



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 30, 2026 – 04:43 PM UTC

PDB ID : 7NPA / pdb_00007npa
Title : Crystal structure of the Coenzyme F420-dependent sulfite reductase from
Methanothermococcus thermolithotrophicus at 1.55-Å resolution
Authors : Jespersen, M.; Wagner, T.
Deposited on : 2021-02-26
Resolution : 1.55 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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

A user guide is available at

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

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:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

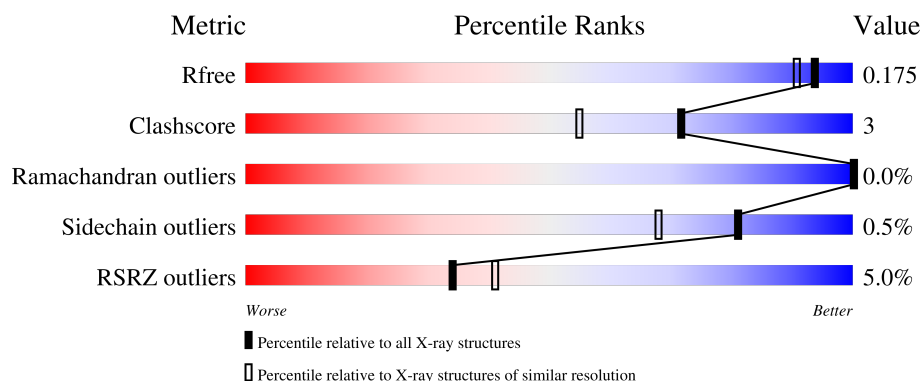
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2145 (1.56-1.56)
Clashscore	190562	2189 (1.56-1.56)
Ramachandran outliers	187476	2153 (1.56-1.56)
Sidechain outliers	187428	2150 (1.56-1.56)
RSRZ outliers	180081	2146 (1.56-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	618	% 94% 6%
1	B	618	% 94% 6%
1	C	618	% 95% 5%
1	D	618	5% 91% 9%
1	E	618	7% 90% 10%

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Mol	Chain	Length	Quality of chain
1	F	618	
1	G	618	
1	H	618	
1	I	618	
1	J	618	
1	K	618	
1	L	618	
1	M	618	
1	N	618	
1	O	618	
1	P	618	

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
2	SF4	N	1006[A]	-	-	X	-
2	SF4	N	1007[A]	-	-	X	-
5	SRM	A	1109	X	-	-	-
5	SRM	B	4210	X	-	-	-
5	SRM	C	3910	X	-	-	-
5	SRM	D	4610	X	-	-	-
5	SRM	E	1109	X	-	-	-
5	SRM	F	1109	X	-	-	-
5	SRM	G	1109	X	-	-	-
5	SRM	H	4410	X	-	-	-
5	SRM	I	1109	X	-	-	-
5	SRM	J	1109	X	-	-	-
5	SRM	K	1109	X	-	-	-
5	SRM	L	1109	X	-	-	-
5	SRM	M	1109	X	-	-	-
5	SRM	N	1012	X	-	-	-
5	SRM	O	1109	X	-	-	-
5	SRM	P	1109	X	-	-	-

2 Entry composition [i](#)

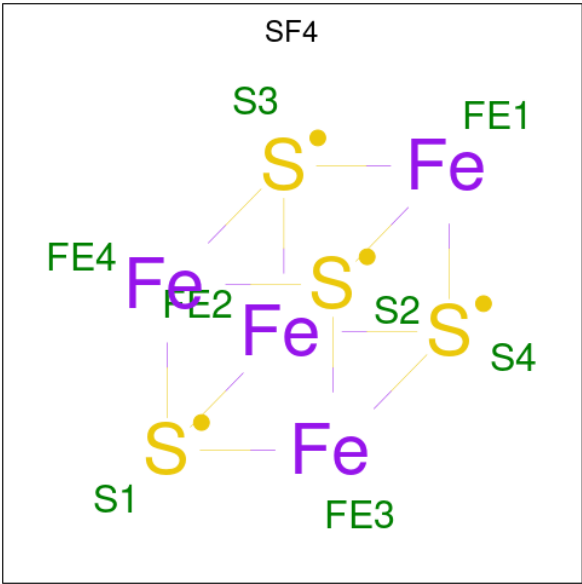
There are 13 unique types of molecules in this entry. The entry contains 93689 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Coenzyme F420-dependent sulfite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	618	Total	C	N	O	S	0	4	0
			4869	3083	820	925	41			
1	B	618	Total	C	N	O	S	0	3	0
			4863	3081	821	920	41			
1	C	618	Total	C	N	O	S	0	3	0
			4862	3079	820	922	41			
1	D	617	Total	C	N	O	S	0	1	0
			4838	3064	816	918	40			
1	E	617	Total	C	N	O	S	0	2	0
			4845	3068	817	920	40			
1	F	618	Total	C	N	O	S	0	5	0
			4877	3090	823	923	41			
1	G	618	Total	C	N	O	S	0	3	0
			4858	3077	819	920	42			
1	H	617	Total	C	N	O	S	0	2	0
			4843	3067	817	918	41			
1	I	618	Total	C	N	O	S	0	3	0
			4863	3081	821	920	41			
1	J	618	Total	C	N	O	S	0	2	0
			4855	3075	819	920	41			
1	K	617	Total	C	N	O	S	0	2	0
			4845	3068	817	920	40			
1	L	617	Total	C	N	O	S	0	2	0
			4847	3070	819	918	40			
1	M	617	Total	C	N	O	S	0	1	0
			4837	3064	816	917	40			
1	N	616	Total	C	N	O	S	0	266	0
			6587	4178	1095	1263	51			
1	O	617	Total	C	N	O	S	0	1	0
			4837	3064	816	917	40			
1	P	617	Total	C	N	O	S	0	1	0
			4837	3064	816	917	40			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	C	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	D	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	E	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	F	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	G	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0
2	H	1	Total 8	Fe 4	S 4	0	0
2	I	1	Total 8	Fe 4	S 4	0	0
2	I	1	Total 8	Fe 4	S 4	0	0
2	I	1	Total 8	Fe 4	S 4	0	0
2	I	1	Total 8	Fe 4	S 4	0	0
2	I	1	Total 8	Fe 4	S 4	0	0
2	I	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	J	1	Total 8	Fe 4	S 4	0	0
2	J	1	Total 8	Fe 4	S 4	0	0
2	J	1	Total 8	Fe 4	S 4	0	0
2	J	1	Total 8	Fe 4	S 4	0	0
2	J	1	Total 8	Fe 4	S 4	0	0
2	J	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	K	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	L	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0

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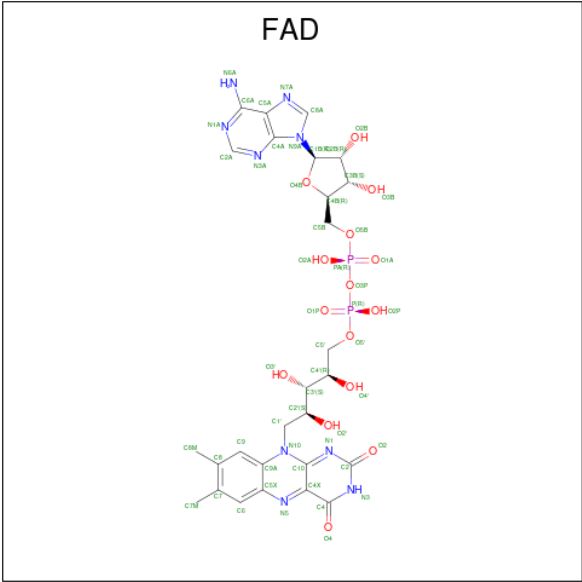
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 16	Fe 8	S 8	0	1
2	N	1	Total 8	Fe 4	S 4	0	1
2	N	1	Total 8	Fe 4	S 4	0	1
2	O	1	Total 8	Fe 4	S 4	0	0
2	O	1	Total 8	Fe 4	S 4	0	0
2	O	1	Total 8	Fe 4	S 4	0	0
2	O	1	Total 8	Fe 4	S 4	0	0
2	O	1	Total 8	Fe 4	S 4	0	0
2	O	1	Total 8	Fe 4	S 4	0	0
2	O	1	Total 8	Fe 4	S 4	0	0
2	P	1	Total 8	Fe 4	S 4	0	0
2	P	1	Total 8	Fe 4	S 4	0	0
2	P	1	Total 8	Fe 4	S 4	0	0
2	P	1	Total 8	Fe 4	S 4	0	0
2	P	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
2	P	1	8	4	4	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂) (labeled as "Ligand of Interest" by depositor).



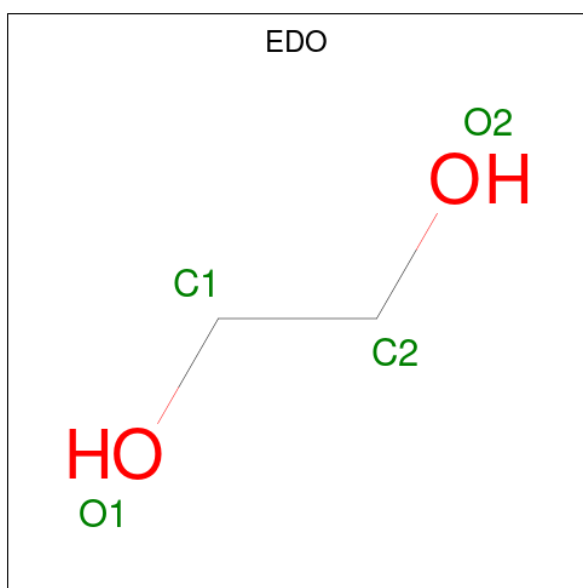
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	53	27	9	15	2	0	0
3	B	1	53	27	9	15	2	0	0
3	C	1	53	27	9	15	2	0	0
3	D	1	53	27	9	15	2	0	0
3	E	1	53	27	9	15	2	0	0
3	F	1	53	27	9	15	2	0	0
3	G	1	53	27	9	15	2	0	0
3	H	1	53	27	9	15	2	0	0
3	I	1	53	27	9	15	2	0	0
3	J	1	53	27	9	15	2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	K	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	L	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	M	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	N	1	Total	C	N	O	P	0	1
			53	27	9	15	2		
3	N	1	Total	C	N	O	P	0	1
			53	27	9	15	2		
3	O	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
3	P	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	1
			4	2	2		
4	B	1	Total	C	O	0	1
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	1
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	1
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	F	1	Total	C	O	0	1
			4	2	2		
4	F	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	G	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	J	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		

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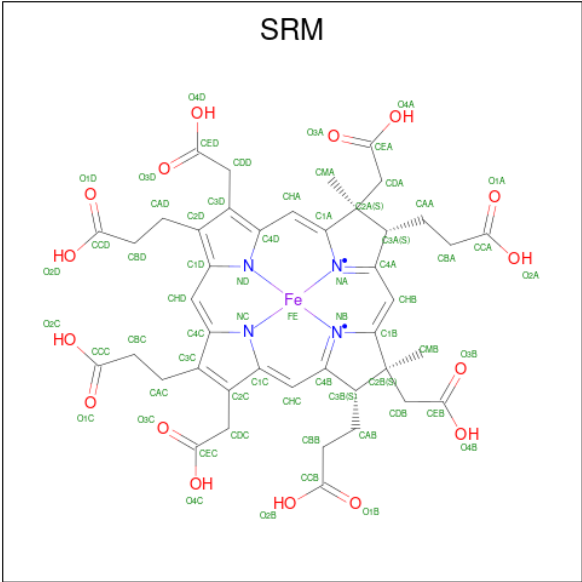
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	K	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	L	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	M	1	Total	C	O	0	0
			4	2	2		
4	N	1	Total	C	O	0	0
			4	2	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	N	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	O	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		
4	P	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is SIROHEME (CCD ID: SRM) (formula: $C_{42}H_{44}FeN_4O_{16}$) (labeled as "Ligand of Interest" by depositor).



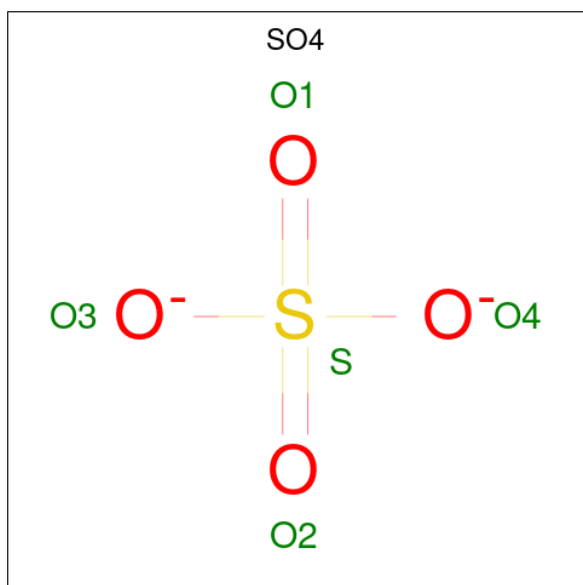
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	B	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	C	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	D	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	E	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	F	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	G	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	H	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	I	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	J	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	K	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	L	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	M	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	N	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	O	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		
5	P	1	Total	C	Fe	N	O	0	0
			63	42	1	4	16		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	E	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		

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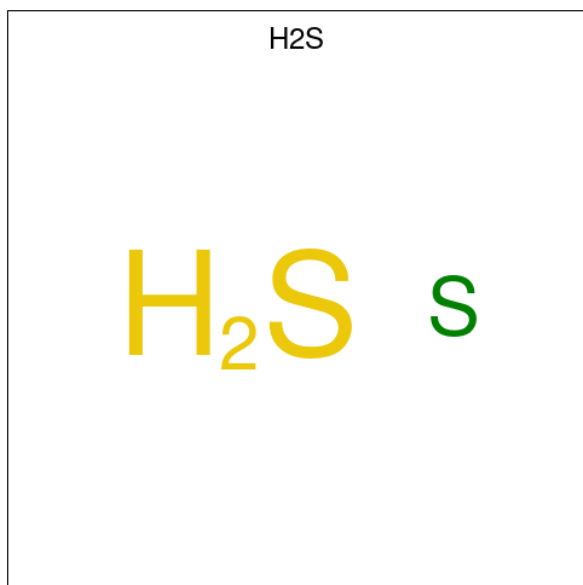
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	K	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	L	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	M	1	Total	O	S	0	0
			5	4	1		
6	N	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		
6	O	1	Total	O	S	0	0
			5	4	1		
6	P	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	S	0	0
			1	1		
7	B	1	Total	S	0	0
			1	1		
7	C	1	Total	S	0	0
			1	1		
7	D	1	Total	S	0	0
			1	1		
7	E	1	Total	S	0	0
			1	1		
7	F	1	Total	S	0	0
			1	1		
7	G	1	Total	S	0	0
			1	1		
7	H	1	Total	S	0	0
			1	1		
7	I	1	Total	S	0	0
			1	1		
7	J	1	Total	S	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	K	1	Total S 1 1	0	0
7	L	1	Total S 1 1	0	0
7	M	1	Total S 1 1	0	0
7	N	1	Total S 1 1	0	0
7	O	1	Total S 1 1	0	0
7	P	1	Total S 1 1	0	0

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

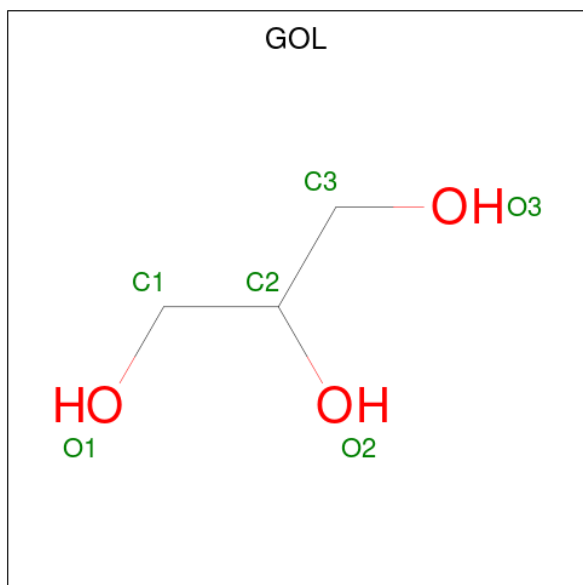
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Cl 2 2	0	1
8	B	2	Total Cl 2 2	0	1
8	C	2	Total Cl 2 2	0	1
8	D	2	Total Cl 2 2	0	1
8	E	2	Total Cl 2 2	0	1
8	F	1	Total Cl 1 1	0	1
8	G	2	Total Cl 2 2	0	1
8	H	2	Total Cl 2 2	0	1
8	I	2	Total Cl 2 2	0	1
8	J	2	Total Cl 2 2	0	1
8	K	2	Total Cl 2 2	0	1
8	L	1	Total Cl 1 1	0	1
8	M	2	Total Cl 2 2	0	1

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	N	1	Total	Cl	0	1
			1	1		
8	O	2	Total	Cl	0	1
			2	2		
8	P	2	Total	Cl	0	1
			2	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	1
			6	3	3		
9	B	1	Total	C	O	0	1
			6	3	3		
9	B	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	C	1	Total	C	O	0	0
			6	3	3		
9	E	1	Total	C	O	0	0
			6	3	3		
9	F	1	Total	C	O	0	0
			6	3	3		
9	G	1	Total	C	O	0	1
			6	3	3		

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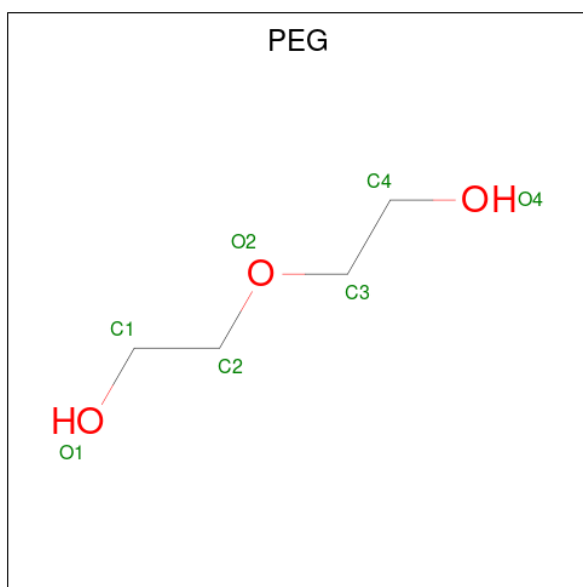
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	1
9	K	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0
9	N	1	Total C O 6 3 3	0	0
9	N	1	Total C O 6 3 3	0	0
9	O	1	Total C O 6 3 3	0	0
9	P	1	Total C O 6 3 3	0	0
9	P	1	Total C O 6 3 3	0	0

- Molecule 10 is LITHIUM ION (CCD ID: LI) (formula: Li).

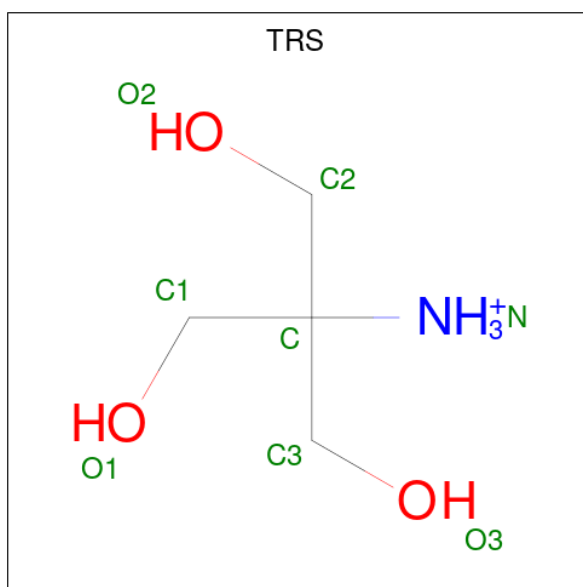
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Li 1 1	0	0
10	F	1	Total Li 1 1	0	0
10	L	1	Total Li 1 1	0	0
10	P	1	Total Li 1 1	0	0

- Molecule 11 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	D	1	Total	C	O	0	0
			7	4	3		
11	K	1	Total	C	O	0	0
			7	4	3		
11	M	1	Total	C	O	0	0
			7	4	3		
11	M	1	Total	C	O	0	0
			7	4	3		
11	N	1	Total	C	O	0	0
			7	4	3		

- Molecule 12 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	H	1	Total	C	N	O	0	0
			8	4	1	3		
12	I	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	800	Total	O	0	6
			800	800		
13	B	744	Total	O	0	4
			744	744		
13	C	762	Total	O	0	0
			762	762		
13	D	713	Total	O	0	5
			713	713		
13	E	645	Total	O	0	0
			645	645		
13	F	605	Total	O	0	0
			605	605		
13	G	748	Total	O	0	3
			748	748		
13	H	685	Total	O	0	0
			685	685		
13	I	704	Total	O	0	7
			704	704		
13	J	567	Total	O	0	1
			567	567		

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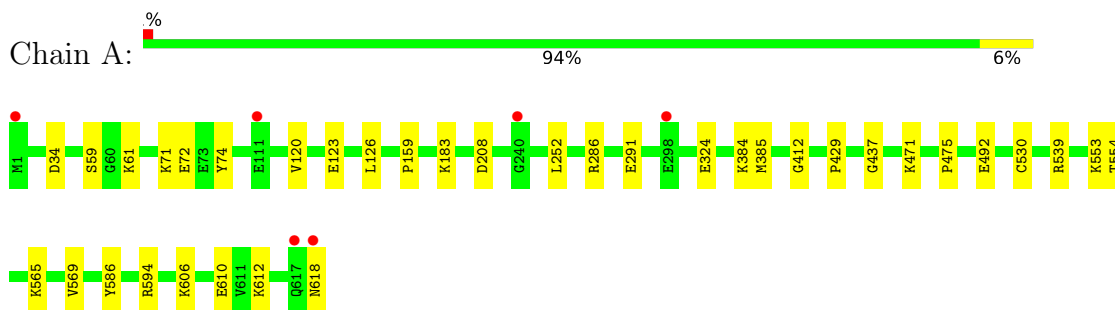
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	K	766	Total 766	O 766	0	1
13	L	681	Total 681	O 681	0	3
13	M	690	Total 690	O 690	0	2
13	N	465	Total 465	O 465	0	12
13	O	665	Total 665	O 665	0	2
13	P	532	Total 532	O 532	0	0

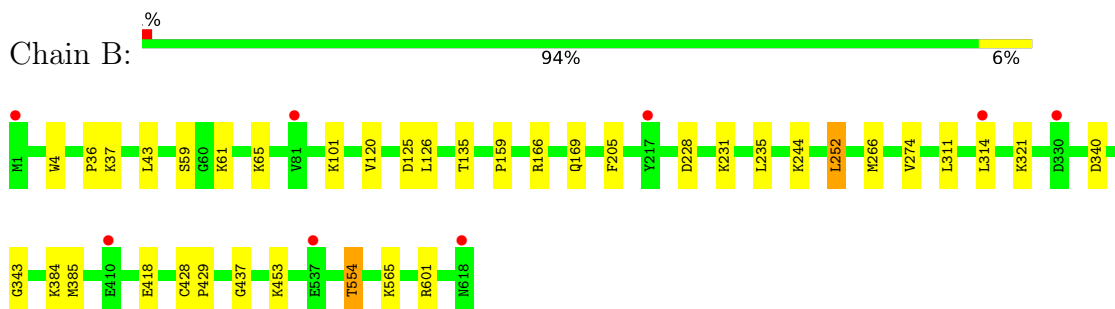
3 Residue-property plots [i](#)

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

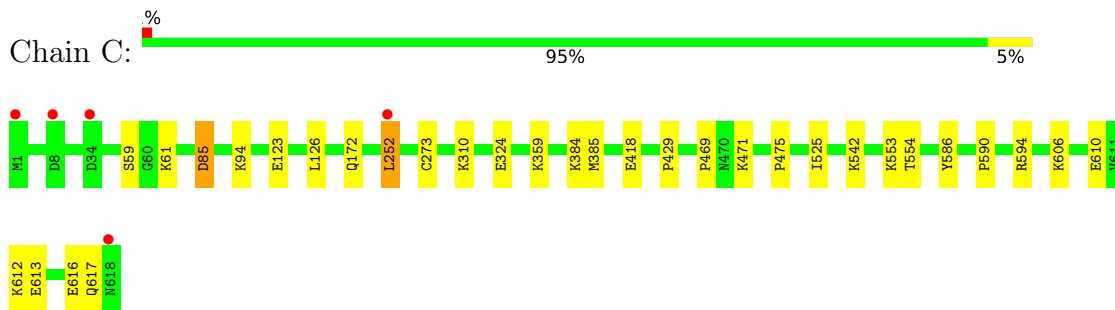
- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase

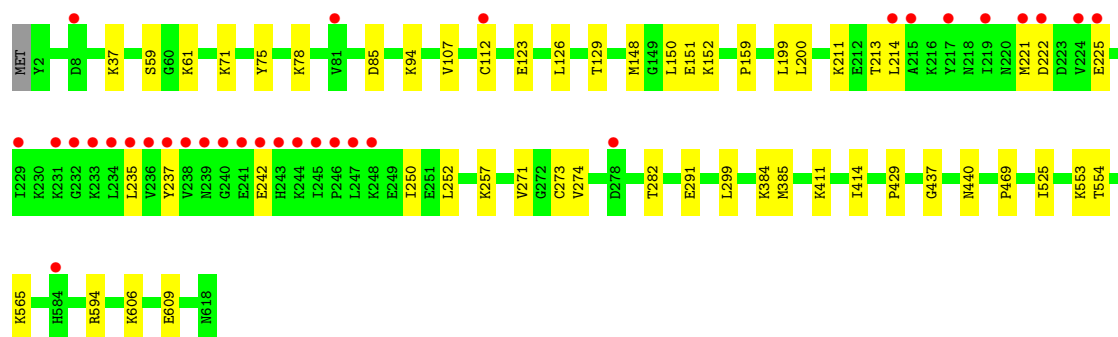


- Molecule 1: Coenzyme F420-dependent sulfite reductase

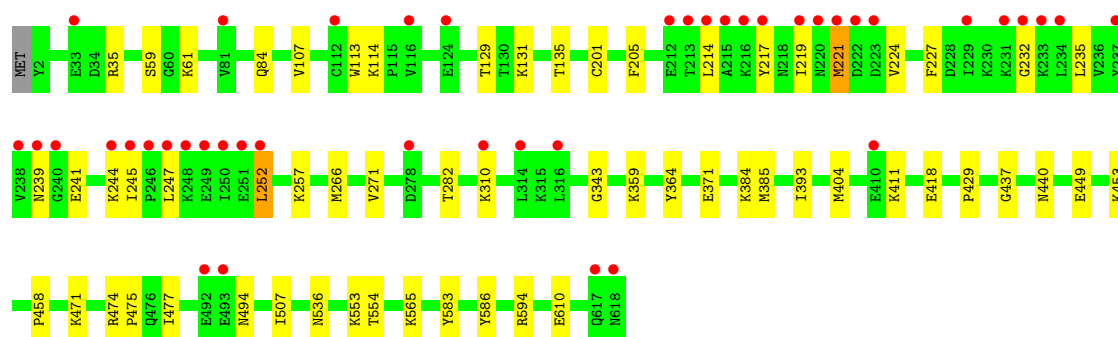
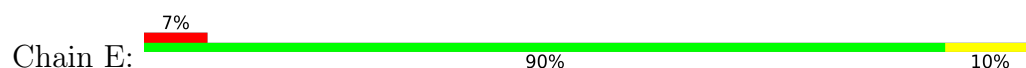


- Molecule 1: Coenzyme F420-dependent sulfite reductase

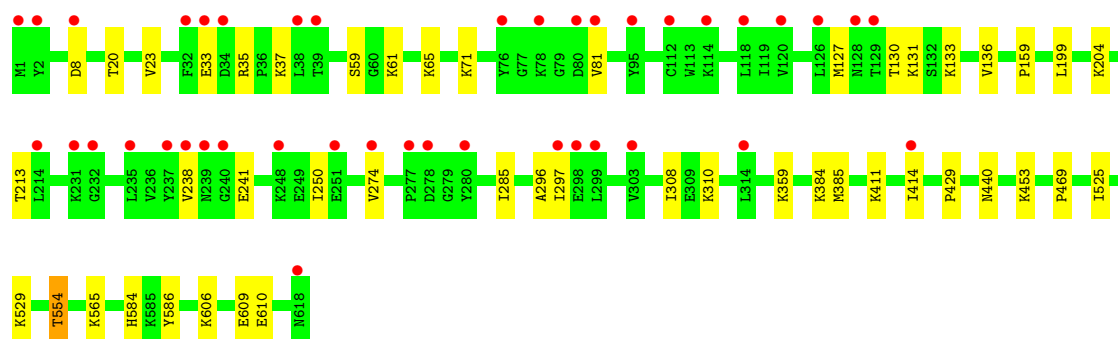
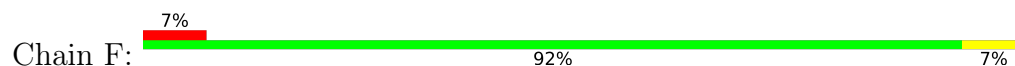




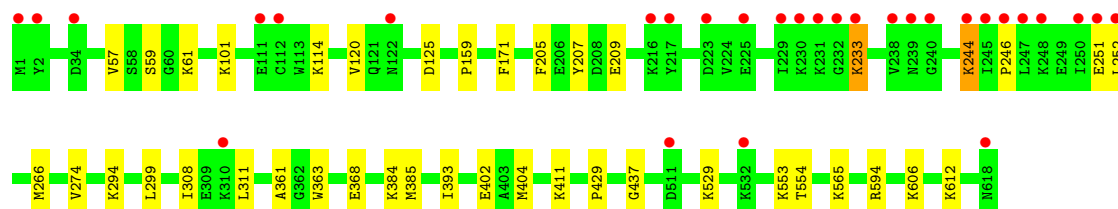
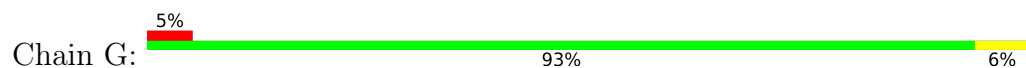
- Molecule 1: Coenzyme F420-dependent sulfite reductase



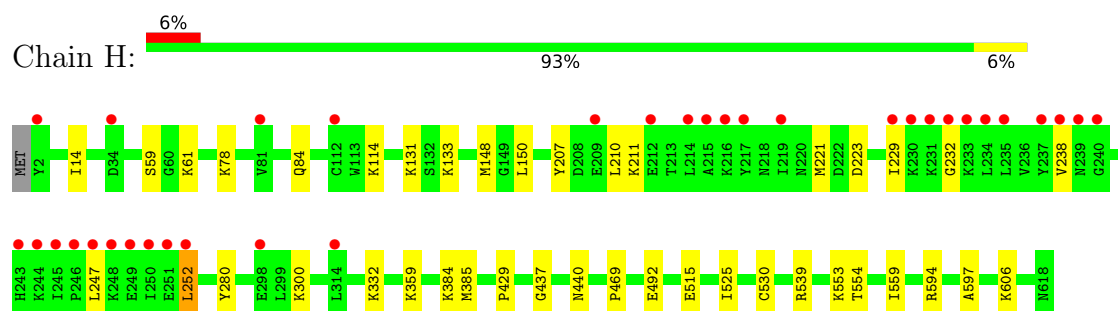
- Molecule 1: Coenzyme F420-dependent sulfite reductase



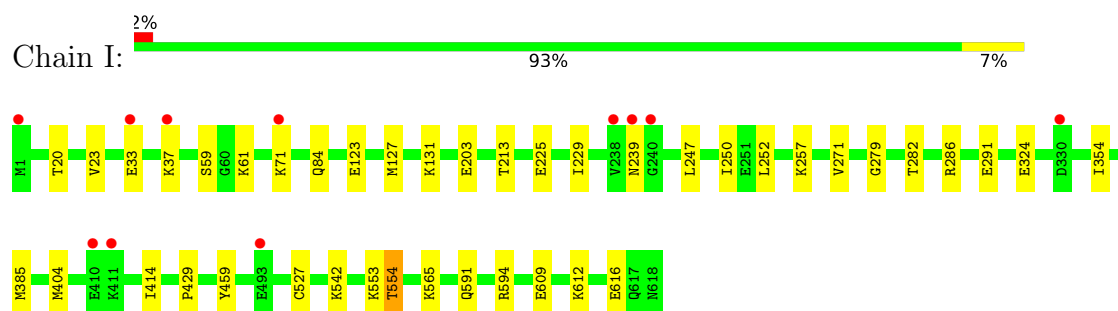
- Molecule 1: Coenzyme F420-dependent sulfite reductase



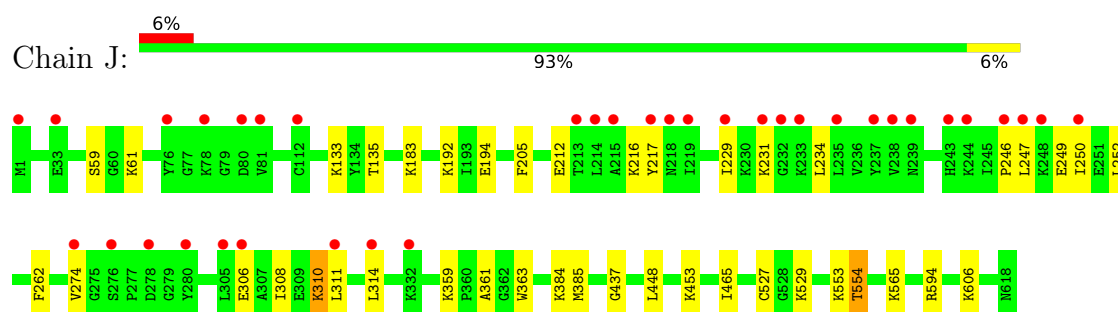
- Molecule 1: Coenzyme F420-dependent sulfite reductase



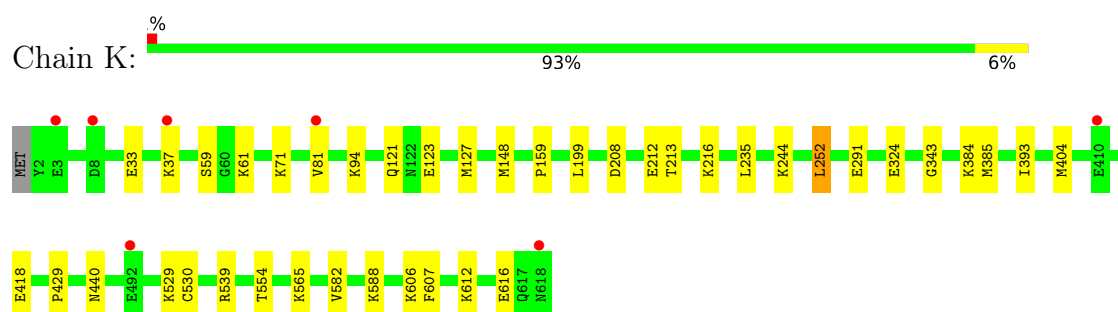
- Molecule 1: Coenzyme F420-dependent sulfite reductase



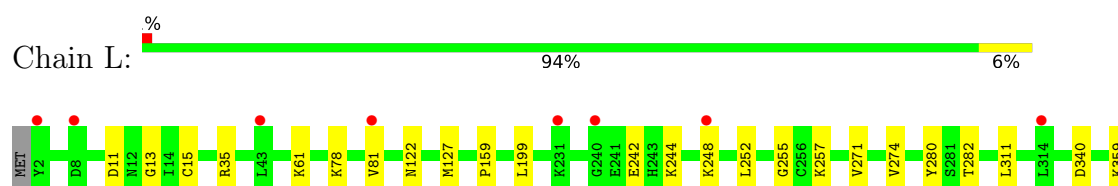
- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase

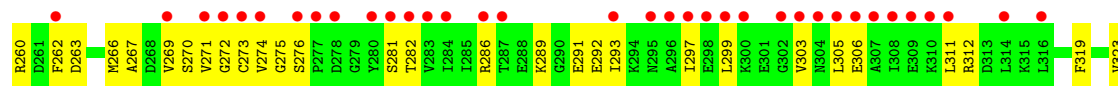
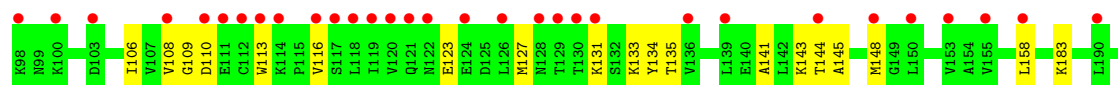
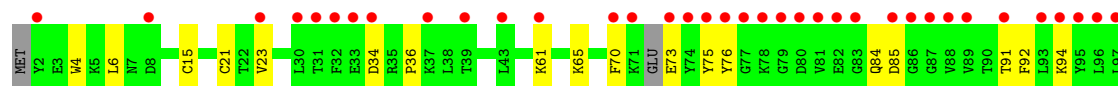
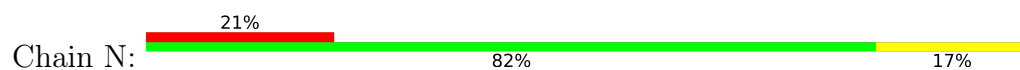




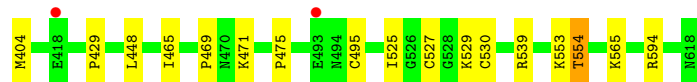
- Molecule 1: Coenzyme F420-dependent sulfite reductase



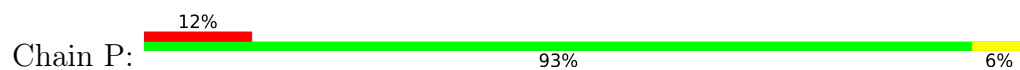
- Molecule 1: Coenzyme F420-dependent sulfite reductase

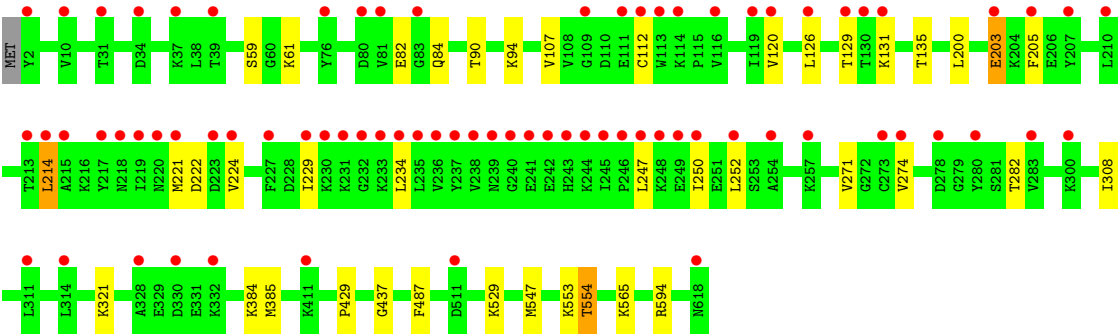


- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	113.15Å 124.16Å 241.06Å 102.28° 95.71° 90.25°	Depositor
Resolution (Å)	77.29 – 1.55 77.29 – 1.55	Depositor EDS
% Data completeness (in resolution range)	75.5 (77.29-1.55) 75.6 (77.29-1.55)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.55Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.159 , 0.171 0.164 , 0.175	Depositor DCC
R_{free} test set	69216 reflections (3.75%)	wwPDB-VP
Wilson B-factor (Å ²)	13.8	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h,k,-k-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	93689	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.18% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: H2S, SF4, EDO, PEG, TRS, SRM, GOL, LI, FAD, SO4, CL

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	0.43	0/4946	0.63	2/6639 (0.0%)
1	B	0.48	0/4940	0.68	0/6628
1	C	0.43	0/4939	0.62	1/6628 (0.0%)
1	D	0.45	0/4915	0.65	0/6596
1	E	0.52	0/4922	0.71	0/6607
1	F	0.44	0/4954	0.64	0/6648
1	G	0.49	0/4935	0.69	1/6624 (0.0%)
1	H	0.45	0/4920	0.63	0/6604
1	I	0.44	0/4940	0.63	0/6628
1	J	0.45	0/4932	0.65	0/6617
1	K	0.40	0/4922	0.61	0/6607
1	L	0.42	0/4925	0.60	0/6612
1	M	0.50	0/4914	0.71	0/6596
1	N	0.54	1/6693 (0.0%)	0.66	1/8982 (0.0%)
1	O	0.45	0/4914	0.65	0/6596
1	P	0.52	0/4914	0.69	1/6596 (0.0%)
All	All	0.47	1/80625 (0.0%)	0.65	6/108208 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	217[A]	TYR	C-N	-5.10	1.26	1.33

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	57	VAL	N-CA-C	-6.33	105.57	111.45
1	A	412	GLY	N-CA-C	5.54	122.97	115.32
1	N	34	ASP	N-CA-C	-5.40	106.70	113.72
1	A	34	ASP	N-CA-C	-5.25	106.92	113.38
1	C	85	ASP	O-C-N	5.07	124.58	120.83

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4869	0	4909	28	0
1	B	4863	0	4917	36	0
1	C	4862	0	4908	22	0
1	D	4838	0	4881	38	0
1	E	4845	0	4884	38	0
1	F	4877	0	4931	32	0
1	G	4858	0	4906	34	0
1	H	4843	0	4885	32	0
1	I	4863	0	4917	32	0
1	J	4855	0	4905	35	0
1	K	4845	0	4884	29	0
1	L	4847	0	4888	28	0
1	M	4837	0	4881	22	0
1	N	6587	0	6651	106	0
1	O	4837	0	4881	31	0
1	P	4837	0	4881	32	0
2	A	48	0	0	2	0
2	B	48	0	0	2	0
2	C	48	0	0	0	0
2	D	48	0	0	1	0
2	E	48	0	0	1	0
2	F	48	0	0	0	0
2	G	48	0	0	2	0
2	H	48	0	0	1	0
2	I	48	0	0	0	0
2	J	48	0	0	1	0
2	K	48	0	0	0	0
2	L	48	0	0	0	0
2	M	48	0	0	2	0
2	N	64	0	0	5	0
2	O	48	0	0	1	0
2	P	48	0	0	1	0
3	A	53	0	31	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	53	0	31	0	0
3	C	53	0	31	0	0
3	D	53	0	31	1	0
3	E	53	0	31	1	0
3	F	53	0	31	0	0
3	G	53	0	31	0	0
3	H	53	0	31	0	0
3	I	53	0	31	1	0
3	J	53	0	31	0	0
3	K	53	0	31	1	0
3	L	53	0	31	0	0
3	M	53	0	31	0	0
3	N	106	0	62	4	0
3	O	53	0	31	0	0
3	P	53	0	31	1	0
4	A	40	0	60	2	0
4	B	52	0	78	2	0
4	C	32	0	48	0	0
4	D	36	0	54	1	0
4	E	32	0	48	1	0
4	F	20	0	30	2	0
4	G	48	0	72	4	0
4	H	16	0	24	4	0
4	I	32	0	48	1	0
4	J	28	0	42	4	0
4	K	28	0	42	1	0
4	L	16	0	24	0	0
4	M	52	0	78	0	0
4	N	8	0	12	0	0
4	O	36	0	54	0	0
4	P	16	0	24	0	0
5	A	63	0	34	0	0
5	B	63	0	34	0	0
5	C	63	0	34	0	0
5	D	63	0	34	0	0
5	E	63	0	34	1	0
5	F	63	0	34	1	0
5	G	63	0	34	0	0
5	H	63	0	34	0	0
5	I	63	0	34	0	0
5	J	63	0	34	0	0
5	K	63	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	L	63	0	34	0	0
5	M	63	0	34	1	0
5	N	63	0	34	1	0
5	O	63	0	34	0	0
5	P	63	0	34	0	0
6	A	5	0	0	0	0
6	B	10	0	0	1	0
6	C	5	0	0	0	0
6	D	15	0	0	0	0
6	E	5	0	0	0	0
6	F	20	0	0	1	0
6	G	5	0	0	0	0
6	H	10	0	0	0	0
6	I	5	0	0	0	0
6	J	10	0	0	0	0
6	K	10	0	0	0	0
6	L	15	0	0	0	0
6	M	15	0	0	0	0
6	N	5	0	0	0	0
6	O	10	0	0	0	0
6	P	10	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
7	I	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	O	1	0	0	0	0
7	P	1	0	0	0	0
8	A	2	0	0	0	0
8	B	2	0	0	0	0
8	C	2	0	0	0	0
8	D	2	0	0	0	0
8	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	1	0	0	0	0
8	G	2	0	0	0	0
8	H	2	0	0	0	0
8	I	2	0	0	0	0
8	J	2	0	0	0	0
8	K	2	0	0	0	0
8	L	1	0	0	0	0
8	M	2	0	0	0	0
8	N	1	0	0	0	0
8	O	2	0	0	0	0
8	P	2	0	0	0	0
9	B	18	0	24	1	0
9	C	12	0	16	2	0
9	E	6	0	8	0	0
9	F	6	0	8	1	0
9	G	6	0	8	0	0
9	I	12	0	16	4	0
9	J	12	0	16	0	0
9	K	6	0	8	0	0
9	M	6	0	8	1	0
9	N	12	0	16	1	0
9	O	6	0	8	0	0
9	P	12	0	16	2	0
10	C	1	0	0	0	0
10	F	1	0	0	0	0
10	L	1	0	0	0	0
10	P	1	0	0	0	0
11	D	7	0	10	0	0
11	K	7	0	10	1	0
11	M	14	0	20	2	0
11	N	7	0	10	0	0
12	H	8	0	12	0	0
12	I	8	0	12	0	0
13	A	800	0	0	5	0
13	B	744	0	0	7	0
13	C	762	0	0	2	0
13	D	713	0	0	2	0
13	E	645	0	0	2	0
13	F	605	0	0	5	0
13	G	748	0	0	3	0
13	H	685	0	0	2	0
13	I	704	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	J	567	0	0	7	0
13	K	766	0	0	3	0
13	L	681	0	0	5	0
13	M	690	0	0	1	0
13	N	465	0	0	2	0
13	O	665	0	0	5	0
13	P	532	0	0	5	0
All	All	93689	0	82144	548	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 3.

The worst 5 of 548 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:B:274:VAL:HG21	1:B:311:LEU:CD1	2.03	0.87
1:N:263[B]:ASP:OD2	1:N:312[B]:ARG:NE	2.16	0.78
1:B:274:VAL:HG21	1:B:311:LEU:HD12	1.70	0.71
1:C:385:MET:HE2	1:D:385:MET:HE2	1.74	0.69
1:J:252:LEU:HD23	1:J:252:LEU:H	1.55	0.69

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	620/618 (100%)	605 (98%)	15 (2%)	0	100	100
1	B	619/618 (100%)	604 (98%)	15 (2%)	0	100	100
1	C	619/618 (100%)	603 (97%)	16 (3%)	0	100	100
1	D	616/618 (100%)	601 (98%)	15 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	617/618 (100%)	604 (98%)	13 (2%)	0	100	100
1	F	621/618 (100%)	606 (98%)	15 (2%)	0	100	100
1	G	619/618 (100%)	606 (98%)	13 (2%)	0	100	100
1	H	617/618 (100%)	605 (98%)	12 (2%)	0	100	100
1	I	619/618 (100%)	604 (98%)	15 (2%)	0	100	100
1	J	618/618 (100%)	603 (98%)	15 (2%)	0	100	100
1	K	617/618 (100%)	602 (98%)	15 (2%)	0	100	100
1	L	617/618 (100%)	603 (98%)	14 (2%)	0	100	100
1	M	616/618 (100%)	602 (98%)	14 (2%)	0	100	100
1	N	836/618 (135%)	800 (96%)	34 (4%)	2 (0%)	43	24
1	O	616/618 (100%)	602 (98%)	14 (2%)	0	100	100
1	P	616/618 (100%)	600 (97%)	16 (3%)	0	100	100
All	All	10103/9888 (102%)	9850 (98%)	251 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	N	243[A]	HIS
1	N	243[B]	HIS

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 X-ray entries followed by that with respect to entries of similar resolution.

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	528/524 (101%)	526 (100%)	2 (0%)	84	73
1	B	527/524 (101%)	525 (100%)	2 (0%)	84	73
1	C	527/524 (101%)	523 (99%)	4 (1%)	73	56
1	D	524/524 (100%)	521 (99%)	3 (1%)	78	64
1	E	525/524 (100%)	519 (99%)	6 (1%)	65	43
1	F	529/524 (101%)	524 (99%)	5 (1%)	70	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	527/524 (101%)	523 (99%)	4 (1%)	73	56
1	H	525/524 (100%)	522 (99%)	3 (1%)	78	64
1	I	527/524 (101%)	525 (100%)	2 (0%)	84	73
1	J	526/524 (100%)	524 (100%)	2 (0%)	84	73
1	K	525/524 (100%)	523 (100%)	2 (0%)	84	73
1	L	525/524 (100%)	524 (100%)	1 (0%)	87	79
1	M	524/524 (100%)	521 (99%)	3 (1%)	78	64
1	N	718/524 (137%)	713 (99%)	5 (1%)	76	59
1	O	524/524 (100%)	522 (100%)	2 (0%)	84	73
1	P	524/524 (100%)	522 (100%)	2 (0%)	84	73
All	All	8605/8384 (103%)	8557 (99%)	48 (1%)	81	64

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	554	THR
1	L	554	THR
1	I	414	ILE
1	J	554	THR
1	M	252	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	239	ASN
1	I	218	ASN
1	N	618	ASN
1	L	99	ASN
1	M	243	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 360 ligands modelled in this entry, 16 are modelled with single atom and 33 are monoatomic - leaving 311 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	GOL	P	1111	-	5,5,5	0.10	0	5,5,5	0.32	0
4	EDO	M	1123	-	3,3,3	0.11	0	2,2,2	0.13	0
2	SF4	L	1105	1	0,12,12	-	-	-		
12	TRS	I	1119	-	7,7,7	0.18	0	9,9,9	0.20	0
5	SRM	E	1109	1	68,70,70	2.52	21 (30%)	86,112,112	1.69	20 (23%)
6	SO4	A	1119	-	4,4,4	0.26	0	6,6,6	0.20	0
2	SF4	P	1102	1	0,12,12	-	-	-		
2	SF4	A	1102	1	0,12,12	-	-	-		
4	EDO	G	1113	-	3,3,3	0.08	0	2,2,2	0.20	0
6	SO4	F	1116	-	4,4,4	0.39	0	6,6,6	0.07	0
2	SF4	B	4206	1	0,12,12	-	-	-		
5	SRM	G	1109	1	68,70,70	2.49	22 (32%)	86,112,112	1.70	18 (20%)
2	SF4	K	1101	1	0,12,12	-	-	-		
2	SF4	C	3906	1	0,12,12	-	-	-		
9	GOL	I	1117	-	5,5,5	0.10	0	5,5,5	0.32	0
2	SF4	D	4603	1	0,12,12	-	-	-		
6	SO4	E	1118	-	4,4,4	0.28	0	6,6,6	0.25	0
2	SF4	G	1103	1	0,12,12	-	-	-		
5	SRM	H	4410	1	68,70,70	2.89	26 (38%)	86,112,112	1.97	26 (30%)
4	EDO	M	1108	-	3,3,3	0.41	0	2,2,2	0.39	0
4	EDO	A	1115	-	3,3,3	0.11	0	2,2,2	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	P	1101	1	0,12,12	-	-	-		
2	SF4	M	1107	1	0,12,12	-	-	-		
11	PEG	D	4601	-	6,6,6	0.14	0	5,5,5	0.08	0
2	SF4	B	4208	1	0,12,12	-	-	-		
2	SF4	P	1103	1	0,12,12	-	-	-		
2	SF4	H	4403	1	0,12,12	-	-	-		
4	EDO	I	1110	-	3,3,3	0.06	0	2,2,2	0.11	0
2	SF4	I	1104	1	0,12,12	-	-	-		
4	EDO	B	4223	-	3,3,3	0.07	0	2,2,2	0.12	0
4	EDO	D	4618	-	3,3,3	0.13	0	2,2,2	0.11	0
5	SRM	B	4210	1	68,70,70	2.61	23 (33%)	86,112,112	1.66	20 (23%)
2	SF4	J	1105	1	0,12,12	-	-	-		
4	EDO	M	1122	-	3,3,3	0.05	0	2,2,2	0.17	0
2	SF4	A	1104	1	0,12,12	-	-	-		
9	GOL	J	1114	-	5,5,5	0.08	0	5,5,5	0.30	0
2	SF4	E	1102	1	0,12,12	-	-	-		
4	EDO	E	1116	-	3,3,3	0.06	0	2,2,2	0.11	0
5	SRM	C	3910	1	68,70,70	2.47	23 (33%)	86,112,112	1.67	19 (22%)
5	SRM	M	1109	1	68,70,70	2.78	23 (33%)	86,112,112	1.87	24 (27%)
2	SF4	N	1008[B]	1	0,12,12	-	-	-		
4	EDO	H	4412	-	3,3,3	0.07	0	2,2,2	0.19	0
2	SF4	B	4205	1	0,12,12	-	-	-		
9	GOL	K	1117	-	5,5,5	0.09	0	5,5,5	0.35	0
4	EDO	E	1115	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	K	1116	-	3,3,3	0.11	0	2,2,2	0.04	0
4	EDO	G	1115	-	3,3,3	0.06	0	2,2,2	0.11	0
6	SO4	N	1016	-	4,4,4	0.26	0	6,6,6	0.25	0
4	EDO	C	3909	-	3,3,3	0.47	0	2,2,2	0.18	0
4	EDO	B	4215	-	3,3,3	0.08	0	2,2,2	0.08	0
4	EDO	J	1110	-	3,3,3	0.06	0	2,2,2	0.09	0
6	SO4	F	1118	-	4,4,4	0.33	0	6,6,6	0.07	0
4	EDO	M	1121	-	3,3,3	0.07	0	2,2,2	0.33	0
4	EDO	I	1113	-	3,3,3	0.06	0	2,2,2	0.11	0
2	SF4	K	1105	1	0,12,12	-	-	-		
4	EDO	P	1110	-	3,3,3	0.08	0	2,2,2	0.20	0
3	FAD	P	1106	-	58,58,58	1.43	10 (17%)	85,89,89	1.58	18 (21%)
4	EDO	F	1113	-	3,3,3	0.10	0	2,2,2	0.03	0
6	SO4	L	1113	-	4,4,4	0.23	0	6,6,6	0.20	0
11	PEG	K	1115	-	6,6,6	0.11	0	5,5,5	0.08	0
4	EDO	K	1113	-	3,3,3	0.05	0	2,2,2	0.11	0
2	SF4	N	1007[A]	1	0,12,12	-	-	-		
2	SF4	M	1102	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	SO4	H	4415	-	4,4,4	0.22	0	6,6,6	0.17	0
4	EDO	O	1112	-	3,3,3	0.10	0	2,2,2	0.18	0
2	SF4	G	1104	1	0,12,12	-	-	-		
2	SF4	N	1002	1	0,12,12	-	-	-		
4	EDO	D	4616	-	3,3,3	0.09	0	2,2,2	0.19	0
4	EDO	B	4219[A]	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	E	1117	-	3,3,3	0.11	0	2,2,2	0.21	0
4	EDO	O	1111	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	K	1114	-	3,3,3	0.06	0	2,2,2	0.11	0
2	SF4	J	1107	1	0,12,12	-	-	-		
3	FAD	M	1106	-	58,58,58	1.49	11 (18%)	85,89,89	1.51	15 (17%)
6	SO4	G	1122	-	4,4,4	0.29	0	6,6,6	0.27	0
4	EDO	M	1116	-	3,3,3	0.05	0	2,2,2	0.11	0
9	GOL	C	3901	-	5,5,5	0.09	0	5,5,5	0.31	0
2	SF4	I	1101	1	0,12,12	-	-	-		
4	EDO	M	1113	-	3,3,3	0.06	0	2,2,2	0.11	0
12	TRS	H	4401	-	7,7,7	0.18	0	9,9,9	0.33	0
6	SO4	M	1125	-	4,4,4	0.26	0	6,6,6	0.09	0
3	FAD	B	4207	-	58,58,58	1.49	10 (17%)	85,89,89	1.39	10 (11%)
9	GOL	O	1116	-	5,5,5	0.11	0	5,5,5	0.40	0
4	EDO	I	1108	-	3,3,3	0.45	0	2,2,2	0.42	0
5	SRM	I	1109	1	68,70,70	2.55	23 (33%)	86,112,112	1.73	17 (19%)
2	SF4	F	1105	1	0,12,12	-	-	-		
6	SO4	B	4226	-	4,4,4	0.25	0	6,6,6	0.24	0
9	GOL	N	1015	-	5,5,5	0.11	0	5,5,5	0.32	0
2	SF4	H	4405	1	0,12,12	-	-	-		
3	FAD	O	1106	-	58,58,58	1.47	9 (15%)	85,89,89	1.46	14 (16%)
4	EDO	M	1118	-	3,3,3	0.06	0	2,2,2	0.04	0
2	SF4	H	4408	1	0,12,12	-	-	-		
2	SF4	A	1101	1	0,12,12	-	-	-		
4	EDO	J	1116	-	3,3,3	0.06	0	2,2,2	0.16	0
9	GOL	P	1112	-	5,5,5	0.10	0	5,5,5	0.30	0
4	EDO	A	1113	-	3,3,3	0.08	0	2,2,2	0.07	0
4	EDO	O	1117	-	3,3,3	0.05	0	2,2,2	0.12	0
4	EDO	I	1112	-	3,3,3	0.06	0	2,2,2	0.18	0
2	SF4	C	3905	1	0,12,12	-	-	-		
2	SF4	L	1103	1	0,12,12	-	-	-		
6	SO4	M	1126	-	4,4,4	0.33	0	6,6,6	0.07	0
4	EDO	B	4221	-	3,3,3	0.08	0	2,2,2	0.01	0
5	SRM	J	1109	1	68,70,70	2.45	22 (32%)	86,112,112	1.63	16 (18%)
2	SF4	L	1102	1	0,12,12	-	-	-		
2	SF4	G	1107	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	EDO	C	3916	-	3,3,3	0.06	0	2,2,2	0.07	0
4	EDO	H	4413	-	3,3,3	0.05	0	2,2,2	0.12	0
2	SF4	M	1104	1	0,12,12	-	-	-		
2	SF4	G	1102	1	0,12,12	-	-	-		
2	SF4	H	4406	1	0,12,12	-	-	-		
2	SF4	J	1103	1	0,12,12	-	-	-		
9	GOL	N	1011	-	5,5,5	0.11	0	5,5,5	0.32	0
4	EDO	O	1110	-	3,3,3	0.39	0	2,2,2	0.58	0
4	EDO	C	3911	-	3,3,3	0.52	0	2,2,2	0.39	0
2	SF4	N	1004	1	0,12,12	-	-	-		
4	EDO	M	1124	-	3,3,3	0.08	0	2,2,2	0.12	0
2	SF4	C	3904	1	0,12,12	-	-	-		
2	SF4	F	1107	1	0,12,12	-	-	-		
4	EDO	J	1115	-	3,3,3	0.12	0	2,2,2	0.04	0
4	EDO	G	1120	-	3,3,3	0.05	0	2,2,2	0.12	0
4	EDO	L	1111	-	3,3,3	0.10	0	2,2,2	0.19	0
4	EDO	K	1112	-	3,3,3	0.08	0	2,2,2	0.10	0
4	EDO	E	1113	-	3,3,3	0.14	0	2,2,2	0.13	0
6	SO4	B	4225	-	4,4,4	0.46	0	6,6,6	0.13	0
4	EDO	B	4213	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	F	1111	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	B	4212	-	3,3,3	0.10	0	2,2,2	0.12	0
4	EDO	C	3915	-	3,3,3	0.06	0	2,2,2	0.12	0
2	SF4	E	1101	1	0,12,12	-	-	-		
4	EDO	N	1013	-	3,3,3	0.05	0	2,2,2	0.09	0
2	SF4	P	1105	1	0,12,12	-	-	-		
2	SF4	J	1104	1	0,12,12	-	-	-		
4	EDO	A	1116	-	3,3,3	0.08	0	2,2,2	0.09	0
3	FAD	C	3907	-	58,58,58	1.47	11 (18%)	85,89,89	1.46	13 (15%)
4	EDO	P	1113	-	3,3,3	0.08	0	2,2,2	0.15	0
2	SF4	K	1107	1	0,12,12	-	-	-		
6	SO4	L	1114	-	4,4,4	0.26	0	6,6,6	0.20	0
6	SO4	I	1120	-	4,4,4	0.21	0	6,6,6	0.31	0
2	SF4	D	4606	1	0,12,12	-	-	-		
4	EDO	B	4211	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	A	1112	-	3,3,3	0.09	0	2,2,2	0.12	0
4	EDO	G	1112	-	3,3,3	0.09	0	2,2,2	0.13	0
3	FAD	L	1106	-	58,58,58	1.46	10 (17%)	85,89,89	1.44	13 (15%)
4	EDO	F	1108	-	3,3,3	0.37	0	2,2,2	0.58	0
4	EDO	G	1118	-	3,3,3	0.06	0	2,2,2	0.12	0
6	SO4	J	1119	-	4,4,4	0.37	0	6,6,6	0.10	0
2	SF4	A	1103	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	J	1106	-	58,58,58	1.47	10 (17%)	85,89,89	1.48	15 (17%)
4	EDO	J	1111	-	3,3,3	0.07	0	2,2,2	0.11	0
4	EDO	D	4611	-	3,3,3	0.10	0	2,2,2	0.22	0
2	SF4	F	1102	1	0,12,12	-	-	-	-	-
4	EDO	D	4609	-	3,3,3	0.37	0	2,2,2	0.59	0
6	SO4	P	1116	-	4,4,4	0.36	0	6,6,6	0.11	0
6	SO4	H	4414	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SF4	O	1101	1	0,12,12	-	-	-	-	-
4	EDO	A	1114	-	3,3,3	0.11	0	2,2,2	0.24	0
4	EDO	A	1108	-	3,3,3	0.42	0	2,2,2	0.43	0
11	PEG	M	1115	-	6,6,6	0.14	0	5,5,5	0.08	0
2	SF4	B	4202	1	0,12,12	-	-	-	-	-
2	SF4	H	4402	1	0,12,12	-	-	-	-	-
4	EDO	L	1110	-	3,3,3	0.39	0	2,2,2	0.63	0
2	SF4	C	3902	1	0,12,12	-	-	-	-	-
5	SRM	F	1109	1	68,70,70	2.49	24 (35%)	86,112,112	1.81	18 (20%)
4	EDO	E	1112	-	3,3,3	0.06	0	2,2,2	0.12	0
4	EDO	B	4220[B]	-	3,3,3	0.07	0	2,2,2	0.11	0
2	SF4	P	1107	1	0,12,12	-	-	-	-	-
2	SF4	O	1105	1	0,12,12	-	-	-	-	-
2	SF4	F	1101	1	0,12,12	-	-	-	-	-
6	SO4	F	1115	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SF4	K	1103	1	0,12,12	-	-	-	-	-
6	SO4	D	4621	-	4,4,4	0.35	0	6,6,6	0.08	0
4	EDO	G	1117	-	3,3,3	0.10	0	2,2,2	0.21	0
2	SF4	C	3903	1	0,12,12	-	-	-	-	-
4	EDO	G	1114	-	3,3,3	0.12	0	2,2,2	0.04	0
4	EDO	G	1116	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	I	1118	-	3,3,3	0.05	0	2,2,2	0.11	0
6	SO4	D	4620	-	4,4,4	0.33	0	6,6,6	0.08	0
4	EDO	F	1112[A]	-	3,3,3	0.13	0	2,2,2	0.27	0
2	SF4	N	1005	1	0,12,12	-	-	-	-	-
9	GOL	B	4217[A]	-	5,5,5	0.11	0	5,5,5	0.35	0
3	FAD	A	1106	-	58,58,58	1.42	10 (17%)	85,89,89	1.49	13 (15%)
4	EDO	G	1111	-	3,3,3	0.06	0	2,2,2	0.11	0
4	EDO	B	4216	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	P	1114	-	3,3,3	0.10	0	2,2,2	0.10	0
4	EDO	A	1110	-	3,3,3	0.44	0	2,2,2	0.33	0
4	EDO	G	1110	-	3,3,3	0.10	0	2,2,2	0.23	0
4	EDO	O	1114	-	3,3,3	0.07	0	2,2,2	0.20	0
4	EDO	A	1117	-	3,3,3	0.04	0	2,2,2	0.05	0
6	SO4	K	1118	-	4,4,4	0.41	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	FAD	N	1001[A]	-	58,58,58	0.56	0	85,89,89	0.59	1 (1%)
4	EDO	E	1111	-	3,3,3	0.09	0	2,2,2	0.11	0
3	FAD	F	1106	-	58,58,58	1.46	10 (17%)	85,89,89	1.56	19 (22%)
5	SRM	P	1109	1	68,70,70	2.41	22 (32%)	86,112,112	1.67	18 (20%)
2	SF4	F	1104	1	0,12,12	-	-	-		
2	SF4	K	1104	1	0,12,12	-	-	-		
2	SF4	I	1102	1	0,12,12	-	-	-		
2	SF4	O	1107	1	0,12,12	-	-	-		
2	SF4	L	1101	1	0,12,12	-	-	-		
4	EDO	K	1111	-	3,3,3	0.09	0	2,2,2	0.20	0
9	GOL	E	1114	-	5,5,5	0.11	0	5,5,5	0.36	0
2	SF4	D	4605	1	0,12,12	-	-	-		
6	SO4	D	4619	-	4,4,4	0.24	0	6,6,6	0.16	0
9	GOL	J	1117[A]	-	5,5,5	0.09	0	5,5,5	0.36	0
9	GOL	F	1114	-	5,5,5	0.11	0	5,5,5	0.31	0
2	SF4	H	4404	1	0,12,12	-	-	-		
6	SO4	F	1117	-	4,4,4	0.37	0	6,6,6	0.08	0
2	SF4	N	1006[A]	1	0,12,12	-	-	-		
4	EDO	D	4617	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	E	1110	-	3,3,3	0.10	0	2,2,2	0.20	0
4	EDO	O	1108	-	3,3,3	0.48	0	2,2,2	0.54	0
6	SO4	J	1118	-	4,4,4	0.24	0	6,6,6	0.13	0
4	EDO	K	1110	-	3,3,3	0.55	0	2,2,2	0.10	0
4	EDO	M	1119	-	3,3,3	0.06	0	2,2,2	0.11	0
2	SF4	I	1103	1	0,12,12	-	-	-		
2	SF4	B	4203	1	0,12,12	-	-	-		
6	SO4	P	1115	-	4,4,4	0.24	0	6,6,6	0.18	0
4	EDO	M	1112	-	3,3,3	0.04	0	2,2,2	0.11	0
11	PEG	N	1014	-	6,6,6	0.12	0	5,5,5	0.08	0
4	EDO	M	1111	-	3,3,3	0.09	0	2,2,2	0.20	0
4	EDO	D	4613	-	3,3,3	0.05	0	2,2,2	0.15	0
2	SF4	P	1104	1	0,12,12	-	-	-		
4	EDO	L	1112	-	3,3,3	0.06	0	2,2,2	0.11	0
5	SRM	D	4610	1	68,70,70	2.41	22 (32%)	86,112,112	1.73	19 (22%)
9	GOL	B	4224	-	5,5,5	0.11	0	5,5,5	0.31	0
2	SF4	D	4608	1	0,12,12	-	-	-		
2	SF4	D	4604	1	0,12,12	-	-	-		
4	EDO	M	1117	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	J	1113	-	3,3,3	0.17	0	2,2,2	0.14	0
5	SRM	O	1109	1	68,70,70	3.67	27 (39%)	86,112,112	2.18	34 (39%)
3	FAD	H	4407	-	58,58,58	1.40	10 (17%)	85,89,89	1.54	17 (20%)
4	EDO	I	1114	-	3,3,3	0.06	0	2,2,2	0.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SF4	G	1101	1	0,12,12	-	-	-		
2	SF4	J	1101	1	0,12,12	-	-	-		
4	EDO	C	3917	-	3,3,3	0.09	0	2,2,2	0.12	0
9	GOL	G	1119[A]	-	5,5,5	0.10	0	5,5,5	0.34	0
2	SF4	E	1103	1	0,12,12	-	-	-		
9	GOL	M	1114	-	5,5,5	0.11	0	5,5,5	0.31	0
4	EDO	L	1108	-	3,3,3	0.42	0	2,2,2	0.44	0
6	SO4	O	1120	-	4,4,4	0.37	0	6,6,6	0.08	0
3	FAD	I	1106	-	58,58,58	0.63	0	85,89,89	0.59	0
2	SF4	D	4602	1	0,12,12	-	-	-		
4	EDO	K	1108	-	3,3,3	0.40	0	2,2,2	0.45	0
2	SF4	A	1105	1	0,12,12	-	-	-		
2	SF4	E	1107	1	0,12,12	-	-	-		
9	GOL	C	3913	-	5,5,5	0.10	0	5,5,5	0.32	0
4	EDO	O	1115	-	3,3,3	0.07	0	2,2,2	0.11	0
2	SF4	B	4204	1	0,12,12	-	-	-		
9	GOL	B	4218[B]	-	5,5,5	0.13	0	5,5,5	0.37	0
4	EDO	C	3918	-	3,3,3	0.10	0	2,2,2	0.02	0
4	EDO	I	1115	-	3,3,3	0.06	0	2,2,2	0.11	0
3	FAD	D	4607	-	58,58,58	1.54	10 (17%)	85,89,89	1.48	17 (20%)
4	EDO	C	3914	-	3,3,3	0.14	0	2,2,2	0.22	0
2	SF4	L	1107	1	0,12,12	-	-	-		
4	EDO	D	4612	-	3,3,3	0.05	0	2,2,2	0.11	0
3	FAD	G	1106	-	58,58,58	0.63	0	85,89,89	0.58	0
4	EDO	O	1118	-	3,3,3	0.13	0	2,2,2	0.06	0
4	EDO	H	4411	-	3,3,3	0.08	0	2,2,2	0.27	0
2	SF4	O	1102	1	0,12,12	-	-	-		
2	SF4	I	1105	1	0,12,12	-	-	-		
2	SF4	O	1104	1	0,12,12	-	-	-		
4	EDO	B	4209	-	3,3,3	0.37	0	2,2,2	0.66	0
5	SRM	K	1109	1	68,70,70	2.48	23 (33%)	86,112,112	1.65	18 (20%)
4	EDO	E	1108	-	3,3,3	0.45	0	2,2,2	0.57	0
4	EDO	M	1110	-	3,3,3	0.39	0	2,2,2	0.74	0
4	EDO	G	1108	-	3,3,3	0.56	0	2,2,2	0.35	0
2	SF4	G	1105	1	0,12,12	-	-	-		
4	EDO	A	1111	-	3,3,3	0.11	0	2,2,2	0.23	0
2	SF4	M	1103	1	0,12,12	-	-	-		
2	SF4	K	1102	1	0,12,12	-	-	-		
6	SO4	O	1119	-	4,4,4	0.25	0	6,6,6	0.21	0
2	SF4	F	1103	1	0,12,12	-	-	-		
5	SRM	L	1109	1	68,70,70	2.57	22 (32%)	86,112,112	1.69	17 (19%)
2	SF4	A	1107	1	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GOL	I	1111	-	5,5,5	0.10	0	5,5,5	0.32	0
2	SF4	N	1003	1	0,12,12	-	-	-		
4	EDO	N	1010	-	3,3,3	0.11	0	2,2,2	0.30	0
2	SF4	M	1101	1	0,12,12	-	-	-		
4	EDO	D	4614	-	3,3,3	0.07	0	2,2,2	0.12	0
2	SF4	O	1103	1	0,12,12	-	-	-		
2	SF4	E	1105	1	0,12,12	-	-	-		
4	EDO	B	4214	-	3,3,3	0.06	0	2,2,2	0.08	0
4	EDO	J	1108	-	3,3,3	0.47	0	2,2,2	0.53	0
11	PEG	M	1120	-	6,6,6	0.13	0	5,5,5	0.10	0
3	FAD	K	1106	-	58,58,58	1.42	10 (17%)	85,89,89	1.48	12 (14%)
2	SF4	J	1102	1	0,12,12	-	-	-		
2	SF4	I	1107	1	0,12,12	-	-	-		
4	EDO	D	4615	-	3,3,3	0.10	0	2,2,2	0.06	0
2	SF4	N	1006[B]	1	0,12,12	-	-	-		
4	EDO	B	4201	-	3,3,3	0.10	0	2,2,2	0.05	0
5	SRM	N	1012	1	68,70,70	2.53	22 (32%)	86,112,112	1.73	20 (23%)
6	SO4	L	1115	-	4,4,4	0.39	0	6,6,6	0.05	0
5	SRM	A	1109	1	68,70,70	2.49	23 (33%)	86,112,112	1.71	21 (24%)
6	SO4	K	1119	-	4,4,4	0.37	0	6,6,6	0.08	0
4	EDO	I	1116	-	3,3,3	0.06	0	2,2,2	0.03	0
2	SF4	L	1104	1	0,12,12	-	-	-		
4	EDO	F	1110[B]	-	3,3,3	0.24	0	2,2,2	0.18	0
4	EDO	G	1121	-	3,3,3	0.06	0	2,2,2	0.04	0
3	FAD	E	1106	-	58,58,58	1.50	10 (17%)	85,89,89	1.49	13 (15%)
4	EDO	H	4409	-	3,3,3	0.50	0	2,2,2	0.18	0
4	EDO	B	4222[A]	-	3,3,3	0.07	0	2,2,2	0.26	0
2	SF4	C	3908	1	0,12,12	-	-	-		
6	SO4	C	3919	-	4,4,4	0.40	0	6,6,6	0.10	0
4	EDO	O	1113	-	3,3,3	0.05	0	2,2,2	0.12	0
2	SF4	M	1105	1	0,12,12	-	-	-		
6	SO4	M	1127	-	4,4,4	0.37	0	6,6,6	0.06	0
3	FAD	N	1009[B]	-	58,58,58	0.55	0	85,89,89	0.56	1 (1%)
2	SF4	E	1104	1	0,12,12	-	-	-		
4	EDO	J	1112	-	3,3,3	0.05	0	2,2,2	0.11	0
4	EDO	C	3912	-	3,3,3	0.10	0	2,2,2	0.25	0
4	EDO	A	1118	-	3,3,3	0.14	0	2,2,2	0.08	0
4	EDO	P	1108	-	3,3,3	0.38	0	2,2,2	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	B	4220[B]	-	-	0/1/1/1	-
4	EDO	K	1108	-	-	0/1/1/1	-
2	SF4	A	1105	1	-	-	0/6/5/5
2	SF4	E	1107	1	-	-	0/6/5/5
9	GOL	N	1015	-	-	1/4/4/4	-
2	SF4	P	1107	1	-	-	0/6/5/5
9	GOL	P	1111	-	-	1/4/4/4	-
4	EDO	M	1123	-	-	1/1/1/1	-
2	SF4	O	1105	1	-	-	0/6/5/5
9	GOL	C	3913	-	-	4/4/4/4	-
2	SF4	L	1105	1	-	-	0/6/5/5
12	TRS	I	1119	-	-	6/9/9/9	-
4	EDO	O	1115	-	-	0/1/1/1	-
2	SF4	F	1101	1	-	-	0/6/5/5
5	SRM	E	1109	1	1/1/19/23	10/38/126/126	-
2	SF4	B	4204	1	-	-	0/6/5/5
2	SF4	H	4405	1	-	-	0/6/5/5
2	SF4	K	1103	1	-	-	0/6/5/5
2	SF4	P	1102	1	-	-	0/6/5/5
3	FAD	O	1106	-	-	2/34/50/50	0/6/6/6
4	EDO	M	1118	-	-	1/1/1/1	-
4	EDO	C	3918	-	-	1/1/1/1	-
9	GOL	B	4218[B]	-	-	2/4/4/4	-
4	EDO	I	1115	-	-	1/1/1/1	-
2	SF4	H	4408	1	-	-	0/6/5/5
4	EDO	J	1116	-	-	0/1/1/1	-
2	SF4	A	1101	1	-	-	0/6/5/5
3	FAD	D	4607	-	-	3/34/50/50	0/6/6/6
4	EDO	C	3914	-	-	0/1/1/1	-
4	EDO	G	1117	-	-	0/1/1/1	-
2	SF4	C	3903	1	-	-	0/6/5/5
2	SF4	L	1107	1	-	-	0/6/5/5
4	EDO	D	4612	-	-	1/1/1/1	-
9	GOL	P	1112	-	-	0/4/4/4	-
3	FAD	G	1106	-	-	2/34/50/50	0/6/6/6
4	EDO	A	1113	-	-	1/1/1/1	-
4	EDO	O	1117	-	-	1/1/1/1	-
4	EDO	I	1112	-	-	1/1/1/1	-
4	EDO	G	1114	-	-	0/1/1/1	-
4	EDO	G	1116	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	1113	-	-	1/1/1/1	-
4	EDO	O	1118	-	-	0/1/1/1	-
2	SF4	A	1102	1	-	-	0/6/5/5
4	EDO	H	4411	-	-	0/1/1/1	-
5	SRM	G	1109	1	1/1/19/23	11/38/126/126	-
2	SF4	B	4206	1	-	-	0/6/5/5
2	SF4	C	3905	1	-	-	0/6/5/5
2	SF4	L	1103	1	-	-	0/6/5/5
4	EDO	I	1118	-	-	1/1/1/1	-
2	SF4	K	1101	1	-	-	0/6/5/5
2	SF4	C	3906	1	-	-	0/6/5/5
4	EDO	B	4221	-	-	1/1/1/1	-
2	SF4	O	1102	1	-	-	0/6/5/5
5	SRM	J	1109	1	1/1/19/23	11/38/126/126	-
2	SF4	L	1102	1	-	-	0/6/5/5
9	GOL	I	1117	-	-	4/4/4/4	-
4	EDO	F	1112[A]	-	-	0/1/1/1	-
2	SF4	D	4603	1	-	-	0/6/5/5
2	SF4	I	1105	1	-	-	0/6/5/5
2	SF4	G	1107	1	-	-	0/6/5/5
2	SF4	N	1005	1	-	-	0/6/5/5
2	SF4	O	1104	1	-	-	0/6/5/5
2	SF4	G	1103	1	-	-	0/6/5/5
5	SRM	H	4410	1	1/1/19/23	11/38/126/126	-
4	EDO	B	4209	-	-	0/1/1/1	-
4	EDO	C	3916	-	-	1/1/1/1	-
4	EDO	H	4413	-	-	1/1/1/1	-
5	SRM	K	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	M	1108	-	-	0/1/1/1	-
2	SF4	M	1104	1	-	-	0/6/5/5
4	EDO	E	1108	-	-	0/1/1/1	-
4	EDO	A	1115	-	-	1/1/1/1	-
4	EDO	M	1110	-	-	1/1/1/1	-
4	EDO	G	1108	-	-	0/1/1/1	-
2	SF4	G	1102	1	-	-	0/6/5/5
9	GOL	B	4217[A]	-	-	2/4/4/4	-
3	FAD	A	1106	-	-	1/34/50/50	0/6/6/6
4	EDO	A	1111	-	-	0/1/1/1	-
2	SF4	G	1105	1	-	-	0/6/5/5
2	SF4	H	4406	1	-	-	0/6/5/5
2	SF4	J	1103	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	P	1101	1	-	-	0/6/5/5
4	EDO	G	1111	-	-	0/1/1/1	-
4	EDO	B	4216	-	-	0/1/1/1	-
4	EDO	P	1114	-	-	1/1/1/1	-
4	EDO	A	1110	-	-	1/1/1/1	-
4	EDO	G	1110	-	-	0/1/1/1	-
4	EDO	O	1114	-	-	1/1/1/1	-
9	GOL	N	1011	-	-	2/4/4/4	-
2	SF4	M	1107	1	-	-	0/6/5/5
2	SF4	M	1103	1	-	-	0/6/5/5
4	EDO	O	1110	-	-	1/1/1/1	-
4	EDO	A	1117	-	-	1/1/1/1	-
3	FAD	N	1001[A]	-	-	8/34/50/50	0/6/6/6
4	EDO	C	3911	-	-	1/1/1/1	-
4	EDO	I	1110	-	-	1/1/1/1	-
11	PEG	D	4601	-	-	3/4/4/4	-
2	SF4	B	4208	1	-	-	0/6/5/5
4	EDO	E	1111	-	-	0/1/1/1	-
2	SF4	H	4403	1	-	-	0/6/5/5
3	FAD	F	1106	-	-	2/34/50/50	0/6/6/6
5	SRM	P	1109	1	1/1/19/23	11/38/126/126	-
2	SF4	N	1004	1	-	-	0/6/5/5
2	SF4	F	1104	1	-	-	0/6/5/5
2	SF4	I	1104	1	-	-	0/6/5/5
4	EDO	M	1124	-	-	0/1/1/1	-
4	EDO	B	4223	-	-	1/1/1/1	-
2	SF4	K	1102	1	-	-	0/6/5/5
2	SF4	K	1104	1	-	-	0/6/5/5
4	EDO	D	4618	-	-	0/1/1/1	-
5	SRM	B	4210	1	1/1/19/23	11/38/126/126	-
2	SF4	J	1105	1	-	-	0/6/5/5
4	EDO	M	1122	-	-	1/1/1/1	-
2	SF4	A	1104	1	-	-	0/6/5/5
2	SF4	C	3904	1	-	-	0/6/5/5
2	SF4	F	1107	1	-	-	0/6/5/5
4	EDO	J	1115	-	-	0/1/1/1	-
9	GOL	J	1114	-	-	4/4/4/4	-
4	EDO	G	1120	-	-	1/1/1/1	-
4	EDO	L	1111	-	-	0/1/1/1	-
2	SF4	I	1102	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SRM	L	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	K	1112	-	-	0/1/1/1	-
2	SF4	F	1103	1	-	-	0/6/5/5
4	EDO	E	1116	-	-	1/1/1/1	-
2	SF4	A	1107	1	-	-	0/6/5/5
2	SF4	E	1102	1	-	-	0/6/5/5
5	SRM	C	3910	1	1/1/19/23	11/38/126/126	-
5	SRM	M	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	E	1113	-	-	1/1/1/1	-
9	GOL	I	1111	-	-	1/4/4/4	-
4	EDO	H	4412	-	-	1/1/1/1	-
2	SF4	N	1008[B]	1	-	-	0/6/5/5
2	SF4	B	4205	1	-	-	0/6/5/5
9	GOL	K	1117	-	-	4/4/4/4	-
4	EDO	E	1115	-	-	1/1/1/1	-
4	EDO	B	4213	-	-	1/1/1/1	-
2	SF4	O	1107	1	-	-	0/6/5/5
4	EDO	K	1116	-	-	1/1/1/1	-
4	EDO	F	1111	-	-	1/1/1/1	-
2	SF4	L	1101	1	-	-	0/6/5/5
4	EDO	B	4212	-	-	0/1/1/1	-
4	EDO	G	1115	-	-	1/1/1/1	-
4	EDO	K	1111	-	-	0/1/1/1	-
9	GOL	E	1114	-	-	4/4/4/4	-
2	SF4	N	1003	1	-	-	0/6/5/5
2	SF4	D	4605	1	-	-	0/6/5/5
4	EDO	C	3915	-	-	1/1/1/1	-
4	EDO	N	1010	-	-	0/1/1/1	-
4	EDO	C	3909	-	-	0/1/1/1	-
9	GOL	J	1117[A]	-	-	2/4/4/4	-
2	SF4	E	1101	1	-	-	0/6/5/5
4	EDO	B	4215	-	-	1/1/1/1	-
2	SF4	M	1101	1	-	-	0/6/5/5
4	EDO	D	4614	-	-	1/1/1/1	-
2	SF4	O	1103	1	-	-	0/6/5/5
9	GOL	F	1114	-	-	1/4/4/4	-
2	SF4	H	4404	1	-	-	0/6/5/5
4	EDO	J	1110	-	-	1/1/1/1	-
4	EDO	N	1013	-	-	0/1/1/1	-
2	SF4	E	1105	1	-	-	0/6/5/5
4	EDO	M	1121	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	N	1006[A]	1	-	-	0/6/5/5
4	EDO	B	4214	-	-	1/1/1/1	-
4	EDO	J	1108	-	-	0/1/1/1	-
4	EDO	I	1113	-	-	0/1/1/1	-
4	EDO	D	4617	-	-	1/1/1/1	-
4	EDO	E	1110	-	-	0/1/1/1	-
11	PEG	M	1120	-	-	1/4/4/4	-
2	SF4	P	1105	1	-	-	0/6/5/5
2	SF4	J	1104	1	-	-	0/6/5/5
4	EDO	O	1108	-	-	0/1/1/1	-
2	SF4	K	1105	1	-	-	0/6/5/5
4	EDO	P	1110	-	-	0/1/1/1	-
4	EDO	A	1116	-	-	0/1/1/1	-
4	EDO	K	1110	-	-	0/1/1/1	-
3	FAD	P	1106	-	-	2/34/50/50	0/6/6/6
3	FAD	K	1106	-	-	0/34/50/50	0/6/6/6
4	EDO	M	1119	-	-	0/1/1/1	-
3	FAD	C	3907	-	-	3/34/50/50	0/6/6/6
4	EDO	F	1113	-	-	0/1/1/1	-
2	SF4	I	1107	1	-	-	0/6/5/5
4	EDO	D	4615	-	-	1/1/1/1	-
4	EDO	P	1113	-	-	1/1/1/1	-
2	SF4	J	1102	1	-	-	0/6/5/5
2	SF4	K	1107	1	-	-	0/6/5/5
11	PEG	K	1115	-	-	3/4/4/4	-
4	EDO	K	1113	-	-	1/1/1/1	-
2	SF4	N	1006[B]	1	-	-	0/6/5/5
2	SF4	N	1007[A]	1	-	-	0/6/5/5
2	SF4	I	1103	1	-	-	0/6/5/5
2	SF4	B	4203	1	-	-	0/6/5/5
4	EDO	B	4211	-	-	0/1/1/1	-
2	SF4	D	4606	1	-	-	0/6/5/5
4	EDO	M	1112	-	-	1/1/1/1	-
2	SF4	M	1102	1	-	-	0/6/5/5
4	EDO	A	1112	-	-	0/1/1/1	-
4	EDO	B	4201	-	-	0/1/1/1	-
4	EDO	G	1112	-	-	1/1/1/1	-
3	FAD	L	1106	-	-	3/34/50/50	0/6/6/6
4	EDO	F	1108	-	-	0/1/1/1	-
11	PEG	N	1014	-	-	3/4/4/4	-
4	EDO	O	1112	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	G	1118	-	-	0/1/1/1	-
5	SRM	N	1012	1	1/1/19/23	14/38/126/126	-
4	EDO	D	4613	-	-	1/1/1/1	-
4	EDO	L	1112	-	-	1/1/1/1	-
4	EDO	M	1111	-	-	0/1/1/1	-
2	SF4	P	1104	1	-	-	0/6/5/5
5	SRM	D	4610	1	1/1/19/23	11/38/126/126	-
9	GOL	B	4224	-	-	3/4/4/4	-
2	SF4	A	1103	1	-	-	0/6/5/5
2	SF4	G	1104	1	-	-	0/6/5/5
3	FAD	J	1106	-	-	2/34/50/50	0/6/6/6
2	SF4	D	4608	1	-	-	0/6/5/5
4	EDO	J	1111	-	-	1/1/1/1	-
4	EDO	D	4611	-	-	0/1/1/1	-
2	SF4	D	4604	1	-	-	0/6/5/5
5	SRM	A	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	E	1117	-	-	1/1/1/1	-
4	EDO	D	4616	-	-	0/1/1/1	-
4	EDO	B	4219[A]	-	-	0/1/1/1	-
4	EDO	M	1117	-	-	1/1/1/1	-
2	SF4	N	1002	1	-	-	0/6/5/5
4	EDO	J	1113	-	-	1/1/1/1	-
4	EDO	O	1111	-	-	0/1/1/1	-
2	SF4	F	1102	1	-	-	0/6/5/5
5	SRM	O	1109	1	1/1/19/23	12/38/126/126	-
3	FAD	H	4407	-	-	1/34/50/50	0/6/6/6
4	EDO	I	1116	-	-	0/1/1/1	-
4	EDO	I	1114	-	-	1/1/1/1	-
4	EDO	D	4609	-	-	0/1/1/1	-
4	EDO	K	1114	-	-	1/1/1/1	-
2	SF4	J	1107	1	-	-	0/6/5/5
2	SF4	G	1101	1	-	-	0/6/5/5
2	SF4	J	1101	1	-	-	0/6/5/5
2	SF4	L	1104	1	-	-	0/6/5/5
3	FAD	M	1106	-	-	2/34/50/50	0/6/6/6
4	EDO	C	3917	-	-	1/1/1/1	-
4	EDO	F	1110[B]	-	-	1/1/1/1	-
4	EDO	G	1121	-	-	0/1/1/1	-
4	EDO	M	1116	-	-	0/1/1/1	-
3	FAD	E	1106	-	-	0/34/50/50	0/6/6/6
4	EDO	H	4409	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	C	3901	-	-	2/4/4/4	-
9	GOL	G	1119[A]	-	-	0/4/4/4	-
2	SF4	O	1101	1	-	-	0/6/5/5
4	EDO	A	1114	-	-	0/1/1/1	-
4	EDO	A	1108	-	-	0/1/1/1	-
4	EDO	B	4222[A]	-	-	1/1/1/1	-
11	PEG	M	1115	-	-	4/4/4/4	-
2	SF4	C	3908	1	-	-	0/6/5/5
2	SF4	I	1101	1	-	-	0/6/5/5
4	EDO	M	1113	-	-	1/1/1/1	-
2	SF4	E	1103	1	-	-	0/6/5/5
2	SF4	B	4202	1	-	-	0/6/5/5
12	TRS	H	4401	-	-	6/9/9/9	-
9	GOL	M	1114	-	-	1/4/4/4	-
2	SF4	P	1103	1	-	-	0/6/5/5
4	EDO	L	1108	-	-	0/1/1/1	-
3	FAD	B	4207	-	-	0/34/50/50	0/6/6/6
9	GOL	O	1116	-	-	4/4/4/4	-
2	SF4	H	4402	1	-	-	0/6/5/5
4	EDO	I	1108	-	-	0/1/1/1	-
4	EDO	O	1113	-	-	1/1/1/1	-
3	FAD	I	1106	-	-	1/34/50/50	0/6/6/6
4	EDO	L	1110	-	-	0/1/1/1	-
2	SF4	M	1105	1	-	-	0/6/5/5
2	SF4	C	3902	1	-	-	0/6/5/5
3	FAD	N	1009[B]	-	-	1/34/50/50	0/6/6/6
5	SRM	F	1109	1	1/1/19/23	10/38/126/126	-
5	SRM	I	1109	1	1/1/19/23	11/38/126/126	-
4	EDO	J	1112	-	-	1/1/1/1	-
2	SF4	E	1104	1	-	-	0/6/5/5
2	SF4	D	4602	1	-	-	0/6/5/5
2	SF4	F	1105	1	-	-	0/6/5/5
4	EDO	C	3912	-	-	0/1/1/1	-
4	EDO	E	1112	-	-	1/1/1/1	-
4	EDO	A	1118	-	-	1/1/1/1	-
4	EDO	P	1108	-	-	0/1/1/1	-

The worst 5 of 499 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1109	SRM	C4A-NA	-19.82	1.21	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1109	SRM	C4A-NA	-15.02	1.24	1.35
5	H	4410	SRM	C4A-NA	-14.89	1.24	1.35
5	B	4210	SRM	C4A-NA	-13.24	1.25	1.35
5	L	1109	SRM	C4A-NA	-13.22	1.25	1.35

The worst 5 of 516 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1109	SRM	C1A-NA-C4A	6.21	113.01	105.34
3	E	1106	FAD	C5A-C4A-N3A	-6.05	118.39	126.72
3	M	1106	FAD	C5A-C4A-N3A	-5.90	118.59	126.72
5	F	1109	SRM	C2A-C1A-CHA	-5.84	118.29	123.54
3	P	1106	FAD	C5A-C4A-N3A	-5.77	118.77	126.72

5 of 16 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1109	SRM	NC
5	B	4210	SRM	NC
5	C	3910	SRM	NC
5	D	4610	SRM	NC
5	E	1109	SRM	NC

5 of 342 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	N	1001[A]	FAD	C2'-C3'-C4'-C5'
3	N	1001[A]	FAD	O3'-C3'-C4'-C5'
3	N	1001[A]	FAD	C5'-O5'-P-O2P
3	N	1001[A]	FAD	C5'-O5'-P-O3P
5	N	1012	SRM	C2C-C3C-CAC-CBC

There are no ring outliers.

56 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	P	1111	GOL	2	0
5	E	1109	SRM	1	0
9	I	1117	GOL	2	0
2	A	1104	SF4	1	0
5	M	1109	SRM	1	0

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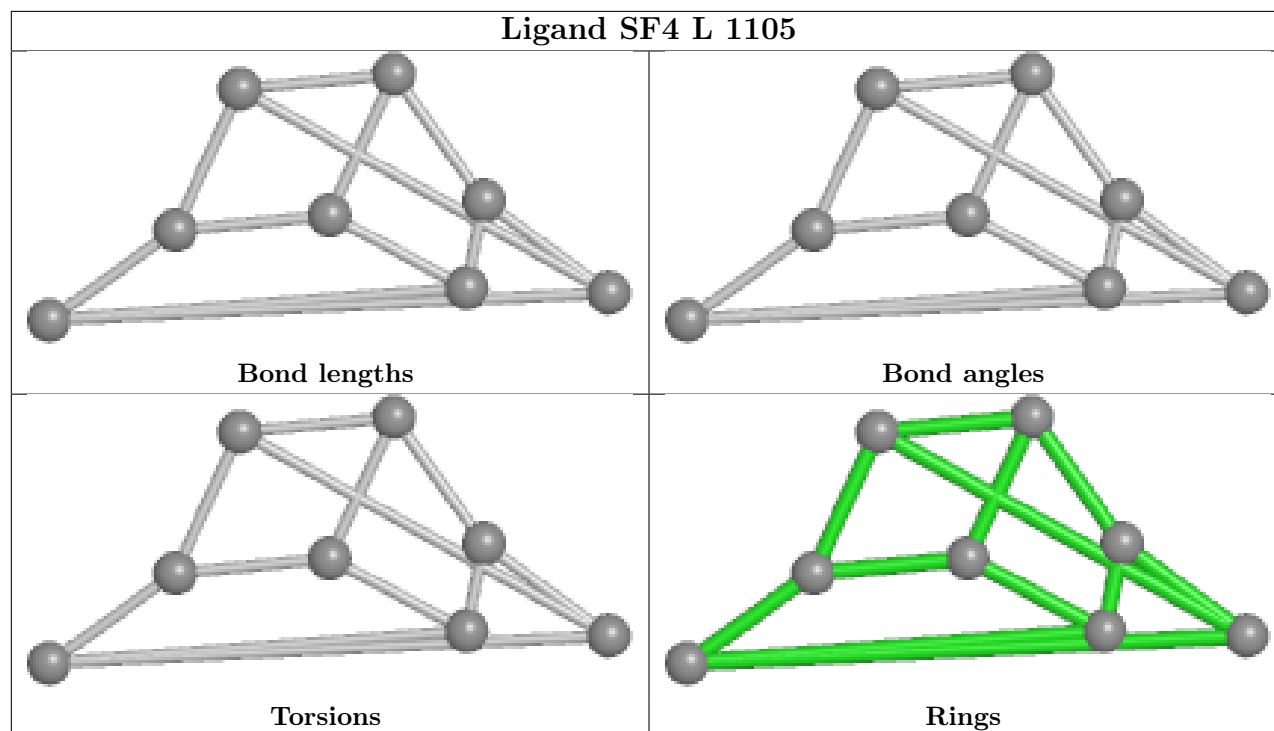
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	4412	EDO	3	0
2	B	4205	SF4	1	0
4	K	1116	EDO	1	0
4	J	1110	EDO	2	0
6	F	1118	SO4	1	0
3	P	1106	FAD	1	0
4	F	1113	EDO	1	0
11	K	1115	PEG	1	0
2	N	1007[A]	SF4	3	0
2	G	1104	SF4	1	0
9	C	3901	GOL	2	0
6	B	4226	SO4	1	0
2	H	4405	SF4	1	0
2	A	1101	SF4	1	0
4	H	4413	EDO	1	0
2	M	1104	SF4	1	0
9	N	1011	GOL	1	0
4	G	1120	EDO	1	0
2	J	1104	SF4	1	0
4	A	1116	EDO	2	0
4	B	4211	EDO	1	0
4	G	1118	EDO	2	0
11	M	1115	PEG	2	0
2	B	4202	SF4	1	0
5	F	1109	SRM	1	0
4	E	1112	EDO	1	0
2	O	1105	SF4	1	0
4	G	1116	EDO	1	0
9	B	4217[A]	GOL	1	0
4	B	4216	EDO	1	0
3	N	1001[A]	FAD	3	0
2	D	4605	SF4	1	0
9	F	1114	GOL	1	0
6	F	1117	SO4	1	0
2	N	1006[A]	SF4	2	0
2	P	1104	SF4	1	0
2	G	1101	SF4	1	0
9	M	1114	GOL	1	0
3	I	1106	FAD	1	0
4	I	1115	EDO	1	0
3	D	4607	FAD	1	0
2	M	1103	SF4	1	0

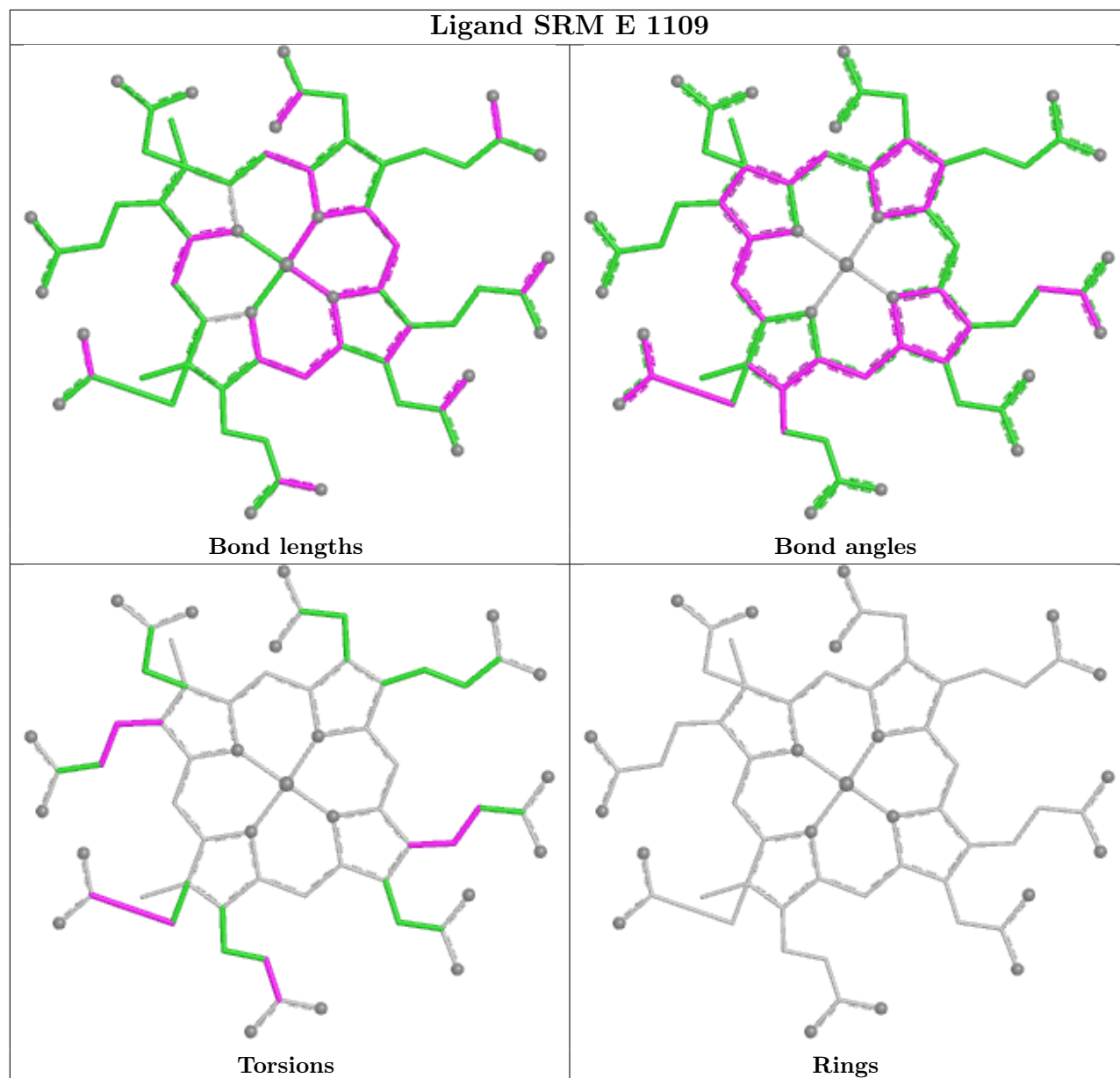
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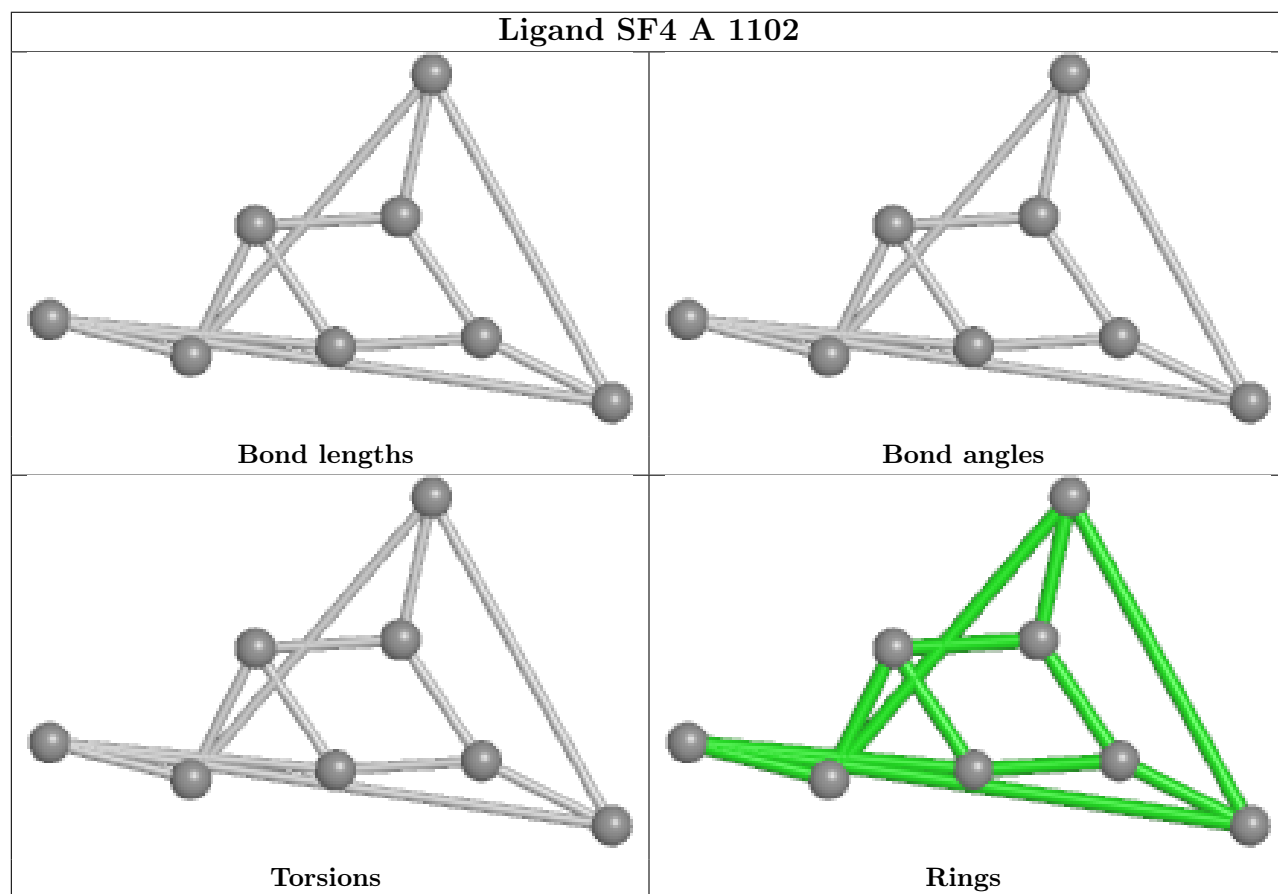
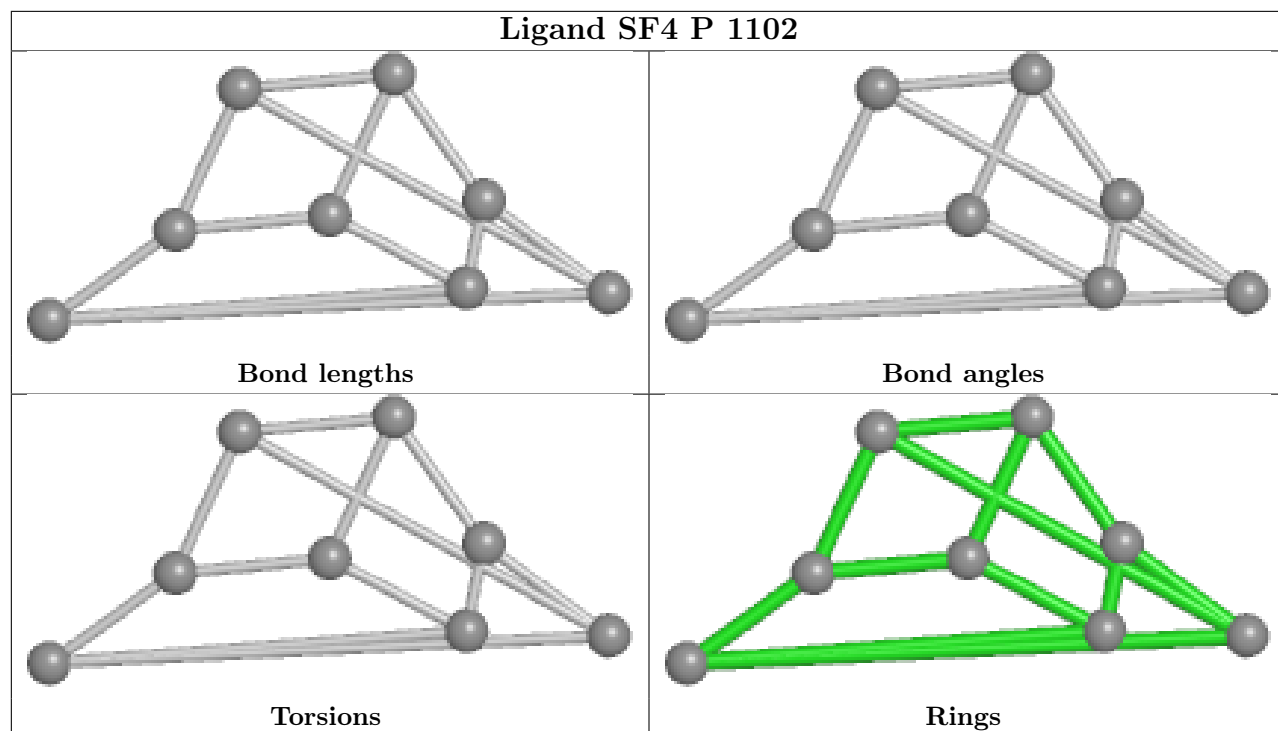
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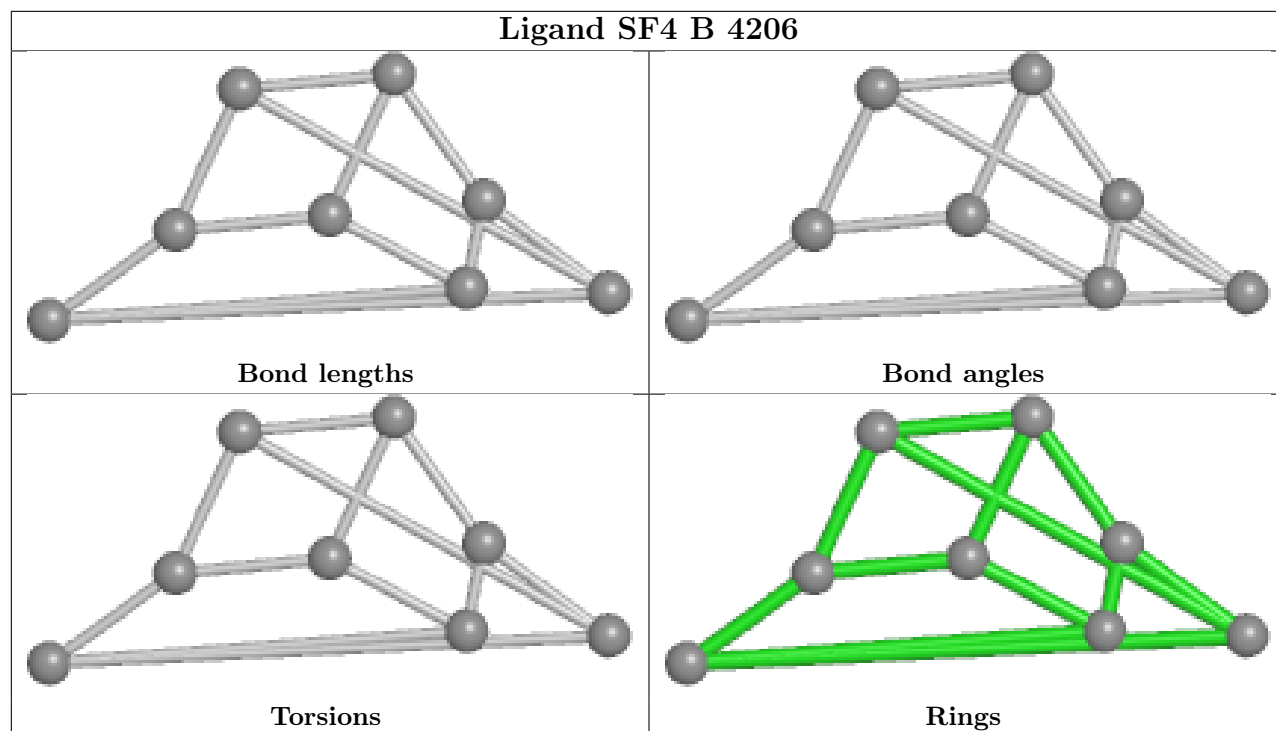
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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3	K	1106	FAD	1	0
4	D	4615	EDO	1	0
5	N	1012	SRM	1	0
4	F	1110[B]	EDO	1	0
3	E	1106	FAD	1	0
3	N	1009[B]	FAD	1	0
2	E	1104	SF4	1	0
4	J	1112	EDO	2	0

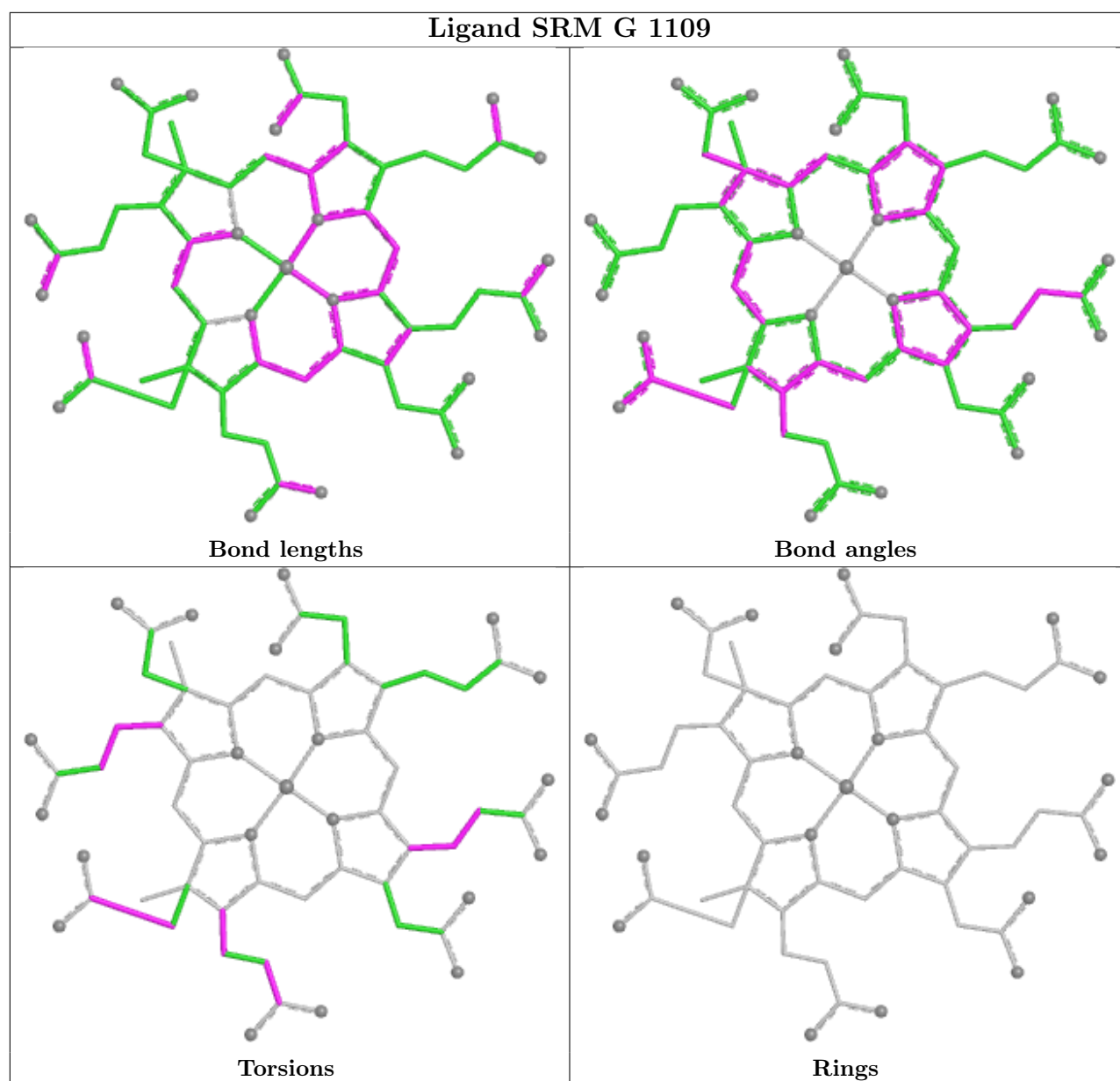
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

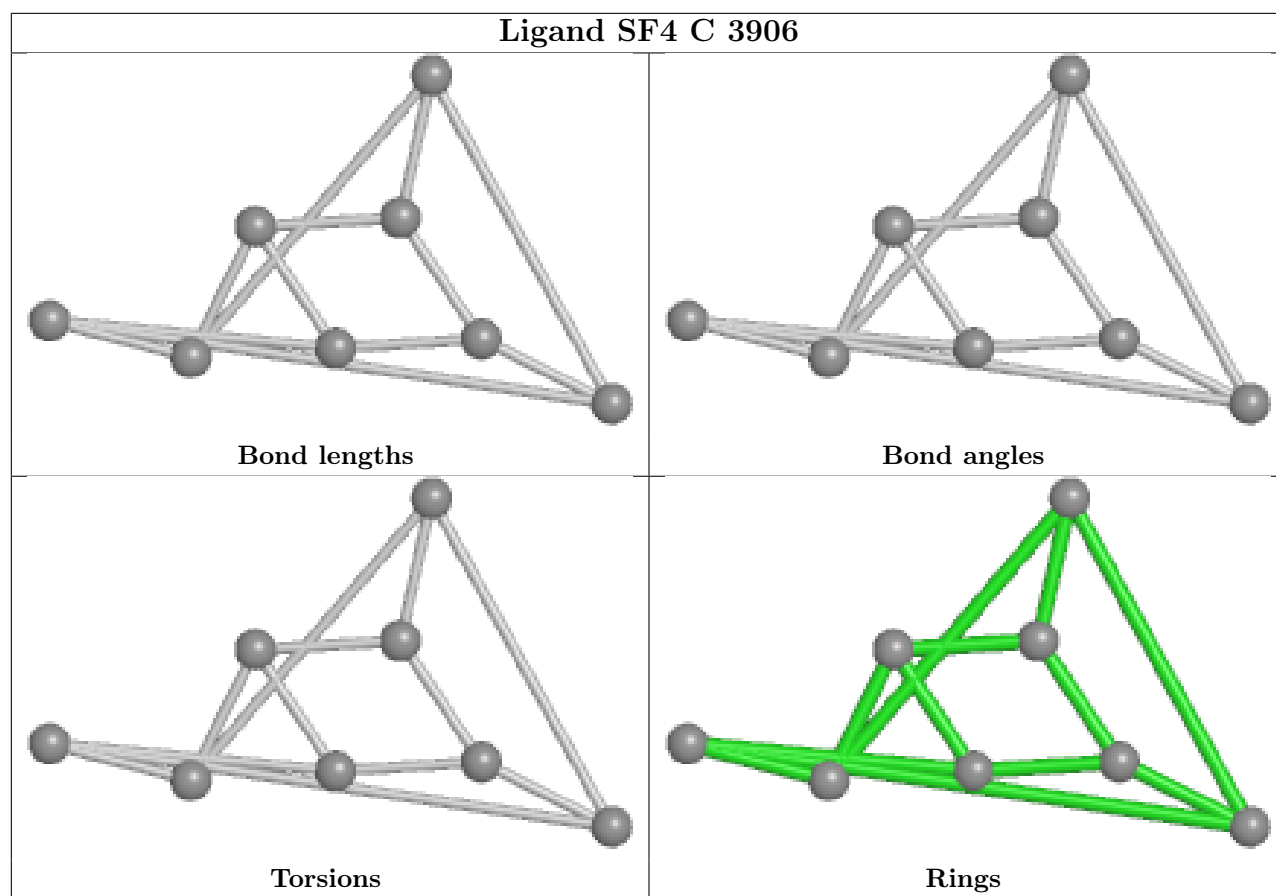
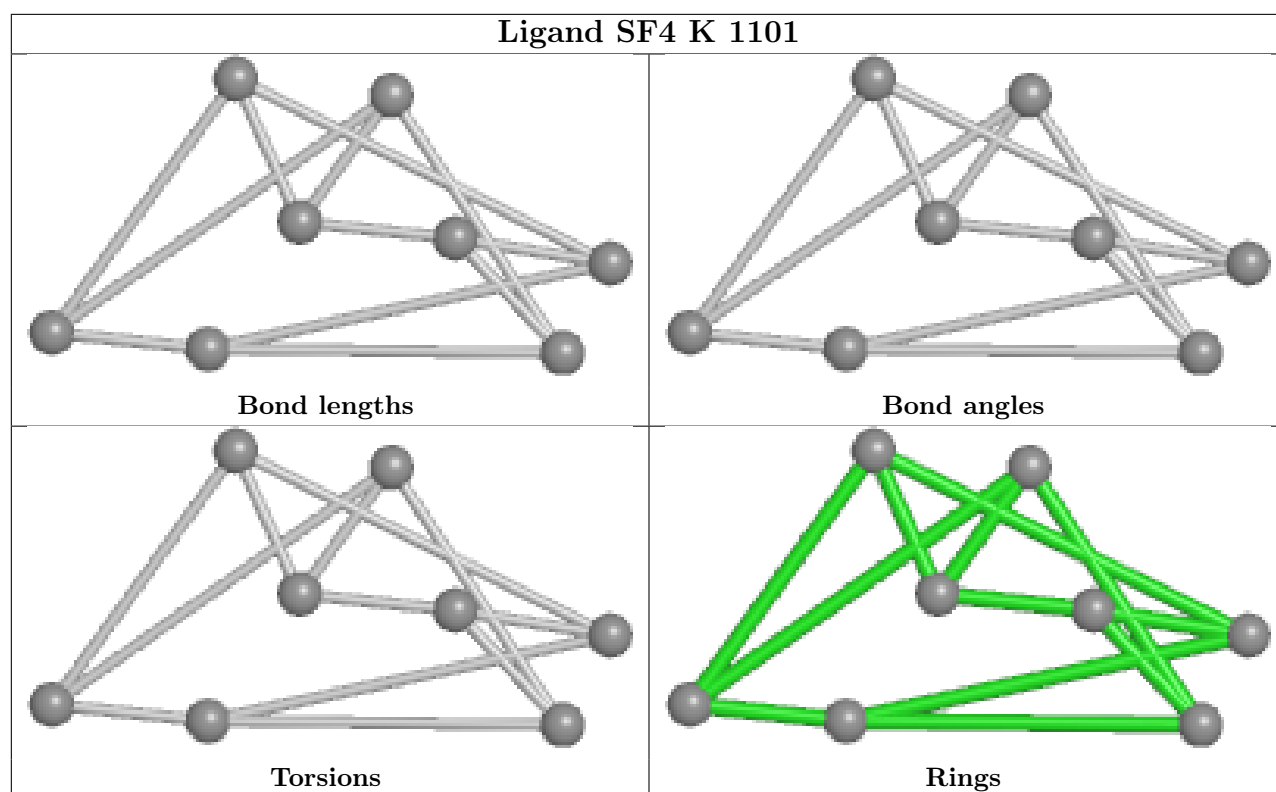


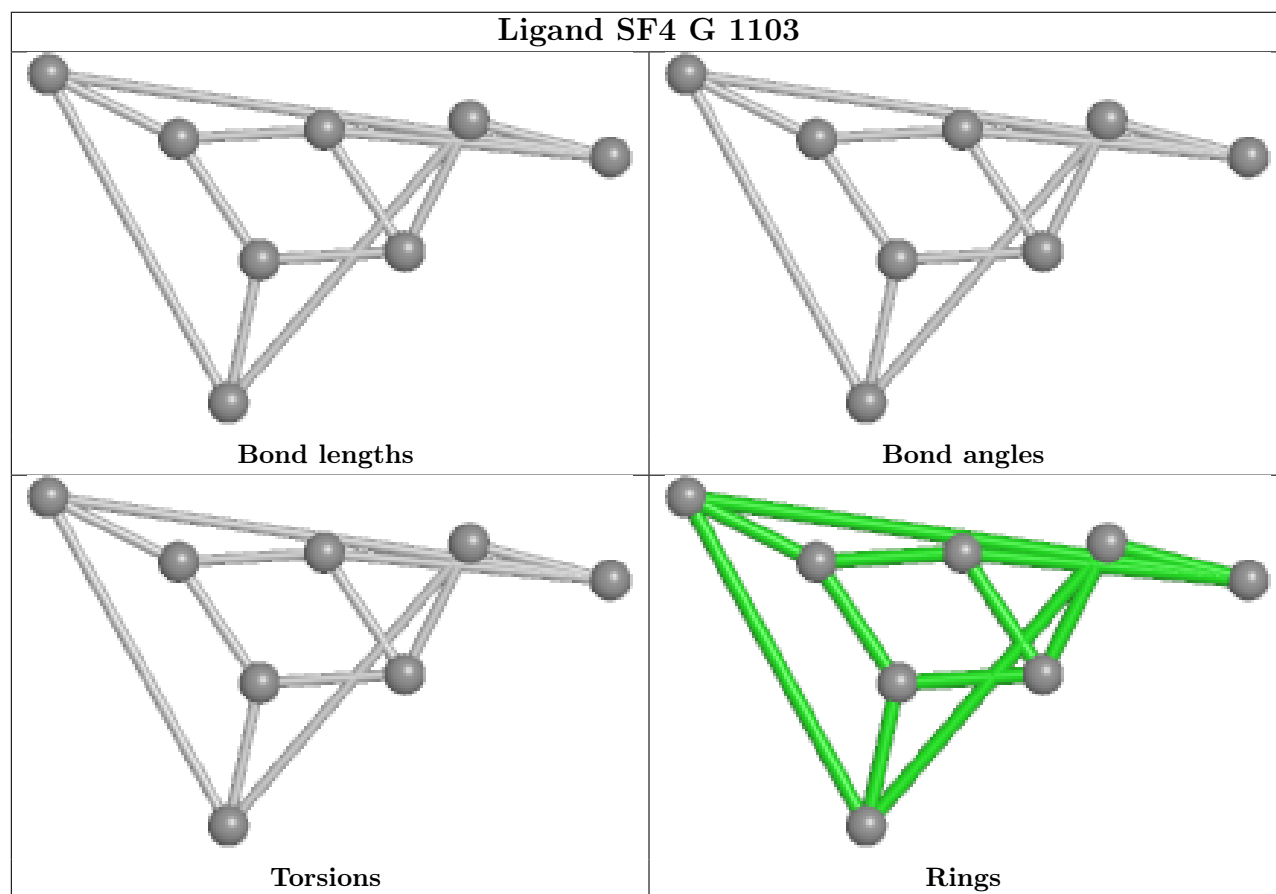
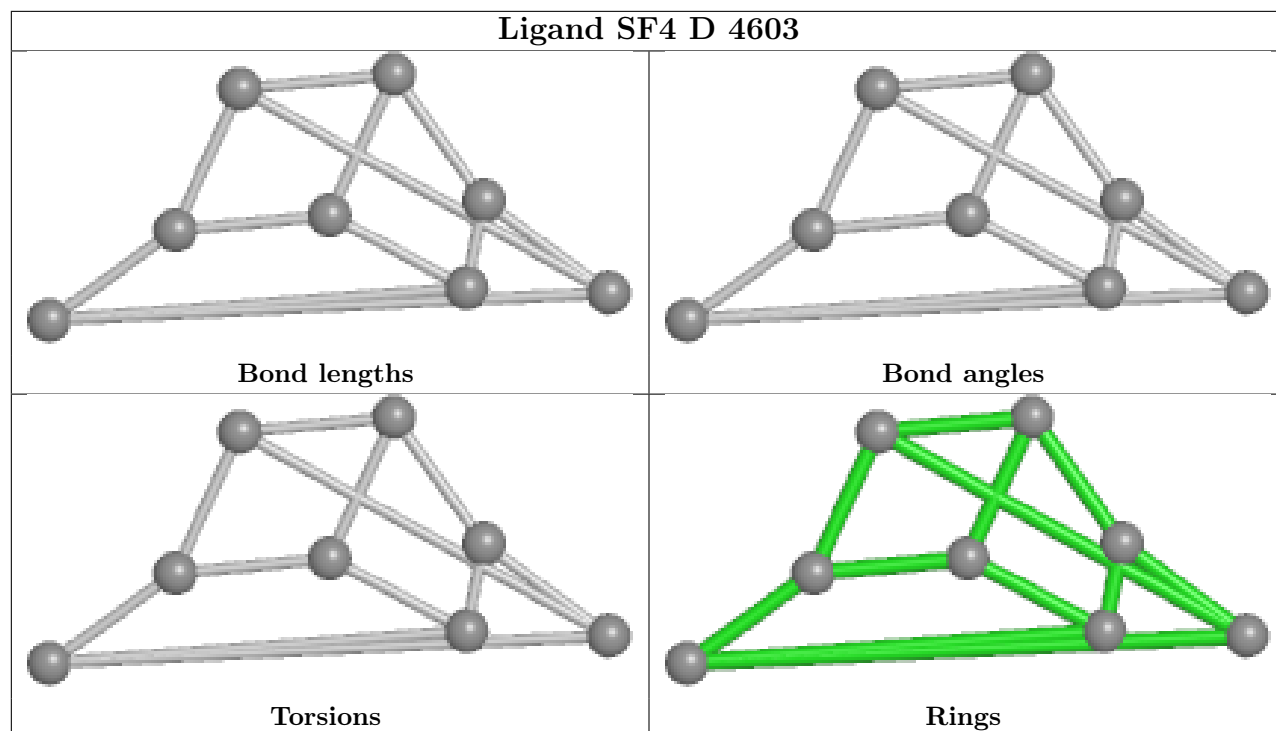


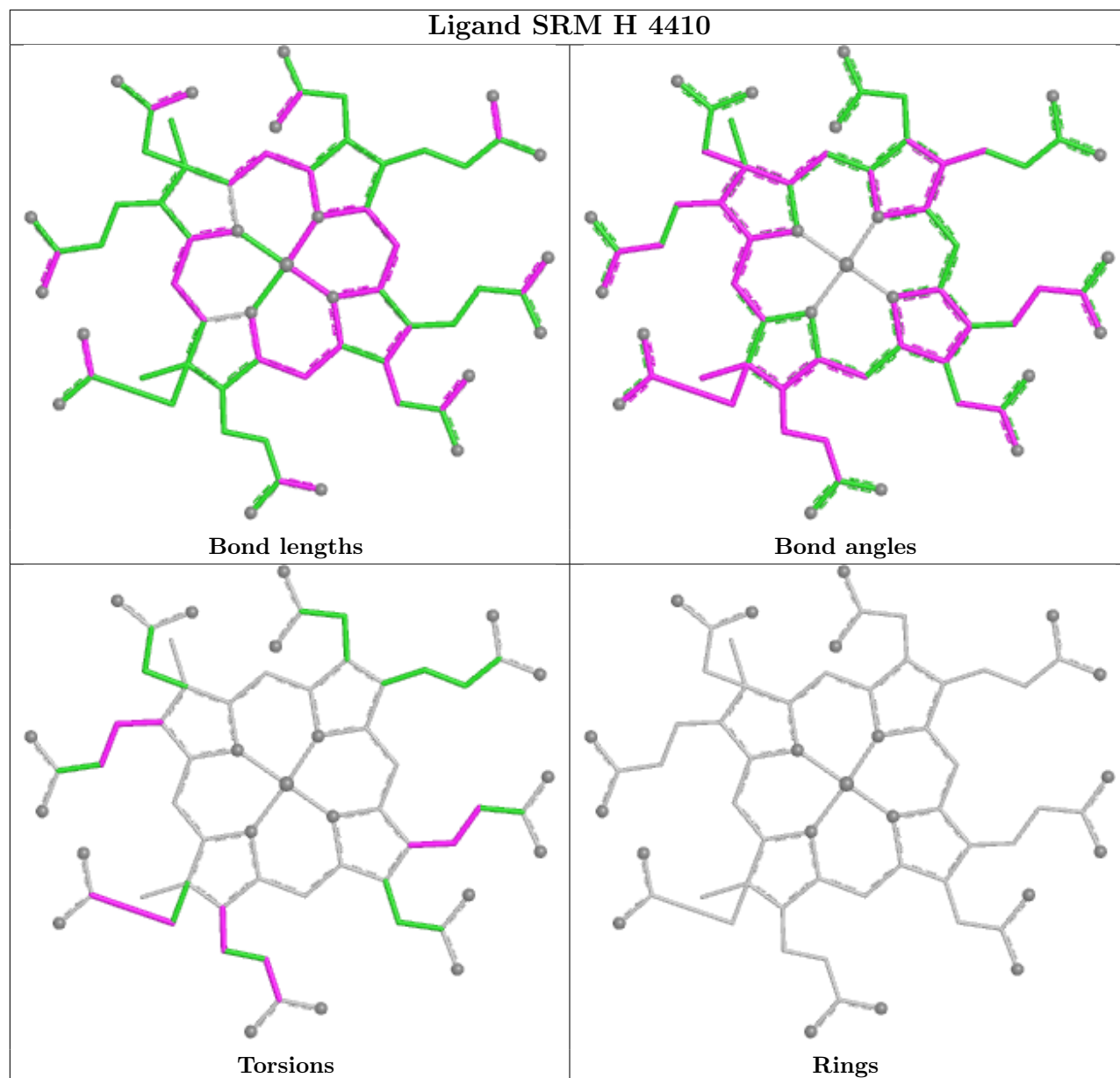


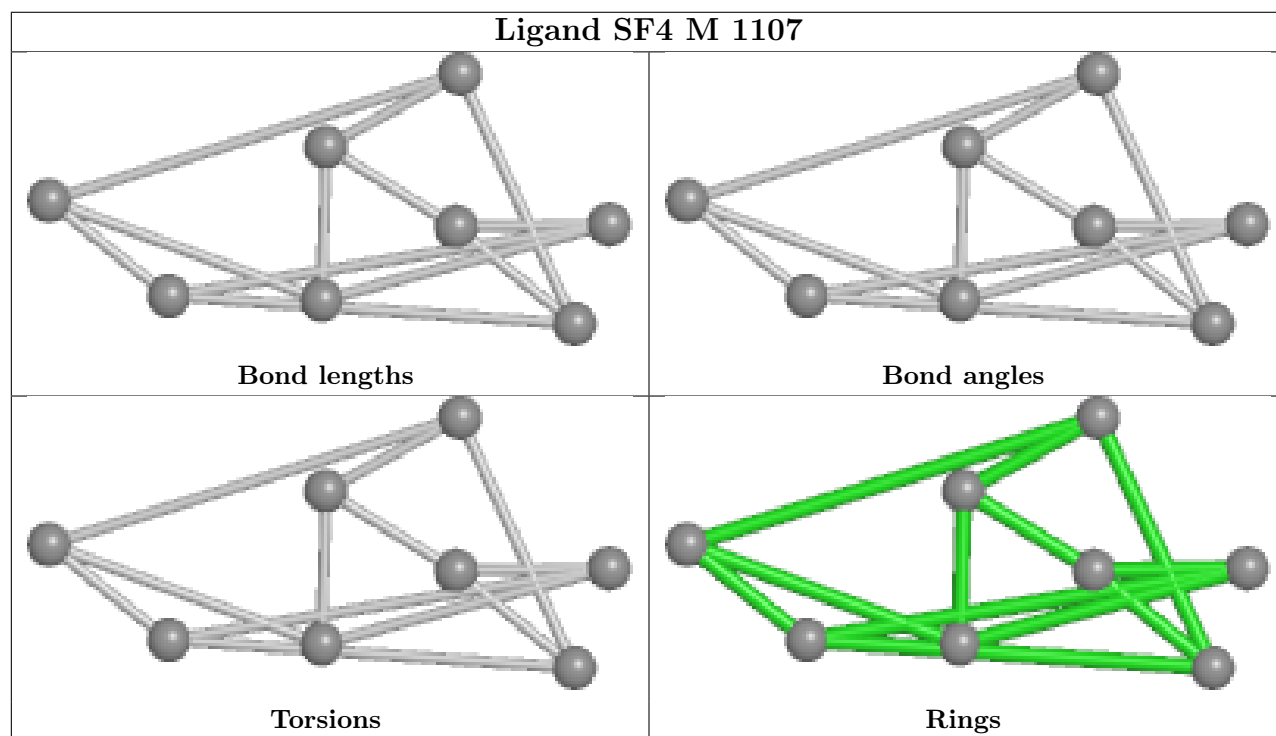
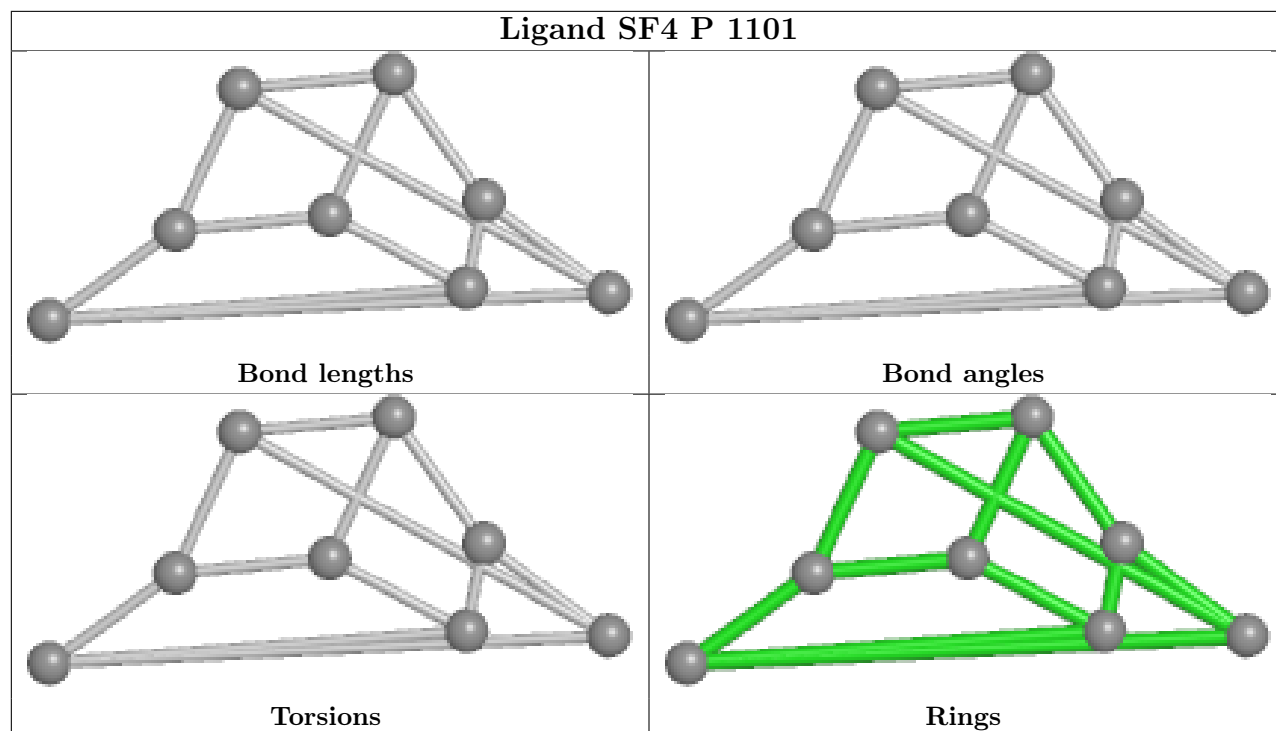


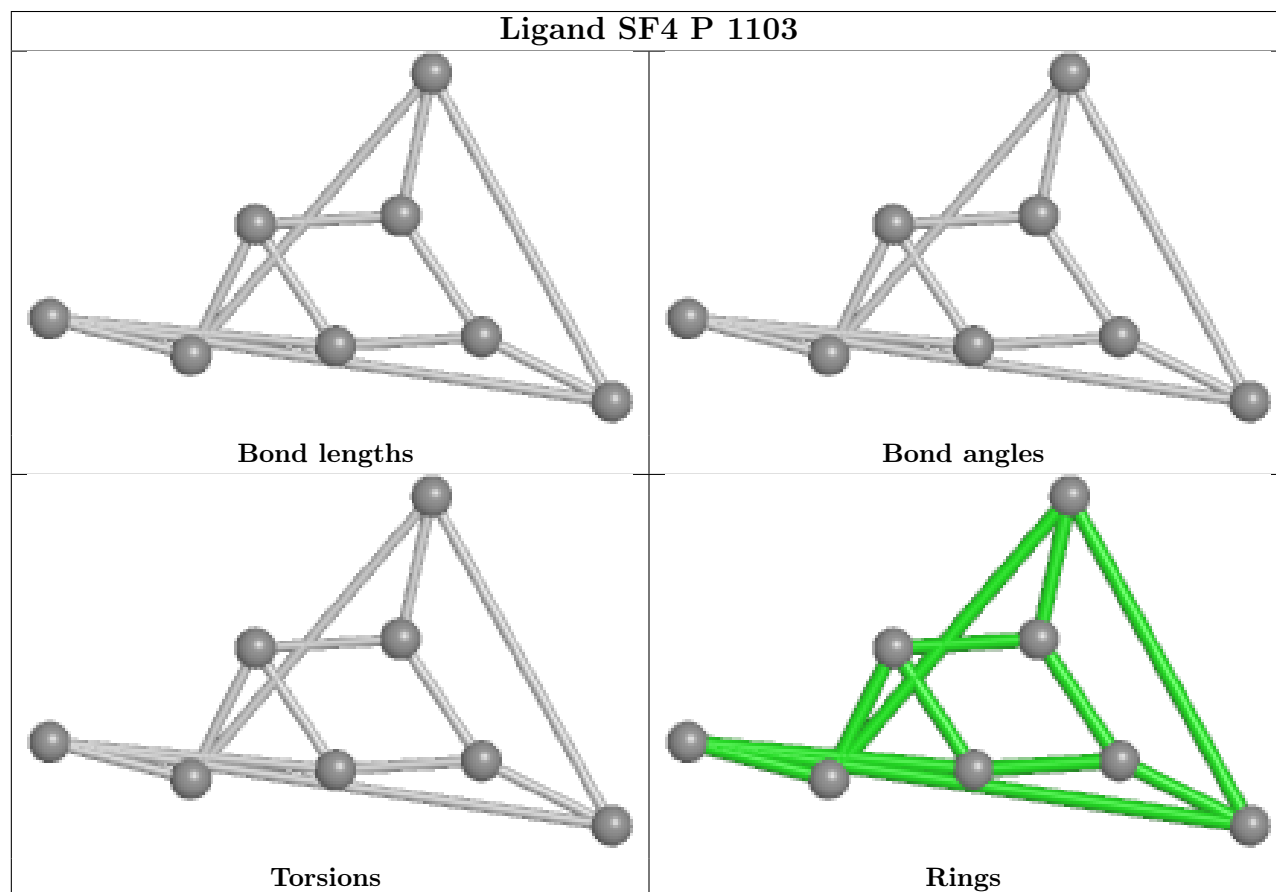
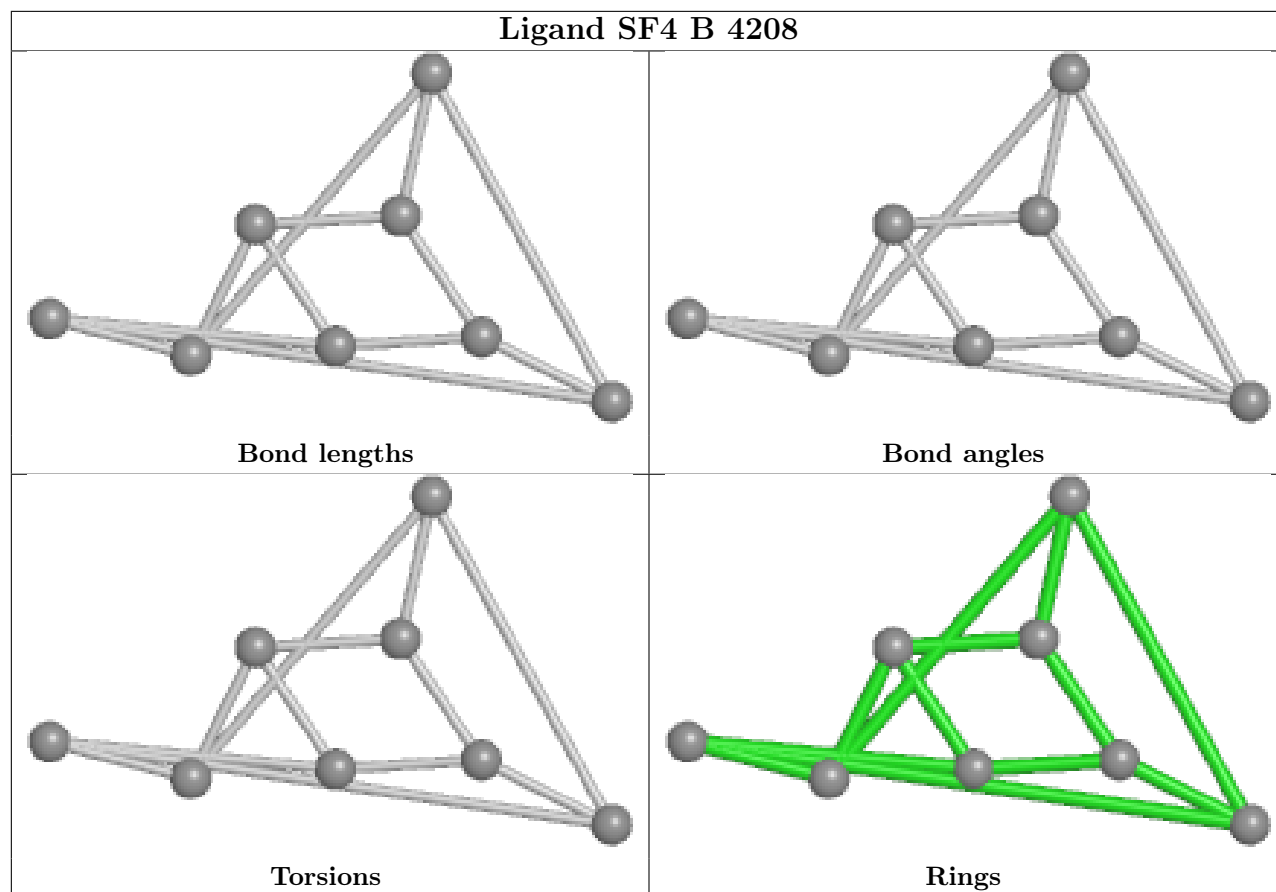


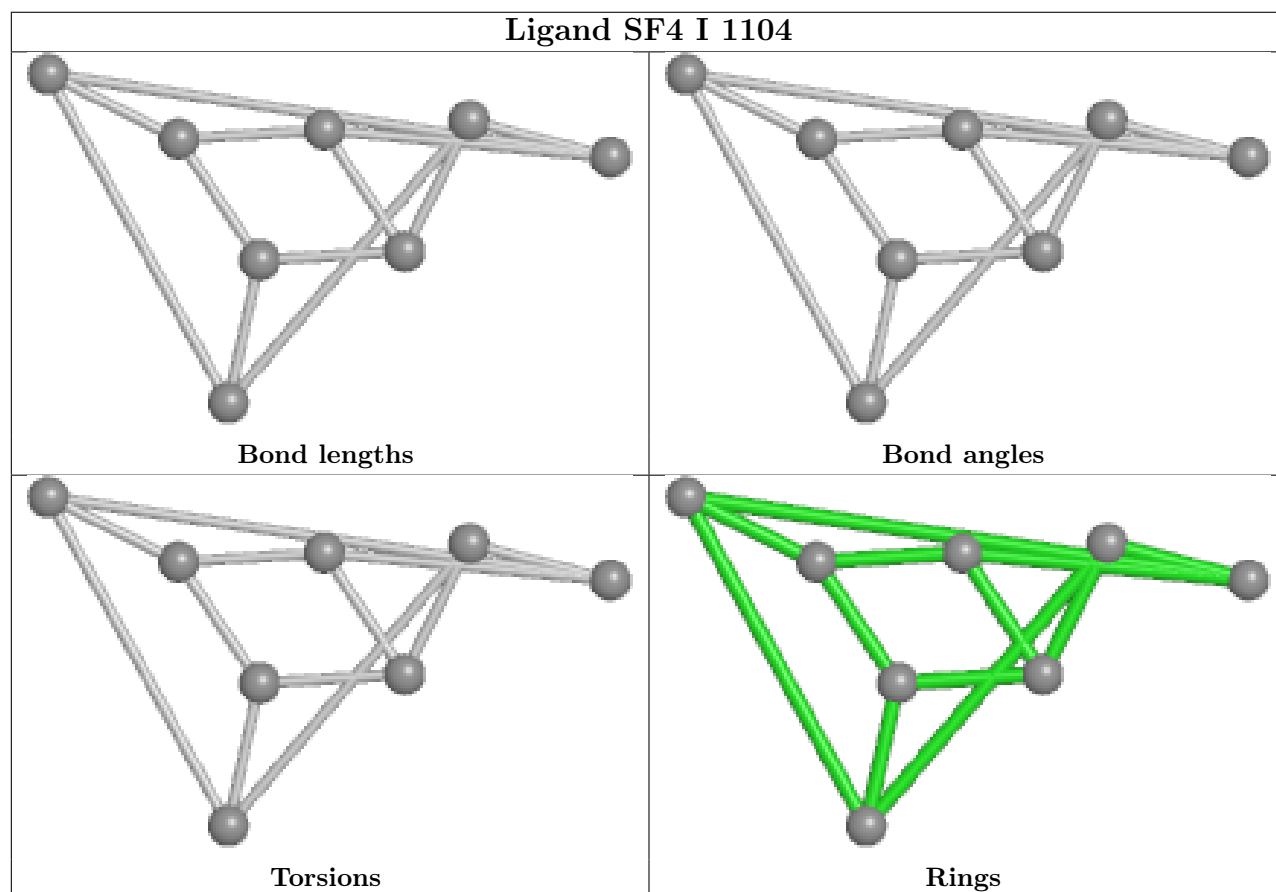
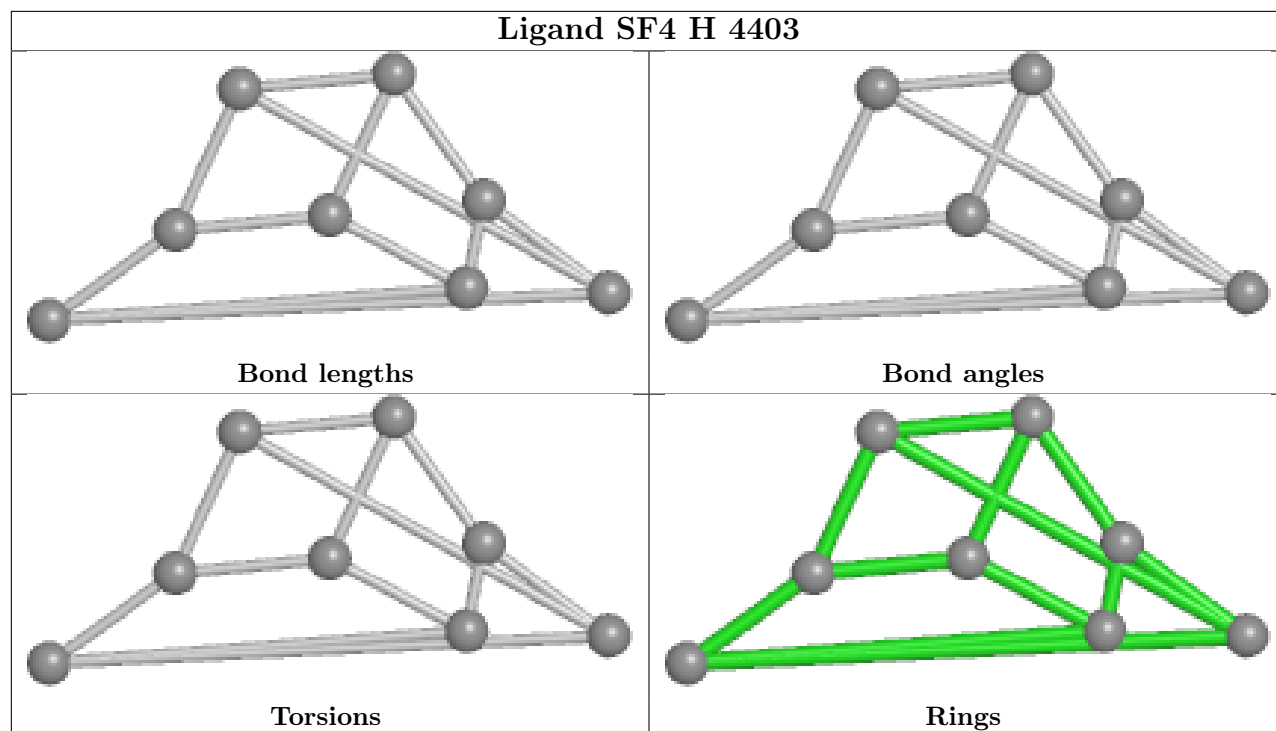


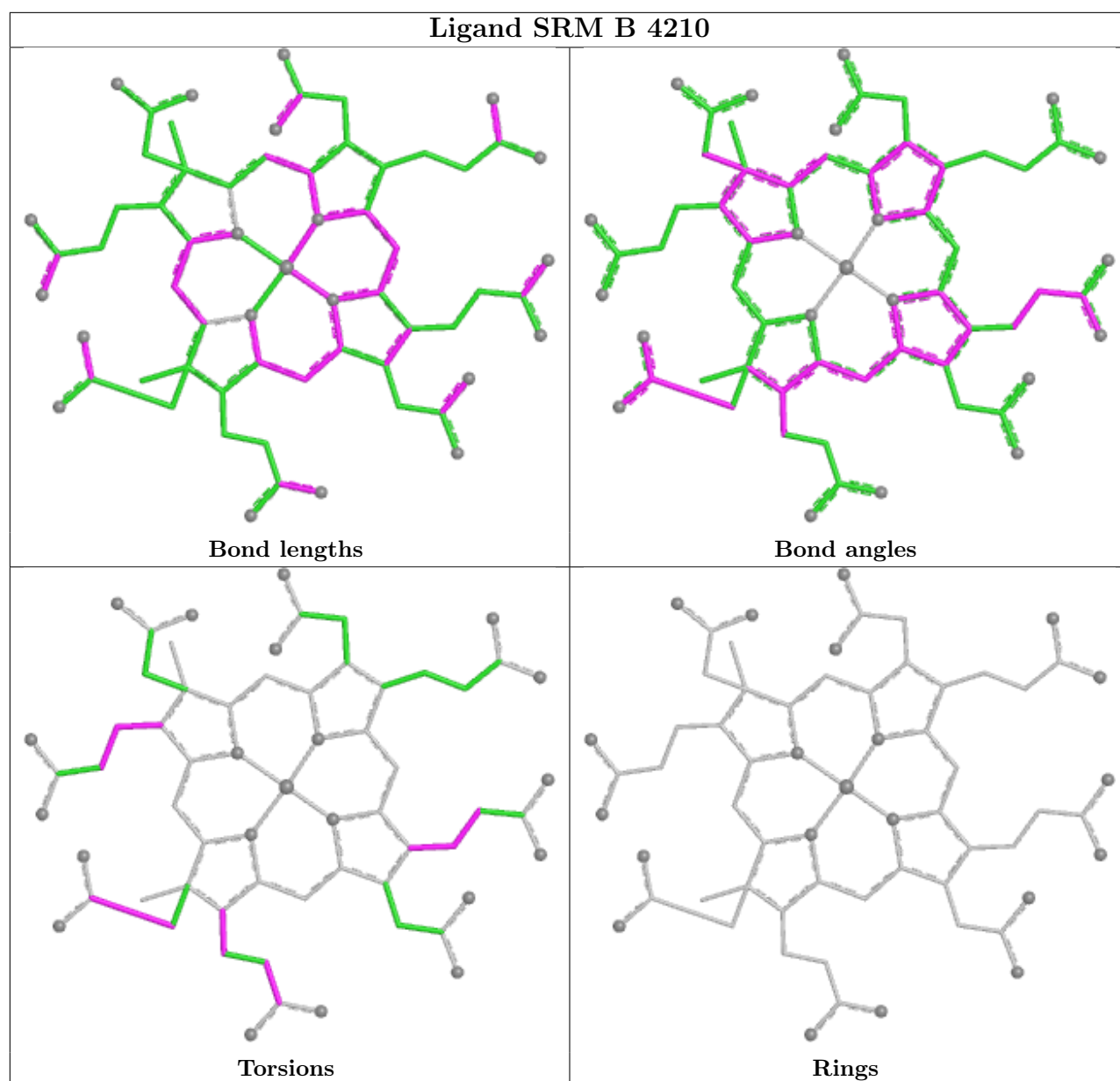




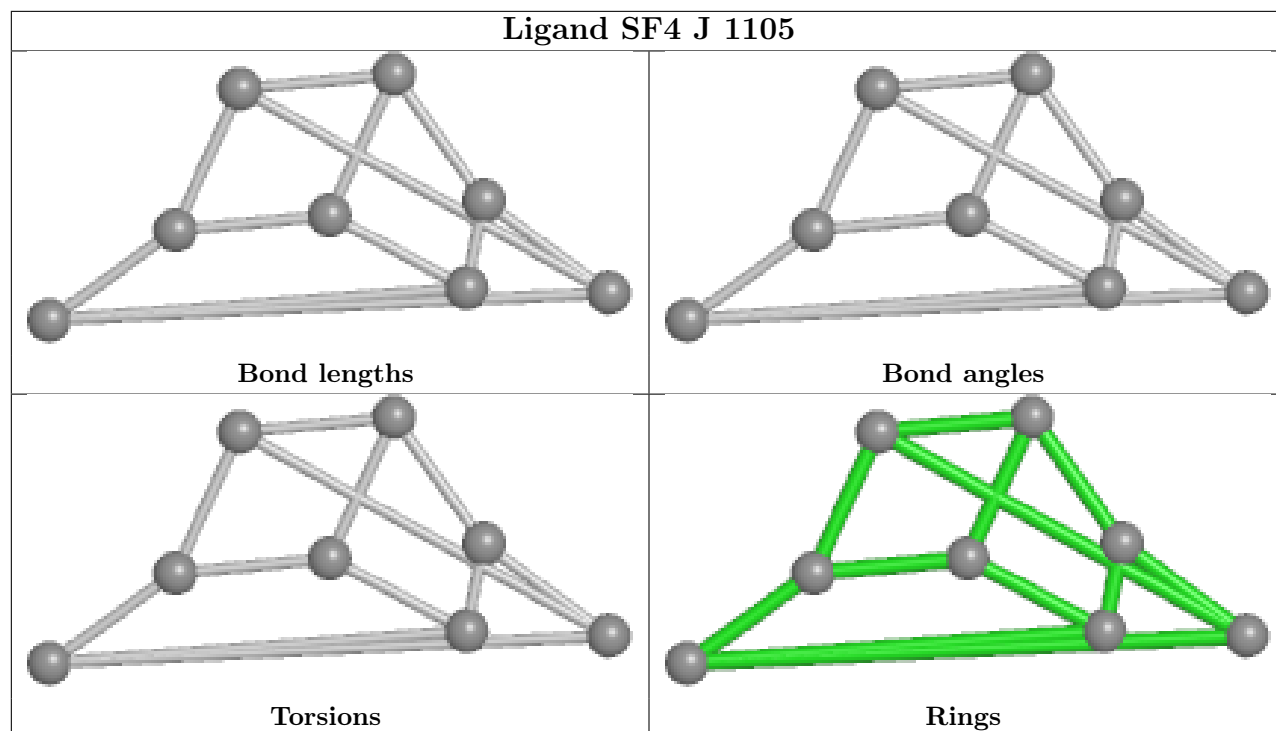




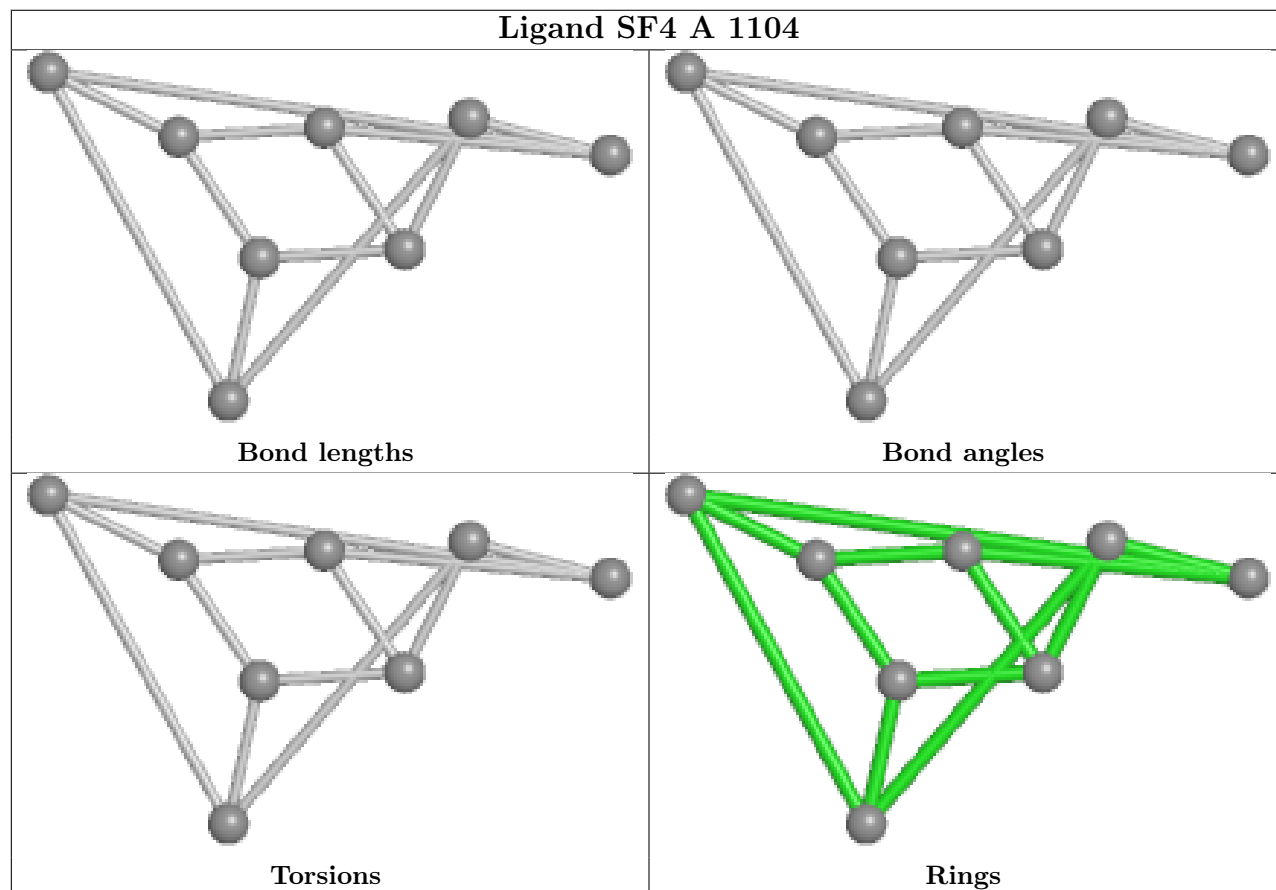


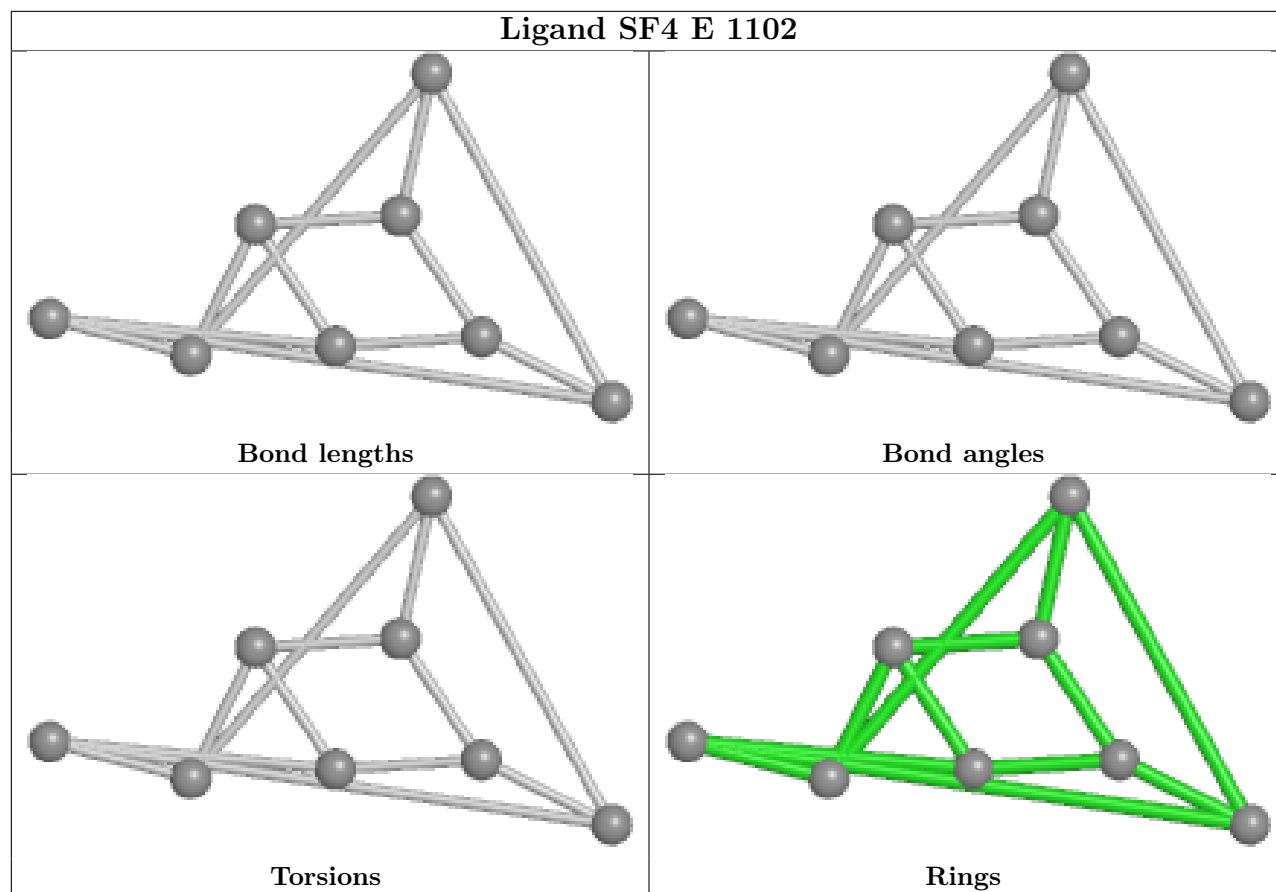


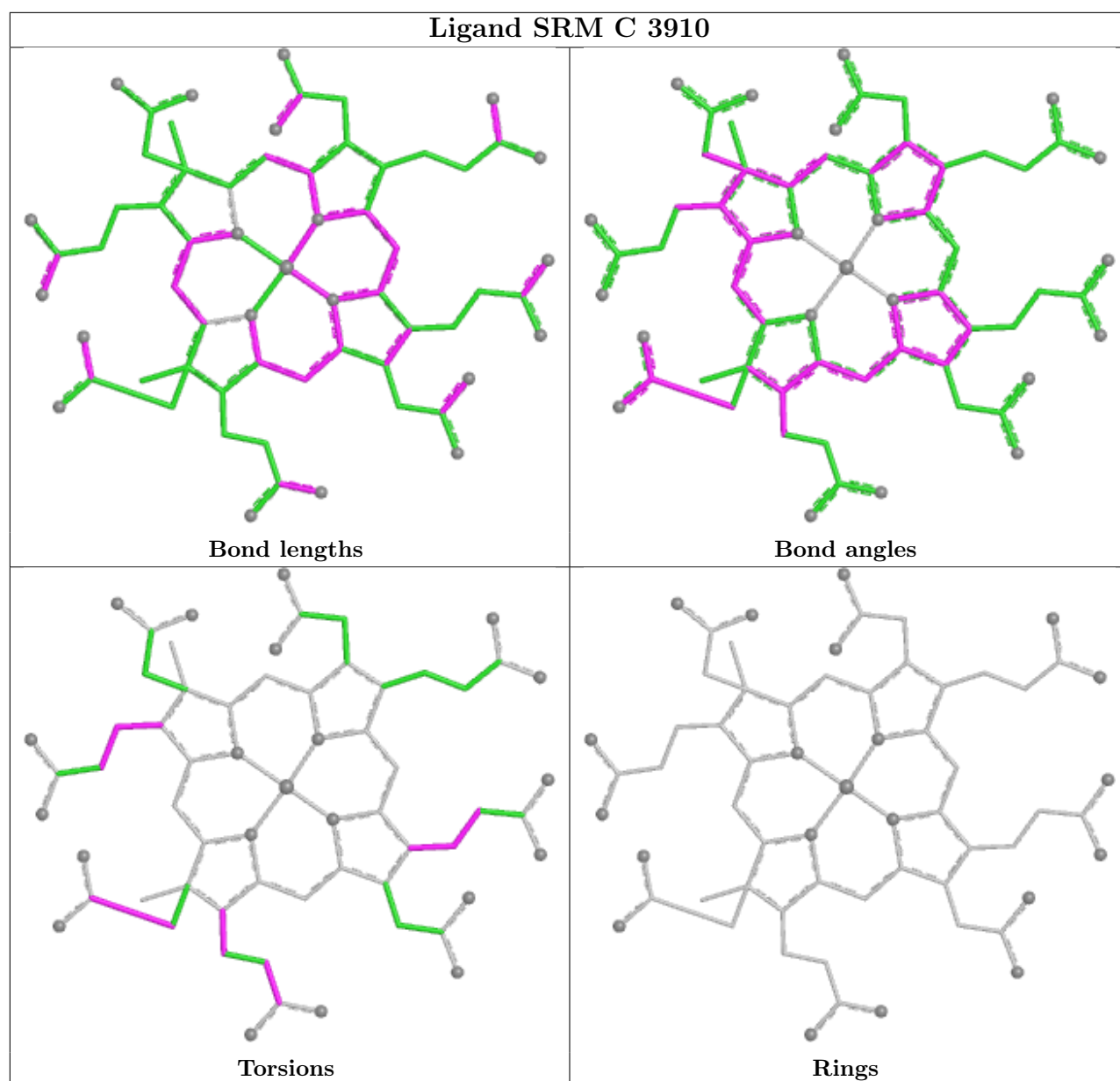
Ligand SF4 J 1105

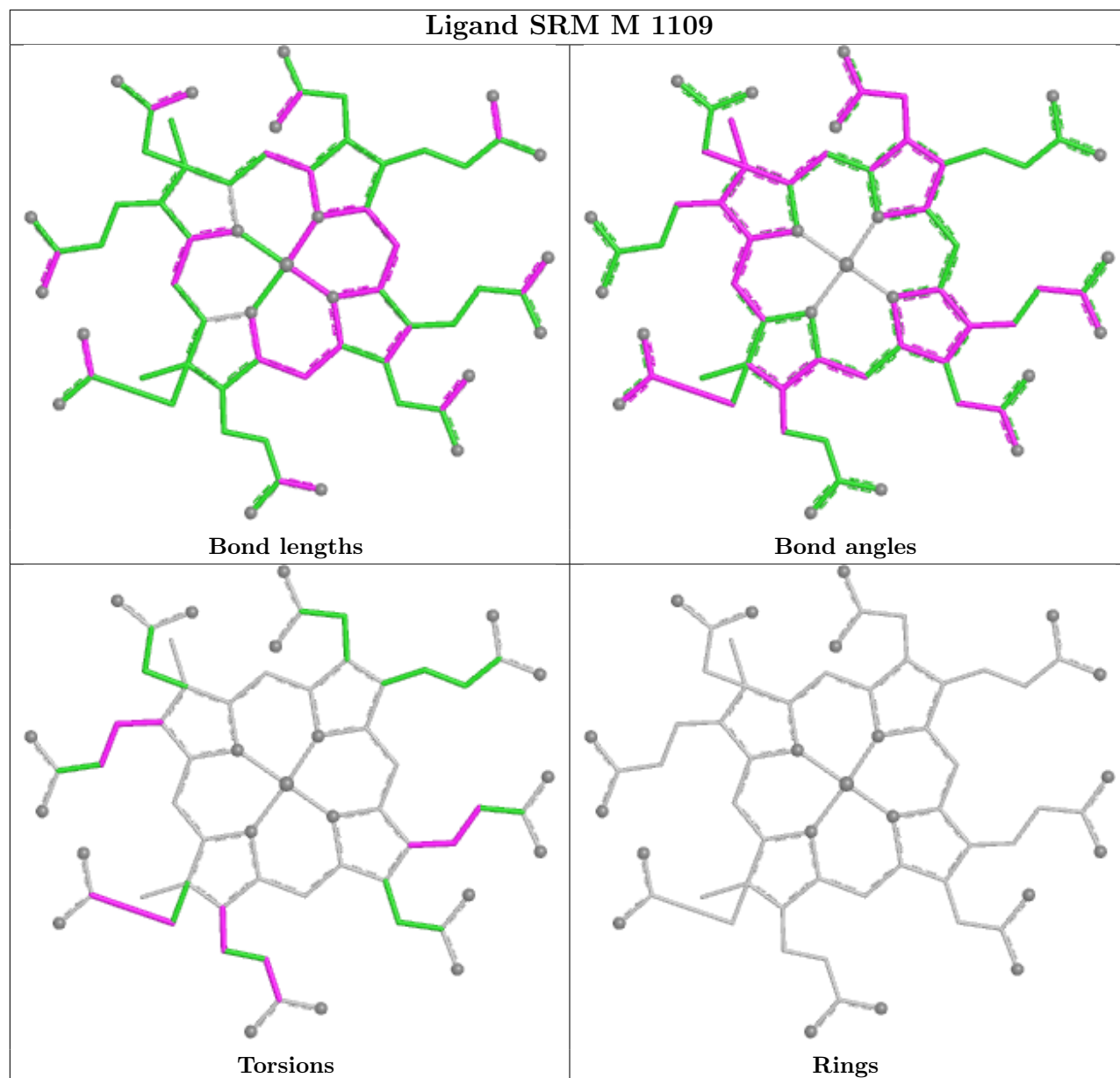


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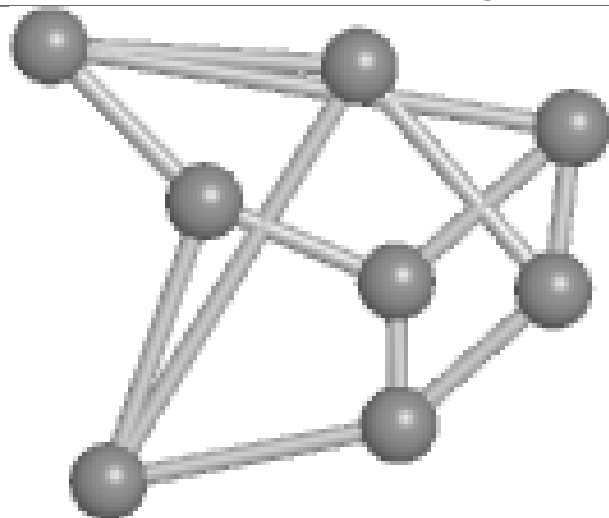




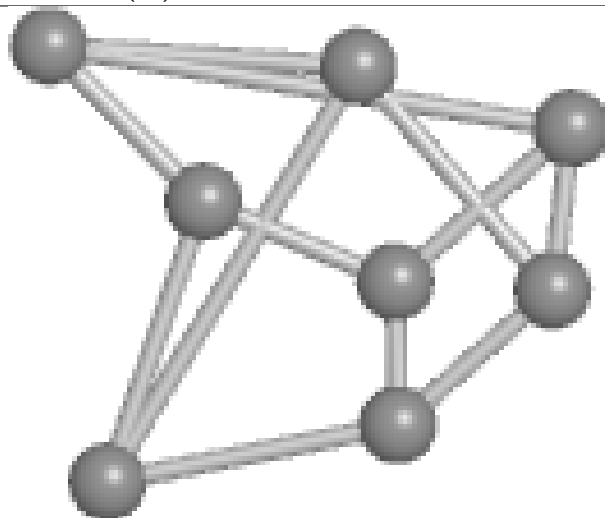




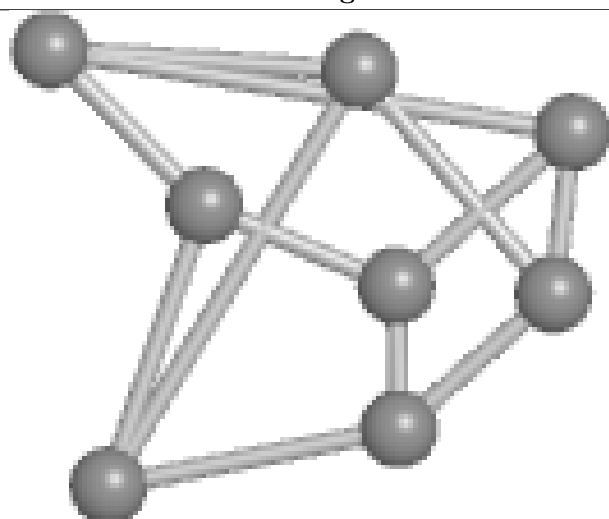
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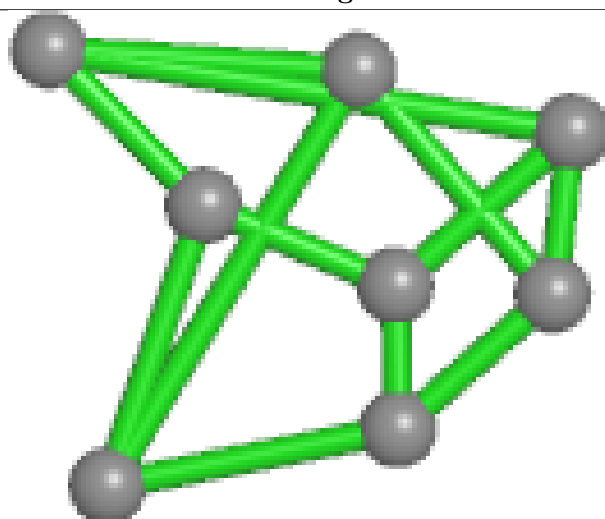
Bond lengths



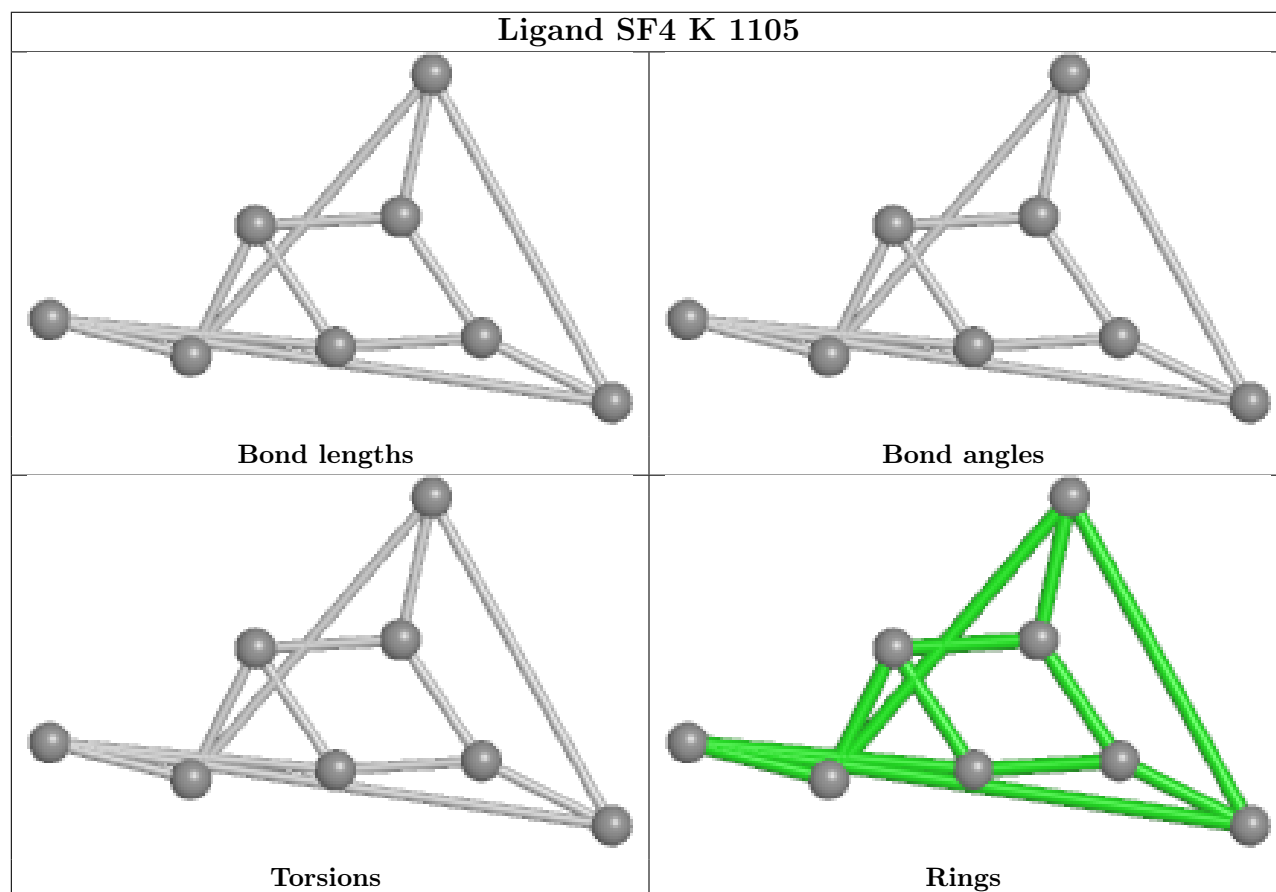
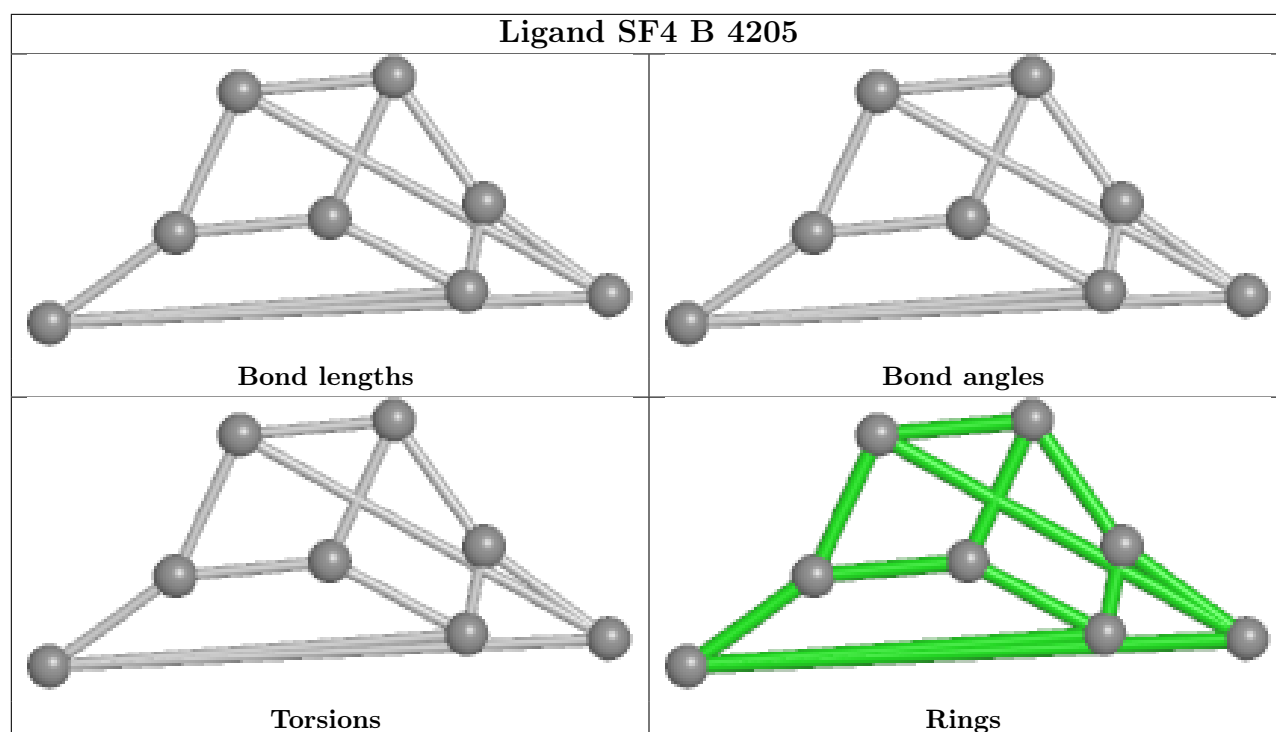
Bond angles

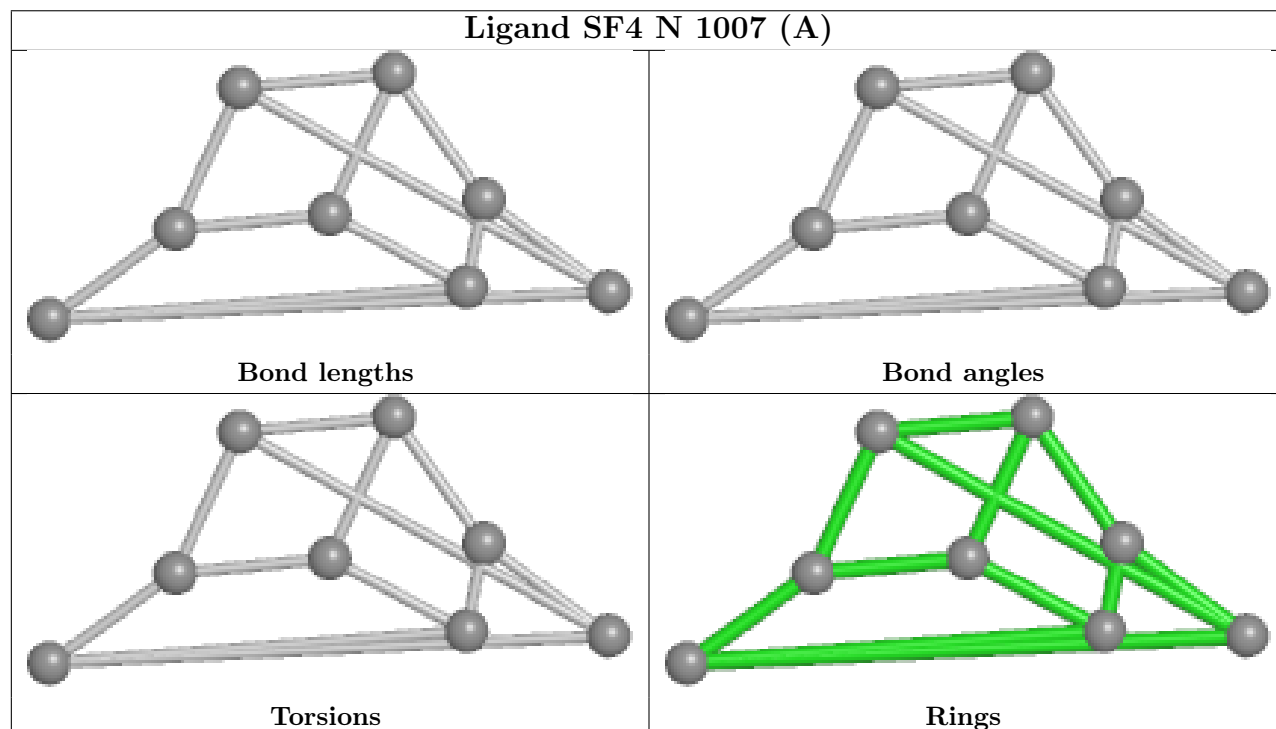
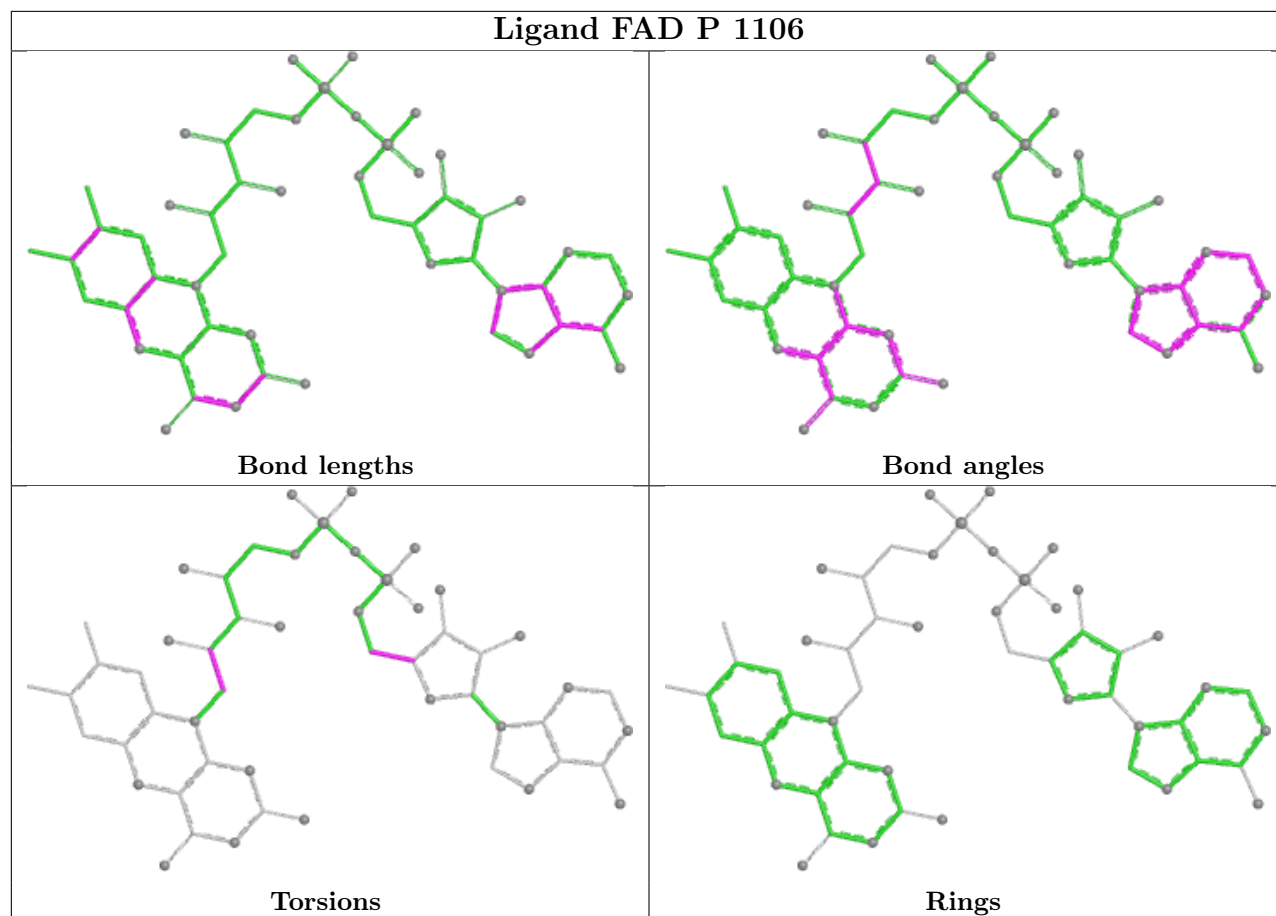


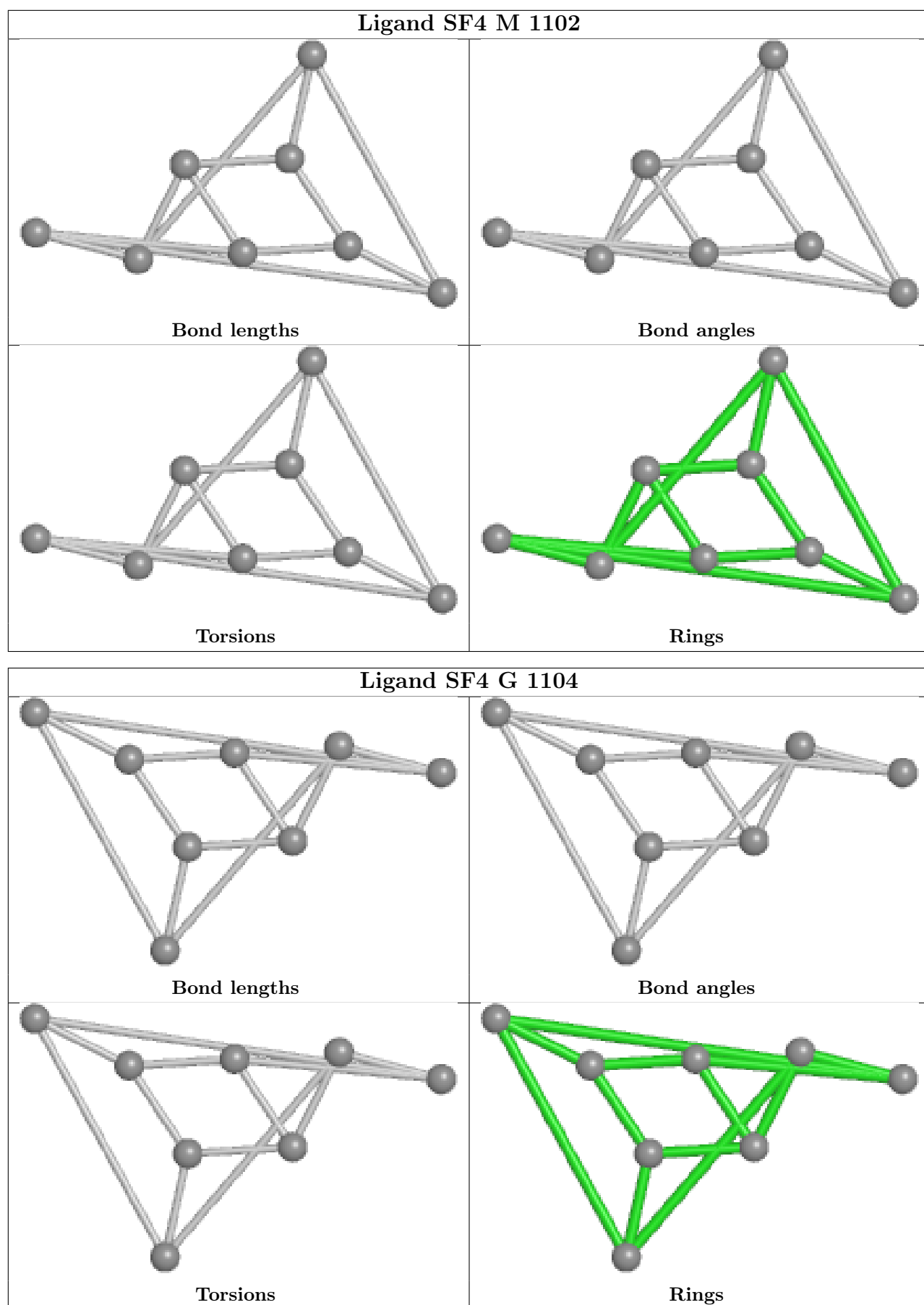
Torsions

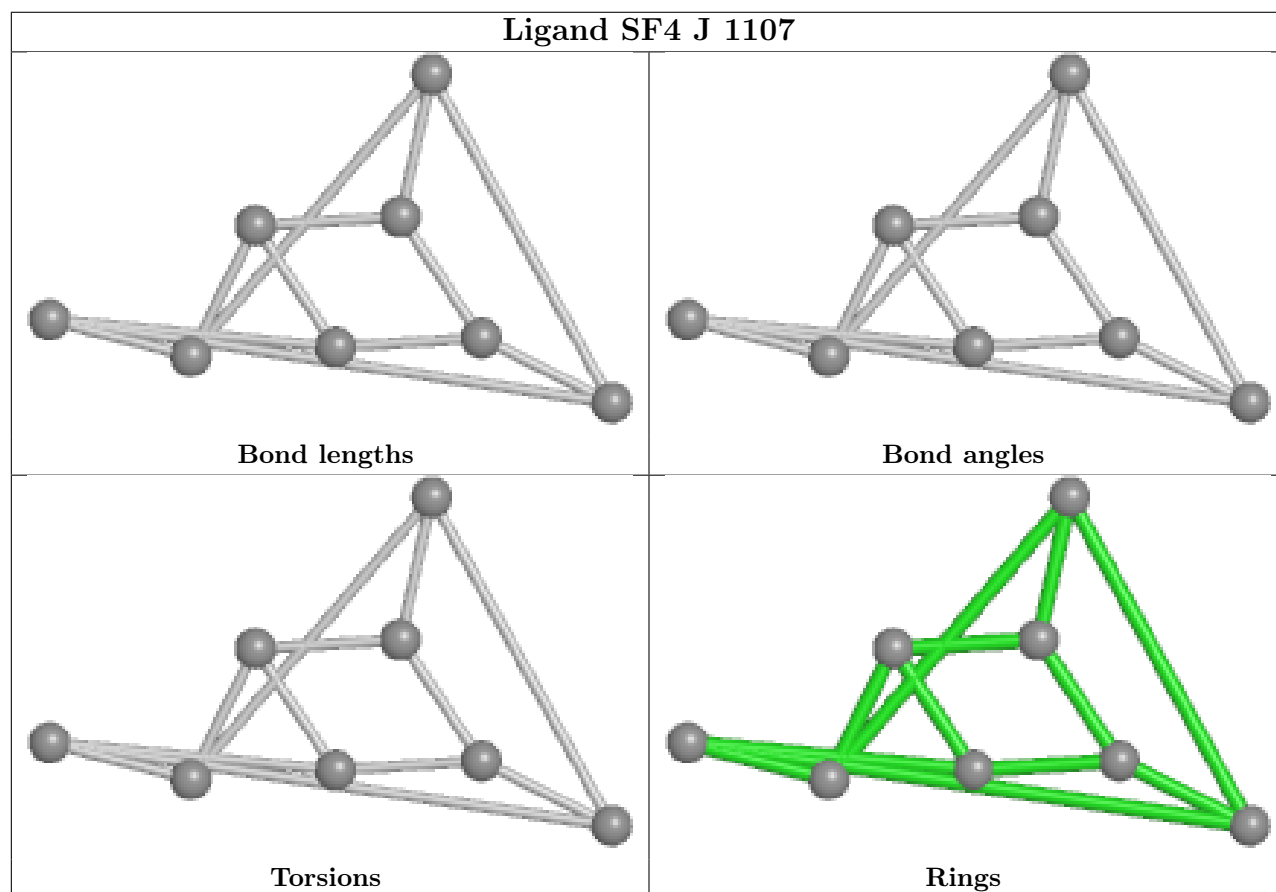
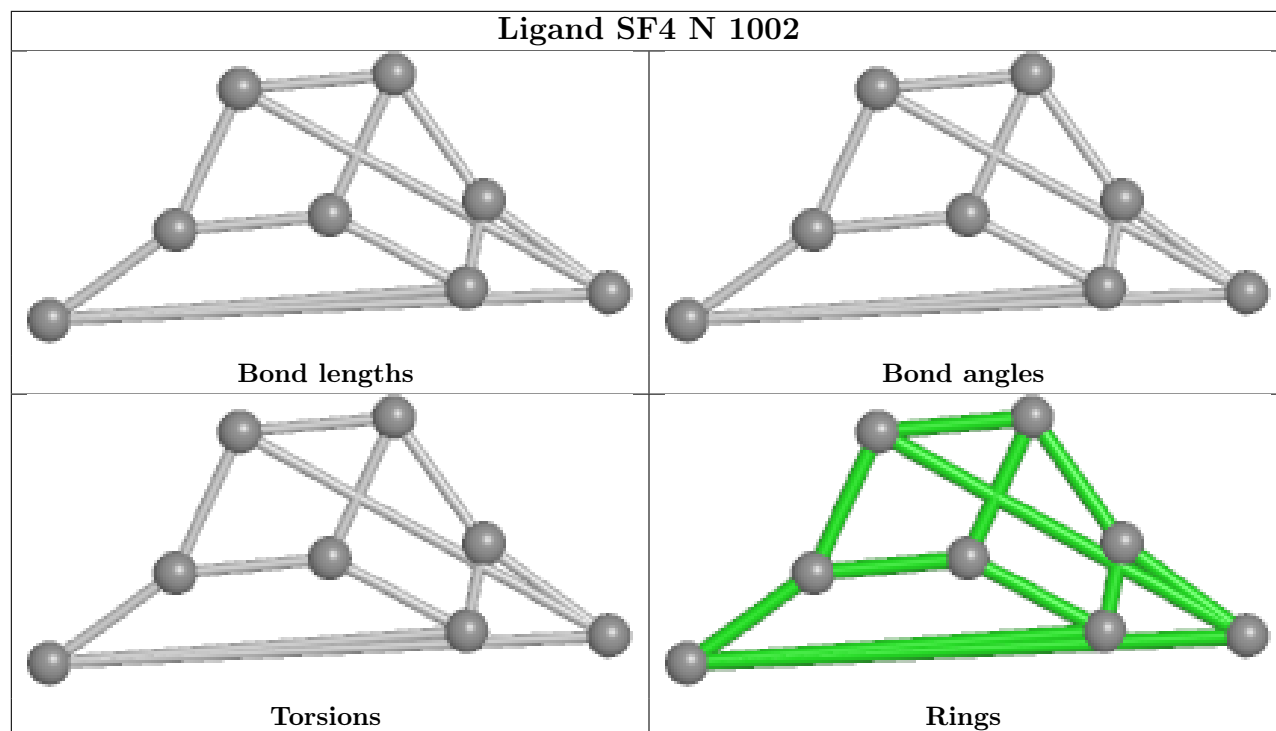


Rings

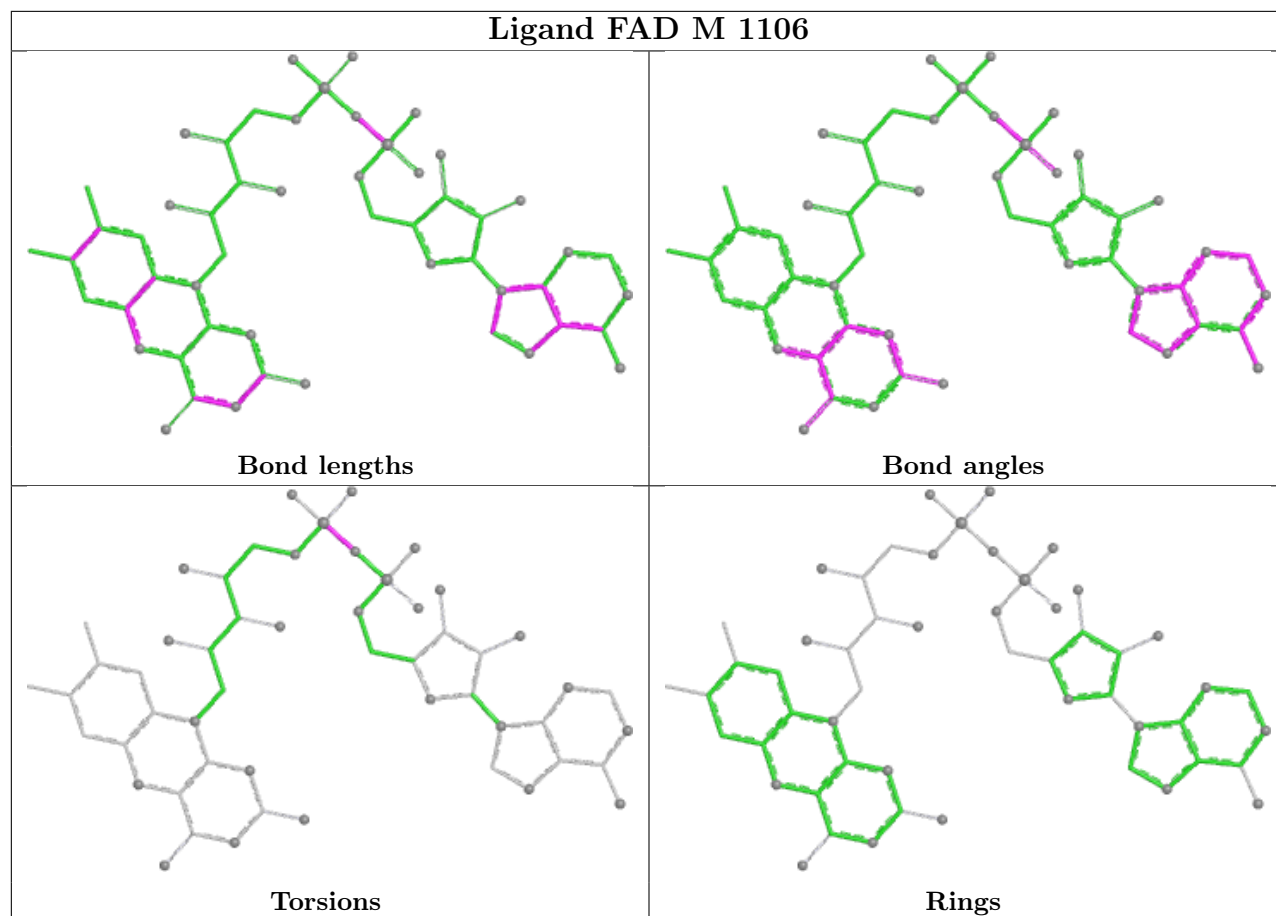




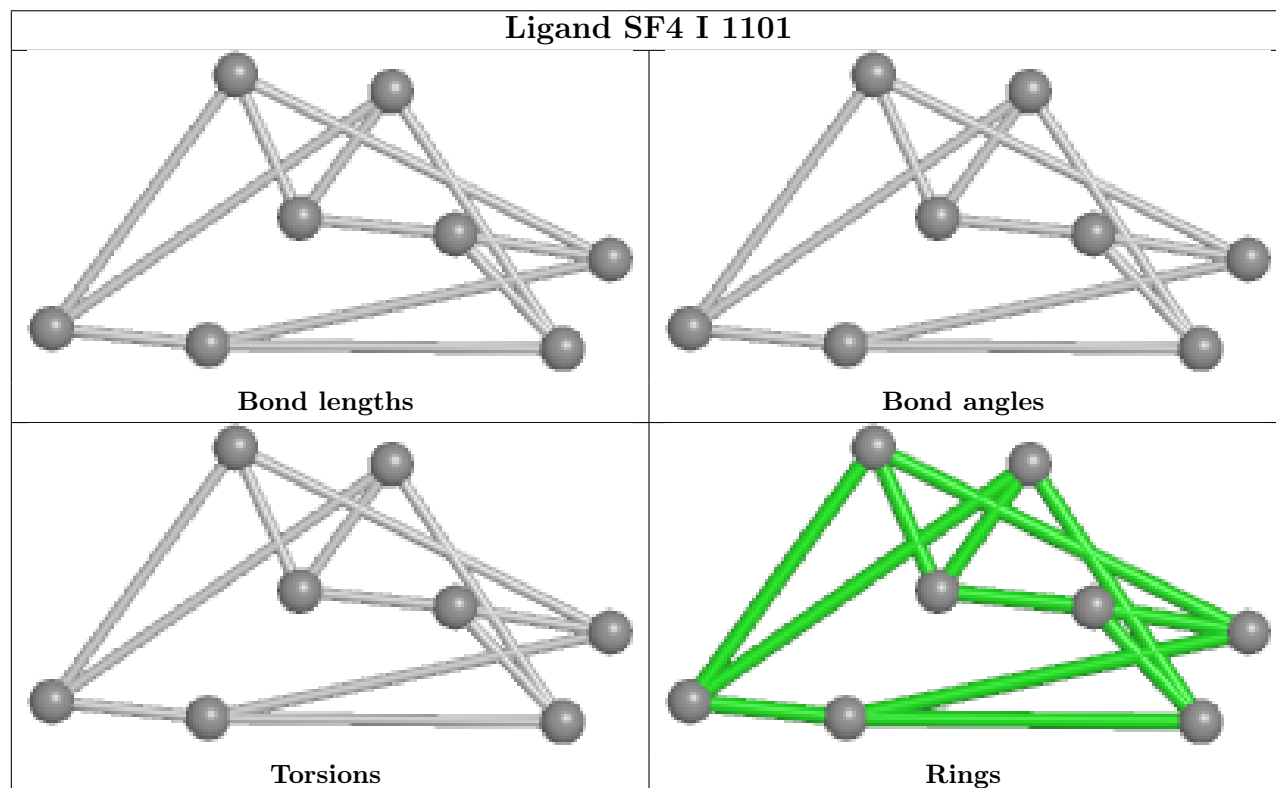


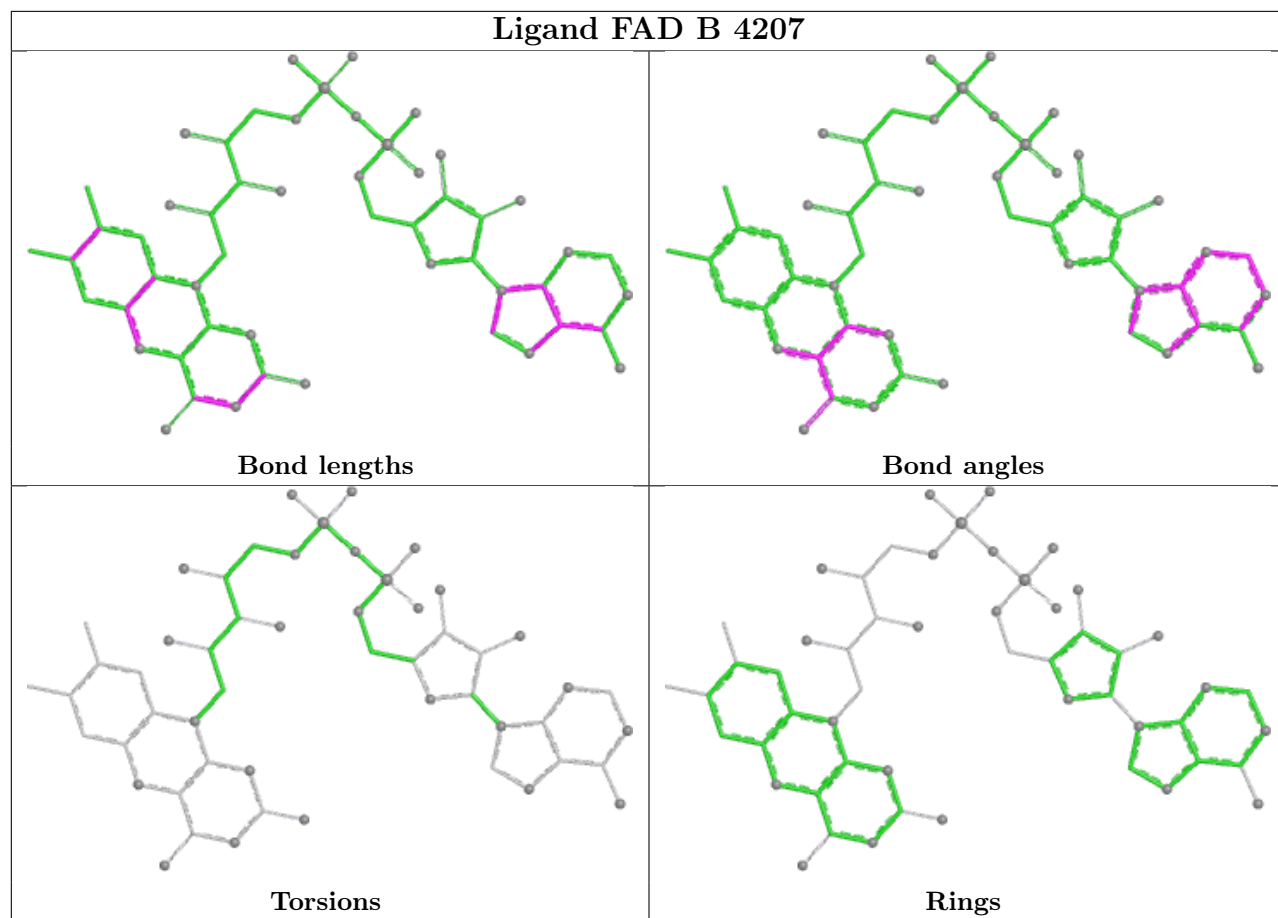


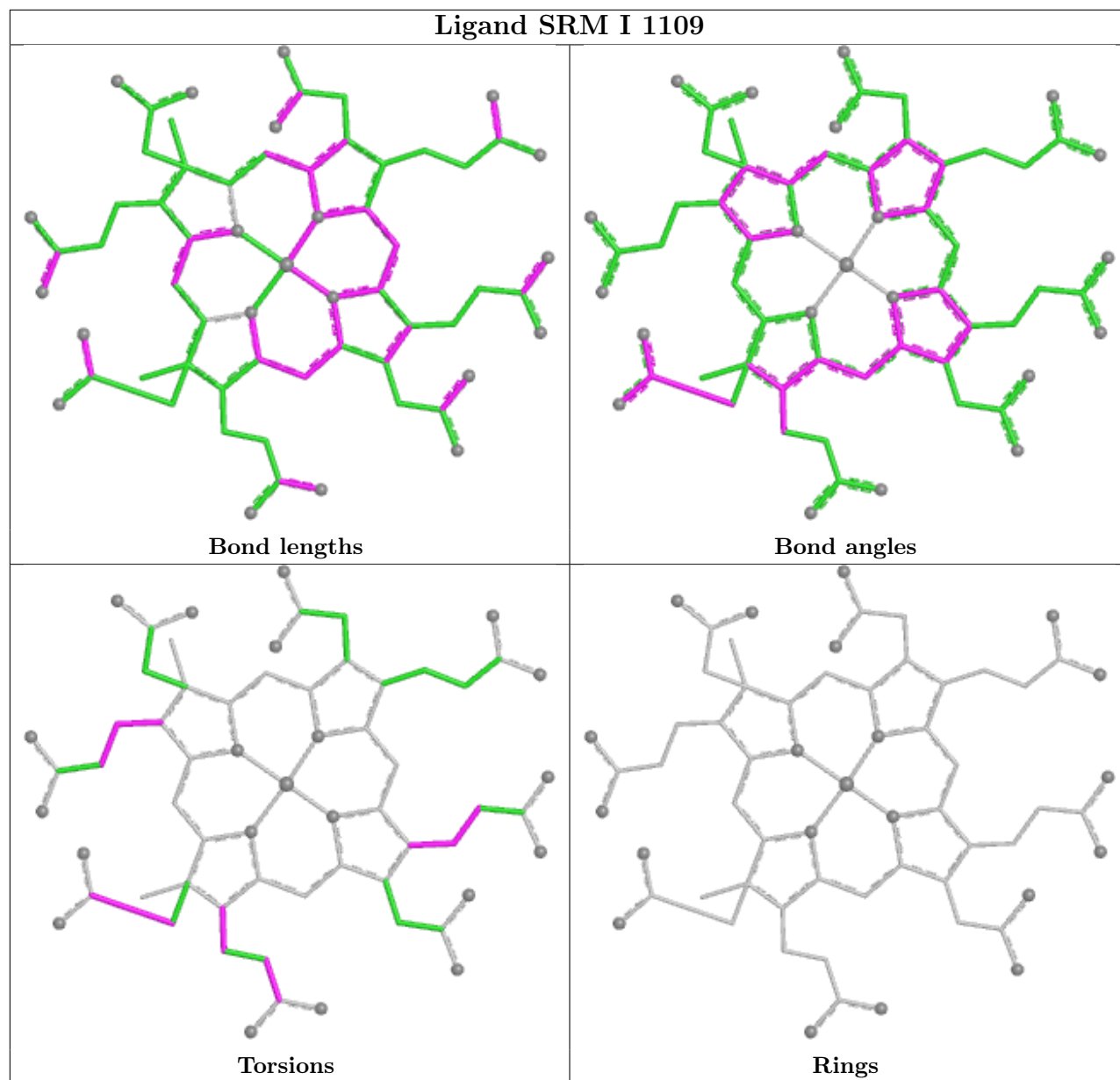
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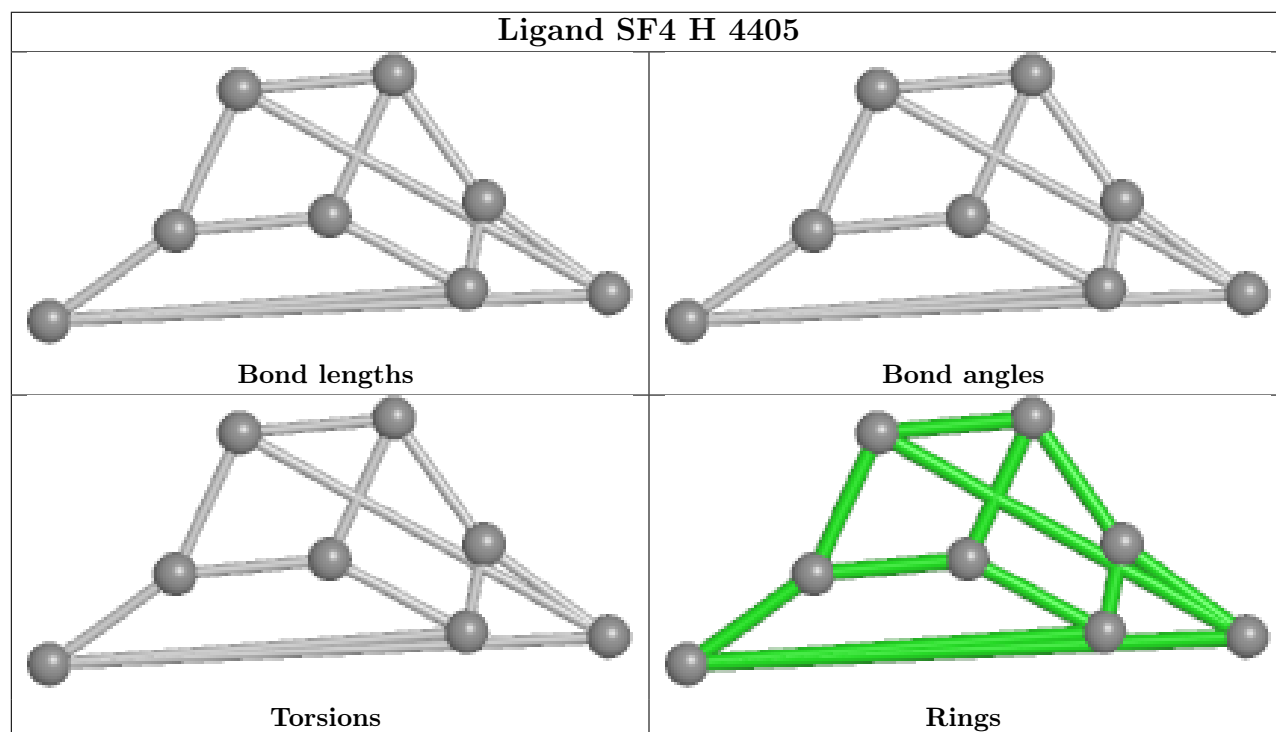
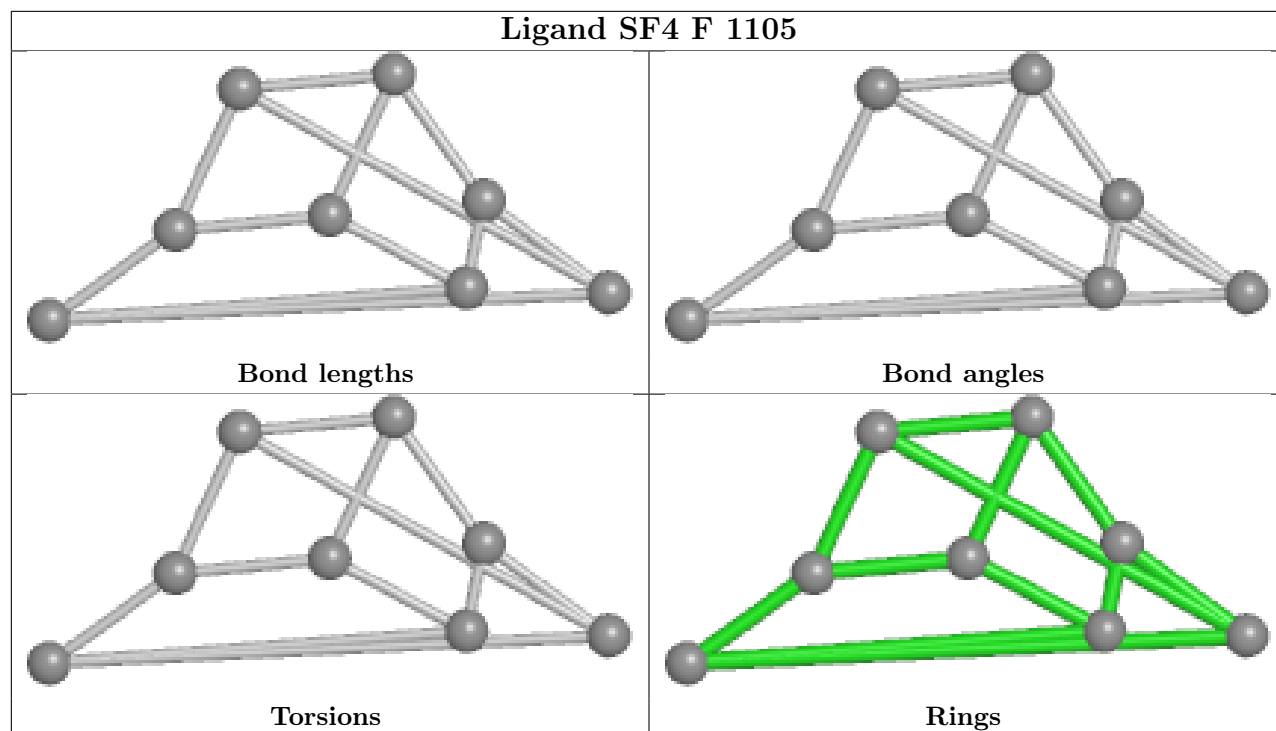


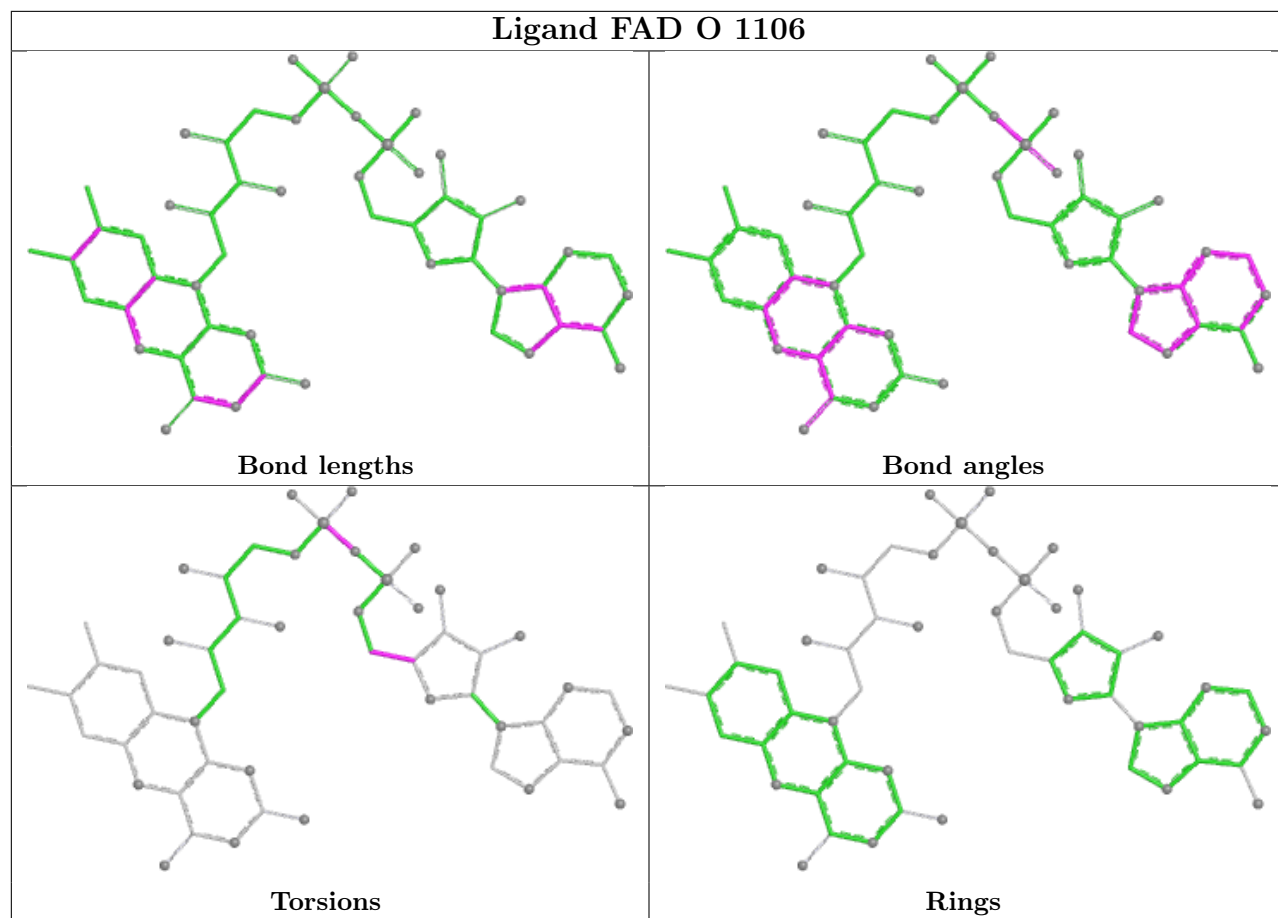
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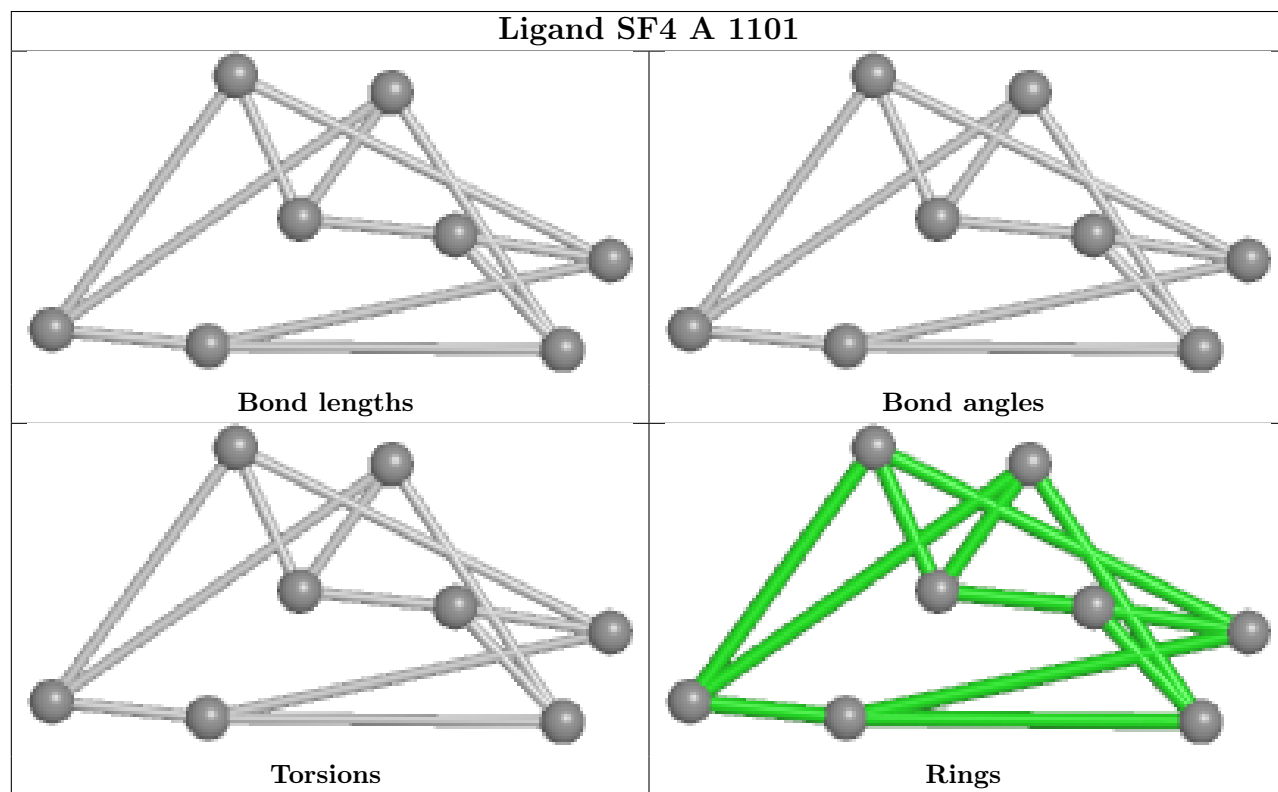
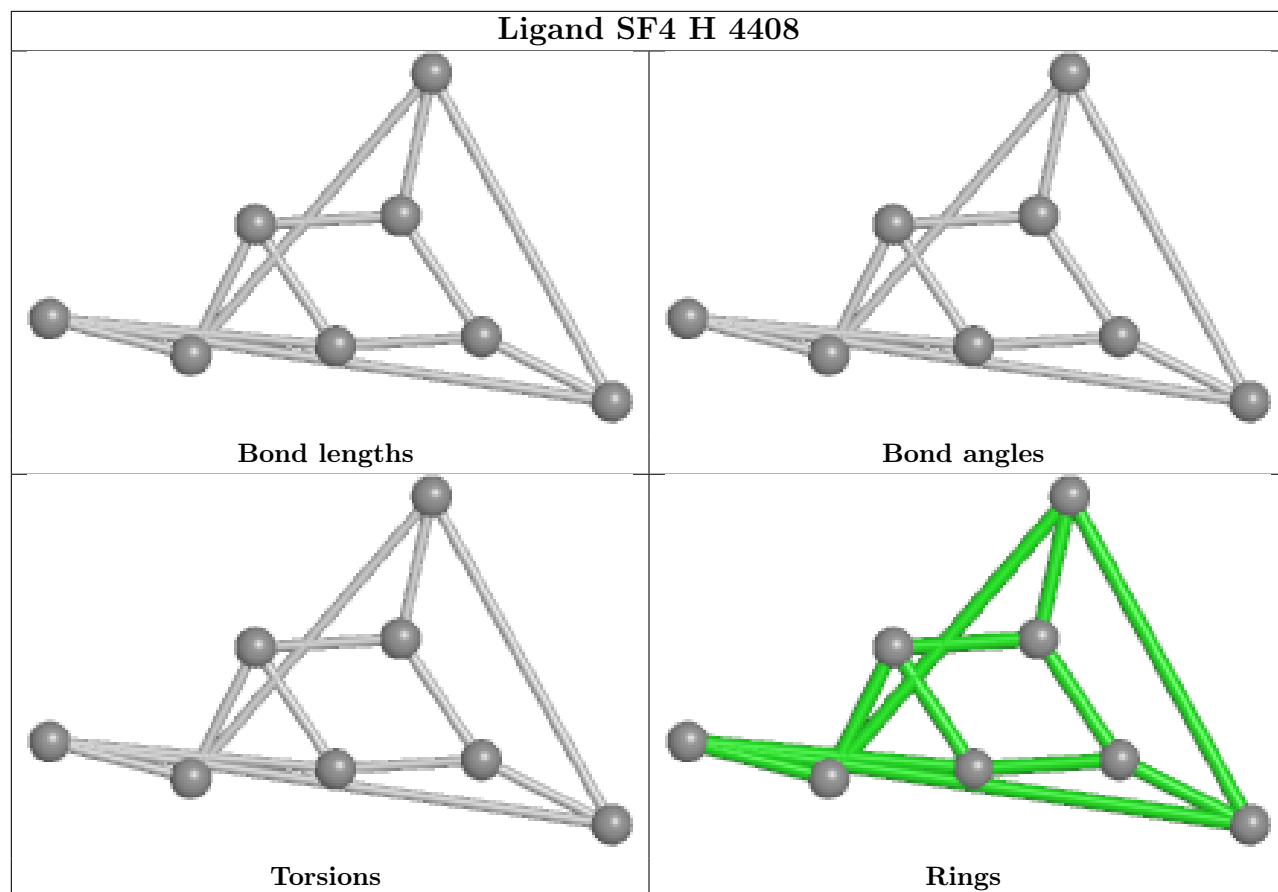


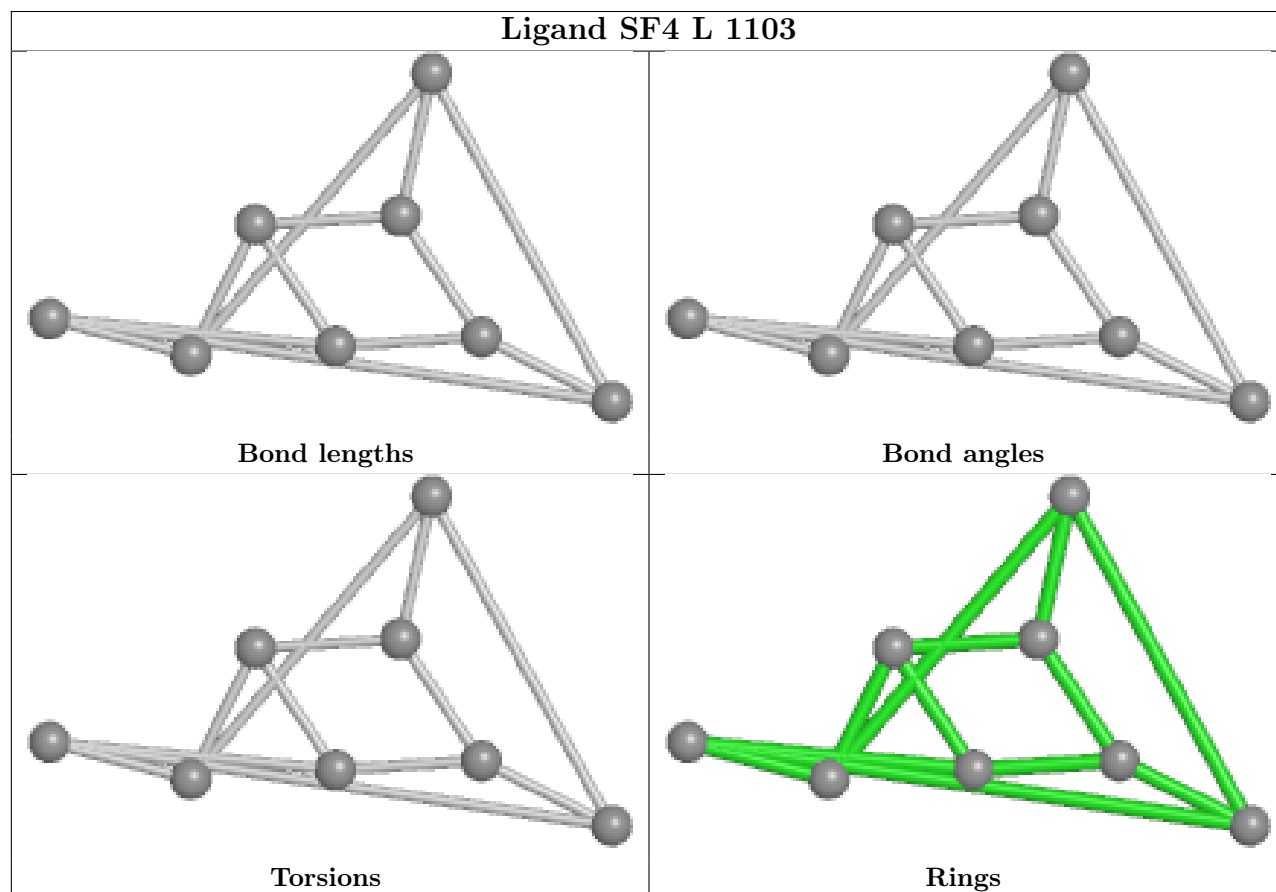
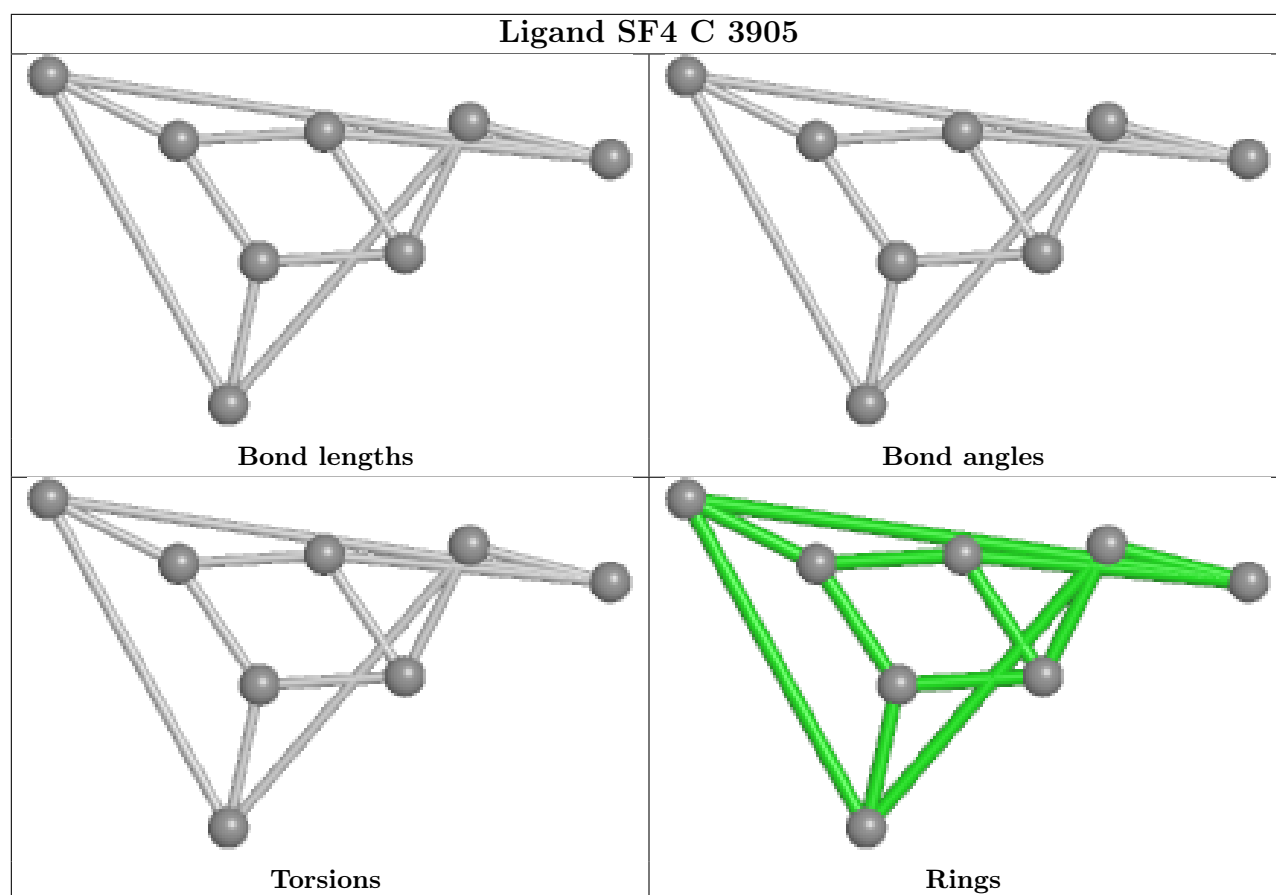


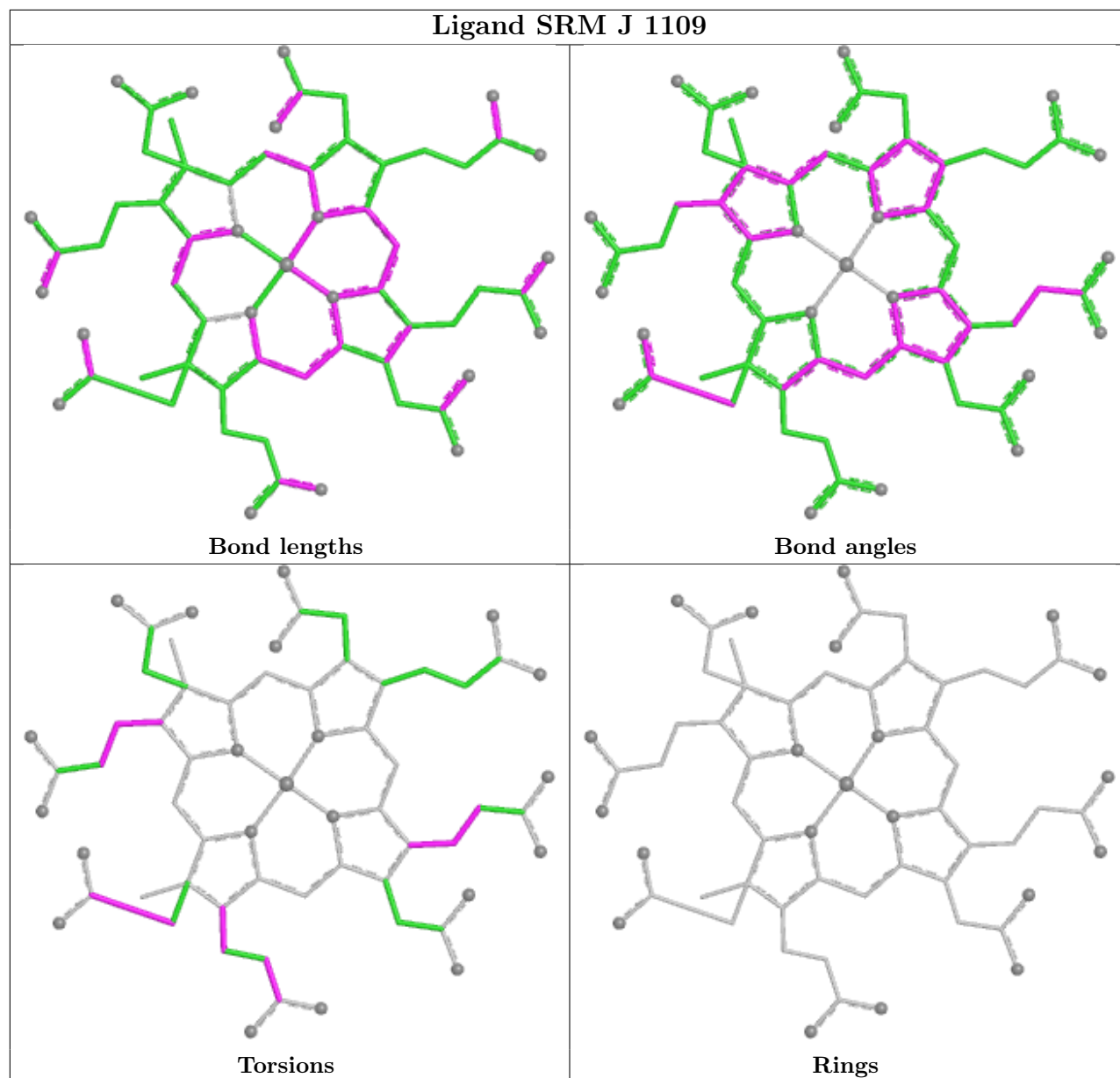




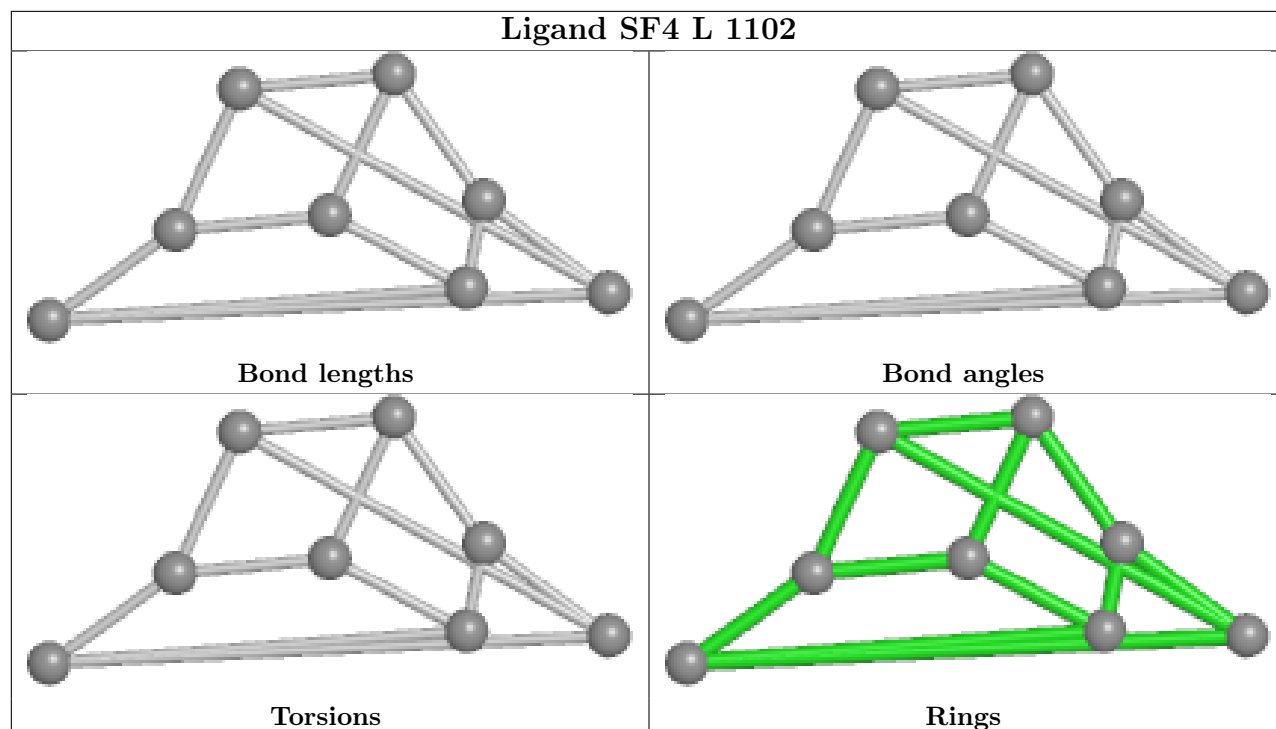




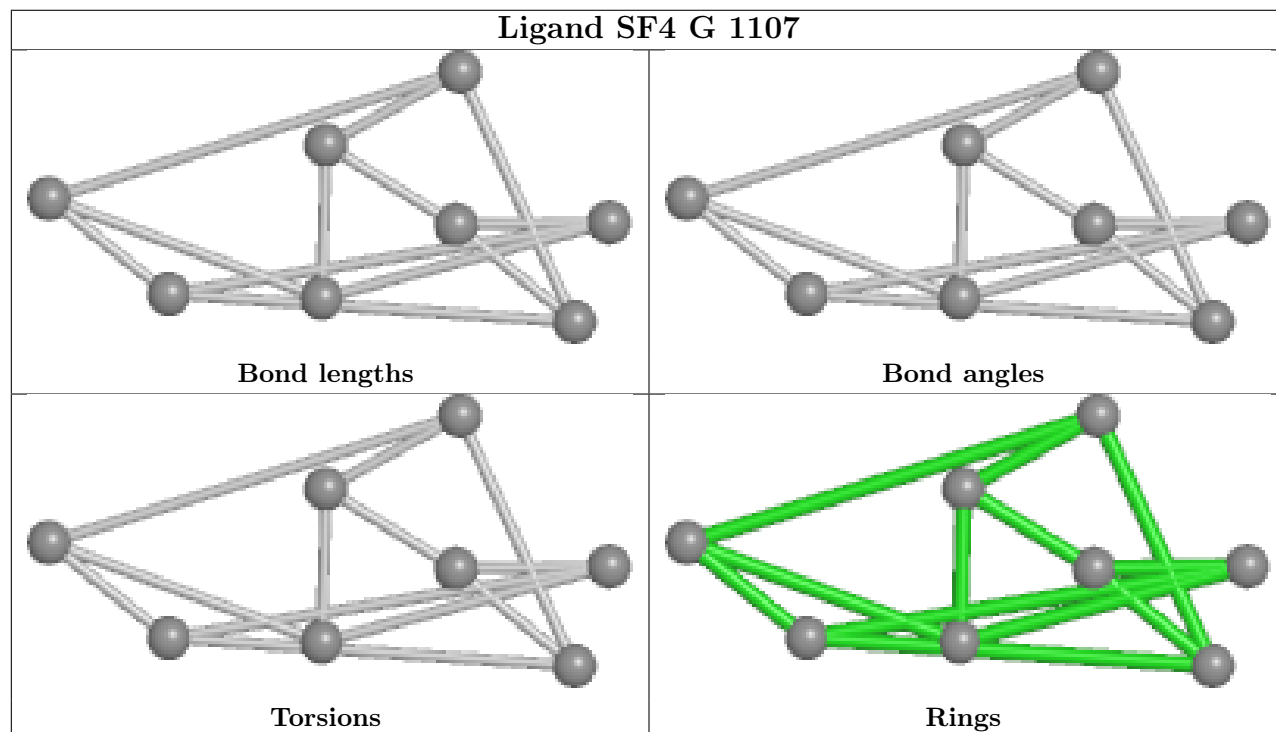


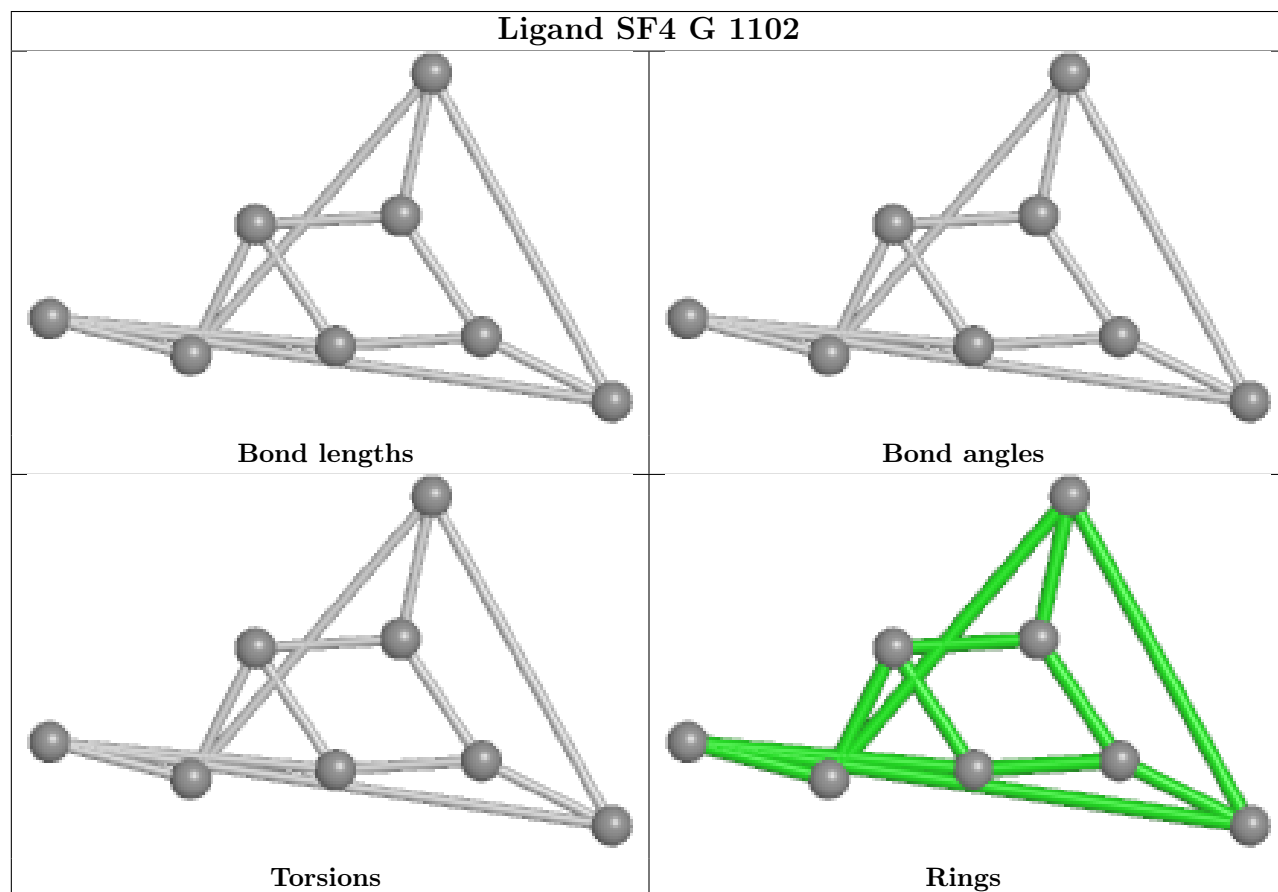
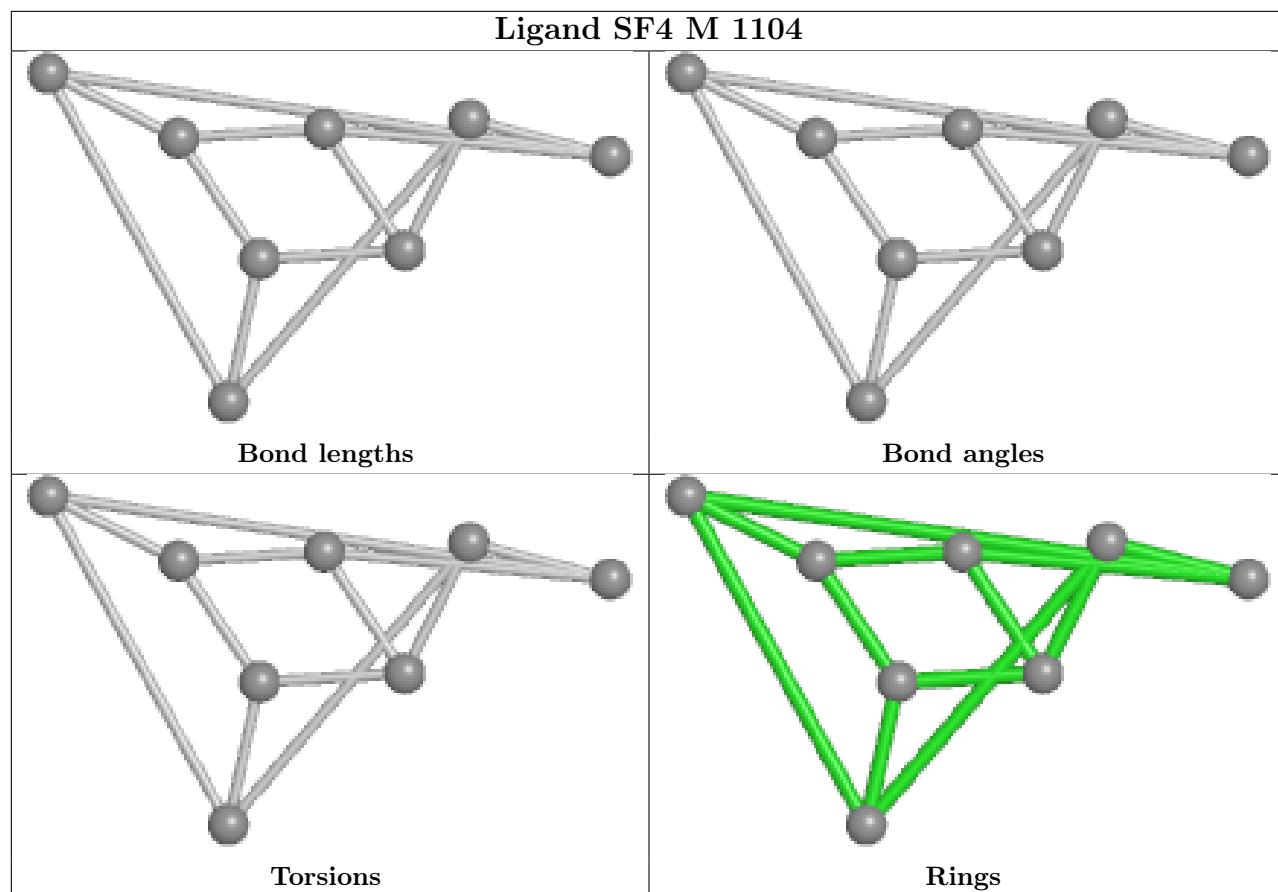


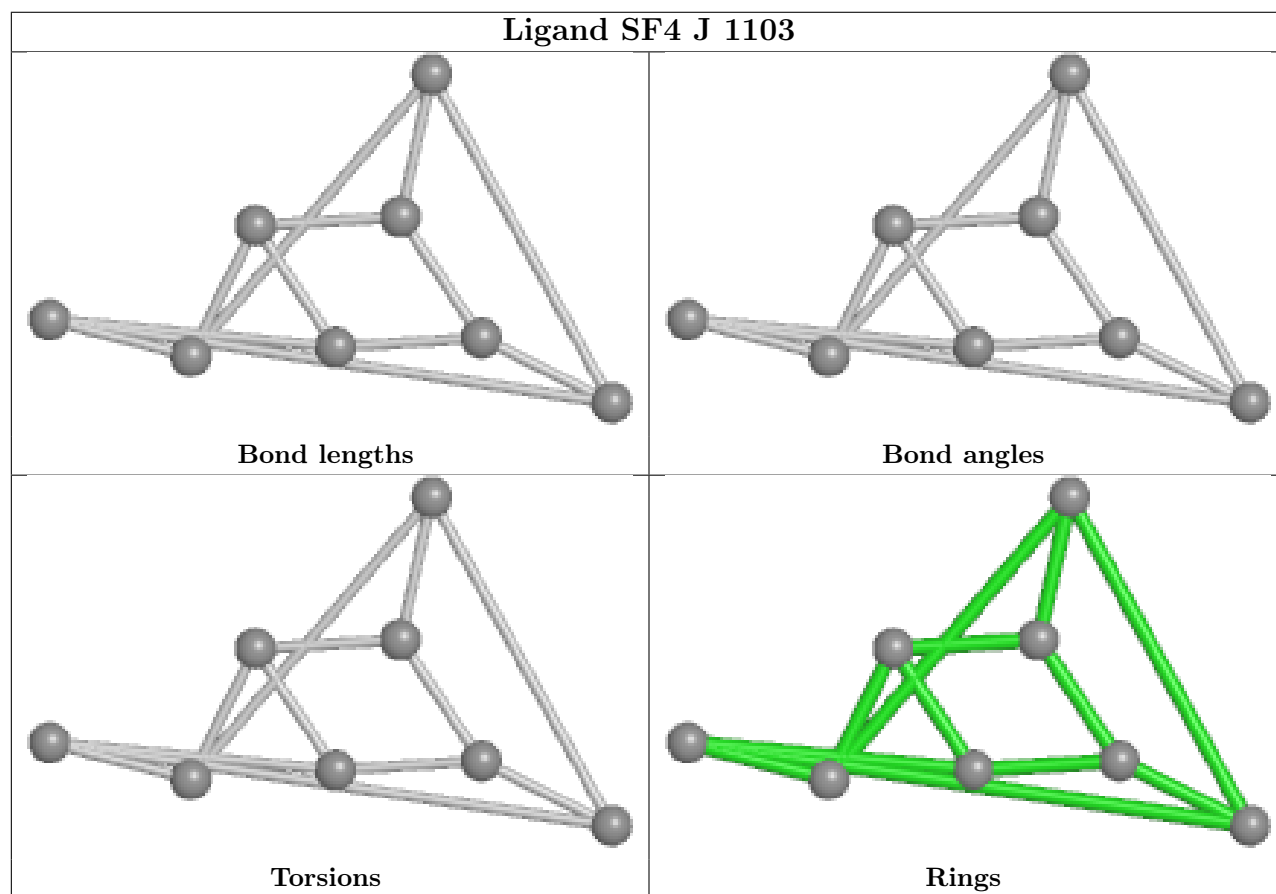
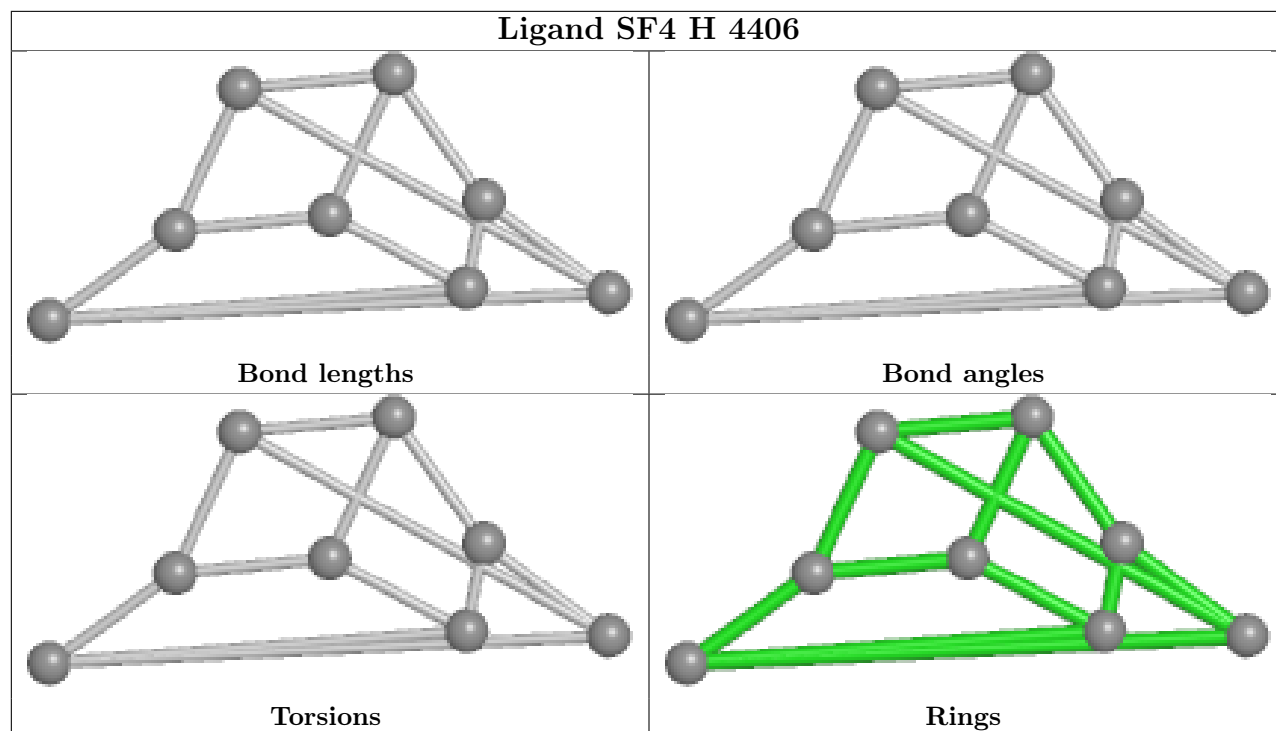
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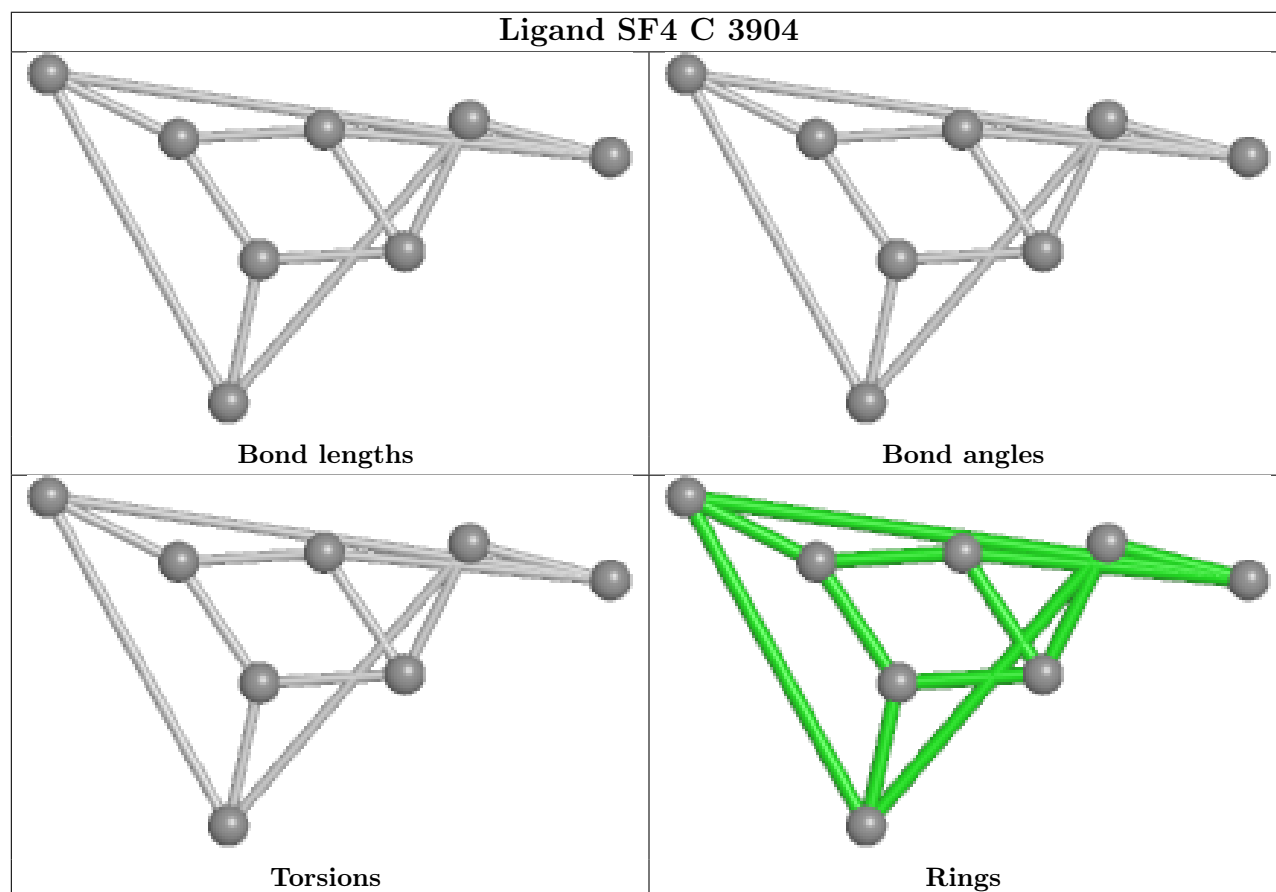
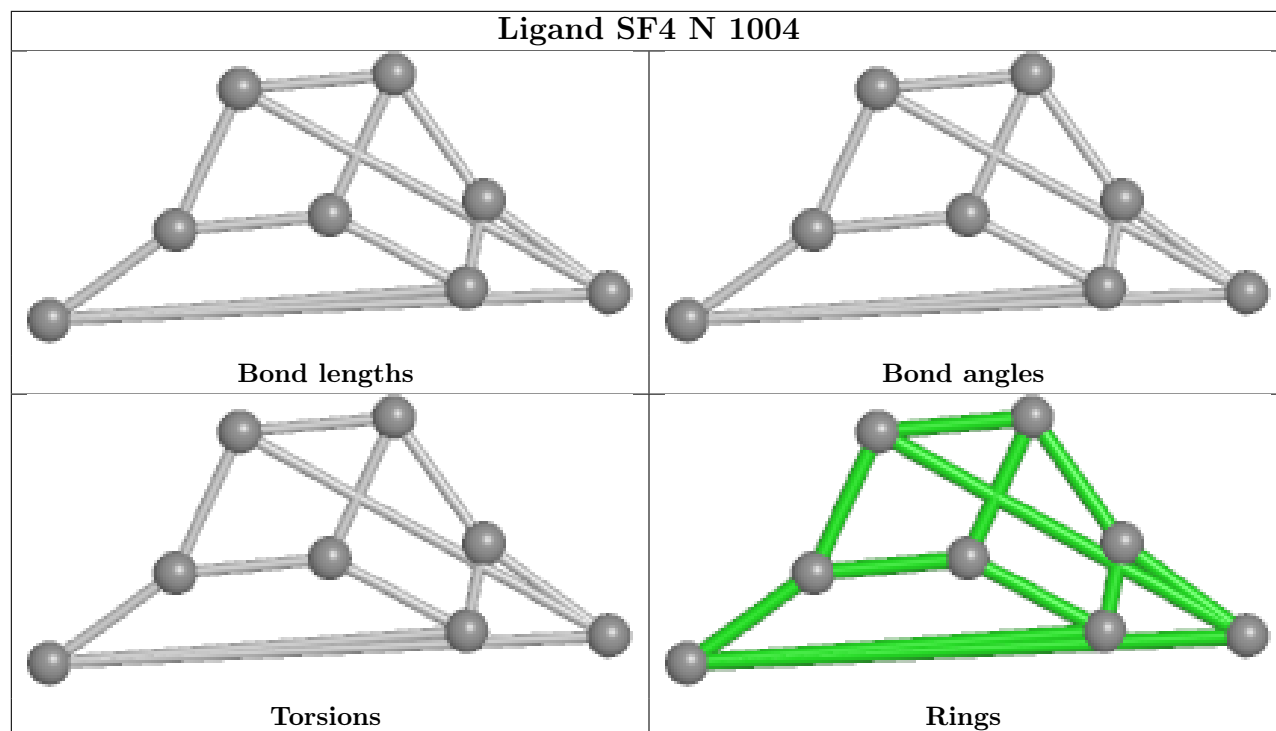


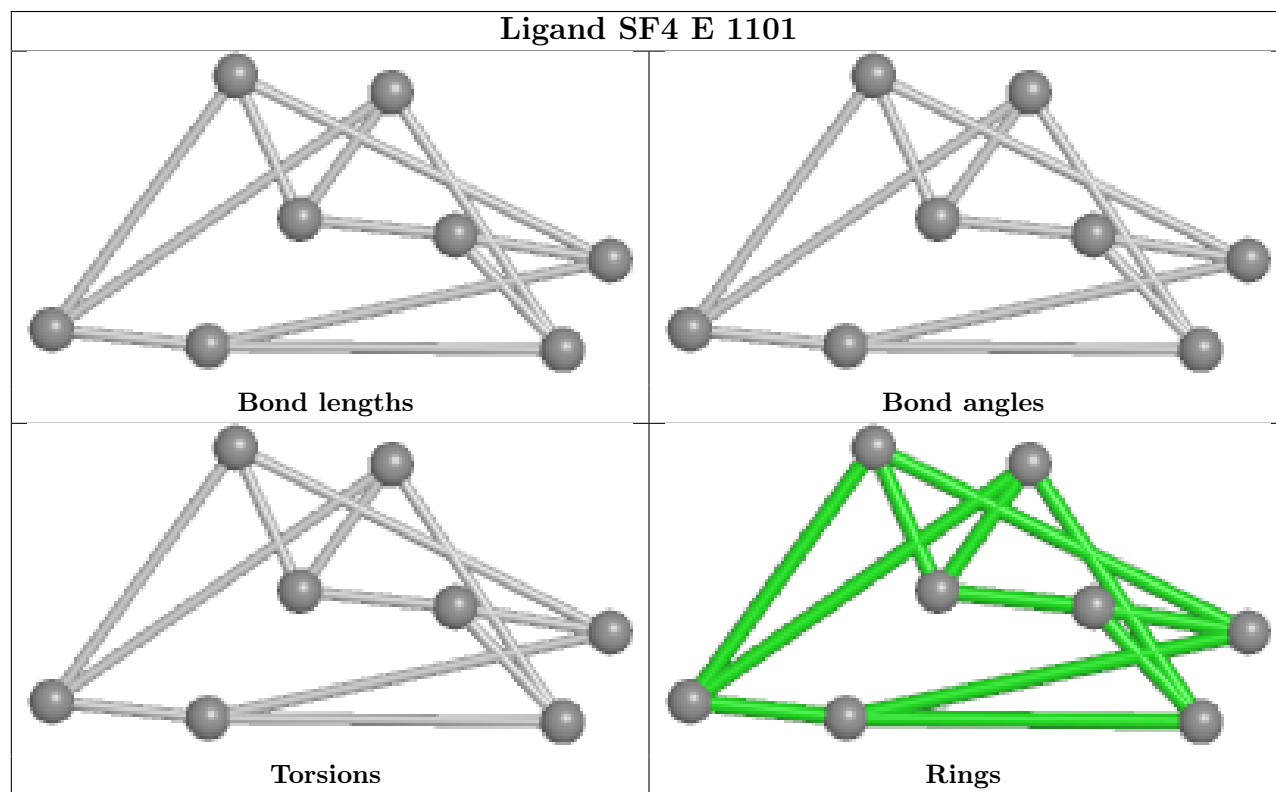
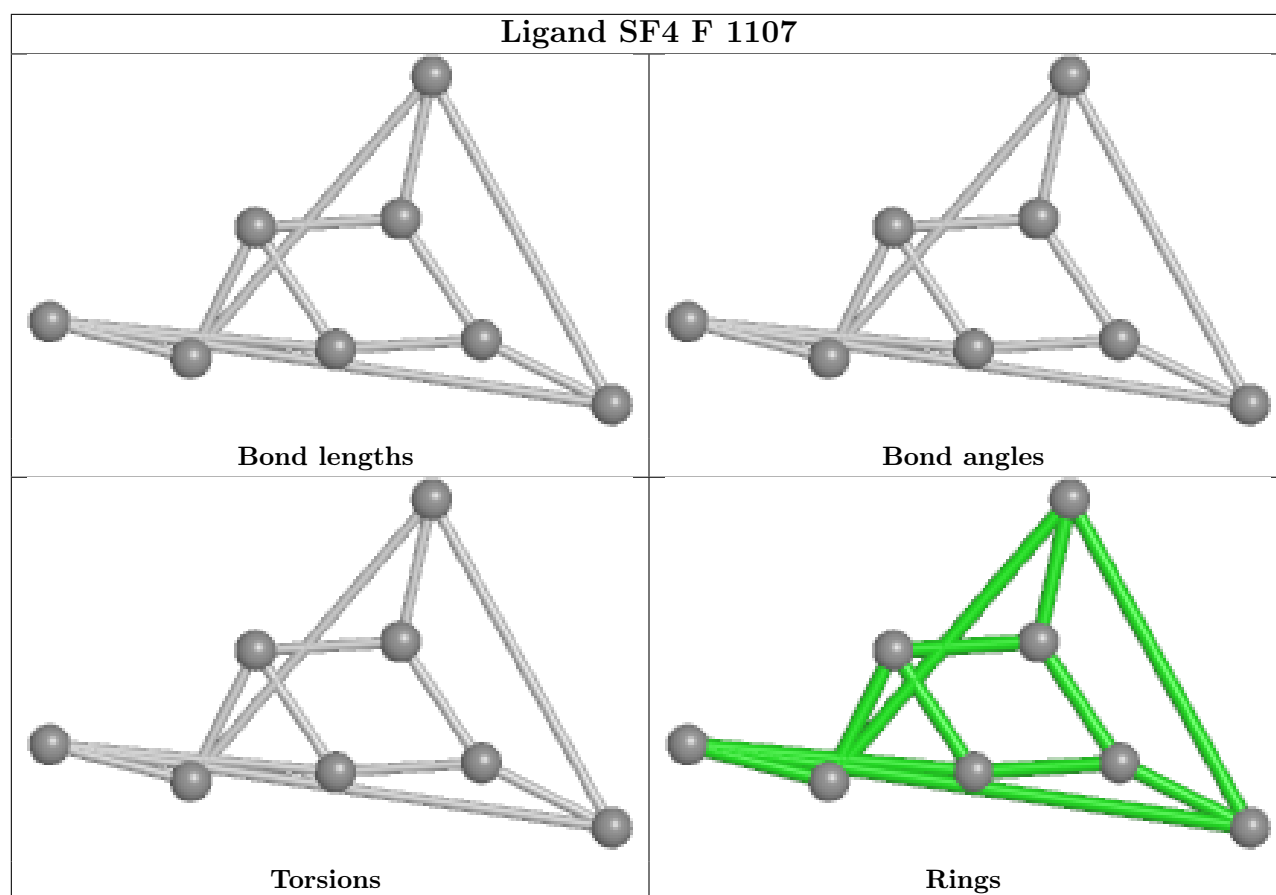
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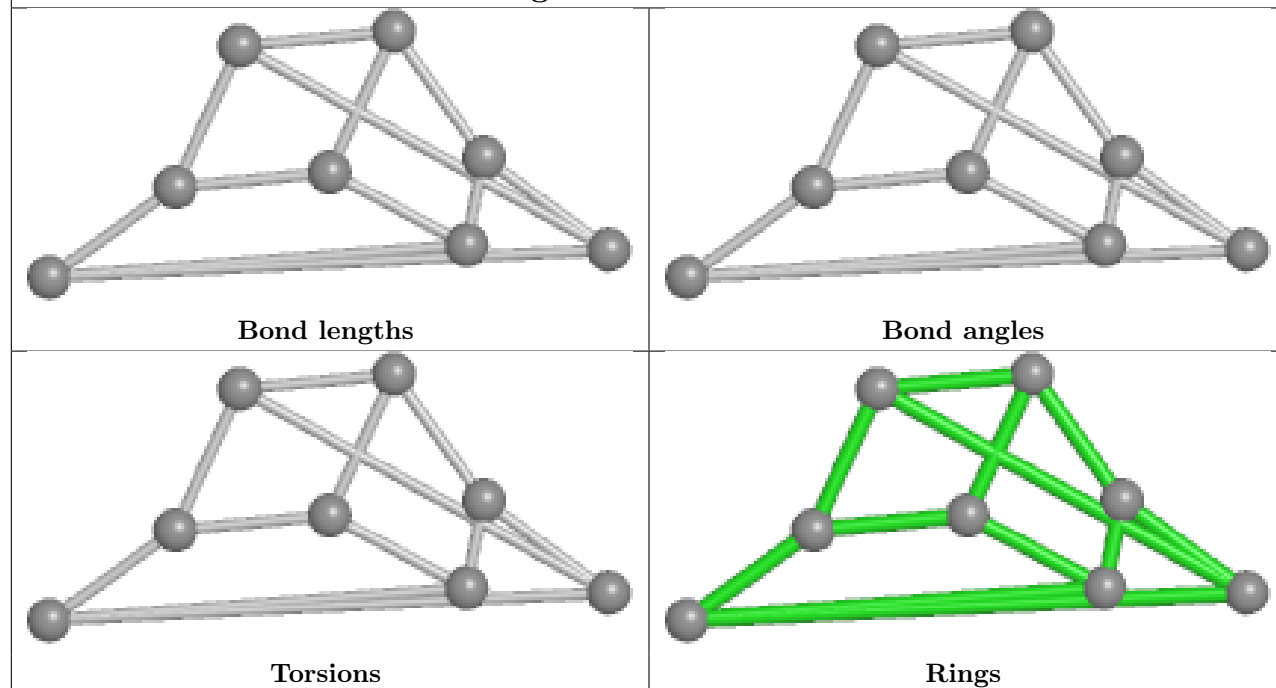




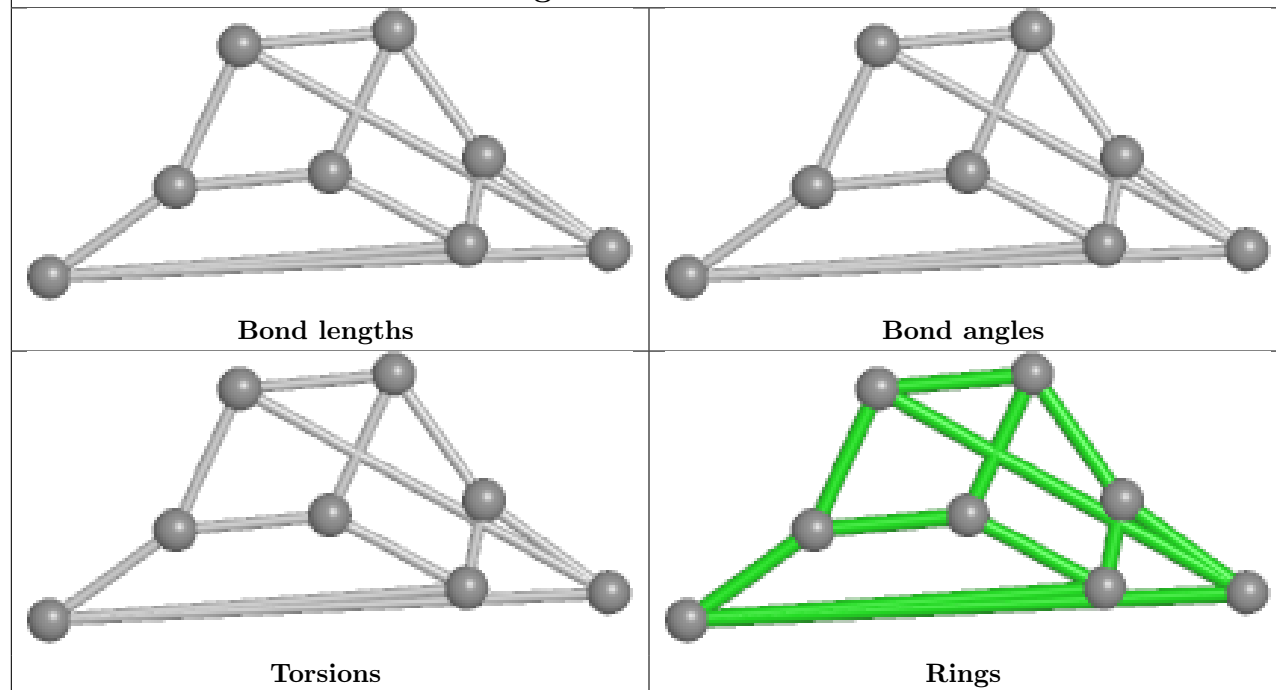


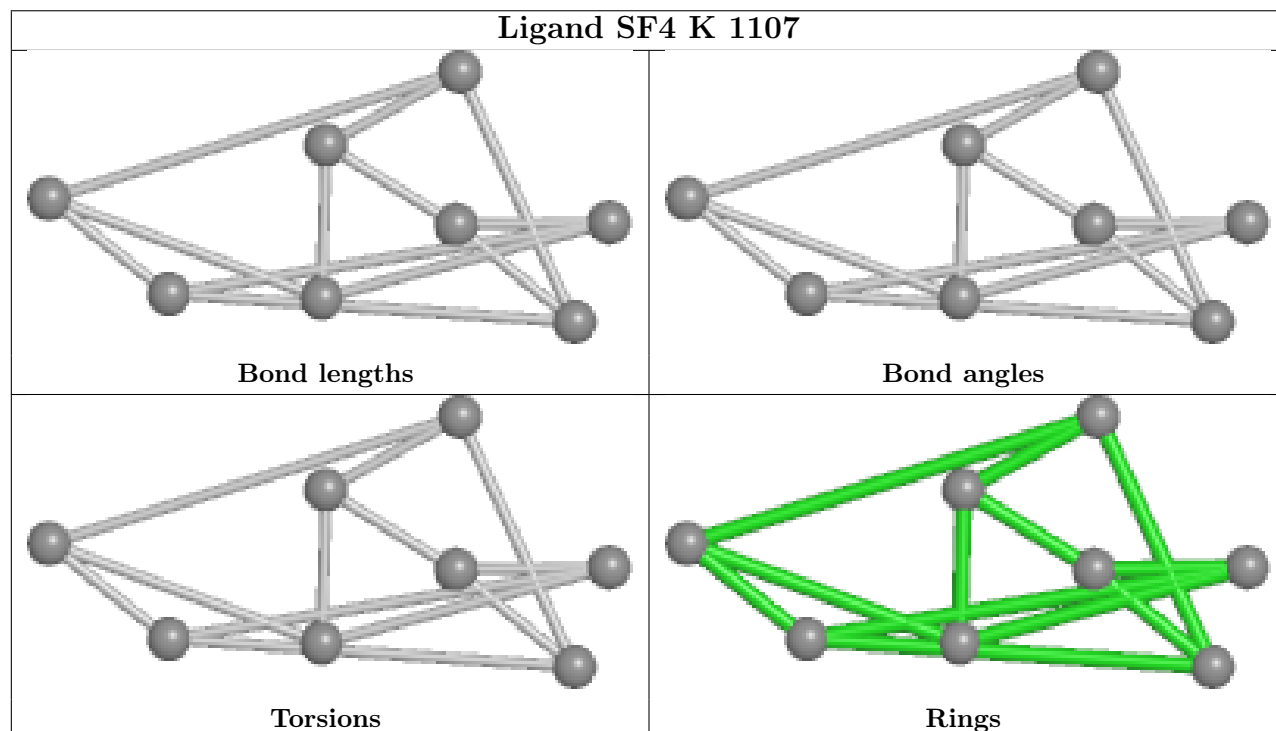
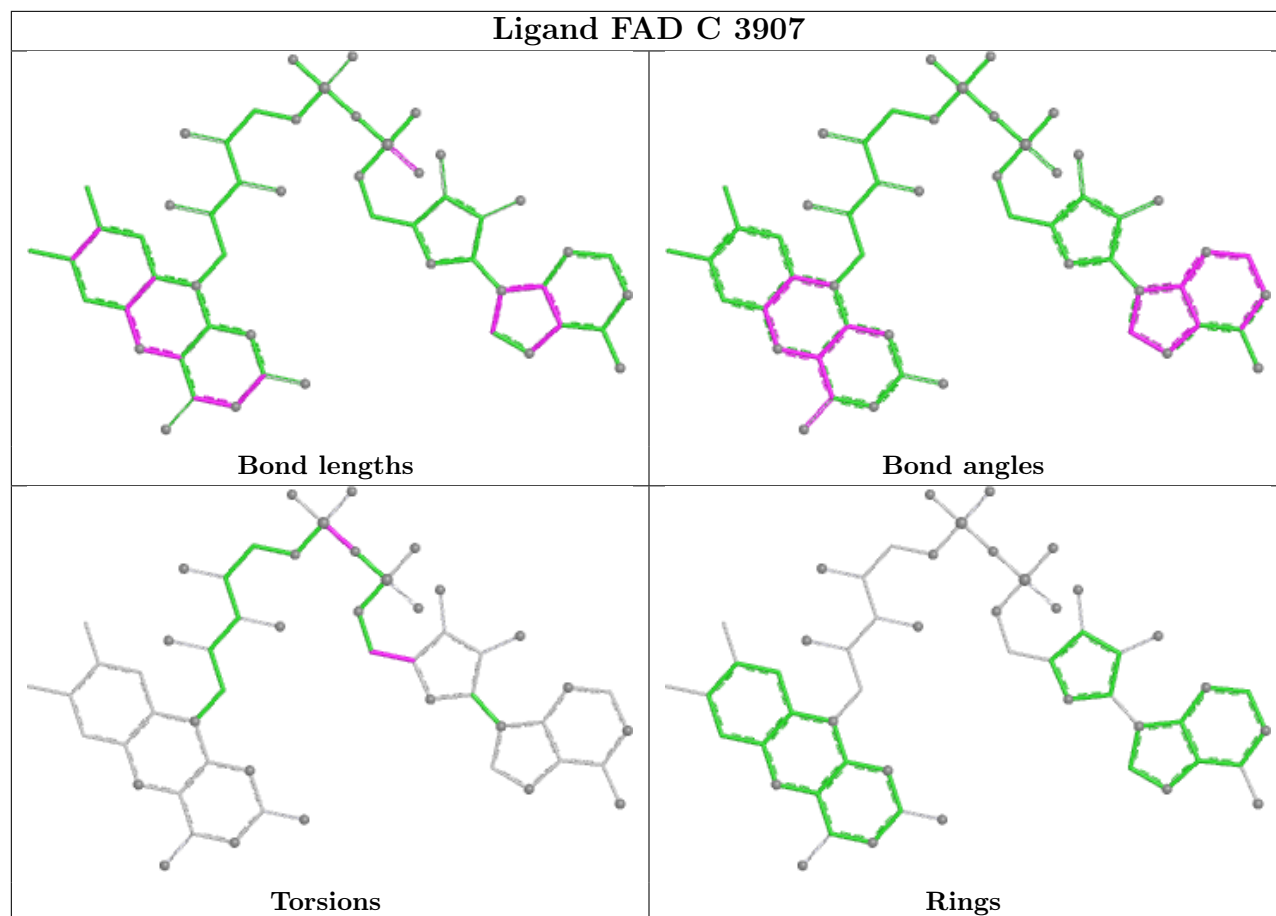


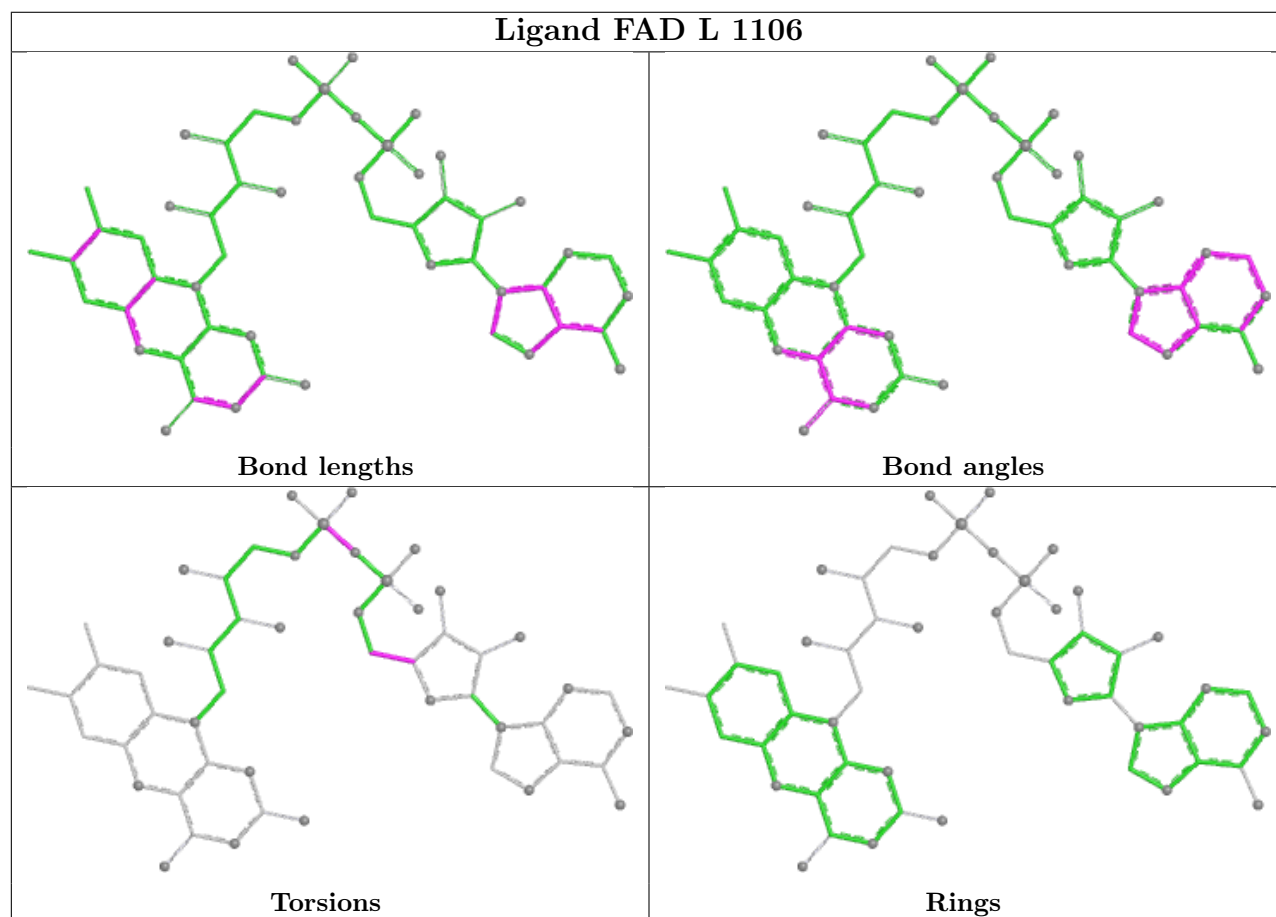
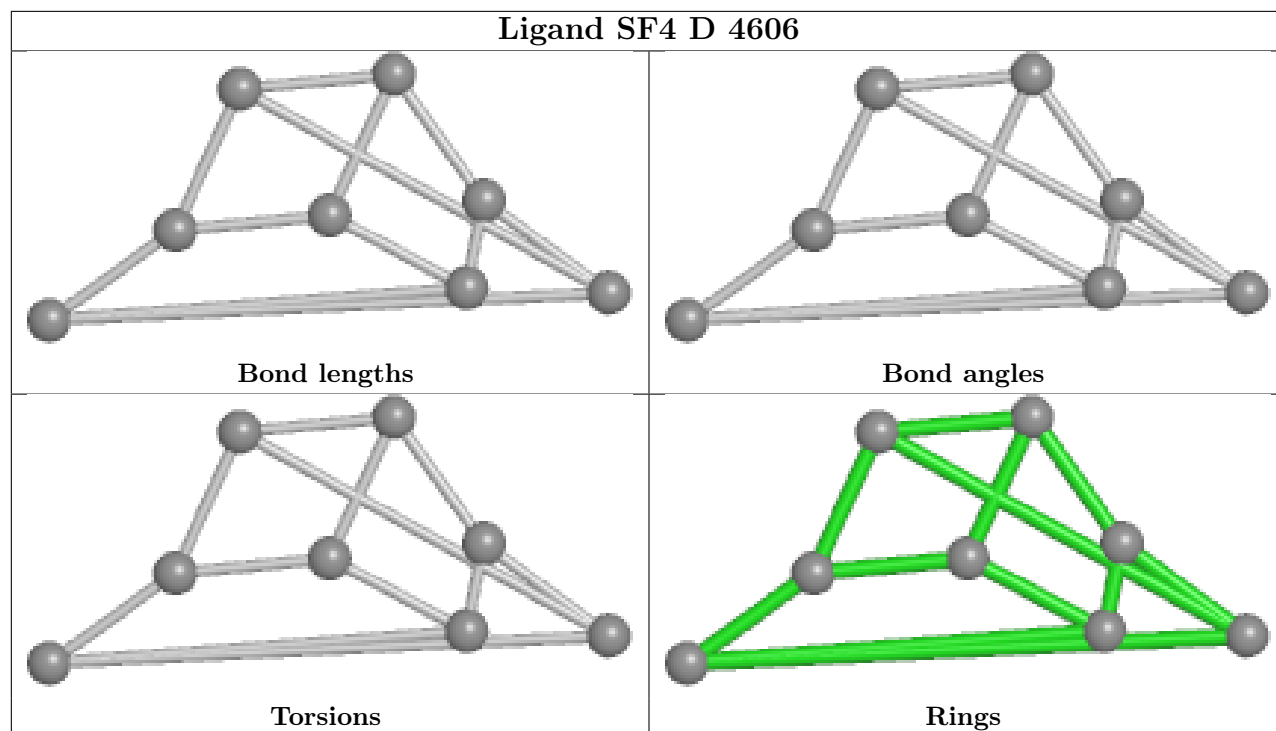
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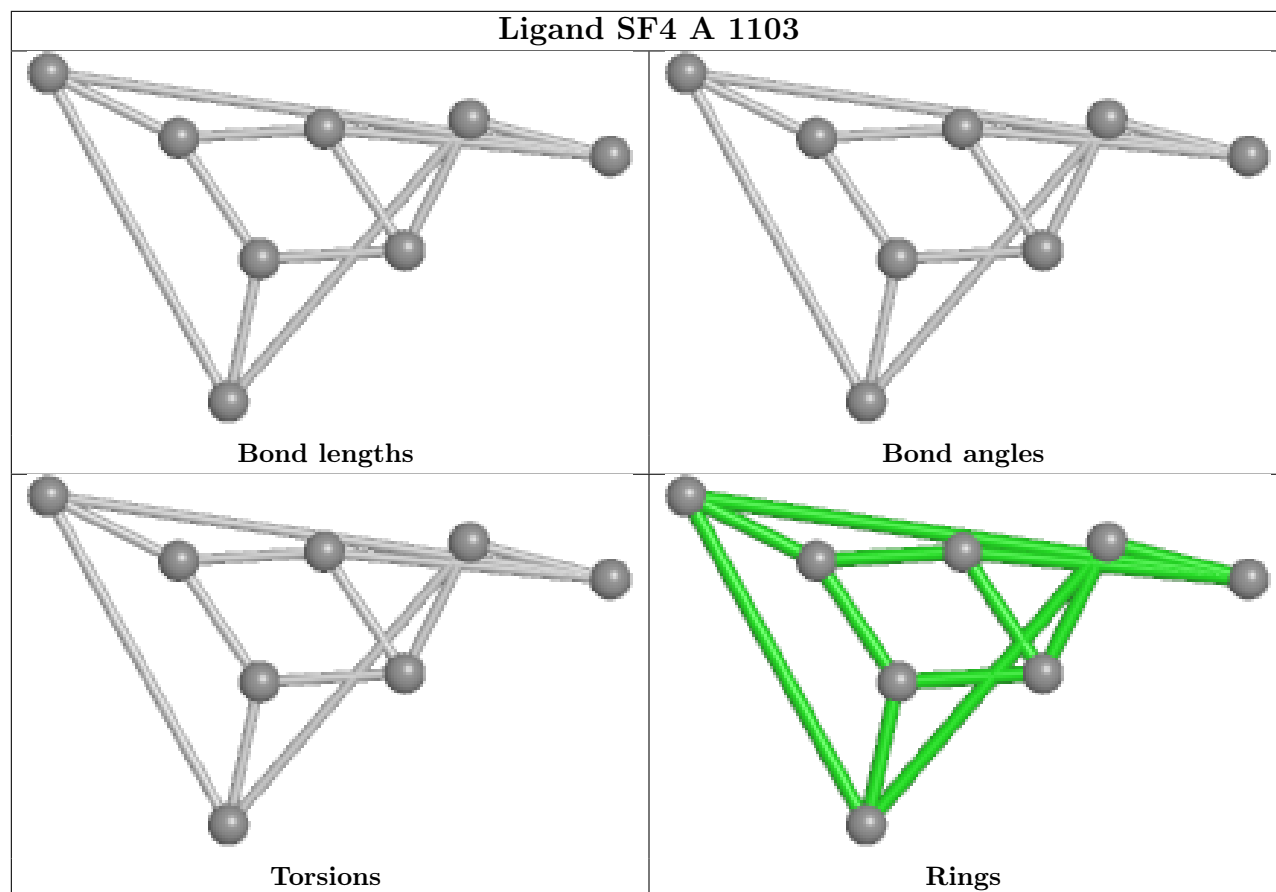


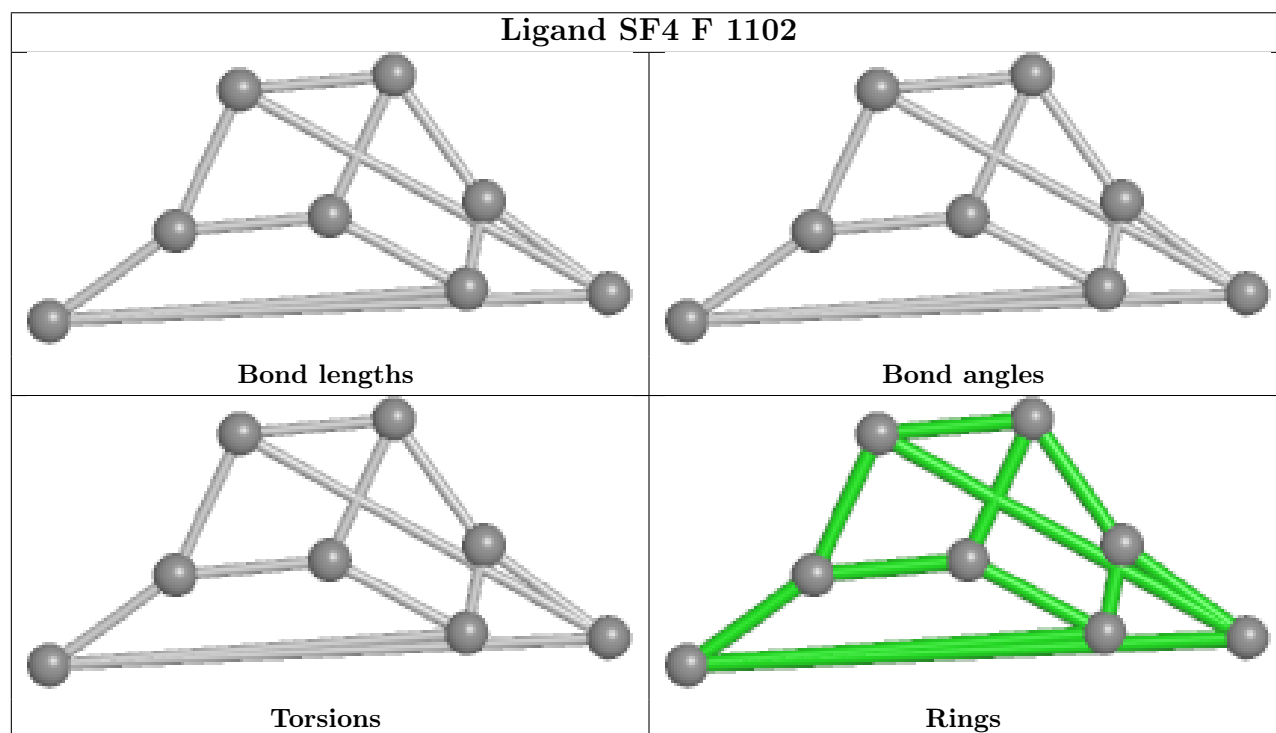
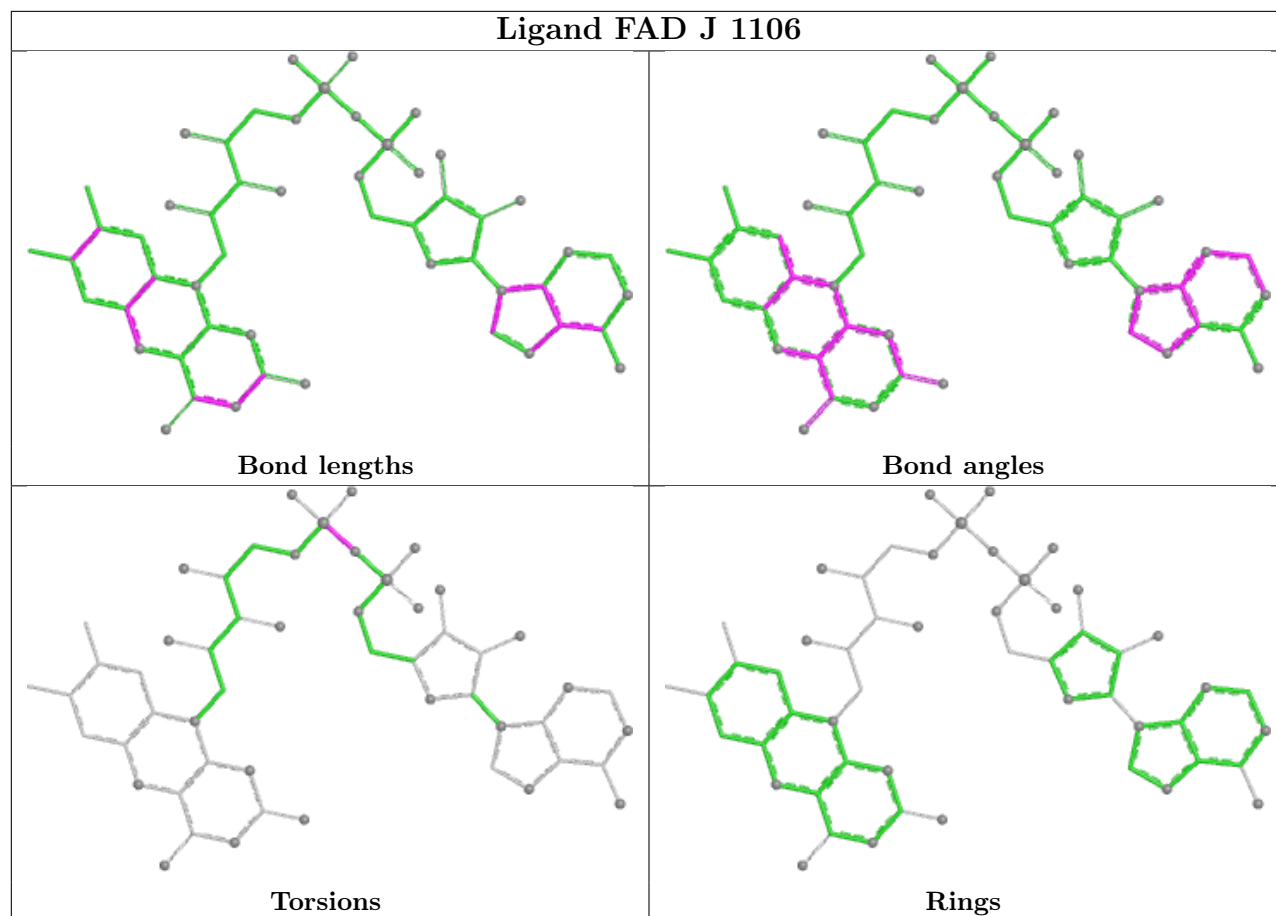
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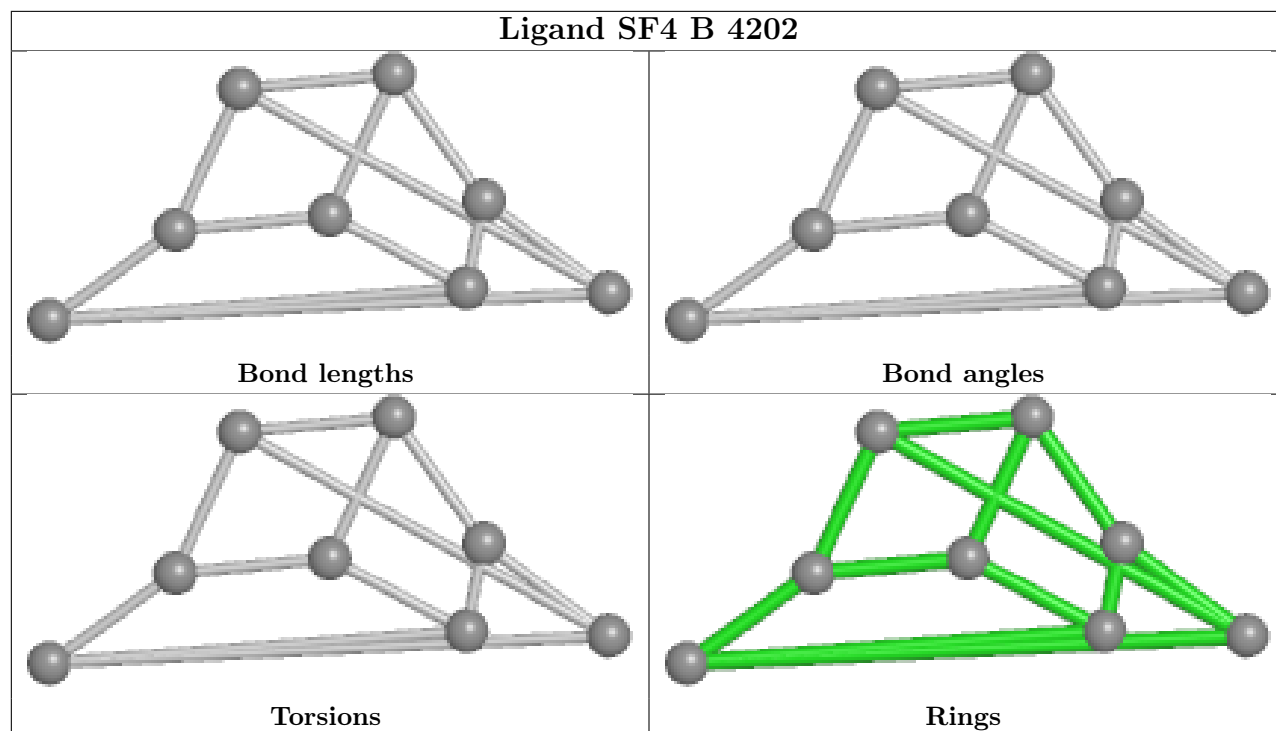
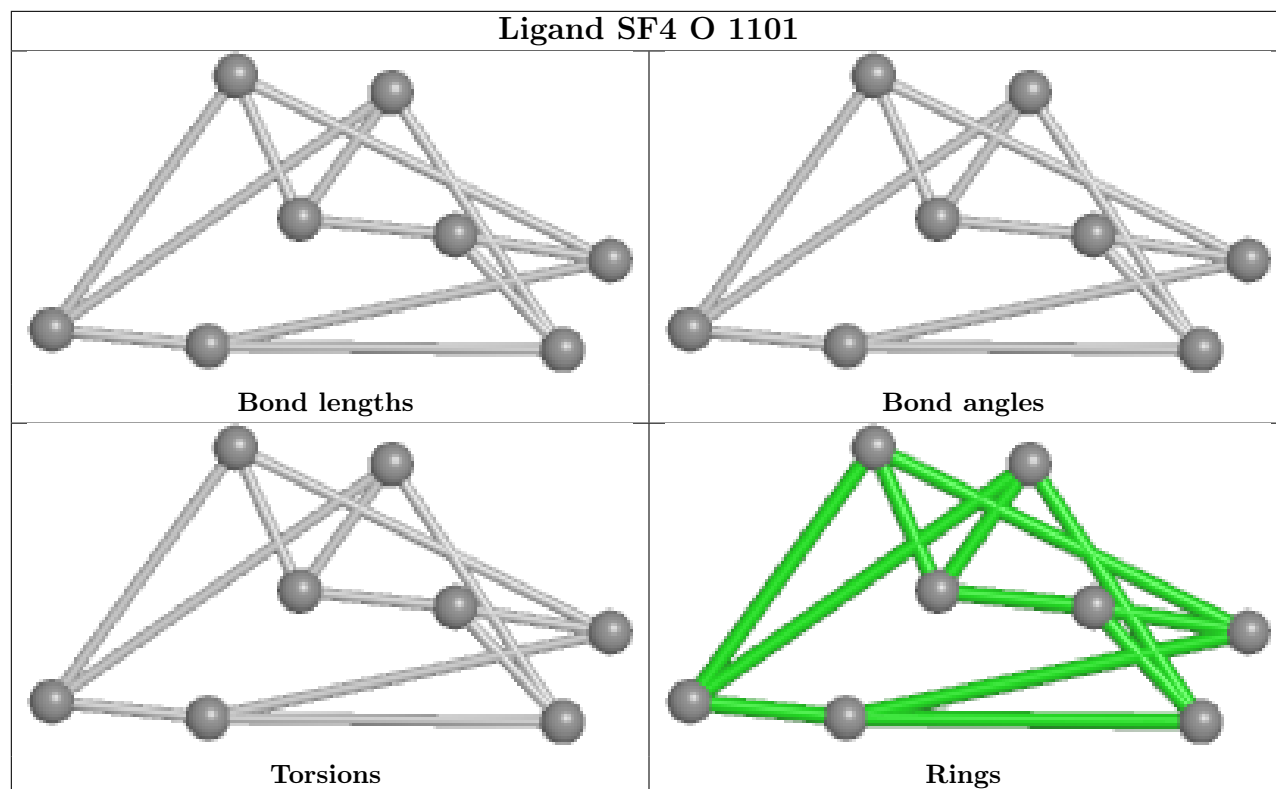


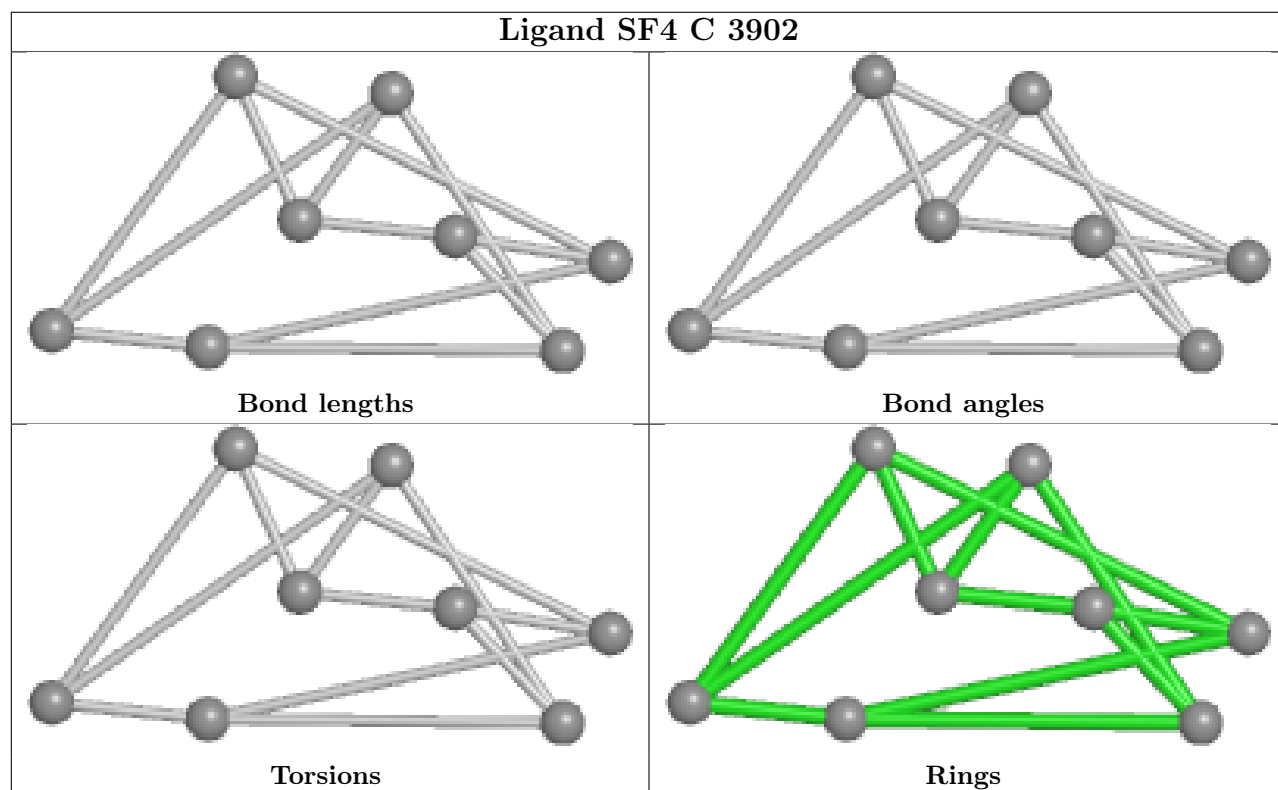
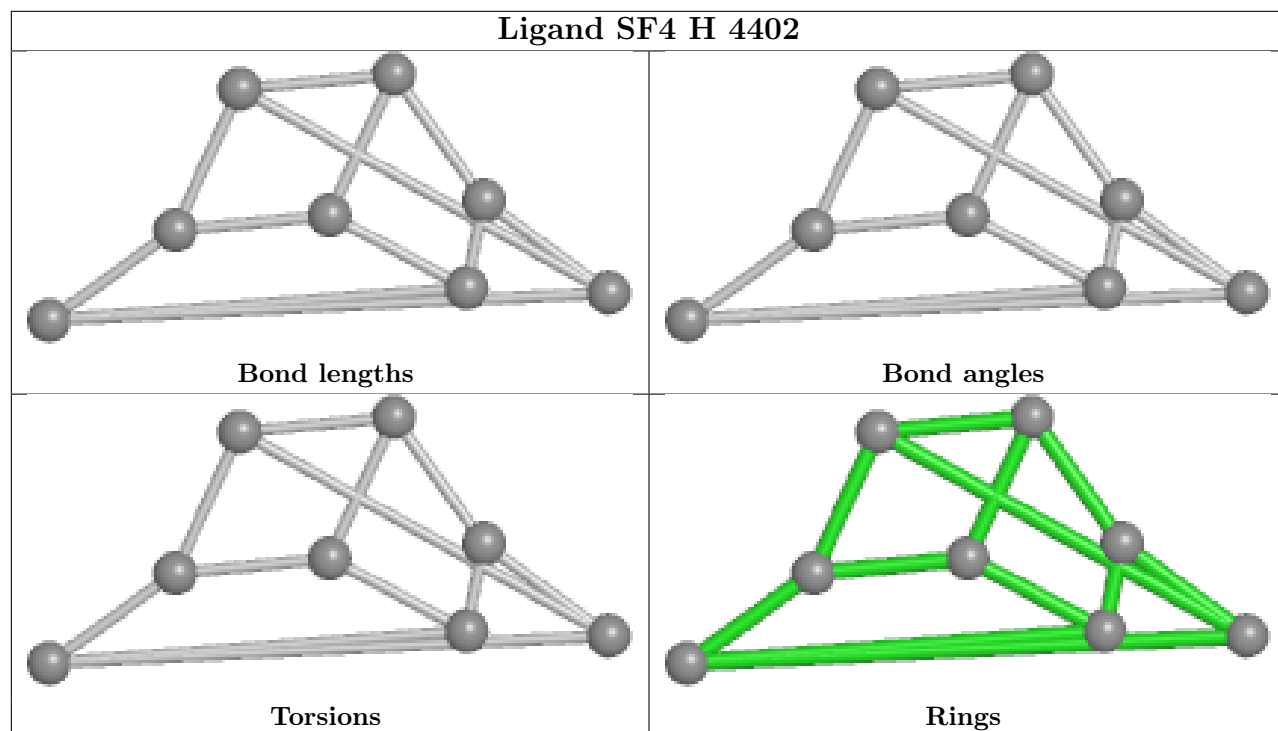


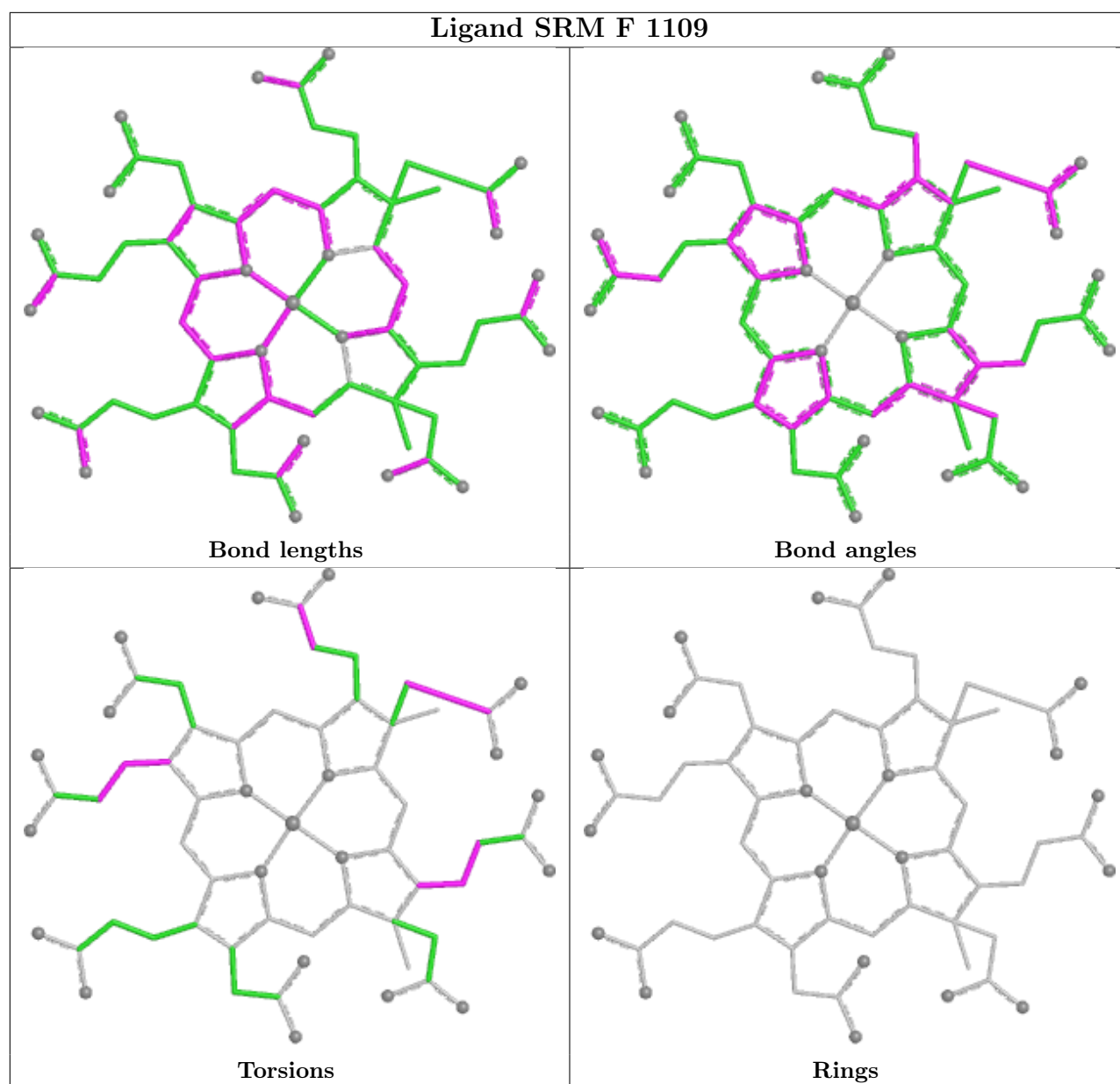




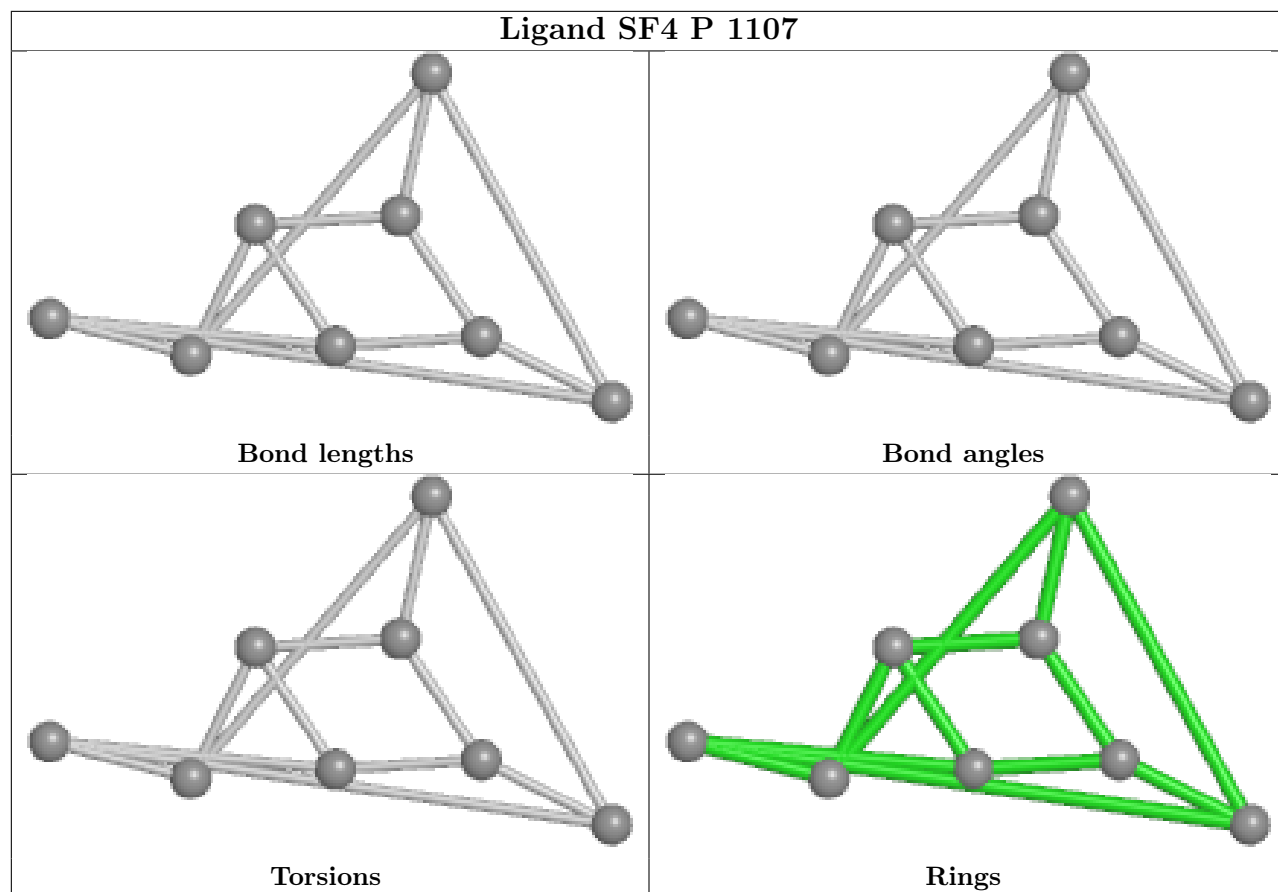




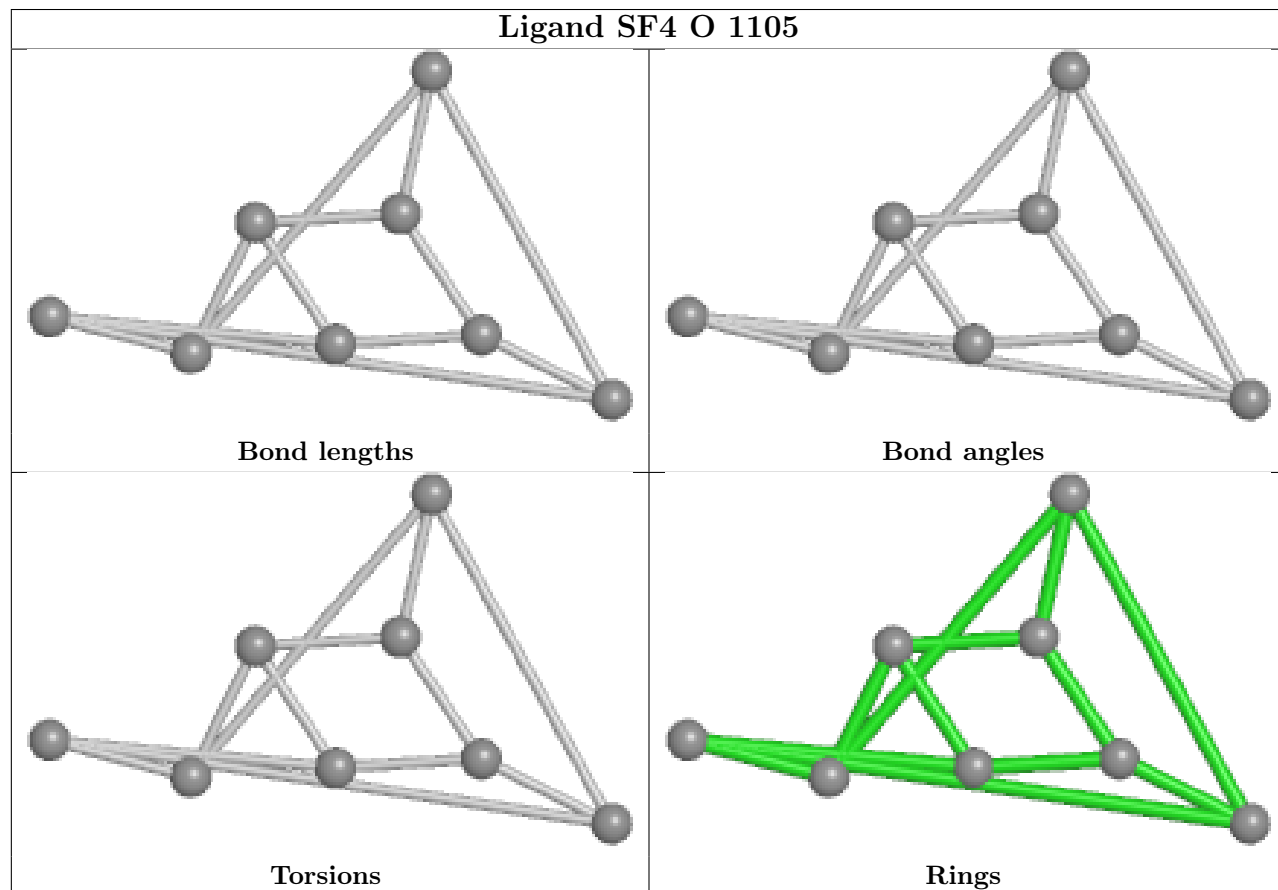




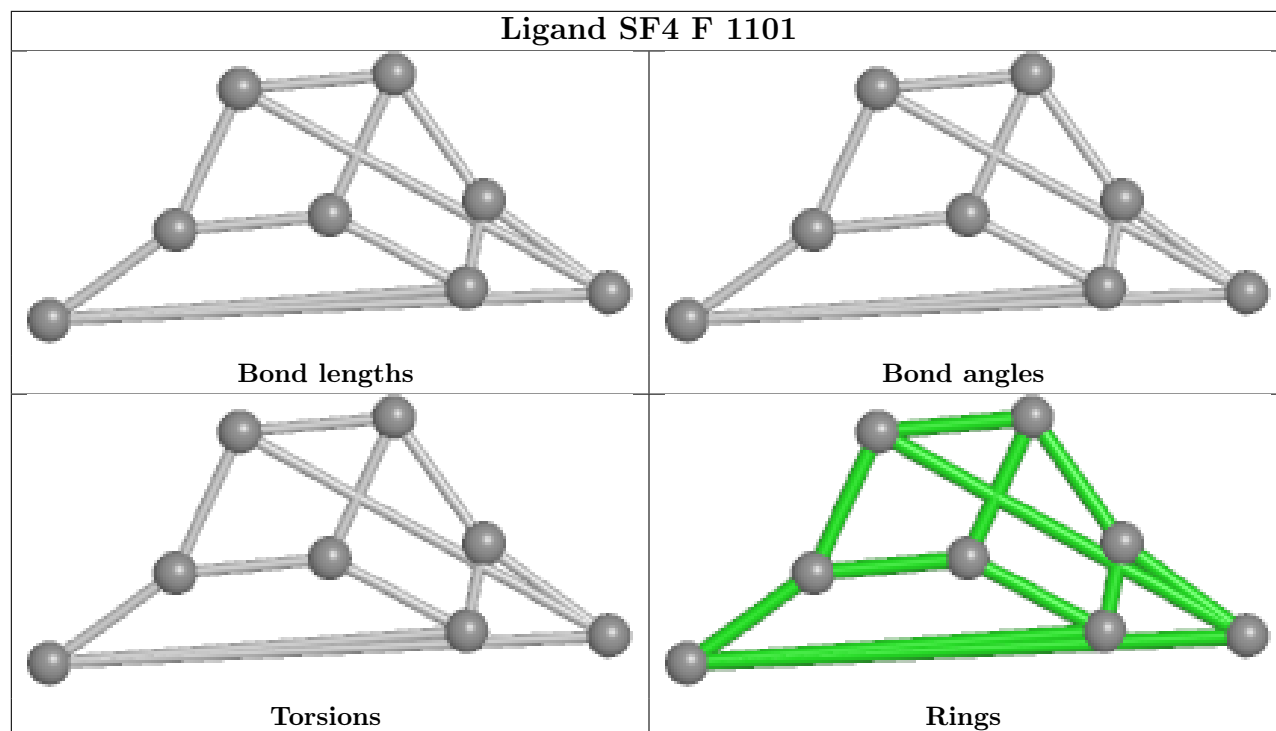
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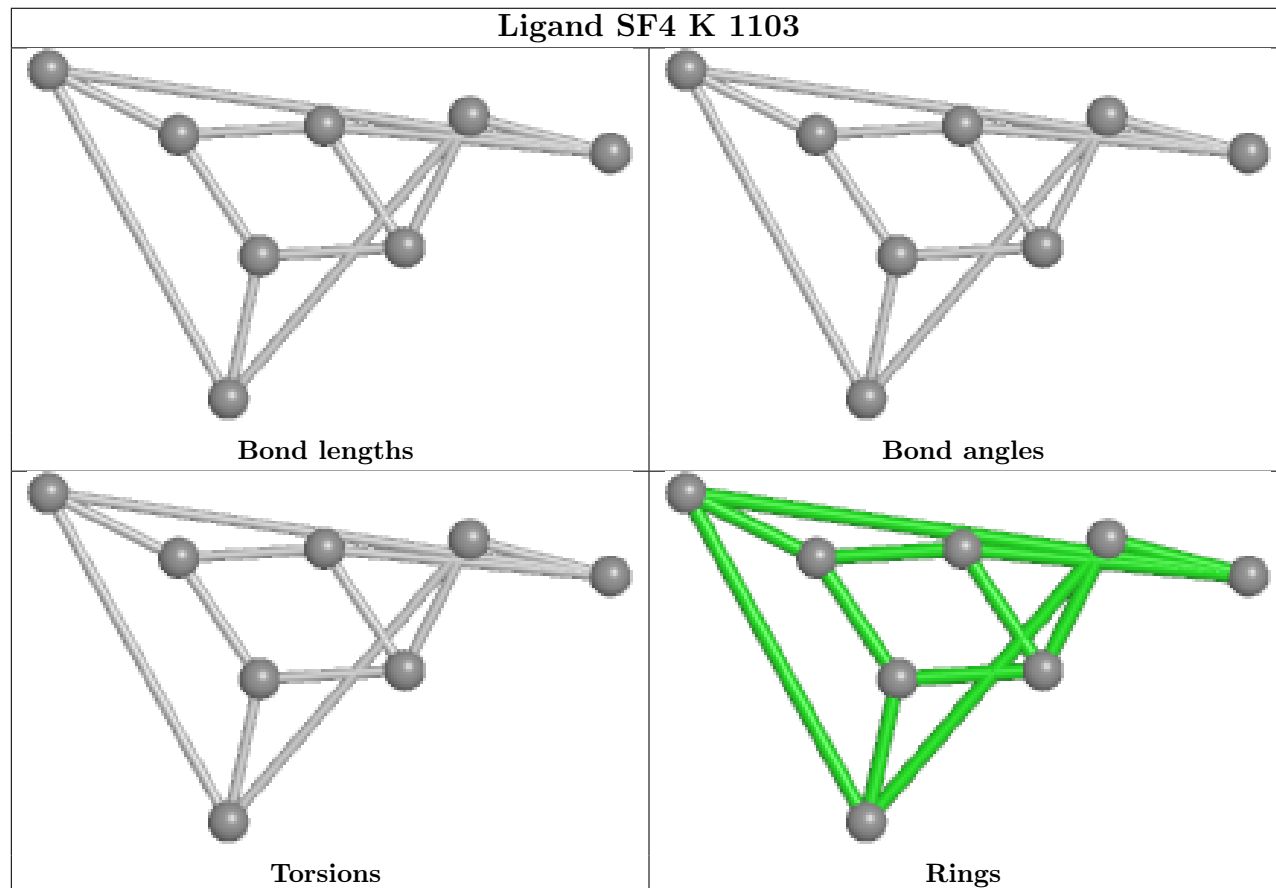
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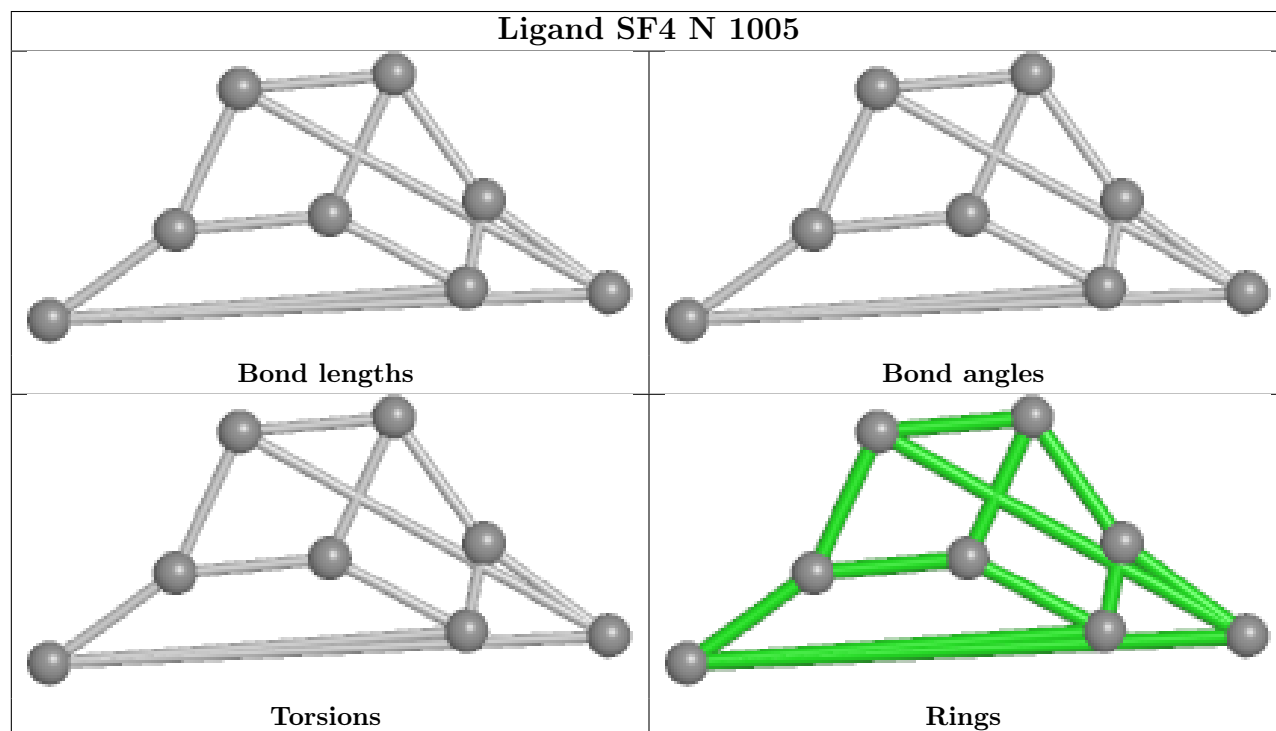
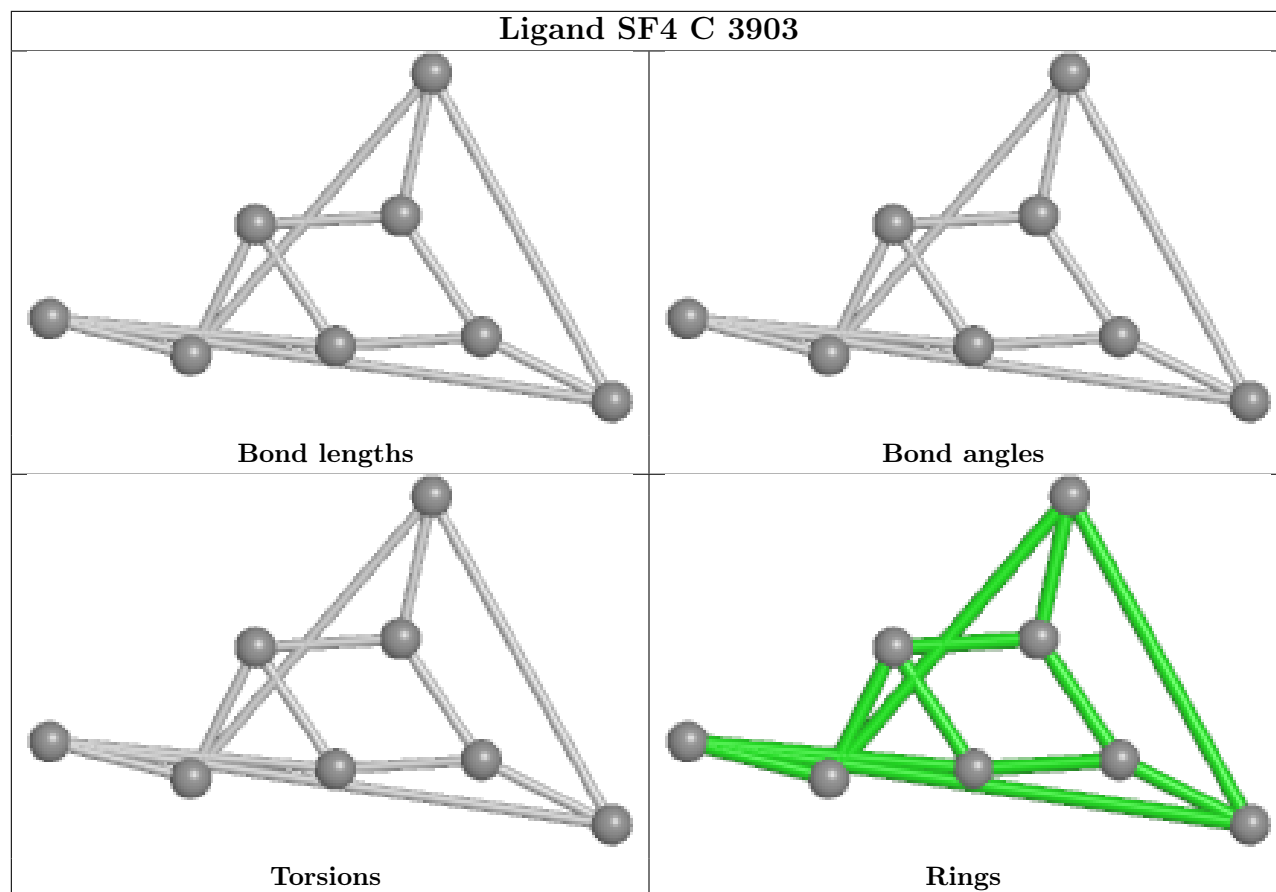


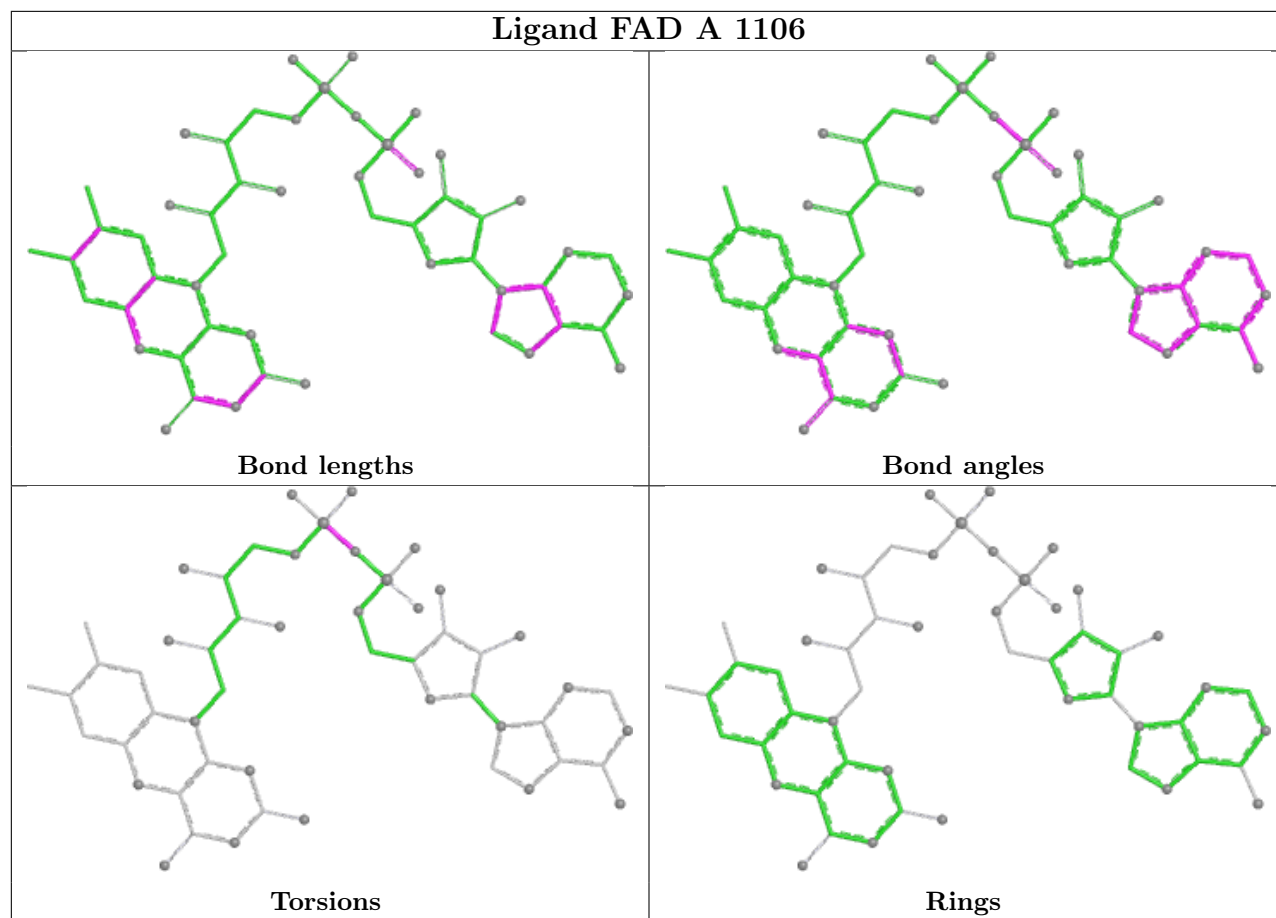
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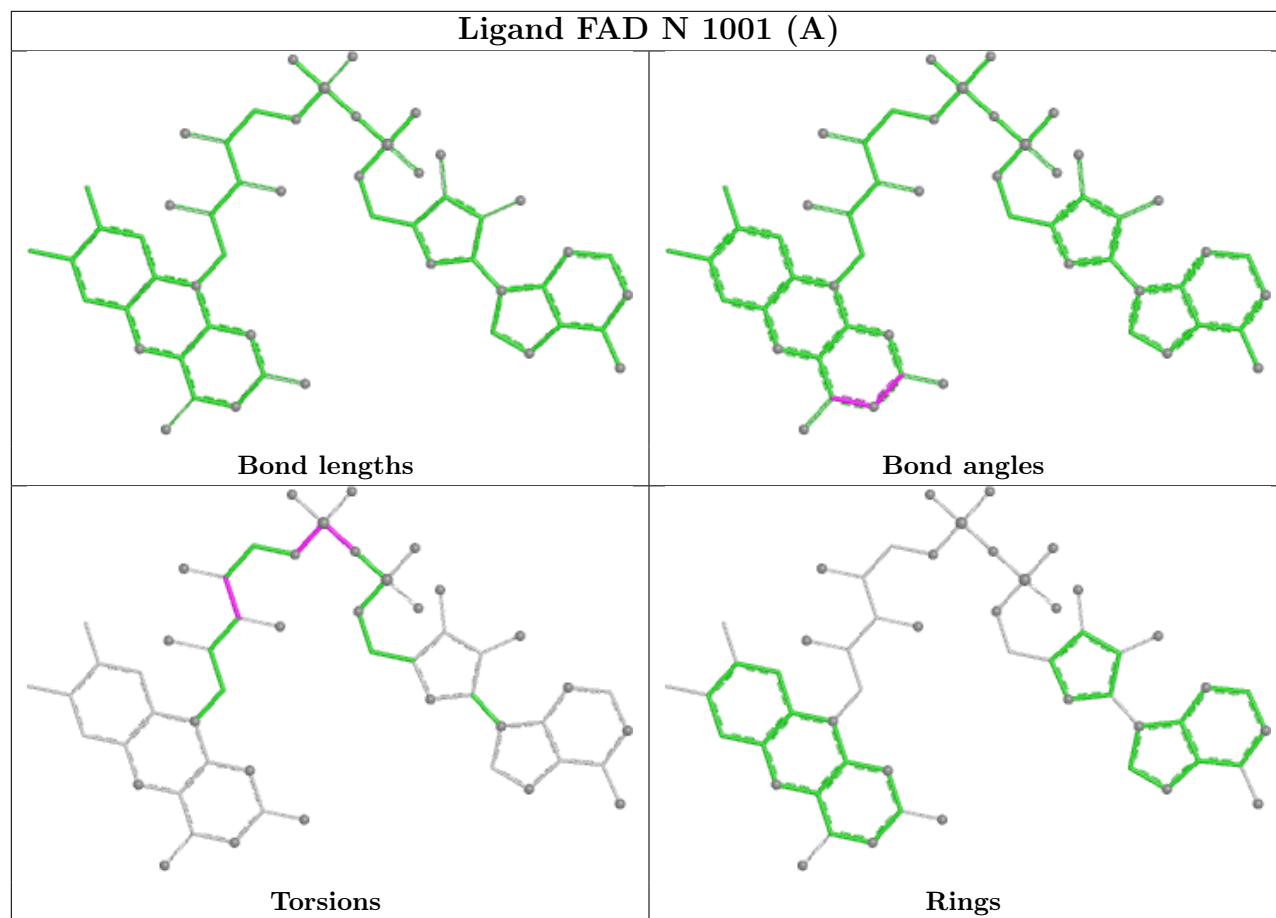


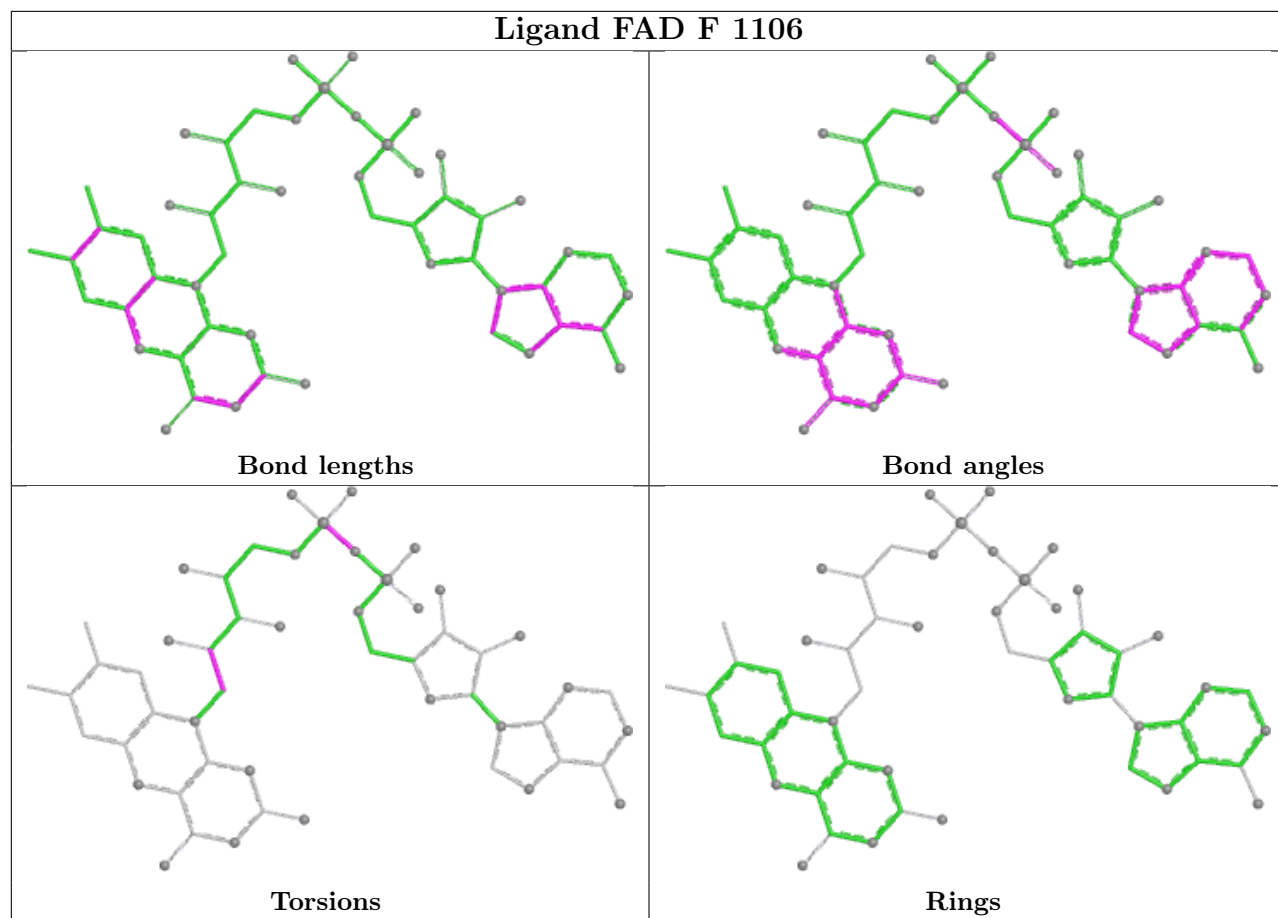
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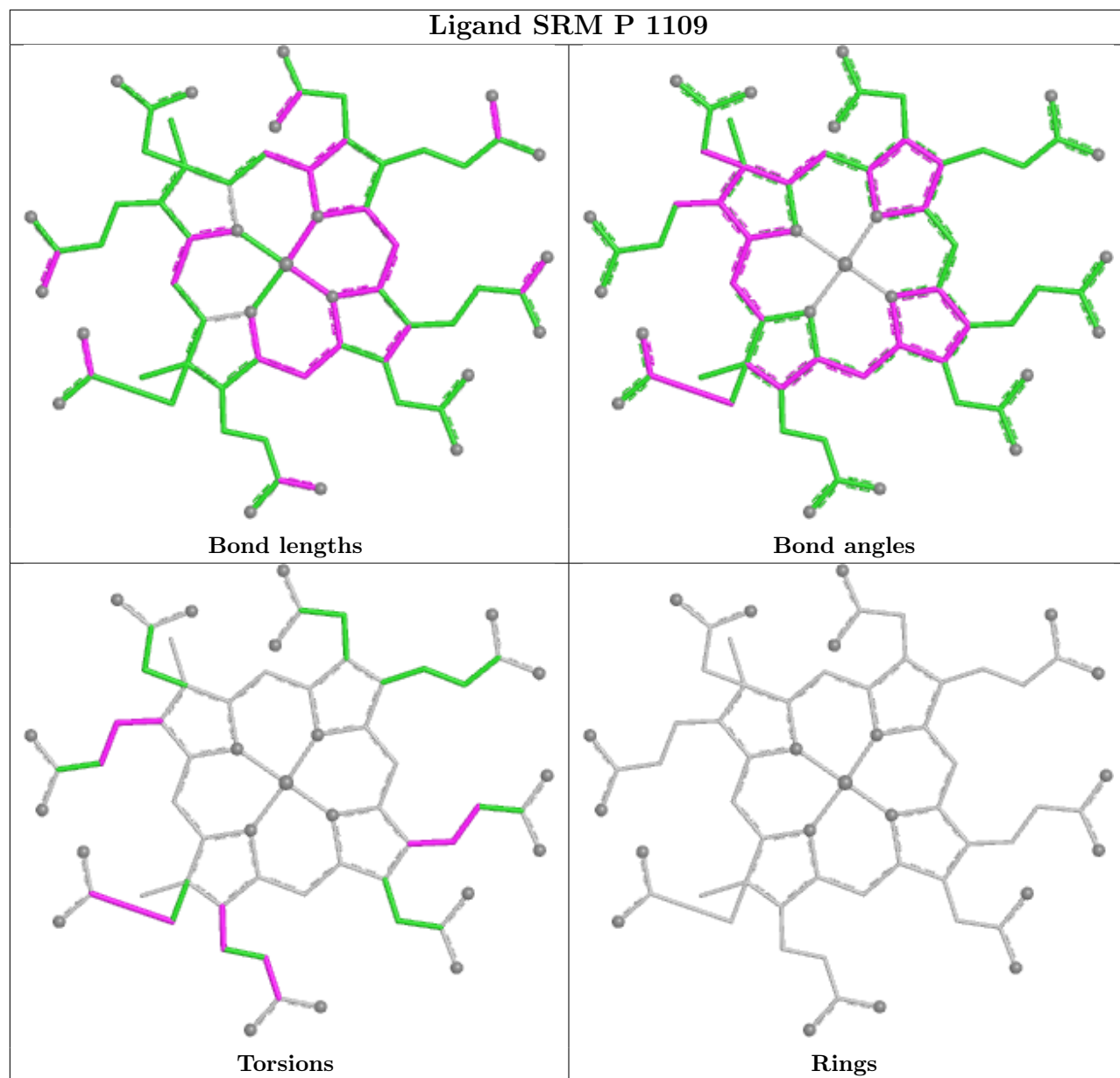




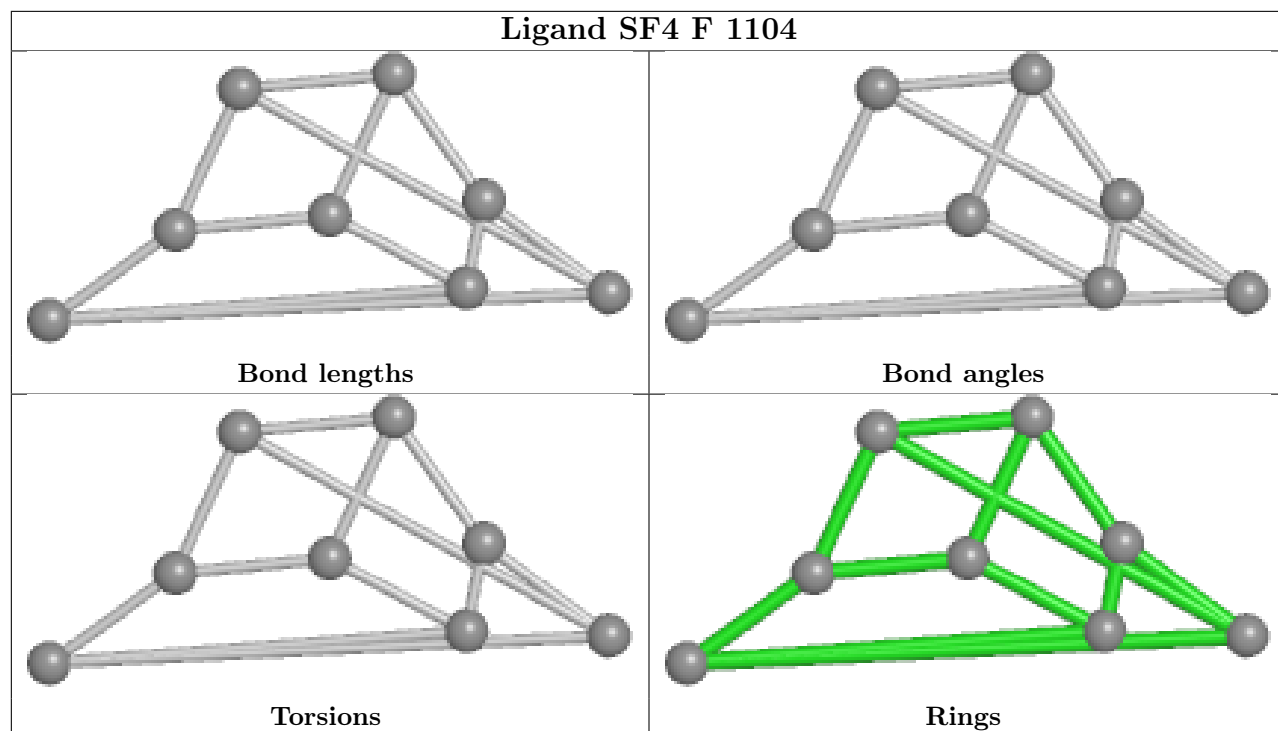




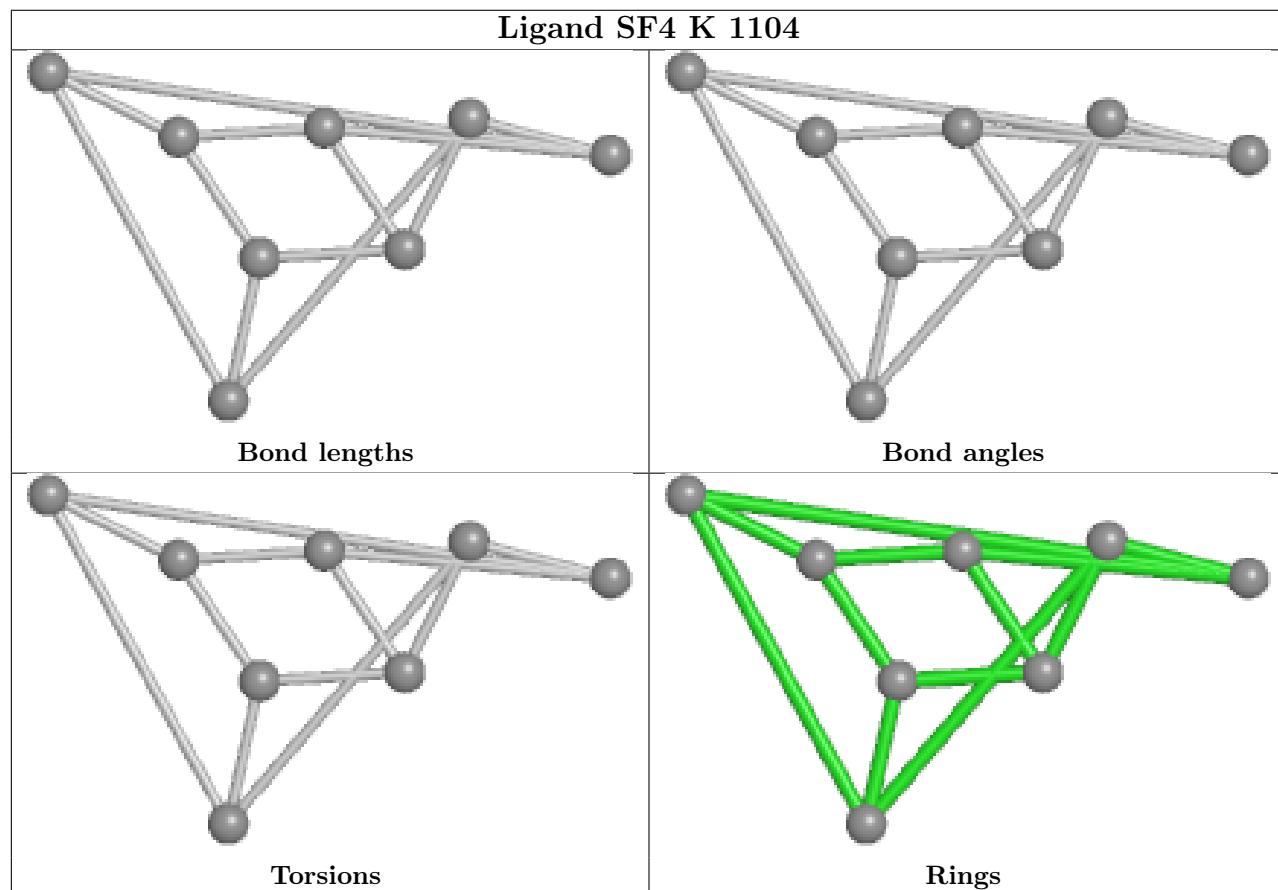




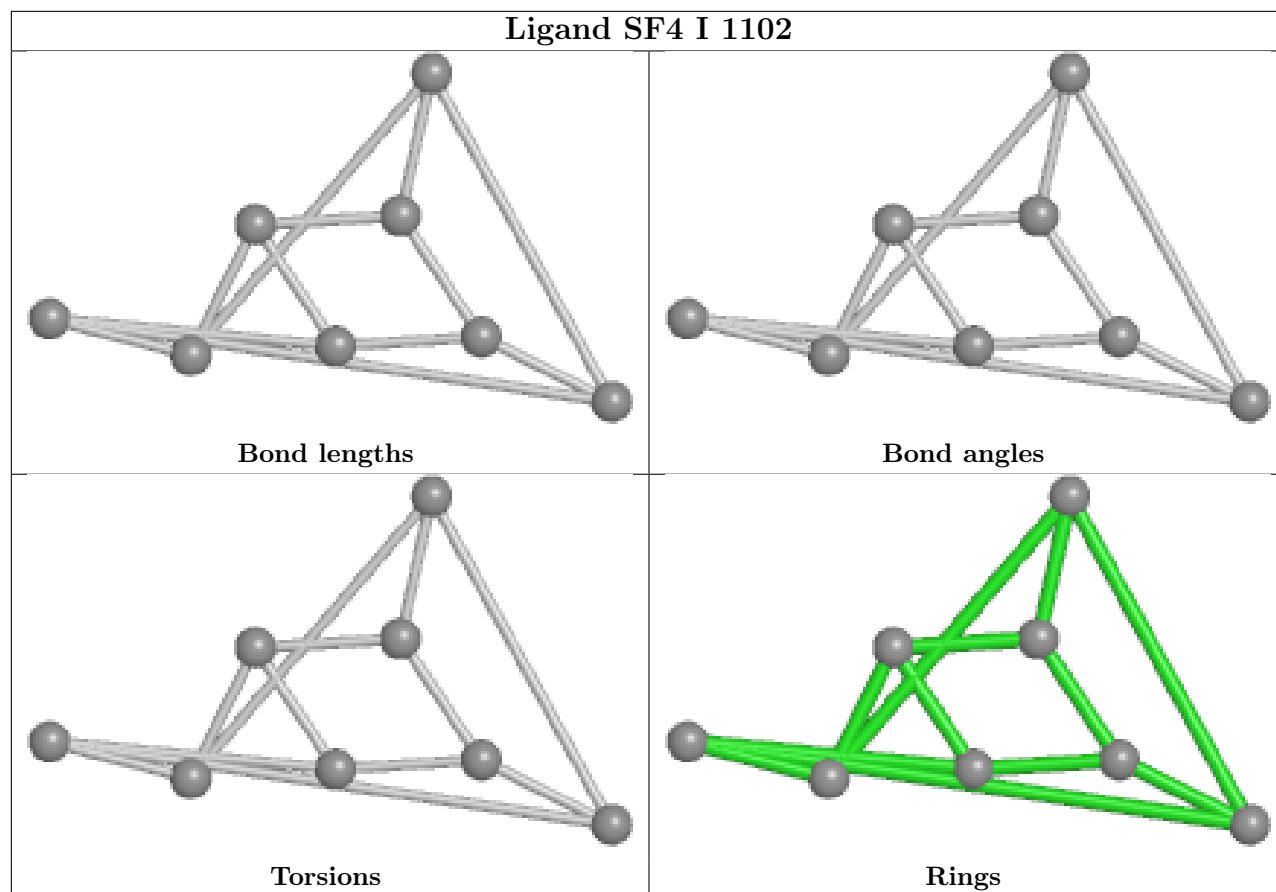
Ligand SF4 F 1104



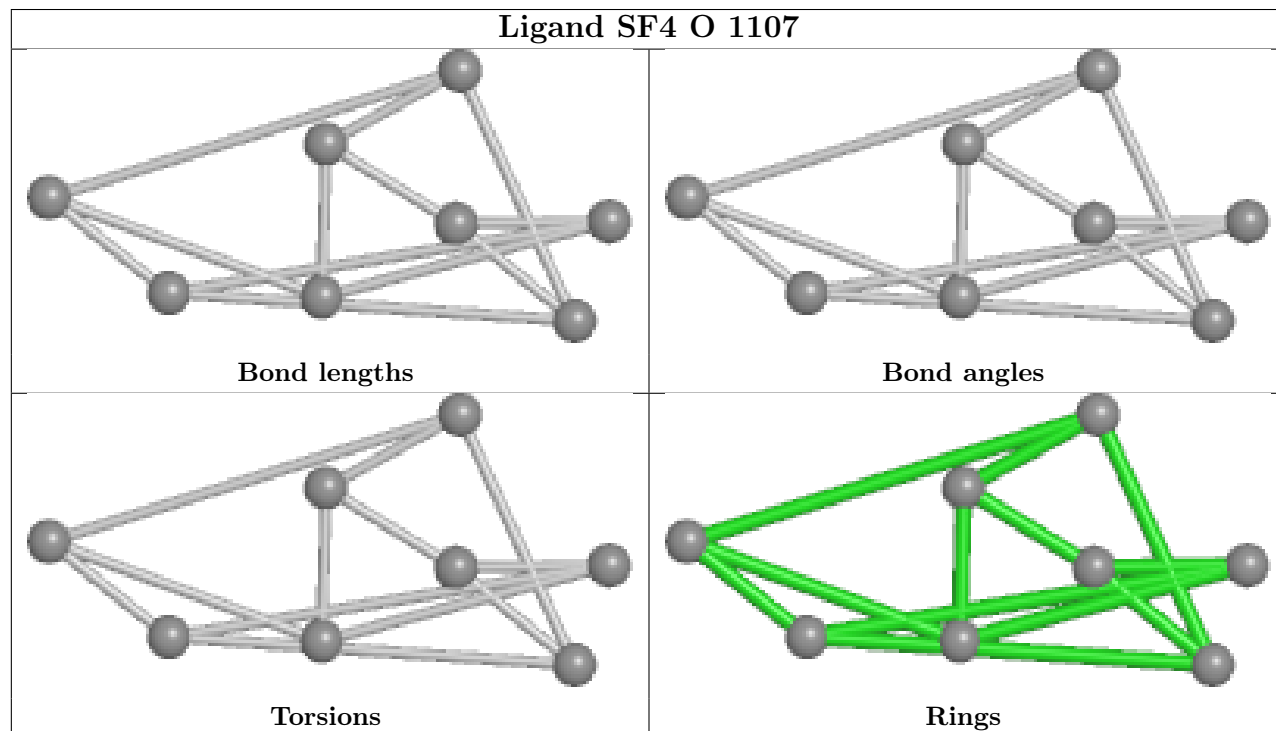
Ligand SF4 K 1104



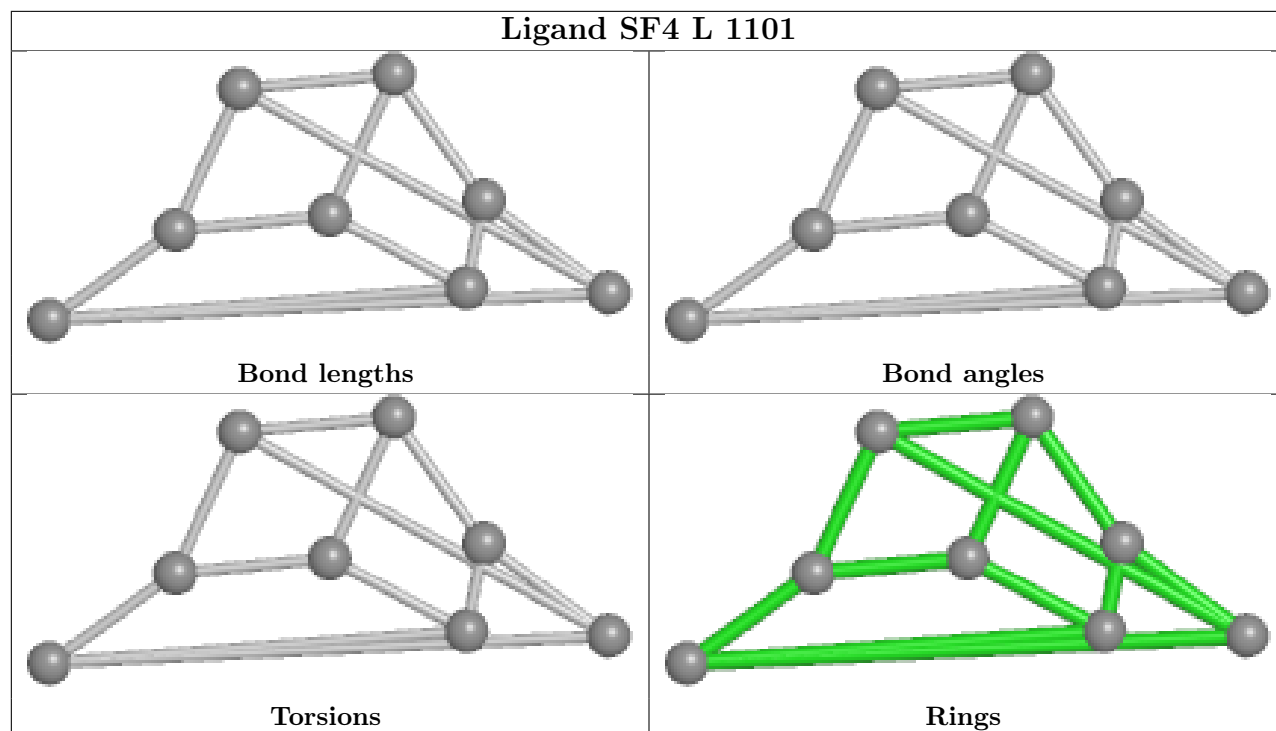
Ligand SF4 I 1102



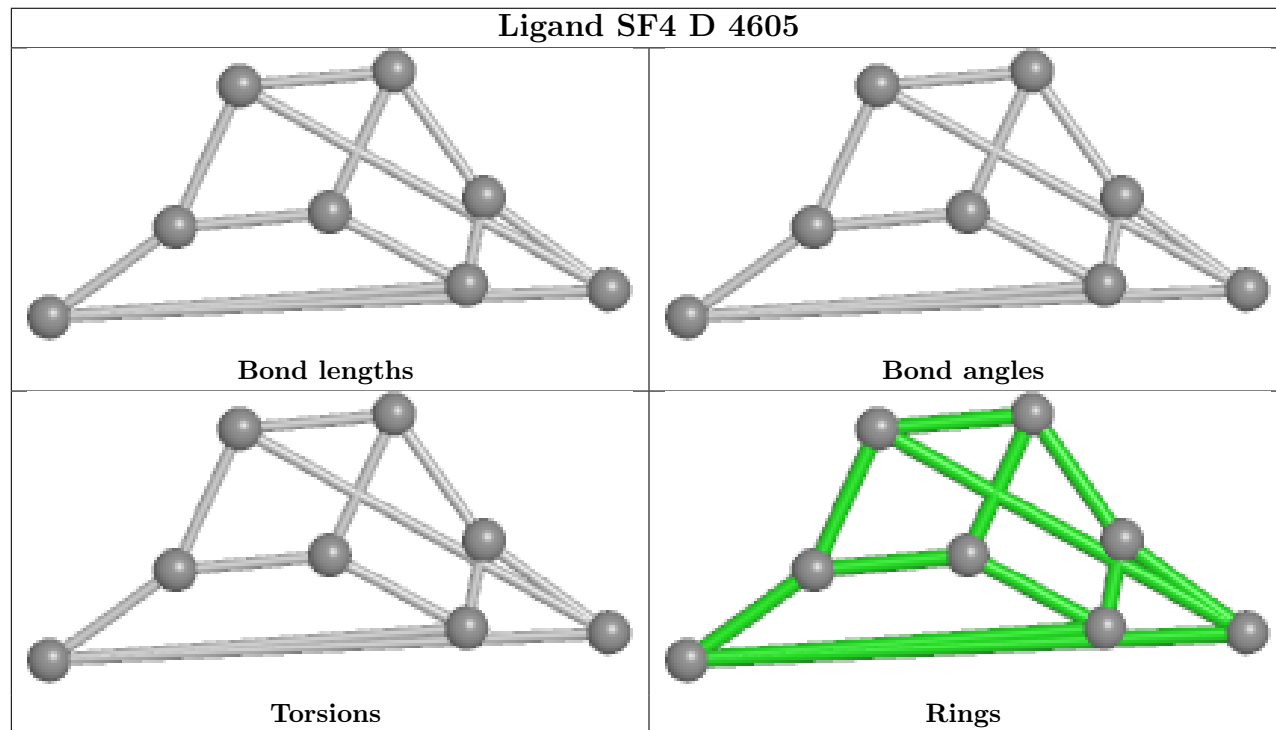
Ligand SF4 O 1107

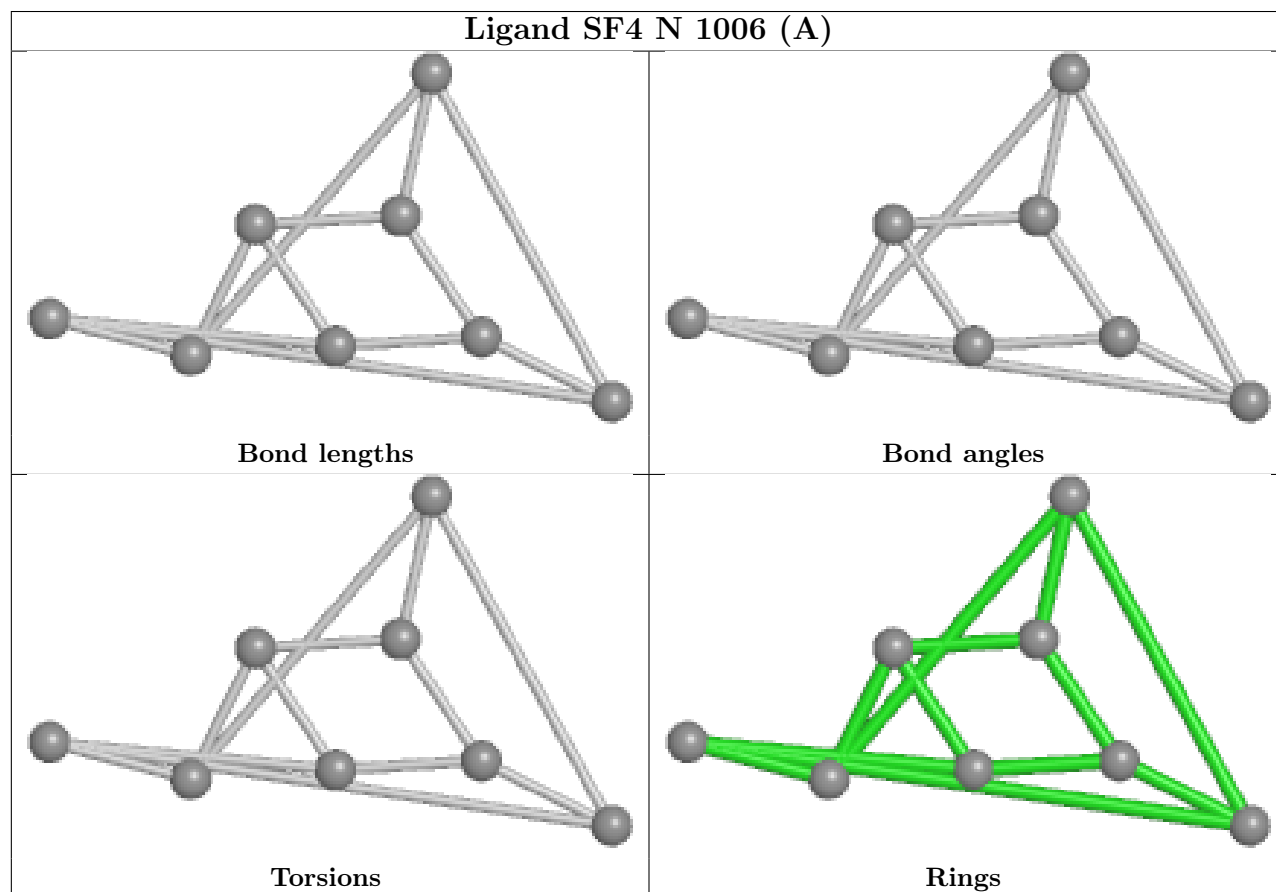
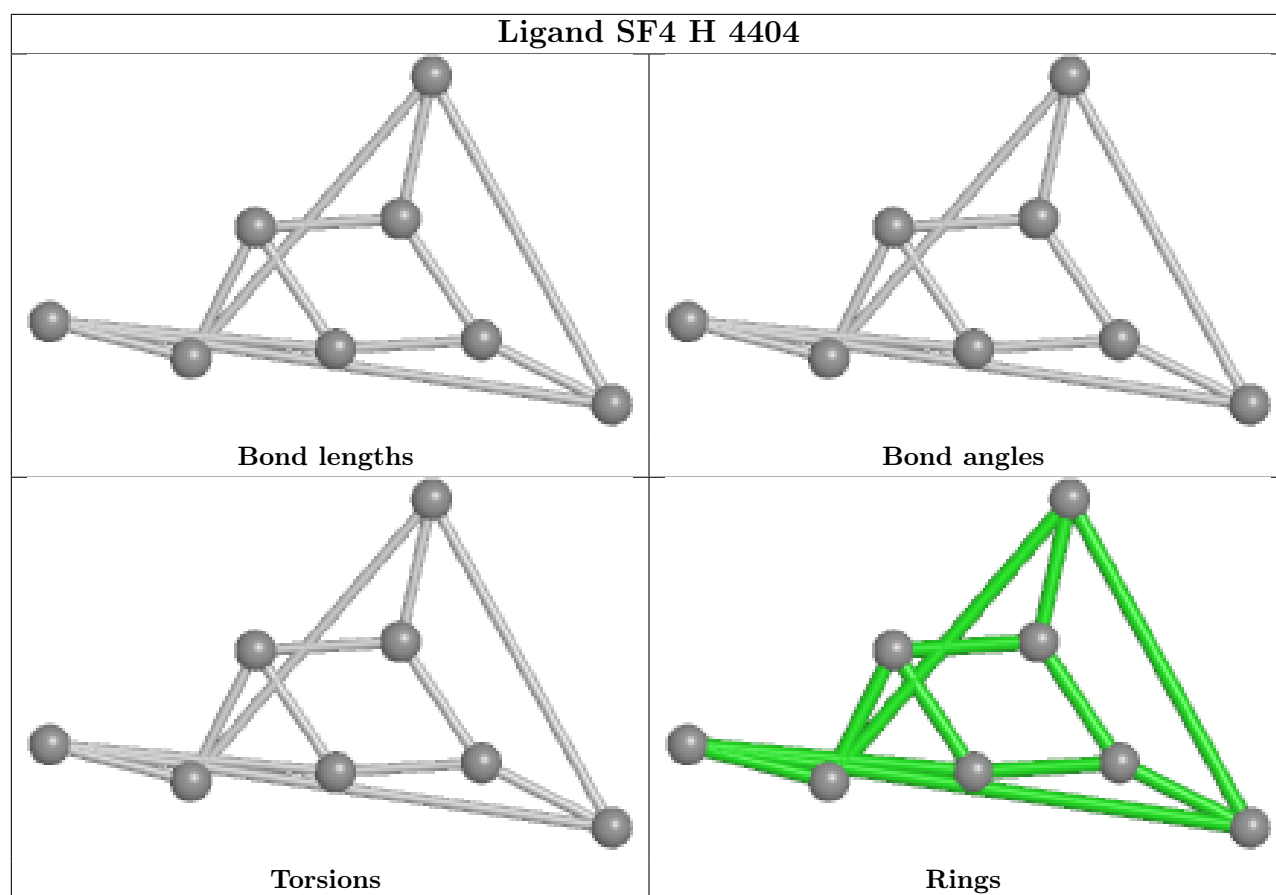


Ligand SF4 L 1101

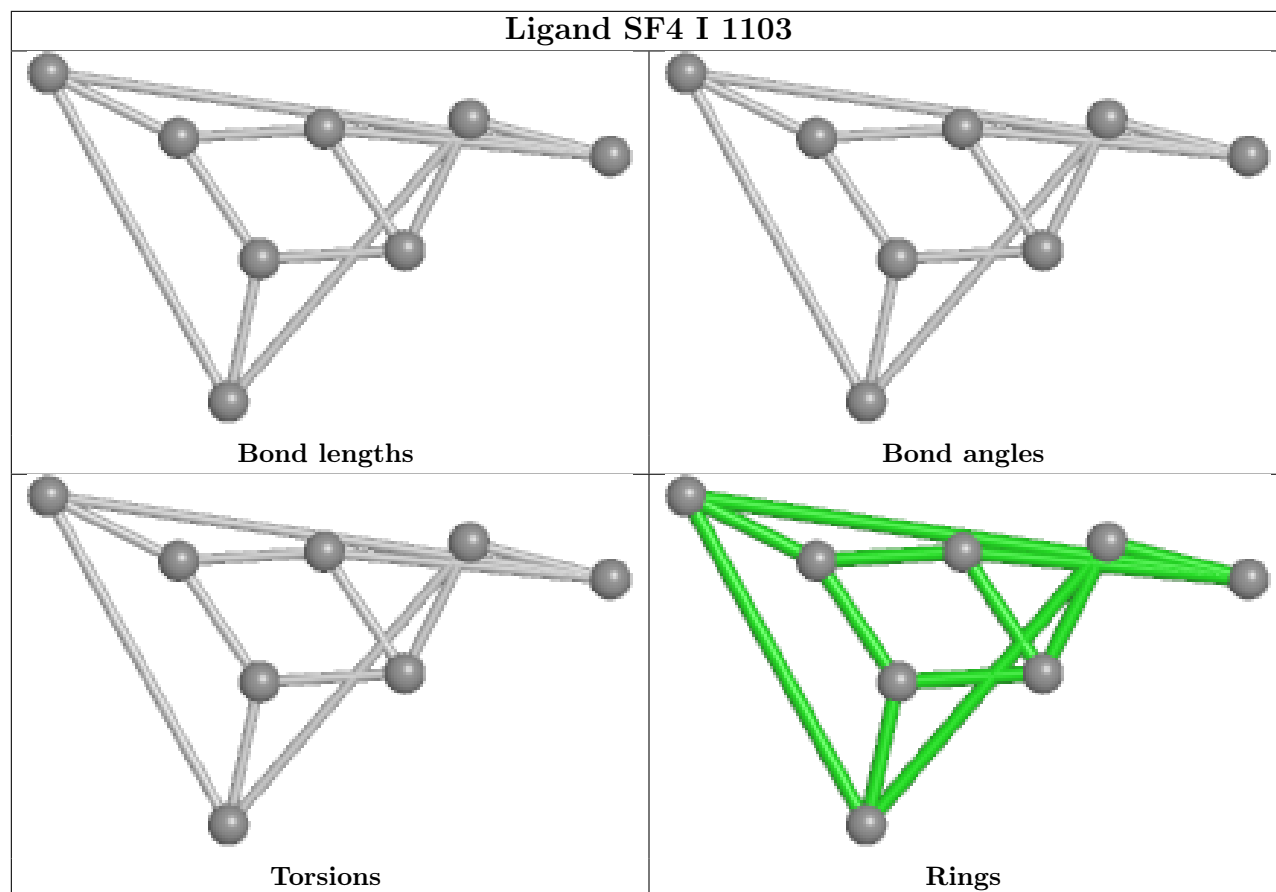


Ligand SF4 D 4605

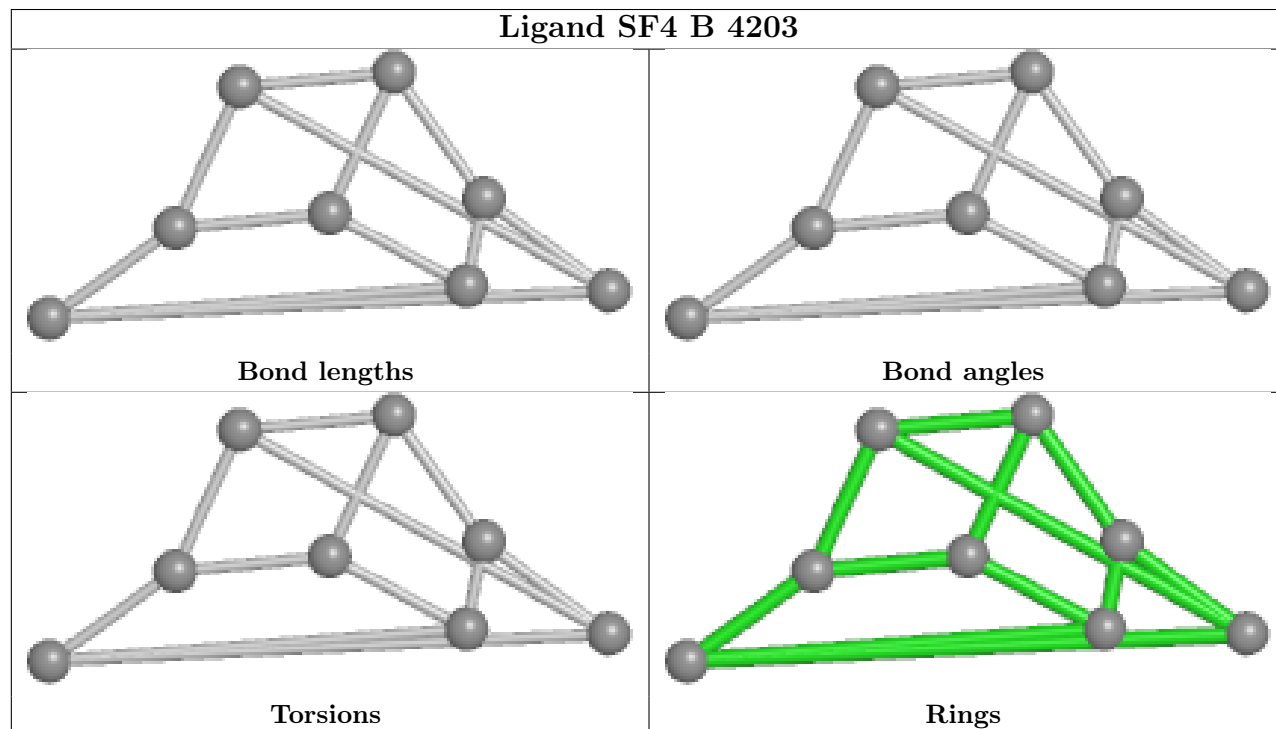


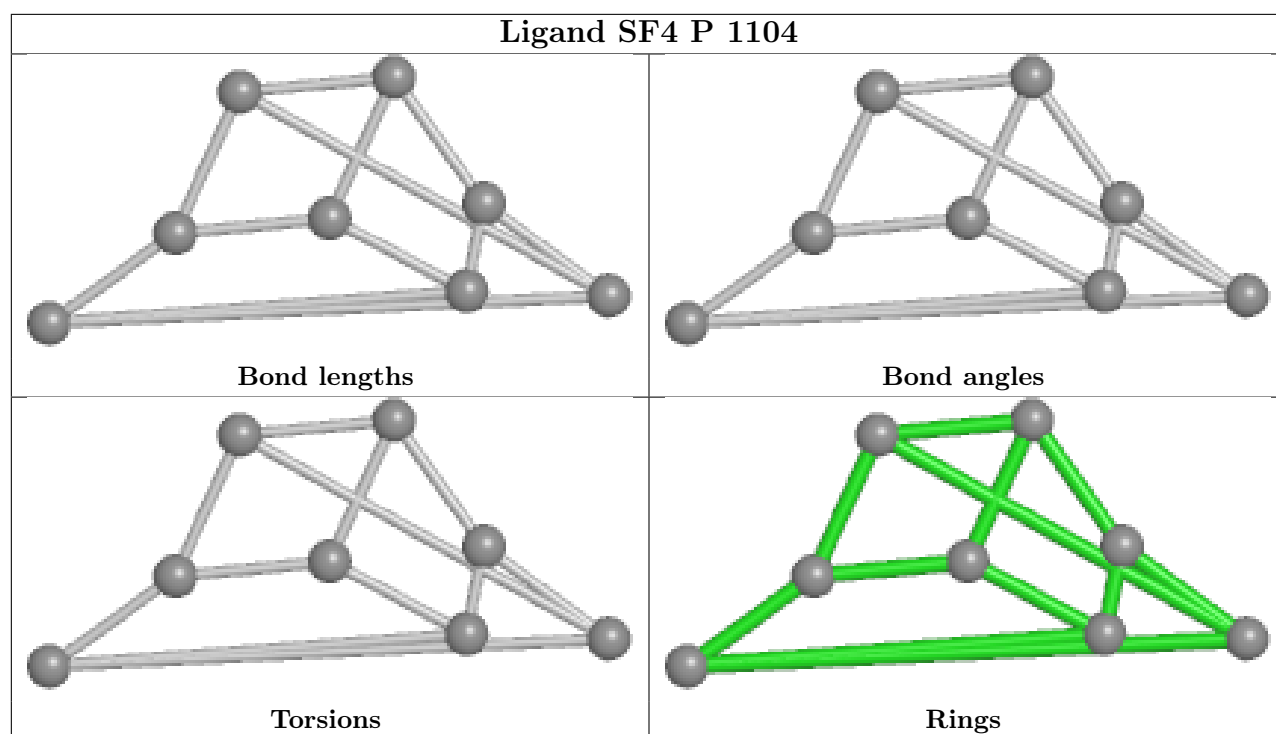


Ligand SF4 I 1103

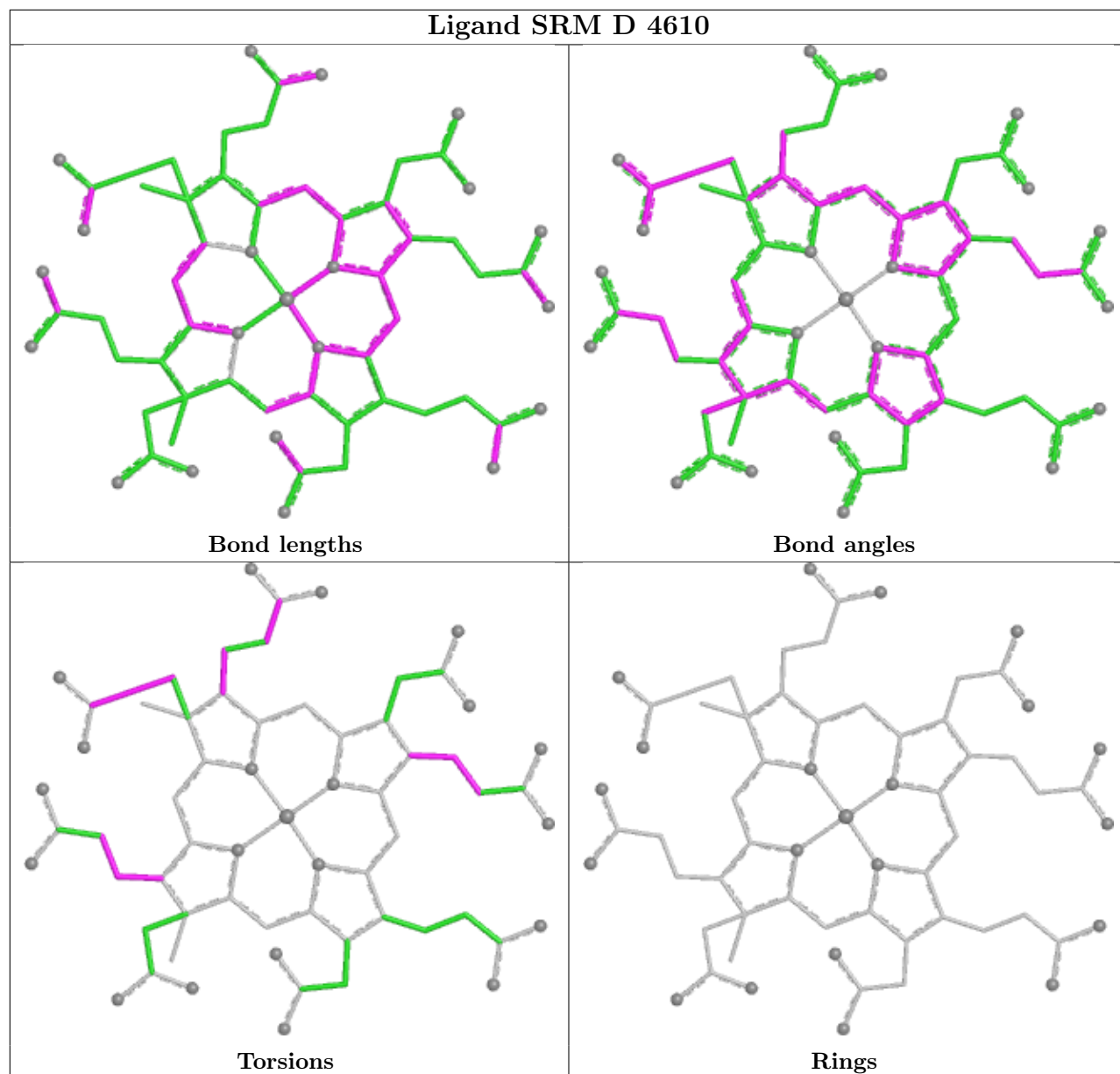


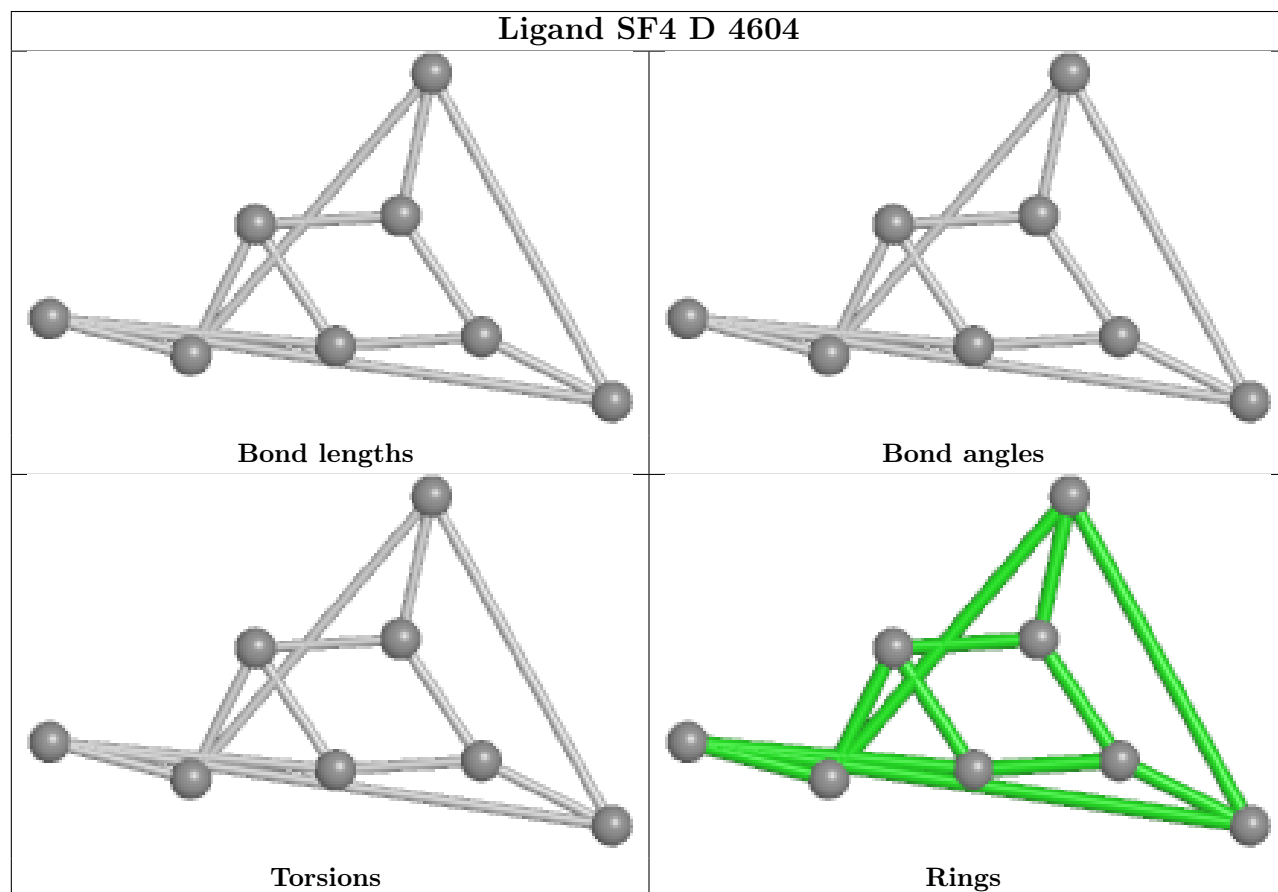
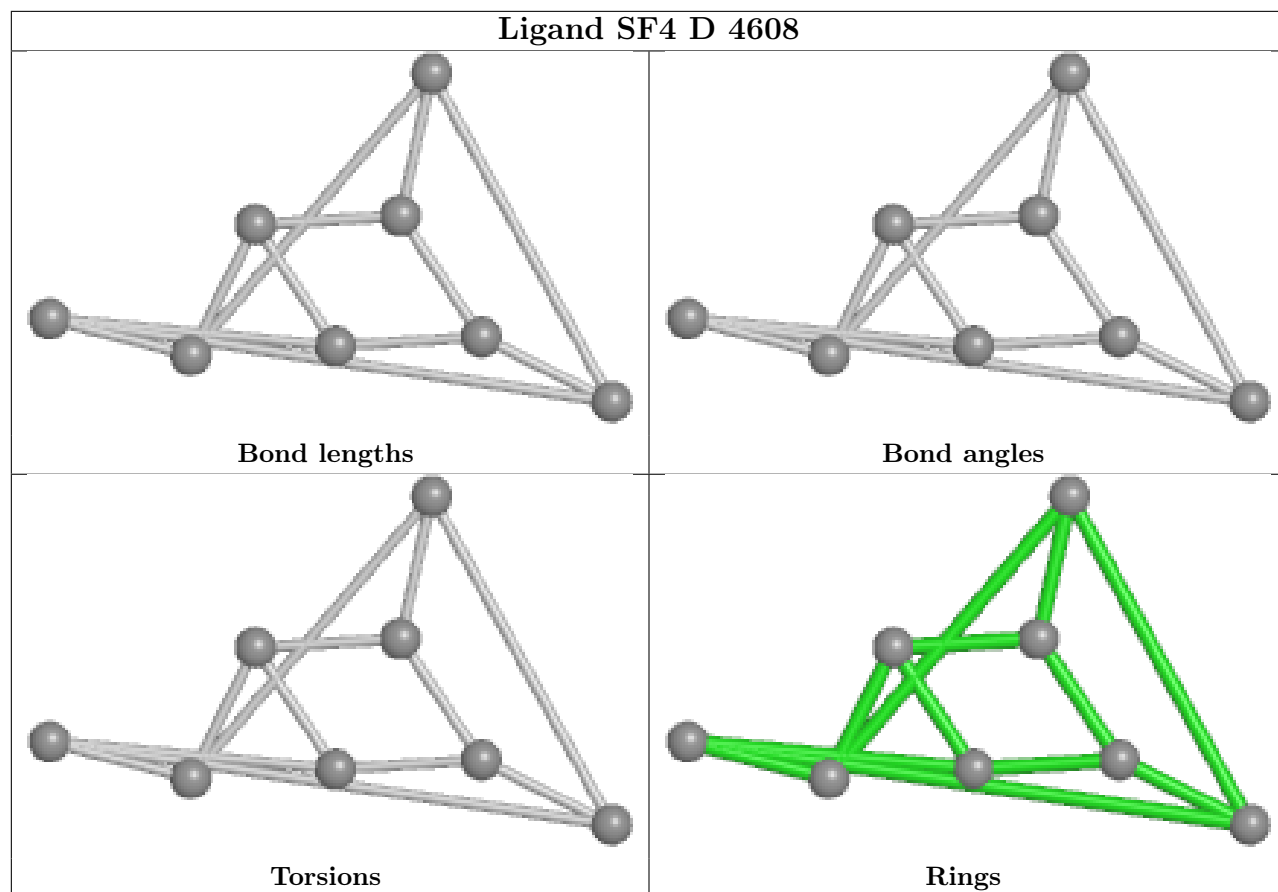
Ligand SF4 B 4203

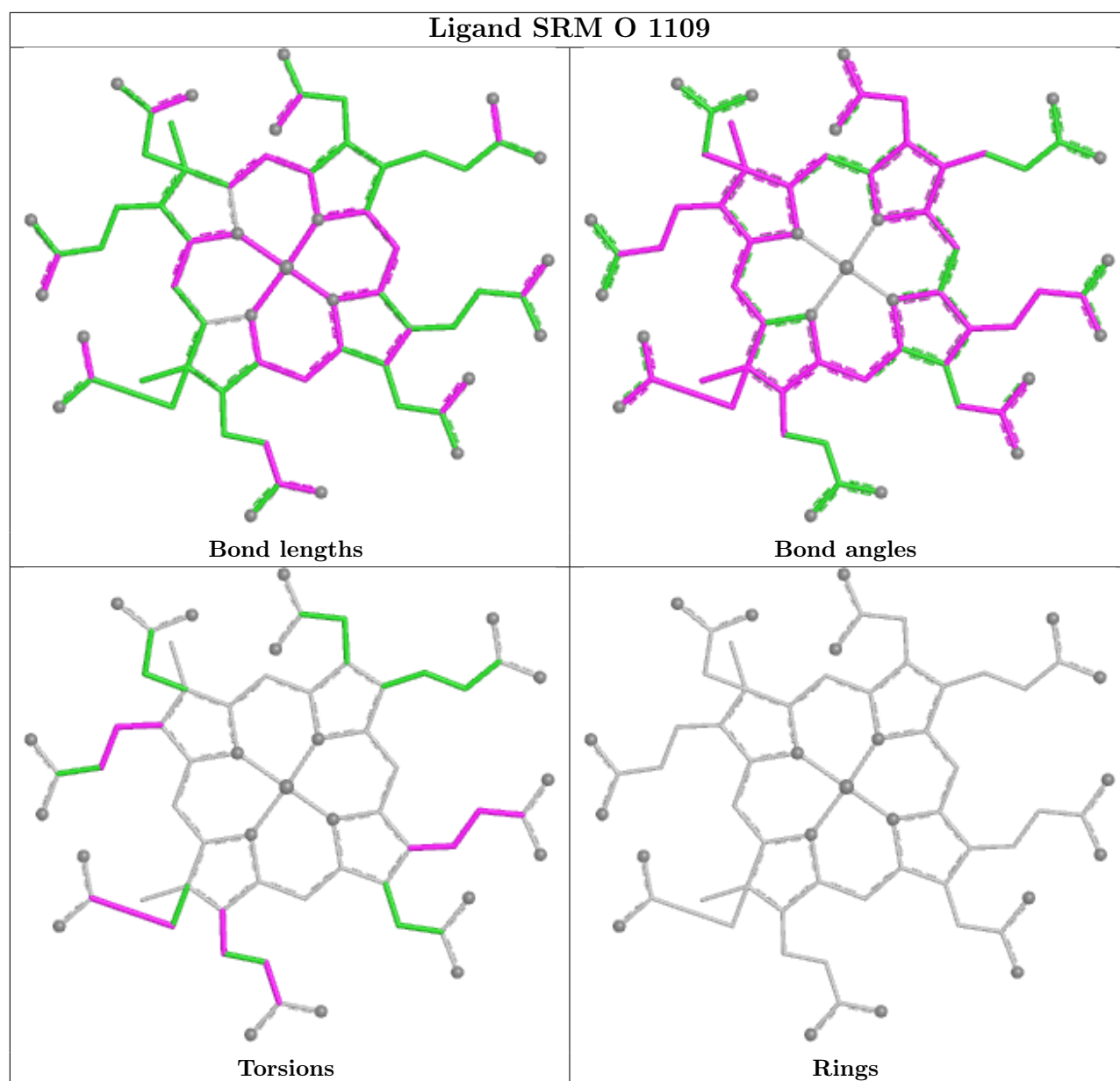




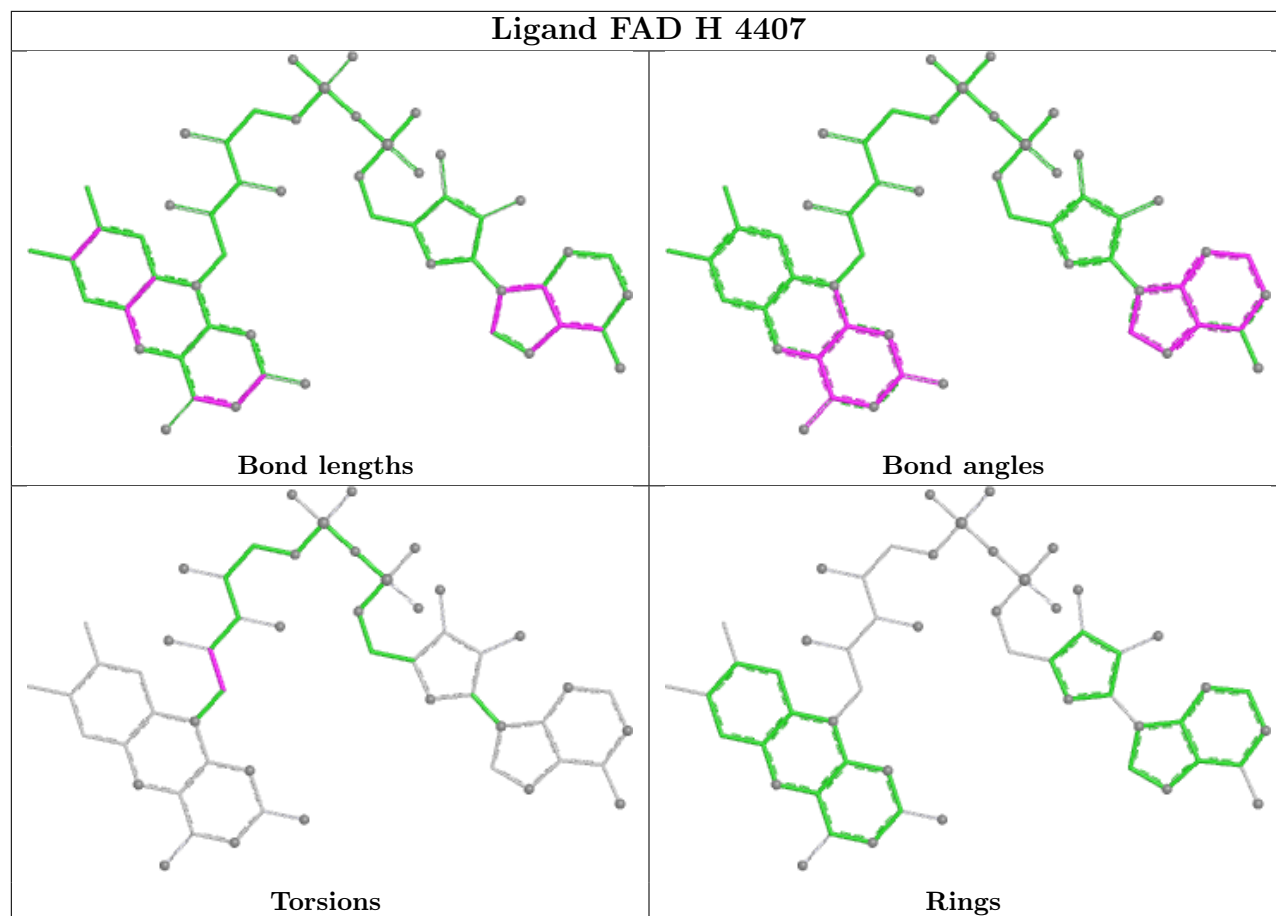
Ligand SRM D 4610



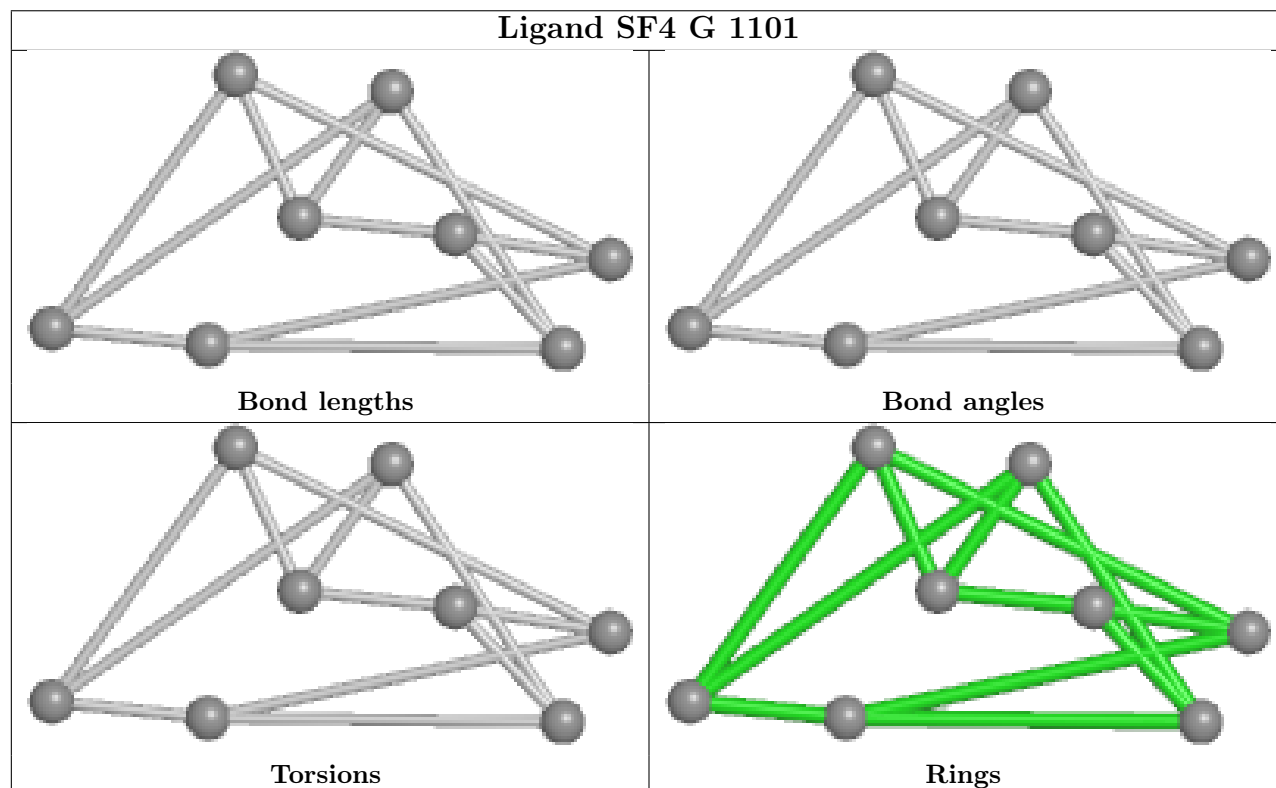




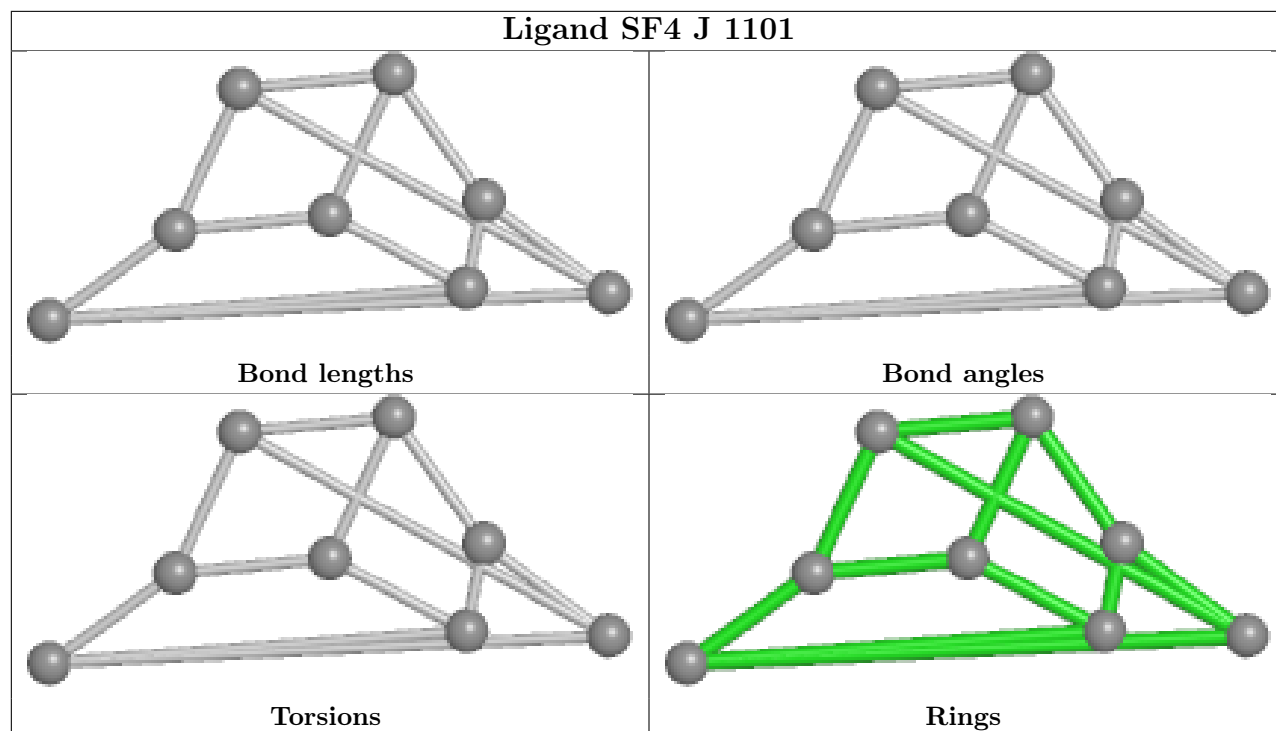
Ligand FAD H 4407



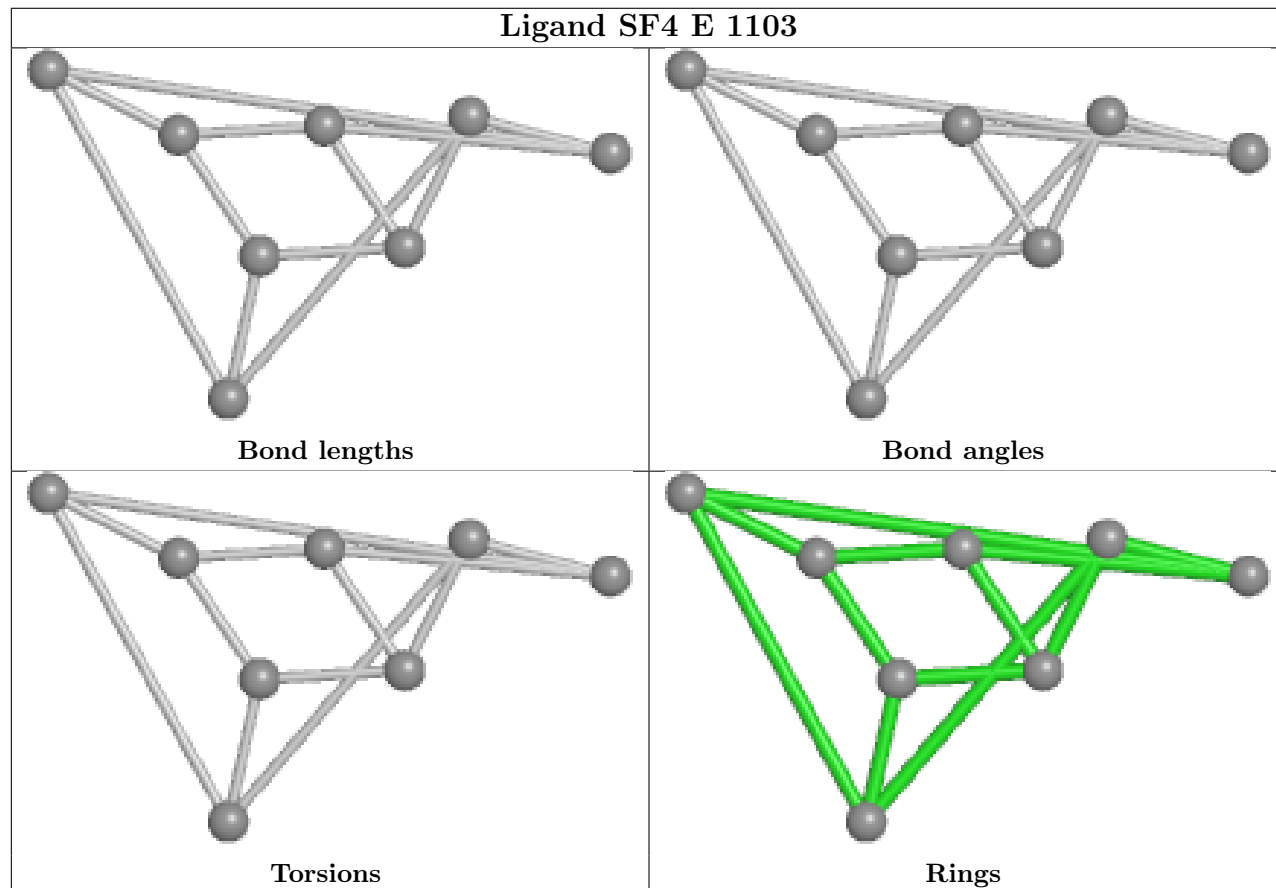
Ligand SF4 G 1101

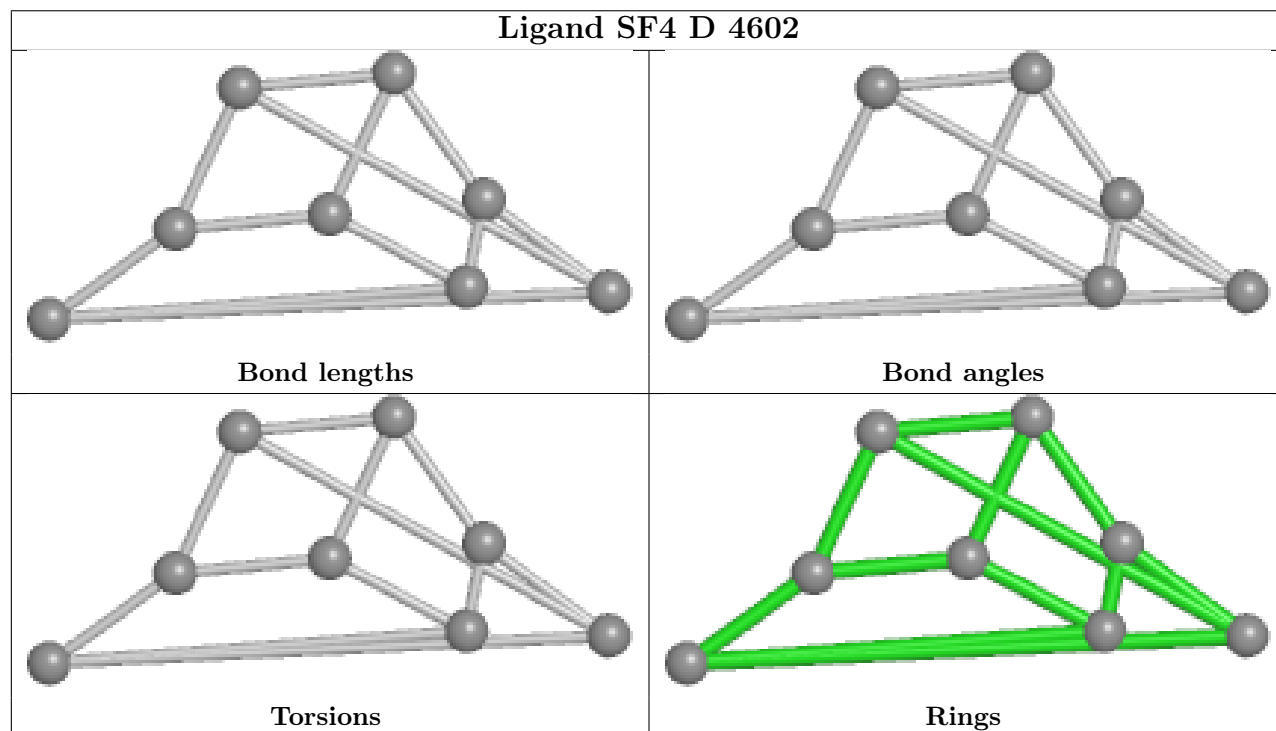
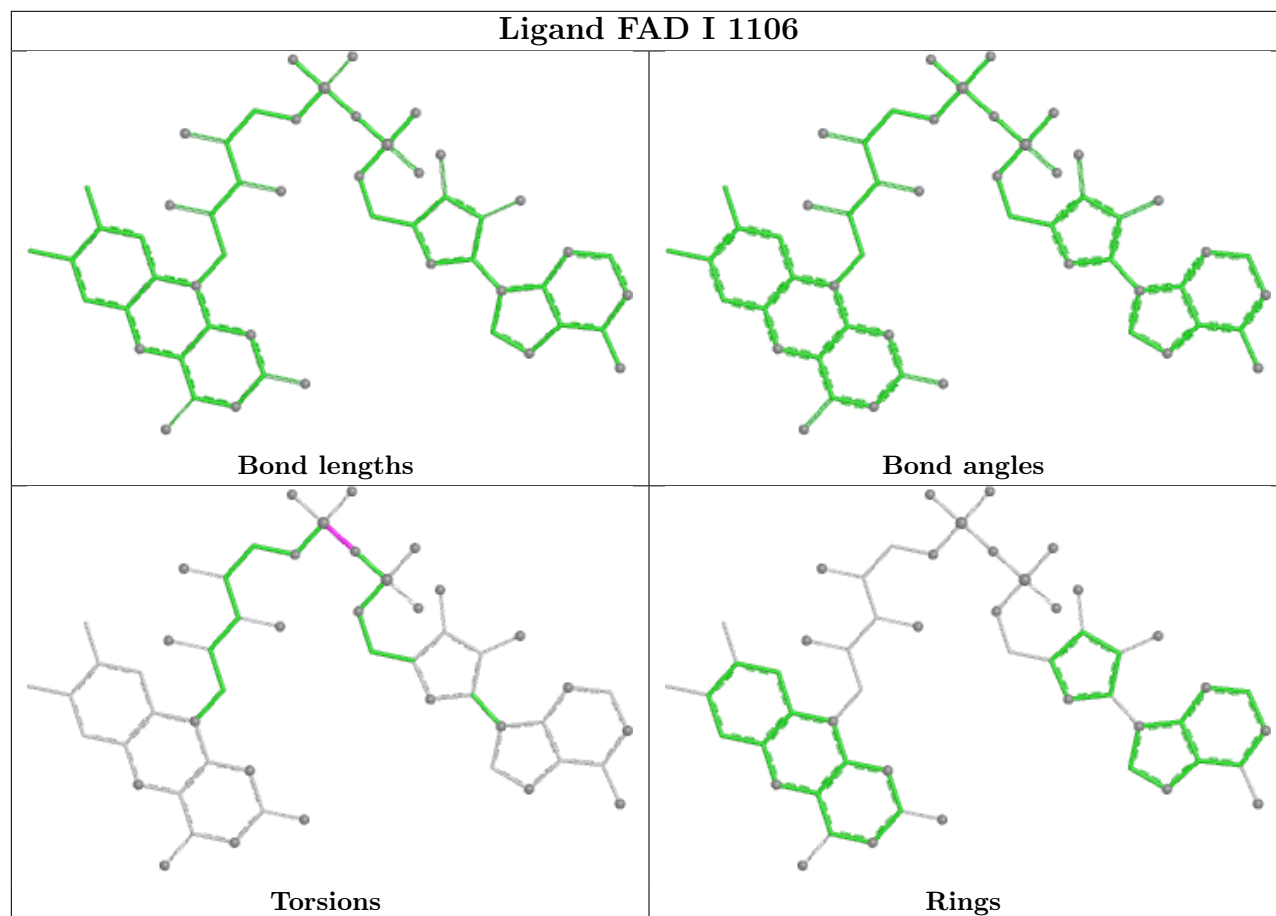


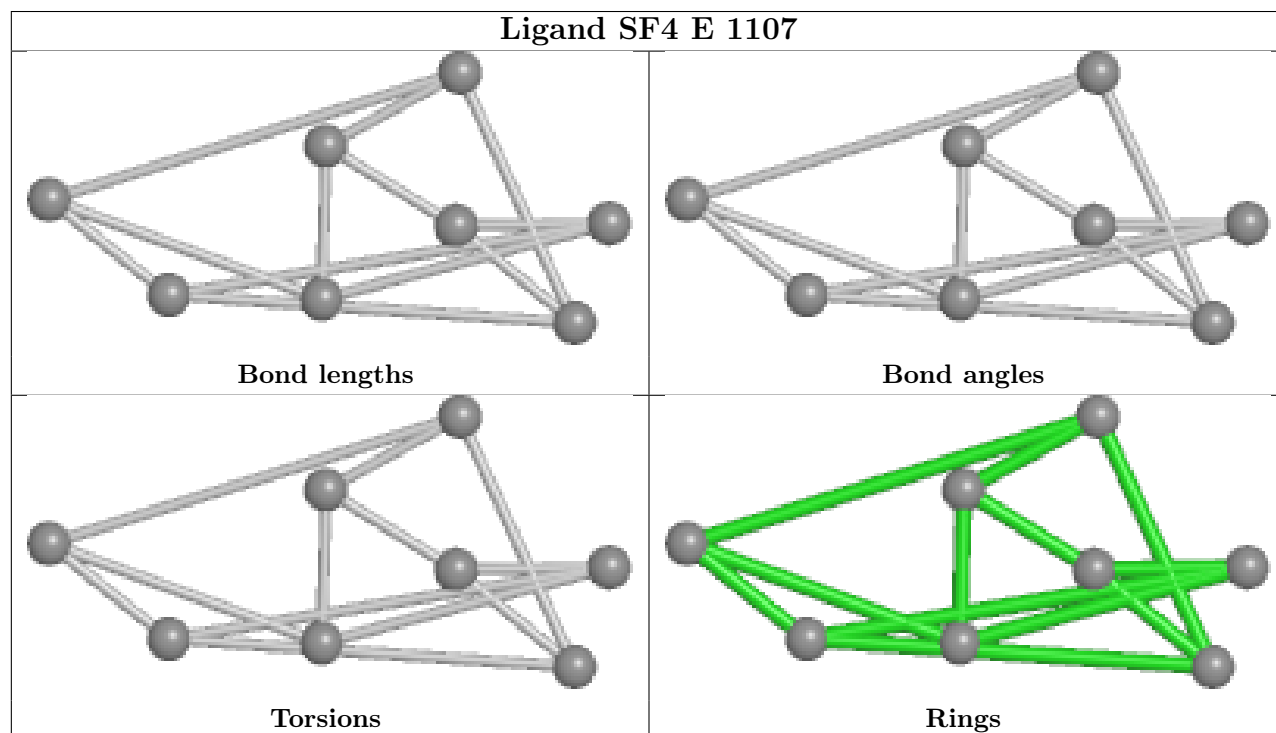
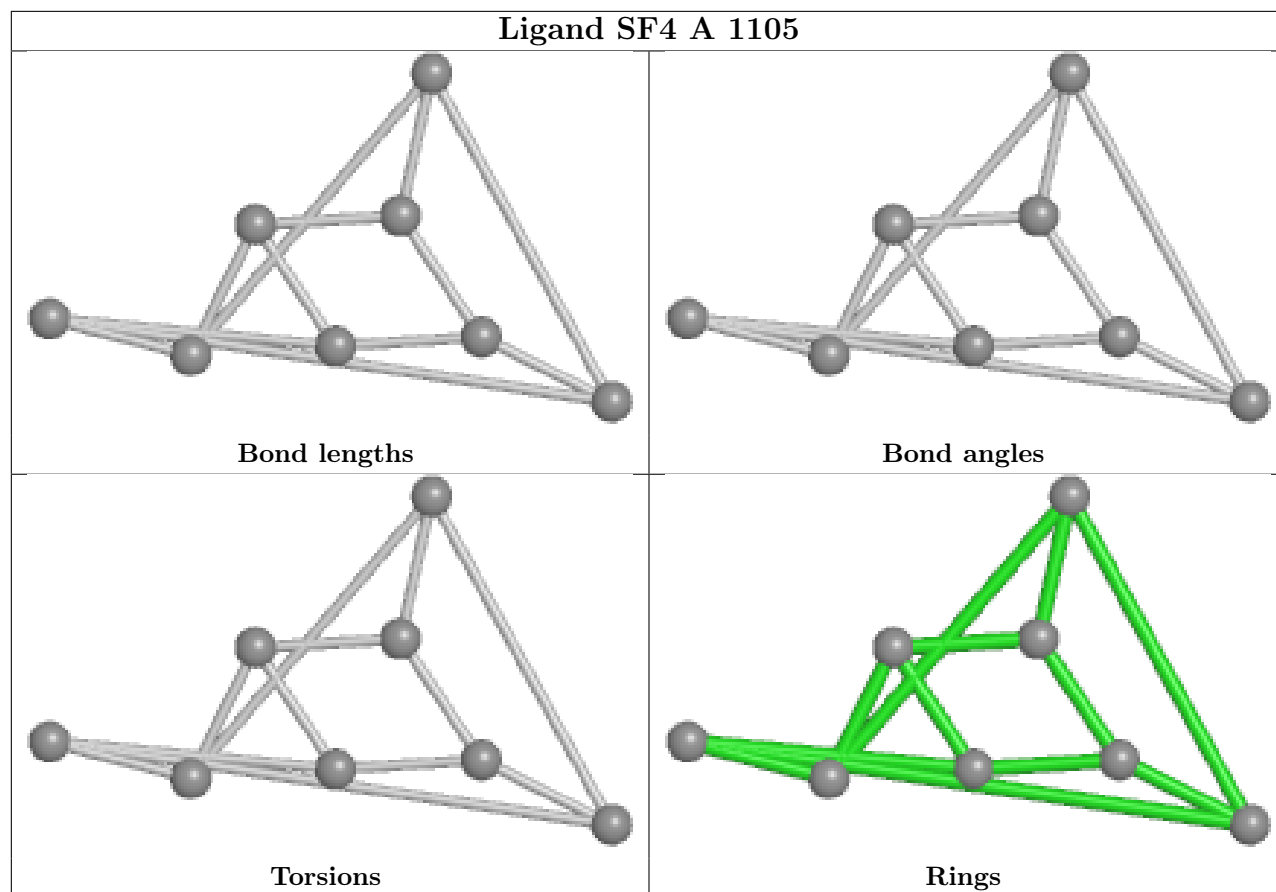
Ligand SF4 J 1101

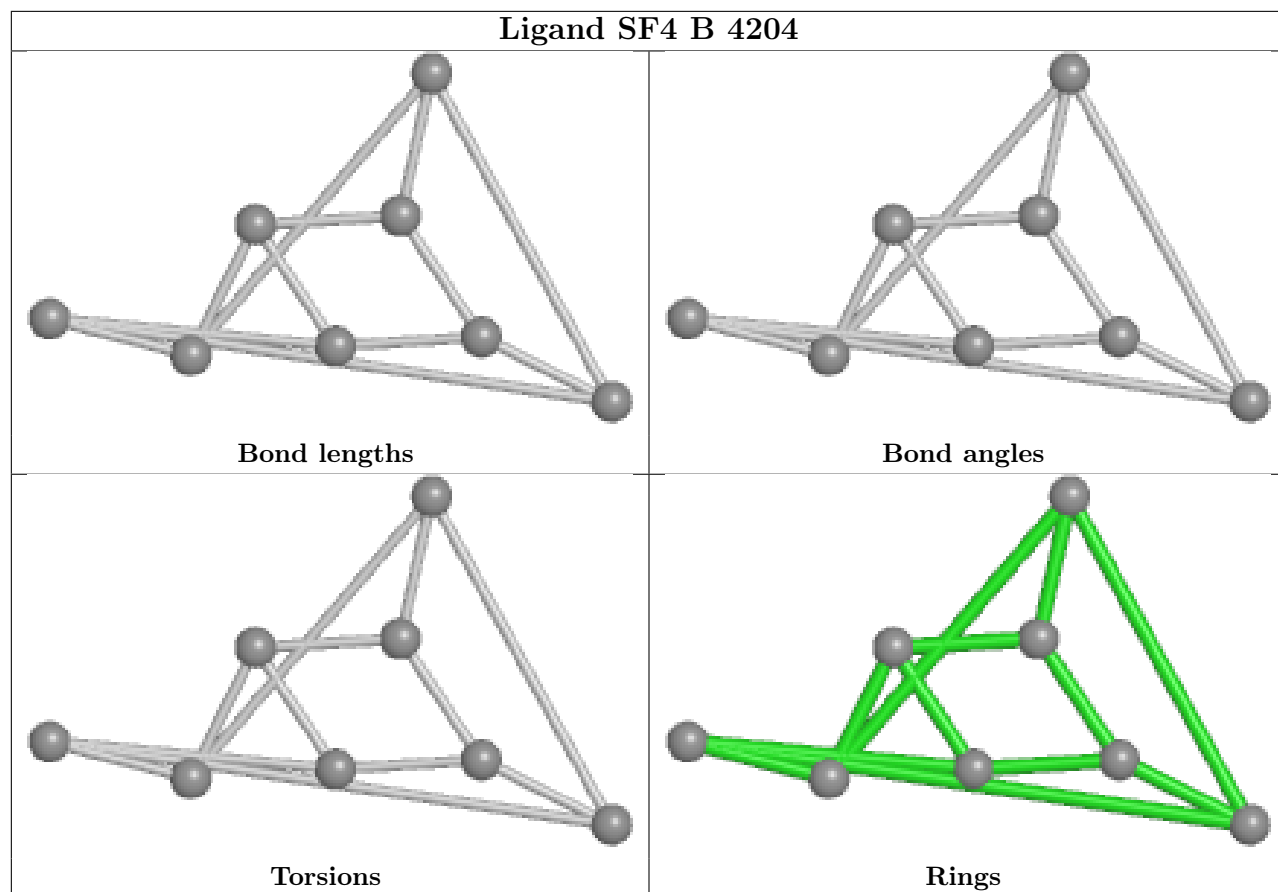


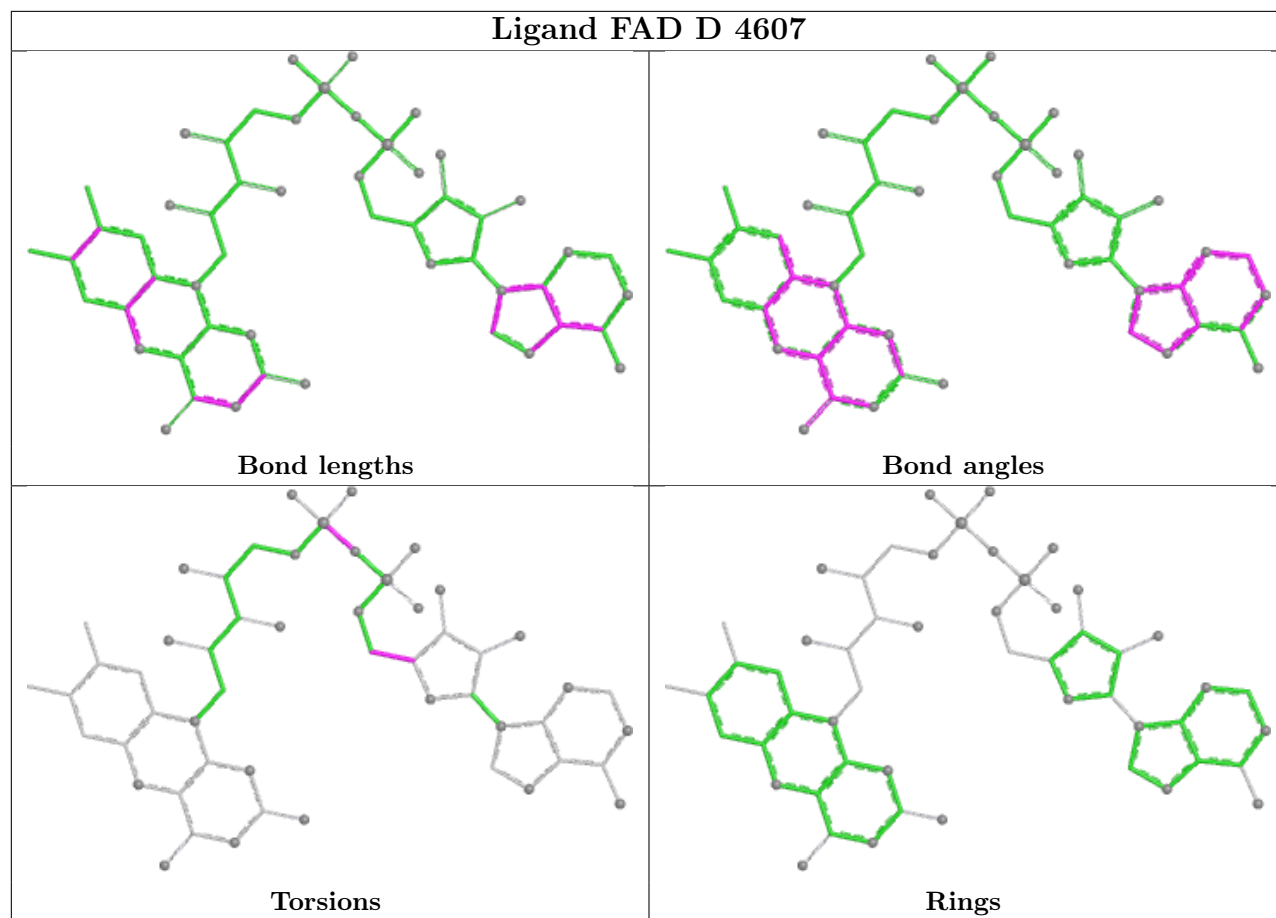
Ligand SF4 E 1103

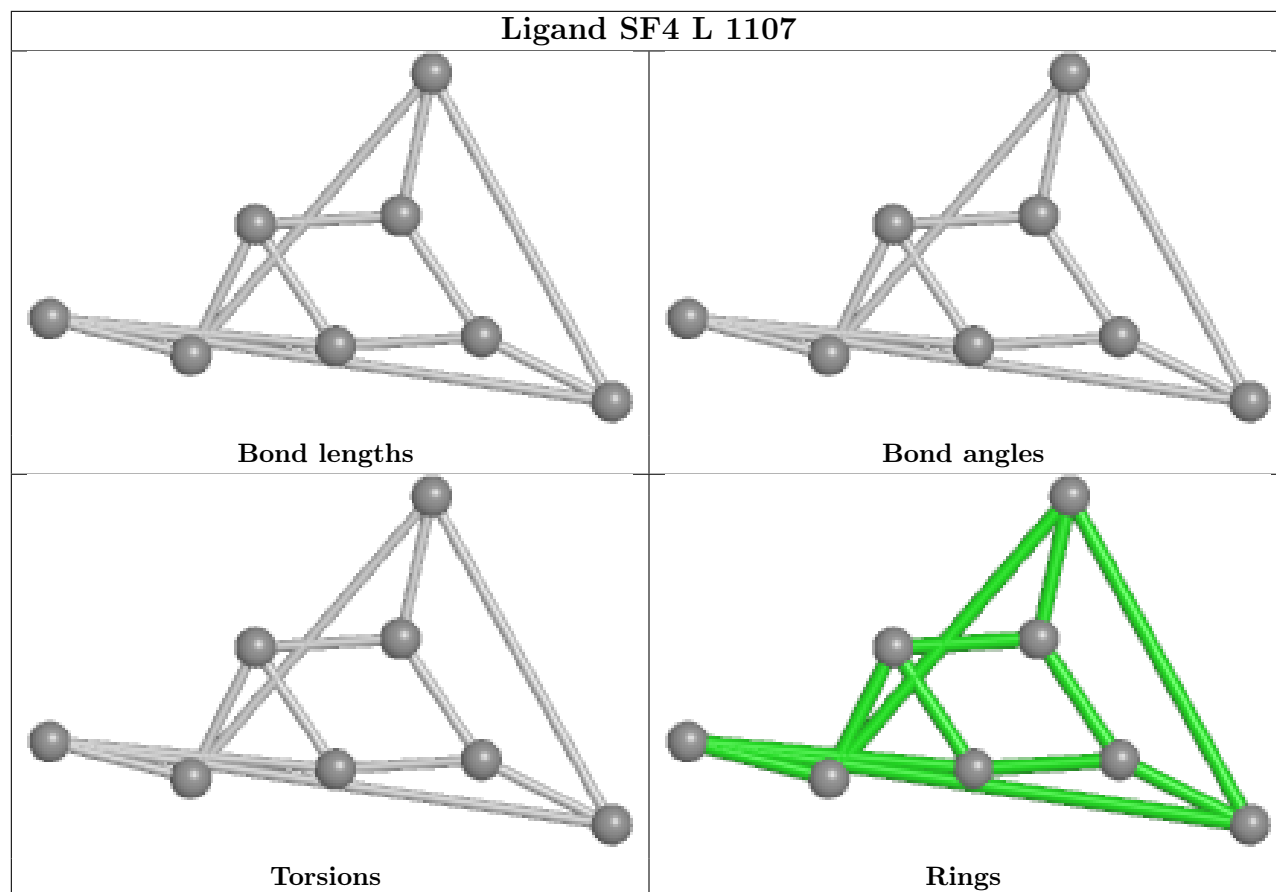


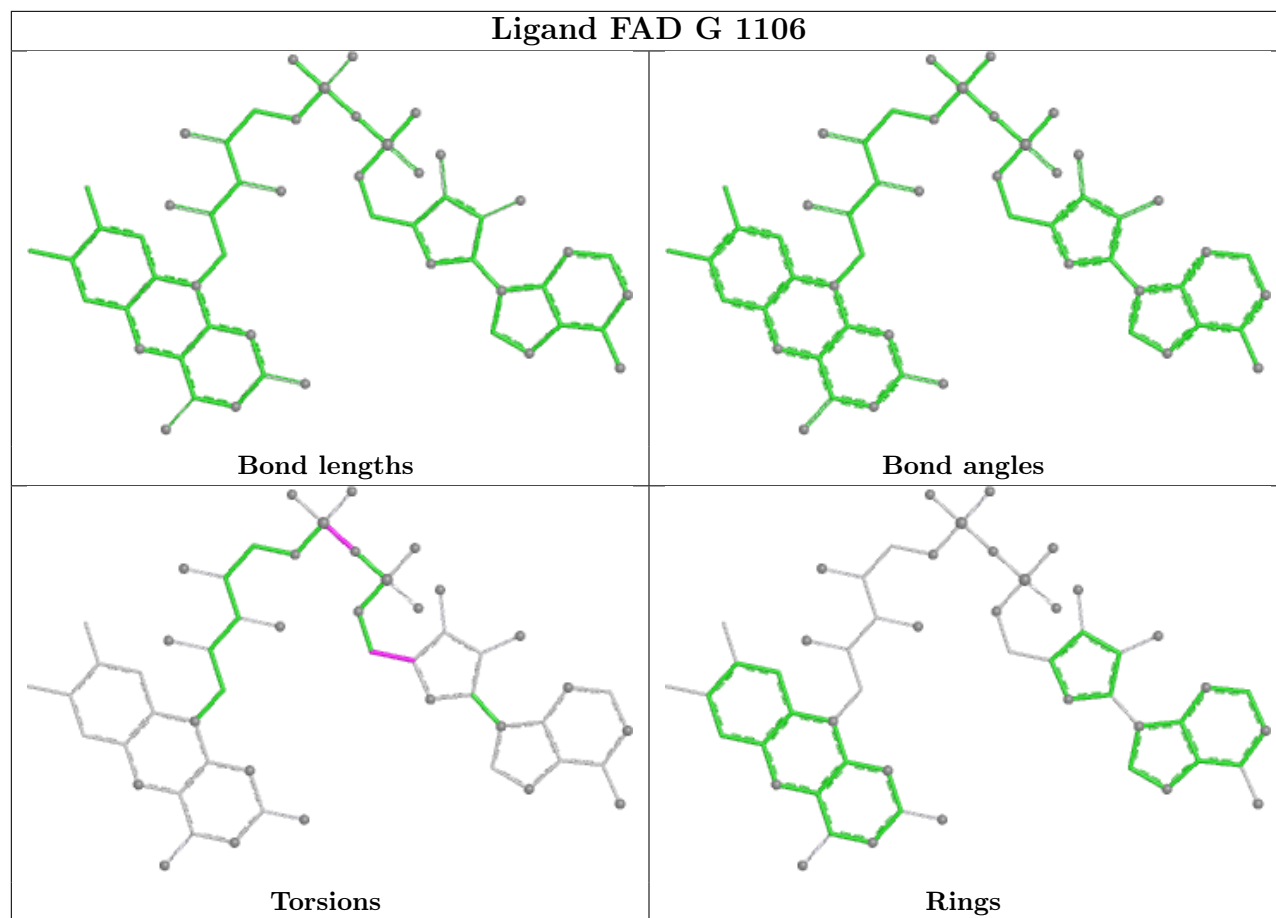


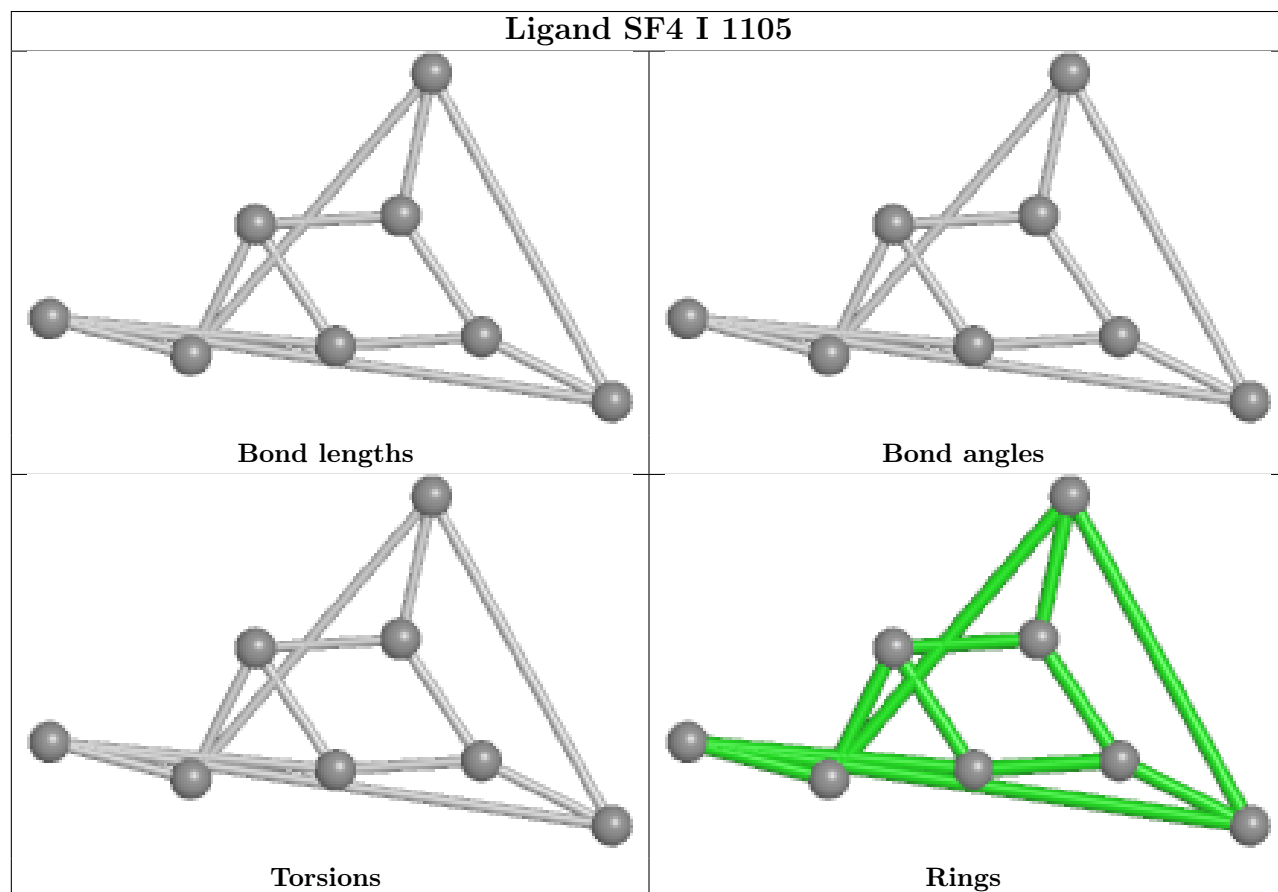
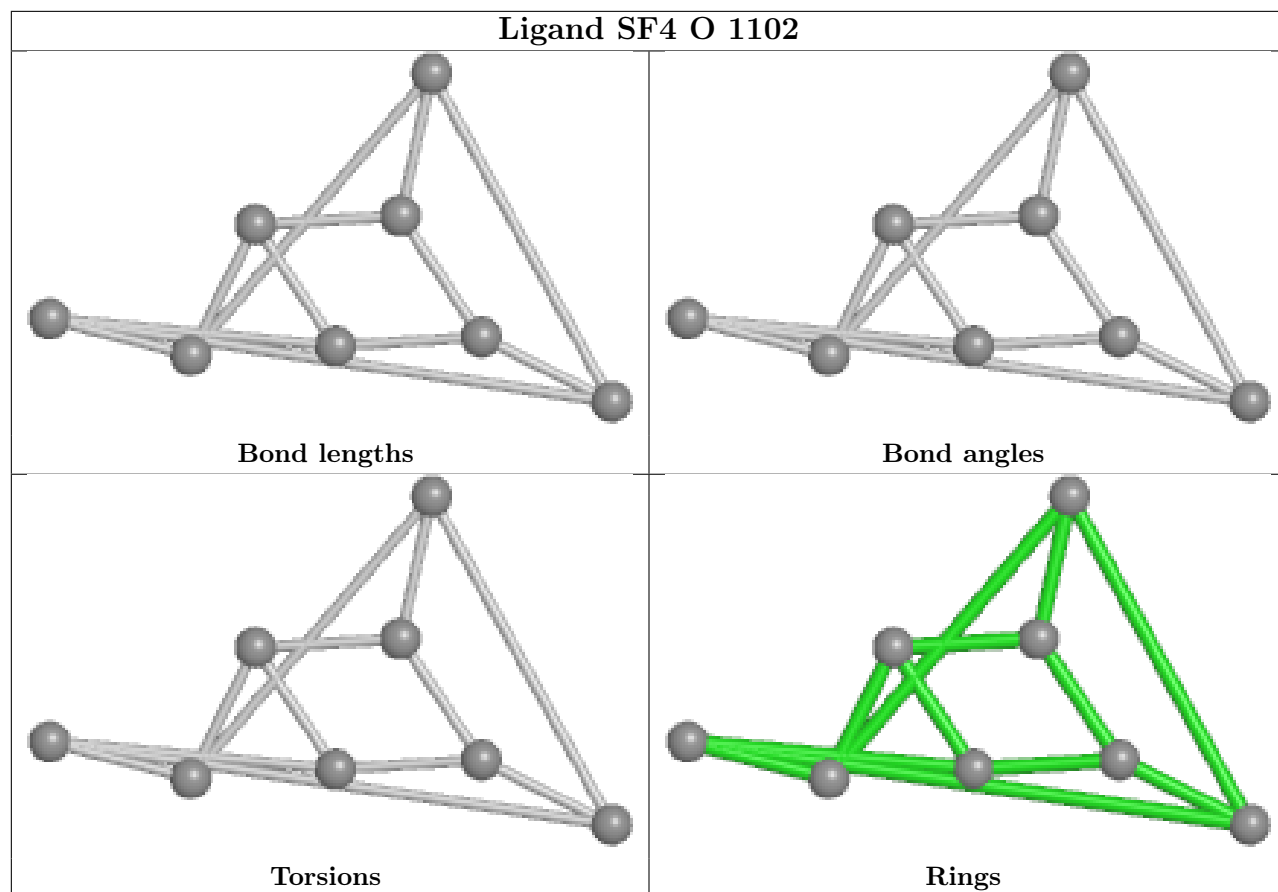


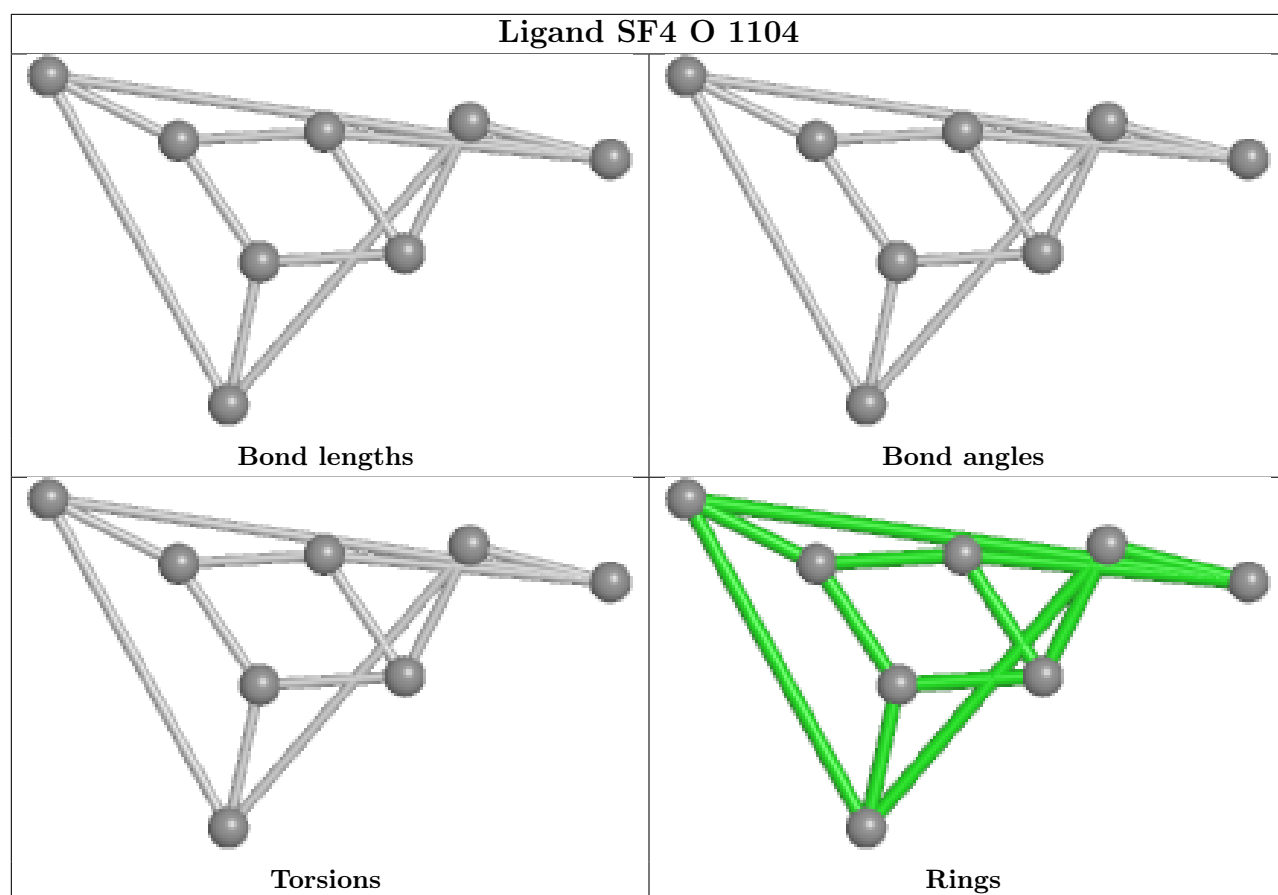


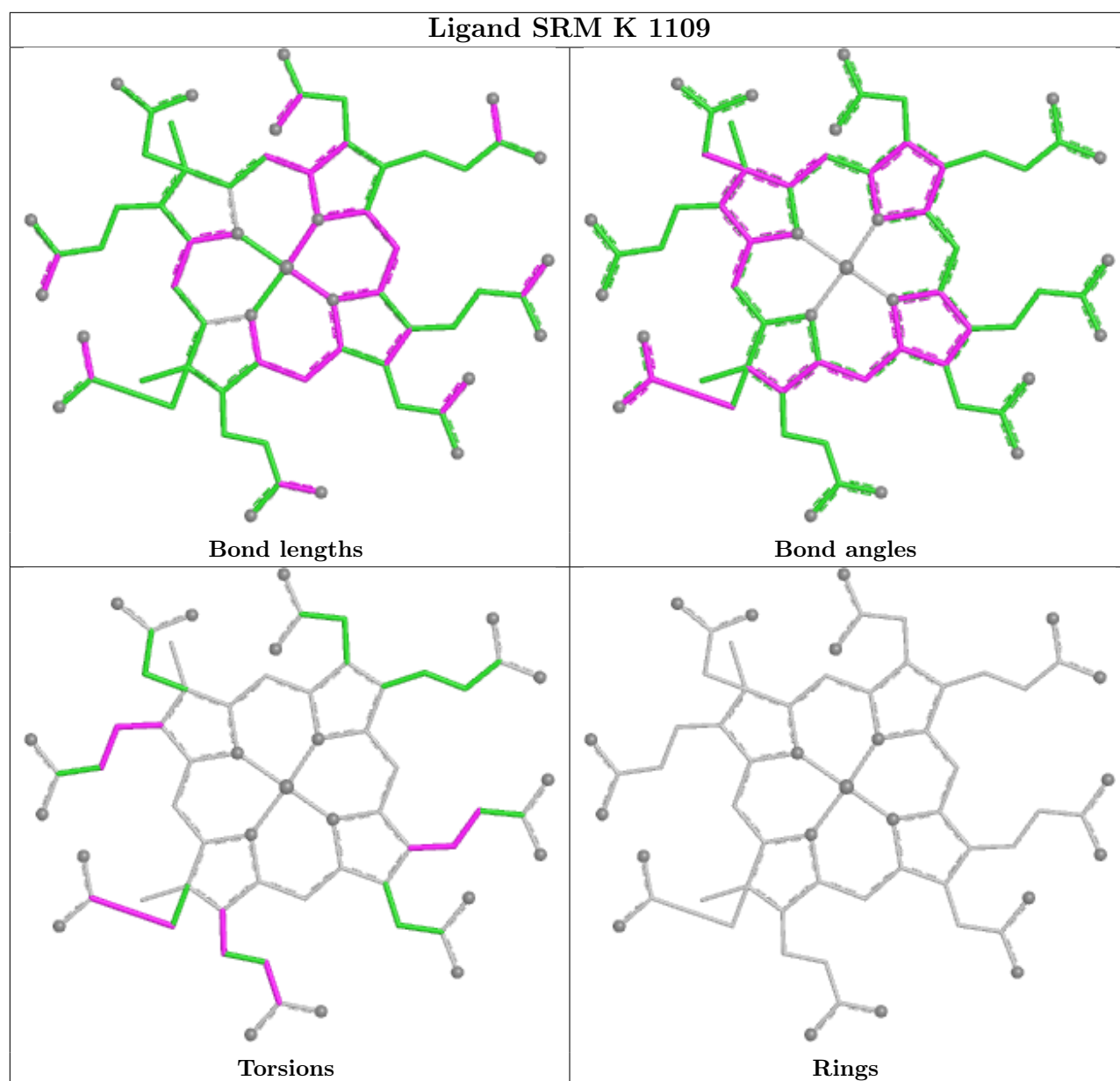


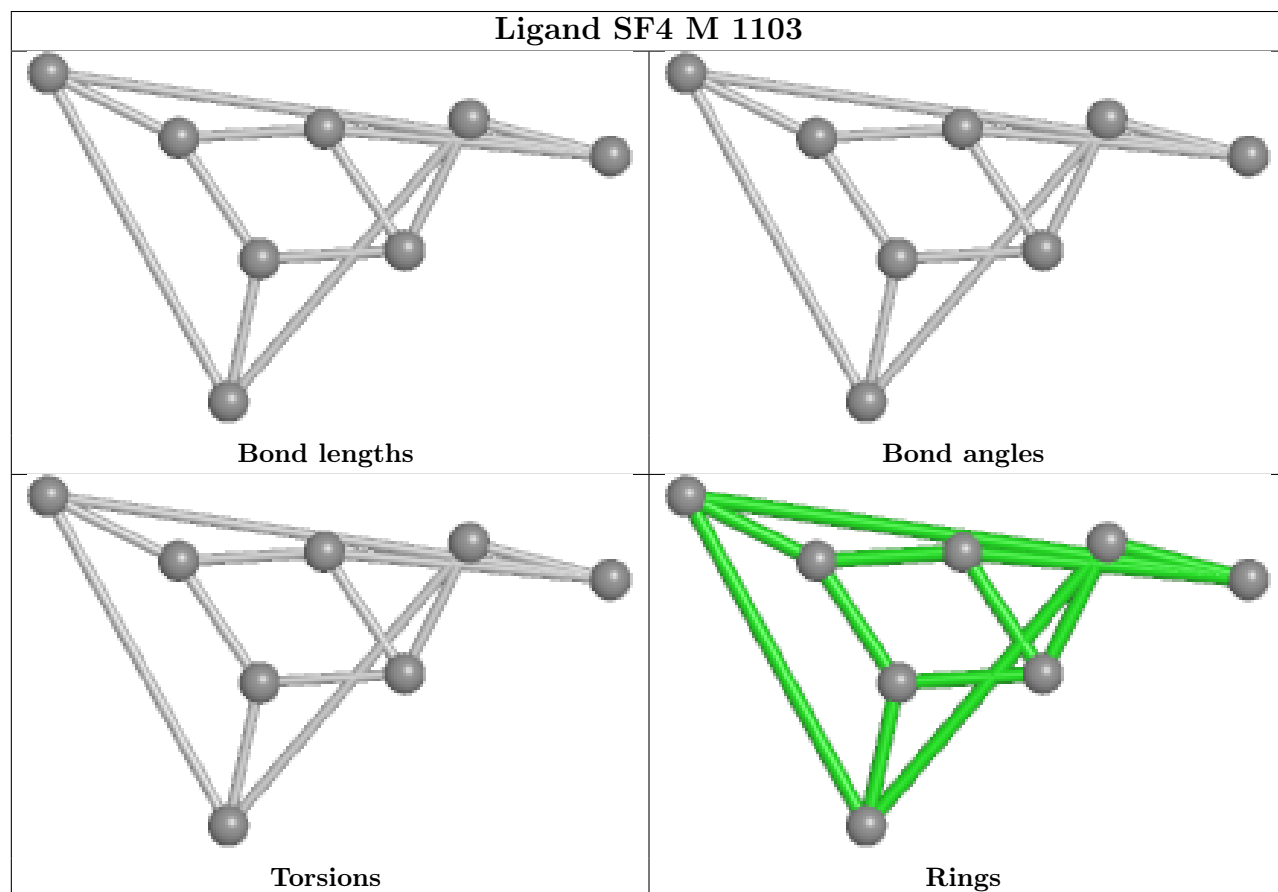
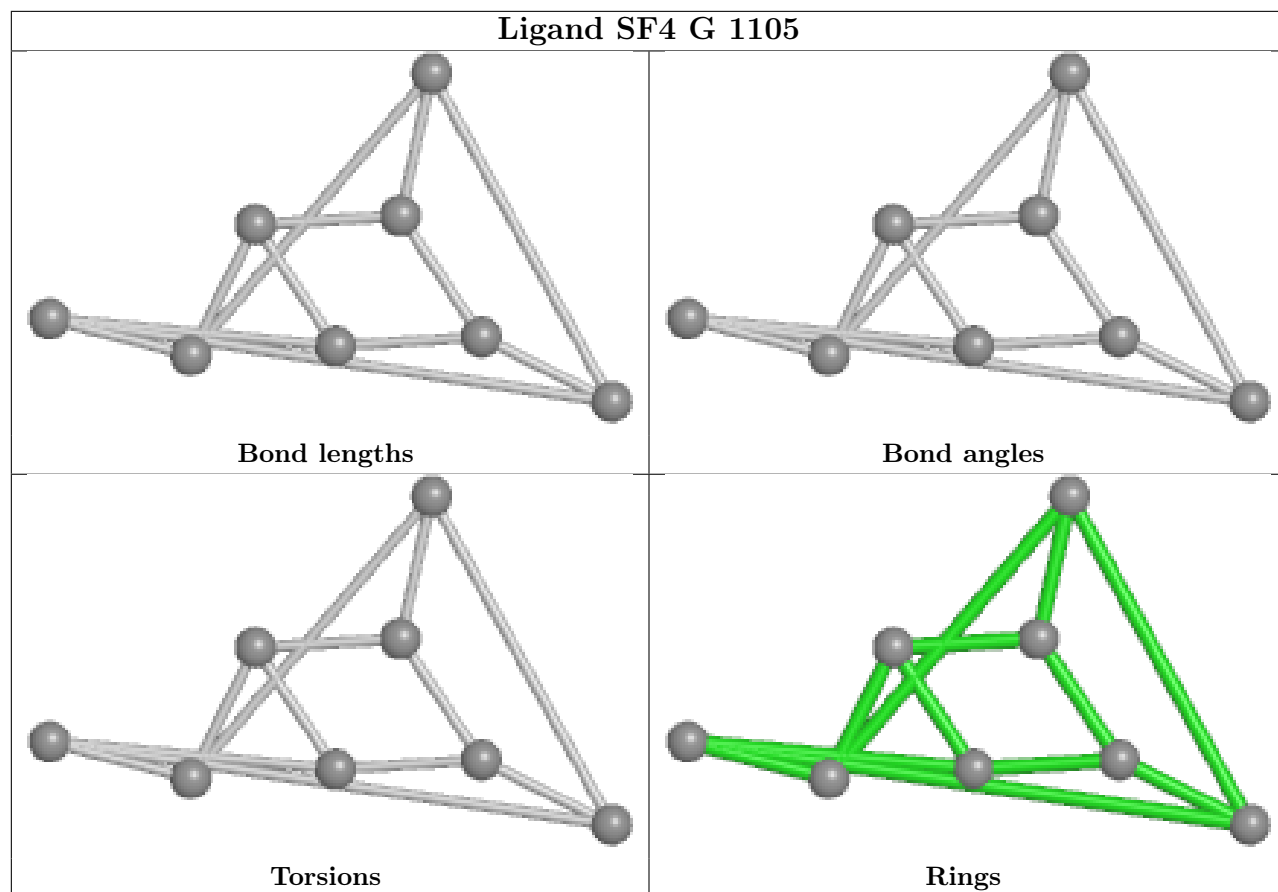


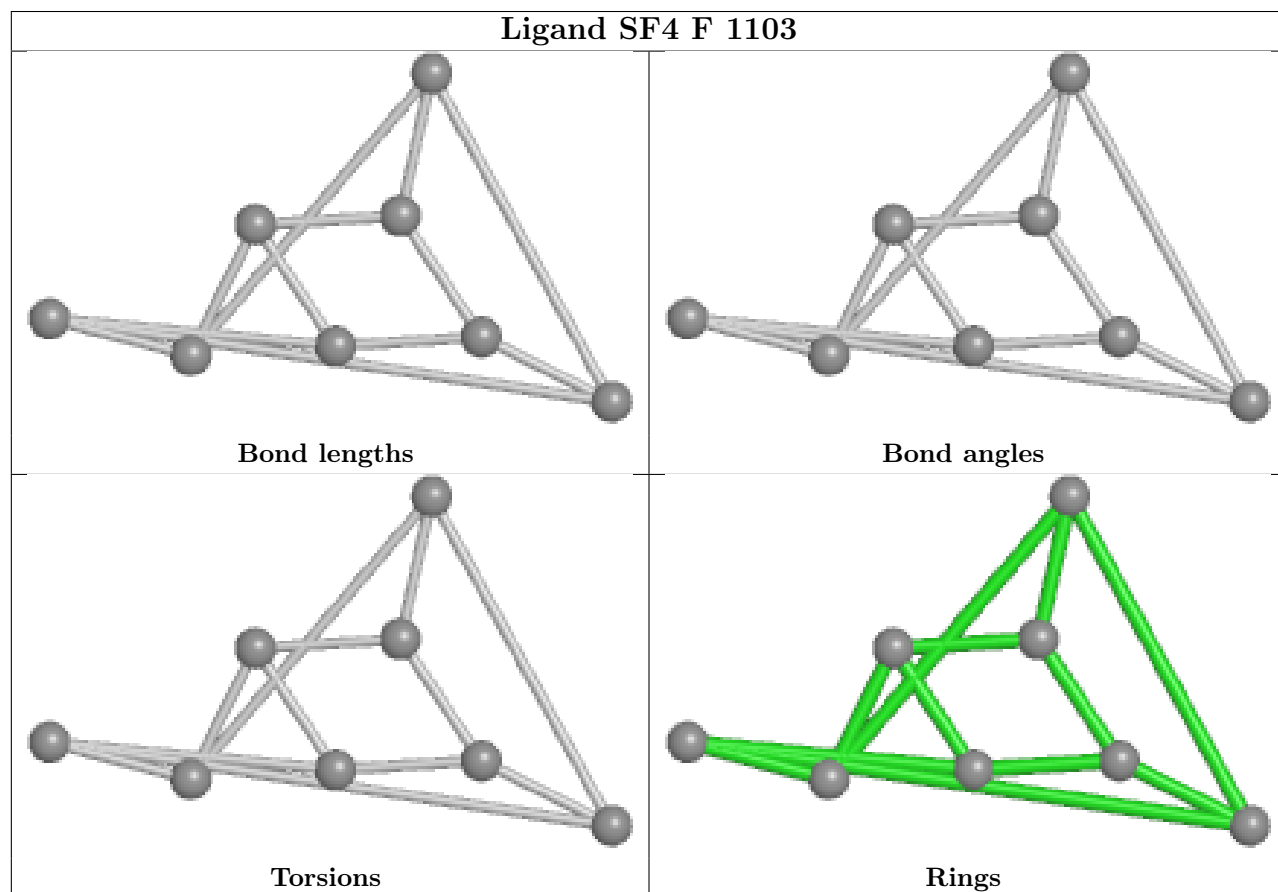
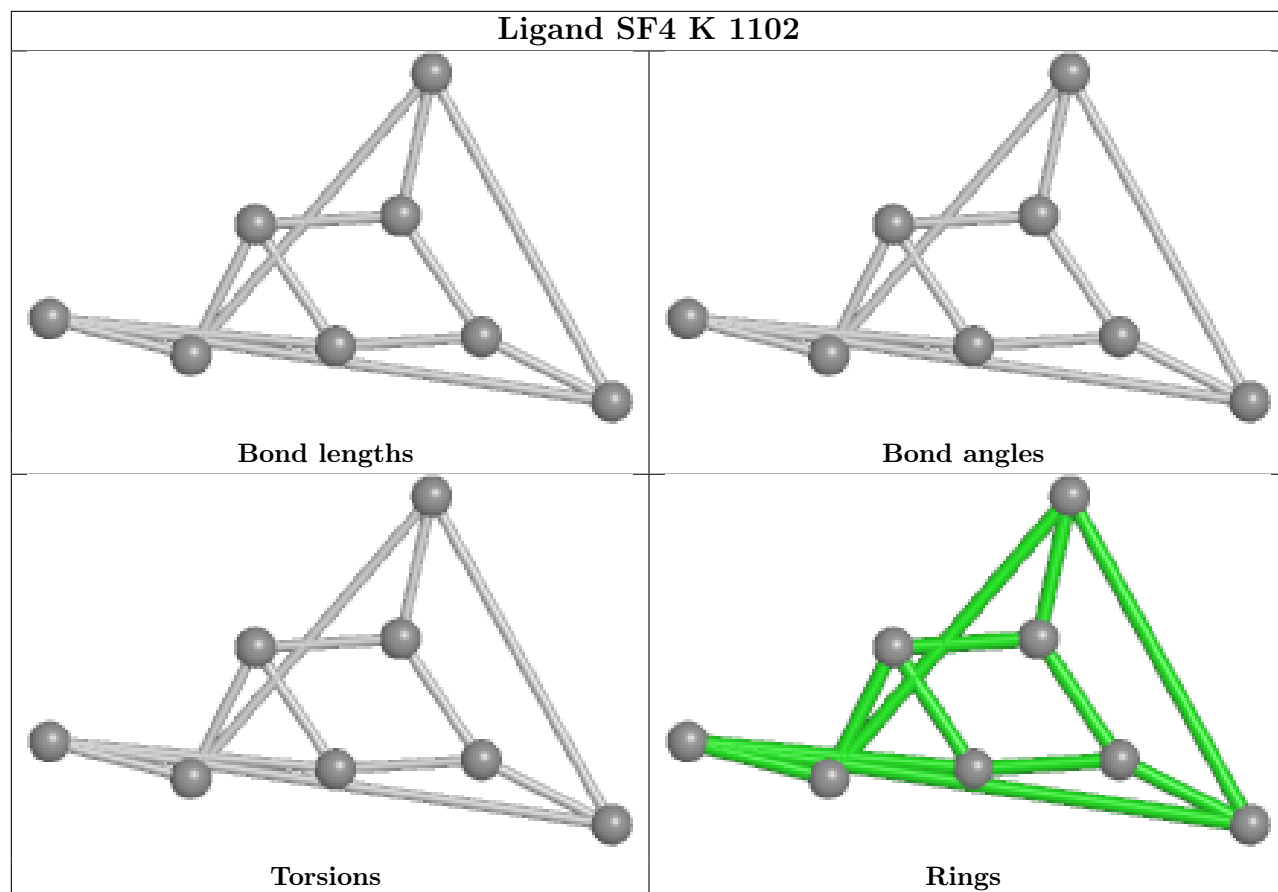


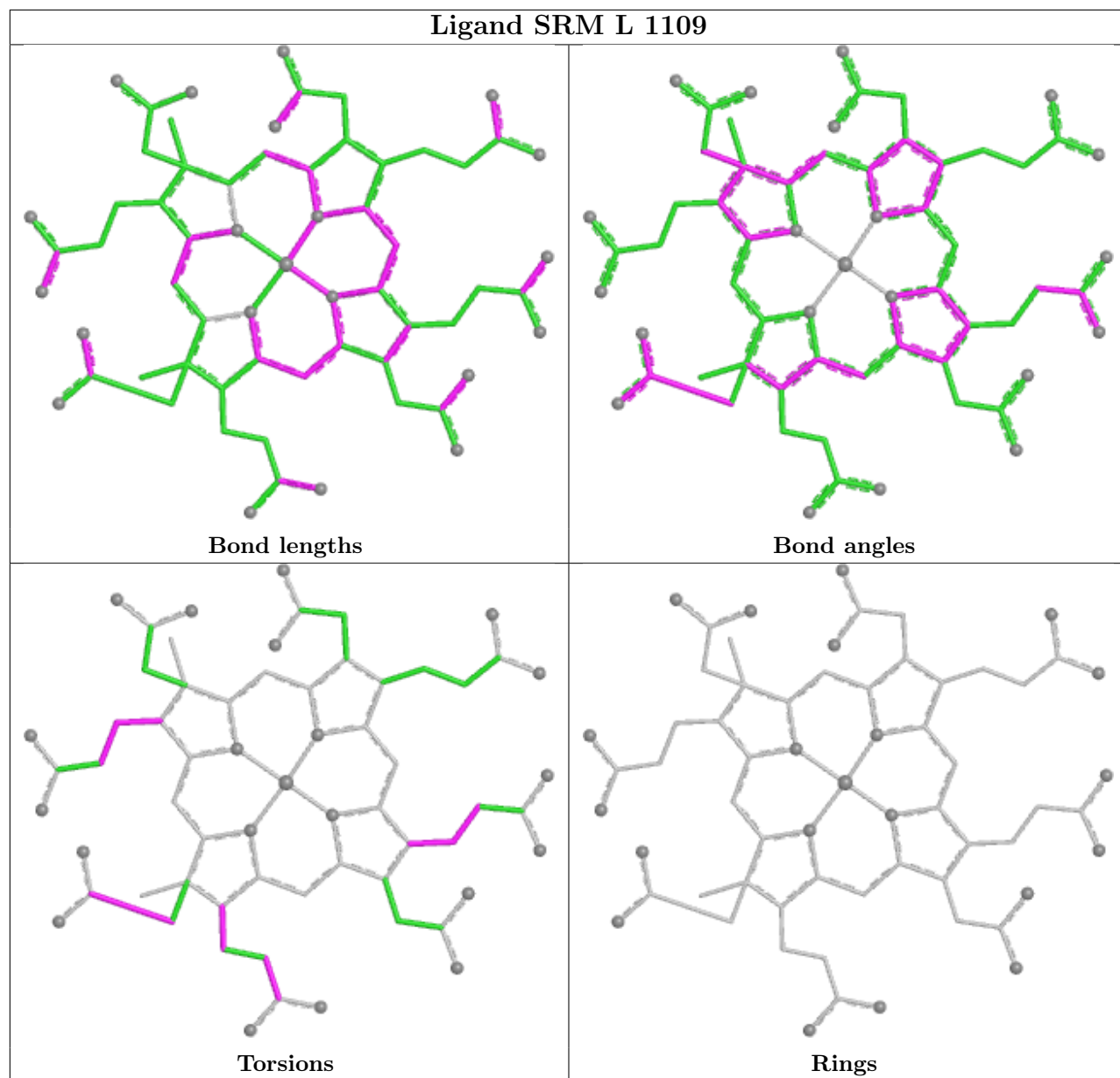


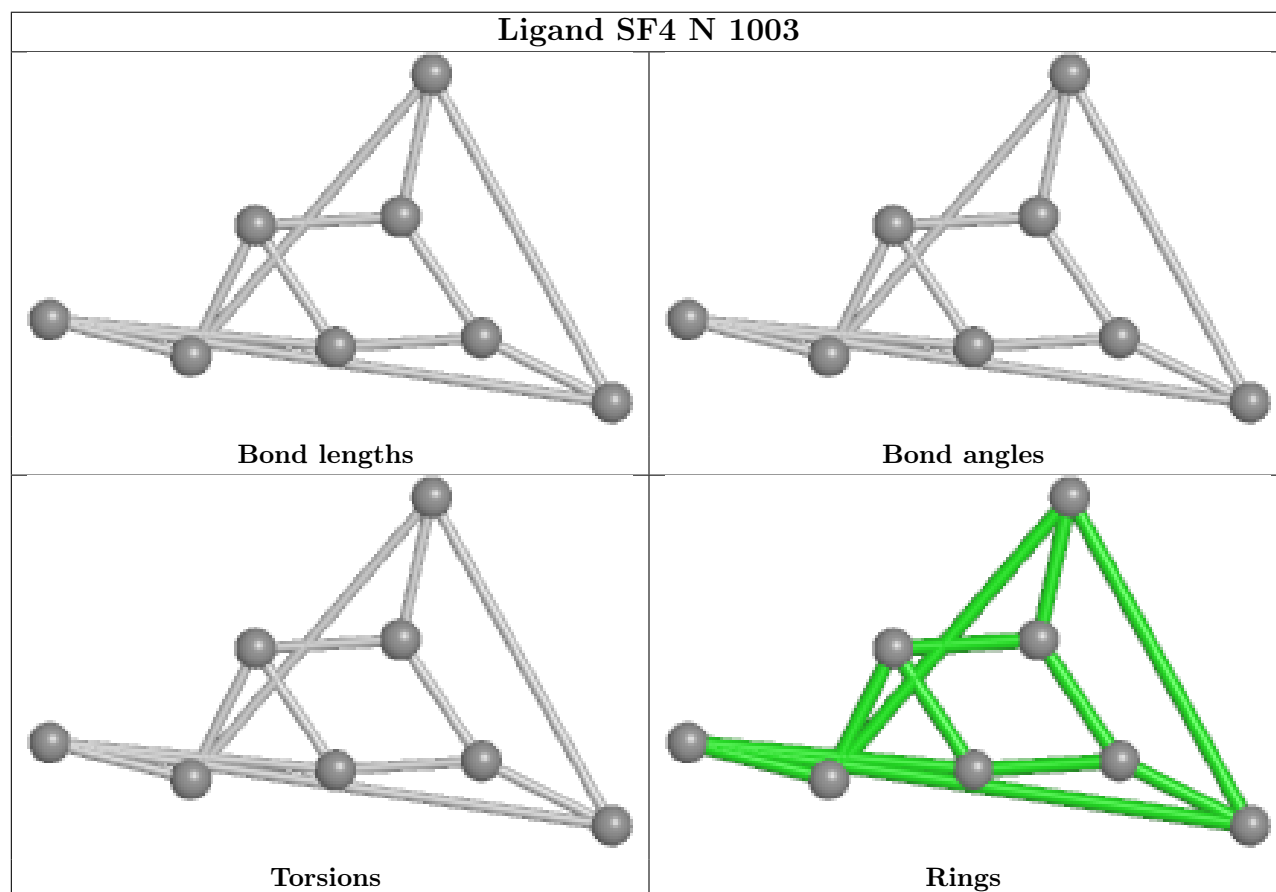
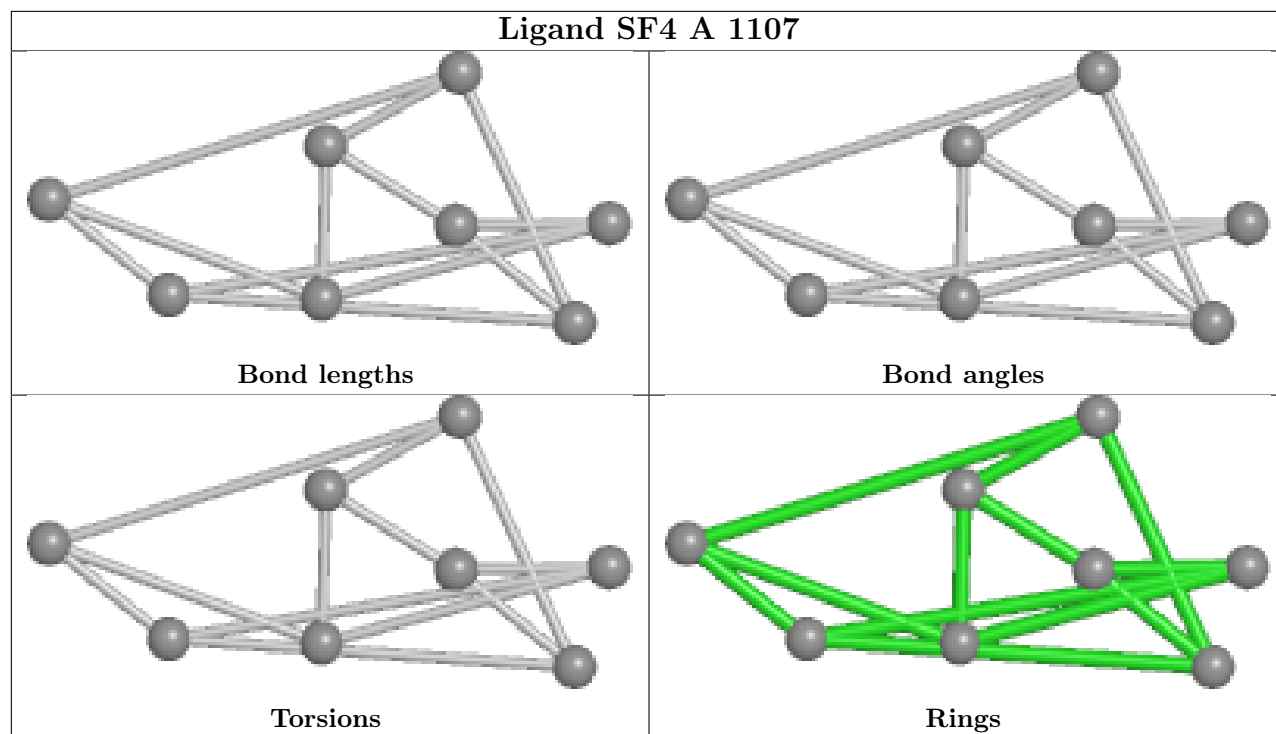


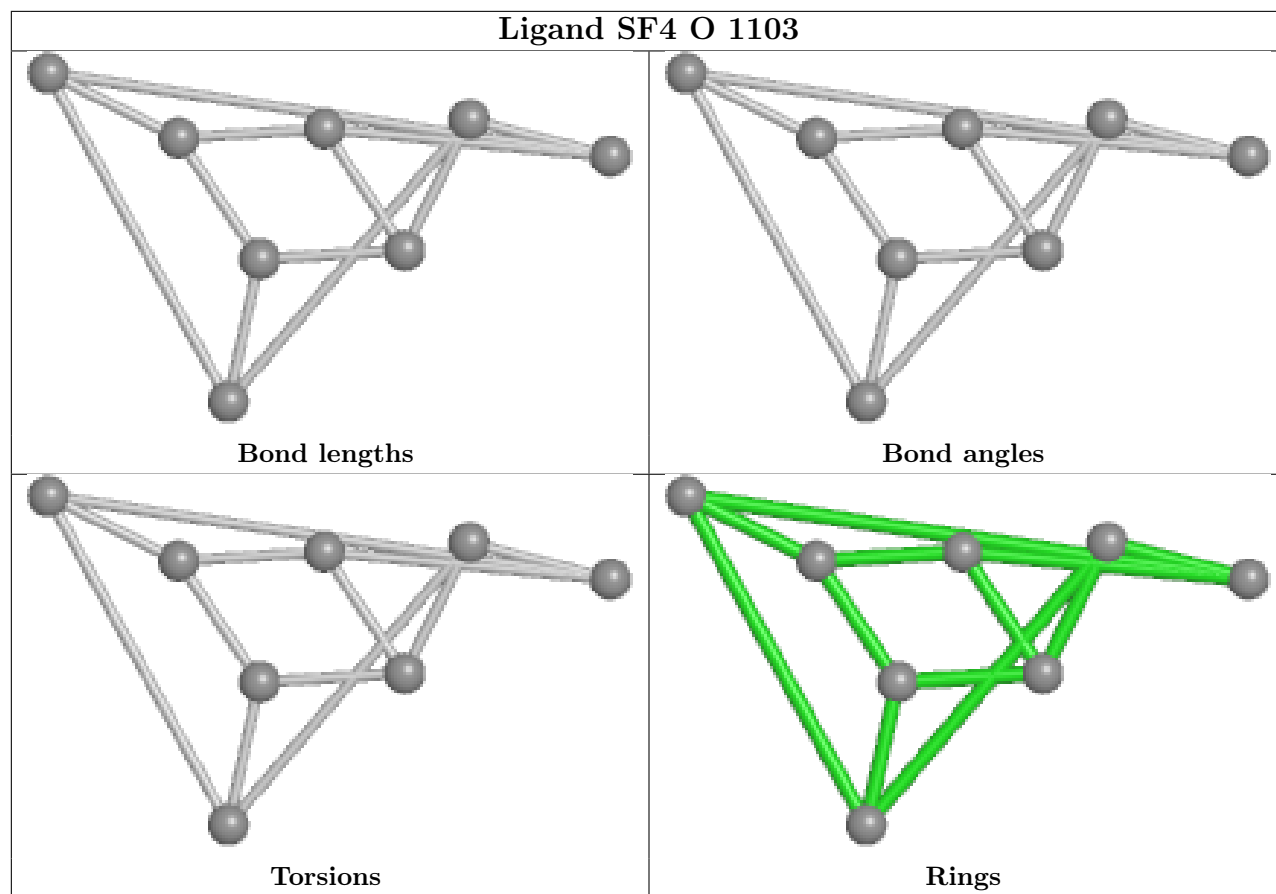
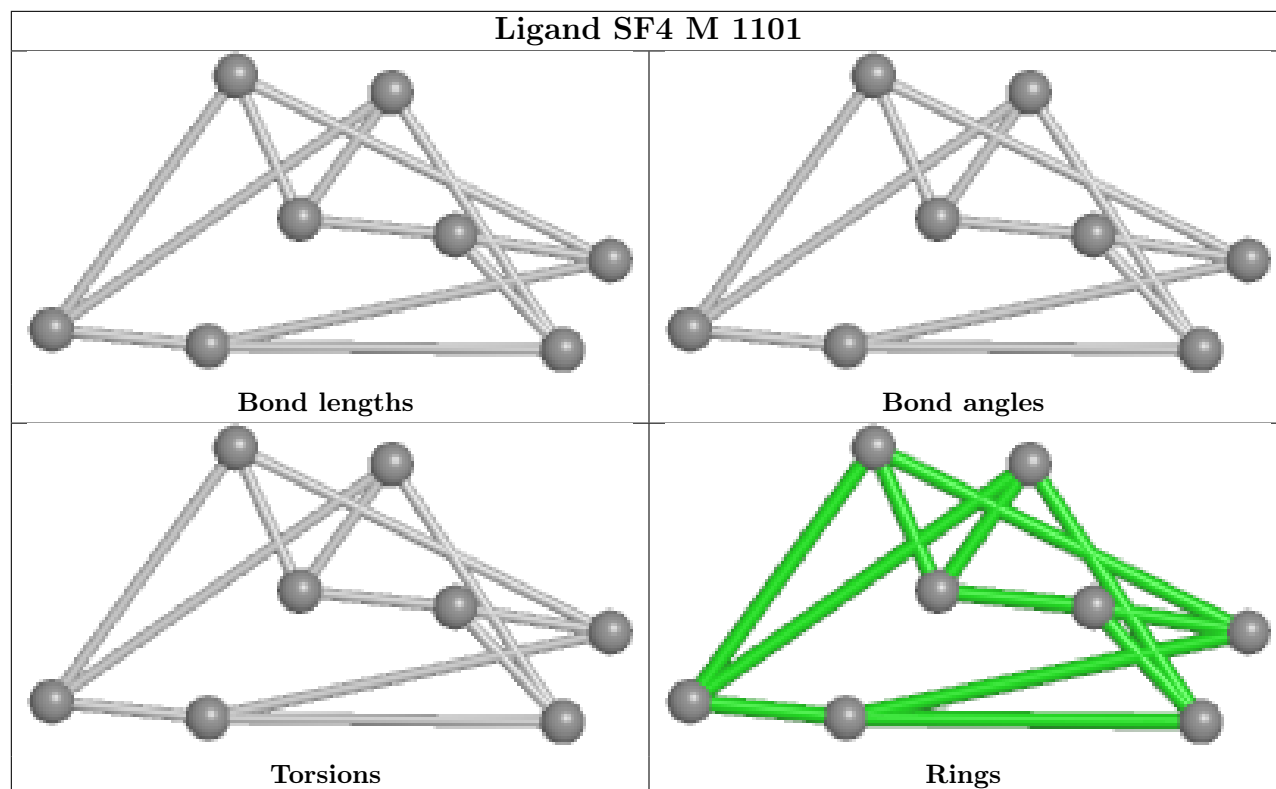


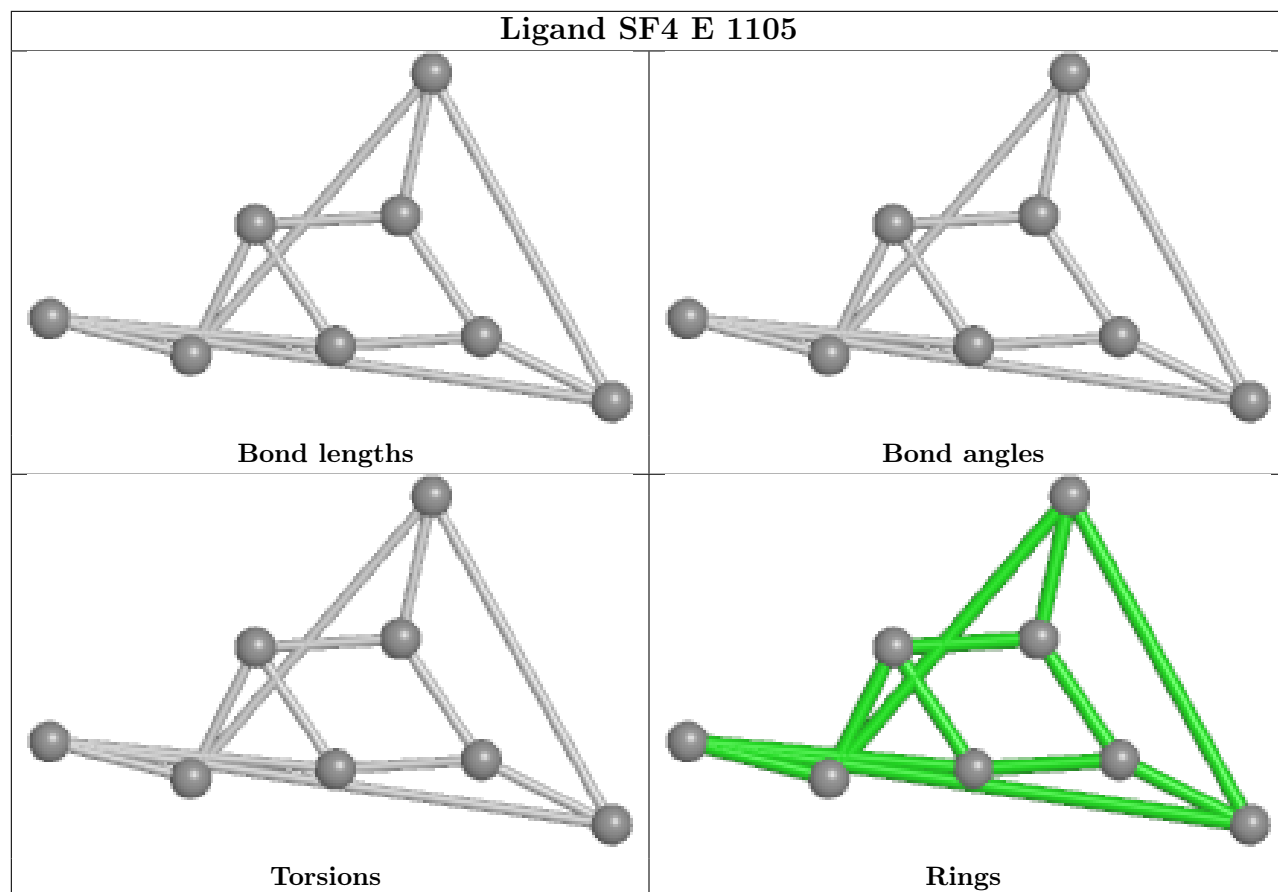


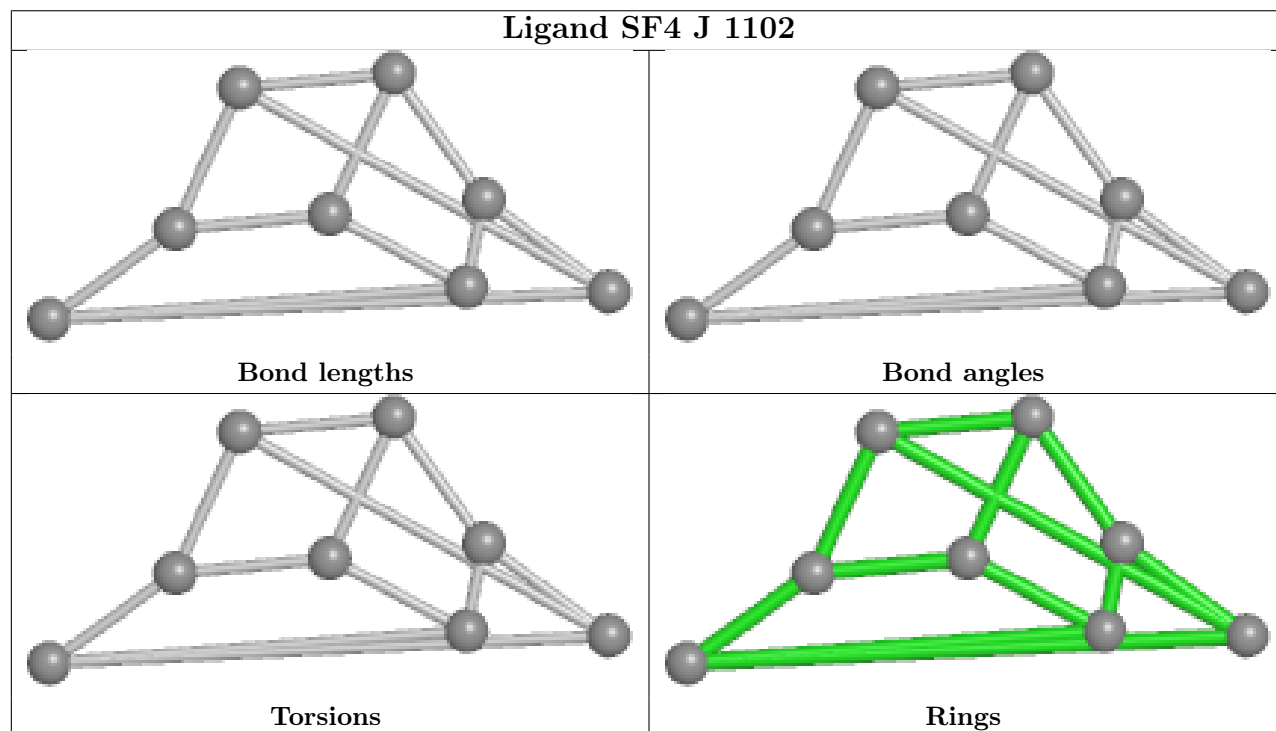
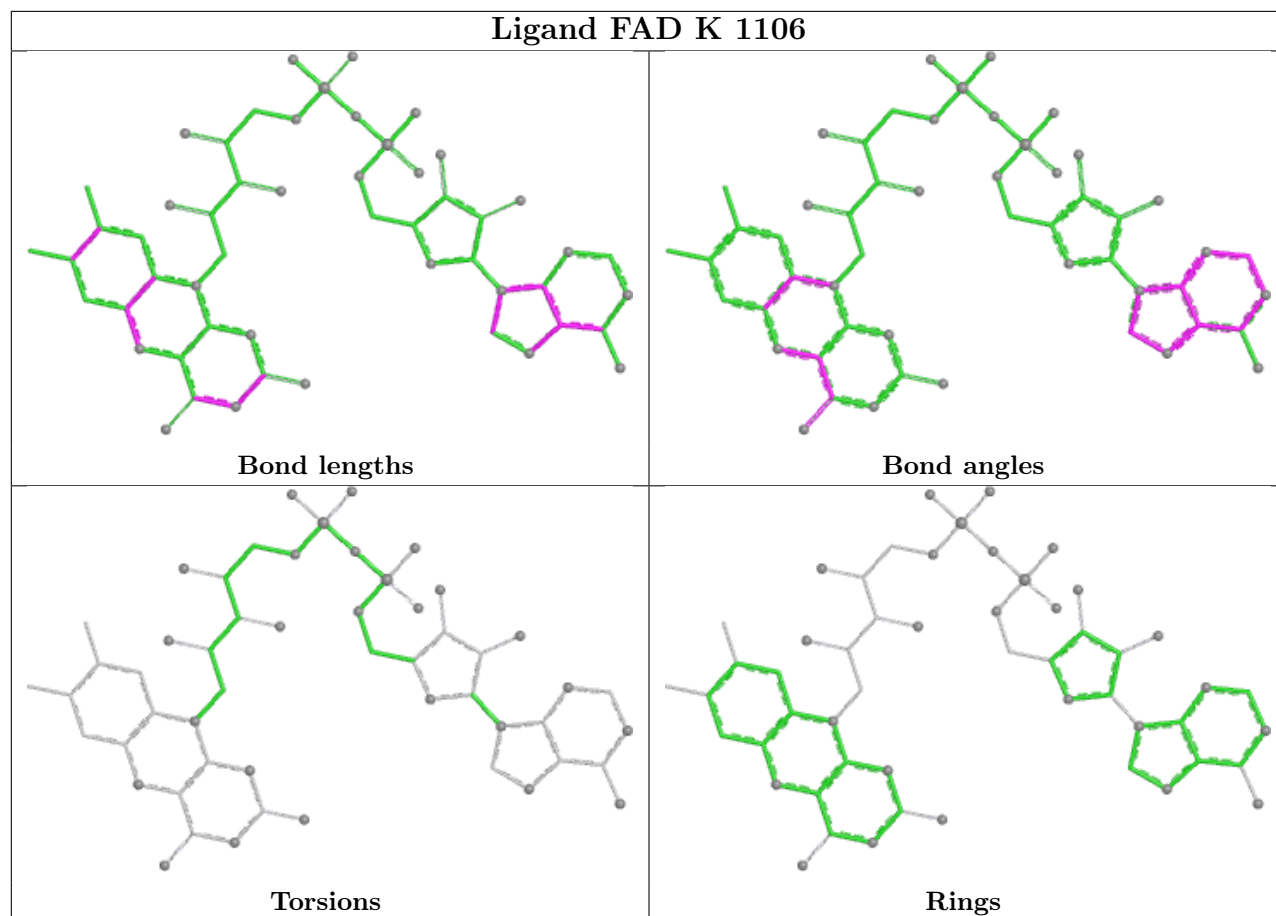


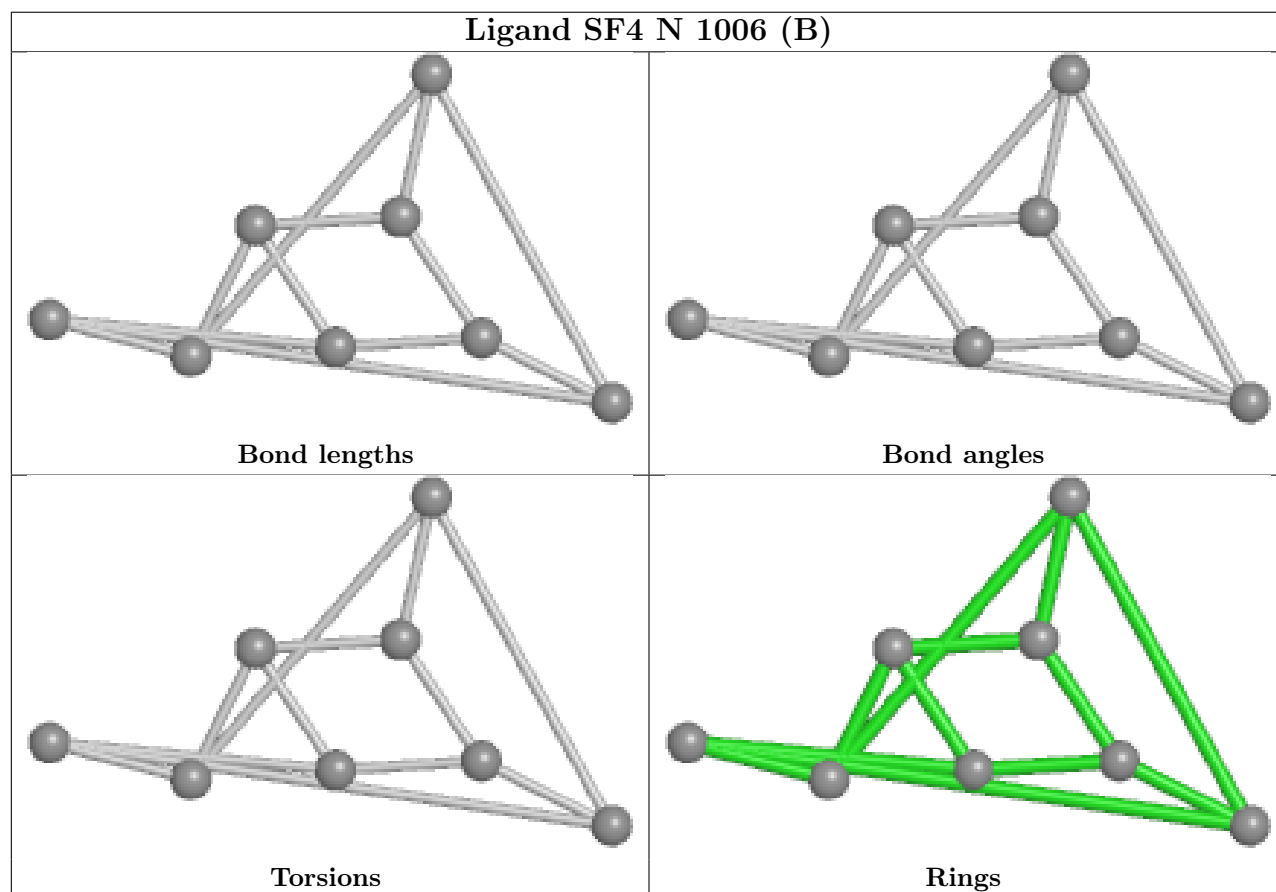
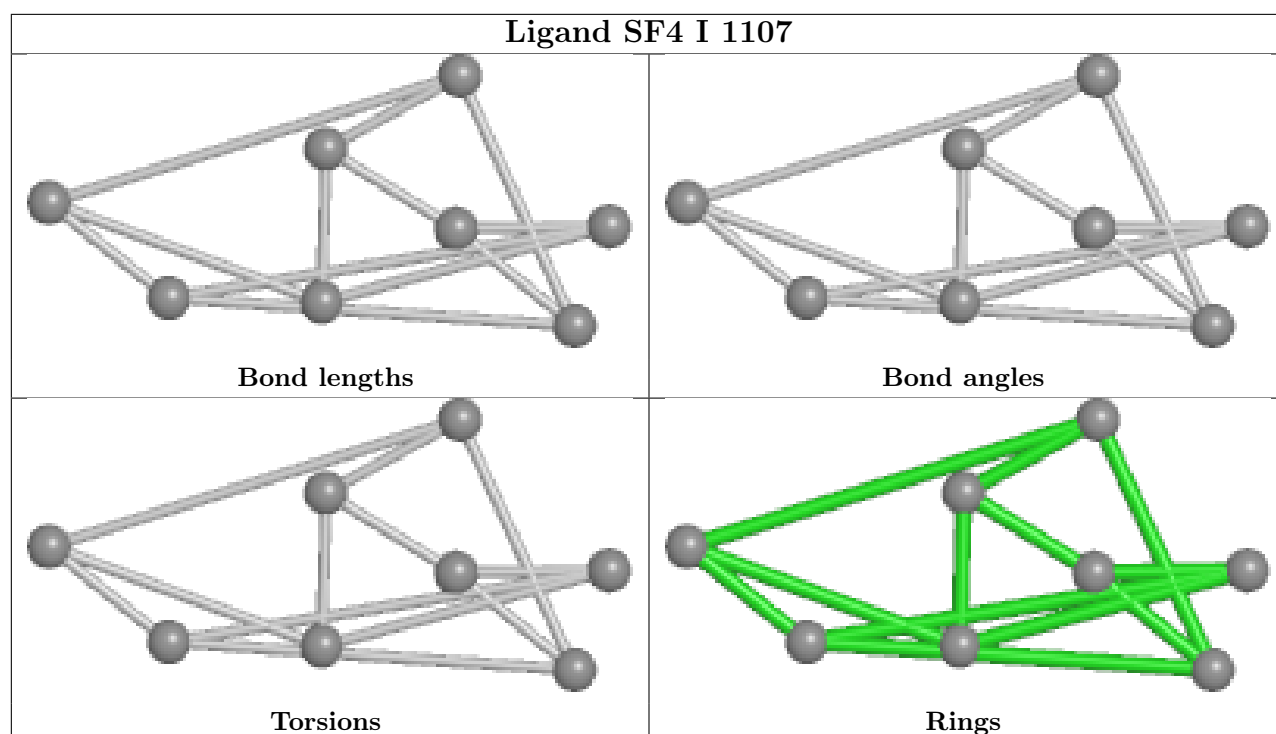




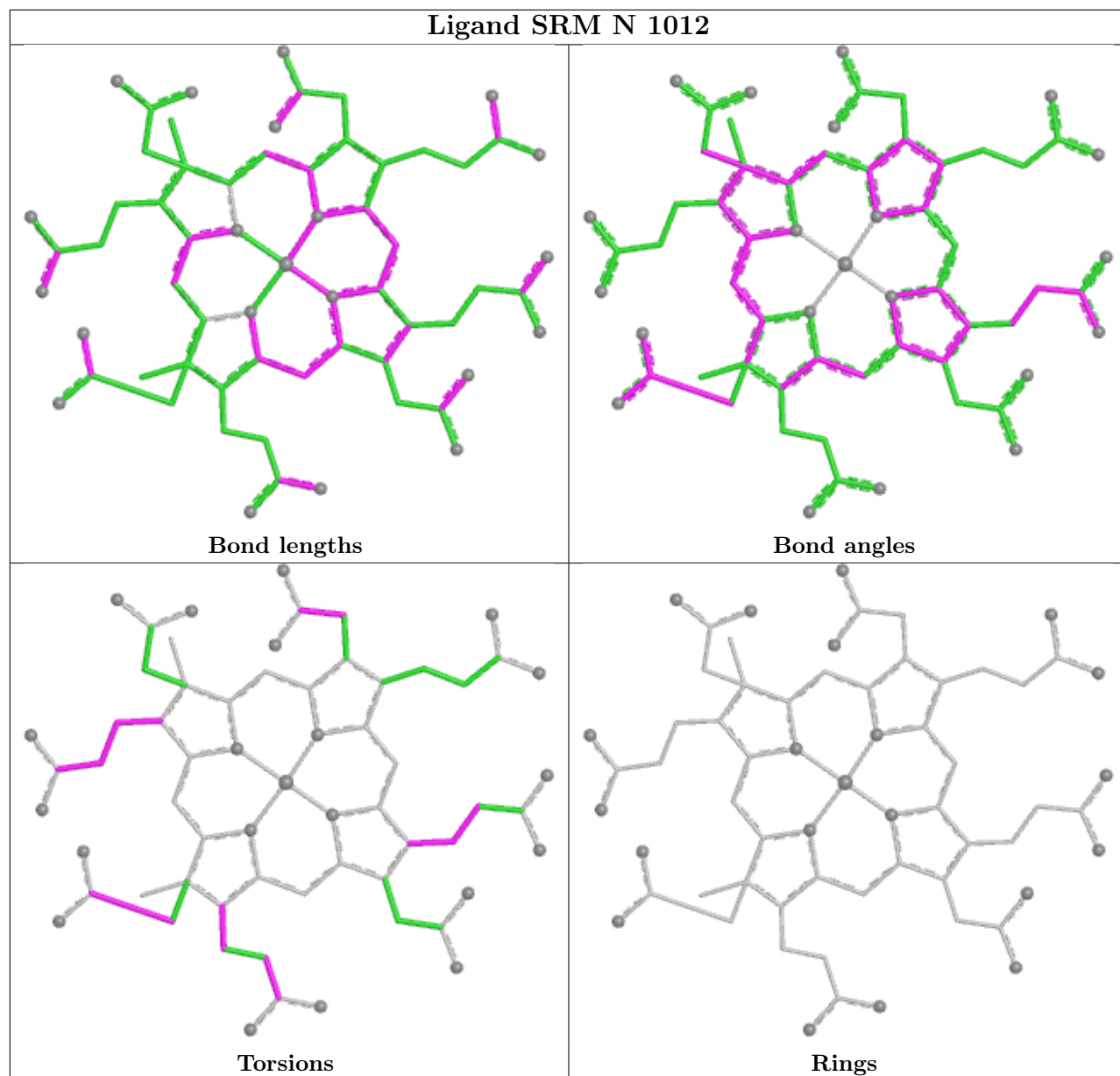




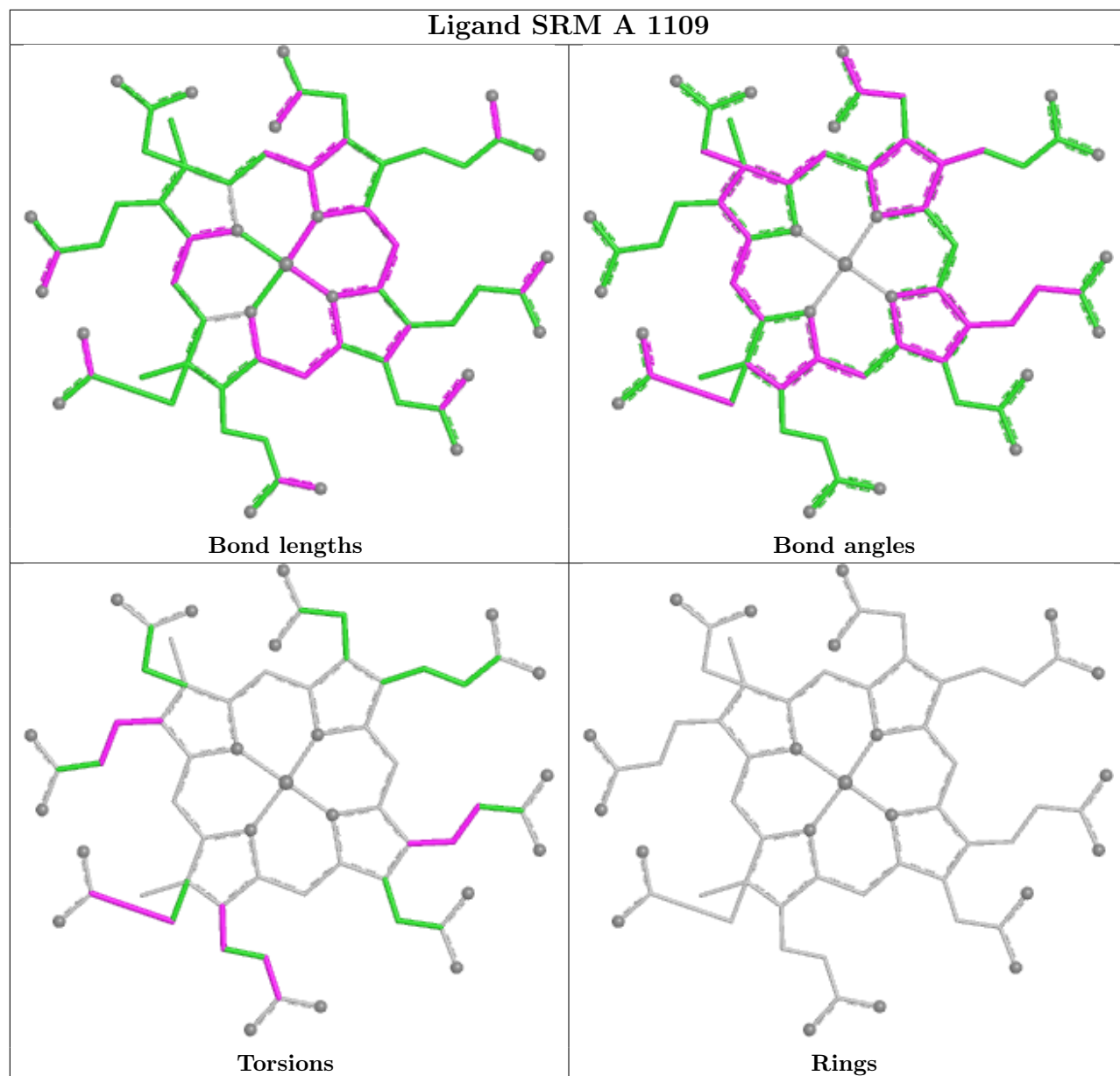




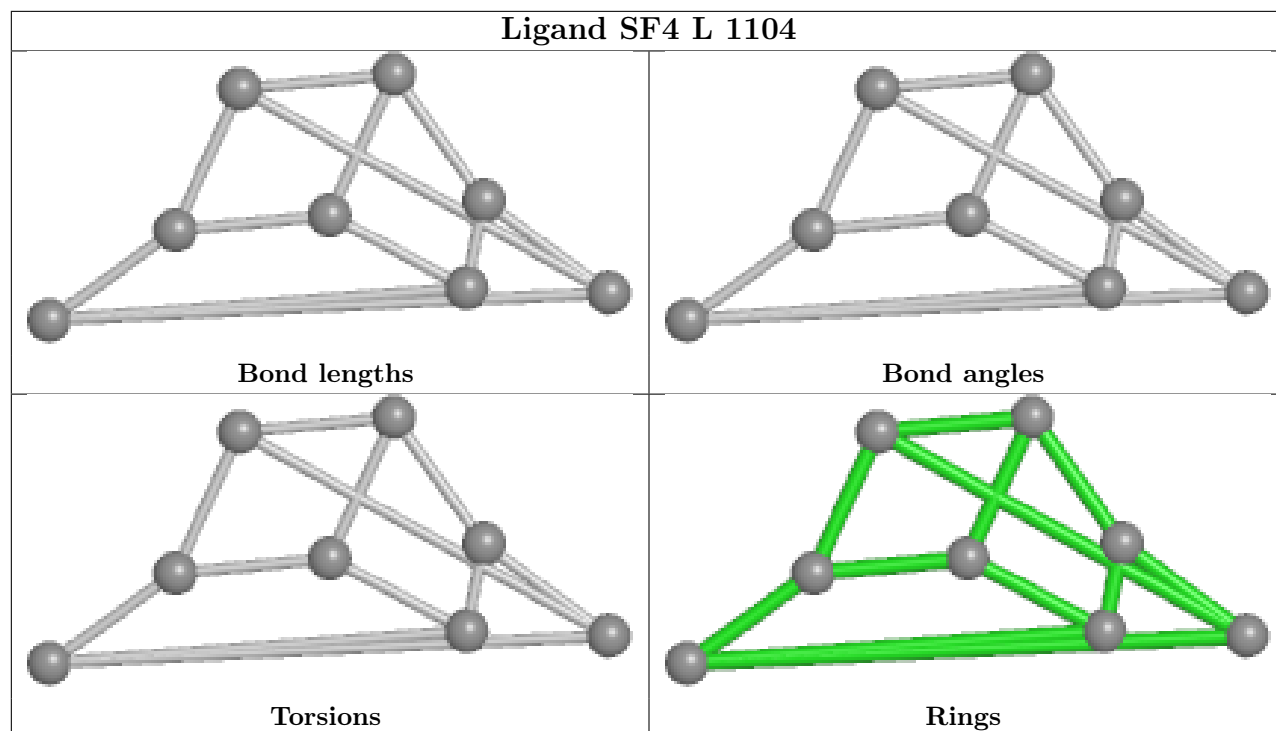
Ligand SRM N 1012



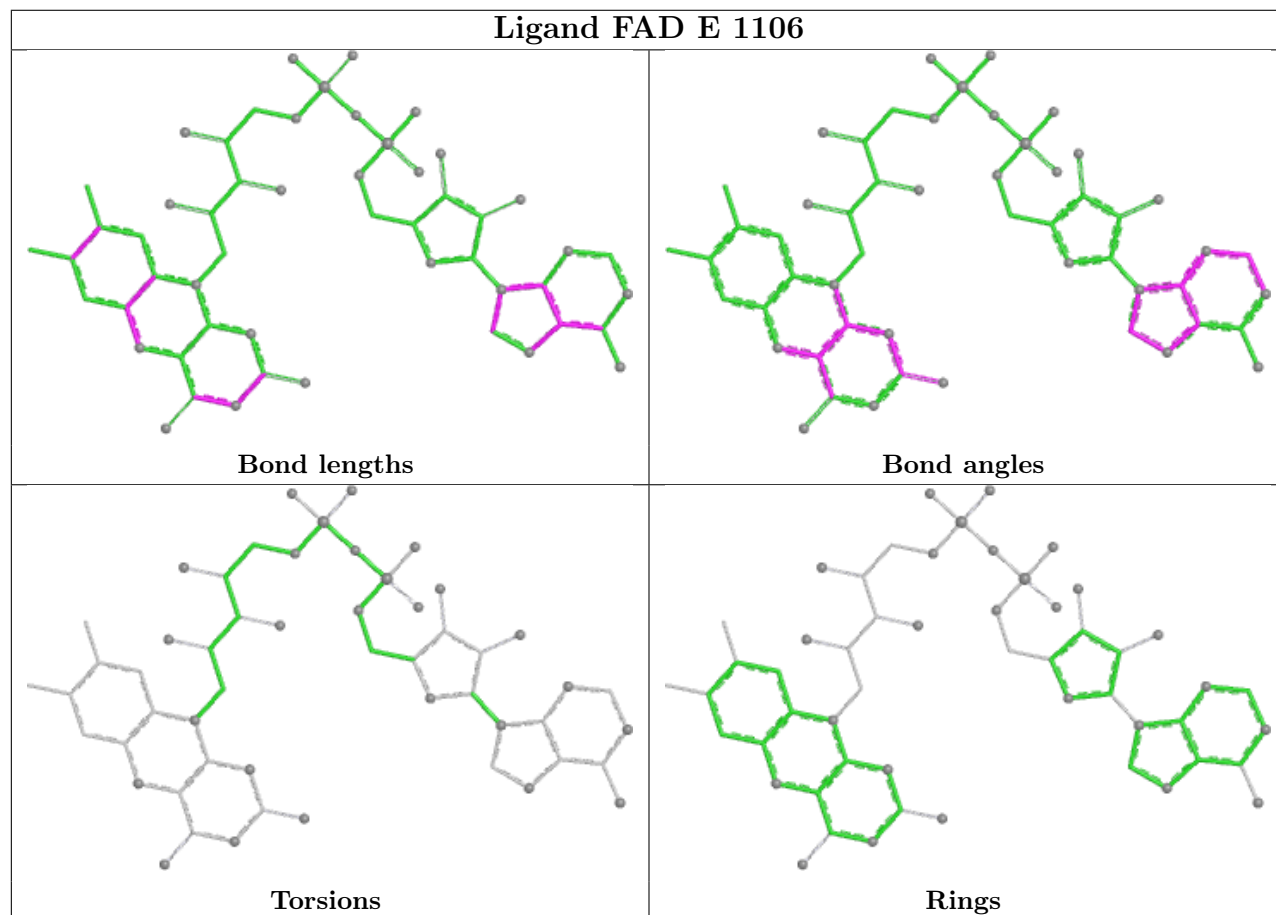
Ligand SRM A 1109

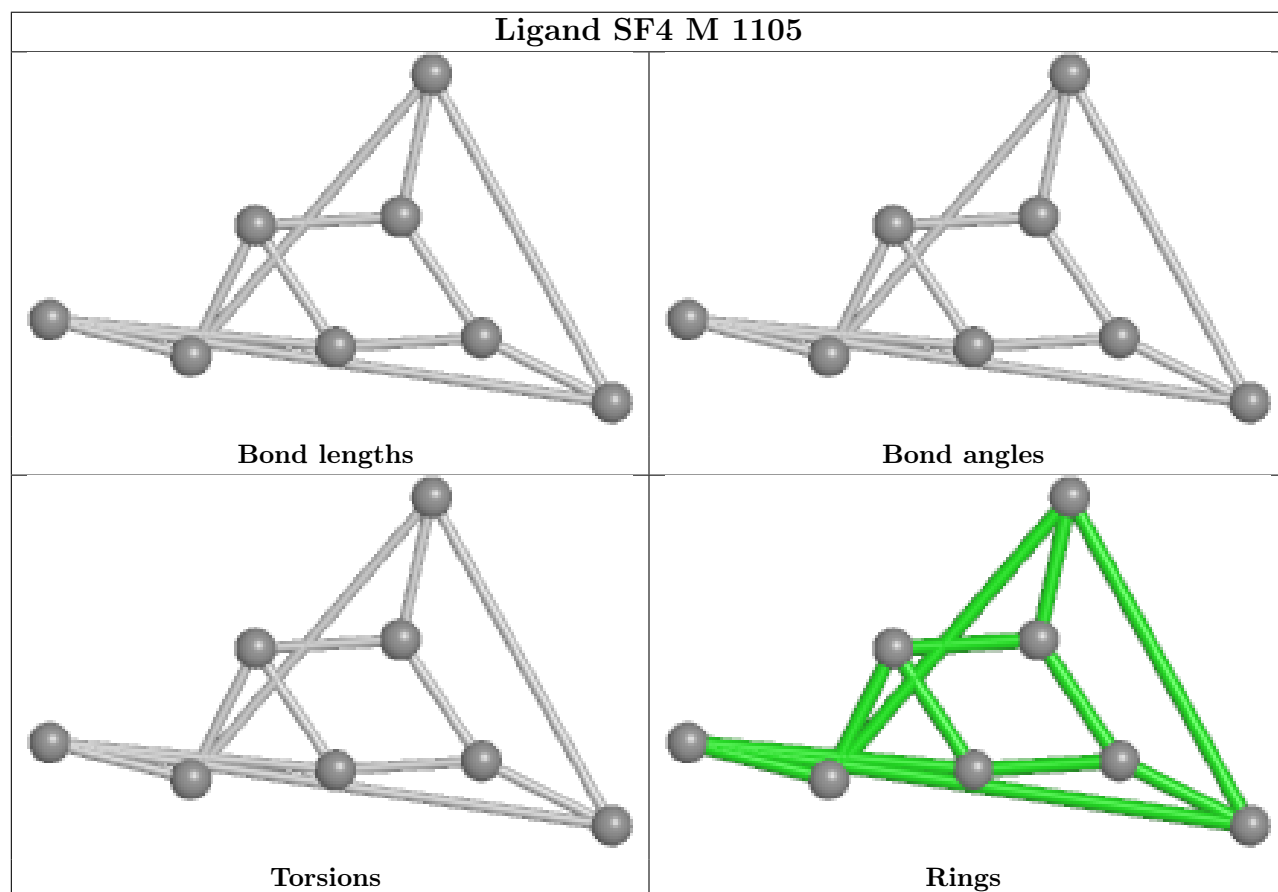
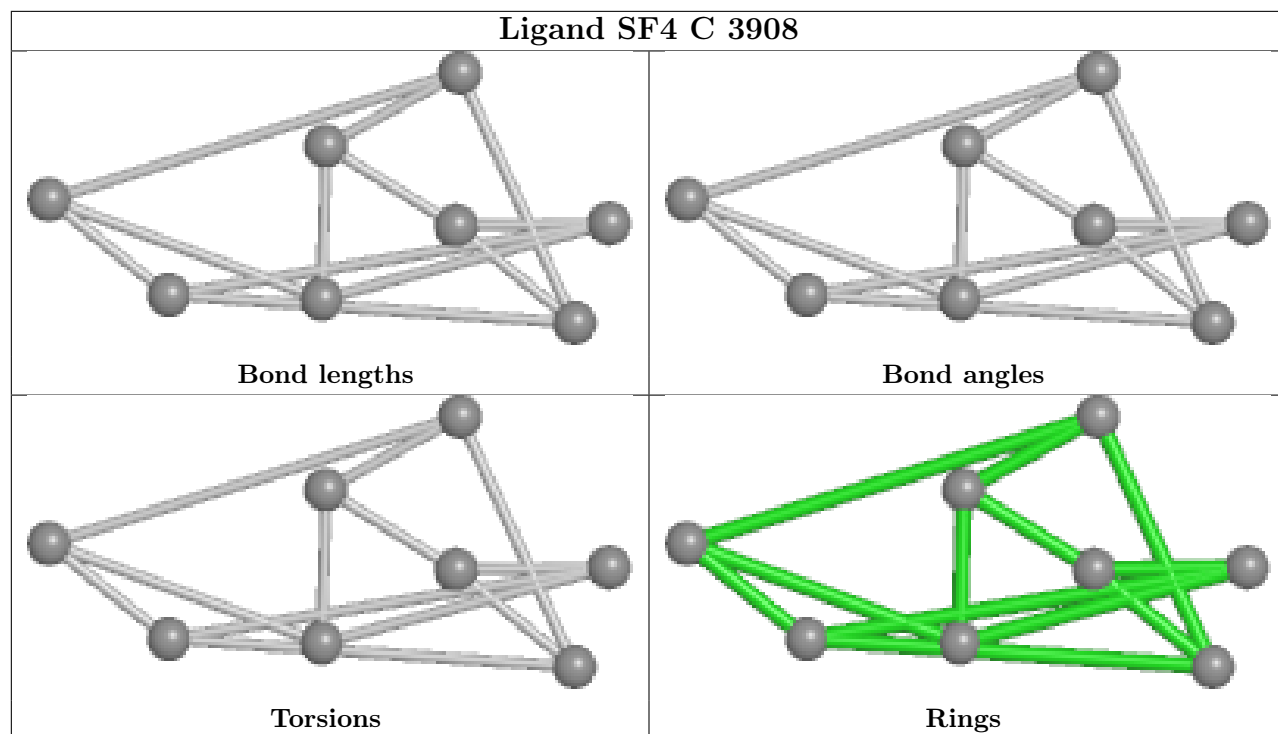


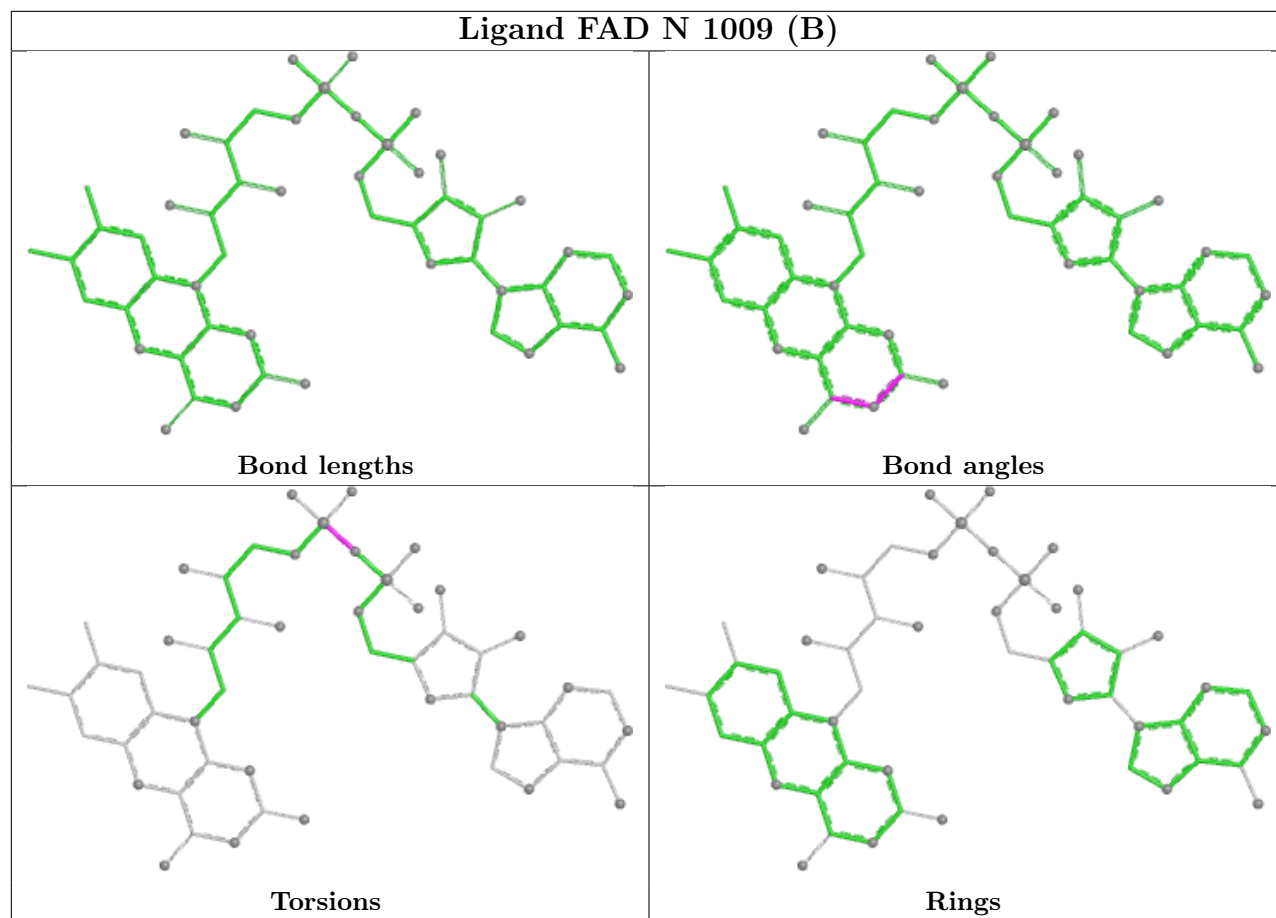
Ligand SF4 L 1104

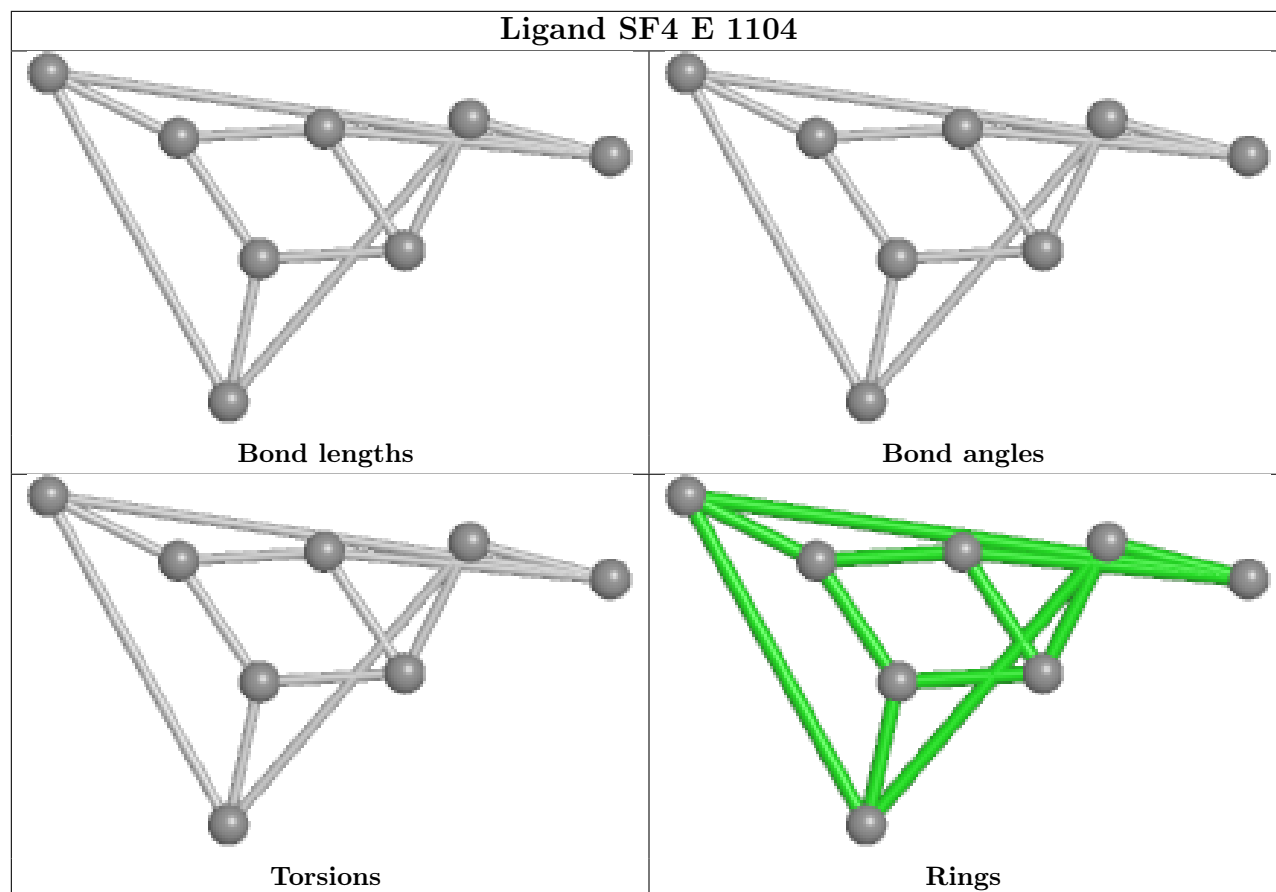


Ligand FAD E 1106









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	618/618 (100%)	-0.26	6 (0%) 79 85	8, 16, 38, 83	4 (0%)
1	B	618/618 (100%)	-0.13	8 (1%) 75 82	9, 18, 42, 83	3 (0%)
1	C	618/618 (100%)	-0.15	5 (0%) 82 87	8, 17, 40, 77	3 (0%)
1	D	617/618 (99%)	0.05	32 (5%) 33 39	9, 20, 53, 94	1 (0%)
1	E	617/618 (99%)	0.25	43 (6%) 22 26	8, 22, 59, 88	2 (0%)
1	F	618/618 (100%)	0.38	41 (6%) 24 29	9, 25, 54, 79	5 (0%)
1	G	618/618 (100%)	-0.07	30 (4%) 35 42	8, 17, 46, 94	3 (0%)
1	H	617/618 (99%)	0.11	34 (5%) 30 37	9, 21, 55, 86	2 (0%)
1	I	618/618 (100%)	-0.03	11 (1%) 67 76	10, 20, 42, 78	3 (0%)
1	J	618/618 (100%)	0.21	36 (5%) 29 34	10, 24, 54, 79	2 (0%)
1	K	617/618 (99%)	-0.20	7 (1%) 78 84	9, 17, 37, 61	2 (0%)
1	L	617/618 (99%)	-0.03	9 (1%) 72 79	9, 20, 45, 61	2 (0%)
1	M	617/618 (99%)	0.02	13 (2%) 63 72	9, 22, 45, 66	1 (0%)
1	N	616/618 (99%)	0.92	130 (21%) 2 3	12, 21, 41, 70	241 (39%)
1	O	617/618 (99%)	0.01	11 (1%) 67 76	9, 21, 44, 65	1 (0%)
1	P	617/618 (99%)	0.53	76 (12%) 8 10	9, 30, 74, 102	1 (0%)
All	All	9878/9888 (99%)	0.10	492 (4%) 34 41	8, 20, 49, 102	276 (2%)

The worst 5 of 492 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	76[A]	TYR	6.2
1	N	305[A]	LEU	6.0
1	N	71[A]	LYS	6.0
1	N	232[A]	GLY	5.8
1	N	97[A]	LEU	5.7

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GOL	J	1114	6/6	0.49	0.28	70,71,72,72	0
9	GOL	B	4217[A]	6/6	0.57	0.25	55,57,57,58	6
11	PEG	N	1014	7/7	0.61	0.24	59,63,65,65	0
9	GOL	B	4218[B]	6/6	0.65	0.23	42,50,52,52	6
12	TRS	I	1119	8/8	0.65	0.19	52,54,56,58	0
4	EDO	A	1117	4/4	0.68	0.25	64,64,64,65	0
9	GOL	P	1112	6/6	0.68	0.22	69,69,71,71	0
4	EDO	L	1112	4/4	0.69	0.32	63,63,64,65	0
6	SO4	F	1117	5/5	0.69	0.18	88,88,89,89	0
4	EDO	J	1111	4/4	0.71	0.23	51,53,55,56	0
9	GOL	F	1114	6/6	0.72	0.20	56,56,57,58	0
9	GOL	I	1117	6/6	0.72	0.23	60,61,62,63	0
4	EDO	A	1114	4/4	0.72	0.28	57,57,57,58	0
6	SO4	P	1116	5/5	0.72	0.19	91,91,92,92	0
4	EDO	M	1122	4/4	0.72	0.21	57,58,58,59	0
6	SO4	D	4621	5/5	0.72	0.19	93,93,94,94	0
9	GOL	M	1114	6/6	0.73	0.22	53,54,54,56	0
4	EDO	F	1110[B]	4/4	0.73	0.15	12,14,14,14	4
10	LI	L	1118	1/1	0.74	0.21	11,11,11,11	0
9	GOL	B	4224	6/6	0.74	0.20	52,55,57,57	0
6	SO4	F	1116	5/5	0.74	0.18	88,88,88,89	0
4	EDO	D	4615	4/4	0.75	0.21	50,50,50,51	0
9	GOL	O	1116	6/6	0.75	0.17	59,60,61,61	0
4	EDO	D	4617	4/4	0.75	0.23	53,53,54,54	0
4	EDO	C	3917	4/4	0.76	0.21	59,60,61,63	0
4	EDO	O	1117	4/4	0.76	0.18	49,50,50,51	0
4	EDO	G	1115	4/4	0.76	0.20	45,45,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	I	1113	4/4	0.77	0.19	41,41,42,43	0
6	SO4	J	1119	5/5	0.77	0.19	86,87,87,87	0
4	EDO	M	1118	4/4	0.77	0.18	51,52,53,53	0
4	EDO	M	1116	4/4	0.78	0.21	45,45,45,46	0
4	EDO	J	1110	4/4	0.78	0.24	53,54,54,55	0
4	EDO	G	1120	4/4	0.78	0.17	37,38,39,40	0
4	EDO	N	1013	4/4	0.78	0.23	49,50,51,53	0
6	SO4	L	1115	5/5	0.78	0.16	86,86,87,87	0
4	EDO	B	4221	4/4	0.78	0.19	58,59,59,60	0
10	LI	F	1121	1/1	0.79	0.32	18,18,18,18	0
6	SO4	K	1119	5/5	0.79	0.16	67,68,70,71	0
4	EDO	M	1113	4/4	0.79	0.21	47,47,48,49	0
9	GOL	E	1114	6/6	0.79	0.20	56,59,60,60	0
6	SO4	H	4414	5/5	0.80	0.17	75,75,76,77	0
9	GOL	C	3901	6/6	0.80	0.20	57,59,61,62	0
4	EDO	E	1112	4/4	0.80	0.17	46,47,47,47	0
10	LI	P	1120	1/1	0.80	0.18	11,11,11,11	0
9	GOL	N	1015	6/6	0.80	0.19	56,56,57,59	0
6	SO4	M	1127	5/5	0.80	0.16	93,93,94,94	0
4	EDO	K	1113	4/4	0.81	0.21	37,39,40,40	0
4	EDO	B	4216	4/4	0.81	0.15	38,38,40,40	0
4	EDO	F	1113	4/4	0.81	0.20	47,47,48,48	0
4	EDO	I	1116	4/4	0.81	0.21	45,46,47,48	0
4	EDO	E	1116	4/4	0.81	0.19	39,40,43,45	0
4	EDO	G	1117	4/4	0.81	0.20	63,63,64,64	0
4	EDO	M	1123	4/4	0.81	0.16	47,47,48,49	0
4	EDO	K	1114	4/4	0.82	0.16	50,51,53,53	0
4	EDO	D	4618	4/4	0.82	0.18	60,60,61,62	0
4	EDO	B	4220[B]	4/4	0.82	0.19	47,47,48,49	4
4	EDO	G	1116	4/4	0.82	0.21	67,67,67,67	0
4	EDO	B	4211	4/4	0.82	0.19	40,42,43,47	0
11	PEG	K	1115	7/7	0.82	0.17	41,45,50,50	0
4	EDO	J	1116	4/4	0.82	0.21	58,60,60,60	0
4	EDO	C	3916	4/4	0.82	0.17	51,51,52,53	0
4	EDO	D	4613	4/4	0.83	0.16	51,53,53,54	0
6	SO4	F	1118	5/5	0.83	0.15	101,102,102,102	0
4	EDO	H	4413	4/4	0.83	0.21	45,45,45,45	0
11	PEG	M	1120	7/7	0.83	0.18	56,58,59,59	0
4	EDO	O	1113	4/4	0.83	0.18	52,53,54,55	0
9	GOL	J	1117[A]	6/6	0.83	0.15	43,49,49,50	0
4	EDO	G	1111	4/4	0.84	0.18	44,45,46,47	0
4	EDO	M	1117	4/4	0.84	0.15	51,51,52,52	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
9	GOL	C	3913	6/6	0.84	0.15	43,45,47,49	0
4	EDO	P	1114	4/4	0.84	0.16	58,58,58,59	0
6	SO4	D	4620	5/5	0.84	0.17	79,79,80,80	0
4	EDO	E	1111	4/4	0.84	0.19	43,43,45,46	0
4	EDO	G	1118	4/4	0.84	0.17	53,54,54,54	0
4	EDO	J	1113	4/4	0.84	0.17	52,52,52,53	0
9	GOL	K	1117	6/6	0.84	0.15	38,41,43,46	0
4	EDO	J	1115	4/4	0.84	0.19	56,56,56,57	0
4	EDO	M	1119	4/4	0.85	0.18	47,47,48,48	0
4	EDO	E	1113	4/4	0.85	0.18	54,54,55,55	0
4	EDO	B	4213	4/4	0.85	0.16	36,37,38,38	0
12	TRS	H	4401	8/8	0.85	0.14	34,46,50,51	0
4	EDO	G	1121	4/4	0.85	0.17	39,39,41,42	0
4	EDO	I	1114	4/4	0.86	0.13	50,50,50,51	0
11	PEG	M	1115	7/7	0.86	0.15	36,39,42,45	0
4	EDO	M	1112	4/4	0.86	0.15	46,46,46,46	0
4	EDO	I	1118	4/4	0.86	0.21	52,52,54,54	0
4	EDO	I	1115	4/4	0.86	0.17	64,64,64,65	0
4	EDO	P	1113	4/4	0.86	0.15	46,47,47,48	0
4	EDO	M	1124	4/4	0.87	0.16	51,51,51,51	0
9	GOL	P	1111	6/6	0.87	0.17	53,54,55,57	0
4	EDO	B	4219[A]	4/4	0.87	0.17	45,45,46,46	4
4	EDO	F	1111	4/4	0.87	0.18	35,37,37,37	0
4	EDO	C	3914	4/4	0.88	0.15	40,41,42,43	0
11	PEG	D	4601	7/7	0.88	0.15	40,45,48,49	0
4	EDO	O	1115	4/4	0.88	0.13	44,46,48,50	0
4	EDO	B	4201	4/4	0.88	0.13	45,46,46,48	0
4	EDO	O	1118	4/4	0.88	0.15	40,40,41,42	0
4	EDO	A	1113	4/4	0.88	0.14	30,31,32,33	0
4	EDO	A	1118	4/4	0.88	0.14	47,48,49,49	0
4	EDO	B	4215	4/4	0.88	0.15	49,50,52,53	0
4	EDO	B	4214	4/4	0.89	0.14	29,30,30,32	0
4	EDO	C	3915	4/4	0.89	0.15	43,43,45,46	0
4	EDO	H	4412	4/4	0.89	0.14	46,46,46,46	0
4	EDO	J	1112	4/4	0.89	0.18	38,39,39,39	0
4	EDO	G	1114	4/4	0.89	0.13	48,48,49,49	0
4	EDO	A	1110	4/4	0.89	0.16	47,48,48,48	0
4	EDO	E	1117	4/4	0.89	0.14	29,31,31,32	0
4	EDO	B	4222[A]	4/4	0.89	0.13	25,28,29,31	4
4	EDO	C	3918	4/4	0.89	0.16	51,52,52,52	0
4	EDO	K	1116	4/4	0.89	0.13	42,42,44,44	0
4	EDO	N	1010	4/4	0.89	0.15	24,24,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	D	4616	4/4	0.90	0.11	52,52,53,53	0
4	EDO	D	4612	4/4	0.90	0.13	46,47,47,47	0
10	LI	C	3923	1/1	0.90	0.25	18,18,18,18	0
4	EDO	A	1116	4/4	0.90	0.12	46,47,48,50	0
9	GOL	G	1119[A]	6/6	0.90	0.12	37,43,45,45	0
9	GOL	I	1111	6/6	0.90	0.16	40,45,46,47	0
6	SO4	M	1126	5/5	0.90	0.13	70,71,72,73	0
4	EDO	A	1115	4/4	0.90	0.13	49,49,50,51	0
4	EDO	O	1111	4/4	0.90	0.14	19,21,24,25	0
4	EDO	O	1112	4/4	0.90	0.12	42,42,42,43	0
4	EDO	G	1112	4/4	0.90	0.13	45,46,47,48	0
4	EDO	G	1113	4/4	0.90	0.12	38,38,39,40	0
4	EDO	M	1110	4/4	0.90	0.13	35,37,39,40	0
4	EDO	B	4223	4/4	0.91	0.12	52,52,52,53	0
4	EDO	A	1111	4/4	0.91	0.12	17,20,23,24	0
4	EDO	D	4614	4/4	0.91	0.12	49,49,49,50	0
4	EDO	I	1112	4/4	0.91	0.13	48,48,49,50	0
6	SO4	H	4415	5/5	0.92	0.12	45,46,46,49	0
8	CL	N	1018[A]	1/1	0.92	0.12	40,40,40,40	1
6	SO4	J	1118	5/5	0.92	0.14	52,53,54,57	0
6	SO4	F	1115	5/5	0.92	0.12	42,42,43,46	0
4	EDO	E	1115	4/4	0.92	0.12	31,35,35,36	0
4	EDO	H	4411	4/4	0.92	0.16	18,24,24,26	0
9	GOL	N	1011	6/6	0.92	0.14	31,33,37,39	0
6	SO4	M	1125	5/5	0.92	0.11	48,50,50,51	0
4	EDO	M	1111	4/4	0.92	0.11	20,21,23,24	0
4	EDO	I	1110	4/4	0.92	0.10	40,41,42,42	0
6	SO4	O	1119	5/5	0.92	0.11	47,47,49,49	0
6	SO4	A	1119	5/5	0.93	0.11	40,40,41,43	0
6	SO4	D	4619	5/5	0.93	0.12	48,48,50,52	0
6	SO4	L	1114	5/5	0.93	0.11	53,54,55,56	0
4	EDO	M	1121	4/4	0.93	0.10	32,33,33,34	0
4	EDO	G	1110	4/4	0.93	0.12	17,19,23,24	0
4	EDO	O	1114	4/4	0.93	0.10	28,32,32,33	0
4	EDO	C	3912	4/4	0.93	0.11	17,20,21,22	0
6	SO4	N	1016	5/5	0.93	0.11	49,51,53,54	0
4	EDO	A	1112	4/4	0.93	0.09	33,33,34,35	0
6	SO4	O	1120	5/5	0.93	0.10	47,48,49,49	0
4	EDO	K	1110	4/4	0.93	0.12	28,29,31,31	0
4	EDO	P	1110	4/4	0.93	0.12	21,22,24,24	0
4	EDO	K	1111	4/4	0.93	0.11	20,21,24,24	0
4	EDO	K	1112	4/4	0.93	0.09	29,29,31,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	EDO	L	1110	4/4	0.94	0.10	31,32,32,35	0
6	SO4	I	1120	5/5	0.94	0.12	47,49,51,52	0
3	FAD	N	1009[B]	53/53	0.94	0.09	15,21,24,28	53
6	SO4	E	1118	5/5	0.94	0.10	40,41,44,44	0
6	SO4	P	1115	5/5	0.94	0.10	46,46,47,48	0
3	FAD	N	1001[A]	53/53	0.94	0.08	16,20,26,27	53
8	CL	B	4229[B]	1/1	0.94	0.09	28,28,28,28	1
8	CL	F	1120[B]	1/1	0.94	0.09	29,29,29,29	1
6	SO4	L	1113	5/5	0.94	0.11	42,44,46,47	0
4	EDO	E	1110	4/4	0.94	0.09	17,20,21,22	0
4	EDO	O	1108	4/4	0.94	0.08	34,34,34,35	0
6	SO4	C	3919	5/5	0.94	0.12	46,47,48,51	0
4	EDO	O	1110	4/4	0.94	0.11	36,38,38,40	0
6	SO4	K	1118	5/5	0.95	0.09	41,42,44,45	0
4	EDO	F	1112[A]	4/4	0.95	0.09	12,18,18,19	4
3	FAD	P	1106	53/53	0.95	0.08	27,31,35,38	0
4	EDO	I	1108	4/4	0.95	0.08	26,27,29,30	0
8	CL	M	1130[B]	1/1	0.95	0.09	32,32,32,32	1
6	SO4	B	4225	5/5	0.95	0.10	43,43,46,46	0
6	SO4	G	1122	5/5	0.95	0.09	34,35,37,37	0
4	EDO	G	1108	4/4	0.95	0.06	22,23,23,24	0
4	EDO	L	1108	4/4	0.95	0.07	28,29,29,31	0
4	EDO	B	4212	4/4	0.95	0.08	18,18,21,22	0
4	EDO	L	1111	4/4	0.95	0.09	18,20,22,23	0
4	EDO	E	1108	4/4	0.95	0.08	27,27,28,29	0
3	FAD	F	1106	53/53	0.96	0.07	21,25,28,30	0
4	EDO	C	3911	4/4	0.96	0.09	28,29,29,30	0
4	EDO	J	1108	4/4	0.96	0.07	26,26,27,27	0
8	CL	K	1122[B]	1/1	0.96	0.07	26,26,26,26	1
4	EDO	D	4609	4/4	0.96	0.07	30,31,32,33	0
4	EDO	D	4611	4/4	0.96	0.08	17,19,21,21	0
4	EDO	F	1108	4/4	0.96	0.07	35,35,35,36	0
4	EDO	B	4209	4/4	0.96	0.07	24,24,25,26	0
4	EDO	P	1108	4/4	0.96	0.08	37,37,37,37	0
8	CL	E	1121[B]	1/1	0.97	0.05	27,27,27,27	1
6	SO4	B	4226	5/5	0.97	0.07	40,40,41,41	0
4	EDO	K	1108	4/4	0.97	0.05	21,21,22,23	0
2	SF4	N	1006[B]	8/8	0.97	0.06	30,33,33,35	8
4	EDO	H	4409	4/4	0.97	0.07	24,25,25,26	0
4	EDO	C	3909	4/4	0.97	0.06	22,22,24,24	0
2	SF4	N	1006[A]	8/8	0.97	0.06	23,26,27,27	8
4	EDO	A	1108	4/4	0.98	0.06	22,25,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FAD	E	1106	53/53	0.98	0.05	20,22,26,29	0
2	SF4	N	1008[B]	8/8	0.98	0.06	29,31,33,34	8
7	H2S	J	1120	1/1	0.98	0.09	22,22,22,22	0
7	H2S	K	1120	1/1	0.98	0.06	16,16,16,16	0
7	H2S	M	1128	1/1	0.98	0.05	19,19,19,19	0
3	FAD	H	4407	53/53	0.98	0.04	17,20,24,26	0
8	CL	C	3922[B]	1/1	0.98	0.05	32,32,32,32	1
8	CL	D	4624[B]	1/1	0.98	0.05	29,29,29,29	1
3	FAD	I	1106	53/53	0.98	0.04	12,18,19,21	0
3	FAD	J	1106	53/53	0.98	0.05	22,26,29,32	0
8	CL	G	1125[A]	1/1	0.98	0.05	31,31,31,31	1
8	CL	H	4418[A]	1/1	0.98	0.05	31,31,31,31	1
8	CL	I	1123[B]	1/1	0.98	0.06	36,36,36,36	1
8	CL	J	1122[A]	1/1	0.98	0.06	40,40,40,40	0
3	FAD	L	1106	53/53	0.98	0.04	14,19,22,26	0
8	CL	L	1117[B]	1/1	0.98	0.05	33,33,33,33	1
3	FAD	M	1106	53/53	0.98	0.04	17,21,24,27	0
3	FAD	B	4207	53/53	0.98	0.04	14,17,21,27	0
8	CL	P	1118[B]	1/1	0.98	0.06	35,35,35,35	1
3	FAD	C	3907	53/53	0.98	0.04	12,16,18,21	0
3	FAD	O	1106	53/53	0.98	0.05	13,18,22,28	0
4	EDO	M	1108	4/4	0.98	0.05	23,26,27,27	0
3	FAD	D	4607	53/53	0.98	0.05	20,22,25,27	0
5	SRM	N	1012	63/63	0.98	0.05	11,15,18,20	0
2	SF4	K	1104	8/8	0.99	0.02	12,12,13,13	0
2	SF4	K	1105	8/8	0.99	0.03	14,16,16,17	0
2	SF4	K	1107	8/8	0.99	0.03	12,12,13,14	0
2	SF4	L	1101	8/8	0.99	0.02	17,17,17,18	0
5	SRM	A	1109	63/63	0.99	0.04	6,9,13,16	0
5	SRM	B	4210	63/63	0.99	0.04	5,10,12,16	0
5	SRM	C	3910	63/63	0.99	0.04	6,10,14,17	0
5	SRM	D	4610	63/63	0.99	0.04	6,10,13,14	0
5	SRM	E	1109	63/63	0.99	0.04	8,11,14,16	0
5	SRM	F	1109	63/63	0.99	0.04	8,12,15,16	0
5	SRM	G	1109	63/63	0.99	0.04	5,9,13,16	0
5	SRM	H	4410	63/63	0.99	0.04	9,11,15,18	0
5	SRM	I	1109	63/63	0.99	0.04	9,13,17,20	0
5	SRM	J	1109	63/63	0.99	0.04	11,14,18,22	0
5	SRM	K	1109	63/63	0.99	0.04	8,11,15,17	0
5	SRM	L	1109	63/63	0.99	0.04	8,11,15,17	0
5	SRM	M	1109	63/63	0.99	0.04	9,13,16,19	0
2	SF4	L	1102	8/8	0.99	0.02	16,17,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SRM	O	1109	63/63	0.99	0.04	8,11,14,17	0
5	SRM	P	1109	63/63	0.99	0.04	11,13,19,20	0
2	SF4	L	1103	8/8	0.99	0.03	12,12,13,13	0
2	SF4	L	1104	8/8	0.99	0.03	11,12,12,12	0
2	SF4	L	1105	8/8	0.99	0.03	12,13,14,14	0
2	SF4	M	1101	8/8	0.99	0.03	16,17,17,18	0
2	SF4	M	1102	8/8	0.99	0.03	14,14,14,15	0
2	SF4	M	1103	8/8	0.99	0.02	15,16,17,17	0
2	SF4	M	1104	8/8	0.99	0.03	14,14,14,15	0
2	SF4	M	1105	8/8	0.99	0.03	19,20,21,21	0
2	SF4	M	1107	8/8	0.99	0.03	14,14,15,15	0
2	SF4	N	1002	8/8	0.99	0.04	25,26,28,28	0
2	SF4	N	1005	8/8	0.99	0.02	12,13,14,14	0
2	SF4	A	1101	8/8	0.99	0.03	10,11,12,12	0
2	SF4	A	1102	8/8	0.99	0.02	12,12,13,13	0
2	SF4	N	1007[A]	8/8	0.99	0.04	17,18,19,22	8
2	SF4	A	1103	8/8	0.99	0.02	10,11,11,12	0
2	SF4	O	1101	8/8	0.99	0.02	13,14,15,15	0
2	SF4	O	1102	8/8	0.99	0.03	12,13,14,14	0
2	SF4	O	1103	8/8	0.99	0.04	19,20,20,20	0
2	SF4	O	1104	8/8	0.99	0.03	14,15,16,17	0
2	SF4	O	1105	8/8	0.99	0.03	23,26,27,27	0
2	SF4	O	1107	8/8	0.99	0.03	13,14,14,14	0
2	SF4	P	1101	8/8	0.99	0.04	30,31,32,32	0
2	SF4	P	1102	8/8	0.99	0.03	27,29,30,30	0
2	SF4	P	1105	8/8	0.99	0.02	12,12,12,13	0
2	SF4	P	1107	8/8	0.99	0.04	29,31,32,33	0
3	FAD	A	1106	53/53	0.99	0.04	10,13,17,21	0
2	SF4	A	1104	8/8	0.99	0.02	10,10,11,12	0
2	SF4	A	1105	8/8	0.99	0.03	12,12,13,13	0
2	SF4	A	1107	8/8	0.99	0.03	11,11,12,13	0
2	SF4	B	4202	8/8	0.99	0.03	14,15,15,15	0
2	SF4	B	4203	8/8	0.99	0.03	12,12,13,14	0
7	H2S	A	1120	1/1	0.99	0.05	15,15,15,15	0
7	H2S	B	4227	1/1	0.99	0.06	18,18,18,18	0
7	H2S	C	3920	1/1	0.99	0.05	16,16,16,16	0
7	H2S	D	4622	1/1	0.99	0.05	16,16,16,16	0
7	H2S	E	1119	1/1	0.99	0.04	17,17,17,17	0
7	H2S	G	1123	1/1	0.99	0.03	15,15,15,15	0
3	FAD	G	1106	53/53	0.99	0.04	11,14,17,21	0
2	SF4	B	4204	8/8	0.99	0.03	10,11,11,12	0
7	H2S	L	1116	1/1	0.99	0.07	18,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	B	4205	8/8	0.99	0.03	9,10,11,11	0
7	H2S	N	1017	1/1	0.99	0.05	20,20,20,20	0
7	H2S	O	1121	1/1	0.99	0.04	17,17,17,17	0
8	CL	A	1122[B]	1/1	0.99	0.05	27,27,27,27	1
8	CL	B	4228	1/1	0.99	0.06	21,21,21,21	0
2	SF4	B	4206	8/8	0.99	0.03	12,12,13,14	0
3	FAD	K	1106	53/53	0.99	0.04	11,14,18,23	0
8	CL	D	4623	1/1	0.99	0.07	21,21,21,21	0
2	SF4	B	4208	8/8	0.99	0.03	12,13,14,14	0
2	SF4	C	3903	8/8	0.99	0.03	12,13,13,13	0
2	SF4	C	3904	8/8	0.99	0.03	11,12,12,12	0
8	CL	G	1124	1/1	0.99	0.04	21,21,21,21	0
2	SF4	C	3905	8/8	0.99	0.03	10,11,11,11	0
2	SF4	C	3906	8/8	0.99	0.03	12,13,14,14	0
8	CL	I	1122	1/1	0.99	0.06	23,23,23,23	0
2	SF4	C	3908	8/8	0.99	0.03	12,13,13,14	0
2	SF4	D	4603	8/8	0.99	0.02	14,15,15,15	0
8	CL	K	1121	1/1	0.99	0.07	19,19,19,19	0
2	SF4	D	4604	8/8	0.99	0.02	10,11,12,12	0
2	SF4	D	4605	8/8	0.99	0.02	9,10,10,11	0
2	SF4	D	4606	8/8	0.99	0.03	11,11,12,12	0
2	SF4	D	4608	8/8	0.99	0.03	14,15,16,16	0
8	CL	O	1122	1/1	0.99	0.03	20,20,20,20	0
8	CL	O	1123[B]	1/1	0.99	0.04	24,24,24,24	1
2	SF4	E	1101	8/8	0.99	0.03	17,17,19,19	0
8	CL	P	1119	1/1	0.99	0.10	34,34,34,34	0
2	SF4	E	1103	8/8	0.99	0.03	13,14,15,15	0
2	SF4	E	1104	8/8	0.99	0.03	12,12,13,13	0
2	SF4	E	1105	8/8	0.99	0.03	18,19,20,21	0
2	SF4	E	1107	8/8	0.99	0.03	14,15,16,16	0
2	SF4	F	1101	8/8	0.99	0.03	19,22,22,23	0
2	SF4	F	1102	8/8	0.99	0.03	20,22,23,23	0
2	SF4	F	1103	8/8	0.99	0.02	11,11,12,12	0
2	SF4	F	1104	8/8	0.99	0.02	9,11,12,12	0
2	SF4	F	1105	8/8	0.99	0.03	12,12,12,13	0
2	SF4	F	1107	8/8	0.99	0.03	20,22,22,23	0
2	SF4	G	1101	8/8	0.99	0.02	12,13,13,13	0
2	SF4	G	1103	8/8	0.99	0.03	13,14,14,14	0
2	SF4	G	1104	8/8	0.99	0.03	11,11,12,12	0
2	SF4	G	1105	8/8	0.99	0.02	15,16,16,17	0
2	SF4	G	1107	8/8	0.99	0.03	10,12,12,12	0
2	SF4	H	4402	8/8	0.99	0.03	17,18,18,18	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	H	4403	8/8	0.99	0.03	17,18,18,19	0
2	SF4	H	4404	8/8	0.99	0.03	10,10,11,11	0
2	SF4	H	4406	8/8	0.99	0.02	10,11,11,12	0
2	SF4	I	1101	8/8	0.99	0.03	15,16,16,16	0
2	SF4	I	1103	8/8	0.99	0.03	14,14,15,15	0
2	SF4	I	1104	8/8	0.99	0.03	14,15,15,16	0
2	SF4	I	1105	8/8	0.99	0.03	15,15,16,16	0
2	SF4	I	1107	8/8	0.99	0.03	15,16,17,18	0
2	SF4	J	1101	8/8	0.99	0.03	19,21,21,22	0
2	SF4	J	1102	8/8	0.99	0.03	17,17,17,18	0
2	SF4	J	1103	8/8	0.99	0.03	13,13,13,13	0
2	SF4	J	1107	8/8	0.99	0.03	18,18,19,19	0
2	SF4	K	1102	8/8	0.99	0.03	12,12,13,13	0
2	SF4	K	1103	8/8	0.99	0.03	13,13,14,15	0
2	SF4	N	1004	8/8	1.00	0.02	12,13,14,15	0
2	SF4	P	1103	8/8	1.00	0.02	11,12,12,13	0
7	H2S	F	1119	1/1	1.00	0.03	20,20,20,20	0
2	SF4	P	1104	8/8	1.00	0.02	10,10,11,12	0
8	CL	H	4417	1/1	1.00	0.07	24,24,24,24	0
7	H2S	H	4416	1/1	1.00	0.03	17,17,17,17	0
7	H2S	I	1121	1/1	1.00	0.05	20,20,20,20	0
2	SF4	J	1105	8/8	1.00	0.02	12,13,13,14	0
8	CL	J	1121	1/1	1.00	0.06	27,27,27,27	0
2	SF4	C	3902	8/8	1.00	0.02	13,14,14,15	0
2	SF4	K	1101	8/8	1.00	0.02	12,13,14,14	0
2	SF4	L	1107	8/8	1.00	0.02	15,16,16,16	0
2	SF4	D	4602	8/8	1.00	0.02	16,17,17,17	0
8	CL	M	1129	1/1	1.00	0.02	24,24,24,24	0
2	SF4	H	4405	8/8	1.00	0.02	9,10,10,10	0
7	H2S	P	1117	1/1	1.00	0.02	21,21,21,21	0
8	CL	A	1121	1/1	1.00	0.04	18,18,18,18	0
2	SF4	G	1102	8/8	1.00	0.02	11,12,13,13	0
2	SF4	H	4408	8/8	1.00	0.02	15,17,18,18	0
2	SF4	E	1102	8/8	1.00	0.02	13,13,14,14	0
8	CL	C	3921	1/1	1.00	0.06	19,19,19,19	0
2	SF4	I	1102	8/8	1.00	0.02	15,15,17,17	0
2	SF4	J	1104	8/8	1.00	0.02	12,13,14,14	0
2	SF4	N	1003	8/8	1.00	0.02	12,13,14,14	0
8	CL	E	1120	1/1	1.00	0.06	25,25,25,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.