



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 6, 2021 – 02:44 pm BST

PDB ID : 7B04  
Title : Structure of Nitrite oxidoreductase (Nxr) from the anammox bacterium *Kuenenia stuttgartiensis*.  
Authors : Moreno-Chicano, T.; Dietl, A.; Akram, M.; Barends, T.R.M.  
Deposited on : 2020-11-18  
Resolution : 2.97 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.22  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.22

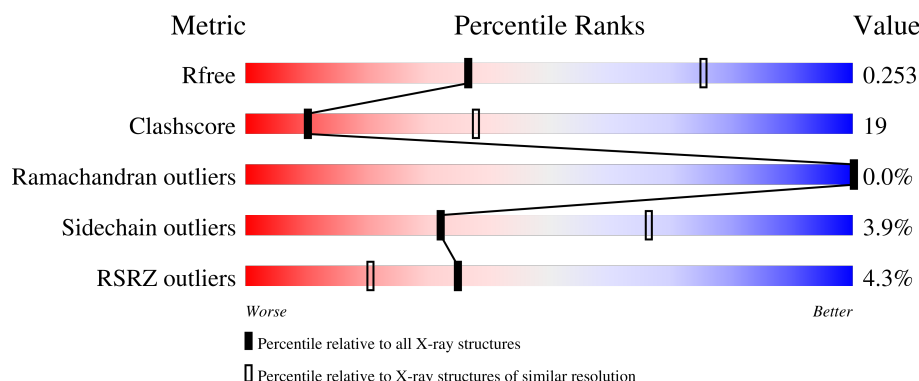
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.97 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))
$R_{free}$	130704	2754 (3.00-2.96)
Clashscore	141614	3103 (3.00-2.96)
Ramachandran outliers	138981	2993 (3.00-2.96)
Sidechain outliers	138945	2996 (3.00-2.96)
RSRZ outliers	127900	2644 (3.00-2.96)

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  $\geq 3$ , 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	410	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>74%</span> <span>25%</span> </div> </div>
1	D	410	<div> <div style="width: 100%; height: 10px; background-color: red; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">26%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>65%</span> <span>32%</span> </div> </div>
1	G	410	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">74%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>74%</span> <span>25%</span> </div> </div>
1	J	410	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">77%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>77%</span> <span>21%</span> </div> </div>
1	M	410	<div> <div style="width: 100%; height: 10px; background-color: green; position: relative;"> <span style="position: absolute; top: -10px; left: 0;">64%</span> </div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>64%</span> <span>34%</span> </div> </div>

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Mol	Chain	Length	Quality of chain
1	P	410	
1	S	410	
1	V	410	
2	B	1148	
2	E	1148	
2	H	1148	
2	K	1148	
2	N	1148	
2	Q	1148	
2	T	1148	
2	W	1148	
3	C	322	
3	F	322	
3	I	322	
3	L	322	
3	O	322	
3	R	322	
3	U	322	
3	X	322	

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	D	501	-	-	X	-
4	SF4	D	502	-	-	X	-
4	SF4	G	503	-	-	X	-
4	SF4	J	503	-	-	X	-
4	SF4	M	503	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	N	5804	-	-	X	-
4	SF4	P	503	-	-	X	-
4	SF4	Q	5804	-	-	X	-
4	SF4	S	503	-	-	X	-
4	SF4	T	5804	-	-	X	-
4	SF4	V	501	-	-	X	-
4	SF4	V	503	-	-	X	-
4	SF4	W	5804	-	-	X	-
5	F3S	D	504	-	-	X	-
5	F3S	M	504	-	-	X	-
5	F3S	V	504	-	-	X	-
6	MD1	E	5801	X	-	-	-
8	HEM	F	401	-	-	X	-
8	HEM	I	401	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 115931 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 Nitrite oxidoreductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3349	2138	579	606	26			
1	D	408	Total	C	N	O	S	0	0	0
			2872	1805	508	534	25			
1	G	409	Total	C	N	O	S	0	0	0
			3344	2138	578	602	26			
1	J	409	Total	C	N	O	S	0	0	0
			3361	2147	580	608	26			
1	M	409	Total	C	N	O	S	0	0	0
			3309	2114	572	597	26			
1	P	409	Total	C	N	O	S	0	0	0
			3321	2121	573	601	26			
1	S	409	Total	C	N	O	S	0	0	0
			3333	2131	577	599	26			
1	V	409	Total	C	N	O	S	0	0	0
			3239	2063	556	594	26			

- Molecule 2 is a protein called Nitrite oxidoreductase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1120	Total	C	N	O	S	0	1	0
			9003	5748	1551	1662	42			
2	E	1111	Total	C	N	O	S	0	1	0
			6871	4264	1247	1334	26			
2	H	1118	Total	C	N	O	S	0	1	0
			9028	5760	1561	1665	42			
2	K	1119	Total	C	N	O	S	0	1	0
			9046	5777	1559	1668	42			
2	N	1117	Total	C	N	O	S	0	3	0
			9052	5773	1564	1672	43			
2	Q	1116	Total	C	N	O	S	0	1	0
			8902	5678	1533	1649	42			

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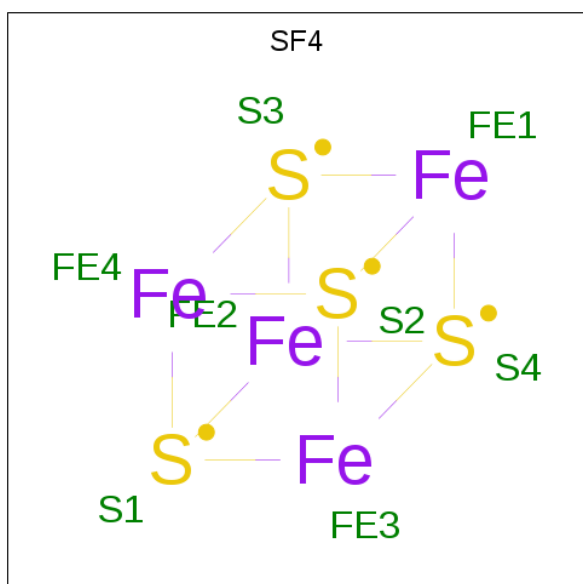
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	1119	Total	C	N	O	S	0	0	0
			9034	5766	1555	1671	42			
2	W	1118	Total	C	N	O	S	0	1	0
			8920	5688	1532	1658	42			

- Molecule 3 is a protein called Nitrite oxidoreductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	292	Total	C	N	O	S	0	1	0
			2281	1435	400	438	8			
3	F	292	Total	C	N	O	S	0	0	0
			2068	1305	358	398	7			
3	I	292	Total	C	N	O	S	0	0	0
			2216	1401	385	422	8			
3	L	292	Total	C	N	O	S	0	1	0
			2274	1431	396	439	8			
3	O	291	Total	C	N	O	S	0	0	0
			2124	1337	369	410	8			
3	R	291	Total	C	N	O	S	0	0	0
			2261	1423	392	438	8			
3	U	292	Total	C	N	O	S	0	0	0
			2267	1428	393	438	8			
3	X	292	Total	C	N	O	S	0	0	0
			2225	1401	387	429	8			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



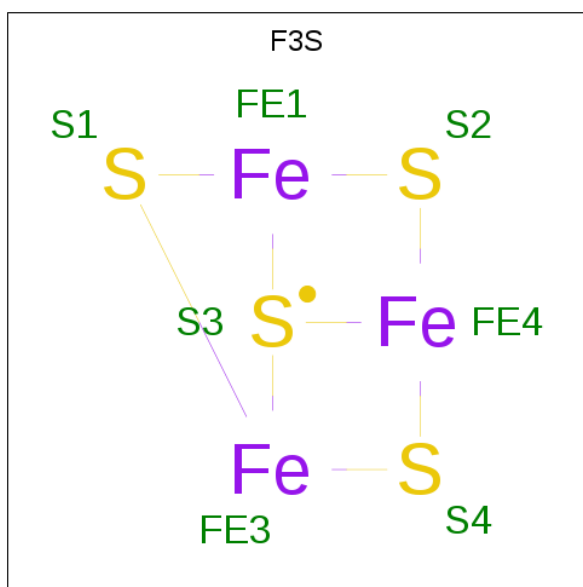
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	A	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	D	1	Total 8	Fe 4	S 4	0	0
4	E	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	G	1	Total 8	Fe 4	S 4	0	0
4	H	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	J	1	Total 8	Fe 4	S 4	0	0
4	K	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	M	1	Total 8	Fe 4	S 4	0	0
4	N	1	Total 8	Fe 4	S 4	0	0
4	P	1	Total 8	Fe 4	S 4	0	0
4	P	1	Total 8	Fe 4	S 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	P	1	Total	Fe	S	0	0
			8	4	4		
4	Q	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	S	1	Total	Fe	S	0	0
			8	4	4		
4	T	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	V	1	Total	Fe	S	0	0
			8	4	4		
4	W	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is FE3-S4 CLUSTER (three-letter code: F3S) (formula:  $\text{Fe}_3\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



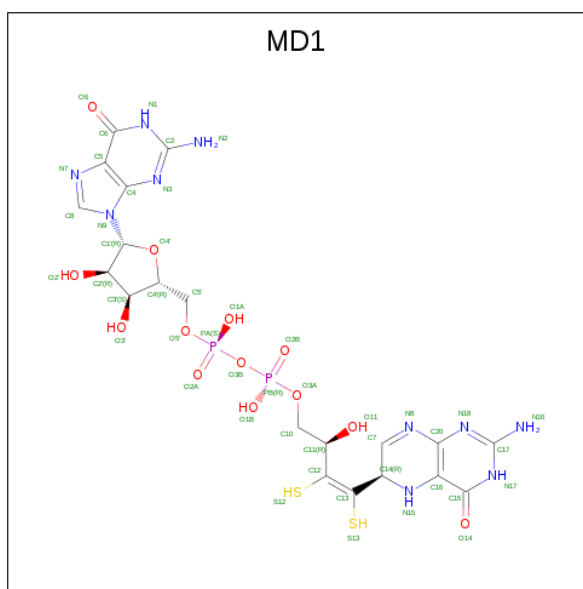
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Fe	S	0	0
			7	3	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	Fe	S	0	0
			7	3	4		
5	G	1	Total	Fe	S	0	0
			7	3	4		
5	J	1	Total	Fe	S	0	0
			7	3	4		
5	M	1	Total	Fe	S	0	0
			7	3	4		
5	P	1	Total	Fe	S	0	0
			7	3	4		
5	S	1	Total	Fe	S	0	0
			7	3	4		
5	V	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 6 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTERIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (three-letter code: MD1) (formula: C<sub>20</sub>H<sub>26</sub>N<sub>10</sub>O<sub>13</sub>P<sub>2</sub>S<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	B	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	E	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	H	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	K	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	N	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	Q	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	T	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0
6	W	1	Total 47	C 20	N 10	O 13	P 2	S 2	0	0

- Molecule 7 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

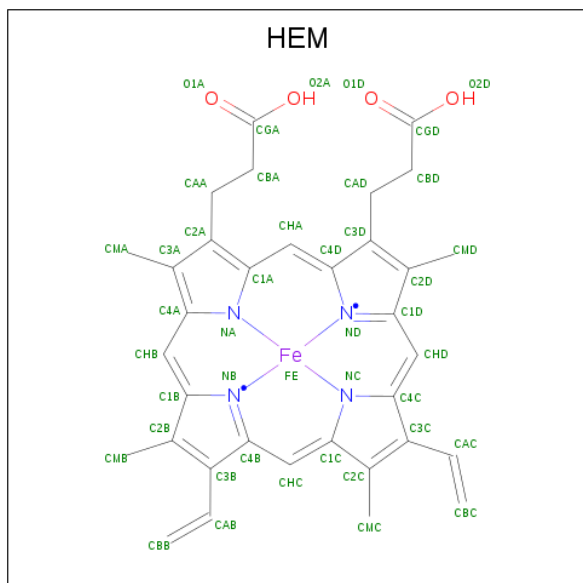
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Mo 1	0	0
7	E	1	Total 1	Mo 1	0	0
7	H	1	Total 1	Mo 1	0	0
7	K	1	Total 1	Mo 1	0	0
7	N	1	Total 1	Mo 1	0	0
7	Q	1	Total 1	Mo 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	T	1	Total	Mo	0	0
			1	1		
7	W	1	Total	Mo	0	0
			1	1		

- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	2	Total 2 Ca 2	0	0
9	F	2	Total 2 Ca 2	0	0
9	I	2	Total 2 Ca 2	0	0
9	L	2	Total 2 Ca 2	0	0
9	O	2	Total 2 Ca 2	0	0
9	R	2	Total 2 Ca 2	0	0
9	U	2	Total 2 Ca 2	0	0
9	X	2	Total 2 Ca 2	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	37	Total 37 O 37	0	0
10	B	72	Total 72 O 72	0	0
10	C	35	Total 35 O 35	0	0
10	D	6	Total 6 O 6	0	0
10	E	13	Total 13 O 13	0	0
10	F	8	Total 8 O 8	0	0
10	G	25	Total 25 O 25	0	0
10	H	83	Total 83 O 83	0	0
10	I	20	Total 20 O 20	0	0
10	J	28	Total 28 O 28	0	0
10	K	74	Total 74 O 74	0	0
10	L	30	Total 30 O 30	0	0

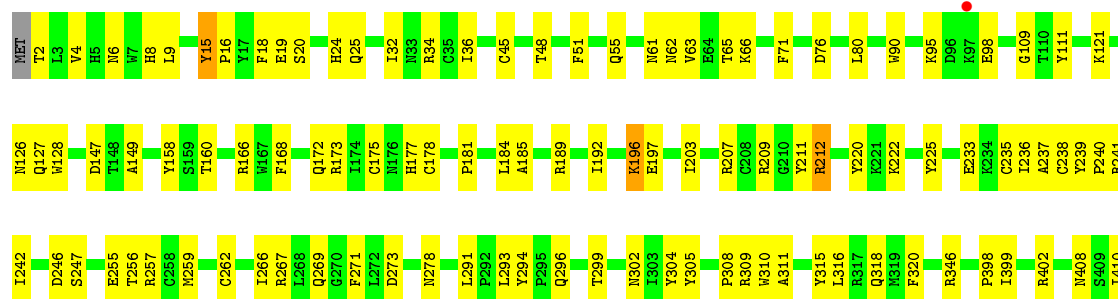
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	M	10	Total 10	O 10	0	0
10	N	76	Total 76	O 76	0	0
10	O	17	Total 17	O 17	0	0
10	P	16	Total 16	O 16	0	0
10	Q	43	Total 43	O 43	0	0
10	R	22	Total 22	O 22	0	0
10	S	20	Total 20	O 20	0	0
10	T	62	Total 62	O 62	0	0
10	U	25	Total 25	O 25	0	0
10	V	12	Total 12	O 12	0	0
10	W	41	Total 41	O 41	0	0
10	X	24	Total 24	O 24	0	0

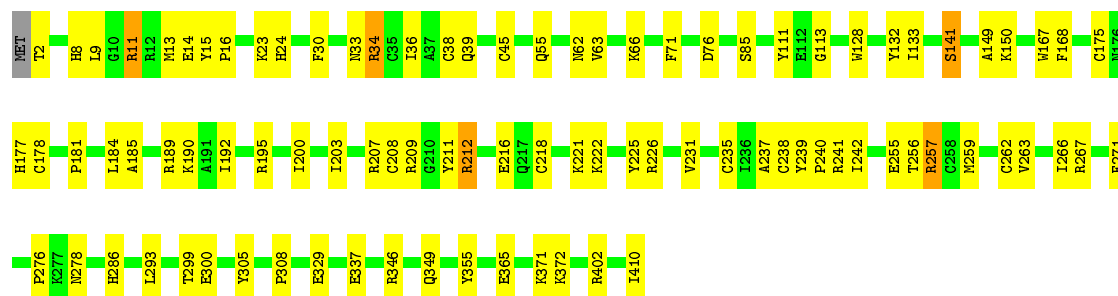


Chain G:  74% 25% .



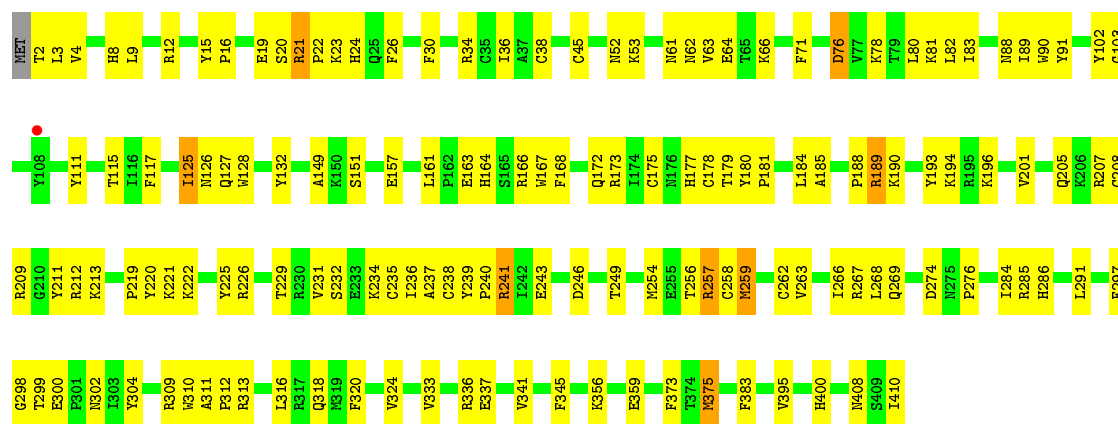
• Molecule 1: Nitrite oxidoreductase subunit B

Chain J:  77% 21% .



• Molecule 1: Nitrite oxidoreductase subunit B

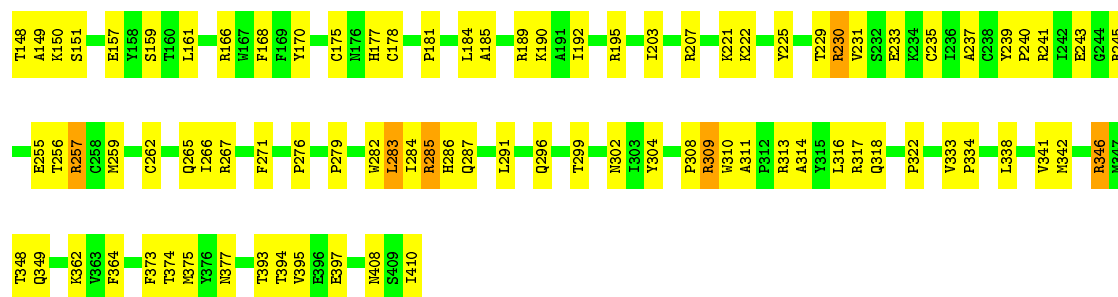
Chain M:  64% 34% .



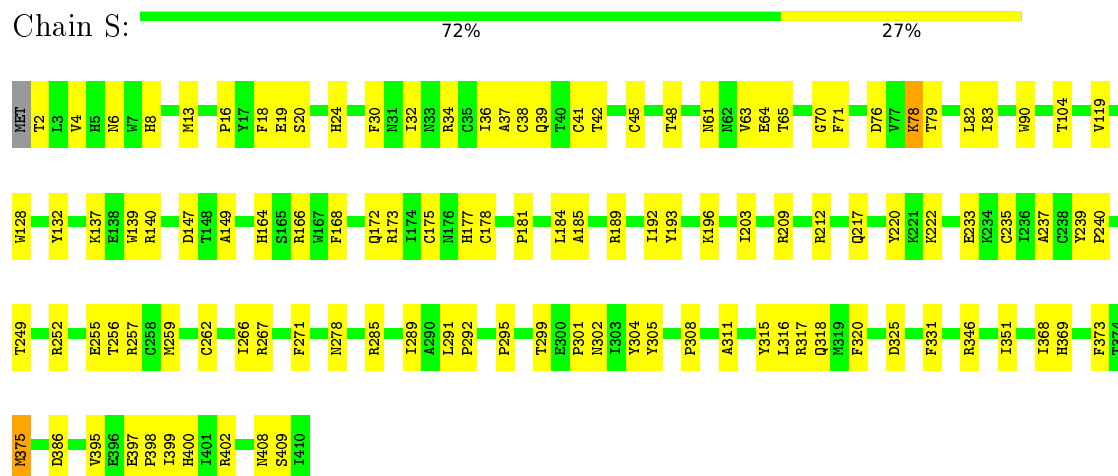
• Molecule 1: Nitrite oxidoreductase subunit B

Chain P:  70% 28% .

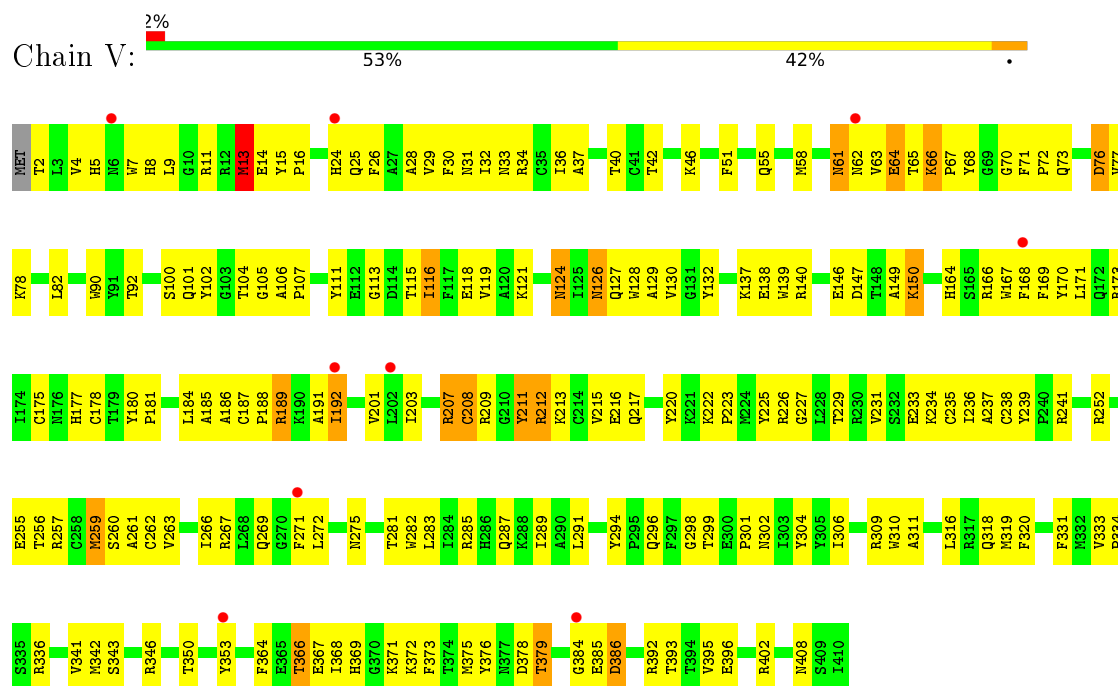




• Molecule 1: Nitrite oxidoreductase subunit B



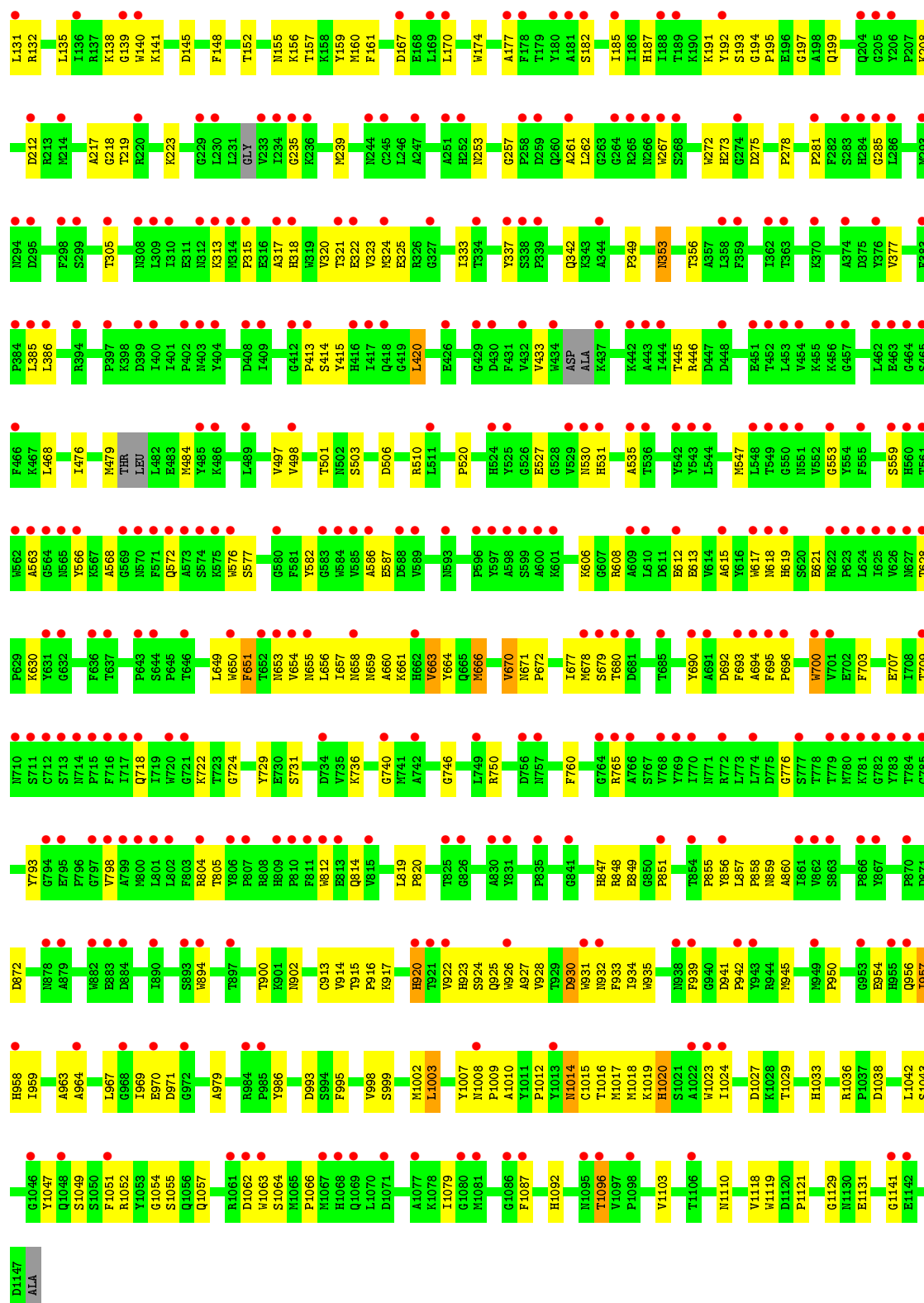
• Molecule 1: Nitrite oxidoreductase subunit B



• Molecule 2: Nitrite oxidoreductase subunit A







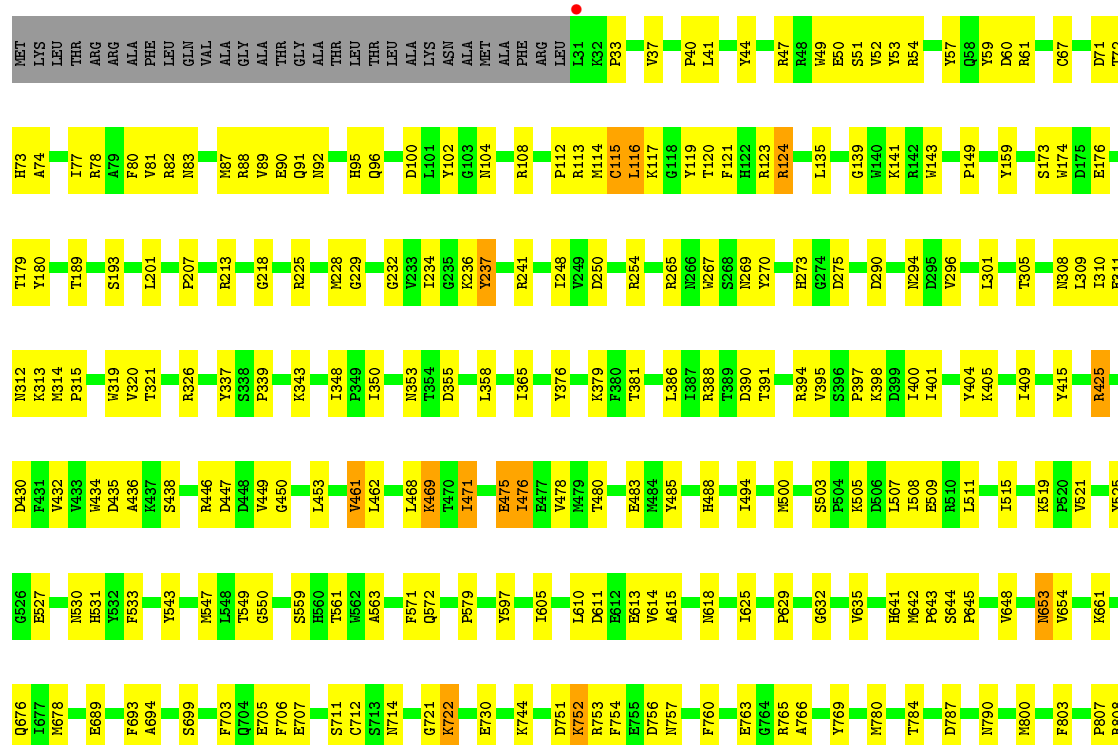
• Molecule 2: Nitrite oxidoreductase subunit A

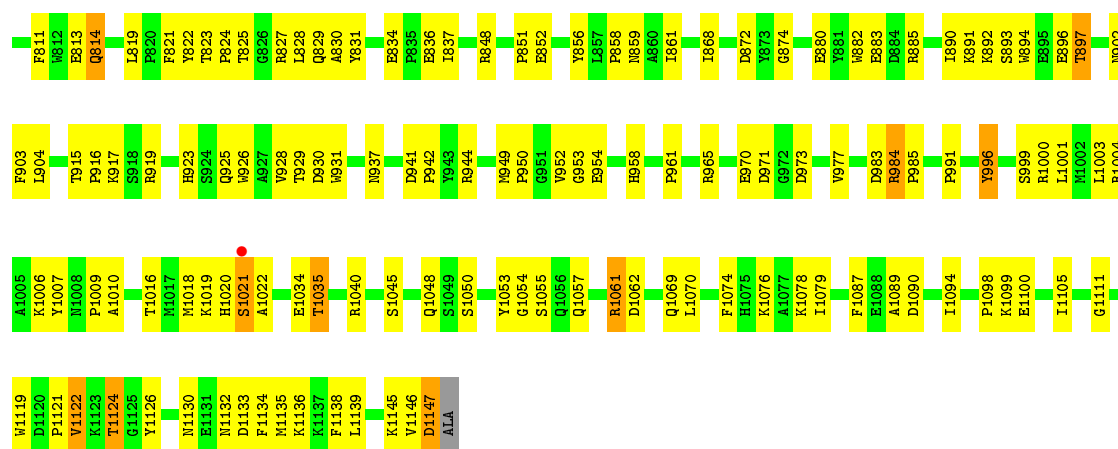
Chain H:

69%

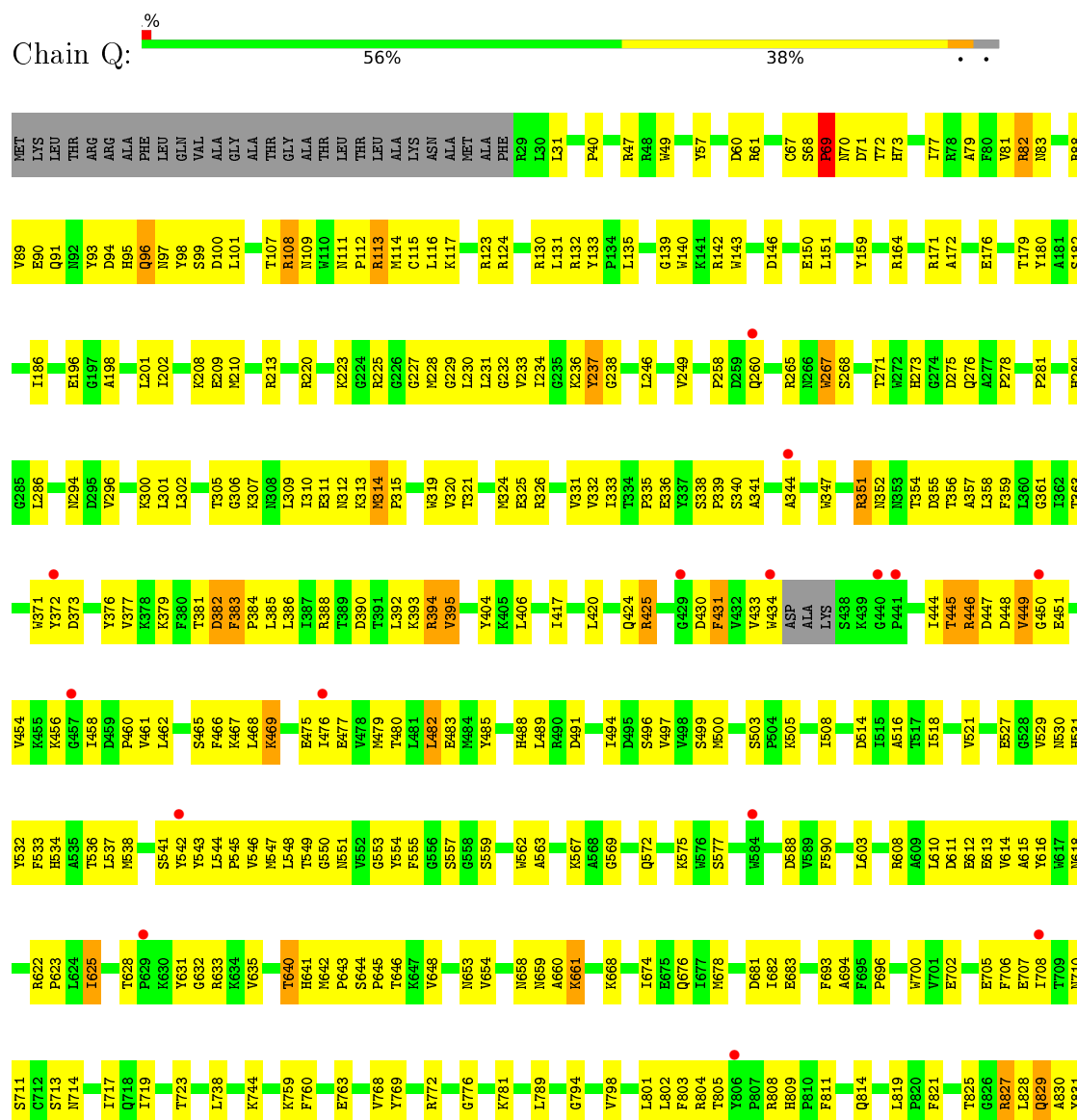
27%

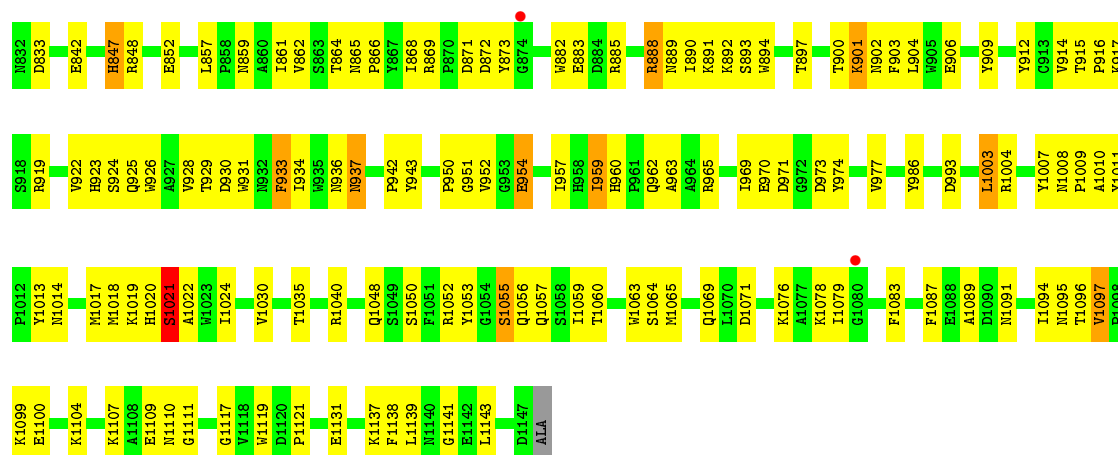






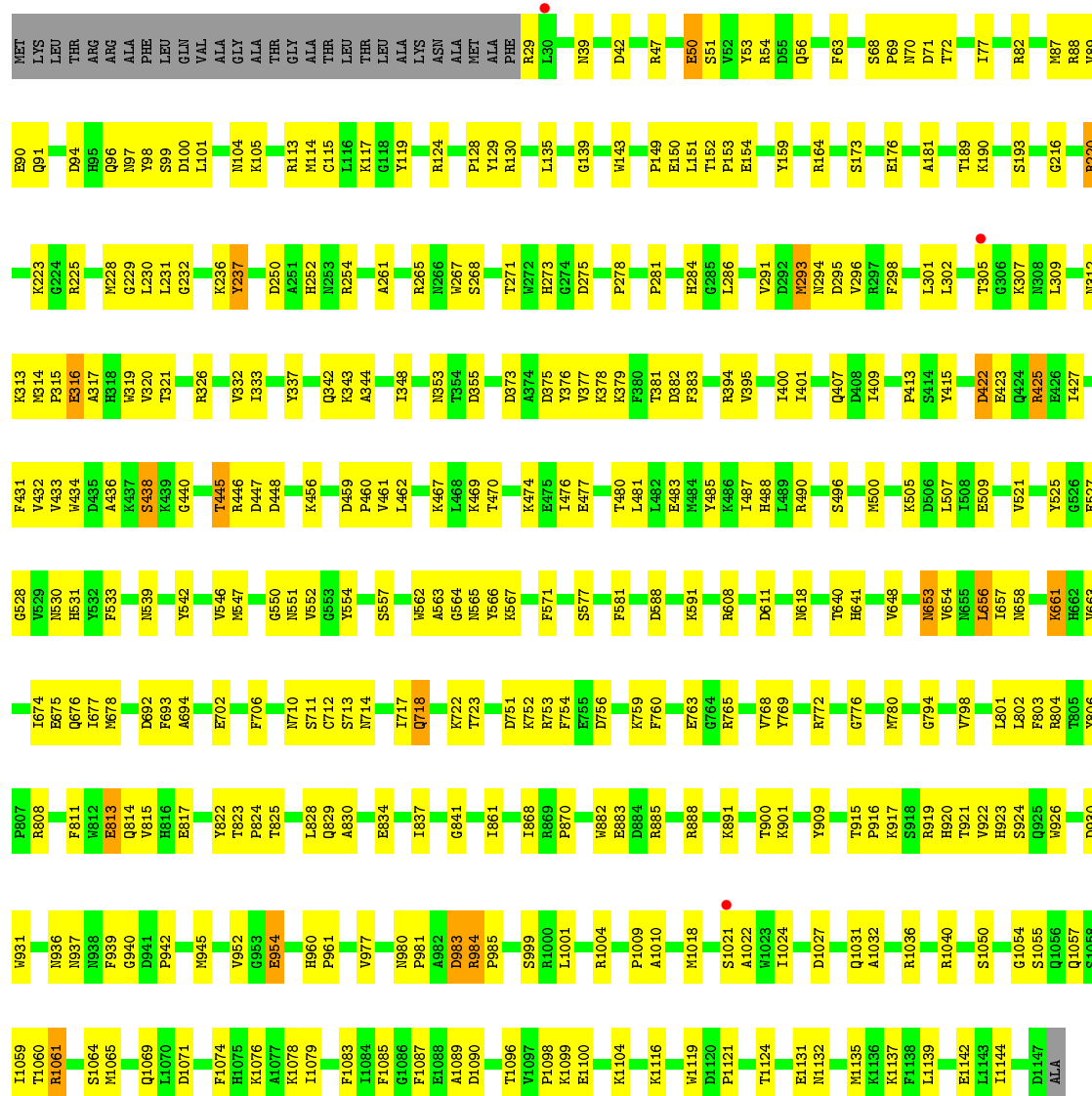
• Molecule 2: Nitrite oxidoreductase subunit A



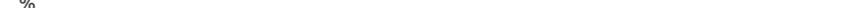


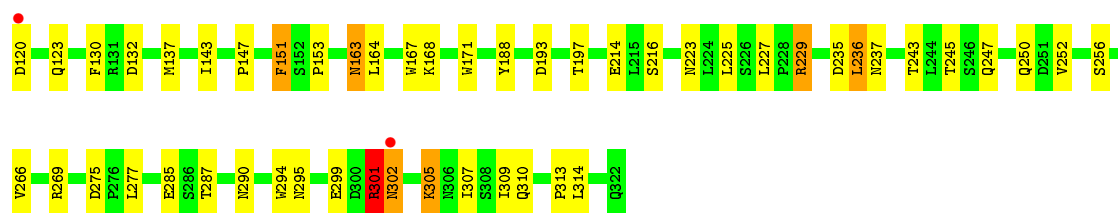
### • Molecule 2: Nitrite oxidoreductase subunit A

Chain T: 67% 29% ••

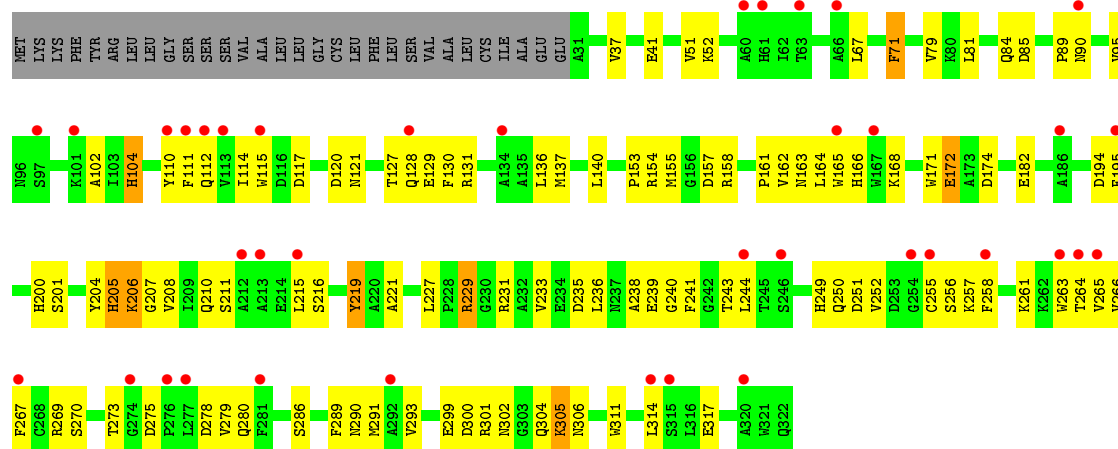


[illegible]

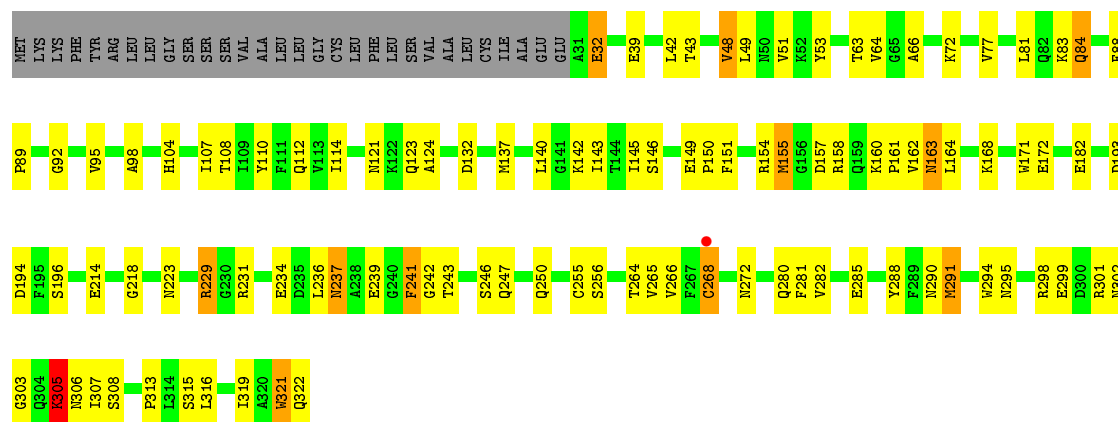
Chain C: 



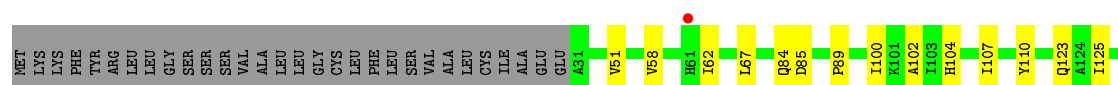
• Molecule 3: Nitrite oxidoreductase subunit C

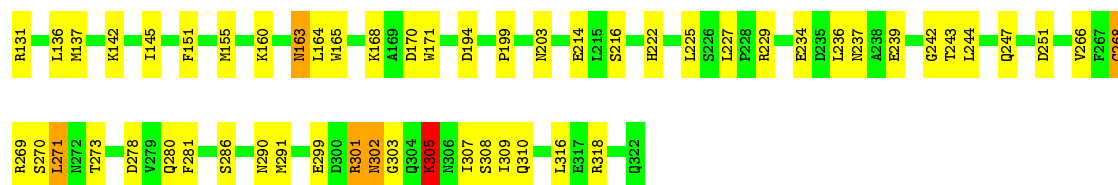


• Molecule 3: Nitrite oxidoreductase subunit C

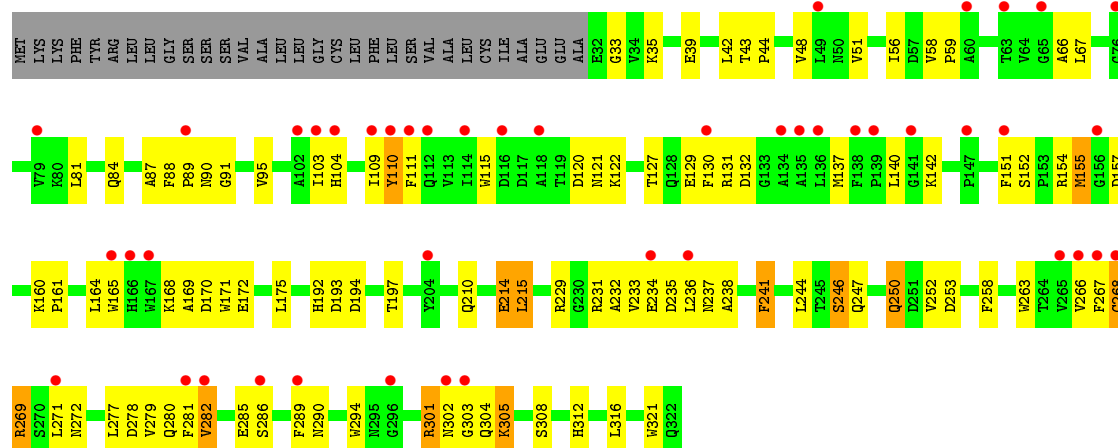


• Molecule 3: Nitrite oxidoreductase subunit C

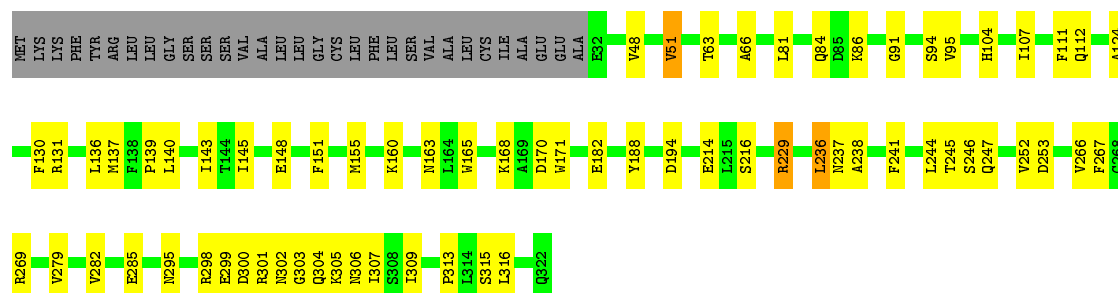




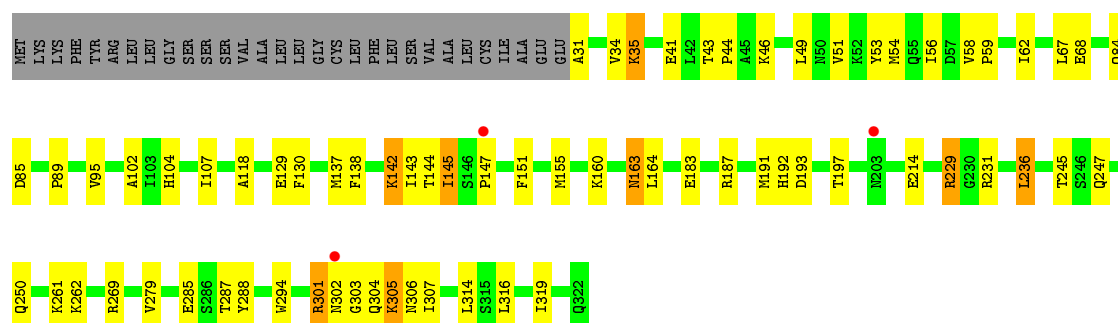
• Molecule 3: Nitrite oxidoreductase subunit C



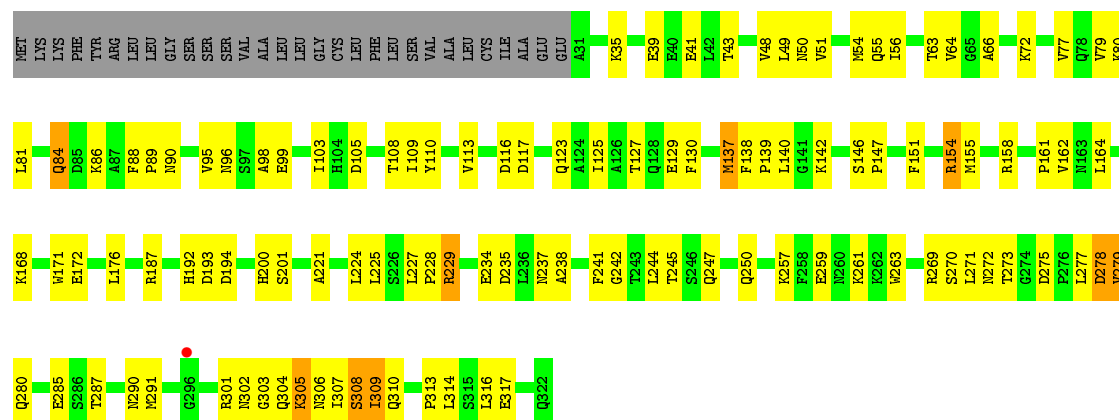
• Molecule 3: Nitrite oxidoreductase subunit C



• Molecule 3: Nitrite oxidoreductase subunit C



Chain X:  56% 32% 9%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	177.63Å 206.47Å 527.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	192.25 – 2.97 192.25 – 2.97	Depositor EDS
% Data completeness (in resolution range)	95.4 (192.25-2.97) 95.4 (192.25-2.97)	Depositor EDS
$R_{merge}$	0.43	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.57 (at 2.96Å)	Xtriage
Refinement program	PHENIX v1.14rc1	Depositor
R, $R_{free}$	0.223 , 0.255 0.222 , 0.253	Depositor DCC
$R_{free}$ test set	21282 reflections (5.64%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	49.7	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 39.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	115931	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MD1, F3S, HEM, SF4, MO, CA

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	0.36	0/3450	0.52	0/4676
1	D	0.33	0/2957	0.53	0/4058
1	G	0.29	0/3445	0.49	0/4670
1	J	0.33	0/3462	0.49	0/4690
1	M	0.34	0/3410	0.56	1/4632 (0.0%)
1	P	0.39	0/3422	0.57	0/4646
1	S	0.31	2/3434 (0.1%)	0.49	0/4657
1	V	0.50	1/3339 (0.0%)	0.68	4/4545 (0.1%)
2	B	0.41	1/9267 (0.0%)	0.59	2/12591 (0.0%)
2	E	0.44	1/7024 (0.0%)	0.69	1/9696 (0.0%)
2	H	0.37	1/9292 (0.0%)	0.57	3/12617 (0.0%)
2	K	0.37	0/9313	0.55	0/12642
2	N	0.39	1/9319 (0.0%)	0.57	2/12649 (0.0%)
2	Q	0.48	1/9165 (0.0%)	0.67	4/12465 (0.0%)
2	T	0.39	3/9298 (0.0%)	0.55	2/12625 (0.0%)
2	W	0.43	1/9187 (0.0%)	0.61	1/12501 (0.0%)
3	C	0.42	2/2338 (0.1%)	0.64	3/3175 (0.1%)
3	F	0.43	0/2123	0.68	0/2911
3	I	0.40	0/2272	0.68	1/3093 (0.0%)
3	L	0.49	3/2331 (0.1%)	0.60	1/3169 (0.0%)
3	O	0.47	1/2179 (0.0%)	0.69	1/2983 (0.0%)
3	R	0.44	1/2318 (0.0%)	0.57	0/3151
3	U	0.39	0/2324	0.58	1/3158 (0.0%)
3	X	0.41	0/2282	0.63	0/3104
All	All	0.40	19/116951 (0.0%)	0.59	27/159104 (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
2	B	0	1
2	H	0	1
2	K	0	2
2	W	0	3
All	All	0	7

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	663	VAL	C-N	15.00	1.68	1.34
2	Q	1097	VAL	CB-CG2	-9.56	1.32	1.52
3	C	214	GLU	CD-OE1	-6.92	1.18	1.25
3	C	214	GLU	CD-OE2	-6.58	1.18	1.25
2	T	954	GLU	CD-OE1	-6.28	1.18	1.25

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	954	GLU	O-C-N	-16.77	95.87	122.70
3	I	305	LYS	CB-CA-C	13.42	137.23	110.40
2	Q	954	GLU	CB-CA-C	9.42	129.23	110.40
2	E	663	VAL	C-N-CA	-9.22	98.64	121.70
2	Q	69	PRO	N-CA-CB	-8.98	92.53	103.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	446	ARG	Sidechain
2	H	954	GLU	Mainchain
2	K	1021	SER	Mainchain
2	K	446	ARG	Sidechain
2	W	111	ASN	Peptide

## 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	3349	0	3216	88	0
1	D	2872	0	2267	142	0
1	G	3344	0	3208	92	0
1	J	3361	0	3242	85	0
1	M	3309	0	3136	155	0
1	P	3321	0	3149	117	0
1	S	3333	0	3198	92	0
1	V	3239	0	2948	264	0
2	B	9003	0	8576	356	0
2	E	6871	0	4598	311	0
2	H	9028	0	8644	244	0
2	K	9046	0	8683	294	0
2	N	9052	0	8682	316	0
2	Q	8902	0	8343	440	0
2	T	9034	0	8643	270	0
2	W	8920	0	8364	432	0
3	C	2281	0	2171	60	0
3	F	2068	0	1752	149	0
3	I	2216	0	2068	149	0
3	L	2274	0	2151	62	0
3	O	2124	0	1863	123	0
3	R	2261	0	2134	59	0
3	U	2267	0	2146	53	0
3	X	2225	0	2060	134	0
4	A	24	0	0	1	0
4	B	8	0	0	0	0
4	D	24	0	0	7	0
4	E	8	0	0	0	0
4	G	24	0	0	3	0
4	H	8	0	0	0	0
4	J	24	0	0	5	0
4	K	8	0	0	1	0
4	M	24	0	0	3	0
4	N	8	0	0	3	0
4	P	24	0	0	3	0
4	Q	8	0	0	3	0
4	S	24	0	0	3	0
4	T	8	0	0	3	0
4	V	24	0	0	6	0
4	W	8	0	0	2	0
5	A	7	0	0	0	0
5	D	7	0	0	3	0
5	G	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	7	0	0	0	0
5	M	7	0	0	2	0
5	P	7	0	0	0	0
5	S	7	0	0	0	0
5	V	7	0	0	5	0
6	B	94	0	43	12	0
6	E	94	0	41	19	0
6	H	94	0	42	13	0
6	K	94	0	43	14	0
6	N	94	0	43	18	0
6	Q	94	0	41	19	0
6	T	94	0	43	13	0
6	W	94	0	44	21	0
7	B	1	0	0	0	0
7	E	1	0	0	0	0
7	H	1	0	0	0	0
7	K	1	0	0	0	0
7	N	1	0	0	0	0
7	Q	1	0	0	0	0
7	T	1	0	0	0	0
7	W	1	0	0	0	0
8	C	43	0	30	8	0
8	F	43	0	30	25	0
8	I	43	0	30	29	0
8	L	43	0	30	6	0
8	O	43	0	30	11	0
8	R	43	0	30	5	0
8	U	43	0	30	4	0
8	X	43	0	30	15	0
9	C	2	0	0	0	0
9	F	2	0	0	0	0
9	I	2	0	0	0	0
9	L	2	0	0	0	0
9	O	2	0	0	0	0
9	R	2	0	0	0	0
9	U	2	0	0	0	0
9	X	2	0	0	1	0
10	A	37	0	0	0	0
10	B	72	0	0	7	0
10	C	35	0	0	1	0
10	D	6	0	0	0	0
10	E	13	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	8	0	0	0	0
10	G	25	0	0	1	0
10	H	83	0	0	3	0
10	I	20	0	0	1	0
10	J	28	0	0	2	0
10	K	74	0	0	3	0
10	L	30	0	0	0	0
10	M	10	0	0	0	0
10	N	76	0	0	5	0
10	O	17	0	0	3	0
10	P	16	0	0	4	0
10	Q	43	0	0	3	0
10	R	22	0	0	1	0
10	S	20	0	0	1	0
10	T	62	0	0	4	0
10	U	25	0	0	3	0
10	V	12	0	0	1	0
10	W	41	0	0	3	0
10	X	24	0	0	3	0
All	All	115931	0	105822	4154	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 19.

The worst 5 of 4154 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)
2:W:939:PHE:CE2	2:W:1004:ARG:CD	1.78	1.66
1:V:16:PRO:CG	1:V:128:TRP:CE2	1.81	1.62
2:W:939:PHE:CE2	2:W:1004:ARG:HD2	1.10	1.59
1:V:16:PRO:HG3	1:V:128:TRP:CZ2	0.98	1.50
1:V:241:ARG:HH12	1:V:257:ARG:CG	1.20	1.50

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	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	D	406/410 (99%)	388 (96%)	18 (4%)	0	100	100
1	G	407/410 (99%)	399 (98%)	8 (2%)	0	100	100
1	J	407/410 (99%)	403 (99%)	4 (1%)	0	100	100
1	M	407/410 (99%)	401 (98%)	6 (2%)	0	100	100
1	P	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	S	407/410 (99%)	400 (98%)	7 (2%)	0	100	100
1	V	407/410 (99%)	395 (97%)	12 (3%)	0	100	100
2	B	1119/1148 (98%)	1078 (96%)	41 (4%)	0	100	100
2	E	1104/1148 (96%)	1034 (94%)	68 (6%)	2 (0%)	47	80
2	H	1117/1148 (97%)	1073 (96%)	43 (4%)	1 (0%)	51	83
2	K	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	N	1118/1148 (97%)	1075 (96%)	43 (4%)	0	100	100
2	Q	1113/1148 (97%)	1071 (96%)	39 (4%)	3 (0%)	41	74
2	T	1117/1148 (97%)	1079 (97%)	38 (3%)	0	100	100
2	W	1117/1148 (97%)	1072 (96%)	44 (4%)	1 (0%)	51	83
3	C	291/322 (90%)	282 (97%)	9 (3%)	0	100	100
3	F	290/322 (90%)	278 (96%)	12 (4%)	0	100	100
3	I	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
3	L	291/322 (90%)	288 (99%)	3 (1%)	0	100	100
3	O	289/322 (90%)	280 (97%)	9 (3%)	0	100	100
3	R	289/322 (90%)	279 (96%)	10 (4%)	0	100	100
3	U	290/322 (90%)	284 (98%)	6 (2%)	0	100	100
3	X	290/322 (90%)	279 (96%)	11 (4%)	0	100	100
All	All	14498/15040 (96%)	13995 (96%)	496 (3%)	7 (0%)	100	100

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	520	PRO
2	H	1021	SER
2	Q	69	PRO
2	Q	113	ARG
2	Q	1021	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	359/365 (98%)	352 (98%)	7 (2%)	57	82
1	D	229/365 (63%)	219 (96%)	10 (4%)	28	63
1	G	356/365 (98%)	348 (98%)	8 (2%)	52	80
1	J	362/365 (99%)	356 (98%)	6 (2%)	60	84
1	M	348/365 (95%)	337 (97%)	11 (3%)	39	72
1	P	350/365 (96%)	339 (97%)	11 (3%)	40	73
1	S	355/365 (97%)	350 (99%)	5 (1%)	67	86
1	V	324/365 (89%)	300 (93%)	24 (7%)	13	42
2	B	943/991 (95%)	902 (96%)	41 (4%)	29	64
2	E	373/991 (38%)	347 (93%)	26 (7%)	15	45
2	H	952/991 (96%)	930 (98%)	22 (2%)	50	79
2	K	956/991 (96%)	934 (98%)	22 (2%)	50	79
2	N	959/991 (97%)	933 (97%)	26 (3%)	44	75
2	Q	913/991 (92%)	868 (95%)	45 (5%)	25	59
2	T	953/991 (96%)	926 (97%)	27 (3%)	43	75
2	W	918/991 (93%)	864 (94%)	54 (6%)	19	52
3	C	238/265 (90%)	229 (96%)	9 (4%)	33	67
3	F	175/265 (66%)	162 (93%)	13 (7%)	13	42
3	I	220/265 (83%)	205 (93%)	15 (7%)	16	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	236/265 (89%)	227 (96%)	9 (4%)	33	67
3	O	196/265 (74%)	178 (91%)	18 (9%)	9	32
3	R	235/265 (89%)	226 (96%)	9 (4%)	33	67
3	U	235/265 (89%)	222 (94%)	13 (6%)	21	55
3	X	223/265 (84%)	205 (92%)	18 (8%)	11	37
All	All	11408/12968 (88%)	10959 (96%)	449 (4%)	32	66

5 of 449 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	O	229	ARG
3	X	259	GLU
2	Q	829	GLN
3	X	146	SER
2	W	468	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	W	244	ASN
2	W	704	GLN
3	I	302	ASN
3	I	104	HIS
2	W	1048	GLN

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry

Of 88 ligands modelled in this entry, 24 are monoatomic - leaving 64 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	501	1	0,12,12	0.00	-	-		
4	SF4	Q	5804	2	0,12,12	0.00	-	-		
5	F3S	S	504	1	0,9,9	0.00	-	-		
4	SF4	J	503	1	0,12,12	0.00	-	-		
6	MD1	H	5802	7	38,51,51	6.87	21 (55%)	35,78,78	1.78	11 (31%)
5	F3S	J	504	1	0,9,9	0.00	-	-		
6	MD1	T	5801	7	38,51,51	6.81	21 (55%)	35,78,78	1.44	4 (11%)
4	SF4	V	501	1	0,12,12	0.00	-	-		
4	SF4	A	503	1	0,12,12	0.00	-	-		
4	SF4	N	5804	2	0,12,12	0.00	-	-		
8	HEM	R	401	3	27,50,50	1.89	5 (18%)	17,82,82	1.52	4 (23%)
8	HEM	L	401	3	27,50,50	1.88	5 (18%)	17,82,82	1.43	3 (17%)
8	HEM	I	401	3	27,50,50	1.96	9 (33%)	17,82,82	1.95	5 (29%)
4	SF4	W	5804	2	0,12,12	0.00	-	-		
4	SF4	D	503	1	0,12,12	0.00	-	-		
4	SF4	P	501	1	0,12,12	0.00	-	-		
6	MD1	Q	5801	7	38,51,51	6.66	21 (55%)	35,78,78	1.65	7 (20%)
8	HEM	F	401	-	27,50,50	1.95	5 (18%)	17,82,82	2.23	7 (41%)
4	SF4	G	502	1	0,12,12	0.00	-	-		
8	HEM	C	401	3	27,50,50	1.86	5 (18%)	17,82,82	1.52	4 (23%)
4	SF4	E	5804	2	0,12,12	0.00	-	-		
5	F3S	M	504	1	0,9,9	0.00	-	-		
4	SF4	A	502	1	0,12,12	0.00	-	-		
4	SF4	D	502	1	0,12,12	0.00	-	-		
4	SF4	J	501	1	0,12,12	0.00	-	-		
5	F3S	V	504	1	0,9,9	0.00	-	-		
6	MD1	E	5801	7,6	38,51,51	6.61	22 (57%)	35,78,78	1.68	8 (22%)
6	MD1	K	5802	7	38,51,51	6.89	21 (55%)	35,78,78	1.64	13 (37%)
6	MD1	N	5801	7	38,51,51	6.78	21 (55%)	35,78,78	1.52	7 (20%)
4	SF4	M	503	1	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	SF4	G	501	1	0,12,12	0.00	-	-		
6	MD1	T	5802	7	38,51,51	6.91	21 (55%)	35,78,78	1.79	12 (34%)
6	MD1	E	5802	7,6	38,51,51	6.93	21 (55%)	35,78,78	1.80	10 (28%)
6	MD1	W	5801	7	38,51,51	6.78	21 (55%)	35,78,78	1.51	5 (14%)
4	SF4	D	501	1	0,12,12	0.00	-	-		
4	SF4	M	501	1	0,12,12	0.00	-	-		
8	HEM	U	401	3	27,50,50	1.88	4 (14%)	17,82,82	1.63	3 (17%)
4	SF4	P	503	1	0,12,12	0.00	-	-		
4	SF4	V	502	1	0,12,12	0.00	-	-		
4	SF4	G	503	1	0,12,12	0.00	-	-		
4	SF4	S	503	1	0,12,12	0.00	-	-		
6	MD1	B	5801	7	38,51,51	6.80	21 (55%)	35,78,78	1.45	5 (14%)
8	HEM	O	401	3	27,50,50	1.83	5 (18%)	17,82,82	1.77	5 (29%)
6	MD1	Q	5802	7	38,51,51	6.87	21 (55%)	35,78,78	1.80	11 (31%)
4	SF4	S	501	1	0,12,12	0.00	-	-		
4	SF4	H	5804	2	0,12,12	0.00	-	-		
4	SF4	S	502	1	0,12,12	0.00	-	-		
4	SF4	P	502	1	0,12,12	0.00	-	-		
5	F3S	G	504	1	0,9,9	0.00	-	-		
6	MD1	N	5802	7	38,51,51	6.89	21 (55%)	35,78,78	1.76	12 (34%)
6	MD1	W	5802	7	38,51,51	6.90	21 (55%)	35,78,78	1.83	11 (31%)
4	SF4	J	502	1	0,12,12	0.00	-	-		
5	F3S	P	504	1	0,9,9	0.00	-	-		
6	MD1	H	5801	7	38,51,51	6.80	21 (55%)	35,78,78	1.52	6 (17%)
6	MD1	B	5802	7	38,51,51	6.89	21 (55%)	35,78,78	1.84	9 (25%)
5	F3S	D	504	1	0,9,9	0.00	-	-		
4	SF4	M	502	1	0,12,12	0.00	-	-		
4	SF4	B	5804	2	0,12,12	0.00	-	-		
4	SF4	T	5804	2	0,12,12	0.00	-	-		
4	SF4	K	5804	2	0,12,12	0.00	-	-		
4	SF4	V	503	1	0,12,12	0.00	-	-		
6	MD1	K	5801	7	38,51,51	6.78	21 (55%)	35,78,78	1.56	7 (20%)
8	HEM	X	401	3	27,50,50	1.95	4 (14%)	17,82,82	1.48	2 (11%)
5	F3S	A	504	1	0,9,9	0.00	-	-		

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	501	1	-	-	0/6/5/5
4	SF4	Q	5804	2	-	-	0/6/5/5
5	F3S	S	504	1	-	-	0/3/3/3
4	SF4	J	503	1	-	-	0/6/5/5
6	MD1	H	5802	7	-	3/21/59/59	0/5/5/5
5	F3S	J	504	1	-	-	0/3/3/3
6	MD1	T	5801	7	-	11/21/59/59	0/5/5/5
4	SF4	V	501	1	-	-	0/6/5/5
8	HEM	R	401	3	-	1/6/54/54	-
4	SF4	A	503	1	-	-	0/6/5/5
4	SF4	N	5804	2	-	-	0/6/5/5
8	HEM	L	401	3	-	0/6/54/54	-
8	HEM	I	401	3	-	3/6/54/54	-
4	SF4	W	5804	2	-	-	0/6/5/5
8	HEM	F	401	-	-	2/6/54/54	-
6	MD1	Q	5801	7	-	10/21/59/59	0/5/5/5
4	SF4	D	503	1	-	-	0/6/5/5
4	SF4	P	501	1	-	-	0/6/5/5
8	HEM	C	401	3	-	1/6/54/54	-
4	SF4	G	502	1	-	-	0/6/5/5
4	SF4	E	5804	2	-	-	0/6/5/5
5	F3S	M	504	1	-	-	0/3/3/3
6	MD1	T	5802	7	-	3/21/59/59	0/5/5/5
6	MD1	E	5801	7,6	1/1/10/12	9/21/59/59	0/5/5/5
4	SF4	A	502	1	-	-	0/6/5/5
6	MD1	K	5802	7	-	3/21/59/59	0/5/5/5
6	MD1	N	5801	7	-	11/21/59/59	0/5/5/5
4	SF4	D	502	1	-	-	0/6/5/5
4	SF4	J	501	1	-	-	0/6/5/5
4	SF4	M	503	1	-	-	0/6/5/5
4	SF4	G	501	1	-	-	0/6/5/5
6	MD1	E	5802	7,6	-	4/21/59/59	0/5/5/5
4	SF4	D	501	1	-	-	0/6/5/5
4	SF4	M	501	1	-	-	0/6/5/5
8	HEM	U	401	3	-	1/6/54/54	-
4	SF4	P	503	1	-	-	0/6/5/5
4	SF4	V	502	1	-	-	0/6/5/5
4	SF4	G	503	1	-	-	0/6/5/5
4	SF4	S	503	1	-	-	0/6/5/5
6	MD1	B	5801	7	-	10/21/59/59	0/5/5/5
8	HEM	O	401	3	-	0/6/54/54	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MD1	Q	5802	7	-	9/21/59/59	0/5/5/5
4	SF4	S	501	1	-	-	0/6/5/5
4	SF4	H	5804	2	-	-	0/6/5/5
5	F3S	V	504	1	-	-	0/3/3/3
4	SF4	S	502	1	-	-	0/6/5/5
4	SF4	P	502	1	-	-	0/6/5/5
5	F3S	G	504	1	-	-	0/3/3/3
6	MD1	N	5802	7	-	3/21/59/59	0/5/5/5
6	MD1	W	5802	7	-	6/21/59/59	0/5/5/5
4	SF4	J	502	1	-	-	0/6/5/5
6	MD1	H	5801	7	-	11/21/59/59	0/5/5/5
5	F3S	P	504	1	-	-	0/3/3/3
6	MD1	B	5802	7	-	3/21/59/59	0/5/5/5
5	F3S	D	504	1	-	-	0/3/3/3
4	SF4	M	502	1	-	-	0/6/5/5
4	SF4	V	503	1	-	-	0/6/5/5
4	SF4	B	5804	2	-	-	0/6/5/5
4	SF4	T	5804	2	-	-	0/6/5/5
4	SF4	K	5804	2	-	-	0/6/5/5
6	MD1	W	5801	7	-	10/21/59/59	0/5/5/5
6	MD1	K	5801	7	-	11/21/59/59	0/5/5/5
8	HEM	X	401	3	-	0/6/54/54	-
5	F3S	A	504	1	-	-	0/3/3/3

The worst 5 of 379 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	5802	MD1	C7-N8	28.72	1.61	1.27
6	T	5802	MD1	C7-N8	28.42	1.61	1.27
6	K	5802	MD1	C7-N8	28.38	1.61	1.27
6	W	5802	MD1	C7-N8	28.25	1.61	1.27
6	N	5802	MD1	C7-N8	28.22	1.61	1.27

The worst 5 of 171 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	Q	5801	MD1	C4-C5-N7	4.25	108.09	102.46
6	H	5801	MD1	C4-C5-N7	4.24	108.08	102.46
6	E	5802	MD1	C4-C5-N7	4.21	108.05	102.46
6	W	5802	MD1	C4-C5-N7	4.21	108.03	102.46
8	F	401	HEM	CMA-C3A-C4A	-4.17	122.06	128.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	E	5801	MD1	C14

5 of 125 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	5801	MD1	C10-O3A-PB-O3B
6	B	5801	MD1	O3A-C10-C11-O11
6	B	5801	MD1	O3A-C10-C11-C12
6	B	5801	MD1	C3'-C4'-C5'-O5'
6	E	5801	MD1	O3A-C10-C11-O11

There are no ring outliers.

48 monomers are involved in 285 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	5804	SF4	3	0
4	J	503	SF4	4	0
6	H	5802	MD1	7	0
6	T	5801	MD1	8	0
4	V	501	SF4	2	0
4	A	503	SF4	1	0
4	N	5804	SF4	3	0
8	R	401	HEM	5	0
8	L	401	HEM	6	0
8	I	401	HEM	29	0
4	W	5804	SF4	2	0
4	D	503	SF4	1	0
6	Q	5801	MD1	12	0
8	F	401	HEM	25	0
8	C	401	HEM	8	0
5	M	504	F3S	2	0
4	D	502	SF4	2	0
4	J	501	SF4	1	0
5	V	504	F3S	5	0
6	E	5801	MD1	14	0
6	K	5802	MD1	5	0
6	N	5801	MD1	10	0
4	M	503	SF4	2	0
4	G	501	SF4	1	0
6	T	5802	MD1	5	0
6	E	5802	MD1	5	0

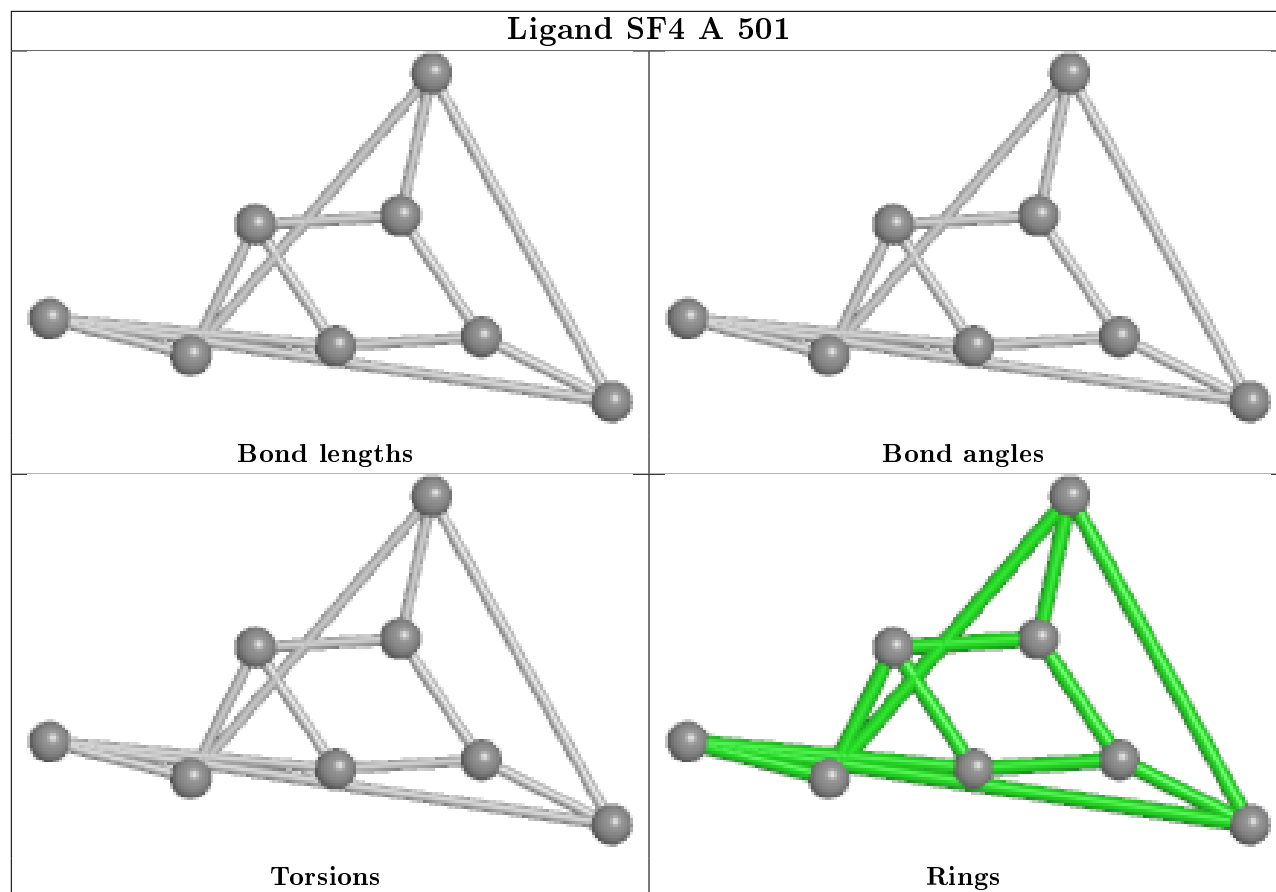
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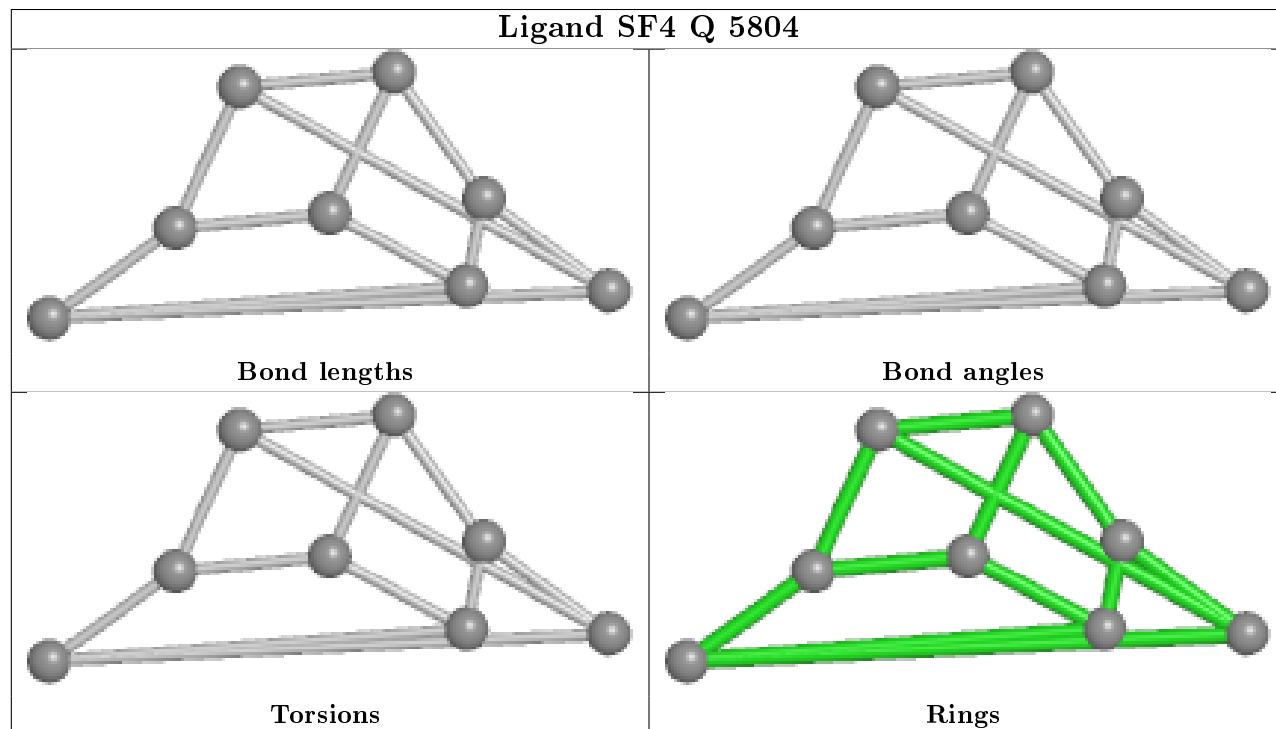
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	W	5801	MD1	13	0
4	D	501	SF4	4	0
4	M	501	SF4	1	0
8	U	401	HEM	4	0
4	P	503	SF4	3	0
4	V	502	SF4	1	0
4	G	503	SF4	2	0
4	S	503	SF4	2	0
6	B	5801	MD1	6	0
8	O	401	HEM	11	0
6	Q	5802	MD1	7	0
4	S	501	SF4	1	0
6	N	5802	MD1	8	0
6	W	5802	MD1	8	0
6	H	5801	MD1	6	0
6	B	5802	MD1	6	0
5	D	504	F3S	3	0
4	T	5804	SF4	3	0
4	K	5804	SF4	1	0
4	V	503	SF4	3	0
6	K	5801	MD1	9	0
8	X	401	HEM	15	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.

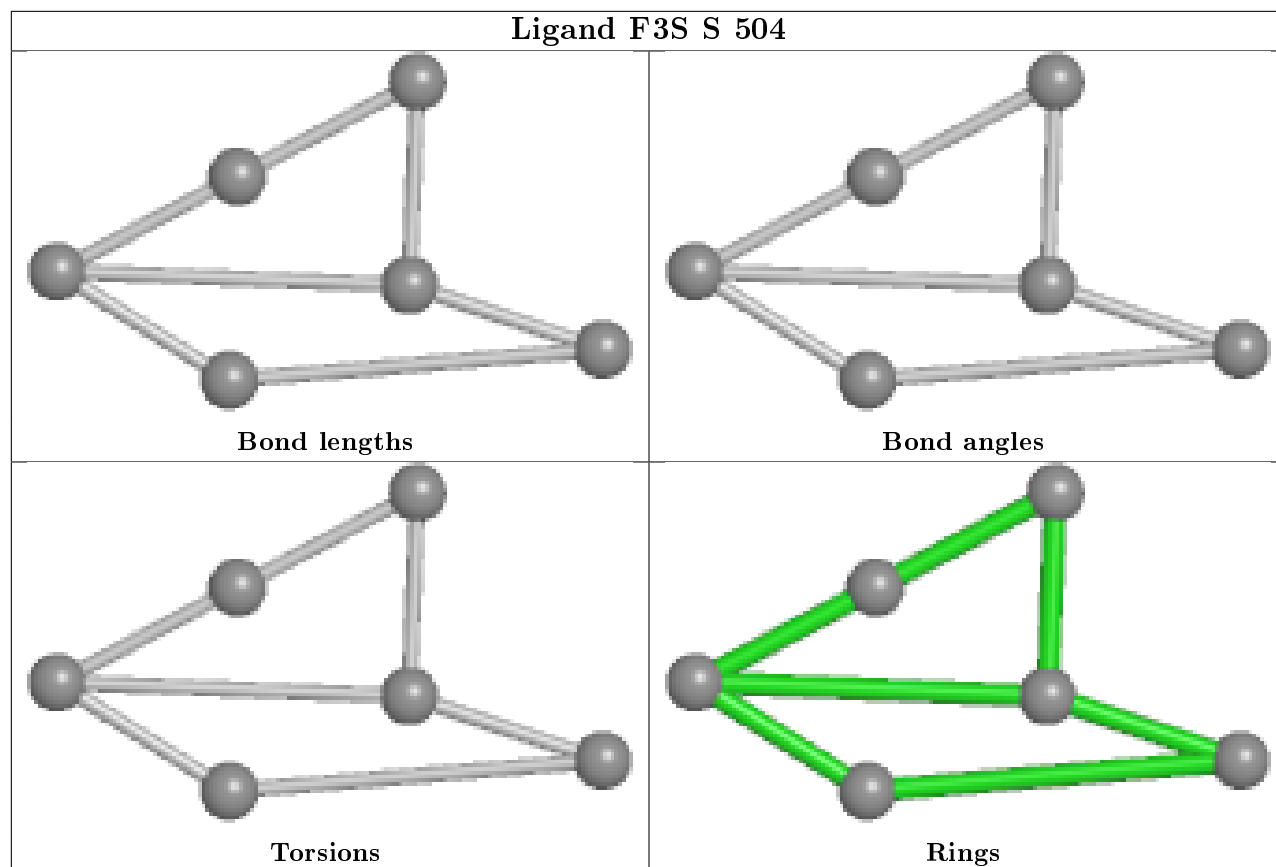
## Ligand SF4 A 501



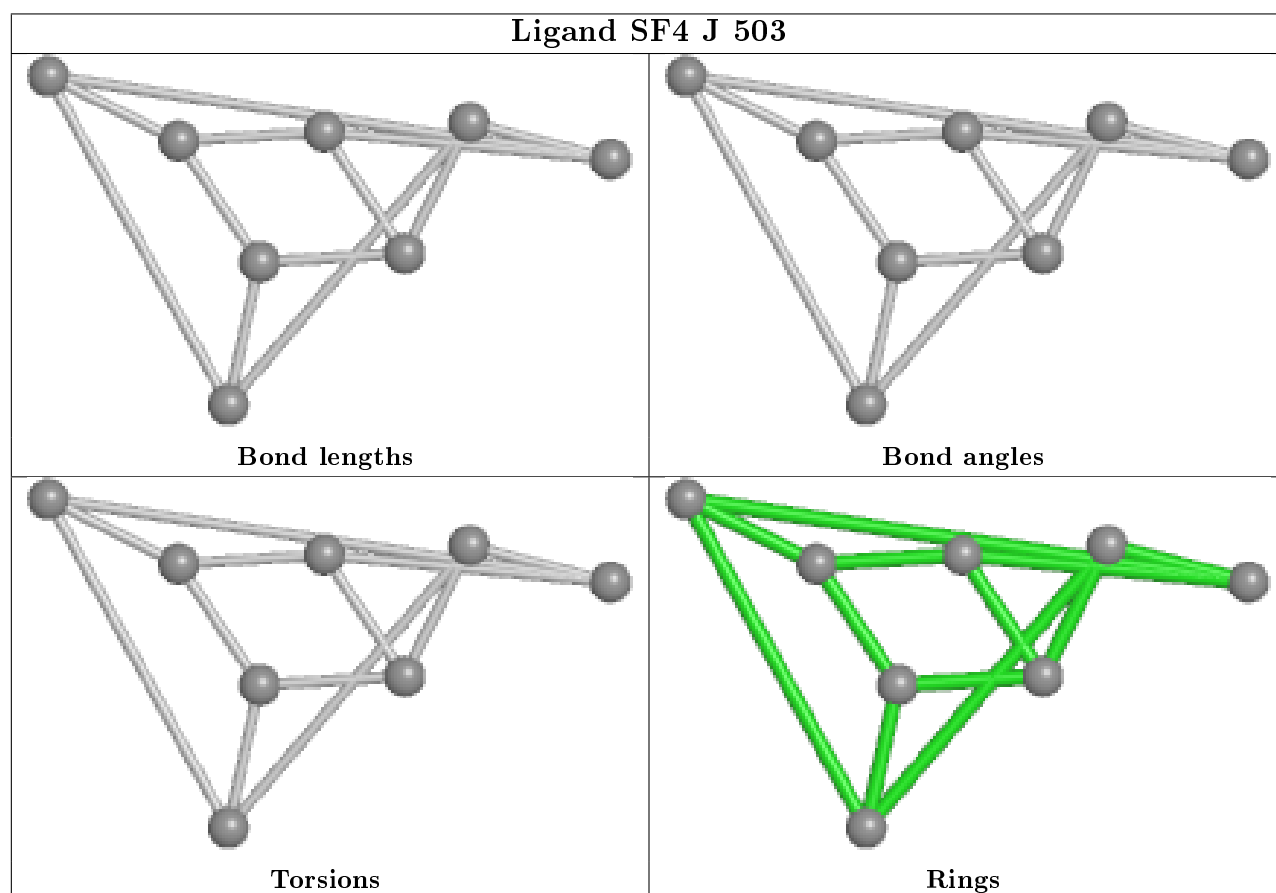
## Ligand SF4 Q 5804



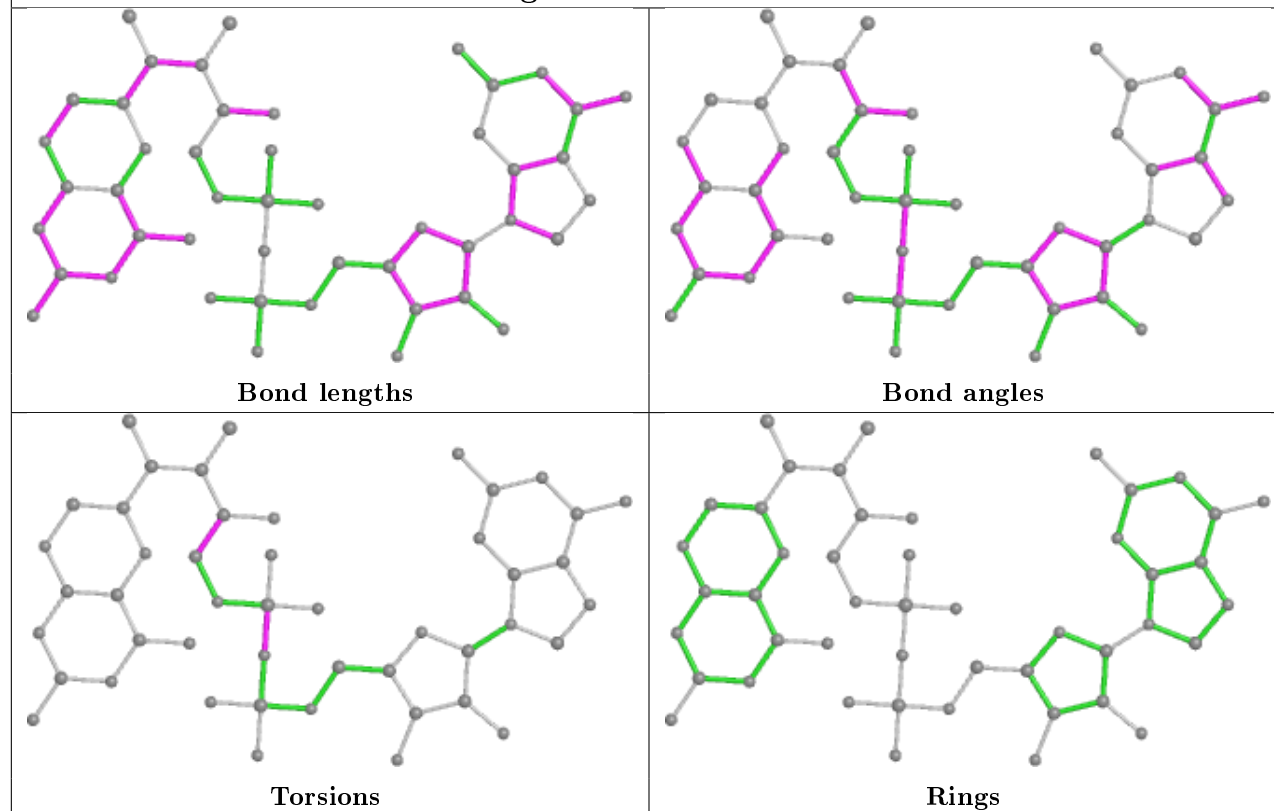
## Ligand F3S S 504



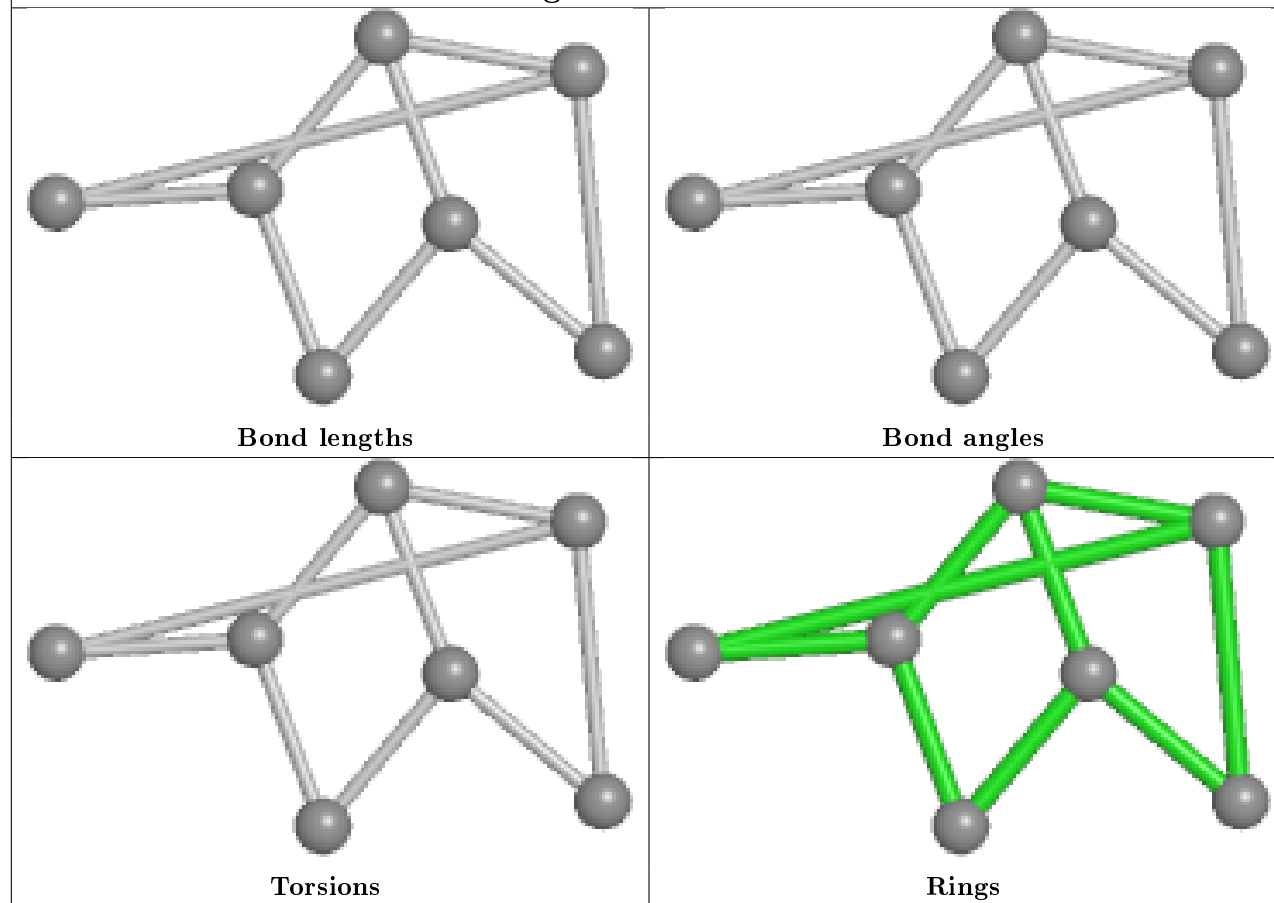
## Ligand SF4 J 503



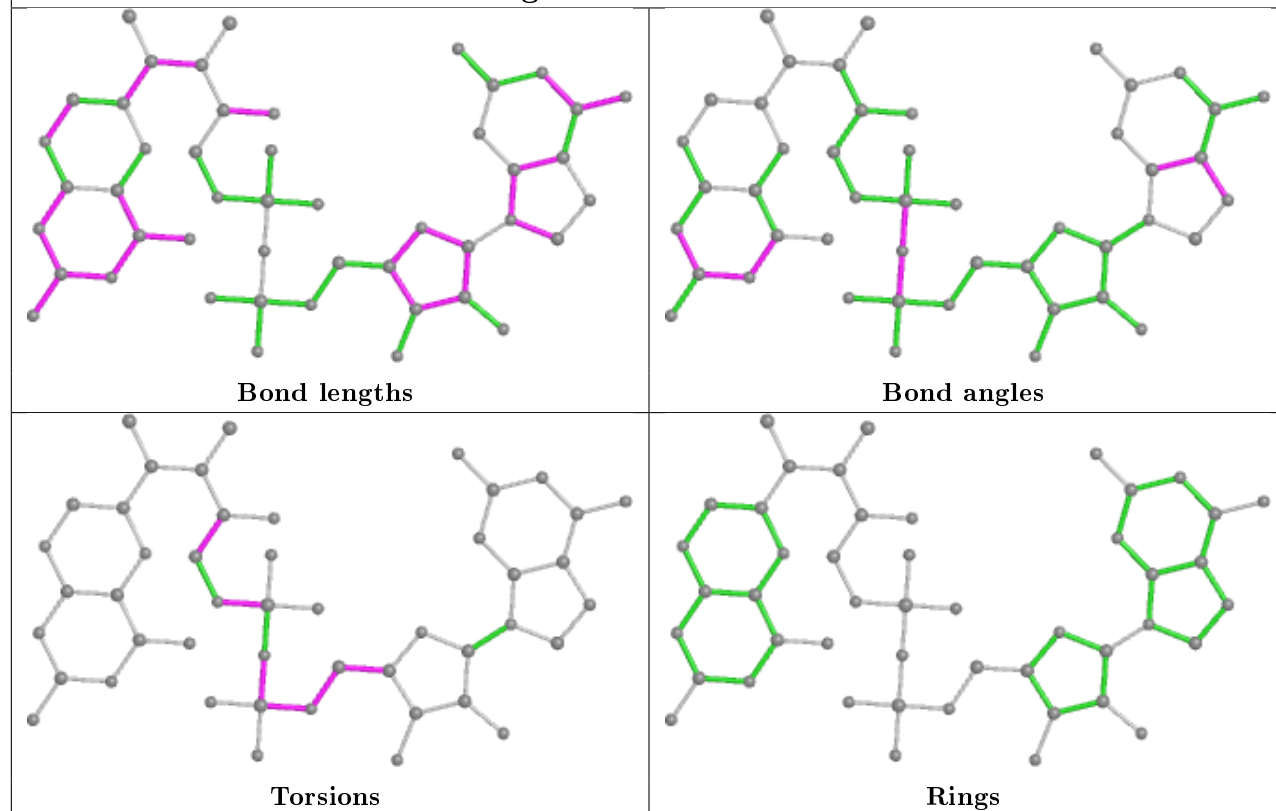
## Ligand MD1 H 5802



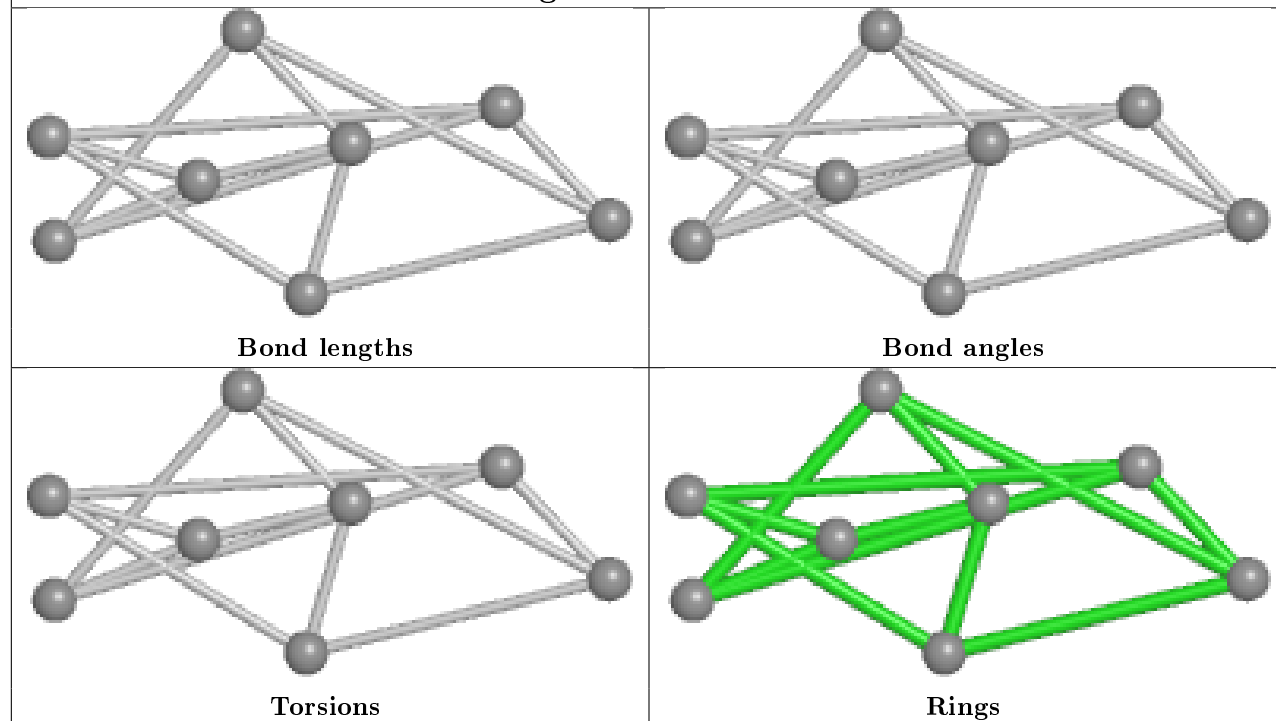
## Ligand F3S J 504

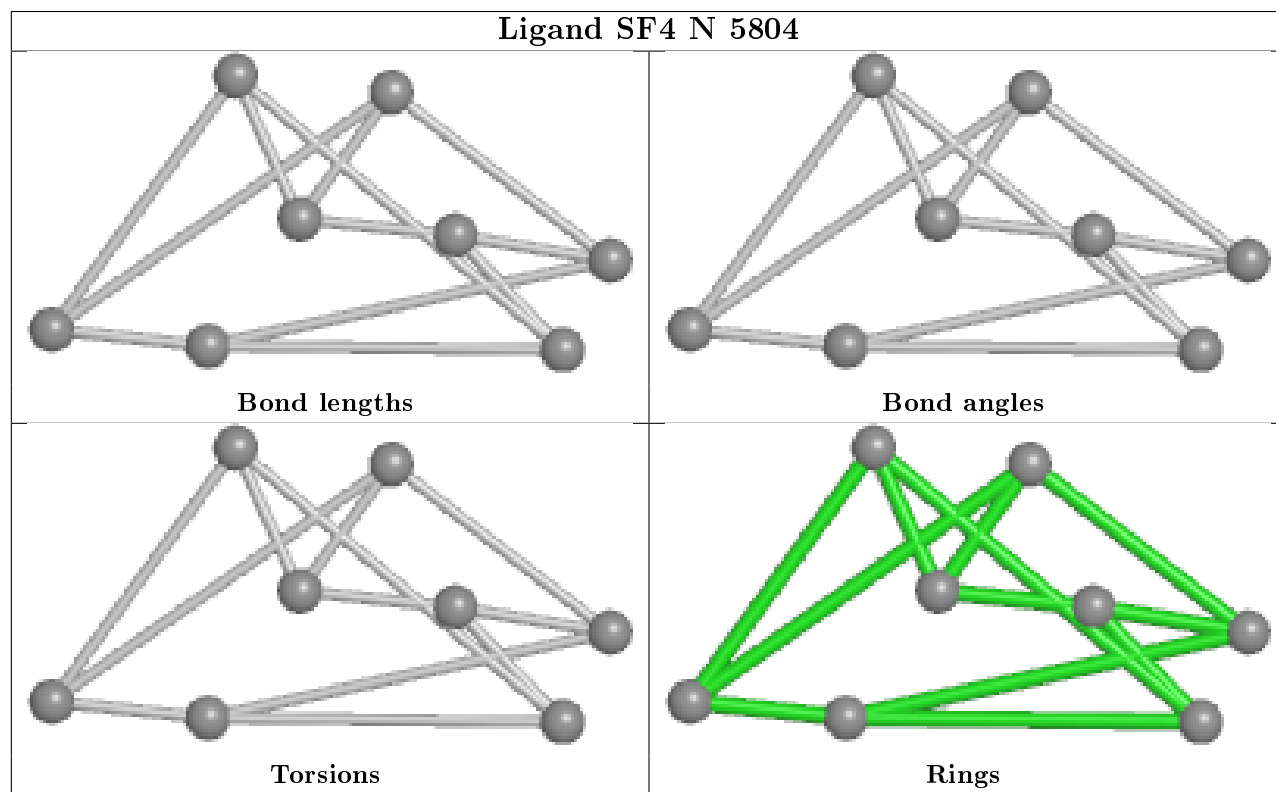
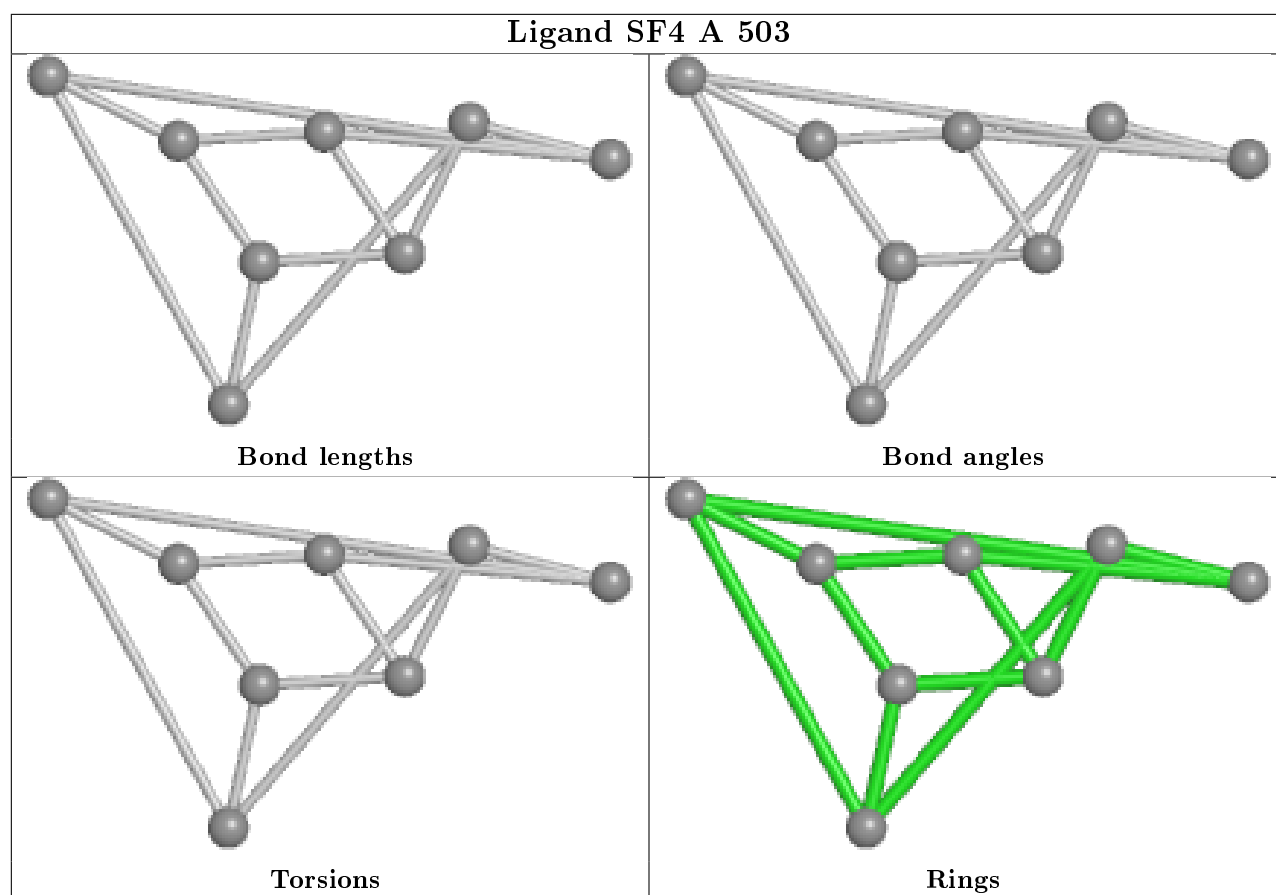


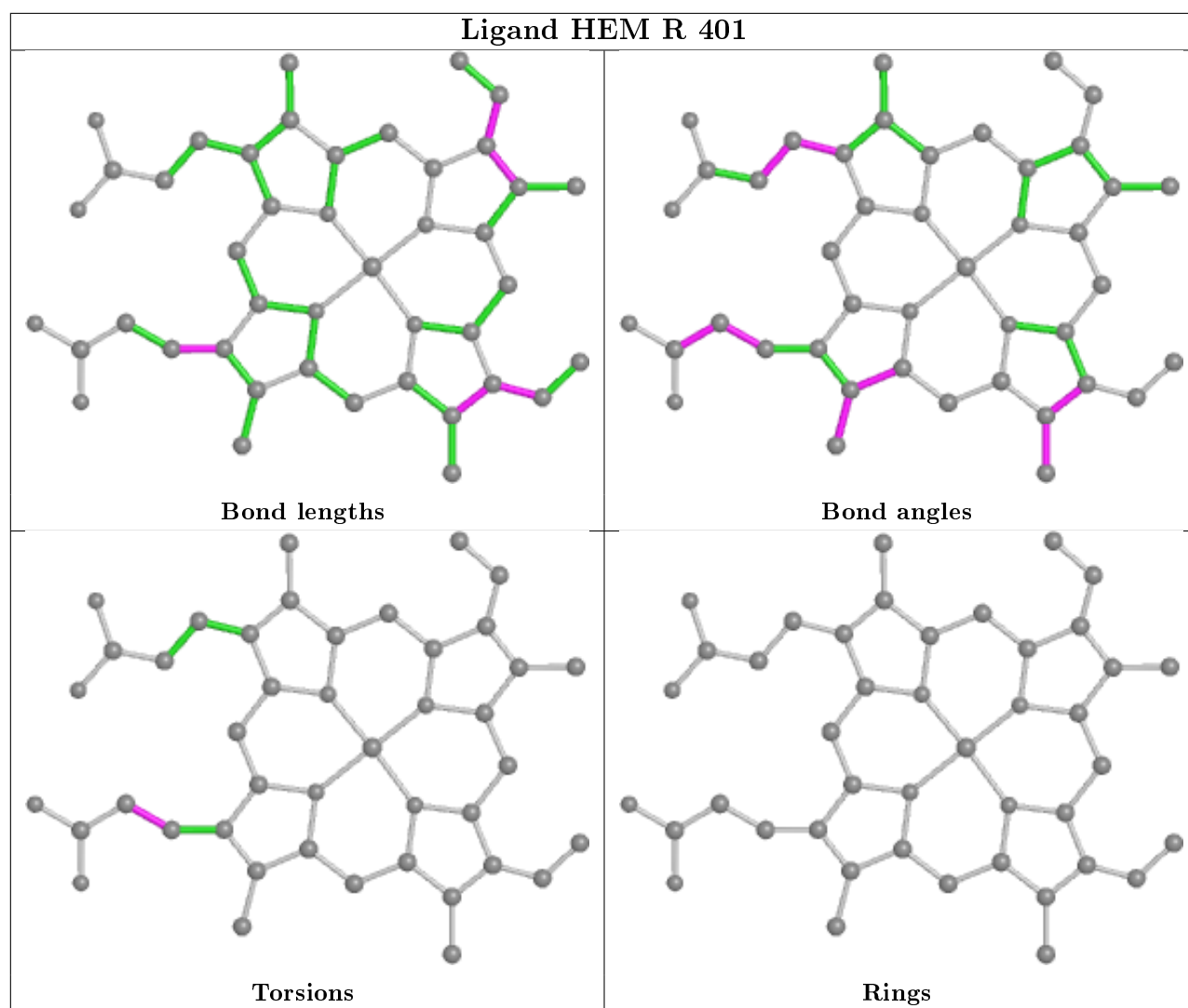
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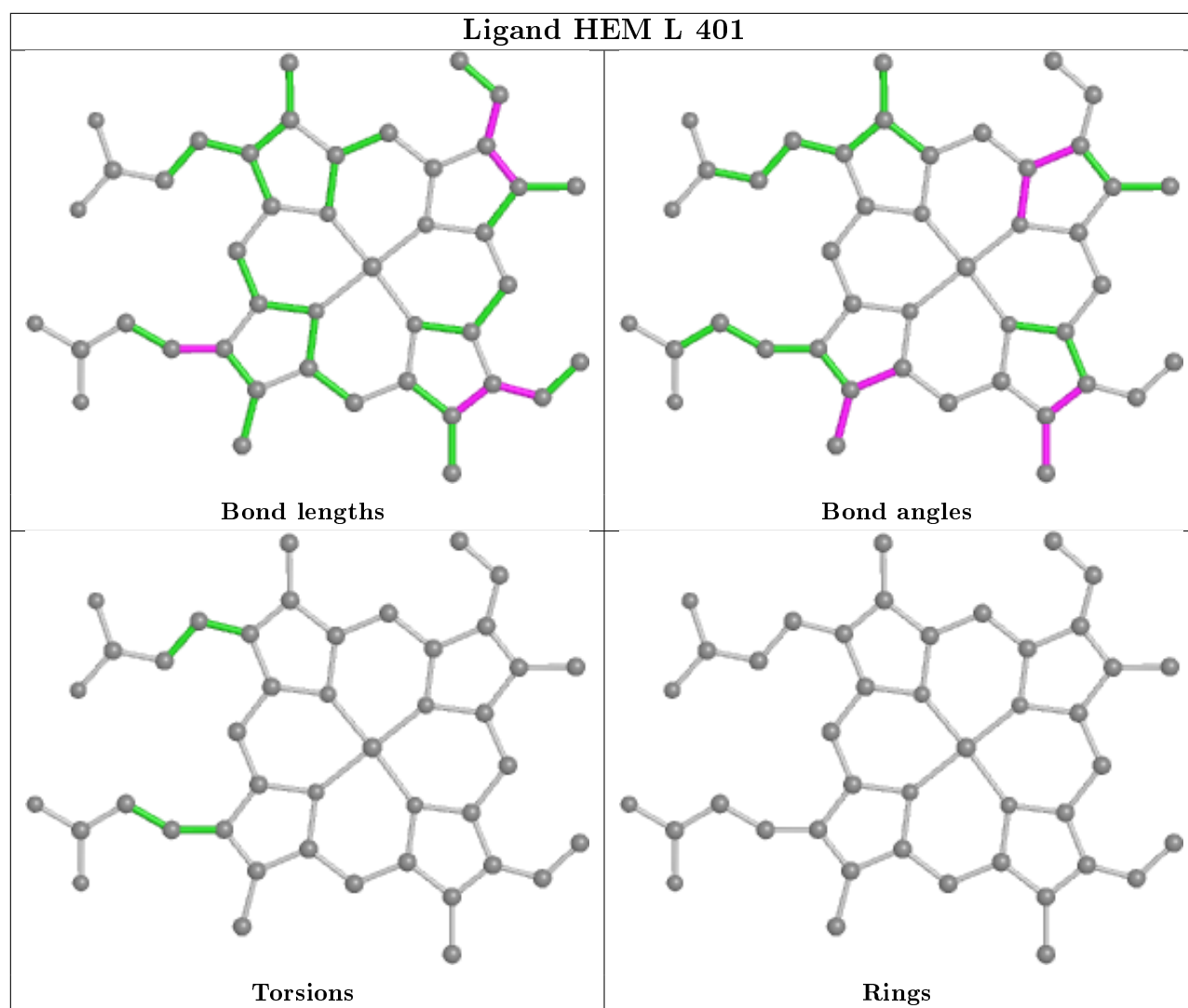


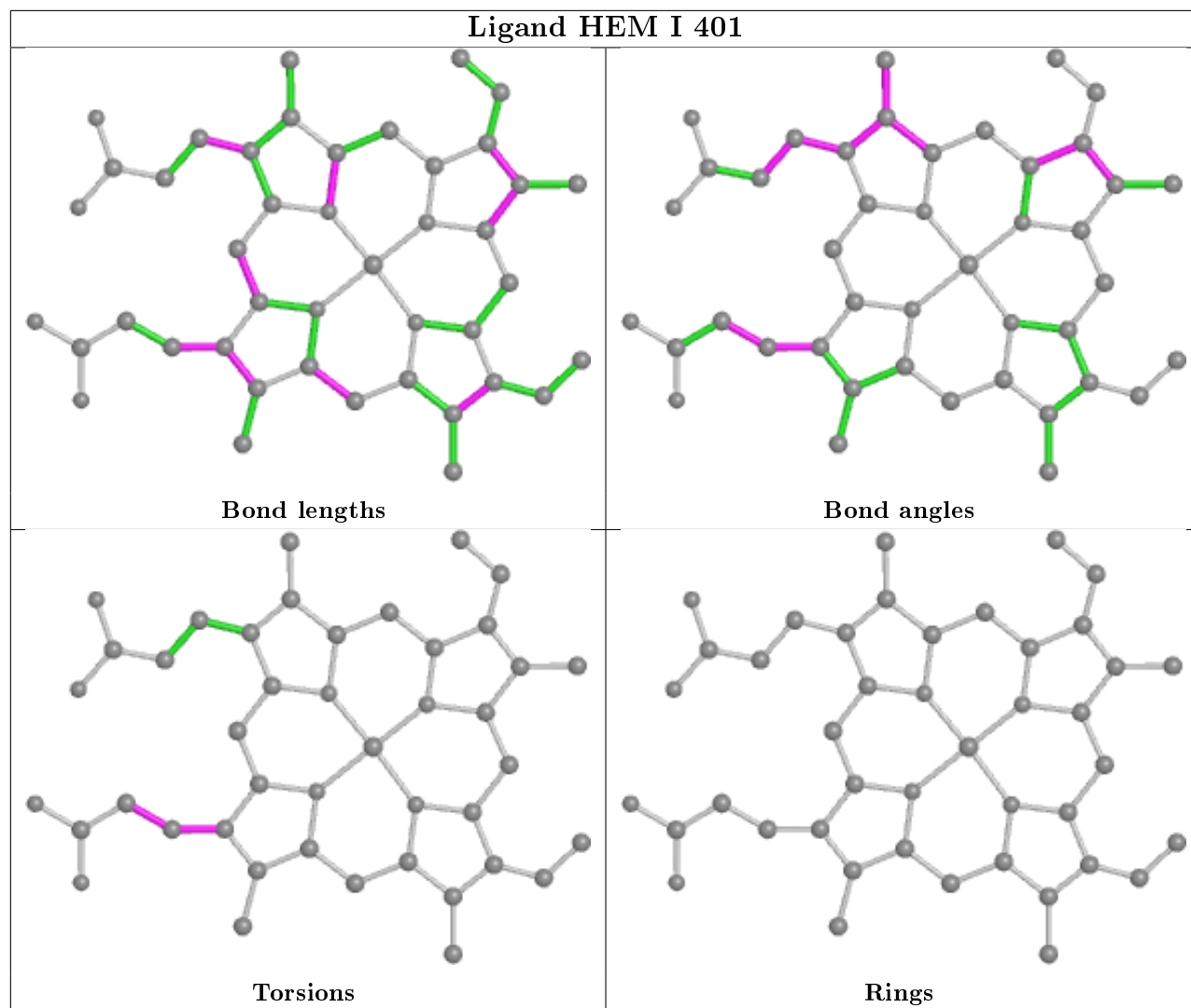
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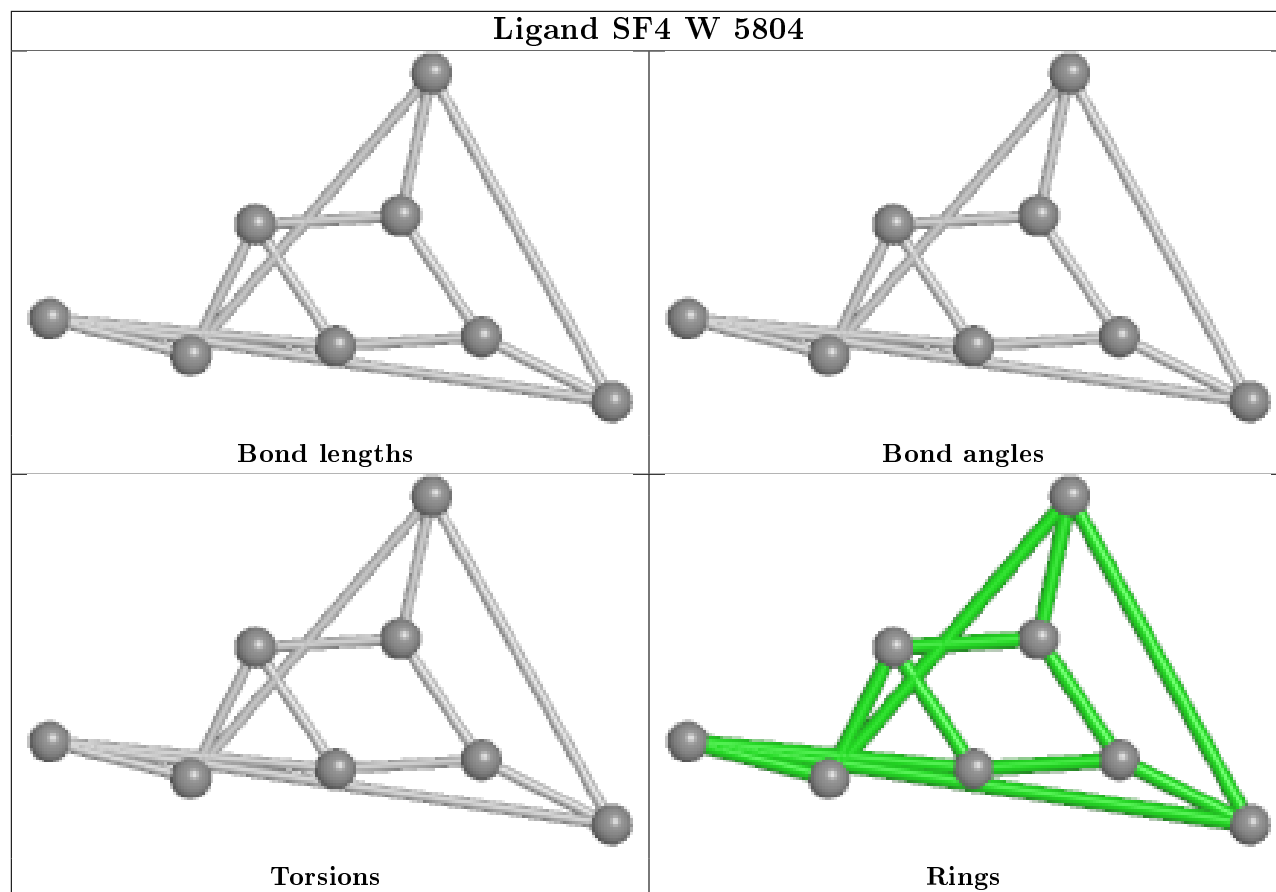




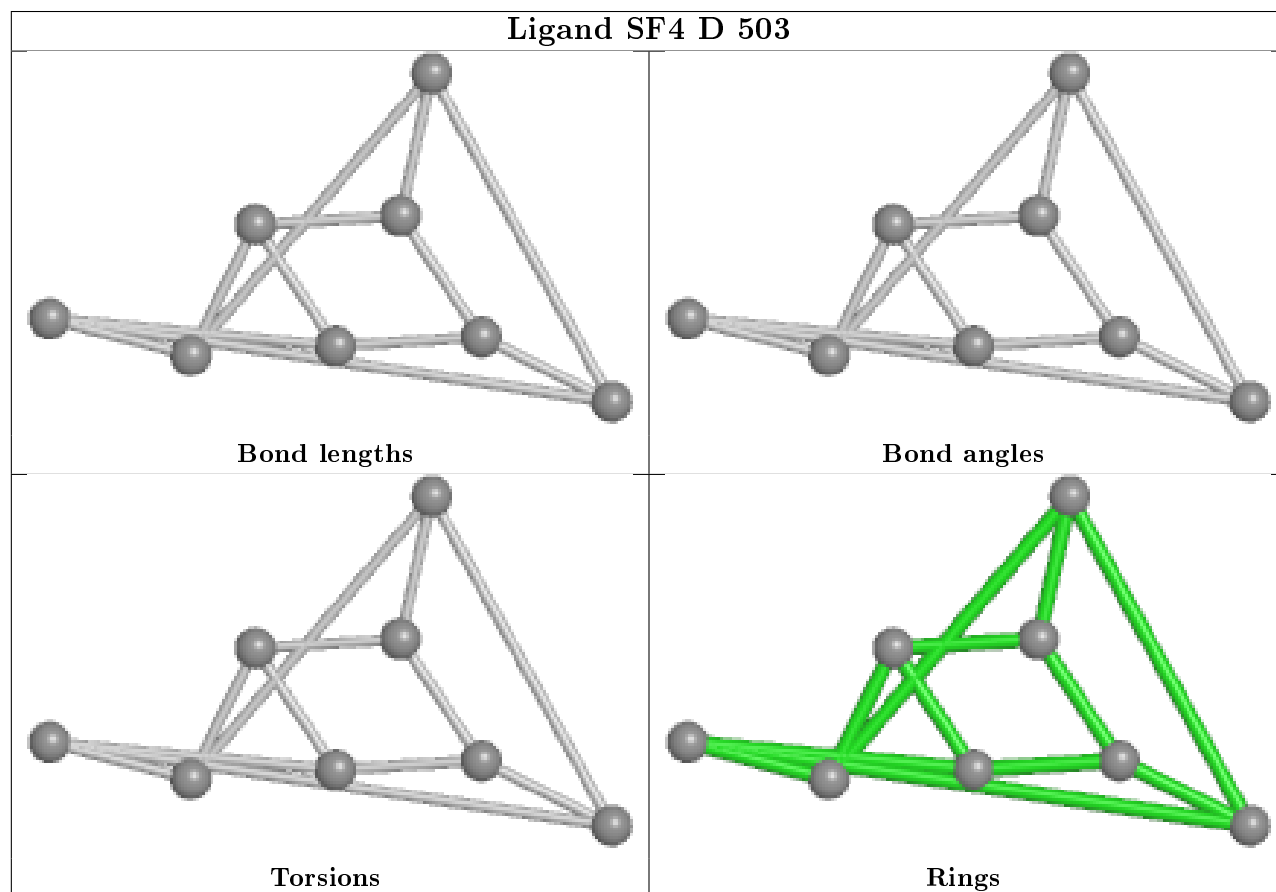




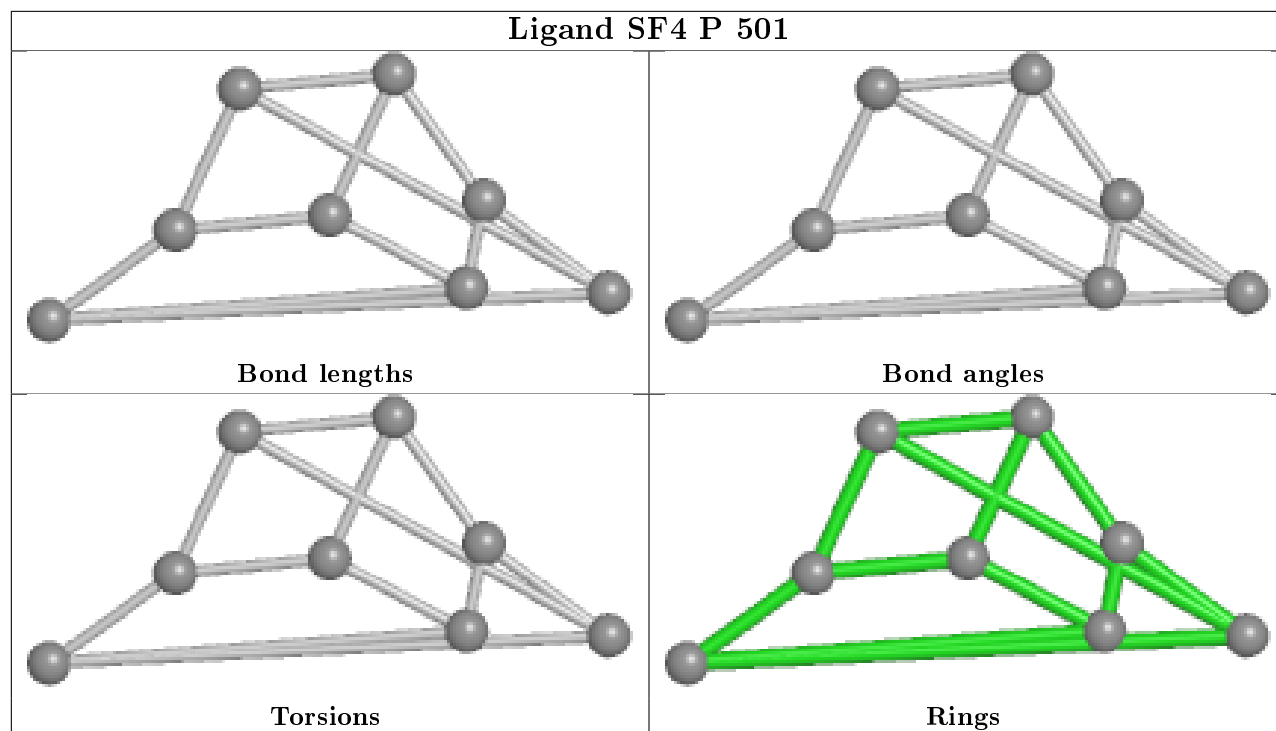
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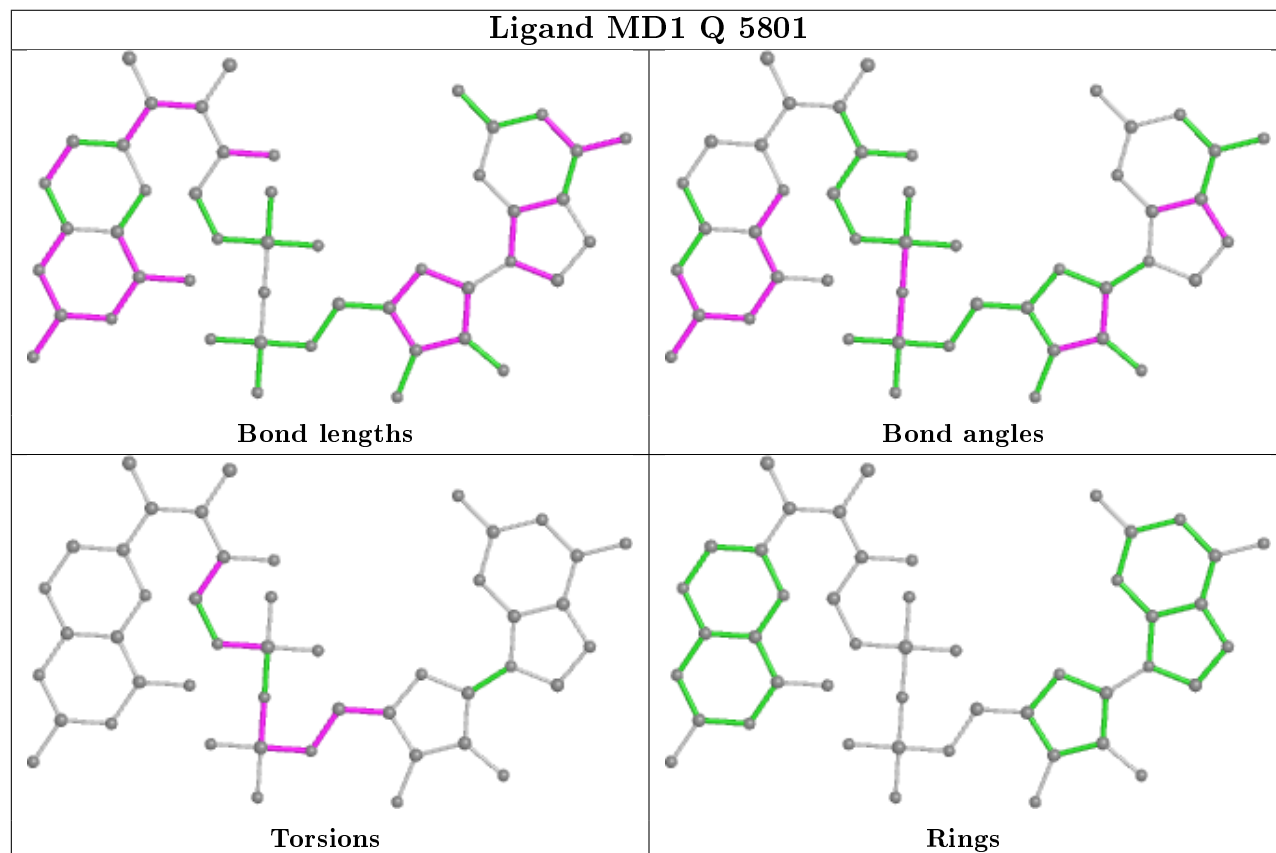
## Ligand SF4 D 503

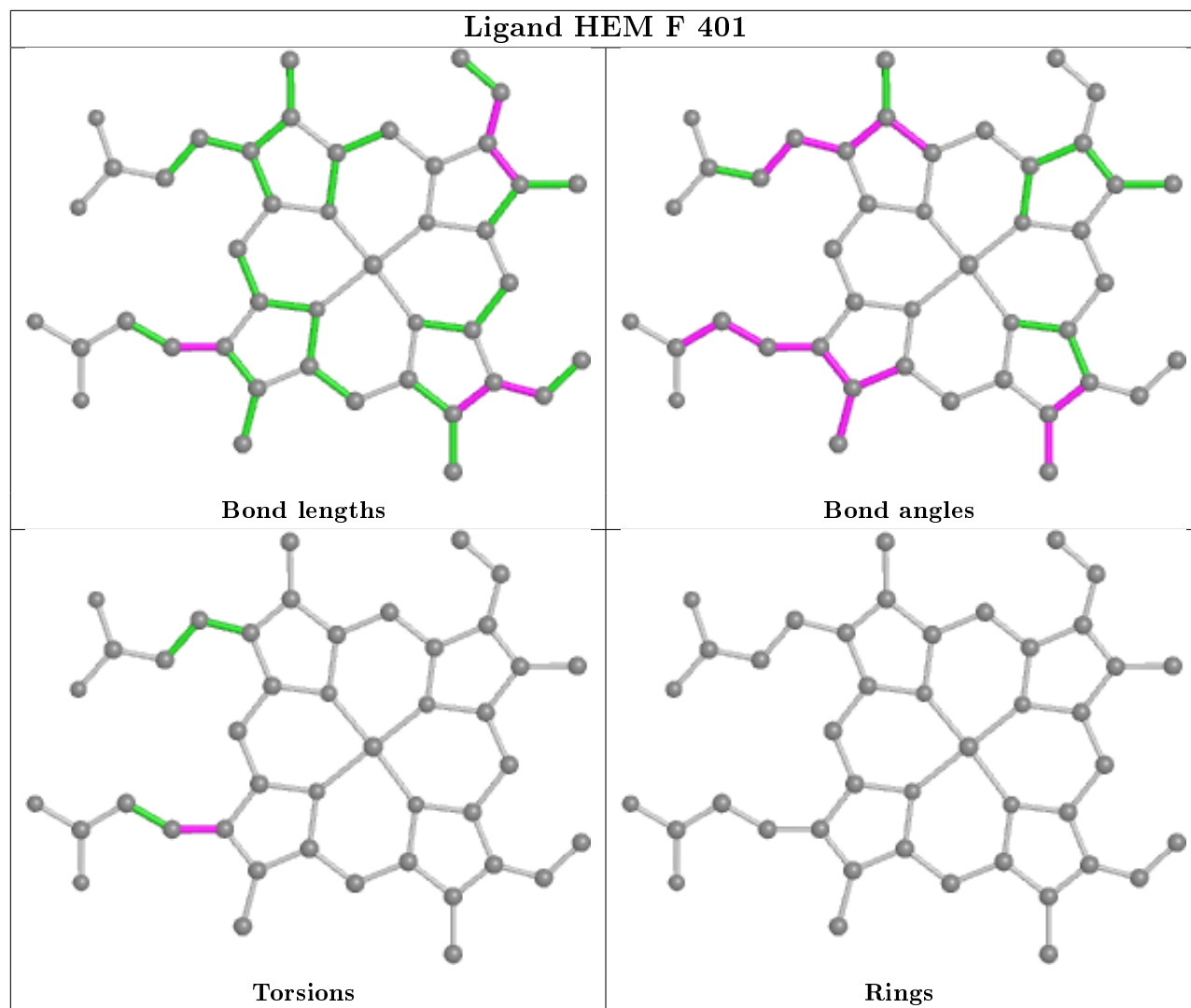


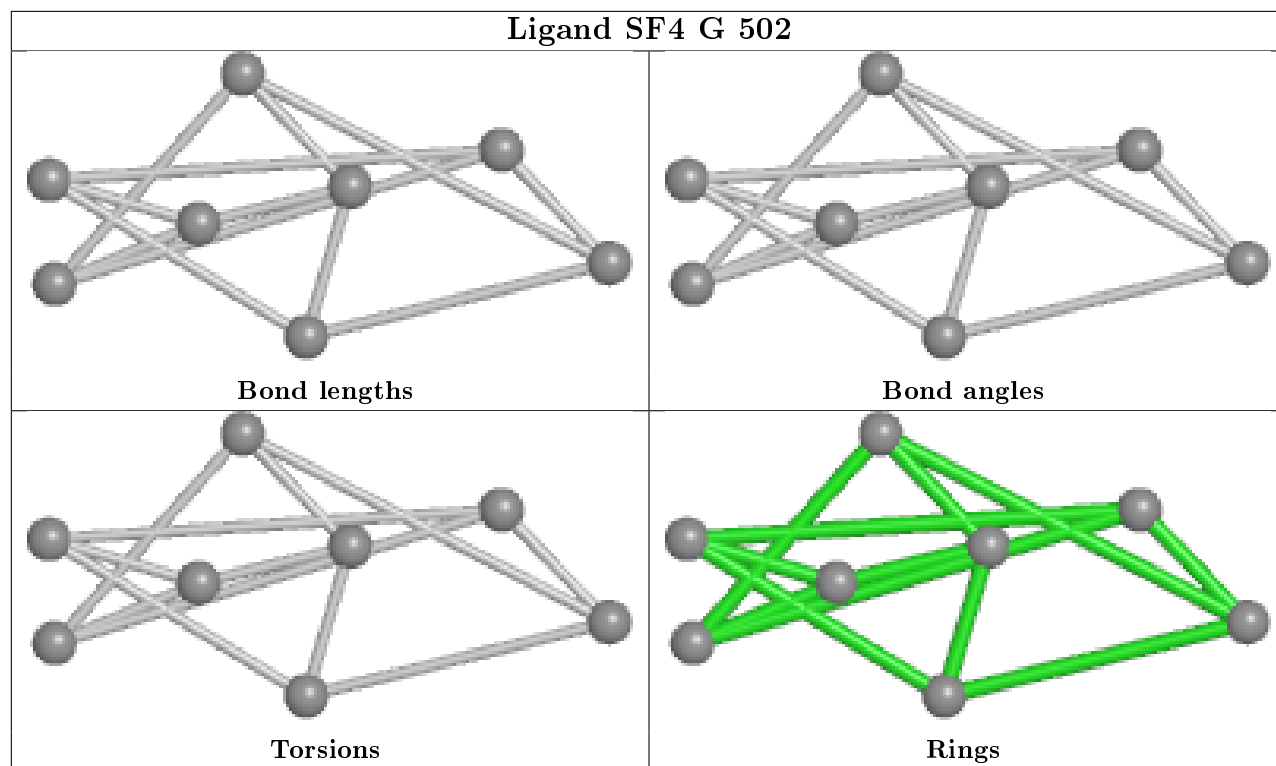
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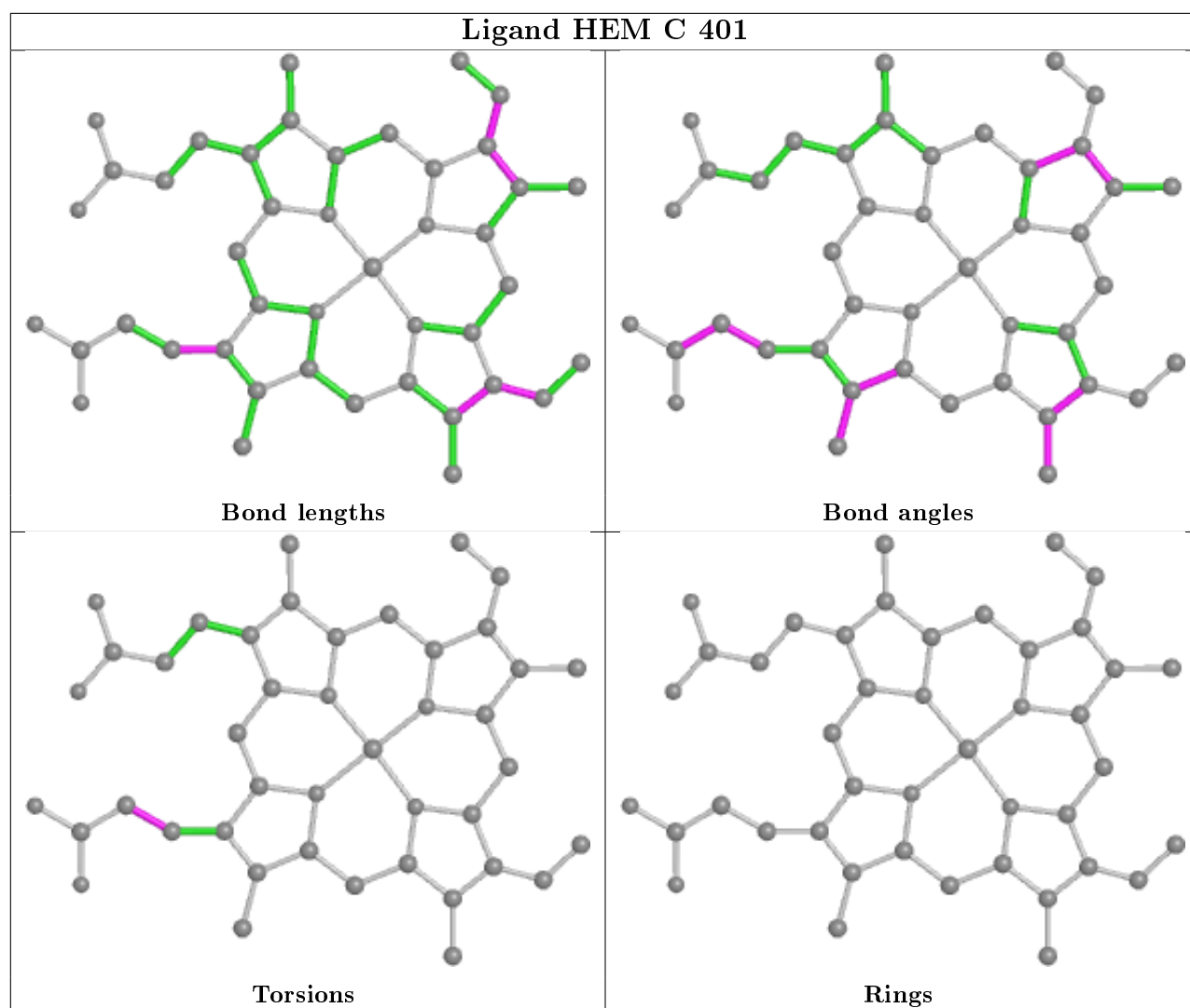


## Ligand MD1 Q 5801

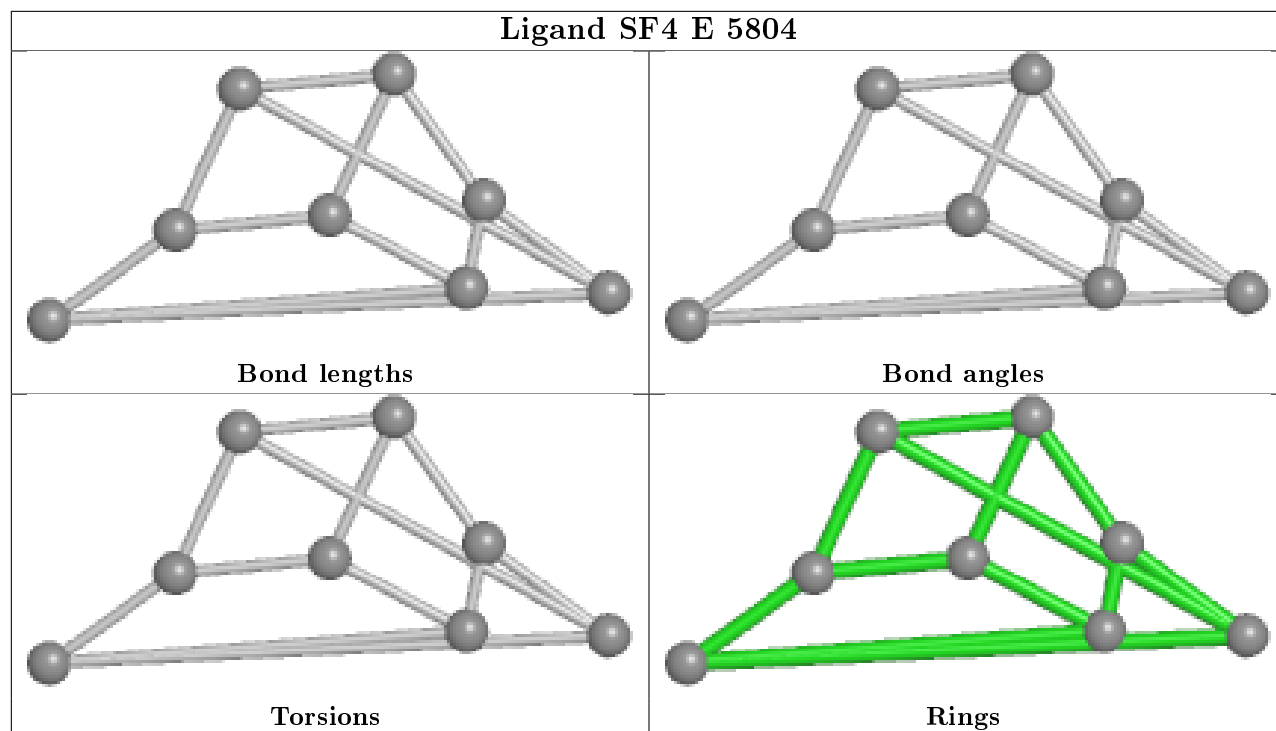




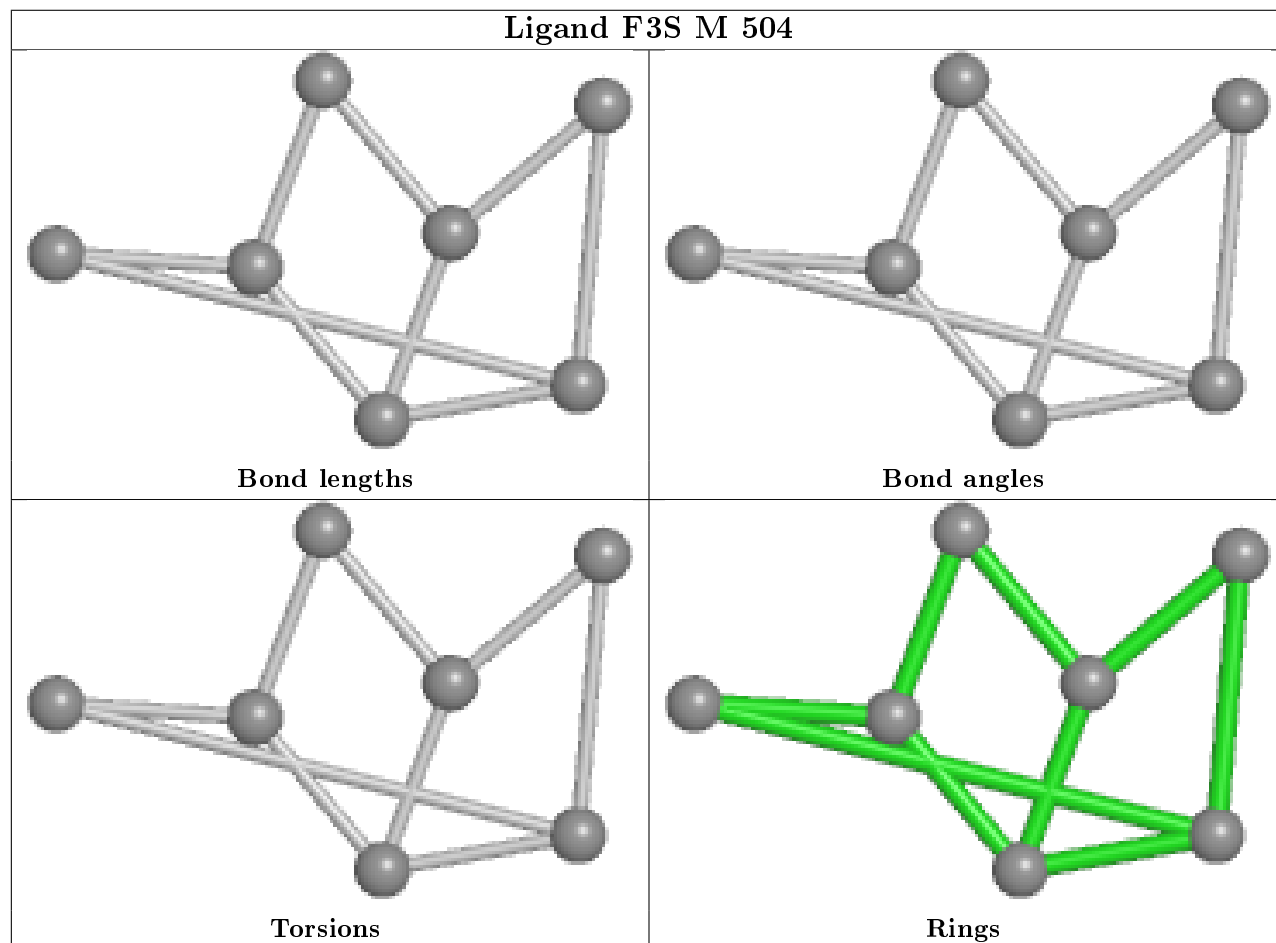


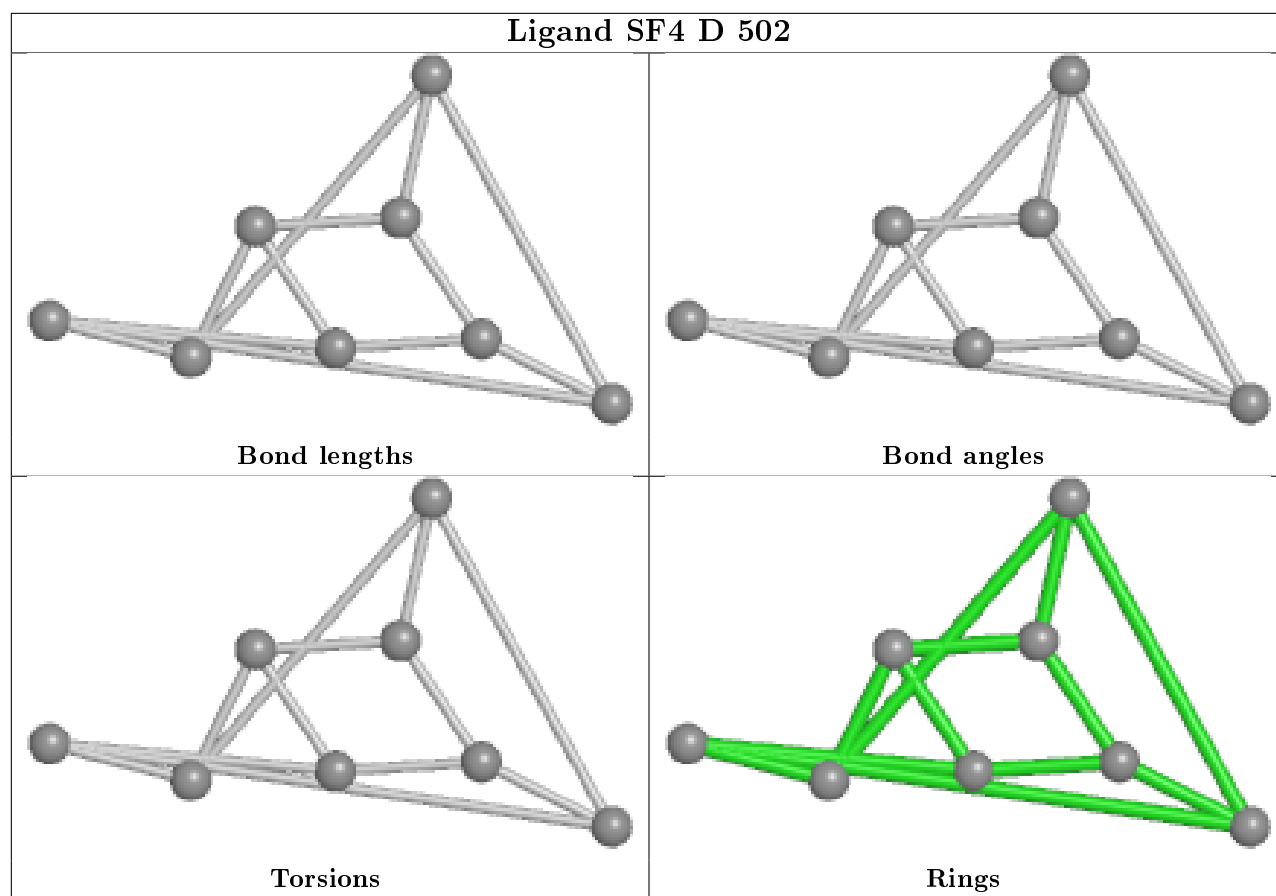
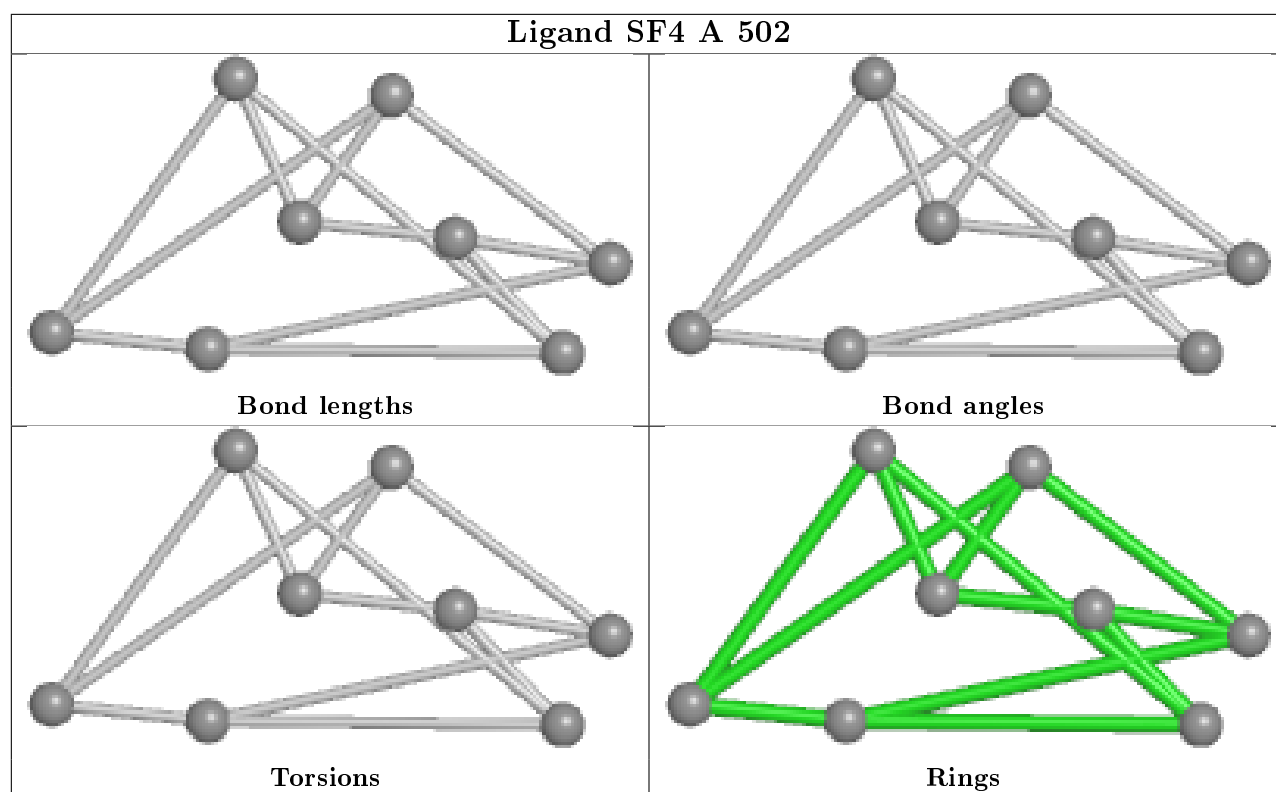


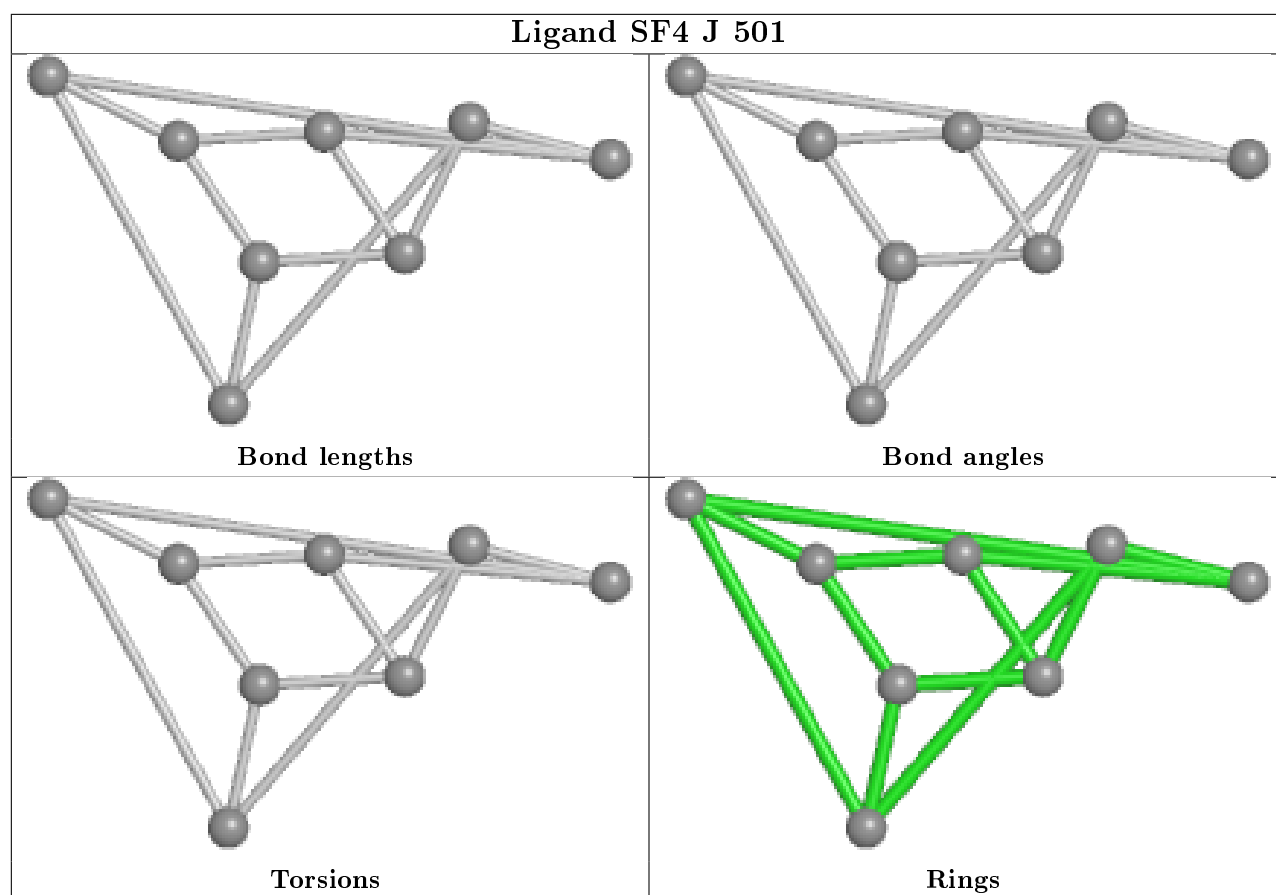
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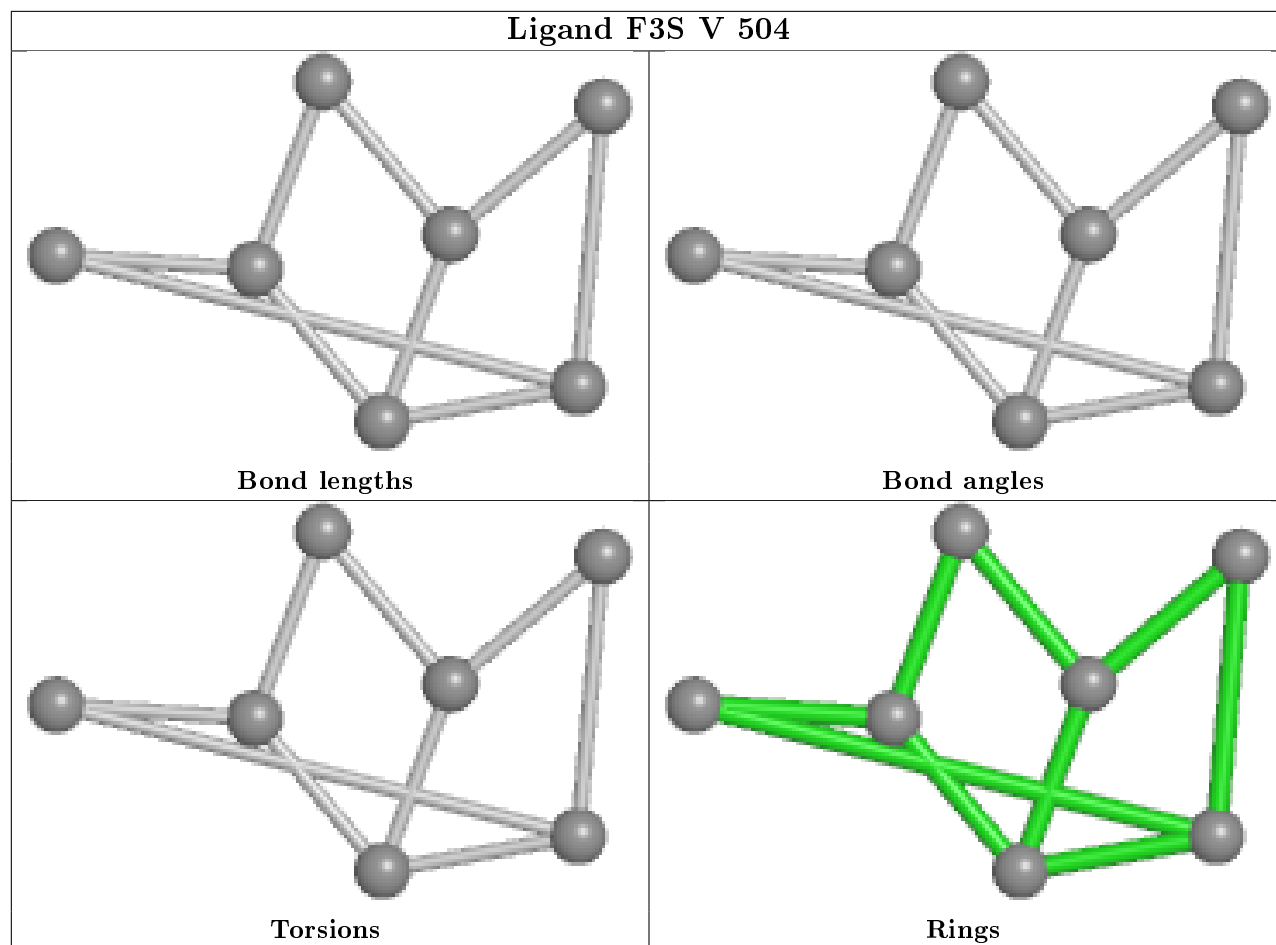
## Ligand F3S M 504



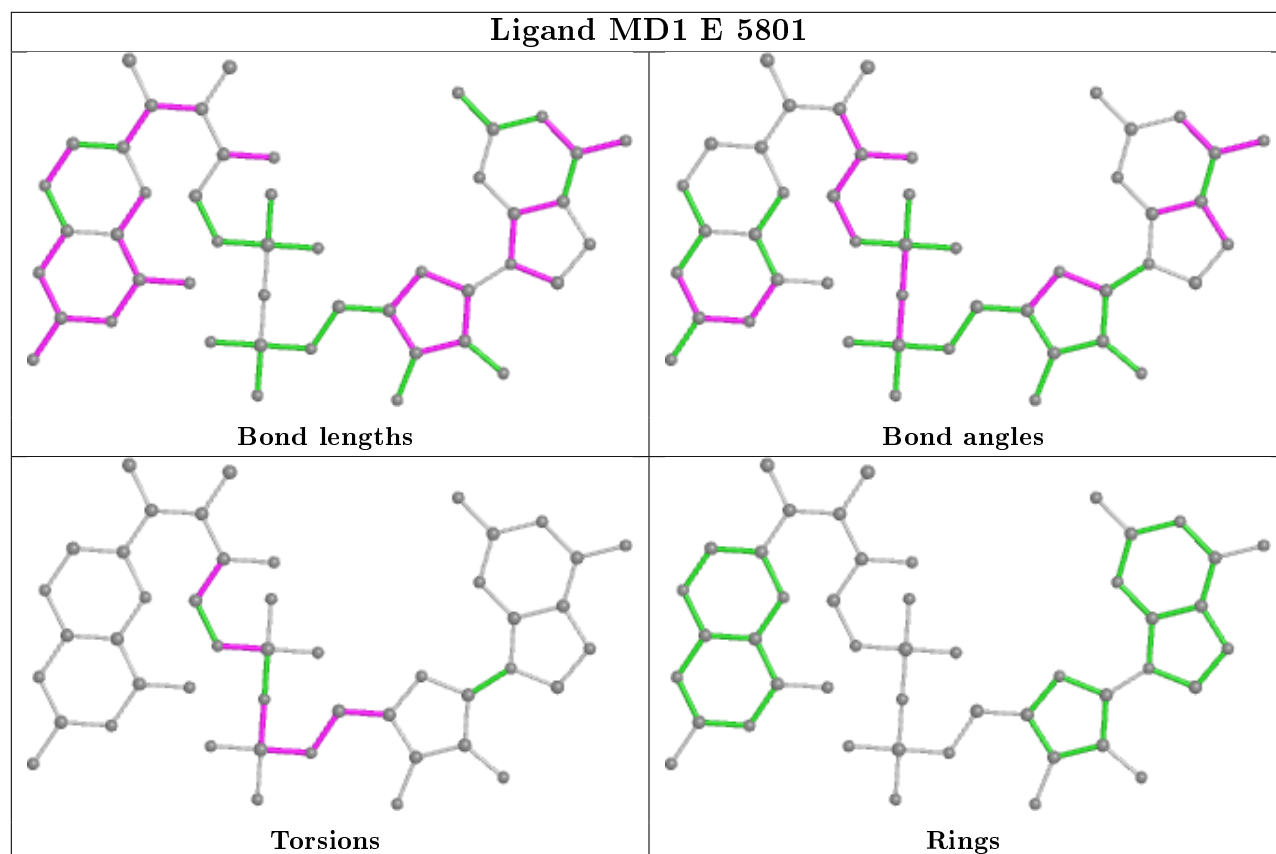




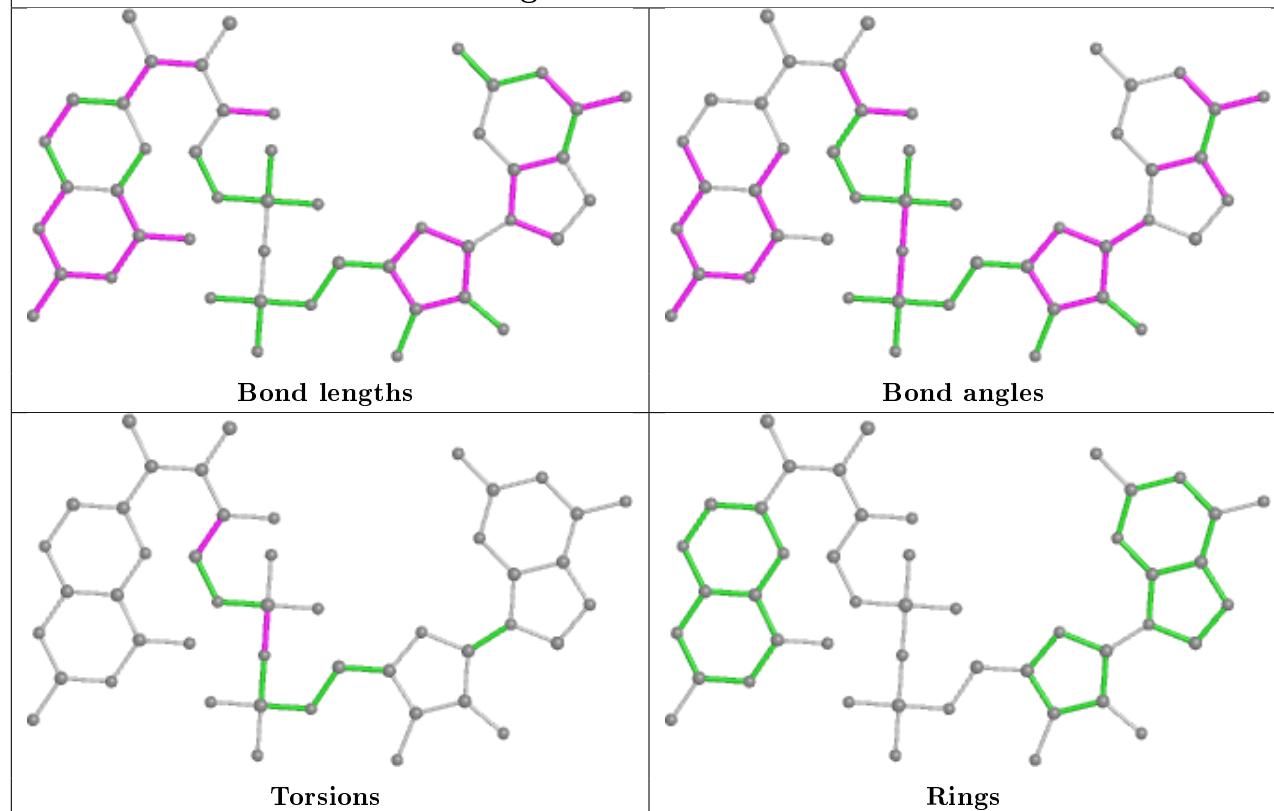
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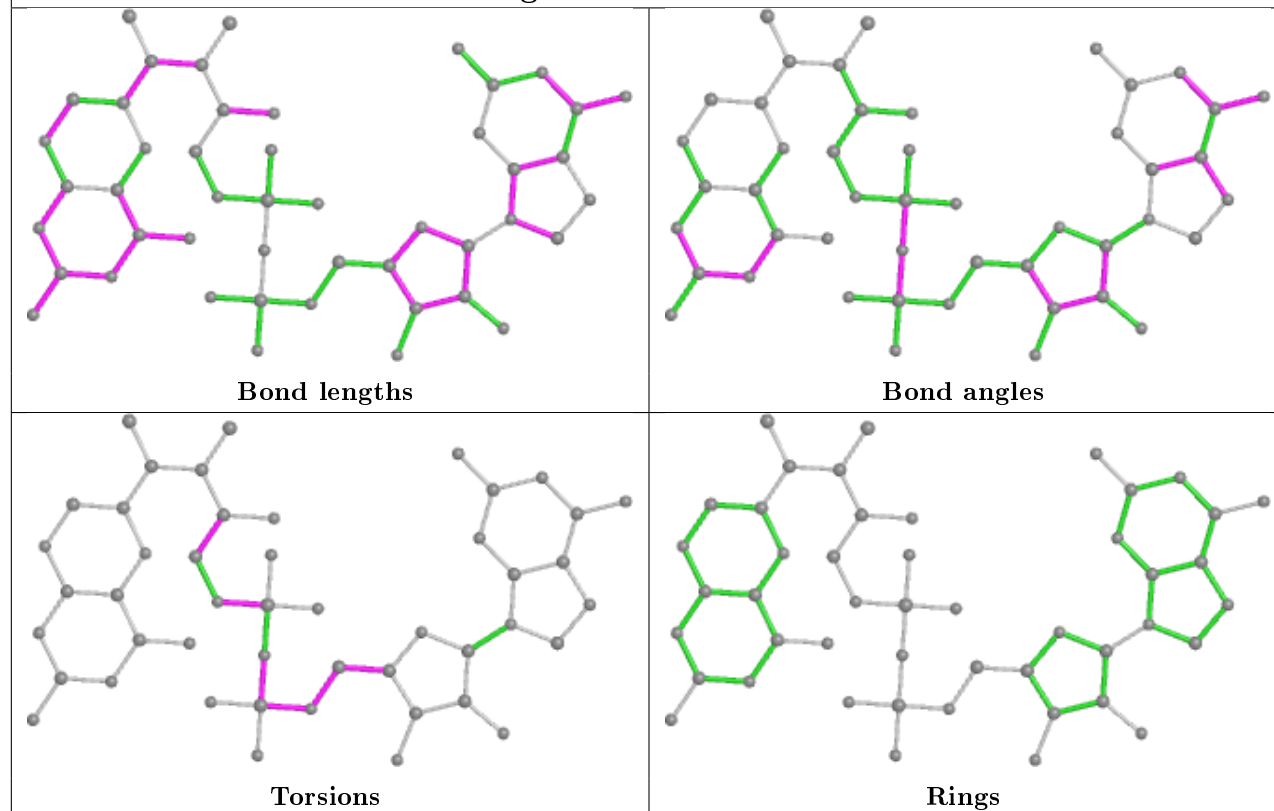
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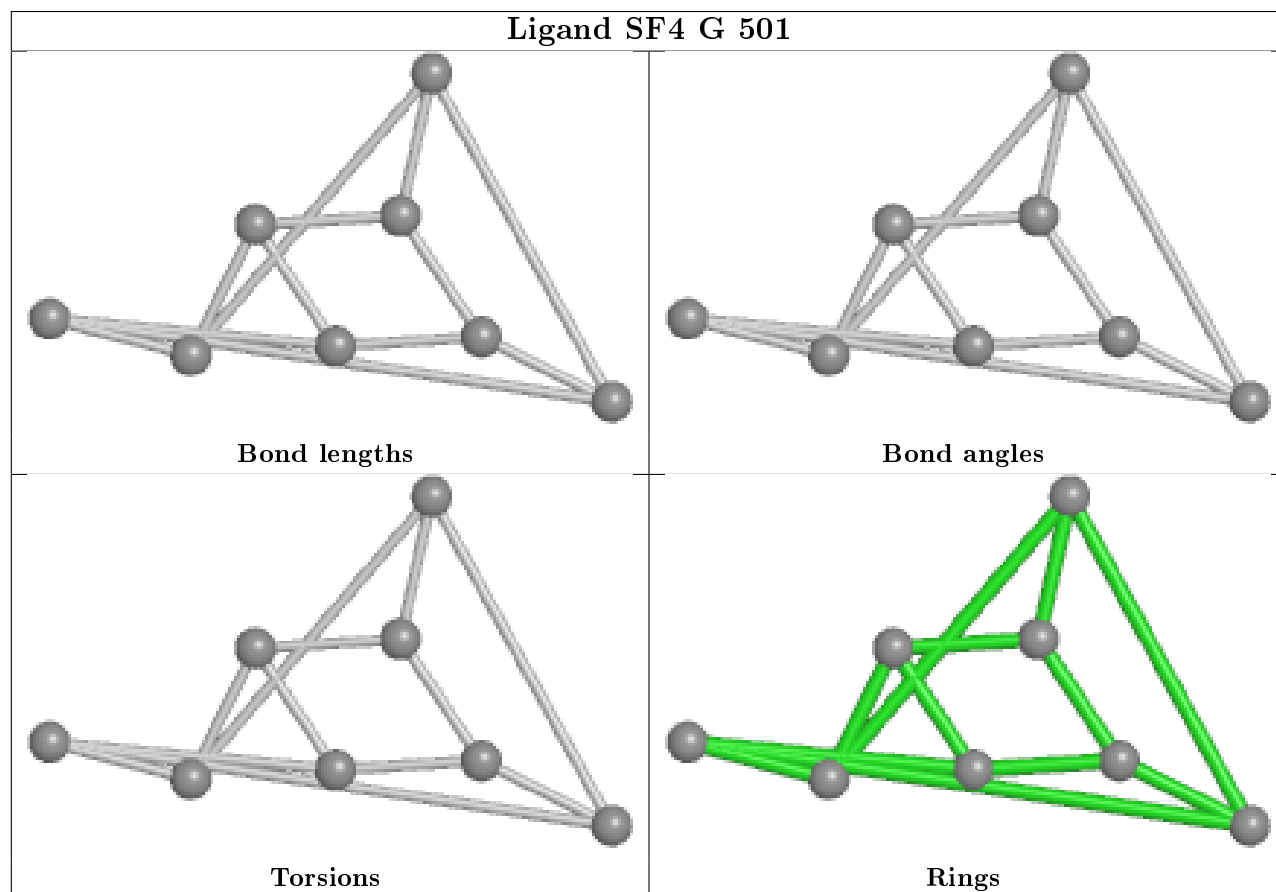
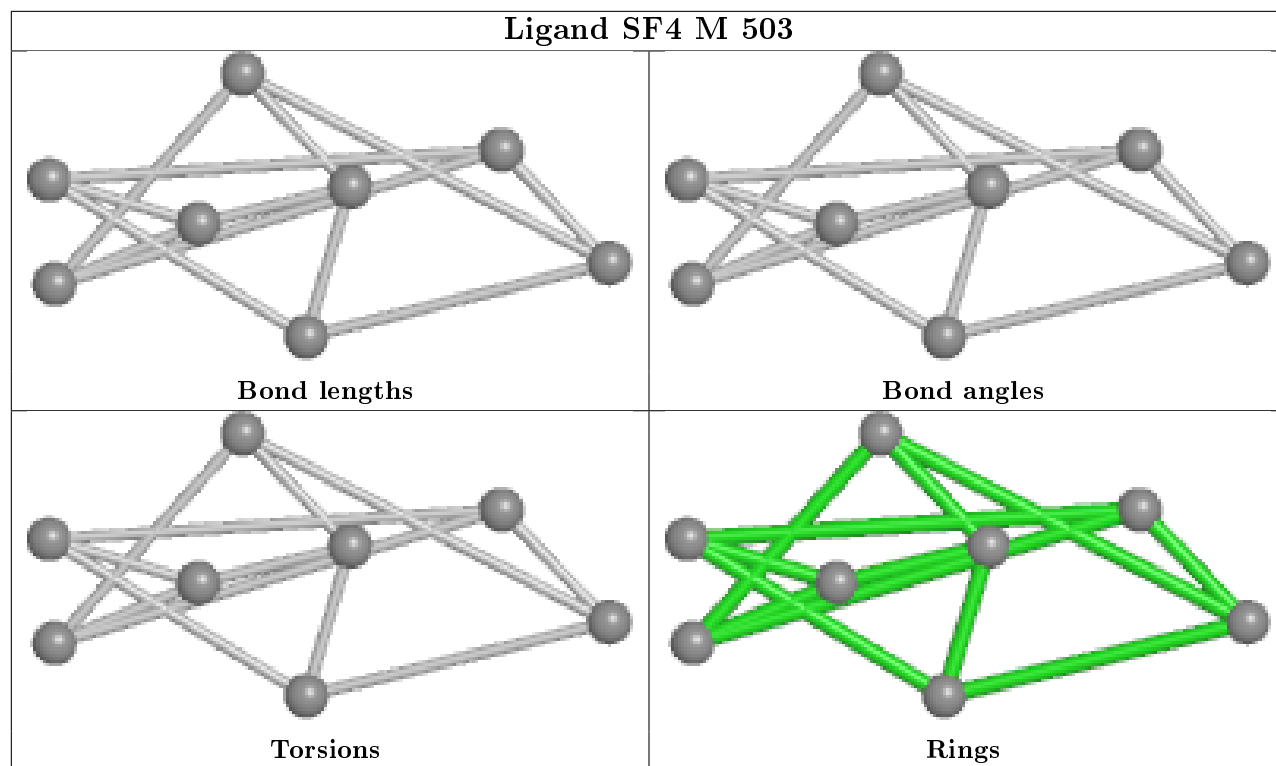


## Ligand MD1 K 5802

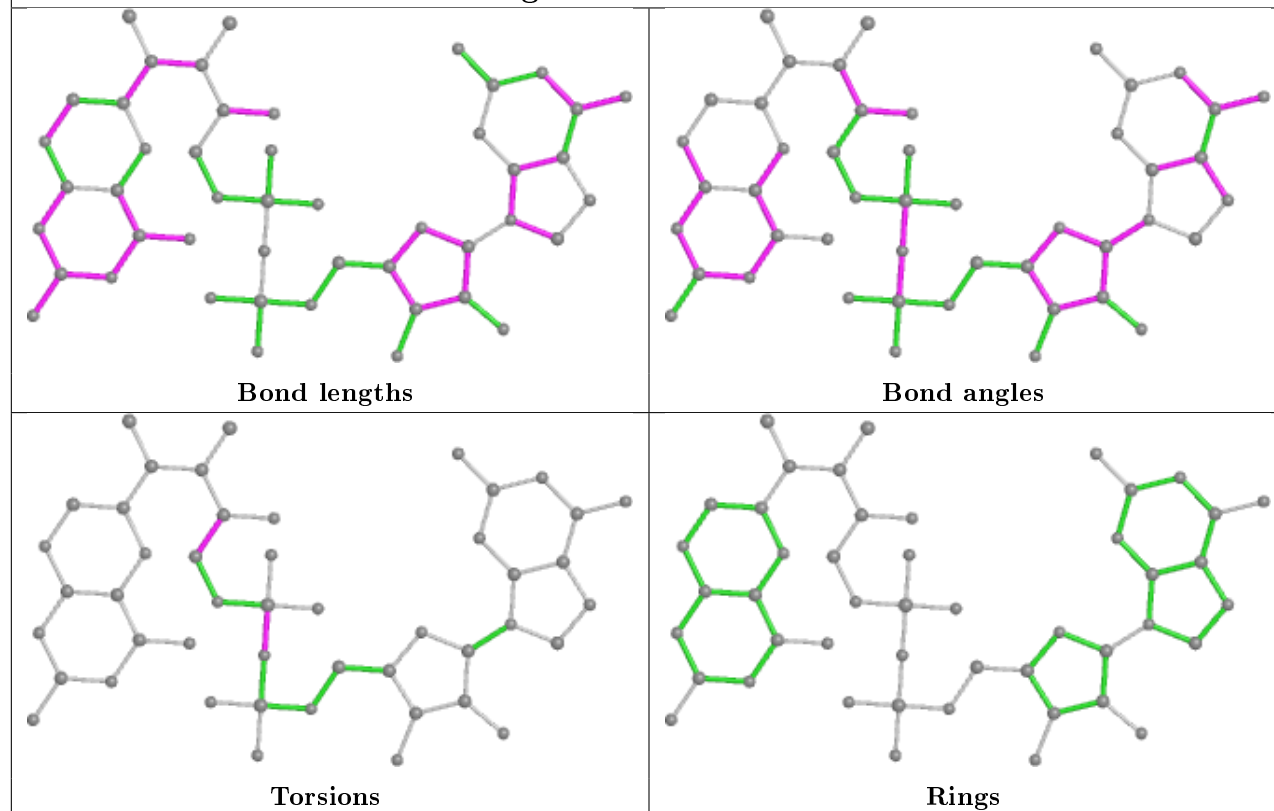


## Ligand MD1 N 5801

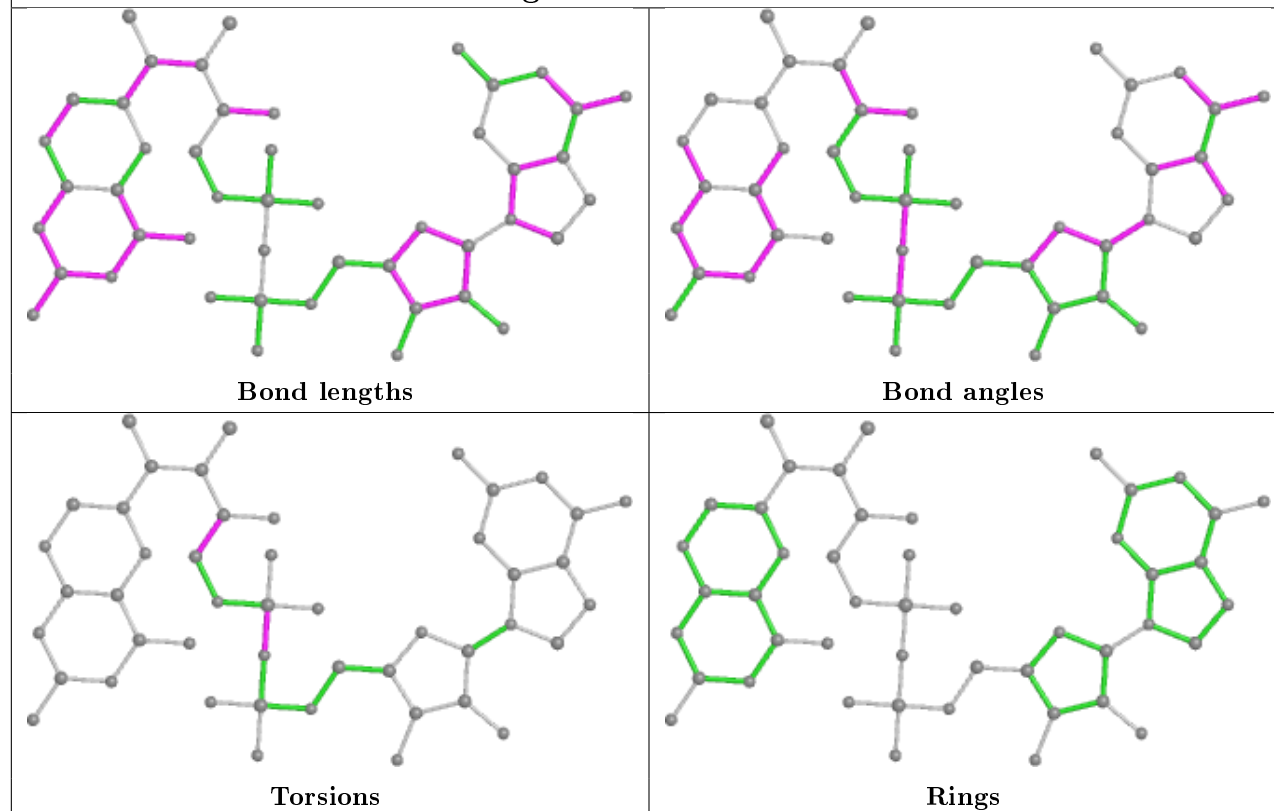




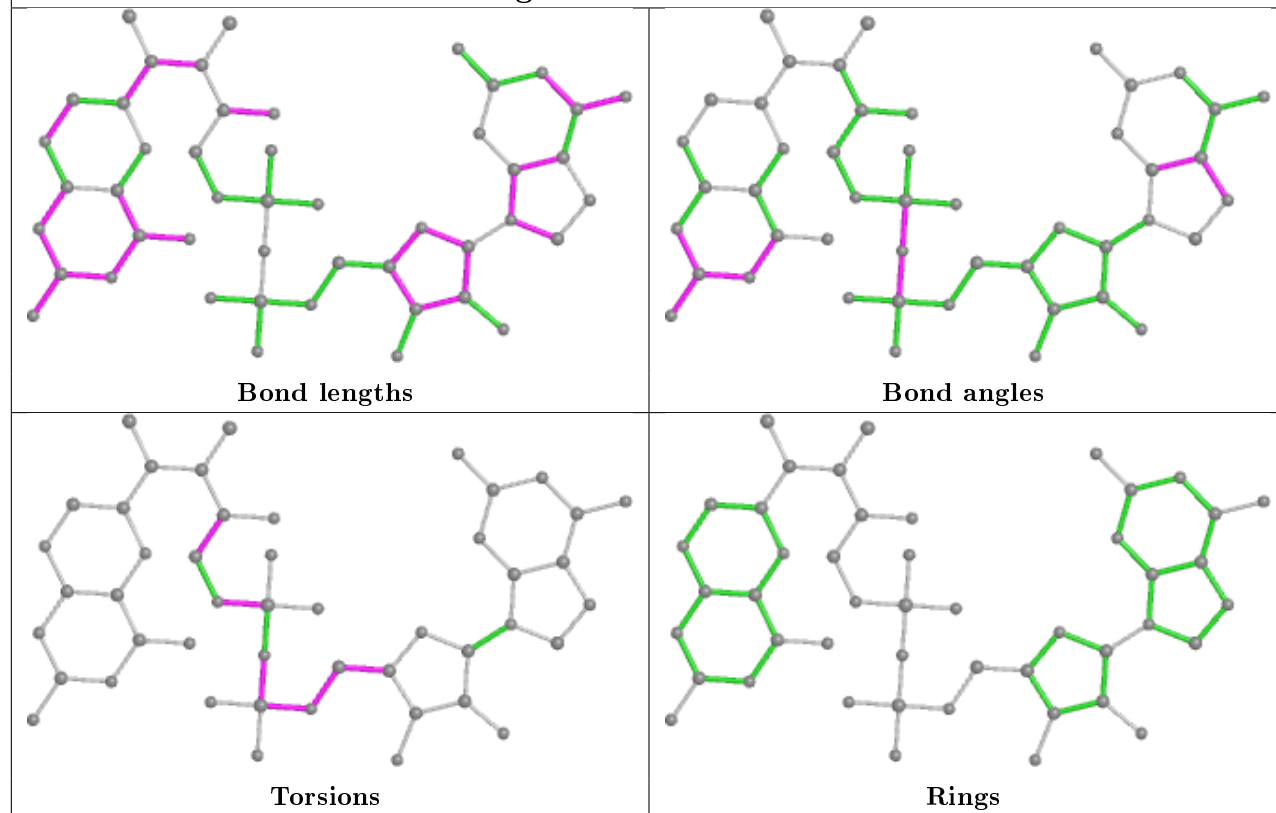
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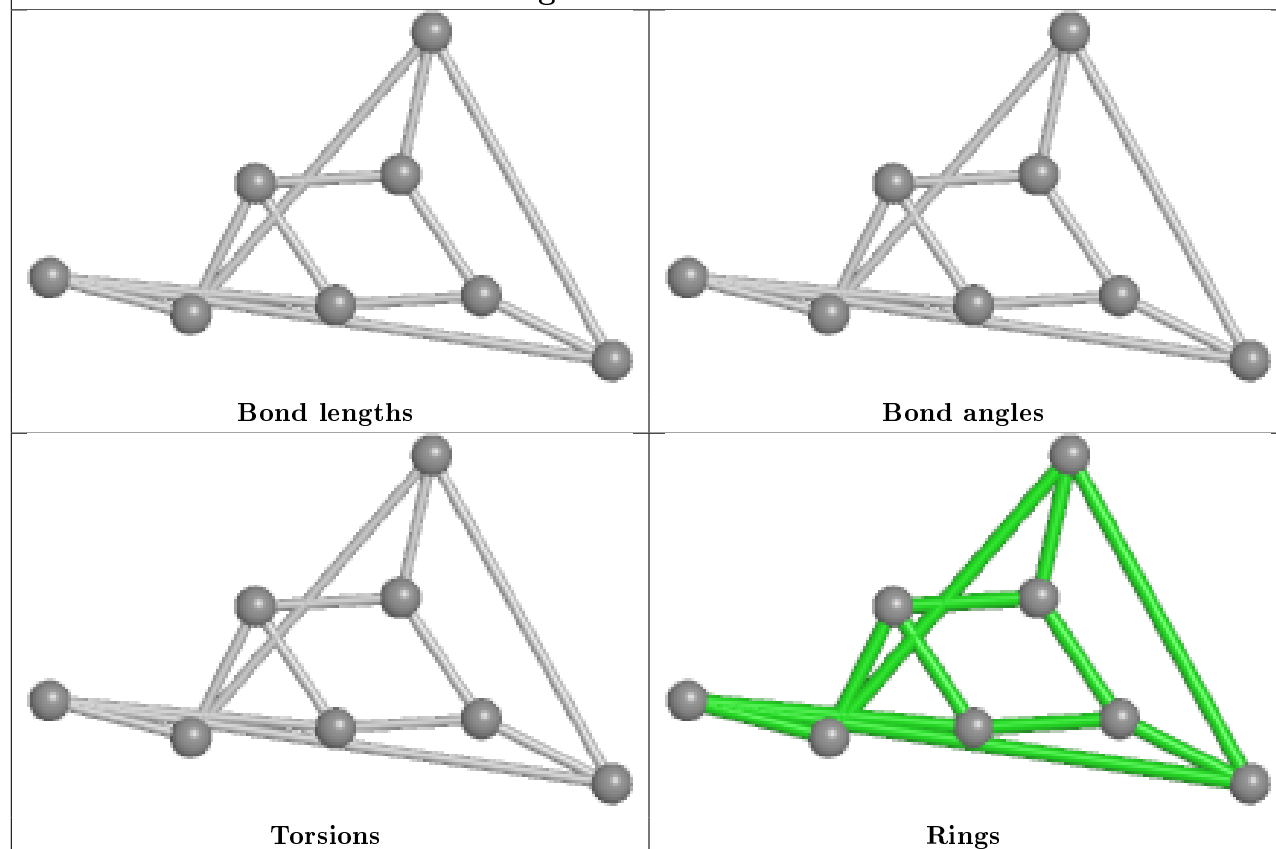
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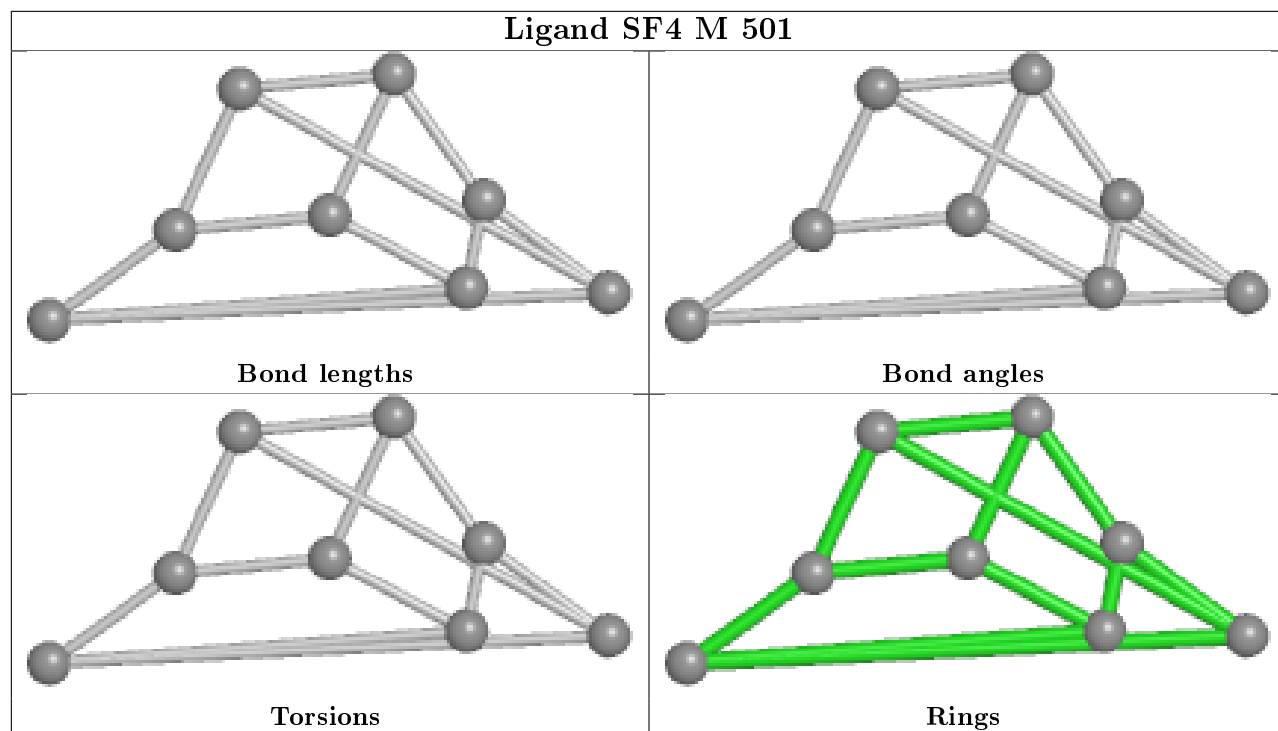


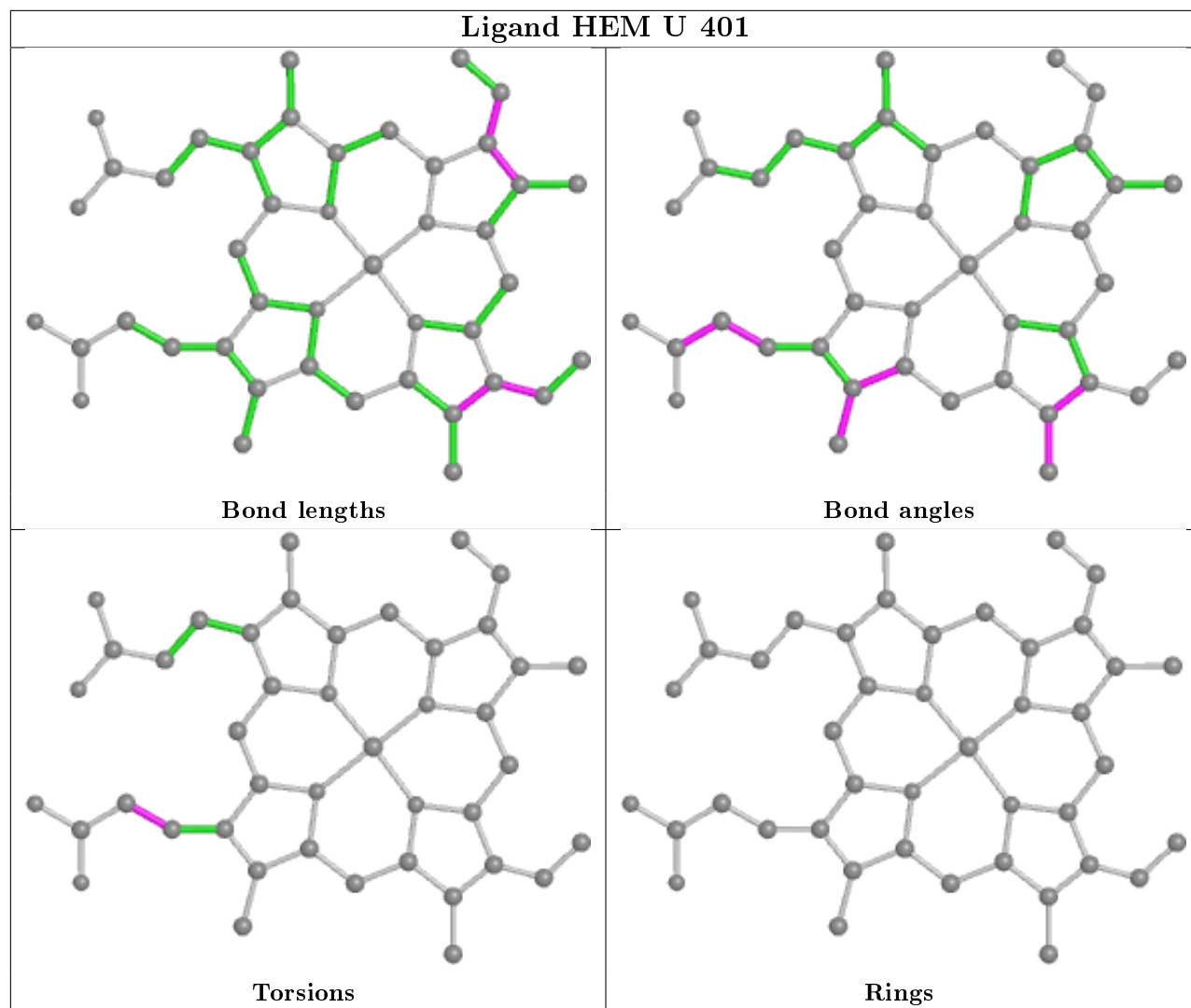
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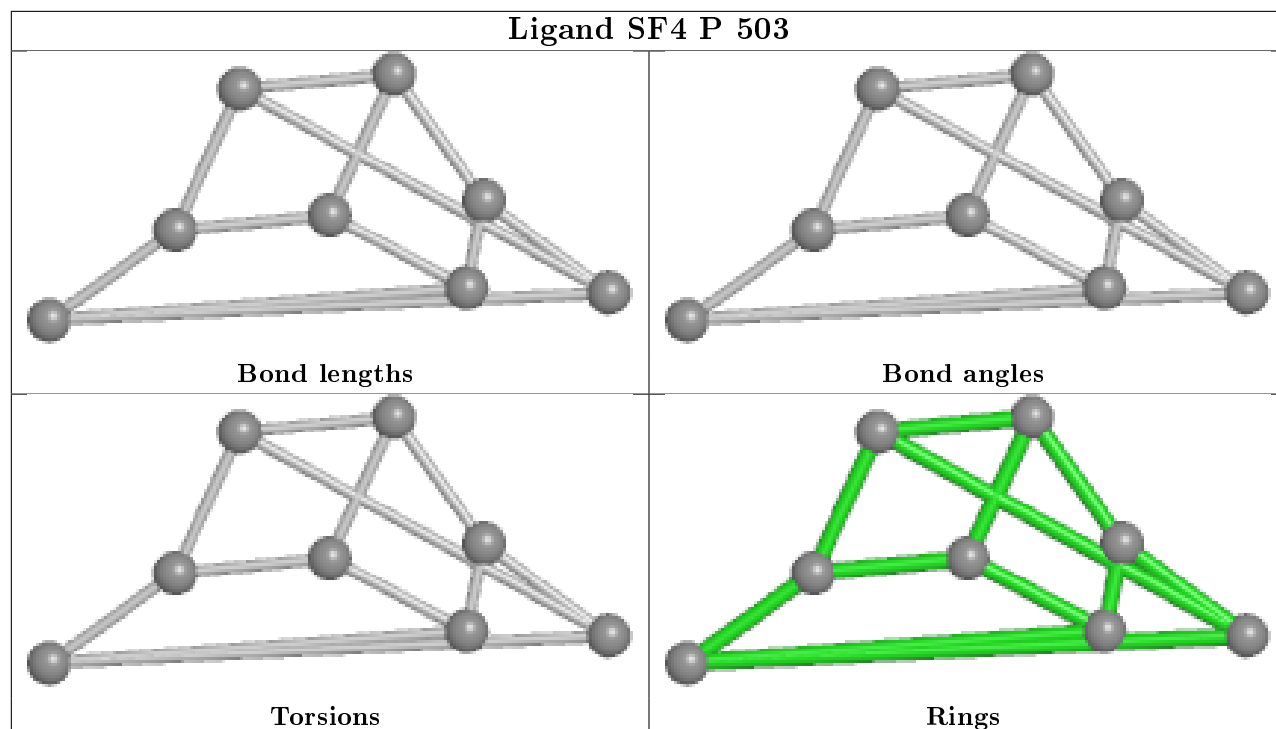
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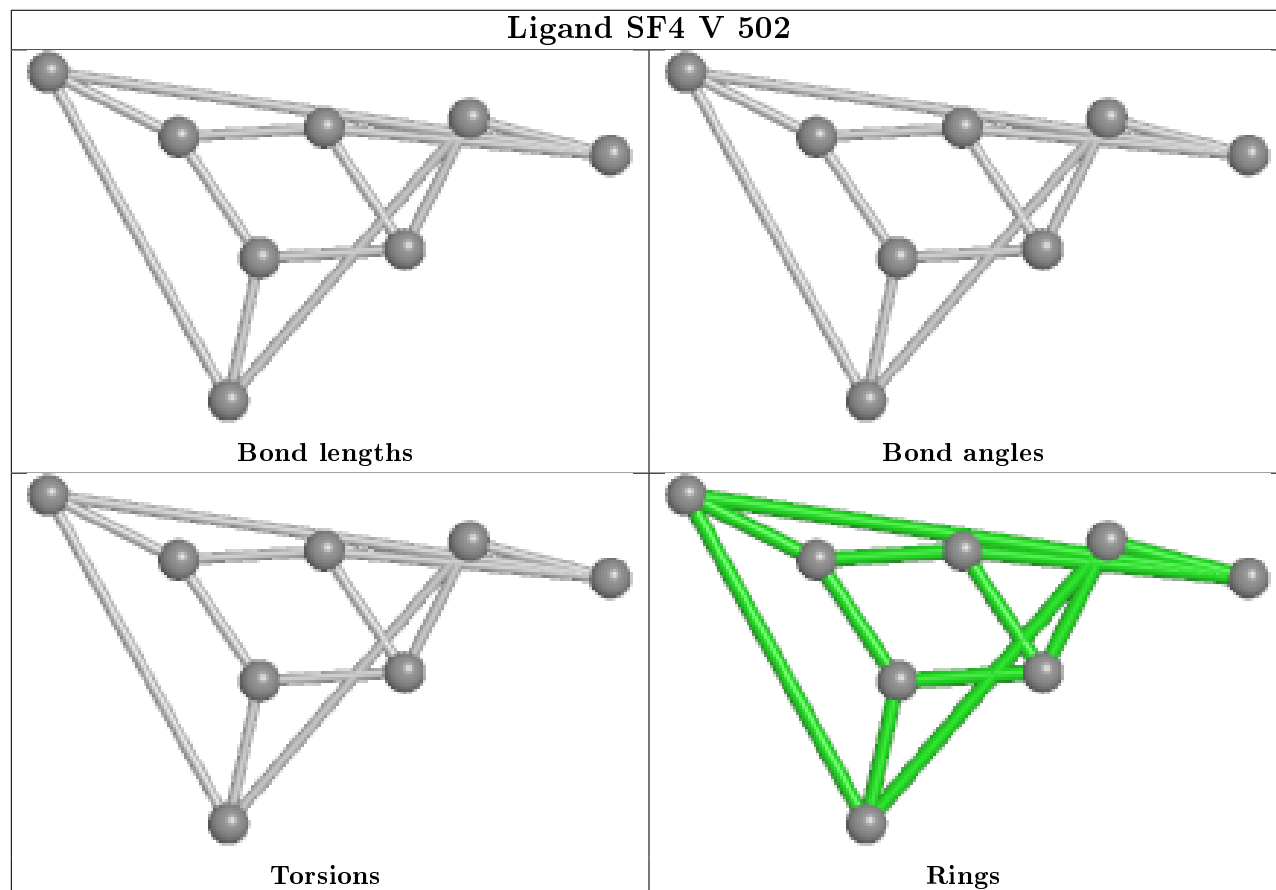




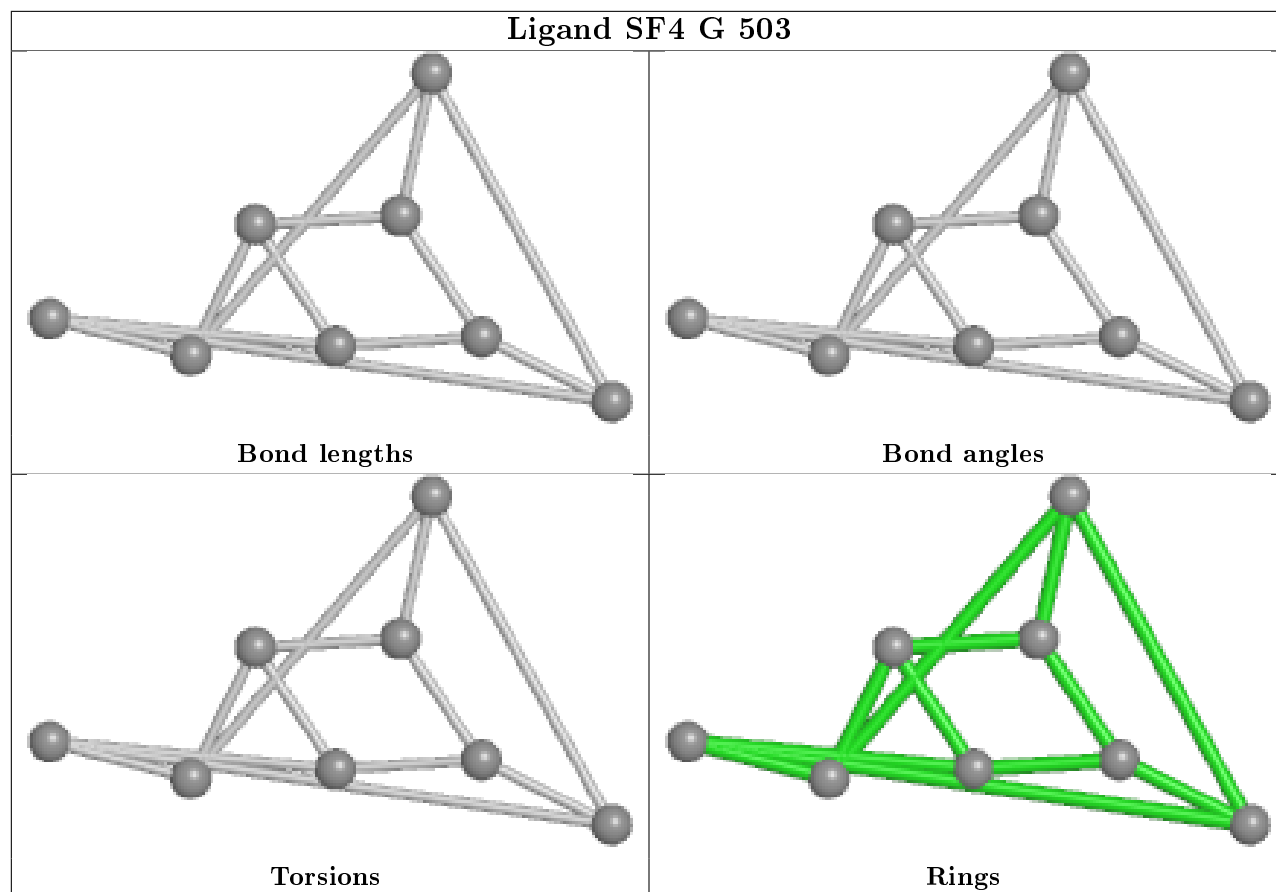
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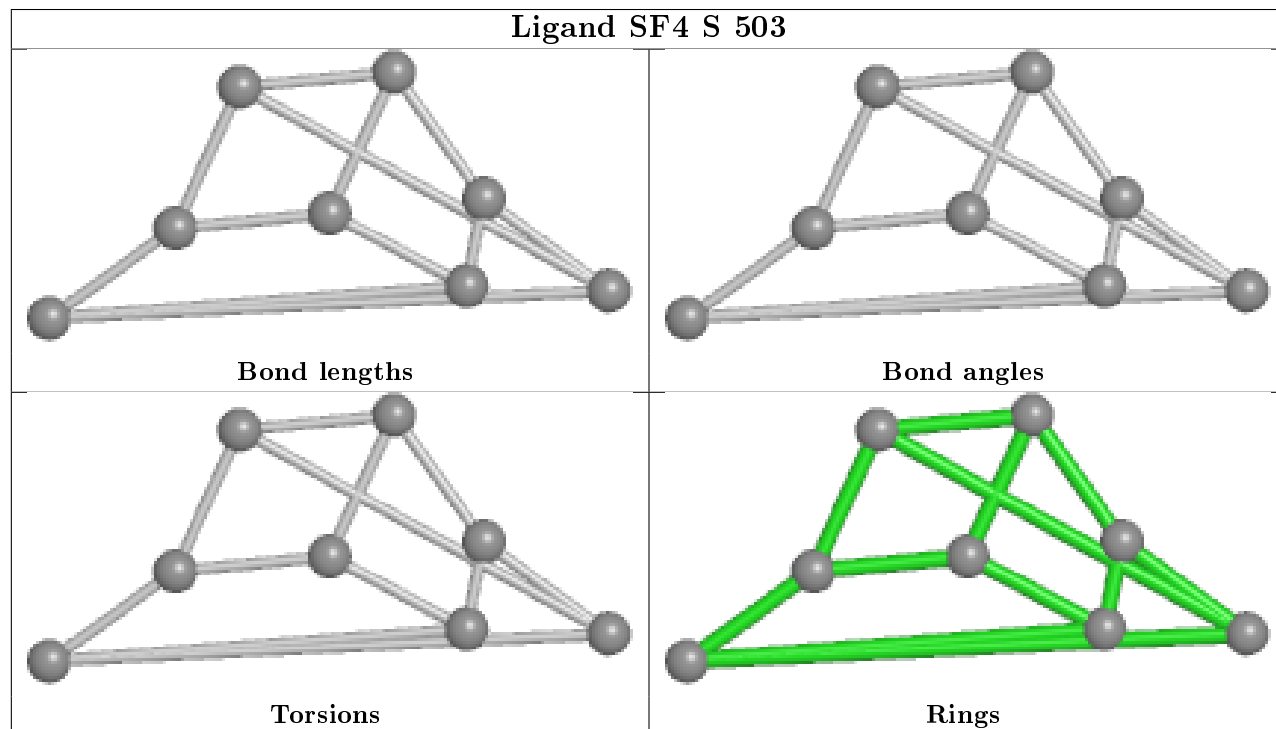
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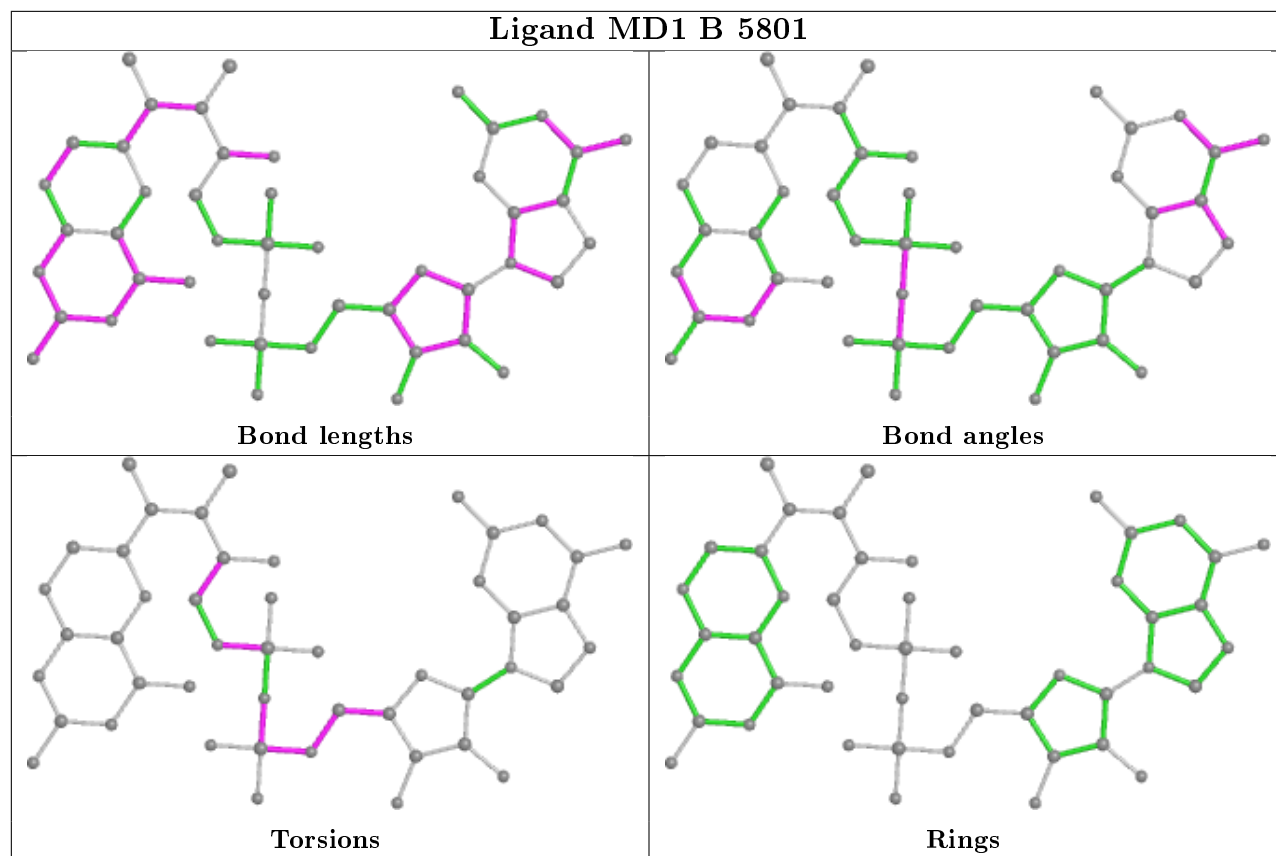


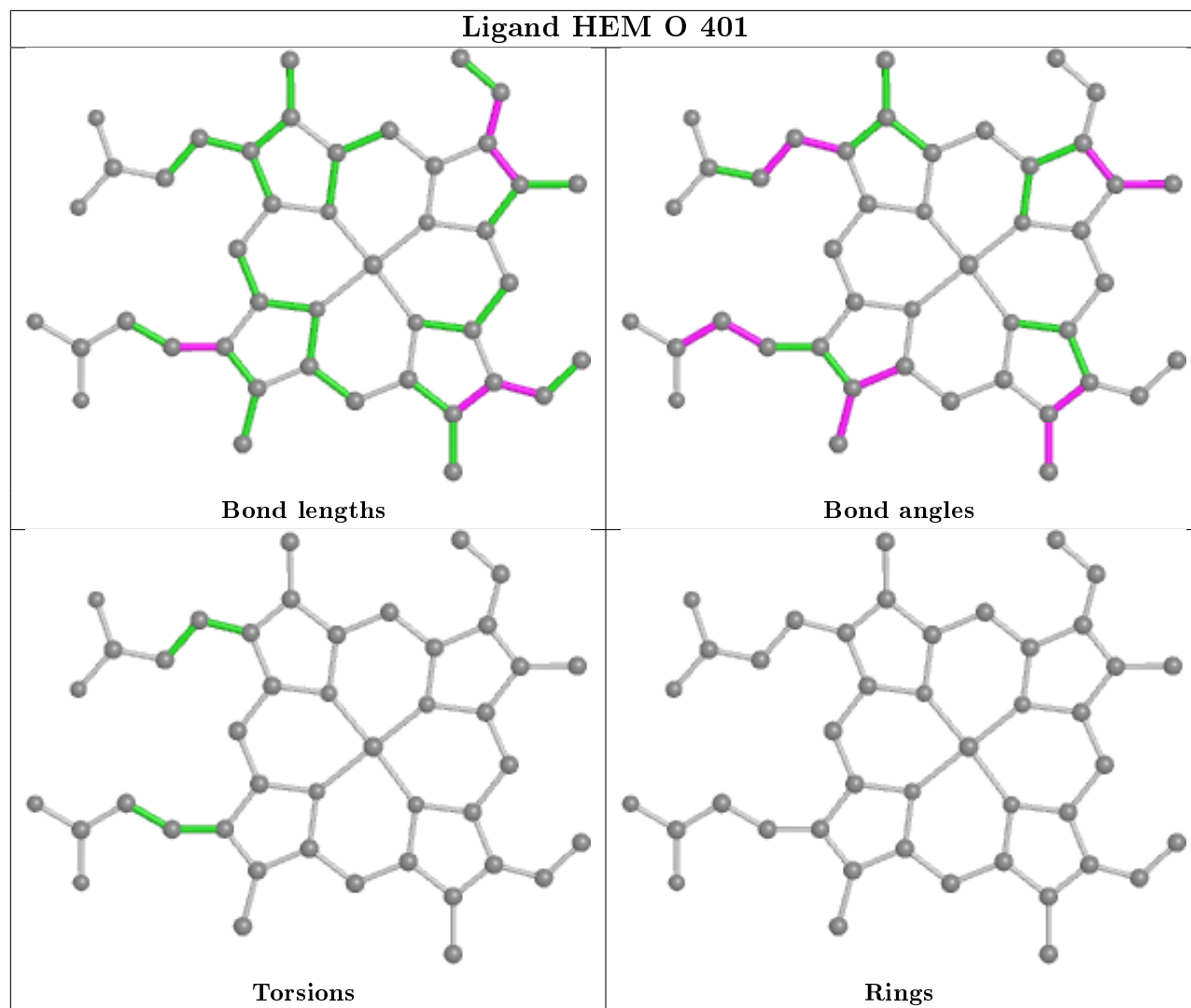
## Ligand SF4 G 503



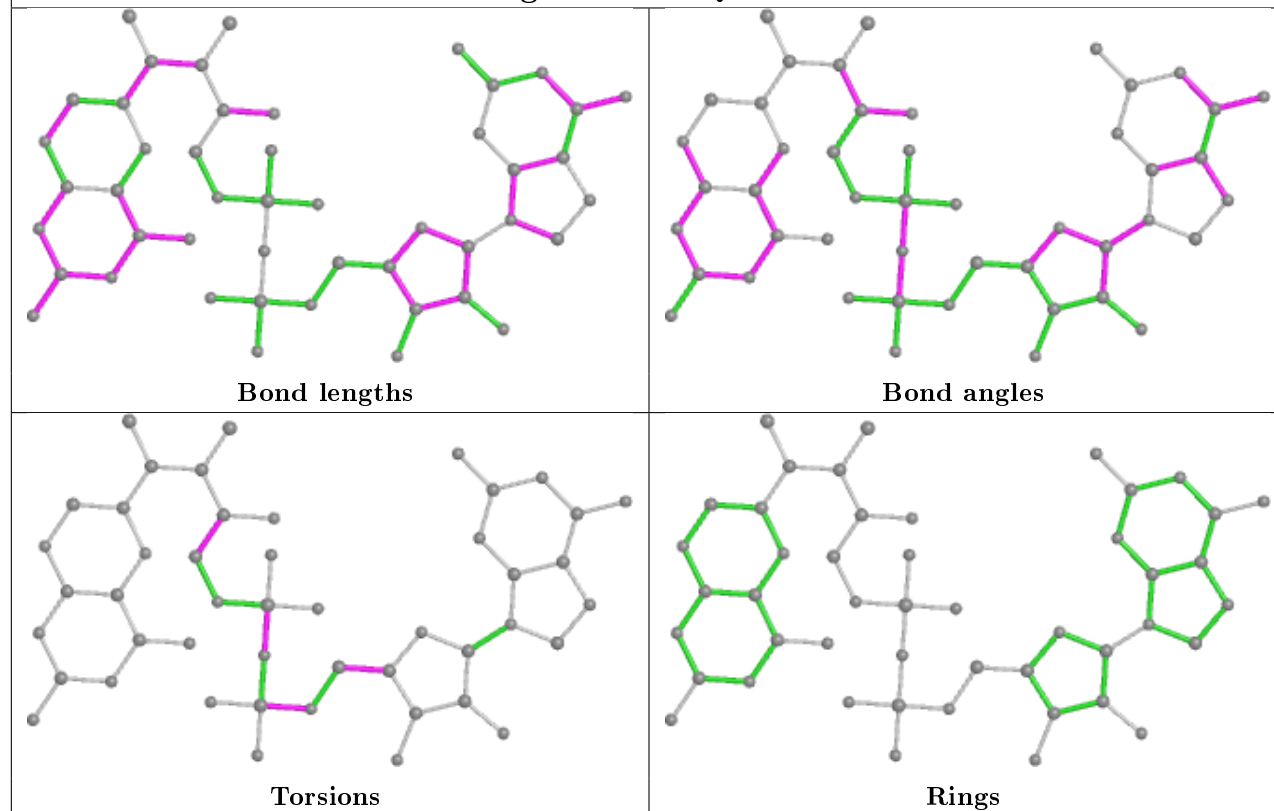
## Ligand SF4 S 503



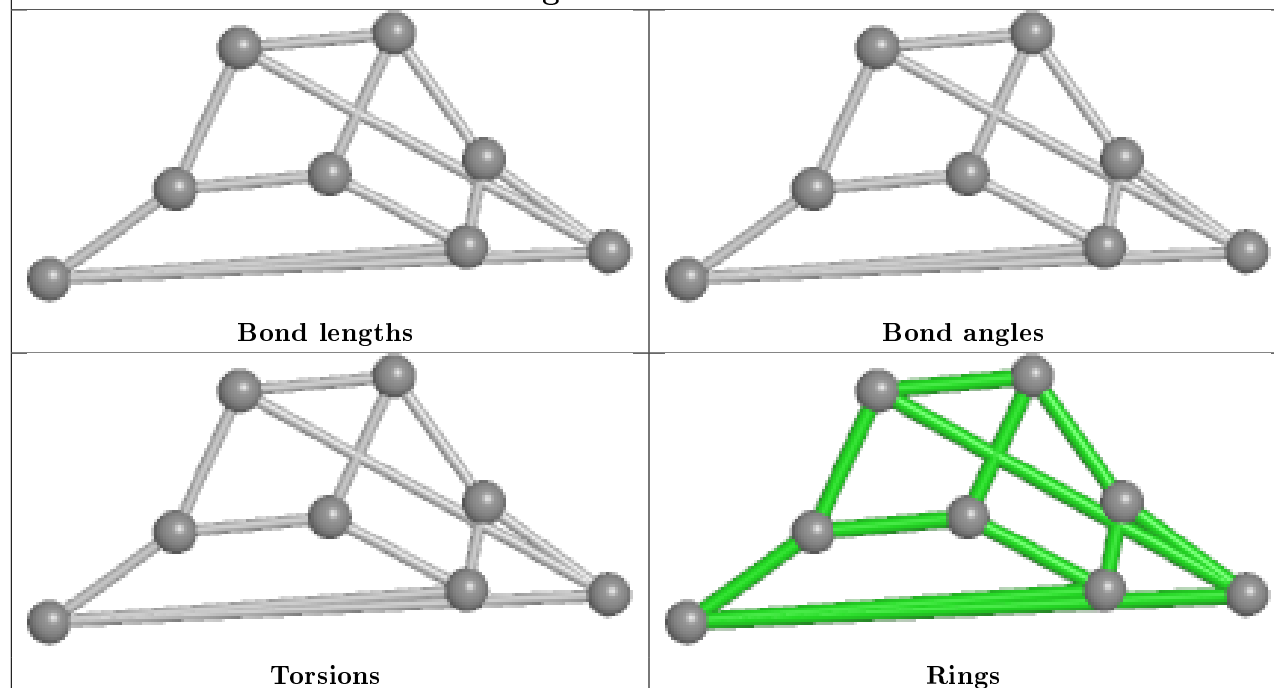




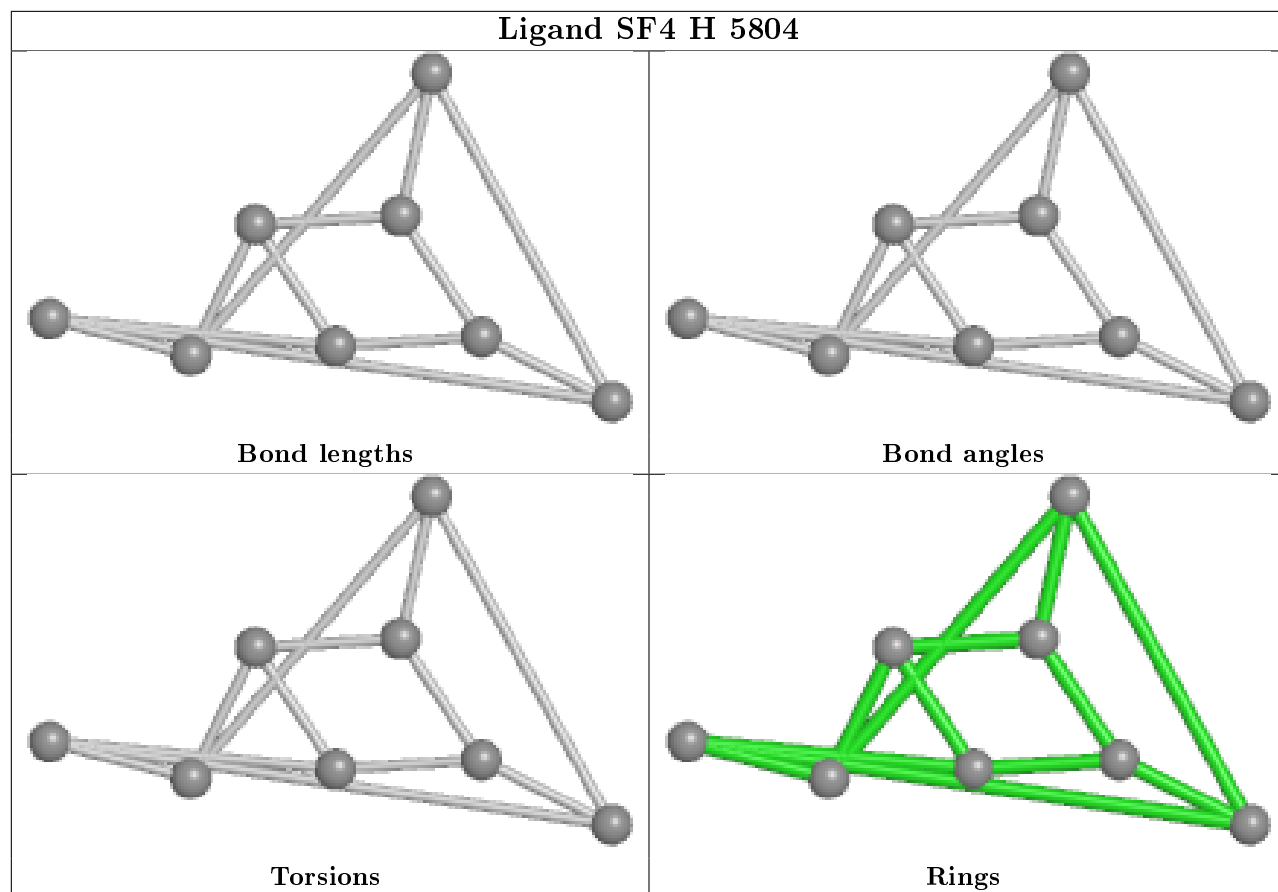
## Ligand MD1 Q 5802



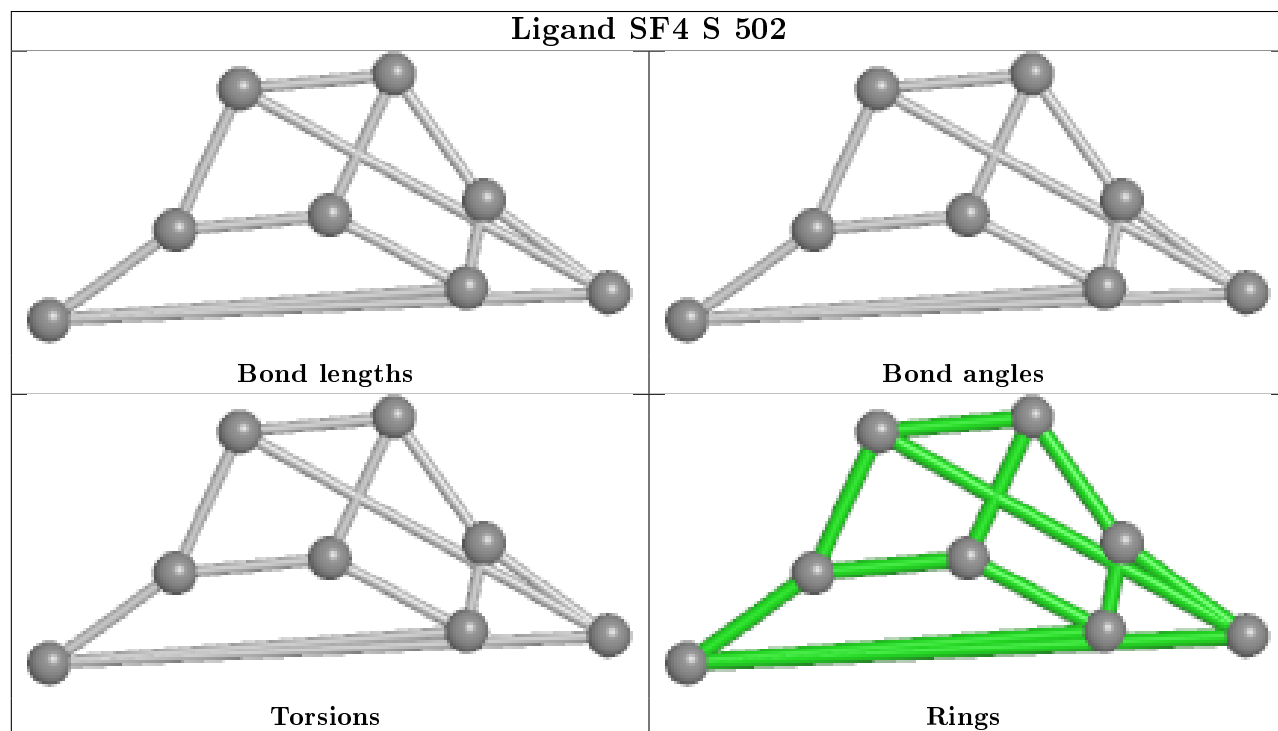
## Ligand SF4 S 501



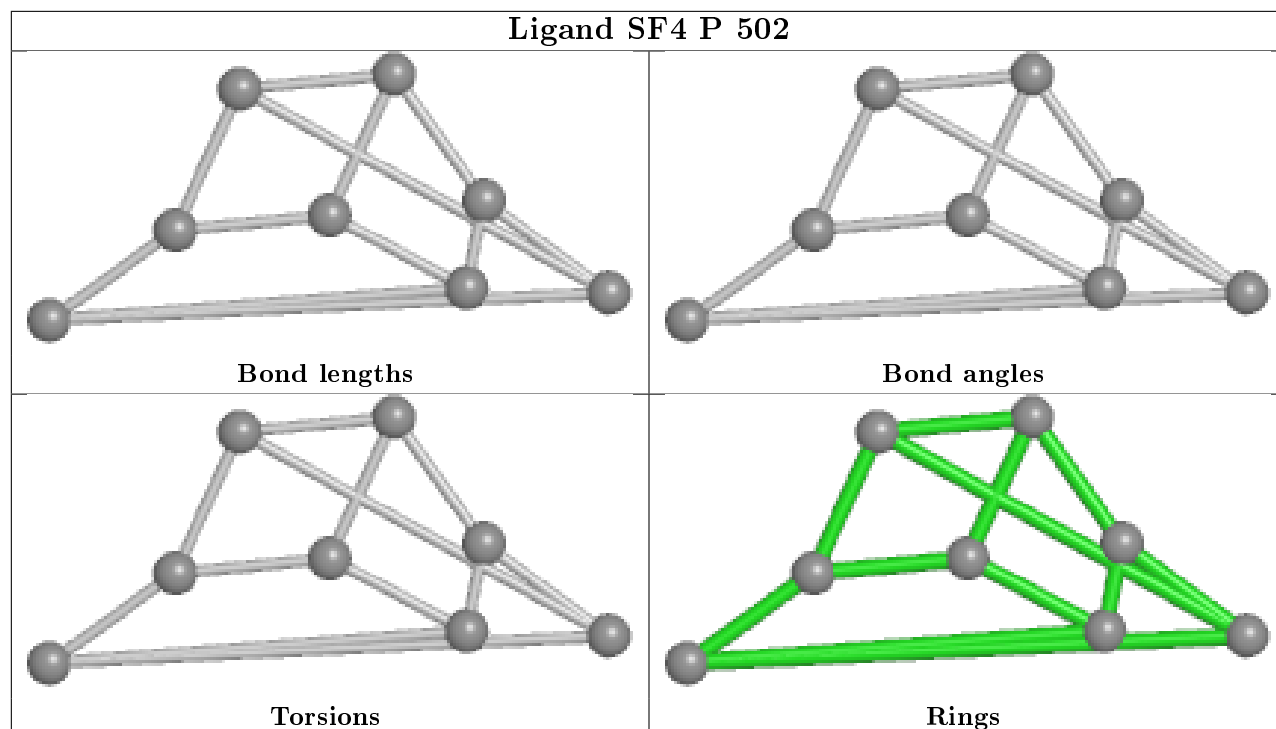
## Ligand SF4 H 5804



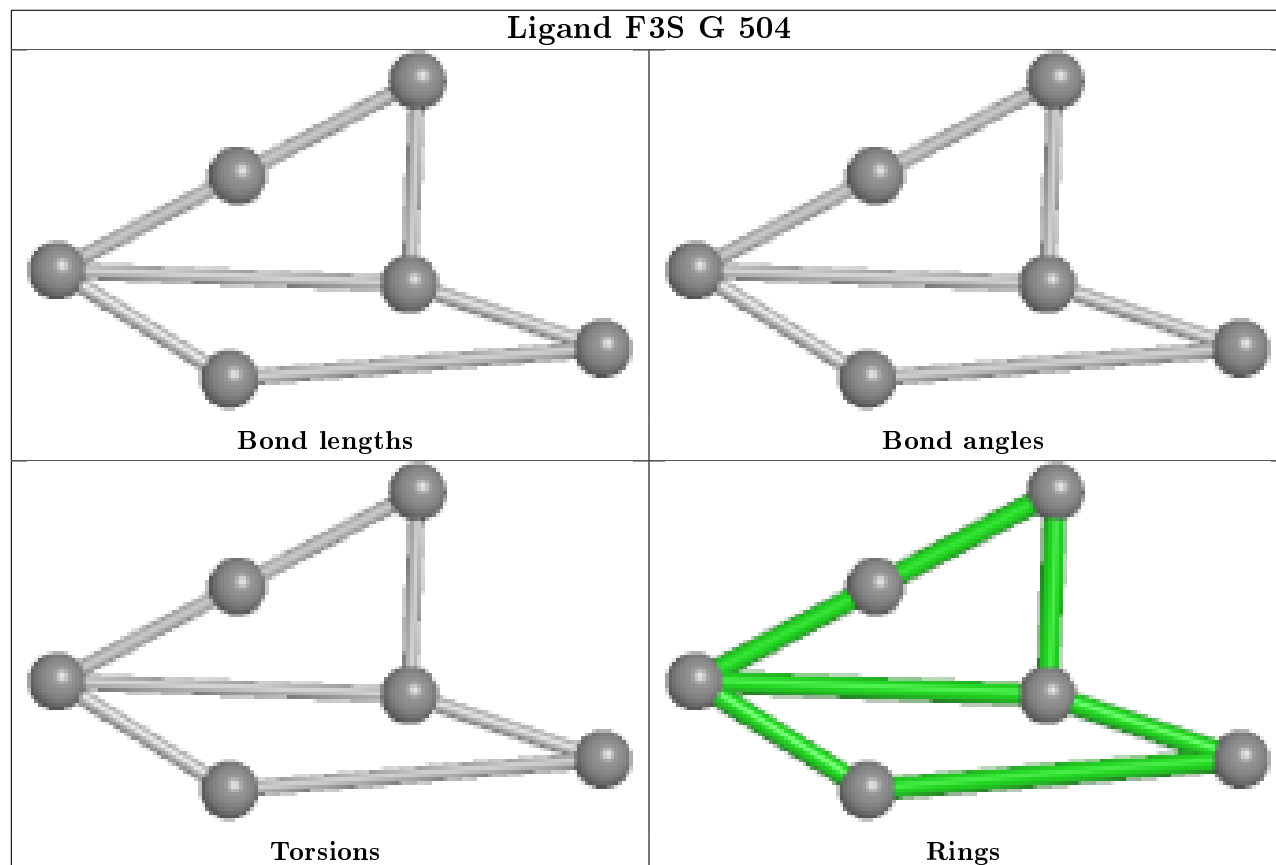
## Ligand SF4 S 502



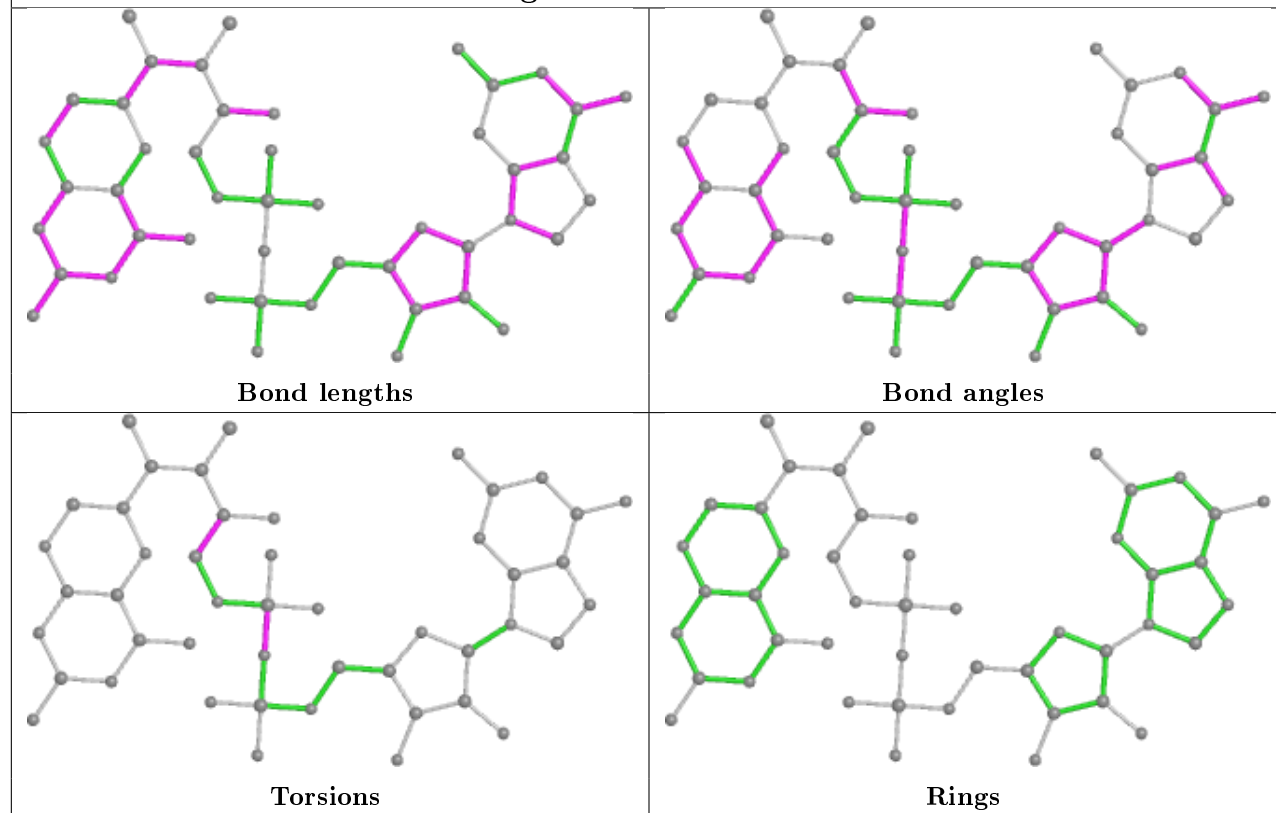
## Ligand SF4 P 502



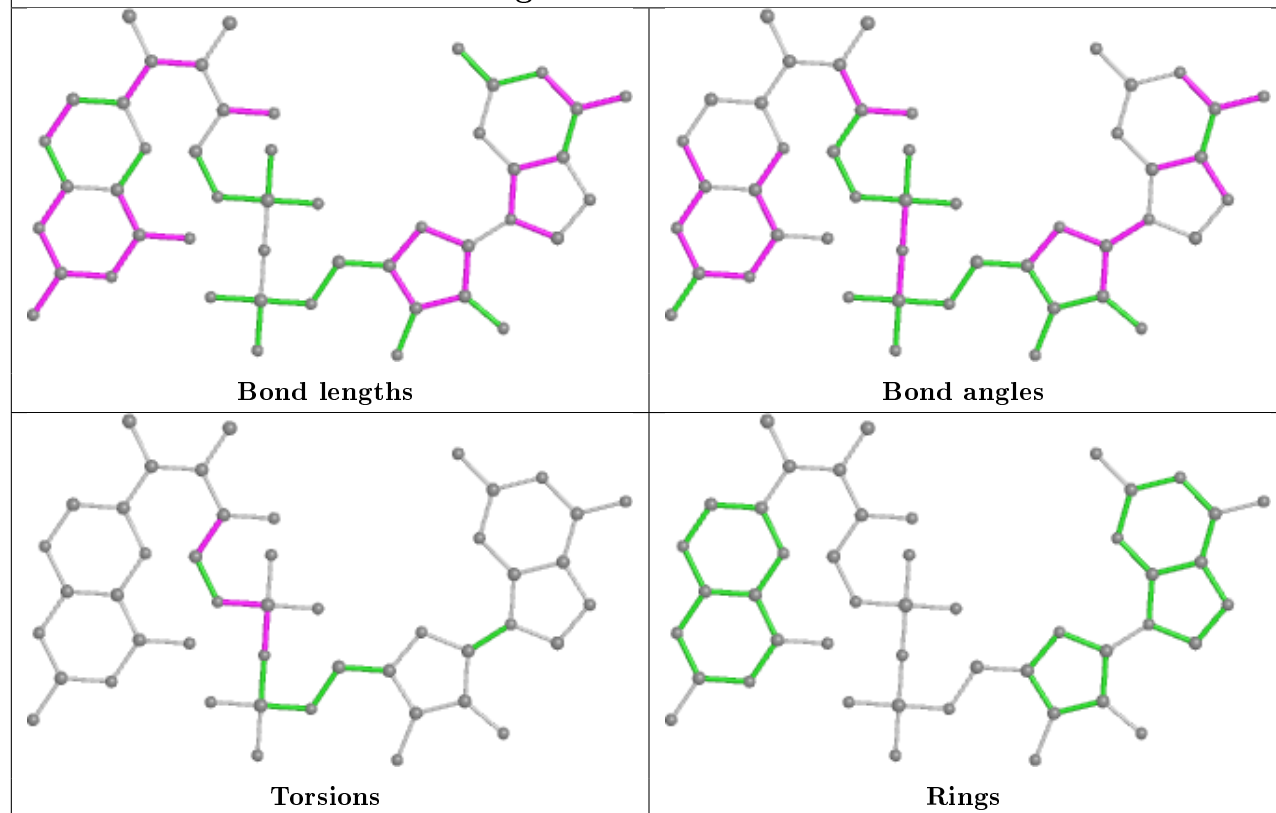
## Ligand F3S G 504



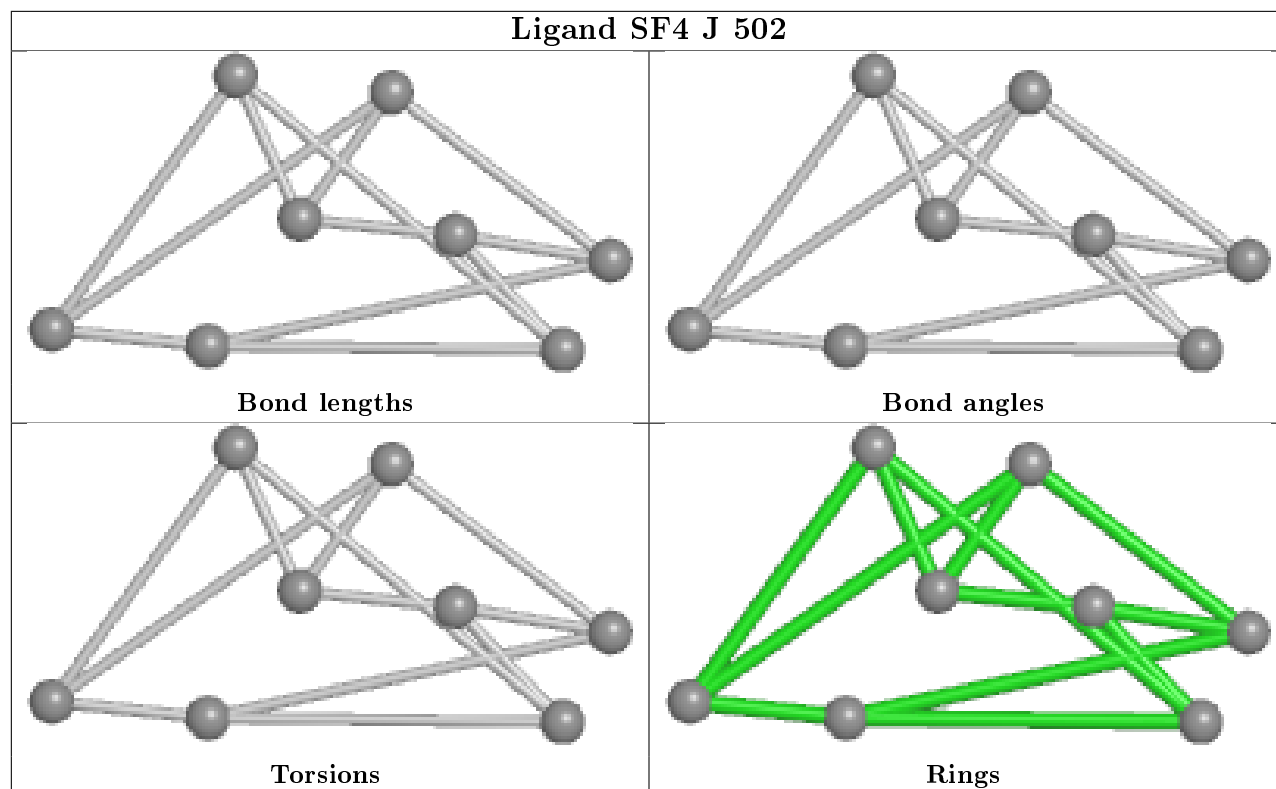
## Ligand MD1 N 5802



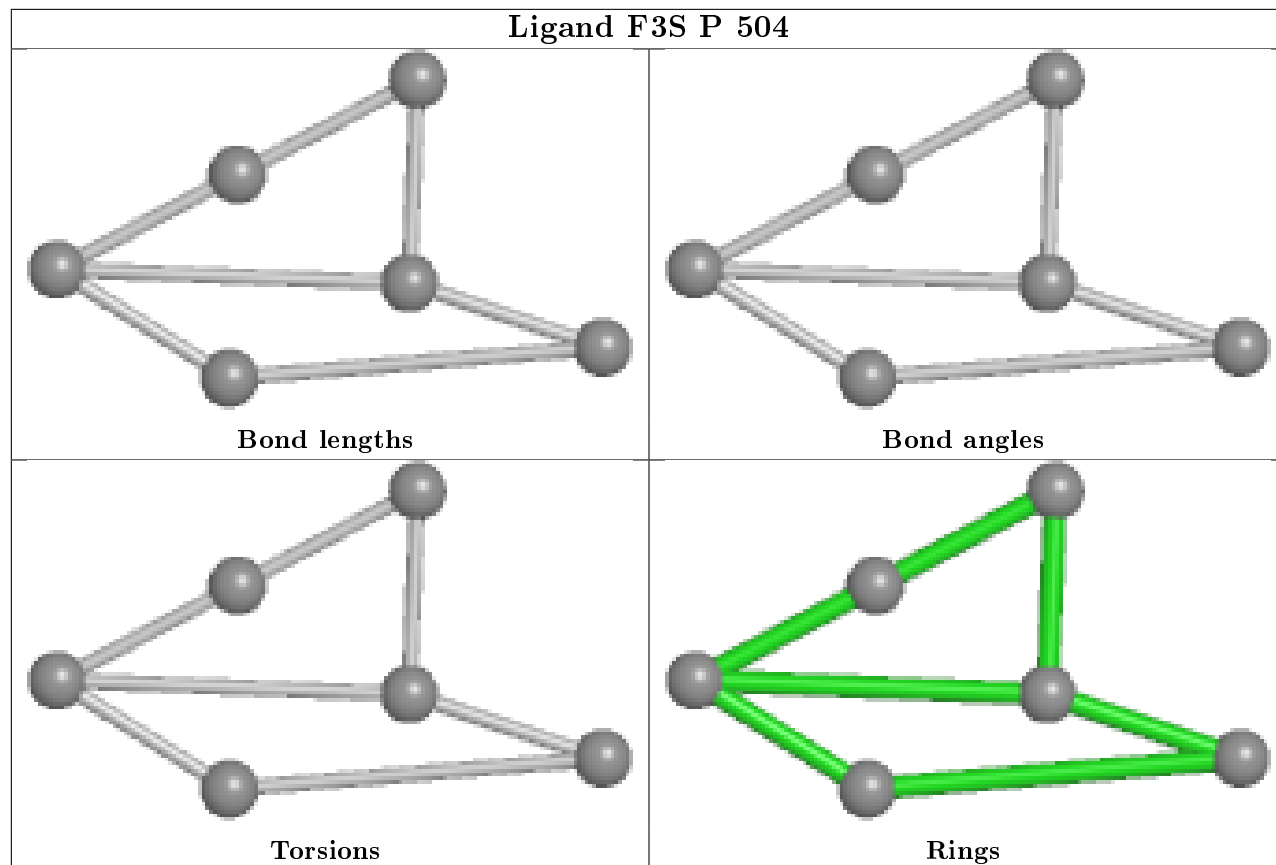
## Ligand MD1 W 5802



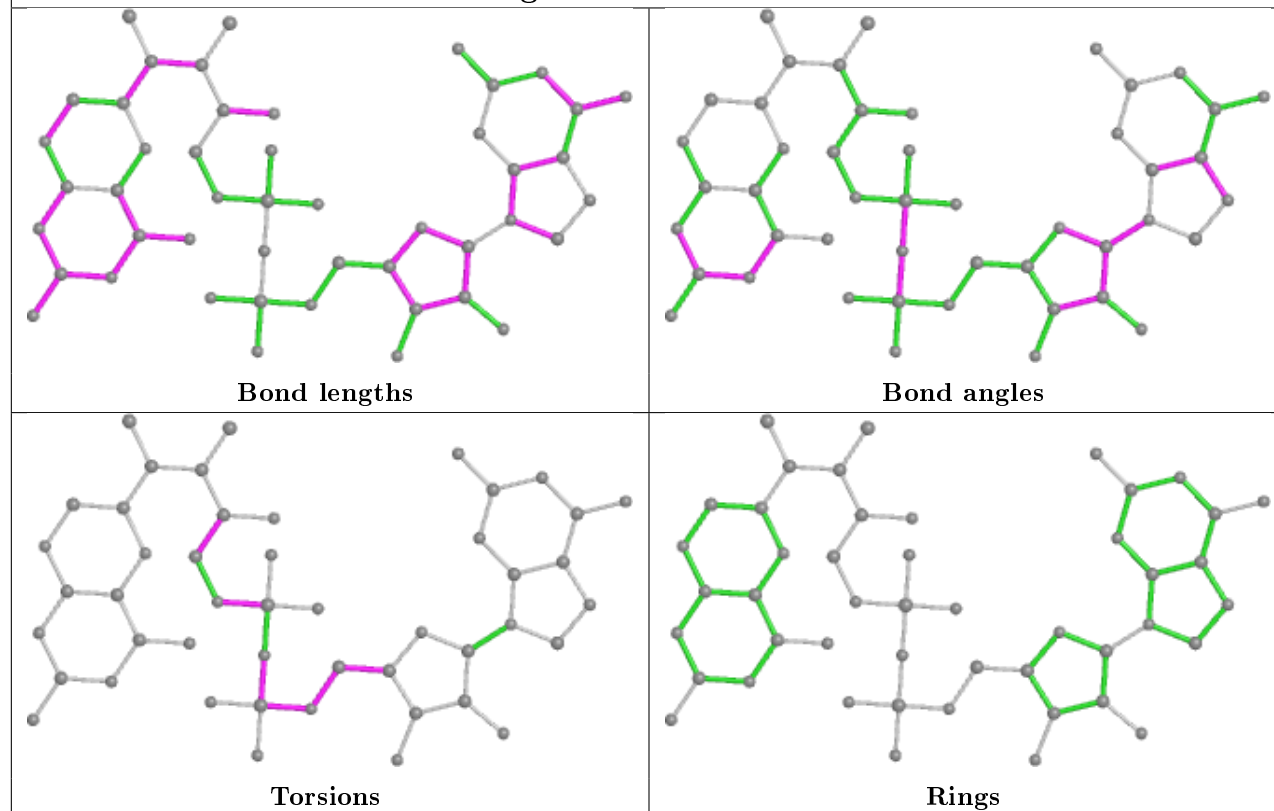
## Ligand SF4 J 502



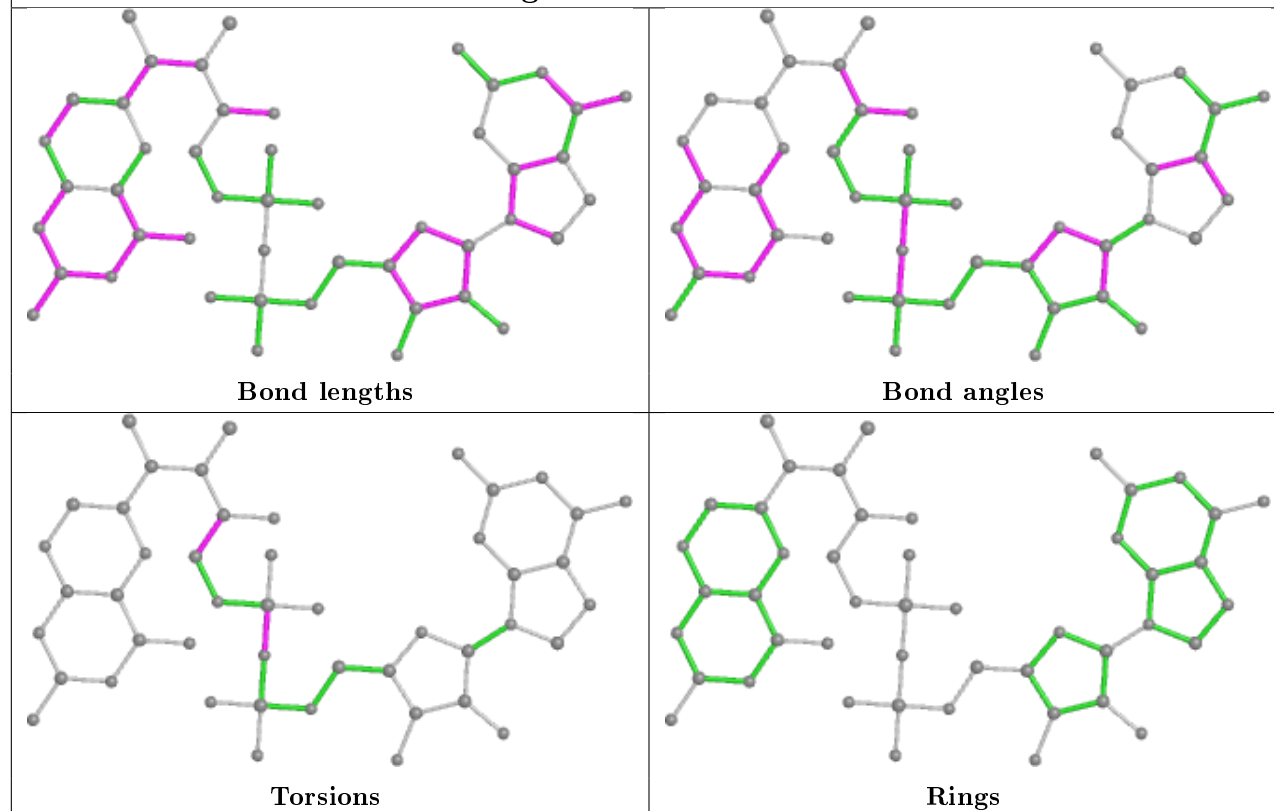
## Ligand F3S P 504



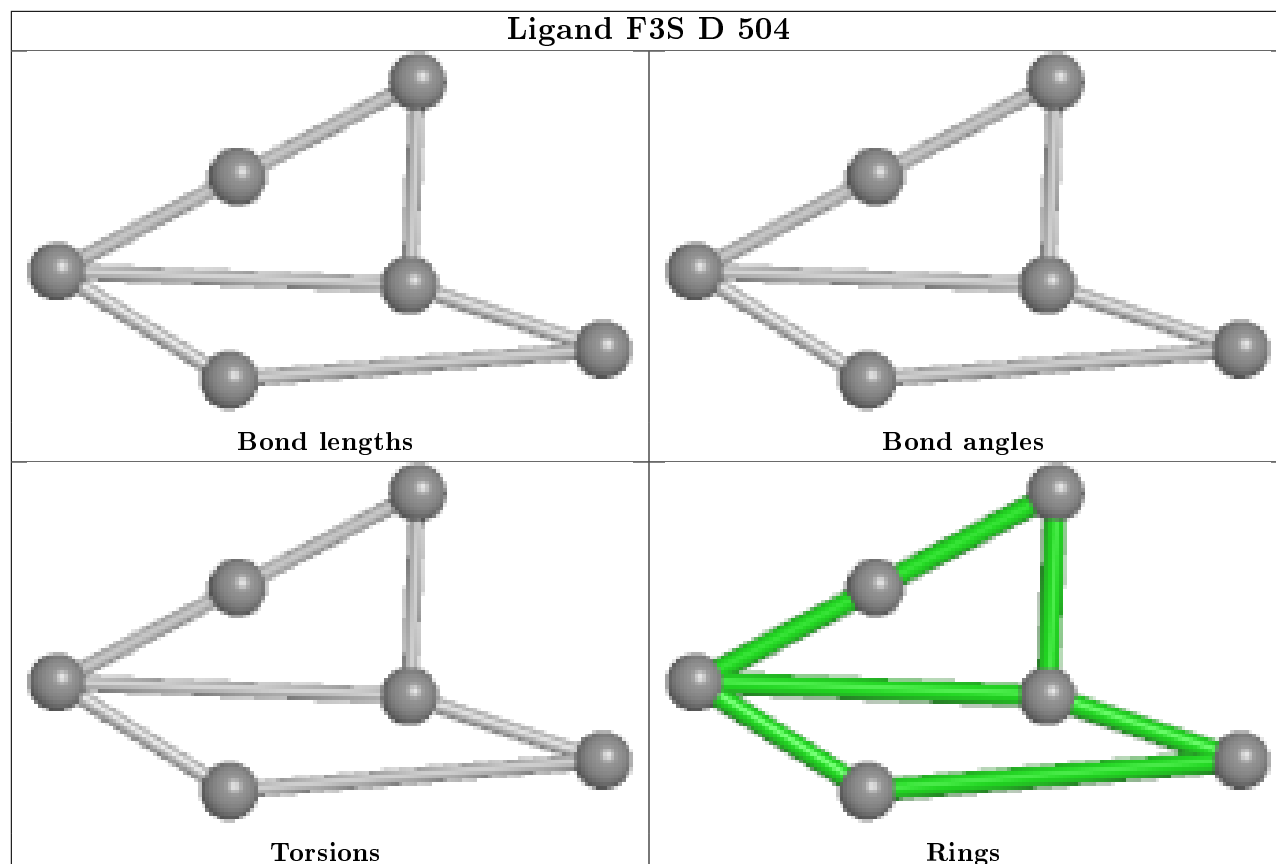
## Ligand MD1 H 5801



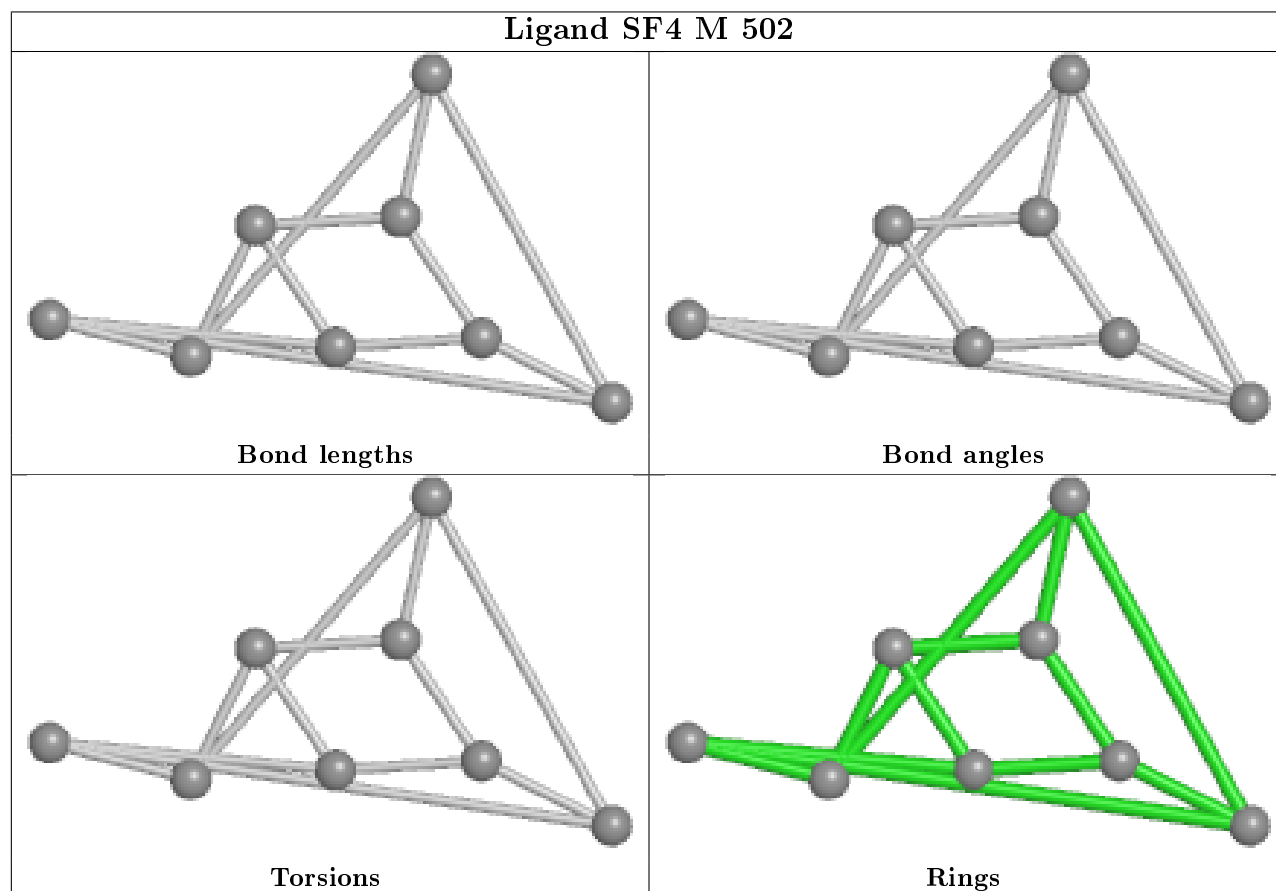
## Ligand MD1 B 5802

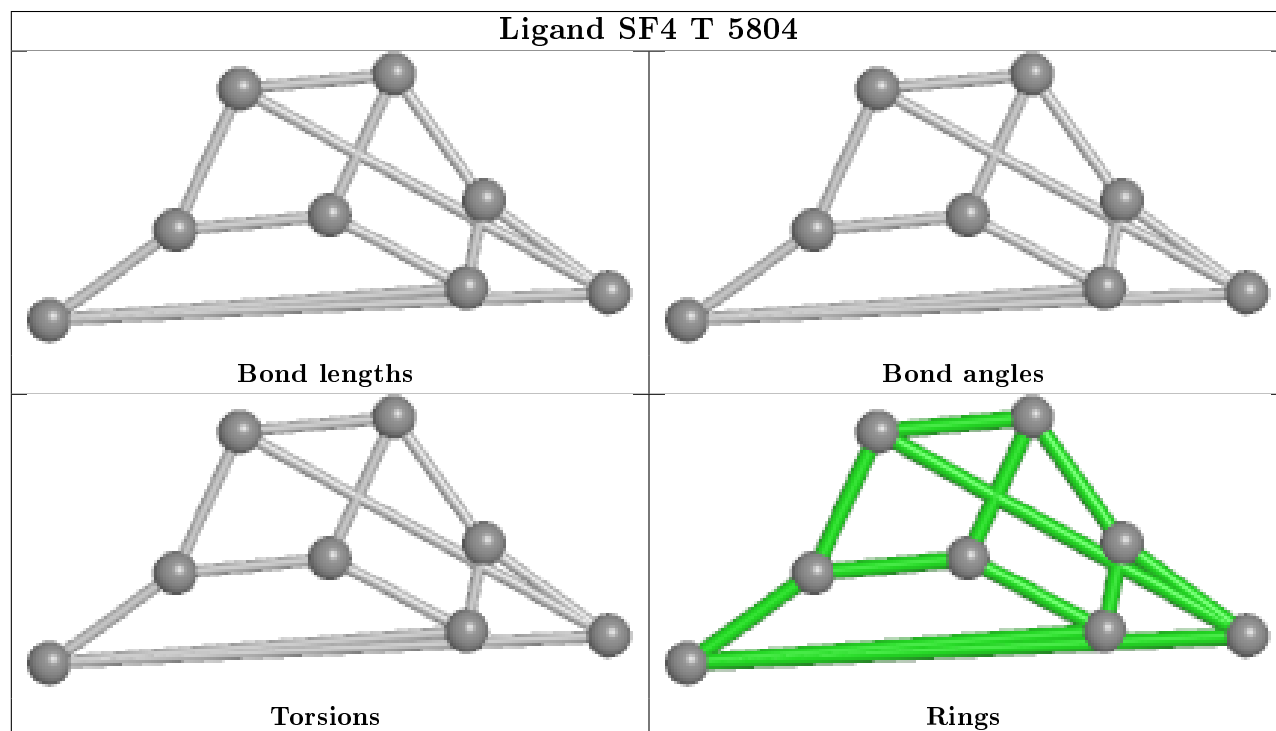
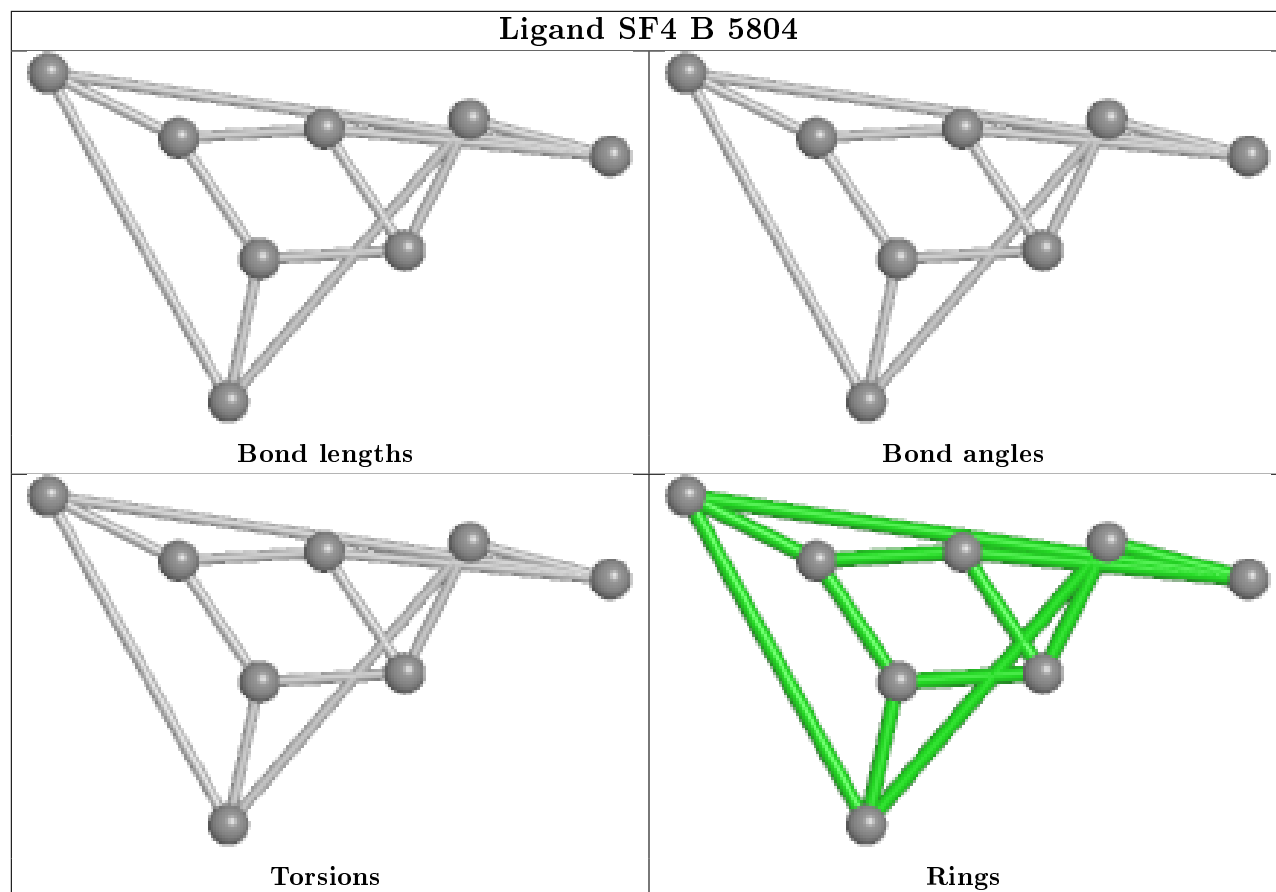


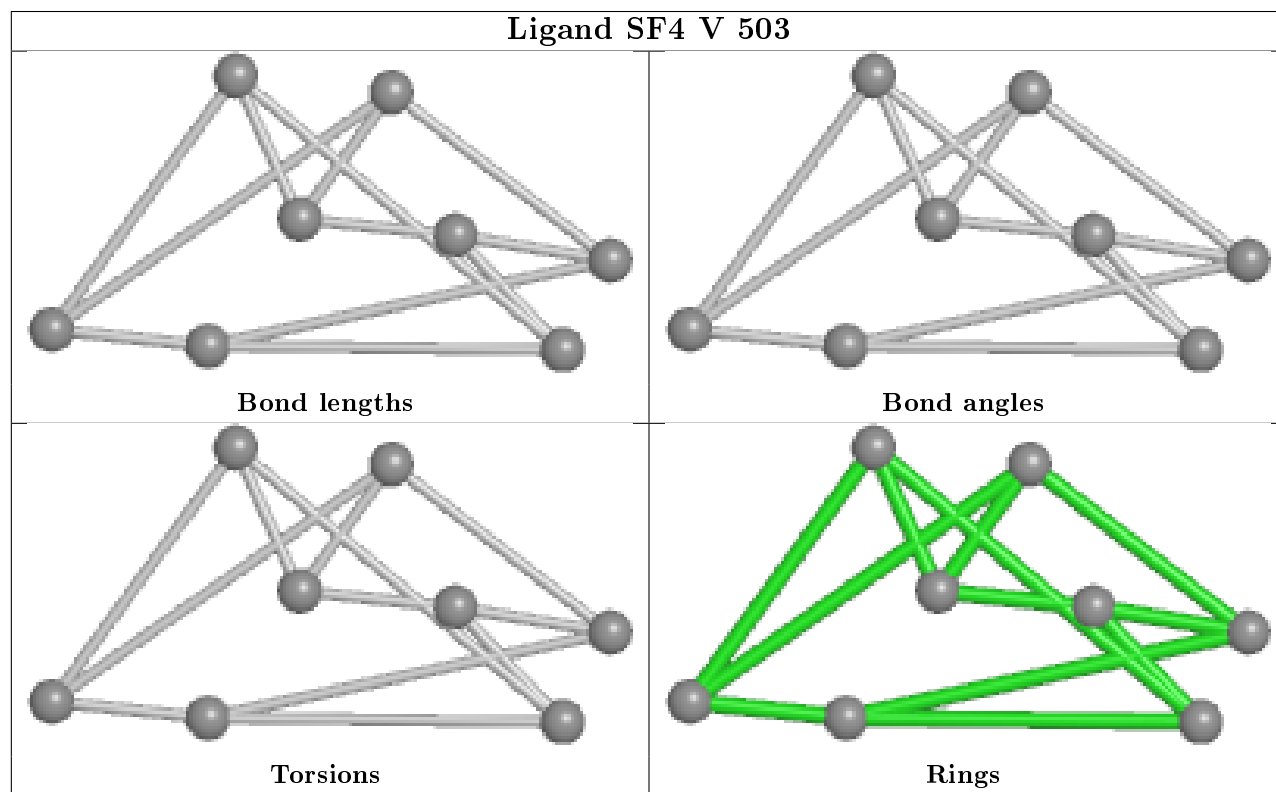
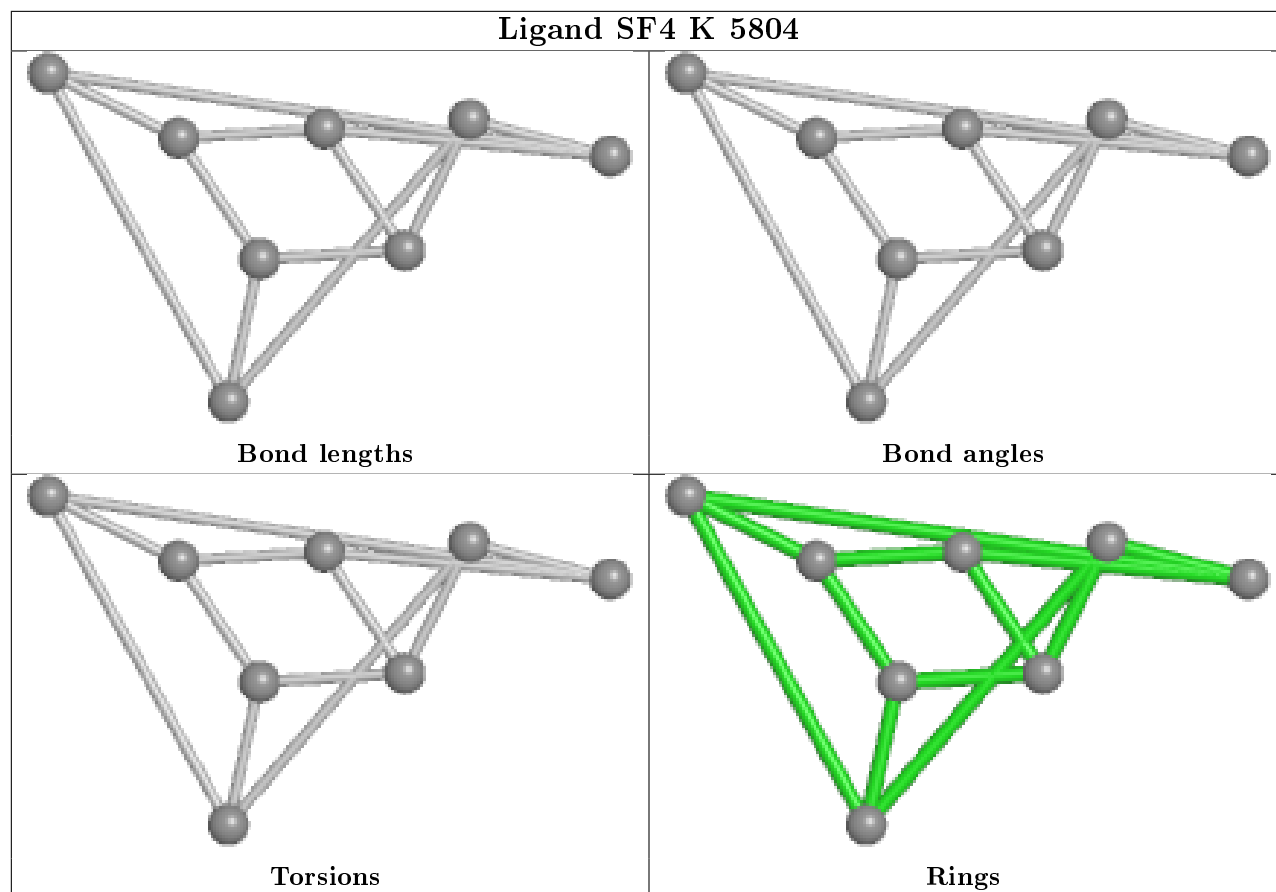
## Ligand F3S D 504

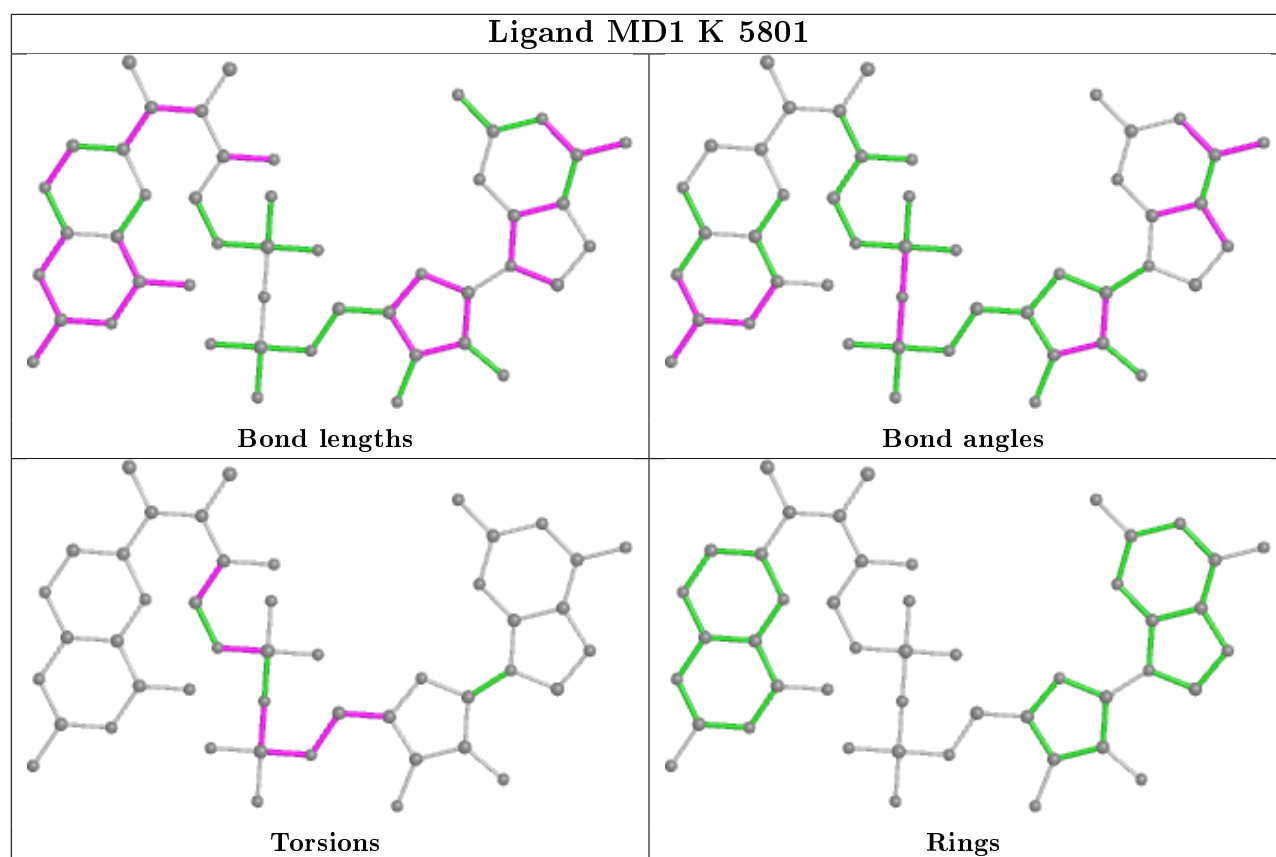


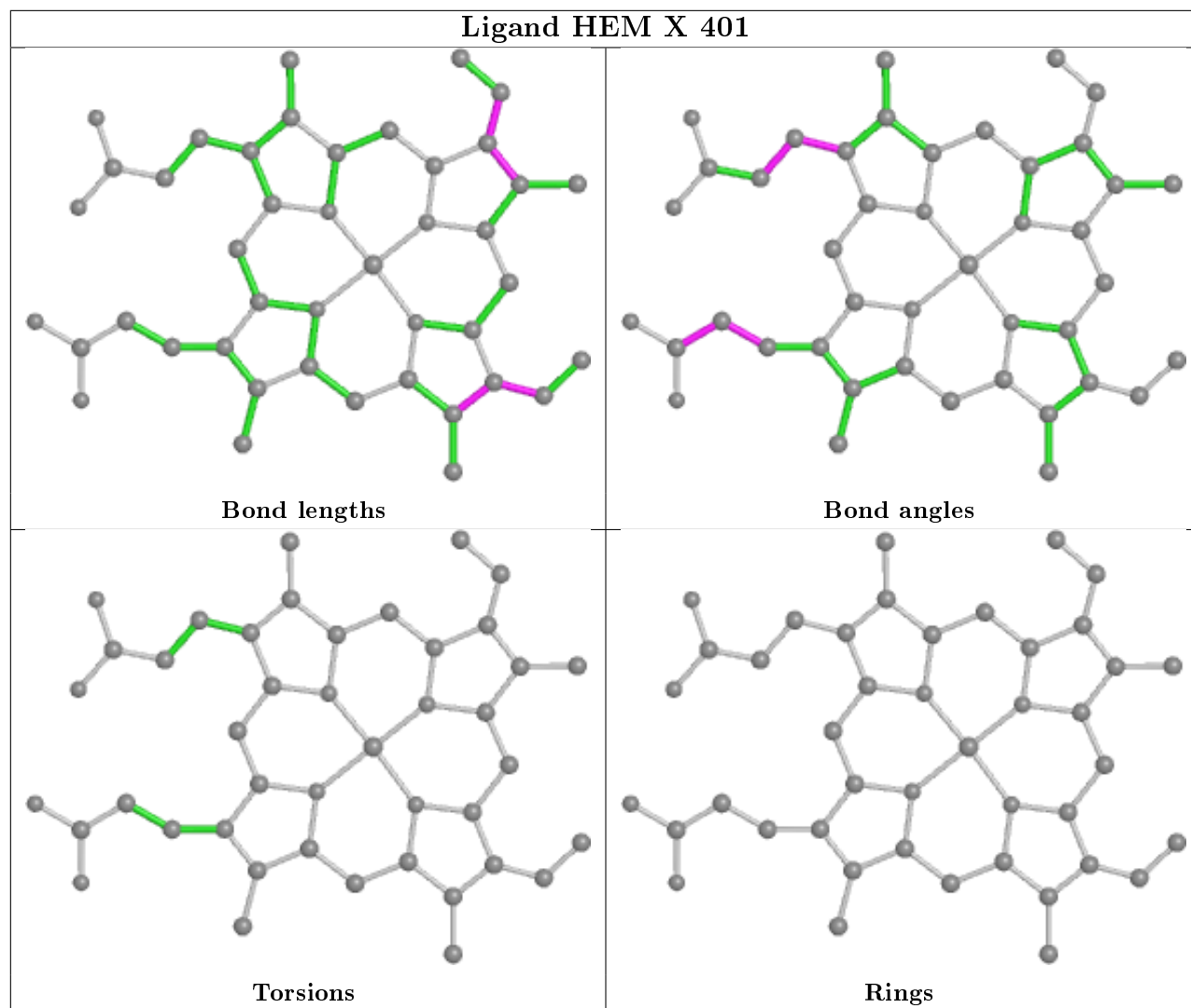
## Ligand SF4 M 502

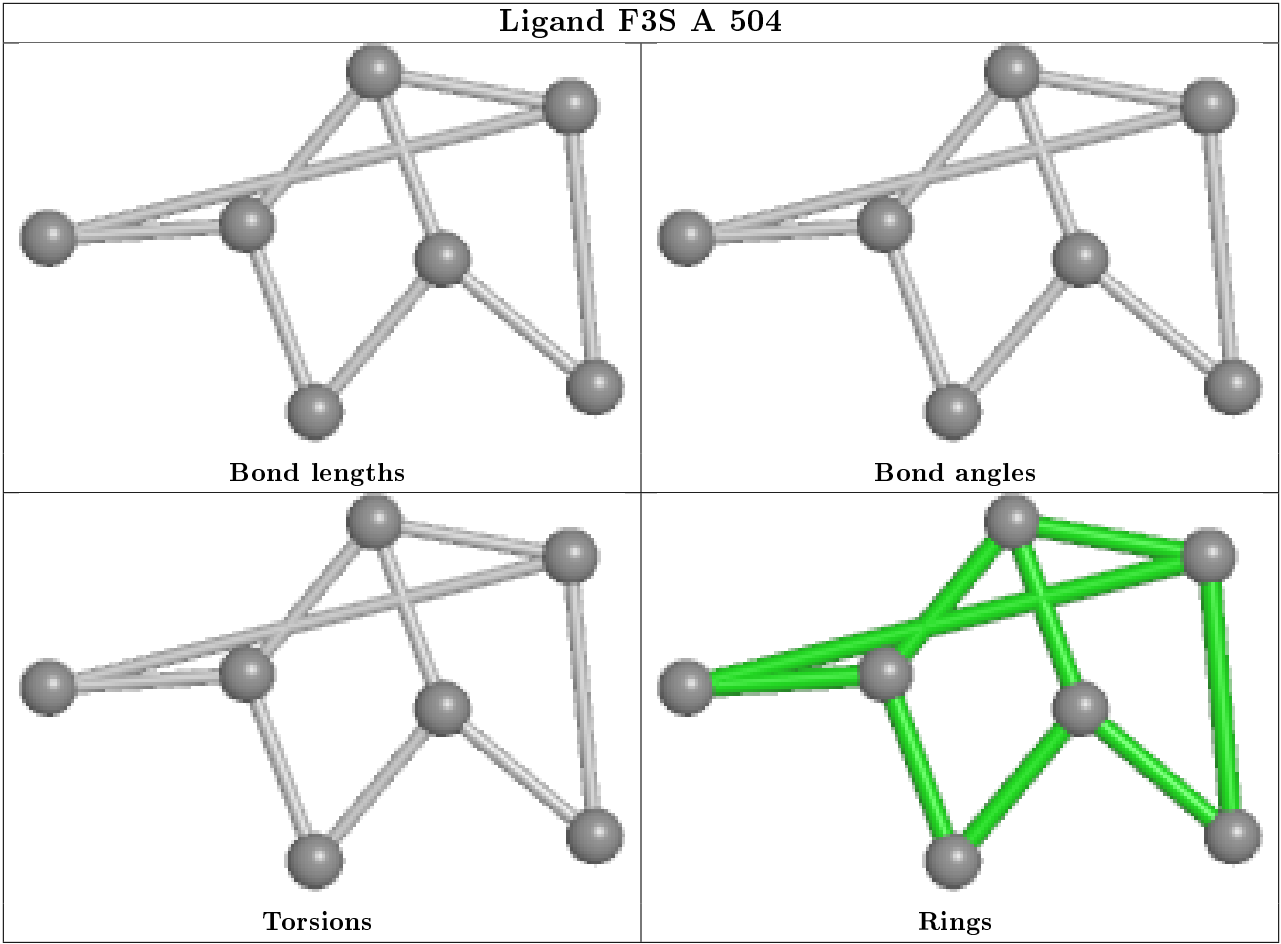












5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	663:VAL	C	664:TYR	N	1.68

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	409/410 (99%)	0.15	3 (0%) 87 74	22, 37, 53, 68	2 (0%)
1	D	408/410 (99%)	1.29	106 (25%) 0 0	66, 97, 117, 133	0
1	G	409/410 (99%)	-0.09	1 (0%) 95 89	21, 32, 45, 93	0
1	J	409/410 (99%)	-0.01	0 100 100	18, 25, 37, 58	0
1	M	409/410 (99%)	0.25	1 (0%) 95 89	27, 48, 65, 79	0
1	P	409/410 (99%)	0.11	0 100 100	26, 46, 64, 77	3 (0%)
1	S	409/410 (99%)	-0.00	0 100 100	21, 33, 47, 61	1 (0%)
1	V	409/410 (99%)	0.28	9 (2%) 62 42	43, 61, 79, 86	1 (0%)
2	B	1120/1148 (97%)	0.10	3 (0%) 94 87	20, 41, 62, 92	1 (0%)
2	E	1111/1148 (96%)	1.57	384 (34%) 0 0	64, 117, 155, 175	0
2	H	1118/1148 (97%)	0.03	1 (0%) 95 91	16, 29, 45, 85	3 (0%)
2	K	1119/1148 (97%)	0.01	1 (0%) 95 91	17, 32, 47, 76	1 (0%)
2	N	1117/1148 (97%)	0.09	2 (0%) 95 89	18, 34, 54, 85	1 (0%)
2	Q	1116/1148 (97%)	0.42	17 (1%) 73 54	24, 47, 70, 92	6 (0%)
2	T	1119/1148 (97%)	0.00	3 (0%) 94 87	21, 37, 57, 88	3 (0%)
2	W	1118/1148 (97%)	0.12	6 (0%) 91 80	29, 49, 66, 95	4 (0%)
3	C	292/322 (90%)	0.21	4 (1%) 75 57	21, 31, 49, 72	0
3	F	292/322 (90%)	0.93	38 (13%) 3 1	57, 83, 104, 121	0
3	I	292/322 (90%)	0.19	1 (0%) 94 87	25, 51, 69, 83	0
3	L	292/322 (90%)	0.06	1 (0%) 94 87	19, 31, 47, 70	0
3	O	291/322 (90%)	1.00	45 (15%) 2 1	35, 69, 89, 102	0
3	R	291/322 (90%)	-0.02	0 100 100	23, 35, 51, 72	1 (0%)
3	U	292/322 (90%)	0.03	3 (1%) 82 66	23, 34, 51, 70	1 (0%)
3	X	292/322 (90%)	0.01	1 (0%) 94 87	30, 62, 76, 81	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
All	All	14543/15040 (96%)	0.28	630 (4%) 35 20	16, 41, 109, 175	28 (0%)

The worst 5 of 630 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	799	ALA	9.0
2	E	626	VAL	8.7
2	E	112	PRO	7.8
2	E	564	GLY	7.0
2	E	417	ILE	6.8

## 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 monosaccharides 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
9	CA	F	403	1/1	0.33	0.13	104,104,104,104	0
6	MD1	E	5801	47/47	0.73	0.29	75,111,136,150	0
9	CA	X	403	1/1	0.73	0.10	71,71,71,71	0
6	MD1	E	5802	47/47	0.82	0.27	80,117,133,137	0
9	CA	F	402	1/1	0.82	0.07	76,76,76,76	0
9	CA	I	403	1/1	0.85	0.10	69,69,69,69	0
8	HEM	F	401	43/43	0.85	0.30	77,97,112,116	0
9	CA	U	403	1/1	0.88	0.12	29,29,29,29	0
4	SF4	D	501	8/8	0.89	0.17	91,115,146,160	0
5	F3S	V	504	7/7	0.89	0.13	65,87,97,112	0
9	CA	O	402	1/1	0.90	0.09	61,61,61,61	0
8	HEM	X	401	43/43	0.91	0.23	59,75,81,89	0
7	MO	E	5803	1/1	0.92	0.06	139,139,139,139	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
9	CA	L	402	1/1	0.92	0.09	27,27,27,27	0
9	CA	C	403	1/1	0.92	0.13	35,35,35,35	0
9	CA	R	403	1/1	0.92	0.09	35,35,35,35	0
5	F3S	D	504	7/7	0.92	0.13	99,113,128,134	0
8	HEM	O	401	43/43	0.92	0.32	57,69,75,84	0
6	MD1	Q	5802	47/47	0.93	0.23	30,43,56,59	0
4	SF4	D	503	8/8	0.93	0.16	107,133,158,166	0
7	MO	T	5803	1/1	0.93	0.14	37,37,37,37	0
4	SF4	E	5804	8/8	0.94	0.12	119,125,139,167	0
7	MO	Q	5803	1/1	0.94	0.11	46,46,46,46	0
9	CA	L	403	1/1	0.94	0.09	29,29,29,29	0
9	CA	C	402	1/1	0.94	0.09	33,33,33,33	0
4	SF4	D	502	8/8	0.94	0.08	112,118,142,149	0
9	CA	U	402	1/1	0.94	0.13	32,32,32,32	0
6	MD1	W	5802	47/47	0.94	0.20	28,47,62,72	0
8	HEM	I	401	43/43	0.94	0.19	38,55,65,66	0
4	SF4	W	5804	8/8	0.95	0.10	40,57,63,72	0
9	CA	O	403	1/1	0.95	0.07	73,73,73,73	0
9	CA	X	402	1/1	0.95	0.07	56,56,56,56	0
6	MD1	Q	5801	47/47	0.95	0.20	21,34,44,54	0
6	MD1	T	5802	47/47	0.96	0.19	22,31,41,45	0
6	MD1	W	5801	47/47	0.96	0.18	31,46,57,69	0
4	SF4	V	501	8/8	0.96	0.10	43,63,75,78	0
9	CA	I	402	1/1	0.96	0.09	46,46,46,46	0
4	SF4	N	5804	8/8	0.96	0.12	40,42,48,51	0
6	MD1	H	5802	47/47	0.96	0.21	15,30,36,47	0
6	MD1	K	5801	47/47	0.96	0.19	20,25,33,37	0
8	HEM	C	401	43/43	0.96	0.23	19,27,32,49	0
6	MD1	K	5802	47/47	0.96	0.22	15,29,38,45	0
6	MD1	N	5801	47/47	0.96	0.19	21,28,34,48	0
8	HEM	L	401	43/43	0.96	0.21	17,24,30,33	0
6	MD1	N	5802	47/47	0.96	0.19	26,34,44,46	0
6	MD1	B	5801	47/47	0.96	0.21	24,34,40,41	0
6	MD1	B	5802	47/47	0.96	0.18	28,42,50,56	0
6	MD1	T	5801	47/47	0.97	0.18	23,29,35,38	0
4	SF4	H	5804	8/8	0.97	0.11	15,35,41,43	0
9	CA	R	402	1/1	0.97	0.10	31,31,31,31	0
6	MD1	H	5801	47/47	0.97	0.19	16,24,36,38	0
8	HEM	R	401	43/43	0.97	0.21	23,33,40,46	0
8	HEM	U	401	43/43	0.97	0.19	23,30,34,43	0
4	SF4	M	502	8/8	0.97	0.08	58,64,82,84	0
7	MO	B	5803	1/1	0.97	0.13	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SF4	J	502	8/8	0.98	0.08	24,36,52,52	0
4	SF4	V	502	8/8	0.98	0.08	62,72,89,95	0
4	SF4	V	503	8/8	0.98	0.09	50,65,72,83	0
4	SF4	K	5804	8/8	0.98	0.14	18,32,40,42	0
4	SF4	B	5804	8/8	0.98	0.12	22,38,47,49	0
5	F3S	M	504	7/7	0.98	0.10	46,67,69,70	0
4	SF4	J	501	8/8	0.98	0.09	16,26,33,33	0
7	MO	H	5803	1/1	0.98	0.14	38,38,38,38	0
7	MO	N	5803	1/1	0.98	0.14	30,30,30,30	0
4	SF4	P	502	8/8	0.98	0.10	37,47,60,63	0
4	SF4	Q	5804	8/8	0.98	0.10	26,43,57,67	0
7	MO	W	5803	1/1	0.98	0.13	61,61,61,61	0
4	SF4	S	503	8/8	0.99	0.07	28,33,41,47	0
4	SF4	T	5804	8/8	0.99	0.11	27,42,48,57	0
4	SF4	A	502	8/8	0.99	0.07	27,43,54,56	0
4	SF4	J	503	8/8	0.99	0.08	25,29,37,38	0
4	SF4	G	501	8/8	0.99	0.10	24,29,42,43	0
4	SF4	M	501	8/8	0.99	0.10	35,47,52,54	0
5	F3S	A	504	7/7	0.99	0.10	24,32,43,44	0
4	SF4	G	502	8/8	0.99	0.09	30,38,54,60	0
5	F3S	G	504	7/7	0.99	0.10	26,42,51,52	0
5	F3S	J	504	7/7	0.99	0.10	14,25,31,32	0
4	SF4	M	503	8/8	0.99	0.07	32,44,56,57	0
5	F3S	P	504	7/7	0.99	0.09	24,34,45,47	0
5	F3S	S	504	7/7	0.99	0.09	19,29,43,43	0
7	MO	K	5803	1/1	0.99	0.12	36,36,36,36	0
4	SF4	G	503	8/8	0.99	0.08	17,27,33,35	0
4	SF4	P	501	8/8	0.99	0.10	30,35,42,42	0
4	SF4	A	503	8/8	0.99	0.09	27,34,49,51	0
4	SF4	P	503	8/8	0.99	0.09	30,39,51,60	0
4	SF4	A	501	8/8	0.99	0.10	26,27,41,46	0
4	SF4	S	501	8/8	0.99	0.11	21,32,42,43	0
4	SF4	S	502	8/8	0.99	0.09	29,39,52,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.