



wwPDB EM Validation Summary Report ⓘ

Mar 19, 2026 – 08:25 PM UTC

PDB ID : 7Q4W / pdb_00007q4w
EMDB ID : EMD-13819
Title : CryoEM structure of electron bifurcating Fe-Fe hydrogenase HydABC complex
A. woodii in the oxidised state
Authors : Kumar, A.; Saura, P.; Poeverlein, M.C.; Gamiz-Hernandez, A.P.; Kaila,
V.R.I.; Mueller, V.; Schuller, J.M.
Deposited on : 2021-11-02
Resolution : 3.78 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

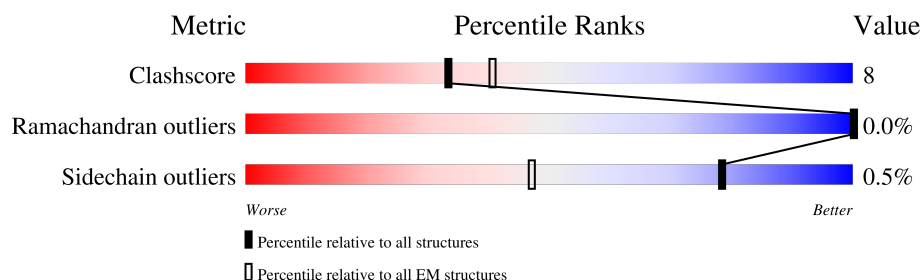
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.78 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	583	78% 21%
1	E	583	83% 17%
2	B	470	77% 23%
2	F	470	79% 21%
3	C	156	72% 11% 17%
3	G	156	69% 13% 17%

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
4	SF4	A	601	-	-	X	-
4	SF4	A	604	-	-	X	-
4	SF4	B	602	-	-	X	-
4	SF4	E	604	-	-	X	-
5	FES	C	201	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18050 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Iron hydrogenase HydA1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	583	Total	C	N	O	S	0	0
			4442	2774	766	865	37		
1	E	583	Total	C	N	O	S	0	0
			4442	2774	766	865	37		

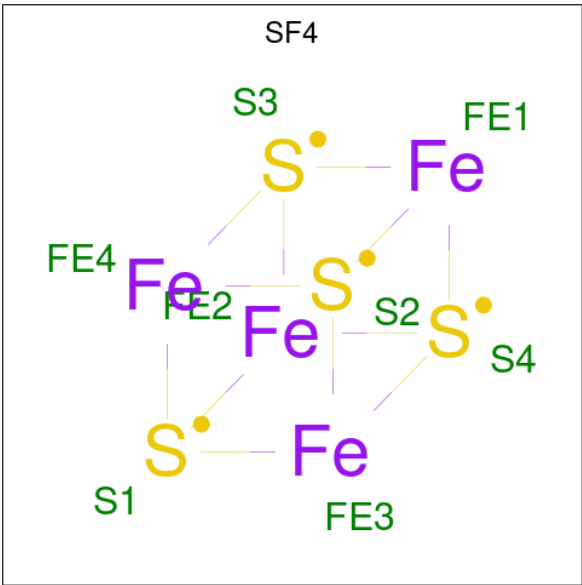
- Molecule 2 is a protein called Iron hydrogenase HydB.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	470	Total	C	N	O	S	0	0
			3513	2216	592	676	29		
2	F	470	Total	C	N	O	S	0	0
			3513	2216	592	676	29		

- Molecule 3 is a protein called Iron hydrogenase HydC.

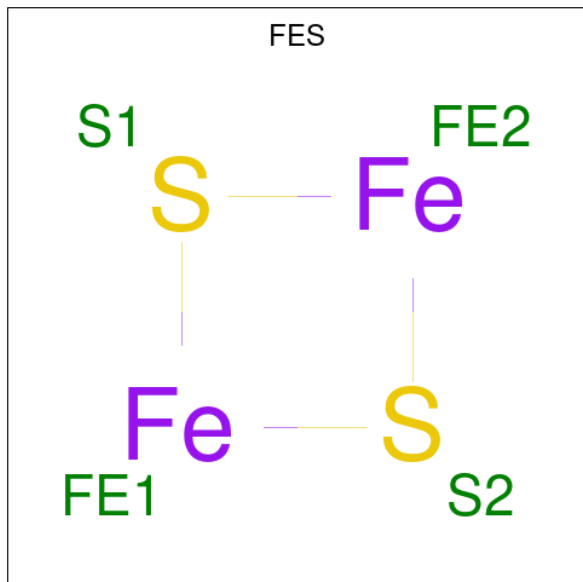
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	129	Total	C	N	O	S	0	0
			974	621	158	188	7		
3	G	129	Total	C	N	O	S	0	0
			974	621	158	188	7		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



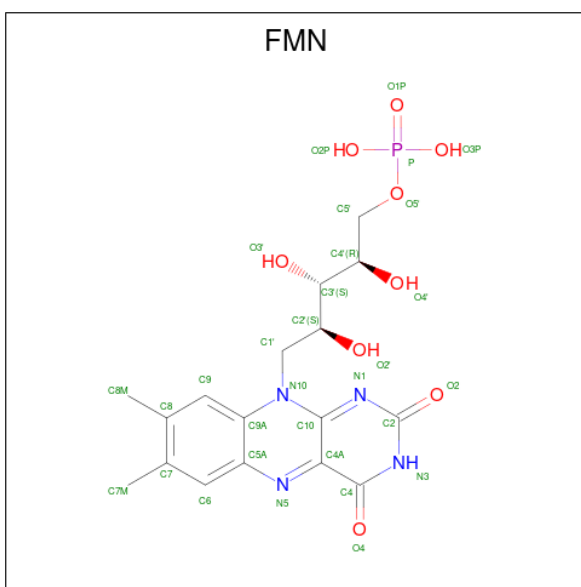
Mol	Chain	Residues	Atoms			AltConf
4	A	1	Total	Fe	S	0
			8	4	4	
4	A	1	Total	Fe	S	
			8	4	4	
4	A	1	Total	Fe	S	0
			8	4	4	
4	A	1	Total	Fe	S	
			8	4	4	
4	B	1	Total	Fe	S	0
			8	4	4	
4	B	1	Total	Fe	S	
			8	4	4	
4	B	1	Total	Fe	S	0
			8	4	4	
4	E	1	Total	Fe	S	
			8	4	4	
4	E	1	Total	Fe	S	0
			8	4	4	
4	E	1	Total	Fe	S	
			8	4	4	
4	F	1	Total	Fe	S	0
			8	4	4	
4	F	1	Total	Fe	S	
			8	4	4	
4	F	1	Total	Fe	S	0
			8	4	4	
4	F	1	Total	Fe	S	
			8	4	4	

- Molecule 5 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	Fe	S	0
			4	2	2	
5	C	1	Total	Fe	S	0
			4	2	2	
5	E	1	Total	Fe	S	0
			4	2	2	
5	G	1	Total	Fe	S	0
			4	2	2	

- Molecule 6 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $\text{C}_{17}\text{H}_{21}\text{N}_4\text{O}_9\text{P}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
6	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
6	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

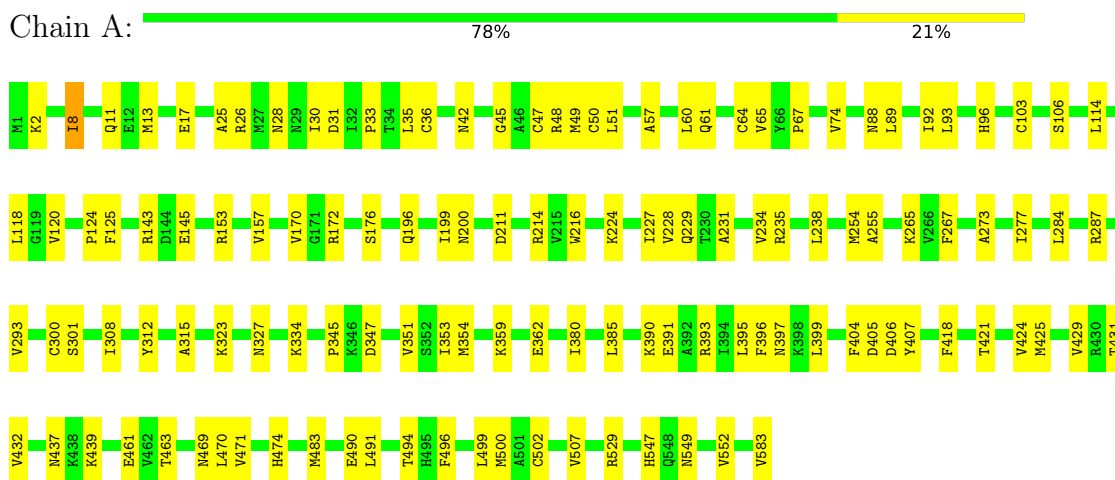
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	B	1	Total	Zn	0
			1	1	
7	F	1	Total	Zn	0
			1	1	

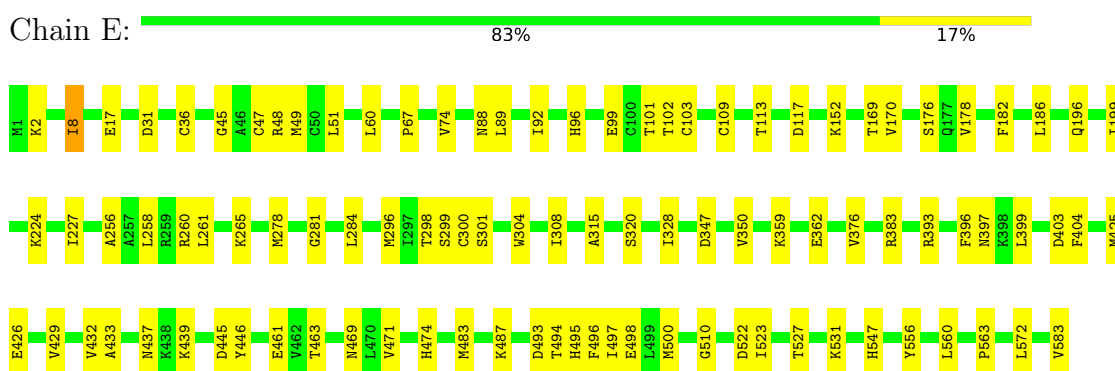
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

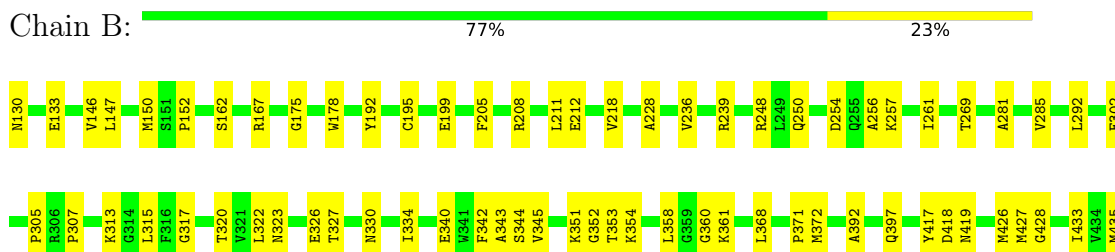
• Molecule 1: Iron hydrogenase HydA1



• Molecule 1: Iron hydrogenase HydA1



• Molecule 2: Iron hydrogenase HydB



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	250709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	55	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, ZN, FES, FMN

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	0.21	0/4507	0.49	1/6105 (0.0%)
1	E	0.19	0/4507	0.44	0/6105
2	B	0.15	0/3577	0.42	0/4825
2	F	0.16	0/3577	0.40	0/4825
3	C	0.18	0/989	0.42	0/1342
3	G	0.14	0/989	0.38	0/1342
All	All	0.18	0/18146	0.44	1/24544 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	G	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	VAL	N-CA-C	-6.06	106.86	112.43

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	G	123	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4442	0	4462	79	0
1	E	4442	0	4462	70	0
2	B	3513	0	3481	73	0
2	F	3513	0	3481	69	0
3	C	974	0	990	15	0
3	G	974	0	990	15	0
4	A	32	0	0	5	0
4	B	24	0	0	5	0
4	E	32	0	0	6	0
4	F	24	0	0	2	0
5	A	4	0	0	1	0
5	C	4	0	0	2	0
5	E	4	0	0	1	0
5	G	4	0	0	1	0
6	B	31	0	19	0	0
6	F	31	0	19	0	0
7	B	1	0	0	0	0
7	F	1	0	0	0	0
All	All	18050	0	17904	299	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 8.

The worst 5 of 299 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:E:170:VAL:O	1:E:176:SER:HA	1.65	0.95
1:A:170:VAL:O	1:A:176:SER:HA	1.70	0.92
1:E:96:HIS:CE1	4:E:604:SF4:S2	2.59	0.90
2:B:503:CYS:HB2	4:B:602:SF4:S2	2.12	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:CE1	4:A:604:SF4:S2	2.58	0.84

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/583 (100%)	556 (96%)	24 (4%)	1 (0%)	43	72
1	E	581/583 (100%)	558 (96%)	23 (4%)	0	100	100
2	B	468/470 (100%)	455 (97%)	13 (3%)	0	100	100
2	F	468/470 (100%)	456 (97%)	12 (3%)	0	100	100
3	C	127/156 (81%)	126 (99%)	1 (1%)	0	100	100
3	G	127/156 (81%)	126 (99%)	1 (1%)	0	100	100
All	All	2352/2418 (97%)	2277 (97%)	74 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	SER

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	492/492 (100%)	490 (100%)	2 (0%)	84	83
1	E	492/492 (100%)	490 (100%)	2 (0%)	84	83
2	B	369/369 (100%)	366 (99%)	3 (1%)	73	76
2	F	369/369 (100%)	368 (100%)	1 (0%)	86	84
3	C	106/130 (82%)	105 (99%)	1 (1%)	70	74
3	G	106/130 (82%)	105 (99%)	1 (1%)	70	74
All	All	1934/1982 (98%)	1924 (100%)	10 (0%)	78	81

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	308	ILE
2	F	576	ILE
3	G	49	ILE
2	B	497	ILE
2	B	576	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	61	GLN
1	E	548	GLN
3	G	9	ASN
1	E	569	HIS
1	E	342	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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
4	SF4	A	602	1	0,12,12	-	-	-		
5	FES	G	201	3	0,4,4	-	-	-		
4	SF4	B	603	2	0,12,12	-	-	-		
4	SF4	A	601	1	0,12,12	-	-	-		
4	SF4	F	603	2	0,12,12	-	-	-		
4	SF4	E	602	1	0,12,12	-	-	-		
5	FES	A	605	1	0,4,4	-	-	-		
4	SF4	E	604	1	0,12,12	-	-	-		
4	SF4	E	601	1	0,12,12	-	-	-		
5	FES	E	605	1	0,4,4	-	-	-		
4	SF4	B	602	2	0,12,12	-	-	-		
4	SF4	E	603	1	0,12,12	-	-	-		
6	FMN	F	602	-	33,33,33	2.20	15 (45%)	48,50,50	2.74	17 (35%)
4	SF4	F	604	2	0,12,12	-	-	-		
4	SF4	A	603	1	0,12,12	-	-	-		
4	SF4	A	604	1	0,12,12	-	-	-		
4	SF4	F	605	2	0,12,12	-	-	-		
5	FES	C	201	3	0,4,4	-	-	-		
4	SF4	B	604	2	0,12,12	-	-	-		
6	FMN	B	601	-	33,33,33	2.19	15 (45%)	48,50,50	2.77	18 (37%)

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	SF4	A	602	1	-	-	0/6/5/5
5	FES	G	201	3	-	-	0/1/1/1
4	SF4	B	603	2	-	-	0/6/5/5
4	SF4	A	601	1	-	-	0/6/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	F	603	2	-	-	0/6/5/5
4	SF4	E	602	1	-	-	0/6/5/5
5	FES	A	605	1	-	-	0/1/1/1
4	SF4	E	604	1	-	-	0/6/5/5
4	SF4	E	601	1	-	-	0/6/5/5
5	FES	E	605	1	-	-	0/1/1/1
4	SF4	B	602	2	-	-	0/6/5/5
4	SF4	E	603	1	-	-	0/6/5/5
6	FMN	F	602	-	-	5/18/18/18	0/3/3/3
4	SF4	F	604	2	-	-	0/6/5/5
4	SF4	A	603	1	-	-	0/6/5/5
4	SF4	A	604	1	-	-	0/6/5/5
4	SF4	F	605	2	-	-	0/6/5/5
5	FES	C	201	3	-	-	0/1/1/1
4	SF4	B	604	2	-	-	0/6/5/5
6	FMN	B	601	-	-	7/18/18/18	0/3/3/3

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	601	FMN	C10-N1	4.79	1.42	1.33
6	F	602	FMN	C10-N1	4.72	1.42	1.33
6	F	602	FMN	C9A-C5A	3.76	1.47	1.41
6	B	601	FMN	C9A-C5A	3.70	1.47	1.41
6	F	602	FMN	C2-N3	-3.41	1.31	1.39

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	601	FMN	C4A-C10-N1	-8.80	103.00	124.59
6	F	602	FMN	C4A-C10-N1	-8.66	103.34	124.59
6	B	601	FMN	C10-N1-C2	8.22	134.64	116.85
6	F	602	FMN	C10-N1-C2	8.20	134.62	116.85
6	B	601	FMN	C4A-C10-N10	7.04	126.55	116.48

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	601	FMN	N10-C1'-C2'-O2'
6	B	601	FMN	C3'-C4'-C5'-O5'

Continued on next page...

Continued from previous page...

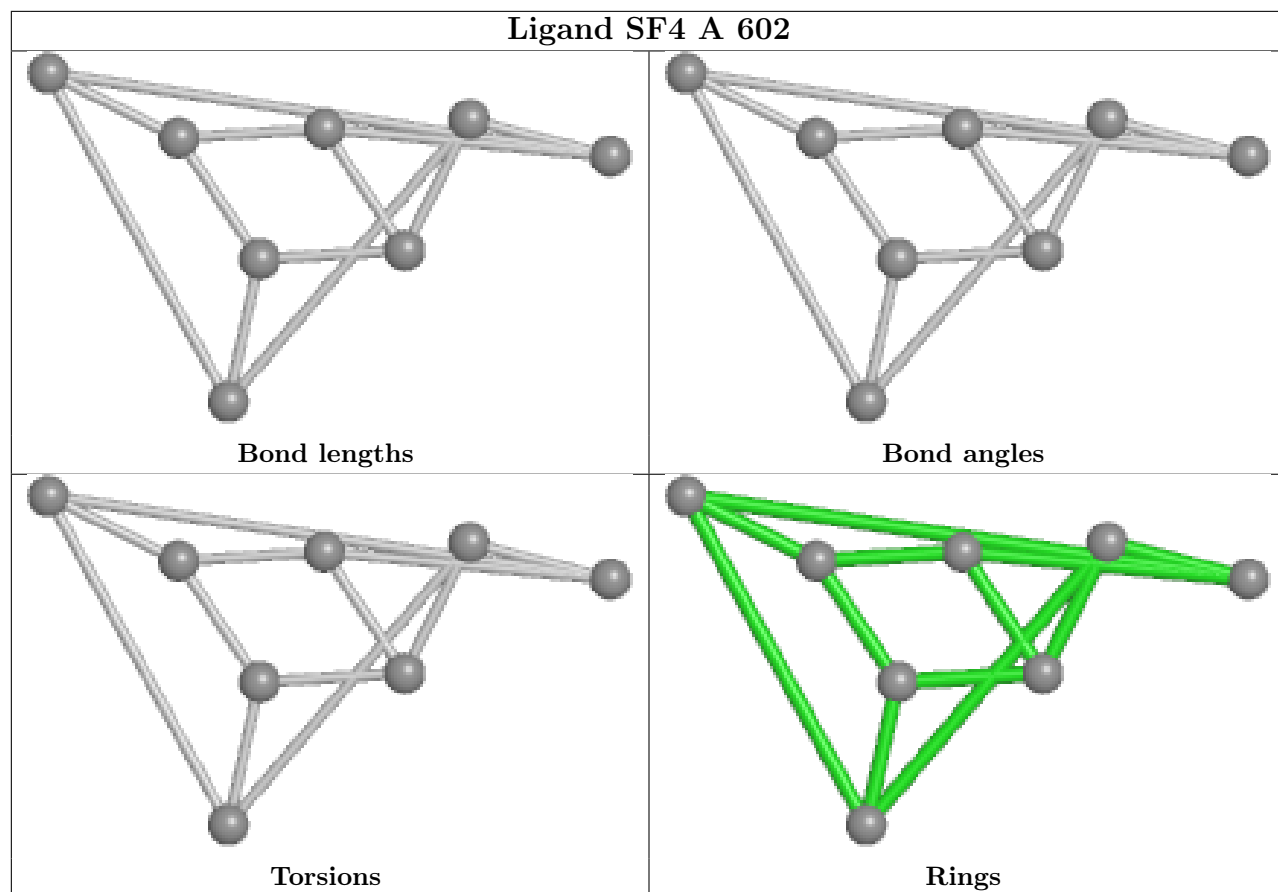
Mol	Chain	Res	Type	Atoms
6	B	601	FMN	O4'-C4'-C5'-O5'
6	B	601	FMN	C5'-O5'-P-O2P
6	B	601	FMN	C5'-O5'-P-O3P

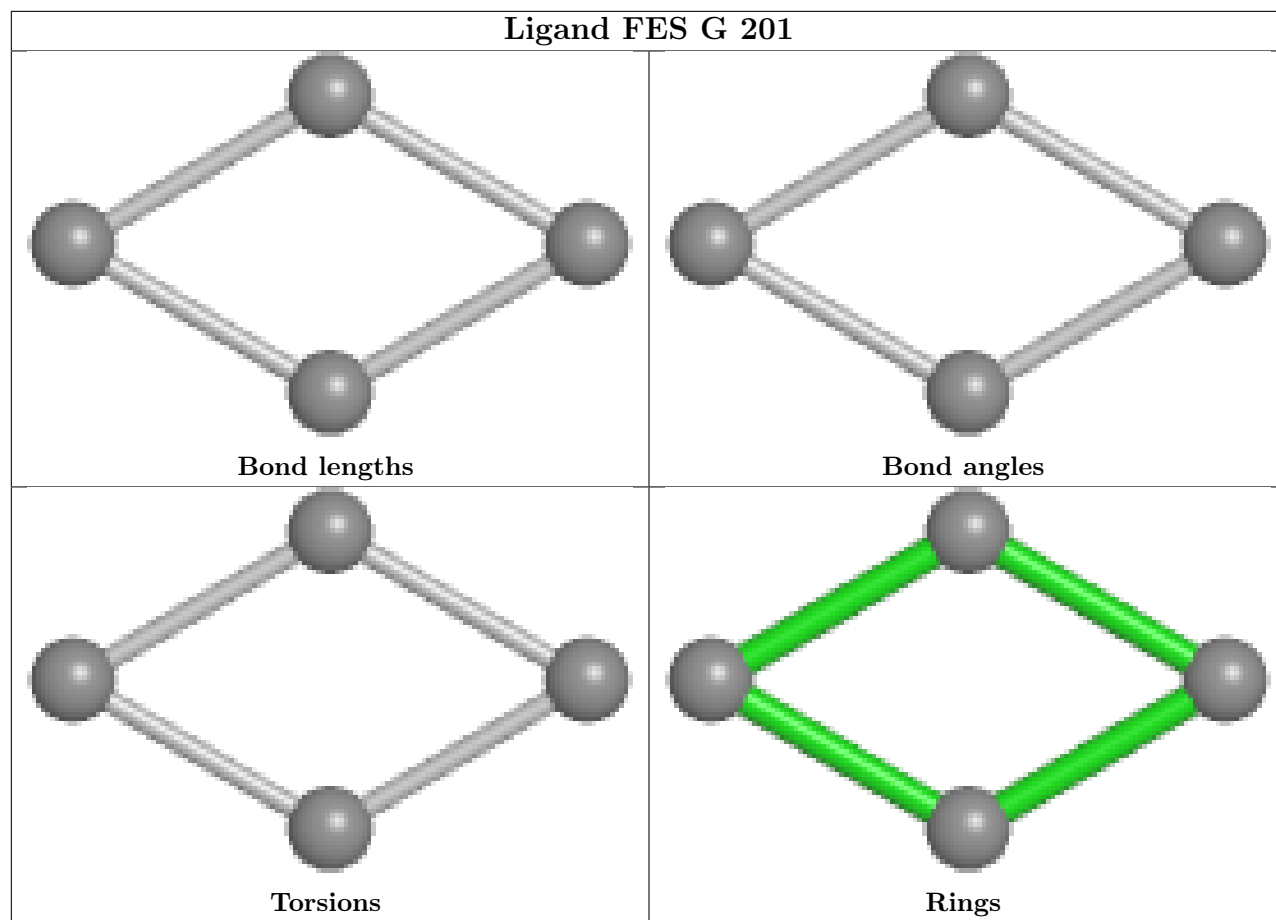
There are no ring outliers.

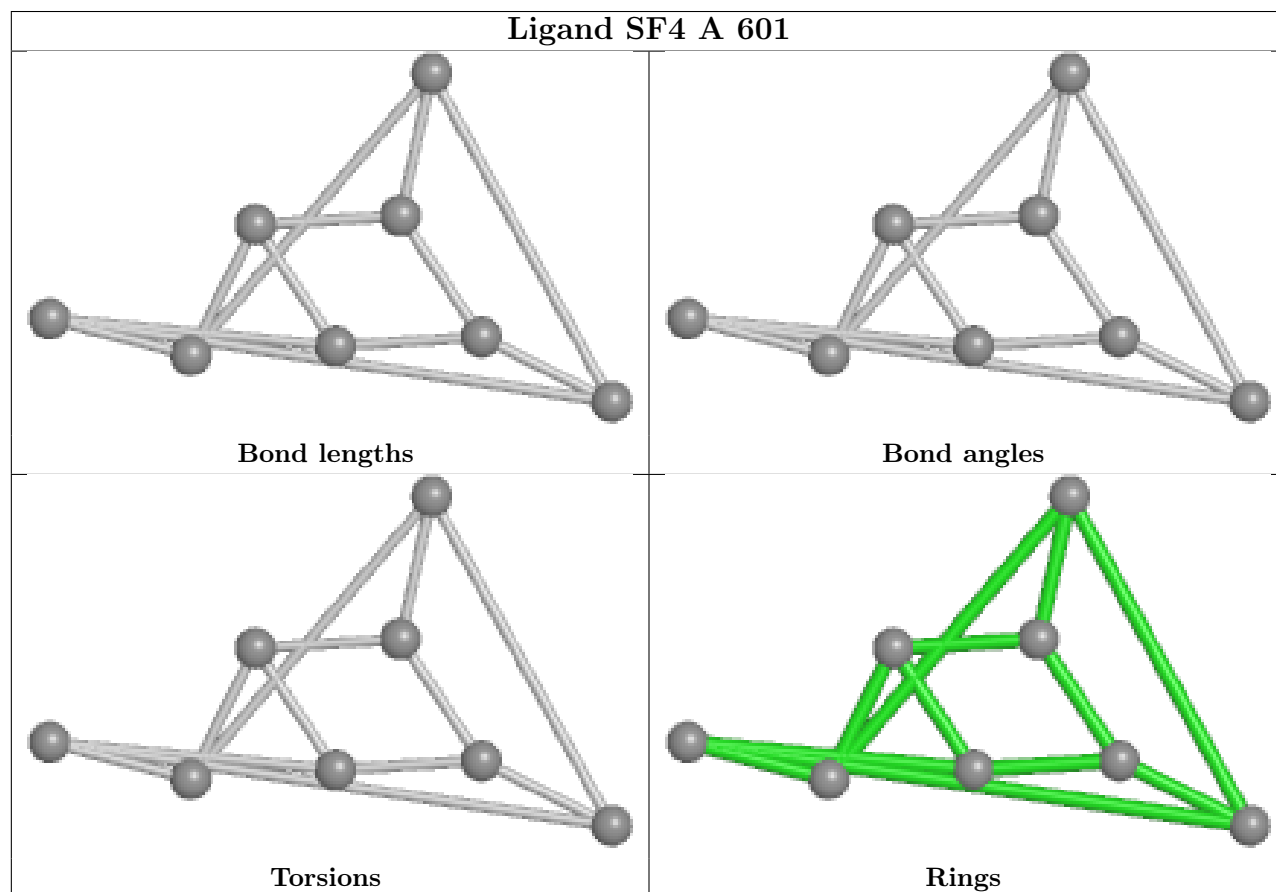
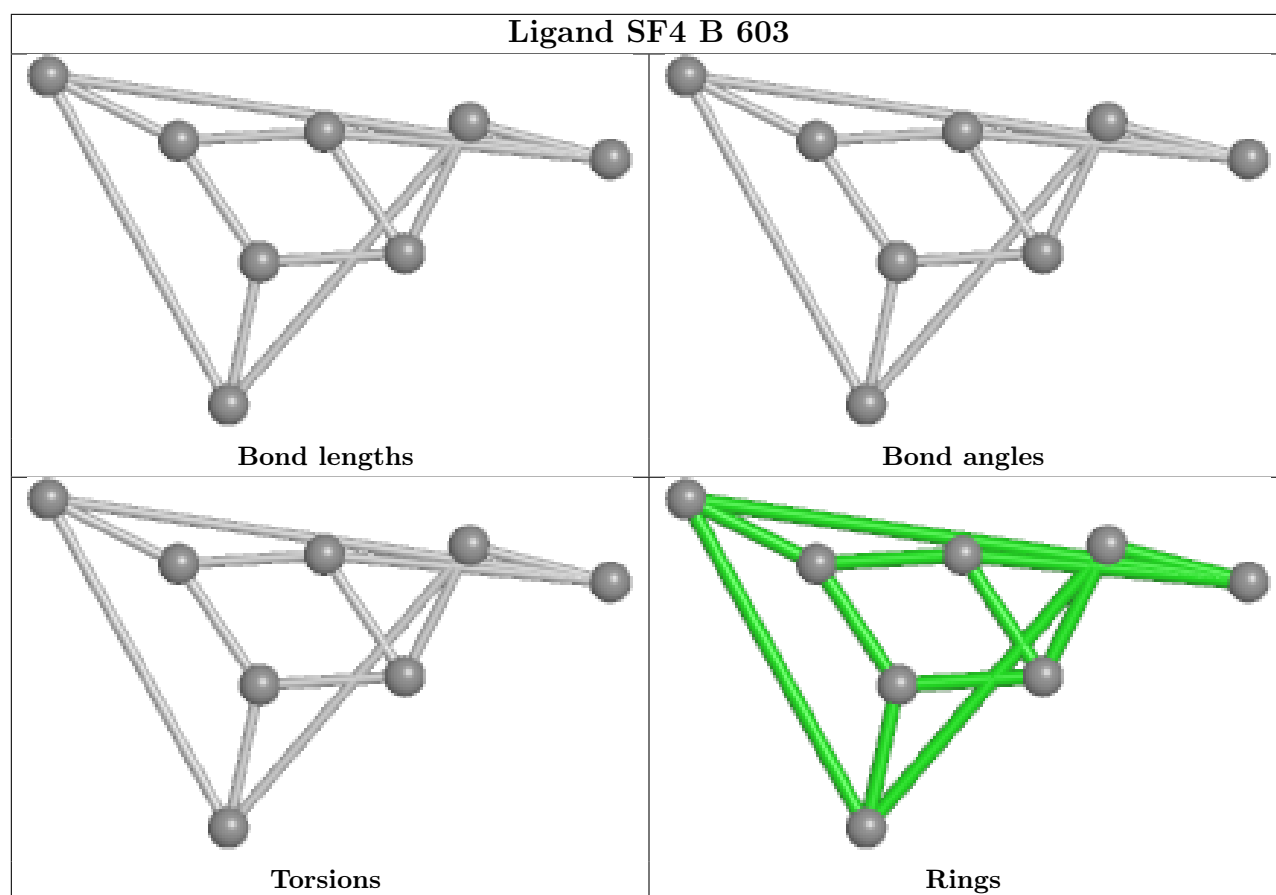
14 monomers are involved in 23 short contacts:

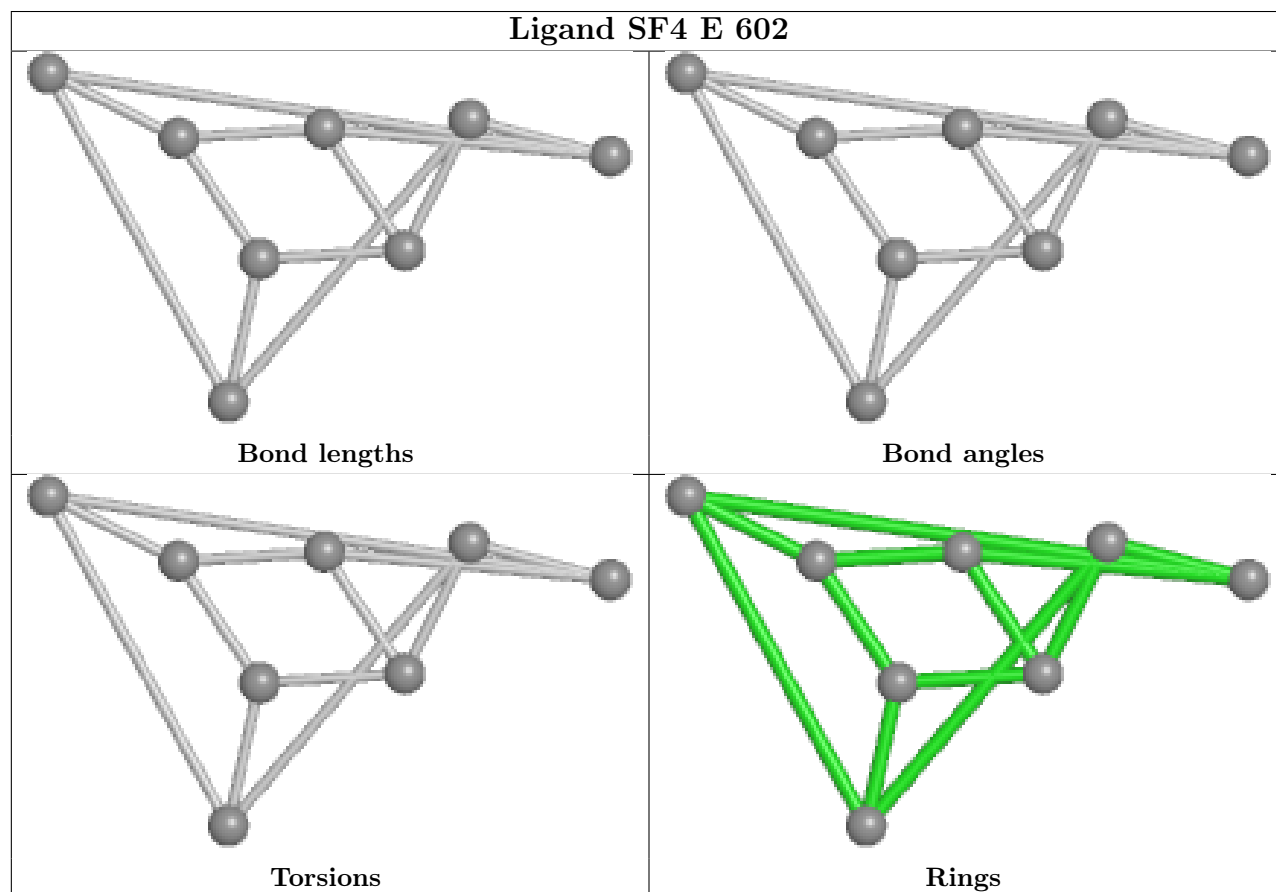
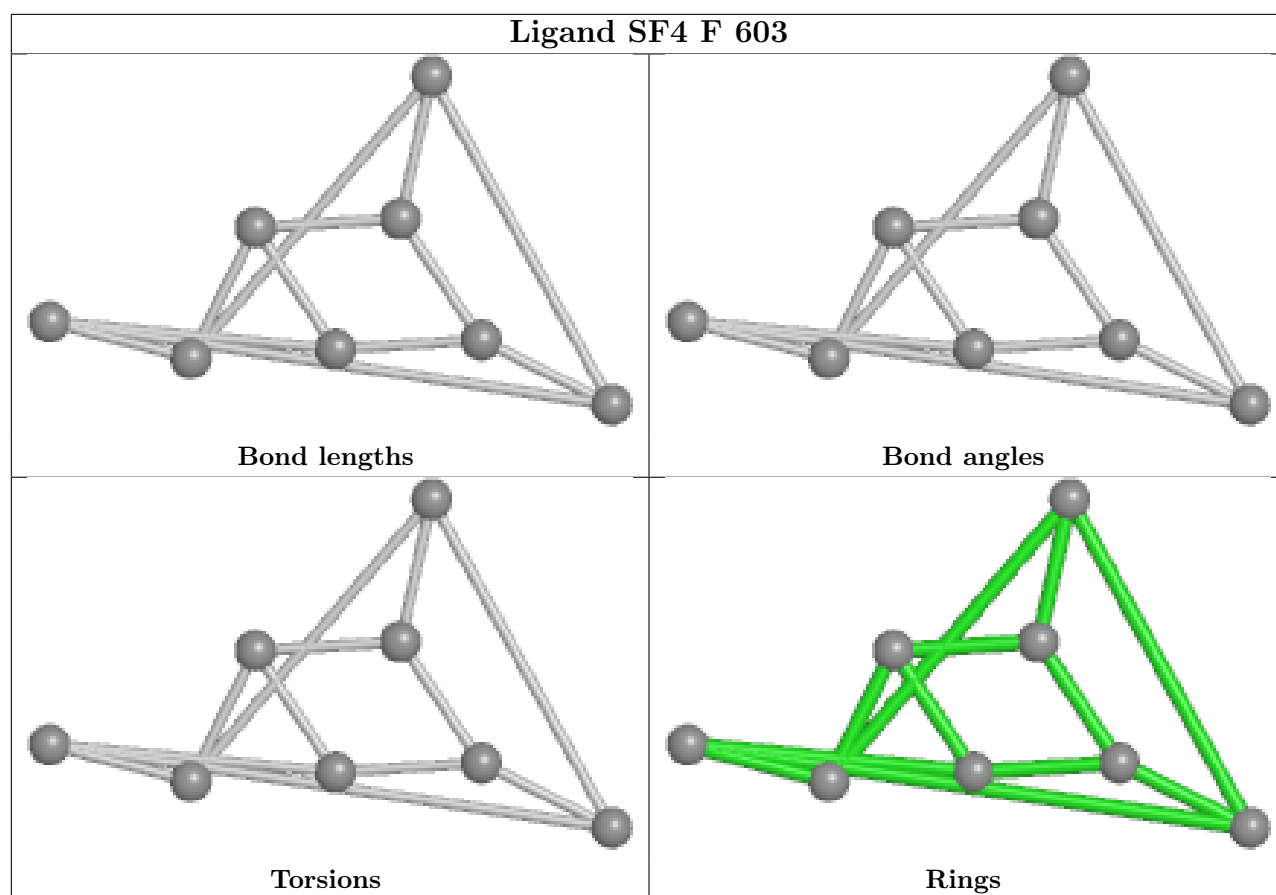
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	201	FES	1	0
4	B	603	SF4	1	0
4	A	601	SF4	2	0
4	F	603	SF4	1	0
5	A	605	FES	1	0
4	E	604	SF4	4	0
4	E	601	SF4	1	0
5	E	605	FES	1	0
4	B	602	SF4	3	0
4	E	603	SF4	1	0
4	A	604	SF4	3	0
4	F	605	SF4	1	0
5	C	201	FES	2	0
4	B	604	SF4	1	0

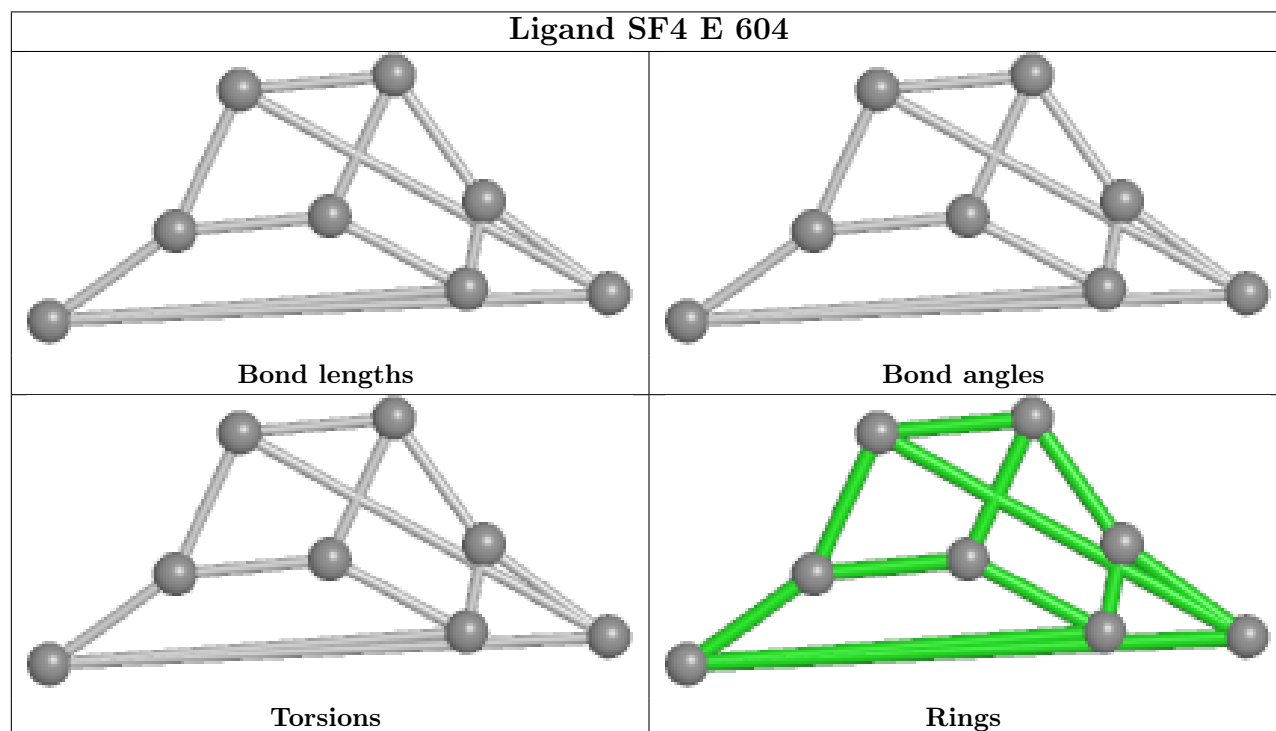
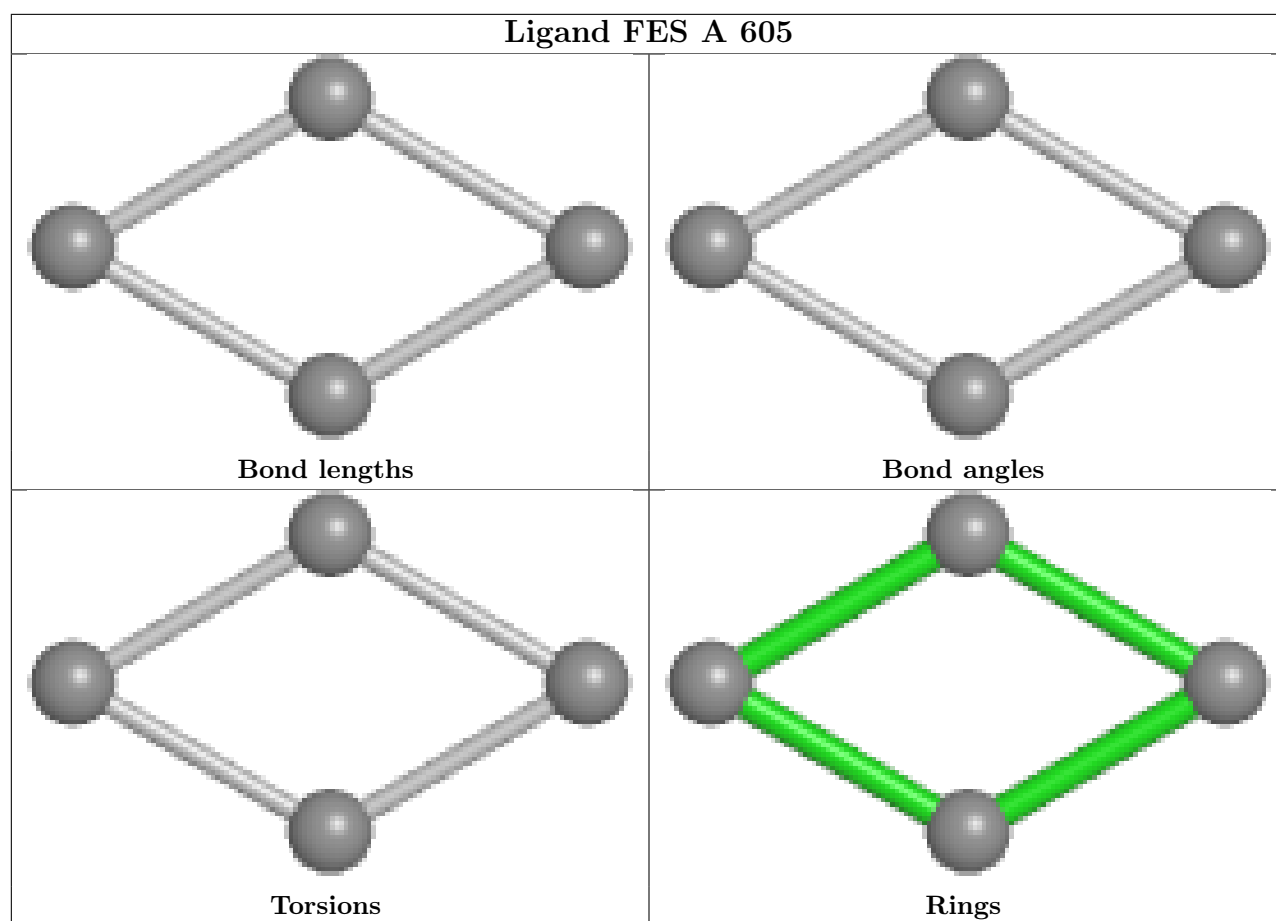
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

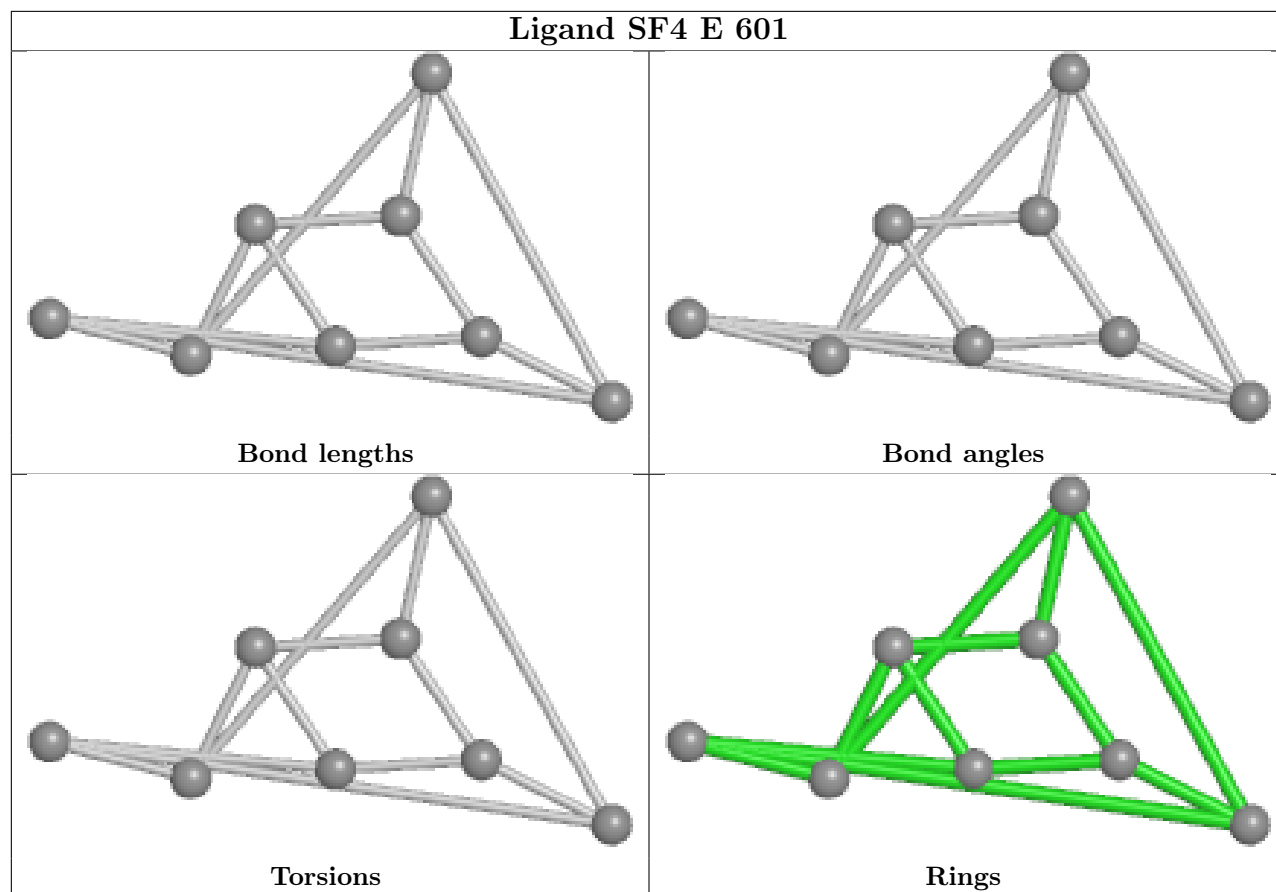


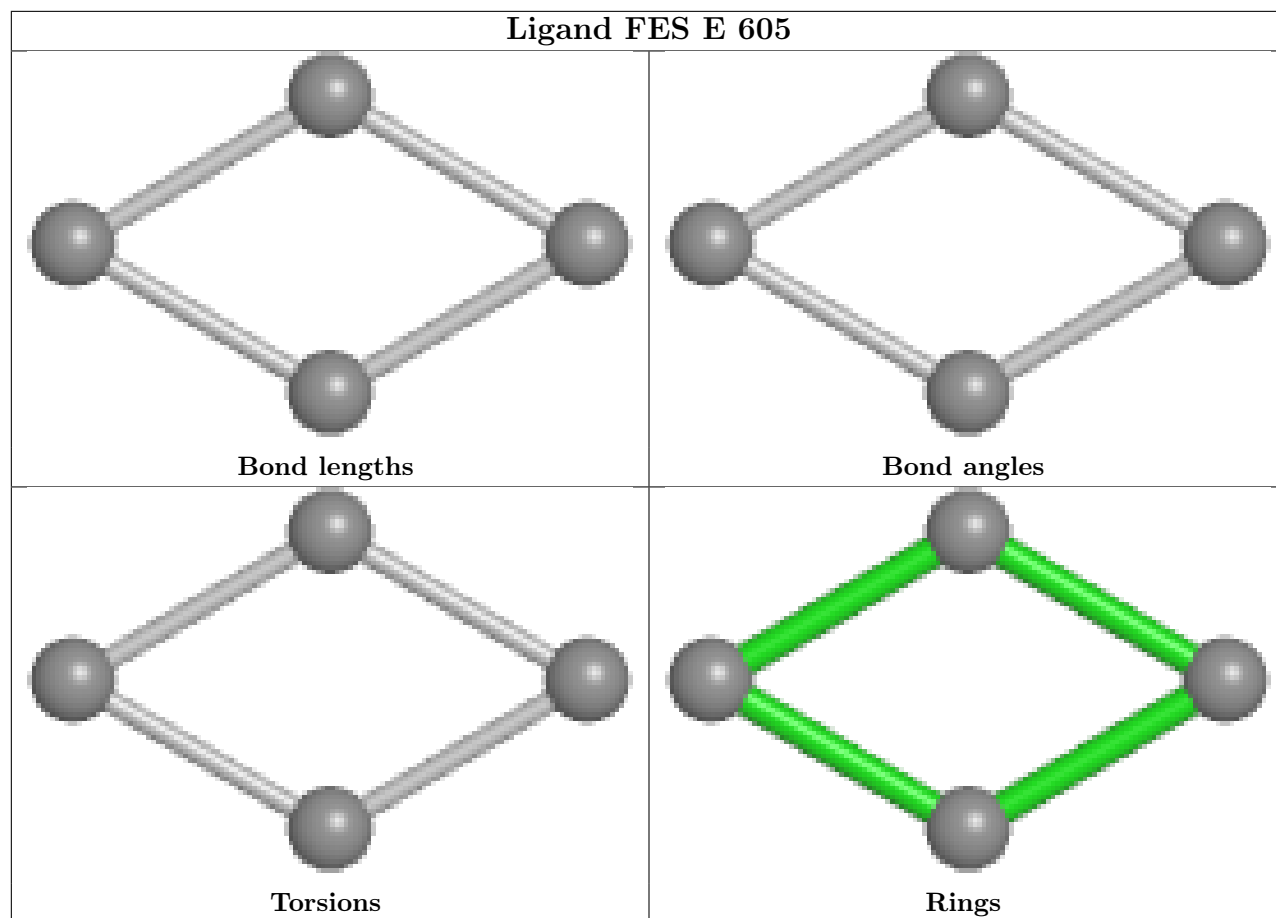




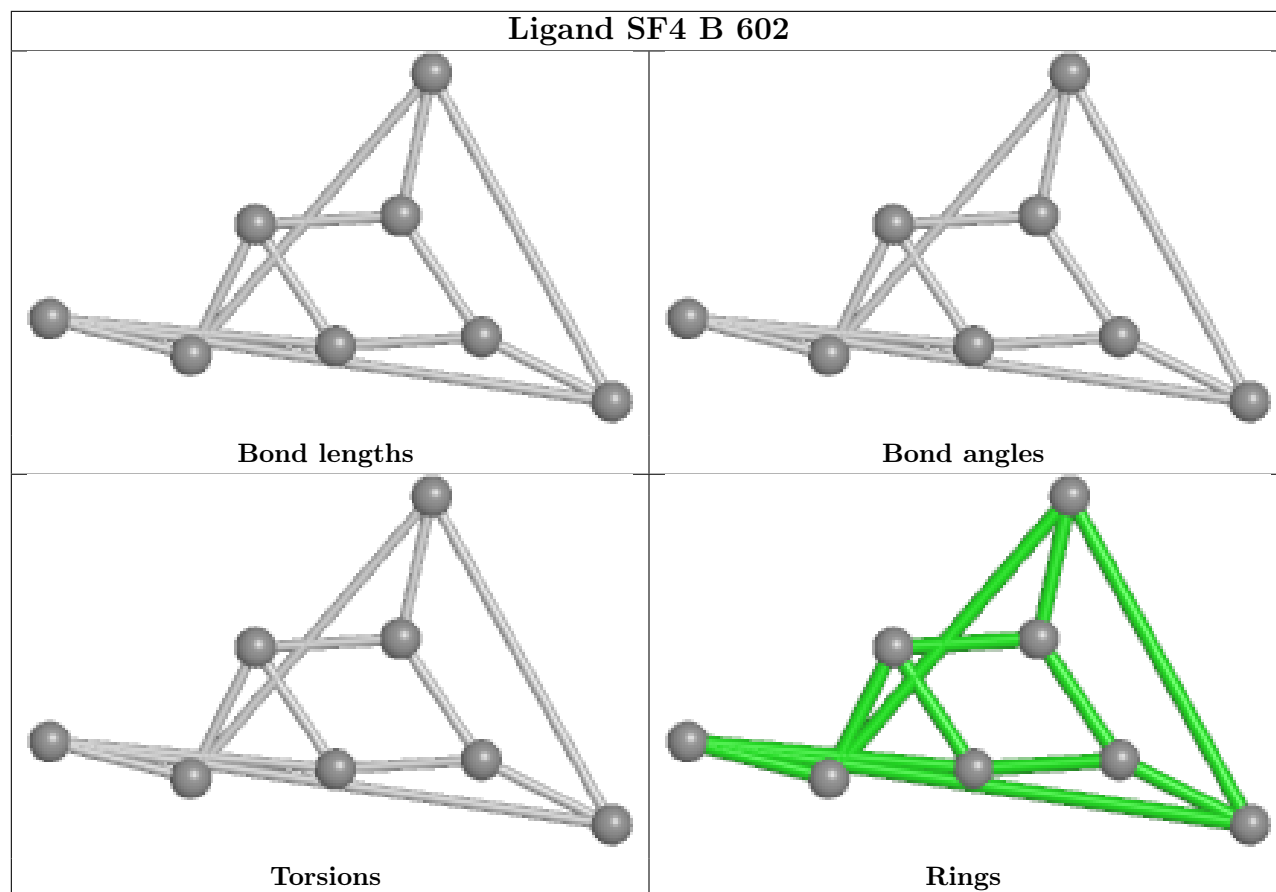




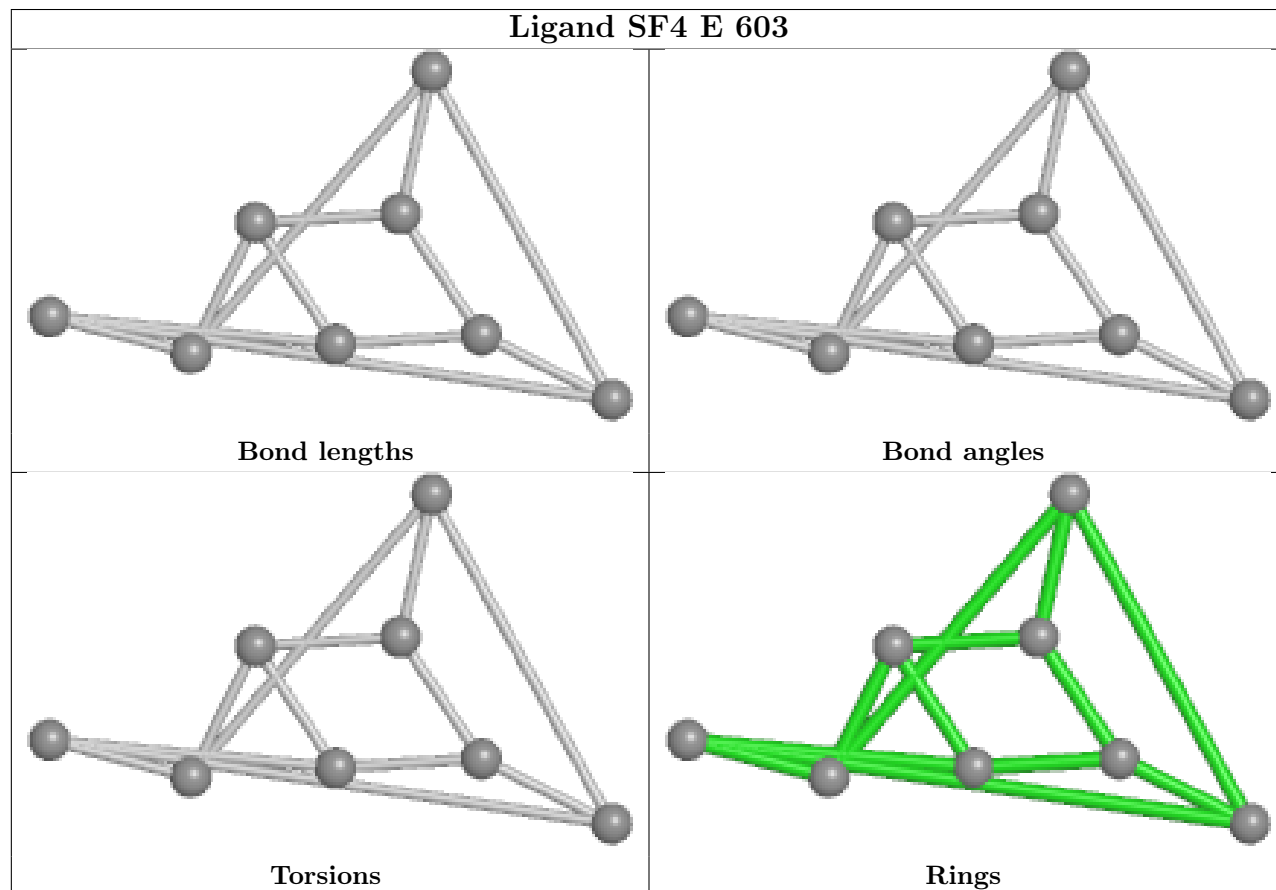


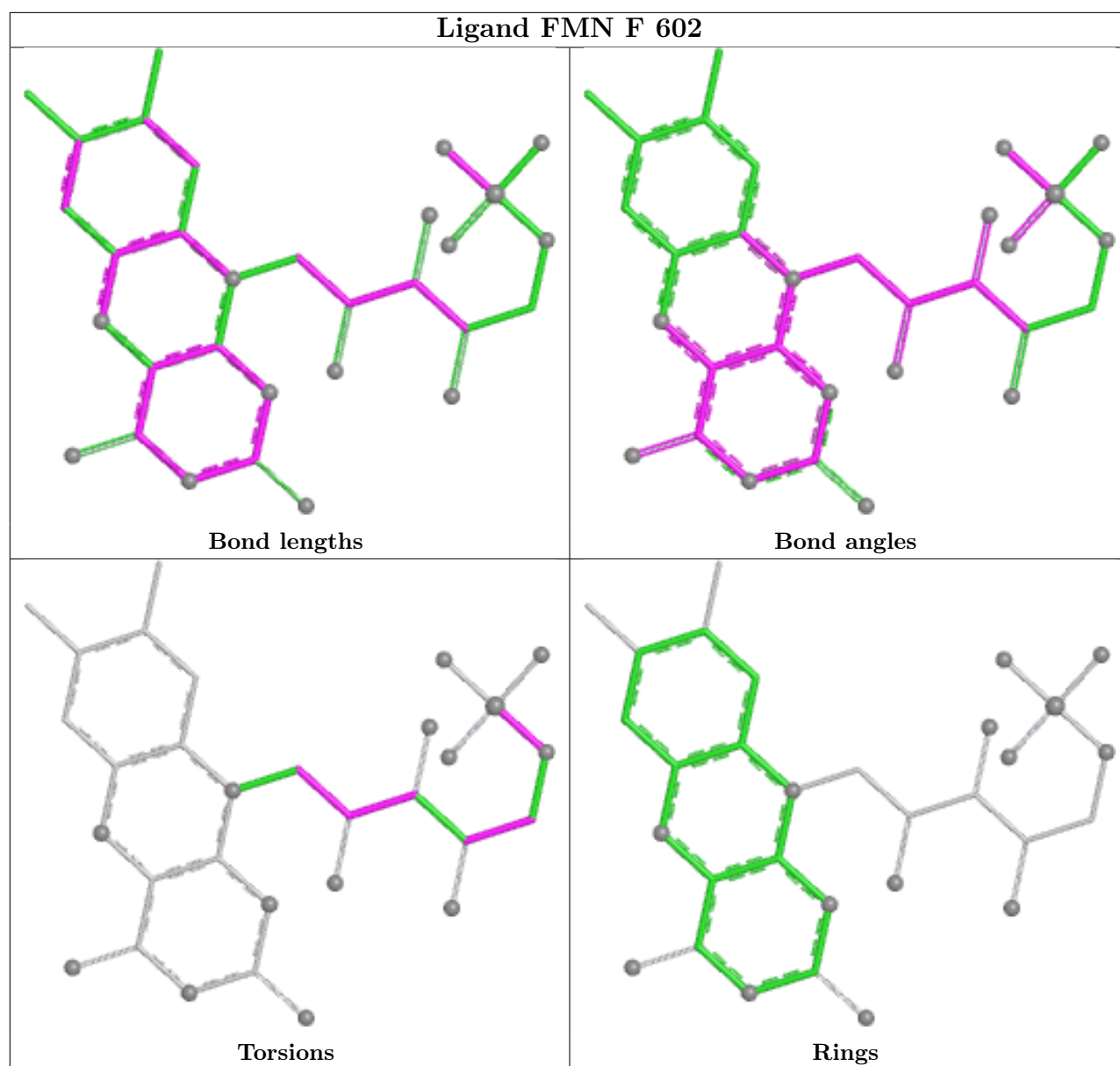


Ligand SF4 B 602

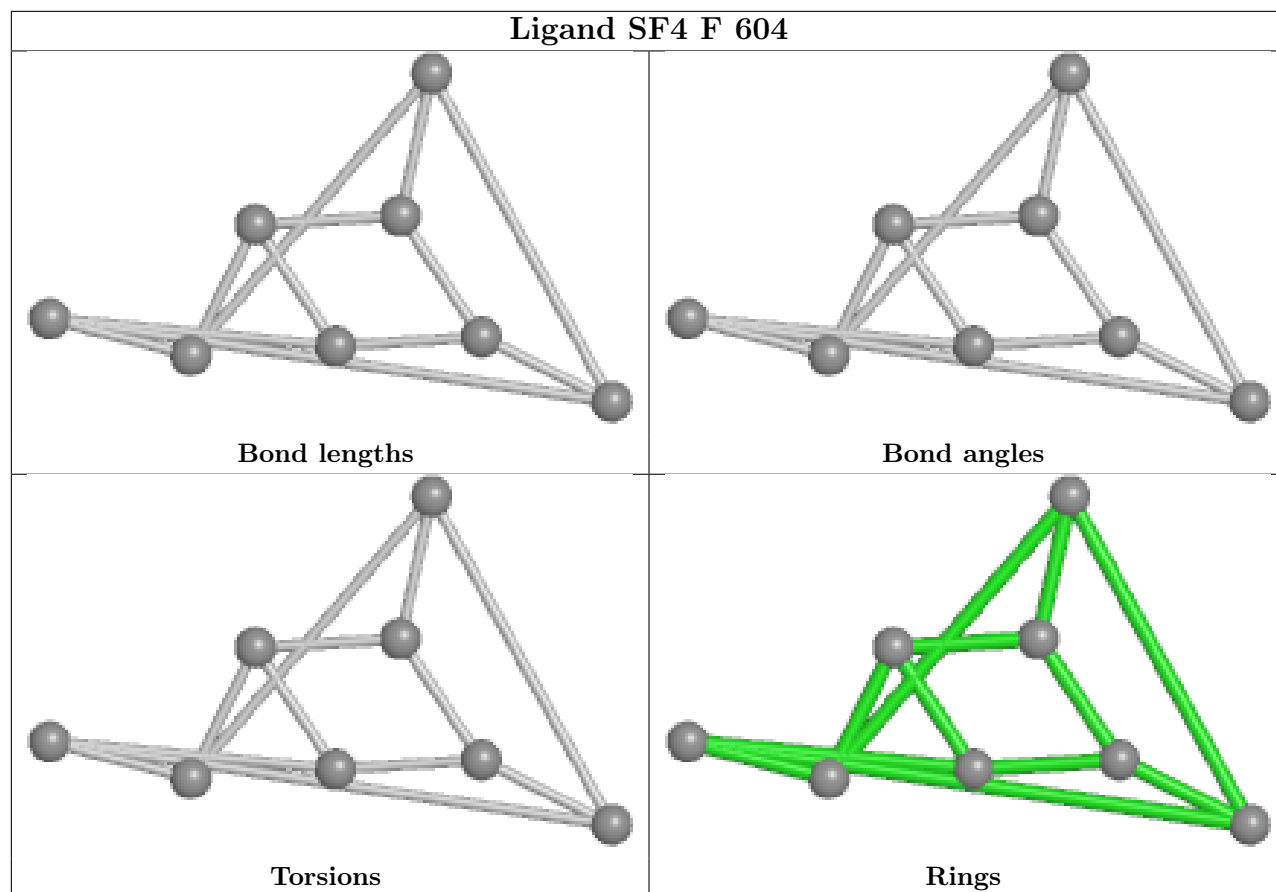


Ligand SF4 E 603

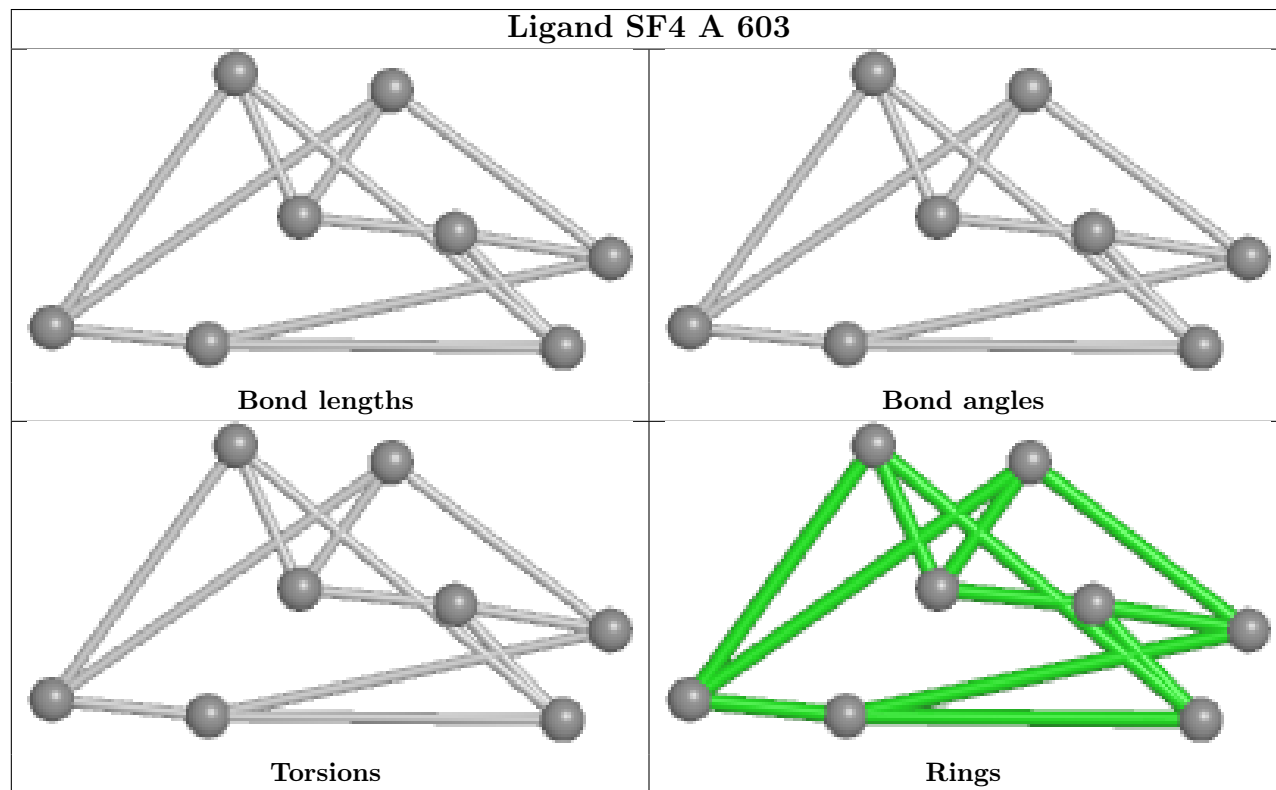


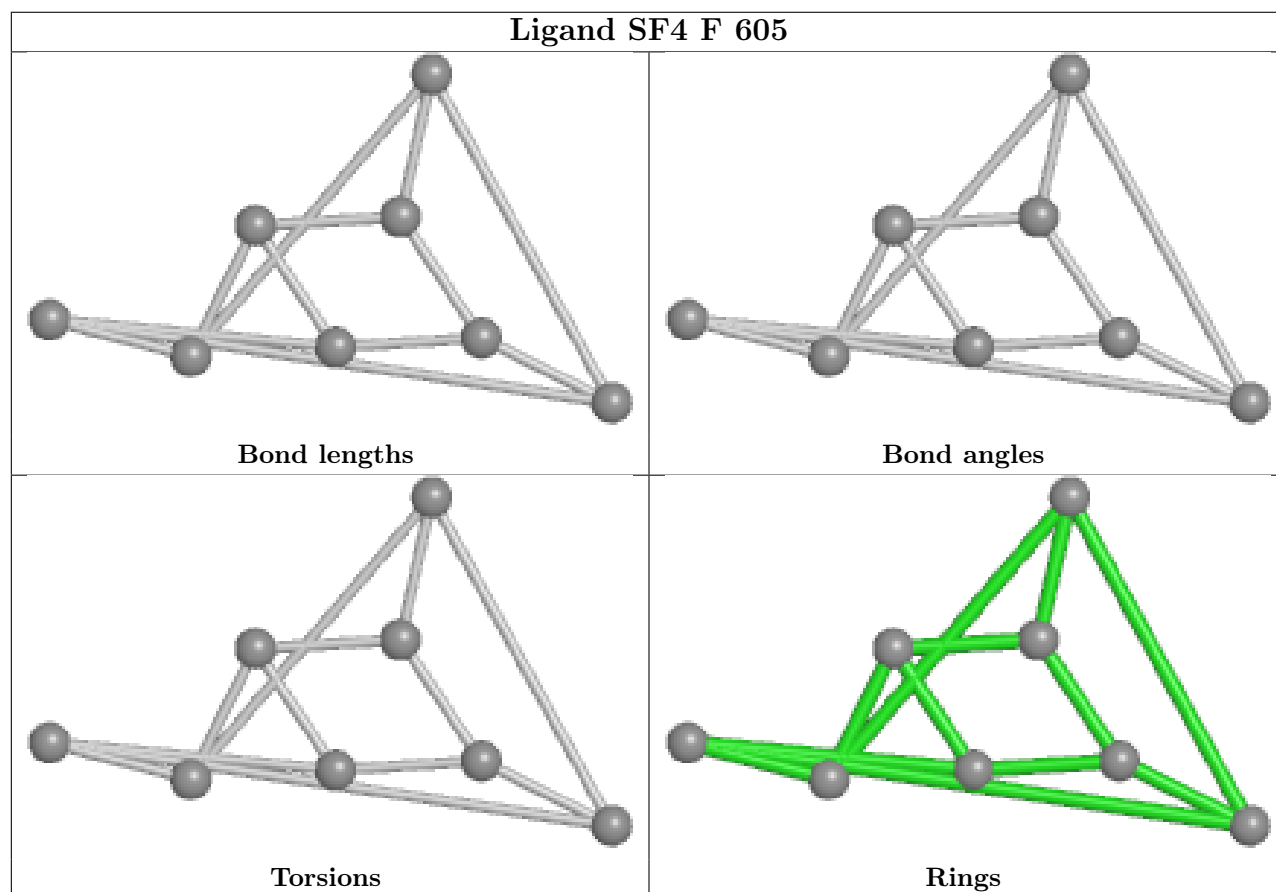
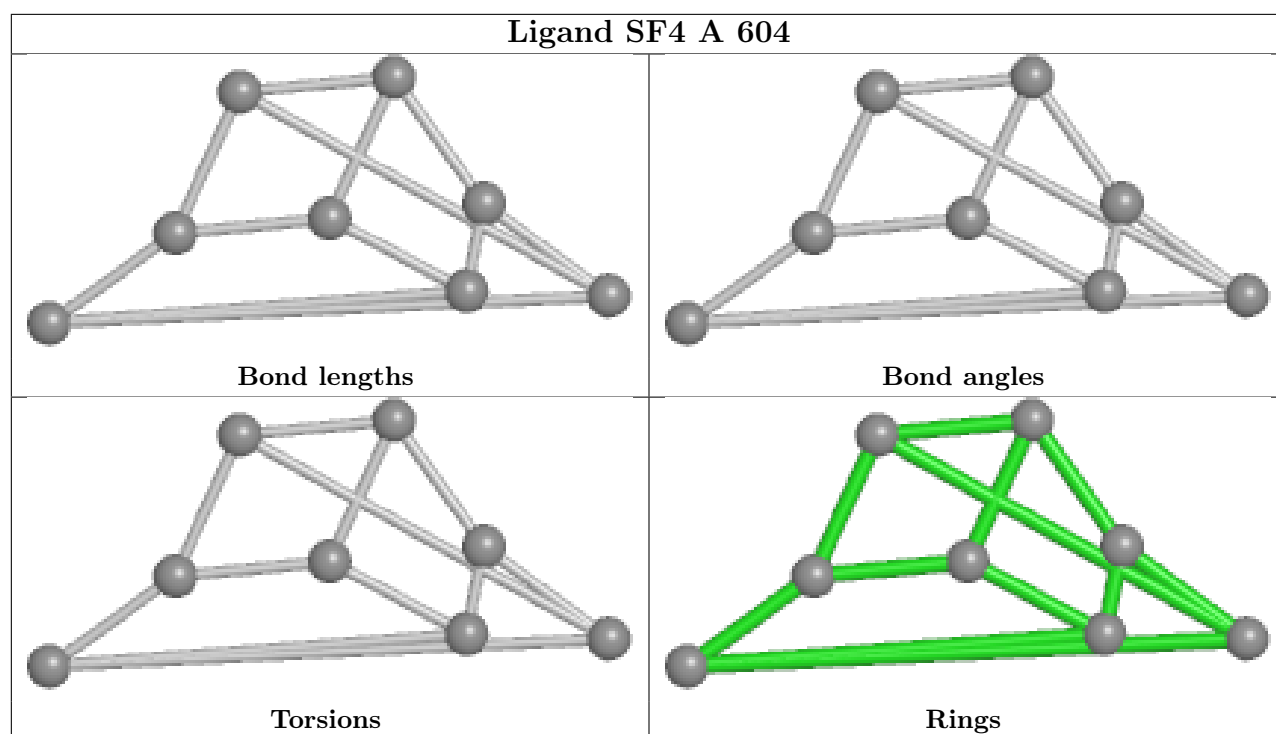


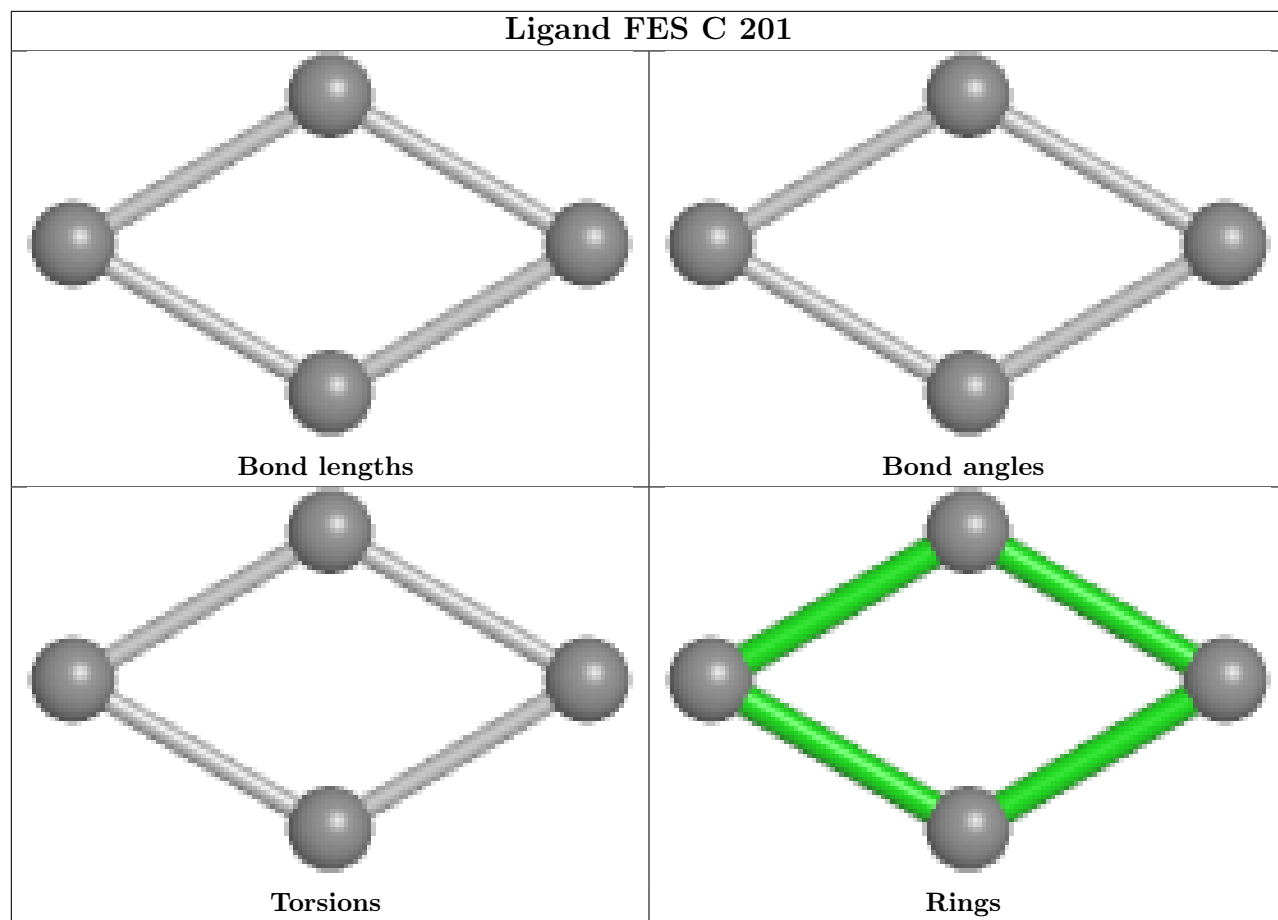
Ligand SF4 F 604

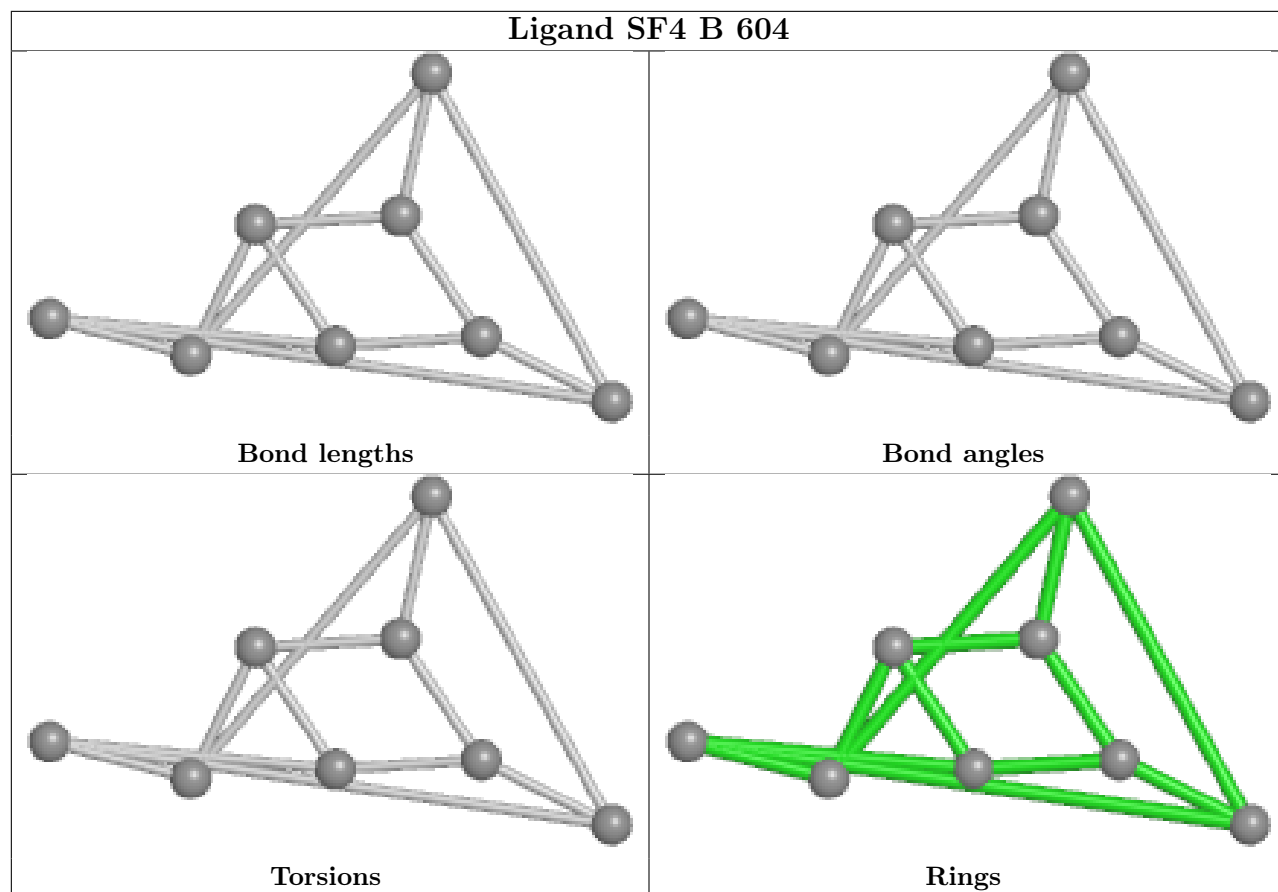


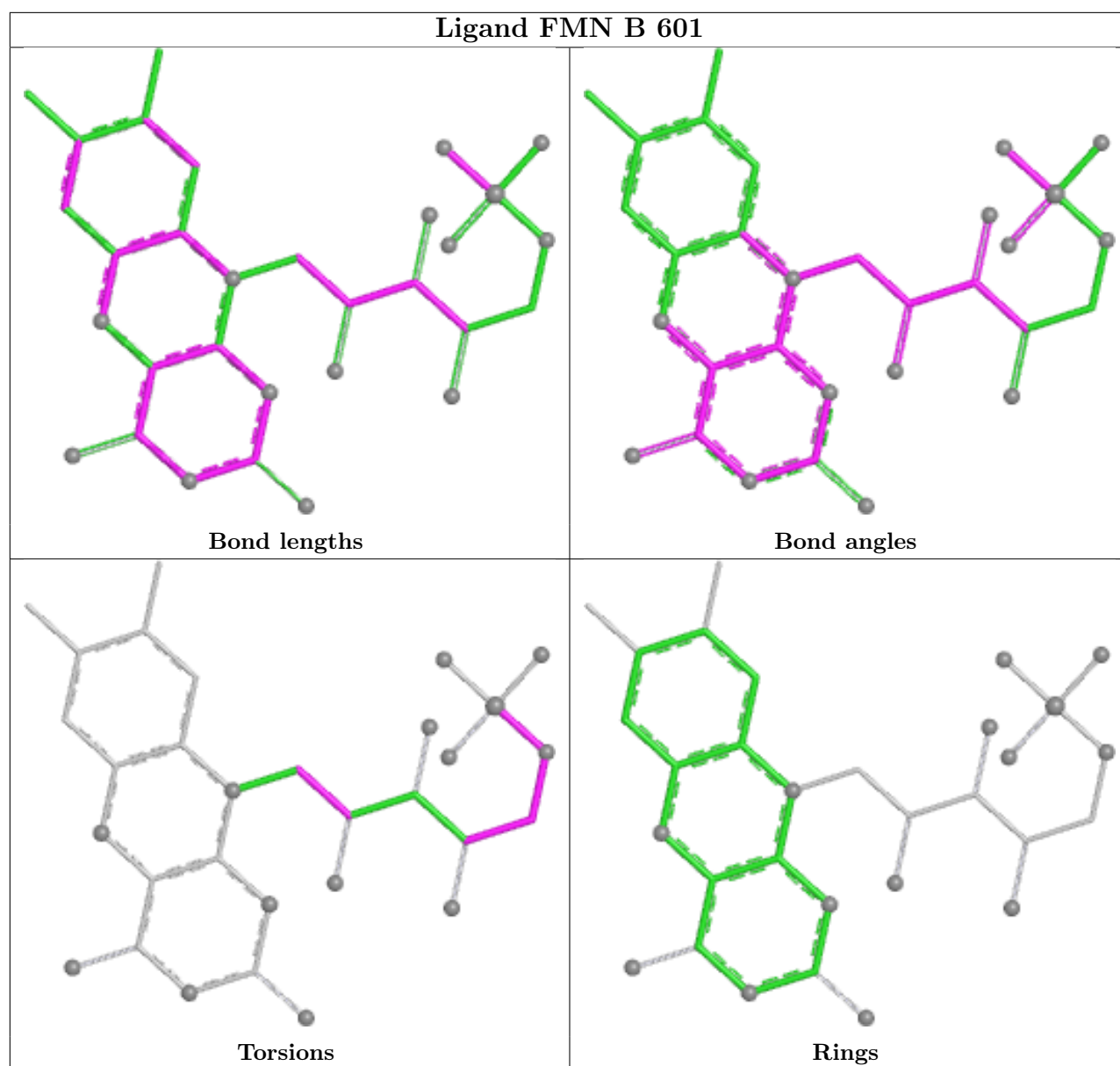
Ligand SF4 A 603











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 Map visualisation

This section contains visualisations of the EMDB entry EMD-13819. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.