



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 14, 2024 – 12:33 pm GMT

PDB ID : 6QPA  
Title : Halothiobacillus neapolitanus sulfur oxygenase reductase  
Authors : Frazao, C.; Klezin, A.; Poell, U.; Veith, A.; Ruehl, P.; Coelho, R.  
Deposited on : 2019-02-13  
Resolution : 2.10 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.

The types of validation reports are described at

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

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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 : 1.8.4, CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : **FAILED**  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

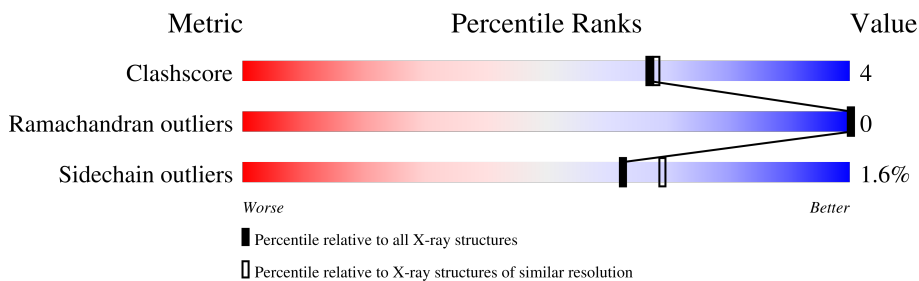
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)











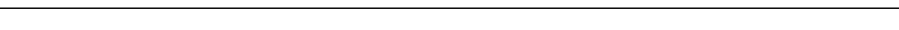
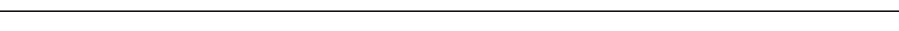
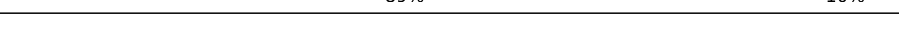

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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  $\leq 5\%$

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	314	
1	B	314	
1	C	314	
1	D	314	
1	E	314	
1	F	314	
1	G	314	
1	H	314	

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Mol	Chain	Length	Quality of chain
1	I	314	 89% 9% ..
1	J	314	 88% 10% ..
1	K	314	 89% 9% ..
1	L	314	 91% 7% ..
1	M	314	 89% 9% ..
1	N	314	 89% 8% ..
1	O	314	 90% 8% .
1	P	314	 87% 11% ..
1	Q	314	 88% 10% ..
1	R	314	 89% 10% .
1	T	314	 90% 8% ..
1	U	314	 87% 11% .
1	V	314	 89% 9% .
1	W	314	 89% 10% .
1	Y	314	 91% 8% .
1	Z	314	 91% 6% ..

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 63067 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 Sulfur oxygenase/reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	310	2447	1561	412	447	27	0	1	0
1	B	310	2447	1561	412	447	27	0	1	0
1	C	310	2451	1563	413	448	27	0	2	0
1	D	310	2456	1566	414	449	27	0	3	0
1	E	310	2447	1561	412	447	27	0	1	0
1	F	310	2452	1564	413	448	27	0	2	0
1	G	310	2452	1564	413	448	27	0	2	0
1	H	310	2452	1564	413	448	27	0	2	0
1	I	310	2456	1566	414	449	27	0	3	0
1	J	310	2451	1564	413	447	27	0	2	0
1	K	310	2447	1561	412	447	27	0	1	0
1	L	310	2456	1567	414	448	27	0	3	0
1	M	310	2451	1564	413	447	27	0	2	0
1	N	310	2452	1564	413	448	27	0	2	0
1	O	309	2454	1565	415	447	27	0	4	0
1	P	310	2460	1569	415	449	27	0	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	310	Total	C	N	O	S	0	3	0
			2456	1567	414	448	27			
1	R	310	Total	C	N	O	S	0	2	0
			2452	1564	413	448	27			
1	T	310	Total	C	N	O	S	0	2	0
			2452	1564	413	448	27			
1	U	310	Total	C	N	O	S	0	3	0
			2456	1566	414	449	27			
1	V	310	Total	C	N	O	S	0	1	0
			2447	1561	412	447	27			
1	W	310	Total	C	N	O	S	0	1	0
			2447	1561	412	447	27			
1	Y	310	Total	C	N	O	S	0	1	0
			2447	1561	412	447	27			
1	Z	310	Total	C	N	O	S	0	4	0
			2460	1569	415	449	27			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe) (labeled as "Ligand of Interest" by depositor).

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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	L	1	Total Fe 1 1	0	0
2	M	1	Total Fe 1 1	0	0
2	N	1	Total Fe 1 1	0	0
2	O	1	Total Fe 1 1	0	0
2	P	1	Total Fe 1 1	0	0
2	Q	1	Total Fe 1 1	0	0
2	R	1	Total Fe 1 1	0	0
2	T	1	Total Fe 1 1	0	0
2	U	1	Total Fe 1 1	0	0
2	V	1	Total Fe 1 1	0	0
2	W	1	Total Fe 1 1	0	0
2	Y	1	Total Fe 1 1	0	0
2	Z	1	Total Fe 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S) (labeled as "Ligand of Interest" by depositor).



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

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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	Q	1	Total 5	O 4	S 1	0	0
3	Q	1	Total 5	O 4	S 1	0	0
3	R	1	Total 5	O 4	S 1	0	0
3	T	1	Total 5	O 4	S 1	0	0
3	U	1	Total 5	O 4	S 1	0	0
3	U	1	Total 5	O 4	S 1	0	0
3	V	1	Total 5	O 4	S 1	0	0
3	V	1	Total 5	O 4	S 1	0	0
3	V	1	Total 5	O 4	S 1	0	0
3	W	1	Total 5	O 4	S 1	0	0
3	W	1	Total 5	O 4	S 1	0	0
3	Y	1	Total 5	O 4	S 1	0	0
3	Z	1	Total 5	O 4	S 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	203	Total 203	O 203	0	0
4	B	191	Total 191	O 191	0	0
4	C	154	Total 154	O 154	0	0
4	D	118	Total 118	O 118	0	0
4	E	160	Total 160	O 160	0	0
4	F	122	Total 122	O 122	0	0

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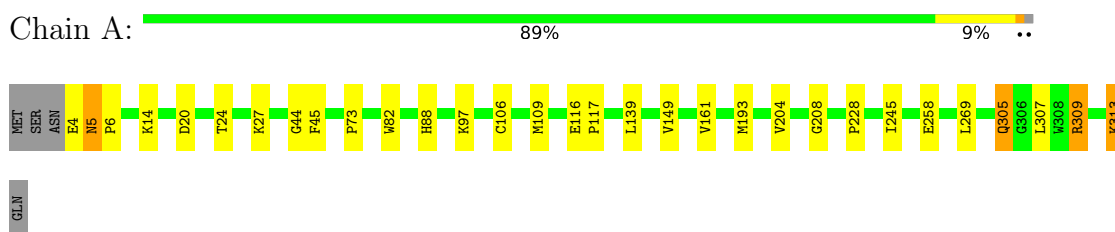
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	215	Total 215	O 215	0	0
4	H	186	Total 186	O 186	0	0
4	I	219	Total 219	O 219	0	0
4	J	204	Total 204	O 204	0	0
4	K	183	Total 183	O 183	0	0
4	L	101	Total 101	O 101	0	0
4	M	203	Total 203	O 203	0	0
4	N	219	Total 219	O 219	0	0
4	O	171	Total 171	O 171	0	0
4	P	153	Total 153	O 153	0	0
4	Q	221	Total 221	O 221	0	0
4	R	169	Total 169	O 169	0	0
4	T	174	Total 174	O 174	0	0
4	U	122	Total 122	O 122	0	0
4	V	116	Total 116	O 116	0	0
4	W	76	Total 76	O 76	0	0
4	Y	96	Total 96	O 96	0	0
4	Z	179	Total 179	O 179	0	0

### 3 Residue-property plots [i](#)

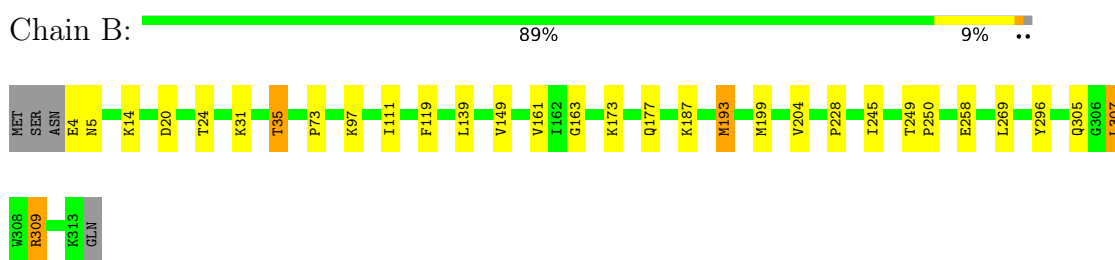
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS failed to run properly.

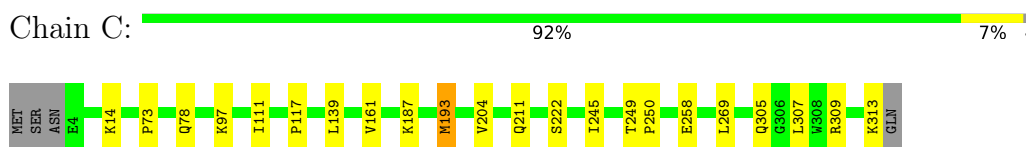
- Molecule 1: Sulfur oxygenase/reductase



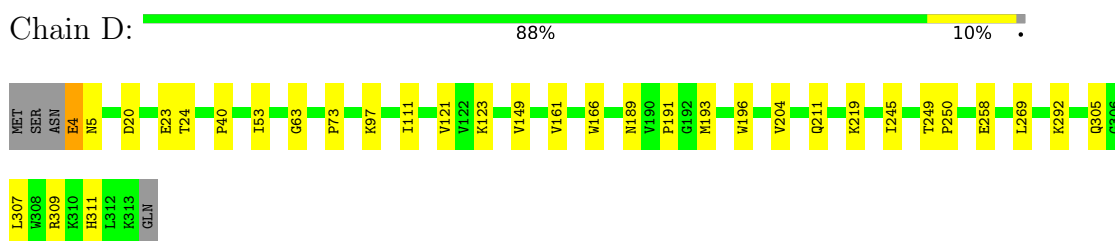
- Molecule 1: Sulfur oxygenase/reductase




- Molecule 1: Sulfur oxygenase/reductase

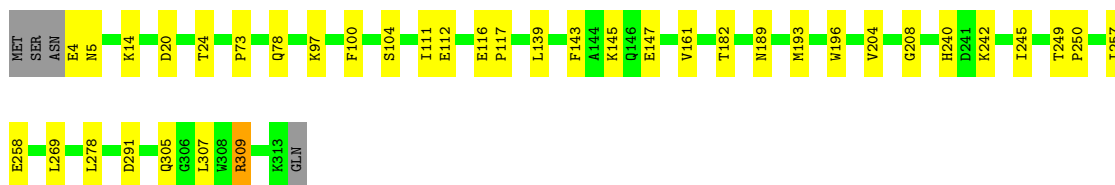


- Molecule 1: Sulfur oxygenase/reductase




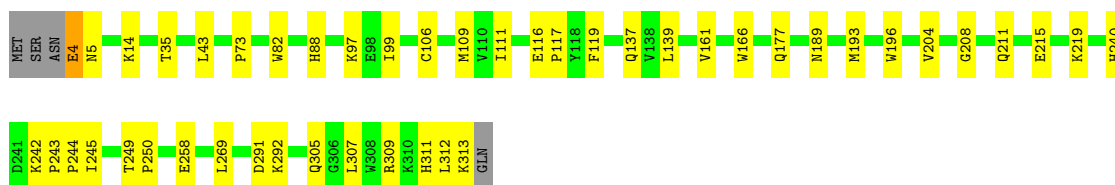
- Molecule 1: Sulfur oxygenase/reductase

Chain E:  87% 12%




- Molecule 1: Sulfur oxygenase/reductase

Chain F:  84% 14%




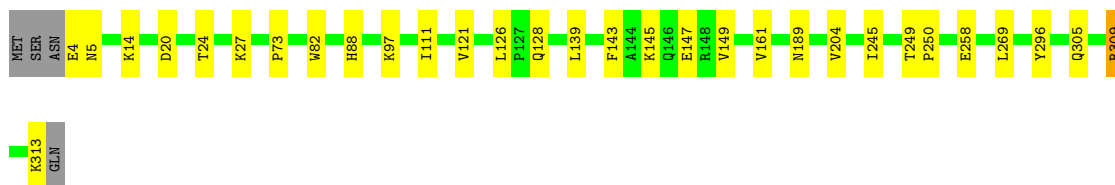
- Molecule 1: Sulfur oxygenase/reductase

Chain G:  89% 8%



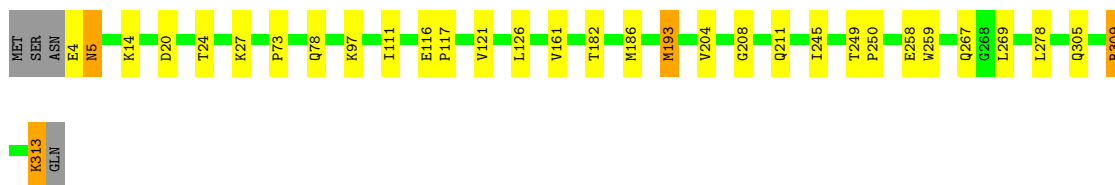
- Molecule 1: Sulfur oxygenase/reductase

Chain H:  89% 10%




- Molecule 1: Sulfur oxygenase/reductase

Chain I:  89% 9%



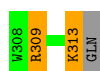
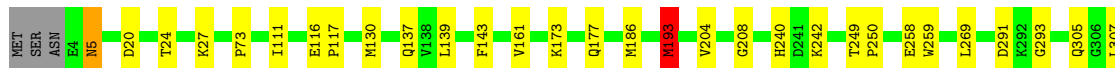
- Molecule 1: Sulfur oxygenase/reductase

Chain J:  88% 10%



- Molecule 1: Sulfur oxygenase/reductase

Chain K: 89% 9% ..



- Molecule 1: Sulfur oxygenase/reductase

Chain L: 91% 7% ..



- Molecule 1: Sulfur oxygenase/reductase

Chain M: 89% 9% ..



- Molecule 1: Sulfur oxygenase/reductase

Chain N: 89% 8% ..




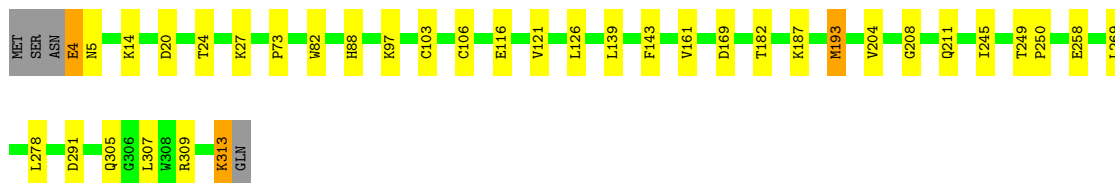
- Molecule 1: Sulfur oxygenase/reductase

Chain O: 90% 8% .




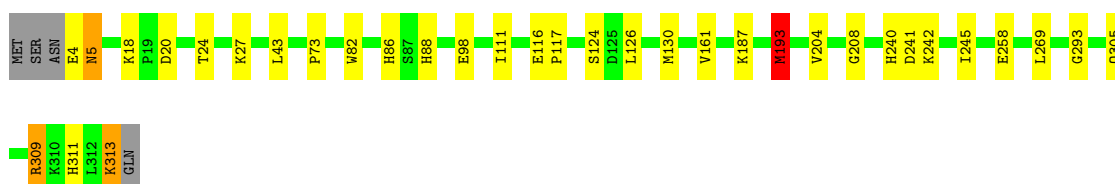
- Molecule 1: Sulfur oxygenase/reductase

Chain P:  87% 11% ..




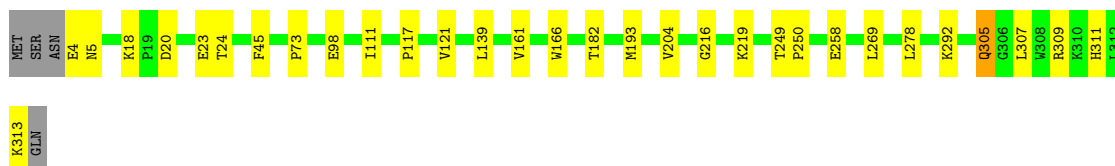
- Molecule 1: Sulfur oxygenase/reductase

Chain Q:  88% 10% ..




- Molecule 1: Sulfur oxygenase/reductase

Chain R:  89% 10% .




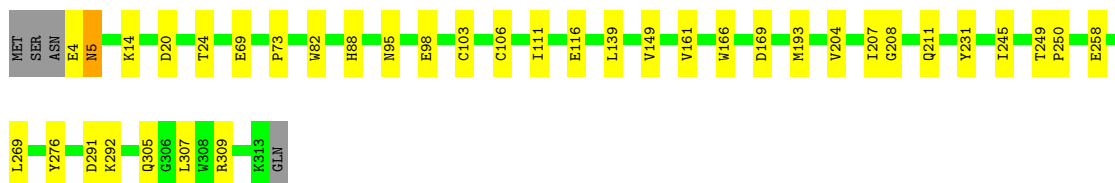
- Molecule 1: Sulfur oxygenase/reductase

Chain T:  90% 8% ..




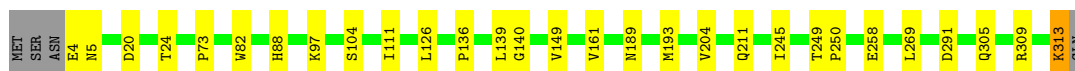
- Molecule 1: Sulfur oxygenase/reductase

Chain U:  87% 11% .




- Molecule 1: Sulfur oxygenase/reductase

Chain V:  89% 9%



- Molecule 1: Sulfur oxygenase/reductase

Chain W:  89% 10%




- Molecule 1: Sulfur oxygenase/reductase

Chain Y:  91% 8%



- Molecule 1: Sulfur oxygenase/reductase

Chain Z:  91% 6%



## 4 Data and refinement statistics i

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	200.84Å 212.45Å 215.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.69 – 2.10	Depositor
% Data completeness (in resolution range)	99.9 (83.69-2.10)	Depositor
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.48 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.162 , 0.200	Depositor
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtrriage
Anisotropy	0.309	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	0.013 for -h,l,k	Xtrriage
Total number of atoms	63067	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FE, CSS

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	0.44	0/2510	0.62	1/3399 (0.0%)
1	B	0.43	0/2510	0.61	1/3399 (0.0%)
1	C	0.40	0/2519	0.58	0/3411
1	D	0.37	0/2527	0.58	0/3423
1	E	0.42	0/2510	0.60	1/3399 (0.0%)
1	F	0.38	0/2518	0.56	0/3411
1	G	0.48	0/2518	0.65	3/3411 (0.1%)
1	H	0.44	0/2518	0.63	1/3411 (0.0%)
1	I	0.49	0/2527	0.65	2/3423 (0.1%)
1	J	0.45	0/2518	0.62	2/3407 (0.1%)
1	K	0.45	0/2510	0.63	2/3399 (0.1%)
1	L	0.37	0/2526	0.57	1/3419 (0.0%)
1	M	0.45	0/2518	0.62	2/3407 (0.1%)
1	N	0.47	0/2518	0.64	3/3411 (0.1%)
1	O	0.43	0/2526	0.60	0/3419
1	P	0.41	0/2535	0.60	0/3431
1	Q	0.44	0/2526	0.64	2/3419 (0.1%)
1	R	0.42	0/2518	0.59	0/3411
1	T	0.42	0/2518	0.58	0/3411
1	U	0.40	0/2527	0.58	0/3423
1	V	0.38	0/2510	0.57	0/3399
1	W	0.36	0/2510	0.57	0/3399
1	Y	0.36	0/2510	0.55	0/3399
1	Z	0.47	1/2535 (0.0%)	0.63	2/3431 (0.1%)
All	All	0.42	1/60462 (0.0%)	0.60	23/81872 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Z	161	VAL	CB-CG1	-5.35	1.41	1.52

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Z	309	ARG	NE-CZ-NH2	-9.14	115.73	120.30
1	J	309	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	G	309	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	N	309	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	Q	309	ARG	NE-CZ-NH2	-7.76	116.42	120.30

There are no chirality outliers.

There are no planarity outliers.

## 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	2447	0	2362	18	0
1	B	2447	0	2362	22	0
1	C	2451	0	2366	17	0
1	D	2456	0	2372	21	0
1	E	2447	0	2362	22	0
1	F	2452	0	2368	36	0
1	G	2452	0	2368	19	0
1	H	2452	0	2368	22	0
1	I	2456	0	2372	22	0
1	J	2451	0	2371	21	0
1	K	2447	0	2362	22	0
1	L	2456	0	2377	16	0
1	M	2451	0	2371	20	0
1	N	2452	0	2368	18	0
1	O	2454	0	2374	15	0
1	P	2460	0	2381	25	0
1	Q	2456	0	2377	24	0
1	R	2452	0	2368	18	0
1	T	2452	0	2368	17	0
1	U	2456	0	2372	25	0
1	V	2447	0	2362	20	0
1	W	2447	0	2362	22	0
1	Y	2447	0	2362	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	2460	0	2381	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
2	M	1	0	0	0	0
2	N	1	0	0	0	0
2	O	1	0	0	0	0
2	P	1	0	0	0	0
2	Q	1	0	0	0	0
2	R	1	0	0	0	0
2	T	1	0	0	0	0
2	U	1	0	0	0	0
2	V	1	0	0	0	0
2	W	1	0	0	0	0
2	Y	1	0	0	0	0
2	Z	1	0	0	0	0
3	A	15	0	0	0	0
3	B	10	0	0	0	0
3	C	15	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	15	0	0	0	0
3	G	10	0	0	1	0
3	H	10	0	0	0	0
3	I	10	0	0	0	0
3	J	10	0	0	1	0
3	K	10	0	0	0	0
3	L	10	0	0	1	0
3	M	10	0	0	0	0
3	N	10	0	0	0	0
3	O	10	0	0	0	0
3	P	10	0	0	0	0
3	Q	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	R	5	0	0	0	0
3	T	5	0	0	0	0
3	U	10	0	0	0	0
3	V	15	0	0	0	0
3	W	10	0	0	0	0
3	Y	5	0	0	0	0
3	Z	5	0	0	0	0
4	A	203	0	0	0	0
4	B	191	0	0	2	0
4	C	154	0	0	2	0
4	D	118	0	0	3	0
4	E	160	0	0	0	0
4	F	122	0	0	3	0
4	G	215	0	0	1	0
4	H	186	0	0	1	1
4	I	219	0	0	3	0
4	J	204	0	0	3	1
4	K	183	0	0	1	0
4	L	101	0	0	1	0
4	M	203	0	0	1	0
4	N	219	0	0	2	0
4	O	171	0	0	2	0
4	P	153	0	0	3	0
4	Q	221	0	0	3	0
4	R	169	0	0	0	0
4	T	174	0	0	1	0
4	U	122	0	0	3	0
4	V	116	0	0	1	0
4	W	76	0	0	0	0
4	Y	96	0	0	1	0
4	Z	179	0	0	0	0
All	All	63067	0	56856	450	1

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 4.

The worst 5 of 450 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:J:145:LYS:NZ	4:J:501:HOH:O	1.96	0.99
1:B:187:LYS:HA	1:B:193:MET:HG2	1.51	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:187:LYS:HA	1:N:193:MET:HG2	1.51	0.89
1:H:126:LEU:H	1:H:313:LYS:HZ1	1.26	0.81
1:P:4:GLU:OE1	4:P:501:HOH:O	1.99	0.79

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:576:HOH:O	4:J:660:HOH:O[4_456]	1.93	0.27

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
1	B	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	C	308/314 (98%)	301 (98%)	7 (2%)	0	100	100
1	D	309/314 (98%)	301 (97%)	8 (3%)	0	100	100
1	E	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	F	308/314 (98%)	299 (97%)	9 (3%)	0	100	100
1	G	308/314 (98%)	301 (98%)	7 (2%)	0	100	100
1	H	308/314 (98%)	302 (98%)	6 (2%)	0	100	100
1	I	309/314 (98%)	302 (98%)	7 (2%)	0	100	100
1	J	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	K	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
1	L	308/314 (98%)	300 (97%)	8 (3%)	0	100	100
1	M	307/314 (98%)	299 (97%)	8 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	308/314 (98%)	300 (97%)	8 (3%)	0	100	100
1	O	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	P	309/314 (98%)	301 (97%)	8 (3%)	0	100	100
1	Q	308/314 (98%)	302 (98%)	6 (2%)	0	100	100
1	R	308/314 (98%)	301 (98%)	7 (2%)	0	100	100
1	T	308/314 (98%)	301 (98%)	7 (2%)	0	100	100
1	U	309/314 (98%)	302 (98%)	7 (2%)	0	100	100
1	V	307/314 (98%)	298 (97%)	9 (3%)	0	100	100
1	W	307/314 (98%)	299 (97%)	8 (3%)	0	100	100
1	Y	307/314 (98%)	300 (98%)	7 (2%)	0	100	100
1	Z	309/314 (98%)	303 (98%)	6 (2%)	0	100	100
All	All	7387/7536 (98%)	7210 (98%)	177 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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 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	263/266 (99%)	258 (98%)	5 (2%)	57	63
1	B	263/266 (99%)	258 (98%)	5 (2%)	57	63
1	C	264/266 (99%)	261 (99%)	3 (1%)	73	79
1	D	265/266 (100%)	261 (98%)	4 (2%)	65	71
1	E	263/266 (99%)	259 (98%)	4 (2%)	65	71
1	F	264/266 (99%)	262 (99%)	2 (1%)	81	86
1	G	264/266 (99%)	260 (98%)	4 (2%)	65	71
1	H	264/266 (99%)	261 (99%)	3 (1%)	73	79
1	I	265/266 (100%)	258 (97%)	7 (3%)	46	50
1	J	264/266 (99%)	260 (98%)	4 (2%)	65	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	263/266 (99%)	257 (98%)	6 (2%)	50	55
1	L	265/266 (100%)	260 (98%)	5 (2%)	57	63
1	M	264/266 (99%)	258 (98%)	6 (2%)	50	55
1	N	264/266 (99%)	260 (98%)	4 (2%)	65	71
1	O	265/266 (100%)	260 (98%)	5 (2%)	57	63
1	P	266/266 (100%)	260 (98%)	6 (2%)	50	55
1	Q	265/266 (100%)	258 (97%)	7 (3%)	46	50
1	R	264/266 (99%)	258 (98%)	6 (2%)	50	55
1	T	264/266 (99%)	259 (98%)	5 (2%)	57	63
1	U	265/266 (100%)	259 (98%)	6 (2%)	50	55
1	V	263/266 (99%)	258 (98%)	5 (2%)	57	63
1	W	263/266 (99%)	261 (99%)	2 (1%)	81	86
1	Y	263/266 (99%)	261 (99%)	2 (1%)	81	86
1	Z	266/266 (100%)	260 (98%)	6 (2%)	50	55
All	All	6339/6384 (99%)	6227 (98%)	112 (2%)	62	65

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	313[B]	LYS
1	Z	313[A]	LYS
1	P	313[A]	LYS
1	Z	305	GLN
1	V	193	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	177	GLN
1	Z	86	HIS
1	W	78	GLN
1	T	78	GLN
1	Y	211	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

48 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	CSS	F	103	1	4,6,7	1.42	0	1,6,8	1.91	0
1	CSS	Z	33	1	4,6,7	1.29	0	1,6,8	1.21	0
1	CSS	Z	103	1	4,6,7	1.30	0	1,6,8	1.58	0
1	CSS	E	33	1	4,6,7	1.20	0	1,6,8	0.66	0
1	CSS	O	33	1	4,6,7	1.43	0	1,6,8	1.48	0
1	CSS	B	103	1	4,6,7	1.39	0	1,6,8	1.48	0
1	CSS	U	103	1	4,6,7	1.38	0	1,6,8	1.75	0
1	CSS	C	33	1	4,6,7	1.19	0	1,6,8	0.66	0
1	CSS	W	33	1	4,6,7	1.31	0	1,6,8	0.40	0
1	CSS	L	33	1	4,6,7	1.46	0	1,6,8	1.84	0
1	CSS	L	103	1	4,6,7	1.31	0	1,6,8	1.53	0
1	CSS	R	103	1	4,6,7	1.43	0	1,6,8	1.85	0
1	CSS	V	33	1	4,6,7	1.40	0	1,6,8	1.02	0
1	CSS	V	103	1	4,6,7	1.35	0	1,6,8	1.16	0
1	CSS	E	103	1	4,6,7	1.39	0	1,6,8	0.92	0
1	CSS	P	33	1	4,6,7	1.25	0	1,6,8	1.06	0
1	CSS	Q	33	1	4,6,7	1.32	0	1,6,8	1.33	0
1	CSS	T	33	1	4,6,7	1.41	0	1,6,8	1.85	0
1	CSS	A	103	1	4,6,7	1.23	0	1,6,8	1.29	0
1	CSS	H	33	1	4,6,7	1.29	0	1,6,8	0.92	0
1	CSS	D	33	1	4,6,7	1.46	0	1,6,8	1.47	0
1	CSS	K	33	1	4,6,7	1.29	0	1,6,8	0.67	0
1	CSS	G	103	1	4,6,7	1.34	0	1,6,8	1.57	0
1	CSS	G	33	1	4,6,7	1.15	0	1,6,8	1.21	0
1	CSS	N	103	1	4,6,7	1.30	0	1,6,8	1.75	0
1	CSS	T	103	1	4,6,7	1.39	0	1,6,8	1.48	0
1	CSS	Y	33	1	4,6,7	1.32	0	1,6,8	0.84	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSS	Y	103	1	4,6,7	1.41	0	1,6,8	1.79	0
1	CSS	P	103	1	4,6,7	1.48	0	1,6,8	1.92	0
1	CSS	J	103	1	4,6,7	1.39	0	1,6,8	1.31	0
1	CSS	A	33	1	4,6,7	1.32	0	1,6,8	0.98	0
1	CSS	R	33	1	4,6,7	1.29	0	1,6,8	0.71	0
1	CSS	W	103	1	4,6,7	1.43	0	1,6,8	1.69	0
1	CSS	D	103	1	4,6,7	1.26	0	1,6,8	1.08	0
1	CSS	I	33	1	4,6,7	1.11	0	1,6,8	0.98	0
1	CSS	N	33	1	4,6,7	1.31	0	1,6,8	0.92	0
1	CSS	C	103	1	4,6,7	1.31	0	1,6,8	1.43	0
1	CSS	O	103	1	4,6,7	1.21	0	1,6,8	1.20	0
1	CSS	Q	103	1	4,6,7	1.27	0	1,6,8	0.90	0
1	CSS	M	33	1	4,6,7	1.34	0	1,6,8	1.15	0
1	CSS	M	103	1	4,6,7	1.26	0	1,6,8	1.47	0
1	CSS	H	103	1	4,6,7	1.25	0	1,6,8	1.59	0
1	CSS	I	103	1	4,6,7	1.24	0	1,6,8	0.94	0
1	CSS	K	103	1	4,6,7	1.22	0	1,6,8	0.90	0
1	CSS	U	33	1	4,6,7	1.33	0	1,6,8	1.37	0
1	CSS	B	33	1	4,6,7	1.36	0	1,6,8	1.41	0
1	CSS	J	33	1	4,6,7	1.29	0	1,6,8	0.76	0
1	CSS	F	33	1	4,6,7	1.39	0	1,6,8	0.99	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
1	CSS	F	103	1	-	0/1/5/7	-
1	CSS	Z	33	1	-	0/1/5/7	-
1	CSS	Z	103	1	-	0/1/5/7	-
1	CSS	E	33	1	-	0/1/5/7	-
1	CSS	O	33	1	-	0/1/5/7	-
1	CSS	B	103	1	-	0/1/5/7	-
1	CSS	U	103	1	-	0/1/5/7	-
1	CSS	C	33	1	-	0/1/5/7	-
1	CSS	W	33	1	-	0/1/5/7	-
1	CSS	L	33	1	-	0/1/5/7	-
1	CSS	L	103	1	-	0/1/5/7	-
1	CSS	R	103	1	-	0/1/5/7	-
1	CSS	V	33	1	-	0/1/5/7	-
1	CSS	V	103	1	-	0/1/5/7	-
1	CSS	E	103	1	-	0/1/5/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSS	P	33	1	-	0/1/5/7	-
1	CSS	Q	33	1	-	0/1/5/7	-
1	CSS	T	33	1	-	0/1/5/7	-
1	CSS	A	103	1	-	0/1/5/7	-
1	CSS	H	33	1	-	0/1/5/7	-
1	CSS	D	33	1	-	0/1/5/7	-
1	CSS	K	33	1	-	0/1/5/7	-
1	CSS	G	103	1	-	0/1/5/7	-
1	CSS	G	33	1	-	0/1/5/7	-
1	CSS	N	103	1	-	0/1/5/7	-
1	CSS	T	103	1	-	0/1/5/7	-
1	CSS	Y	33	1	-	0/1/5/7	-
1	CSS	Y	103	1	-	0/1/5/7	-
1	CSS	P	103	1	-	0/1/5/7	-
1	CSS	J	103	1	-	0/1/5/7	-
1	CSS	A	33	1	-	0/1/5/7	-
1	CSS	R	33	1	-	0/1/5/7	-
1	CSS	W	103	1	-	0/1/5/7	-
1	CSS	D	103	1	-	0/1/5/7	-
1	CSS	I	33	1	-	0/1/5/7	-
1	CSS	N	33	1	-	0/1/5/7	-
1	CSS	C	103	1	-	0/1/5/7	-
1	CSS	O	103	1	-	0/1/5/7	-
1	CSS	Q	103	1	-	0/1/5/7	-
1	CSS	M	33	1	-	0/1/5/7	-
1	CSS	M	103	1	-	0/1/5/7	-
1	CSS	H	103	1	-	0/1/5/7	-
1	CSS	I	103	1	-	0/1/5/7	-
1	CSS	K	103	1	-	0/1/5/7	-
1	CSS	U	33	1	-	0/1/5/7	-
1	CSS	B	33	1	-	0/1/5/7	-
1	CSS	J	33	1	-	0/1/5/7	-
1	CSS	F	33	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	U	103	CSS	2	0
1	W	33	CSS	1	0
1	T	33	CSS	1	0
1	Y	103	CSS	1	0
1	P	103	CSS	1	0
1	J	103	CSS	1	0
1	J	33	CSS	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 72 ligands modelled in this entry, 24 are monoatomic - leaving 48 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	$\# Z  > 2$
3	SO4	R	402	-	4,4,4	0.13	0	6,6,6	0.14	0
3	SO4	A	403	-	4,4,4	0.10	0	6,6,6	0.33	0
3	SO4	B	402	-	4,4,4	0.11	0	6,6,6	0.13	0
3	SO4	I	402	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	N	403	-	4,4,4	0.16	0	6,6,6	0.30	0
3	SO4	M	403	-	4,4,4	0.17	0	6,6,6	0.29	0
3	SO4	N	402	-	4,4,4	0.13	0	6,6,6	0.18	0
3	SO4	Y	402	-	4,4,4	0.14	0	6,6,6	0.08	0
3	SO4	E	402	-	4,4,4	0.15	0	6,6,6	0.05	0
3	SO4	P	402	-	4,4,4	0.15	0	6,6,6	0.10	0
3	SO4	P	403	-	4,4,4	0.12	0	6,6,6	0.17	0
3	SO4	K	403	-	4,4,4	0.14	0	6,6,6	0.19	0
3	SO4	J	403	-	4,4,4	0.13	0	6,6,6	0.20	0
3	SO4	J	402	-	4,4,4	0.15	0	6,6,6	0.20	0
3	SO4	G	403	-	4,4,4	0.14	0	6,6,6	0.25	0
3	SO4	A	404	-	4,4,4	0.11	0	6,6,6	0.23	0
3	SO4	L	402	-	4,4,4	0.15	0	6,6,6	0.10	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	E	403	-	4,4,4	0.13	0	6,6,6	0.25	0
3	SO4	V	401	-	4,4,4	0.16	0	6,6,6	0.20	0
3	SO4	K	402	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	G	402	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	C	403	-	4,4,4	0.11	0	6,6,6	0.18	0
3	SO4	U	403	-	4,4,4	0.11	0	6,6,6	0.23	0
3	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.14	0
3	SO4	F	404	-	4,4,4	0.16	0	6,6,6	0.13	0
3	SO4	W	402	-	4,4,4	0.15	0	6,6,6	0.11	0
3	SO4	V	403	-	4,4,4	0.12	0	6,6,6	0.12	0
3	SO4	W	403	-	4,4,4	0.17	0	6,6,6	0.10	0
3	SO4	M	402	-	4,4,4	0.15	0	6,6,6	0.08	0
3	SO4	H	403	-	4,4,4	0.18	0	6,6,6	0.27	0
3	SO4	C	404	-	4,4,4	0.17	0	6,6,6	0.18	0
3	SO4	Q	403	-	4,4,4	0.21	0	6,6,6	0.19	0
3	SO4	Q	402	-	4,4,4	0.13	0	6,6,6	0.16	0
3	SO4	T	402	-	4,4,4	0.13	0	6,6,6	0.15	0
3	SO4	V	404	-	4,4,4	0.17	0	6,6,6	0.14	0
3	SO4	H	402	-	4,4,4	0.15	0	6,6,6	0.09	0
3	SO4	B	403	-	4,4,4	0.15	0	6,6,6	0.24	0
3	SO4	F	403	-	4,4,4	0.16	0	6,6,6	0.10	0
3	SO4	F	402	-	4,4,4	0.16	0	6,6,6	0.12	0
3	SO4	A	402	-	4,4,4	0.12	0	6,6,6	0.14	0
3	SO4	L	403	-	4,4,4	0.15	0	6,6,6	0.18	0
3	SO4	D	402	-	4,4,4	0.15	0	6,6,6	0.06	0
3	SO4	D	403	-	4,4,4	0.12	0	6,6,6	0.18	0
3	SO4	O	402	-	4,4,4	0.12	0	6,6,6	0.13	0
3	SO4	U	402	-	4,4,4	0.12	0	6,6,6	0.11	0
3	SO4	Z	402	-	4,4,4	0.17	0	6,6,6	0.12	0
3	SO4	I	403	-	4,4,4	0.11	0	6,6,6	0.44	0
3	SO4	O	403	-	4,4,4	0.11	0	6,6,6	0.27	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

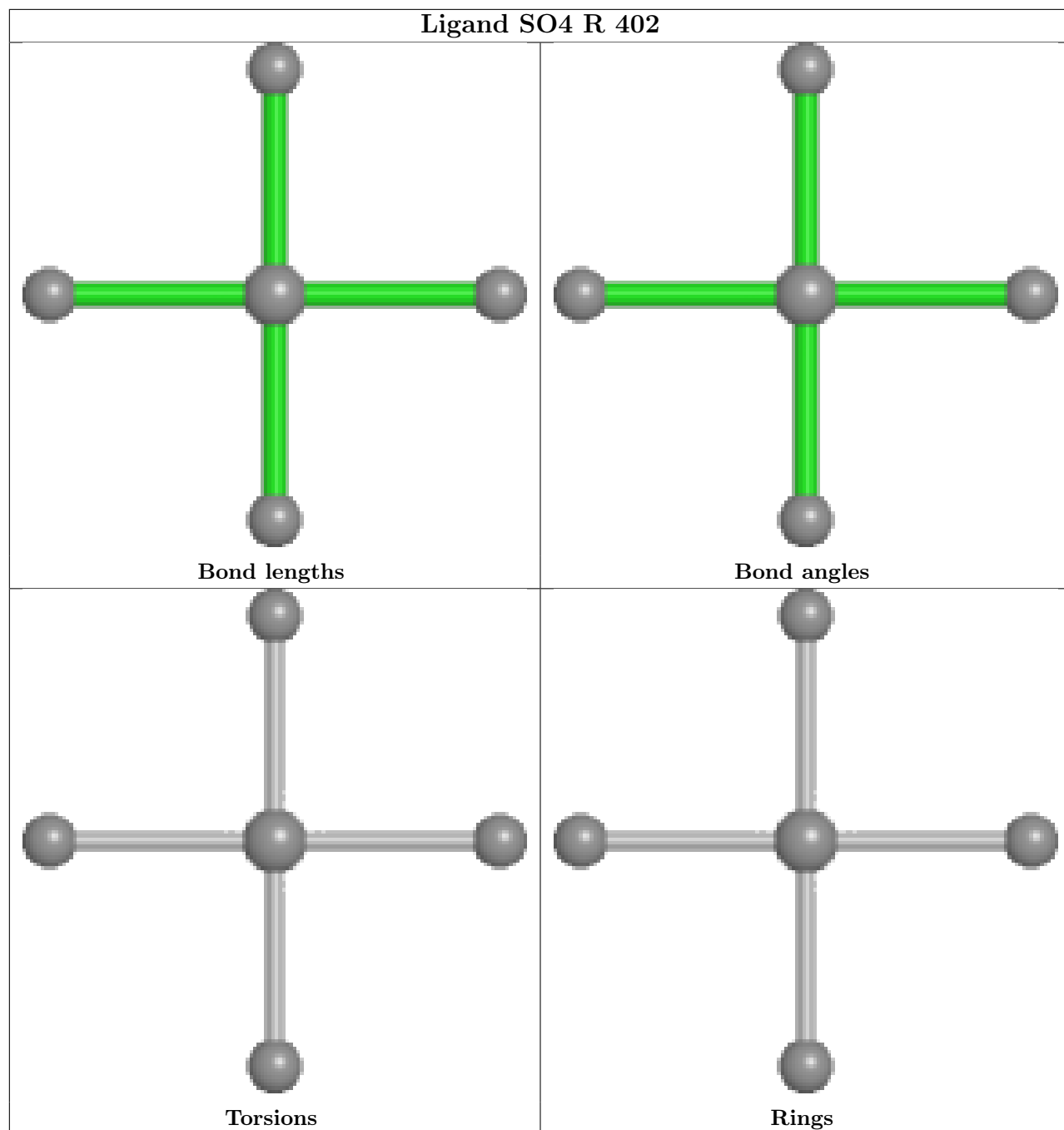
There are no torsion outliers.

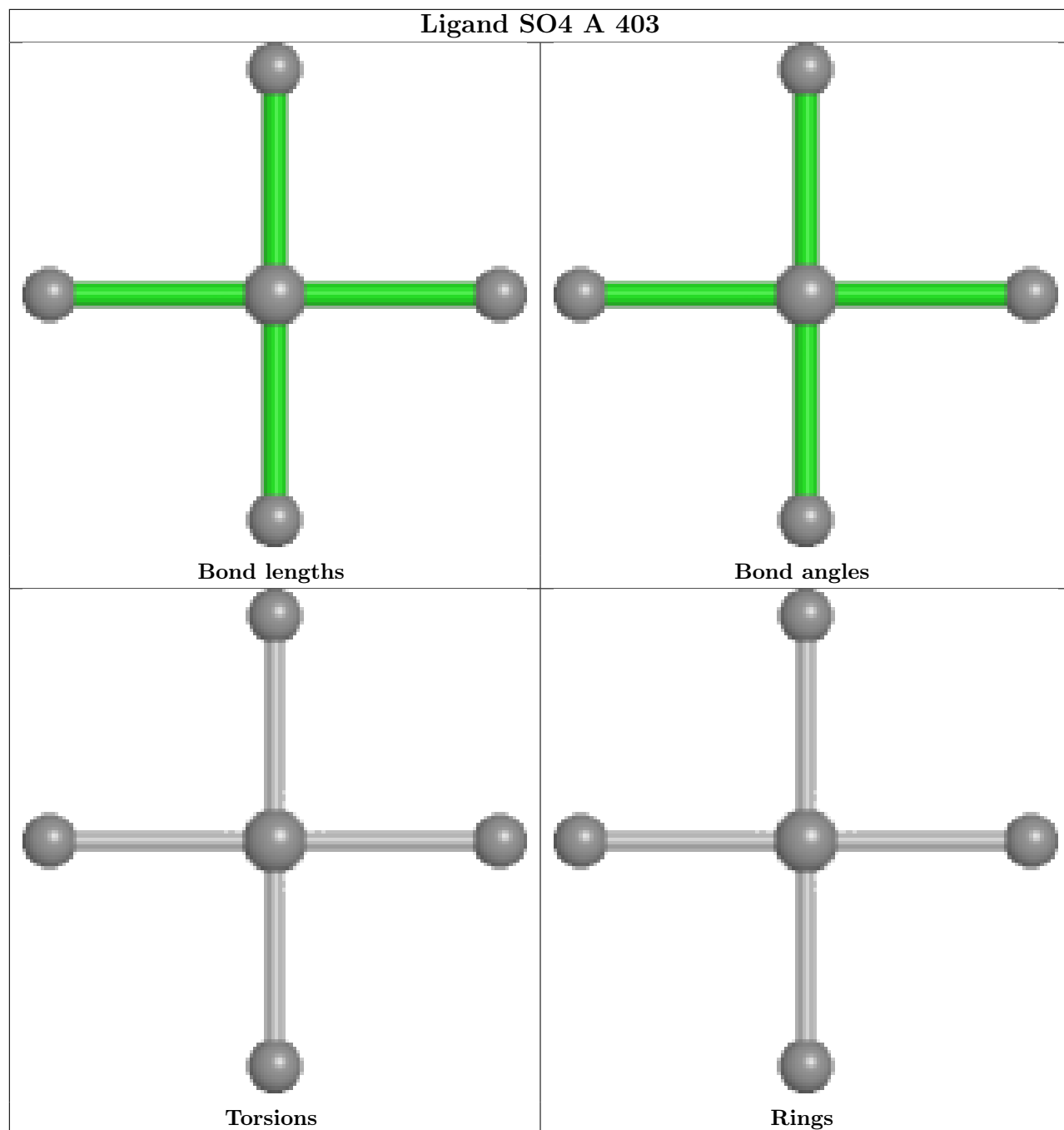
There are no ring outliers.

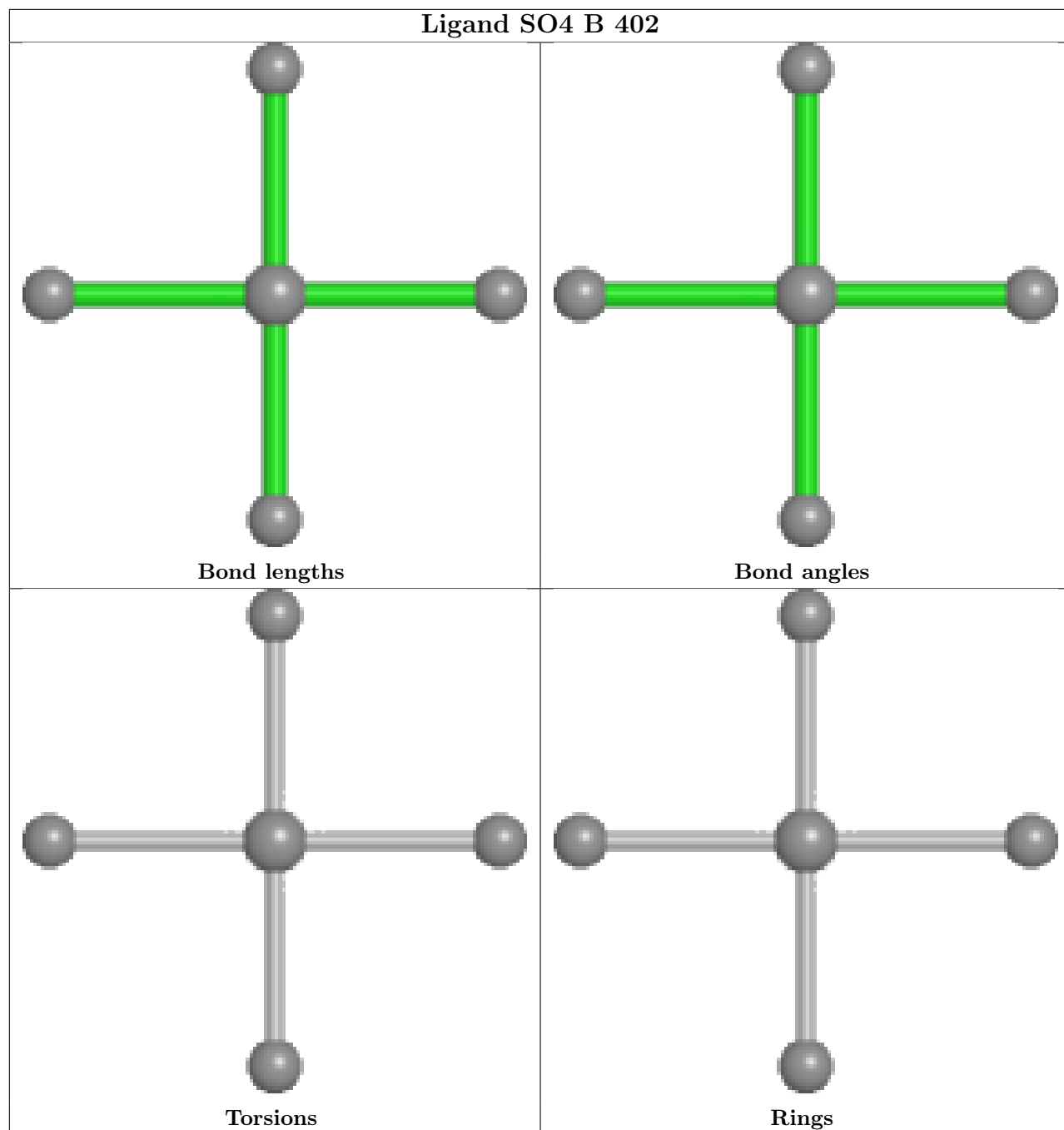
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	J	402	SO4	1	0
3	L	402	SO4	1	0
3	G	402	SO4	1	0

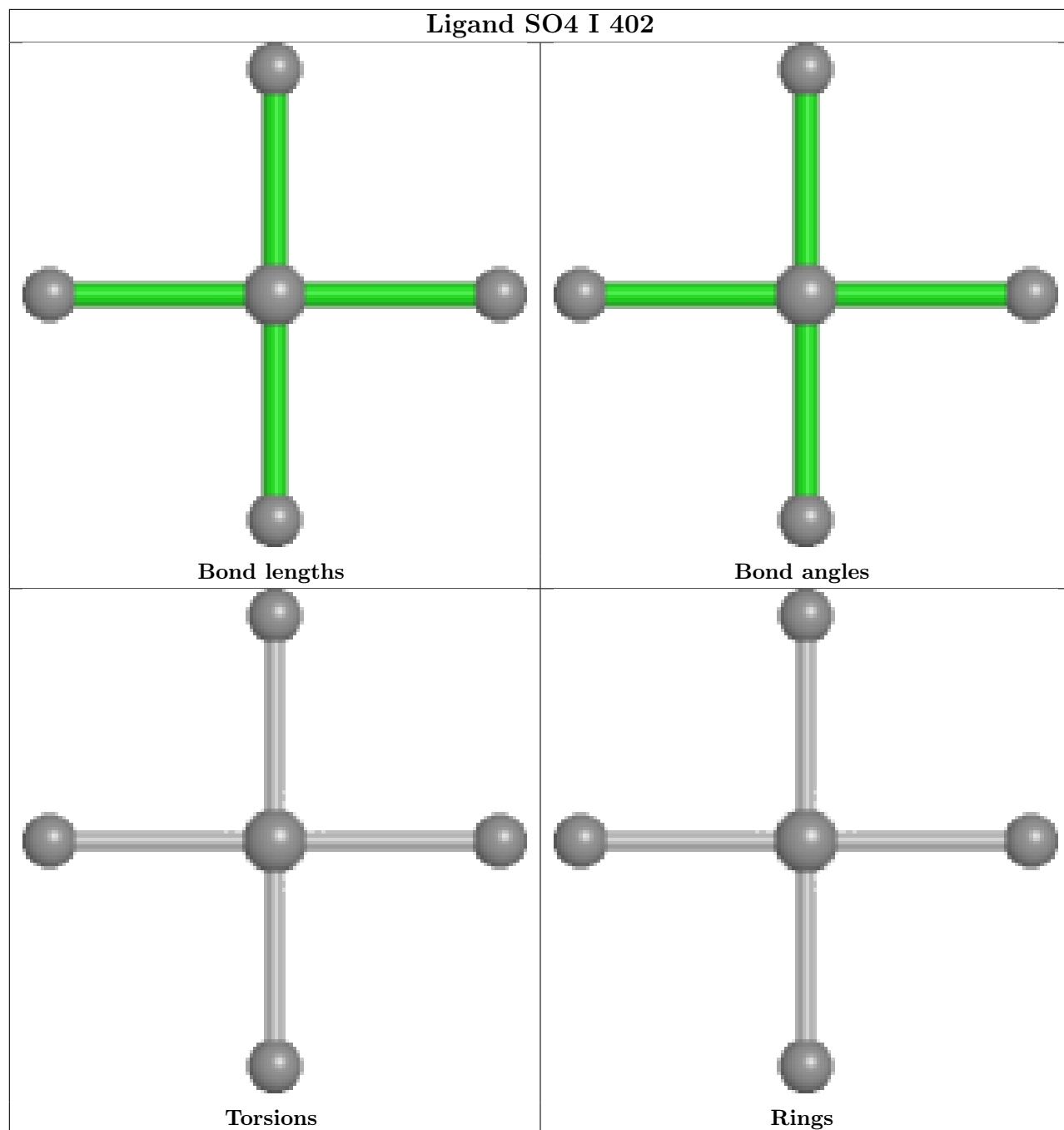
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

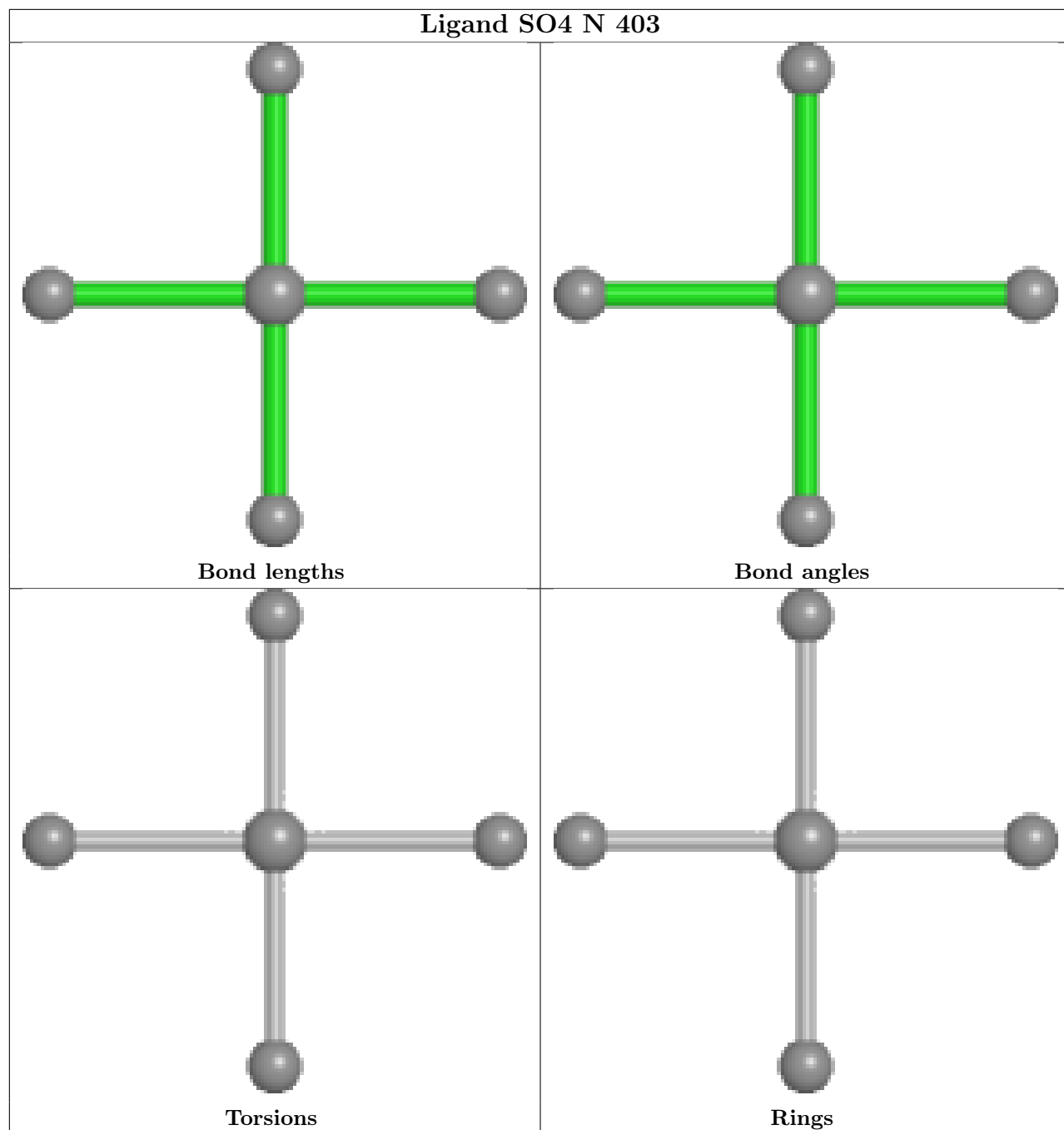


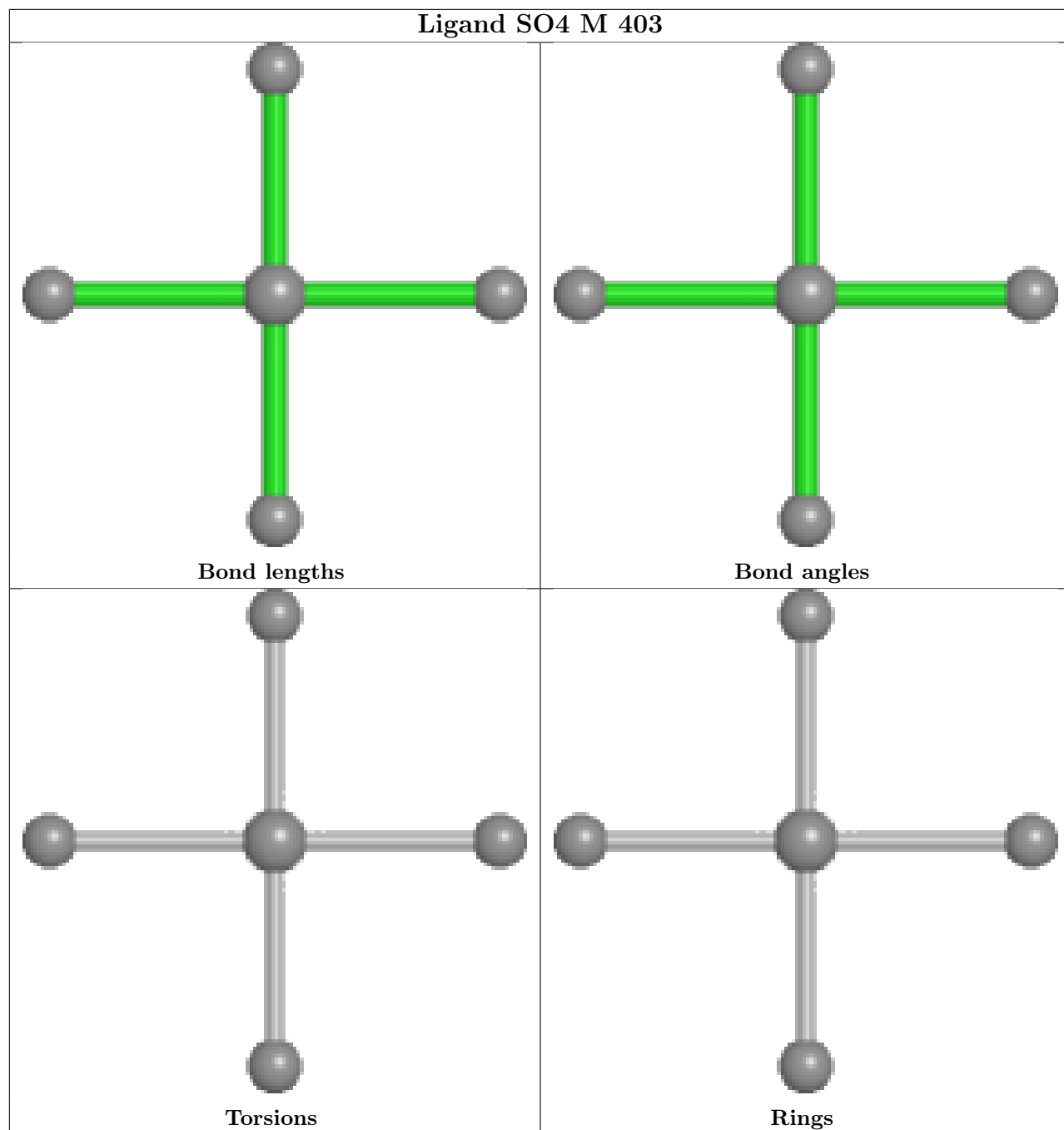


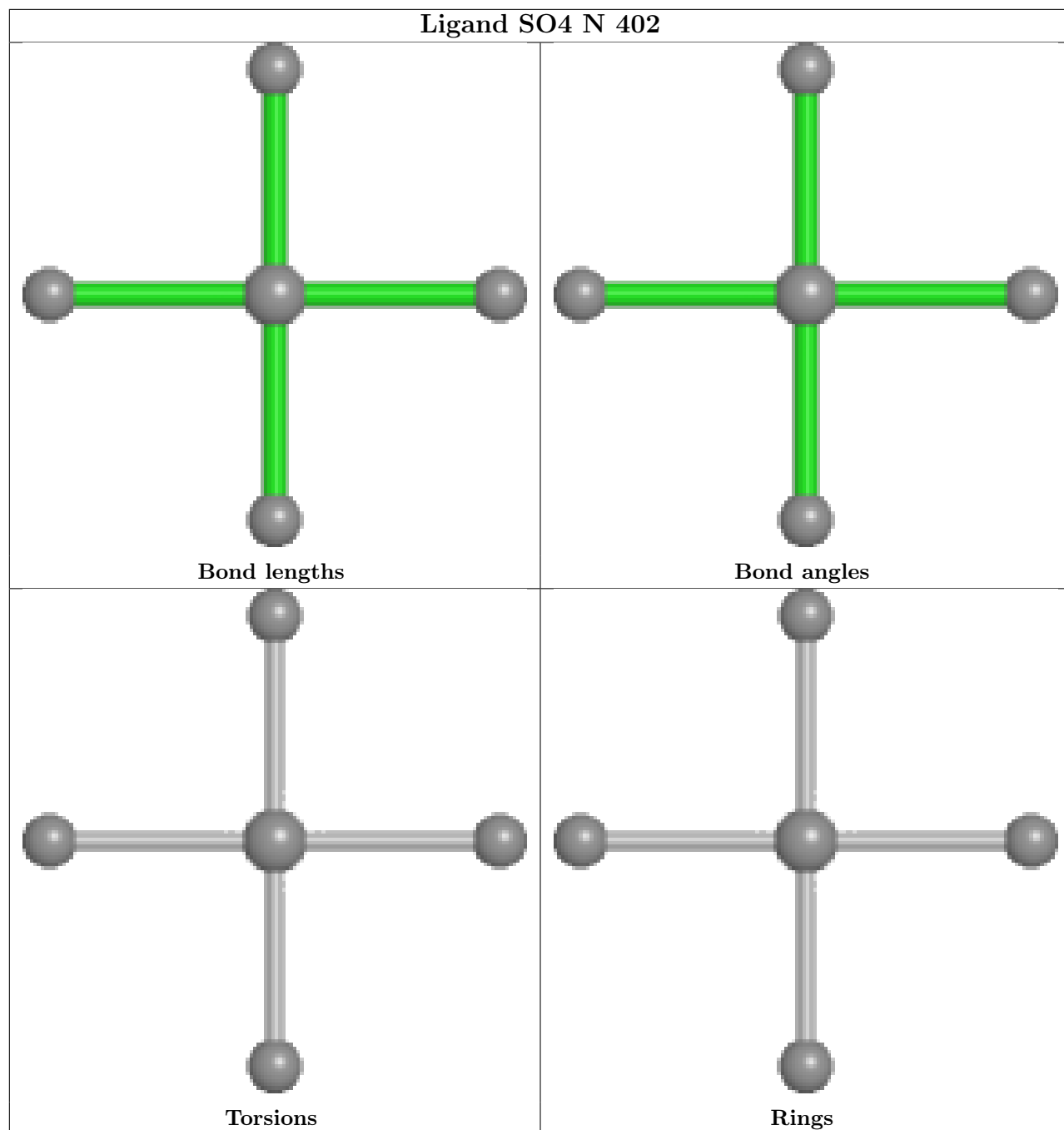


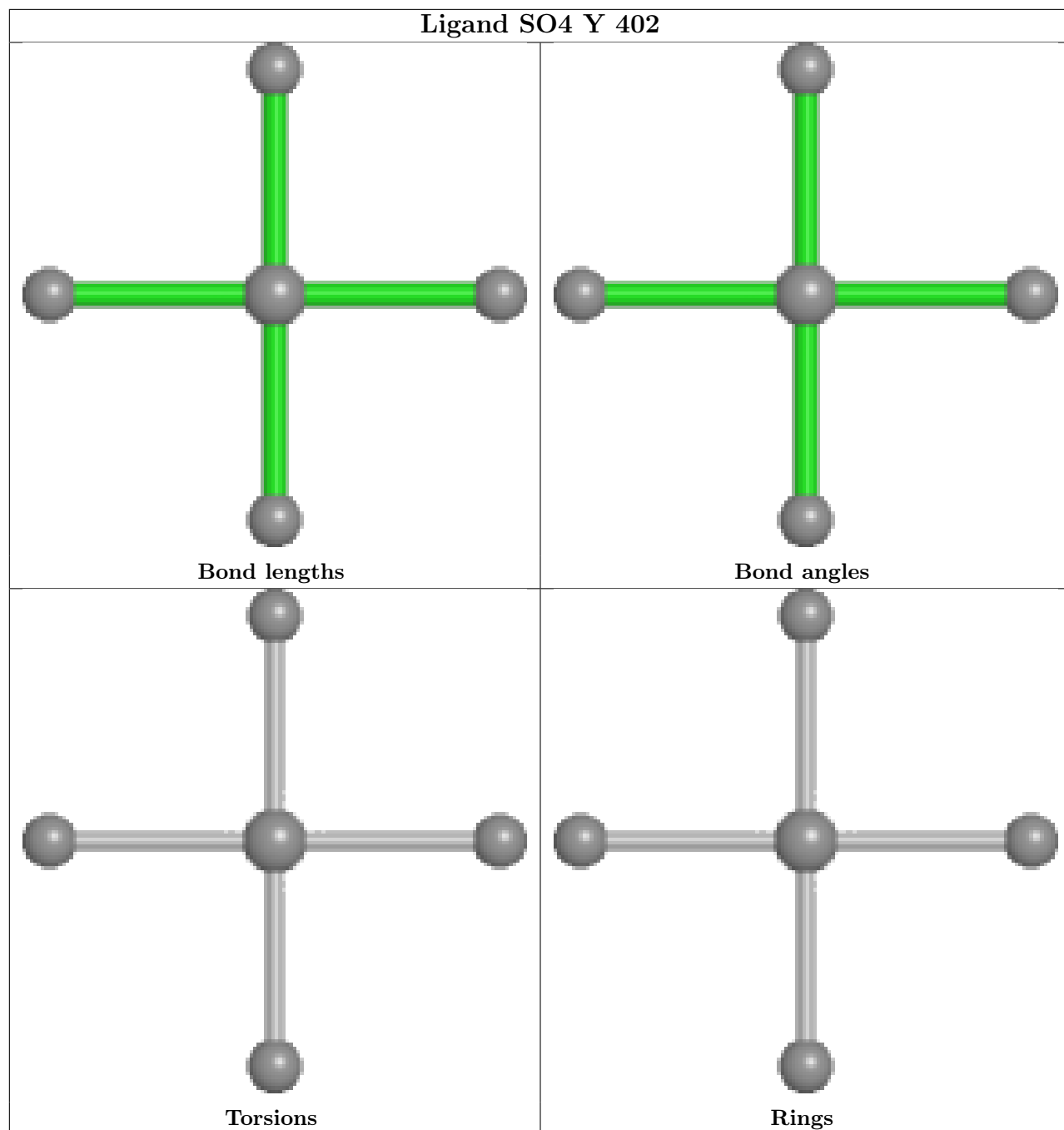


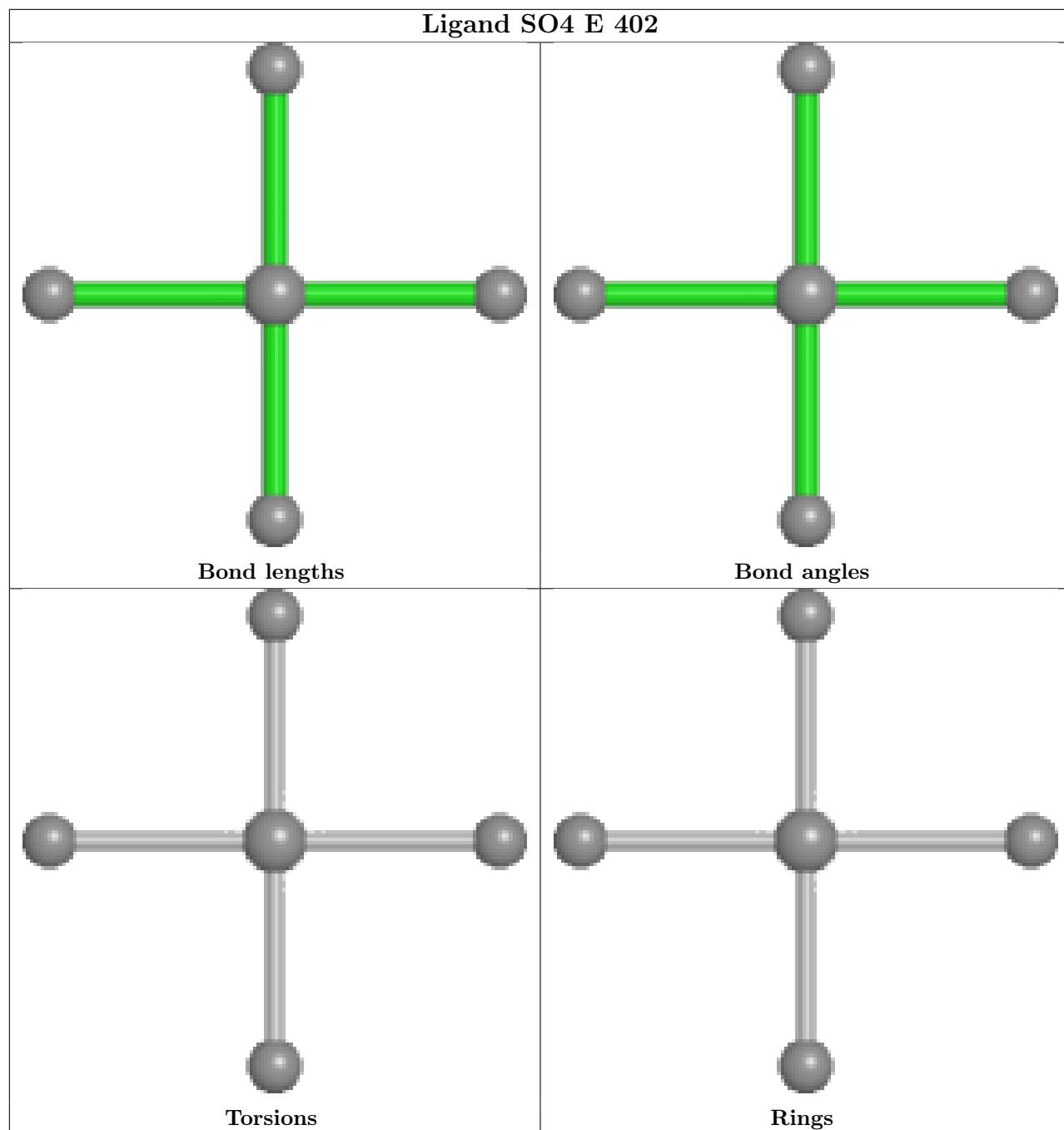


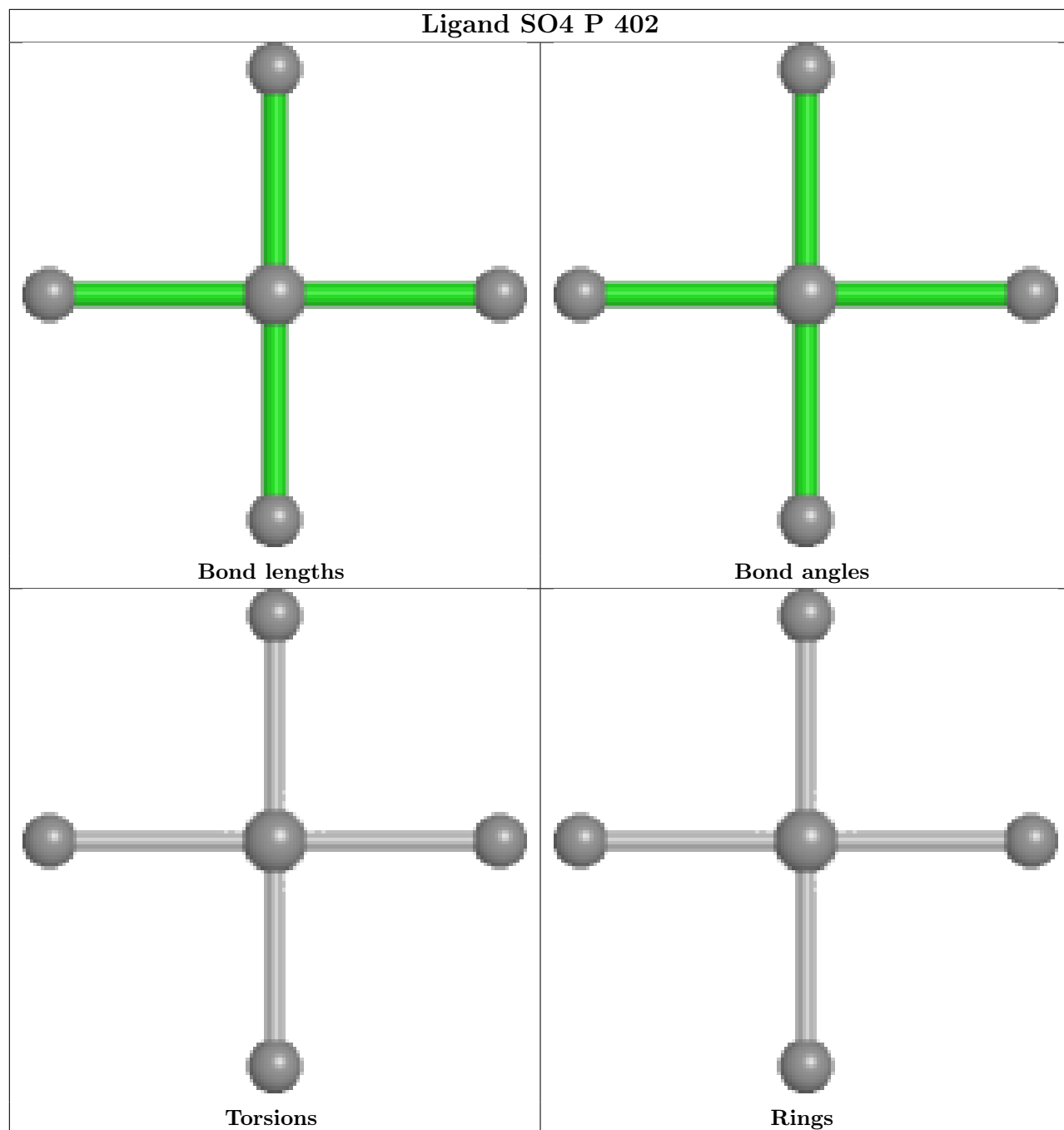


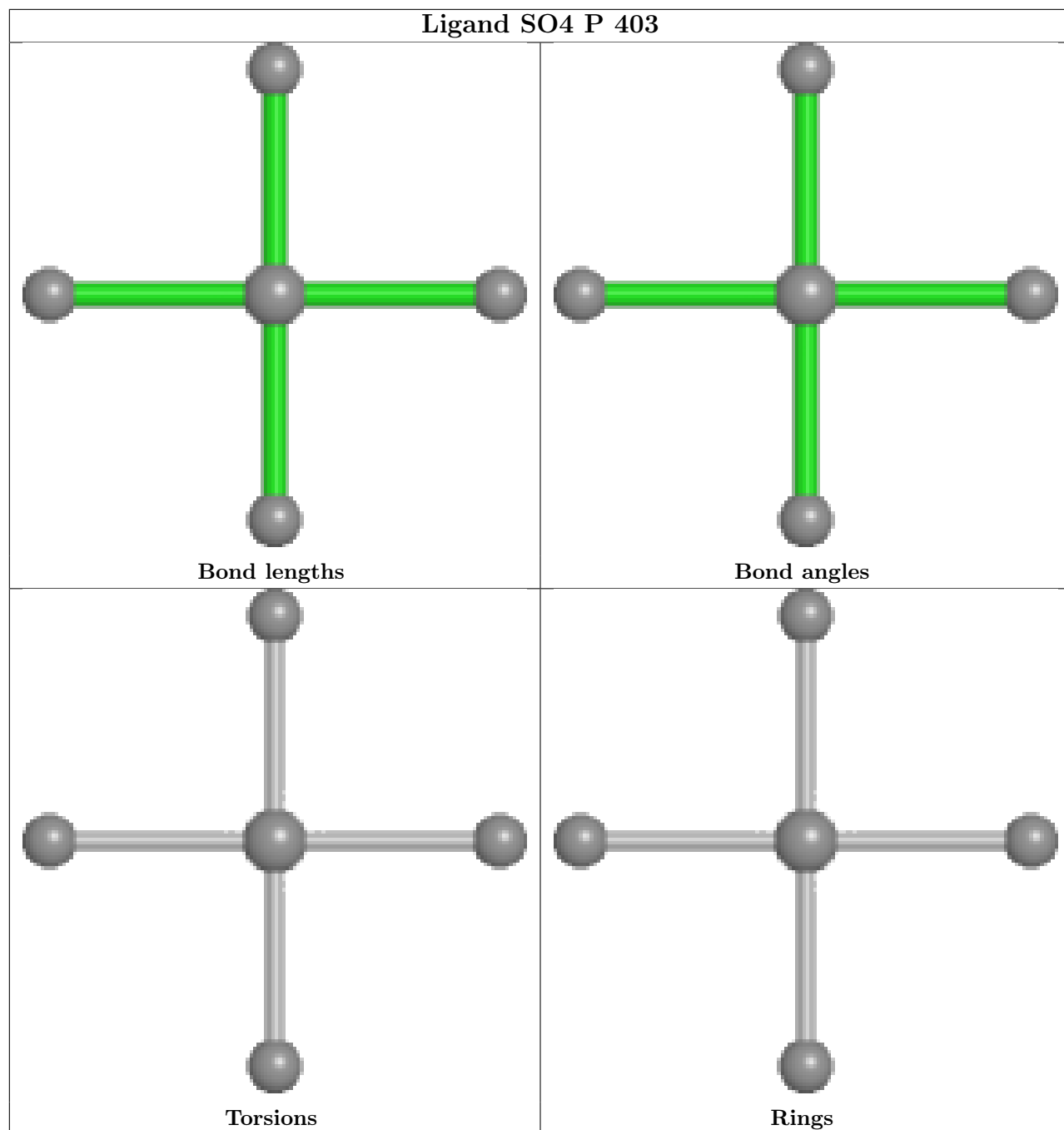




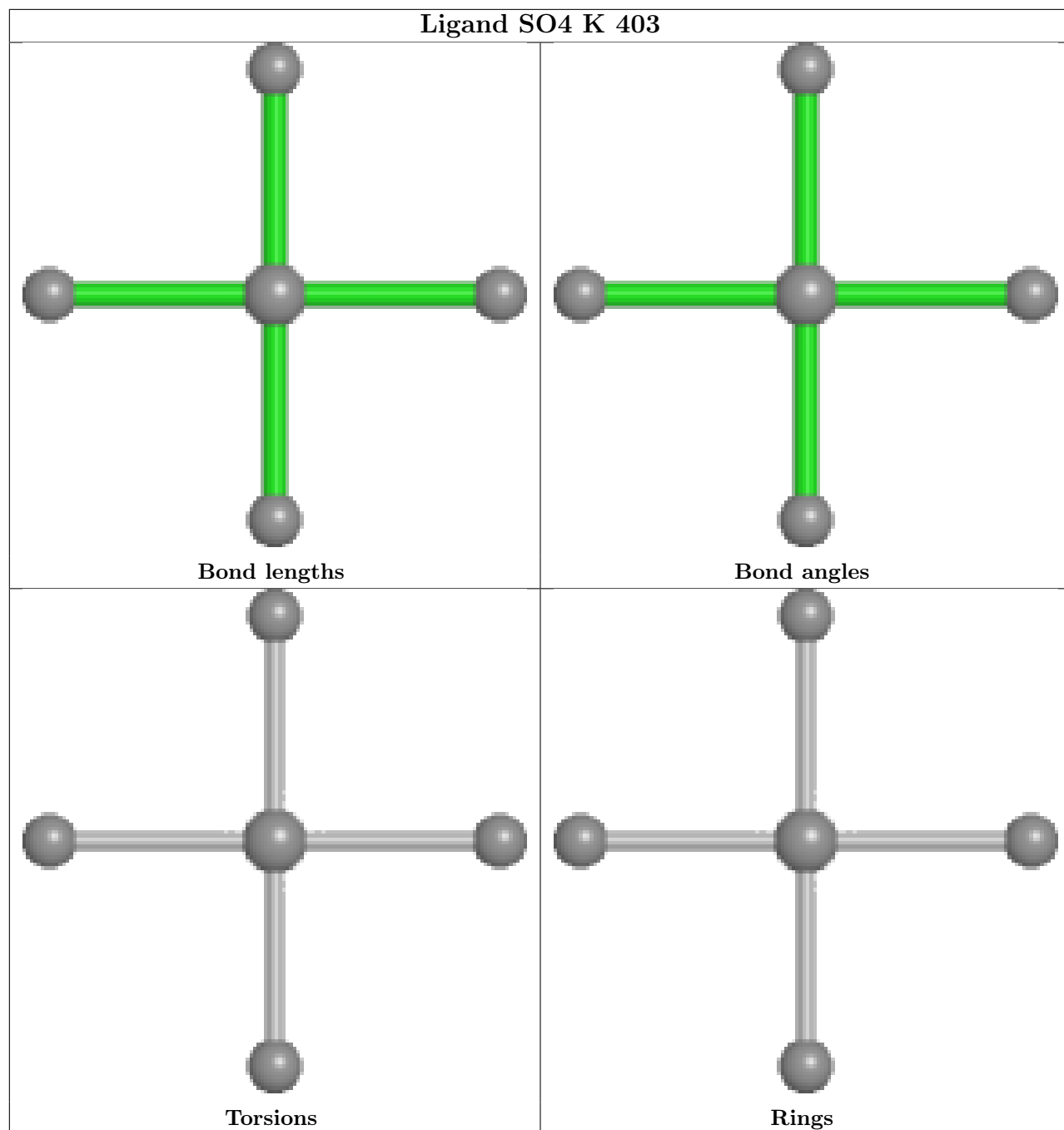


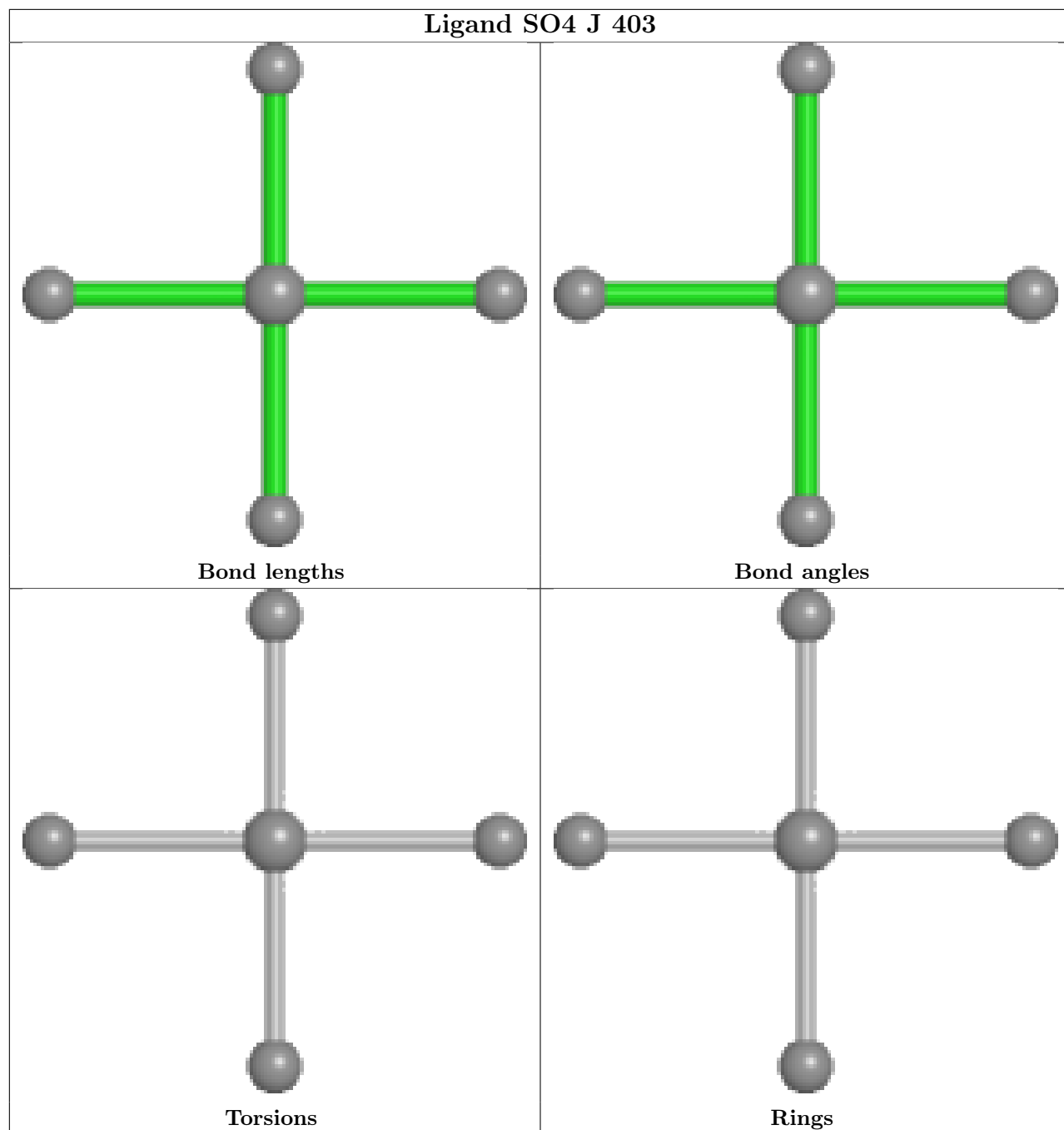


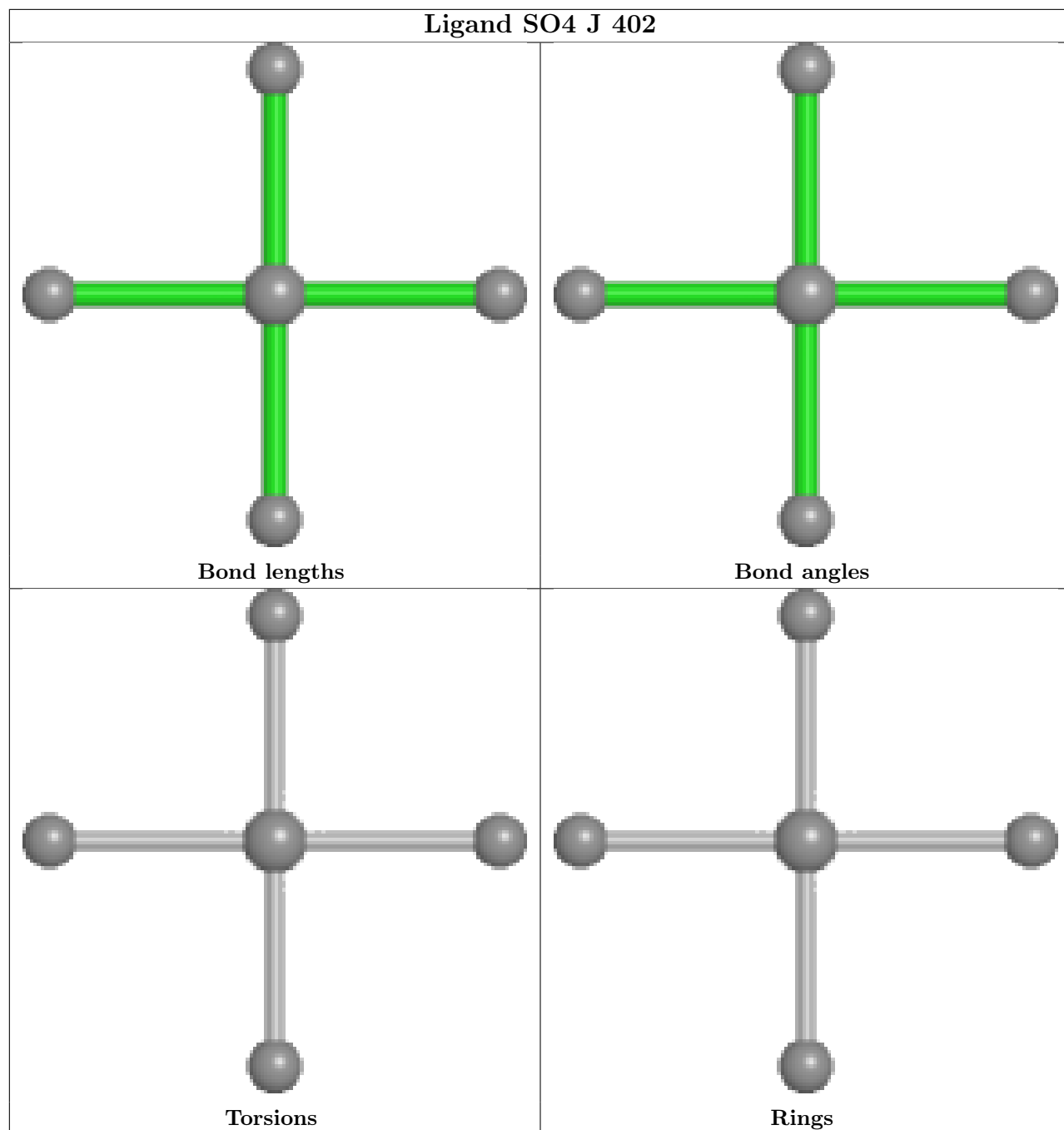


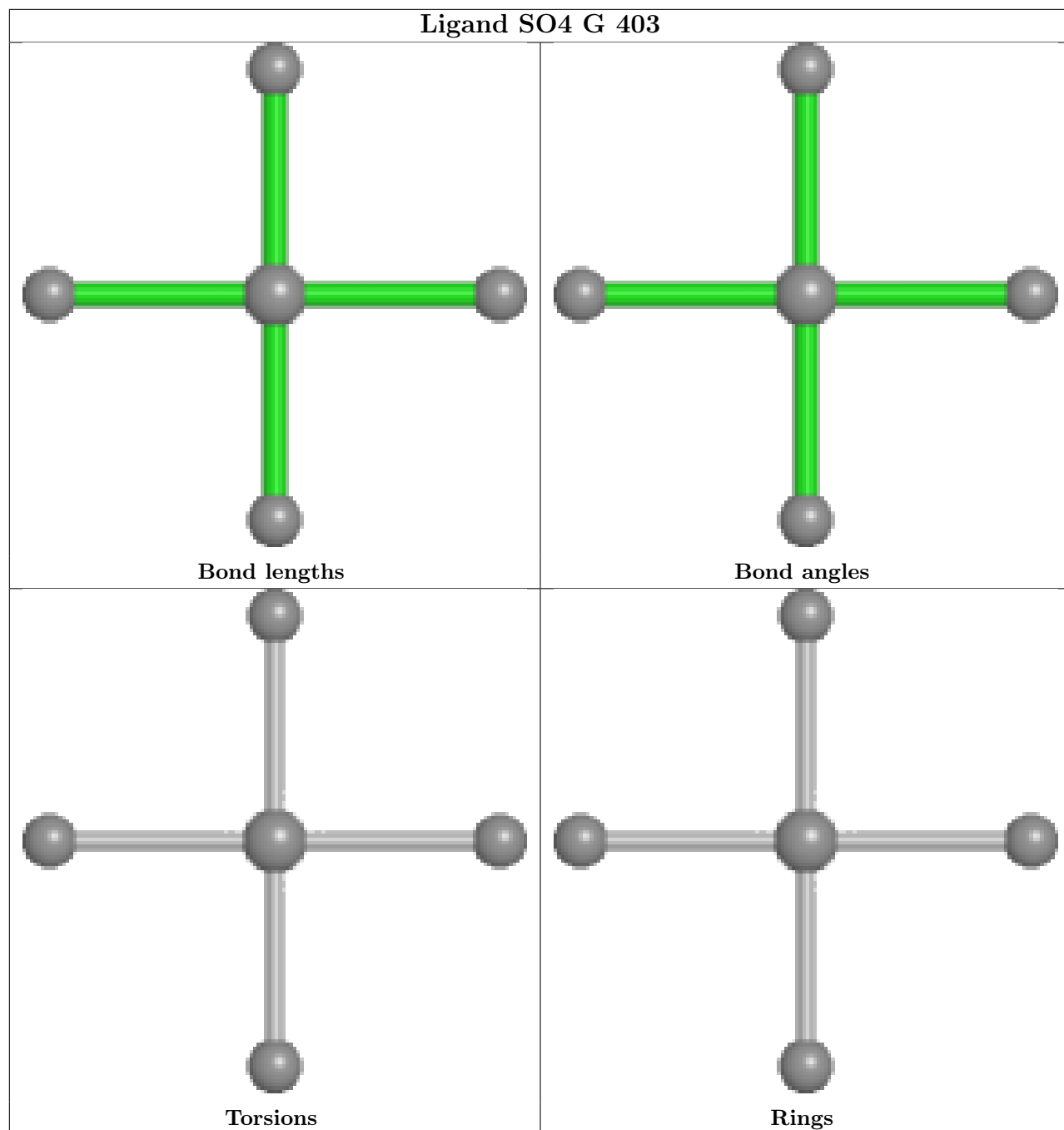


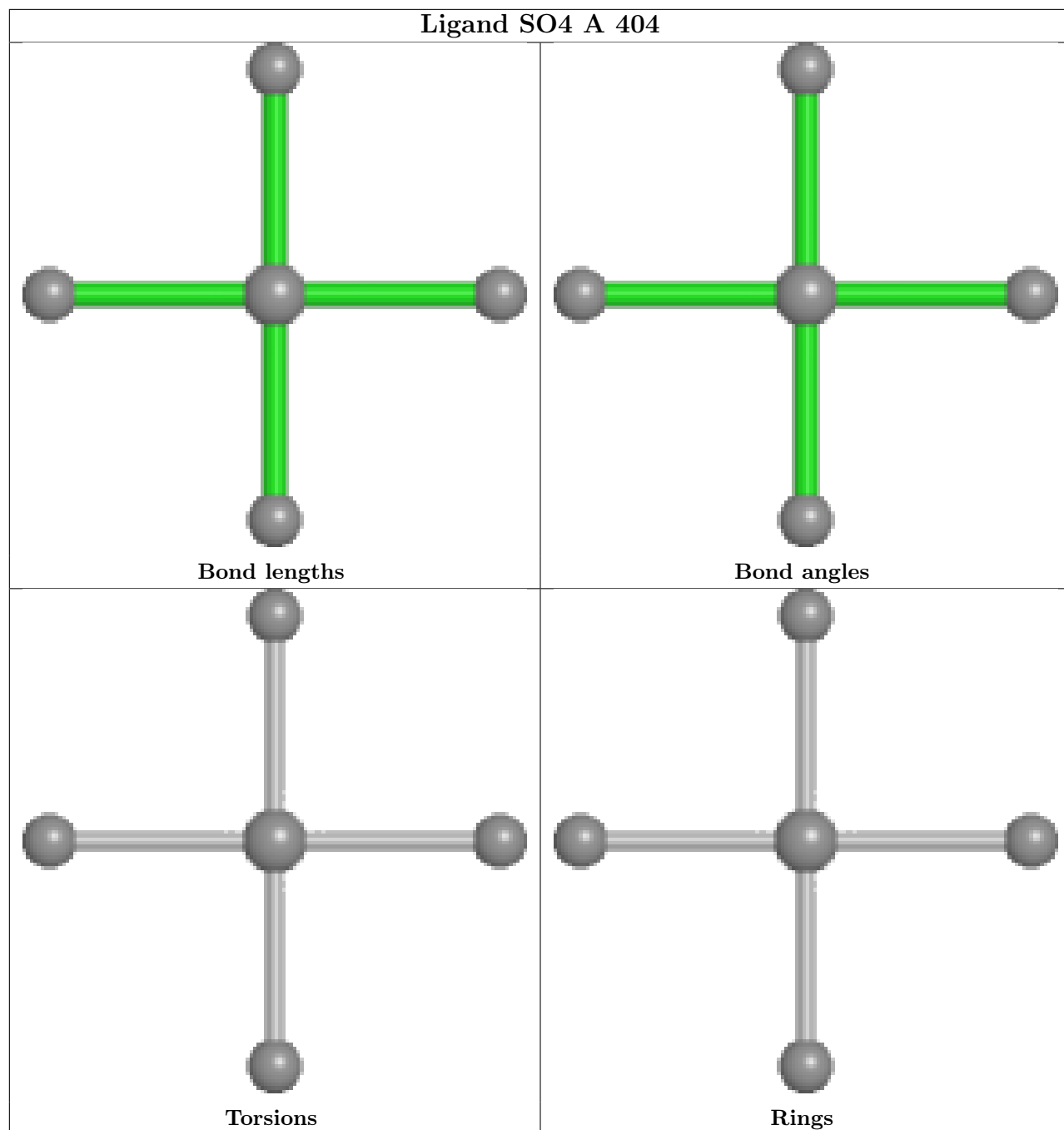


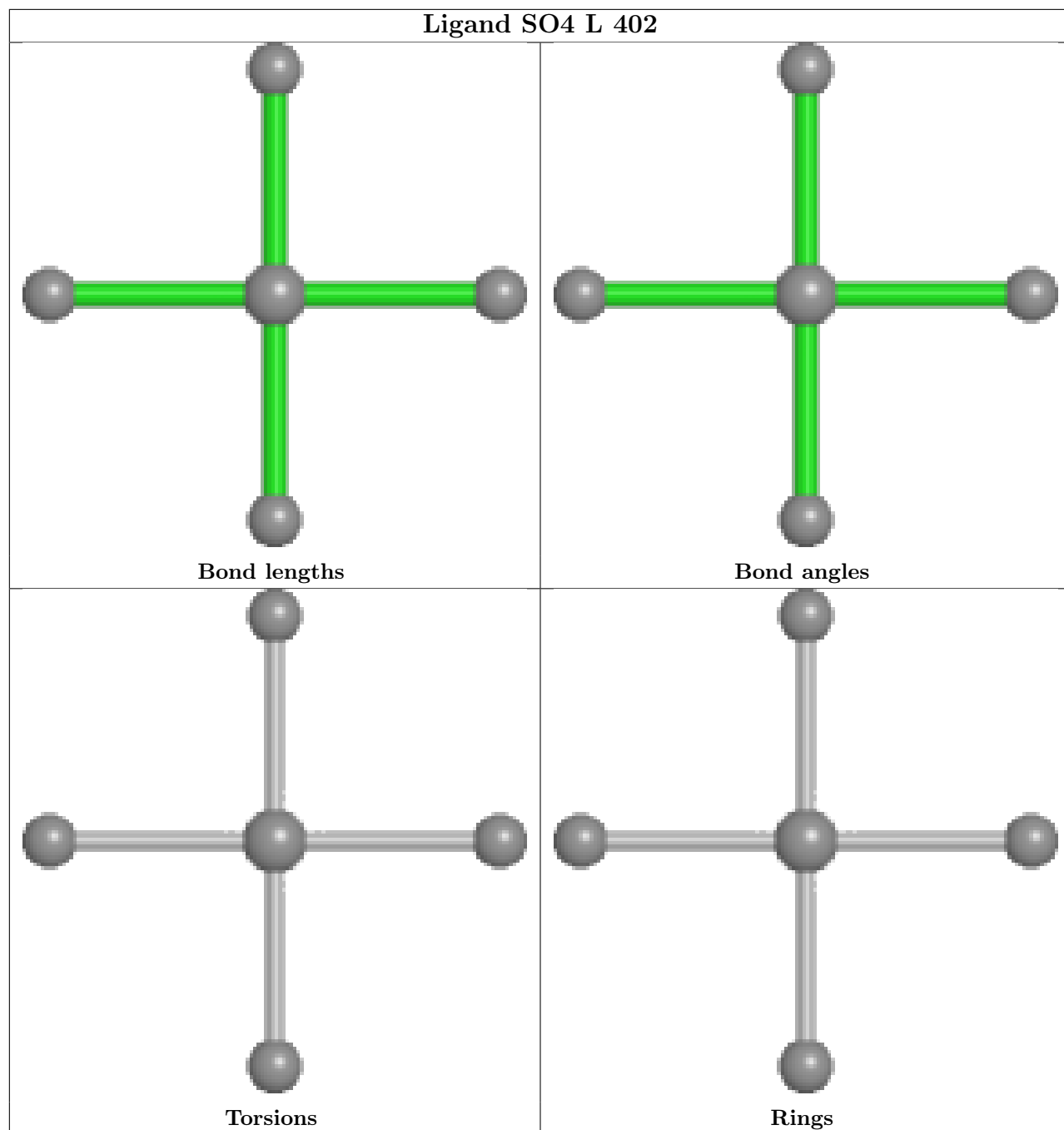


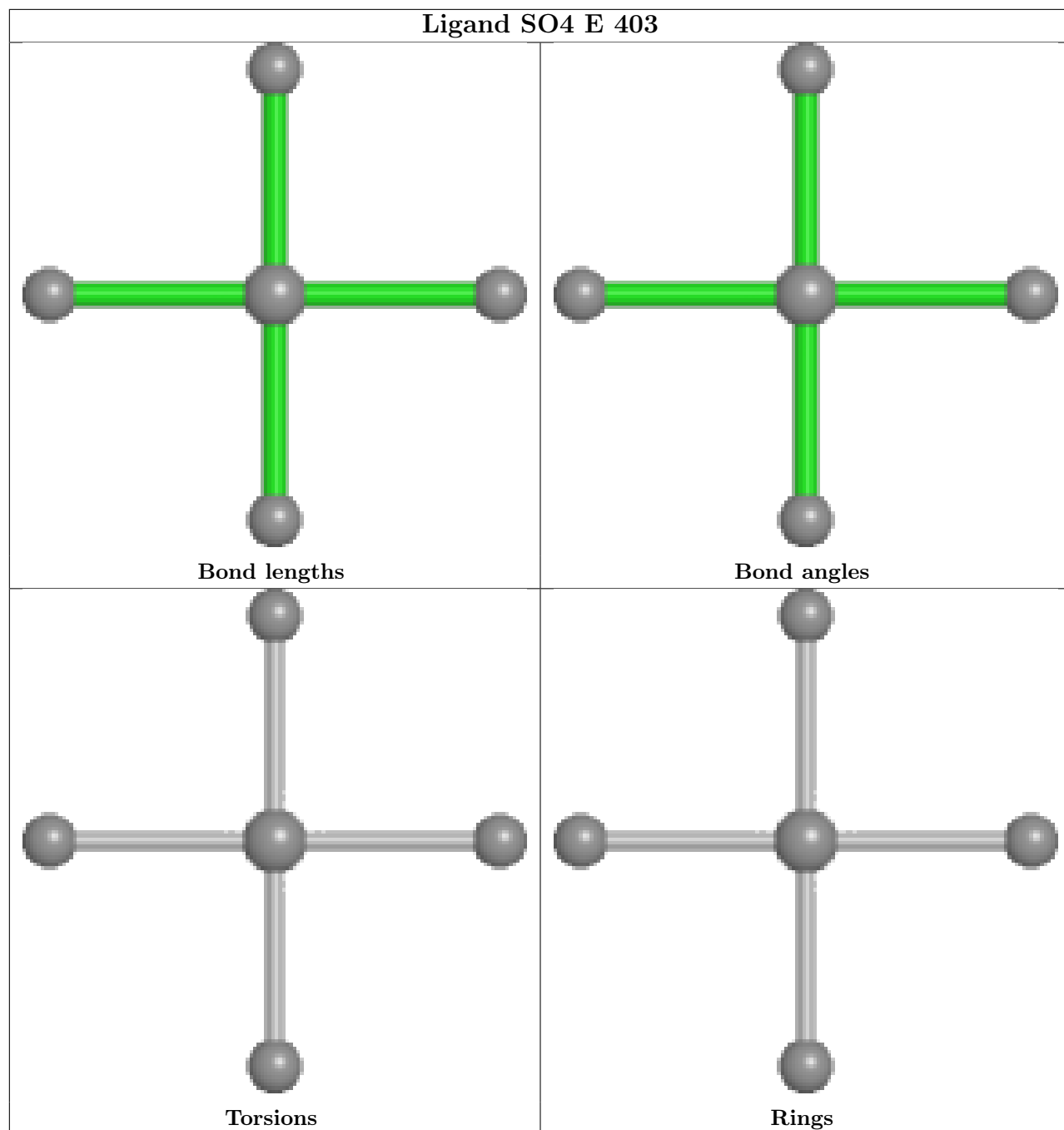


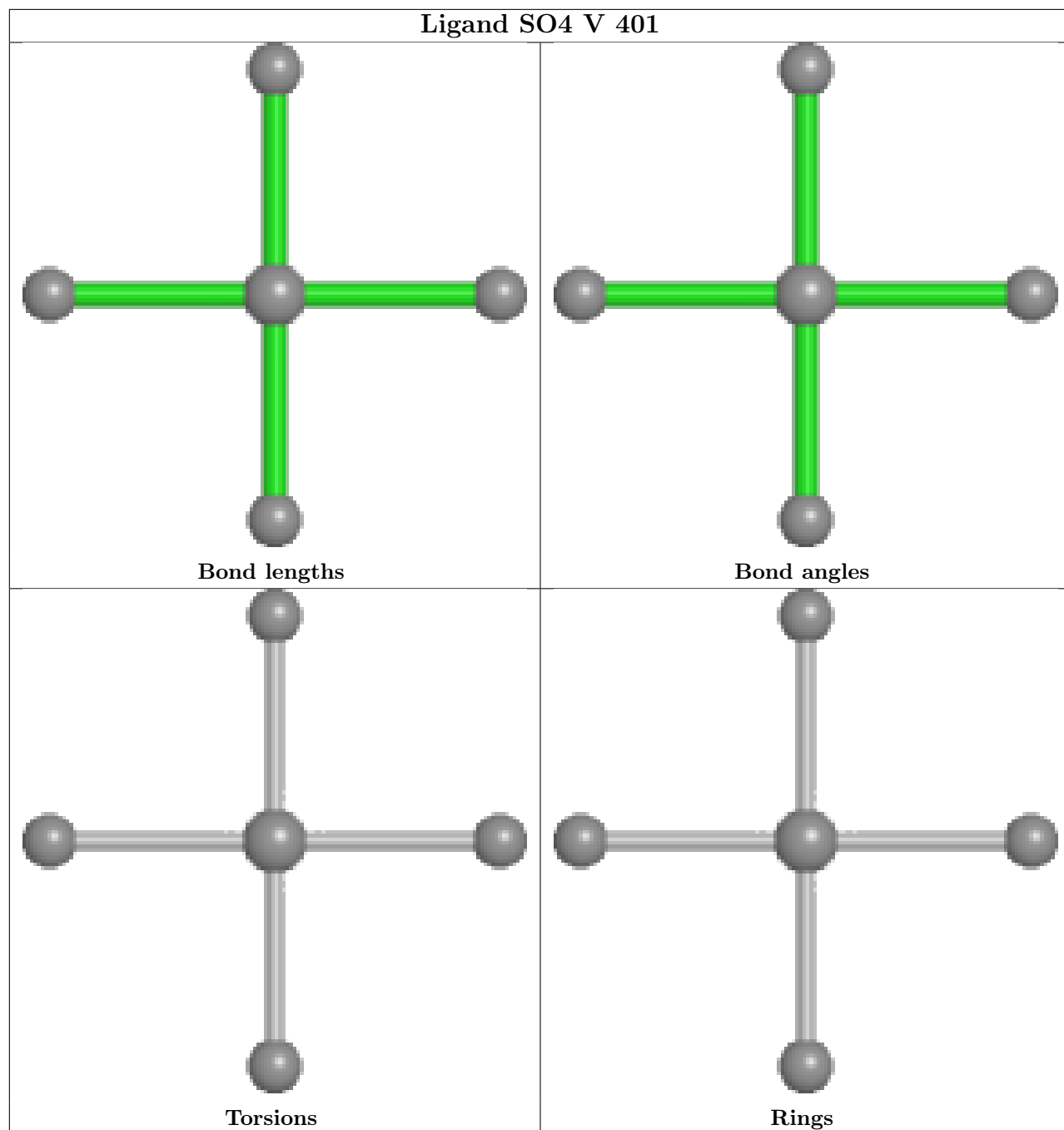




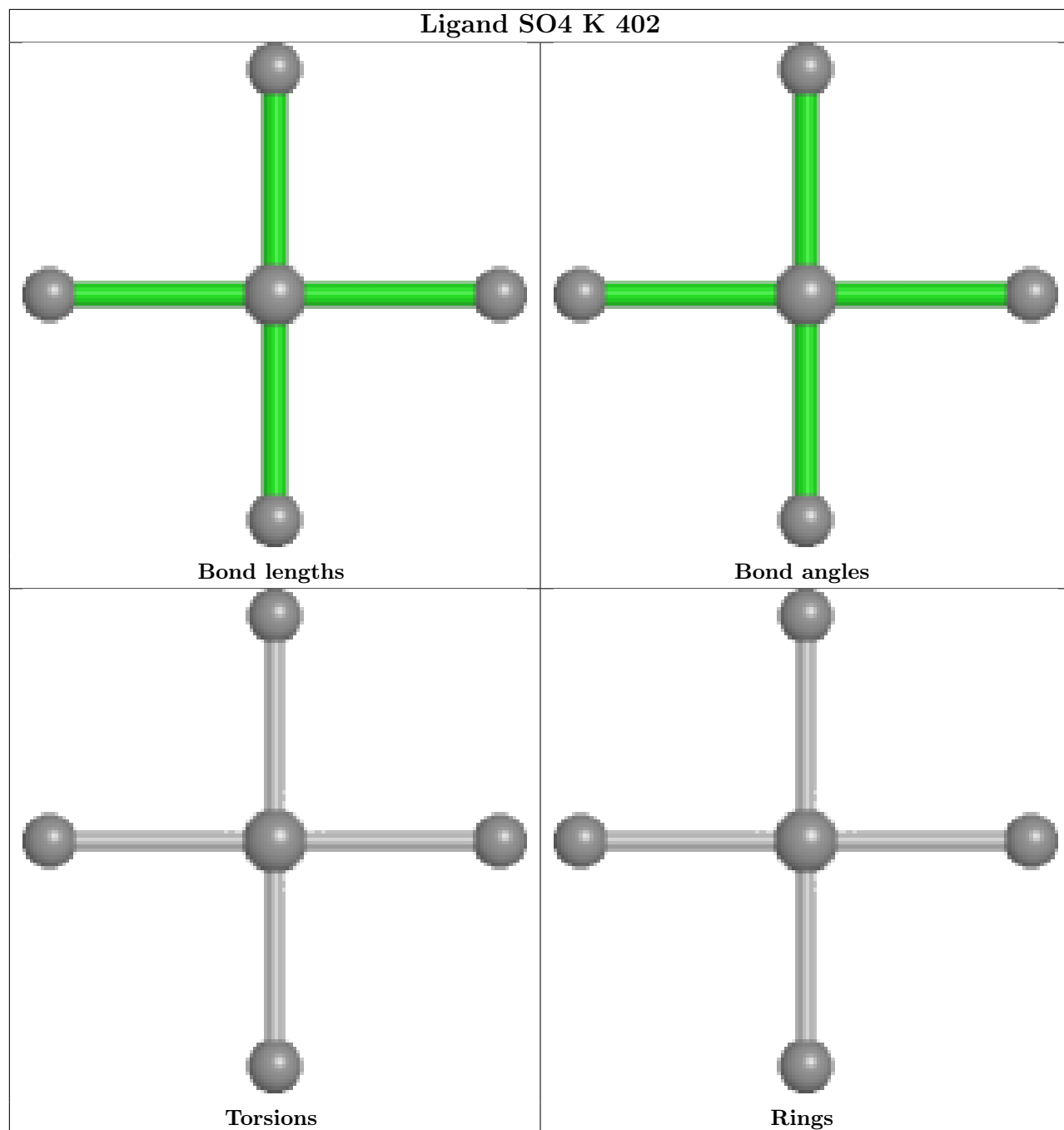


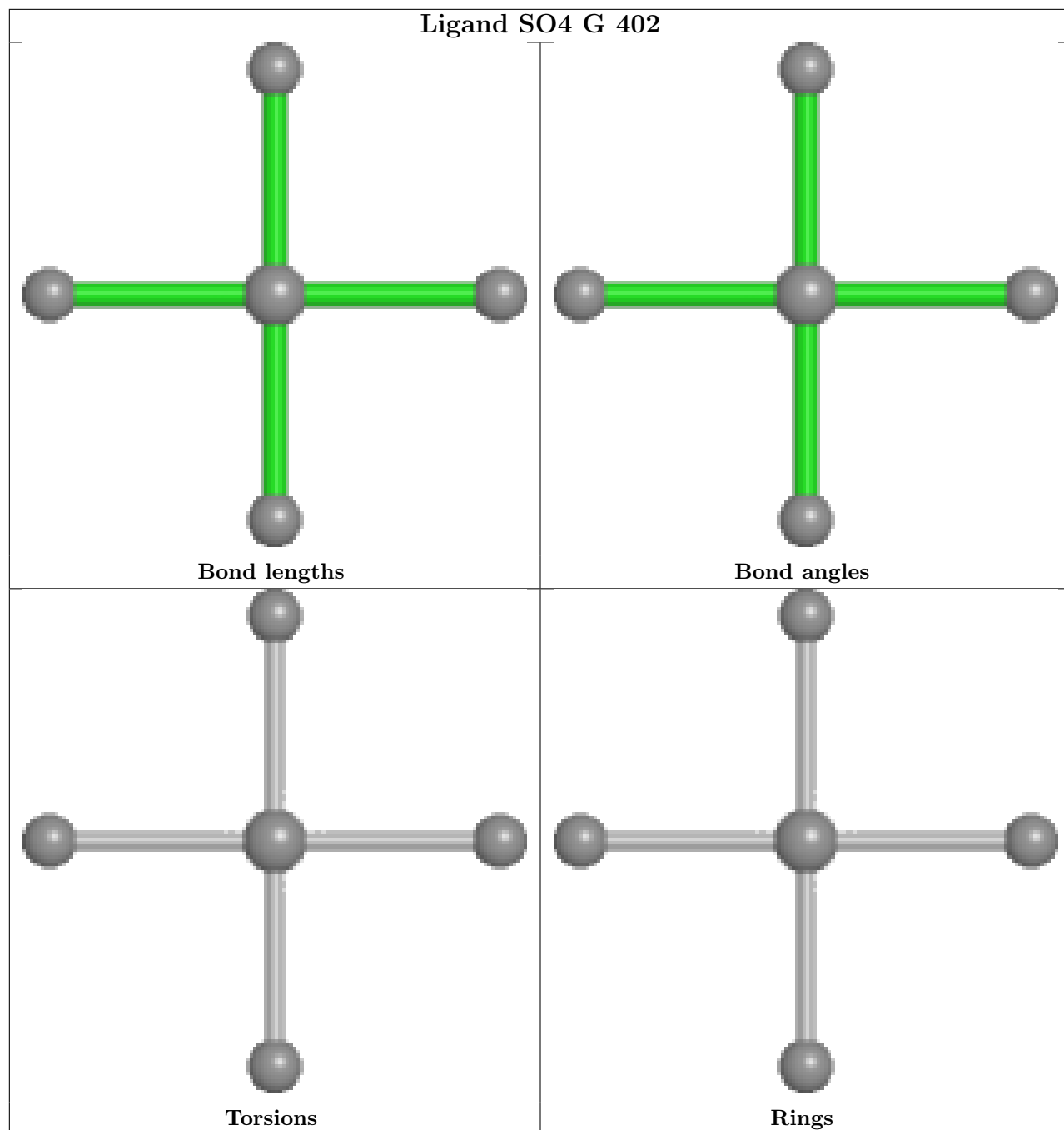


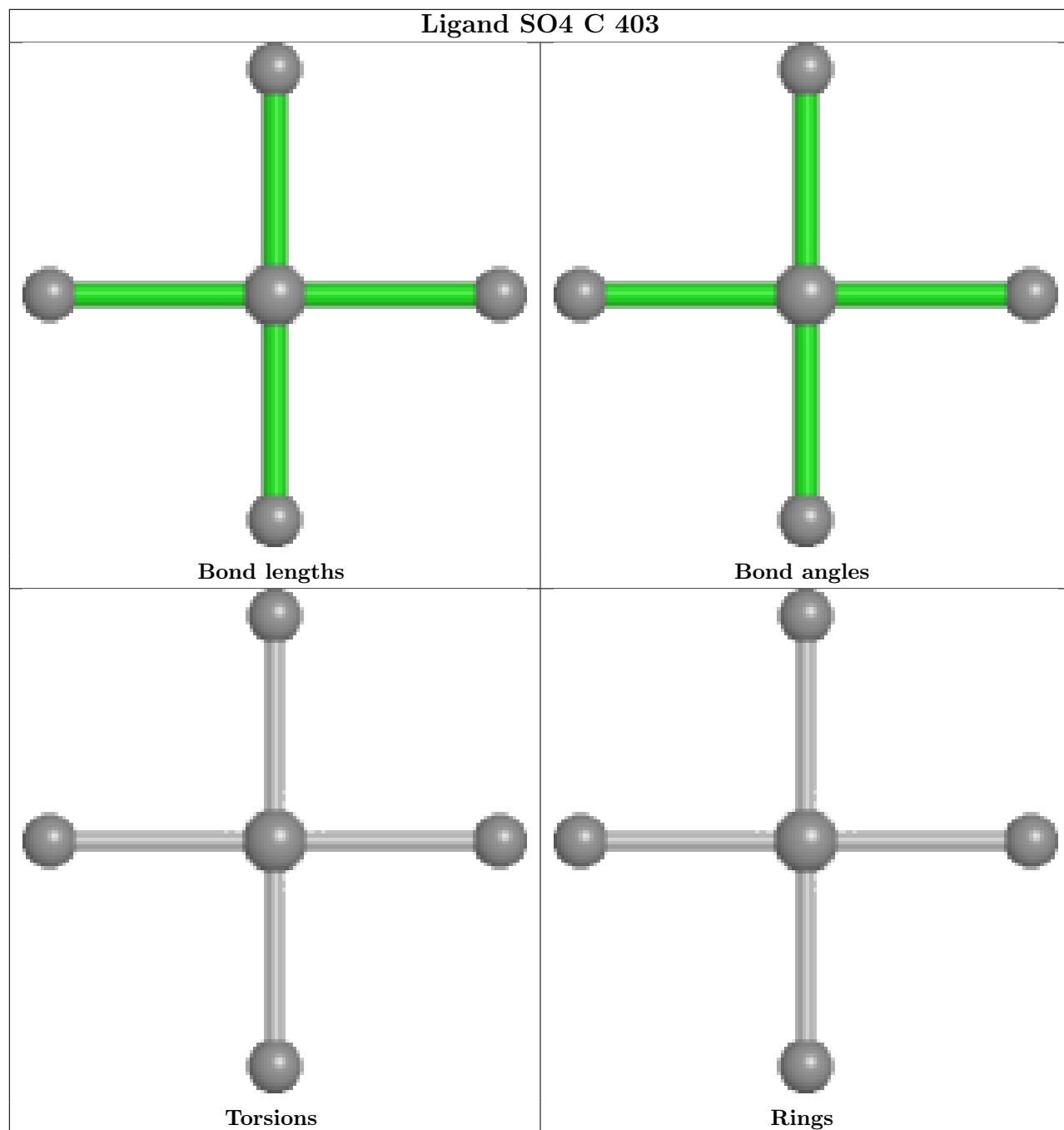


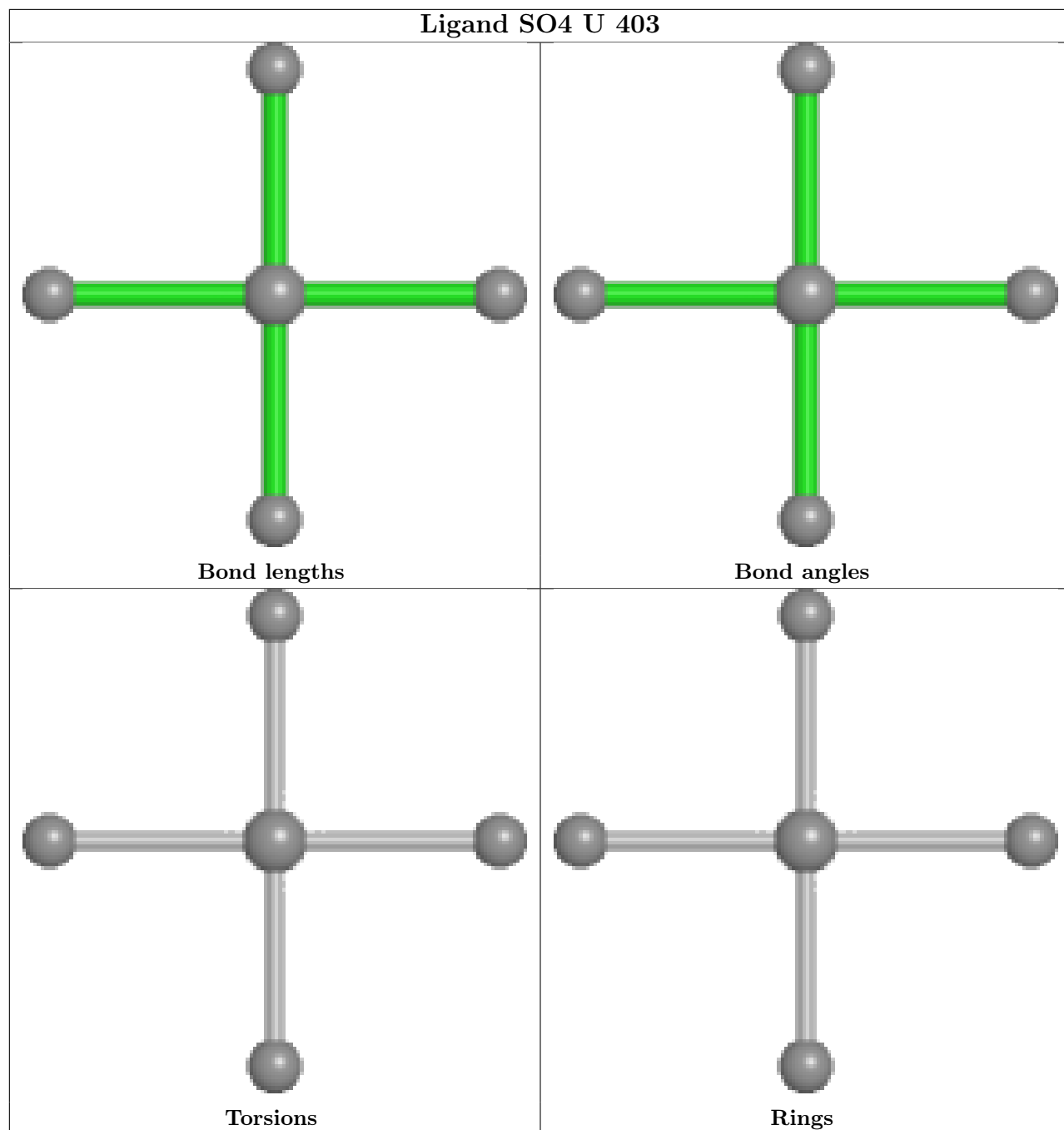


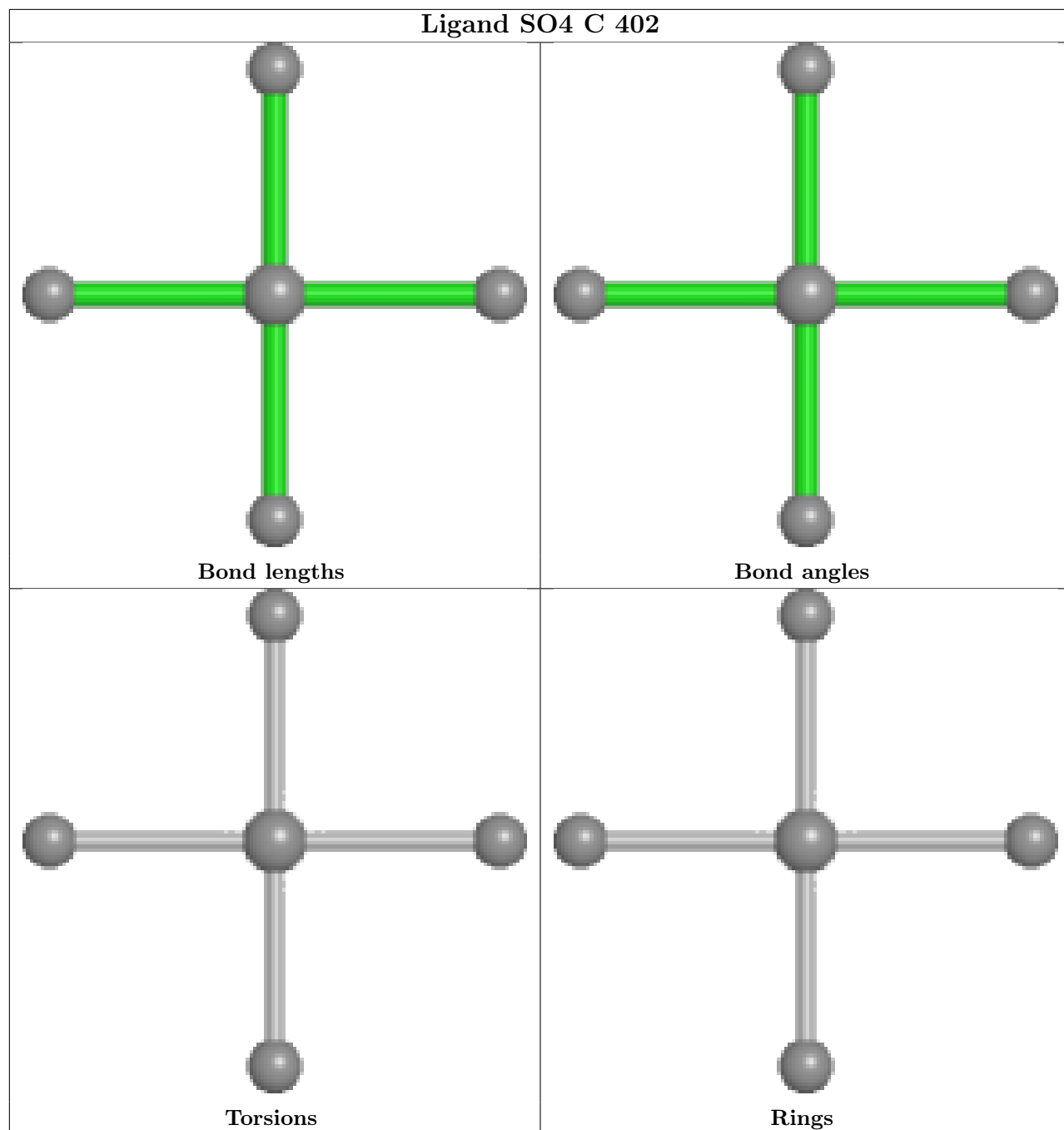


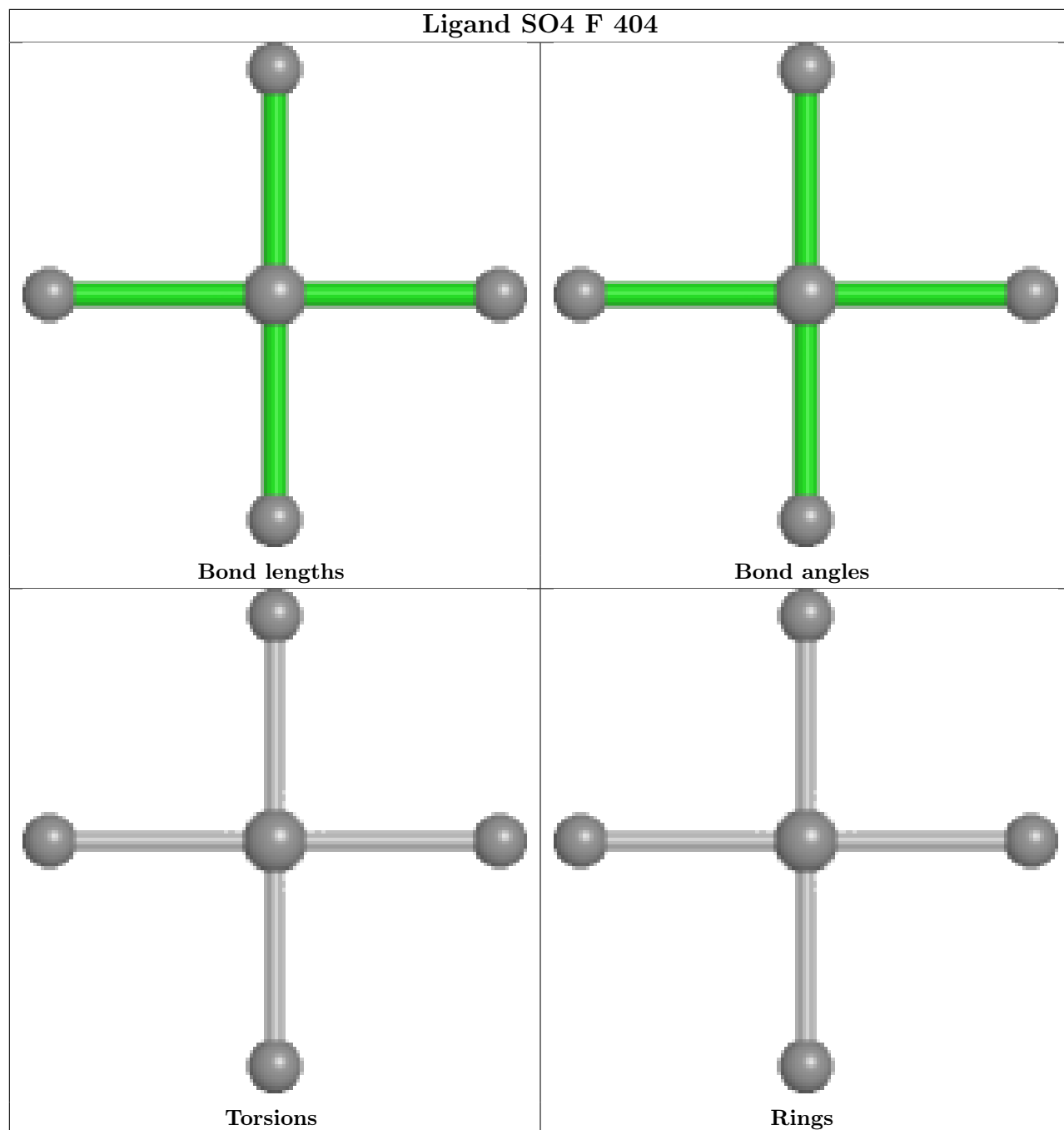


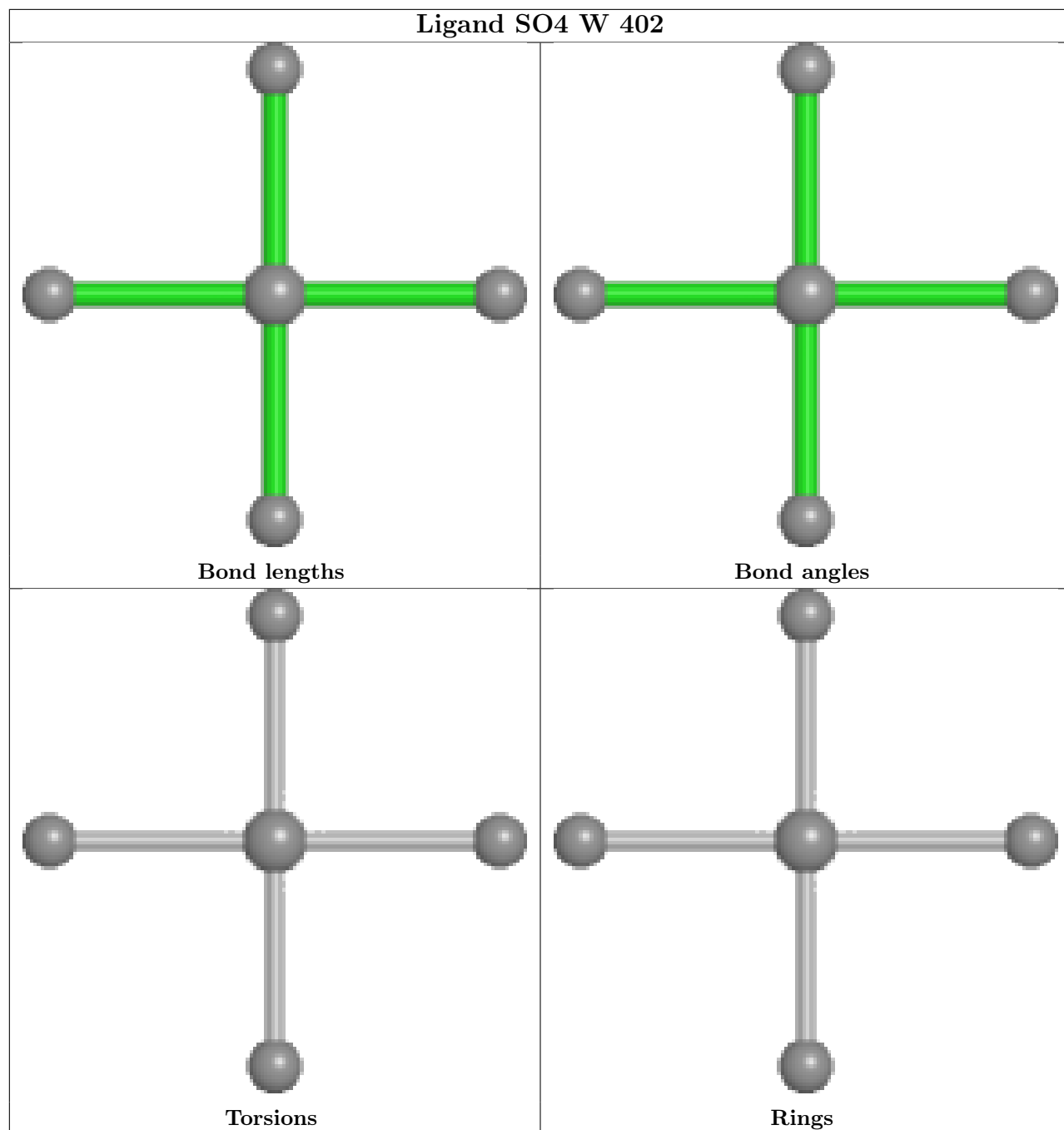


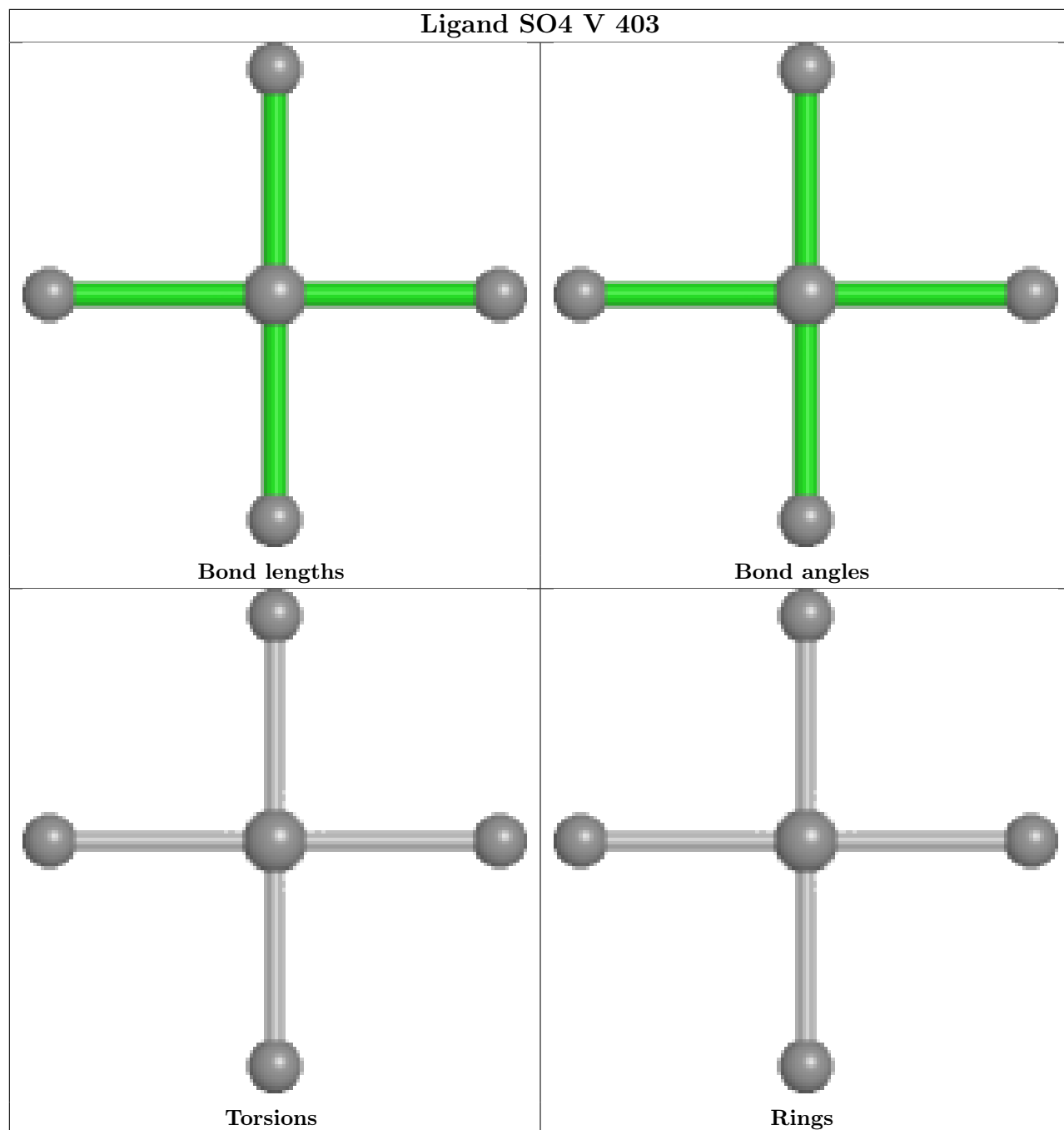




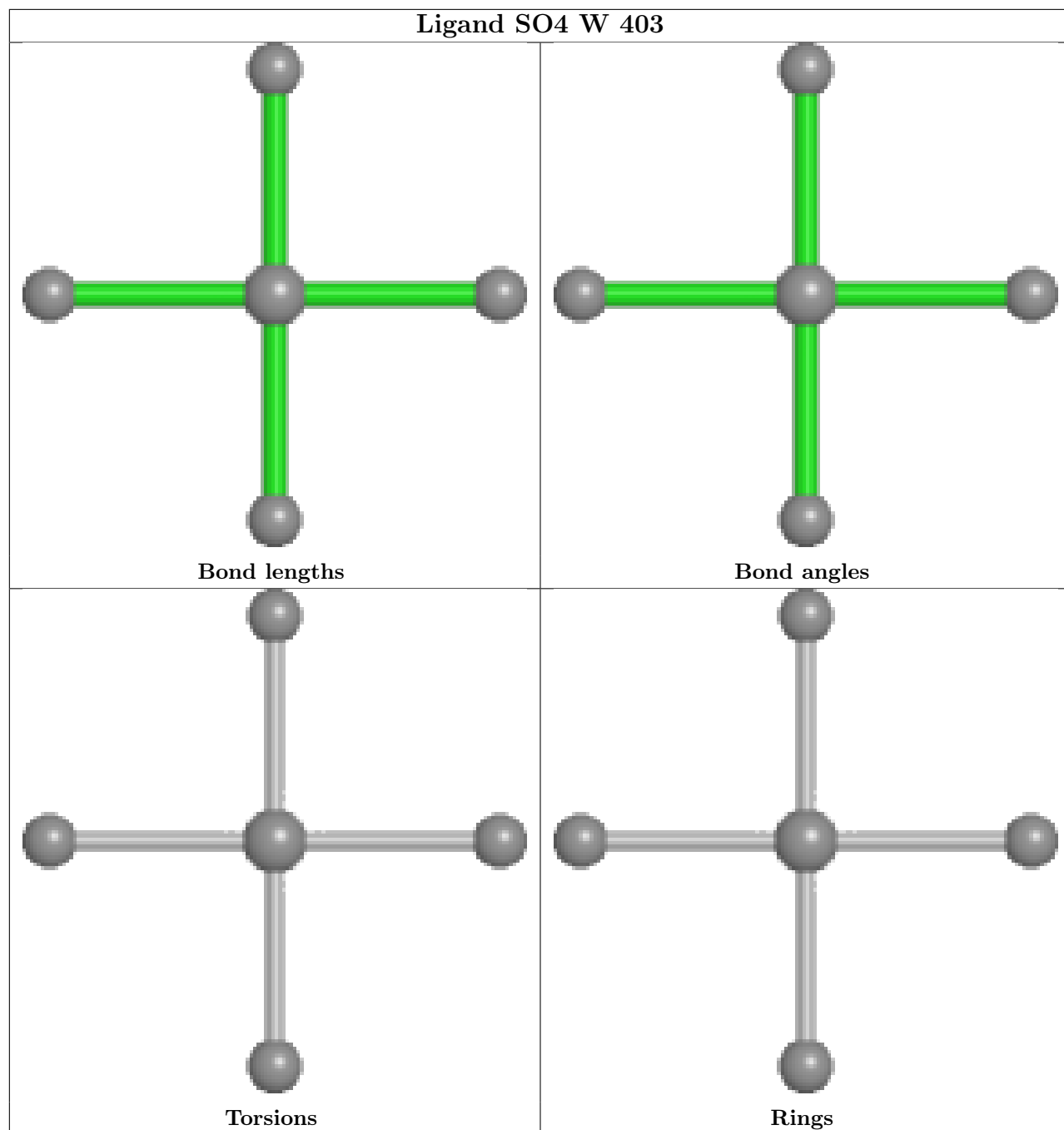


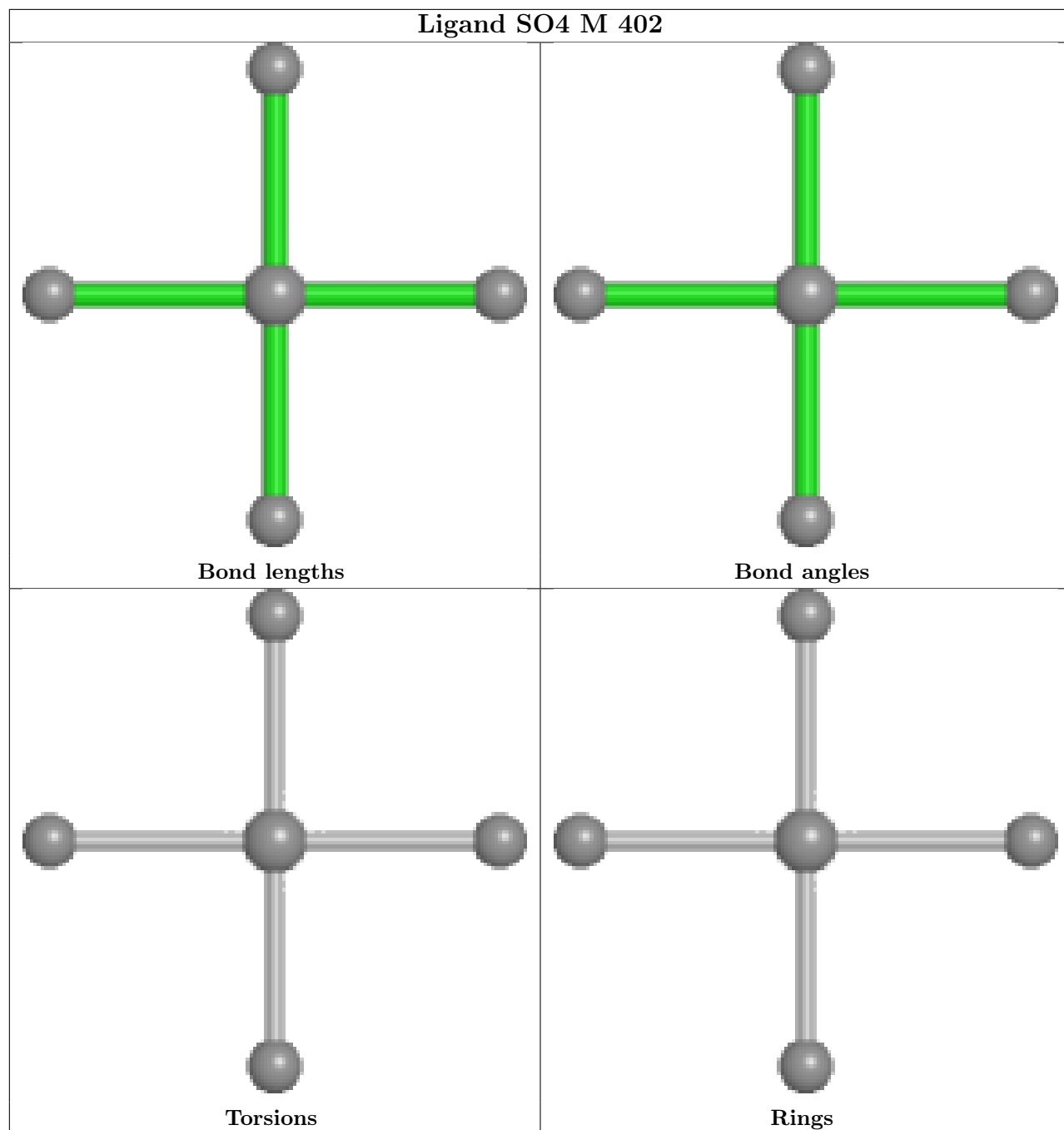


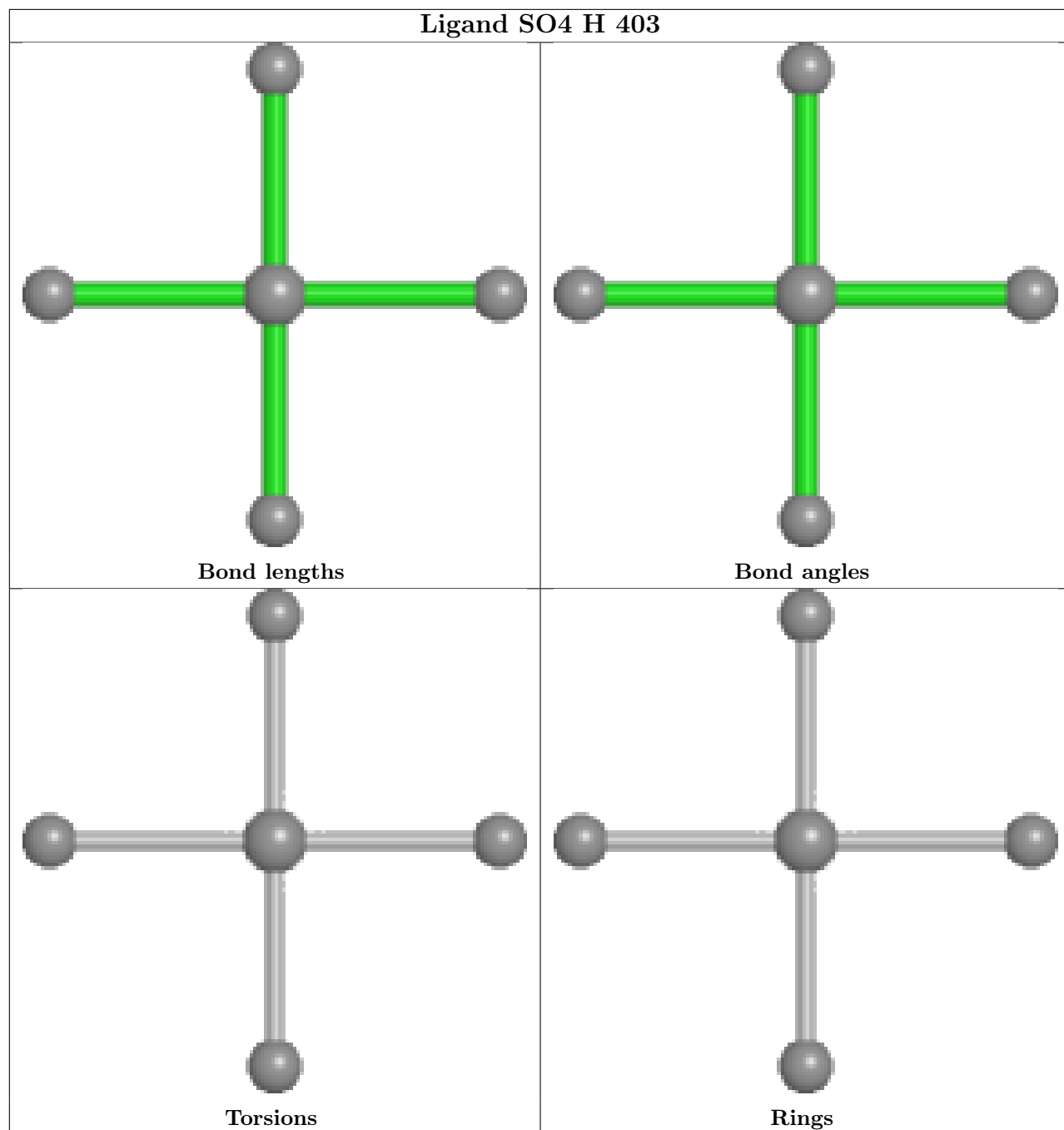


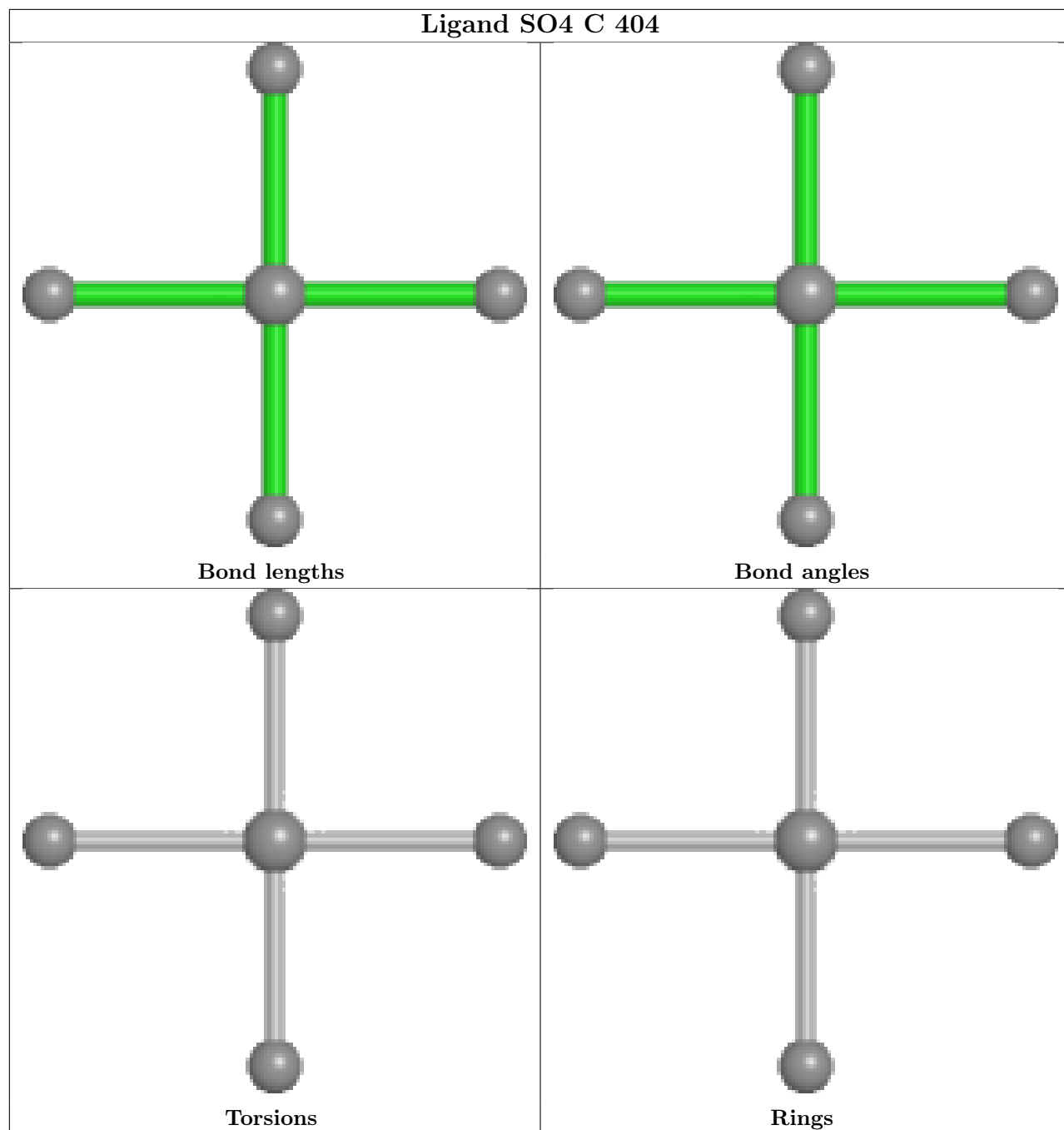


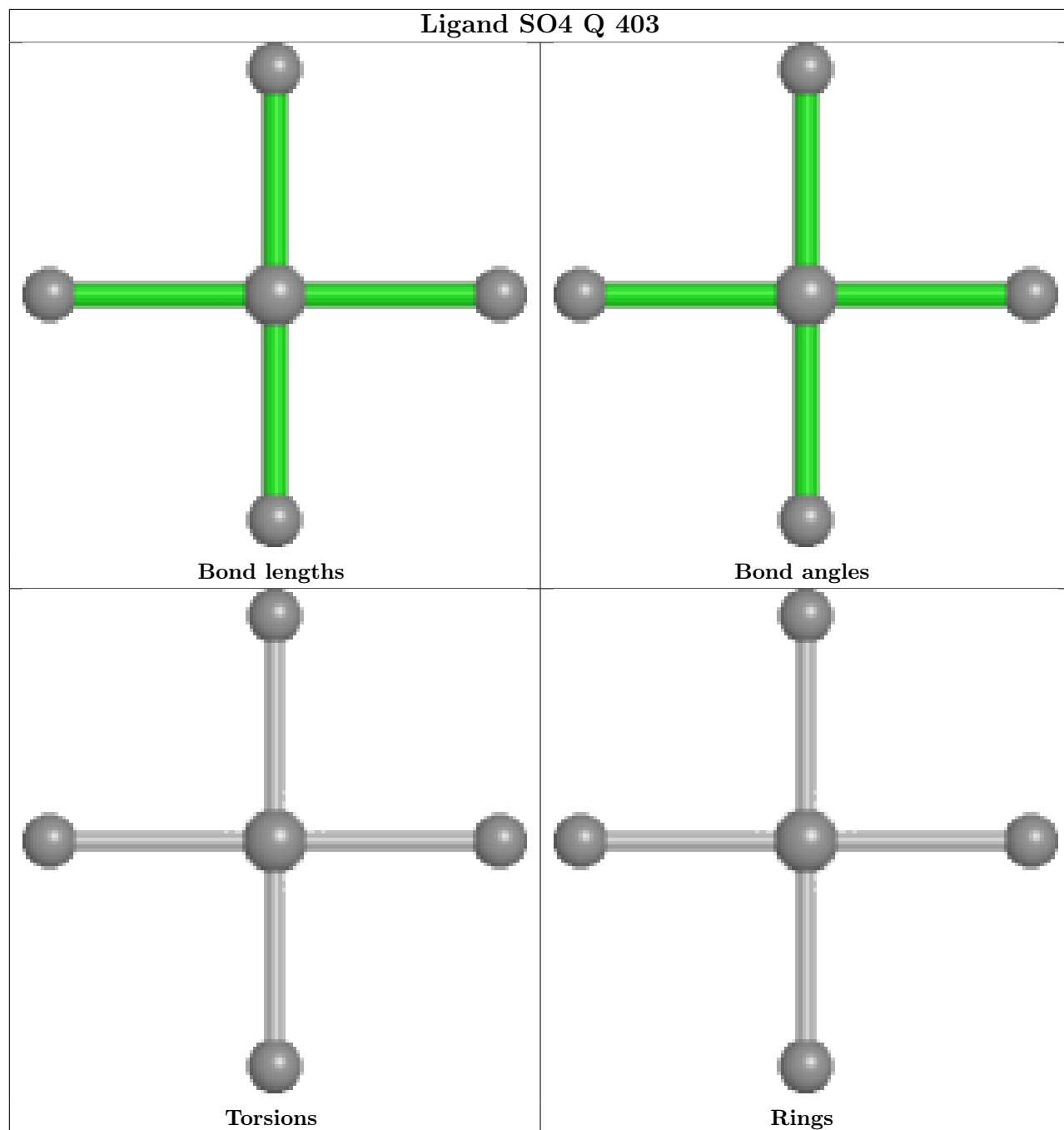


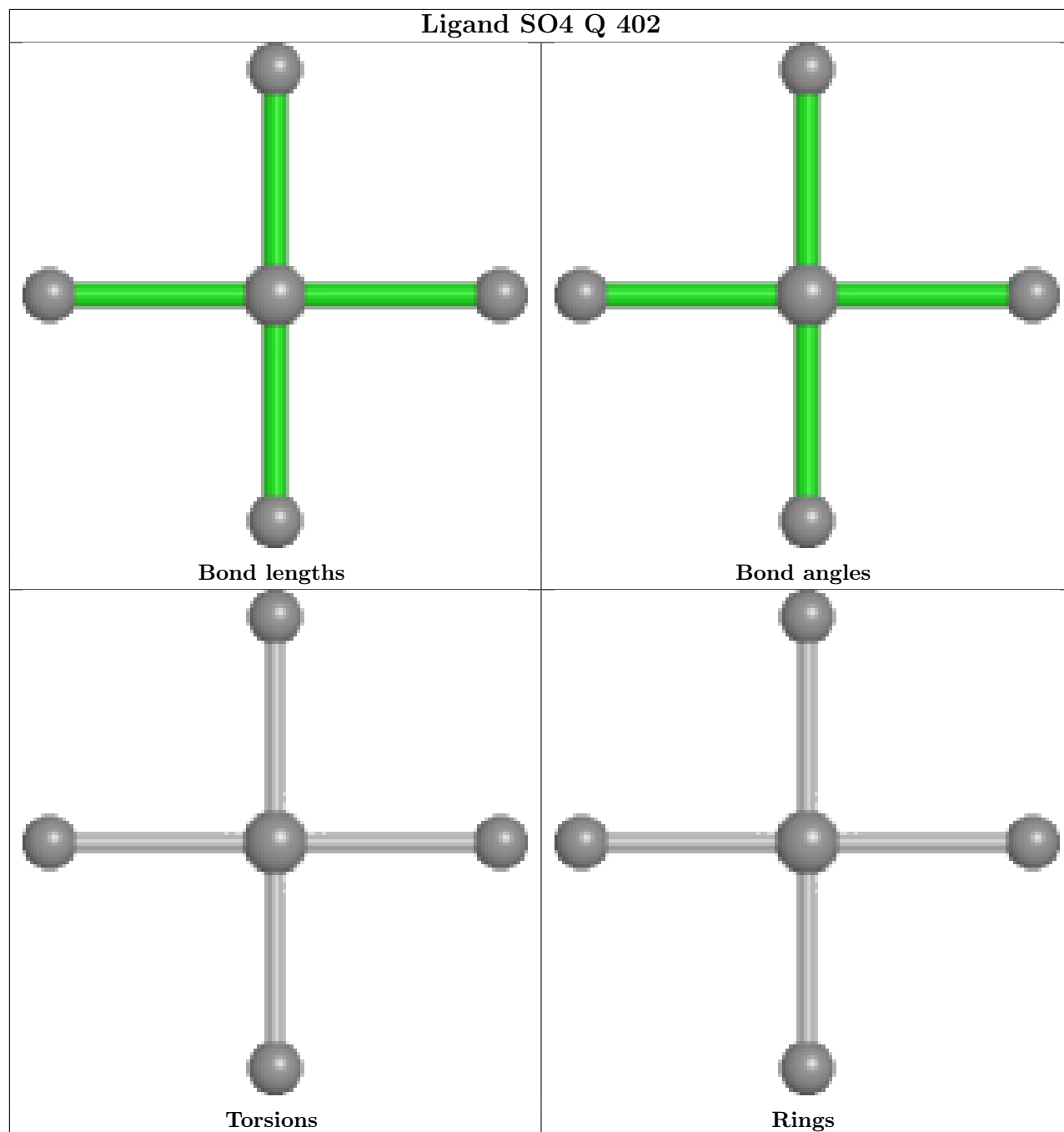


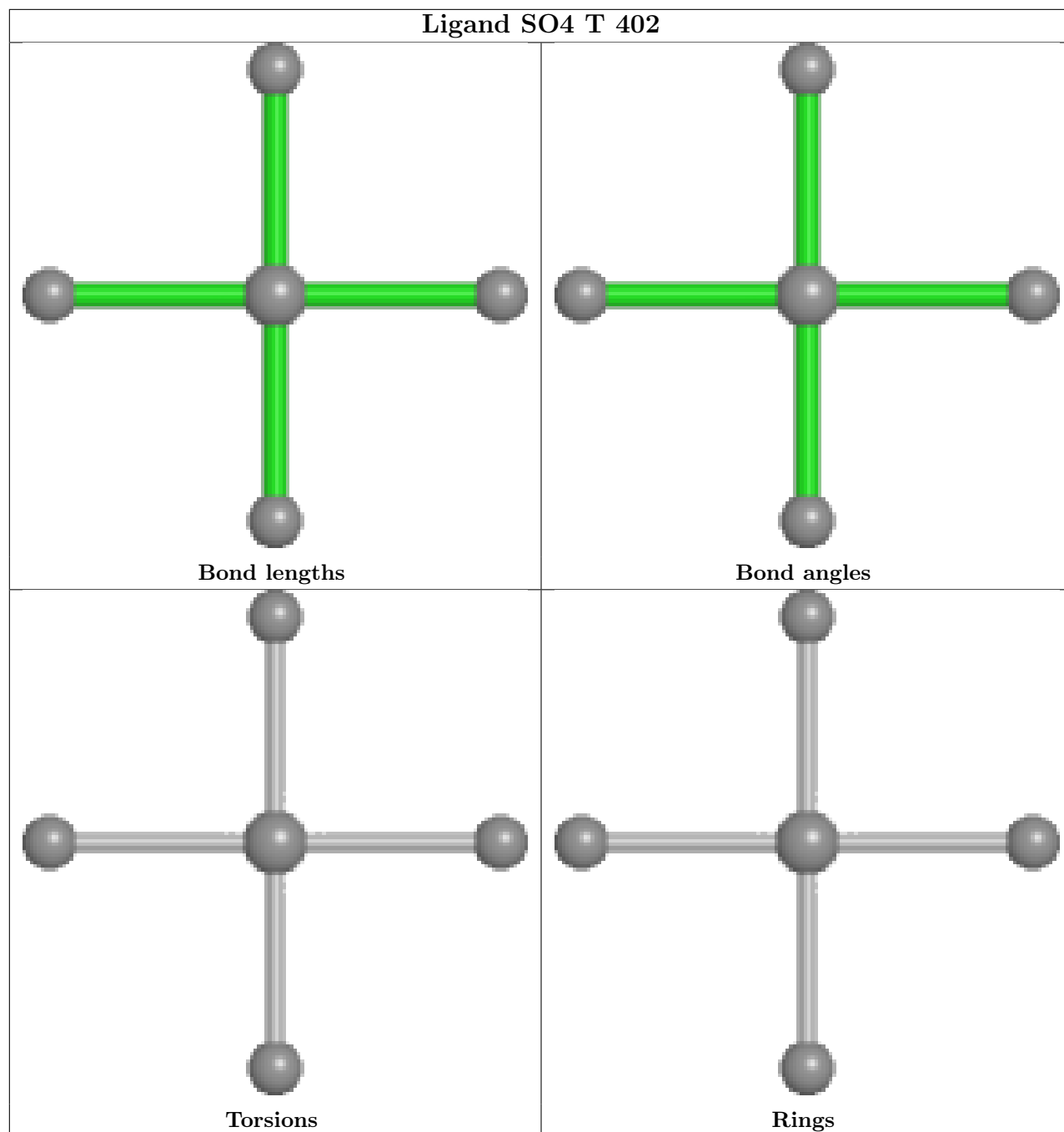


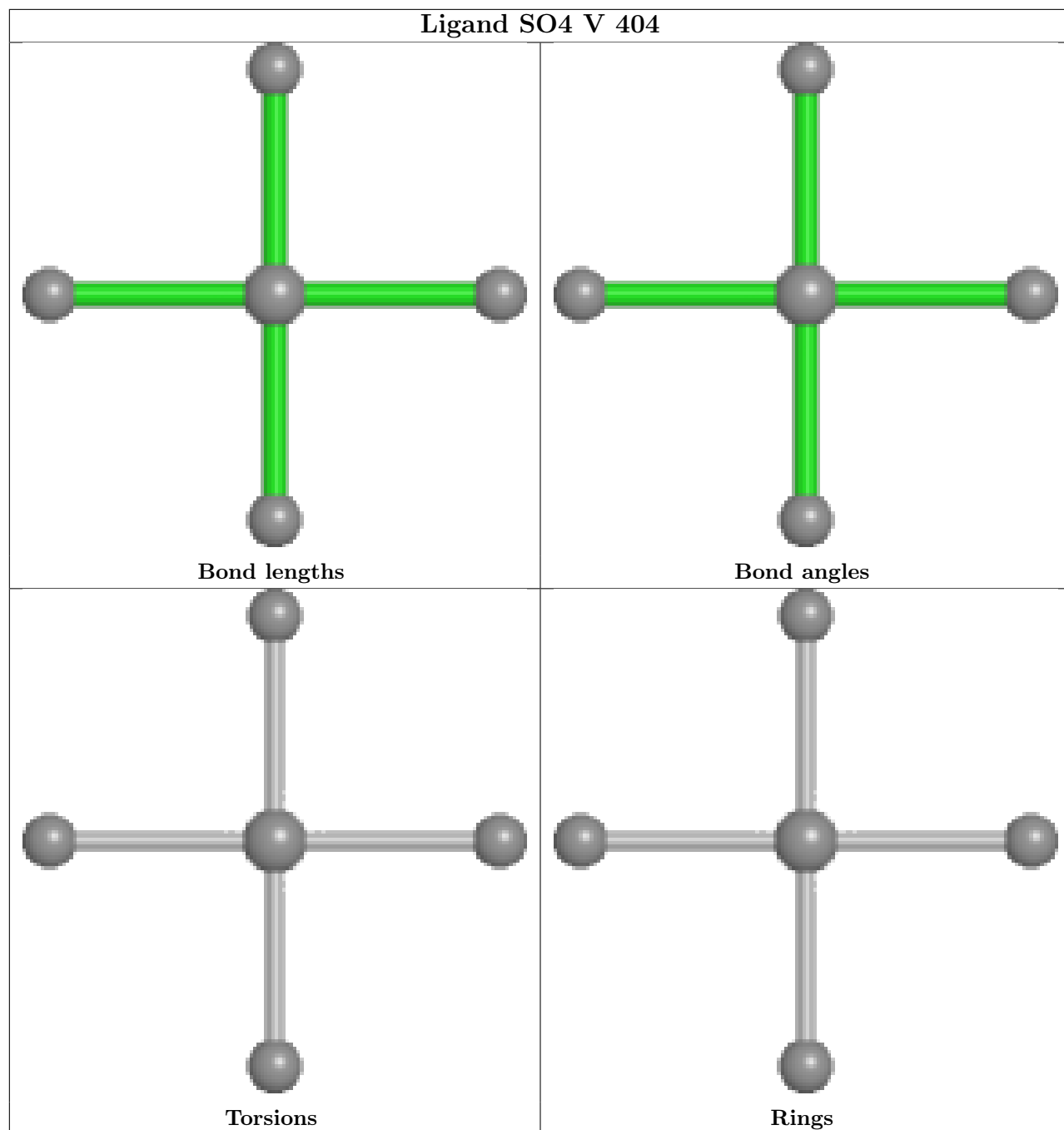




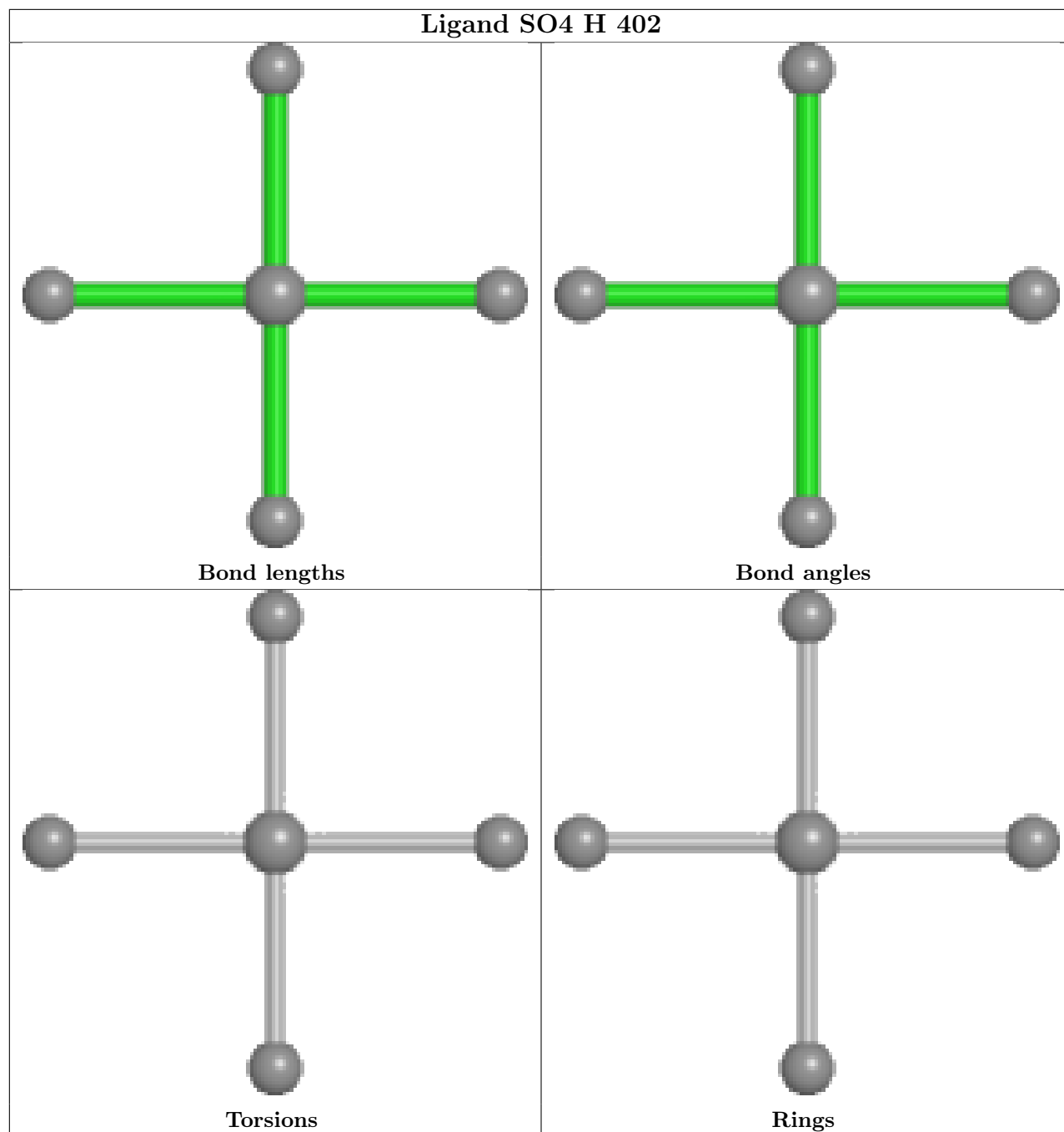


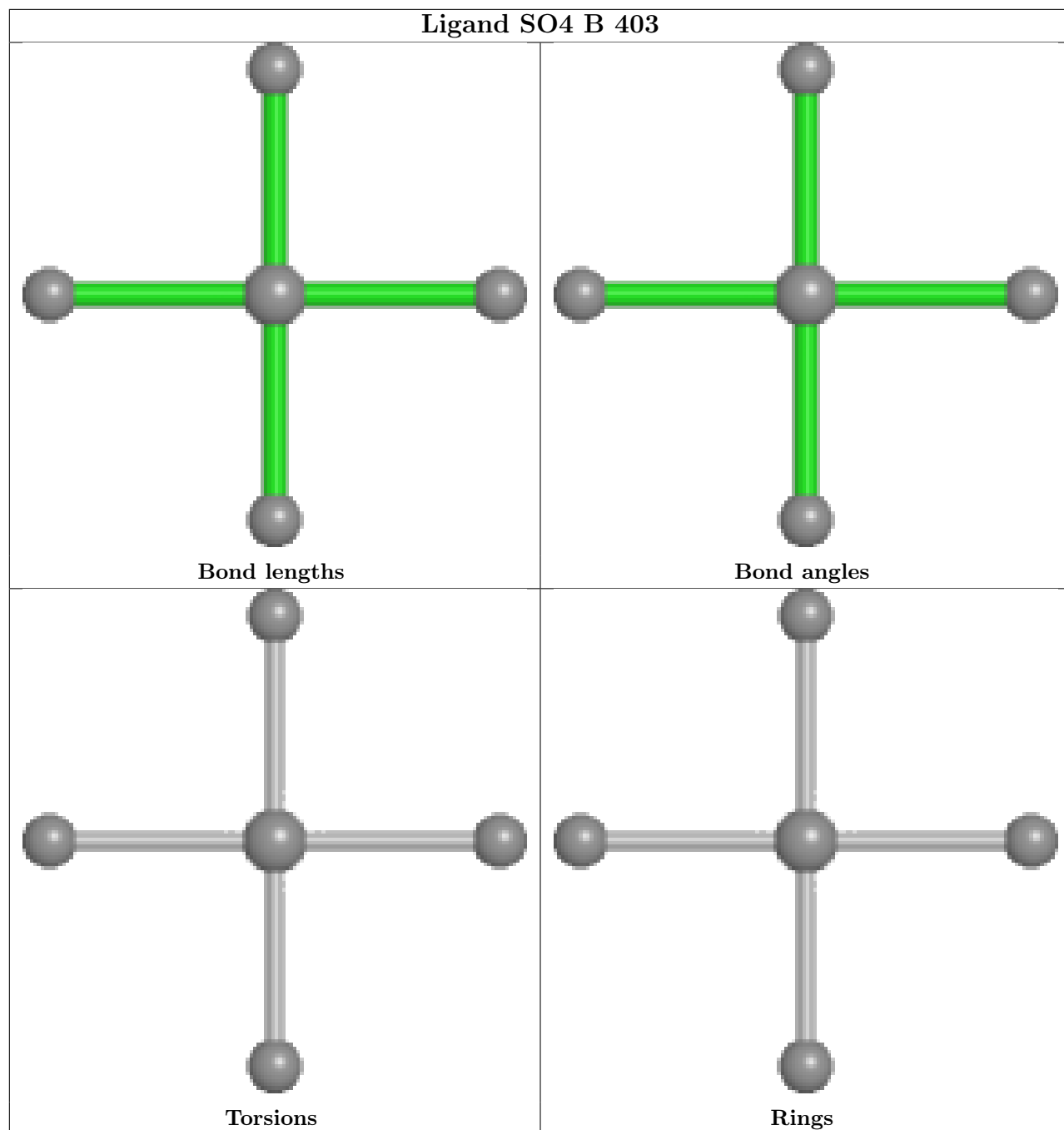


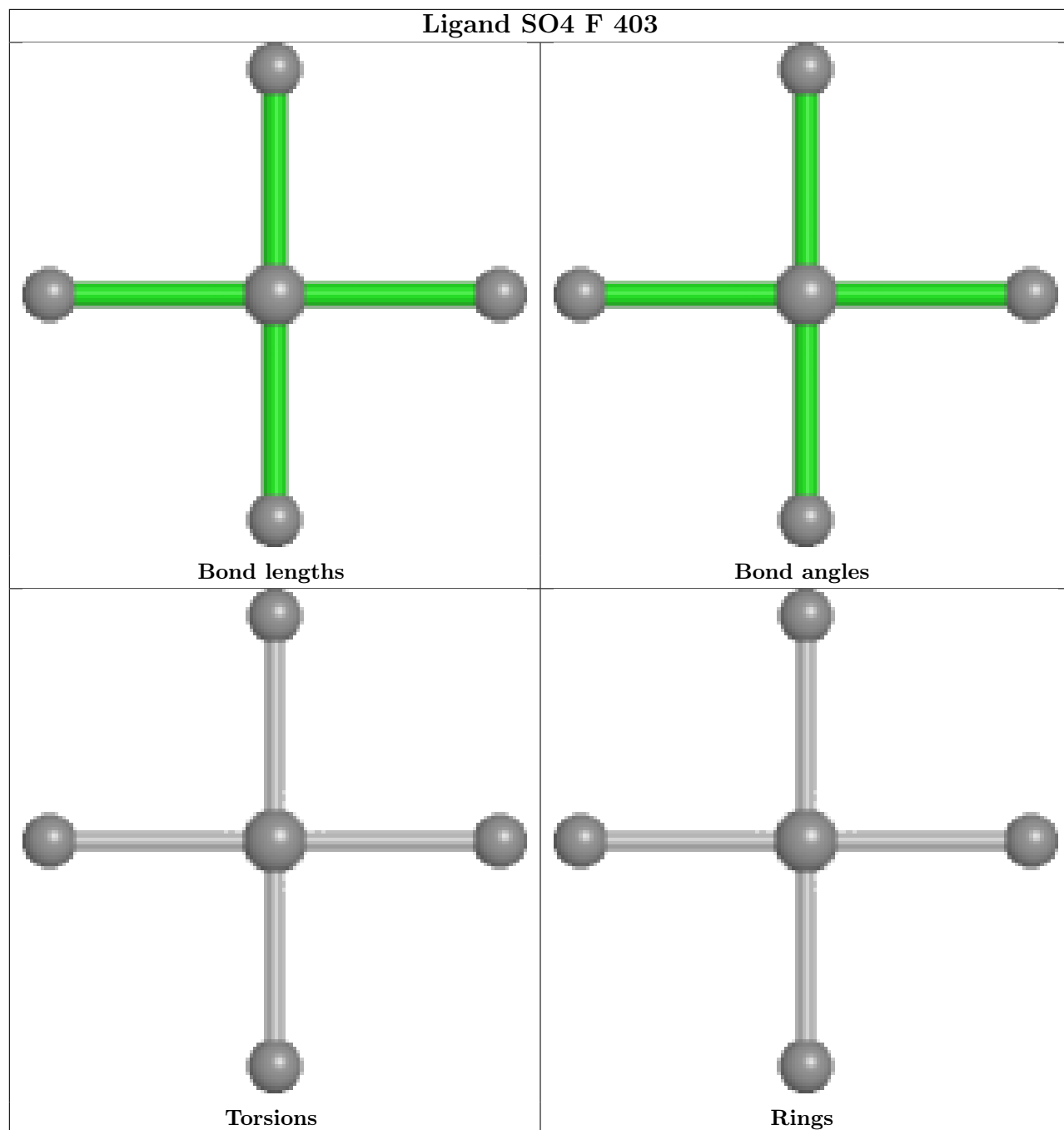


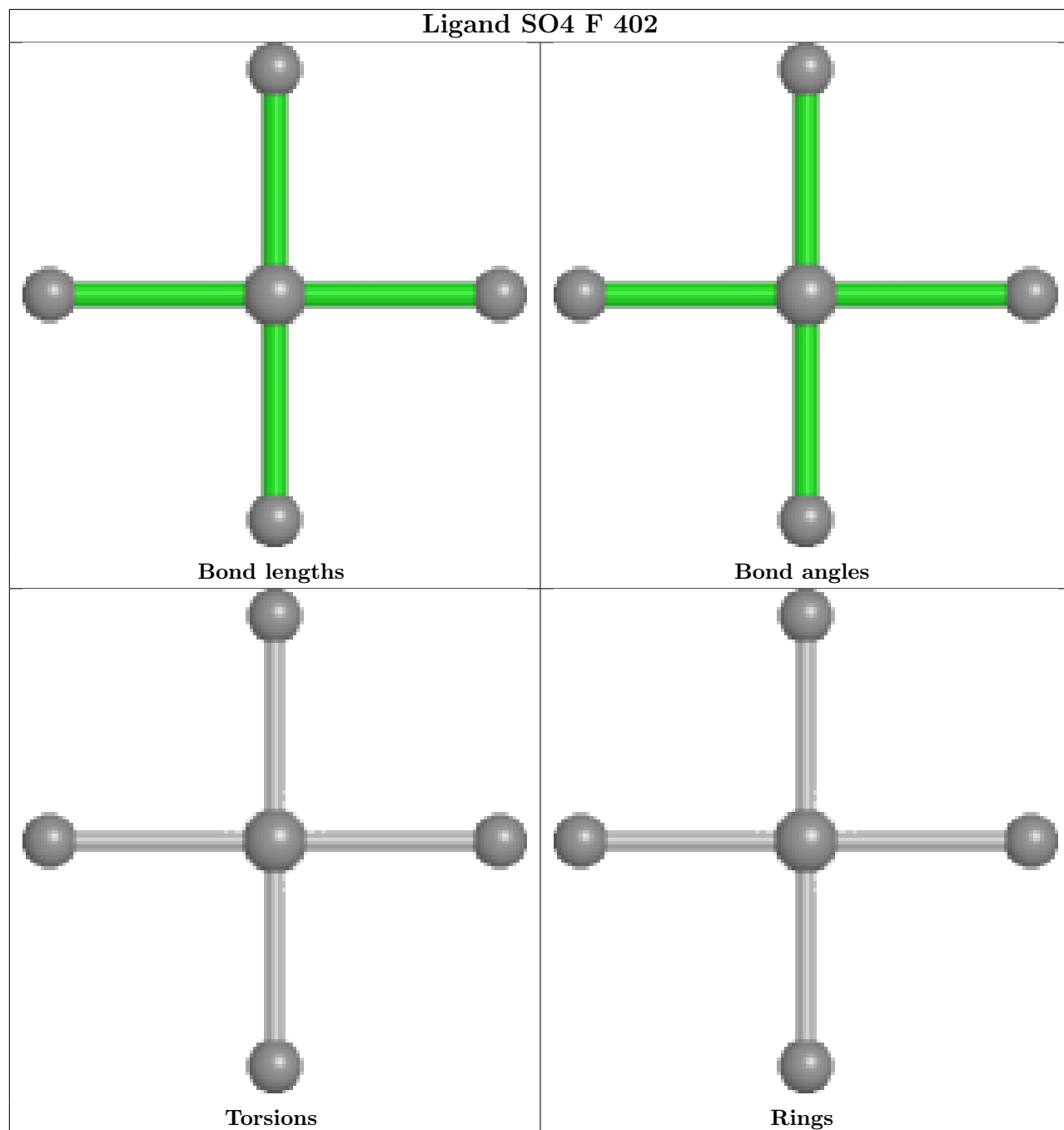


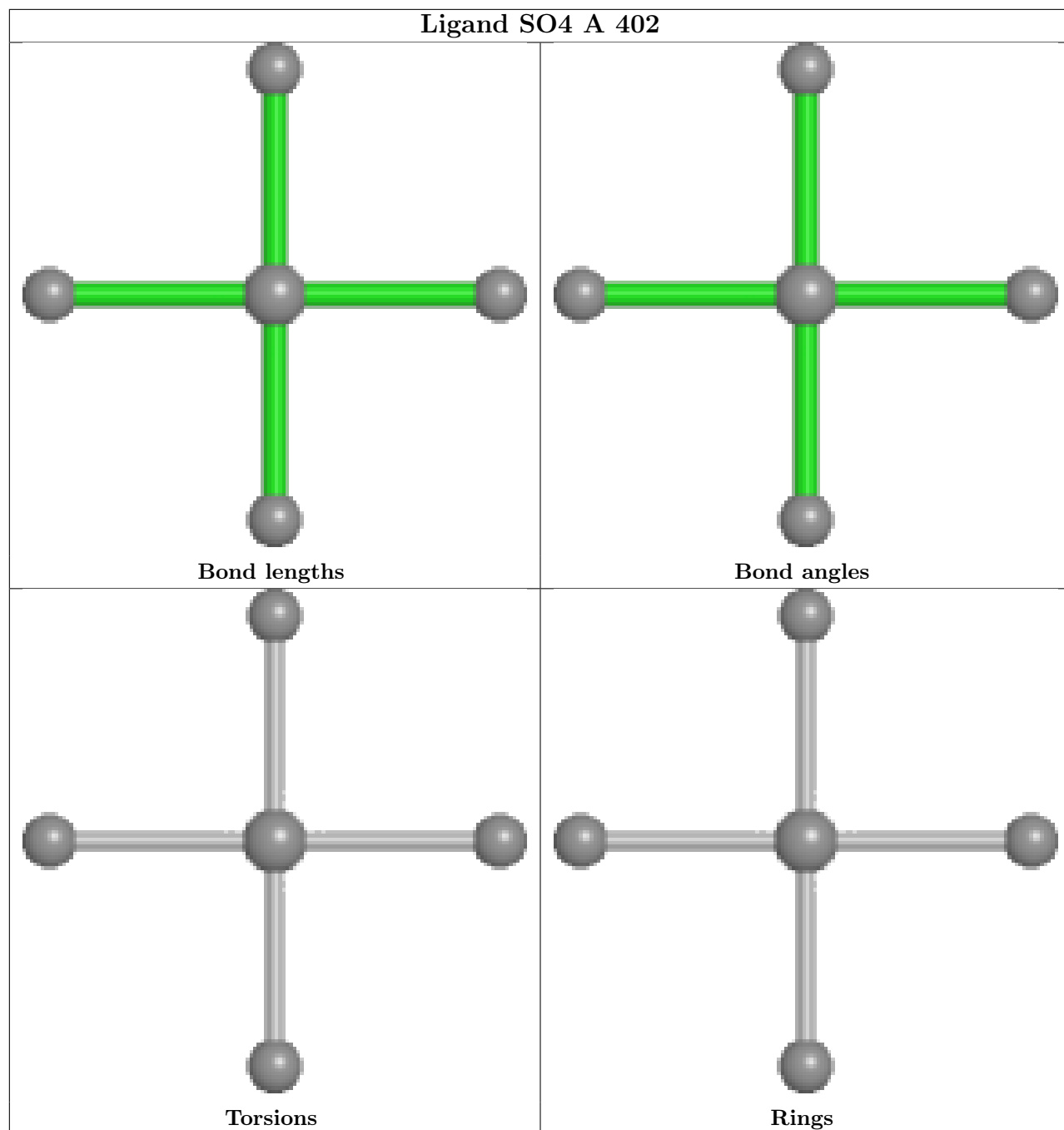


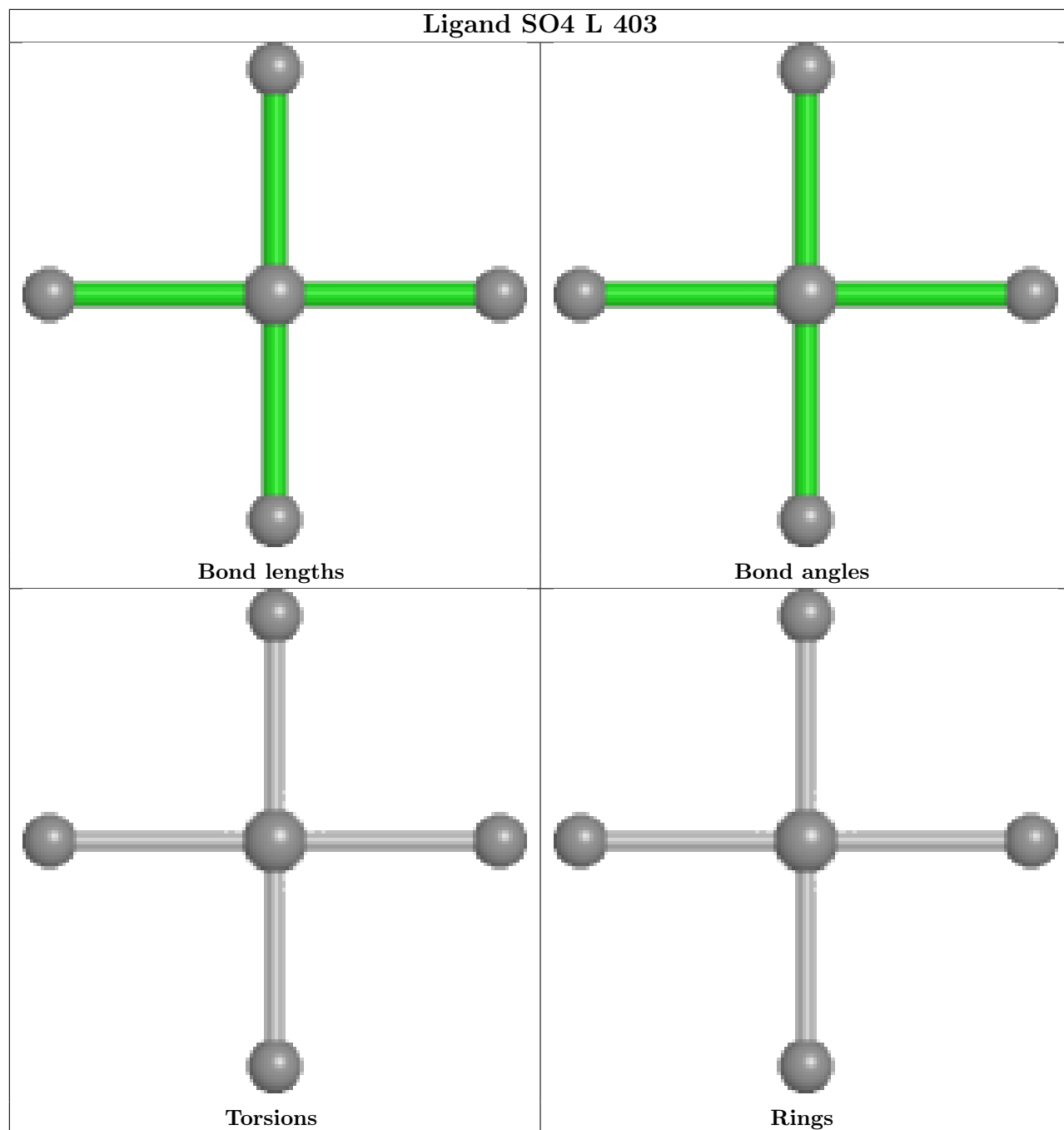


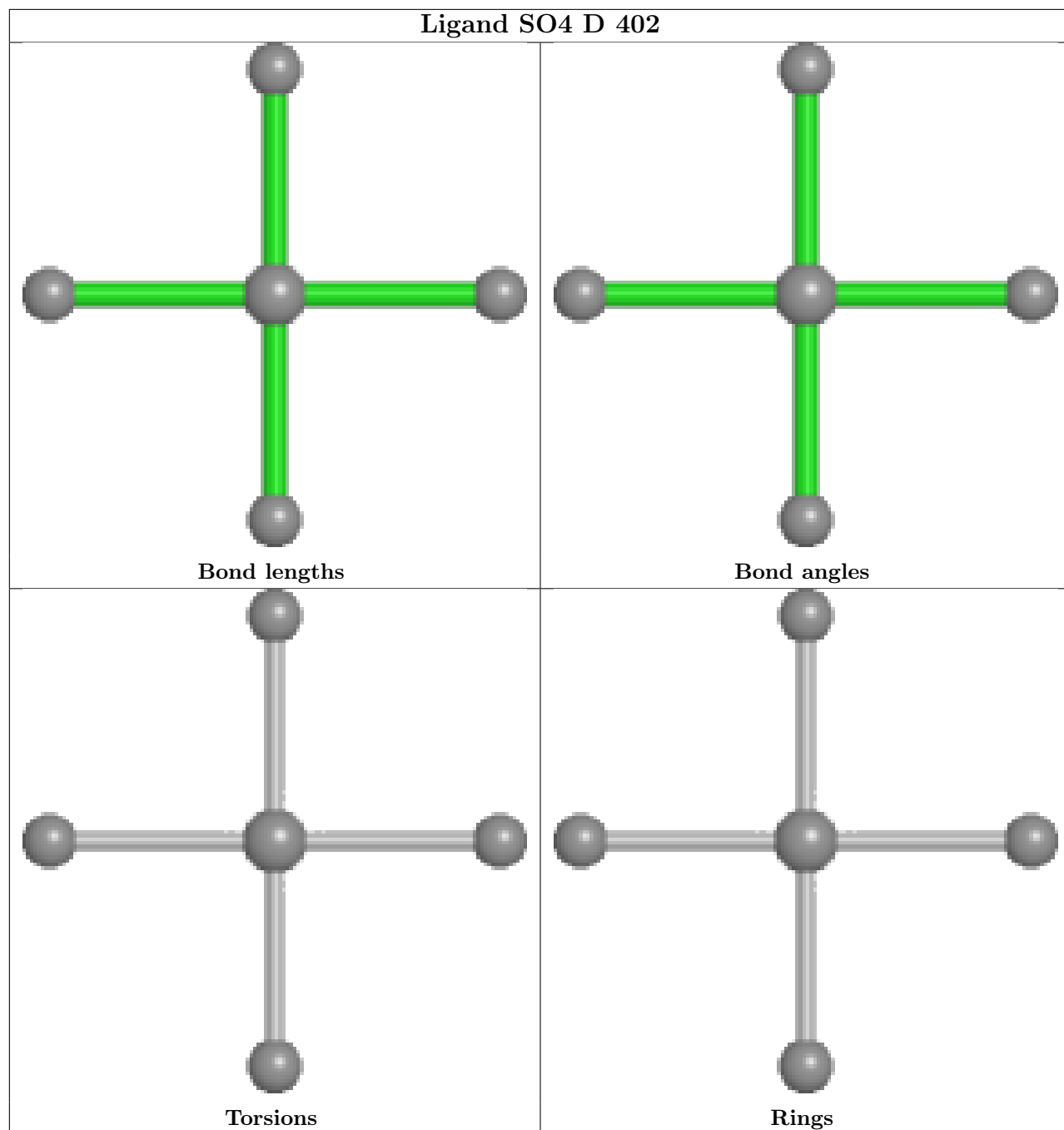


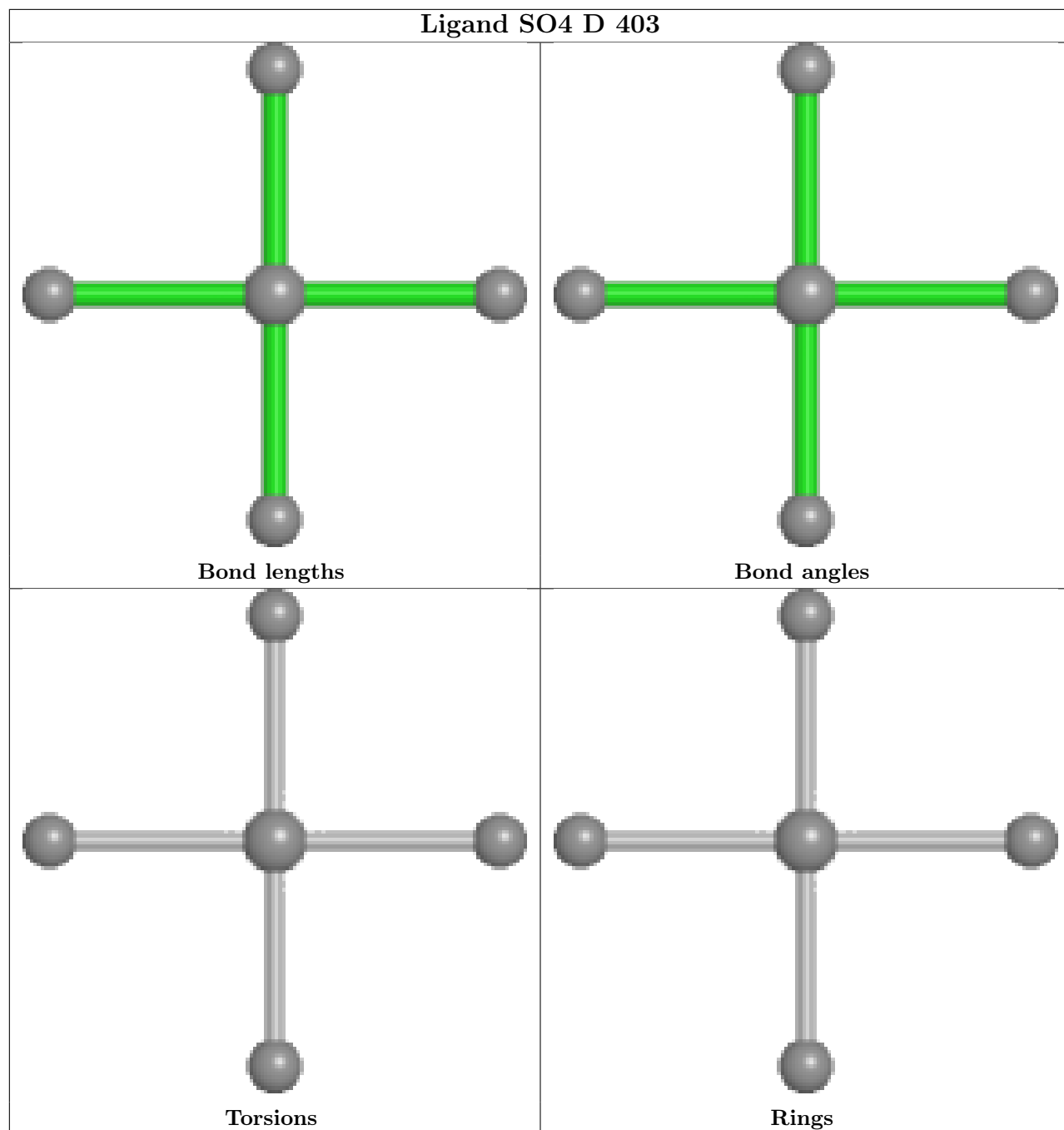




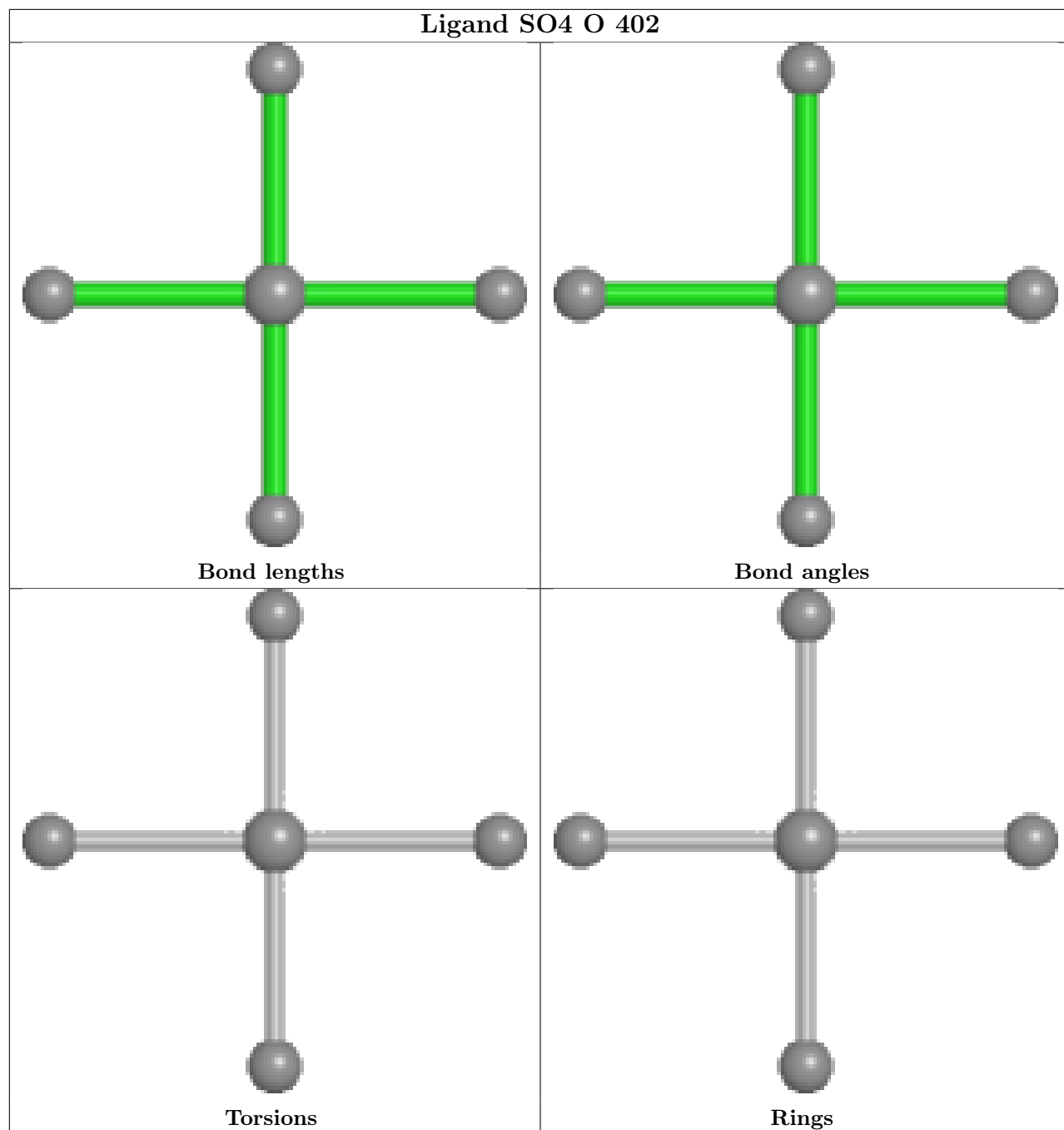


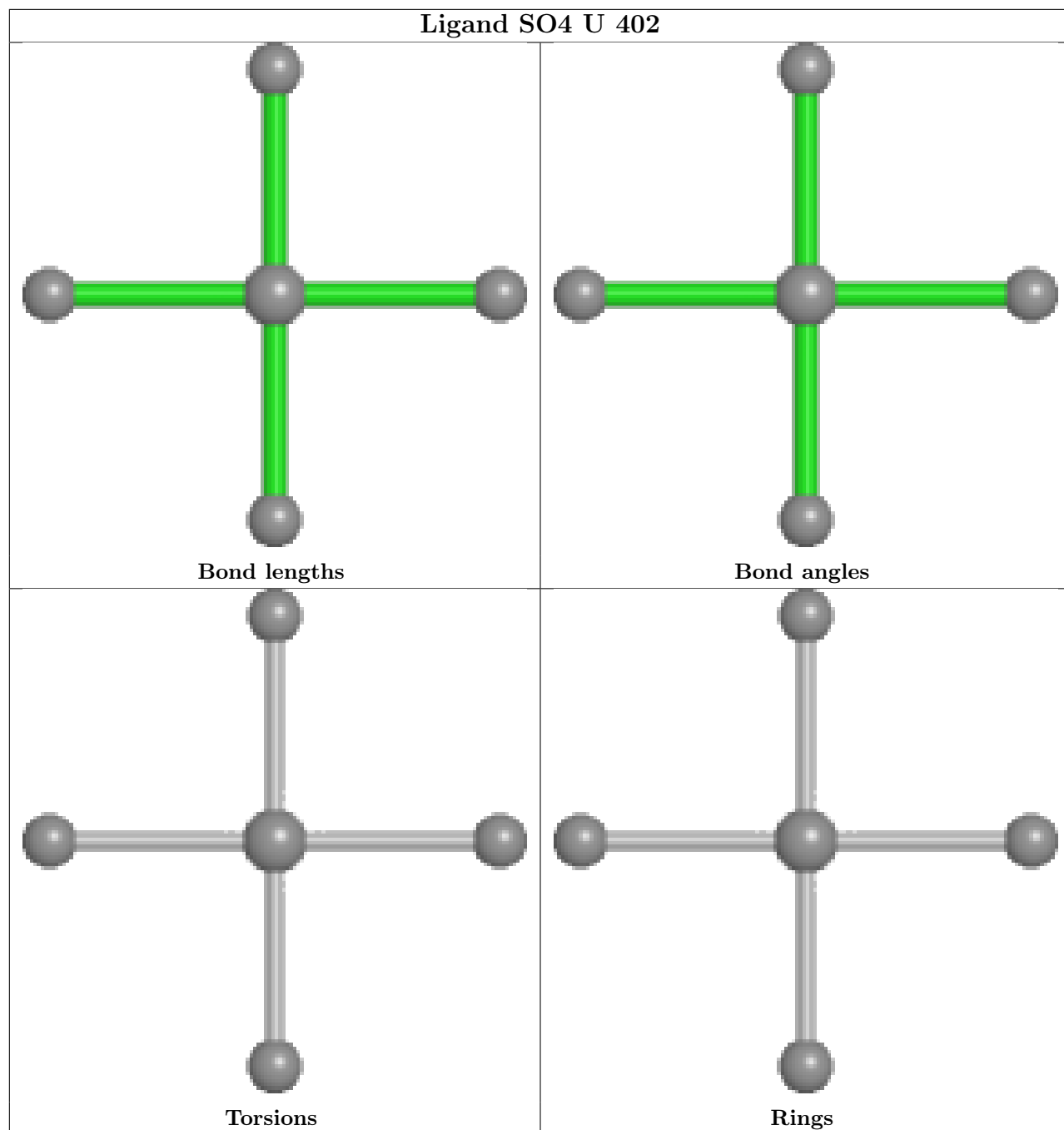


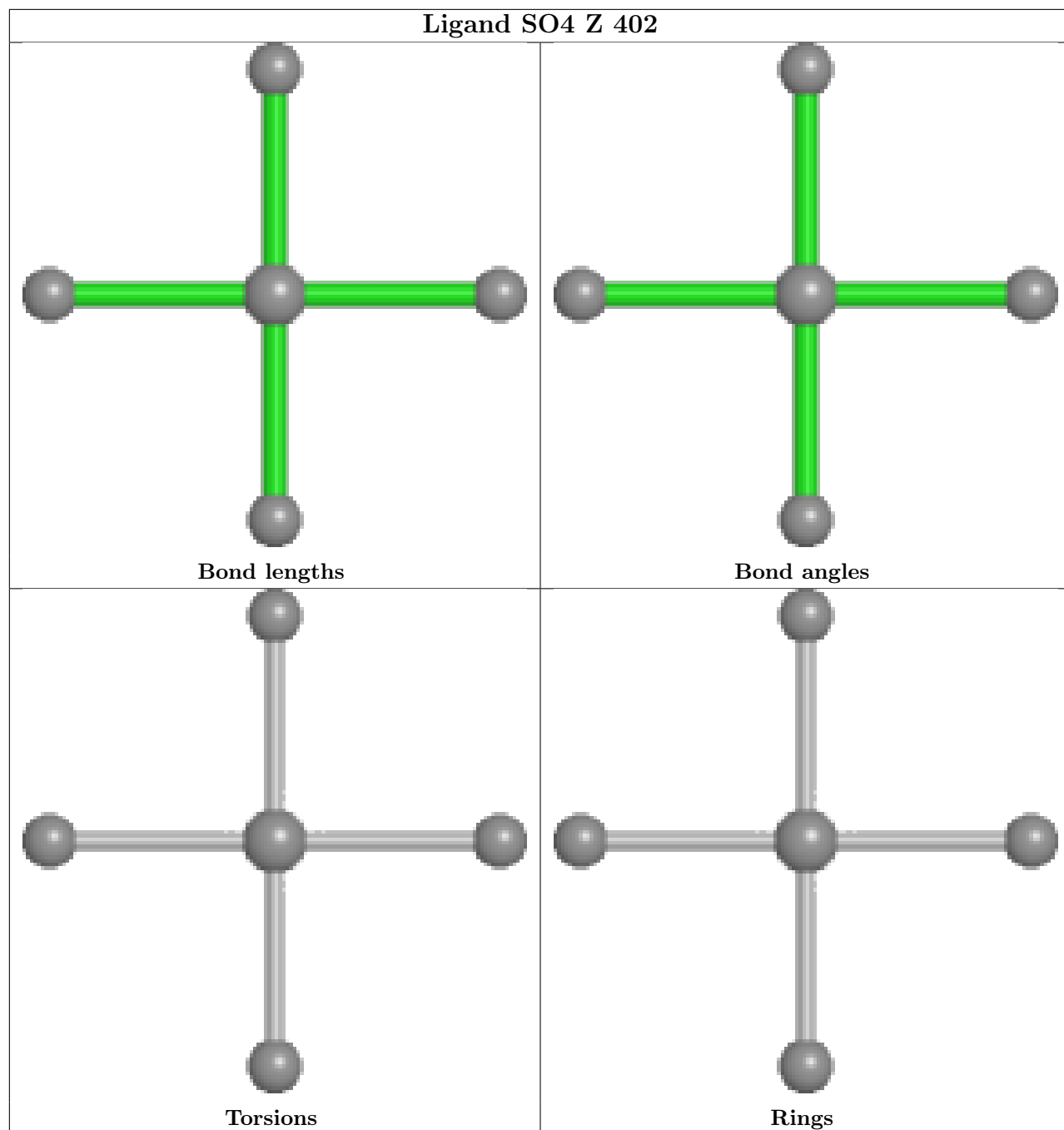


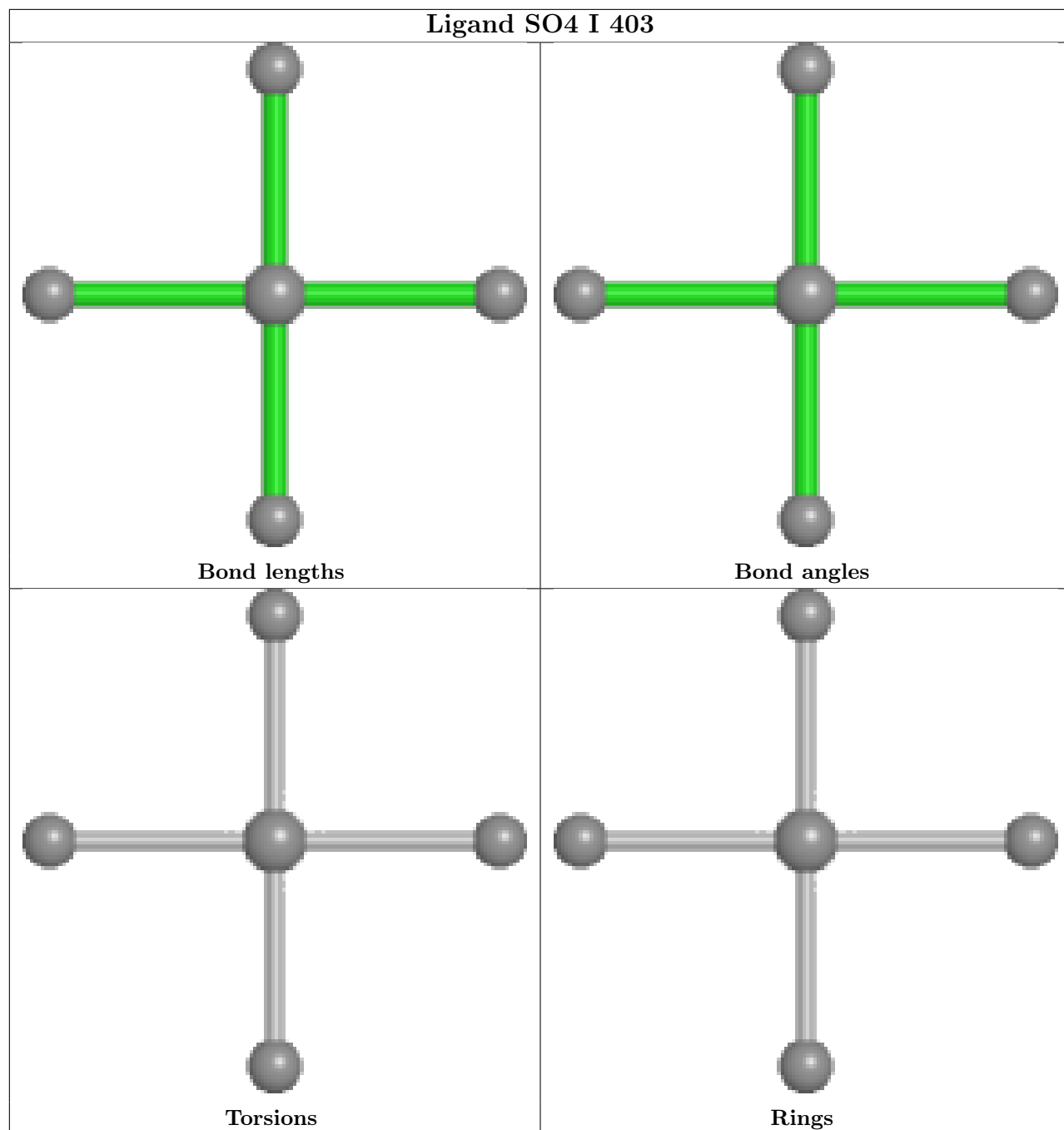


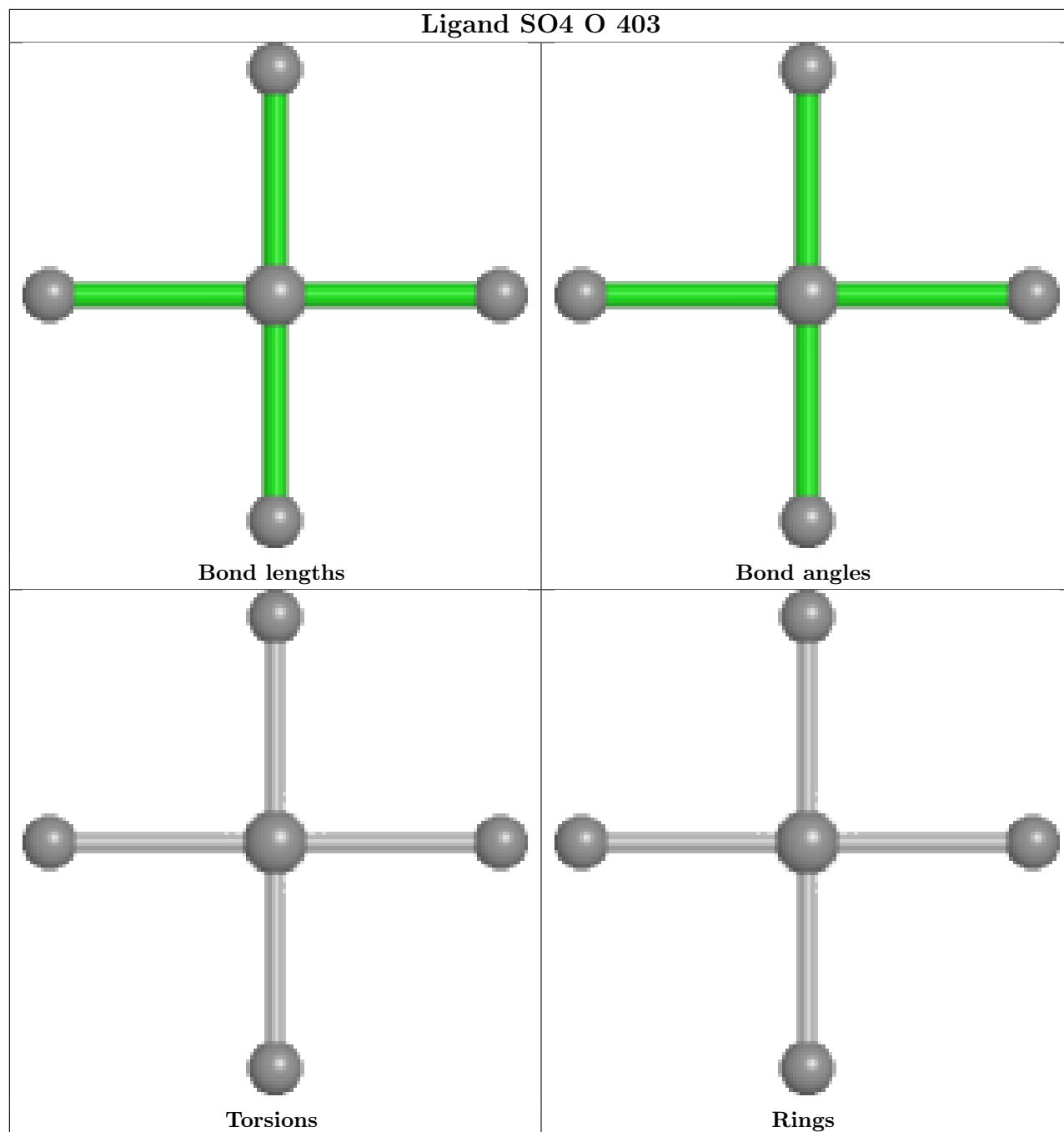












### 5.7 Other polymers [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers

EDS failed to run properly - this section is therefore empty.