



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 05:17 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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

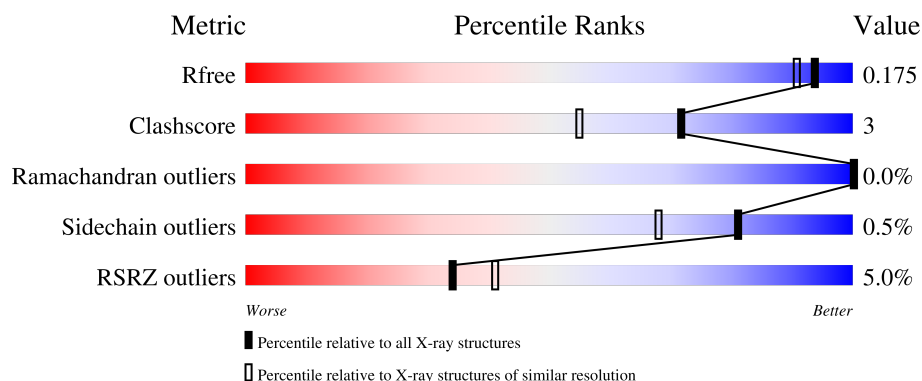
1 Overall quality at a glance

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	
1	B	618	
1	C	618	
1	D	618	
1	E	618	

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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

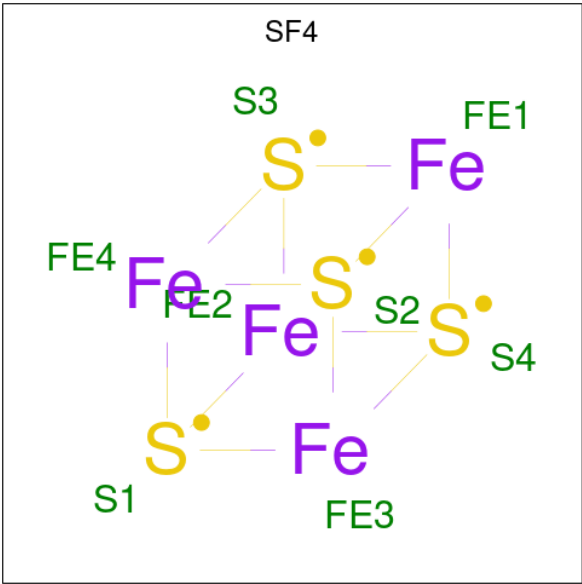
There are 13 unique types of molecules in this entry. The entry contains 93689 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	Fe	S	0	0
			8	4	4		
2	J	1	Total	Fe	S	0	0
			8	4	4		
2	J	1	Total	Fe	S	0	0
			8	4	4		
2	J	1	Total	Fe	S	0	0
			8	4	4		
2	J	1	Total	Fe	S	0	0
			8	4	4		
2	K	1	Total	Fe	S	0	0
			8	4	4		
2	K	1	Total	Fe	S	0	0
			8	4	4		
2	K	1	Total	Fe	S	0	0
			8	4	4		
2	K	1	Total	Fe	S	0	0
			8	4	4		
2	K	1	Total	Fe	S	0	0
			8	4	4		
2	K	1	Total	Fe	S	0	0
			8	4	4		
2	L	1	Total	Fe	S	0	0
			8	4	4		
2	L	1	Total	Fe	S	0	0
			8	4	4		
2	L	1	Total	Fe	S	0	0
			8	4	4		
2	L	1	Total	Fe	S	0	0
			8	4	4		
2	L	1	Total	Fe	S	0	0
			8	4	4		
2	M	1	Total	Fe	S	0	0
			8	4	4		
2	M	1	Total	Fe	S	0	0
			8	4	4		
2	M	1	Total	Fe	S	0	0
			8	4	4		

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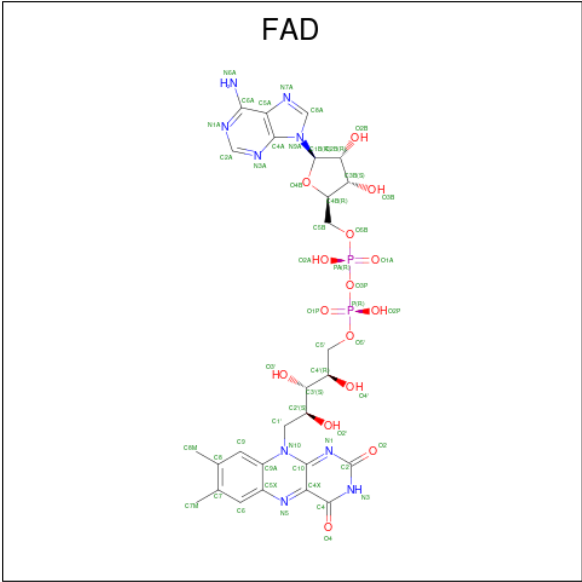
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	M	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0
2	M	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 8	Fe 4	S 4	0	0
2	N	1	Total 16	Fe 8	S 8	0	1
2	N	1	Total 8	Fe 4	S 4	0	1
2	N	1	Total 8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



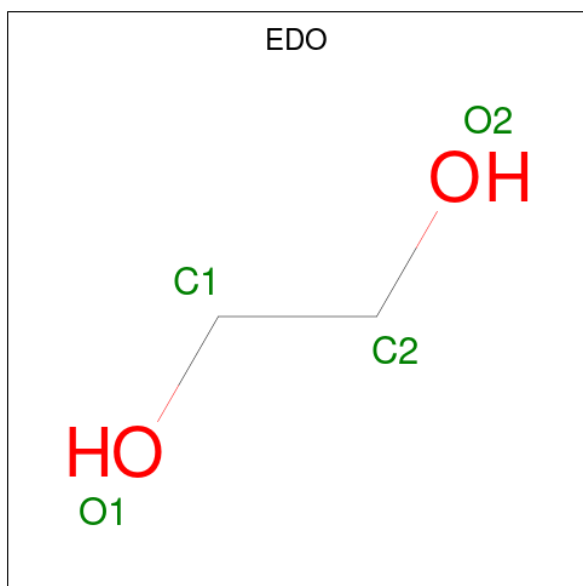
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 53	27	9	15	2	0	0
3	B	1	Total 53	27	9	15	2	0	0
3	C	1	Total 53	27	9	15	2	0	0
3	D	1	Total 53	27	9	15	2	0	0
3	E	1	Total 53	27	9	15	2	0	0
3	F	1	Total 53	27	9	15	2	0	0
3	G	1	Total 53	27	9	15	2	0	0
3	H	1	Total 53	27	9	15	2	0	0
3	I	1	Total 53	27	9	15	2	0	0
3	J	1	Total 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 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	C	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	D	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0
4	E	1	Total 4	C 2	O 2	0	0

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

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

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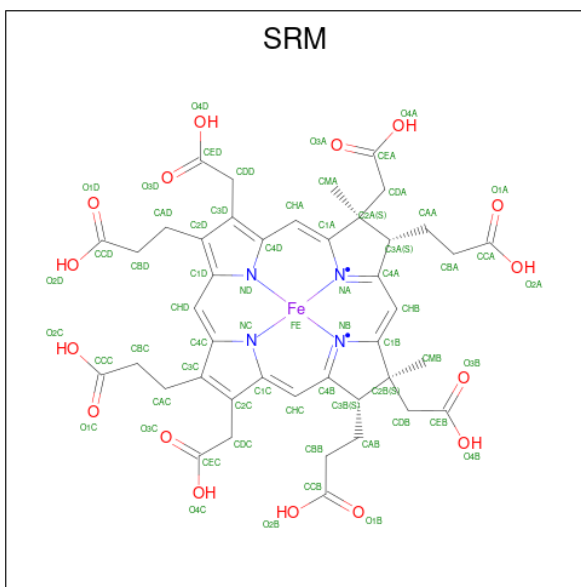
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	K	1	Total 4	C 2	O 2	0	0
4	K	1	Total 4	C 2	O 2	0	0
4	K	1	Total 4	C 2	O 2	0	0
4	L	1	Total 4	C 2	O 2	0	0
4	L	1	Total 4	C 2	O 2	0	0
4	L	1	Total 4	C 2	O 2	0	0
4	L	1	Total 4	C 2	O 2	0	0
4	M	1	Total 4	C 2	O 2	0	0
4	M	1	Total 4	C 2	O 2	0	0
4	M	1	Total 4	C 2	O 2	0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

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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).



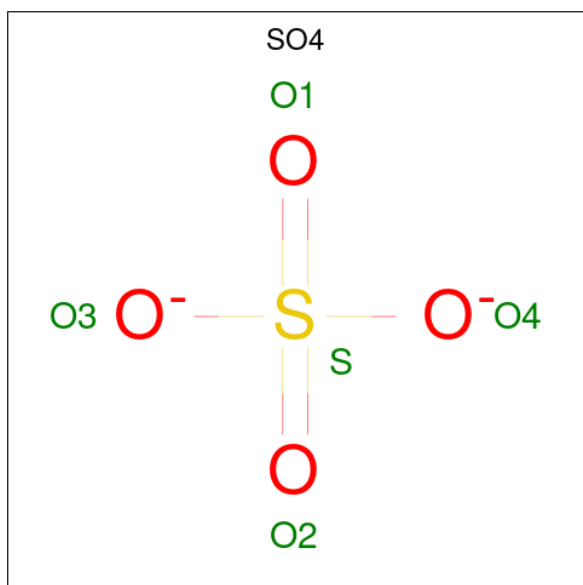
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
5	B	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
5	C	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
5	D	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
5	E	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
5	F	1	Total 63	C 42	Fe 1	N 4	O 16	0	0
5	G	1	Total 63	C 42	Fe 1	N 4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

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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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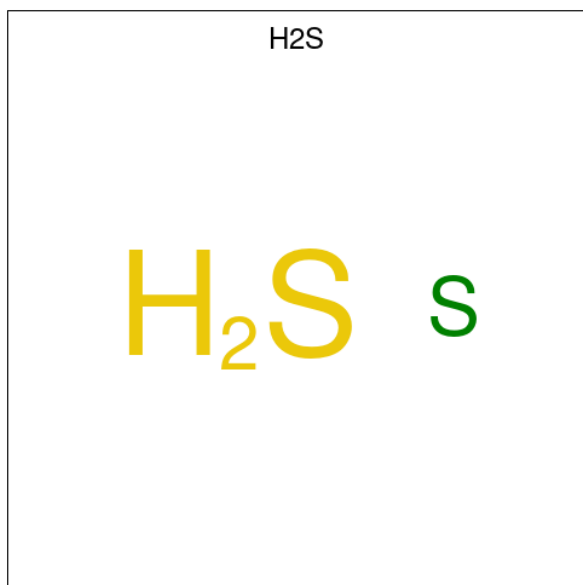
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	F	1	Total	O	S	0	0
			5	4	1		
6	G	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	H	1	Total	O	S	0	0
			5	4	1		
6	I	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	O	S	0	0
			5	4	1		
6	J	1	Total	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).

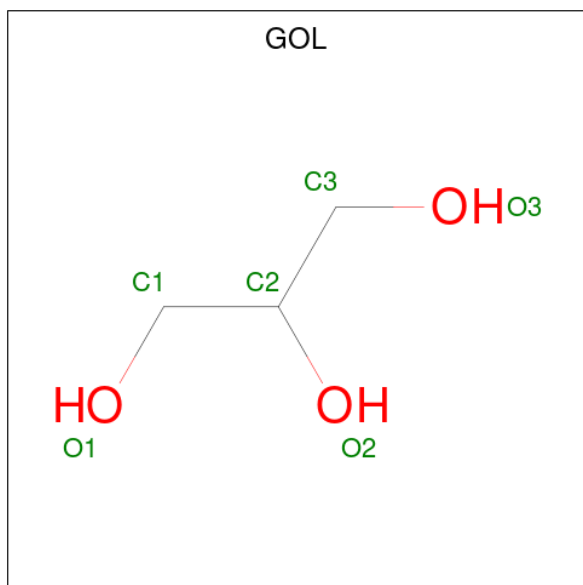
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	2	Total Cl 2 2	0	1
8	B	2	Total Cl 2 2	0	1
8	C	2	Total Cl 2 2	0	1
8	D	2	Total Cl 2 2	0	1
8	E	2	Total Cl 2 2	0	1
8	F	1	Total Cl 1 1	0	1
8	G	2	Total Cl 2 2	0	1
8	H	2	Total Cl 2 2	0	1
8	I	2	Total Cl 2 2	0	1
8	J	2	Total Cl 2 2	0	1
8	K	2	Total Cl 2 2	0	1
8	L	1	Total 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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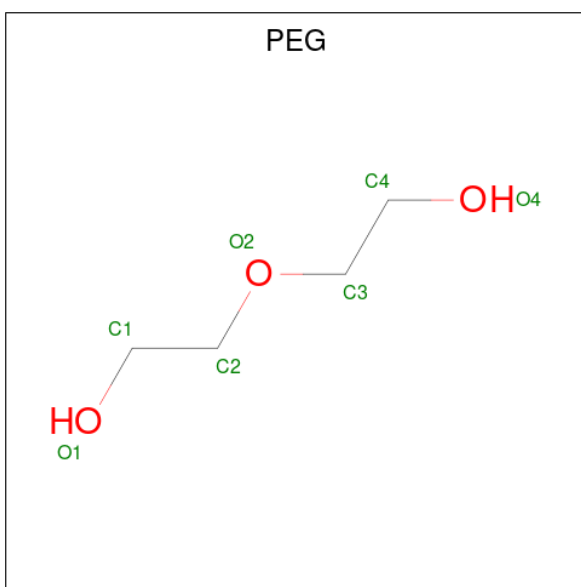
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	I	1	Total C O 6 3 3	0	0
9	I	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	0
9	J	1	Total C O 6 3 3	0	1
9	K	1	Total C O 6 3 3	0	0
9	M	1	Total C O 6 3 3	0	0
9	N	1	Total C O 6 3 3	0	0
9	N	1	Total C O 6 3 3	0	0
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).

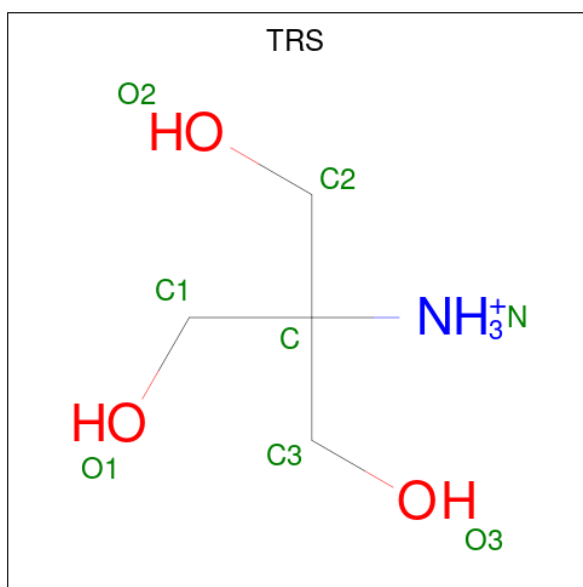
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	C	1	Total Li 1 1	0	0
10	F	1	Total Li 1 1	0	0
10	L	1	Total Li 1 1	0	0
10	P	1	Total Li 1 1	0	0

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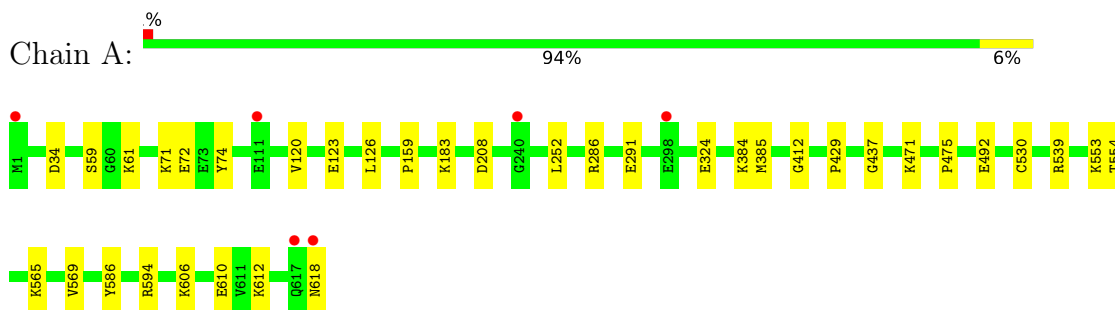
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	K	766	Total 766	O 766	0	1
13	L	681	Total 681	O 681	0	3
13	M	690	Total 690	O 690	0	2
13	N	465	Total 465	O 465	0	12
13	O	665	Total 665	O 665	0	2
13	P	532	Total 532	O 532	0	0

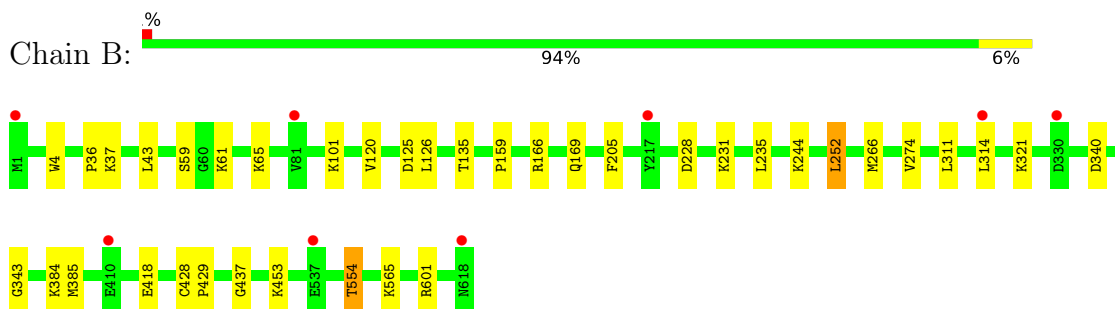
3 Residue-property plots [i](#)

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.

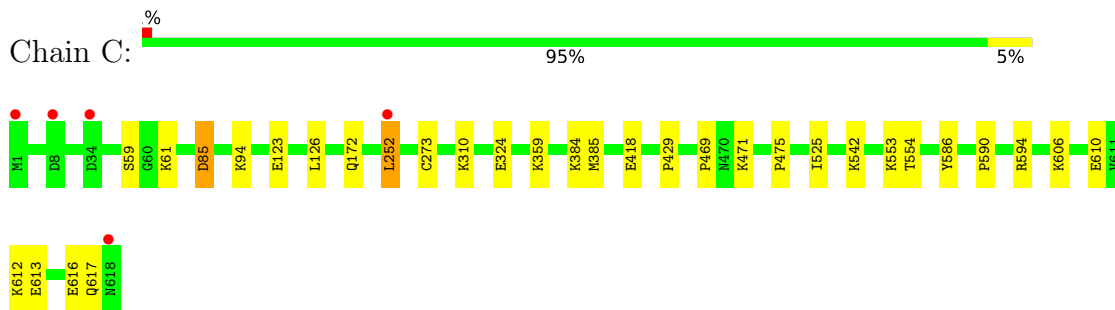
- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase

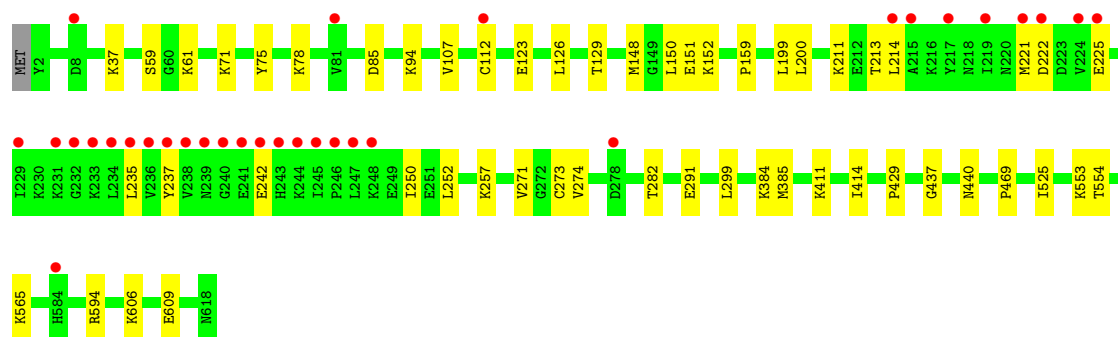


- Molecule 1: Coenzyme F420-dependent sulfite reductase

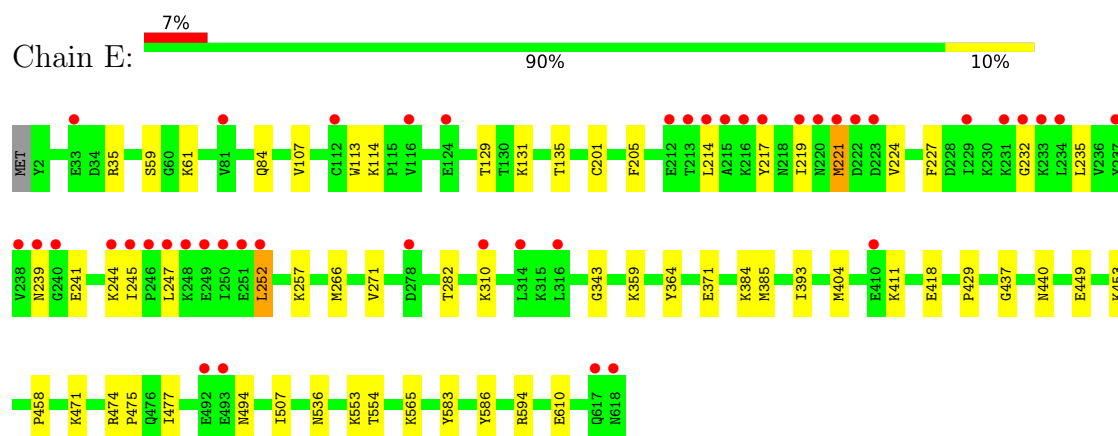


- Molecule 1: Coenzyme F420-dependent sulfite reductase

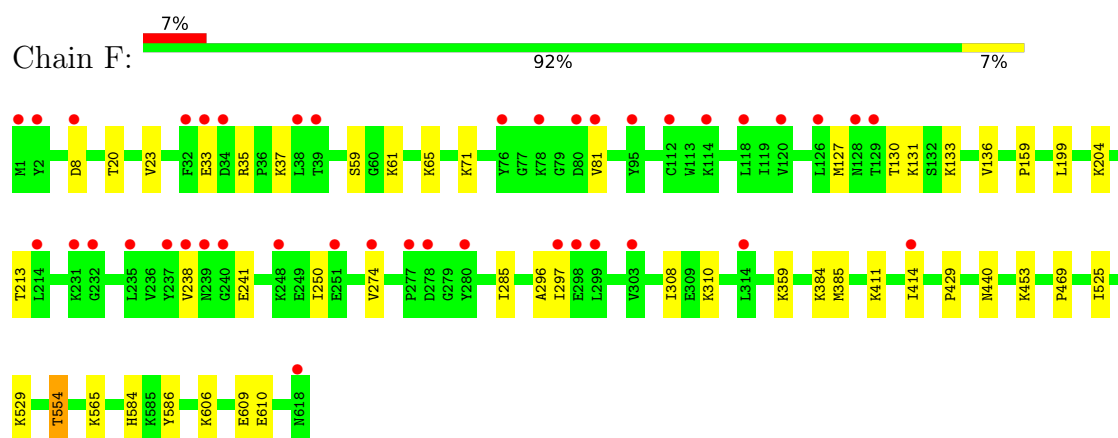




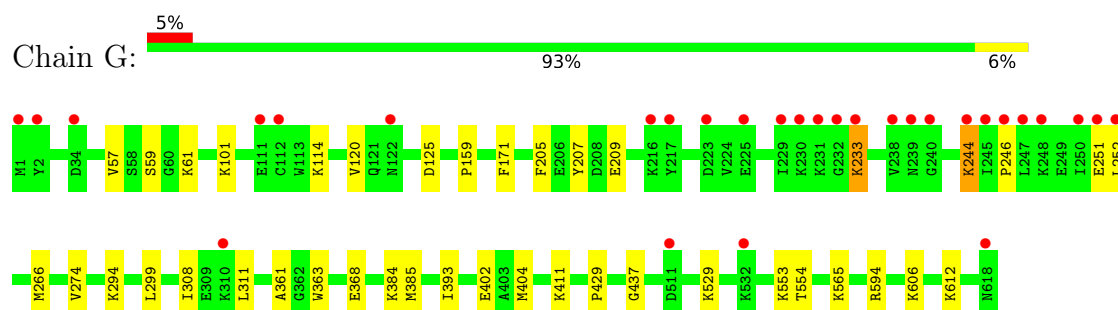
- Molecule 1: Coenzyme F420-dependent sulfite reductase



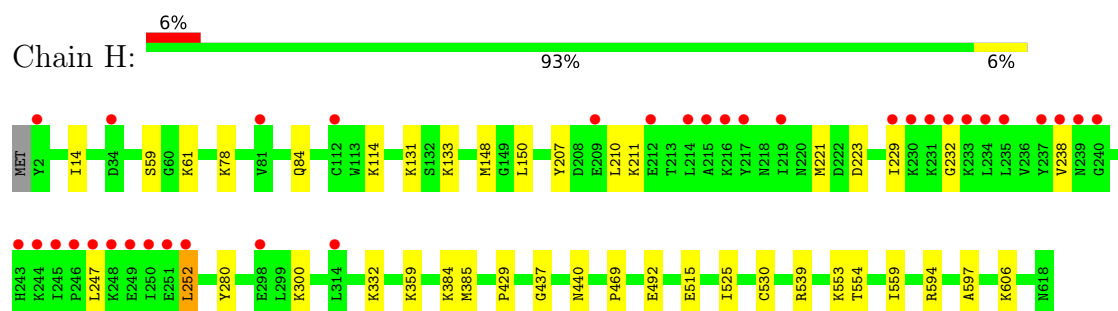
- Molecule 1: Coenzyme F420-dependent sulfite reductase



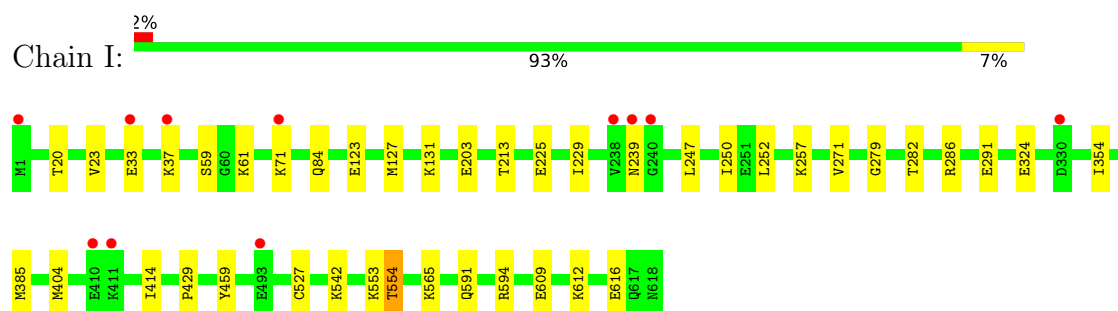
- Molecule 1: Coenzyme F420-dependent sulfite reductase



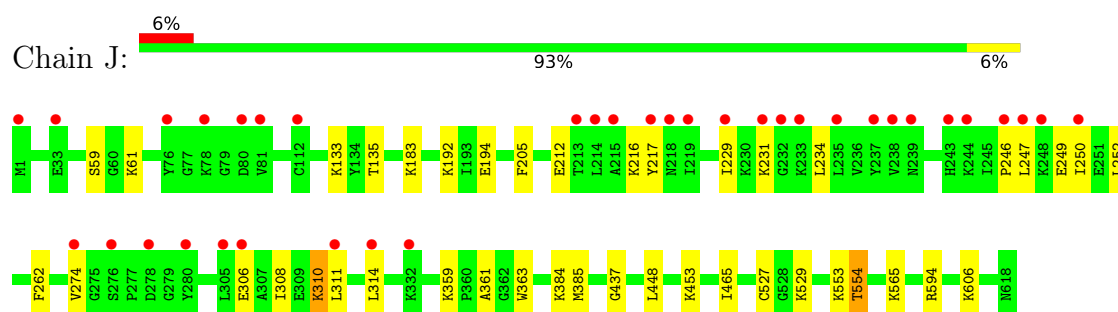
- Molecule 1: Coenzyme F420-dependent sulfite reductase



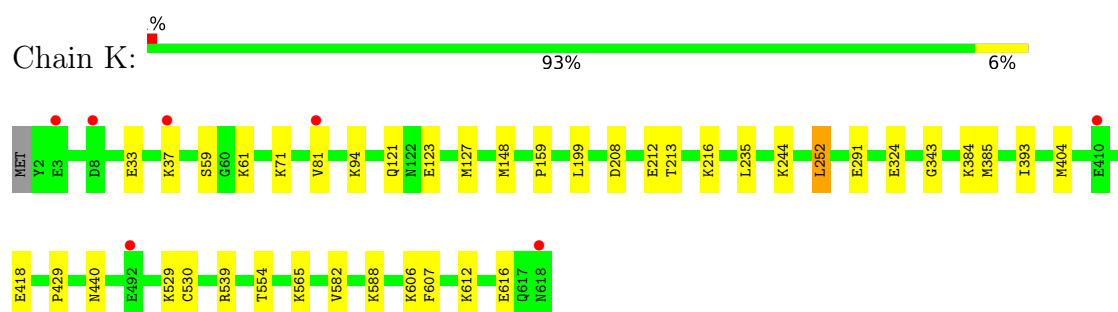
- Molecule 1: Coenzyme F420-dependent sulfite reductase



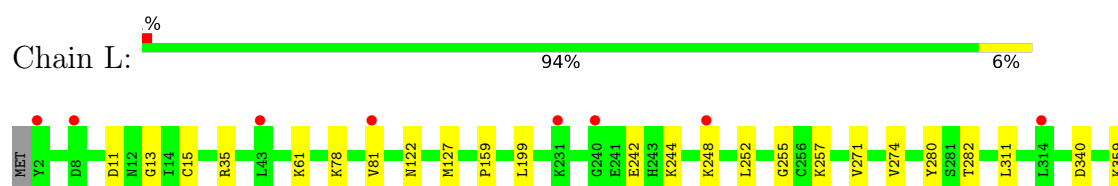
- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase



- Molecule 1: Coenzyme F420-dependent sulfite reductase

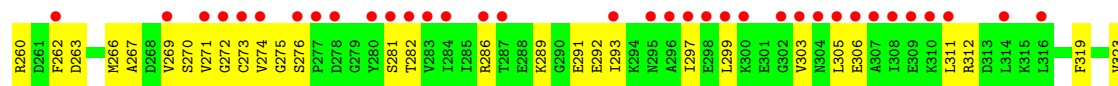
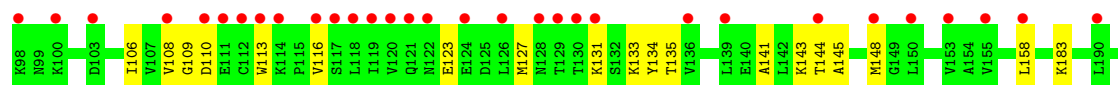
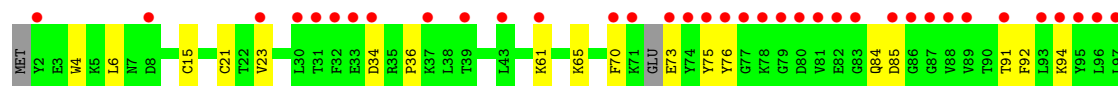
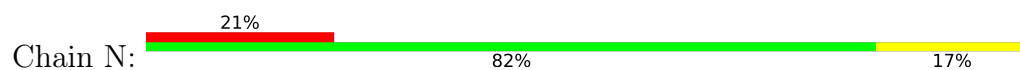




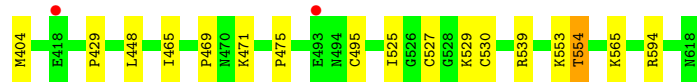
- Molecule 1: Coenzyme F420-dependent sulfite reductase



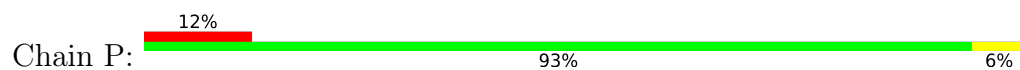
- Molecule 1: Coenzyme F420-dependent sulfite reductase

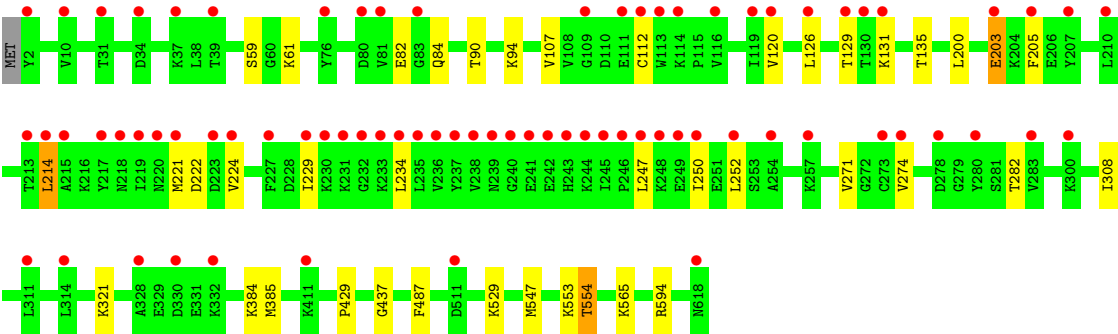


- Molecule 1: Coenzyme F420-dependent sulfite reductase



- 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

All (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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	85	ASP	O-C-N	5.07	124.58	120.83
1	P	203	GLU	CB-CA-C	-5.02	102.00	110.43

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

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

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

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

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

All (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
1:J:252:LEU:H	1:J:252:LEU:CD2	2.05	0.68
1:N:263[B]:ASP:CG	1:N:312[B]:ARG:HE	2.01	0.67
1:O:252:LEU:H	1:O:252:LEU:CD2	2.08	0.67
1:O:252:LEU:H	1:O:252:LEU:HD23	1.60	0.66
1:A:385:MET:HE2	1:B:385:MET:HE2	1.78	0.65
1:N:131[B]:LYS:HD2	1:N:226[B]:LYS:HD2	1.80	0.64
1:G:274[A]:VAL:HG21	1:G:311:LEU:CD1	2.27	0.64
1:G:274[B]:VAL:HG11	1:G:311:LEU:CD1	2.28	0.63
1:L:359:LYS:NZ	13:L:1201:HOH:O	2.30	0.63
1:O:385:MET:HE2	1:P:385:MET:HE2	1.80	0.63
1:J:252:LEU:HD23	1:J:252:LEU:N	2.13	0.63
1:N:252[A]:LEU:H	1:N:252[A]:LEU:HD23	1.62	0.63
1:I:252:LEU:HD12	1:I:252:LEU:O	1.99	0.62
1:A:612:LYS:NZ	1:D:609:GLU:CD	2.59	0.61
1:H:78:LYS:HG3	1:H:280:TYR:CD2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:229:ILE:HG22	1:P:229:ILE:O	2.01	0.60
1:M:84:GLN:HB2	1:M:131:LYS:HA	1.83	0.60
1:B:59:SER:HB2	1:B:61[A]:LYS:HG3	1.83	0.60
1:N:73[B]:GLU:HB3	1:N:75[B]:TYR:CE2	2.38	0.59
1:N:214[A]:LEU:HD12	1:N:221[A]:MET:HE3	1.83	0.59
1:K:385:MET:HE2	1:L:385:MET:HE2	1.84	0.59
1:O:59:SER:HB2	1:O:61:LYS:HG3	1.84	0.59
1:G:59:SER:HB2	1:G:61:LYS:HG3	1.85	0.59
1:N:305[A]:LEU:HD12	1:N:305[A]:LEU:C	2.27	0.59
1:E:385:MET:HE2	1:F:385:MET:HE2	1.85	0.58
1:B:274:VAL:HG21	1:B:311:LEU:HD11	1.84	0.58
1:N:259[B]:CYS:O	1:N:319[B]:PHE:HB2	2.03	0.58
1:C:94:LYS:HD2	1:C:123:GLU:HG3	1.86	0.58
1:F:71:LYS:HE3	1:F:285:ILE:HG22	1.86	0.58
1:N:73[B]:GLU:HB3	1:N:75[B]:TYR:HE2	1.68	0.58
1:N:262[B]:PHE:HB3	1:N:312[B]:ARG:HA	1.86	0.58
1:N:525:ILE:HD11	9:N:1011:GOL:H32	1.85	0.58
1:O:189:LYS:NZ	13:O:1203:HOH:O	2.37	0.58
1:P:84:GLN:HB2	1:P:131:LYS:HA	1.86	0.58
1:N:84[B]:GLN:HB2	1:N:131[B]:LYS:HA	1.85	0.58
1:N:198[B]:GLY:O	1:N:270[B]:SER:HA	2.03	0.58
1:N:145[B]:ALA:HA	1:N:148[B]:MET:HE2	1.86	0.57
1:N:214[B]:LEU:HD11	1:N:227[B]:PHE:CE1	2.39	0.57
1:L:248:LYS:HA	1:L:248:LYS:HE3	1.84	0.57
1:O:61:LYS:HE2	1:O:266:MET:CG	2.35	0.57
1:G:429:PRO:HG3	1:H:384:LYS:HE2	1.86	0.57
1:N:195[B]:TYR:CD1	1:N:289[B]:LYS:HB3	2.39	0.57
1:F:59:SER:HB2	1:F:61:LYS:HG3	1.86	0.57
1:O:527:CYS:SG	1:O:529:LYS:HB2	2.44	0.57
1:D:151:GLU:HG2	1:D:152:LYS:HG3	1.85	0.57
1:J:453:LYS:NZ	13:J:1204:HOH:O	2.37	0.57
1:N:134[B]:TYR:CE1	1:N:229[B]:ILE:HG13	2.40	0.57
1:F:35:ARG:HD3	13:F:1290:HOH:O	2.05	0.56
1:N:23:VAL:HG12	1:N:143[B]:LYS:HE2	1.86	0.56
1:P:547:MET:SD	9:P:1111:GOL:O3	2.62	0.56
1:G:385:MET:HE2	1:H:385:MET:HE2	1.86	0.56
1:E:371:GLU:OE2	1:E:411:LYS:HD2	2.06	0.56
1:L:81:VAL:HB	1:L:127:MET:HE1	1.88	0.56
1:N:113[B]:TRP:NE1	1:N:224[B]:VAL:O	2.35	0.56
1:H:559:ILE:CD1	4:H:4412:EDO:H22	2.35	0.56
1:N:209[B]:GLU:HG2	1:N:251[B]:GLU:HB3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:108[B]:VAL:HG21	3:N:1009[B]:FAD:C2A	2.35	0.56
1:O:252:LEU:HD23	1:O:252:LEU:N	2.21	0.56
1:E:214:LEU:HD11	1:E:227:PHE:HZ	1.69	0.56
9:F:1114:GOL:H31	4:G:1116:EDO:H11	1.88	0.56
1:B:231:LYS:HE2	6:B:4226:SO4:O1	2.06	0.56
1:H:211:LYS:HA	1:H:221:MET:HE3	1.88	0.56
1:J:359:LYS:HE2	13:J:1343:HOH:O	2.05	0.56
1:M:384:LYS:HE2	1:N:429:PRO:HG3	1.88	0.56
1:C:429:PRO:HG3	1:D:384:LYS:HE2	1.88	0.55
1:J:453:LYS:HE3	13:J:1249:HOH:O	2.06	0.55
1:N:299[B]:LEU:N	1:N:299[B]:LEU:HD23	2.21	0.55
1:N:61:LYS:O	1:N:65:LYS:HB3	2.06	0.55
1:N:210[A]:LEU:HD23	1:N:221[A]:MET:HE1	1.87	0.55
1:E:217:TYR:CE2	1:E:245:ILE:HD13	2.42	0.55
1:G:209:GLU:HG2	1:G:251:GLU:CD	2.32	0.55
13:I:1430:HOH:O	1:J:554:THR:HG22	2.06	0.55
1:E:113:TRP:HB2	1:E:221:MET:HG2	1.89	0.55
1:H:559:ILE:HD11	4:H:4412:EDO:H22	1.88	0.55
1:K:33:GLU:HG3	1:K:37:LYS:HE2	1.88	0.55
1:D:112:CYS:SG	1:D:222:ASP:HA	2.47	0.55
1:I:429:PRO:HG3	1:J:384:LYS:HE2	1.87	0.55
1:K:429:PRO:HG3	1:L:384:LYS:HE2	1.89	0.55
1:N:214[B]:LEU:HD11	1:N:227[B]:PHE:HE1	1.71	0.55
1:B:453:LYS:NZ	13:B:4310:HOH:O	2.39	0.54
1:G:114:LYS:HG3	1:G:207:TYR:CZ	2.43	0.54
1:J:231:LYS:HG3	4:J:1110:EDO:H21	1.88	0.54
1:O:127:MET:HE3	1:O:127:MET:HA	1.89	0.54
1:N:36:PRO:HG3	2:N:1006[A]:SF4:S3	2.47	0.54
1:N:200[A]:LEU:HG	1:N:263[A]:ASP:HA	1.89	0.54
1:N:299[A]:LEU:HD23	1:N:299[A]:LEU:N	2.21	0.54
1:N:106[B]:ILE:HG23	1:N:141[B]:ALA:HB3	1.90	0.54
1:N:276[A]:SER:HB3	1:N:282[A]:THR:OG1	2.07	0.54
1:J:192:LYS:HE2	1:J:194:GLU:OE1	2.08	0.54
1:N:214[A]:LEU:HD11	1:N:227[A]:PHE:CE1	2.43	0.54
1:P:203:GLU:OE1	1:P:247:LEU:HD13	2.08	0.54
1:P:120:VAL:HG21	1:P:126:LEU:HD13	1.89	0.54
1:F:81:VAL:HB	1:F:127:MET:HE1	1.89	0.54
1:L:242:GLU:OE1	1:L:244:LYS:HE3	2.08	0.53
13:G:1223:HOH:O	1:H:515:GLU:HG3	2.07	0.53
1:K:393:ILE:HG21	1:K:404:MET:HE1	1.91	0.53
1:N:289[B]:LYS:O	1:N:292[B]:GLU:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:213:THR:HG21	1:F:250:ILE:HG12	1.89	0.53
1:I:612[B]:LYS:O	1:I:616:GLU:HG3	2.09	0.53
1:I:324:GLU:HG2	13:I:1203:HOH:O	2.09	0.53
1:E:235:LEU:HD22	1:E:244:LYS:HG2	1.91	0.53
1:B:101:LYS:NZ	13:B:4313:HOH:O	2.42	0.53
1:D:237:TYR:CE2	1:D:242:GLU:HB3	2.43	0.53
1:J:183:LYS:NZ	13:J:1207:HOH:O	2.41	0.53
1:K:252:LEU:HD12	1:K:252:LEU:O	2.09	0.53
1:N:209[A]:GLU:HG2	1:N:251[A]:GLU:HB3	1.89	0.53
1:D:211:LYS:HA	1:D:221:MET:HE3	1.91	0.53
1:P:107:VAL:CG2	1:P:129:THR:HG21	2.39	0.53
1:A:324:GLU:HG2	13:A:1225:HOH:O	2.08	0.53
1:N:232[B]:GLY:C	1:N:247[B]:LEU:HG	2.34	0.53
1:N:200[B]:LEU:HG	1:N:263[B]:ASP:HA	1.90	0.53
1:P:321:LYS:NZ	13:P:1201:HOH:O	2.30	0.53
1:B:37:LYS:HA	4:B:4216:EDO:H12	1.90	0.52
1:N:94[A]:LYS:HG3	1:N:123[A]:GLU:HG2	1.92	0.52
1:G:411:LYS:HE2	13:G:1209:HOH:O	2.08	0.52
1:L:11:ASP:OD1	1:L:35:ARG:NH2	2.42	0.52
1:N:612:LYS:NZ	13:N:1106:HOH:O	2.41	0.52
1:O:393:ILE:HG21	1:O:404:MET:HE1	1.90	0.52
1:F:33:GLU:HB2	1:F:37:LYS:HE3	1.91	0.52
1:L:61:LYS:HE2	13:L:1238:HOH:O	2.10	0.52
1:I:59:SER:HB2	1:I:61:LYS:HG3	1.92	0.52
1:N:291[A]:GLU:HA	1:N:291[A]:GLU:OE1	2.10	0.52
1:D:213:THR:HG21	1:D:250:ILE:HG12	1.92	0.52
1:E:429:PRO:HG3	1:F:384:LYS:HE2	1.92	0.52
1:I:385:MET:HE2	1:J:385:MET:HE2	1.92	0.52
1:N:134[B]:TYR:HE2	1:N:227[B]:PHE:O	1.93	0.52
1:C:359:LYS:NZ	13:C:4018:HOH:O	2.42	0.51
1:N:267[A]:ALA:O	1:N:286[A]:ARG:HD2	2.11	0.51
1:D:94:LYS:HG3	1:D:126:LEU:HD23	1.92	0.51
1:F:274:VAL:HG13	1:F:308:ILE:HG12	1.92	0.51
1:I:612[A]:LYS:O	1:I:616:GLU:HG3	2.09	0.51
1:L:61:LYS:HB3	1:L:340:ASP:HA	1.93	0.51
1:N:327[A]:LYS:NZ	13:N:1108:HOH:O	2.43	0.51
1:D:414:ILE:N	1:D:414:ILE:HD12	2.25	0.51
1:I:542:LYS:HZ3	9:I:1117:GOL:H32	1.76	0.51
1:A:59:SER:HB2	1:A:61:LYS:HG3	1.91	0.51
1:C:252:LEU:HD12	1:C:252:LEU:O	2.10	0.51
1:K:121:GLN:OE1	1:K:148:MET:HE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:232:GLY:O	1:H:247:LEU:HB2	2.10	0.51
1:N:275[B]:GLY:O	1:N:303[B]:VAL:HG13	2.10	0.51
1:A:606:LYS:HB2	1:D:565:LYS:HB3	1.92	0.51
1:I:33:GLU:HB2	1:I:37:LYS:HE2	1.93	0.51
1:B:252:LEU:HD12	1:B:252:LEU:O	2.11	0.51
1:J:527:CYS:SG	4:J:1112:EDO:H11	2.51	0.51
1:N:197[A]:ILE:HG23	1:N:269[A]:VAL:HG13	1.94	0.51
1:D:85:ASP:OD2	1:D:273:CYS:HB3	2.12	0.50
1:L:252:LEU:CD2	1:L:252:LEU:H	2.23	0.50
1:N:606:LYS:HB2	1:O:565:LYS:HB3	1.93	0.50
1:A:159:PRO:HD2	2:A:1101:SF4:S2	2.52	0.50
1:N:232[A]:GLY:C	1:N:247[A]:LEU:HG	2.36	0.50
1:B:120:VAL:HG13	1:B:125:ASP:HB2	1.94	0.50
1:G:294:LYS:HG2	1:G:299:LEU:HD12	1.93	0.50
1:J:274:VAL:HG13	1:J:308:ILE:HG12	1.92	0.50
1:N:70:PHE:CZ	1:N:266[B]:MET:O	2.64	0.50
1:N:204[A]:LYS:NZ	2:N:1007[A]:SF4:S1	2.82	0.50
1:I:252:LEU:HD12	1:I:252:LEU:C	2.36	0.50
1:O:61:LYS:HE2	1:O:266:MET:HG3	1.94	0.50
1:P:529:LYS:HD3	13:P:1547:HOH:O	2.12	0.50
1:N:134[B]:TYR:CZ	1:N:229[B]:ILE:HG13	2.47	0.50
1:N:21:CYS:HB3	2:N:1006[A]:SF4:S1	2.52	0.50
1:D:469:PRO:HB2	1:D:525:ILE:HD12	1.94	0.50
1:H:229:ILE:CG2	1:H:247:LEU:HD11	2.42	0.50
1:J:216:LYS:HD3	1:J:216:LYS:N	2.27	0.50
1:O:120:VAL:HG13	1:O:125:ASP:HB2	1.94	0.50
1:O:384:LYS:HE2	1:P:429:PRO:HG3	1.93	0.50
1:D:71:LYS:HZ1	1:D:291:GLU:CD	2.19	0.50
1:E:232:GLY:HA2	1:E:247:LEU:HD12	1.94	0.50
1:F:411:LYS:NZ	13:F:1213:HOH:O	2.43	0.50
1:M:393:ILE:HG21	1:M:404:MET:HE1	1.92	0.50
1:P:84:GLN:HG2	3:P:1106:FAD:H3'	1.93	0.50
1:B:565:LYS:HB3	1:C:606:LYS:HB2	1.94	0.50
1:E:449:GLU:O	1:E:453:LYS:HB3	2.11	0.50
1:K:59:SER:HB2	1:K:61:LYS:HG3	1.93	0.50
1:A:252:LEU:HD23	1:A:252:LEU:H	1.77	0.49
1:F:565:LYS:HB3	1:G:606:LYS:HB2	1.94	0.49
1:A:384:LYS:HE2	1:B:429:PRO:HG3	1.94	0.49
1:B:65:LYS:HD3	13:B:4393:HOH:O	2.12	0.49
6:F:1117:SO4:O2	6:F:1118:SO4:O4	2.29	0.49
1:H:84:GLN:HB2	1:H:131:LYS:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:133[B]:LYS:HD3	1:N:133[B]:LYS:N	2.27	0.49
1:O:495:CYS:HA	2:O:1105:SF4:S4	2.51	0.49
1:A:252:LEU:H	1:A:252:LEU:CD2	2.25	0.49
1:K:588:LYS:NZ	13:K:1218:HOH:O	2.45	0.49
1:N:214[A]:LEU:CD1	1:N:221[A]:MET:HE3	2.41	0.49
1:P:112:CYS:SG	1:P:222:ASP:HA	2.52	0.49
1:B:61[B]:LYS:HB3	1:B:340:ASP:HA	1.93	0.49
1:E:214:LEU:HD11	1:E:227:PHE:CZ	2.47	0.49
1:E:252:LEU:CD1	1:E:252:LEU:C	2.86	0.49
1:I:71:LYS:O	1:I:286:ARG:HA	2.12	0.49
1:K:94:LYS:CD	1:K:123:GLU:HG3	2.42	0.49
1:E:384:LYS:HE2	1:F:429:PRO:HG3	1.95	0.49
1:H:300:LYS:NZ	13:H:4510:HOH:O	2.42	0.49
1:H:553:LYS:HE3	1:H:594:ARG:HG3	1.93	0.49
1:M:252:LEU:CD1	1:M:252:LEU:C	2.85	0.49
1:F:136:VAL:HA	1:F:204:LYS:HD2	1.94	0.49
1:M:252:LEU:N	1:M:252:LEU:HD12	2.27	0.49
1:P:214:LEU:HD12	1:P:221:MET:HB2	1.94	0.49
1:G:384:LYS:HE2	1:H:429:PRO:HG3	1.95	0.49
1:O:189:LYS:NZ	13:O:1208:HOH:O	2.43	0.49
1:F:609:GLU:OE1	1:G:612:LYS:HE3	2.13	0.49
1:L:367:ASP:O	1:L:371:GLU:HG3	2.13	0.49
1:F:440:ASN:HB3	4:F:1113:EDO:H11	1.94	0.49
1:N:489:VAL:HB	1:N:542:LYS:HB2	1.95	0.49
1:F:469:PRO:HB2	1:F:525:ILE:HD12	1.95	0.48
1:H:440:ASN:HB3	4:H:4413:EDO:H11	1.95	0.48
1:K:81:VAL:HB	1:K:127:MET:HE1	1.94	0.48
1:N:94[B]:LYS:HG3	1:N:123[B]:GLU:HG2	1.95	0.48
1:D:237:TYR:CD2	1:D:242:GLU:HB3	2.48	0.48
1:M:213:THR:HG21	1:M:250:ILE:HG12	1.95	0.48
1:E:553:LYS:HE3	1:E:594:ARG:HG3	1.95	0.48
1:N:133[A]:LYS:HD3	1:N:133[A]:LYS:N	2.28	0.48
1:N:252[A]:LEU:H	1:N:252[A]:LEU:CD2	2.25	0.48
1:A:429:PRO:HG3	1:B:384:LYS:HE2	1.94	0.48
1:F:359:LYS:NZ	13:F:1223:HOH:O	2.47	0.48
1:M:601:ARG:HH11	9:M:1114:GOL:H31	1.77	0.48
1:N:106[A]:ILE:HG23	1:N:141[A]:ALA:HB3	1.95	0.48
9:B:4217[A]:GOL:H32	13:B:4412:HOH:O	2.14	0.48
1:D:440:ASN:HB3	4:D:4615:EDO:H11	1.96	0.48
1:O:246:PRO:HD2	1:O:249:GLU:OE1	2.14	0.48
1:D:59:SER:HB2	1:D:61:LYS:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:LYS:NZ	13:I:1223:HOH:O	2.47	0.48
1:N:4:TRP:CZ2	1:N:6:LEU:HD12	2.49	0.48
1:N:123[B]:GLU:O	1:N:127[B]:MET:HG2	2.13	0.48
1:H:252:LEU:HD23	1:H:252:LEU:H	1.79	0.48
1:C:252:LEU:HD12	1:C:252:LEU:N	2.28	0.47
1:E:507:ILE:HG22	4:F:1110[B]:EDO:H12	1.95	0.47
1:P:487:PHE:CE1	9:P:1111:GOL:H32	2.48	0.47
1:H:59:SER:HB2	1:H:61:LYS:HG3	1.96	0.47
1:I:203:GLU:OE2	1:I:252:LEU:HB3	2.14	0.47
1:L:252:LEU:H	1:L:252:LEU:HD23	1.79	0.47
1:N:274[B]:VAL:HG21	1:N:311:LEU:HD11	1.96	0.47
5:N:1012:SRM:HMA1	5:N:1012:SRM:O3A	2.14	0.47
1:F:606:LYS:HB2	1:G:565:LYS:HB3	1.97	0.47
1:G:553:LYS:HE3	1:G:594:ARG:HG3	1.96	0.47
1:N:319[B]:PHE:O	1:N:323[B]:VAL:HG23	2.12	0.47
1:O:84:GLN:HB2	1:O:131:LYS:HA	1.97	0.47
1:K:440:ASN:HB3	4:K:1116:EDO:H22	1.96	0.47
1:P:553:LYS:HE3	1:P:594:ARG:HG3	1.96	0.47
1:B:61[A]:LYS:HE2	1:B:266:MET:SD	2.54	0.47
1:E:586:TYR:OH	1:E:610:GLU:OE2	2.30	0.47
1:F:310:LYS:HE3	13:F:1477:HOH:O	2.15	0.47
1:H:597:ALA:HA	4:H:4412:EDO:H21	1.95	0.47
5:M:1109:SRM:O3A	5:M:1109:SRM:HMA1	2.14	0.47
1:D:200:LEU:HD23	1:D:274:VAL:HG12	1.97	0.47
1:H:229:ILE:HG23	1:H:247:LEU:HD11	1.95	0.47
1:A:71:LYS:HG2	1:A:286:ARG:O	2.14	0.47
1:B:135:THR:HA	1:B:205:PHE:O	2.15	0.47
1:C:384:LYS:HE2	1:D:429:PRO:HG3	1.97	0.47
1:K:213:THR:HA	1:K:216:LYS:HE2	1.97	0.47
13:M:1819:HOH:O	1:N:183[A]:LYS:HG3	2.14	0.47
1:M:159:PRO:HD3	1:M:199:LEU:O	2.15	0.47
1:N:135[A]:THR:HA	1:N:205[A]:PHE:O	2.15	0.47
1:N:297[B]:ILE:HB	1:N:299[B]:LEU:HD21	1.96	0.47
1:A:612:LYS:HZ2	1:D:609:GLU:CD	2.22	0.47
1:C:613:GLU:O	1:C:617:GLN:HG3	2.14	0.47
1:E:393:ILE:HG21	1:E:404:MET:HE1	1.95	0.47
1:N:92[B]:PHE:CG	1:N:293[B]:ILE:HG13	2.50	0.47
1:N:109[B]:GLY:N	1:N:116[B]:VAL:O	2.35	0.47
1:D:225:GLU:HB2	1:D:237:TYR:O	2.15	0.47
1:G:233:LYS:HD2	1:G:244:LYS:CD	2.45	0.47
1:I:609:GLU:HG2	1:L:612:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:235:LEU:HD22	1:K:244:LYS:HG2	1.97	0.47
1:N:108[A]:VAL:HG21	3:N:1001[A]:FAD:C2A	2.45	0.47
1:P:107:VAL:HG23	1:P:129:THR:HG21	1.95	0.47
1:J:212:GLU:O	1:J:216:LYS:HE2	2.14	0.46
1:K:71:LYS:HZ1	1:K:291:GLU:CD	2.23	0.46
1:A:553:LYS:HE3	1:A:594:ARG:HG3	1.97	0.46
1:J:246:PRO:O	1:J:249:GLU:HB3	2.15	0.46
1:O:359:LYS:NZ	13:O:1219:HOH:O	2.49	0.46
1:B:252:LEU:HD12	1:B:252:LEU:C	2.40	0.46
1:I:554:THR:HG22	13:J:1321:HOH:O	2.16	0.46
1:P:90:THR:O	1:P:94:LYS:HG3	2.16	0.46
1:E:252:LEU:HD12	1:E:252:LEU:O	2.16	0.46
1:N:75[B]:TYR:HB3	1:N:299[B]:LEU:HB3	1.97	0.46
1:A:612:LYS:HZ3	1:D:609:GLU:CD	2.24	0.46
1:C:59:SER:HB2	1:C:61:LYS:HG3	1.98	0.46
1:F:65:LYS:NZ	13:F:1207:HOH:O	2.39	0.46
1:A:618:ASN:ND2	13:A:1214:HOH:O	2.43	0.46
1:J:231:LYS:CG	4:J:1110:EDO:H21	2.45	0.46
1:G:402:GLU:OE1	4:G:1120:EDO:H22	2.15	0.46
1:I:542:LYS:NZ	9:I:1117:GOL:H32	2.30	0.46
1:K:384:LYS:HE2	1:L:429:PRO:HG3	1.97	0.46
1:N:233[B]:LYS:HG2	1:N:246[B]:PRO:HA	1.98	0.46
1:N:276[A]:SER:CB	1:N:282[A]:THR:OG1	2.63	0.46
1:J:310:LYS:O	1:J:314:LEU:HD23	2.16	0.46
1:P:135:THR:HA	1:P:205:PHE:O	2.16	0.46
1:C:586:TYR:OH	1:C:610:GLU:OE2	2.30	0.46
1:D:242:GLU:O	1:D:242:GLU:HG3	2.15	0.46
1:G:171:PHE:HB3	4:G:1118:EDO:C2	2.46	0.46
1:I:20:THR:O	1:I:23:VAL:HG22	2.16	0.46
1:N:197[B]:ILE:HG23	1:N:269[B]:VAL:HG13	1.98	0.45
1:N:219[A]:ILE:HG21	1:N:236[A]:VAL:HG11	1.98	0.45
1:P:221:MET:HA	1:P:224:VAL:HG23	1.97	0.45
1:H:148:MET:CE	1:H:150:LEU:HD11	2.46	0.45
1:J:448:LEU:HD12	1:J:465:ILE:HD11	1.97	0.45
1:M:252:LEU:HD12	1:M:252:LEU:H	1.81	0.45
1:N:214[A]:LEU:HD11	1:N:227[A]:PHE:CZ	2.51	0.45
1:C:553:LYS:HE3	1:C:594:ARG:HG3	1.97	0.45
1:E:84:GLN:HB2	1:E:131:LYS:HA	1.98	0.45
1:H:437:GLY:HA2	2:H:4405:SF4:S2	2.56	0.45
11:K:1115:PEG:H11	11:K:1115:PEG:H31	1.36	0.45
1:L:418:GLU:HG2	13:L:1214:HOH:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:252[B]:LEU:HD23	1:N:252[B]:LEU:H	1.81	0.45
1:A:565:LYS:HB3	1:D:606:LYS:HB2	1.99	0.45
1:B:601:ARG:HH11	9:C:3901:GOL:H2	1.81	0.45
1:G:274[A]:VAL:HG21	1:G:311:LEU:HD11	1.96	0.45
1:D:159:PRO:HD3	1:D:199:LEU:O	2.16	0.45
1:M:59:SER:HB2	1:M:61:LYS:HG3	1.99	0.45
1:N:260[A]:ARG:HD2	1:N:319[A]:PHE:CZ	2.52	0.45
1:B:554:THR:HG22	13:B:4413:HOH:O	2.16	0.45
1:H:247:LEU:HD23	1:H:247:LEU:HA	1.85	0.45
1:O:374:GLU:HG2	13:O:1388:HOH:O	2.16	0.45
1:D:107:VAL:CG2	1:D:129:THR:HG21	2.47	0.45
1:G:233:LYS:HG2	1:G:246:PRO:HA	1.99	0.45
1:J:262:PHE:CZ	1:J:311:LEU:HD12	2.51	0.45
1:L:274:VAL:HG21	1:L:311:LEU:HD12	1.98	0.45
1:N:272[A]:GLY:HA2	3:N:1001[A]:FAD:O4'	2.17	0.45
1:J:361:ALA:HB3	1:J:363:TRP:CD1	2.52	0.45
1:K:324:GLU:HG2	13:K:1215:HOH:O	2.16	0.45
1:N:274[B]:VAL:HG21	1:N:311:LEU:CD1	2.47	0.45
1:F:59:SER:CB	1:F:61:LYS:HG3	2.47	0.45
1:G:205:PHE:HA	1:G:252:LEU:HA	1.97	0.45
1:D:94:LYS:HG2	1:D:123:GLU:HG2	1.99	0.45
1:D:214:LEU:HD12	1:D:221:MET:CE	2.47	0.45
1:G:120:VAL:HG13	1:G:125:ASP:HB2	1.99	0.45
1:N:297[A]:ILE:HB	1:N:299[A]:LEU:HD21	1.99	0.45
1:O:554:THR:HG22	13:P:1340:HOH:O	2.17	0.45
1:B:314:LEU:HG	13:B:4456:HOH:O	2.18	0.44
1:C:85:ASP:OD2	1:C:273:CYS:HB3	2.17	0.44
1:E:201:CYS:HA	3:E:1106:FAD:N5	2.32	0.44
1:E:239:ASN:O	1:E:241:GLU:HG3	2.17	0.44
5:E:1109:SRM:HMA1	5:E:1109:SRM:O3A	2.16	0.44
1:I:229:ILE:HG23	1:I:247:LEU:HD11	1.99	0.44
1:N:76[B]:TYR:O	1:N:76[B]:TYR:CD1	2.70	0.44
1:P:271:VAL:HA	1:P:282:THR:O	2.16	0.44
1:D:257:LYS:NZ	13:D:4712:HOH:O	2.42	0.44
1:I:279:GLY:HA3	4:I:1115:EDO:H21	1.98	0.44
1:L:252:LEU:HD21	1:L:257:LYS:HE2	1.99	0.44
1:M:135:THR:HA	1:M:205:PHE:O	2.17	0.44
1:N:85[B]:ASP:OD2	1:N:273[B]:CYS:HB2	2.17	0.44
1:N:271[A]:VAL:CG1	1:N:281[A]:SER:HB3	2.47	0.44
1:O:553:LYS:HE3	1:O:594:ARG:HG3	1.99	0.44
1:I:527:CYS:SG	9:I:1111:GOL:H2	2.58	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76[A]:TYR:O	1:N:76[A]:TYR:CD1	2.71	0.44
1:N:361:ALA:HB3	1:N:363:TRP:CD1	2.52	0.44
1:O:429:PRO:HG3	1:P:384:LYS:HE2	2.00	0.44
1:P:82:GLU:N	13:P:1231:HOH:O	2.50	0.44
1:D:235:LEU:N	1:D:235:LEU:HD23	2.31	0.44
5:F:1109:SRM:HMA1	5:F:1109:SRM:O3A	2.17	0.44
1:J:529:LYS:HD3	4:J:1112:EDO:H22	2.00	0.44
1:M:429:PRO:HG3	1:N:384:LYS:HE2	1.98	0.44
1:M:437:GLY:HA2	2:M:1104:SF4:S2	2.57	0.44
1:N:469:PRO:HB2	1:N:525:ILE:HD12	2.00	0.44
1:D:75:TYR:HB3	1:D:299:LEU:HB3	1.98	0.44
1:F:238:VAL:O	1:F:241:GLU:HG2	2.17	0.44
1:F:296:ALA:O	1:F:297:ILE:HD13	2.17	0.44
1:F:609:GLU:CD	1:G:612:LYS:HE3	2.43	0.44
1:G:274[B]:VAL:HG11	1:G:311:LEU:HD11	1.98	0.44
1:I:123:GLU:O	1:I:127:MET:HG2	2.18	0.44
1:I:553:LYS:HE3	1:I:594:ARG:HG3	1.99	0.44
11:M:1115:PEG:H21	11:M:1115:PEG:H42	1.74	0.44
1:A:471:LYS:HB3	1:A:475:PRO:HD2	1.99	0.44
1:J:217:TYR:OH	1:J:249:GLU:OE2	2.35	0.44
1:J:606:LYS:HB2	1:K:565:LYS:HB3	1.99	0.44
1:N:91[A]:THR:HB	1:N:297[A]:ILE:HD11	2.00	0.44
1:P:59:SER:HB2	1:P:61:LYS:HG3	2.00	0.44
1:C:471:LYS:HB3	1:C:475:PRO:HD2	2.00	0.44
1:C:542:LYS:NZ	9:C:3901:GOL:H32	2.33	0.44
1:E:437:GLY:HA2	2:E:1104:SF4:S2	2.58	0.44
1:H:14:ILE:HD12	1:H:332:LYS:HE3	1.99	0.44
1:H:469:PRO:HB2	1:H:525:ILE:HD12	2.00	0.44
1:M:252:LEU:HD22	1:M:256:CYS:HB2	1.99	0.44
1:N:231[B]:LYS:HA	1:N:231[B]:LYS:HD3	1.66	0.44
1:A:291:GLU:O	1:A:291:GLU:HG3	2.18	0.43
1:G:101:LYS:HA	1:G:101:LYS:HD2	1.89	0.43
1:J:453:LYS:CE	13:J:1249:HOH:O	2.66	0.43
1:B:159:PRO:HD2	2:B:4202:SF4:S2	2.59	0.43
1:C:252:LEU:CD1	1:C:252:LEU:C	2.90	0.43
1:C:469:PRO:HB2	1:C:525:ILE:HD12	2.00	0.43
1:L:375:ILE:HD11	1:L:411:LYS:HE2	2.00	0.43
1:N:15:CYS:O	1:N:255[A]:GLY:HA3	2.17	0.43
1:H:210:LEU:HG	1:H:221:MET:HE2	1.99	0.43
1:I:565:LYS:HB3	1:L:606:LYS:HB2	1.99	0.43
1:P:252:LEU:O	1:P:252:LEU:HD23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:OE2	1:A:74:TYR:OH	2.29	0.43
1:B:252:LEU:C	1:B:252:LEU:CD1	2.91	0.43
1:I:213:THR:HG21	1:I:250:ILE:HG12	1.99	0.43
1:J:565:LYS:HB3	1:K:606:LYS:HB2	2.00	0.43
1:A:569[B]:VAL:HG21	4:A:1116:EDO:H22	1.99	0.43
1:A:586:TYR:OH	1:A:610:GLU:OE2	2.35	0.43
1:G:209:GLU:OE1	1:G:209:GLU:N	2.51	0.43
1:J:553:LYS:HE3	1:J:594:ARG:HG3	2.00	0.43
1:P:234:LEU:HD22	1:P:250:ILE:CD1	2.48	0.43
1:A:437:GLY:HA2	2:A:1104:SF4:S2	2.58	0.43
1:E:135:THR:HA	1:E:205:PHE:O	2.19	0.43
1:G:393:ILE:HG21	1:G:404:MET:HE1	2.00	0.43
1:I:84:GLN:HB2	1:I:131:LYS:HA	2.01	0.43
1:J:59:SER:HB2	1:J:61:LYS:HG3	2.00	0.43
1:K:612:LYS:O	1:K:616:GLU:HG3	2.18	0.43
1:N:158[A]:LEU:HD13	2:N:1007[A]:SF4:S1	2.58	0.43
1:N:271[B]:VAL:CG1	1:N:281[B]:SER:HB3	2.48	0.43
1:B:343:GLY:HA2	1:B:418:GLU:HG2	2.00	0.43
1:E:235:LEU:CD2	1:E:244:LYS:HG2	2.49	0.43
1:G:437:GLY:HA2	2:G:1104:SF4:S2	2.59	0.43
1:P:200:LEU:HD23	1:P:274:VAL:HG12	2.01	0.43
1:A:123:GLU:CG	13:A:1213:HOH:O	2.66	0.43
1:J:437:GLY:HA2	2:J:1104:SF4:S2	2.59	0.43
1:L:78:LYS:HD3	1:L:280:TYR:CE2	2.53	0.43
1:F:414:ILE:HD13	1:F:453[A]:LYS:HE2	2.00	0.43
1:J:133:LYS:HD3	1:J:133:LYS:N	2.34	0.43
1:J:229:ILE:HG23	1:J:247:LEU:HD11	2.00	0.43
1:A:208:ASP:HB2	13:A:1725:HOH:O	2.19	0.42
1:H:148:MET:HE2	1:H:150:LEU:HD11	2.00	0.42
1:H:530:CYS:SG	1:H:539:ARG:HD3	2.59	0.42
1:L:252:LEU:HD23	1:L:252:LEU:N	2.34	0.42
1:N:76[B]:TYR:O	1:N:76[B]:TYR:CG	2.71	0.42
1:N:135[B]:THR:HA	1:N:205[B]:PHE:O	2.19	0.42
1:O:448:LEU:HD12	1:O:465:ILE:HD11	2.01	0.42
1:A:492:GLU:HG3	13:A:1512:HOH:O	2.19	0.42
1:B:228:ASP:HB3	1:B:235:LEU:HB2	2.01	0.42
1:E:343:GLY:HA2	1:E:418:GLU:CG	2.49	0.42
1:H:359:LYS:NZ	13:H:4535:HOH:O	2.52	0.42
1:L:15:CYS:O	1:L:255:GLY:HA3	2.19	0.42
1:C:172:GLN:OE1	1:C:590:PRO:HD2	2.18	0.42
1:I:225:GLU:OE2	1:I:239:ASN:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:135:THR:HA	1:J:205:PHE:O	2.19	0.42
1:K:235:LEU:CD2	1:K:244:LYS:HG2	2.50	0.42
1:M:274:VAL:HG13	1:M:308:ILE:HG12	2.01	0.42
1:G:171:PHE:HB3	4:G:1118:EDO:H22	2.01	0.42
1:E:59:SER:HB2	1:E:61:LYS:HG3	2.01	0.42
1:E:494:ASN:HB3	1:E:536:ASN:O	2.19	0.42
1:H:133:LYS:N	1:H:133:LYS:HD3	2.35	0.42
1:K:94:LYS:HD3	1:K:123:GLU:HG3	2.01	0.42
1:L:13:GLY:HA2	13:L:1554:HOH:O	2.19	0.42
1:K:252:LEU:CD1	1:K:252:LEU:C	2.92	0.42
1:N:134[A]:TYR:HA	3:N:1001[A]:FAD:HM73	2.02	0.42
1:I:71:LYS:HD2	1:I:291:GLU:OE1	2.19	0.42
1:M:20:THR:O	1:M:23:VAL:HG22	2.20	0.42
1:N:76[A]:TYR:HD2	1:N:303[A]:VAL:HG22	1.83	0.42
1:N:85[A]:ASP:OD2	1:N:273[A]:CYS:HB2	2.19	0.42
1:E:310:LYS:HB3	1:E:310:LYS:HE3	1.82	0.42
1:G:361:ALA:HB3	1:G:363:TRP:CD1	2.54	0.42
1:L:248:LYS:HE3	1:L:248:LYS:CA	2.49	0.42
1:N:204[A]:LYS:HD3	2:N:1007[A]:SF4:S1	2.60	0.42
1:A:120:VAL:HG21	1:A:126:LEU:HD13	2.01	0.42
1:A:530:CYS:SG	1:A:539:ARG:HD3	2.60	0.42
13:E:1359:HOH:O	1:F:554:THR:HG22	2.20	0.42
1:G:159:PRO:HD2	2:G:1101:SF4:S2	2.60	0.42
1:H:114:LYS:HG3	1:H:207:TYR:CZ	2.55	0.42
1:E:257:LYS:NZ	13:E:1242:HOH:O	2.53	0.42
1:F:130:THR:O	1:F:131:LYS:HB2	2.20	0.42
1:N:110[B]:ASP:OD1	1:N:110[B]:ASP:N	2.53	0.42
1:B:428:CYS:HB2	1:B:429:PRO:CD	2.49	0.41
1:C:252:LEU:HD12	1:C:252:LEU:H	1.85	0.41
1:E:271:VAL:HA	1:E:282:THR:O	2.20	0.41
1:K:343:GLY:HA2	1:K:418:GLU:HG2	2.01	0.41
1:L:271:VAL:HA	1:L:282:THR:O	2.19	0.41
1:M:278:ASP:OD1	1:M:279:GLY:N	2.53	0.41
1:N:269[B]:VAL:HG13	1:N:269[B]:VAL:O	2.20	0.41
3:D:4607:FAD:H9	3:D:4607:FAD:H1'1	1.81	0.41
1:E:565:LYS:HB3	1:H:606:LYS:HB2	2.01	0.41
1:F:159:PRO:HD3	1:F:199:LEU:O	2.20	0.41
1:F:586:TYR:OH	1:F:610:GLU:OE2	2.36	0.41
1:I:459:TYR:CD1	1:I:591:GLN:HA	2.54	0.41
1:K:582:VAL:HG12	1:K:607:PHE:CE2	2.55	0.41
1:O:252:LEU:CD2	1:O:252:LEU:N	2.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:78:LYS:HG3	1:H:280:TYR:CE2	2.56	0.41
3:I:1106:FAD:H1'1	3:I:1106:FAD:H9	1.84	0.41
1:O:530:CYS:SG	1:O:539:ARG:HD3	2.61	0.41
1:P:205:PHE:CD1	1:P:250:ILE:HG21	2.56	0.41
1:E:458:PRO:HD2	1:E:583:TYR:CE2	2.55	0.41
1:G:274[B]:VAL:HG23	1:G:308:ILE:HG12	2.02	0.41
1:J:306:GLU:O	1:J:310:LYS:HG3	2.20	0.41
1:K:208:ASP:O	1:K:212:GLU:HG3	2.21	0.41
1:L:159:PRO:HD3	1:L:199:LEU:O	2.20	0.41
1:M:252:LEU:HD11	1:M:257:LYS:HE3	2.02	0.41
1:B:321:LYS:HE3	13:B:4944:HOH:O	2.20	0.41
1:K:159:PRO:HD3	1:K:199:LEU:O	2.21	0.41
1:B:437:GLY:HA2	2:B:4205:SF4:S2	2.61	0.41
1:D:271:VAL:HA	1:D:282:THR:O	2.21	0.41
1:D:411:LYS:HE3	13:D:5084:HOH:O	2.19	0.41
1:E:474:ARG:HD3	1:E:477:ILE:HD11	2.03	0.41
1:G:233:LYS:CD	1:G:244:LYS:HB3	2.51	0.41
1:M:507:ILE:HD11	2:M:1103:SF4:S3	2.61	0.41
1:N:195[A]:TYR:OH	1:N:292[A]:GLU:OE2	2.34	0.41
1:P:274:VAL:HG13	1:P:308:ILE:HG12	2.03	0.41
1:B:61[A]:LYS:HE2	1:B:266:MET:CG	2.51	0.41
1:D:252:LEU:H	1:D:252:LEU:HD23	1.85	0.41
1:E:61:LYS:HE2	1:E:266:MET:CG	2.51	0.41
1:E:440:ASN:HB3	4:E:1112:EDO:H22	2.02	0.41
1:B:235:LEU:HD22	1:B:244:LYS:HG2	2.03	0.41
1:B:343:GLY:CA	1:B:418:GLU:HG2	2.51	0.41
1:D:437:GLY:HA2	2:D:4605:SF4:S2	2.61	0.41
1:F:20:THR:O	1:F:23:VAL:HG22	2.21	0.41
1:G:529:LYS:HE2	13:G:1702:HOH:O	2.20	0.41
1:H:223:ASP:C	1:H:238:VAL:HG23	2.46	0.41
1:I:612[A]:LYS:NZ	1:L:609:GLU:OE1	2.54	0.41
3:K:1106:FAD:H9	3:K:1106:FAD:H1'1	1.89	0.41
1:N:144[B]:THR:O	1:N:148[B]:MET:HG3	2.20	0.41
1:N:305[A]:LEU:HD12	1:N:306[A]:GLU:N	2.36	0.41
1:O:82:GLU:O	1:O:82:GLU:HG3	2.21	0.41
1:O:216:LYS:HE3	1:O:216:LYS:HB3	1.93	0.41
1:O:469:PRO:HB2	1:O:525:ILE:HD12	2.03	0.41
1:P:529:LYS:NZ	13:P:1240:HOH:O	2.54	0.41
1:B:43:LEU:HG	4:B:4211:EDO:H11	2.04	0.41
1:C:324:GLU:HG2	13:C:4008:HOH:O	2.20	0.41
9:I:1111:GOL:H32	13:J:1370:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:252:LEU:HD12	1:M:252:LEU:O	2.21	0.41
13:O:1441:HOH:O	1:P:554:THR:HG22	2.20	0.41
1:B:166:ARG:HD3	1:B:169:GLN:OE1	2.21	0.40
1:F:133:LYS:HD3	1:F:133:LYS:N	2.36	0.40
1:K:343:GLY:CA	1:K:418:GLU:HG2	2.52	0.40
1:N:311:LEU:HD23	1:N:311:LEU:HA	1.89	0.40
1:B:120:VAL:HG11	1:B:126:LEU:HG	2.03	0.40
1:C:612:LYS:O	1:C:616:GLU:HG3	2.21	0.40
1:D:214:LEU:HD12	1:D:221:MET:HE3	2.02	0.40
1:E:107:VAL:CG2	1:E:129:THR:HG21	2.52	0.40
1:E:471:LYS:HB3	1:E:475:PRO:HD2	2.03	0.40
1:F:8:ASP:OD1	1:F:8:ASP:N	2.55	0.40
1:I:252:LEU:C	1:I:252:LEU:CD1	2.94	0.40
1:K:529:LYS:HE3	13:K:1804:HOH:O	2.20	0.40
1:L:122:ASN:HB3	13:L:1670:HOH:O	2.21	0.40
1:P:437:GLY:HA2	2:P:1104:SF4:S2	2.61	0.40
1:B:4:TRP:CH2	1:B:36:PRO:HB2	2.55	0.40
1:D:148:MET:HE2	1:D:150:LEU:HD11	2.03	0.40
1:D:553:LYS:HE3	1:D:594:ARG:HG3	2.04	0.40
1:E:224:VAL:HG11	1:E:227:PHE:CE2	2.56	0.40
1:G:61:LYS:HG2	1:G:266:MET:HE2	2.03	0.40
1:I:271:VAL:HA	1:I:282:THR:O	2.21	0.40
1:M:606:LYS:HB2	1:P:565:LYS:HB3	2.04	0.40
1:O:271:VAL:HA	1:O:282:THR:O	2.20	0.40
1:E:359:LYS:HG2	1:E:364:TYR:CE2	2.56	0.40
1:M:385:MET:HE2	1:N:385:MET:HE2	2.04	0.40
1:N:91[B]:THR:HB	1:N:297[B]:ILE:HD11	2.02	0.40
1:N:198[A]:GLY:O	1:N:270[A]:SER:HA	2.22	0.40
1:A:569[B]:VAL:HG21	4:A:1116:EDO:C2	2.52	0.40
1:C:94:LYS:HG3	1:C:126:LEU:HD23	2.03	0.40
1:I:354:ILE:HD12	1:I:404:MET:HE2	2.03	0.40
1:J:234:LEU:HD22	1:J:250:ILE:CD1	2.51	0.40
1:K:530:CYS:SG	1:K:539:ARG:HD3	2.62	0.40
11:M:1115:PEG:H32	11:M:1115:PEG:H12	1.77	0.40
1:N:257[B]:LYS:O	1:N:319[B]:PHE:HA	2.21	0.40
1:O:471:LYS:HB3	1:O:475:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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
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
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

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	183	LYS
1	A	554	THR
1	B	252	LEU
1	B	554	THR
1	C	252	LEU
1	C	310	LYS
1	C	418	GLU
1	C	554	THR

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Mol	Chain	Res	Type
1	D	37	LYS
1	D	78	LYS
1	D	554	THR
1	E	35	ARG
1	E	114	LYS
1	E	219	ILE
1	E	221	MET
1	E	252	LEU
1	E	554	THR
1	F	529[A]	LYS
1	F	529[B]	LYS
1	F	554	THR
1	F	584[A]	HIS
1	F	584[B]	HIS
1	G	233	LYS
1	G	244	LYS
1	G	368	GLU
1	G	554	THR
1	H	252	LEU
1	H	492	GLU
1	H	554	THR
1	I	414	ILE
1	I	554	THR
1	J	310	LYS
1	J	554	THR
1	K	252	LEU
1	K	554	THR
1	L	554	THR
1	M	238	VAL
1	M	252	LEU
1	M	554	THR
1	N	202[A]	THR
1	N	202[B]	THR
1	N	217[A]	TYR
1	N	242[A]	GLU
1	N	554	THR
1	O	346	LYS
1	O	554	THR
1	P	214	LEU
1	P	554	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	239	ASN
1	D	243	HIS
1	D	618	ASN
1	E	99	ASN
1	E	494	ASN
1	F	239	ASN
1	H	12	ASN
1	H	239	ASN
1	I	218	ASN
1	J	239	ASN
1	K	239	ASN
1	L	99	ASN
1	M	243	HIS
1	N	618	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
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

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

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

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

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

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

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

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-

All (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
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
5	N	1012	SRM	C4A-NA	-12.98	1.25	1.35
5	I	1109	SRM	C4A-NA	-12.96	1.25	1.35
5	E	1109	SRM	C4A-NA	-12.57	1.26	1.35
5	F	1109	SRM	C4A-NA	-12.00	1.26	1.35
5	K	1109	SRM	C4A-NA	-11.94	1.26	1.35
5	C	3910	SRM	C4A-NA	-11.93	1.26	1.35
5	G	1109	SRM	C4A-NA	-11.88	1.26	1.35
5	A	1109	SRM	C4A-NA	-11.52	1.27	1.35
5	J	1109	SRM	C4A-NA	-11.44	1.27	1.35
5	D	4610	SRM	C4A-NA	-11.18	1.27	1.35
5	P	1109	SRM	C4A-NA	-11.10	1.27	1.35
5	O	1109	SRM	C4B-NB	-10.37	1.27	1.35
5	O	1109	SRM	C4D-ND	-6.61	1.27	1.39
5	O	1109	SRM	FE-NC	6.23	2.15	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1109	SRM	C1C-NC	-5.48	1.29	1.39
5	F	1109	SRM	C3C-C2C	5.25	1.47	1.36
5	H	4410	SRM	C1C-NC	-5.19	1.29	1.39
5	G	1109	SRM	C3C-C2C	5.12	1.47	1.36
5	L	1109	SRM	C3C-C2C	5.05	1.47	1.36
5	H	4410	SRM	C4D-ND	-5.01	1.30	1.39
5	H	4410	SRM	C4B-NB	-5.01	1.31	1.35
5	O	1109	SRM	FE-ND	4.97	2.11	1.95
5	M	1109	SRM	C3C-C2C	4.95	1.47	1.36
5	B	4210	SRM	C3C-C2C	4.93	1.47	1.36
5	H	4410	SRM	C4C-NC	-4.92	1.30	1.39
5	E	1109	SRM	FE-ND	4.91	2.11	1.95
5	A	1109	SRM	FE-ND	4.89	2.11	1.95
5	A	1109	SRM	C3C-C2C	4.87	1.46	1.36
5	I	1109	SRM	FE-NC	4.86	2.11	1.95
5	J	1109	SRM	C3C-C2C	4.86	1.46	1.36
5	B	4210	SRM	FE-NC	4.82	2.11	1.95
5	D	4610	SRM	C3C-C2C	4.80	1.46	1.36
3	E	1106	FAD	C9A-C5X	4.80	1.48	1.41
5	K	1109	SRM	C3C-C2C	4.76	1.46	1.36
5	J	1109	SRM	FE-ND	4.75	2.10	1.95
5	G	1109	SRM	FE-ND	4.73	2.10	1.95
5	C	3910	SRM	C3C-C2C	4.72	1.46	1.36
5	D	4610	SRM	FE-NC	4.72	2.10	1.95
3	D	4607	FAD	C9A-C5X	4.71	1.48	1.41
5	K	1109	SRM	FE-ND	4.70	2.10	1.95
5	P	1109	SRM	C3C-C2C	4.70	1.46	1.36
5	N	1012	SRM	C3C-C2C	4.70	1.46	1.36
5	K	1109	SRM	FE-NC	4.68	2.10	1.95
5	E	1109	SRM	C3C-C2C	4.67	1.46	1.36
5	I	1109	SRM	FE-ND	4.67	2.10	1.95
5	G	1109	SRM	CHD-C4C	4.65	1.47	1.38
5	O	1109	SRM	C3C-C2C	4.65	1.46	1.36
5	L	1109	SRM	FE-ND	4.65	2.10	1.95
5	E	1109	SRM	CHD-C4C	4.64	1.47	1.38
3	F	1106	FAD	C9A-C5X	4.62	1.48	1.41
5	A	1109	SRM	FE-NC	4.62	2.10	1.95
5	A	1109	SRM	CHD-C4C	4.62	1.47	1.38
5	C	3910	SRM	FE-NC	4.61	2.10	1.95
5	E	1109	SRM	CHC-C1C	4.60	1.47	1.38
5	P	1109	SRM	CHD-C4C	4.60	1.47	1.38
5	D	4610	SRM	CHC-C1C	4.59	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	1109	SRM	C4D-ND	-4.59	1.31	1.39
5	K	1109	SRM	CHD-C4C	4.58	1.47	1.38
5	C	3910	SRM	CHD-C4C	4.55	1.47	1.38
5	I	1109	SRM	C3C-C2C	4.54	1.46	1.36
5	I	1109	SRM	CHD-C4C	4.54	1.47	1.38
5	N	1012	SRM	CHD-C4C	4.53	1.47	1.38
5	P	1109	SRM	FE-NC	4.53	2.10	1.95
5	E	1109	SRM	FE-NC	4.53	2.10	1.95
3	O	1106	FAD	C9A-C5X	4.50	1.48	1.41
5	H	4410	SRM	C3C-C2C	4.50	1.46	1.36
5	B	4210	SRM	FE-ND	4.49	2.10	1.95
5	B	4210	SRM	CHC-C1C	4.49	1.47	1.38
5	J	1109	SRM	FE-NC	4.49	2.10	1.95
5	B	4210	SRM	CHD-C4C	4.49	1.47	1.38
3	M	1106	FAD	C9A-C5X	4.47	1.48	1.41
5	M	1109	SRM	FE-NC	4.47	2.09	1.95
5	G	1109	SRM	FE-NC	4.46	2.09	1.95
5	L	1109	SRM	CHD-C4C	4.44	1.47	1.38
5	O	1109	SRM	O4B-CEB	-4.43	1.16	1.30
5	M	1109	SRM	CHC-C1C	4.41	1.47	1.38
5	F	1109	SRM	FE-NC	4.40	2.09	1.95
5	J	1109	SRM	CHC-C1C	4.39	1.47	1.38
5	N	1012	SRM	FE-ND	4.37	2.09	1.95
5	H	4410	SRM	FE-NC	4.37	2.09	1.95
5	J	1109	SRM	CHD-C4C	4.37	1.46	1.38
5	P	1109	SRM	CHC-C1C	4.37	1.46	1.38
3	J	1106	FAD	C5A-C4A	4.37	1.46	1.39
3	C	3907	FAD	C9A-C5X	4.35	1.48	1.41
5	L	1109	SRM	FE-NC	4.34	2.09	1.95
5	C	3910	SRM	CHC-C1C	4.33	1.46	1.38
3	O	1106	FAD	C5A-C4A	4.32	1.46	1.39
5	P	1109	SRM	C1C-NC	-4.32	1.31	1.39
3	B	4207	FAD	C9A-C5X	4.30	1.48	1.41
5	N	1012	SRM	FE-NC	4.30	2.09	1.95
5	M	1109	SRM	FE-ND	4.29	2.09	1.95
5	C	3910	SRM	FE-ND	4.28	2.09	1.95
3	D	4607	FAD	C5A-C4A	4.26	1.46	1.39
5	H	4410	SRM	FE-ND	4.26	2.09	1.95
3	H	4407	FAD	C5A-C4A	4.25	1.46	1.39
3	F	1106	FAD	C5A-C4A	4.24	1.46	1.39
5	P	1109	SRM	FE-ND	4.24	2.09	1.95
3	P	1106	FAD	C9A-C5X	4.23	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	1109	SRM	CHC-C1C	4.22	1.46	1.38
5	A	1109	SRM	CHA-C4D	4.21	1.48	1.39
5	O	1109	SRM	CHC-C1C	4.21	1.46	1.38
5	F	1109	SRM	FE-ND	4.21	2.09	1.95
3	H	4407	FAD	C9A-C5X	4.19	1.47	1.41
3	E	1106	FAD	C5A-C4A	4.19	1.46	1.39
3	A	1106	FAD	C9A-C5X	4.18	1.47	1.41
5	F	1109	SRM	CHD-C4C	4.18	1.46	1.38
5	I	1109	SRM	CHC-C1C	4.18	1.46	1.38
3	L	1106	FAD	C5A-C4A	4.18	1.46	1.39
3	B	4207	FAD	C5A-C4A	4.17	1.46	1.39
5	B	4210	SRM	CHA-C4D	4.17	1.48	1.39
5	H	4410	SRM	CHD-C4C	4.15	1.46	1.38
5	D	4610	SRM	FE-ND	4.14	2.08	1.95
5	G	1109	SRM	CHC-C1C	4.14	1.46	1.38
3	L	1106	FAD	C9A-C5X	4.14	1.47	1.41
3	P	1106	FAD	C5A-C4A	4.13	1.46	1.39
5	M	1109	SRM	C4B-NB	-4.13	1.32	1.35
5	O	1109	SRM	CHD-C4C	4.11	1.46	1.38
5	N	1012	SRM	CHA-C4D	4.11	1.48	1.39
5	H	4410	SRM	CHA-C4D	4.11	1.48	1.39
3	M	1106	FAD	C5A-C4A	4.10	1.46	1.39
5	F	1109	SRM	C4D-ND	-4.10	1.31	1.39
5	L	1109	SRM	CHC-C1C	4.09	1.46	1.38
3	C	3907	FAD	C5A-C4A	4.09	1.46	1.39
5	K	1109	SRM	CHA-C4D	4.08	1.48	1.39
5	O	1109	SRM	CHA-C4D	4.07	1.48	1.39
5	E	1109	SRM	CHA-C4D	4.07	1.48	1.39
5	C	3910	SRM	CHA-C4D	4.06	1.48	1.39
5	D	4610	SRM	CHD-C4C	4.05	1.46	1.38
5	A	1109	SRM	CHC-C1C	4.05	1.46	1.38
5	N	1012	SRM	C4D-ND	-4.04	1.32	1.39
5	L	1109	SRM	CHA-C4D	4.03	1.48	1.39
5	J	1109	SRM	C1C-NC	-4.00	1.32	1.39
5	D	4610	SRM	CHA-C4D	4.00	1.48	1.39
5	B	4210	SRM	C1C-NC	-4.00	1.32	1.39
5	O	1109	SRM	O2B-CCB	-3.98	1.17	1.30
3	A	1106	FAD	C5A-C4A	3.98	1.46	1.39
3	K	1106	FAD	C9A-C5X	3.98	1.47	1.41
5	J	1109	SRM	CHA-C4D	3.97	1.48	1.39
5	M	1109	SRM	C1D-ND	-3.93	1.32	1.39
3	J	1106	FAD	C9A-C5X	3.92	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	P	1109	SRM	C4D-ND	-3.91	1.32	1.39
5	P	1109	SRM	CHA-C4D	3.89	1.48	1.39
5	C	3910	SRM	C1C-NC	-3.89	1.32	1.39
5	E	1109	SRM	CHD-C1D	3.86	1.48	1.39
5	K	1109	SRM	CHC-C1C	3.86	1.45	1.38
5	L	1109	SRM	C1C-NC	-3.85	1.32	1.39
5	E	1109	SRM	C1C-NC	-3.83	1.32	1.39
5	O	1109	SRM	O4D-CED	-3.79	1.18	1.30
3	L	1106	FAD	C4-N3	-3.79	1.31	1.38
3	K	1106	FAD	C5A-C4A	3.78	1.45	1.39
5	M	1109	SRM	C1C-NC	-3.78	1.32	1.39
5	K	1109	SRM	C1C-NC	-3.77	1.32	1.39
5	B	4210	SRM	CHD-C1D	3.77	1.47	1.39
5	G	1109	SRM	C4D-ND	-3.76	1.32	1.39
5	O	1109	SRM	CHD-C1D	3.76	1.47	1.39
5	N	1012	SRM	C1C-NC	-3.74	1.32	1.39
5	I	1109	SRM	CHA-C4D	3.73	1.47	1.39
5	A	1109	SRM	CHD-C1D	3.73	1.47	1.39
5	H	4410	SRM	C1D-ND	-3.73	1.32	1.39
5	F	1109	SRM	CHD-C1D	3.72	1.47	1.39
5	K	1109	SRM	CHD-C1D	3.72	1.47	1.39
5	M	1109	SRM	CHD-C4C	3.71	1.45	1.38
5	G	1109	SRM	CHA-C4D	3.70	1.47	1.39
5	N	1012	SRM	CHC-C1C	3.70	1.45	1.38
5	A	1109	SRM	C4D-ND	-3.69	1.32	1.39
5	C	3910	SRM	C4D-ND	-3.69	1.32	1.39
5	B	4210	SRM	C4C-NC	-3.69	1.32	1.39
5	L	1109	SRM	C4C-NC	-3.68	1.32	1.39
5	O	1109	SRM	C4C-NC	-3.68	1.32	1.39
5	N	1012	SRM	C4C-NC	-3.67	1.32	1.39
5	I	1109	SRM	C1C-NC	-3.67	1.32	1.39
5	L	1109	SRM	CHD-C1D	3.66	1.47	1.39
5	D	4610	SRM	C4D-ND	-3.65	1.32	1.39
5	F	1109	SRM	C1C-NC	-3.64	1.32	1.39
5	M	1109	SRM	CHA-C4D	3.63	1.47	1.39
5	I	1109	SRM	CHD-C1D	3.63	1.47	1.39
5	G	1109	SRM	C4C-NC	-3.63	1.32	1.39
5	D	4610	SRM	C1C-NC	-3.62	1.32	1.39
5	F	1109	SRM	C4C-NC	-3.59	1.32	1.39
5	N	1012	SRM	CHD-C1D	3.58	1.47	1.39
5	I	1109	SRM	C4C-NC	-3.57	1.32	1.39
5	A	1109	SRM	C1C-NC	-3.55	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1109	SRM	C4D-ND	-3.54	1.32	1.39
5	A	1109	SRM	C4C-NC	-3.53	1.33	1.39
5	C	3910	SRM	CHD-C1D	3.52	1.47	1.39
5	F	1109	SRM	CHA-C4D	3.52	1.47	1.39
5	I	1109	SRM	C4D-ND	-3.51	1.33	1.39
5	G	1109	SRM	C1C-NC	-3.50	1.33	1.39
5	B	4210	SRM	C4D-ND	-3.49	1.33	1.39
5	J	1109	SRM	C1D-ND	-3.49	1.33	1.39
5	J	1109	SRM	CHD-C1D	3.48	1.47	1.39
5	P	1109	SRM	CHD-C1D	3.46	1.47	1.39
5	G	1109	SRM	CHD-C1D	3.46	1.47	1.39
3	A	1106	FAD	C5A-N7A	-3.46	1.32	1.39
5	O	1109	SRM	C1D-ND	-3.46	1.33	1.39
5	O	1109	SRM	O4C-CEC	-3.45	1.19	1.30
5	K	1109	SRM	C4D-ND	-3.44	1.33	1.39
3	J	1106	FAD	C5X-N5	-3.43	1.33	1.39
5	H	4410	SRM	CHC-C1C	3.43	1.45	1.38
5	H	4410	SRM	O2B-CCB	-3.42	1.19	1.30
5	M	1109	SRM	CHD-C1D	3.41	1.47	1.39
5	P	1109	SRM	C4C-NC	-3.40	1.33	1.39
5	M	1109	SRM	C4C-NC	-3.40	1.33	1.39
3	B	4207	FAD	C4-N3	-3.40	1.32	1.38
5	L	1109	SRM	C4D-ND	-3.40	1.33	1.39
3	O	1106	FAD	C4-N3	-3.40	1.32	1.38
3	D	4607	FAD	C5X-N5	-3.39	1.33	1.39
5	D	4610	SRM	CHD-C1D	3.36	1.47	1.39
5	J	1109	SRM	C4D-ND	-3.36	1.33	1.39
5	F	1109	SRM	C4B-NB	-3.34	1.32	1.35
5	K	1109	SRM	C4C-NC	-3.34	1.33	1.39
5	C	3910	SRM	C4C-NC	-3.33	1.33	1.39
5	O	1109	SRM	O2C-CCC	-3.31	1.19	1.30
5	D	4610	SRM	C4C-NC	-3.28	1.33	1.39
3	J	1106	FAD	C4-N3	-3.27	1.32	1.38
5	E	1109	SRM	C4C-NC	-3.25	1.33	1.39
3	C	3907	FAD	C5A-N7A	-3.25	1.33	1.39
5	H	4410	SRM	CHD-C1D	3.21	1.46	1.39
3	K	1106	FAD	C5A-N7A	-3.21	1.33	1.39
3	E	1106	FAD	C4-N3	-3.20	1.32	1.38
5	O	1109	SRM	O2A-CCA	-3.19	1.20	1.30
3	M	1106	FAD	C5A-N7A	-3.18	1.33	1.39
5	J	1109	SRM	C4C-NC	-3.13	1.33	1.39
5	G	1109	SRM	C1D-ND	-3.13	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4210	SRM	C4B-NB	-3.12	1.33	1.35
3	B	4207	FAD	C5X-N5	-3.11	1.33	1.39
3	F	1106	FAD	C5A-N7A	-3.09	1.33	1.39
3	P	1106	FAD	C5A-N7A	-3.08	1.33	1.39
3	H	4407	FAD	C8-C7	3.08	1.48	1.40
3	M	1106	FAD	C4-N3	-3.08	1.33	1.38
3	C	3907	FAD	C5X-N5	-3.06	1.33	1.39
3	J	1106	FAD	C5A-N7A	-3.05	1.33	1.39
3	D	4607	FAD	C4-N3	-3.05	1.33	1.38
5	D	4610	SRM	C1D-ND	-3.04	1.33	1.39
3	C	3907	FAD	C8-C7	3.01	1.48	1.40
3	B	4207	FAD	C5A-N7A	-2.99	1.33	1.39
5	K	1109	SRM	C4B-NB	-2.99	1.33	1.35
5	B	4210	SRM	C1D-ND	-2.98	1.34	1.39
5	H	4410	SRM	O4D-CED	-2.98	1.21	1.30
5	C	3910	SRM	C1D-ND	-2.98	1.34	1.39
3	K	1106	FAD	C5X-N5	-2.95	1.34	1.39
3	B	4207	FAD	C8-C7	2.94	1.48	1.40
3	M	1106	FAD	C5X-N5	-2.94	1.34	1.39
5	I	1109	SRM	C1D-ND	-2.92	1.34	1.39
5	H	4410	SRM	O2D-CCD	-2.92	1.21	1.30
3	B	4207	FAD	C4A-N9A	-2.92	1.31	1.37
3	L	1106	FAD	C5X-N5	-2.91	1.34	1.39
3	K	1106	FAD	C4-N3	-2.91	1.33	1.38
3	E	1106	FAD	C5X-N5	-2.89	1.34	1.39
5	E	1109	SRM	C1D-ND	-2.89	1.34	1.39
5	P	1109	SRM	C1D-ND	-2.88	1.34	1.39
5	A	1109	SRM	C4B-NB	-2.87	1.33	1.35
3	P	1106	FAD	C4A-N9A	-2.87	1.31	1.37
5	H	4410	SRM	O2C-CCC	-2.86	1.21	1.30
3	P	1106	FAD	C4-N3	-2.85	1.33	1.38
5	F	1109	SRM	C1D-ND	-2.85	1.34	1.39
5	L	1109	SRM	C1D-ND	-2.85	1.34	1.39
3	M	1106	FAD	C8-C7	2.84	1.47	1.40
3	F	1106	FAD	C8-C7	2.83	1.47	1.40
3	D	4607	FAD	C5A-N7A	-2.83	1.33	1.39
5	M	1109	SRM	O4D-CED	-2.83	1.21	1.30
3	L	1106	FAD	C5A-N7A	-2.82	1.33	1.39
3	C	3907	FAD	C4-N3	-2.81	1.33	1.38
5	A	1109	SRM	CHB-C4A	2.81	1.47	1.39
3	F	1106	FAD	C4-N3	-2.81	1.33	1.38
5	O	1109	SRM	O4A-CEA	-2.79	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1106	FAD	C8-C7	2.78	1.47	1.40
3	D	4607	FAD	C8-C7	2.78	1.47	1.40
5	M	1109	SRM	O2D-CCD	-2.76	1.21	1.30
3	D	4607	FAD	C4A-N9A	-2.76	1.32	1.37
3	O	1106	FAD	C8-C7	2.75	1.47	1.40
3	L	1106	FAD	C8-C7	2.75	1.47	1.40
3	L	1106	FAD	C2-N3	-2.75	1.32	1.39
3	F	1106	FAD	C5X-N5	-2.74	1.34	1.39
5	M	1109	SRM	CHC-C4B	-2.74	1.31	1.39
5	O	1109	SRM	CHB-C4A	2.73	1.46	1.39
3	L	1106	FAD	C4A-N9A	-2.71	1.32	1.37
3	E	1106	FAD	C5A-N7A	-2.70	1.34	1.39
5	P	1109	SRM	O4B-CEB	-2.70	1.21	1.30
3	E	1106	FAD	C8-C7	2.69	1.47	1.40
3	O	1106	FAD	C5A-N7A	-2.68	1.34	1.39
3	K	1106	FAD	C4A-N9A	-2.68	1.32	1.37
5	G	1109	SRM	CHB-C4A	2.67	1.46	1.39
5	D	4610	SRM	O2B-CCB	-2.67	1.22	1.30
5	M	1109	SRM	O4B-CEB	-2.67	1.22	1.30
3	K	1106	FAD	C8A-N9A	-2.66	1.33	1.37
3	P	1106	FAD	C2-N3	-2.65	1.33	1.39
3	A	1106	FAD	C8A-N9A	-2.64	1.33	1.37
3	H	4407	FAD	C5A-N7A	-2.64	1.34	1.39
3	A	1106	FAD	C4A-N9A	-2.64	1.32	1.37
5	J	1109	SRM	CHB-C4A	2.63	1.46	1.39
5	N	1012	SRM	O4D-CED	-2.63	1.22	1.30
3	O	1106	FAD	C5X-N5	-2.63	1.34	1.39
5	A	1109	SRM	C1D-ND	-2.62	1.34	1.39
3	F	1106	FAD	C4A-N9A	-2.62	1.32	1.37
3	O	1106	FAD	C2-N3	-2.61	1.33	1.39
5	H	4410	SRM	O4B-CEB	-2.61	1.22	1.30
3	A	1106	FAD	C8-C7	2.61	1.47	1.40
5	O	1109	SRM	O2D-CCD	-2.60	1.22	1.30
5	G	1109	SRM	O4B-CEB	-2.59	1.22	1.30
3	A	1106	FAD	C4-N3	-2.59	1.34	1.38
3	H	4407	FAD	C4-N3	-2.59	1.34	1.38
5	K	1109	SRM	CHC-C4B	-2.58	1.31	1.39
5	M	1109	SRM	O2B-CCB	-2.57	1.22	1.30
5	J	1109	SRM	O4B-CEB	-2.57	1.22	1.30
5	A	1109	SRM	O4B-CEB	-2.54	1.22	1.30
3	O	1106	FAD	C4A-N9A	-2.54	1.32	1.37
5	M	1109	SRM	CHB-C4A	2.53	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	1109	SRM	O2D-CCD	-2.53	1.22	1.30
3	B	4207	FAD	C2-N3	-2.53	1.33	1.39
5	H	4410	SRM	O4C-CEC	-2.52	1.22	1.30
5	K	1109	SRM	O4B-CEB	-2.51	1.22	1.30
5	L	1109	SRM	O2A-CCA	-2.50	1.22	1.30
5	H	4410	SRM	O2A-CCA	-2.50	1.22	1.30
5	H	4410	SRM	CHC-C4B	-2.50	1.32	1.39
5	A	1109	SRM	C4D-C3D	2.49	1.49	1.44
3	C	3907	FAD	C4A-N9A	-2.48	1.32	1.37
3	J	1106	FAD	C8-C7	2.48	1.46	1.40
5	D	4610	SRM	CHB-C4A	2.48	1.46	1.39
5	L	1109	SRM	CHC-C4B	-2.48	1.32	1.39
3	J	1106	FAD	C2-N3	-2.47	1.33	1.39
3	K	1106	FAD	C8-C7	2.47	1.46	1.40
5	A	1109	SRM	O2C-CCC	-2.47	1.22	1.30
5	L	1109	SRM	O4D-CED	-2.47	1.22	1.30
3	E	1106	FAD	C5A-C6A	2.46	1.47	1.41
3	K	1106	FAD	C2-N3	-2.46	1.33	1.39
5	K	1109	SRM	C1D-ND	-2.46	1.35	1.39
5	L	1109	SRM	O2D-CCD	-2.45	1.22	1.30
3	M	1106	FAD	C4A-N9A	-2.45	1.32	1.37
5	P	1109	SRM	O2B-CCB	-2.45	1.22	1.30
3	D	4607	FAD	C2-N3	-2.44	1.33	1.39
5	I	1109	SRM	O2B-CCB	-2.44	1.22	1.30
3	E	1106	FAD	C8A-N9A	-2.44	1.33	1.37
3	C	3907	FAD	C2-N3	-2.44	1.33	1.39
5	M	1109	SRM	O2C-CCC	-2.43	1.22	1.30
5	E	1109	SRM	O2B-CCB	-2.43	1.22	1.30
5	N	1012	SRM	CHB-C4A	2.43	1.46	1.39
5	P	1109	SRM	CHB-C4A	2.43	1.46	1.39
5	F	1109	SRM	O2B-CCB	-2.43	1.22	1.30
3	J	1106	FAD	C4A-N9A	-2.43	1.32	1.37
5	M	1109	SRM	O4C-CEC	-2.42	1.22	1.30
5	E	1109	SRM	O4D-CED	-2.42	1.22	1.30
5	C	3910	SRM	O2D-CCD	-2.41	1.22	1.30
5	K	1109	SRM	O2D-CCD	-2.40	1.22	1.30
5	C	3910	SRM	O4D-CED	-2.40	1.22	1.30
5	O	1109	SRM	CBB-CCB	2.40	1.56	1.50
5	B	4210	SRM	O4D-CED	-2.39	1.22	1.30
5	G	1109	SRM	O2B-CCB	-2.39	1.22	1.30
5	A	1109	SRM	O2D-CCD	-2.39	1.22	1.30
5	A	1109	SRM	O2B-CCB	-2.38	1.22	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	1109	SRM	CHC-C4B	-2.38	1.32	1.39
5	G	1109	SRM	O4D-CED	-2.38	1.23	1.30
5	B	4210	SRM	O2D-CCD	-2.37	1.23	1.30
5	D	4610	SRM	O2C-CCC	-2.37	1.23	1.30
5	E	1109	SRM	C4B-NB	-2.37	1.33	1.35
5	G	1109	SRM	O2C-CCC	-2.37	1.23	1.30
5	L	1109	SRM	O2B-CCB	-2.37	1.23	1.30
3	E	1106	FAD	C4A-N9A	-2.36	1.32	1.37
5	C	3910	SRM	CHB-C4A	2.36	1.45	1.39
5	F	1109	SRM	CHB-C4A	2.36	1.45	1.39
5	F	1109	SRM	O4B-CEB	-2.36	1.23	1.30
3	H	4407	FAD	C5A-C6A	2.36	1.47	1.41
5	B	4210	SRM	O2A-CCA	-2.36	1.23	1.30
5	I	1109	SRM	O2D-CCD	-2.36	1.23	1.30
5	K	1109	SRM	CHB-C4A	2.35	1.45	1.39
5	I	1109	SRM	CHB-C4A	2.35	1.45	1.39
3	A	1106	FAD	C5X-N5	-2.35	1.35	1.39
5	D	4610	SRM	CHC-C4B	-2.35	1.32	1.39
5	M	1109	SRM	O2A-CCA	-2.34	1.23	1.30
3	H	4407	FAD	C4A-N9A	-2.34	1.32	1.37
5	F	1109	SRM	O2C-CCC	-2.34	1.23	1.30
3	P	1106	FAD	C5A-C6A	2.34	1.47	1.41
5	J	1109	SRM	O2D-CCD	-2.33	1.23	1.30
3	H	4407	FAD	C5X-N5	-2.33	1.35	1.39
5	F	1109	SRM	O2D-CCD	-2.32	1.23	1.30
5	K	1109	SRM	C4D-C3D	2.32	1.49	1.44
3	L	1106	FAD	C5A-C6A	2.32	1.47	1.41
5	E	1109	SRM	CHB-C4A	2.32	1.45	1.39
5	P	1109	SRM	O2A-CCA	-2.32	1.23	1.30
5	I	1109	SRM	O4D-CED	-2.31	1.23	1.30
3	H	4407	FAD	C8A-N9A	-2.31	1.33	1.37
5	K	1109	SRM	O4D-CED	-2.31	1.23	1.30
5	C	3910	SRM	O2C-CCC	-2.31	1.23	1.30
5	C	3910	SRM	O4B-CEB	-2.31	1.23	1.30
5	N	1012	SRM	O2D-CCD	-2.30	1.23	1.30
5	B	4210	SRM	O4C-CEC	-2.30	1.23	1.30
5	E	1109	SRM	O2C-CCC	-2.30	1.23	1.30
5	D	4610	SRM	O2D-CCD	-2.30	1.23	1.30
5	D	4610	SRM	O2A-CCA	-2.29	1.23	1.30
5	J	1109	SRM	O4D-CED	-2.29	1.23	1.30
5	M	1109	SRM	O4A-CEA	-2.29	1.23	1.30
5	N	1012	SRM	C1D-ND	-2.28	1.35	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	P	1106	FAD	C8A-N9A	-2.28	1.33	1.37
5	G	1109	SRM	C4B-NB	-2.28	1.33	1.35
5	N	1012	SRM	O2C-CCC	-2.27	1.23	1.30
5	J	1109	SRM	O4C-CEC	-2.27	1.23	1.30
5	A	1109	SRM	O4D-CED	-2.27	1.23	1.30
5	F	1109	SRM	CHC-C4B	-2.27	1.32	1.39
5	I	1109	SRM	O4C-CEC	-2.27	1.23	1.30
5	A	1109	SRM	CHC-C4B	-2.26	1.32	1.39
5	N	1012	SRM	O4B-CEB	-2.26	1.23	1.30
5	J	1109	SRM	C4B-NB	-2.26	1.33	1.35
5	N	1012	SRM	O4C-CEC	-2.26	1.23	1.30
5	B	4210	SRM	CHC-C4B	-2.25	1.32	1.39
5	K	1109	SRM	O2C-CCC	-2.25	1.23	1.30
5	B	4210	SRM	O4B-CEB	-2.25	1.23	1.30
3	O	1106	FAD	C5A-C6A	2.24	1.47	1.41
5	O	1109	SRM	FE-NA	2.24	2.01	1.94
5	N	1012	SRM	CHC-C4B	-2.24	1.32	1.39
5	J	1109	SRM	O2C-CCC	-2.24	1.23	1.30
5	D	4610	SRM	O4B-CEB	-2.24	1.23	1.30
5	I	1109	SRM	O2C-CCC	-2.23	1.23	1.30
5	C	3910	SRM	C4B-NB	-2.23	1.33	1.35
3	F	1106	FAD	C5A-C6A	2.23	1.47	1.41
5	A	1109	SRM	O4C-CEC	-2.23	1.23	1.30
5	J	1109	SRM	O2B-CCB	-2.22	1.23	1.30
5	C	3910	SRM	CHC-C4B	-2.22	1.32	1.39
5	L	1109	SRM	O4C-CEC	-2.22	1.23	1.30
5	I	1109	SRM	O4B-CEB	-2.21	1.23	1.30
3	E	1106	FAD	C2-N3	-2.21	1.34	1.39
5	C	3910	SRM	O4C-CEC	-2.21	1.23	1.30
5	N	1012	SRM	C4B-NB	-2.19	1.33	1.35
5	E	1109	SRM	CHC-C4B	-2.19	1.32	1.39
5	F	1109	SRM	O4D-CED	-2.19	1.23	1.30
3	D	4607	FAD	C8A-N9A	-2.19	1.33	1.37
3	J	1106	FAD	C8A-N9A	-2.18	1.33	1.37
3	K	1106	FAD	C5A-C6A	2.18	1.47	1.41
5	B	4210	SRM	O2B-CCB	-2.18	1.23	1.30
5	O	1109	SRM	FE-NB	2.18	2.01	1.94
5	L	1109	SRM	O2C-CCC	-2.18	1.23	1.30
5	I	1109	SRM	CHC-C4B	-2.18	1.32	1.39
5	P	1109	SRM	O2D-CCD	-2.17	1.23	1.30
3	F	1106	FAD	C8A-N9A	-2.17	1.33	1.37
3	A	1106	FAD	C2-N3	-2.17	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	4407	FAD	C2-N3	-2.17	1.34	1.39
3	P	1106	FAD	C5X-N5	-2.16	1.35	1.39
5	L	1109	SRM	C4B-NB	-2.16	1.33	1.35
5	H	4410	SRM	CDC-C2C	-2.16	1.47	1.51
5	L	1109	SRM	CHB-C4A	2.16	1.45	1.39
5	E	1109	SRM	O2D-CCD	-2.16	1.23	1.30
5	K	1109	SRM	O2B-CCB	-2.15	1.23	1.30
5	P	1109	SRM	C4D-C3D	2.15	1.48	1.44
3	M	1106	FAD	C2-N3	-2.15	1.34	1.39
3	B	4207	FAD	C8A-N9A	-2.15	1.33	1.37
5	O	1109	SRM	CHA-C1A	-2.15	1.31	1.37
5	B	4210	SRM	O2C-CCC	-2.15	1.23	1.30
5	F	1109	SRM	C4D-C3D	2.15	1.48	1.44
5	I	1109	SRM	C4B-NB	-2.14	1.33	1.35
3	C	3907	FAD	C8A-N9A	-2.14	1.33	1.37
3	B	4207	FAD	C5A-C6A	2.14	1.47	1.41
3	M	1106	FAD	C8A-N9A	-2.14	1.33	1.37
5	N	1012	SRM	O2B-CCB	-2.14	1.23	1.30
5	K	1109	SRM	O2A-CCA	-2.14	1.23	1.30
5	A	1109	SRM	O2A-CCA	-2.13	1.23	1.30
5	P	1109	SRM	O2C-CCC	-2.13	1.23	1.30
5	C	3910	SRM	O2B-CCB	-2.12	1.23	1.30
3	J	1106	FAD	C5A-C6A	2.12	1.46	1.41
5	B	4210	SRM	CHB-C4A	2.12	1.45	1.39
5	F	1109	SRM	O2A-CCA	-2.12	1.23	1.30
3	D	4607	FAD	C5A-C6A	2.12	1.46	1.41
5	K	1109	SRM	O4C-CEC	-2.11	1.23	1.30
5	H	4410	SRM	CHB-C4A	2.11	1.45	1.39
5	L	1109	SRM	O4B-CEB	-2.11	1.23	1.30
3	C	3907	FAD	PA-O2A	-2.11	1.45	1.55
3	C	3907	FAD	C4X-N5	2.11	1.35	1.30
5	N	1012	SRM	O2A-CCA	-2.10	1.23	1.30
5	P	1109	SRM	C4B-NB	-2.10	1.33	1.35
5	I	1109	SRM	C4D-C3D	2.10	1.48	1.44
5	F	1109	SRM	CHB-C1B	-2.10	1.31	1.37
5	C	3910	SRM	CHB-C1B	-2.09	1.31	1.37
5	E	1109	SRM	O4B-CEB	-2.09	1.23	1.30
5	H	4410	SRM	CHB-C1B	-2.09	1.31	1.37
3	M	1106	FAD	C5A-C6A	2.09	1.46	1.41
5	I	1109	SRM	O2A-CCA	-2.08	1.23	1.30
5	B	4210	SRM	CHB-C1B	-2.07	1.31	1.37
5	D	4610	SRM	C4C-C3C	2.06	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	1109	SRM	CHC-C4B	-2.06	1.33	1.39
5	P	1109	SRM	CHC-C4B	-2.06	1.33	1.39
5	C	3910	SRM	O2A-CCA	-2.05	1.24	1.30
5	D	4610	SRM	CHB-C1B	-2.05	1.31	1.37
3	L	1106	FAD	C8A-N9A	-2.05	1.34	1.37
5	D	4610	SRM	O4D-CED	-2.05	1.24	1.30
5	E	1109	SRM	O4C-CEC	-2.04	1.24	1.30
5	G	1109	SRM	O2A-CCA	-2.04	1.24	1.30
5	G	1109	SRM	CHC-C4B	-2.04	1.33	1.39
3	M	1106	FAD	PA-O3P	-2.04	1.57	1.59
3	F	1106	FAD	C2-N3	-2.03	1.34	1.39
5	H	4410	SRM	CHA-C1A	-2.03	1.31	1.37
5	F	1109	SRM	O4A-CEA	-2.02	1.24	1.30
5	J	1109	SRM	O2A-CCA	-2.02	1.24	1.30
5	H	4410	SRM	O4A-CEA	-2.01	1.24	1.30
3	A	1106	FAD	PA-O2A	-2.01	1.46	1.55
5	G	1109	SRM	C4D-C3D	2.00	1.48	1.44
5	P	1109	SRM	O4D-CED	-2.00	1.24	1.30

All (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
3	F	1106	FAD	C5A-C4A-N3A	-5.60	119.01	126.72
3	J	1106	FAD	C5A-C4A-N3A	-5.57	119.05	126.72
3	A	1106	FAD	C5A-C4A-N3A	-5.54	119.09	126.72
5	O	1109	SRM	C2A-C1A-CHA	-5.45	118.65	123.54
3	H	4407	FAD	C5A-C4A-N3A	-5.44	119.22	126.72
5	H	4410	SRM	C1D-C2D-C3D	-5.35	101.20	106.81
3	K	1106	FAD	C5A-C4A-N3A	-5.33	119.37	126.72
5	O	1109	SRM	CAB-C3B-C4B	5.30	120.44	111.19
3	C	3907	FAD	C5A-C4A-N3A	-5.23	119.52	126.72
5	L	1109	SRM	C2A-C1A-CHA	-5.15	118.92	123.54
3	O	1106	FAD	C5A-C4A-N3A	-5.14	119.63	126.72
5	H	4410	SRM	C2A-C1A-CHA	-5.14	118.92	123.54
5	G	1109	SRM	C2A-C1A-CHA	-5.14	118.93	123.54
3	L	1106	FAD	C5A-C4A-N3A	-5.08	119.72	126.72
5	N	1012	SRM	C2A-C1A-CHA	-5.03	119.02	123.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	4607	FAD	C5A-C4A-N3A	-4.97	119.87	126.72
3	E	1106	FAD	N3A-C4A-N9A	4.88	135.47	127.17
5	K	1109	SRM	C2C-C1C-NC	4.81	114.96	110.32
3	M	1106	FAD	N3A-C4A-N9A	4.74	135.22	127.17
5	C	3910	SRM	C2A-C1A-CHA	-4.70	119.32	123.54
5	I	1109	SRM	C2C-C1C-NC	4.70	114.86	110.32
3	C	3907	FAD	N3A-C4A-N9A	4.70	135.16	127.17
3	A	1106	FAD	N3A-C4A-N9A	4.62	135.02	127.17
3	F	1106	FAD	N3A-C4A-N9A	4.55	134.91	127.17
5	M	1109	SRM	C1D-C2D-C3D	-4.53	102.06	106.81
5	D	4610	SRM	C3C-C4C-NC	4.52	114.69	110.32
5	F	1109	SRM	C1D-C2D-C3D	-4.50	102.09	106.81
3	B	4207	FAD	C5A-C4A-N3A	-4.45	120.59	126.72
3	O	1106	FAD	N3A-C4A-N9A	4.44	134.72	127.17
3	L	1106	FAD	N3A-C4A-N9A	4.43	134.70	127.17
3	H	4407	FAD	N3A-C4A-N9A	4.39	134.63	127.17
5	J	1109	SRM	C4C-C3C-C2C	-4.38	101.94	106.84
5	M	1109	SRM	C2A-C1A-CHA	-4.37	119.62	123.54
5	E	1109	SRM	C2A-C1A-CHA	-4.36	119.62	123.54
3	P	1106	FAD	C4A-C5A-N7A	-4.35	105.61	110.58
3	K	1106	FAD	N3A-C4A-N9A	4.34	134.56	127.17
5	D	4610	SRM	C4C-C3C-C2C	-4.34	101.98	106.84
5	A	1109	SRM	C1D-C2D-C3D	-4.34	102.26	106.81
5	L	1109	SRM	C1D-C2D-C3D	-4.34	102.26	106.81
3	J	1106	FAD	N3A-C4A-N9A	4.33	134.52	127.17
5	A	1109	SRM	C2A-C1A-CHA	-4.31	119.67	123.54
5	D	4610	SRM	C2A-C1A-CHA	-4.30	119.68	123.54
3	B	4207	FAD	N3A-C4A-N9A	4.30	134.48	127.17
5	K	1109	SRM	C2A-C1A-CHA	-4.29	119.69	123.54
5	P	1109	SRM	C1D-C2D-C3D	-4.28	102.32	106.81
5	N	1012	SRM	C1D-C2D-C3D	-4.28	102.32	106.81
5	J	1109	SRM	C3C-C4C-NC	4.26	114.43	110.32
3	D	4607	FAD	N3A-C4A-N9A	4.26	134.41	127.17
5	D	4610	SRM	C2C-C1C-NC	4.23	114.41	110.32
5	M	1109	SRM	C2C-C1C-NC	4.17	114.34	110.32
5	L	1109	SRM	C2C-C1C-NC	4.14	114.31	110.32
5	I	1109	SRM	C3C-C4C-NC	4.14	114.31	110.32
3	P	1106	FAD	N3A-C4A-N9A	4.13	134.19	127.17
5	I	1109	SRM	C1D-C2D-C3D	-4.11	102.50	106.81
5	H	4410	SRM	C4C-C3C-C2C	-4.10	102.26	106.84
5	D	4610	SRM	C1D-C2D-C3D	-4.08	102.53	106.81
5	O	1109	SRM	C4C-C3C-C2C	-4.08	102.28	106.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	P	1109	SRM	C4C-C3C-C2C	-4.07	102.29	106.84
5	F	1109	SRM	C2C-C1C-NC	4.07	114.25	110.32
5	B	4210	SRM	C2A-C1A-CHA	-4.07	119.89	123.54
5	N	1012	SRM	C2C-C1C-NC	4.05	114.23	110.32
3	M	1106	FAD	C4-C4X-N5	4.03	123.78	118.21
5	H	4410	SRM	CAA-C3A-C4A	4.01	118.18	111.19
5	C	3910	SRM	C3C-C4C-NC	3.96	114.14	110.32
5	C	3910	SRM	C1D-C2D-C3D	-3.95	102.66	106.81
5	A	1109	SRM	C2C-C1C-NC	3.95	114.13	110.32
5	B	4210	SRM	C3C-C4C-NC	3.94	114.13	110.32
5	B	4210	SRM	C1D-C2D-C3D	-3.94	102.67	106.81
5	J	1109	SRM	C2C-C1C-NC	3.92	114.10	110.32
5	B	4210	SRM	C4C-C3C-C2C	-3.91	102.47	106.84
5	E	1109	SRM	C1D-C2D-C3D	-3.90	102.72	106.81
5	G	1109	SRM	C1D-C2D-C3D	-3.88	102.74	106.81
5	M	1109	SRM	C1C-C2C-C3C	-3.87	102.51	106.84
5	N	1012	SRM	C1C-C2C-C3C	-3.83	102.55	106.84
5	I	1109	SRM	C2A-C1A-CHA	-3.83	120.10	123.54
5	O	1109	SRM	C3B-C4B-CHC	-3.83	115.18	123.33
5	F	1109	SRM	C3C-C4C-NC	3.83	114.02	110.32
5	I	1109	SRM	C1C-C2C-C3C	-3.82	102.57	106.84
5	I	1109	SRM	C2D-C1D-ND	3.81	114.38	110.15
5	C	3910	SRM	C4C-C3C-C2C	-3.80	102.59	106.84
5	J	1109	SRM	C1D-C2D-C3D	-3.80	102.82	106.81
5	P	1109	SRM	C3C-C4C-NC	3.79	113.98	110.32
5	J	1109	SRM	C2A-C1A-CHA	-3.79	120.14	123.54
5	K	1109	SRM	C1C-C2C-C3C	-3.78	102.62	106.84
5	O	1109	SRM	C4C-NC-C1C	3.77	111.97	105.82
3	P	1106	FAD	C4-C4X-N5	3.76	123.40	118.21
5	C	3910	SRM	C2C-C1C-NC	3.74	113.94	110.32
5	F	1109	SRM	C4C-C3C-C2C	-3.74	102.66	106.84
5	G	1109	SRM	C4C-C3C-C2C	-3.73	102.66	106.84
5	K	1109	SRM	C1D-C2D-C3D	-3.73	102.90	106.81
5	O	1109	SRM	C4D-ND-C1D	3.71	111.88	105.82
3	P	1106	FAD	C2A-N3A-C4A	3.71	120.88	111.83
5	I	1109	SRM	C4D-C3D-C2D	-3.70	102.93	106.81
5	K	1109	SRM	C3C-C4C-NC	3.70	113.89	110.32
5	B	4210	SRM	C2C-C1C-NC	3.69	113.89	110.32
3	E	1106	FAD	C2A-N3A-C4A	3.69	120.84	111.83
5	F	1109	SRM	C1C-C2C-C3C	-3.68	102.72	106.84
5	G	1109	SRM	C3C-C4C-NC	3.66	113.86	110.32
3	K	1106	FAD	C2A-N3A-C4A	3.65	120.74	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1109	SRM	C1C-C2C-C3C	-3.64	102.77	106.84
3	K	1106	FAD	N3A-C2A-N1A	-3.64	123.07	128.58
5	L	1109	SRM	C4C-C3C-C2C	-3.63	102.78	106.84
3	H	4407	FAD	C4A-C5A-N7A	-3.63	106.43	110.58
5	O	1109	SRM	CED-CDD-C3D	3.60	122.82	113.76
5	P	1109	SRM	C2A-C1A-CHA	-3.60	120.31	123.54
5	F	1109	SRM	C2D-C1D-ND	3.60	114.15	110.15
5	I	1109	SRM	C4C-C3C-C2C	-3.60	102.81	106.84
5	I	1109	SRM	C3D-C4D-ND	3.60	114.14	110.15
5	K	1109	SRM	C4C-C3C-C2C	-3.57	102.85	106.84
3	B	4207	FAD	C4A-N9A-C8A	3.56	109.48	105.74
5	H	4410	SRM	C3A-C4A-CHB	-3.56	115.75	123.33
5	P	1109	SRM	C2C-C1C-NC	3.56	113.75	110.32
5	A	1109	SRM	C4C-C3C-C2C	-3.55	102.87	106.84
5	A	1109	SRM	C1C-C2C-C3C	-3.55	102.87	106.84
5	J	1109	SRM	C4D-C3D-C2D	-3.55	103.09	106.81
5	O	1109	SRM	O4C-CEC-O3C	3.53	132.42	123.33
5	A	1109	SRM	C3C-C4C-NC	3.53	113.73	110.32
3	F	1106	FAD	C4A-C5A-N7A	-3.53	106.55	110.58
5	P	1109	SRM	C2D-C1D-ND	3.52	114.06	110.15
5	M	1109	SRM	C3C-C4C-NC	3.50	113.70	110.32
3	H	4407	FAD	C2A-N3A-C4A	3.49	120.37	111.83
5	E	1109	SRM	C3C-C4C-NC	3.48	113.68	110.32
5	L	1109	SRM	C2D-C1D-ND	3.47	114.00	110.15
5	N	1012	SRM	C2D-C1D-ND	3.47	114.00	110.15
5	B	4210	SRM	C1C-C2C-C3C	-3.46	102.97	106.84
5	H	4410	SRM	C2B-C3B-C4B	-3.46	96.51	100.89
5	J	1109	SRM	C2D-C1D-ND	3.46	113.99	110.15
5	E	1109	SRM	C4C-C3C-C2C	-3.45	102.98	106.84
5	A	1109	SRM	C2D-C1D-ND	3.44	113.97	110.15
5	H	4410	SRM	C3A-C2A-C1A	-3.42	95.11	100.92
5	O	1109	SRM	C2B-C3B-C4B	-3.42	96.56	100.89
5	H	4410	SRM	C3B-C4B-CHC	-3.42	116.06	123.33
3	F	1106	FAD	C4-C4X-N5	3.41	122.92	118.21
5	H	4410	SRM	C4A-CHB-C1B	-3.41	120.83	125.84
3	B	4207	FAD	N3A-C2A-N1A	-3.38	123.47	128.58
5	L	1109	SRM	C3C-C4C-NC	3.37	113.58	110.32
3	C	3907	FAD	C2A-N3A-C4A	3.36	120.04	111.83
3	M	1106	FAD	C2A-N3A-C4A	3.36	120.04	111.83
5	H	4410	SRM	CAB-C3B-C4B	3.36	117.04	111.19
3	A	1106	FAD	C2A-N3A-C4A	3.35	120.01	111.83
3	D	4607	FAD	N3A-C2A-N1A	-3.35	123.52	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	3910	SRM	C1C-C2C-C3C	-3.33	103.11	106.84
5	O	1109	SRM	O4D-CED-O3D	3.33	131.89	123.33
5	P	1109	SRM	C4D-C3D-C2D	-3.32	103.33	106.81
5	E	1109	SRM	C2C-C1C-NC	3.32	113.52	110.32
5	E	1109	SRM	C1C-C2C-C3C	-3.29	103.16	106.84
5	M	1109	SRM	C4C-C3C-C2C	-3.29	103.16	106.84
3	C	3907	FAD	N3A-C2A-N1A	-3.29	123.61	128.58
3	L	1106	FAD	C4A-N9A-C8A	3.28	109.19	105.74
3	A	1106	FAD	C4A-C5A-N7A	-3.28	106.83	110.58
5	G	1109	SRM	C1C-C2C-C3C	-3.28	103.17	106.84
5	O	1109	SRM	C4D-C3D-C2D	-3.28	103.37	106.81
5	M	1109	SRM	CAB-C3B-C4B	3.28	116.90	111.19
5	N	1012	SRM	C3D-C4D-ND	3.28	113.79	110.15
3	L	1106	FAD	C2A-N3A-C4A	3.26	119.79	111.83
3	F	1106	FAD	C2A-N3A-C4A	3.25	119.76	111.83
3	A	1106	FAD	N3A-C2A-N1A	-3.24	123.68	128.58
3	H	4407	FAD	N3A-C2A-N1A	-3.24	123.69	128.58
5	M	1109	SRM	C2B-C3B-C4B	-3.22	96.81	100.89
3	E	1106	FAD	C4A-C5A-N7A	-3.22	106.90	110.58
5	N	1012	SRM	C4C-C3C-C2C	-3.21	103.25	106.84
3	O	1106	FAD	C2A-N3A-C4A	3.21	119.66	111.83
3	D	4607	FAD	C5X-C9A-N10	3.20	120.86	117.97
3	P	1106	FAD	N3A-C2A-N1A	-3.19	123.75	128.58
5	E	1109	SRM	C4D-C3D-C2D	-3.19	103.47	106.81
3	M	1106	FAD	N3A-C2A-N1A	-3.18	123.77	128.58
3	J	1106	FAD	C2A-N3A-C4A	3.18	119.59	111.83
3	D	4607	FAD	C2A-N3A-C4A	3.17	119.58	111.83
3	A	1106	FAD	C4-C4X-N5	3.17	122.59	118.21
5	H	4410	SRM	C1C-C2C-C3C	-3.17	103.30	106.84
3	L	1106	FAD	C4A-C5A-N7A	-3.17	106.96	110.58
5	M	1109	SRM	O4B-CEB-CDB	3.13	124.27	114.35
5	N	1012	SRM	C3C-C4C-NC	3.12	113.33	110.32
5	N	1012	SRM	C4D-C3D-C2D	-3.11	103.55	106.81
5	D	4610	SRM	C1C-C2C-C3C	-3.09	103.39	106.84
3	K	1106	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
3	J	1106	FAD	C4A-C5A-N7A	-3.08	107.06	110.58
5	G	1109	SRM	C4D-C3D-C2D	-3.07	103.59	106.81
3	J	1106	FAD	C5X-C9A-N10	3.06	120.73	117.97
5	O	1109	SRM	CAA-C3A-C4A	3.06	116.52	111.19
3	F	1106	FAD	N3A-C2A-N1A	-3.06	123.96	128.58
5	K	1109	SRM	C4D-C3D-C2D	-3.05	103.61	106.81
5	P	1109	SRM	C1C-C2C-C3C	-3.05	103.42	106.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1109	SRM	C2D-C1D-ND	3.04	113.53	110.15
5	J	1109	SRM	C3D-C4D-ND	3.04	113.53	110.15
3	C	3907	FAD	C4A-N9A-C8A	3.04	108.92	105.74
3	P	1106	FAD	C5A-N7A-C8A	3.03	108.21	103.45
3	B	4207	FAD	C2A-N1A-C6A	3.03	123.70	118.73
5	O	1109	SRM	O3D-CED-CDD	-3.02	113.50	122.11
5	G	1109	SRM	C2C-C1C-NC	3.02	113.24	110.32
5	L	1109	SRM	O4B-CEB-CDB	3.02	123.91	114.35
3	D	4607	FAD	C4A-C5A-N7A	-3.01	107.14	110.58
5	P	1109	SRM	C3D-C4D-ND	3.00	113.48	110.15
3	O	1106	FAD	N3A-C2A-N1A	-3.00	124.04	128.58
5	O	1109	SRM	C3A-C2A-C1A	-2.99	95.84	100.92
3	O	1106	FAD	C4A-N9A-C8A	2.99	108.88	105.74
3	F	1106	FAD	C4A-N9A-C8A	2.98	108.87	105.74
5	E	1109	SRM	C2D-C1D-ND	2.98	113.46	110.15
3	D	4607	FAD	C4A-N9A-C8A	2.98	108.87	105.74
3	L	1106	FAD	N3A-C2A-N1A	-2.98	124.08	128.58
5	M	1109	SRM	C3B-C4B-CHC	-2.97	117.02	123.33
3	H	4407	FAD	O2-C2-N1	-2.96	116.88	121.80
5	D	4610	SRM	C2D-C1D-ND	2.96	113.44	110.15
3	E	1106	FAD	C4-C4X-N5	2.95	122.28	118.21
5	O	1109	SRM	O3B-CEB-CDB	-2.95	114.60	122.95
3	E	1106	FAD	N3A-C2A-N1A	-2.94	124.13	128.58
3	H	4407	FAD	C4A-N9A-C8A	2.94	108.82	105.74
5	O	1109	SRM	CAA-CBA-CCA	2.94	120.32	112.49
5	M	1109	SRM	O1C-CCC-CBC	-2.94	113.78	123.09
5	L	1109	SRM	C4D-C3D-C2D	-2.92	103.74	106.81
3	K	1106	FAD	C4-C4X-N5	2.92	122.25	118.21
3	B	4207	FAD	C2A-N3A-C4A	2.92	118.96	111.83
5	J	1109	SRM	C1C-C2C-C3C	-2.90	103.60	106.84
5	H	4410	SRM	CDA-C2A-C3A	2.89	115.99	108.37
5	E	1109	SRM	CAB-C3B-C4B	2.89	116.22	111.19
5	H	4410	SRM	O4B-CEB-CDB	2.88	123.48	114.35
5	E	1109	SRM	C3D-C4D-ND	2.88	113.34	110.15
3	O	1106	FAD	C4-C4X-N5	2.88	122.18	118.21
3	K	1106	FAD	C4A-N9A-C8A	2.87	108.75	105.74
5	F	1109	SRM	O4B-CEB-CDB	2.86	123.42	114.35
5	G	1109	SRM	C2D-C1D-ND	2.86	113.32	110.15
5	O	1109	SRM	C1D-C2D-C3D	-2.85	103.82	106.81
5	B	4210	SRM	C2D-C1D-ND	2.85	113.31	110.15
3	P	1106	FAD	C4A-N9A-C8A	2.84	108.72	105.74
3	M	1106	FAD	C4A-N9A-C8A	2.84	108.72	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	1109	SRM	CDA-C2A-C1A	2.83	115.87	107.11
5	B	4210	SRM	C4D-C3D-C2D	-2.82	103.85	106.81
5	M	1109	SRM	C3A-C2A-C1A	-2.82	96.14	100.92
5	H	4410	SRM	O1C-CCC-CBC	-2.81	114.18	123.09
3	O	1106	FAD	C4A-C5A-N7A	-2.80	107.38	110.58
5	C	3910	SRM	O4B-CEB-CDB	2.80	123.22	114.35
3	J	1106	FAD	N3A-C2A-N1A	-2.80	124.34	128.58
5	M	1109	SRM	C3A-C4A-CHB	-2.80	117.38	123.33
5	F	1109	SRM	C4D-C3D-C2D	-2.80	103.88	106.81
5	C	3910	SRM	C4D-C3D-C2D	-2.79	103.89	106.81
3	D	4607	FAD	C2A-N1A-C6A	2.78	123.30	118.73
5	L	1109	SRM	C3D-C4D-ND	2.76	113.22	110.15
5	H	4410	SRM	C2C-C1C-NC	2.76	112.98	110.32
5	A	1109	SRM	C4D-C3D-C2D	-2.76	103.92	106.81
5	E	1109	SRM	O4B-CEB-CDB	2.74	123.03	114.35
5	C	3910	SRM	C2D-C1D-ND	2.73	113.19	110.15
5	G	1109	SRM	O4B-CEB-CDB	2.73	123.00	114.35
5	I	1109	SRM	O4B-CEB-CDB	2.73	122.99	114.35
5	B	4210	SRM	CAC-CBC-CCC	-2.71	106.48	113.67
3	J	1106	FAD	C4A-N9A-C8A	2.71	108.58	105.74
3	H	4407	FAD	O4-C4-C4X	-2.71	119.39	126.53
5	M	1109	SRM	C4D-C3D-C2D	-2.69	103.99	106.81
5	H	4410	SRM	C2D-C1D-ND	2.69	113.14	110.15
5	G	1109	SRM	C4A-CHB-C1B	-2.68	121.89	125.84
3	F	1106	FAD	C5A-N7A-C8A	2.67	107.65	103.45
5	B	4210	SRM	O4B-CEB-CDB	2.67	122.81	114.35
5	D	4610	SRM	O4B-CEB-CDB	2.67	122.81	114.35
5	G	1109	SRM	C3D-C4D-ND	2.67	113.11	110.15
5	H	4410	SRM	C3C-C4C-NC	2.67	112.89	110.32
3	D	4607	FAD	C4-C4X-N5	2.66	121.88	118.21
3	C	3907	FAD	C5X-C9A-N10	2.65	120.37	117.97
5	M	1109	SRM	C2D-C1D-ND	2.64	113.08	110.15
3	M	1106	FAD	C4A-C5A-N7A	-2.64	107.56	110.58
5	D	4610	SRM	C4D-C3D-C2D	-2.64	104.04	106.81
5	D	4610	SRM	C2B-C3B-C4B	-2.64	97.55	100.89
5	B	4210	SRM	CHC-C1C-NC	-2.62	121.60	124.45
5	C	3910	SRM	C3B-C4B-CHC	-2.62	117.75	123.33
3	H	4407	FAD	C4-C4X-N5	2.62	121.82	118.21
5	C	3910	SRM	C2B-C3B-C4B	-2.62	97.58	100.89
5	D	4610	SRM	O3B-CEB-CDB	-2.61	115.55	122.95
3	P	1106	FAD	C6A-C5A-N7A	2.60	137.11	132.09
5	H	4410	SRM	C3A-C4A-NA	2.60	115.91	110.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1109	SRM	CAB-C3B-C4B	2.60	115.72	111.19
5	L	1109	SRM	C2B-C3B-C4B	-2.60	97.60	100.89
5	F	1109	SRM	C3A-C2A-C1A	-2.60	96.51	100.92
3	A	1106	FAD	O4-C4-C4X	-2.60	119.68	126.53
3	C	3907	FAD	O4-C4-C4X	-2.59	119.69	126.53
3	B	4207	FAD	C4-C4X-N5	2.58	121.77	118.21
3	L	1106	FAD	O4-C4-C4X	-2.58	119.73	126.53
3	A	1106	FAD	C4A-N9A-C8A	2.58	108.44	105.74
5	E	1109	SRM	C2B-C3B-C4B	-2.58	97.63	100.89
5	A	1109	SRM	CDA-C2A-C3A	2.57	115.16	108.37
5	A	1109	SRM	C3B-C4B-CHC	-2.57	117.85	123.33
3	H	4407	FAD	C5A-N7A-C8A	2.56	107.48	103.45
3	P	1106	FAD	O2-C2-N1	-2.56	117.55	121.80
5	G	1109	SRM	C3A-C2A-C1A	-2.56	96.58	100.92
5	K	1109	SRM	O4B-CEB-CDB	2.56	122.45	114.35
5	C	3910	SRM	CDA-C2A-C3A	2.56	115.11	108.37
5	P	1109	SRM	CHC-C1C-NC	-2.54	121.69	124.45
5	P	1109	SRM	C4A-CHB-C1B	-2.54	122.11	125.84
5	E	1109	SRM	C3A-C4A-NA	2.53	115.76	110.83
5	O	1109	SRM	C3B-C4B-NB	2.53	115.76	110.83
5	A	1109	SRM	O4B-CEB-CDB	2.52	122.34	114.35
5	F	1109	SRM	C3B-C4B-CHC	-2.52	117.96	123.33
3	P	1106	FAD	N9A-C8A-N7A	-2.51	110.37	113.94
5	I	1109	SRM	CHC-C1C-NC	-2.51	121.72	124.45
5	A	1109	SRM	C3A-C2A-C1A	-2.51	96.66	100.92
5	M	1109	SRM	CED-CDD-C3D	2.51	120.06	113.76
5	O	1109	SRM	C3A-C4A-CHB	-2.50	118.01	123.33
5	B	4210	SRM	C3A-C4A-NA	2.50	115.70	110.83
5	O	1109	SRM	O3C-CEC-CDC	-2.49	115.02	122.11
5	K	1109	SRM	C3D-C4D-ND	2.47	112.89	110.15
3	H	4407	FAD	C2A-N1A-C6A	2.46	122.77	118.73
5	E	1109	SRM	C3A-C4A-CHB	-2.46	118.09	123.33
3	K	1106	FAD	O4-C4-C4X	-2.46	120.04	126.53
3	A	1106	FAD	C2A-N1A-C6A	2.46	122.77	118.73
3	C	3907	FAD	C4A-C5A-N7A	-2.46	107.77	110.58
5	B	4210	SRM	C2B-C3B-C4B	-2.46	97.78	100.89
3	L	1106	FAD	C4X-C10-N1	-2.45	118.58	124.59
3	J	1106	FAD	C4-C4X-N5	2.45	121.59	118.21
3	A	1106	FAD	C5A-N7A-C8A	2.45	107.30	103.45
5	F	1109	SRM	C3D-C4D-ND	2.45	112.86	110.15
5	P	1109	SRM	O4B-CEB-CDB	2.44	122.09	114.35
3	M	1106	FAD	O2A-PA-O3P	2.44	113.88	107.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	1109	SRM	CDA-C2A-C3A	2.44	114.80	108.37
3	F	1106	FAD	C4X-C10-N1	-2.44	118.61	124.59
5	G	1109	SRM	CAB-C3B-C4B	2.44	115.44	111.19
5	K	1109	SRM	CHC-C1C-NC	-2.43	121.81	124.45
5	F	1109	SRM	CAA-C3A-C4A	2.42	115.41	111.19
5	H	4410	SRM	CAC-CBC-CCC	-2.42	107.24	113.67
5	H	4410	SRM	C4D-ND-C1D	2.42	109.76	105.82
5	O	1109	SRM	CDB-C2B-C3B	2.41	114.74	108.37
5	E	1109	SRM	CHC-C1C-NC	-2.41	121.83	124.45
5	N	1012	SRM	O4B-CEB-CDB	2.40	121.96	114.35
3	L	1106	FAD	C4-C4X-N5	2.40	121.53	118.21
3	E	1106	FAD	C4A-N9A-C8A	2.40	108.26	105.74
5	B	4210	SRM	CDA-C2A-C3A	2.40	114.70	108.37
5	L	1109	SRM	C3B-C4B-CHC	-2.40	118.22	123.33
5	O	1109	SRM	CHD-C1D-ND	2.39	128.20	123.86
5	A	1109	SRM	C3D-C4D-ND	2.39	112.81	110.15
5	B	4210	SRM	CAB-C3B-C4B	2.39	115.36	111.19
5	A	1109	SRM	C2B-C3B-C4B	-2.38	97.87	100.89
5	A	1109	SRM	C4A-CHB-C1B	-2.38	122.33	125.84
5	I	1109	SRM	C3A-C4A-NA	2.38	115.47	110.83
3	O	1106	FAD	O4-C4-C4X	-2.38	120.25	126.53
5	P	1109	SRM	C3A-C4A-NA	2.38	115.46	110.83
5	D	4610	SRM	C3D-C4D-ND	2.37	112.79	110.15
3	O	1106	FAD	O2A-PA-O3P	2.37	113.68	107.27
5	E	1109	SRM	C3B-C4B-CHC	-2.37	118.28	123.33
5	D	4610	SRM	CHC-C1C-NC	-2.37	121.87	124.45
3	F	1106	FAD	C4X-C10-N10	2.37	119.87	116.48
5	H	4410	SRM	O3B-CEB-CDB	-2.36	116.25	122.95
3	L	1106	FAD	C5A-N7A-C8A	2.36	107.17	103.45
3	J	1106	FAD	C9A-N10-C10	-2.36	117.16	120.75
5	L	1109	SRM	O3B-CEB-CDB	-2.35	116.29	122.95
5	G	1109	SRM	CAC-CBC-CCC	-2.35	107.44	113.67
5	K	1109	SRM	CDA-C2A-C3A	2.34	114.55	108.37
5	P	1109	SRM	C3B-C4B-CHC	-2.34	118.34	123.33
5	M	1109	SRM	O4D-CED-O3D	2.34	129.35	123.33
5	M	1109	SRM	CAC-C3C-C4C	2.34	129.61	124.85
5	G	1109	SRM	CDA-C2A-C3A	2.33	114.53	108.37
5	B	4210	SRM	C3D-C4D-ND	2.33	112.74	110.15
3	D	4607	FAD	O4-C4-C4X	-2.33	120.39	126.53
5	G	1109	SRM	C2B-C3B-C4B	-2.33	97.94	100.89
5	O	1109	SRM	CHC-C1C-NC	2.33	126.98	124.45
3	E	1106	FAD	C4X-C10-N1	-2.32	118.89	124.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	1109	SRM	CAC-CBC-CCC	-2.32	107.51	113.67
5	M	1109	SRM	O3C-CEC-CDC	-2.31	115.52	122.11
5	B	4210	SRM	C3A-C2A-C1A	-2.31	96.99	100.92
5	O	1109	SRM	CDA-C2A-C3A	2.31	114.46	108.37
3	H	4407	FAD	C4X-C10-N10	2.31	119.78	116.48
5	P	1109	SRM	C3A-C4A-CHB	-2.31	118.42	123.33
5	C	3910	SRM	C3A-C4A-CHB	-2.30	118.43	123.33
5	K	1109	SRM	C3B-C4B-CHC	-2.30	118.43	123.33
5	I	1109	SRM	C3B-C4B-CHC	-2.30	118.43	123.33
5	P	1109	SRM	C2B-C3B-C4B	-2.30	97.98	100.89
5	C	3910	SRM	C3A-C4A-NA	2.30	115.32	110.83
3	H	4407	FAD	C4X-C10-N1	-2.29	118.97	124.59
5	D	4610	SRM	CAB-C3B-C4B	2.29	115.18	111.19
5	N	1012	SRM	C4A-CHB-C1B	-2.29	122.48	125.84
5	D	4610	SRM	C3B-C4B-CHC	-2.29	118.46	123.33
3	B	4207	FAD	C4A-C5A-N7A	-2.29	107.97	110.58
5	L	1109	SRM	C3A-C2A-C1A	-2.29	97.04	100.92
3	P	1106	FAD	O4-C4-C4X	-2.28	120.51	126.53
5	I	1109	SRM	C3A-C2A-C1A	-2.28	97.05	100.92
3	C	3907	FAD	C2A-N1A-C6A	2.28	122.47	118.73
3	P	1106	FAD	C4X-C10-N10	2.27	119.73	116.48
3	J	1106	FAD	C4X-C10-N1	-2.26	119.04	124.59
5	N	1012	SRM	C3A-C4A-NA	2.26	115.24	110.83
3	E	1106	FAD	C10-N1-C2	2.26	121.75	116.85
3	F	1106	FAD	N9A-C8A-N7A	-2.26	110.73	113.94
3	H	4407	FAD	C6A-C5A-N7A	2.26	136.44	132.09
5	B	4210	SRM	C3B-C4B-CHC	-2.26	118.52	123.33
5	L	1109	SRM	C3A-C4A-NA	2.26	115.23	110.83
3	D	4607	FAD	C9A-C5X-N5	-2.26	120.06	122.45
3	K	1106	FAD	C6A-C5A-N7A	2.26	136.44	132.09
3	J	1106	FAD	C5A-N7A-C8A	2.26	107.00	103.45
5	F	1109	SRM	O3B-CEB-CDB	-2.26	116.56	122.95
5	A	1109	SRM	CAC-CBC-CCC	-2.25	107.69	113.67
5	I	1109	SRM	C2B-C3B-C4B	-2.25	98.04	100.89
3	A	1106	FAD	N6A-C6A-N1A	2.25	123.38	118.38
3	D	4607	FAD	C4X-C10-N1	-2.25	119.08	124.59
5	N	1012	SRM	C3B-C4B-CHC	-2.24	118.55	123.33
5	K	1109	SRM	C3A-C2A-C1A	-2.24	97.11	100.92
5	K	1109	SRM	O3B-CEB-CDB	-2.23	116.62	122.95
5	J	1109	SRM	CAA-C3A-C4A	2.23	115.08	111.19
3	B	4207	FAD	C4X-C10-N1	-2.23	119.11	124.59
3	F	1106	FAD	C10-N1-C2	2.23	121.68	116.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	4610	SRM	CDA-C2A-C3A	2.23	114.26	108.37
5	O	1109	SRM	CBC-CAC-C3C	2.23	118.70	112.53
5	C	3910	SRM	CAB-C3B-C4B	2.23	115.07	111.19
5	N	1012	SRM	C3A-C2A-C1A	-2.23	97.14	100.92
5	E	1109	SRM	O3B-CEB-CDB	-2.22	116.65	122.95
3	B	4207	FAD	O4-C4-C4X	-2.22	120.67	126.53
3	F	1106	FAD	O4-C4-C4X	-2.22	120.67	126.53
3	O	1106	FAD	C5X-C9A-N10	2.22	119.97	117.97
5	J	1109	SRM	C3A-C4A-NA	2.22	115.15	110.83
5	M	1109	SRM	CAA-C3A-C4A	2.21	115.05	111.19
5	P	1109	SRM	CAA-C3A-C4A	2.21	115.05	111.19
5	C	3910	SRM	C4A-CHB-C1B	-2.21	122.59	125.84
3	P	1106	FAD	C4X-C10-N1	-2.21	119.18	124.59
5	G	1109	SRM	C3B-C4B-CHC	-2.20	118.64	123.33
5	O	1109	SRM	O1C-CCC-CBC	-2.20	116.11	123.09
5	L	1109	SRM	CDA-C2A-C3A	2.20	114.17	108.37
5	H	4410	SRM	O2A-CCA-CBA	2.19	120.93	114.00
5	O	1109	SRM	C2B-C1B-CHB	-2.19	121.57	123.54
5	C	3910	SRM	CAA-C3A-C4A	2.19	115.00	111.19
5	O	1109	SRM	CMA-C2A-CDA	-2.18	107.03	110.74
5	K	1109	SRM	C2B-C3B-C4B	-2.18	98.13	100.89
5	M	1109	SRM	O3B-CEB-CDB	-2.18	116.78	122.95
5	M	1109	SRM	C4A-CHB-C1B	-2.18	122.64	125.84
3	P	1106	FAD	C10-N1-C2	2.18	121.56	116.85
3	F	1106	FAD	O2-C2-N1	-2.18	118.19	121.80
3	K	1106	FAD	C5A-N7A-C8A	2.17	106.87	103.45
5	K	1109	SRM	C3A-C4A-CHB	-2.17	118.70	123.33
3	H	4407	FAD	C10-N1-C2	2.17	121.55	116.85
5	O	1109	SRM	CAD-C2D-C1D	2.17	129.18	124.94
3	A	1106	FAD	C10-N1-C2	2.17	121.54	116.85
3	M	1106	FAD	C10-N1-C2	2.17	121.54	116.85
5	H	4410	SRM	CAD-C2D-C1D	2.17	129.17	124.94
3	F	1106	FAD	C2A-N1A-C6A	2.16	122.28	118.73
5	J	1109	SRM	C3B-C4B-CHC	-2.16	118.73	123.33
3	E	1106	FAD	C4X-C10-N10	2.16	119.57	116.48
3	K	1106	FAD	C2A-N1A-C6A	2.16	122.27	118.73
5	L	1109	SRM	O1C-CCC-CBC	-2.16	116.26	123.09
5	J	1109	SRM	C3A-C2A-C1A	-2.15	97.26	100.92
3	C	3907	FAD	C4-C4X-N5	2.15	121.18	118.21
5	N	1012	SRM	O3B-CEB-CDB	-2.15	116.86	122.95
3	D	4607	FAD	C9A-N10-C10	-2.15	117.47	120.75
3	M	1106	FAD	C5A-N7A-C8A	2.15	106.83	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	1106	FAD	C2A-N1A-C6A	2.15	122.25	118.73
5	I	1109	SRM	CAB-C3B-C4B	2.14	114.93	111.19
3	J	1106	FAD	O2-C2-N1	-2.14	118.24	121.80
3	A	1106	FAD	O2A-PA-O3P	2.14	113.06	107.27
3	C	3907	FAD	C9A-C5X-N5	-2.14	120.19	122.45
5	F	1109	SRM	O1C-CCC-CBC	-2.13	116.33	123.09
5	F	1109	SRM	C2B-C3B-C4B	-2.13	98.19	100.89
5	H	4410	SRM	CMB-C2B-CDB	-2.13	107.11	110.74
5	A	1109	SRM	C3A-C4A-CHB	-2.13	118.80	123.33
3	D	4607	FAD	C9-C9A-N10	-2.12	119.00	121.85
3	F	1106	FAD	C10-C4X-N5	-2.12	120.48	124.81
3	M	1106	FAD	O2-C2-N1	-2.12	118.29	121.80
3	M	1106	FAD	O4-C4-C4X	-2.11	120.95	126.53
5	J	1109	SRM	CHC-C1C-NC	-2.11	122.15	124.45
3	C	3907	FAD	C4X-C10-N1	-2.11	119.41	124.59
3	L	1106	FAD	C4X-C4-N3	2.11	118.62	113.25
3	O	1106	FAD	C4X-C10-N1	-2.11	119.42	124.59
5	D	4610	SRM	CAC-CBC-CCC	-2.10	108.08	113.67
3	H	4407	FAD	C4-N3-C2	-2.10	121.91	125.64
3	P	1106	FAD	C4'-C3'-C2'	-2.10	110.07	113.57
3	J	1106	FAD	O4-C4-C4X	-2.10	120.99	126.53
5	E	1109	SRM	C3A-C2A-C1A	-2.10	97.36	100.92
5	A	1109	SRM	CAC-C3C-C4C	2.10	129.11	124.85
5	D	4610	SRM	C3A-C4A-CHB	-2.09	118.87	123.33
5	N	1012	SRM	CAC-CBC-CCC	-2.09	108.12	113.67
5	E	1109	SRM	O1C-CCC-CBC	-2.09	116.46	123.09
3	N	1001[A]	FAD	C4-N3-C2	-2.09	121.93	125.64
5	O	1109	SRM	CMB-C2B-CDB	-2.09	107.19	110.74
3	J	1106	FAD	C4X-C10-N10	2.08	119.46	116.48
3	N	1009[B]	FAD	C4-N3-C2	-2.08	121.95	125.64
5	K	1109	SRM	C3A-C4A-NA	2.07	114.88	110.83
5	D	4610	SRM	CAA-CBA-CCA	2.07	118.01	112.49
5	N	1012	SRM	C3A-C4A-CHB	-2.07	118.93	123.33
5	M	1109	SRM	C3A-C4A-NA	2.07	114.86	110.83
3	E	1106	FAD	O2-C2-N1	-2.07	118.37	121.80
5	E	1109	SRM	C4A-CHB-C1B	-2.07	122.80	125.84
5	C	3910	SRM	O3B-CEB-CDB	-2.06	117.10	122.95
5	A	1109	SRM	C3B-C4B-NB	2.06	114.86	110.83
3	C	3907	FAD	C5A-N7A-C8A	2.06	106.69	103.45
3	O	1106	FAD	C5A-N7A-C8A	2.06	106.69	103.45
3	L	1106	FAD	N9A-C8A-N7A	-2.06	111.02	113.94
5	B	4210	SRM	O1C-CCC-CBC	-2.06	116.56	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	4410	SRM	O3C-CEC-CDC	-2.05	116.27	122.11
3	D	4607	FAD	C10-N1-C2	2.05	121.28	116.85
3	F	1106	FAD	C4X-C4-N3	2.05	118.46	113.25
3	D	4607	FAD	C5A-N7A-C8A	2.05	106.67	103.45
3	K	1106	FAD	C5X-C9A-N10	2.05	119.82	117.97
5	C	3910	SRM	CHC-C1C-NC	-2.04	122.23	124.45
5	B	4210	SRM	O3B-CEB-CDB	-2.04	117.17	122.95
5	J	1109	SRM	O4B-CEB-CDB	2.04	120.80	114.35
3	E	1106	FAD	C5A-N7A-C8A	2.04	106.65	103.45
3	P	1106	FAD	C2A-N1A-C6A	2.03	122.07	118.73
5	P	1109	SRM	CDA-C2A-C3A	2.03	113.73	108.37
3	P	1106	FAD	C10-C4X-N5	-2.03	120.67	124.81
5	A	1109	SRM	O3D-CED-CDD	-2.03	116.33	122.11
3	O	1106	FAD	C9A-C5X-N5	-2.03	120.30	122.45
5	G	1109	SRM	O3B-CEB-CDB	-2.03	117.22	122.95
5	N	1012	SRM	C2B-C1B-CHB	-2.02	121.73	123.54
3	F	1106	FAD	C4-N3-C2	-2.02	122.06	125.64
3	M	1106	FAD	C4X-C10-N1	-2.02	119.65	124.59
3	D	4607	FAD	C4X-C4-N3	2.02	118.39	113.25
5	N	1012	SRM	O1C-CCC-CBC	-2.02	116.70	123.09
3	M	1106	FAD	N6A-C6A-N1A	2.02	122.87	118.38
5	I	1109	SRM	O3B-CEB-CDB	-2.01	117.24	122.95
5	M	1109	SRM	CMA-C2A-CDA	-2.01	107.31	110.74
3	O	1106	FAD	C2A-N1A-C6A	2.01	122.04	118.73
3	H	4407	FAD	C4X-C4-N3	2.01	118.37	113.25
5	O	1109	SRM	O4B-CEB-CDB	2.01	120.72	114.35
3	J	1106	FAD	C9-C9A-N10	-2.01	119.15	121.85
5	N	1012	SRM	CDA-C2A-C3A	2.01	113.66	108.37
3	F	1106	FAD	O2A-PA-O3P	2.01	112.69	107.27
5	O	1109	SRM	C1C-CHC-C4B	-2.00	121.79	126.62
3	E	1106	FAD	C10-C4X-N5	-2.00	120.72	124.81
5	A	1109	SRM	CAD-C2D-C1D	2.00	128.85	124.94
5	H	4410	SRM	CAB-CBB-CCB	2.00	117.83	112.49
3	M	1106	FAD	C10-C4X-N5	-2.00	120.72	124.81

All (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

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Mol	Chain	Res	Type	Atom
5	E	1109	SRM	NC
5	F	1109	SRM	NC
5	G	1109	SRM	NC
5	H	4410	SRM	NC
5	I	1109	SRM	NC
5	J	1109	SRM	NC
5	K	1109	SRM	NC
5	L	1109	SRM	NC
5	M	1109	SRM	NC
5	N	1012	SRM	NC
5	O	1109	SRM	NC
5	P	1109	SRM	NC

All (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
5	O	1109	SRM	C2C-C3C-CAC-CBC
5	O	1109	SRM	C4C-C3C-CAC-CBC
9	B	4218[B]	GOL	O1-C1-C2-C3
9	B	4224	GOL	C1-C2-C3-O3
9	B	4224	GOL	O2-C2-C3-O3
9	C	3901	GOL	C1-C2-C3-O3
9	C	3913	GOL	C1-C2-C3-O3
9	C	3913	GOL	O2-C2-C3-O3
9	E	1114	GOL	O2-C2-C3-O3
9	I	1117	GOL	O1-C1-C2-O2
9	I	1117	GOL	O1-C1-C2-C3
9	J	1114	GOL	O1-C1-C2-O2
9	J	1114	GOL	O1-C1-C2-C3
9	J	1117[A]	GOL	C1-C2-C3-O3
9	O	1116	GOL	O1-C1-C2-C3
9	O	1116	GOL	C1-C2-C3-O3
12	H	4401	TRS	N-C-C2-O2
12	I	1119	TRS	N-C-C1-O1
5	B	4210	SRM	C2C-C3C-CAC-CBC
5	H	4410	SRM	C2C-C3C-CAC-CBC
5	I	1109	SRM	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
5	J	1109	SRM	C2C-C3C-CAC-CBC
11	K	1115	PEG	C1-C2-O2-C3
11	D	4601	PEG	C1-C2-O2-C3
5	B	4210	SRM	C4C-C3C-CAC-CBC
5	C	3910	SRM	C4C-C3C-CAC-CBC
5	I	1109	SRM	C4C-C3C-CAC-CBC
5	J	1109	SRM	C4C-C3C-CAC-CBC
5	N	1012	SRM	C4C-C3C-CAC-CBC
3	N	1001[A]	FAD	C2'-C3'-C4'-O4'
5	B	4210	SRM	C4A-C3A-CAA-CBA
5	E	1109	SRM	C4A-C3A-CAA-CBA
5	G	1109	SRM	C4A-C3A-CAA-CBA
5	L	1109	SRM	C4A-C3A-CAA-CBA
5	M	1109	SRM	C4A-C3A-CAA-CBA
5	F	1109	SRM	C2C-C3C-CAC-CBC
5	K	1109	SRM	C2C-C3C-CAC-CBC
5	A	1109	SRM	C4C-C3C-CAC-CBC
5	D	4610	SRM	C4C-C3C-CAC-CBC
5	F	1109	SRM	C4C-C3C-CAC-CBC
5	G	1109	SRM	C4C-C3C-CAC-CBC
5	H	4410	SRM	C4C-C3C-CAC-CBC
5	K	1109	SRM	C4C-C3C-CAC-CBC
5	L	1109	SRM	C4C-C3C-CAC-CBC
5	P	1109	SRM	C4C-C3C-CAC-CBC
11	M	1115	PEG	O1-C1-C2-O2
5	A	1109	SRM	C2C-C3C-CAC-CBC
5	C	3910	SRM	C2C-C3C-CAC-CBC
5	E	1109	SRM	C2C-C3C-CAC-CBC
5	G	1109	SRM	C2C-C3C-CAC-CBC
5	L	1109	SRM	C2C-C3C-CAC-CBC
5	M	1109	SRM	C2C-C3C-CAC-CBC
5	P	1109	SRM	C2C-C3C-CAC-CBC
3	N	1001[A]	FAD	O3'-C3'-C4'-O4'
9	I	1117	GOL	O2-C2-C3-O3
5	G	1109	SRM	C2A-C3A-CAA-CBA
5	H	4410	SRM	C2A-C3A-CAA-CBA
5	N	1012	SRM	C2A-C3A-CAA-CBA
11	D	4601	PEG	O2-C3-C4-O4
4	J	1110	EDO	O1-C1-C2-O2
5	A	1109	SRM	C4A-C3A-CAA-CBA
5	D	4610	SRM	C4A-C3A-CAA-CBA
5	H	4410	SRM	C4A-C3A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
5	K	1109	SRM	C4A-C3A-CAA-CBA
5	N	1012	SRM	C4A-C3A-CAA-CBA
5	P	1109	SRM	C4A-C3A-CAA-CBA
5	D	4610	SRM	C2C-C3C-CAC-CBC
5	G	1109	SRM	C3A-CAA-CBA-CCA
5	H	4410	SRM	C3A-CAA-CBA-CCA
5	E	1109	SRM	C4C-C3C-CAC-CBC
5	M	1109	SRM	C4C-C3C-CAC-CBC
11	D	4601	PEG	O1-C1-C2-O2
11	K	1115	PEG	O1-C1-C2-O2
11	M	1120	PEG	O1-C1-C2-O2
11	N	1014	PEG	O2-C3-C4-O4
5	O	1109	SRM	C3A-CAA-CBA-CCA
11	M	1115	PEG	C4-C3-O2-C2
5	C	3910	SRM	C4A-C3A-CAA-CBA
5	I	1109	SRM	C4A-C3A-CAA-CBA
5	J	1109	SRM	C4A-C3A-CAA-CBA
5	O	1109	SRM	C4A-C3A-CAA-CBA
5	C	3910	SRM	C3A-CAA-CBA-CCA
5	D	4610	SRM	C3A-CAA-CBA-CCA
5	E	1109	SRM	C3A-CAA-CBA-CCA
5	L	1109	SRM	C3A-CAA-CBA-CCA
5	M	1109	SRM	C3A-CAA-CBA-CCA
5	P	1109	SRM	C3A-CAA-CBA-CCA
9	B	4217[A]	GOL	O1-C1-C2-C3
9	C	3913	GOL	O1-C1-C2-C3
9	E	1114	GOL	O1-C1-C2-C3
9	E	1114	GOL	C1-C2-C3-O3
9	I	1111	GOL	O1-C1-C2-C3
9	I	1117	GOL	C1-C2-C3-O3
9	J	1114	GOL	C1-C2-C3-O3
9	K	1117	GOL	C1-C2-C3-O3
9	N	1011	GOL	C1-C2-C3-O3
11	K	1115	PEG	O2-C3-C4-O4
9	C	3901	GOL	O2-C2-C3-O3
9	C	3913	GOL	O1-C1-C2-O2
9	K	1117	GOL	O2-C2-C3-O3
5	A	1109	SRM	C2A-C3A-CAA-CBA
5	B	4210	SRM	C2A-C3A-CAA-CBA
5	E	1109	SRM	C2A-C3A-CAA-CBA
5	L	1109	SRM	C2A-C3A-CAA-CBA
12	H	4401	TRS	C3-C-C2-O2

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Mol	Chain	Res	Type	Atoms
12	I	1119	TRS	C3-C-C1-O1
4	B	4223	EDO	O1-C1-C2-O2
4	F	1110[B]	EDO	O1-C1-C2-O2
4	J	1112	EDO	O1-C1-C2-O2
4	J	1113	EDO	O1-C1-C2-O2
4	M	1113	EDO	O1-C1-C2-O2
4	P	1113	EDO	O1-C1-C2-O2
5	D	4610	SRM	C2B-CDB-CEB-O4B
5	E	1109	SRM	C2B-CDB-CEB-O3B
5	L	1109	SRM	C2B-CDB-CEB-O3B
11	M	1115	PEG	C1-C2-O2-C3
5	F	1109	SRM	C3A-CAA-CBA-CCA
5	D	4610	SRM	C2A-C3A-CAA-CBA
5	F	1109	SRM	C2A-C3A-CAA-CBA
5	J	1109	SRM	C2A-C3A-CAA-CBA
5	M	1109	SRM	C2A-C3A-CAA-CBA
5	O	1109	SRM	C2A-C3A-CAA-CBA
5	P	1109	SRM	C2A-C3A-CAA-CBA
5	F	1109	SRM	C4A-C3A-CAA-CBA
5	I	1109	SRM	C3A-CAA-CBA-CCA
9	B	4218[B]	GOL	O1-C1-C2-O2
9	N	1011	GOL	O2-C2-C3-O3
9	O	1116	GOL	O2-C2-C3-O3
5	K	1109	SRM	C2A-C3A-CAA-CBA
5	N	1012	SRM	C3A-CAA-CBA-CCA
4	A	1118	EDO	O1-C1-C2-O2
4	E	1116	EDO	O1-C1-C2-O2
4	G	1113	EDO	O1-C1-C2-O2
4	I	1118	EDO	O1-C1-C2-O2
5	A	1109	SRM	C3A-CAA-CBA-CCA
5	B	4210	SRM	C3A-CAA-CBA-CCA
9	M	1114	GOL	C1-C2-C3-O3
5	C	3910	SRM	C2B-CDB-CEB-O4B
5	F	1109	SRM	C2B-CDB-CEB-O4B
5	L	1109	SRM	C2B-CDB-CEB-O4B
5	N	1012	SRM	C2B-CDB-CEB-O4B
5	P	1109	SRM	C2B-CDB-CEB-O4B
5	I	1109	SRM	C2A-C3A-CAA-CBA
5	J	1109	SRM	C3A-CAA-CBA-CCA
9	O	1116	GOL	O1-C1-C2-O2
5	A	1109	SRM	C3C-CAC-CBC-CCC
5	C	3910	SRM	C3C-CAC-CBC-CCC

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Mol	Chain	Res	Type	Atoms
5	E	1109	SRM	C3C-CAC-CBC-CCC
5	I	1109	SRM	C3C-CAC-CBC-CCC
5	N	1012	SRM	C3C-CAC-CBC-CCC
12	H	4401	TRS	C2-C-C1-O1
12	H	4401	TRS	C3-C-C1-O1
12	I	1119	TRS	C1-C-C2-O2
12	I	1119	TRS	N-C-C2-O2
5	K	1109	SRM	C3A-CAA-CBA-CCA
4	L	1112	EDO	O1-C1-C2-O2
4	O	1114	EDO	O1-C1-C2-O2
5	B	4210	SRM	C3C-CAC-CBC-CCC
5	G	1109	SRM	C3C-CAC-CBC-CCC
5	H	4410	SRM	C3C-CAC-CBC-CCC
5	A	1109	SRM	C2B-CDB-CEB-O4B
5	B	4210	SRM	C2B-CDB-CEB-O4B
5	C	3910	SRM	C2B-CDB-CEB-O3B
5	D	4610	SRM	C2B-CDB-CEB-O3B
5	E	1109	SRM	C2B-CDB-CEB-O4B
5	G	1109	SRM	C2B-CDB-CEB-O4B
5	H	4410	SRM	C2B-CDB-CEB-O3B
5	I	1109	SRM	C2B-CDB-CEB-O4B
5	J	1109	SRM	C2B-CDB-CEB-O4B
5	K	1109	SRM	C2B-CDB-CEB-O4B
5	M	1109	SRM	C2B-CDB-CEB-O3B
5	N	1012	SRM	C2B-CDB-CEB-O3B
9	B	4224	GOL	O1-C1-C2-O2
9	F	1114	GOL	O1-C1-C2-O2
9	J	1114	GOL	O2-C2-C3-O3
9	J	1117[A]	GOL	O2-C2-C3-O3
5	D	4610	SRM	C3C-CAC-CBC-CCC
5	F	1109	SRM	C3C-CAC-CBC-CCC
5	J	1109	SRM	C3C-CAC-CBC-CCC
5	K	1109	SRM	C3C-CAC-CBC-CCC
5	M	1109	SRM	C3C-CAC-CBC-CCC
5	O	1109	SRM	C3C-CAC-CBC-CCC
5	P	1109	SRM	C3C-CAC-CBC-CCC
5	L	1109	SRM	C3C-CAC-CBC-CCC
5	A	1109	SRM	C2B-CDB-CEB-O3B
5	B	4210	SRM	C2B-CDB-CEB-O3B
5	F	1109	SRM	C2B-CDB-CEB-O3B
5	G	1109	SRM	C2B-CDB-CEB-O3B
5	H	4410	SRM	C2B-CDB-CEB-O4B

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Mol	Chain	Res	Type	Atoms
5	I	1109	SRM	C2B-CDB-CEB-O3B
5	J	1109	SRM	C2B-CDB-CEB-O3B
5	K	1109	SRM	C2B-CDB-CEB-O3B
5	M	1109	SRM	C2B-CDB-CEB-O4B
5	O	1109	SRM	C2B-CDB-CEB-O3B
5	P	1109	SRM	C2B-CDB-CEB-O3B
3	H	4407	FAD	N10-C1'-C2'-O2'
5	C	3910	SRM	C2A-C3A-CAA-CBA
12	H	4401	TRS	C1-C-C2-O2
12	I	1119	TRS	C2-C-C1-O1
12	I	1119	TRS	C3-C-C2-O2
4	C	3916	EDO	O1-C1-C2-O2
4	I	1112	EDO	O1-C1-C2-O2
4	O	1117	EDO	O1-C1-C2-O2
5	M	1109	SRM	C4B-C3B-CAB-CBB
5	N	1012	SRM	C4B-C3B-CAB-CBB
9	N	1015	GOL	C1-C2-C3-O3
3	N	1001[A]	FAD	PA-O3P-P-O2P
3	O	1106	FAD	PA-O3P-P-O1P
4	B	4222[A]	EDO	O1-C1-C2-O2
4	C	3917	EDO	O1-C1-C2-O2
4	D	4614	EDO	O1-C1-C2-O2
4	E	1112	EDO	O1-C1-C2-O2
4	E	1113	EDO	O1-C1-C2-O2
4	E	1115	EDO	O1-C1-C2-O2
4	I	1110	EDO	O1-C1-C2-O2
4	I	1114	EDO	O1-C1-C2-O2
4	M	1112	EDO	O1-C1-C2-O2
4	M	1117	EDO	O1-C1-C2-O2
5	N	1012	SRM	C3D-CDD-CED-O3D
5	O	1109	SRM	C2B-CDB-CEB-O4B
5	B	4210	SRM	C4B-C3B-CAB-CBB
5	K	1109	SRM	C4B-C3B-CAB-CBB
5	P	1109	SRM	C4B-C3B-CAB-CBB
12	H	4401	TRS	N-C-C1-O1
5	E	1109	SRM	CAB-CBB-CCB-O2B
11	N	1014	PEG	C4-C3-O2-C2
5	G	1109	SRM	CAB-CBB-CCB-O2B
5	B	4210	SRM	CAB-CBB-CCB-O2B
5	F	1109	SRM	CAB-CBB-CCB-O1B
5	P	1109	SRM	CAB-CBB-CCB-O2B
4	A	1110	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	4213	EDO	O1-C1-C2-O2
4	K	1114	EDO	O1-C1-C2-O2
4	M	1122	EDO	O1-C1-C2-O2
4	P	1114	EDO	O1-C1-C2-O2
9	B	4217[A]	GOL	O1-C1-C2-O2
5	C	3910	SRM	CAB-CBB-CCB-O1B
5	H	4410	SRM	CAB-CBB-CCB-O1B
5	J	1109	SRM	CAB-CBB-CCB-O2B
5	F	1109	SRM	CAB-CBB-CCB-O2B
5	I	1109	SRM	CAB-CBB-CCB-O2B
5	L	1109	SRM	CAB-CBB-CCB-O1B
5	A	1109	SRM	CAB-CBB-CCB-O1B
5	L	1109	SRM	CAB-CBB-CCB-O2B
5	H	4410	SRM	CAB-CBB-CCB-O2B
5	K	1109	SRM	CAB-CBB-CCB-O2B
5	O	1109	SRM	CAB-CBB-CCB-O1B
5	A	1109	SRM	CAB-CBB-CCB-O2B
5	C	3910	SRM	CAB-CBB-CCB-O2B
5	D	4610	SRM	CAB-CBB-CCB-O2B
5	O	1109	SRM	CAB-CBB-CCB-O2B
5	D	4610	SRM	CAB-CBB-CCB-O1B
5	I	1109	SRM	CAB-CBB-CCB-O1B
5	P	1109	SRM	CAB-CBB-CCB-O1B
5	N	1012	SRM	C3D-CDD-CED-O4D
3	C	3907	FAD	PA-O3P-P-O1P
3	D	4607	FAD	PA-O3P-P-O1P
3	J	1106	FAD	PA-O3P-P-O1P
3	M	1106	FAD	PA-O3P-P-O1P
5	J	1109	SRM	C4B-C3B-CAB-CBB
5	G	1109	SRM	CAB-CBB-CCB-O1B
5	K	1109	SRM	CAB-CBB-CCB-O1B
5	E	1109	SRM	CAB-CBB-CCB-O1B
5	B	4210	SRM	CAB-CBB-CCB-O1B
5	J	1109	SRM	CAB-CBB-CCB-O1B
9	E	1114	GOL	O1-C1-C2-O2
9	K	1117	GOL	O1-C1-C2-O2
4	A	1113	EDO	O1-C1-C2-O2
4	A	1115	EDO	O1-C1-C2-O2
4	B	4214	EDO	O1-C1-C2-O2
4	C	3911	EDO	O1-C1-C2-O2
4	D	4613	EDO	O1-C1-C2-O2
4	D	4617	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	E	1117	EDO	O1-C1-C2-O2
4	F	1111	EDO	O1-C1-C2-O2
4	G	1112	EDO	O1-C1-C2-O2
4	G	1120	EDO	O1-C1-C2-O2
4	H	4412	EDO	O1-C1-C2-O2
4	I	1115	EDO	O1-C1-C2-O2
4	J	1111	EDO	O1-C1-C2-O2
4	M	1121	EDO	O1-C1-C2-O2
4	M	1123	EDO	O1-C1-C2-O2
11	N	1014	PEG	C1-C2-O2-C3
5	C	3910	SRM	C4B-C3B-CAB-CBB
5	G	1109	SRM	C4B-C3B-CAB-CBB
5	H	4410	SRM	C4B-C3B-CAB-CBB
5	I	1109	SRM	C4B-C3B-CAB-CBB
5	L	1109	SRM	C4B-C3B-CAB-CBB
5	A	1109	SRM	C4B-C3B-CAB-CBB
5	O	1109	SRM	C4B-C3B-CAB-CBB
9	P	1111	GOL	O1-C1-C2-O2
5	N	1012	SRM	CAB-CBB-CCB-O2B
4	A	1117	EDO	O1-C1-C2-O2
4	B	4215	EDO	O1-C1-C2-O2
4	B	4221	EDO	O1-C1-C2-O2
4	C	3915	EDO	O1-C1-C2-O2
4	D	4612	EDO	O1-C1-C2-O2
4	G	1116	EDO	O1-C1-C2-O2
4	H	4413	EDO	O1-C1-C2-O2
4	K	1116	EDO	O1-C1-C2-O2
4	O	1110	EDO	O1-C1-C2-O2
5	M	1109	SRM	CAB-CBB-CCB-O1B
5	N	1012	SRM	CAB-CBB-CCB-O1B
5	M	1109	SRM	CAB-CBB-CCB-O2B
5	D	4610	SRM	C4B-C3B-CAB-CBB
3	L	1106	FAD	O4B-C4B-C5B-O5B
3	O	1106	FAD	O4B-C4B-C5B-O5B
3	C	3907	FAD	PA-O3P-P-O2P
3	F	1106	FAD	PA-O3P-P-O1P
3	N	1001[A]	FAD	PA-O3P-P-O1P
3	N	1009[B]	FAD	PA-O3P-P-O2P
3	C	3907	FAD	O4B-C4B-C5B-O5B
4	C	3918	EDO	O1-C1-C2-O2
4	D	4615	EDO	O1-C1-C2-O2
4	G	1115	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	K	1113	EDO	O1-C1-C2-O2
4	M	1110	EDO	O1-C1-C2-O2
4	M	1118	EDO	O1-C1-C2-O2
4	O	1112	EDO	O1-C1-C2-O2
4	O	1113	EDO	O1-C1-C2-O2
3	F	1106	FAD	N10-C1'-C2'-O2'
3	P	1106	FAD	N10-C1'-C2'-O2'
9	K	1117	GOL	O1-C1-C2-C3
3	G	1106	FAD	O4B-C4B-C5B-O5B
3	P	1106	FAD	O4B-C4B-C5B-O5B
5	O	1109	SRM	CAC-CBC-CCC-O2C
5	N	1012	SRM	CAA-CBA-CCA-O2A
11	M	1115	PEG	O2-C3-C4-O4
3	A	1106	FAD	PA-O3P-P-O2P
3	D	4607	FAD	PA-O3P-P-O2P
3	G	1106	FAD	PA-O3P-P-O2P
3	I	1106	FAD	PA-O3P-P-O2P
3	J	1106	FAD	PA-O3P-P-O2P
3	L	1106	FAD	PA-O3P-P-O1P
3	L	1106	FAD	PA-O3P-P-O2P
3	M	1106	FAD	PA-O3P-P-O2P
3	D	4607	FAD	O4B-C4B-C5B-O5B

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
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

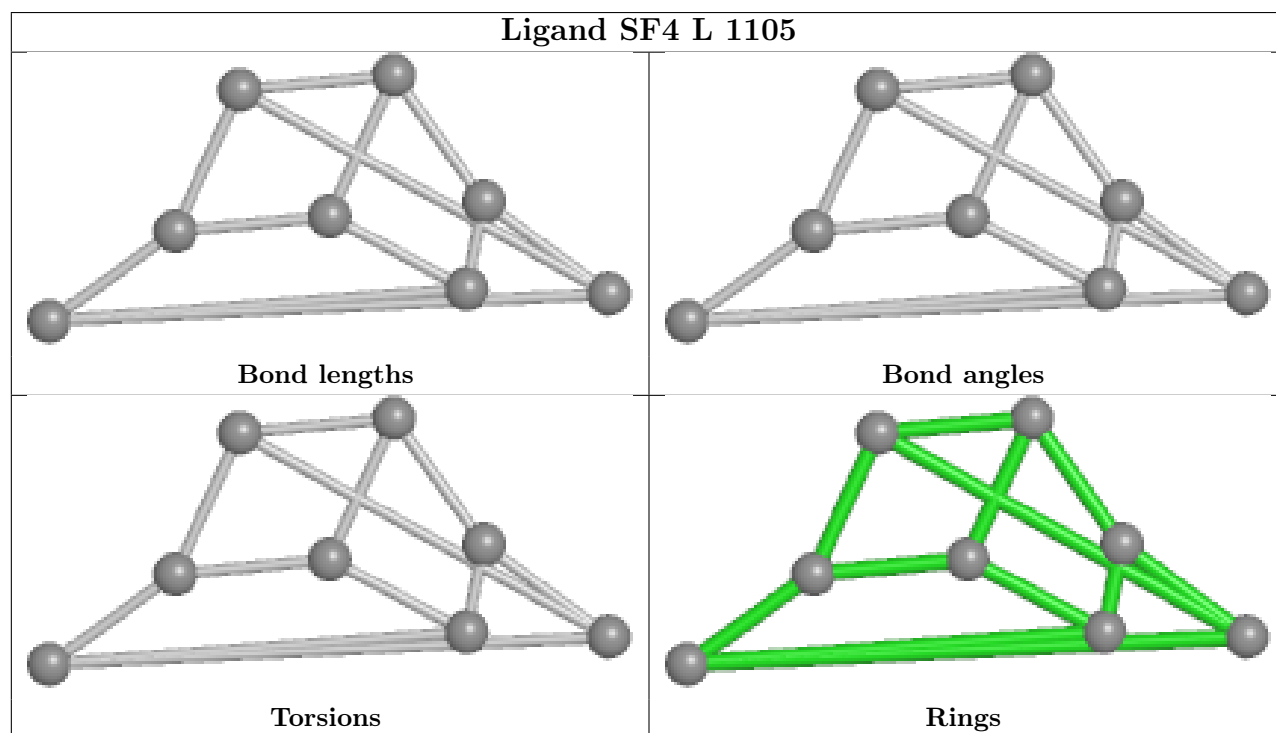
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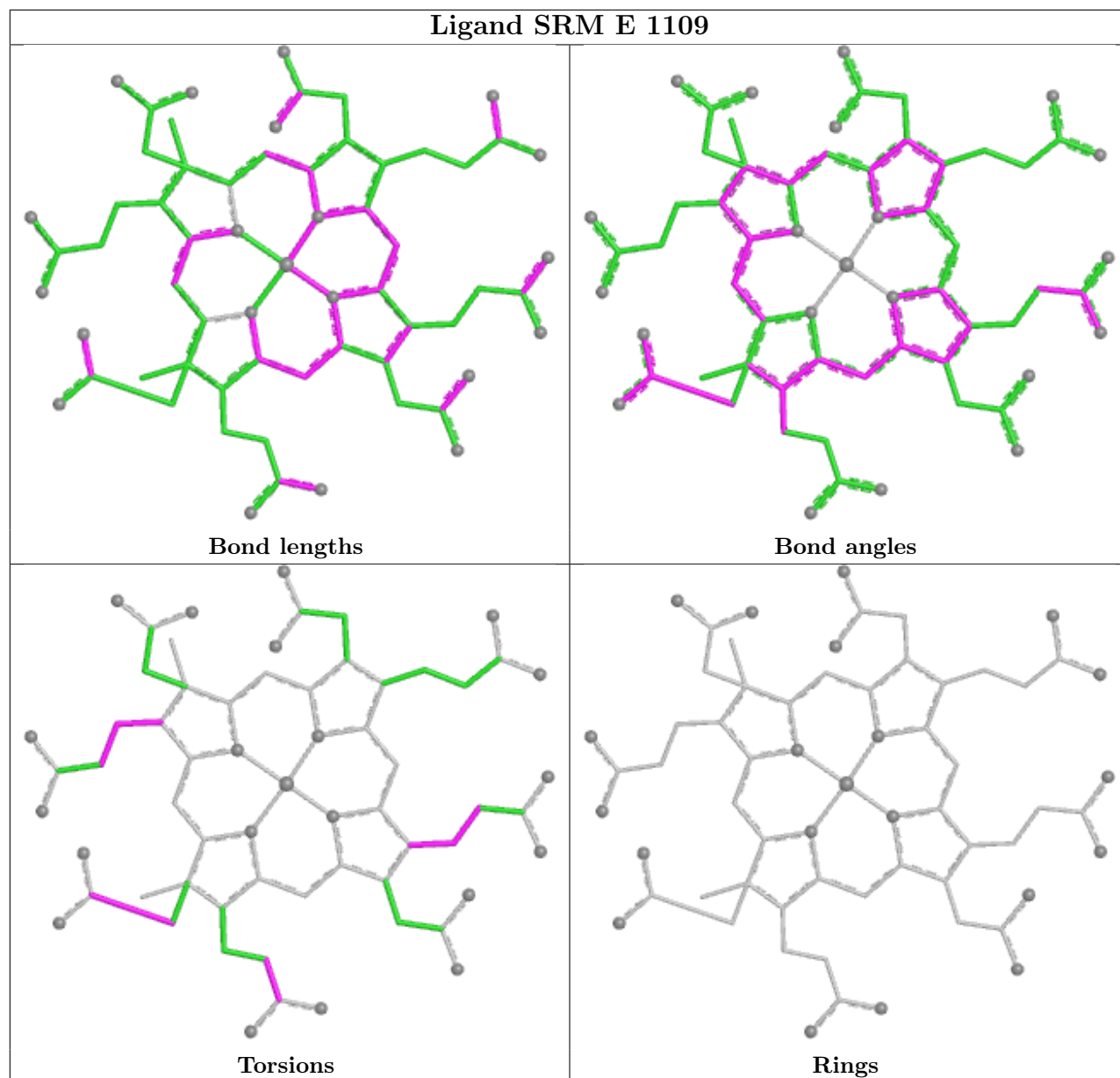
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	C	3901	GOL	2	0
6	B	4226	SO4	1	0
2	H	4405	SF4	1	0
2	A	1101	SF4	1	0
4	H	4413	EDO	1	0
2	M	1104	SF4	1	0
9	N	1011	GOL	1	0
4	G	1120	EDO	1	0
2	J	1104	SF4	1	0
4	A	1116	EDO	2	0
4	B	4211	EDO	1	0
4	G	1118	EDO	2	0
11	M	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
9	I	1111	GOL	2	0
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

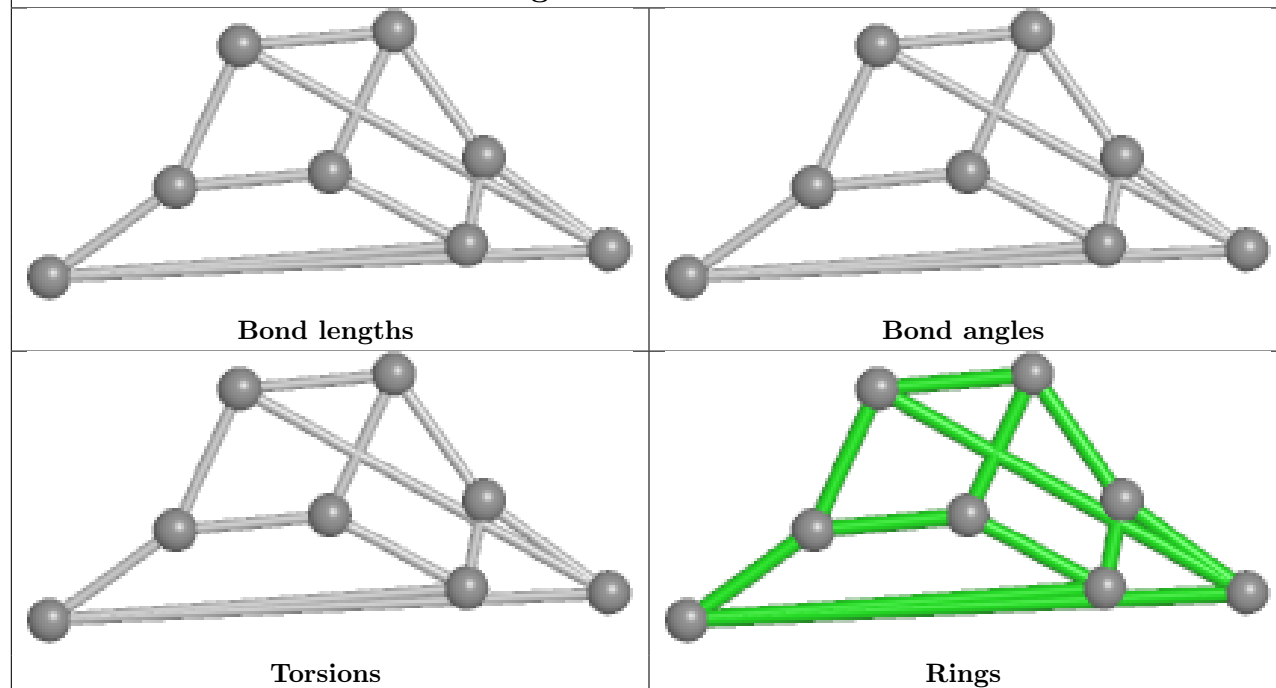
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

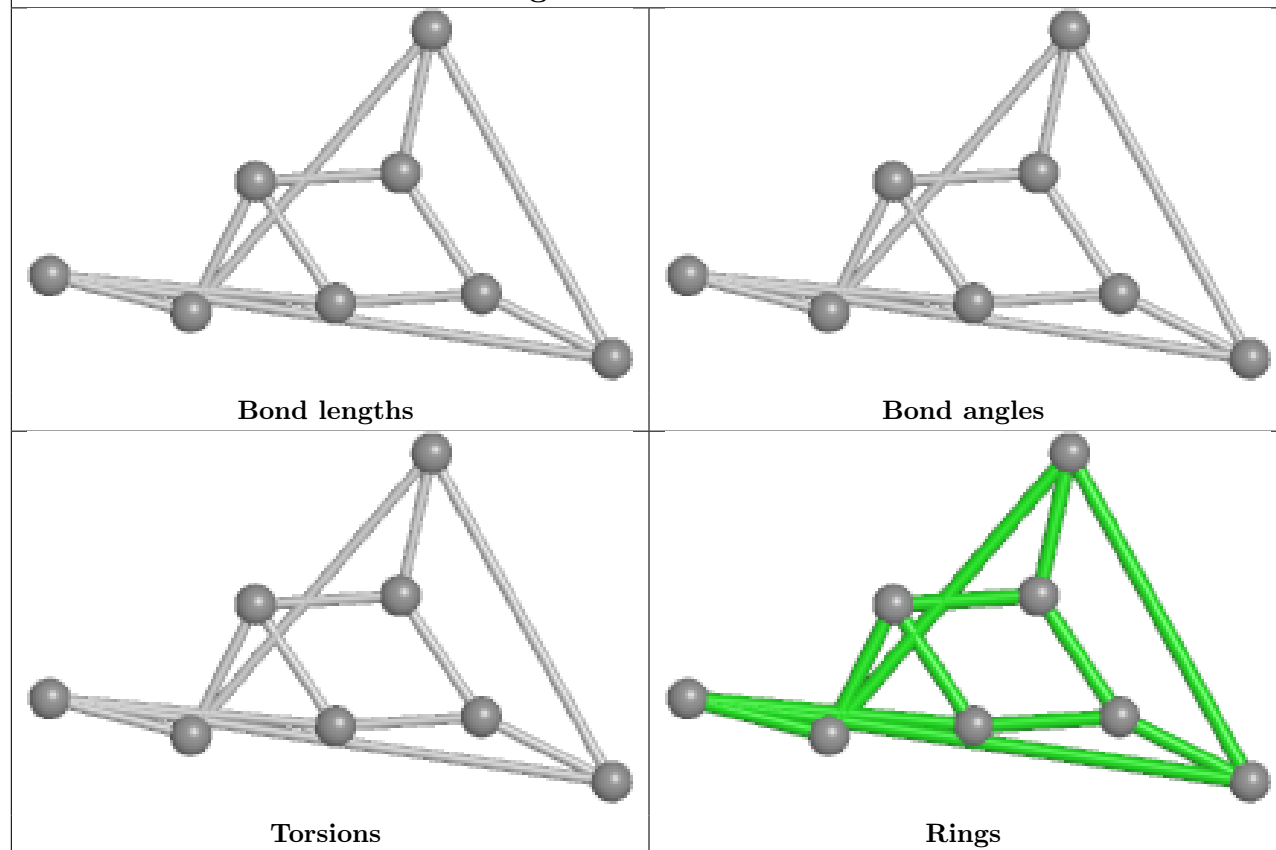


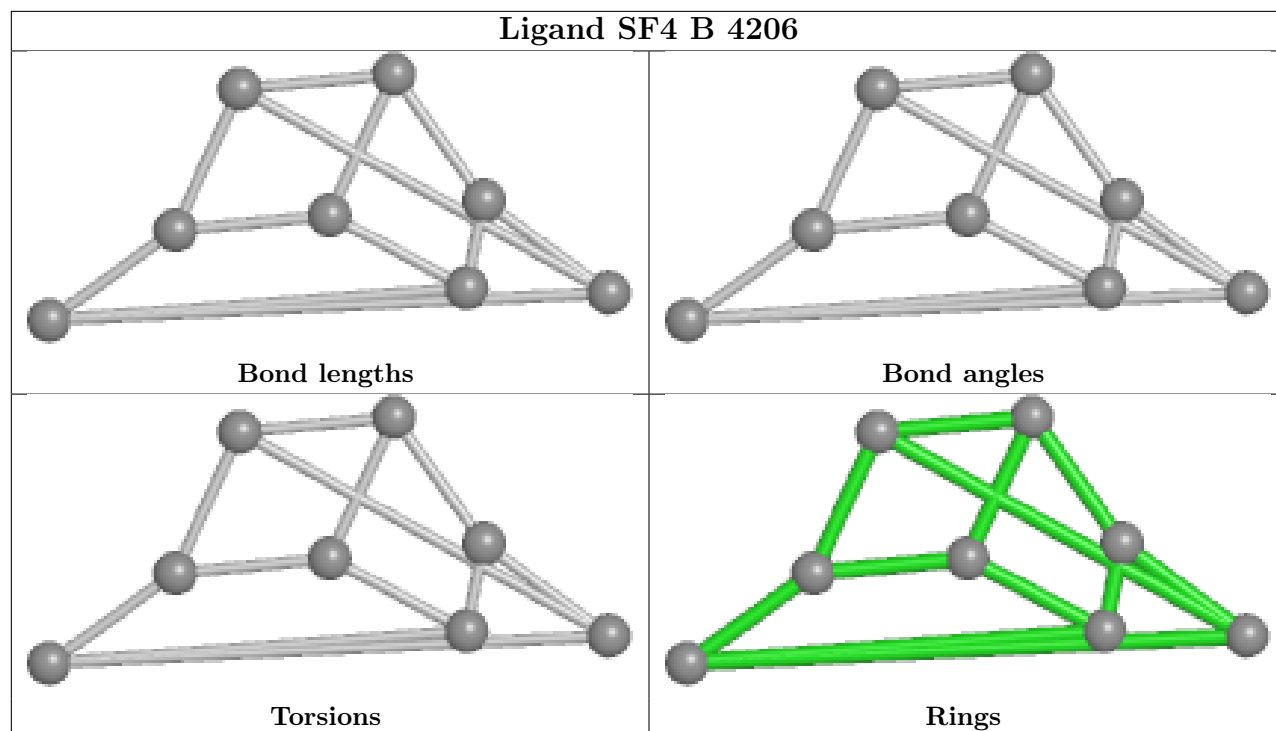


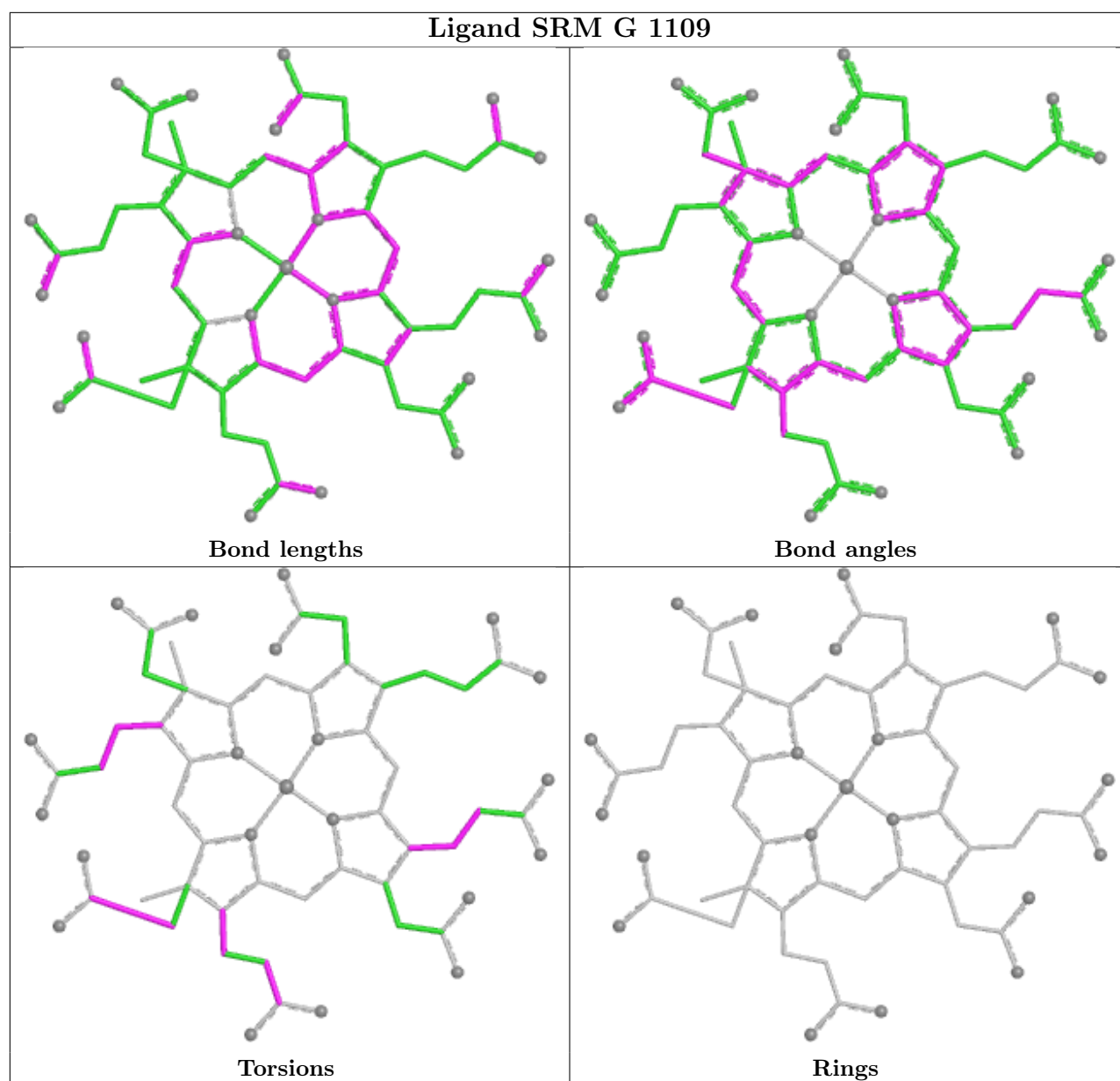
Ligand SF4 P 1102

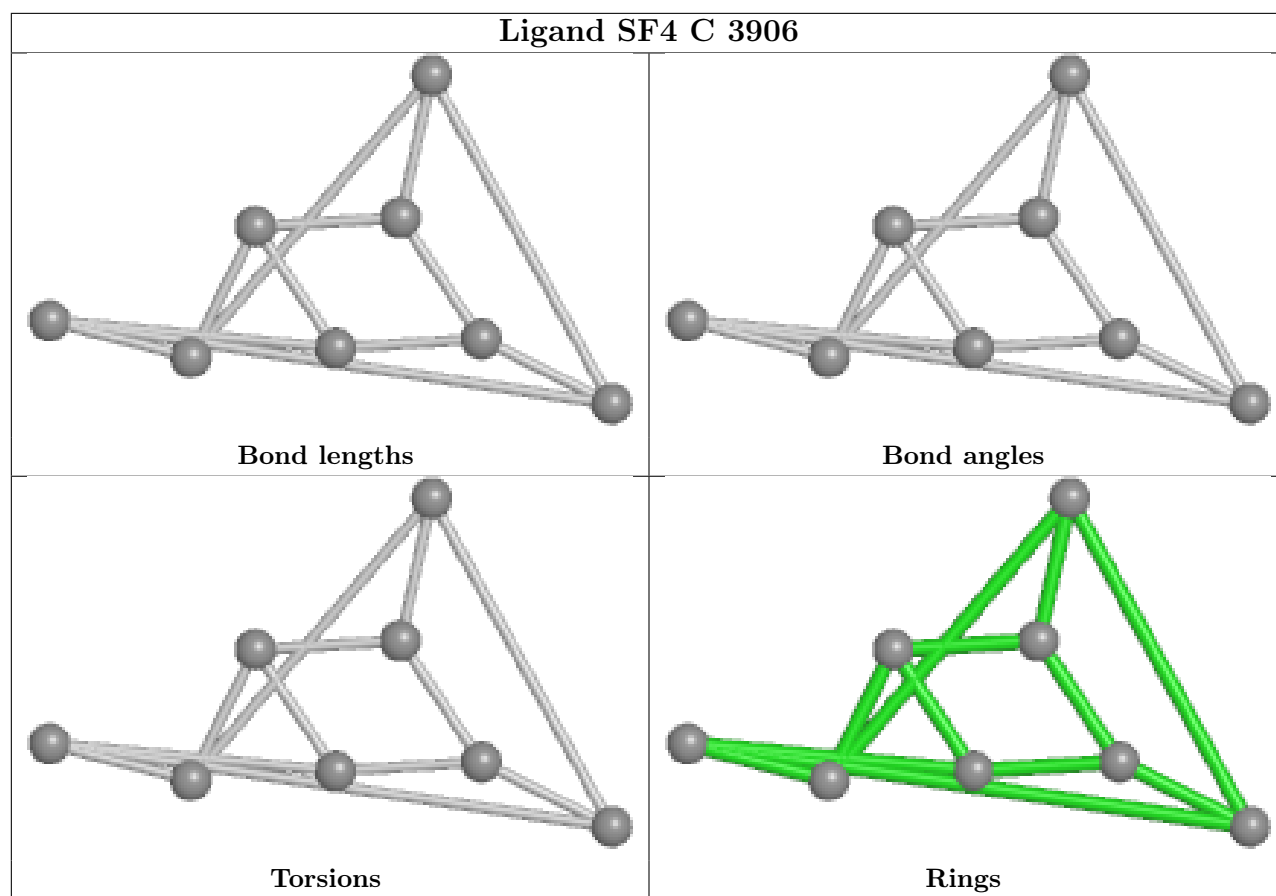
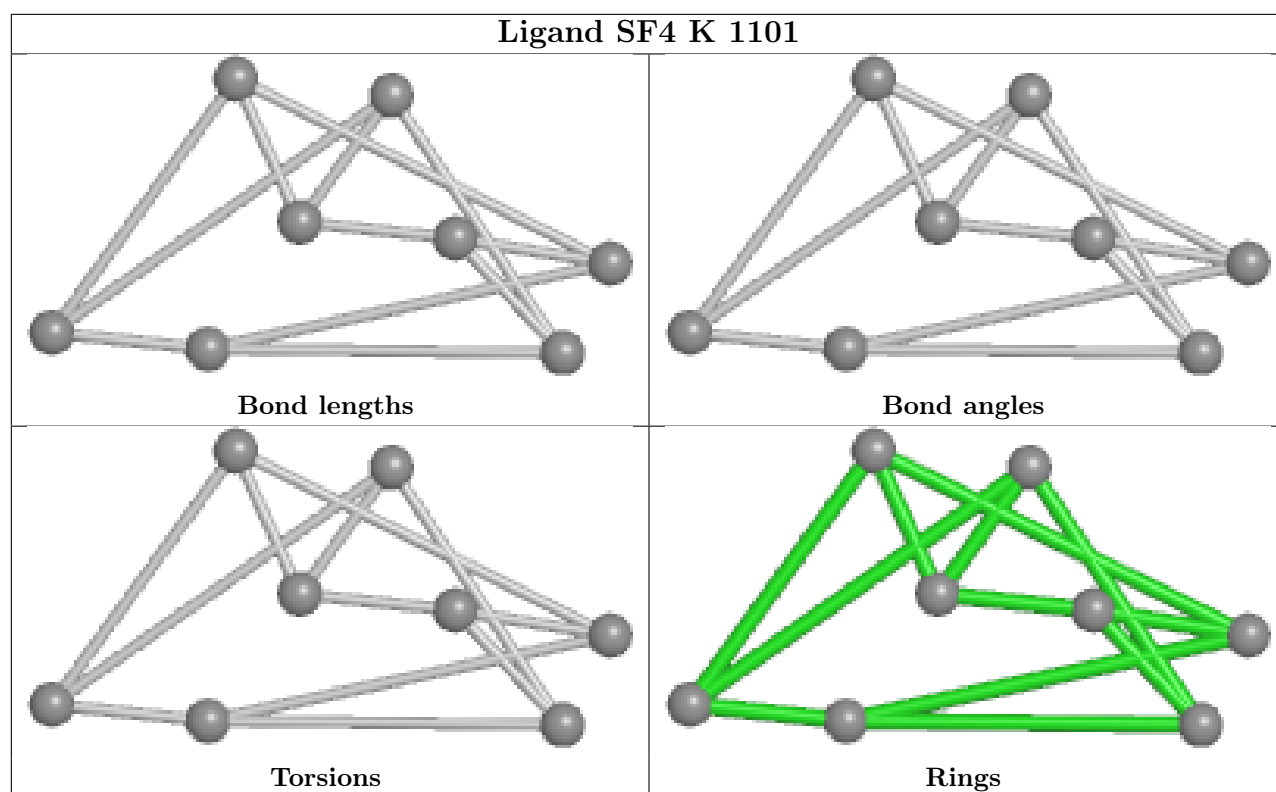


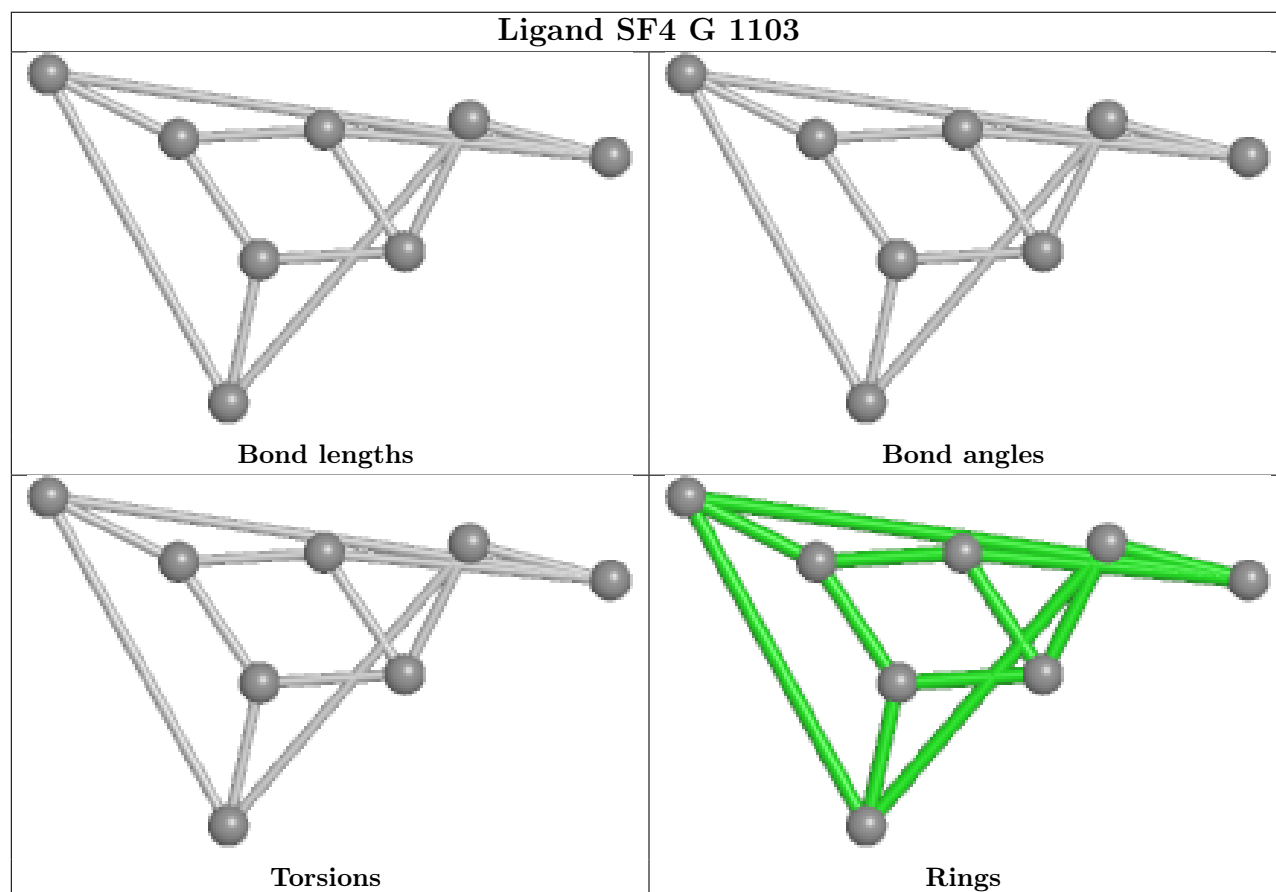
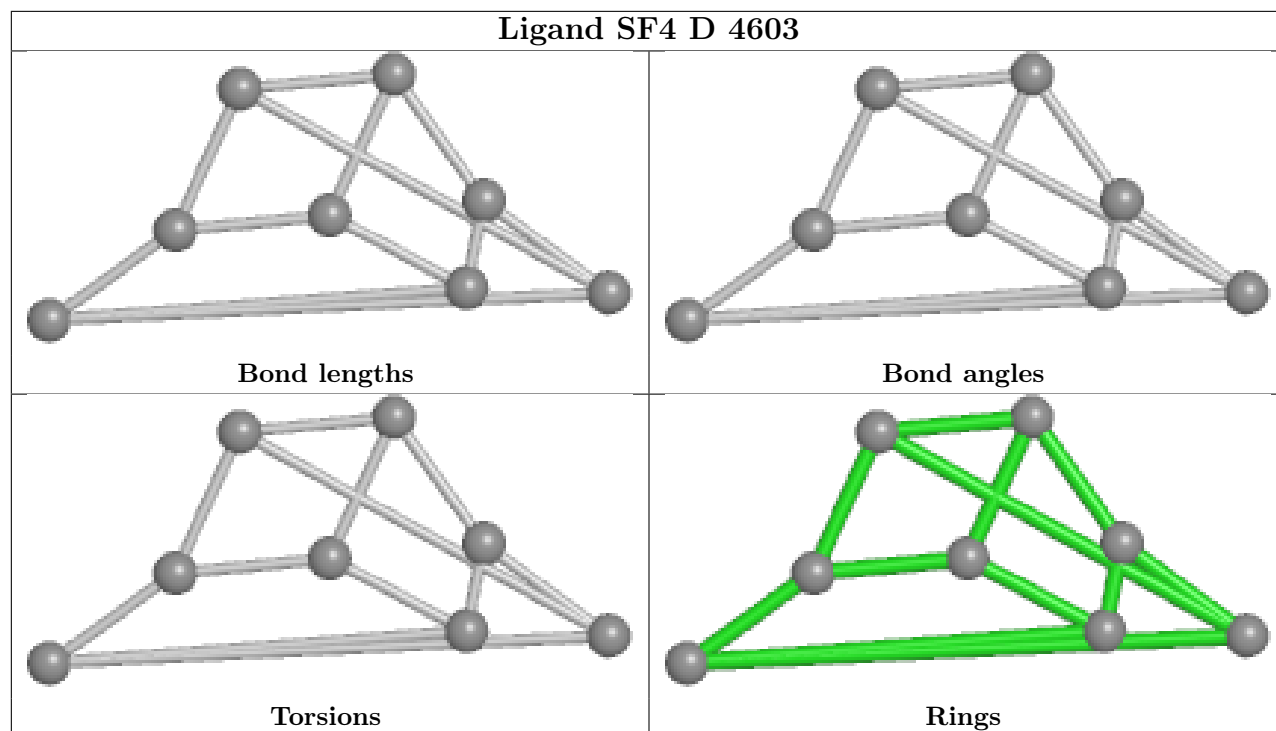
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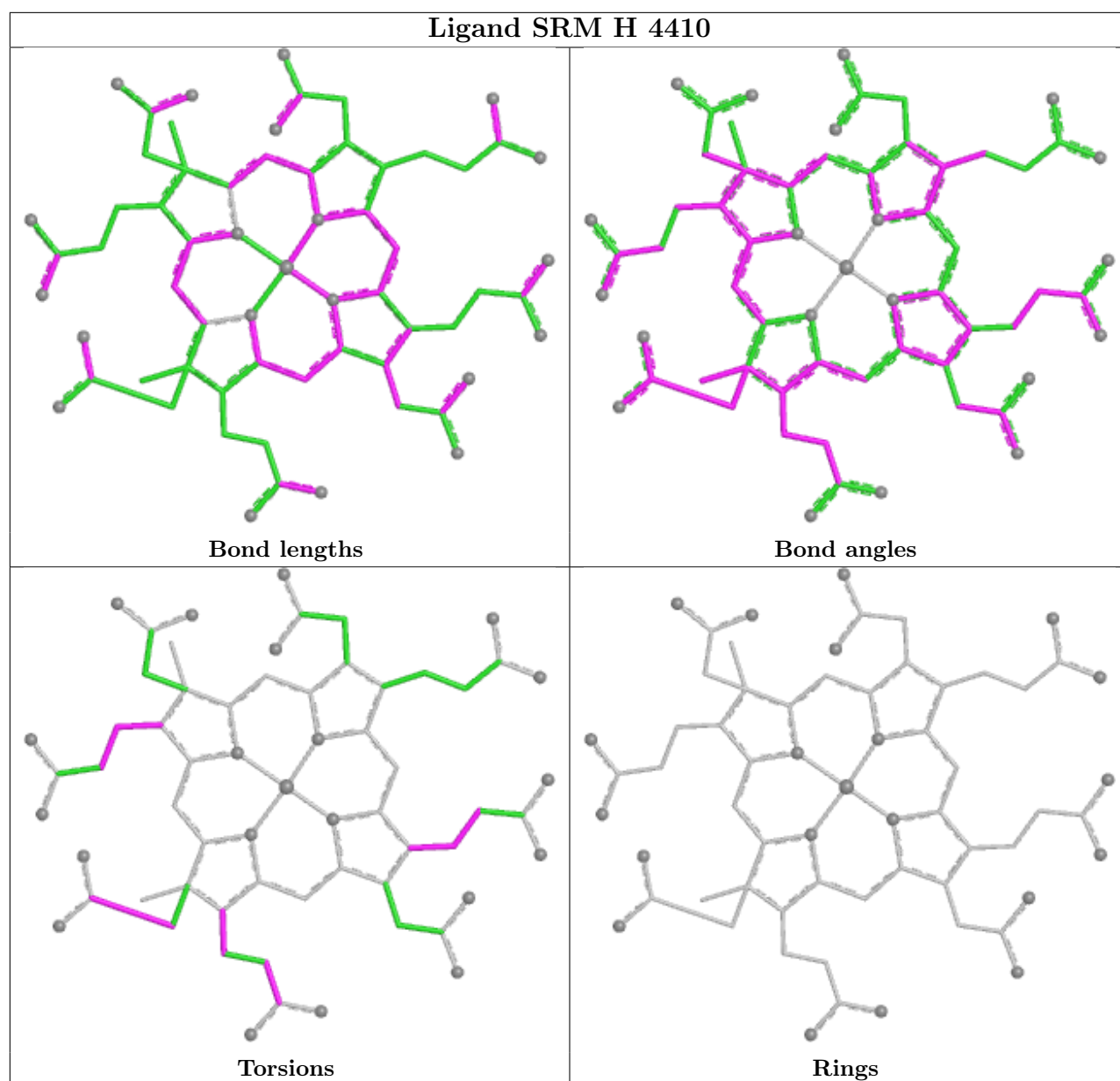




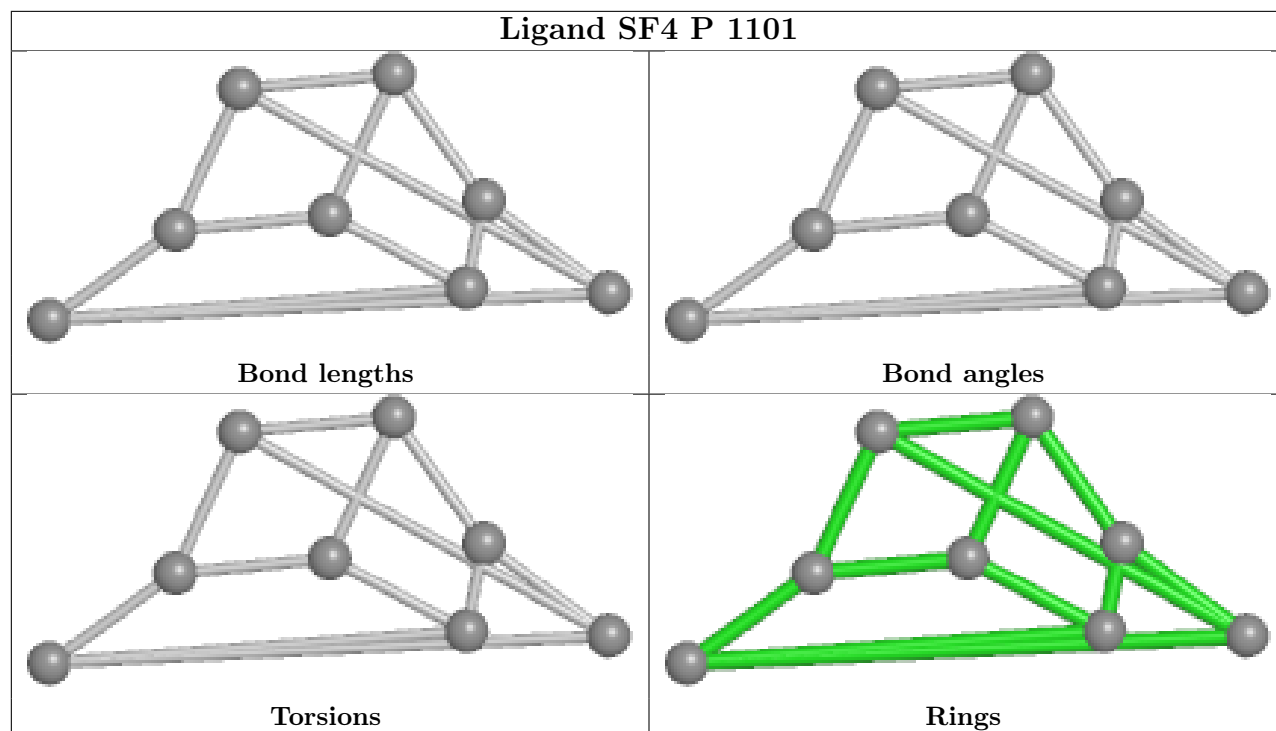




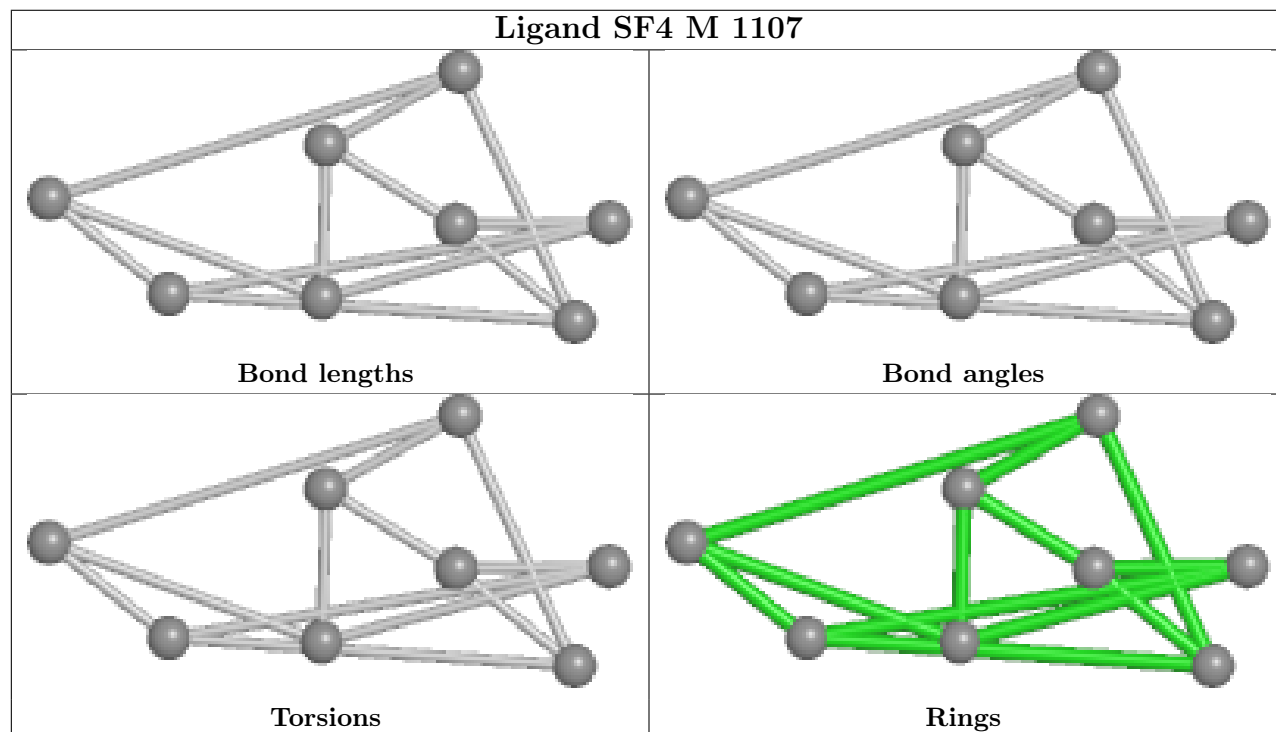




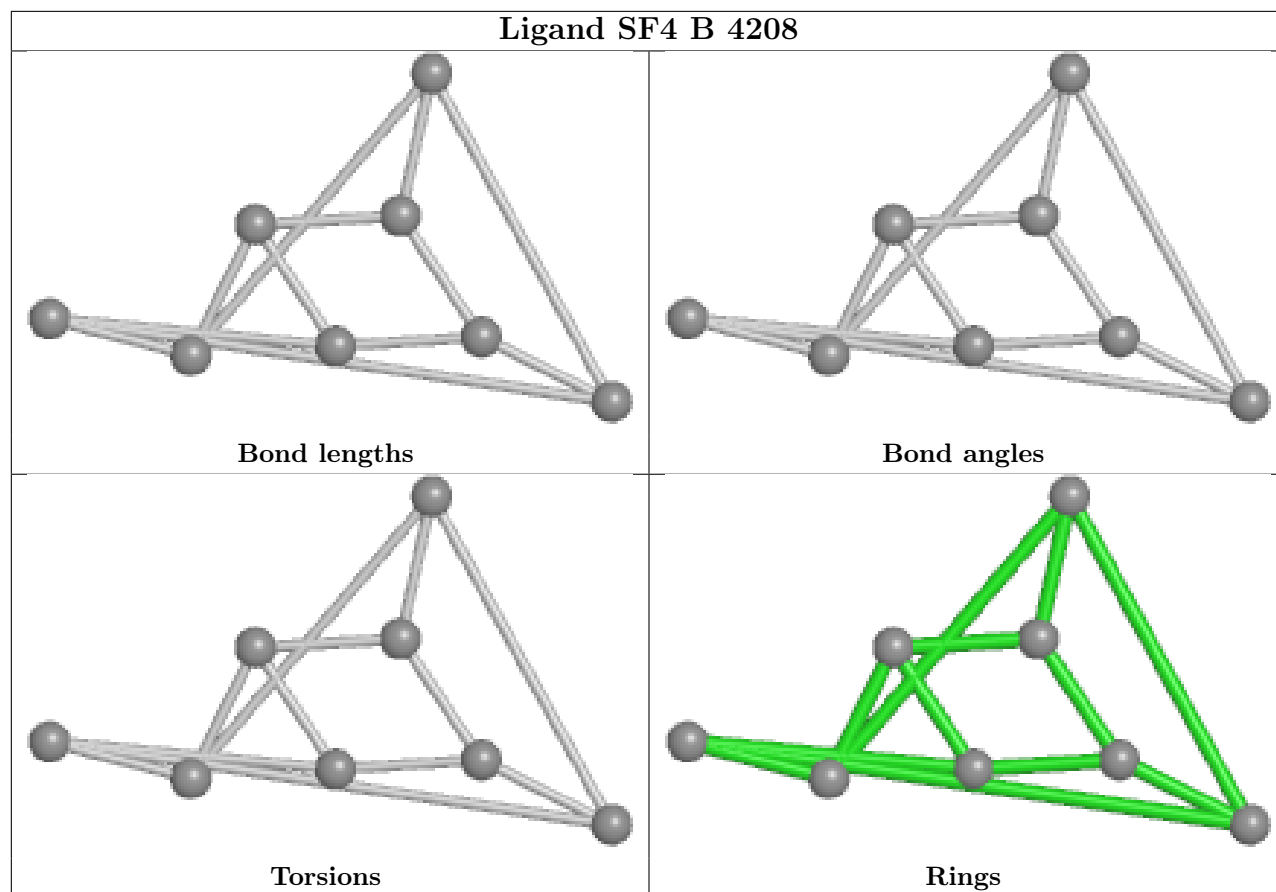
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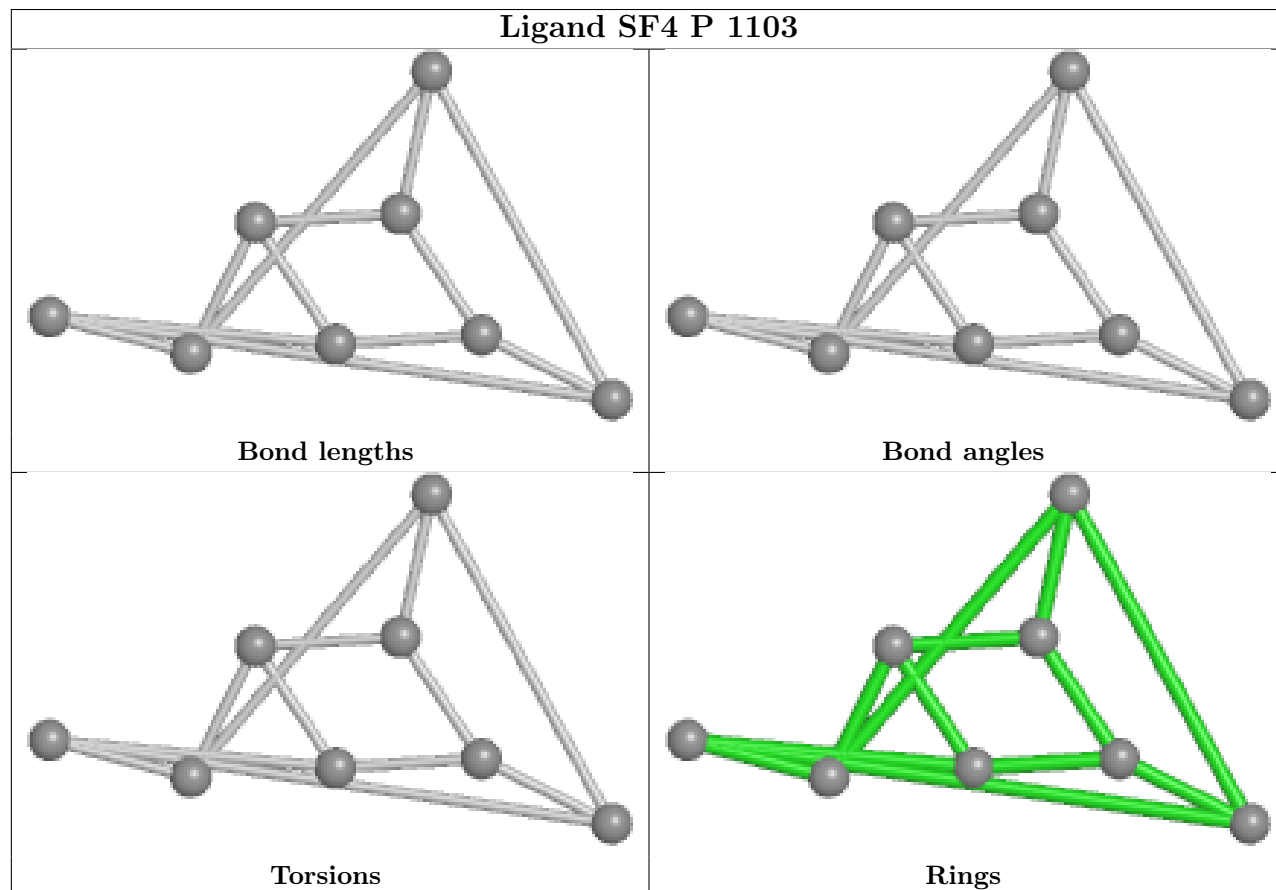
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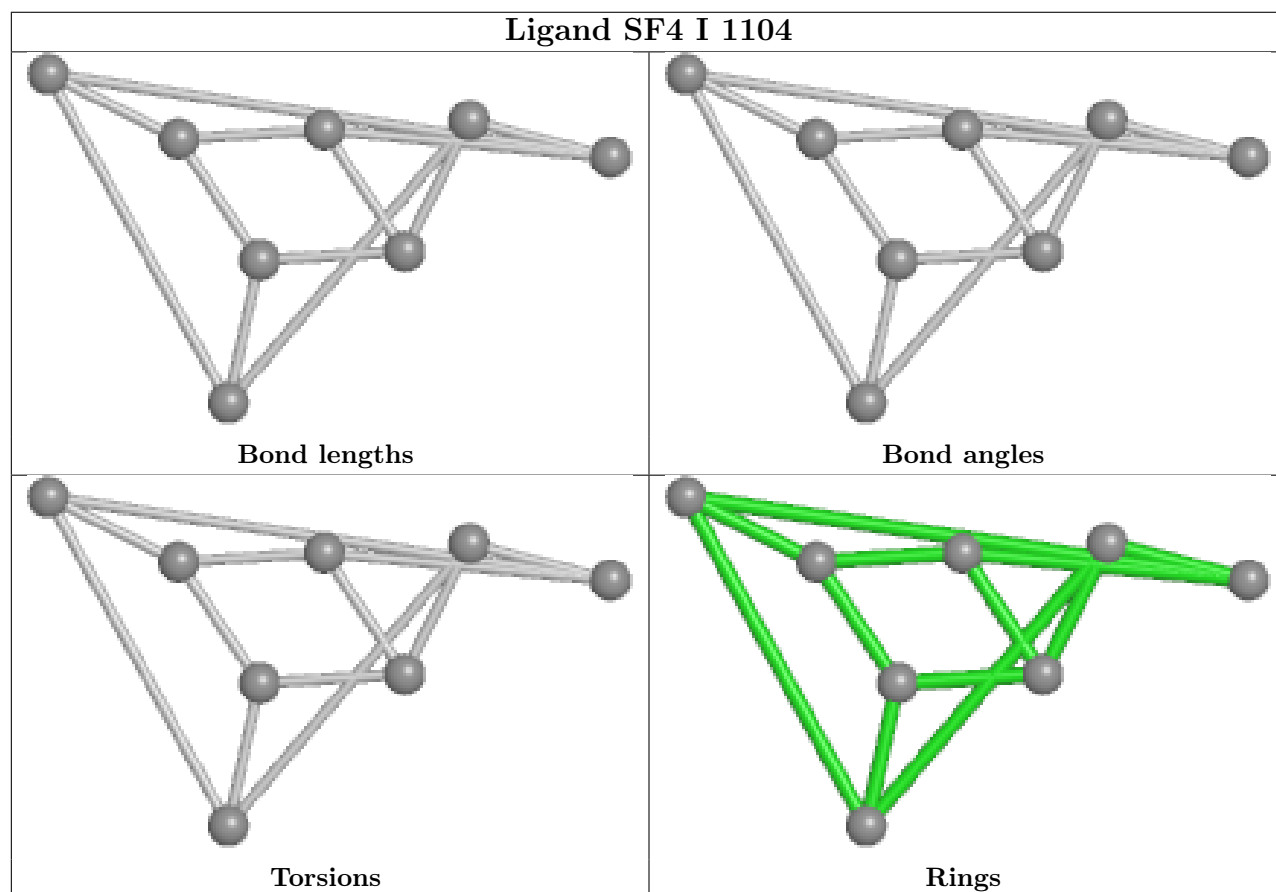
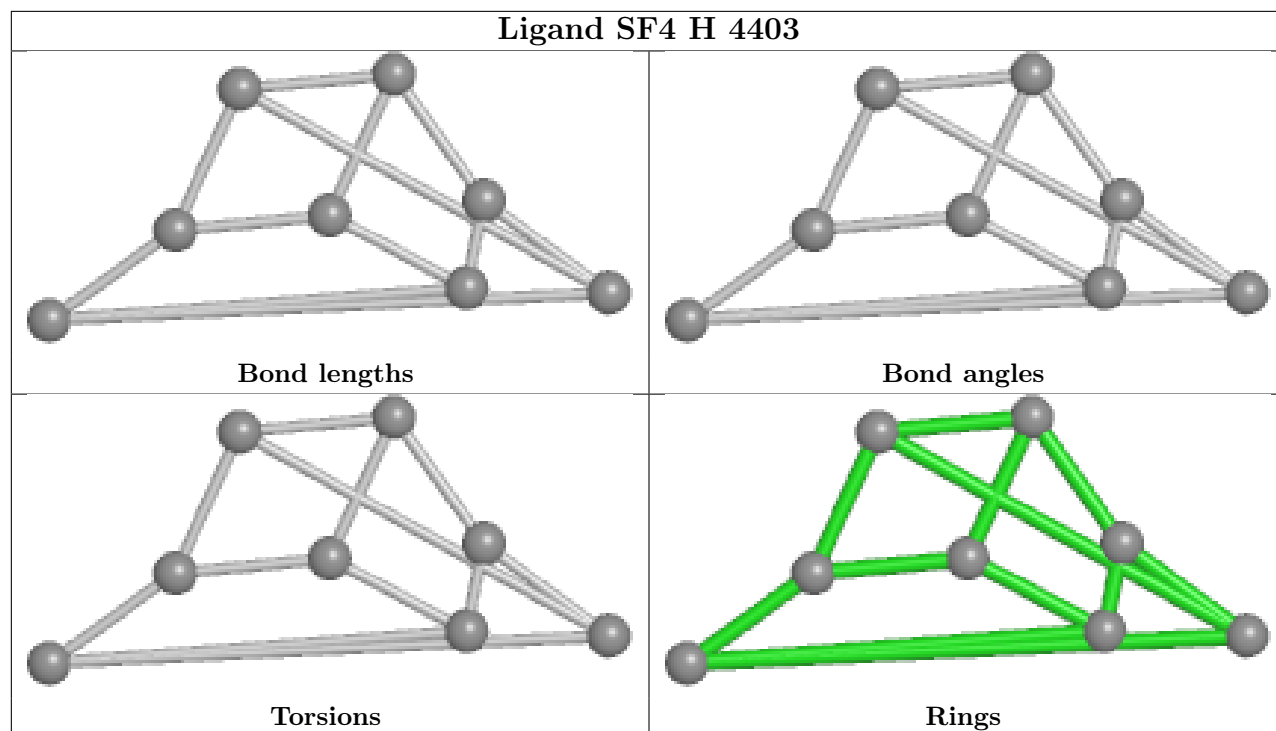


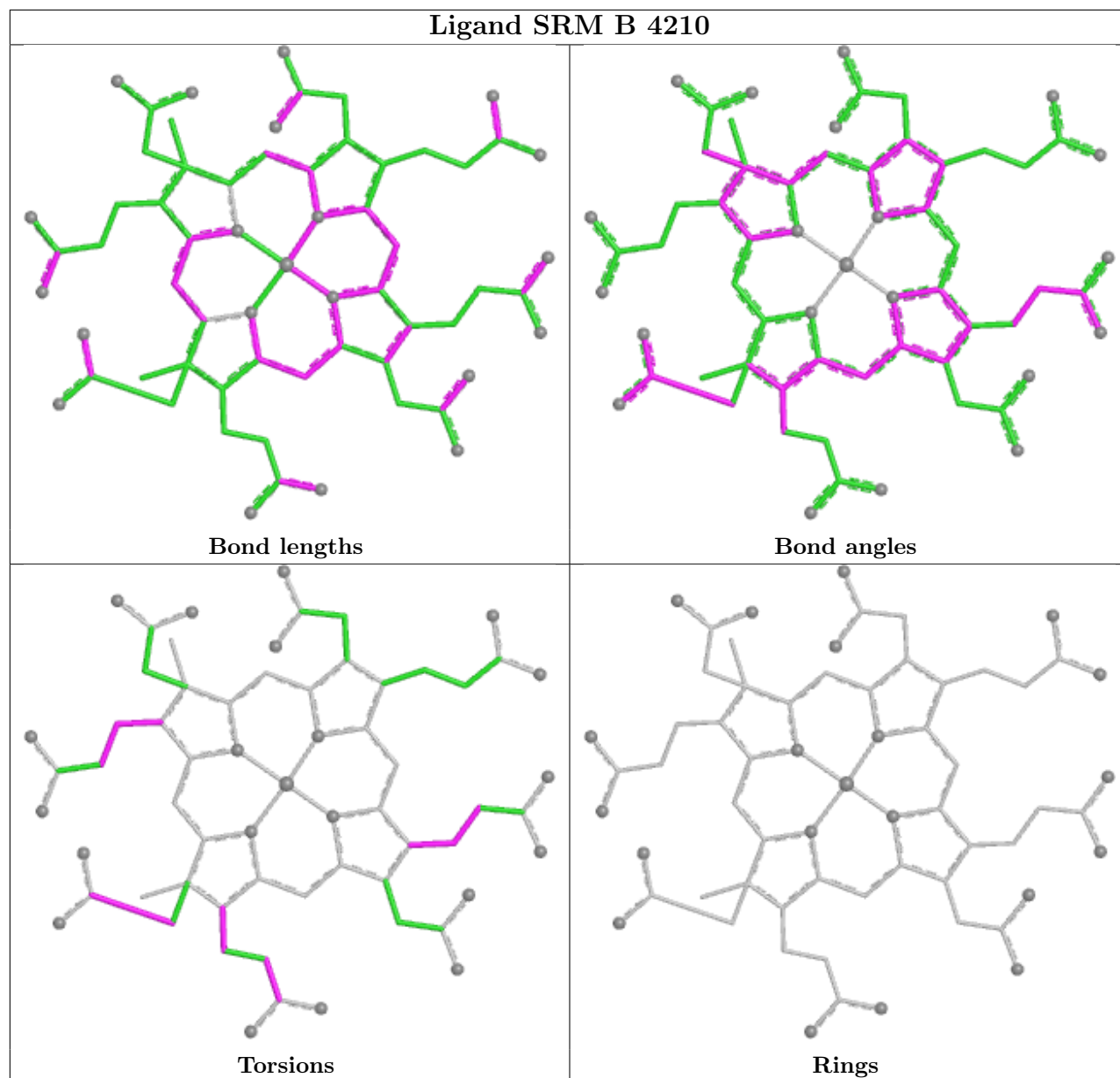
Ligand SF4 B 4208



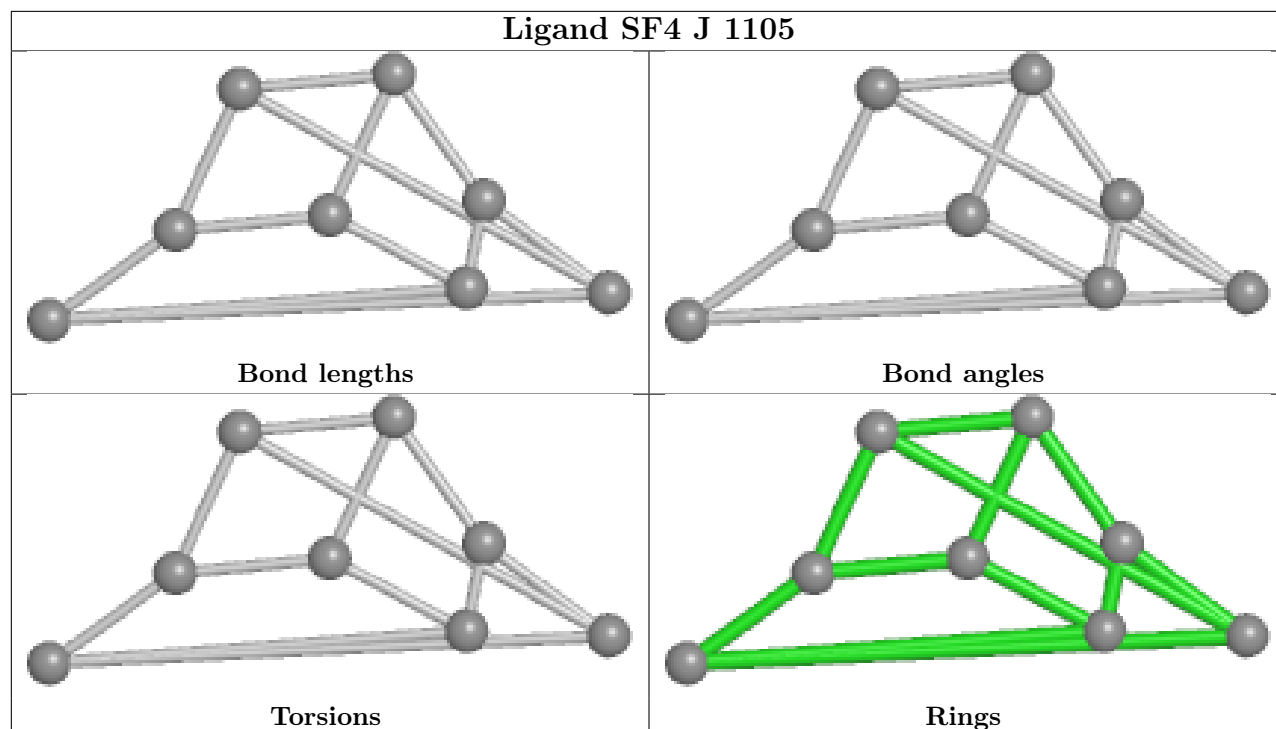
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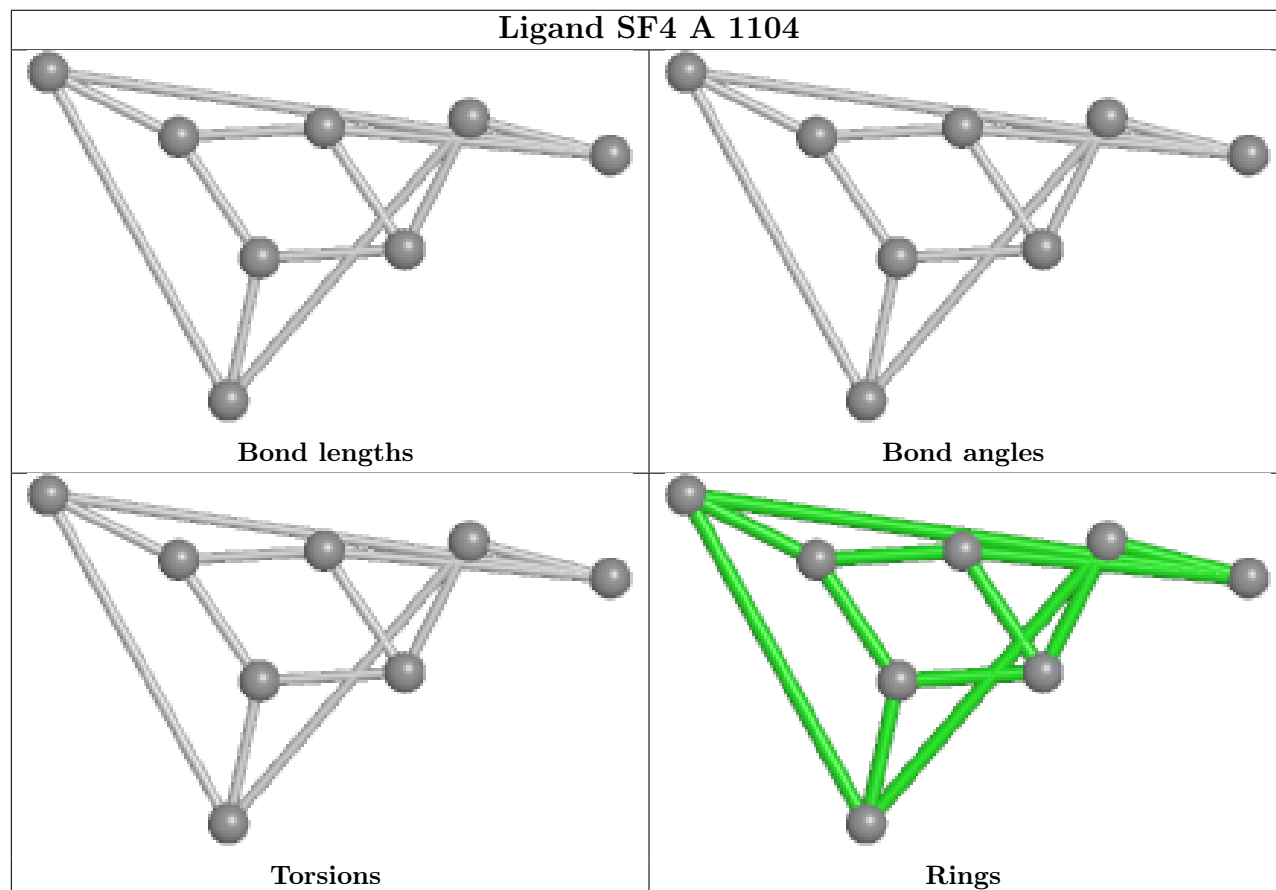


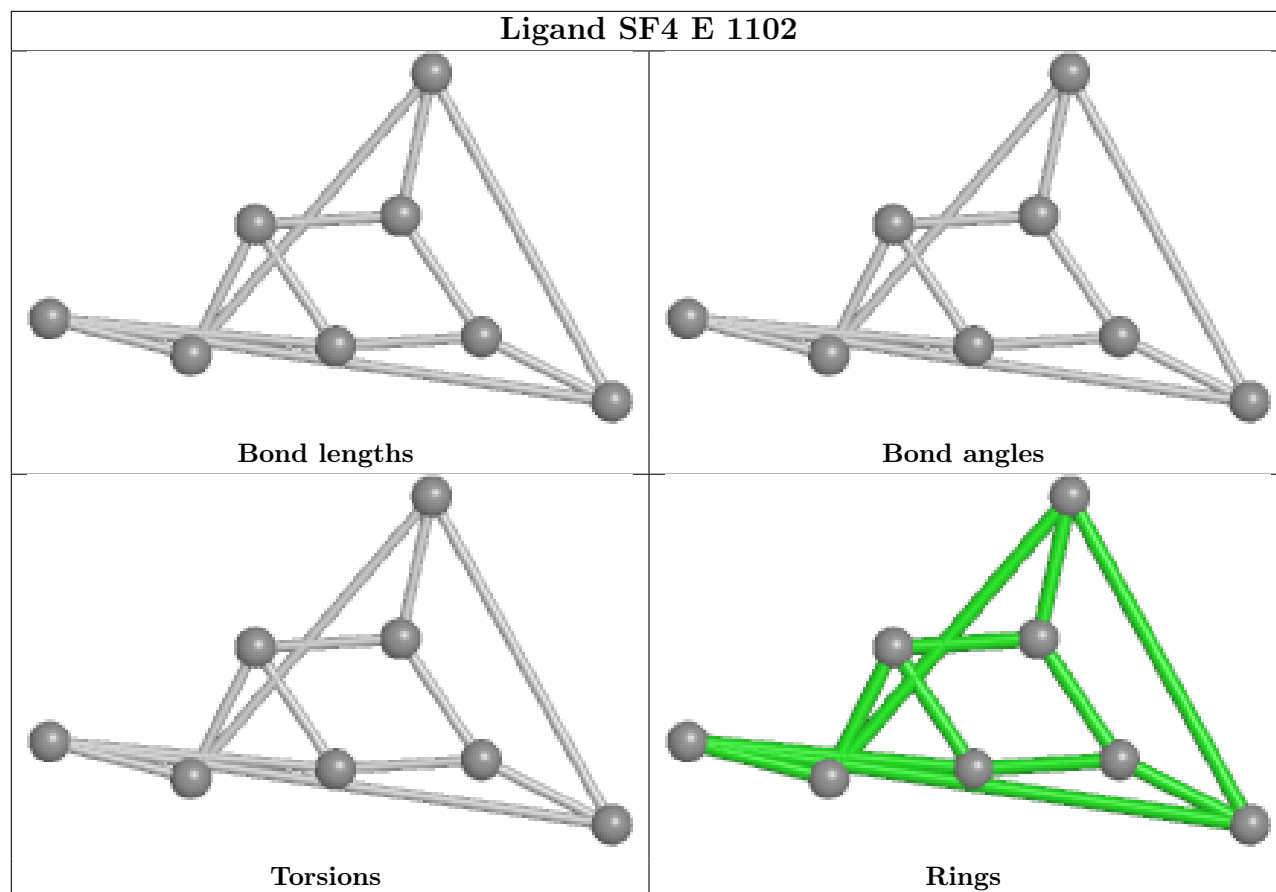


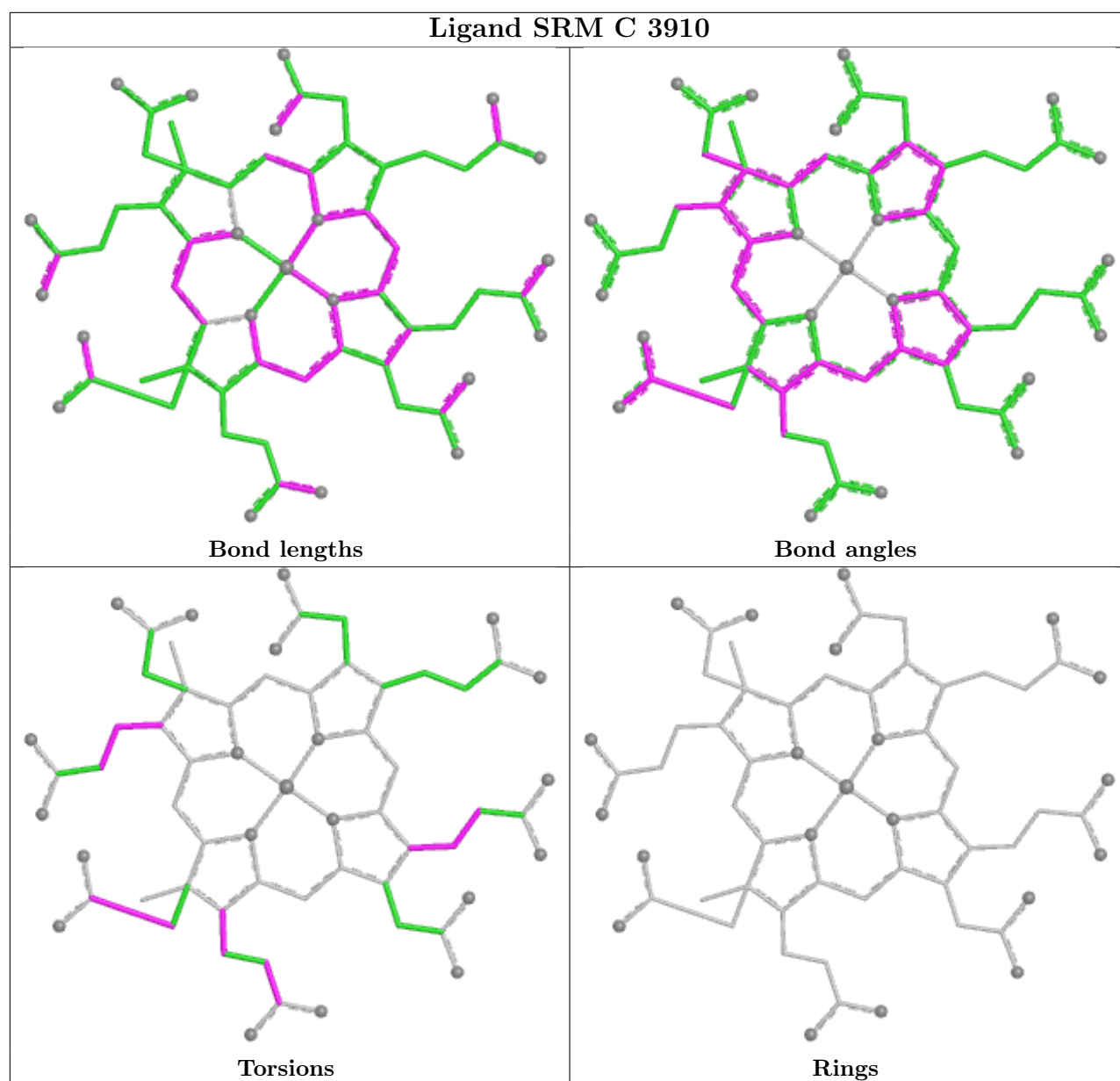
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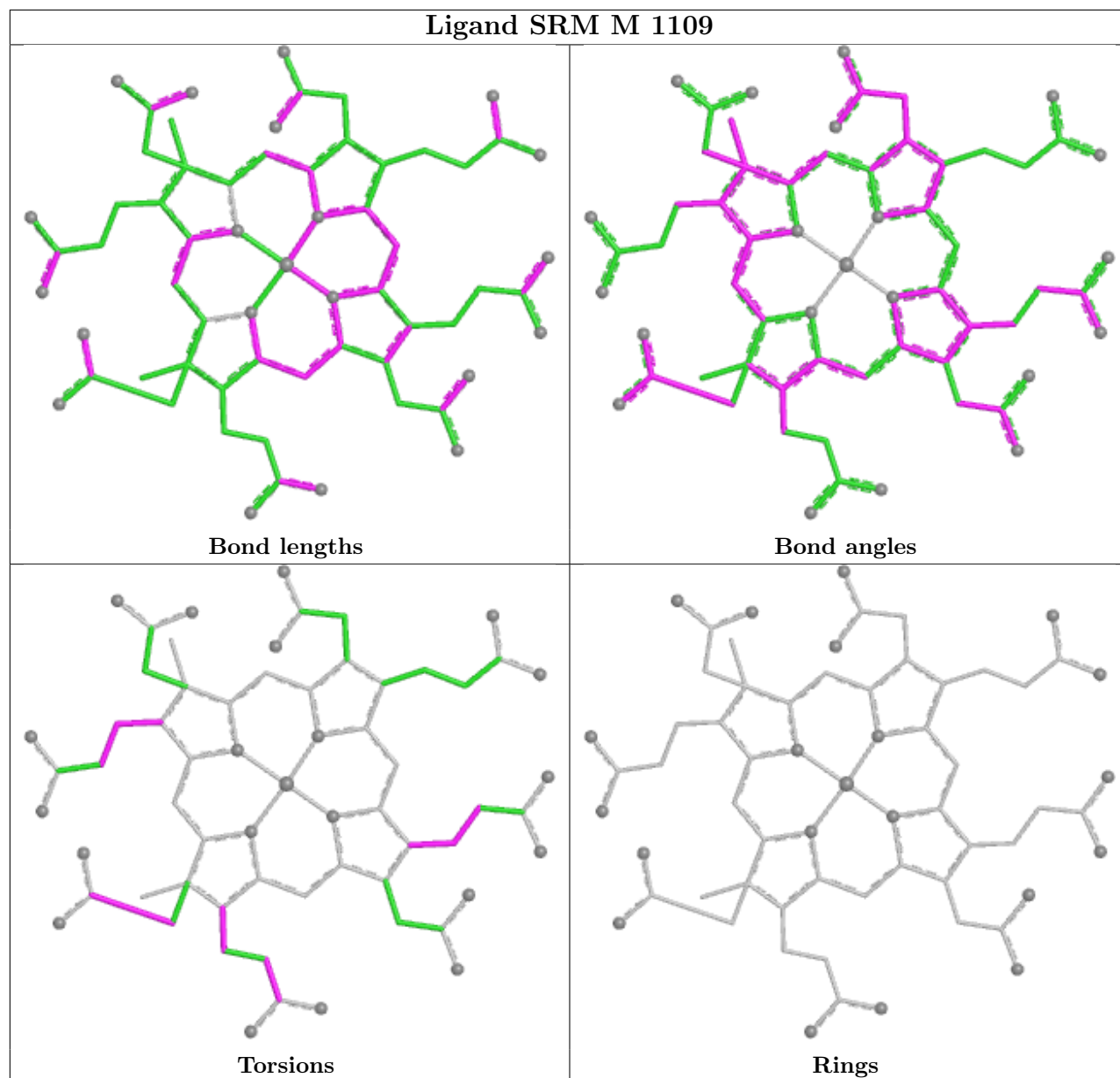
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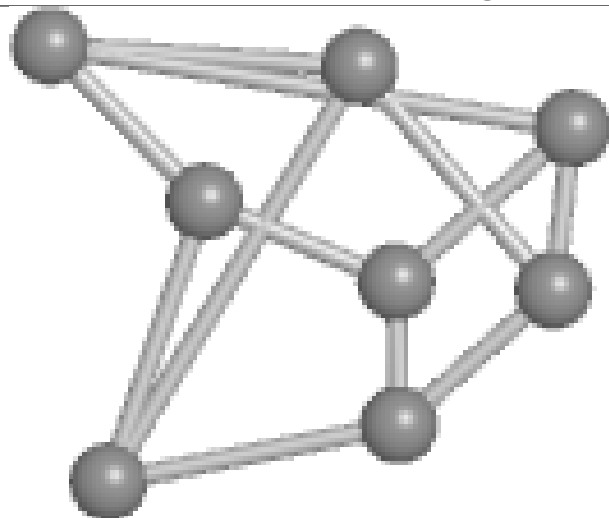




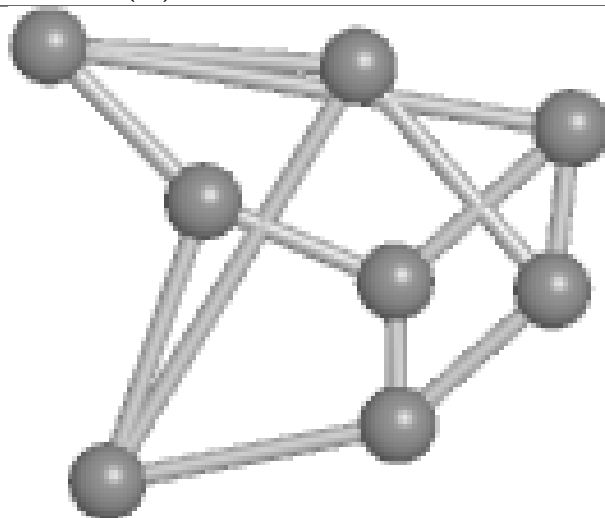
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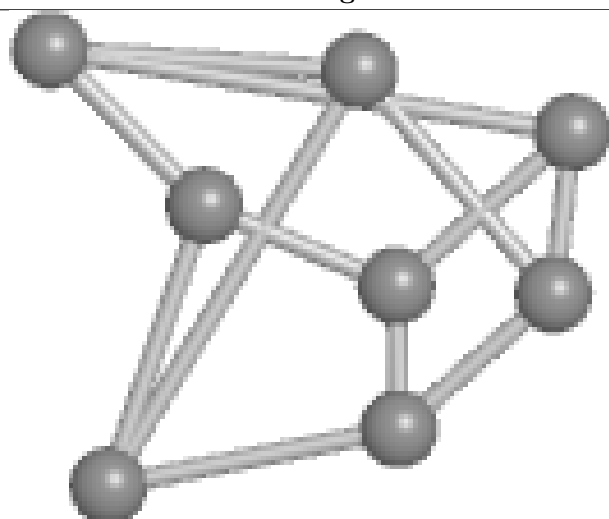
Ligand SF4 N 1008 (B)



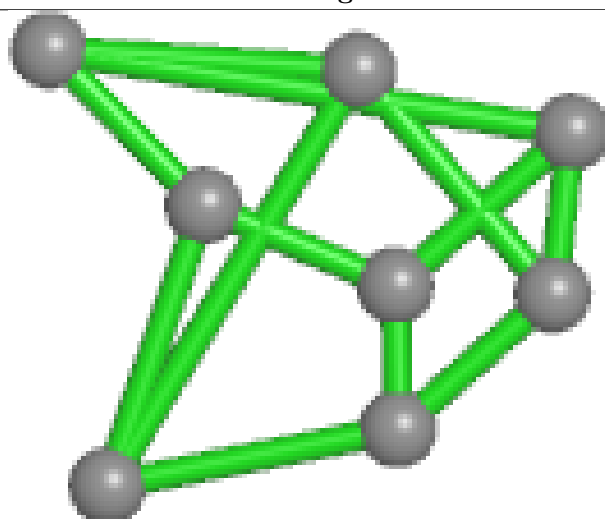
Bond lengths



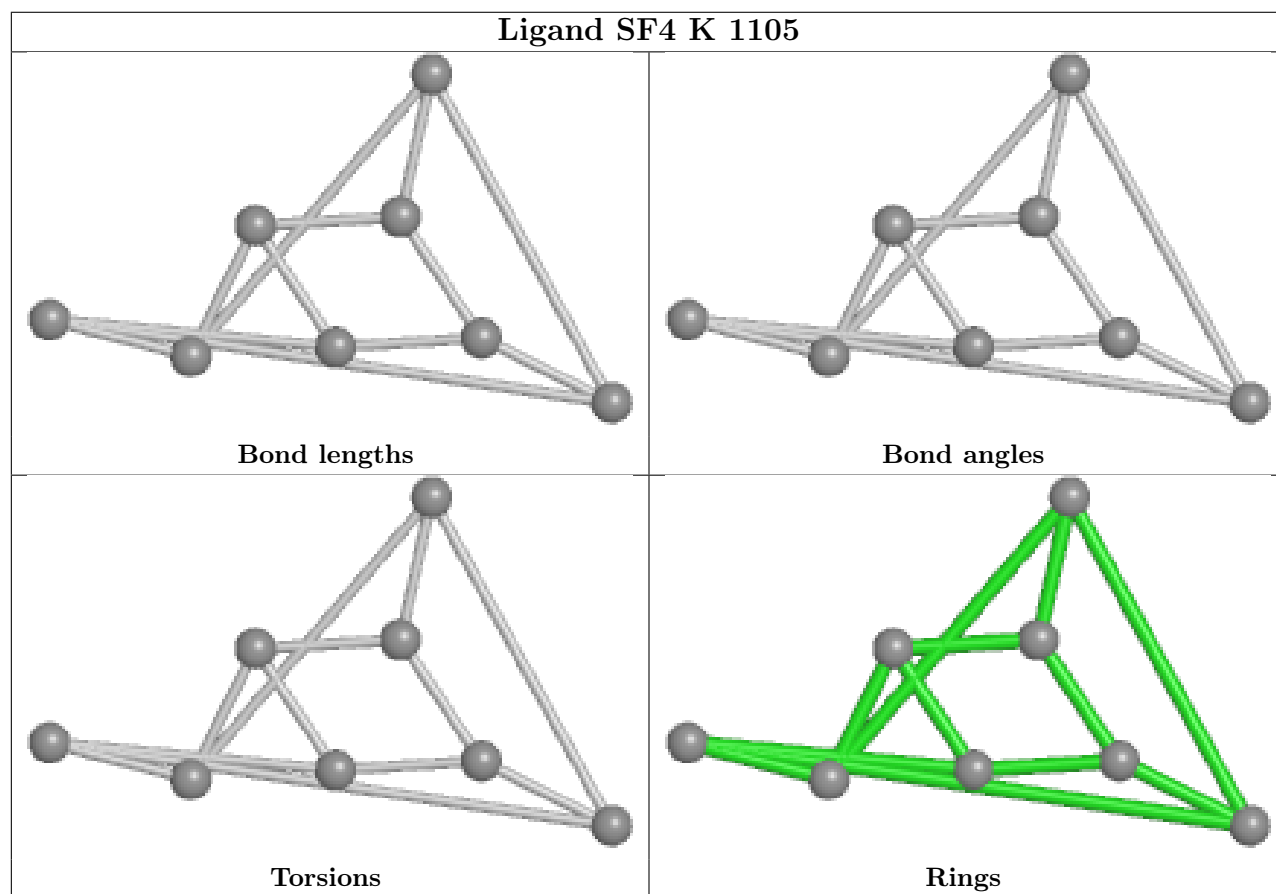
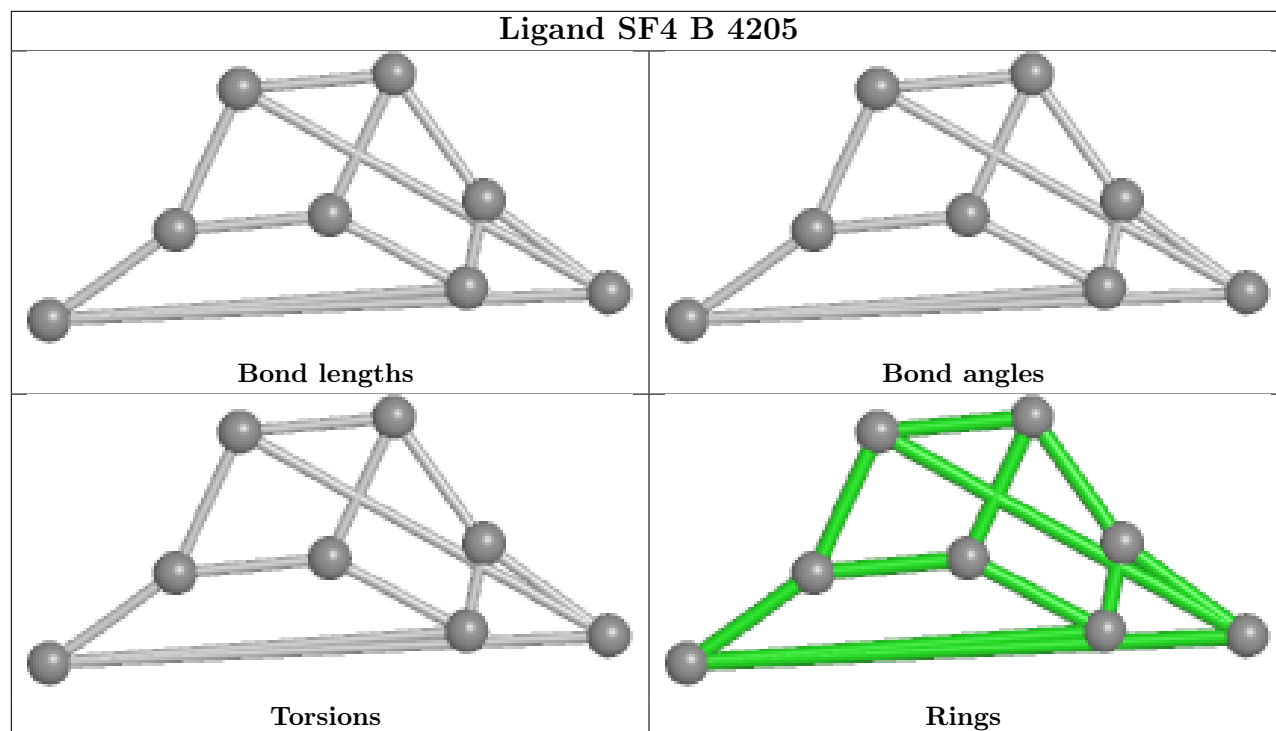
Bond angles

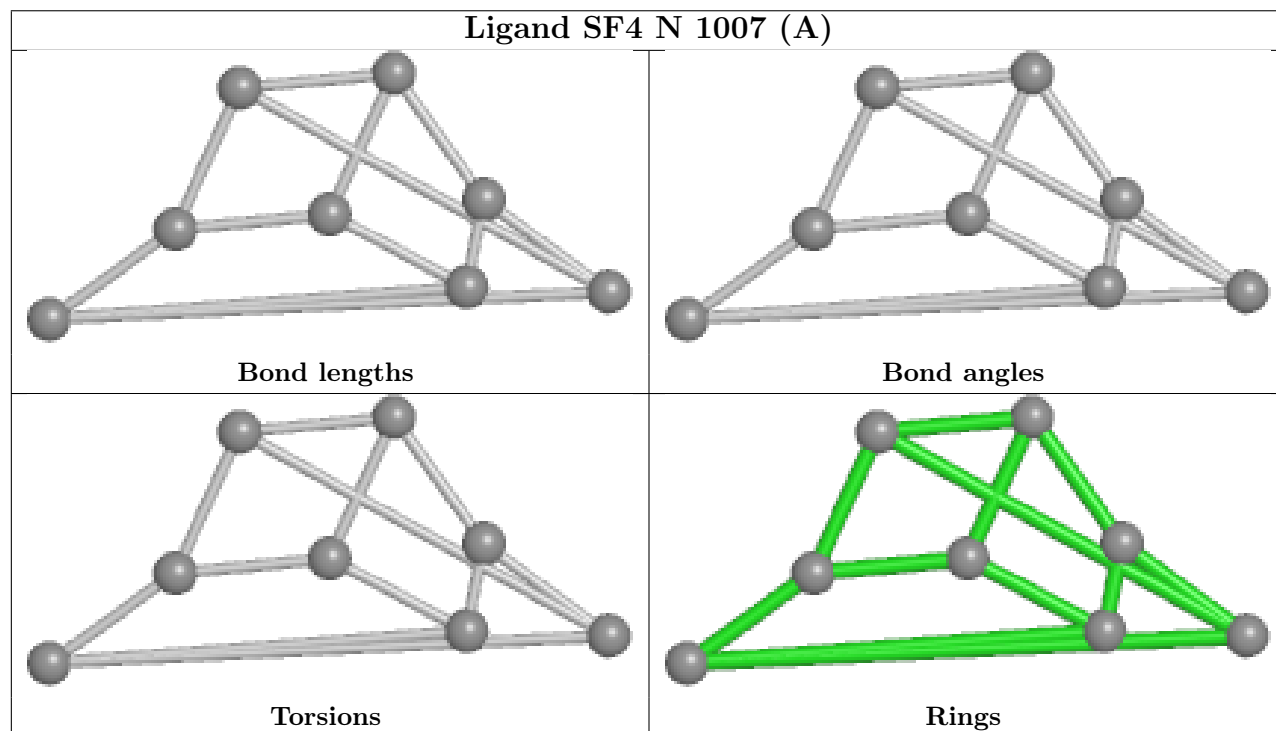
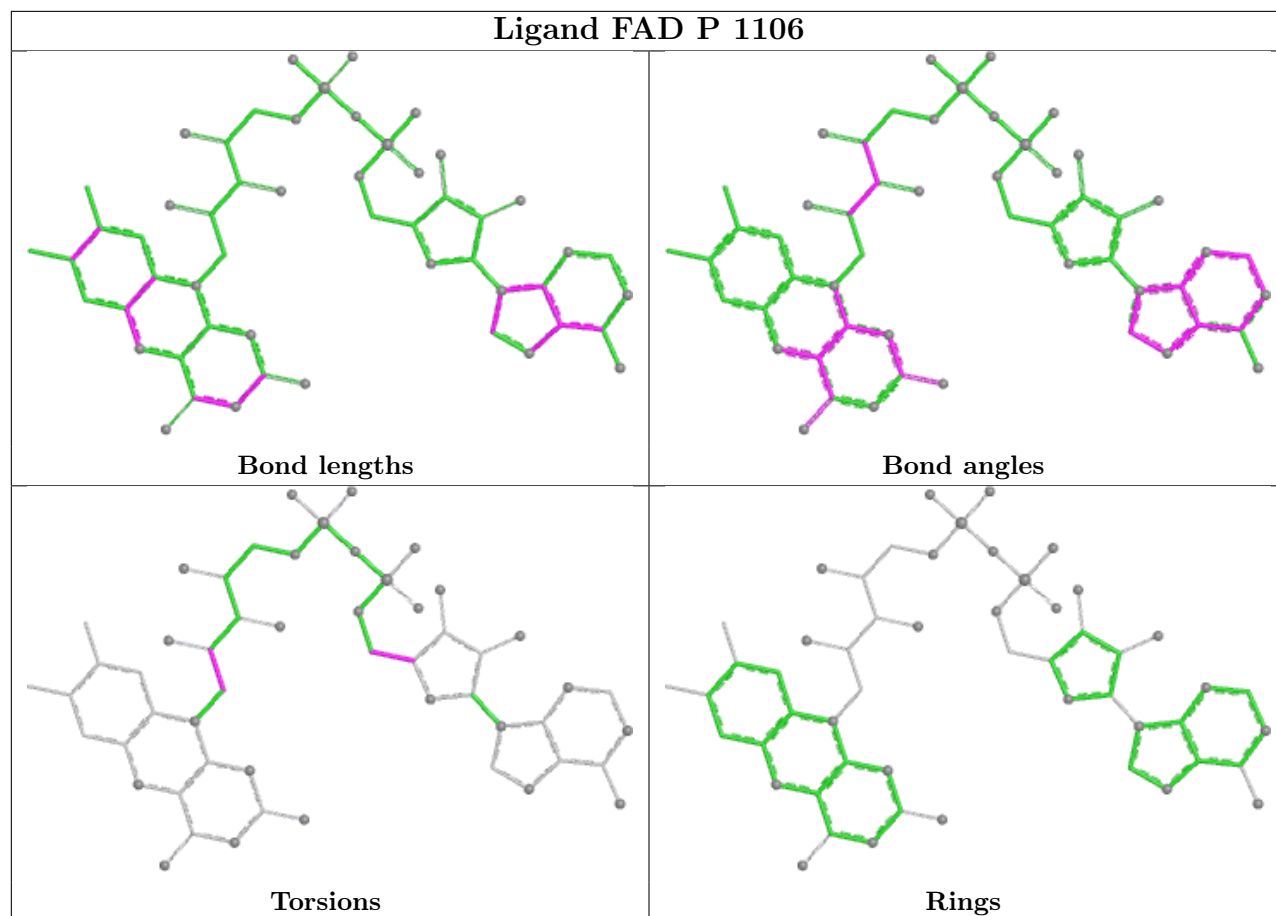


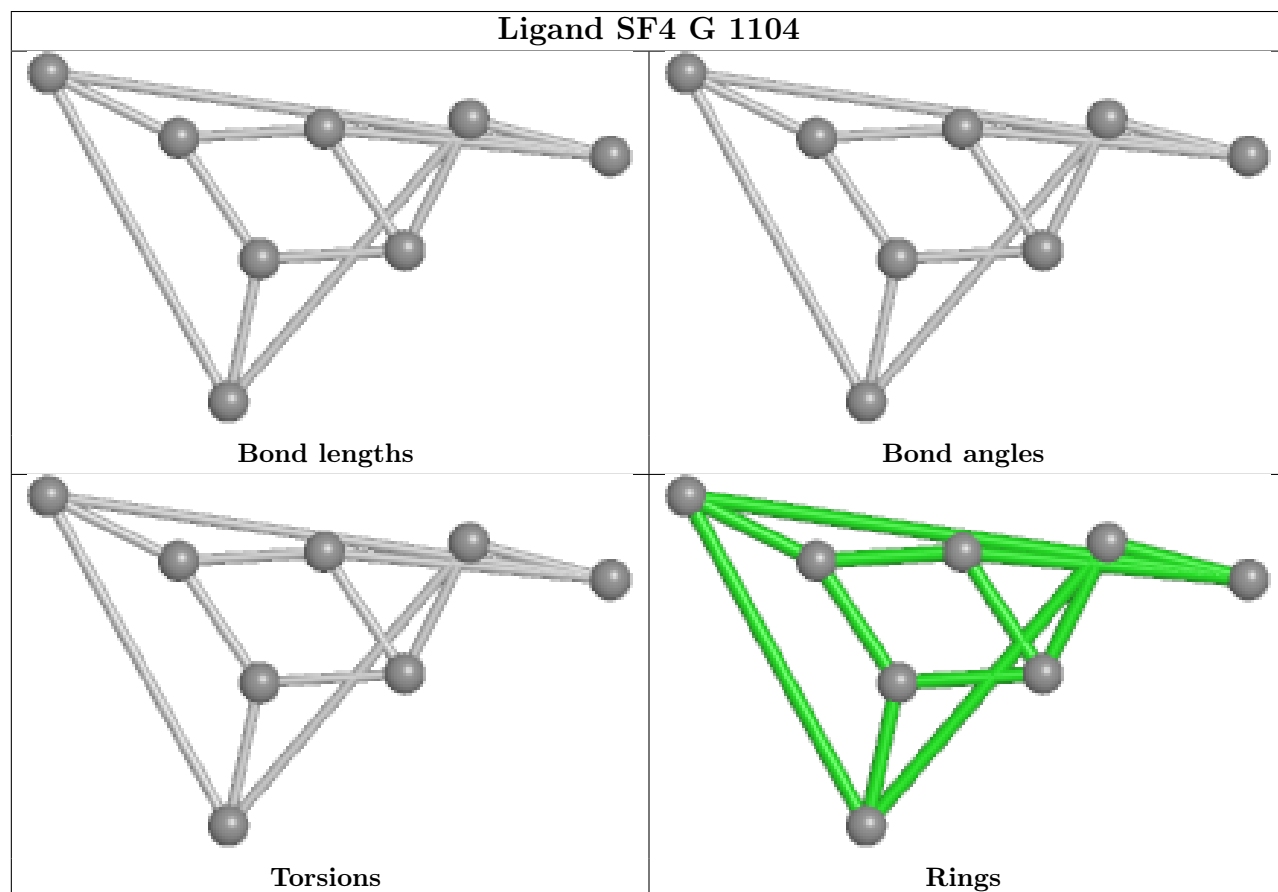
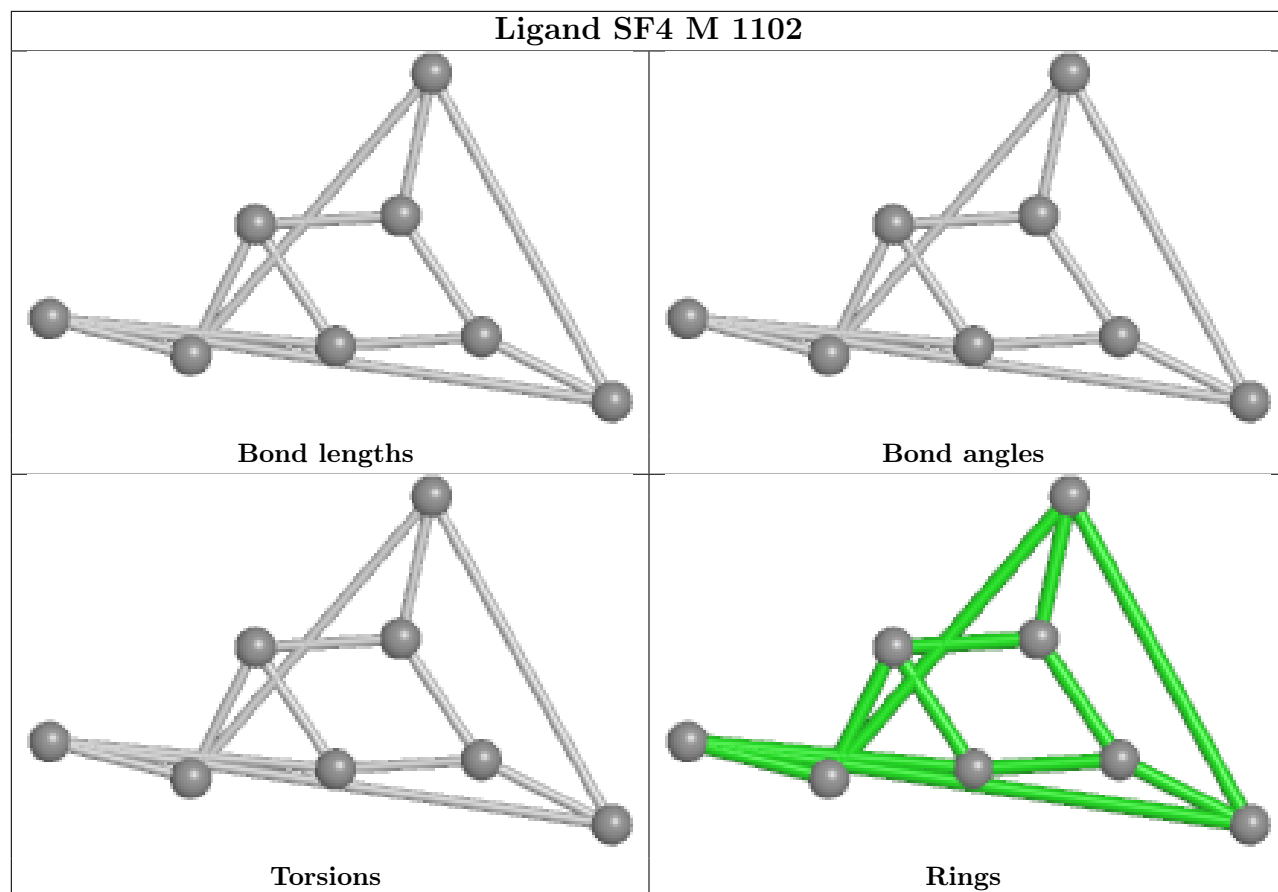
Torsions

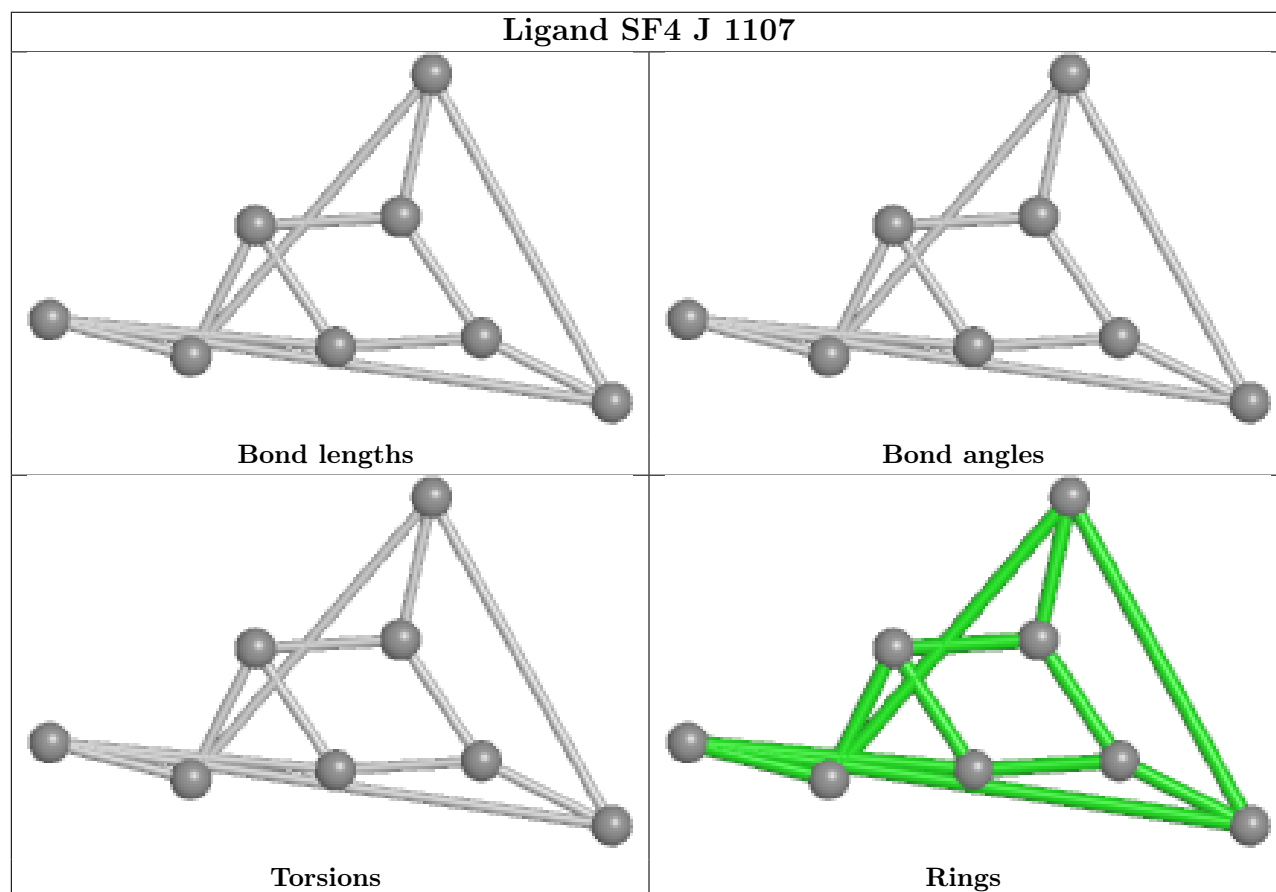
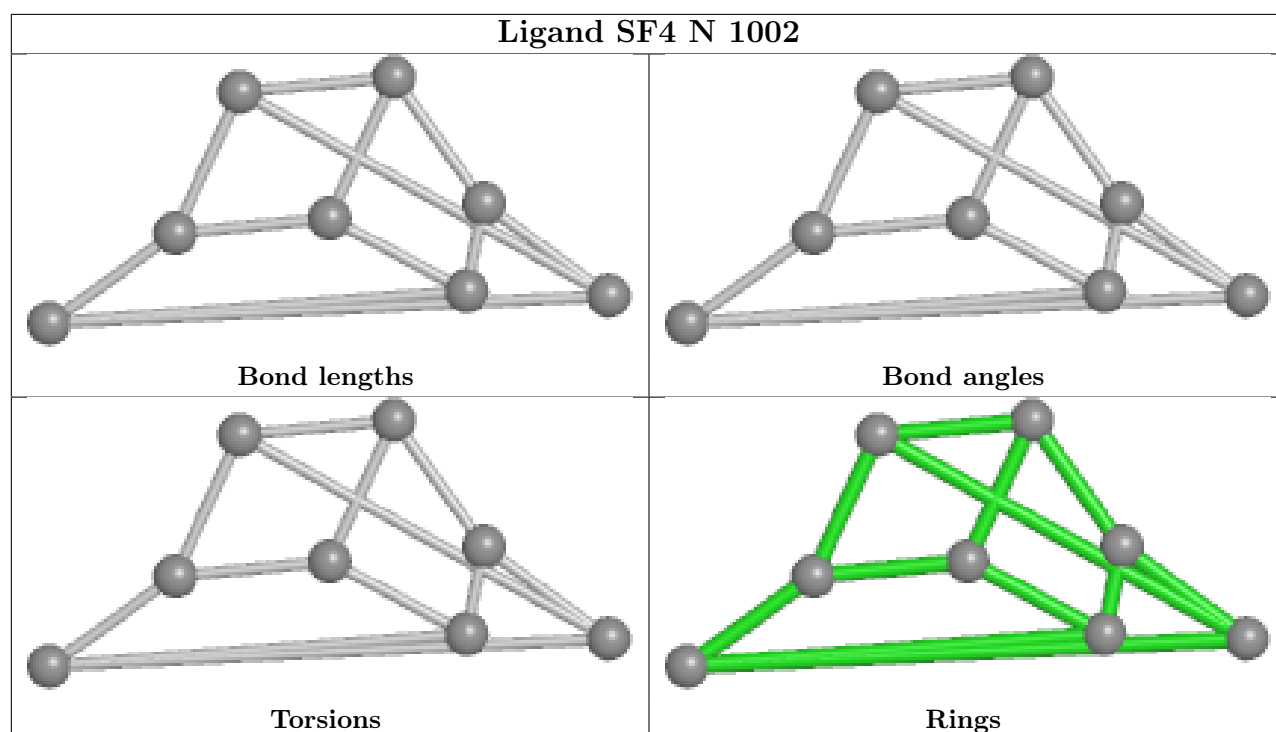


Rings

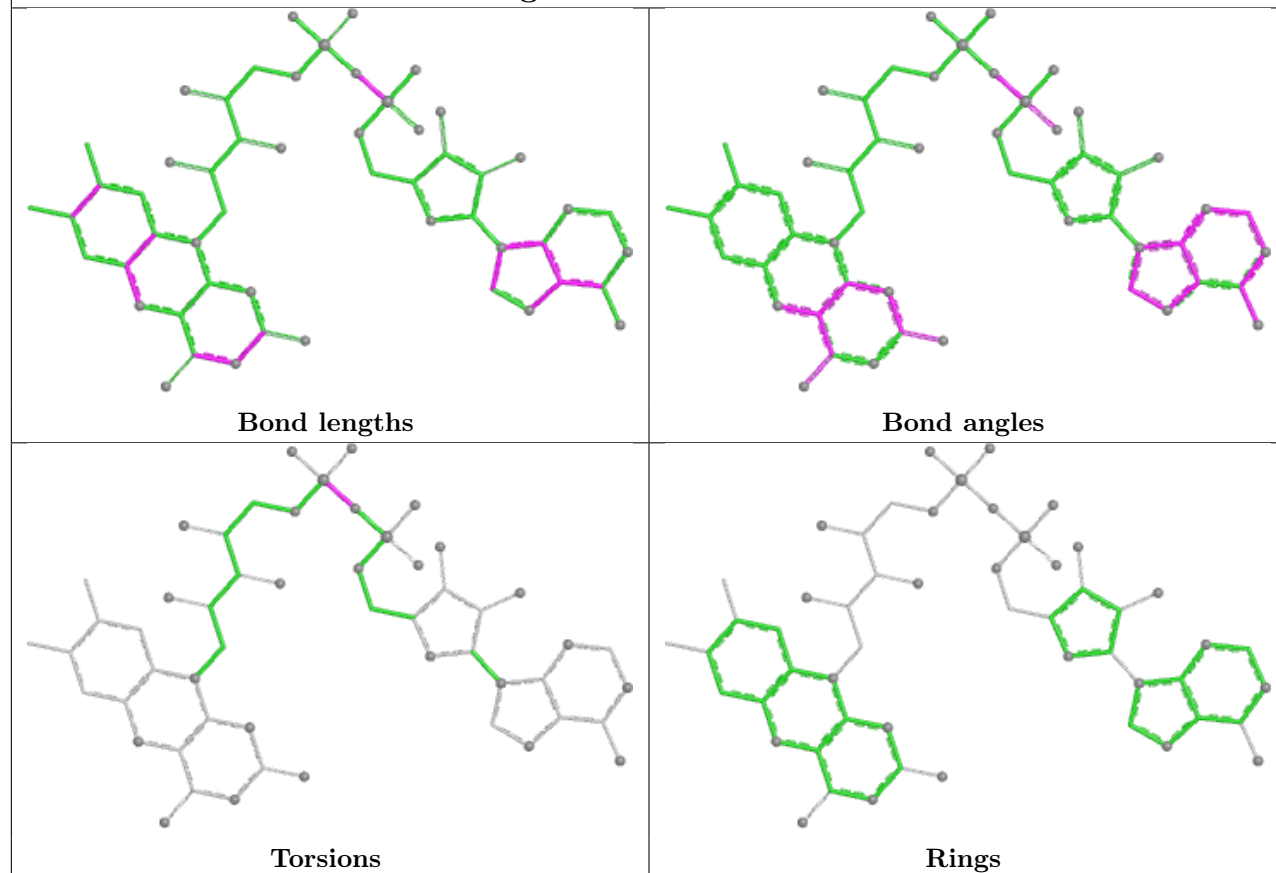




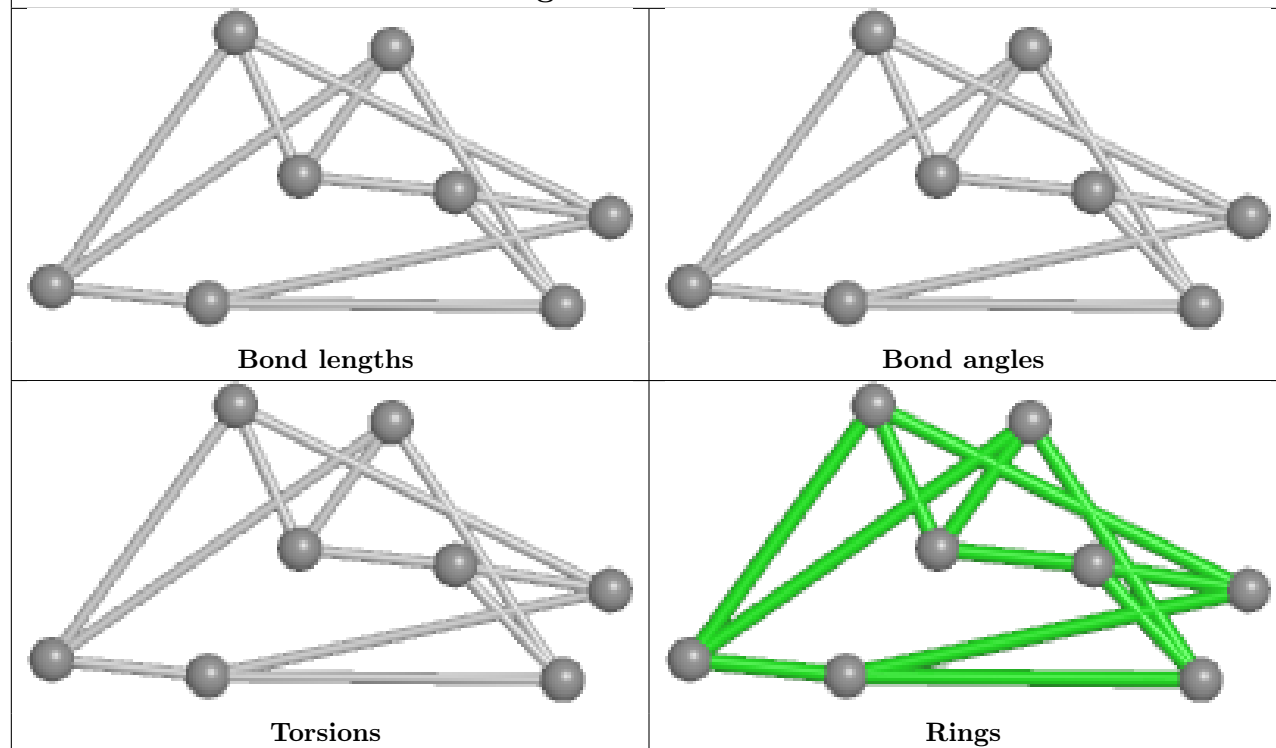


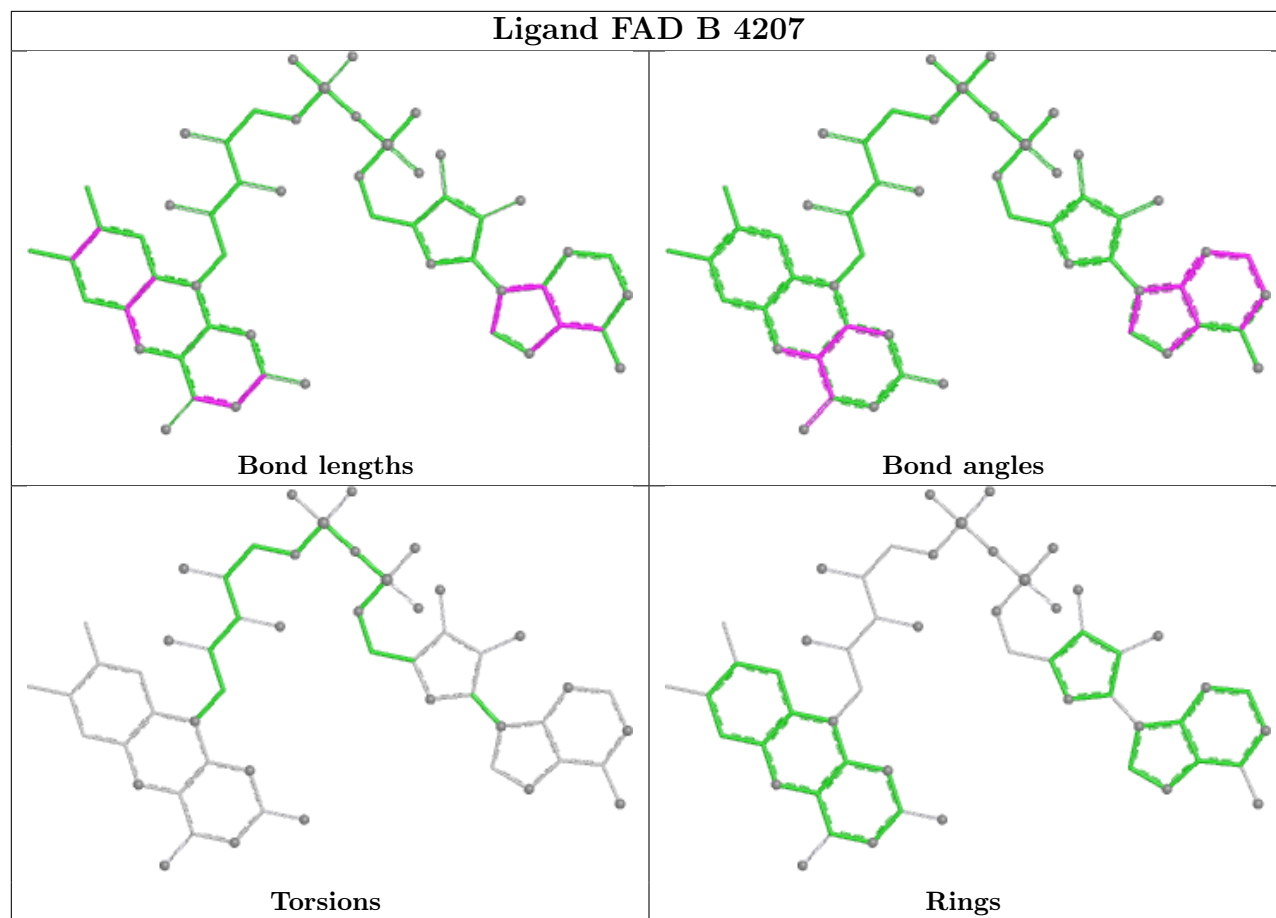


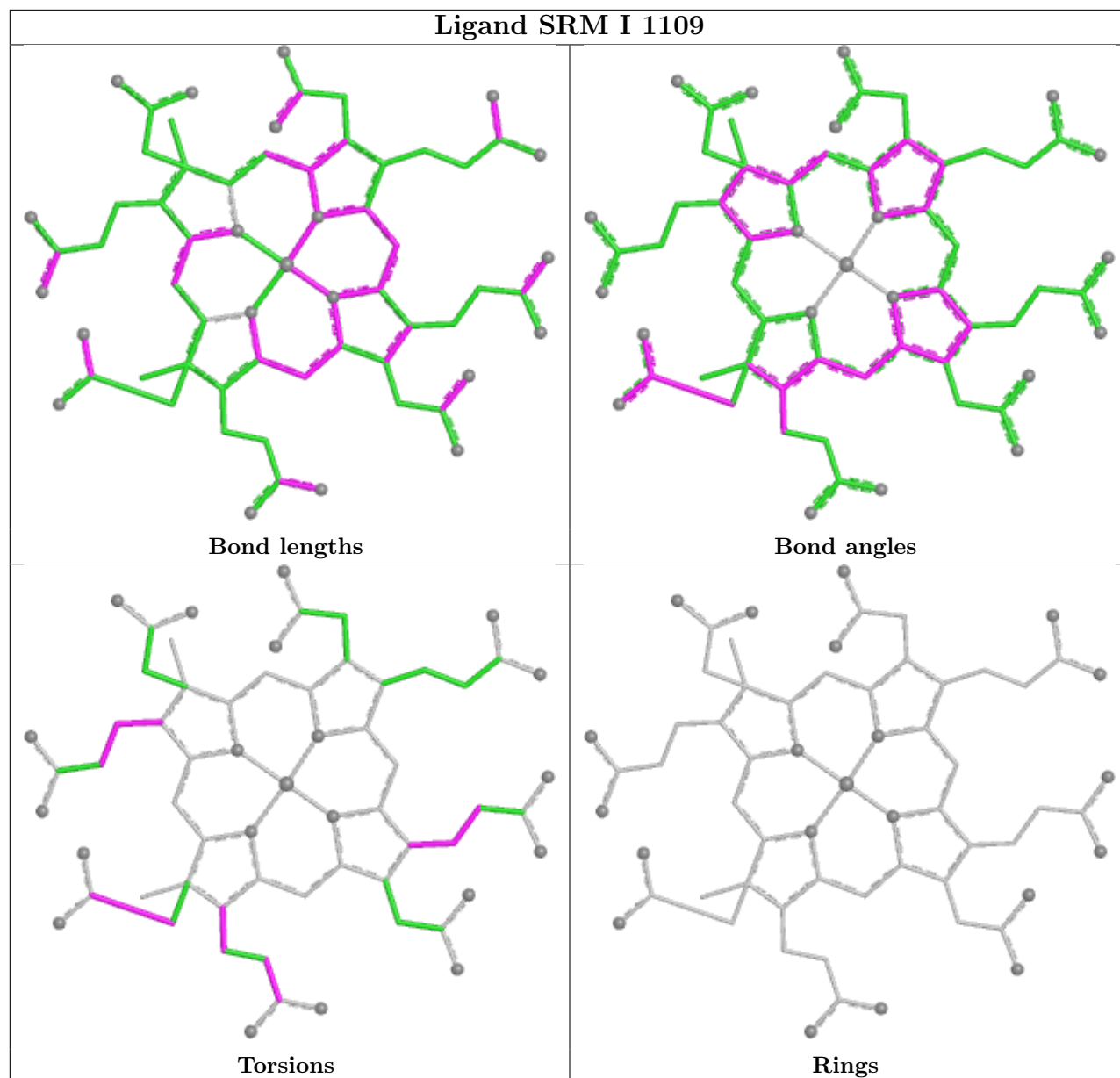
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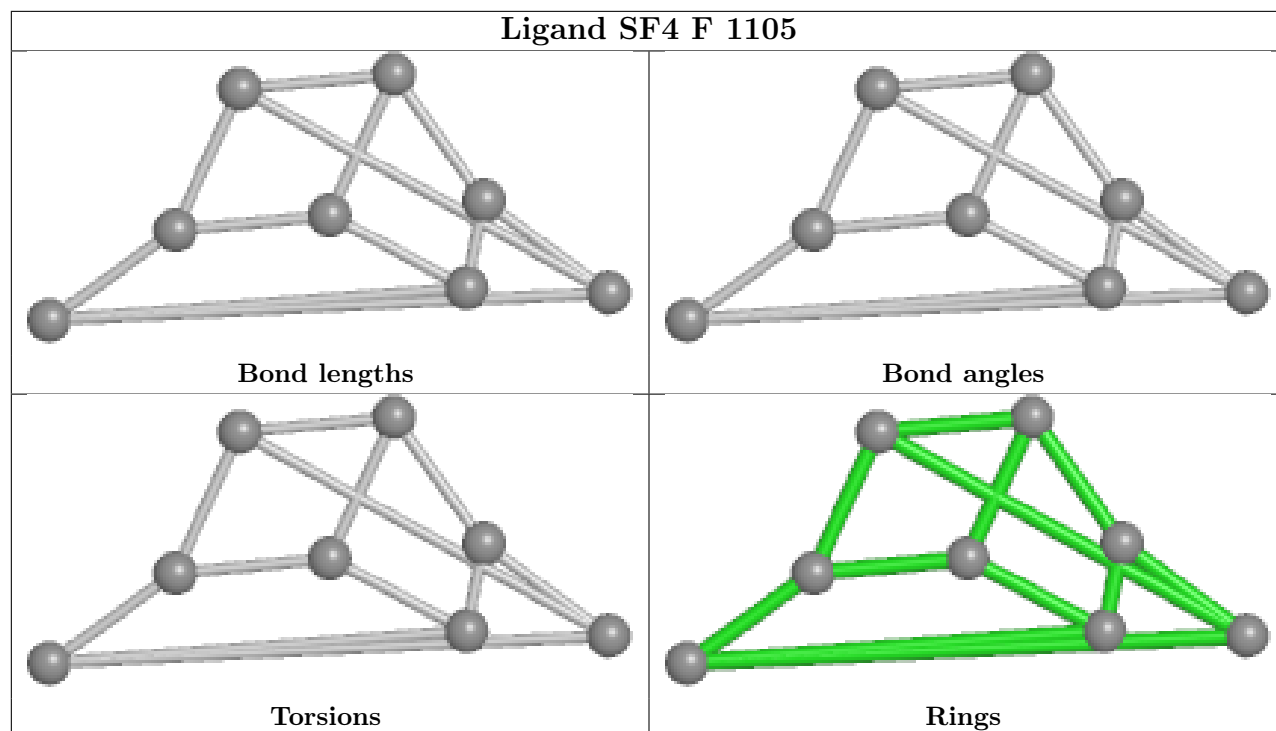
Ligand SF4 I 1101



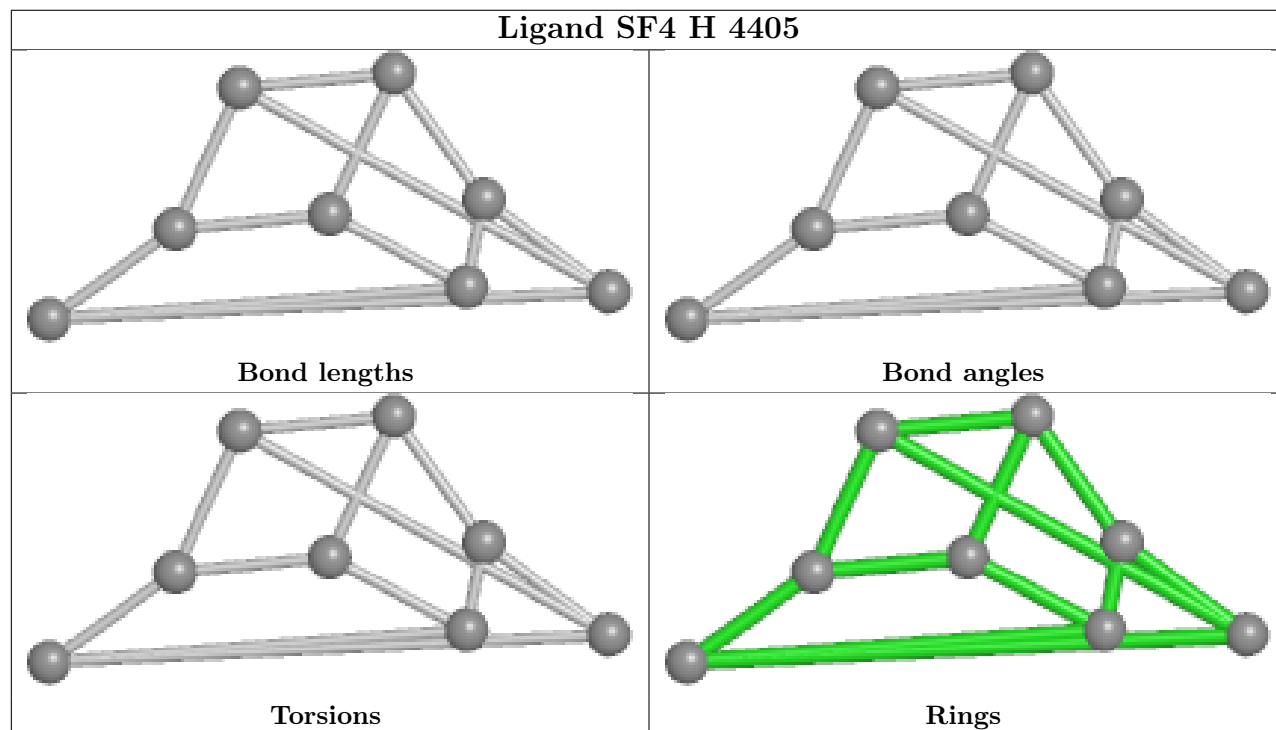


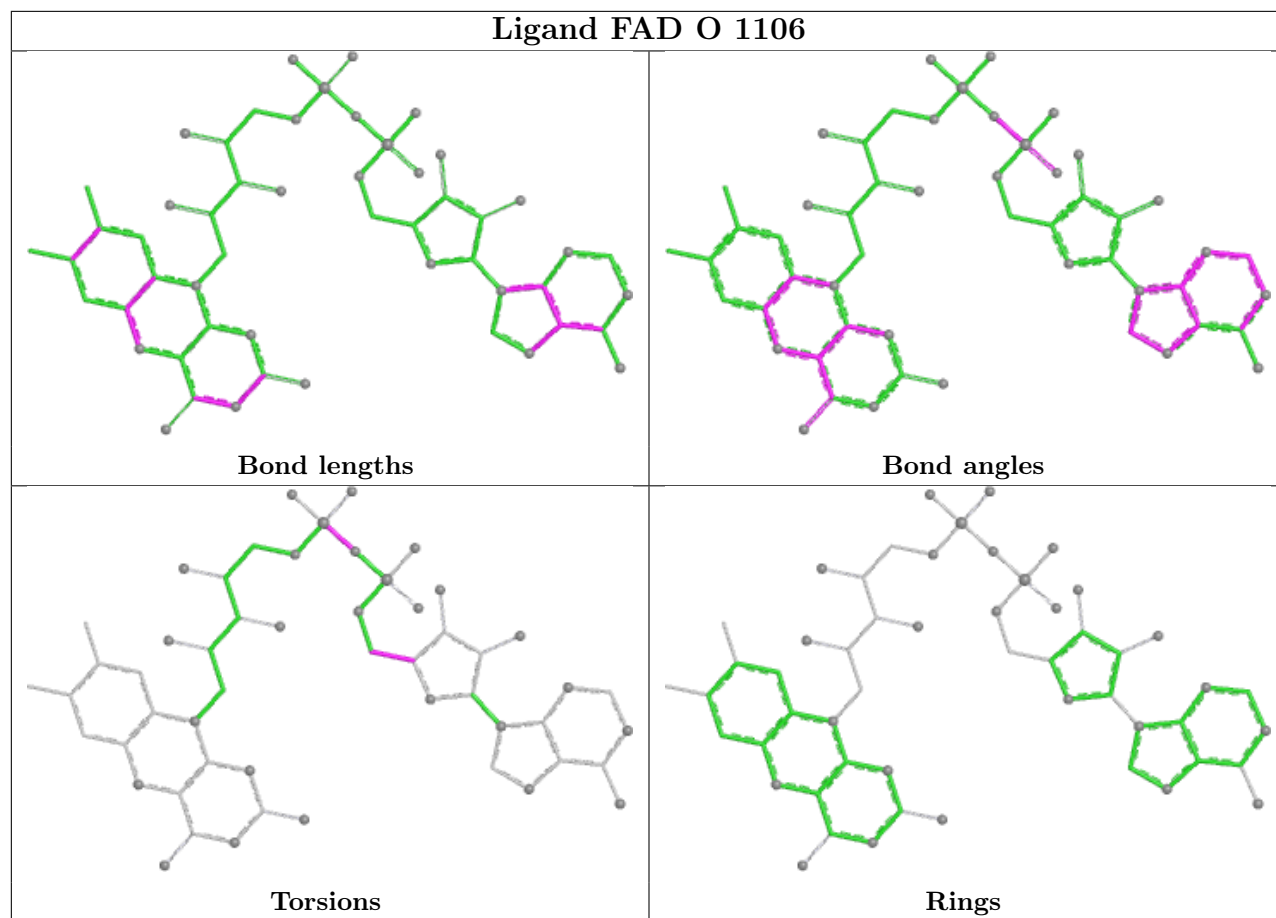


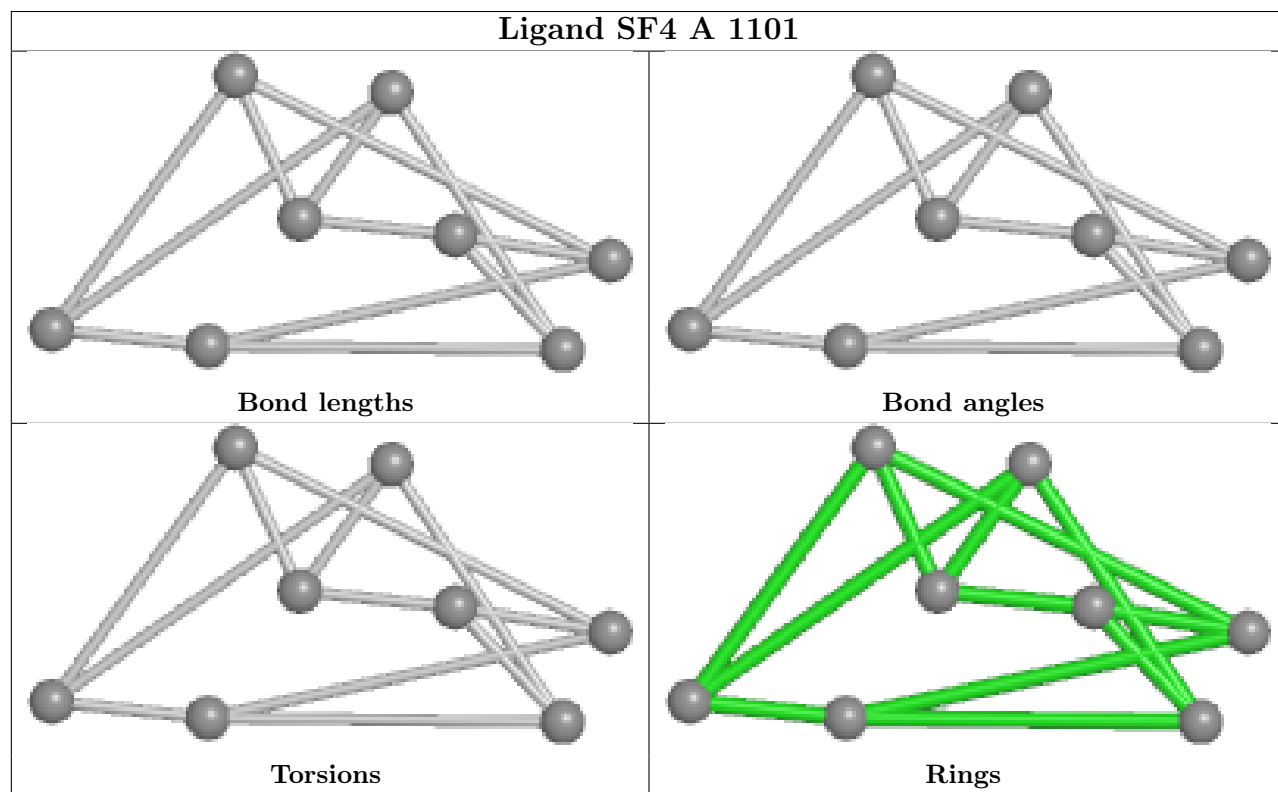
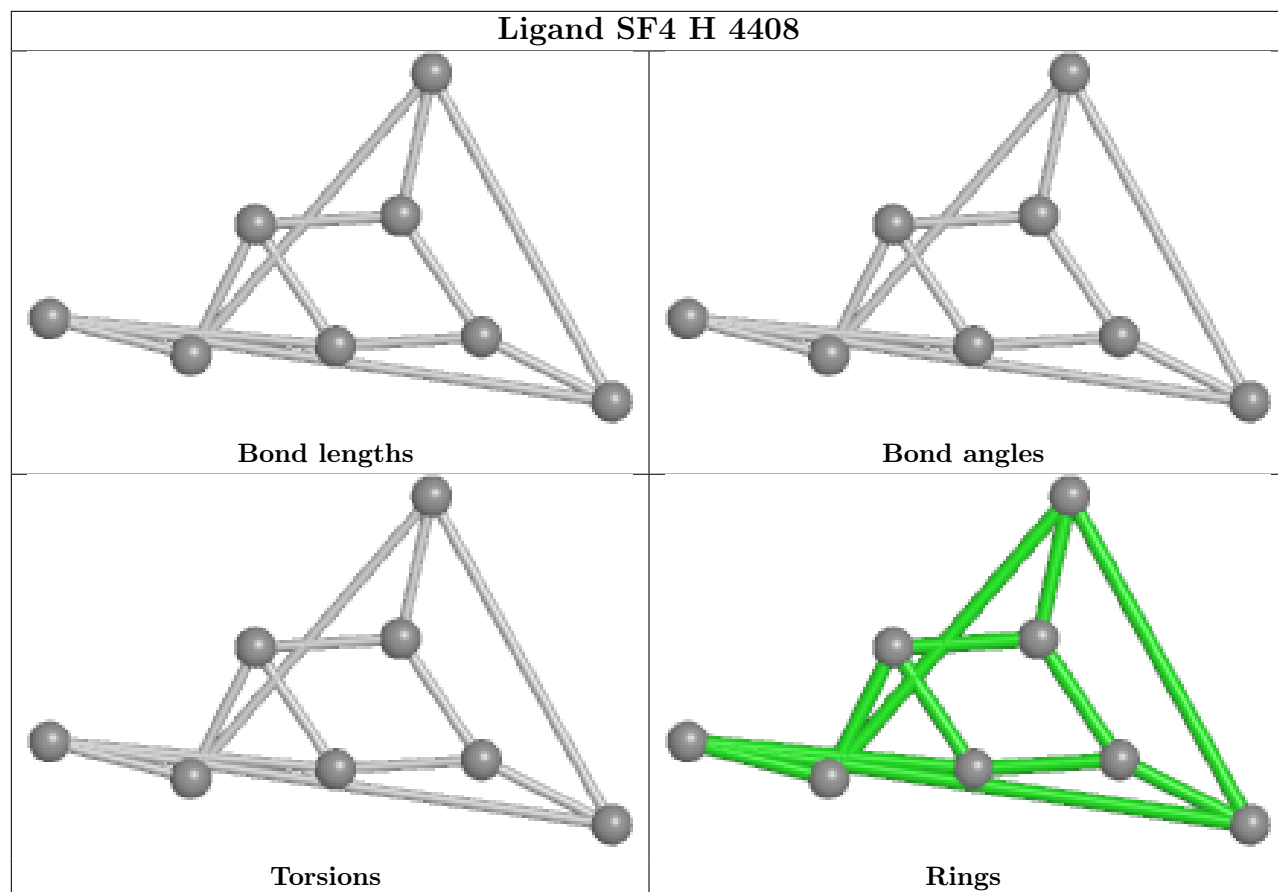
Ligand SF4 F 1105

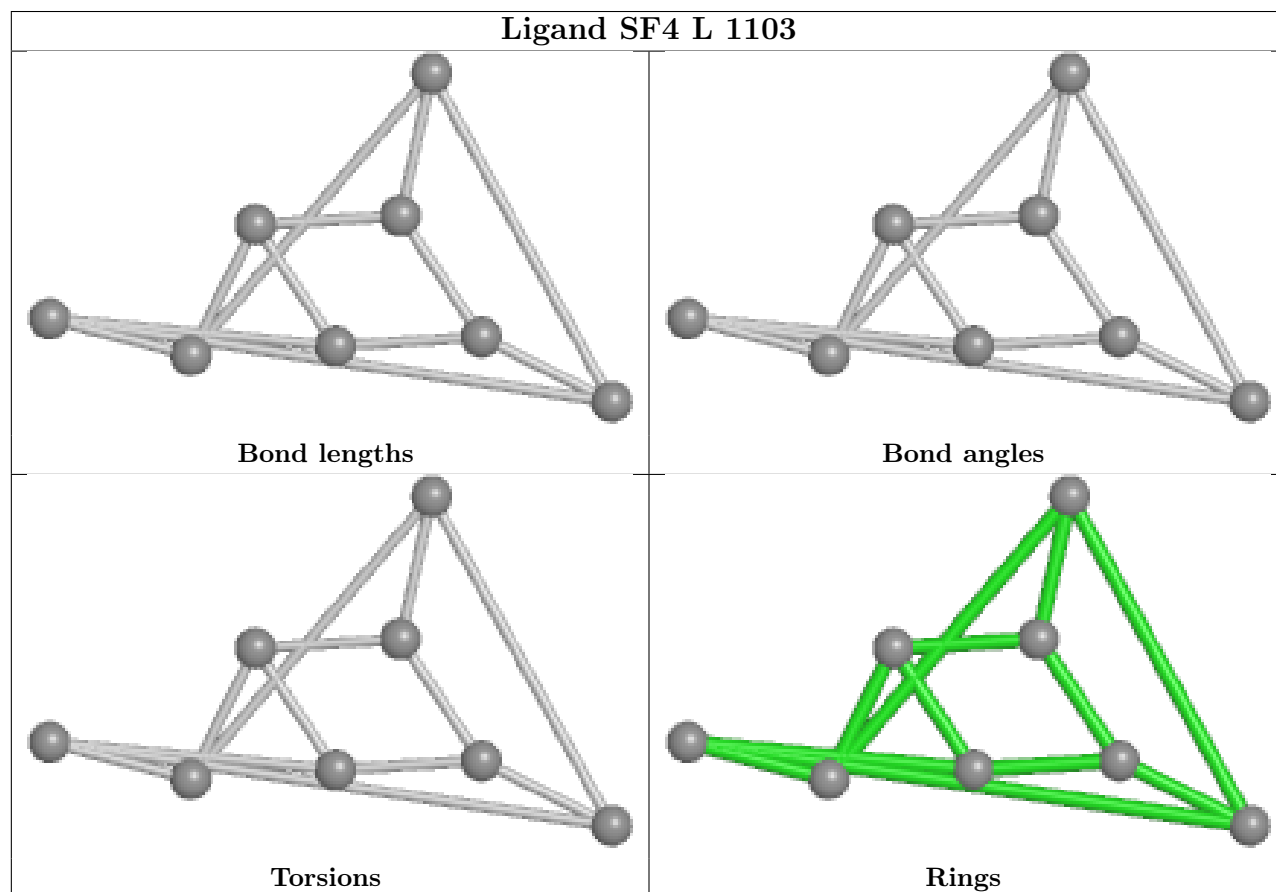
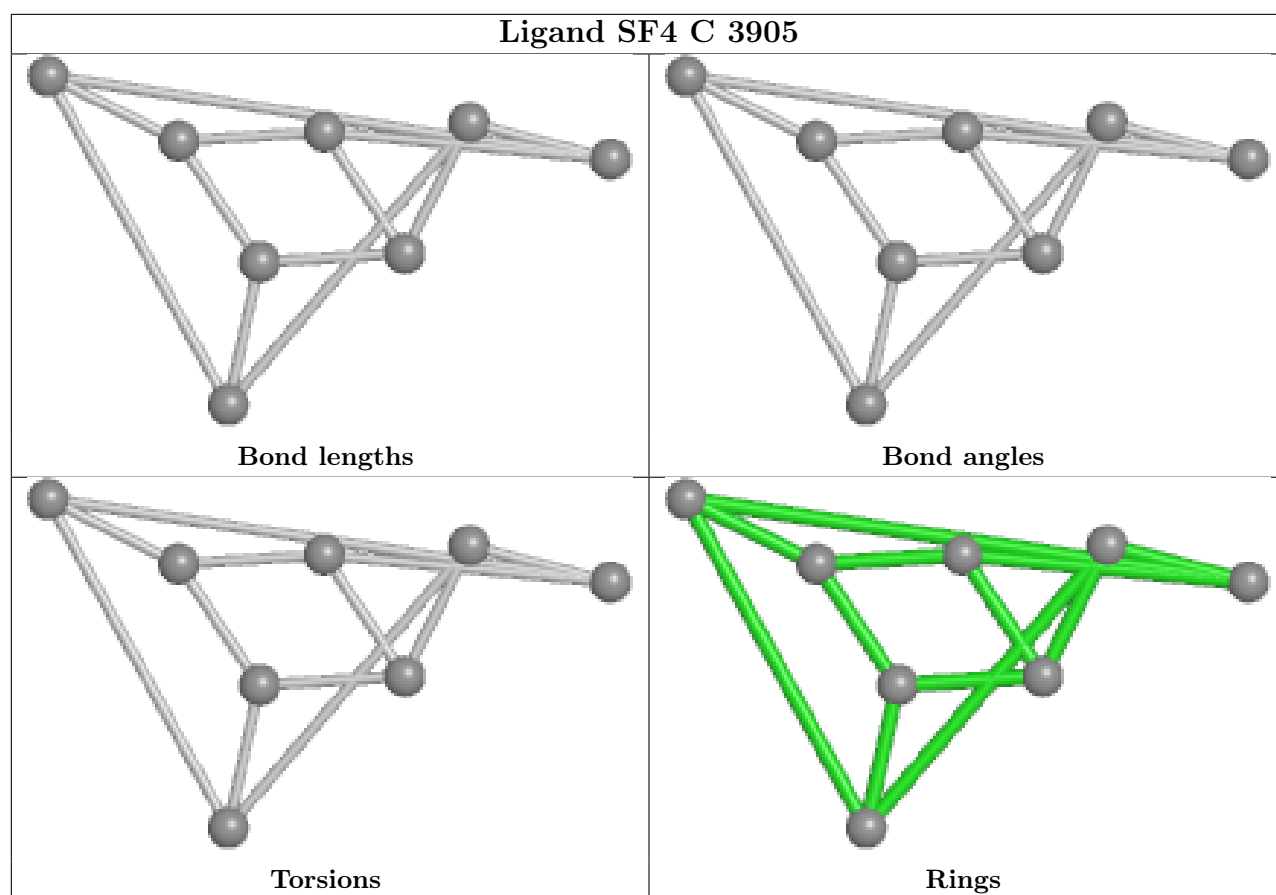


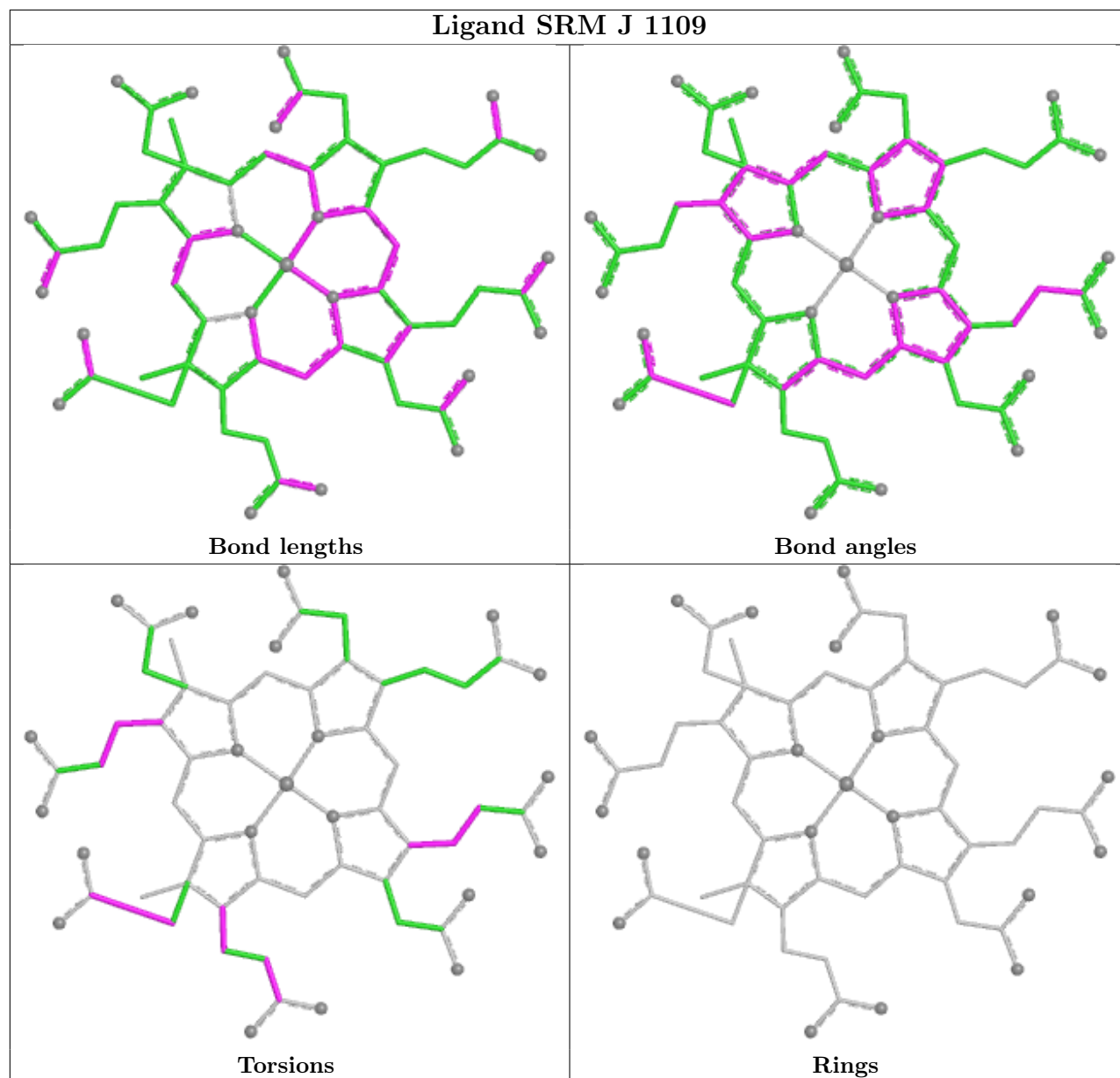
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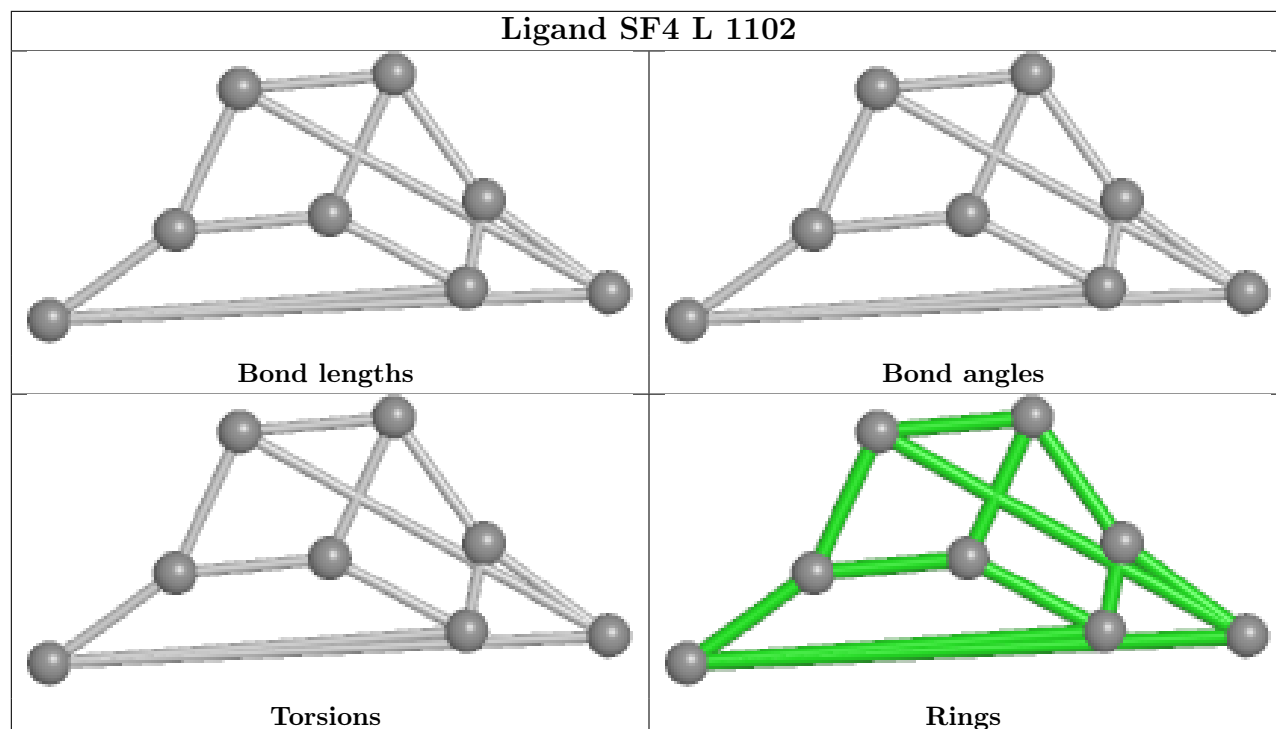




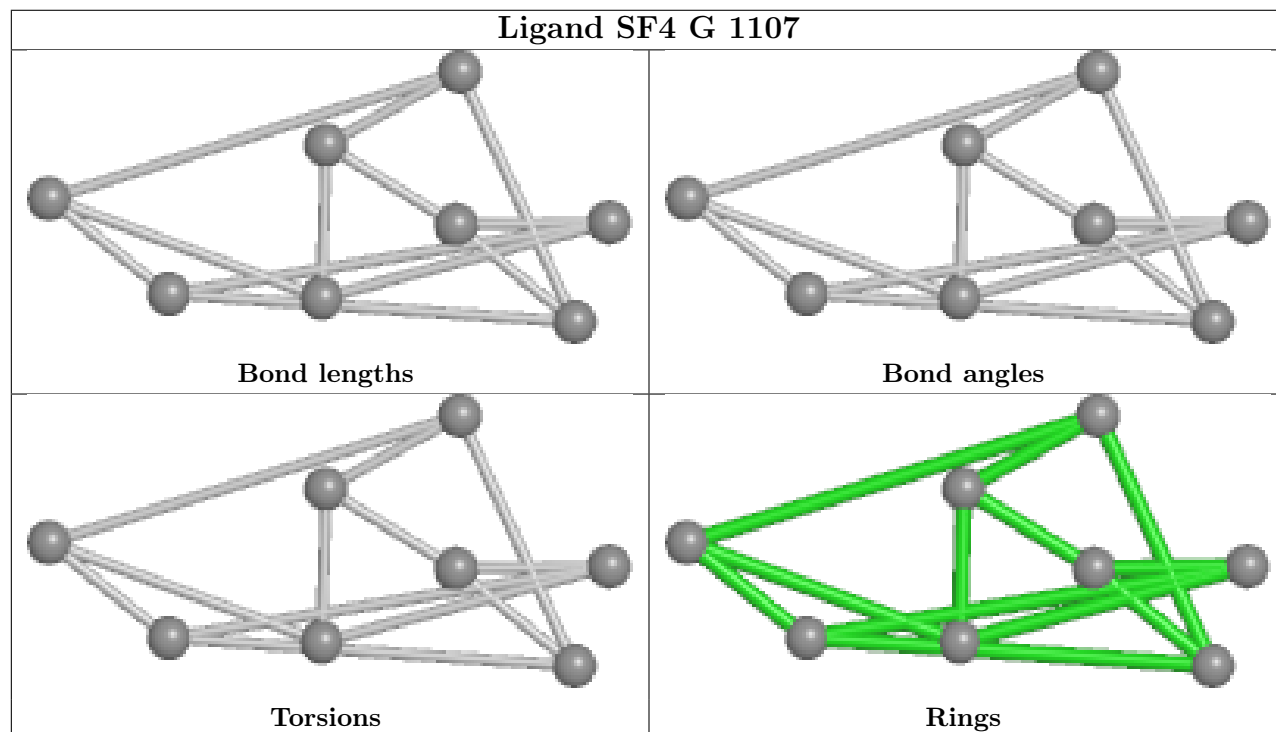


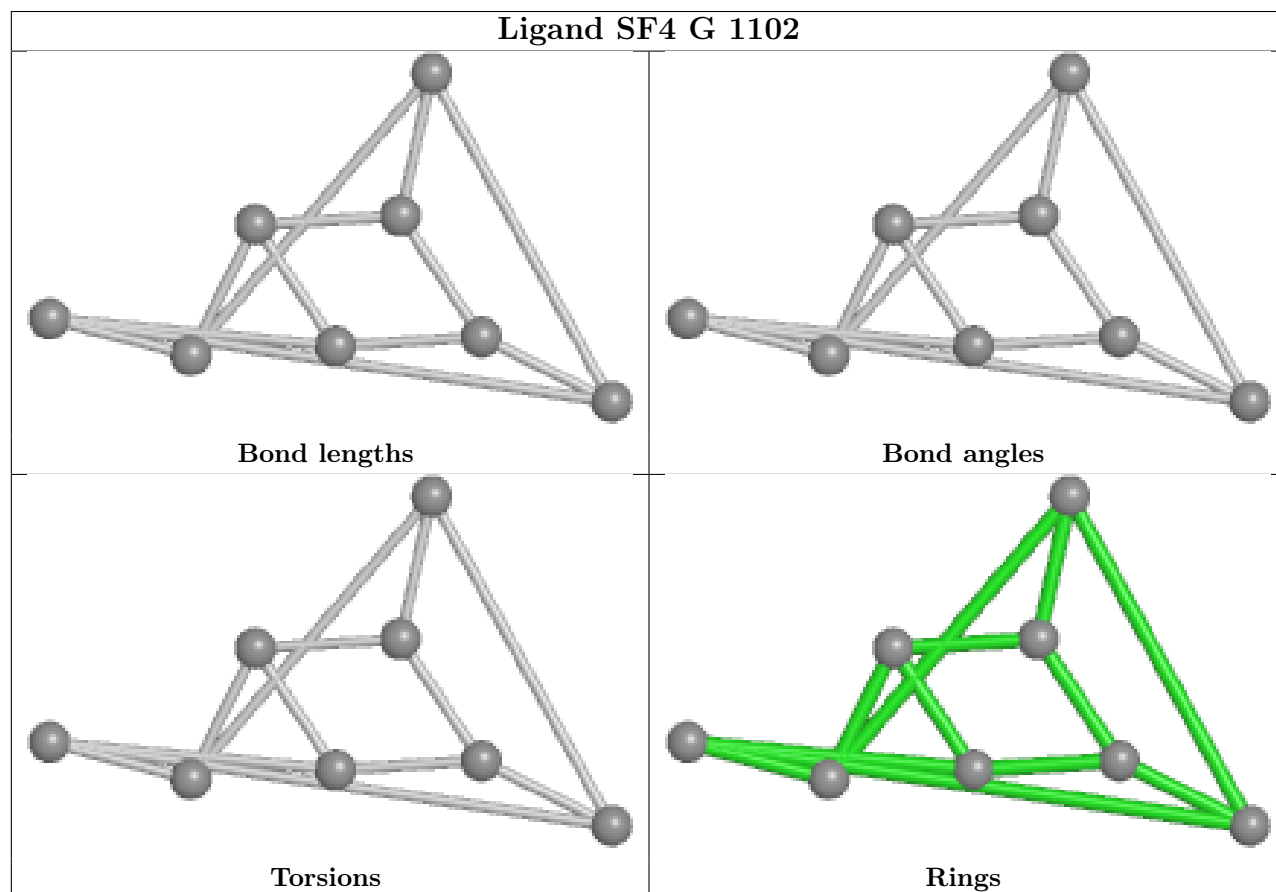
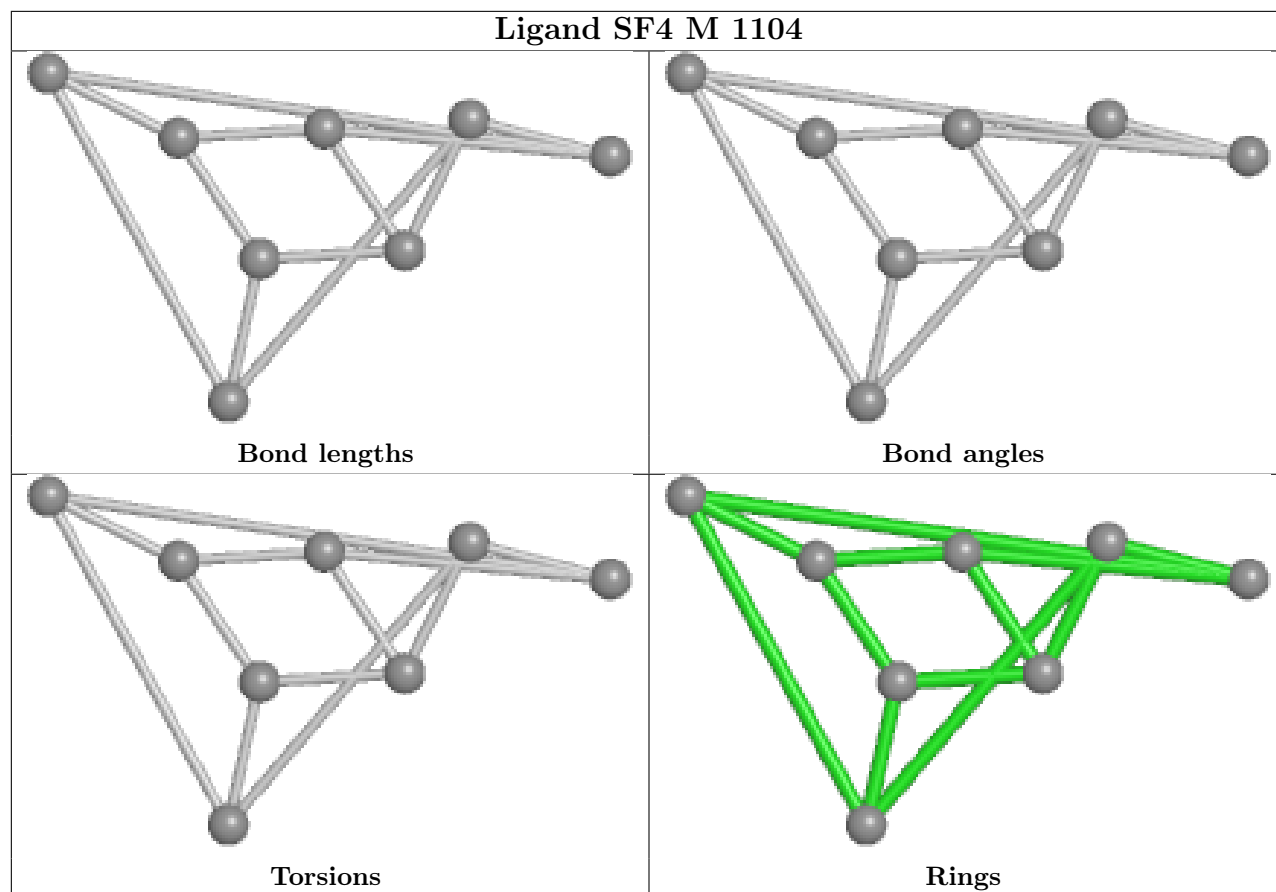


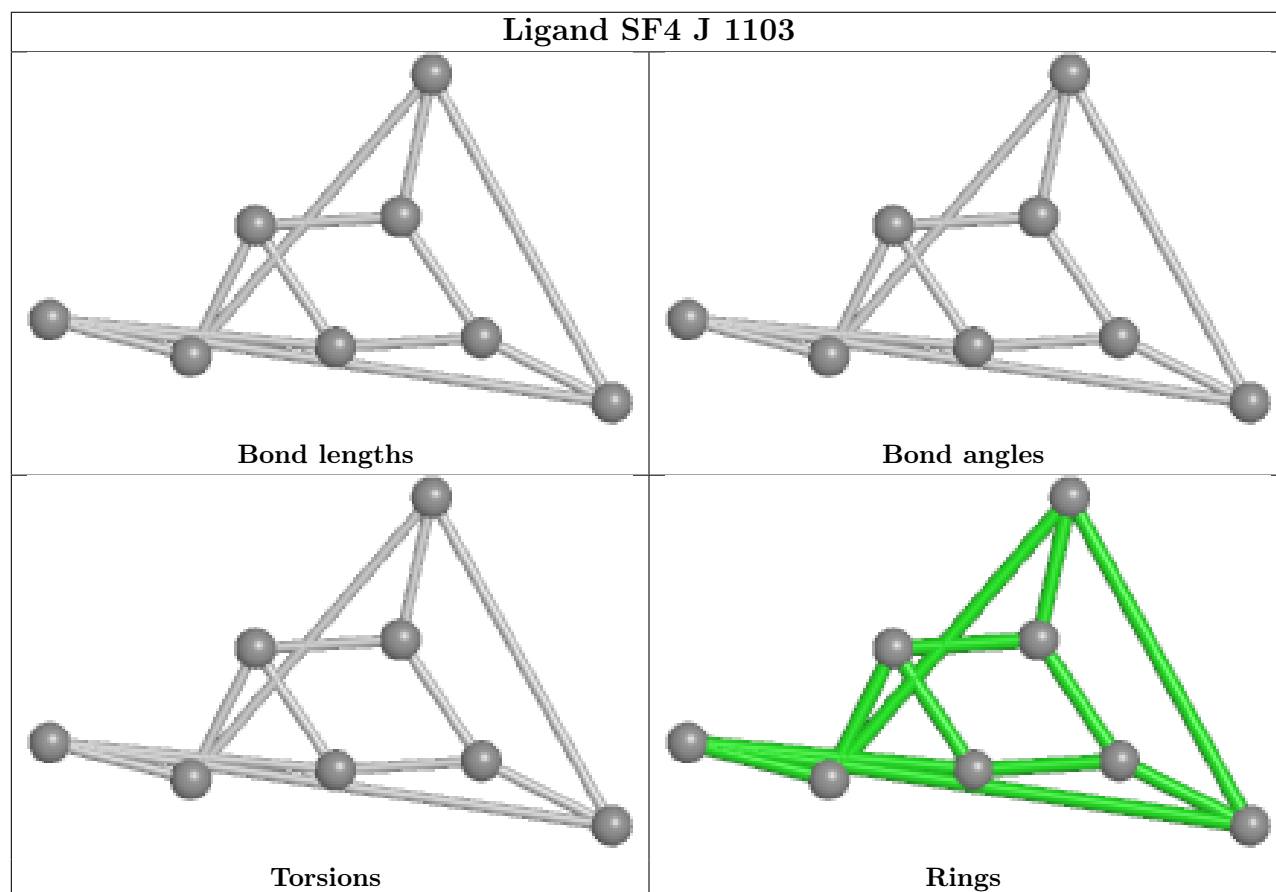
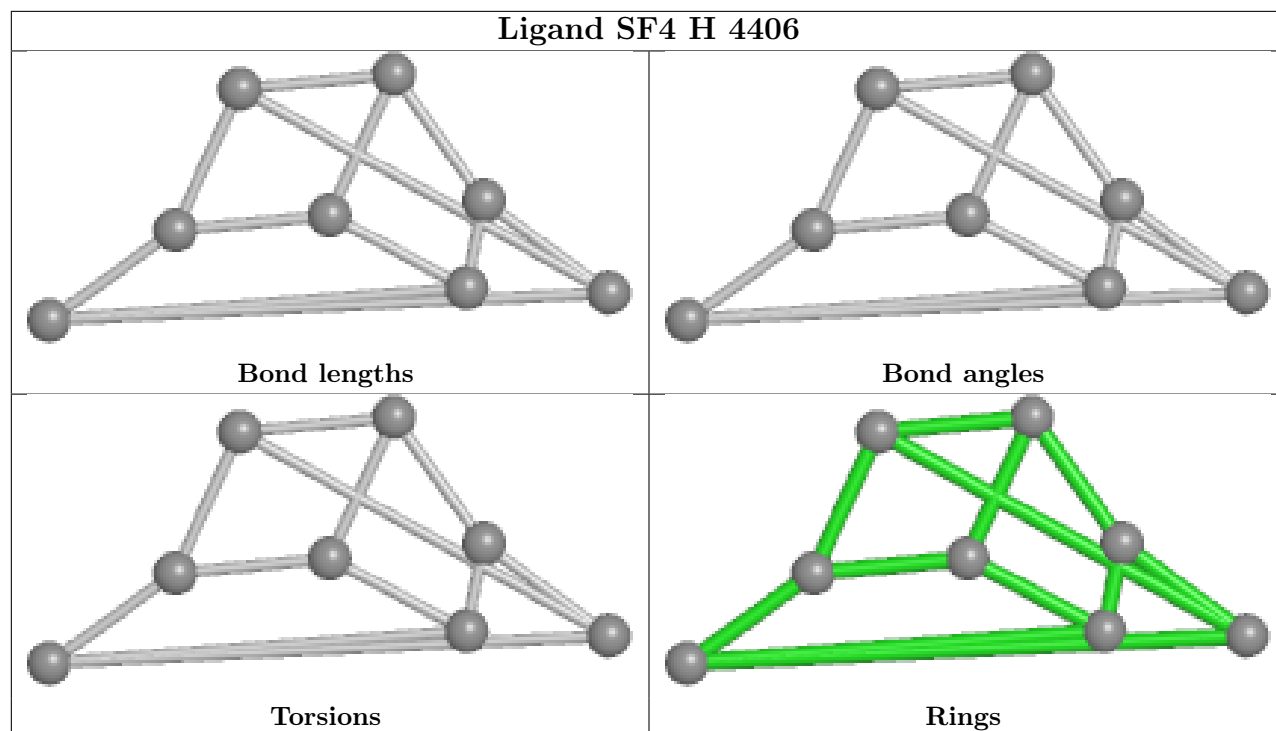
Ligand SF4 L 1102

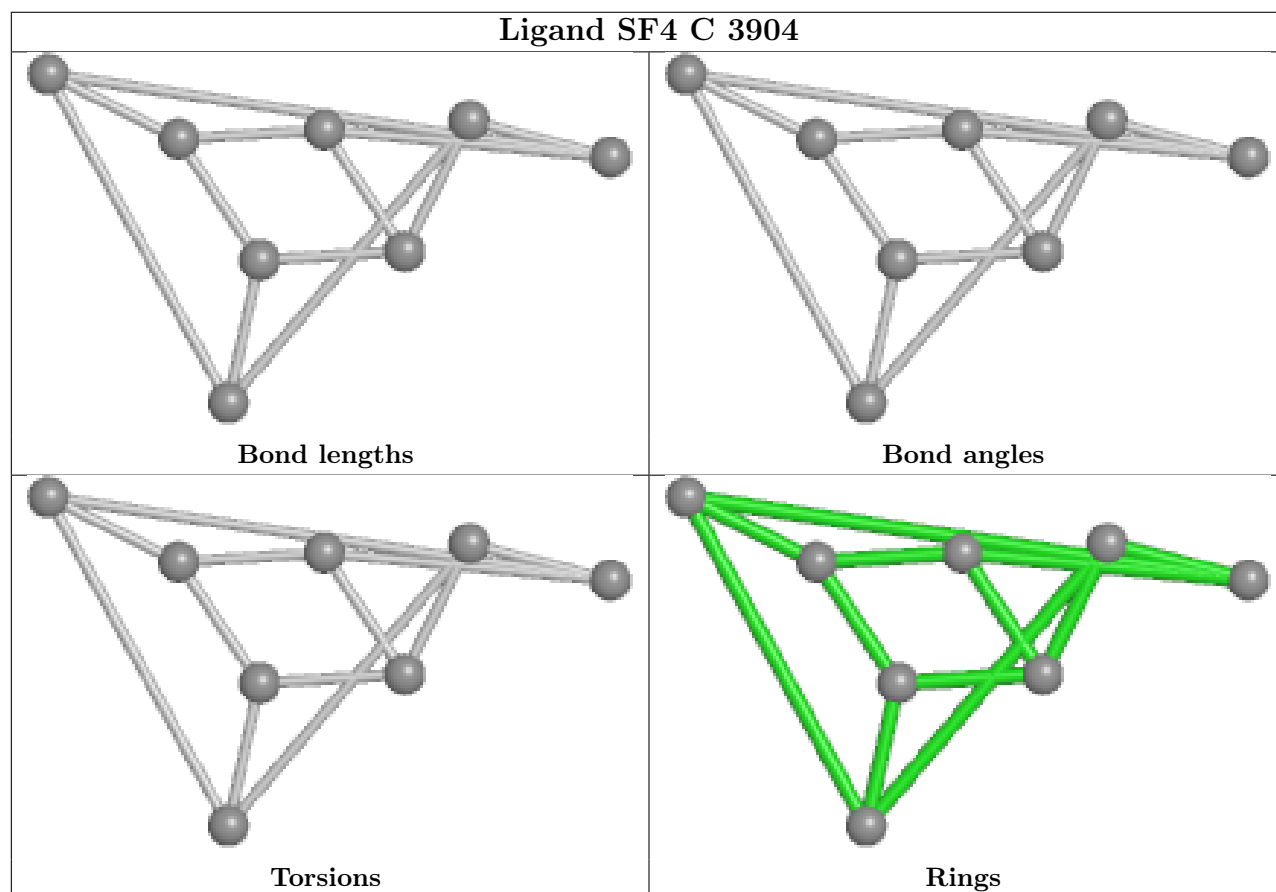
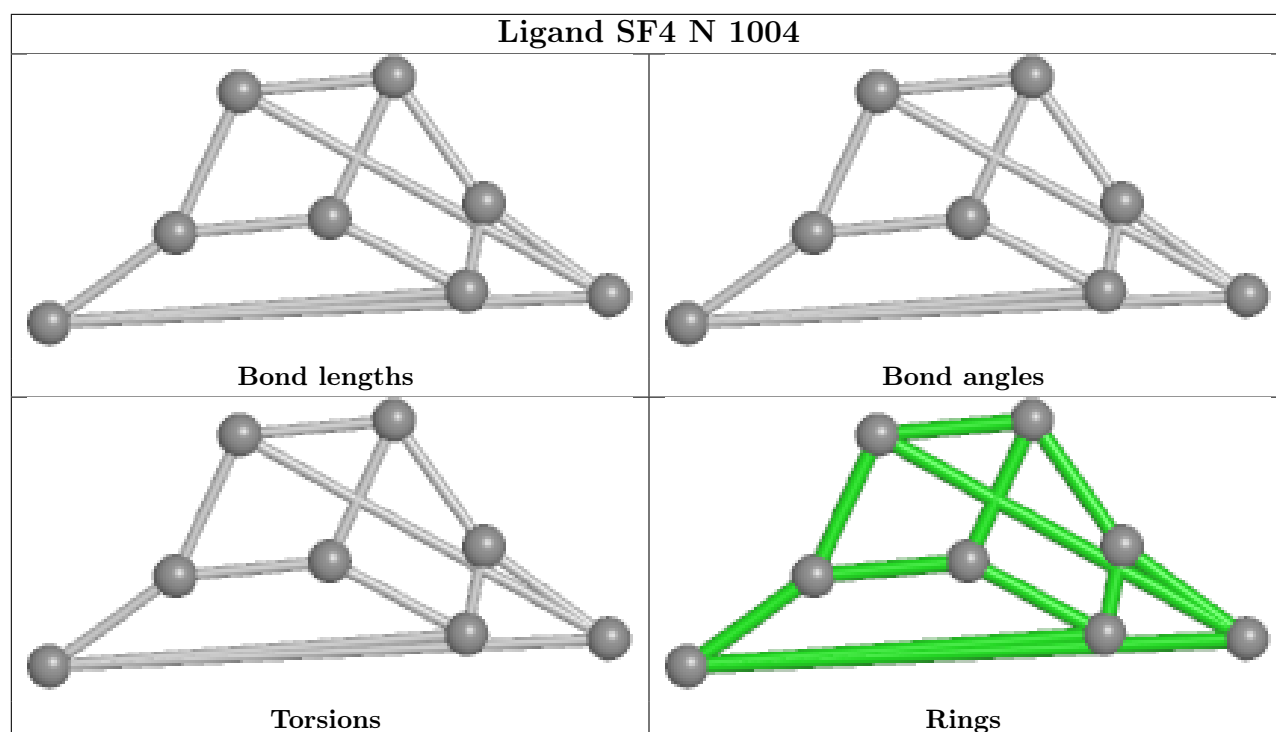


Ligand SF4 G 1107

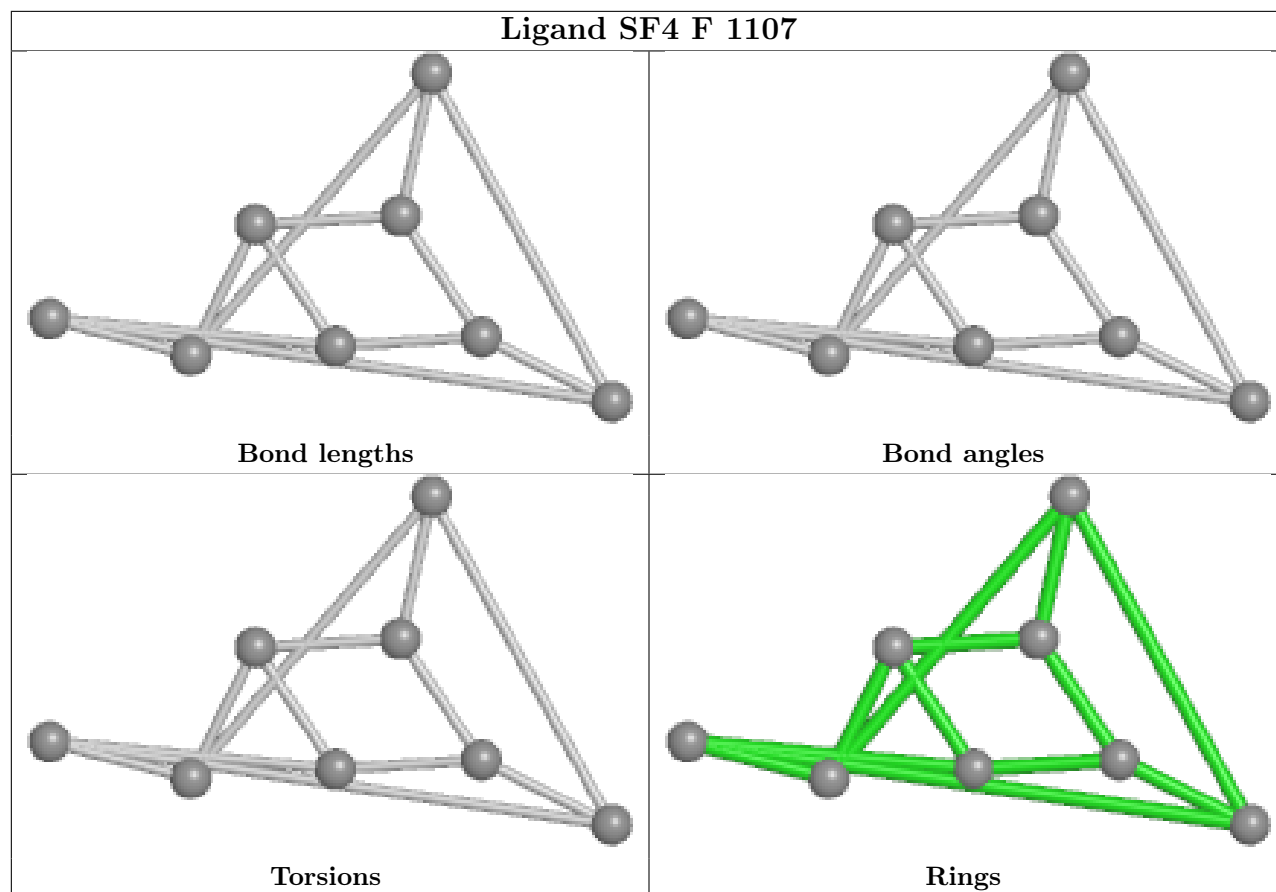




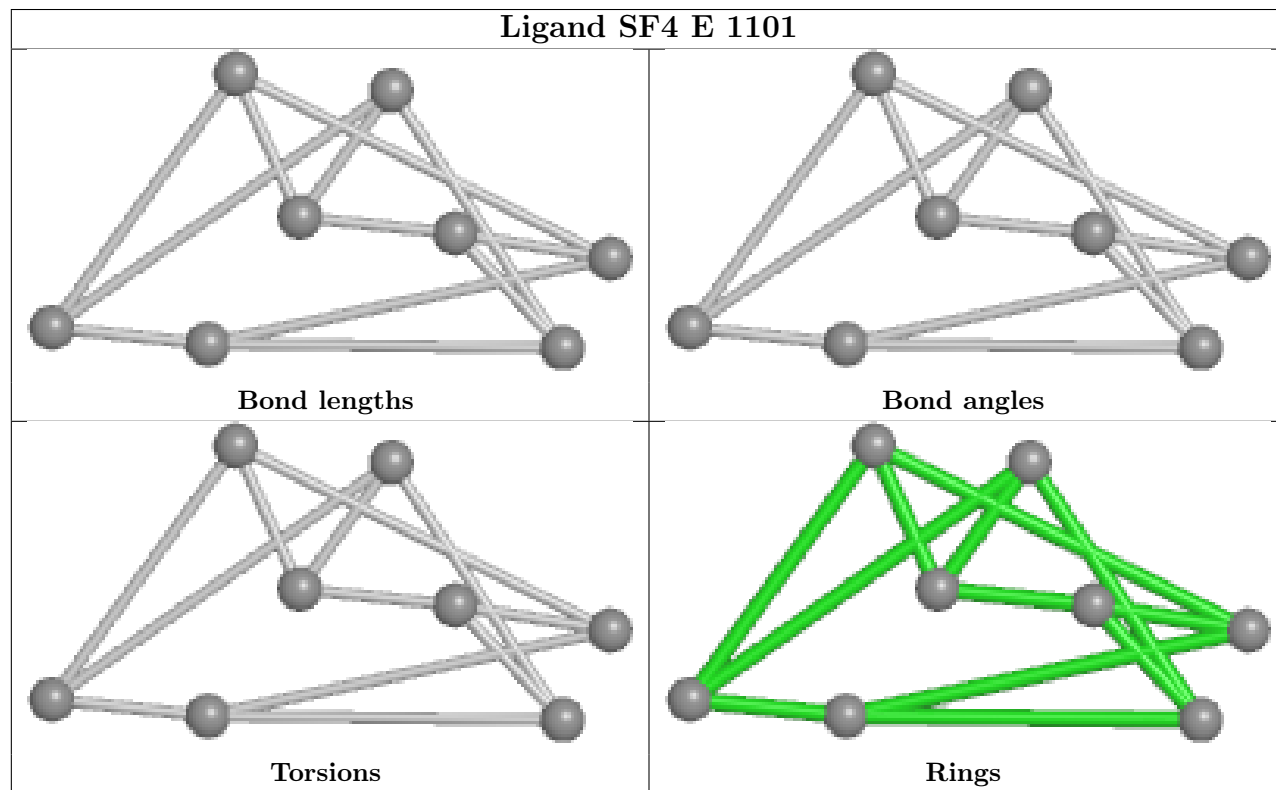




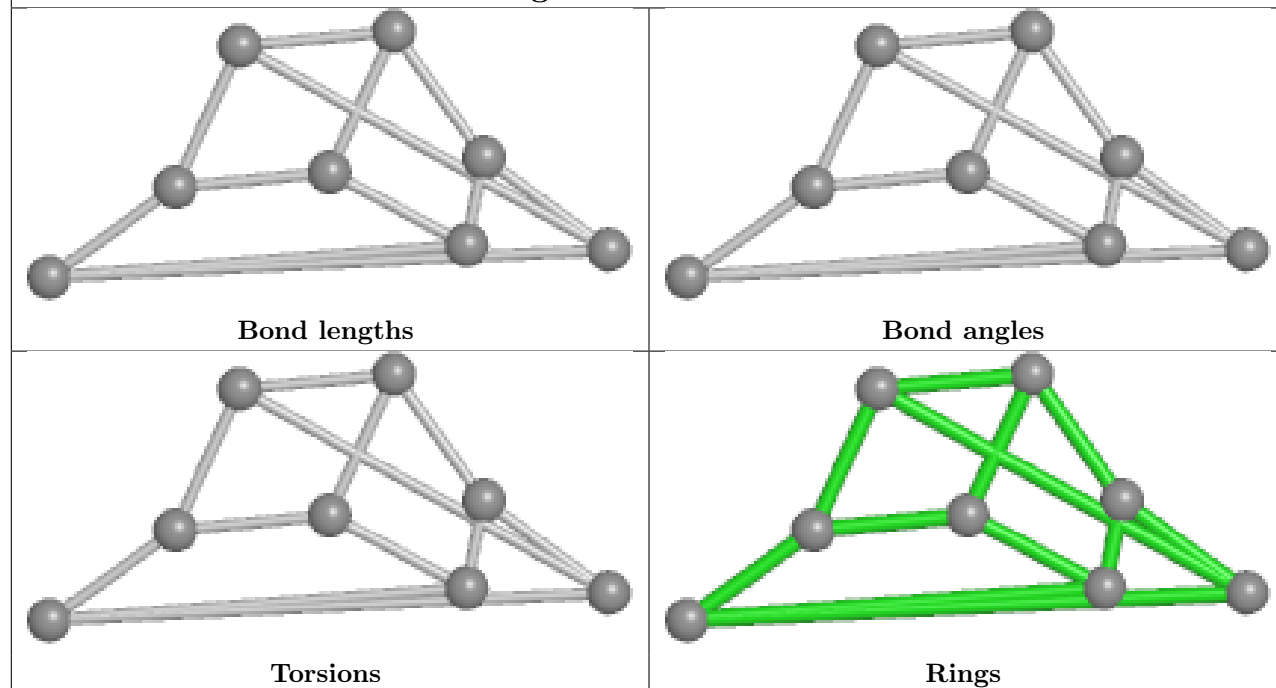
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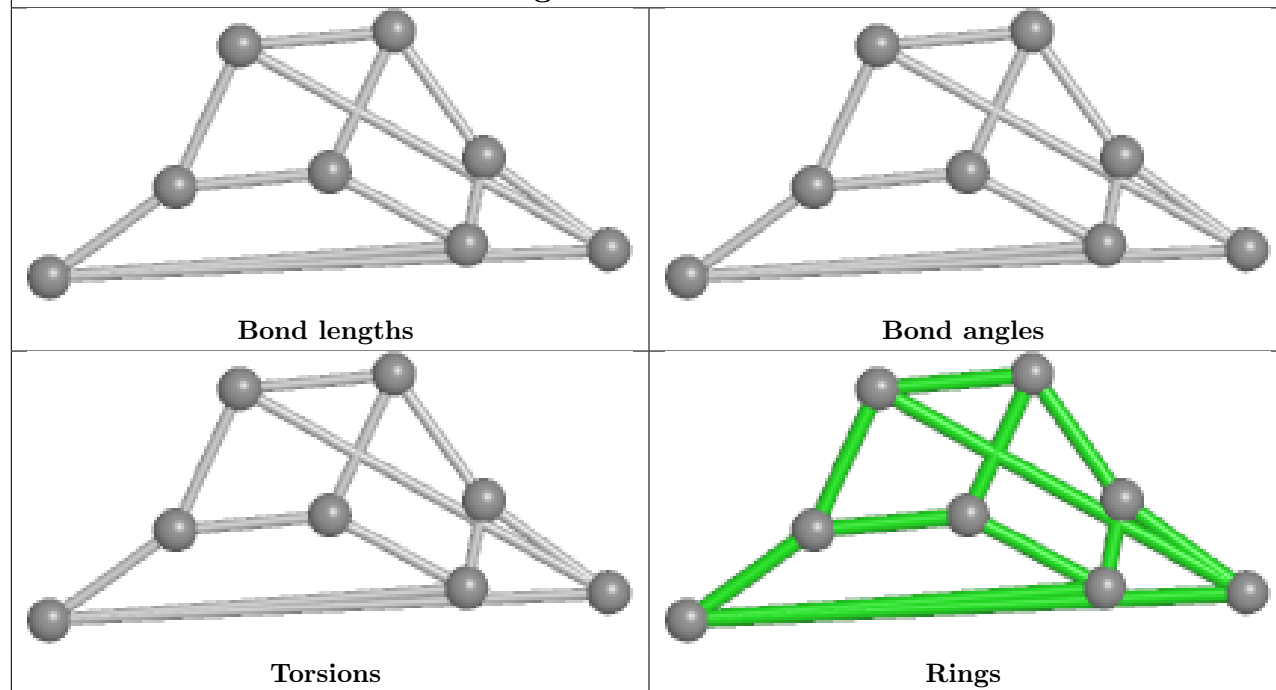
Ligand SF4 E 1101

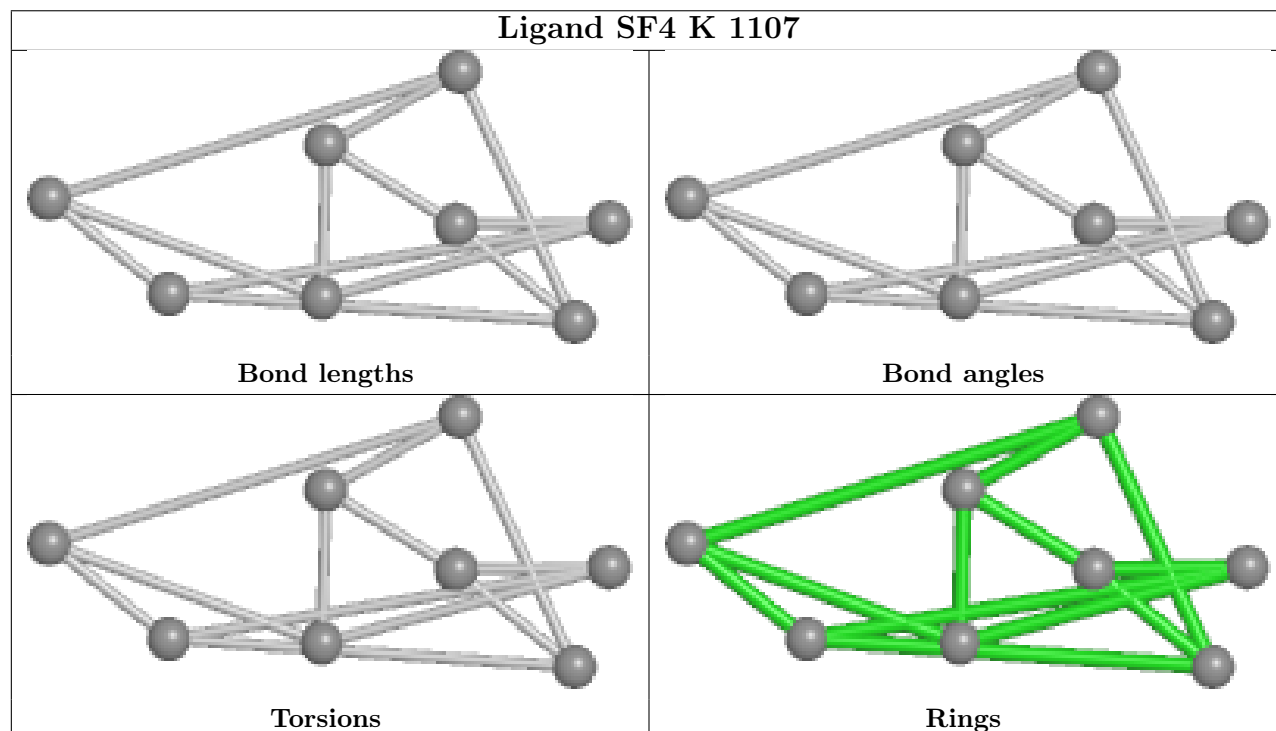
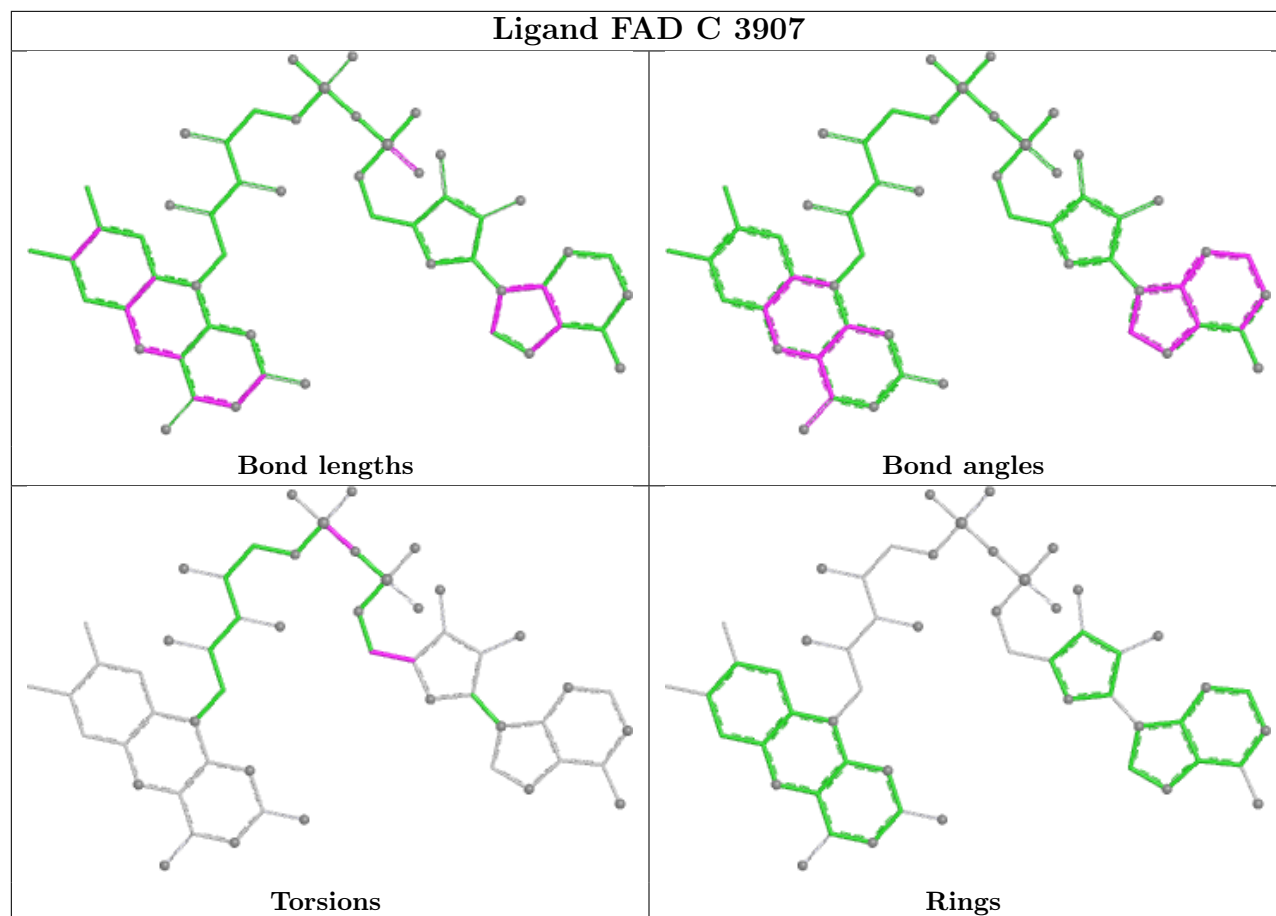


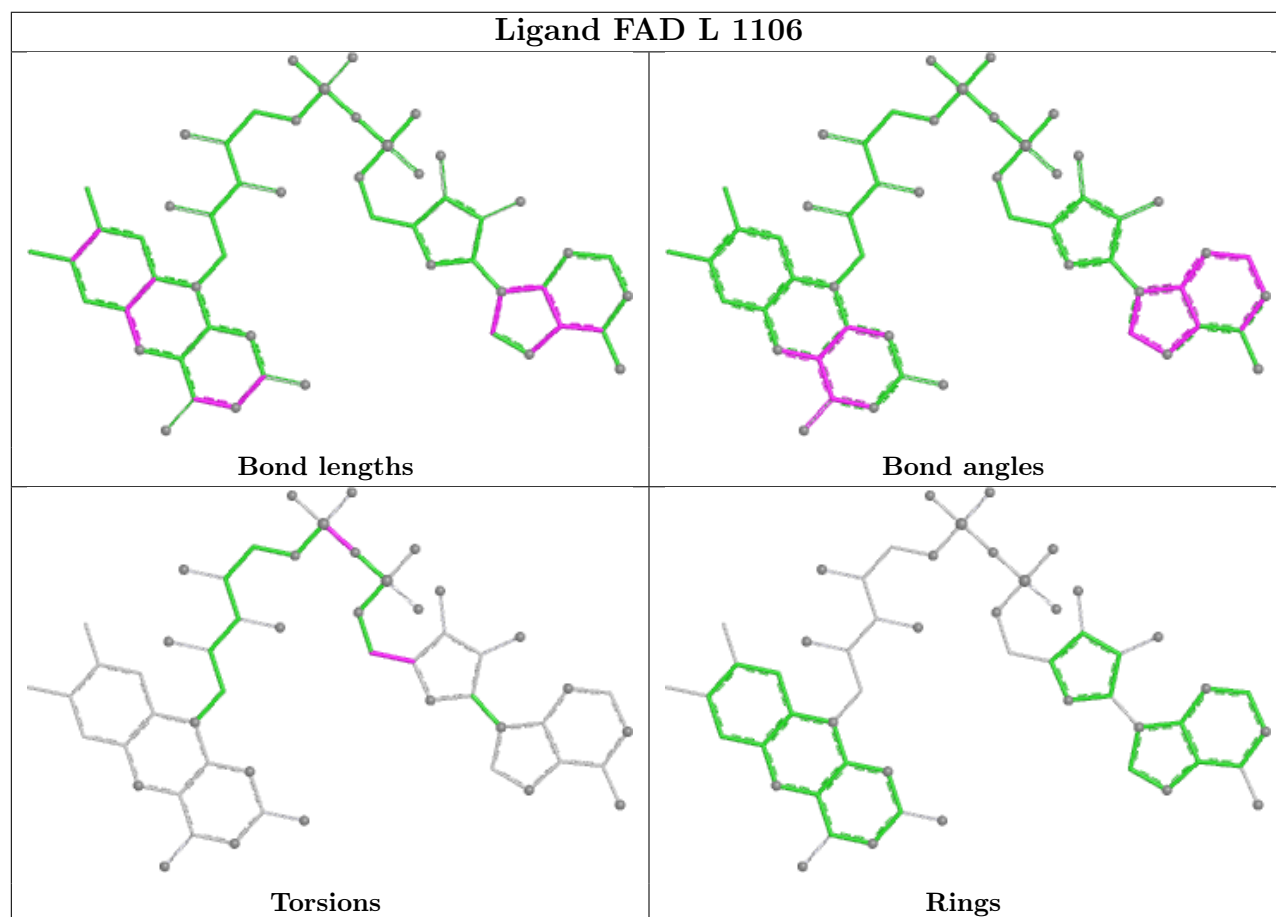
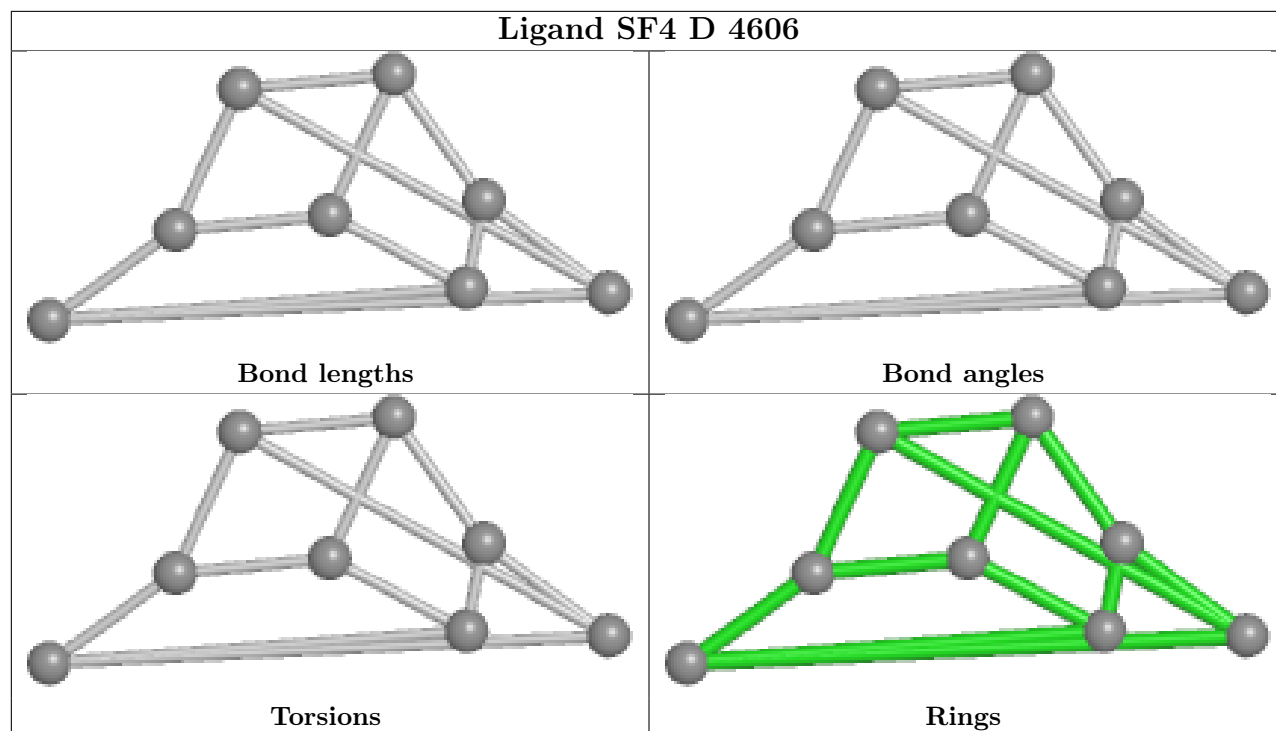
Ligand SF4 P 1105

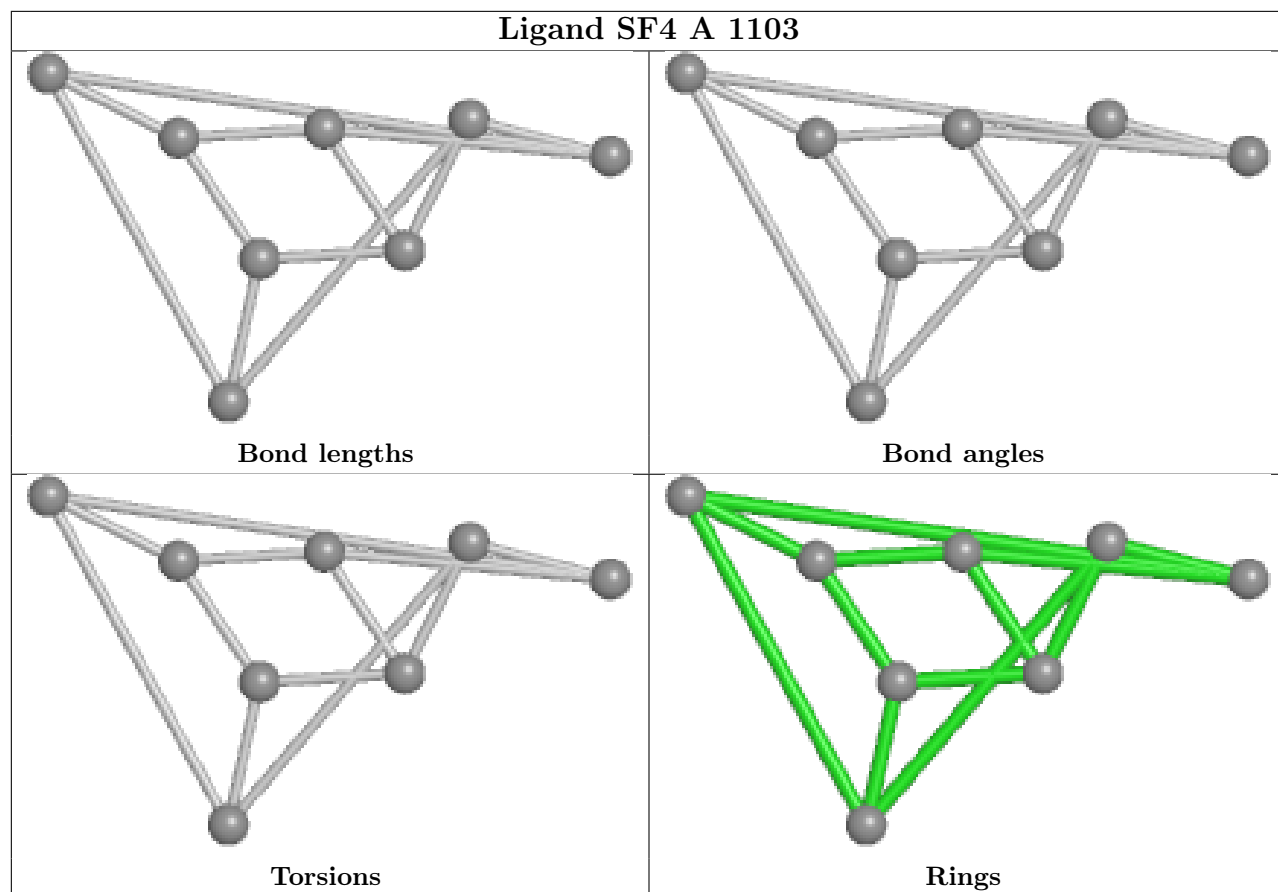


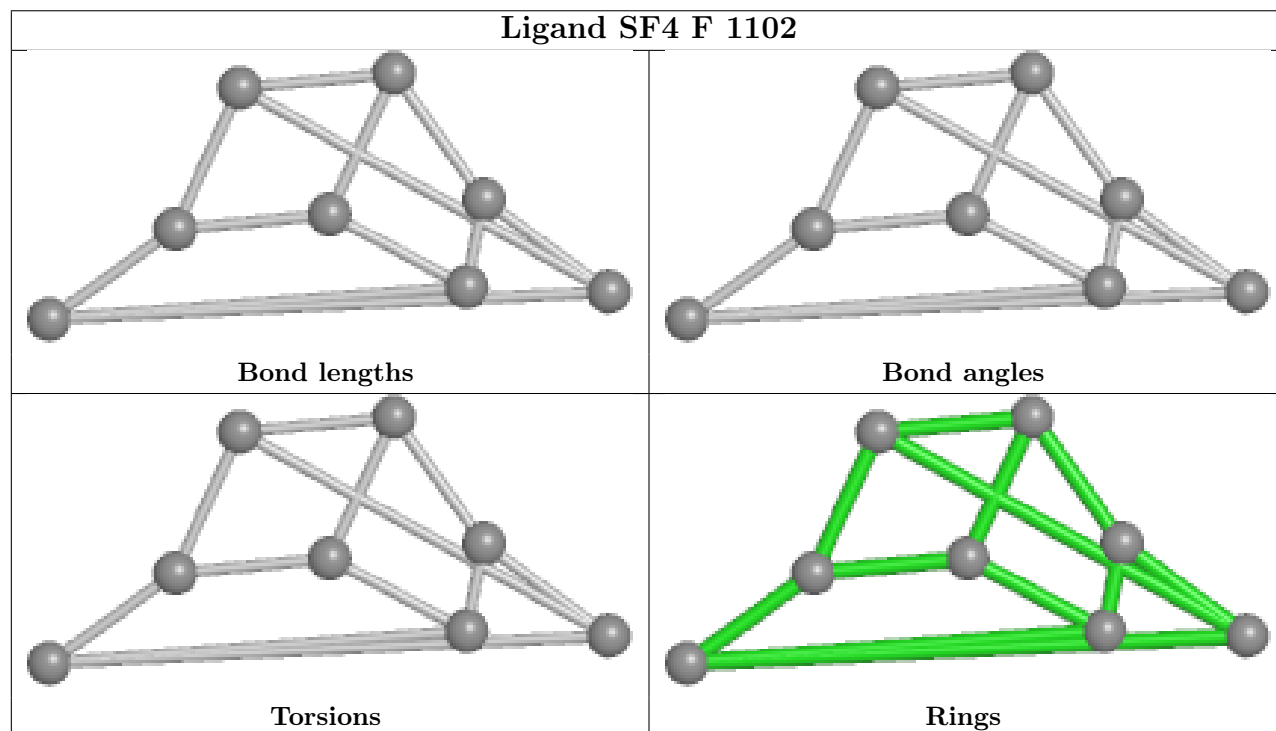
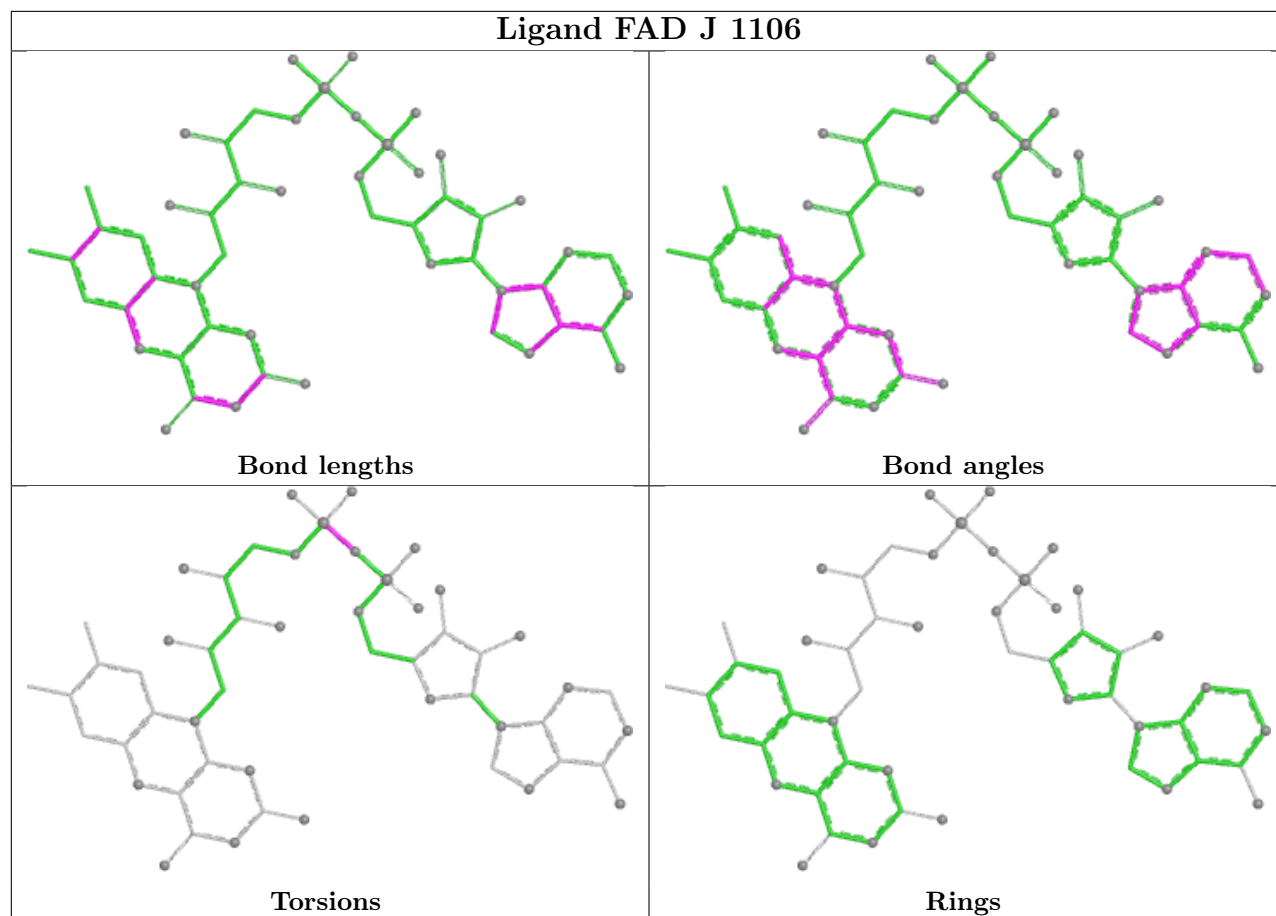
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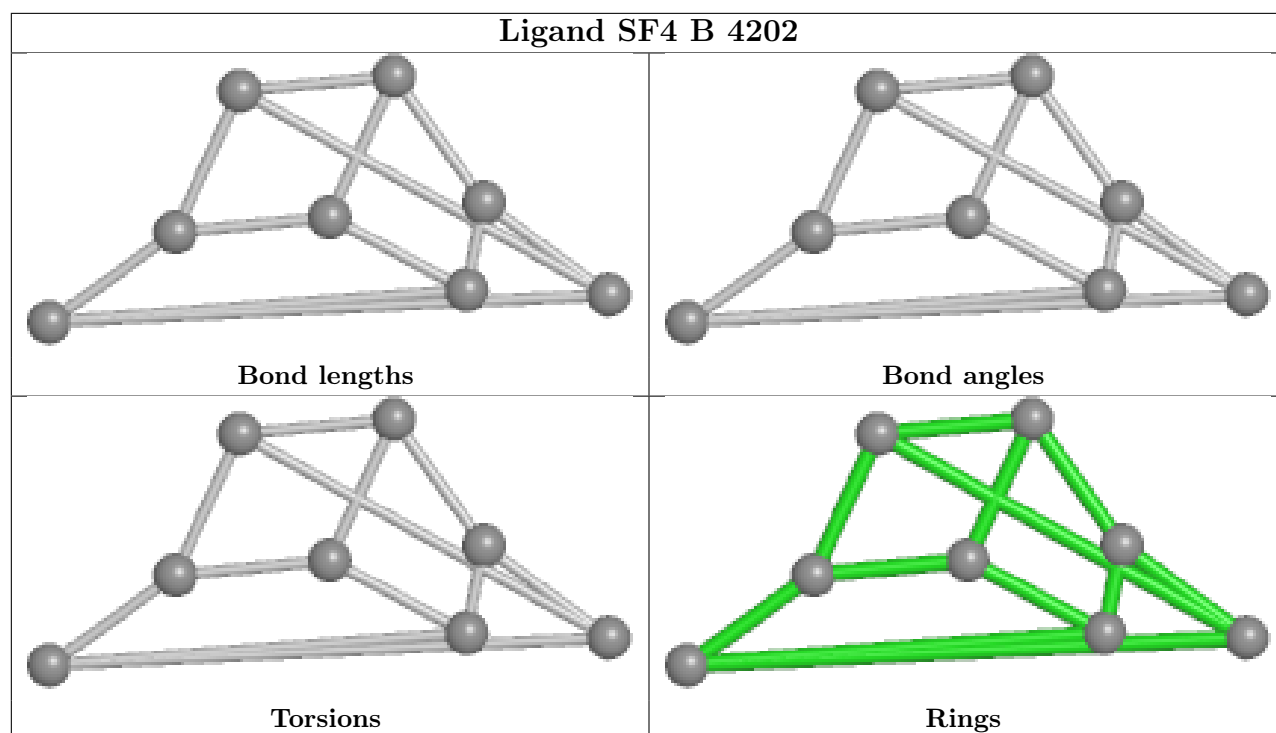
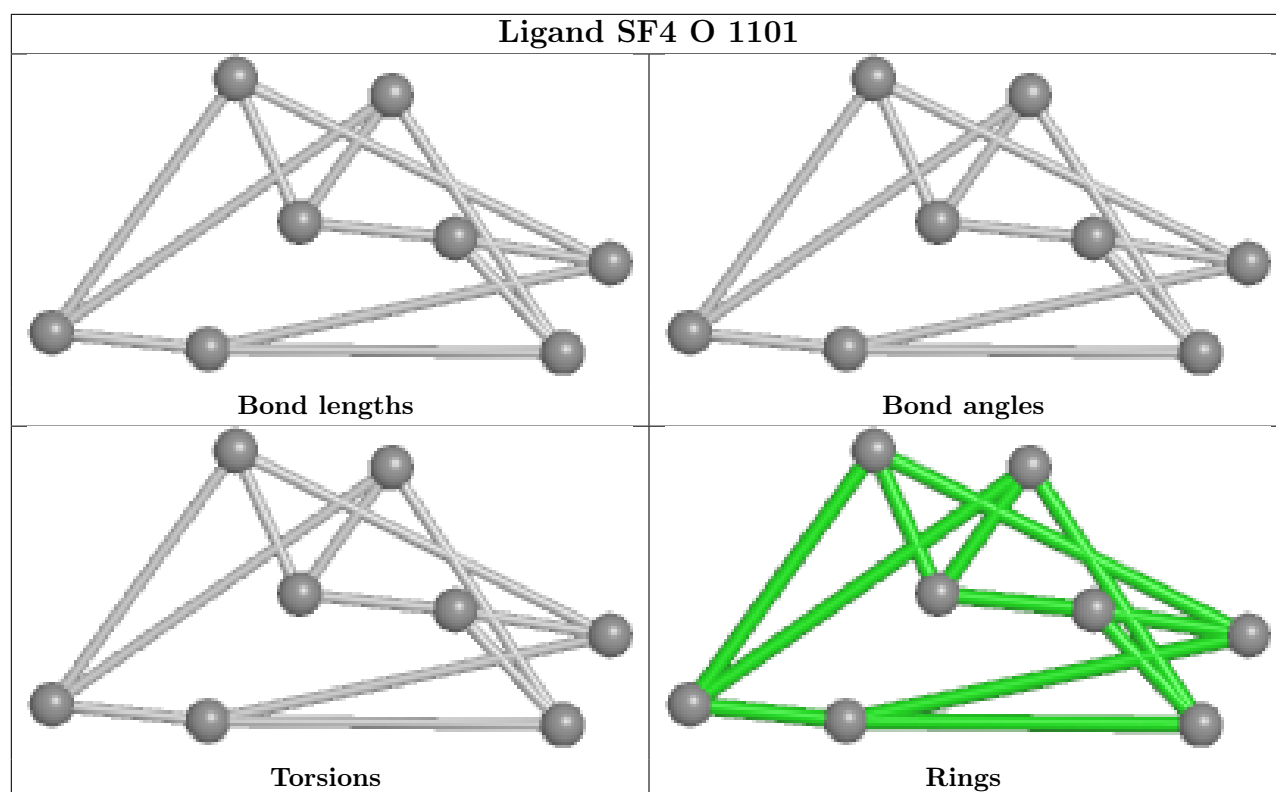


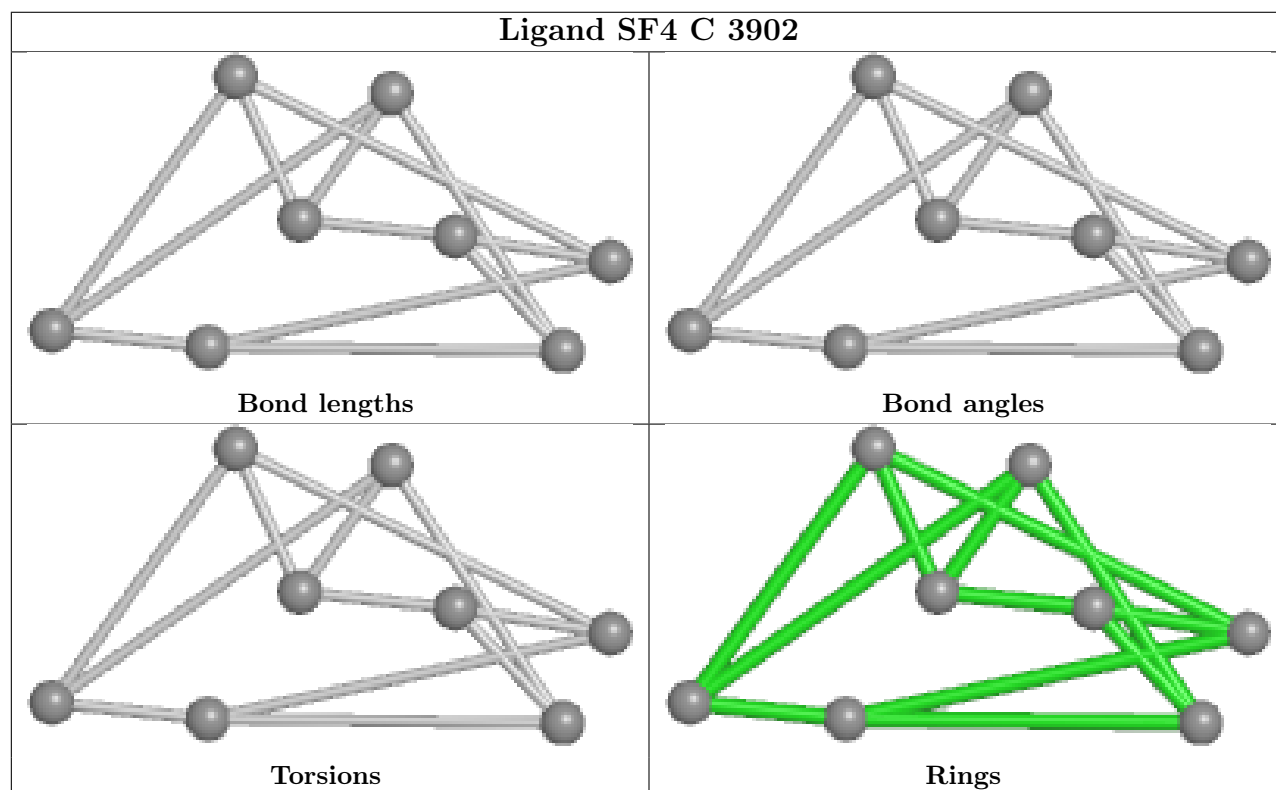
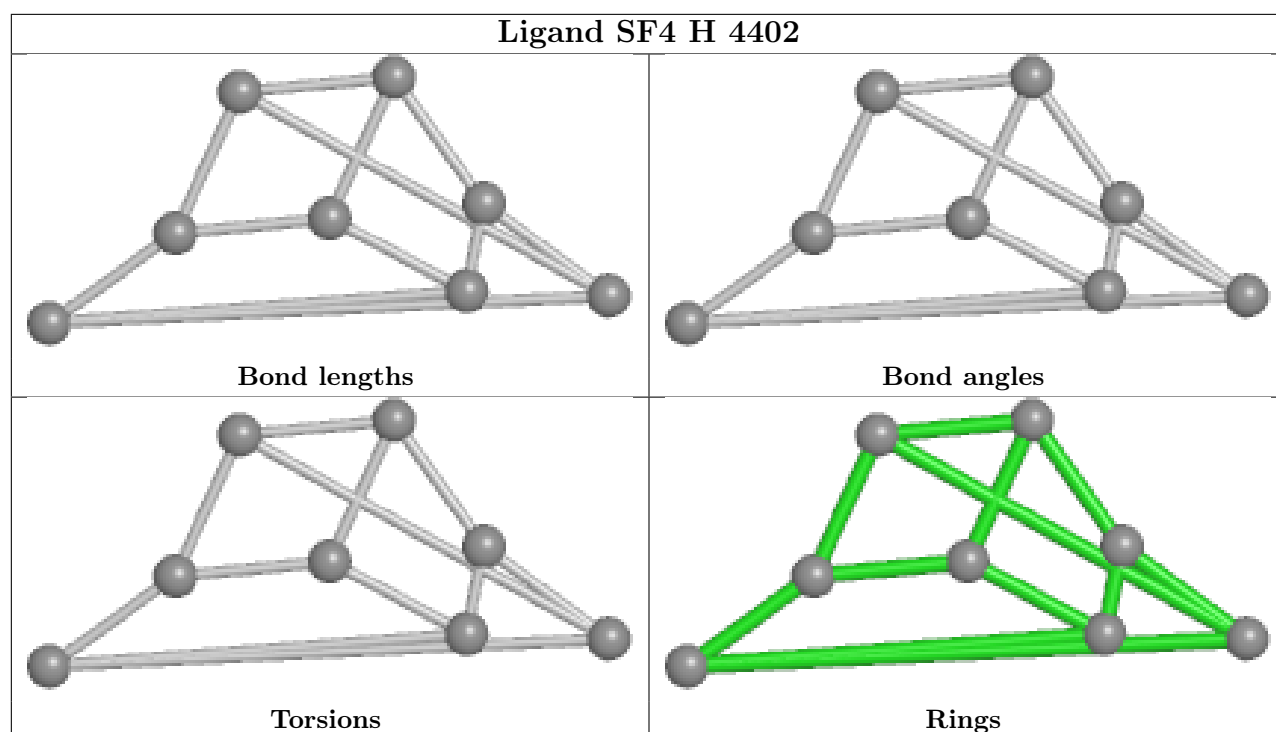


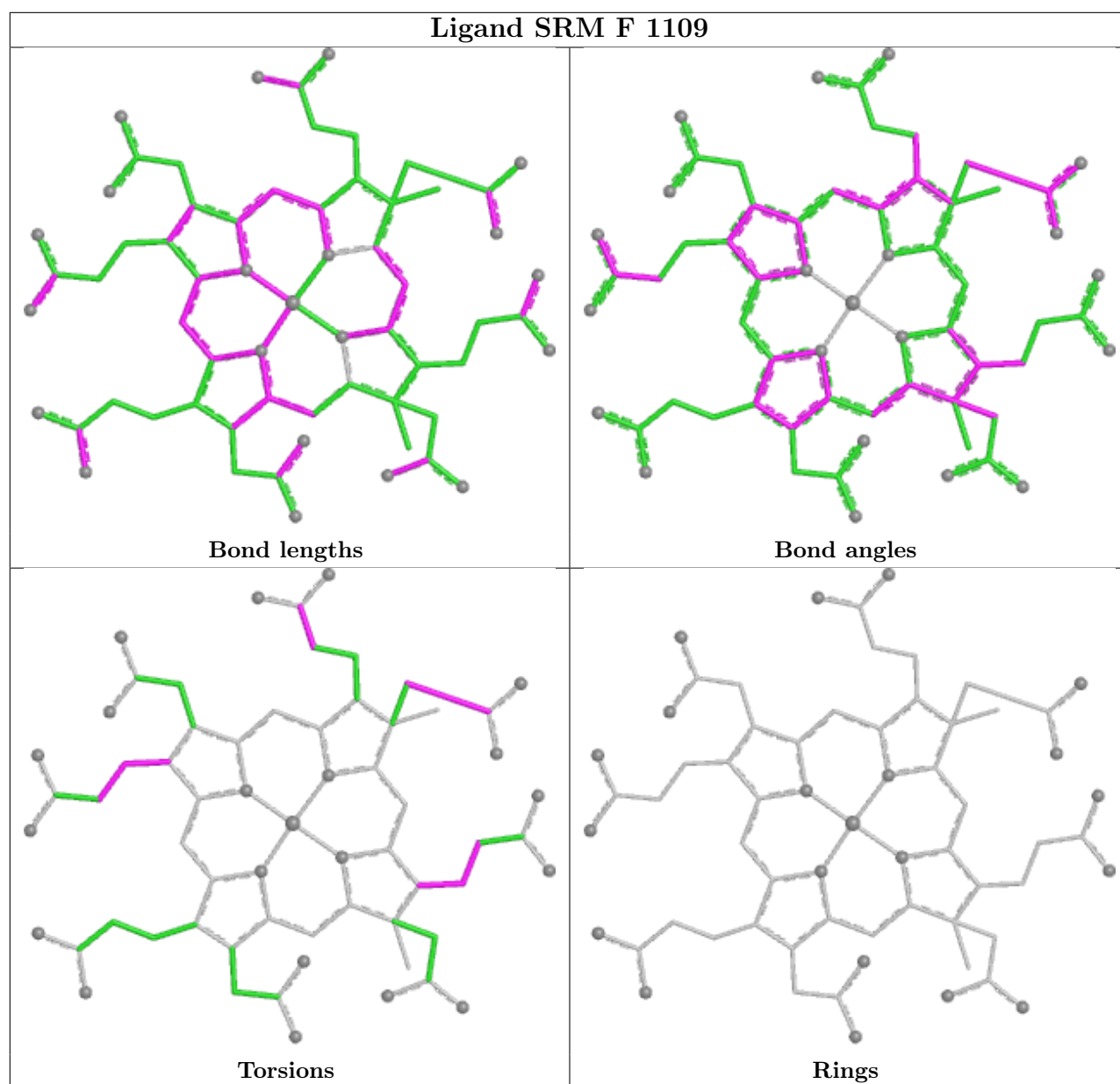




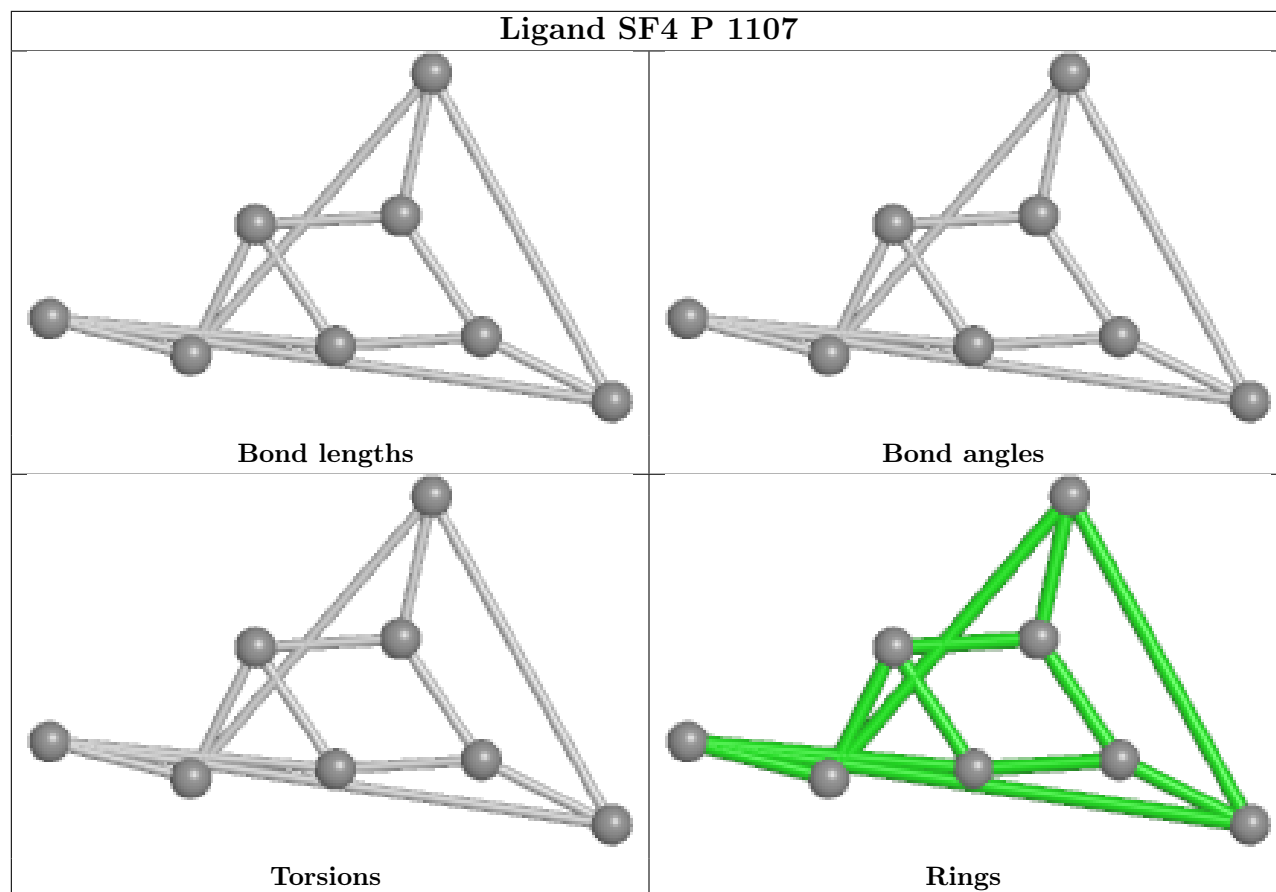




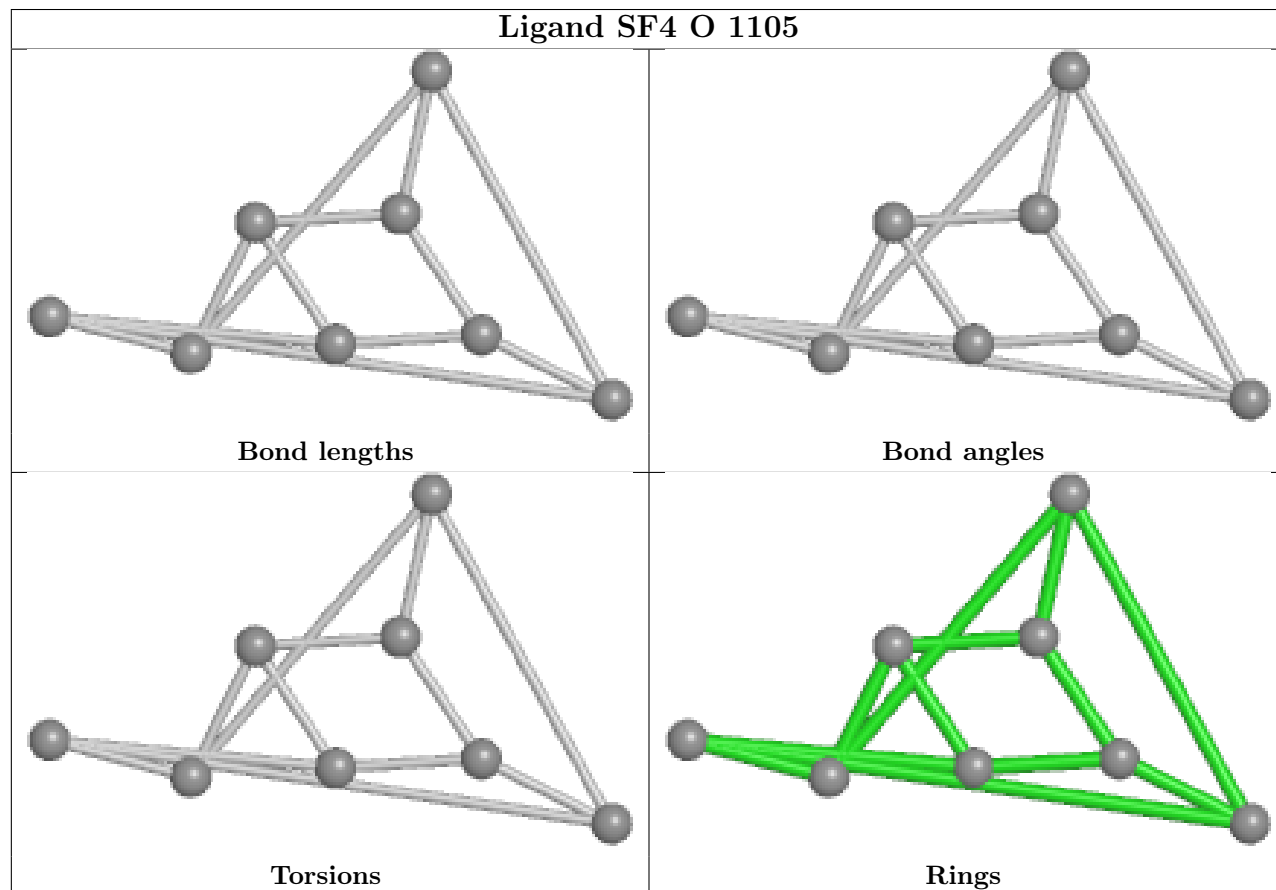




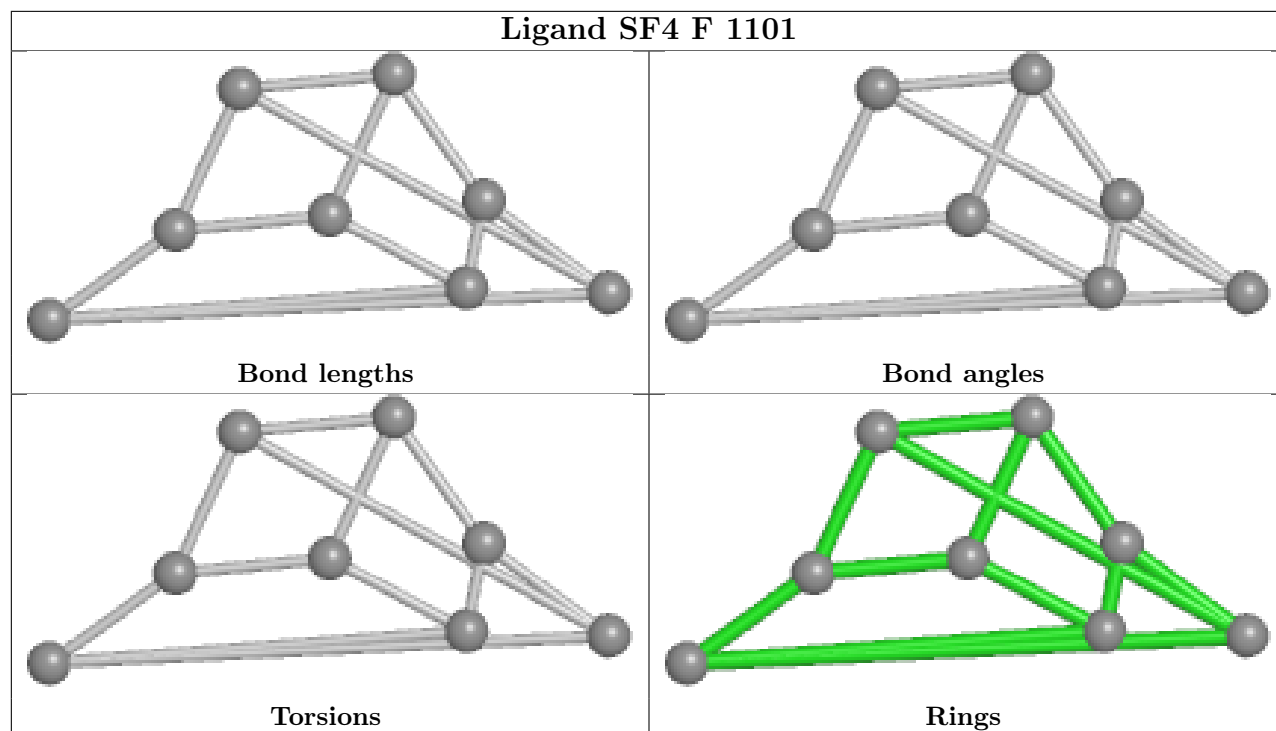
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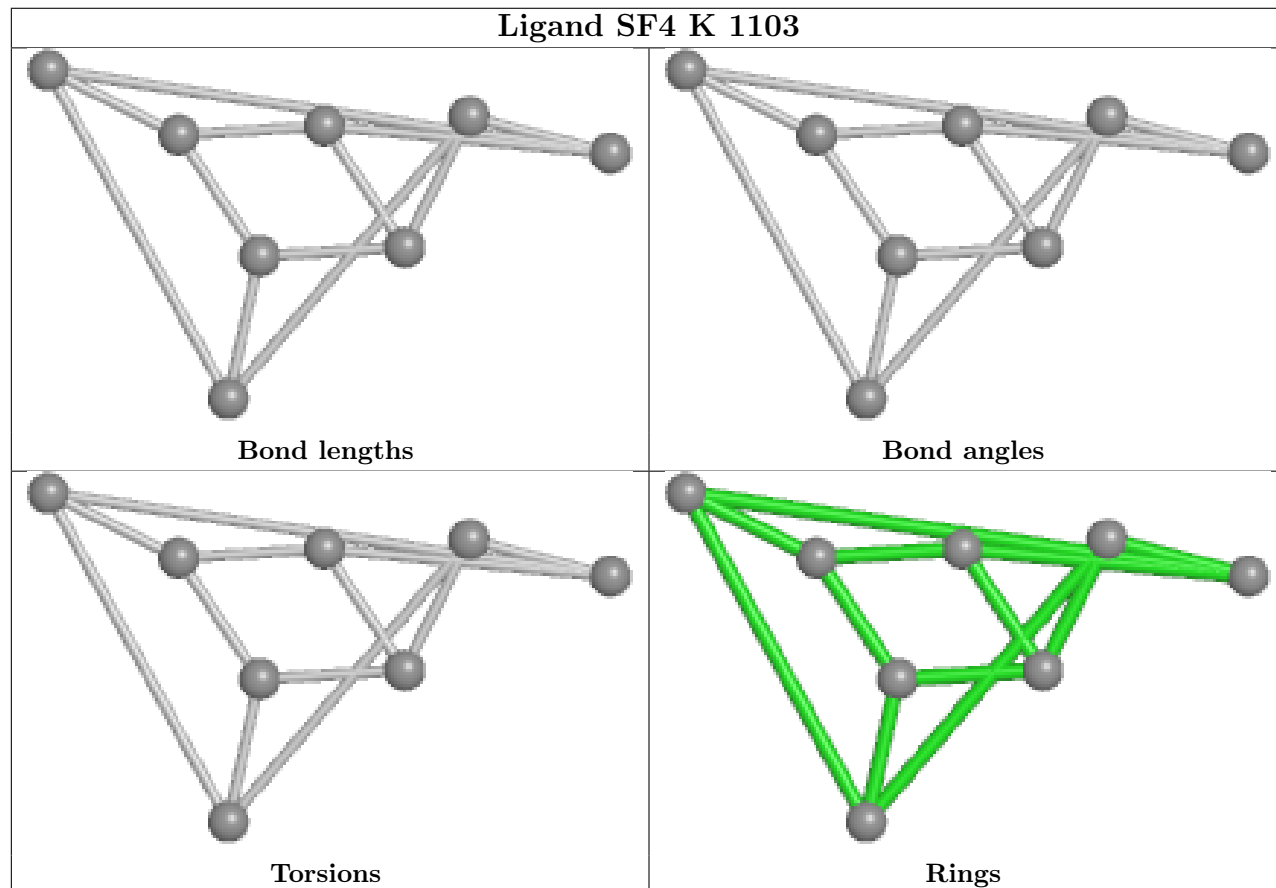
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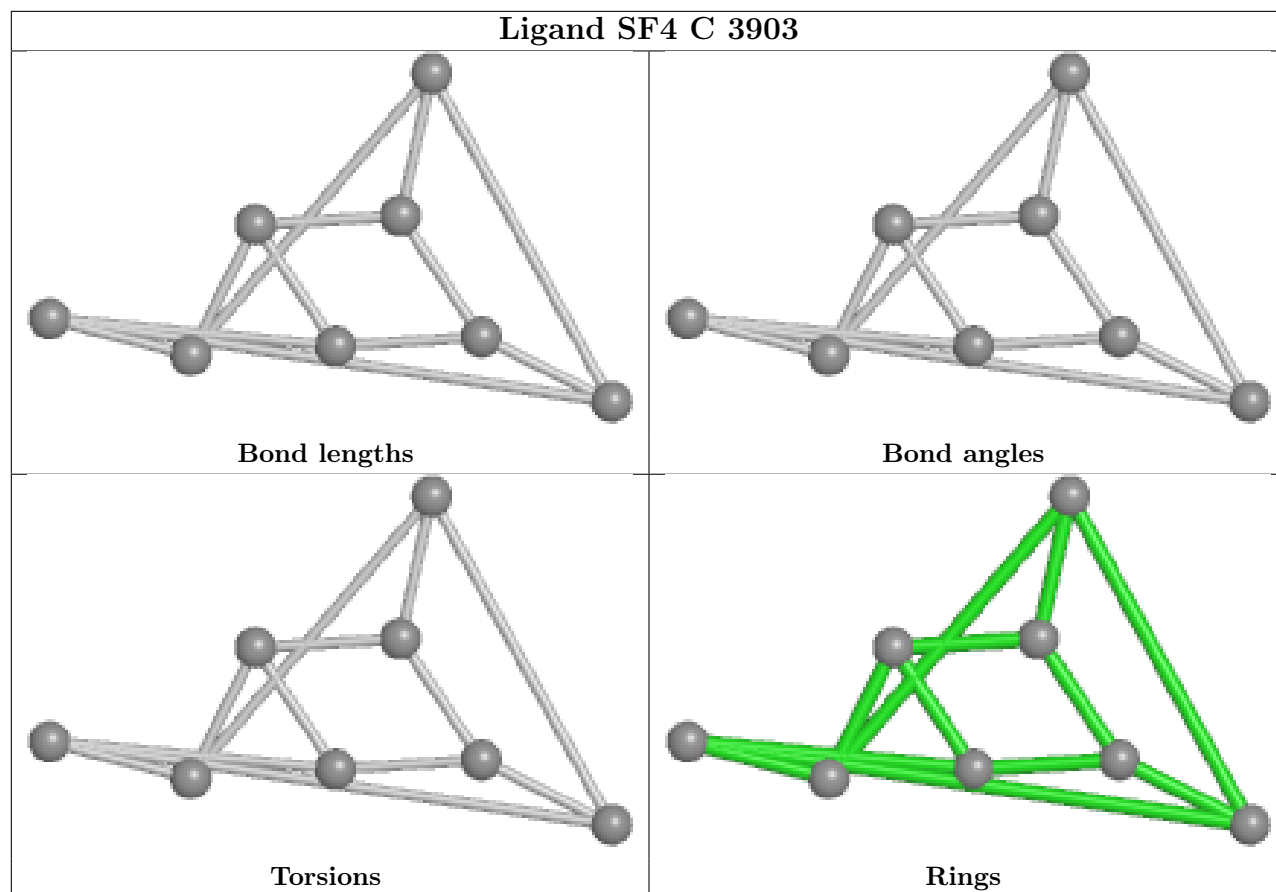
Ligand SF4 F 1101



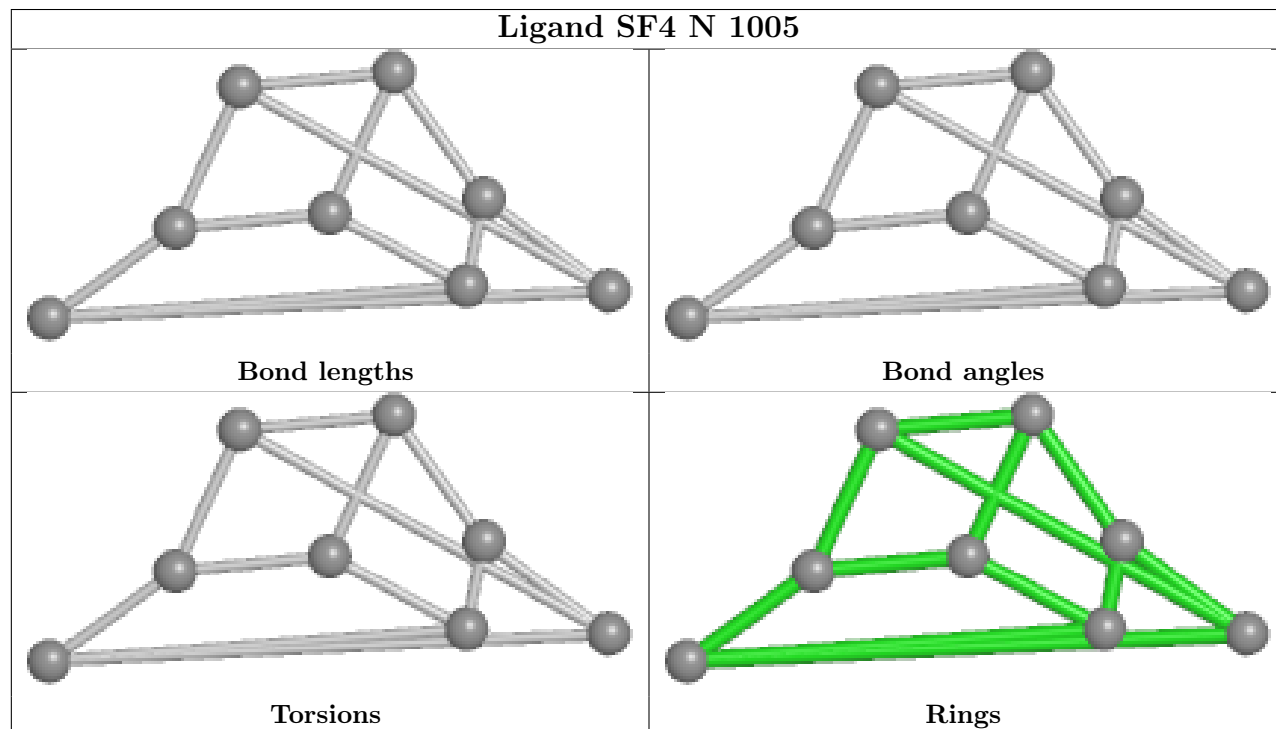
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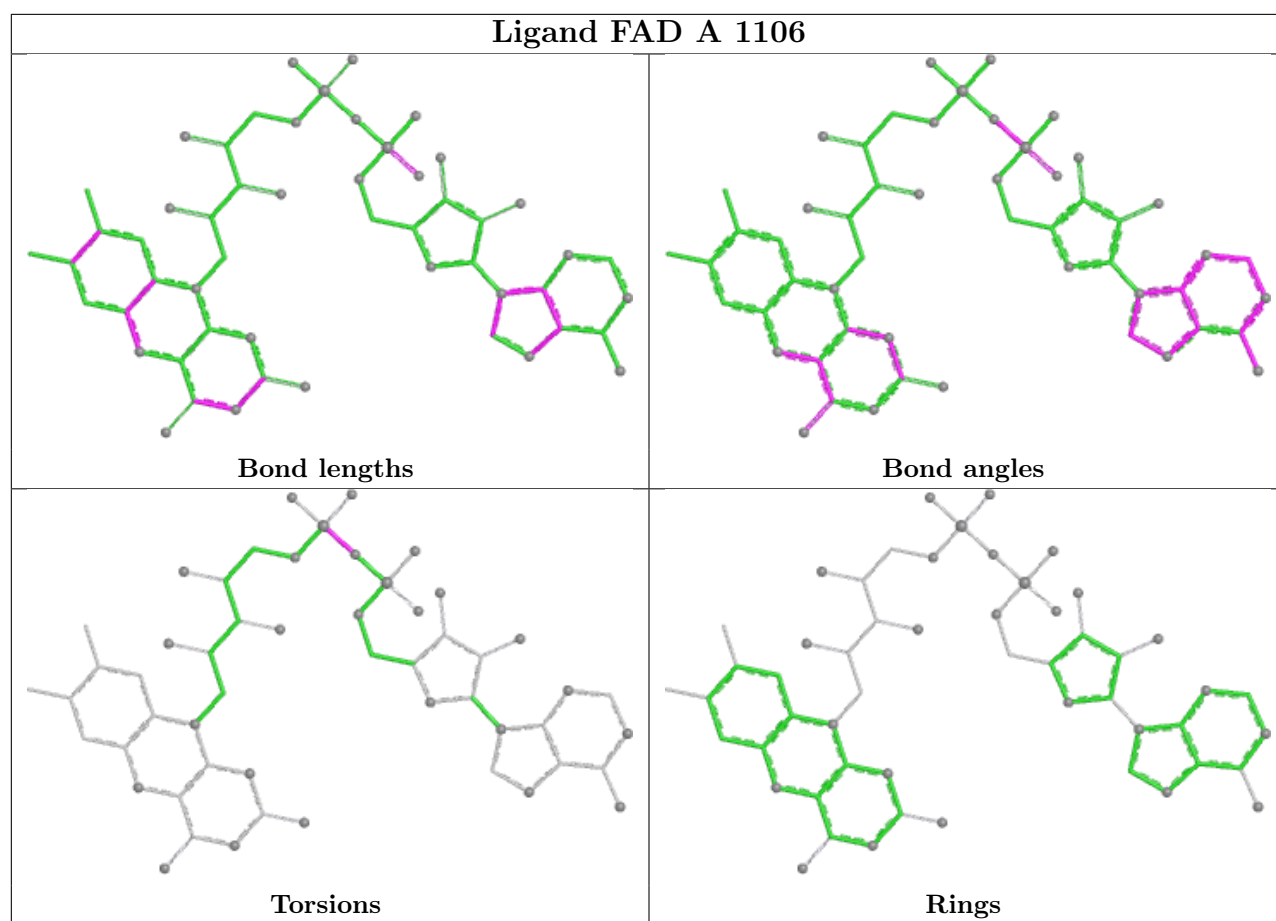


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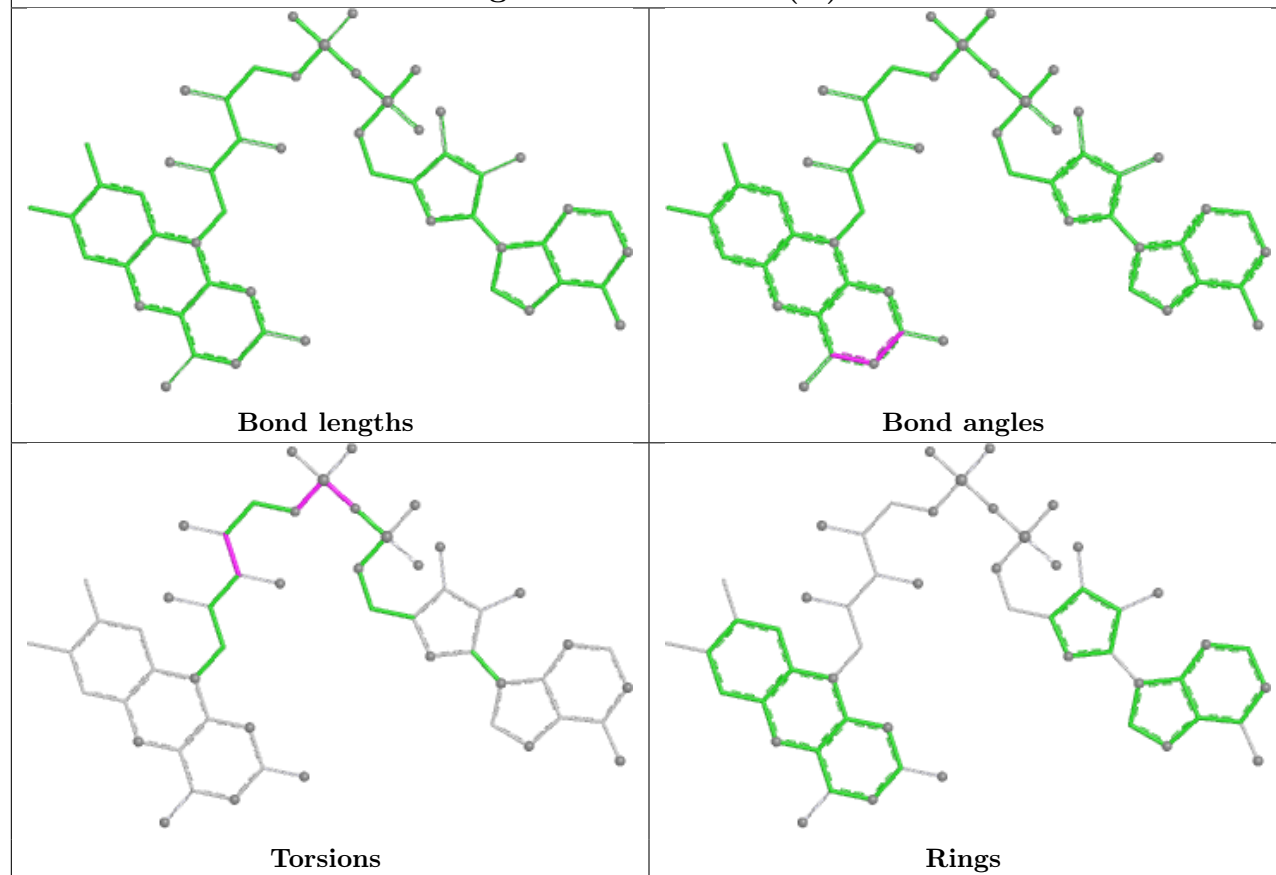


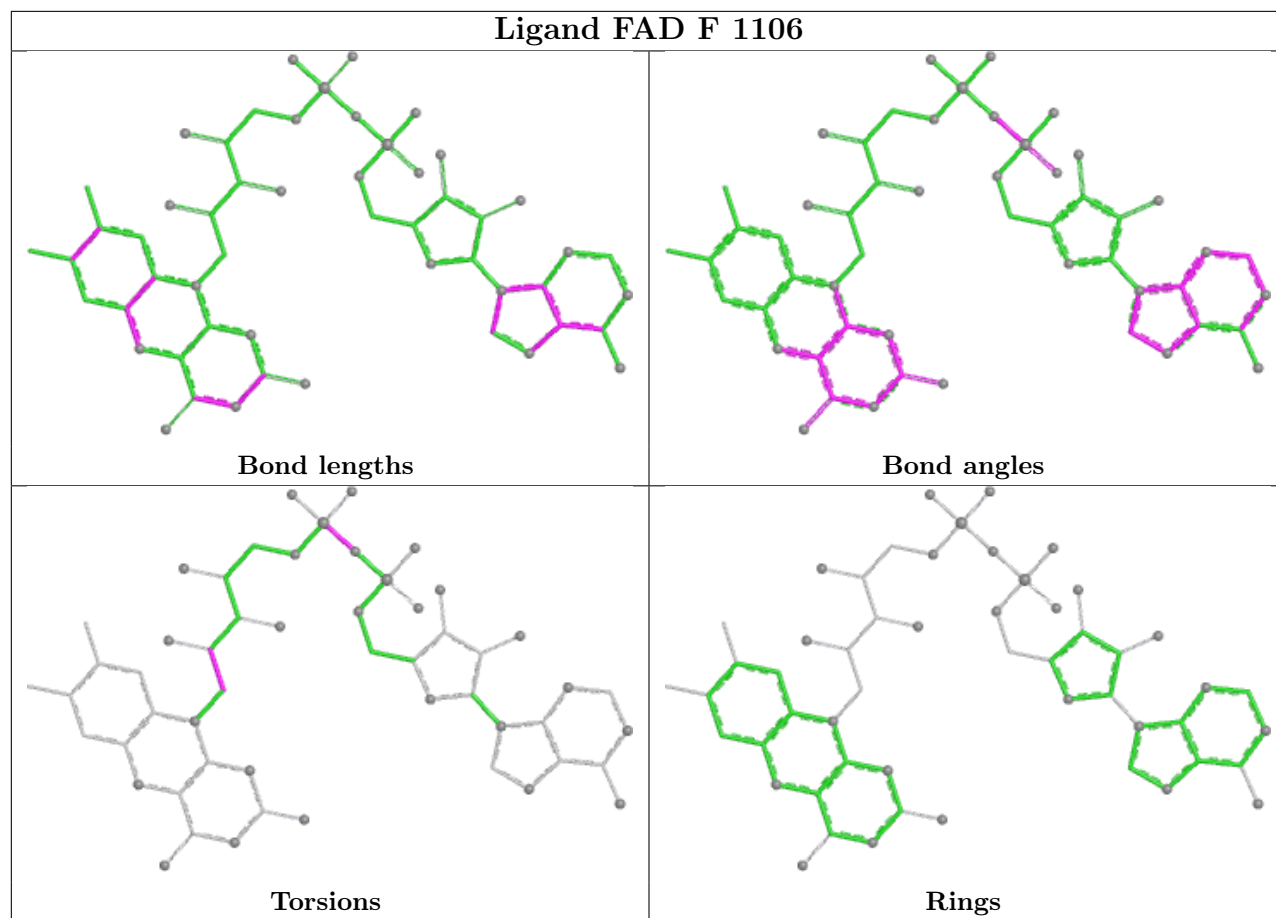
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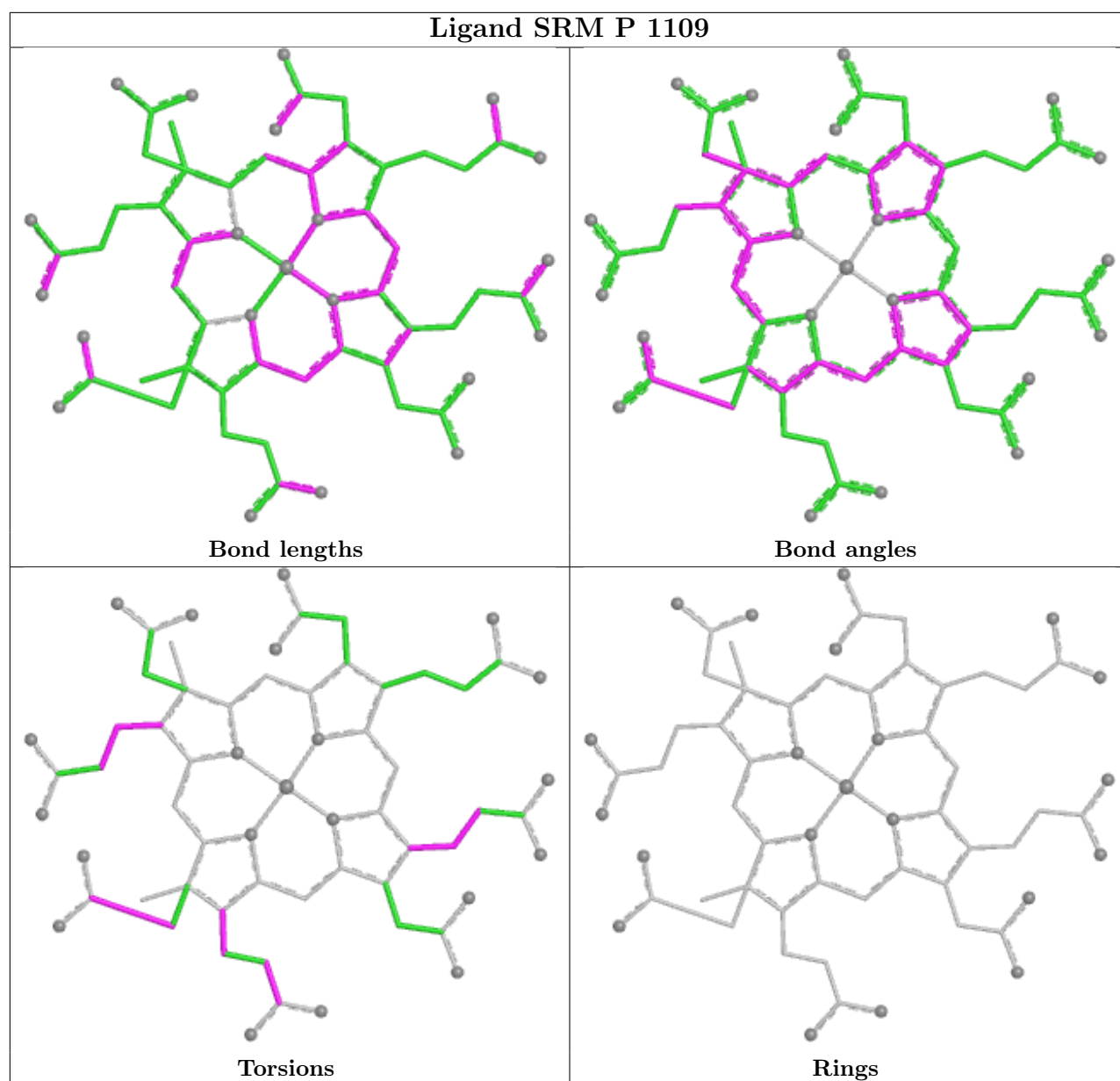




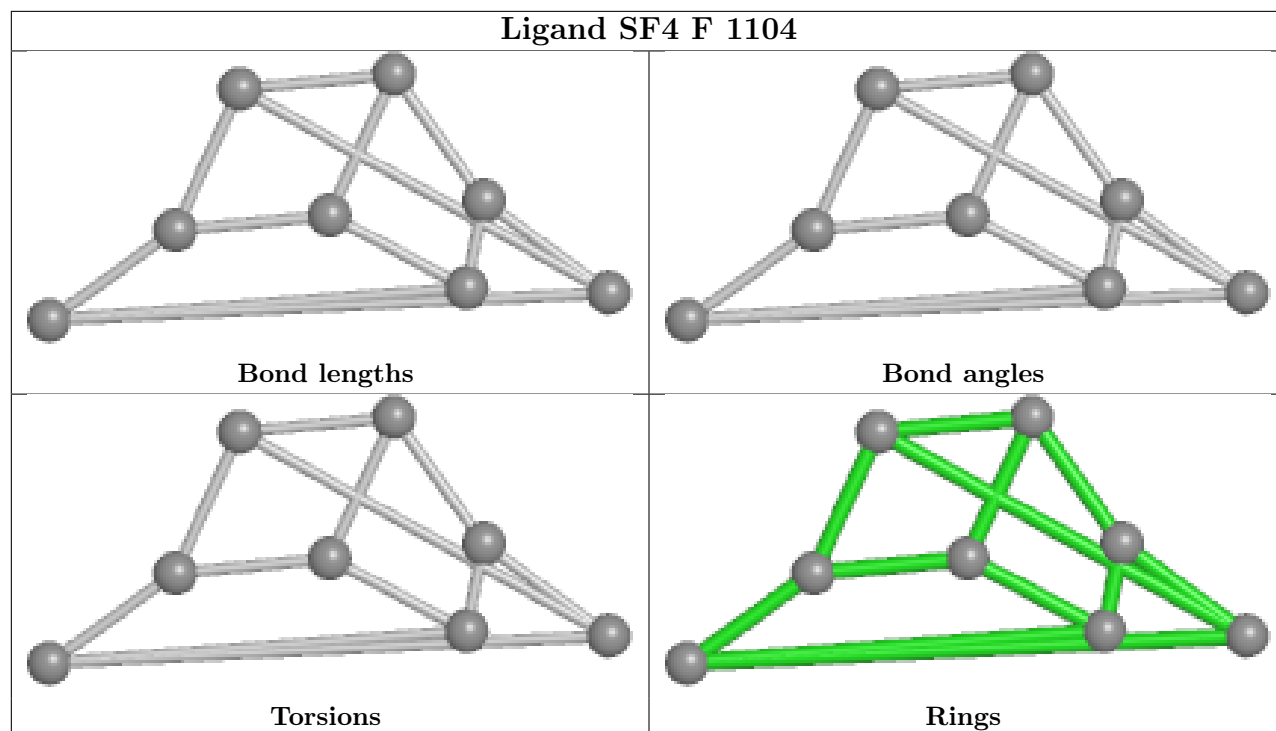
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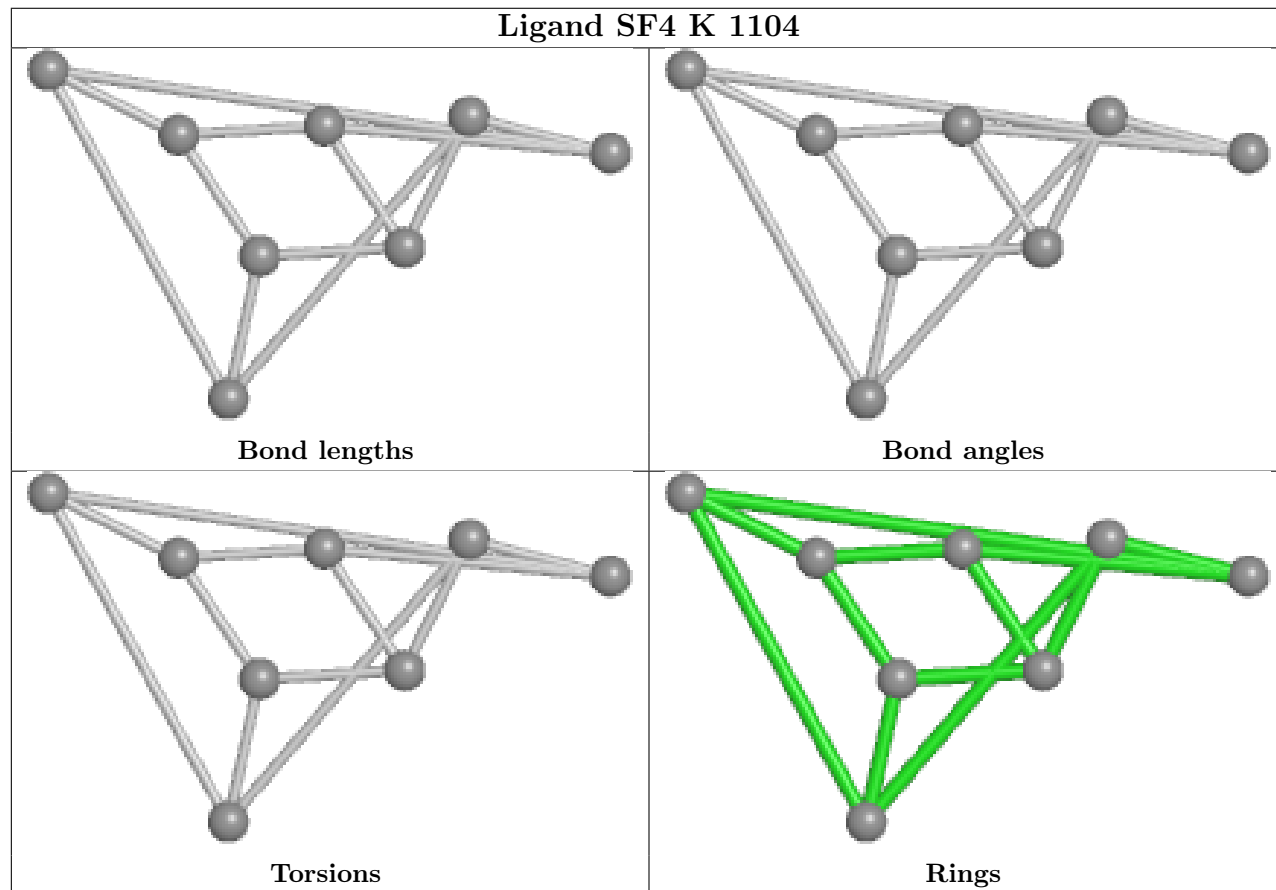




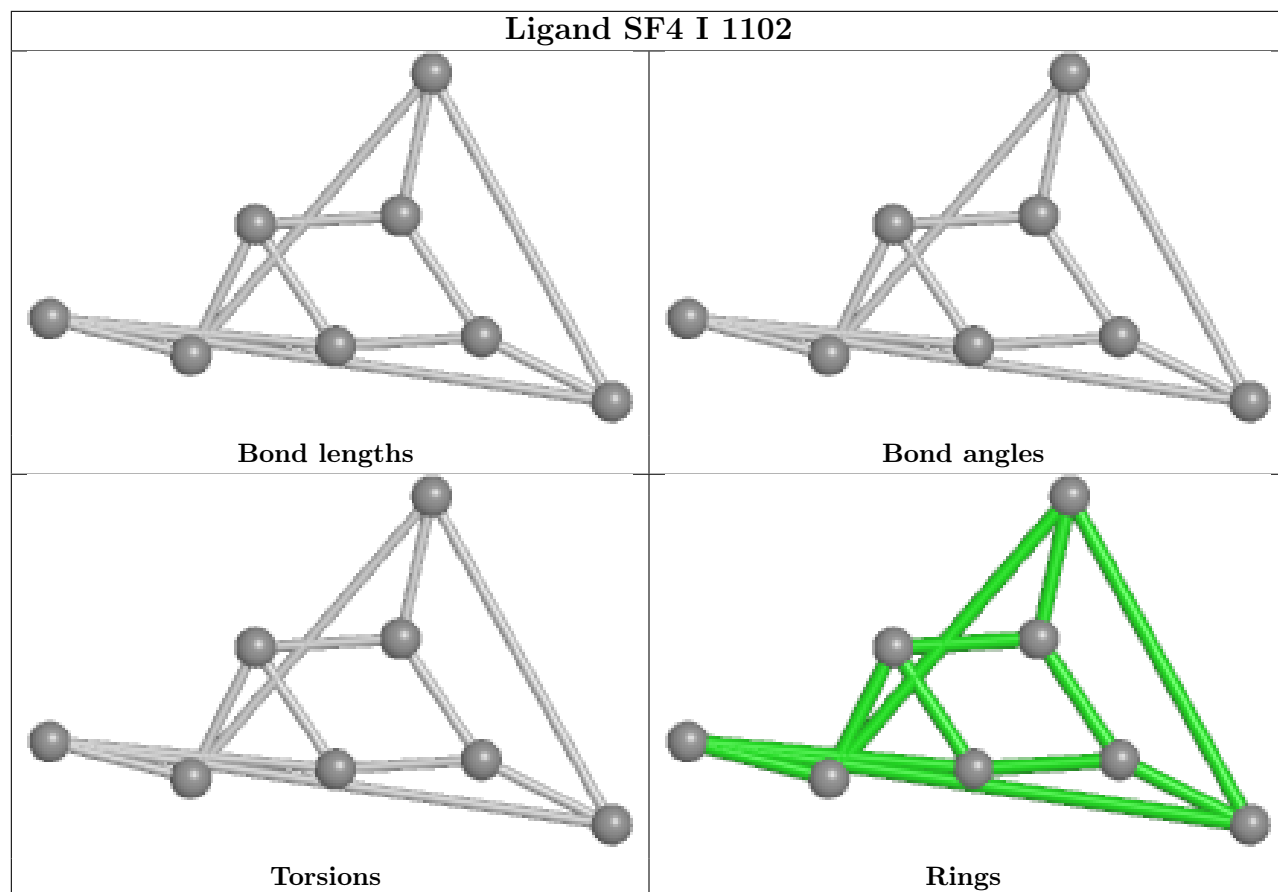
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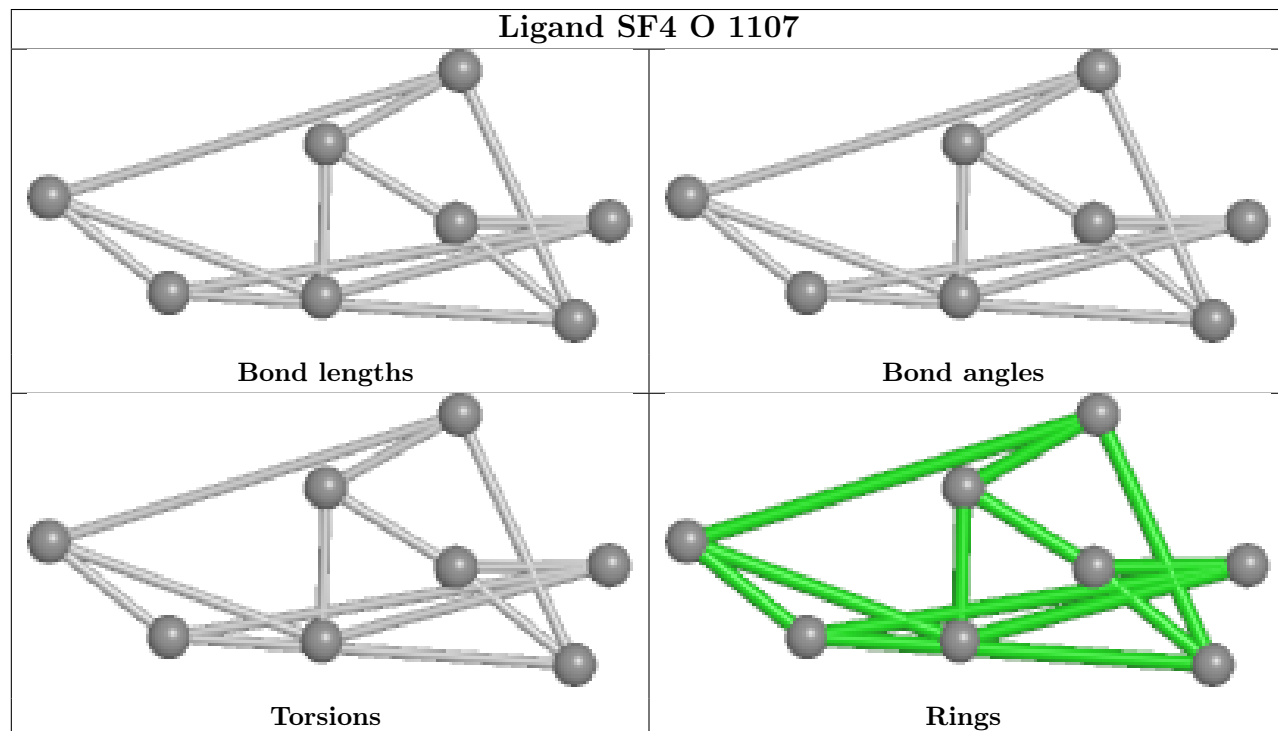
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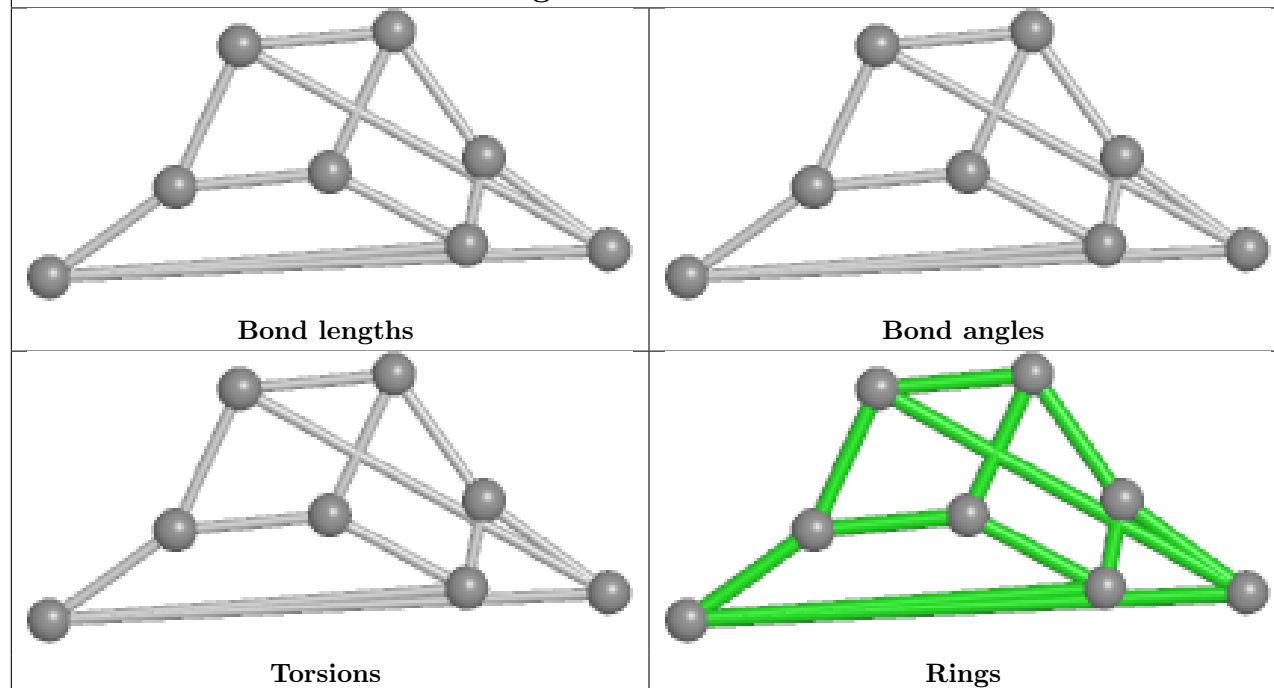
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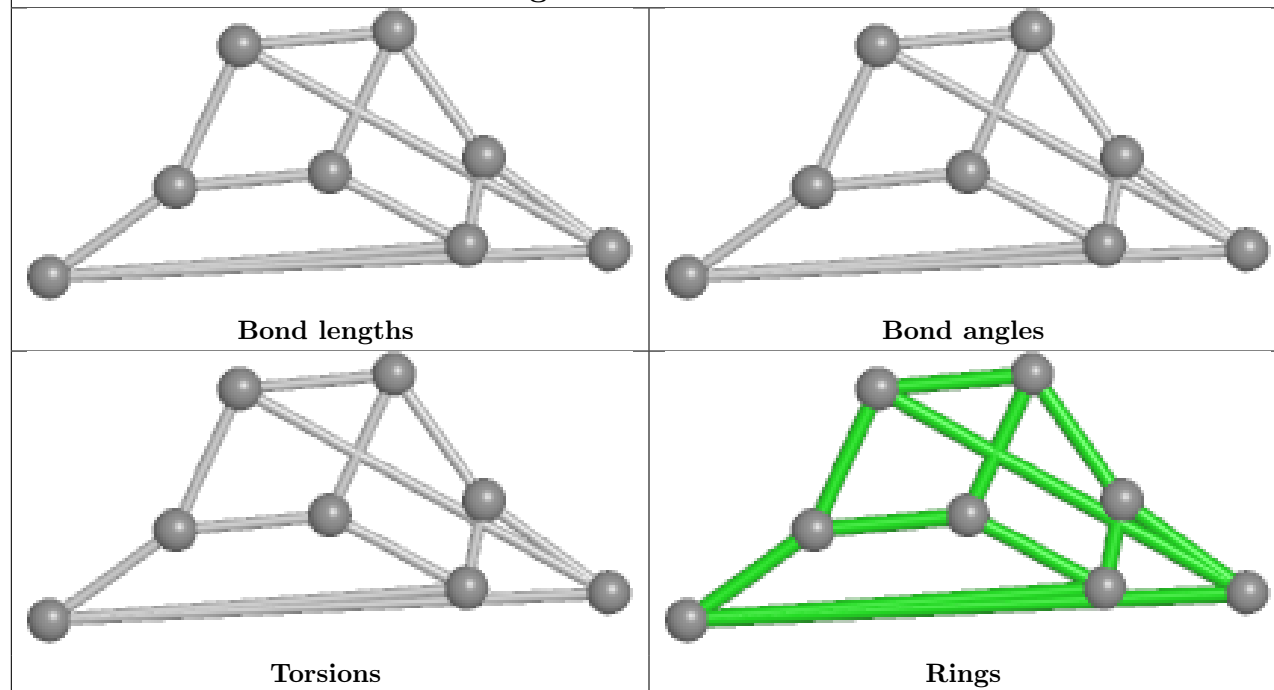
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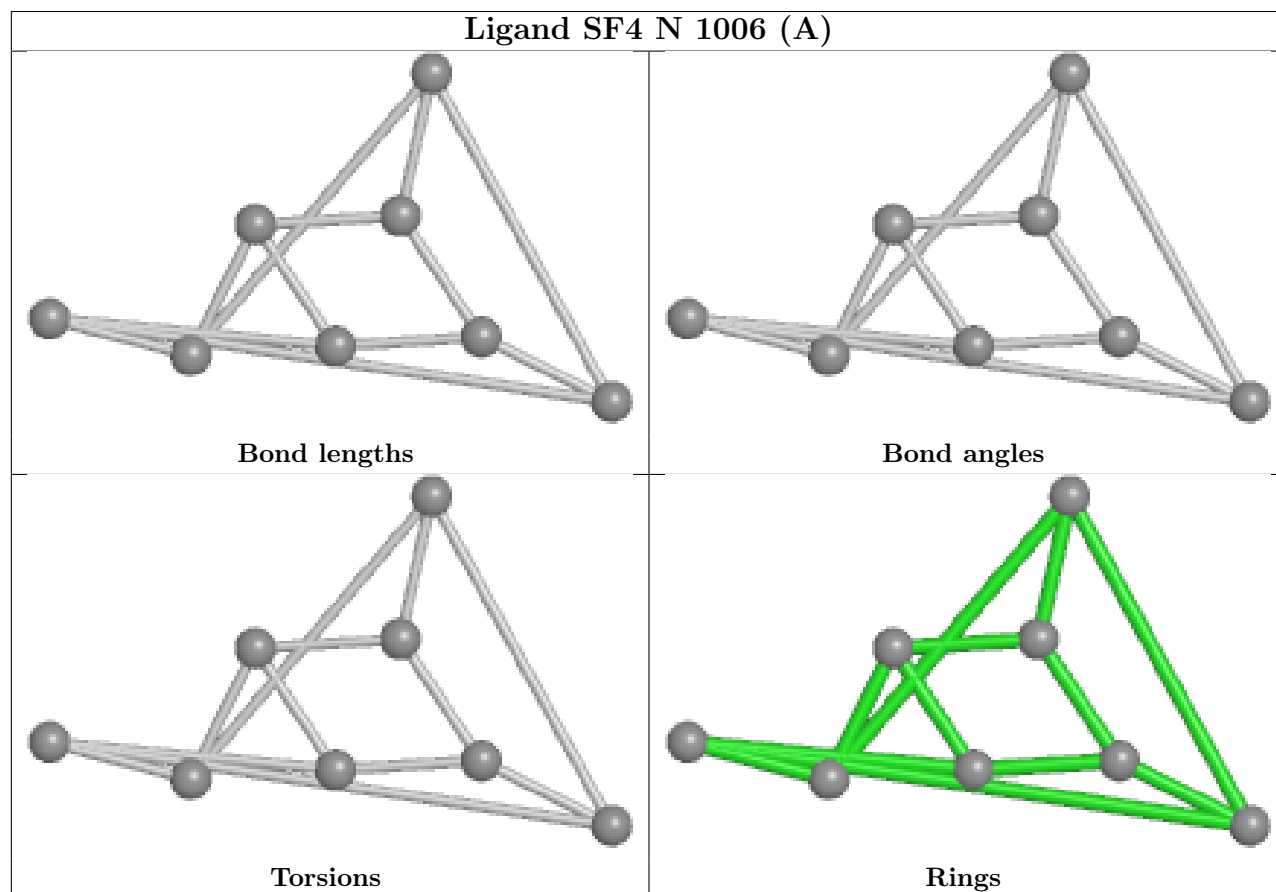
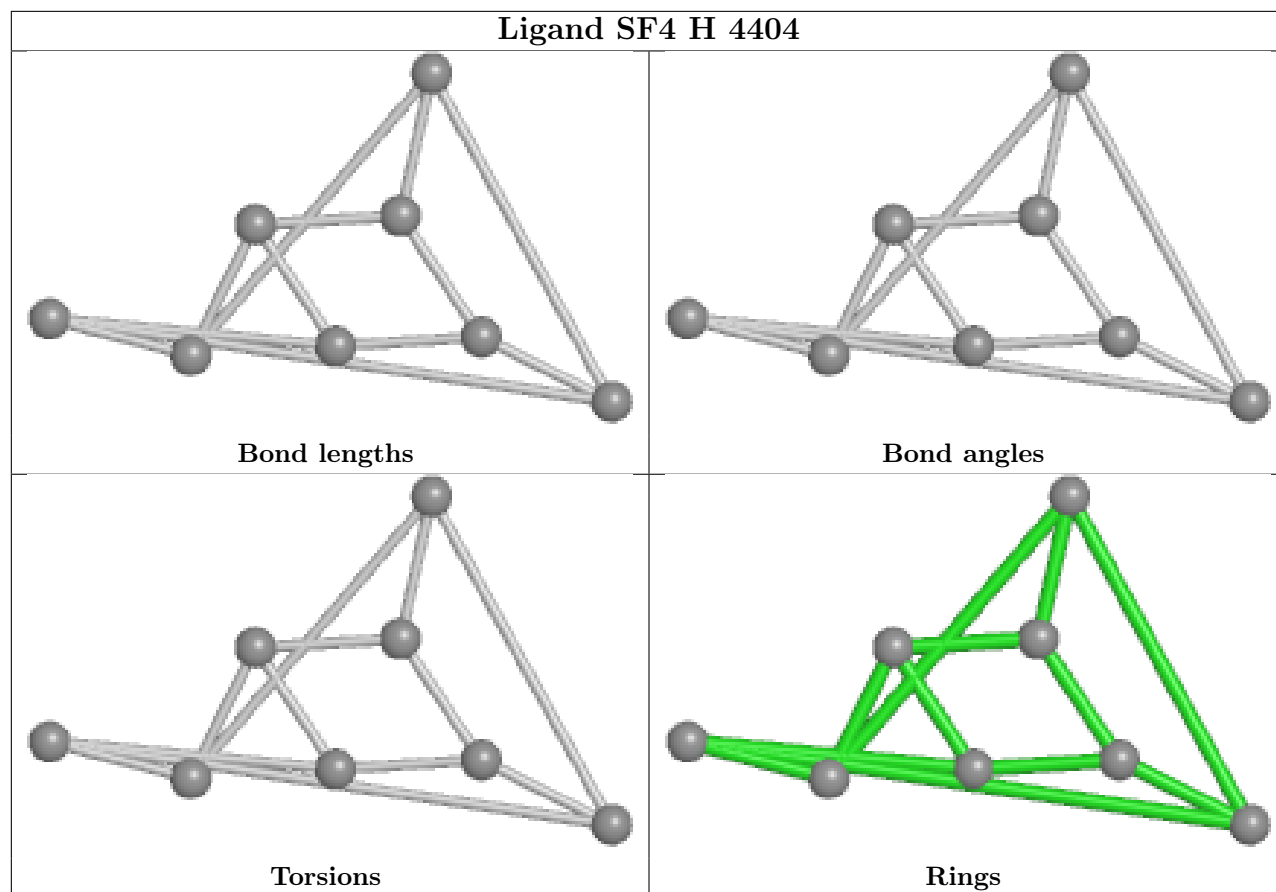


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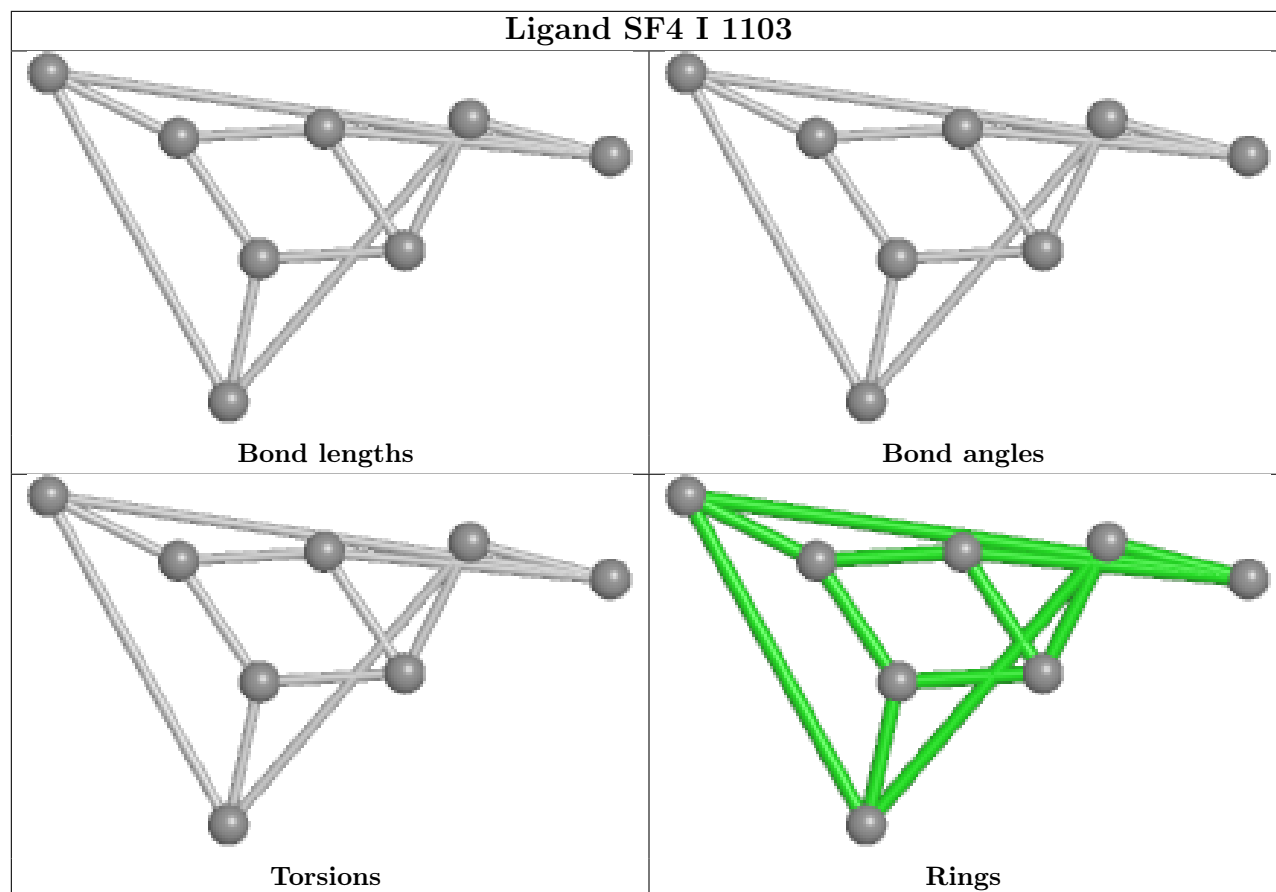


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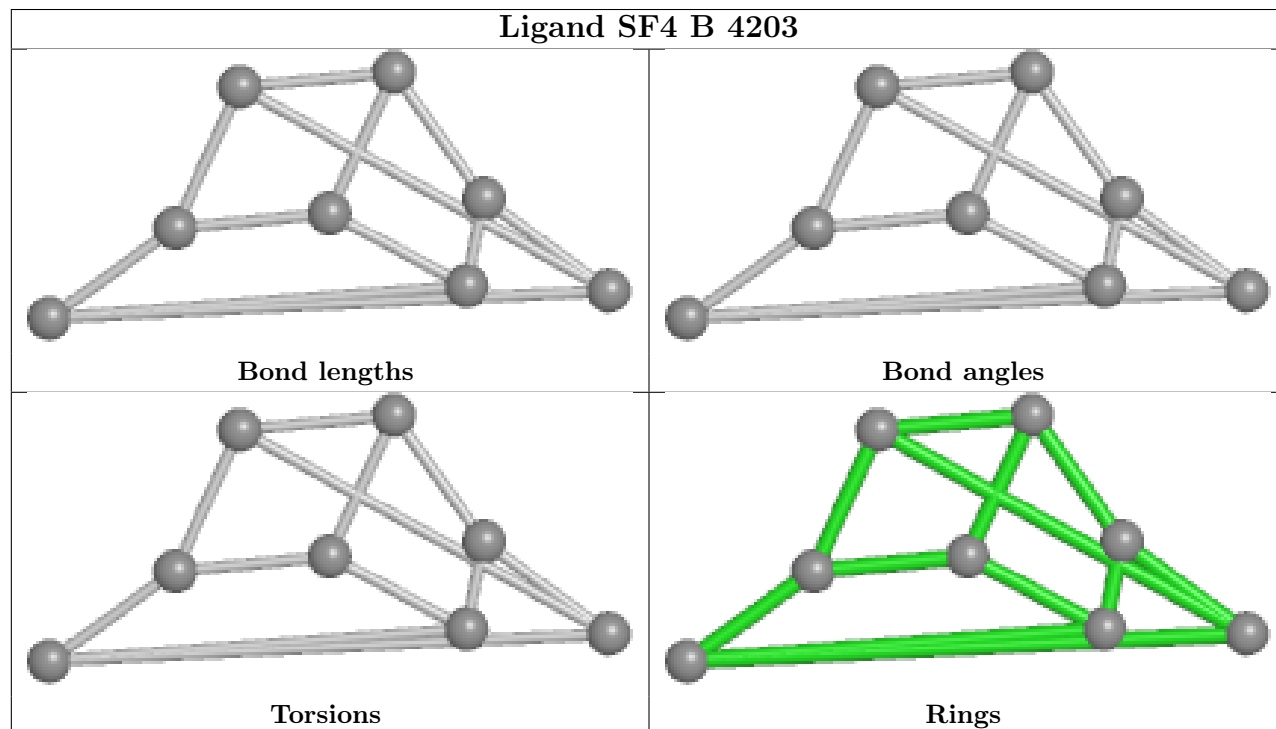


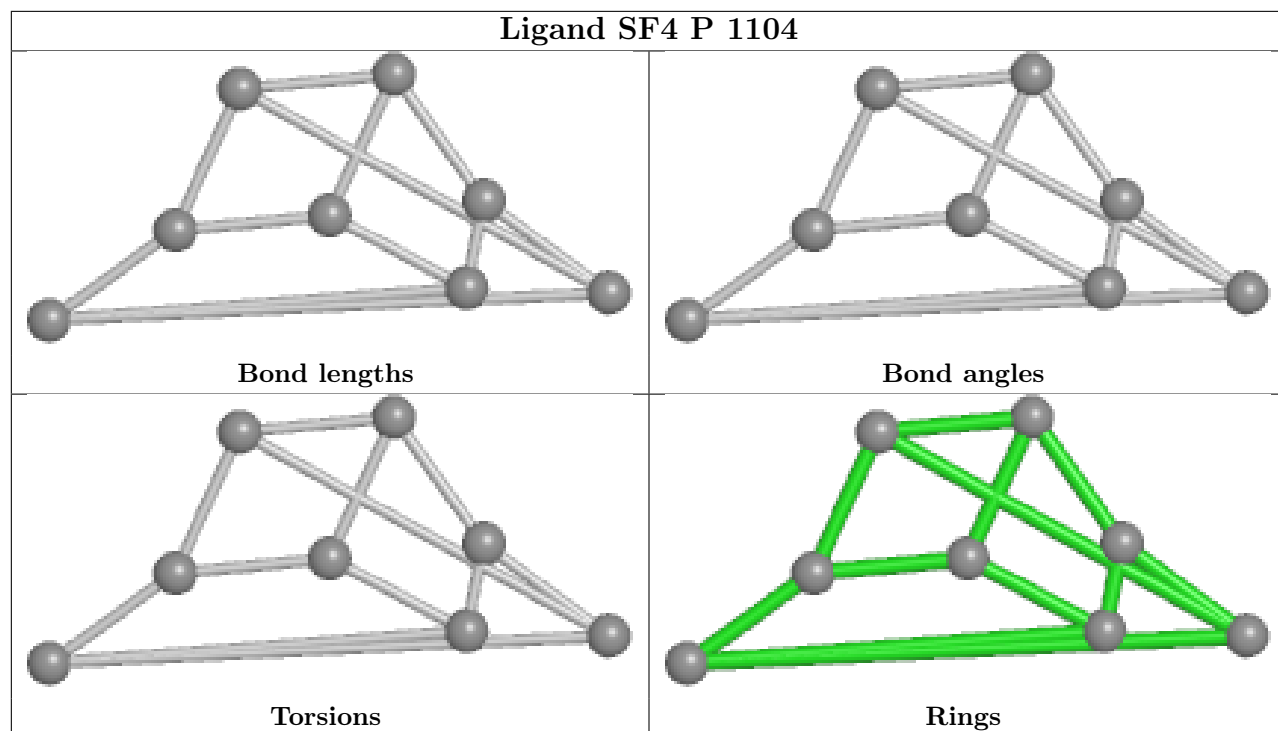


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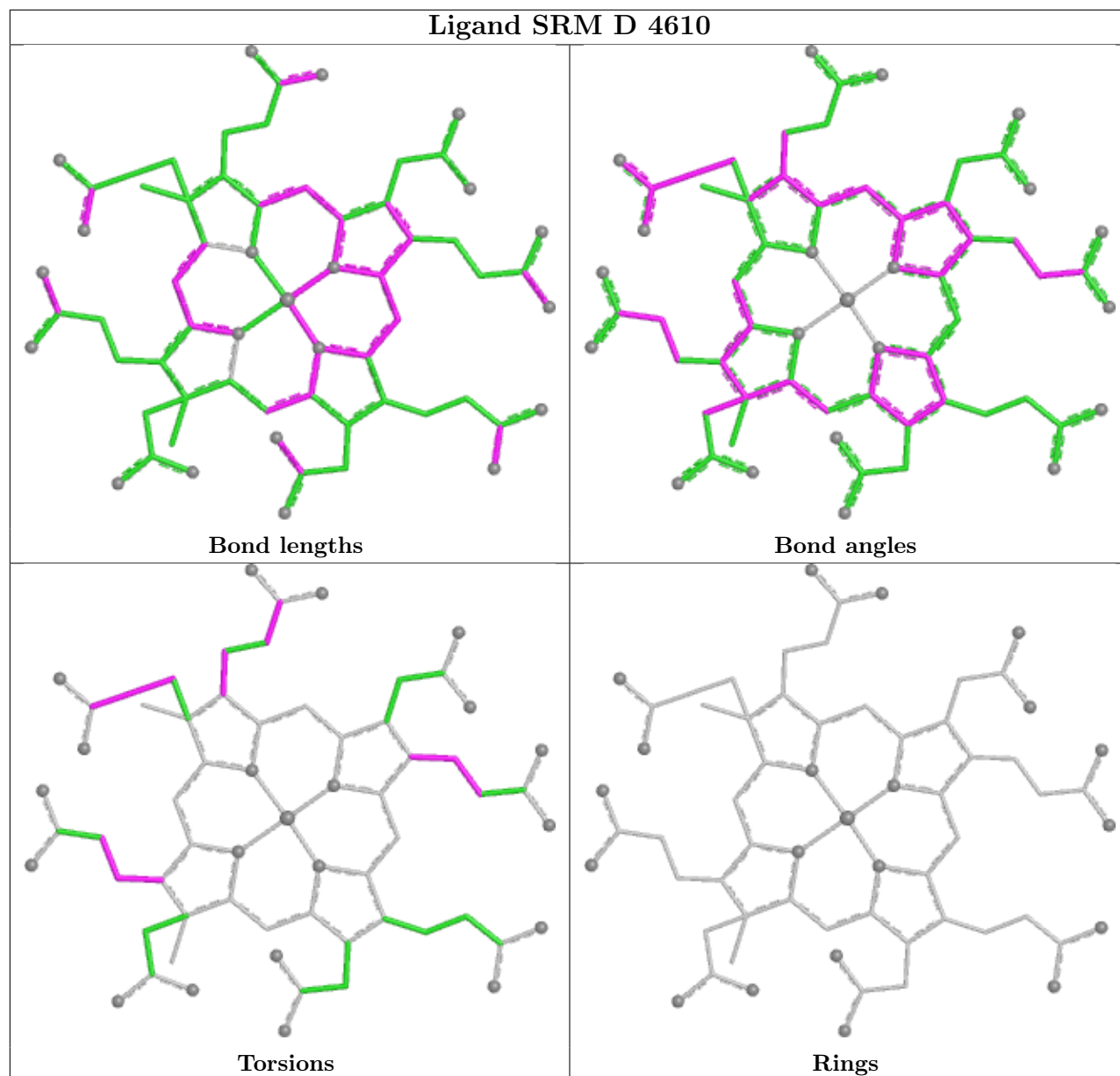


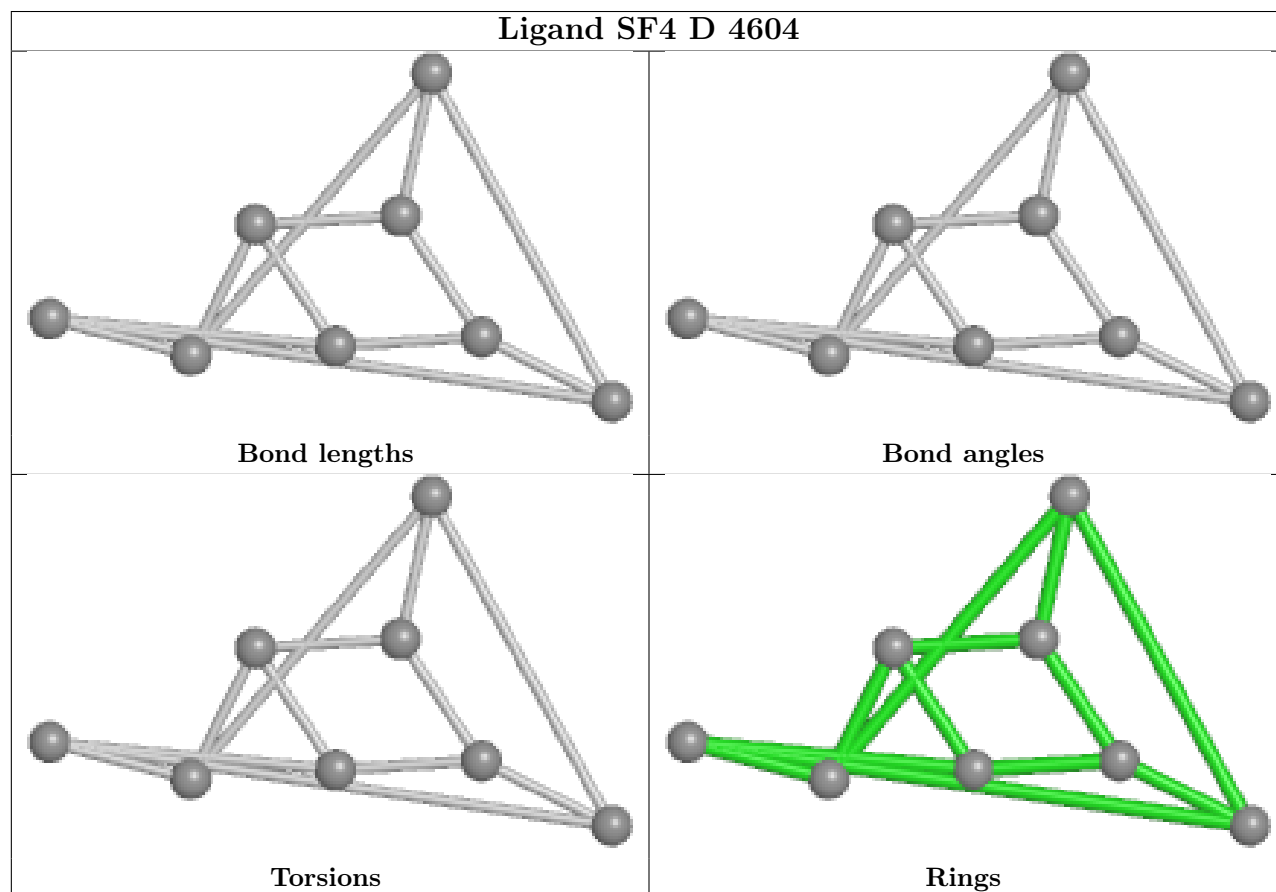
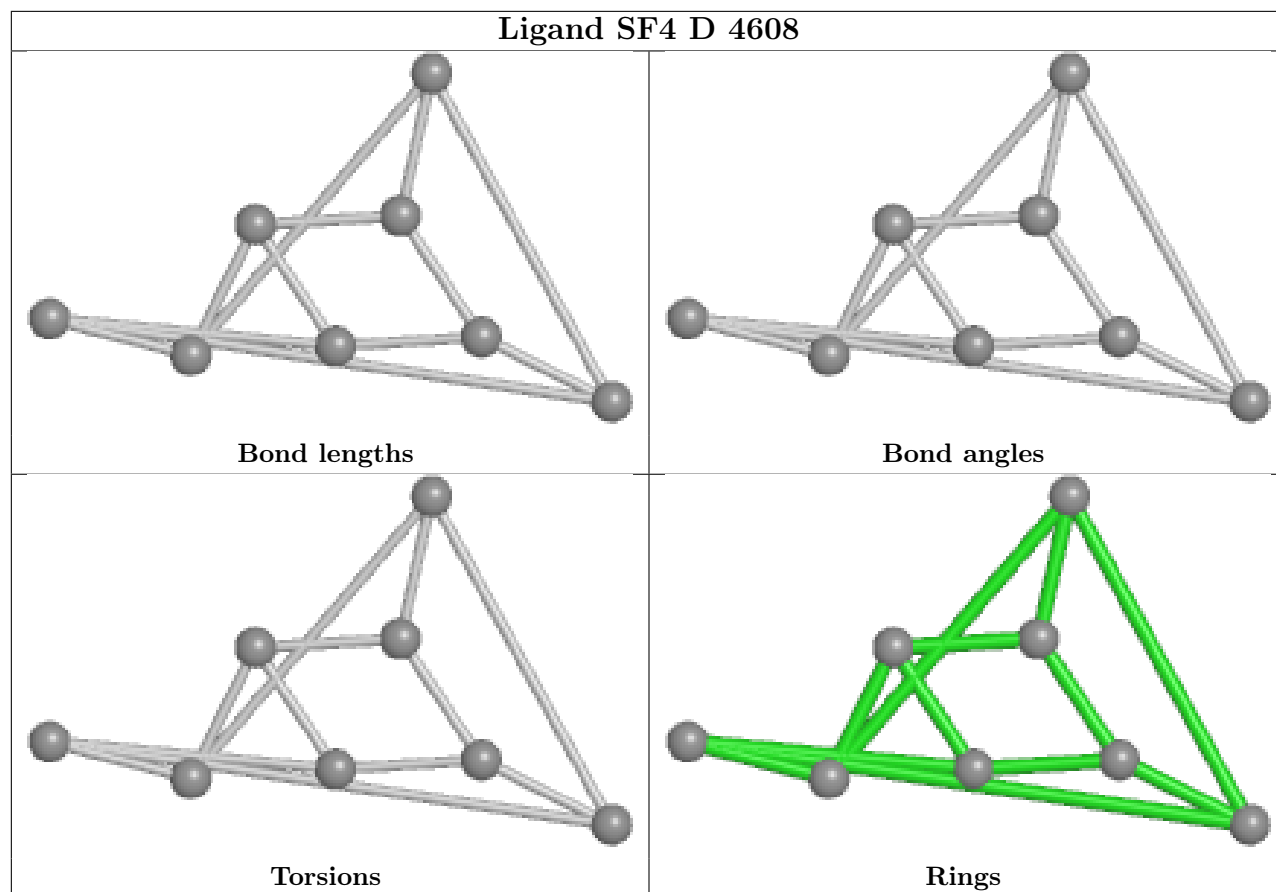
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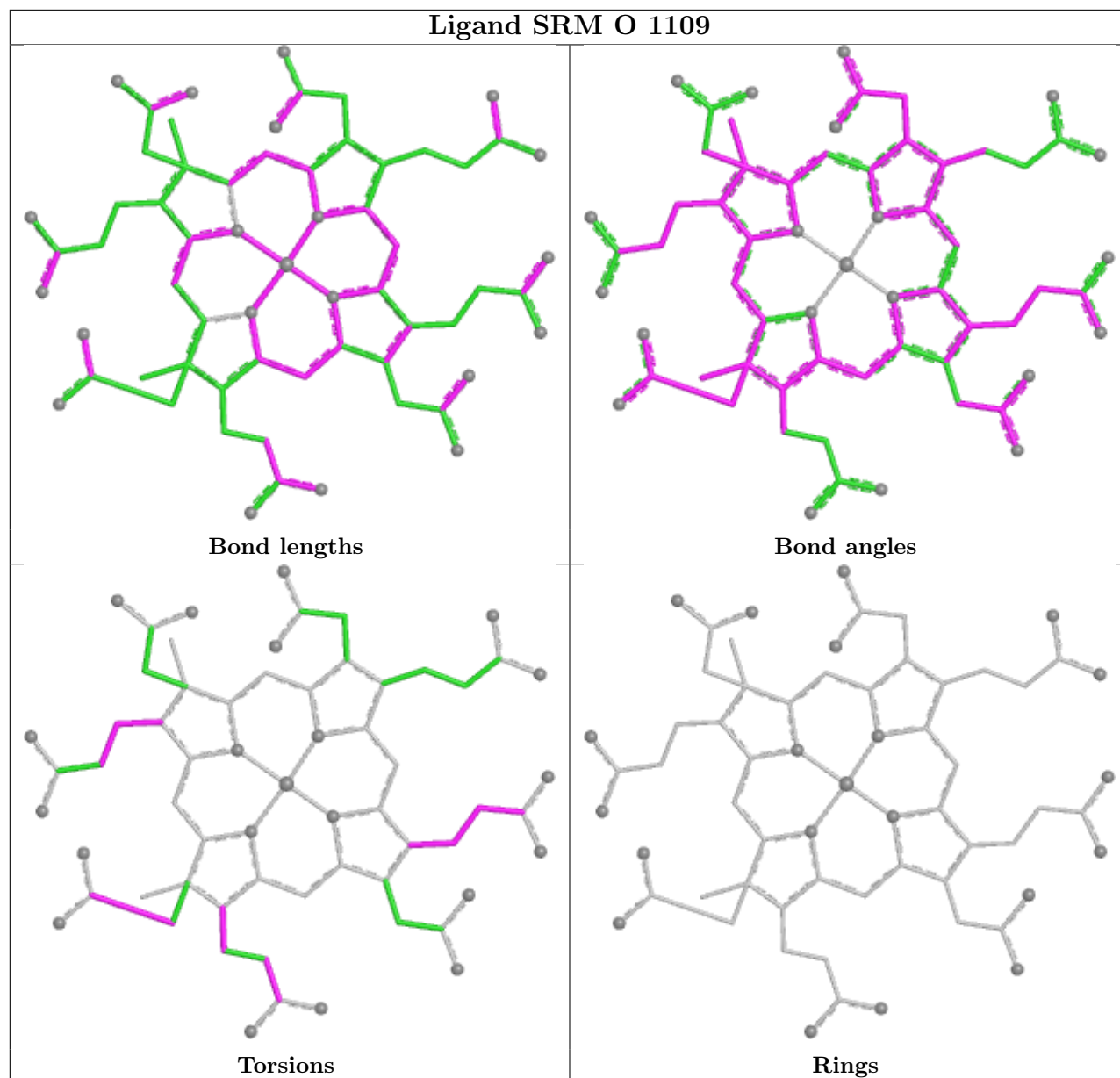




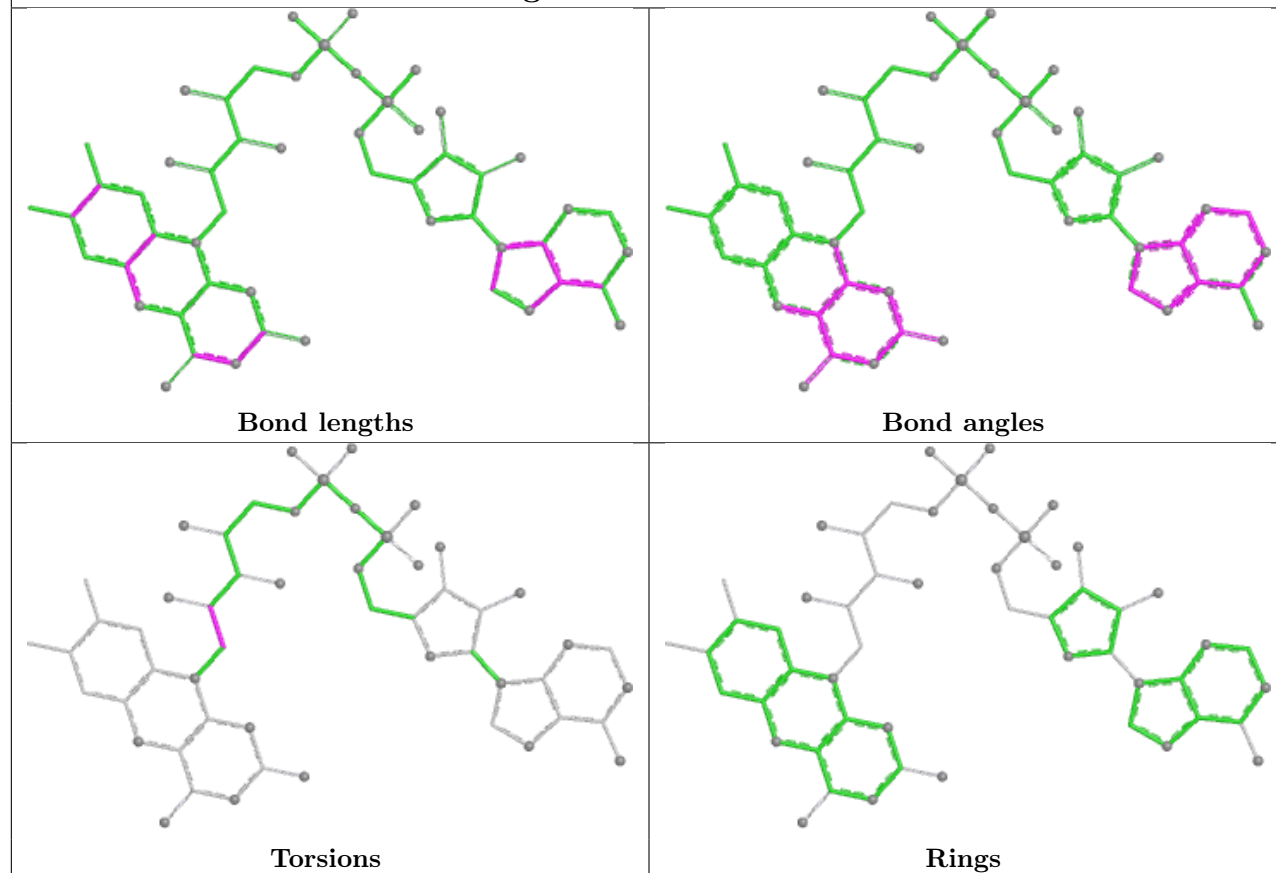
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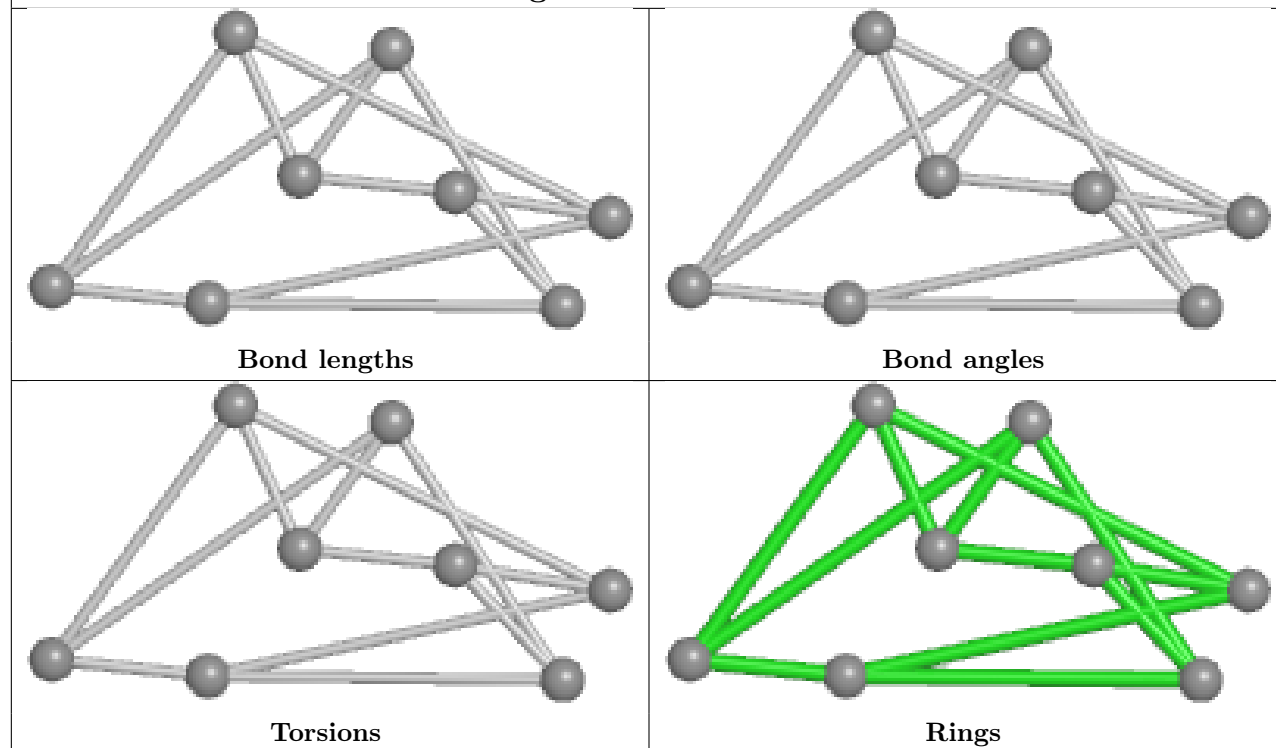




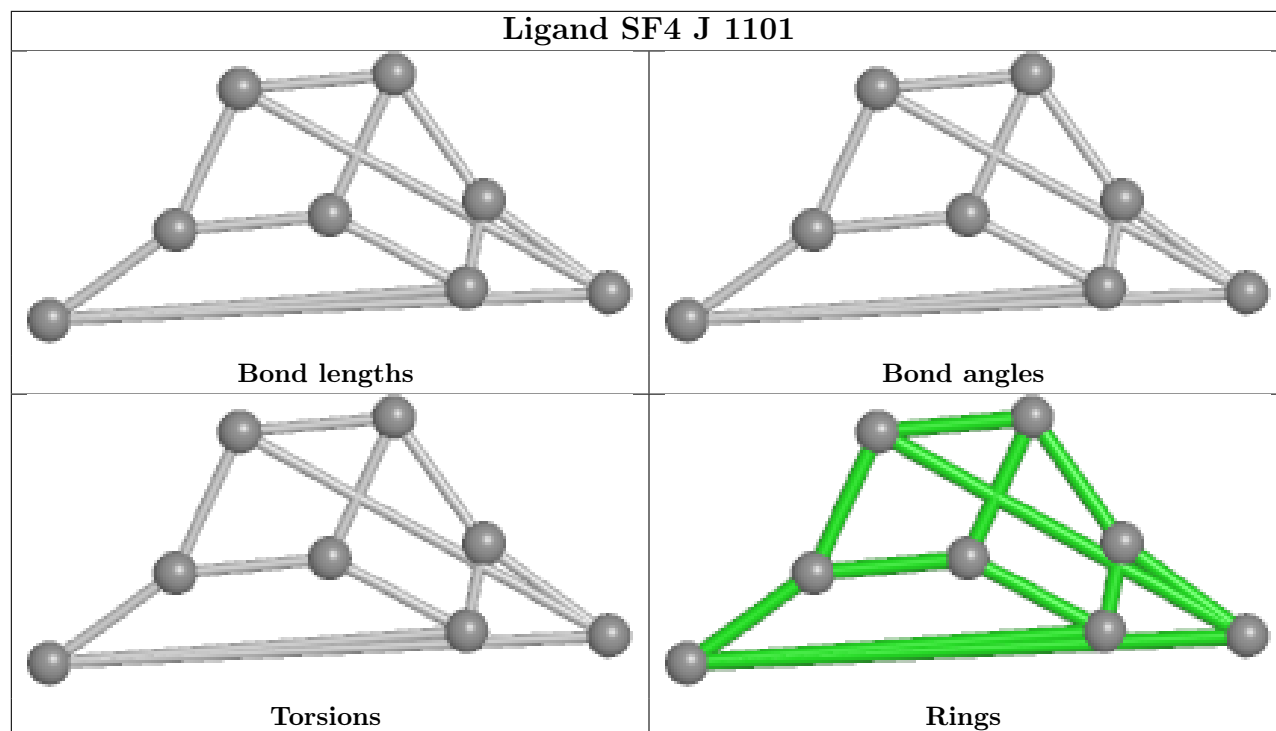
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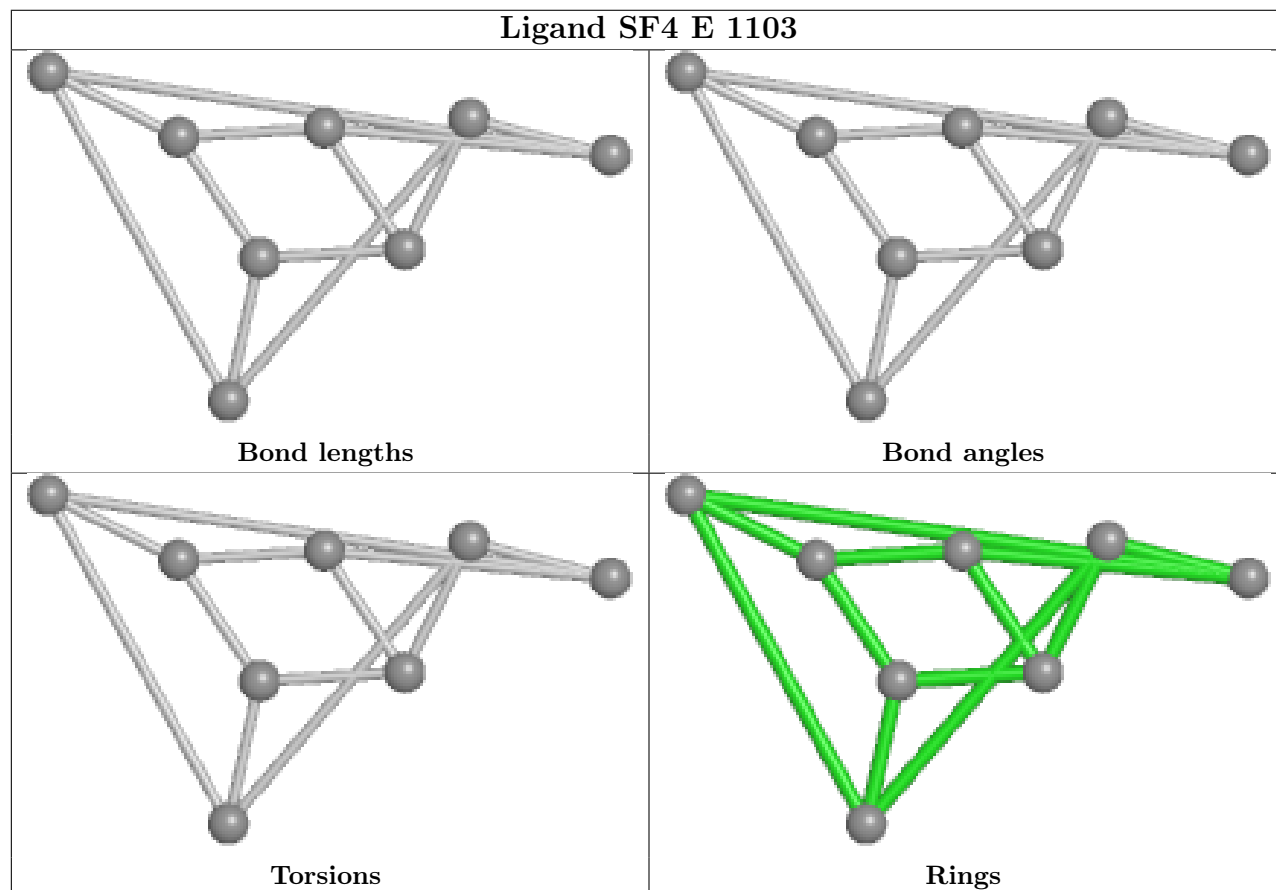
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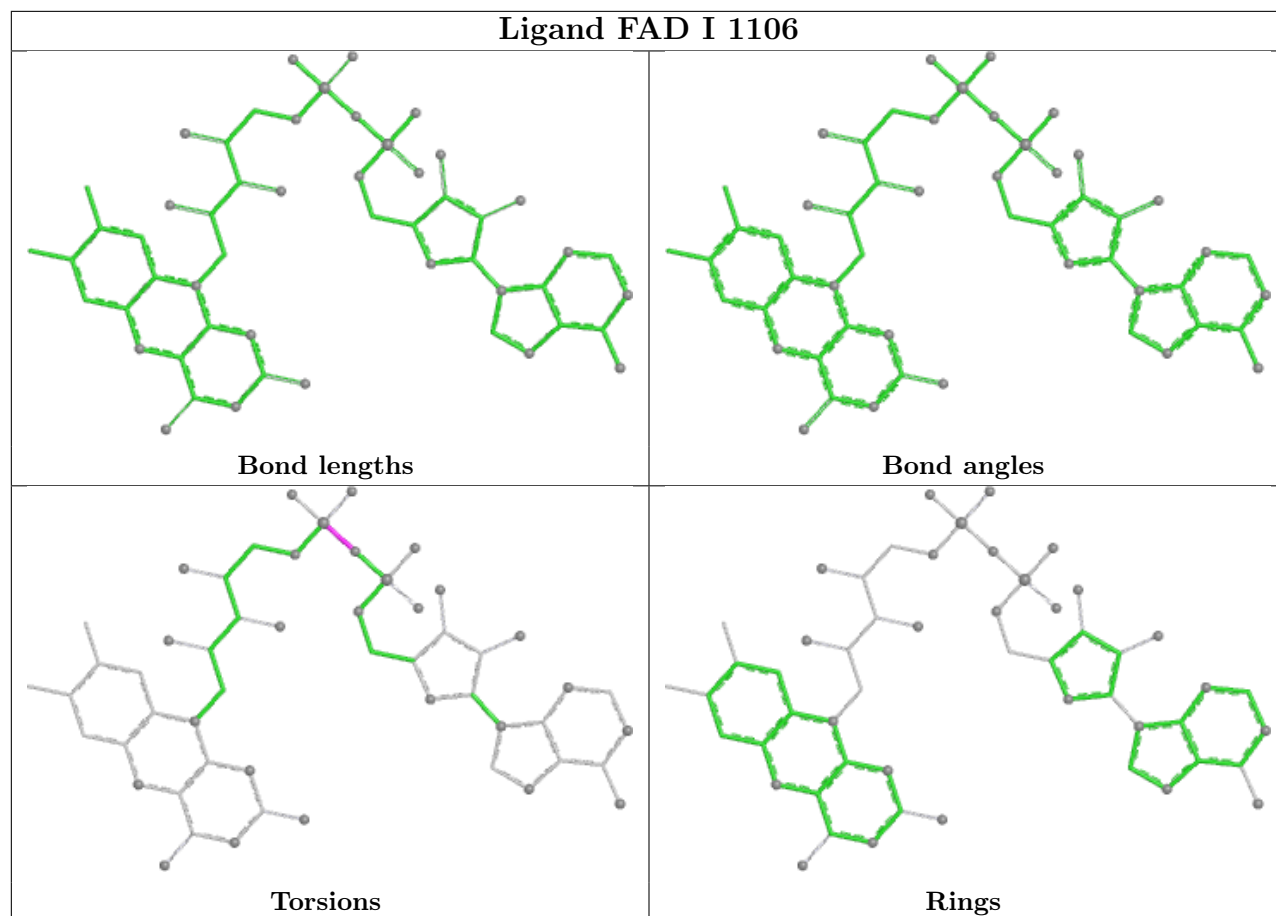
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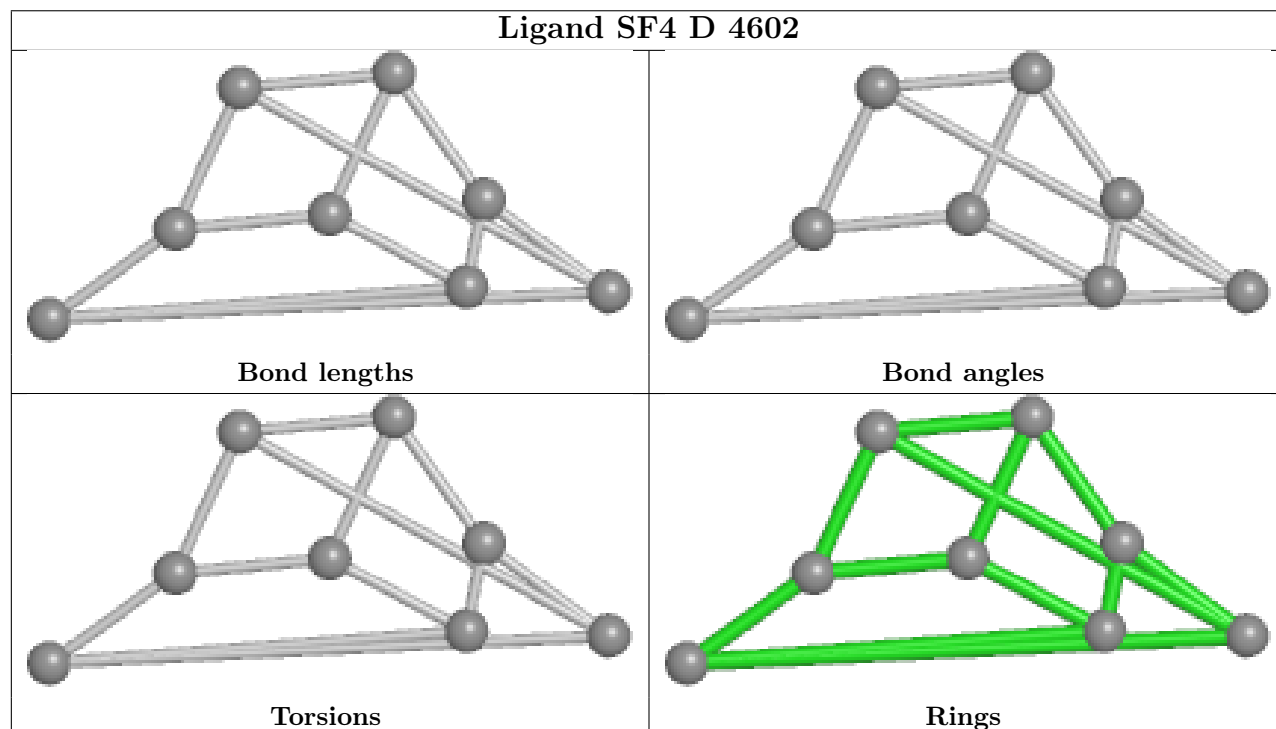
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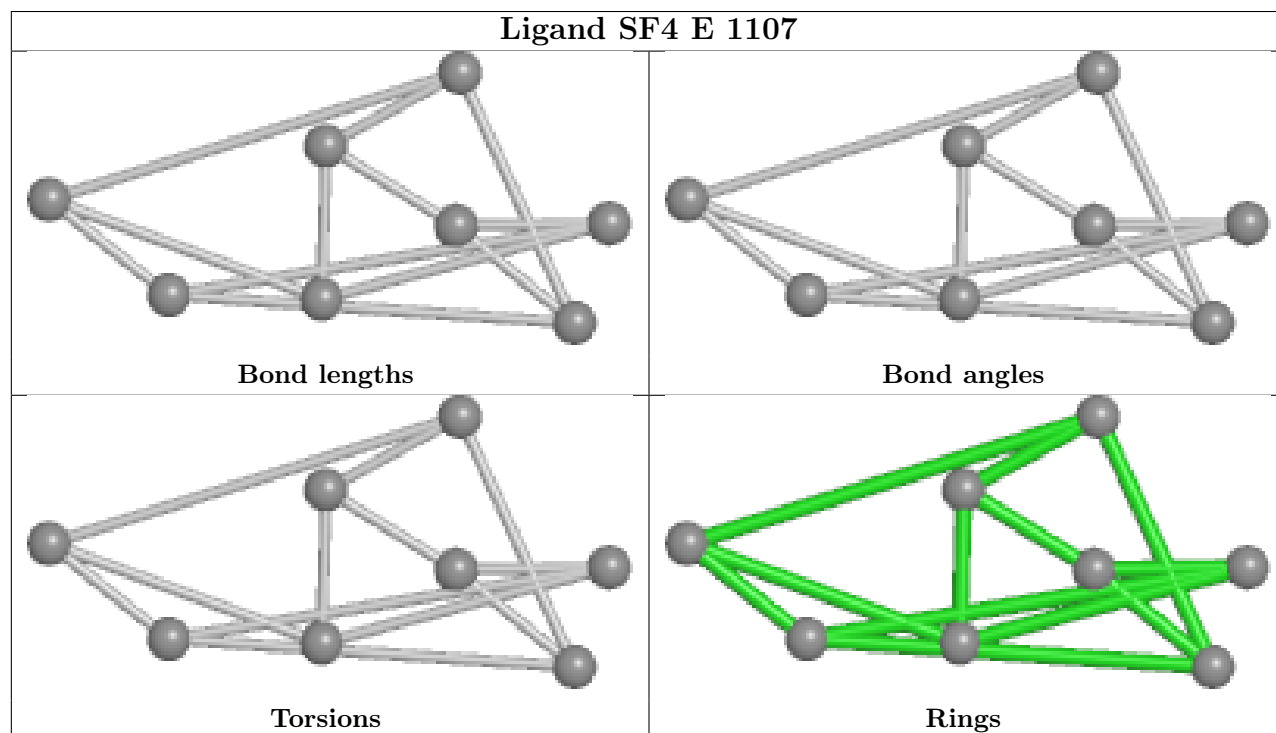
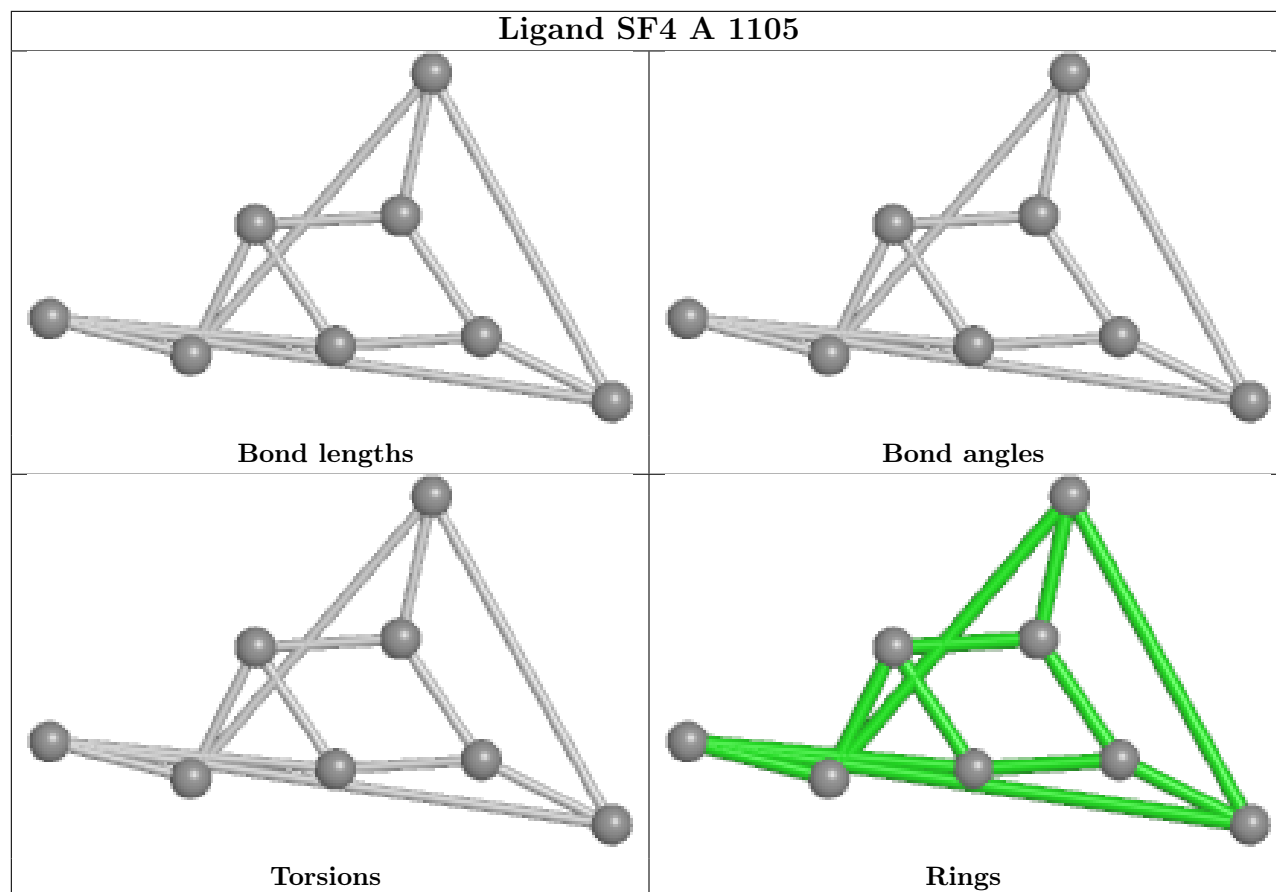


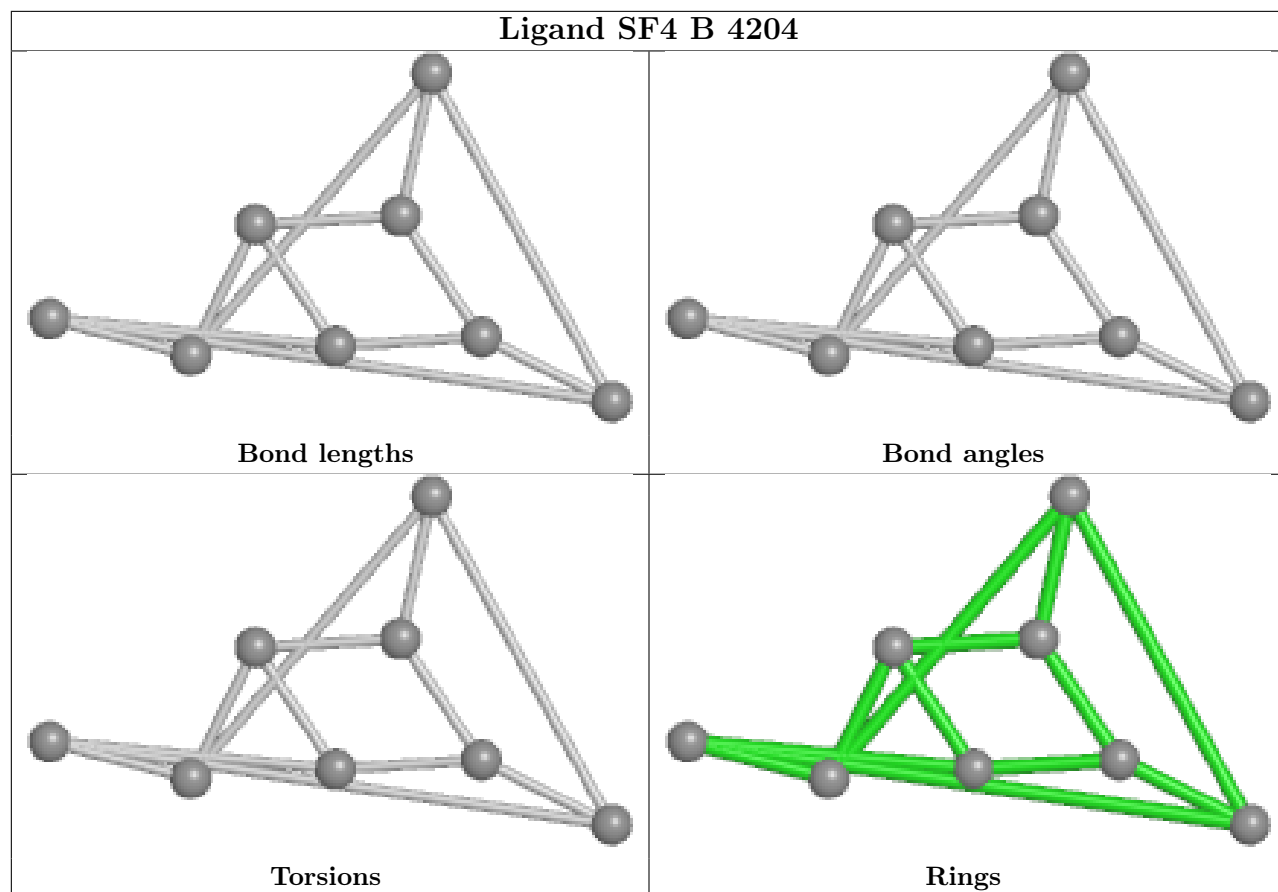
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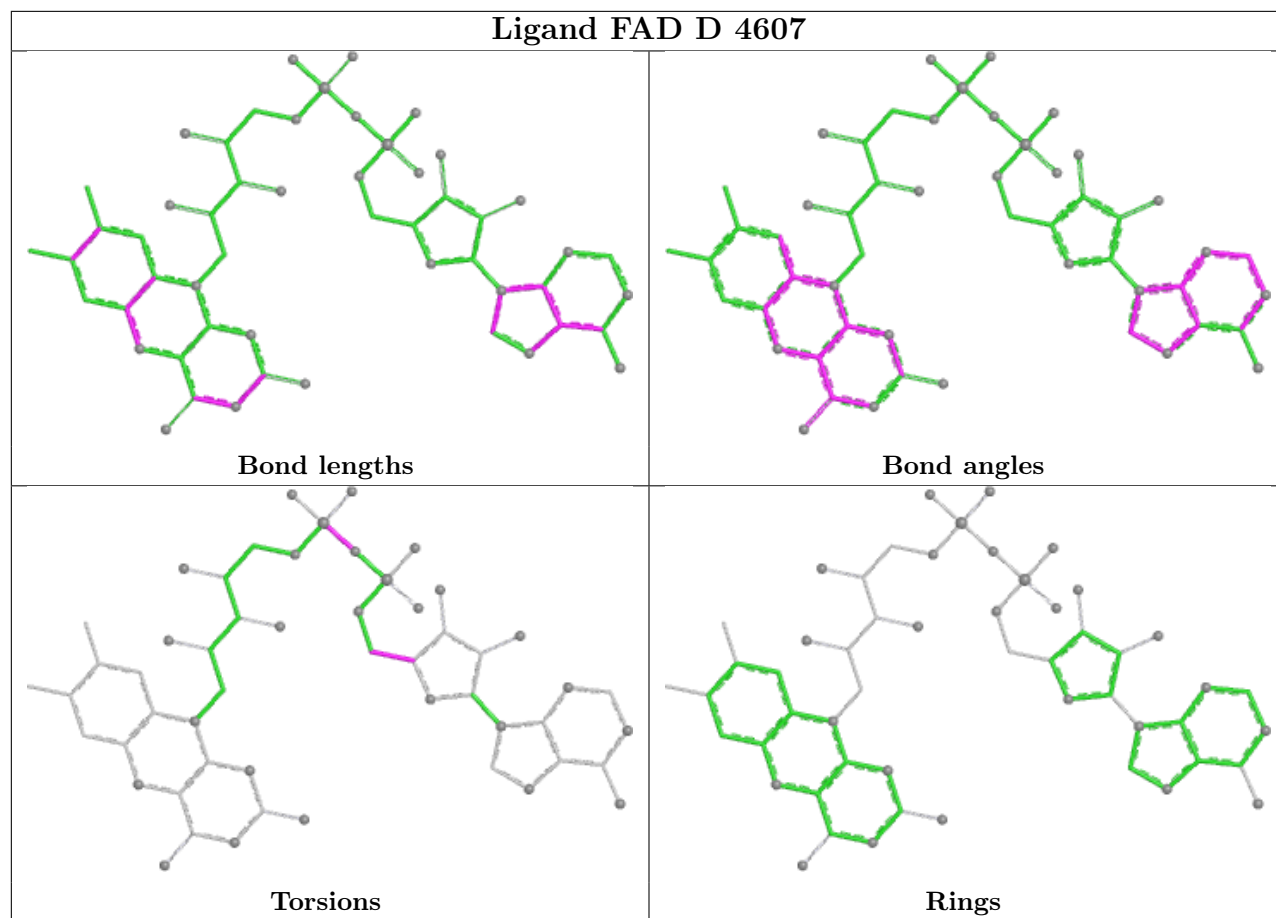


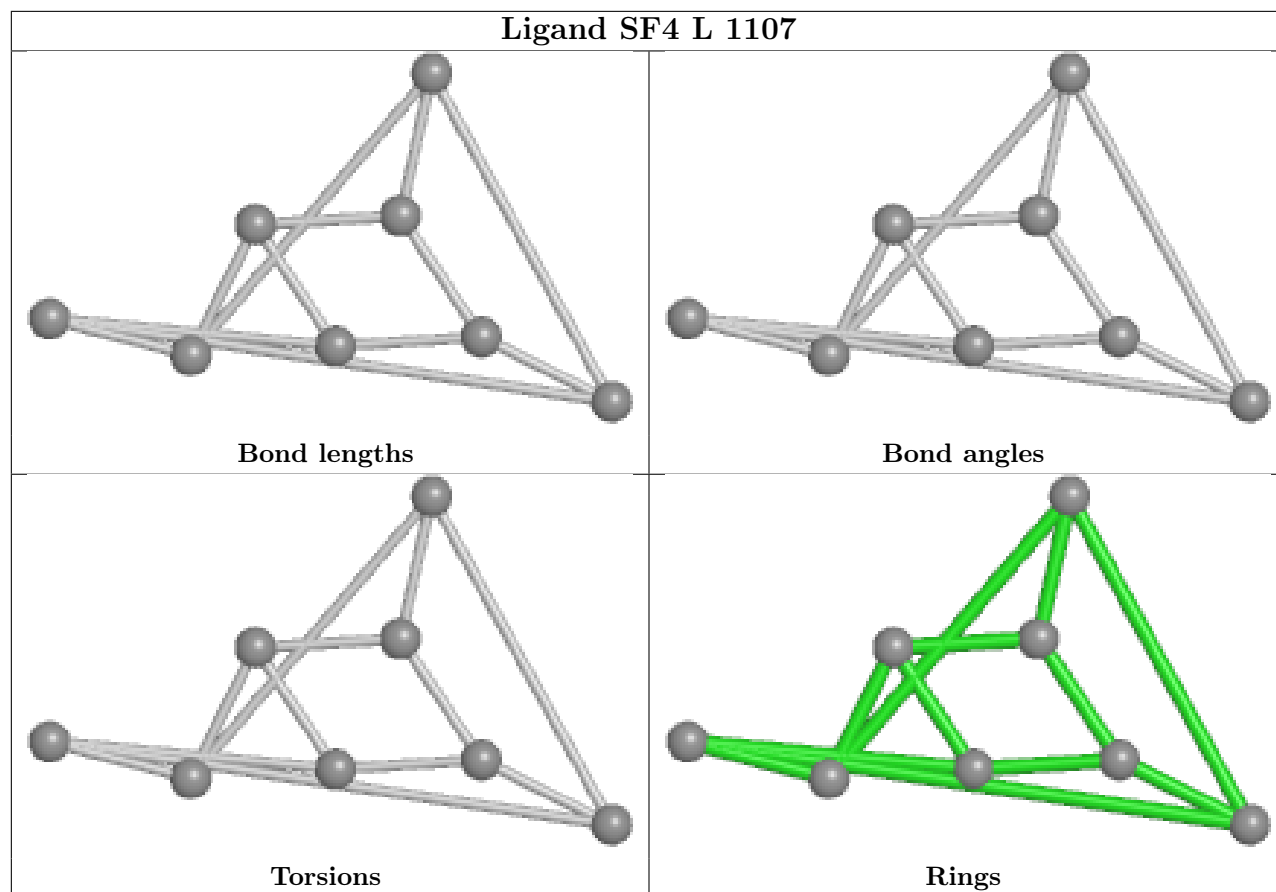
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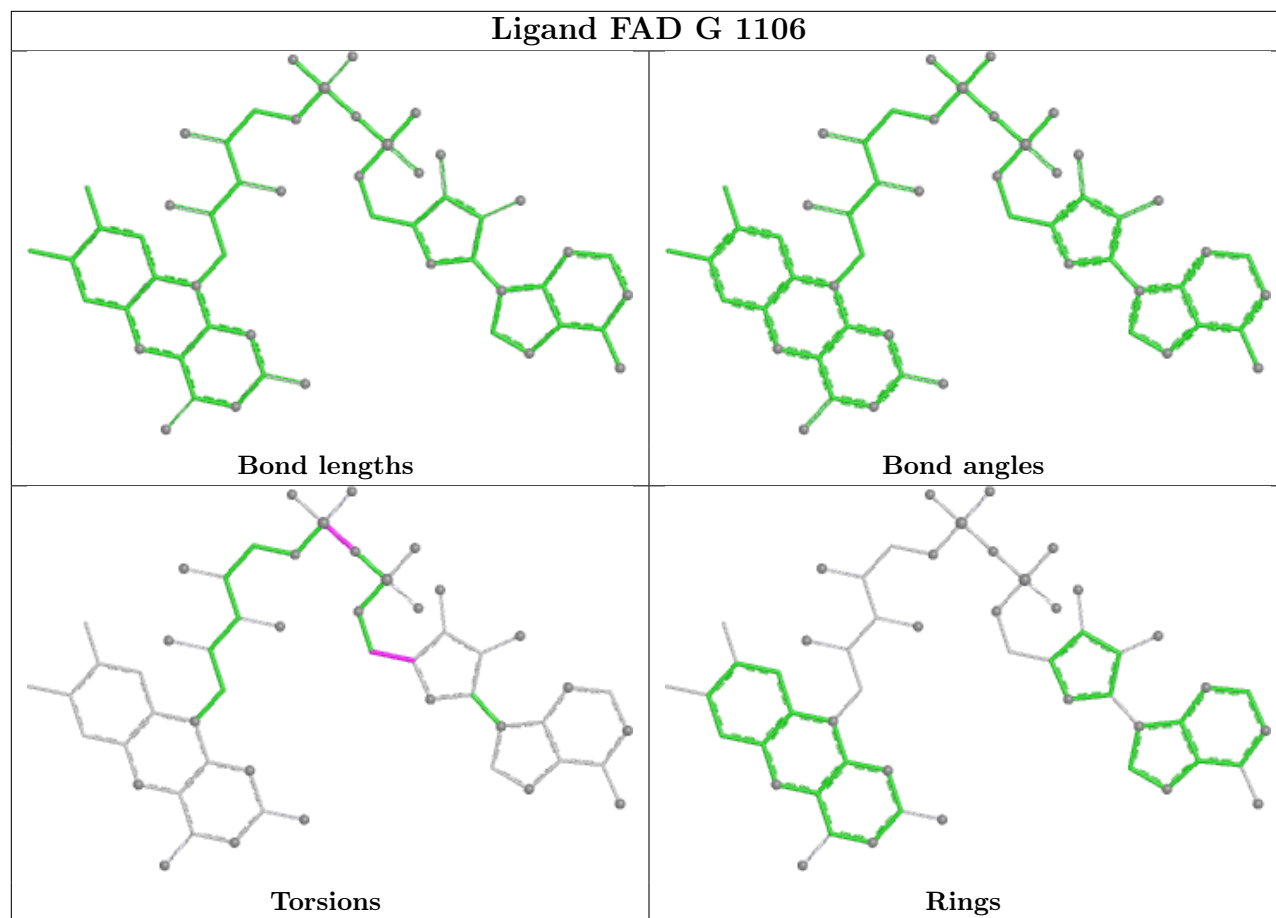


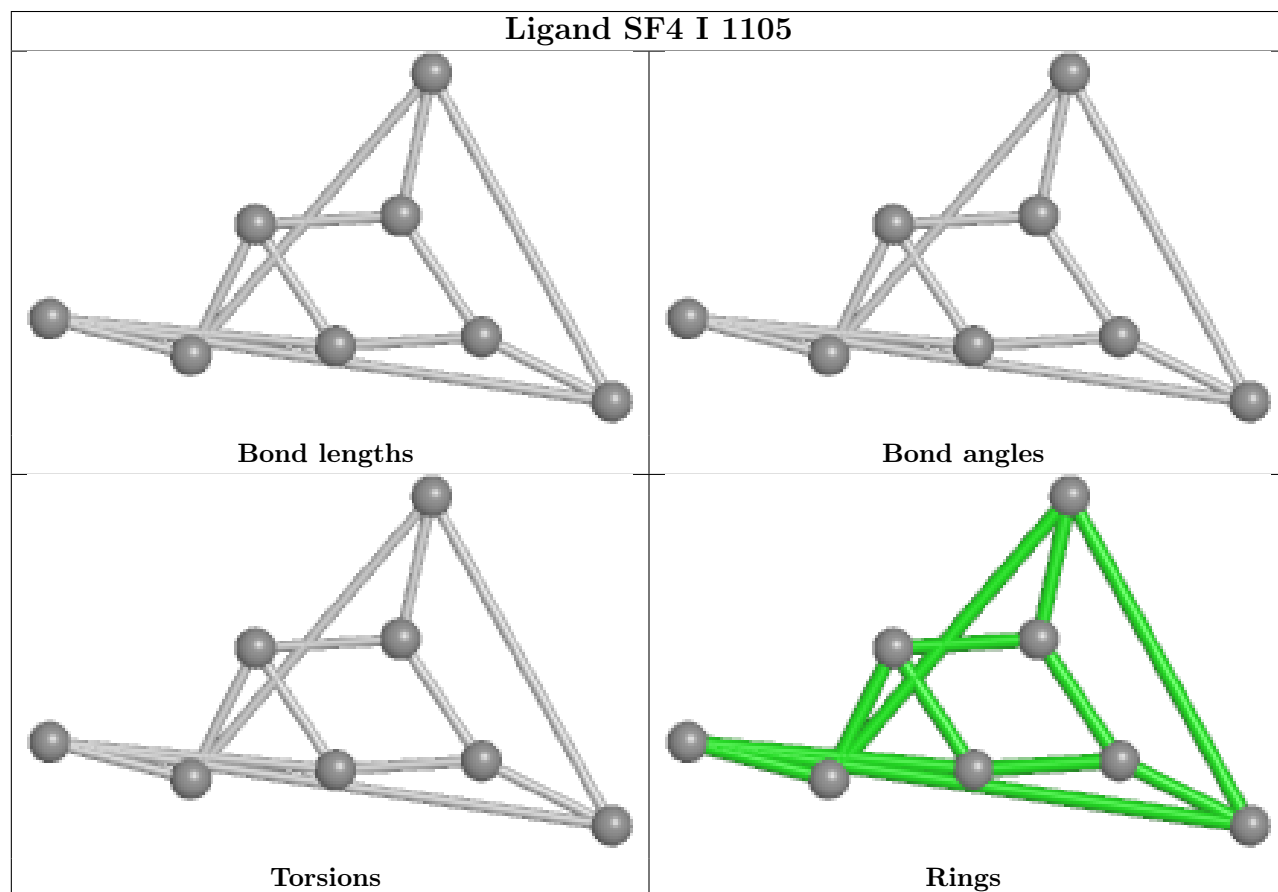
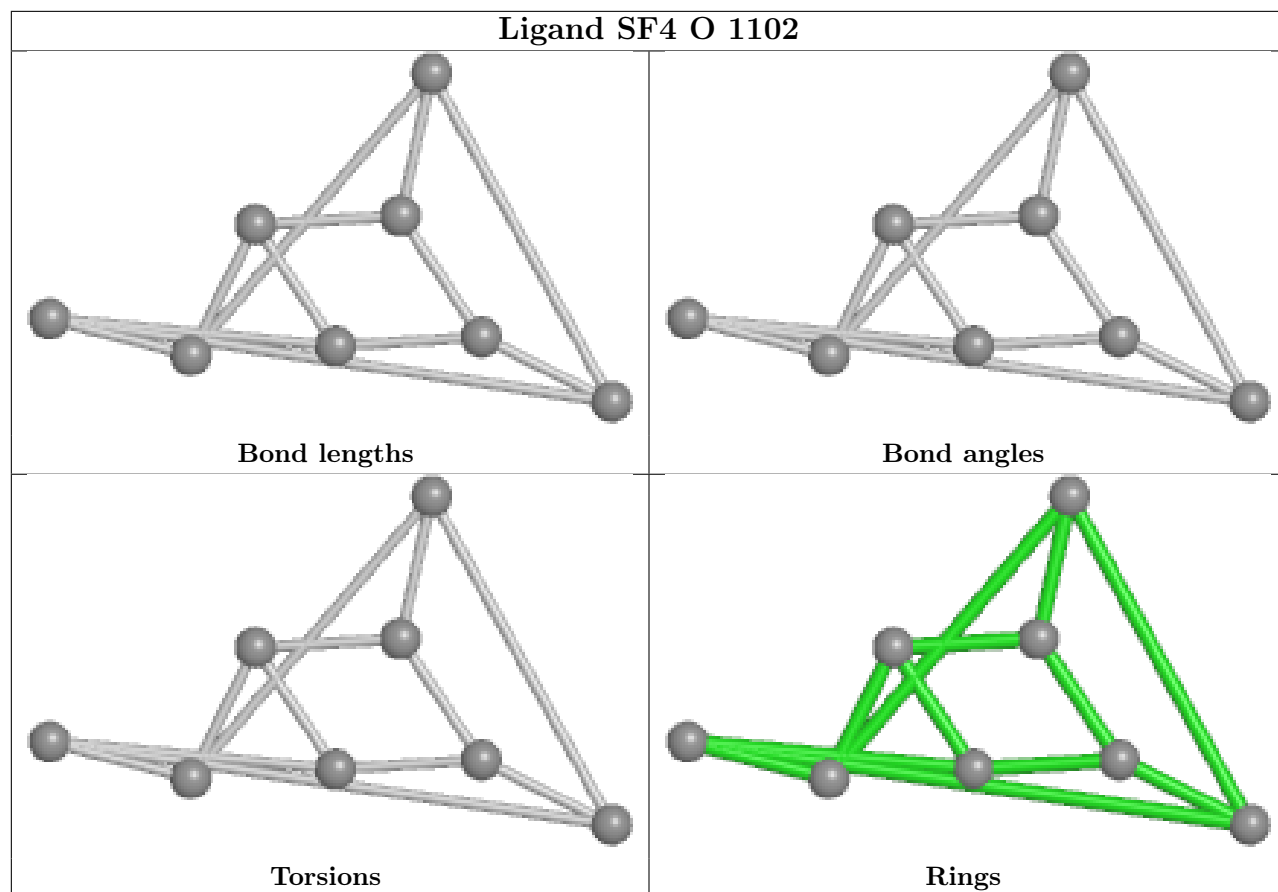


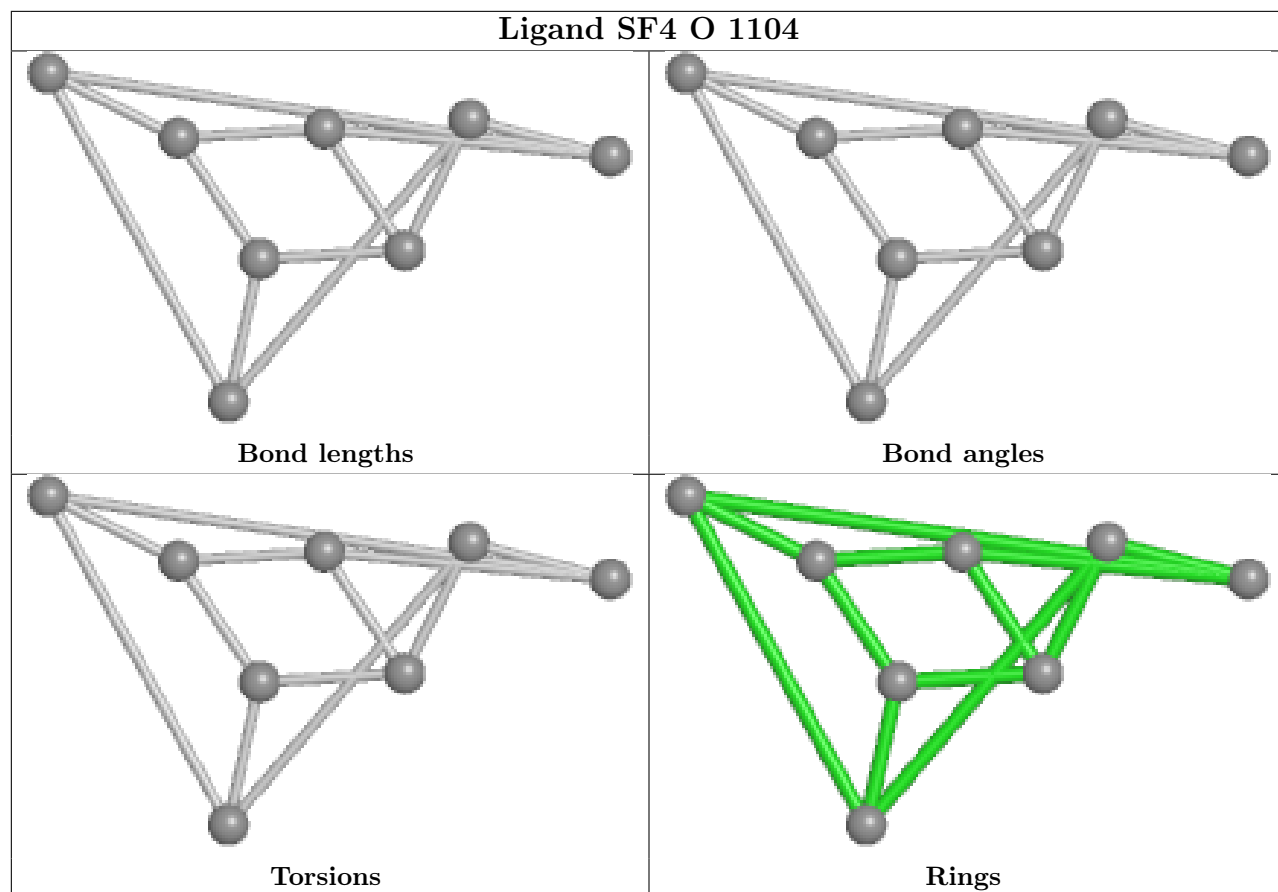


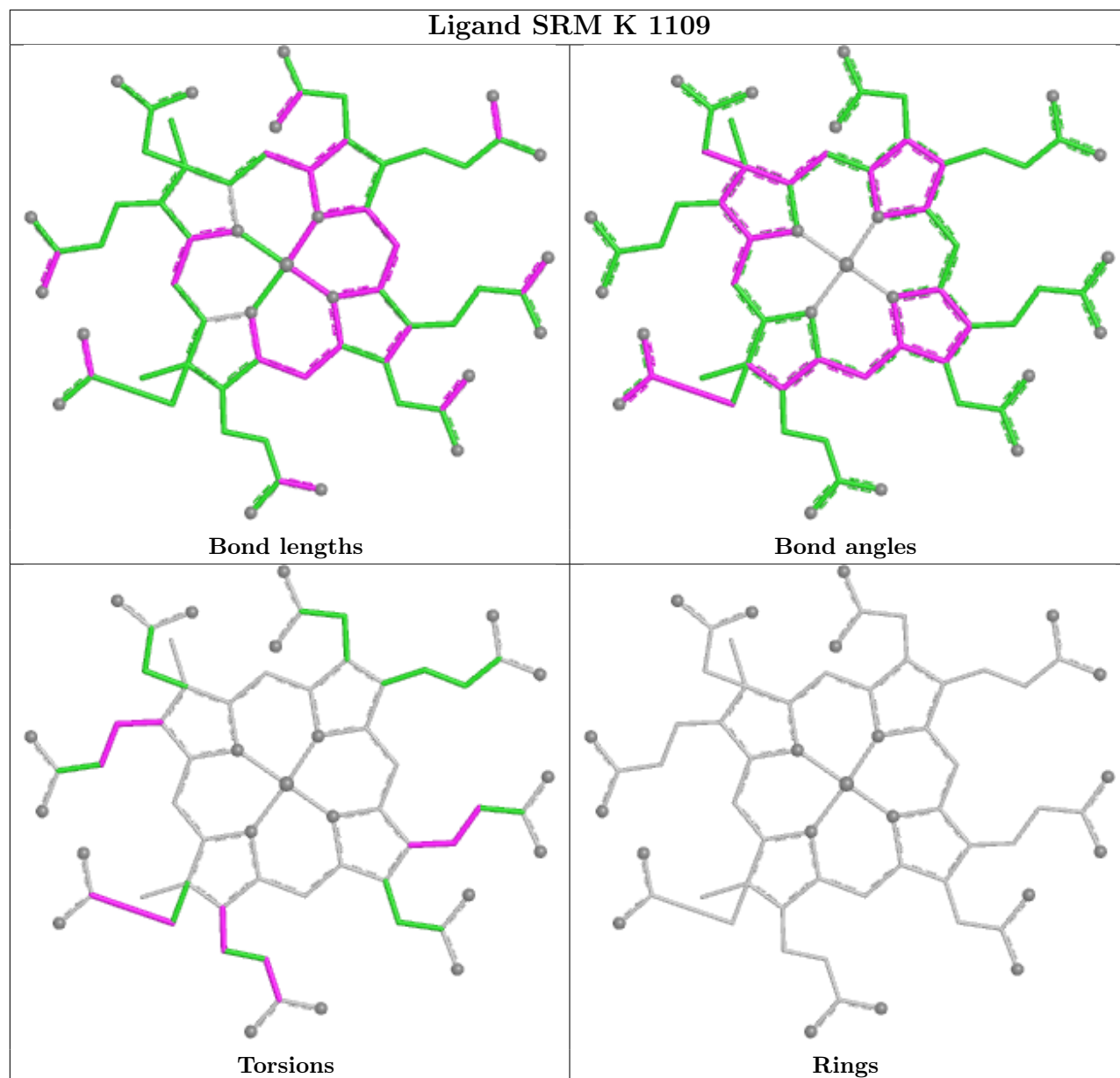


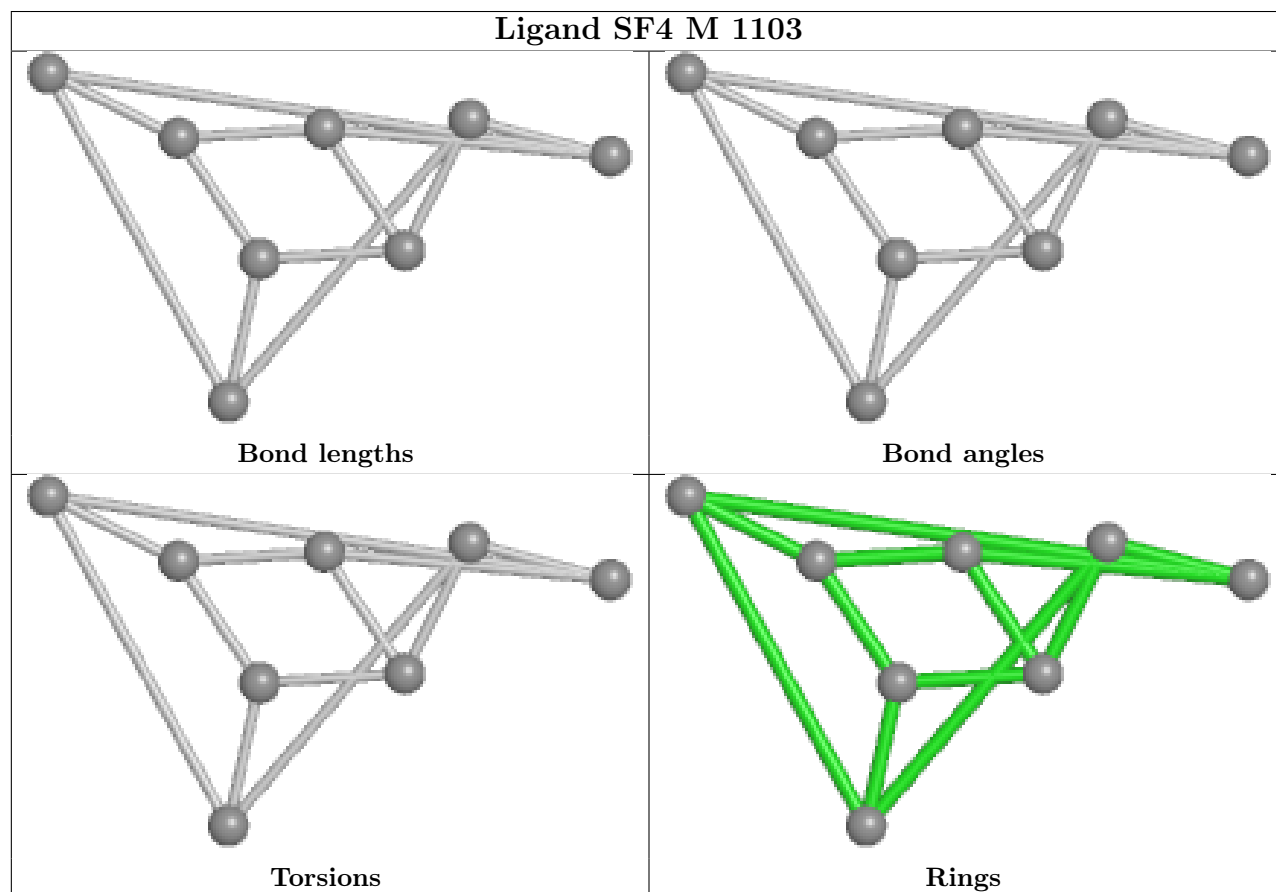
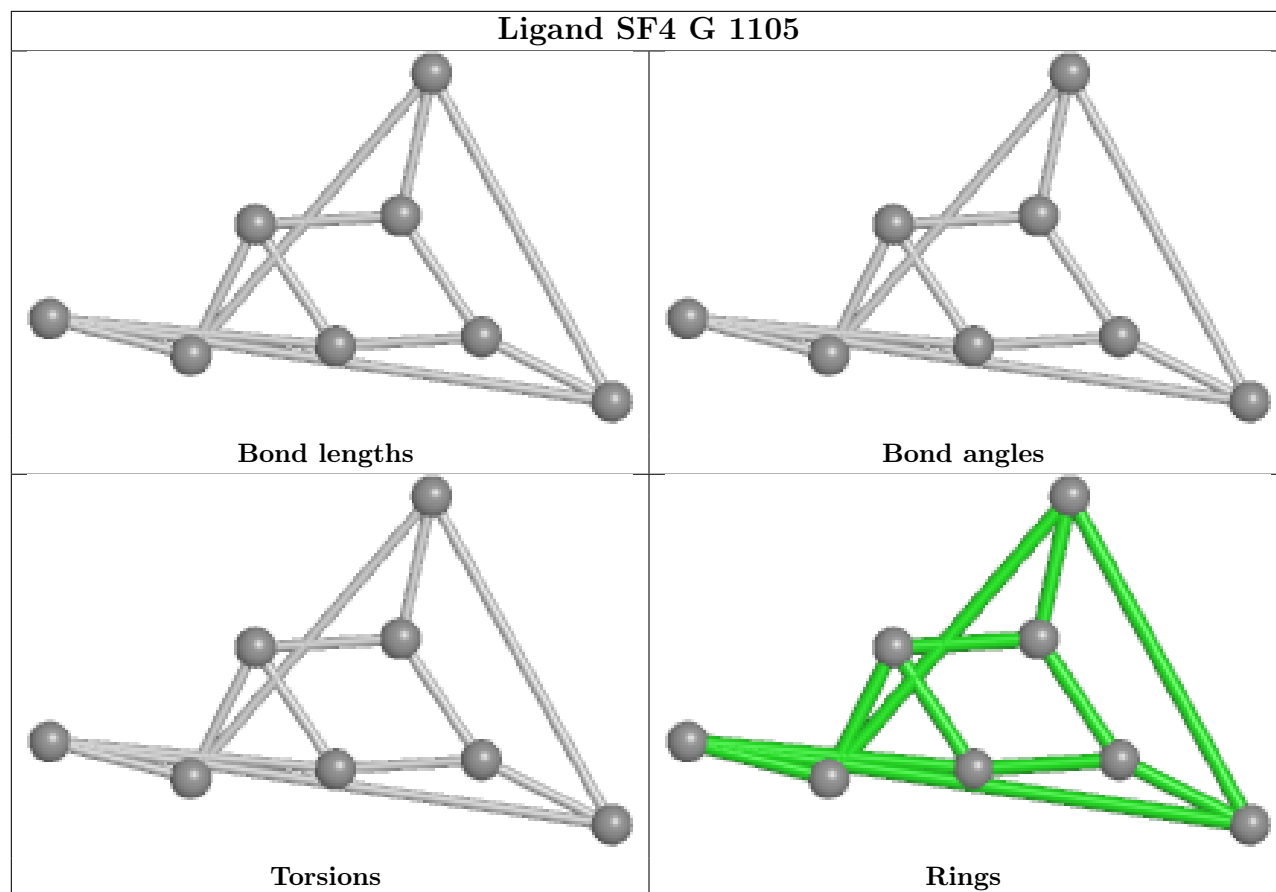


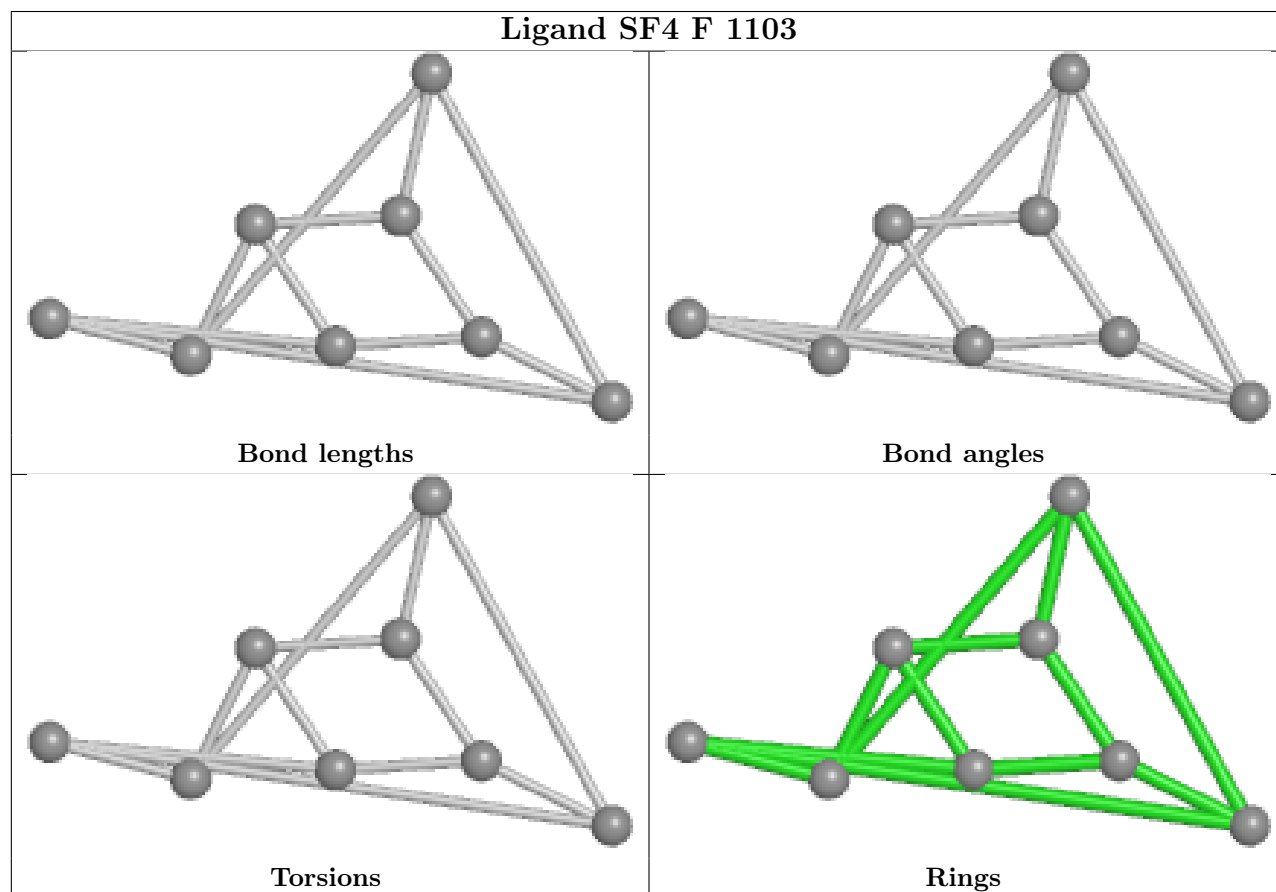
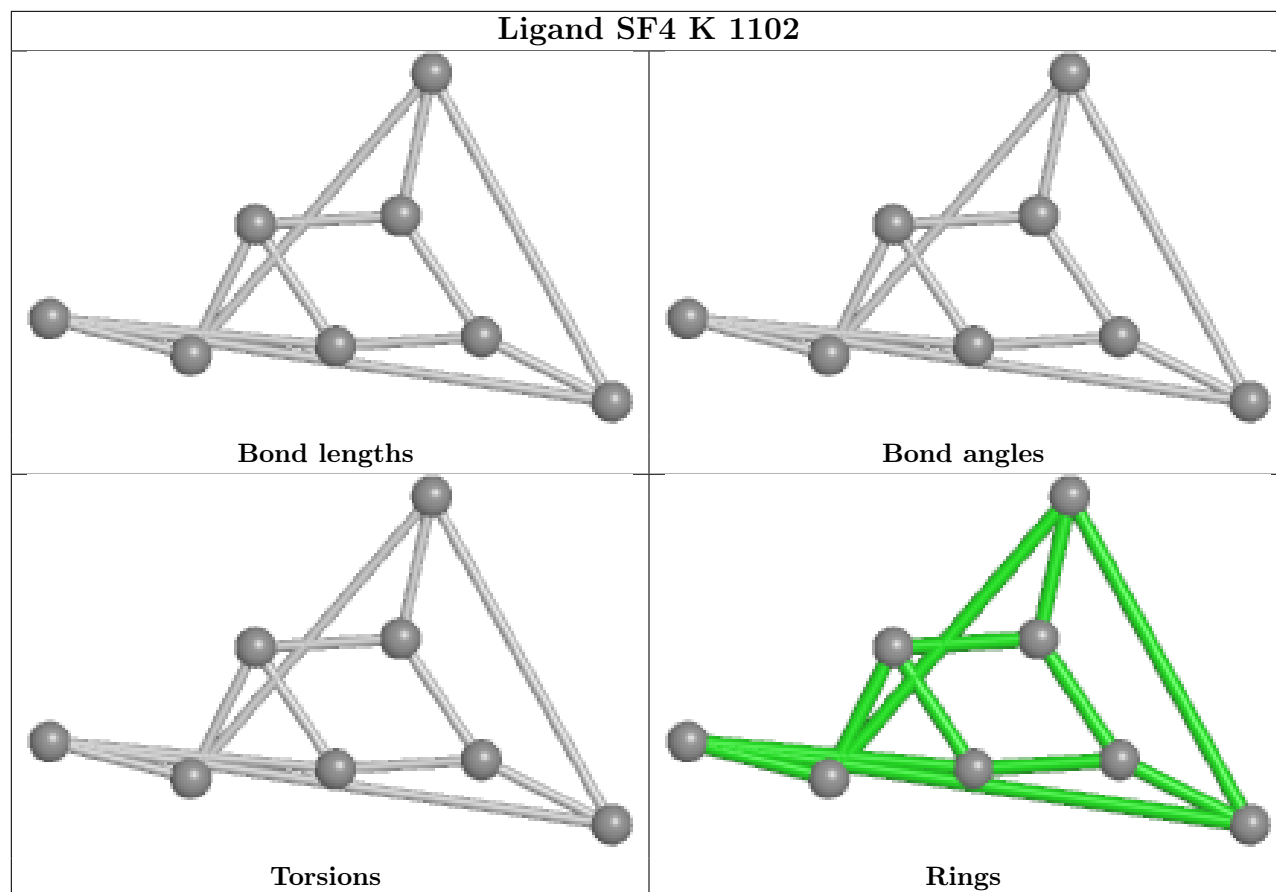


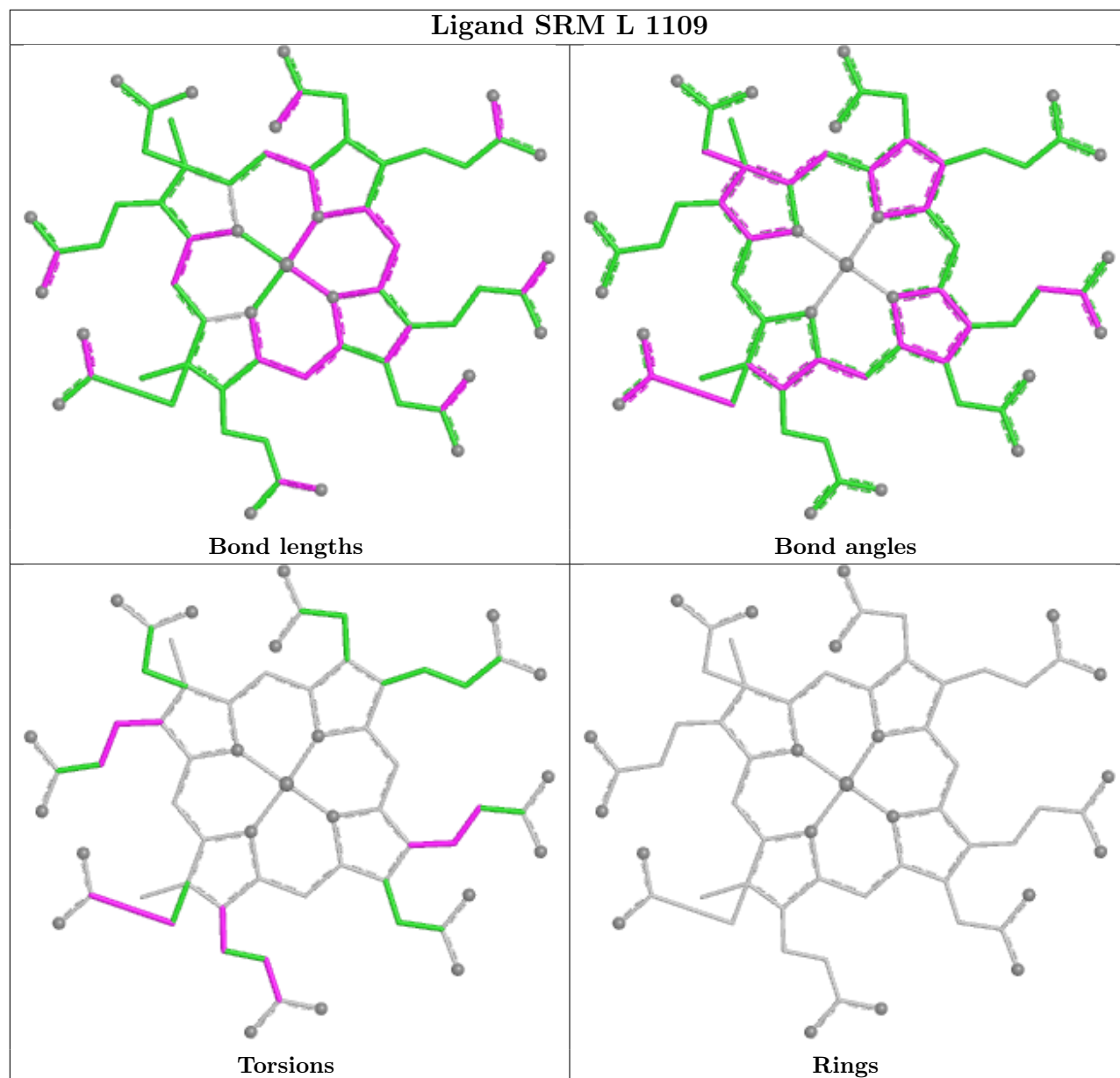


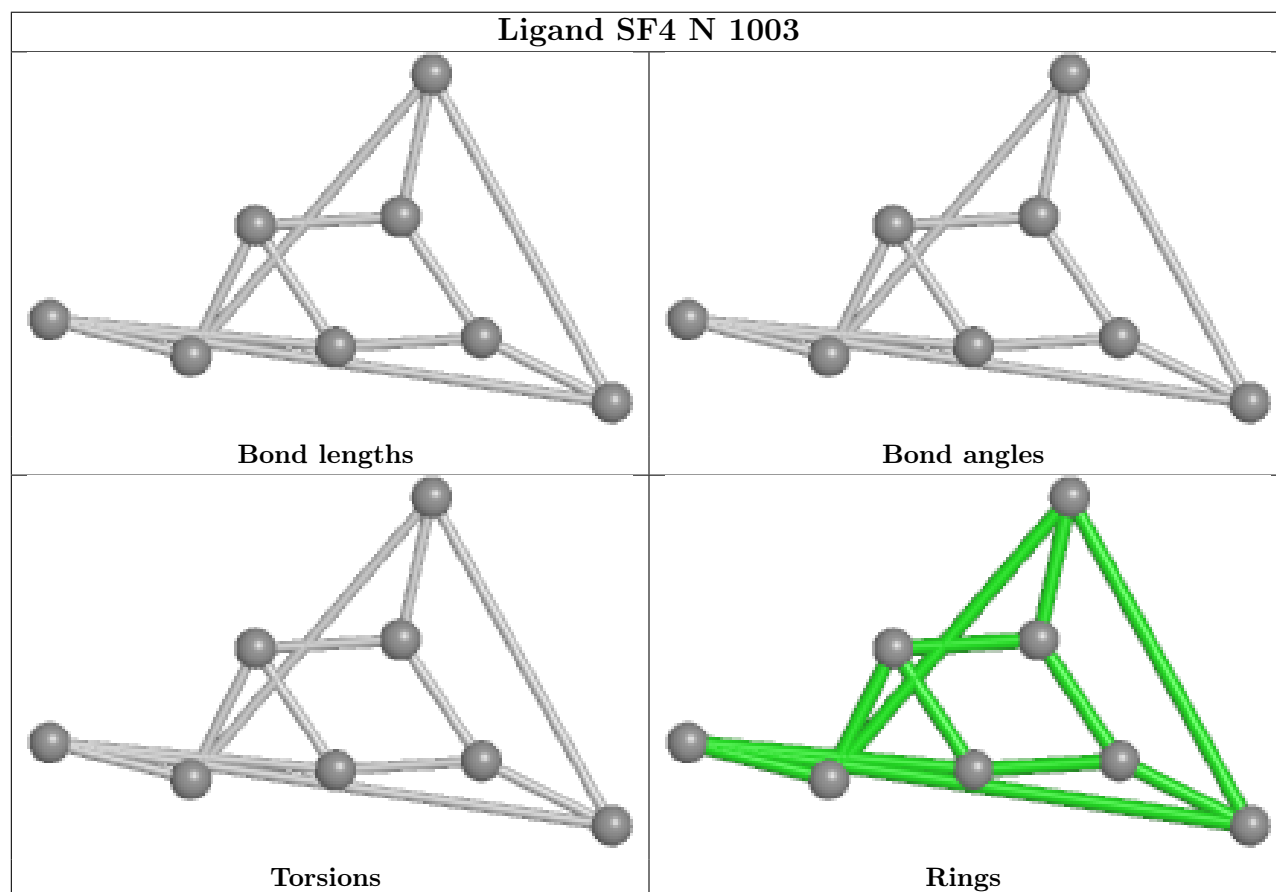
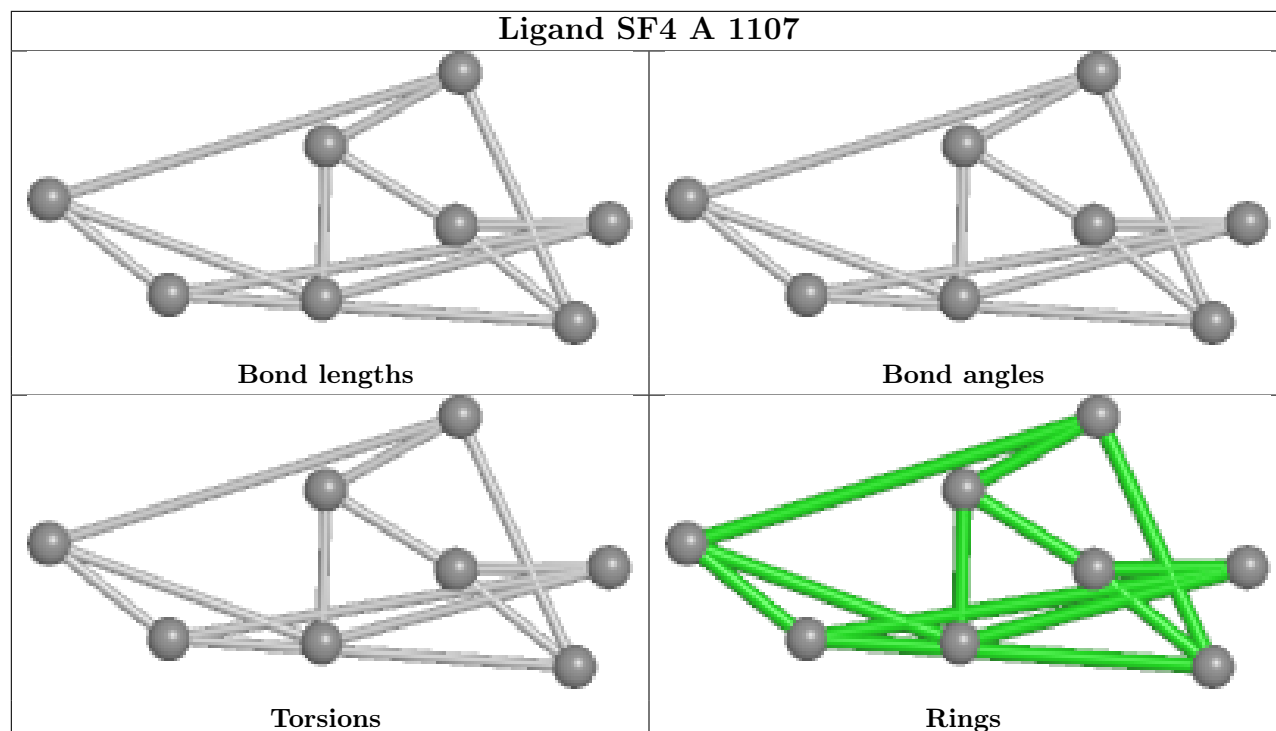


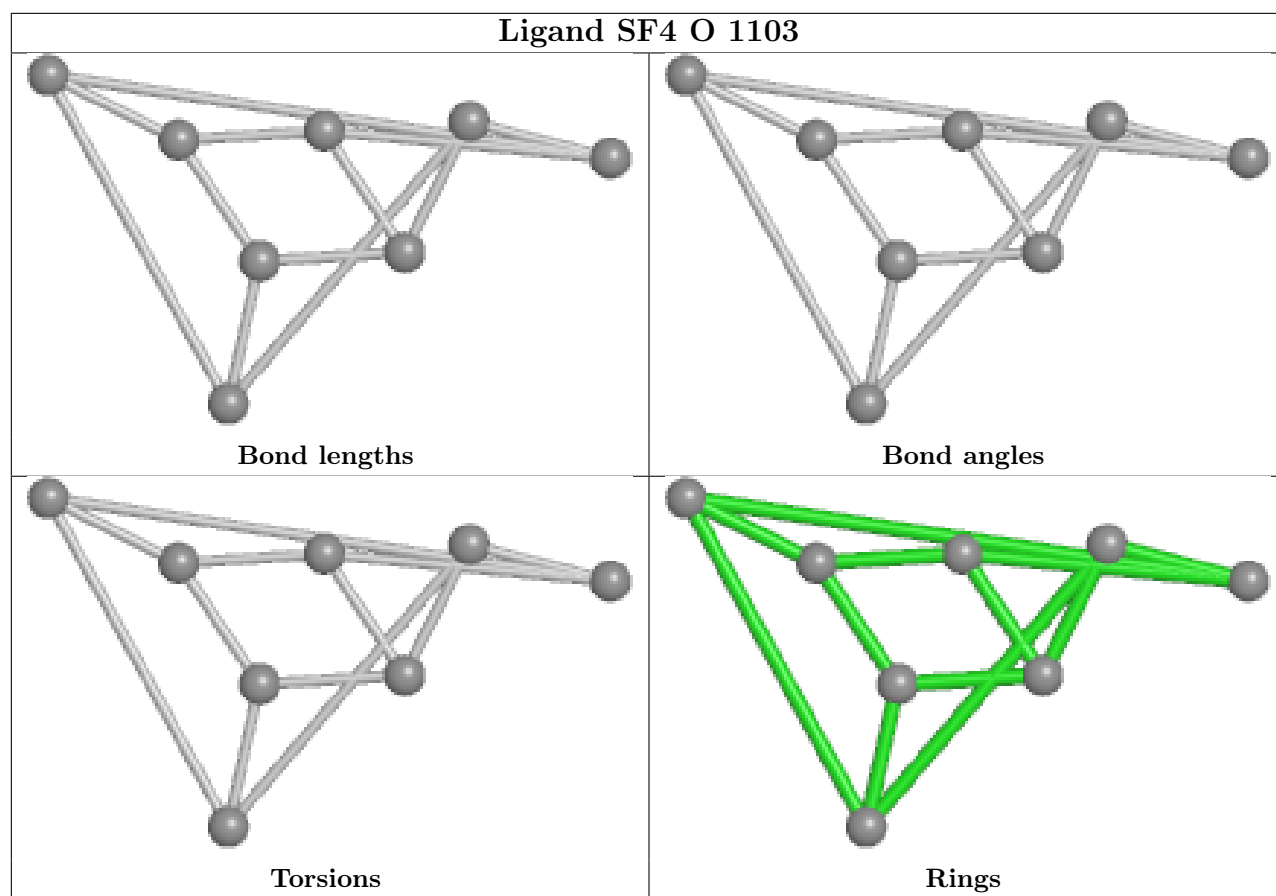
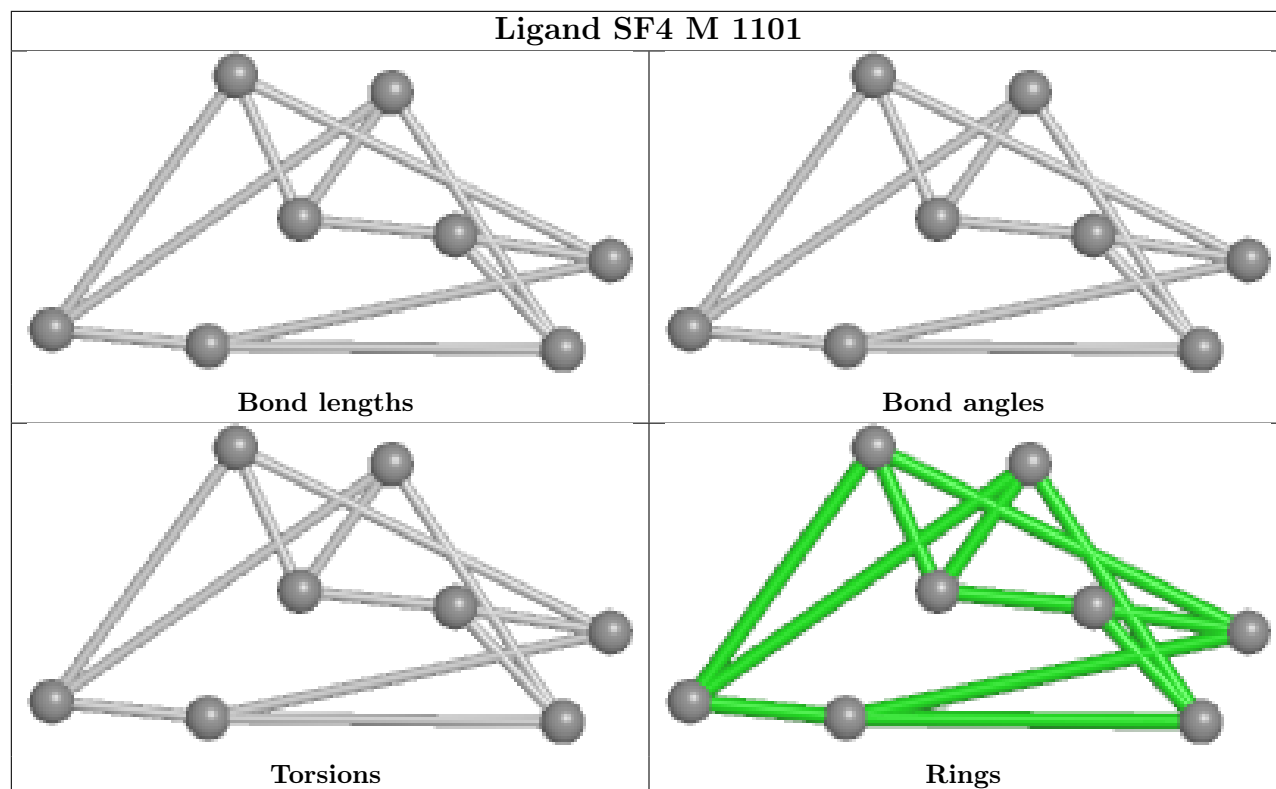


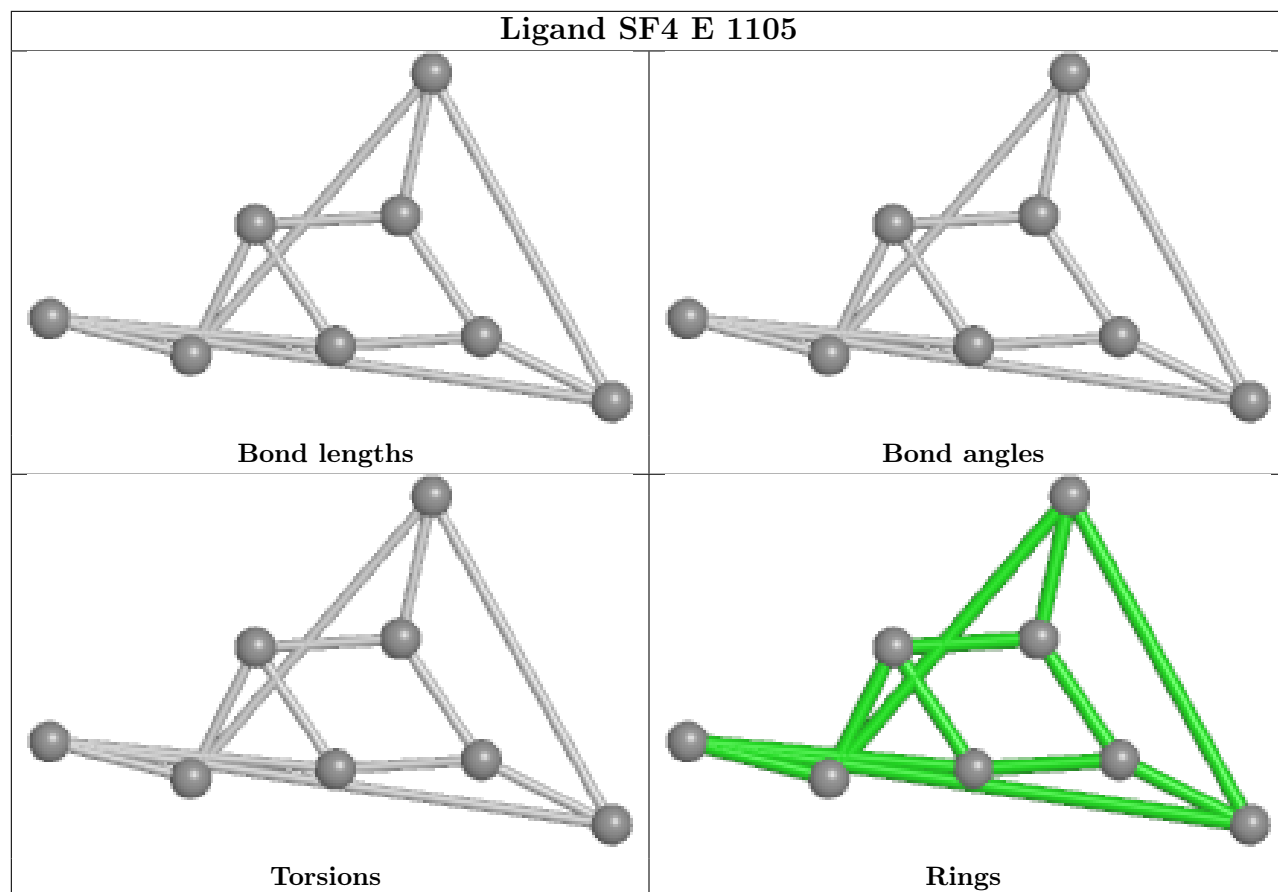




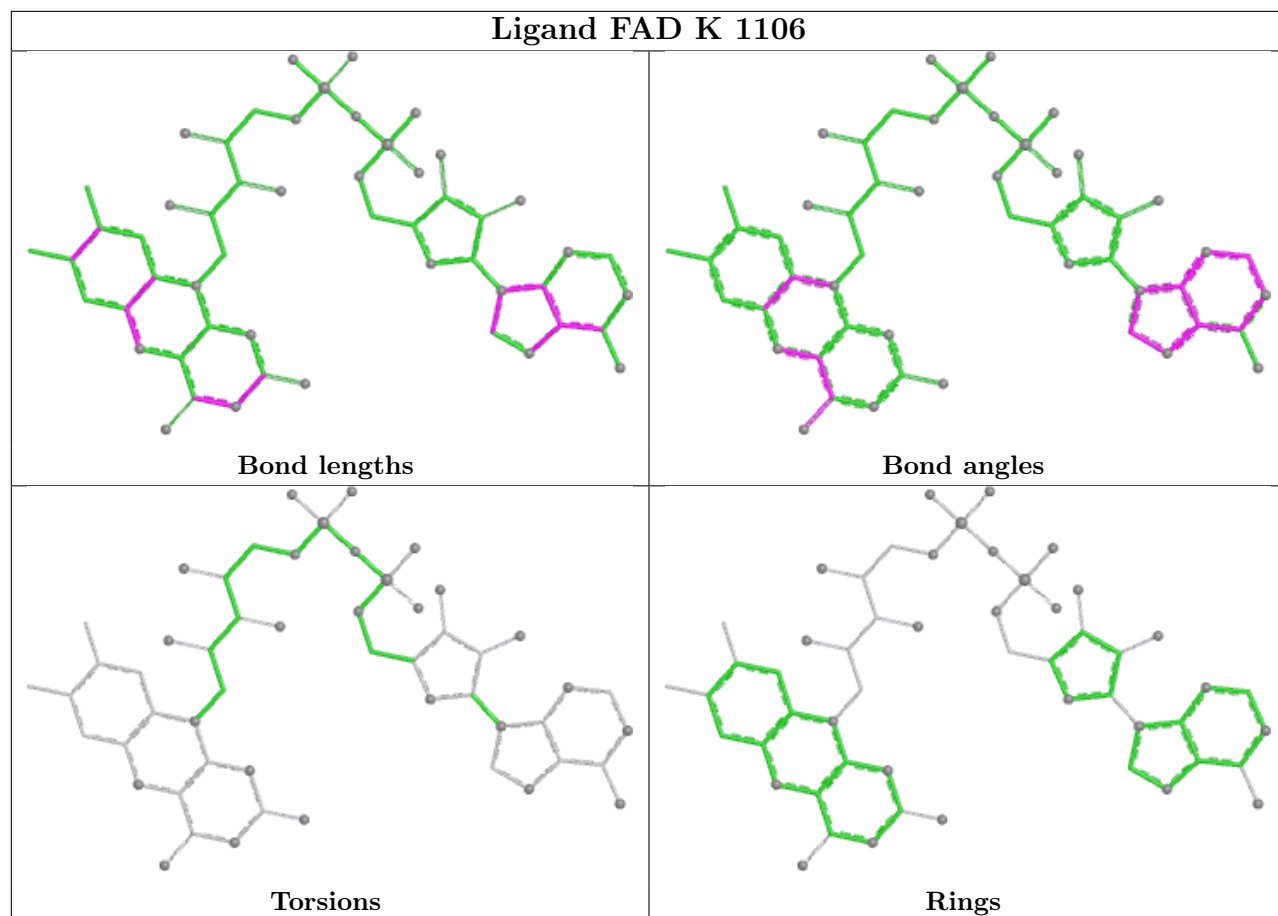




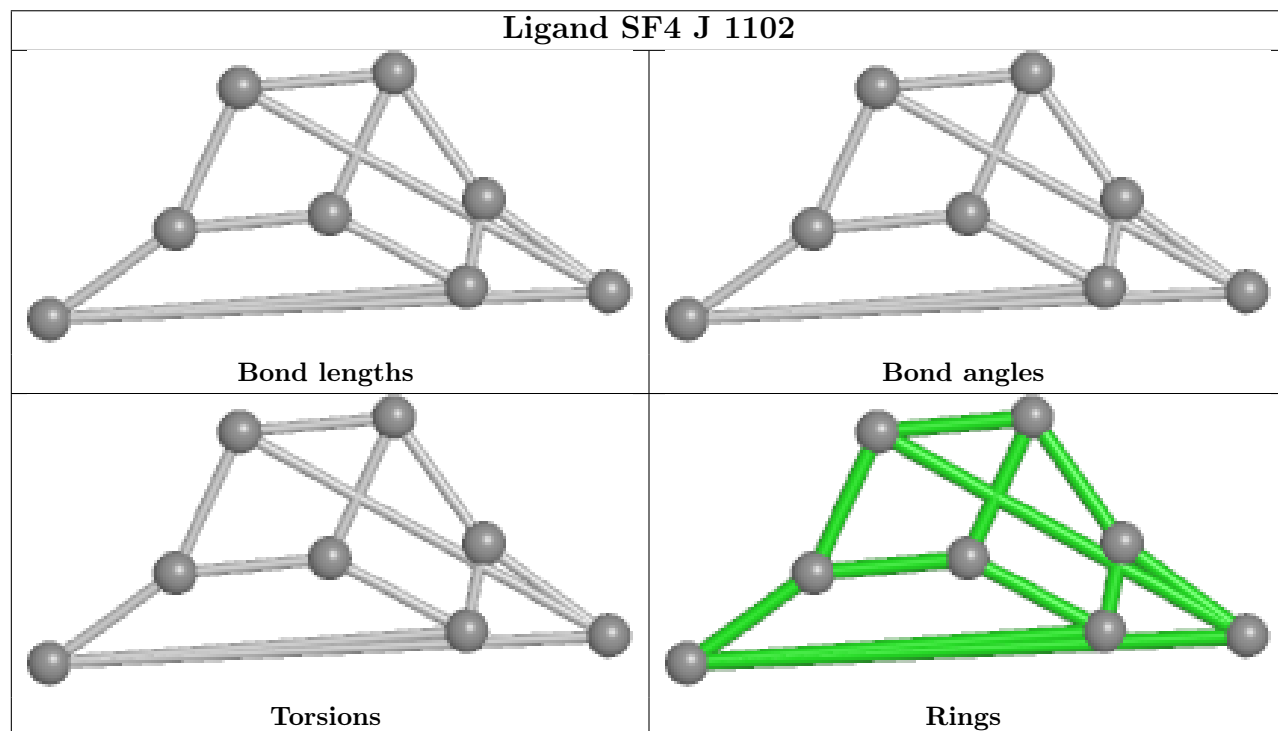


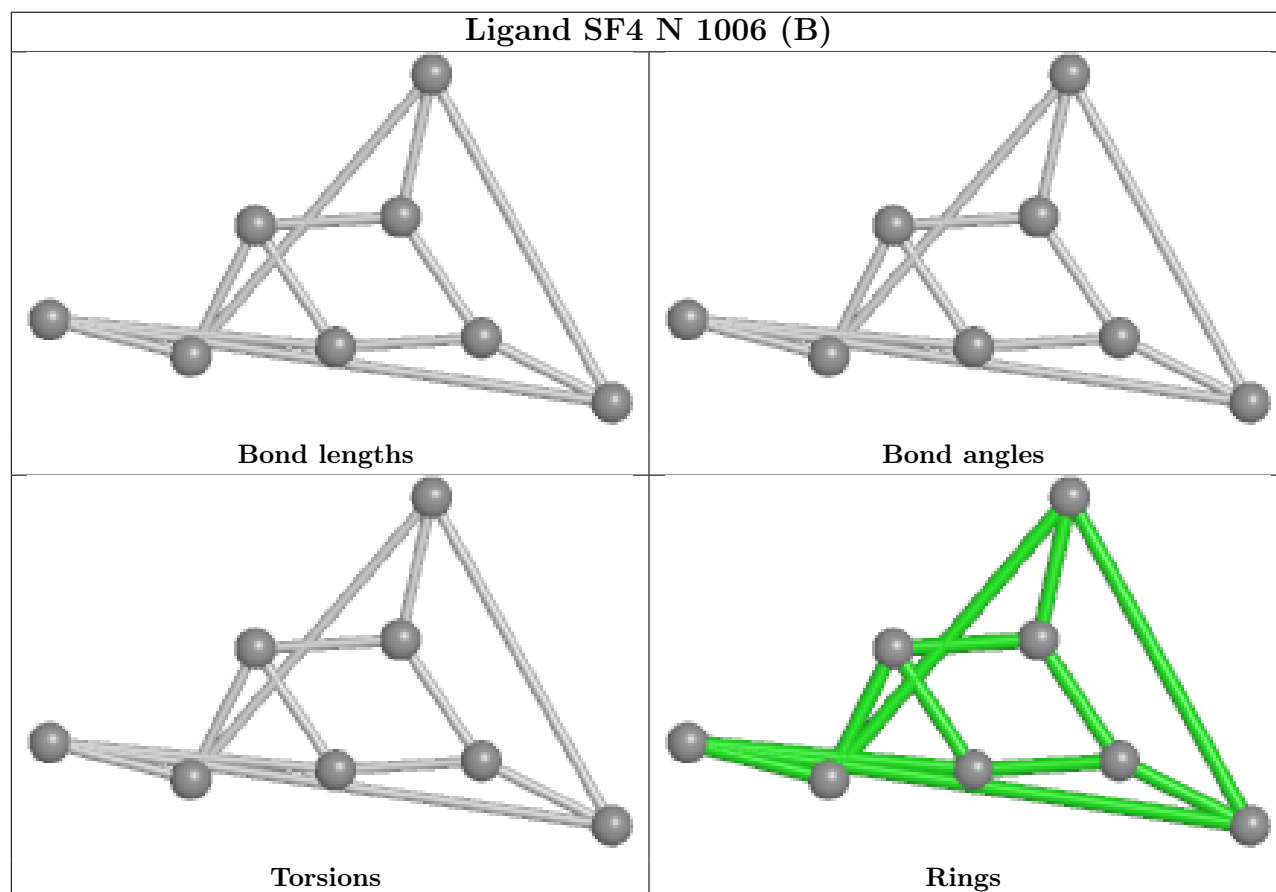
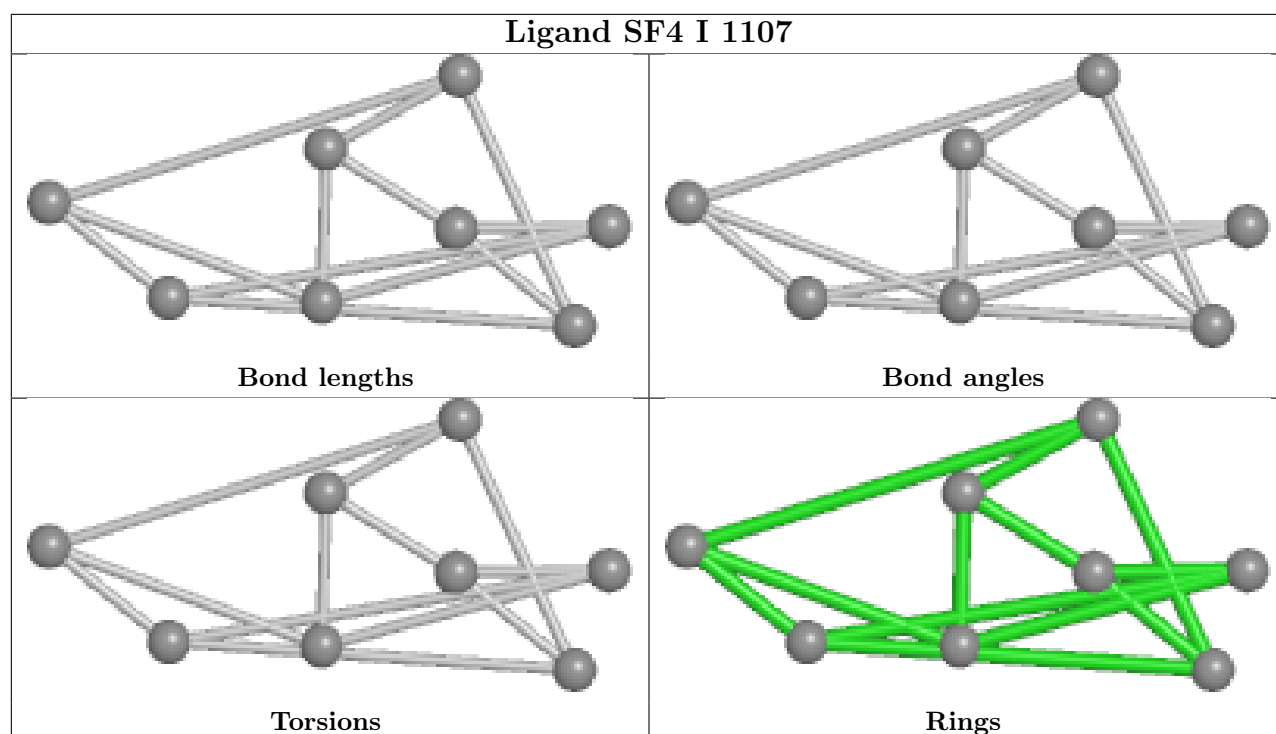


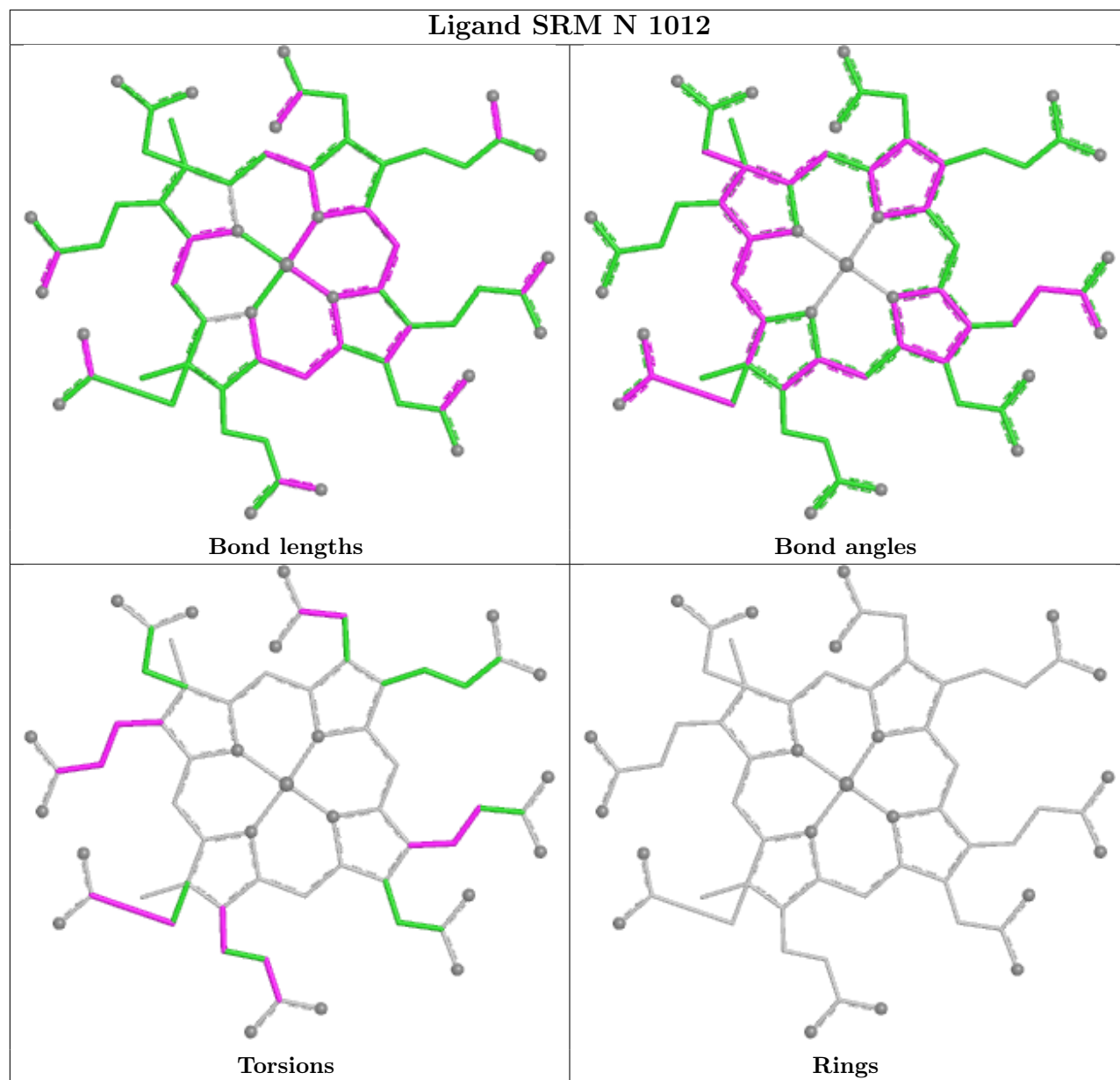
Ligand FAD K 1106

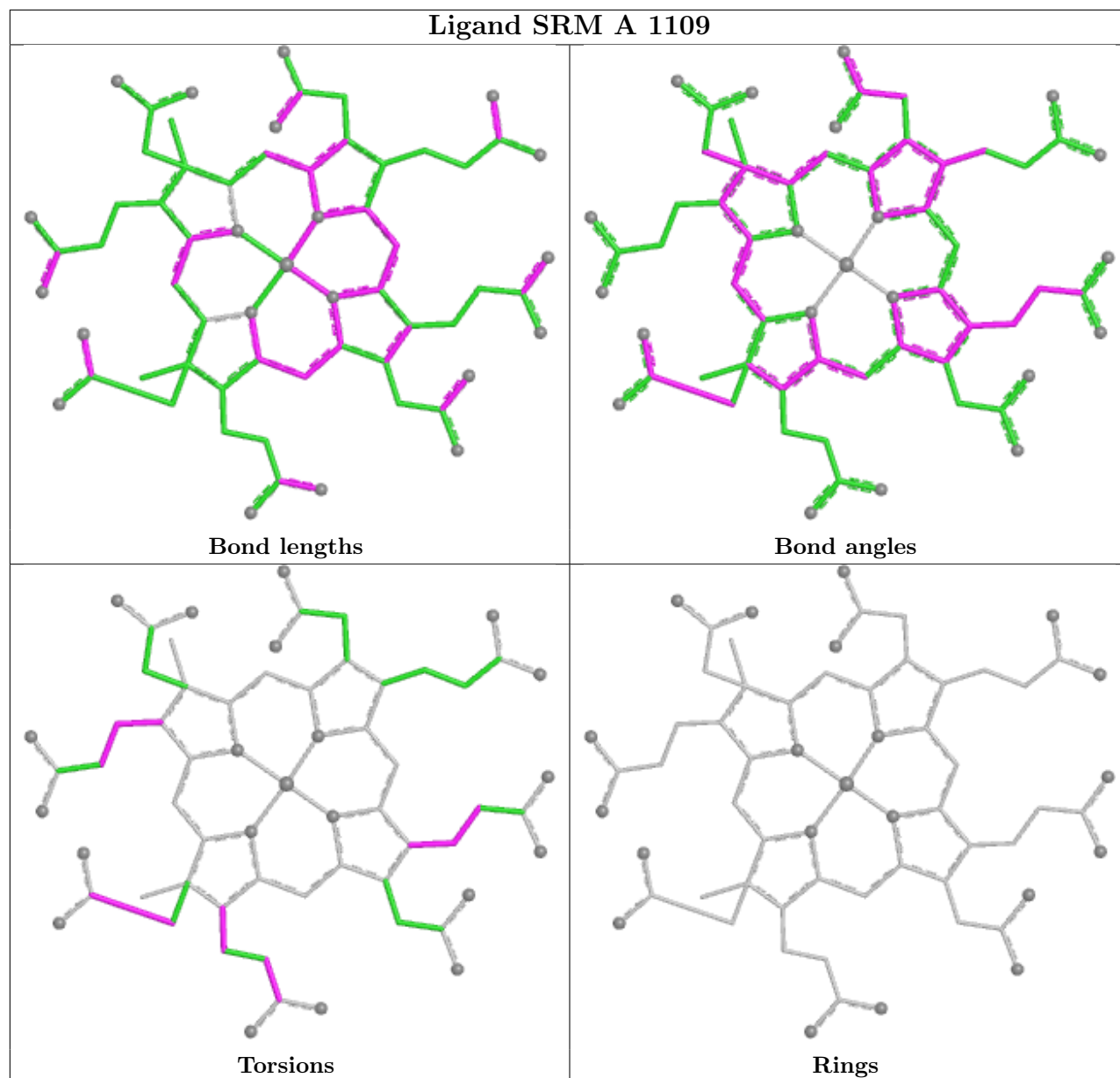


Ligand SF4 J 1102

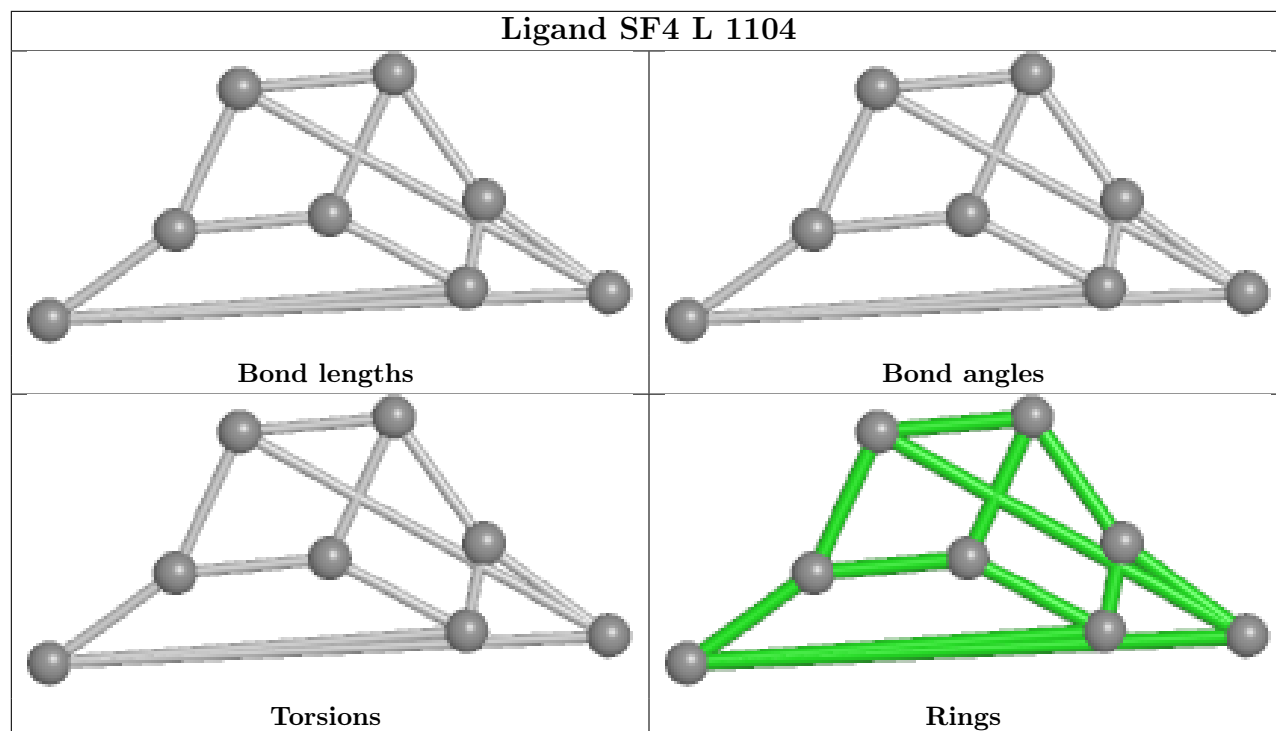




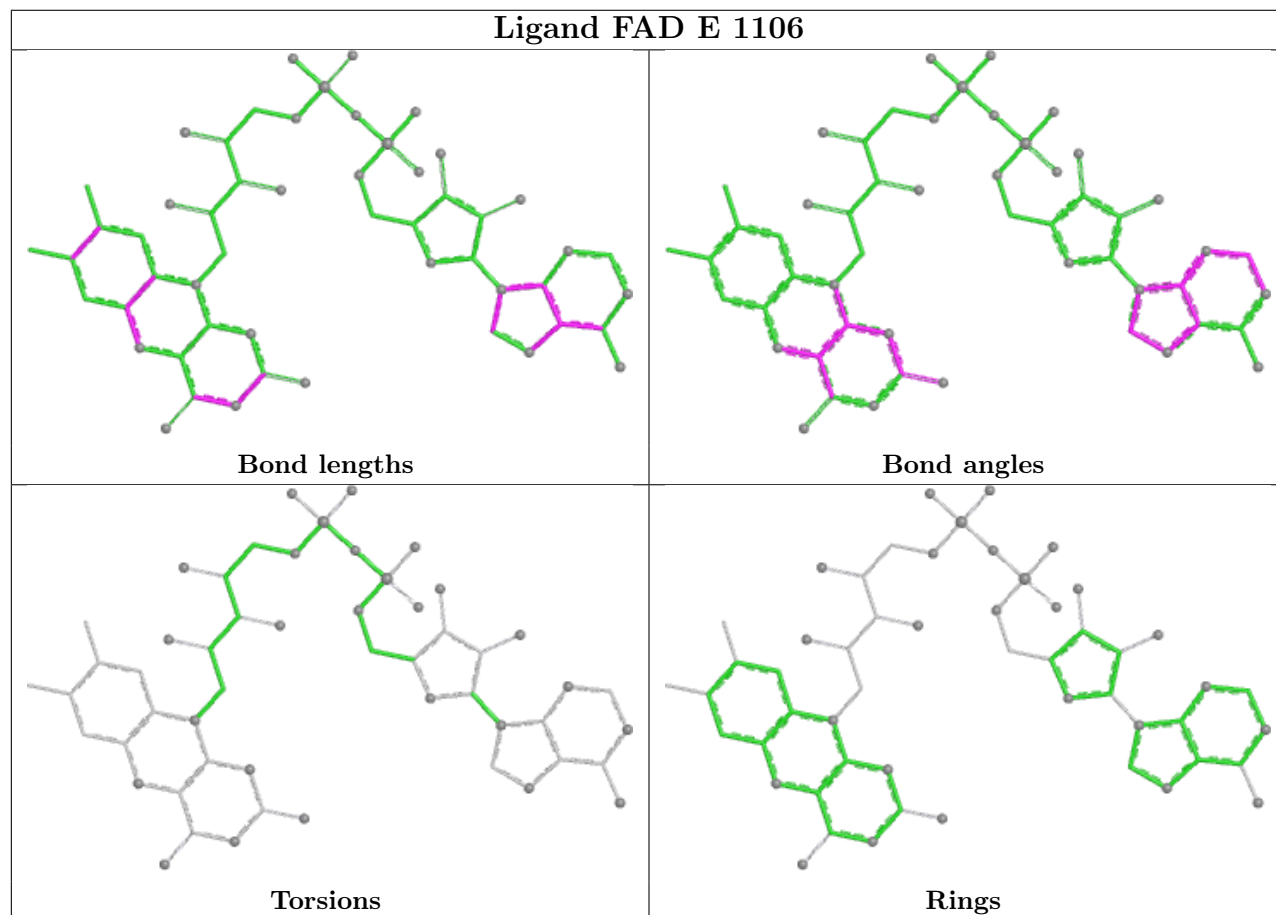


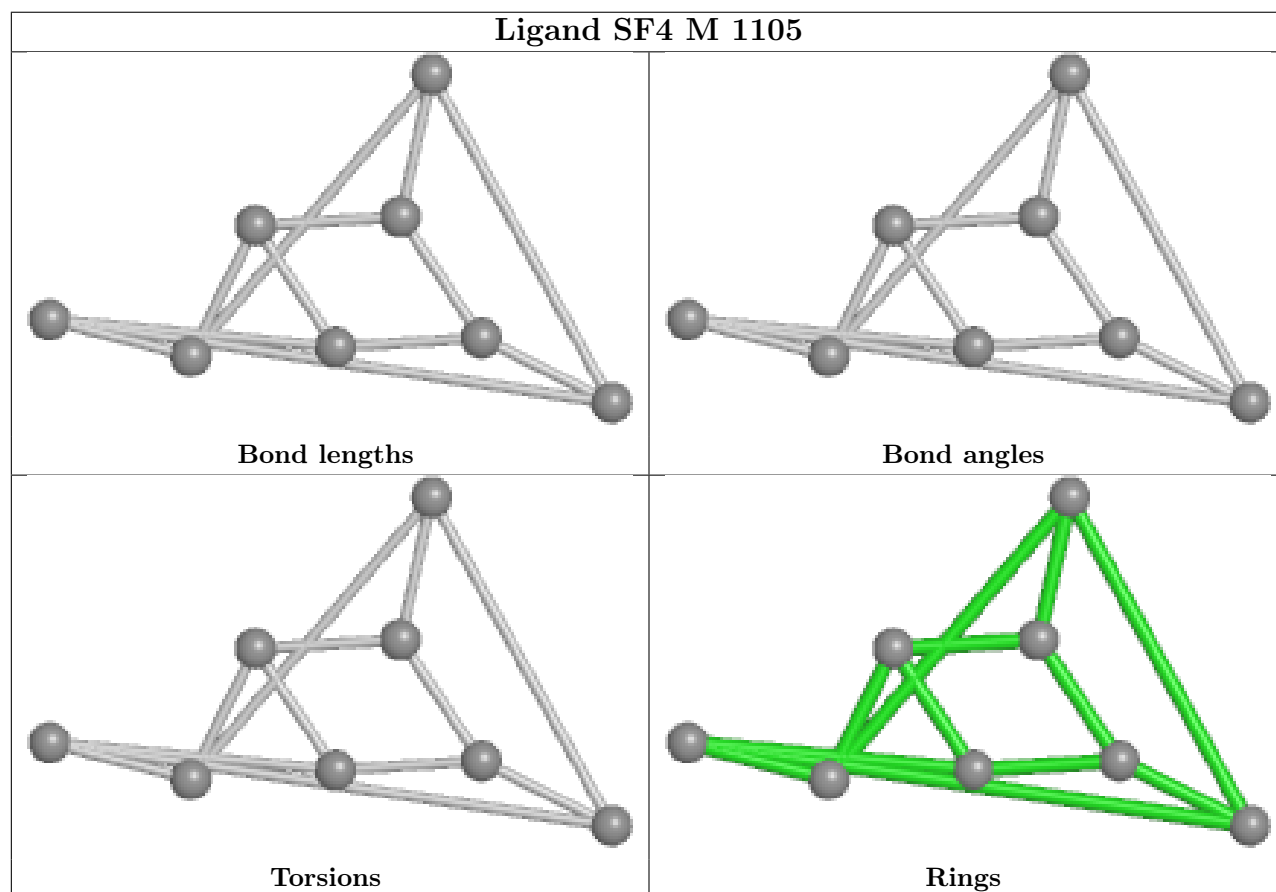
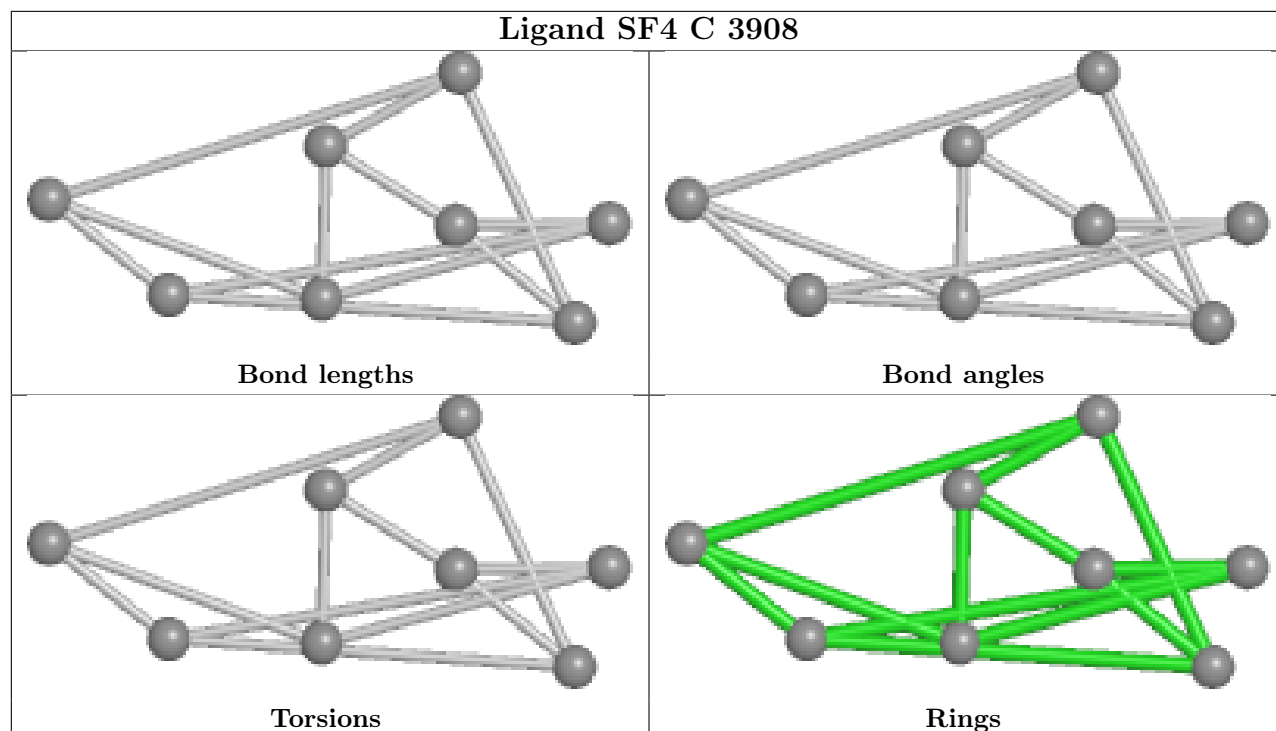


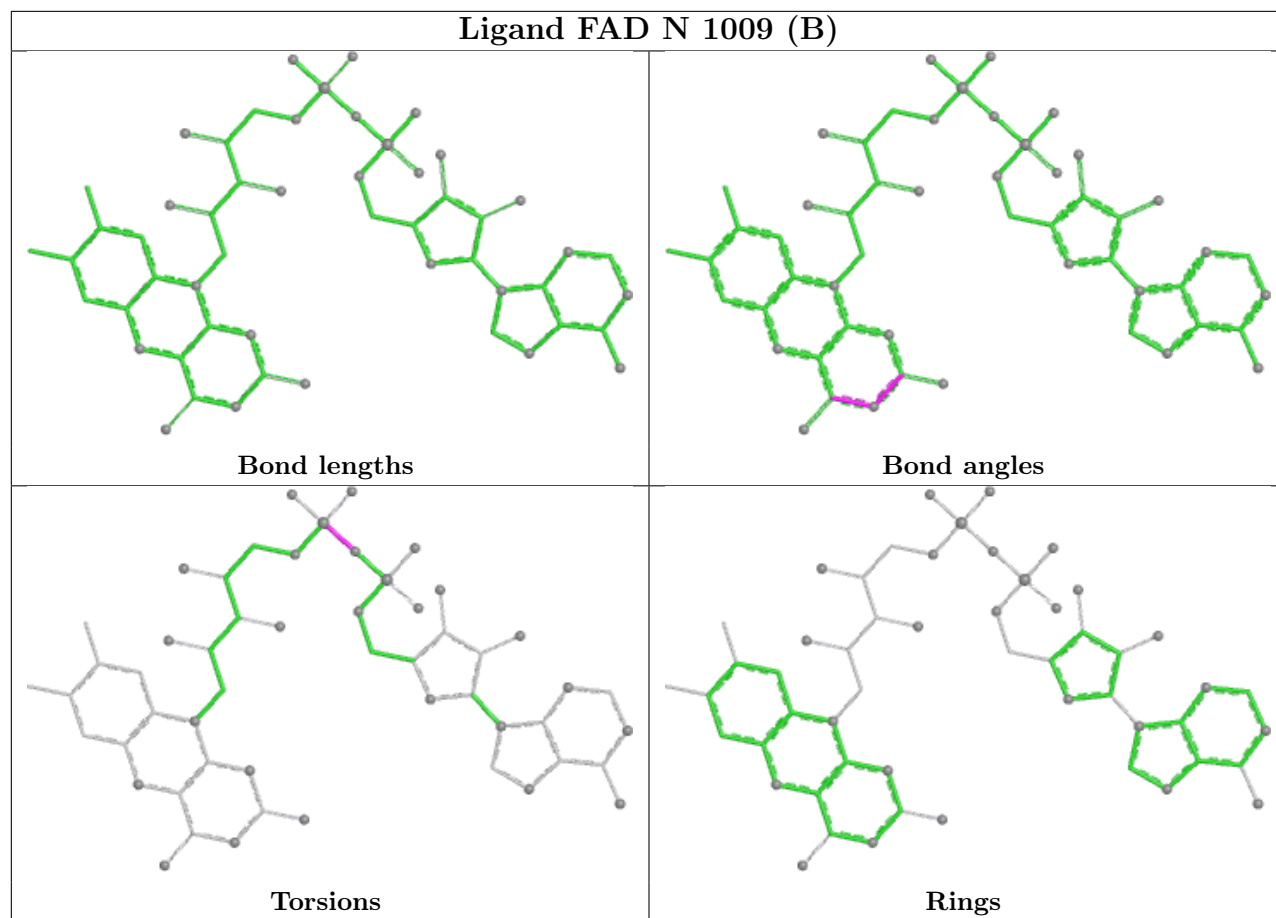
Ligand SF4 L 1104

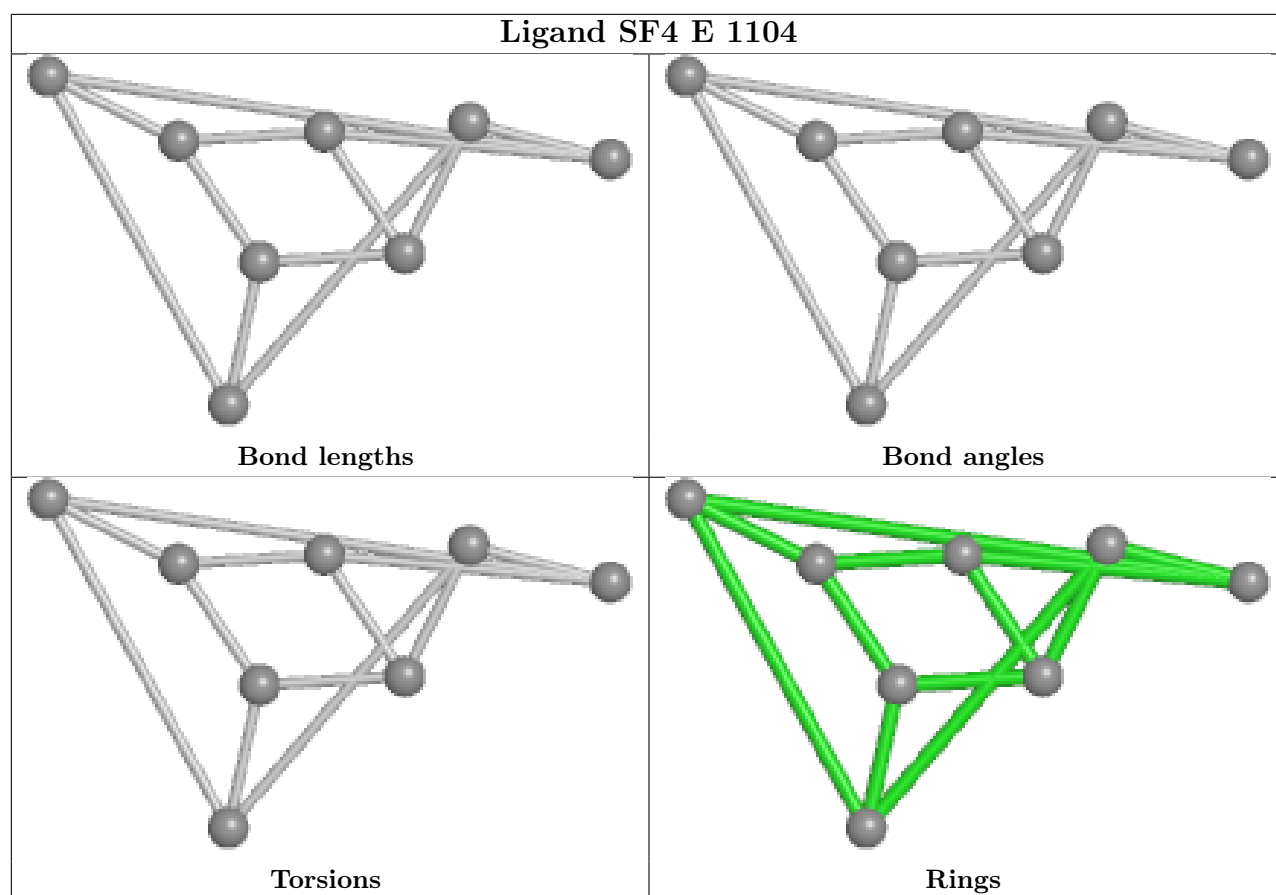


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5.7 Other polymers [i](#)

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%)

All (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

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Mol	Chain	Res	Type	RSRZ
1	G	252	LEU	5.7
1	N	74[A]	TYR	5.5
1	D	238	VAL	5.4
1	P	238	VAL	5.3
1	P	250	ILE	5.3
1	N	75[A]	TYR	5.2
1	P	229	ILE	5.2
1	N	81[A]	VAL	5.2
1	P	247	LEU	5.2
1	N	276[A]	SER	5.0
1	N	110[A]	ASP	5.0
1	N	307[A]	ALA	5.0
1	G	231	LYS	4.9
1	P	252	LEU	4.9
1	E	214	LEU	4.8
1	H	252	LEU	4.8
1	P	232	GLY	4.8
1	E	216	LYS	4.8
1	H	229	ILE	4.7
1	N	300[A]	LYS	4.7
1	N	238[A]	VAL	4.7
1	A	1	MET	4.7
1	E	247	LEU	4.7
1	N	296[A]	ALA	4.7
1	B	1	MET	4.6
1	N	78[A]	LYS	4.6
1	N	248[A]	LYS	4.5
1	E	215	ALA	4.5
1	N	308[A]	ILE	4.4
1	G	232	GLY	4.4
1	P	219	ILE	4.4
1	N	122[A]	ASN	4.3
1	E	232	GLY	4.3
1	E	238	VAL	4.3
1	P	217	TYR	4.2
1	N	274[A]	VAL	4.2
1	N	240[A]	GLY	4.1
1	E	217	TYR	4.1
1	N	310[A]	LYS	4.1
1	P	130	THR	4.1
1	E	245	ILE	4.1
1	H	232	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	N	302[A]	GLY	4.0
1	H	247	LEU	4.0
1	C	1	MET	4.0
1	H	231	LYS	3.9
1	J	1	MET	3.9
1	D	231	LYS	3.9
1	E	219	ILE	3.9
1	H	240	GLY	3.9
1	N	272[A]	GLY	3.8
1	N	94[A]	LYS	3.8
1	N	299[A]	LEU	3.8
1	G	1	MET	3.8
1	P	213	THR	3.8
1	H	230	LYS	3.8
1	P	39	THR	3.8
1	H	245	ILE	3.7
1	N	227[A]	PHE	3.7
1	N	303[A]	VAL	3.7
1	F	238	VAL	3.7
1	D	240	GLY	3.7
1	N	215[A]	ALA	3.7
1	G	247	LEU	3.6
1	M	314	LEU	3.6
1	J	231	LYS	3.6
1	N	202[A]	THR	3.6
1	N	229[A]	ILE	3.6
1	N	283[A]	VAL	3.6
1	F	78	LYS	3.6
1	E	246	PRO	3.6
1	P	240	GLY	3.6
1	N	100[A]	LYS	3.5
1	N	111[A]	GLU	3.5
1	G	246	PRO	3.5
1	D	214	LEU	3.5
1	F	126	LEU	3.5
1	P	221	MET	3.5
1	N	271[A]	VAL	3.5
1	N	112[A]	CYS	3.4
1	F	239	ASN	3.4
1	E	213	THR	3.4
1	P	81	VAL	3.4
1	J	217	TYR	3.4

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Mol	Chain	Res	Type	RSRZ
1	N	114[A]	LYS	3.4
1	P	214	LEU	3.4
1	H	219	ILE	3.4
1	N	273[A]	CYS	3.4
1	H	235	LEU	3.4
1	P	233	LYS	3.3
1	N	73[A]	GLU	3.3
1	F	76	TYR	3.3
1	N	95[A]	TYR	3.3
1	N	130[A]	THR	3.3
1	H	246	PRO	3.3
1	P	248	LYS	3.3
1	F	1	MET	3.3
1	N	282[A]	THR	3.3
1	E	314	LEU	3.3
1	N	234[A]	LEU	3.3
1	H	244	LYS	3.3
1	I	238	VAL	3.3
1	N	39	THR	3.3
1	P	236	VAL	3.3
1	N	82[A]	GLU	3.3
1	N	280[A]	TYR	3.3
1	D	8	ASP	3.2
1	E	233	LYS	3.2
1	G	245	ILE	3.2
1	N	236[A]	VAL	3.2
1	P	273	CYS	3.2
1	D	217	TYR	3.2
1	N	278[A]	ASP	3.2
1	N	87[A]	GLY	3.2
1	E	229	ILE	3.2
1	H	238	VAL	3.2
1	N	2	TYR	3.2
1	H	216	LYS	3.2
1	P	246	PRO	3.2
1	P	245	ILE	3.2
1	P	218	ASN	3.2
1	F	237	TYR	3.2
1	N	190[A]	LEU	3.1
1	I	330	ASP	3.1
1	I	1	MET	3.1
1	G	238	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	N	33	GLU	3.1
1	M	248	LYS	3.1
1	N	98[A]	LYS	3.1
1	O	2	TYR	3.1
1	P	34	ASP	3.1
1	P	207	TYR	3.1
1	N	129[A]	THR	3.1
1	N	311	LEU	3.1
1	N	314[A]	LEU	3.1
1	N	61	LYS	3.1
1	N	34	ASP	3.1
1	D	112	CYS	3.1
1	N	269[A]	VAL	3.0
1	G	217	TYR	3.0
1	H	217	TYR	3.0
1	P	314	LEU	3.0
1	E	222	ASP	3.0
1	N	85[A]	ASP	3.0
1	N	77[A]	GLY	3.0
1	P	227	PHE	3.0
1	E	112	CYS	3.0
1	E	492	GLU	3.0
1	D	235	LEU	3.0
1	P	126	LEU	3.0
1	H	215	ALA	3.0
1	H	250	ILE	3.0
1	P	234	LEU	3.0
1	P	231	LYS	3.0
1	F	8	ASP	2.9
1	H	214	LEU	2.9
1	P	203	GLU	2.9
1	N	31	THR	2.9
1	J	243	HIS	2.9
1	J	229	ILE	2.9
1	E	231	LYS	2.9
1	I	411	LYS	2.9
1	F	81	VAL	2.9
1	F	38	LEU	2.9
1	A	240	GLY	2.9
1	E	223	ASP	2.9
1	N	293[A]	ILE	2.9
1	P	2	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	213	THR	2.9
1	N	239[A]	ASN	2.9
1	P	224	VAL	2.9
1	J	214	LEU	2.9
1	G	230	LYS	2.9
1	N	230[A]	LYS	2.9
1	P	332	LYS	2.9
1	F	278	ASP	2.8
1	P	215	ALA	2.8
1	D	219	ILE	2.8
1	D	239	ASN	2.8
1	E	239	ASN	2.8
1	P	243	HIS	2.8
1	N	242[A]	GLU	2.8
1	N	244[A]	LYS	2.8
1	P	114	LYS	2.8
1	F	232	GLY	2.8
1	N	281[A]	SER	2.8
1	L	8	ASP	2.8
1	F	112	CYS	2.8
1	N	277[A]	PRO	2.8
1	P	300	LYS	2.8
1	M	278	ASP	2.8
1	H	209	GLU	2.8
1	E	220	ASN	2.8
1	J	244	LYS	2.8
1	M	231	LYS	2.8
1	P	244	LYS	2.8
1	E	250	ILE	2.8
1	E	221	MET	2.8
1	E	618	ASN	2.8
1	J	218	ASN	2.8
1	N	93[A]	LEU	2.8
1	D	584[A]	HIS	2.8
1	H	248	LYS	2.8
1	N	116[A]	VAL	2.7
1	P	278	ASP	2.7
1	N	241[A]	GLU	2.7
1	P	241	GLU	2.7
1	J	239	ASN	2.7
1	H	233	LYS	2.7
1	J	248	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	P	112	CYS	2.7
1	N	150[A]	LEU	2.7
1	G	240	GLY	2.7
1	M	240	GLY	2.7
1	N	83[A]	GLY	2.7
1	P	109	GLY	2.7
1	N	295[A]	ASN	2.7
1	N	37	LYS	2.7
1	D	241	GLU	2.7
1	E	124	GLU	2.7
1	N	306[A]	GLU	2.7
1	P	237	TYR	2.7
1	P	280	TYR	2.7
1	F	299	LEU	2.7
1	P	311	LEU	2.7
1	J	238	VAL	2.7
1	E	244	LYS	2.7
1	G	122	ASN	2.7
1	I	37	LYS	2.7
1	D	229	ILE	2.7
1	P	254	ALA	2.6
1	J	233	LYS	2.6
1	N	195[A]	TYR	2.6
1	J	305	LEU	2.6
1	N	43	LEU	2.6
1	P	618	ASN	2.6
1	D	236	VAL	2.6
1	M	511	ASP	2.6
1	N	89[A]	VAL	2.6
1	N	330[A]	ASP	2.6
1	P	119	ILE	2.6
1	F	32	PHE	2.6
1	N	118[A]	LEU	2.6
1	D	224	VAL	2.6
1	N	155[A]	VAL	2.6
1	M	346	LYS	2.6
1	P	37	LYS	2.6
1	N	128[A]	ASN	2.6
1	P	239	ASN	2.6
1	H	249	GLU	2.6
1	F	214	LEU	2.6
1	O	314	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	248	LYS	2.6
1	N	225[A]	GLU	2.6
1	N	304[A]	ASN	2.6
1	N	410	GLU	2.6
1	H	81	VAL	2.6
1	J	246	PRO	2.6
1	E	240	GLY	2.6
1	F	297	ILE	2.5
1	N	219[A]	ILE	2.5
1	H	251	GLU	2.5
1	K	618	ASN	2.5
1	M	2	TYR	2.5
1	P	116	VAL	2.5
1	N	91[A]	THR	2.5
1	N	119[A]	ILE	2.5
1	E	237	TYR	2.5
1	N	207[A]	TYR	2.5
1	D	232	GLY	2.5
1	F	240	GLY	2.5
1	O	124	GLU	2.5
1	J	81	VAL	2.5
1	J	332	LYS	2.5
1	L	248	LYS	2.5
1	N	131[A]	LYS	2.5
1	N	224[A]	VAL	2.5
1	G	112	CYS	2.5
1	B	330	ASP	2.5
1	N	79[A]	GLY	2.5
1	J	235	LEU	2.5
1	N	199[A]	LEU	2.5
1	N	32	PHE	2.5
1	E	278	ASP	2.5
1	N	80[A]	ASP	2.5
1	E	248	LYS	2.4
1	N	297[A]	ILE	2.4
1	F	314	LEU	2.4
1	H	2	TYR	2.4
1	N	316[A]	LEU	2.4
1	G	511	ASP	2.4
1	H	34	ASP	2.4
1	N	262[A]	PHE	2.4
1	F	39	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	120	VAL	2.4
1	F	303	VAL	2.4
1	L	81	VAL	2.4
1	N	136[A]	VAL	2.4
1	P	274	VAL	2.4
1	D	248	LYS	2.4
1	G	310	LYS	2.4
1	N	86[A]	GLY	2.4
1	N	221[A]	MET	2.4
1	H	239	ASN	2.4
1	L	618	ASN	2.4
1	G	229	ILE	2.4
1	B	314	LEU	2.4
1	H	234	LEU	2.4
1	F	280	TYR	2.4
1	P	76	TYR	2.4
1	D	233	LYS	2.4
1	K	37	LYS	2.4
1	N	113[A]	TRP	2.4
1	J	215	ALA	2.4
1	I	239	ASN	2.4
1	G	251	GLU	2.4
1	I	33	GLU	2.4
1	F	231	LYS	2.4
1	G	216	LYS	2.4
1	N	126[A]	LEU	2.4
1	N	286[A]	ARG	2.4
1	P	131	LYS	2.4
1	P	230	LYS	2.4
1	M	618	ASN	2.4
1	N	70	PHE	2.4
1	P	205	PHE	2.4
1	N	148[A]	MET	2.3
1	N	197[A]	ILE	2.3
1	D	247	LEU	2.3
1	E	493	GLU	2.3
1	N	124[A]	GLU	2.3
1	N	298[A]	GLU	2.3
1	O	418	GLU	2.3
1	B	618	ASN	2.3
1	F	95	TYR	2.3
1	J	76	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	O	239	ASN	2.3
1	C	34	ASP	2.3
1	E	617	GLN	2.3
1	P	328	ALA	2.3
1	D	244	LYS	2.3
1	D	221	MET	2.3
1	N	88[A]	VAL	2.3
1	P	120	VAL	2.3
1	P	113	TRP	2.3
1	J	306	GLU	2.3
1	M	306	GLU	2.3
1	L	240	GLY	2.3
1	P	330	ASP	2.3
1	E	234	LEU	2.3
1	G	250	ILE	2.3
1	N	139[A]	LEU	2.3
1	N	158[A]	LEU	2.3
1	N	235[A]	LEU	2.3
1	N	284[A]	ILE	2.3
1	G	2	TYR	2.3
1	H	237	TYR	2.3
1	A	298	GLU	2.3
1	H	212	GLU	2.3
1	J	276	SER	2.3
1	F	274	VAL	2.3
1	M	81	VAL	2.3
1	O	81	VAL	2.3
1	F	129	THR	2.3
1	J	80	ASP	2.3
1	N	287[A]	THR	2.3
1	D	243	HIS	2.3
1	E	252	LEU	2.3
1	F	414	ILE	2.3
1	J	311	LEU	2.3
1	L	314	LEU	2.3
1	B	217	TYR	2.3
1	F	2	TYR	2.3
1	E	116	VAL	2.2
1	J	274	VAL	2.2
1	N	23	VAL	2.2
1	A	111	GLU	2.2
1	E	33	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	212	GLU	2.2
1	J	247	LEU	2.2
1	G	239	ASN	2.2
1	J	112	CYS	2.2
1	E	249	GLU	2.2
1	E	251	GLU	2.2
1	E	410	GLU	2.2
1	F	251	GLU	2.2
1	H	243	HIS	2.2
1	K	3	GLU	2.2
1	G	233	LYS	2.2
1	L	231	LYS	2.2
1	N	144[A]	THR	2.2
1	N	120[A]	VAL	2.2
1	F	128	ASN	2.2
1	G	618	ASN	2.2
1	G	223	ASP	2.2
1	K	8	ASP	2.2
1	N	103[A]	ASP	2.2
1	C	252	LEU	2.2
1	H	314	LEU	2.2
1	P	210	LEU	2.2
1	B	537	GLU	2.2
1	D	242	GLU	2.2
1	D	245	ILE	2.2
1	N	309[A]	GLU	2.2
1	P	249	GLU	2.2
1	L	2	TYR	2.2
1	D	246	PRO	2.2
1	N	216[A]	LYS	2.2
1	P	411	LYS	2.2
1	O	218	ASN	2.2
1	F	80	ASP	2.2
1	N	8	ASP	2.2
1	N	108[A]	VAL	2.2
1	G	244	LYS	2.2
1	J	78	LYS	2.2
1	E	316	LEU	2.1
1	J	314	LEU	2.1
1	N	200[A]	LEU	2.1
1	J	280	TYR	2.1
1	N	121[A]	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	225	GLU	2.1
1	P	111	GLU	2.1
1	P	223	ASP	2.1
1	P	283	VAL	2.1
1	L	43	LEU	2.1
1	N	96[A]	LEU	2.1
1	O	214	LEU	2.1
1	B	410	GLU	2.1
1	C	618	ASN	2.1
1	F	298	GLU	2.1
1	M	418	GLU	2.1
1	J	219	ILE	2.1
1	A	617	GLN	2.1
1	D	225	GLU	2.1
1	I	240	GLY	2.1
1	J	232	GLY	2.1
1	M	33	GLU	2.1
1	G	34	ASP	2.1
1	P	31	THR	2.1
1	D	234	LEU	2.1
1	F	235	LEU	2.1
1	P	235	LEU	2.1
1	F	114	LYS	2.1
1	G	532	LYS	2.1
1	J	237	TYR	2.1
1	J	250	ILE	2.1
1	F	33	GLU	2.1
1	I	410	GLU	2.1
1	K	410	GLU	2.1
1	K	492	GLU	2.1
1	P	242	GLU	2.1
1	D	222	ASP	2.1
1	D	278	ASP	2.1
1	P	511	ASP	2.1
1	E	310	LYS	2.0
1	P	129	THR	2.0
1	D	81	VAL	2.0
1	E	81	VAL	2.0
1	K	81	VAL	2.0
1	D	215	ALA	2.0
1	H	112	CYS	2.0
1	G	111	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	298	GLU	2.0
1	J	33	GLU	2.0
1	O	493	GLU	2.0
1	D	237	TYR	2.0
1	A	618	ASN	2.0
1	F	618	ASN	2.0
1	J	278	ASP	2.0
1	O	122	ASN	2.0
1	P	80	ASP	2.0
1	P	83	GLY	2.0
1	G	248	LYS	2.0
1	I	71	LYS	2.0
1	P	257	LYS	2.0
1	F	277	PRO	2.0
1	I	493	GLU	2.0
1	B	81	VAL	2.0
1	N	153[A]	VAL	2.0
1	P	10	VAL	2.0
1	F	118	LEU	2.0
1	N	30	LEU	2.0
1	N	117[A]	SER	2.0
1	C	8	ASP	2.0
1	F	34	ASP	2.0
1	P	220	ASN	2.0
1	O	237	TYR	2.0

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($\text{\AA}^2$)	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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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
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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
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.