9	A1AIO	A	2021	4	11,11,12	5.60	6 (54%)	13,15,17	1.36	2 (15%)
9	A1AIO	A	2020	4	11,11,12	5.60	6 (54%)	13,15,17	1.39	2 (15%)
9	A1AIO	B	2012	4	11,11,12	5.60	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	B	2042	4	11,11,12	5.61	6 (54%)	13,15,17	1.42	2 (15%)
9	A1AIO	A	2027	4	11,11,12	5.58	6 (54%)	13,15,17	1.49	2 (15%)
9	A1AIO	B	2045	4	11,11,12	5.60	6 (54%)	13,15,17	1.42	2 (15%)
9	A1AIO	A	2015	4	11,11,12	5.59	6 (54%)	13,15,17	1.37	2 (15%)
10	GLA	A	2066	1	11,11,12	1.67	3 (27%)	15,15,17	0.84	0
9	A1AIO	B	2016	4	11,11,12	5.54	6 (54%)	13,15,17	1.38	2 (15%)
9	A1AIO	B	2022	4	11,11,12	5.56	6 (54%)	13,15,17	1.41	2 (15%)
9	A1AIO	A	2013	4	11,11,12	5.57	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	B	2023	4	11,11,12	5.56	6 (54%)	13,15,17	1.33	2 (15%)
9	A1AIO	B	2050	4	11,11,12	5.57	6 (54%)	13,15,17	1.41	2 (15%)
10	GLA	B	2060	-	11,11,12	1.68	3 (27%)	15,15,17	0.91	1 (6%)
9	A1AIO	A	2039	6	11,11,12	5.59	6 (54%)	13,15,17	1.47	2 (15%)
9	A1AIO	A	2018	4	11,11,12	5.57	6 (54%)	13,15,17	1.49	2 (15%)
9	A1AIO	B	2049	4	11,11,12	5.59	6 (54%)	13,15,17	1.49	2 (15%)
9	A1AIO	B	2038	4	11,11,12	5.61	6 (54%)	13,15,17	1.47	2 (15%)
10	GLA	B	2059	1	11,11,12	0.42	0	15,15,17	0.74	1 (6%)
9	A1AIO	A	2007	4	11,11,12	5.60	6 (54%)	13,15,17	1.50	2 (15%)
9	A1AIO	A	2045	4	11,11,12	5.58	6 (54%)	13,15,17	1.50	2 (15%)
9	A1AIO	B	2024	4	11,11,12	5.59	6 (54%)	13,15,17	1.38	1 (7%)
10	GLA	A	2067	1	11,11,12	1.71	3 (27%)	15,15,17	0.88	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A1AIO	A	2047	4	11,11,12	5.58	6 (54%)	13,15,17	1.50	2 (15%)
9	A1AIO	A	2046	4	11,11,12	5.59	6 (54%)	13,15,17	1.45	2 (15%)
9	A1AIO	B	2002	4	11,11,12	5.57	6 (54%)	13,15,17	1.53	2 (15%)
9	A1AIO	A	2034	4	11,11,12	5.59	6 (54%)	13,15,17	1.51	2 (15%)
9	A1AIO	B	2053	5	11,11,12	5.57	6 (54%)	13,15,17	1.50	2 (15%)
9	A1AIO	B	2029	4	11,11,12	5.61	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	B	2040	5	11,11,12	5.56	6 (54%)	13,15,17	1.56	2 (15%)
9	A1AIO	B	2051	5	11,11,12	5.58	6 (54%)	13,15,17	1.34	2 (15%)
9	A1AIO	A	2002	4	11,11,12	5.60	6 (54%)	13,15,17	1.47	2 (15%)
10	GLA	A	2064	1	11,11,12	1.68	3 (27%)	15,15,17	0.90	1 (6%)
9	A1AIO	B	2010	4	11,11,12	5.59	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	A	2041	4	11,11,12	5.61	6 (54%)	13,15,17	1.32	2 (15%)
9	A1AIO	B	2041	4	11,11,12	5.57	6 (54%)	13,15,17	1.53	2 (15%)
10	GLA	A	2062	1	11,11,12	1.68	3 (27%)	15,15,17	0.86	1 (6%)
9	A1AIO	B	2046	4	11,11,12	5.53	6 (54%)	13,15,17	1.68	2 (15%)
9	A1AIO	A	2052	5	11,11,12	5.58	6 (54%)	13,15,17	1.49	2 (15%)
9	A1AIO	B	2033	4	11,11,12	5.56	6 (54%)	13,15,17	1.62	2 (15%)
9	A1AIO	B	2054	8	11,11,12	5.59	6 (54%)	13,15,17	1.19	2 (15%)
9	A1AIO	B	2032	4	11,11,12	5.59	6 (54%)	13,15,17	1.57	2 (15%)
9	A1AIO	A	2004	4	11,11,12	5.58	6 (54%)	13,15,17	1.46	2 (15%)
9	A1AIO	A	2035	4	11,11,12	5.61	6 (54%)	13,15,17	1.34	1 (7%)
9	A1AIO	A	2030	4	11,11,12	5.59	6 (54%)	13,15,17	1.32	2 (15%)
10	GLA	A	2058	1	11,11,12	1.67	3 (27%)	15,15,17	0.85	1 (6%)
9	A1AIO	B	2020	4	11,11,12	5.56	6 (54%)	13,15,17	1.30	2 (15%)
9	A1AIO	B	2028	4	11,11,12	5.60	6 (54%)	13,15,17	1.24	2 (15%)
10	GLA	B	2066	-	11,11,12	1.69	3 (27%)	15,15,17	0.87	0
9	A1AIO	A	2048	4	11,11,12	5.59	6 (54%)	13,15,17	1.50	2 (15%)
9	A1AIO	A	2026	4	11,11,12	5.59	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	B	2004	4	11,11,12	5.59	6 (54%)	13,15,17	1.57	2 (15%)
9	A1AIO	A	2008	4	11,11,12	5.59	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	B	2043	4	11,11,12	5.60	6 (54%)	13,15,17	1.43	2 (15%)
10	GLA	B	2063	-	11,11,12	1.70	3 (27%)	15,15,17	1.10	1 (6%)
9	A1AIO	A	2014	4	11,11,12	5.59	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	B	2056	5	11,11,12	5.61	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	B	2019	4	11,11,12	5.57	6 (54%)	13,15,17	1.53	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GLA	A	2069	1	11,11,12	1.68	3 (27%)	15,15,17	0.84	0
9	A1AIO	A	2055	6	11,11,12	5.60	6 (54%)	13,15,17	1.36	2 (15%)
9	A1AIO	B	2057	5	11,11,12	5.57	6 (54%)	13,15,17	1.51	2 (15%)
9	A1AIO	A	2001	4	11,11,12	5.61	6 (54%)	13,15,17	1.47	2 (15%)
9	A1AIO	B	2044	4	11,11,12	5.60	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	A	2037	4	11,11,12	5.59	6 (54%)	13,15,17	1.42	2 (15%)
9	A1AIO	A	2038	4	11,11,12	5.56	6 (54%)	13,15,17	1.54	2 (15%)
9	A1AIO	B	2048	4	11,11,12	5.59	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	A	2006	4	11,11,12	5.56	6 (54%)	13,15,17	1.67	2 (15%)
10	GLA	B	2067	1	11,11,12	1.68	3 (27%)	15,15,17	0.85	0
9	A1AIO	B	2035	8	11,11,12	5.61	6 (54%)	13,15,17	1.47	2 (15%)
9	A1AIO	B	2006	4	11,11,12	5.61	6 (54%)	13,15,17	1.61	2 (15%)
9	A1AIO	A	2042	4	11,11,12	5.60	6 (54%)	13,15,17	1.49	2 (15%)
10	GLA	B	2064	1	11,11,12	1.67	3 (27%)	15,15,17	0.85	0
9	A1AIO	B	2007	4	11,11,12	5.59	6 (54%)	13,15,17	1.52	2 (15%)
9	A1AIO	A	2036	4	11,11,12	5.58	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	A	2016	4	11,11,12	5.56	6 (54%)	13,15,17	1.55	2 (15%)
9	A1AIO	A	2022	4	11,11,12	5.59	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	A	2056	5	11,11,12	5.58	6 (54%)	13,15,17	1.53	2 (15%)
9	A1AIO	B	2021	4	11,11,12	5.60	6 (54%)	13,15,17	1.30	1 (7%)
9	A1AIO	B	2013	4	11,11,12	5.58	6 (54%)	13,15,17	1.36	2 (15%)
9	A1AIO	B	2008	4	11,11,12	5.59	6 (54%)	13,15,17	1.53	2 (15%)
9	A1AIO	A	2057	5	11,11,12	5.60	6 (54%)	13,15,17	1.38	2 (15%)
9	A1AIO	B	2052	5	11,11,12	5.56	6 (54%)	13,15,17	1.55	2 (15%)
10	GLA	A	2061	1	11,11,12	1.70	3 (27%)	15,15,17	0.86	0
10	GLA	B	2065	1	11,11,12	1.65	3 (27%)	15,15,17	0.90	1 (6%)
9	A1AIO	A	2049	4	11,11,12	5.58	6 (54%)	13,15,17	1.49	2 (15%)
9	A1AIO	B	2039	5	11,11,12	5.61	6 (54%)	13,15,17	1.44	1 (7%)
9	A1AIO	A	2003	5	11,11,12	5.59	6 (54%)	13,15,17	1.47	2 (15%)
9	A1AIO	B	2009	4	11,11,12	5.55	6 (54%)	13,15,17	1.73	2 (15%)
10	GLA	B	2058	-	11,11,12	1.67	3 (27%)	15,15,17	0.92	0
10	GLA	B	2062	1	11,11,12	1.68	3 (27%)	15,15,17	0.85	0
9	A1AIO	B	2055	8	11,11,12	5.56	6 (54%)	13,15,17	1.54	2 (15%)
9	A1AIO	B	2018	4	11,11,12	5.60	6 (54%)	13,15,17	1.35	2 (15%)
9	A1AIO	A	2029	4	11,11,12	5.60	6 (54%)	13,15,17	1.27	2 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	A1AIO	B	2047	4	11,11,12	5.57	6 (54%)	13,15,17	1.62	2 (15%)
10	GLA	A	2059	1	11,11,12	0.41	0	15,15,17	0.74	1 (6%)
9	A1AIO	B	2034	4	11,11,12	5.53	6 (54%)	13,15,17	1.67	2 (15%)
9	A1AIO	B	2001	7	11,11,12	5.58	6 (54%)	13,15,17	1.59	2 (15%)
9	A1AIO	B	2003	5	11,11,12	5.59	6 (54%)	13,15,17	1.42	1 (7%)
9	A1AIO	A	2025	4	11,11,12	5.59	6 (54%)	13,15,17	1.42	2 (15%)
9	A1AIO	A	2012	4	11,11,12	5.56	6 (54%)	13,15,17	1.54	2 (15%)
10	GLA	A	2070	1	11,11,12	1.68	3 (27%)	15,15,17	0.85	0
10	GLA	B	2070	-	11,11,12	1.68	3 (27%)	15,15,17	0.86	0
9	A1AIO	A	2028	4	11,11,12	5.60	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	A	2033	4	11,11,12	5.61	6 (54%)	13,15,17	1.36	1 (7%)
9	A1AIO	B	2017	4	11,11,12	5.57	6 (54%)	13,15,17	1.46	2 (15%)
9	A1AIO	A	2023	4	11,11,12	5.59	6 (54%)	13,15,17	1.44	2 (15%)
9	A1AIO	A	2050	5	11,11,12	5.61	6 (54%)	13,15,17	1.29	2 (15%)
9	A1AIO	A	2032	4	11,11,12	5.57	6 (54%)	13,15,17	1.47	2 (15%)
9	A1AIO	B	2027	4	11,11,12	5.60	6 (54%)	13,15,17	1.49	2 (15%)
10	GLA	A	2068	1	11,11,12	1.70	3 (27%)	15,15,17	0.81	0
10	GLA	A	2060	1	11,11,12	0.42	0	15,15,17	0.75	1 (6%)
9	A1AIO	B	2030	4	11,11,12	5.55	6 (54%)	13,15,17	1.51	2 (15%)
9	A1AIO	B	2036	4	11,11,12	5.60	6 (54%)	13,15,17	1.43	2 (15%)
10	GLA	B	2068	1	11,11,12	1.69	3 (27%)	15,15,17	0.81	0
9	A1AIO	A	2009	4	11,11,12	5.58	6 (54%)	13,15,17	1.59	2 (15%)
9	A1AIO	A	2024	4	11,11,12	5.60	6 (54%)	13,15,17	1.49	2 (15%)
10	GLA	A	2063	1	11,11,12	1.69	3 (27%)	15,15,17	0.89	0
9	A1AIO	A	2043	5	11,11,12	5.62	6 (54%)	13,15,17	1.48	1 (7%)
10	GLA	A	2065	1	11,11,12	1.69	3 (27%)	15,15,17	0.84	0
9	A1AIO	A	2053	6	11,11,12	5.59	6 (54%)	13,15,17	1.51	2 (15%)
10	GLA	B	2061	1	11,11,12	1.70	3 (27%)	15,15,17	0.82	0
9	A1AIO	A	2005	5	11,11,12	5.63	6 (54%)	13,15,17	1.42	2 (15%)
9	A1AIO	A	2051	5	11,11,12	5.61	6 (54%)	13,15,17	1.48	2 (15%)
9	A1AIO	B	2014	4	11,11,12	5.56	6 (54%)	13,15,17	1.43	2 (15%)
9	A1AIO	A	2017	4	11,11,12	5.60	6 (54%)	13,15,17	1.36	1 (7%)
9	A1AIO	A	2044	5	11,11,12	5.60	6 (54%)	13,15,17	1.61	2 (15%)
9	A1AIO	B	2026	4	11,11,12	5.58	6 (54%)	13,15,17	1.56	2 (15%)
9	A1AIO	B	2015	4	11,11,12	5.57	6 (54%)	13,15,17	1.45	2 (15%)

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
9	A1AIO	A	2010	4	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2005	5	-	6/6/19/22	0/1/1/1
10	GLA	B	2069	1	-	2/2/19/22	0/1/1/1
9	A1AIO	B	2031	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2011	5	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2019	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2037	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2031	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2054	6	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2040	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	B	2025	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2011	5	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2021	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2012	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2020	4	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2042	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2027	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2045	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2015	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2066	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2016	4	1/1/4/5	6/6/19/22	0/1/1/1
9	A1AIO	B	2022	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2013	4	-	1/6/19/22	0/1/1/1
9	A1AIO	B	2023	4	-	4/6/19/22	0/1/1/1
9	A1AIO	B	2050	4	-	0/6/19/22	0/1/1/1
10	GLA	B	2060	-	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2039	6	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2018	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	B	2049	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2038	4	-	0/6/19/22	0/1/1/1
10	GLA	B	2059	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2007	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2045	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2024	4	-	1/6/19/22	0/1/1/1
10	GLA	A	2067	1	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2047	4	-	2/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	A	2046	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2002	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2034	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2053	5	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	B	2029	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2040	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2051	5	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2002	4	-	2/6/19/22	0/1/1/1
10	GLA	A	2064	1	-	2/2/19/22	0/1/1/1
9	A1AIO	B	2010	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2041	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2041	4	-	2/6/19/22	0/1/1/1
10	GLA	A	2062	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2046	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2052	5	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	B	2033	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	B	2054	8	-	6/6/19/22	0/1/1/1
9	A1AIO	B	2032	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2004	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2035	4	1/1/4/5	5/6/19/22	0/1/1/1
9	A1AIO	A	2030	4	-	2/6/19/22	0/1/1/1
10	GLA	A	2058	1	-	1/2/19/22	0/1/1/1
9	A1AIO	B	2020	4	-	4/6/19/22	0/1/1/1
9	A1AIO	B	2028	4	-	4/6/19/22	0/1/1/1
10	GLA	B	2066	-	-	1/2/19/22	0/1/1/1
9	A1AIO	A	2048	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2026	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2004	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2008	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2043	4	-	2/6/19/22	0/1/1/1
10	GLA	B	2063	-	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2014	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	B	2056	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2019	4	-	2/6/19/22	0/1/1/1
10	GLA	A	2069	1	-	1/2/19/22	0/1/1/1
9	A1AIO	A	2055	6	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2057	5	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2001	4	-	2/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	A1AIO	B	2044	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2037	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2038	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	B	2048	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2006	4	1/1/4/5	1/6/19/22	0/1/1/1
10	GLA	B	2067	1	-	2/2/19/22	0/1/1/1
9	A1AIO	B	2035	8	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2006	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	A	2042	4	-	0/6/19/22	0/1/1/1
10	GLA	B	2064	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2007	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2036	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2016	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2022	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2056	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2021	4	-	3/6/19/22	0/1/1/1
9	A1AIO	B	2013	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2008	4	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2057	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2052	5	-	2/6/19/22	0/1/1/1
10	GLA	A	2061	1	-	0/2/19/22	0/1/1/1
10	GLA	B	2065	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2049	4	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2039	5	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2003	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2009	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	B	2058	-	-	2/2/19/22	0/1/1/1
10	GLA	B	2062	1	-	1/2/19/22	0/1/1/1
9	A1AIO	B	2055	8	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2029	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2018	4	-	4/6/19/22	0/1/1/1
9	A1AIO	B	2047	4	1/1/4/5	0/6/19/22	0/1/1/1
10	GLA	A	2059	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2034	4	1/1/4/5	2/6/19/22	0/1/1/1
9	A1AIO	B	2001	7	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2003	5	-	3/6/19/22	0/1/1/1
9	A1AIO	A	2025	4	1/1/4/5	0/6/19/22	0/1/1/1
9	A1AIO	A	2012	4	1/1/4/5	0/6/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GLA	A	2070	1	-	0/2/19/22	0/1/1/1
10	GLA	B	2070	-	-	0/2/19/22	0/1/1/1
9	A1AIO	A	2028	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2033	4	-	1/6/19/22	0/1/1/1
9	A1AIO	A	2023	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2050	5	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2017	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2032	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2027	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2068	1	-	0/2/19/22	0/1/1/1
10	GLA	A	2060	1	-	0/2/19/22	0/1/1/1
9	A1AIO	B	2030	4	1/1/4/5	4/6/19/22	0/1/1/1
9	A1AIO	B	2036	4	-	2/6/19/22	0/1/1/1
10	GLA	B	2068	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2009	4	1/1/4/5	1/6/19/22	0/1/1/1
9	A1AIO	A	2024	4	-	0/6/19/22	0/1/1/1
10	GLA	A	2063	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2043	5	-	0/6/19/22	0/1/1/1
10	GLA	A	2065	1	-	2/2/19/22	0/1/1/1
9	A1AIO	A	2053	6	-	0/6/19/22	0/1/1/1
10	GLA	B	2061	1	-	2/2/19/22	0/1/1/1
9	A1AIO	B	2014	4	1/1/4/5	3/6/19/22	0/1/1/1
9	A1AIO	A	2005	5	-	2/6/19/22	0/1/1/1
9	A1AIO	A	2051	5	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2017	4	-	0/6/19/22	0/1/1/1
9	A1AIO	A	2044	5	-	2/6/19/22	0/1/1/1
9	A1AIO	B	2026	4	-	0/6/19/22	0/1/1/1
9	A1AIO	B	2015	4	-	1/6/19/22	0/1/1/1

The worst 5 of 753 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2043	A1AIO	C05-C04	-15.09	1.28	1.53
9	B	2039	A1AIO	C05-C04	-15.06	1.28	1.53
9	A	2005	A1AIO	C05-C04	-15.06	1.28	1.53
9	A	2029	A1AIO	C05-C04	-15.04	1.28	1.53
9	A	2033	A1AIO	C05-C04	-15.03	1.28	1.53

The worst 5 of 229 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2026	A1AIO	C02-C03-C04	-4.68	109.23	115.95
9	A	2044	A1AIO	C02-C03-C04	-4.56	109.40	115.95
9	B	2033	A1AIO	C02-C03-C04	-4.55	109.42	115.95
9	B	2047	A1AIO	C02-C03-C04	-4.53	109.44	115.95
9	B	2006	A1AIO	C02-C03-C04	-4.46	109.54	115.95

5 of 29 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	2004	A1AIO	C06
9	A	2006	A1AIO	C06
9	A	2009	A1AIO	C06
9	A	2011	A1AIO	C06
9	A	2012	A1AIO	C06

5 of 169 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	A	2002	A1AIO	O12-C01-C02-O11
9	A	2005	A1AIO	O12-C01-C02-O11
9	A	2030	A1AIO	C01-C02-C03-O07
9	A	2033	A1AIO	C01-C02-C03-O07
9	A	2035	A1AIO	O12-C01-C02-C03

There are no ring outliers.

103 monomers are involved in 123 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2010	A1AIO	1	0
9	B	2005	A1AIO	1	0
9	B	2031	A1AIO	1	0
9	A	2011	A1AIO	1	0
9	A	2019	A1AIO	1	0
9	A	2031	A1AIO	1	0
9	A	2054	A1AIO	1	0
9	A	2040	A1AIO	2	0
9	B	2025	A1AIO	2	0
9	B	2011	A1AIO	1	0
9	A	2021	A1AIO	1	0
9	A	2020	A1AIO	1	0
9	B	2012	A1AIO	1	0
9	A	2027	A1AIO	1	0
9	B	2016	A1AIO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	2022	A1AIO	1	0
9	A	2013	A1AIO	1	0
9	B	2023	A1AIO	2	0
9	B	2050	A1AIO	1	0
10	B	2060	GLA	6	0
9	A	2039	A1AIO	1	0
9	A	2018	A1AIO	1	0
9	B	2049	A1AIO	1	0
9	B	2038	A1AIO	1	0
9	A	2007	A1AIO	1	0
9	A	2045	A1AIO	1	0
9	B	2024	A1AIO	2	0
9	A	2047	A1AIO	1	0
9	A	2046	A1AIO	1	0
9	B	2002	A1AIO	1	0
9	B	2053	A1AIO	1	0
9	B	2029	A1AIO	2	0
9	B	2040	A1AIO	1	0
9	B	2051	A1AIO	1	0
9	B	2010	A1AIO	1	0
9	A	2041	A1AIO	1	0
9	B	2041	A1AIO	1	0
9	B	2046	A1AIO	1	0
9	A	2052	A1AIO	1	0
9	B	2033	A1AIO	1	0
9	B	2054	A1AIO	1	0
9	B	2032	A1AIO	1	0
9	A	2004	A1AIO	2	0
9	A	2035	A1AIO	1	0
9	A	2030	A1AIO	1	0
9	B	2020	A1AIO	1	0
9	B	2028	A1AIO	1	0
9	A	2048	A1AIO	1	0
9	A	2026	A1AIO	1	0
9	B	2004	A1AIO	1	0
9	A	2008	A1AIO	1	0
9	A	2014	A1AIO	1	0
9	B	2056	A1AIO	1	0
9	B	2019	A1AIO	2	0
9	A	2055	A1AIO	2	0
9	B	2057	A1AIO	1	0
9	A	2001	A1AIO	1	0

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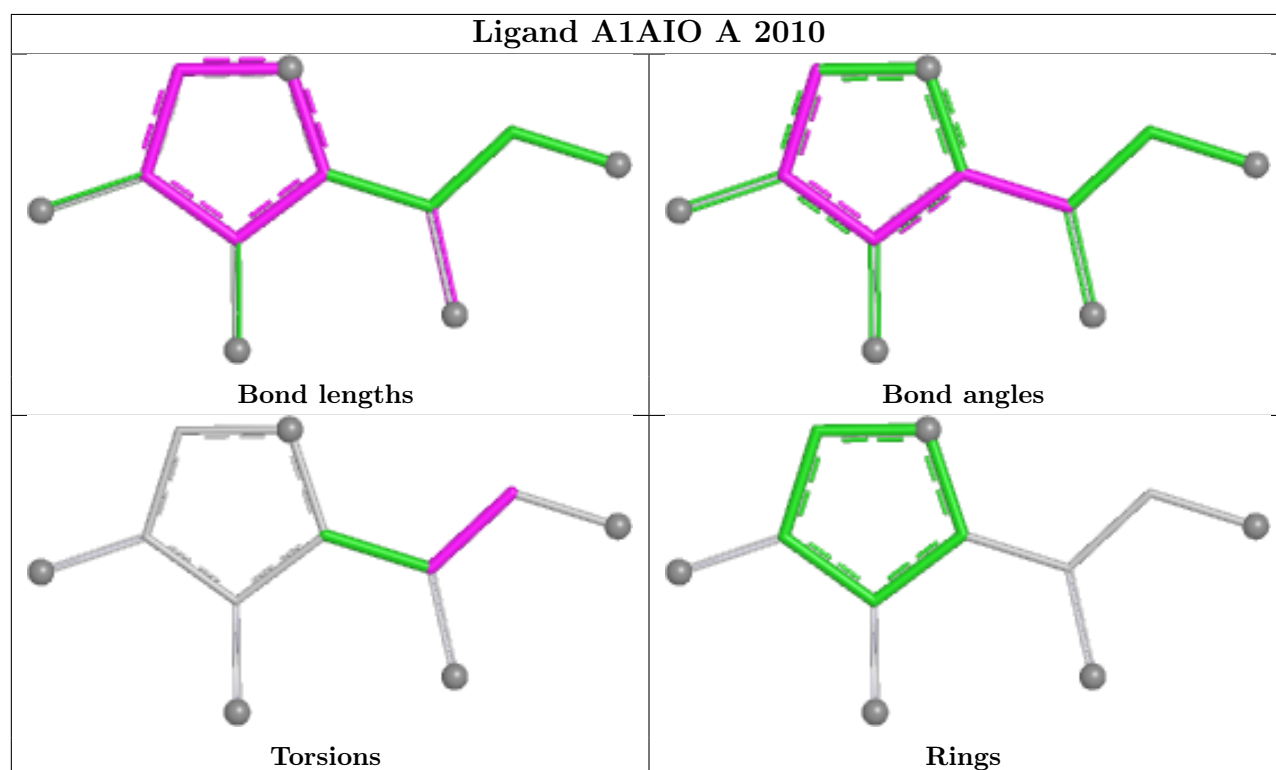
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	2037	A1AIO	1	0
9	A	2038	A1AIO	1	0
9	A	2006	A1AIO	1	0
10	B	2067	GLA	1	0
9	B	2035	A1AIO	1	0
9	B	2006	A1AIO	1	0
9	A	2042	A1AIO	1	0
9	B	2007	A1AIO	1	0
9	A	2036	A1AIO	1	0
9	A	2016	A1AIO	1	0
9	A	2022	A1AIO	1	0
9	A	2056	A1AIO	1	0
9	B	2021	A1AIO	1	0
9	B	2013	A1AIO	1	0
9	B	2008	A1AIO	1	0
9	A	2057	A1AIO	1	0
10	A	2061	GLA	1	0
9	A	2049	A1AIO	1	0
9	B	2039	A1AIO	1	0
9	A	2003	A1AIO	1	0
10	B	2058	GLA	1	0
9	B	2055	A1AIO	2	0
9	B	2018	A1AIO	2	0
9	A	2029	A1AIO	1	0
9	B	2047	A1AIO	1	0
10	A	2059	GLA	2	0
9	B	2034	A1AIO	2	0
9	B	2001	A1AIO	1	0
9	B	2003	A1AIO	1	0
9	A	2025	A1AIO	1	0
9	A	2012	A1AIO	1	0
9	A	2028	A1AIO	1	0
9	A	2033	A1AIO	2	0
9	B	2017	A1AIO	1	0
9	A	2023	A1AIO	1	0
9	A	2050	A1AIO	2	0
9	A	2032	A1AIO	1	0
9	B	2027	A1AIO	1	0
9	B	2030	A1AIO	1	0
9	A	2009	A1AIO	1	0
9	A	2043	A1AIO	1	0
9	A	2051	A1AIO	1	0

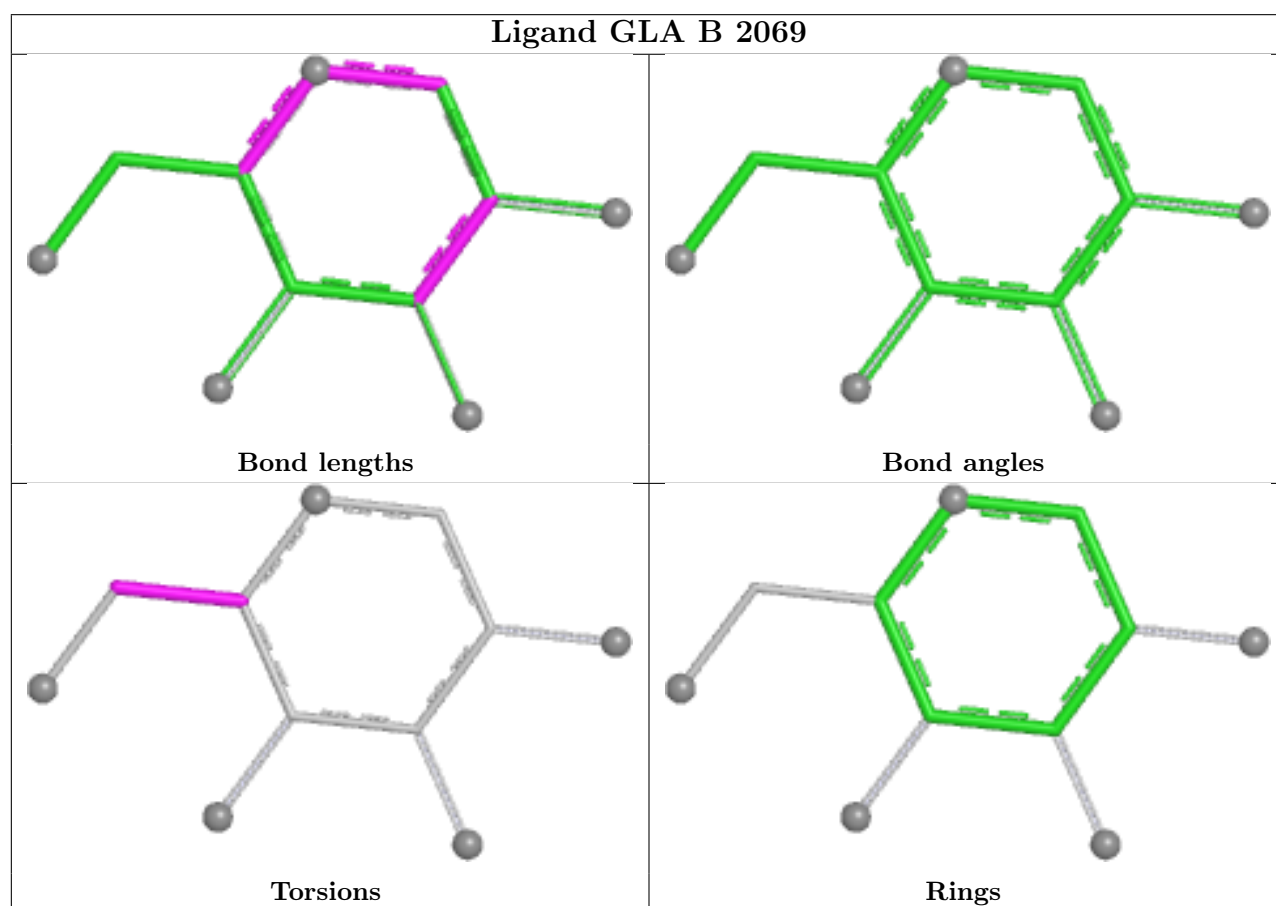
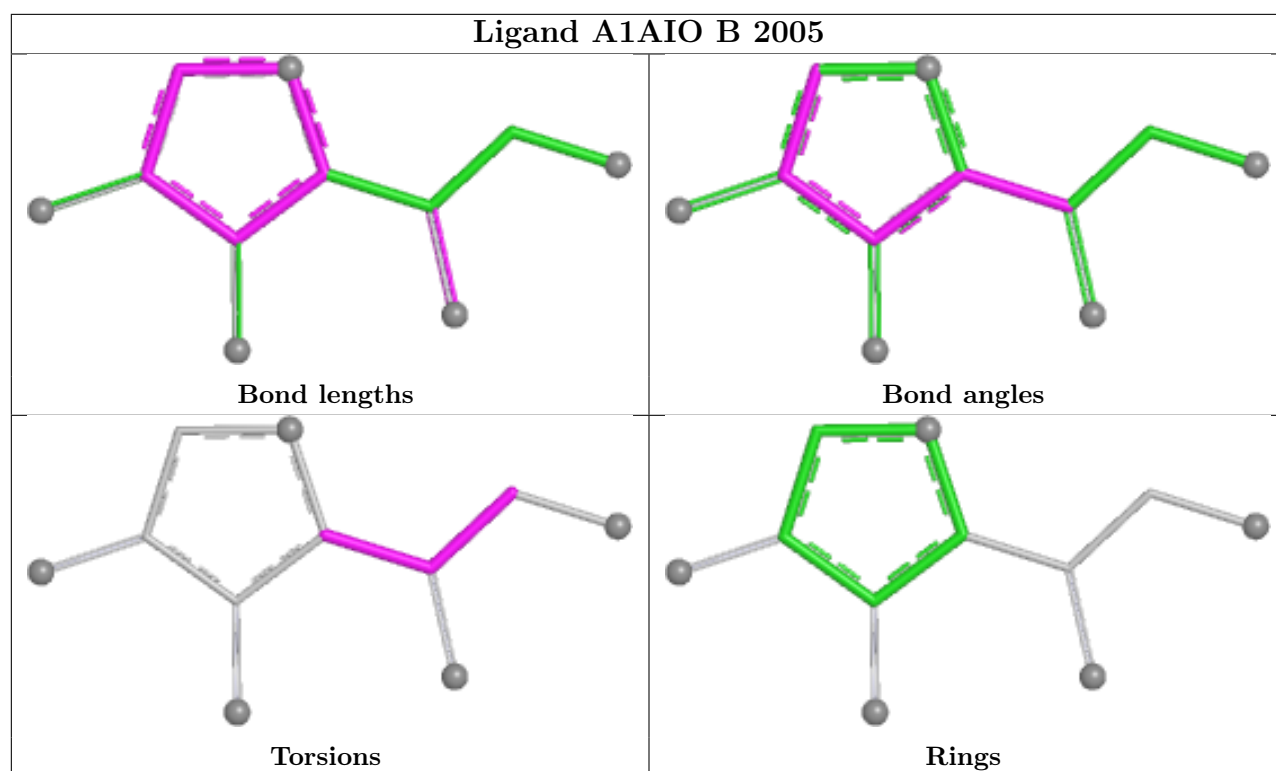
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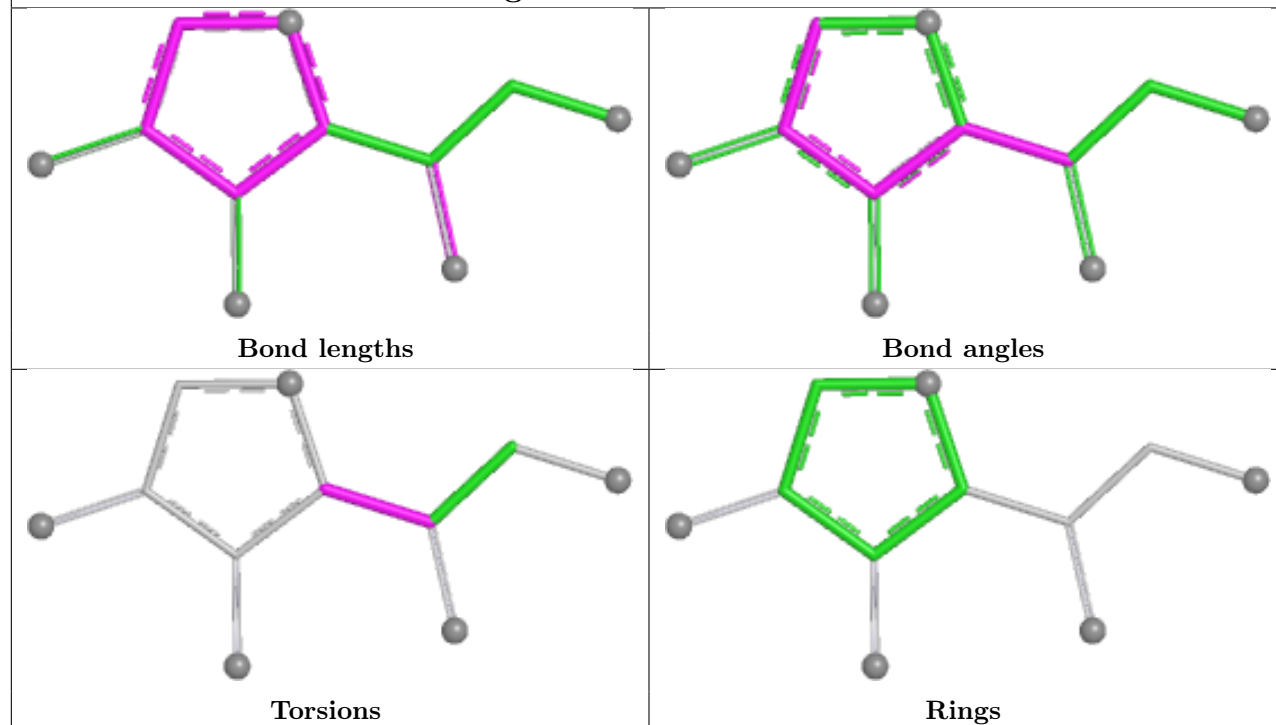
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	2014	A1AIO	1	0
9	A	2017	A1AIO	1	0
9	B	2026	A1AIO	1	0
9	B	2015	A1AIO	2	0

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

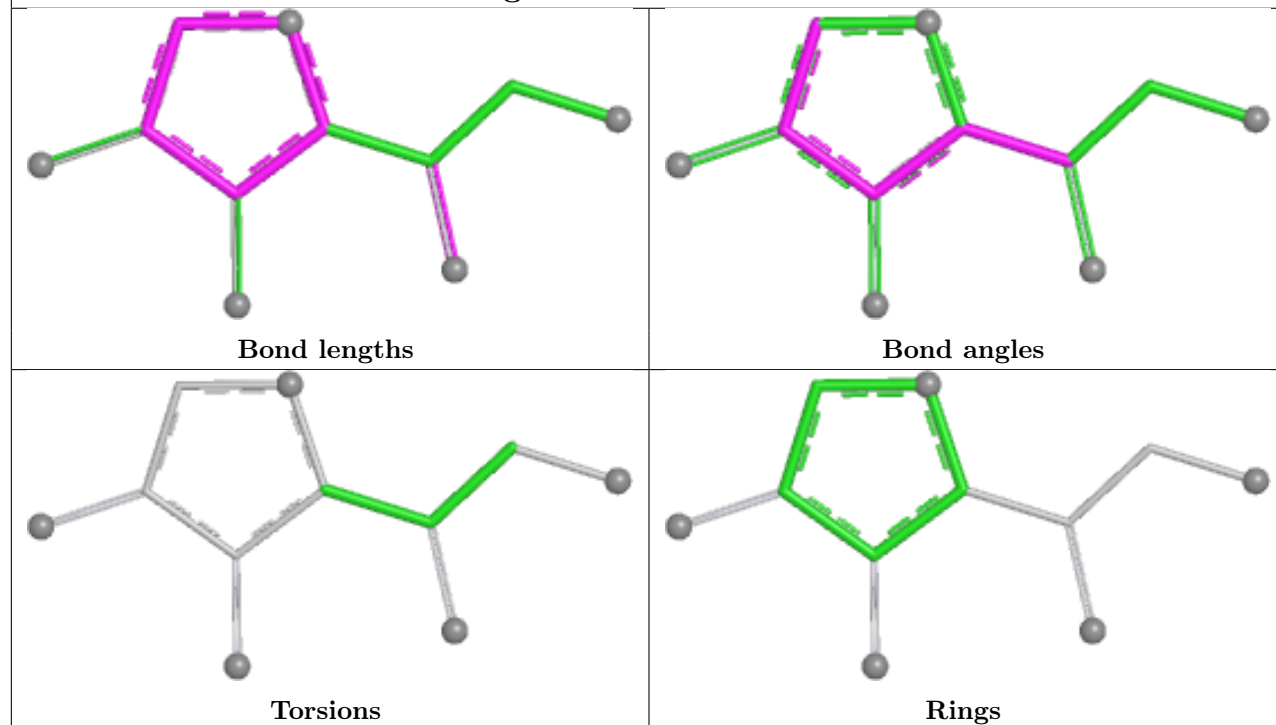




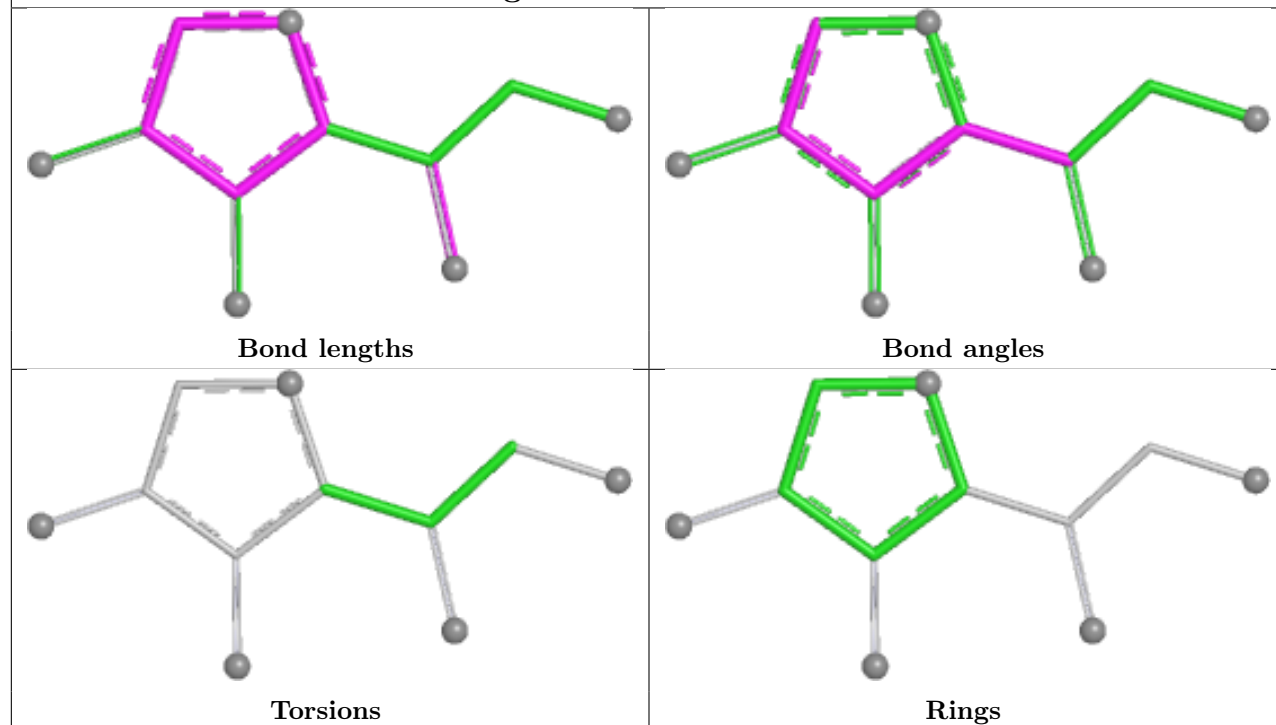
Ligand A1AIO B 2031



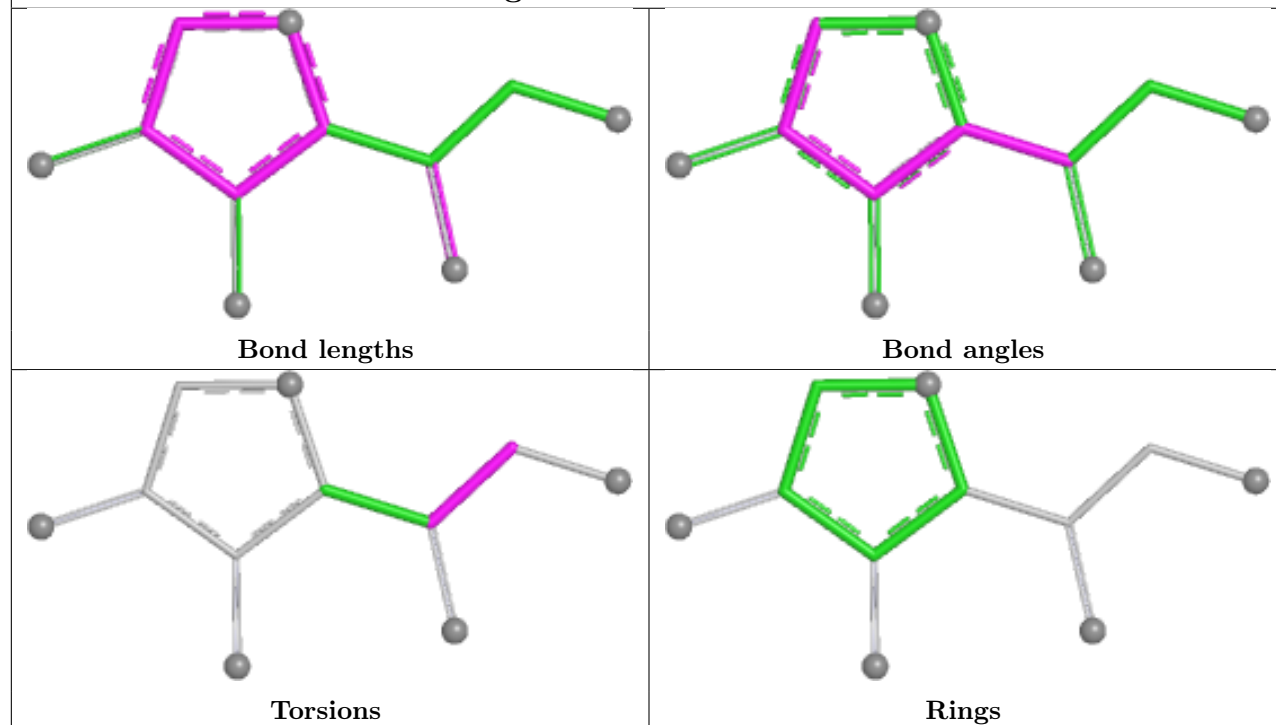
Ligand A1AIO A 2011



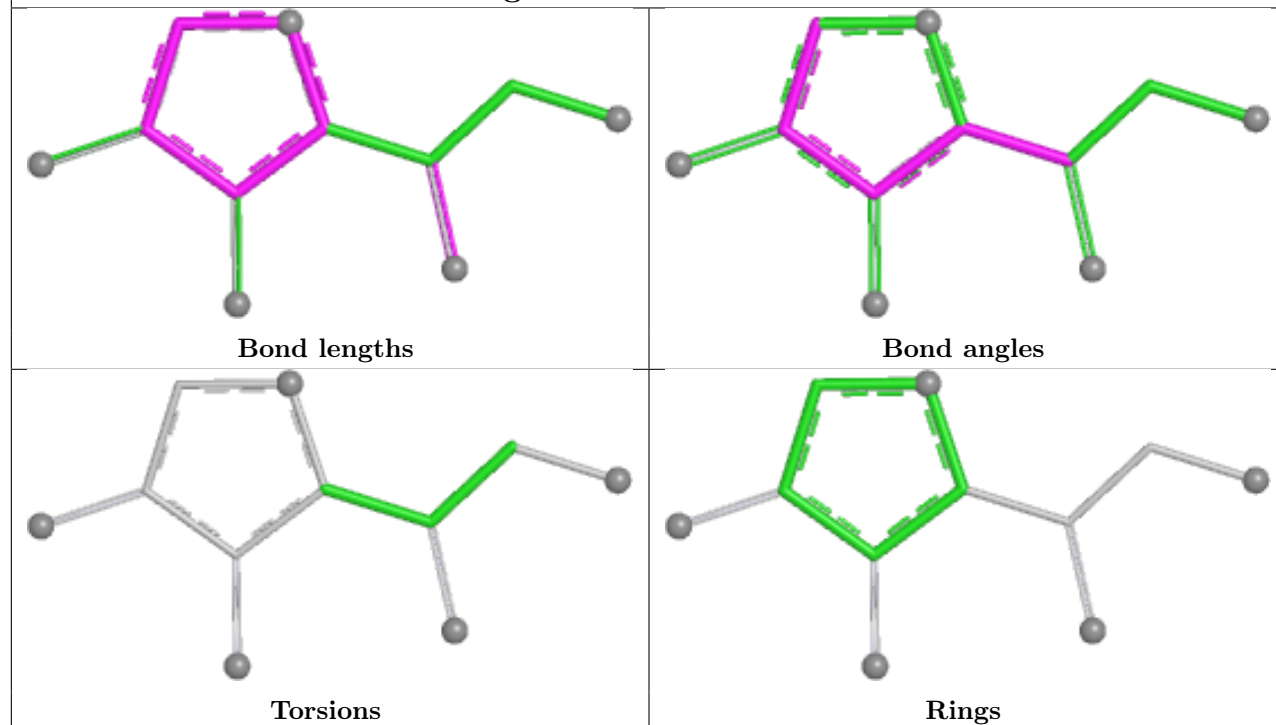
Ligand A1AIO A 2019



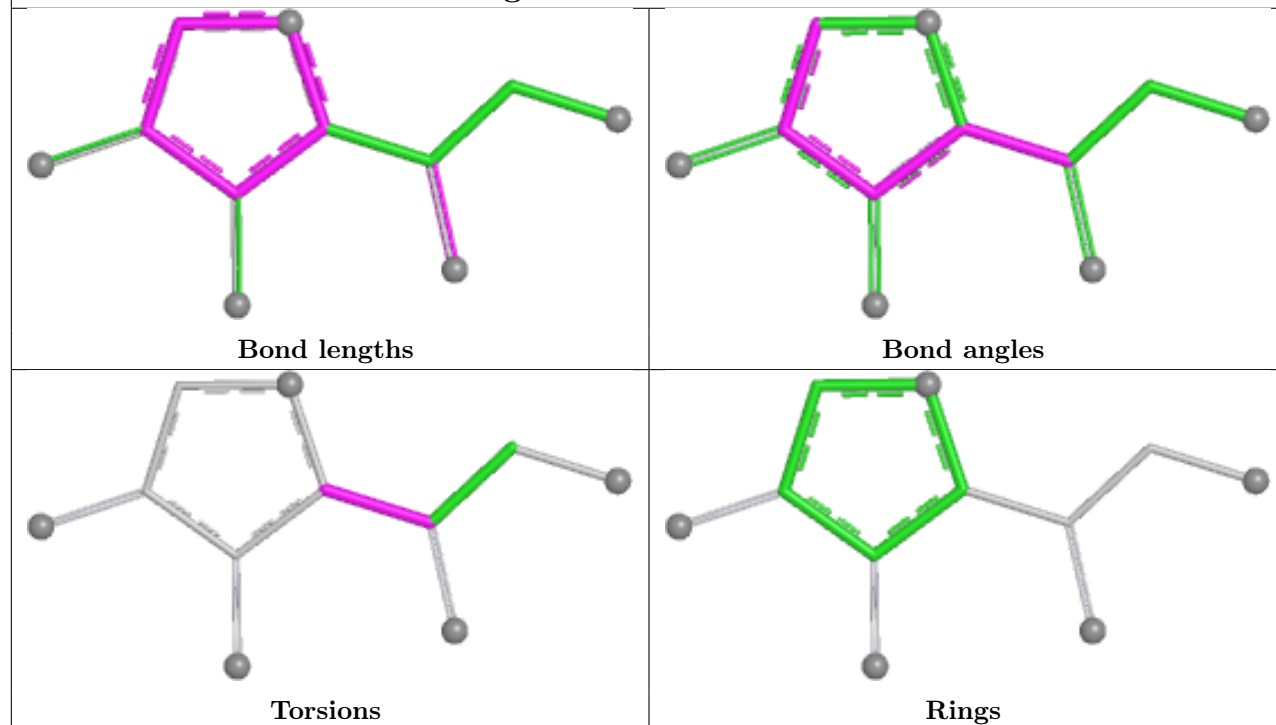
Ligand A1AIO B 2037

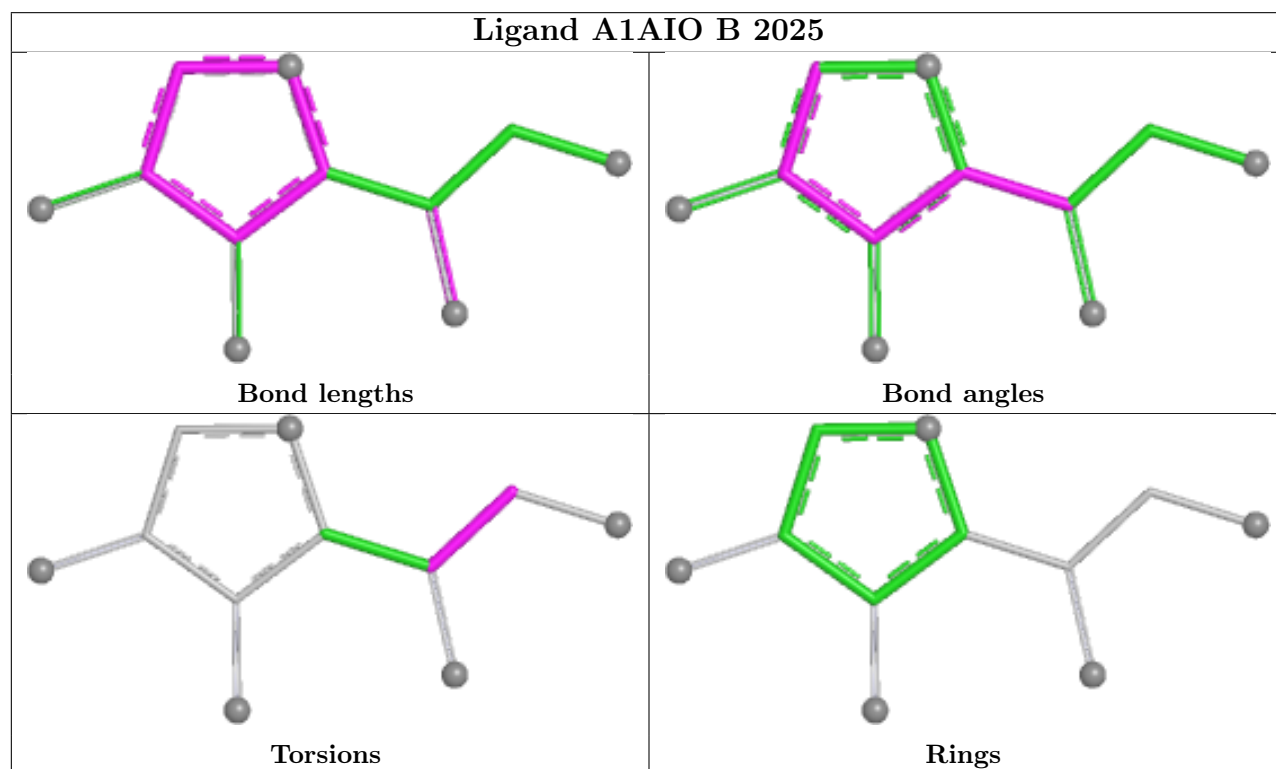
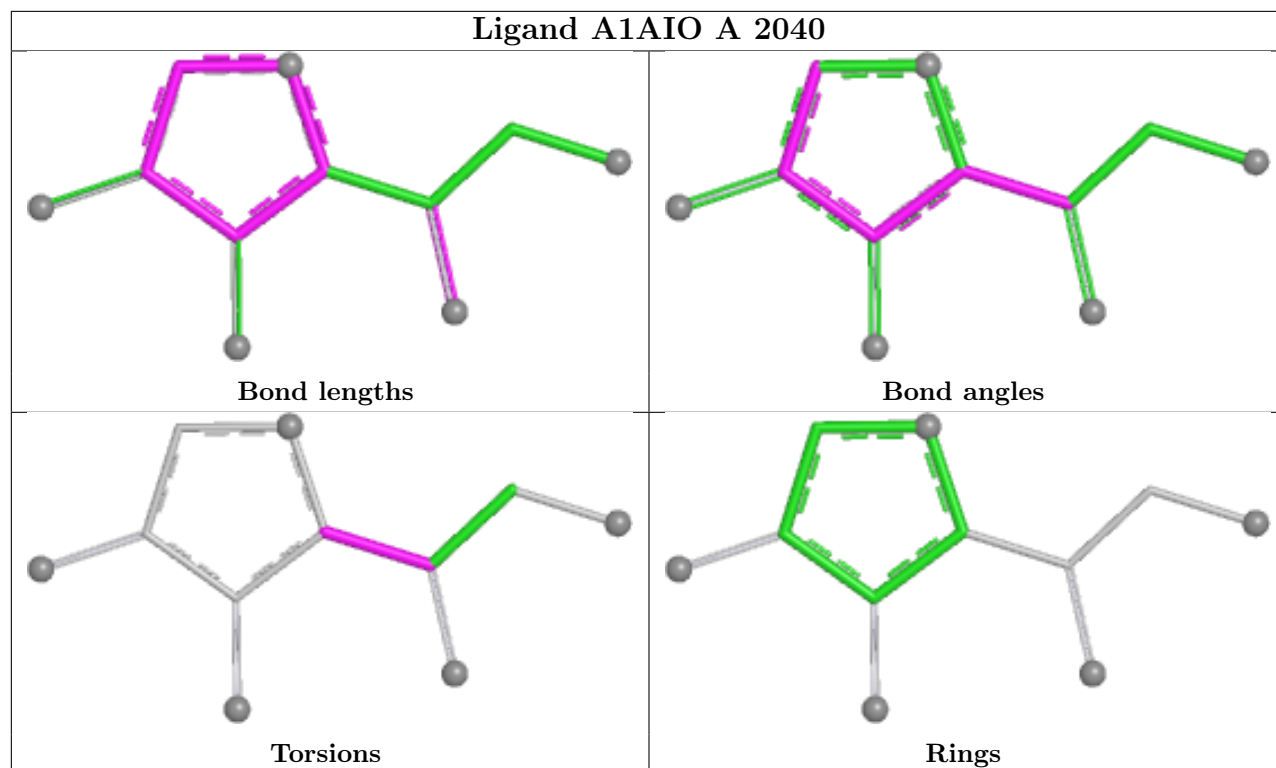


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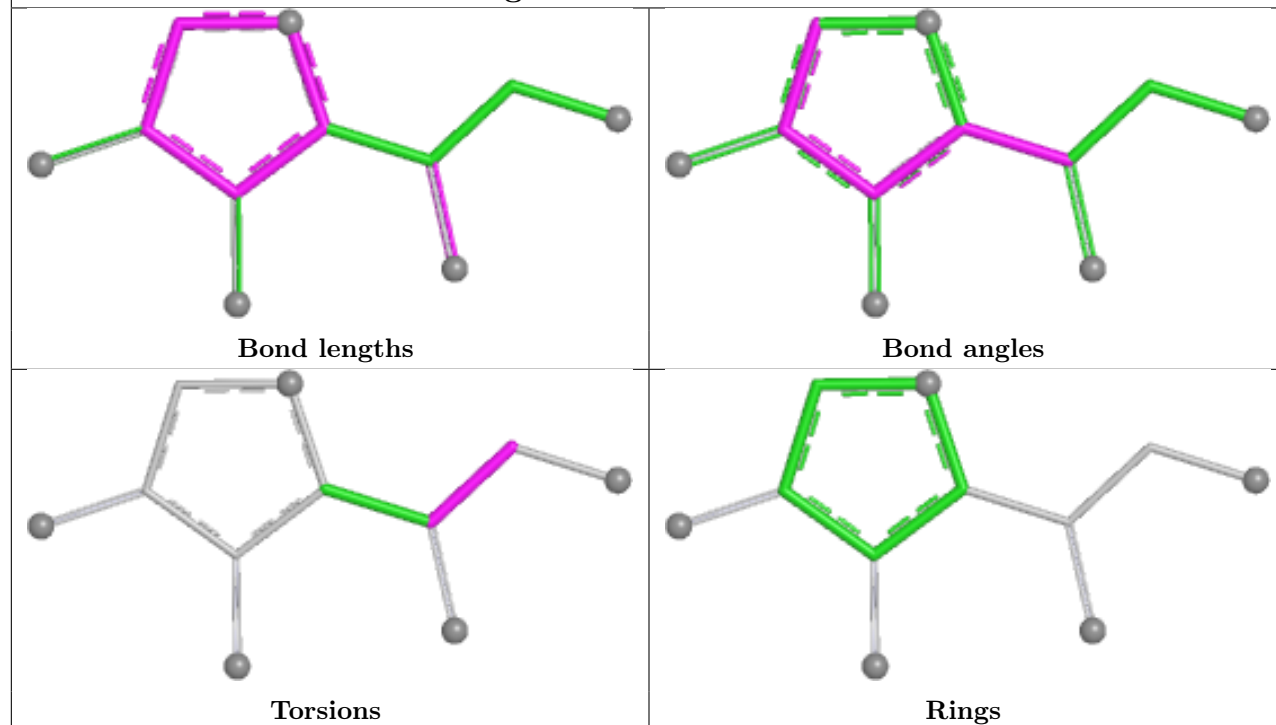


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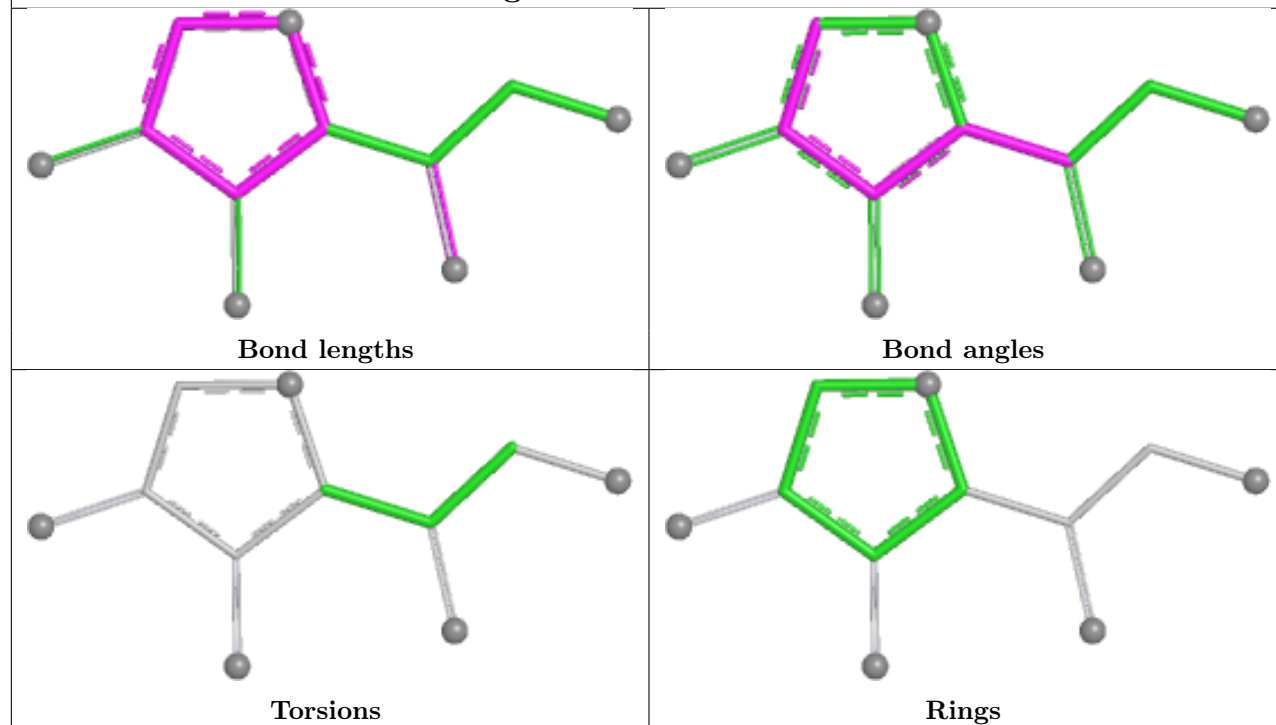


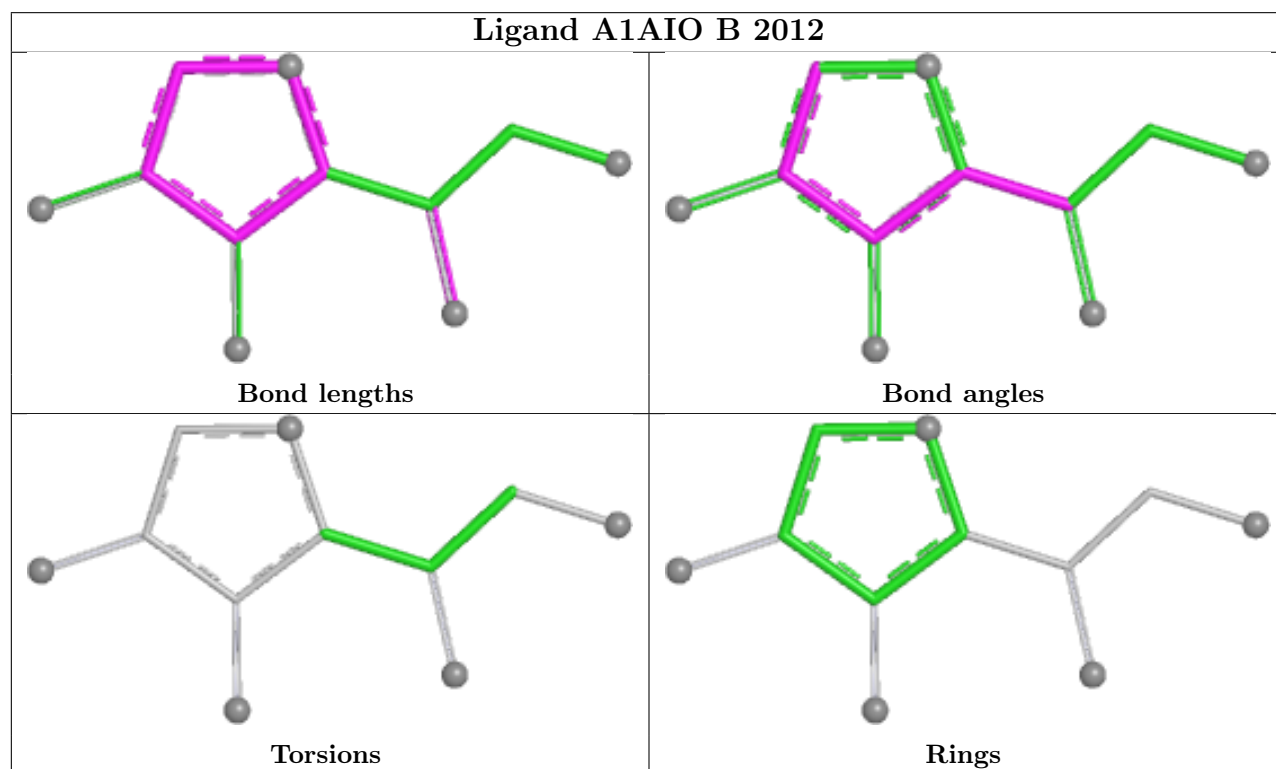
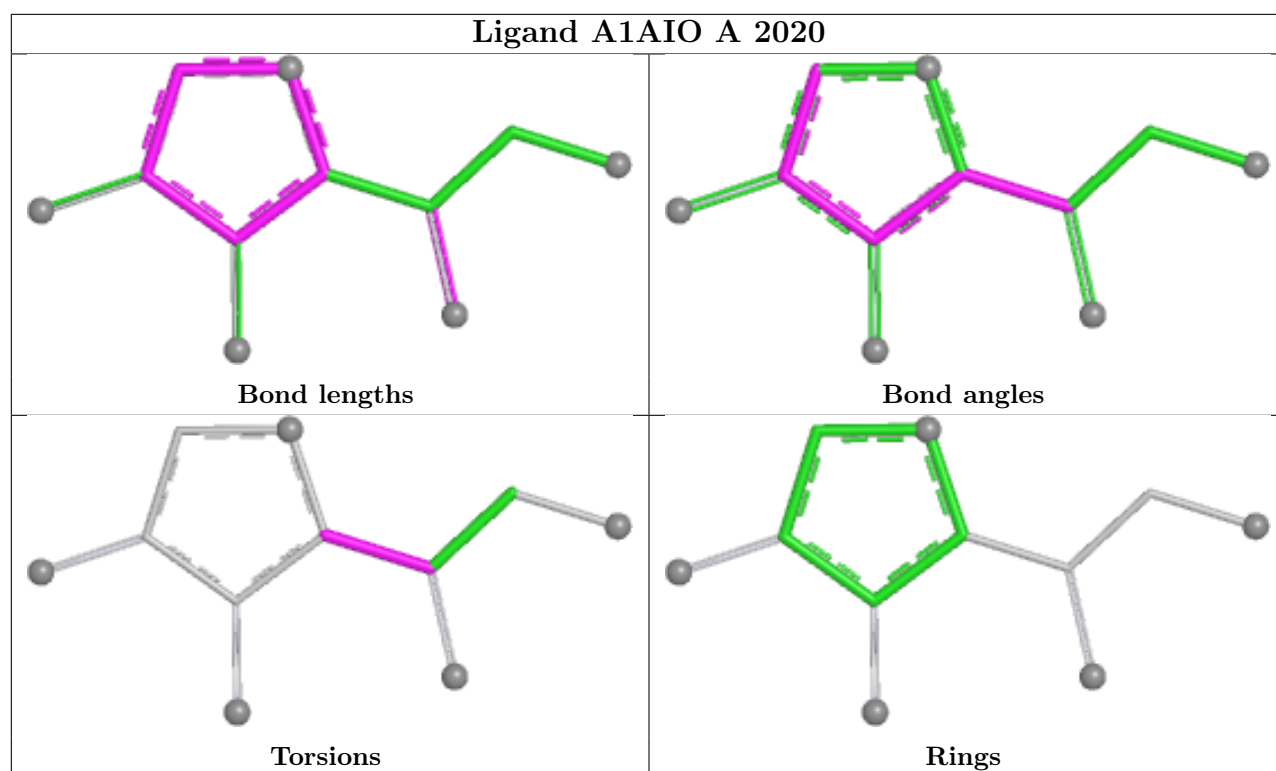


Ligand A1AIO B 2011

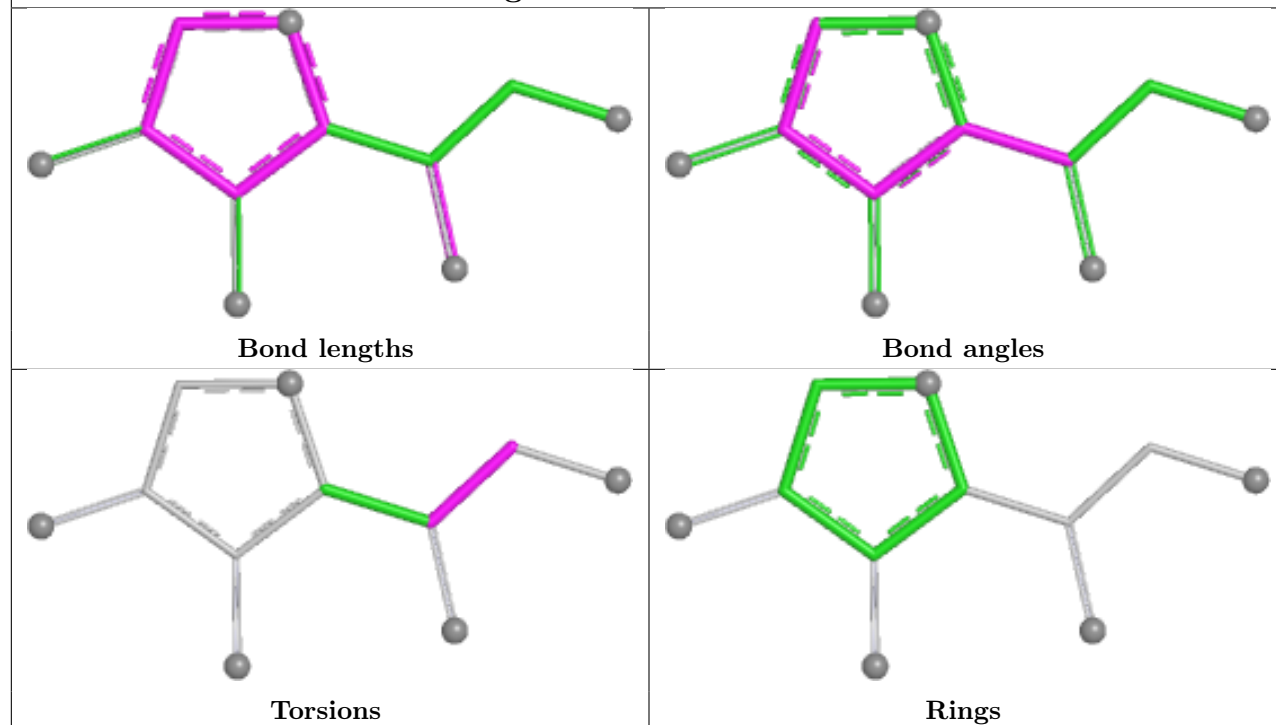


Ligand A1AIO A 2021

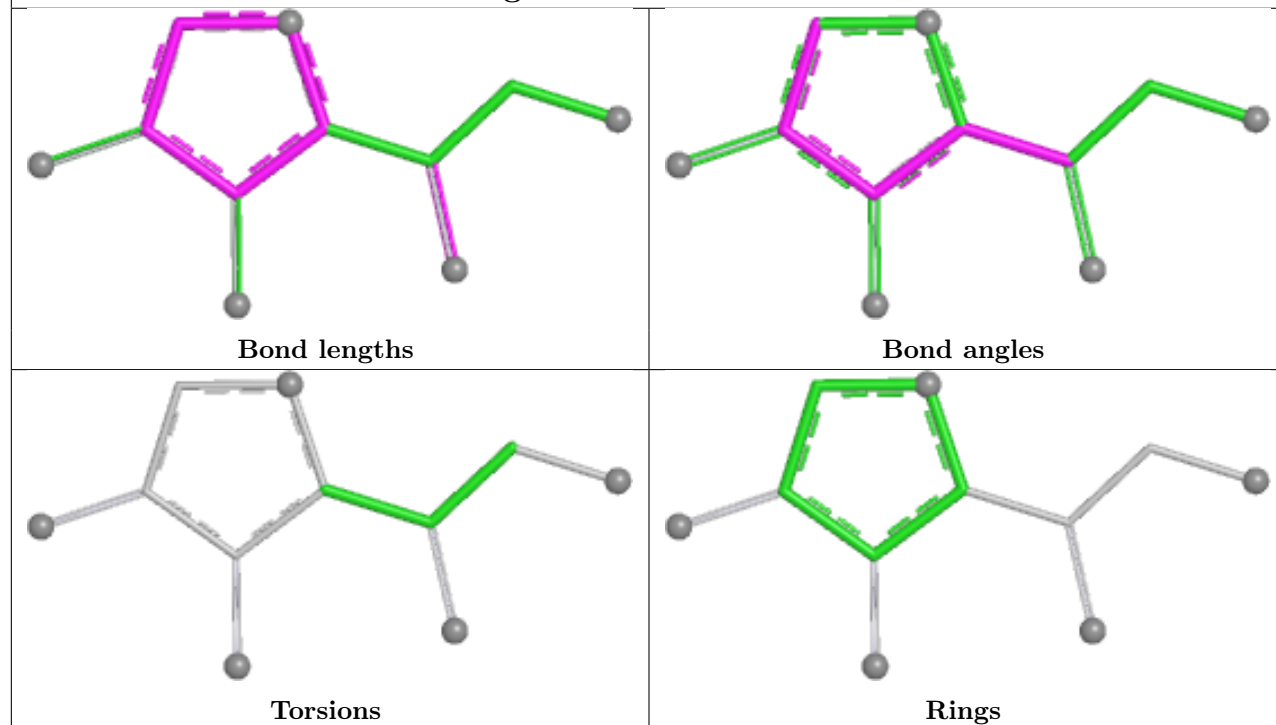


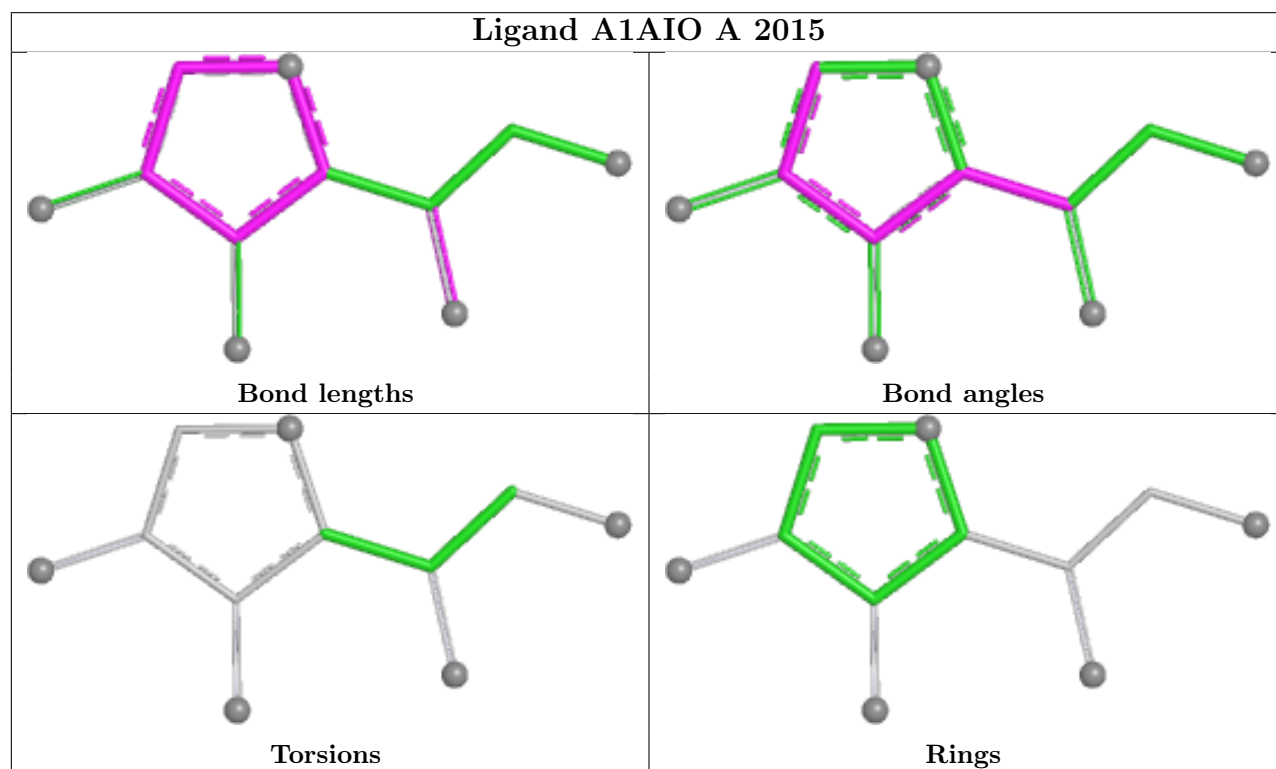
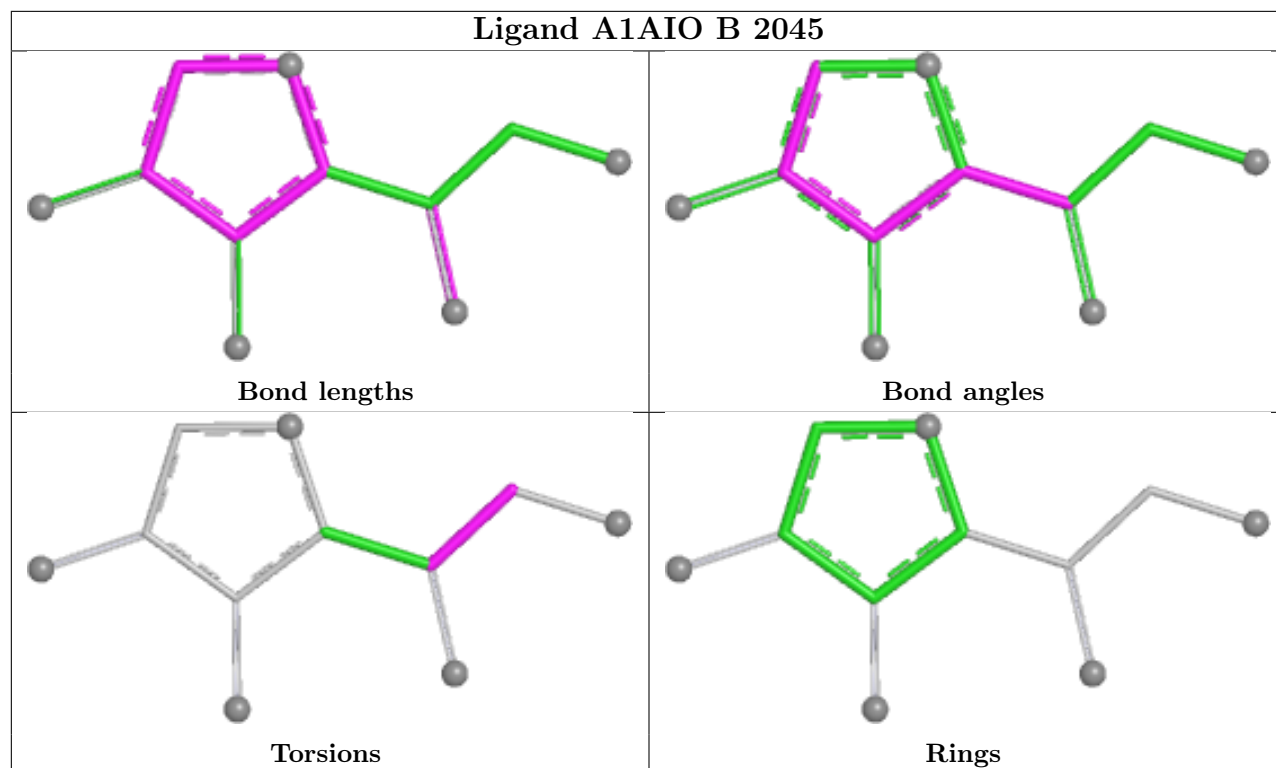


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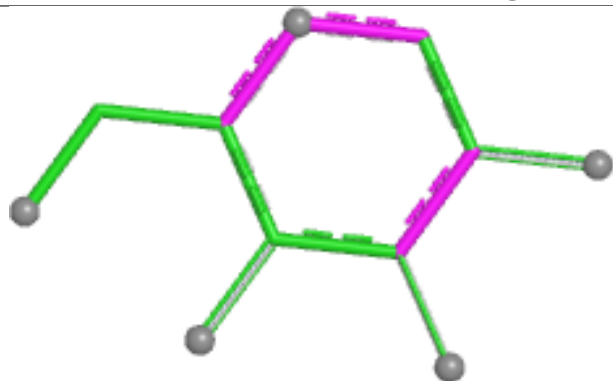


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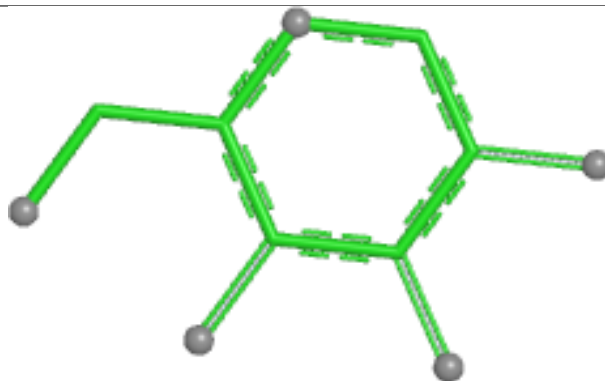




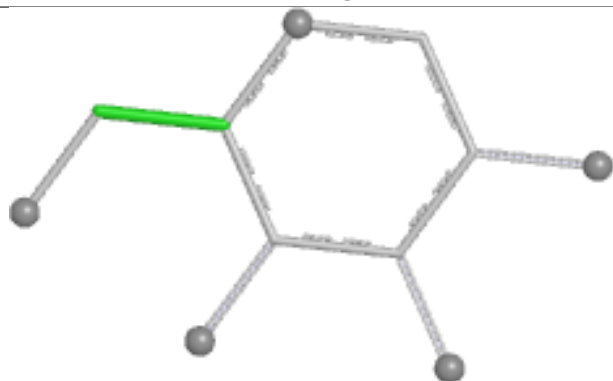
Ligand GLA A 2066



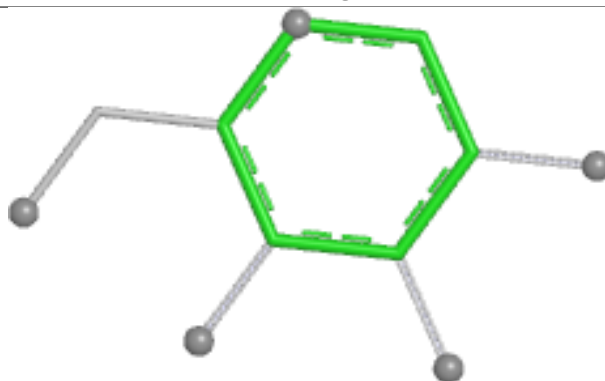
Bond lengths



Bond angles

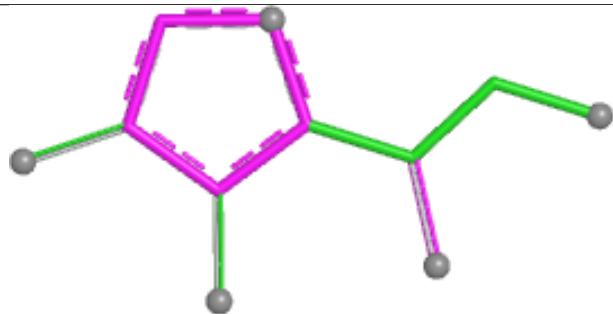


Torsions

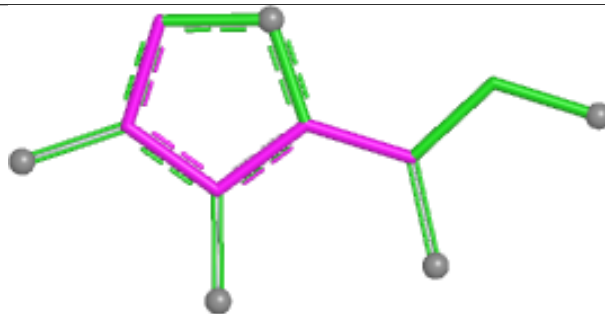


Rings

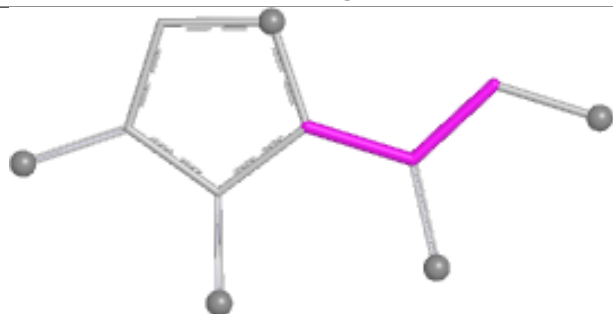
Ligand A1AIO B 2016



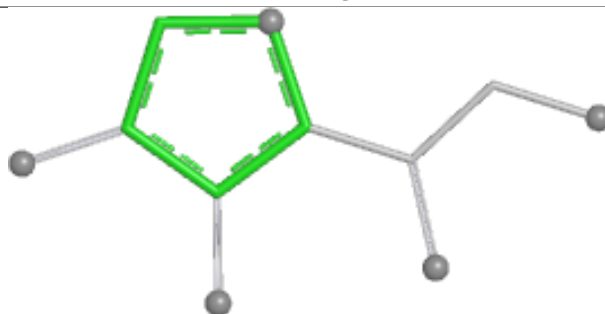
Bond lengths



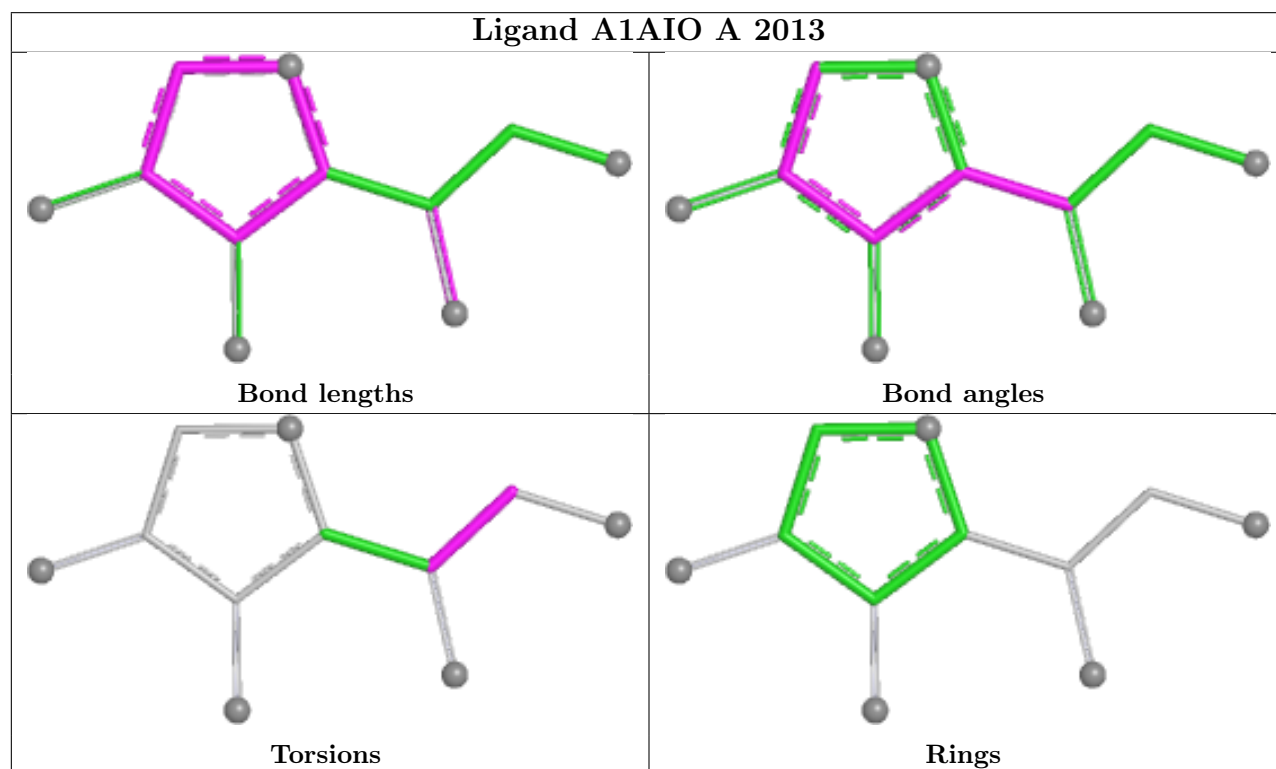
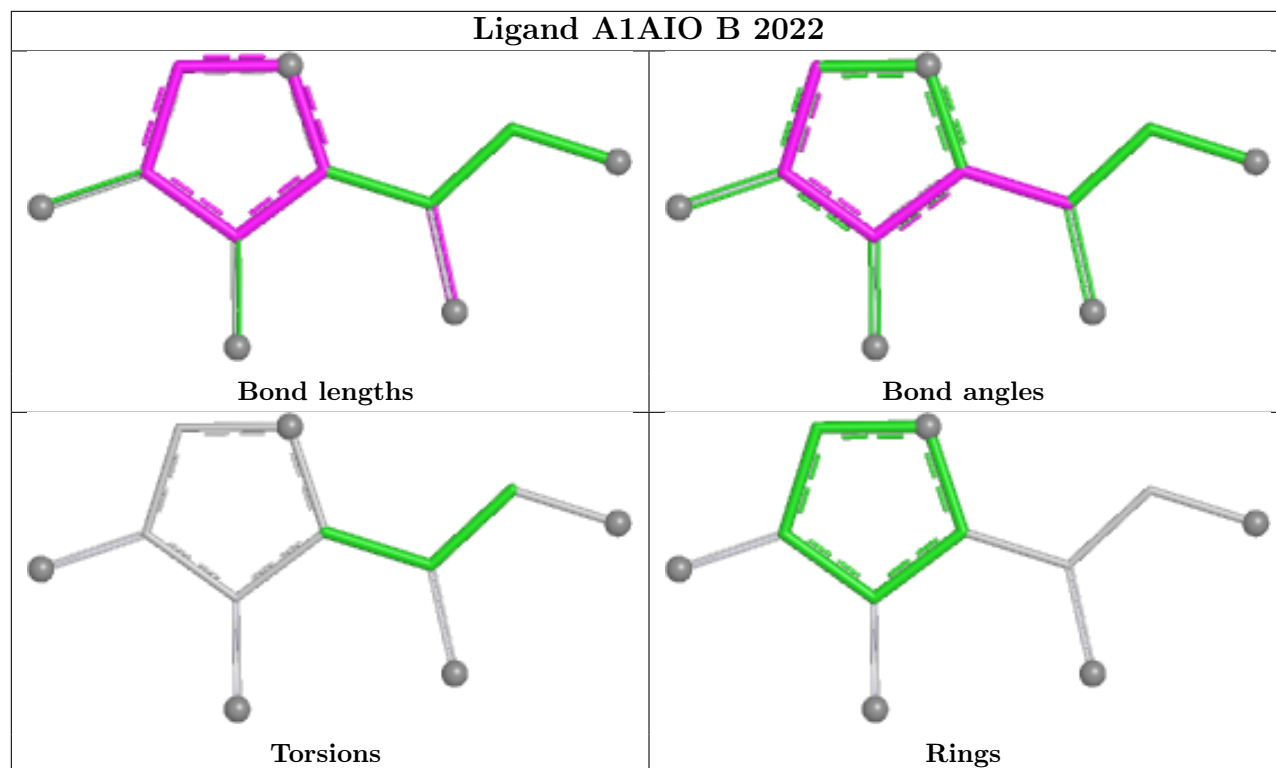
Bond angles

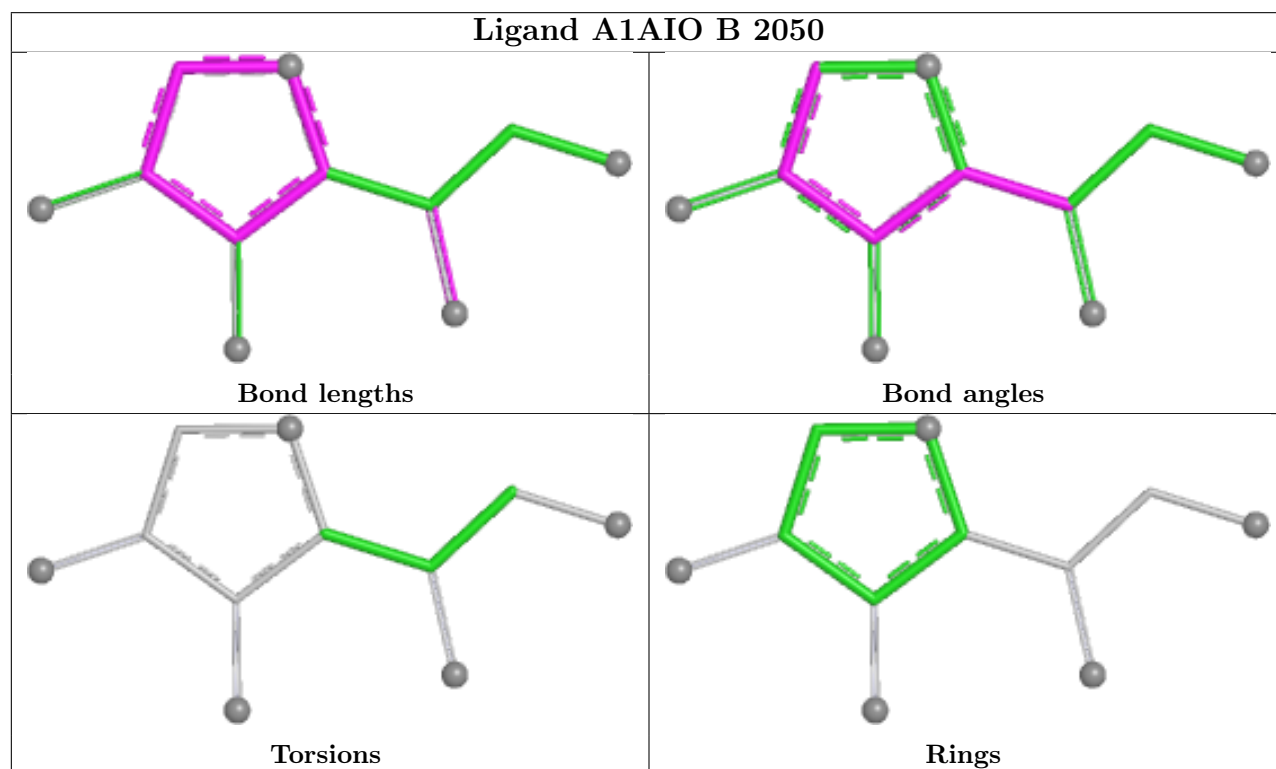
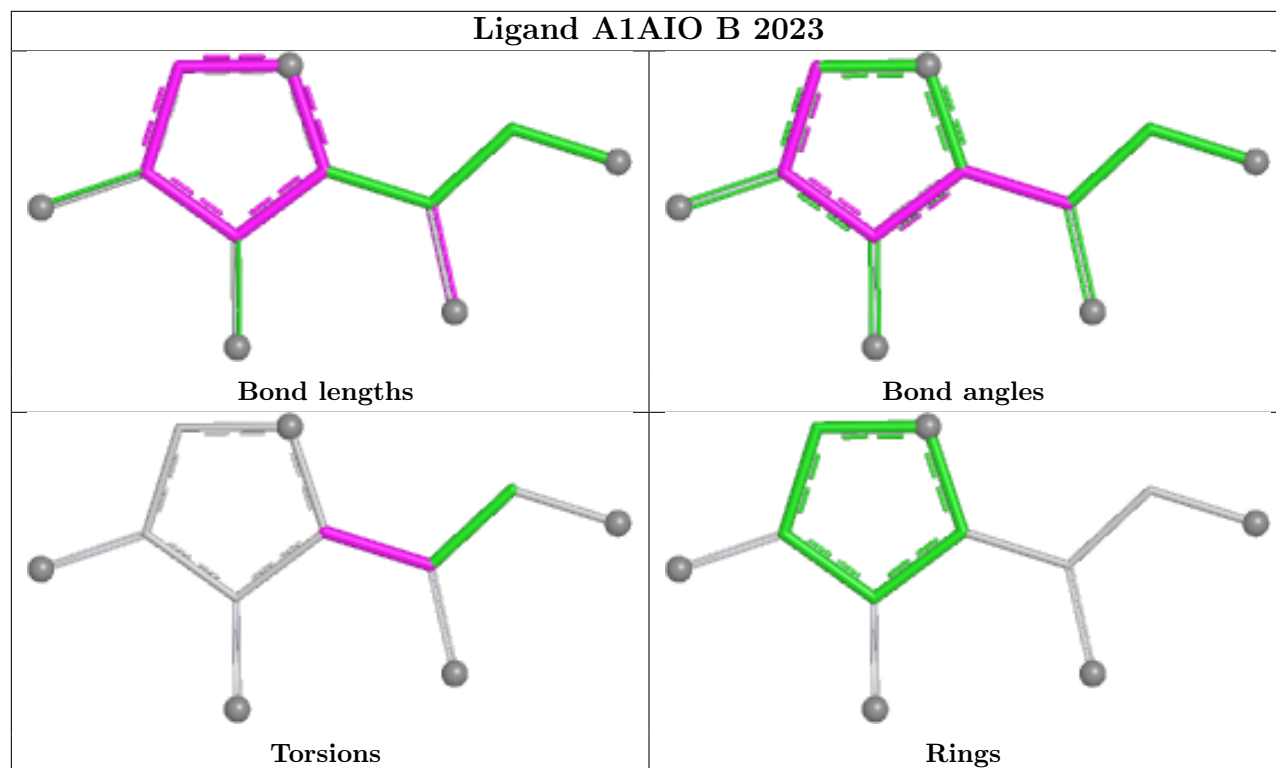


Torsions

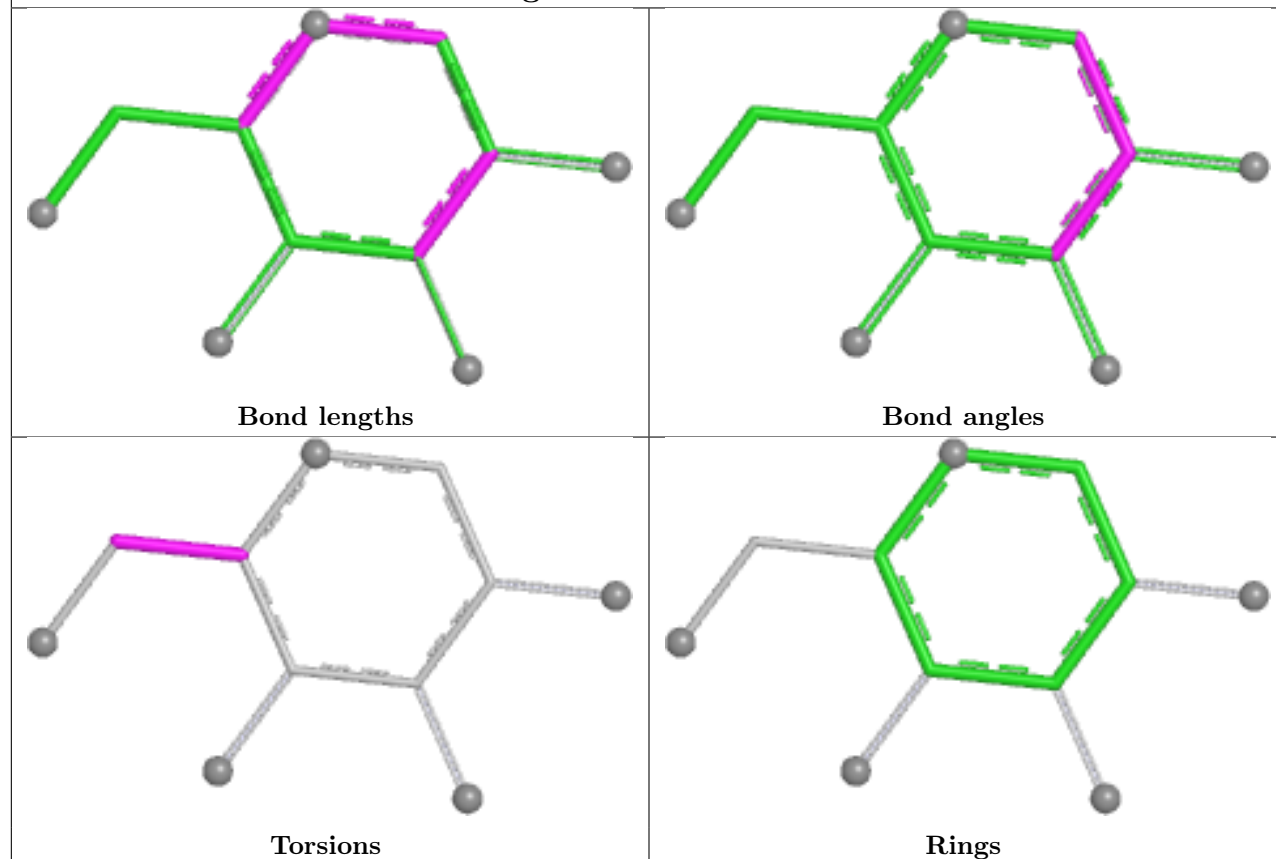


Rings

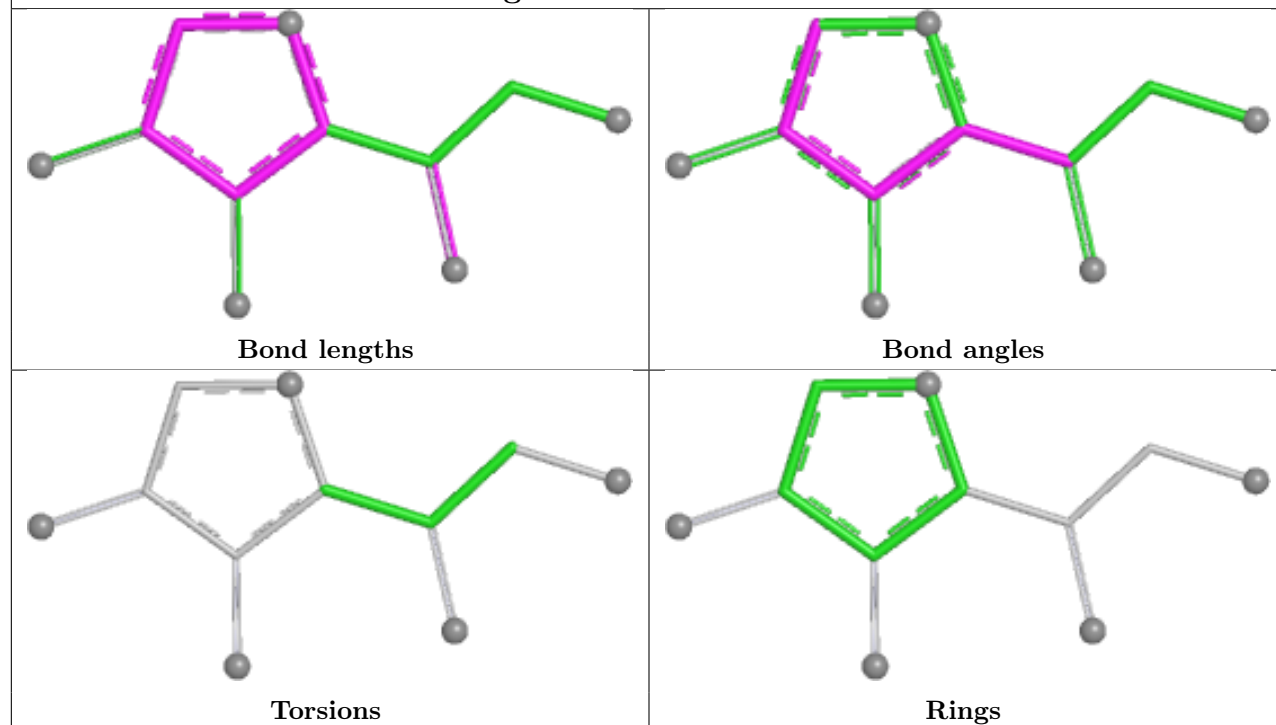




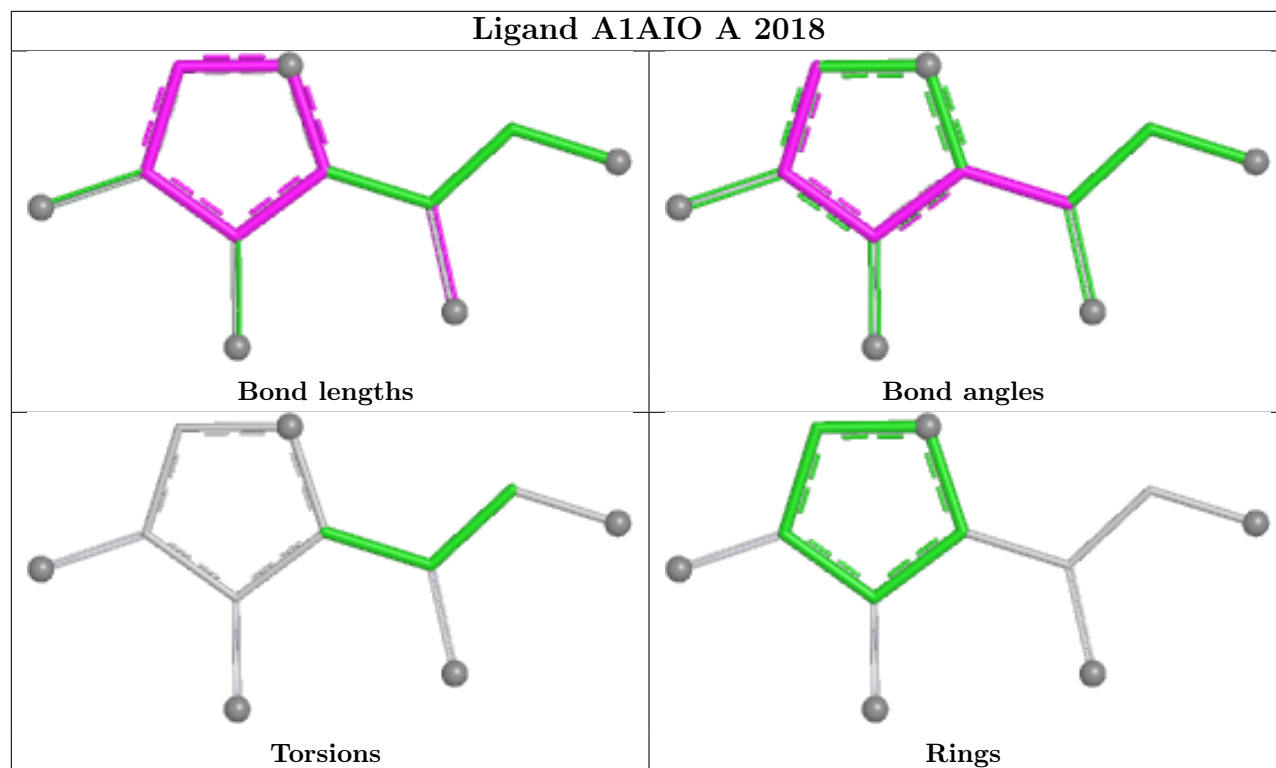
Ligand GLA B 2060



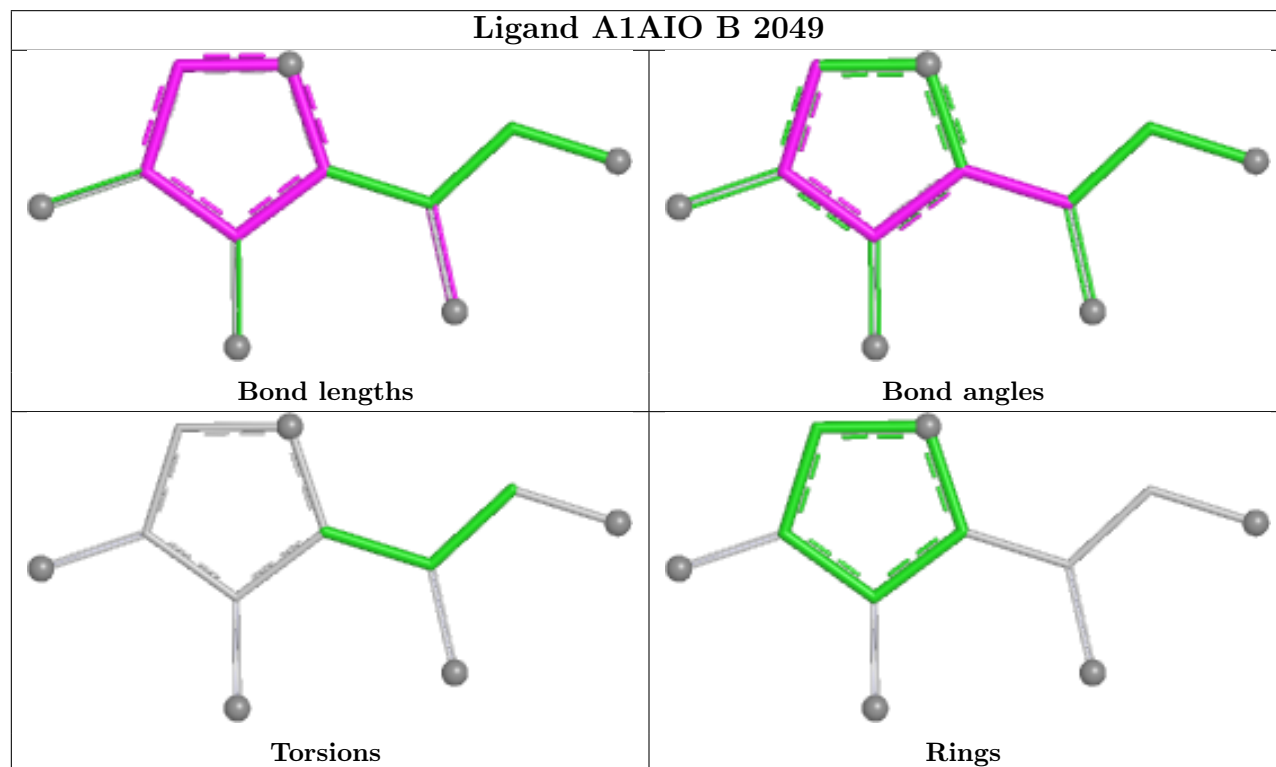
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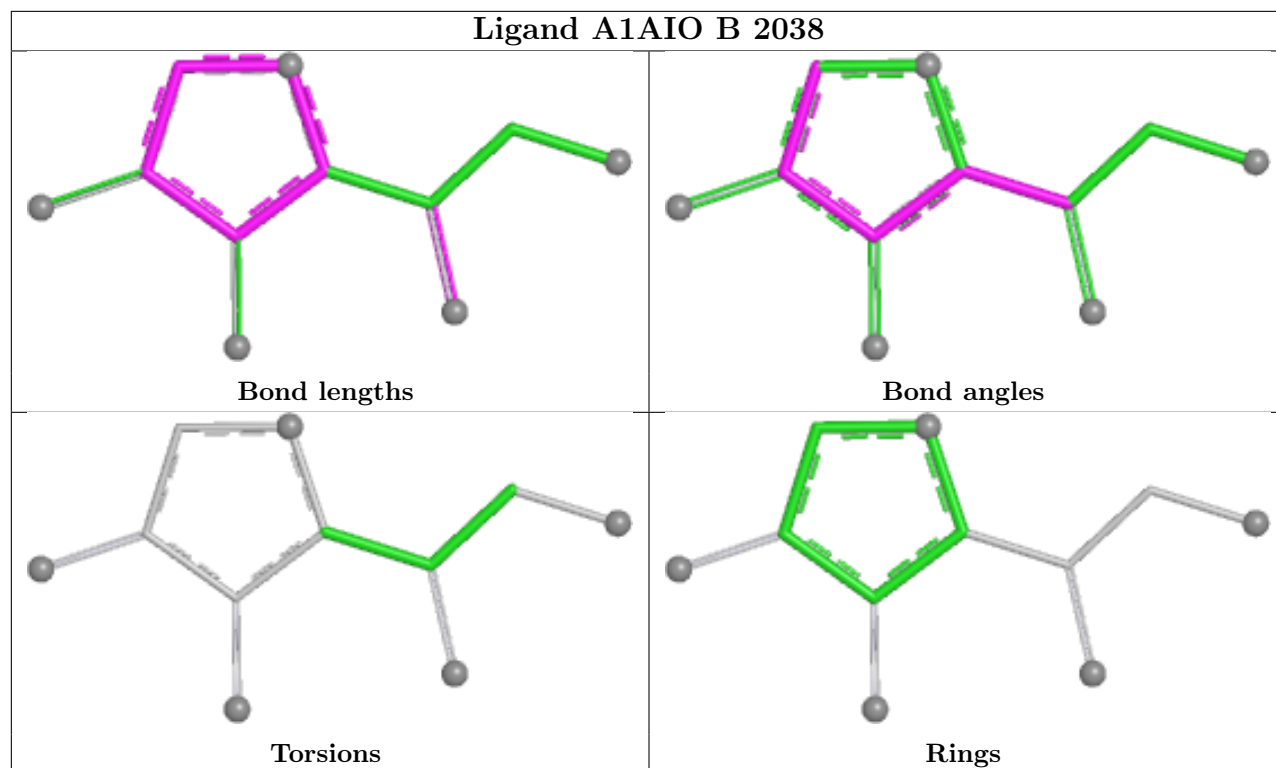
Ligand A1AIO A 2018



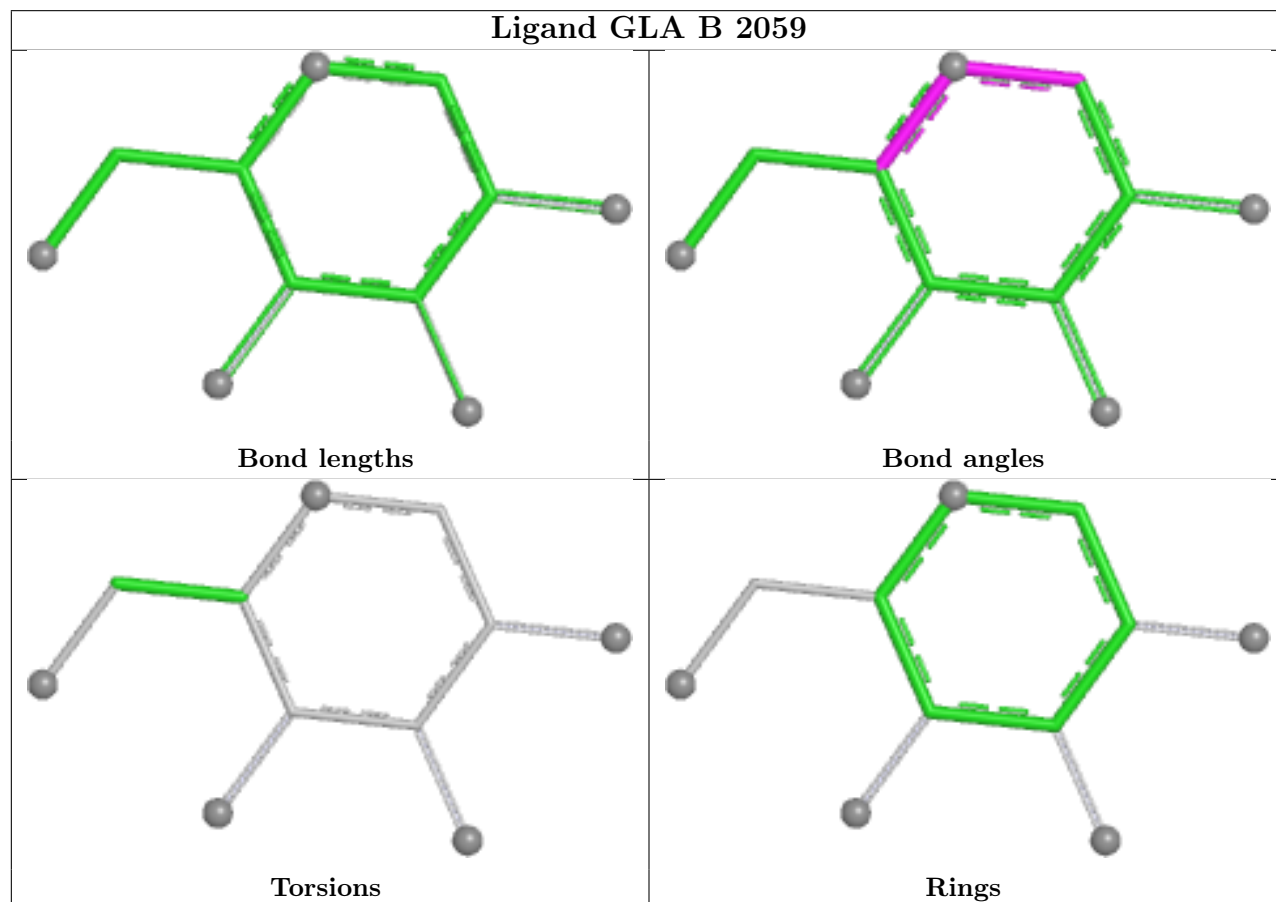
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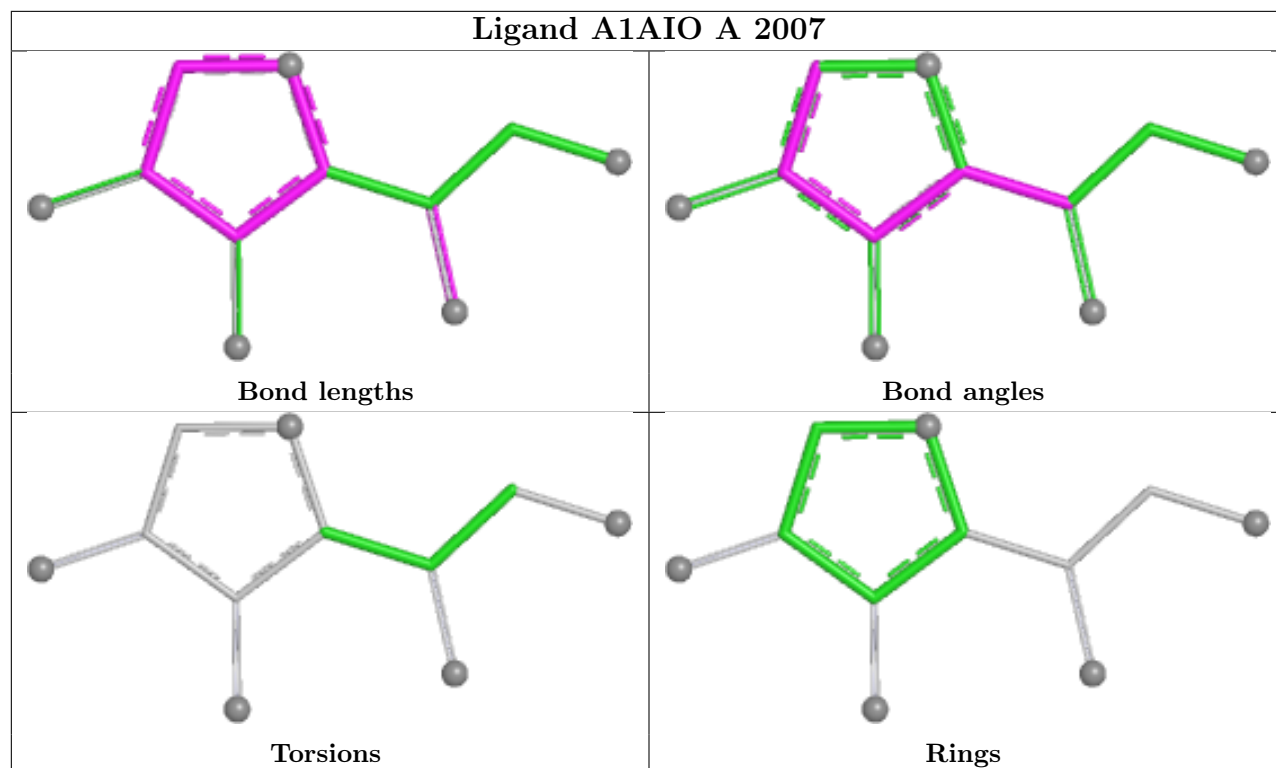
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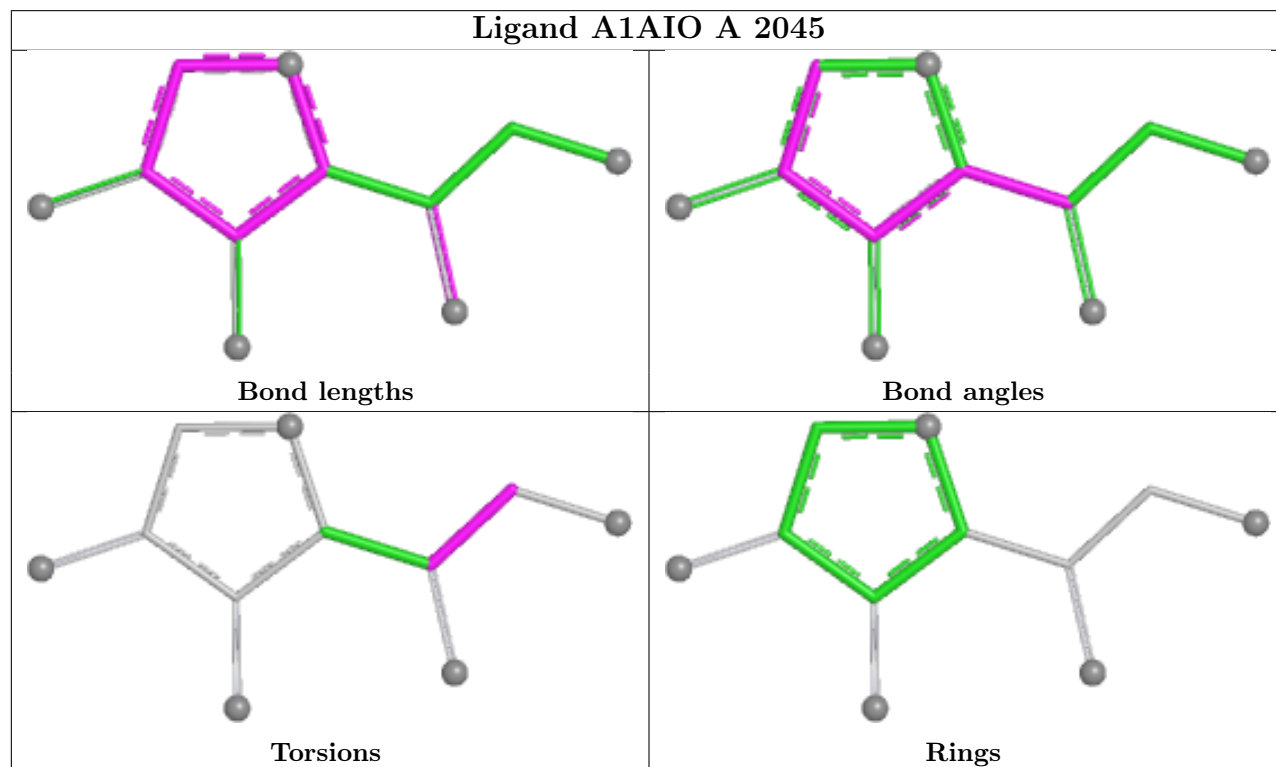
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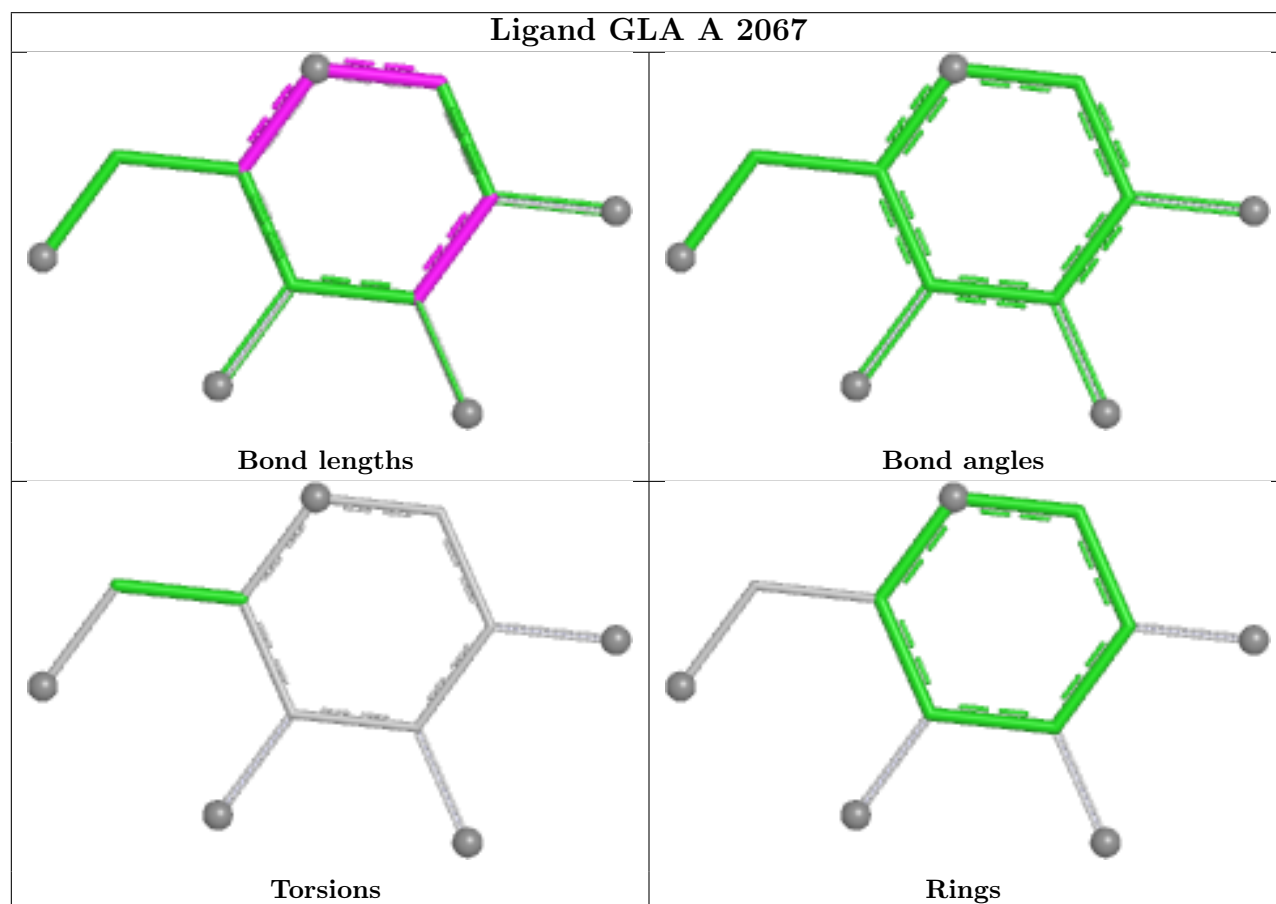
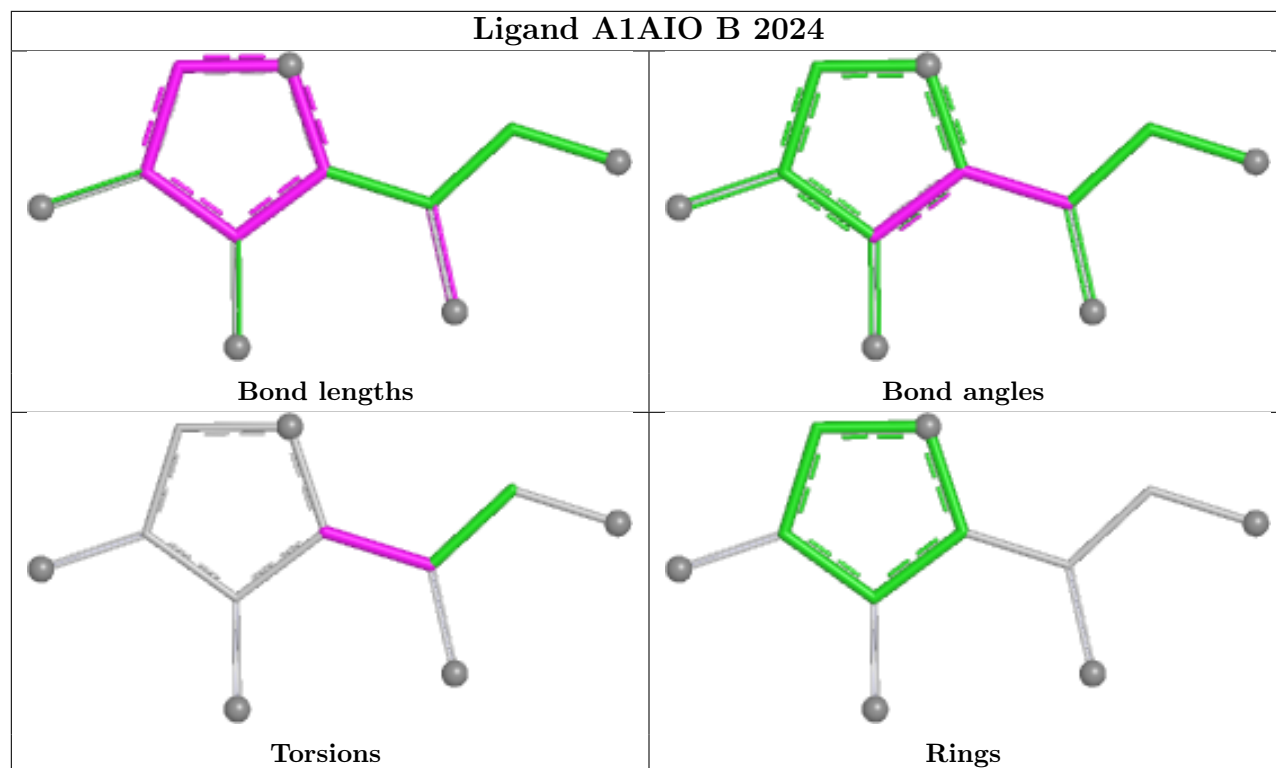


Ligand A1AIO A 2007

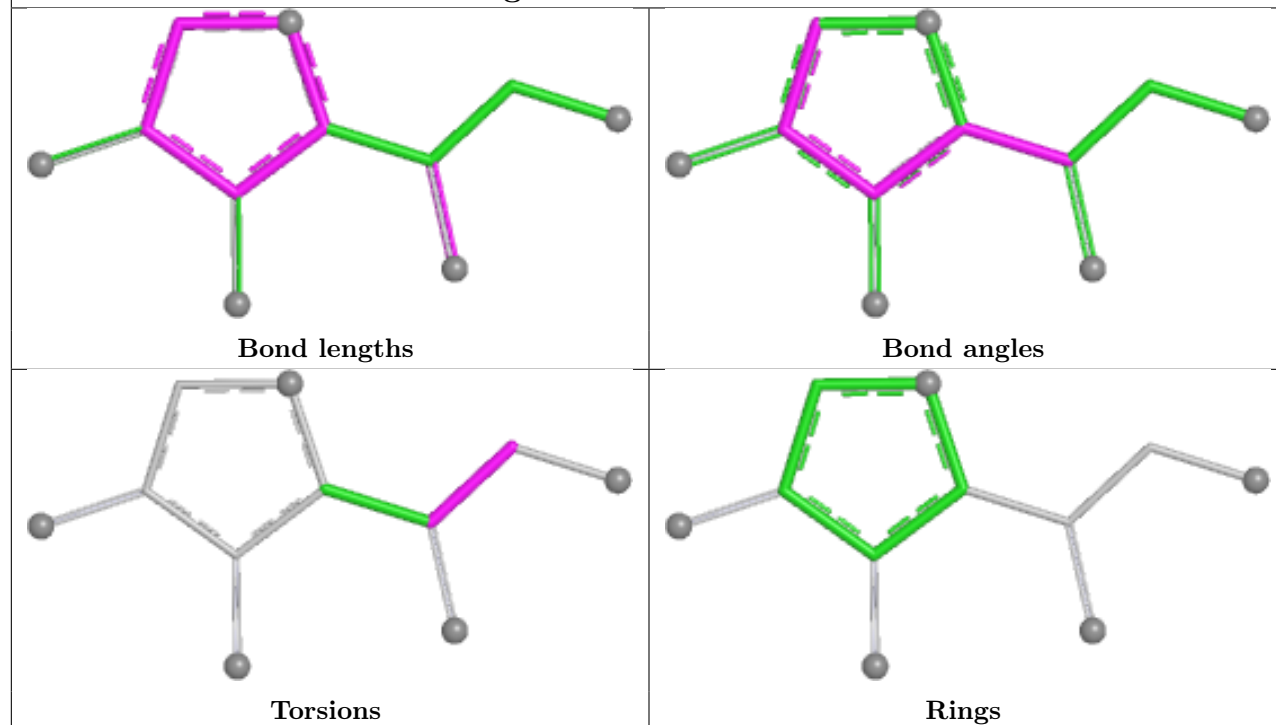


Ligand A1AIO A 2045

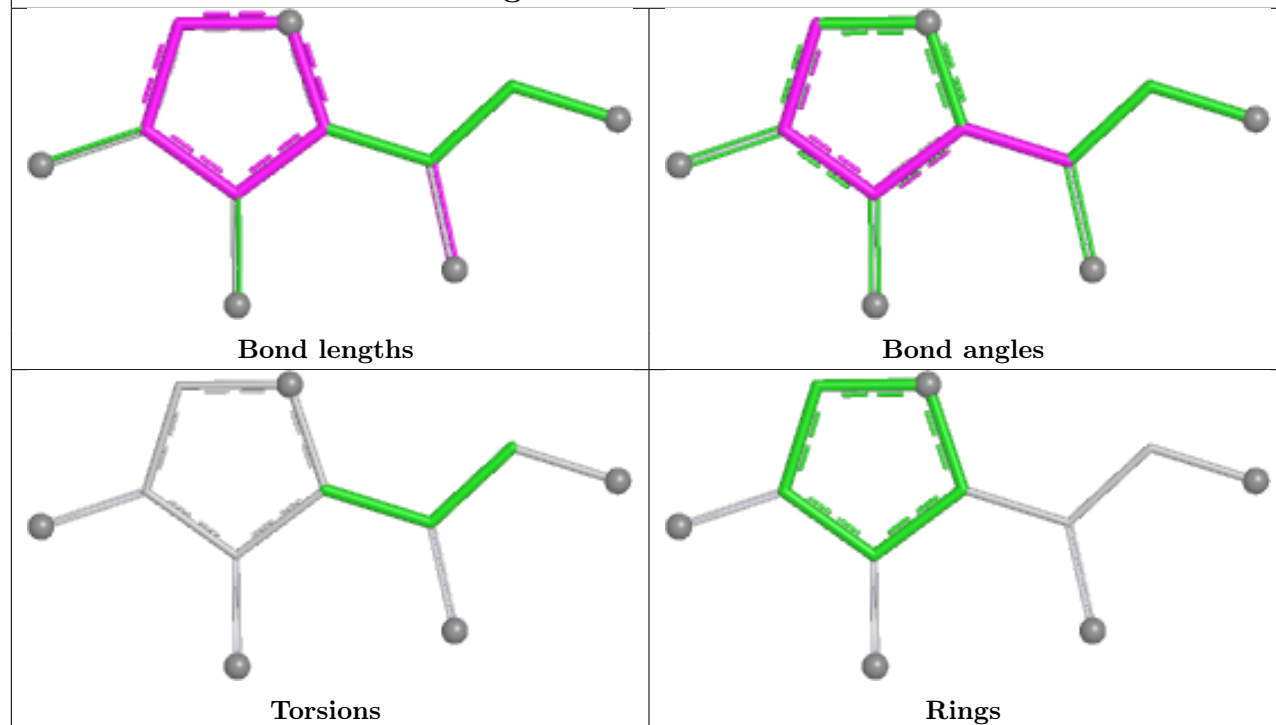




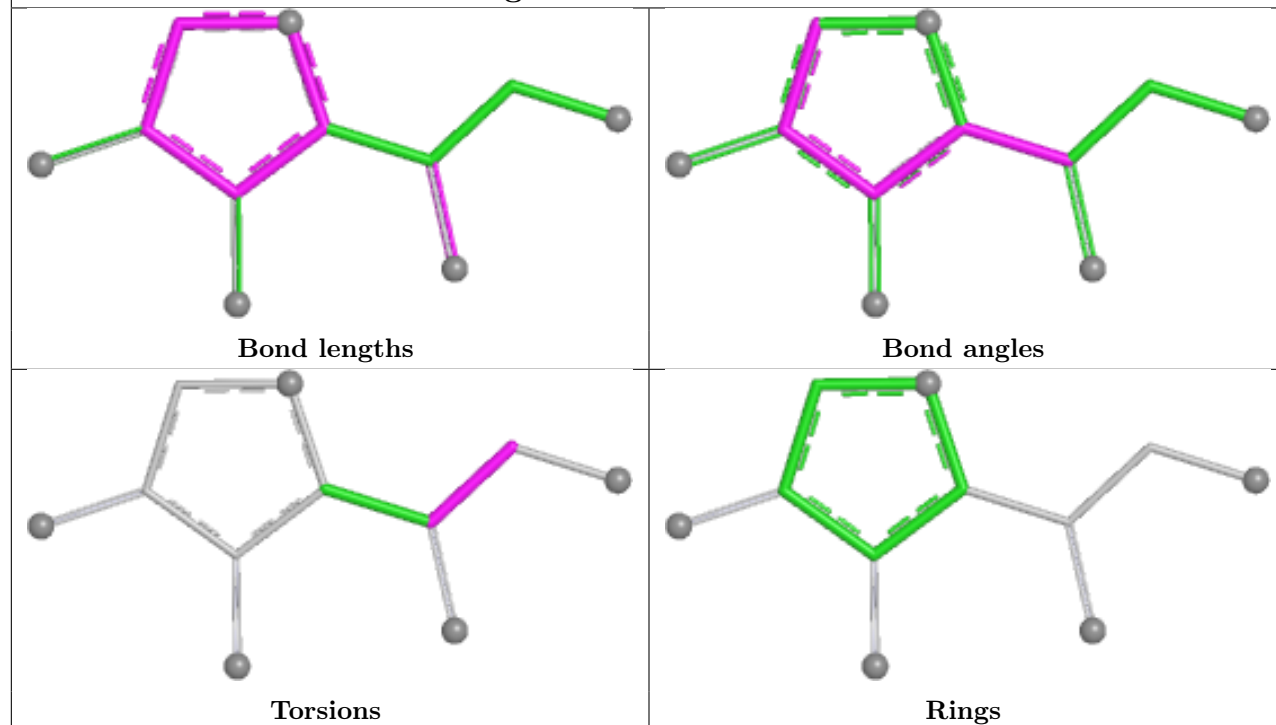
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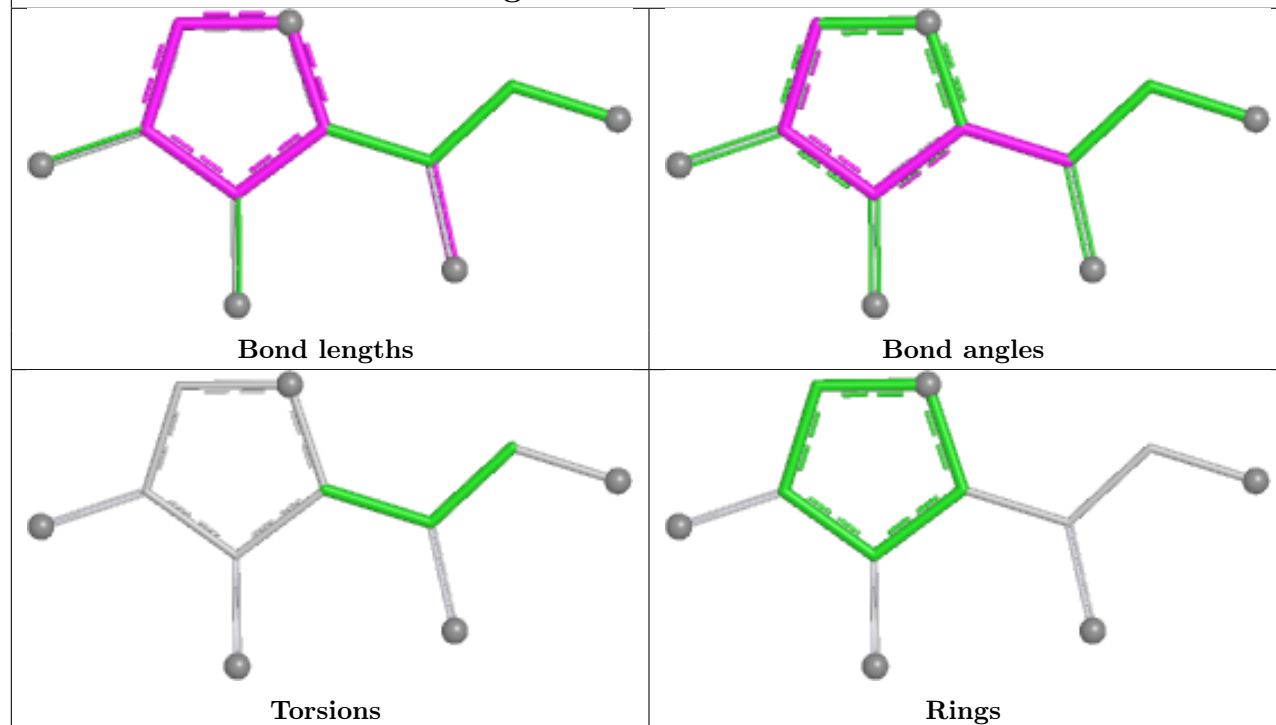
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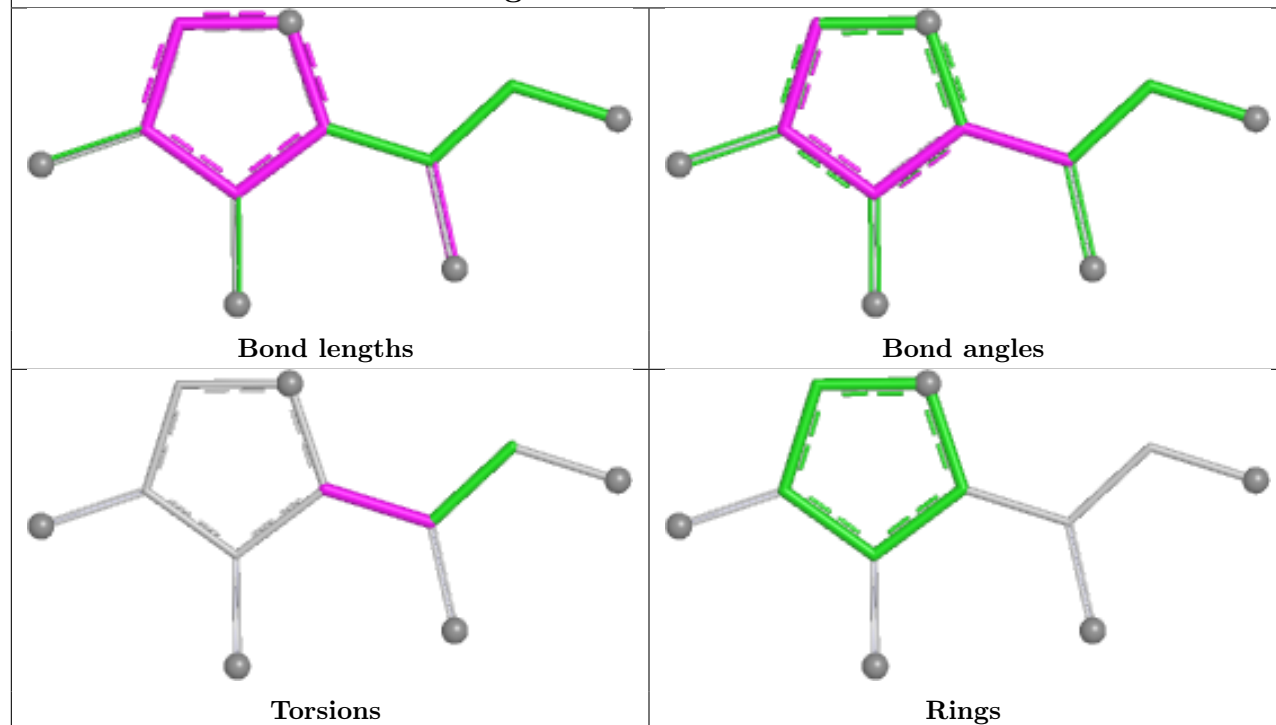
Ligand A1AIO B 2002



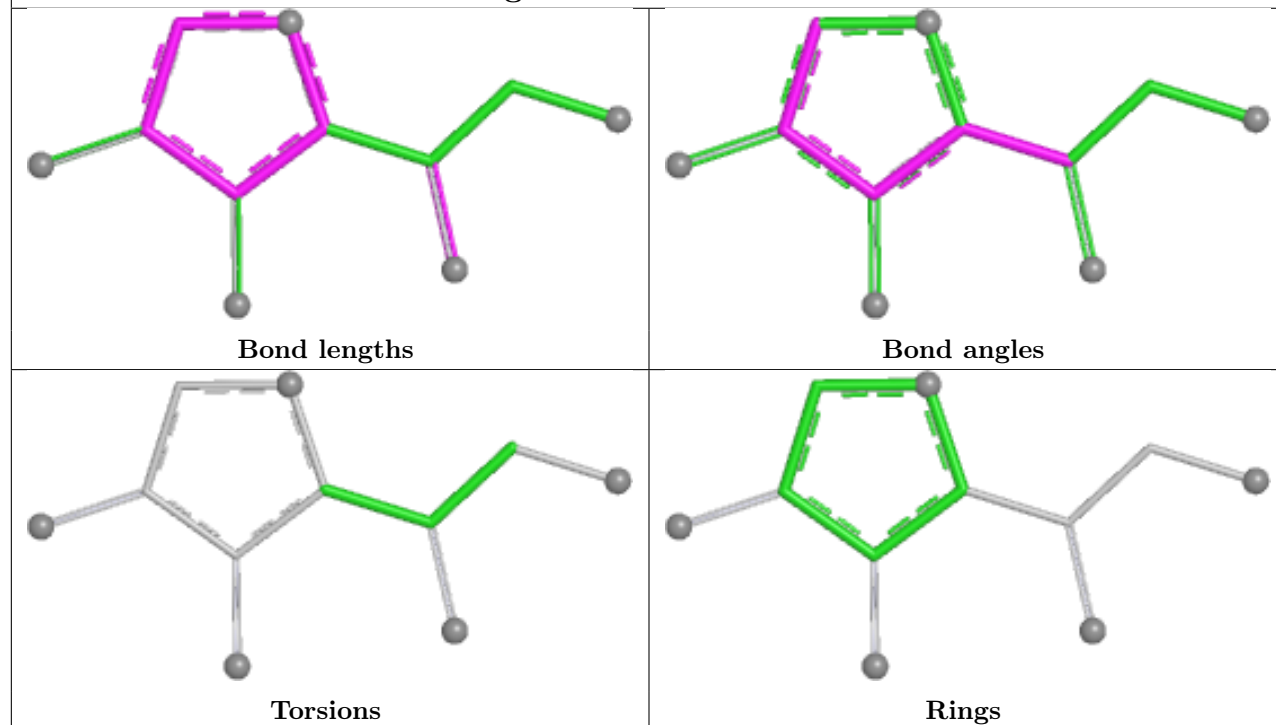
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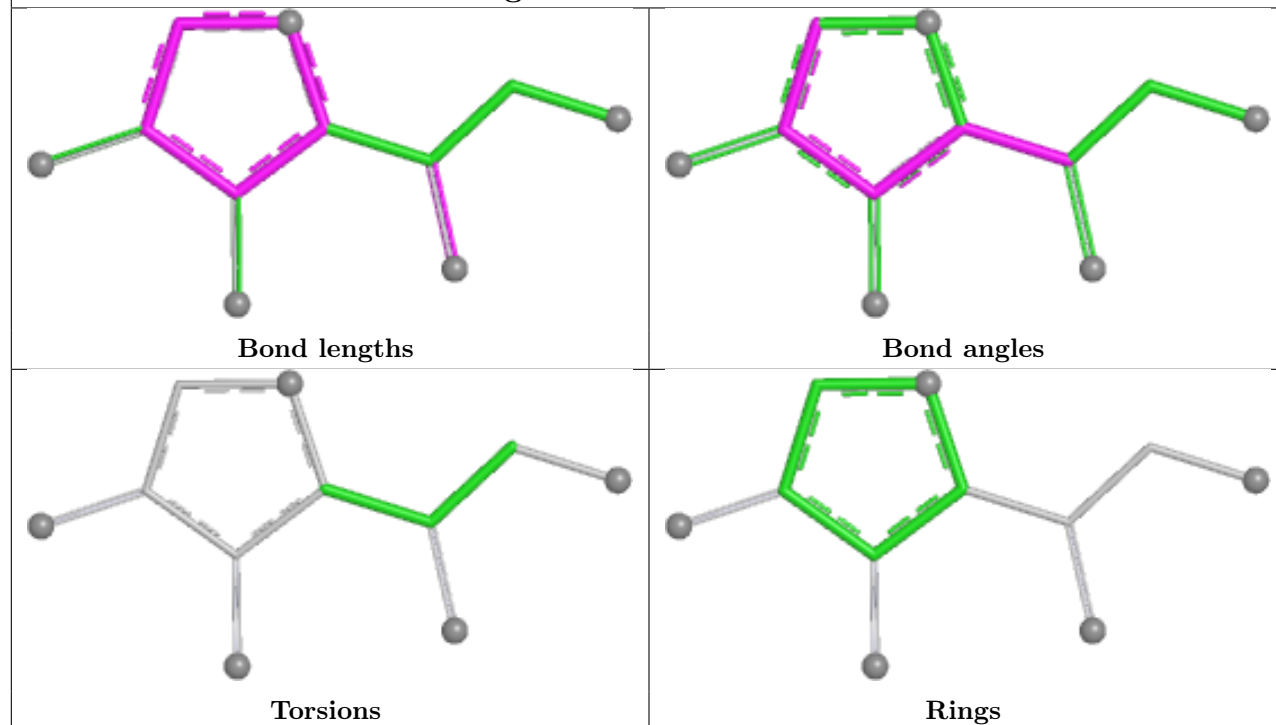
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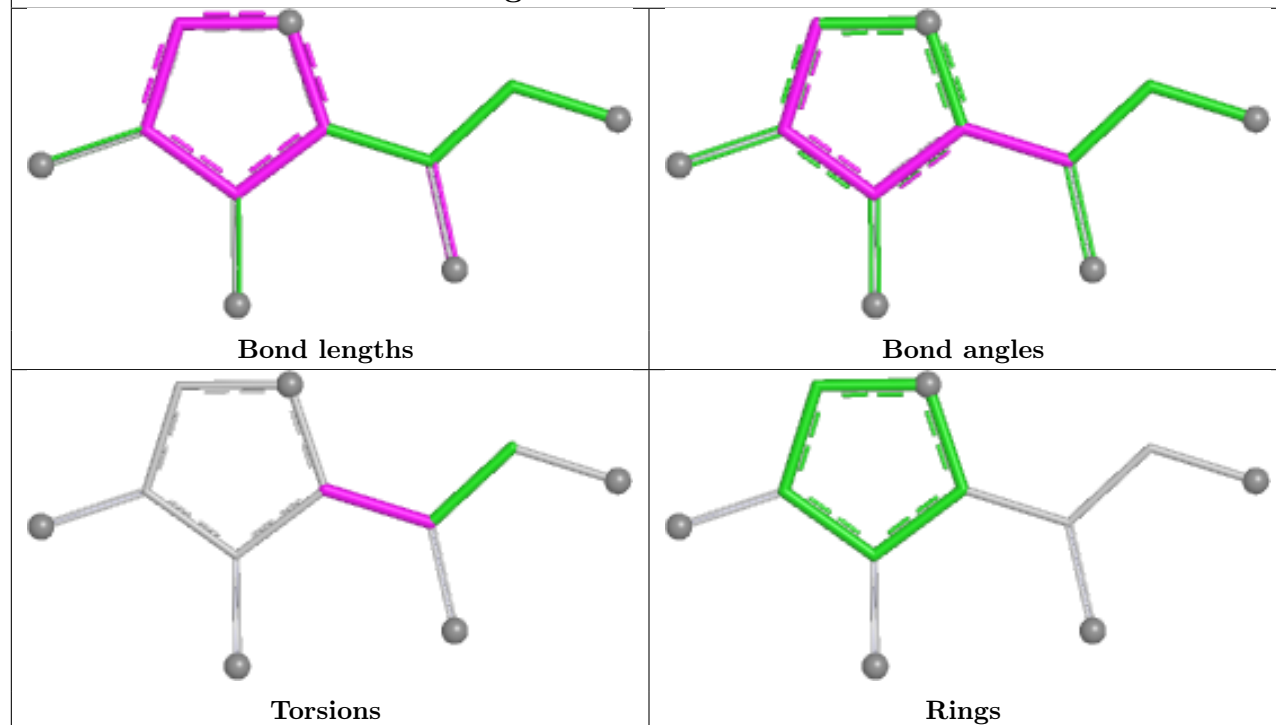
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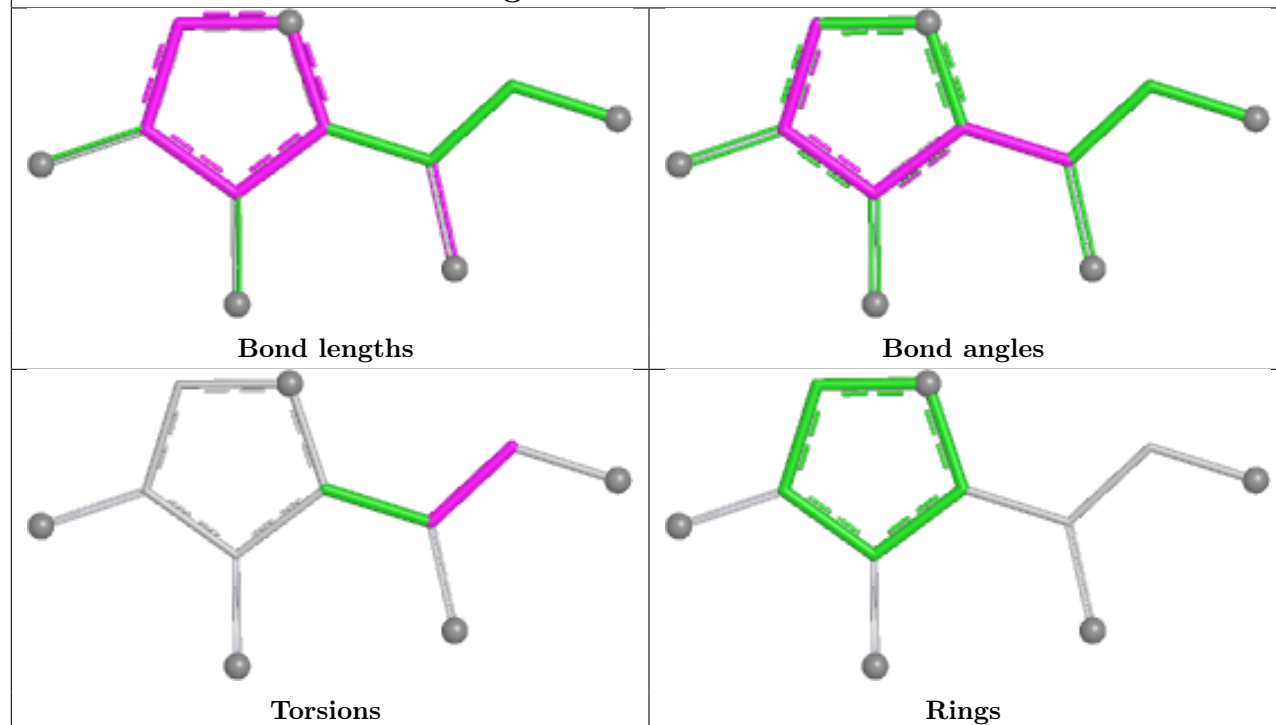
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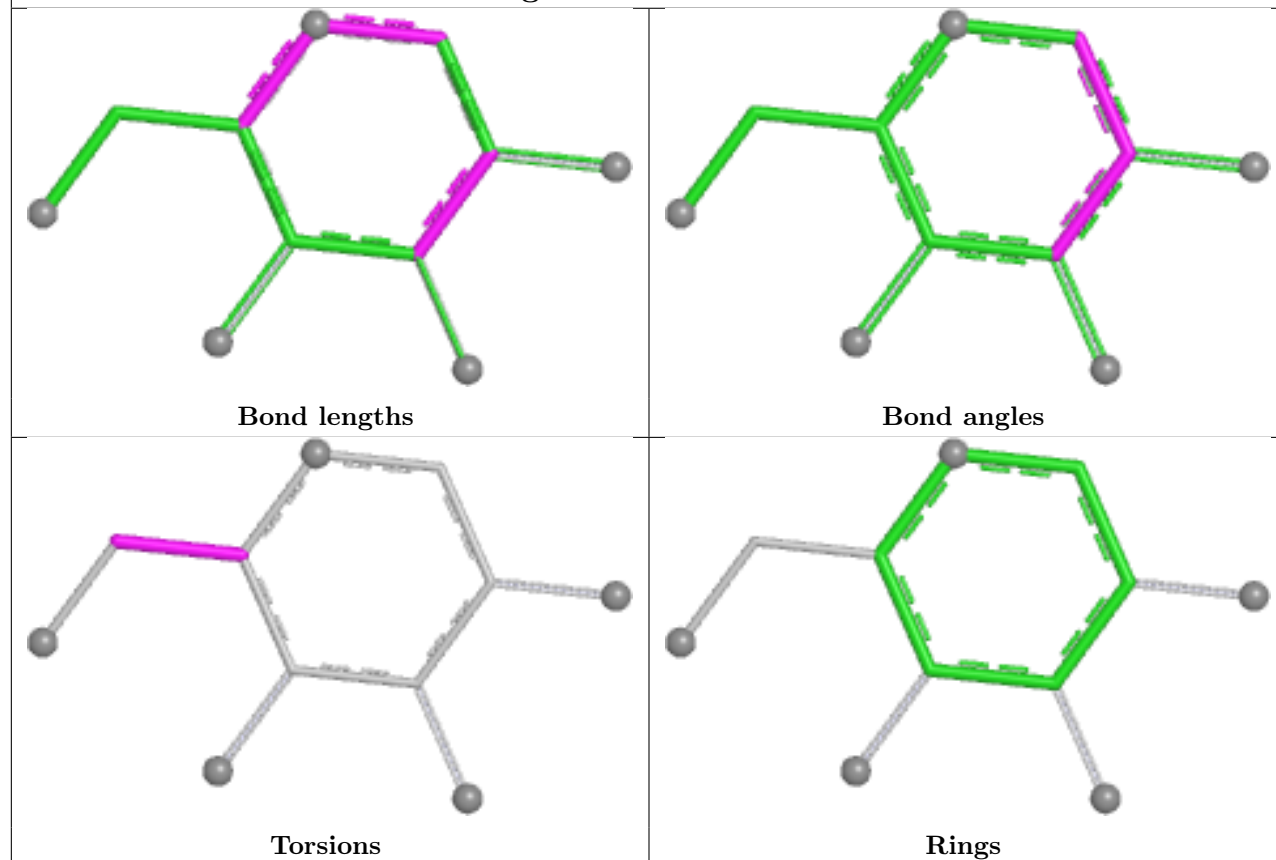
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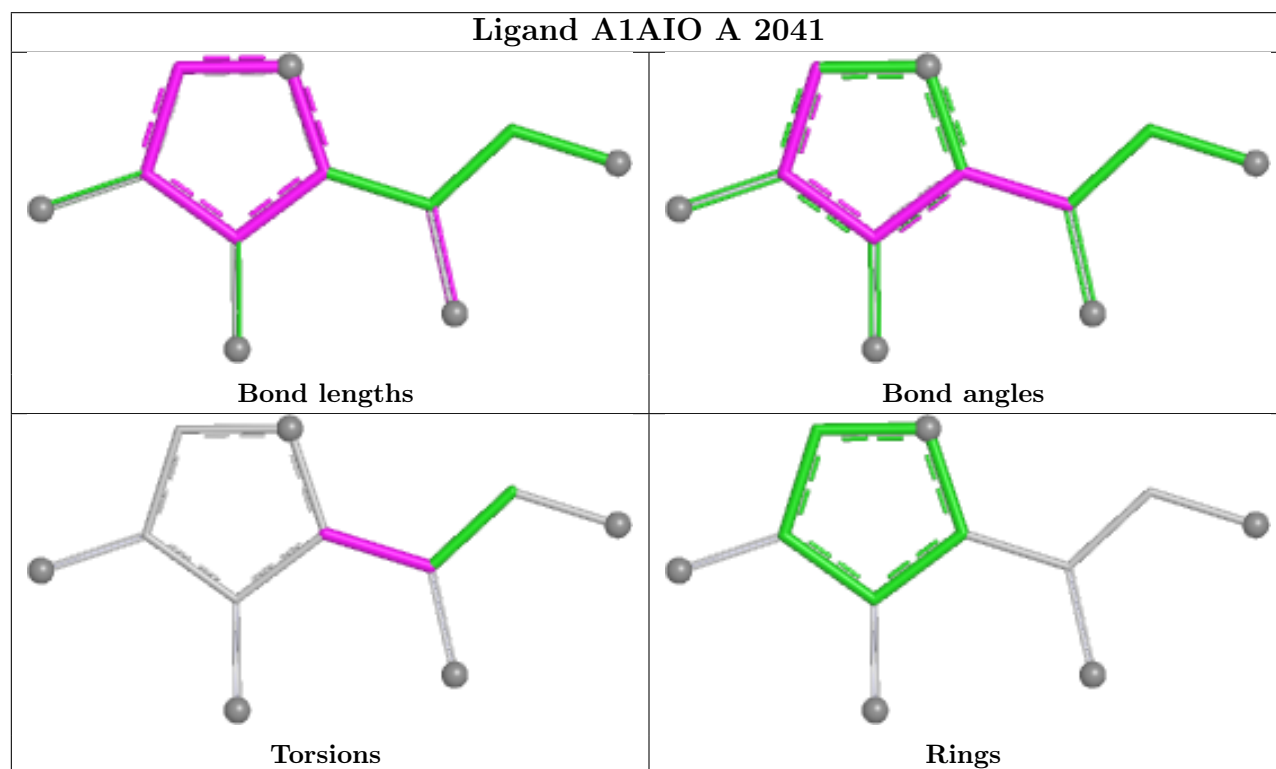
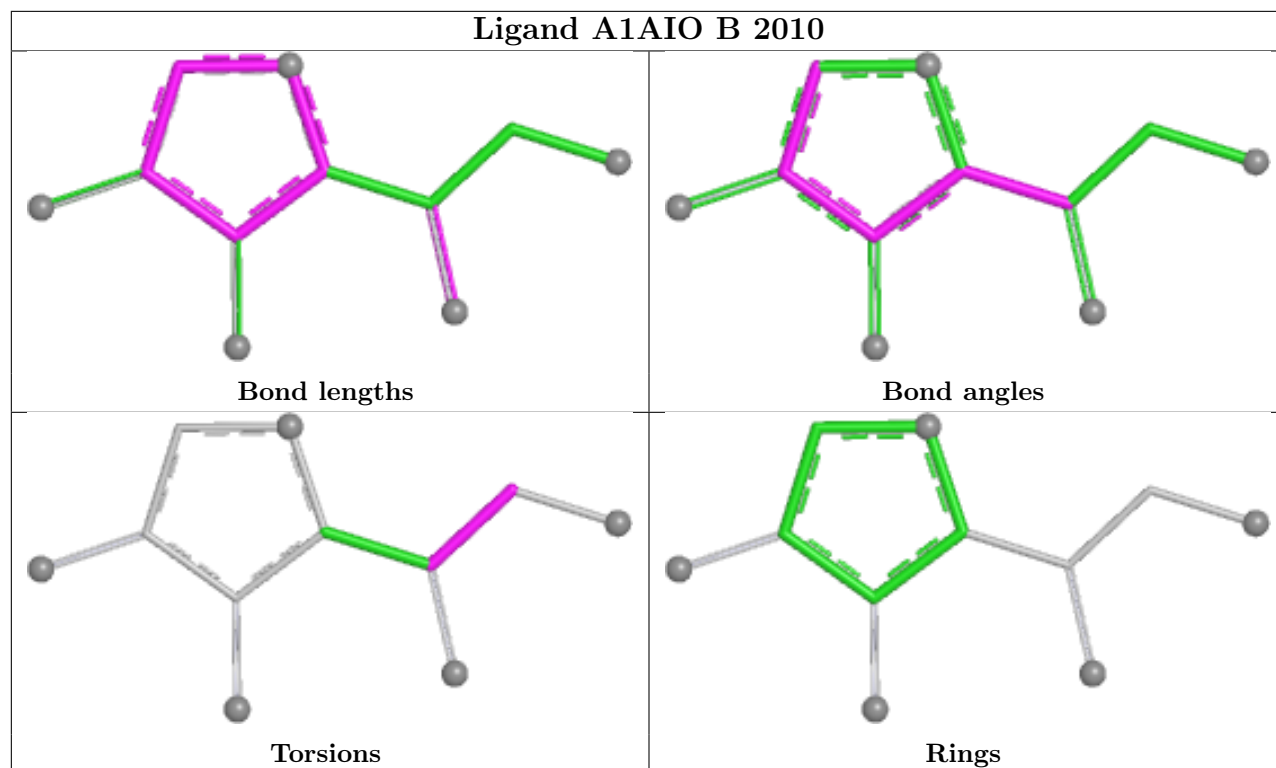


Ligand A1AIO A 2002

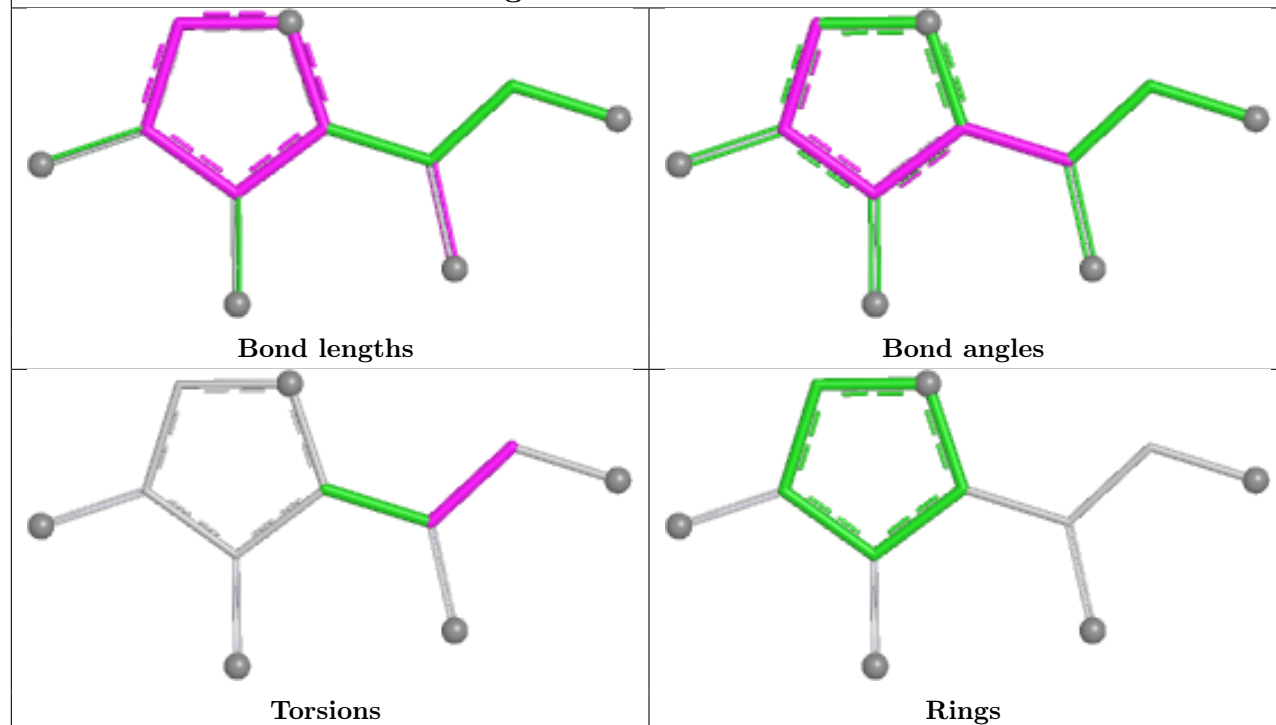


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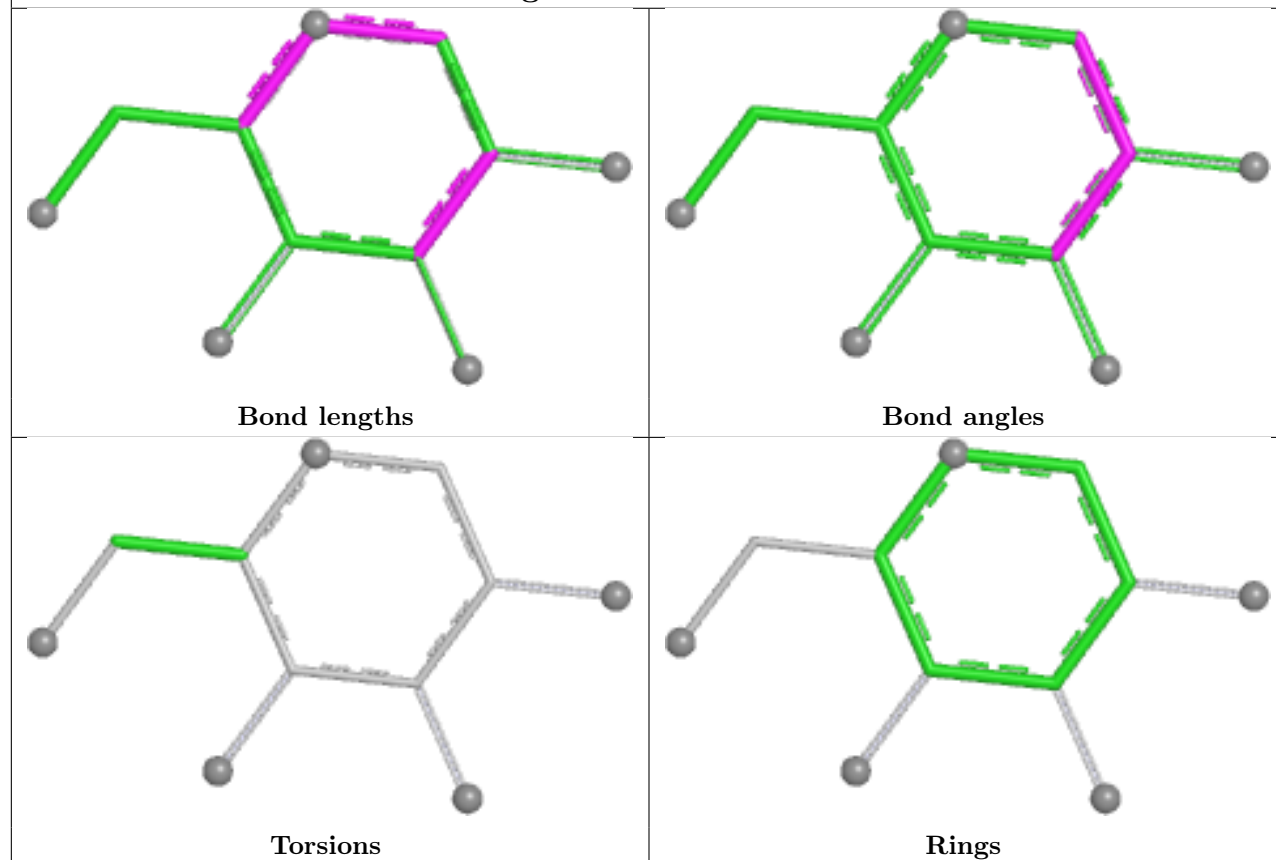




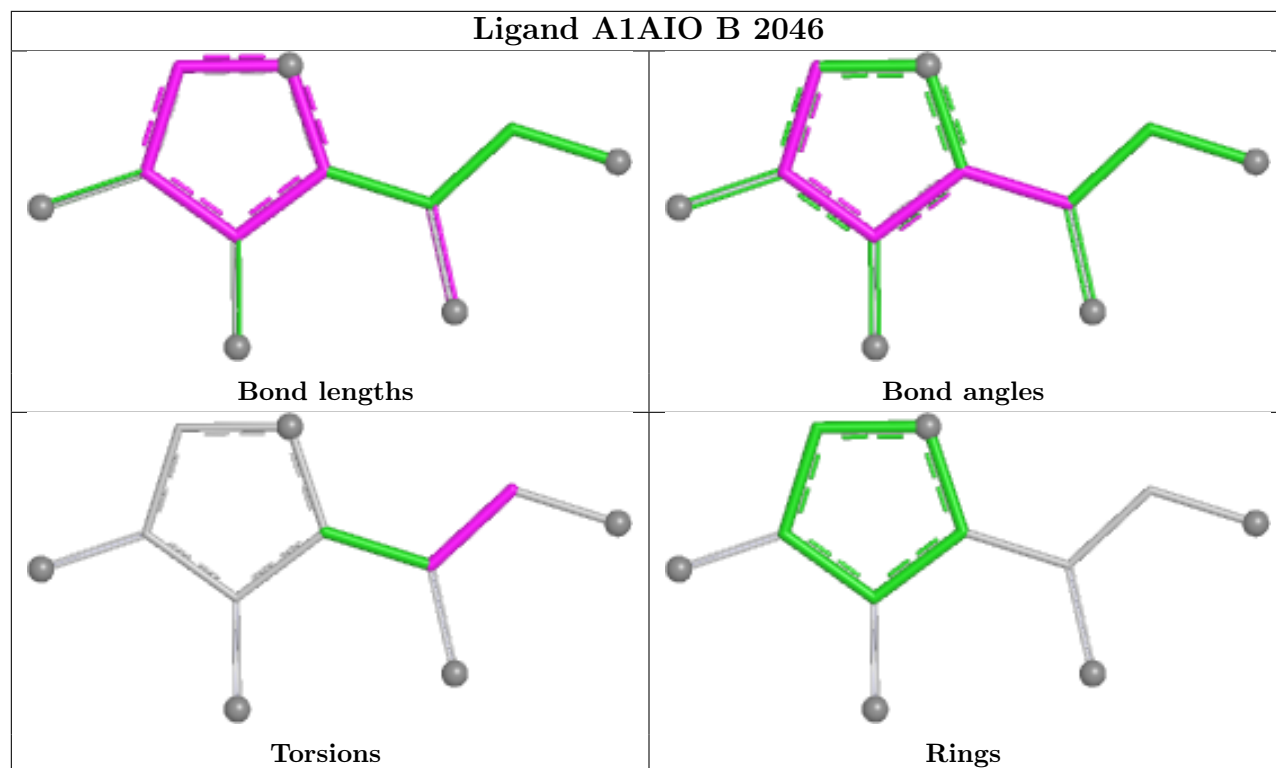
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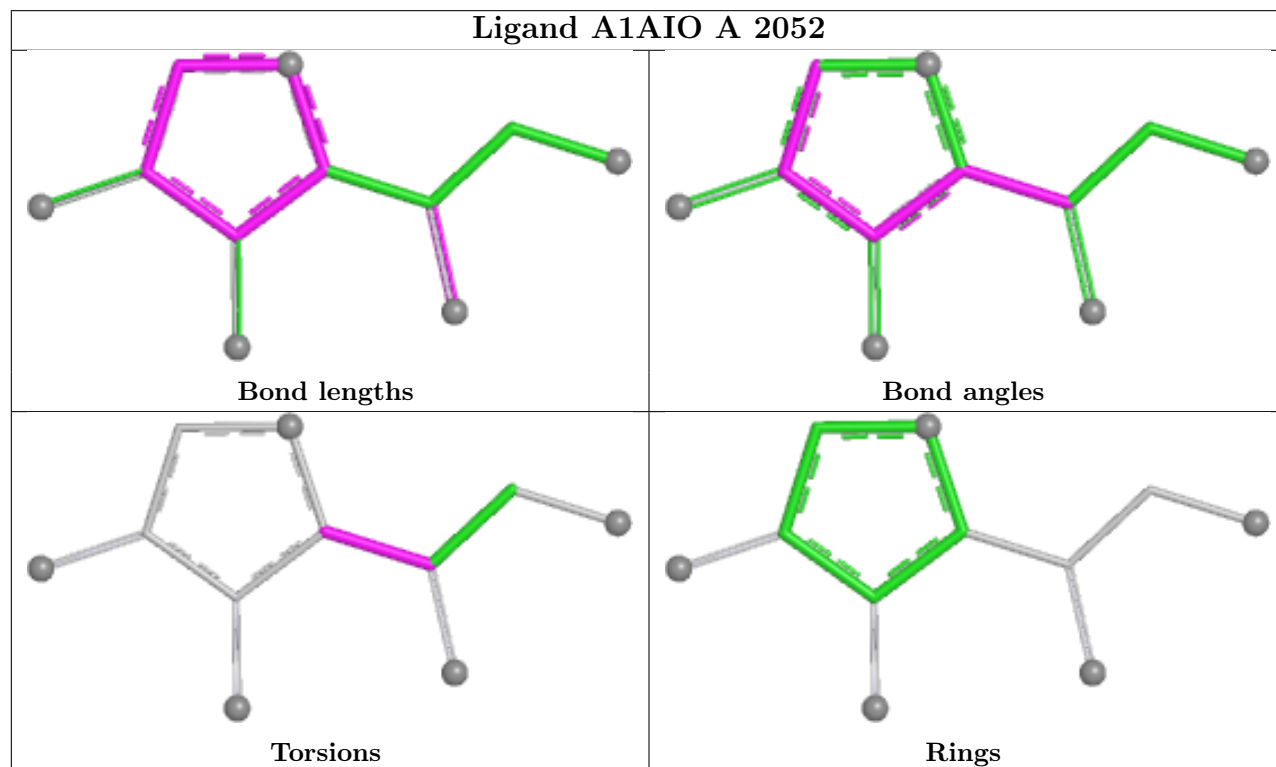
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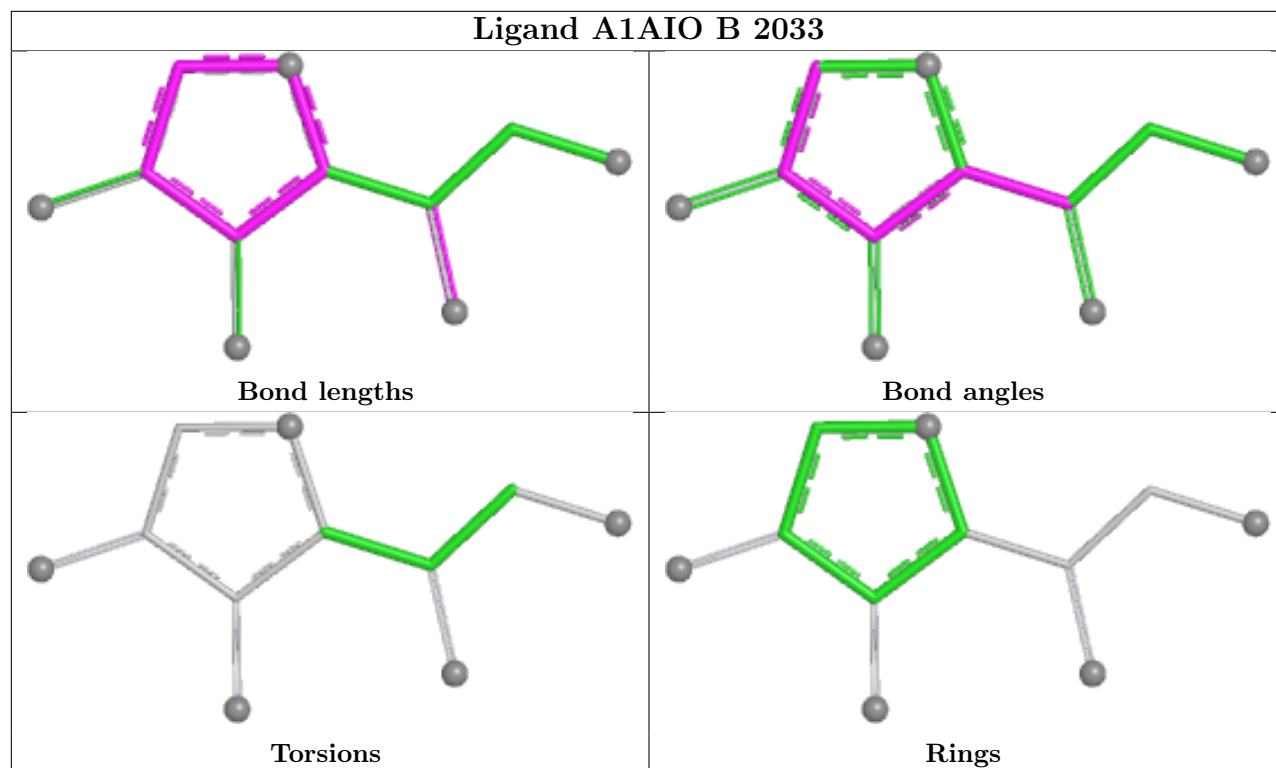
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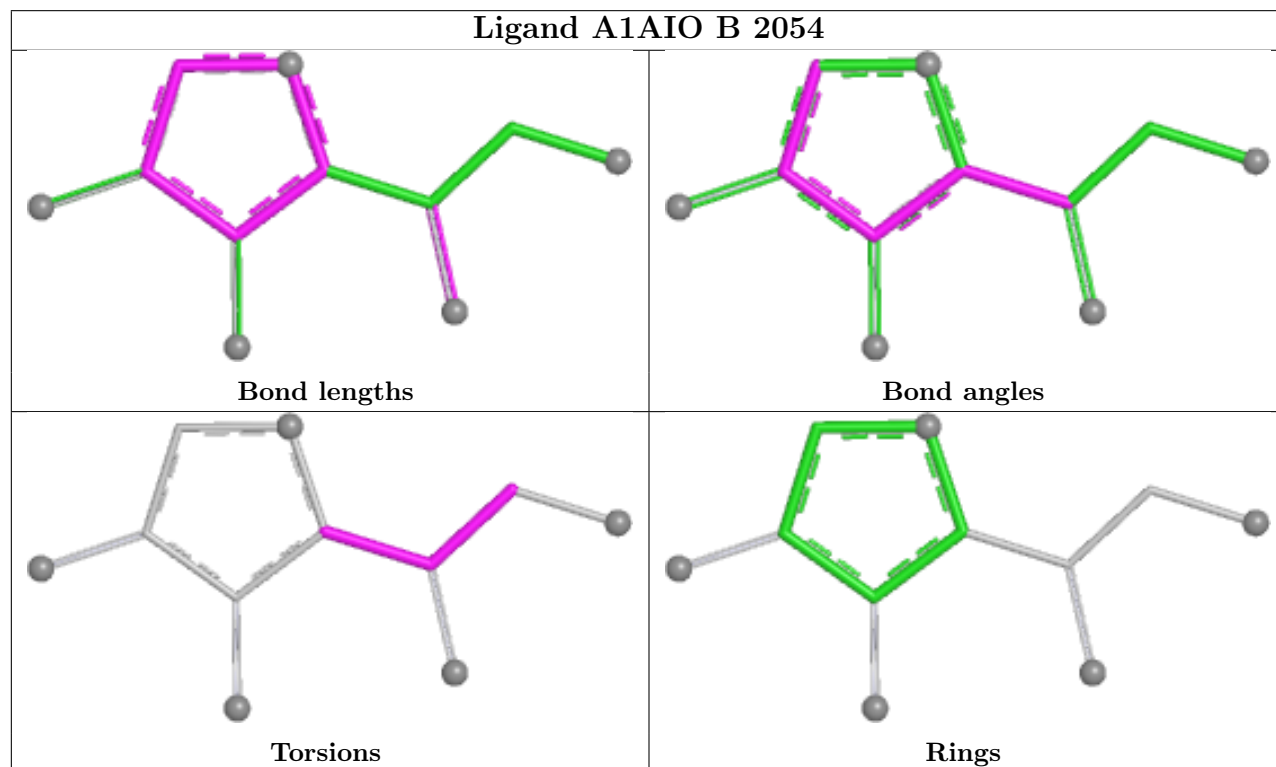
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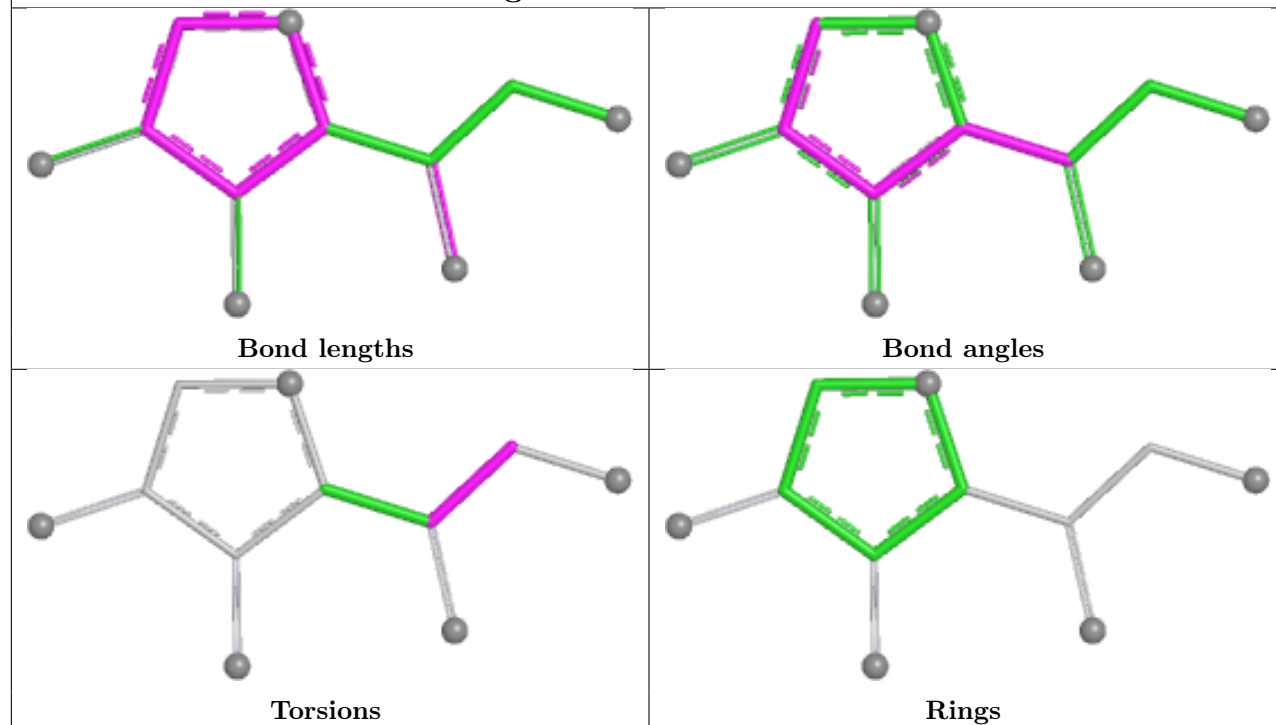
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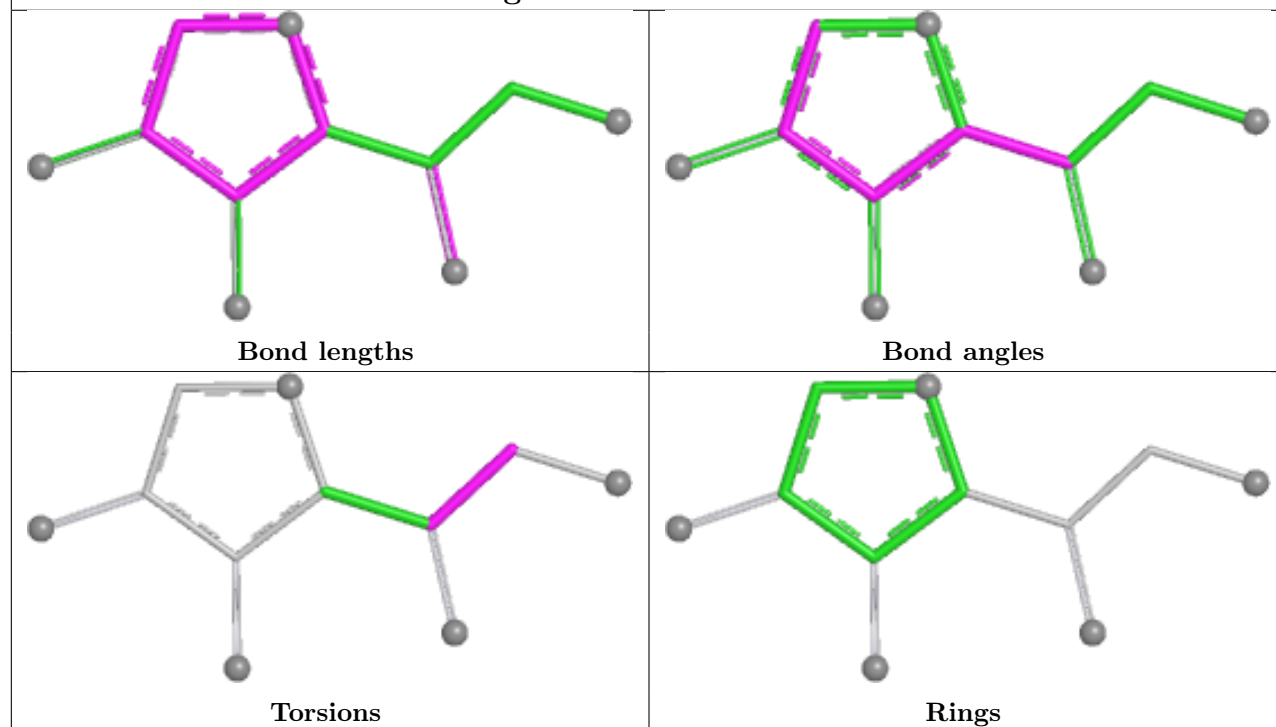
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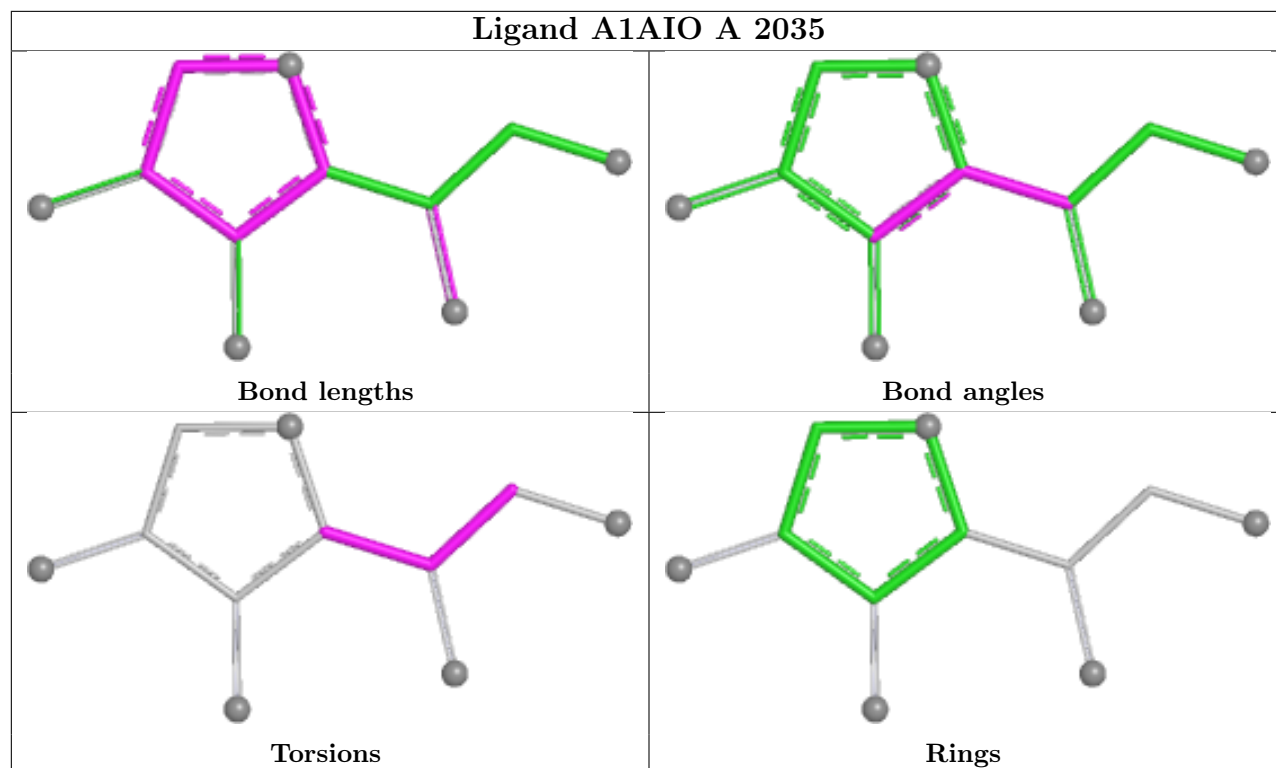
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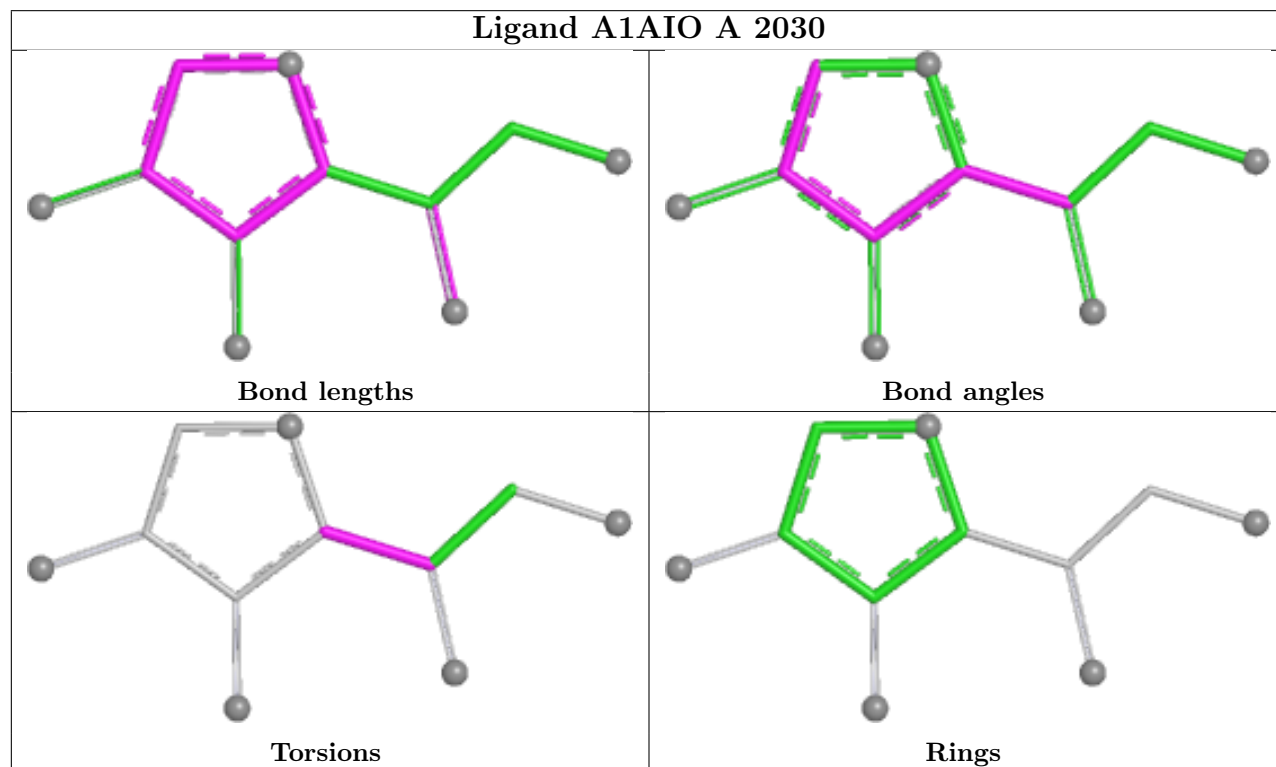
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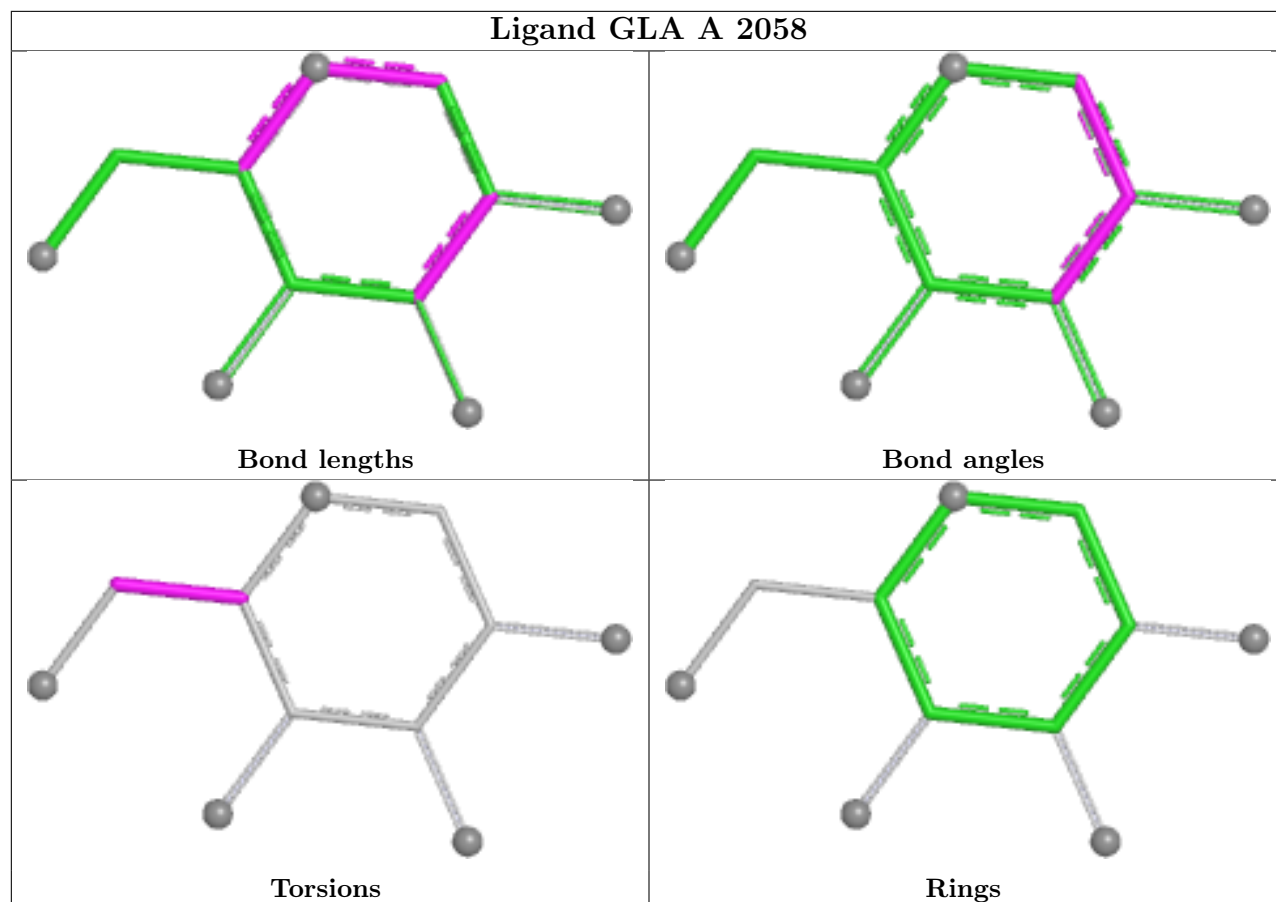
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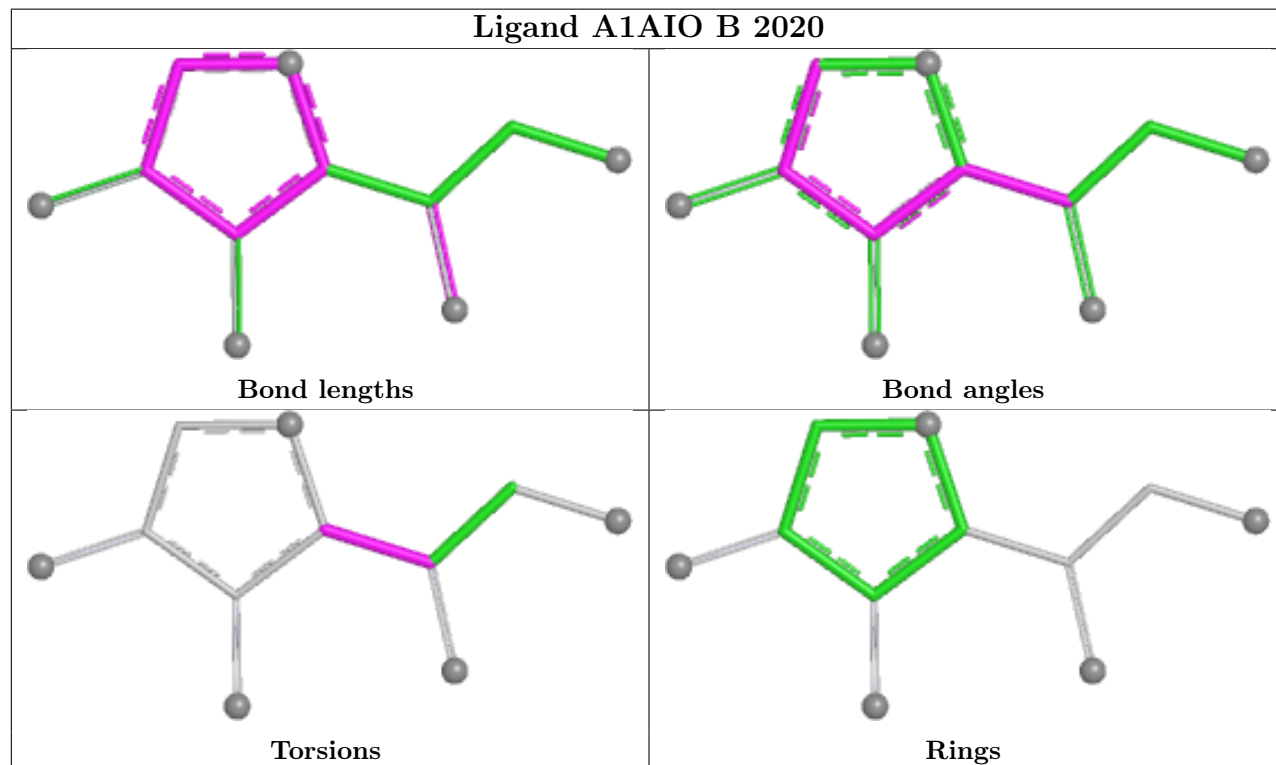
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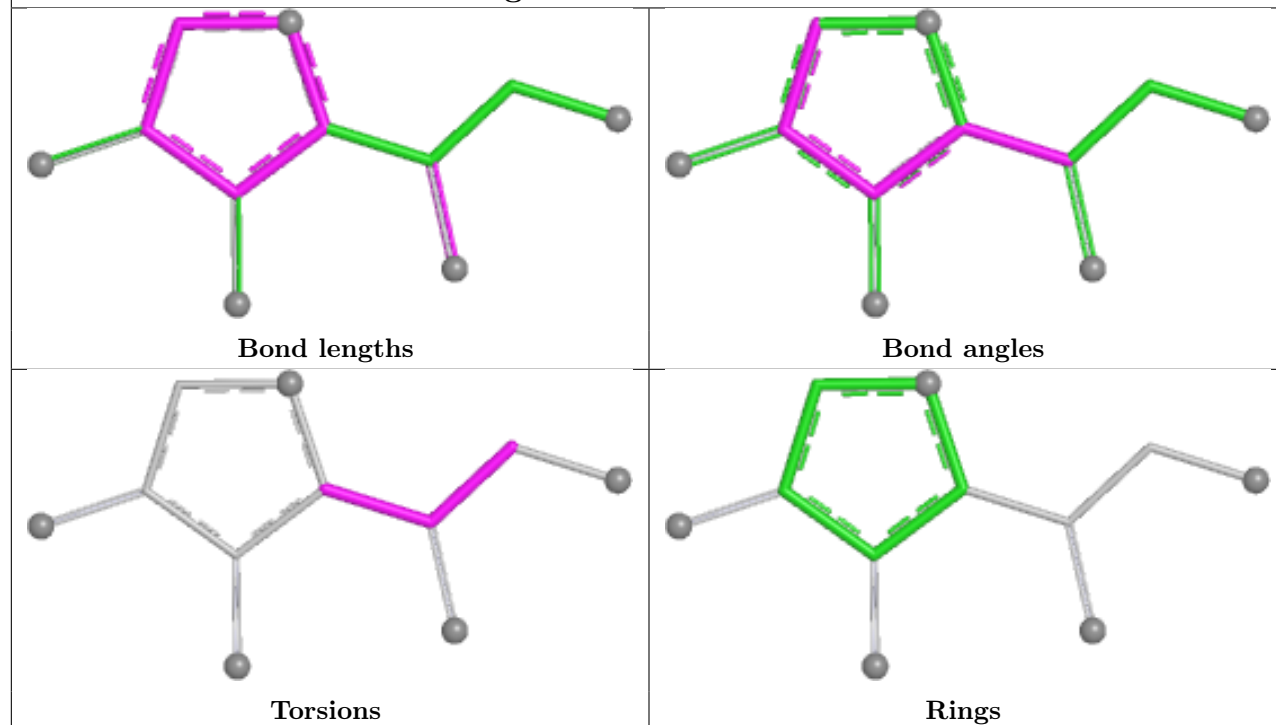
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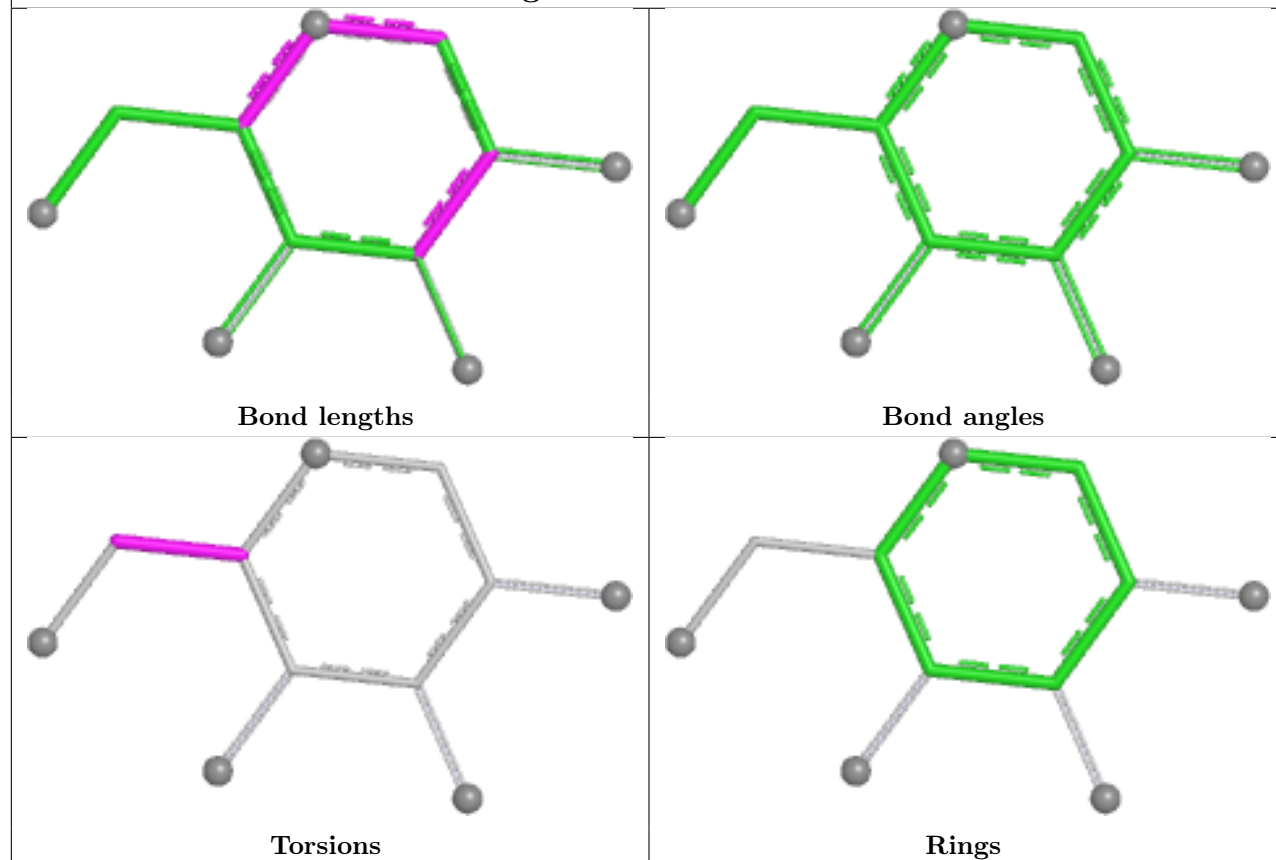
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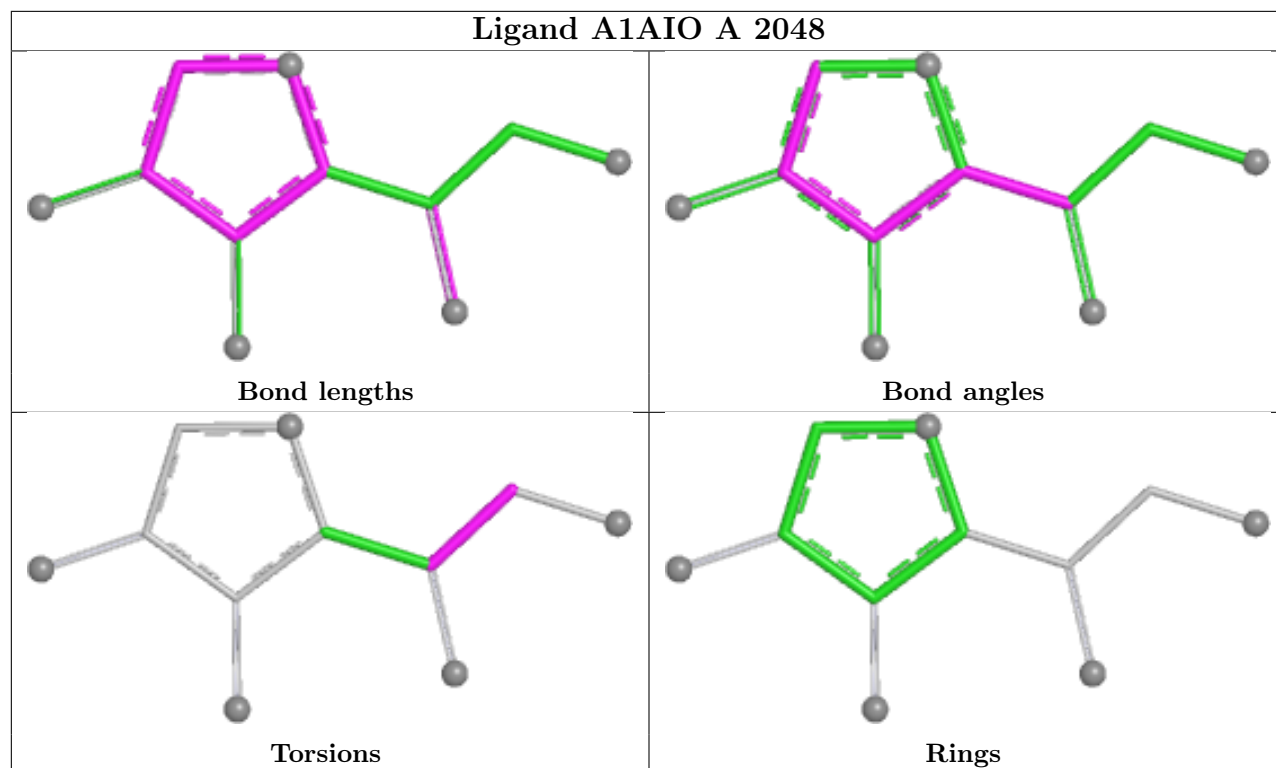
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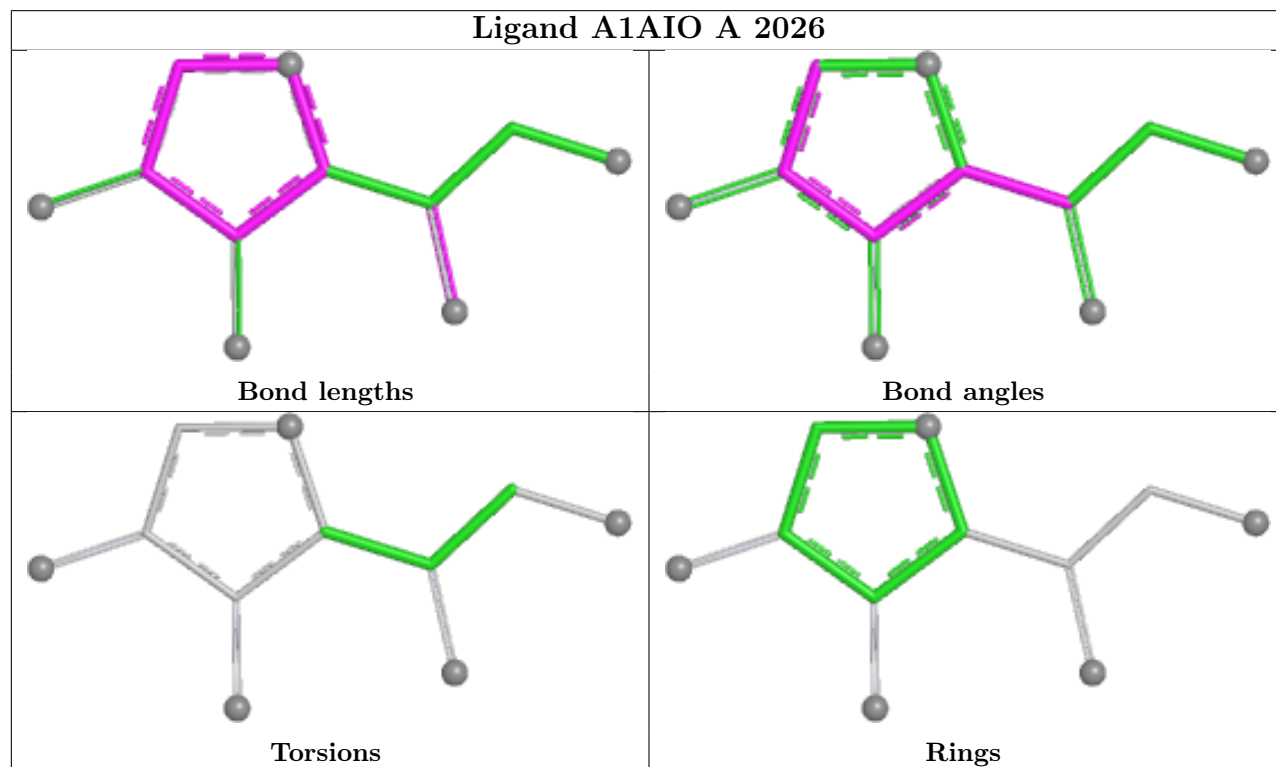
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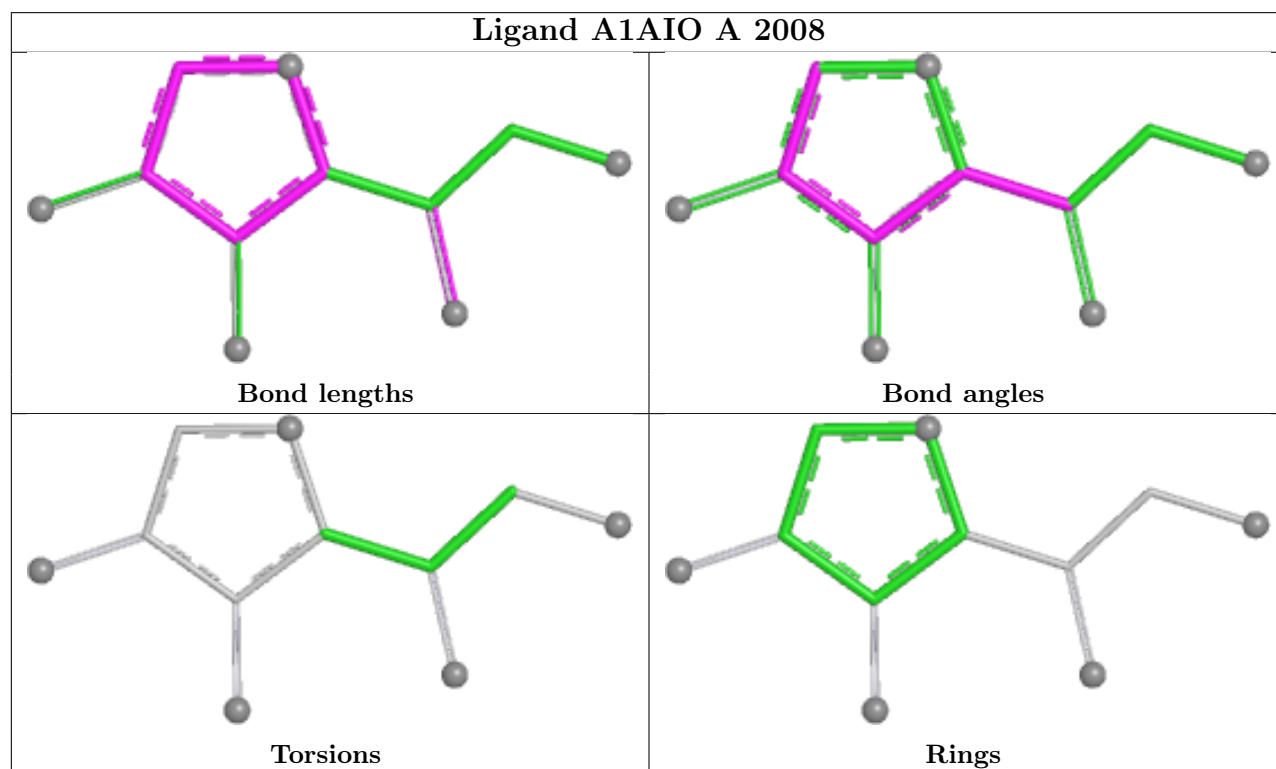
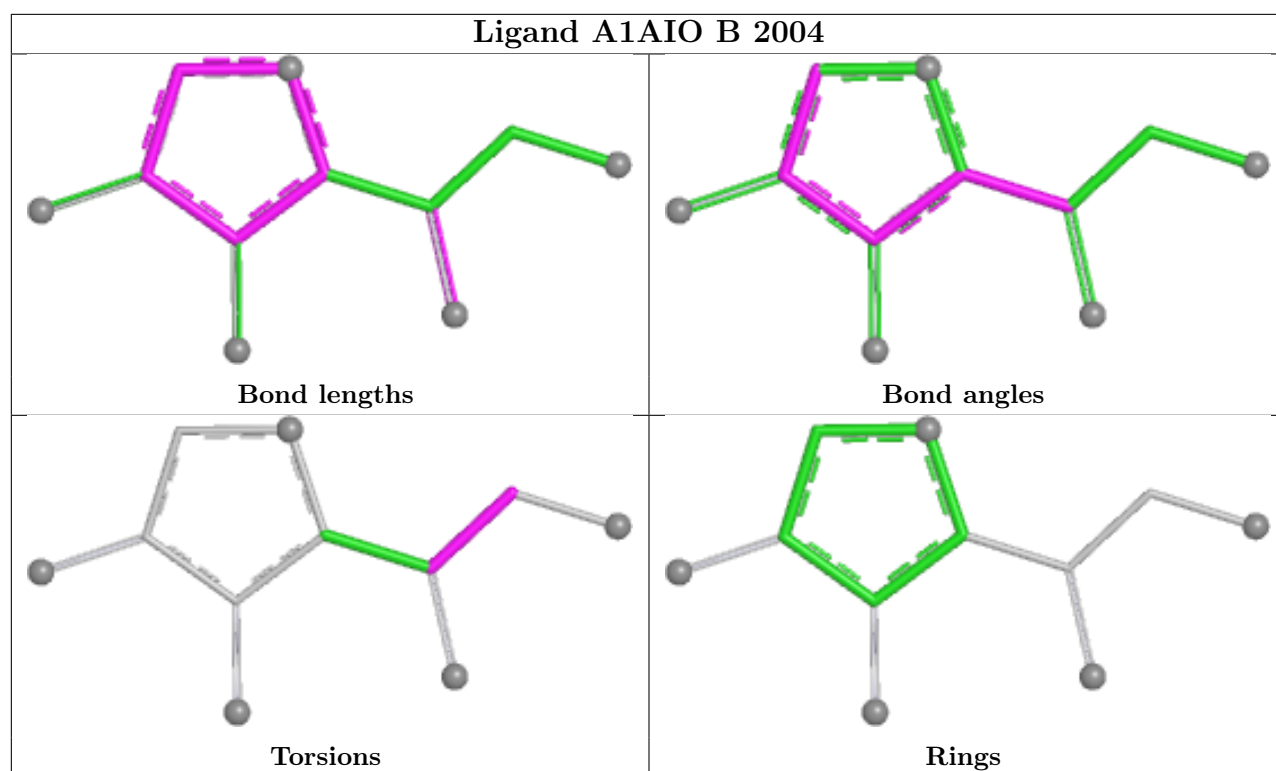


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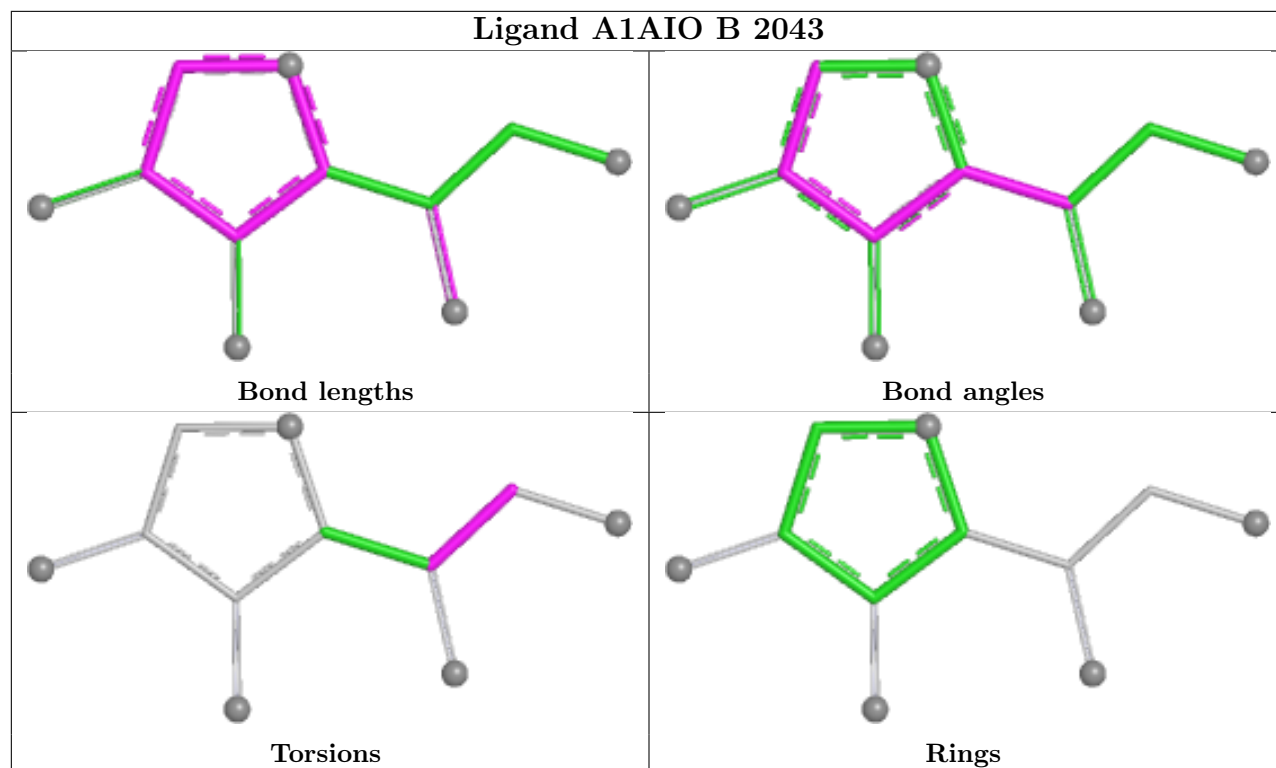


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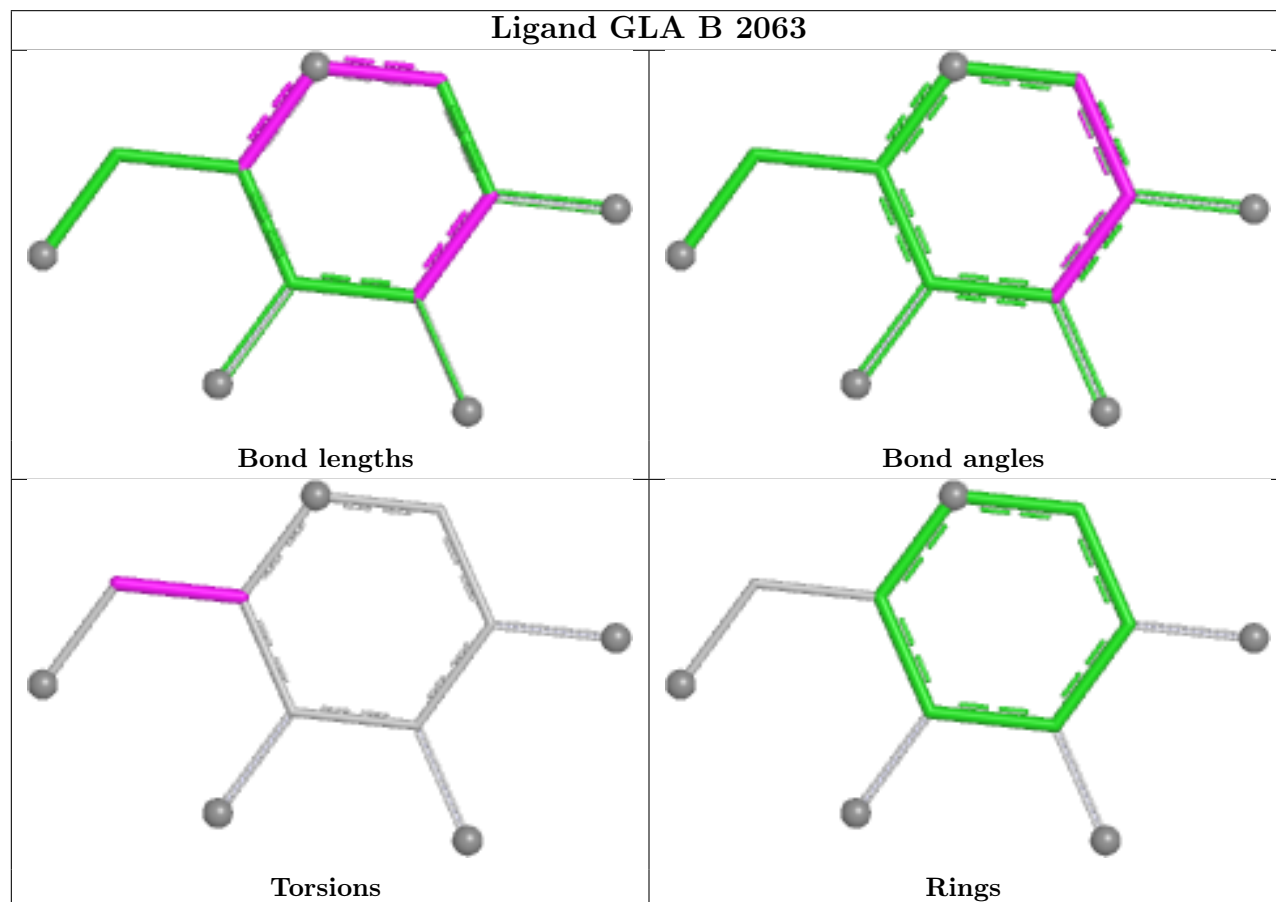




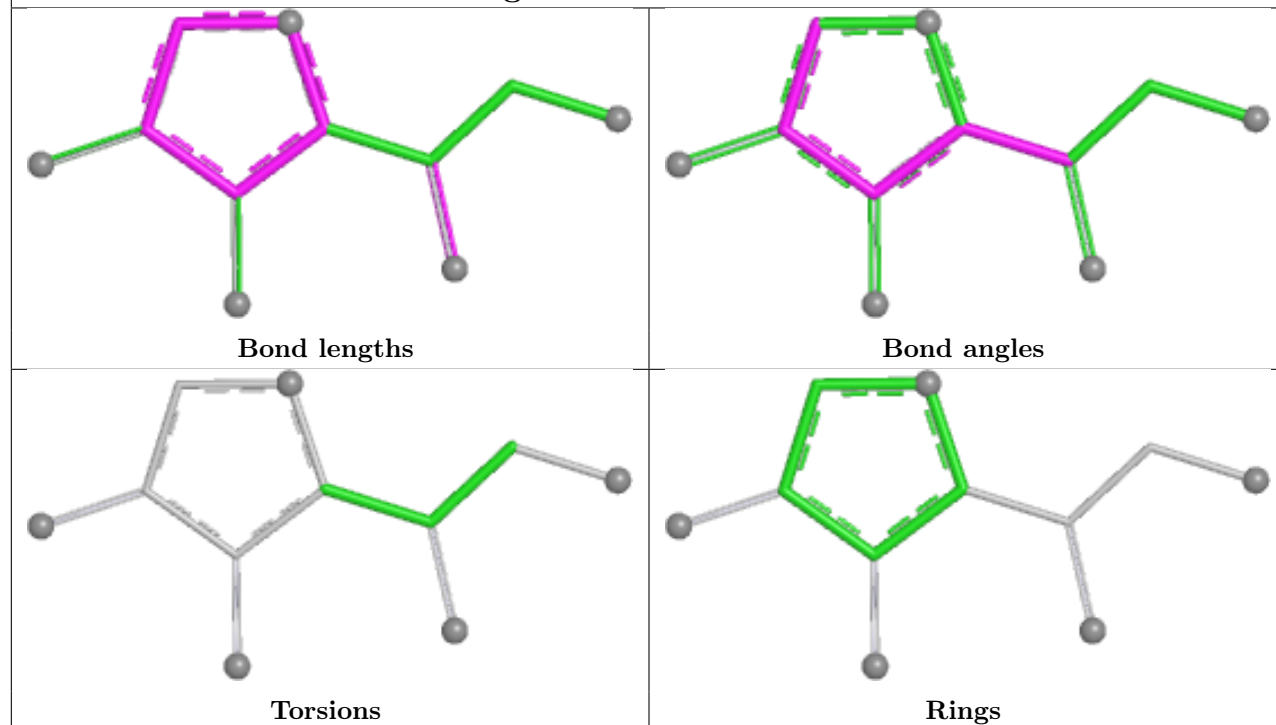
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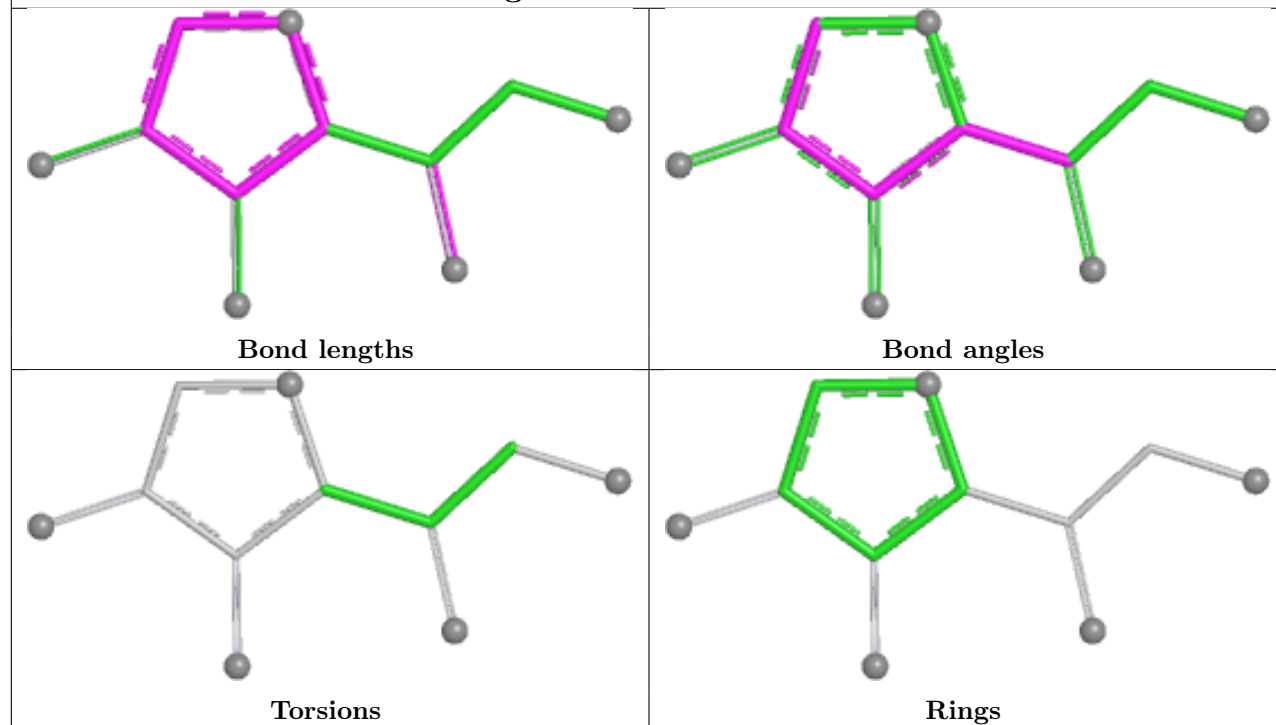
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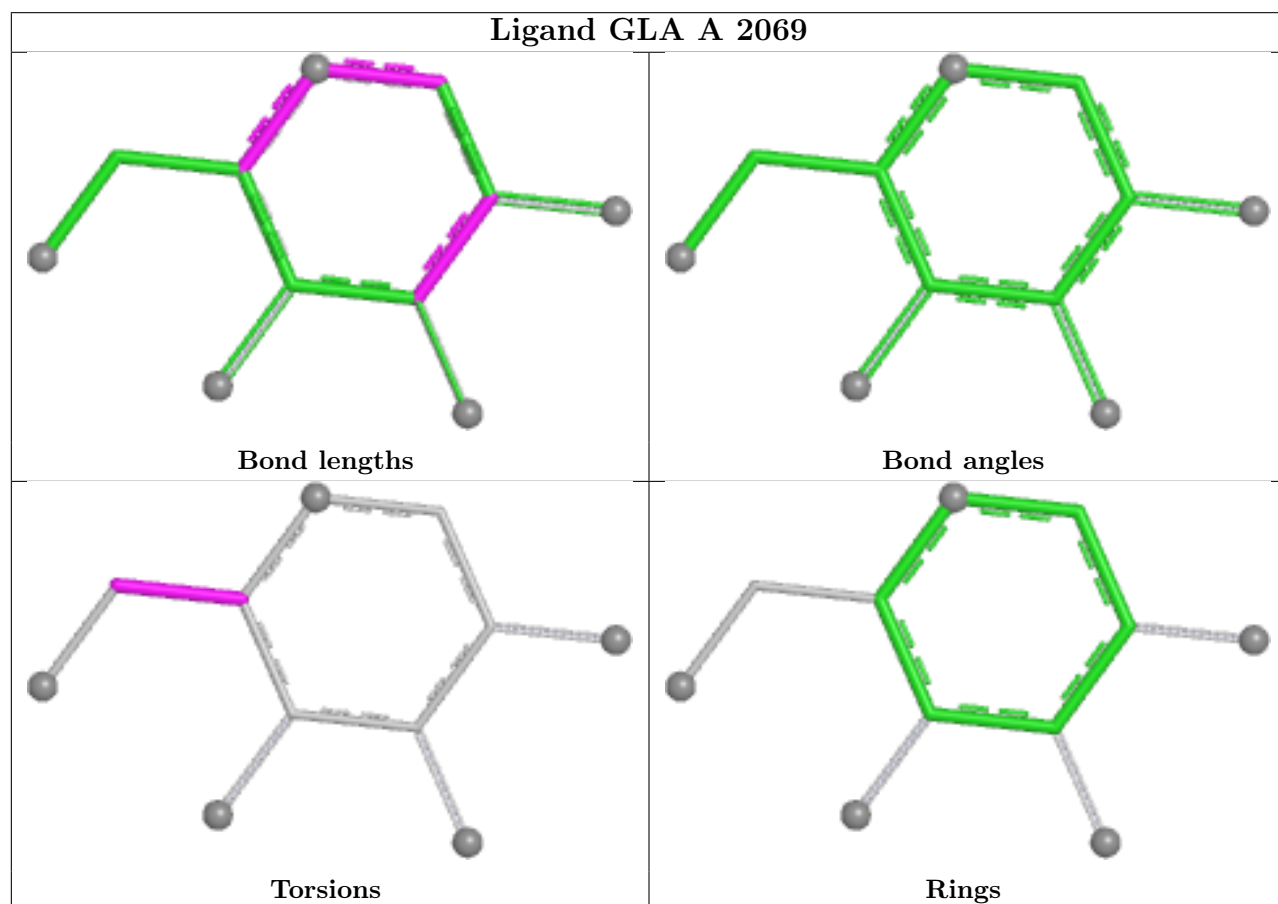
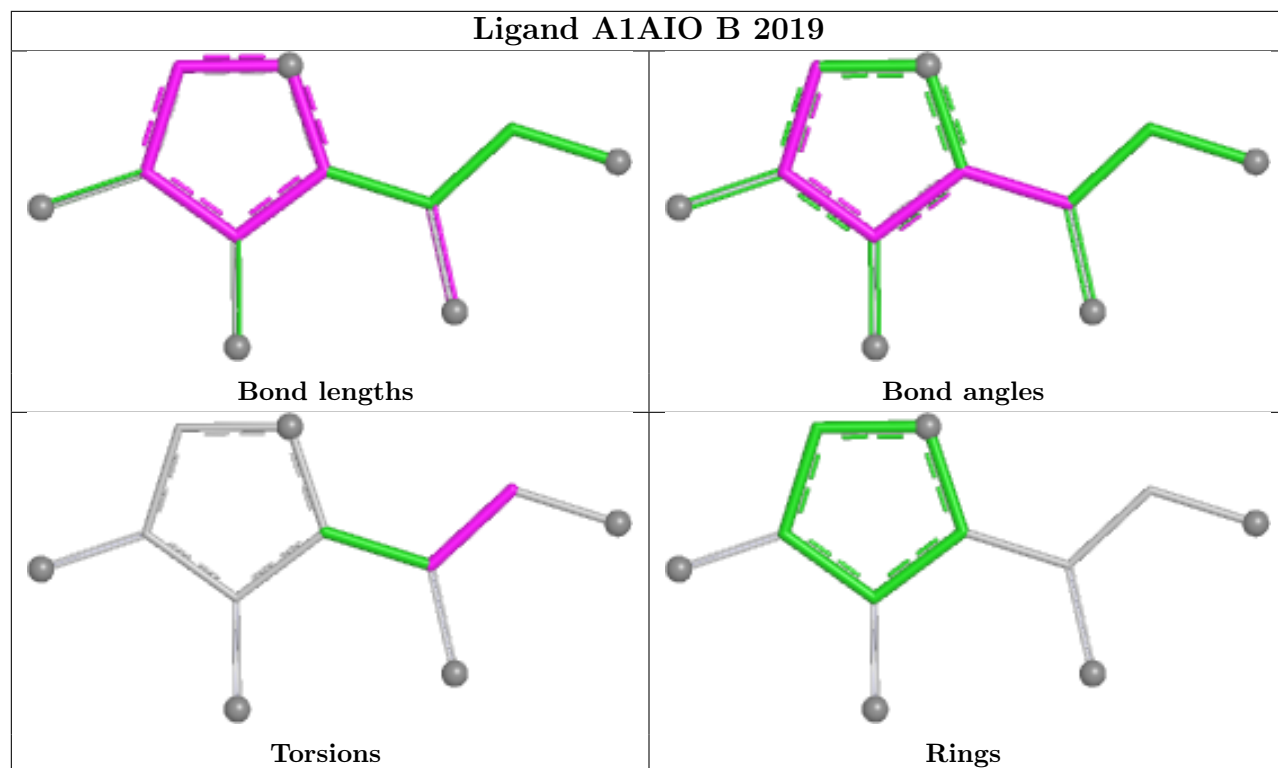


Ligand A1AIO A 2014

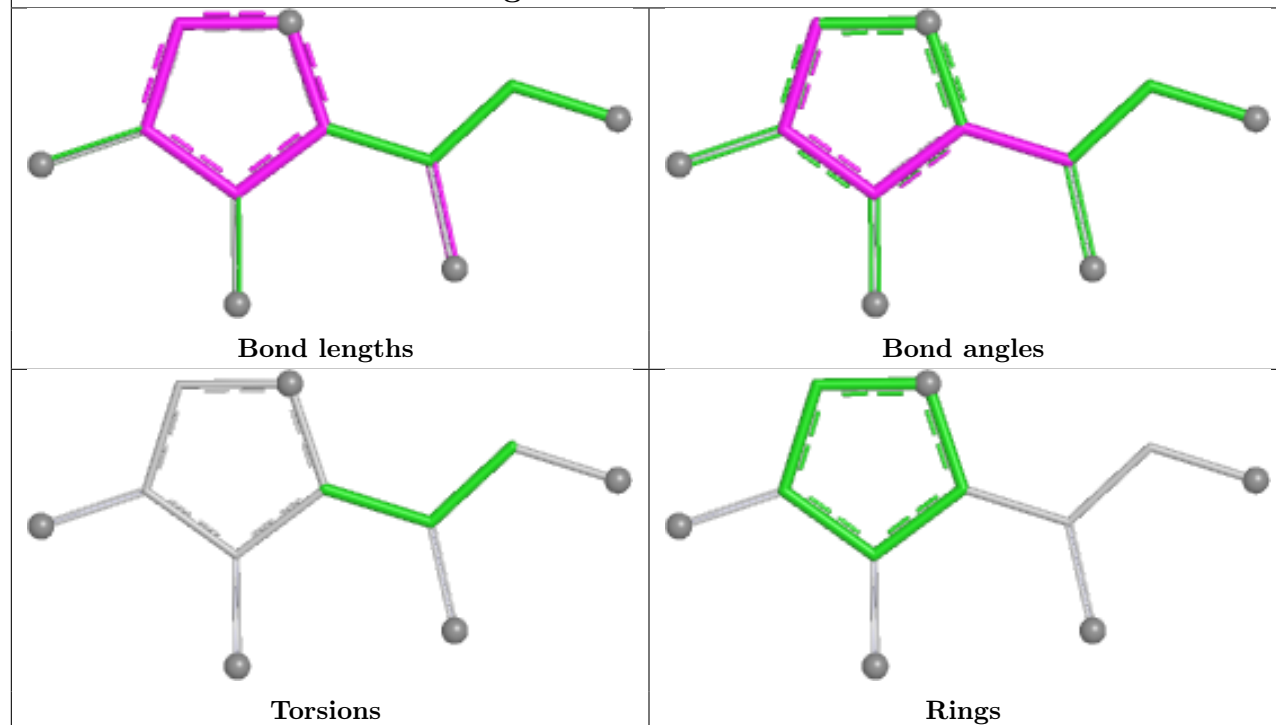


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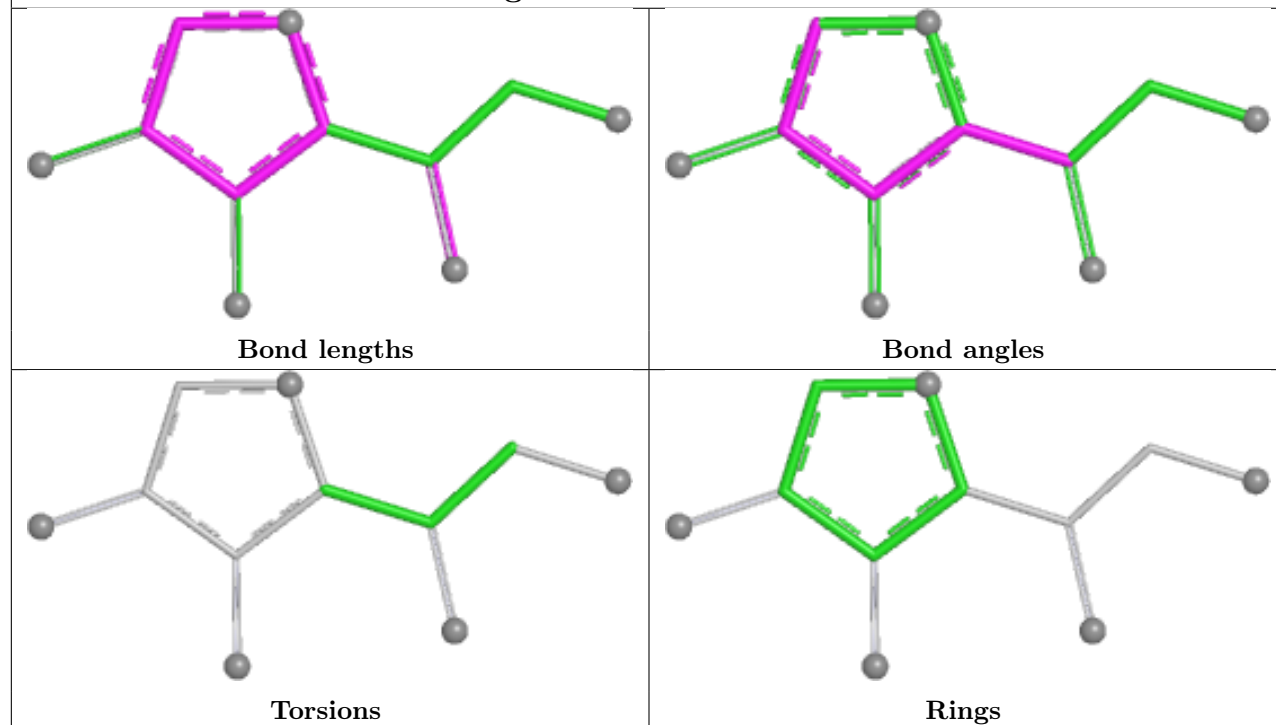




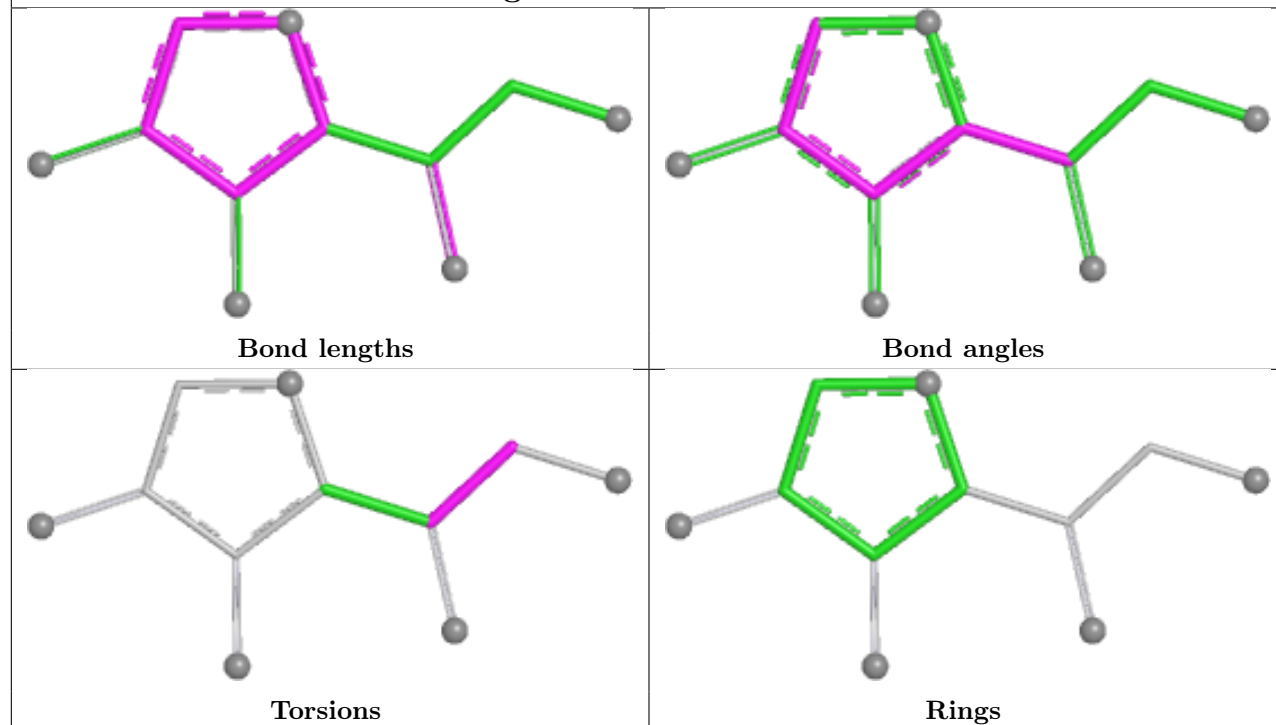
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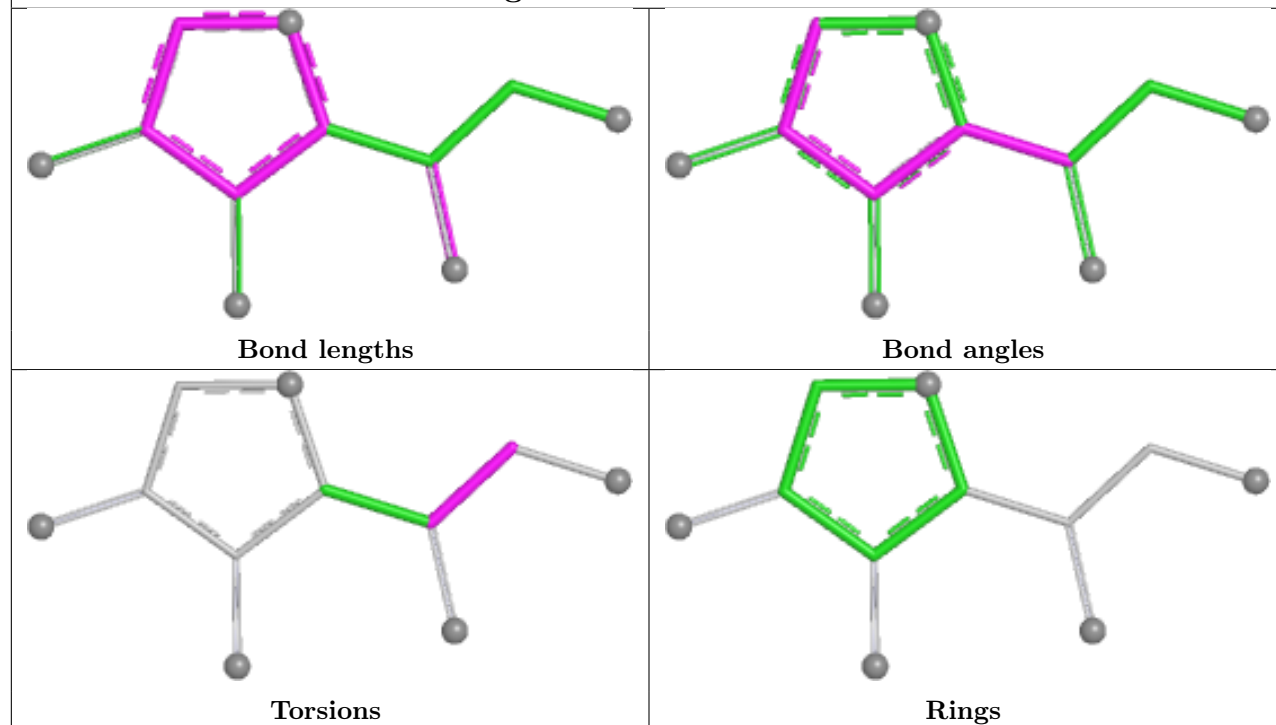
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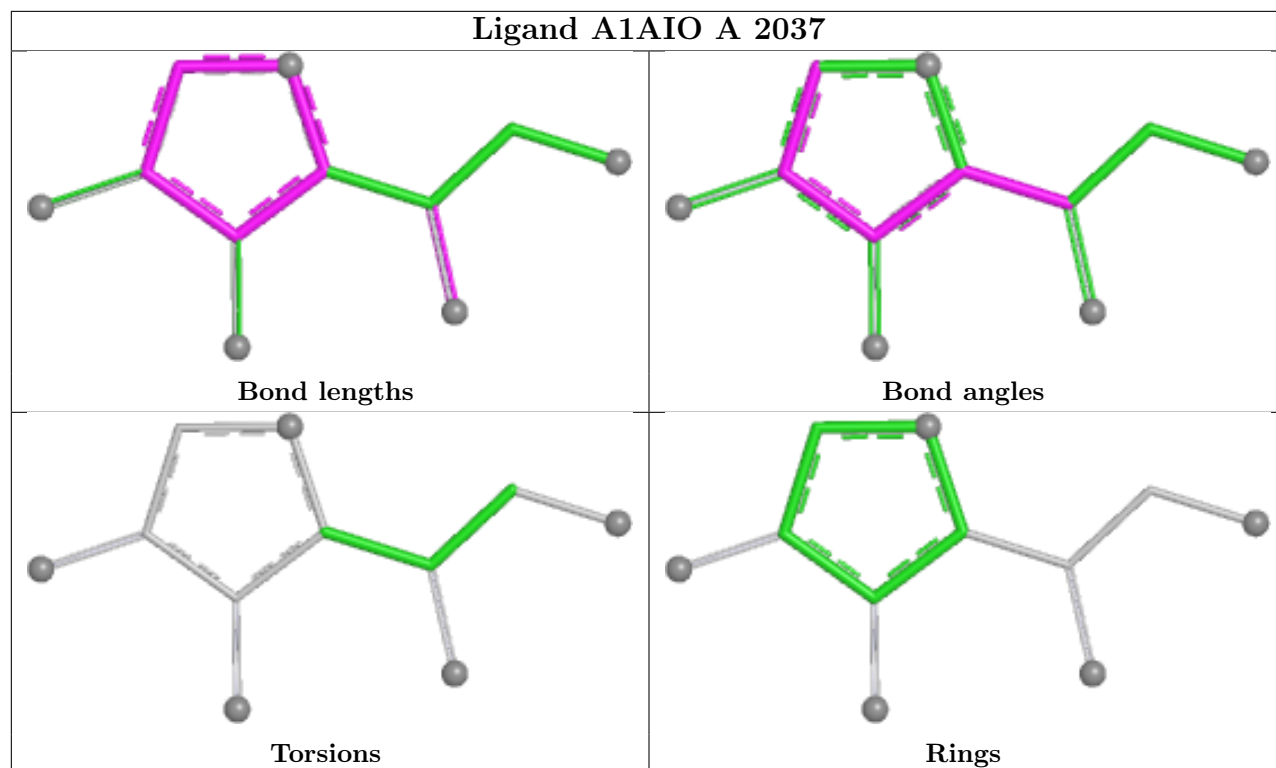
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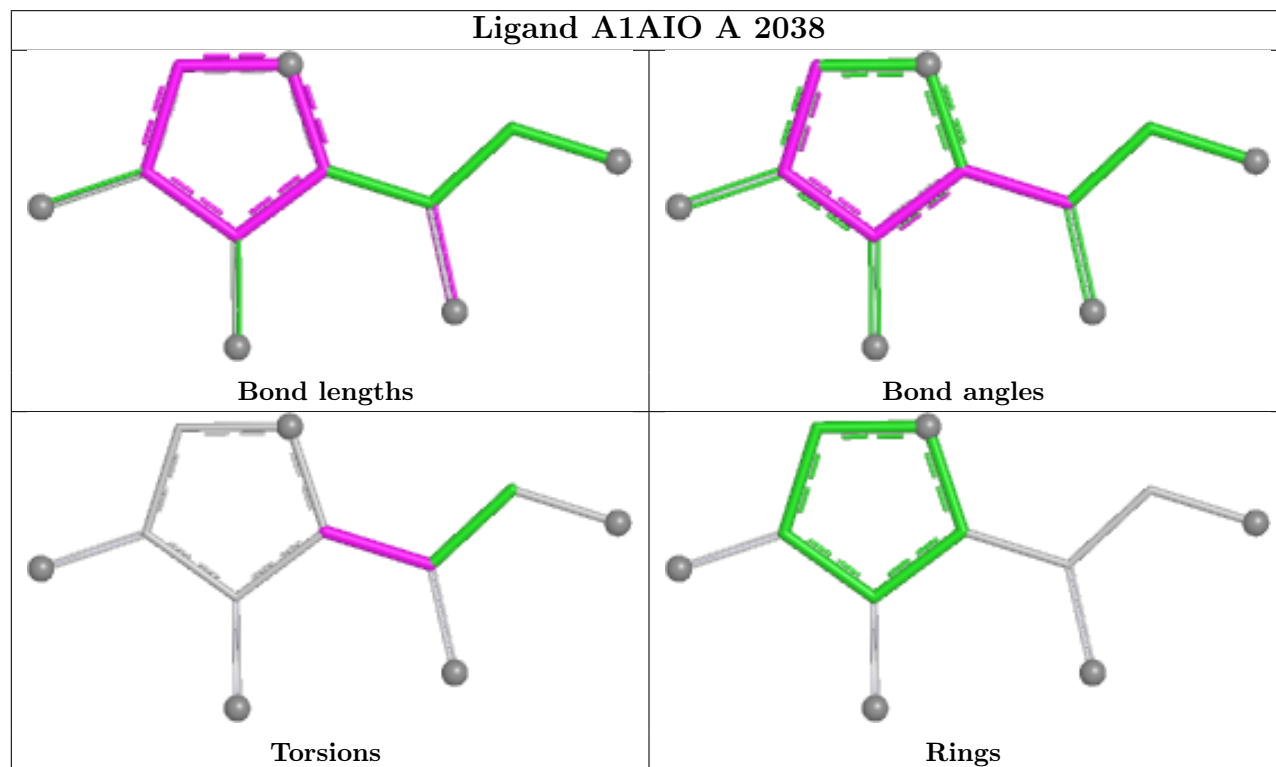
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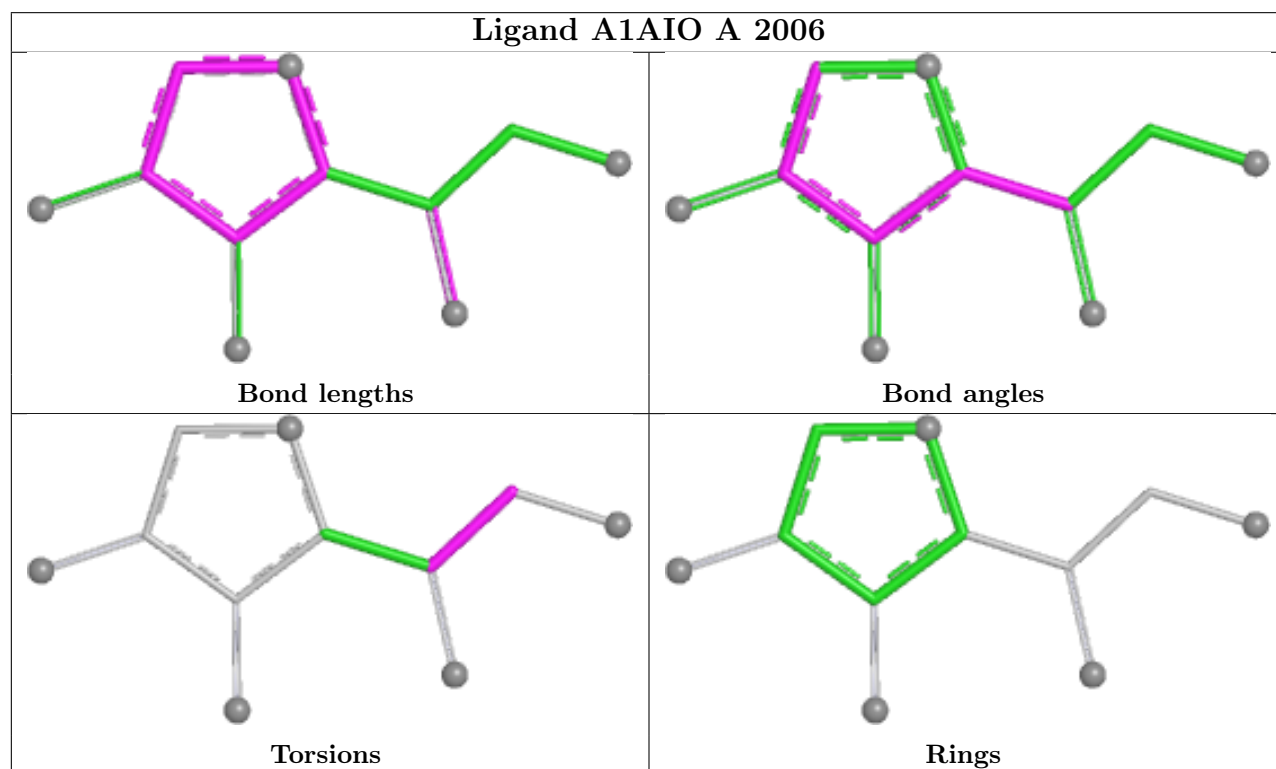
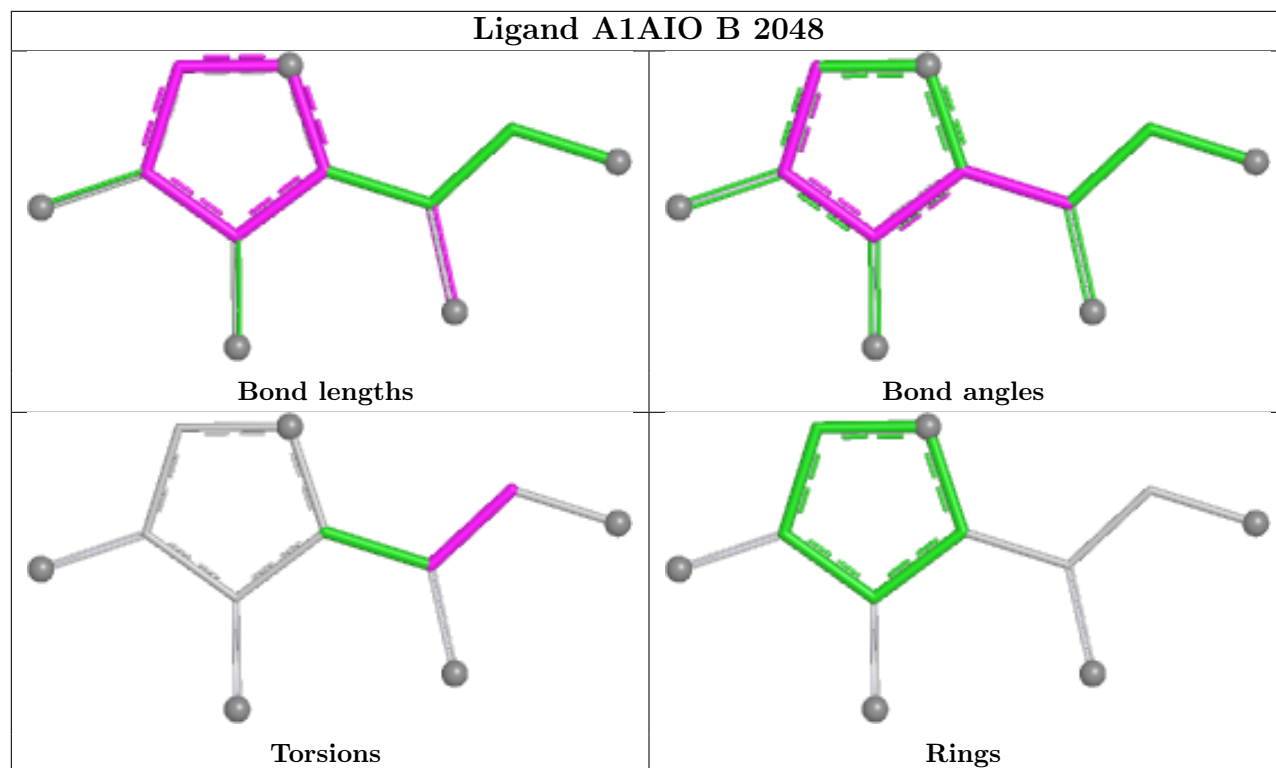


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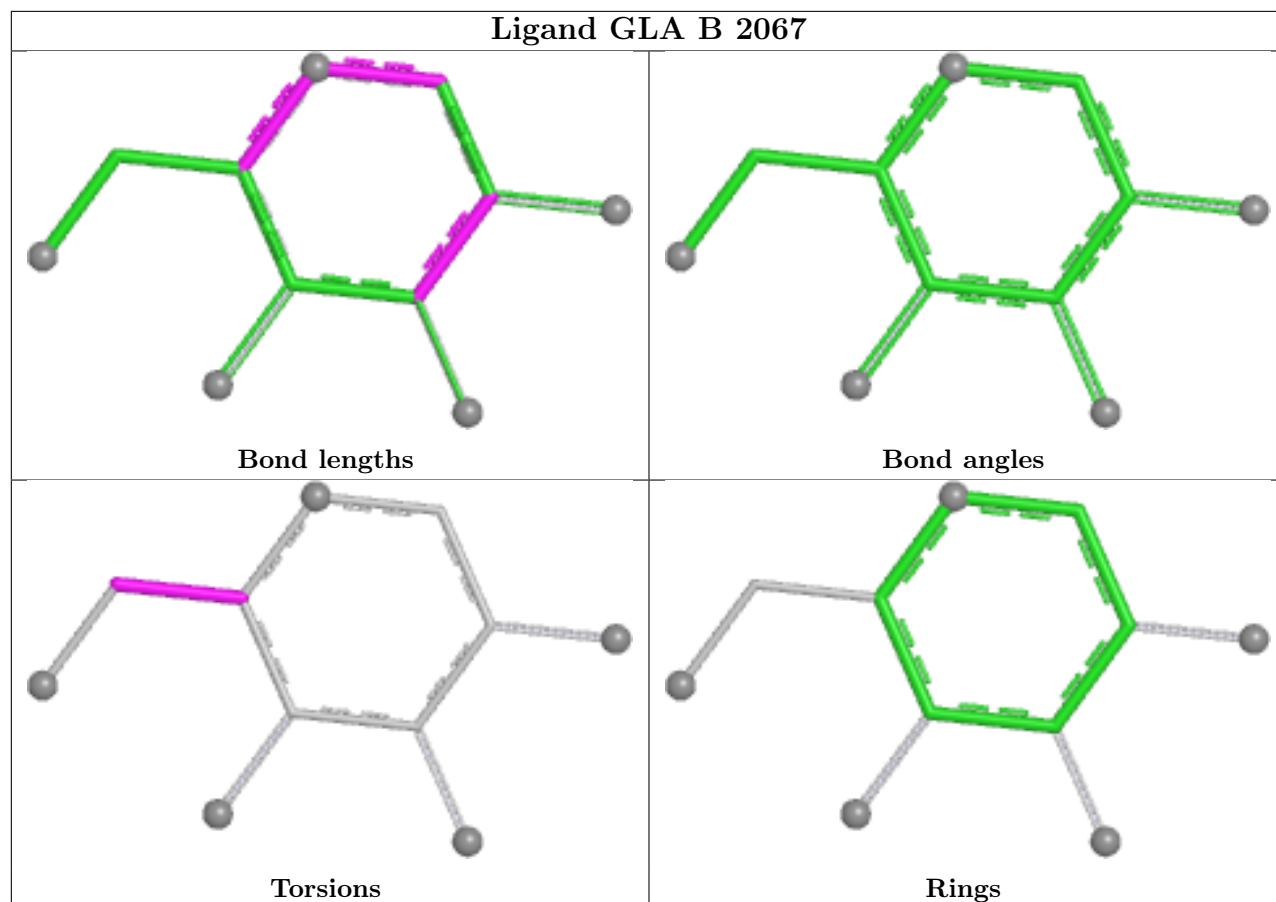


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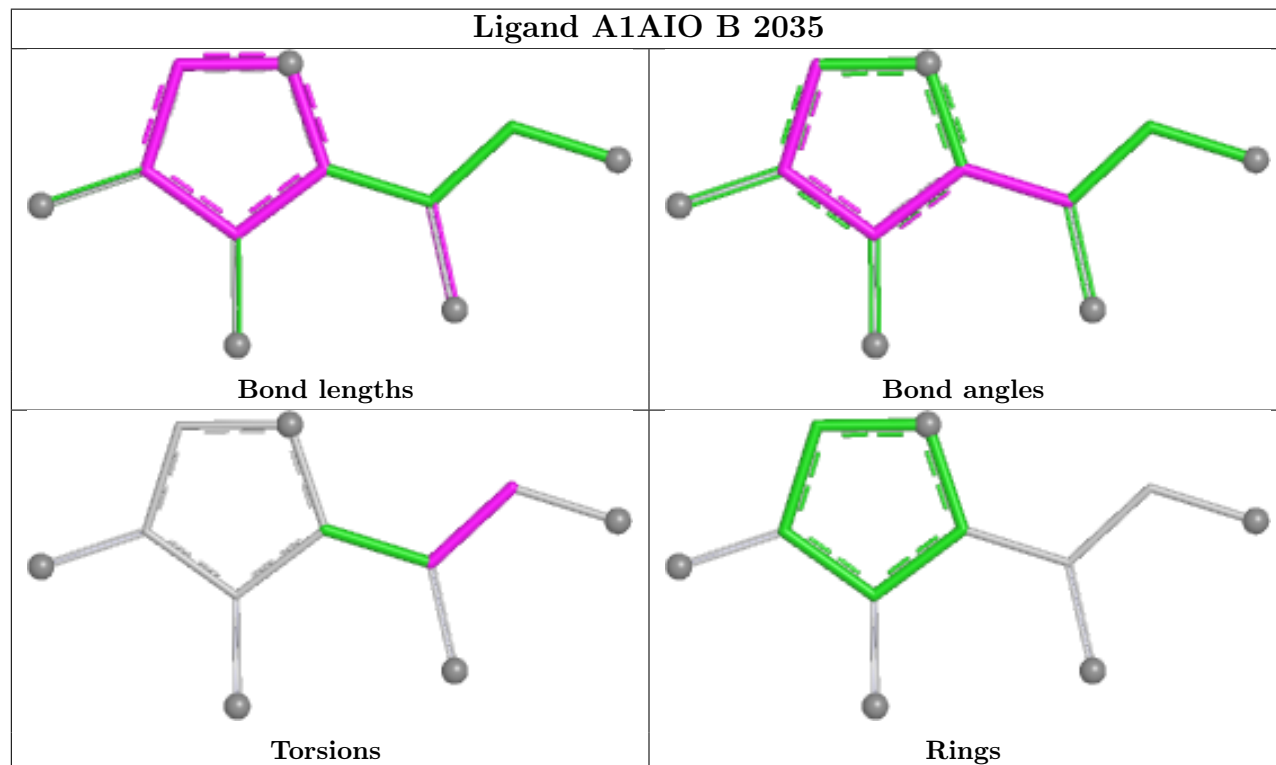




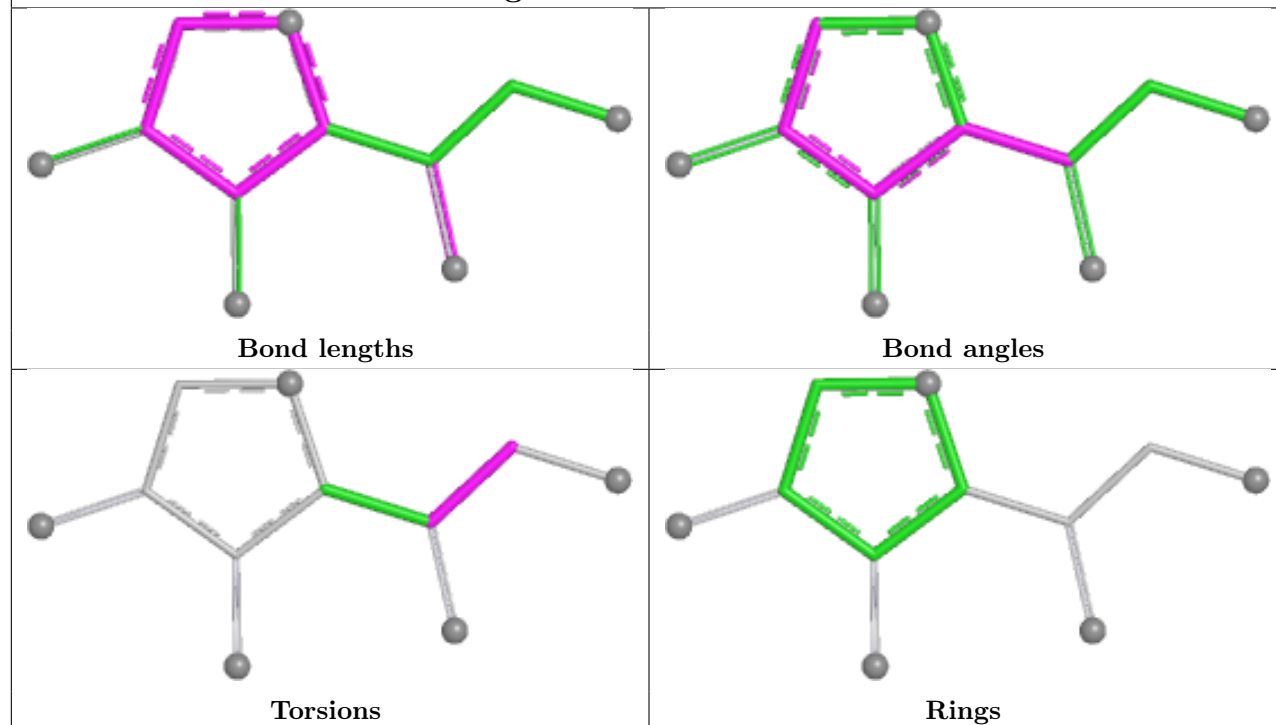
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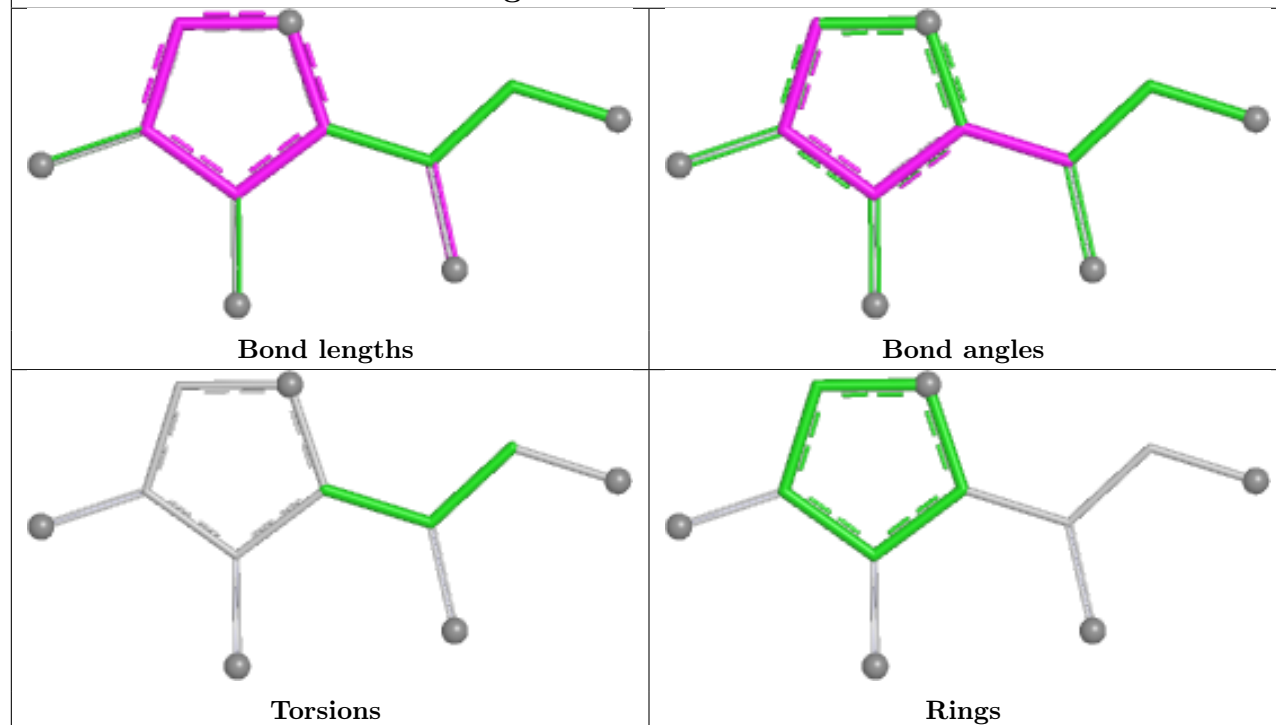
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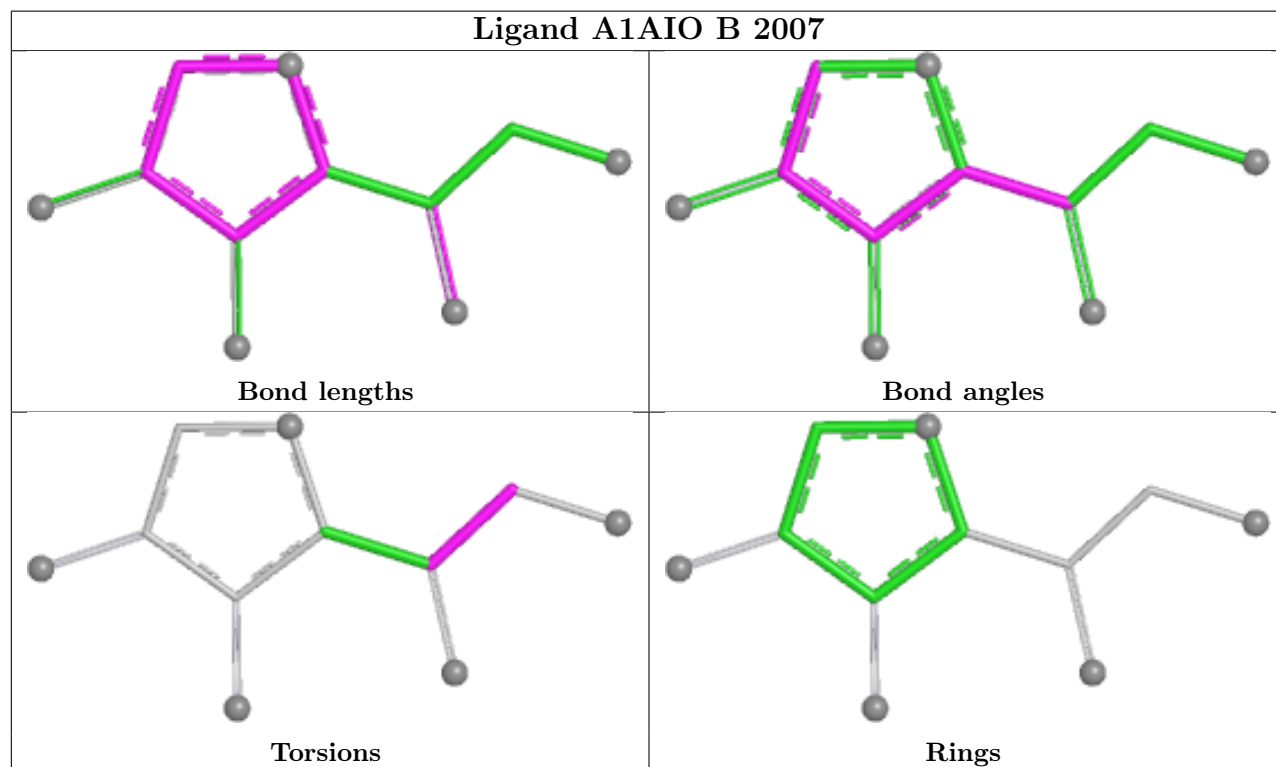
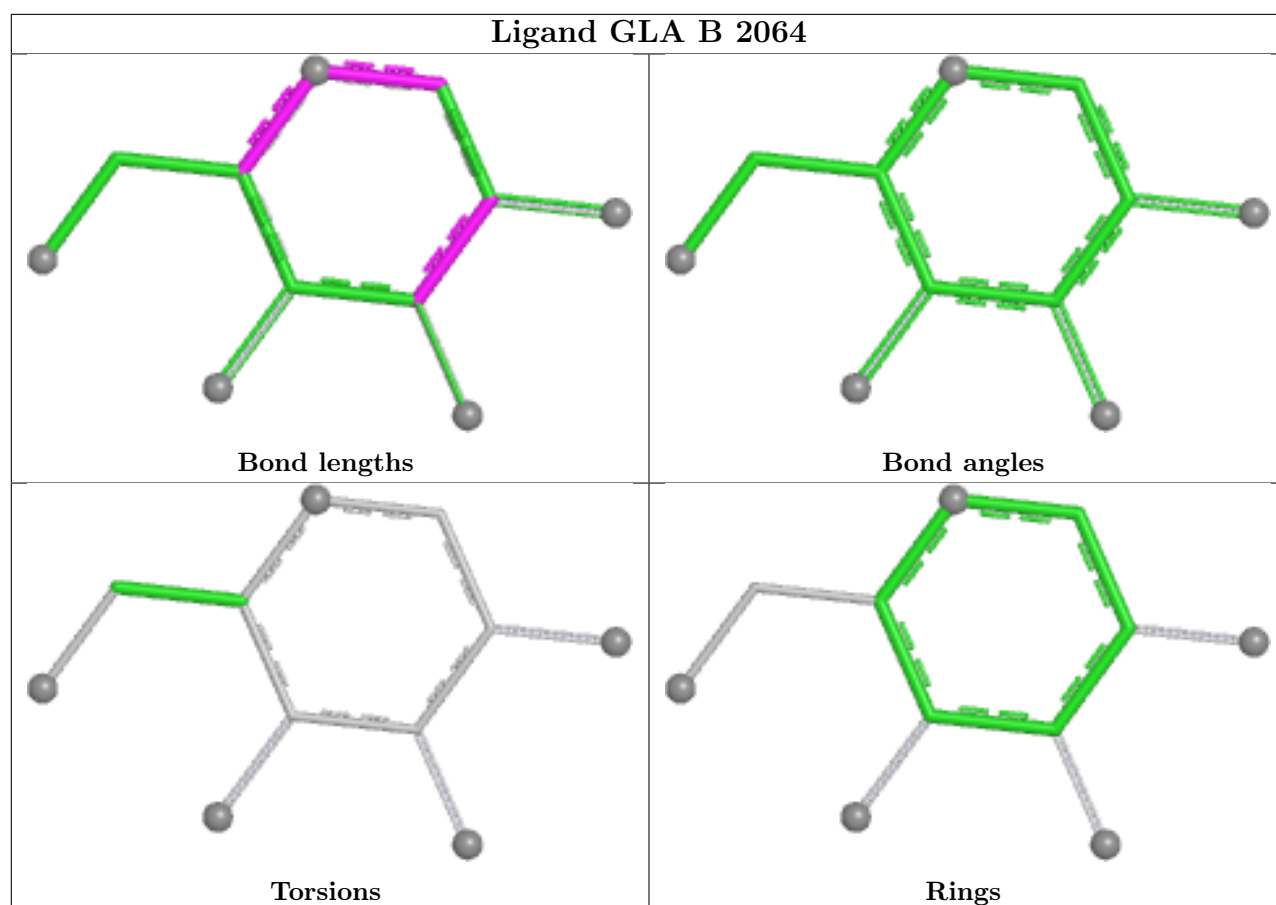


Ligand A1AIO B 2006

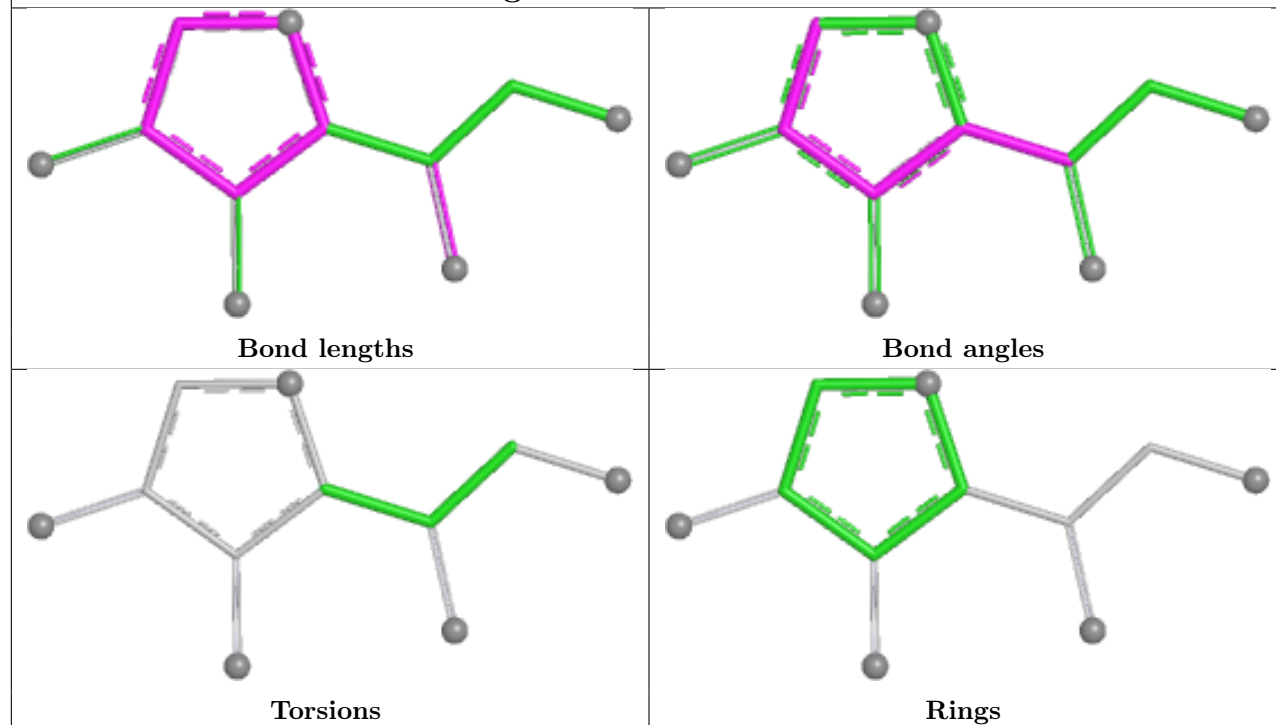


Ligand A1AIO A 2042

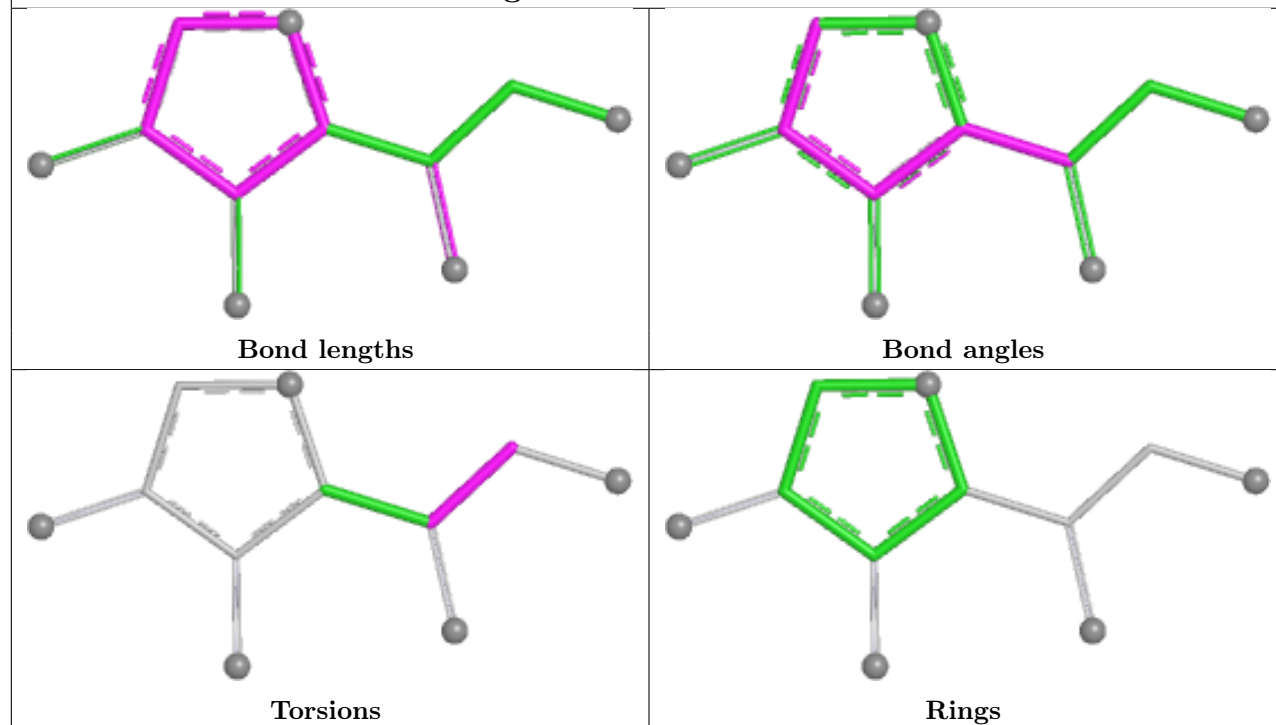




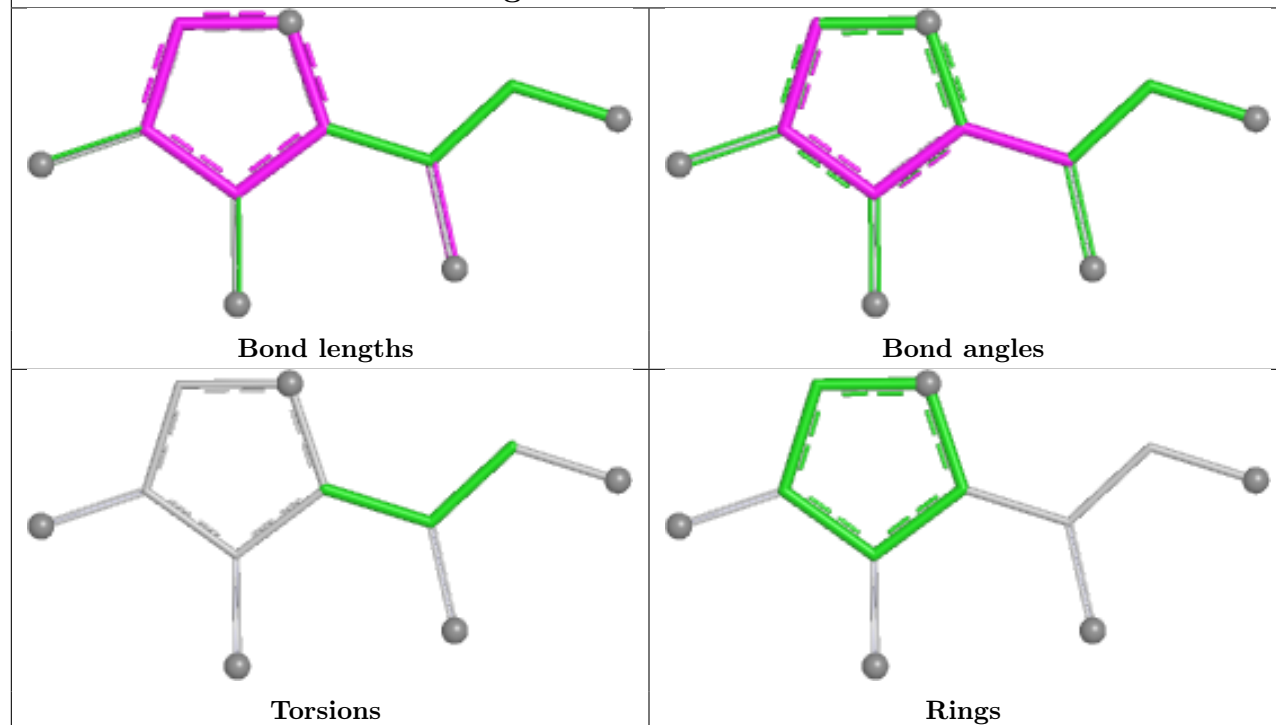
Ligand A1AIO A 2036



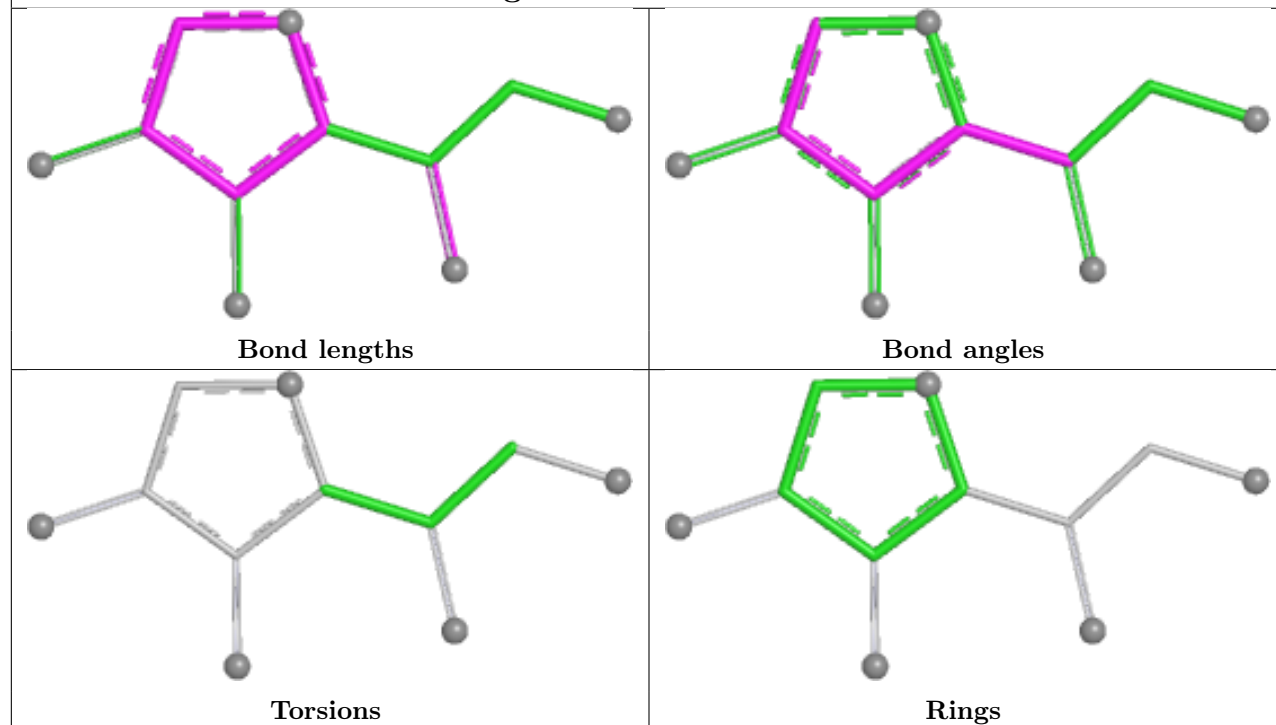
Ligand A1AIO A 2016

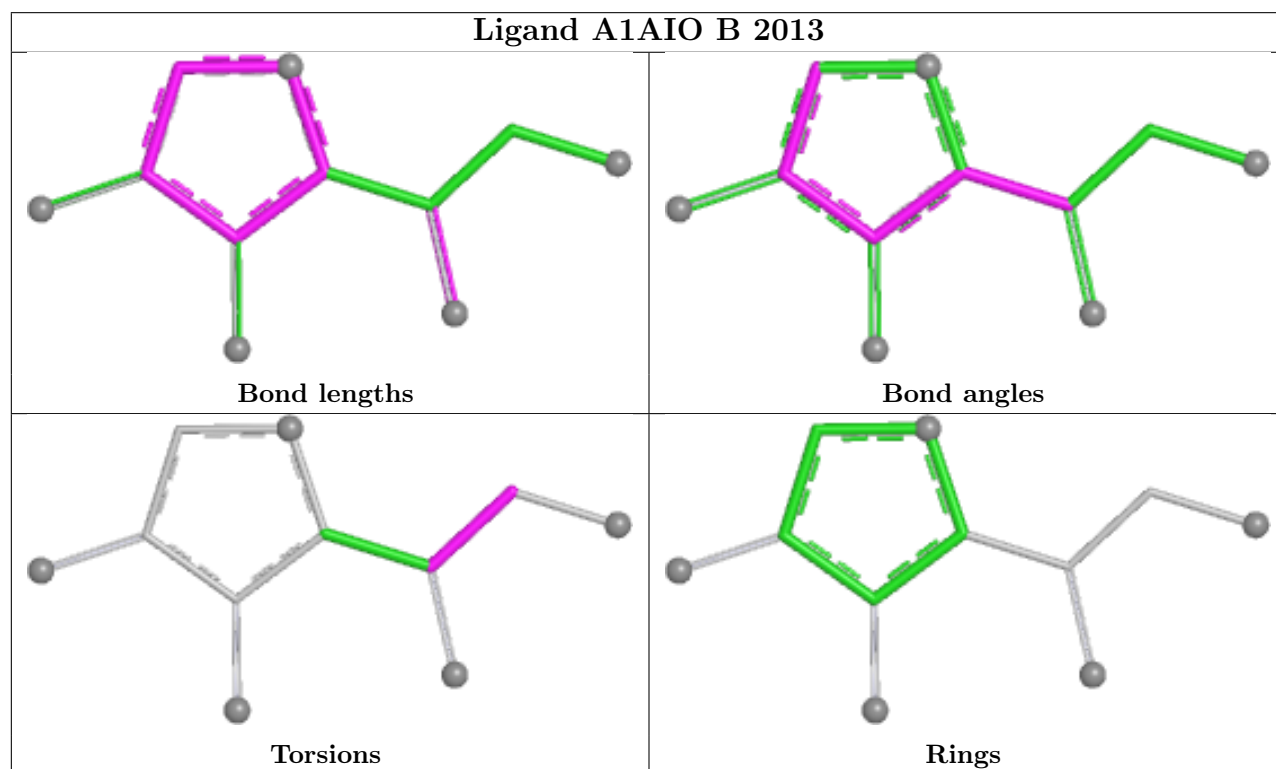
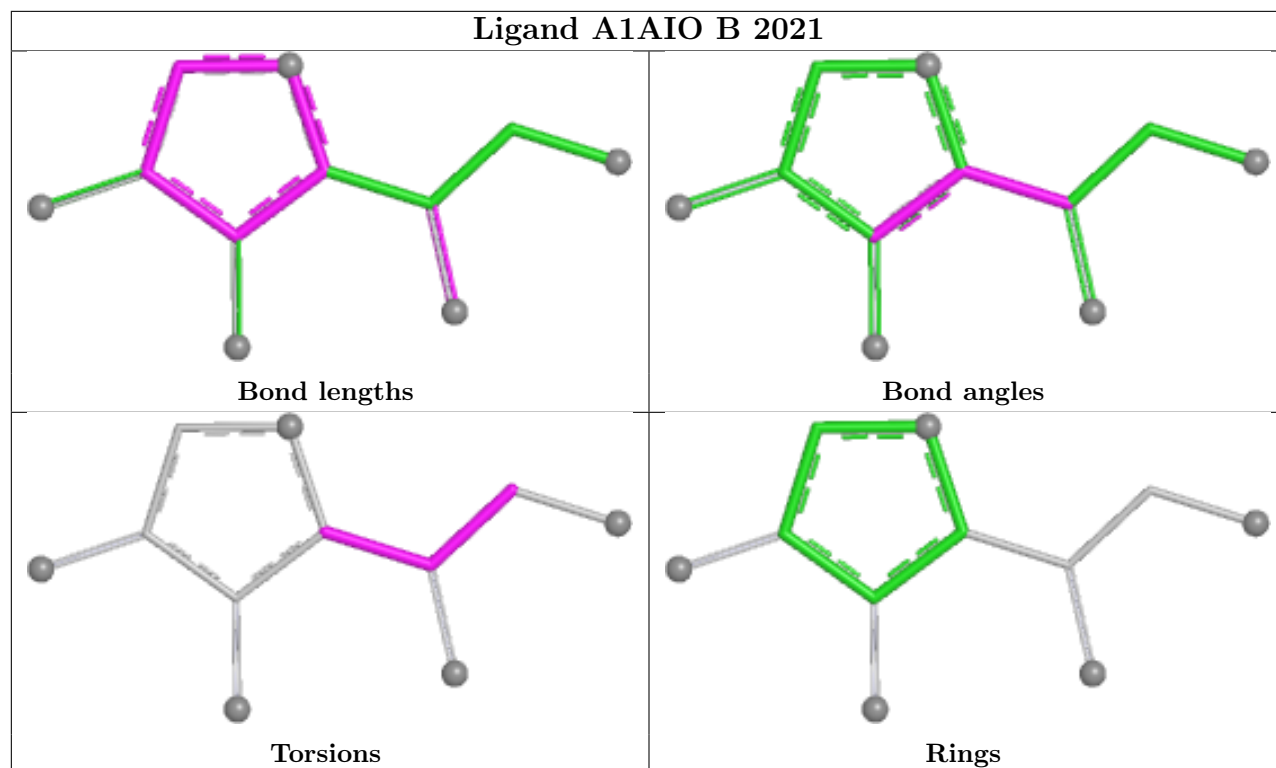


Ligand A1AIO A 2022

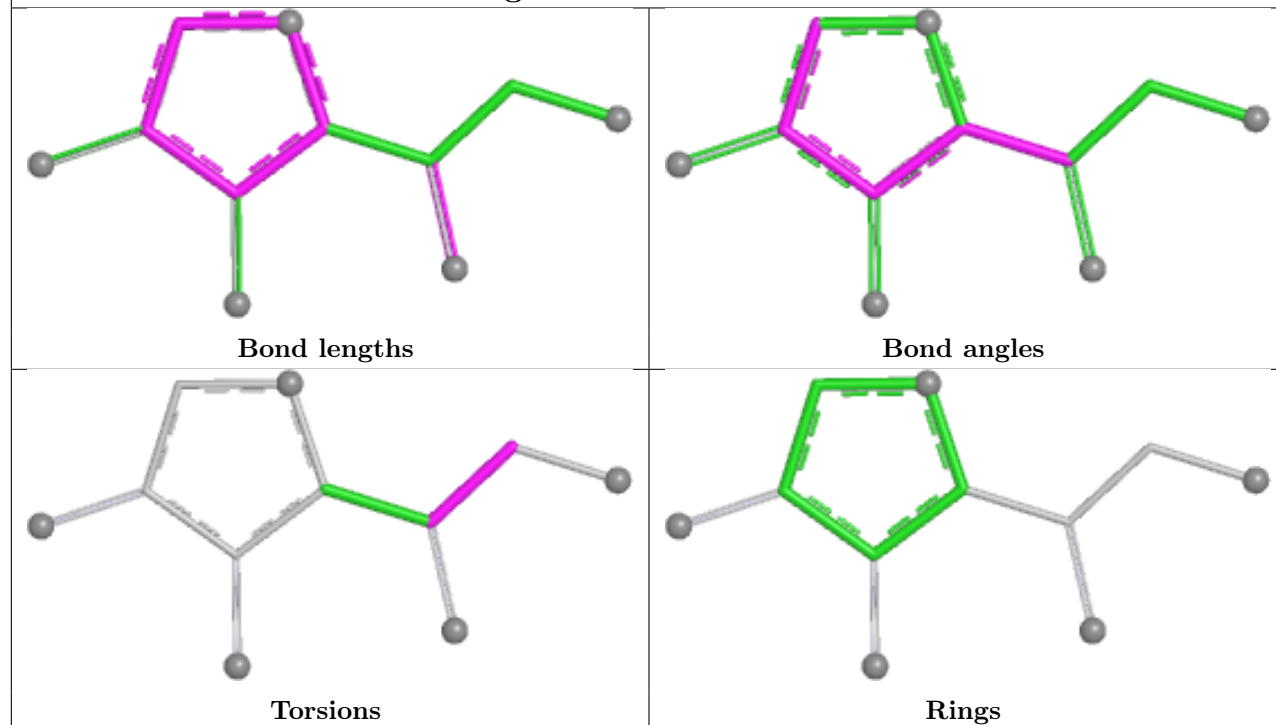


Ligand A1AIO A 2056

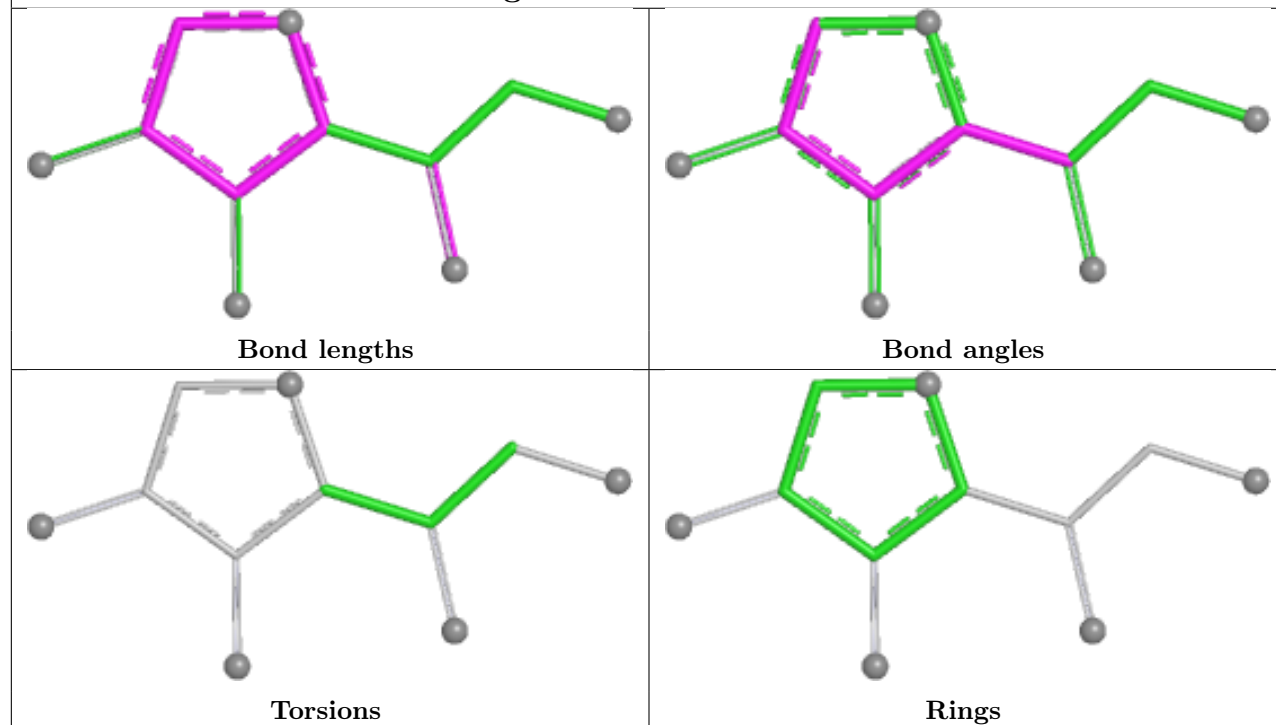




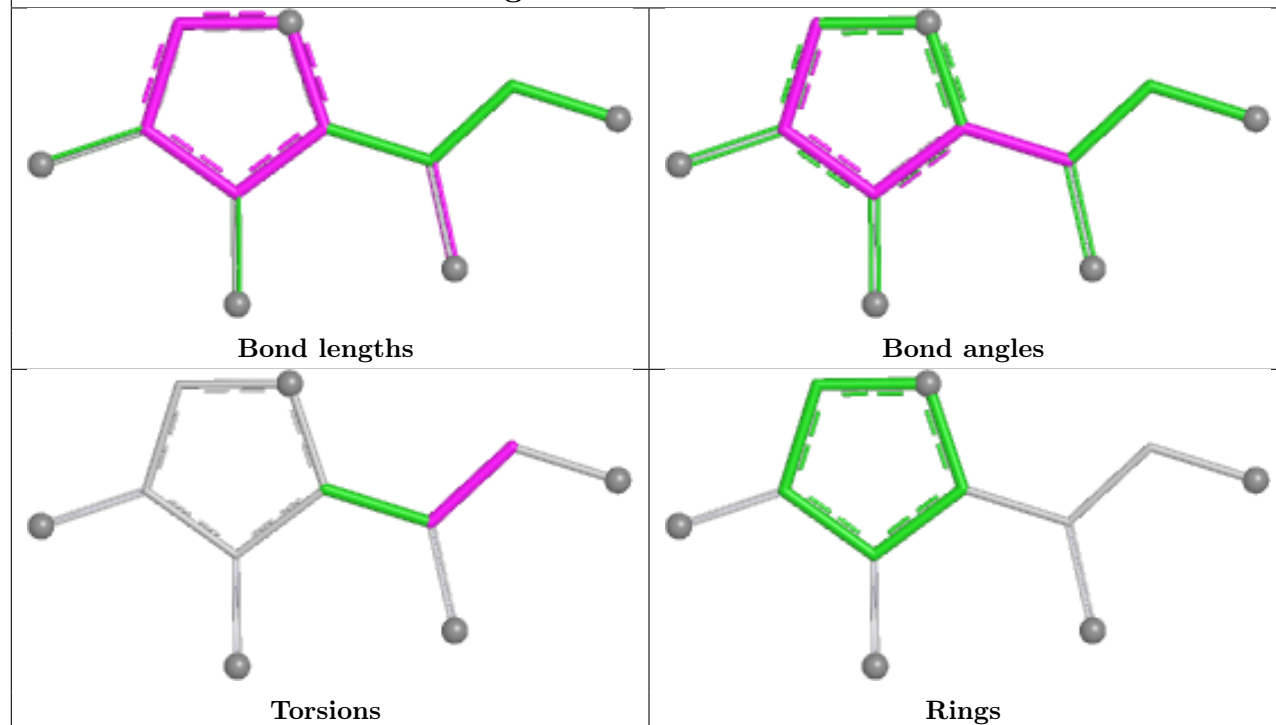
Ligand A1AIO B 2008



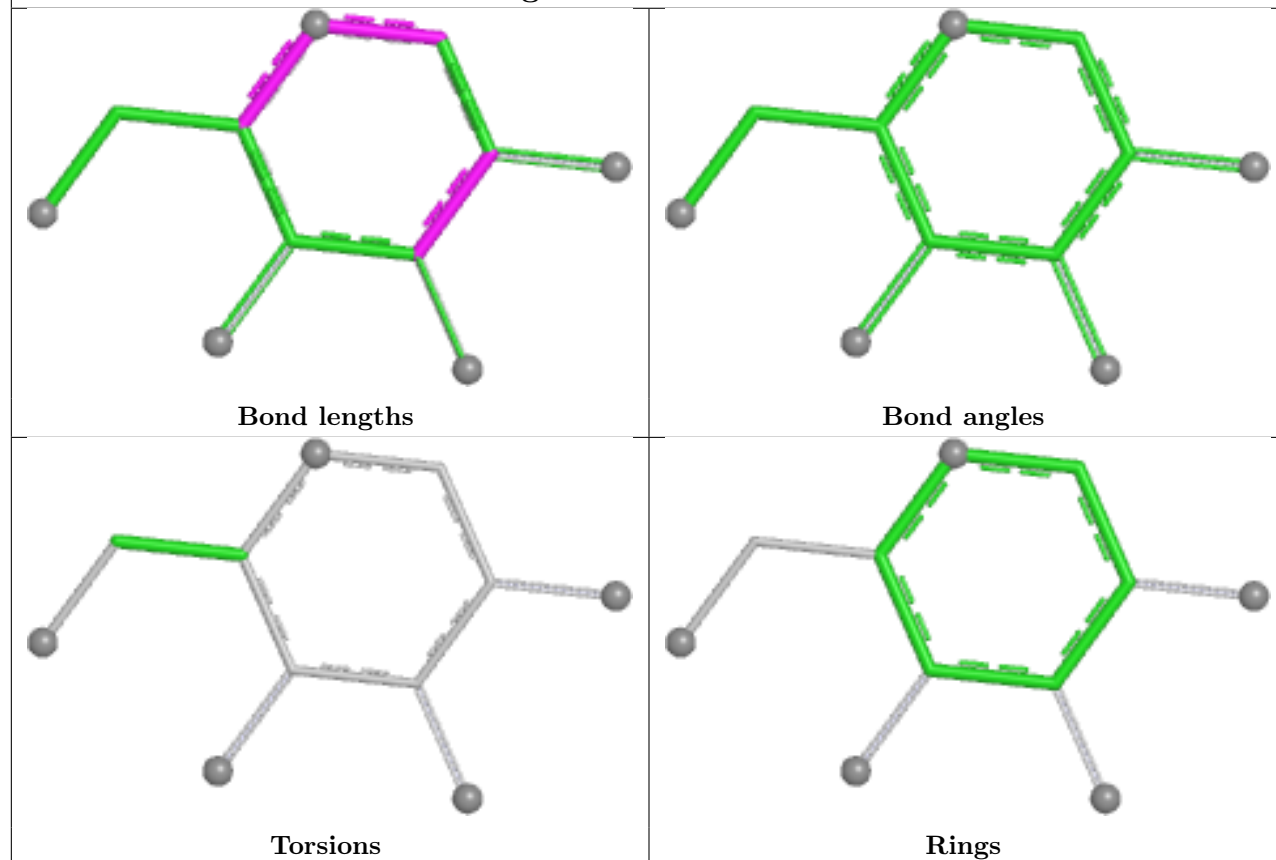
Ligand A1AIO A 2057



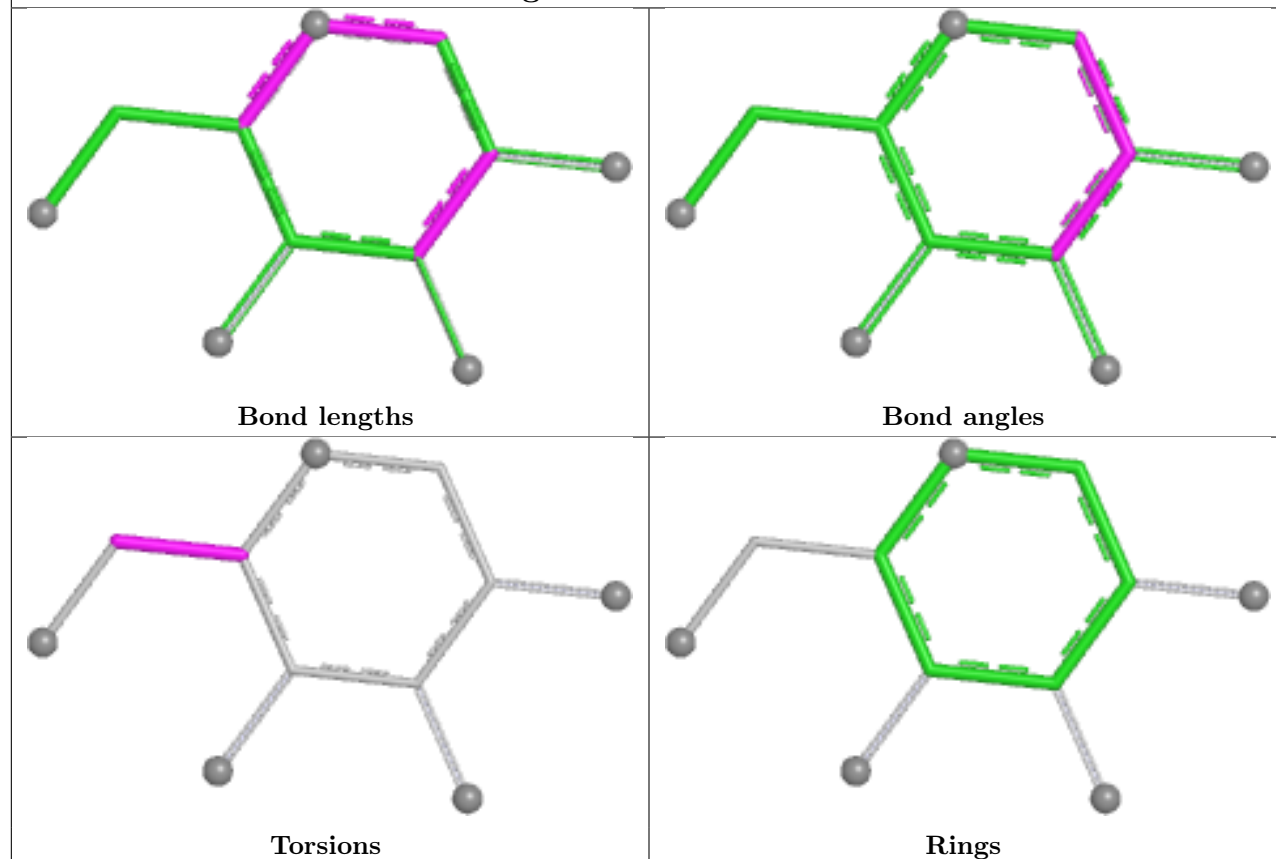
Ligand A1AIO B 2052



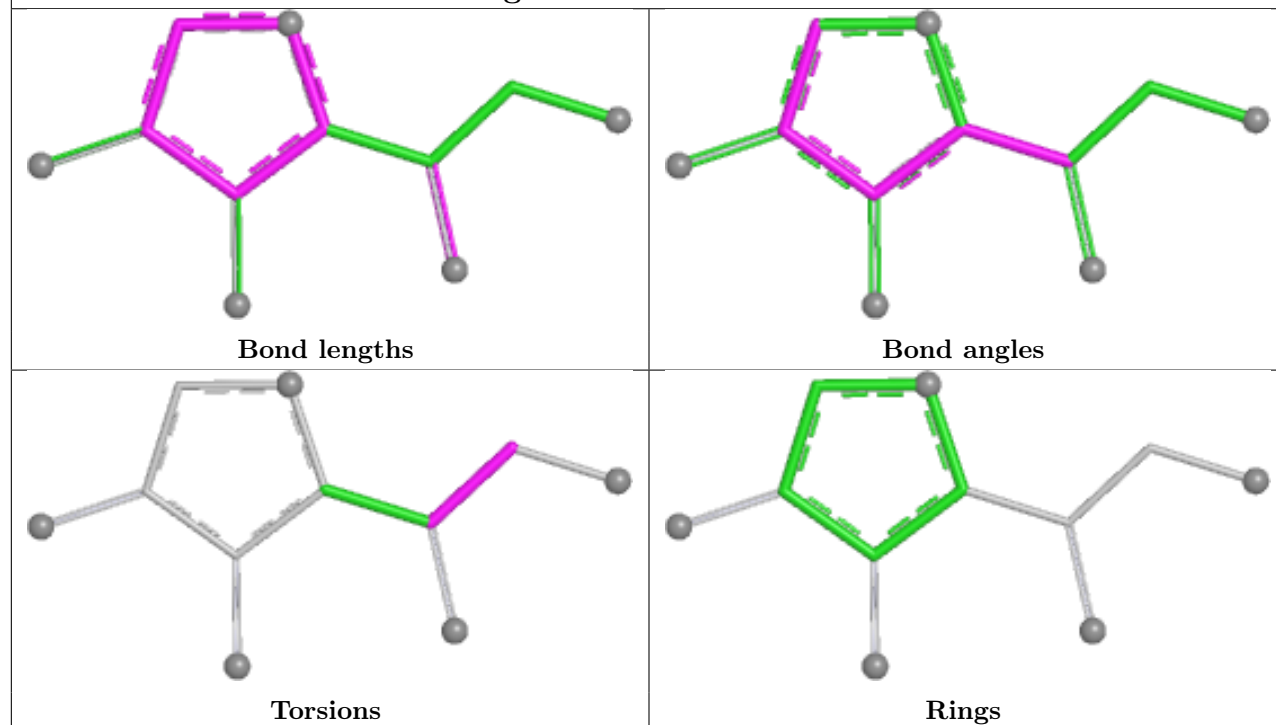
Ligand GLA A 2061



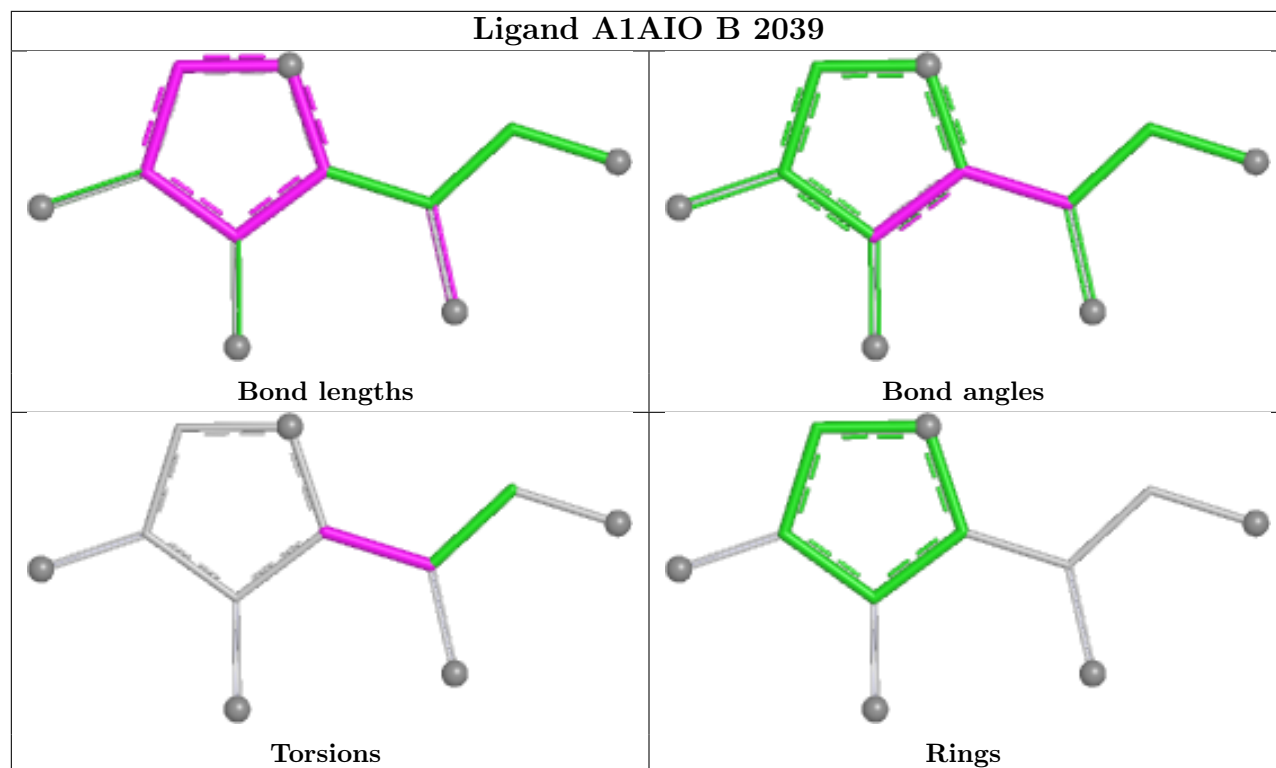
Ligand GLA B 2065



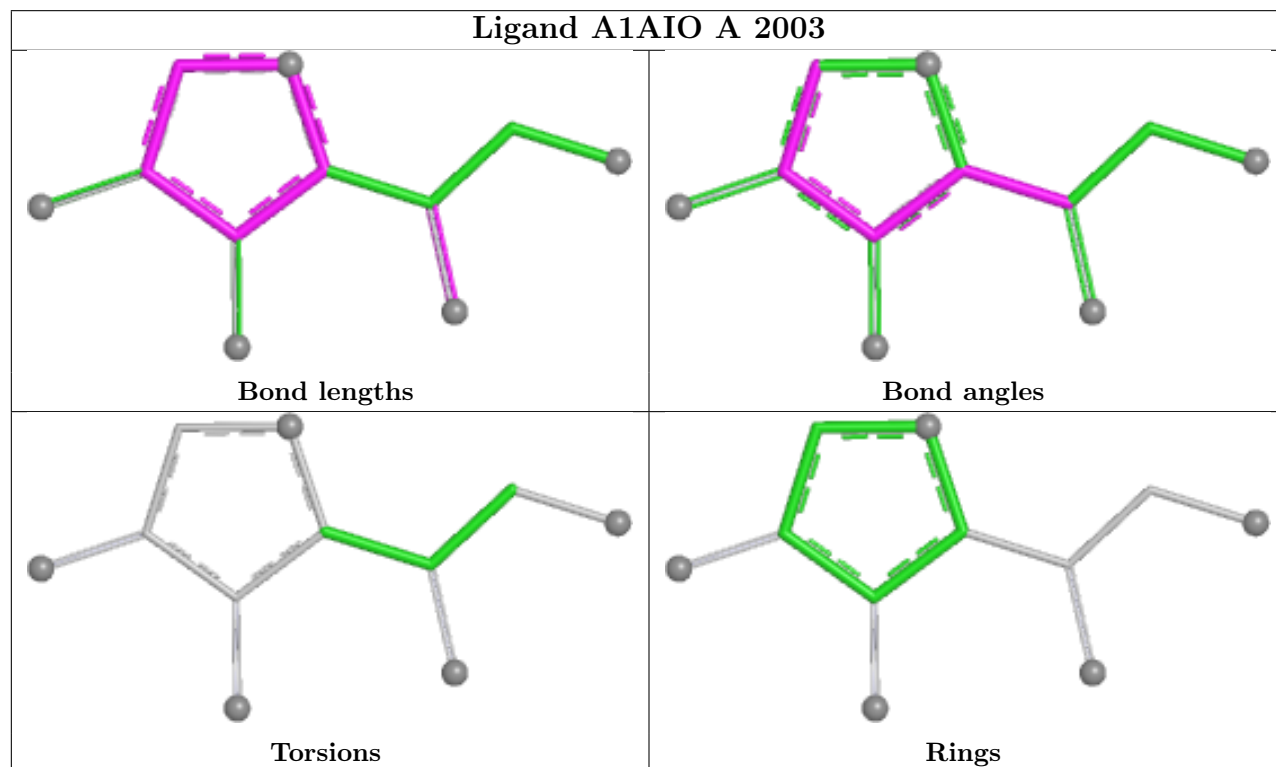
Ligand A1AIO A 2049

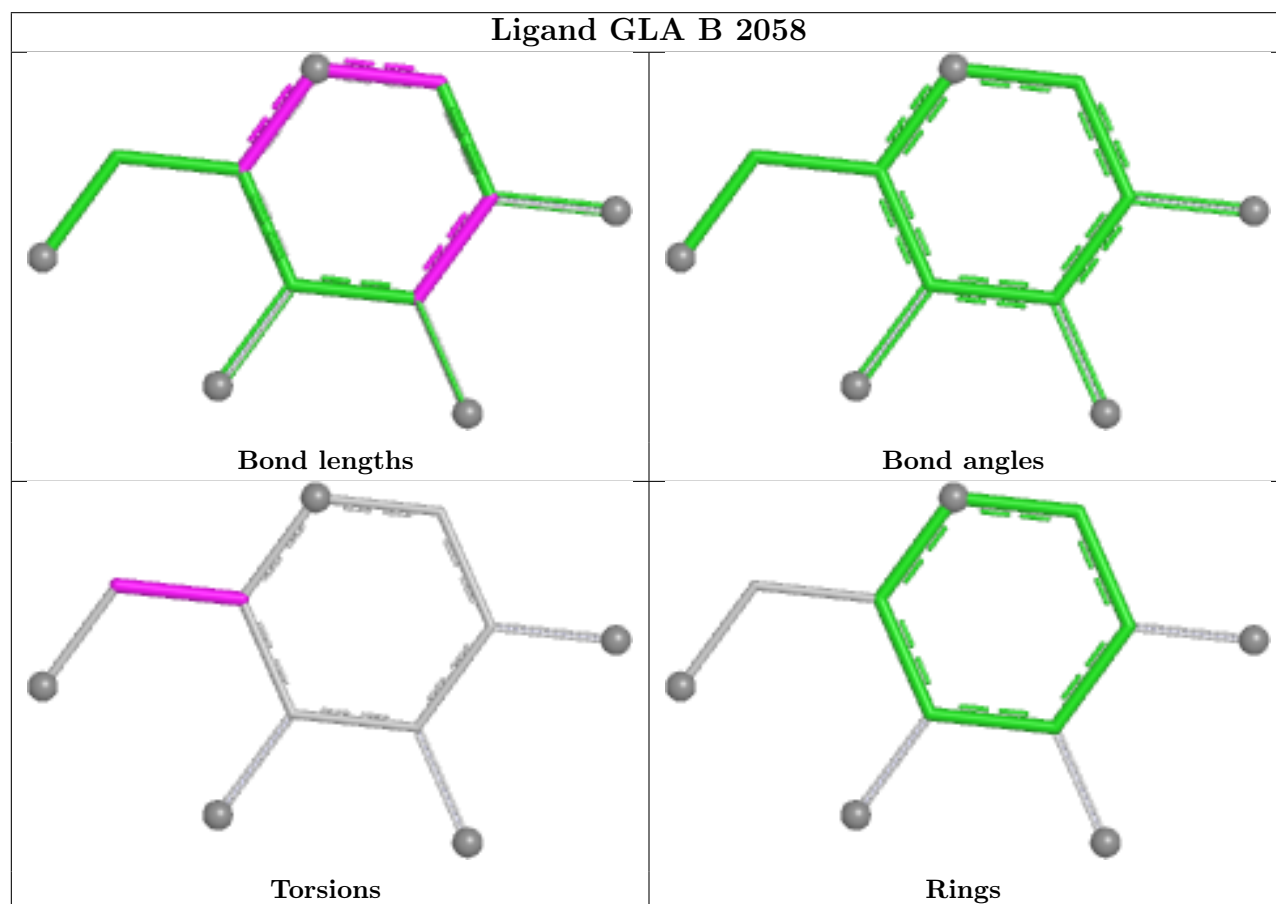
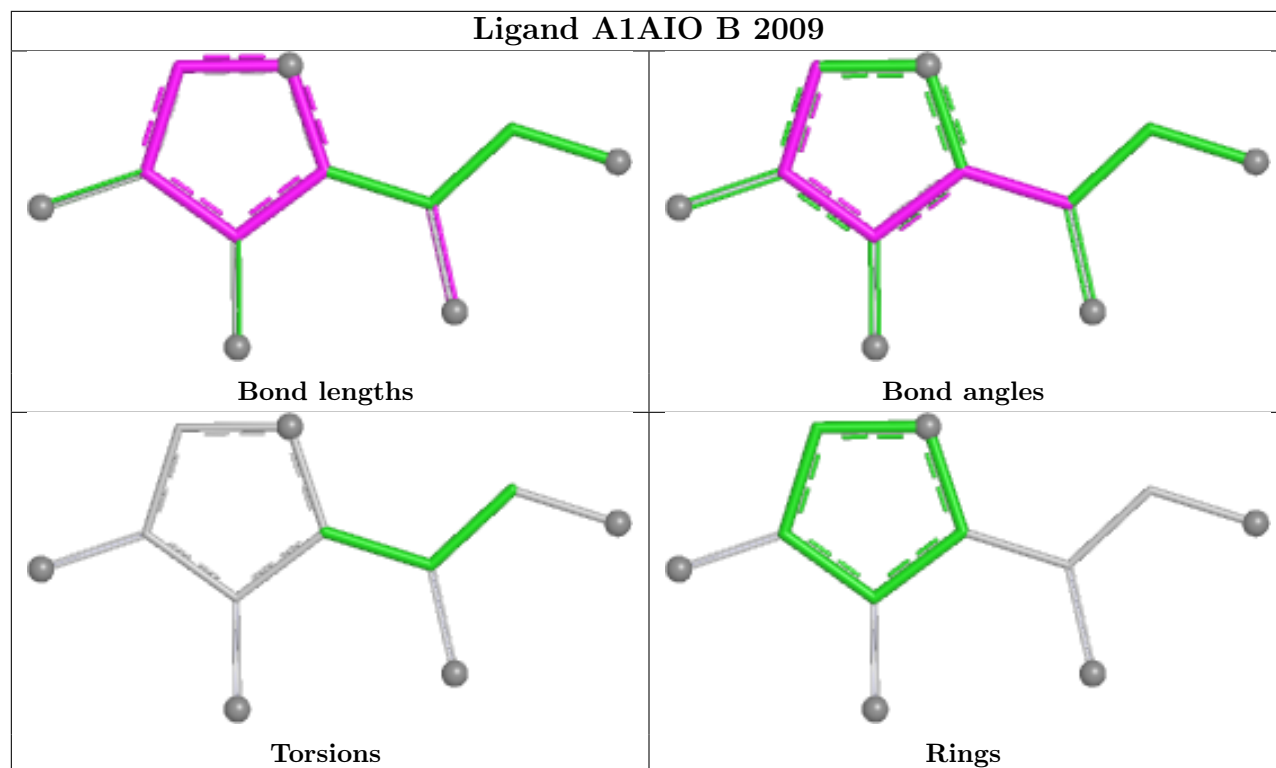


Ligand A1AIO B 2039

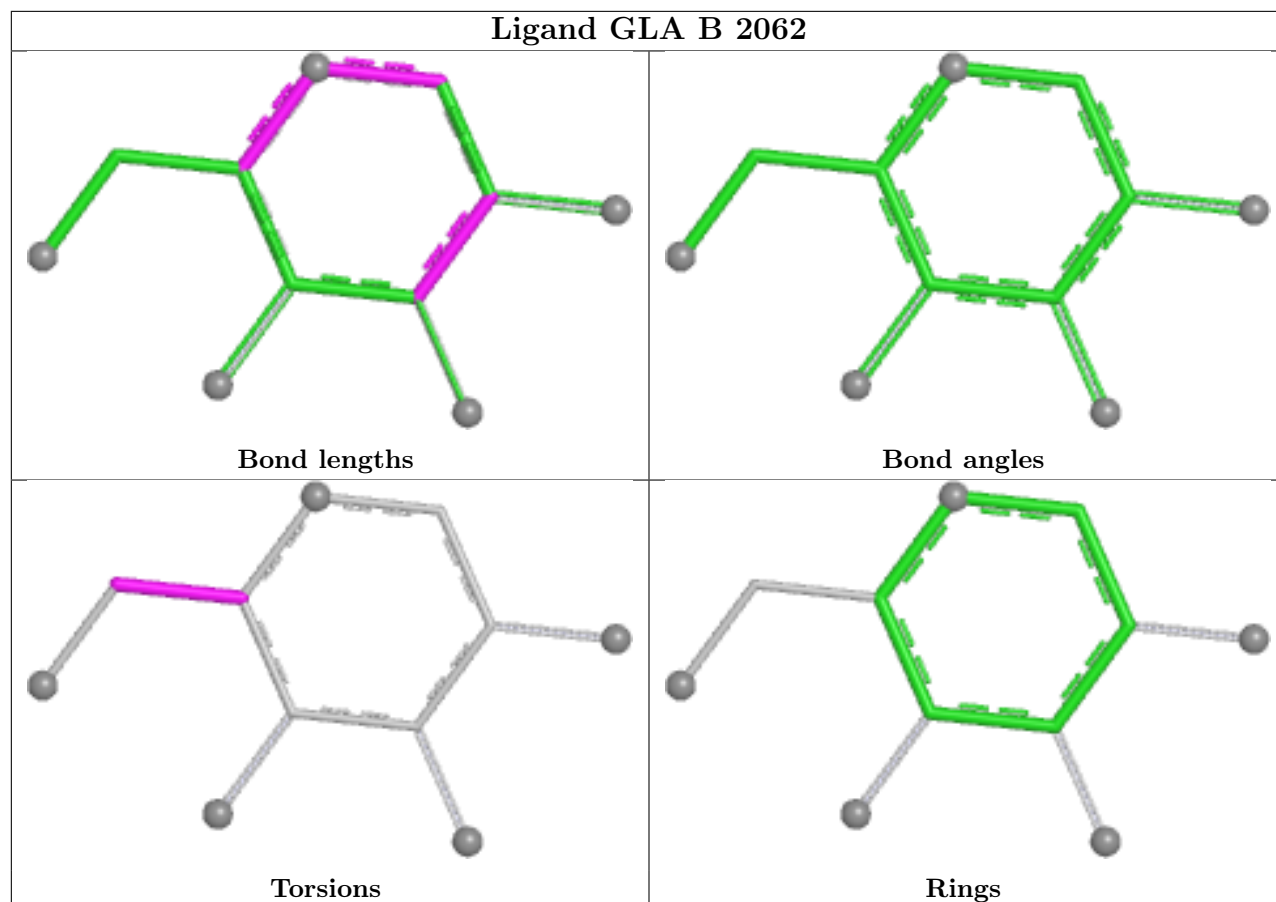


Ligand A1AIO A 2003

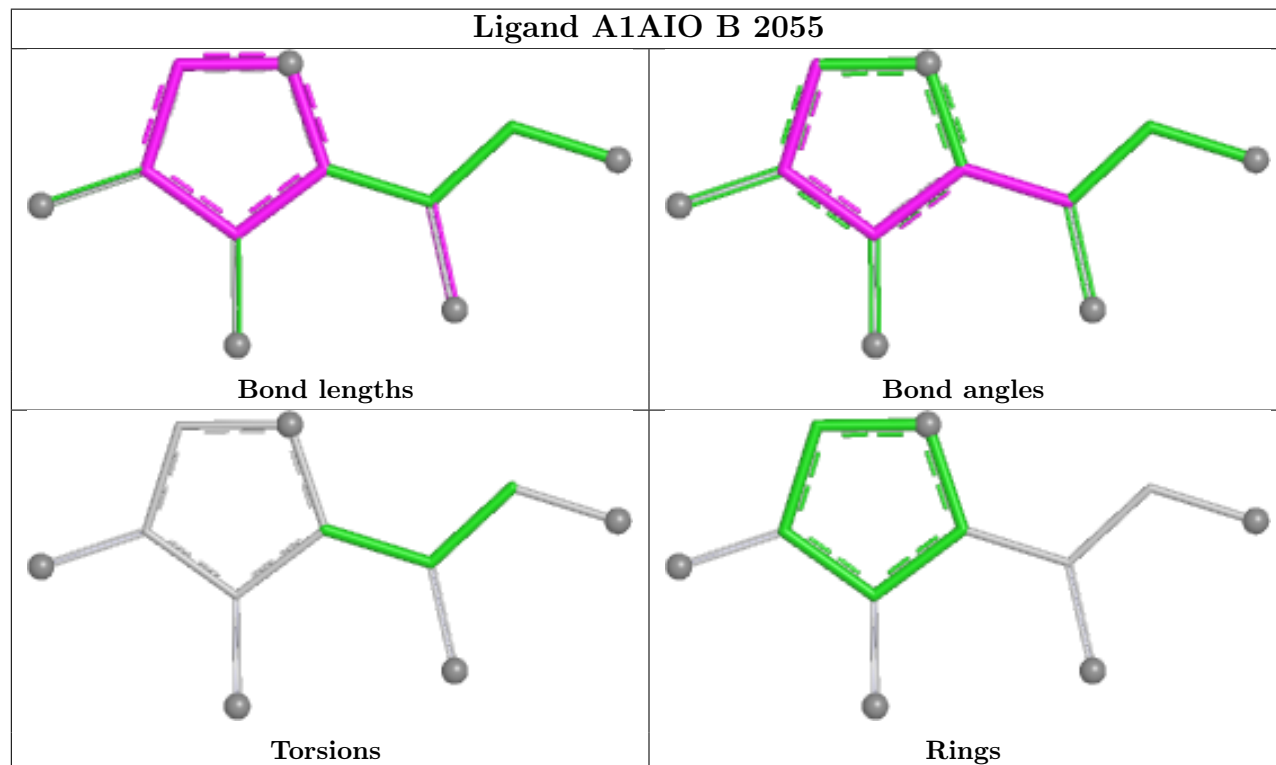




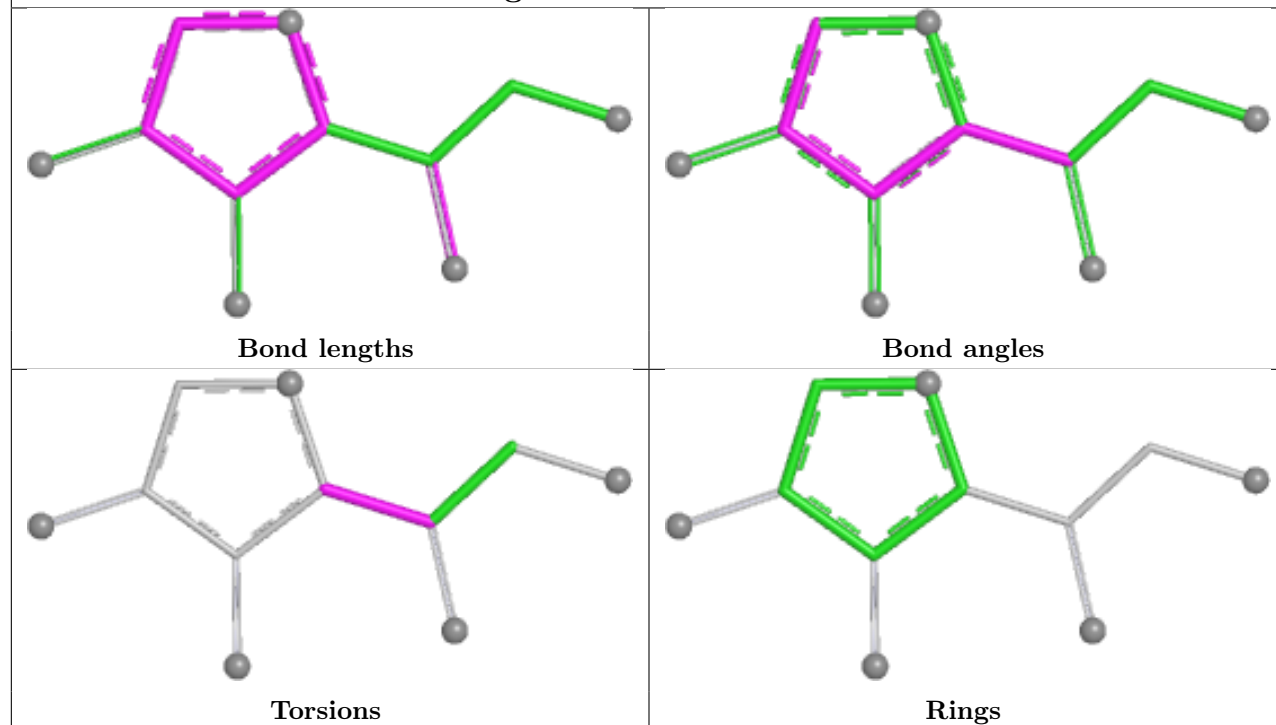
Ligand GLA B 2062



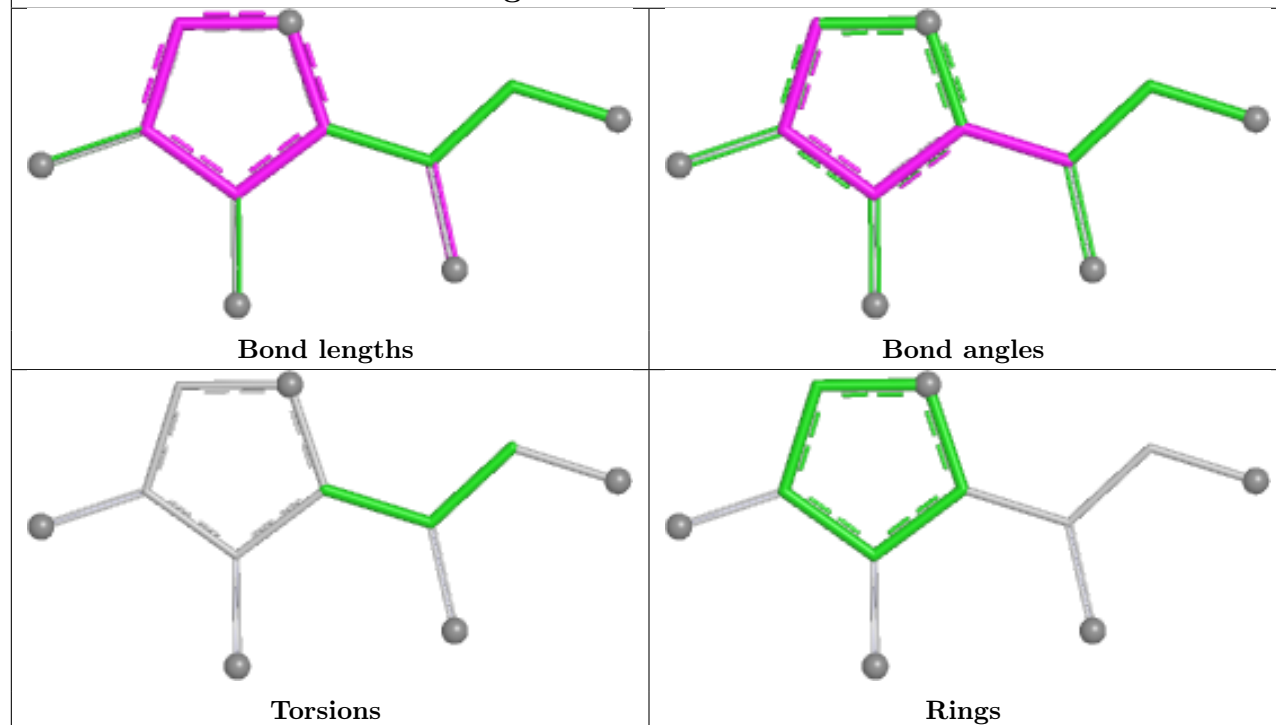
Ligand A1AIO B 2055

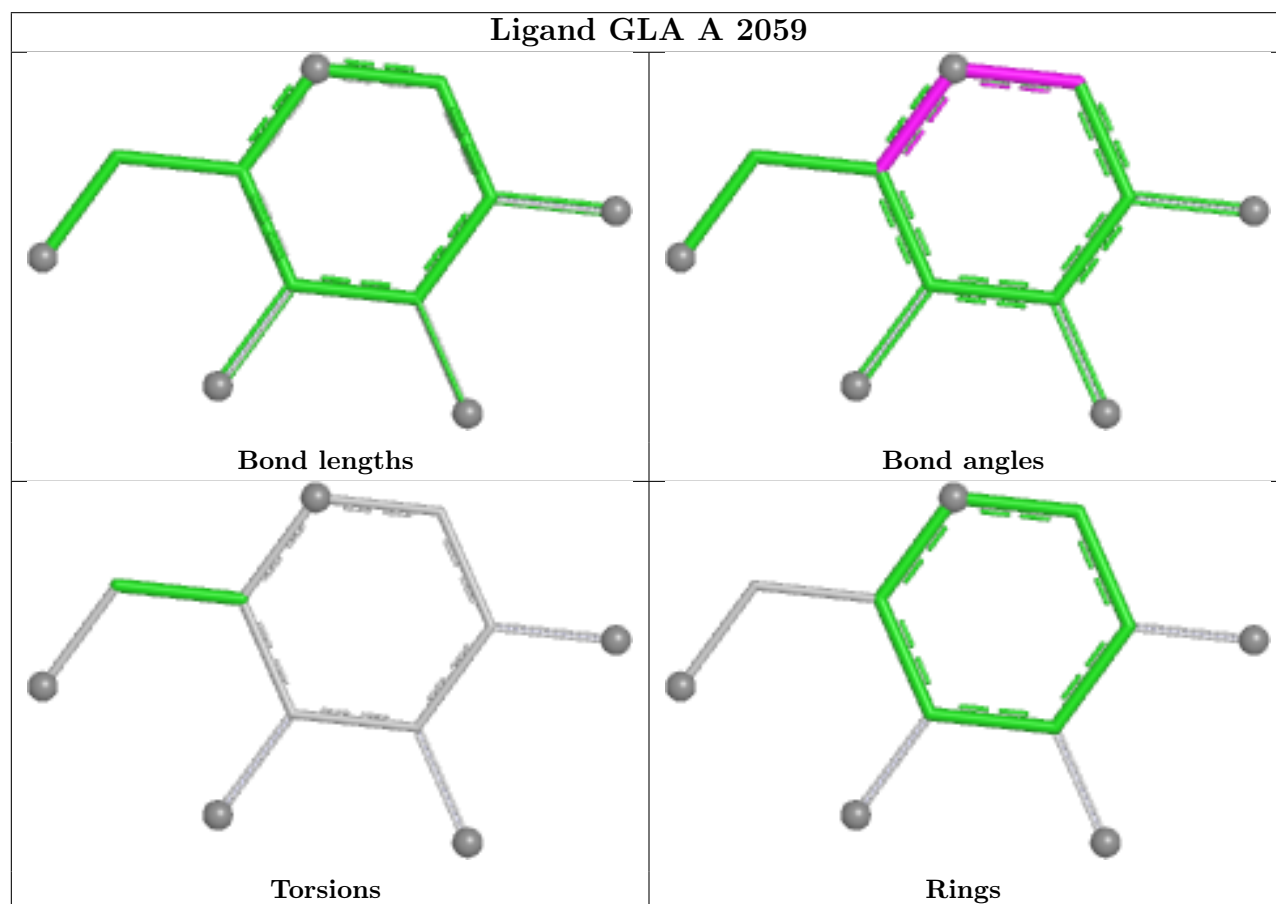
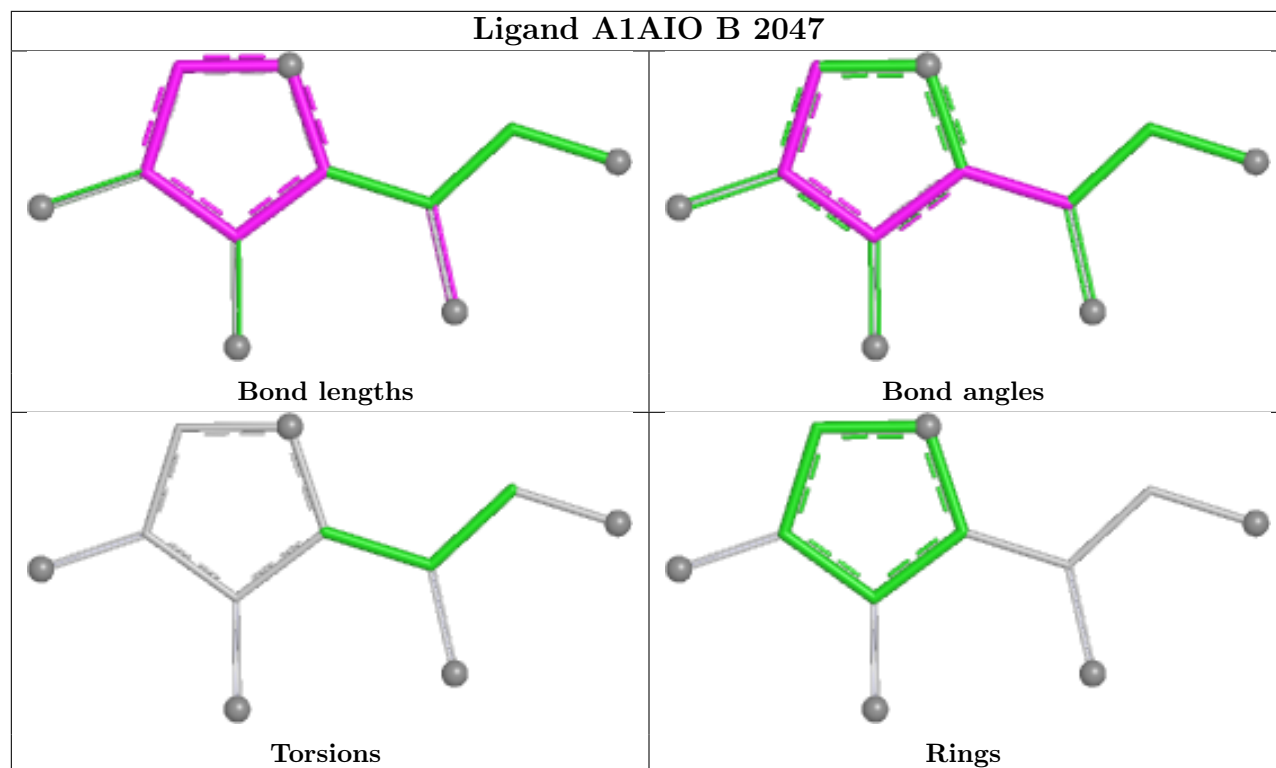


Ligand A1AIO B 2018

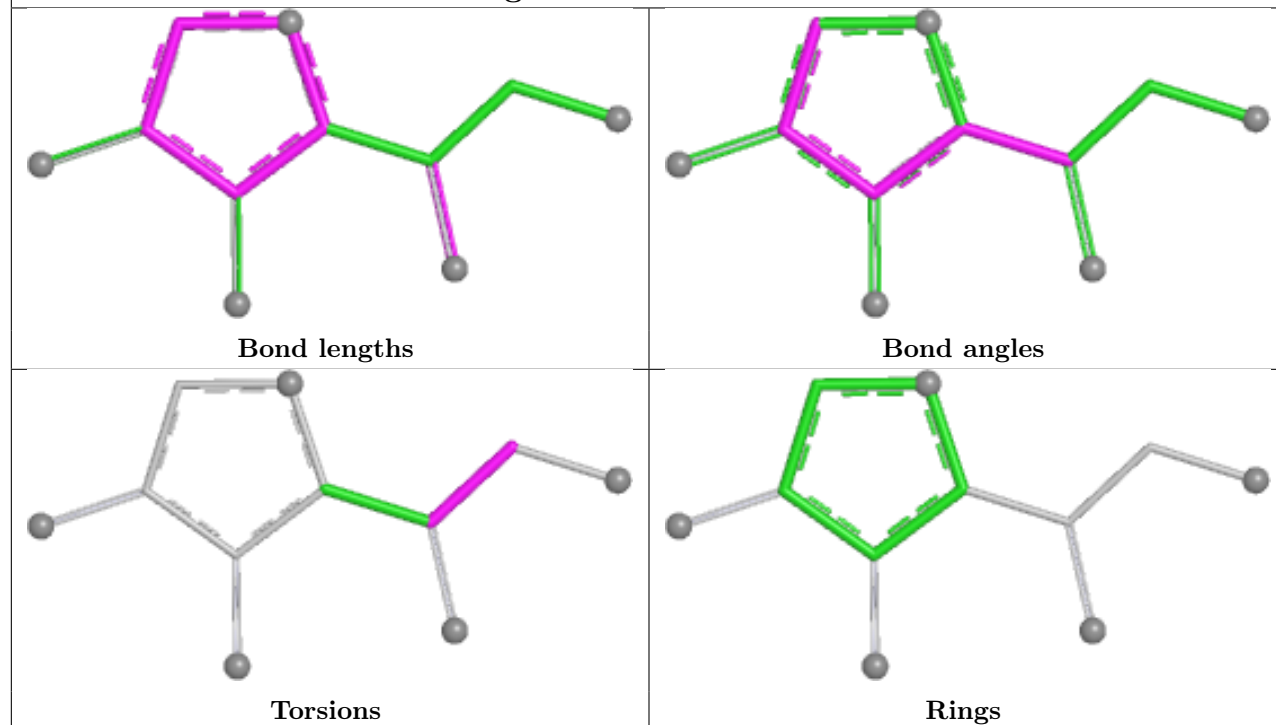


Ligand A1AIO A 2029

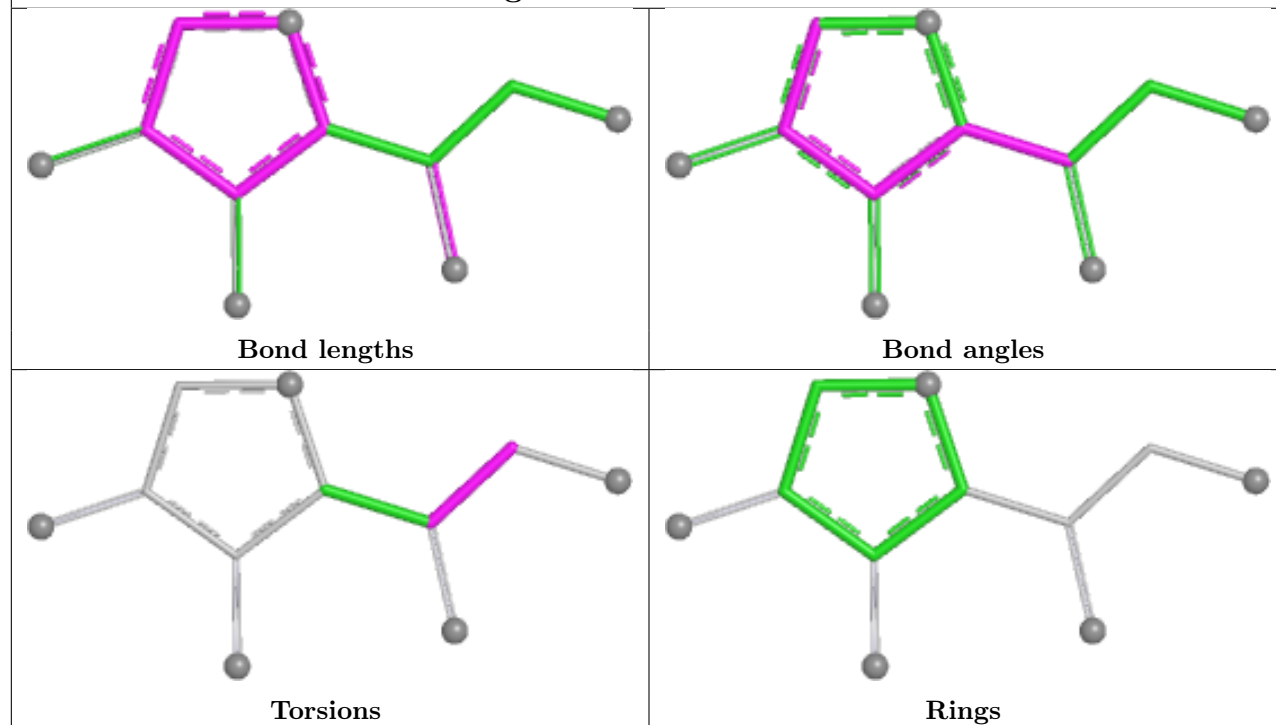




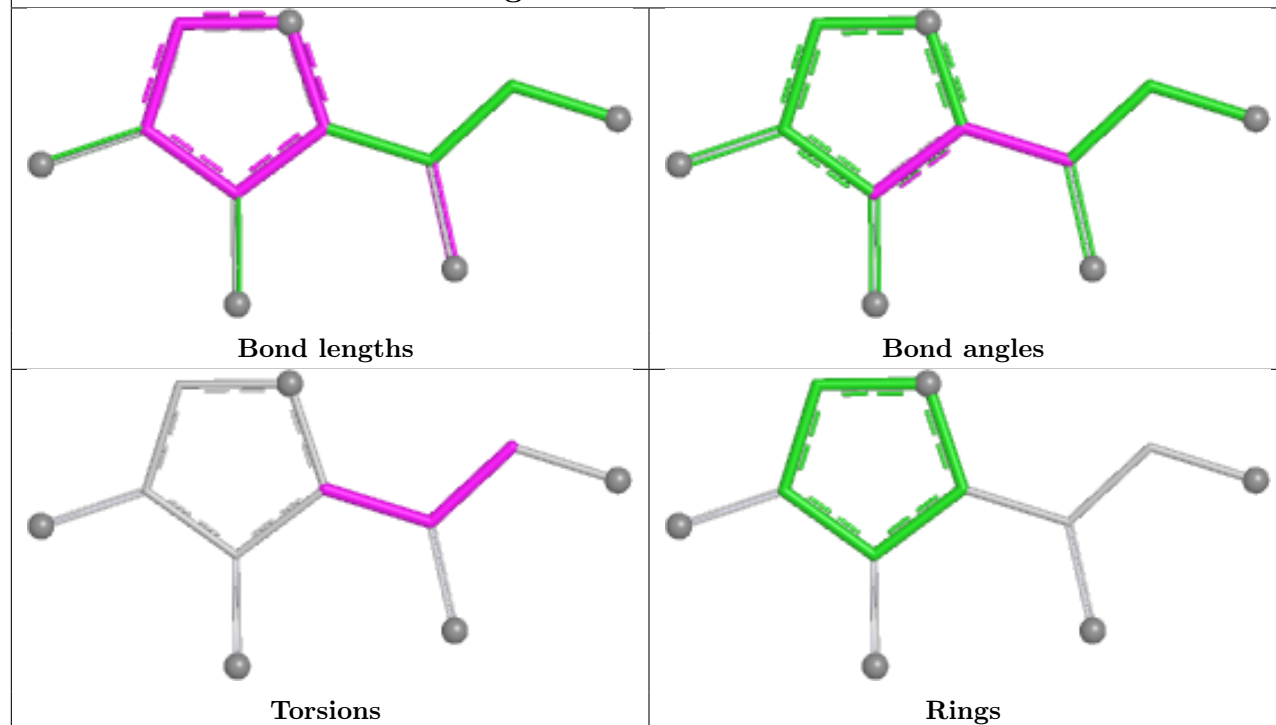
Ligand A1AIO B 2034



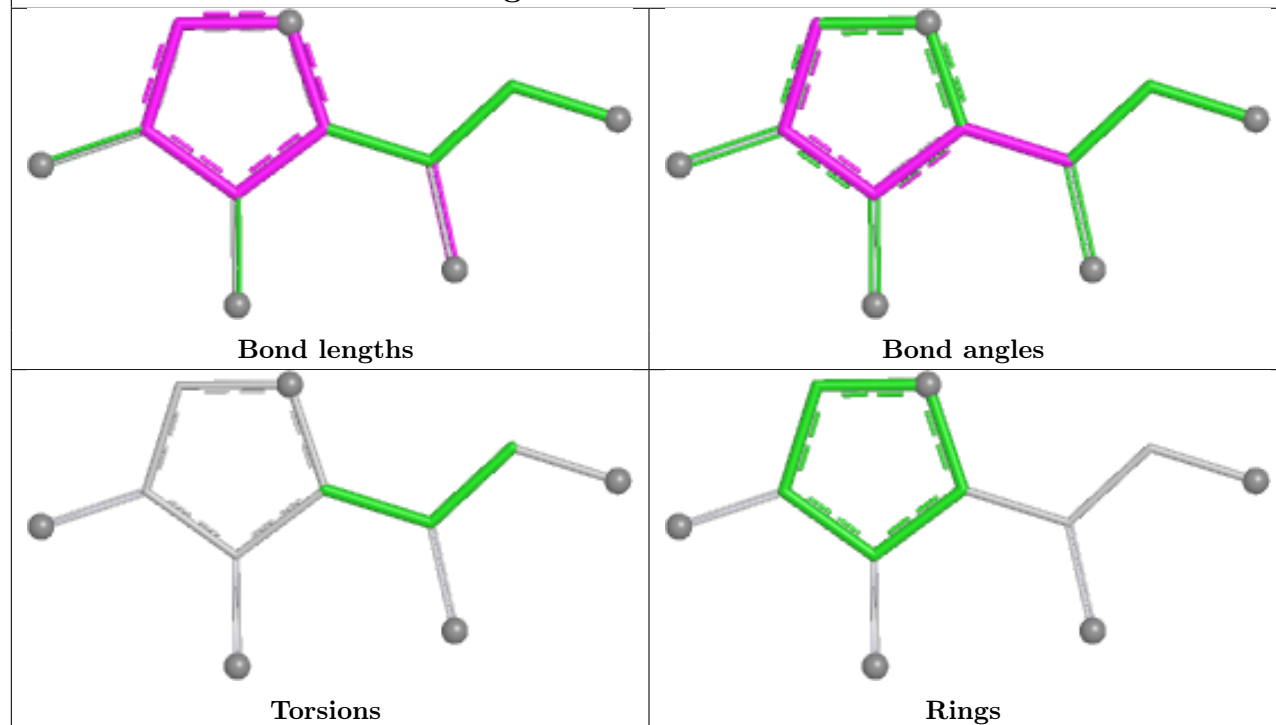
Ligand A1AIO B 2001



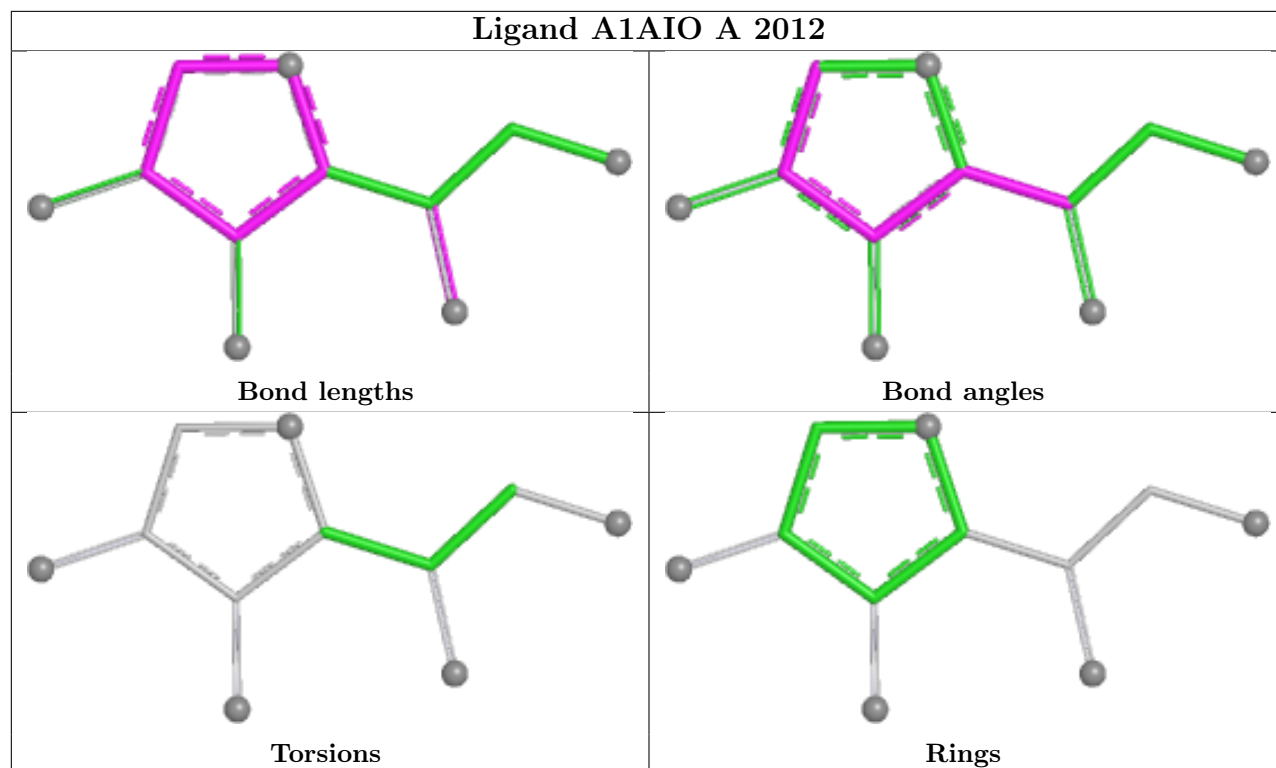
Ligand A1AIO B 2003



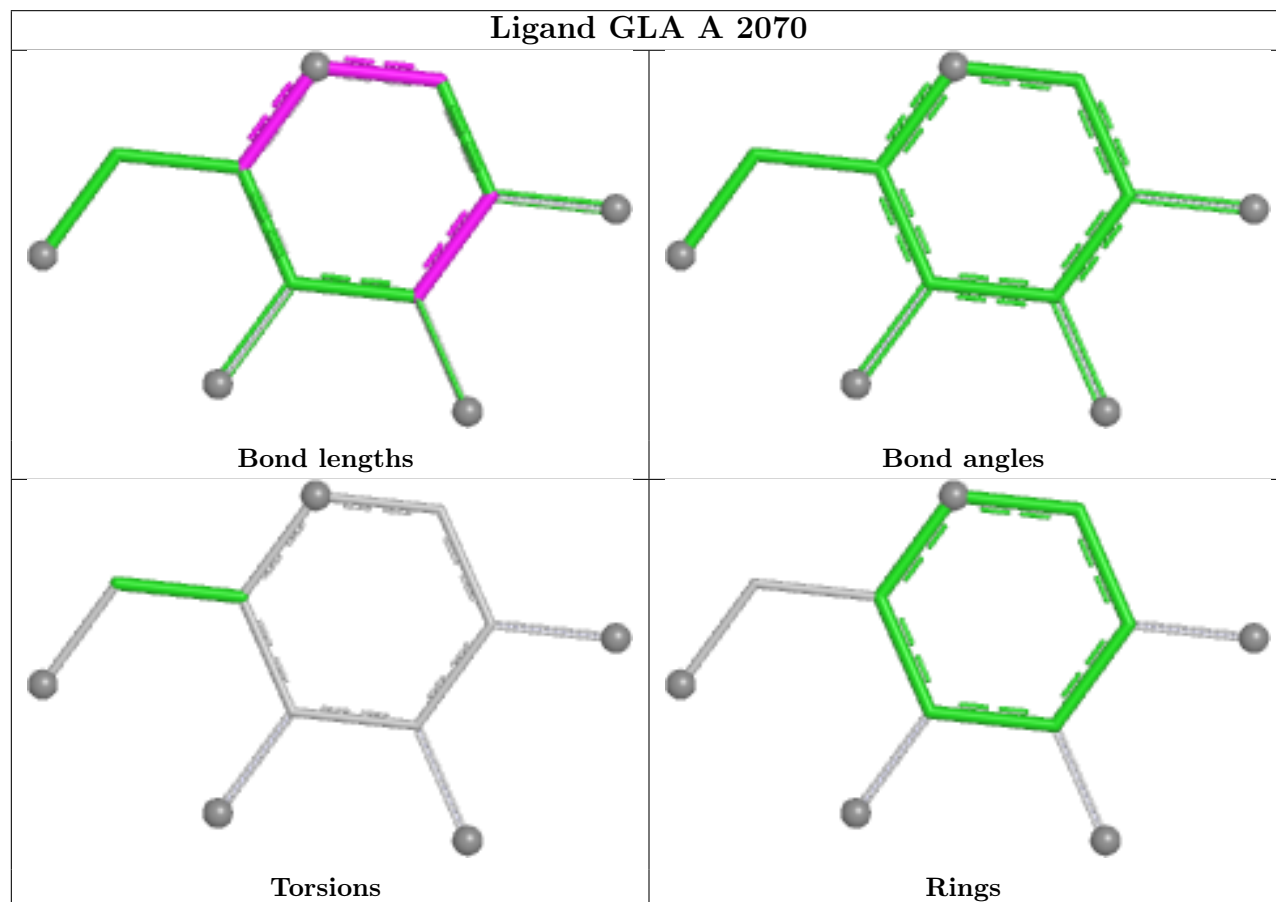
Ligand A1AIO A 2025



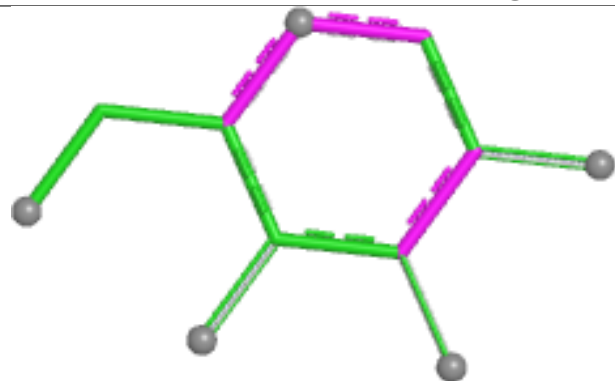
Ligand A1AIO A 2012



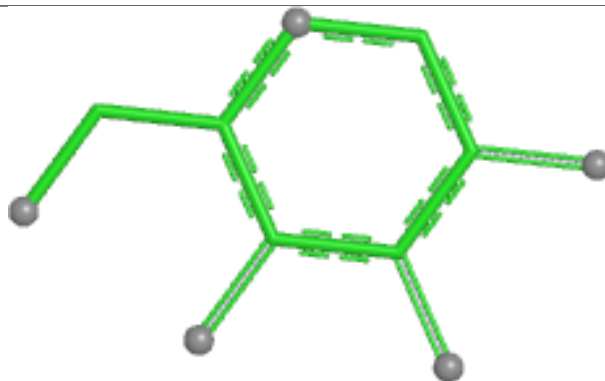
Ligand GLA A 2070



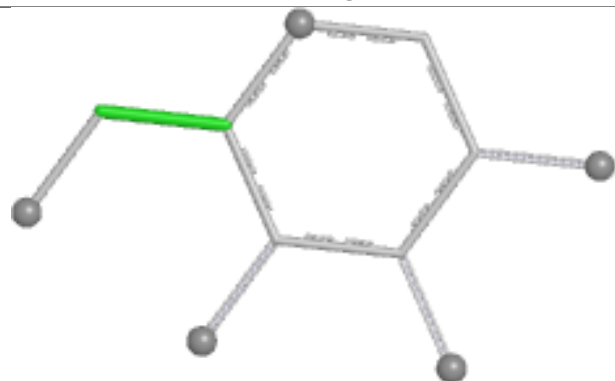
Ligand GLA B 2070



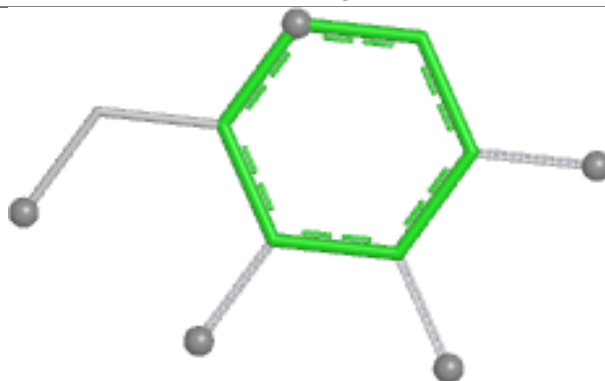
Bond lengths



Bond angles

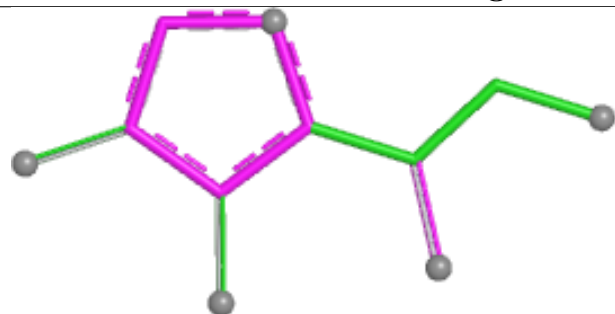


Torsions

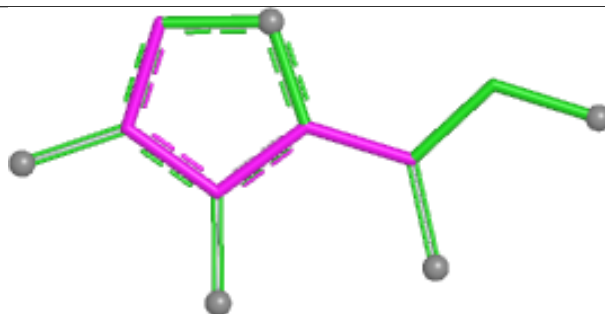


Rings

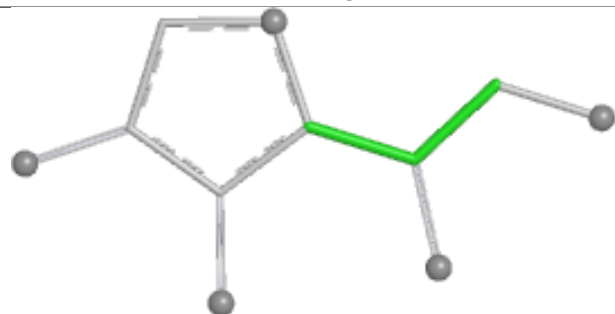
Ligand A1AIO A 2028



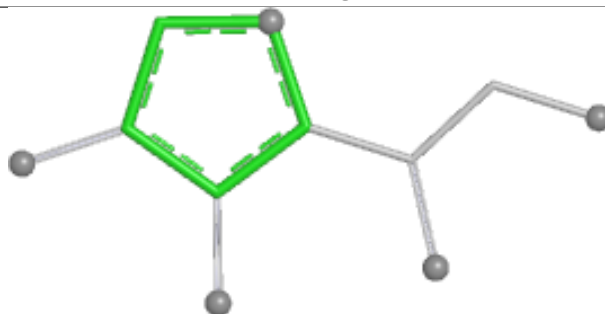
Bond lengths



Bond angles

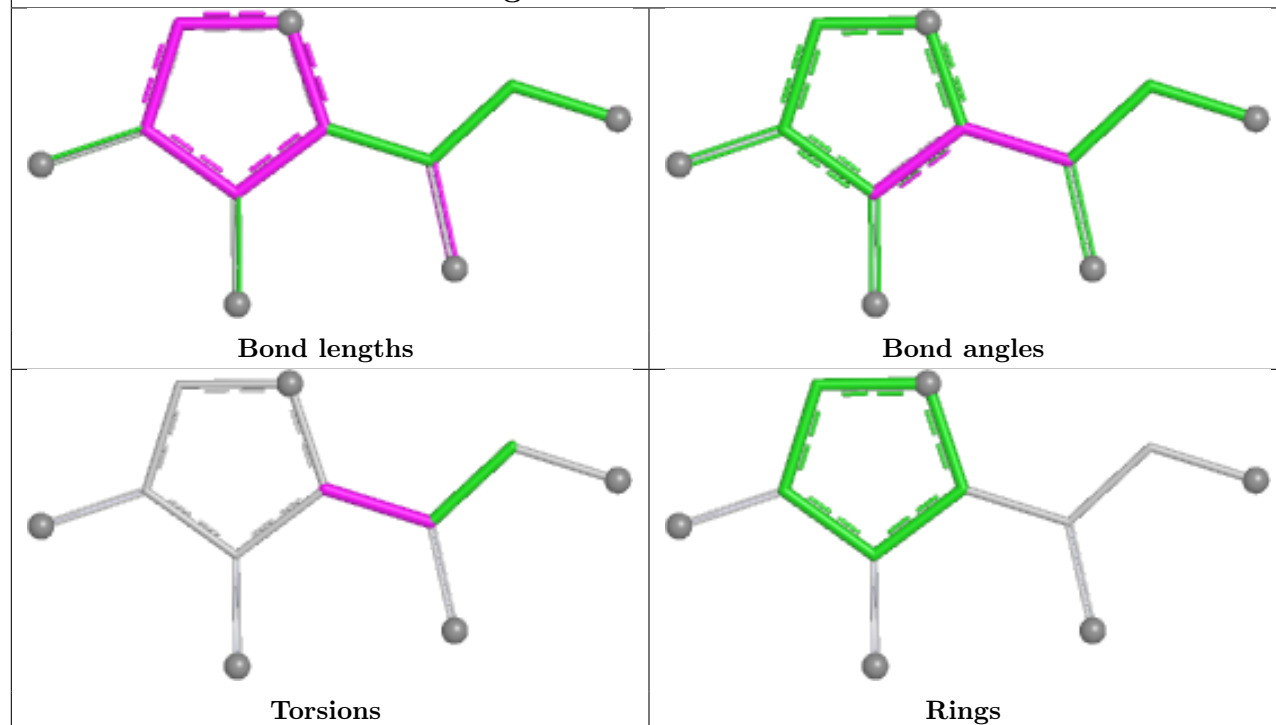


Torsions

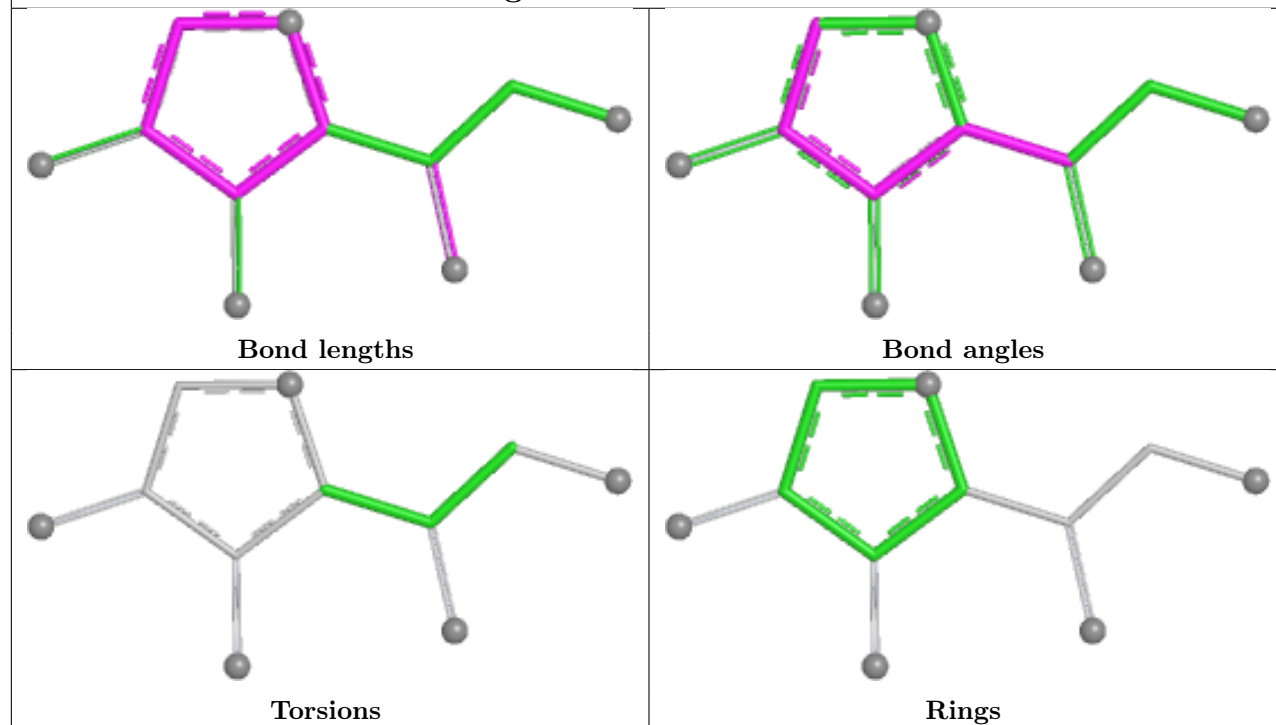


Rings

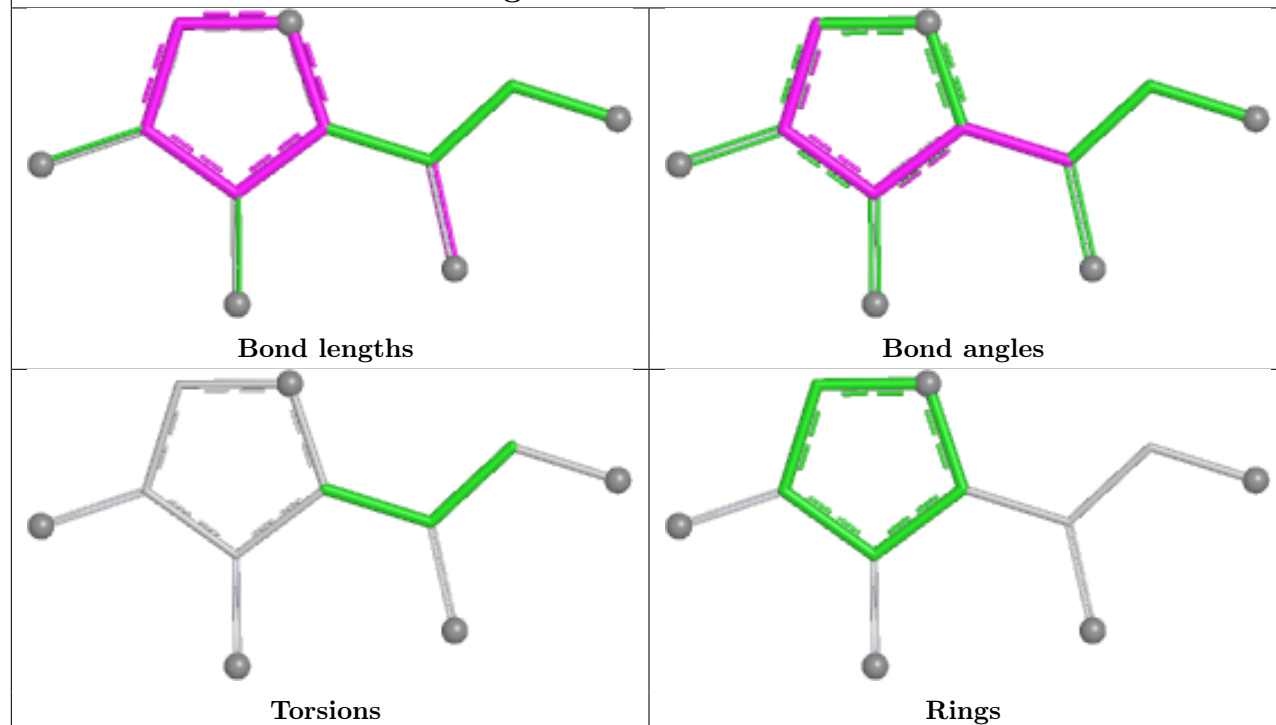
Ligand A1AIO A 2033



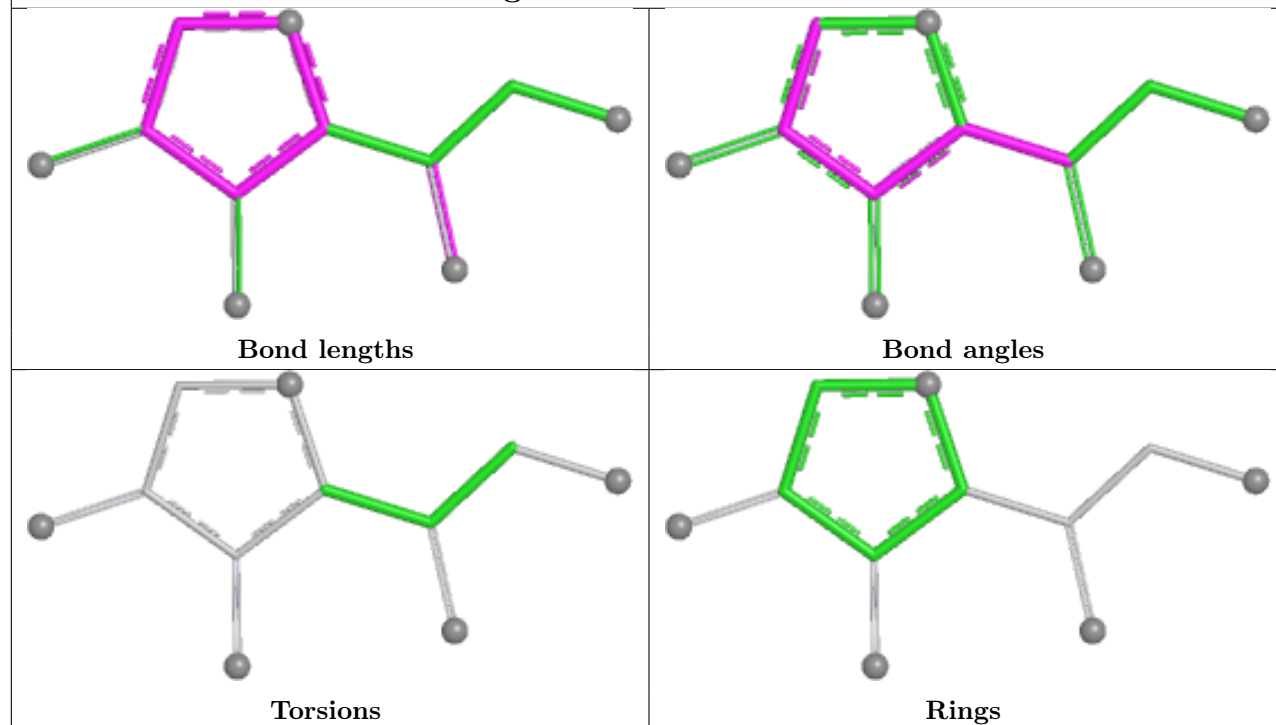
Ligand A1AIO B 2017



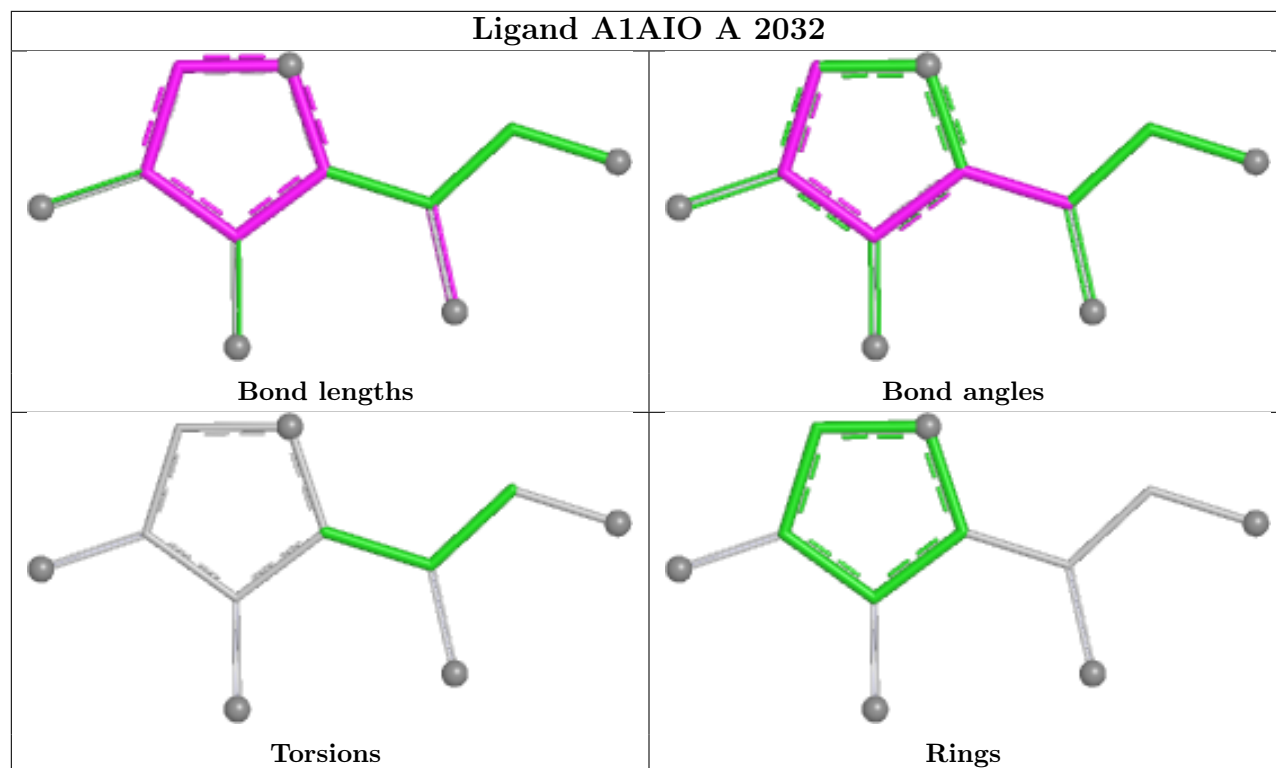
Ligand A1AIO A 2023



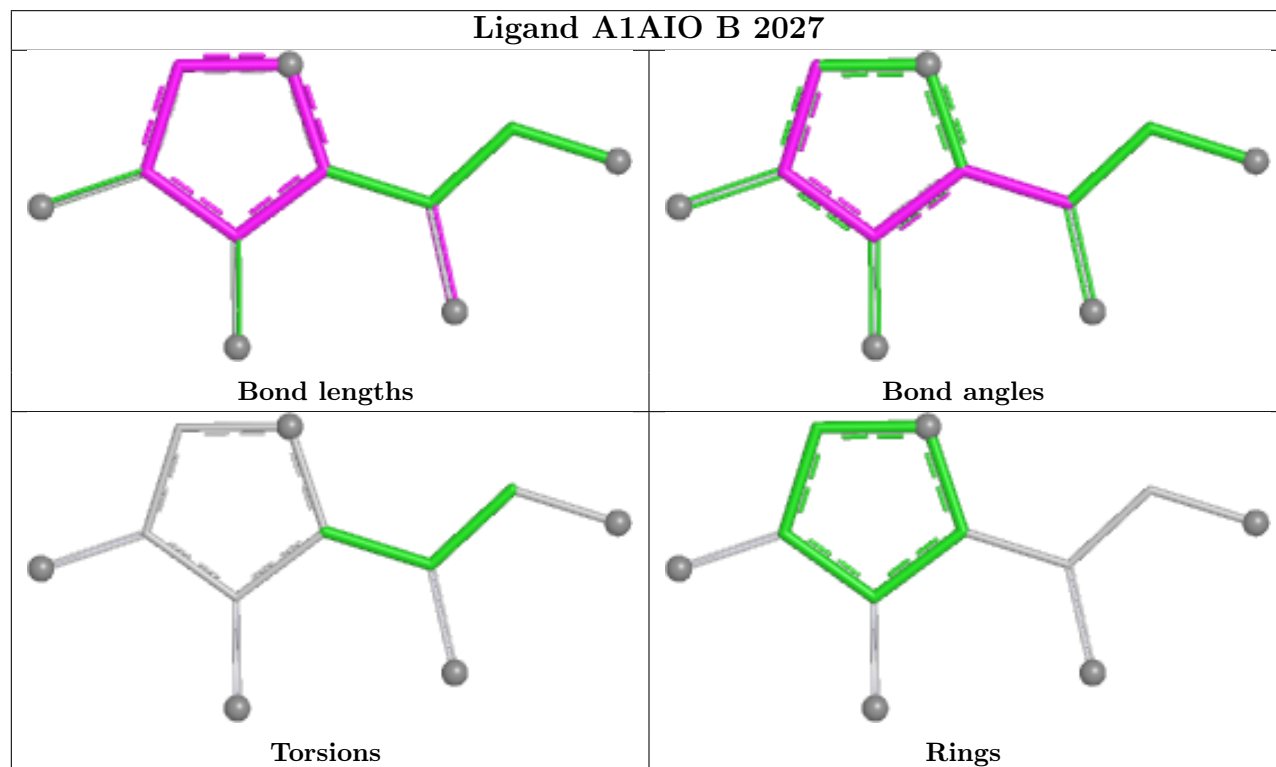
Ligand A1AIO A 2050

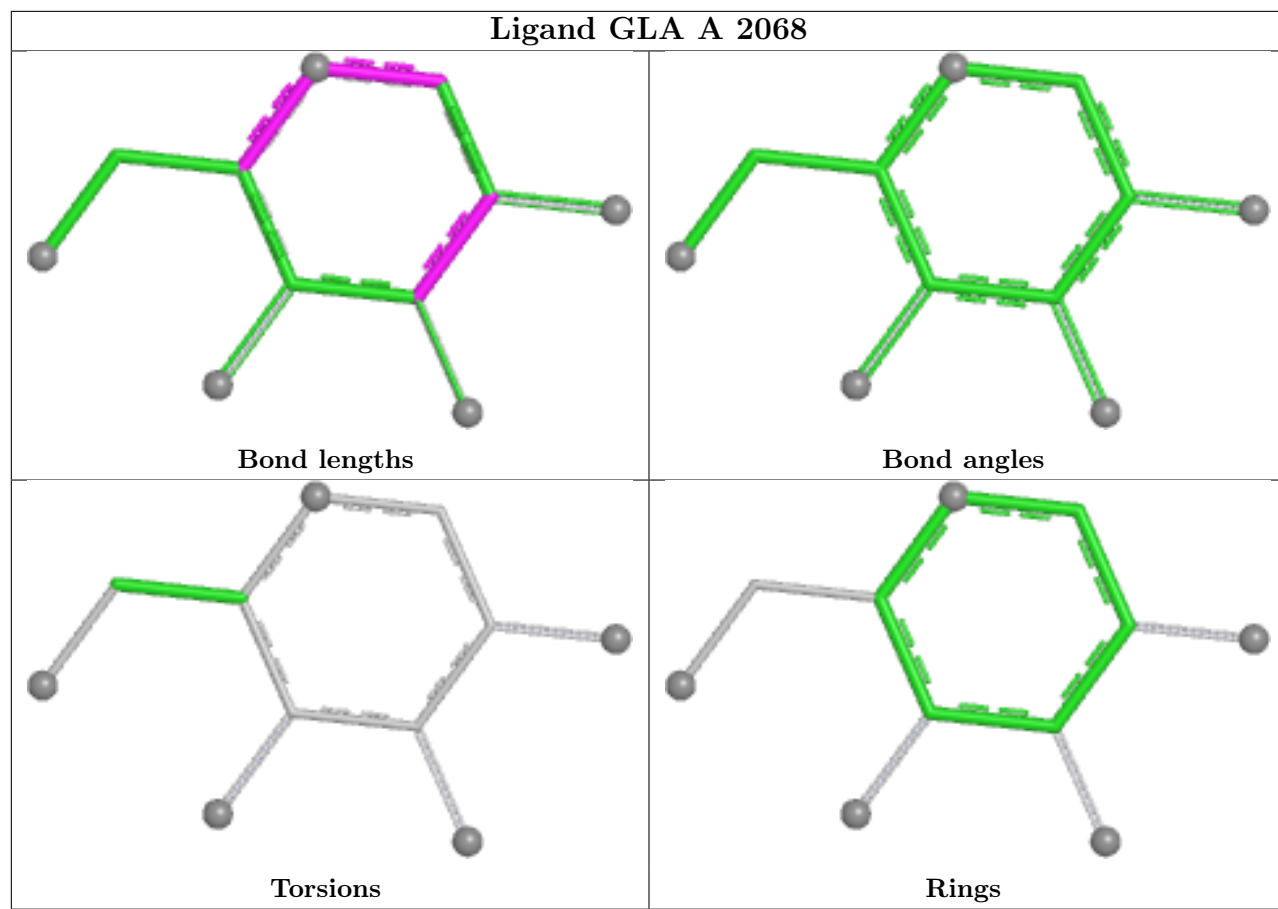


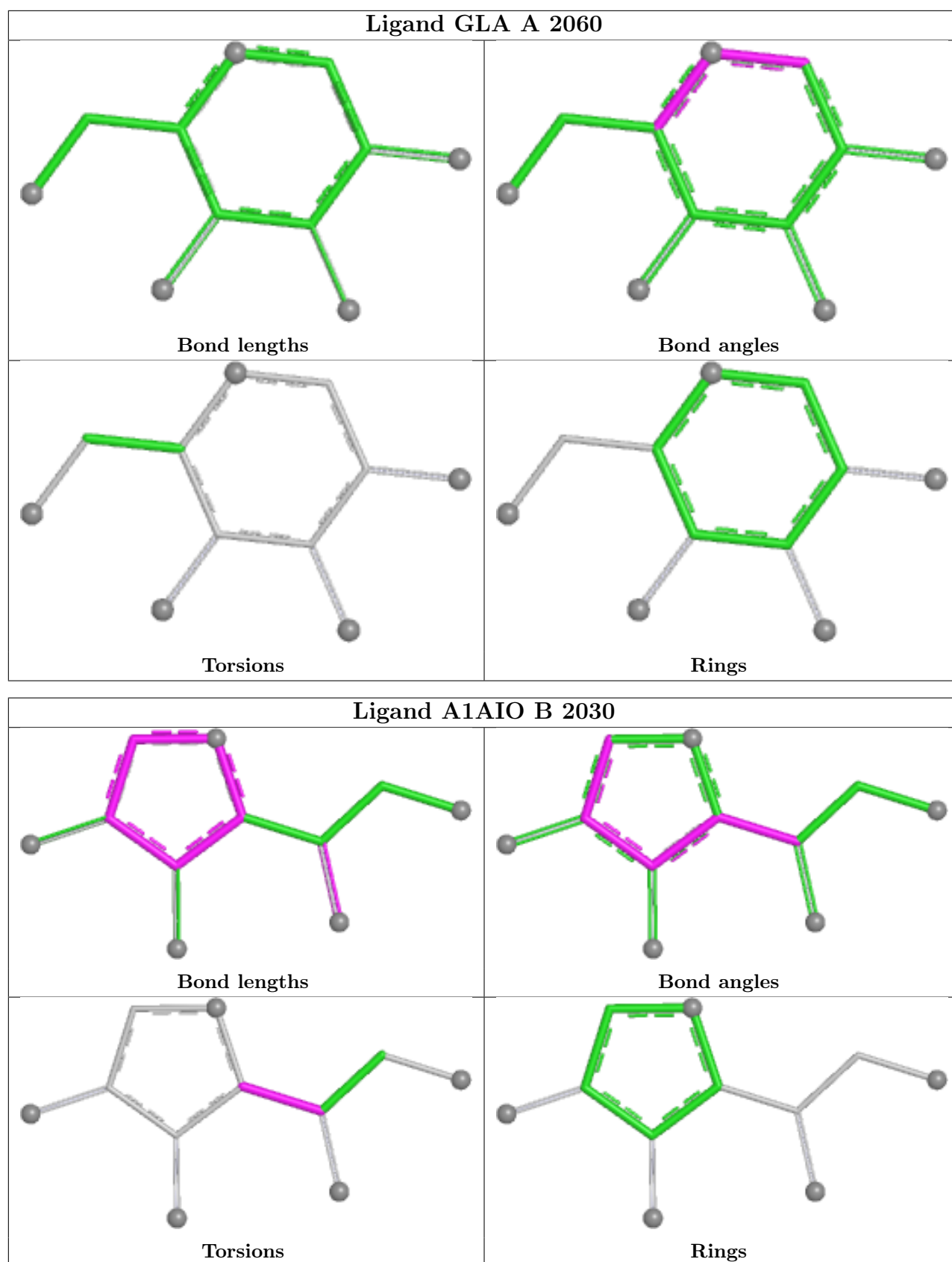
Ligand A1AIO A 2032



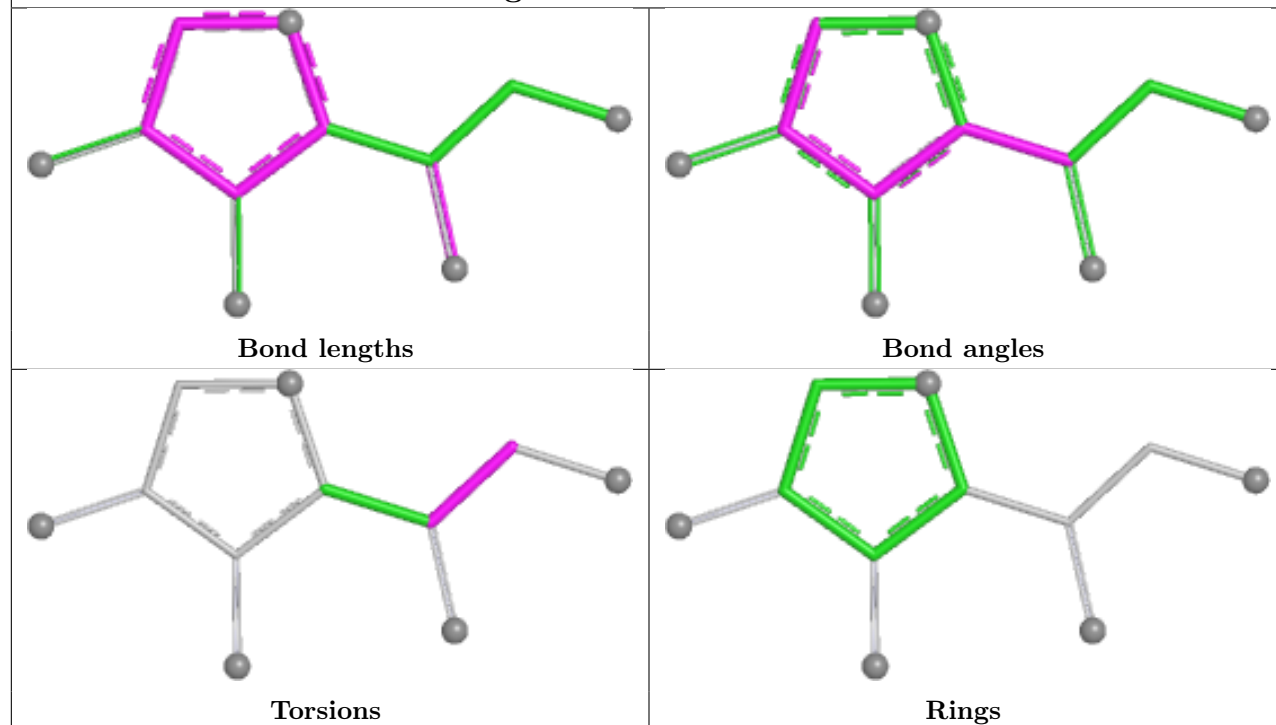
Ligand A1AIO B 2027



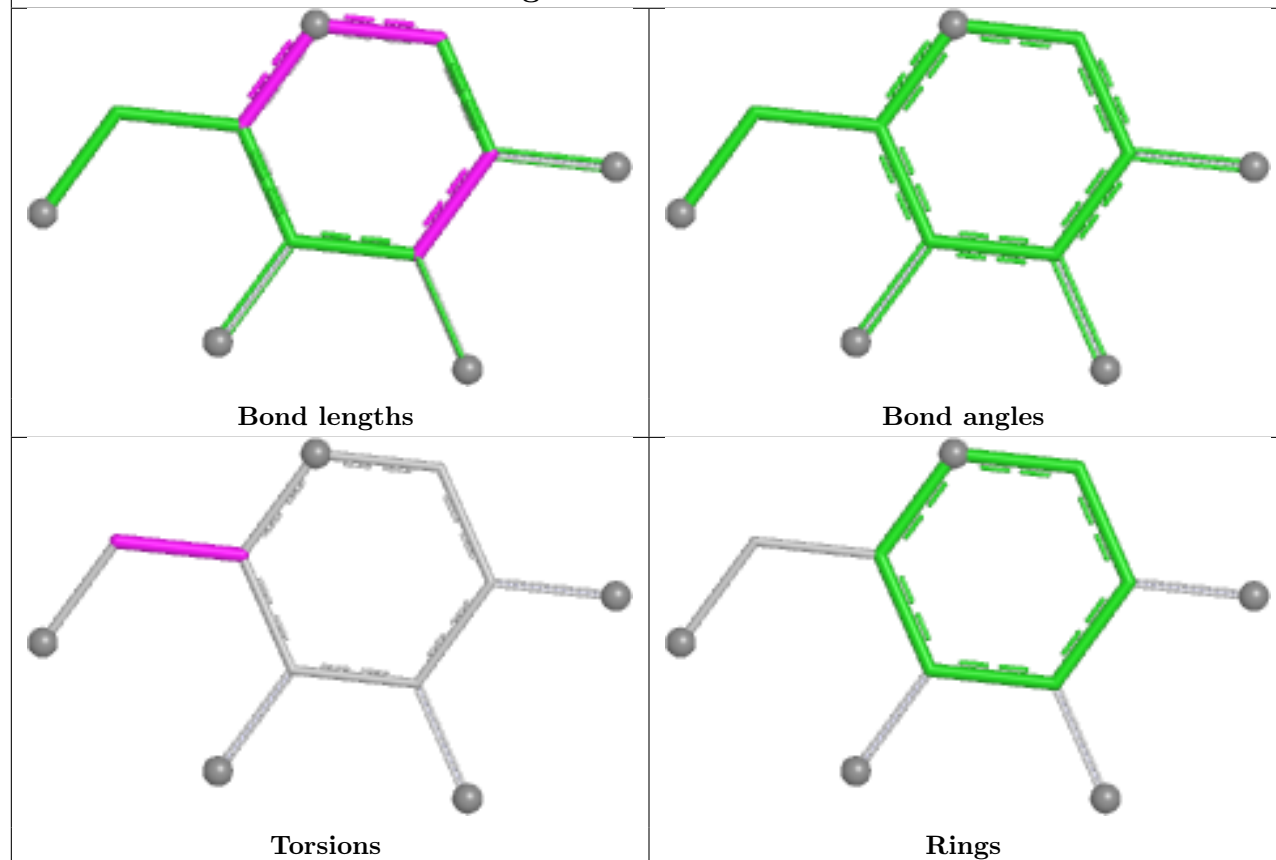




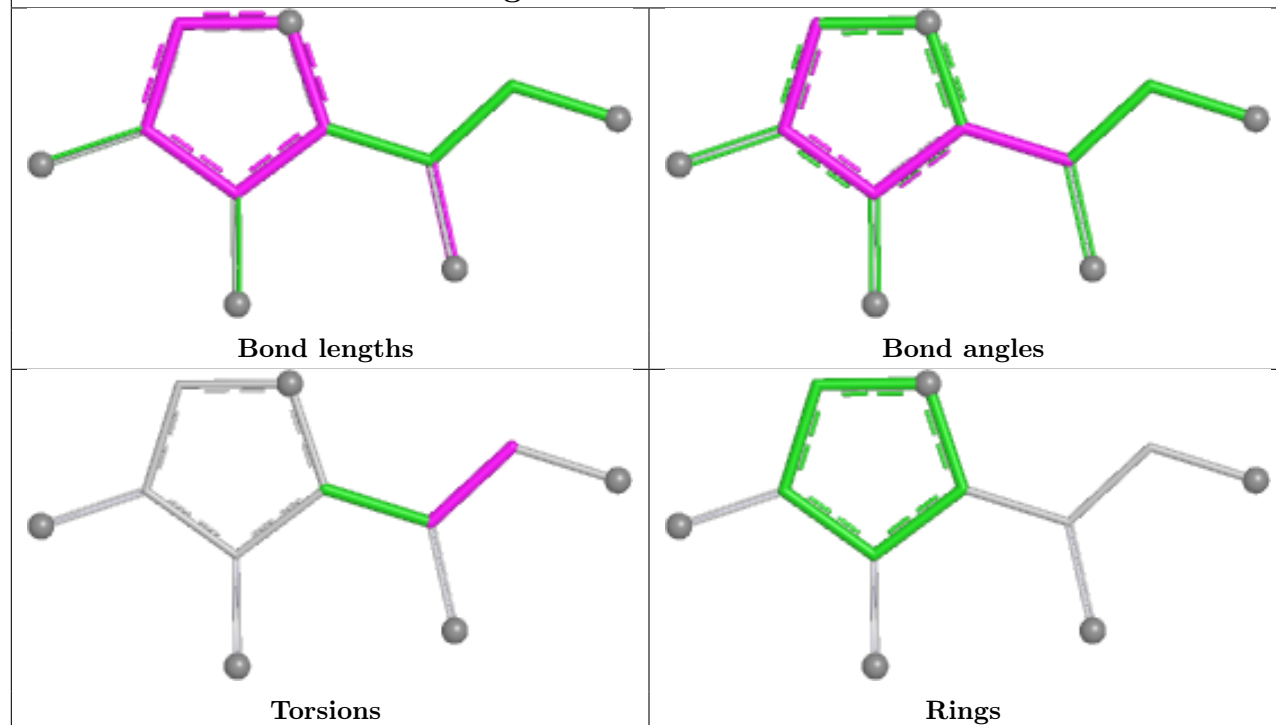
Ligand A1AIO B 2036



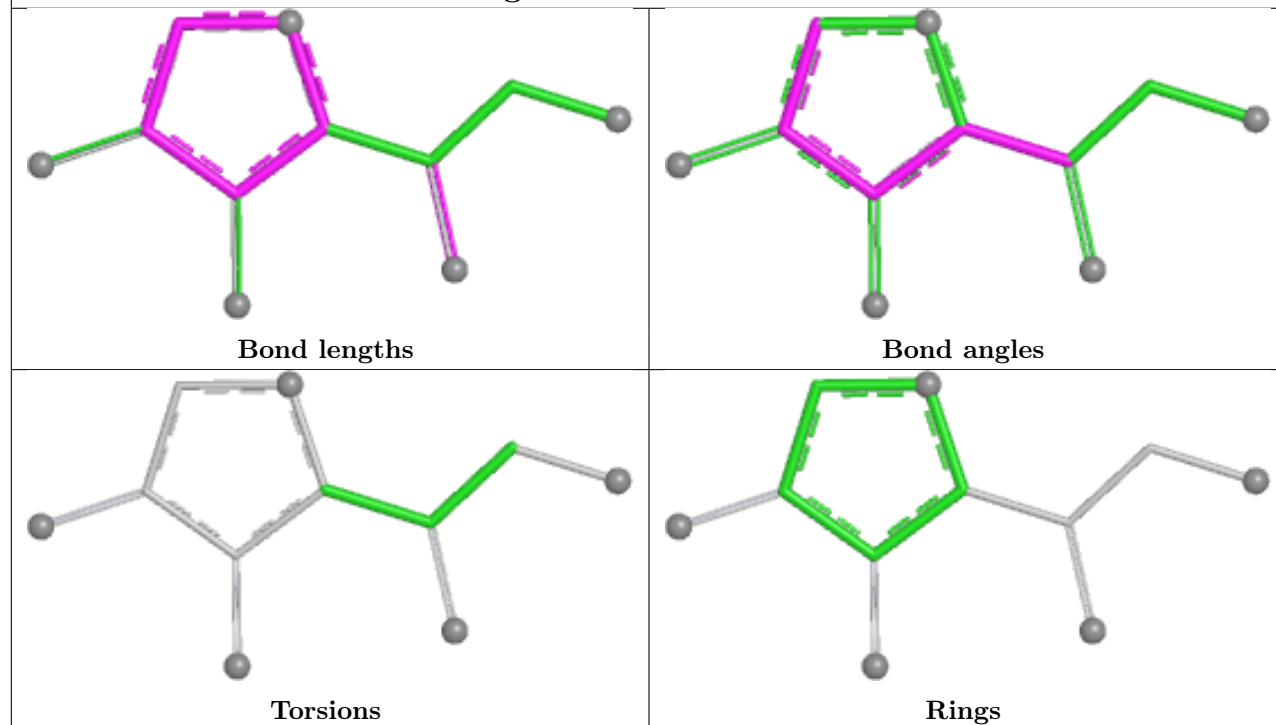
Ligand GLA B 2068



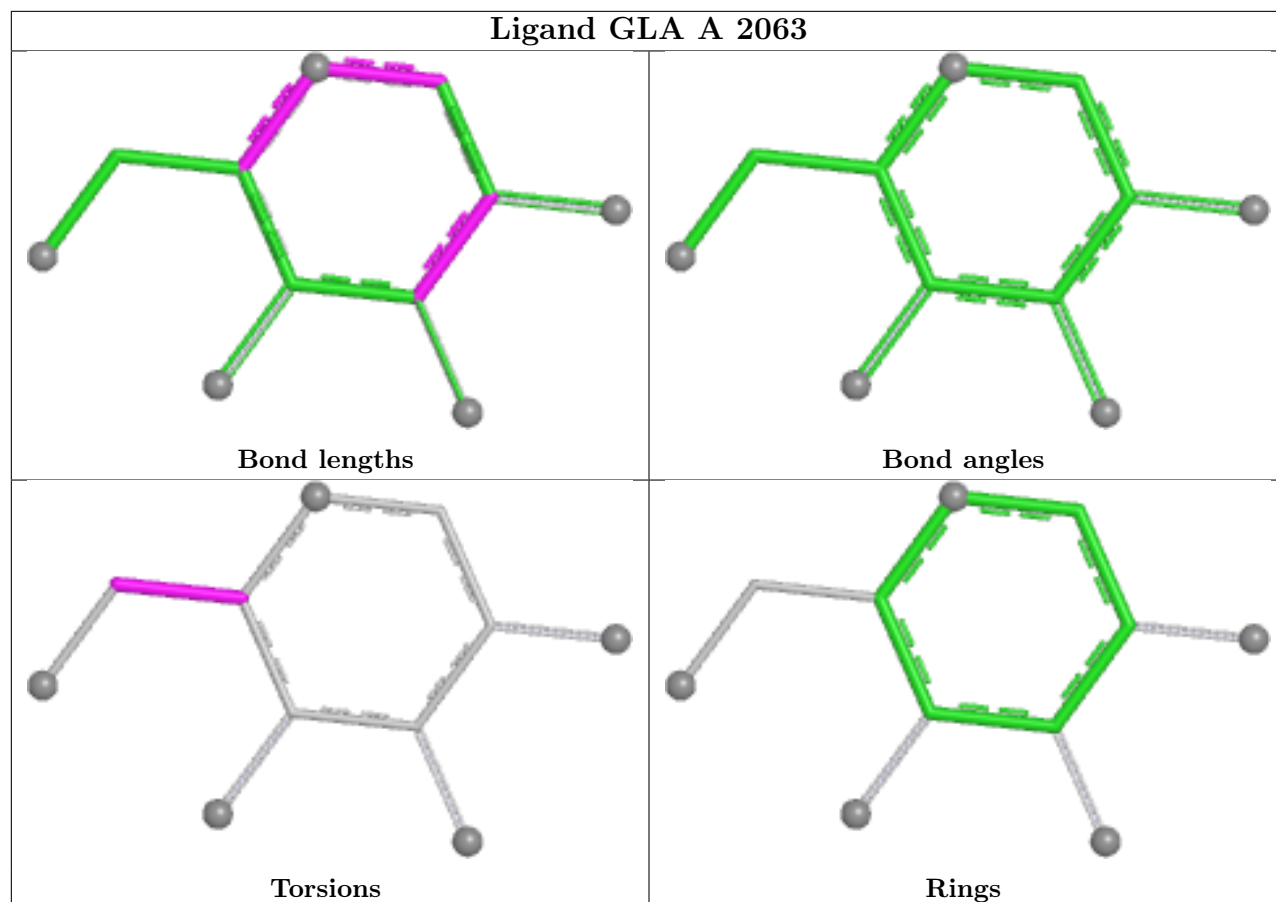
Ligand A1AIO A 2009



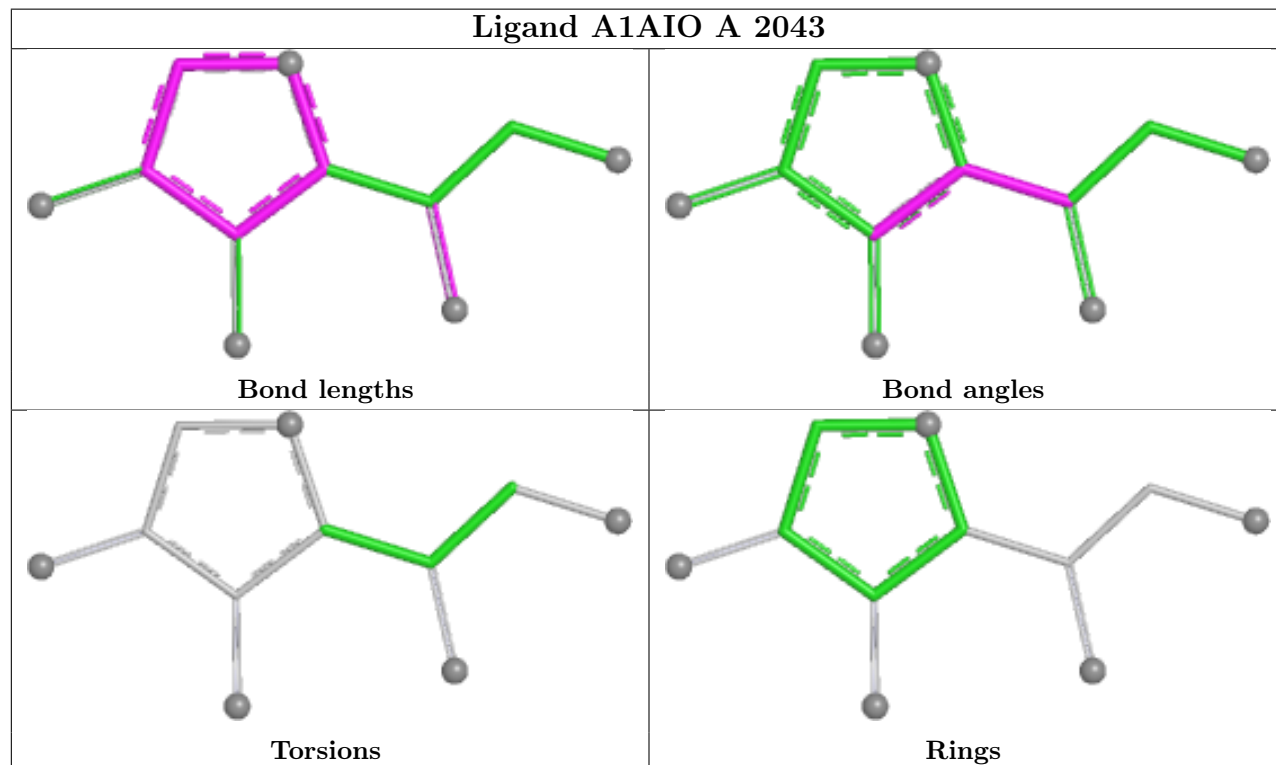
Ligand A1AIO A 2024



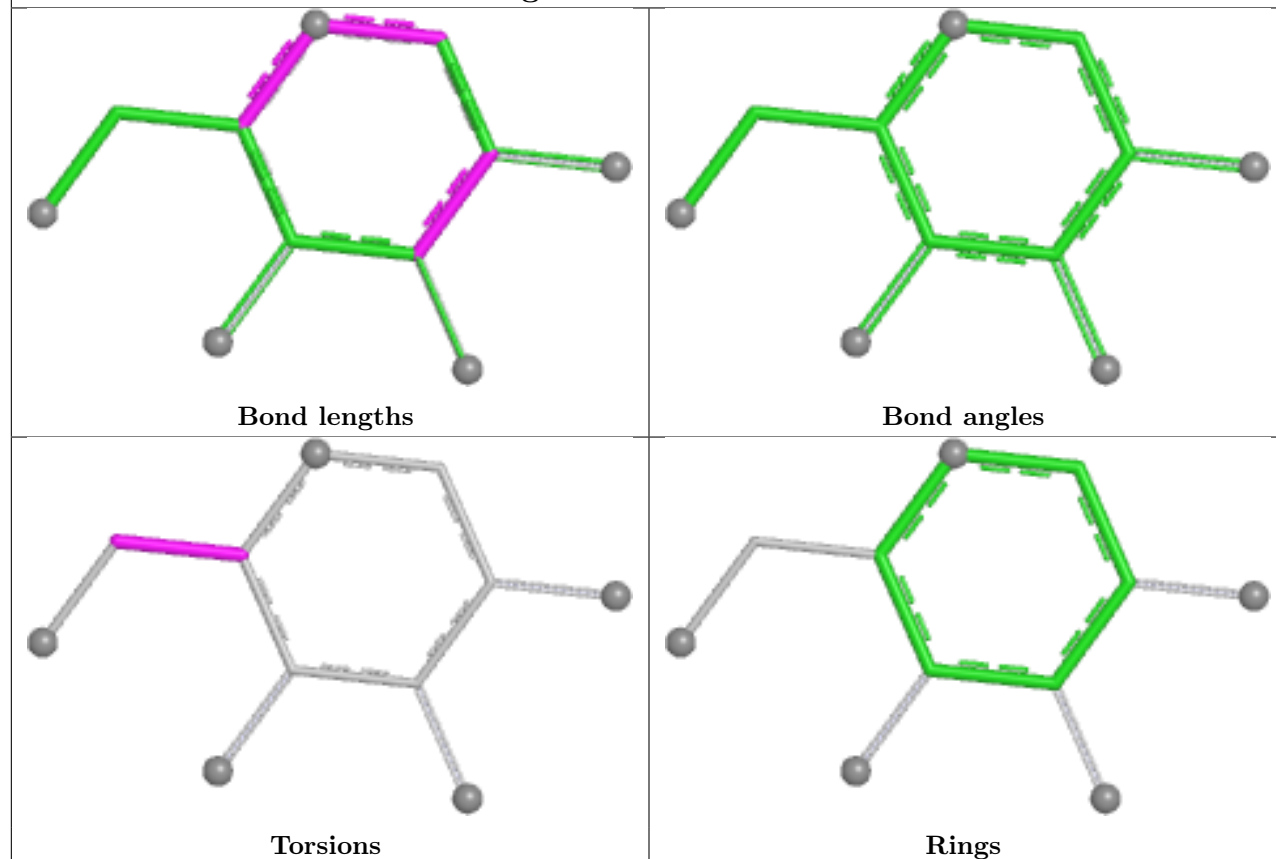
Ligand GLA A 2063



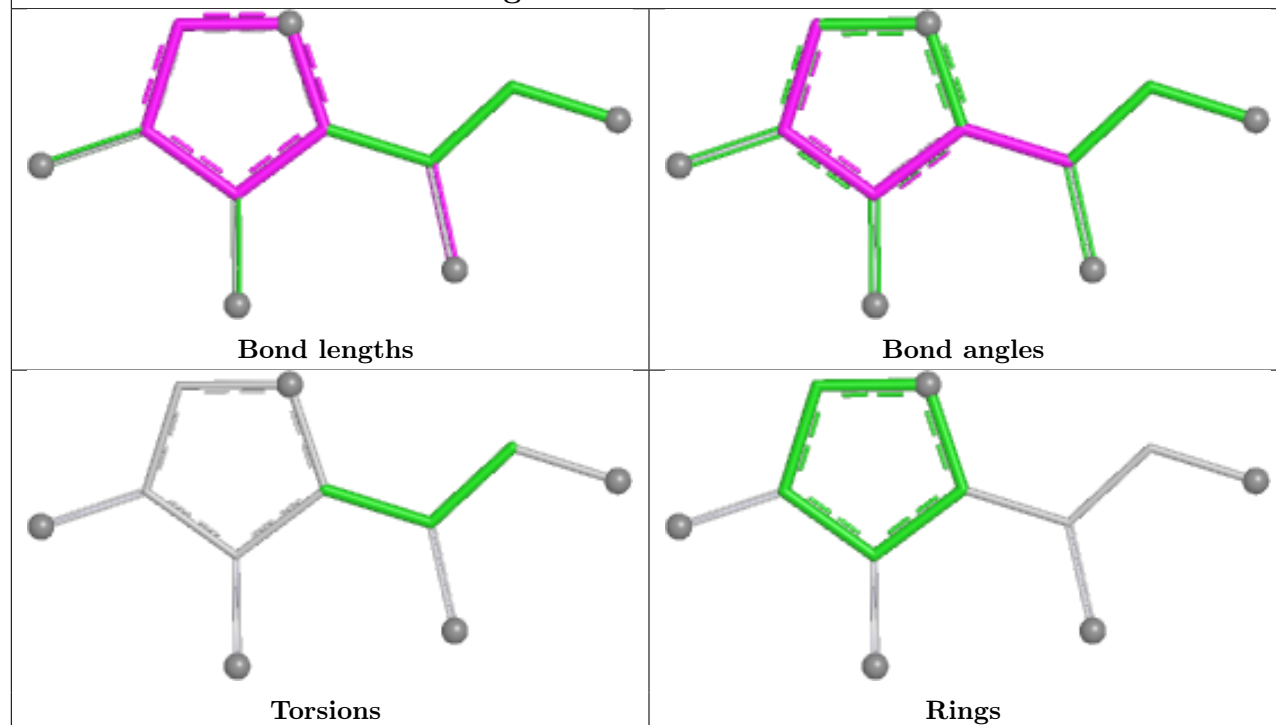
Ligand A1AIO A 2043

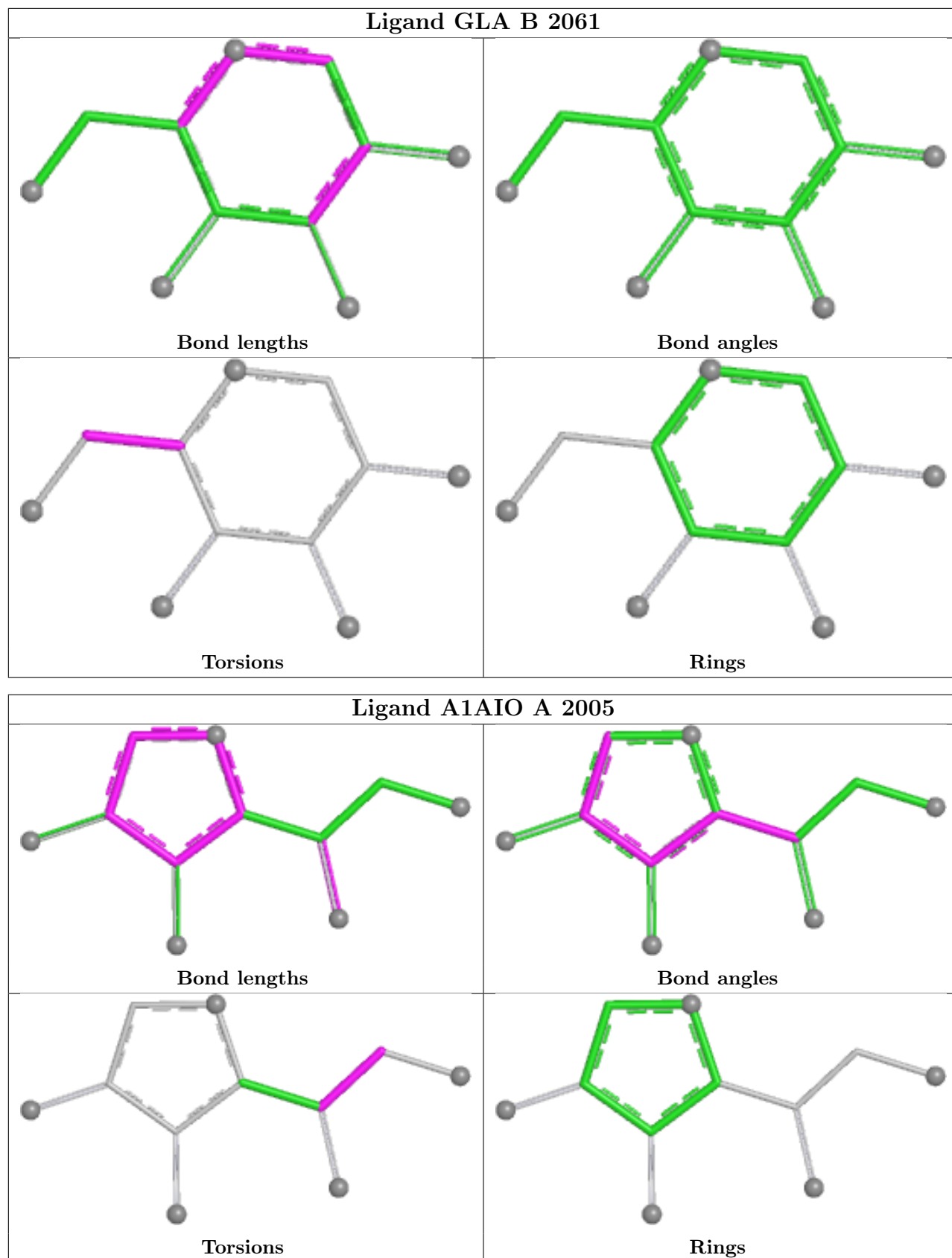


Ligand GLA A 2065

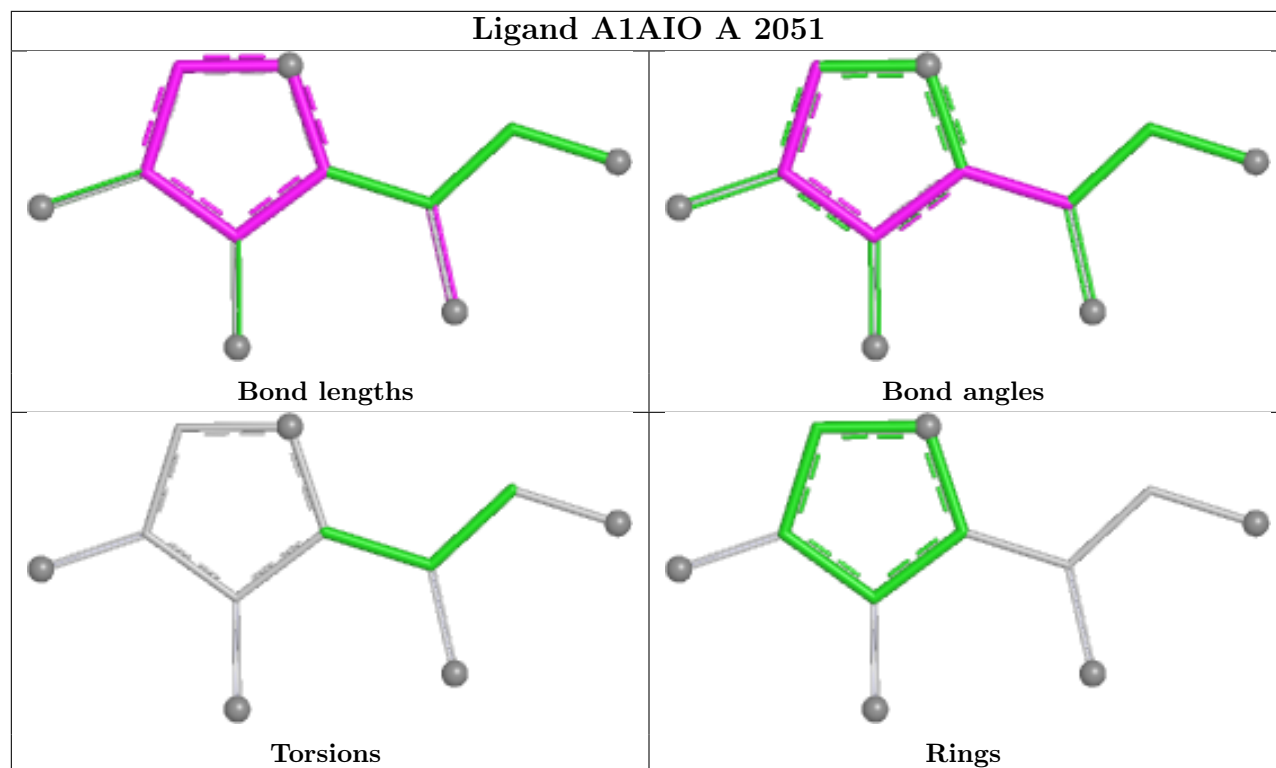


Ligand A1AIO A 2053

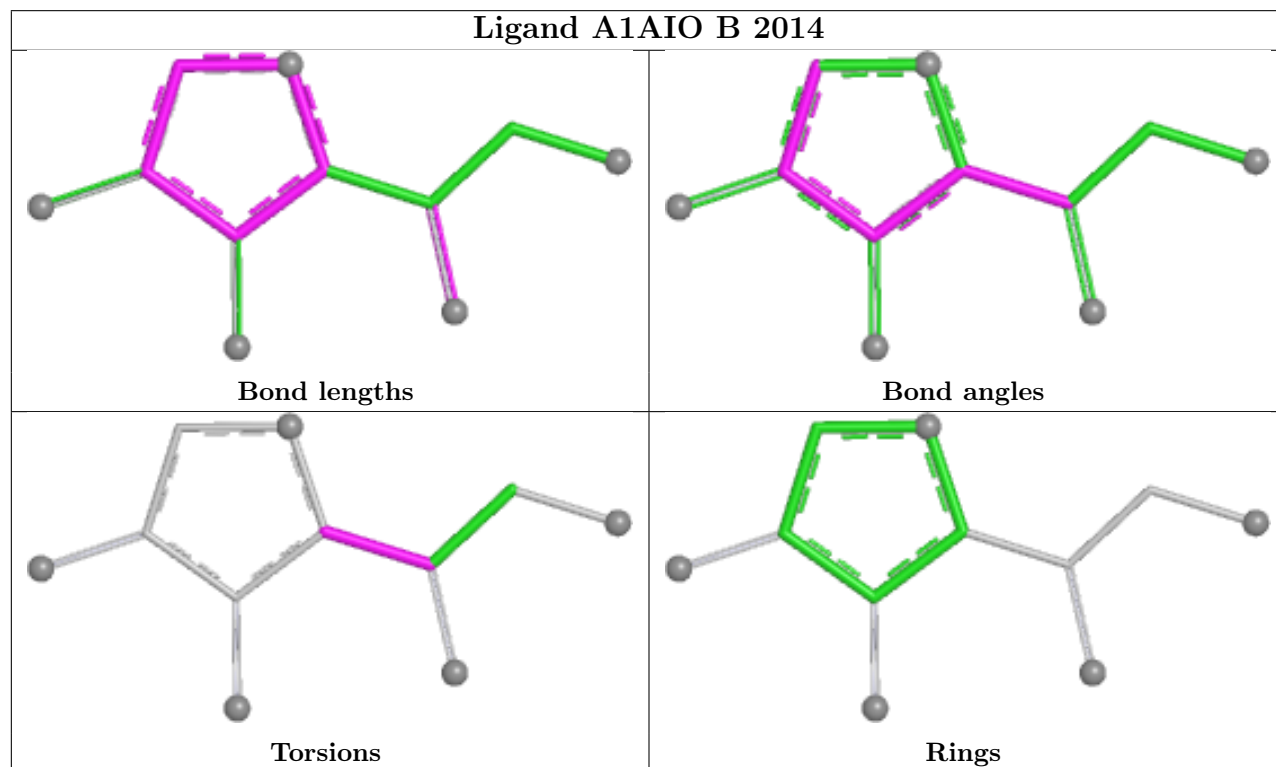




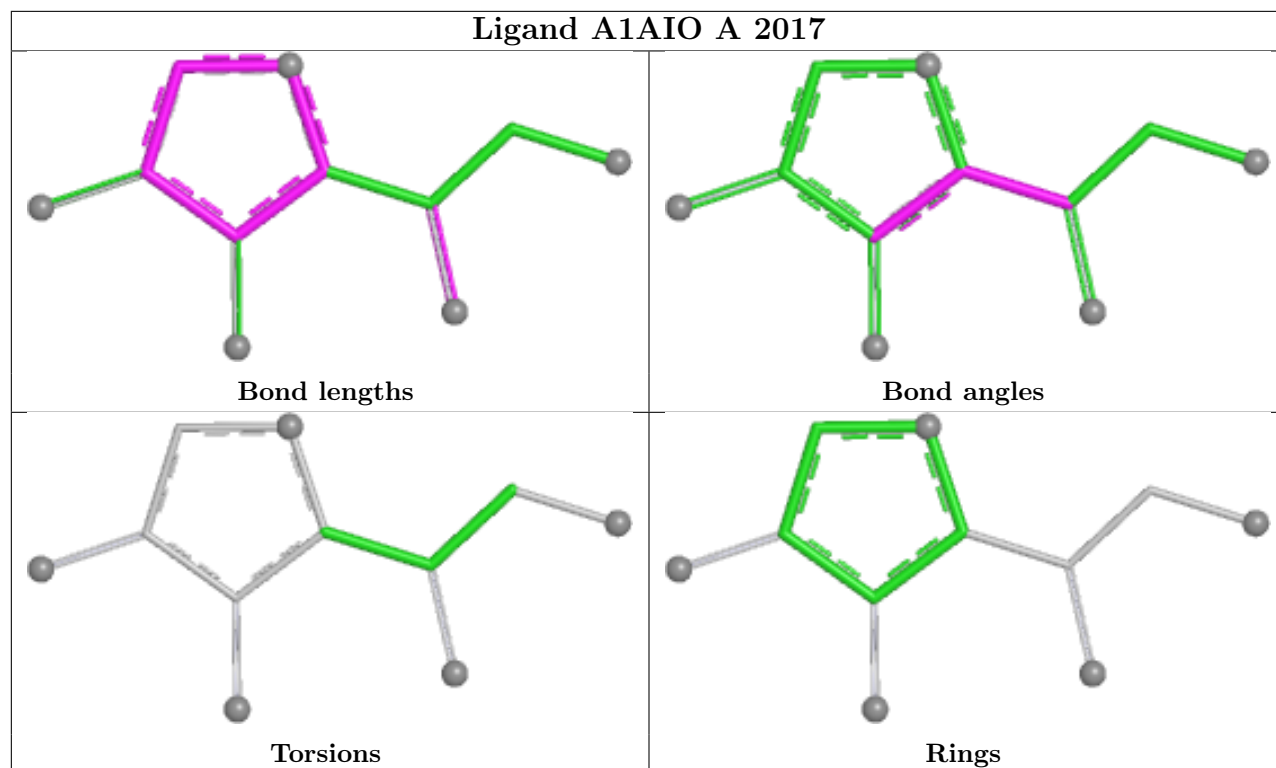
Ligand A1AIO A 2051



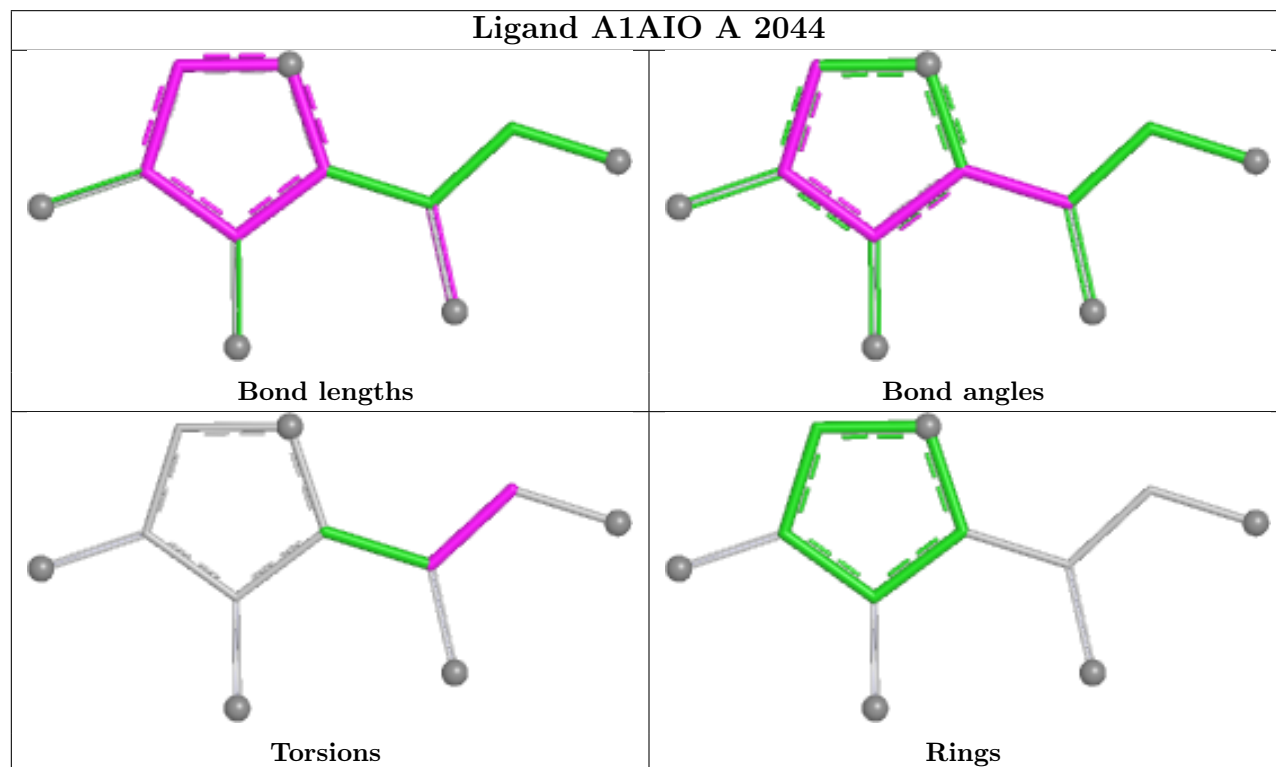
Ligand A1AIO B 2014

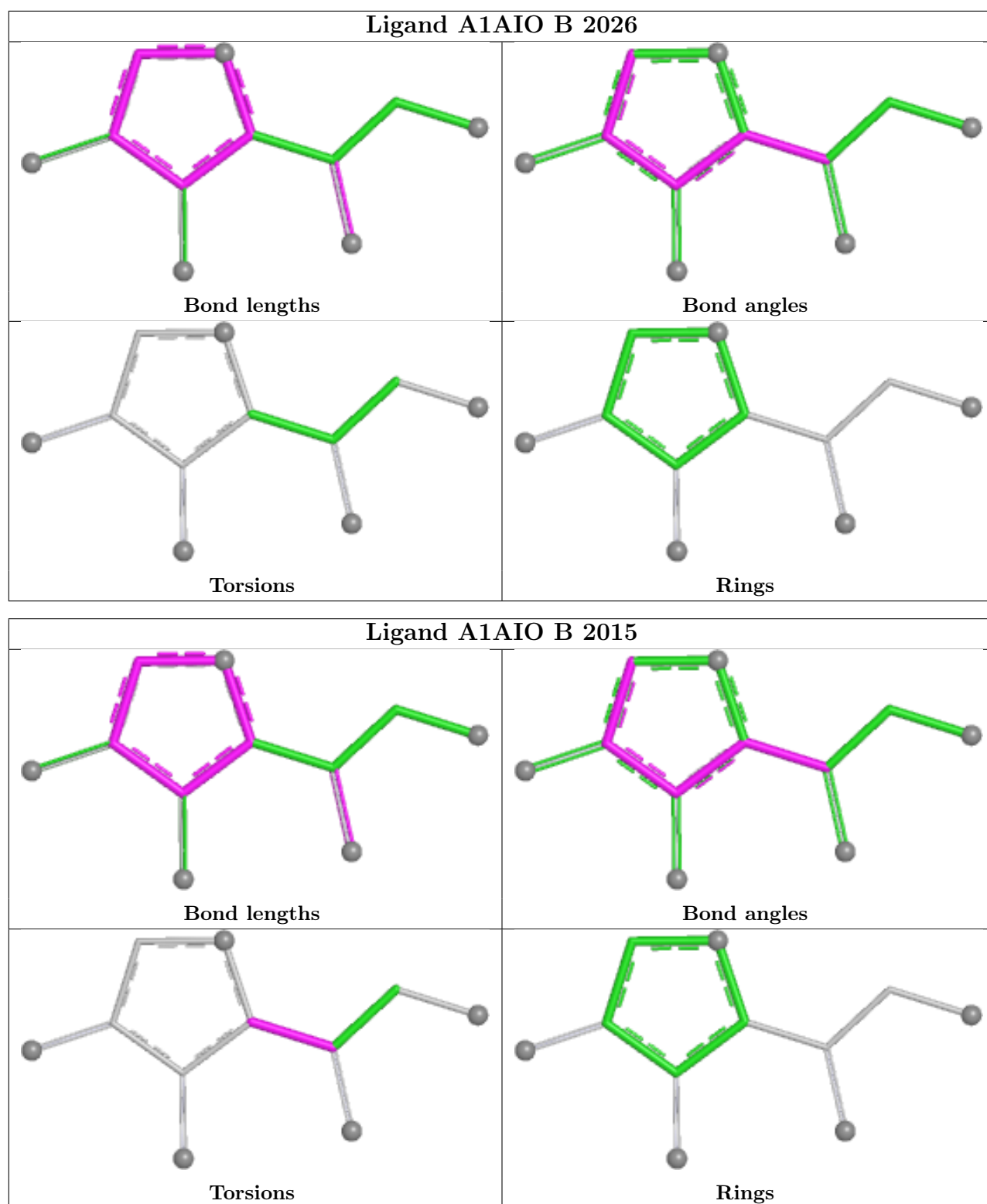


Ligand A1AIO A 2017



Ligand A1AIO A 2044





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

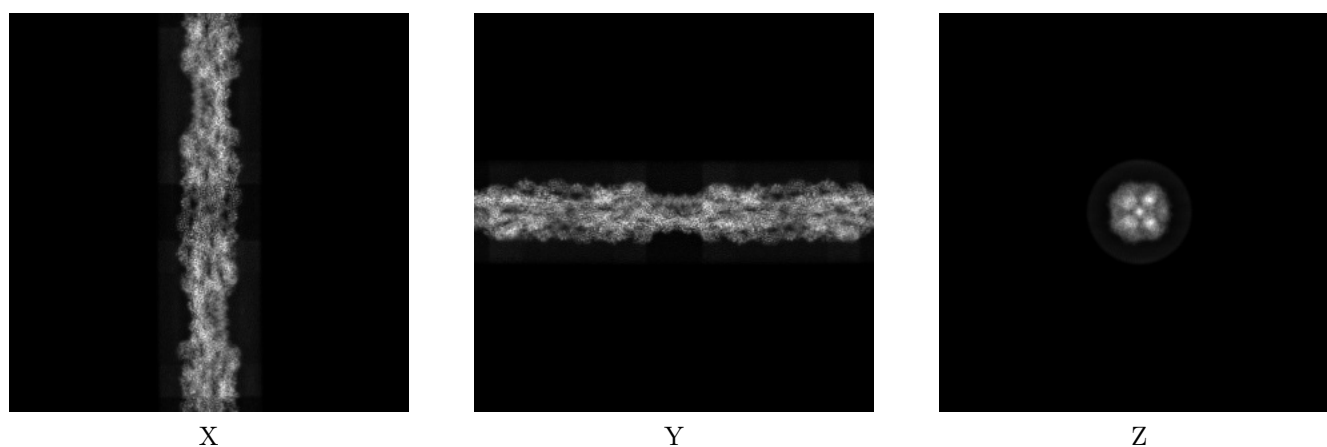
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43892. 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 [i](#)

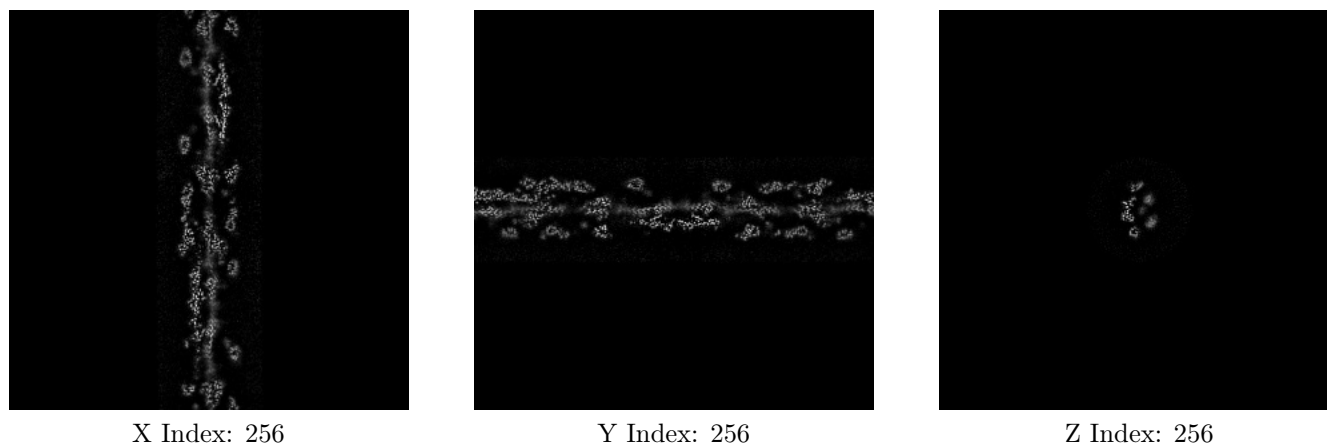
6.1.1 Primary map



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

6.2 Central slices [i](#)

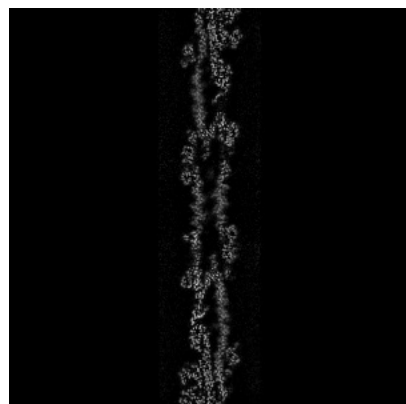
6.2.1 Primary map



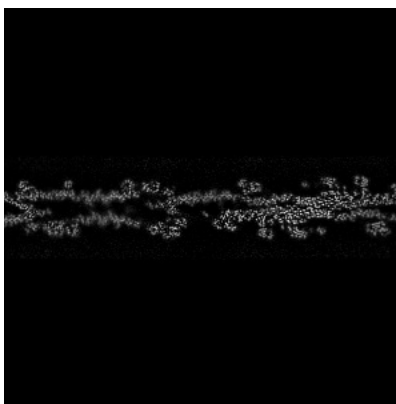
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

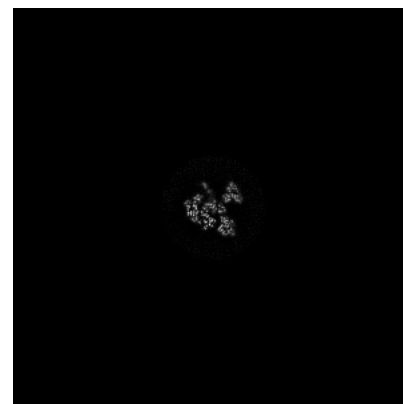
6.3.1 Primary map



X Index: 270



Y Index: 271

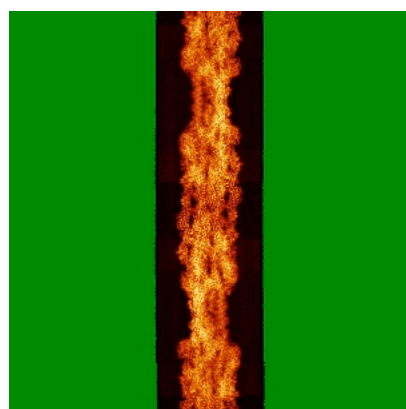


Z Index: 161

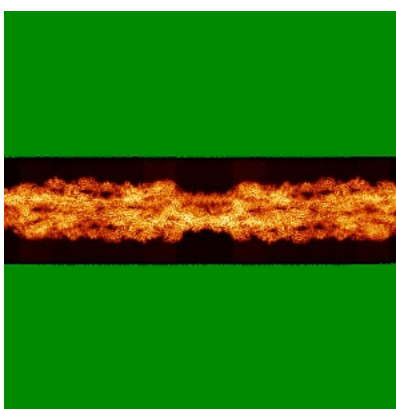
The images above show the largest variance slices of the map in three orthogonal directions.

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

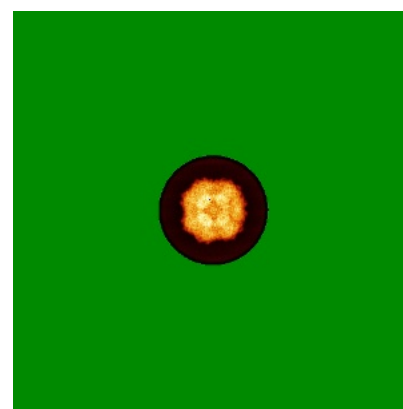
6.4.1 Primary map



X



Y



Z

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

This section was not generated.

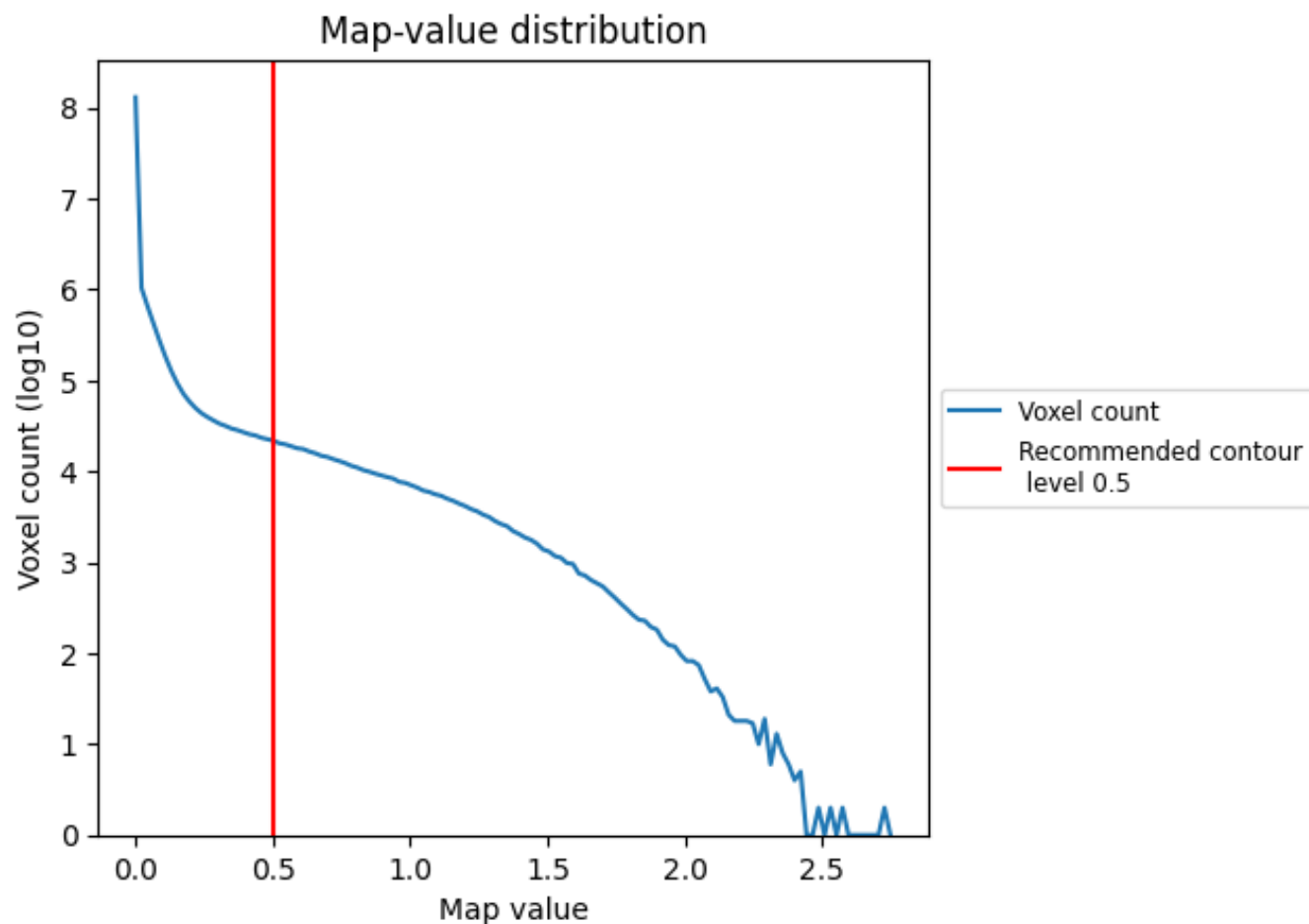
6.6 Mask visualisation

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

7 Map analysis [i](#)

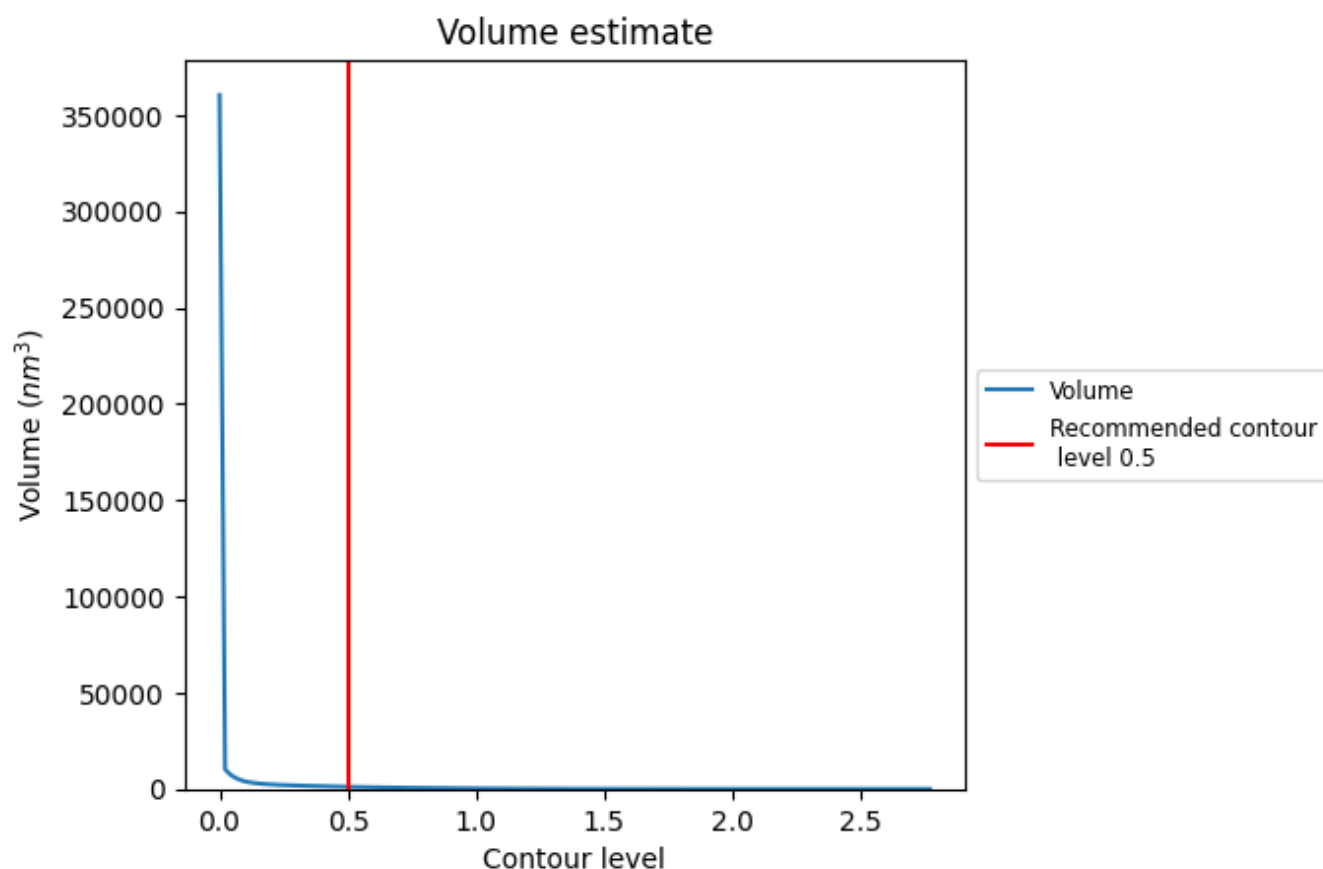
This section contains the results of statistical analysis of the map.

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.

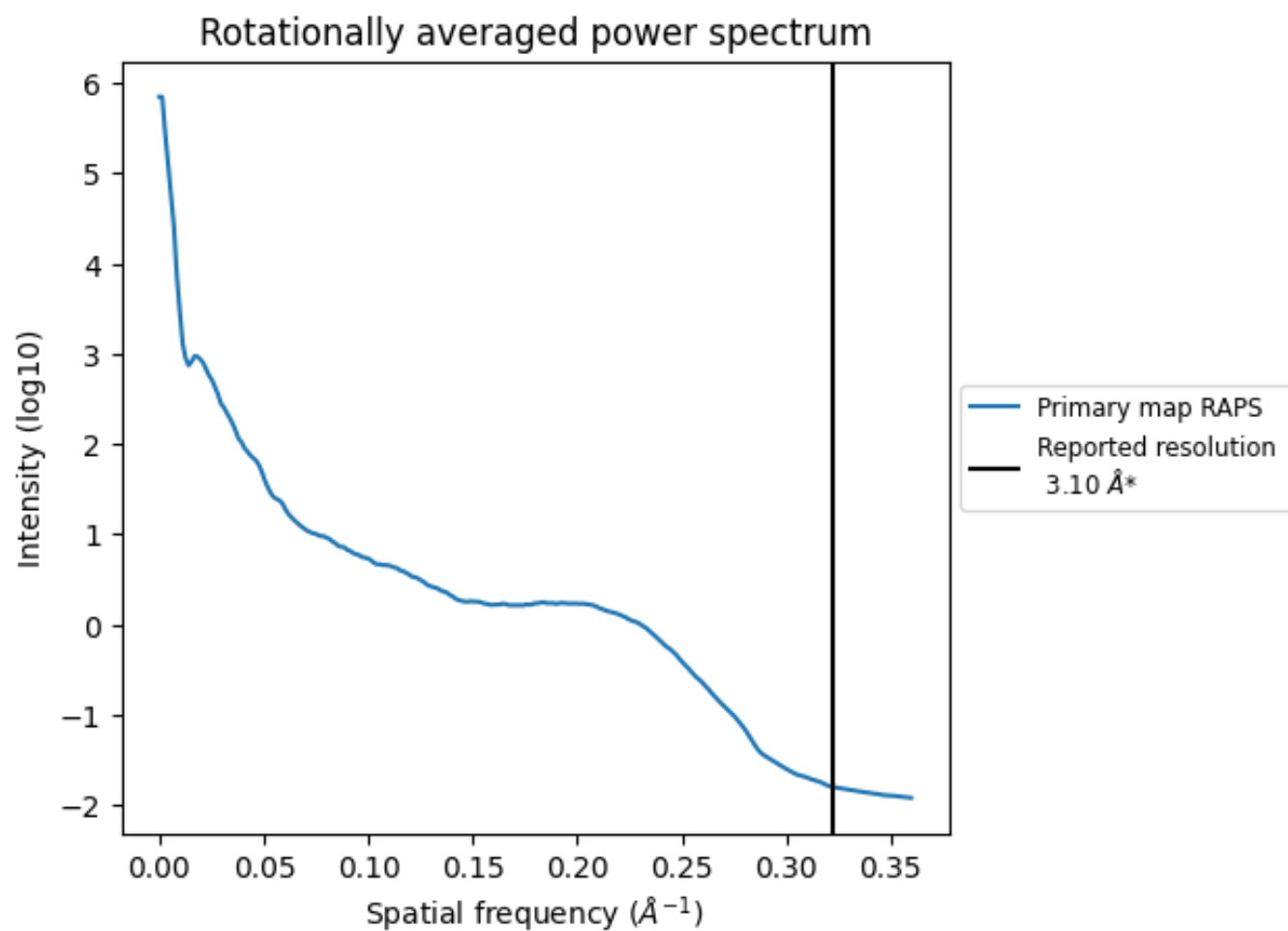
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1110 nm^3 ; this corresponds to an approximate mass of 1002 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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-43892 and PDB model 9B4H. Per-residue inclusion information can be found in section 3 on page 23.

9.1 Map-model overlay [i](#)

This section was not generated.

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



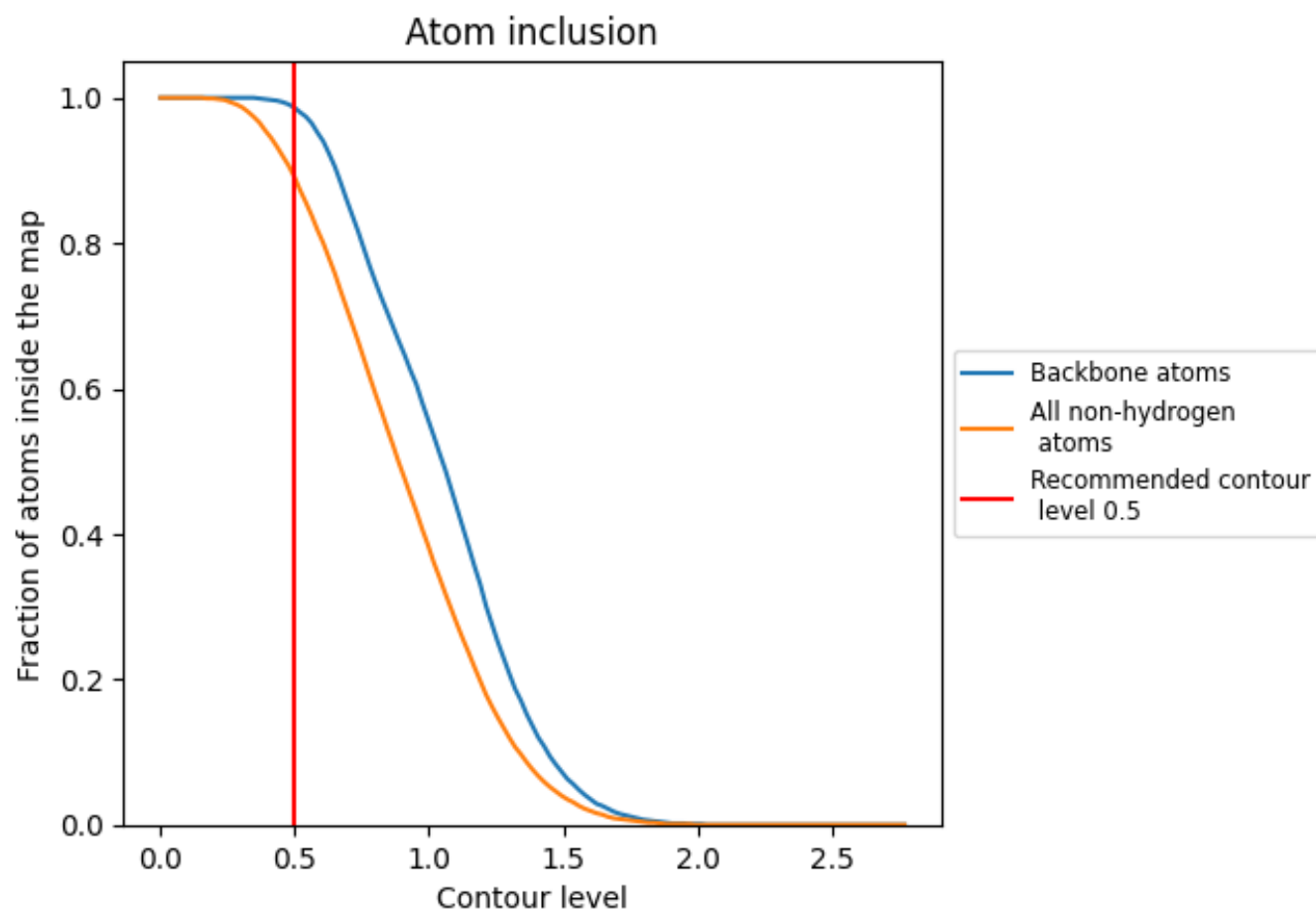
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 89% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8900	 0.4880
A	 0.8940	 0.4900
A1	 0.7140	 0.4580
A2	 0.8210	 0.4630
A3	 0.8930	 0.5310
A4	 0.8330	 0.5290
A5	 0.8330	 0.4860
A6	 0.8330	 0.4760
A7	 1.0000	 0.5530
A9	 0.8060	 0.4870
B	 0.8900	 0.4890
B0	 0.8890	 0.4180
B1	 0.7780	 0.4140
B3	 0.8330	 0.4690
B4	 0.7220	 0.4660
B5	 0.7220	 0.5070
B6	 0.8060	 0.4670
B7	 0.8890	 0.4520
B9	 0.6670	 0.5150
C0	 0.8330	 0.4270
C1	 0.7780	 0.4790
C2	 0.6670	 0.4470
C3	 0.9440	 0.4330
C4	 0.8330	 0.4900
C5	 0.7220	 0.4670
C6	 1.0000	 0.4270
C7	 0.8890	 0.4860
C8	 0.7780	 0.4280
C9	 0.7780	 0.4180
D0	 0.8890	 0.4360
D1	 0.5560	 0.3560
D2	 0.6670	 0.4780
D3	 0.8330	 0.5100
D4	 0.8330	 0.4810
D5	 0.7780	 0.4830



Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
D6	 0.9440	 0.5310
D7	 0.8890	 0.4730
D8	 0.8330	 0.4470
D9	 0.8890	 0.4850
E0	 0.8330	 0.4820
E1	 0.7780	 0.4790
E2	 0.6670	 0.4360
E3	 0.8330	 0.4660
E4	 0.7220	 0.3750
E5	 0.7780	 0.4620
E6	 0.7780	 0.4810
E7	 0.7220	 0.5030
E8	 0.8330	 0.4950
F0	 0.7780	 0.4980
F2	 0.9440	 0.5270
F3	 0.9440	 0.4910
F5	 0.6670	 0.4890
F6	 0.8890	 0.5040
F7	 0.9170	 0.5100
F8	 0.9440	 0.5430
X	 0.9770	 0.4900
a1	 0.7500	 0.4670
a2	 0.7860	 0.4180
a3	 0.8570	 0.5080
a4	 0.8330	 0.5080
a5	 0.8330	 0.4650
a6	 0.8330	 0.4790
a7	 1.0000	 0.5850
a9	 0.8060	 0.4960
b0	 0.9440	 0.4330
b1	 0.6670	 0.4610
b3	 0.9440	 0.5280
b4	 0.8330	 0.4610
b5	 0.7780	 0.4880
b6	 0.8610	 0.4400
b7	 0.9440	 0.4880
b9	 0.8330	 0.4850
c0	 0.8330	 0.4050
c1	 0.8330	 0.4300
c2	 0.6670	 0.4130
c3	 0.9440	 0.4320
c4	 0.8330	 0.4440

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Chain	Atom inclusion	Q-score
c5	 0.7780	 0.4640
c6	 1.0000	 0.3930
c7	 0.8890	 0.4920
c8	 0.8330	 0.4650
c9	 0.8330	 0.4250
d0	 0.7780	 0.4100
d1	 0.6670	 0.3850
d2	 0.7220	 0.4600
d3	 0.8890	 0.5220
d4	 0.8330	 0.4840
d5	 0.9440	 0.5030
d6	 0.9440	 0.4680
d7	 0.8890	 0.4480
d8	 0.7780	 0.4470
d9	 0.6670	 0.4410
e0	 0.8890	 0.5090
e1	 0.7780	 0.5230
e2	 0.7780	 0.4800
e3	 0.8330	 0.4630
e4	 0.7780	 0.3930
e5	 0.7780	 0.4600
e6	 0.8330	 0.4700
e7	 0.8330	 0.4670
e8	 0.8330	 0.5300
e9	 0.8330	 0.4940
f0	 0.8330	 0.4820
f2	 0.8890	 0.4740
f3	 0.9440	 0.5090
f5	 0.7220	 0.5210
f6	 0.9440	 0.5080
f7	 0.9170	 0.5290
f8	 1.0000	 0.5210