



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 08:08 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

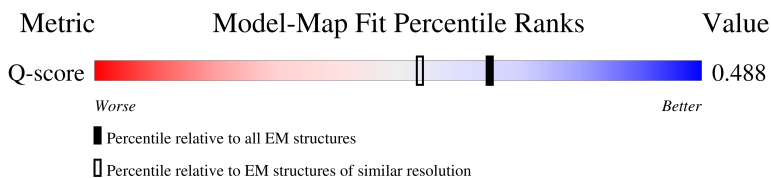
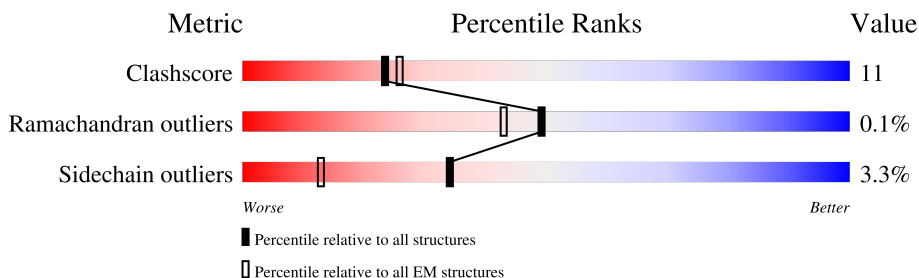
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 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.



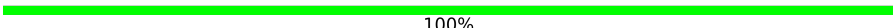
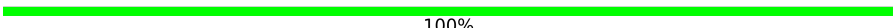
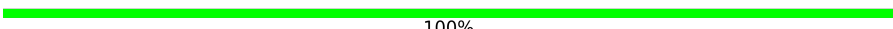
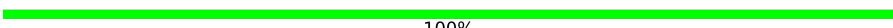
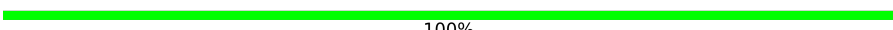
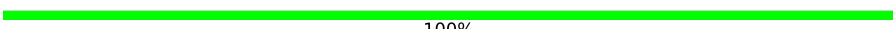
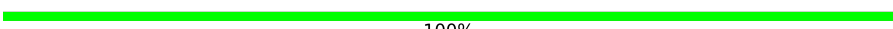
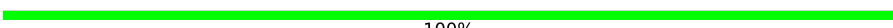
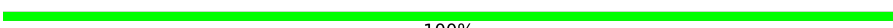
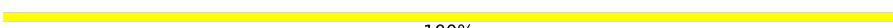
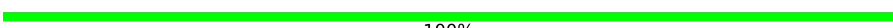
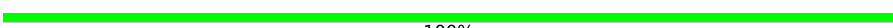
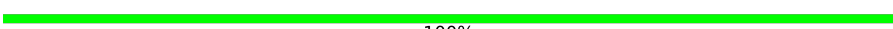
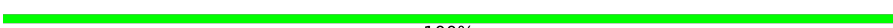
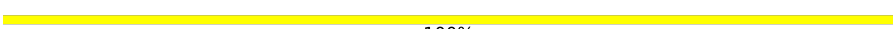
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	 72% 22% . .
1	B	1987	 72% 22% . .
2	X	8572	 99%
3	A1	2	 100%

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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%

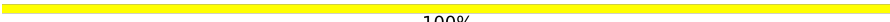
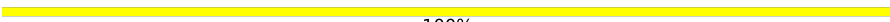
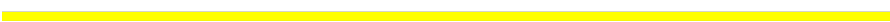
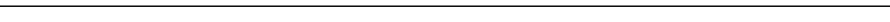
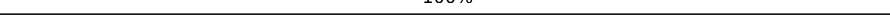
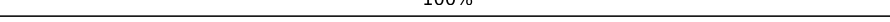
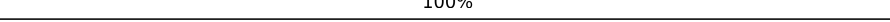
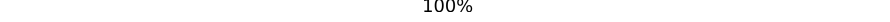
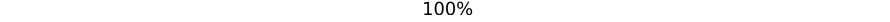
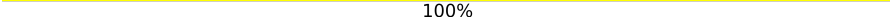
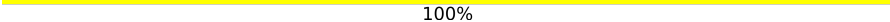
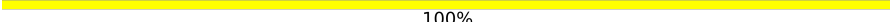
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Mol	Chain	Length	Quality of chain
4	D0	2	100%
4	D1	2	50%
4	D2	2	100%
4	D3	2	100%
4	D4	2	100%
4	D5	2	100%
4	D6	2	100%
4	D7	2	100%
4	D8	2	100%
4	D9	2	50%
4	E0	2	100%
4	E1	2	100%
4	E2	2	100%
4	E3	2	100%
4	E4	2	50%
4	E5	2	100%
4	E7	2	100%
4	E8	2	100%
4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

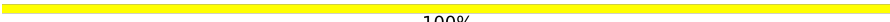
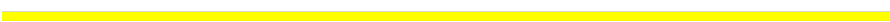
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Mol	Chain	Length	Quality of chain
4	d8	2	100%
4	d9	2	50% 50%
4	e0	2	100%
4	e1	2	100%
4	e2	2	100%
4	e3	2	50% 50%
4	e4	2	50% 50%
4	e5	2	100%
4	e6	2	50% 50%
4	e7	2	50% 50%
4	e8	2	100%
4	f0	2	50% 50%
4	f2	2	50% 50%
4	f3	2	100%
4	f5	2	100%
4	f8	2	100%
5	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		

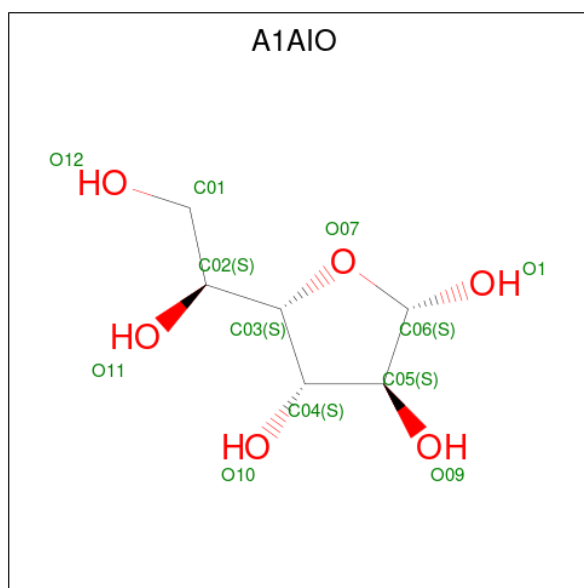
- Molecule 7 is an oligosaccharide called beta-L-arabinofuranose-(1-4)-beta-L-ribulofuranose.

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	

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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	

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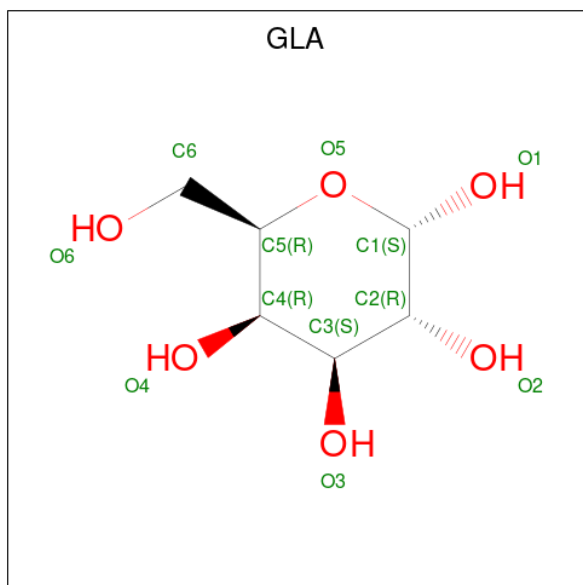
Mol	Chain	Residues	Atoms			AltConf
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1	Total	C	O	0
			11	6	5	
9	B	1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

- 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
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	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	A	1	Total	C	O	0
			11	6	5	
10	A	1	Total	C	O	0
			11	6	5	

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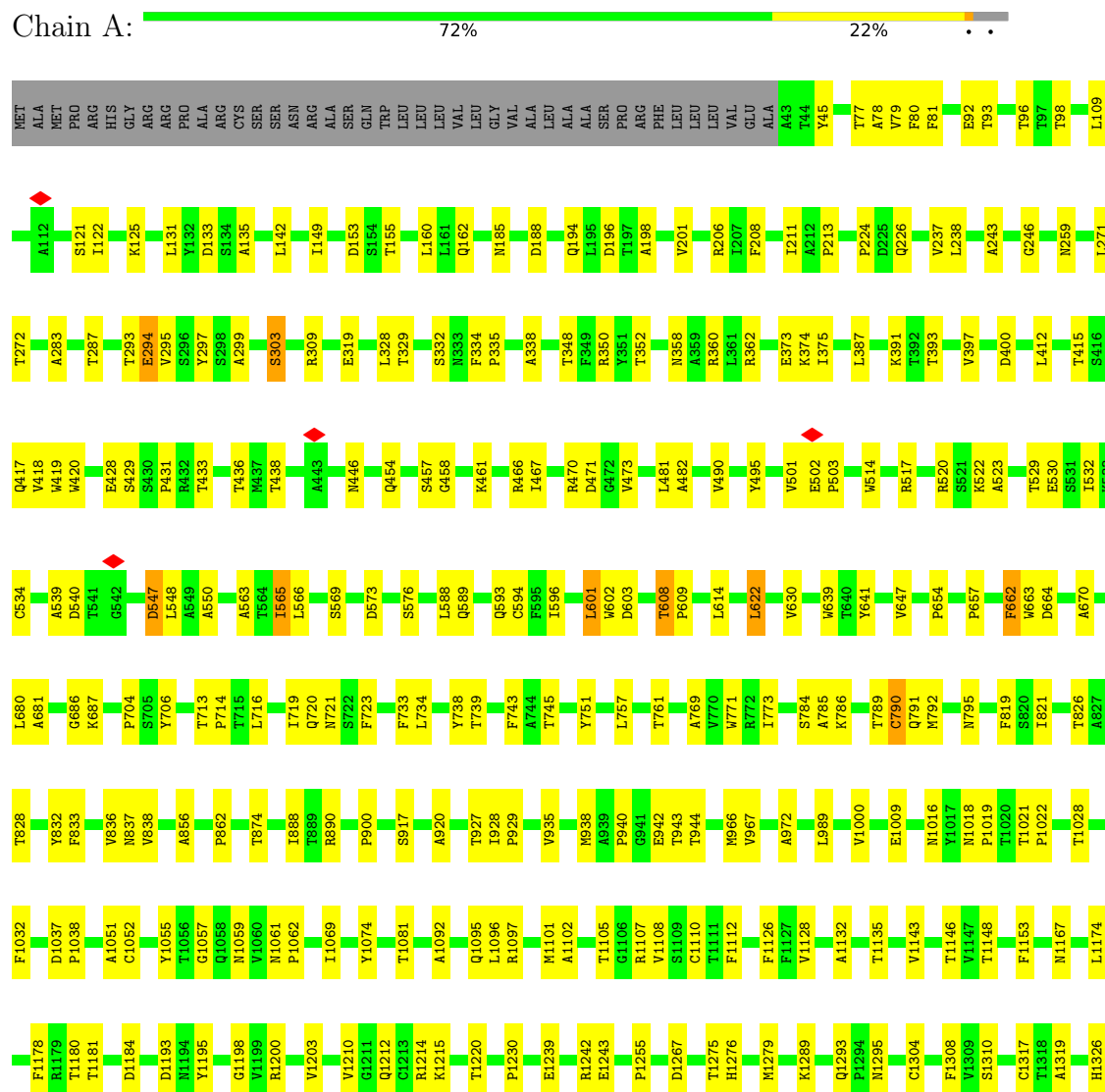
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Mol	Chain	Residues	Atoms			AltConf
10	A	1	Total	C	O	0
			11	6	5	
10	A	1	Total	C	O	0
			11	6	5	
10	A	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10	B	1	Total	C	O	0
			11	6	5	
10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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

















- 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%

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:  100%

FUB1
FUB2

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

Chain F3:  100%

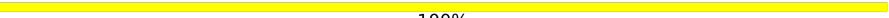
FUB1
FUB2

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

Chain F8:  100%

FUB1
FUB2

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

Chain a5:  100%

FUB1
FUB2

- 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%

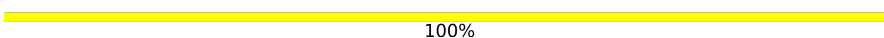


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d9:  50% 50%

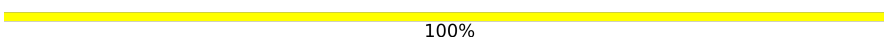


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

Chain d7:  100%

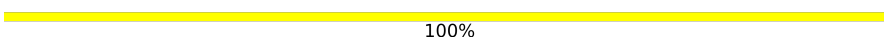


- Molecule 4: beta-L-arabinofuranose-(1-2)-beta-L-arabinofuranose

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%

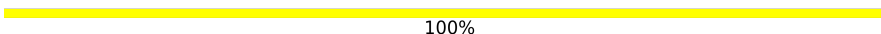
FUB1
FUB2
FUB3
FUB4

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

Chain a9:  25% 75%

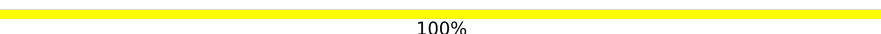
FUB1
FUB2
FUB3
FUB4

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

Chain b6:  100%

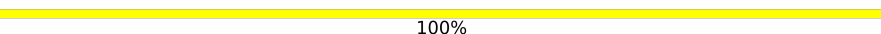
FUB1
FUB2
FUB3
FUB4

- 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%

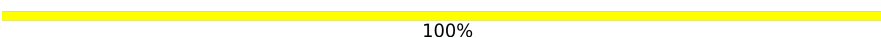
FUB1
FUB2
FUB3
FUB4

- 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.

All (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
1:B:1914:HYP:HG	4:e6:1:FUB:C1	1.84	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1776:TYR:CE1	10:B:2060:GLA:H62	1.93	1.03
4:e6:2:FUB:C5	4:e3:1:FUB:O5	2.07	1.01
1:B:1905:HYP:OD1	4:d8:1:FUB:O4	1.80	0.98
1:B:1861:SER:OG	10:B:2060:GLA:C1	2.11	0.97
1:B:1914:HYP:CG	4:e6:1:FUB:C1	2.44	0.94
1:B:1893:HYP:HD1	4:d0:1:FUB:C1	1.69	0.93
1:B:1914:HYP:HG	4:e6:1:FUB:O4	1.75	0.87
4:e6:2:FUB:O5	4:e3:1:FUB:C5	2.25	0.85
4:e6:2:FUB:O5	4:e3:1:FUB:O5	1.95	0.82
4:e1:2:FUB:O3	4:d8:1:FUB:O5	1.97	0.82
1:B:1905:HYP:OD1	4:d8:1:FUB:C1	2.27	0.82
1:B:1914:HYP:OD1	4:e6:1:FUB:O2	2.00	0.80
1:A:1909:ARG:CD	4:E4:2:FUB:O3	2.30	0.79
4:f0:2:FUB:C4	4:e7:1:FUB:O5	2.31	0.79
1:A:1927:HYP:HG	4:F5:1:FUB:C1	2.13	0.79
1:B:1861:SER:CB	10:B:2060:GLA:C1	2.61	0.78
2:X:1560:SER:OG	2:X:1561:THR:N	2.18	0.77
1:A:1909:ARG:HB3	4:E4:2:FUB:O3	1.85	0.76
1:B:1914:HYP:OD1	4:e6:1:FUB:C1	2.33	0.76
1:A:1909:ARG:HD3	4:E4:2:FUB:O3	1.86	0.76
1:A:1909:ARG:CB	4:E4:2:FUB:O3	2.35	0.75
4:f0:1:FUB:O5	4:f2:2:FUB:O5	2.05	0.73
1:B:1776:TYR:HE1	10:B:2060:GLA:H62	1.50	0.73
4:f0:2:FUB:O5	4:e7:1:FUB:O5	2.06	0.73
1:A:1310:SER:HB3	1:A:1317:CYS:HB3	1.71	0.73
1:A:900:PRO:HB3	1:A:940:PRO:HD3	1.71	0.72
1:B:1773:TYR:OH	4:a7:2:FUB:O5	2.07	0.71
1:B:1779:ALA:HB1	1:B:1793:GLY:HA2	1.71	0.71
1:B:249:LEU:HD21	1:B:252:THR:HG23	1.71	0.71
1:B:1398:SER:HB2	1:B:1405:CYS:HB3	1.72	0.71
1:B:793:PRO:HD2	1:B:835:THR:HG23	1.73	0.71
1:A:1198:GLY:HA3	1:A:1215:LYS:HG3	1.73	0.70
1:A:1293:GLN:NE2	1:A:1295:ASN:OD1	2.24	0.70
1:B:927:THR:HG22	1:B:929:PRO:HD2	1.73	0.68
1:A:935:VAL:HG11	1:A:972:ALA:HB2	1.75	0.68
1:A:1779:ALA:HB1	1:A:1793:GLY:HA2	1.75	0.68
1:B:156:LEU:HB2	1:B:186:ARG:HH12	1.57	0.68
1:A:1366:TYR:HB2	1:A:1403:ALA:HA	1.76	0.68
9:B:2016:A1AIO:O11	9:B:2016:A1AIO:O10	2.11	0.68
1:B:196:ASP:HB3	1:B:201:VAL:HG21	1.76	0.67
9:B:2005:A1AIO:O10	9:B:2005:A1AIO:O11	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:593:GLN:NE2	1:B:602:TRP:O	2.29	0.66
4:f0:2:FUB:C5	4:e7:1:FUB:O5	2.44	0.66
1:A:789:THR:HG22	1:A:791:GLN:HE21	1.60	0.65
1:B:1672:GLN:HB2	1:B:1680:CYS:HB3	1.76	0.65
1:B:1921:HYP:HD23	4:f2:1:FUB:C1	2.27	0.65
1:B:1255:PRO:HB2	1:B:1276:HIS:HB3	1.79	0.65
1:A:657:PRO:HB2	1:A:721:ASN:HB2	1.78	0.65
1:A:1484:PRO:HD3	1:A:1558:ASP:HB3	1.78	0.65
1:B:1219:GLY:HA3	1:B:1277:LEU:HB2	1.77	0.65
1:B:1490:MET:HE3	1:B:1538:PHE:HB2	1.78	0.65
1:B:777:ARG:NH1	1:B:779:ALA:O	2.30	0.65
1:A:757:LEU:HD11	1:A:769:ALA:HB1	1.78	0.64
1:A:828:THR:HB	1:A:832:TYR:HE1	1.62	0.64
9:B:2030:A1AIO:O11	9:B:2030:A1AIO:O10	2.14	0.64
1:B:178:ARG:NE	1:B:218:ASN:OD1	2.30	0.64
9:A:2038:A1AIO:O10	9:A:2038:A1AIO:O11	2.16	0.64
1:B:274:THR:H	1:B:293:THR:HG22	1.63	0.63
1:A:1815:PRO:O	1:A:1827:GLN:NE2	2.28	0.63
1:A:589:GLN:NE2	1:A:608:THR:O	2.31	0.63
4:f0:1:FUB:O5	4:f2:2:FUB:C5	2.46	0.63
1:B:1310:SER:HB3	1:B:1317:CYS:HB3	1.80	0.63
9:A:2040:A1AIO:O10	9:A:2040:A1AIO:O11	2.17	0.62
9:B:2054:A1AIO:O10	9:B:2054:A1AIO:O11	2.17	0.62
4:f0:2:FUB:O5	4:e7:1:FUB:C5	2.47	0.62
1:B:1326:HIS:NE2	1:B:1355:PRO:O	2.28	0.62
1:B:1396:THR:HG22	1:B:1407:LYS:HA	1.82	0.62
1:B:681:ALA:HA	1:B:686:GLY:HA3	1.82	0.62
9:B:2003:A1AIO:O11	9:B:2003:A1AIO:O10	2.18	0.62
1:A:1820:GLY:O	1:A:1823:ASN:ND2	2.33	0.61
1:B:536:PHE:HB2	1:B:592:LEU:HD23	1.82	0.61
1:B:900:PRO:HB3	1:B:940:PRO:HD3	1.81	0.61
1:A:1101:MET:HG2	1:A:1108:VAL:HB	1.82	0.61
9:B:2028:A1AIO:O10	9:B:2028:A1AIO:O11	2.17	0.61
1:A:358:ASN:HB3	1:A:375:ILE:HD12	1.82	0.61
1:A:1912:HYP:HG	4:E4:1:FUB:C1	2.29	0.61
1:A:1927:HYP:OD1	4:F5:1:FUB:C2	2.45	0.61
1:A:1576:THR:HG22	1:A:1588:VAL:H	1.64	0.61
1:B:507:ILE:HG23	1:B:510:VAL:HB	1.82	0.61
9:B:2020:A1AIO:O10	9:B:2020:A1AIO:O11	2.18	0.61
9:B:2023:A1AIO:O10	9:B:2023:A1AIO:O11	2.17	0.61
1:A:1644:ALA:HB2	1:A:1656:LEU:HB2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ARG:NH1	1:B:530:GLU:OE2	2.31	0.61
1:B:1125:LYS:HG3	1:B:1147:VAL:HG21	1.83	0.61
1:B:1322:GLU:OE2	1:B:1370:ARG:NH1	2.34	0.60
9:B:2046:A1AIO:O10	9:B:2046:A1AIO:O11	2.19	0.60
4:e1:1:FUB:O5	4:e3:2:FUB:O5	2.19	0.60
1:B:1293:GLN:NE2	1:B:1300:VAL:O	2.34	0.60
1:A:428:GLU:OE2	1:A:466:ARG:NH1	2.34	0.60
1:B:1378:MET:SD	1:B:1378:MET:N	2.75	0.60
9:B:2014:A1AIO:O10	9:B:2014:A1AIO:O11	2.19	0.60
1:B:432:ARG:NH1	1:B:470:ARG:O	2.34	0.60
1:B:666:LYS:HD3	1:B:712:ALA:HB2	1.84	0.60
1:B:1565:PRO:HB3	1:B:1606:SER:HB3	1.83	0.59
1:B:1773:TYR:HD2	1:B:1810:GLN:HA	1.66	0.59
1:A:1242:ARG:HG3	1:A:1243:GLU:HG3	1.84	0.59
1:B:1037:ASP:CG	1:B:1038:PRO:HD3	2.28	0.59
9:B:2034:A1AIO:O10	9:B:2034:A1AIO:O11	2.19	0.59
9:B:2051:A1AIO:O11	9:B:2051:A1AIO:O10	2.21	0.59
1:A:1803:ALA:HB1	1:A:1808:VAL:HG11	1.83	0.59
1:B:540:ASP:OD1	1:B:540:ASP:N	2.34	0.59
1:B:311:ASN:HB3	1:B:319:GLU:HB2	1.85	0.59
1:A:1443:SER:OG	1:A:1445:CYS:SG	2.60	0.59
1:B:1452:THR:HG22	1:B:1464:PRO:HA	1.84	0.58
1:A:1471:ALA:HB2	1:A:1479:CYS:HB3	1.84	0.58
1:A:1637:ASN:HB3	1:A:1678:THR:HB	1.84	0.58
1:B:1776:TYR:CE1	10:B:2060:GLA:C6	2.79	0.58
1:B:1308:PHE:HA	1:B:1319:ALA:HA	1.84	0.58
9:B:2053:A1AIO:O10	9:B:2053:A1AIO:O11	2.21	0.58
1:A:1009:GLU:OE1	1:A:1107:ARG:NH1	2.36	0.58
1:A:1308:PHE:HA	1:A:1319:ALA:HA	1.85	0.58
1:A:1802:PHE:HB2	1:A:1835:GLN:HA	1.85	0.58
1:B:166:PRO:HG2	1:B:263:VAL:HG12	1.86	0.58
1:B:155:THR:OG1	1:B:186:ARG:NH2	2.37	0.58
1:A:522:LYS:NZ	1:A:523:ALA:O	2.36	0.58
9:A:2030:A1AIO:O10	9:A:2030:A1AIO:O11	2.20	0.58
1:B:206:ARG:HH22	1:B:246:GLY:HA2	1.69	0.58
9:B:2018:A1AIO:O11	9:B:2018:A1AIO:O10	2.21	0.58
1:A:400:ASP:O	1:A:454:GLN:NE2	2.36	0.57
1:A:1255:PRO:HB2	1:A:1276:HIS:HB3	1.86	0.57
9:A:2046:A1AIO:O11	9:A:2046:A1AIO:O10	2.22	0.57
1:B:185:ASN:HA	1:B:213:PRO:HA	1.86	0.57
1:B:1465:CYS:SG	1:B:1469:THR:OG1	2.59	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1180:THR:HG23	1:B:1181:THR:HG23	1.85	0.57
1:A:1143:VAL:O	1:A:1146:THR:OG1	2.23	0.57
1:B:756:TYR:HA	1:B:899:ILE:HG21	1.84	0.57
1:A:1757:ASN:OD1	1:A:1764:SER:N	2.36	0.57
1:A:1326:HIS:NE2	1:A:1355:PRO:O	2.27	0.57
1:A:1421:GLN:NE2	1:A:1438:LEU:O	2.38	0.57
9:A:2033:A1AIO:O10	9:A:2033:A1AIO:O11	2.23	0.57
1:B:918:ALA:HB1	1:B:966:MET:HE2	1.85	0.57
1:A:1603:ASP:OD1	1:A:1611:LYS:NZ	2.38	0.57
1:B:206:ARG:NH1	1:B:243:ALA:O	2.37	0.57
1:B:1081:THR:HG22	1:B:1097:ARG:HA	1.87	0.57
1:A:566:LEU:O	1:A:569:SER:OG	2.21	0.56
1:B:1741:LYS:O	1:B:1744:SER:OG	2.22	0.56
1:A:1193:ASP:OD2	1:A:1200:ARG:NH2	2.39	0.56
1:B:609:PRO:HB2	1:B:654:PRO:HD3	1.88	0.56
1:A:160:LEU:HB2	1:A:238:LEU:HD12	1.88	0.56
9:A:2035:A1AIO:O10	9:A:2035:A1AIO:O11	2.22	0.56
1:B:603:ASP:OD1	1:B:603:ASP:N	2.38	0.56
1:B:1914:HYP:OD1	4:e6:1:FUB:C2	2.53	0.56
9:B:2022:A1AIO:O11	9:B:2022:A1AIO:O10	2.24	0.56
9:B:2015:A1AIO:O10	9:B:2015:A1AIO:O11	2.23	0.56
1:A:1081:THR:HG22	1:A:1097:ARG:HA	1.87	0.56
1:B:866:VAL:HG22	1:B:888:ILE:HG13	1.88	0.56
1:A:761:THR:OG1	1:A:890:ARG:NH2	2.39	0.55
1:A:283:ALA:O	1:A:350:ARG:NH1	2.37	0.55
1:B:911:GLU:OE2	1:B:954:THR:OG1	2.20	0.55
1:B:1198:GLY:HA3	1:B:1215:LYS:HG3	1.88	0.55
1:A:1239:GLU:OE1	1:A:1239:GLU:N	2.30	0.55
1:A:1565:PRO:HB3	1:A:1606:SER:HB3	1.88	0.55
1:A:1587:THR:O	1:A:1594:TYR:OH	2.22	0.55
1:B:398:THR:HG23	1:B:400:ASP:H	1.70	0.55
1:B:658:ILE:HD11	1:B:691:MET:HE2	1.88	0.55
9:B:2031:A1AIO:O10	9:B:2031:A1AIO:O11	2.24	0.55
1:A:1037:ASP:HB3	1:A:1038:PRO:HD3	1.88	0.55
1:A:1200:ARG:NH1	1:A:1267:ASP:OD2	2.40	0.55
9:A:2054:A1AIO:O10	9:A:2054:A1AIO:O11	2.24	0.55
1:B:214:THR:HG23	1:B:217:THR:HG21	1.89	0.55
1:A:1102:ALA:O	1:A:1105:THR:OG1	2.21	0.55
1:A:928:ILE:HG13	1:A:929:PRO:HD3	1.88	0.55
1:B:502:GLU:HB3	1:B:503:PRO:HD3	1.89	0.55
9:B:2039:A1AIO:O11	9:B:2039:A1AIO:O10	2.25	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:B:2050:A1AIO:O10	9:B:2050:A1AIO:O11	2.24	0.54
9:A:2029:A1AIO:O10	9:A:2029:A1AIO:O11	2.25	0.54
1:B:1672:GLN:NE2	1:B:1679:THR:O	2.41	0.54
1:B:1935:SER:OG	1:B:1936:ALA:N	2.41	0.54
1:B:1218:GLY:O	1:B:1237:SER:OG	2.25	0.54
1:A:609:PRO:HB2	1:A:654:PRO:HD3	1.89	0.54
1:A:1912:HYP:OD1	4:E4:1:FUB:O2	2.24	0.54
1:A:1132:ALA:O	1:A:1135:THR:OG1	2.25	0.54
1:A:1617:SER:OG	1:A:1627:CYS:SG	2.60	0.54
1:A:1733:CYS:SG	1:A:1737:THR:OG1	2.54	0.54
9:B:2002:A1AIO:O10	9:B:2002:A1AIO:O11	2.26	0.54
1:A:1021:THR:HB	1:A:1153:PHE:HB2	1.90	0.54
1:A:1180:THR:HG23	1:A:1181:THR:HG23	1.89	0.54
9:A:2052:A1AIO:O11	9:A:2052:A1AIO:O10	2.26	0.54
1:B:224:PRO:O	1:B:226:GLN:NE2	2.34	0.54
1:B:1006:VAL:HB	1:B:1036:ARG:HG3	1.90	0.54
1:B:428:GLU:OE2	1:B:466:ARG:NH1	2.41	0.54
9:B:2011:A1AIO:O10	9:B:2011:A1AIO:O11	2.25	0.54
9:B:2021:A1AIO:O10	9:B:2021:A1AIO:O11	2.25	0.54
1:A:206:ARG:NH1	1:A:243:ALA:O	2.41	0.54
9:B:2017:A1AIO:O10	9:B:2017:A1AIO:O11	2.26	0.54
1:A:287:THR:HG22	1:A:348:THR:HG22	1.88	0.54
9:A:2009:A1AIO:O10	9:A:2009:A1AIO:O11	2.26	0.54
9:A:2041:A1AIO:O10	9:A:2041:A1AIO:O11	2.25	0.54
1:B:1921:HYP:HG	9:B:2055:A1AIO:O07	2.07	0.54
9:B:2038:A1AIO:O10	9:B:2038:A1AIO:O11	2.26	0.54
1:A:502:GLU:HB3	1:A:503:PRO:HD3	1.90	0.53
1:A:1022:PRO:HB2	1:A:1028:THR:HG21	1.89	0.53
1:A:1488:SER:O	1:A:1488:SER:OG	2.25	0.53
1:B:288:PHE:HE1	1:B:293:THR:HG21	1.73	0.53
1:B:1304:CYS:SG	1:B:1308:PHE:HB2	2.48	0.53
1:A:594:CYS:HB3	1:A:601:LEU:HD23	1.89	0.53
1:A:942:GLU:OE2	4:D9:2:FUB:O3	2.25	0.53
9:A:2037:A1AIO:O10	9:A:2037:A1AIO:O11	2.25	0.53
1:B:1289:LYS:HB3	1:B:1356:ASN:HD21	1.72	0.53
1:A:206:ARG:HH22	1:A:246:GLY:HA2	1.72	0.53
1:A:664:ASP:OD1	1:A:664:ASP:N	2.41	0.53
1:A:1672:GLN:NE2	1:A:1679:THR:O	2.41	0.53
1:B:589:GLN:NE2	1:B:608:THR:O	2.37	0.53
1:A:1598:THR:O	1:A:1658:LYS:NZ	2.36	0.53
1:B:1421:GLN:OE1	1:B:1436:THR:OG1	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1220:THR:HG22	1:A:1230:PRO:HA	1.91	0.53
9:A:2016:A1AIO:O10	9:A:2016:A1AIO:O11	2.27	0.53
1:B:458:GLY:O	1:B:461:LYS:NZ	2.42	0.53
1:A:400:ASP:OD2	1:A:520:ARG:NH2	2.41	0.53
1:A:1051:ALA:HB1	1:A:1096:LEU:HD11	1.90	0.53
1:A:1483:LYS:O	1:A:1486:THR:OG1	2.27	0.53
1:A:1615:SER:HB2	1:A:1637:ASN:HA	1.91	0.53
9:A:2020:A1AIO:O10	9:A:2020:A1AIO:O11	2.25	0.53
1:B:80:PHE:HB3	1:B:95:ARG:HG2	1.90	0.53
1:B:309:ARG:HD3	1:B:319:GLU:HG3	1.90	0.53
1:B:516:PHE:HB2	1:B:575:ILE:HG12	1.90	0.53
1:A:630:VAL:HG22	1:A:745:THR:HB	1.90	0.53
1:B:874:THR:HG23	1:B:1000:VAL:H	1.74	0.53
9:B:2040:A1AIO:O10	9:B:2040:A1AIO:O11	2.27	0.53
1:A:1948:ASP:N	1:A:1948:ASP:OD1	2.36	0.52
9:A:2003:A1AIO:O10	9:A:2003:A1AIO:O11	2.27	0.52
9:A:2006:A1AIO:O10	9:A:2006:A1AIO:O11	2.25	0.52
9:B:2012:A1AIO:O10	9:B:2012:A1AIO:O11	2.27	0.52
1:A:573:ASP:N	1:A:573:ASP:OD1	2.42	0.52
1:B:1270:THR:OG1	1:B:1271:TYR:N	2.42	0.52
1:B:437:MET:HE3	1:B:437:MET:HA	1.91	0.52
1:B:1469:THR:HG22	1:B:1481:GLN:HA	1.91	0.52
1:B:1773:TYR:CD2	1:B:1810:GLN:HA	2.44	0.52
1:B:462:LEU:HB3	1:B:487:THR:HG22	1.91	0.52
1:B:631:VAL:HG23	1:B:746:VAL:HG23	1.90	0.52
1:B:1200:ARG:NH2	1:B:1267:ASP:OD2	2.42	0.52
9:B:2055:A1AIO:O10	9:B:2055:A1AIO:O11	2.28	0.52
1:B:1484:PRO:HD3	1:B:1558:ASP:HB3	1.92	0.52
9:B:2024:A1AIO:O11	9:B:2024:A1AIO:O10	2.27	0.52
9:B:2041:A1AIO:O10	9:B:2041:A1AIO:O11	2.28	0.52
1:A:271:LEU:O	1:A:374:LYS:NZ	2.43	0.52
1:A:1529:ILE:HG23	1:A:1530:VAL:HG23	1.92	0.52
1:B:593:GLN:NE2	1:B:604:PRO:O	2.36	0.52
1:A:1126:PHE:HB3	1:A:1148:THR:HB	1.92	0.52
9:A:2008:A1AIO:O10	9:A:2008:A1AIO:O11	2.28	0.52
1:B:49:LEU:HD21	1:B:127:VAL:HG12	1.92	0.52
1:B:1739:ALA:HB2	1:B:1747:CYS:HB3	1.91	0.52
1:B:494:LEU:N	1:B:521:SER:OG	2.43	0.51
1:B:1883:HYP:HA	9:B:2018:A1AIO:O09	2.10	0.51
9:A:2012:A1AIO:O10	9:A:2012:A1AIO:O11	2.28	0.51
1:B:1392:CYS:SG	1:B:1396:THR:OG1	2.63	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LEU:HD13	1:A:467:ILE:HD13	1.93	0.51
1:B:1412:THR:HG21	1:B:1440:GLU:HB2	1.90	0.51
1:B:1575:ASP:OD1	1:B:1576:THR:N	2.43	0.51
9:B:2056:A1AIO:O10	9:B:2056:A1AIO:O11	2.28	0.51
1:B:1921:HYP:CD	4:f2:1:FUB:C1	2.88	0.51
1:A:196:ASP:HB3	1:A:201:VAL:HG21	1.92	0.51
1:B:501:VAL:HG22	1:B:503:PRO:HD2	1.93	0.51
1:A:681:ALA:HA	1:A:686:GLY:HA3	1.92	0.51
1:A:1556:ASP:N	1:A:1556:ASP:OD1	2.43	0.51
1:B:1327:THR:OG1	1:B:1328:ASP:N	2.44	0.51
9:B:2032:A1AIO:O10	9:B:2032:A1AIO:O11	2.28	0.51
1:A:1804:ASP:OD1	1:A:1804:ASP:N	2.36	0.51
1:B:194:GLN:OE1	1:B:239:ARG:NH1	2.42	0.51
1:A:784:SER:OG	1:A:785:ALA:N	2.43	0.51
9:A:2019:A1AIO:O11	9:A:2019:A1AIO:O10	2.28	0.51
1:A:1671:PHE:HD2	1:A:1696:ALA:HA	1.76	0.51
9:A:2007:A1AIO:O10	9:A:2007:A1AIO:O11	2.29	0.51
9:A:2021:A1AIO:O10	9:A:2021:A1AIO:O11	2.29	0.51
1:B:1675:ALA:O	1:B:1676:GLU:HG2	2.11	0.51
9:B:2027:A1AIO:O10	9:B:2027:A1AIO:O11	2.29	0.51
1:A:362:ARG:HG2	1:A:373:GLU:HG2	1.92	0.51
1:A:943:THR:HG22	1:A:944:THR:HG23	1.93	0.51
9:B:2057:A1AIO:O10	9:B:2057:A1AIO:O11	2.28	0.51
1:B:277:PRO:HG2	1:B:280:VAL:HG12	1.93	0.50
1:B:325:PRO:HB2	1:B:328:LEU:HD12	1.93	0.50
9:B:2008:A1AIO:O10	9:B:2008:A1AIO:O11	2.29	0.50
1:A:224:PRO:O	1:A:226:GLN:NE2	2.43	0.50
1:B:905:CYS:HB3	1:B:965:LEU:HD11	1.93	0.50
1:B:1617:SER:OG	1:B:1627:CYS:SG	2.60	0.50
9:B:2047:A1AIO:O10	9:B:2047:A1AIO:O11	2.26	0.50
1:A:188:ASP:HB2	1:A:208:PHE:HE1	1.75	0.50
1:A:1495:GLN:HG2	1:A:1509:PRO:HB2	1.92	0.50
1:B:1829:THR:OG1	1:B:1830:GLU:N	2.45	0.50
1:B:1852:GLU:HB2	10:B:2058:GLA:O6	2.12	0.50
9:A:2014:A1AIO:O10	9:A:2014:A1AIO:O11	2.30	0.50
1:A:391:LYS:NZ	1:A:393:THR:O	2.43	0.50
9:B:2049:A1AIO:O10	9:B:2049:A1AIO:O11	2.29	0.50
1:A:771:TRP:HD1	1:A:821:ILE:HD13	1.76	0.50
1:B:714:PRO:HD2	1:B:740:ALA:HB3	1.94	0.50
4:C8:1:FUB:O3	4:C8:2:FUB:O5	2.30	0.50
1:B:1905:HYP:HG	9:B:2029:A1AIO:O07	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:309:ARG:NH1	1:B:319:GLU:OE2	2.45	0.50
1:B:1802:PHE:HB2	1:B:1835:GLN:HA	1.94	0.50
1:A:133:ASP:OD1	1:A:133:ASP:N	2.45	0.50
1:A:329:THR:O	1:A:332:SER:OG	2.30	0.50
1:A:1856:HYP:HG	9:A:2004:A1AIO:O07	2.12	0.50
1:A:467:ILE:HD11	1:A:482:ALA:HB3	1.92	0.49
1:B:1365:THR:HG22	1:B:1391:PRO:HA	1.94	0.49
1:B:674:ASP:OD2	1:B:732:GLY:N	2.39	0.49
1:B:771:TRP:HB2	1:B:819:PHE:HB2	1.93	0.49
1:A:92:GLU:OE2	1:A:93:THR:N	2.45	0.49
1:B:771:TRP:HD1	1:B:821:ILE:HD13	1.77	0.49
1:A:397:VAL:HB	1:A:490:VAL:HG12	1.94	0.49
9:A:2036:A1AIO:O10	9:A:2036:A1AIO:O11	2.30	0.49
9:A:2042:A1AIO:O10	9:A:2042:A1AIO:O11	2.31	0.49
1:B:467:ILE:HD11	1:B:482:ALA:HB3	1.94	0.49
1:B:1220:THR:HG1	1:B:1229:ILE:C	2.19	0.49
1:B:1397:TRP:HZ3	1:B:1399:LYS:HE3	1.77	0.49
9:B:2033:A1AIO:O10	9:B:2033:A1AIO:O11	2.26	0.49
1:A:1675:ALA:O	1:A:1676:GLU:HG2	2.13	0.49
1:B:760:VAL:HG12	1:B:761:THR:HG23	1.95	0.49
1:B:1220:THR:OG1	1:B:1221:ALA:N	2.45	0.49
9:A:2056:A1AIO:O10	9:A:2056:A1AIO:O11	2.30	0.49
1:B:300:SER:OG	1:B:301:ALA:N	2.46	0.49
9:B:2004:A1AIO:O10	9:B:2004:A1AIO:O11	2.29	0.49
1:A:98:THR:HG23	1:A:109:LEU:HD13	1.94	0.49
1:B:1671:PHE:HD2	1:B:1696:ALA:HA	1.78	0.49
9:A:2048:A1AIO:O10	9:A:2048:A1AIO:O11	2.31	0.49
1:B:1456:THR:HG22	1:B:1459:MET:HE3	1.95	0.49
1:B:1897:HYP:HA	9:B:2025:A1AIO:O09	2.12	0.49
1:B:268:LYS:HG3	1:B:299:ALA:HB2	1.95	0.48
1:A:495:TYR:OH	1:A:530:GLU:OE2	2.31	0.48
1:B:111:SER:OG	1:B:112:ALA:N	2.44	0.48
1:A:540:ASP:OD1	1:A:540:ASP:N	2.41	0.48
1:B:1576:THR:HG22	1:B:1588:VAL:H	1.77	0.48
1:A:608:THR:HG22	1:A:609:PRO:HD2	1.96	0.48
1:A:1916:HYP:HA	9:A:2040:A1AIO:O09	2.13	0.48
1:B:803:ASP:N	1:B:803:ASP:OD1	2.46	0.48
1:B:1502:THR:HG23	1:B:1509:PRO:HG3	1.94	0.48
1:A:194:GLN:HB3	1:A:237:VAL:HG22	1.94	0.48
1:A:1198:GLY:HA2	1:A:1214:ARG:HA	1.95	0.48
9:A:2043:A1AIO:O10	9:A:2043:A1AIO:O11	2.31	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:1625:GLN:HG2	2:X:1626:HYP:HD22	1.96	0.48
1:B:657:PRO:HB2	1:B:721:ASN:HB3	1.94	0.48
1:B:1558:ASP:OD1	1:B:1558:ASP:N	2.39	0.48
1:A:77:THR:OG1	1:A:78:ALA:N	2.43	0.48
1:A:1052:CYS:HB2	1:A:1112:PHE:HZ	1.78	0.48
1:A:1580:ASN:OD1	1:A:1580:ASN:N	2.46	0.48
9:A:2032:A1AIO:O10	9:A:2032:A1AIO:O11	2.31	0.48
9:A:2050:A1AIO:O11	9:A:2050:A1AIO:O10	2.31	0.48
1:B:95:ARG:HH12	1:B:137:ALA:HB2	1.79	0.48
1:B:663:TRP:CZ3	1:B:665:GLY:HA2	2.49	0.48
1:A:458:GLY:O	1:A:461:LYS:NZ	2.46	0.48
1:A:539:ALA:HB3	1:A:588:LEU:HD13	1.96	0.48
1:A:791:GLN:OE1	1:A:837:ASN:ND2	2.44	0.48
1:B:1912:HYP:HG	4:e4:1:FUB:O4	2.14	0.48
1:A:1935:SER:OG	1:A:1936:ALA:N	2.47	0.48
9:A:2055:A1AIO:O10	9:A:2055:A1AIO:O11	2.32	0.48
9:A:2057:A1AIO:O10	9:A:2057:A1AIO:O11	2.32	0.48
1:B:365:ASP:OD2	1:B:369:ASN:ND2	2.46	0.48
1:B:1421:GLN:NE2	1:B:1438:LEU:O	2.47	0.48
1:A:603:ASP:N	1:A:603:ASP:OD1	2.47	0.48
1:A:938:MET:HE3	1:A:938:MET:HB2	1.74	0.48
1:A:1799:TYR:HE1	1:A:1831:ASP:HA	1.76	0.48
9:A:2045:A1AIO:O10	9:A:2045:A1AIO:O11	2.31	0.48
10:A:2059:GLA:H62	4:A5:1:FUB:O5	2.14	0.48
1:B:1132:ALA:O	1:B:1135:THR:OG1	2.32	0.48
9:A:2018:A1AIO:O10	9:A:2018:A1AIO:O11	2.32	0.48
1:B:1636:THR:HG22	1:B:1663:PRO:HA	1.95	0.48
1:A:352:THR:HA	1:A:470:ARG:HH22	1.79	0.47
1:A:1069:ILE:HA	1:A:1074:TYR:HE1	1.79	0.47
1:B:757:LEU:HD11	1:B:769:ALA:HB1	1.96	0.47
1:B:935:VAL:HG21	1:B:972:ALA:HB2	1.96	0.47
1:B:1097:ARG:HG3	1:B:1112:PHE:CE1	2.48	0.47
1:A:272:THR:O	1:A:293:THR:HA	2.14	0.47
1:A:1439:THR:HG22	1:A:1446:SER:HA	1.96	0.47
1:B:709:THR:HA	1:B:746:VAL:HG13	1.96	0.47
1:B:1058:GLN:HG3	1:B:1060:VAL:HG23	1.95	0.47
1:B:1861:SER:HB2	10:B:2060:GLA:C1	2.43	0.47
9:A:2051:A1AIO:O10	9:A:2051:A1AIO:O11	2.31	0.47
9:B:2019:A1AIO:O10	9:B:2019:A1AIO:O11	2.31	0.47
1:A:1496:GLN:HG3	1:A:1550:LEU:HD21	1.96	0.47
1:B:225:ASP:N	1:B:225:ASP:OD1	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1174:LEU:HD13	1:A:1178:PHE:HD2	1.80	0.47
9:A:2027:A1AIO:O10	9:A:2027:A1AIO:O11	2.33	0.47
1:B:1492:ASP:N	1:B:1492:ASP:OD1	2.46	0.47
1:A:888:ILE:O	1:A:944:THR:HA	2.14	0.47
1:A:1327:THR:OG1	1:A:1328:ASP:N	2.48	0.47
9:A:2017:A1AIO:O10	9:A:2017:A1AIO:O11	2.32	0.47
9:A:2049:A1AIO:O10	9:A:2049:A1AIO:O11	2.31	0.47
1:B:1127:PHE:CZ	1:B:1147:VAL:HB	2.50	0.47
1:B:1890:HYP:HG	9:B:2023:A1AIO:O07	2.15	0.47
1:A:593:GLN:NE2	1:A:602:TRP:O	2.34	0.47
1:A:662:PHE:HZ	1:A:704:PRO:HG3	1.78	0.47
1:A:1293:GLN:NE2	1:A:1295:ASN:H	2.13	0.47
1:A:1489:LEU:O	1:A:1542:LYS:NZ	2.47	0.47
1:B:548:LEU:HD21	1:B:600:PRO:HG3	1.96	0.47
1:B:622:LEU:HD21	1:B:718:LEU:HD11	1.96	0.47
1:B:659:LEU:HD11	1:B:681:ALA:HB1	1.97	0.47
1:B:1576:THR:HG22	1:B:1588:VAL:HG22	1.97	0.47
1:B:1733:CYS:SG	1:B:1737:THR:OG1	2.55	0.47
1:B:1831:ASP:OD1	1:B:1831:ASP:N	2.44	0.47
1:A:1906:HYP:HA	9:A:2033:A1AIO:O09	2.14	0.47
9:A:2001:A1AIO:O10	9:A:2001:A1AIO:O11	2.31	0.47
9:A:2004:A1AIO:O11	9:A:2004:A1AIO:O10	2.31	0.47
1:B:1443:SER:OG	1:B:1444:GLY:N	2.46	0.47
1:A:211:ILE:HD12	1:A:211:ILE:H	1.80	0.47
1:A:436:THR:O	1:A:446:ASN:ND2	2.48	0.47
9:A:2047:A1AIO:O10	9:A:2047:A1AIO:O11	2.31	0.47
1:B:280:VAL:HB	1:B:284:ASP:HB2	1.97	0.47
1:B:664:ASP:OD1	1:B:664:ASP:N	2.47	0.47
1:A:792:MET:HB2	1:A:836:VAL:HG22	1.97	0.47
1:A:547:ASP:OD2	1:A:550:ALA:N	2.45	0.46
1:A:734:LEU:HD21	1:A:738:TYR:HB2	1.97	0.46
1:A:828:THR:HB	1:A:832:TYR:CE1	2.47	0.46
9:A:2025:A1AIO:O11	9:A:2025:A1AIO:O10	2.33	0.46
1:B:1687:THR:HG22	1:B:1699:PRO:HA	1.97	0.46
9:B:2006:A1AIO:O10	9:B:2006:A1AIO:O11	2.33	0.46
1:B:1898:HYP:O	10:B:2067:GLA:O6	2.30	0.46
1:A:271:LEU:HG	1:A:295:VAL:HG12	1.96	0.46
1:A:360:ARG:HD2	1:A:362:ARG:NE	2.29	0.46
1:A:1061:ASN:HB3	1:A:1062:PRO:HD3	1.97	0.46
9:A:2010:A1AIO:O11	9:A:2010:A1AIO:O10	2.33	0.46
1:B:1495:GLN:HB3	1:B:1511:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:PHE:HB2	1:A:716:LEU:HD12	1.97	0.46
1:A:1342:ASP:OD1	1:A:1342:ASP:N	2.33	0.46
1:B:1224:ASP:OD1	1:B:1225:GLY:N	2.48	0.46
1:B:1443:SER:OG	1:B:1445:CYS:SG	2.70	0.46
4:e1:2:FUB:C4	4:d8:1:FUB:O5	2.64	0.46
1:A:622:LEU:HD21	1:A:641:TYR:HD2	1.81	0.46
1:A:1800:ASP:N	1:A:1829:THR:OG1	2.42	0.46
1:B:1051:ALA:HB1	1:B:1096:LEU:HD11	1.98	0.46
9:A:2023:A1AIO:O11	9:A:2023:A1AIO:O10	2.33	0.46
1:B:1220:THR:HG21	1:B:1228:CYS:HB3	1.98	0.46
1:B:1938:ASN:OD1	1:B:1938:ASN:N	2.49	0.46
1:A:687:LYS:HD3	1:A:687:LYS:HA	1.80	0.46
1:A:328:LEU:HD11	1:A:335:PRO:HD3	1.98	0.46
1:A:419:TRP:CE2	1:A:471:ASP:HB2	2.51	0.46
1:A:773:ILE:HD13	1:A:836:VAL:HG11	1.97	0.46
1:B:1878:HYP:HA	9:B:2015:A1AIO:O09	2.16	0.46
9:B:2029:A1AIO:O10	9:B:2029:A1AIO:O11	2.34	0.46
9:B:2035:A1AIO:O10	9:B:2035:A1AIO:O11	2.34	0.46
1:A:1857:HYP:HD22	10:A:2059:GLA:O6	2.16	0.46
1:B:1496:GLN:HA	1:B:1511:LEU:HB2	1.98	0.46
4:e1:1:FUB:O5	4:e3:2:FUB:C5	2.64	0.46
1:A:387:LEU:HD22	1:A:467:ILE:HG12	1.98	0.45
1:A:826:THR:HG21	1:A:856:ALA:HA	1.98	0.45
1:A:1293:GLN:HE21	1:A:1295:ASN:H	1.64	0.45
1:A:1805:ARG:NH2	2:X:1520:HYP:OD1	2.49	0.45
1:B:907:PHE:HE1	1:B:963:ALA:HB1	1.80	0.45
1:B:1218:GLY:HA2	1:B:1239:GLU:HA	1.98	0.45
1:B:1803:ALA:HB1	1:B:1808:VAL:HG21	1.96	0.45
1:A:663:TRP:CE3	1:A:670:ALA:HB2	2.51	0.45
9:B:2010:A1AIO:O10	9:B:2010:A1AIO:O11	2.34	0.45
1:A:1580:ASN:HD21	1:A:1609:VAL:HG21	1.81	0.45
9:A:2013:A1AIO:O10	9:A:2013:A1AIO:O11	2.34	0.45
1:B:1913:HYP:HA	1:B:1914:HYP:HD23	1.76	0.45
1:A:438:THR:N	1:A:446:ASN:HD21	2.15	0.45
1:A:1092:ALA:H	1:A:1095:GLN:HE21	1.62	0.45
1:B:1698:LYS:H	1:B:1698:LYS:HG2	1.55	0.45
1:A:1374:ALA:HA	1:A:1388:PRO:HD3	1.99	0.45
1:A:1476:ALA:C	1:A:1478:ALA:H	2.24	0.45
1:B:1912:HYP:OD1	4:e4:1:FUB:O2	2.34	0.45
1:A:1304:CYS:SG	1:A:1308:PHE:HB2	2.57	0.45
1:A:419:TRP:CZ2	1:A:471:ASP:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1755:TYR:CD2	1:A:1781:ALA:HB2	2.52	0.45
2:X:1594:HYP:HA	2:X:1595:HYP:HD22	1.77	0.45
1:B:1026:ILE:HD13	1:B:1026:ILE:HA	1.83	0.45
1:B:1068:ALA:HB3	1:B:1070:THR:HG22	1.98	0.45
2:X:1593:HYP:HA	2:X:1594:HYP:HD22	1.69	0.44
1:A:297:TYR:CE2	1:A:299:ALA:HB3	2.53	0.44
1:A:751:TYR:OH	1:A:786:LYS:NZ	2.47	0.44
1:A:1018:ASN:OD1	1:A:1021:THR:HG22	2.17	0.44
1:A:1913:HYP:HA	1:A:1914:HYP:HD23	1.68	0.44
1:B:1876:ASN:OD1	1:B:1876:ASN:N	2.49	0.44
1:A:966:MET:SD	1:A:967:VAL:N	2.90	0.44
1:A:1701:GLN:HB2	1:A:1702:PRO:HD2	1.99	0.44
1:B:307:GLN:HG3	1:B:322:LEU:HD13	1.99	0.44
1:B:466:ARG:HG2	1:B:483:SER:HB2	2.00	0.44
4:c7:1:FUB:O3	4:c7:2:FUB:O5	2.35	0.44
1:A:420:TRP:CE2	1:A:433:THR:HB	2.53	0.44
1:A:1687:THR:HG22	1:A:1699:PRO:HA	1.98	0.44
1:B:457:SER:OG	1:B:458:GLY:N	2.50	0.44
1:B:930:ASP:N	1:B:930:ASP:OD1	2.50	0.44
1:A:429:SER:OG	1:A:431:PRO:HD2	2.17	0.44
1:A:1514:TYR:HB2	1:A:1550:LEU:HD13	2.00	0.44
1:A:45:TYR:HE2	1:A:142:LEU:HD12	1.82	0.44
1:A:532:ILE:HG22	1:A:596:ILE:HB	1.99	0.44
1:A:792:MET:SD	1:A:795:ASN:HB3	2.58	0.44
1:B:92:GLU:OE2	1:B:93:THR:N	2.50	0.44
1:B:1799:TYR:HE2	1:B:1850:ARG:HB3	1.83	0.44
1:A:927:THR:HG23	1:A:929:PRO:HD2	2.00	0.44
1:A:1741:LYS:O	1:A:1744:SER:OG	2.36	0.44
1:B:228:TYR:CG	1:B:263:VAL:HG11	2.52	0.44
1:B:1261:ARG:H	1:B:1261:ARG:HG3	1.54	0.44
1:B:1409:PRO:O	1:B:1412:THR:OG1	2.34	0.44
1:A:1897:HYP:HA	9:A:2026:A1AIO:O09	2.17	0.44
9:A:2028:A1AIO:O10	9:A:2028:A1AIO:O11	2.36	0.44
1:B:586:ALA:HA	1:B:612:GLN:HE21	1.83	0.44
1:B:840:ASP:O	1:B:843:VAL:HG12	2.18	0.44
1:A:1558:ASP:OD1	1:A:1558:ASP:N	2.50	0.43
9:A:2022:A1AIO:O10	9:A:2022:A1AIO:O11	2.36	0.43
1:B:932:ASP:OD1	1:B:933:THR:N	2.51	0.43
1:A:153:ASP:OD2	1:A:155:THR:OG1	2.32	0.43
1:A:989:LEU:HD12	1:A:989:LEU:HA	1.84	0.43
1:A:1506:ASN:OD1	1:A:1506:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1581:LEU:HD23	1:A:1581:LEU:HA	1.74	0.43
2:X:1600:MET:HA	2:X:1601:HYP:HD23	1.82	0.43
1:B:364:TYR:HD2	1:B:368:ASN:HA	1.82	0.43
1:B:1476:ALA:C	1:B:1478:ALA:H	2.25	0.43
9:B:2025:A1AIO:O10	9:B:2025:A1AIO:O11	2.36	0.43
1:B:259:ASN:OD1	1:B:259:ASN:N	2.51	0.43
1:B:1728:GLU:HG3	1:B:1729:LEU:HD22	2.00	0.43
1:B:1856:HYP:OD1	4:a5:1:FUB:O4	2.35	0.43
1:A:79:VAL:HG21	1:A:131:LEU:HD23	2.00	0.43
1:A:819:PHE:HB3	1:A:821:ILE:HD11	1.99	0.43
1:A:185:ASN:HA	1:A:213:PRO:HA	2.01	0.43
1:B:154:SER:HA	1:B:251:ARG:HH22	1.83	0.43
1:B:387:LEU:HD13	1:B:467:ILE:HD13	2.00	0.43
9:B:2013:A1AIO:O10	9:B:2013:A1AIO:O11	2.37	0.43
1:A:874:THR:HG23	1:A:1000:VAL:H	1.84	0.43
1:A:1544:GLU:N	1:A:1544:GLU:OE1	2.51	0.43
1:A:1573:PRO:HG2	1:A:1588:VAL:HG11	1.99	0.43
2:X:1520:HYP:HA	2:X:1521:HYP:HD23	1.86	0.43
1:B:453:ASN:OD1	1:B:454:GLN:N	2.52	0.43
1:B:1885:HYP:HA	9:B:2019:A1AIO:O09	2.19	0.43
1:B:1927:HYP:HA	1:B:1928:HYP:HD22	1.84	0.43
1:A:1167:ASN:OD1	1:A:1167:ASN:N	2.51	0.43
1:B:43:ALA:N	1:B:74:ASP:OD2	2.52	0.43
1:B:122:ILE:HG13	1:B:153:ASP:HB3	2.01	0.43
1:B:1016:ASN:HD22	1:B:1019:PRO:HA	1.84	0.43
1:B:1515:THR:HB	1:B:1530:VAL:HB	2.01	0.43
1:B:1769:PRO:HG3	1:B:1788:PHE:CD2	2.52	0.43
4:f0:1:FUB:O5	4:f2:2:FUB:C4	2.66	0.43
1:A:664:ASP:HB2	1:A:706:TYR:CE1	2.54	0.43
1:A:719:ILE:HG22	1:A:720:GLN:H	1.83	0.43
1:B:51:LYS:HE3	1:B:51:LYS:HB3	1.69	0.43
1:B:165:VAL:HG22	1:B:365:ASP:HB2	1.99	0.43
1:B:354:THR:O	1:B:357:LYS:NZ	2.49	0.43
1:B:451:LEU:HD23	1:B:451:LEU:HA	1.77	0.43
1:A:81:PHE:CE1	1:A:96:THR:HB	2.54	0.43
1:A:417:GLN:NE2	1:A:418:VAL:O	2.52	0.43
1:B:1186:TYR:CE1	1:B:1215:LYS:HG2	2.54	0.43
1:B:1624:LEU:HD23	1:B:1624:LEU:HA	1.81	0.43
1:A:309:ARG:HD3	1:A:319:GLU:HG3	2.00	0.43
1:A:1412:THR:HG21	1:A:1440:GLU:HB2	2.01	0.43
1:A:1909:ARG:HD2	4:E4:2:FUB:O3	2.14	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1921:HYP:HG	9:A:2055:A1AIO:O07	2.19	0.42
1:B:152:GLU:HB3	1:B:250:LEU:O	2.19	0.42
1:B:1249:ALA:HB2	1:B:1296:ILE:HD13	2.00	0.42
1:B:666:LYS:NZ	1:B:711:THR:O	2.41	0.42
1:B:1011:THR:HG21	1:B:1150:LEU:HD11	2.01	0.42
1:B:1013:ILE:HG21	1:B:1022:PRO:HB3	2.01	0.42
1:B:1328:ASP:N	1:B:1328:ASP:OD1	2.51	0.42
4:e4:1:FUB:C5	4:e7:2:FUB:O3	2.67	0.42
1:A:662:PHE:HE1	1:A:714:PRO:HB3	1.84	0.42
1:A:1397:TRP:HZ3	1:A:1399:LYS:HE3	1.85	0.42
10:A:2061:GLA:O4	4:B3:1:FUB:O5	2.28	0.42
1:B:1573:PRO:HG2	1:B:1588:VAL:HG11	2.01	0.42
1:B:1864:HYP:OD1	9:B:2007:A1AIO:O09	2.37	0.42
1:B:624:ALA:HB3	1:B:741:PRO:HD2	2.01	0.42
1:B:1895:THR:OG1	1:B:1896:SER:N	2.52	0.42
1:A:1016:ASN:OD1	1:A:1016:ASN:N	2.53	0.42
9:A:2031:A1AIO:O11	9:A:2031:A1AIO:O10	2.37	0.42
1:B:265:ASP:OD2	1:B:268:LYS:HG2	2.18	0.42
1:B:1061:ASN:HB3	1:B:1062:PRO:HD3	2.01	0.42
1:B:1905:HYP:HD23	4:d8:1:FUB:C1	2.50	0.42
1:A:790:CYS:HB3	1:A:838:VAL:HG22	2.02	0.42
1:A:1289:LYS:HB2	1:A:1338:ALA:HB2	2.02	0.42
1:B:400:ASP:OD1	1:B:400:ASP:N	2.50	0.42
1:B:505:SER:OG	1:B:645:ARG:NH2	2.49	0.42
1:B:960:GLY:HA3	1:B:998:PRO:HB2	2.02	0.42
1:B:1139:ASN:ND2	1:B:1146:THR:H	2.18	0.42
1:B:1855:HYP:HA	9:B:2001:A1AIO:O09	2.18	0.42
1:B:198:ALA:HB3	1:B:201:VAL:HG23	2.02	0.42
1:B:962:THR:O	1:B:962:THR:OG1	2.37	0.42
1:A:1195:TYR:HB2	1:A:1212:GLN:OE1	2.20	0.42
1:A:1421:GLN:OE1	1:A:1438:LEU:N	2.49	0.42
1:B:999:MET:HE2	1:B:999:MET:HB2	1.94	0.42
1:A:259:ASN:OD1	1:A:259:ASN:N	2.52	0.42
1:A:917:SER:H	1:A:920:ALA:HB3	1.85	0.42
1:B:195:LEU:HD21	1:B:226:GLN:HB3	2.00	0.42
1:B:1800:ASP:OD1	1:B:1800:ASP:N	2.51	0.42
1:A:294:GLU:HG3	1:A:338:ALA:HB1	2.02	0.42
1:A:458:GLY:HA2	1:A:490:VAL:HG23	2.02	0.42
1:A:713:THR:HG22	1:A:743:PHE:HB3	2.02	0.42
1:A:1379:ASN:N	1:A:1379:ASN:OD1	2.53	0.42
1:B:458:GLY:HA2	1:B:490:VAL:HG23	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:639:TRP:NE1	1:A:706:TYR:OH	2.52	0.41
1:B:828:THR:OG1	1:B:832:TYR:OH	2.33	0.41
1:B:1893:HYP:CG	4:d0:1:FUB:C1	2.88	0.41
4:C2:1:FUB:O3	4:C2:2:FUB:O5	2.38	0.41
1:A:614:LEU:HD21	1:A:647:VAL:HG11	2.01	0.41
1:A:1487:ASN:OD1	1:A:1547:SER:OG	2.30	0.41
1:A:1694:LEU:HD23	1:A:1694:LEU:HA	1.91	0.41
1:B:893:ALA:HA	1:B:943:THR:HG22	2.01	0.41
1:B:1614:TRP:HA	3:a3:1:NAG:H83	2.01	0.41
1:A:80:PHE:CE1	1:A:135:ALA:HB2	2.55	0.41
1:A:360:ARG:HH11	1:A:362:ARG:HD2	1.84	0.41
1:A:514:TRP:O	1:A:576:SER:HA	2.20	0.41
9:A:2011:A1AIO:O10	9:A:2011:A1AIO:O11	2.36	0.41
1:B:306:LEU:HD13	1:B:371:ILE:HG21	2.02	0.41
1:B:1179:ARG:NH2	1:B:1181:THR:O	2.53	0.41
1:A:1862:HYP:HA	1:A:1863:HYP:HD23	1.88	0.41
1:A:1937:ILE:HD12	1:A:1937:ILE:H	1.84	0.41
2:X:1495:GLN:HG2	2:X:1496:HYP:HD22	2.01	0.41
2:X:1601:HYP:HA	2:X:1602:HYP:HD23	1.88	0.41
1:B:1862:HYP:HA	1:B:1863:HYP:HD23	1.88	0.41
1:B:1863:HYP:HA	1:B:1864:HYP:HD23	1.75	0.41
1:B:1865:HYP:HA	1:B:1866:HYP:HD23	1.93	0.41
1:A:532:ILE:HG13	1:A:563:ALA:HB3	2.02	0.41
1:B:536:PHE:O	1:B:579:ARG:NH1	2.54	0.41
1:B:1129:PHE:HD1	1:B:1139:ASN:HA	1.86	0.41
1:B:1688:TYR:O	1:B:1697:CYS:HB2	2.21	0.41
1:A:121:SER:O	1:A:125:LYS:NZ	2.45	0.41
1:A:1773:TYR:CE1	1:A:1795:TYR:HB2	2.56	0.41
1:B:570:ILE:HD12	1:B:570:ILE:H	1.85	0.41
1:B:1840:CYS:HB3	1:B:1843:LEU:HD22	2.02	0.41
1:A:1184:ASP:OD2	1:A:1242:ARG:NE	2.53	0.41
1:A:1617:SER:OG	1:A:1628:GLU:O	2.39	0.41
1:A:1712:ARG:NH2	1:B:1591:THR:OG1	2.54	0.41
9:A:2039:A1AIO:O11	9:A:2039:A1AIO:O10	2.39	0.41
1:B:717:GLN:OE1	1:B:718:LEU:N	2.48	0.41
1:A:1032:PHE:HB2	1:A:1110:CYS:SG	2.61	0.41
1:A:1178:PHE:HA	1:A:1210:VAL:HG13	2.02	0.41
1:A:1721:THR:HG22	1:A:1732:LYS:HA	2.03	0.41
1:B:1515:THR:OG1	1:B:1528:PRO:HB2	2.21	0.41
1:A:1826:GLU:HG2	1:A:1840:CYS:SG	2.60	0.41
2:X:1487:HYP:HA	2:X:1488:HYP:HD23	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:PRO:HB3	1:B:371:ILE:O	2.20	0.41
1:B:689:THR:OG1	1:B:690:SER:N	2.54	0.41
1:B:901:GLN:HB3	1:B:938:MET:HB3	2.02	0.41
1:B:1016:ASN:HB2	1:B:1018:ASN:O	2.20	0.41
1:B:1489:LEU:HD13	1:B:1539:MET:HE2	2.02	0.41
1:A:198:ALA:HB3	1:A:201:VAL:HG23	2.03	0.41
1:A:1101:MET:HE2	1:A:1101:MET:HB3	1.80	0.41
1:B:574:ILE:HD13	1:B:724:ALA:HB2	2.03	0.41
1:B:1840:CYS:HB3	1:B:1843:LEU:HD13	2.03	0.41
1:A:303:SER:HB2	1:A:334:PHE:HB3	2.03	0.40
1:B:412:LEU:HA	1:B:412:LEU:HD12	1.87	0.40
1:B:1219:GLY:HA2	1:B:1278:ALA:O	2.21	0.40
1:B:1916:HYP:HA	9:B:2034:A1AIO:O09	2.21	0.40
1:A:457:SER:OG	1:A:458:GLY:N	2.55	0.40
1:A:862:PRO:HG3	1:A:890:ARG:HH21	1.86	0.40
2:X:1453:HYP:HA	2:X:1454:HYP:HD22	1.67	0.40
1:B:794:ASP:HB3	1:B:835:THR:HG22	2.03	0.40
1:B:1178:PHE:HD2	1:B:1210:VAL:HG22	1.87	0.40
1:B:1250:GLY:HA2	1:B:1293:GLN:HB3	2.03	0.40
1:B:1894:HYP:HA	9:B:2024:A1AIO:O09	2.21	0.40
1:A:520:ARG:HD3	1:A:565:ILE:HD13	2.03	0.40
1:A:662:PHE:CE1	1:A:714:PRO:HB3	2.57	0.40
1:A:1490:MET:H	1:A:1490:MET:HG3	1.66	0.40
1:A:1607:GLN:HA	1:A:1608:PRO:HD3	1.94	0.40
1:A:1858:HYP:HB3	9:A:2050:A1AIO:O07	2.22	0.40
1:A:1911:HYP:HA	1:A:1912:HYP:HD23	1.85	0.40
1:A:1912:HYP:CG	4:E4:1:FUB:C1	2.97	0.40
2:X:1454:HYP:HA	2:X:1455:HYP:HD23	1.82	0.40
1:B:1055:TYR:CZ	1:B:1057:GLY:HA2	2.56	0.40
1:A:122:ILE:HG21	1:A:153:ASP:HB3	2.04	0.40
1:A:309:ARG:NH1	1:A:319:GLU:OE2	2.55	0.40
1:A:1016:ASN:HB2	1:A:1018:ASN:O	2.22	0.40
1:A:1018:ASN:HB2	1:A:1019:PRO:HD2	2.04	0.40
1:A:1055:TYR:CZ	1:A:1057:GLY:HA2	2.56	0.40
1:A:1560:LEU:HD23	1:A:1560:LEU:HA	1.93	0.40
9:B:2026:A1AIO:O10	9:B:2026:A1AIO:O11	2.38	0.40
1:A:481:LEU:HD23	1:A:481:LEU:HA	1.96	0.40
1:A:517:ARG:HB2	1:A:723:PHE:CE2	2.57	0.40
1:A:534:CYS:HA	1:A:594:CYS:HA	2.04	0.40
1:B:1189:ILE:HD13	1:B:1214:ARG:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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 ⓘ

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

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	ILE
1	A	162	GLN
1	A	294	GLU
1	A	303	SER
1	A	412	LEU
1	A	415	THR
1	A	473	VAL
1	A	501	VAL
1	A	529	THR
1	A	547	ASP
1	A	548	LEU
1	A	565	ILE
1	A	601	LEU
1	A	608	THR
1	A	622	LEU
1	A	662	PHE
1	A	680	LEU
1	A	733	PHE
1	A	739	THR
1	A	790	CYS
1	A	833	PHE
1	A	1059	ASN
1	A	1128	VAL
1	A	1203	VAL
1	A	1275	THR
1	A	1279	MET
1	A	1342	ASP
1	A	1379	ASN
1	A	1380	LEU
1	A	1434	VAL
1	A	1493	ARG
1	A	1534	ASP
1	A	1557	VAL
1	A	1563	GLN
1	A	1598	THR
1	A	1621	LYS
1	A	1638	VAL
1	A	1676	GLU
1	A	1677	THR
1	A	1715	LYS
1	A	1723	SER
1	A	1741	LYS
1	A	1748	THR

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Mol	Chain	Res	Type
1	A	1805	ARG
1	A	1843	LEU
1	A	1943	VAL
1	A	1945	GLN
2	X	1492	THR
2	X	1561	THR
2	X	1624	ASP
1	B	211	ILE
1	B	214	THR
1	B	263	VAL
1	B	281	THR
1	B	386	THR
1	B	403	ILE
1	B	415	THR
1	B	430	SER
1	B	473	VAL
1	B	528	VAL
1	B	660	CYS
1	B	745	THR
1	B	913	THR
1	B	967	VAL
1	B	1011	THR
1	B	1070	THR
1	B	1081	THR
1	B	1134	SER
1	B	1147	VAL
1	B	1162	ILE
1	B	1170	GLN
1	B	1277	LEU
1	B	1339	THR
1	B	1367	LEU
1	B	1441	LEU
1	B	1459	MET
1	B	1534	ASP
1	B	1580	ASN
1	B	1591	THR
1	B	1629	ILE
1	B	1654	THR
1	B	1677	THR
1	B	1800	ASP
1	B	1808	VAL
1	B	1840	CYS

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Mol	Chain	Res	Type
1	B	1852	GLU
1	B	1853	GLN
1	B	1854	SER
1	B	1859	SER
1	B	1861	SER
1	B	1876	ASN
1	B	1895	THR
1	B	1938	ASN
1	B	1945	GLN
1	B	1946	ASN
1	B	1948	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	720	GLN
1	A	1293	GLN
1	A	1946	ASN
1	B	333	ASN
1	B	369	ASN
1	B	556	ASN
1	B	612	GLN
1	B	642	ASN
1	B	1661	GLN
1	B	1853	GLN

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%)
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%)

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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.

All (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
1	A	1863	HYP	CB-CG-CD	-4.11	98.58	103.16
1	B	1868	HYP	CB-CG-CD	-4.07	98.62	103.16
1	B	1877	HYP	CG-CB-CA	-4.07	99.05	103.75
1	A	1923	HYP	CB-CG-CD	-4.06	98.63	103.16
1	B	1932	HYP	CB-CG-CD	-3.99	98.71	103.16
1	A	1918	HYP	CB-CG-CD	-3.90	98.82	103.16
1	B	1866	HYP	CB-CG-CD	-3.86	98.86	103.16
1	A	1922	HYP	CB-CG-CD	-3.81	98.92	103.16
1	B	1910	HYP	CB-CG-CD	-3.77	98.96	103.16
1	A	1927	HYP	CB-CG-CD	-3.76	98.96	103.16
1	A	1864	HYP	CB-CG-CD	-3.73	99.00	103.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1920	HYP	CB-CG-CD	-3.73	99.00	103.16
1	B	1908	HYP	CB-CG-CD	-3.71	99.02	103.16
1	B	1863	HYP	CB-CG-CD	-3.70	99.03	103.16
1	B	1885	HYP	CB-CG-CD	-3.67	99.07	103.16
2	X	1597	HYP	CB-CG-CD	-3.64	99.10	103.16
1	A	1910	HYP	CB-CG-CD	-3.61	99.13	103.16
1	A	1928	HYP	CB-CG-CD	-3.58	99.17	103.16
2	X	1548	HYP	CB-CG-CD	-3.57	99.18	103.16
2	X	1596	HYP	CB-CG-CD	-3.56	99.19	103.16
1	A	1894	HYP	CG-CB-CA	-3.55	99.65	103.75
1	A	1903	HYP	CB-CG-CD	-3.51	99.24	103.16
1	B	1870	HYP	CB-CG-CD	-3.51	99.25	103.16
2	X	1610	HYP	CB-CG-CD	-3.51	99.25	103.16
2	X	1601	HYP	CB-CG-CD	-3.49	99.26	103.16
1	A	1908	HYP	CB-CG-CD	-3.49	99.27	103.16
1	B	1885	HYP	CG-CB-CA	-3.48	99.73	103.75
1	A	1868	HYP	CB-CG-CD	-3.45	99.31	103.16
2	X	1549	HYP	CB-CG-CD	-3.45	99.31	103.16
1	B	1912	HYP	CB-CG-CD	-3.45	99.32	103.16
2	X	1623	HYP	CB-CG-CD	-3.44	99.33	103.16
2	X	1615	HYP	CB-CG-CD	-3.43	99.33	103.16
2	X	1620	HYP	CB-CG-CD	-3.43	99.34	103.16
1	A	1860	HYP	CB-CG-CD	-3.43	99.34	103.16
2	X	1546	HYP	CB-CG-CD	-3.42	99.35	103.16
1	A	1913	HYP	CB-CG-CD	-3.41	99.36	103.16
1	A	1864	HYP	CG-CB-CA	-3.41	99.81	103.75
2	X	1556	HYP	CB-CG-CD	-3.40	99.37	103.16
2	X	1611	HYP	CB-CG-CD	-3.39	99.39	103.16
1	B	1855	HYP	CG-CB-CA	3.38	107.66	103.75
1	B	1894	HYP	CB-CG-CD	-3.37	99.40	103.16
2	X	1562	HYP	CB-CG-CD	-3.37	99.41	103.16
2	X	1551	HYP	CB-CG-CD	-3.36	99.42	103.16
2	X	1490	HYP	CB-CG-CD	-3.36	99.42	103.16
2	X	1547	HYP	CB-CG-CD	-3.35	99.43	103.16
1	A	1890	HYP	CB-CG-CD	-3.33	99.45	103.16
1	A	1870	HYP	CB-CG-CD	-3.33	99.45	103.16
1	A	1878	HYP	CB-CG-CD	-3.32	99.46	103.16
2	X	1526	HYP	CB-CG-CD	-3.31	99.47	103.16
1	A	1885	HYP	CG-CB-CA	-3.30	99.93	103.75
1	B	1927	HYP	CB-CG-CD	-3.30	99.48	103.16
2	X	1593	HYP	CB-CG-CD	-3.30	99.49	103.16
2	X	1488	HYP	CB-CG-CD	-3.29	99.49	103.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1856	HYP	CG-CB-CA	-3.28	99.96	103.75
2	X	1481	HYP	CB-CG-CD	-3.28	99.51	103.16
2	X	1612	HYP	CB-CG-CD	-3.27	99.51	103.16
1	B	1864	HYP	CB-CG-CD	-3.25	99.54	103.16
1	B	1903	HYP	CB-CG-CD	-3.24	99.55	103.16
1	A	1880	HYP	CB-CG-CD	-3.24	99.55	103.16
1	B	1923	HYP	CB-CG-CD	-3.23	99.56	103.16
2	X	1592	HYP	CB-CG-CD	-3.22	99.57	103.16
2	X	1619	HYP	CB-CG-CD	-3.21	99.58	103.16
2	X	1530	HYP	CB-CG-CD	-3.21	99.59	103.16
2	X	1550	HYP	CB-CG-CD	-3.20	99.59	103.16
1	B	1931	HYP	CG-CB-CA	3.20	107.45	103.75
1	B	1882	HYP	CG-CB-CA	3.19	107.44	103.75
2	X	1590	HYP	CB-CG-CD	-3.19	99.61	103.16
1	A	1894	HYP	CB-CG-CD	-3.18	99.61	103.16
1	B	1887	HYP	CG-CB-CA	3.17	107.41	103.75
1	A	1873	HYP	CB-CG-CD	-3.16	99.63	103.16
2	X	1489	HYP	CB-CG-CD	-3.16	99.63	103.16
2	X	1480	HYP	CB-CG-CD	-3.16	99.63	103.16
2	X	1613	HYP	CB-CG-CD	-3.15	99.64	103.16
2	X	1531	HYP	CB-CG-CD	-3.15	99.65	103.16
1	A	1906	HYP	CG-CB-CA	3.14	107.39	103.75
2	X	1468	HYP	CB-CG-CD	-3.13	99.67	103.16
1	A	1877	HYP	CB-CG-CD	-3.13	99.67	103.16
2	X	1462	HYP	CG-CB-CA	3.13	107.38	103.75
2	X	1522	HYP	CG-CB-CA	3.13	107.37	103.75
1	B	1899	HYP	CB-CG-CD	-3.12	99.68	103.16
1	B	1930	HYP	CG-CB-CA	3.12	107.36	103.75
2	X	1559	HYP	CB-CG-CD	-3.12	99.68	103.16
2	X	1591	HYP	CG-CB-CA	3.11	107.35	103.75
1	A	1898	HYP	CG-CB-CA	3.10	107.34	103.75
1	B	1888	HYP	CB-CG-CD	-3.08	99.72	103.16
1	A	1902	HYP	CG-CB-CA	3.06	107.29	103.75
2	X	1493	HYP	CB-CG-CD	-3.05	99.76	103.16
2	X	1523	HYP	CG-CB-CA	3.05	107.28	103.75
1	A	1932	HYP	CB-CG-CD	-3.04	99.77	103.16
1	A	1907	HYP	CG-CB-CA	3.04	107.27	103.75
1	A	1855	HYP	CG-CB-CA	3.04	107.26	103.75
1	A	1866	HYP	CG-CB-CA	3.03	107.26	103.75
1	B	1913	HYP	CB-CG-CD	-3.03	99.78	103.16
1	B	1875	HYP	CB-CG-CD	-3.03	99.79	103.16
2	X	1589	HYP	CG-CB-CA	3.02	107.24	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1857	HYP	CG-CB-CA	3.02	107.24	103.75
2	X	1499	HYP	CG-CB-CA	3.01	107.24	103.75
2	X	1528	HYP	CG-CB-CA	3.01	107.24	103.75
2	X	1486	HYP	CG-CB-CA	3.01	107.23	103.75
1	B	1862	HYP	CG-CB-CA	3.00	107.22	103.75
2	X	1465	HYP	CG-CB-CA	3.00	107.22	103.75
1	B	1929	HYP	CG-CB-CA	2.99	107.21	103.75
1	B	1911	HYP	CB-CG-CD	-2.99	99.83	103.16
2	X	1588	HYP	CG-CB-CA	2.99	107.21	103.75
1	B	1893	HYP	CG-CB-CA	2.98	107.20	103.75
2	X	1553	HYP	CG-CB-CA	2.98	107.19	103.75
2	X	1458	HYP	CG-CB-CA	2.98	107.19	103.75
1	B	1901	HYP	CG-CB-CA	2.98	107.19	103.75
1	A	1916	HYP	CG-CB-CA	2.97	107.19	103.75
1	B	1907	HYP	CG-CB-CA	2.97	107.19	103.75
2	X	1464	HYP	CG-CB-CA	2.97	107.19	103.75
2	X	1483	HYP	CB-CG-CD	-2.96	99.85	103.16
2	X	1455	HYP	CG-CB-CA	2.96	107.17	103.75
2	X	1527	HYP	CG-CB-CA	2.96	107.17	103.75
2	X	1457	HYP	CB-CG-CD	-2.96	99.86	103.16
2	X	1602	HYP	CG-CB-CA	2.96	107.17	103.75
2	X	1461	HYP	CG-CB-CA	2.96	107.17	103.75
1	A	1901	HYP	CG-CB-CA	2.95	107.17	103.75
2	X	1460	HYP	CG-CB-CA	2.95	107.16	103.75
1	B	1867	HYP	CB-CG-CD	-2.94	99.88	103.16
1	A	1857	HYP	CG-CB-CA	2.94	107.15	103.75
2	X	1554	HYP	CG-CB-CA	2.94	107.15	103.75
1	B	1922	HYP	CB-CG-CD	-2.94	99.89	103.16
2	X	1453	HYP	CB-CG-CD	-2.93	99.90	103.16
2	X	1521	HYP	CB-CG-CD	-2.92	99.90	103.16
1	B	1872	HYP	CG-CB-CA	2.92	107.13	103.75
1	A	1897	HYP	CB-CG-CD	-2.92	99.91	103.16
2	X	1482	HYP	CB-CG-CD	-2.91	99.92	103.16
2	X	1456	HYP	CG-CB-CA	2.90	107.11	103.75
1	B	1864	HYP	CG-CB-CA	-2.90	100.41	103.75
1	B	1902	HYP	CB-CG-CD	-2.89	99.94	103.16
1	A	1905	HYP	CG-CB-CA	2.89	107.09	103.75
2	X	1487	HYP	CG-CB-CA	2.89	107.09	103.75
2	X	1587	HYP	CG-CB-CA	2.88	107.08	103.75
2	X	1459	HYP	CG-CB-CA	2.87	107.07	103.75
1	A	1867	HYP	CB-CG-CD	-2.87	99.96	103.16
1	A	1931	HYP	CG-CB-CA	2.86	107.06	103.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1882	HYP	CG-CB-CA	2.86	107.05	103.75
1	B	1883	HYP	CB-CG-CD	-2.84	99.99	103.16
1	B	1880	HYP	CB-CG-CD	-2.84	100.00	103.16
2	X	1617	HYP	CG-CB-CA	2.82	107.01	103.75
1	A	1893	HYP	CG-CB-CA	2.80	107.00	103.75
1	B	1918	HYP	CB-CG-CD	-2.80	100.03	103.16
1	A	1877	HYP	CG-CB-CA	-2.80	100.52	103.75
2	X	1595	HYP	CG-CB-CA	2.80	106.99	103.75
2	X	1552	HYP	CG-CB-CA	2.80	106.99	103.75
2	X	1524	HYP	CG-CB-CA	2.79	106.98	103.75
2	X	1616	HYP	CG-CB-CA	2.79	106.98	103.75
1	B	1855	HYP	OD1-CG-CD	2.79	116.00	110.30
2	X	1525	HYP	CG-CB-CA	2.79	106.97	103.75
2	X	1485	HYP	CG-CB-CA	2.79	106.97	103.75
2	X	1555	HYP	CB-CG-CD	-2.78	100.06	103.16
1	B	1878	HYP	CB-CG-CD	-2.77	100.07	103.16
1	B	1897	HYP	CG-CB-CA	2.76	106.95	103.75
1	B	1917	HYP	CB-CG-CD	-2.76	100.08	103.16
1	A	1863	HYP	CG-CB-CA	-2.75	100.57	103.75
1	A	1875	HYP	CB-CG-CD	-2.75	100.09	103.16
1	A	1899	HYP	CB-CG-CD	-2.75	100.09	103.16
2	X	1598	HYP	CG-CB-CA	-2.74	100.58	103.75
1	A	1865	HYP	CB-CG-CD	-2.74	100.11	103.16
1	B	1906	HYP	CB-CG-CD	-2.74	100.11	103.16
2	X	1586	HYP	CB-CG-CD	-2.74	100.11	103.16
2	X	1520	HYP	CB-CG-CD	-2.74	100.11	103.16
1	A	1887	HYP	CG-CB-CA	2.73	106.91	103.75
2	X	1618	HYP	CB-CG-CD	-2.72	100.13	103.16
2	X	1626	HYP	CG-CB-CA	-2.71	100.62	103.75
1	B	1920	HYP	CB-CG-CD	-2.70	100.15	103.16
2	X	1529	HYP	CG-CB-CA	2.69	106.87	103.75
1	A	1888	HYP	CB-CG-CD	-2.69	100.16	103.16
2	X	1598	HYP	CB-CG-CD	-2.69	100.16	103.16
1	A	1929	HYP	CB-CG-CD	-2.69	100.17	103.16
2	X	1484	HYP	CG-CB-CA	2.68	106.85	103.75
2	X	1614	HYP	CG-CB-CA	2.66	106.83	103.75
2	X	1463	HYP	CG-CB-CA	2.65	106.82	103.75
2	X	1532	HYP	CB-CG-CD	-2.65	100.21	103.16
1	A	1856	HYP	CG-CB-CA	-2.63	100.71	103.75
1	A	1915	HYP	CG-CB-CA	2.62	106.78	103.75
1	A	1887	HYP	CB-CG-CD	-2.62	100.24	103.16
2	X	1529	HYP	CB-CG-CD	-2.61	100.25	103.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1916	HYP	CB-CG-CD	-2.58	100.28	103.16
1	B	1916	HYP	CG-CB-CA	2.58	106.73	103.75
2	X	1618	HYP	CG-CB-CA	2.56	106.72	103.75
1	B	1858	HYP	CB-CG-CD	2.56	106.00	103.16
1	A	1883	HYP	CB-CG-CD	-2.53	100.34	103.16
2	X	1484	HYP	CB-CG-CD	-2.52	100.35	103.16
1	B	1898	HYP	CG-CB-CA	2.52	106.66	103.75
2	X	1463	HYP	CB-CG-CD	-2.51	100.36	103.16
1	A	1862	HYP	CB-CG-CD	-2.51	100.36	103.16
1	A	1929	HYP	CG-CB-CA	2.50	106.64	103.75
1	B	1906	HYP	CG-CB-CA	2.49	106.63	103.75
1	B	1920	HYP	CG-CB-CA	2.49	106.63	103.75
1	A	1865	HYP	CG-CB-CA	2.47	106.61	103.75
2	X	1521	HYP	CG-CB-CA	2.47	106.61	103.75
1	B	1922	HYP	CG-CB-CA	2.46	106.60	103.75
2	X	1614	HYP	CB-CG-CD	-2.46	100.41	103.16
1	A	1897	HYP	CG-CB-CA	2.46	106.59	103.75
1	B	1905	HYP	CB-CG-CD	-2.45	100.42	103.16
2	X	1552	HYP	CB-CG-CD	-2.44	100.44	103.16
2	X	1525	HYP	CB-CG-CD	-2.43	100.45	103.16
2	X	1555	HYP	CG-CB-CA	2.43	106.56	103.75
1	B	1898	HYP	CB-CG-CD	-2.42	100.46	103.16
2	X	1524	HYP	CB-CG-CD	-2.42	100.46	103.16
1	A	1914	HYP	CG-CB-CA	-2.41	100.97	103.75
2	X	1482	HYP	CG-CB-CA	2.40	106.53	103.75
1	A	1911	HYP	CG-CB-CA	2.40	106.53	103.75
2	X	1496	HYP	CB-CG-CD	-2.39	100.49	103.16
1	A	1917	HYP	CB-CG-CD	-2.39	100.50	103.16
1	B	1877	HYP	CB-CG-CD	-2.37	100.52	103.16
1	A	1917	HYP	CG-CB-CA	2.37	106.49	103.75
1	B	1915	HYP	CB-CG-CD	-2.36	100.53	103.16
1	A	1862	HYP	CG-CB-CA	2.36	106.48	103.75
1	B	1856	HYP	O-C-CA	-2.36	118.70	124.77
1	B	1867	HYP	CG-CB-CA	2.34	106.46	103.75
1	A	1920	HYP	O-C-CA	-2.34	118.75	124.77
1	A	1888	HYP	CG-CB-CA	2.34	106.45	103.75
1	B	1911	HYP	CG-CB-CA	2.34	106.45	103.75
2	X	1586	HYP	CG-CB-CA	2.33	106.45	103.75
1	A	1911	HYP	CB-CG-CD	-2.33	100.56	103.16
1	A	1875	HYP	CG-CB-CA	2.32	106.44	103.75
1	B	1912	HYP	CG-CB-CA	-2.32	101.07	103.75
1	B	1902	HYP	O-C-CA	-2.31	118.83	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1910	HYP	CG-CB-CA	2.31	106.42	103.75
2	X	1485	HYP	CB-CG-CD	-2.31	100.58	103.16
1	B	1921	HYP	CG-CB-CA	-2.30	101.09	103.75
2	X	1469	HYP	O-C-CA	-2.30	118.85	124.77
1	A	1856	HYP	CB-CG-CD	-2.28	100.61	103.16
1	A	1897	HYP	O-C-CA	-2.28	118.91	124.77
1	A	1898	HYP	O-C-CA	-2.28	118.92	124.77
1	A	1872	HYP	O-C-CA	-2.27	118.92	124.77
1	B	1867	HYP	O-C-CA	-2.27	118.93	124.77
1	B	1864	HYP	O-C-CA	-2.27	118.93	124.77
1	B	1887	HYP	O-C-CA	-2.27	118.94	124.77
2	X	1594	HYP	CG-CB-CA	2.27	106.38	103.75
2	X	1499	HYP	O-C-CA	-2.27	118.94	124.77
2	X	1597	HYP	O-C-CA	-2.27	118.94	124.77
2	X	1617	HYP	CB-CG-CD	-2.26	100.64	103.16
2	X	1483	HYP	CG-CB-CA	2.26	106.36	103.75
1	A	1887	HYP	O-C-CA	-2.25	118.99	124.77
1	A	1867	HYP	CG-CB-CA	2.25	106.35	103.75
2	X	1468	HYP	CG-CB-CA	2.25	106.35	103.75
1	A	1902	HYP	O-C-CA	-2.24	119.02	124.77
1	B	1914	HYP	CG-CB-CA	-2.23	101.18	103.75
2	X	1587	HYP	CB-CG-CD	-2.23	100.67	103.16
1	B	1898	HYP	O-C-CA	-2.23	119.04	124.77
1	A	1917	HYP	O-C-CA	-2.22	119.05	124.77
2	X	1616	HYP	CB-CG-CD	-2.22	100.68	103.16
2	X	1590	HYP	CG-CB-CA	2.22	106.32	103.75
1	B	1902	HYP	CG-CB-CA	2.22	106.32	103.75
2	X	1459	HYP	CB-CG-CD	-2.22	100.68	103.16
1	B	1928	HYP	O-C-CA	-2.22	119.07	124.77
1	A	1893	HYP	O-C-CA	-2.20	119.10	124.77
2	X	1531	HYP	CG-CB-CA	2.20	106.30	103.75
1	B	1893	HYP	O-C-CA	-2.20	119.11	124.77
1	B	1930	HYP	O-C-CA	-2.20	119.12	124.77
1	A	1901	HYP	O-C-CA	-2.19	119.13	124.77
1	B	1907	HYP	O-C-CA	-2.19	119.13	124.77
2	X	1456	HYP	CB-CG-CD	-2.19	100.71	103.16
1	A	1882	HYP	O-C-CA	-2.19	119.14	124.77
1	B	1921	HYP	O-C-CA	-2.19	119.14	124.77
1	B	1866	HYP	O-C-CA	-2.19	119.14	124.77
1	B	1897	HYP	O-C-CA	-2.19	119.14	124.77
1	A	1907	HYP	O-C-CA	-2.19	119.14	124.77
1	A	1931	HYP	O-C-CA	-2.18	119.16	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1532	HYP	CG-CB-CA	-2.18	101.23	103.75
2	X	1457	HYP	CG-CB-CA	2.18	106.27	103.75
1	A	1856	HYP	O-C-CA	-2.17	119.18	124.77
2	X	1520	HYP	CG-CB-CA	2.17	106.26	103.75
1	A	1930	HYP	O-C-CA	-2.17	119.20	124.77
2	X	1453	HYP	O-C-CA	-2.17	119.20	124.77
1	B	1892	HYP	O-C-CA	-2.17	119.20	124.77
1	B	1855	HYP	O-C-CA	-2.15	119.24	124.77
1	B	1882	HYP	O-C-CA	-2.15	119.25	124.77
1	A	1905	HYP	O-C-CA	-2.14	119.26	124.77
1	B	1872	HYP	O-C-CA	-2.14	119.27	124.77
2	X	1526	HYP	CG-CB-CA	2.13	106.22	103.75
2	X	1454	HYP	CG-CB-CA	2.13	106.22	103.75
2	X	1489	HYP	O-C-CA	-2.12	119.32	124.77
1	B	1931	HYP	O-C-CA	-2.12	119.32	124.77
1	A	1858	HYP	CB-CG-CD	-2.12	100.80	103.16
1	A	1892	HYP	O-C-CA	-2.11	119.35	124.77
1	B	1932	HYP	O-C-CA	-2.10	119.36	124.77
2	X	1554	HYP	O-C-CA	-2.10	119.38	124.77
1	A	1882	HYP	CB-CG-CD	-2.09	100.82	103.16
1	B	1928	HYP	CB-CG-CD	2.09	105.48	103.16
1	A	1915	HYP	O-C-CA	-2.09	119.40	124.77
1	A	1892	HYP	CB-CG-CD	-2.09	100.83	103.16
1	B	1888	HYP	CG-CB-CA	2.09	106.17	103.75
1	A	1878	HYP	CG-CB-CA	2.08	106.16	103.75
1	A	1932	HYP	O-C-CA	-2.08	119.43	124.77
2	X	1469	HYP	CB-CG-CD	-2.08	100.84	103.16
1	A	1867	HYP	O-C-CA	-2.08	119.43	124.77
2	X	1613	HYP	CG-CB-CA	2.07	106.15	103.75
2	X	1555	HYP	O-C-CA	-2.07	119.45	124.77
1	A	1911	HYP	O-C-CA	-2.07	119.45	124.77
1	B	1901	HYP	O-C-CA	-2.07	119.45	124.77
2	X	1487	HYP	CB-CG-CD	-2.07	100.85	103.16
1	A	1857	HYP	O-C-CA	-2.07	119.46	124.77
2	X	1461	HYP	CB-CG-CD	-2.06	100.86	103.16
1	A	1915	HYP	CB-CG-CD	-2.06	100.87	103.16
1	B	1905	HYP	O-C-CA	-2.05	119.49	124.77
1	B	1872	HYP	CB-CG-CD	-2.05	100.88	103.16
1	A	1928	HYP	O-C-CA	-2.05	119.50	124.77
1	A	1906	HYP	O-C-CA	-2.05	119.51	124.77
1	B	1865	HYP	CB-CG-CD	2.04	105.43	103.16
1	B	1917	HYP	O-C-CA	-2.04	119.52	124.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1929	HYP	O-C-CA	-2.04	119.52	124.77
2	X	1524	HYP	O-C-CA	-2.04	119.52	124.77
2	X	1553	HYP	O-C-CA	-2.04	119.52	124.77
1	B	1929	HYP	O-C-CA	-2.04	119.53	124.77
1	B	1915	HYP	CG-CB-CA	2.04	106.11	103.75
1	A	1916	HYP	O-C-CA	-2.04	119.53	124.77
1	A	1865	HYP	O-C-CA	-2.03	119.55	124.77
1	A	1877	HYP	O-C-CA	-2.03	119.55	124.77
2	X	1486	HYP	O-C-CA	-2.03	119.56	124.77
2	X	1530	HYP	O-C-CA	-2.03	119.56	124.77
2	X	1460	HYP	O-C-CA	-2.03	119.56	124.77
1	A	1922	HYP	O-C-CA	-2.03	119.56	124.77
2	X	1554	HYP	CB-CG-CD	-2.02	100.91	103.16
1	B	1878	HYP	O-C-CA	-2.02	119.57	124.77
1	B	1922	HYP	O-C-CA	-2.02	119.58	124.77
2	X	1618	HYP	O-C-CA	-2.02	119.58	124.77
2	X	1592	HYP	O-C-CA	-2.02	119.58	124.77
2	X	1619	HYP	O-C-CA	-2.02	119.58	124.77
2	X	1465	HYP	O-C-CA	-2.02	119.59	124.77
2	X	1522	HYP	O-C-CA	-2.02	119.59	124.77
2	X	1457	HYP	O-C-CA	-2.01	119.59	124.77
2	X	1488	HYP	O-C-CA	-2.01	119.60	124.77
2	X	1484	HYP	O-C-CA	-2.01	119.61	124.77
2	X	1550	HYP	O-C-CA	-2.01	119.61	124.77
2	X	1590	HYP	O-C-CA	-2.01	119.61	124.77

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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1912	HYP	2	0
1	B	1928	HYP	1	0
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

All (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
4	c0	1	FUB	O4-C1	-2.45	1.38	1.43
4	f3	2	FUB	C2-C3	-2.40	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b3	2	FUB	O4-C1	-2.39	1.38	1.43
4	d7	1	FUB	C2-C3	-2.37	1.49	1.53
4	c3	1	FUB	O4-C1	-2.36	1.38	1.43
4	e5	1	FUB	C2-C3	-2.35	1.49	1.53
4	d9	2	FUB	C2-C3	-2.34	1.49	1.53
4	c8	2	FUB	C2-C3	-2.34	1.49	1.53
4	c9	2	FUB	O4-C1	-2.33	1.38	1.43
4	e8	2	FUB	C2-C3	-2.33	1.49	1.53
4	b4	2	FUB	C2-C3	-2.33	1.49	1.53
4	d0	2	FUB	C2-C3	-2.32	1.49	1.53
4	c3	2	FUB	C2-C3	-2.32	1.49	1.53
4	b0	1	FUB	C2-C3	-2.31	1.49	1.53
4	e5	1	FUB	O4-C1	-2.28	1.39	1.43
5	f6	4	FUB	O4-C1	-2.28	1.39	1.43
4	d7	1	FUB	O4-C1	-2.27	1.39	1.43
4	c6	1	FUB	C2-C3	-2.27	1.49	1.53
5	b6	2	FUB	C2-C3	-2.26	1.49	1.53
4	e4	1	FUB	O4-C1	-2.26	1.39	1.43
4	f8	2	FUB	O4-C1	-2.25	1.39	1.43
7	a4	2	FUB	O4-C1	-2.25	1.39	1.43
4	c2	1	FUB	C2-C3	-2.23	1.49	1.53
4	c1	1	FUB	C2-C3	-2.22	1.50	1.53
4	e6	2	FUB	C2-C3	-2.22	1.50	1.53
4	b4	1	FUB	C2-C3	-2.21	1.50	1.53
4	e1	2	FUB	C2-C3	-2.21	1.50	1.53
5	a6	1	FUB	O4-C1	-2.21	1.39	1.43
4	d5	2	FUB	O4-C1	-2.21	1.39	1.43
4	e3	2	FUB	C2-C3	-2.19	1.50	1.53
5	b6	1	FUB	O4-C1	-2.18	1.39	1.43
4	d0	2	FUB	C1-C2	2.18	1.55	1.51
4	d8	2	FUB	C2-C3	-2.17	1.50	1.53
4	d5	2	FUB	C2-C3	-2.17	1.50	1.53
4	e7	2	FUB	C2-C3	-2.17	1.50	1.53
4	e0	2	FUB	O4-C1	-2.16	1.39	1.43
4	f0	2	FUB	C2-C3	-2.16	1.50	1.53
4	f2	2	FUB	C2-C3	-2.16	1.50	1.53
4	b1	1	FUB	C2-C3	-2.16	1.50	1.53
4	b0	2	FUB	C2-C3	-2.15	1.50	1.53
4	c8	2	FUB	C1-C2	2.14	1.55	1.51
4	c6	1	FUB	O4-C1	-2.12	1.39	1.43
4	e4	2	FUB	C2-C3	-2.12	1.50	1.53
4	a5	2	FUB	C2-C3	-2.12	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	c7	1	FUB	C2-C3	-2.11	1.50	1.53
4	b7	2	FUB	C2-C3	-2.10	1.50	1.53
5	a6	4	FUB	C1-C2	2.10	1.55	1.51
4	c1	1	FUB	O4-C1	-2.09	1.39	1.43
4	d4	2	FUB	C2-C3	-2.09	1.50	1.53
4	d6	2	FUB	C2-C3	-2.08	1.50	1.53
4	f5	2	FUB	O4-C1	-2.08	1.39	1.43
5	f7	3	FUB	O4-C1	-2.07	1.39	1.43
4	e2	2	FUB	C2-C3	-2.07	1.50	1.53
5	a9	1	FUB	C2-C3	-2.07	1.50	1.53
5	f7	1	FUB	C2-C3	-2.07	1.50	1.53
4	d1	1	FUB	O4-C1	-2.06	1.39	1.43
5	f7	3	FUB	C2-C3	-2.06	1.50	1.53
4	c3	2	FUB	C1-C2	2.06	1.55	1.51
4	c0	2	FUB	C1-C2	2.05	1.55	1.51
5	f7	1	FUB	O4-C1	-2.04	1.39	1.43
4	f8	2	FUB	C2-C3	-2.04	1.50	1.53
4	d7	2	FUB	C2-C3	-2.03	1.50	1.53
4	c4	2	FUB	O4-C1	-2.03	1.39	1.43
4	B0	1	FUB	O4-C1	-2.03	1.39	1.43
4	c9	1	FUB	O4-C1	-2.03	1.39	1.43
4	e5	2	FUB	C2-C3	-2.01	1.50	1.53
5	a9	2	FUB	C2-C3	-2.01	1.50	1.53
4	c4	2	FUB	C2-C3	-2.00	1.50	1.53

All (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
3	A2	1	NAG	C2-N2-C7	3.19	127.18	122.90
3	a2	1	NAG	C2-N2-C7	3.13	127.09	122.90
4	b0	1	FUB	C5-C4-C3	-3.10	107.79	115.10
5	a6	2	FUB	O4-C4-C3	-3.06	101.81	104.63
5	f6	4	FUB	O4-C4-C3	2.99	107.40	104.63
4	e5	1	FUB	C5-C4-C3	-2.97	108.07	115.10
4	d7	1	FUB	C5-C4-C3	-2.97	108.08	115.10
5	f7	2	FUB	O4-C4-C3	-2.93	101.93	104.63
5	f7	4	FUB	O4-C4-C3	-2.90	101.96	104.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a3	1	NAG	C4-C3-C2	-2.88	106.80	111.02
4	b3	2	FUB	O4-C4-C3	2.84	107.26	104.63
4	d1	2	FUB	C1-O4-C4	2.83	114.30	108.06
4	b1	1	FUB	C5-C4-C3	-2.80	108.48	115.10
4	e1	2	FUB	C5-C4-C3	-2.78	108.52	115.10
4	c6	1	FUB	C5-C4-C3	-2.77	108.56	115.10
7	a4	2	FUB	C5-C4-C3	-2.73	108.64	115.10
4	c7	1	FUB	O4-C4-C3	2.72	107.15	104.63
4	e2	1	FUB	C5-C4-C3	-2.69	108.75	115.10
4	c4	1	FUB	C5-C4-C3	-2.67	108.80	115.10
4	f8	1	FUB	C5-C4-C3	-2.66	108.81	115.10
4	c9	2	FUB	O4-C4-C3	2.66	107.09	104.63
4	c9	2	FUB	C5-C4-C3	-2.65	108.83	115.10
5	f7	1	FUB	C5-C4-C3	-2.64	108.86	115.10
3	a3	2	NAG	O5-C1-C2	-2.64	107.21	111.29
4	f8	2	FUB	C5-C4-C3	-2.63	108.89	115.10
4	b3	2	FUB	C5-C4-C3	-2.63	108.89	115.10
4	b4	2	FUB	C5-C4-C3	-2.63	108.90	115.10
5	a9	1	FUB	C5-C4-C3	-2.62	108.91	115.10
4	d1	2	FUB	C1-C2-C3	2.61	105.79	101.63
4	b5	2	FUB	C5-C4-C3	-2.60	108.95	115.10
4	f5	1	FUB	C5-C4-C3	-2.60	108.96	115.10
4	c9	1	FUB	C5-C4-C3	-2.60	108.96	115.10
4	f3	2	FUB	C5-C4-C3	-2.59	108.98	115.10
4	c0	2	FUB	O4-C4-C3	-2.59	102.24	104.63
4	f5	2	FUB	O4-C4-C3	2.58	107.02	104.63
5	f6	4	FUB	C5-C4-C3	-2.58	109.02	115.10
4	c0	1	FUB	C5-C4-C3	-2.57	109.03	115.10
5	b6	3	FUB	C5-C4-C3	-2.57	109.04	115.10
4	d2	2	FUB	C5-C4-C3	-2.56	109.04	115.10
4	b5	1	FUB	C5-C4-C3	-2.56	109.06	115.10
5	b6	4	FUB	C5-C4-C3	-2.56	109.06	115.10
4	c3	1	FUB	O4-C4-C3	2.56	106.99	104.63
4	e7	2	FUB	C5-C4-C3	-2.55	109.08	115.10
5	f7	3	FUB	C5-C4-C3	-2.55	109.08	115.10
4	e3	2	FUB	C5-C4-C3	-2.54	109.09	115.10
4	d8	2	FUB	C5-C4-C3	-2.54	109.09	115.10
4	f0	2	FUB	C5-C4-C3	-2.54	109.09	115.10
3	A3	1	NAG	O5-C1-C2	-2.54	107.36	111.29
4	f5	2	FUB	C5-C4-C3	-2.54	109.11	115.10
4	d0	2	FUB	C5-C4-C3	-2.54	109.11	115.10
4	c8	2	FUB	C5-C4-C3	-2.53	109.12	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	e6	2	FUB	C5-C4-C3	-2.53	109.12	115.10
4	f2	2	FUB	C5-C4-C3	-2.53	109.13	115.10
4	e8	2	FUB	C5-C4-C3	-2.52	109.14	115.10
4	b0	2	FUB	C5-C4-C3	-2.52	109.14	115.10
4	c1	2	FUB	C5-C4-C3	-2.51	109.16	115.10
4	b7	2	FUB	C5-C4-C3	-2.51	109.16	115.10
4	d9	2	FUB	C5-C4-C3	-2.51	109.16	115.10
4	c0	1	FUB	O4-C4-C3	2.51	106.95	104.63
4	e0	2	FUB	C5-C4-C3	-2.51	109.18	115.10
4	b1	2	FUB	C5-C4-C3	-2.50	109.19	115.10
4	b7	1	FUB	C5-C4-C3	-2.50	109.20	115.10
4	c4	2	FUB	C5-C4-C3	-2.49	109.21	115.10
4	d3	1	FUB	C5-C4-C3	-2.49	109.22	115.10
4	c7	2	FUB	C5-C4-C3	-2.48	109.23	115.10
4	a7	2	FUB	C5-C4-C3	-2.48	109.24	115.10
5	f6	2	FUB	C5-C4-C3	-2.48	109.25	115.10
8	e9	6	FUB	O4-C4-C3	-2.47	102.36	104.63
5	f6	1	FUB	C5-C4-C3	-2.46	109.28	115.10
4	f8	2	FUB	O4-C4-C3	2.46	106.90	104.63
4	c1	1	FUB	C5-C4-C3	-2.45	109.32	115.10
4	d5	2	FUB	C5-C4-C3	-2.43	109.35	115.10
4	c2	2	FUB	C5-C4-C3	-2.43	109.36	115.10
4	c6	2	FUB	C5-C4-C3	-2.43	109.36	115.10
4	e0	2	FUB	O4-C4-C3	2.43	106.88	104.63
4	c2	1	FUB	C5-C4-C3	-2.42	109.38	115.10
4	b1	1	FUB	O4-C4-C3	2.42	106.87	104.63
4	c3	1	FUB	C5-C4-C3	-2.41	109.41	115.10
4	e0	1	FUB	C5-C4-C3	-2.40	109.42	115.10
4	d4	2	FUB	C5-C4-C3	-2.40	109.44	115.10
4	d6	2	FUB	C5-C4-C3	-2.39	109.45	115.10
5	b6	1	FUB	C5-C4-C3	-2.39	109.47	115.10
8	e9	5	FUB	C5-C4-C3	-2.38	109.47	115.10
4	c7	1	FUB	C5-C4-C3	-2.38	109.49	115.10
4	b9	1	FUB	C5-C4-C3	-2.36	109.51	115.10
4	c3	2	FUB	C5-C4-C3	-2.36	109.51	115.10
4	d2	1	FUB	C5-C4-C3	-2.34	109.58	115.10
4	c5	1	FUB	C5-C4-C3	-2.33	109.59	115.10
4	b3	1	FUB	C5-C4-C3	-2.33	109.60	115.10
5	a6	4	FUB	O4-C4-C3	-2.32	102.49	104.63
4	E4	1	FUB	O5-C5-C4	2.32	119.24	111.33
4	b9	2	FUB	C5-C4-C3	-2.31	109.64	115.10
4	a5	2	FUB	C5-C4-C3	-2.31	109.65	115.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	a6	3	FUB	O4-C4-C3	2.30	106.76	104.63
4	B0	1	FUB	O4-C4-C3	2.30	106.76	104.63
8	e9	1	FUB	C5-C4-C3	-2.29	109.70	115.10
4	d3	2	FUB	C5-C4-C3	-2.28	109.70	115.10
4	e8	1	FUB	C5-C4-C3	-2.27	109.73	115.10
4	D1	1	FUB	O4-C4-C3	2.27	106.73	104.63
3	A1	1	NAG	O5-C1-C2	-2.26	107.79	111.29
4	d9	1	FUB	C5-C4-C3	-2.26	109.77	115.10
4	e5	2	FUB	C5-C4-C3	-2.23	109.83	115.10
4	d7	2	FUB	C5-C4-C3	-2.22	109.85	115.10
4	d1	2	FUB	C5-C4-C3	-2.22	109.85	115.10
5	a9	4	FUB	C5-C4-C3	-2.22	109.86	115.10
4	e1	1	FUB	C5-C4-C3	-2.21	109.87	115.10
4	f3	1	FUB	C5-C4-C3	-2.21	109.88	115.10
4	c5	2	FUB	C5-C4-C3	-2.20	109.89	115.10
8	e9	3	FUB	C5-C4-C3	-2.19	109.93	115.10
4	b0	1	FUB	O4-C4-C3	2.18	106.65	104.63
4	d5	1	FUB	C5-C4-C3	-2.17	109.97	115.10
3	A2	1	NAG	O5-C1-C2	-2.17	107.93	111.29
4	e4	2	FUB	O4-C4-C3	2.16	106.63	104.63
4	d0	1	FUB	C5-C4-C3	-2.15	110.02	115.10
4	b5	1	FUB	C1-O4-C4	2.15	112.80	108.06
4	e2	2	FUB	C5-C4-C3	-2.14	110.04	115.10
4	c8	1	FUB	C5-C4-C3	-2.14	110.05	115.10
4	b4	1	FUB	C5-C4-C3	-2.13	110.06	115.10
5	b6	2	FUB	C5-C4-C3	-2.13	110.06	115.10
5	f6	3	FUB	C5-C4-C3	-2.12	110.09	115.10
4	e4	2	FUB	O4-C1-C2	-2.12	102.11	105.76
4	c9	1	FUB	O4-C4-C3	2.11	106.58	104.63
4	c9	1	FUB	C1-O4-C4	2.10	112.70	108.06
4	d4	1	FUB	C5-C4-C3	-2.09	110.17	115.10
3	a1	1	NAG	O5-C1-C2	-2.09	108.06	111.29
4	c0	2	FUB	C5-C4-C3	-2.08	110.17	115.10
4	d6	1	FUB	C5-C4-C3	-2.08	110.19	115.10
7	a4	2	FUB	O4-C4-C3	2.08	106.55	104.63
8	e9	6	FUB	C5-C4-C3	-2.06	110.23	115.10
4	e4	1	FUB	O4-C4-C3	2.03	106.51	104.63
4	a7	1	FUB	C5-C4-C3	-2.02	110.32	115.10
8	e9	2	FUB	O4-C4-C5	2.02	113.04	109.36
4	d1	2	FUB	O4-C4-C3	2.00	106.48	104.63
3	A1	2	NAG	O5-C1-C2	-2.00	108.20	111.29

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	a4	1	34V	C3

All (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
4	d1	2	FUB	O4-C4-C5-O5
4	d4	1	FUB	C3-C4-C5-O5
4	d6	1	FUB	C3-C4-C5-O5
5	b6	1	FUB	C3-C4-C5-O5
5	b6	4	FUB	O4-C4-C5-O5
5	f6	4	FUB	O4-C4-C5-O5
4	c3	1	FUB	O4-C4-C5-O5
4	d4	1	FUB	O4-C4-C5-O5
4	d6	1	FUB	O4-C4-C5-O5
5	b6	1	FUB	O4-C4-C5-O5
4	a7	2	FUB	C3-C4-C5-O5
4	c1	1	FUB	C3-C4-C5-O5
4	c7	2	FUB	C3-C4-C5-O5
4	d1	2	FUB	C3-C4-C5-O5
4	e1	1	FUB	C3-C4-C5-O5
5	a9	3	FUB	C3-C4-C5-O5
5	b6	3	FUB	C3-C4-C5-O5
5	f6	3	FUB	C3-C4-C5-O5
8	e9	3	FUB	C3-C4-C5-O5
8	e9	5	FUB	C3-C4-C5-O5
4	C9	1	FUB	O4-C4-C5-O5
4	b9	2	FUB	O4-C4-C5-O5
4	c8	1	FUB	O4-C4-C5-O5
4	e1	2	FUB	O4-C4-C5-O5
4	f5	1	FUB	O4-C4-C5-O5
4	d0	1	FUB	O4-C4-C5-O5
5	a9	3	FUB	O4-C4-C5-O5
5	b6	3	FUB	O4-C4-C5-O5
5	f6	3	FUB	O4-C4-C5-O5
5	f7	2	FUB	O4-C4-C5-O5
5	f7	4	FUB	O4-C4-C5-O5
8	e9	3	FUB	O4-C4-C5-O5
4	b9	2	FUB	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
4	c1	2	FUB	C3-C4-C5-O5
4	e8	1	FUB	C3-C4-C5-O5
4	f5	1	FUB	C3-C4-C5-O5
4	d9	1	FUB	C3-C4-C5-O5
5	a6	2	FUB	C3-C4-C5-O5
5	b6	4	FUB	C3-C4-C5-O5
5	f6	4	FUB	C3-C4-C5-O5
4	d4	2	FUB	O4-C4-C5-O5
4	e8	1	FUB	O4-C4-C5-O5
4	f0	2	FUB	O4-C4-C5-O5
4	f2	2	FUB	O4-C4-C5-O5
4	e7	2	FUB	O4-C4-C5-O5
4	e6	2	FUB	O4-C4-C5-O5
4	e3	2	FUB	O4-C4-C5-O5
4	d9	1	FUB	O4-C4-C5-O5
4	d8	2	FUB	O4-C4-C5-O5
4	d6	2	FUB	O4-C4-C5-O5
4	b7	2	FUB	C3-C4-C5-O5
4	c9	2	FUB	C3-C4-C5-O5
4	d3	2	FUB	C3-C4-C5-O5
4	d4	2	FUB	C3-C4-C5-O5
4	d5	2	FUB	C3-C4-C5-O5
4	f0	2	FUB	C3-C4-C5-O5
4	f2	2	FUB	C3-C4-C5-O5
4	e7	2	FUB	C3-C4-C5-O5
4	e6	2	FUB	C3-C4-C5-O5
4	e3	2	FUB	C3-C4-C5-O5
4	d8	2	FUB	C3-C4-C5-O5
4	d6	2	FUB	C3-C4-C5-O5
5	F7	2	FUB	C3-C4-C5-O5
5	f7	2	FUB	C3-C4-C5-O5
5	f7	4	FUB	C3-C4-C5-O5
8	e9	4	FUB	C3-C4-C5-O5
4	a7	2	FUB	O4-C4-C5-O5
4	c1	1	FUB	O4-C4-C5-O5
4	c1	2	FUB	O4-C4-C5-O5
4	c7	2	FUB	O4-C4-C5-O5
4	e1	1	FUB	O4-C4-C5-O5
4	f0	1	FUB	O4-C4-C5-O5
4	f2	1	FUB	O4-C4-C5-O5
4	e7	1	FUB	O4-C4-C5-O5
4	e6	1	FUB	O4-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
4	e3	1	FUB	O4-C4-C5-O5
4	d8	1	FUB	O4-C4-C5-O5
8	e9	5	FUB	O4-C4-C5-O5
4	C9	1	FUB	C3-C4-C5-O5
4	b1	1	FUB	C3-C4-C5-O5
4	e1	2	FUB	C3-C4-C5-O5
4	c3	2	FUB	C3-C4-C5-O5
4	c8	1	FUB	C3-C4-C5-O5
4	e5	1	FUB	C3-C4-C5-O5
4	d7	1	FUB	C3-C4-C5-O5
4	d0	1	FUB	C3-C4-C5-O5
6	E6	8	FUB	C3-C4-C5-O5
4	a5	1	FUB	O4-C4-C5-O5
4	c2	1	FUB	O4-C4-C5-O5
4	d5	2	FUB	O4-C4-C5-O5
5	F7	2	FUB	O4-C4-C5-O5
5	a6	2	FUB	O4-C4-C5-O5
5	a9	4	FUB	O4-C4-C5-O5
8	e9	6	FUB	O4-C4-C5-O5
4	d1	1	FUB	C3-C4-C5-O5
4	E0	1	FUB	O4-C4-C5-O5
4	c9	2	FUB	O4-C4-C5-O5
6	E6	5	FUB	O4-C4-C5-O5
3	a3	1	NAG	C4-C5-C6-O6
4	D6	2	FUB	O4-C4-C5-O5
4	b7	2	FUB	O4-C4-C5-O5
4	c0	2	FUB	O4-C4-C5-O5
4	d3	2	FUB	O4-C4-C5-O5
4	f3	1	FUB	O4-C4-C5-O5
5	a9	2	FUB	O4-C4-C5-O5
6	E6	8	FUB	O4-C4-C5-O5
8	e9	4	FUB	O4-C4-C5-O5
4	a5	1	FUB	C3-C4-C5-O5
4	f0	1	FUB	C3-C4-C5-O5
4	f2	1	FUB	C3-C4-C5-O5
4	e7	1	FUB	C3-C4-C5-O5
4	e6	1	FUB	C3-C4-C5-O5
4	e3	1	FUB	C3-C4-C5-O5
4	d8	1	FUB	C3-C4-C5-O5
4	c3	2	FUB	O4-C4-C5-O5
4	D6	2	FUB	C3-C4-C5-O5
4	E0	1	FUB	C3-C4-C5-O5

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Mol	Chain	Res	Type	Atoms
4	c5	2	FUB	C3-C4-C5-O5
4	e5	2	FUB	C3-C4-C5-O5
4	d7	2	FUB	C3-C4-C5-O5
5	b6	2	FUB	C3-C4-C5-O5
6	E6	5	FUB	C3-C4-C5-O5
4	a5	2	FUB	O4-C4-C5-O5
4	b1	1	FUB	O4-C4-C5-O5
4	e2	2	FUB	C3-C4-C5-O5
5	a9	4	FUB	C3-C4-C5-O5
4	E4	1	FUB	O4-C4-C5-O5
4	c2	1	FUB	C3-C4-C5-O5
4	e5	1	FUB	O4-C4-C5-O5
4	d7	1	FUB	O4-C4-C5-O5
4	D4	1	FUB	O4-C4-C5-O5
4	D4	1	FUB	C3-C4-C5-O5
6	E6	4	FUB	O4-C4-C5-O5
8	e9	2	FUB	O4-C4-C5-O5
8	e9	6	FUB	C3-C4-C5-O5
4	c5	2	FUB	O4-C4-C5-O5
4	b3	1	FUB	O4-C4-C5-O5
4	e5	2	FUB	O4-C4-C5-O5
4	d7	2	FUB	O4-C4-C5-O5
4	f3	2	FUB	O4-C4-C5-O5
5	b6	2	FUB	O4-C4-C5-O5
4	d1	1	FUB	O4-C4-C5-O5
4	D8	2	FUB	O4-C4-C5-O5
5	F6	2	FUB	O4-C4-C5-O5
6	E6	4	FUB	C3-C4-C5-O5
3	A1	2	NAG	O5-C5-C6-O6
4	e2	2	FUB	O4-C4-C5-O5
5	f6	2	FUB	O4-C4-C5-O5
3	A2	1	NAG	C1-C2-N2-C7
3	a2	1	NAG	C1-C2-N2-C7
5	a6	1	FUB	C3-C4-C5-O5
3	a3	1	NAG	O5-C5-C6-O6
4	E4	1	FUB	C3-C4-C5-O5
4	b7	1	FUB	C3-C4-C5-O5
4	c0	2	FUB	C3-C4-C5-O5
3	a2	1	NAG	C3-C2-N2-C7
5	a9	2	FUB	C3-C4-C5-O5
8	e9	1	FUB	C3-C4-C5-O5
4	C5	2	FUB	O4-C4-C5-O5

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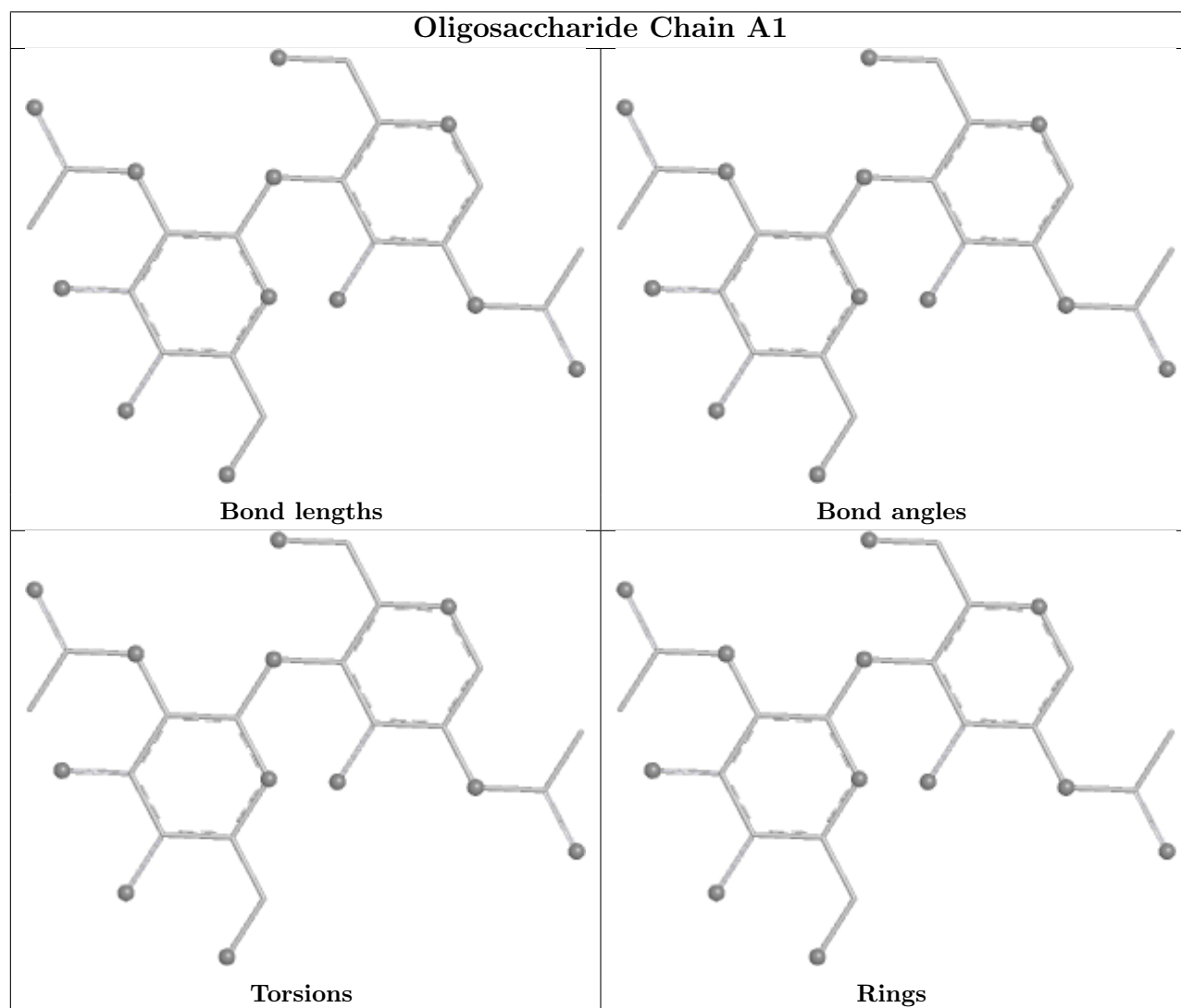
Mol	Chain	Res	Type	Atoms
3	A2	1	NAG	C3-C2-N2-C7
4	d3	1	FUB	C3-C4-C5-O5
5	F6	2	FUB	C3-C4-C5-O5
4	D8	2	FUB	C3-C4-C5-O5
4	f8	1	FUB	O4-C4-C5-O5
4	d5	1	FUB	C3-C4-C5-O5

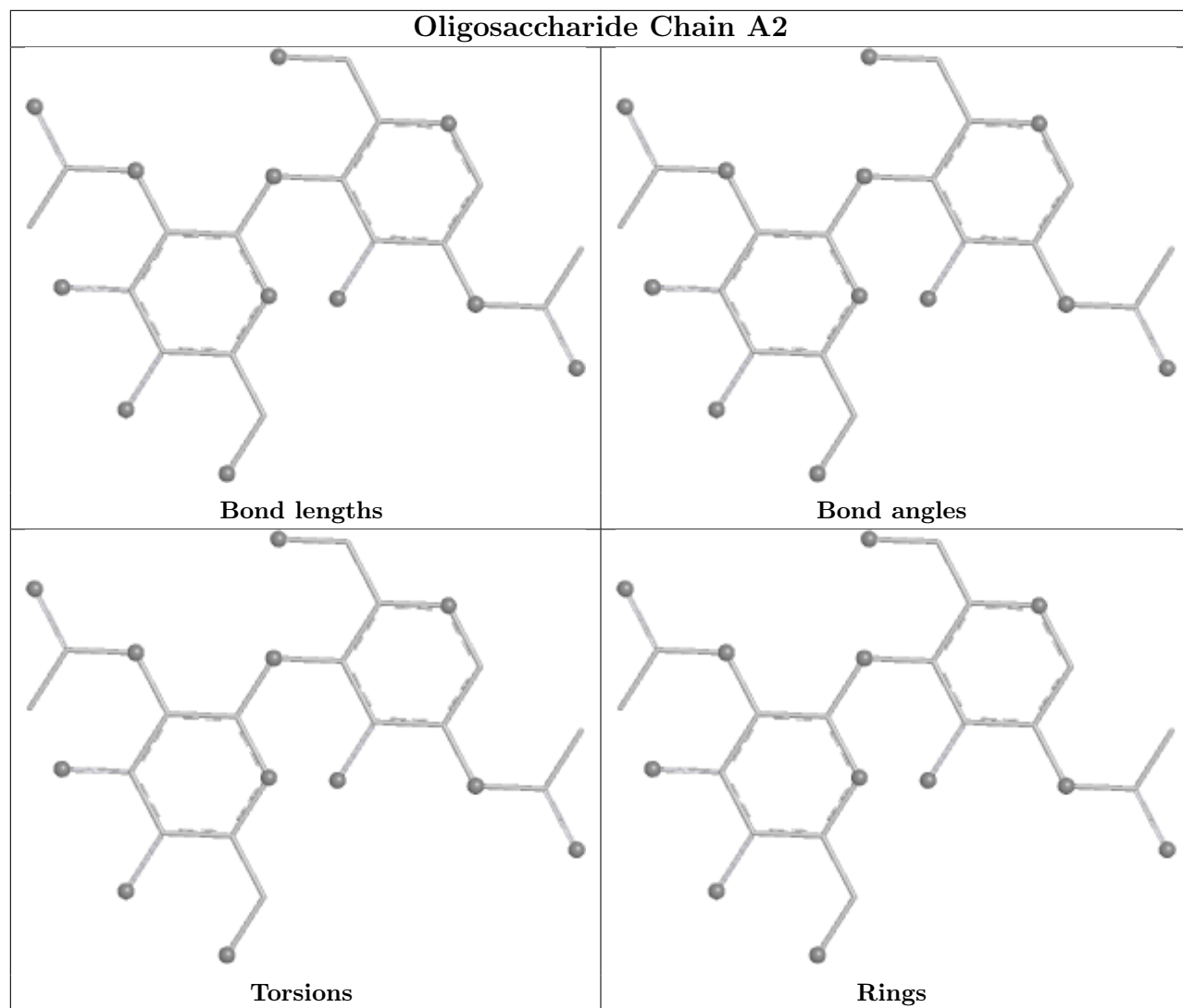
There are no ring outliers.

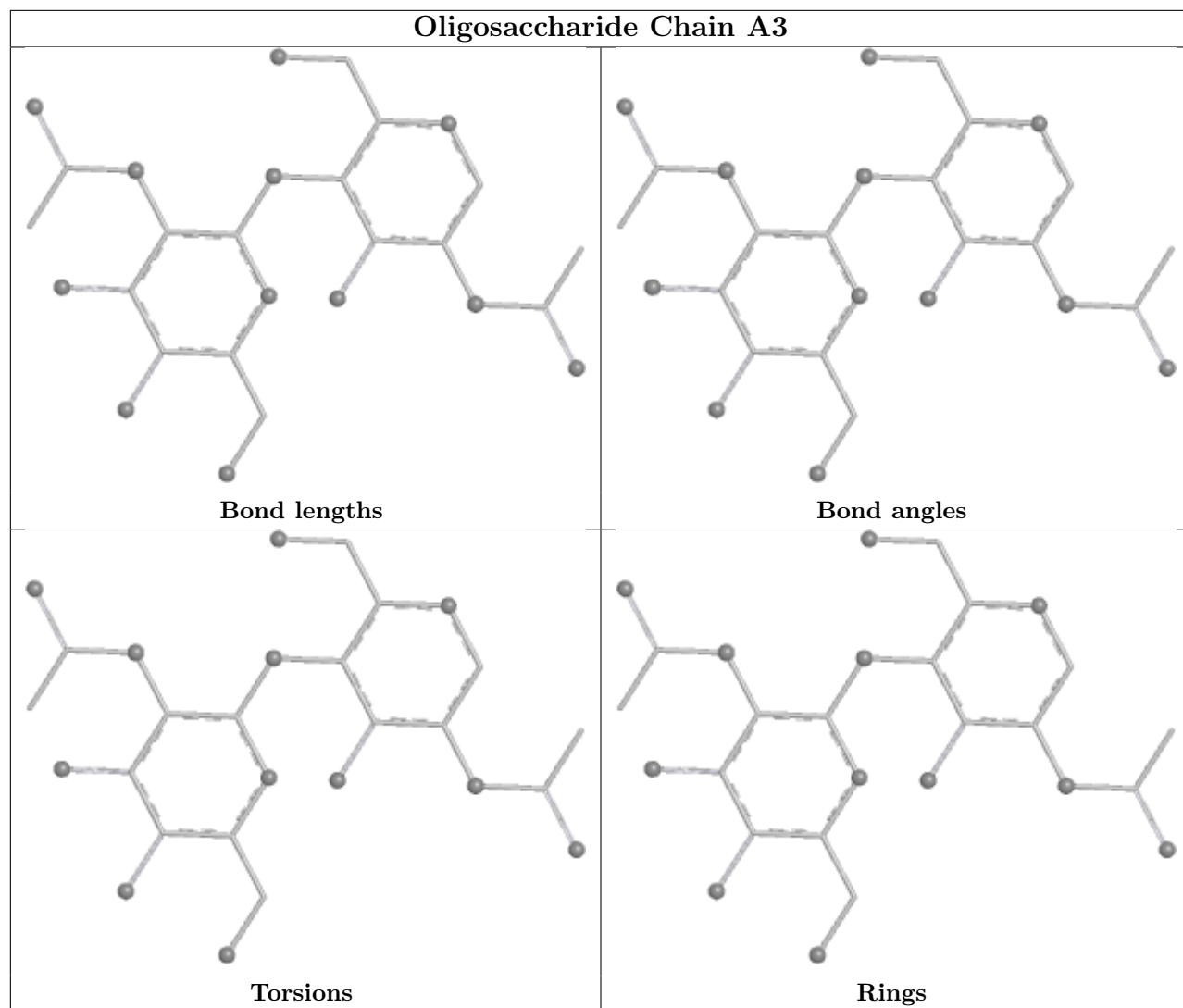
31 monomers are involved in 54 short contacts:

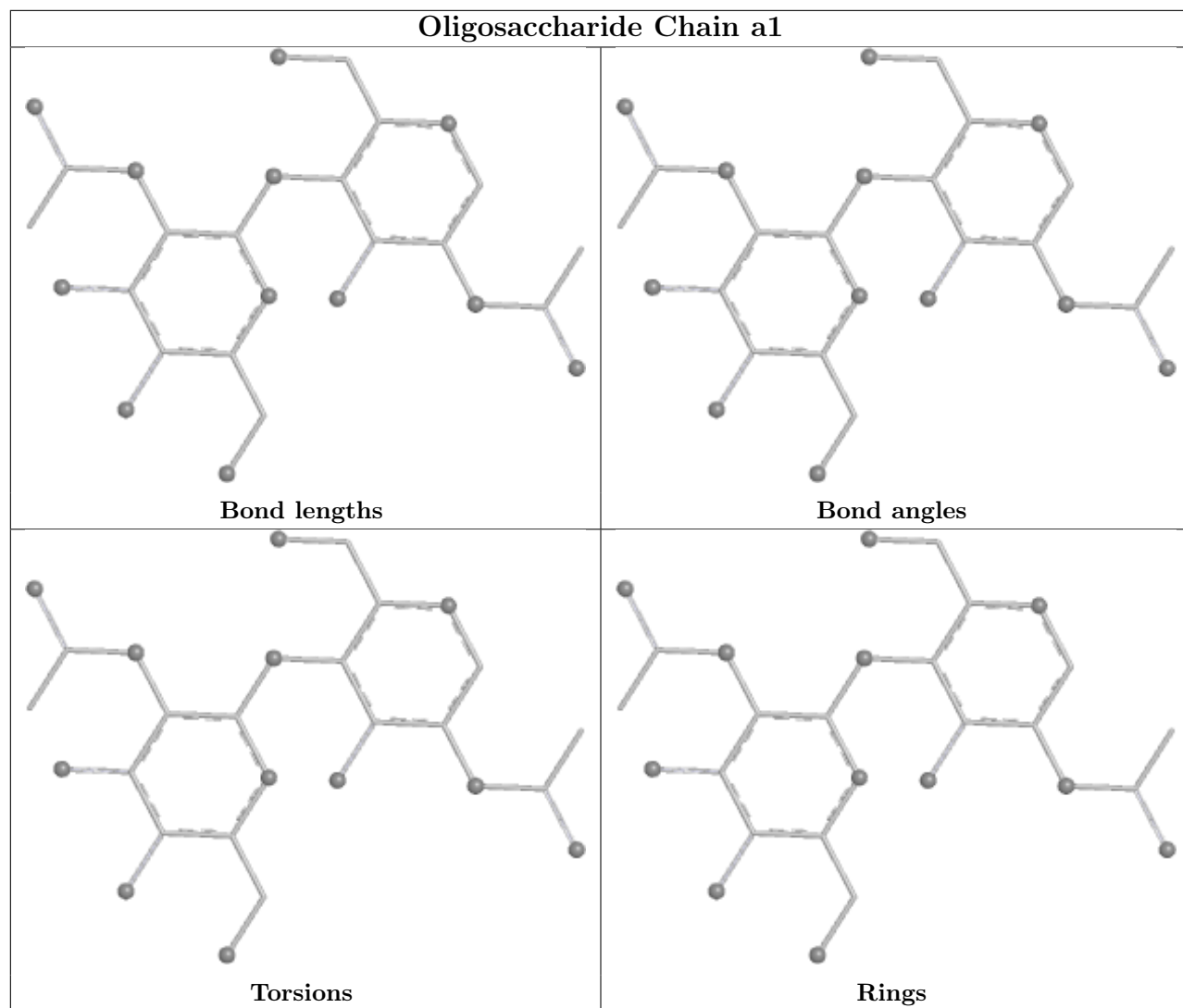
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	e4	1	FUB	3	0
4	f2	1	FUB	2	0
3	a3	1	NAG	1	0
4	a5	1	FUB	1	0
4	e7	2	FUB	1	0
4	d0	1	FUB	3	0
4	C2	2	FUB	1	0
4	D9	2	FUB	1	0
4	B3	1	FUB	1	0
4	f0	1	FUB	3	0
4	f0	2	FUB	4	0
4	C8	2	FUB	1	0
4	c7	2	FUB	1	0
4	e1	1	FUB	2	0
4	a7	2	FUB	1	0
4	f2	2	FUB	3	0
4	C8	1	FUB	1	0
4	c7	1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

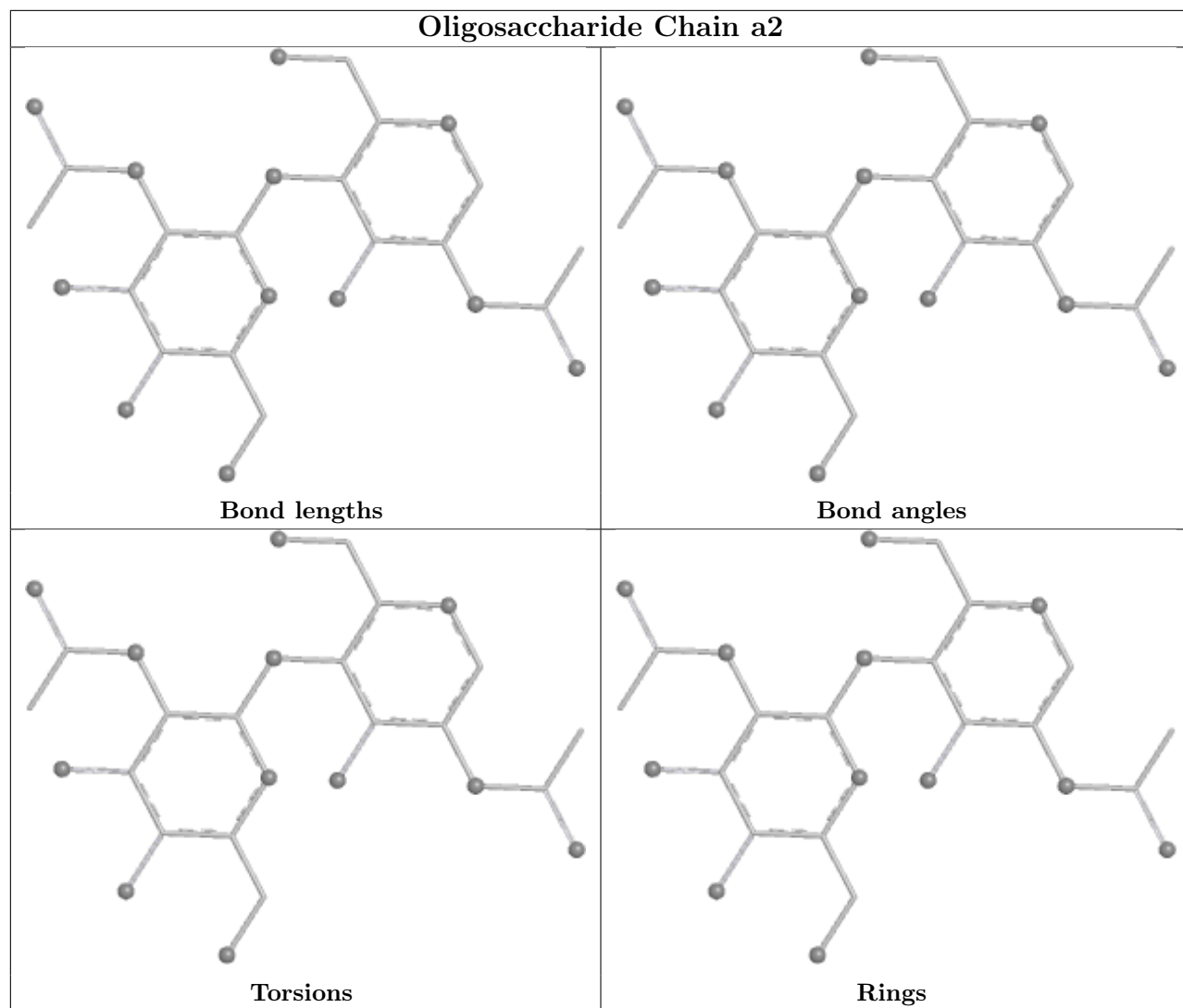
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



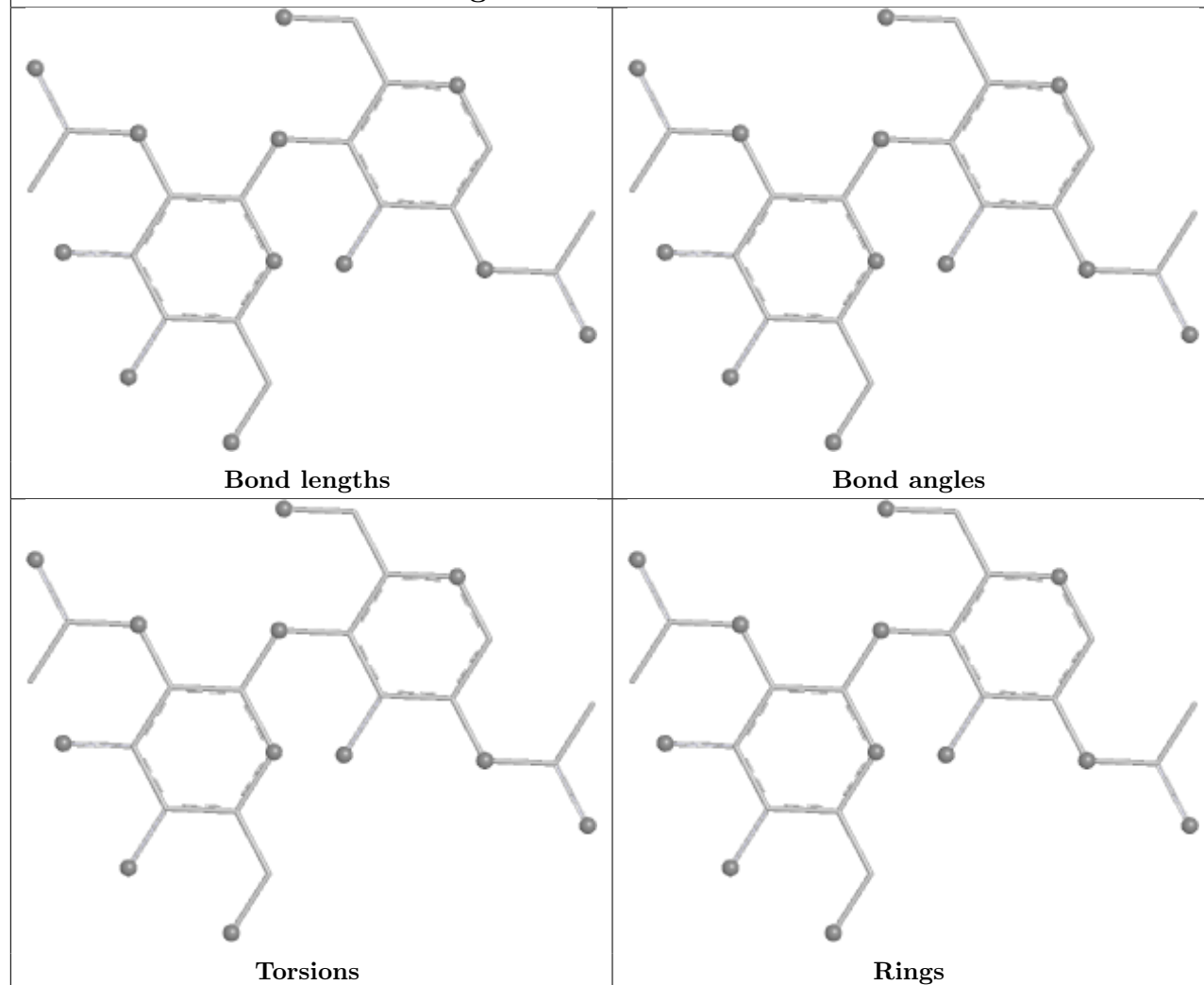




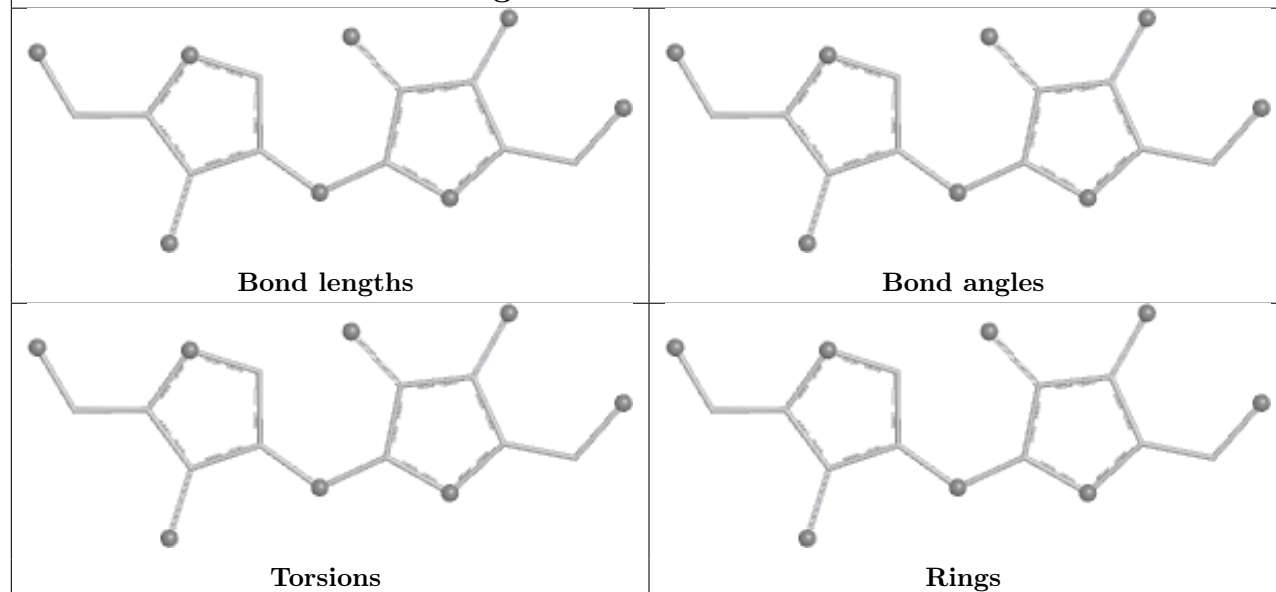


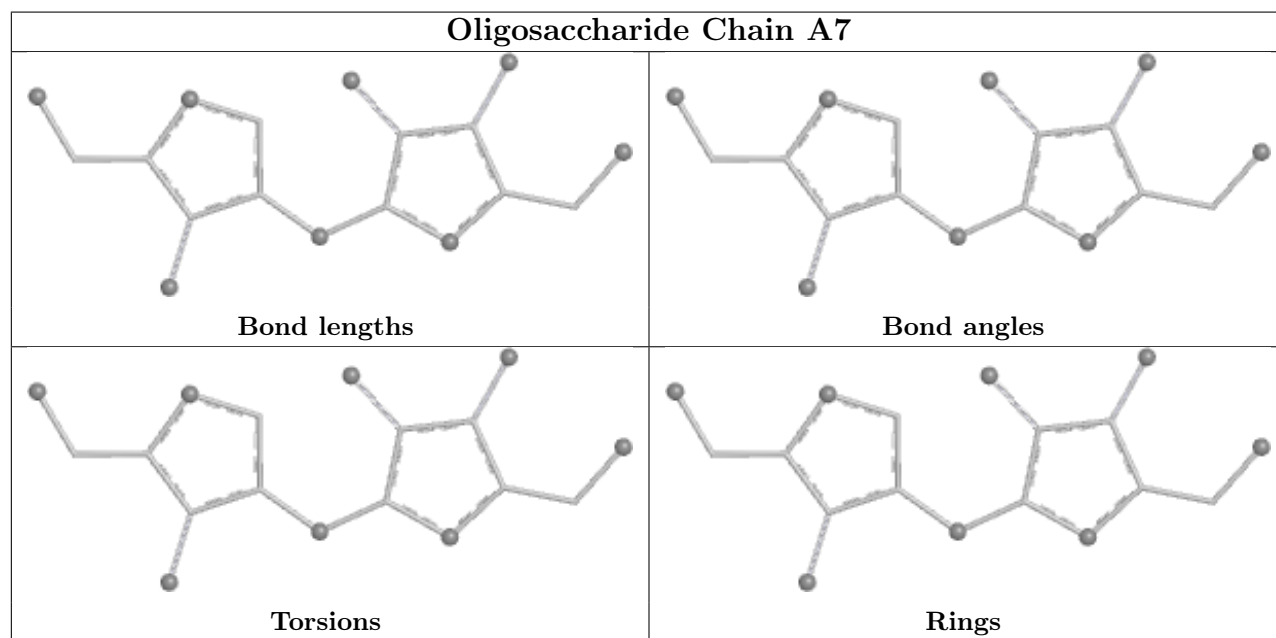
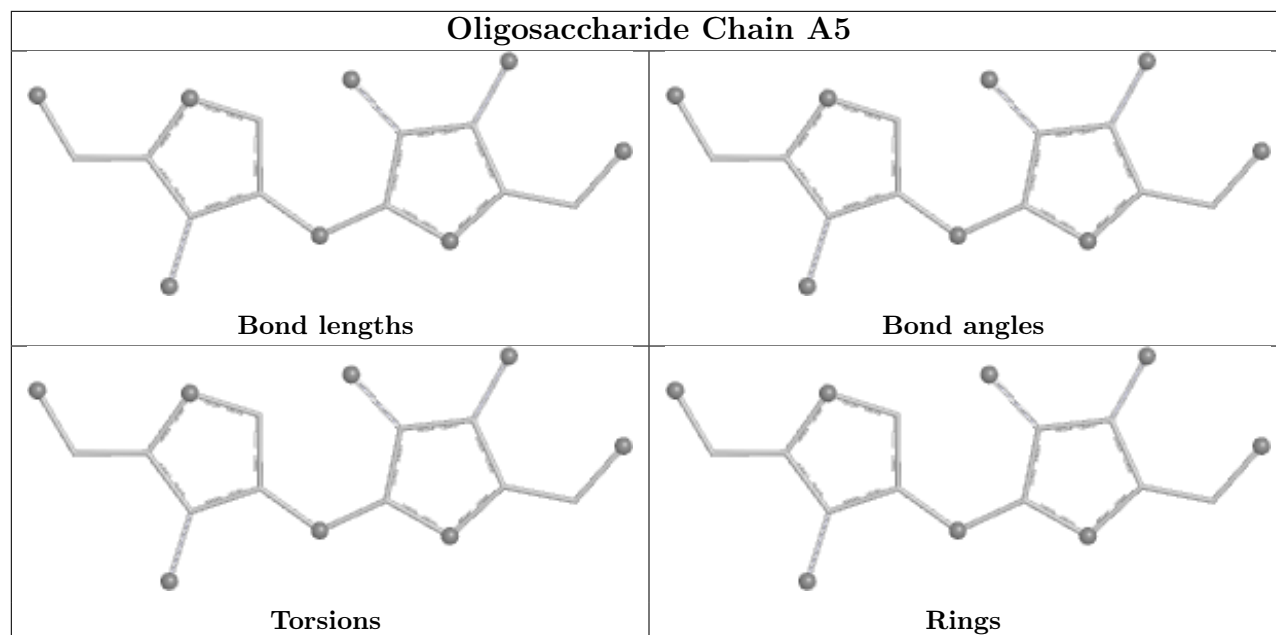


Oligosaccharide Chain a3

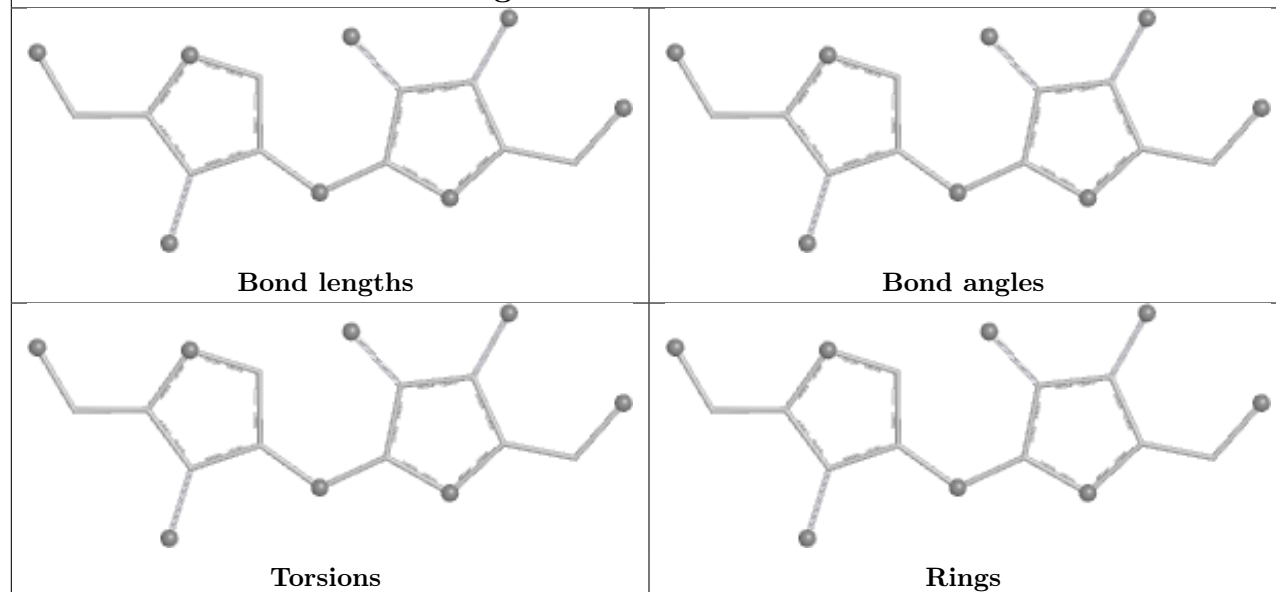


Oligosaccharide Chain A4

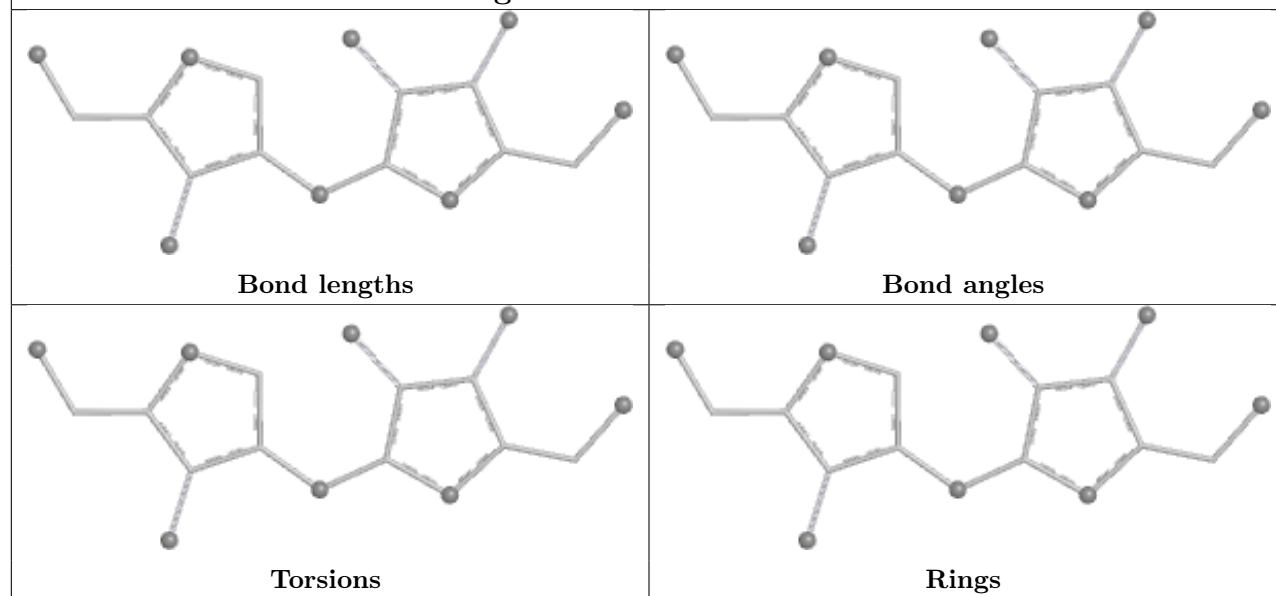


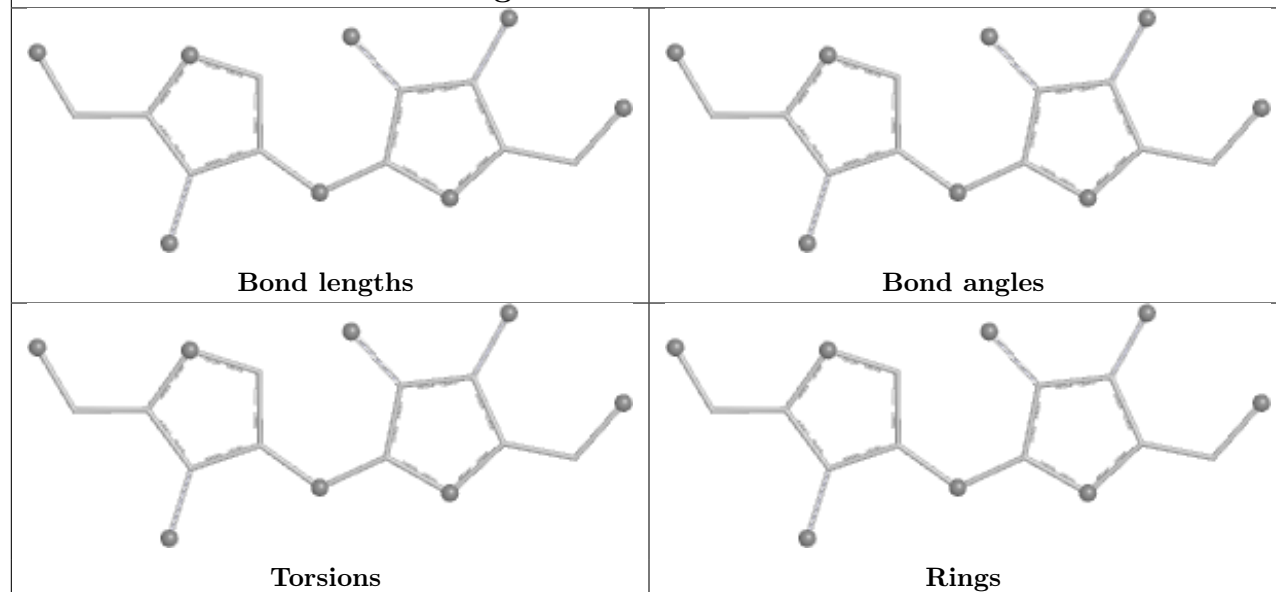
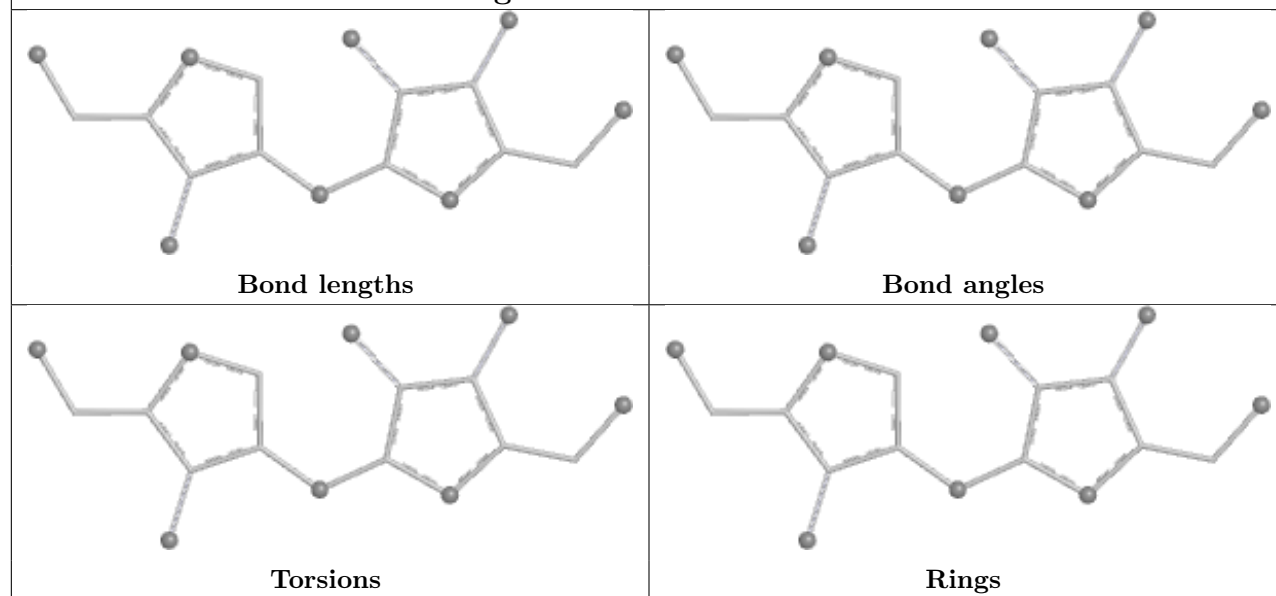


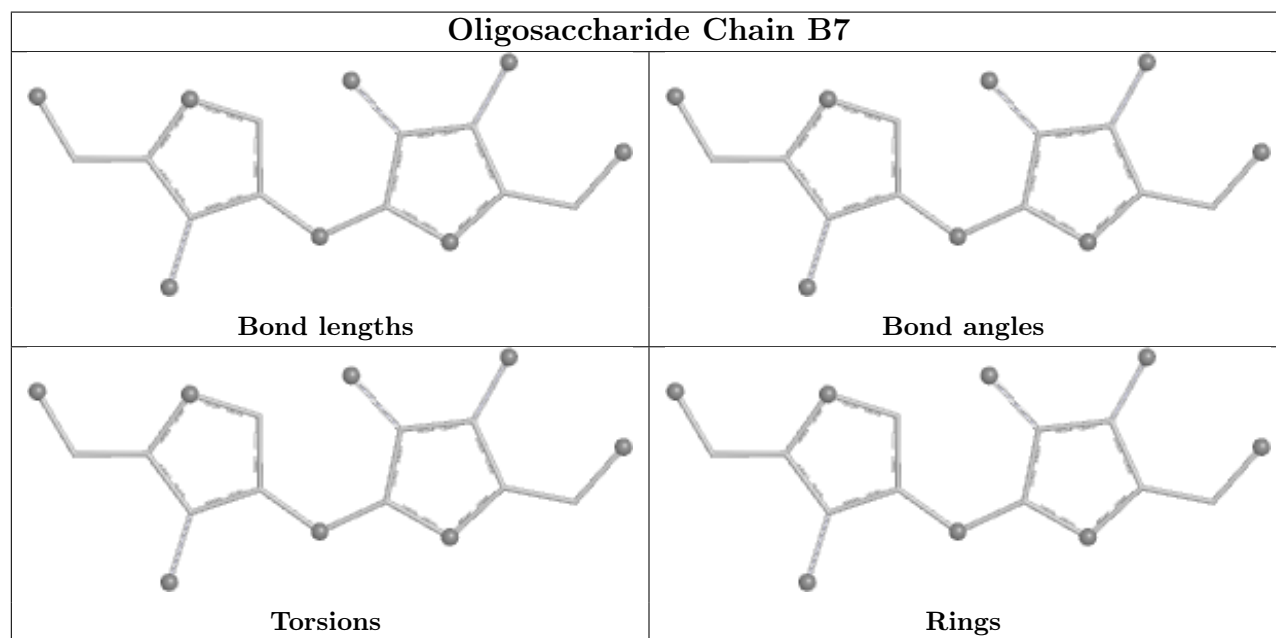
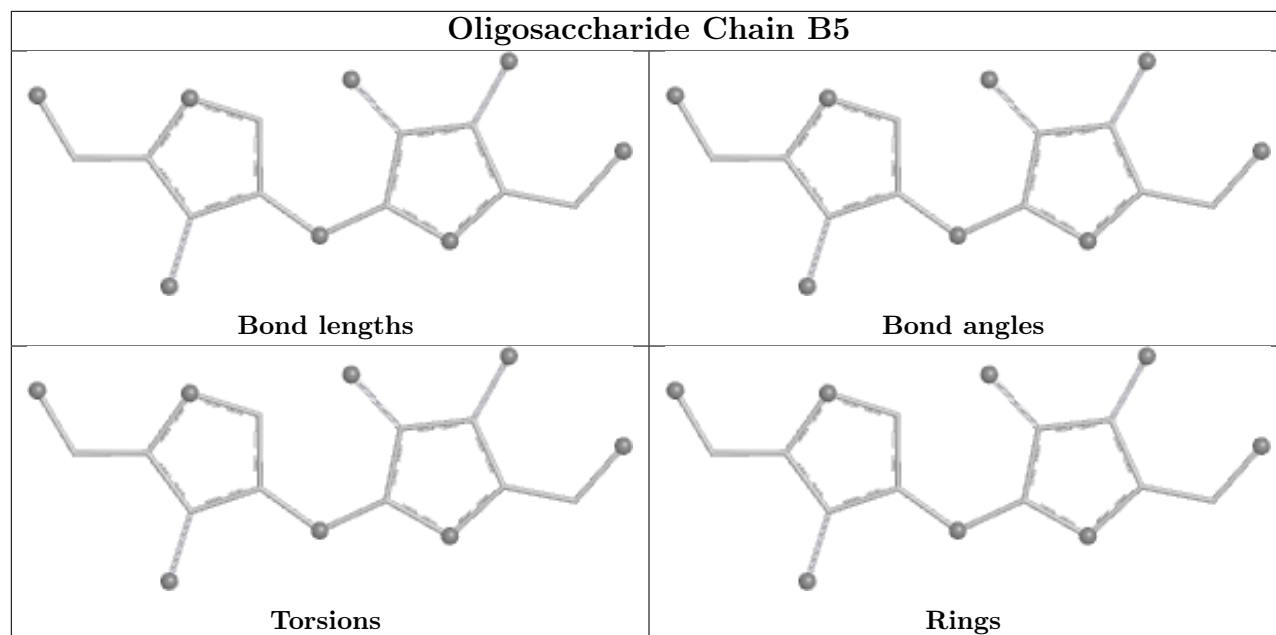
Oligosaccharide Chain B0

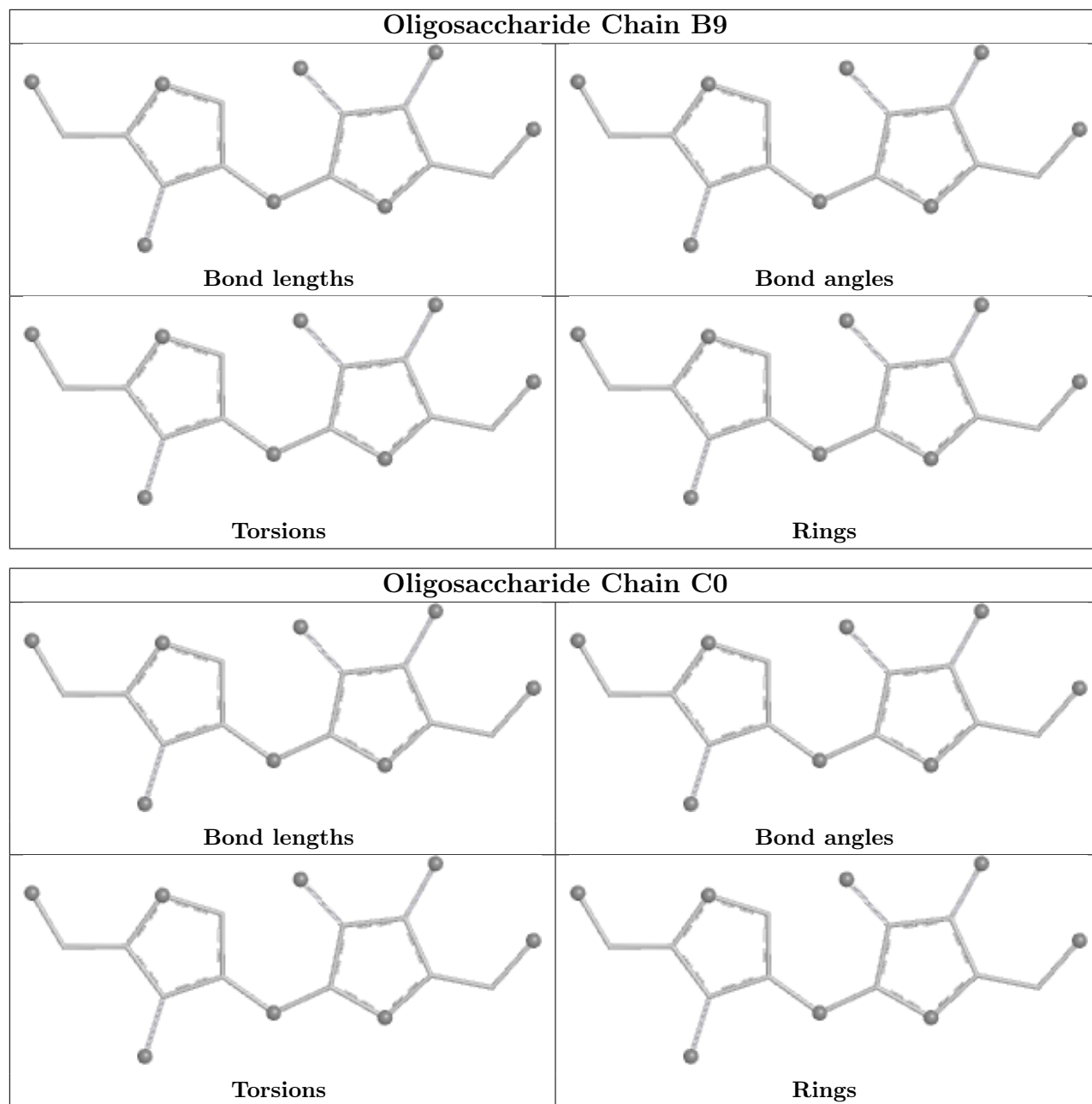


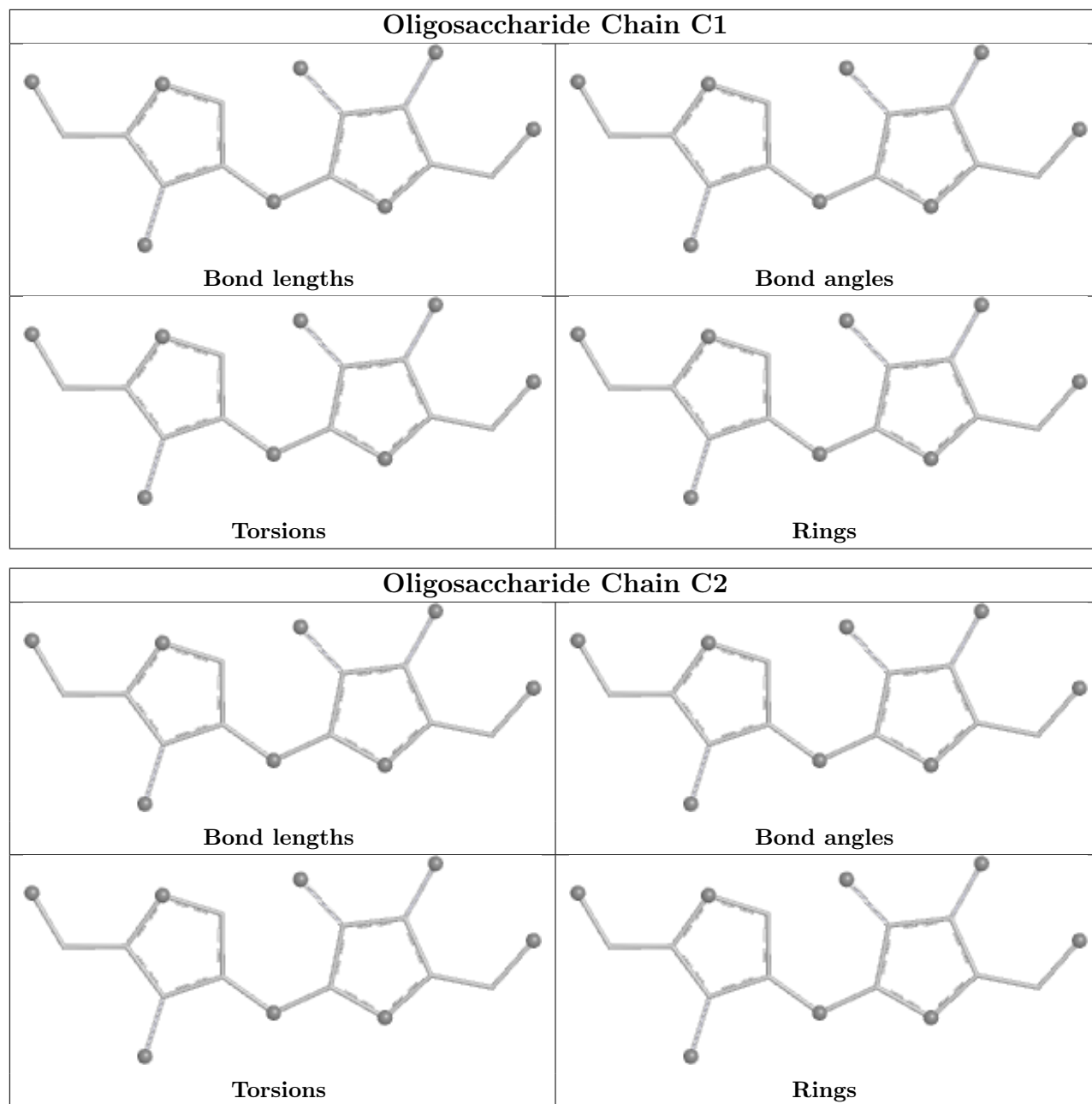
Oligosaccharide Chain B1



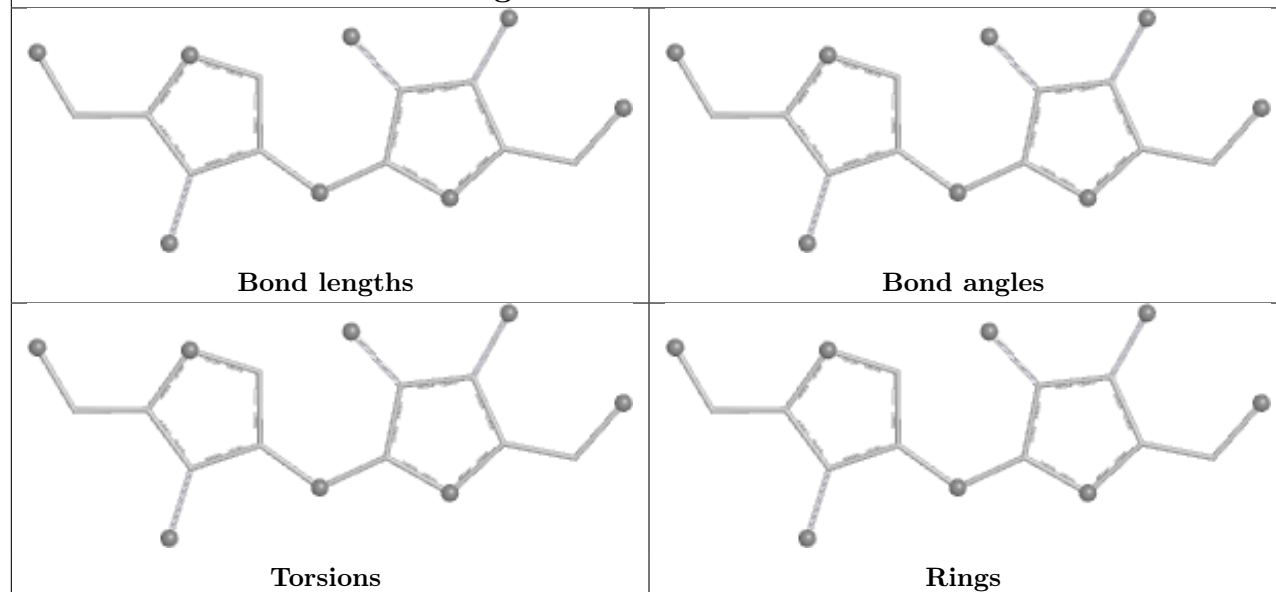
Oligosaccharide Chain B3**Oligosaccharide Chain B4**



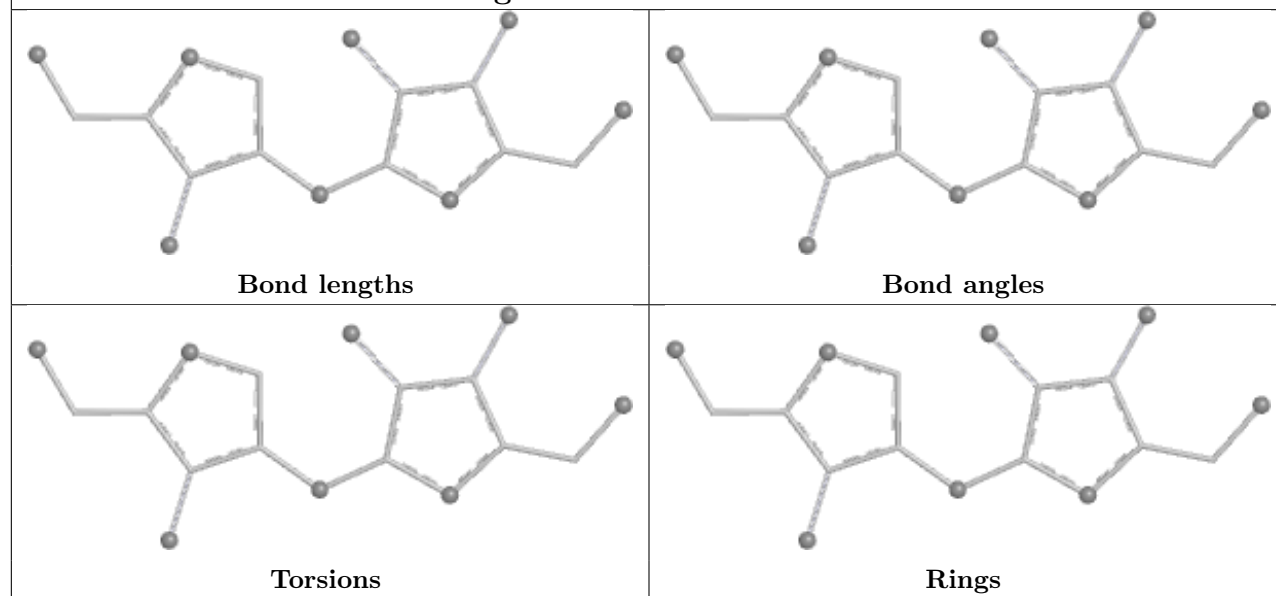




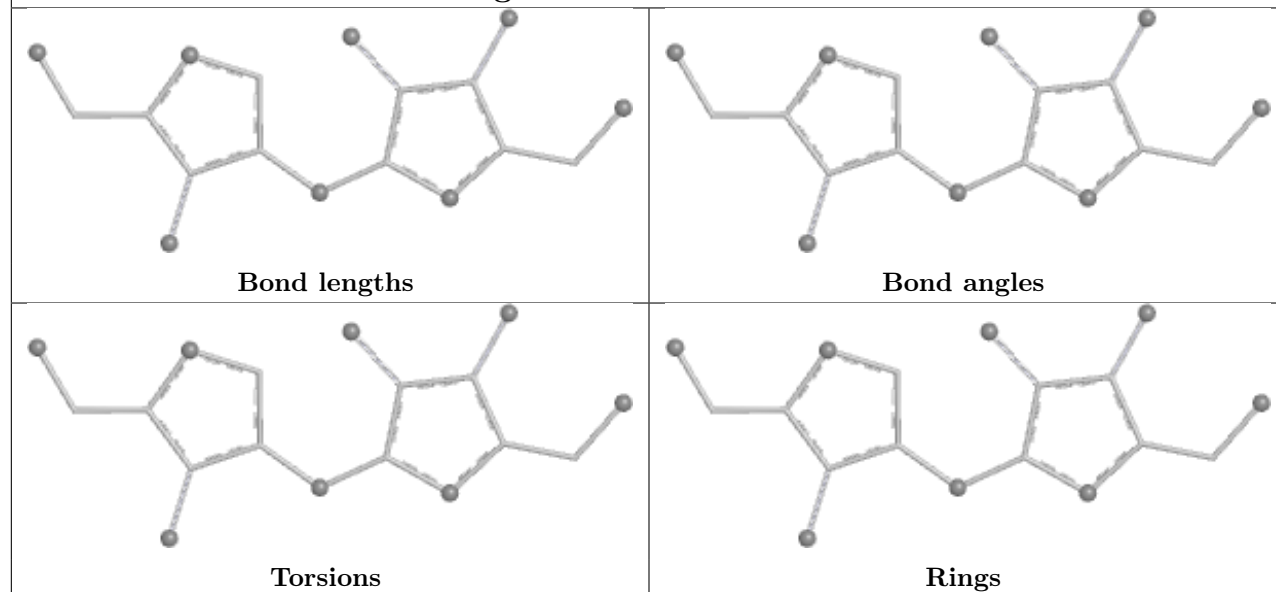
Oligosaccharide Chain C3



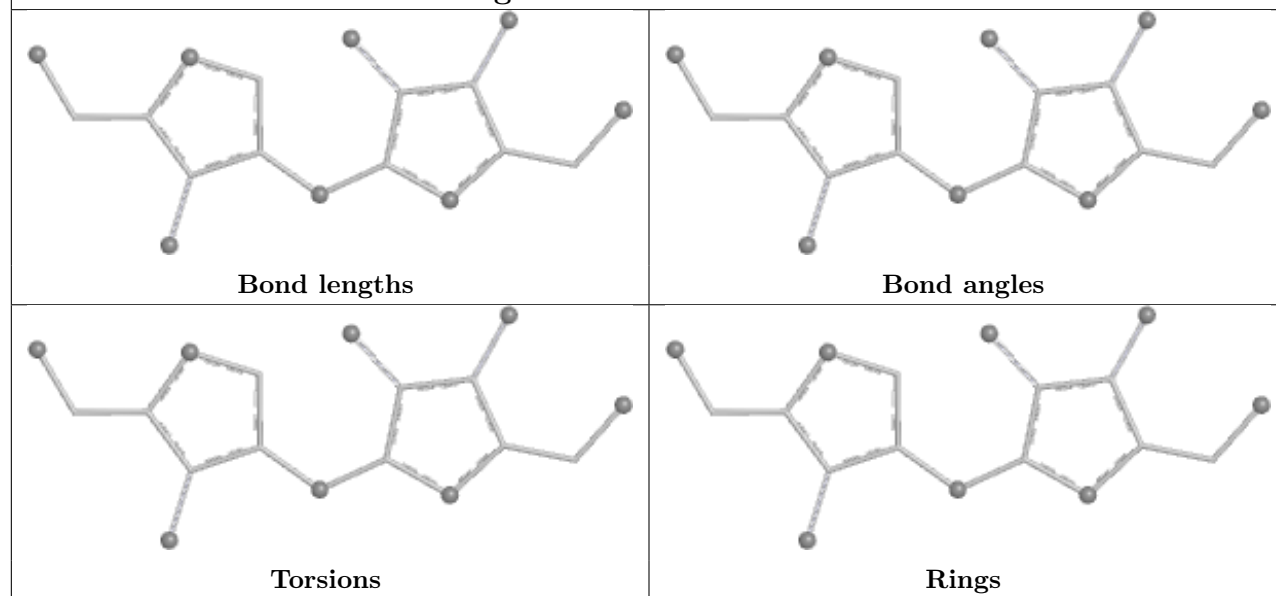
Oligosaccharide Chain C4

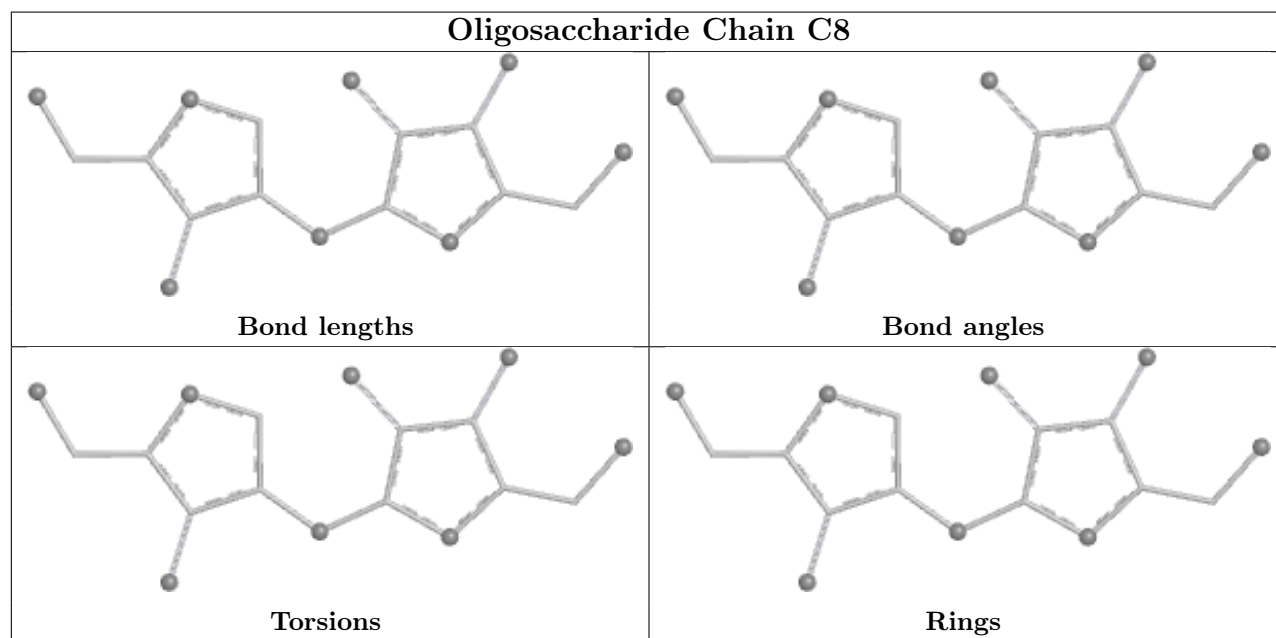
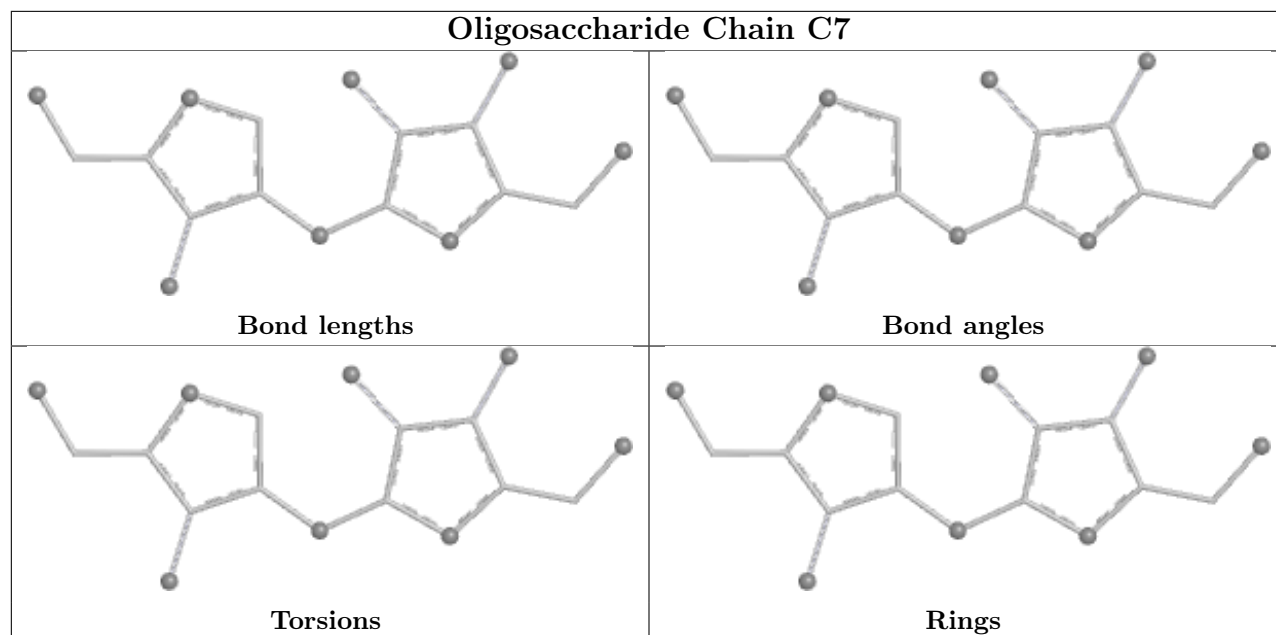


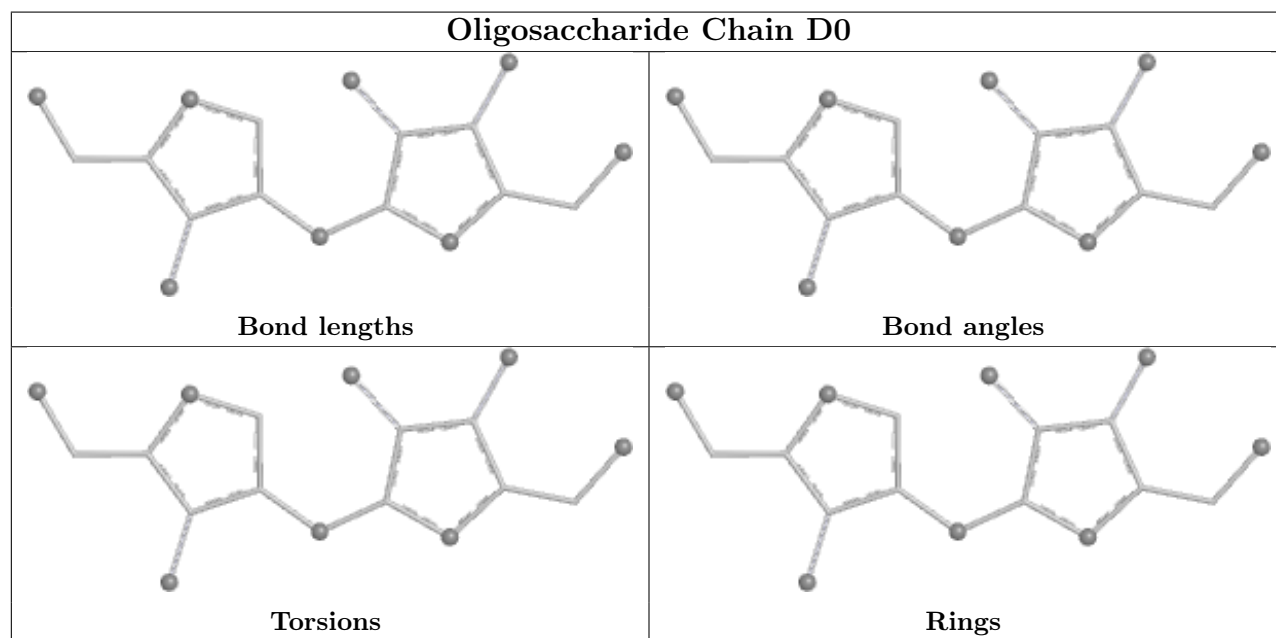
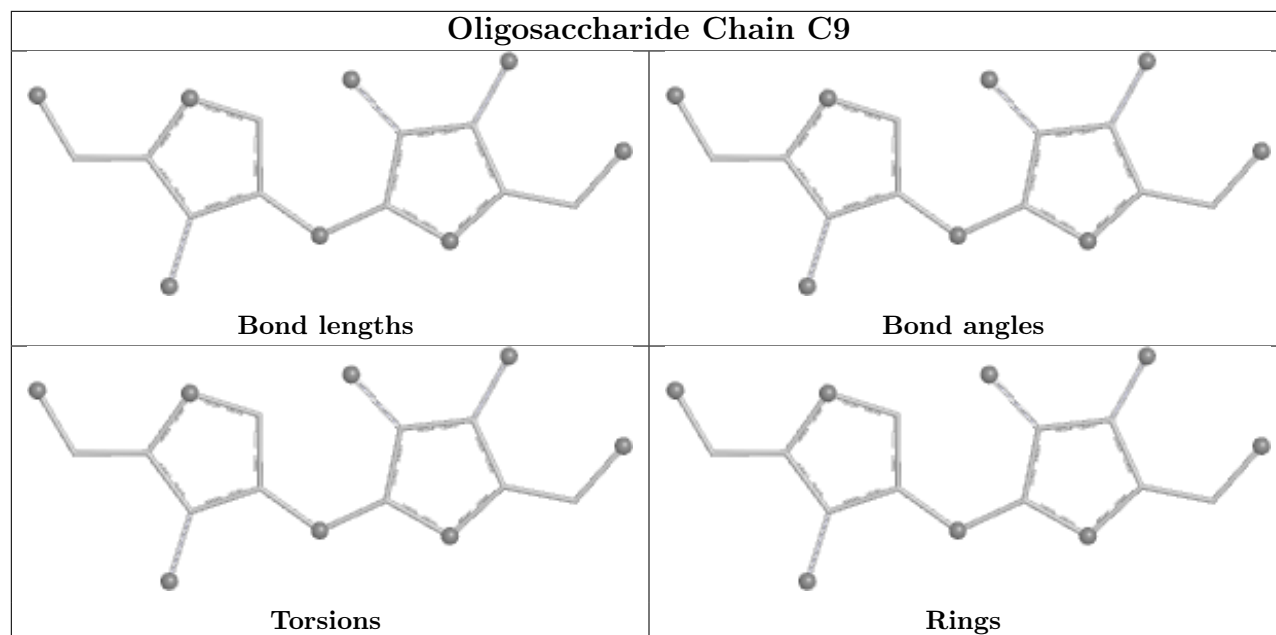
Oligosaccharide Chain C5

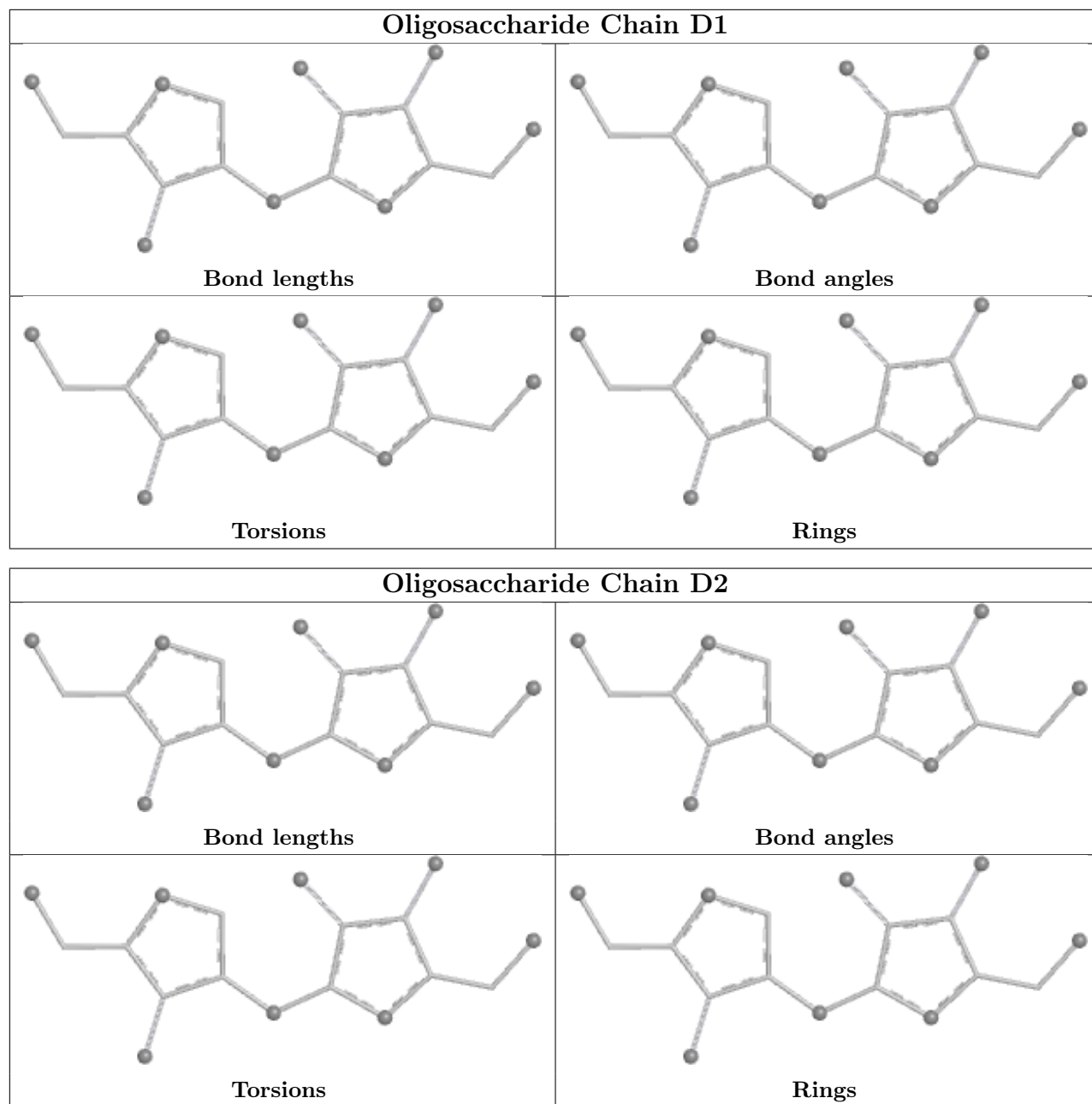


Oligosaccharide Chain C6

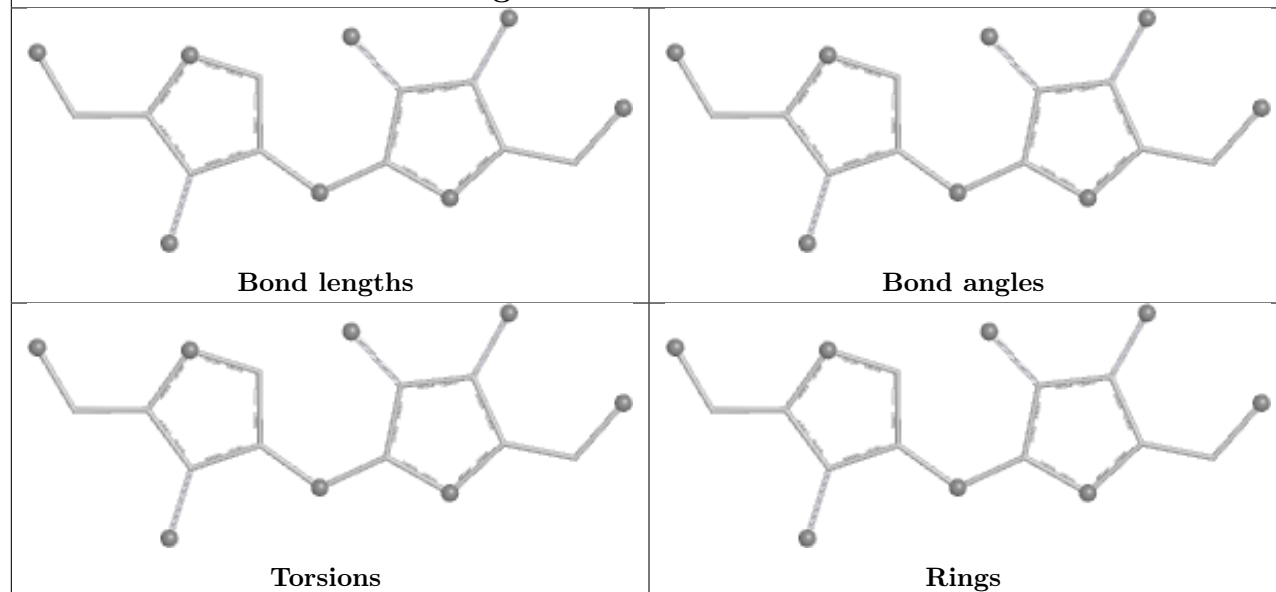




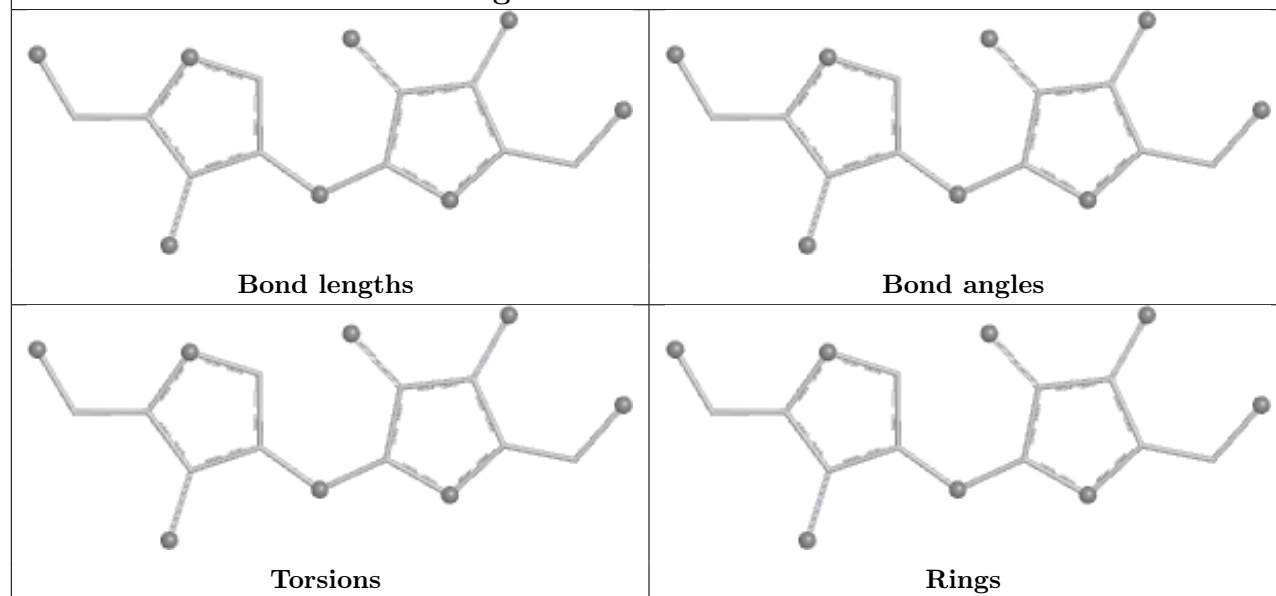


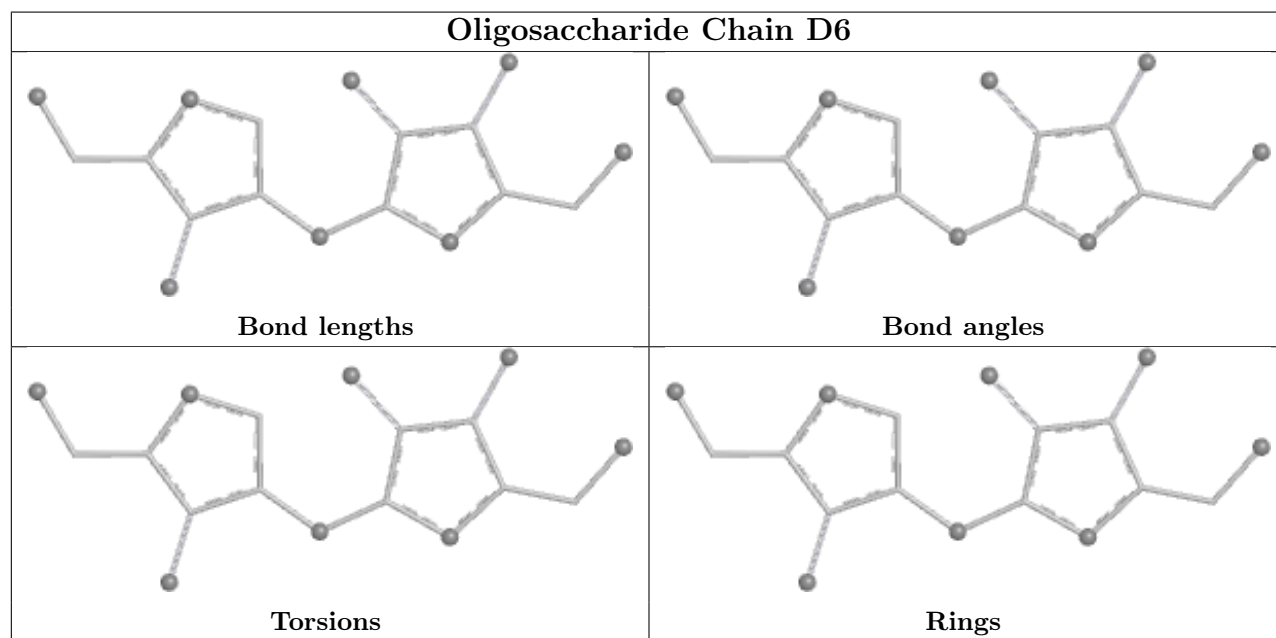
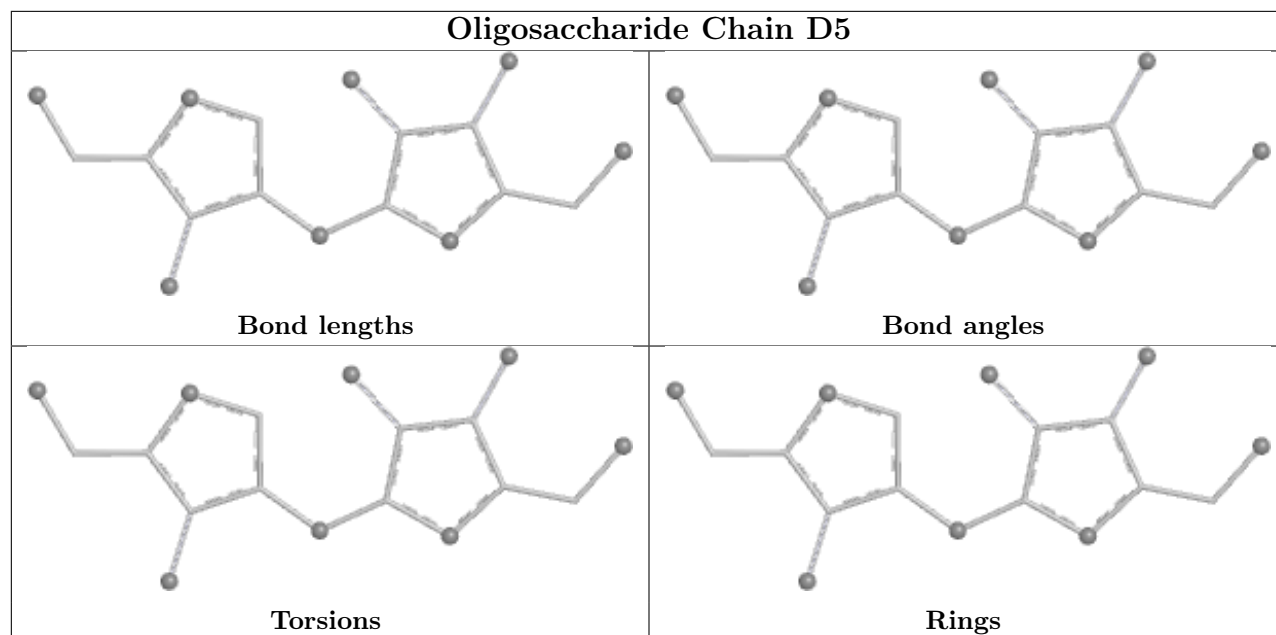


Oligosaccharide Chain D3

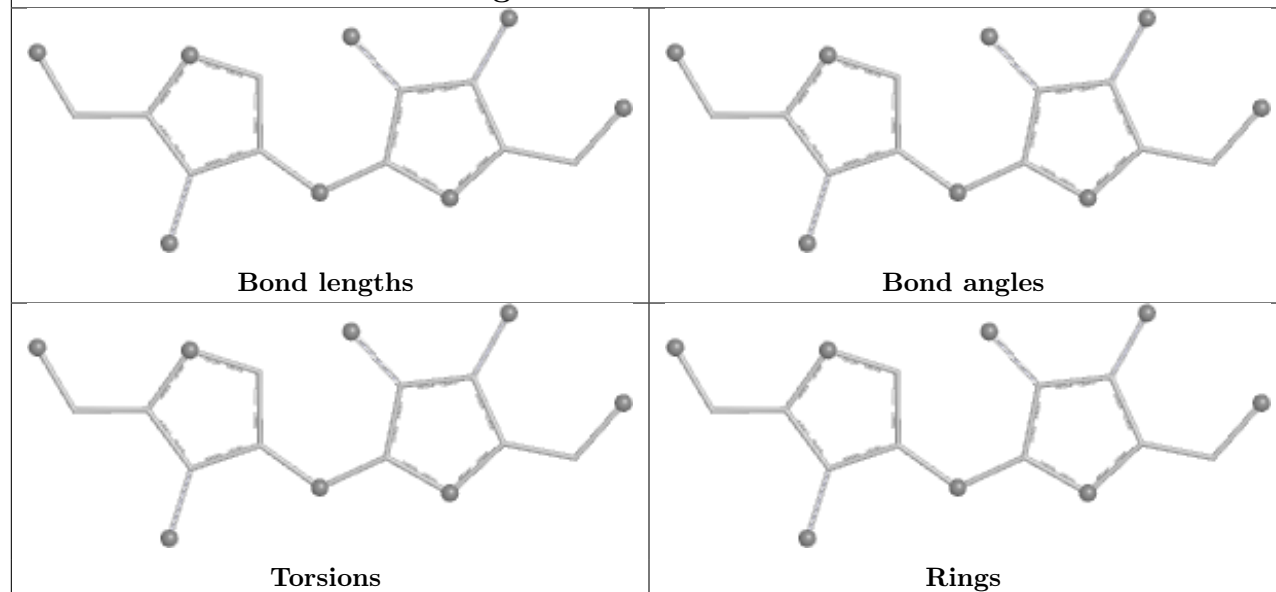


Oligosaccharide Chain D4

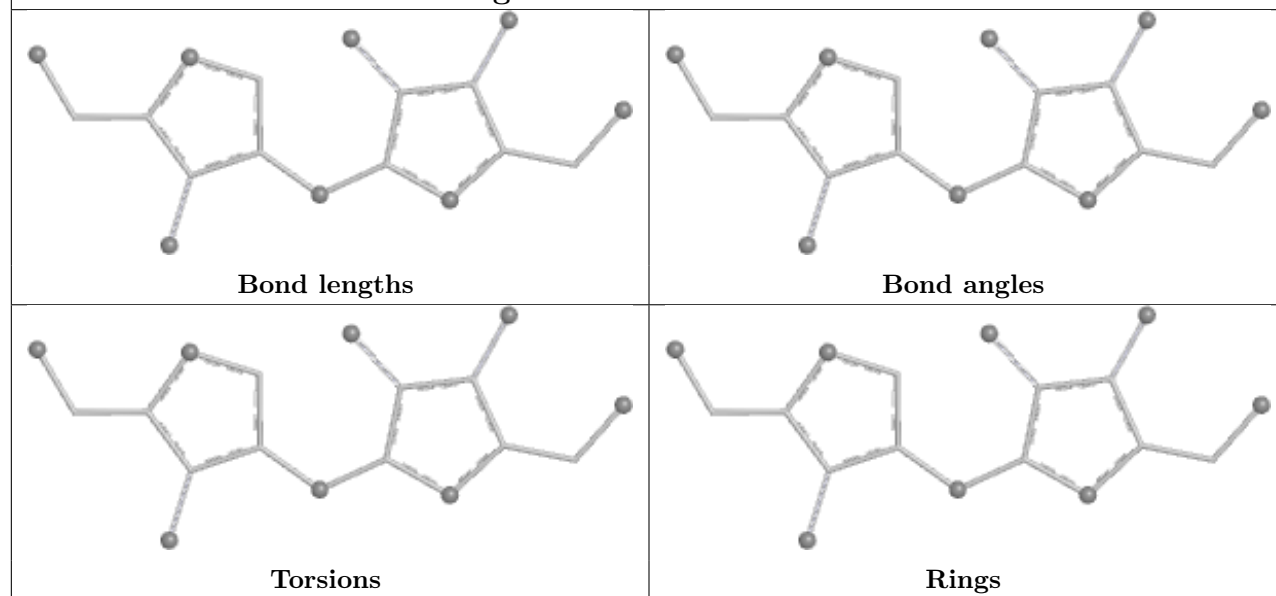




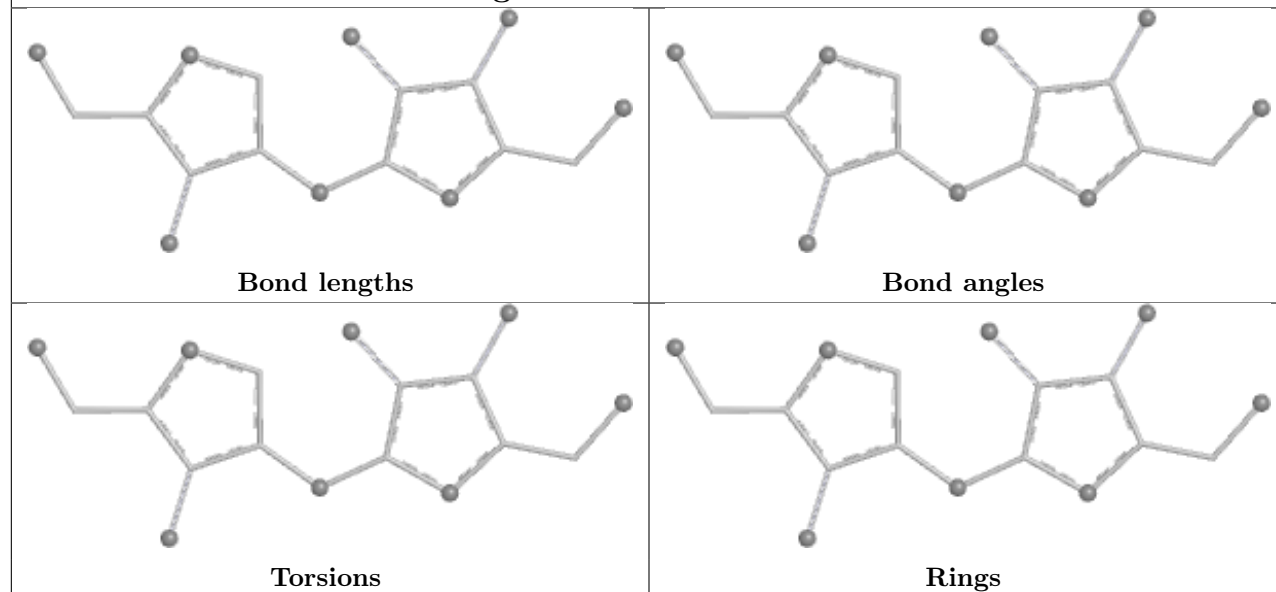
Oligosaccharide Chain D7



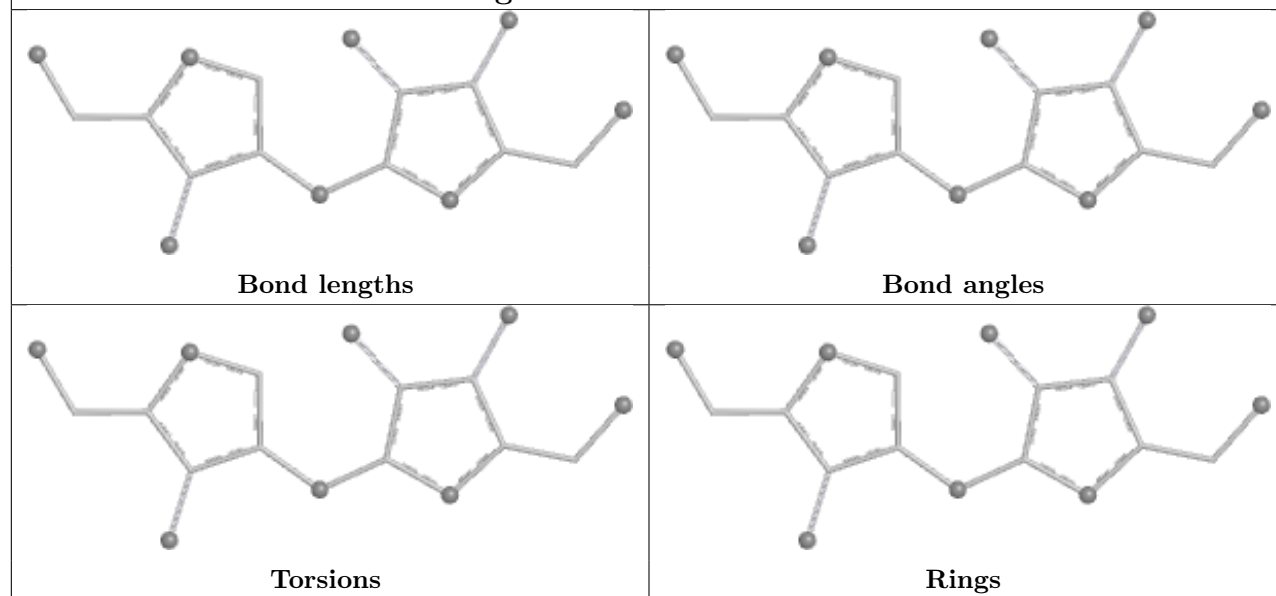
Oligosaccharide Chain D8

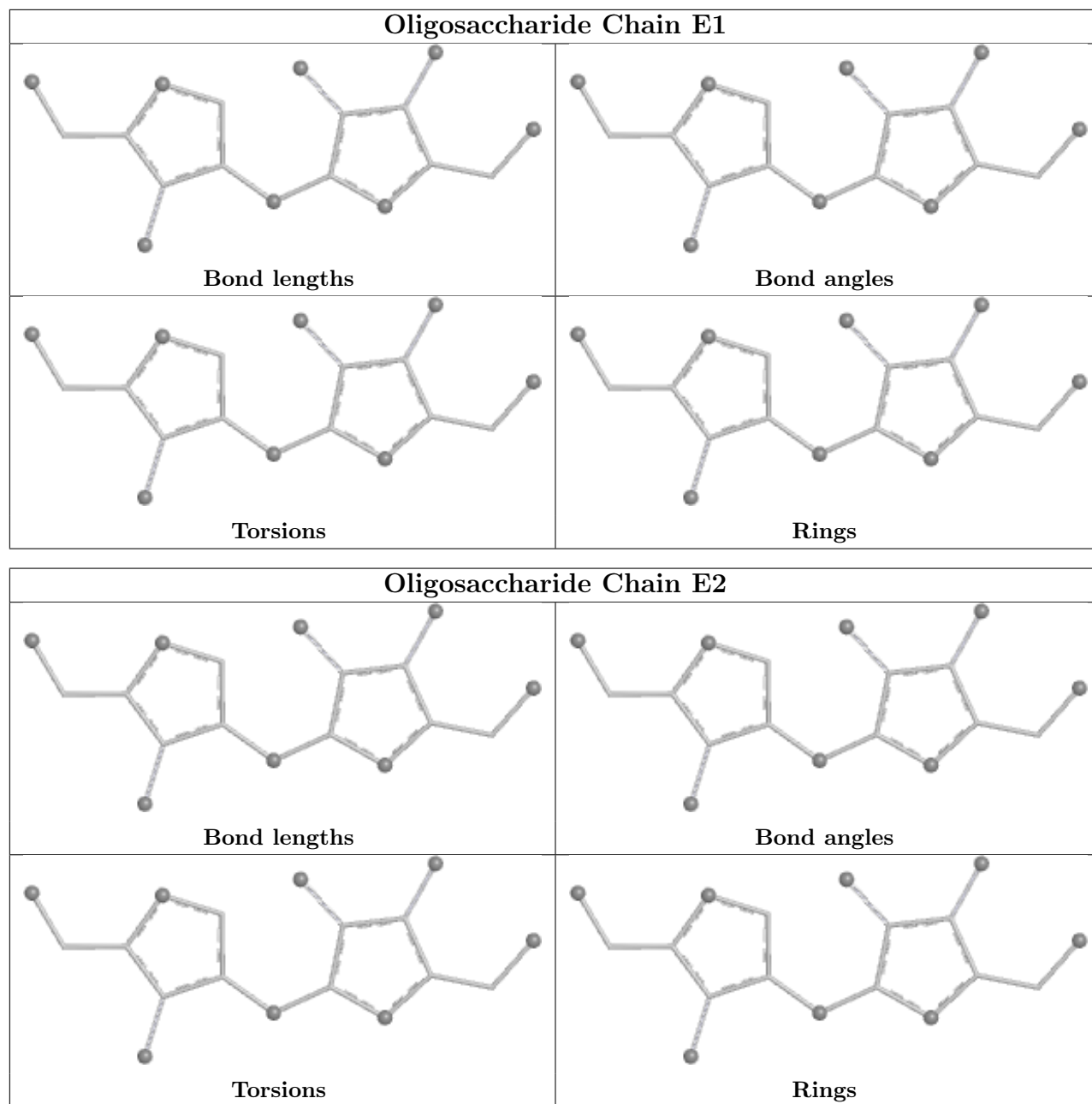


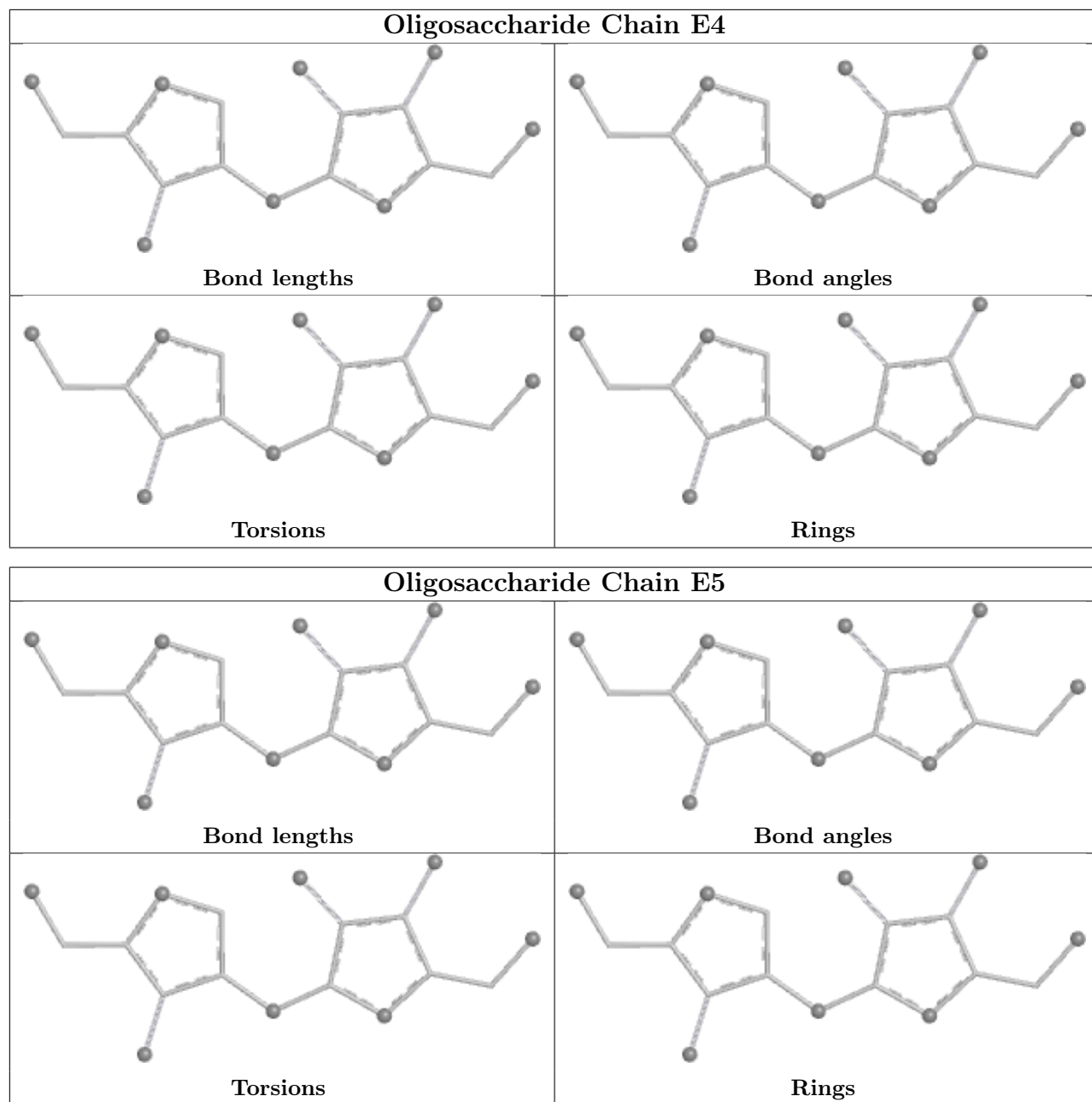
Oligosaccharide Chain D9

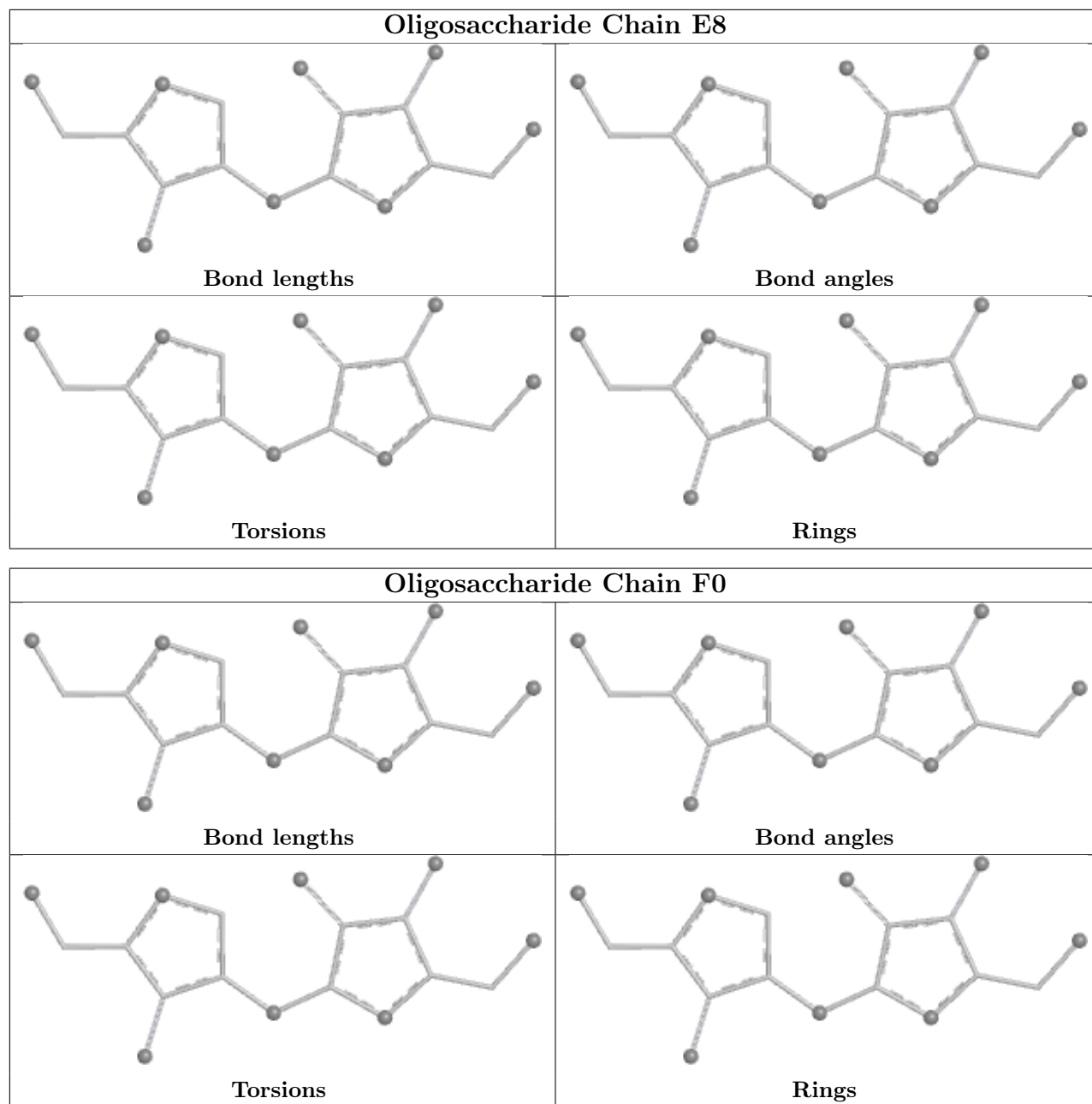


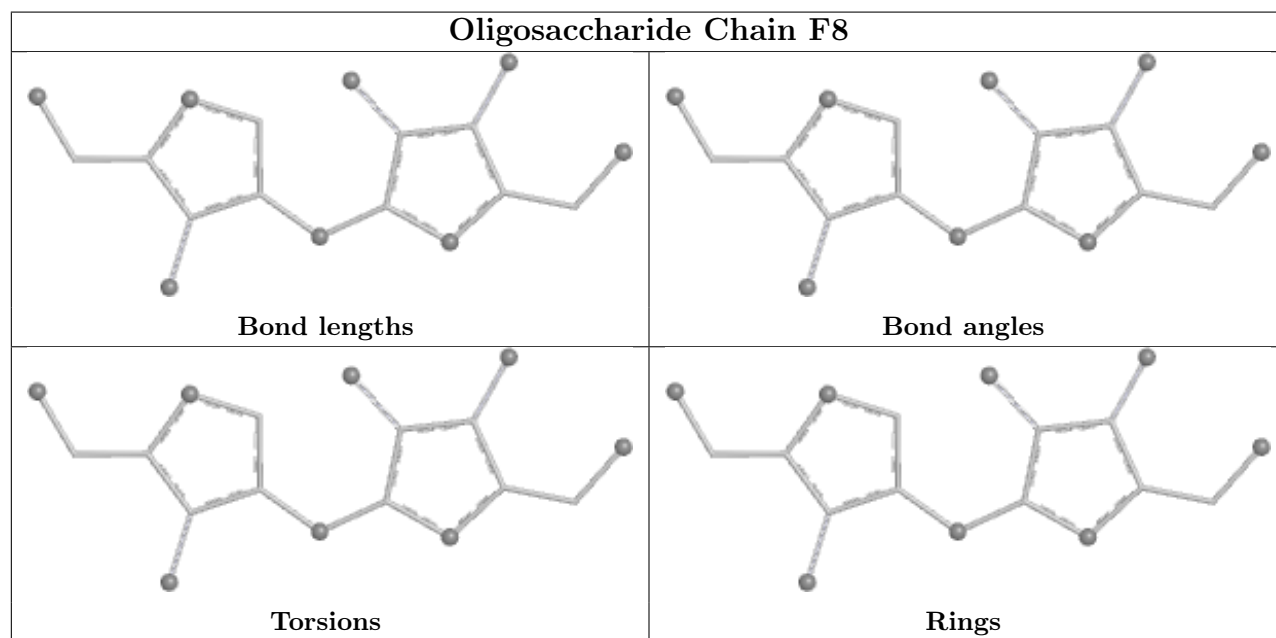
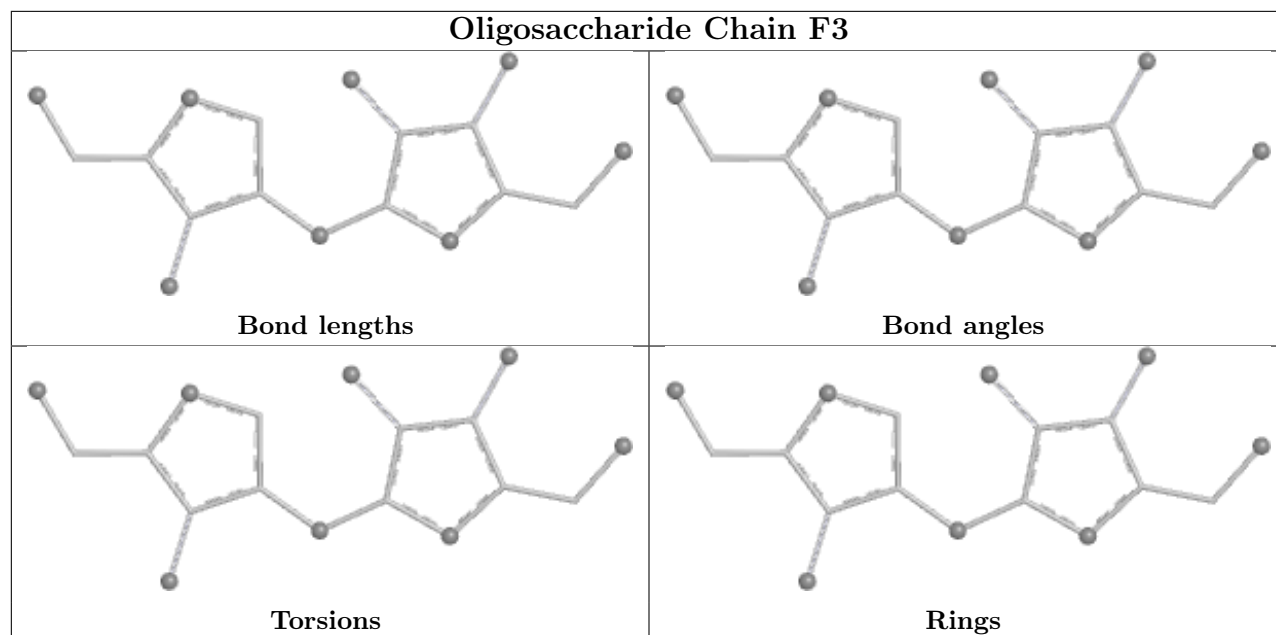
Oligosaccharide Chain E0

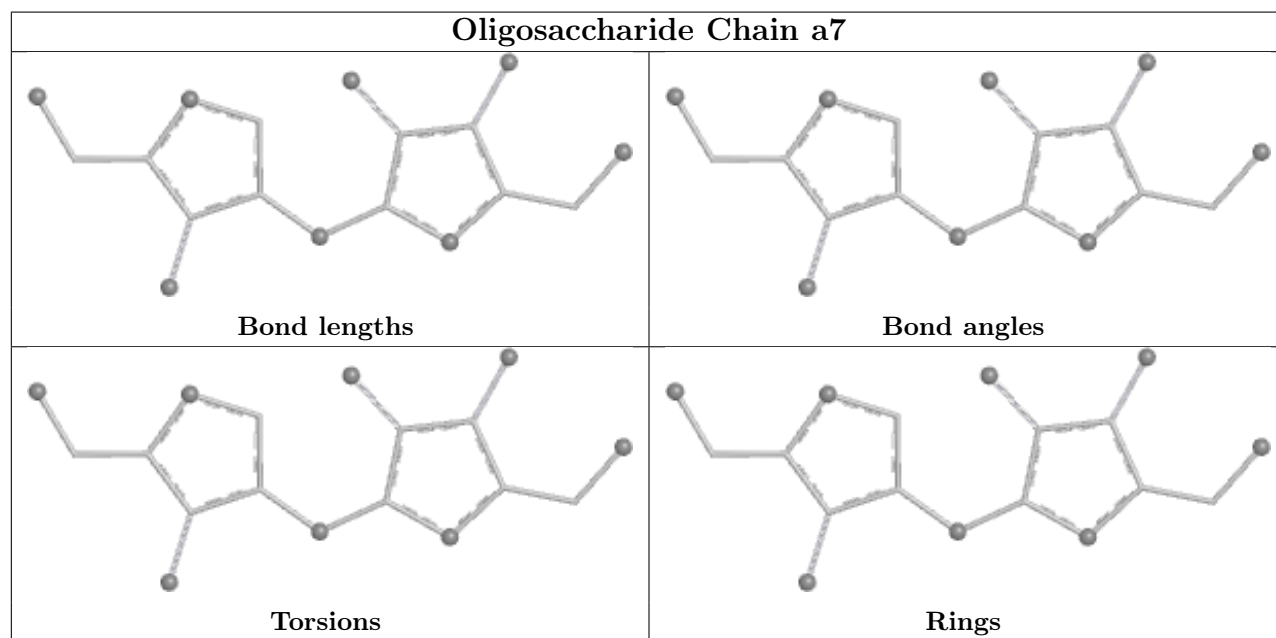
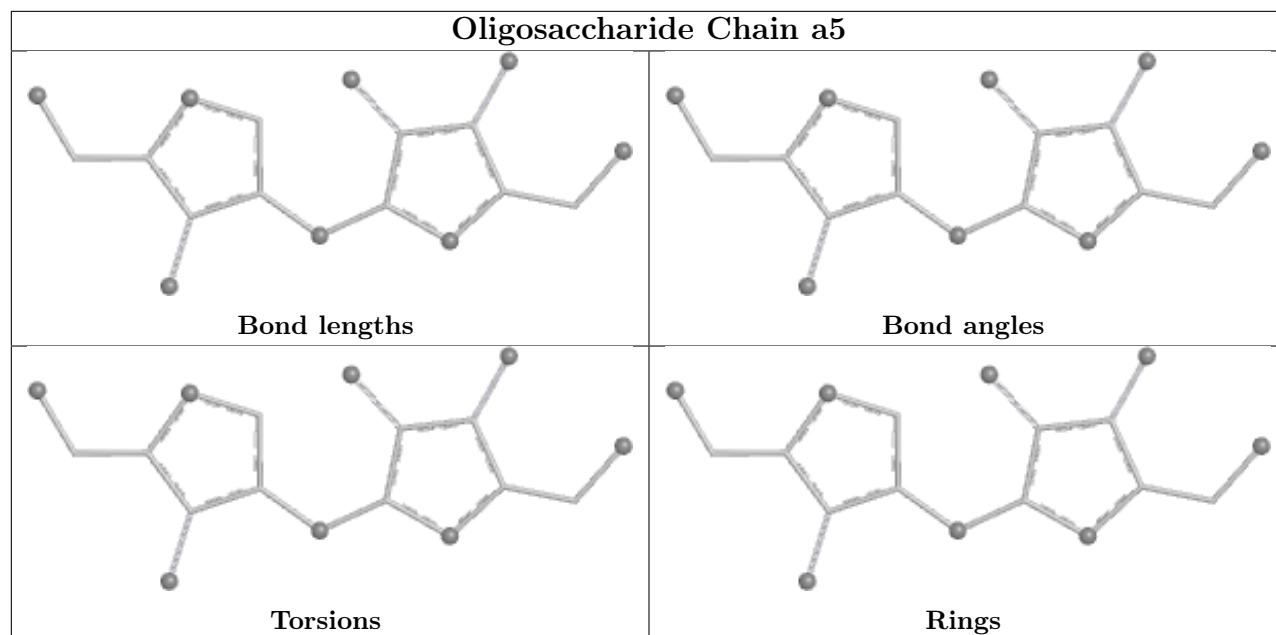


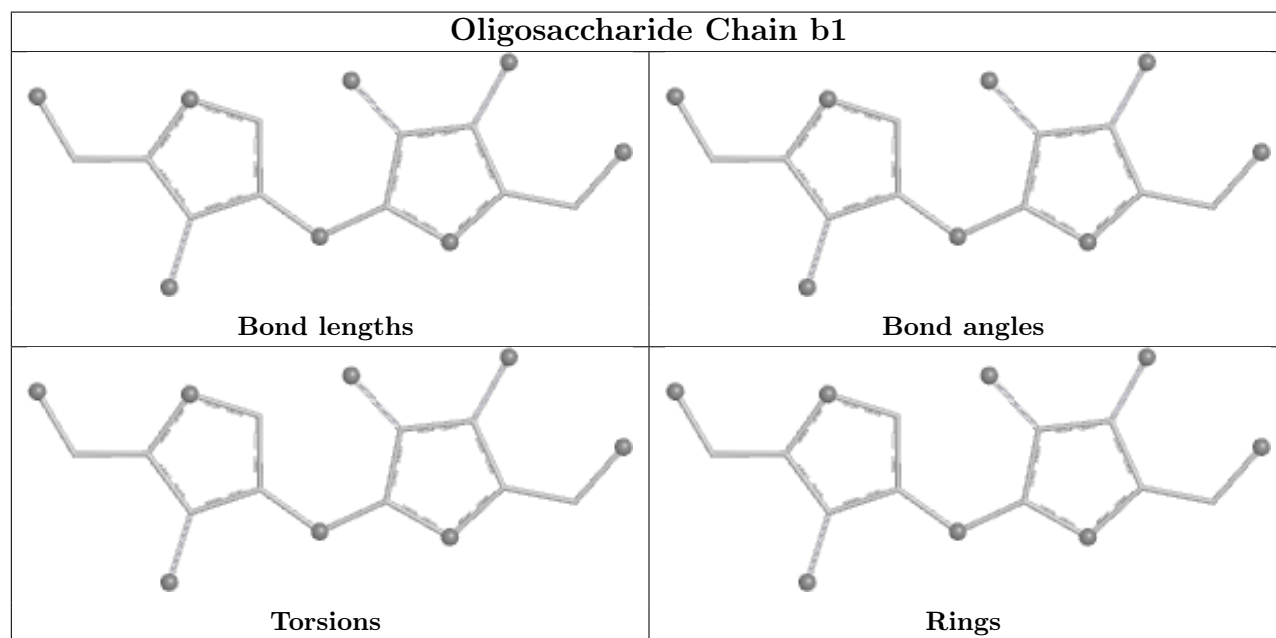
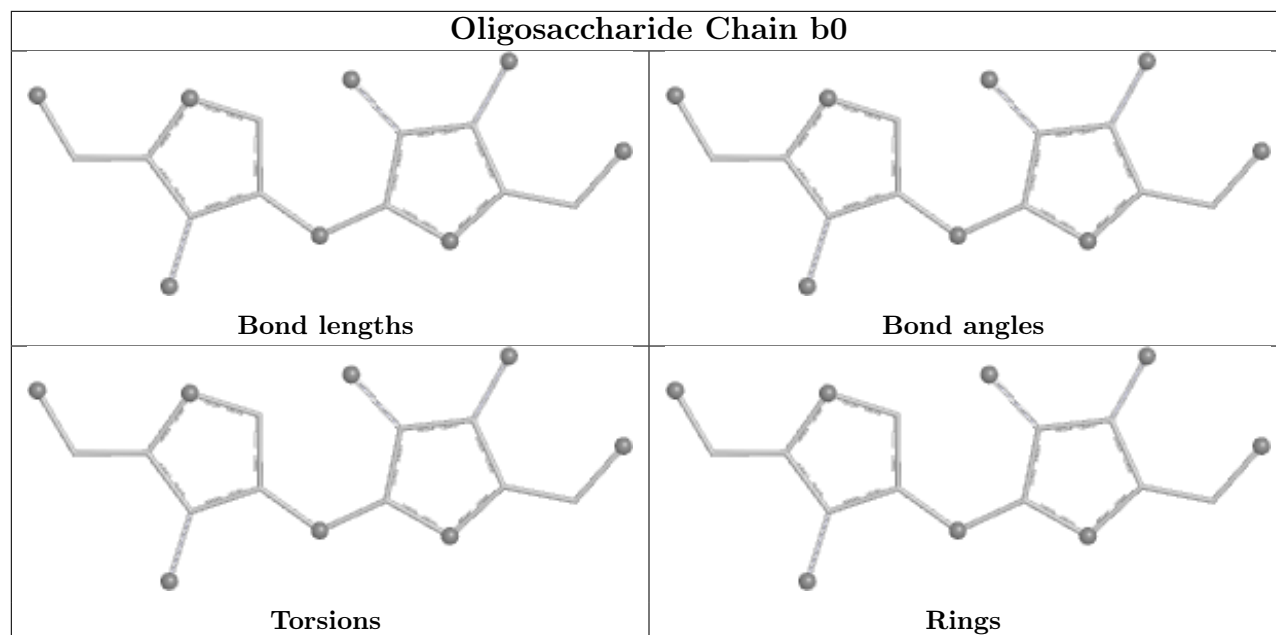


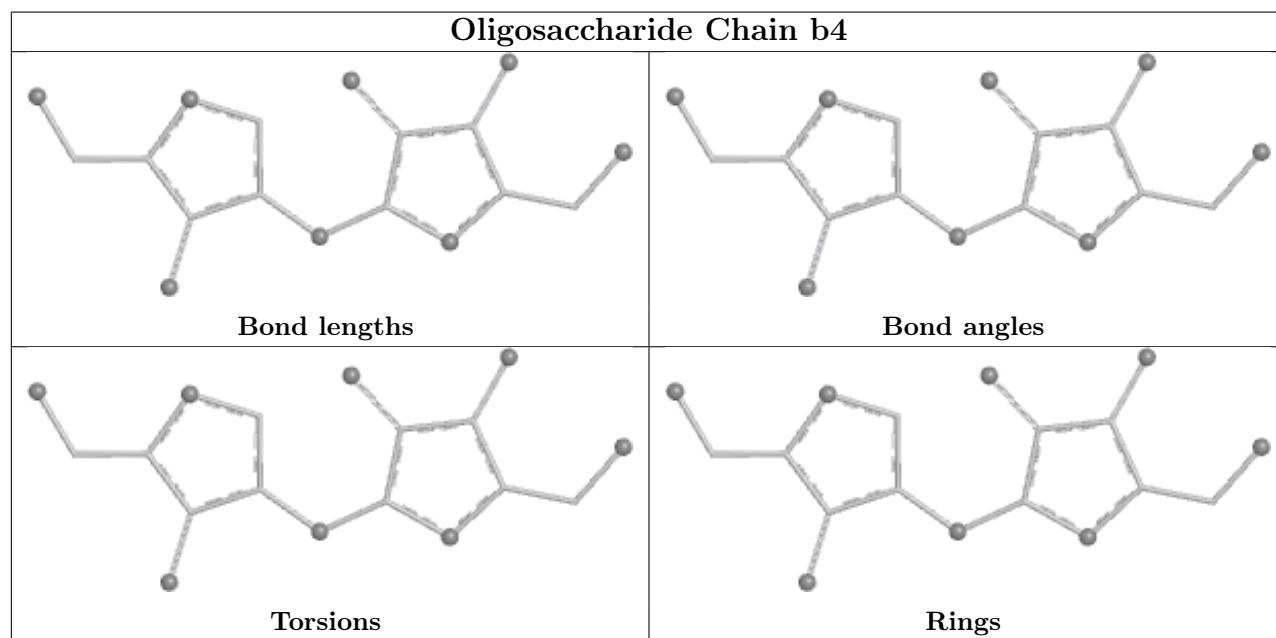
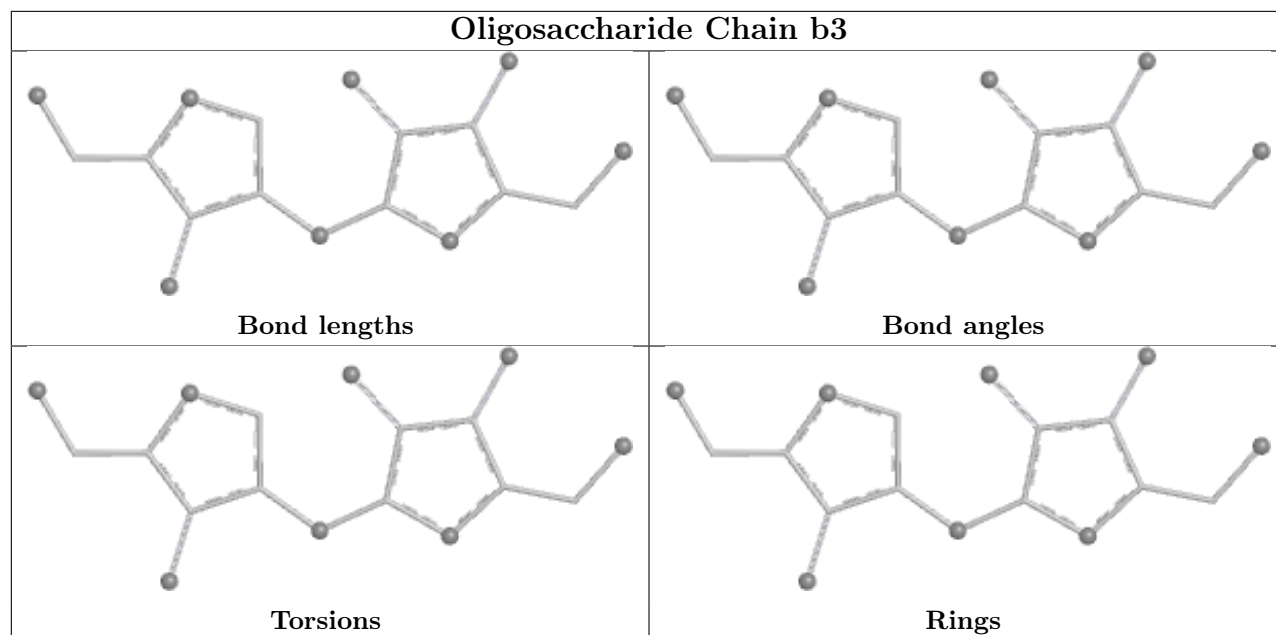


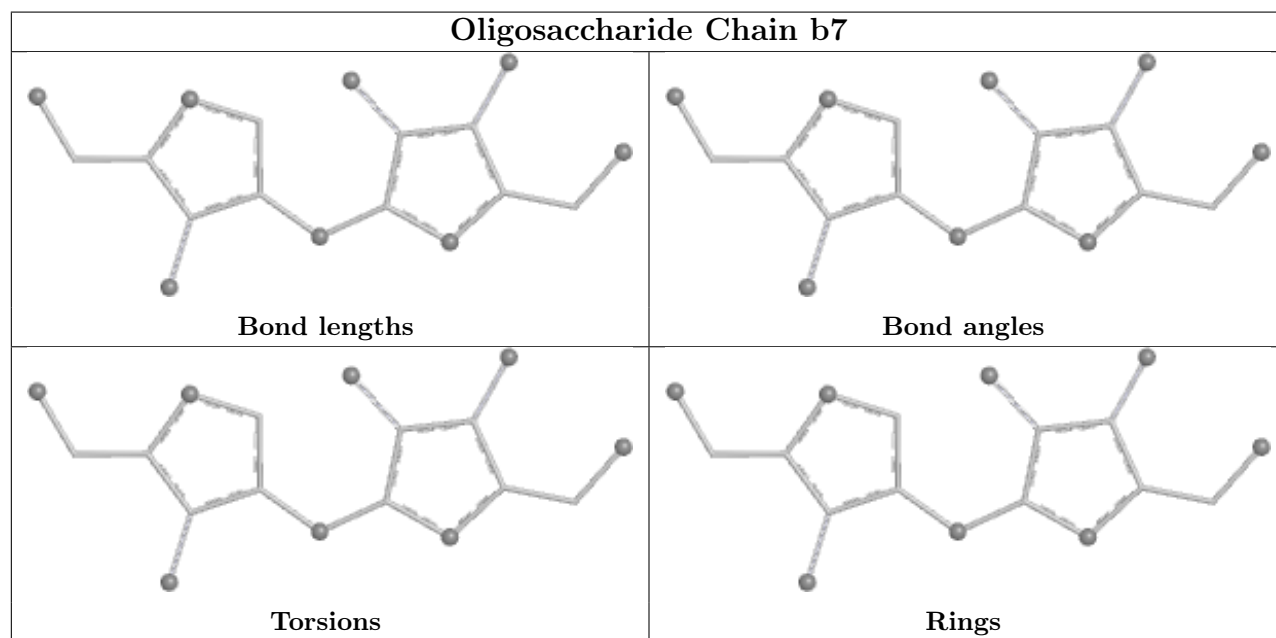
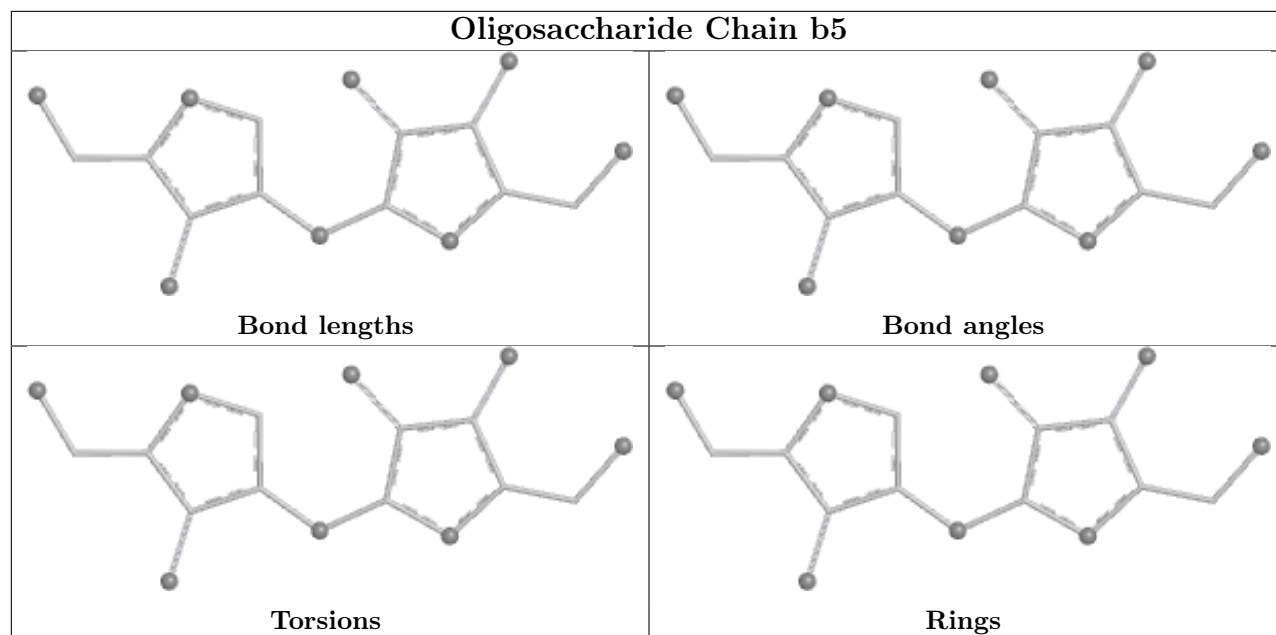


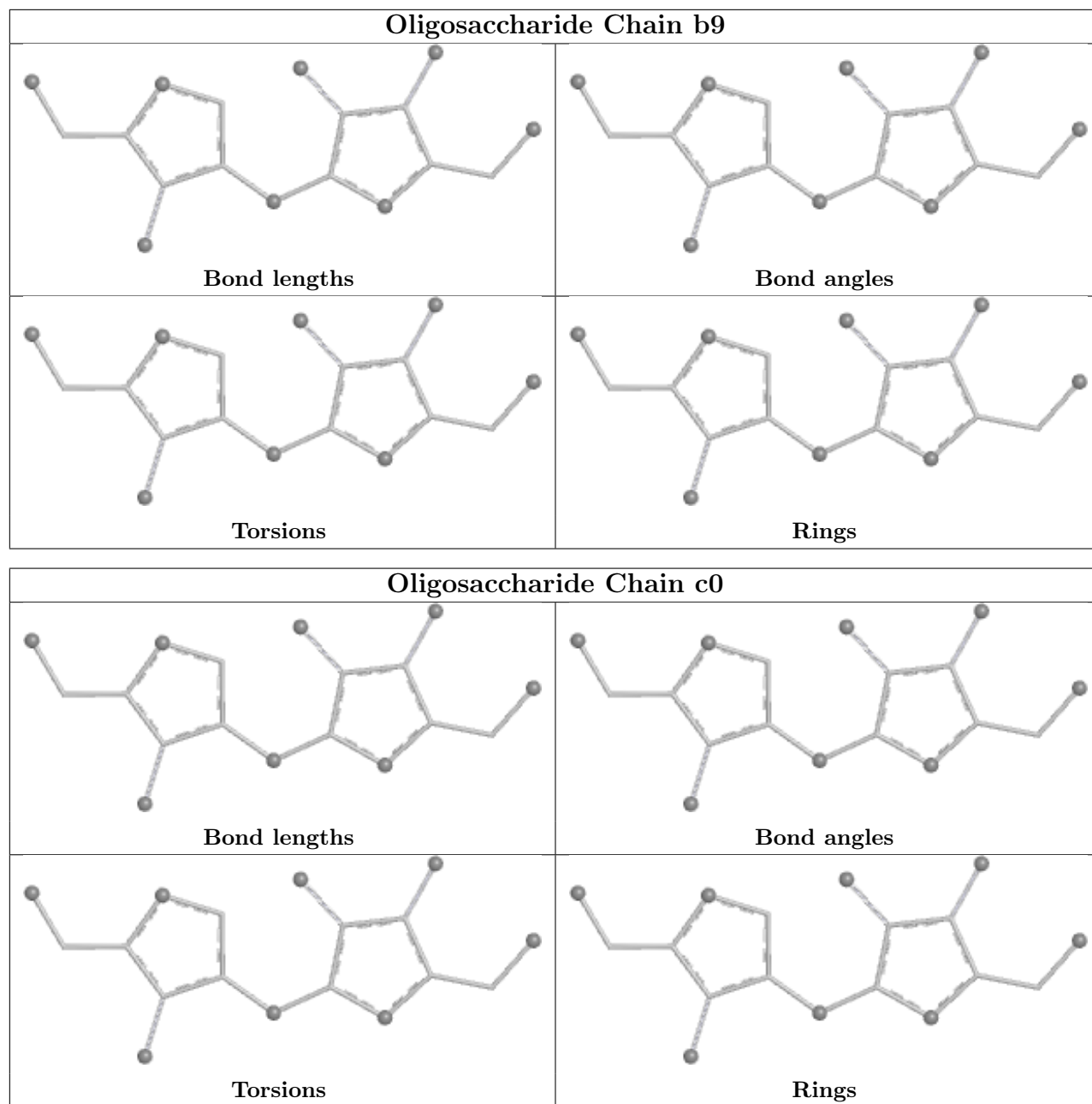


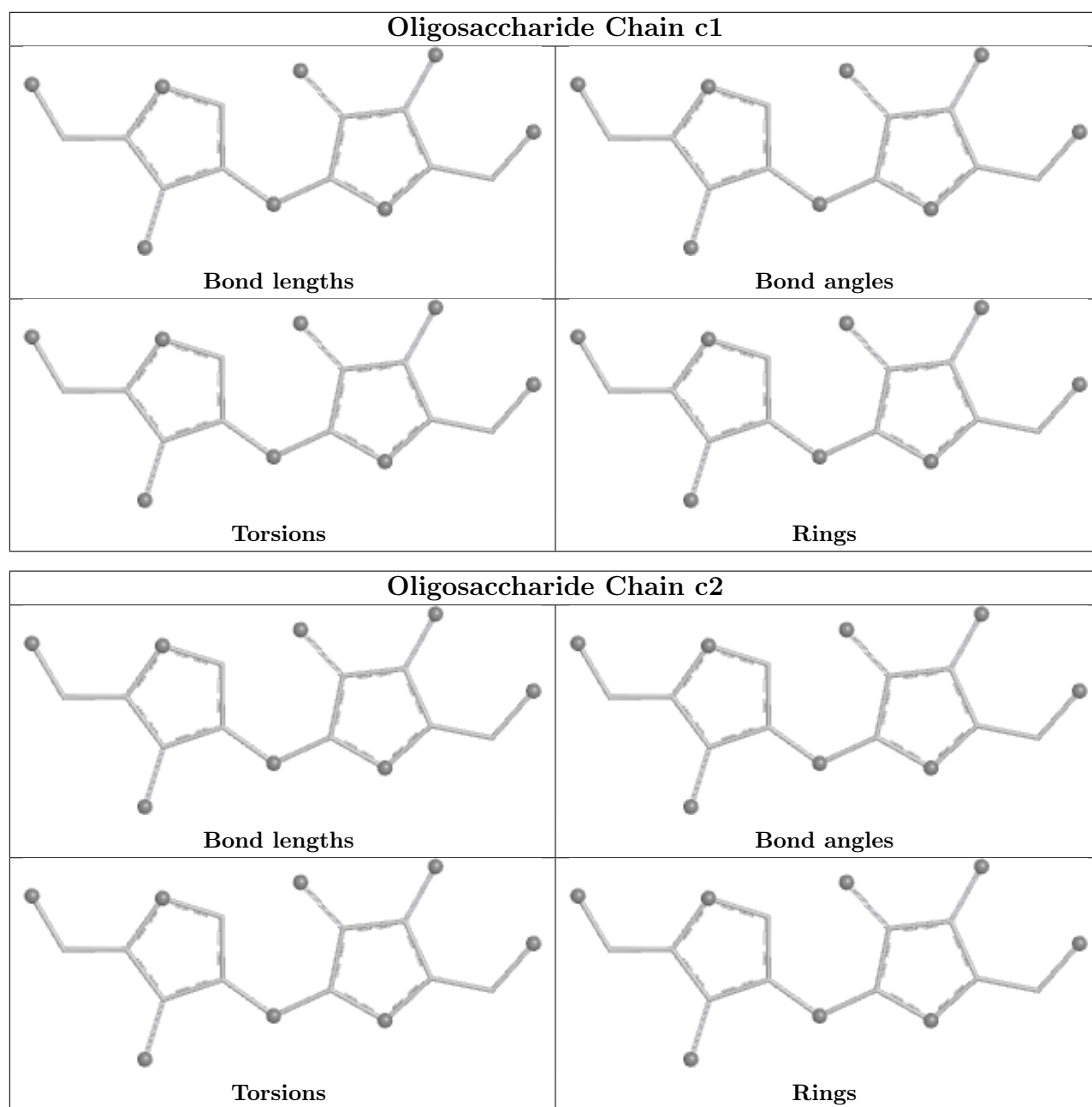


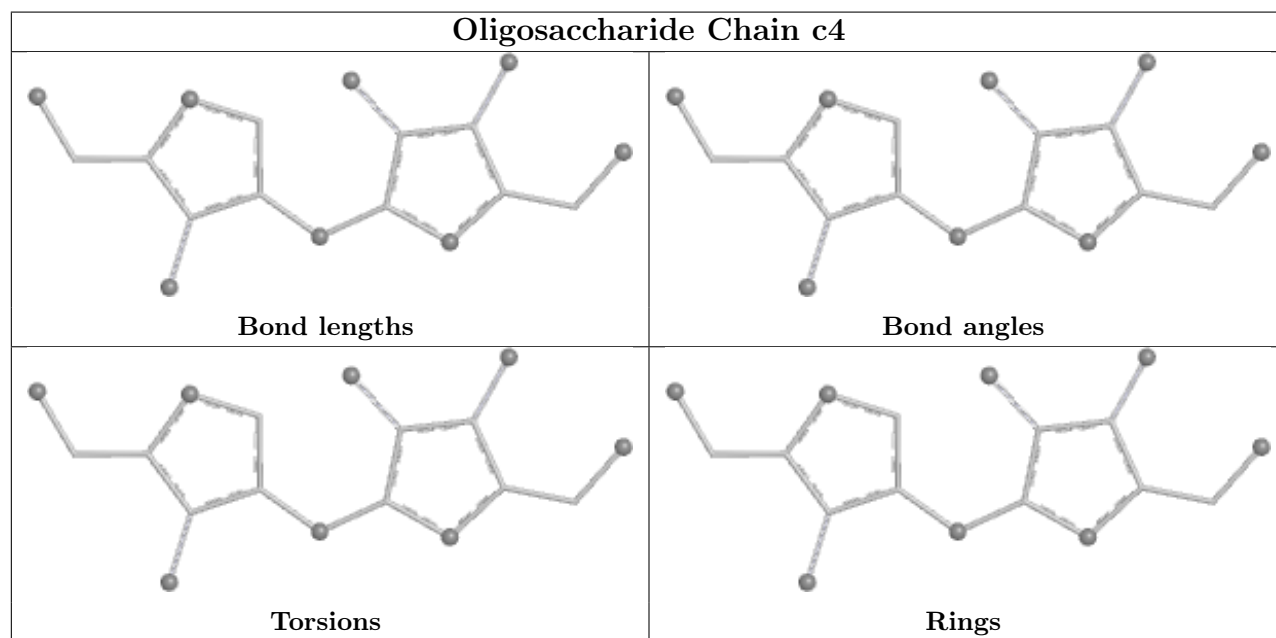
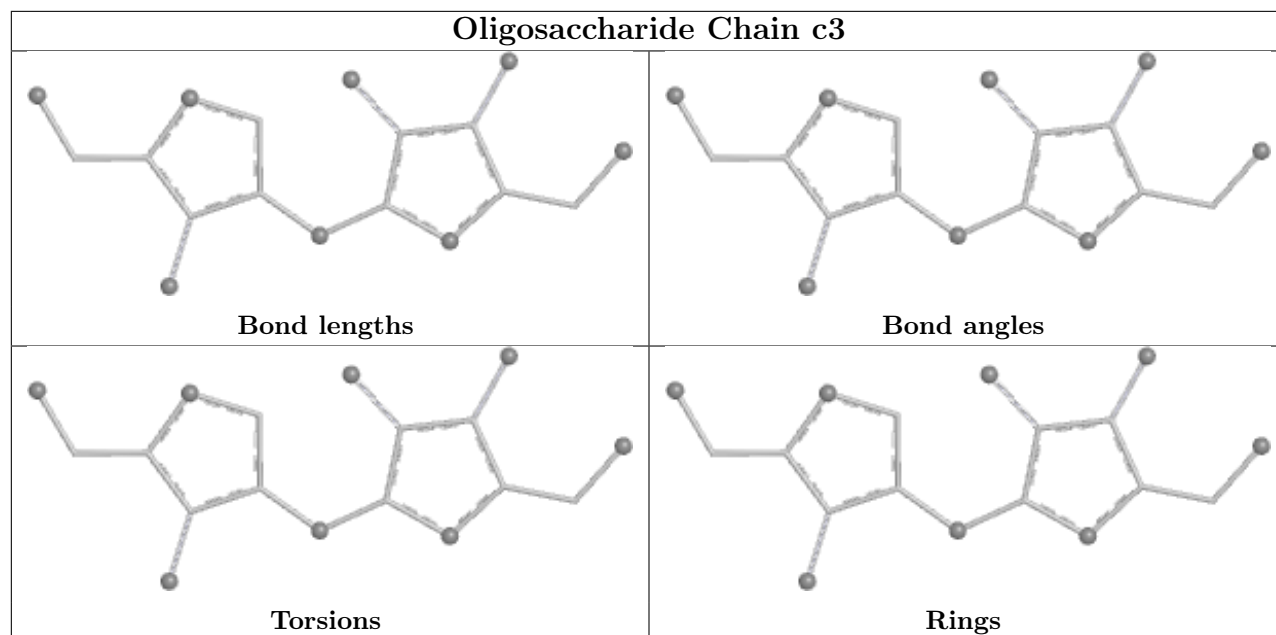


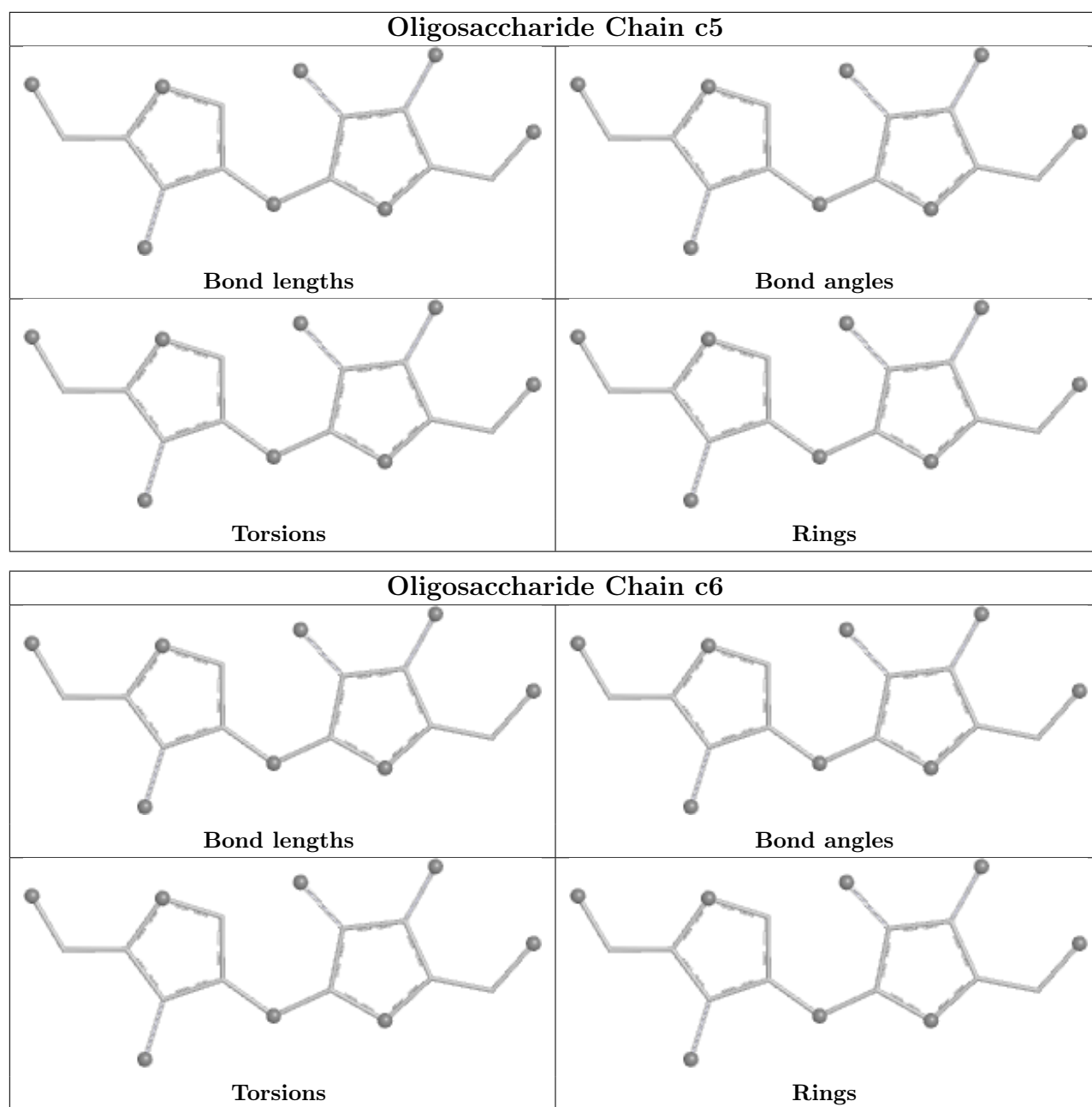


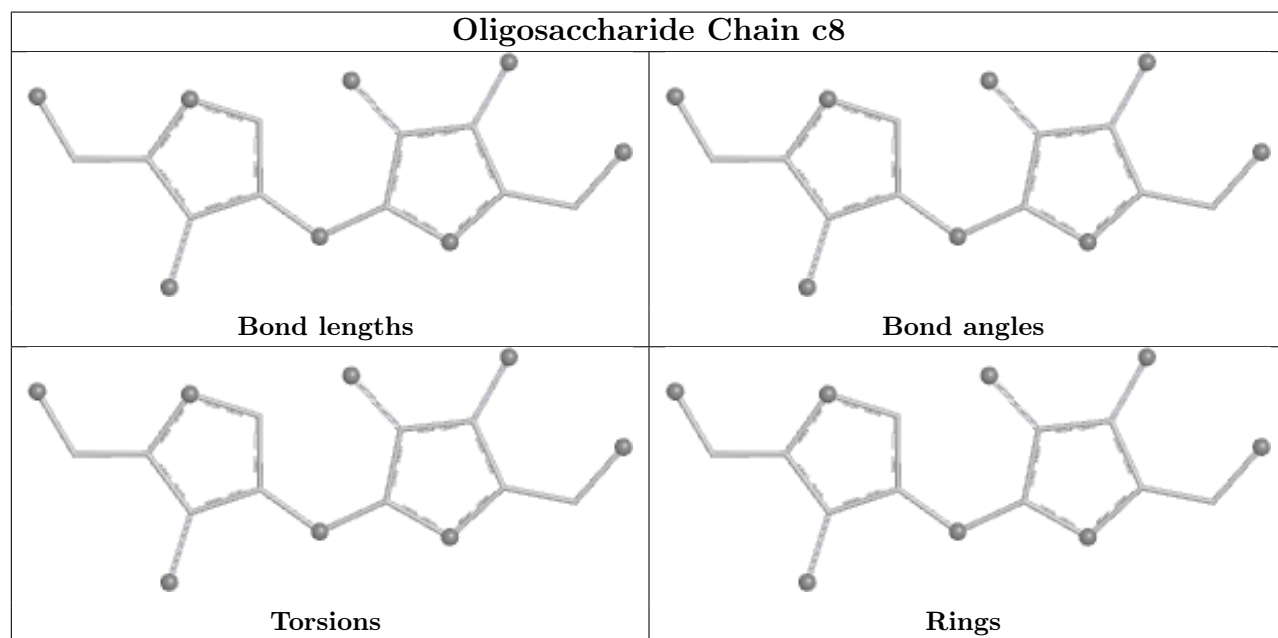
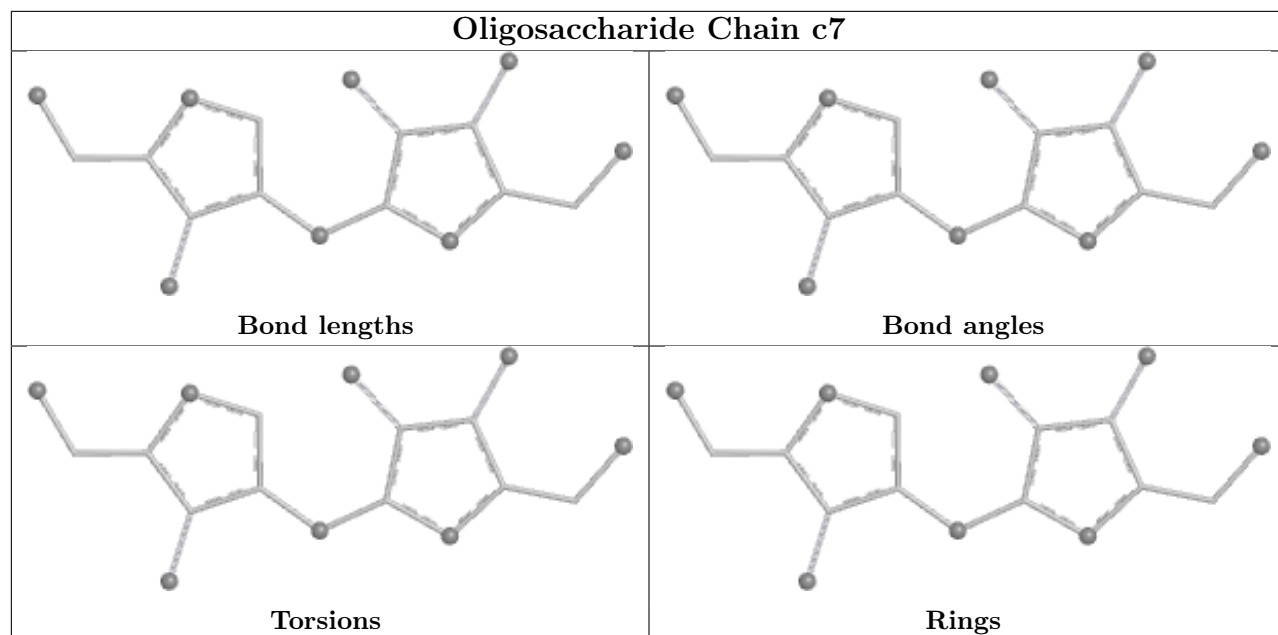


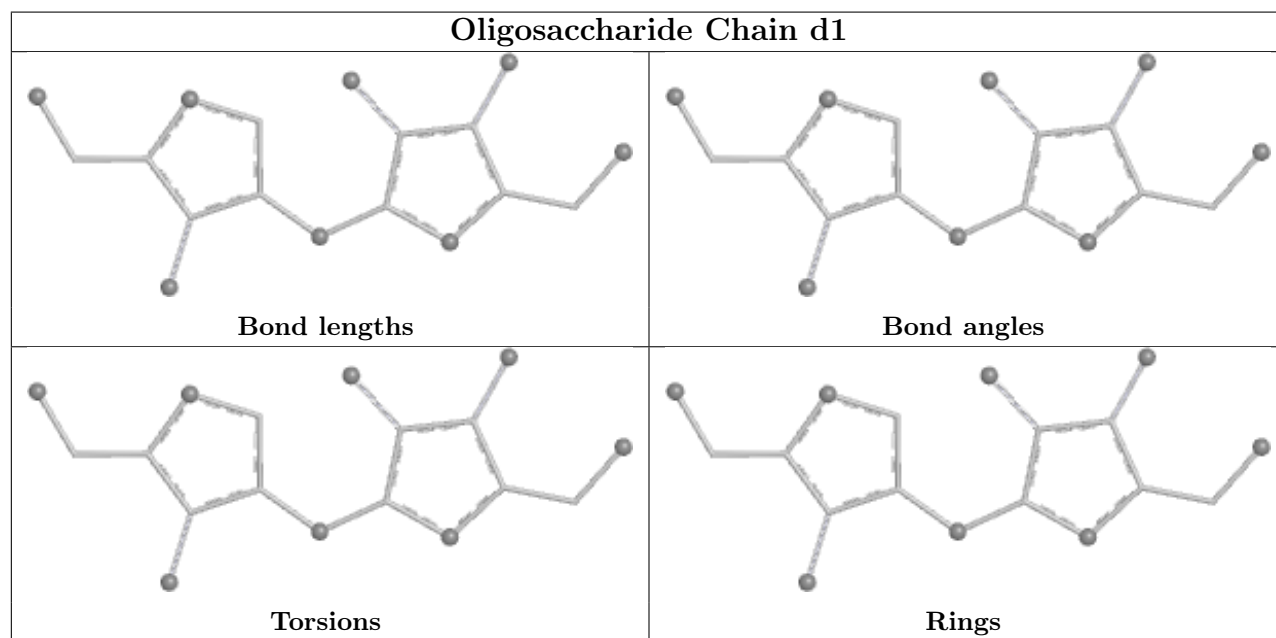
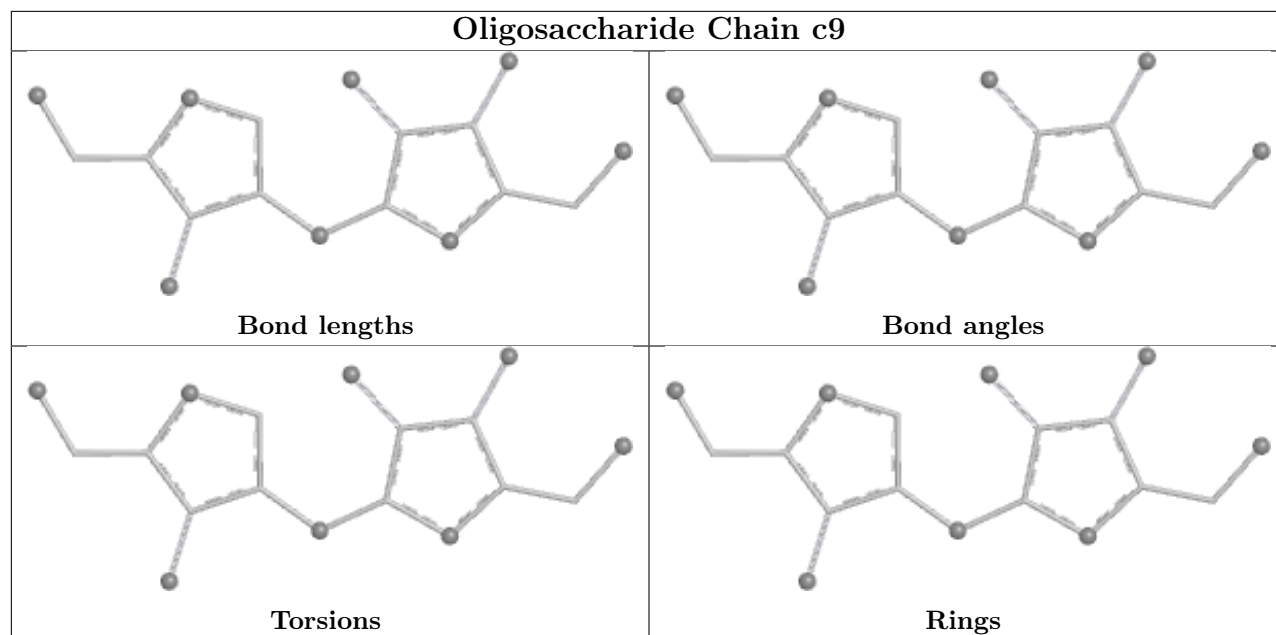


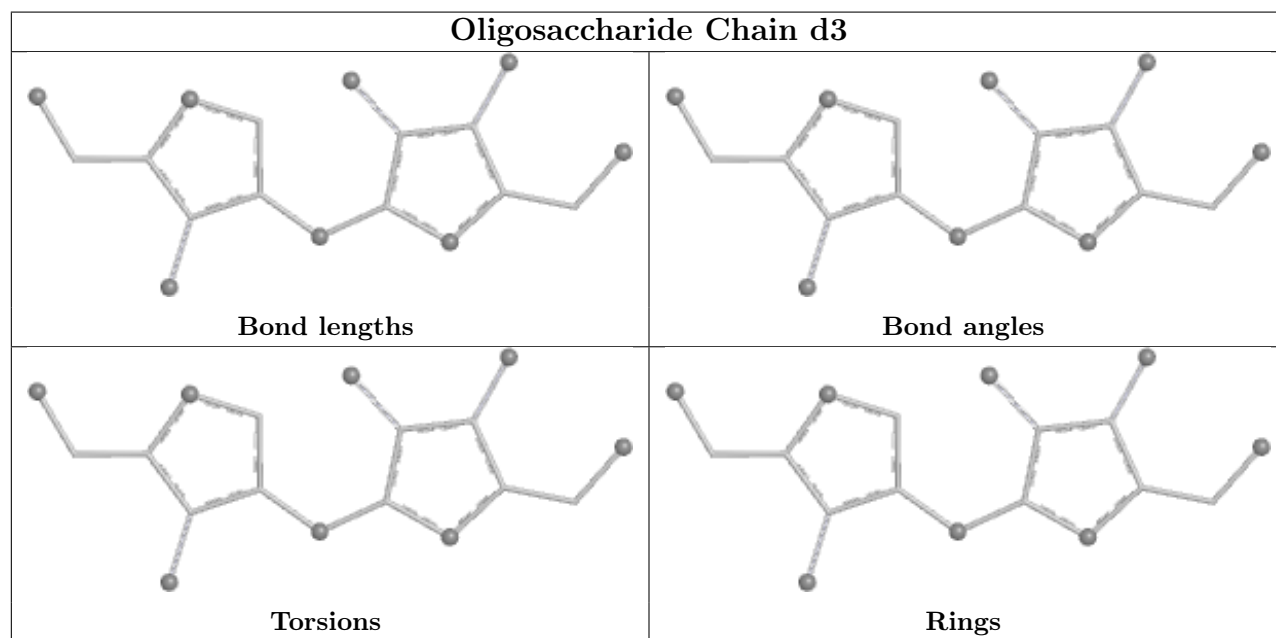
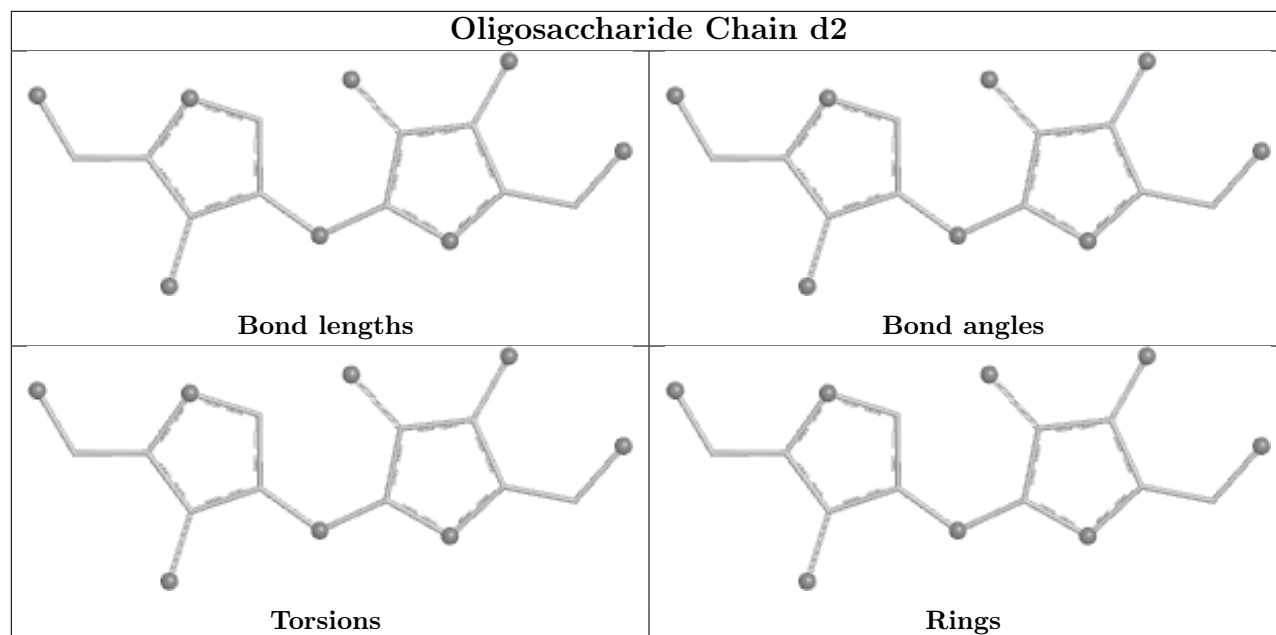


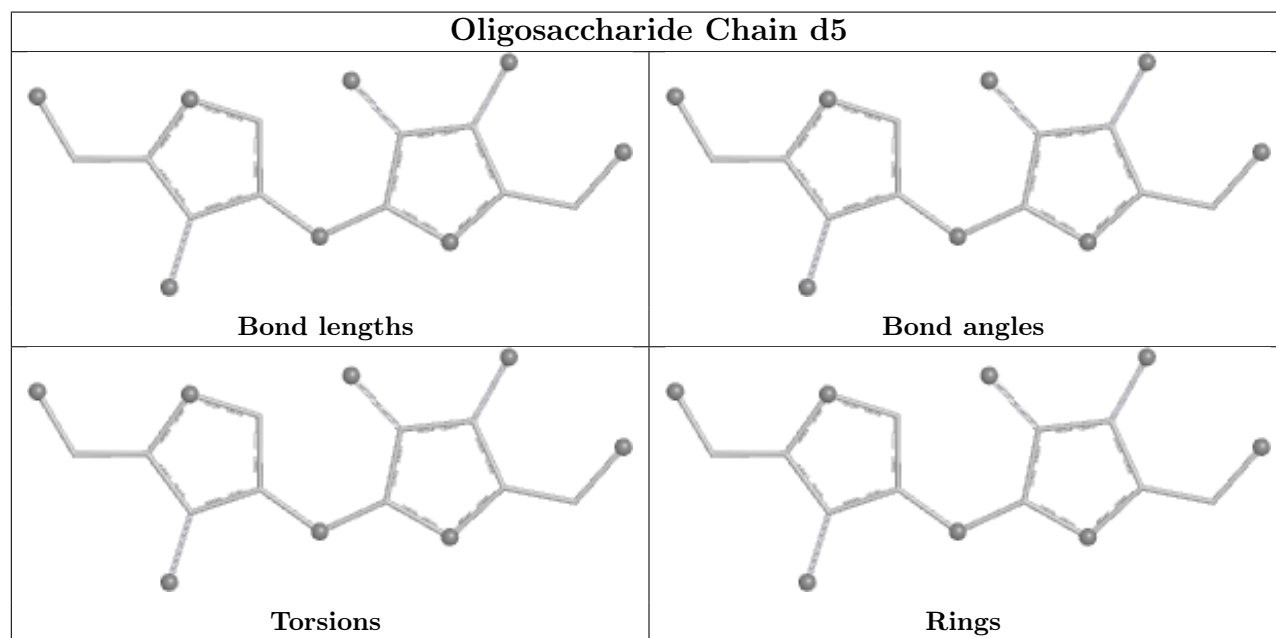
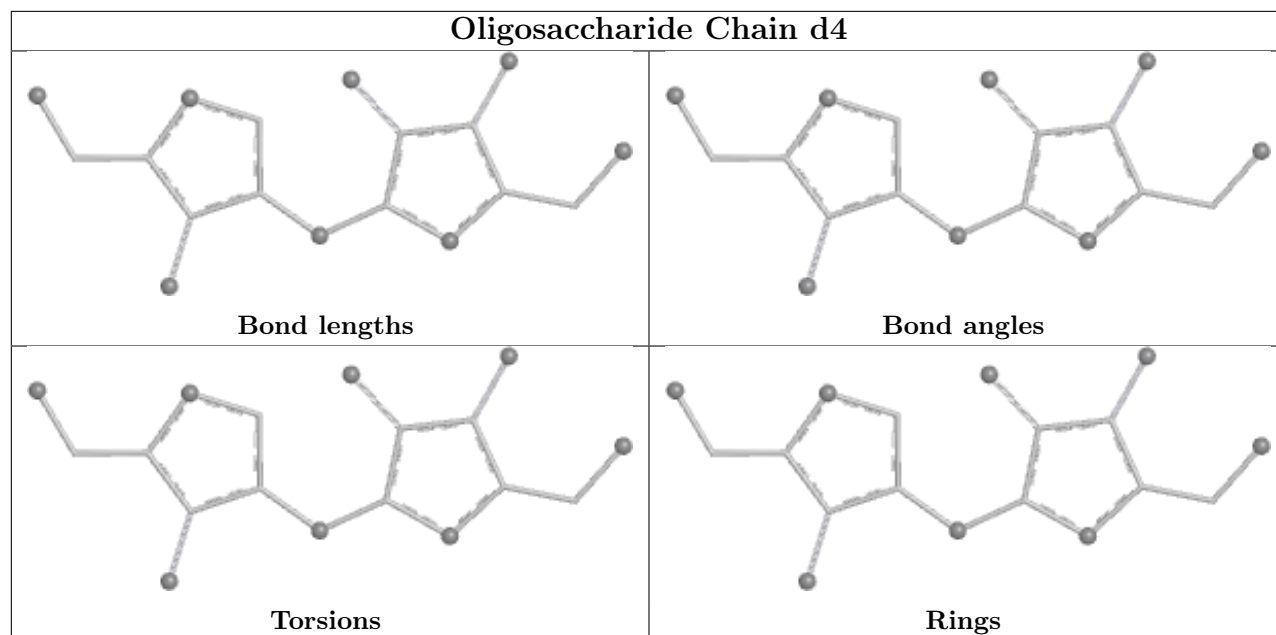


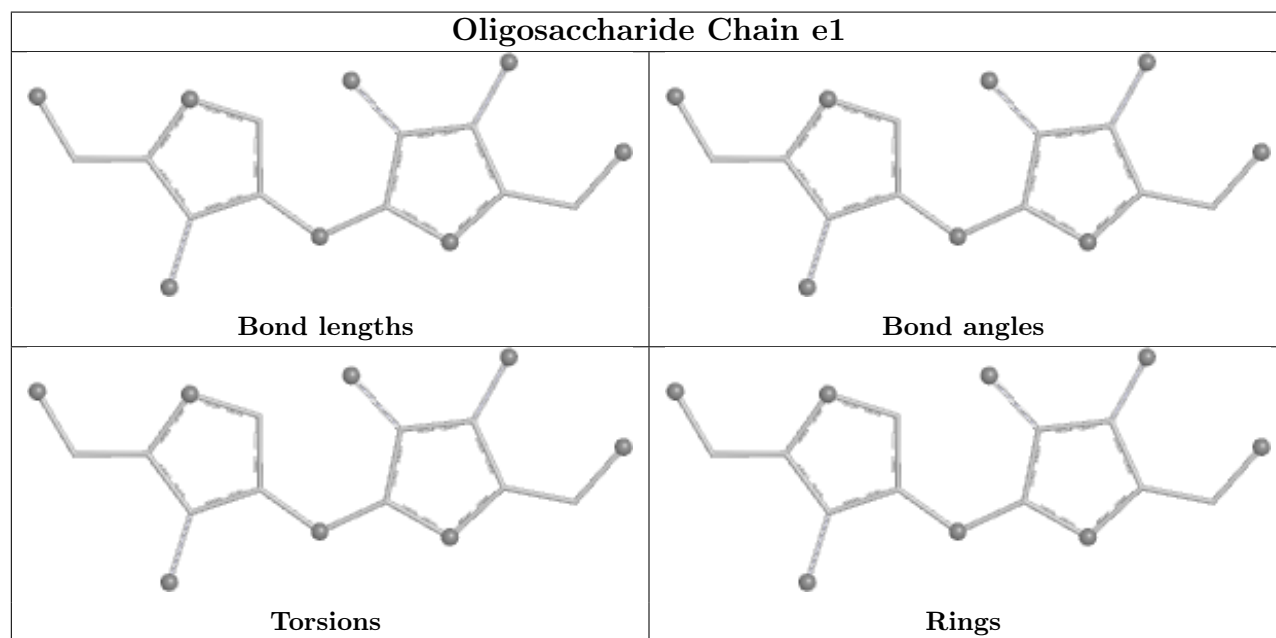
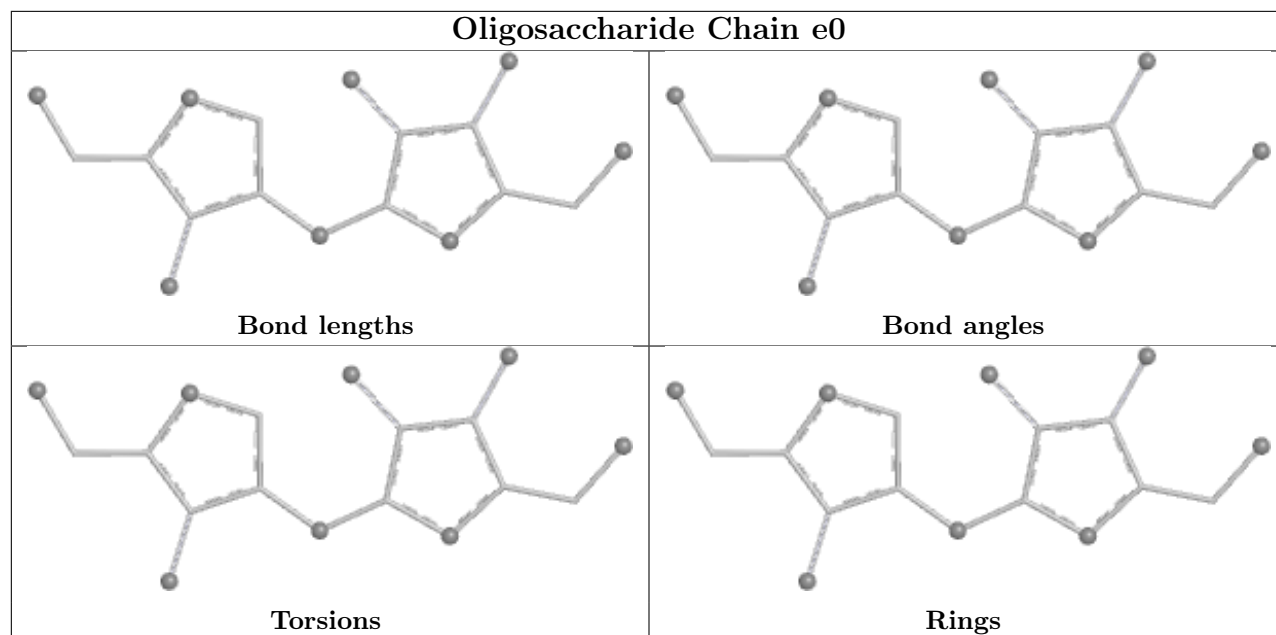


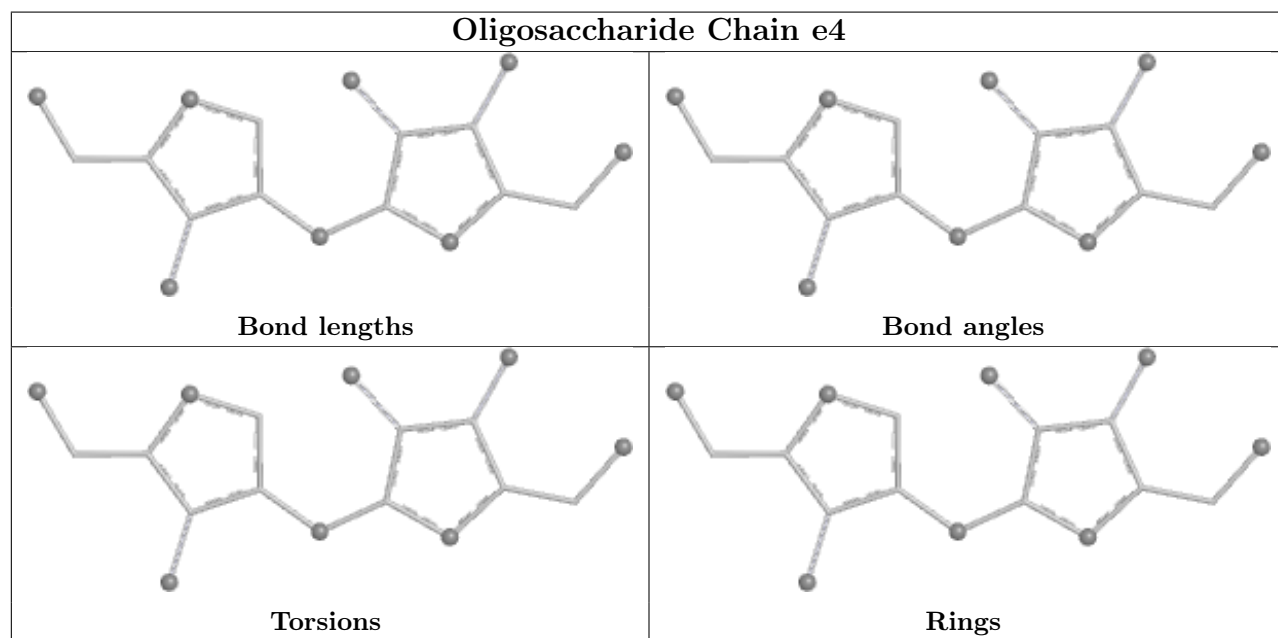
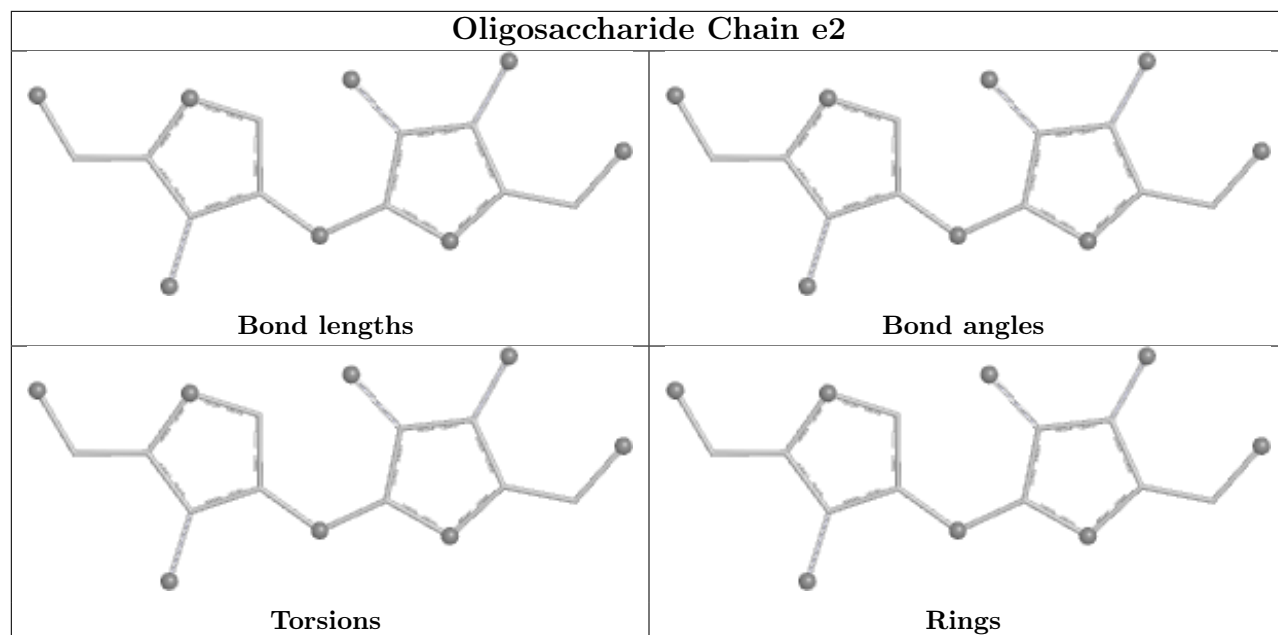


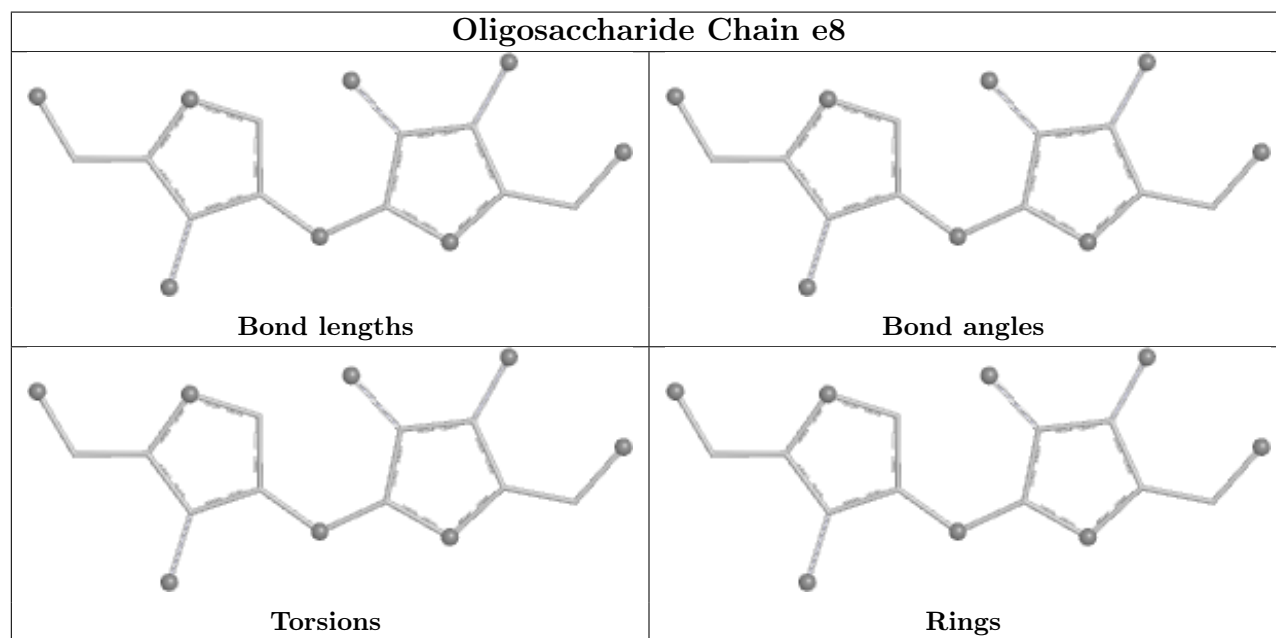
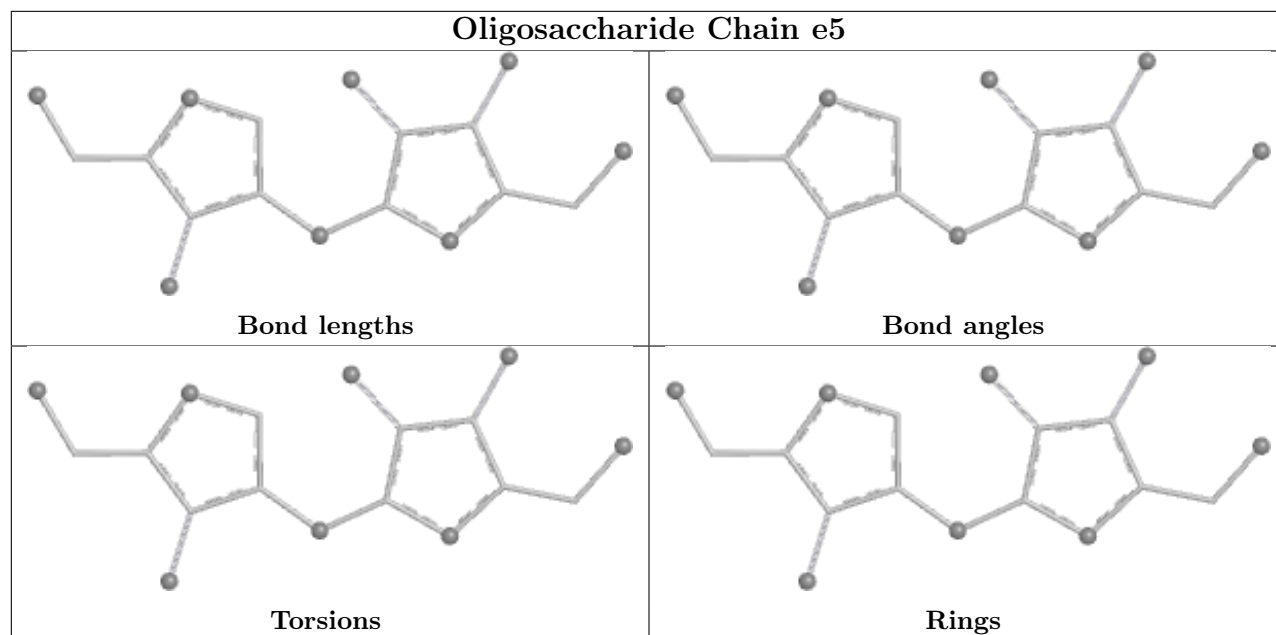


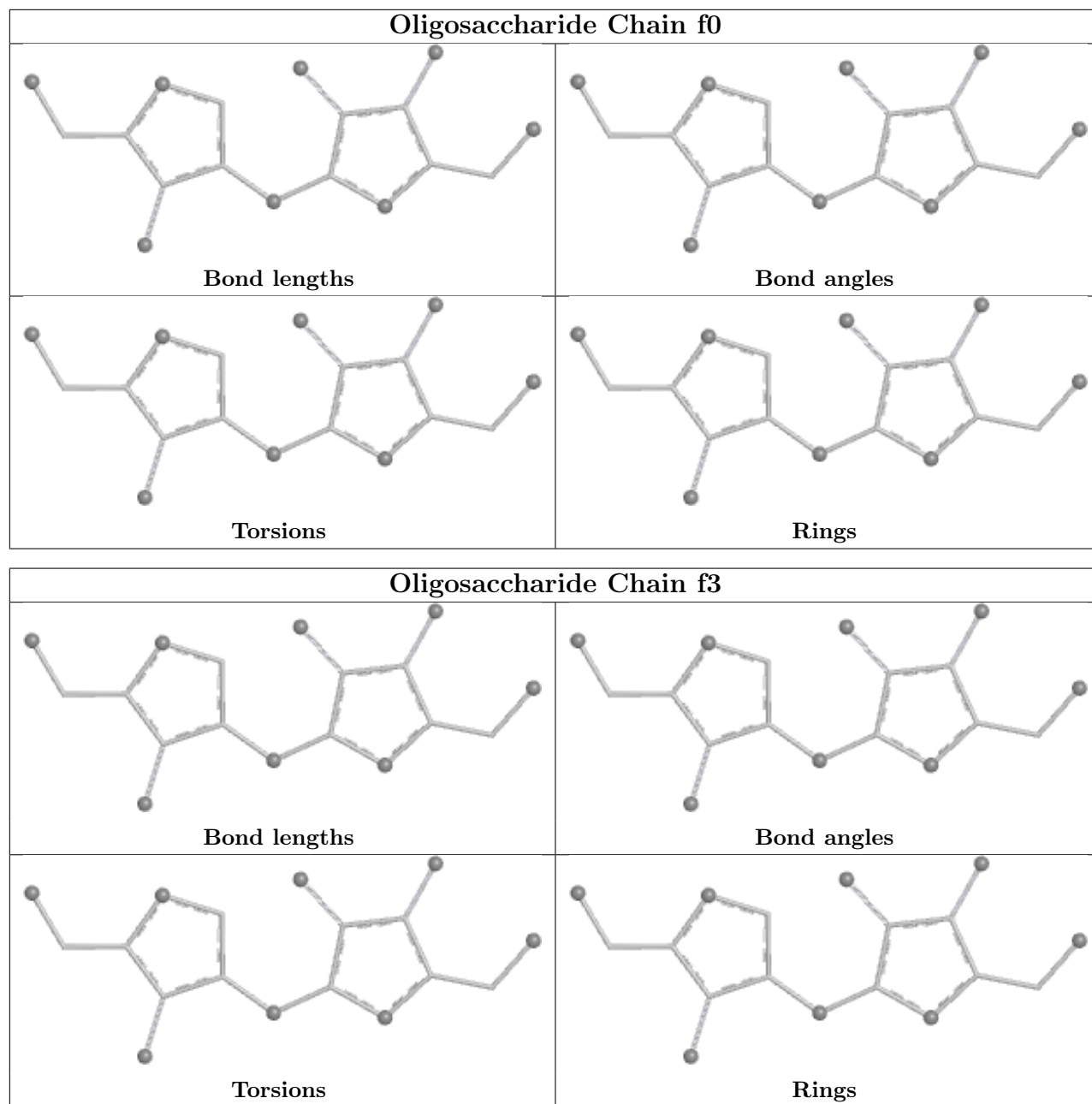


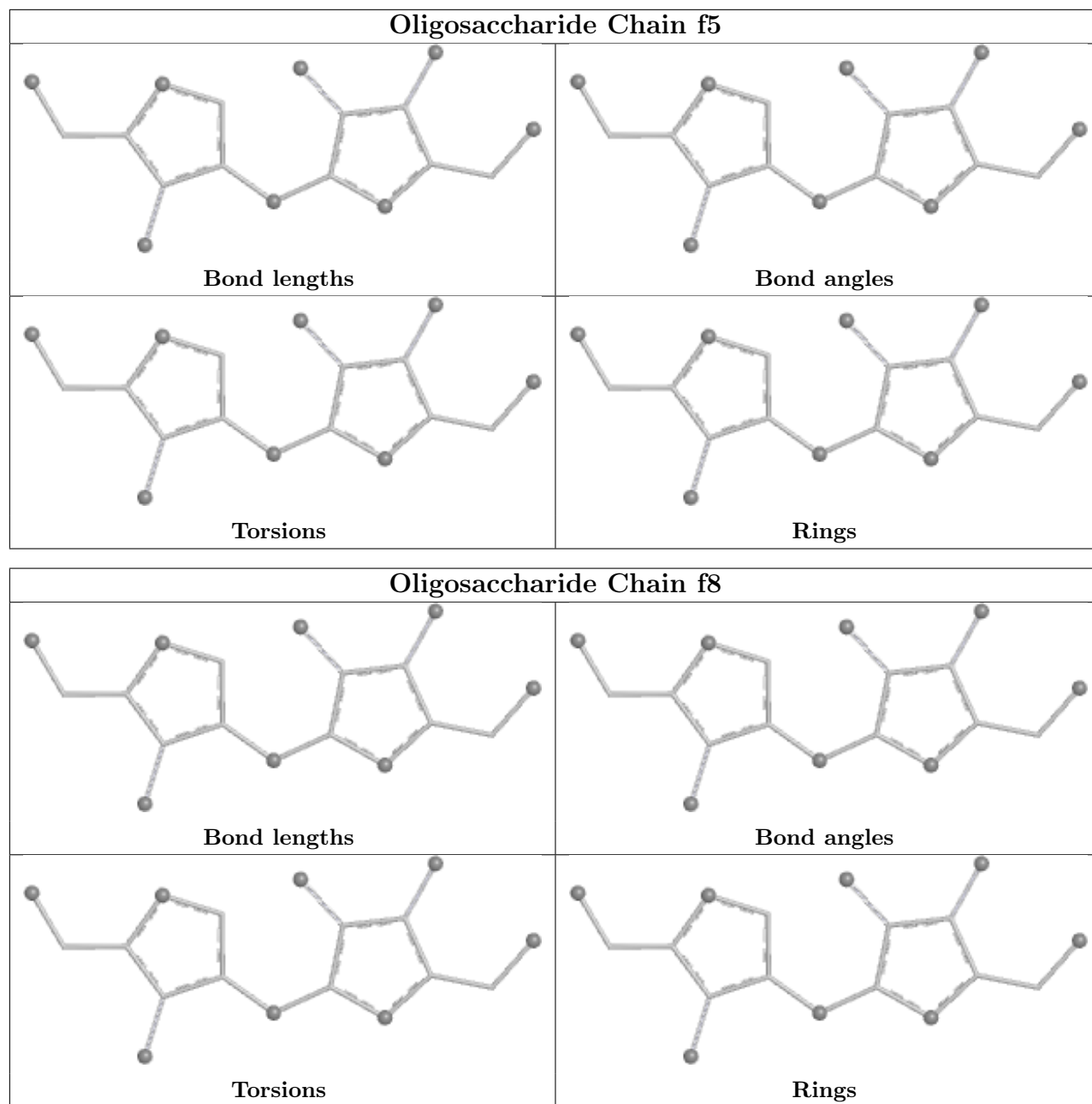


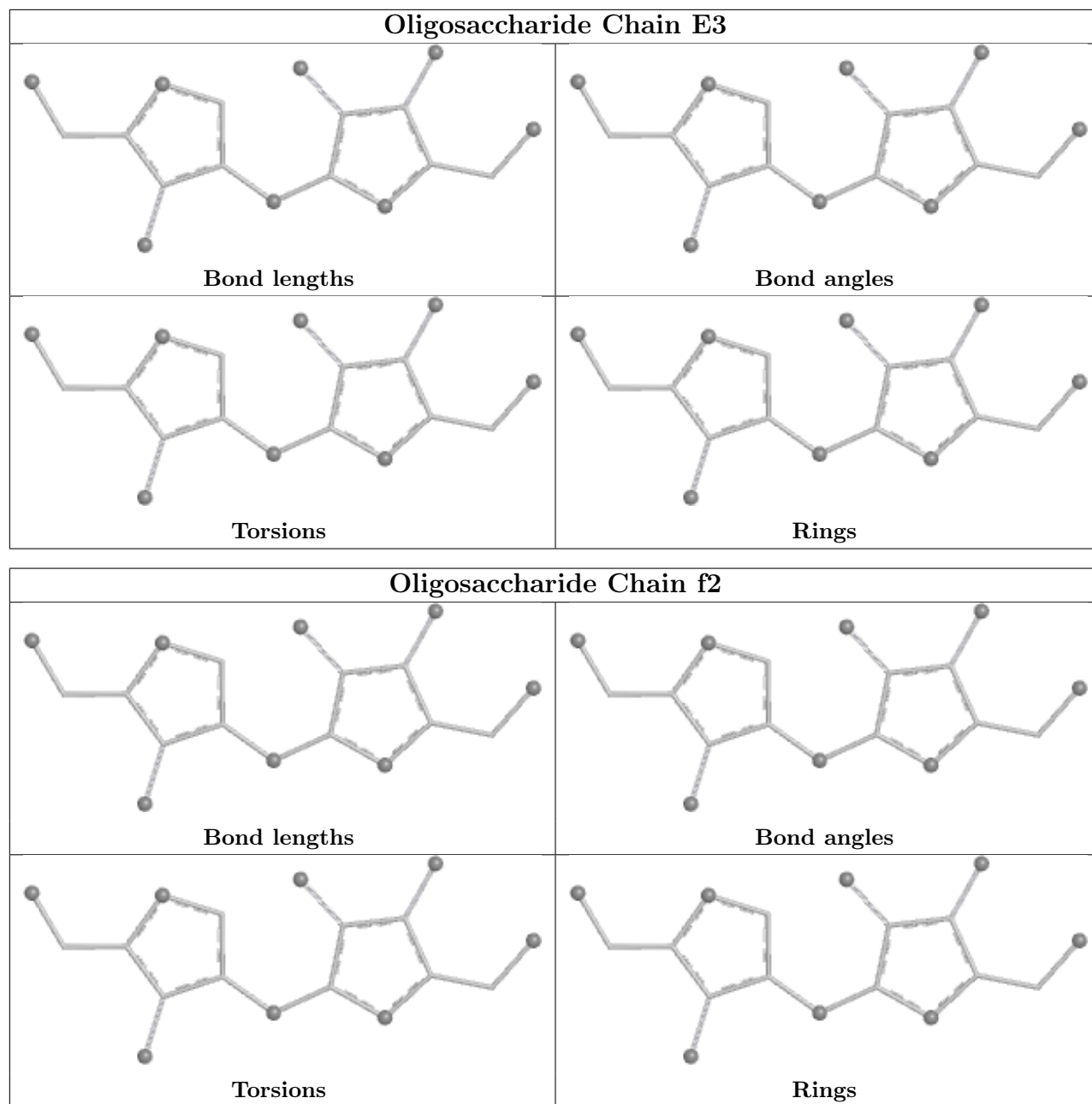


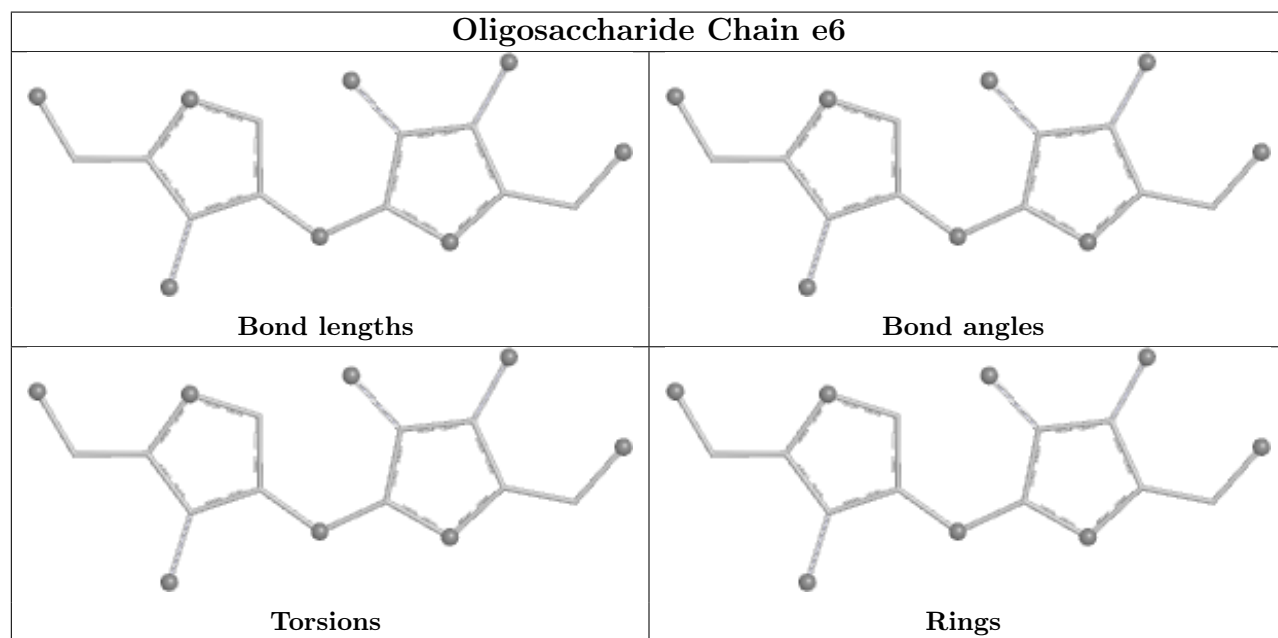
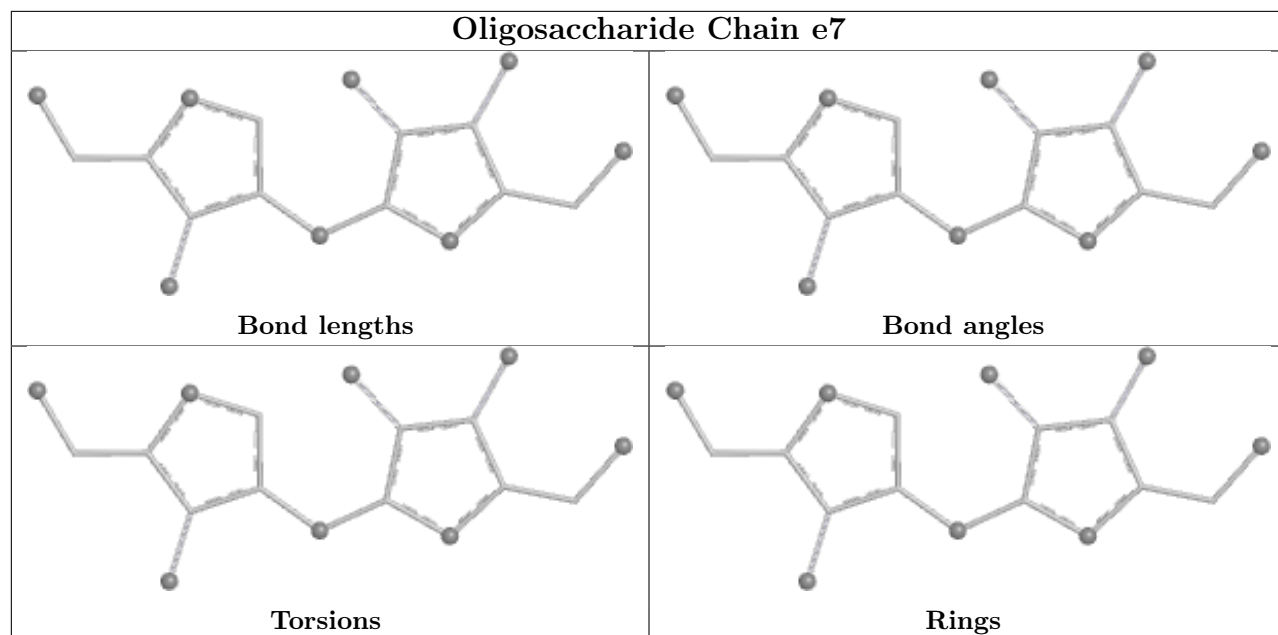


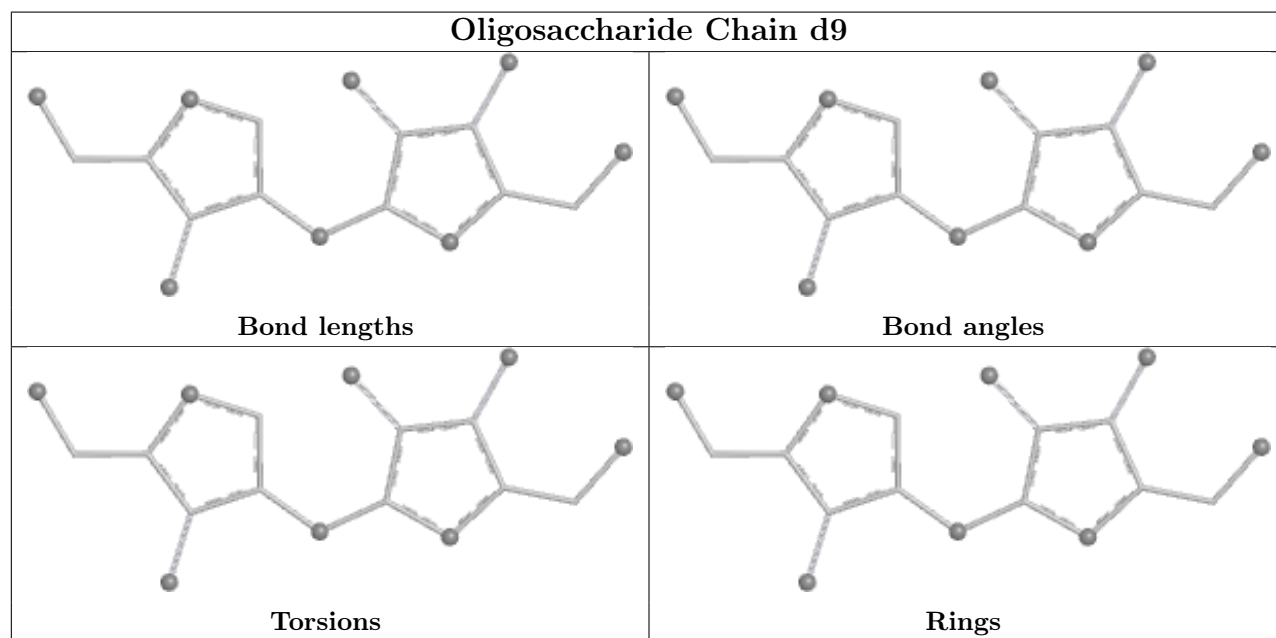
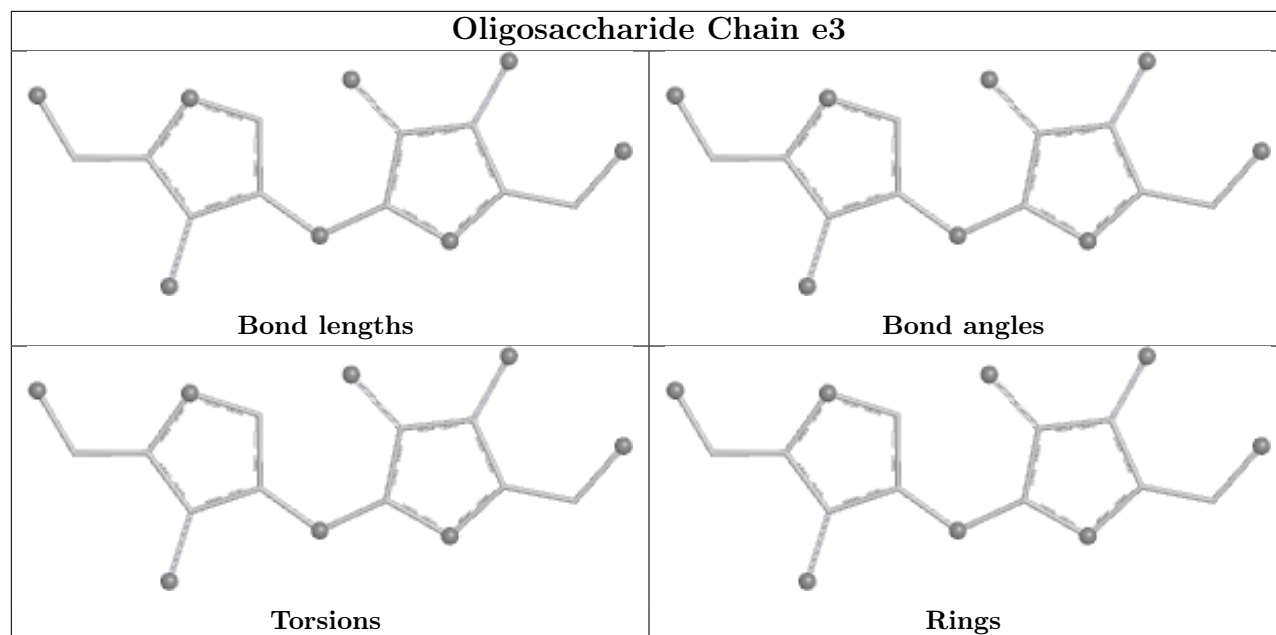


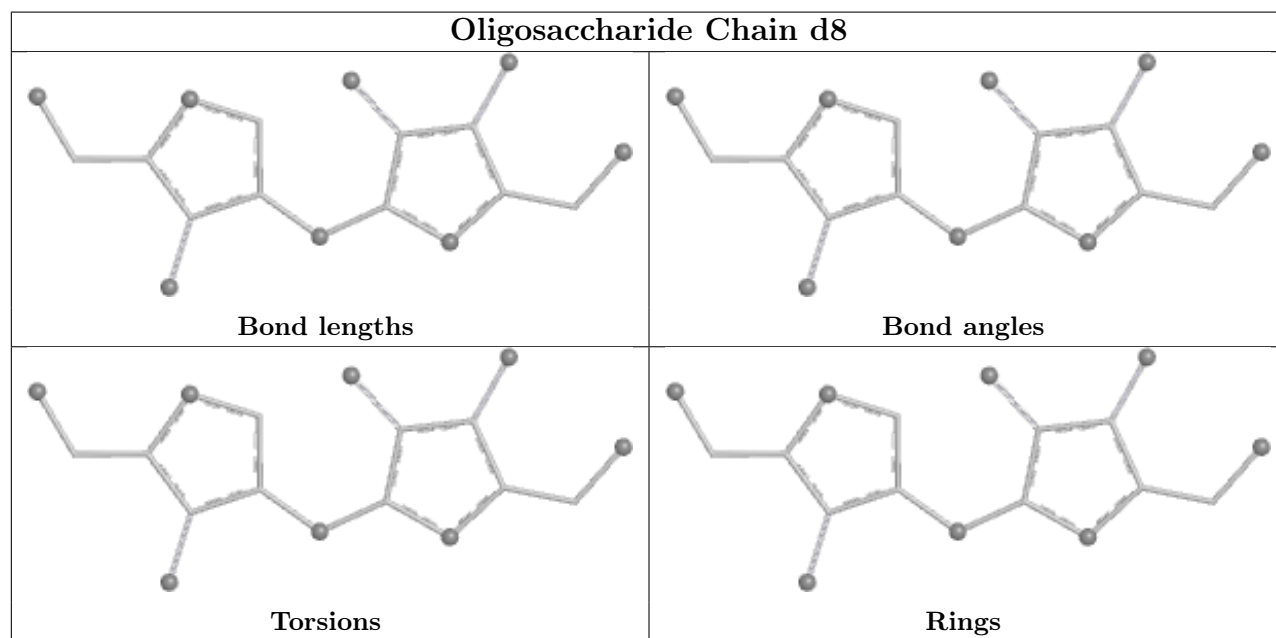
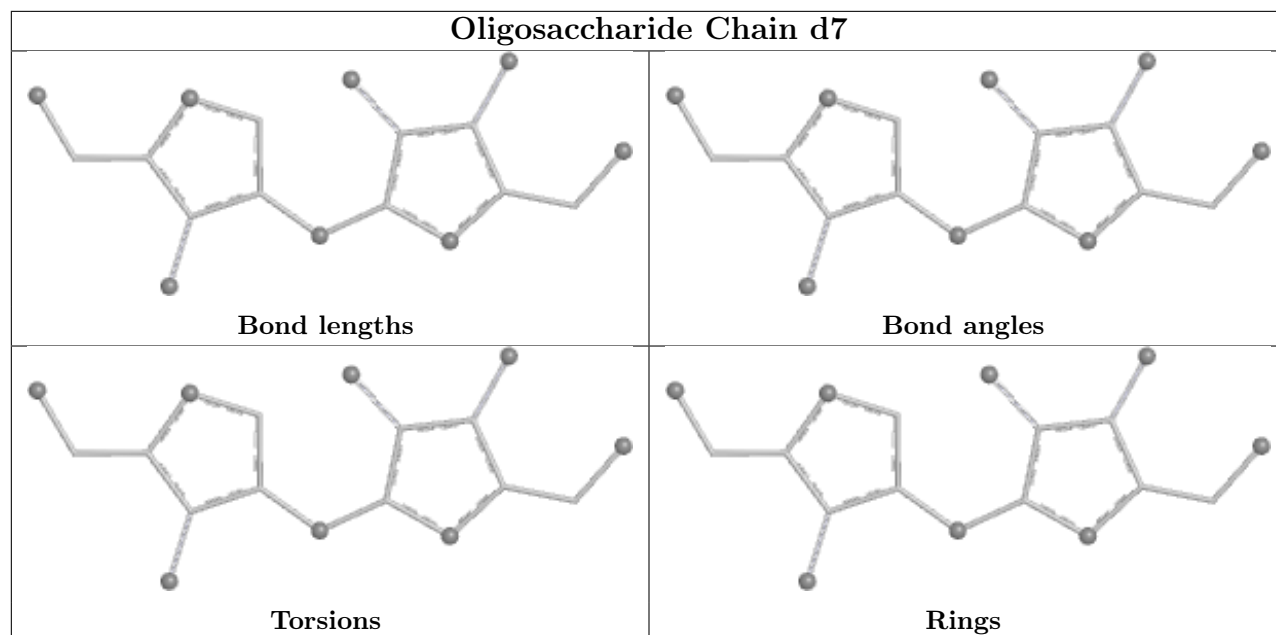


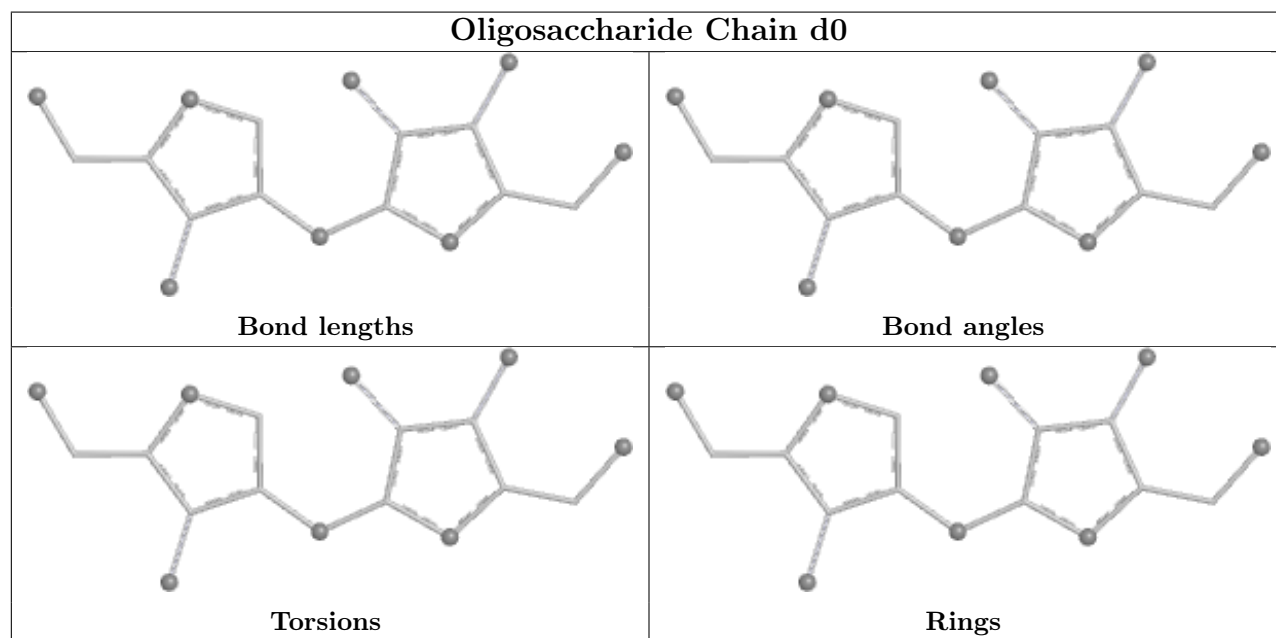
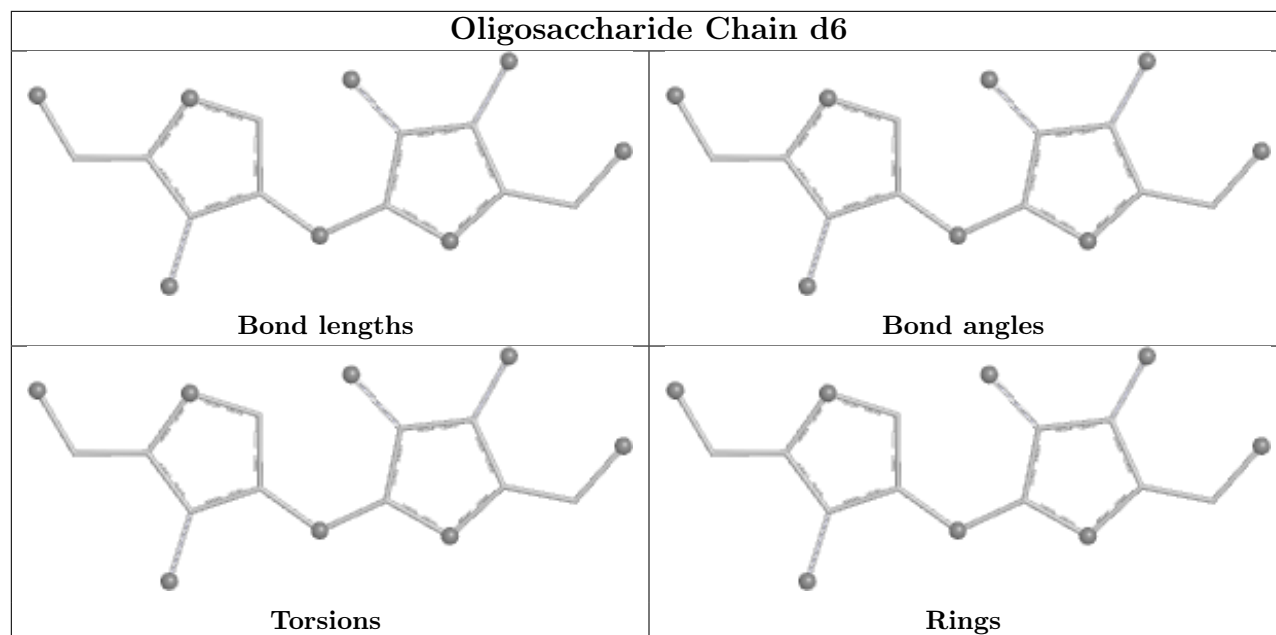


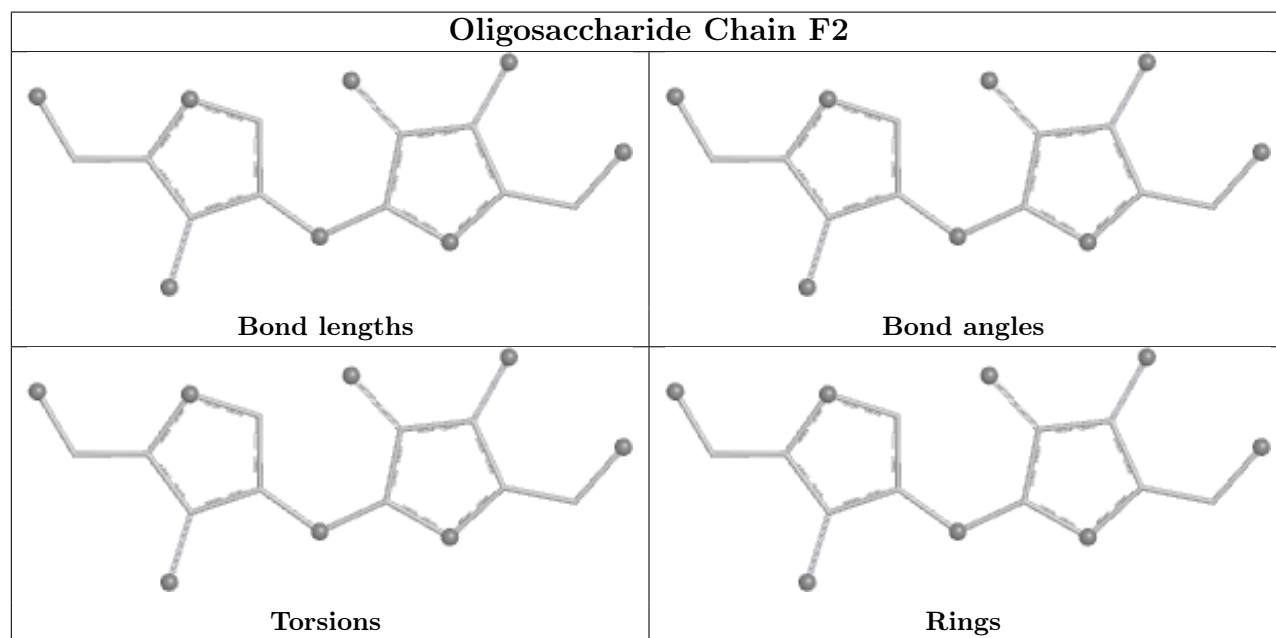
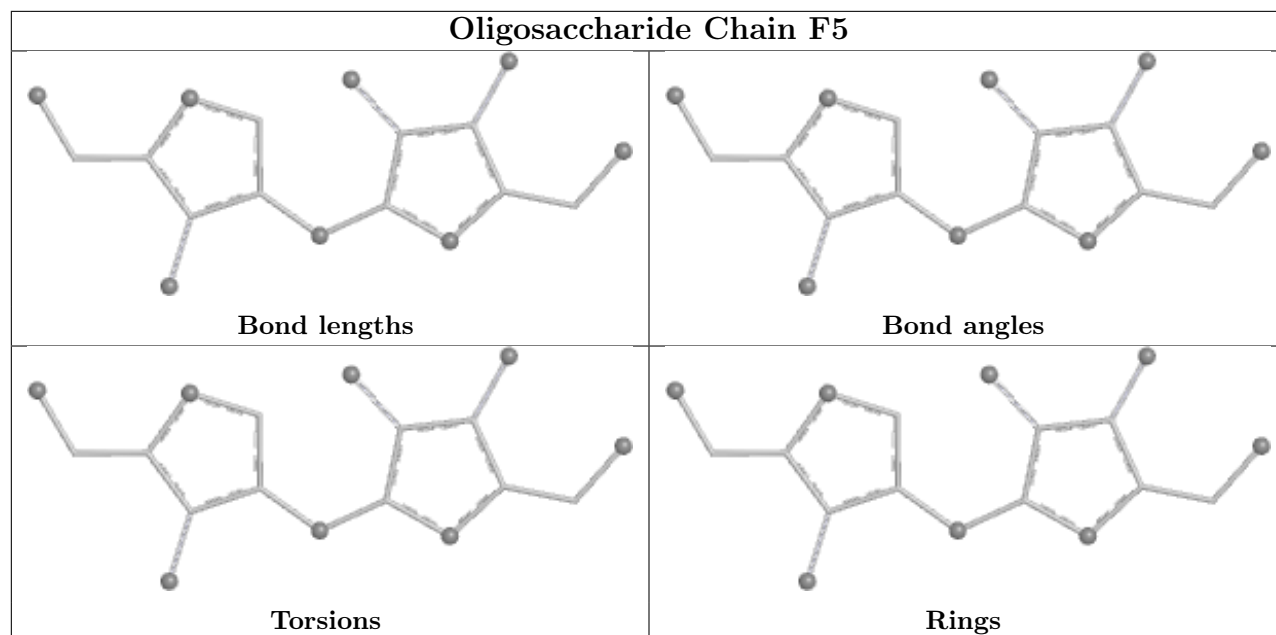


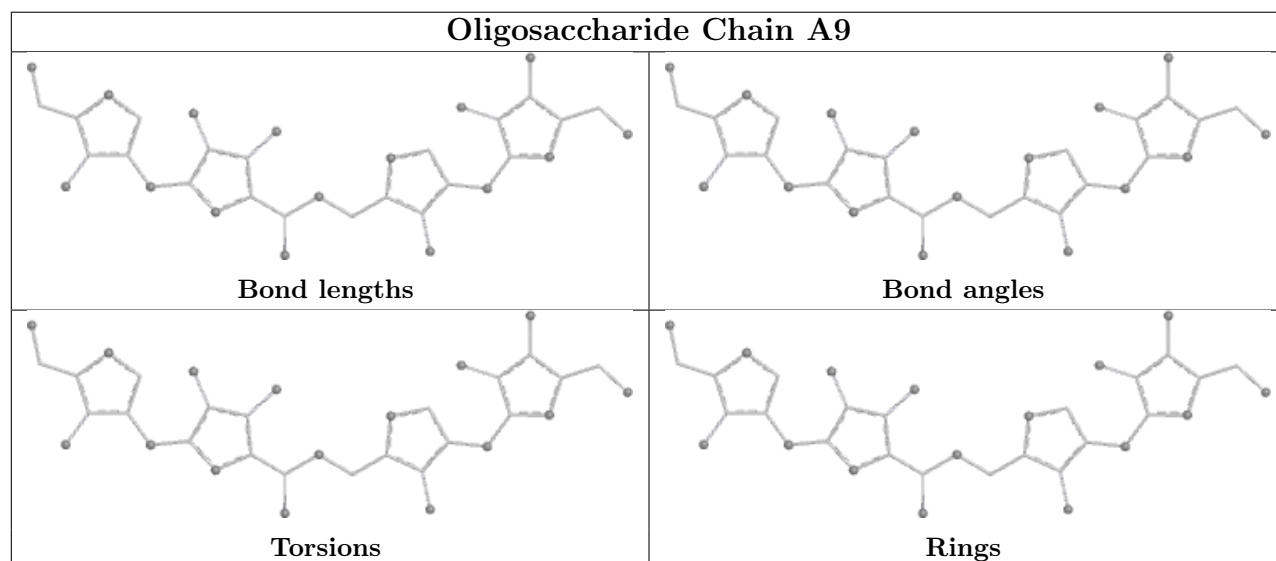
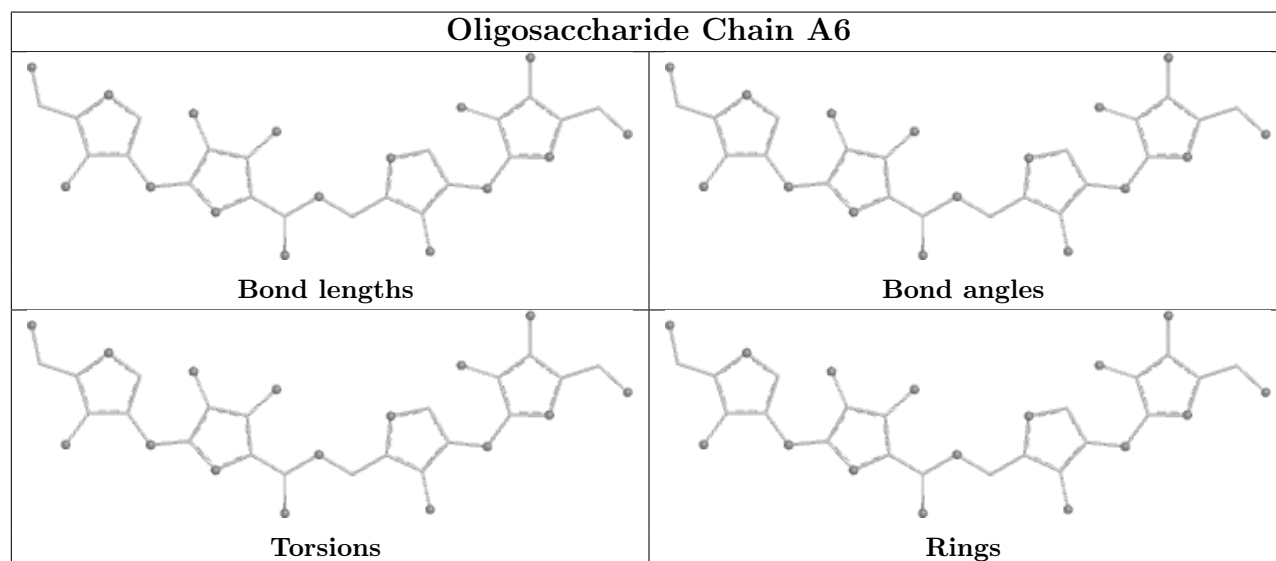
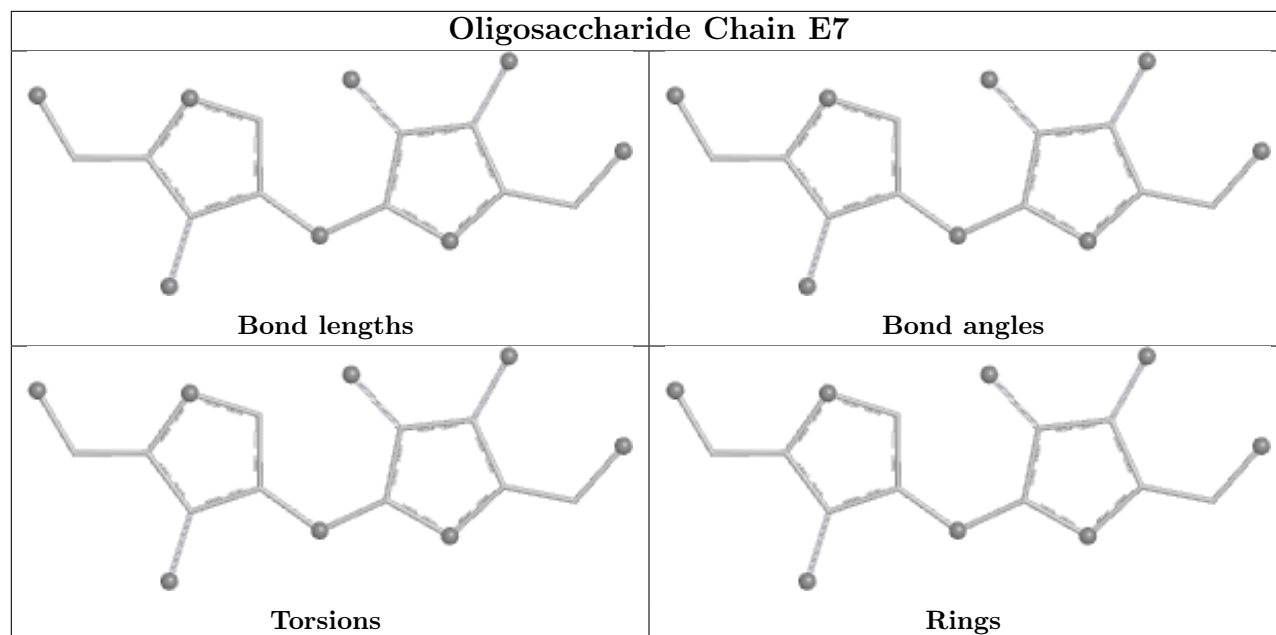


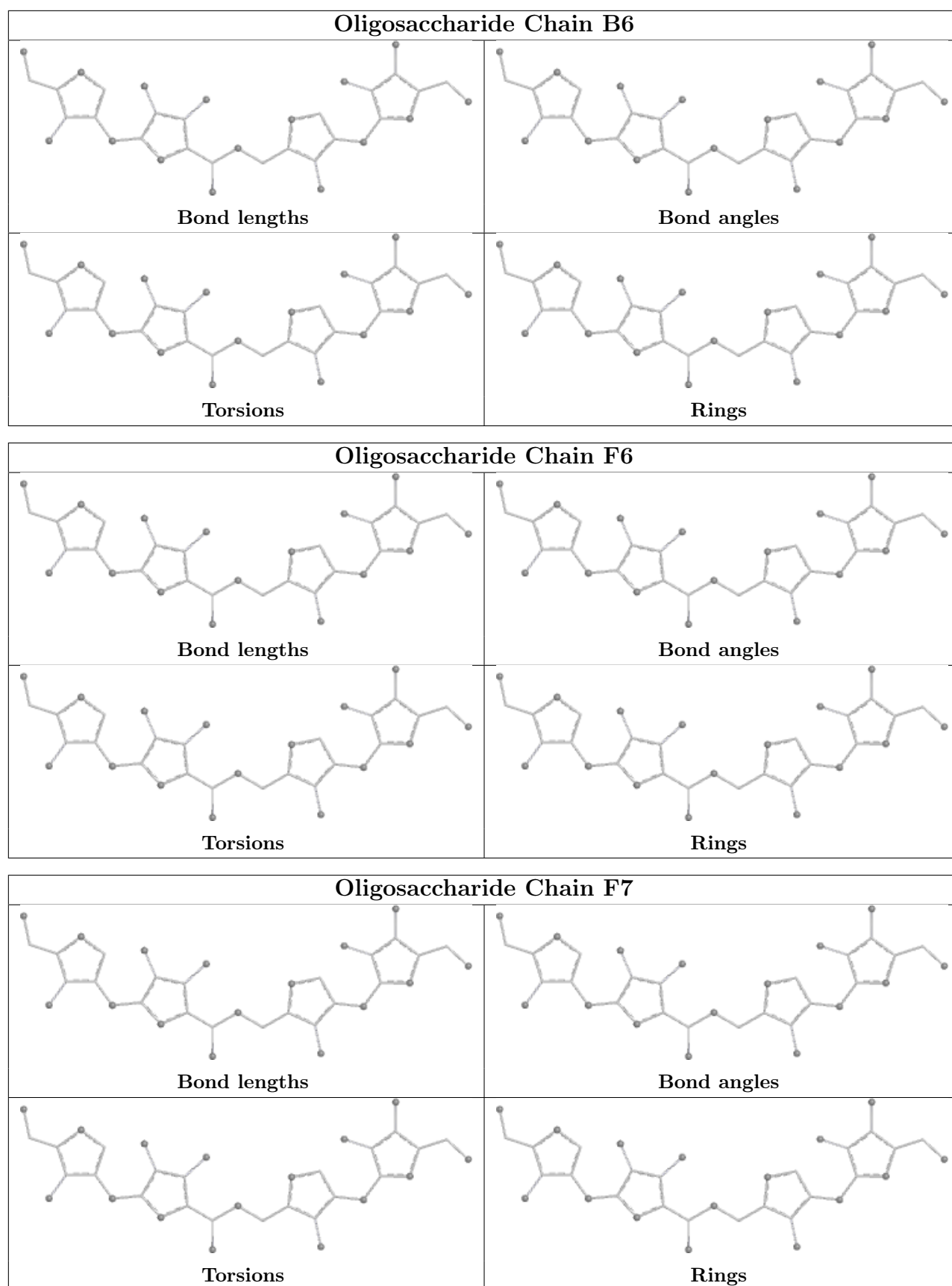


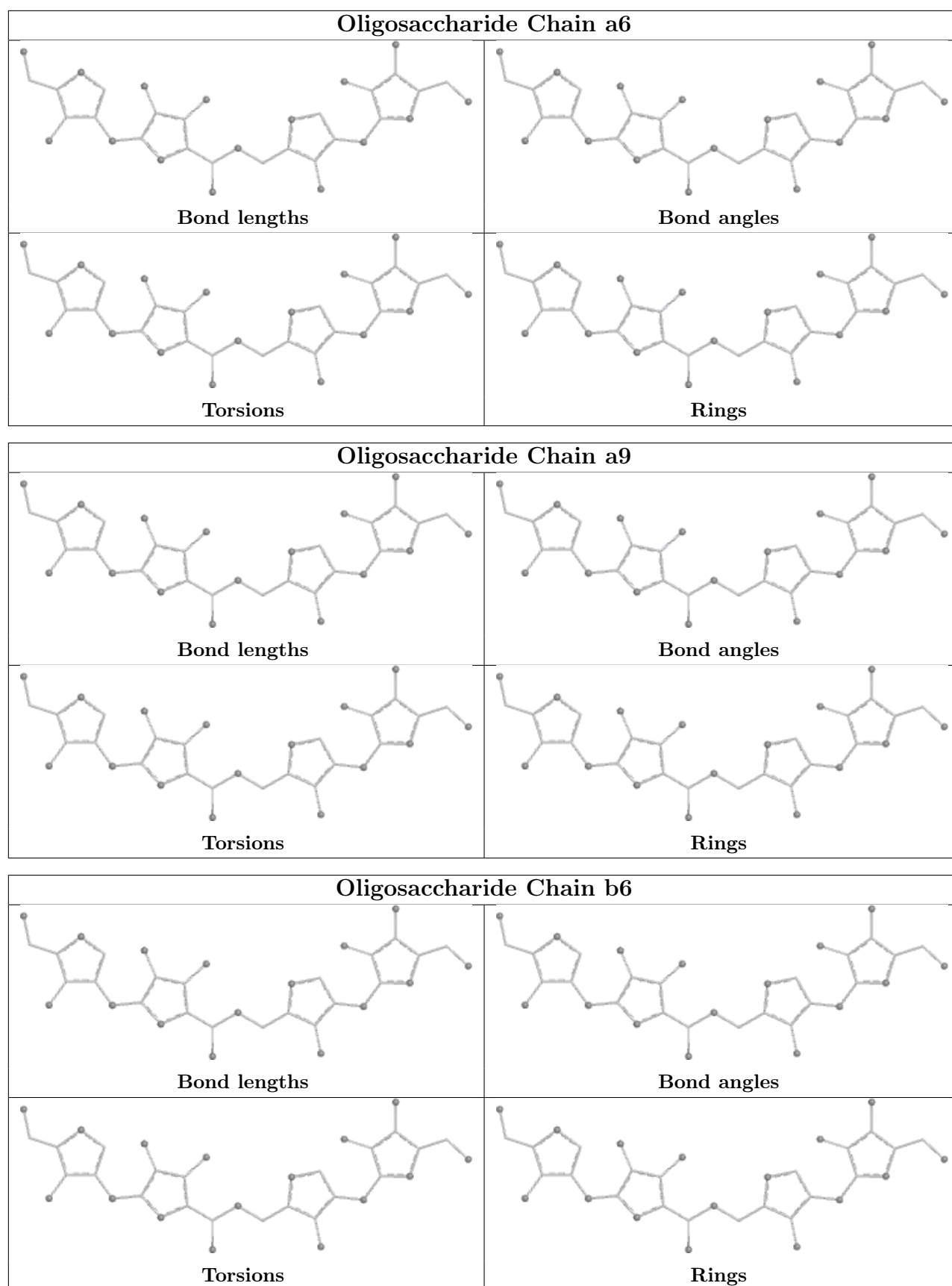


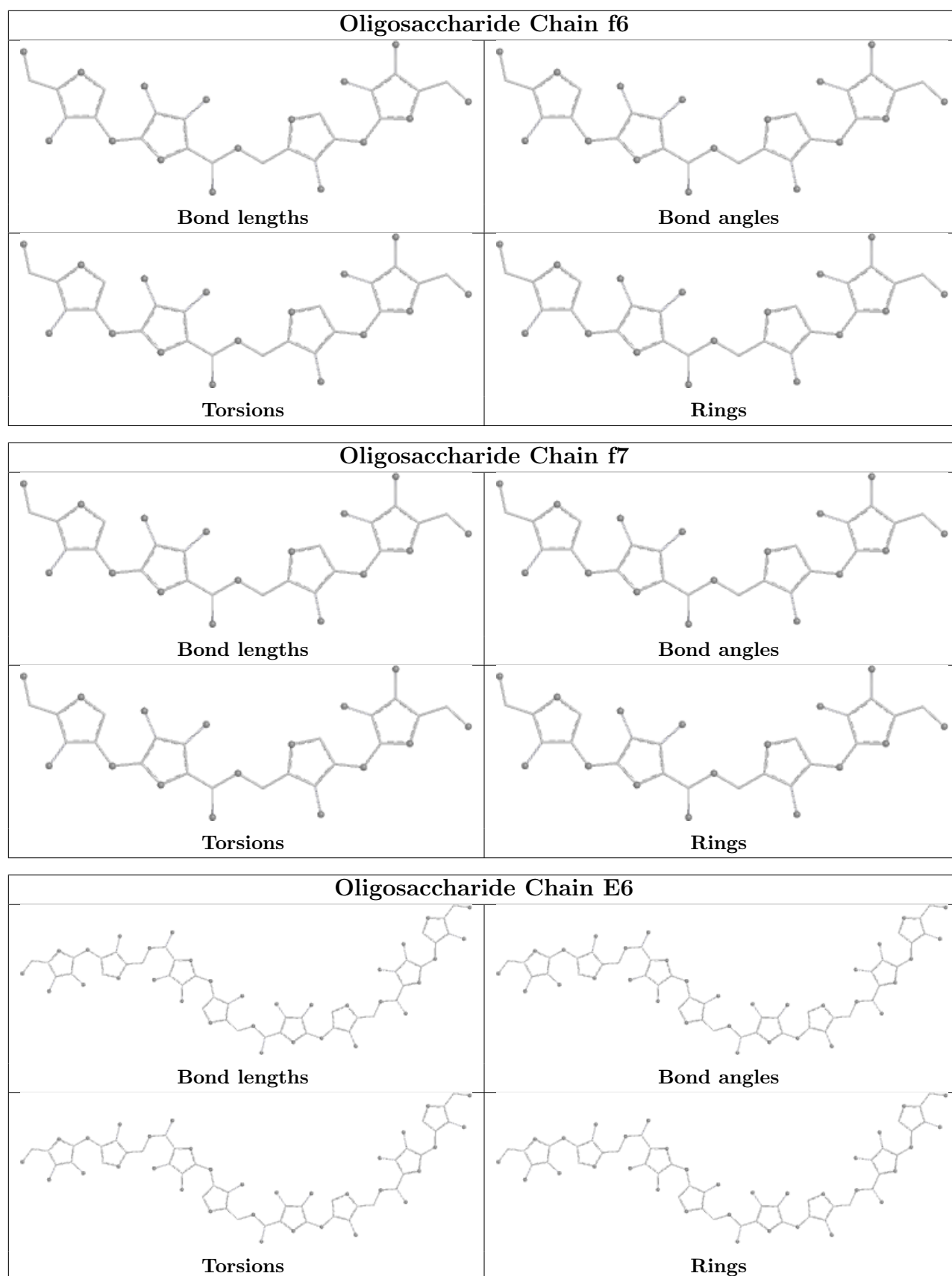


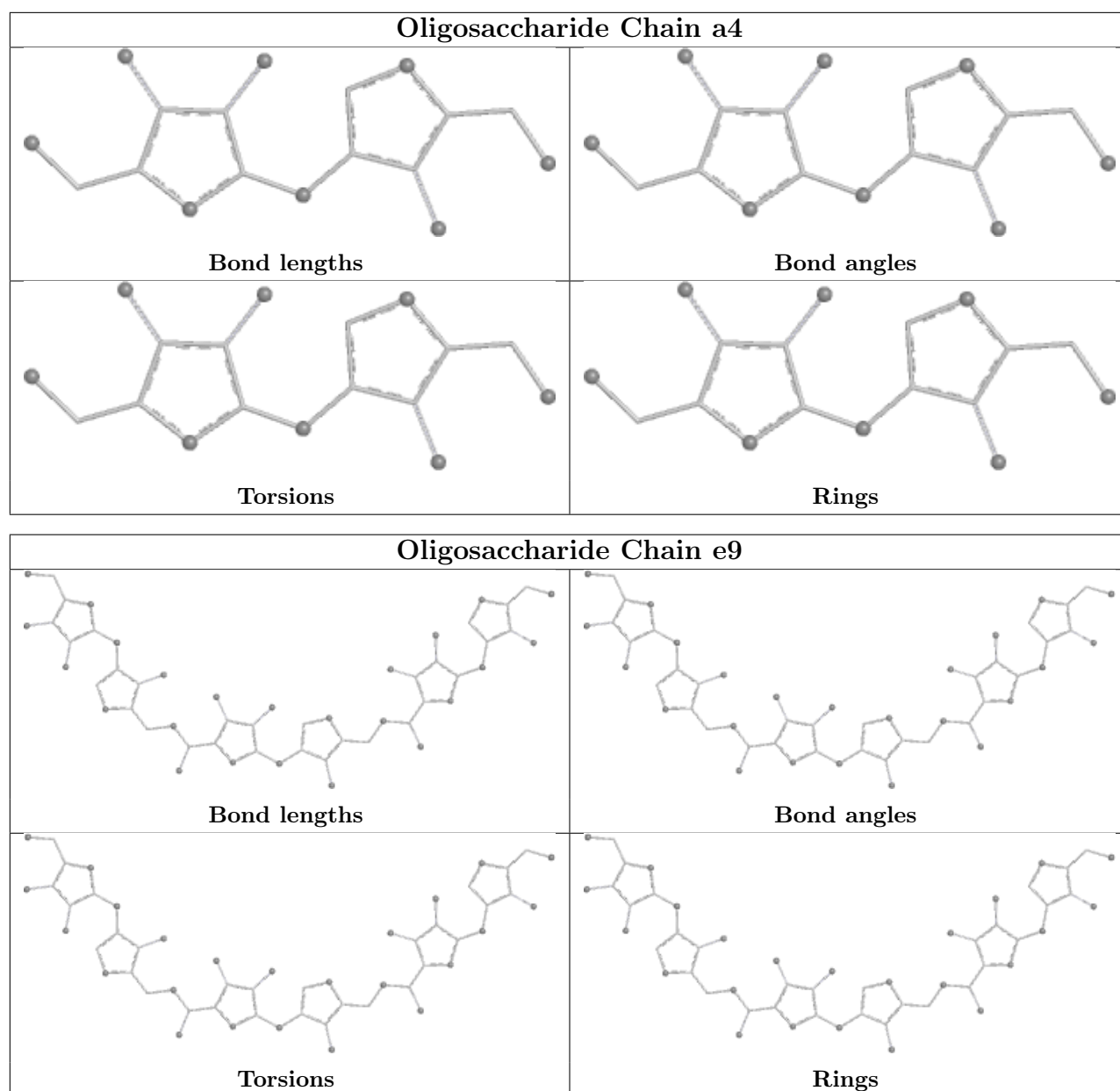












5.6 Ligand geometry [i](#)

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

All (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
9	B	2035	A1AIO	C05-C04	-15.03	1.28	1.53
9	B	2003	A1AIO	C05-C04	-15.02	1.28	1.53
9	A	2044	A1AIO	C05-C04	-15.01	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2038	A1AIO	C05-C04	-15.01	1.28	1.53
9	B	2042	A1AIO	C05-C04	-15.00	1.28	1.53
9	B	2056	A1AIO	C05-C04	-14.99	1.28	1.53
9	B	2006	A1AIO	C05-C04	-14.99	1.28	1.53
9	B	2044	A1AIO	C05-C04	-14.98	1.28	1.53
9	A	2054	A1AIO	C05-C04	-14.97	1.28	1.53
9	A	2035	A1AIO	C05-C04	-14.97	1.28	1.53
9	A	2002	A1AIO	C05-C04	-14.97	1.28	1.53
9	A	2041	A1AIO	C05-C04	-14.97	1.28	1.53
9	B	2045	A1AIO	C05-C04	-14.96	1.28	1.53
9	B	2043	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2050	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2037	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2048	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2004	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2051	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2001	A1AIO	C05-C04	-14.96	1.28	1.53
9	A	2027	A1AIO	C05-C04	-14.95	1.28	1.53
9	B	2026	A1AIO	C05-C04	-14.95	1.28	1.53
9	A	2039	A1AIO	C05-C04	-14.95	1.28	1.53
9	B	2029	A1AIO	C05-C04	-14.95	1.28	1.53
9	A	2034	A1AIO	C05-C04	-14.95	1.28	1.53
9	B	2036	A1AIO	C05-C04	-14.95	1.28	1.53
9	B	2028	A1AIO	C05-C04	-14.95	1.28	1.53
9	A	2017	A1AIO	C05-C04	-14.95	1.28	1.53
9	A	2057	A1AIO	C05-C04	-14.94	1.28	1.53
9	B	2025	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2053	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2003	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2030	A1AIO	C05-C04	-14.94	1.28	1.53
9	B	2048	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2046	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2047	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2008	A1AIO	C05-C04	-14.94	1.28	1.53
9	A	2042	A1AIO	C05-C04	-14.93	1.28	1.53
9	A	2045	A1AIO	C05-C04	-14.93	1.28	1.53
9	A	2055	A1AIO	C05-C04	-14.92	1.28	1.53
9	B	2010	A1AIO	C05-C04	-14.92	1.28	1.53
9	A	2026	A1AIO	C05-C04	-14.92	1.28	1.53
9	A	2049	A1AIO	C05-C04	-14.91	1.28	1.53
9	B	2021	A1AIO	C05-C04	-14.91	1.28	1.53
9	A	2028	A1AIO	C05-C04	-14.91	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2027	A1AIO	C05-C04	-14.91	1.28	1.53
9	A	2021	A1AIO	C05-C04	-14.91	1.28	1.53
9	B	2041	A1AIO	C05-C04	-14.91	1.28	1.53
9	A	2024	A1AIO	C05-C04	-14.91	1.28	1.53
9	A	2031	A1AIO	C05-C04	-14.90	1.28	1.53
9	B	2054	A1AIO	C05-C04	-14.90	1.28	1.53
9	A	2007	A1AIO	C05-C04	-14.90	1.28	1.53
9	B	2008	A1AIO	C05-C04	-14.90	1.28	1.53
9	B	2012	A1AIO	C05-C04	-14.90	1.28	1.53
9	B	2018	A1AIO	C05-C04	-14.89	1.28	1.53
9	B	2024	A1AIO	C05-C04	-14.89	1.28	1.53
9	B	2007	A1AIO	C05-C04	-14.89	1.28	1.53
9	B	2049	A1AIO	C05-C04	-14.89	1.28	1.53
9	B	2004	A1AIO	C05-C04	-14.89	1.28	1.53
9	B	2032	A1AIO	C05-C04	-14.88	1.28	1.53
9	A	2020	A1AIO	C05-C04	-14.88	1.28	1.53
9	A	2014	A1AIO	C05-C04	-14.88	1.28	1.53
9	A	2015	A1AIO	C05-C04	-14.87	1.28	1.53
9	A	2019	A1AIO	C05-C04	-14.87	1.28	1.53
9	A	2056	A1AIO	C05-C04	-14.87	1.28	1.53
9	B	2051	A1AIO	C05-C04	-14.87	1.28	1.53
9	B	2037	A1AIO	C05-C04	-14.86	1.28	1.53
9	A	2010	A1AIO	C05-C04	-14.86	1.28	1.53
9	A	2022	A1AIO	C05-C04	-14.86	1.28	1.53
9	A	2025	A1AIO	C05-C04	-14.86	1.28	1.53
9	B	2001	A1AIO	C05-C04	-14.85	1.28	1.53
9	A	2052	A1AIO	C05-C04	-14.85	1.28	1.53
9	B	2005	A1AIO	C05-C04	-14.84	1.28	1.53
9	B	2047	A1AIO	C05-C04	-14.84	1.28	1.53
9	B	2040	A1AIO	C05-C04	-14.83	1.28	1.53
9	A	2023	A1AIO	C05-C04	-14.83	1.28	1.53
9	B	2002	A1AIO	C05-C04	-14.83	1.28	1.53
9	B	2057	A1AIO	C05-C04	-14.82	1.28	1.53
9	A	2006	A1AIO	C05-C04	-14.82	1.28	1.53
9	A	2036	A1AIO	C05-C04	-14.81	1.28	1.53
9	A	2013	A1AIO	C05-C04	-14.81	1.28	1.53
9	B	2013	A1AIO	C05-C04	-14.81	1.28	1.53
9	A	2009	A1AIO	C05-C04	-14.80	1.28	1.53
9	B	2052	A1AIO	C05-C04	-14.80	1.28	1.53
9	B	2033	A1AIO	C05-C04	-14.80	1.28	1.53
9	B	2015	A1AIO	C05-C04	-14.79	1.28	1.53
9	B	2017	A1AIO	C05-C04	-14.79	1.28	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2011	A1AIO	C05-C04	-14.78	1.29	1.53
9	A	2018	A1AIO	C05-C04	-14.78	1.29	1.53
9	B	2050	A1AIO	C05-C04	-14.77	1.29	1.53
9	A	2032	A1AIO	C05-C04	-14.76	1.29	1.53
9	B	2055	A1AIO	C05-C04	-14.76	1.29	1.53
9	B	2019	A1AIO	C05-C04	-14.75	1.29	1.53
9	B	2020	A1AIO	C05-C04	-14.75	1.29	1.53
9	A	2012	A1AIO	C05-C04	-14.73	1.29	1.53
9	B	2022	A1AIO	C05-C04	-14.73	1.29	1.53
9	B	2023	A1AIO	C05-C04	-14.73	1.29	1.53
9	A	2016	A1AIO	C05-C04	-14.73	1.29	1.53
9	B	2053	A1AIO	C05-C04	-14.72	1.29	1.53
9	B	2014	A1AIO	C05-C04	-14.72	1.29	1.53
9	B	2009	A1AIO	C05-C04	-14.71	1.29	1.53
9	B	2030	A1AIO	C05-C04	-14.70	1.29	1.53
9	A	2040	A1AIO	C05-C04	-14.70	1.29	1.53
9	B	2031	A1AIO	C05-C04	-14.69	1.29	1.53
9	A	2038	A1AIO	C05-C04	-14.69	1.29	1.53
9	B	2011	A1AIO	C05-C04	-14.64	1.29	1.53
9	B	2034	A1AIO	C05-C04	-14.64	1.29	1.53
9	B	2046	A1AIO	C05-C04	-14.63	1.29	1.53
9	B	2016	A1AIO	C05-C04	-14.62	1.29	1.53
9	B	2023	A1AIO	C04-C03	6.29	1.66	1.53
9	B	2016	A1AIO	C04-C03	6.27	1.66	1.53
9	B	2015	A1AIO	C04-C03	6.23	1.66	1.53
9	B	2031	A1AIO	C04-C03	6.18	1.66	1.53
9	B	2005	A1AIO	C04-C03	6.17	1.66	1.53
9	B	2047	A1AIO	C04-C03	6.15	1.66	1.53
9	B	2033	A1AIO	C04-C03	6.12	1.66	1.53
9	B	2011	A1AIO	C04-C03	6.10	1.66	1.53
9	B	2030	A1AIO	C04-C03	6.09	1.66	1.53
9	B	2050	A1AIO	C04-C03	6.09	1.66	1.53
9	B	2017	A1AIO	C04-C03	6.08	1.66	1.53
9	B	2046	A1AIO	C04-C03	6.07	1.66	1.53
9	B	2028	A1AIO	C04-C03	6.06	1.66	1.53
9	B	2022	A1AIO	C04-C03	6.06	1.66	1.53
9	B	2008	A1AIO	C04-C03	6.06	1.66	1.53
9	B	2034	A1AIO	C04-C03	6.04	1.66	1.53
9	B	2051	A1AIO	C04-C03	6.03	1.66	1.53
9	B	2020	A1AIO	C04-C03	6.03	1.66	1.53
9	B	2013	A1AIO	C04-C03	6.03	1.66	1.53
9	A	2039	A1AIO	C04-C03	6.03	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2014	A1AIO	C04-C03	6.02	1.66	1.53
9	B	2054	A1AIO	C04-C03	6.02	1.66	1.53
9	B	2019	A1AIO	C04-C03	6.01	1.66	1.53
9	A	2046	A1AIO	C04-C03	6.00	1.66	1.53
9	B	2021	A1AIO	C04-C03	5.99	1.66	1.53
9	B	2053	A1AIO	C04-C03	5.99	1.66	1.53
9	A	2012	A1AIO	C04-C03	5.99	1.66	1.53
9	B	2041	A1AIO	C04-C03	5.99	1.66	1.53
9	A	2016	A1AIO	C04-C03	5.98	1.66	1.53
9	B	2009	A1AIO	C04-C03	5.98	1.66	1.53
9	A	2038	A1AIO	C04-C03	5.98	1.66	1.53
9	A	2023	A1AIO	C04-C03	5.97	1.66	1.53
9	A	2020	A1AIO	C04-C03	5.97	1.66	1.53
9	A	2019	A1AIO	C04-C03	5.97	1.66	1.53
9	A	2018	A1AIO	C04-C03	5.97	1.66	1.53
9	B	2012	A1AIO	C04-C03	5.97	1.66	1.53
9	A	2025	A1AIO	C04-C03	5.97	1.66	1.53
9	A	2040	A1AIO	C04-C03	5.96	1.66	1.53
9	B	2055	A1AIO	C04-C03	5.96	1.66	1.53
9	A	2032	A1AIO	C04-C03	5.96	1.66	1.53
9	A	2014	A1AIO	C04-C03	5.96	1.66	1.53
9	B	2052	A1AIO	C04-C03	5.96	1.66	1.53
9	A	2056	A1AIO	C04-C03	5.95	1.66	1.53
9	B	2018	A1AIO	C04-C03	5.95	1.66	1.53
9	A	2021	A1AIO	C04-C03	5.95	1.66	1.53
9	A	2026	A1AIO	C04-C03	5.95	1.66	1.53
9	A	2022	A1AIO	C04-C03	5.94	1.66	1.53
9	A	2015	A1AIO	C04-C03	5.94	1.66	1.53
9	A	2029	A1AIO	C04-C03	5.94	1.66	1.53
9	A	2041	A1AIO	C04-C03	5.94	1.66	1.53
9	A	2024	A1AIO	C04-C03	5.93	1.66	1.53
9	A	2054	A1AIO	C04-C03	5.93	1.66	1.53
9	A	2009	A1AIO	C04-C03	5.93	1.66	1.53
9	B	2001	A1AIO	C04-C03	5.93	1.65	1.53
9	B	2032	A1AIO	C04-C03	5.93	1.65	1.53
9	A	2035	A1AIO	C04-C03	5.92	1.65	1.53
9	A	2030	A1AIO	C04-C03	5.92	1.65	1.53
9	A	2044	A1AIO	C04-C03	5.92	1.65	1.53
9	A	2017	A1AIO	C04-C03	5.91	1.65	1.53
9	A	2037	A1AIO	C04-C03	5.91	1.65	1.53
9	A	2052	A1AIO	C04-C03	5.91	1.65	1.53
9	A	2011	A1AIO	C04-C03	5.91	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2008	A1AIO	C04-C03	5.91	1.65	1.53
9	A	2034	A1AIO	C04-C03	5.90	1.65	1.53
9	B	2057	A1AIO	C04-C03	5.90	1.65	1.53
9	A	2050	A1AIO	C04-C03	5.90	1.65	1.53
9	A	2053	A1AIO	C04-C03	5.90	1.65	1.53
9	A	2010	A1AIO	C04-C03	5.90	1.65	1.53
9	A	2055	A1AIO	C04-C03	5.90	1.65	1.53
9	B	2004	A1AIO	C04-C03	5.89	1.65	1.53
9	A	2031	A1AIO	C04-C03	5.89	1.65	1.53
9	B	2024	A1AIO	C04-C03	5.89	1.65	1.53
9	A	2013	A1AIO	C04-C03	5.89	1.65	1.53
9	A	2028	A1AIO	C04-C03	5.89	1.65	1.53
9	B	2035	A1AIO	C04-C03	5.89	1.65	1.53
9	B	2029	A1AIO	C04-C03	5.89	1.65	1.53
9	A	2036	A1AIO	C04-C03	5.89	1.65	1.53
9	B	2002	A1AIO	C04-C03	5.88	1.65	1.53
9	A	2033	A1AIO	C04-C03	5.88	1.65	1.53
9	A	2048	A1AIO	C04-C03	5.88	1.65	1.53
9	A	2038	A1AIO	O07-C03	-5.88	1.31	1.43
9	A	2001	A1AIO	C04-C03	5.87	1.65	1.53
9	B	2037	A1AIO	O07-C03	-5.87	1.31	1.43
9	B	2040	A1AIO	C04-C03	5.87	1.65	1.53
9	A	2009	A1AIO	O07-C03	-5.87	1.31	1.43
9	B	2049	A1AIO	C04-C03	5.87	1.65	1.53
9	A	2007	A1AIO	C04-C03	5.87	1.65	1.53
9	A	2057	A1AIO	C04-C03	5.87	1.65	1.53
9	A	2047	A1AIO	C04-C03	5.87	1.65	1.53
9	A	2045	A1AIO	C04-C03	5.86	1.65	1.53
9	B	2027	A1AIO	C04-C03	5.86	1.65	1.53
9	B	2026	A1AIO	C04-C03	5.86	1.65	1.53
9	A	2051	A1AIO	C04-C03	5.85	1.65	1.53
9	A	2049	A1AIO	C04-C03	5.85	1.65	1.53
9	B	2025	A1AIO	C04-C03	5.85	1.65	1.53
9	B	2006	A1AIO	O07-C03	-5.85	1.31	1.43
9	B	2010	A1AIO	C04-C03	5.85	1.65	1.53
9	A	2007	A1AIO	O07-C03	-5.85	1.31	1.43
9	B	2007	A1AIO	O07-C03	-5.85	1.31	1.43
9	A	2003	A1AIO	C04-C03	5.85	1.65	1.53
9	B	2037	A1AIO	C04-C03	5.85	1.65	1.53
9	B	2055	A1AIO	O07-C03	-5.84	1.31	1.43
9	B	2053	A1AIO	O07-C03	-5.84	1.31	1.43
9	B	2044	A1AIO	C04-C03	5.84	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2046	A1AIO	O07-C03	-5.83	1.31	1.43
9	A	2005	A1AIO	C04-C03	5.83	1.65	1.53
9	B	2038	A1AIO	C04-C03	5.83	1.65	1.53
9	A	2006	A1AIO	O07-C03	-5.83	1.31	1.43
9	A	2027	A1AIO	C04-C03	5.83	1.65	1.53
9	B	2056	A1AIO	C04-C03	5.83	1.65	1.53
9	A	2002	A1AIO	C04-C03	5.83	1.65	1.53
9	A	2042	A1AIO	O07-C03	-5.82	1.31	1.43
9	B	2004	A1AIO	O07-C03	-5.82	1.31	1.43
9	A	2010	A1AIO	O07-C03	-5.82	1.31	1.43
9	A	2006	A1AIO	C04-C03	5.82	1.65	1.53
9	A	2011	A1AIO	O07-C03	-5.82	1.31	1.43
9	B	2042	A1AIO	O07-C03	-5.81	1.31	1.43
9	B	2036	A1AIO	C04-C03	5.81	1.65	1.53
9	B	2040	A1AIO	O07-C03	-5.81	1.31	1.43
9	B	2042	A1AIO	C04-C03	5.81	1.65	1.53
9	A	2042	A1AIO	C04-C03	5.81	1.65	1.53
9	B	2009	A1AIO	O07-C03	-5.81	1.31	1.43
9	B	2043	A1AIO	C04-C03	5.81	1.65	1.53
9	B	2048	A1AIO	C04-C03	5.81	1.65	1.53
9	B	2034	A1AIO	O07-C03	-5.81	1.31	1.43
9	B	2036	A1AIO	O07-C03	-5.81	1.31	1.43
9	A	2001	A1AIO	O07-C03	-5.81	1.31	1.43
9	B	2003	A1AIO	C04-C03	5.80	1.65	1.53
9	B	2043	A1AIO	O07-C03	-5.80	1.31	1.43
9	B	2045	A1AIO	O07-C03	-5.80	1.31	1.43
9	A	2049	A1AIO	O07-C03	-5.80	1.31	1.43
9	B	2044	A1AIO	O07-C03	-5.80	1.31	1.43
9	B	2049	A1AIO	O07-C03	-5.80	1.31	1.43
9	A	2016	A1AIO	O07-C03	-5.80	1.31	1.43
9	A	2013	A1AIO	O07-C03	-5.79	1.31	1.43
9	A	2048	A1AIO	O07-C03	-5.79	1.31	1.43
9	B	2039	A1AIO	C04-C03	5.79	1.65	1.53
9	A	2051	A1AIO	O07-C03	-5.79	1.31	1.43
9	B	2030	A1AIO	O07-C03	-5.79	1.31	1.43
9	A	2047	A1AIO	O07-C03	-5.79	1.31	1.43
9	B	2048	A1AIO	O07-C03	-5.79	1.31	1.43
9	A	2050	A1AIO	O07-C03	-5.79	1.31	1.43
9	A	2002	A1AIO	O07-C03	-5.79	1.31	1.43
9	B	2045	A1AIO	C04-C03	5.78	1.65	1.53
9	B	2056	A1AIO	O07-C03	-5.78	1.31	1.43
9	A	2045	A1AIO	O07-C03	-5.78	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2052	A1AIO	O07-C03	-5.78	1.31	1.43
9	A	2004	A1AIO	C04-C03	5.78	1.65	1.53
9	A	2040	A1AIO	O07-C03	-5.78	1.31	1.43
9	B	2029	A1AIO	O07-C03	-5.78	1.31	1.43
9	A	2043	A1AIO	C04-C03	5.78	1.65	1.53
9	A	2036	A1AIO	O07-C03	-5.78	1.31	1.43
9	A	2004	A1AIO	O07-C03	-5.78	1.31	1.43
9	A	2057	A1AIO	O07-C03	-5.78	1.31	1.43
9	A	2023	A1AIO	O07-C03	-5.78	1.31	1.43
9	B	2007	A1AIO	C04-C03	5.77	1.65	1.53
9	B	2027	A1AIO	O07-C03	-5.77	1.31	1.43
9	A	2028	A1AIO	O07-C03	-5.77	1.31	1.43
9	B	2035	A1AIO	O07-C03	-5.77	1.31	1.43
9	A	2055	A1AIO	O07-C03	-5.77	1.31	1.43
9	B	2002	A1AIO	O07-C03	-5.76	1.31	1.43
9	B	2019	A1AIO	O07-C03	-5.76	1.31	1.43
9	A	2005	A1AIO	O07-C03	-5.76	1.31	1.43
9	A	2054	A1AIO	O07-C03	-5.76	1.31	1.43
9	A	2018	A1AIO	O07-C03	-5.76	1.31	1.43
9	B	2057	A1AIO	O07-C03	-5.76	1.31	1.43
9	A	2012	A1AIO	O07-C03	-5.76	1.31	1.43
9	B	2011	A1AIO	O07-C03	-5.76	1.31	1.43
9	A	2056	A1AIO	O07-C03	-5.75	1.31	1.43
9	A	2032	A1AIO	O07-C03	-5.75	1.31	1.43
9	B	2010	A1AIO	O07-C03	-5.75	1.31	1.43
9	B	2052	A1AIO	O07-C03	-5.75	1.31	1.43
9	A	2031	A1AIO	O07-C03	-5.75	1.31	1.43
9	A	2003	A1AIO	O07-C03	-5.75	1.31	1.43
9	B	2006	A1AIO	C04-C03	5.74	1.65	1.53
9	A	2015	A1AIO	O07-C03	-5.74	1.31	1.43
9	B	2038	A1AIO	O07-C03	-5.74	1.31	1.43
9	B	2039	A1AIO	O07-C03	-5.74	1.31	1.43
9	A	2041	A1AIO	O07-C03	-5.74	1.31	1.43
9	B	2001	A1AIO	O07-C03	-5.74	1.31	1.43
9	B	2032	A1AIO	O07-C03	-5.74	1.31	1.43
9	B	2012	A1AIO	O07-C03	-5.73	1.31	1.43
9	A	2024	A1AIO	O07-C03	-5.73	1.31	1.43
9	A	2008	A1AIO	O07-C03	-5.73	1.31	1.43
9	A	2019	A1AIO	O07-C03	-5.73	1.31	1.43
9	B	2014	A1AIO	O07-C03	-5.73	1.31	1.43
9	A	2043	A1AIO	O07-C03	-5.72	1.31	1.43
9	A	2022	A1AIO	O07-C03	-5.72	1.31	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2041	A1AIO	O07-C03	-5.71	1.31	1.43
9	B	2025	A1AIO	O07-C03	-5.71	1.31	1.43
9	A	2035	A1AIO	O07-C03	-5.71	1.31	1.43
9	B	2024	A1AIO	O07-C03	-5.71	1.31	1.43
9	A	2053	A1AIO	O07-C03	-5.71	1.31	1.43
9	A	2025	A1AIO	O07-C03	-5.70	1.31	1.43
9	A	2030	A1AIO	O07-C03	-5.70	1.31	1.43
9	B	2020	A1AIO	O07-C03	-5.69	1.31	1.43
9	B	2033	A1AIO	O07-C03	-5.69	1.31	1.43
9	B	2018	A1AIO	O07-C03	-5.69	1.31	1.43
9	B	2008	A1AIO	O07-C03	-5.69	1.31	1.43
9	B	2013	A1AIO	O07-C03	-5.69	1.31	1.43
9	A	2021	A1AIO	O07-C03	-5.68	1.31	1.43
9	A	2017	A1AIO	O07-C03	-5.68	1.31	1.43
9	A	2026	A1AIO	O07-C03	-5.68	1.31	1.43
9	A	2020	A1AIO	O07-C03	-5.68	1.31	1.43
9	B	2047	A1AIO	O07-C03	-5.68	1.31	1.43
9	A	2027	A1AIO	O07-C03	-5.67	1.31	1.43
9	A	2029	A1AIO	O07-C03	-5.67	1.31	1.43
9	A	2034	A1AIO	O07-C03	-5.67	1.31	1.43
9	B	2026	A1AIO	O07-C03	-5.67	1.31	1.43
9	B	2017	A1AIO	O07-C03	-5.67	1.31	1.43
9	A	2033	A1AIO	O07-C03	-5.67	1.31	1.43
9	B	2021	A1AIO	O07-C03	-5.67	1.31	1.43
9	A	2014	A1AIO	O07-C03	-5.66	1.31	1.43
9	B	2003	A1AIO	O07-C03	-5.66	1.31	1.43
9	B	2054	A1AIO	O07-C03	-5.66	1.31	1.43
9	B	2022	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2050	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2031	A1AIO	O07-C03	-5.65	1.31	1.43
9	B	2051	A1AIO	O07-C03	-5.64	1.31	1.43
9	B	2028	A1AIO	O07-C03	-5.64	1.31	1.43
9	A	2046	A1AIO	O07-C03	-5.63	1.31	1.43
9	B	2016	A1AIO	O07-C03	-5.62	1.31	1.43
9	A	2044	A1AIO	O07-C03	-5.60	1.31	1.43
9	A	2037	A1AIO	O07-C03	-5.60	1.31	1.43
9	B	2005	A1AIO	O07-C03	-5.59	1.31	1.43
9	B	2015	A1AIO	O07-C03	-5.58	1.31	1.43
9	B	2023	A1AIO	O07-C03	-5.57	1.31	1.43
9	A	2039	A1AIO	O07-C03	-5.57	1.31	1.43
9	A	2020	A1AIO	O07-C06	5.19	1.55	1.43
9	B	2018	A1AIO	O07-C06	5.19	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2017	A1AIO	O07-C06	5.18	1.55	1.43
9	B	2024	A1AIO	O07-C06	5.17	1.55	1.43
9	A	2035	A1AIO	O07-C06	5.16	1.55	1.43
9	A	2025	A1AIO	O07-C06	5.16	1.55	1.43
9	A	2021	A1AIO	O07-C06	5.16	1.54	1.43
9	A	2037	A1AIO	O07-C06	5.15	1.54	1.43
9	B	2013	A1AIO	O07-C06	5.15	1.54	1.43
9	A	2024	A1AIO	O07-C06	5.14	1.54	1.43
9	A	2014	A1AIO	O07-C06	5.14	1.54	1.43
9	A	2033	A1AIO	O07-C06	5.14	1.54	1.43
9	A	2036	A1AIO	O07-C06	5.14	1.54	1.43
9	A	2019	A1AIO	O07-C06	5.14	1.54	1.43
9	A	2018	A1AIO	O07-C06	5.13	1.54	1.43
9	B	2012	A1AIO	O07-C06	5.13	1.54	1.43
9	A	2054	A1AIO	O07-C06	5.12	1.54	1.43
9	B	2025	A1AIO	O07-C06	5.12	1.54	1.43
9	A	2022	A1AIO	O07-C06	5.12	1.54	1.43
9	A	2046	A1AIO	O07-C06	5.12	1.54	1.43
9	A	2055	A1AIO	O07-C06	5.12	1.54	1.43
9	A	2041	A1AIO	O07-C06	5.11	1.54	1.43
9	A	2051	A1AIO	O07-C06	5.11	1.54	1.43
9	A	2050	A1AIO	O07-C06	5.11	1.54	1.43
9	B	2021	A1AIO	O07-C06	5.11	1.54	1.43
9	A	2023	A1AIO	O07-C06	5.11	1.54	1.43
9	A	2030	A1AIO	O07-C06	5.11	1.54	1.43
9	B	2004	A1AIO	O07-C06	5.11	1.54	1.43
9	A	2015	A1AIO	O07-C06	5.10	1.54	1.43
9	B	2056	A1AIO	O07-C06	5.10	1.54	1.43
9	B	2020	A1AIO	O07-C06	5.10	1.54	1.43
9	B	2003	A1AIO	O07-C06	5.10	1.54	1.43
9	A	2039	A1AIO	O07-C06	5.10	1.54	1.43
9	B	2049	A1AIO	O07-C06	5.10	1.54	1.43
9	A	2011	A1AIO	O07-C06	5.10	1.54	1.43
9	B	2022	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2044	A1AIO	O07-C06	5.09	1.54	1.43
9	B	2014	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2027	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2032	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2001	A1AIO	O07-C06	5.09	1.54	1.43
9	B	2027	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2042	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2010	A1AIO	O07-C06	5.09	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2026	A1AIO	O07-C06	5.09	1.54	1.43
9	B	2017	A1AIO	O07-C06	5.09	1.54	1.43
9	B	2054	A1AIO	O07-C06	5.09	1.54	1.43
9	A	2052	A1AIO	O07-C06	5.08	1.54	1.43
9	A	2002	A1AIO	O07-C06	5.08	1.54	1.43
9	A	2053	A1AIO	O07-C06	5.08	1.54	1.43
9	A	2028	A1AIO	O07-C06	5.08	1.54	1.43
9	A	2005	A1AIO	O07-C06	5.08	1.54	1.43
9	B	2050	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2006	A1AIO	O07-C06	5.07	1.54	1.43
9	A	2008	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2029	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2026	A1AIO	O07-C06	5.07	1.54	1.43
9	A	2007	A1AIO	O07-C06	5.07	1.54	1.43
9	A	2013	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2019	A1AIO	O07-C06	5.07	1.54	1.43
9	A	2047	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2032	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2039	A1AIO	O07-C06	5.07	1.54	1.43
9	A	2031	A1AIO	O07-C06	5.07	1.54	1.43
9	B	2007	A1AIO	O07-C06	5.06	1.54	1.43
9	A	2043	A1AIO	O07-C06	5.06	1.54	1.43
9	A	2016	A1AIO	O07-C06	5.06	1.54	1.43
9	B	2051	A1AIO	O07-C06	5.06	1.54	1.43
9	B	2010	A1AIO	O07-C06	5.06	1.54	1.43
9	B	2048	A1AIO	O07-C06	5.06	1.54	1.43
9	A	2012	A1AIO	O07-C06	5.06	1.54	1.43
9	A	2034	A1AIO	O07-C06	5.05	1.54	1.43
9	B	2001	A1AIO	O07-C06	5.05	1.54	1.43
9	B	2044	A1AIO	O07-C06	5.05	1.54	1.43
9	B	2036	A1AIO	O07-C06	5.05	1.54	1.43
9	B	2038	A1AIO	O07-C06	5.05	1.54	1.43
9	B	2028	A1AIO	O07-C06	5.05	1.54	1.43
9	B	2052	A1AIO	O07-C06	5.04	1.54	1.43
9	A	2057	A1AIO	O07-C06	5.04	1.54	1.43
9	B	2045	A1AIO	O07-C06	5.04	1.54	1.43
9	B	2043	A1AIO	O07-C06	5.04	1.54	1.43
9	A	2045	A1AIO	O07-C06	5.04	1.54	1.43
9	B	2053	A1AIO	O07-C06	5.04	1.54	1.43
9	A	2003	A1AIO	O07-C06	5.04	1.54	1.43
9	B	2042	A1AIO	O07-C06	5.04	1.54	1.43
9	B	2002	A1AIO	O07-C06	5.04	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2009	A1AIO	O07-C06	5.04	1.54	1.43
9	B	2037	A1AIO	O07-C06	5.03	1.54	1.43
9	B	2035	A1AIO	O07-C06	5.03	1.54	1.43
9	B	2057	A1AIO	O07-C06	5.03	1.54	1.43
9	A	2038	A1AIO	O07-C06	5.02	1.54	1.43
9	A	2049	A1AIO	O07-C06	5.02	1.54	1.43
9	A	2048	A1AIO	O07-C06	5.01	1.54	1.43
9	B	2008	A1AIO	O07-C06	5.01	1.54	1.43
9	B	2011	A1AIO	O07-C06	5.00	1.54	1.43
9	B	2023	A1AIO	O07-C06	4.99	1.54	1.43
9	B	2015	A1AIO	O07-C06	4.99	1.54	1.43
9	B	2016	A1AIO	O07-C06	4.99	1.54	1.43
9	A	2056	A1AIO	O07-C06	4.99	1.54	1.43
9	A	2006	A1AIO	O07-C06	4.99	1.54	1.43
9	A	2040	A1AIO	O07-C06	4.99	1.54	1.43
9	B	2040	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2005	A1AIO	O07-C06	4.98	1.54	1.43
9	A	2029	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2009	A1AIO	O07-C06	4.98	1.54	1.43
9	A	2004	A1AIO	O07-C06	4.98	1.54	1.43
9	B	2046	A1AIO	O07-C06	4.96	1.54	1.43
9	B	2031	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2034	A1AIO	O07-C06	4.95	1.54	1.43
9	B	2047	A1AIO	O07-C06	4.94	1.54	1.43
9	B	2041	A1AIO	O07-C06	4.94	1.54	1.43
9	B	2033	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2030	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2055	A1AIO	O07-C06	4.93	1.54	1.43
9	B	2053	A1AIO	C06-C05	4.14	1.59	1.51
9	B	2007	A1AIO	C06-C05	4.13	1.59	1.51
9	A	2023	A1AIO	C06-C05	4.12	1.59	1.51
9	A	2028	A1AIO	C06-C05	4.12	1.58	1.51
9	B	2021	A1AIO	C06-C05	4.12	1.58	1.51
9	A	2040	A1AIO	C06-C05	4.11	1.58	1.51
9	B	2027	A1AIO	C06-C05	4.10	1.58	1.51
9	B	2002	A1AIO	C06-C05	4.10	1.58	1.51
9	B	2049	A1AIO	C06-C05	4.09	1.58	1.51
9	A	2019	A1AIO	C06-C05	4.09	1.58	1.51
9	A	2036	A1AIO	C06-C05	4.09	1.58	1.51
9	B	2014	A1AIO	C06-C05	4.09	1.58	1.51
9	A	2010	A1AIO	C06-C05	4.09	1.58	1.51
9	A	2011	A1AIO	C06-C05	4.09	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2029	A1AIO	C06-C05	4.08	1.58	1.51
9	A	2012	A1AIO	C06-C05	4.08	1.58	1.51
9	A	2052	A1AIO	C06-C05	4.07	1.58	1.51
9	B	2001	A1AIO	C06-C05	4.07	1.58	1.51
9	B	2006	A1AIO	C06-C05	4.06	1.58	1.51
9	B	2010	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2013	A1AIO	C06-C05	4.06	1.58	1.51
9	B	2037	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2038	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2005	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2016	A1AIO	C06-C05	4.06	1.58	1.51
9	B	2020	A1AIO	C06-C05	4.06	1.58	1.51
9	B	2011	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2018	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2035	A1AIO	C06-C05	4.06	1.58	1.51
9	A	2022	A1AIO	C06-C05	4.05	1.58	1.51
9	A	2001	A1AIO	C06-C05	4.05	1.58	1.51
9	B	2018	A1AIO	C06-C05	4.05	1.58	1.51
9	A	2042	A1AIO	C06-C05	4.05	1.58	1.51
9	A	2009	A1AIO	C06-C05	4.04	1.58	1.51
9	B	2024	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2024	A1AIO	C06-C05	4.04	1.58	1.51
9	B	2042	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2032	A1AIO	C06-C05	4.04	1.58	1.51
9	B	2038	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2007	A1AIO	C06-C05	4.04	1.58	1.51
9	B	2043	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2041	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2020	A1AIO	C06-C05	4.04	1.58	1.51
9	A	2015	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2012	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2030	A1AIO	C06-C05	4.03	1.58	1.51
9	A	2054	A1AIO	C06-C05	4.03	1.58	1.51
9	A	2017	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2032	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2019	A1AIO	C06-C05	4.03	1.58	1.51
9	B	2057	A1AIO	C06-C05	4.03	1.58	1.51
9	A	2014	A1AIO	C06-C05	4.02	1.58	1.51
9	A	2002	A1AIO	C06-C05	4.02	1.58	1.51
9	B	2036	A1AIO	C06-C05	4.02	1.58	1.51
9	A	2031	A1AIO	C06-C05	4.02	1.58	1.51
9	B	2025	A1AIO	C06-C05	4.02	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2055	A1AIO	C06-C05	4.02	1.58	1.51
9	B	2055	A1AIO	C06-C05	4.02	1.58	1.51
9	B	2048	A1AIO	C06-C05	4.01	1.58	1.51
9	A	2051	A1AIO	C06-C05	4.01	1.58	1.51
9	A	2053	A1AIO	C06-C05	4.01	1.58	1.51
9	A	2003	A1AIO	C06-C05	4.01	1.58	1.51
9	A	2021	A1AIO	C06-C05	4.01	1.58	1.51
9	B	2045	A1AIO	C06-C05	4.01	1.58	1.51
9	A	2006	A1AIO	C06-C05	4.00	1.58	1.51
9	A	2008	A1AIO	C06-C05	4.00	1.58	1.51
9	B	2013	A1AIO	C06-C05	4.00	1.58	1.51
9	A	2026	A1AIO	C06-C05	4.00	1.58	1.51
9	B	2022	A1AIO	C06-C05	4.00	1.58	1.51
9	A	2057	A1AIO	C06-C05	4.00	1.58	1.51
9	B	2017	A1AIO	C06-C05	4.00	1.58	1.51
9	B	2044	A1AIO	C06-C05	4.00	1.58	1.51
9	A	2025	A1AIO	C06-C05	3.99	1.58	1.51
9	B	2050	A1AIO	C06-C05	3.99	1.58	1.51
9	A	2056	A1AIO	C06-C05	3.99	1.58	1.51
9	B	2040	A1AIO	C06-C05	3.99	1.58	1.51
9	B	2056	A1AIO	C06-C05	3.99	1.58	1.51
9	A	2043	A1AIO	C06-C05	3.98	1.58	1.51
9	B	2009	A1AIO	C06-C05	3.98	1.58	1.51
9	B	2016	A1AIO	C06-C05	3.97	1.58	1.51
9	A	2034	A1AIO	C06-C05	3.97	1.58	1.51
9	B	2004	A1AIO	C06-C05	3.96	1.58	1.51
9	A	2027	A1AIO	C06-C05	3.95	1.58	1.51
9	A	2033	A1AIO	C06-C05	3.95	1.58	1.51
9	B	2015	A1AIO	C06-C05	3.94	1.58	1.51
9	B	2035	A1AIO	C06-C05	3.94	1.58	1.51
9	A	2050	A1AIO	C06-C05	3.94	1.58	1.51
9	B	2051	A1AIO	C06-C05	3.94	1.58	1.51
9	B	2039	A1AIO	C06-C05	3.94	1.58	1.51
9	A	2030	A1AIO	C06-C05	3.93	1.58	1.51
9	B	2008	A1AIO	C06-C05	3.93	1.58	1.51
9	B	2031	A1AIO	C06-C05	3.92	1.58	1.51
9	A	2037	A1AIO	C06-C05	3.91	1.58	1.51
9	A	2046	A1AIO	C06-C05	3.91	1.58	1.51
9	B	2026	A1AIO	C06-C05	3.91	1.58	1.51
9	A	2004	A1AIO	C06-C05	3.90	1.58	1.51
9	B	2034	A1AIO	C06-C05	3.89	1.58	1.51
9	A	2049	A1AIO	C06-C05	3.89	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2044	A1AIO	C06-C05	3.89	1.58	1.51
9	A	2045	A1AIO	C06-C05	3.88	1.58	1.51
9	B	2023	A1AIO	C06-C05	3.88	1.58	1.51
9	A	2048	A1AIO	C06-C05	3.88	1.58	1.51
9	B	2046	A1AIO	C06-C05	3.88	1.58	1.51
9	B	2054	A1AIO	C06-C05	3.88	1.58	1.51
9	A	2047	A1AIO	C06-C05	3.88	1.58	1.51
9	B	2052	A1AIO	C06-C05	3.87	1.58	1.51
9	A	2039	A1AIO	C06-C05	3.86	1.58	1.51
9	B	2003	A1AIO	C06-C05	3.85	1.58	1.51
9	B	2028	A1AIO	C06-C05	3.85	1.58	1.51
9	A	2029	A1AIO	C06-C05	3.85	1.58	1.51
9	B	2041	A1AIO	C06-C05	3.85	1.58	1.51
9	B	2005	A1AIO	C06-C05	3.82	1.58	1.51
9	B	2033	A1AIO	C06-C05	3.81	1.58	1.51
9	B	2047	A1AIO	C06-C05	3.76	1.58	1.51
10	B	2069	GLA	C2-C3	-3.43	1.47	1.52
10	A	2068	GLA	C2-C3	-3.41	1.47	1.52
10	B	2061	GLA	C2-C3	-3.40	1.47	1.52
10	B	2068	GLA	C2-C3	-3.40	1.47	1.52
10	A	2069	GLA	C2-C3	-3.37	1.47	1.52
10	A	2067	GLA	C2-C3	-3.36	1.47	1.52
10	B	2070	GLA	C2-C3	-3.36	1.47	1.52
10	A	2061	GLA	C2-C3	-3.36	1.47	1.52
10	A	2070	GLA	C2-C3	-3.33	1.47	1.52
10	B	2066	GLA	C2-C3	-3.32	1.47	1.52
10	A	2065	GLA	C2-C3	-3.31	1.47	1.52
10	A	2063	GLA	C2-C3	-3.30	1.47	1.52
10	A	2066	GLA	C2-C3	-3.28	1.47	1.52
10	B	2067	GLA	C2-C3	-3.27	1.47	1.52
10	B	2058	GLA	C2-C3	-3.27	1.47	1.52
10	B	2060	GLA	C2-C3	-3.27	1.47	1.52
10	A	2062	GLA	C2-C3	-3.26	1.47	1.52
10	A	2064	GLA	C2-C3	-3.26	1.47	1.52
10	B	2062	GLA	C2-C3	-3.26	1.47	1.52
10	B	2063	GLA	C2-C3	-3.25	1.47	1.52
10	B	2064	GLA	C2-C3	-3.24	1.47	1.52
10	A	2058	GLA	C2-C3	-3.20	1.47	1.52
10	B	2065	GLA	C2-C3	-3.15	1.47	1.52
10	B	2063	GLA	O5-C1	3.11	1.48	1.43
10	A	2063	GLA	O5-C1	3.10	1.48	1.43
10	A	2067	GLA	O5-C1	3.10	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	2062	GLA	O5-C1	3.08	1.48	1.43
10	A	2061	GLA	O5-C1	3.07	1.48	1.43
10	B	2066	GLA	O5-C1	3.07	1.48	1.43
10	A	2058	GLA	O5-C1	3.06	1.48	1.43
10	A	2064	GLA	O5-C1	3.06	1.48	1.43
10	B	2060	GLA	O5-C1	3.06	1.48	1.43
10	A	2062	GLA	O5-C1	3.06	1.48	1.43
10	B	2058	GLA	O5-C1	3.06	1.48	1.43
10	B	2067	GLA	O5-C1	3.05	1.48	1.43
10	B	2068	GLA	O5-C1	3.04	1.48	1.43
10	A	2065	GLA	O5-C1	3.04	1.48	1.43
10	B	2070	GLA	O5-C1	3.03	1.48	1.43
10	B	2064	GLA	O5-C1	3.02	1.48	1.43
10	A	2068	GLA	O5-C1	3.02	1.48	1.43
10	A	2066	GLA	O5-C1	3.01	1.48	1.43
10	B	2065	GLA	O5-C1	3.00	1.48	1.43
10	B	2061	GLA	O5-C1	3.00	1.48	1.43
10	A	2070	GLA	O5-C1	2.98	1.48	1.43
10	A	2069	GLA	O5-C1	2.98	1.48	1.43
10	B	2069	GLA	O5-C1	2.96	1.48	1.43
10	B	2063	GLA	O5-C5	2.53	1.48	1.43
10	A	2065	GLA	O5-C5	2.50	1.48	1.43
10	A	2066	GLA	O5-C5	2.47	1.48	1.43
10	B	2064	GLA	O5-C5	2.44	1.48	1.43
10	A	2061	GLA	O5-C5	2.43	1.48	1.43
10	B	2061	GLA	O5-C5	2.43	1.48	1.43
10	A	2068	GLA	O5-C5	2.43	1.48	1.43
10	A	2070	GLA	O5-C5	2.43	1.48	1.43
10	A	2067	GLA	O5-C5	2.43	1.48	1.43
10	B	2066	GLA	O5-C5	2.43	1.48	1.43
10	A	2058	GLA	O5-C5	2.41	1.48	1.43
10	B	2062	GLA	O5-C5	2.41	1.48	1.43
10	A	2064	GLA	O5-C5	2.41	1.48	1.43
10	B	2067	GLA	O5-C5	2.40	1.48	1.43
10	A	2062	GLA	O5-C5	2.40	1.48	1.43
10	A	2063	GLA	O5-C5	2.39	1.48	1.43
10	B	2058	GLA	O5-C5	2.38	1.48	1.43
10	B	2065	GLA	O5-C5	2.37	1.48	1.43
10	A	2069	GLA	O5-C5	2.37	1.48	1.43
10	B	2060	GLA	O5-C5	2.36	1.48	1.43
10	B	2069	GLA	O5-C5	2.36	1.48	1.43
10	B	2068	GLA	O5-C5	2.35	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	2070	GLA	O5-C5	2.34	1.48	1.43
9	B	2039	A1AIO	O11-C02	-2.27	1.38	1.43
9	B	2042	A1AIO	O11-C02	-2.27	1.38	1.43
9	A	2029	A1AIO	O11-C02	-2.27	1.38	1.43
9	A	2003	A1AIO	O11-C02	-2.26	1.38	1.43
9	A	2056	A1AIO	O11-C02	-2.25	1.38	1.43
9	A	2057	A1AIO	O11-C02	-2.24	1.38	1.43
9	B	2028	A1AIO	O11-C02	-2.24	1.38	1.43
9	B	2003	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2038	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2044	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2043	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2036	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2045	A1AIO	O11-C02	-2.23	1.38	1.43
9	B	2048	A1AIO	O11-C02	-2.23	1.38	1.43
9	A	2048	A1AIO	O11-C02	-2.22	1.38	1.43
9	A	2055	A1AIO	O11-C02	-2.22	1.38	1.43
9	A	2043	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2051	A1AIO	O11-C02	-2.22	1.38	1.43
9	A	2007	A1AIO	O11-C02	-2.22	1.38	1.43
9	B	2035	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2051	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2055	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2030	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2049	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2010	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2050	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2033	A1AIO	O11-C02	-2.21	1.38	1.43
9	A	2054	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2005	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2027	A1AIO	O11-C02	-2.21	1.38	1.43
9	B	2013	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2004	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2057	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2047	A1AIO	O11-C02	-2.20	1.38	1.43
9	A	2045	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2008	A1AIO	O11-C02	-2.20	1.38	1.43
9	A	2004	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2056	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2052	A1AIO	O11-C02	-2.20	1.38	1.43
9	B	2010	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2034	A1AIO	O11-C02	-2.19	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	2021	A1AIO	O11-C02	-2.19	1.38	1.43
9	A	2049	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2016	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2054	A1AIO	O11-C02	-2.19	1.38	1.43
9	A	2005	A1AIO	O11-C02	-2.19	1.38	1.43
9	B	2032	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2023	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2006	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2033	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2040	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2008	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2013	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2046	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2032	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2009	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2016	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2028	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2020	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2011	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2041	A1AIO	O11-C02	-2.18	1.38	1.43
9	A	2041	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2012	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2050	A1AIO	O11-C02	-2.18	1.38	1.43
9	B	2006	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2031	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2011	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2022	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2001	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2015	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2022	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2002	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2024	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2026	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2047	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2040	A1AIO	O11-C02	-2.17	1.38	1.43
9	B	2037	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2053	A1AIO	O11-C02	-2.17	1.38	1.43
9	A	2012	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2053	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2019	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2023	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2036	A1AIO	O11-C02	-2.16	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	2009	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2030	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2046	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2018	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2014	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2029	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2025	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2031	A1AIO	O11-C02	-2.16	1.38	1.43
9	B	2021	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2001	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2034	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2037	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2042	A1AIO	O11-C02	-2.16	1.38	1.43
9	A	2052	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2039	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2025	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2017	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2015	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2002	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2019	A1AIO	O11-C02	-2.15	1.38	1.43
9	B	2007	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2038	A1AIO	O11-C02	-2.15	1.38	1.43
9	A	2024	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2018	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2014	A1AIO	O11-C02	-2.14	1.38	1.43
9	A	2027	A1AIO	O11-C02	-2.14	1.38	1.43
9	B	2020	A1AIO	O11-C02	-2.13	1.38	1.43
9	A	2035	A1AIO	O11-C02	-2.13	1.38	1.43
9	B	2026	A1AIO	O11-C02	-2.12	1.38	1.43
9	B	2017	A1AIO	O11-C02	-2.12	1.38	1.43
9	A	2044	A1AIO	O11-C02	-2.11	1.38	1.43

All (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
9	A	2027	A1AIO	C02-C03-C04	-4.44	109.58	115.95
9	B	2009	A1AIO	C02-C03-C04	-4.43	109.58	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2006	A1AIO	C02-C03-C04	-4.42	109.60	115.95
9	A	2034	A1AIO	C02-C03-C04	-4.42	109.61	115.95
9	A	2053	A1AIO	C02-C03-C04	-4.40	109.63	115.95
9	B	2004	A1AIO	C02-C03-C04	-4.37	109.67	115.95
9	B	2025	A1AIO	C02-C03-C04	-4.37	109.68	115.95
9	A	2043	A1AIO	C02-C03-C04	-4.34	109.72	115.95
9	A	2039	A1AIO	C02-C03-C04	-4.32	109.74	115.95
9	A	2031	A1AIO	C02-C03-C04	-4.30	109.77	115.95
9	B	2037	A1AIO	C02-C03-C04	-4.30	109.78	115.95
9	B	2035	A1AIO	C02-C03-C04	-4.29	109.79	115.95
9	A	2026	A1AIO	C02-C03-C04	-4.27	109.82	115.95
9	A	2042	A1AIO	C02-C03-C04	-4.27	109.82	115.95
9	A	2024	A1AIO	C02-C03-C04	-4.27	109.83	115.95
9	B	2038	A1AIO	C02-C03-C04	-4.26	109.83	115.95
9	B	2008	A1AIO	C02-C03-C04	-4.26	109.84	115.95
9	B	2041	A1AIO	C02-C03-C04	-4.25	109.84	115.95
9	B	2001	A1AIO	C02-C03-C04	-4.25	109.84	115.95
9	A	2003	A1AIO	C02-C03-C04	-4.24	109.86	115.95
9	B	2039	A1AIO	C02-C03-C04	-4.24	109.86	115.95
9	B	2003	A1AIO	C02-C03-C04	-4.23	109.87	115.95
9	B	2032	A1AIO	C02-C03-C04	-4.22	109.88	115.95
9	B	2027	A1AIO	C02-C03-C04	-4.21	109.90	115.95
9	B	2040	A1AIO	C02-C03-C04	-4.21	109.90	115.95
9	B	2049	A1AIO	C02-C03-C04	-4.21	109.90	115.95
9	A	2048	A1AIO	C02-C03-C04	-4.19	109.93	115.95
9	A	2047	A1AIO	C02-C03-C04	-4.19	109.94	115.95
9	A	2049	A1AIO	C02-C03-C04	-4.19	109.94	115.95
9	B	2046	A1AIO	C02-C03-C04	-4.18	109.94	115.95
9	B	2052	A1AIO	C02-C03-C04	-4.18	109.94	115.95
9	A	2045	A1AIO	C02-C03-C04	-4.18	109.94	115.95
9	A	2011	A1AIO	C02-C03-C04	-4.18	109.95	115.95
9	B	2002	A1AIO	C02-C03-C04	-4.18	109.95	115.95
9	B	2034	A1AIO	C02-C03-C04	-4.18	109.95	115.95
9	A	2004	A1AIO	C02-C03-C04	-4.17	109.95	115.95
9	A	2002	A1AIO	C02-C03-C04	-4.17	109.96	115.95
9	A	2046	A1AIO	C02-C03-C04	-4.16	109.98	115.95
9	B	2007	A1AIO	C02-C03-C04	-4.16	109.98	115.95
9	A	2001	A1AIO	C02-C03-C04	-4.16	109.98	115.95
9	A	2051	A1AIO	C02-C03-C04	-4.14	110.00	115.95
9	A	2007	A1AIO	C02-C03-C04	-4.13	110.01	115.95
9	B	2048	A1AIO	C02-C03-C04	-4.12	110.03	115.95
9	B	2019	A1AIO	C02-C03-C04	-4.12	110.03	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2044	A1AIO	C02-C03-C04	-4.12	110.03	115.95
9	A	2036	A1AIO	C02-C03-C04	-4.11	110.05	115.95
9	B	2036	A1AIO	C02-C03-C04	-4.11	110.05	115.95
9	B	2043	A1AIO	C02-C03-C04	-4.11	110.05	115.95
9	A	2028	A1AIO	C02-C03-C04	-4.10	110.07	115.95
9	B	2045	A1AIO	C02-C03-C04	-4.09	110.08	115.95
9	B	2056	A1AIO	C02-C03-C04	-4.09	110.08	115.95
9	A	2025	A1AIO	C02-C03-C04	-4.08	110.09	115.95
9	B	2042	A1AIO	C02-C03-C04	-4.08	110.09	115.95
9	A	2056	A1AIO	C02-C03-C04	-4.08	110.10	115.95
9	A	2009	A1AIO	C02-C03-C04	-4.07	110.10	115.95
9	A	2018	A1AIO	C02-C03-C04	-4.07	110.11	115.95
9	A	2052	A1AIO	C02-C03-C04	-4.04	110.15	115.95
9	B	2012	A1AIO	C02-C03-C04	-4.04	110.15	115.95
9	A	2014	A1AIO	C02-C03-C04	-4.04	110.15	115.95
9	B	2029	A1AIO	C02-C03-C04	-4.04	110.15	115.95
9	B	2010	A1AIO	C02-C03-C04	-4.03	110.16	115.95
9	A	2037	A1AIO	C02-C03-C04	-4.03	110.16	115.95
9	A	2012	A1AIO	C02-C03-C04	-4.03	110.17	115.95
9	A	2017	A1AIO	C02-C03-C04	-4.01	110.19	115.95
9	B	2024	A1AIO	C02-C03-C04	-4.01	110.19	115.95
9	B	2057	A1AIO	C02-C03-C04	-4.01	110.20	115.95
9	A	2008	A1AIO	C02-C03-C04	-4.00	110.20	115.95
9	A	2022	A1AIO	C02-C03-C04	-4.00	110.20	115.95
9	A	2005	A1AIO	C02-C03-C04	-4.00	110.21	115.95
9	A	2033	A1AIO	C02-C03-C04	-4.00	110.21	115.95
9	A	2013	A1AIO	C02-C03-C04	-3.94	110.30	115.95
9	A	2057	A1AIO	C02-C03-C04	-3.92	110.32	115.95
9	A	2016	A1AIO	C02-C03-C04	-3.92	110.32	115.95
9	A	2032	A1AIO	C02-C03-C04	-3.92	110.33	115.95
9	B	2017	A1AIO	C02-C03-C04	-3.89	110.36	115.95
9	A	2040	A1AIO	C02-C03-C04	-3.88	110.38	115.95
9	A	2054	A1AIO	C02-C03-C04	-3.87	110.39	115.95
9	A	2010	A1AIO	C02-C03-C04	-3.86	110.41	115.95
9	A	2023	A1AIO	C02-C03-C04	-3.86	110.41	115.95
9	A	2021	A1AIO	C02-C03-C04	-3.86	110.41	115.95
9	B	2011	A1AIO	C02-C03-C04	-3.85	110.43	115.95
9	B	2055	A1AIO	C02-C03-C04	-3.85	110.43	115.95
9	A	2020	A1AIO	C02-C03-C04	-3.85	110.43	115.95
9	A	2019	A1AIO	C02-C03-C04	-3.84	110.44	115.95
9	B	2015	A1AIO	C02-C03-C04	-3.83	110.45	115.95
9	A	2038	A1AIO	C02-C03-C04	-3.81	110.48	115.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	2031	A1AIO	C02-C03-C04	-3.79	110.51	115.95
9	B	2053	A1AIO	C02-C03-C04	-3.78	110.52	115.95
9	A	2030	A1AIO	C02-C03-C04	-3.76	110.55	115.95
9	B	2013	A1AIO	C02-C03-C04	-3.76	110.55	115.95
9	A	2015	A1AIO	C02-C03-C04	-3.74	110.58	115.95
9	A	2041	A1AIO	C02-C03-C04	-3.72	110.60	115.95
9	B	2018	A1AIO	C02-C03-C04	-3.71	110.62	115.95
9	A	2055	A1AIO	C02-C03-C04	-3.70	110.64	115.95
9	A	2035	A1AIO	C02-C03-C04	-3.69	110.65	115.95
9	B	2050	A1AIO	C02-C03-C04	-3.69	110.65	115.95
9	B	2022	A1AIO	C02-C03-C04	-3.66	110.70	115.95
9	B	2021	A1AIO	C02-C03-C04	-3.64	110.73	115.95
9	A	2050	A1AIO	C02-C03-C04	-3.57	110.82	115.95
9	B	2014	A1AIO	C02-C03-C04	-3.52	110.90	115.95
9	B	2051	A1AIO	C02-C03-C04	-3.50	110.93	115.95
9	A	2029	A1AIO	C02-C03-C04	-3.48	110.95	115.95
9	B	2030	A1AIO	C02-C03-C04	-3.41	111.05	115.95
9	B	2016	A1AIO	C06-C05-C04	3.38	107.04	101.63
9	B	2028	A1AIO	C02-C03-C04	-3.32	111.18	115.95
9	B	2046	A1AIO	C06-C05-C04	3.30	106.91	101.63
9	B	2009	A1AIO	C06-C05-C04	3.30	106.91	101.63
9	B	2023	A1AIO	C02-C03-C04	-3.28	111.24	115.95
9	B	2034	A1AIO	C06-C05-C04	3.26	106.85	101.63
9	B	2031	A1AIO	C06-C05-C04	3.22	106.78	101.63
9	B	2030	A1AIO	C06-C05-C04	3.22	106.77	101.63
9	B	2011	A1AIO	C06-C05-C04	3.21	106.76	101.63
9	B	2020	A1AIO	C02-C03-C04	-3.17	111.39	115.95
9	B	2005	A1AIO	C02-C03-C04	-3.12	111.47	115.95
9	B	2054	A1AIO	C02-C03-C04	-3.12	111.47	115.95
9	B	2055	A1AIO	C06-C05-C04	3.06	106.53	101.63
9	A	2016	A1AIO	C06-C05-C04	3.01	106.44	101.63
9	A	2040	A1AIO	C06-C05-C04	3.00	106.43	101.63
9	A	2038	A1AIO	C06-C05-C04	2.98	106.40	101.63
9	A	2009	A1AIO	C06-C05-C04	2.97	106.38	101.63
9	A	2006	A1AIO	C06-C05-C04	2.97	106.38	101.63
9	B	2052	A1AIO	C06-C05-C04	2.92	106.30	101.63
9	B	2001	A1AIO	C06-C05-C04	2.92	106.30	101.63
9	B	2016	A1AIO	C02-C03-C04	-2.92	111.76	115.95
9	B	2014	A1AIO	C06-C05-C04	2.90	106.26	101.63
9	A	2056	A1AIO	C06-C05-C04	2.89	106.25	101.63
9	B	2050	A1AIO	C06-C05-C04	2.89	106.24	101.63
9	B	2022	A1AIO	C06-C05-C04	2.88	106.23	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2012	A1AIO	C06-C05-C04	2.87	106.22	101.63
9	B	2017	A1AIO	C06-C05-C04	2.86	106.19	101.63
9	B	2053	A1AIO	C06-C05-C04	2.84	106.17	101.63
9	B	2019	A1AIO	C06-C05-C04	2.83	106.16	101.63
9	A	2032	A1AIO	C06-C05-C04	2.83	106.16	101.63
9	B	2041	A1AIO	C06-C05-C04	2.83	106.15	101.63
9	B	2023	A1AIO	C06-C05-C04	2.80	106.10	101.63
9	B	2015	A1AIO	C06-C05-C04	2.78	106.08	101.63
9	B	2040	A1AIO	C06-C05-C04	2.77	106.05	101.63
9	B	2032	A1AIO	C06-C05-C04	2.76	106.04	101.63
9	B	2008	A1AIO	C06-C05-C04	2.74	106.02	101.63
9	B	2002	A1AIO	C06-C05-C04	2.70	105.95	101.63
9	B	2057	A1AIO	C06-C05-C04	2.70	105.95	101.63
10	B	2063	GLA	C1-C2-C3	2.69	113.56	109.64
9	B	2005	A1AIO	C06-C05-C04	2.68	105.91	101.63
9	B	2051	A1AIO	C06-C05-C04	2.67	105.90	101.63
9	B	2020	A1AIO	C06-C05-C04	2.63	105.83	101.63
9	A	2011	A1AIO	C06-C05-C04	2.58	105.75	101.63
9	A	2023	A1AIO	C06-C05-C04	2.57	105.74	101.63
9	A	2018	A1AIO	C06-C05-C04	2.57	105.73	101.63
9	B	2004	A1AIO	C06-C05-C04	2.57	105.73	101.63
9	A	2044	A1AIO	C06-C05-C04	2.53	105.67	101.63
9	A	2048	A1AIO	C06-C05-C04	2.50	105.63	101.63
9	B	2037	A1AIO	C06-C05-C04	2.50	105.62	101.63
9	A	2045	A1AIO	C06-C05-C04	2.48	105.59	101.63
9	A	2047	A1AIO	C06-C05-C04	2.48	105.59	101.63
9	B	2047	A1AIO	C06-C05-C04	2.46	105.57	101.63
9	A	2049	A1AIO	C06-C05-C04	2.45	105.55	101.63
9	B	2033	A1AIO	C06-C05-C04	2.45	105.54	101.63
9	A	2052	A1AIO	C06-C05-C04	2.40	105.47	101.63
9	A	2008	A1AIO	C06-C05-C04	2.39	105.45	101.63
9	A	2014	A1AIO	C06-C05-C04	2.39	105.45	101.63
9	A	2022	A1AIO	C06-C05-C04	2.38	105.44	101.63
9	A	2007	A1AIO	C06-C05-C04	2.38	105.43	101.63
9	A	2013	A1AIO	C06-C05-C04	2.35	105.38	101.63
9	A	2053	A1AIO	C06-C05-C04	2.32	105.33	101.63
9	B	2012	A1AIO	C06-C05-C04	2.31	105.33	101.63
9	B	2013	A1AIO	C06-C05-C04	2.31	105.33	101.63
10	A	2060	GLA	C1-O5-C5	2.30	115.27	112.19
9	B	2006	A1AIO	C06-C05-C04	2.29	105.29	101.63
9	A	2036	A1AIO	C06-C05-C04	2.29	105.29	101.63
10	A	2059	GLA	C1-O5-C5	2.29	115.25	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2046	A1AIO	C06-C05-C04	2.29	105.29	101.63
9	B	2054	A1AIO	C06-C05-C04	2.29	105.28	101.63
10	B	2059	GLA	C1-O5-C5	2.28	115.25	112.19
9	A	2034	A1AIO	C06-C05-C04	2.28	105.28	101.63
9	B	2028	A1AIO	C06-C05-C04	2.27	105.25	101.63
9	A	2029	A1AIO	C06-C05-C04	2.26	105.24	101.63
9	B	2007	A1AIO	C06-C05-C04	2.25	105.22	101.63
9	A	2051	A1AIO	C06-C05-C04	2.24	105.22	101.63
9	A	2010	A1AIO	C06-C05-C04	2.24	105.21	101.63
9	B	2029	A1AIO	C06-C05-C04	2.24	105.20	101.63
9	A	2024	A1AIO	C06-C05-C04	2.23	105.20	101.63
9	A	2015	A1AIO	C06-C05-C04	2.23	105.19	101.63
9	A	2020	A1AIO	C06-C05-C04	2.23	105.19	101.63
9	A	2054	A1AIO	C06-C05-C04	2.22	105.18	101.63
9	A	2055	A1AIO	C06-C05-C04	2.21	105.17	101.63
9	A	2037	A1AIO	C06-C05-C04	2.19	105.14	101.63
9	B	2026	A1AIO	C06-C05-C04	2.19	105.13	101.63
9	B	2027	A1AIO	C06-C05-C04	2.19	105.12	101.63
9	B	2049	A1AIO	C06-C05-C04	2.19	105.12	101.63
9	A	2004	A1AIO	C06-C05-C04	2.18	105.12	101.63
9	B	2035	A1AIO	C06-C05-C04	2.17	105.10	101.63
10	A	2058	GLA	C1-C2-C3	2.17	112.80	109.64
9	A	2002	A1AIO	C06-C05-C04	2.16	105.08	101.63
9	B	2018	A1AIO	C06-C05-C04	2.14	105.05	101.63
9	B	2056	A1AIO	C06-C05-C04	2.14	105.05	101.63
9	A	2042	A1AIO	C06-C05-C04	2.13	105.04	101.63
9	A	2019	A1AIO	C06-C05-C04	2.13	105.04	101.63
9	B	2010	A1AIO	C06-C05-C04	2.12	105.02	101.63
9	A	2025	A1AIO	C06-C05-C04	2.12	105.02	101.63
9	B	2025	A1AIO	C06-C05-C04	2.11	105.00	101.63
9	B	2038	A1AIO	C06-C05-C04	2.10	104.99	101.63
9	B	2044	A1AIO	C06-C05-C04	2.10	104.98	101.63
10	B	2065	GLA	C1-C2-C3	2.09	112.69	109.64
9	B	2043	A1AIO	C06-C05-C04	2.09	104.97	101.63
9	A	2001	A1AIO	C06-C05-C04	2.09	104.97	101.63
9	A	2003	A1AIO	C06-C05-C04	2.09	104.97	101.63
9	A	2005	A1AIO	C06-C05-C04	2.08	104.96	101.63
9	A	2039	A1AIO	C06-C05-C04	2.08	104.95	101.63
9	B	2045	A1AIO	C06-C05-C04	2.07	104.94	101.63
9	B	2036	A1AIO	C06-C05-C04	2.07	104.94	101.63
9	B	2048	A1AIO	C06-C05-C04	2.07	104.94	101.63
9	B	2042	A1AIO	C06-C05-C04	2.06	104.92	101.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	2026	A1AIO	C06-C05-C04	2.06	104.92	101.63
9	A	2041	A1AIO	C06-C05-C04	2.06	104.92	101.63
9	A	2050	A1AIO	C06-C05-C04	2.04	104.89	101.63
10	A	2062	GLA	C1-C2-C3	2.03	112.60	109.64
10	A	2064	GLA	C1-C2-C3	2.03	112.60	109.64
9	A	2028	A1AIO	C06-C05-C04	2.03	104.87	101.63
9	A	2021	A1AIO	C06-C05-C04	2.03	104.87	101.63
10	B	2060	GLA	C1-C2-C3	2.01	112.58	109.64
9	A	2027	A1AIO	C06-C05-C04	2.01	104.85	101.63
9	A	2031	A1AIO	C06-C05-C04	2.01	104.84	101.63
9	A	2030	A1AIO	C06-C05-C04	2.01	104.84	101.63
9	A	2057	A1AIO	C06-C05-C04	2.00	104.83	101.63

All (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
9	A	2014	A1AIO	C06
9	A	2016	A1AIO	C06
9	A	2018	A1AIO	C06
9	A	2025	A1AIO	C06
9	A	2035	A1AIO	C06
9	A	2037	A1AIO	C06
9	A	2038	A1AIO	C06
9	A	2040	A1AIO	C06
9	A	2052	A1AIO	C06
9	B	2004	A1AIO	C06
9	B	2006	A1AIO	C06
9	B	2009	A1AIO	C06
9	B	2011	A1AIO	C06
9	B	2012	A1AIO	C06
9	B	2014	A1AIO	C06
9	B	2016	A1AIO	C06
9	B	2030	A1AIO	C06
9	B	2031	A1AIO	C06
9	B	2032	A1AIO	C06
9	B	2033	A1AIO	C06
9	B	2034	A1AIO	C06

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Mol	Chain	Res	Type	Atom
9	B	2046	A1AIO	C06
9	B	2047	A1AIO	C06
9	B	2053	A1AIO	C06

All (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
9	A	2035	A1AIO	C01-C02-C03-O07
9	A	2038	A1AIO	C01-C02-C03-O07
9	A	2040	A1AIO	C01-C02-C03-O07
9	A	2041	A1AIO	C01-C02-C03-O07
9	A	2054	A1AIO	C01-C02-C03-O07
9	B	2001	A1AIO	O12-C01-C02-C03
9	B	2003	A1AIO	C01-C02-C03-O07
9	B	2005	A1AIO	O12-C01-C02-C03
9	B	2005	A1AIO	O12-C01-C02-O11
9	B	2005	A1AIO	C01-C02-C03-O07
9	B	2013	A1AIO	O12-C01-C02-O11
9	B	2014	A1AIO	C01-C02-C03-O07
9	B	2016	A1AIO	O12-C01-C02-O11
9	B	2016	A1AIO	C01-C02-C03-C04
9	B	2016	A1AIO	C01-C02-C03-O07
9	B	2016	A1AIO	O11-C02-C03-O07
9	B	2018	A1AIO	C01-C02-C03-O07
9	B	2019	A1AIO	O12-C01-C02-O11
9	B	2020	A1AIO	C01-C02-C03-C04
9	B	2020	A1AIO	C01-C02-C03-O07
9	B	2020	A1AIO	O11-C02-C03-C04
9	B	2020	A1AIO	O11-C02-C03-O07
9	B	2021	A1AIO	C01-C02-C03-O07
9	B	2023	A1AIO	C01-C02-C03-C04
9	B	2023	A1AIO	C01-C02-C03-O07
9	B	2023	A1AIO	O11-C02-C03-C04
9	B	2023	A1AIO	O11-C02-C03-O07
9	B	2028	A1AIO	O12-C01-C02-O11
9	B	2028	A1AIO	C01-C02-C03-O07
9	B	2030	A1AIO	C01-C02-C03-O07

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Mol	Chain	Res	Type	Atoms
9	B	2032	A1AIO	O12-C01-C02-C03
9	B	2032	A1AIO	O12-C01-C02-O11
9	B	2034	A1AIO	O12-C01-C02-O11
9	B	2036	A1AIO	O12-C01-C02-O11
9	B	2037	A1AIO	O12-C01-C02-C03
9	B	2037	A1AIO	O12-C01-C02-O11
9	B	2041	A1AIO	O12-C01-C02-O11
9	B	2042	A1AIO	O12-C01-C02-O11
9	B	2043	A1AIO	O12-C01-C02-O11
9	B	2044	A1AIO	O12-C01-C02-O11
9	B	2045	A1AIO	O12-C01-C02-O11
9	B	2046	A1AIO	O12-C01-C02-O11
9	B	2048	A1AIO	O12-C01-C02-O11
9	B	2051	A1AIO	C01-C02-C03-O07
9	B	2052	A1AIO	O12-C01-C02-O11
9	B	2053	A1AIO	C01-C02-C03-O07
9	B	2054	A1AIO	O12-C01-C02-C03
9	B	2054	A1AIO	O12-C01-C02-O11
9	B	2054	A1AIO	C01-C02-C03-O07
9	B	2054	A1AIO	O11-C02-C03-O07
10	B	2068	GLA	O5-C5-C6-O6
9	A	2035	A1AIO	O12-C01-C02-O11
9	A	2044	A1AIO	O12-C01-C02-O11
9	B	2001	A1AIO	O12-C01-C02-O11
9	B	2010	A1AIO	O12-C01-C02-O11
9	B	2021	A1AIO	O12-C01-C02-O11
9	B	2025	A1AIO	O12-C01-C02-O11
9	B	2035	A1AIO	O12-C01-C02-O11
9	B	2013	A1AIO	O12-C01-C02-C03
9	B	2016	A1AIO	O12-C01-C02-C03
9	B	2019	A1AIO	O12-C01-C02-C03
9	B	2028	A1AIO	O12-C01-C02-C03
9	B	2034	A1AIO	O12-C01-C02-C03
9	B	2036	A1AIO	O12-C01-C02-C03
9	B	2041	A1AIO	O12-C01-C02-C03
9	B	2042	A1AIO	O12-C01-C02-C03
9	B	2043	A1AIO	O12-C01-C02-C03
9	B	2044	A1AIO	O12-C01-C02-C03
9	B	2045	A1AIO	O12-C01-C02-C03
9	B	2046	A1AIO	O12-C01-C02-C03
9	B	2048	A1AIO	O12-C01-C02-C03
9	B	2052	A1AIO	O12-C01-C02-C03

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Mol	Chain	Res	Type	Atoms
10	B	2068	GLA	C4-C5-C6-O6
10	A	2063	GLA	O5-C5-C6-O6
10	B	2067	GLA	C4-C5-C6-O6
10	B	2058	GLA	O5-C5-C6-O6
10	B	2067	GLA	O5-C5-C6-O6
9	A	2004	A1AIO	O12-C01-C02-O11
9	B	2002	A1AIO	O12-C01-C02-O11
10	B	2060	GLA	O5-C5-C6-O6
9	A	2002	A1AIO	O12-C01-C02-C03
9	A	2005	A1AIO	O12-C01-C02-C03
9	A	2044	A1AIO	O12-C01-C02-C03
9	B	2021	A1AIO	O12-C01-C02-C03
9	B	2025	A1AIO	O12-C01-C02-C03
10	B	2060	GLA	C4-C5-C6-O6
10	B	2065	GLA	C4-C5-C6-O6
10	A	2064	GLA	O5-C5-C6-O6
10	A	2063	GLA	C4-C5-C6-O6
10	B	2063	GLA	O5-C5-C6-O6
10	B	2063	GLA	C4-C5-C6-O6
10	B	2058	GLA	C4-C5-C6-O6
9	B	2010	A1AIO	O12-C01-C02-C03
9	B	2035	A1AIO	O12-C01-C02-C03
10	B	2065	GLA	O5-C5-C6-O6
10	A	2065	GLA	O5-C5-C6-O6
9	A	2004	A1AIO	O12-C01-C02-C03
9	B	2002	A1AIO	O12-C01-C02-C03
9	B	2007	A1AIO	O12-C01-C02-O11
9	B	2011	A1AIO	O12-C01-C02-O11
10	B	2069	GLA	O5-C5-C6-O6
10	A	2064	GLA	C4-C5-C6-O6
9	B	2005	A1AIO	O11-C02-C03-C04
9	B	2016	A1AIO	O11-C02-C03-C04
9	B	2018	A1AIO	O11-C02-C03-C04
9	B	2030	A1AIO	O11-C02-C03-C04
9	B	2054	A1AIO	O11-C02-C03-C04
9	A	2038	A1AIO	O11-C02-C03-O07
9	A	2040	A1AIO	O11-C02-C03-O07
9	B	2005	A1AIO	O11-C02-C03-O07
9	B	2014	A1AIO	O11-C02-C03-O07
9	B	2018	A1AIO	O11-C02-C03-O07
9	B	2030	A1AIO	O11-C02-C03-O07
9	B	2005	A1AIO	C01-C02-C03-C04

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Mol	Chain	Res	Type	Atoms
9	B	2054	A1AIO	C01-C02-C03-C04
10	B	2066	GLA	O5-C5-C6-O6
9	A	2020	A1AIO	C01-C02-C03-O07
10	A	2069	GLA	O5-C5-C6-O6
9	B	2006	A1AIO	O12-C01-C02-O11
9	B	2008	A1AIO	O12-C01-C02-O11
10	B	2061	GLA	C4-C5-C6-O6
9	A	2038	A1AIO	O11-C02-C03-C04
9	A	2040	A1AIO	O11-C02-C03-C04
9	B	2014	A1AIO	O11-C02-C03-C04
9	A	2045	A1AIO	O12-C01-C02-O11
9	A	2047	A1AIO	O12-C01-C02-O11
9	A	2048	A1AIO	O12-C01-C02-O11
9	A	2049	A1AIO	O12-C01-C02-O11
10	A	2058	GLA	C4-C5-C6-O6
9	B	2011	A1AIO	O12-C01-C02-C03
9	B	2007	A1AIO	O12-C01-C02-C03
10	B	2061	GLA	O5-C5-C6-O6
9	A	2052	A1AIO	C01-C02-C03-O07
9	B	2006	A1AIO	O12-C01-C02-C03
9	B	2008	A1AIO	O12-C01-C02-C03
9	A	2035	A1AIO	O11-C02-C03-C04
9	B	2028	A1AIO	O11-C02-C03-C04
9	A	2035	A1AIO	O11-C02-C03-O07
10	A	2065	GLA	C4-C5-C6-O6
9	A	2001	A1AIO	O12-C01-C02-O11
9	B	2004	A1AIO	O12-C01-C02-O11
9	A	2030	A1AIO	O11-C02-C03-C04
9	A	2016	A1AIO	O12-C01-C02-O11
9	B	2003	A1AIO	O12-C01-C02-O11
9	A	2048	A1AIO	O12-C01-C02-C03
9	A	2049	A1AIO	O12-C01-C02-C03
9	A	2006	A1AIO	O12-C01-C02-O11
9	B	2018	A1AIO	C01-C02-C03-C04
9	B	2030	A1AIO	C01-C02-C03-C04
9	A	2045	A1AIO	O12-C01-C02-C03
9	A	2047	A1AIO	O12-C01-C02-C03
9	B	2015	A1AIO	C01-C02-C03-O07
9	B	2024	A1AIO	C01-C02-C03-O07
9	B	2031	A1AIO	C01-C02-C03-O07
9	B	2039	A1AIO	C01-C02-C03-O07
10	B	2069	GLA	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	2004	A1AIO	O12-C01-C02-C03
9	A	2041	A1AIO	O11-C02-C03-C04
9	B	2003	A1AIO	O11-C02-C03-C04
10	B	2062	GLA	C4-C5-C6-O6
9	A	2009	A1AIO	O12-C01-C02-O11
9	A	2013	A1AIO	O12-C01-C02-O11
9	A	2010	A1AIO	O12-C01-C02-O11
9	A	2001	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
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

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
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
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

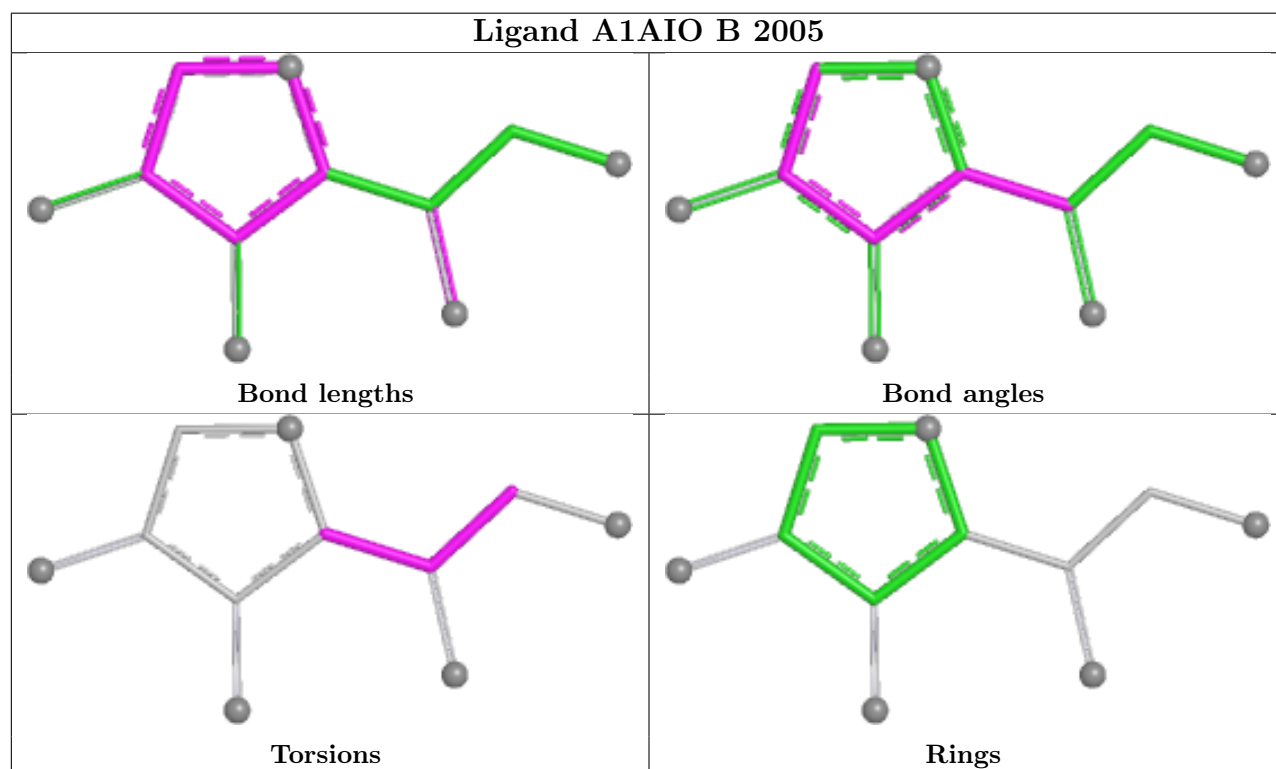
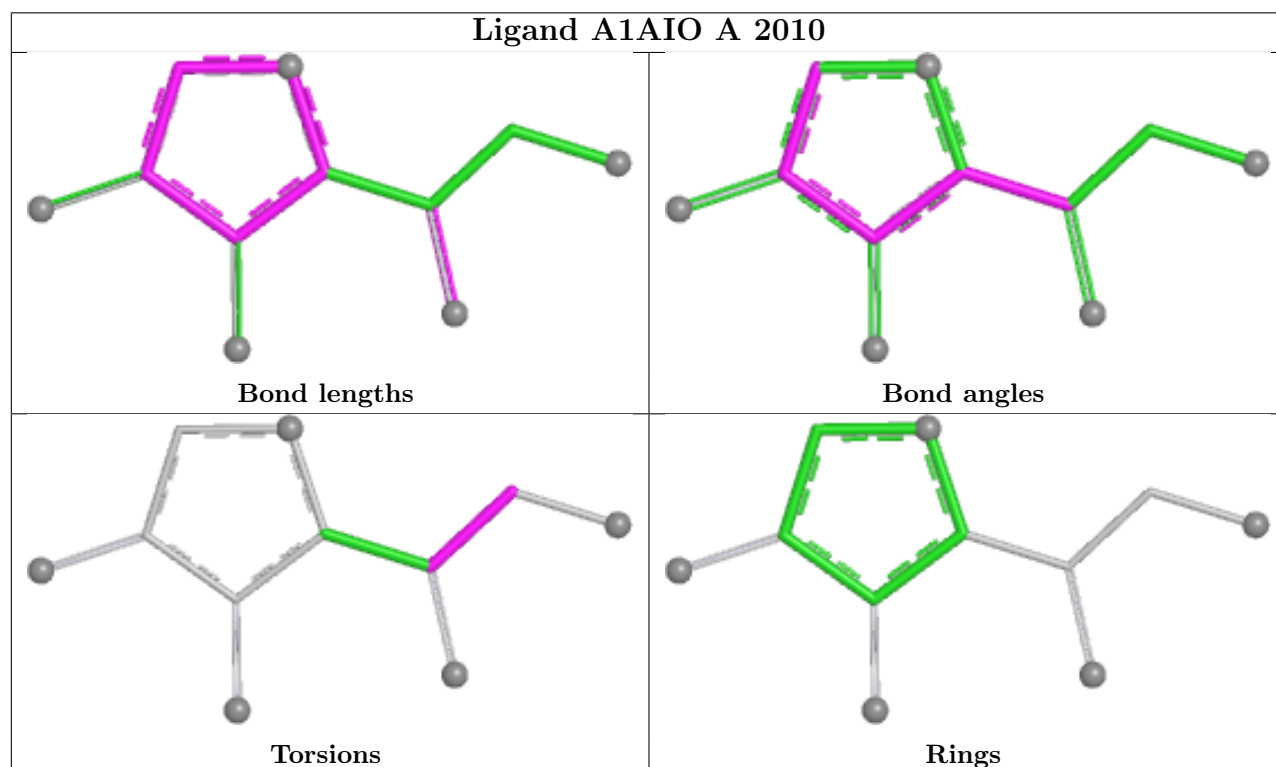
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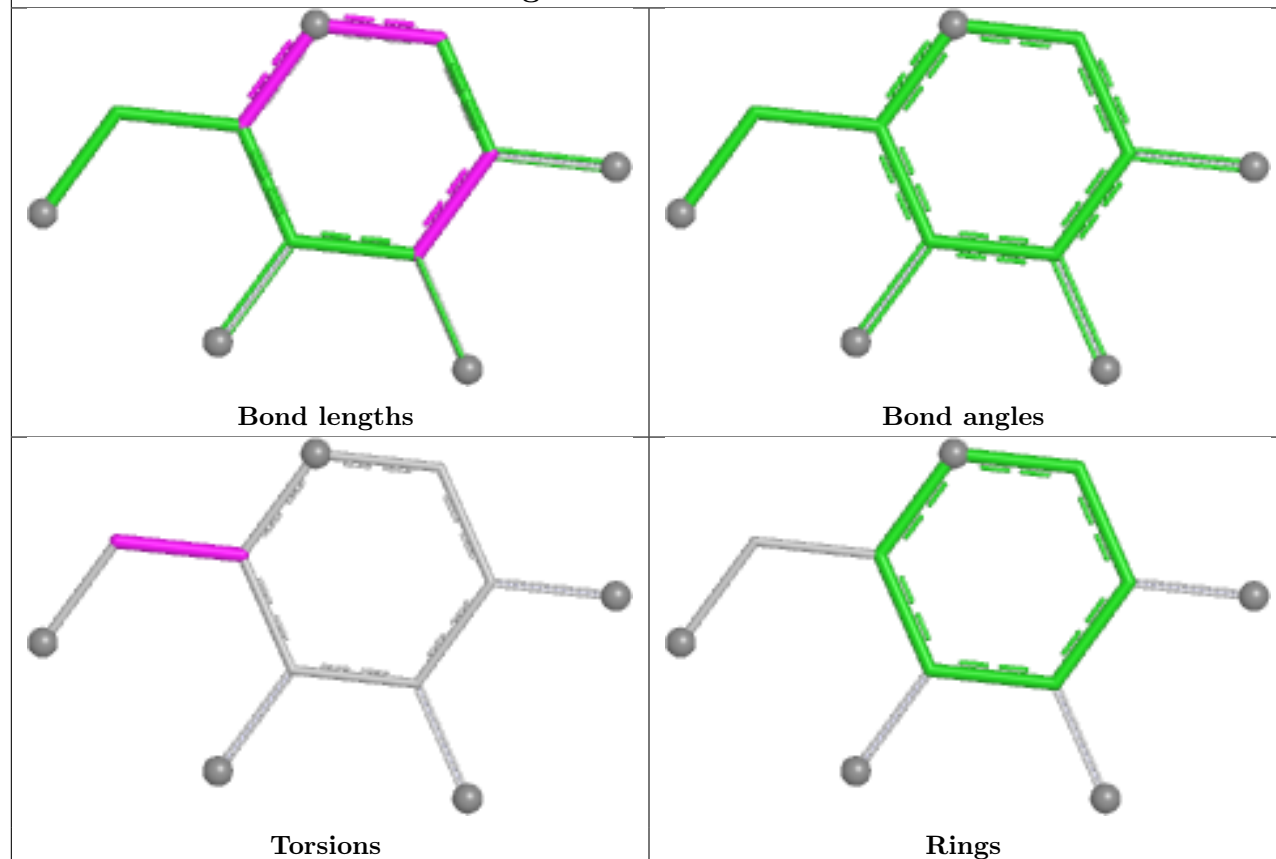
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	2008	A1AIO	1	0
9	A	2057	A1AIO	1	0
10	A	2061	GLA	1	0
9	A	2049	A1AIO	1	0
9	B	2039	A1AIO	1	0
9	A	2003	A1AIO	1	0
10	B	2058	GLA	1	0
9	B	2055	A1AIO	2	0
9	B	2018	A1AIO	2	0
9	A	2029	A1AIO	1	0
9	B	2047	A1AIO	1	0
10	A	2059	GLA	2	0
9	B	2034	A1AIO	2	0
9	B	2001	A1AIO	1	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
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.

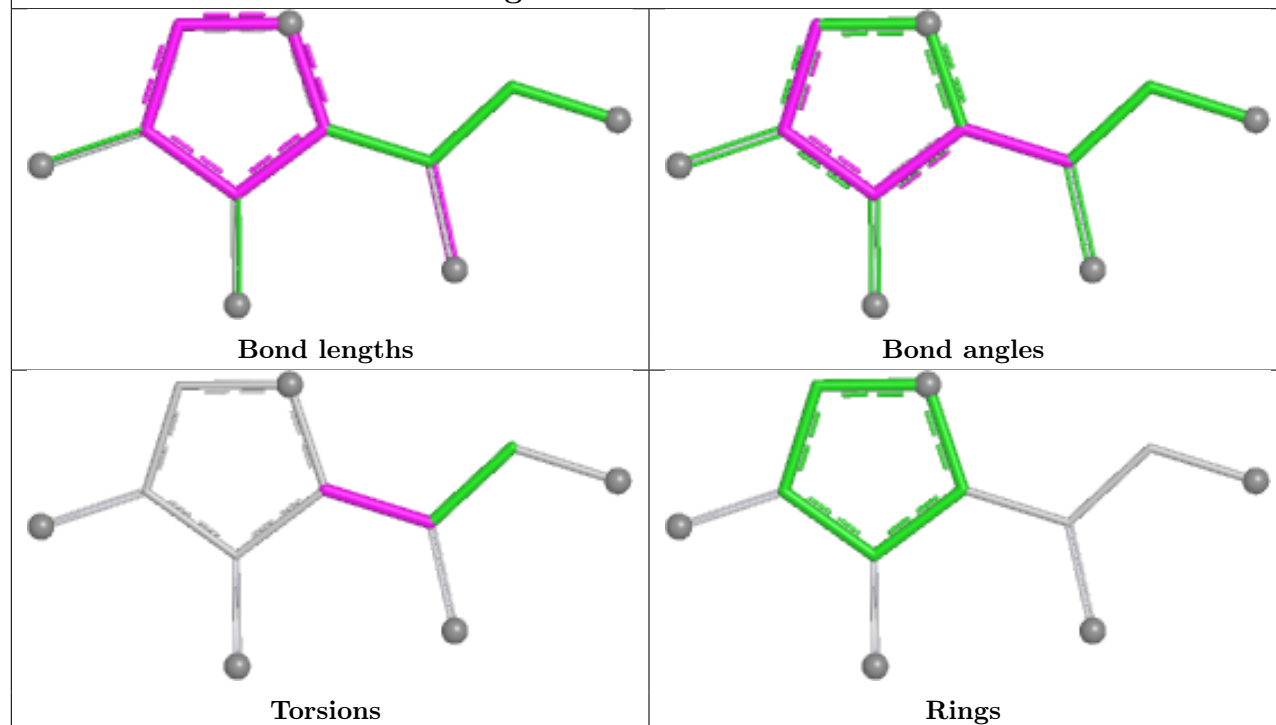
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



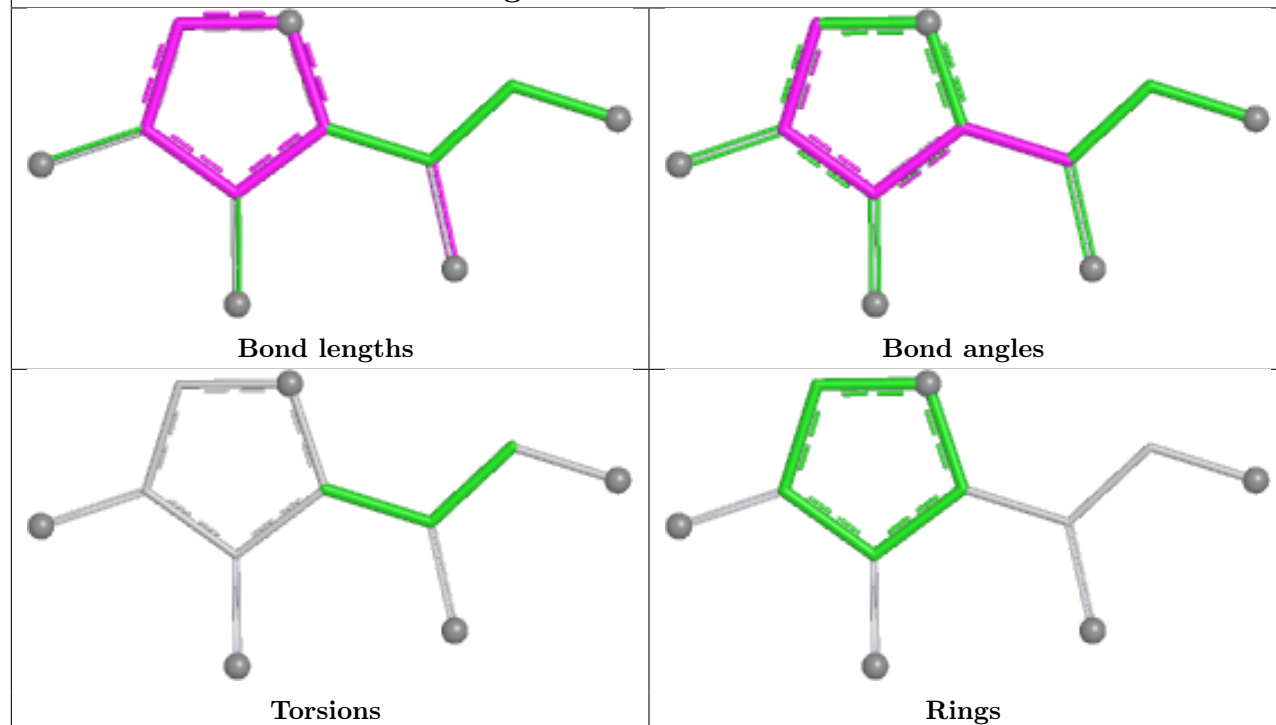
Ligand GLA B 2069



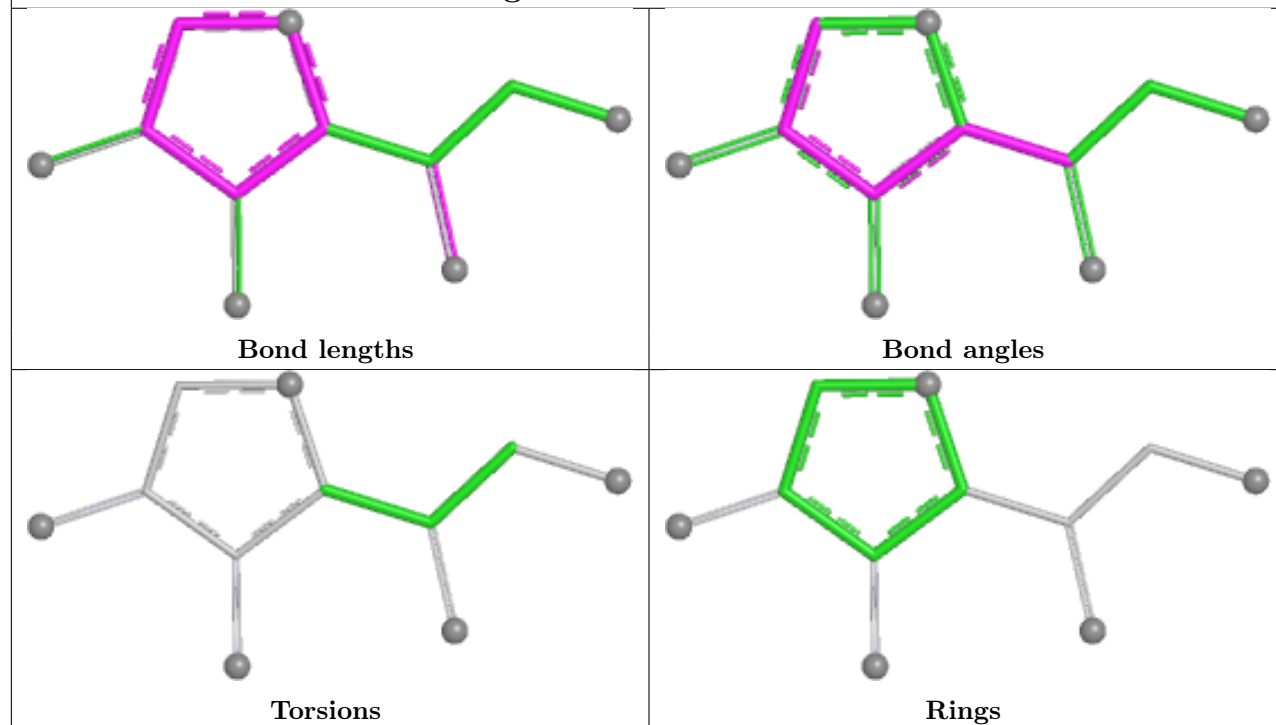
Ligand A1AIO B 2031



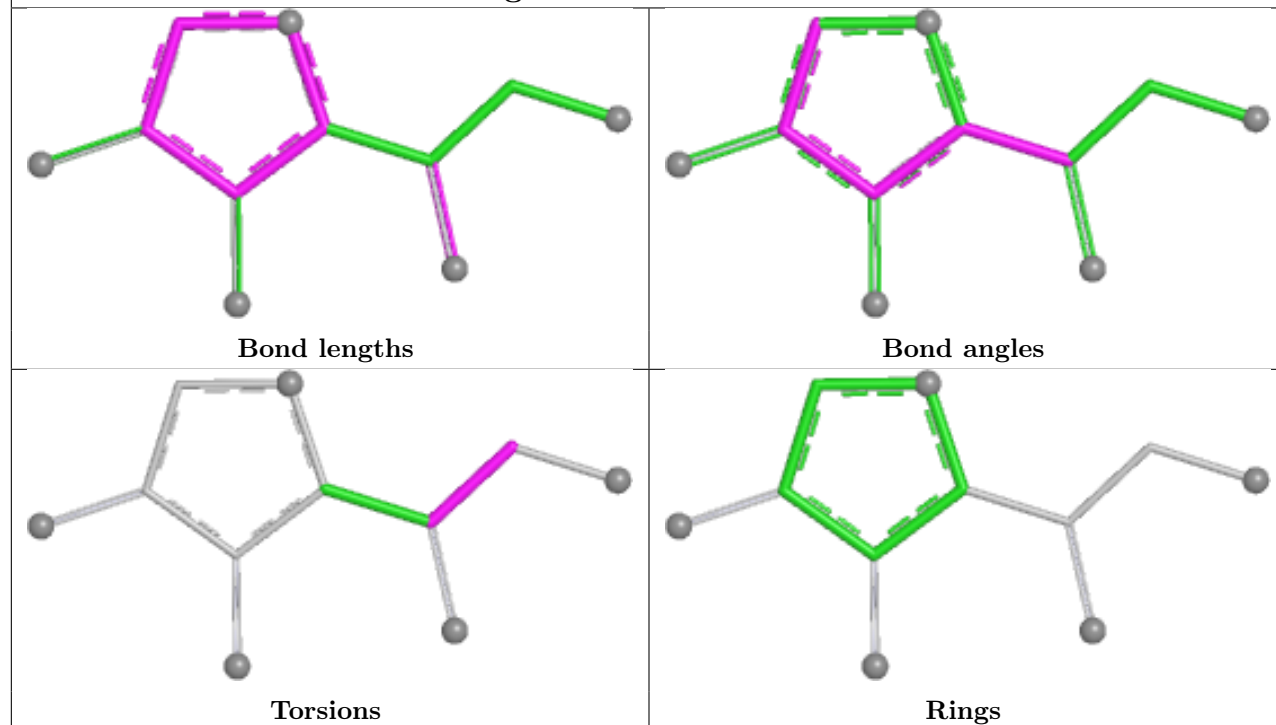
Ligand A1AIO A 2011



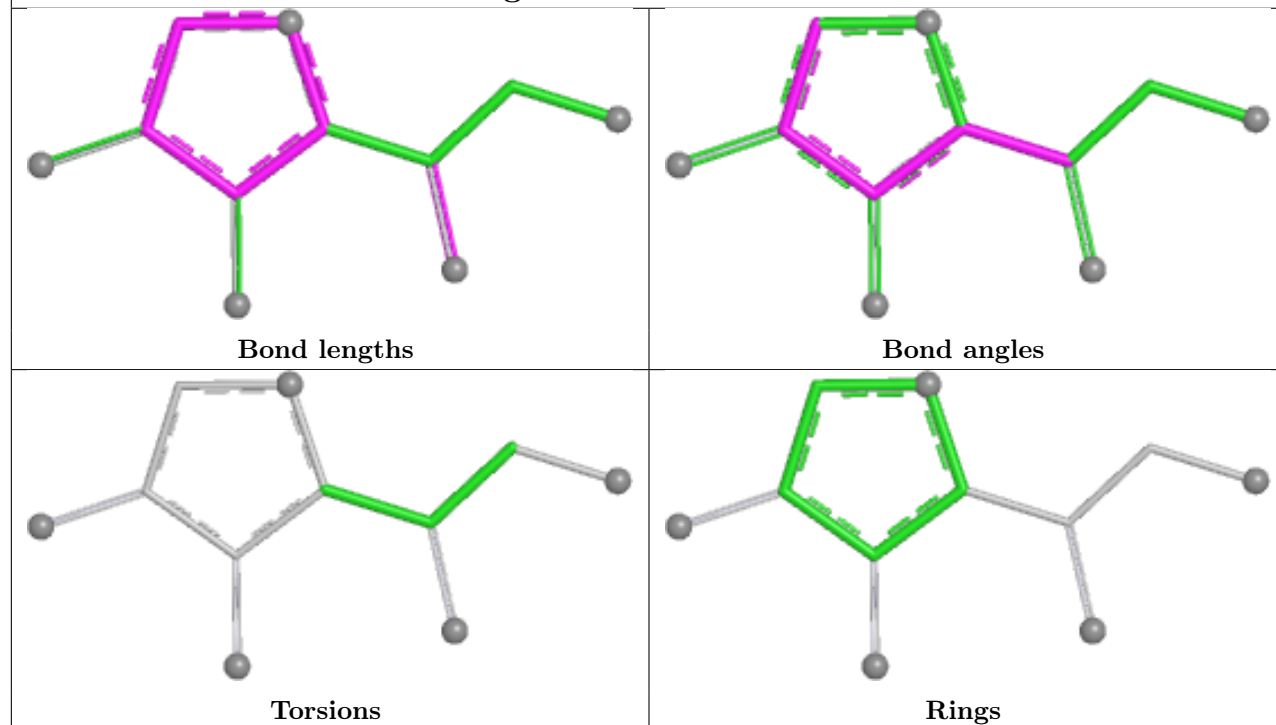
Ligand A1AIO A 2019



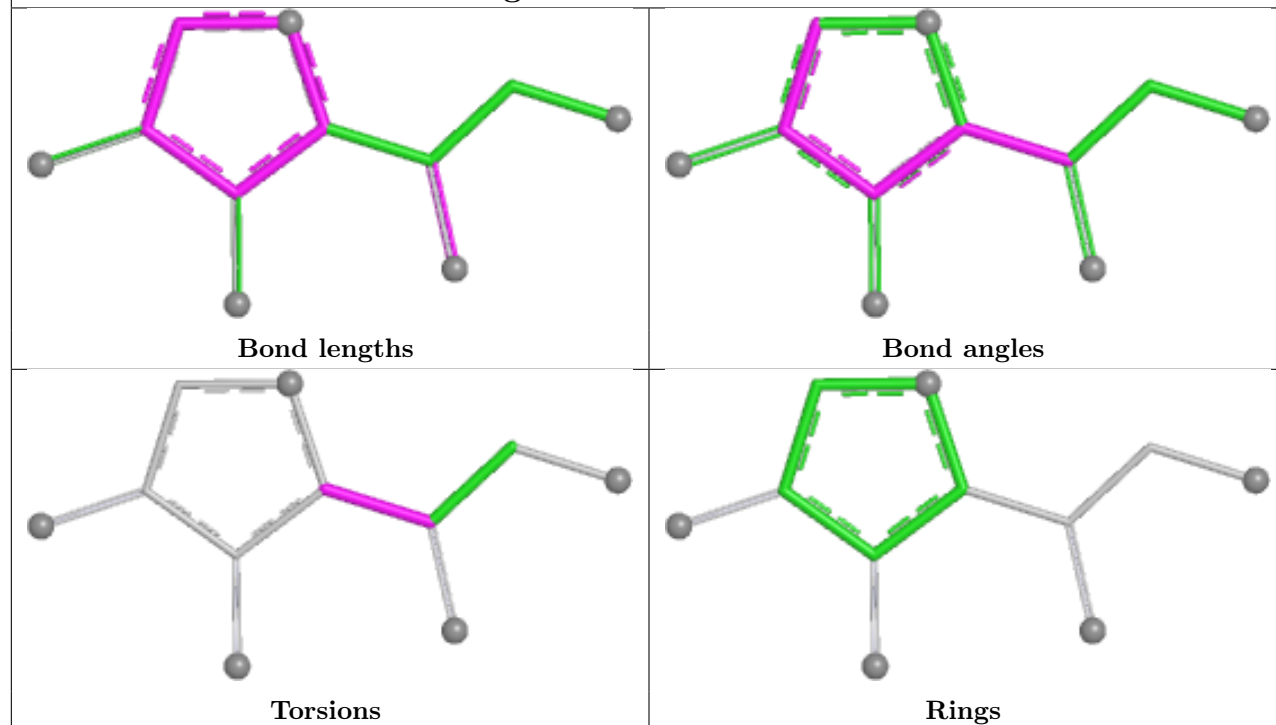
Ligand A1AIO B 2037



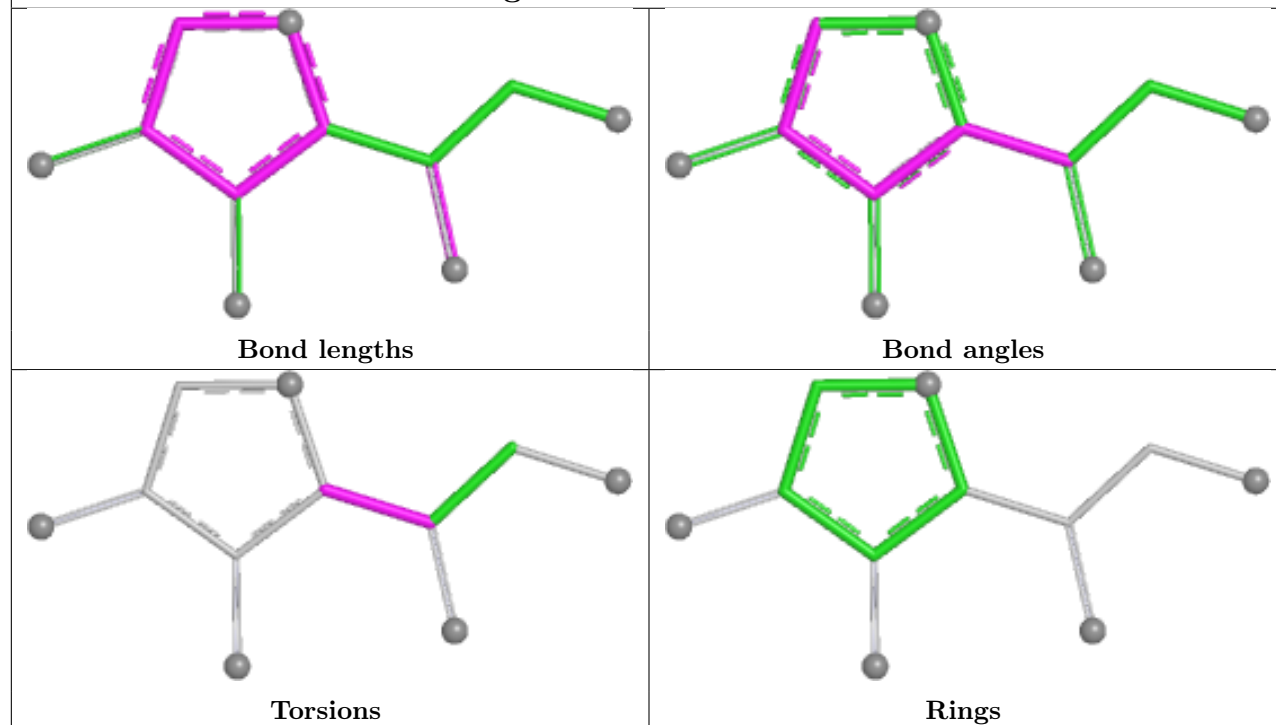
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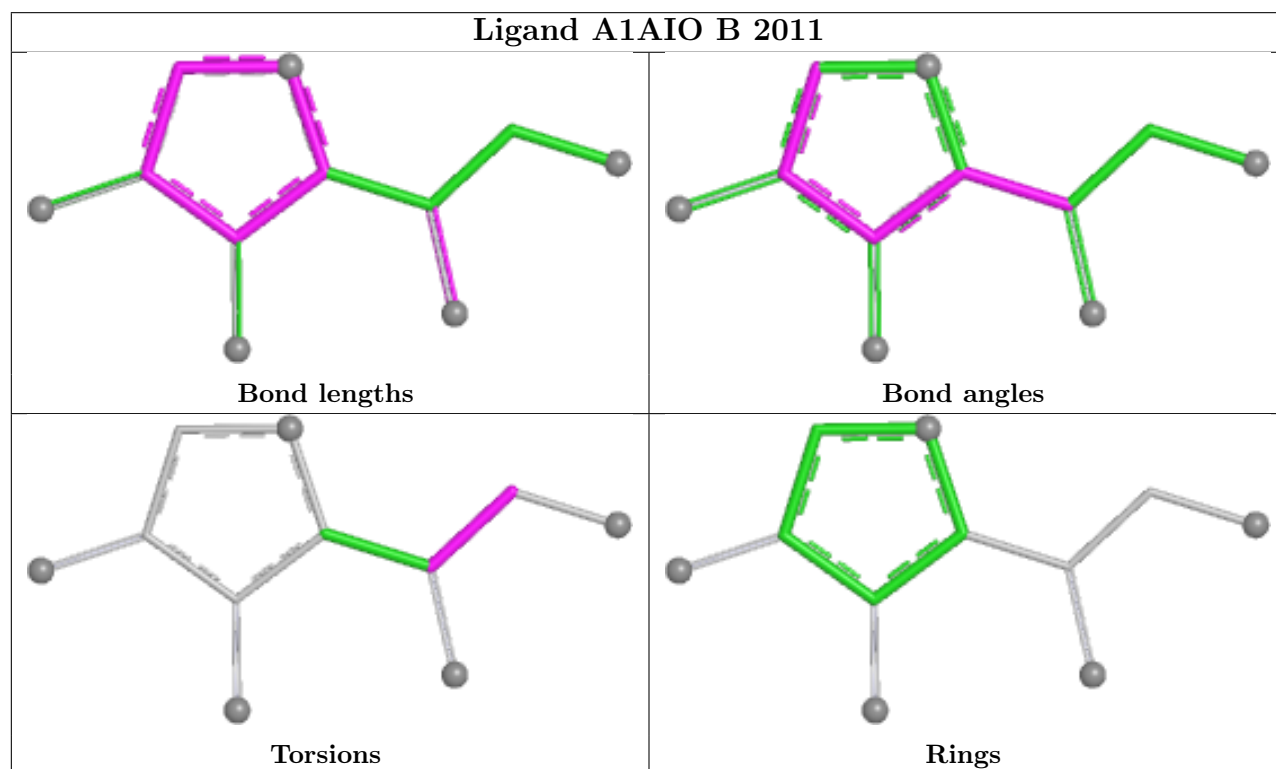
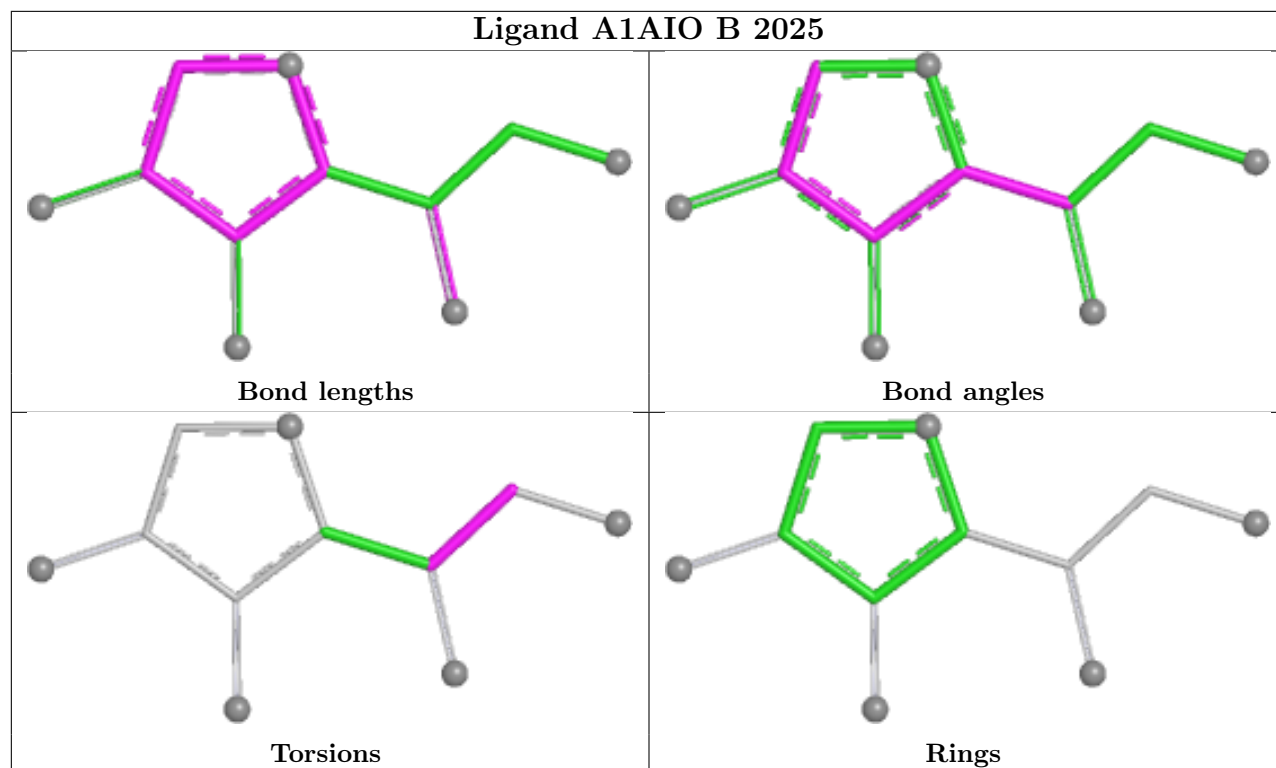


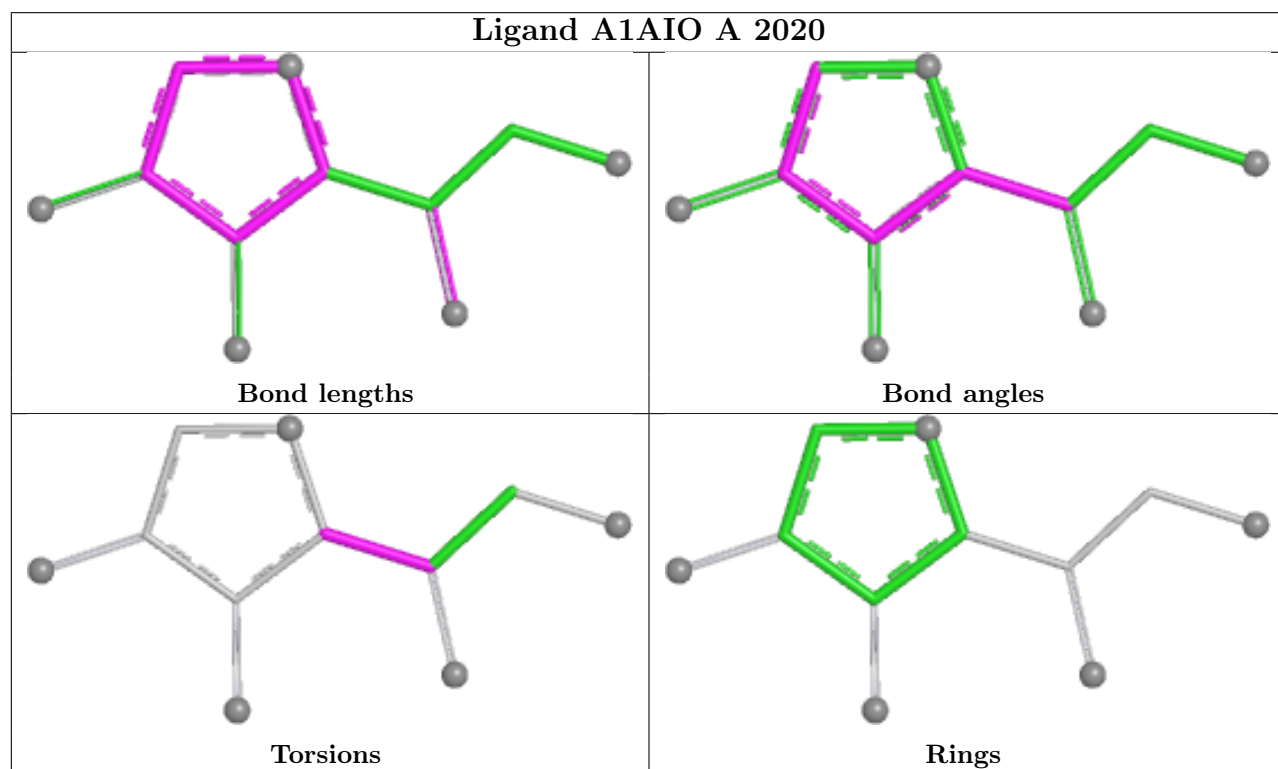
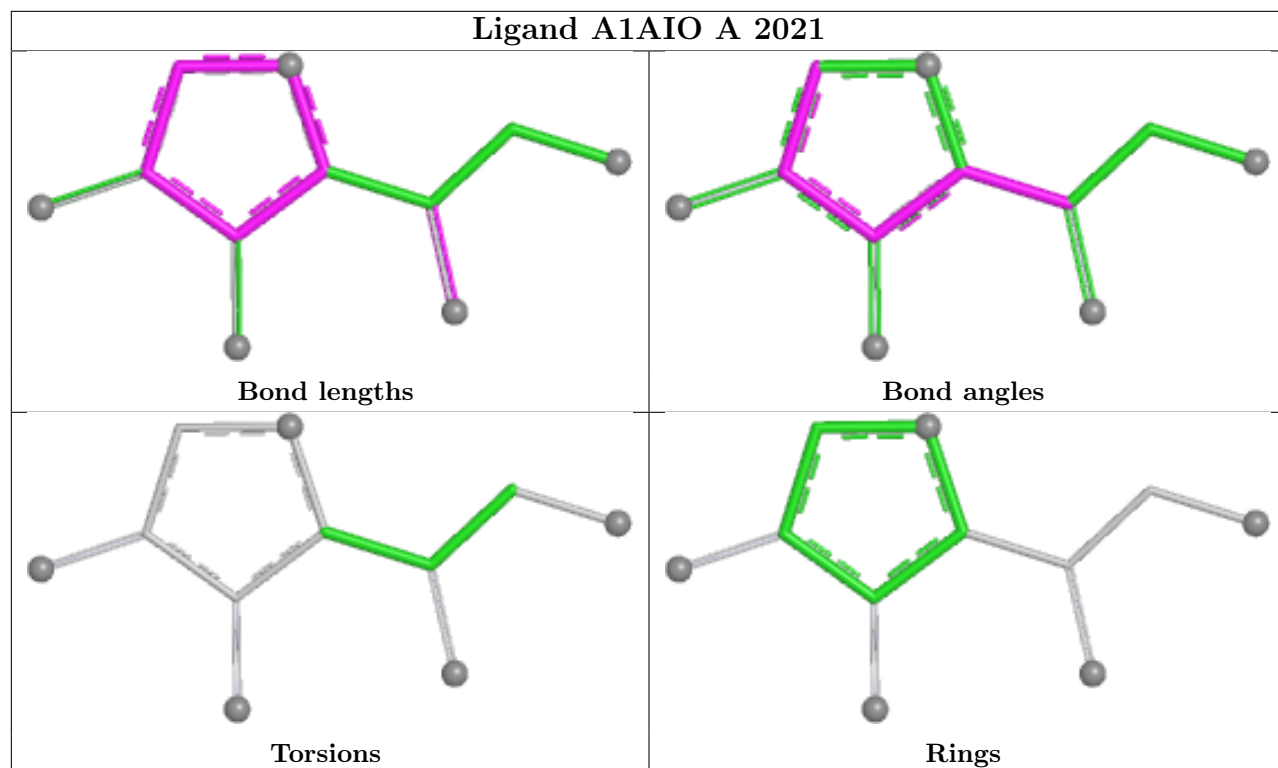
Ligand A1AIO A 2054

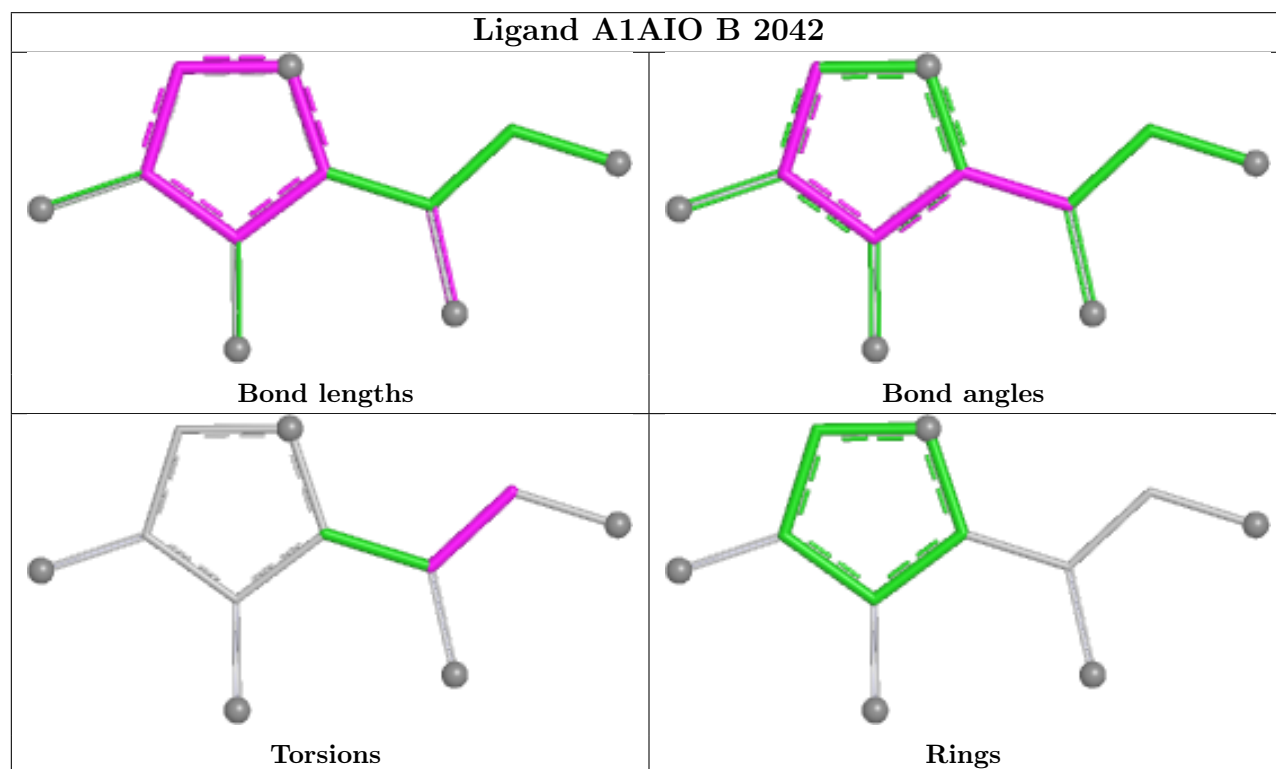
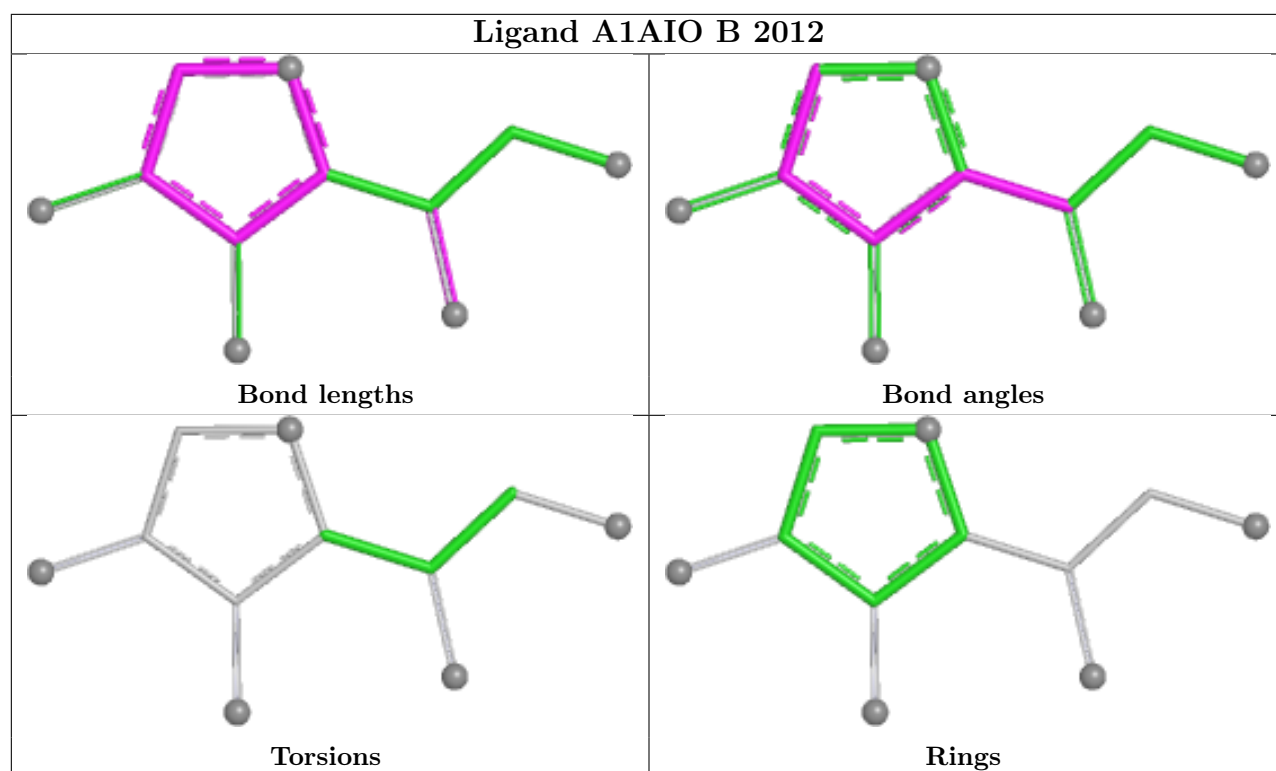


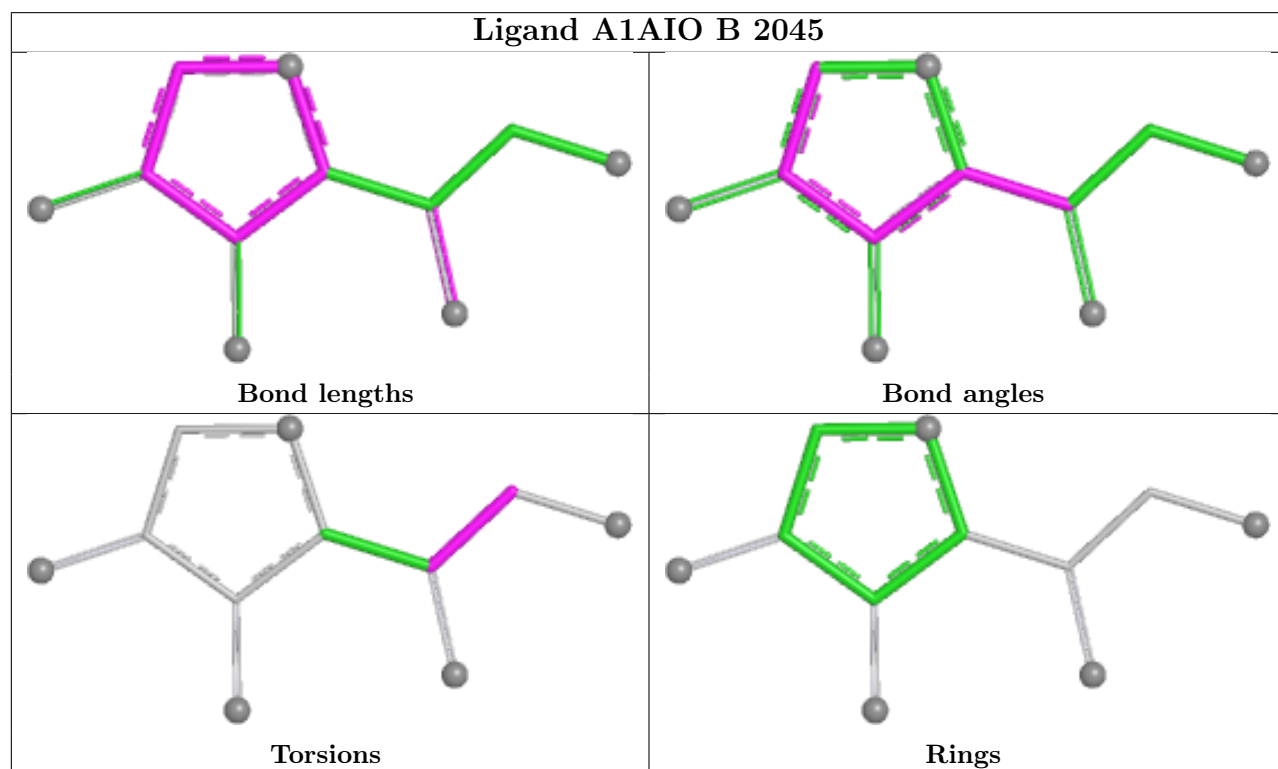
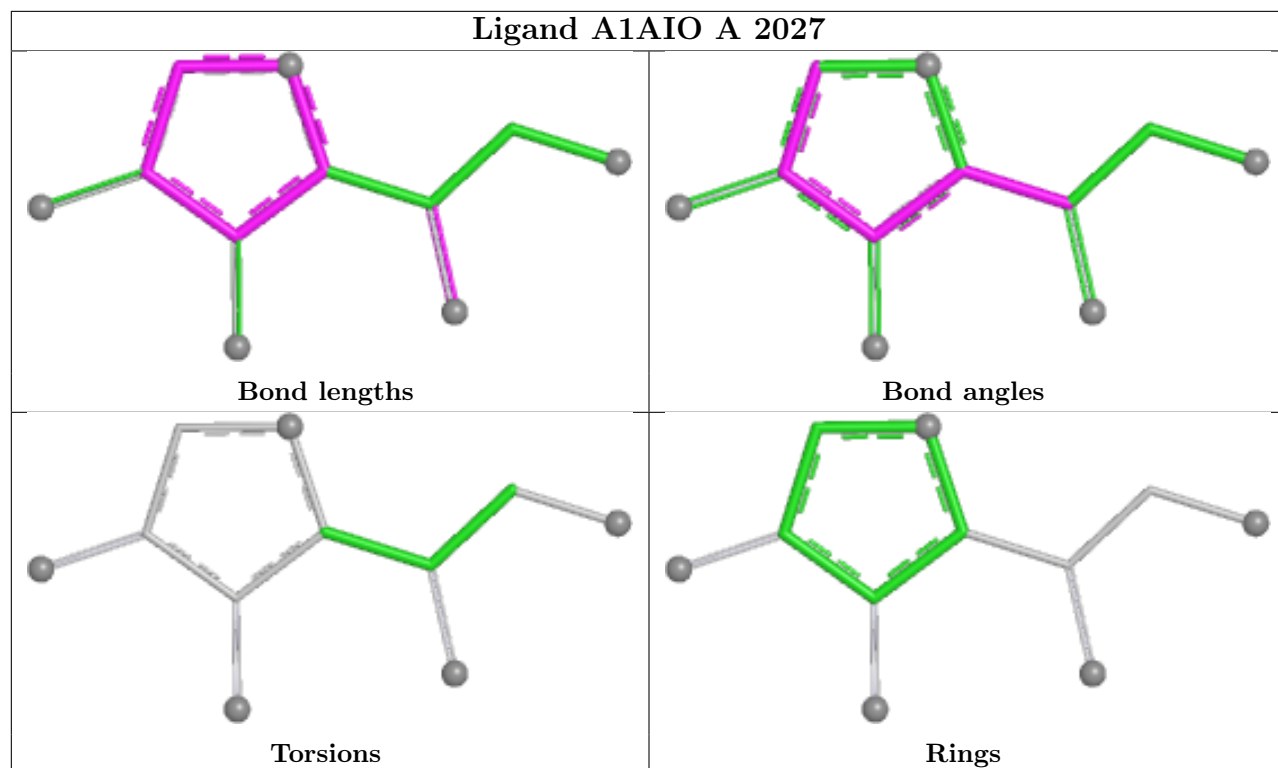
Ligand A1AIO A 2040



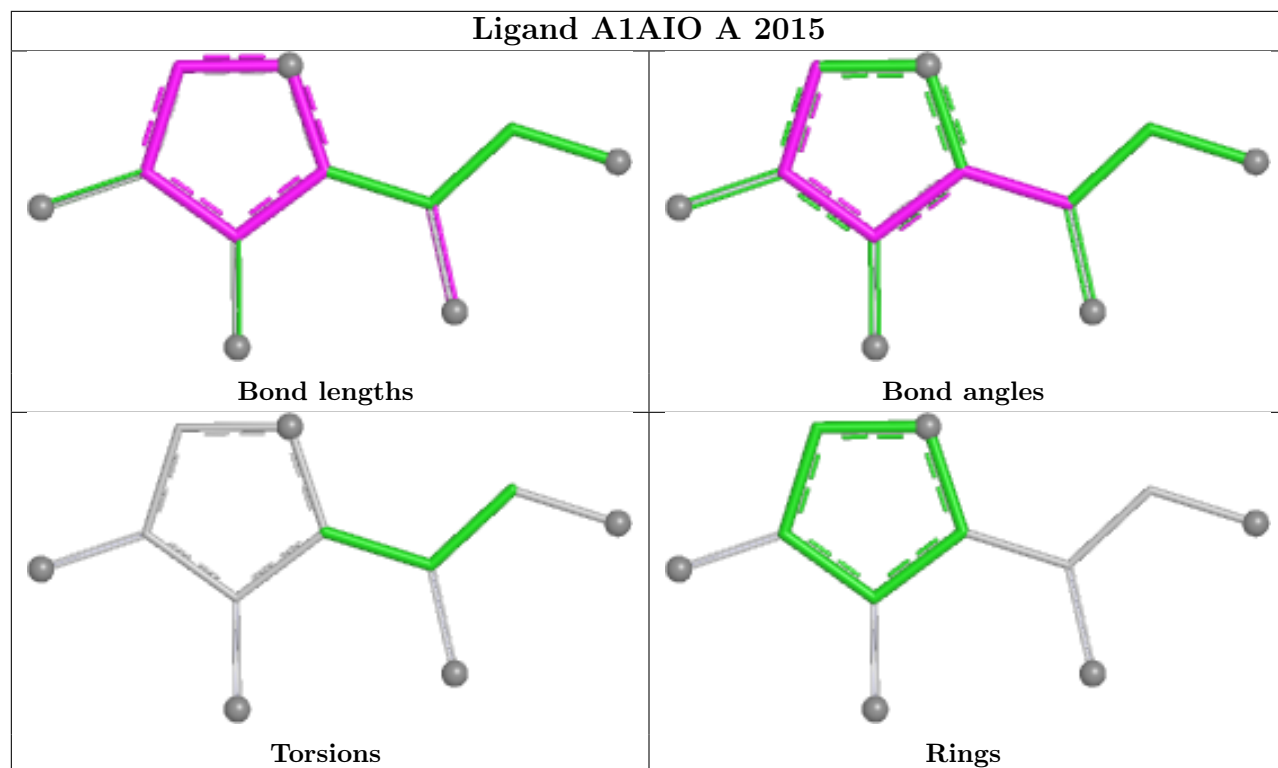




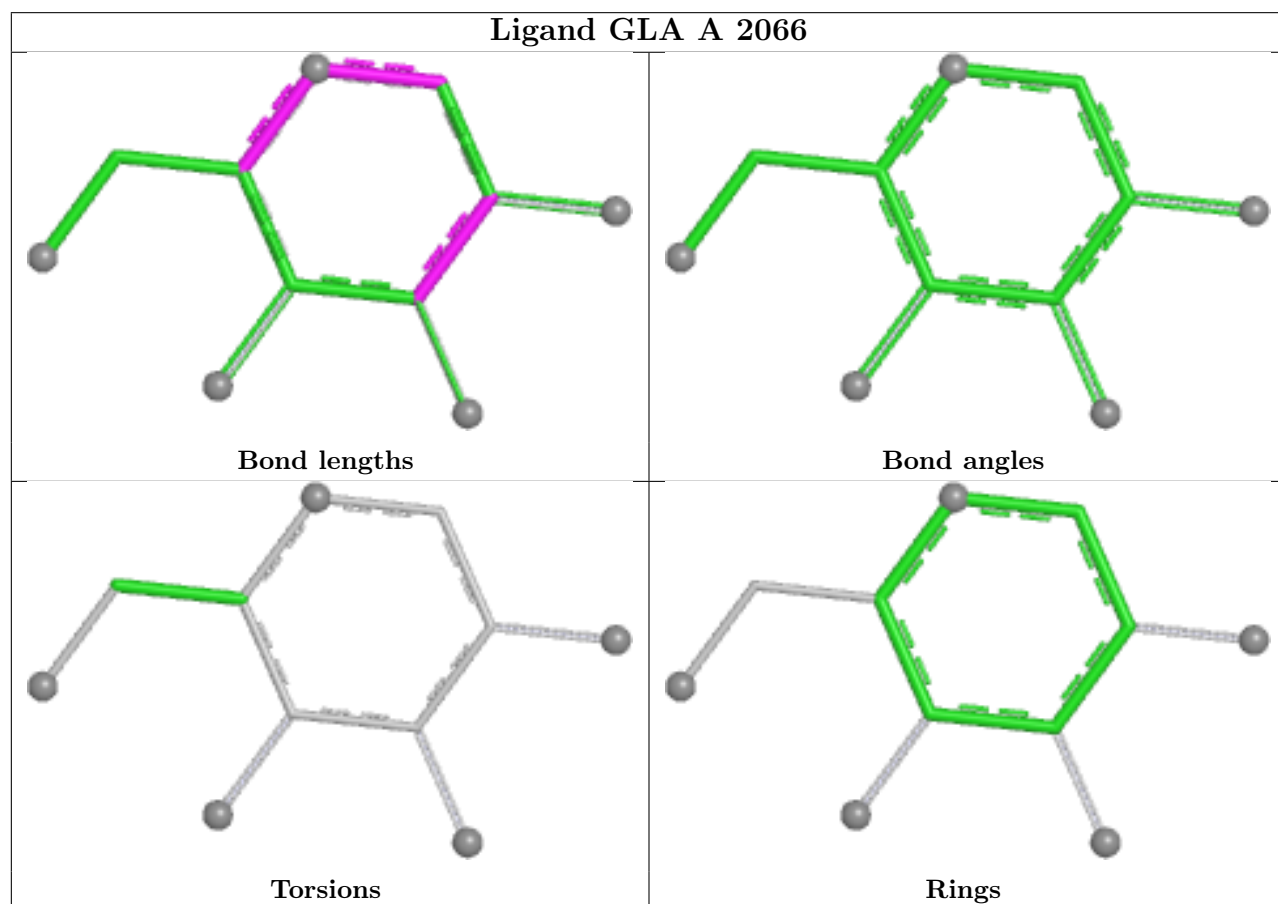


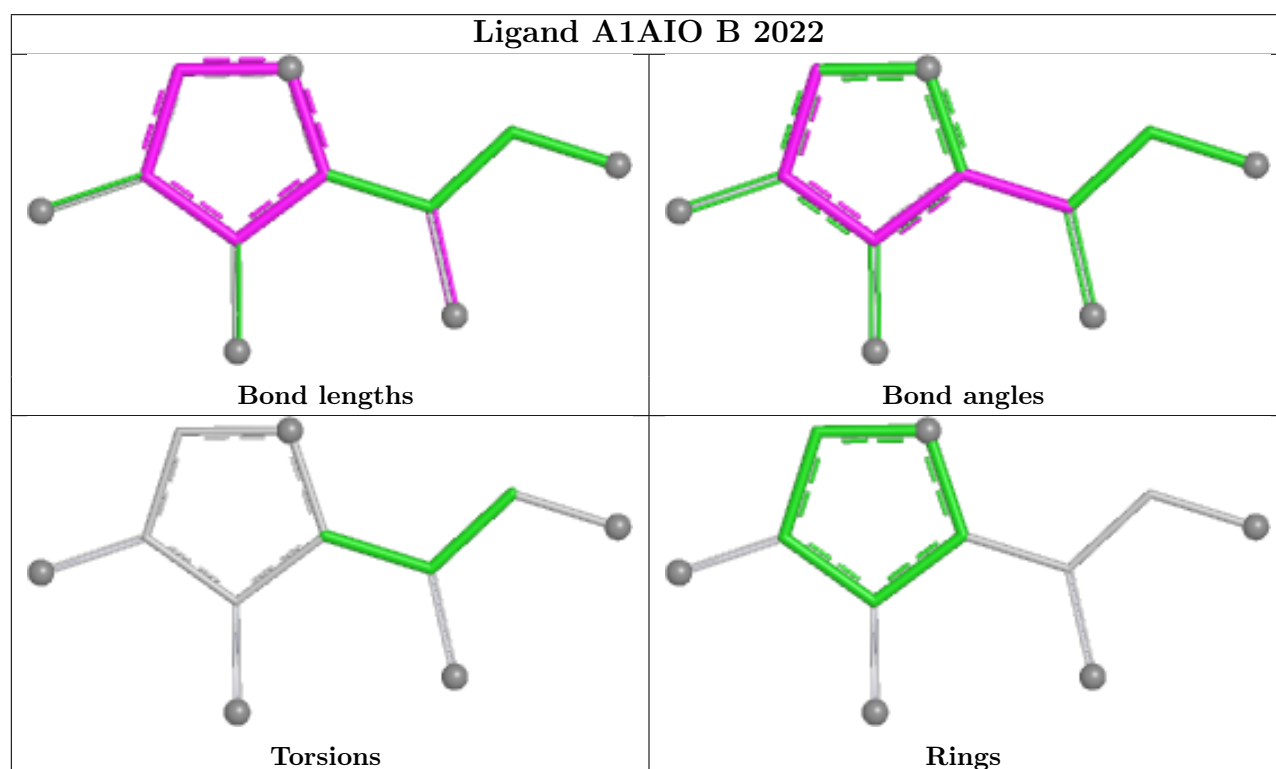
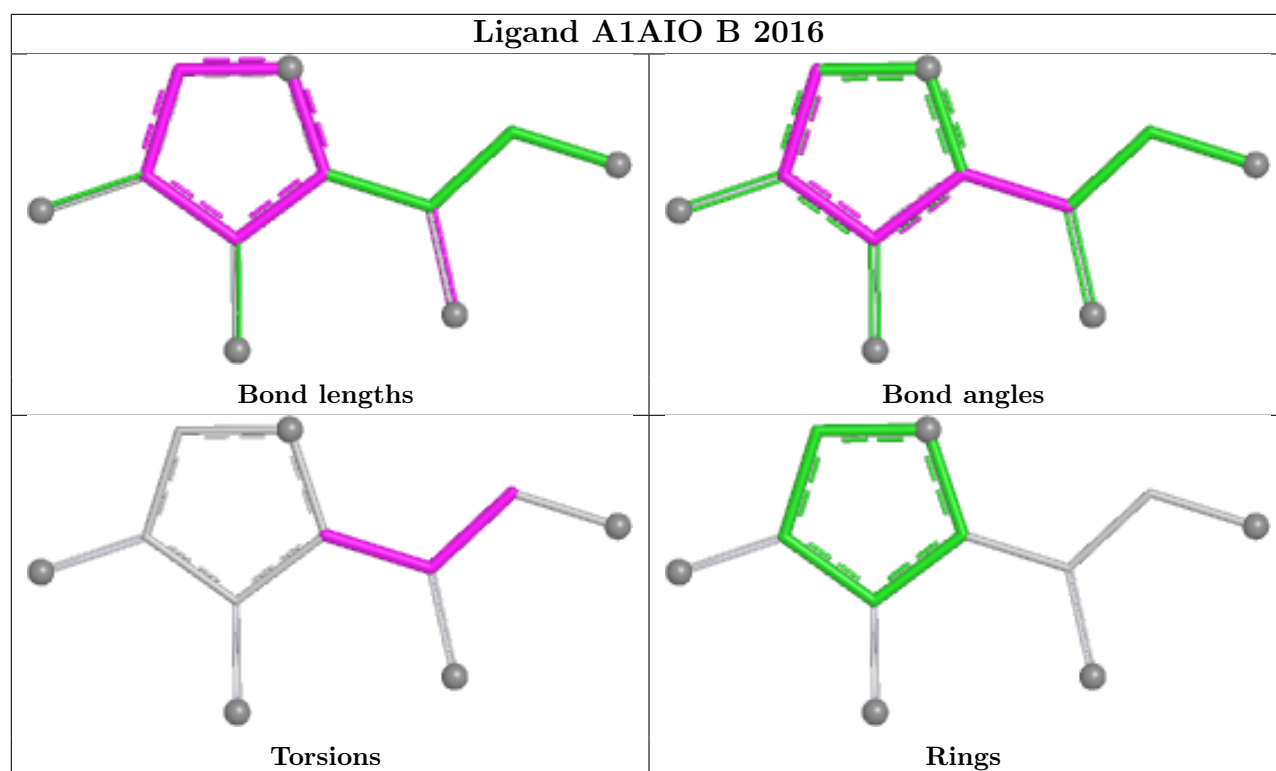


Ligand A1AIO A 2015

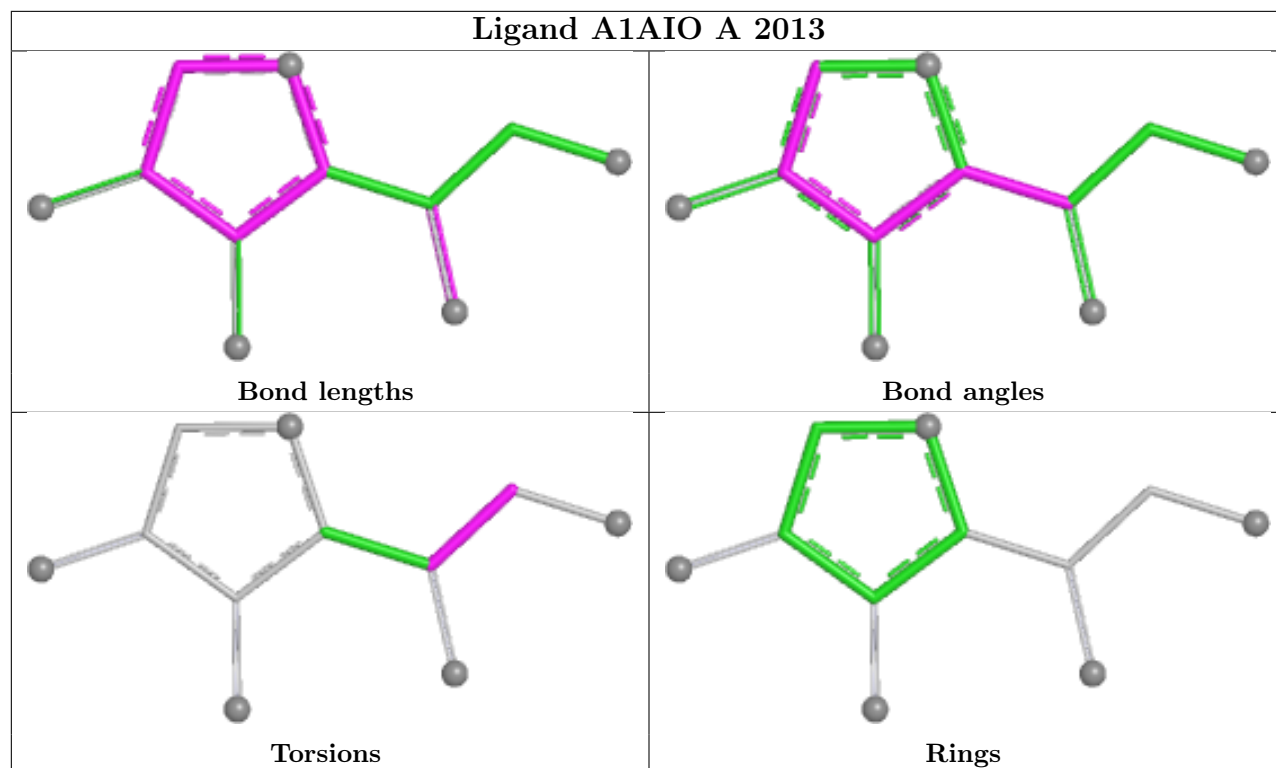


Ligand GLA A 2066

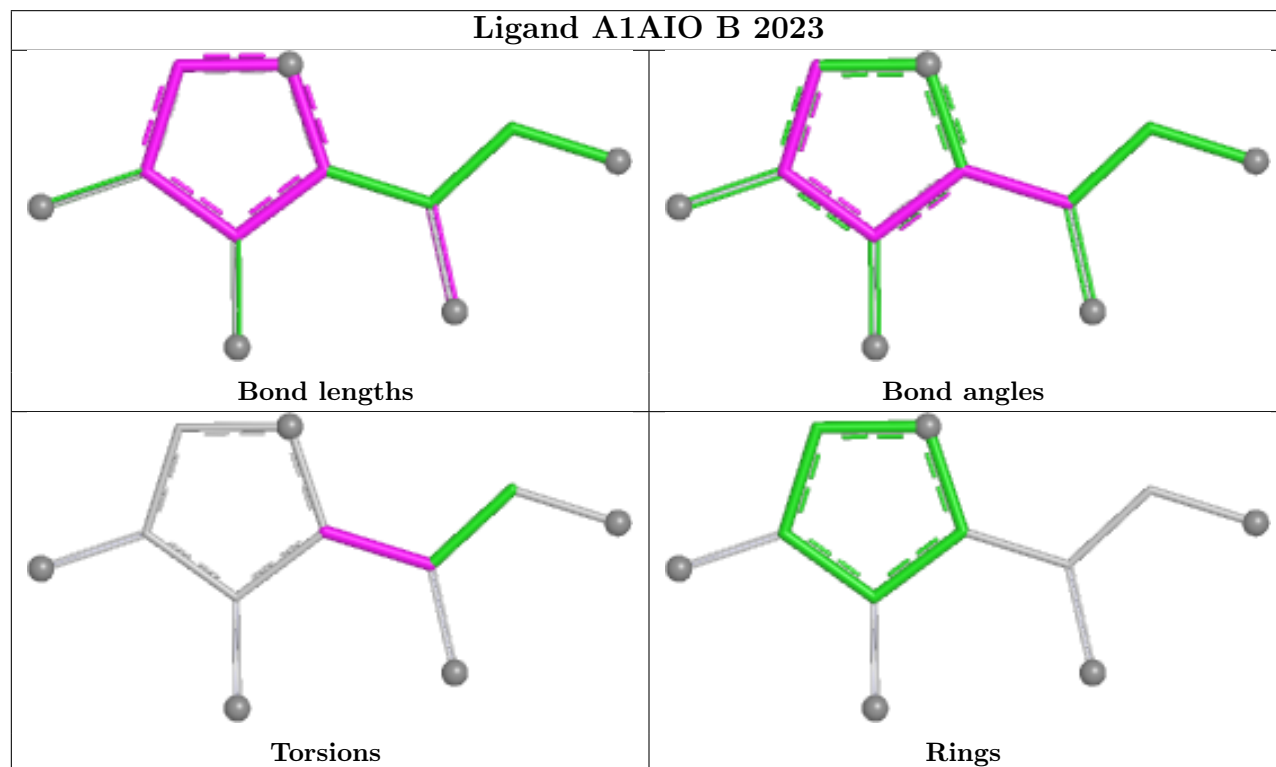




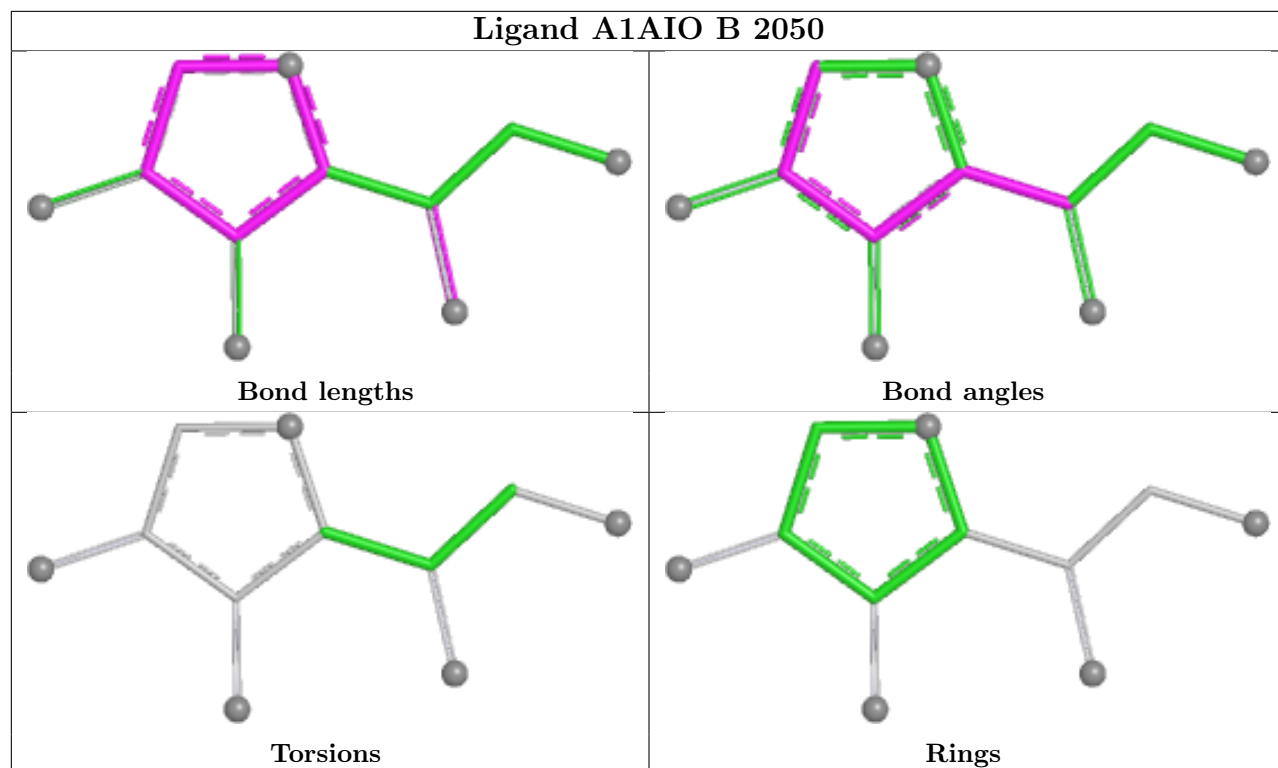
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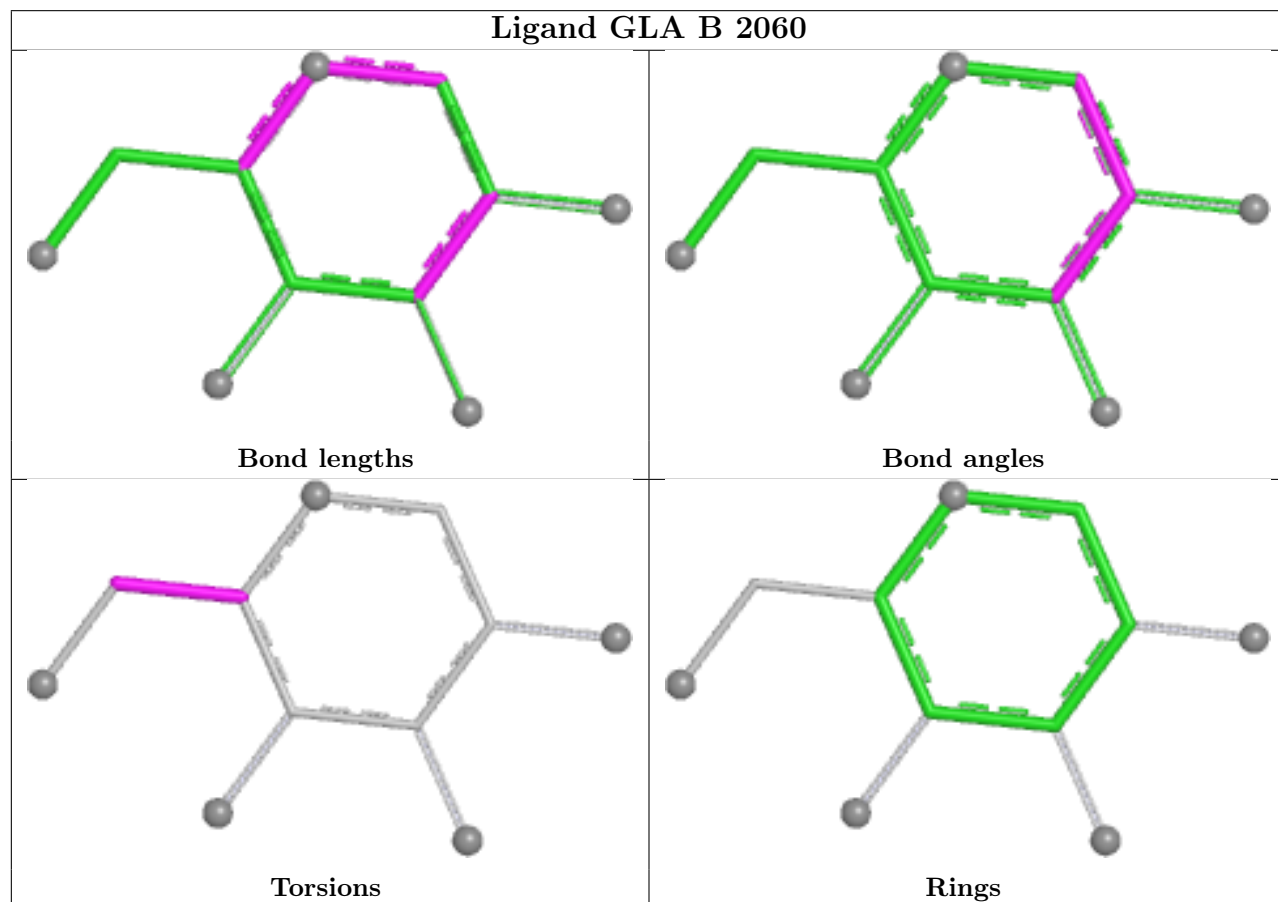
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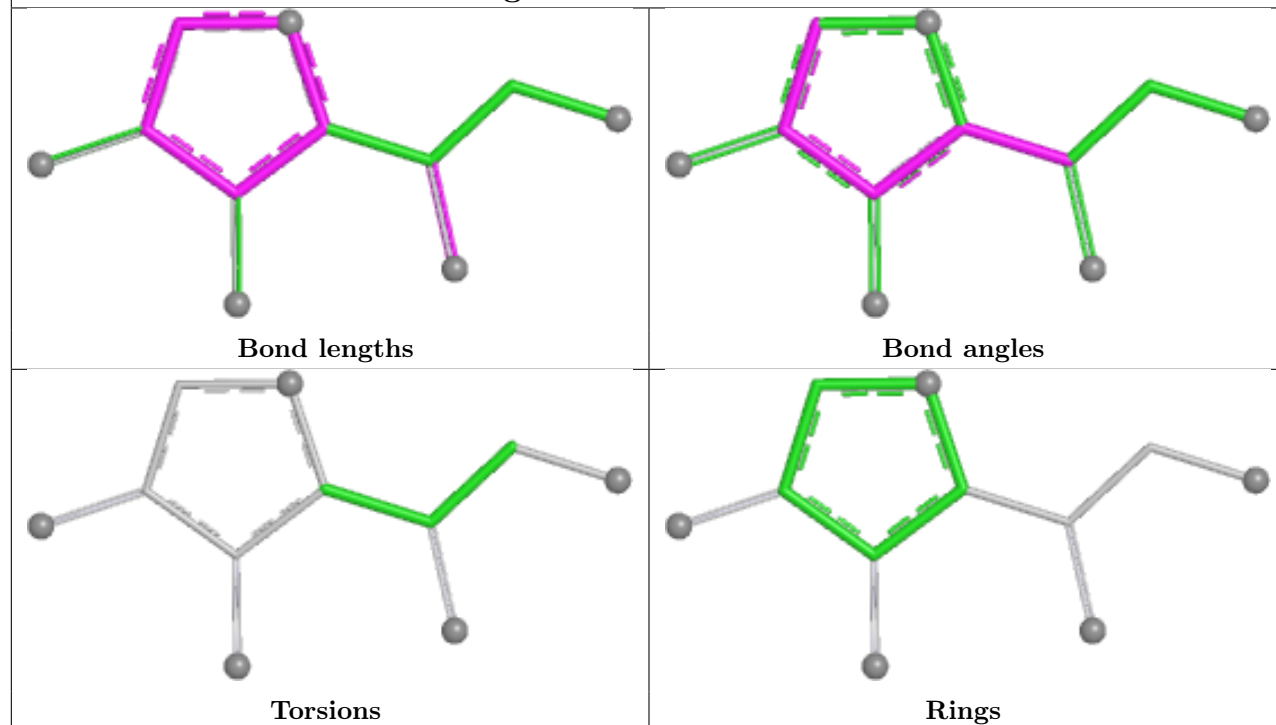
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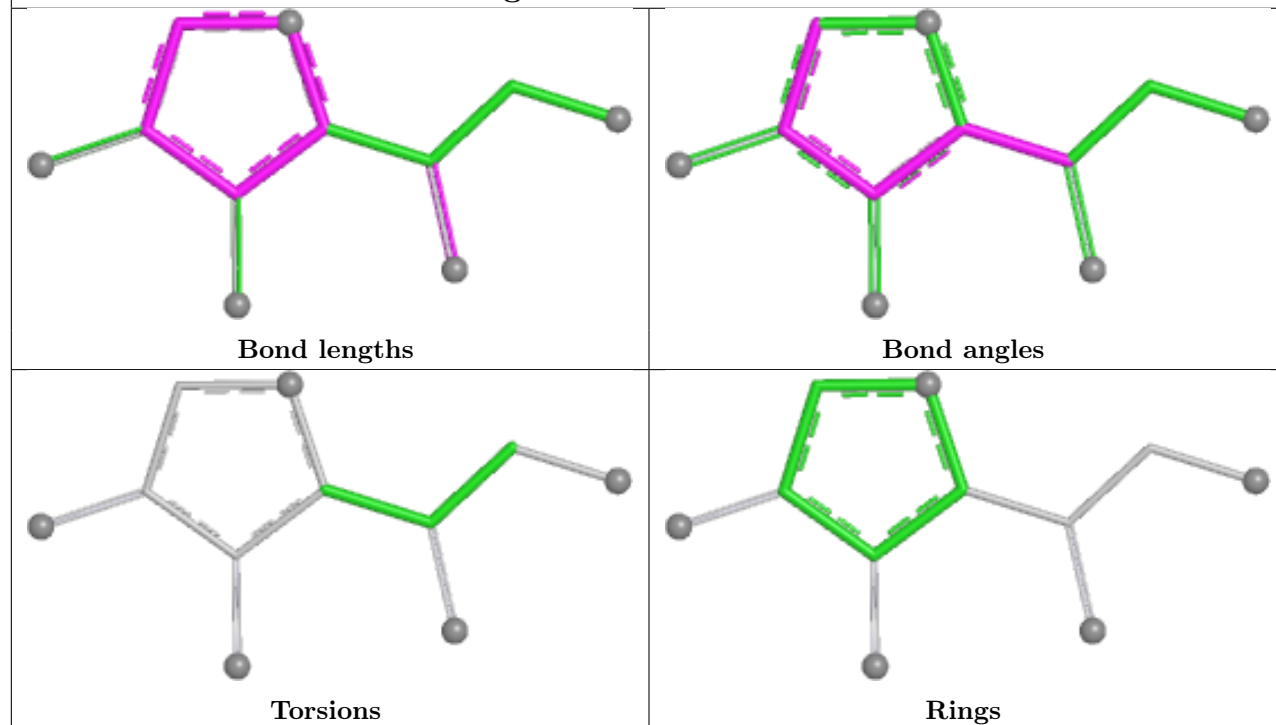
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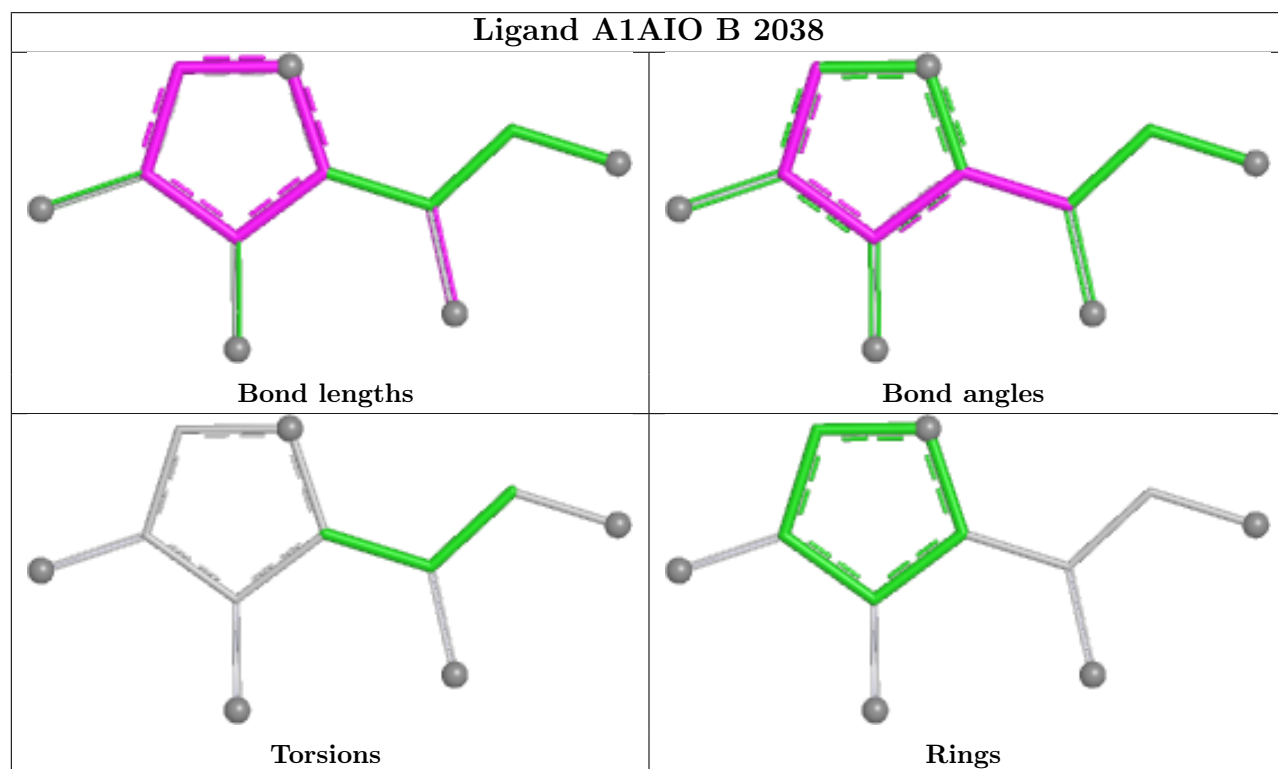
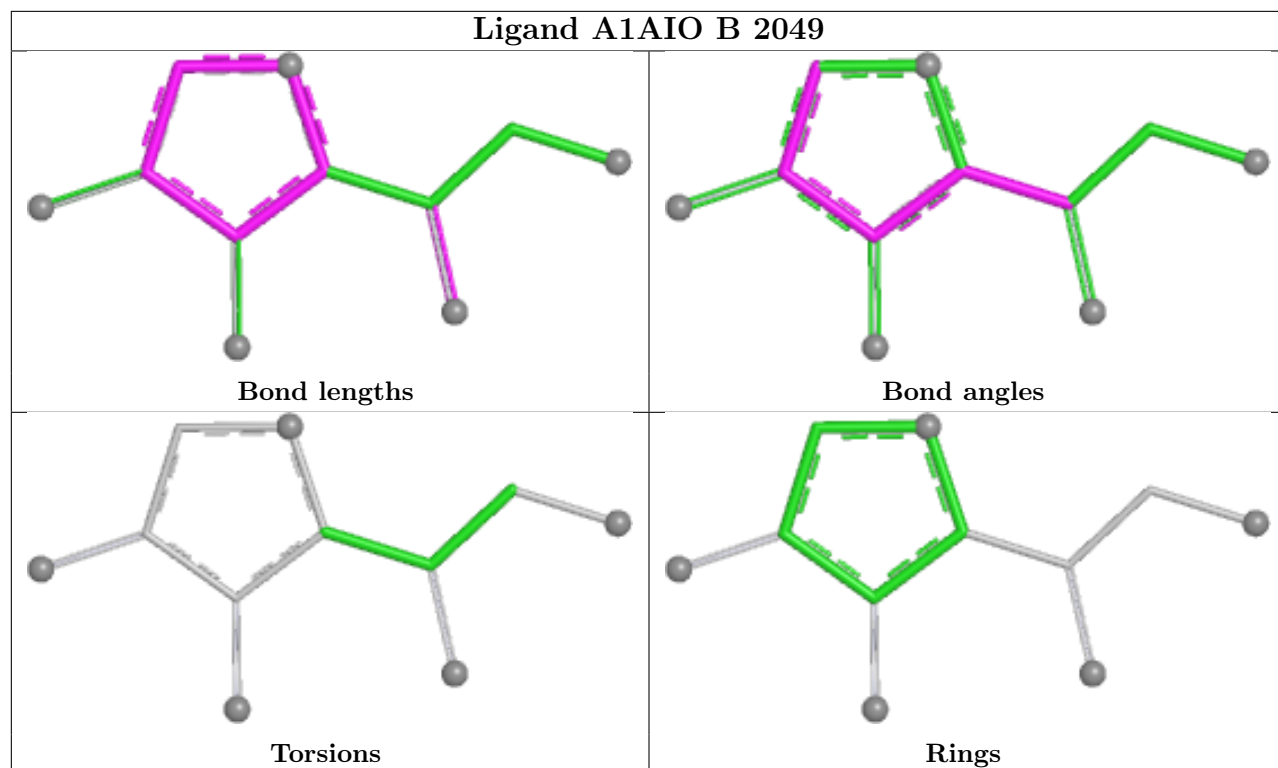


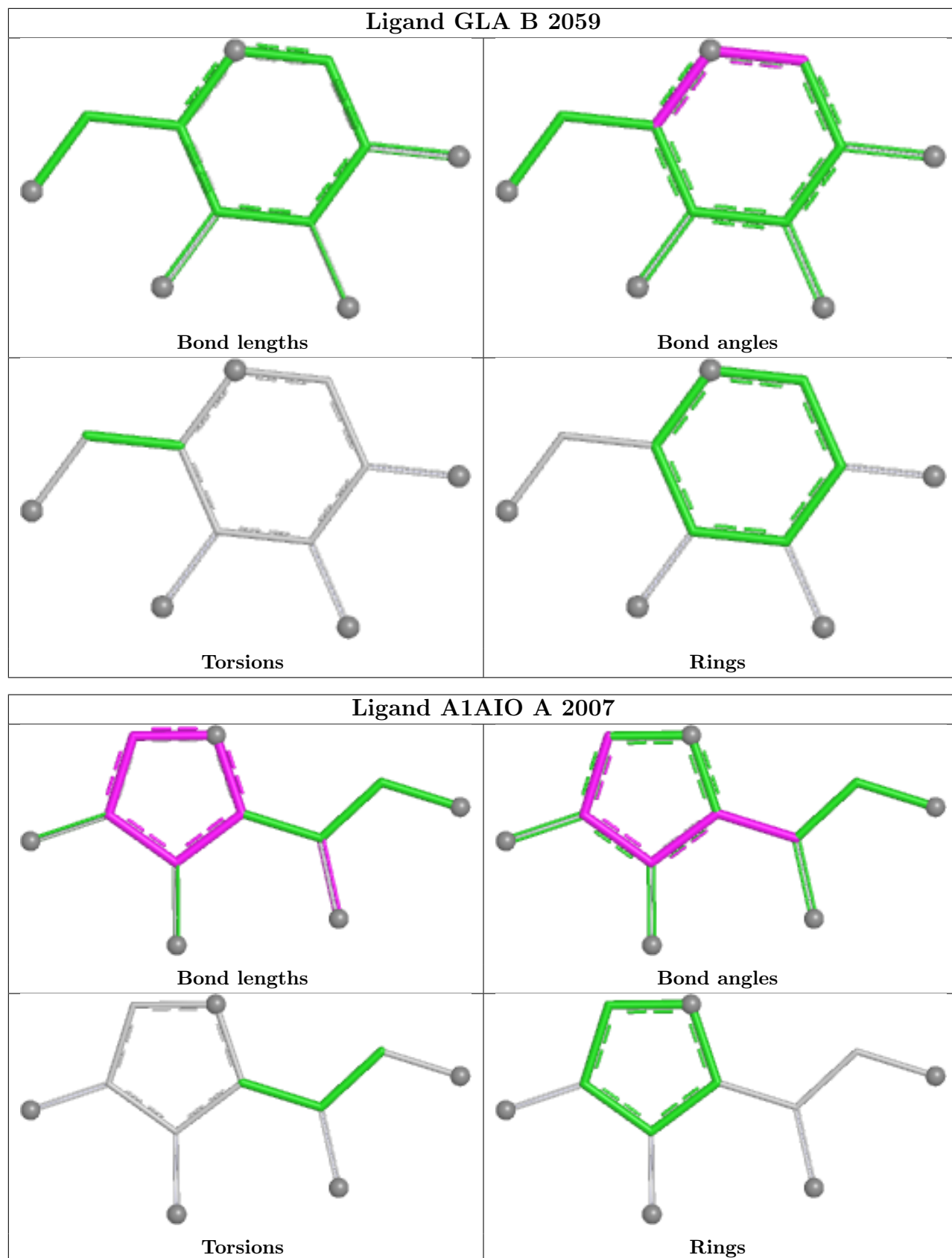
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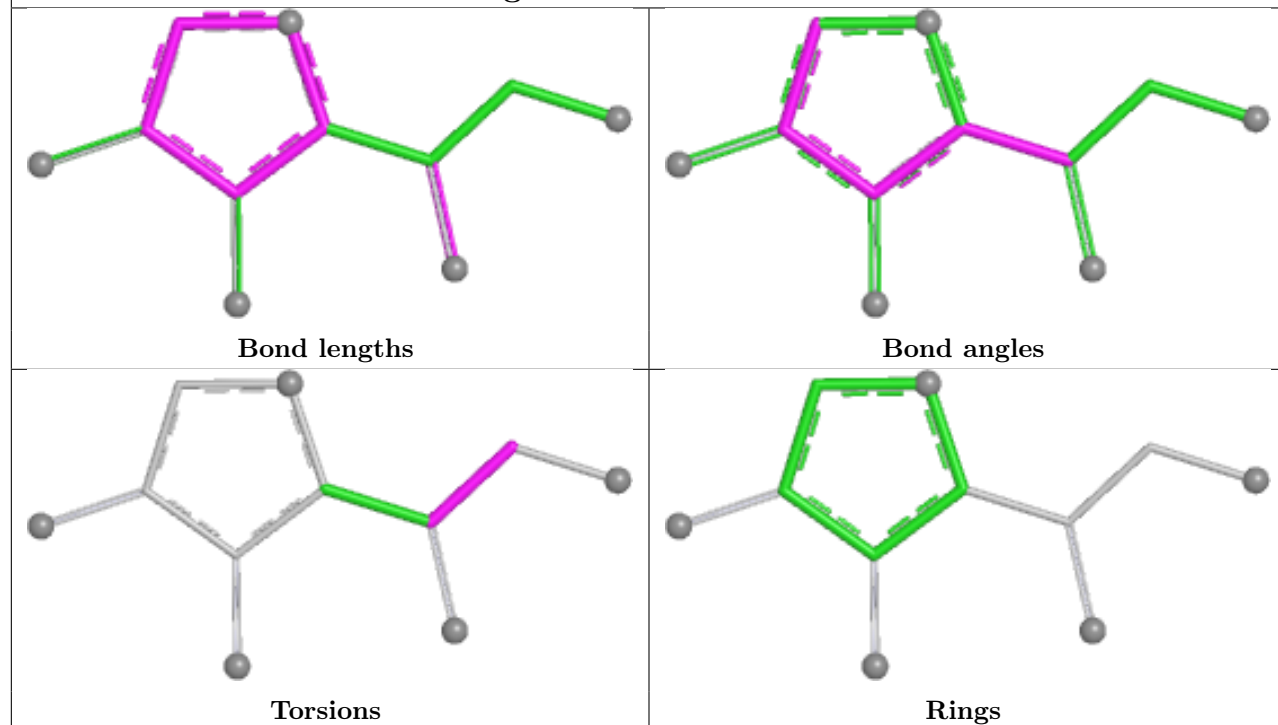
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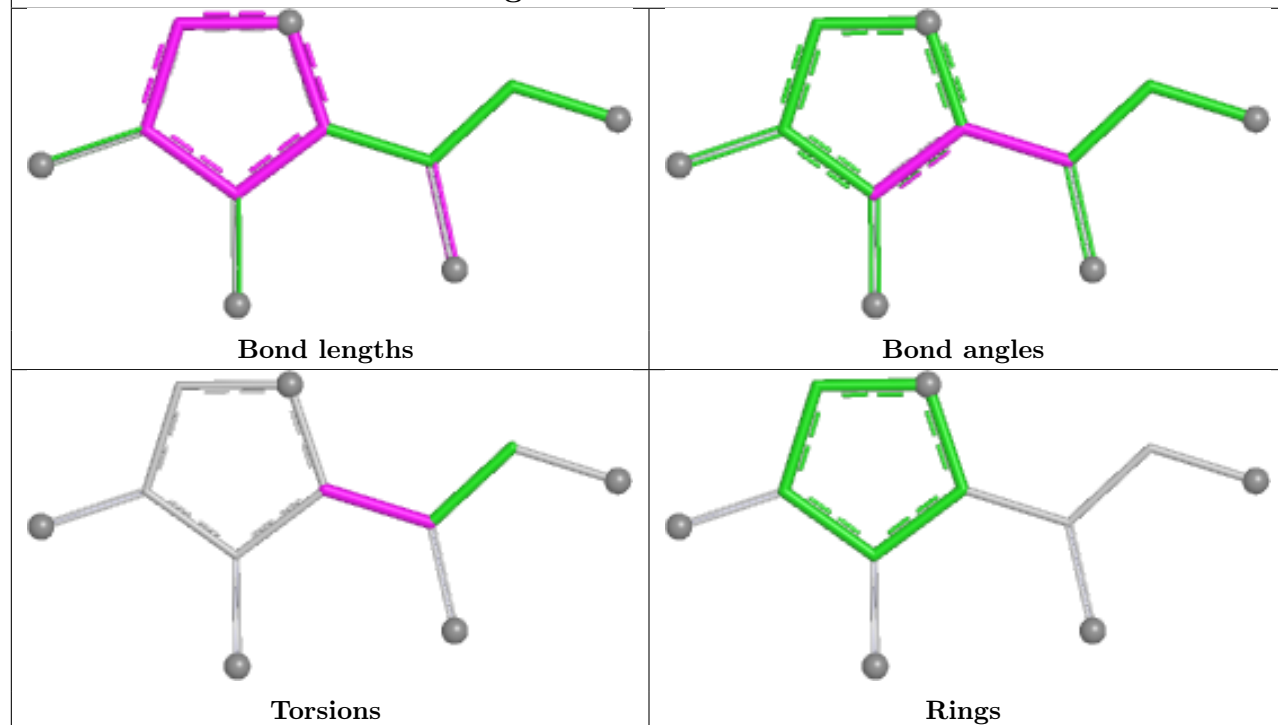




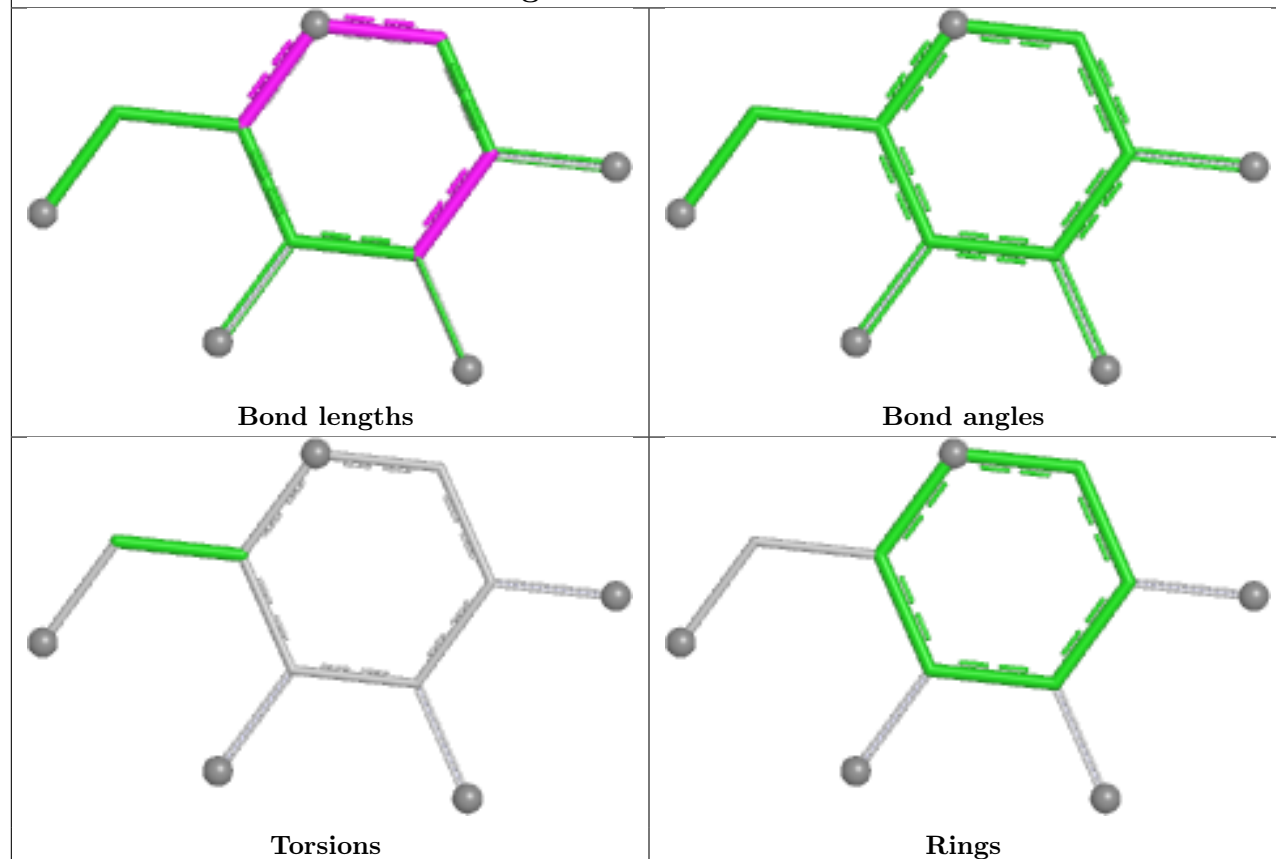
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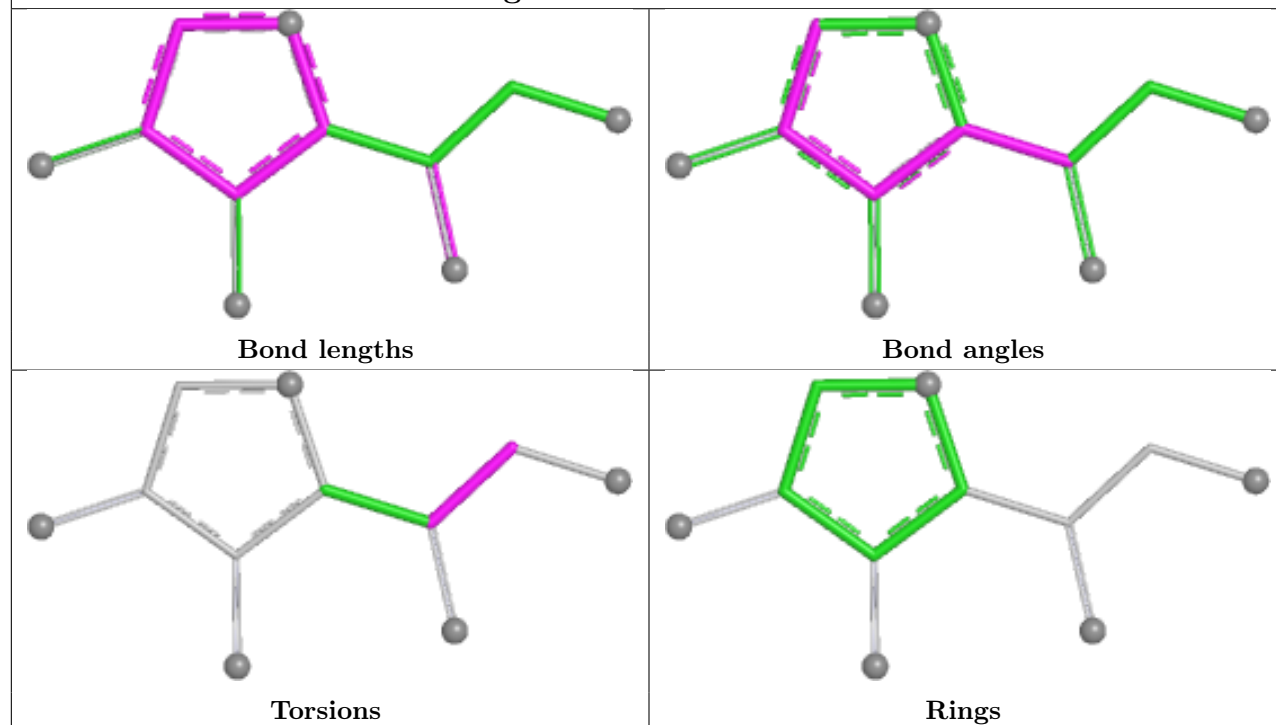
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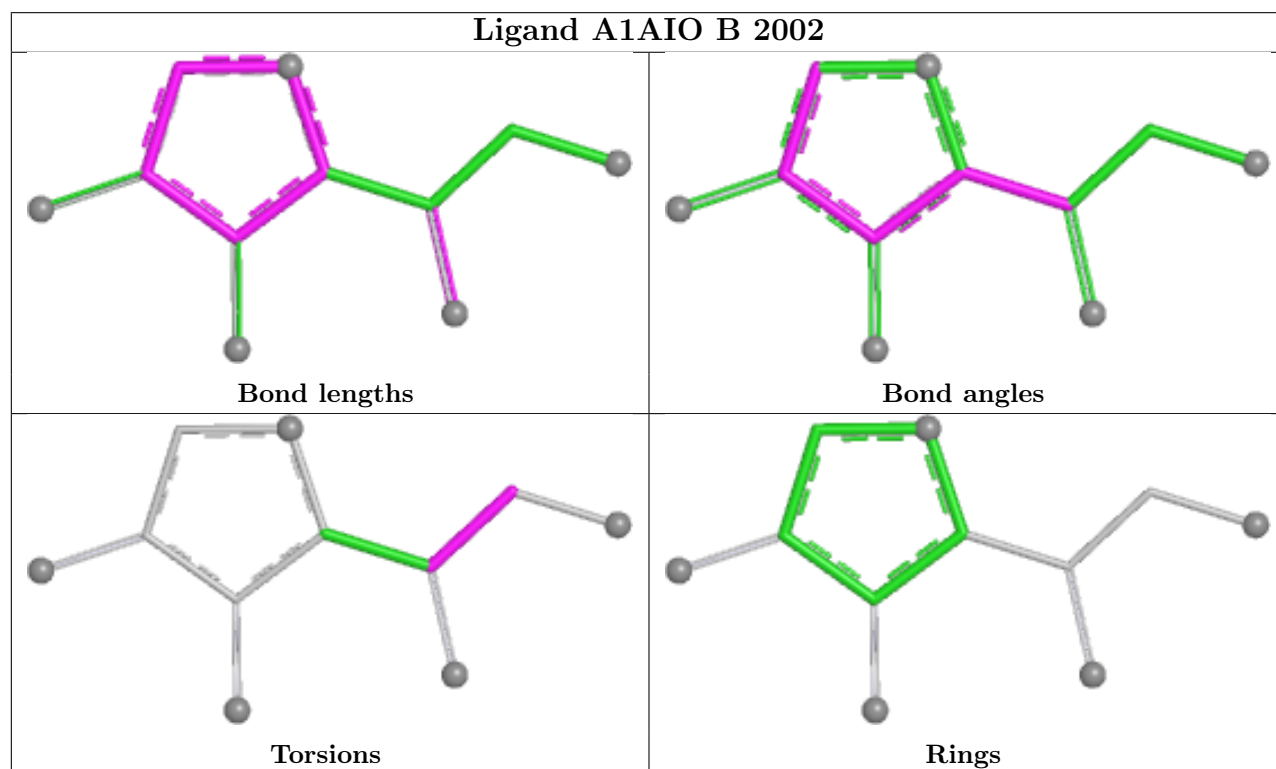
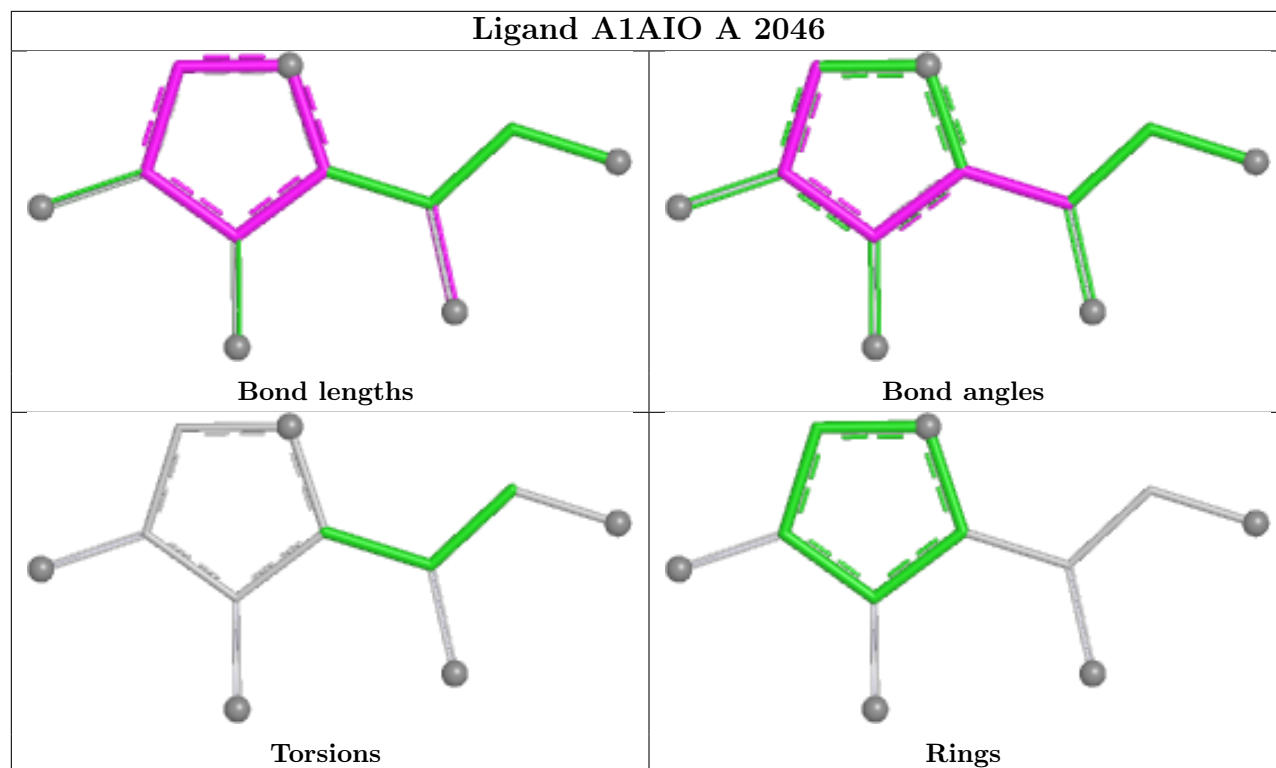


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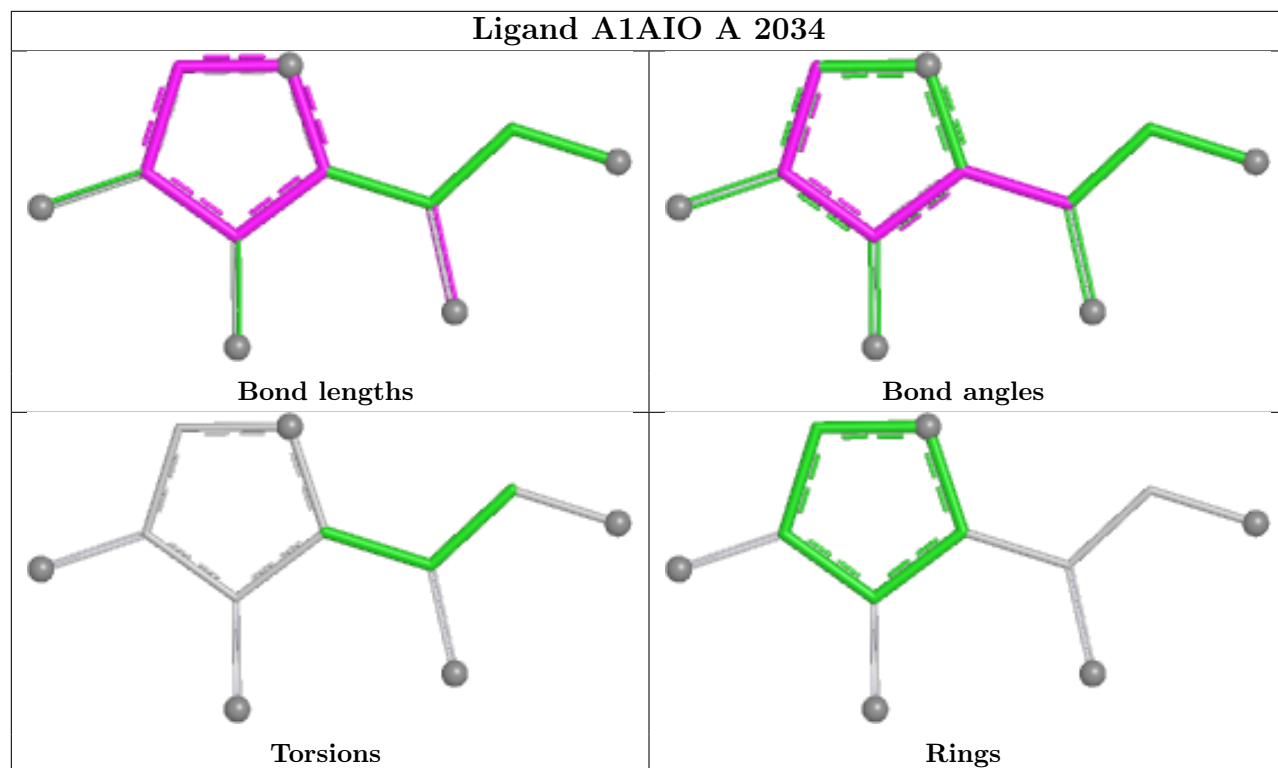


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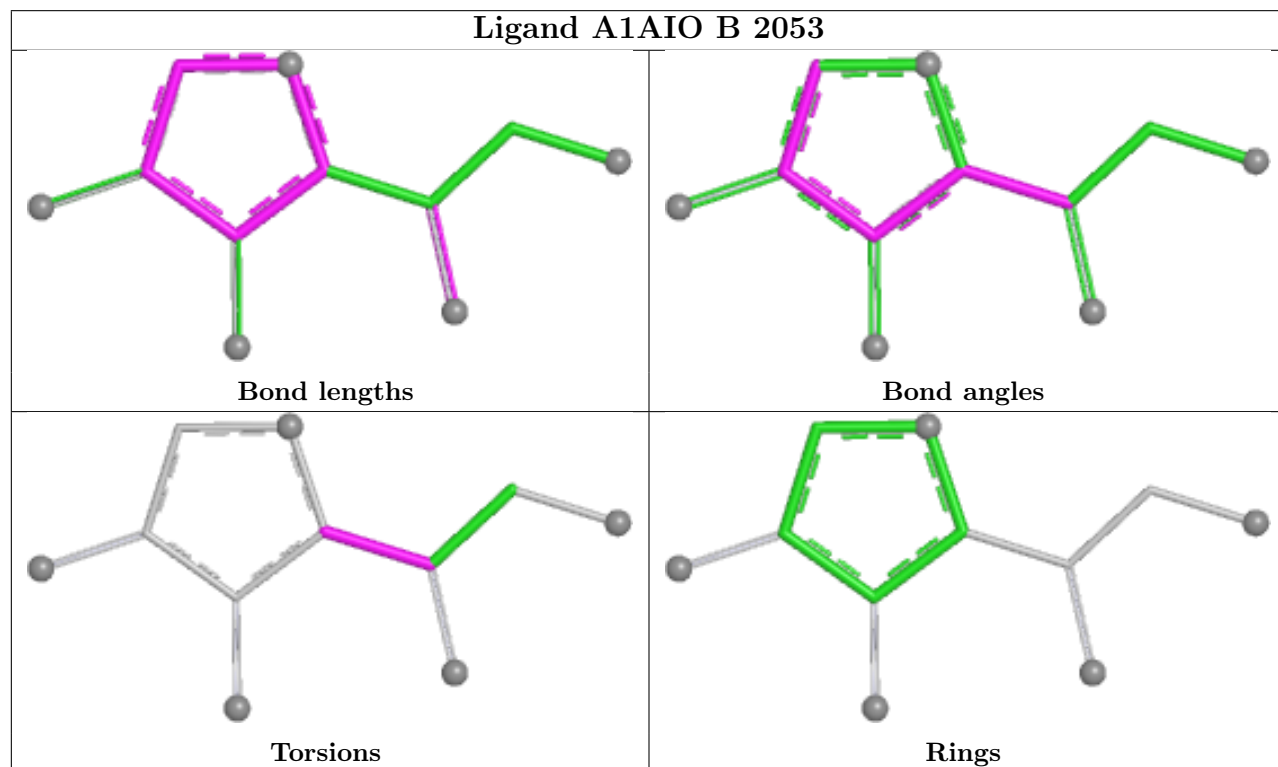


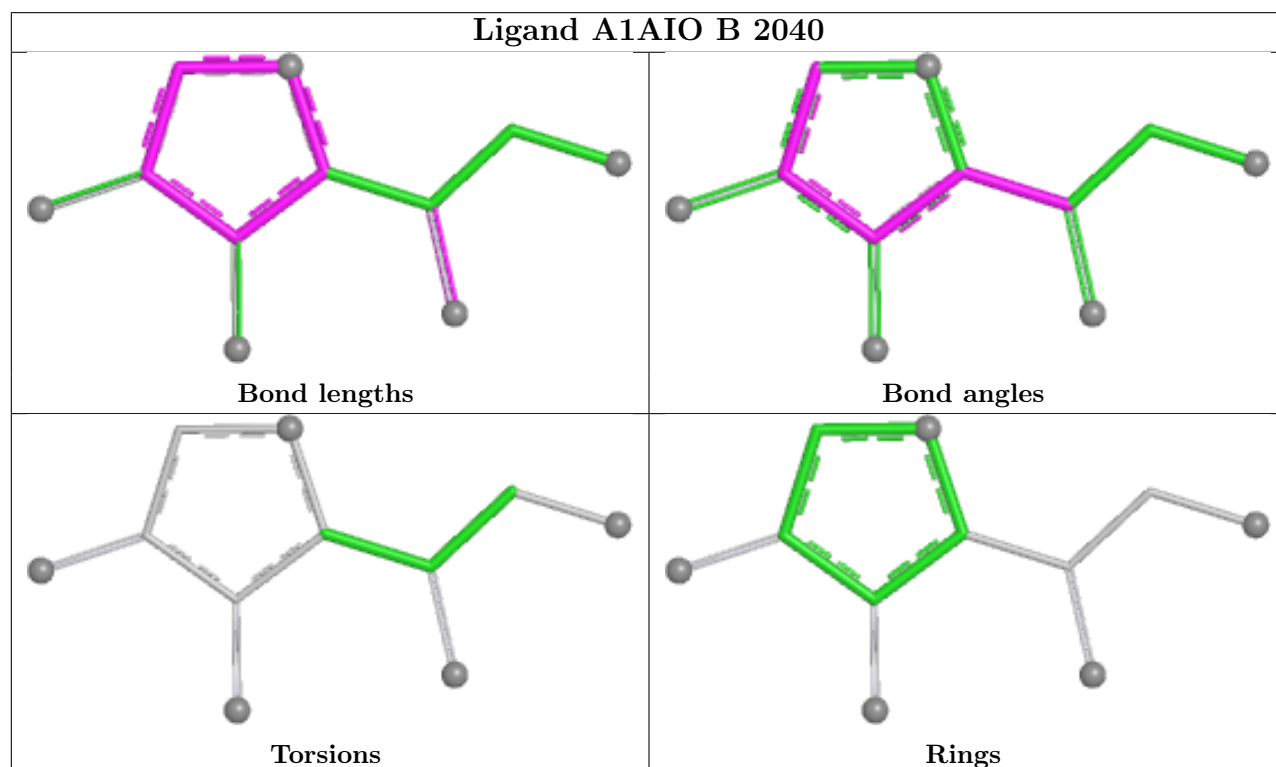
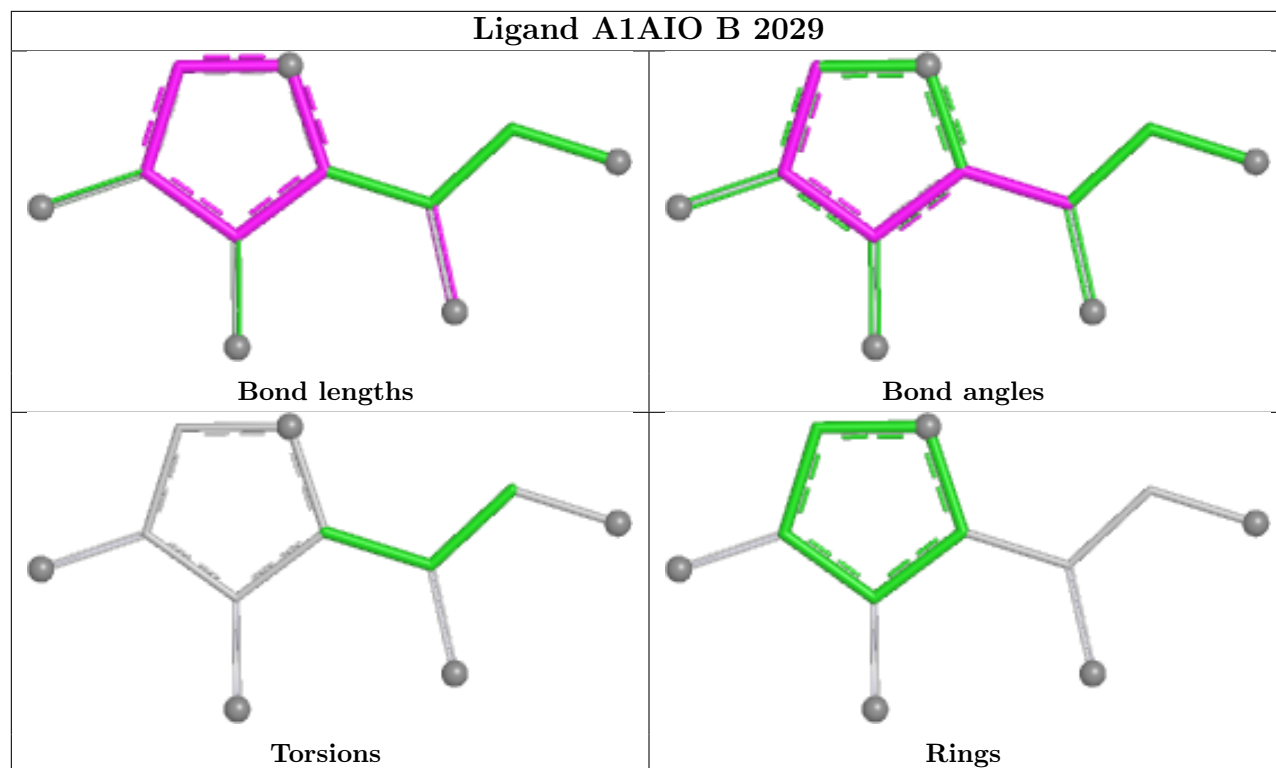


Ligand A1AIO A 2034

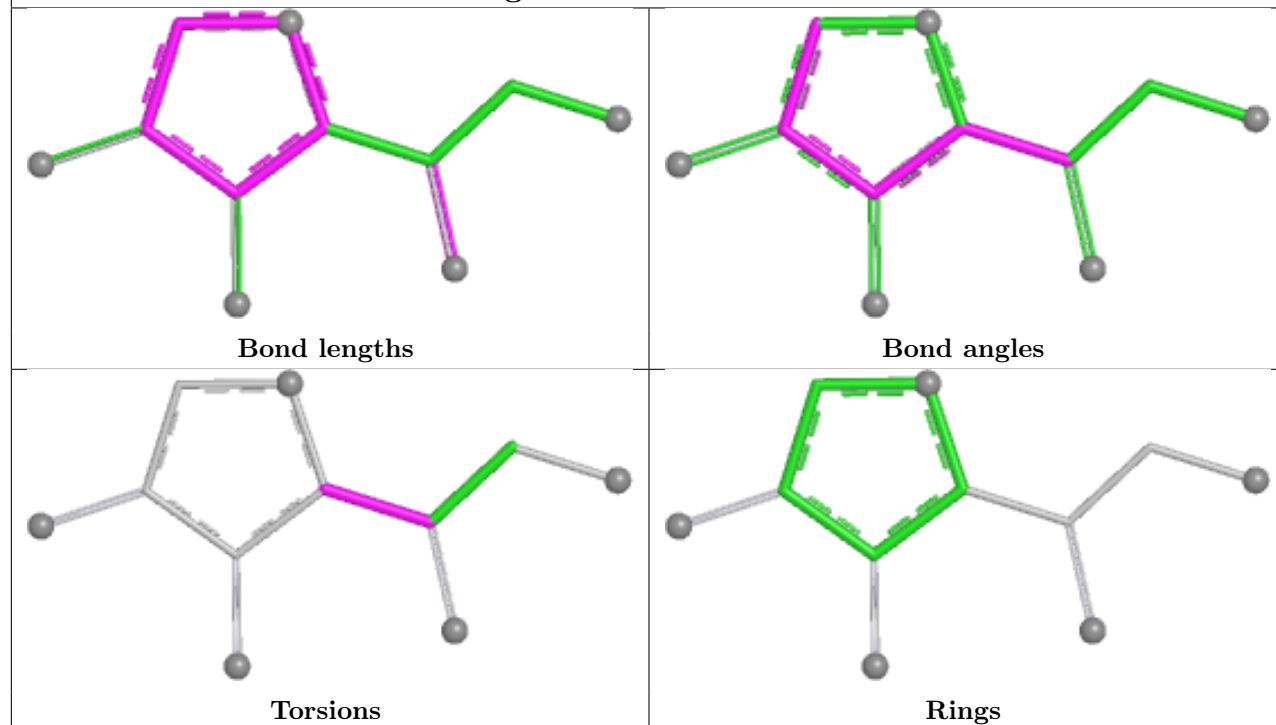


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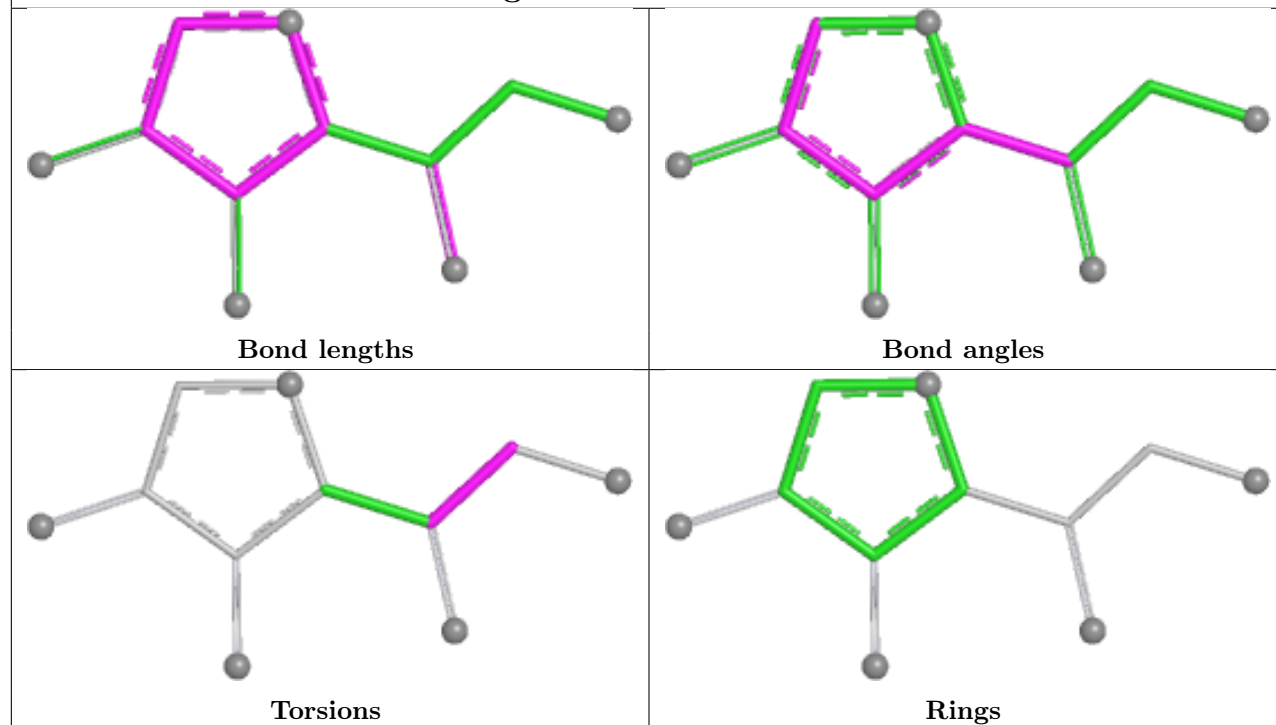




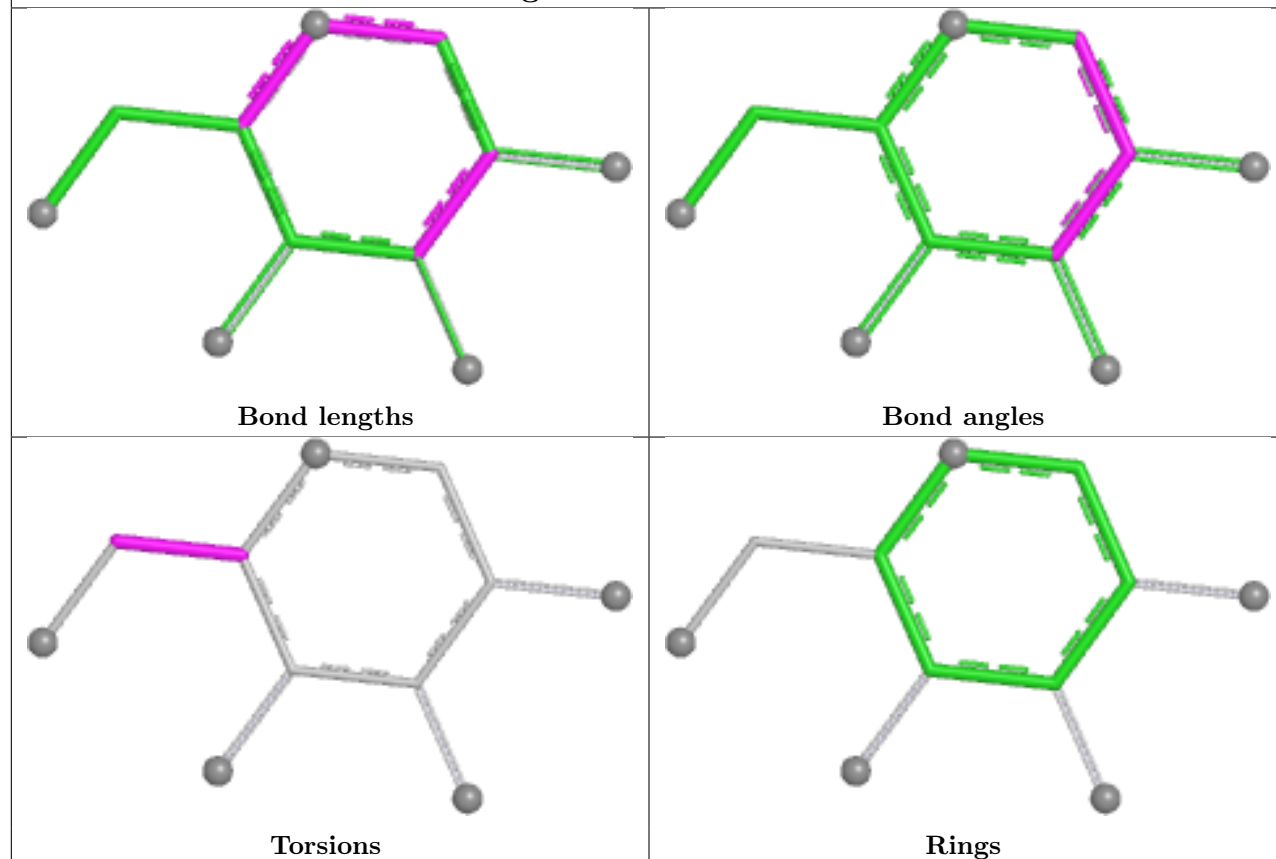
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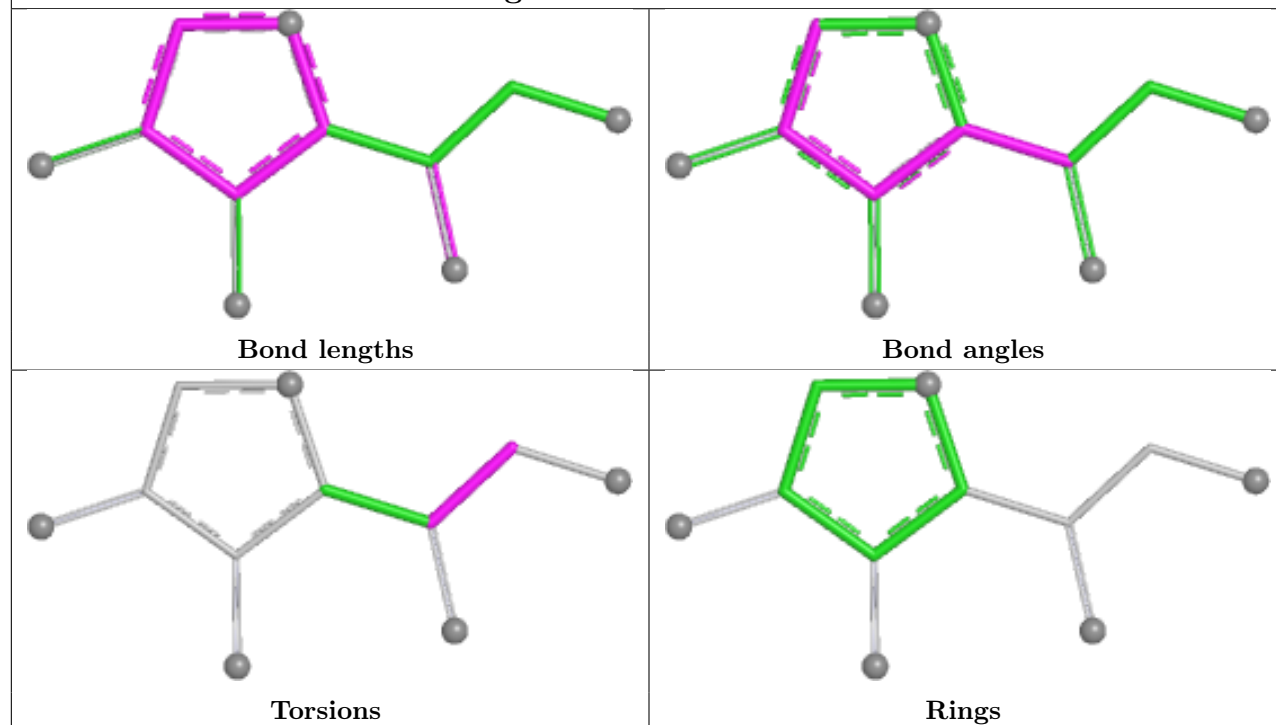
Ligand A1AIO A 2002



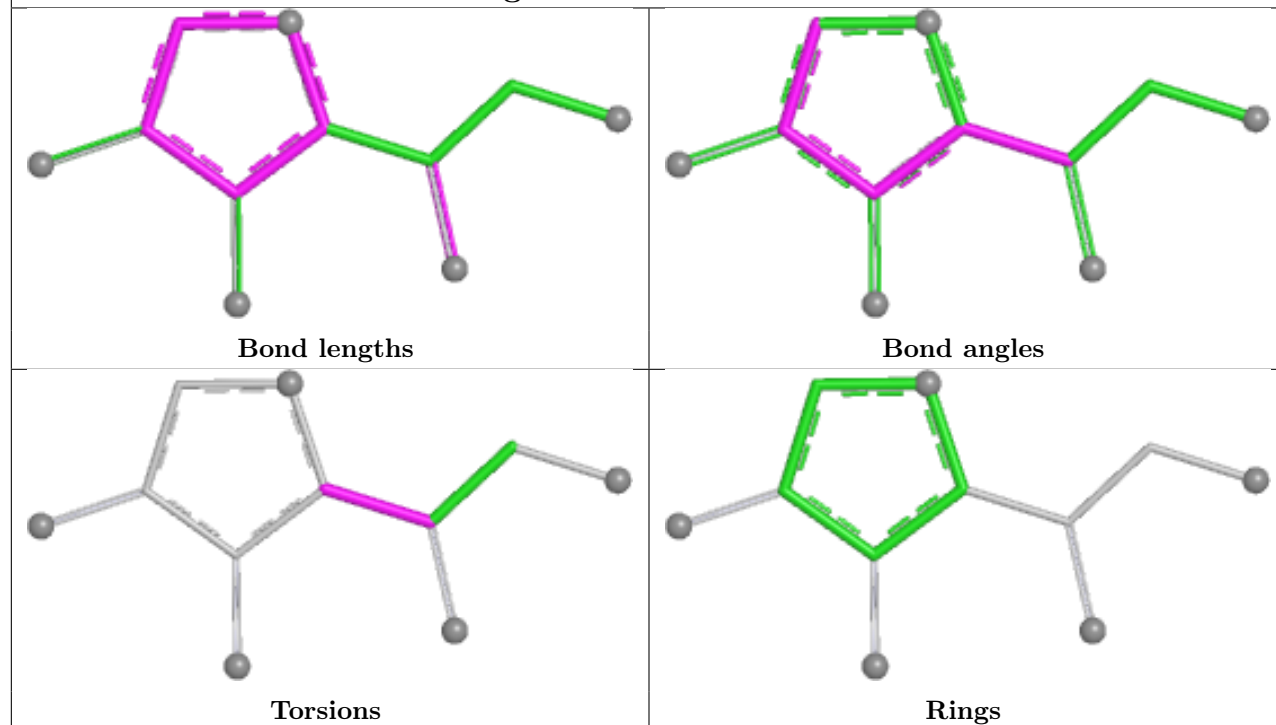
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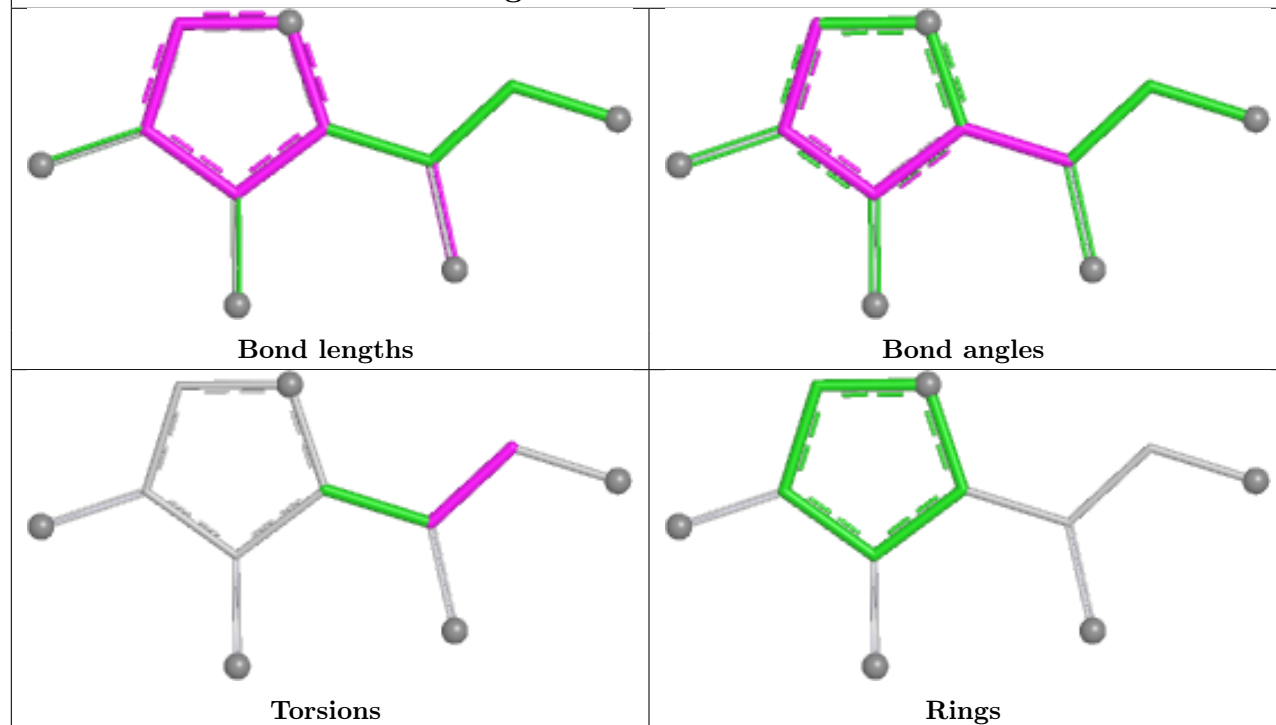
Ligand A1AIO B 2010



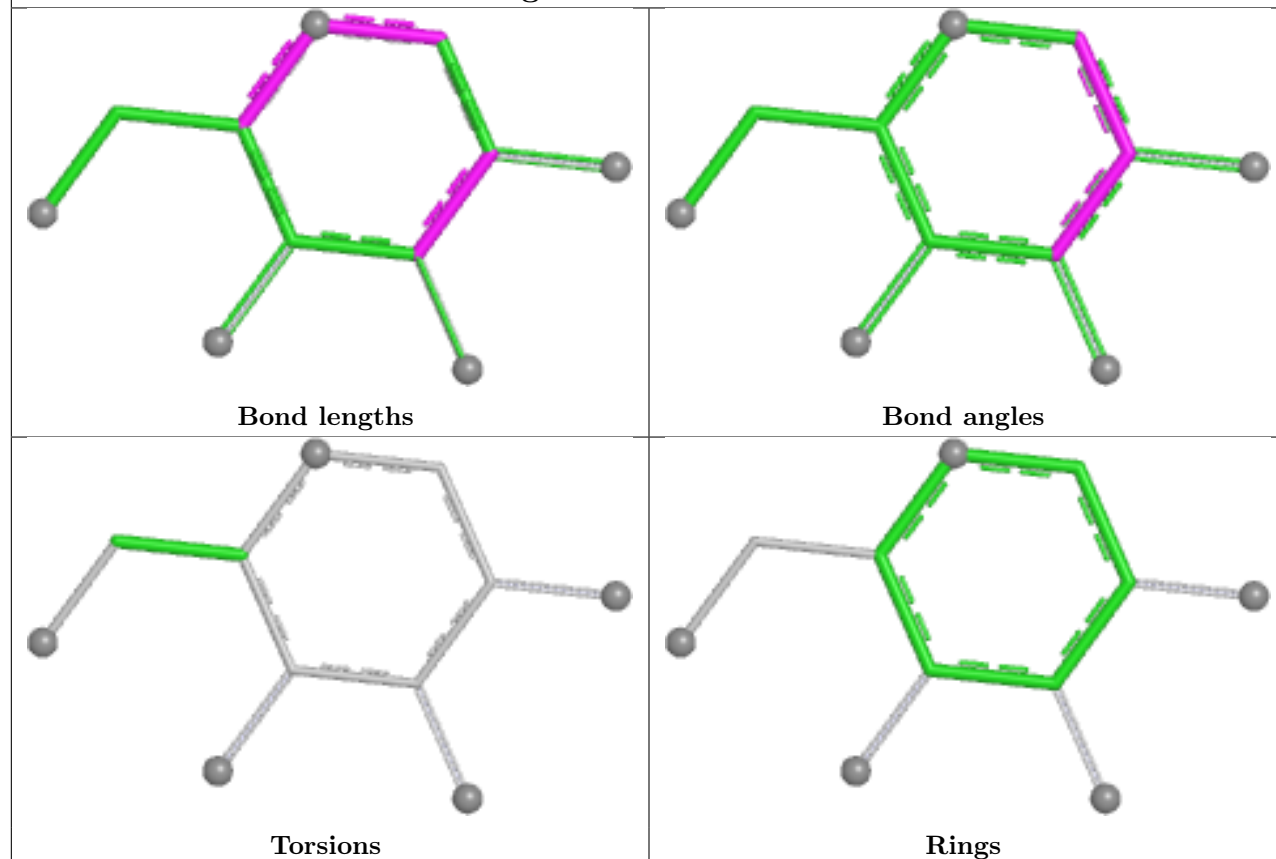
Ligand A1AIO A 2041



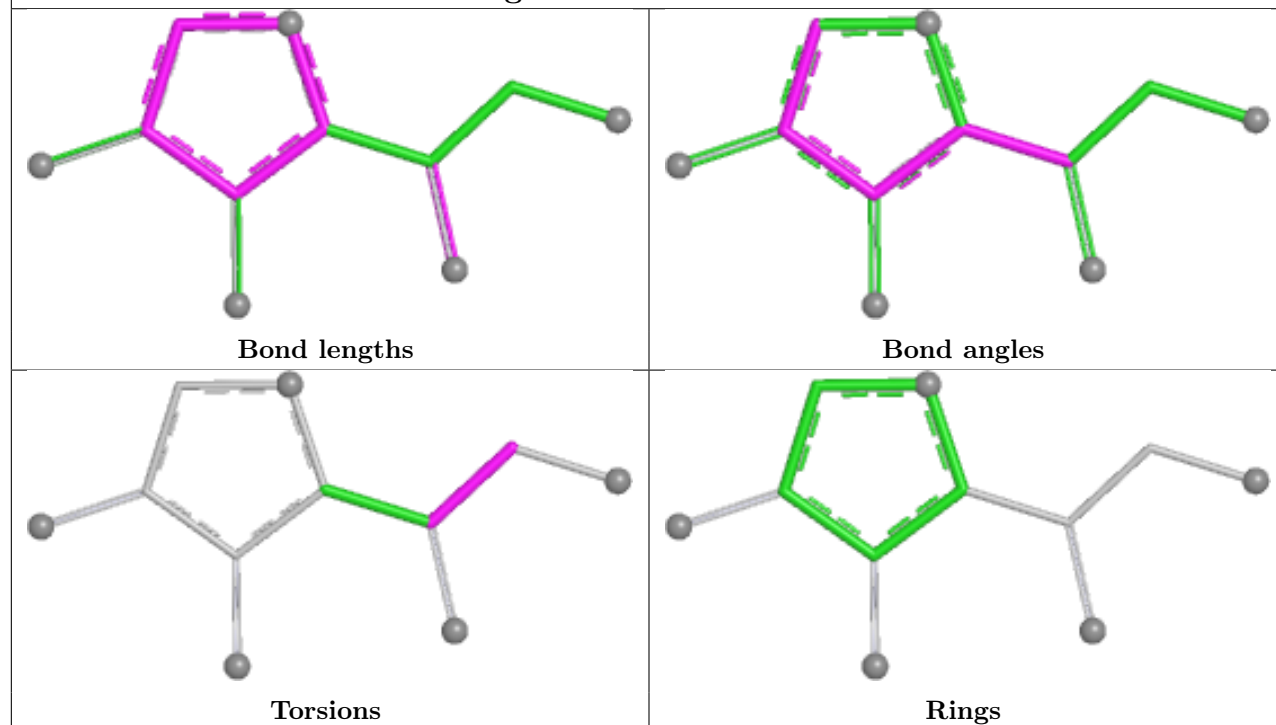
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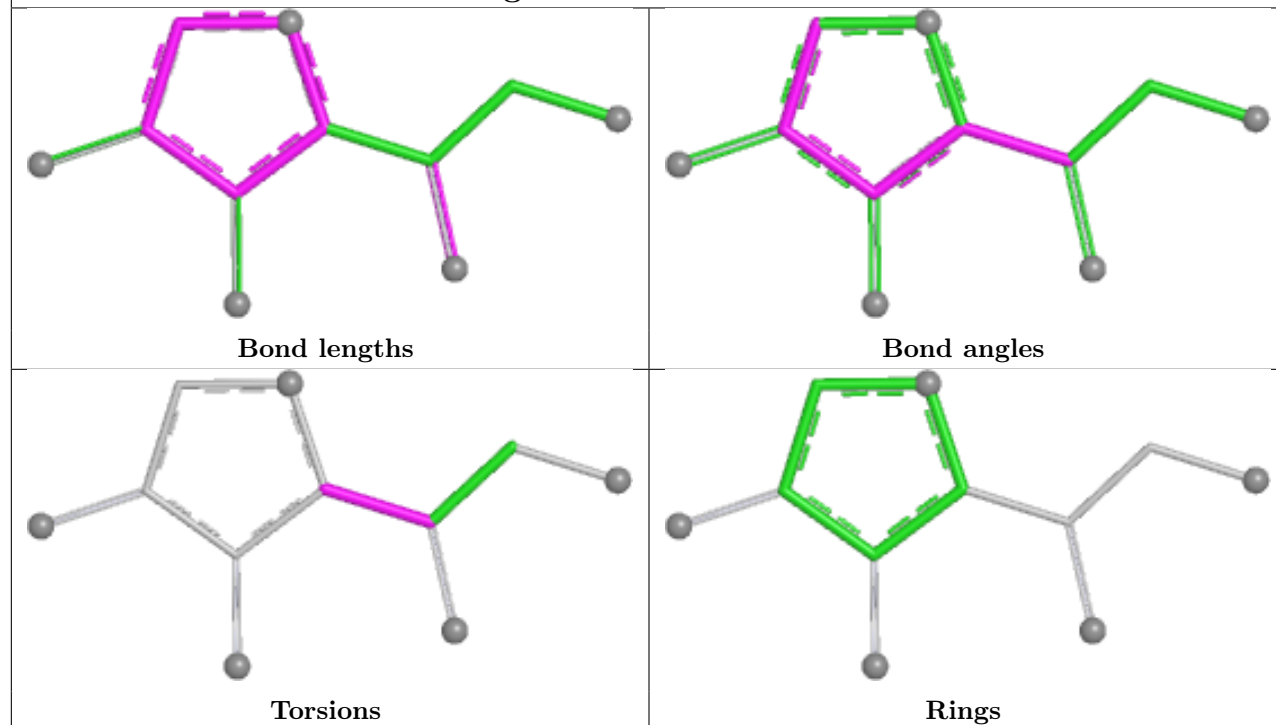
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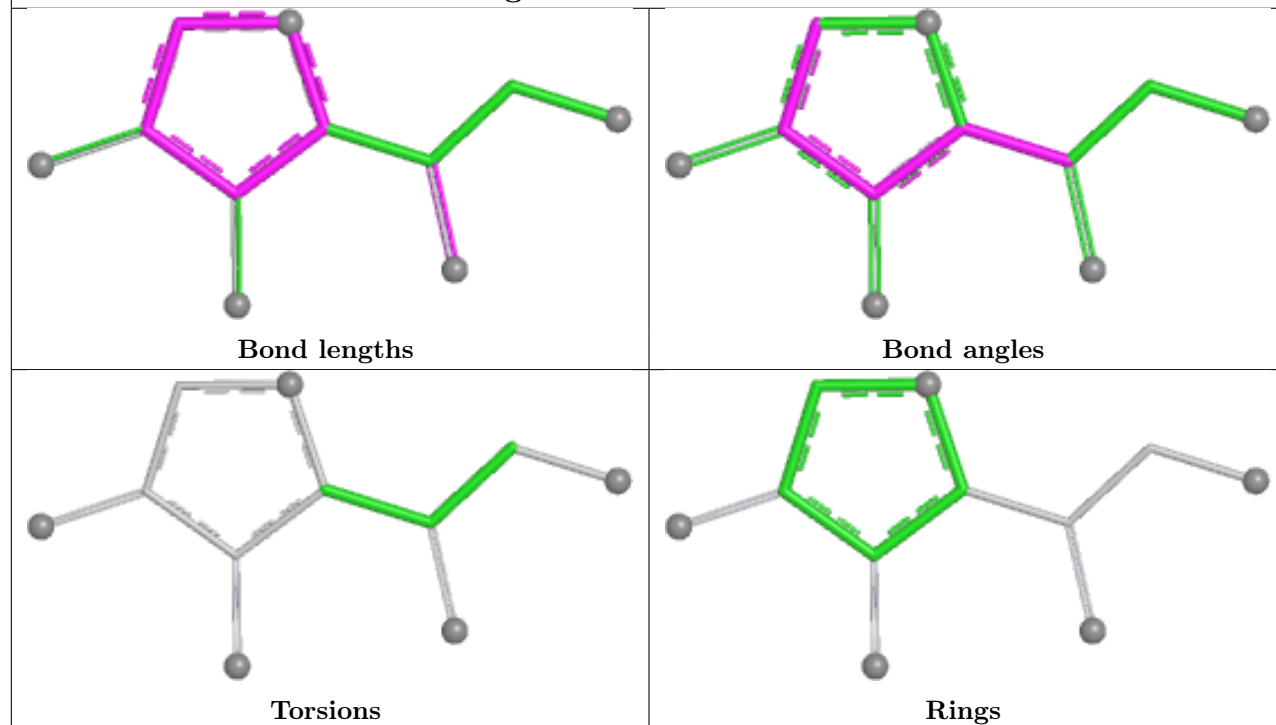
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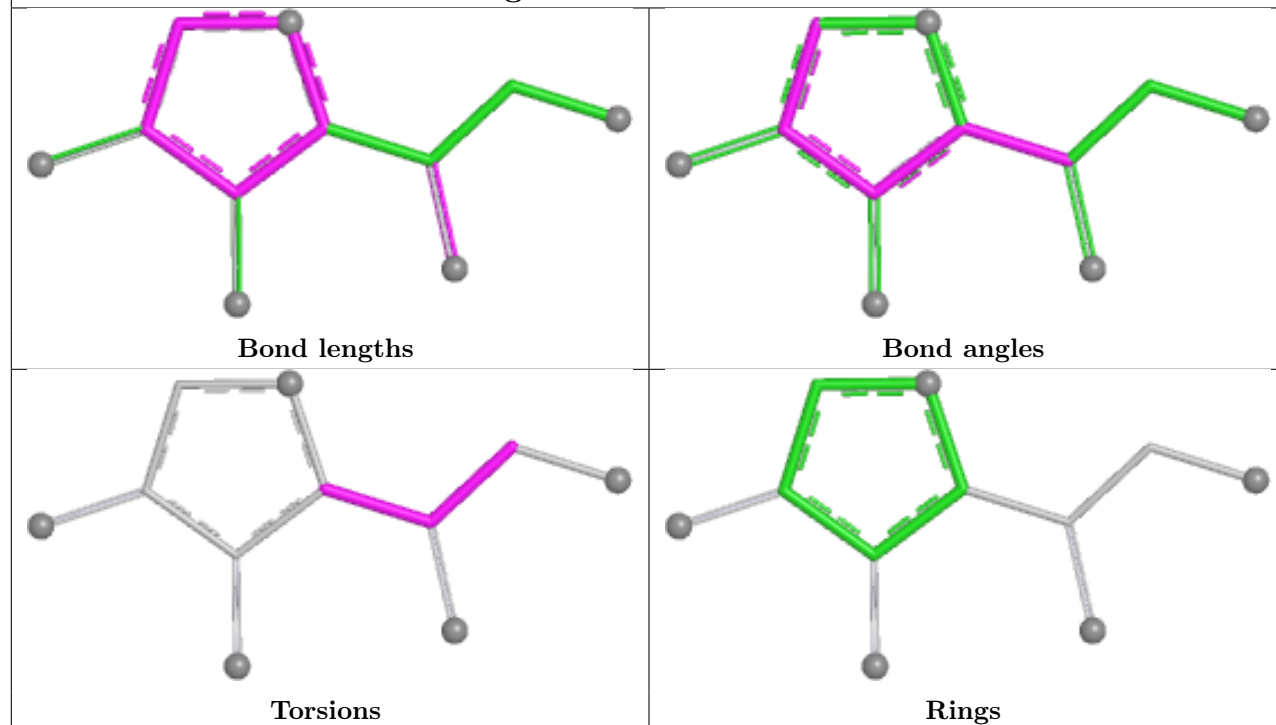
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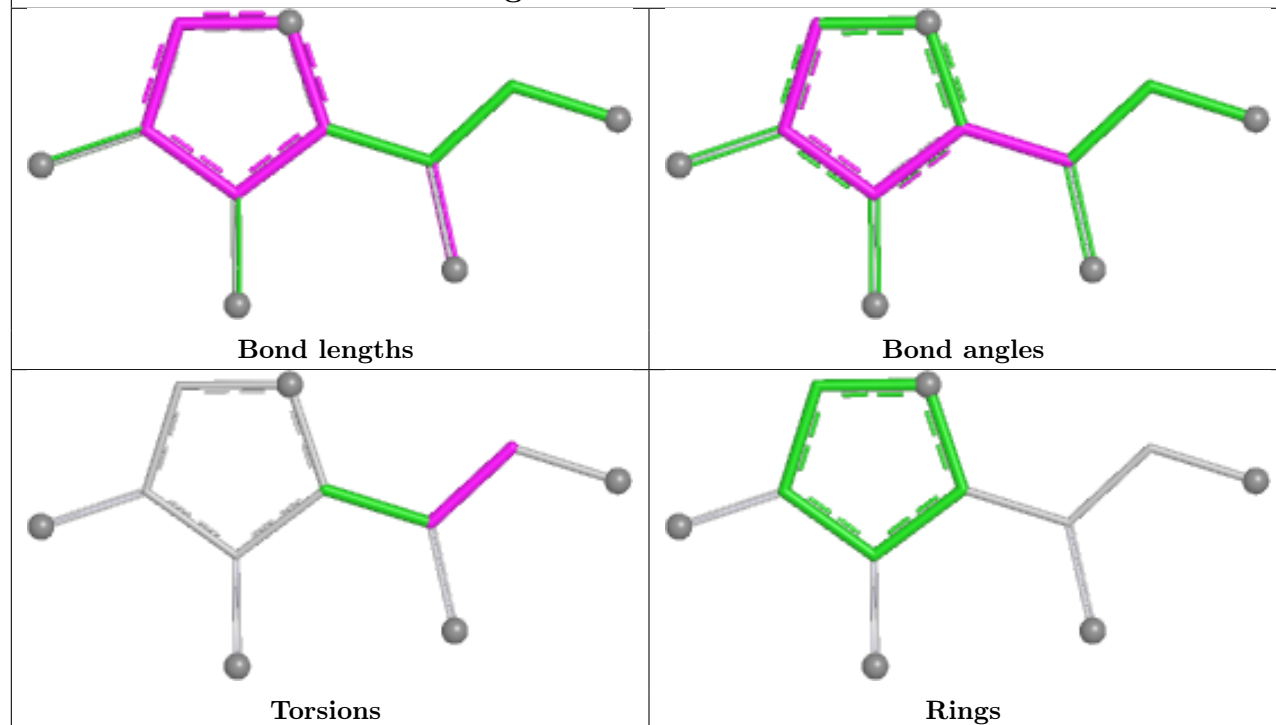
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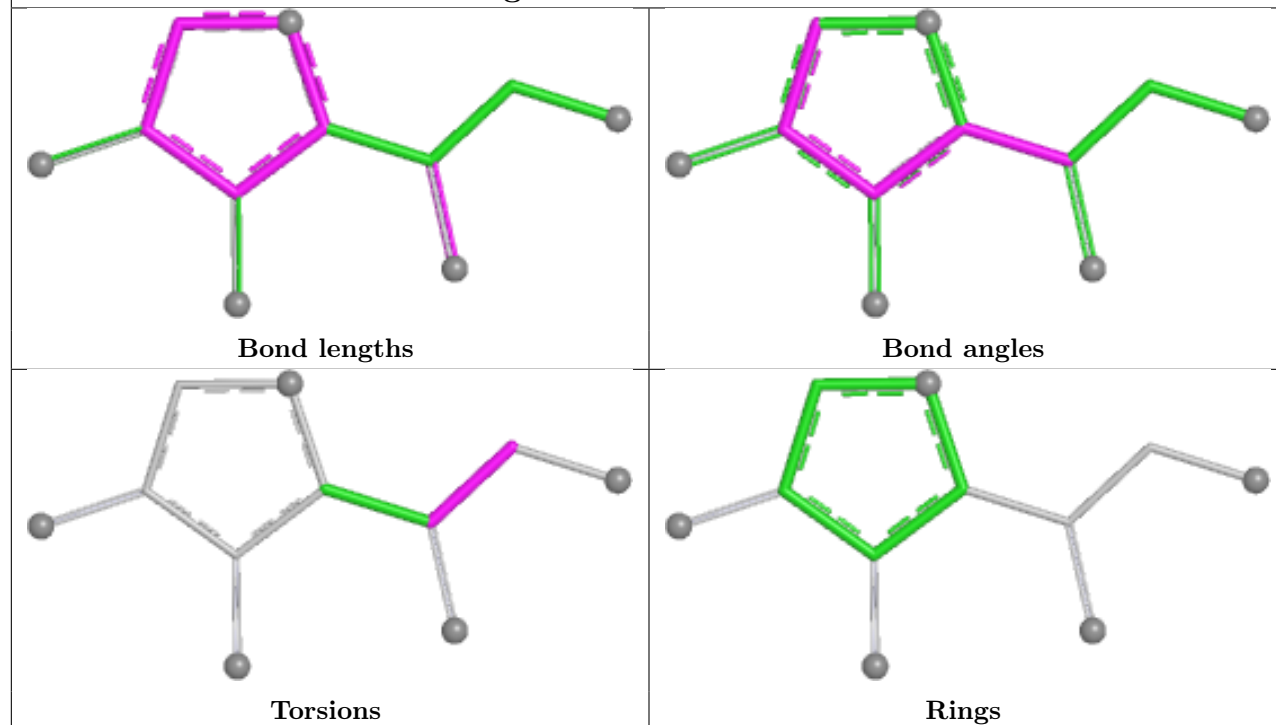
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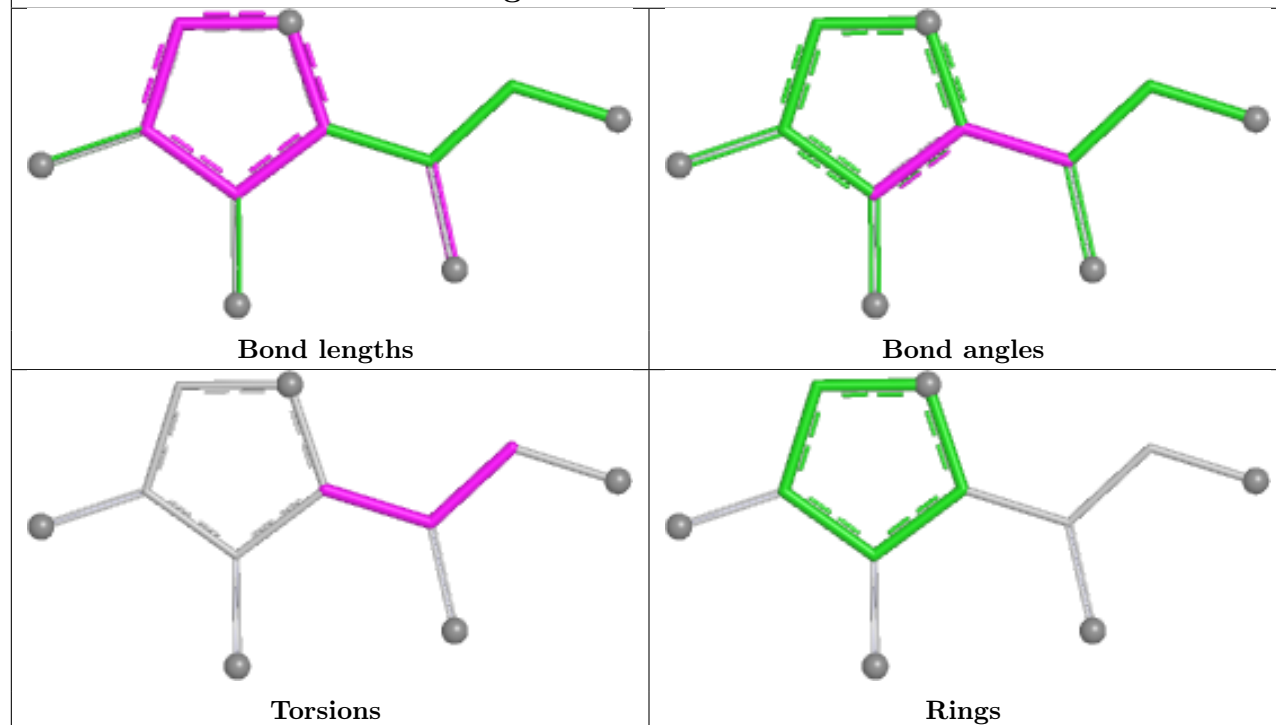
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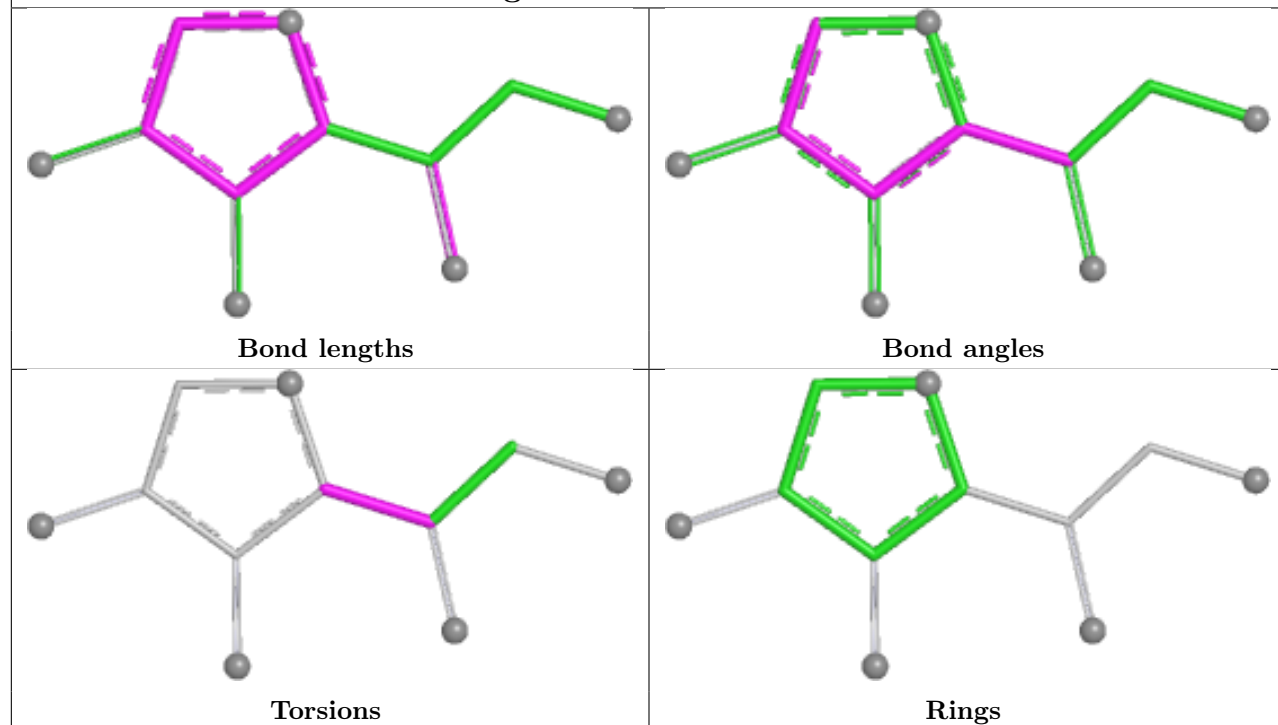
Ligand A1AIO A 2004



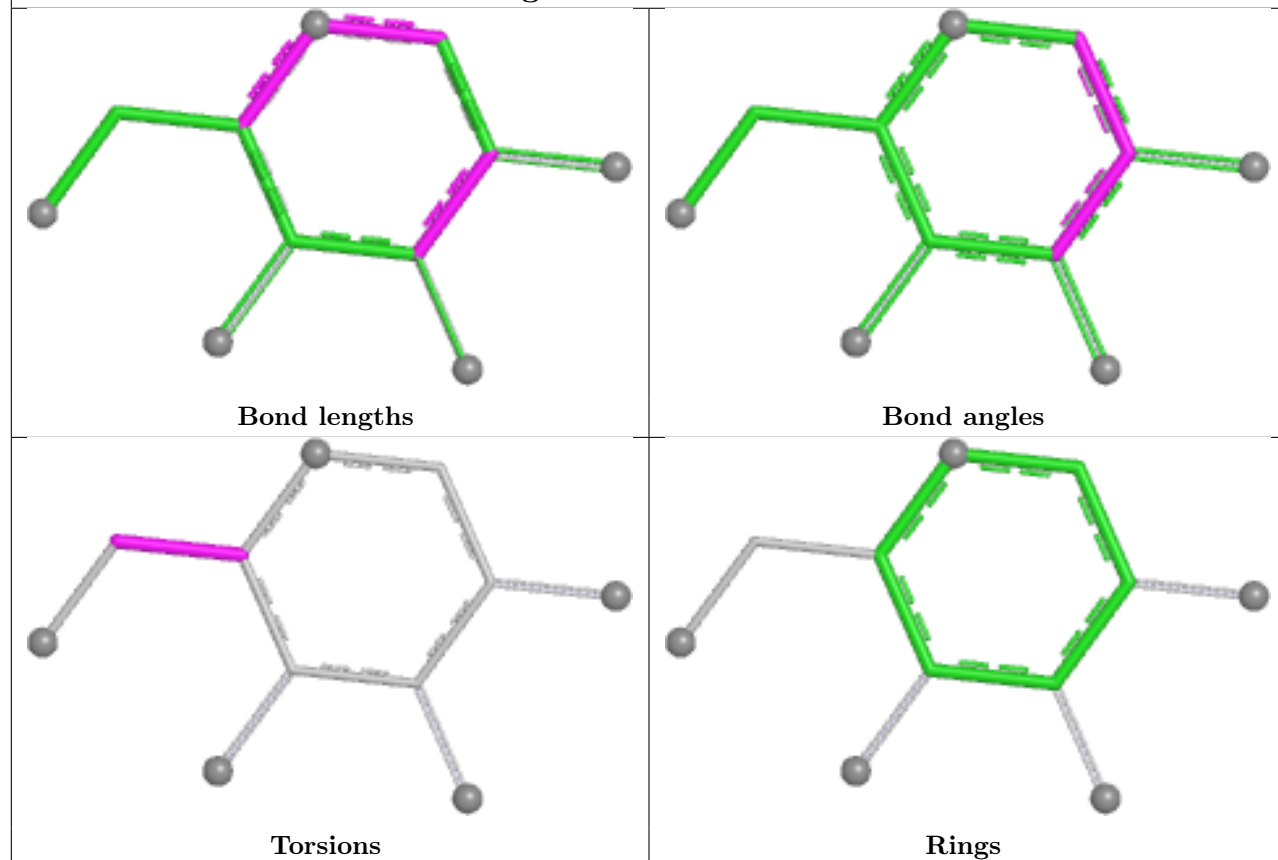
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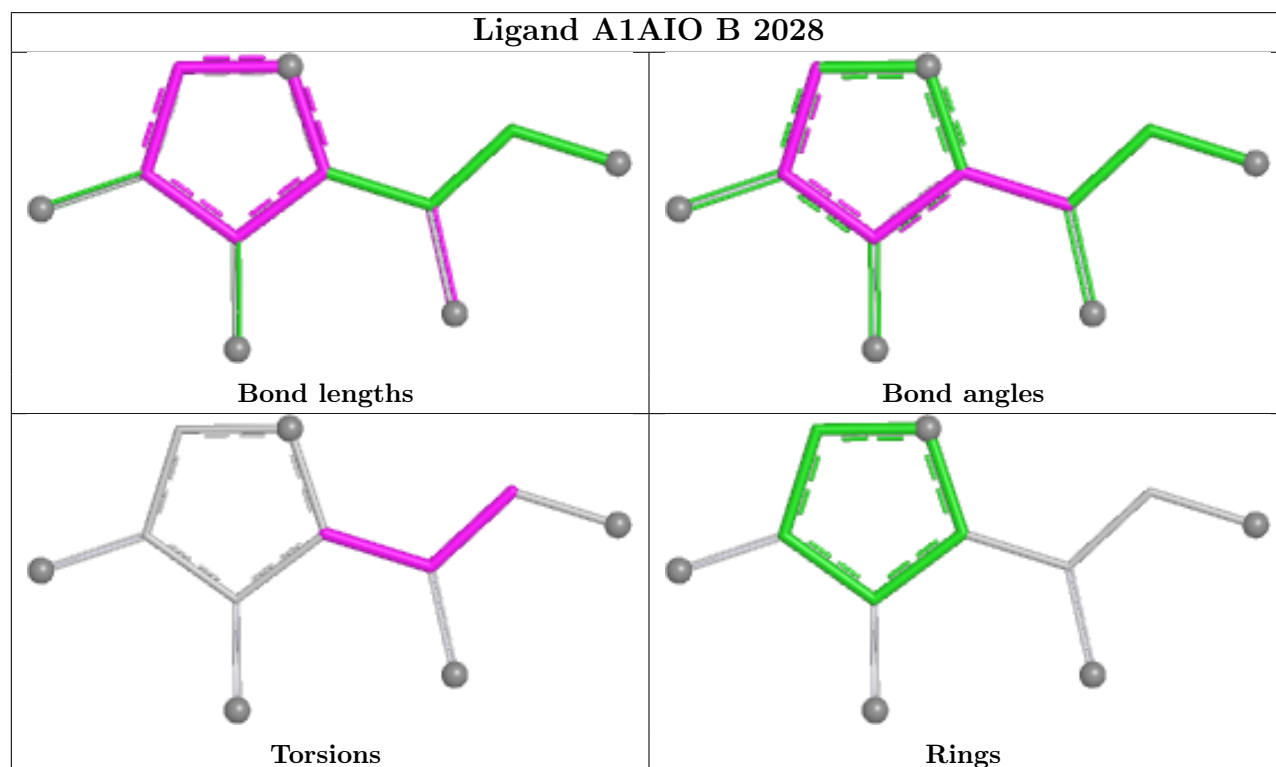
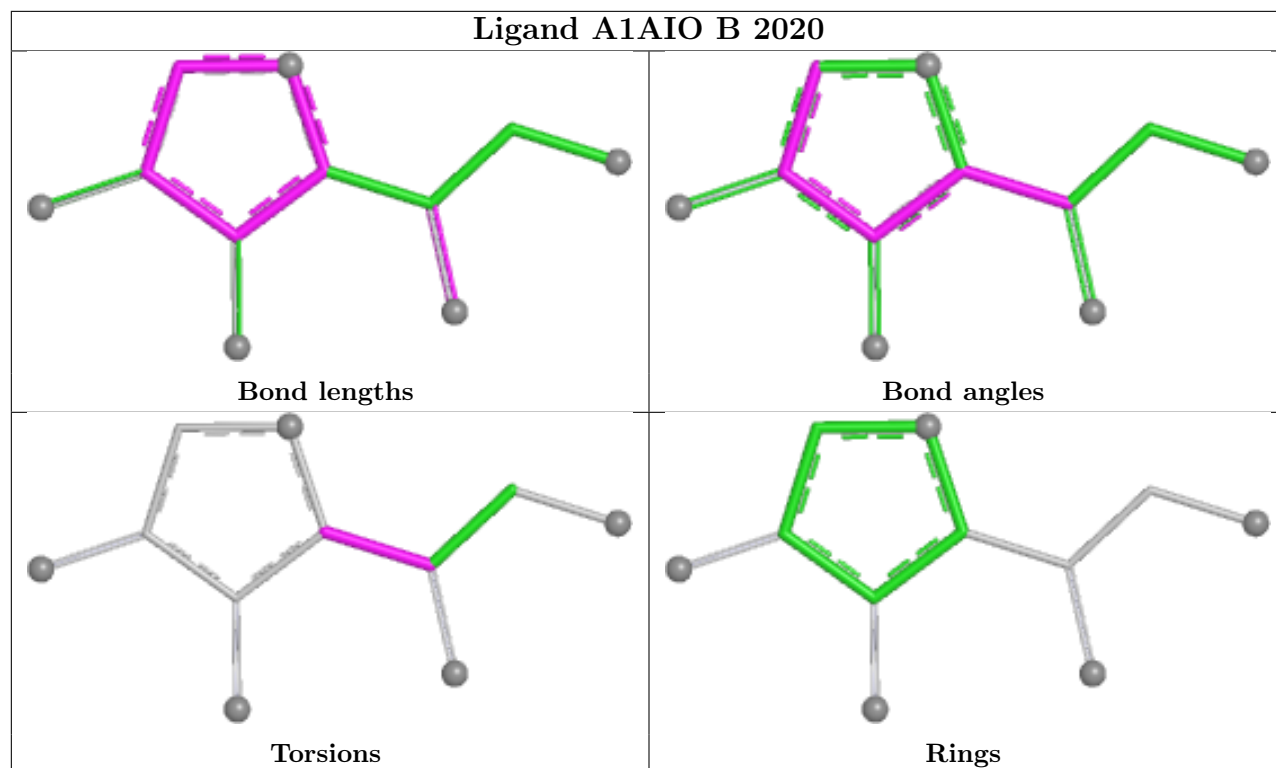


Ligand A1AIO A 2030

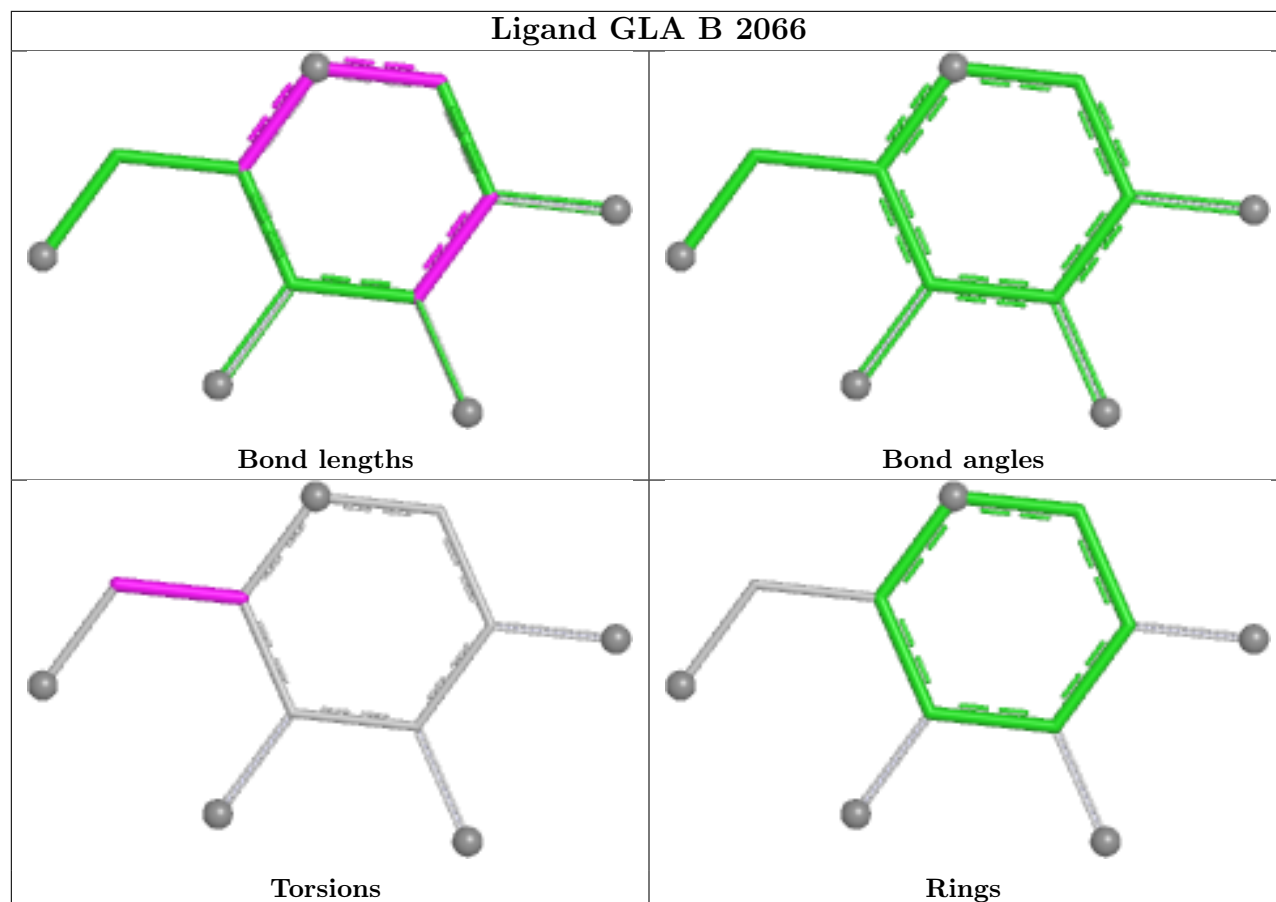


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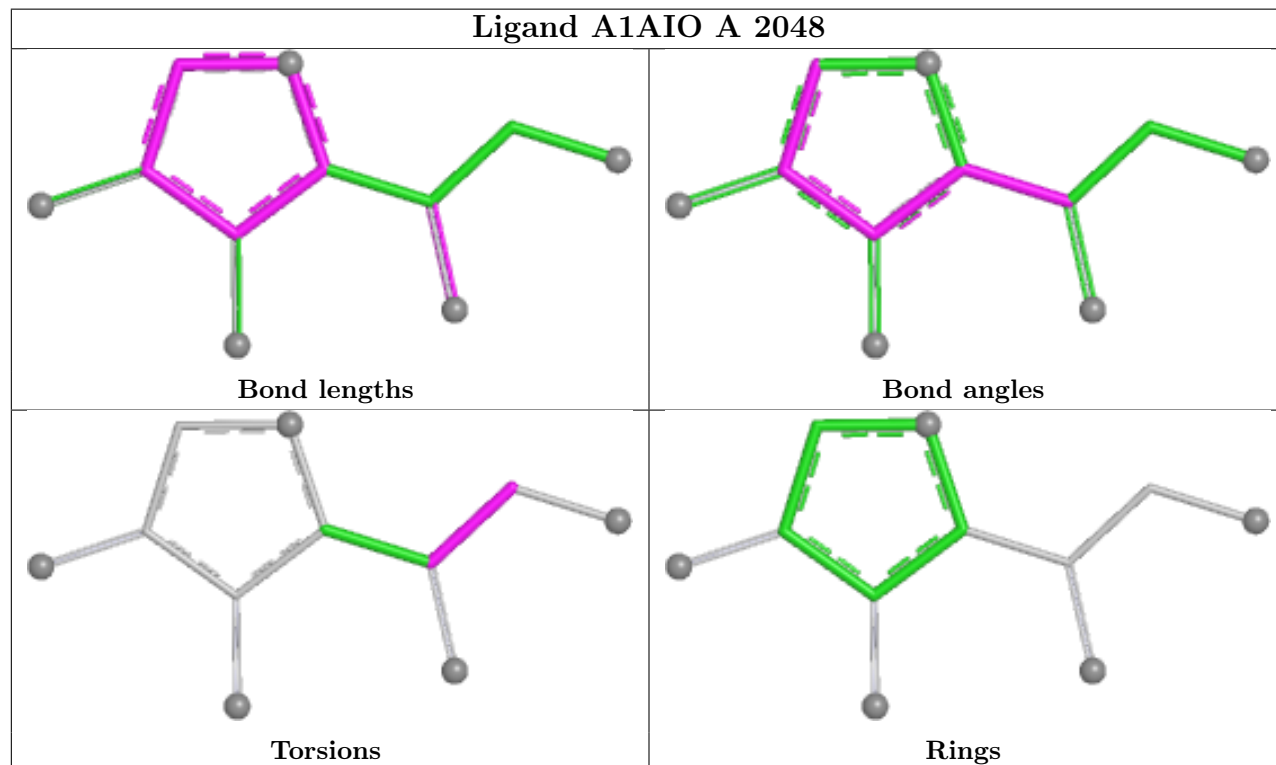




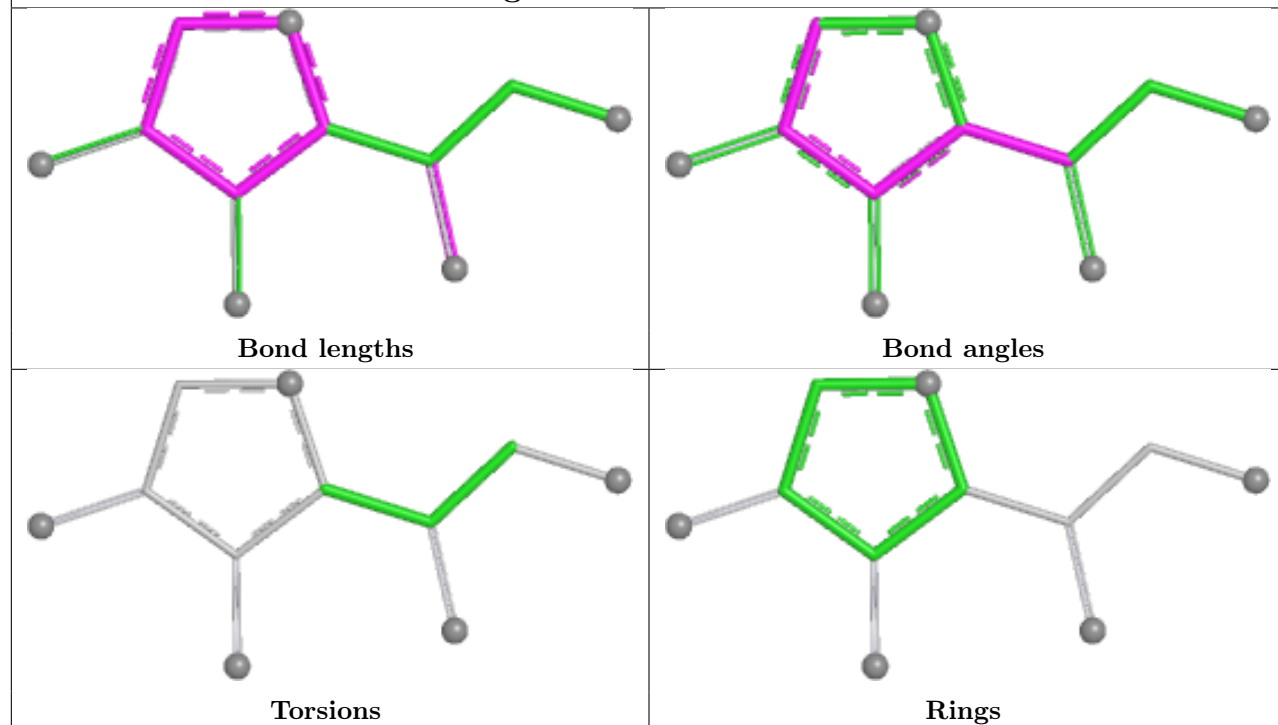
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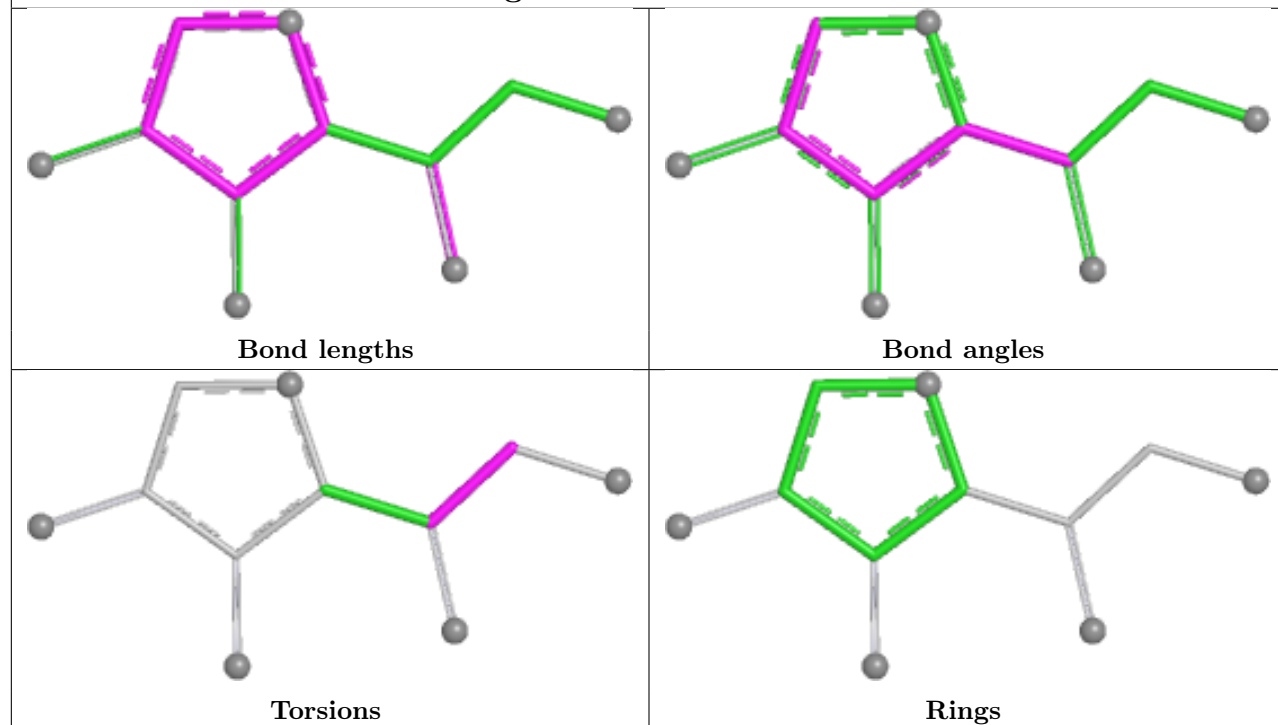
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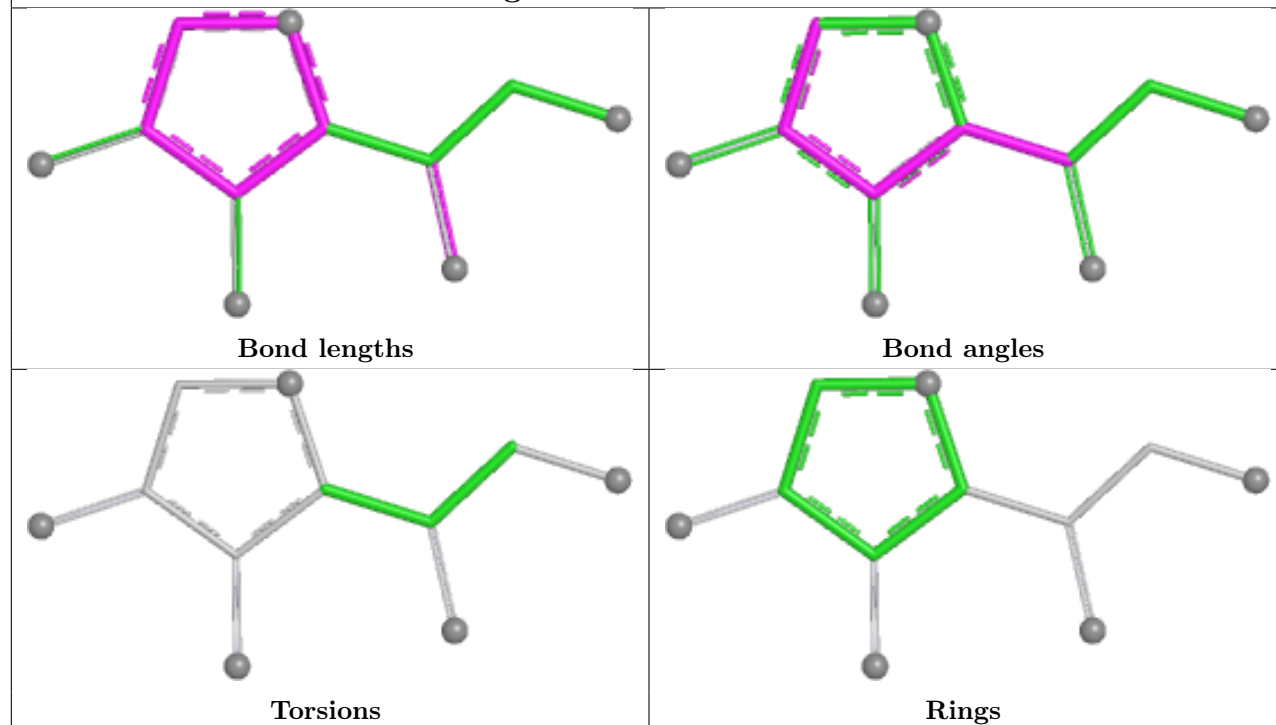
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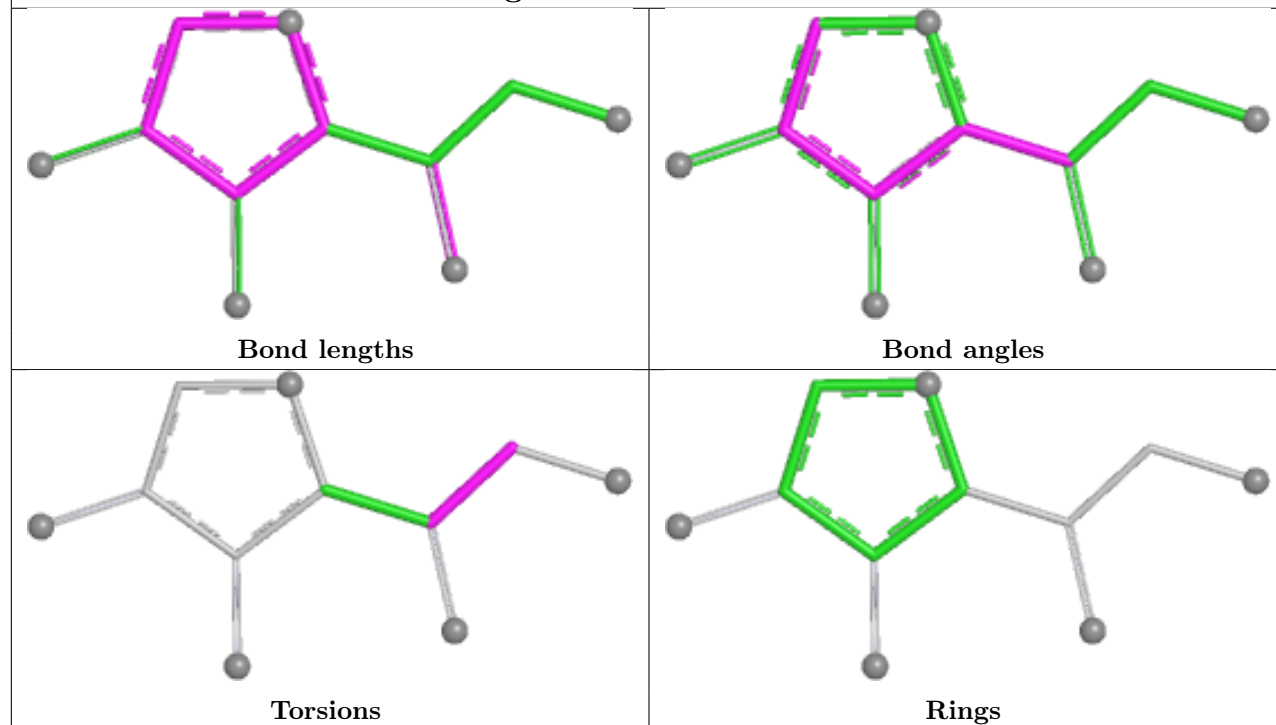
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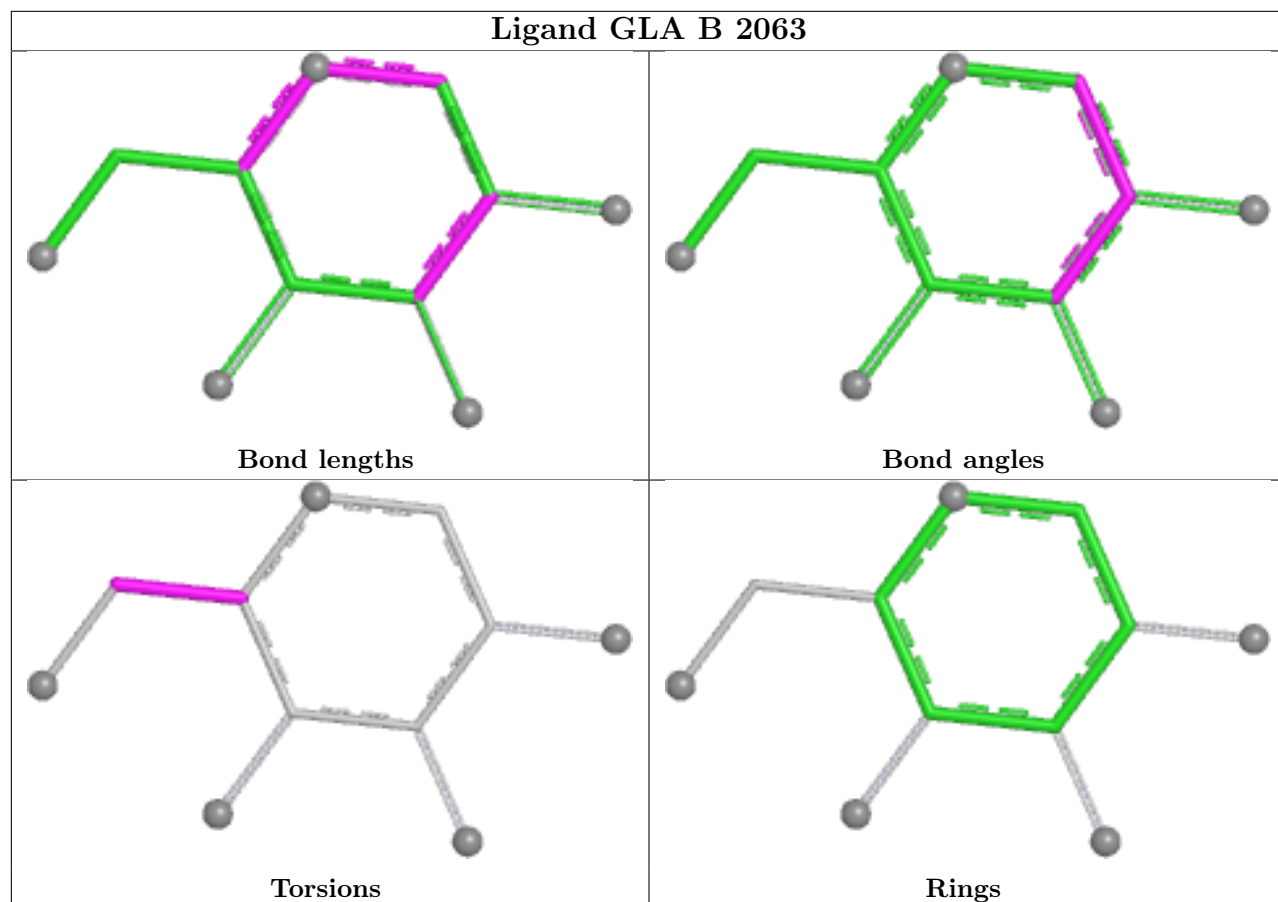
Ligand A1AIO A 2008



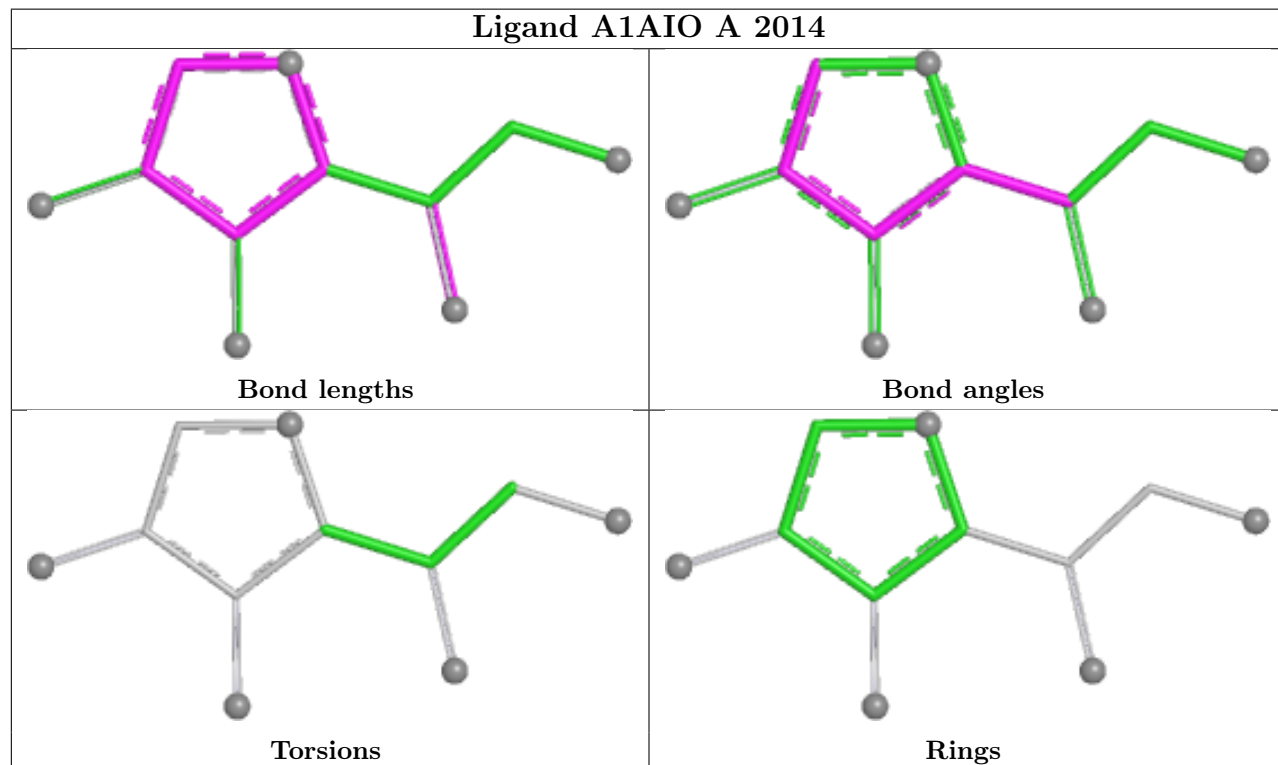
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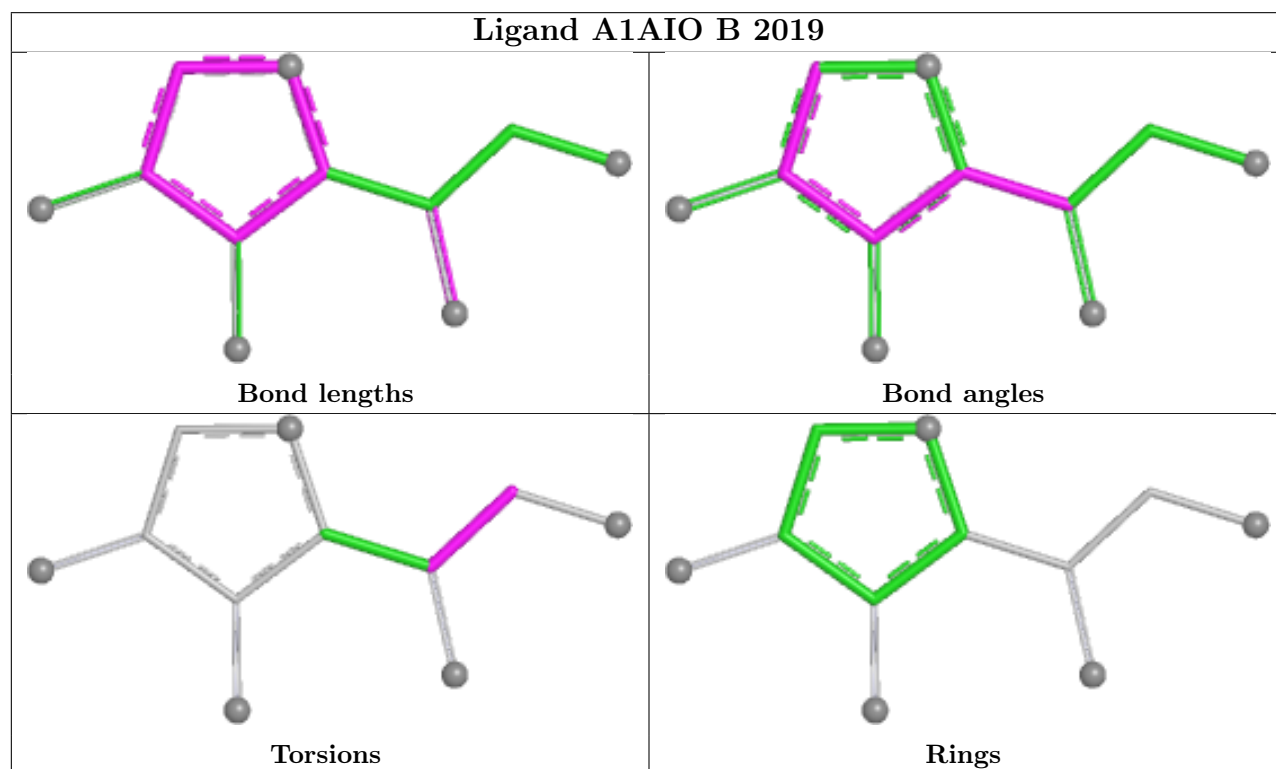
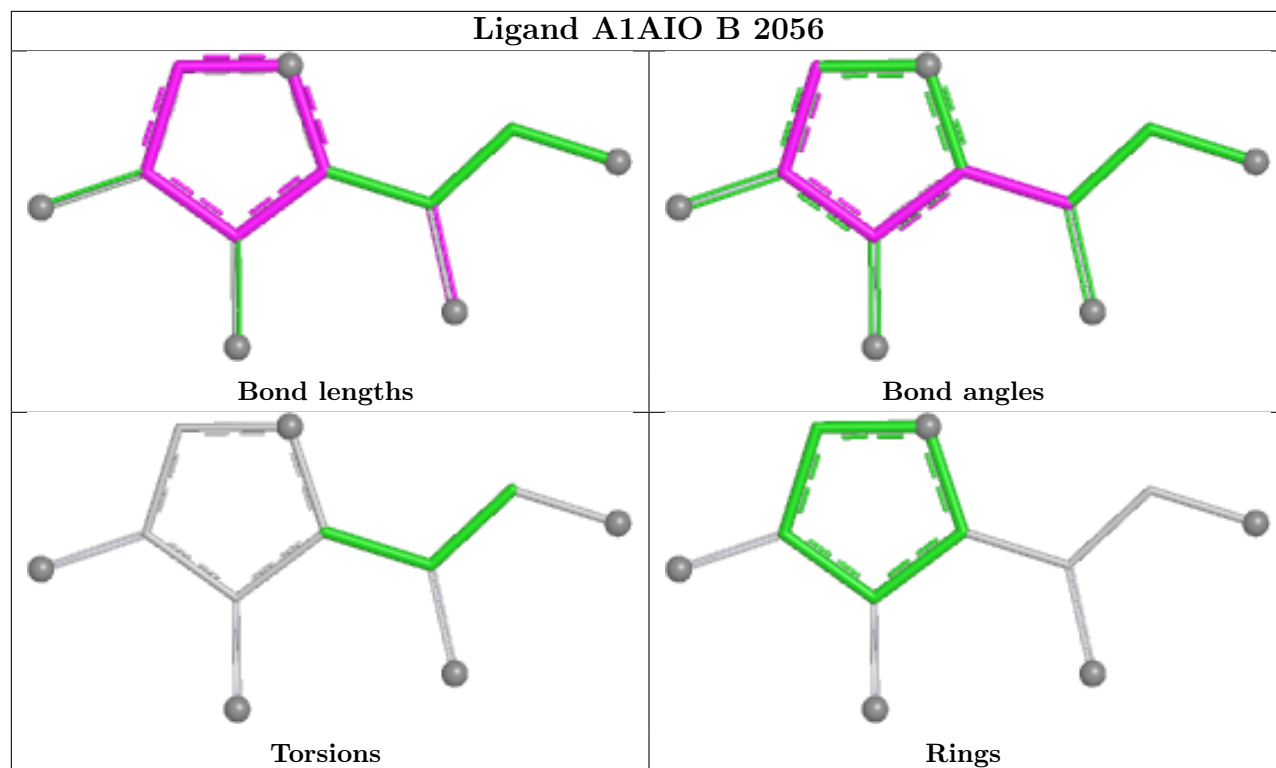


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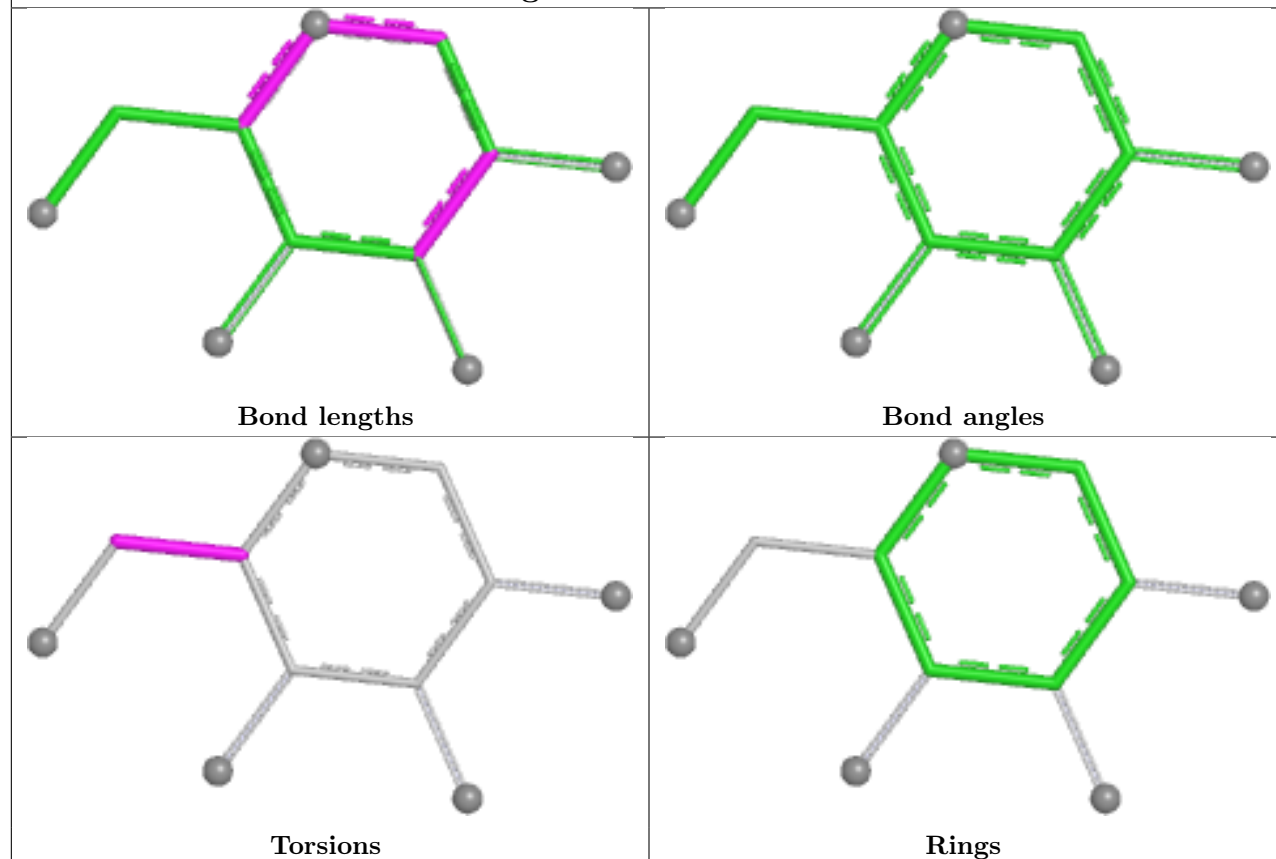


Ligand A1AIO A 2014

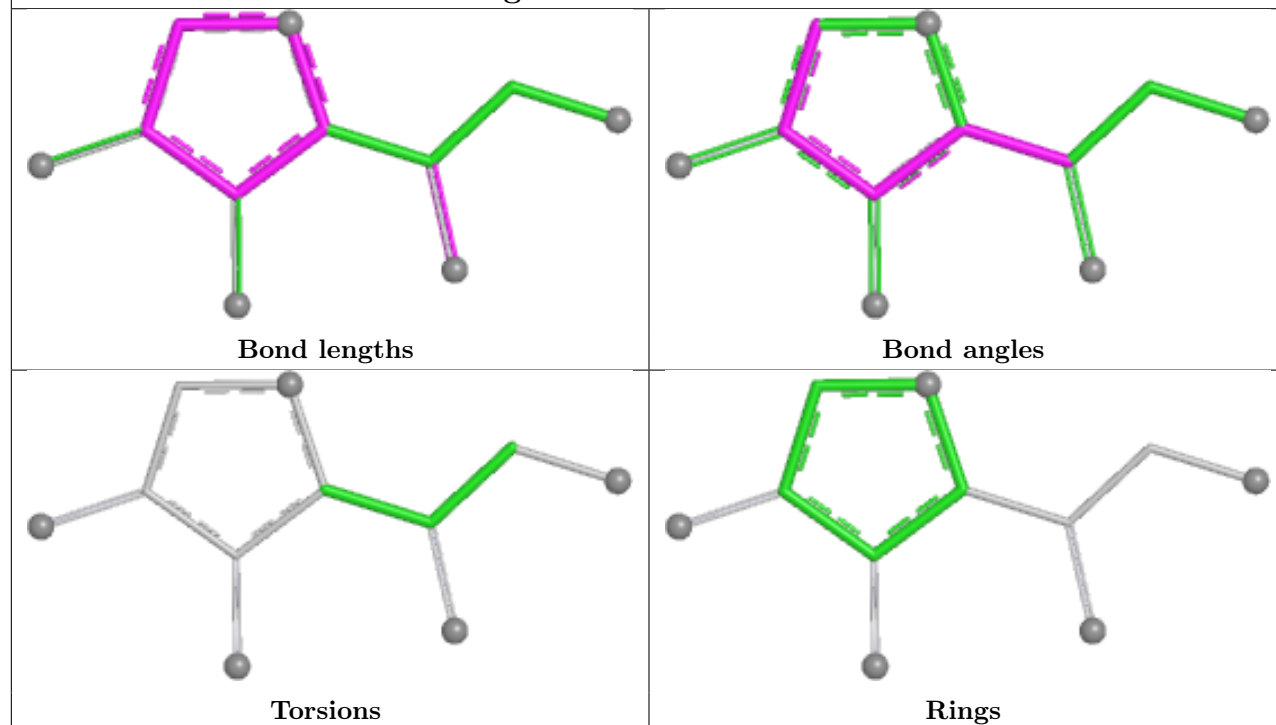




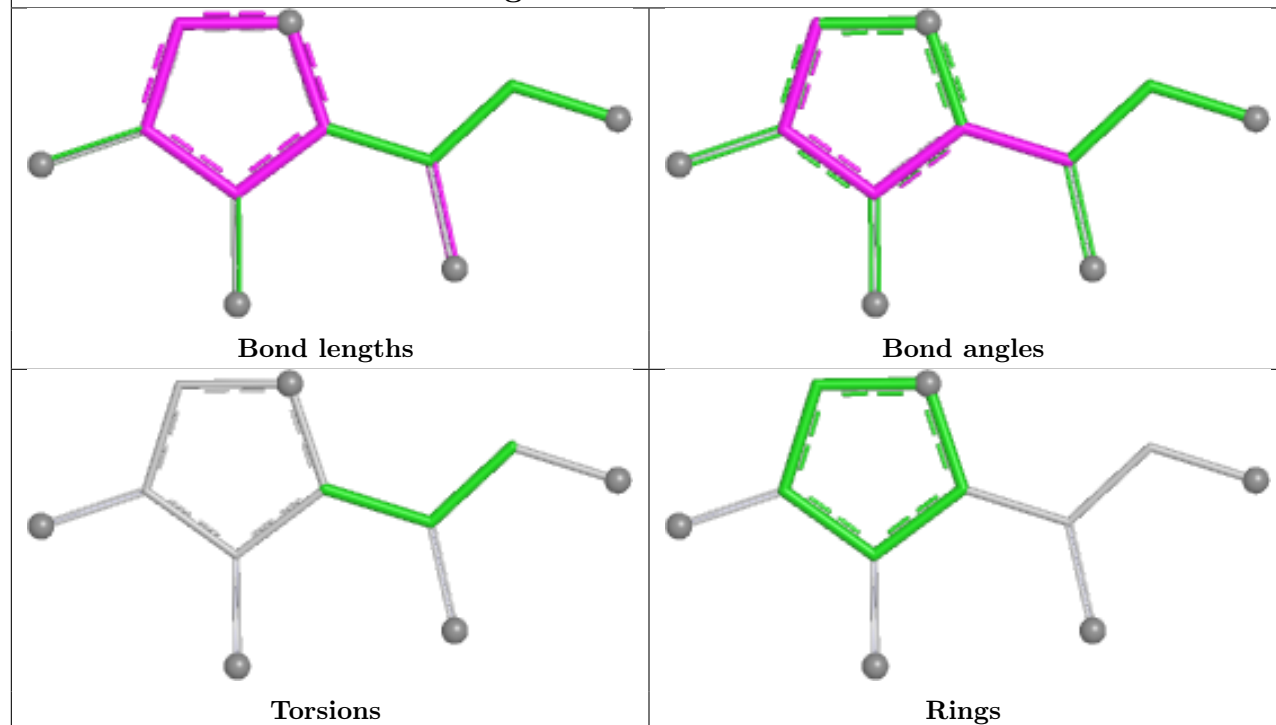
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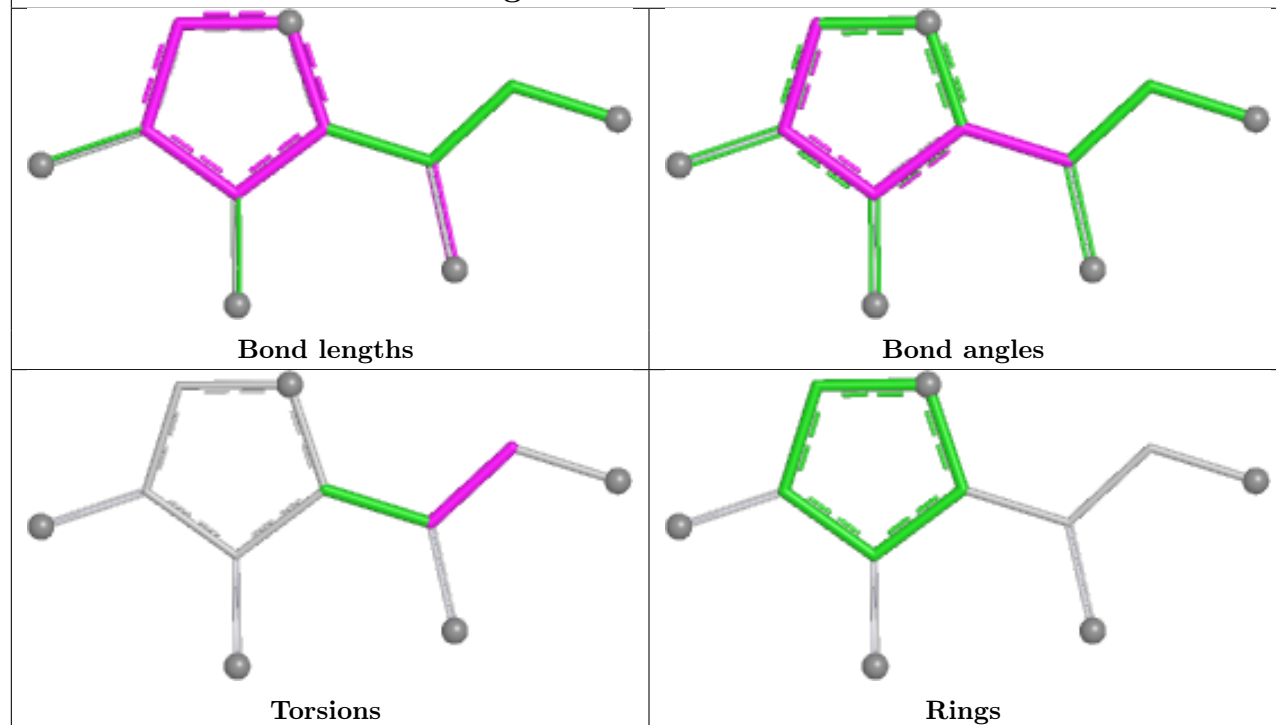
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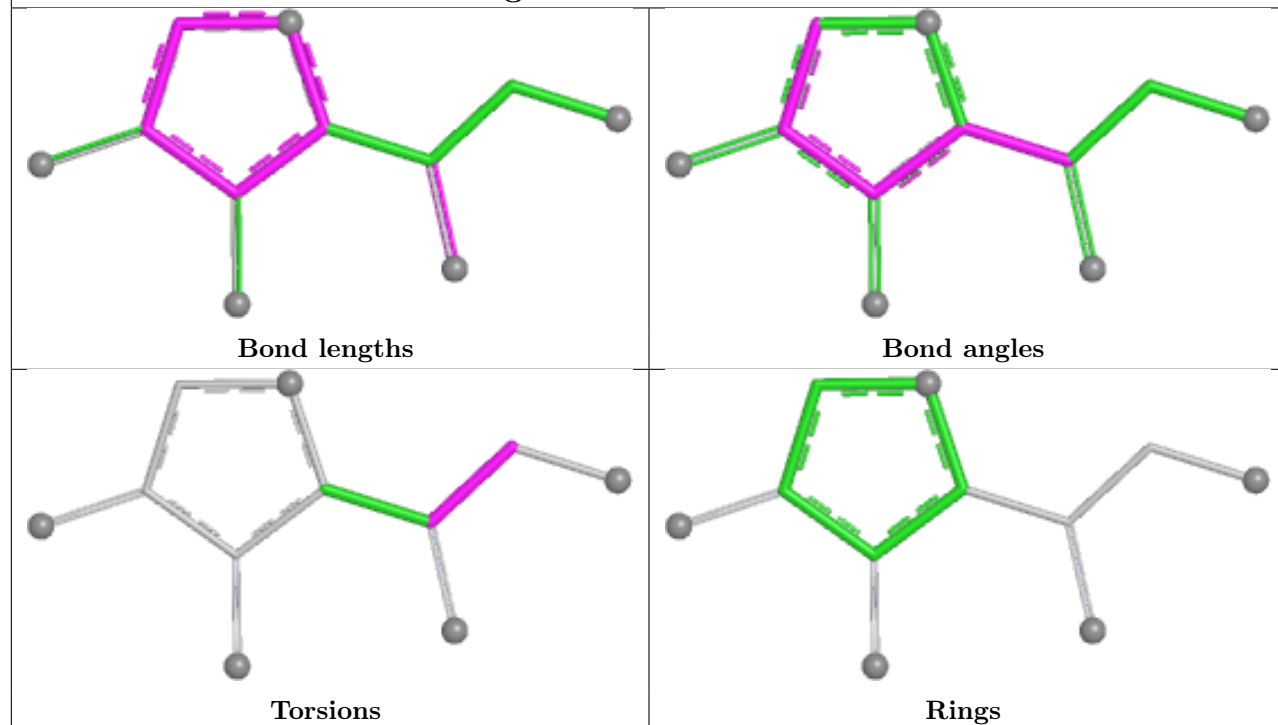
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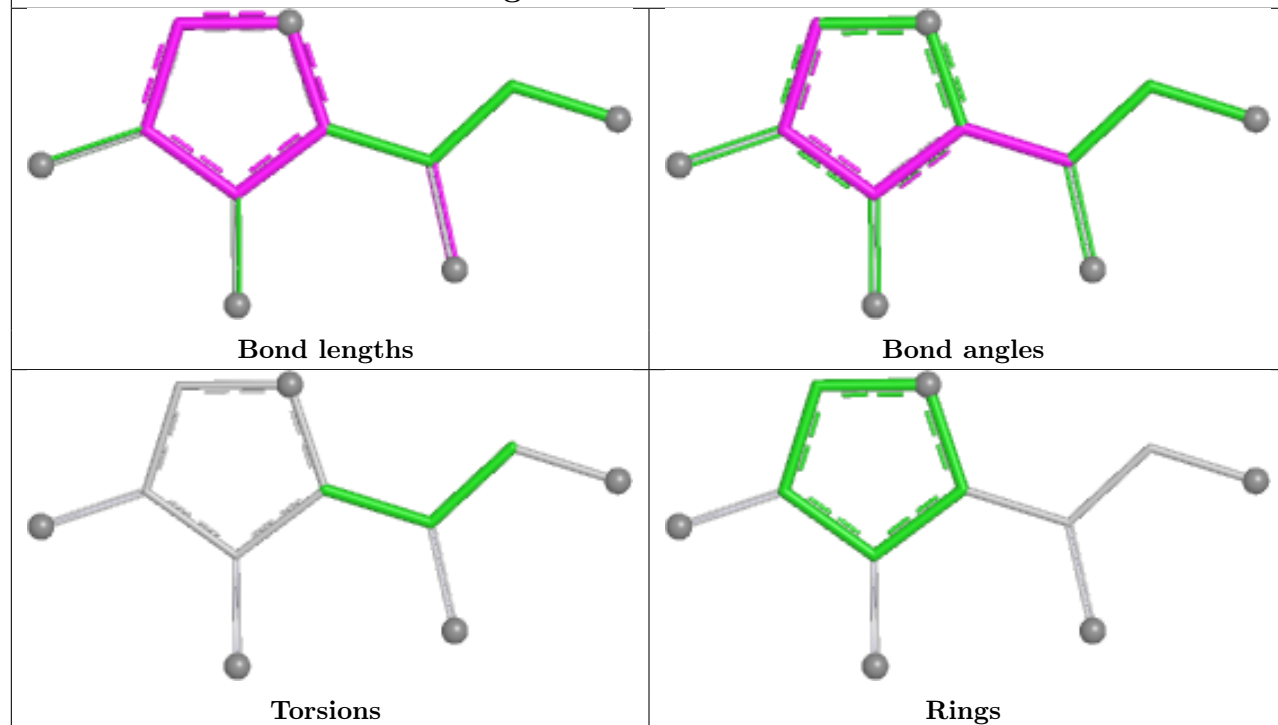
Ligand A1AIO A 2001



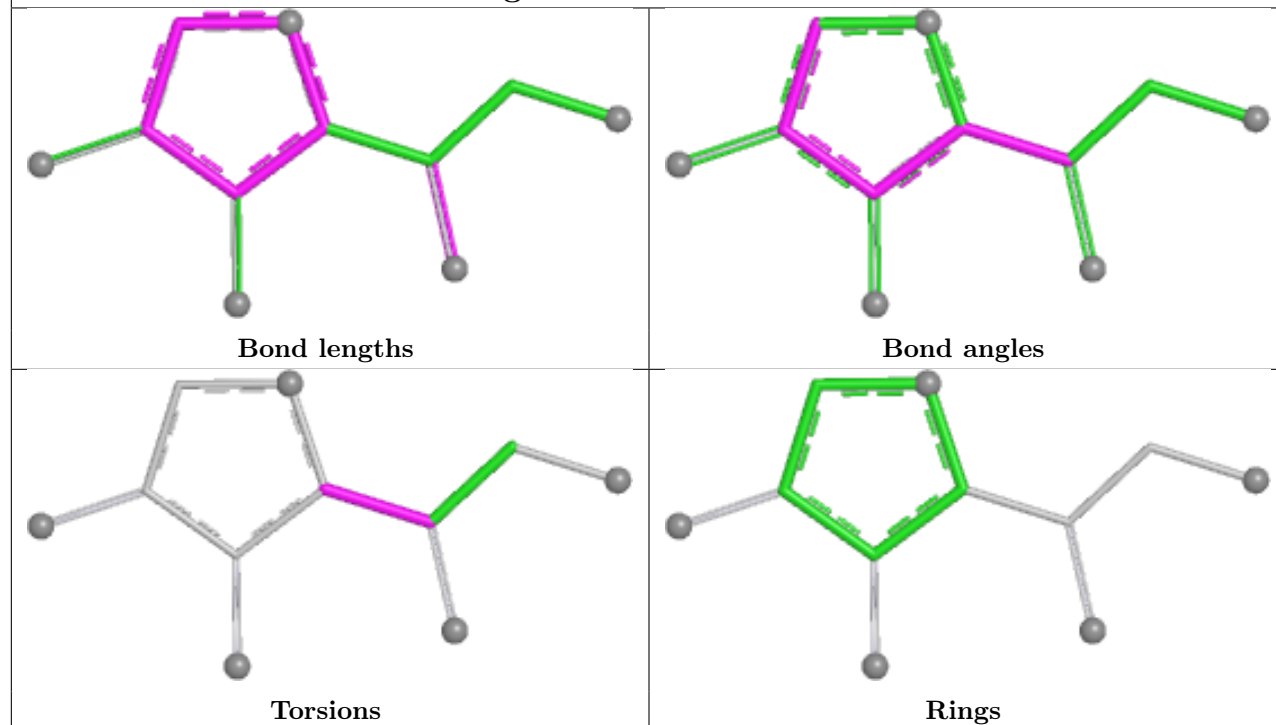
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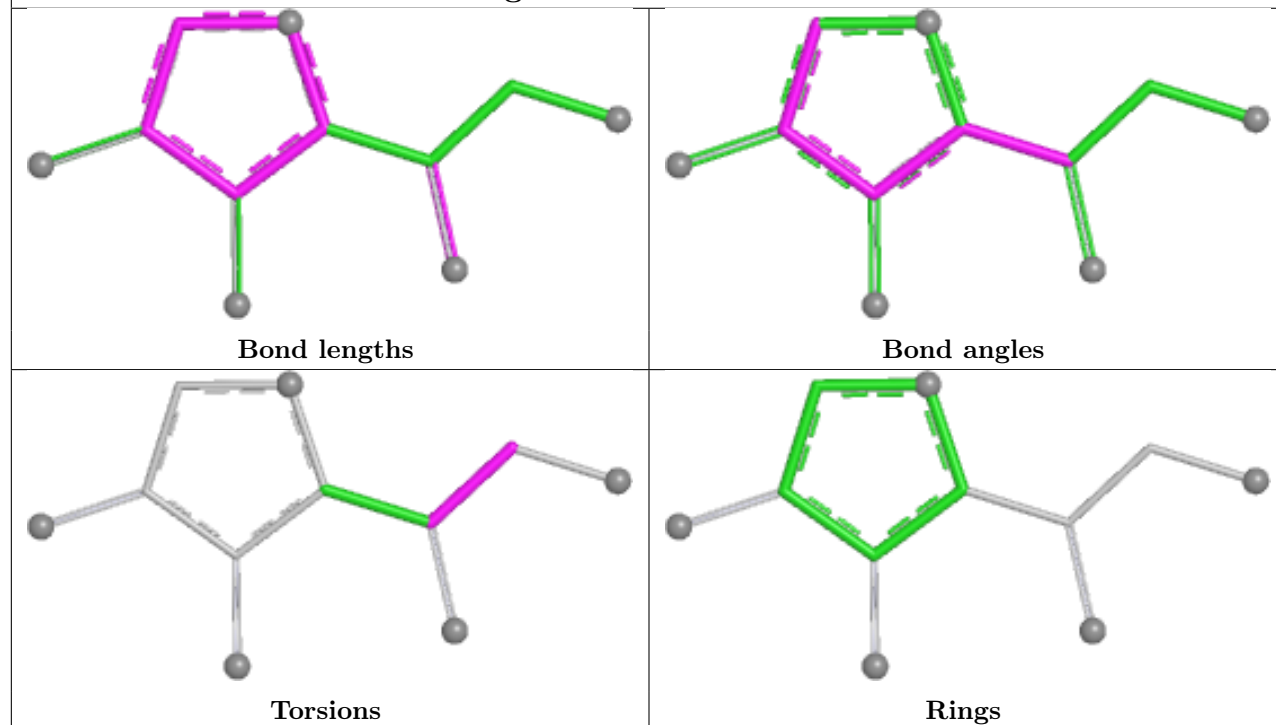
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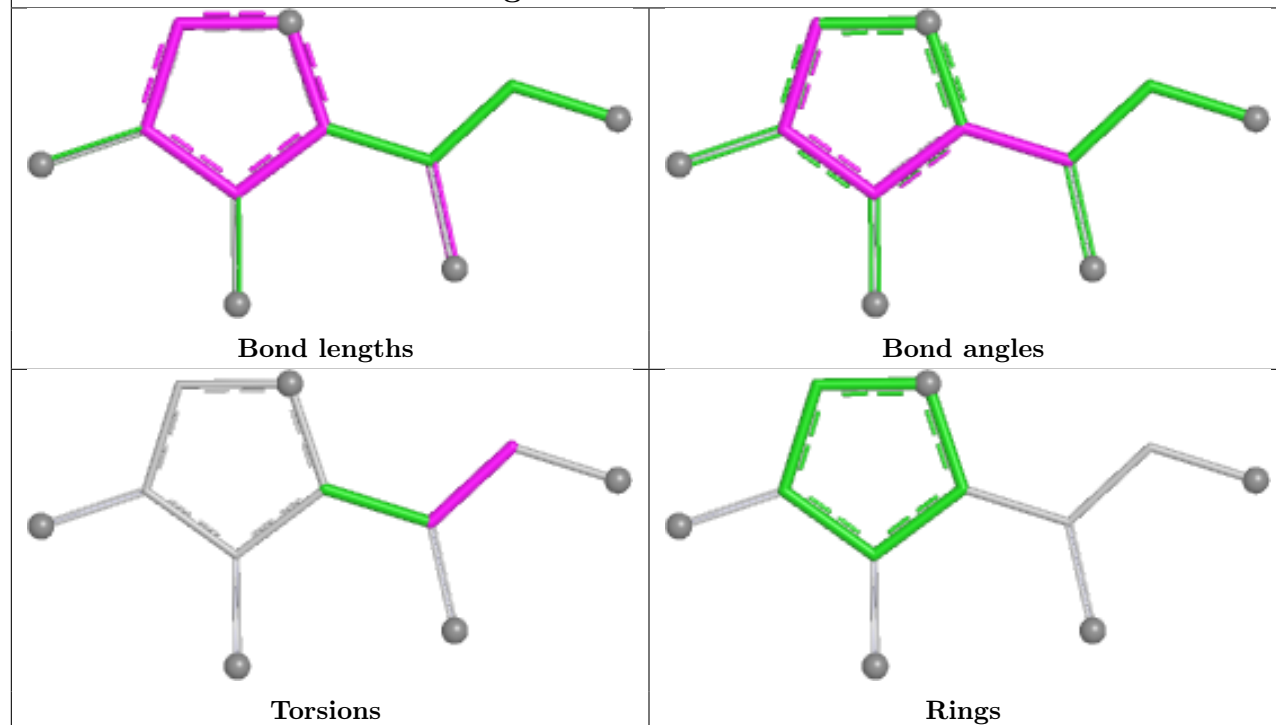
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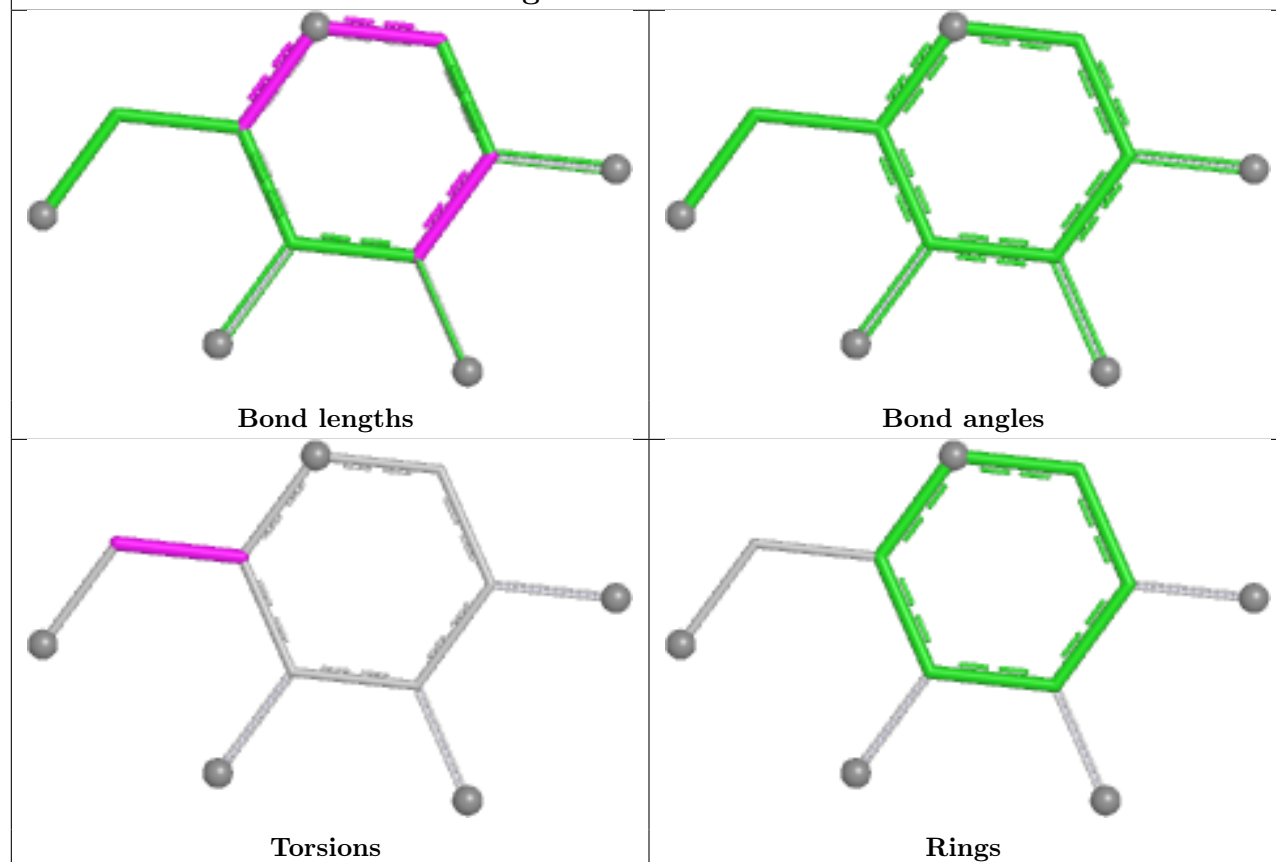
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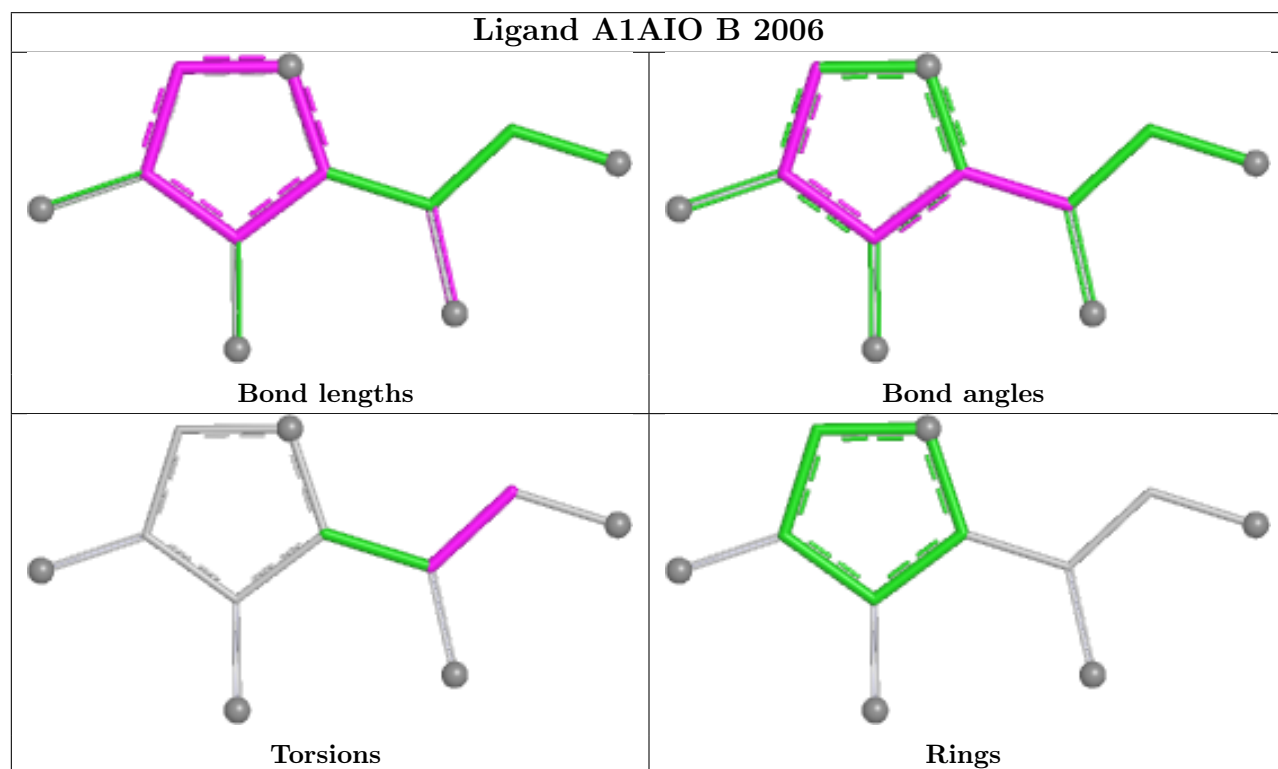
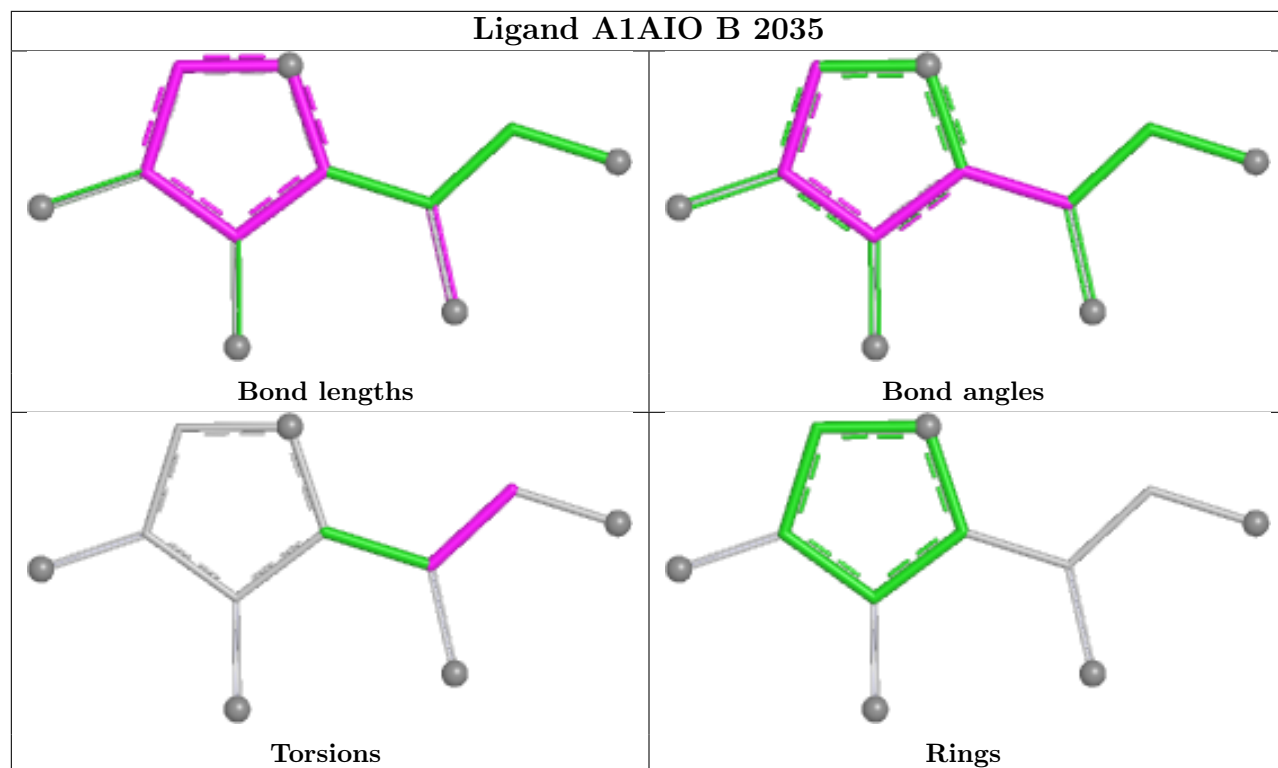


Ligand A1AIO A 2006

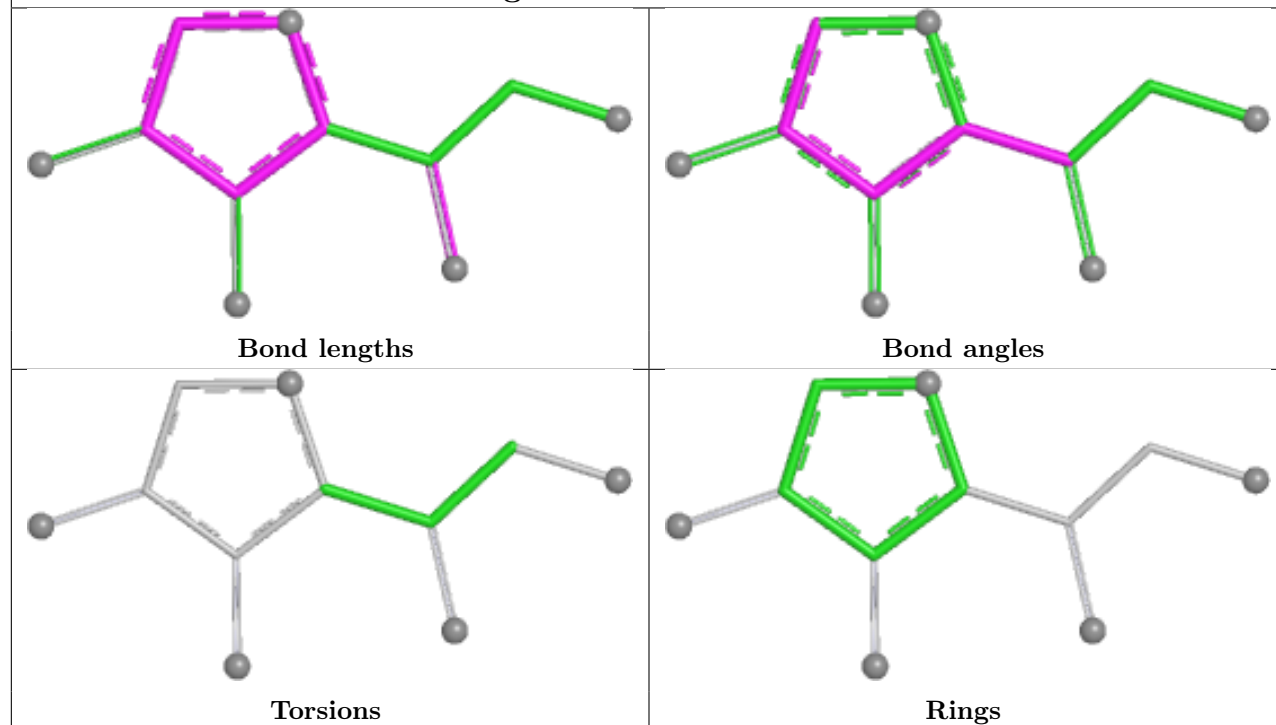


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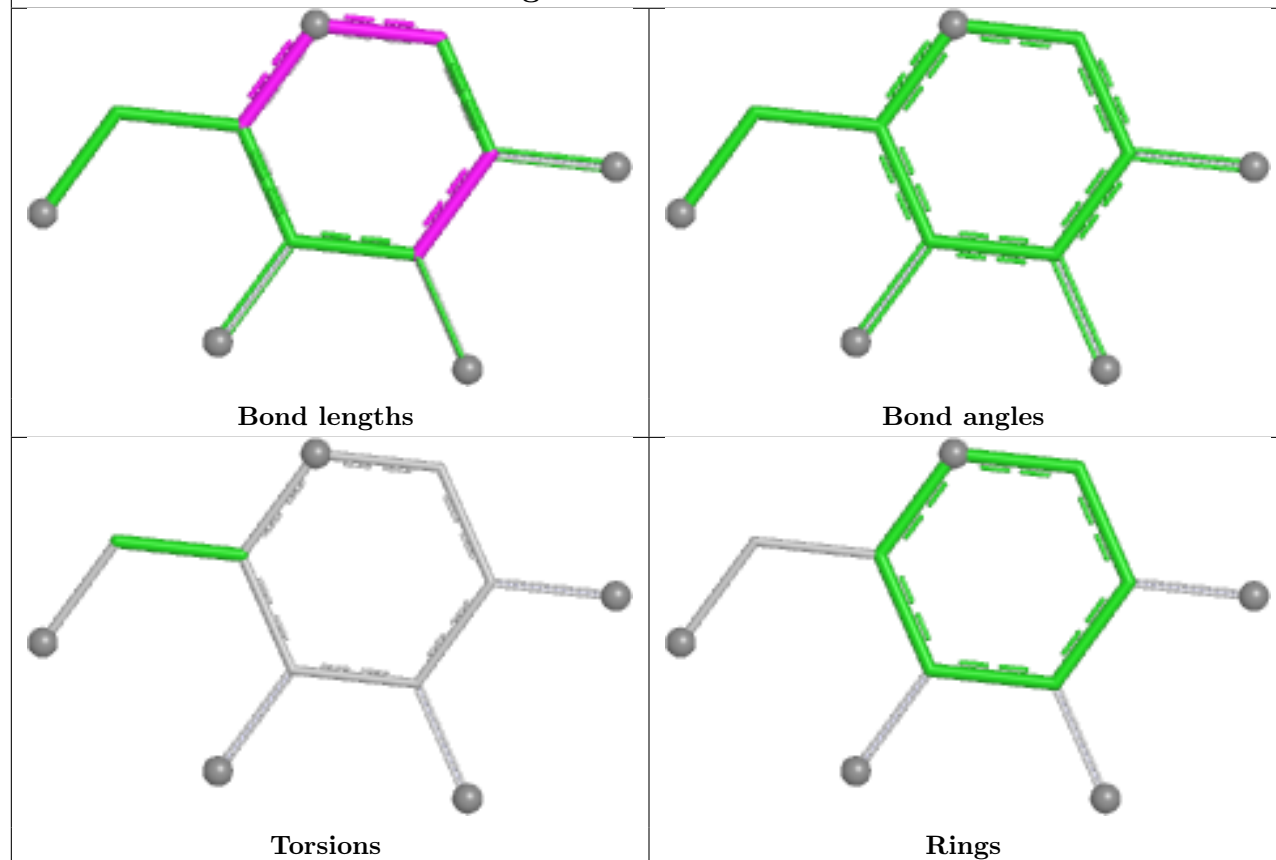




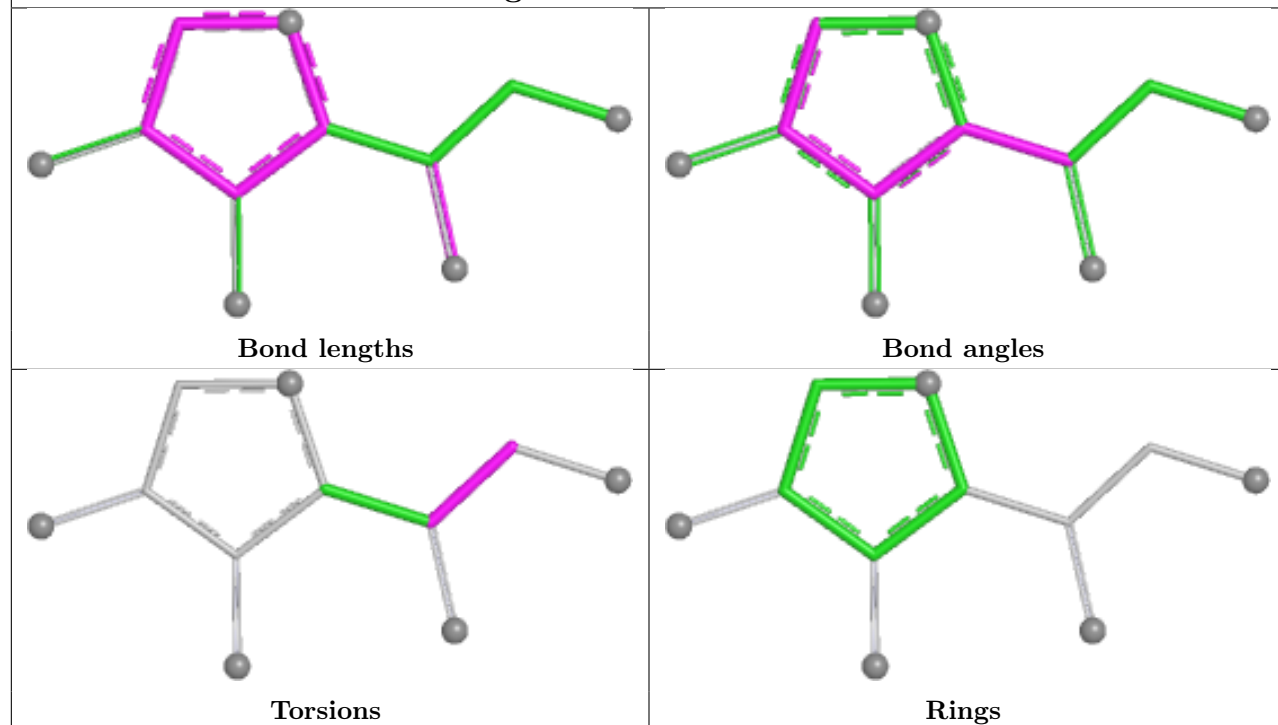
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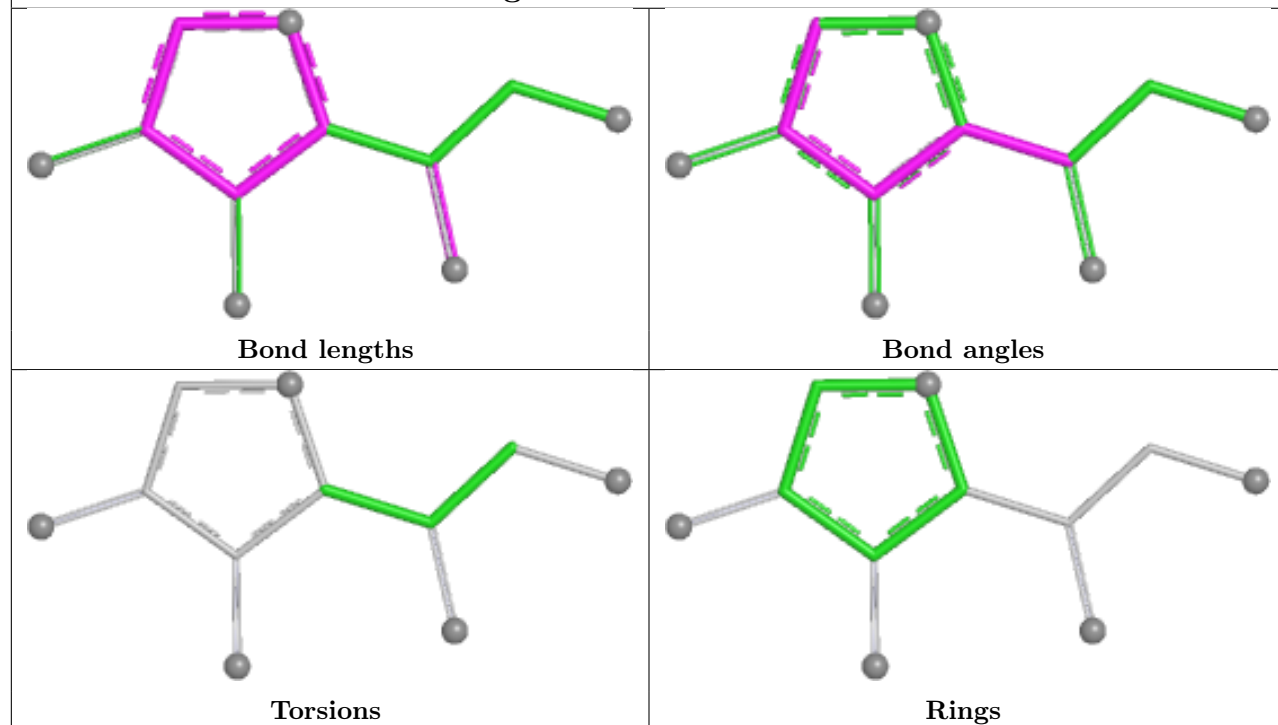
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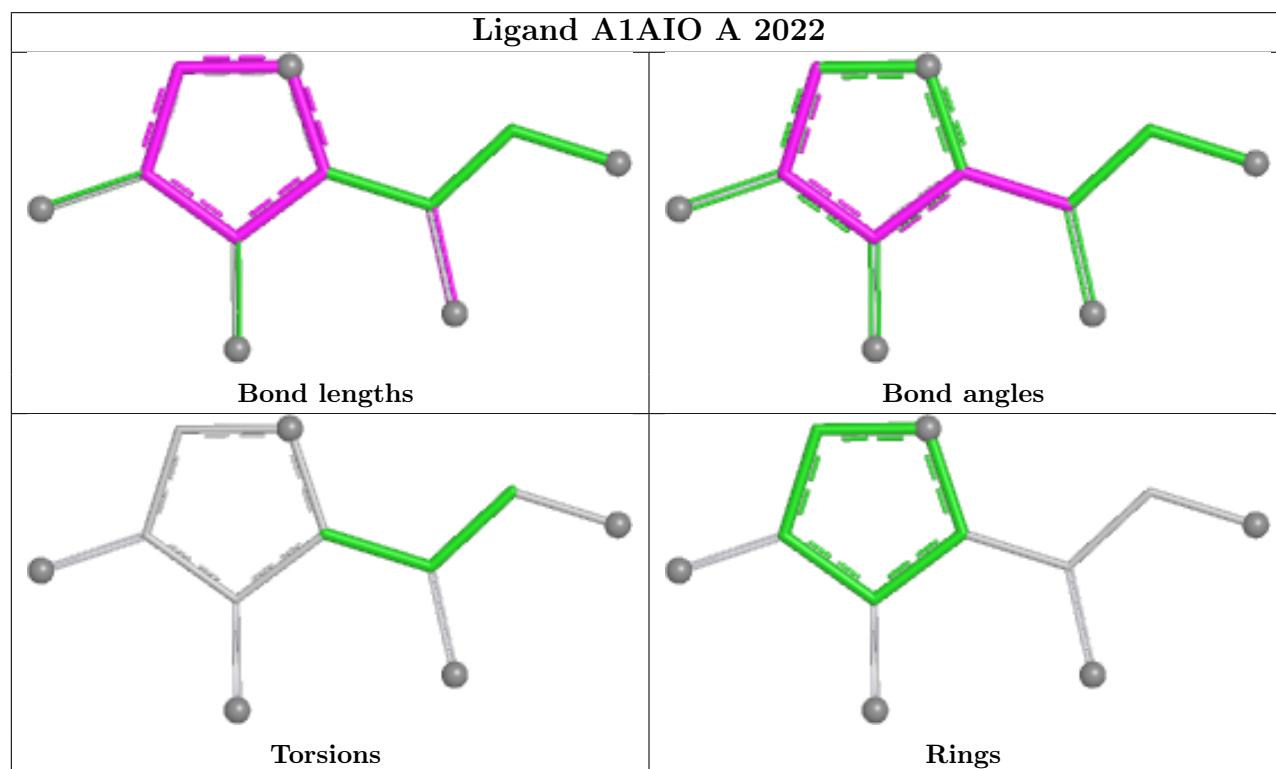
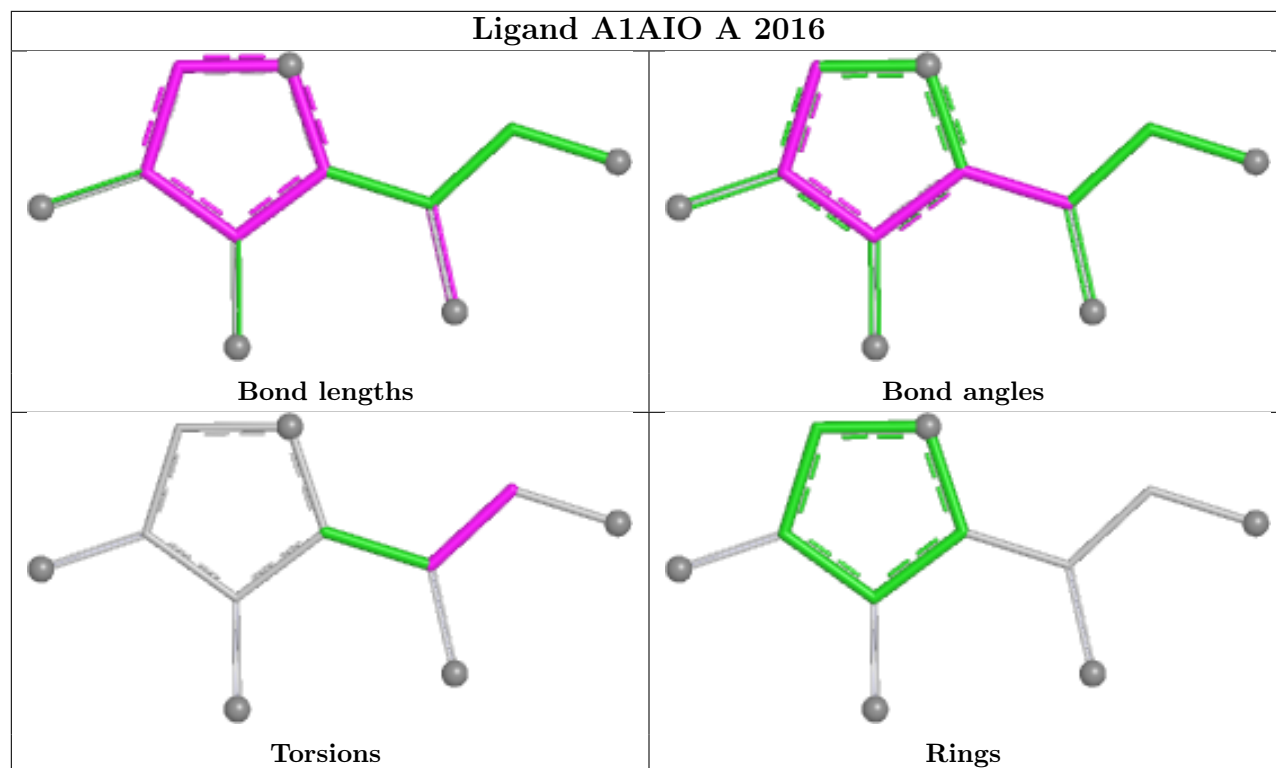


Ligand A1AIO B 2007

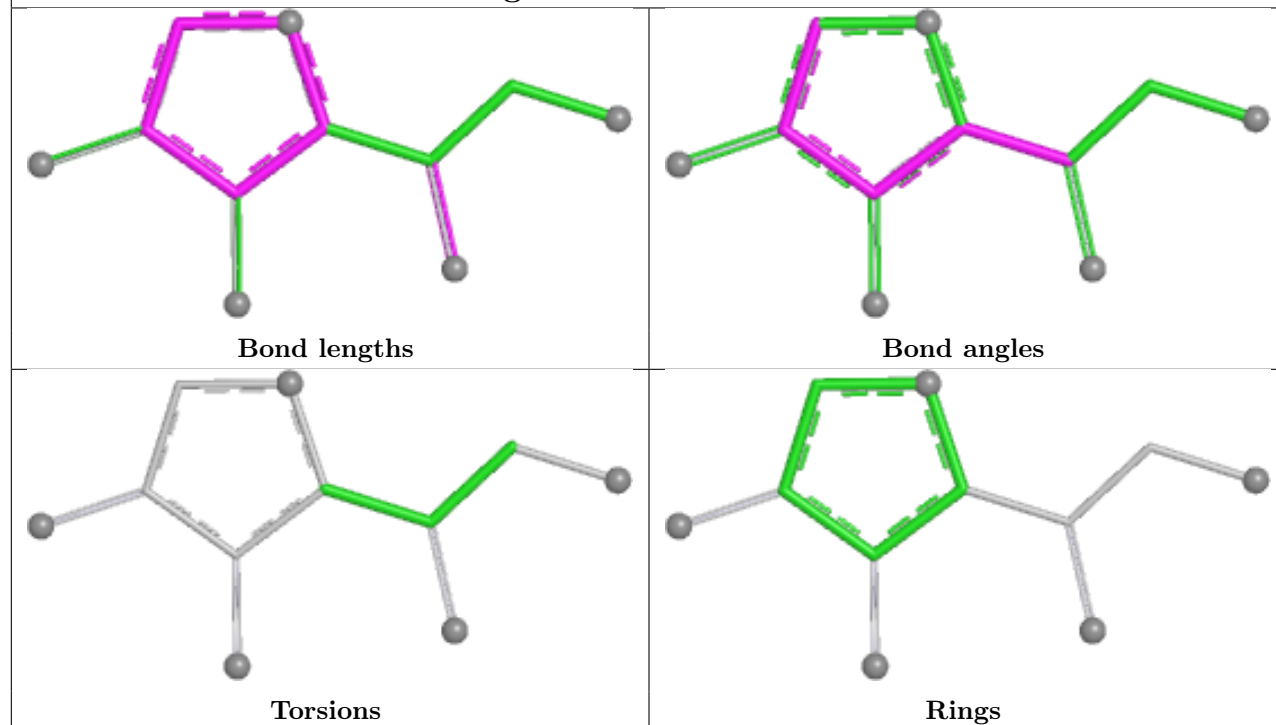


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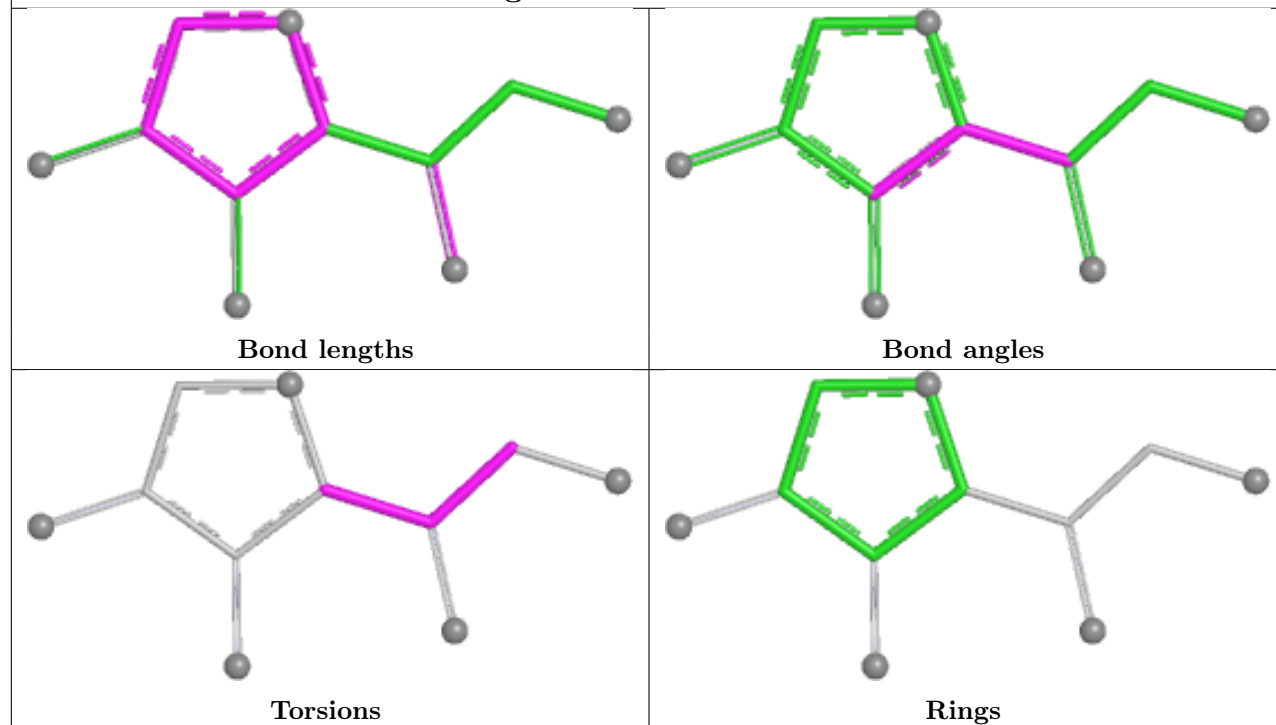


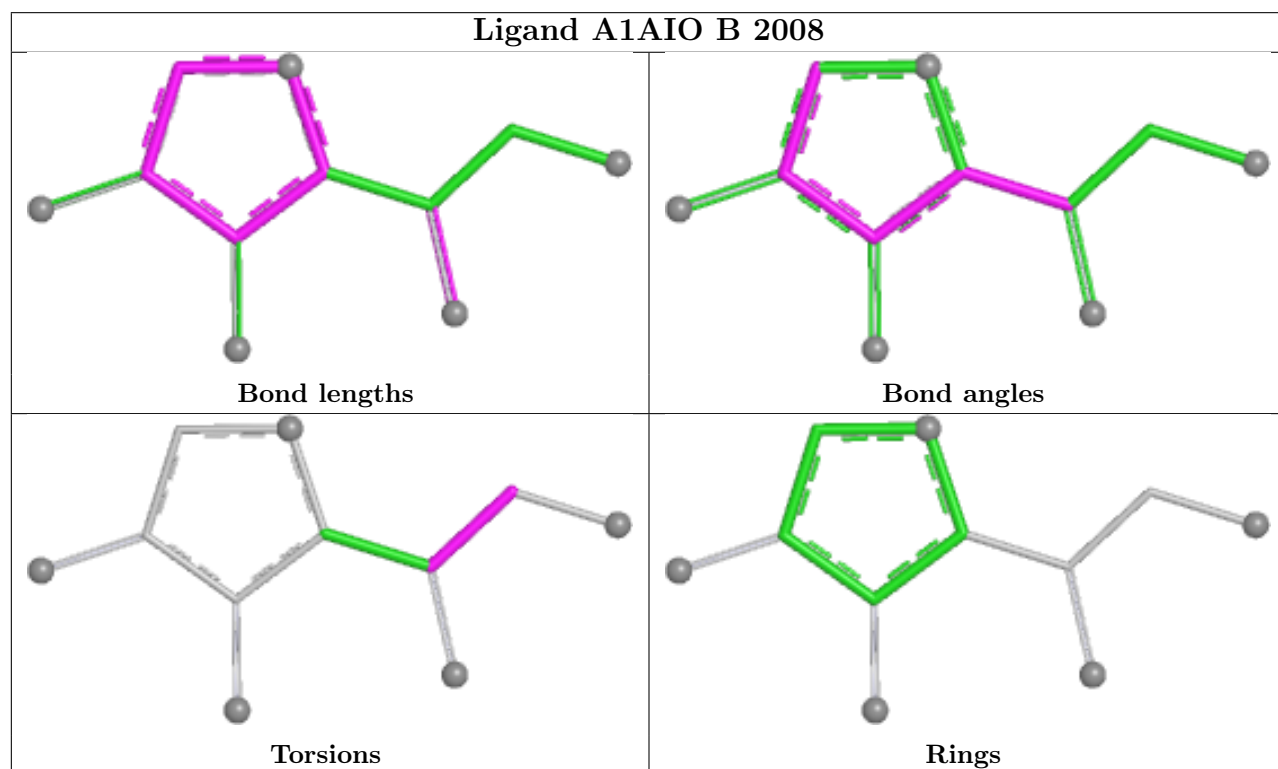
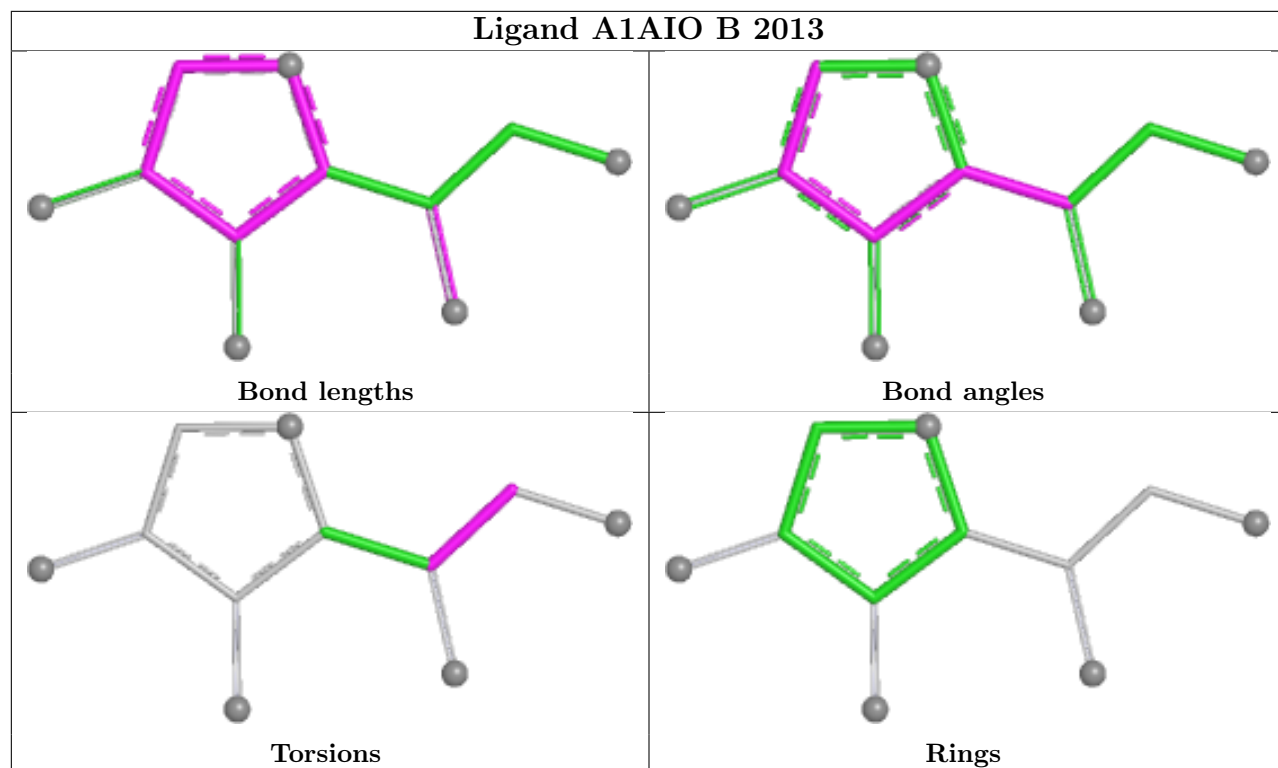


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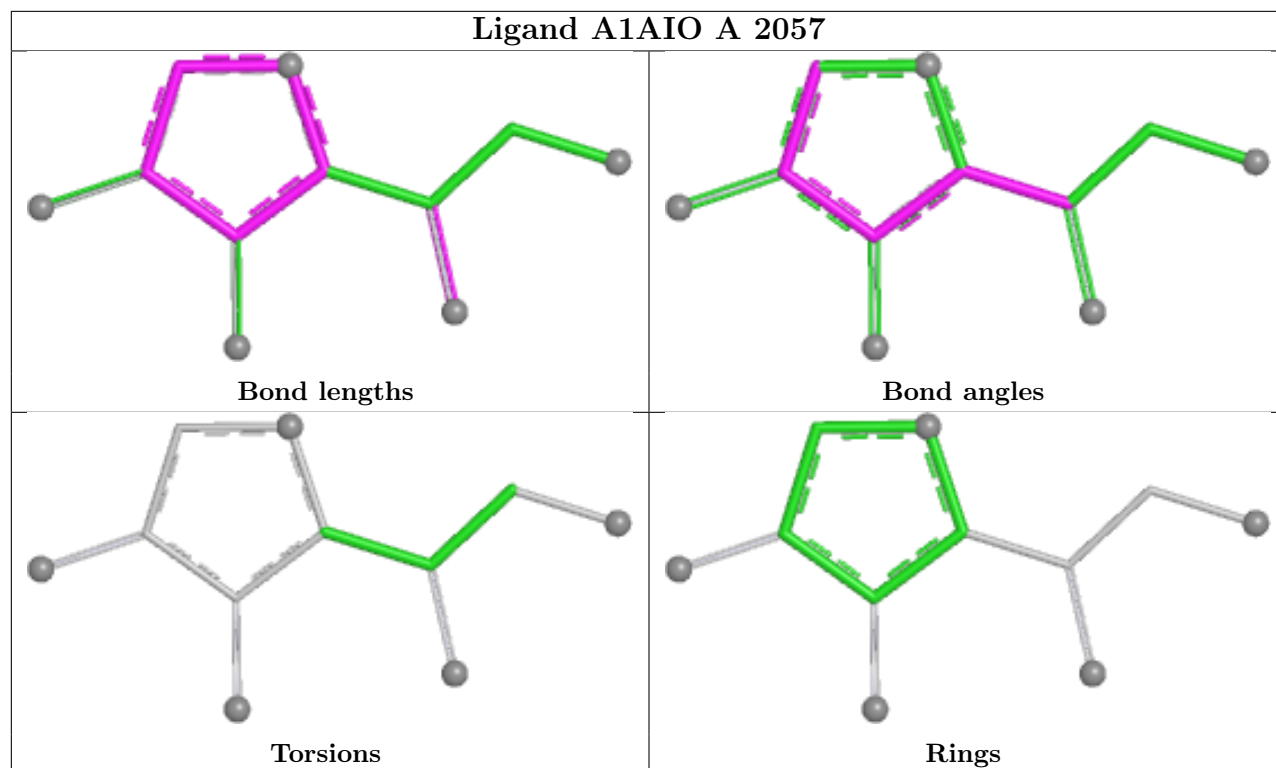


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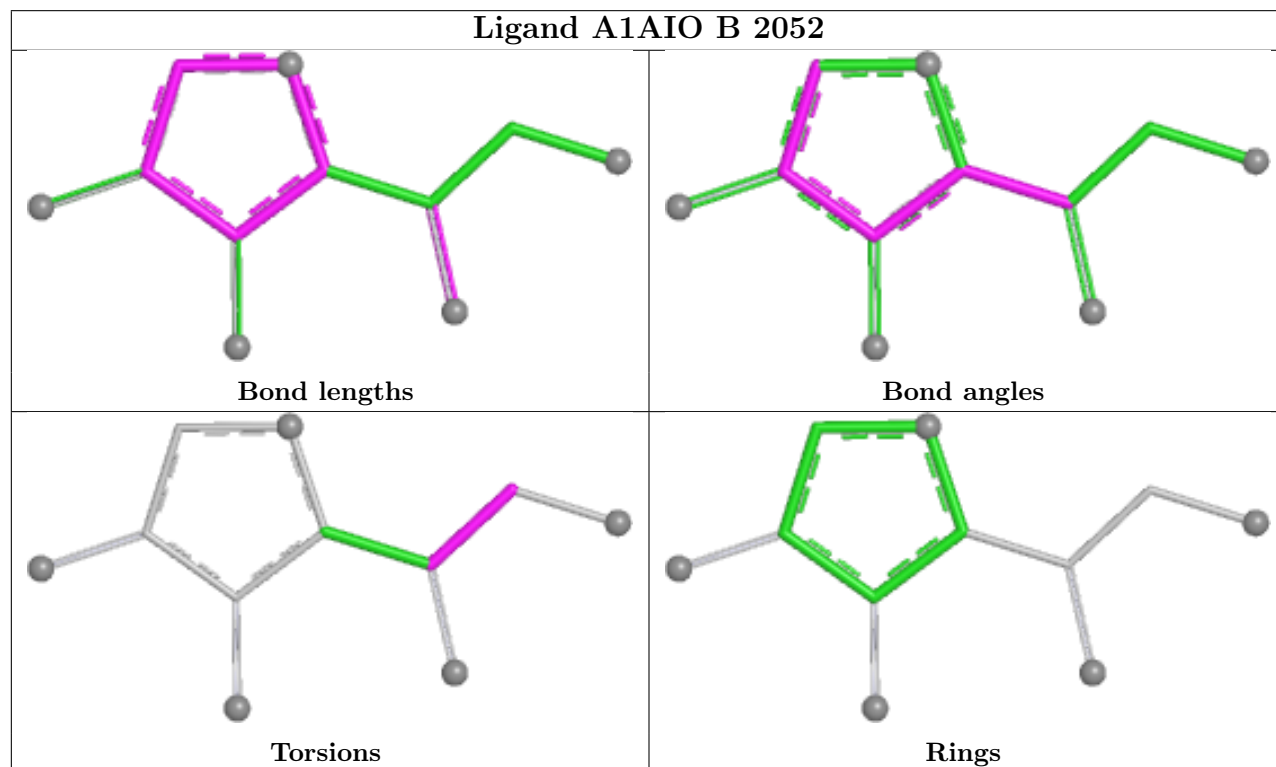


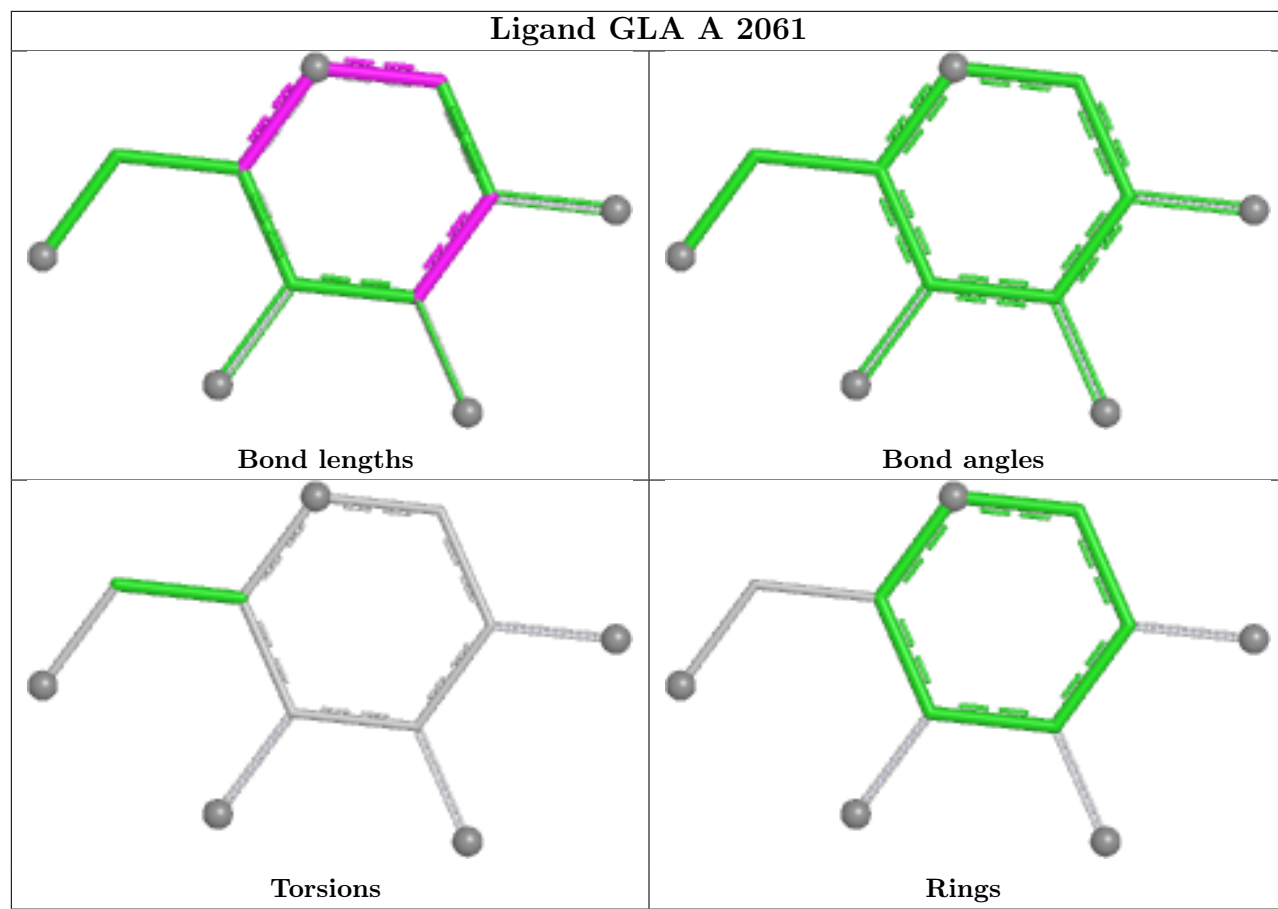


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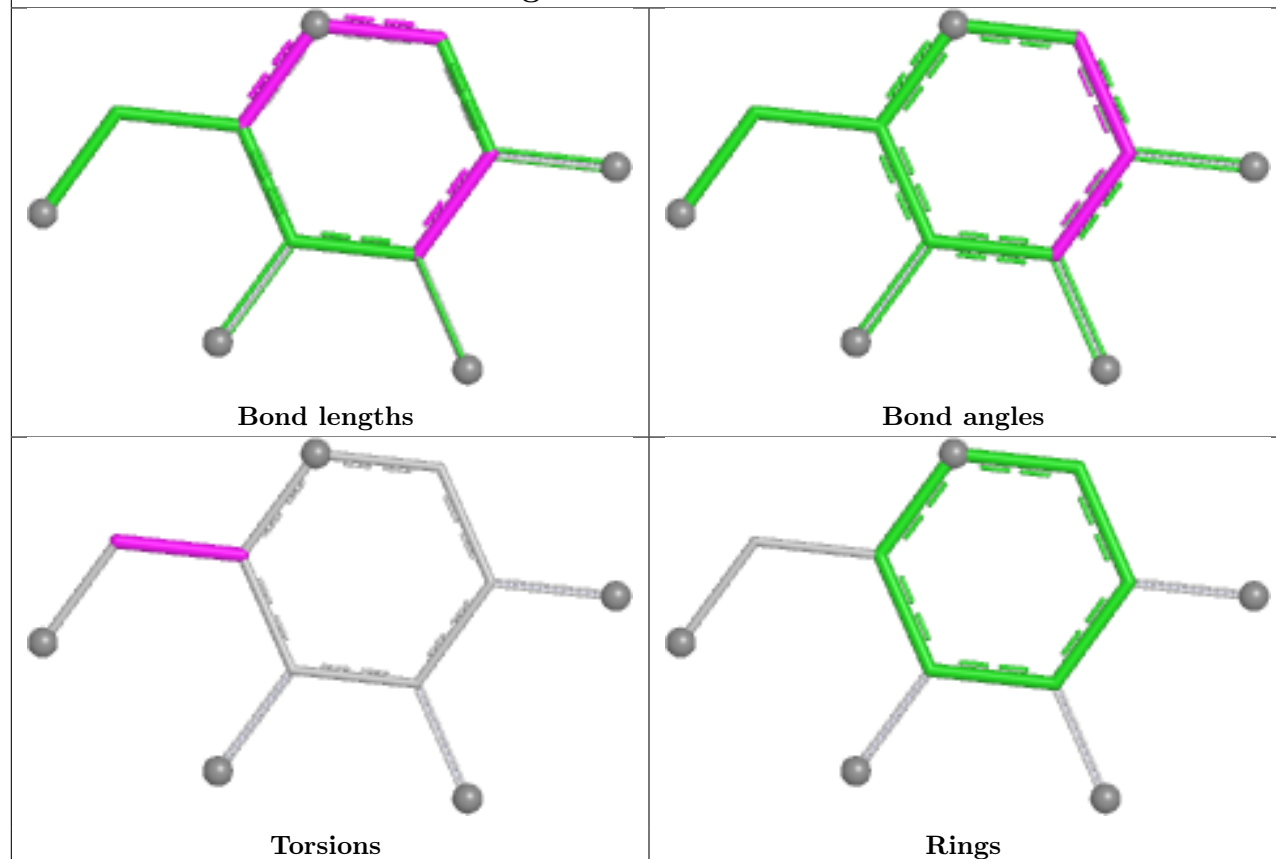


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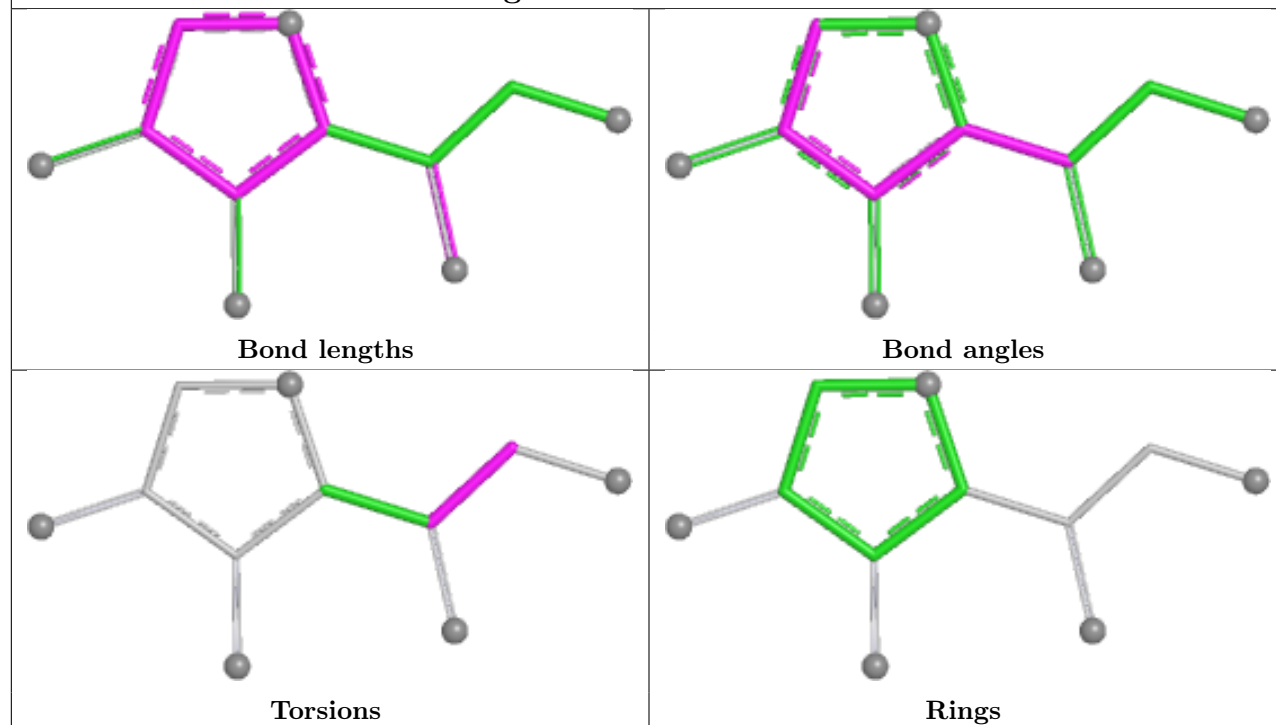




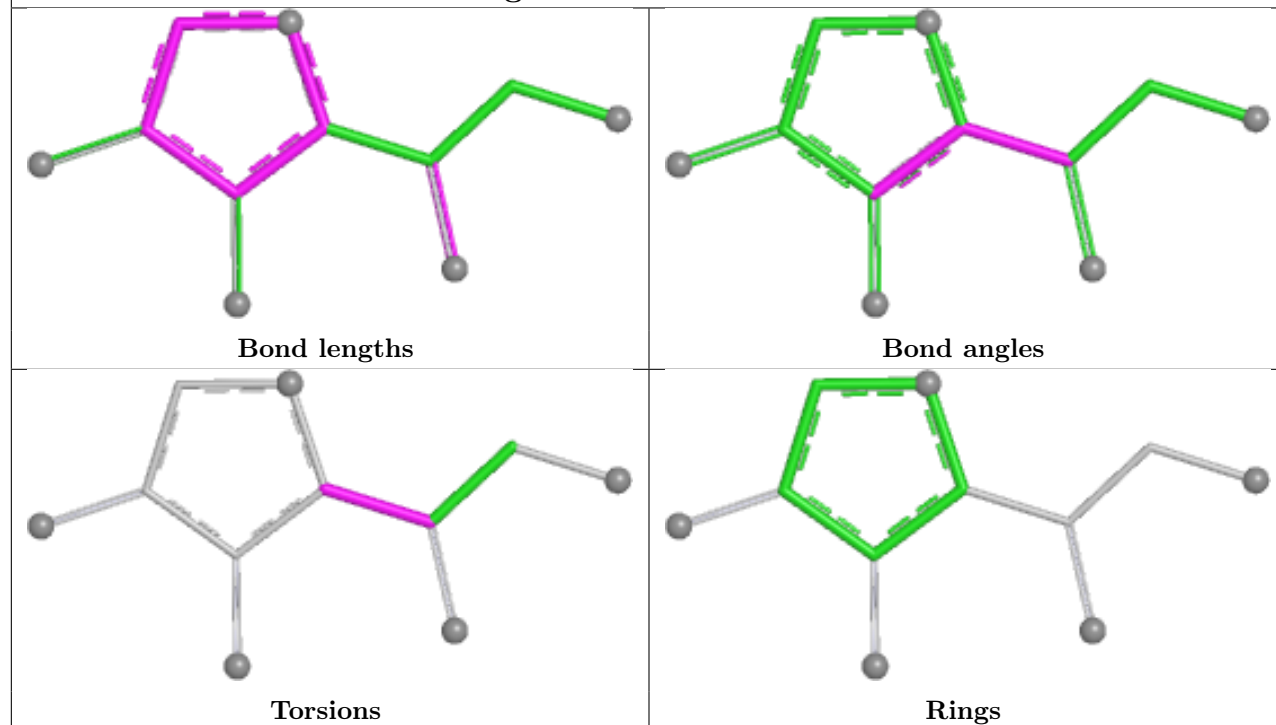
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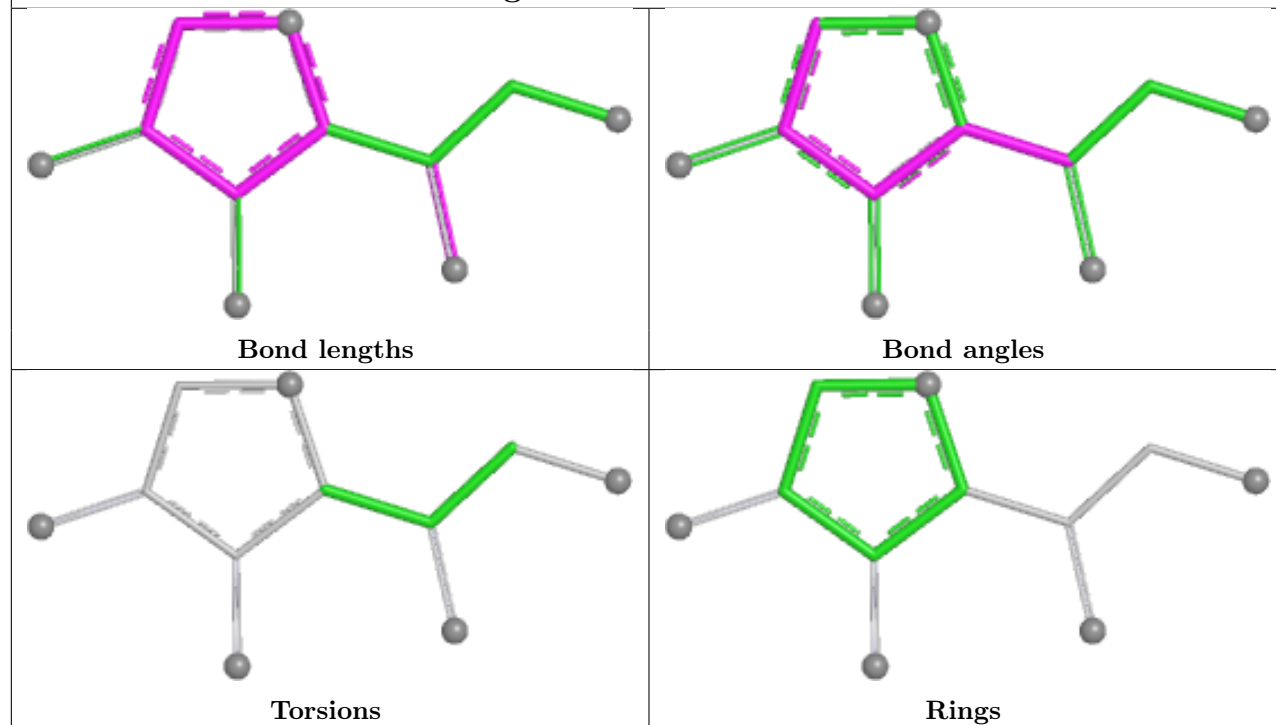
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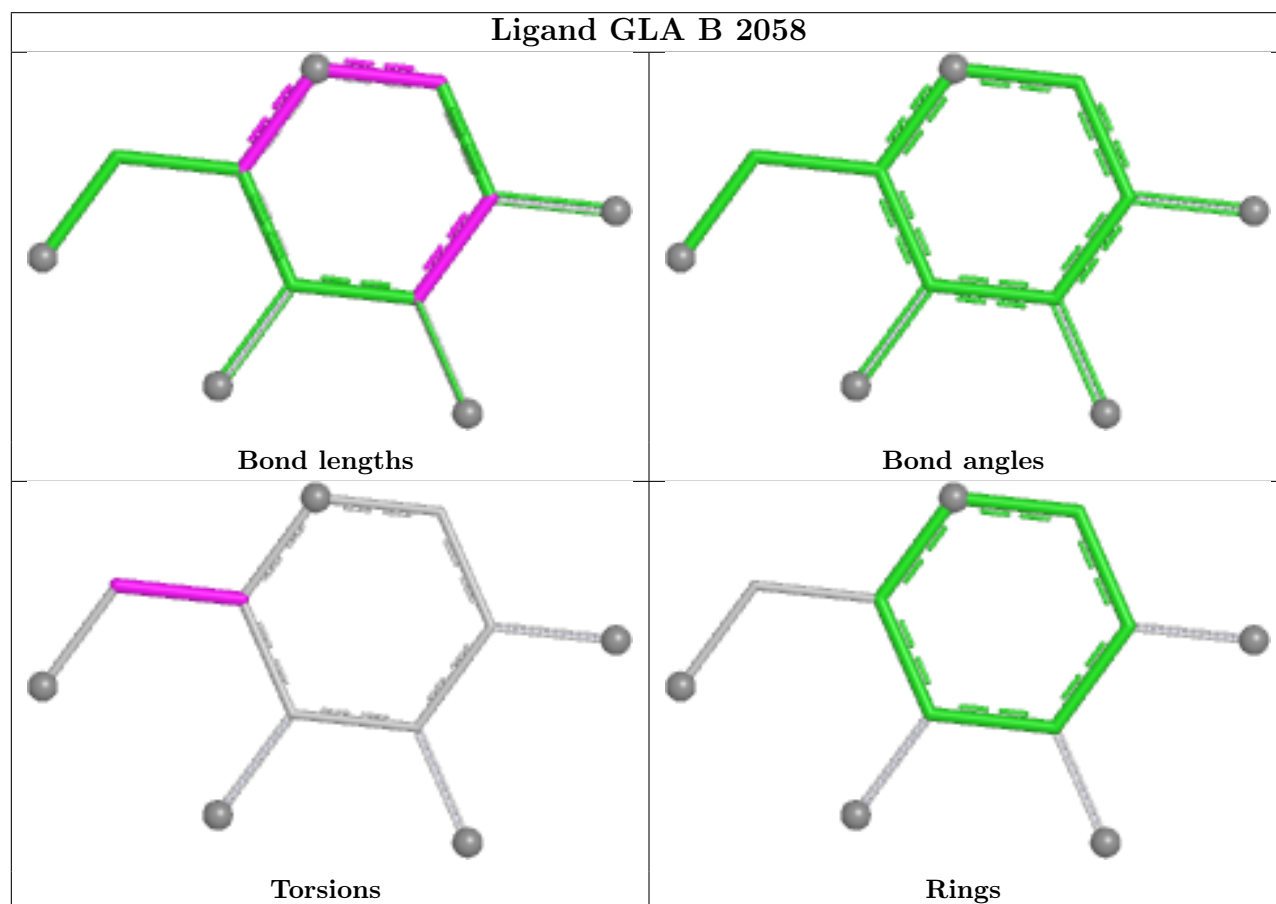
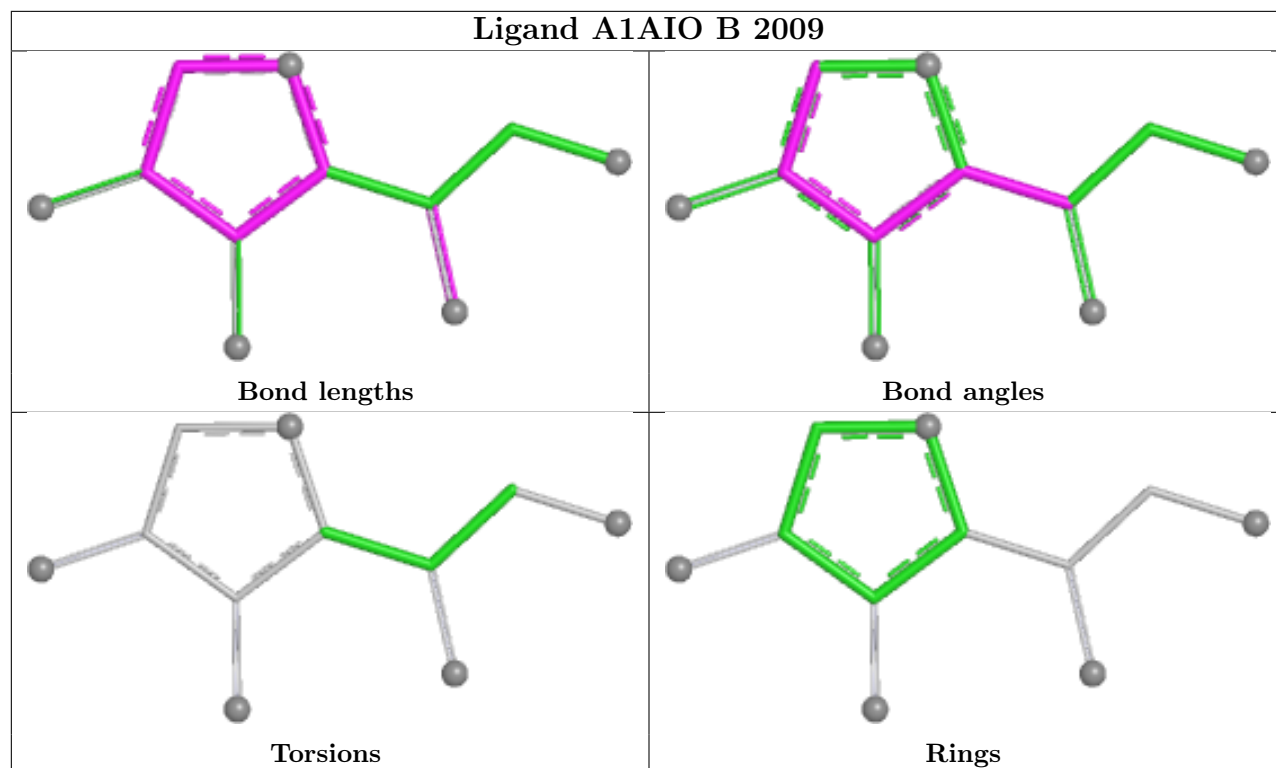


Ligand A1AIO B 2039

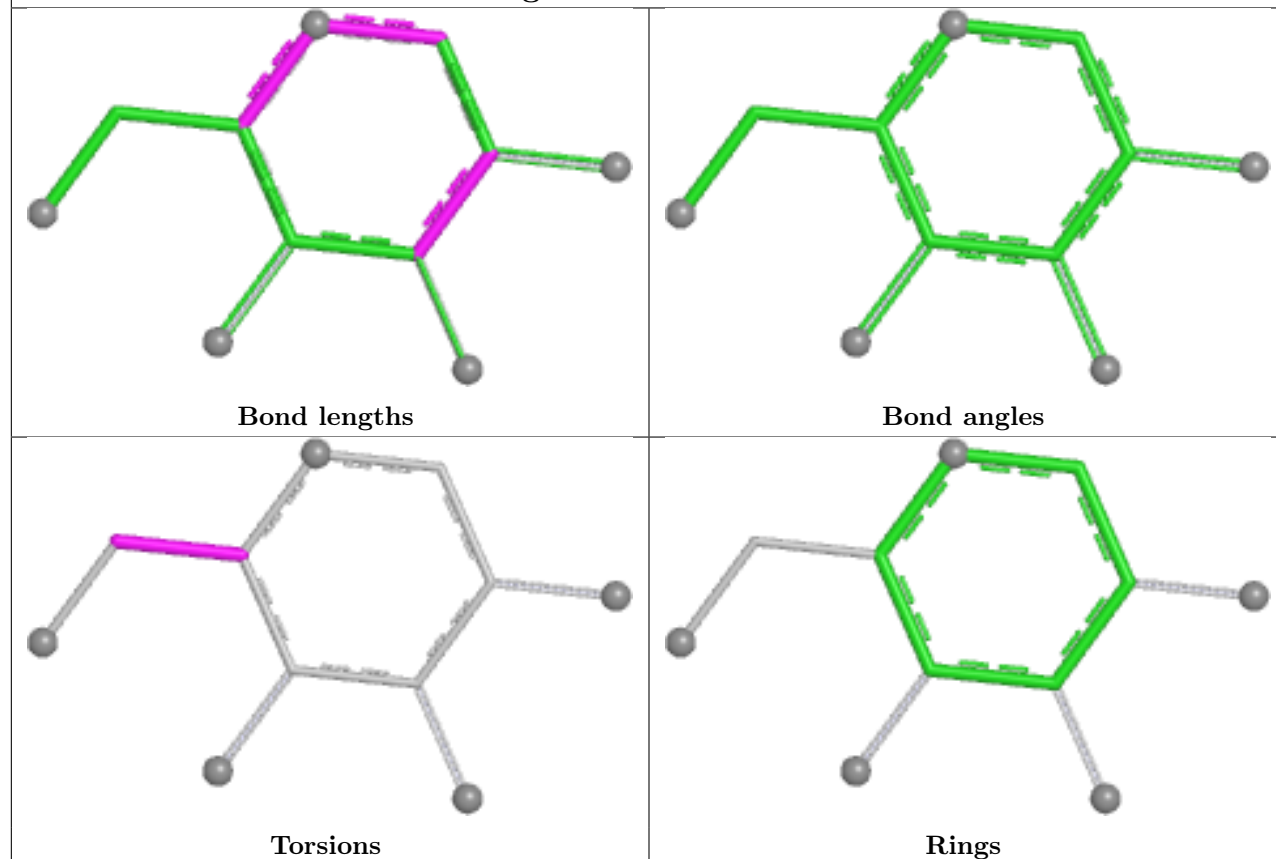


Ligand A1AIO A 2003

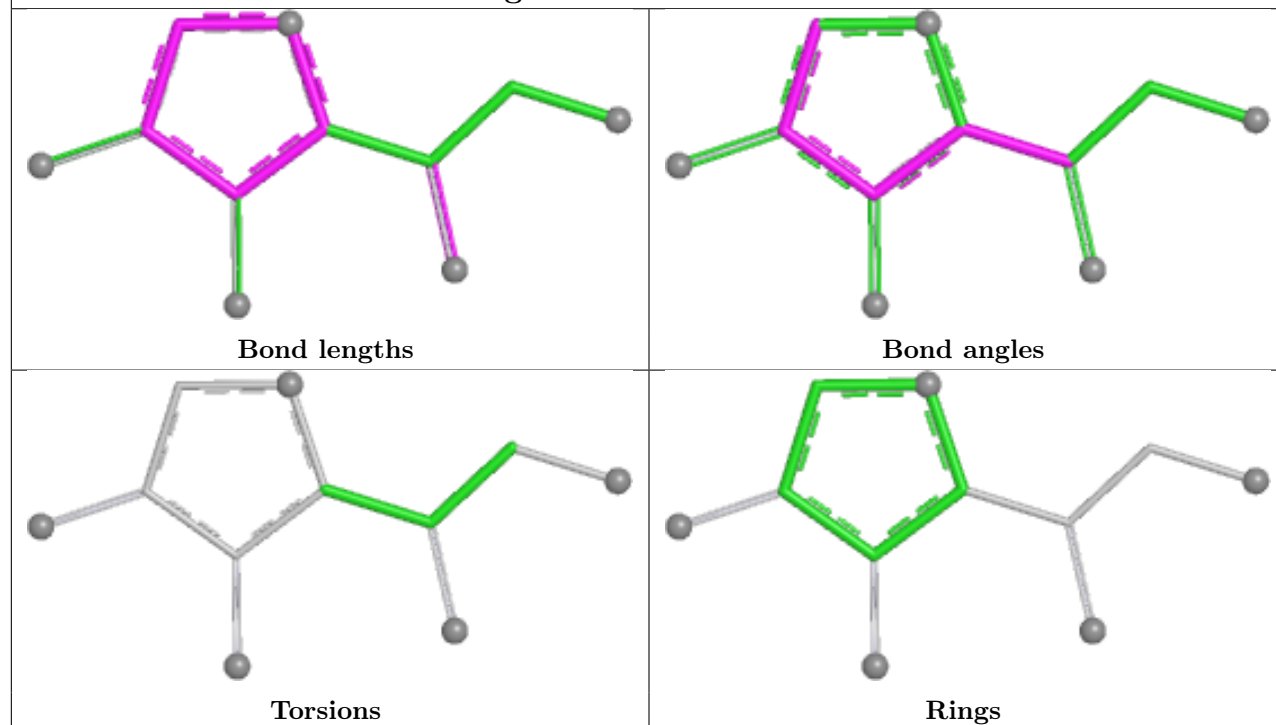




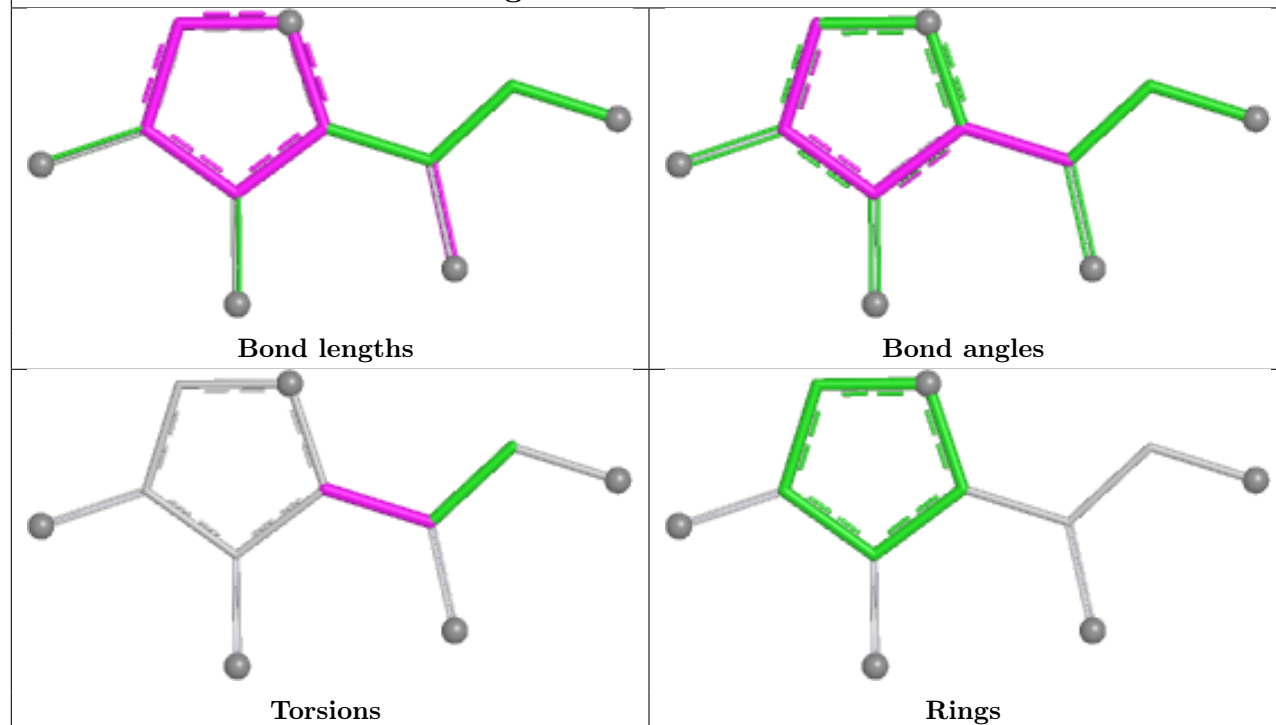
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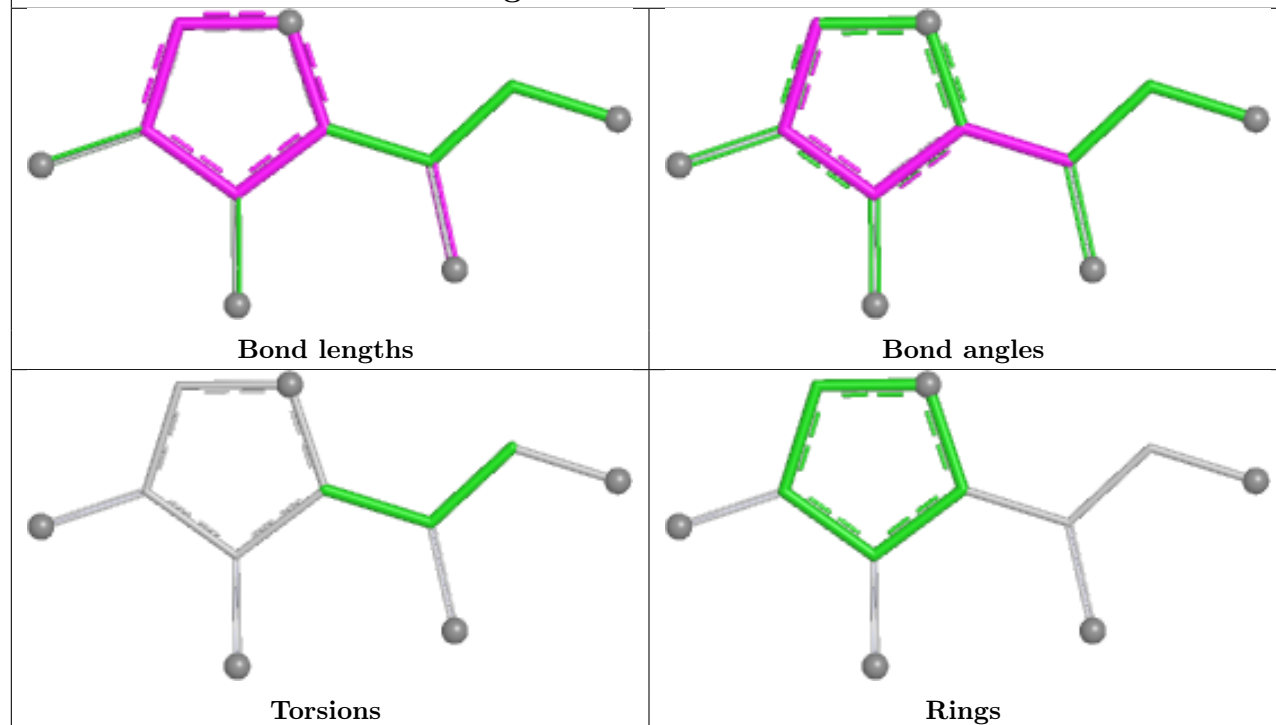
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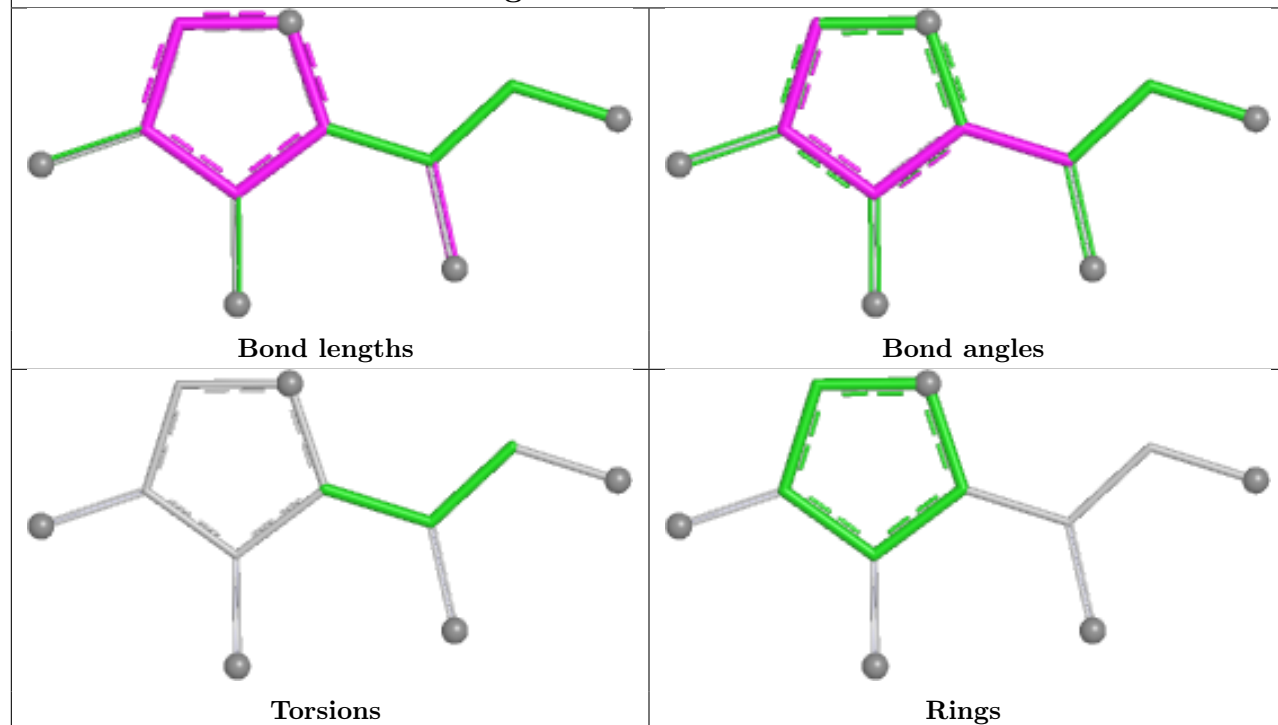
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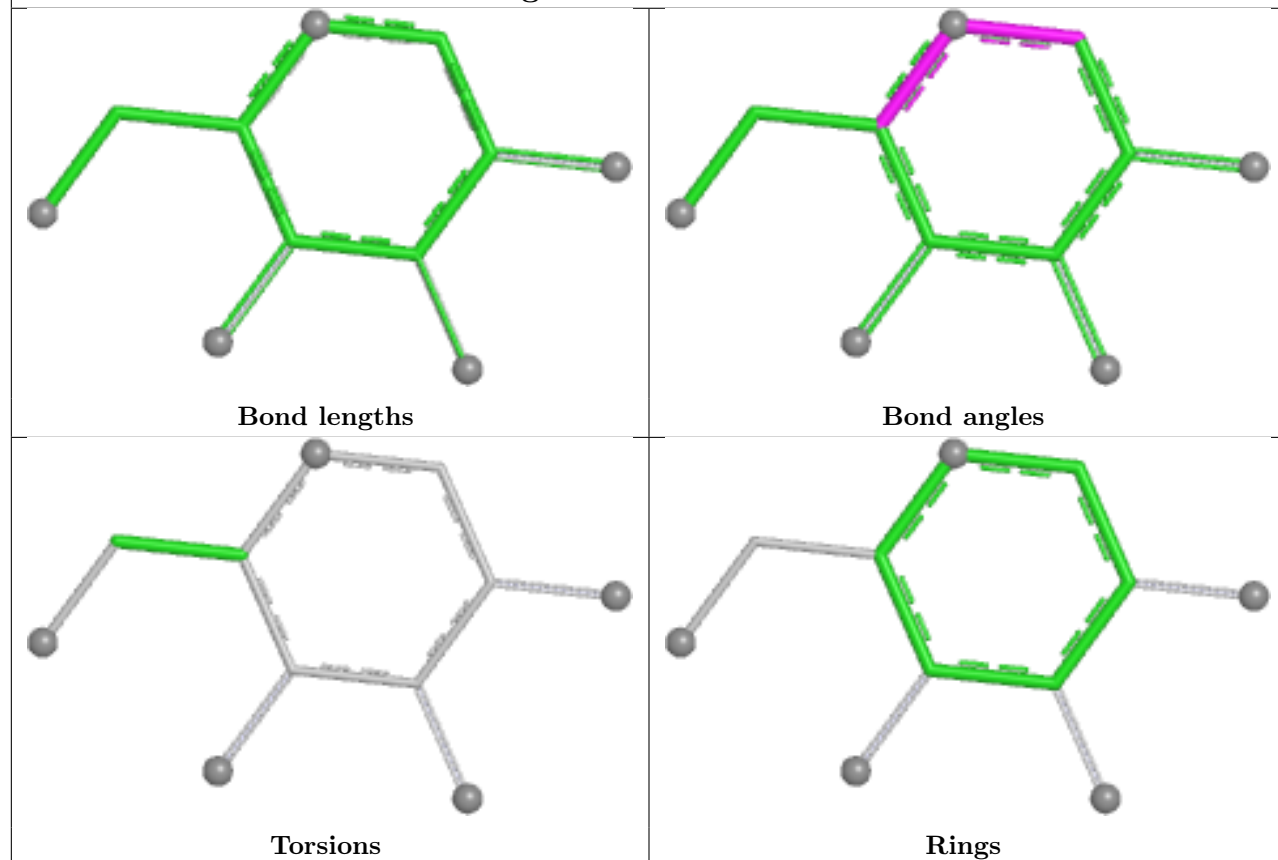
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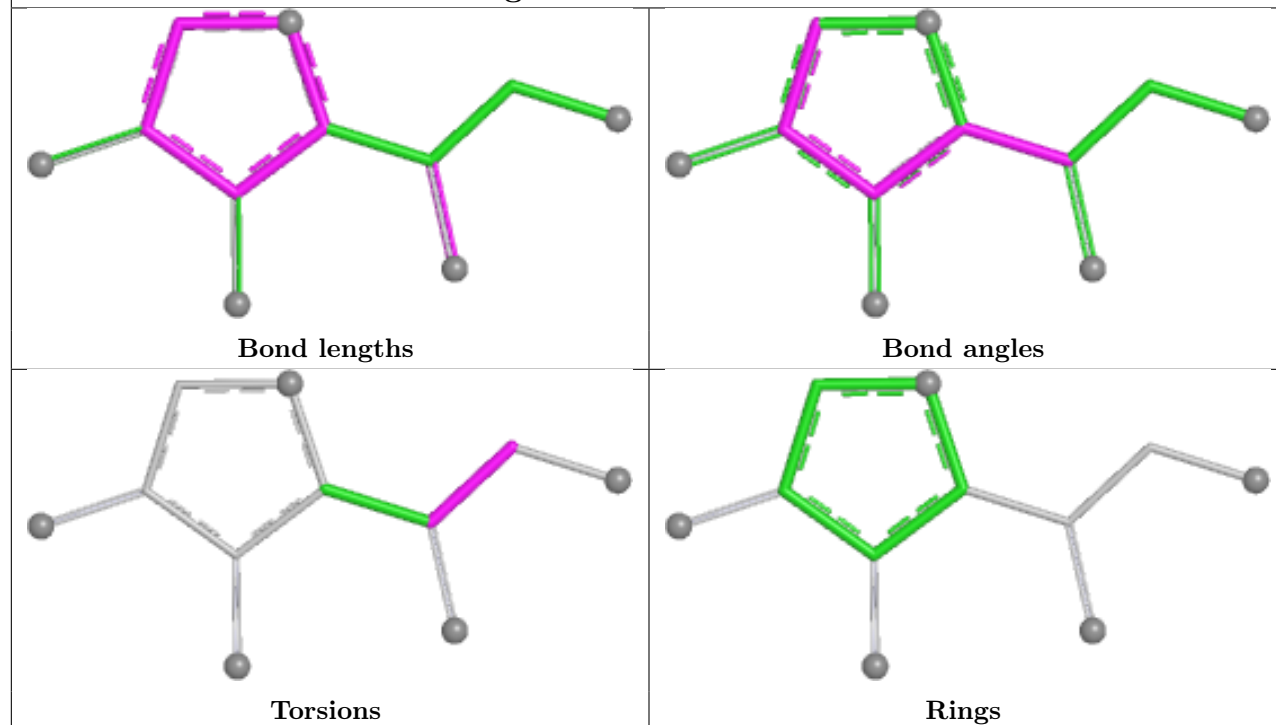
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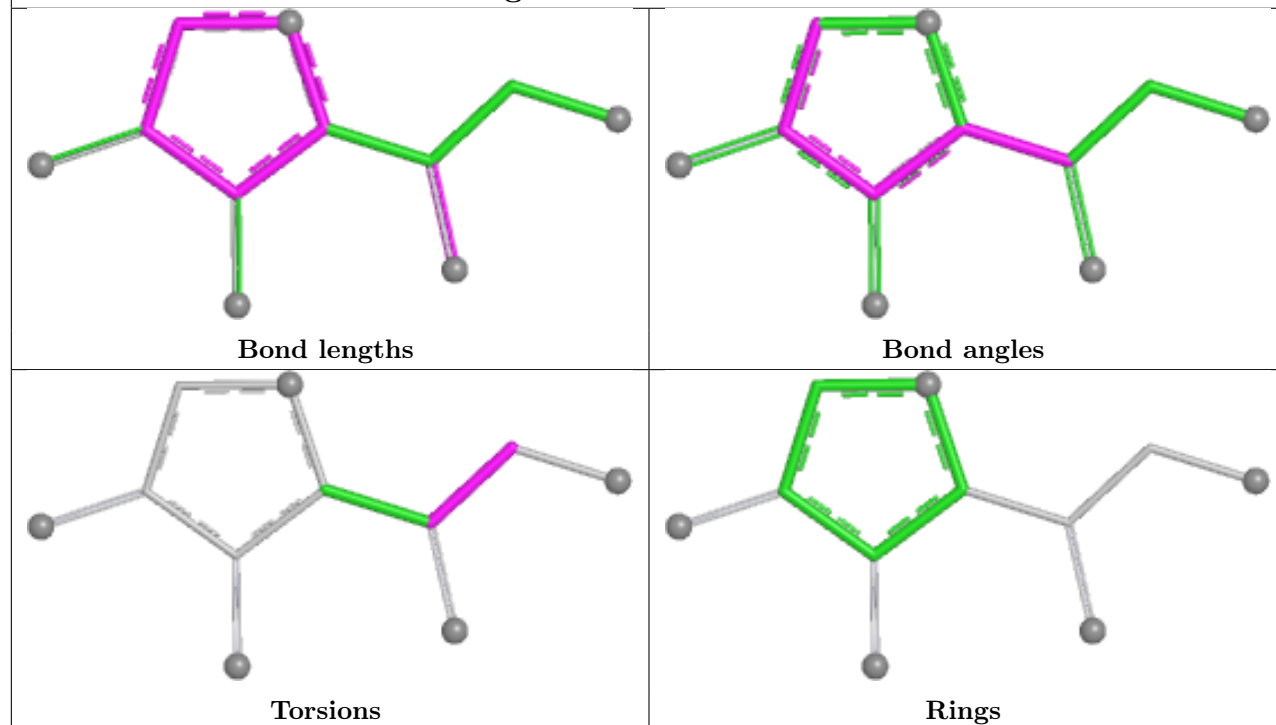
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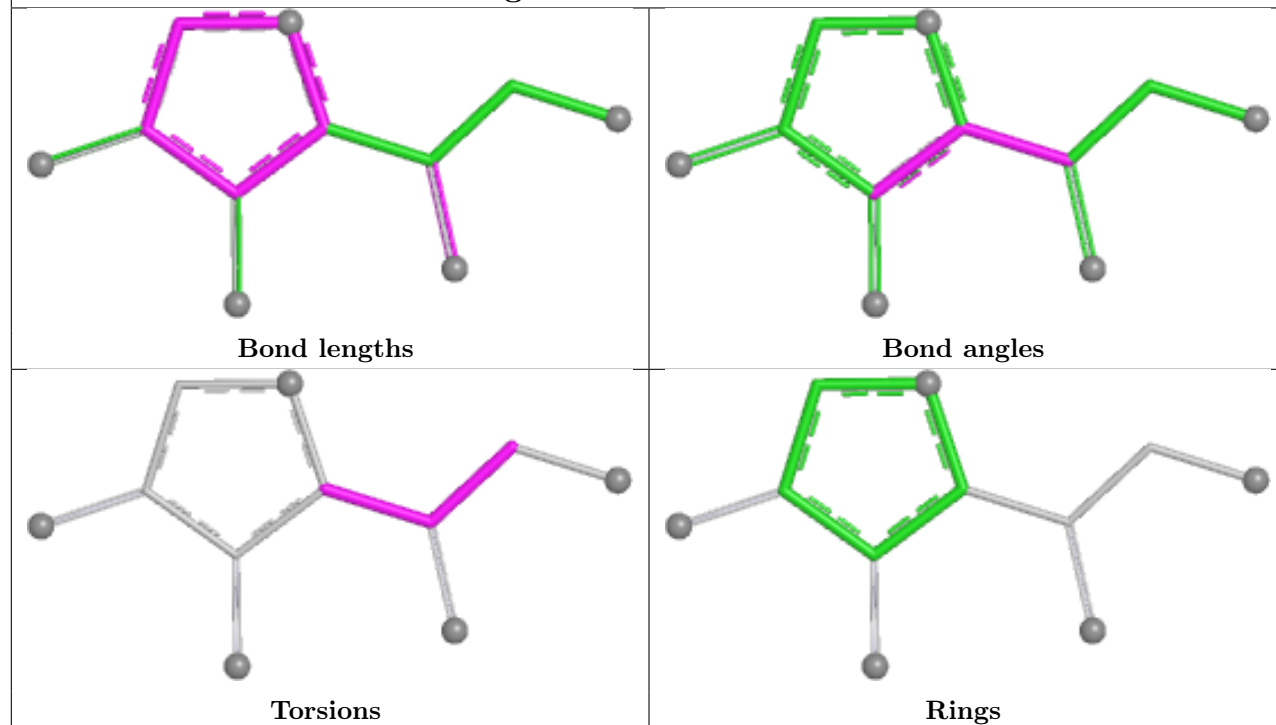
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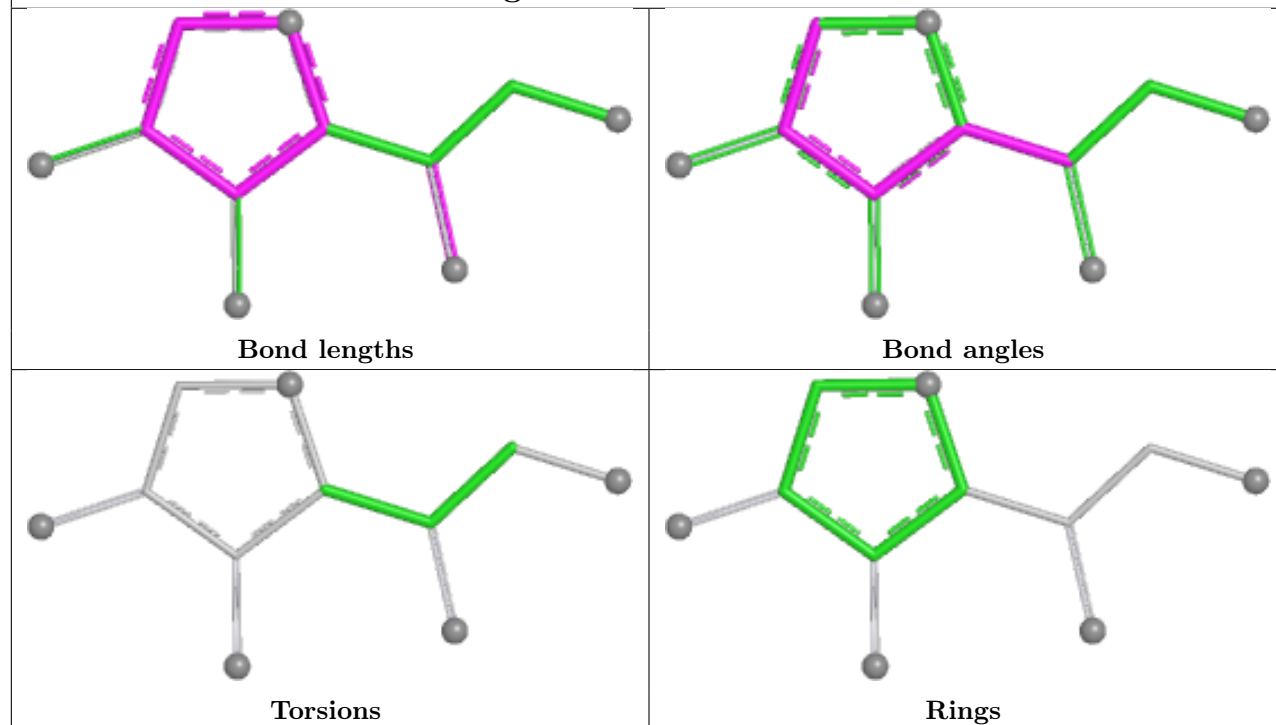
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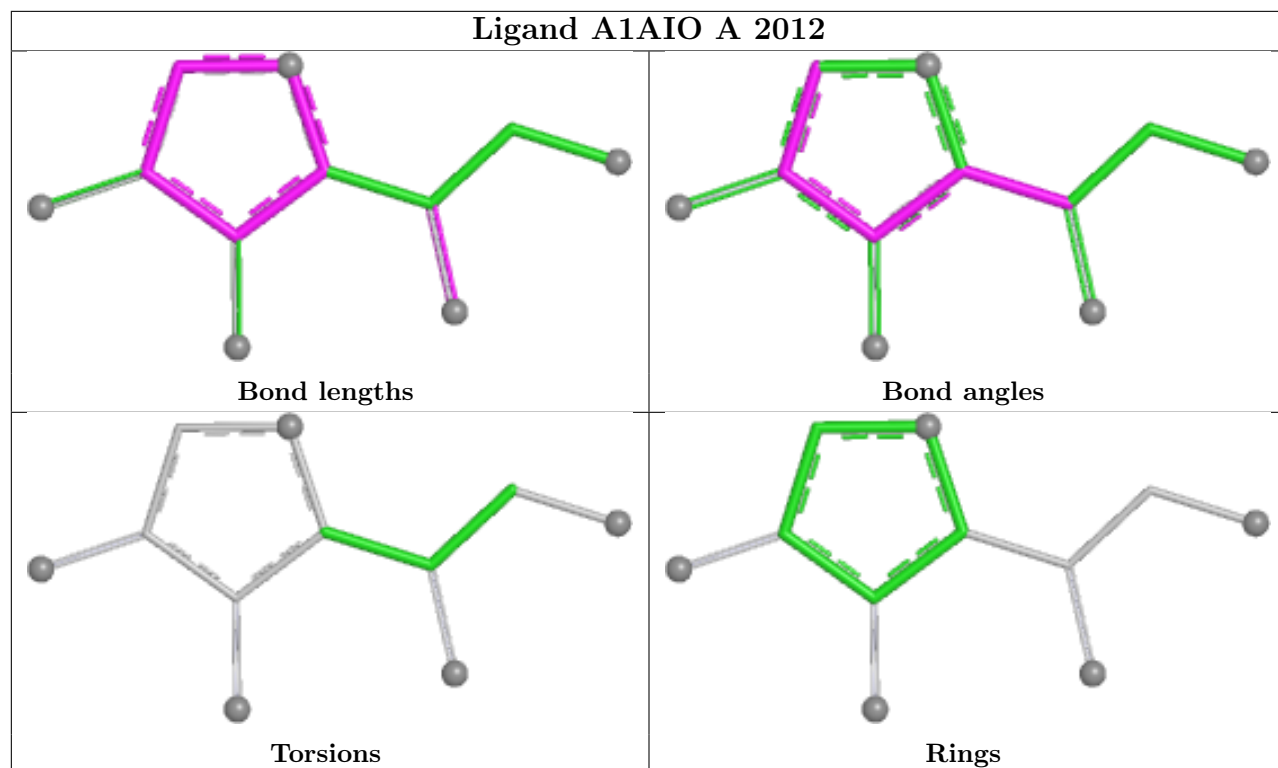
Ligand A1AIO B 2003



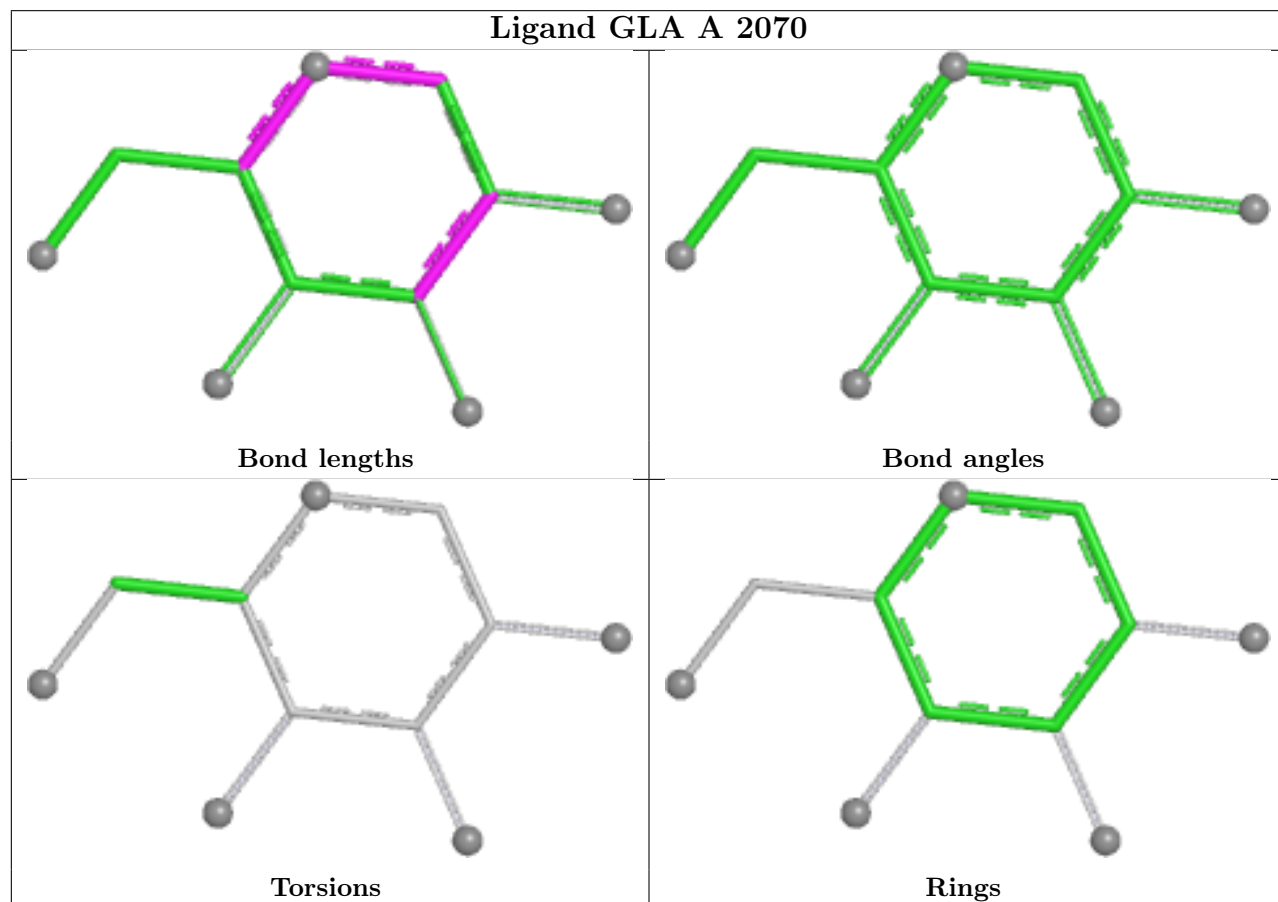
Ligand A1AIO A 2025



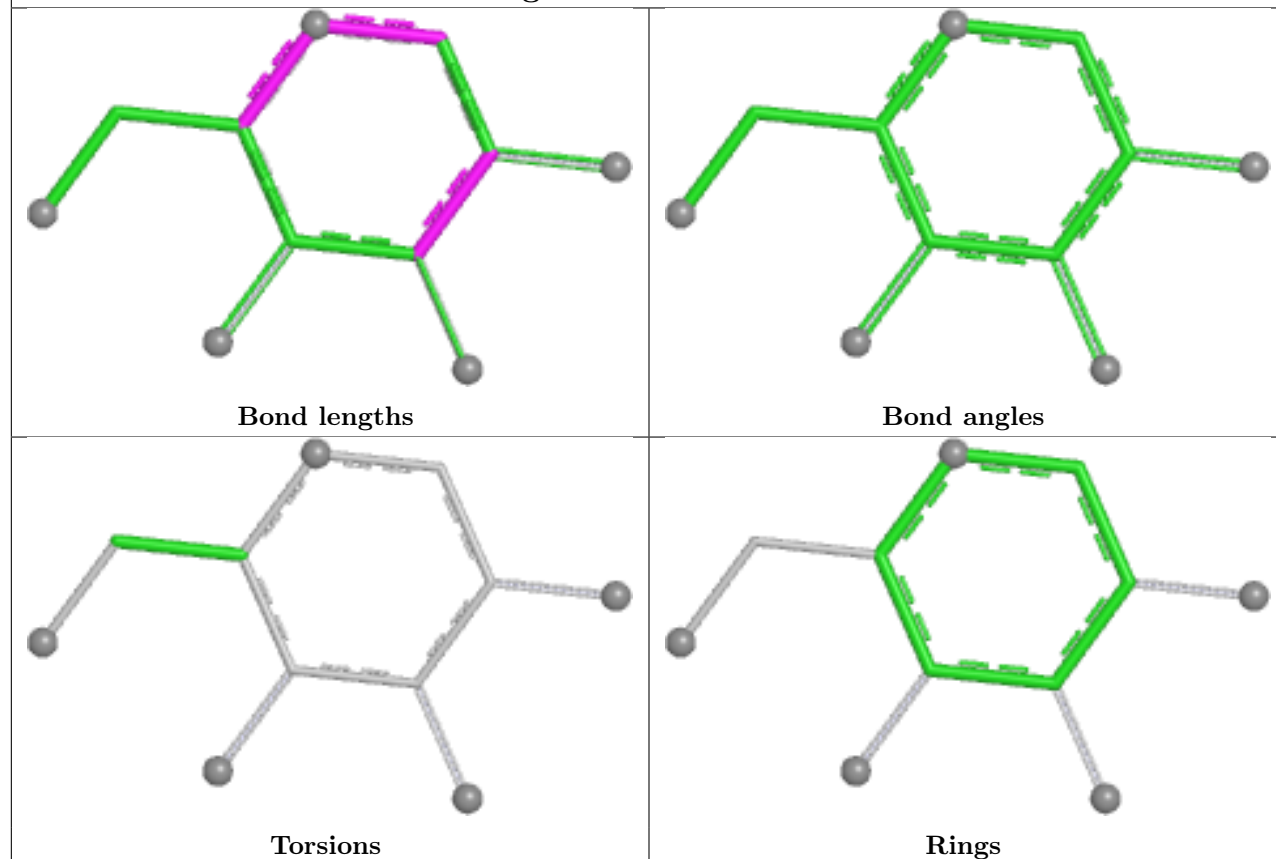
Ligand A1AIO A 2012



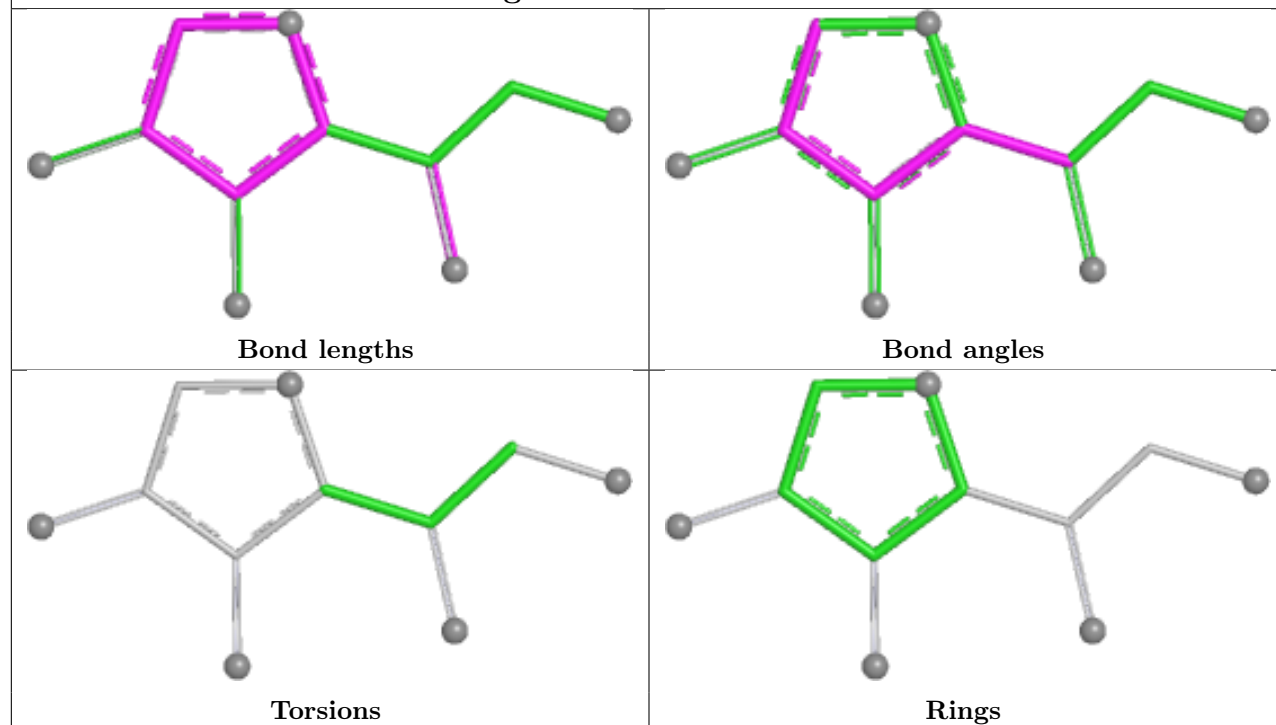
Ligand GLA A 2070



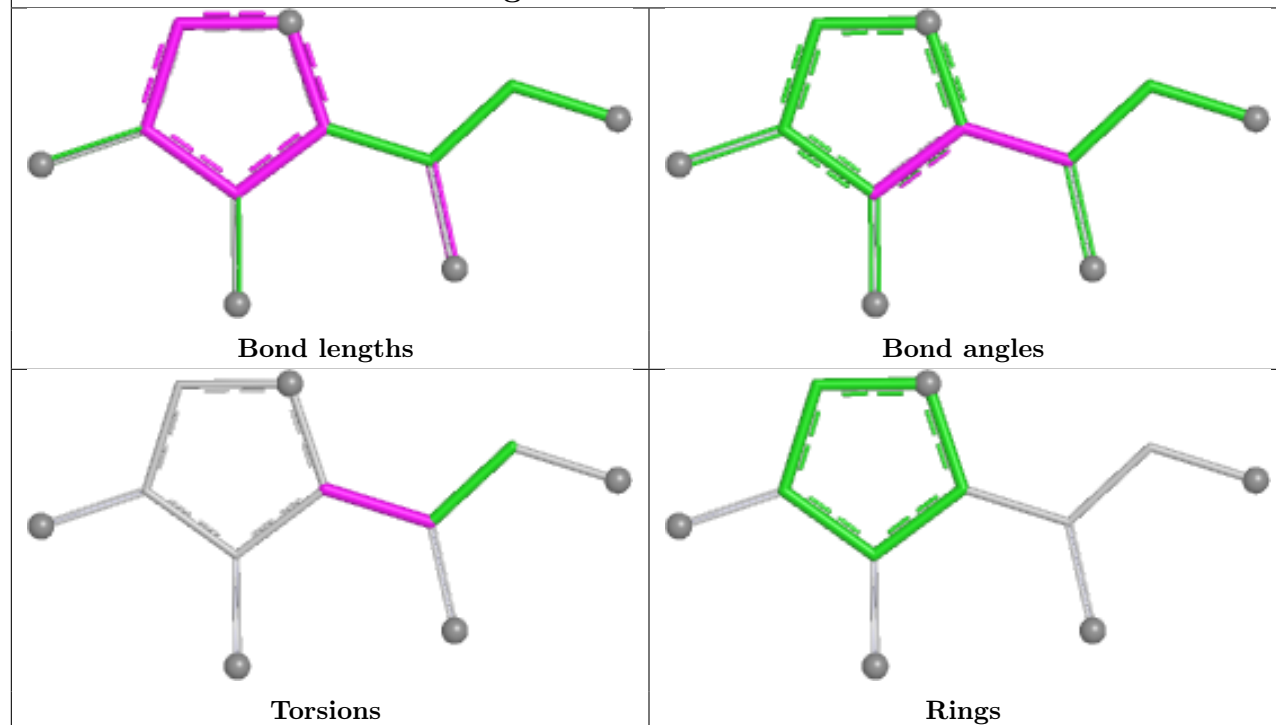
Ligand GLA B 2070



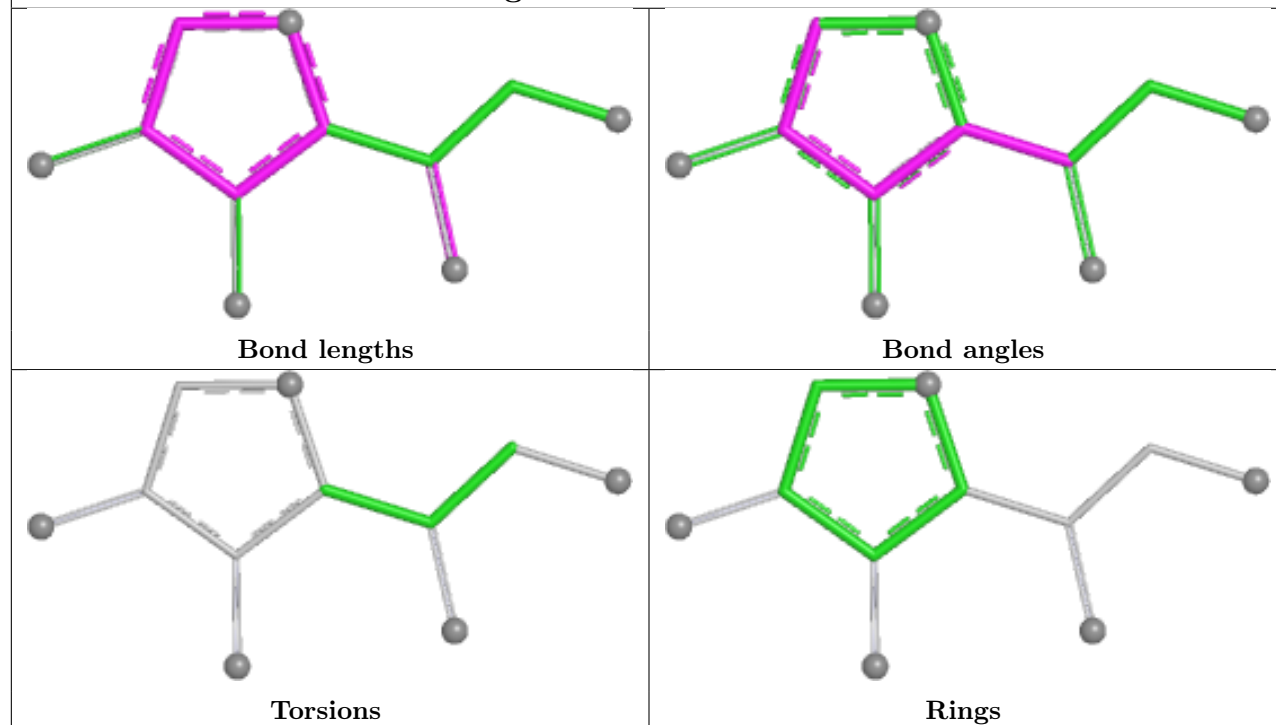
Ligand A1AIO A 2028



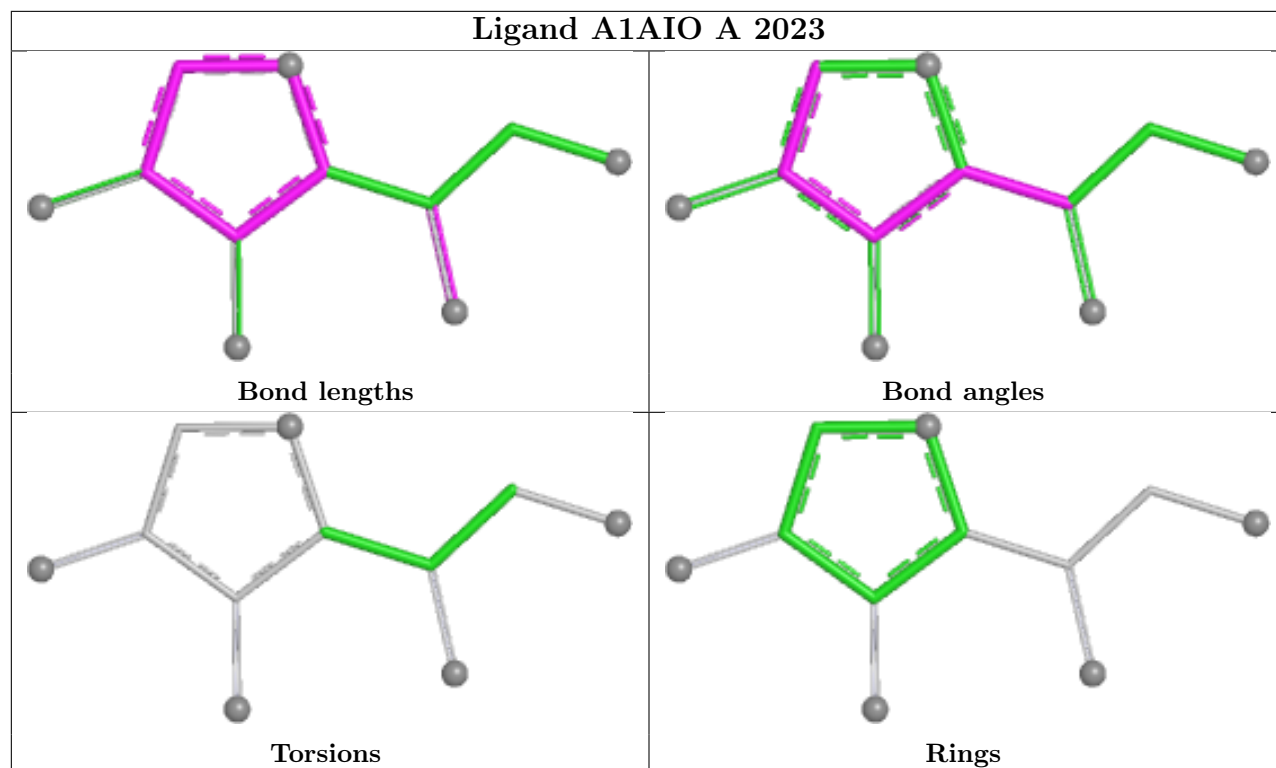
Ligand A1AIO A 2033



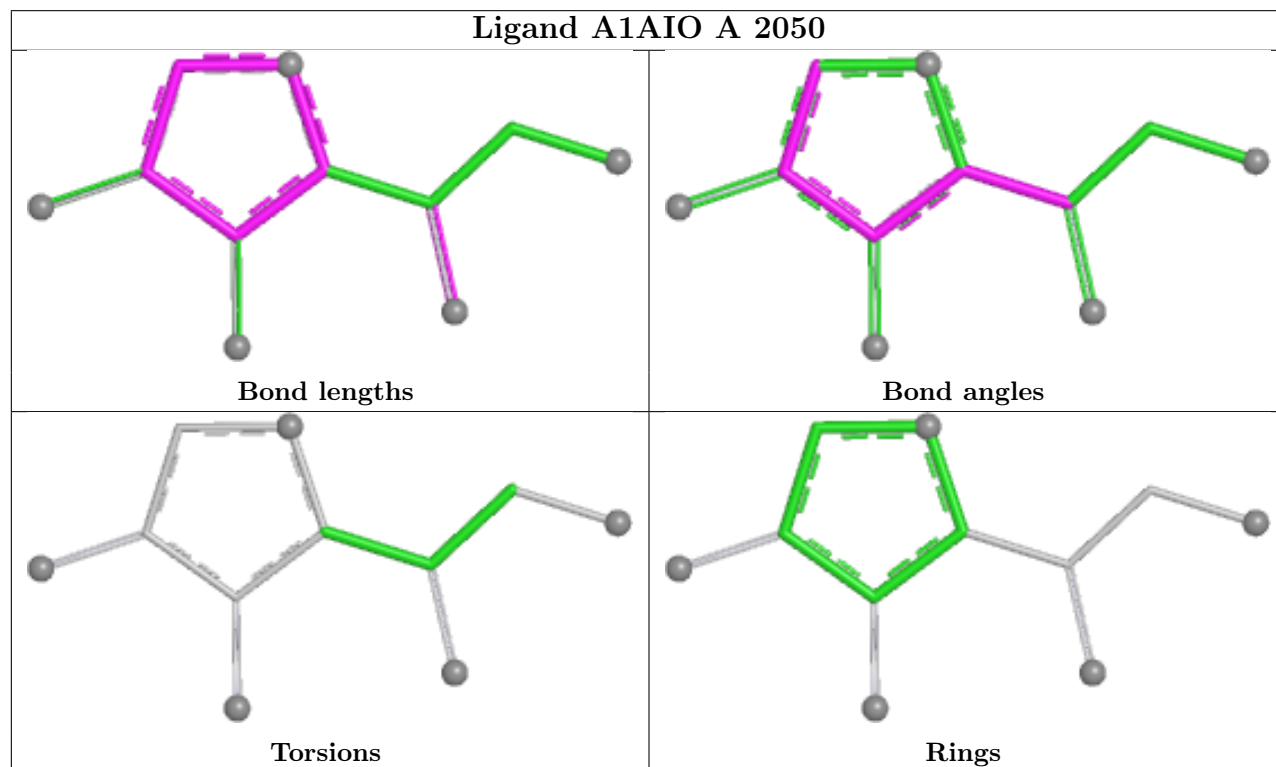
Ligand A1AIO B 2017



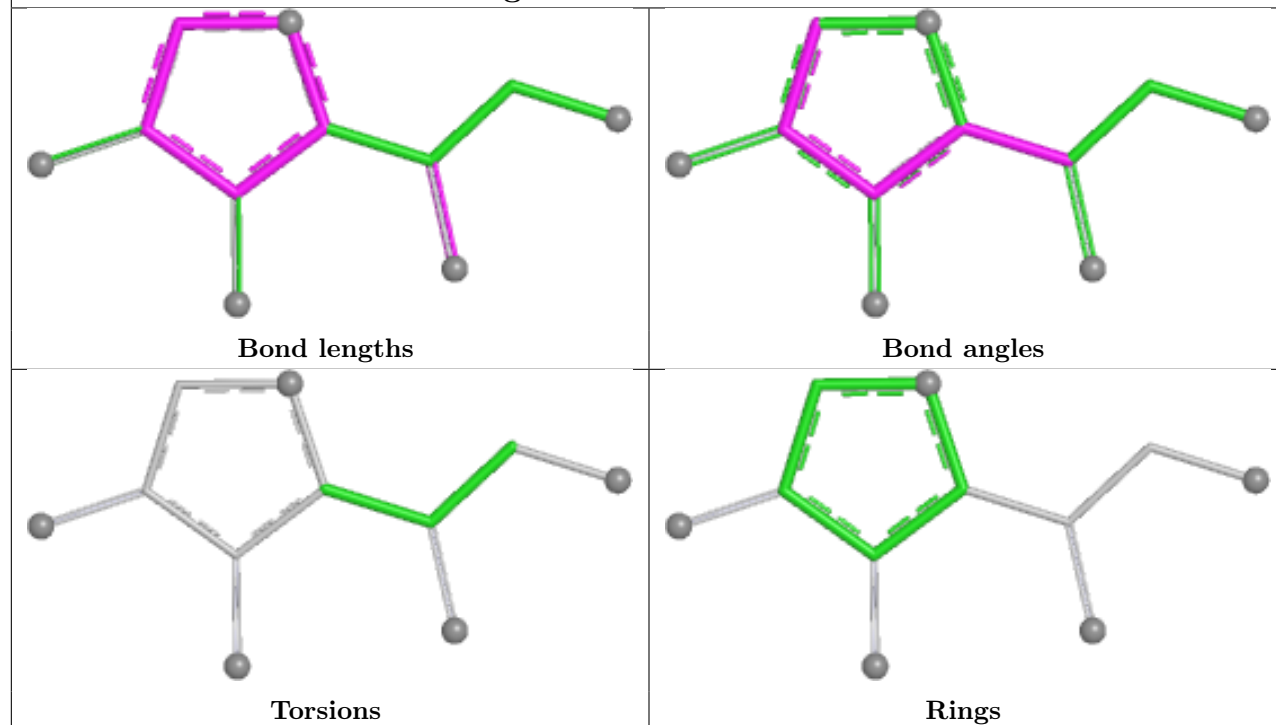
Ligand A1AIO A 2023



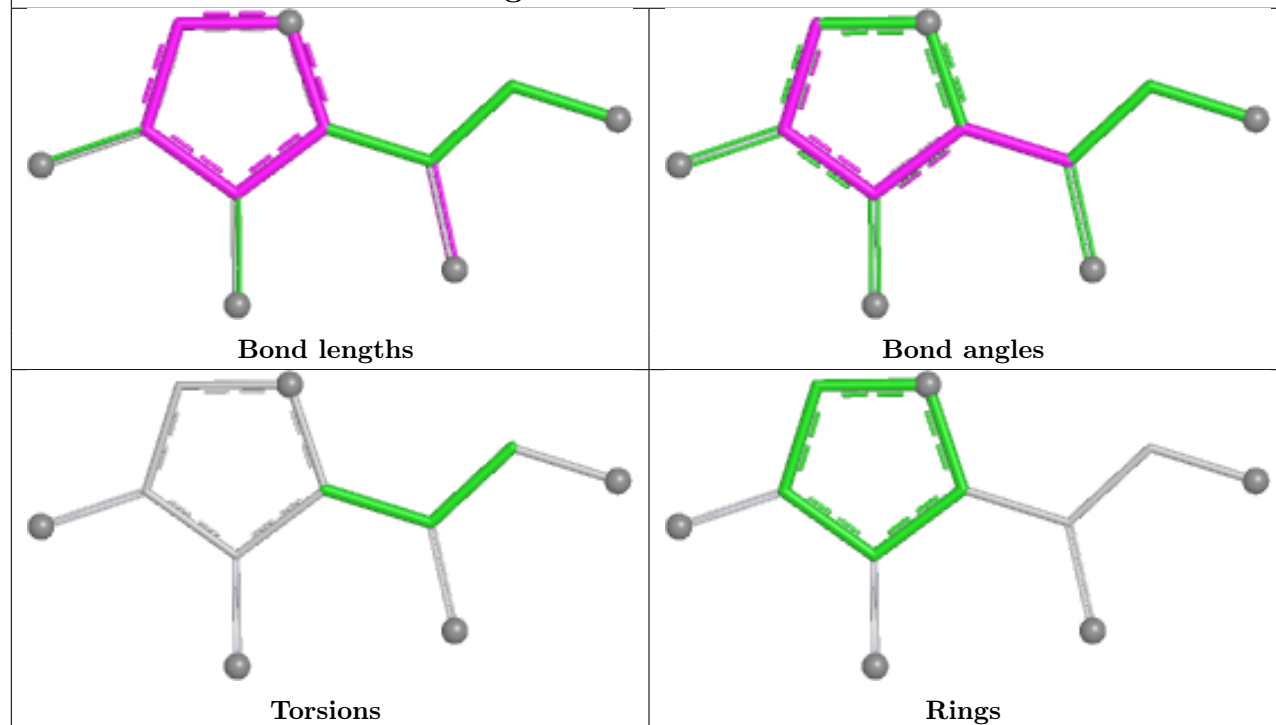
Ligand A1AIO A 2050

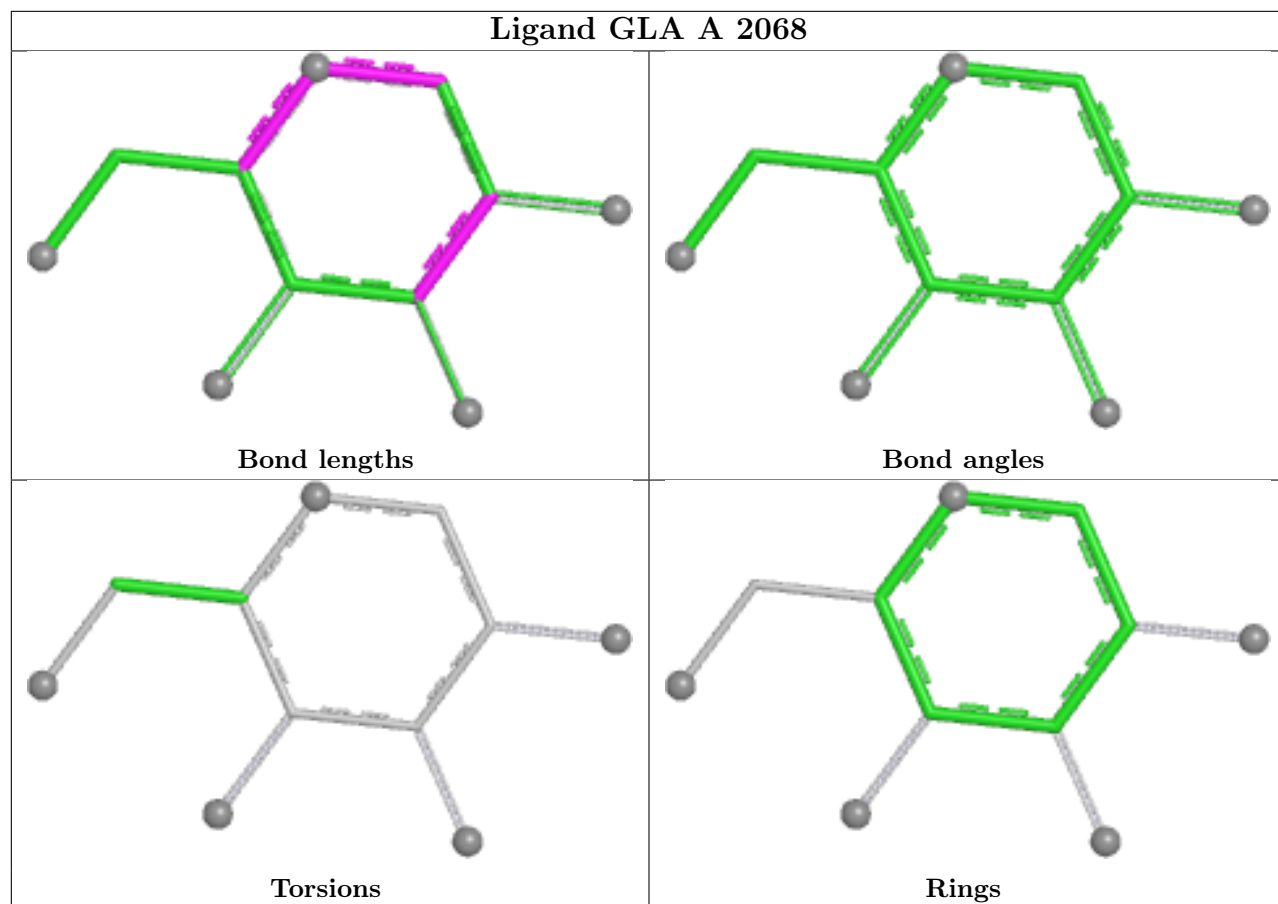


Ligand A1AIO A 2032

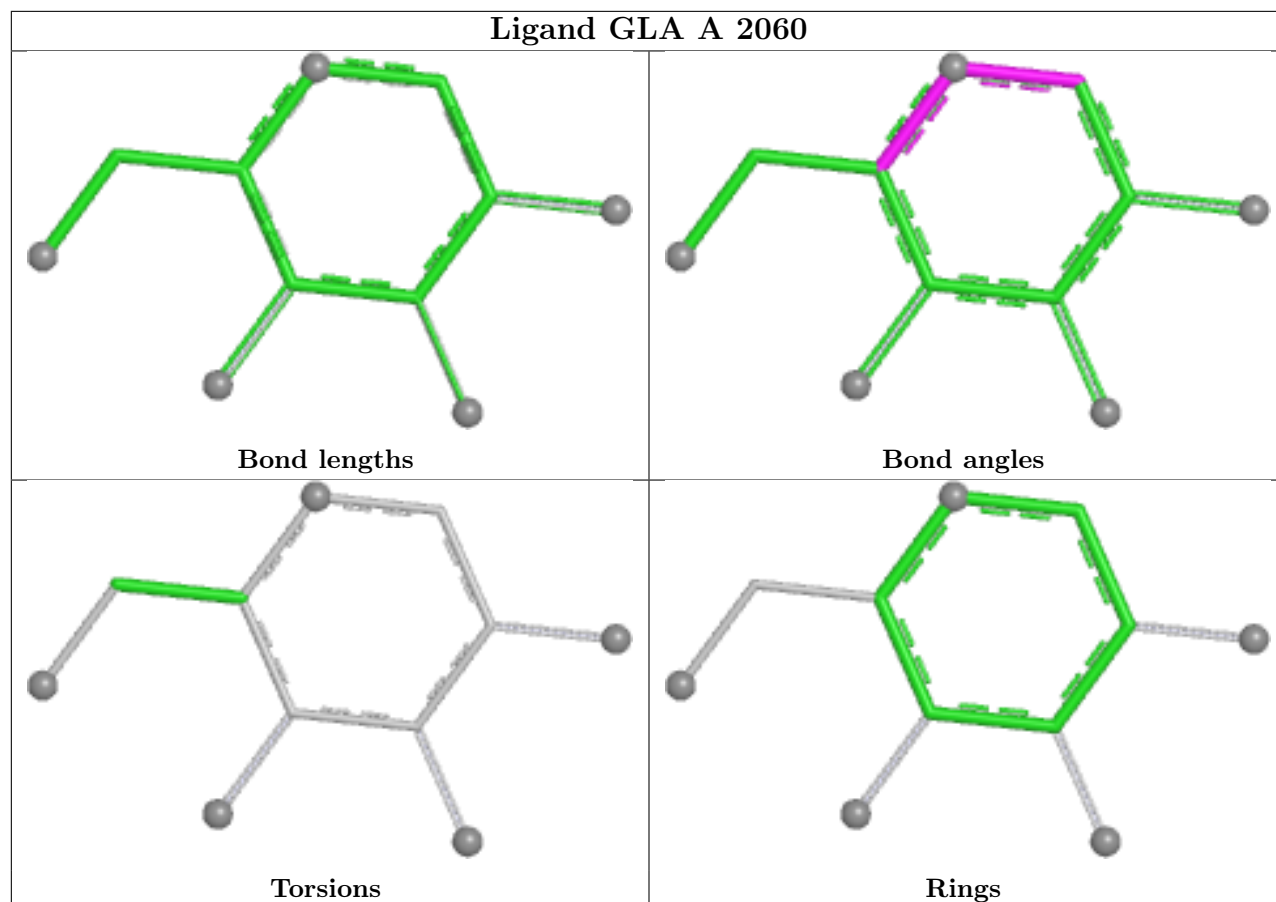


Ligand A1AIO B 2027

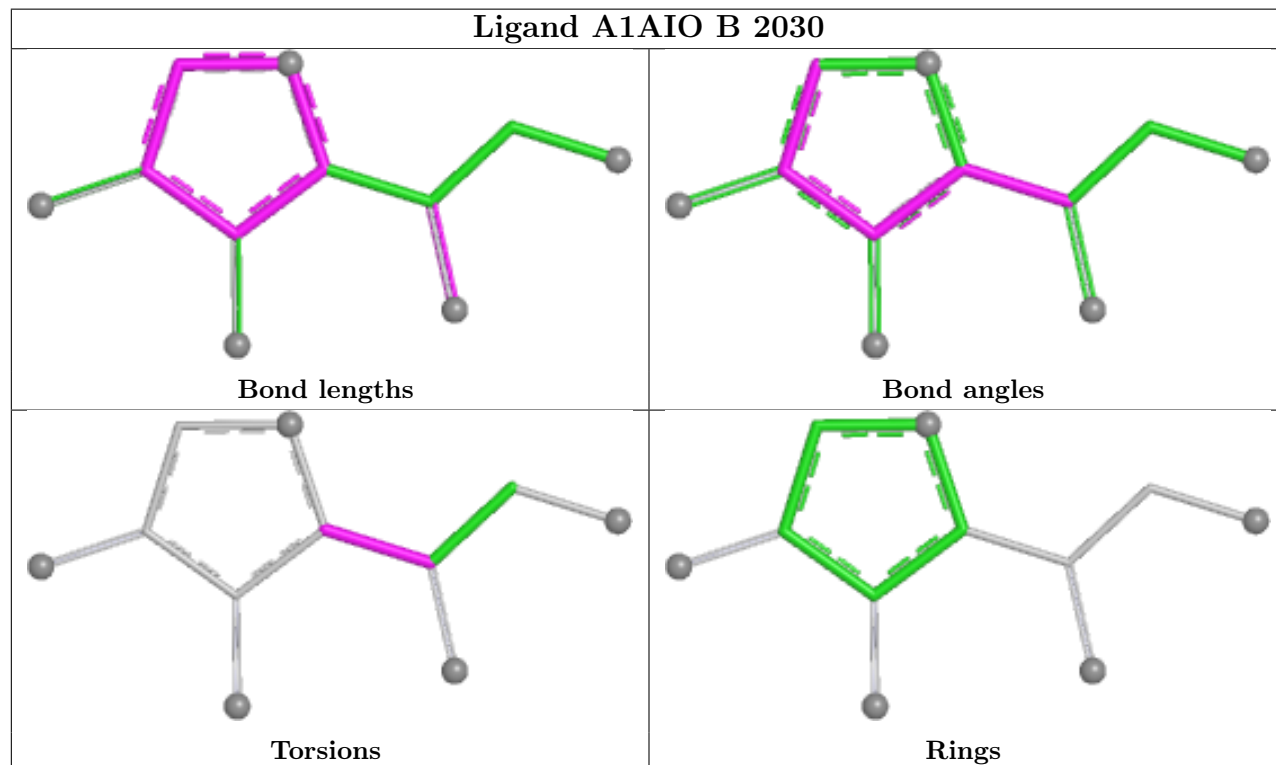




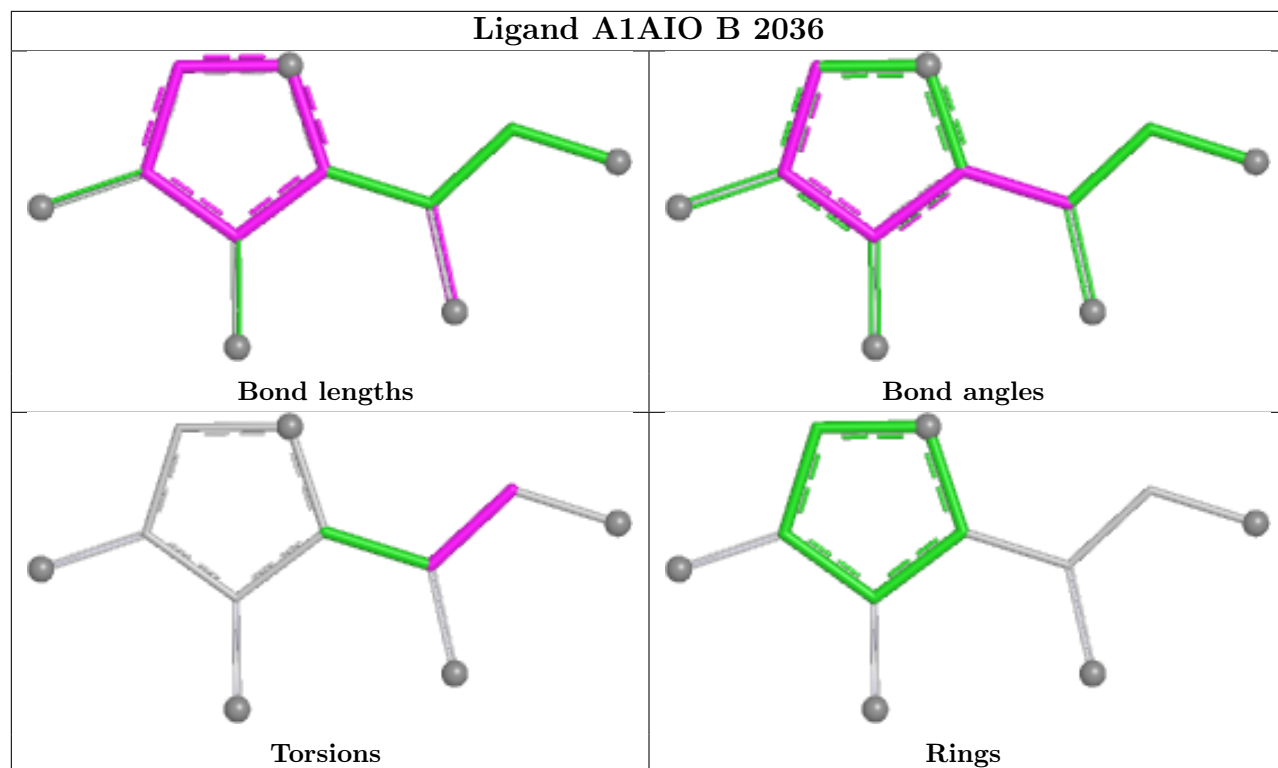
Ligand GLA A 2060



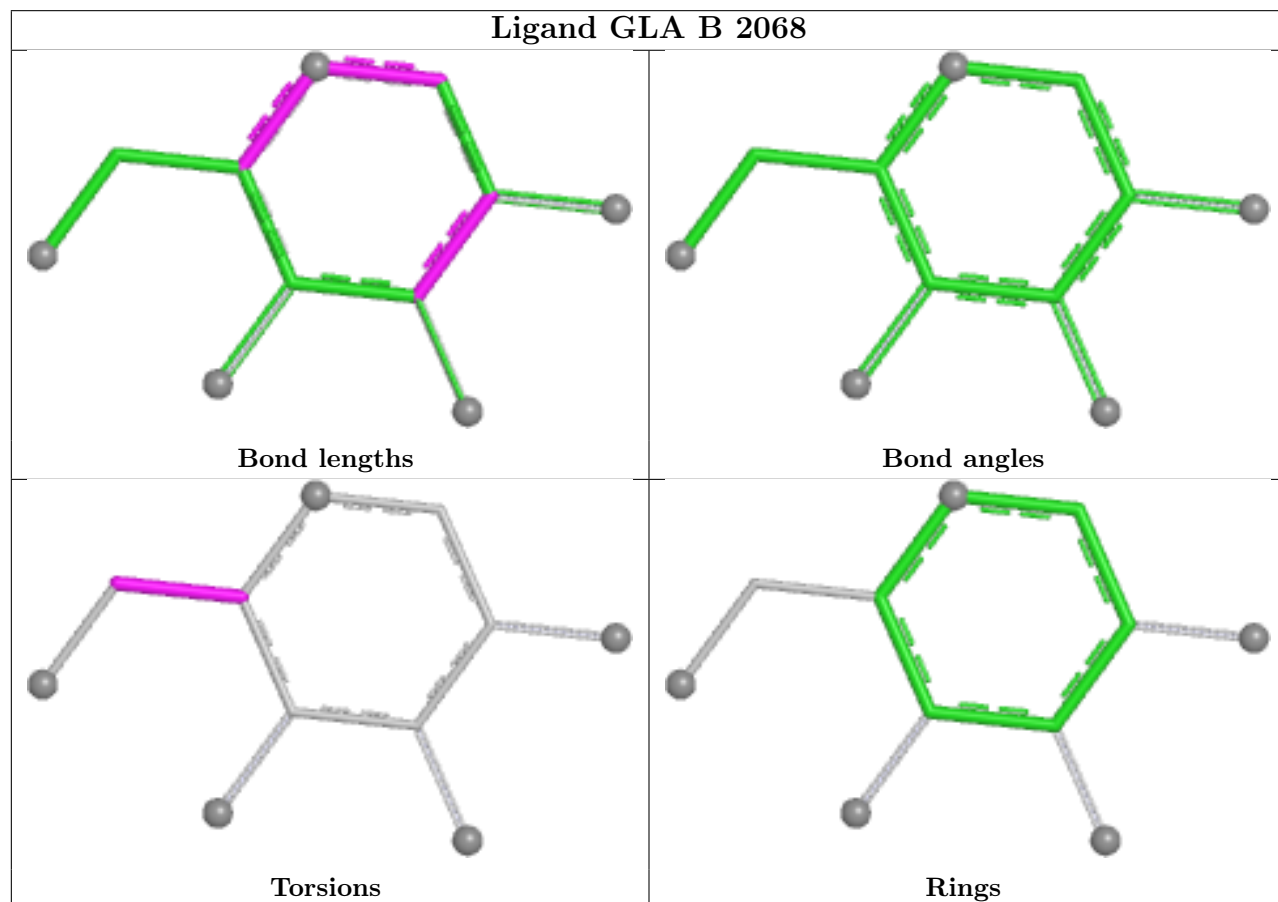
Ligand A1AIO B 2030



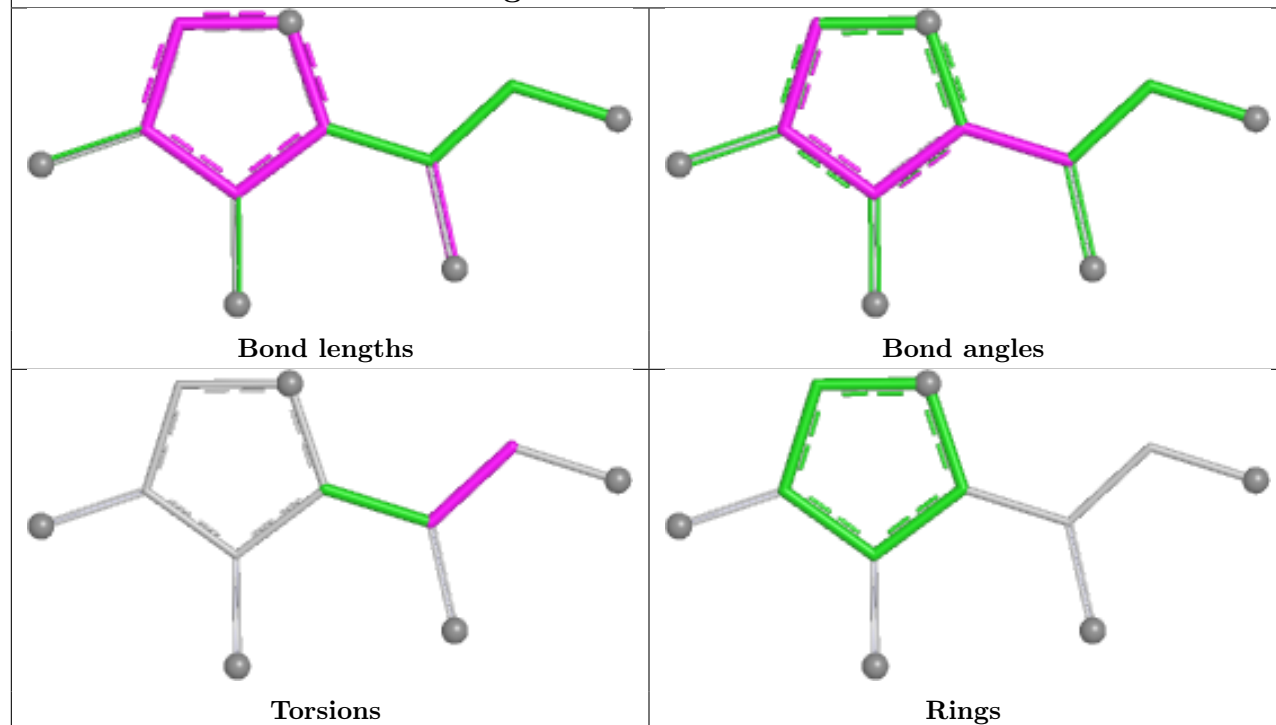
Ligand A1AIO B 2036



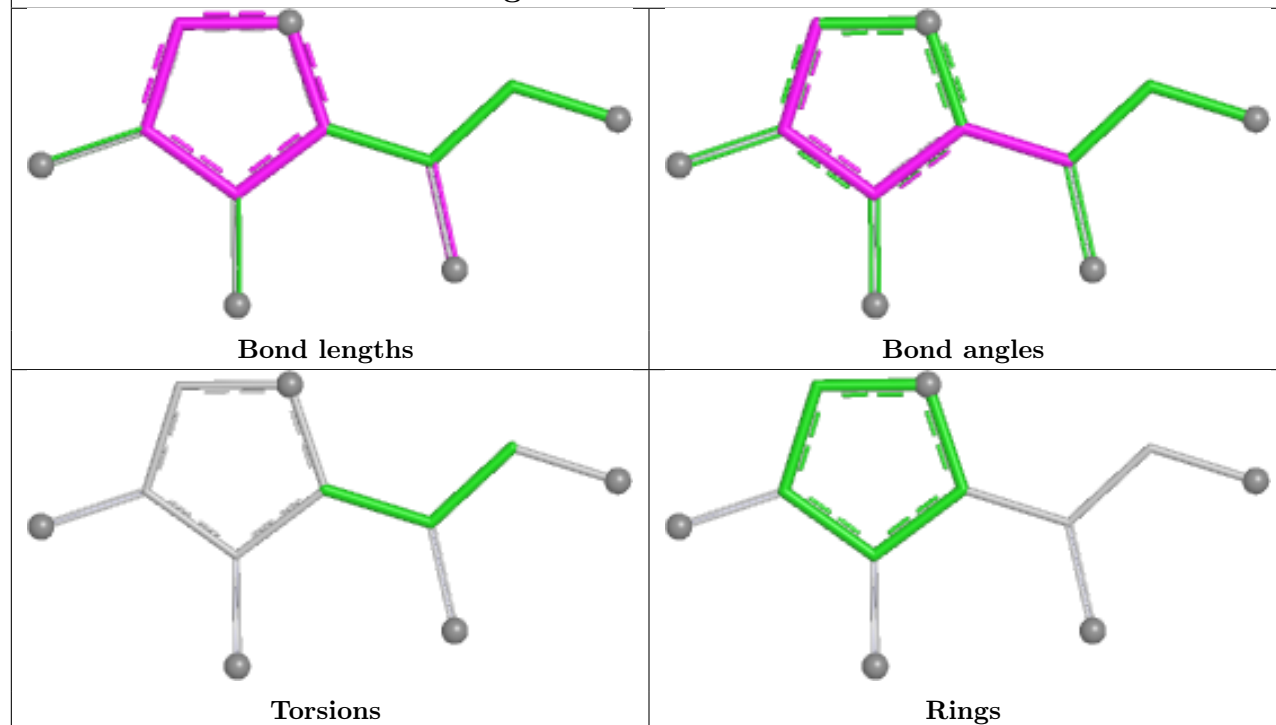
Ligand GLA B 2068



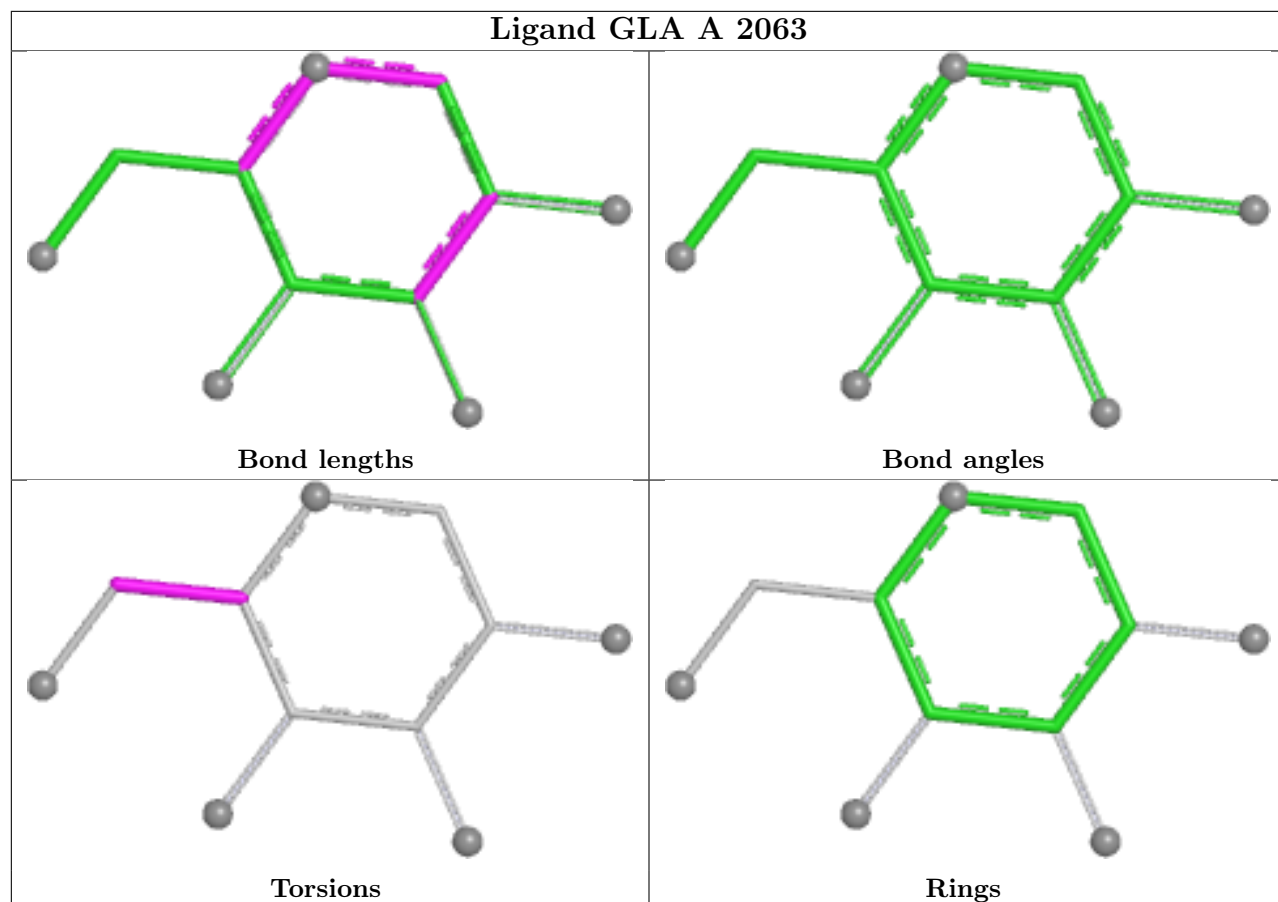
Ligand A1AIO A 2009



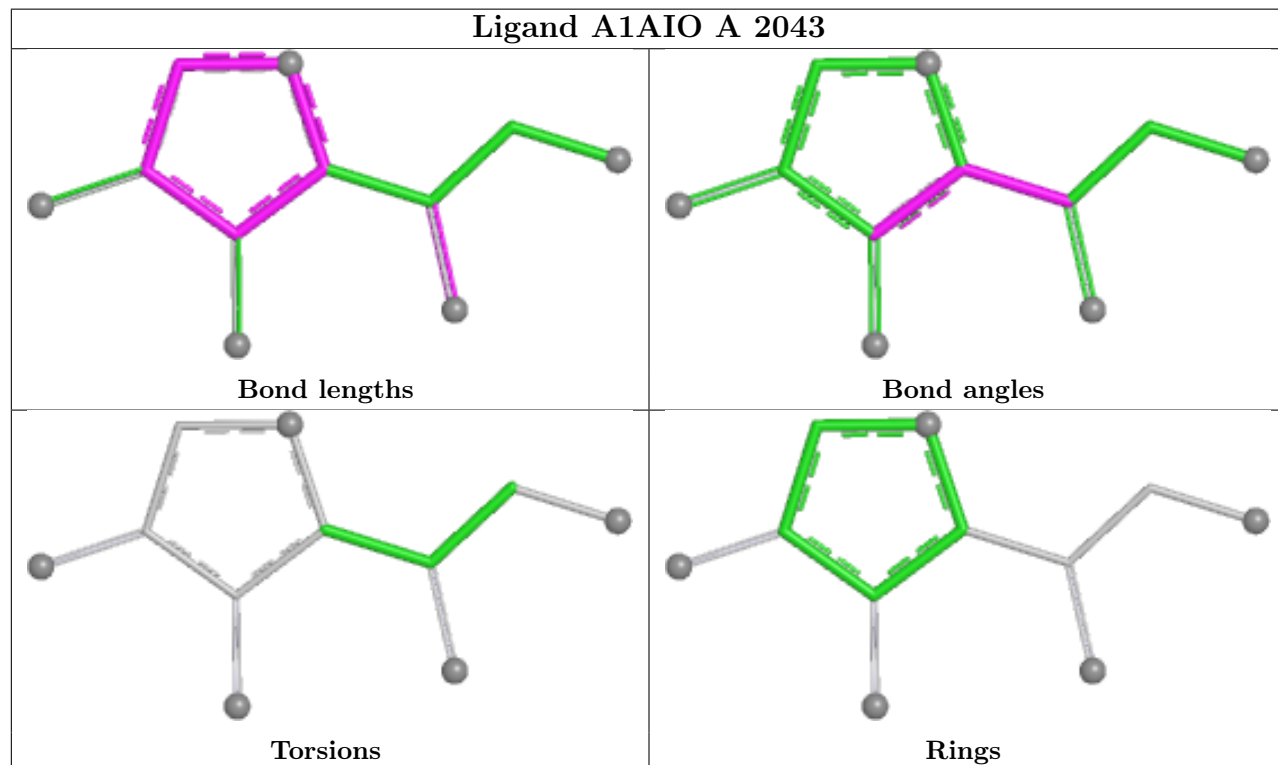
Ligand A1AIO A 2024



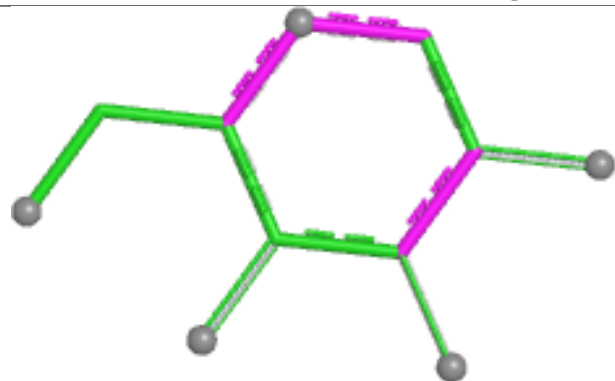
Ligand GLA A 2063



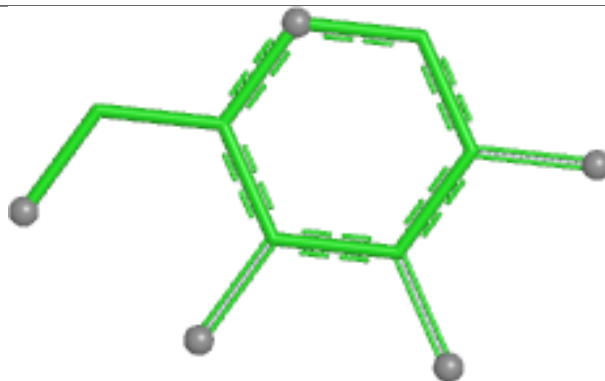
Ligand A1AIO A 2043



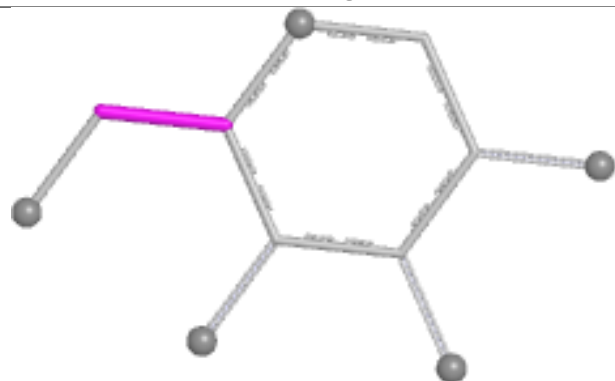
Ligand GLA A 2065



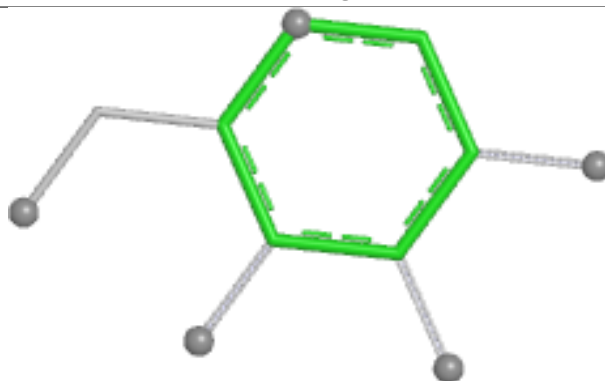
Bond lengths



Bond angles

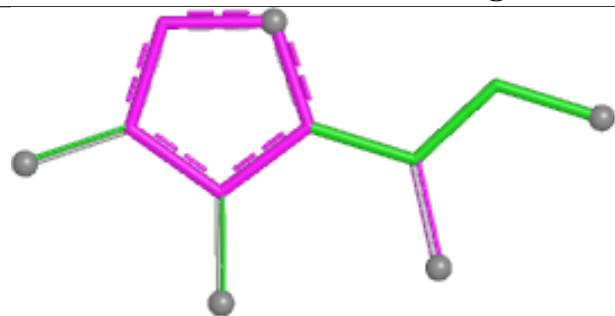


Torsions

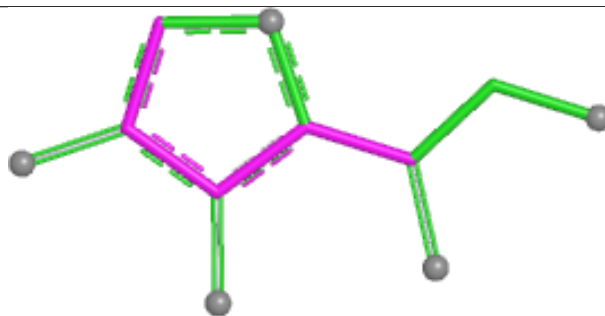


Rings

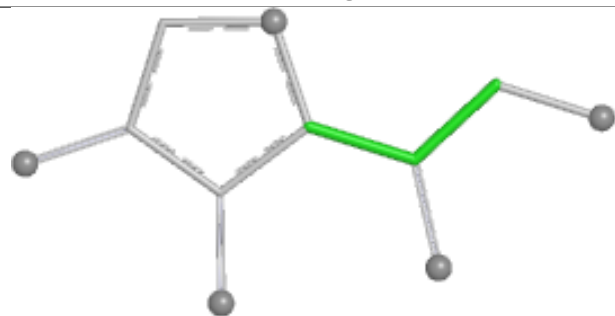
Ligand A1AIO A 2053



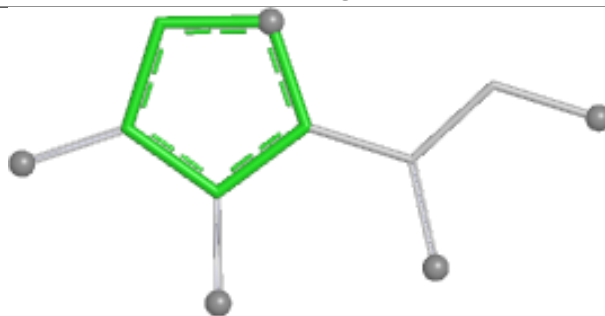
Bond lengths



Bond angles

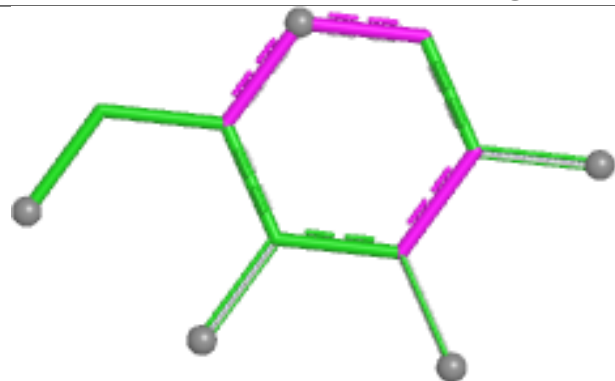


Torsions

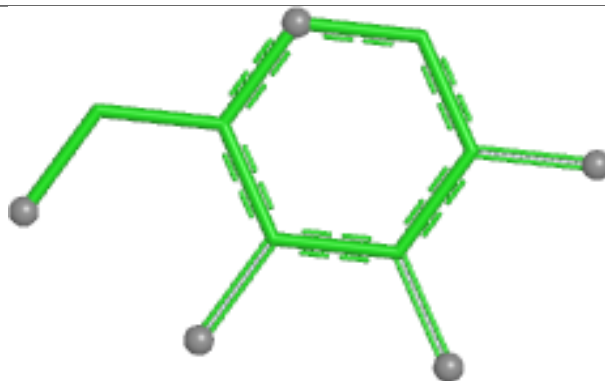


Rings

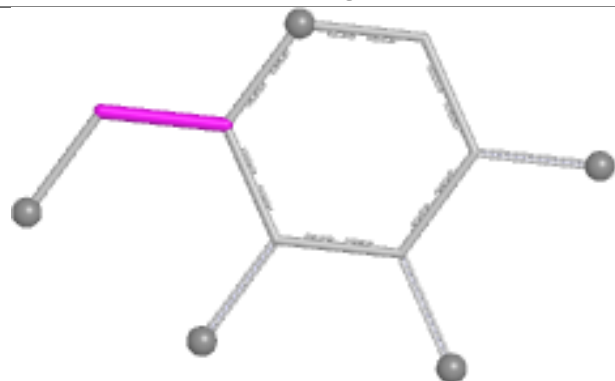
Ligand GLA B 2061



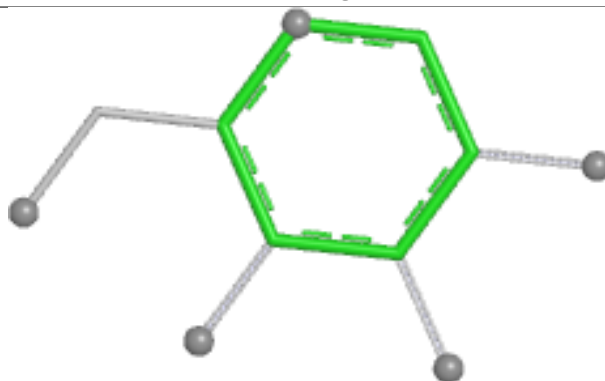
Bond lengths



Bond angles

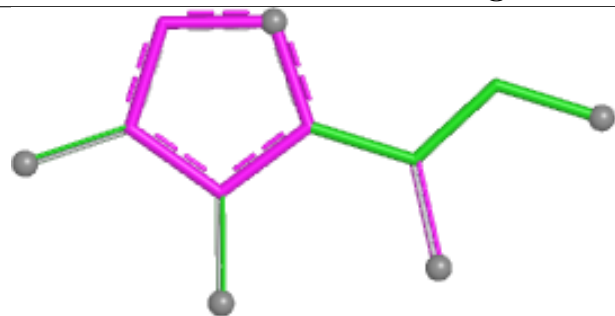


Torsions

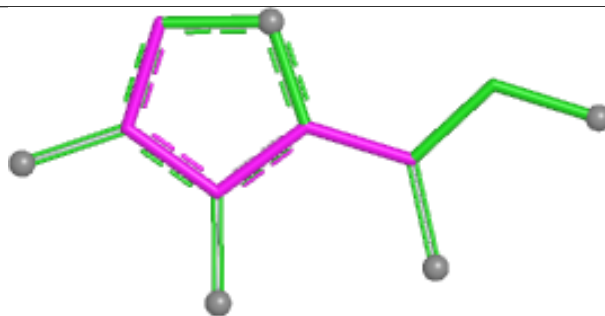


Rings

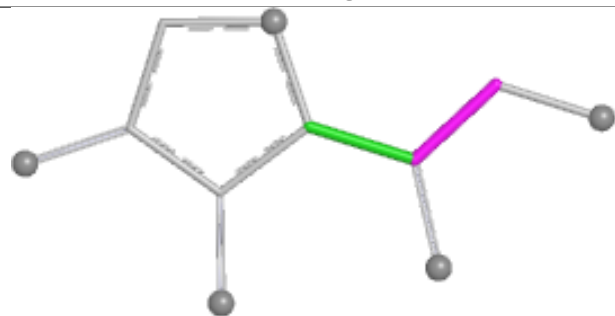
Ligand A1AIO A 2005



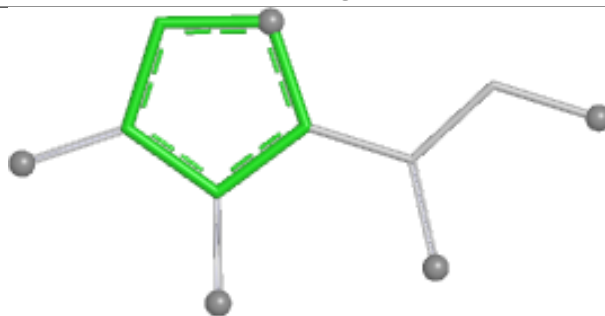
Bond lengths



Bond angles

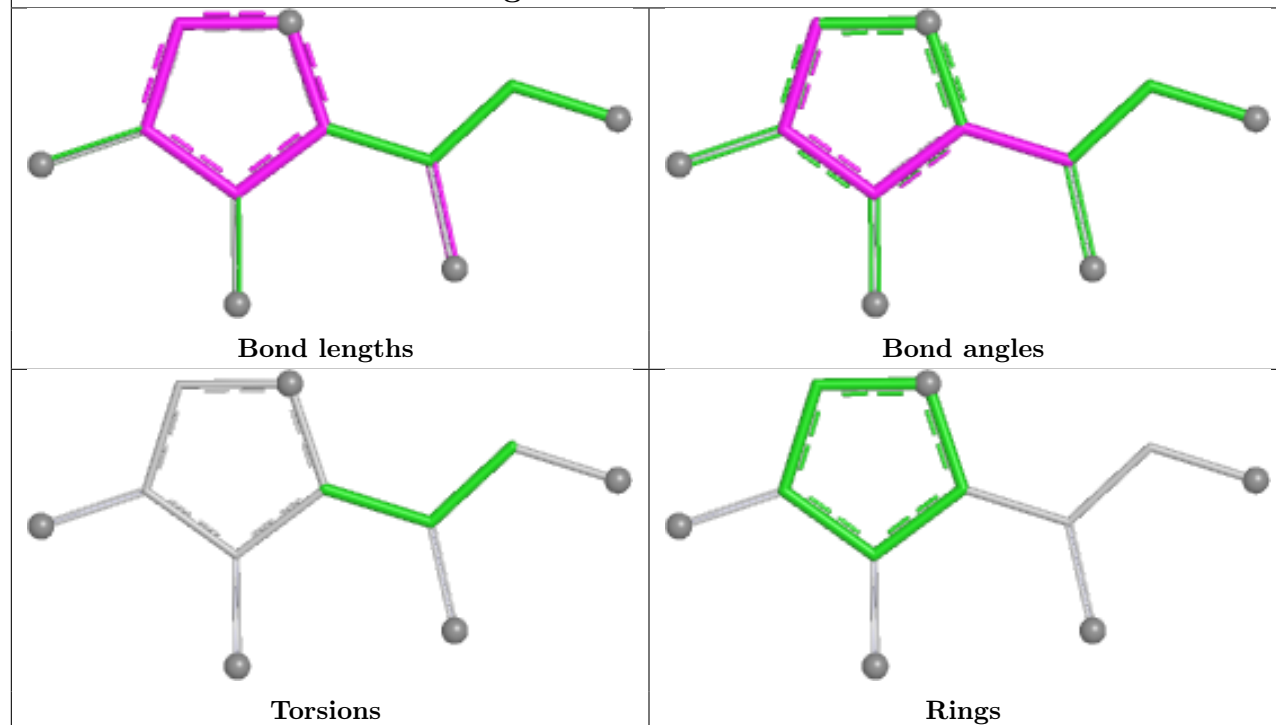


Torsions

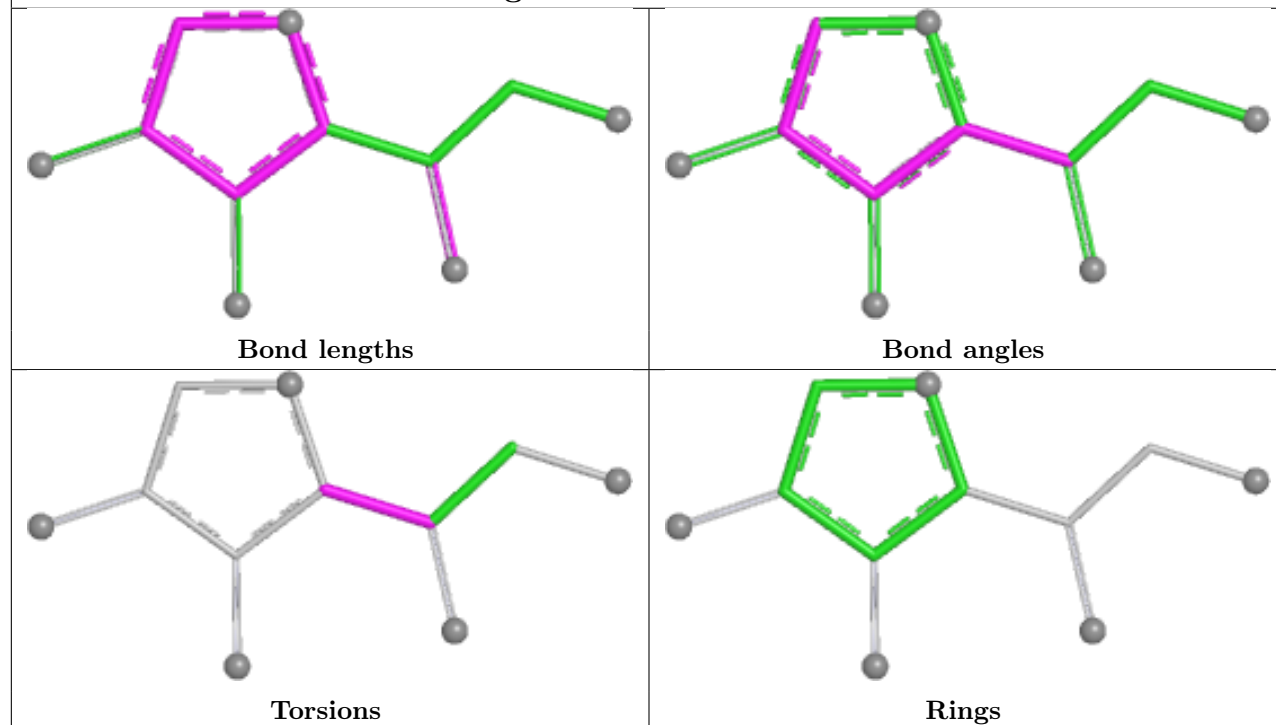


Rings

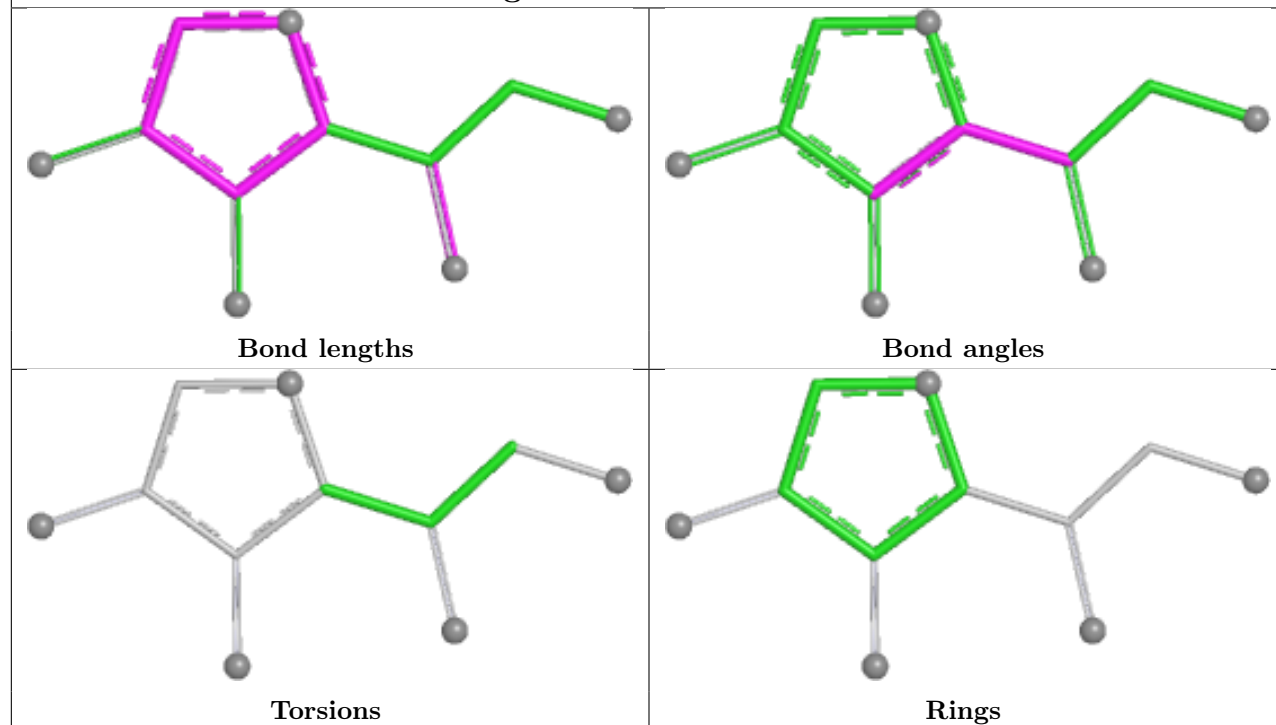
Ligand A1AIO A 2051



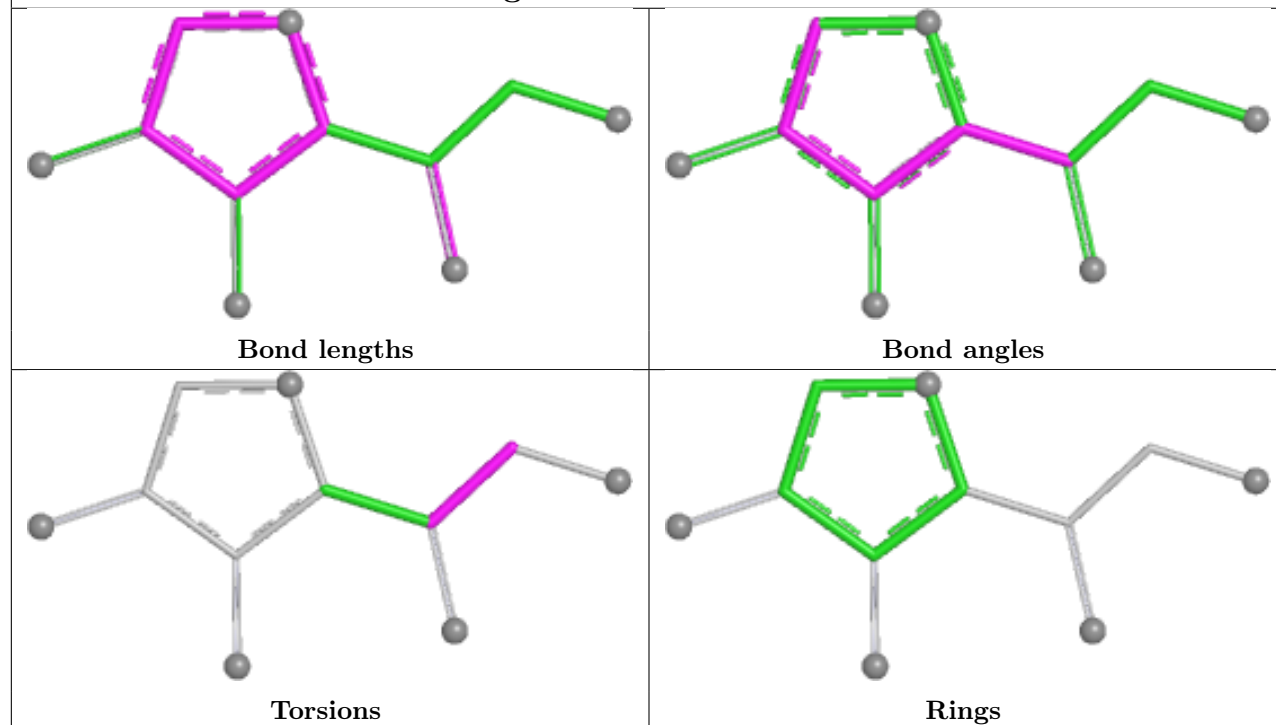
Ligand A1AIO B 2014

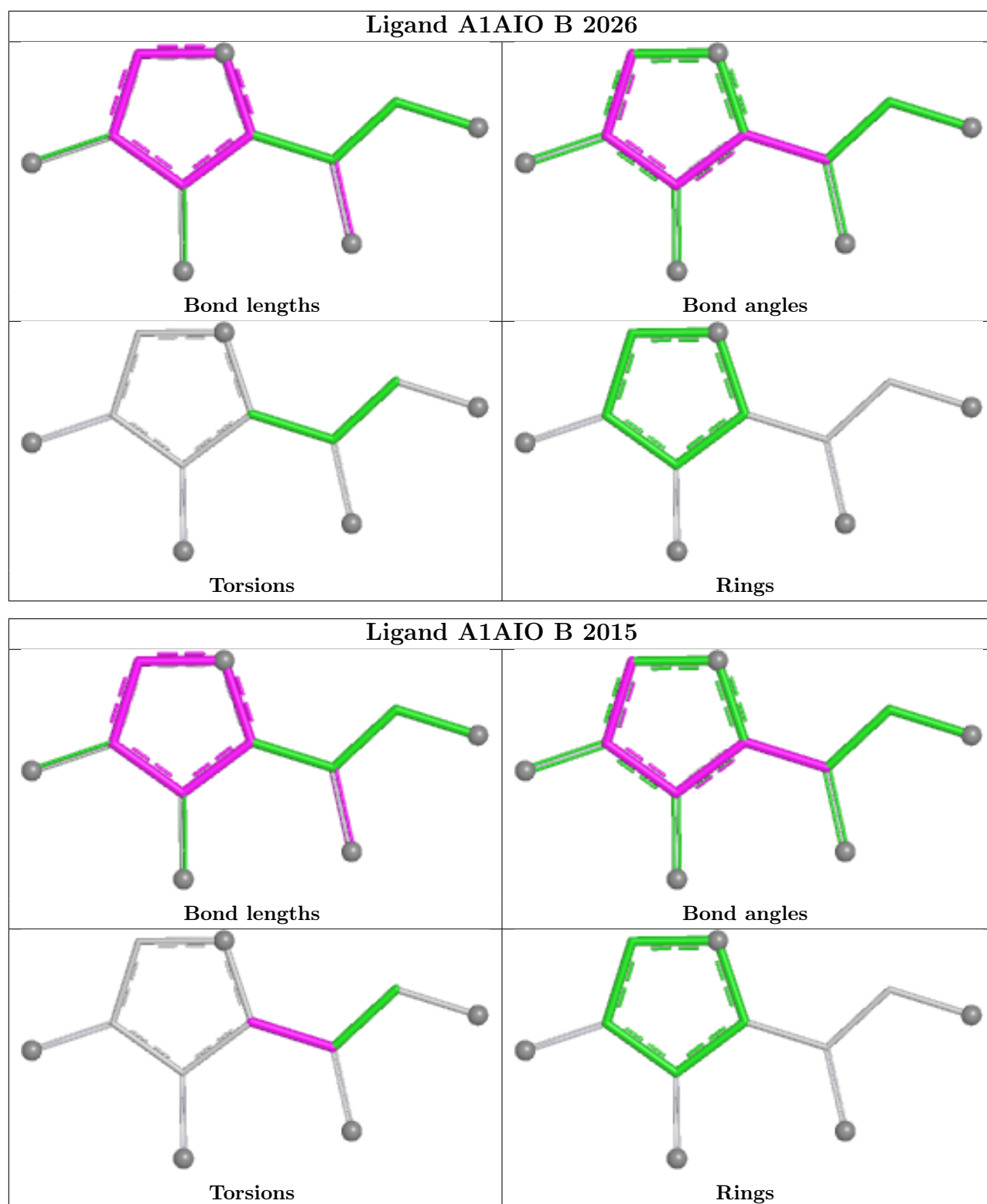


Ligand A1AIO A 2017



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.

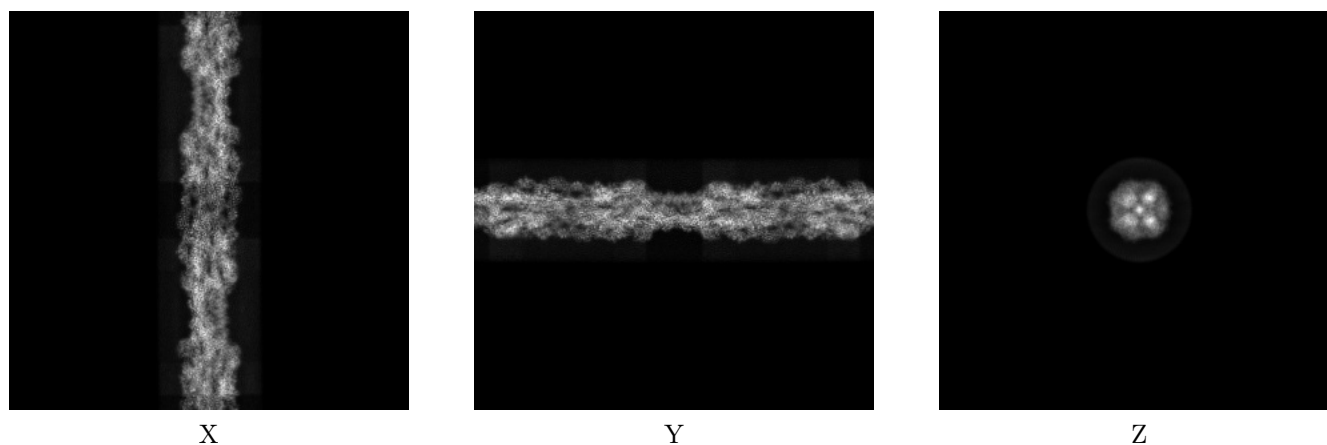
6 Map visualisation [i](#)

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](#)

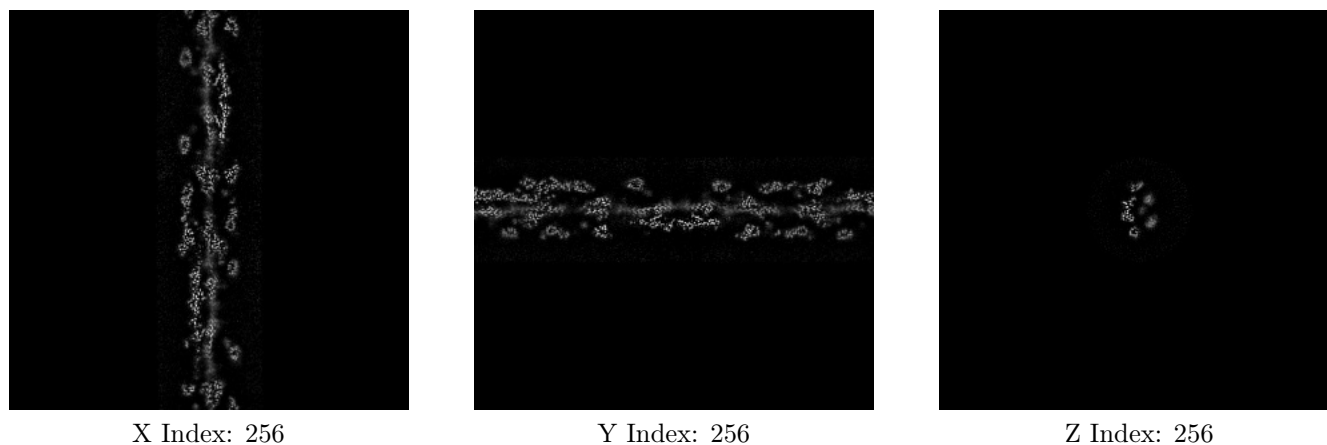
6.1.1 Primary map



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

6.2 Central slices [i](#)

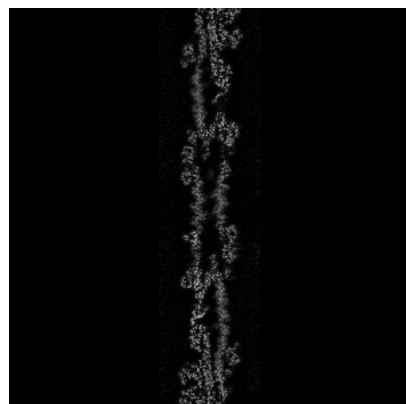
6.2.1 Primary map



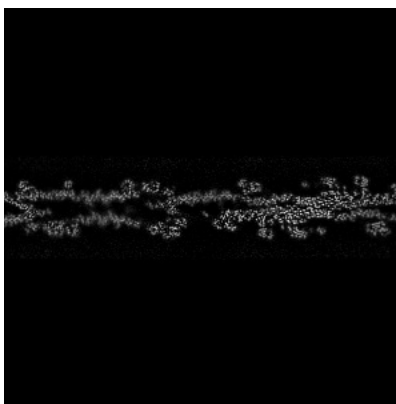
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

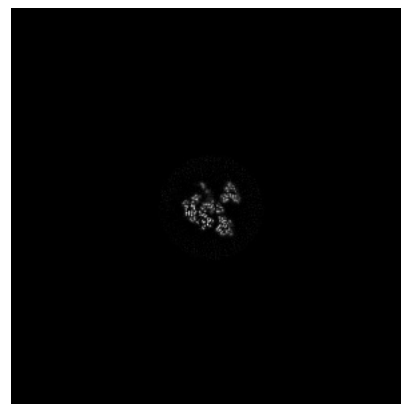
6.3.1 Primary map



X Index: 270



Y Index: 271

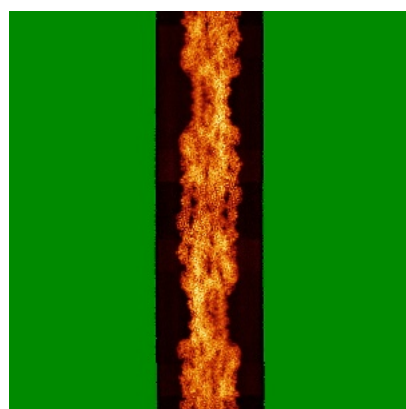


Z Index: 161

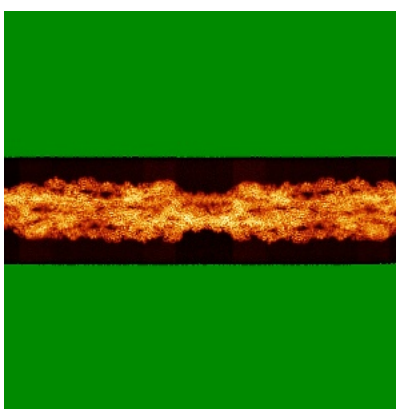
The images above show the largest variance slices of the map in three orthogonal directions.

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

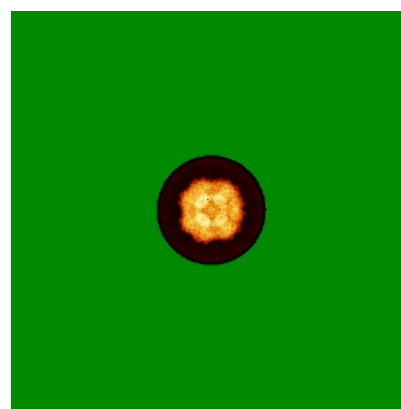
6.4.1 Primary map



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.

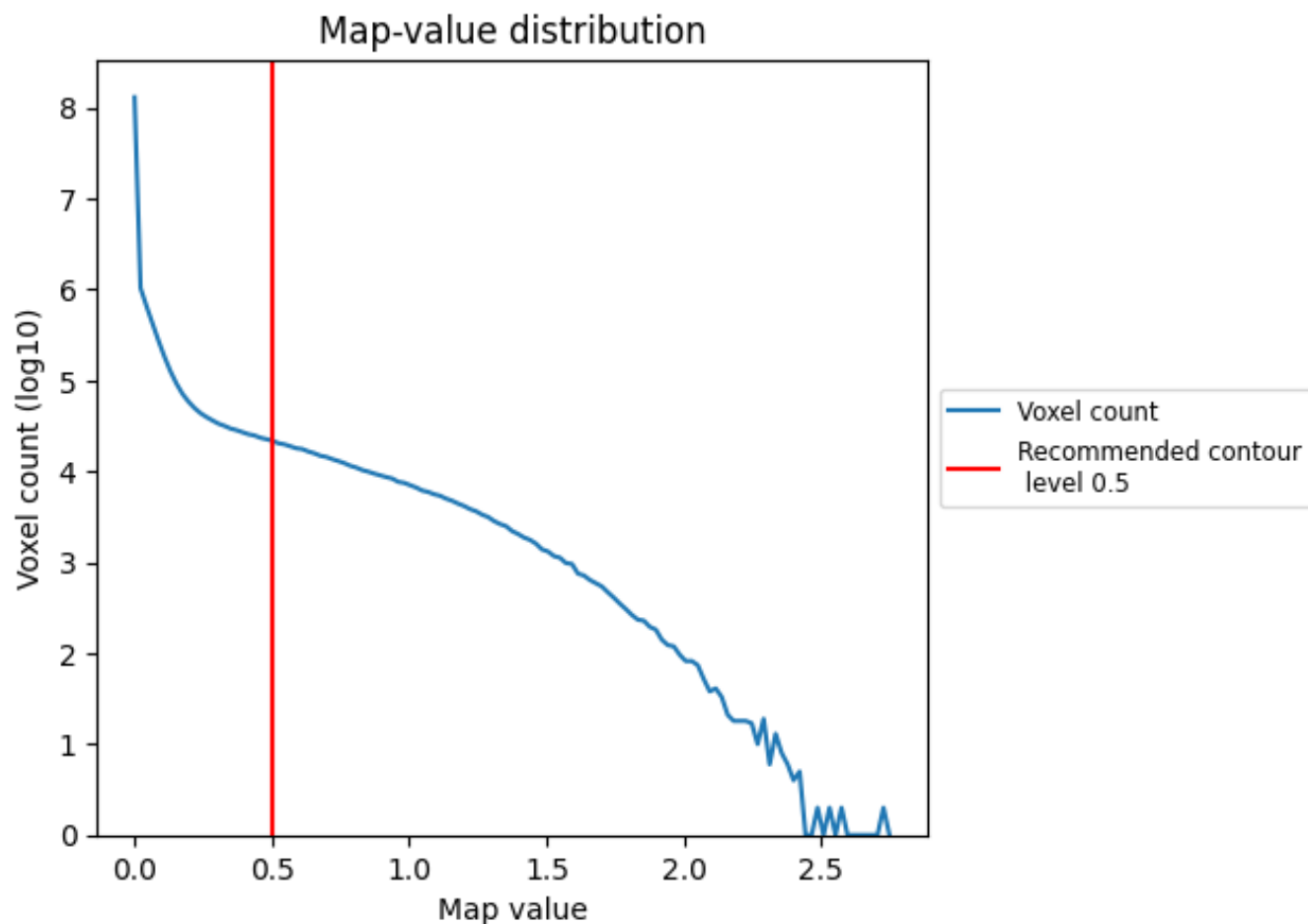
6.6 Mask visualisation

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

7 Map analysis [i](#)

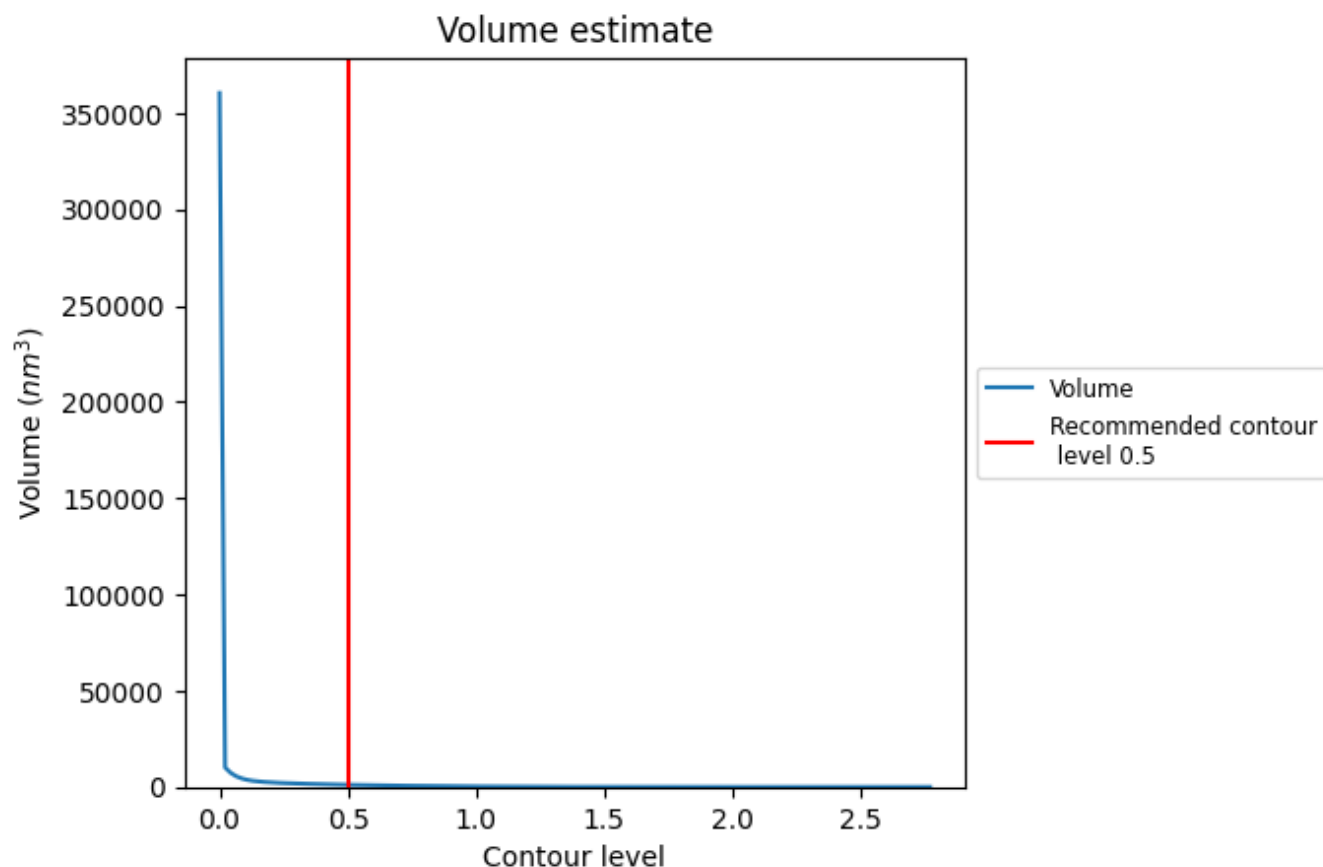
This section contains the results of statistical analysis of the map.

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.

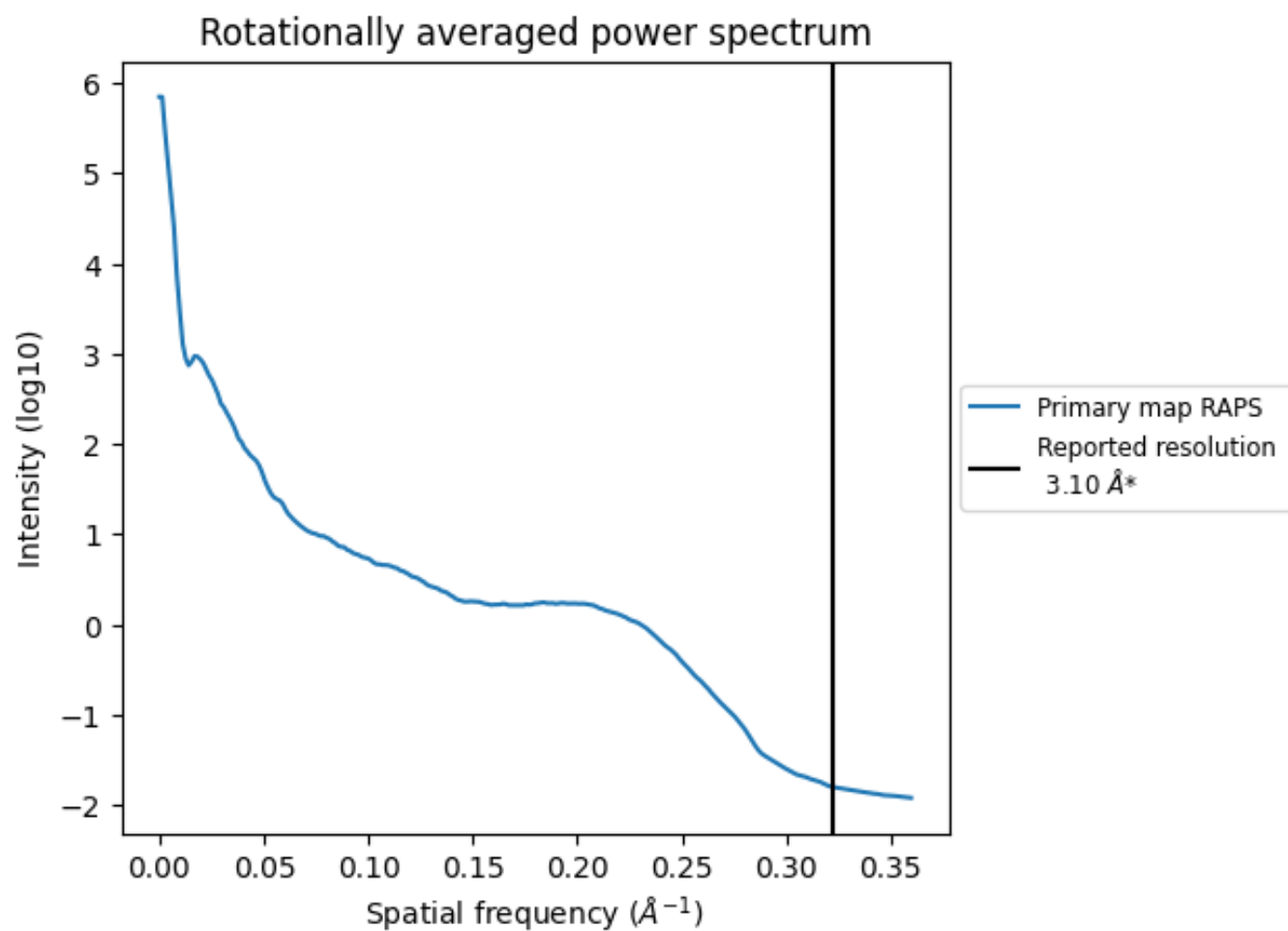
7.2 Volume estimate [i](#)



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 $\text{\AA}^{-1}$

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](#)



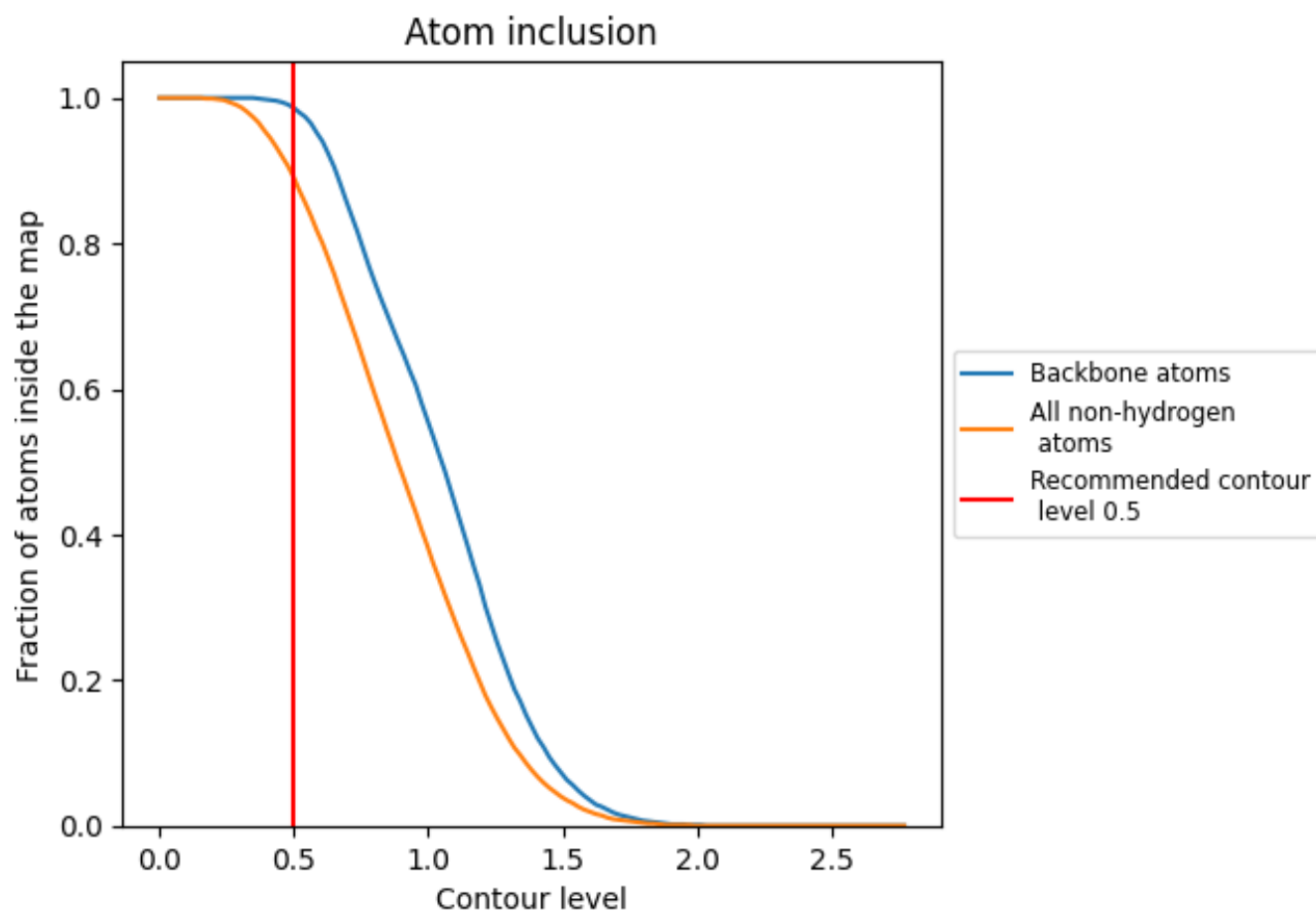
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



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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