



wwPDB EM Validation Summary Report ⓘ

Jul 2, 2026 – 05:31 pm BST

PDB ID : 9SFI / pdb_00009sf1
EMDB ID : EMD-54825
Title : Heterodisulfide reductase-Formylmethanofuran dehydrogenase super-assembly
Authors : Paul, S.; Schuller, J.M.
Deposited on : 2025-08-19
Resolution : 4.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

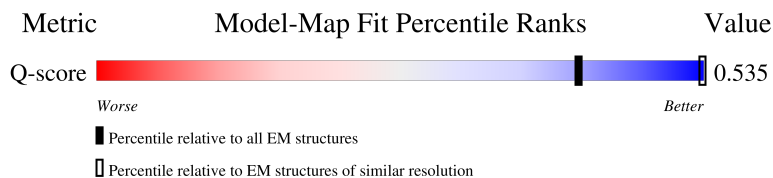
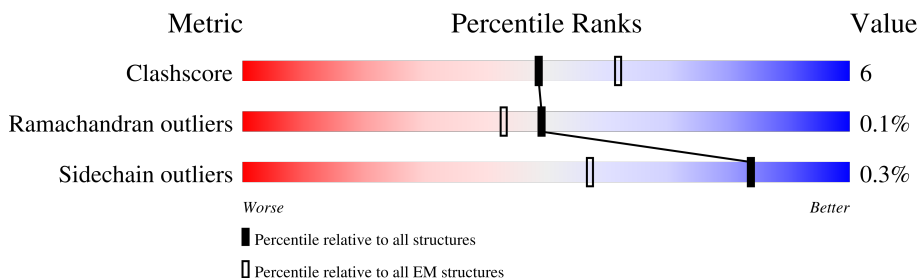
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 4.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	658	86% (Green), 13% (Yellow)
1	B	658	88% (Green), 12% (Yellow)
1	a	658	88% (Green), 12% (Yellow)
1	b	658	89% (Green), 11% (Yellow)





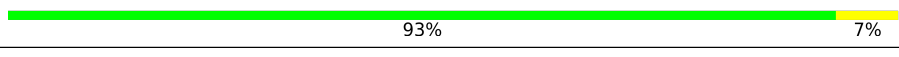
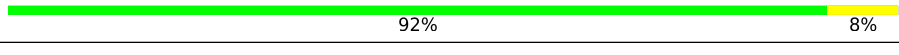
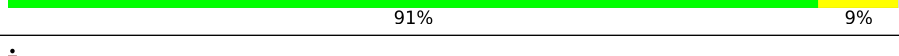

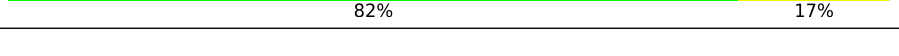

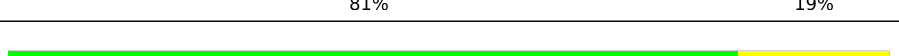
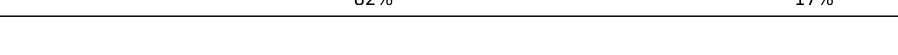
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Mol	Chain	Length	Quality of chain
2	C	293	90% 10%
2	D	293	94% 6%
2	c	293	89% 11%
2	d	293	90% 10%
3	E	184	89% 11%
3	F	184	94% 6%
3	e	184	91% 9%
3	f	184	89% 11%
4	I	288	86% 14%
4	J	288	88% 12%
4	i	288	88% 11%
4	j	288	88% 11%
5	K	134	88% 12%
5	L	134	88% 12%
5	k	134	88% 11%
5	l	134	87% 13%
6	M	27	63% 37%
6	N	27	78% 22%
6	m	27	63% 37%
6	n	27	56% 44%
7	O	394	89% 11%
7	o	394	87% 13%
8	P	567	90% 10%
8	p	567	91% 9%
9	Q	436	88% 12%

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Mol	Chain	Length	Quality of chain
9	q	436	 87% 12%
10	R	272	 83% 17%
10	r	272	 83% 16%
11	S	128	 81% 19%
11	s	128	 93% 7%
12	T	352	 92% 8%
12	t	352	 95% 5%
13	U	80	 91% 9%
13	u	80	 82% 18%
14	G	418	 82% 17%
14	H	418	 83% 17%
14	g	418	 81% 19%
14	h	418	 82% 17%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	SF4	B	705	-	-	X	-
22	NFU	G	501	-	-	X	-
22	NFU	H	501	-	-	X	-
22	NFU	g	501	-	-	X	-
22	NFU	h	501	-	-	X	-

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 96248 atoms, of which 128 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CoB–CoM heterodisulfide reductase iron-sulfur subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	S			Se
1	A	658	4970	3126	834	957	52	1	0	0
1	B	658	4970	3126	834	957	52	1	0	0
1	a	658	4970	3126	834	957	52	1	0	0
1	b	658	4970	3126	834	957	52	1	0	0

- Molecule 2 is a protein called H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit B2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	293	2236	1420	373	419	24	0	0
2	D	293	2236	1420	373	419	24	0	0
2	c	293	2236	1420	373	419	24	0	0
2	d	293	2236	1420	373	419	24	0	0

- Molecule 3 is a protein called H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	184	1426	892	252	268	14	0	0
3	F	184	1426	892	252	268	14	0	0
3	e	184	1426	892	252	268	14	0	0
3	f	184	1426	892	252	268	14	0	0

- Molecule 4 is a protein called F420-non-reducing hydrogenase small subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	I	288	Total	C	N	O	S	0	0
			2149	1360	354	416	19		
4	J	288	Total	C	N	O	S	0	0
			2149	1360	354	416	19		
4	i	288	Total	C	N	O	S	0	0
			2149	1360	354	416	19		
4	j	288	Total	C	N	O	S	0	0
			2149	1360	354	416	19		

- Molecule 5 is a protein called F420-non-reducing hydrogenase subunit delta.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	N	O	S	Se		
5	K	134	Total	C	N	O	S	Se	0	0
			1018	647	173	187	9	2		
5	L	134	Total	C	N	O	S	Se	0	0
			1018	647	173	187	9	2		
5	k	134	Total	C	N	O	S	Se	0	0
			1018	647	173	187	9	2		
5	l	134	Total	C	N	O	S	Se	0	0
			1018	647	173	187	9	2		

- Molecule 6 is a protein called F420 non-reducing hydrogenase subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	N	O	S			Se
6	M	27	Total	C	N	O	S	Se	0	0
			211	134	34	39	3	1		
6	N	27	Total	C	N	O	S	Se	0	0
			211	134	34	39	3	1		
6	m	27	Total	C	N	O	S	Se	0	0
			211	134	34	39	3	1		
6	n	27	Total	C	N	O	S	Se	0	0
			211	134	34	39	3	1		

- Molecule 7 is a protein called Ferredoxin.

Mol	Chain	Residues	Atoms				AltConf	Trace	
			Total	C	N	O			S
7	O	394	Total	C	N	O	S	0	0
			2901	1818	473	556	54		
7	o	394	Total	C	N	O	S	0	0
			2897	1815	472	556	54		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	220	LYS	ALA	conflict	UNP A0A2L1CB03
o	220	LYS	ALA	conflict	UNP A0A2L1CB03

- Molecule 8 is a protein called Formylmethanofuran dehydrogenase subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	567	Total	C	N	O	S	0	0
			4456	2834	746	852	24		
8	p	567	Total	C	N	O	S	0	0
			4456	2834	746	852	24		

- Molecule 9 is a protein called Molybdopterin oxidoreductase.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	Q	436	Total	C	N	O	S	Se	0	0
			3401	2150	596	630	24	1		
9	q	436	Total	C	N	O	S	Se	0	0
			3401	2150	596	630	24	1		

- Molecule 10 is a protein called Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	R	272	Total	C	N	O	S	0	0
			2041	1288	341	399	13		
10	r	272	Total	C	N	O	S	0	0
			2041	1288	341	399	13		

- Molecule 11 is a protein called Formylmethanofuran dehydrogenase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	S	128	Total	C	N	O	S	0	0
			986	625	157	193	11		
11	s	128	Total	C	N	O	S	0	0
			986	625	157	193	11		

- Molecule 12 is a protein called 4Fe-4S ferredoxin.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	T	352	Total	C	N	O	S	0	0
			2640	1653	435	507	45		
12	t	352	Total	C	N	O	S	0	0
			2640	1653	435	507	45		

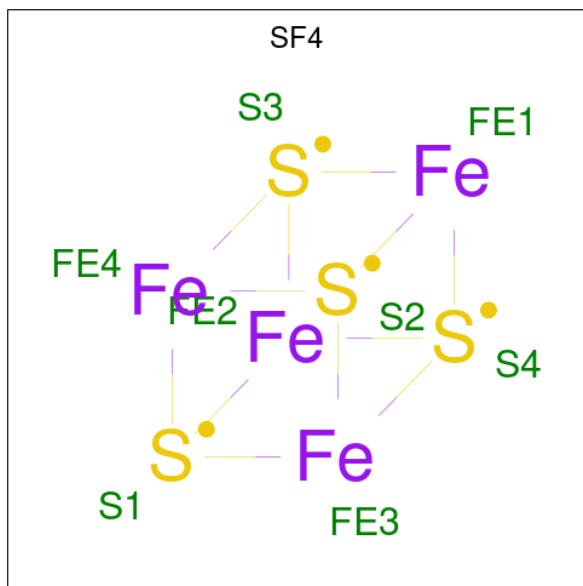
- Molecule 13 is a protein called 4Fe-4S binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	U	80	Total 576	C 358	N 96	O 112	S 10	0	0
13	u	80	Total 576	C 358	N 96	O 112	S 10	0	0

- Molecule 14 is a protein called Coenzyme F420-reducing hydrogenase, alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	g	418	Total 3207	C 2033	N 553	O 604	S 17	0	0
14	G	418	Total 3207	C 2033	N 553	O 604	S 17	0	0
14	H	418	Total 3207	C 2033	N 553	O 604	S 17	0	0
14	h	418	Total 3207	C 2033	N 553	O 604	S 17	0	0

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
15	A	1	Total 8	Fe 4	S 4	0
15	A	1	Total 8	Fe 4	S 4	0

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

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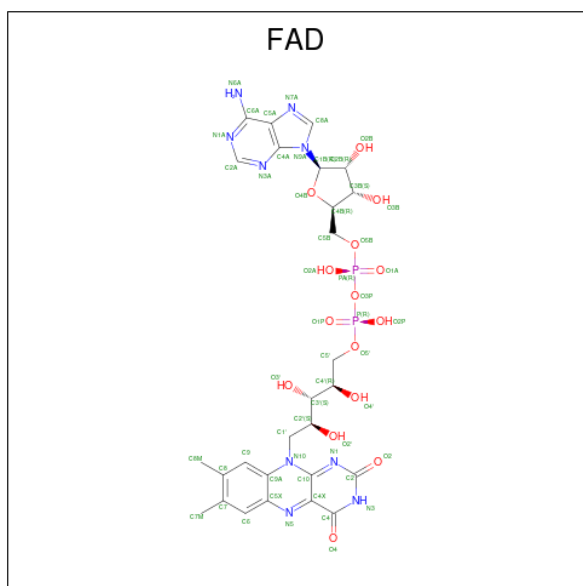
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
15	U	1	8	4	4	0
15	U	1	8	4	4	0
15	a	1	8	4	4	0
15	a	1	8	4	4	0
15	a	1	8	4	4	0
15	a	1	8	4	4	0
15	a	1	8	4	4	0
15	a	1	8	4	4	0
15	a	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	b	1	8	4	4	0
15	e	1	8	4	4	0
15	e	1	8	4	4	0
15	f	1	8	4	4	0
15	f	1	8	4	4	0
15	i	1	8	4	4	0
15	i	1	8	4	4	0
15	i	1	8	4	4	0

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Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
15	t	1	8	4	4	0
15	t	1	8	4	4	0
15	t	1	8	4	4	0
15	t	1	8	4	4	0
15	u	1	8	4	4	0
15	u	1	8	4	4	0

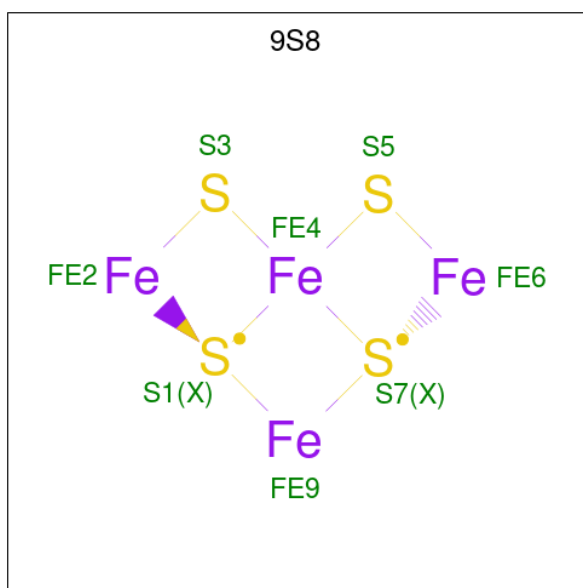
- Molecule 16 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
			Total	C	H	N	O	P	
16	A	1	84	27	31	9	15	2	0
16	B	1	84	27	31	9	15	2	0
16	a	1	84	27	31	9	15	2	0
16	b	1	84	27	31	9	15	2	0

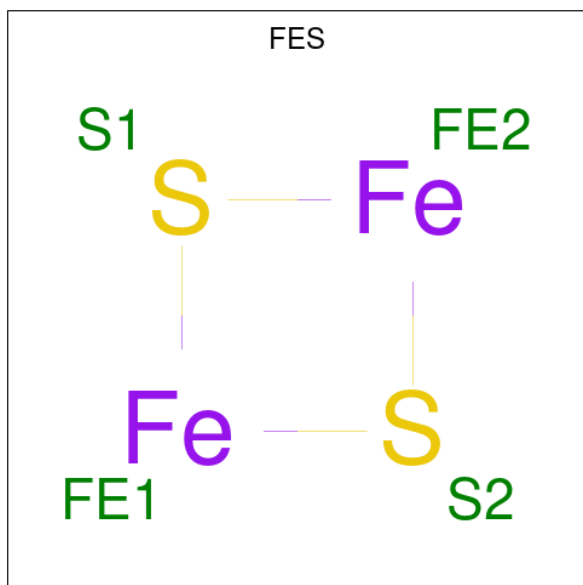
- Molecule 17 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe_4S_4) (labeled as

"Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	D	1	Total	Fe	S	0
			8	4	4	
17	D	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	
17	d	1	Total	Fe	S	0
			8	4	4	
17	d	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe₂S₂) (labeled as "Ligand of Interest" by depositor).

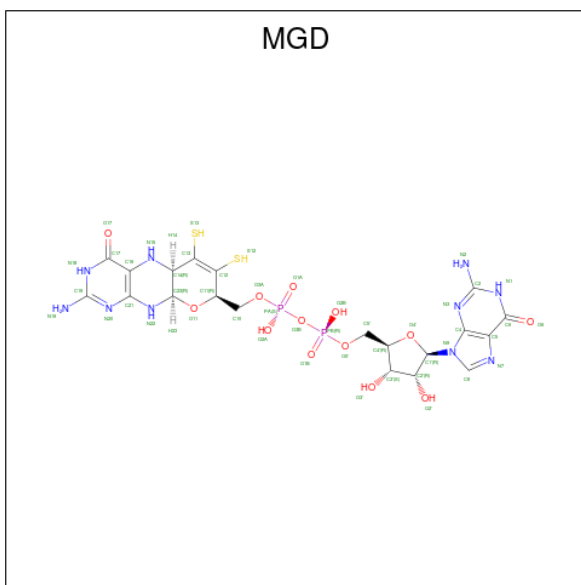


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	K	1	4	2	2	0
18	L	1	4	2	2	0
18	k	1	4	2	2	0
18	l	1	4	2	2	0

- Molecule 19 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
19	P	2	2	2	0
19	p	2	2	2	0

- Molecule 20 is 2-AMINO-5,6-DIMERCAPTO-7-METHYL-3,7,8A,9-TETRAHYDRO-8-OXA-1,3,9,10-TETRAAZA-ANTHRACEN-4-ONE GUANOSINE DINUCLEOTIDE (CCD ID: MGD) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂) (labeled as "Ligand of Interest" by depositor).

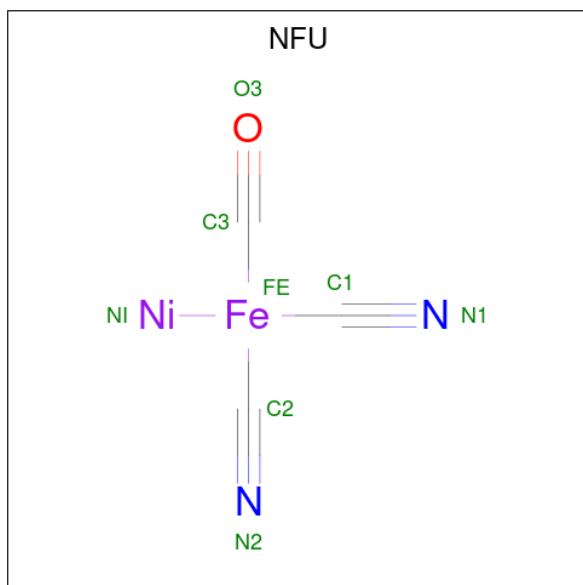


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
20	Q	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
20	Q	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
20	q	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	
20	q	1	Total	C	N	O	P	S	0
			47	20	10	13	2	2	

- Molecule 21 is TUNGSTEN ION (CCD ID: W) (formula: W) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	W	
21	Q	1	Total	W	0
			1	1	
21	q	1	Total	W	0
			1	1	

- Molecule 22 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula: C₃FeN₂NiO) (labeled as "Ligand of Interest" by depositor).

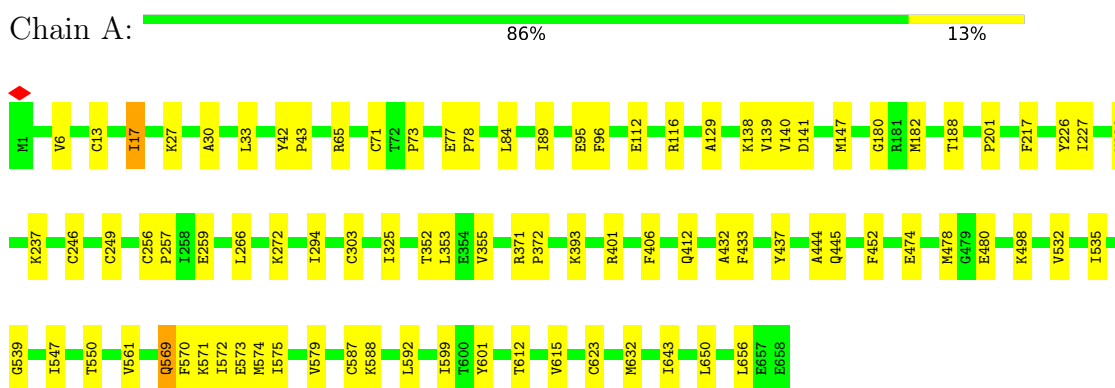


Mol	Chain	Residues	Atoms							AltConf
			Total	C	Fe	H	N	Ni	O	
22	g	1	Total	C	Fe	H	N	Ni	O	0
			9	3	1	1	2	1	1	
22	G	1	Total	C	Fe	H	N	Ni	O	0
			9	3	1	1	2	1	1	
22	H	1	Total	C	Fe	H	N	Ni	O	0
			9	3	1	1	2	1	1	
22	h	1	Total	C	Fe	H	N	Ni	O	0
			9	3	1	1	2	1	1	

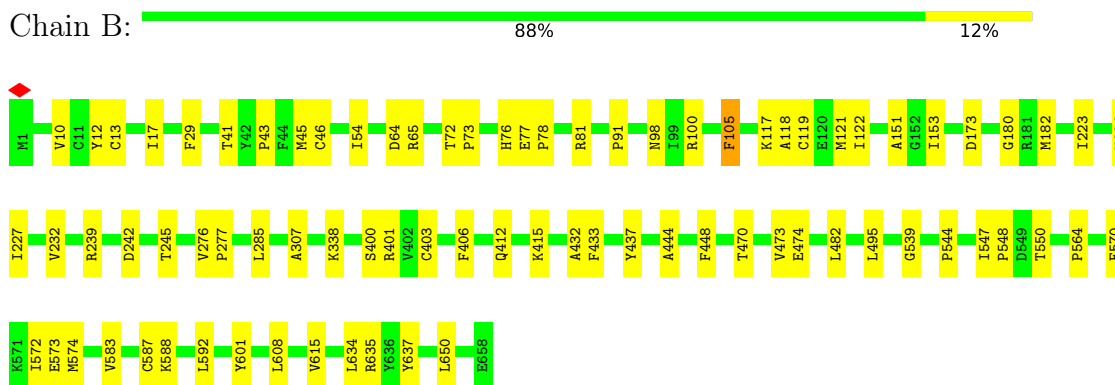
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

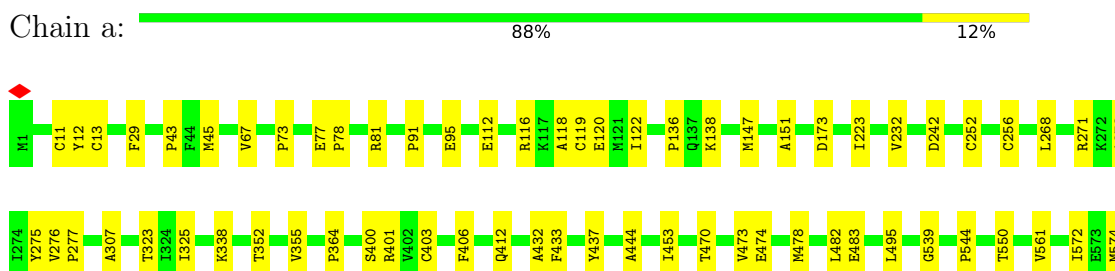
- Molecule 1: CoB-CoM heterodisulfide reductase iron-sulfur subunit A



- Molecule 1: CoB-CoM heterodisulfide reductase iron-sulfur subunit A



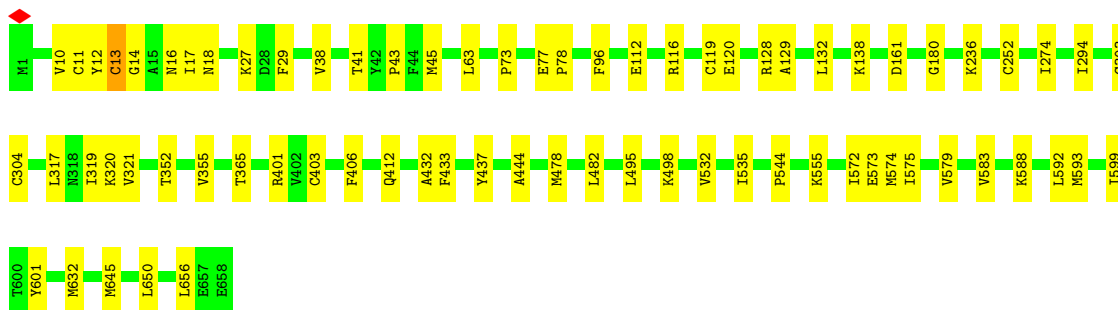
- Molecule 1: CoB-CoM heterodisulfide reductase iron-sulfur subunit A





- Molecule 1: CoB-CoM heterodisulfide reductase iron-sulfur subunit A

Chain b: 89% 11%



- Molecule 2: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit B2

Chain C: 90% 10%



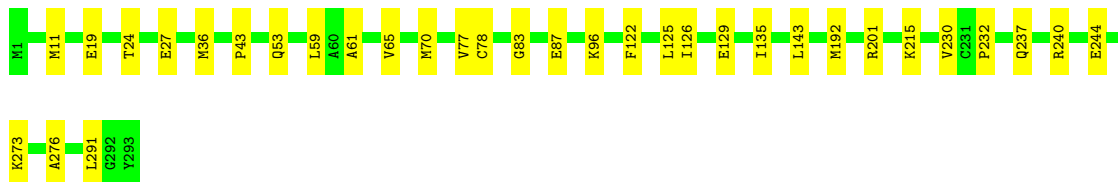
- Molecule 2: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit B2

Chain D: 94% 6%



- Molecule 2: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit B2

Chain c: 89% 11%




- Molecule 2: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit B2

Chain d: 90% 10%



- Molecule 3: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2

Chain E:  89% 11%

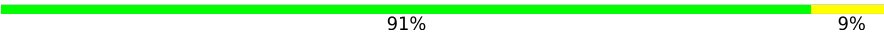


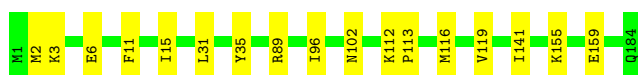
- Molecule 3: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2

Chain F:  94% 6%




- Molecule 3: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2

Chain e:  91% 9%




- Molecule 3: H(2)/formate:CoB-CoM heterodisulfide,ferredoxin reductase subunit C2

Chain f:  89% 11%




- Molecule 4: F420-non-reducing hydrogenase small subunit

Chain I:  86% 14%

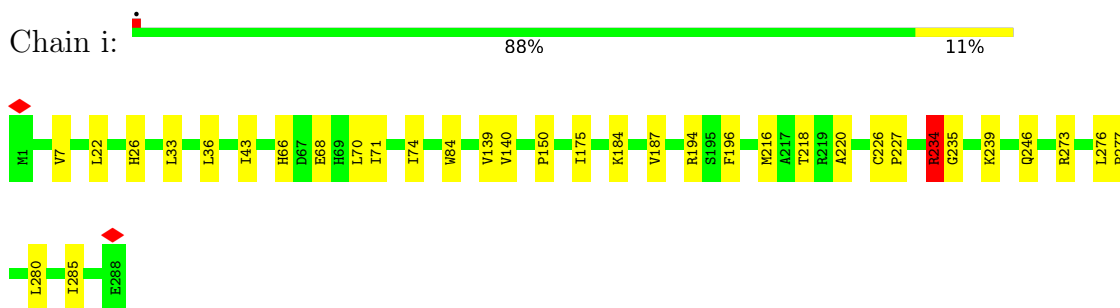


- Molecule 4: F420-non-reducing hydrogenase small subunit

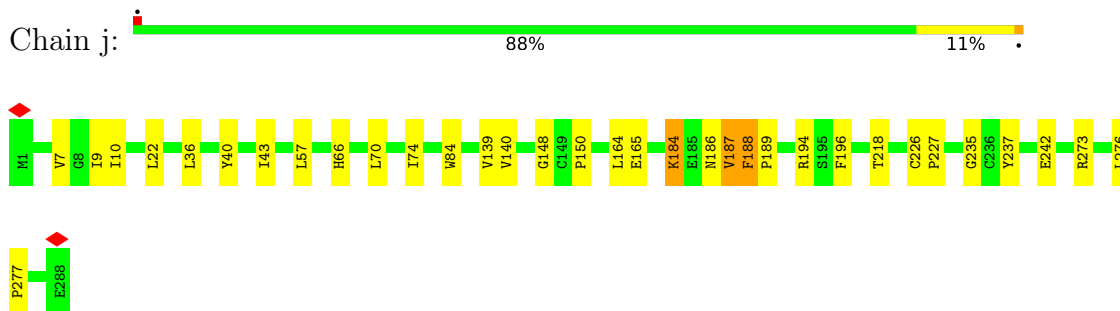
Chain J:  88% 12%



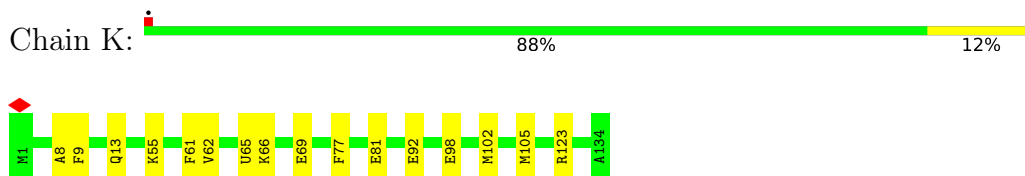
- Molecule 4: F420-non-reducing hydrogenase small subunit



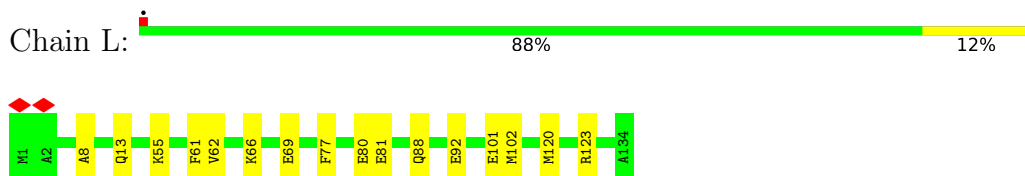
- Molecule 4: F420-non-reducing hydrogenase small subunit



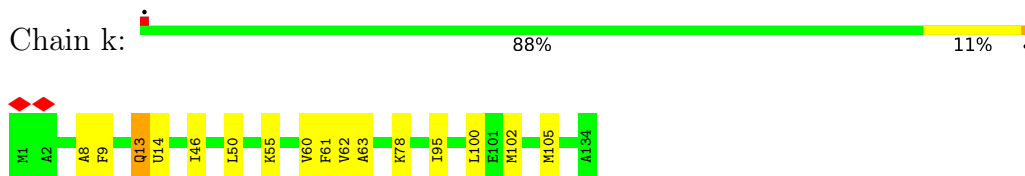
- Molecule 5: F420-non-reducing hydrogenase subunit delta



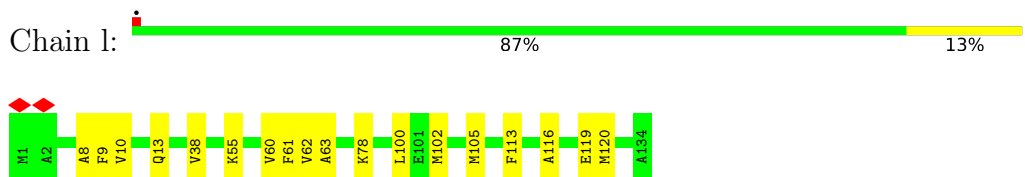
- Molecule 5: F420-non-reducing hydrogenase subunit delta



- Molecule 5: F420-non-reducing hydrogenase subunit delta



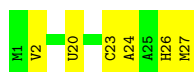
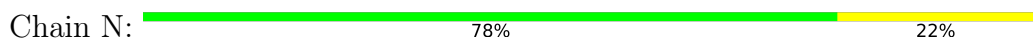
- Molecule 5: F420-non-reducing hydrogenase subunit delta



• Molecule 6: F420 non-reducing hydrogenase subunit



• Molecule 6: F420 non-reducing hydrogenase subunit



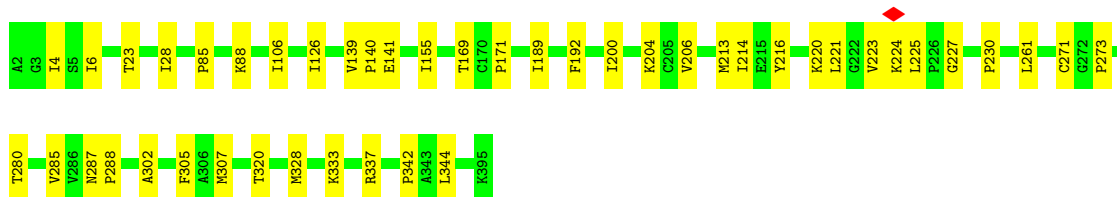
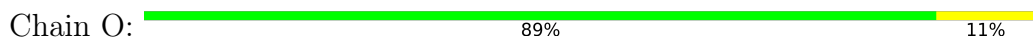
• Molecule 6: F420 non-reducing hydrogenase subunit



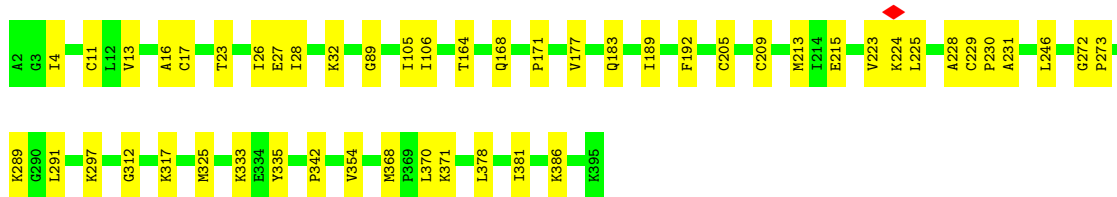
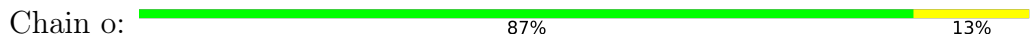
• Molecule 6: F420 non-reducing hydrogenase subunit



• Molecule 7: Ferredoxin

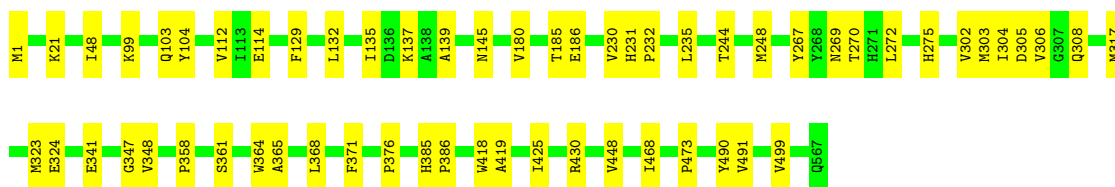


• Molecule 7: Ferredoxin




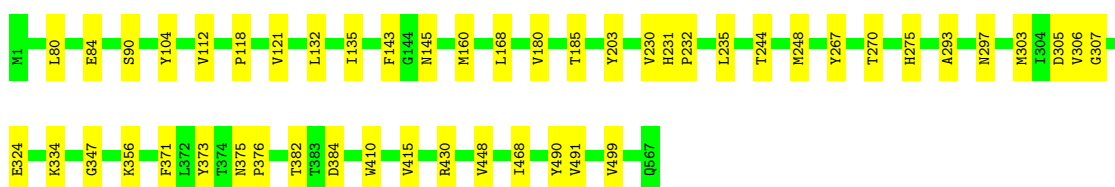
- Molecule 8: Formylmethanofuran dehydrogenase subunit A

Chain P:  90% 10%




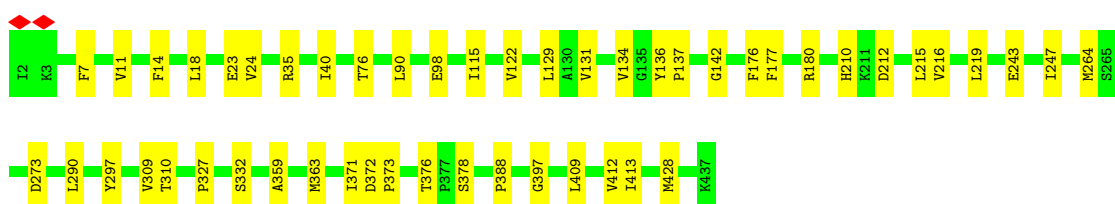
- Molecule 8: Formylmethanofuran dehydrogenase subunit A

Chain p:  91% 9%




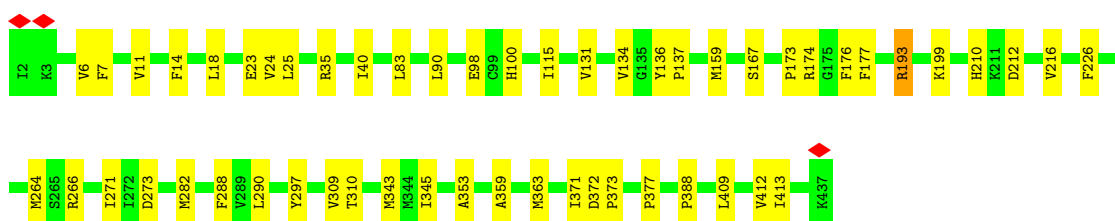
- Molecule 9: Molybdopterin oxidoreductase

Chain Q:  88% 12%




- Molecule 9: Molybdopterin oxidoreductase

Chain q:  87% 12%



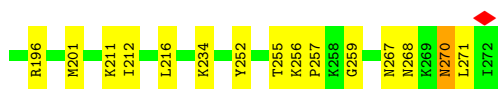
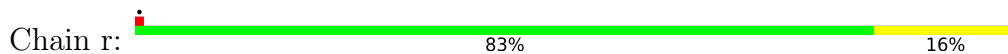
- Molecule 10: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C

Chain R:  83% 17%

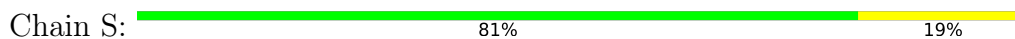




- Molecule 10: Tungsten-containing formylmethanofuran dehydrogenase 2 subunit C



- Molecule 11: Formylmethanofuran dehydrogenase subunit D



- Molecule 11: Formylmethanofuran dehydrogenase subunit D



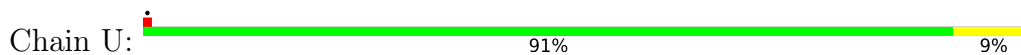
- Molecule 12: 4Fe-4S ferredoxin




- Molecule 12: 4Fe-4S ferredoxin



- Molecule 13: 4Fe-4S binding protein




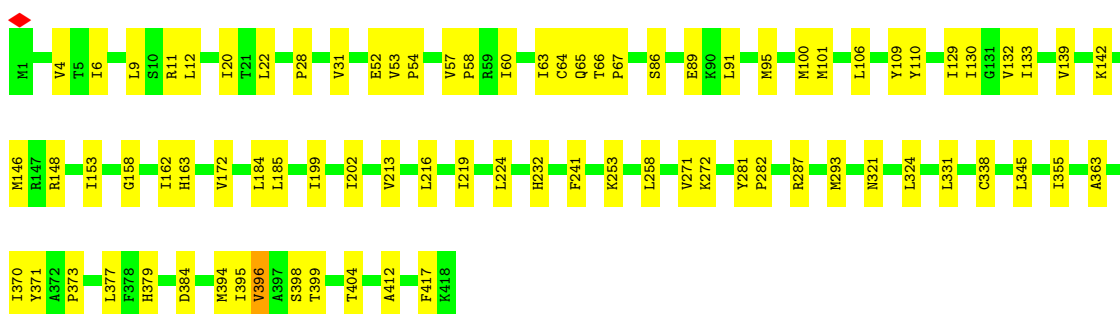
- Molecule 13: 4Fe-4S binding protein

Chain u:  82% 18%




- Molecule 14: Coenzyme F420-reducing hydrogenase, alpha subunit

Chain g:  81% 19%




- Molecule 14: Coenzyme F420-reducing hydrogenase, alpha subunit

Chain G:  82% 17%

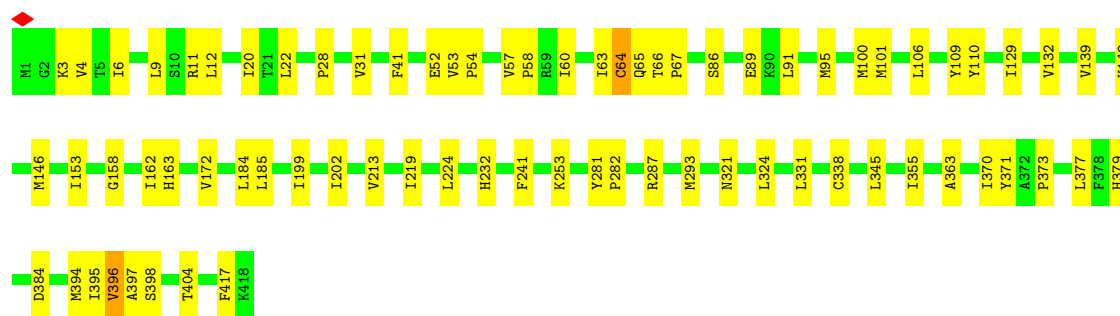
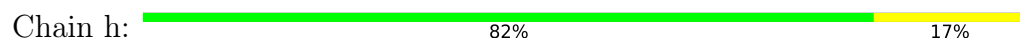


- Molecule 14: Coenzyme F420-reducing hydrogenase, alpha subunit

Chain H:  83% 17%



- Molecule 14: Coenzyme F420-reducing hydrogenase, alpha subunit



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	110231	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	2.000	Depositor
Minimum map value	0.000	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.034	Depositor
Recommended contour level	0.084	Depositor
Map size (Å)	760.0, 760.0, 760.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.95, 0.95, 0.95	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: FES, SEC, FAD, 9S8, ZN, MGD, SF4, W, NFU

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	0.14	0/5052	0.29	0/6830
1	B	0.13	0/5052	0.29	0/6830
1	a	0.13	0/5052	0.25	0/6830
1	b	0.13	0/5052	0.29	0/6830
2	C	0.12	0/2277	0.24	0/3073
2	D	0.13	0/2277	0.24	0/3073
2	c	0.13	0/2277	0.26	0/3073
2	d	0.12	0/2277	0.25	0/3073
3	E	0.11	0/1447	0.21	0/1944
3	F	0.12	0/1447	0.22	0/1944
3	e	0.12	0/1447	0.21	0/1944
3	f	0.12	0/1447	0.22	0/1944
4	I	0.11	0/2192	0.24	0/2982
4	J	0.11	0/2192	0.25	0/2982
4	i	0.11	0/2192	0.25	0/2982
4	j	0.11	0/2192	0.25	0/2982
5	K	0.10	0/1023	0.21	0/1367
5	L	0.10	0/1023	0.22	0/1367
5	k	0.10	0/1023	0.23	0/1367
5	l	0.10	0/1023	0.21	0/1367
6	M	0.18	0/207	0.37	0/278
6	N	0.17	0/207	0.39	0/278
6	m	0.18	0/207	0.40	0/278
6	n	0.17	0/207	0.35	0/278
7	O	0.14	0/2948	0.28	0/3981
7	o	0.13	0/2944	0.30	0/3977
8	P	0.10	0/4563	0.24	0/6190
8	p	0.10	0/4563	0.26	0/6190
9	Q	0.10	0/3468	0.25	0/4695
9	q	0.10	0/3468	0.24	0/4695
10	R	0.08	0/2065	0.21	0/2767
10	r	0.08	0/2065	0.21	0/2767

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	S	0.10	0/1004	0.26	0/1358
11	s	0.09	0/1004	0.23	0/1358
12	T	0.11	0/2682	0.26	0/3630
12	t	0.10	0/2682	0.25	0/3630
13	U	0.13	0/584	0.31	0/789
13	u	0.11	0/584	0.29	0/789
14	G	0.12	0/3275	0.28	0/4435
14	H	0.12	0/3275	0.28	0/4435
14	g	0.12	0/3275	0.28	0/4435
14	h	0.12	0/3275	0.28	1/4435 (0.0%)
All	All	0.12	0/96516	0.26	1/130452 (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
4	i	0	1
9	q	0	1
All	All	0	2

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	h	64	CYS	CA-CB-SG	5.00	125.91	114.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	i	234	ARG	Sidechain
9	q	193	ARG	Sidechain

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	4970	0	4902	69	0
1	B	4970	0	4902	61	0
1	a	4970	0	4902	59	0
1	b	4970	0	4902	64	0
2	C	2236	0	2236	19	0
2	D	2236	0	2236	12	0
2	c	2236	0	2236	20	0
2	d	2236	0	2236	19	0
3	E	1426	0	1460	17	0
3	F	1426	0	1460	10	0
3	e	1426	0	1460	12	0
3	f	1426	0	1460	17	0
4	I	2149	0	2155	39	0
4	J	2149	0	2155	32	0
4	i	2149	0	2155	27	0
4	j	2149	0	2155	29	0
5	K	1018	0	1010	11	0
5	L	1018	0	1010	14	0
5	k	1018	0	1010	14	0
5	l	1018	0	1010	13	0
6	M	211	0	207	19	0
6	N	211	0	207	13	0
6	m	211	0	207	19	0
6	n	211	0	207	18	0
7	O	2901	0	2913	34	0
7	o	2897	0	2902	34	0
8	P	4456	0	4369	42	0
8	p	4456	0	4369	31	0
9	Q	3401	0	3379	34	0
9	q	3401	0	3379	35	0
10	R	2041	0	2105	31	0
10	r	2041	0	2105	32	0
11	S	986	0	984	21	0
11	s	986	0	984	6	0
12	T	2640	0	2648	24	0
12	t	2640	0	2648	12	0
13	U	576	0	570	8	0
13	u	576	0	570	14	0
14	G	3207	0	3217	71	0
14	H	3207	0	3217	67	0
14	g	3207	0	3217	75	0
14	h	3207	0	3217	71	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	A	48	0	0	2	0
15	B	48	0	0	2	0
15	E	16	0	0	0	0
15	F	16	0	0	0	0
15	I	24	0	0	0	0
15	J	24	0	0	0	0
15	O	96	0	0	1	0
15	Q	8	0	0	0	0
15	T	72	0	0	0	0
15	U	16	0	0	1	0
15	a	48	0	0	2	0
15	b	48	0	0	2	0
15	e	16	0	0	0	0
15	f	16	0	0	0	0
15	i	24	0	0	0	0
15	j	24	0	0	0	0
15	o	96	0	0	4	0
15	q	8	0	0	0	0
15	t	72	0	0	1	0
15	u	16	0	0	2	0
16	A	53	31	31	3	0
16	B	53	31	31	2	0
16	a	53	31	31	0	0
16	b	53	31	31	2	0
17	C	16	0	0	0	0
17	D	16	0	0	0	0
17	c	16	0	0	0	0
17	d	16	0	0	0	0
18	K	4	0	0	0	0
18	L	4	0	0	0	0
18	k	4	0	0	0	0
18	l	4	0	0	0	0
19	P	2	0	0	0	0
19	p	2	0	0	0	0
20	Q	94	0	44	3	0
20	q	94	0	44	2	0
21	Q	1	0	0	0	0
21	q	1	0	0	0	0
22	G	8	1	0	3	0
22	H	8	1	0	3	0
22	g	8	1	0	3	0
22	h	8	1	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	96120	128	94885	1106	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 6.

The worst 5 of 1106 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)
5:k:62:VAL:HG23	5:k:102:MET:HG3	1.40	1.02
1:A:139:VAL:HG12	1:A:571:LYS:HG2	1.45	0.98
4:J:112:THR:HG21	14:H:393:ASN:HD22	1.36	0.90
9:Q:131:VAL:HG13	9:Q:136:TYR:HB2	1.56	0.88
1:a:13:CYS:HB2	15:a:701:SF4:S4	2.14	0.88

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	655/658 (100%)	624 (95%)	30 (5%)	1 (0%)	43	75
1	B	655/658 (100%)	609 (93%)	45 (7%)	1 (0%)	43	75
1	a	655/658 (100%)	621 (95%)	34 (5%)	0	100	100
1	b	655/658 (100%)	620 (95%)	34 (5%)	1 (0%)	43	75
2	C	291/293 (99%)	281 (97%)	10 (3%)	0	100	100
2	D	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
2	c	291/293 (99%)	280 (96%)	11 (4%)	0	100	100
2	d	291/293 (99%)	282 (97%)	9 (3%)	0	100	100
3	E	182/184 (99%)	179 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	182/184 (99%)	178 (98%)	4 (2%)	0	100	100
3	e	182/184 (99%)	178 (98%)	4 (2%)	0	100	100
3	f	182/184 (99%)	176 (97%)	6 (3%)	0	100	100
4	I	286/288 (99%)	277 (97%)	9 (3%)	0	100	100
4	J	286/288 (99%)	275 (96%)	11 (4%)	0	100	100
4	i	286/288 (99%)	276 (96%)	10 (4%)	0	100	100
4	j	286/288 (99%)	273 (96%)	11 (4%)	2 (1%)	18	54
5	K	130/134 (97%)	128 (98%)	1 (1%)	1 (1%)	16	52
5	L	130/134 (97%)	128 (98%)	1 (1%)	1 (1%)	16	52
5	k	130/134 (97%)	128 (98%)	1 (1%)	1 (1%)	16	52
5	l	130/134 (97%)	127 (98%)	2 (2%)	1 (1%)	16	52
6	M	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
6	N	24/27 (89%)	22 (92%)	2 (8%)	0	100	100
6	m	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
6	n	24/27 (89%)	23 (96%)	1 (4%)	0	100	100
7	O	392/394 (100%)	375 (96%)	17 (4%)	0	100	100
7	o	392/394 (100%)	368 (94%)	23 (6%)	1 (0%)	36	70
8	P	565/567 (100%)	548 (97%)	17 (3%)	0	100	100
8	p	565/567 (100%)	550 (97%)	15 (3%)	0	100	100
9	Q	433/436 (99%)	420 (97%)	13 (3%)	0	100	100
9	q	433/436 (99%)	417 (96%)	16 (4%)	0	100	100
10	R	270/272 (99%)	259 (96%)	11 (4%)	0	100	100
10	r	270/272 (99%)	261 (97%)	9 (3%)	0	100	100
11	S	126/128 (98%)	125 (99%)	1 (1%)	0	100	100
11	s	126/128 (98%)	124 (98%)	2 (2%)	0	100	100
12	T	350/352 (99%)	344 (98%)	6 (2%)	0	100	100
12	t	350/352 (99%)	345 (99%)	5 (1%)	0	100	100
13	U	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
13	u	78/80 (98%)	77 (99%)	1 (1%)	0	100	100
14	G	416/418 (100%)	408 (98%)	8 (2%)	0	100	100
14	H	416/418 (100%)	407 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	g	416/418 (100%)	408 (98%)	8 (2%)	0	100	100
14	h	416/418 (100%)	408 (98%)	8 (2%)	0	100	100
All	All	12364/12466 (99%)	11932 (96%)	422 (3%)	10 (0%)	49	81

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	105	PHE
5	K	13	GLN
5	L	13	GLN
1	b	304	CYS
4	j	186	ASN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	525/525 (100%)	519 (99%)	6 (1%)	65	74
1	B	525/525 (100%)	525 (100%)	0	100	100
1	a	525/525 (100%)	525 (100%)	0	100	100
1	b	525/525 (100%)	523 (100%)	2 (0%)	84	84
2	C	239/239 (100%)	238 (100%)	1 (0%)	84	84
2	D	239/239 (100%)	239 (100%)	0	100	100
2	c	239/239 (100%)	239 (100%)	0	100	100
2	d	239/239 (100%)	239 (100%)	0	100	100
3	E	155/155 (100%)	155 (100%)	0	100	100
3	F	155/155 (100%)	155 (100%)	0	100	100
3	e	155/155 (100%)	155 (100%)	0	100	100
3	f	155/155 (100%)	155 (100%)	0	100	100
4	I	236/236 (100%)	236 (100%)	0	100	100
4	J	236/236 (100%)	236 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	i	236/236 (100%)	234 (99%)	2 (1%)	73	77
4	j	236/236 (100%)	234 (99%)	2 (1%)	73	77
5	K	100/100 (100%)	100 (100%)	0	100	100
5	L	100/100 (100%)	100 (100%)	0	100	100
5	k	100/100 (100%)	100 (100%)	0	100	100
5	l	100/100 (100%)	100 (100%)	0	100	100
6	M	22/22 (100%)	22 (100%)	0	100	100
6	N	22/22 (100%)	22 (100%)	0	100	100
6	m	22/22 (100%)	22 (100%)	0	100	100
6	n	22/22 (100%)	22 (100%)	0	100	100
7	O	330/330 (100%)	329 (100%)	1 (0%)	86	85
7	o	329/330 (100%)	329 (100%)	0	100	100
8	P	484/484 (100%)	484 (100%)	0	100	100
8	p	484/484 (100%)	484 (100%)	0	100	100
9	Q	369/369 (100%)	369 (100%)	0	100	100
9	q	369/369 (100%)	368 (100%)	1 (0%)	86	85
10	R	221/221 (100%)	221 (100%)	0	100	100
10	r	221/221 (100%)	220 (100%)	1 (0%)	81	82
11	S	106/106 (100%)	106 (100%)	0	100	100
11	s	106/106 (100%)	106 (100%)	0	100	100
12	T	304/304 (100%)	303 (100%)	1 (0%)	86	85
12	t	304/304 (100%)	304 (100%)	0	100	100
13	U	65/65 (100%)	65 (100%)	0	100	100
13	u	65/65 (100%)	65 (100%)	0	100	100
14	G	341/341 (100%)	338 (99%)	3 (1%)	70	76
14	H	341/341 (100%)	339 (99%)	2 (1%)	78	81
14	g	341/341 (100%)	339 (99%)	2 (1%)	78	81
14	h	341/341 (100%)	339 (99%)	2 (1%)	78	81
All	All	10229/10230 (100%)	10203 (100%)	26 (0%)	84	85

5 of 26 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	i	234	ARG
9	q	193	ARG
14	h	63	ILE
4	j	188	PHE
10	r	270	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 82 such sidechains are listed below:

Mol	Chain	Res	Type
10	r	27	GLN
14	G	260	ASN
10	r	88	ASN
12	t	234	GLN
14	H	328	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 122 ligands modelled in this entry, 6 are monoatomic - leaving 116 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
17	9S8	C	302	2	2,10,10	1.28	0	-		
16	FAD	A	704	-	56,58,58	0.37	0	81,89,89	0.38	0
17	9S8	D	302	2	2,10,10	1.26	0	-		
15	SF4	i	303	4	0,12,12	-	-	-		
15	SF4	B	706	1	0,12,12	-	-	-		
17	9S8	c	301	2	2,10,10	1.25	0	-		
15	SF4	f	201	3	0,12,12	-	-	-		
20	MGD	Q	501	21	45,52,52	0.73	0	54,81,81	1.09	6 (11%)
15	SF4	j	302	4	0,12,12	-	-	-		
16	FAD	b	704	-	56,58,58	0.37	0	81,89,89	0.40	0
15	SF4	B	702	1	0,12,12	-	-	-		
15	SF4	O	404	7	0,12,12	-	-	-		
15	SF4	t	407	12	0,12,12	-	-	-		
15	SF4	A	705	1	0,12,12	-	-	-		
15	SF4	A	706	1	0,12,12	-	-	-		
15	SF4	o	401	7	0,12,12	-	-	-		
15	SF4	b	702	1	0,12,12	-	-	-		
15	SF4	e	202	3	0,12,12	-	-	-		
15	SF4	o	410	7	0,12,12	-	-	-		
15	SF4	t	405	12	0,12,12	-	-	-		
15	SF4	i	301	4	0,12,12	-	-	-		
15	SF4	q	504	9	0,12,12	-	-	-		
15	SF4	F	202	3	0,12,12	-	-	-		
15	SF4	A	701	1	0,12,12	-	-	-		
15	SF4	a	702	1	0,12,12	-	-	-		
15	SF4	O	411	7	0,12,12	-	-	-		
22	NFU	H	501	6,14	3,7,7	1.06	0	-		
15	SF4	O	412	7	0,12,12	-	-	-		
15	SF4	o	404	7	0,12,12	-	-	-		
15	SF4	T	408	12	0,12,12	-	-	-		
15	SF4	t	406	12	0,12,12	-	-	-		
15	SF4	A	702	1	0,12,12	-	-	-		
15	SF4	O	403	7	0,12,12	-	-	-		
15	SF4	E	202	3	0,12,12	-	-	-		
15	SF4	I	303	4	0,12,12	-	-	-		
15	SF4	T	409	12	0,12,12	-	-	-		
15	SF4	T	405	12	0,12,12	-	-	-		
15	SF4	a	701	1	0,12,12	-	-	-		
15	SF4	b	705	1	0,12,12	-	-	-		
17	9S8	d	301	2	2,10,10	1.16	0	-		
22	NFU	h	501	6,14	3,7,7	1.03	0	-		
15	SF4	a	703	1	0,12,12	-	-	-		
18	FES	l	201	5	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SF4	O	408	7	0,12,12	-	-	-		
15	SF4	i	302	4	0,12,12	-	-	-		
15	SF4	U	101	13	0,12,12	-	-	-		
15	SF4	b	707	1	0,12,12	-	-	-		
15	SF4	o	408	7	0,12,12	-	-	-		
22	NFU	g	501	14,6	3,7,7	1.06	0	-		
15	SF4	T	407	12	0,12,12	-	-	-		
15	SF4	j	301	4	0,12,12	-	-	-		
20	MGD	Q	502	21	45,52,52	0.71	0	54,81,81	1.04	6 (11%)
15	SF4	f	202	3	0,12,12	-	-	-		
15	SF4	O	401	7	0,12,12	-	-	-		
15	SF4	J	302	4	0,12,12	-	-	-		
15	SF4	B	703	1	0,12,12	-	-	-		
15	SF4	E	201	3	0,12,12	-	-	-		
15	SF4	T	403	12	0,12,12	-	-	-		
15	SF4	O	407	7	0,12,12	-	-	-		
17	9S8	c	302	2	2,10,10	1.24	0	-		
15	SF4	t	404	12	0,12,12	-	-	-		
15	SF4	O	406	7	0,12,12	-	-	-		
22	NFU	G	501	6,14	3,7,7	1.04	0	-		
16	FAD	a	704	-	56,58,58	0.37	0	81,89,89	0.39	0
15	SF4	F	201	3	0,12,12	-	-	-		
15	SF4	J	301	4	0,12,12	-	-	-		
15	SF4	u	101	13	0,12,12	-	-	-		
17	9S8	D	301	2	2,10,10	1.24	0	-		
15	SF4	O	409	7	0,12,12	-	-	-		
15	SF4	t	409	12	0,12,12	-	-	-		
15	SF4	O	402	7	0,12,12	-	-	-		
15	SF4	T	401	12	0,12,12	-	-	-		
15	SF4	o	402	7	0,12,12	-	-	-		
15	SF4	J	303	4	0,12,12	-	-	-		
15	SF4	B	705	1	0,12,12	-	-	-		
18	FES	K	201	5	0,4,4	-	-	-		
15	SF4	T	406	12	0,12,12	-	-	-		
15	SF4	b	701	1	0,12,12	-	-	-		
15	SF4	O	410	7	0,12,12	-	-	-		
16	FAD	B	701	-	56,58,58	0.37	0	81,89,89	0.39	0
15	SF4	Q	504	9	0,12,12	-	-	-		
15	SF4	a	705	1	0,12,12	-	-	-		
15	SF4	b	703	1	0,12,12	-	-	-		
15	SF4	t	403	12	0,12,12	-	-	-		
15	SF4	o	405	7	0,12,12	-	-	-		
15	SF4	j	303	4	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	SF4	T	402	12	0,12,12	-	-	-		
15	SF4	T	404	12	0,12,12	-	-	-		
18	FES	k	201	5	0,4,4	-	-	-		
15	SF4	B	707	1	0,12,12	-	-	-		
15	SF4	u	102	13	0,12,12	-	-	-		
15	SF4	o	409	7	0,12,12	-	-	-		
15	SF4	o	407	7	0,12,12	-	-	-		
15	SF4	t	408	12	0,12,12	-	-	-		
17	9S8	C	301	2	2,10,10	1.24	0	-		
15	SF4	U	102	13	0,12,12	-	-	-		
15	SF4	a	706	1	0,12,12	-	-	-		
15	SF4	O	405	7	0,12,12	-	-	-		
15	SF4	I	301	4	0,12,12	-	-	-		
15	SF4	b	706	1	0,12,12	-	-	-		
15	SF4	o	406	7	0,12,12	-	-	-		
15	SF4	e	201	3	0,12,12	-	-	-		
15	SF4	A	703	1	0,12,12	-	-	-		
15	SF4	o	403	7	0,12,12	-	-	-		
15	SF4	A	707	1	0,12,12	-	-	-		
15	SF4	t	401	12	0,12,12	-	-	-		
15	SF4	o	411	7	0,12,12	-	-	-		
15	SF4	I	302	4	0,12,12	-	-	-		
17	9S8	d	302	2	2,10,10	1.28	0	-		
15	SF4	a	707	1	0,12,12	-	-	-		
20	MGD	q	502	21	45,52,52	0.72	0	54,81,81	1.03	6 (11%)
15	SF4	o	412	7	0,12,12	-	-	-		
15	SF4	B	704	1	0,12,12	-	-	-		
20	MGD	q	501	21	45,52,52	0.72	0	54,81,81	1.09	6 (11%)
18	FES	L	201	5	0,4,4	-	-	-		
15	SF4	t	402	12	0,12,12	-	-	-		

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
17	9S8	C	302	2	-	-	0/3/3/3
16	FAD	A	704	-	-	16/34/50/50	0/6/6/6
17	9S8	D	302	2	-	-	0/3/3/3
15	SF4	i	303	4	-	-	0/6/5/5
15	SF4	B	706	1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	9S8	c	301	2	-	-	0/3/3/3
15	SF4	f	201	3	-	-	0/6/5/5
20	MGD	Q	501	21	-	8/22/66/66	0/6/6/6
16	FAD	b	704	-	-	16/34/50/50	0/6/6/6
15	SF4	j	302	4	-	-	0/6/5/5
15	SF4	B	702	1	-	-	0/6/5/5
15	SF4	O	404	7	-	-	0/6/5/5
15	SF4	t	407	12	-	-	0/6/5/5
15	SF4	A	705	1	-	-	0/6/5/5
15	SF4	A	706	1	-	-	0/6/5/5
15	SF4	o	401	7	-	-	0/6/5/5
15	SF4	b	702	1	-	-	0/6/5/5
15	SF4	e	202	3	-	-	0/6/5/5
15	SF4	o	410	7	-	-	0/6/5/5
15	SF4	t	405	12	-	-	0/6/5/5
15	SF4	i	301	4	-	-	0/6/5/5
15	SF4	q	504	9	-	-	0/6/5/5
15	SF4	F	202	3	-	-	0/6/5/5
15	SF4	A	701	1	-	-	0/6/5/5
15	SF4	a	702	1	-	-	0/6/5/5
15	SF4	O	411	7	-	-	0/6/5/5
15	SF4	O	412	7	-	-	0/6/5/5
15	SF4	o	404	7	-	-	0/6/5/5
15	SF4	T	408	12	-	-	0/6/5/5
15	SF4	t	406	12	-	-	0/6/5/5
15	SF4	A	702	1	-	-	0/6/5/5
15	SF4	O	403	7	-	-	0/6/5/5
15	SF4	E	202	3	-	-	0/6/5/5
15	SF4	I	303	4	-	-	0/6/5/5
15	SF4	T	409	12	-	-	0/6/5/5
15	SF4	T	405	12	-	-	0/6/5/5
15	SF4	a	701	1	-	-	0/6/5/5
15	SF4	b	705	1	-	-	0/6/5/5
17	9S8	d	301	2	-	-	0/3/3/3
15	SF4	a	703	1	-	-	0/6/5/5
18	FES	l	201	5	-	-	0/1/1/1
15	SF4	O	408	7	-	-	0/6/5/5
15	SF4	i	302	4	-	-	0/6/5/5
15	SF4	U	101	13	-	-	0/6/5/5
15	SF4	b	707	1	-	-	0/6/5/5
15	SF4	o	408	7	-	-	0/6/5/5
15	SF4	T	407	12	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	j	301	4	-	-	0/6/5/5
20	MGD	Q	502	21	-	5/22/66/66	0/6/6/6
15	SF4	f	202	3	-	-	0/6/5/5
15	SF4	O	401	7	-	-	0/6/5/5
15	SF4	J	302	4	-	-	0/6/5/5
15	SF4	E	201	3	-	-	0/6/5/5
15	SF4	B	703	1	-	-	0/6/5/5
15	SF4	T	403	12	-	-	0/6/5/5
15	SF4	O	407	7	-	-	0/6/5/5
17	9S8	c	302	2	-	-	0/3/3/3
15	SF4	t	404	12	-	-	0/6/5/5
15	SF4	O	406	7	-	-	0/6/5/5
16	FAD	a	704	-	-	16/34/50/50	0/6/6/6
15	SF4	F	201	3	-	-	0/6/5/5
15	SF4	J	301	4	-	-	0/6/5/5
15	SF4	u	101	13	-	-	0/6/5/5
17	9S8	D	301	2	-	-	0/3/3/3
15	SF4	O	409	7	-	-	0/6/5/5
15	SF4	t	409	12	-	-	0/6/5/5
15	SF4	O	402	7	-	-	0/6/5/5
15	SF4	T	401	12	-	-	0/6/5/5
15	SF4	o	402	7	-	-	0/6/5/5
15	SF4	J	303	4	-	-	0/6/5/5
15	SF4	B	705	1	-	-	0/6/5/5
18	FES	K	201	5	-	-	0/1/1/1
15	SF4	T	406	12	-	-	0/6/5/5
16	FAD	B	701	-	-	16/34/50/50	0/6/6/6
15	SF4	O	410	7	-	-	0/6/5/5
15	SF4	b	701	1	-	-	0/6/5/5
15	SF4	Q	504	9	-	-	0/6/5/5
15	SF4	a	705	1	-	-	0/6/5/5
15	SF4	b	703	1	-	-	0/6/5/5
15	SF4	t	403	12	-	-	0/6/5/5
15	SF4	o	405	7	-	-	0/6/5/5
15	SF4	j	303	4	-	-	0/6/5/5
15	SF4	T	402	12	-	-	0/6/5/5
15	SF4	T	404	12	-	-	0/6/5/5
18	FES	k	201	5	-	-	0/1/1/1
15	SF4	B	707	1	-	-	0/6/5/5
15	SF4	u	102	13	-	-	0/6/5/5
15	SF4	o	409	7	-	-	0/6/5/5
15	SF4	o	407	7	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	SF4	t	408	12	-	-	0/6/5/5
17	9S8	C	301	2	-	-	0/3/3/3
15	SF4	U	102	13	-	-	0/6/5/5
15	SF4	a	706	1	-	-	0/6/5/5
15	SF4	O	405	7	-	-	0/6/5/5
15	SF4	I	301	4	-	-	0/6/5/5
15	SF4	b	706	1	-	-	0/6/5/5
15	SF4	o	406	7	-	-	0/6/5/5
15	SF4	e	201	3	-	-	0/6/5/5
15	SF4	A	703	1	-	-	0/6/5/5
15	SF4	o	403	7	-	-	0/6/5/5
15	SF4	A	707	1	-	-	0/6/5/5
15	SF4	t	401	12	-	-	0/6/5/5
15	SF4	o	411	7	-	-	0/6/5/5
15	SF4	I	302	4	-	-	0/6/5/5
17	9S8	d	302	2	-	-	0/3/3/3
15	SF4	a	707	1	-	-	0/6/5/5
20	MGD	q	502	21	-	4/22/66/66	0/6/6/6
15	SF4	o	412	7	-	-	0/6/5/5
15	SF4	B	704	1	-	-	0/6/5/5
20	MGD	q	501	21	-	7/22/66/66	0/6/6/6
18	FES	L	201	5	-	-	0/1/1/1
15	SF4	t	402	12	-	-	0/6/5/5

There are no bond length outliers.

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Q	501	MGD	C19-N20-C21	3.21	119.22	113.43
20	Q	502	MGD	C19-N20-C21	3.19	119.18	113.43
20	q	501	MGD	C19-N20-C21	3.18	119.16	113.43
20	q	502	MGD	C19-N20-C21	3.14	119.10	113.43
20	Q	501	MGD	C17-C16-N15	2.31	122.97	116.76

There are no chirality outliers.

5 of 88 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	A	704	FAD	C5B-O5B-PA-O1A
16	A	704	FAD	C3B-C4B-C5B-O5B
16	A	704	FAD	C2'-C1'-N10-C10

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Mol	Chain	Res	Type	Atoms
16	A	704	FAD	N10-C1'-C2'-O2'
16	A	704	FAD	N10-C1'-C2'-C3'

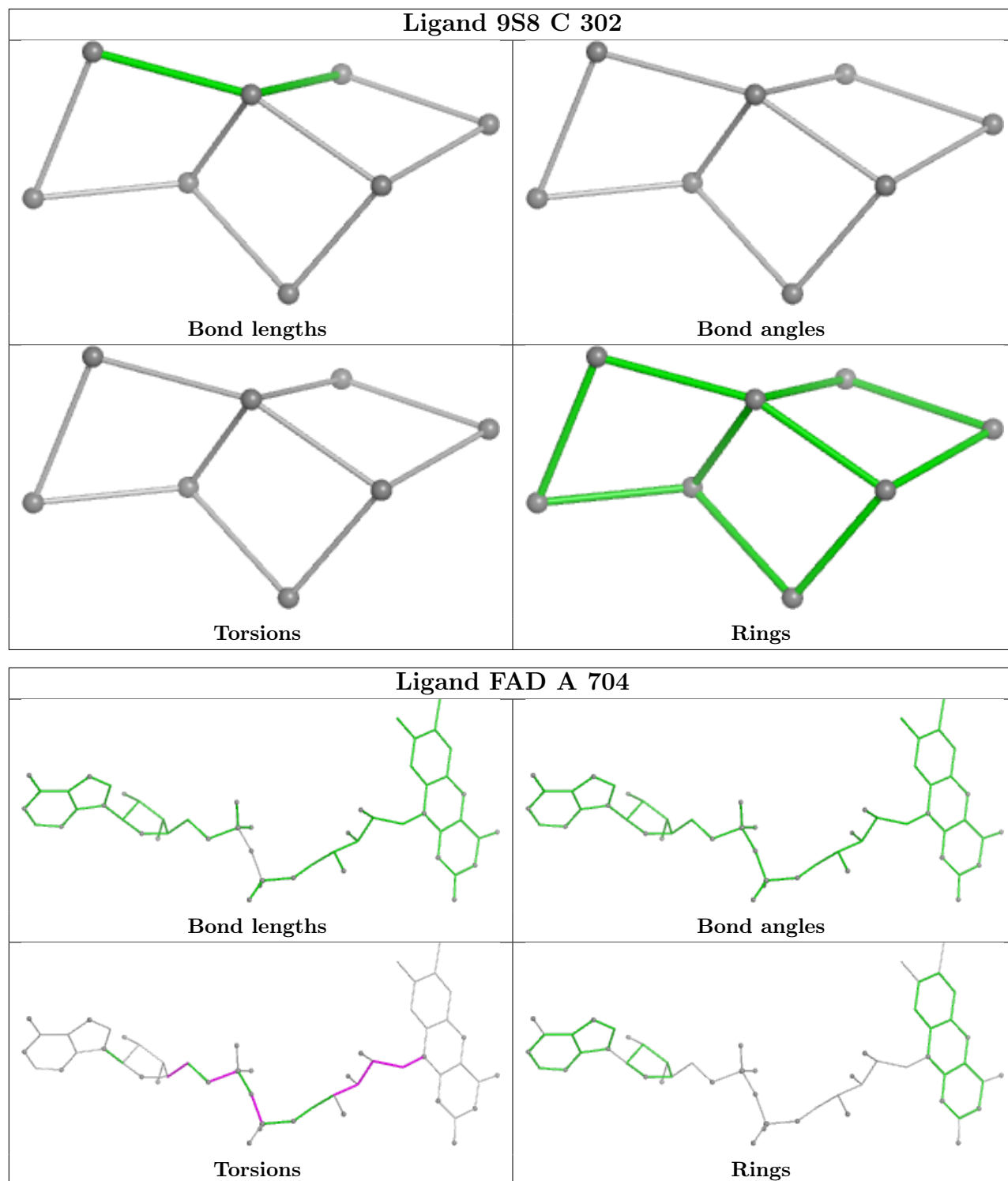
There are no ring outliers.

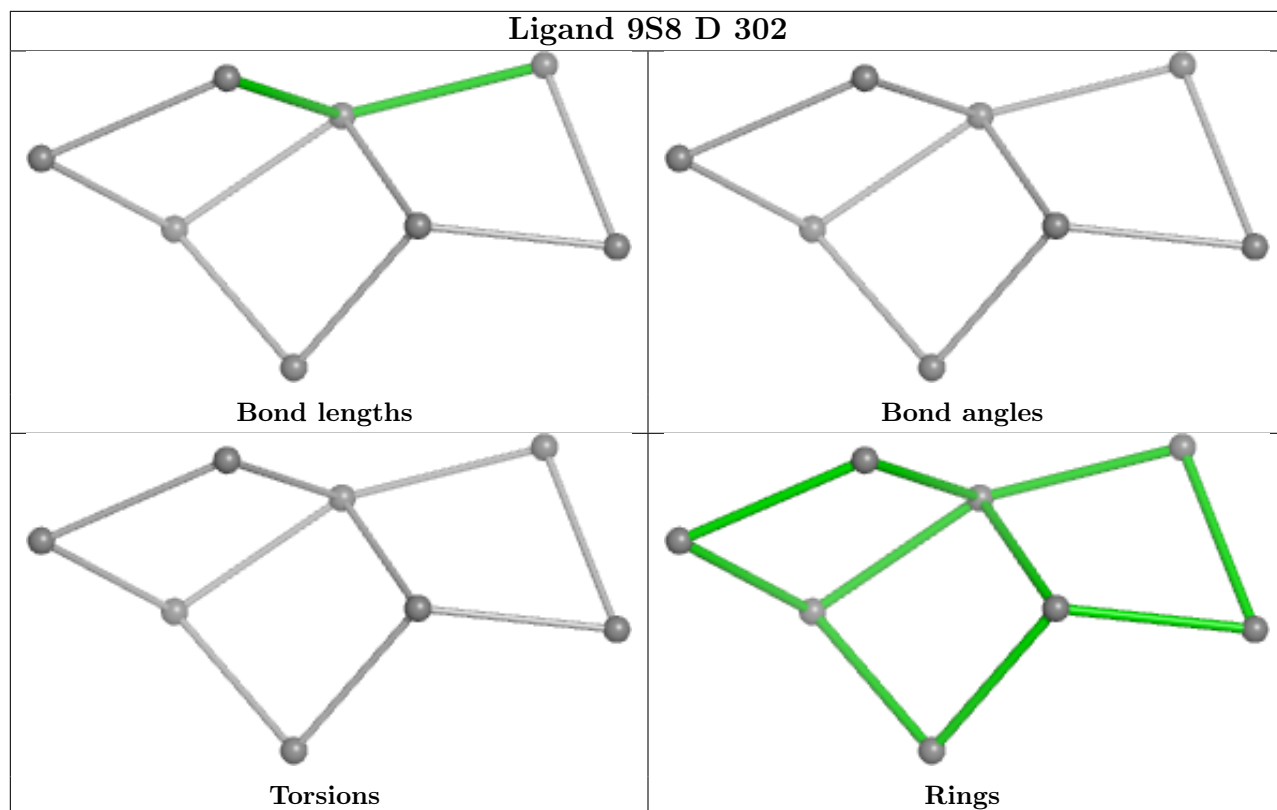
25 monomers are involved in 42 short contacts:

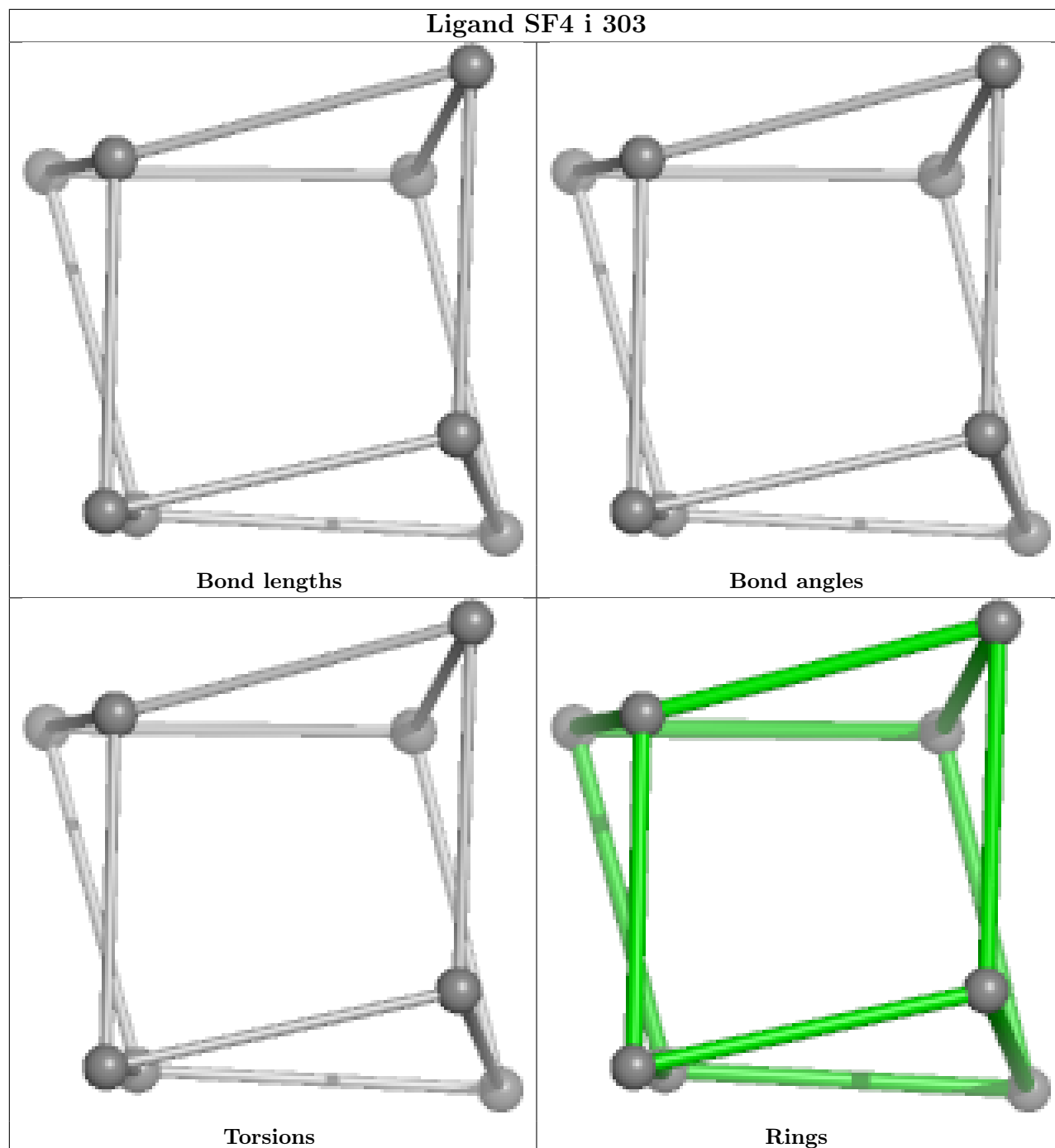
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	704	FAD	3	0
20	Q	501	MGD	3	0
16	b	704	FAD	2	0
15	o	410	SF4	1	0
22	H	501	NFU	3	0
15	O	412	SF4	1	0
15	a	701	SF4	1	0
22	h	501	NFU	4	0
15	b	707	SF4	1	0
15	o	408	SF4	1	0
22	g	501	NFU	3	0
22	G	501	NFU	3	0
15	u	101	SF4	1	0
15	o	402	SF4	1	0
15	B	705	SF4	2	0
16	B	701	FAD	2	0
15	b	703	SF4	1	0
15	u	102	SF4	1	0
15	o	407	SF4	1	0
15	U	102	SF4	1	0
15	a	706	SF4	1	0
15	A	703	SF4	1	0
15	A	707	SF4	1	0
20	q	501	MGD	2	0
15	t	402	SF4	1	0

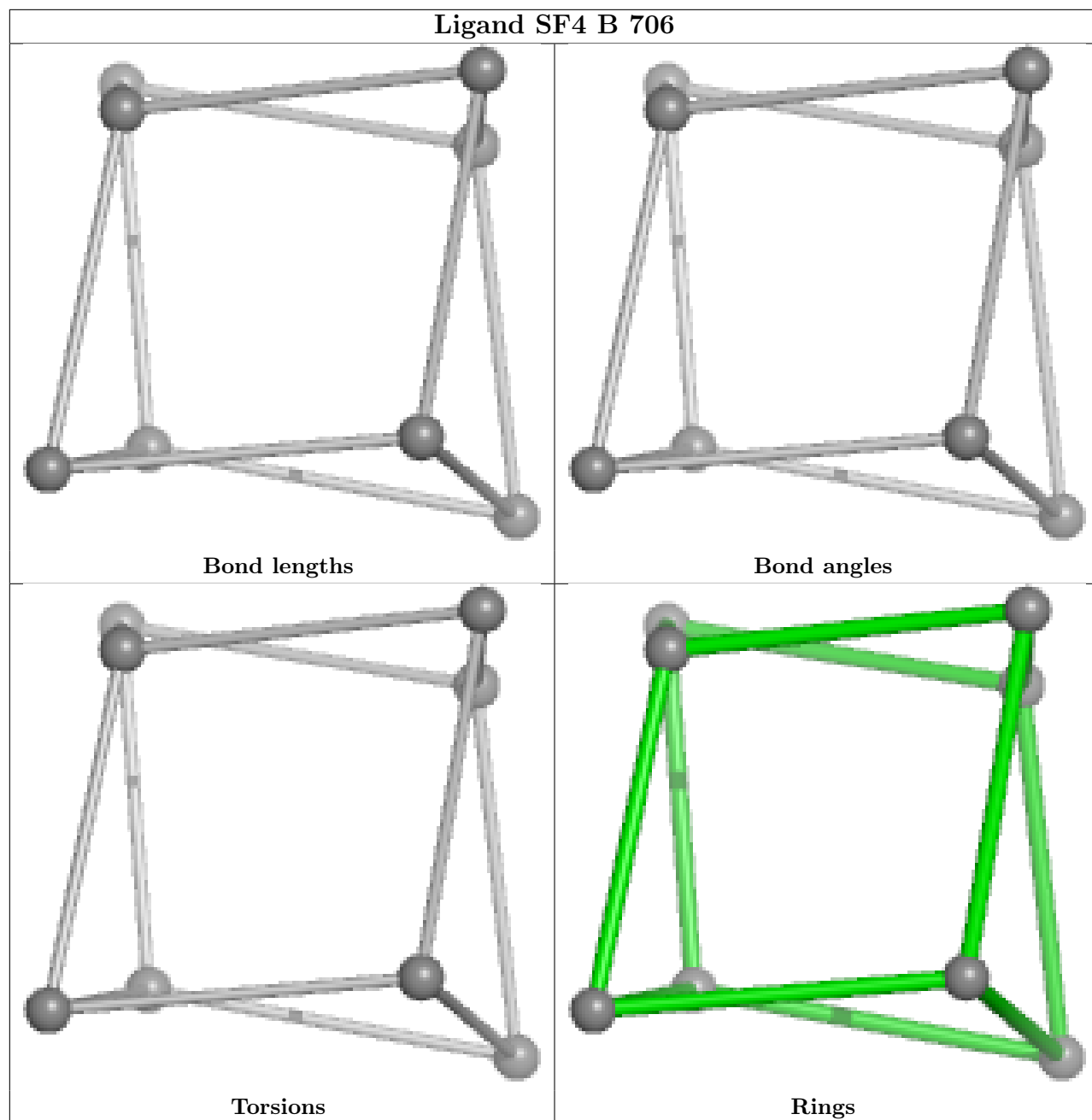
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

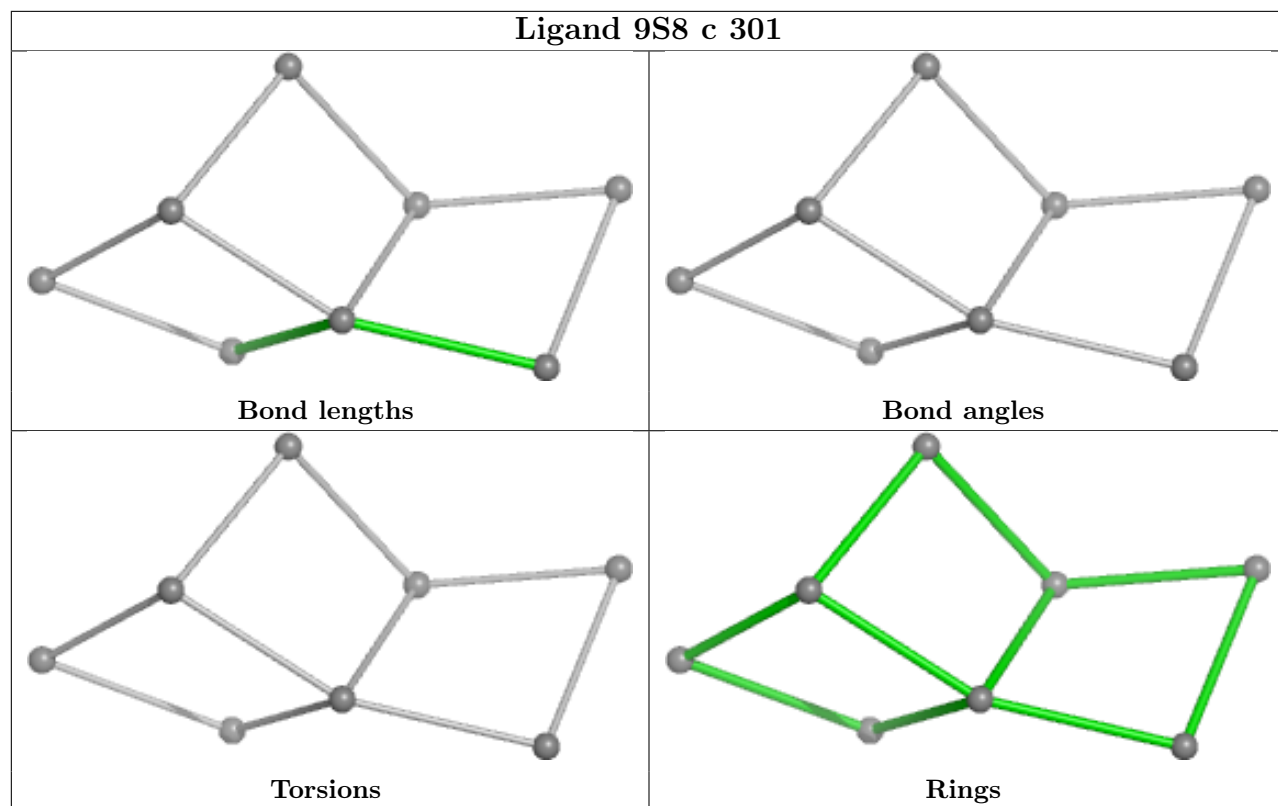
any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

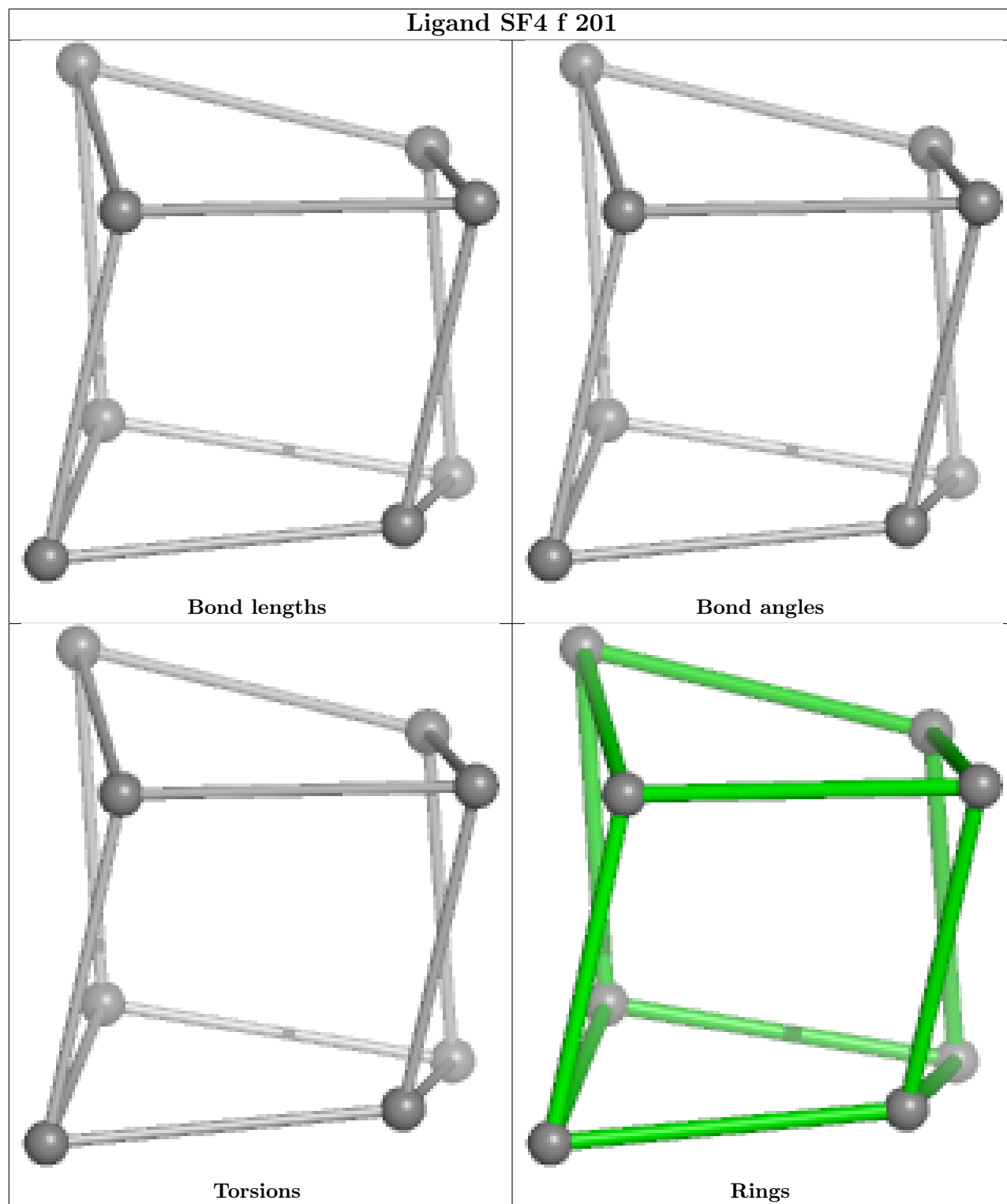


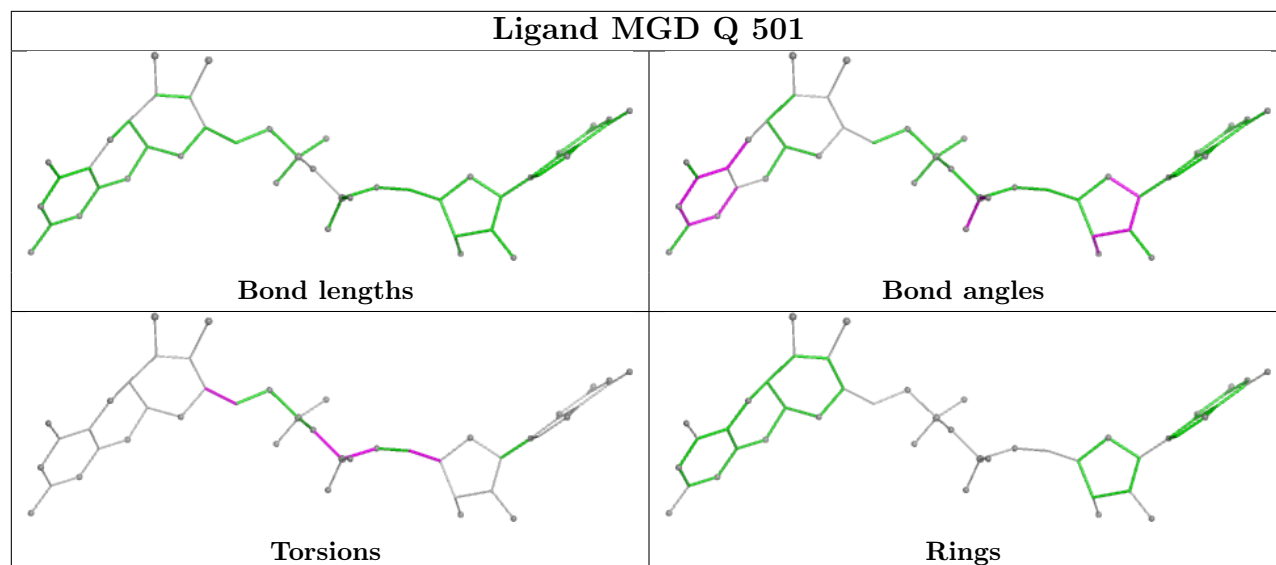


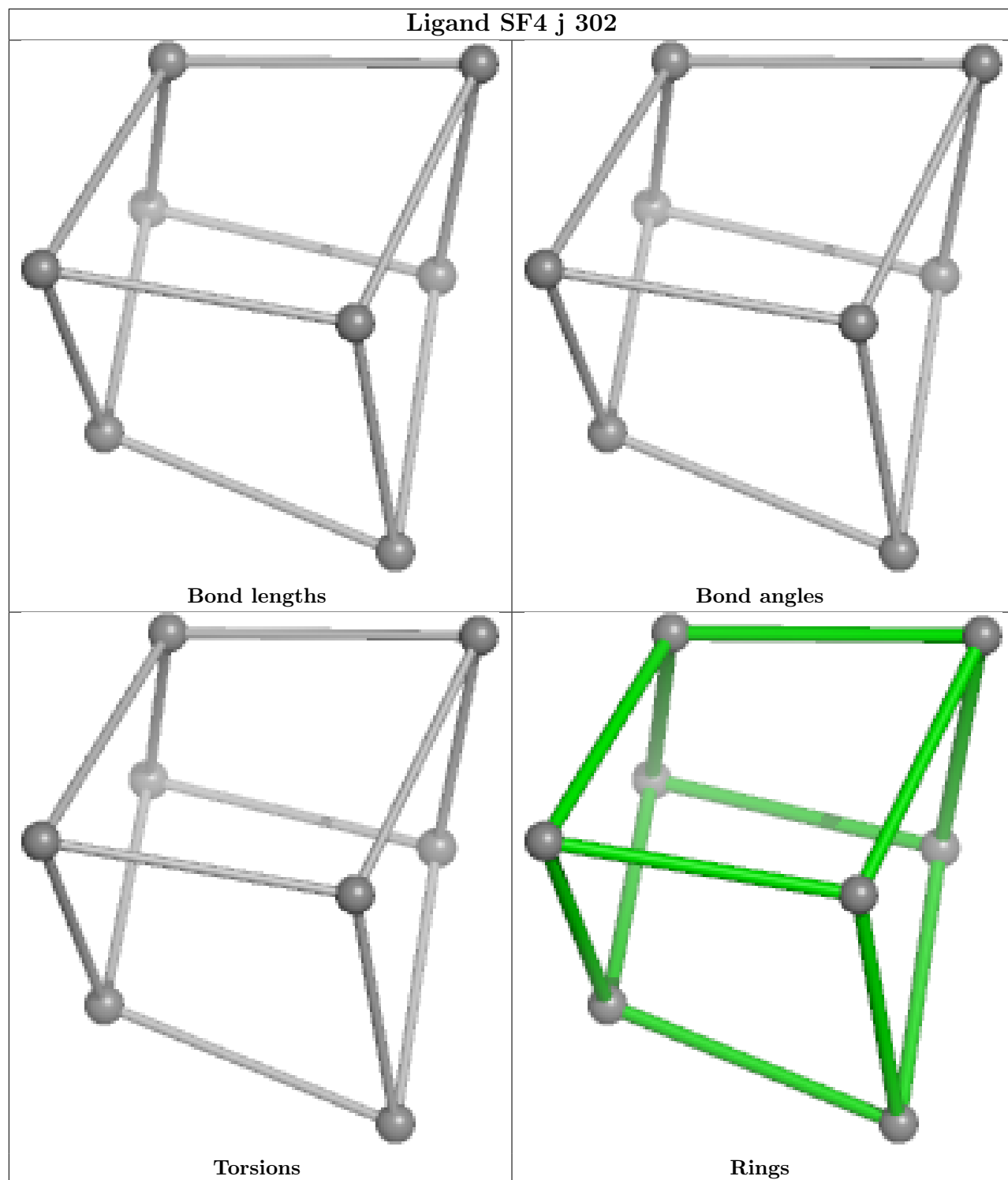


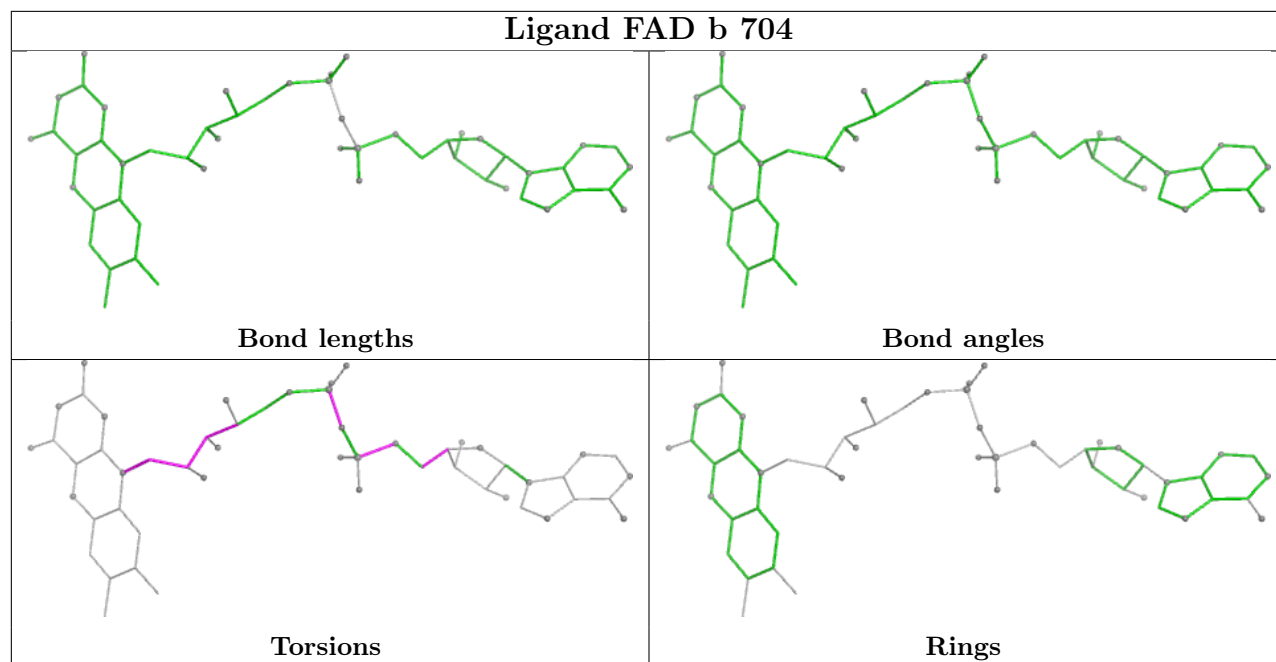


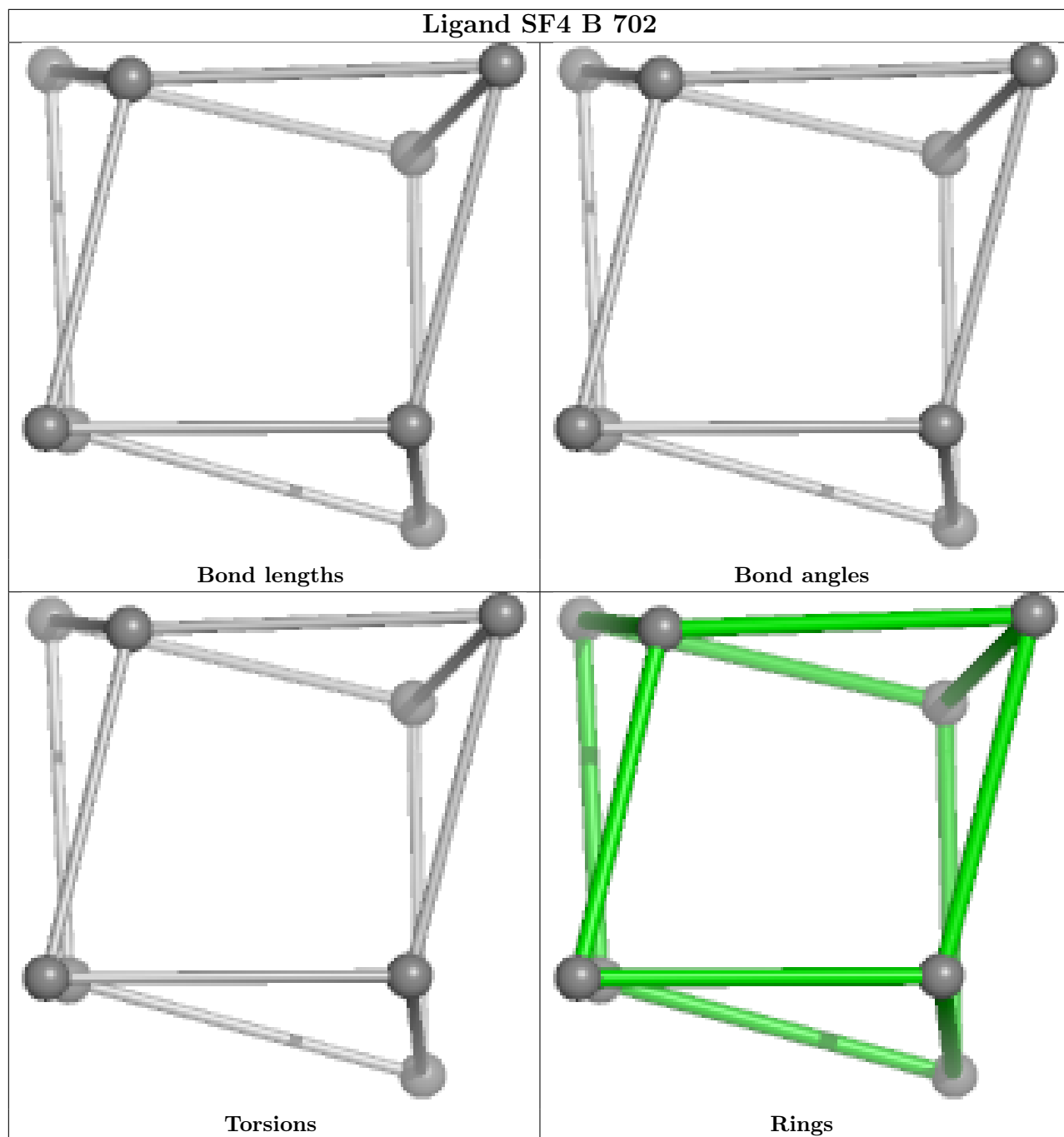


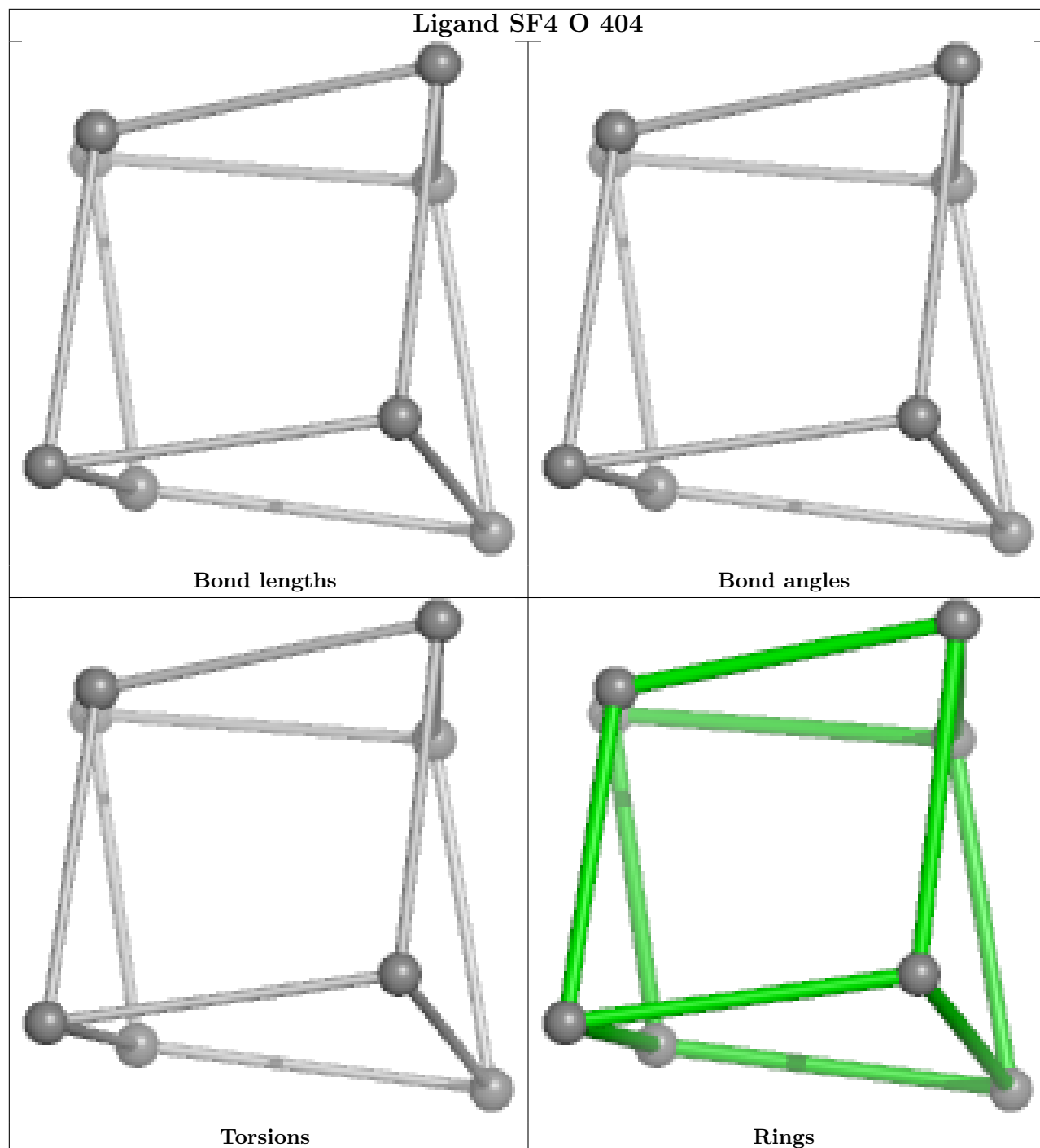


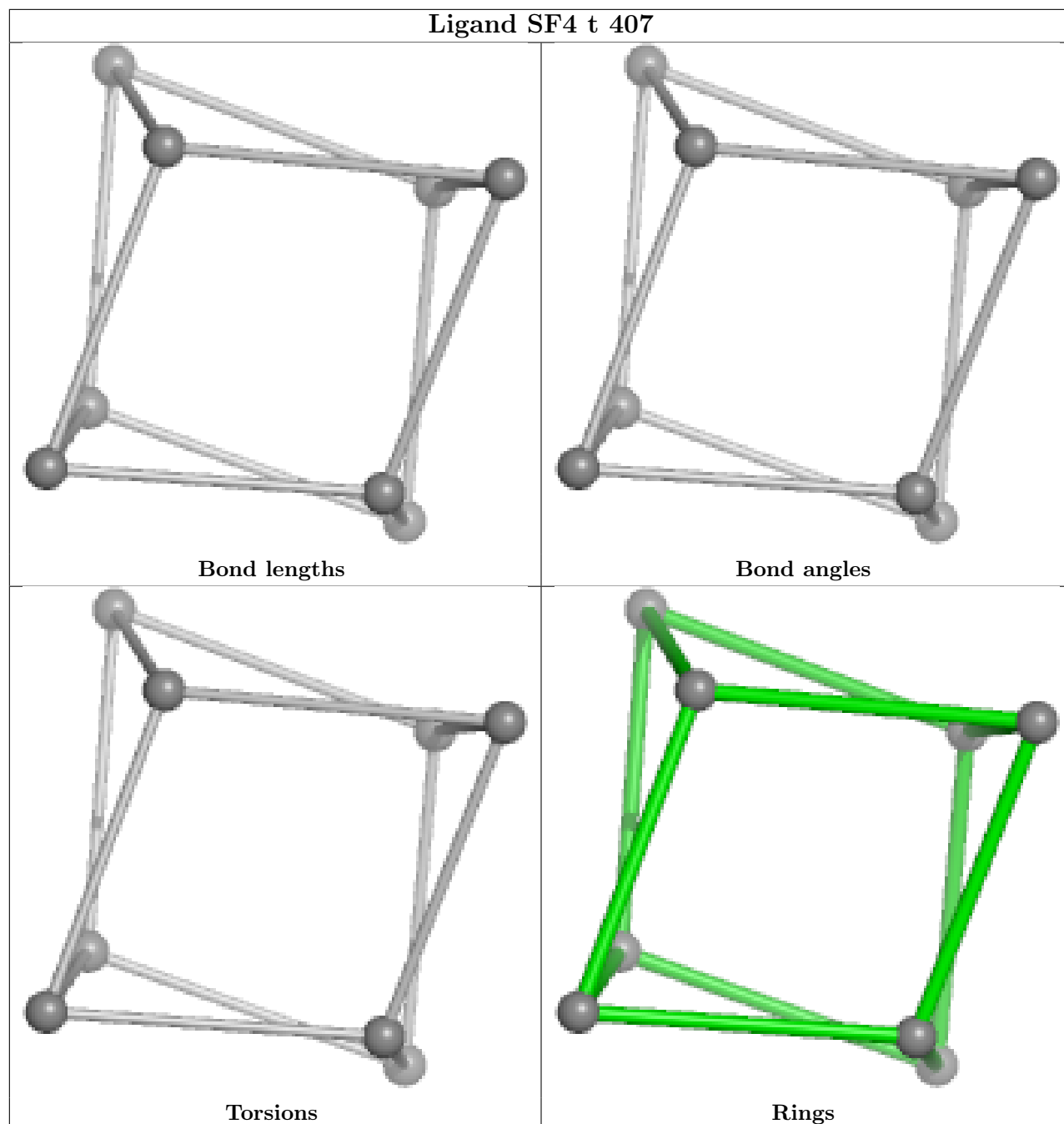


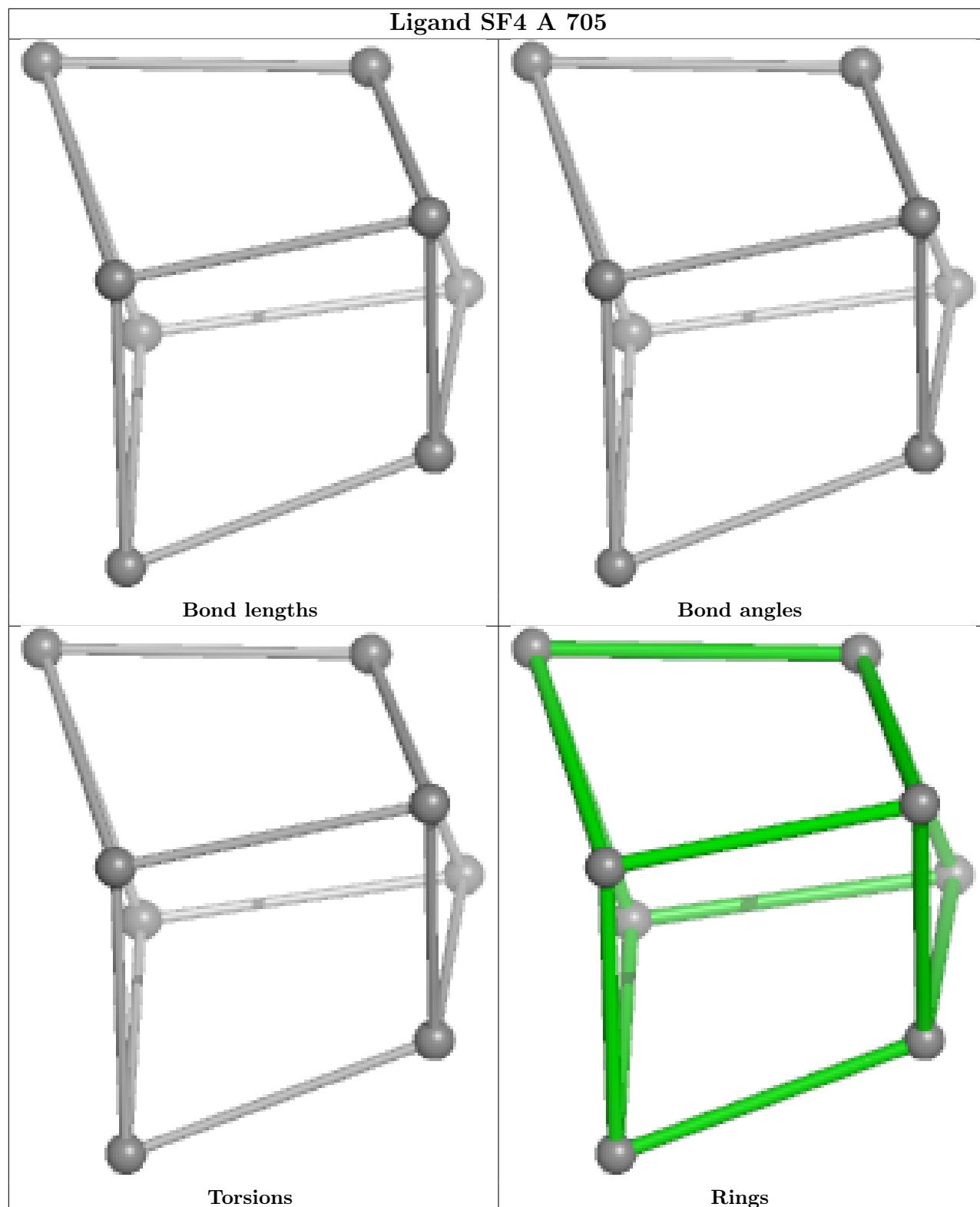


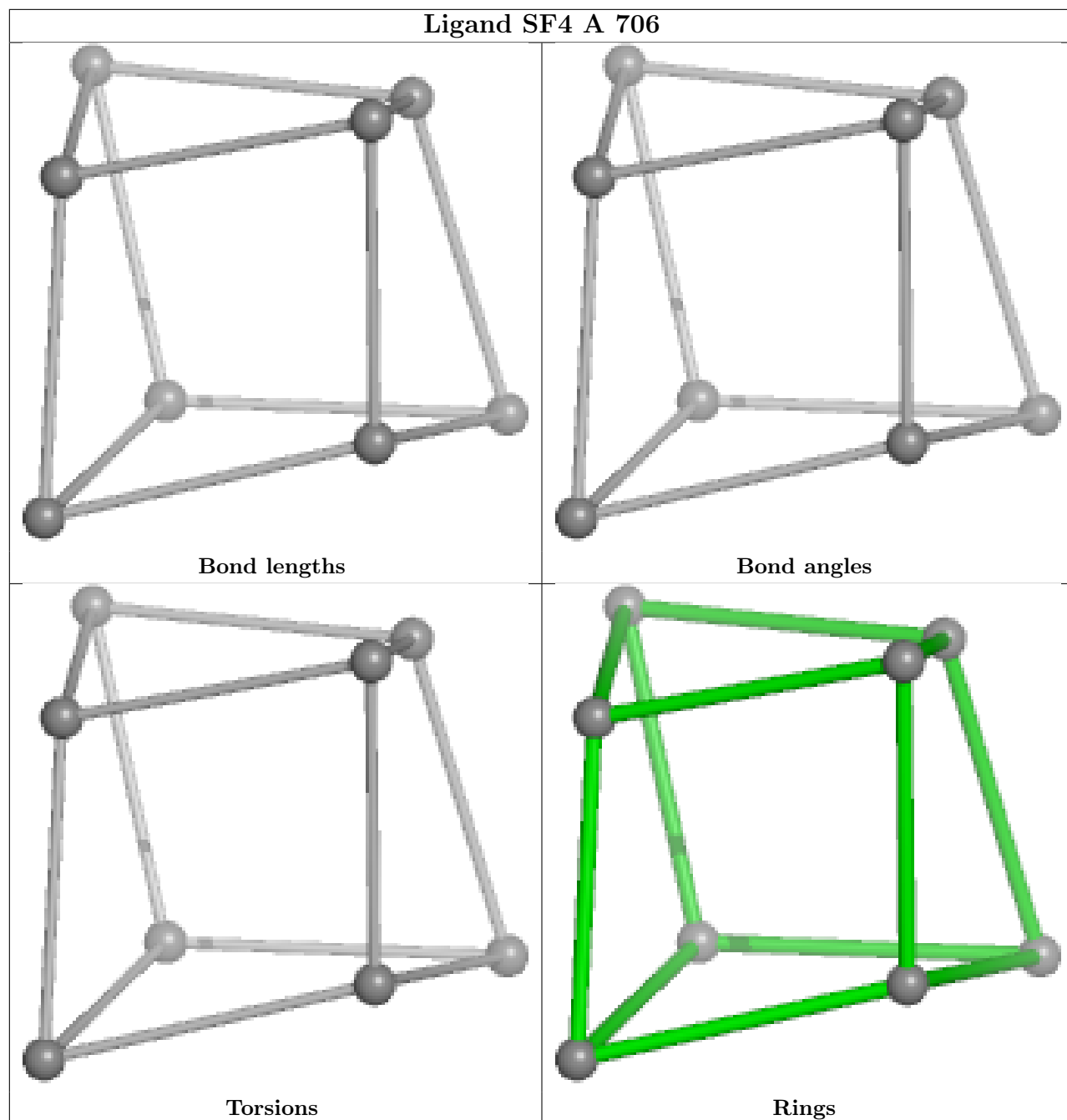


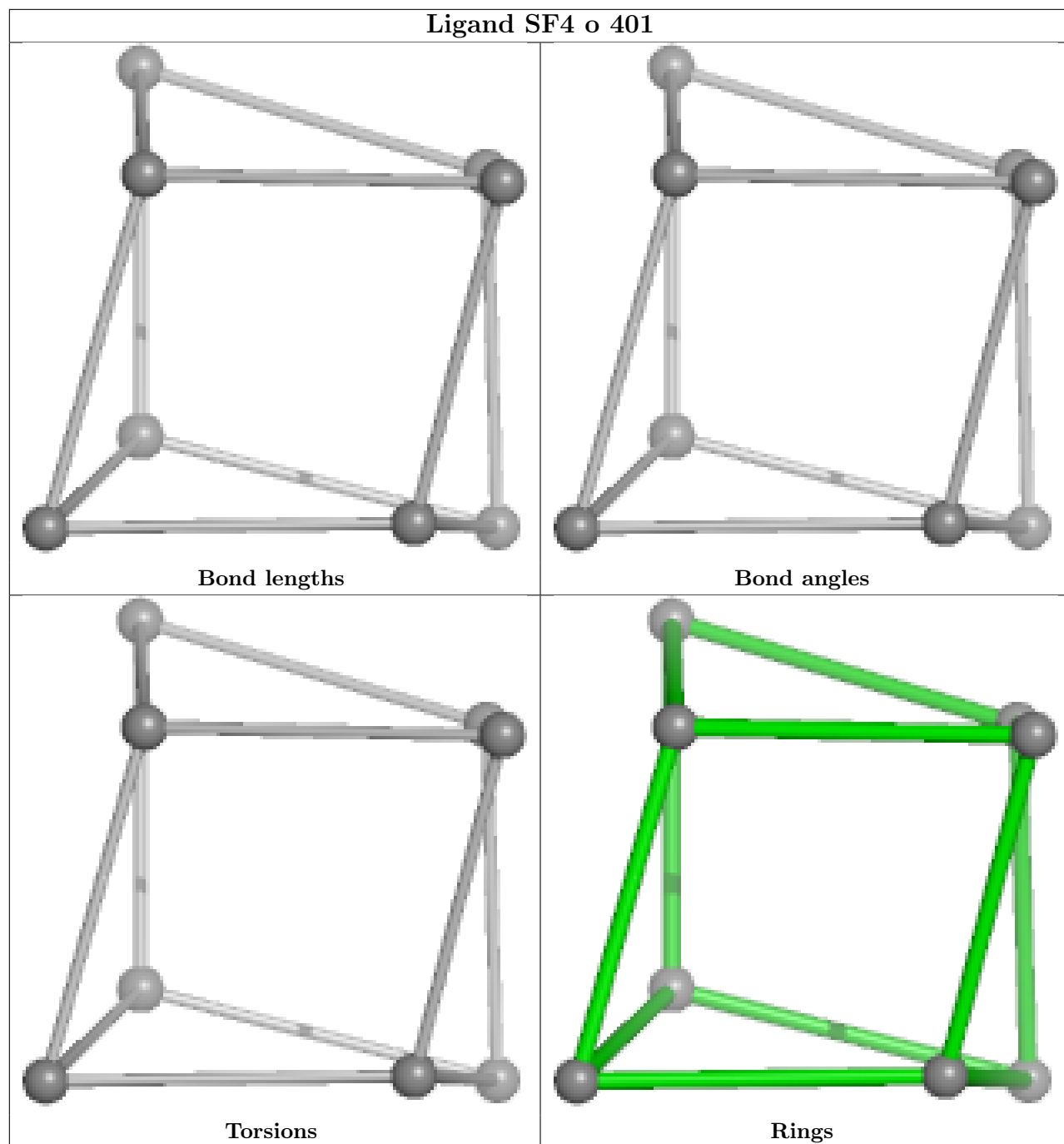


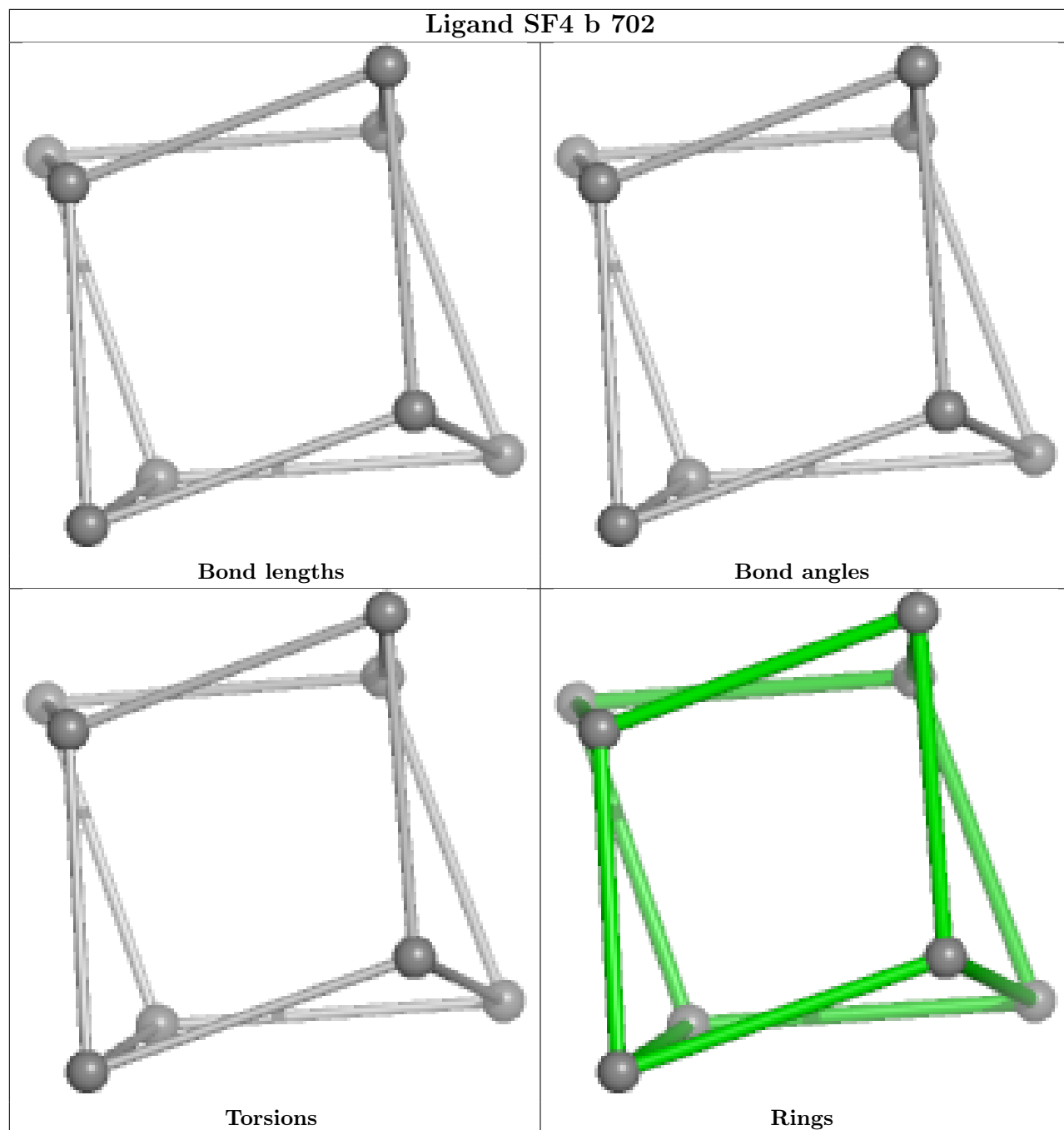


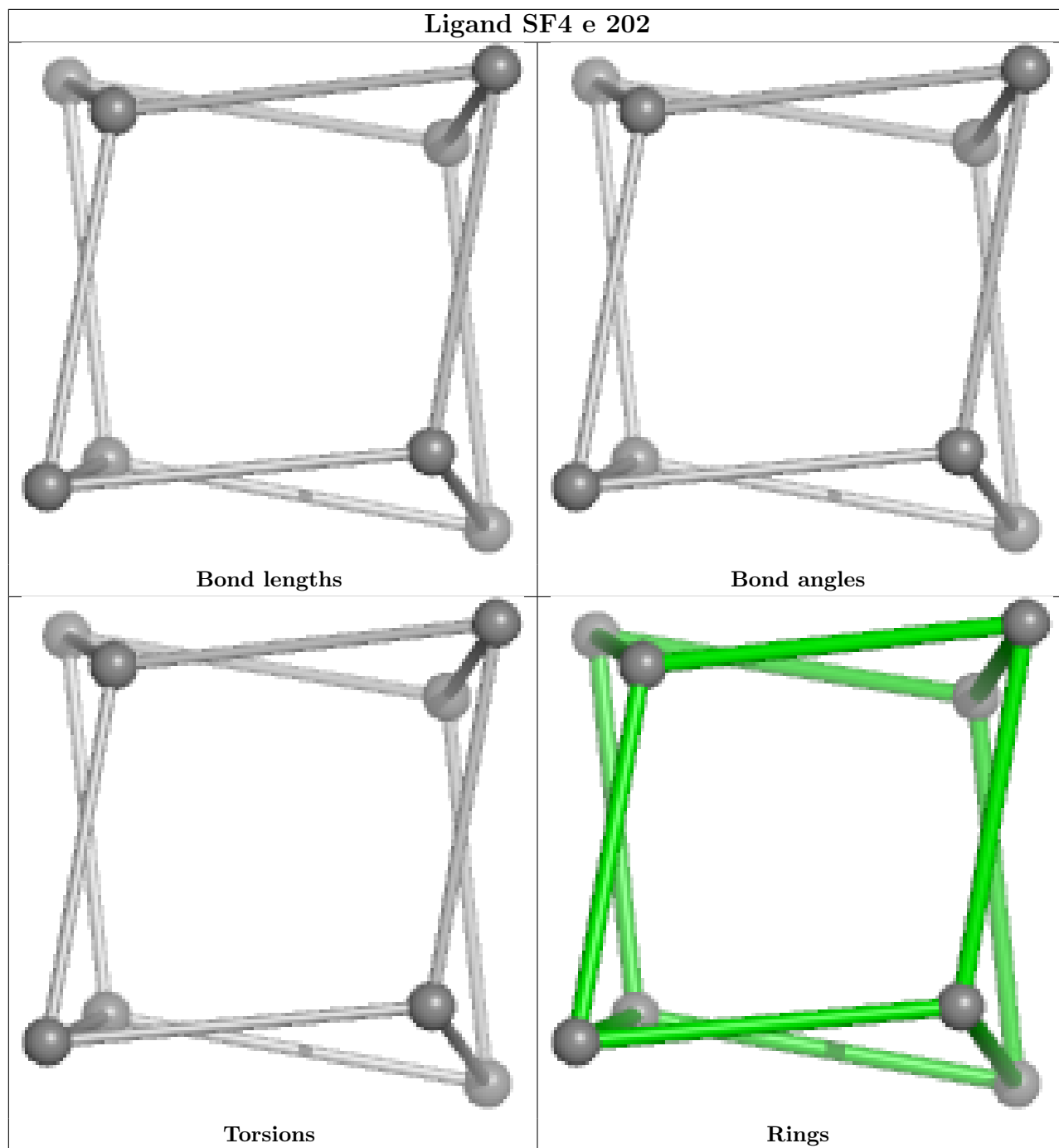


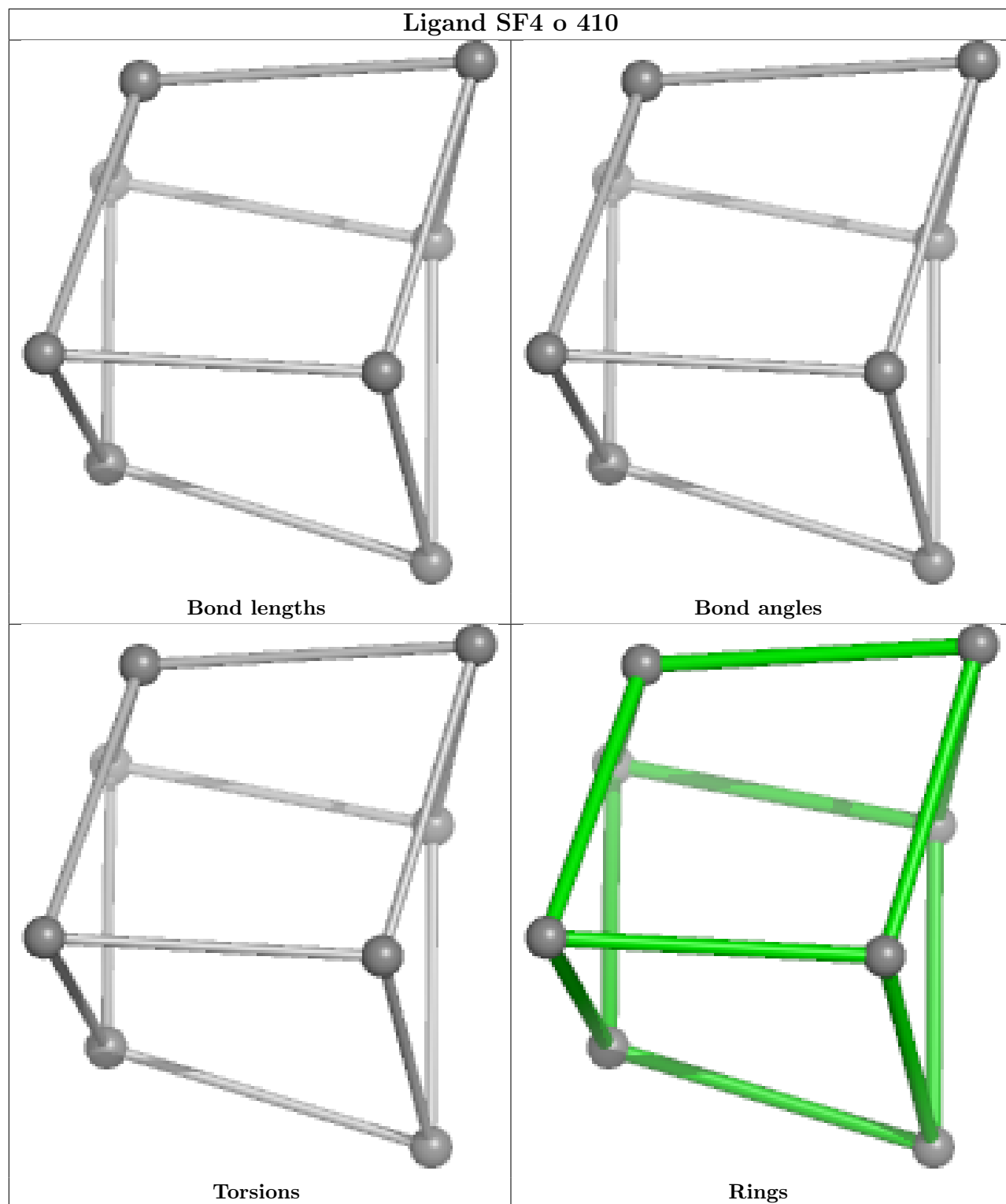


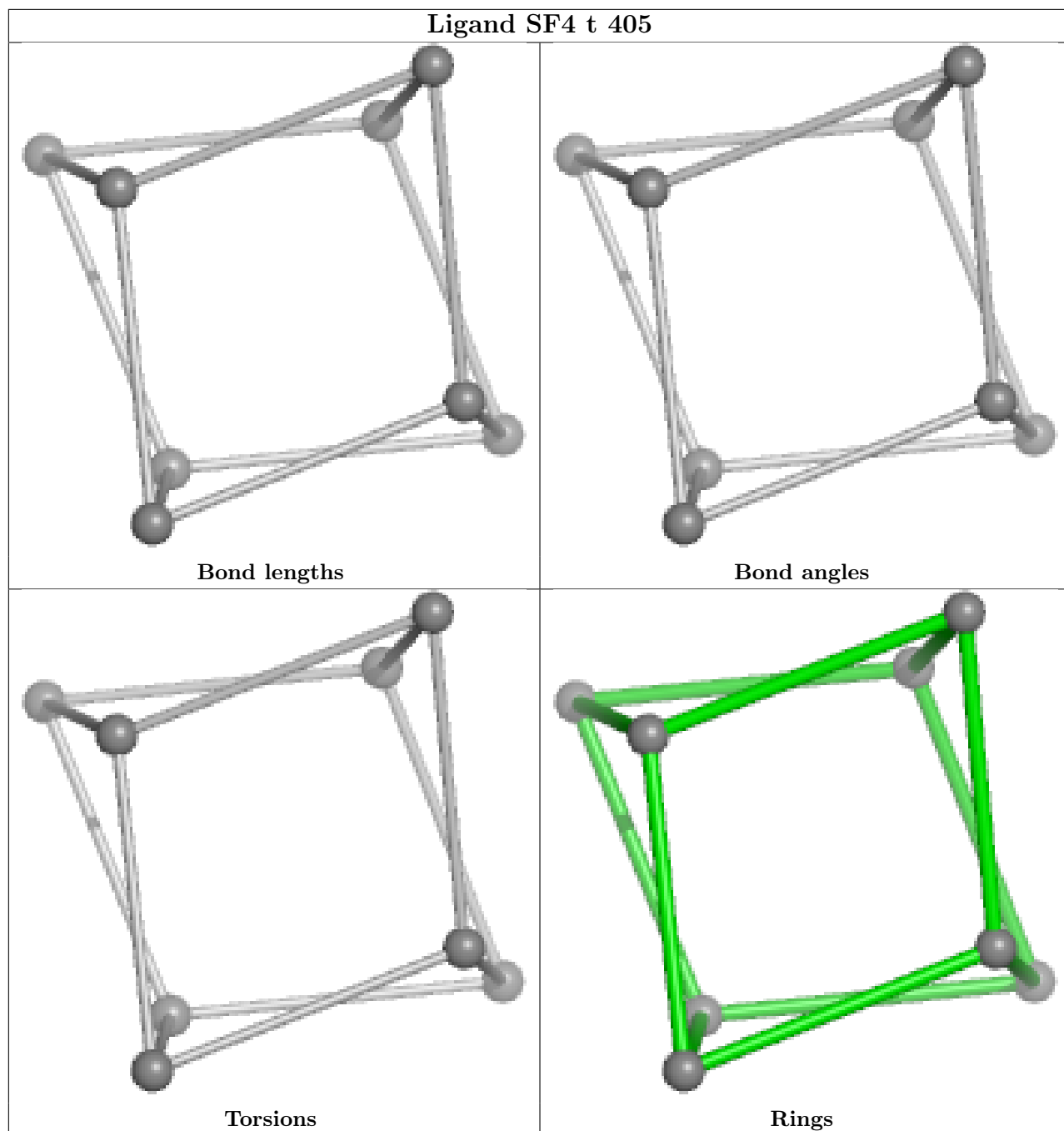


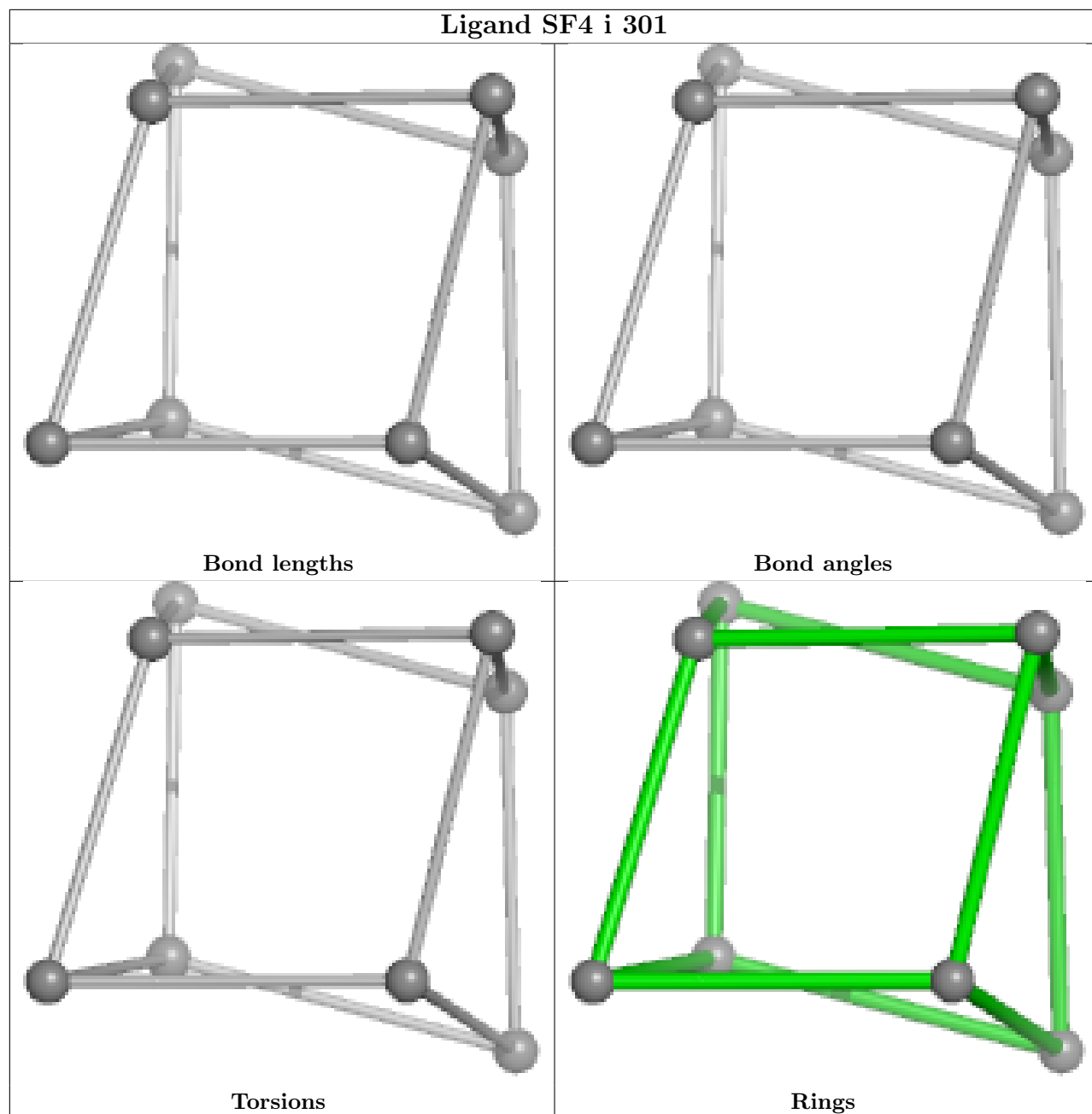


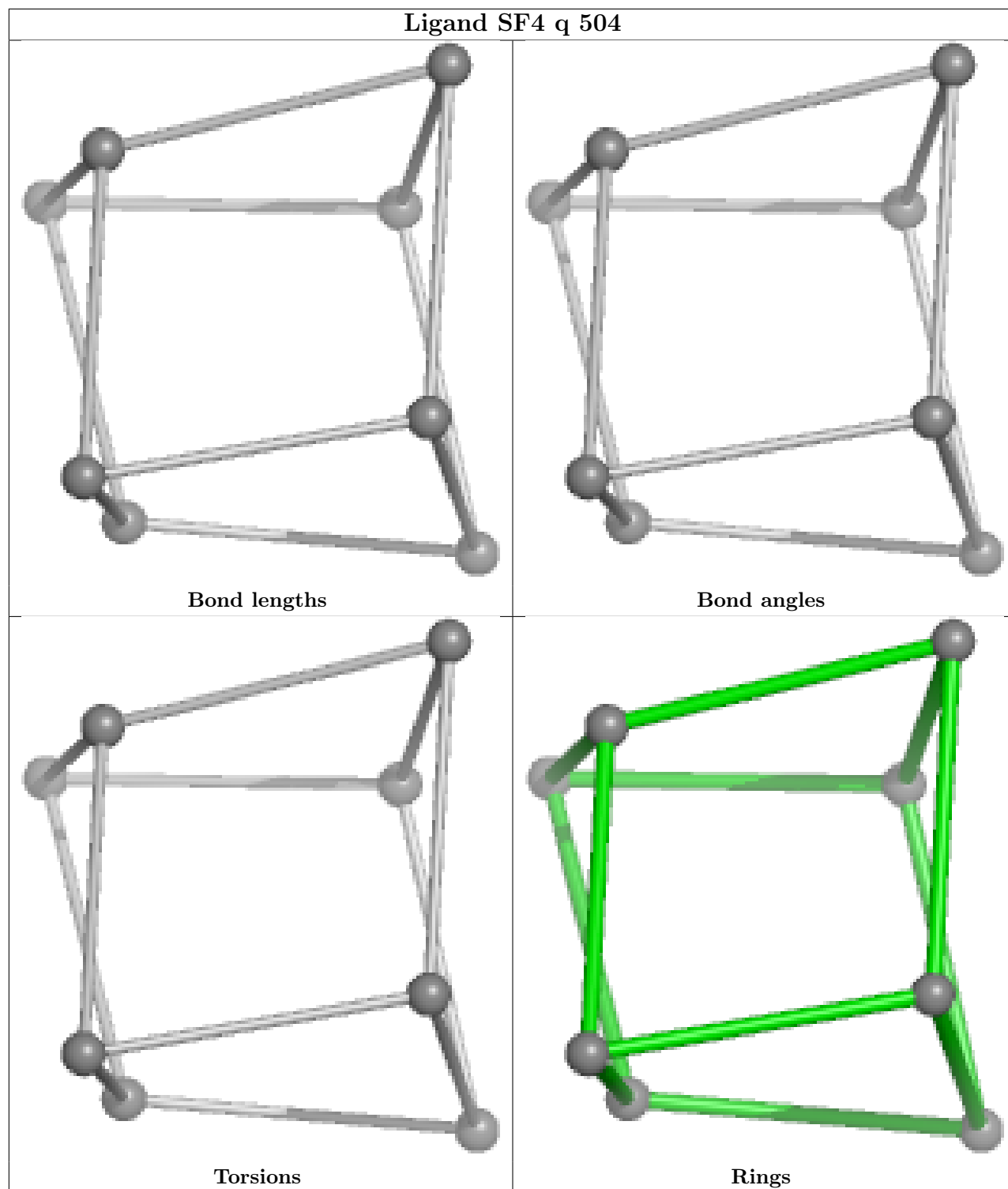


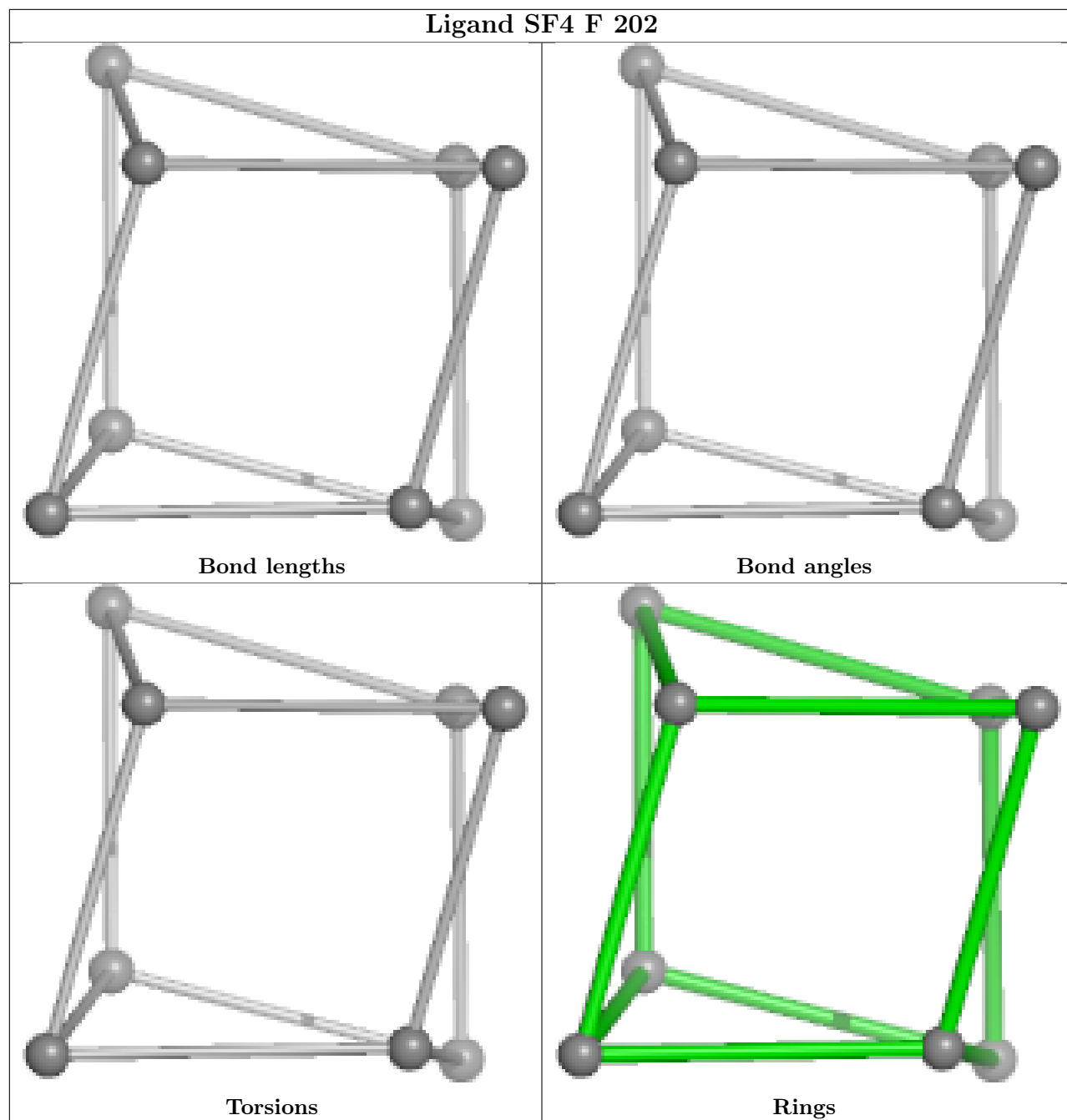




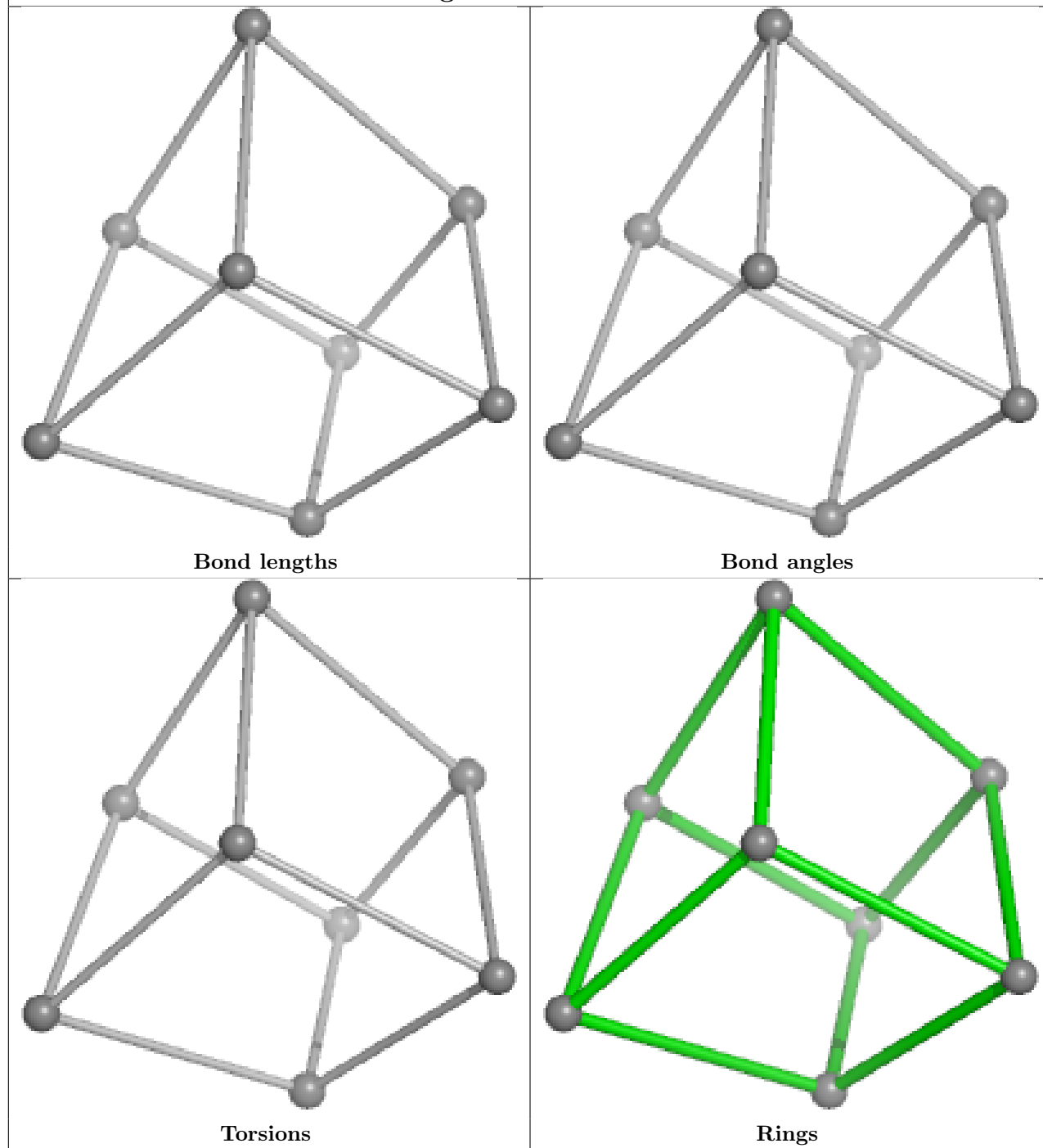


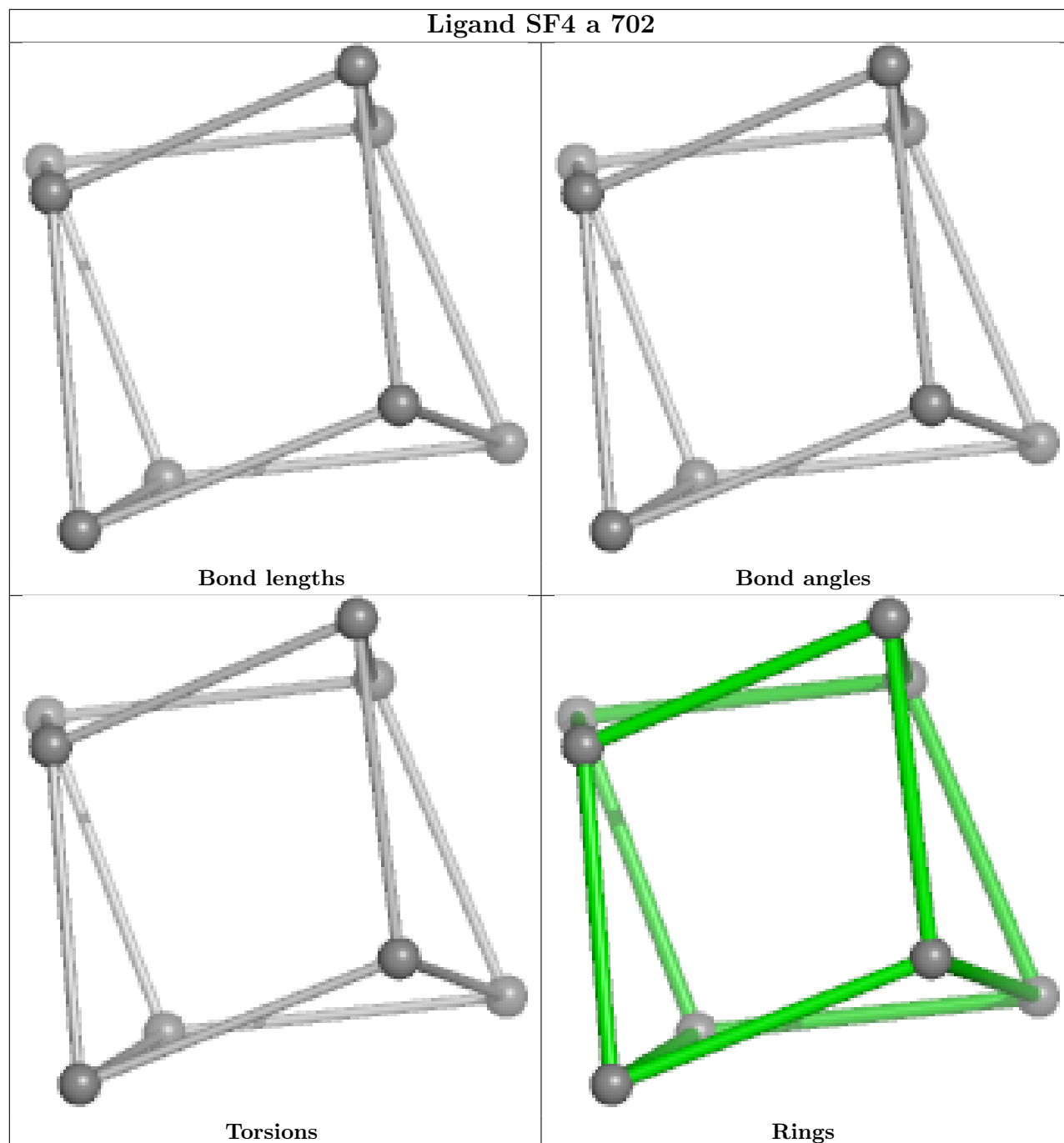




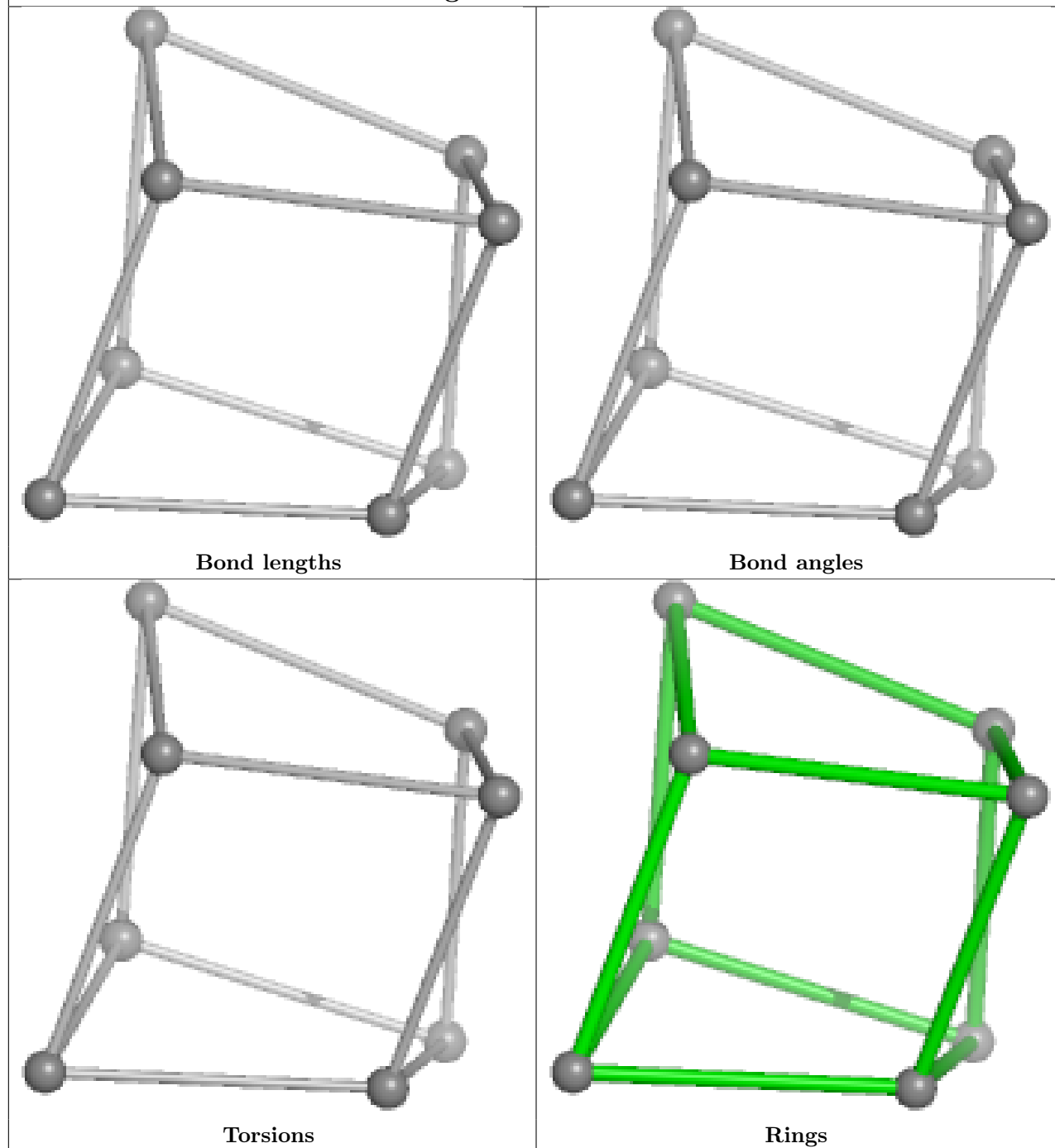


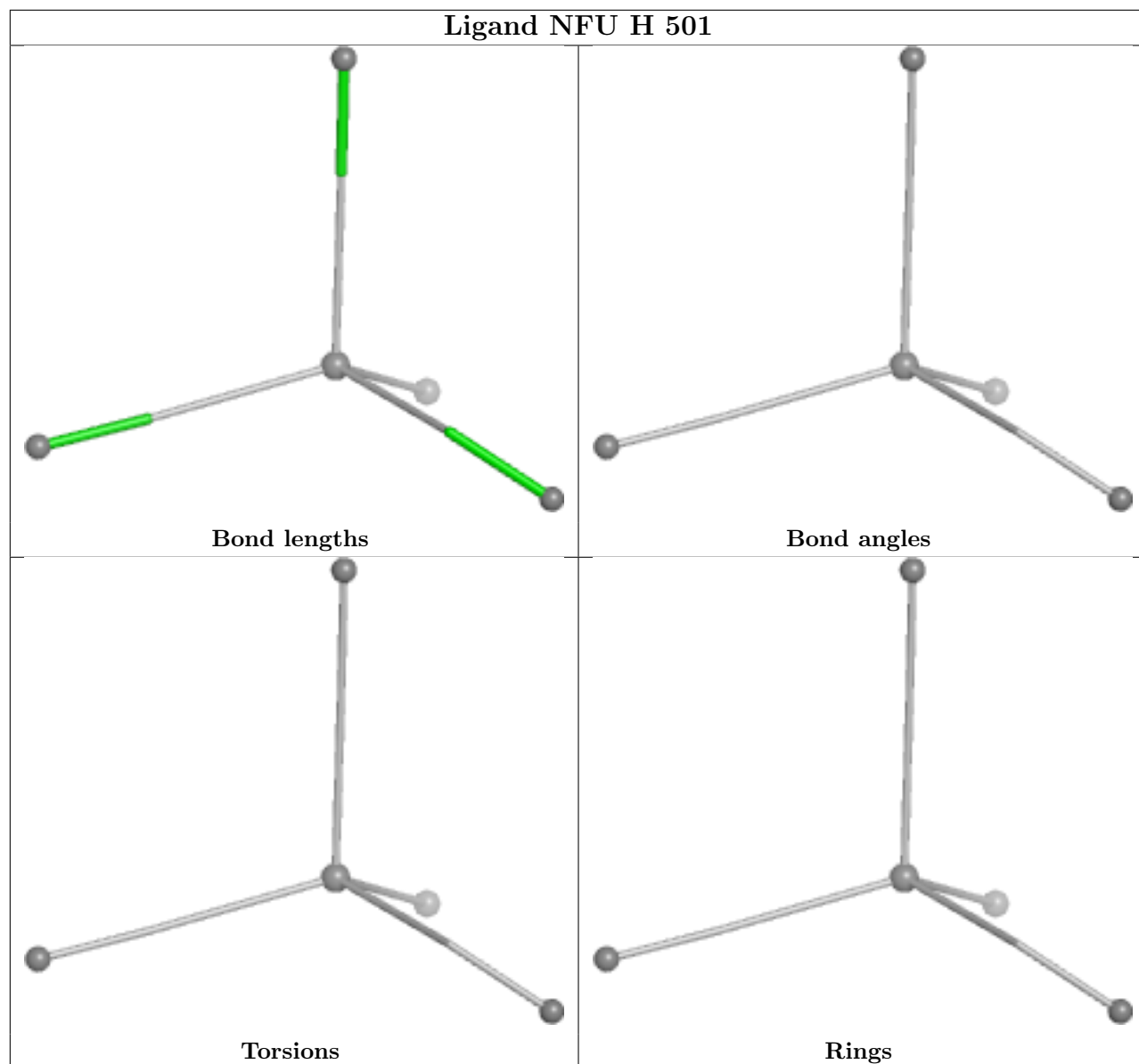
Ligand SF4 A 701

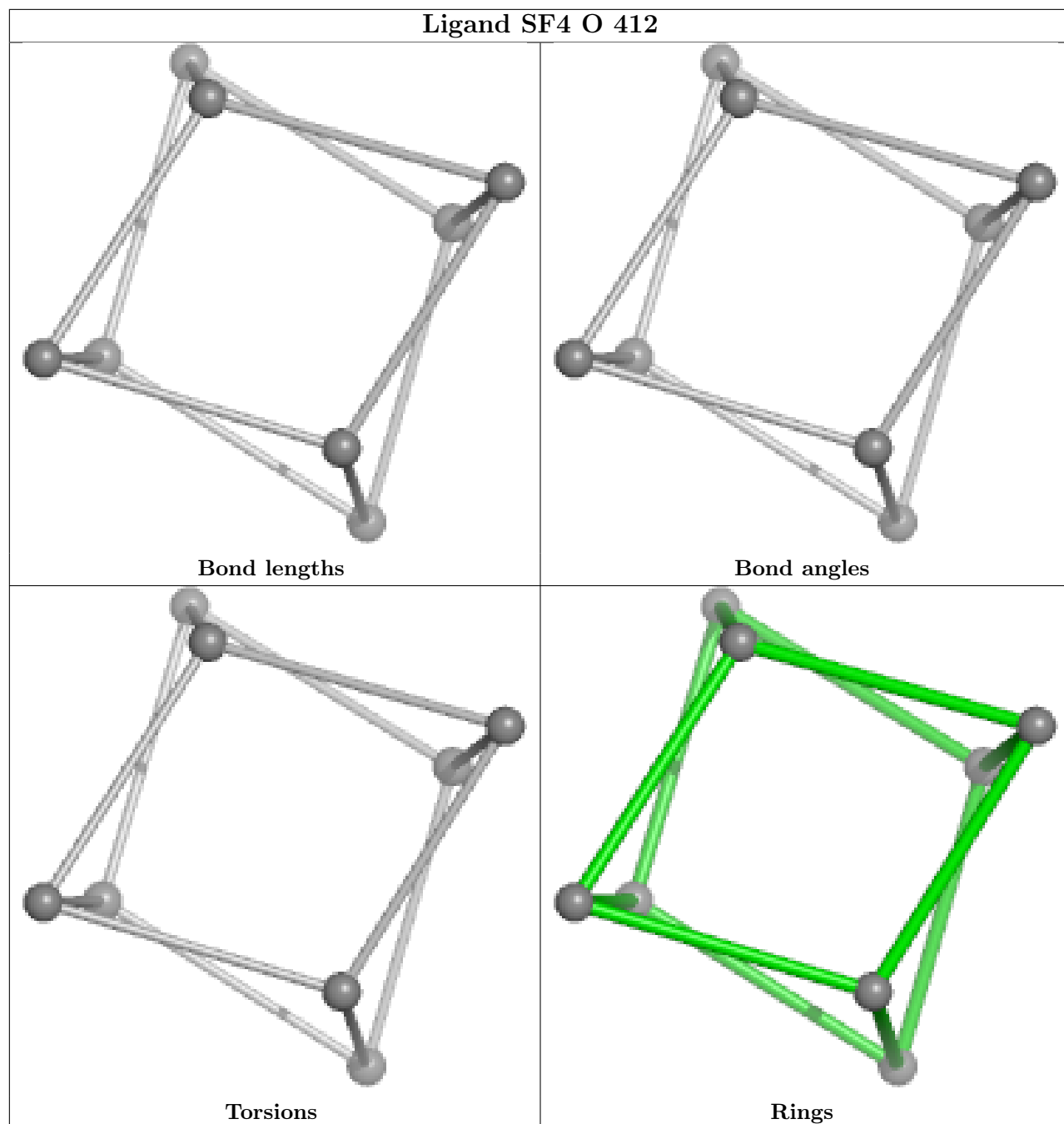


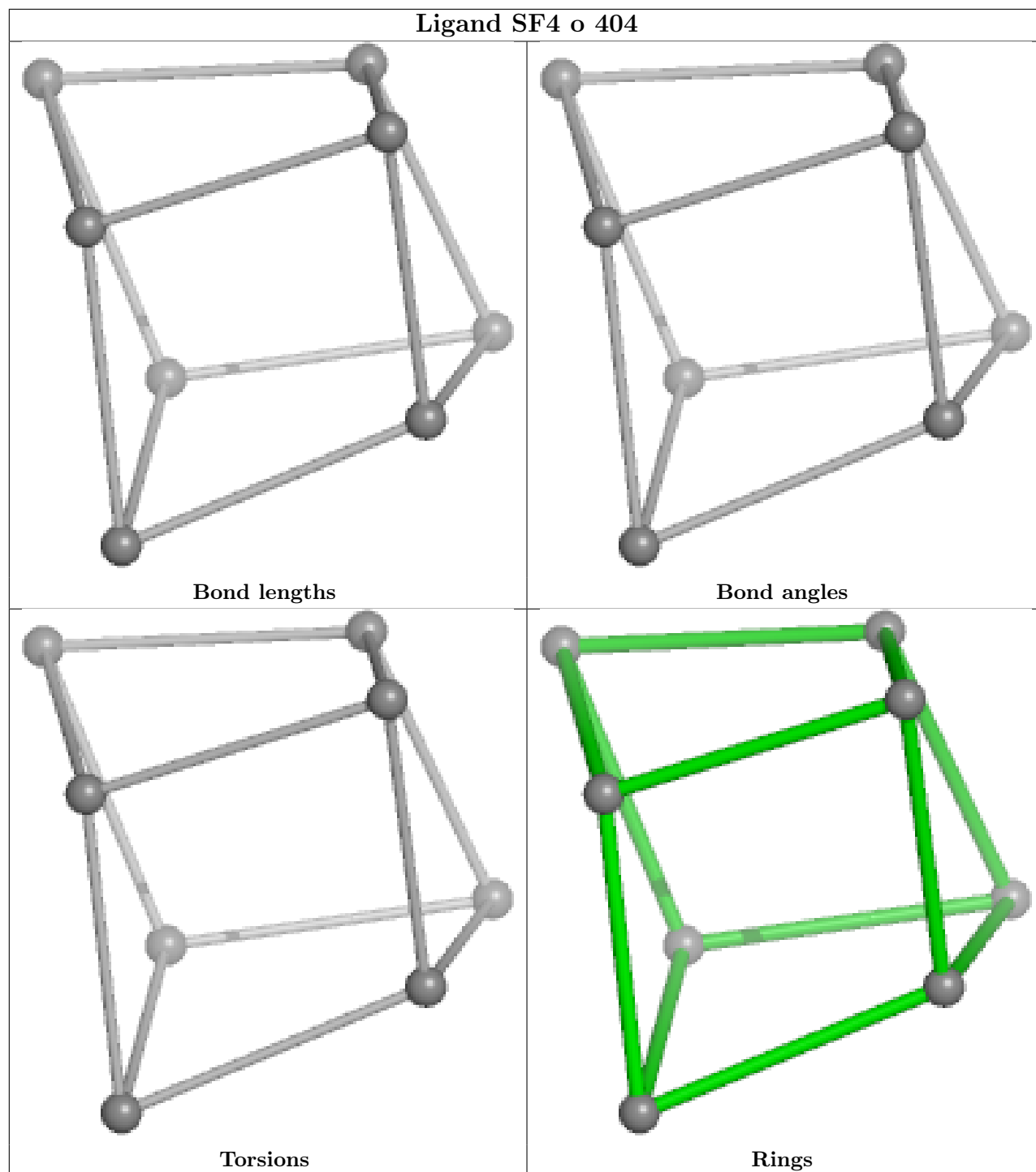


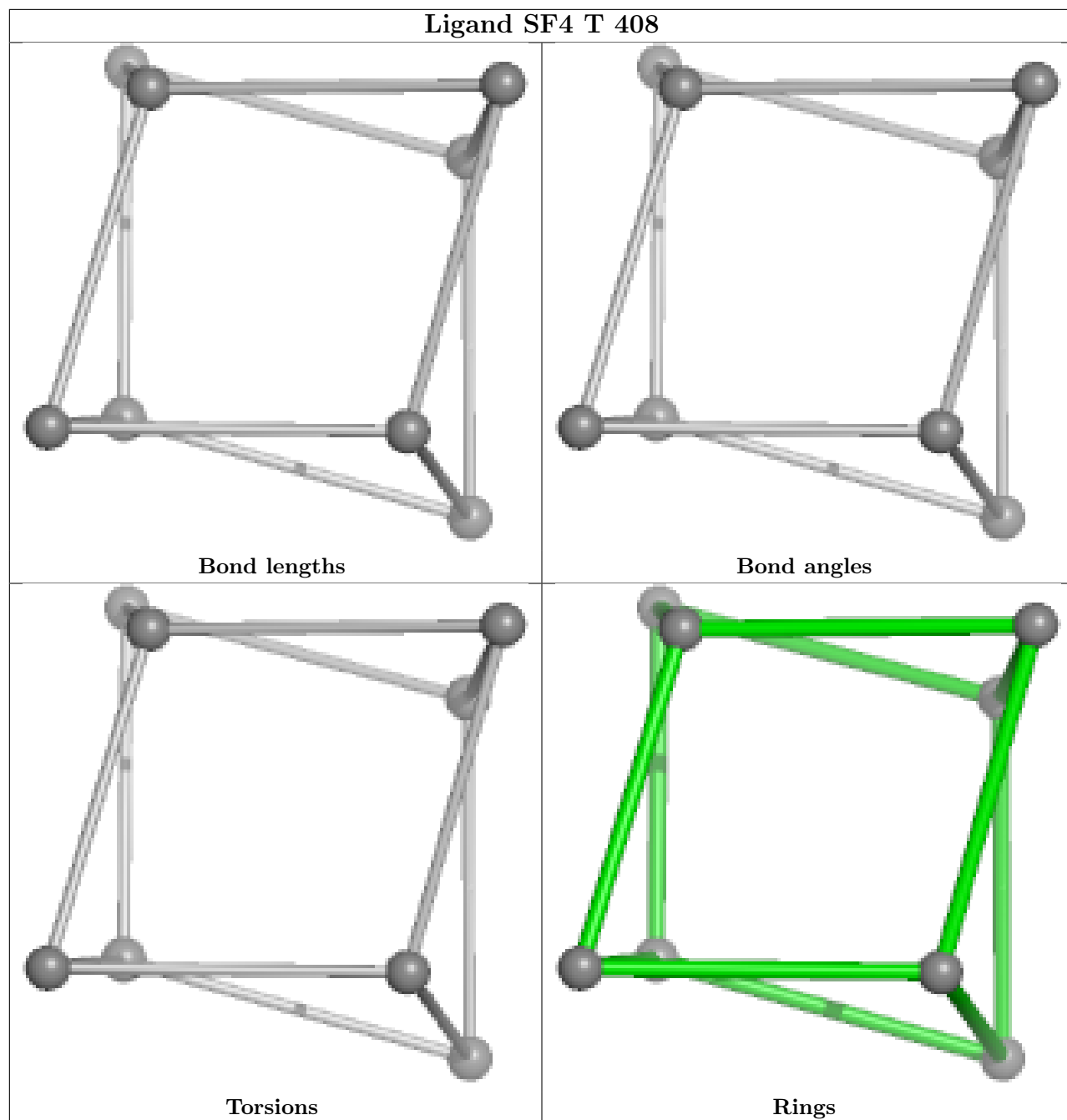
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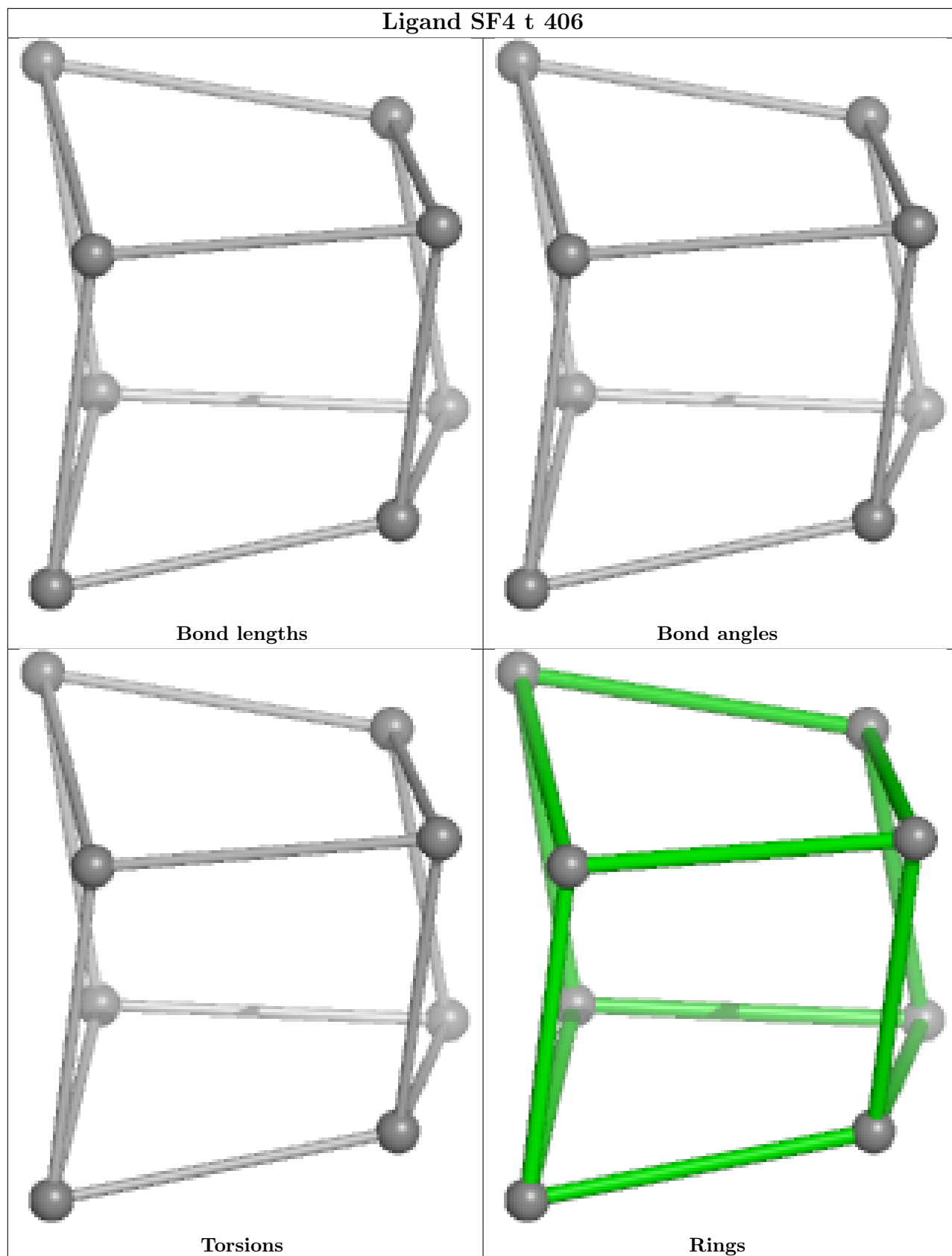


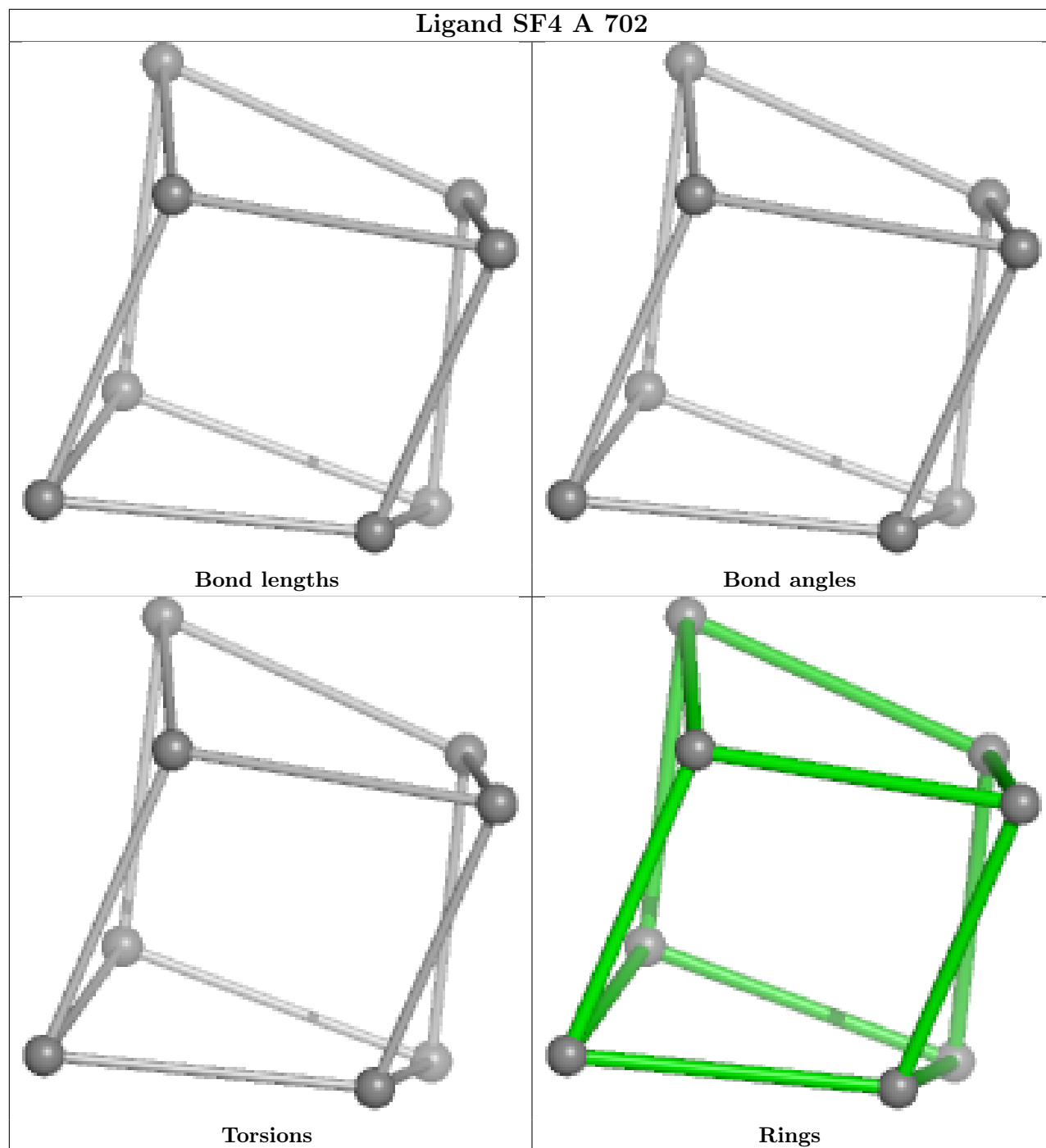


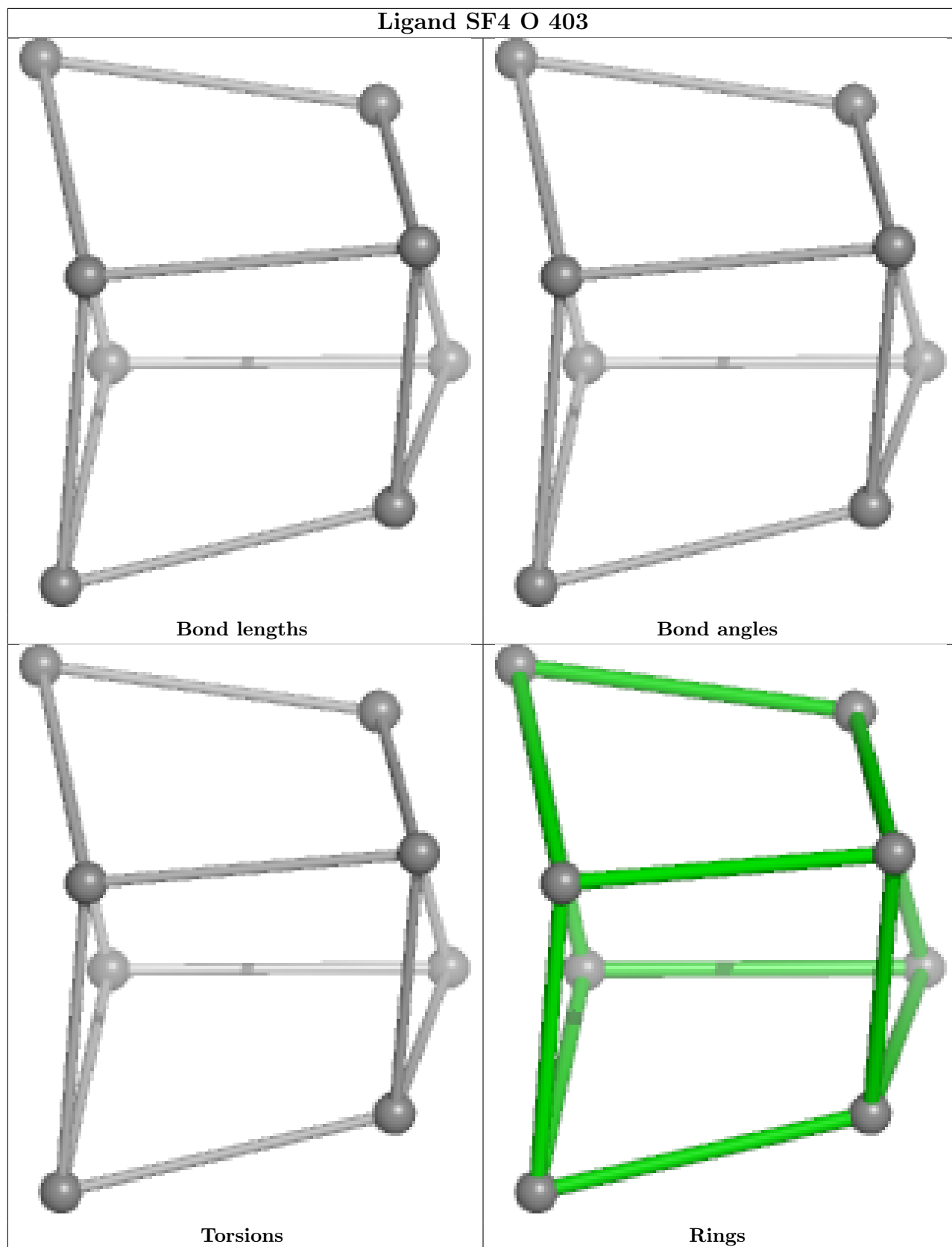


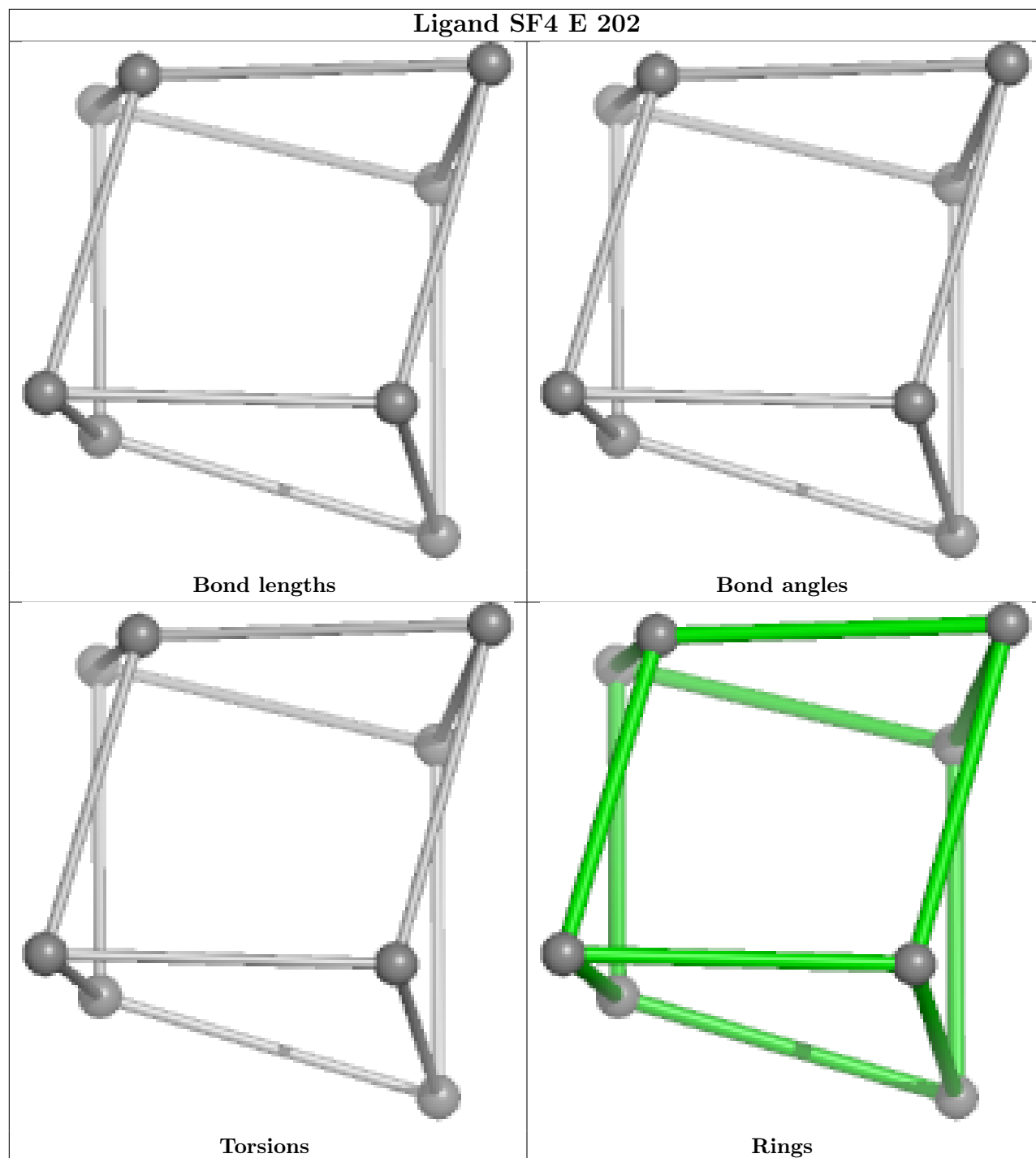


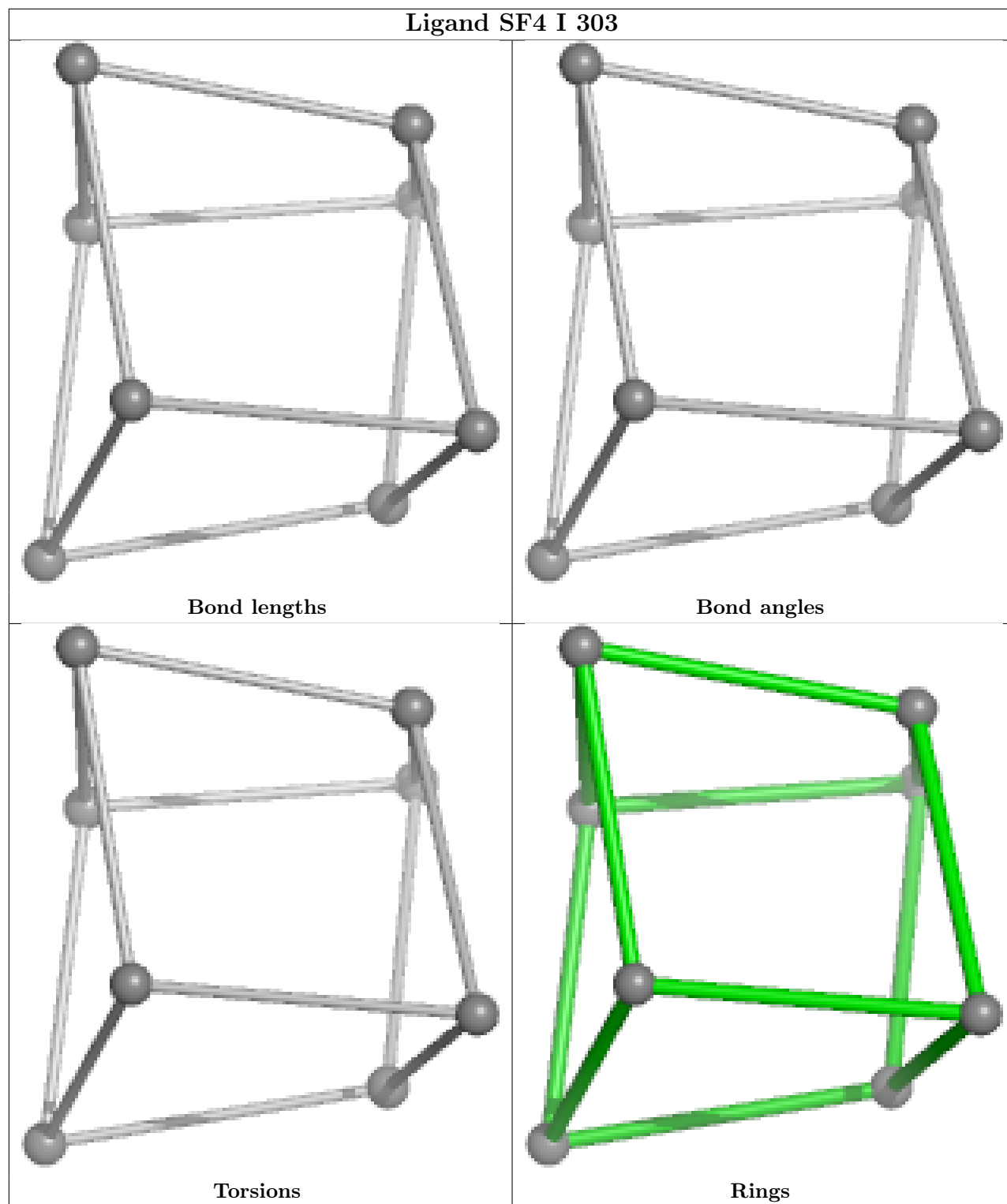


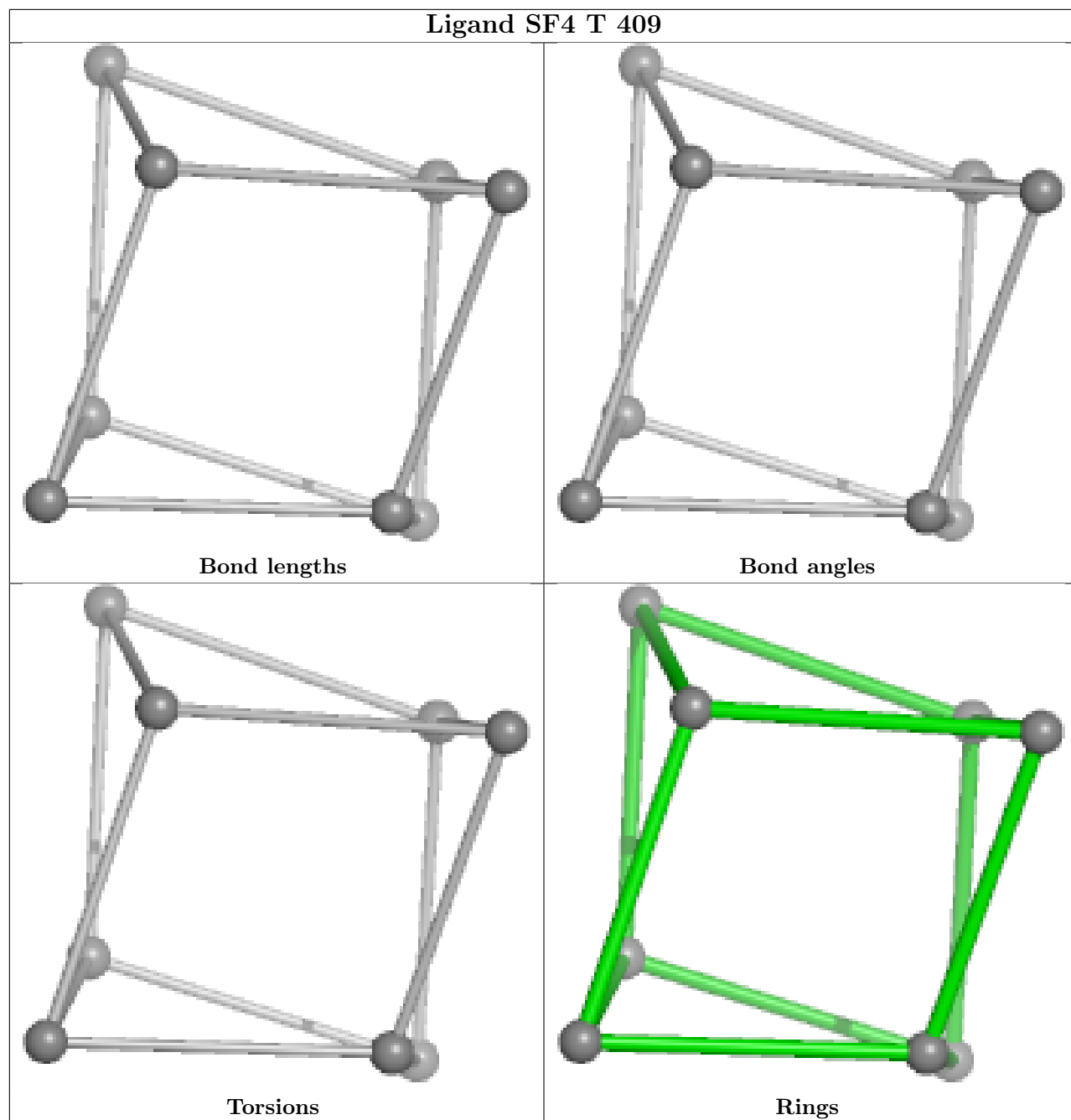


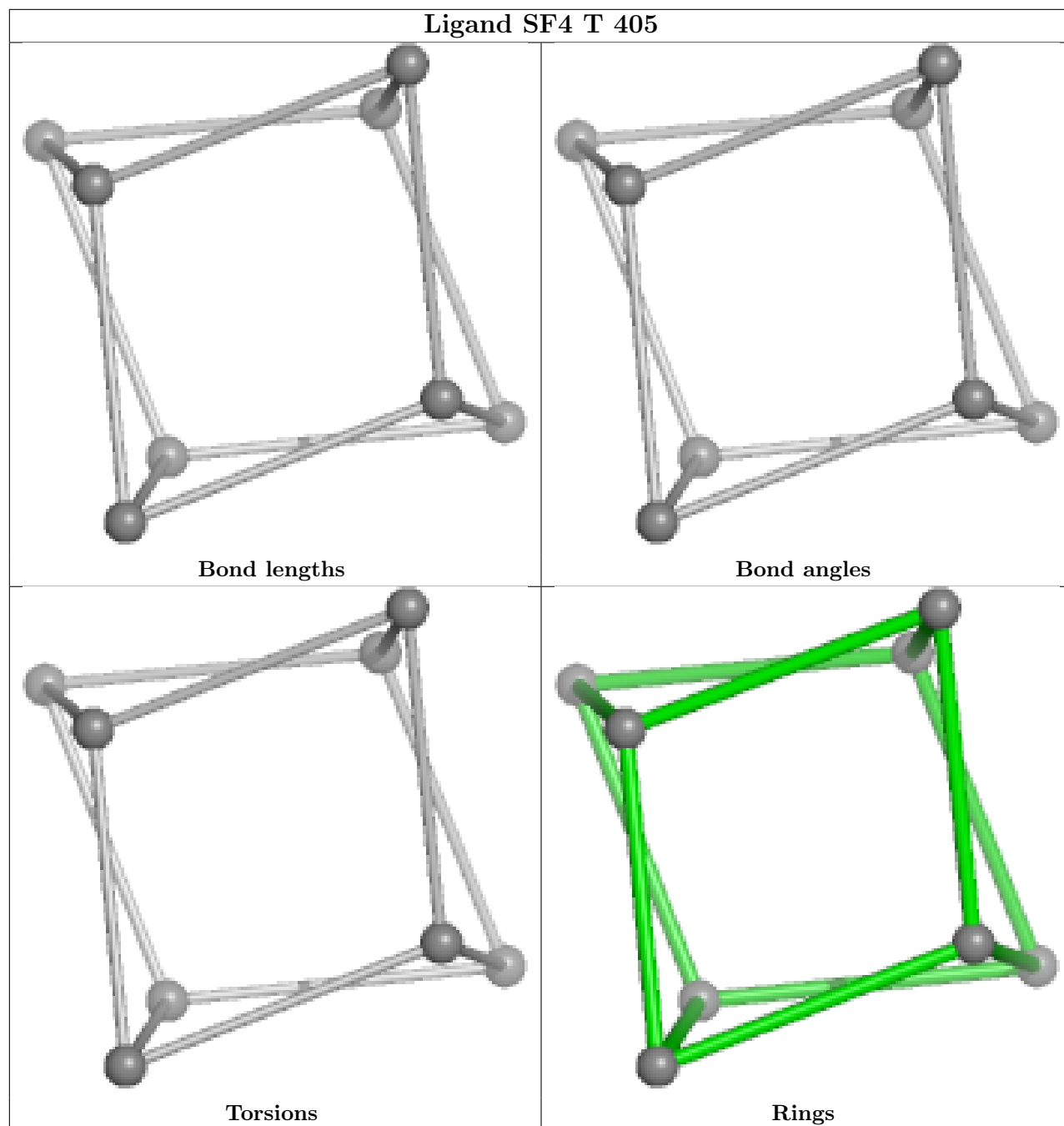


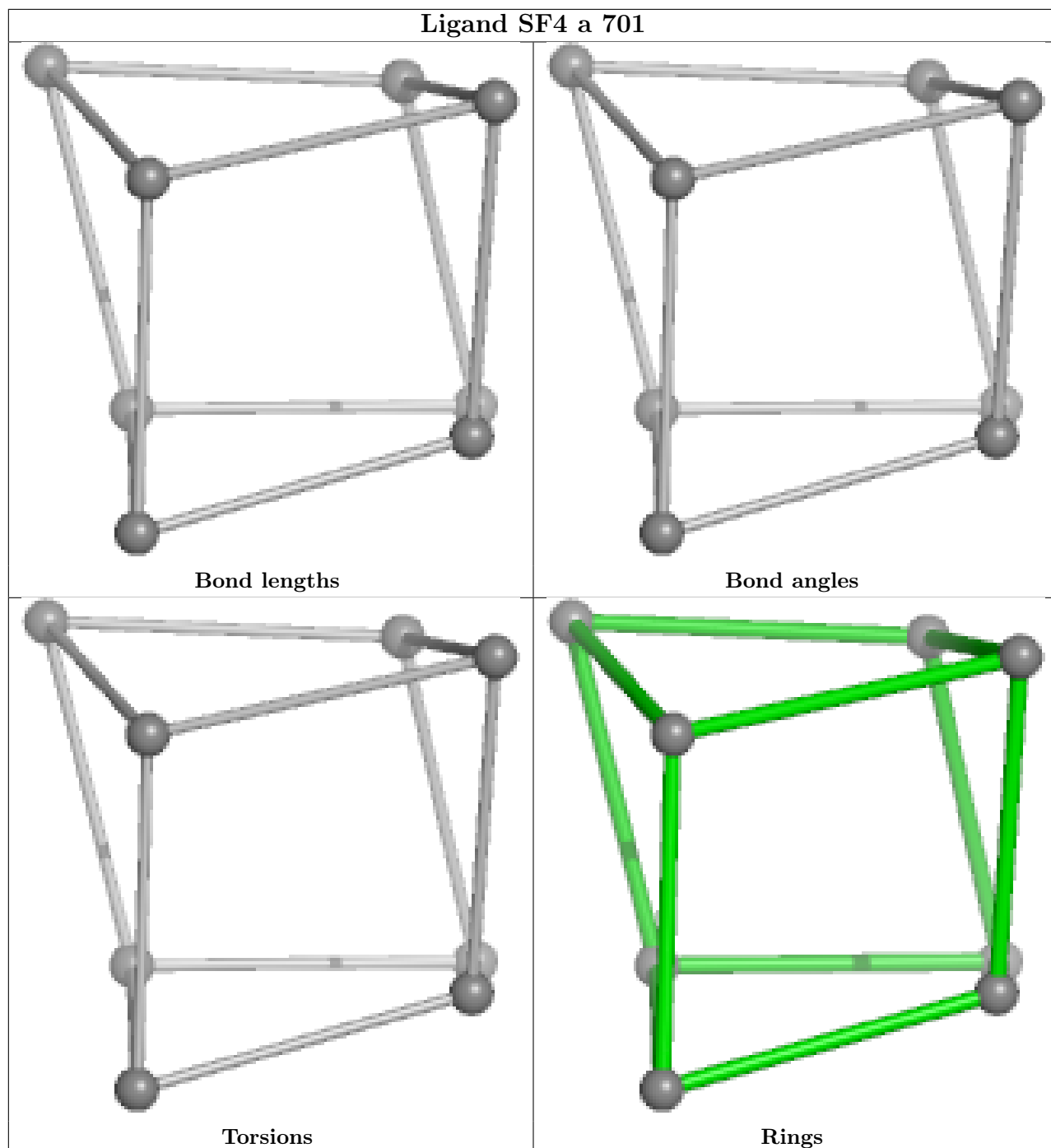


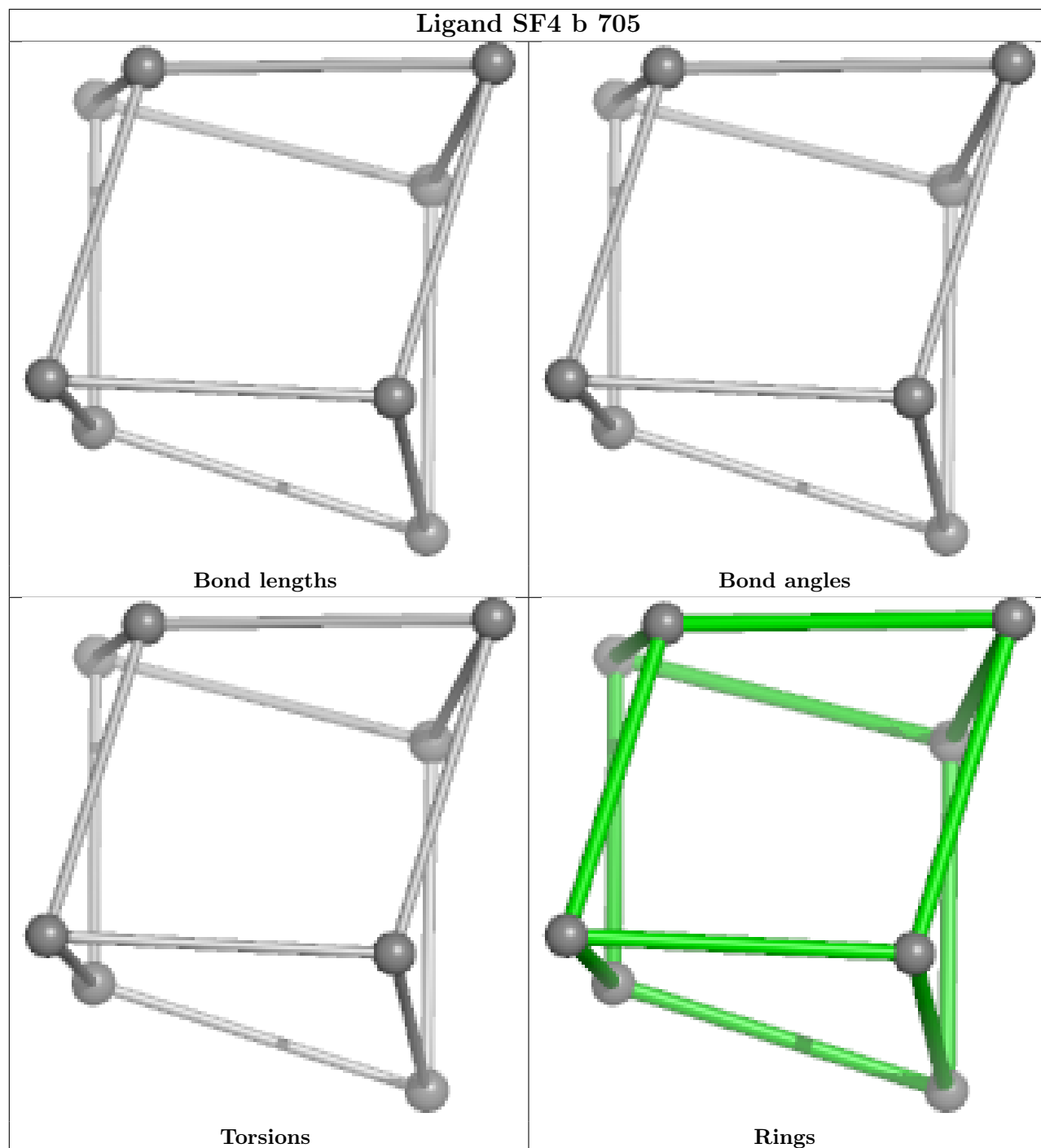


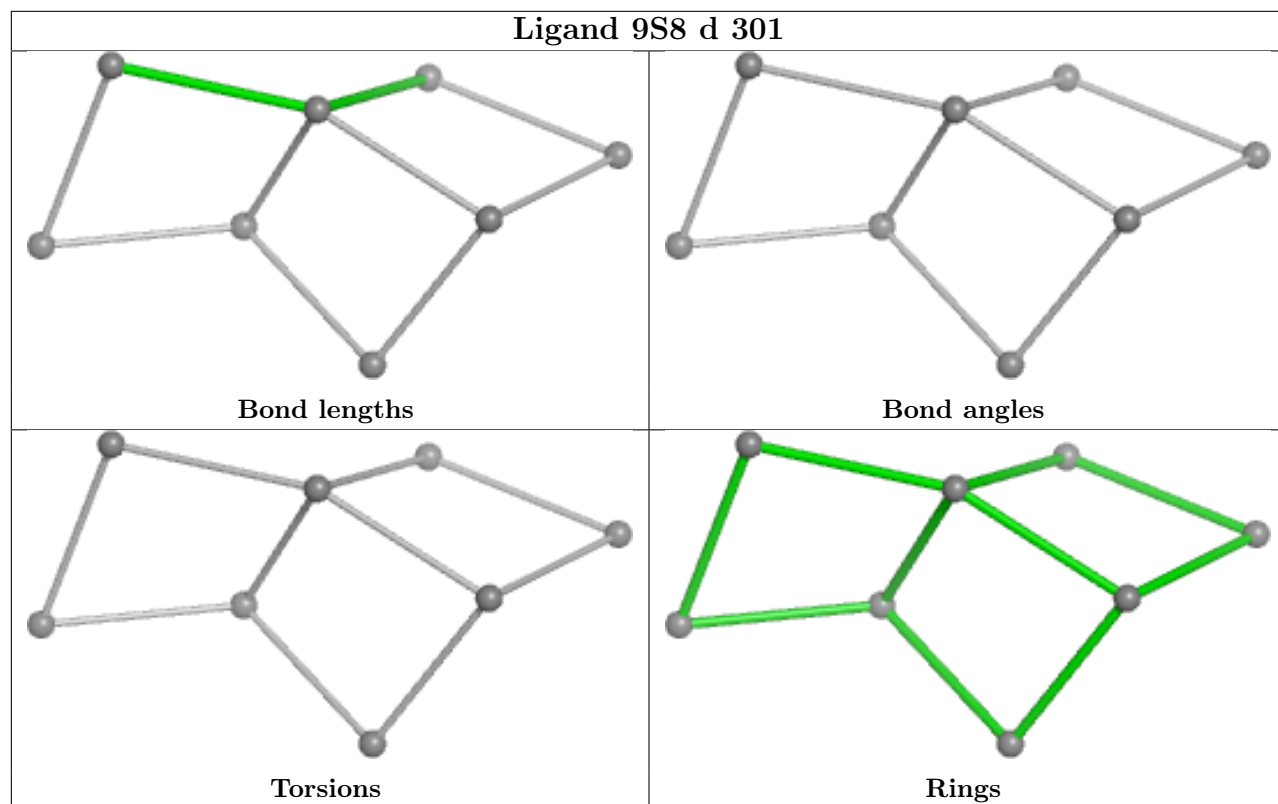


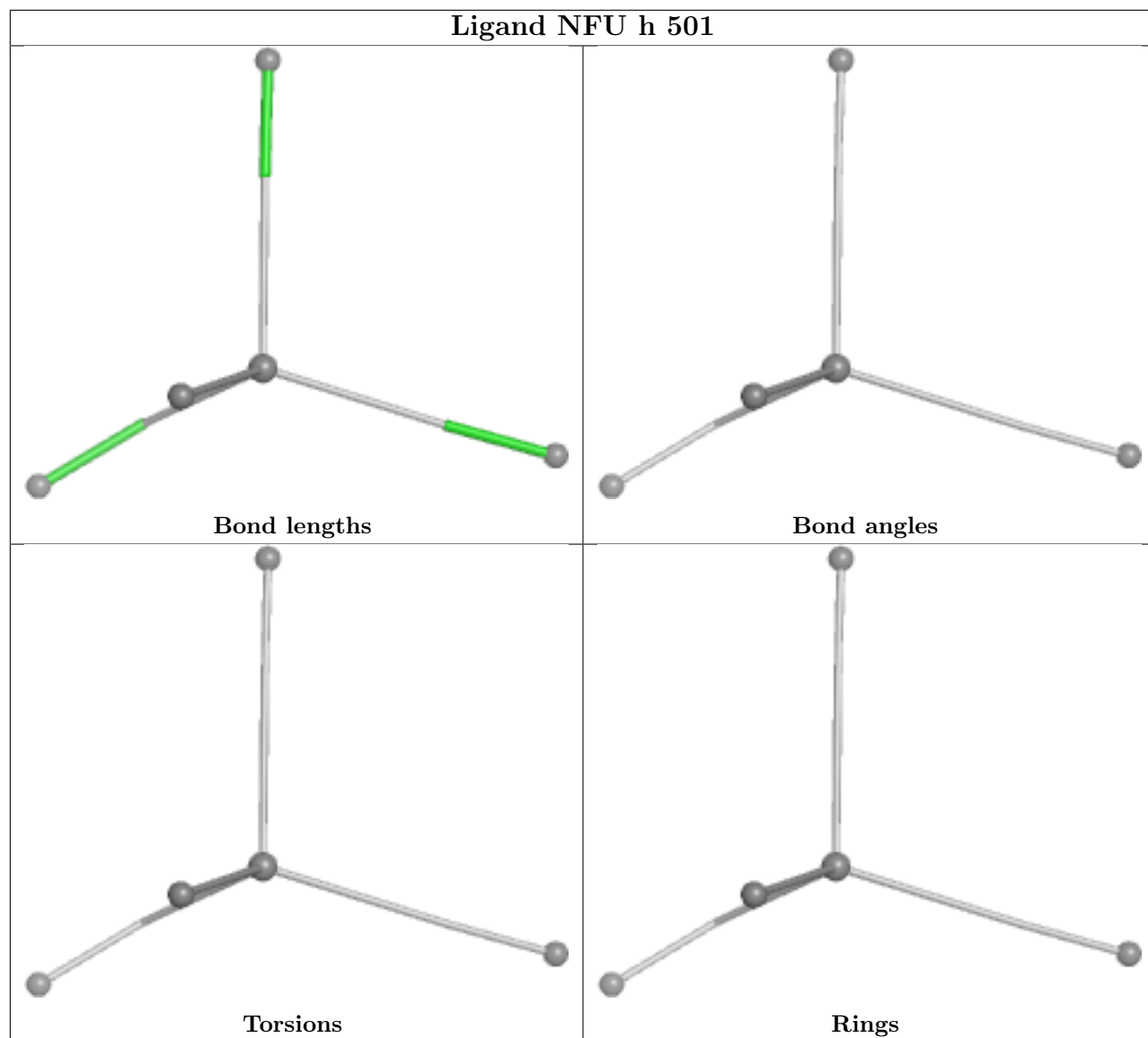


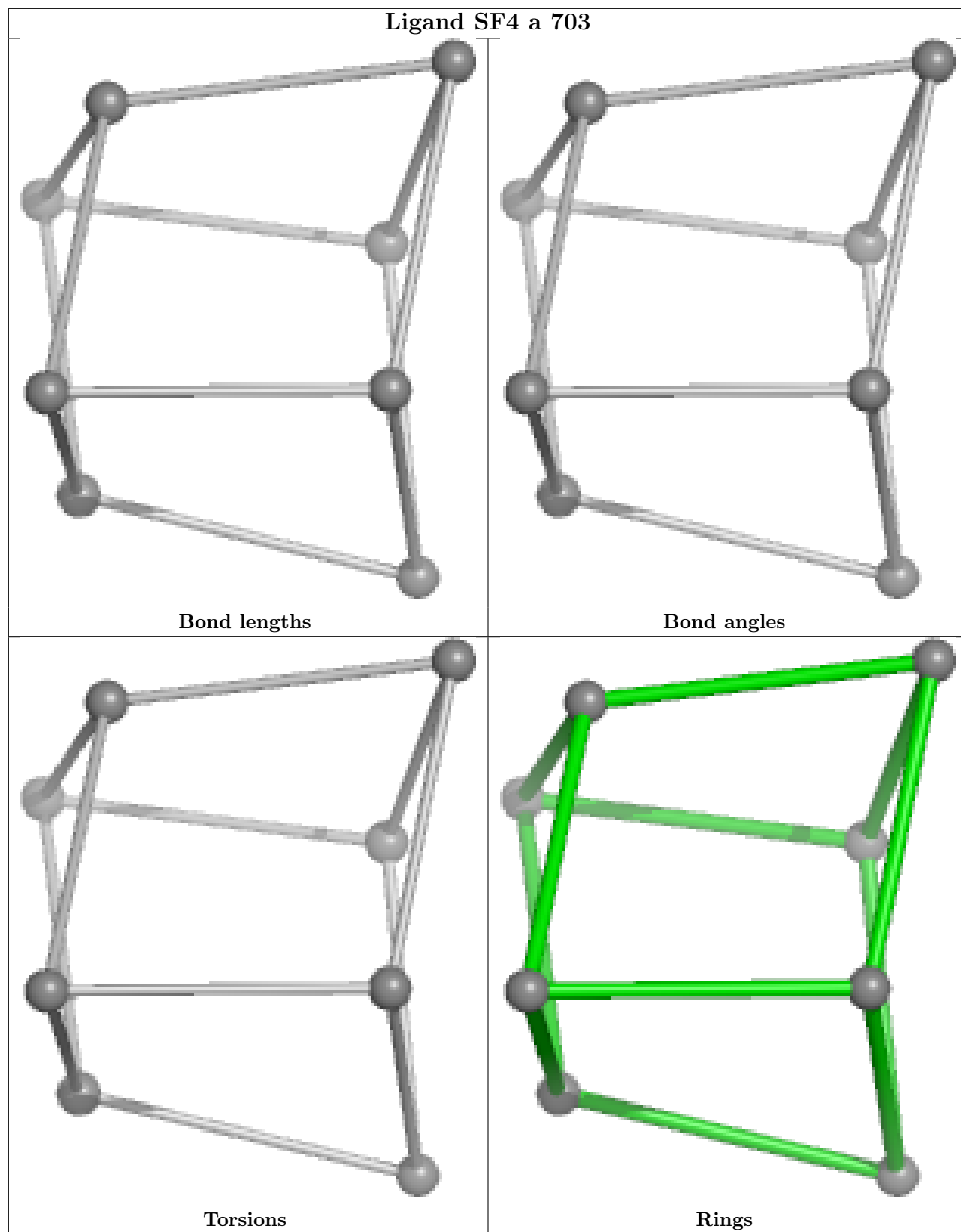


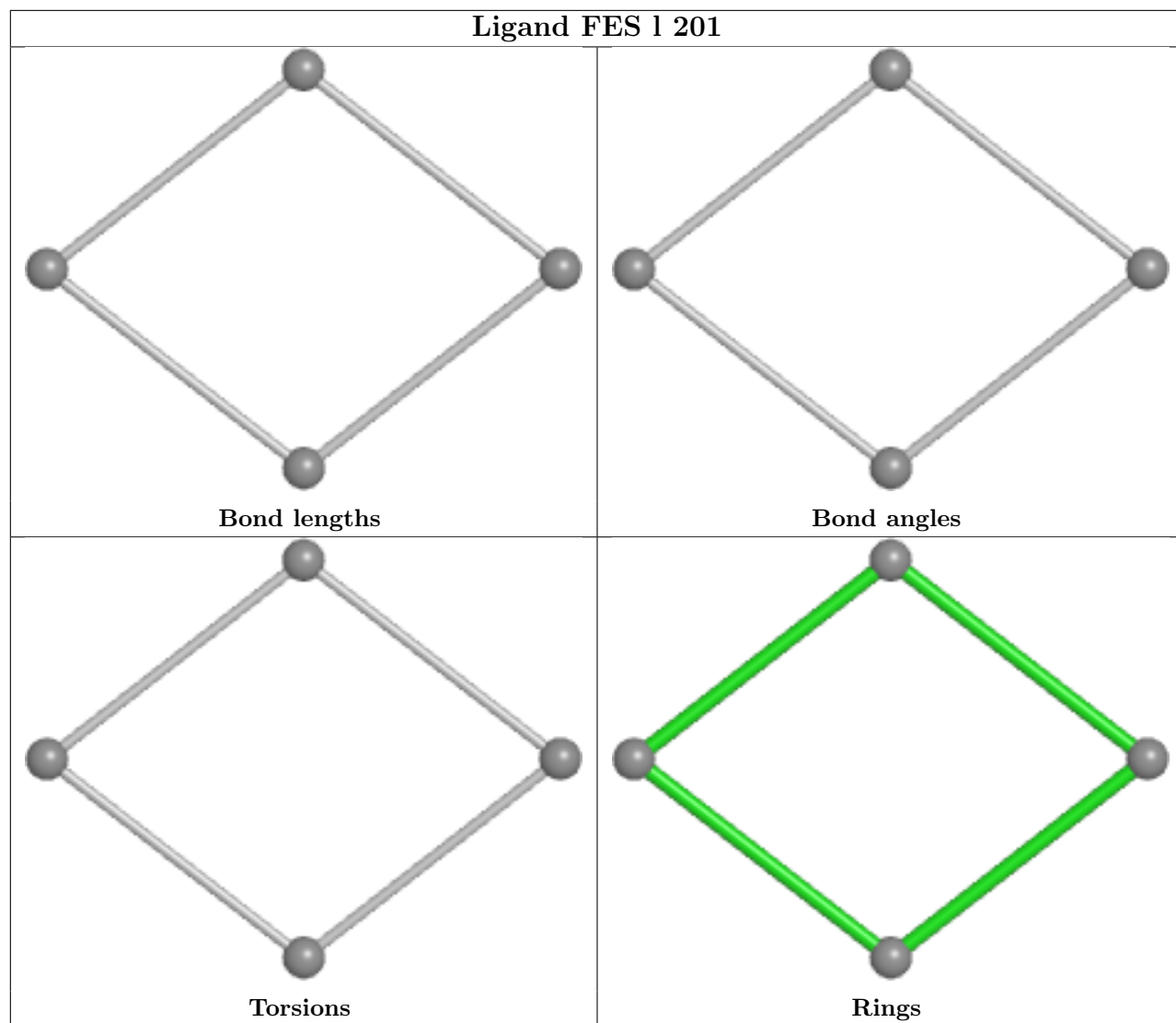


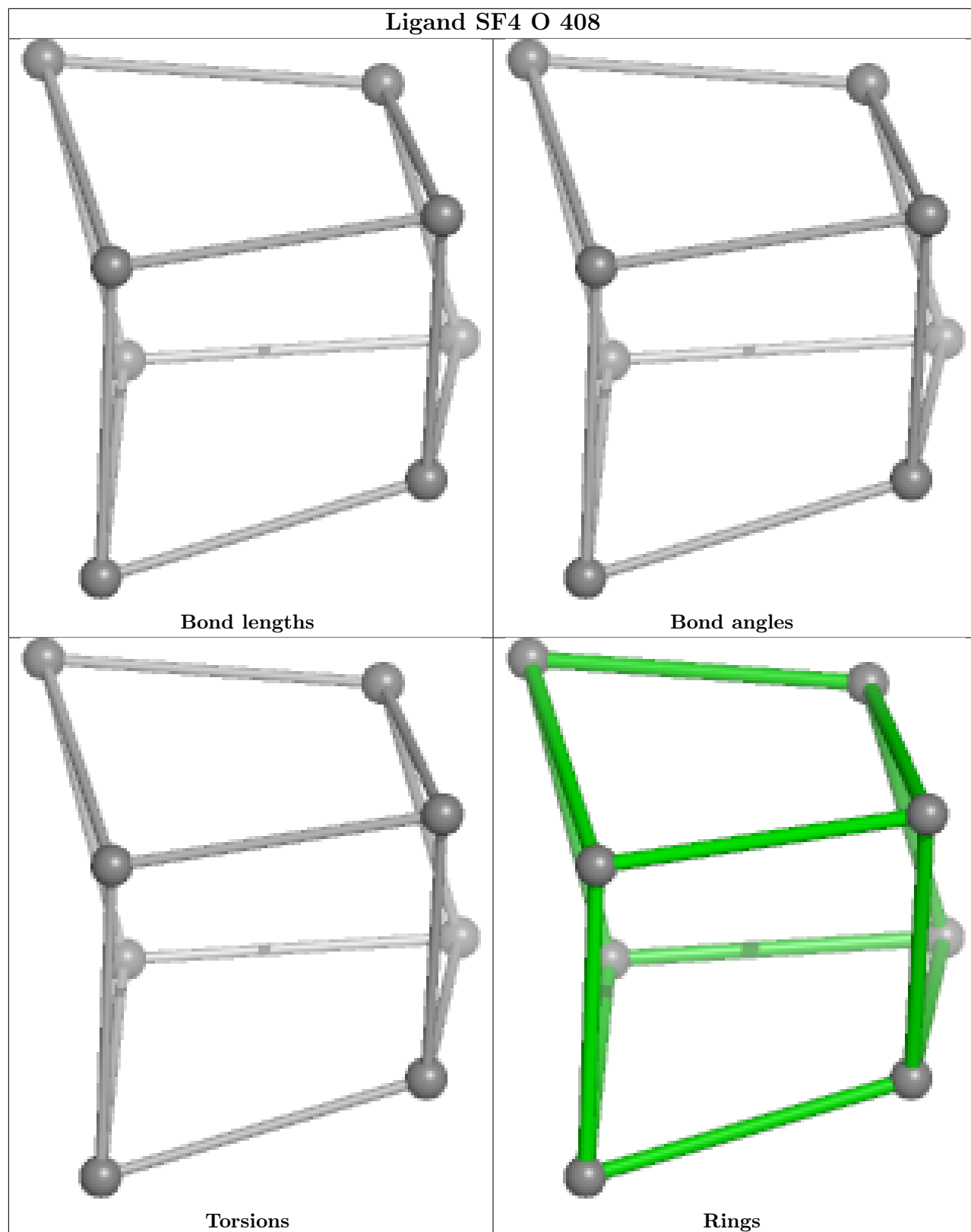


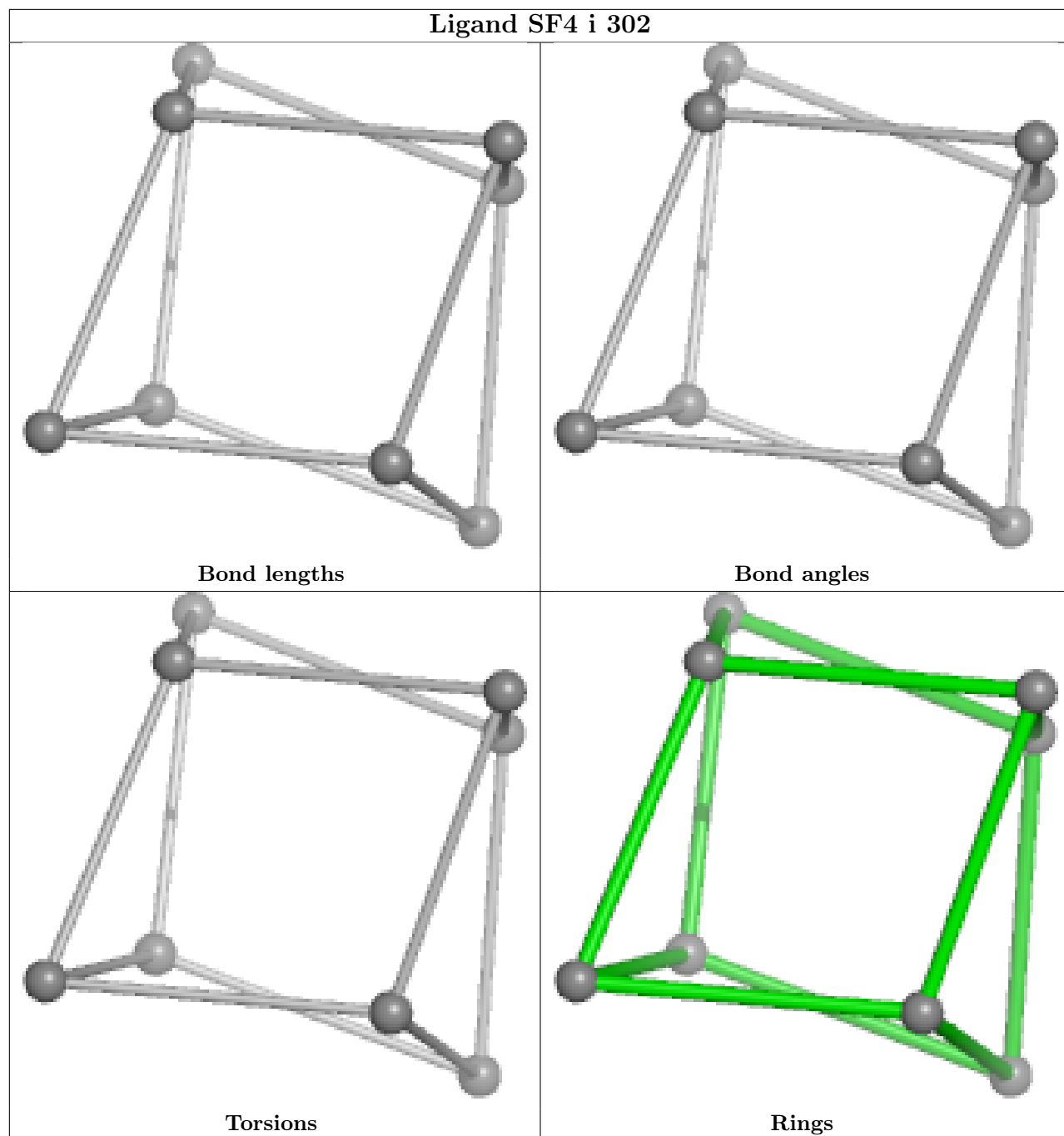


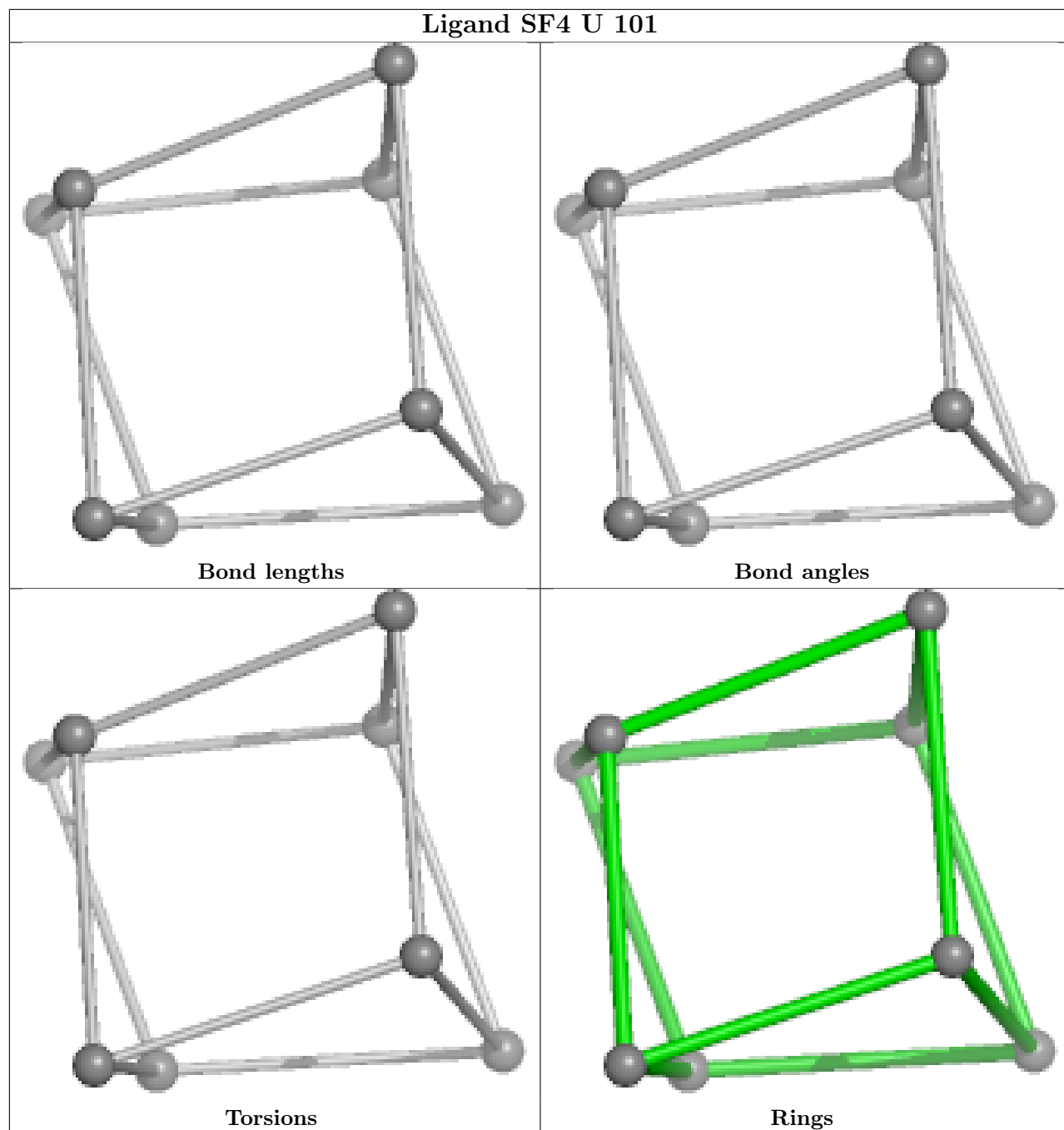


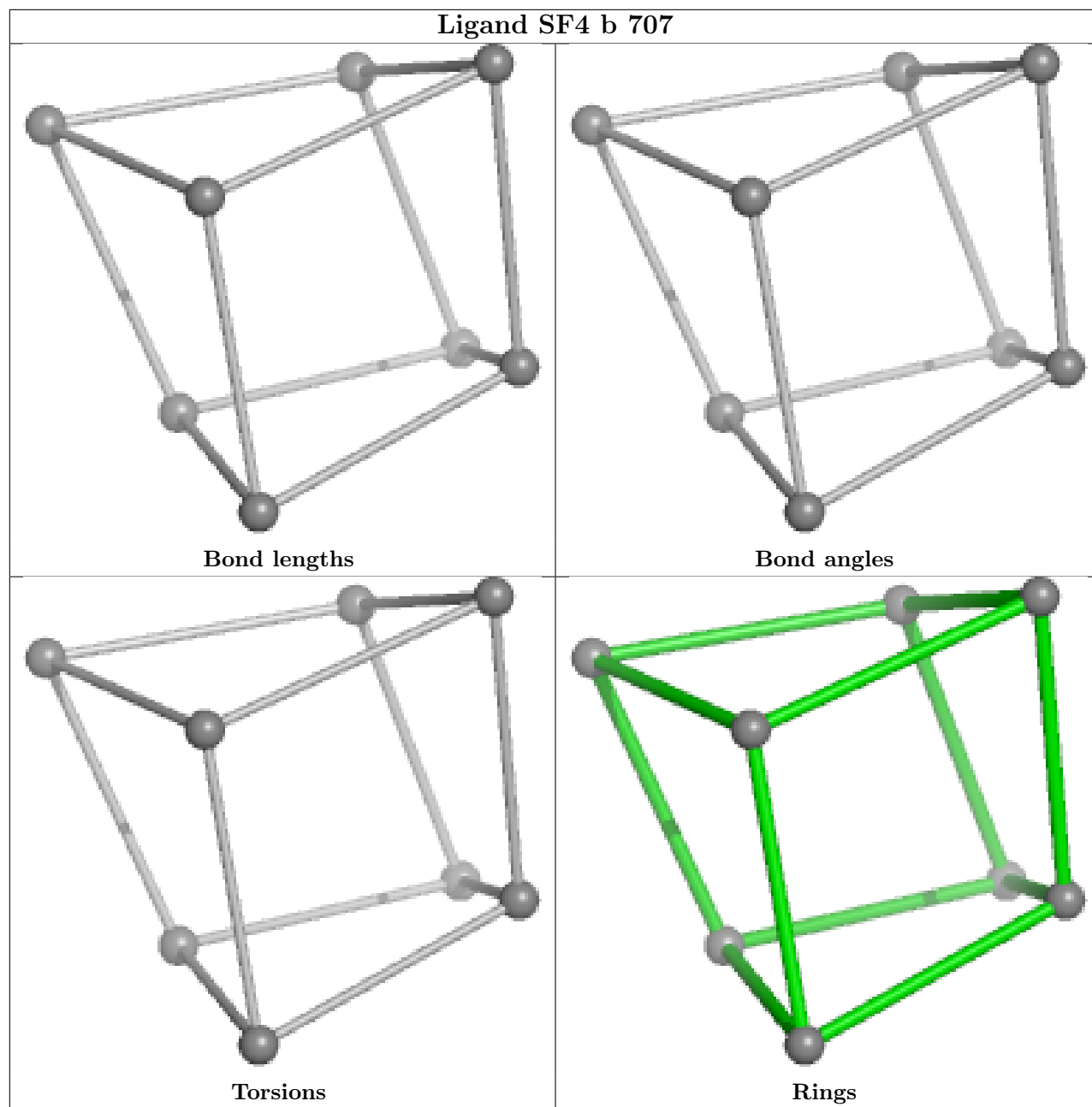


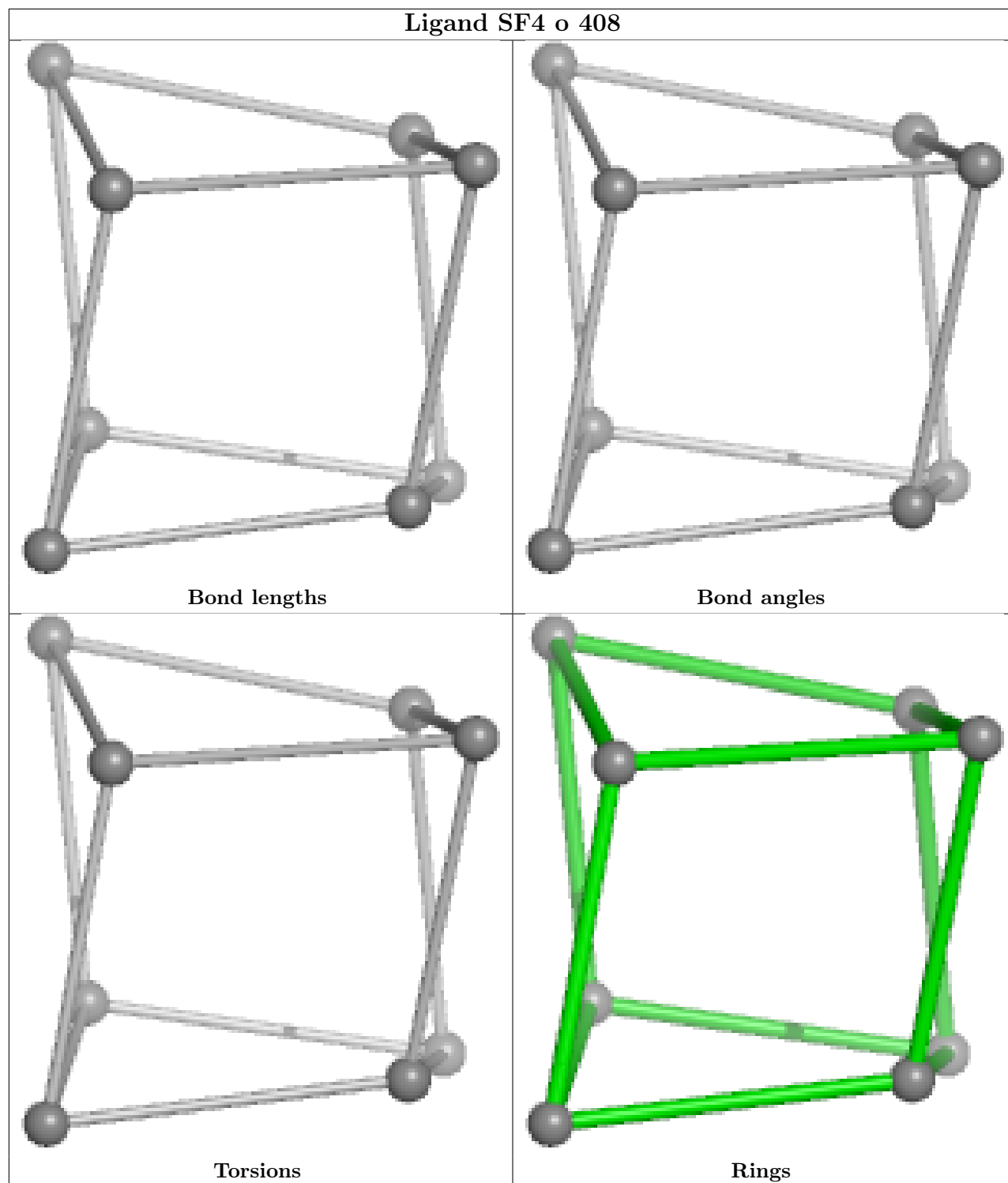


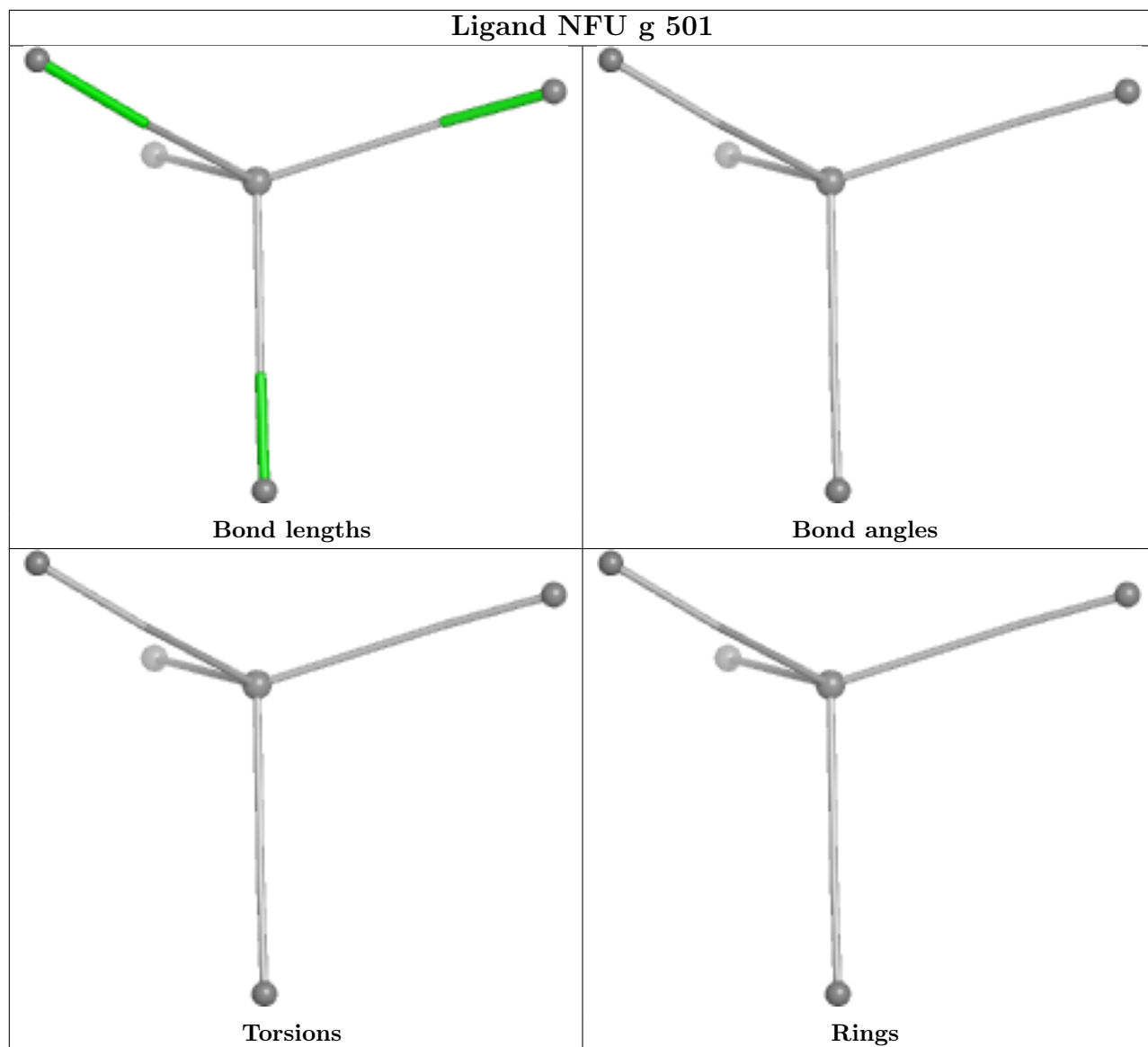


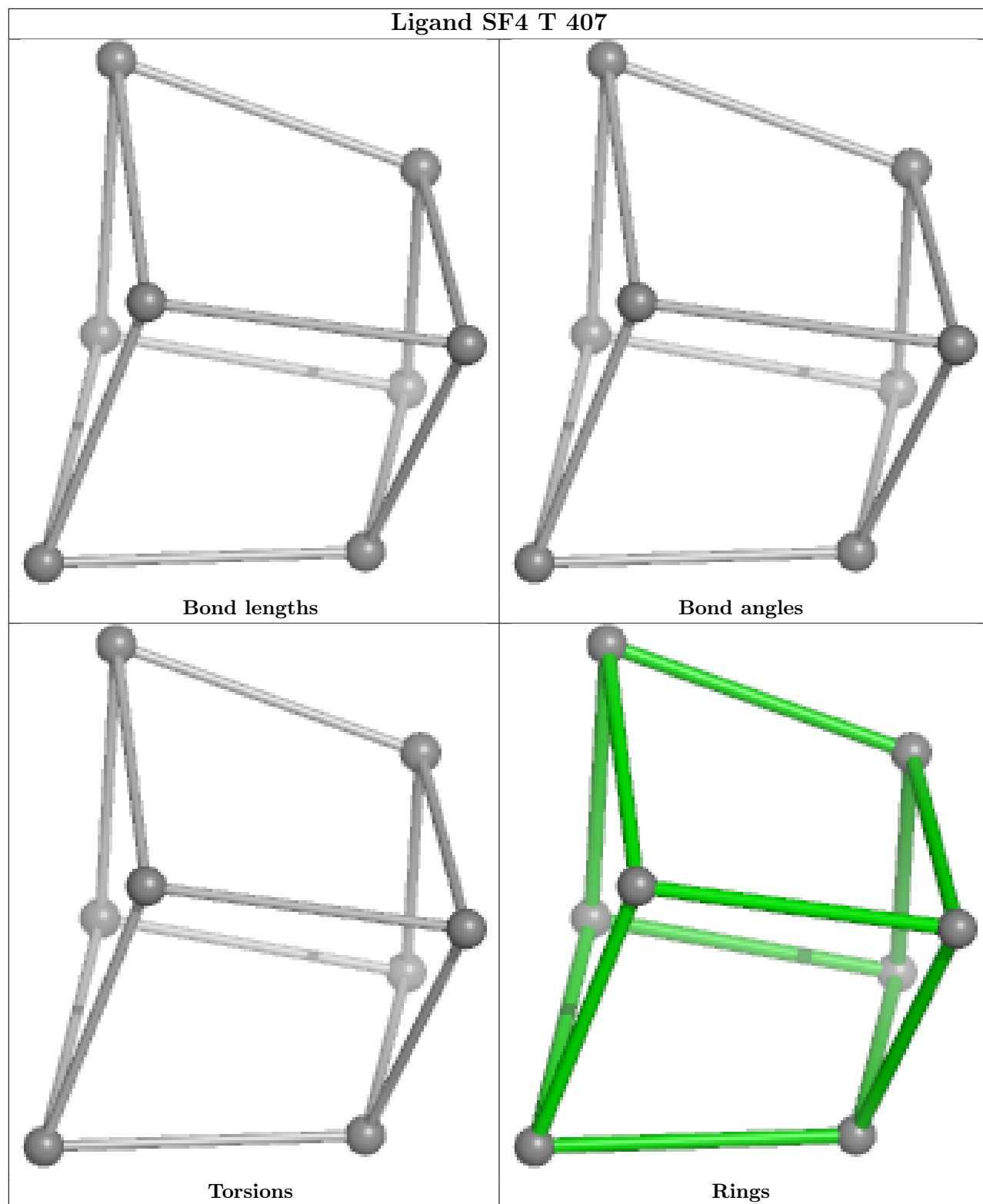


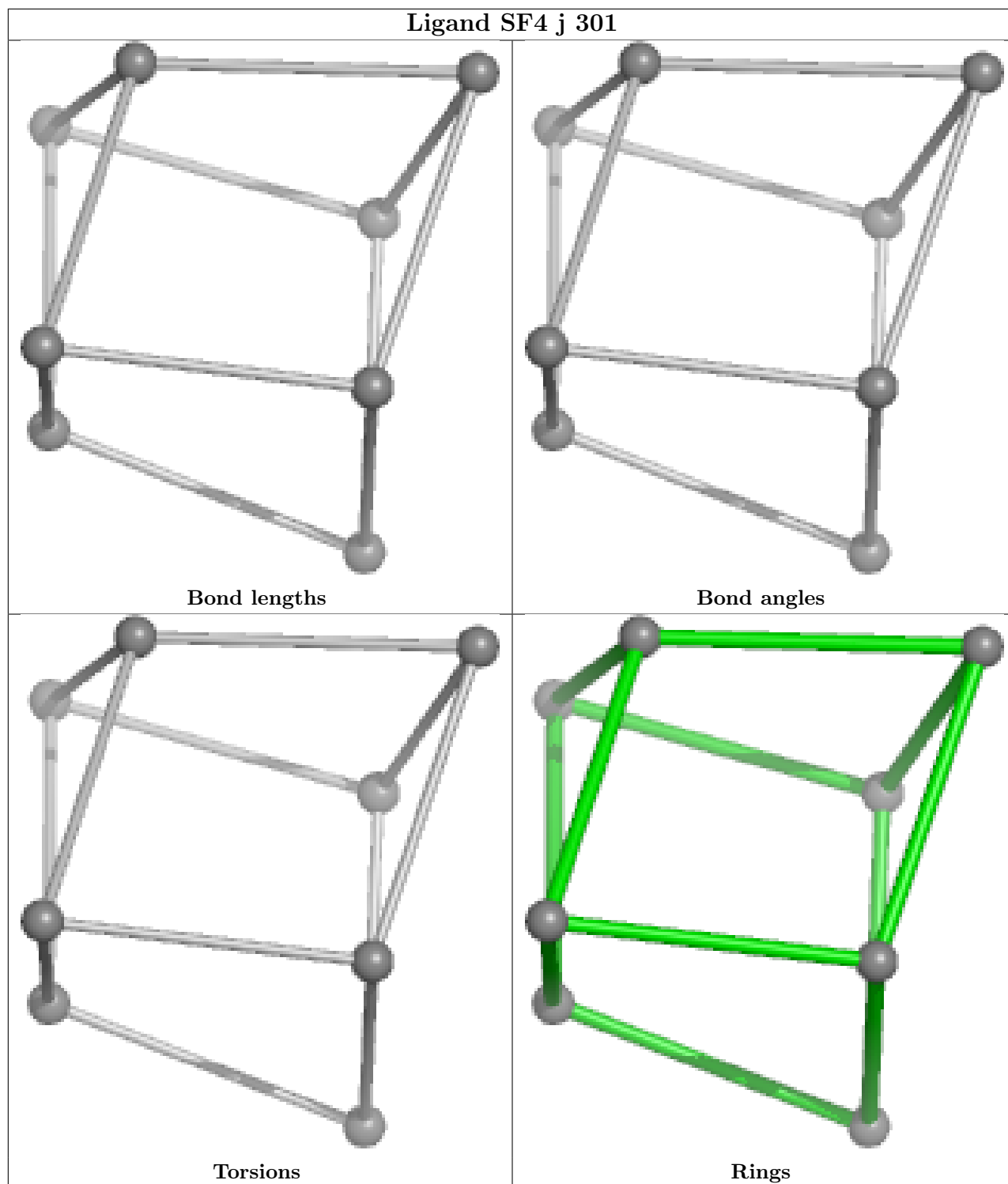


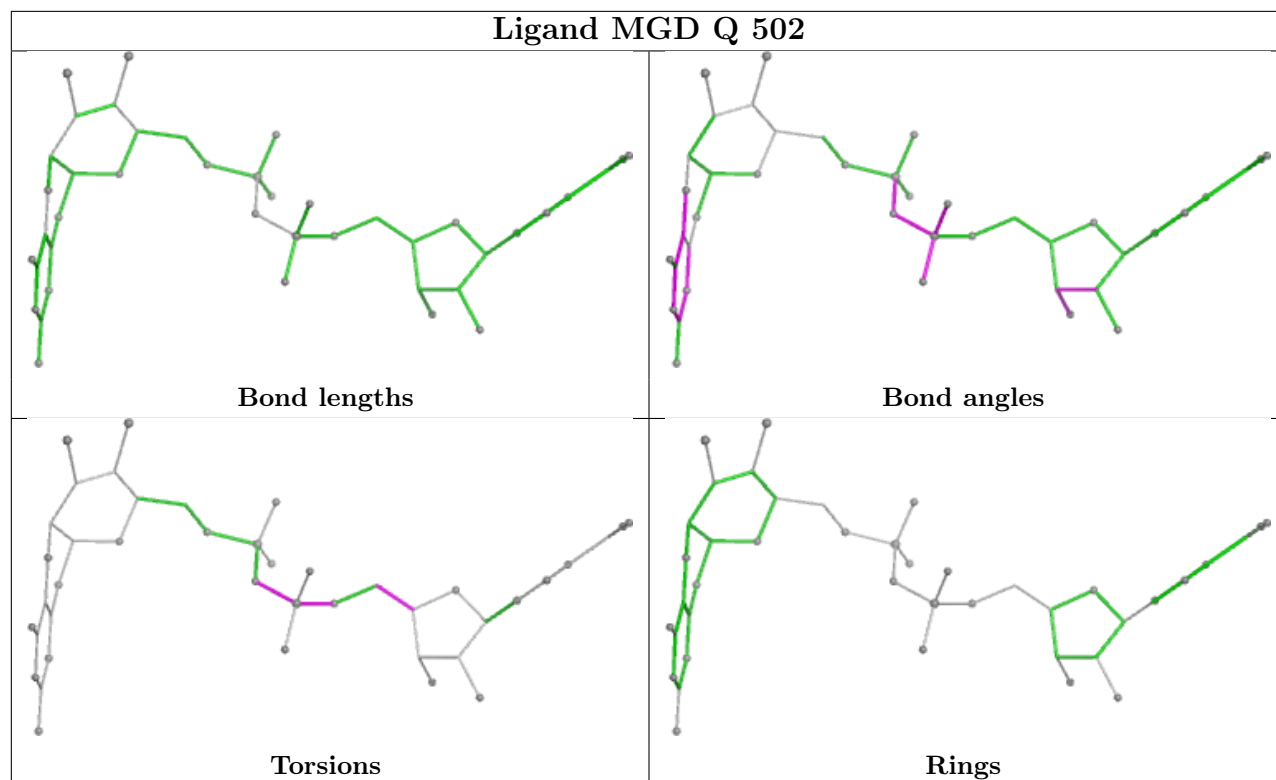


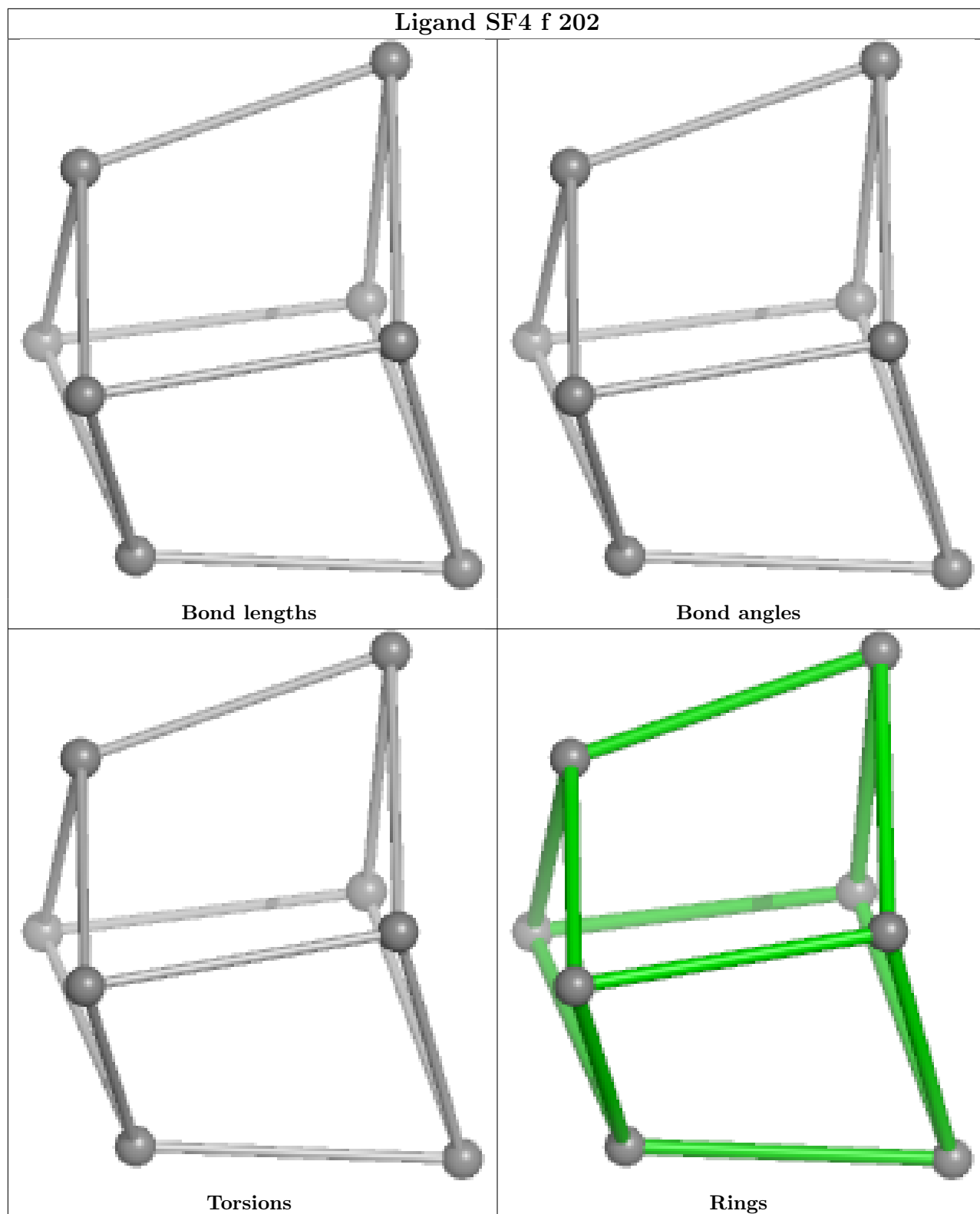


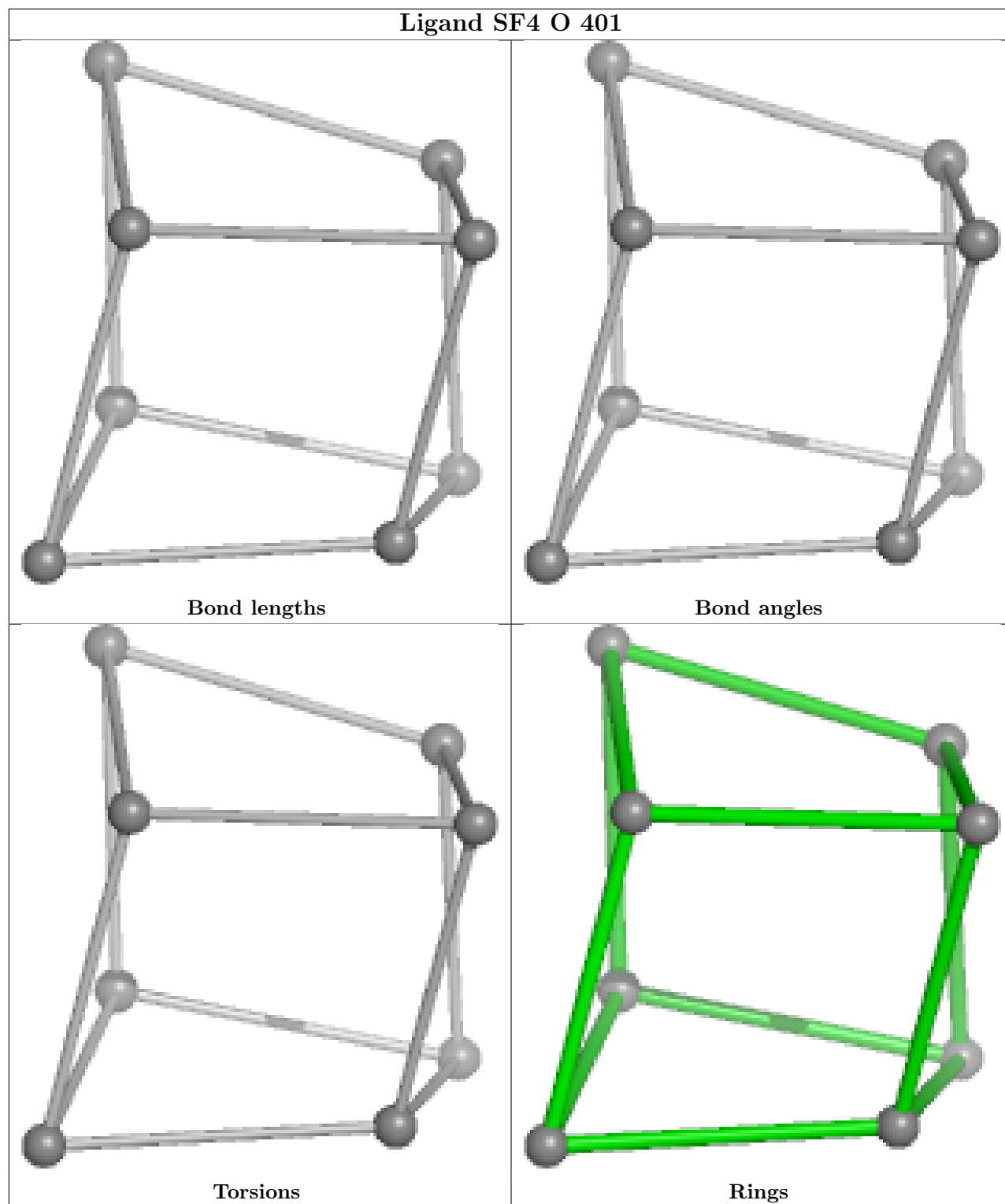


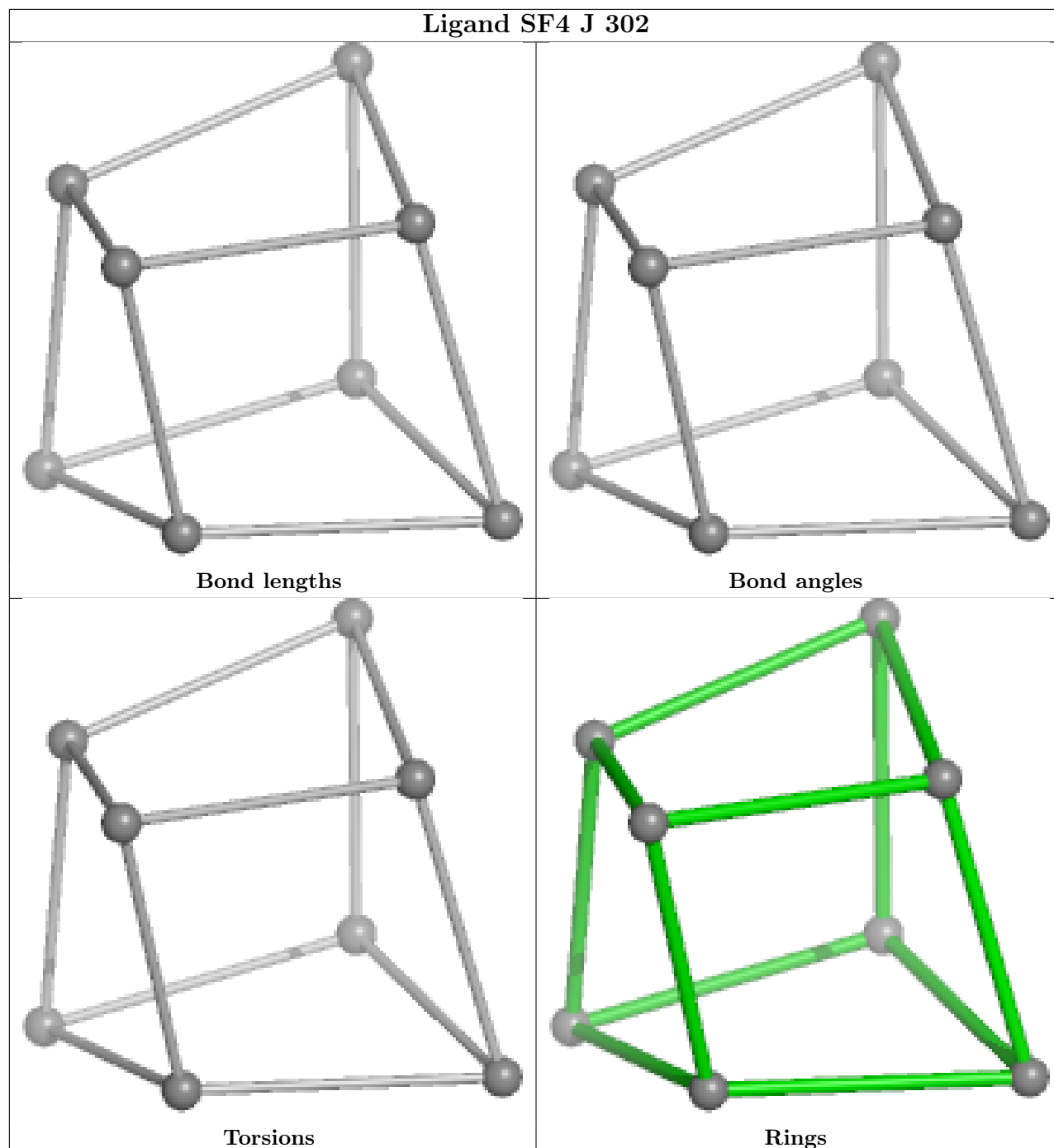


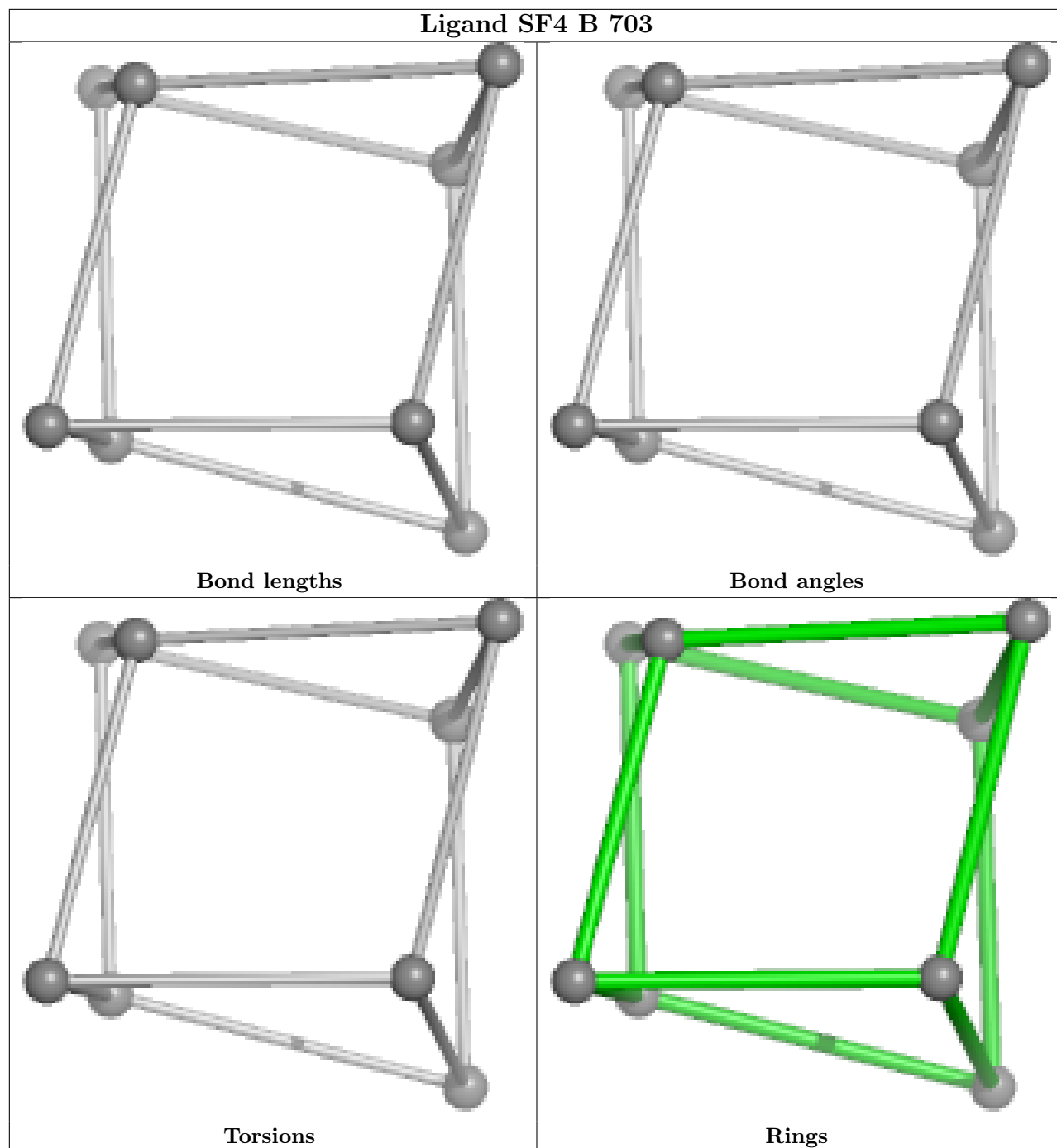


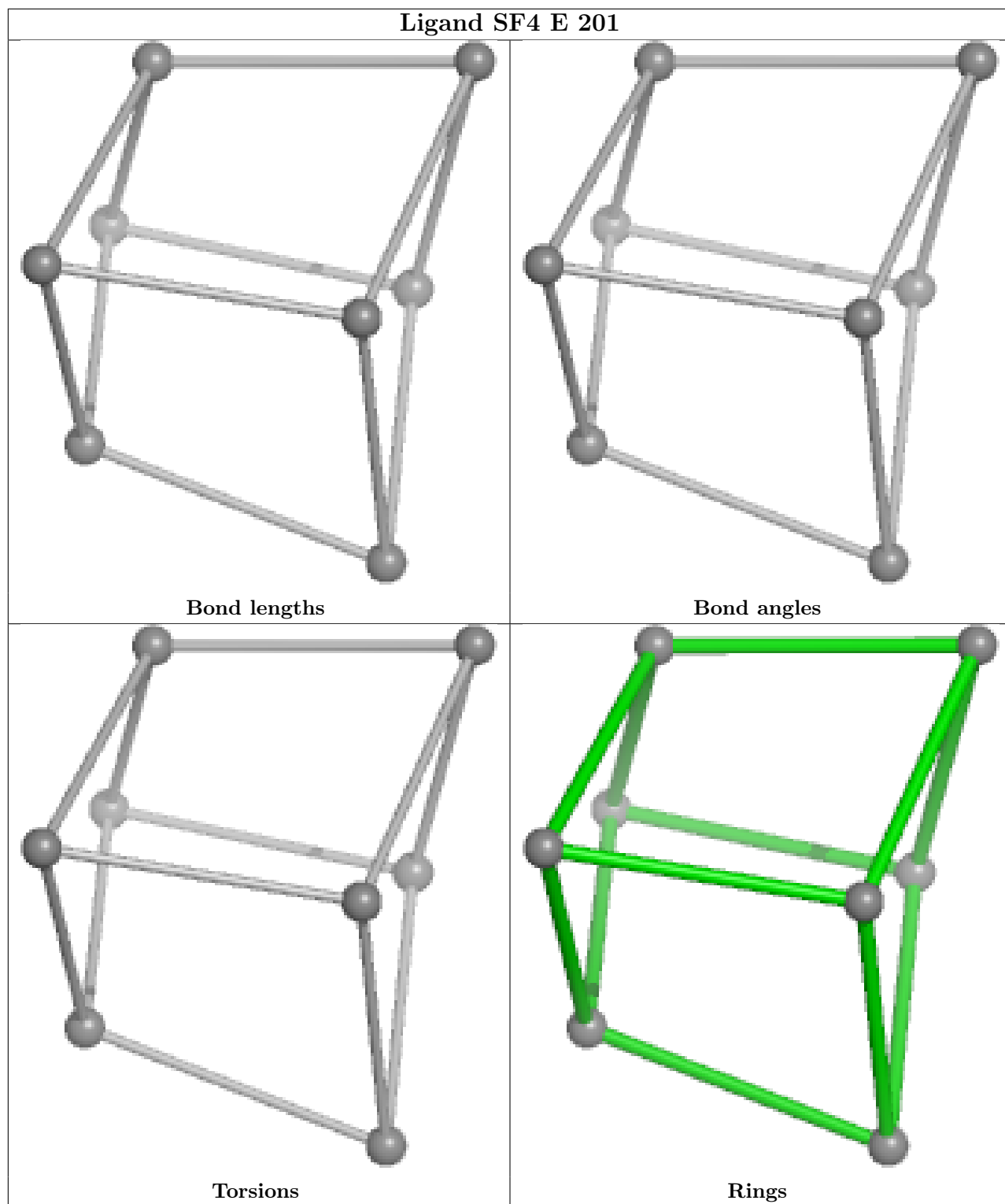


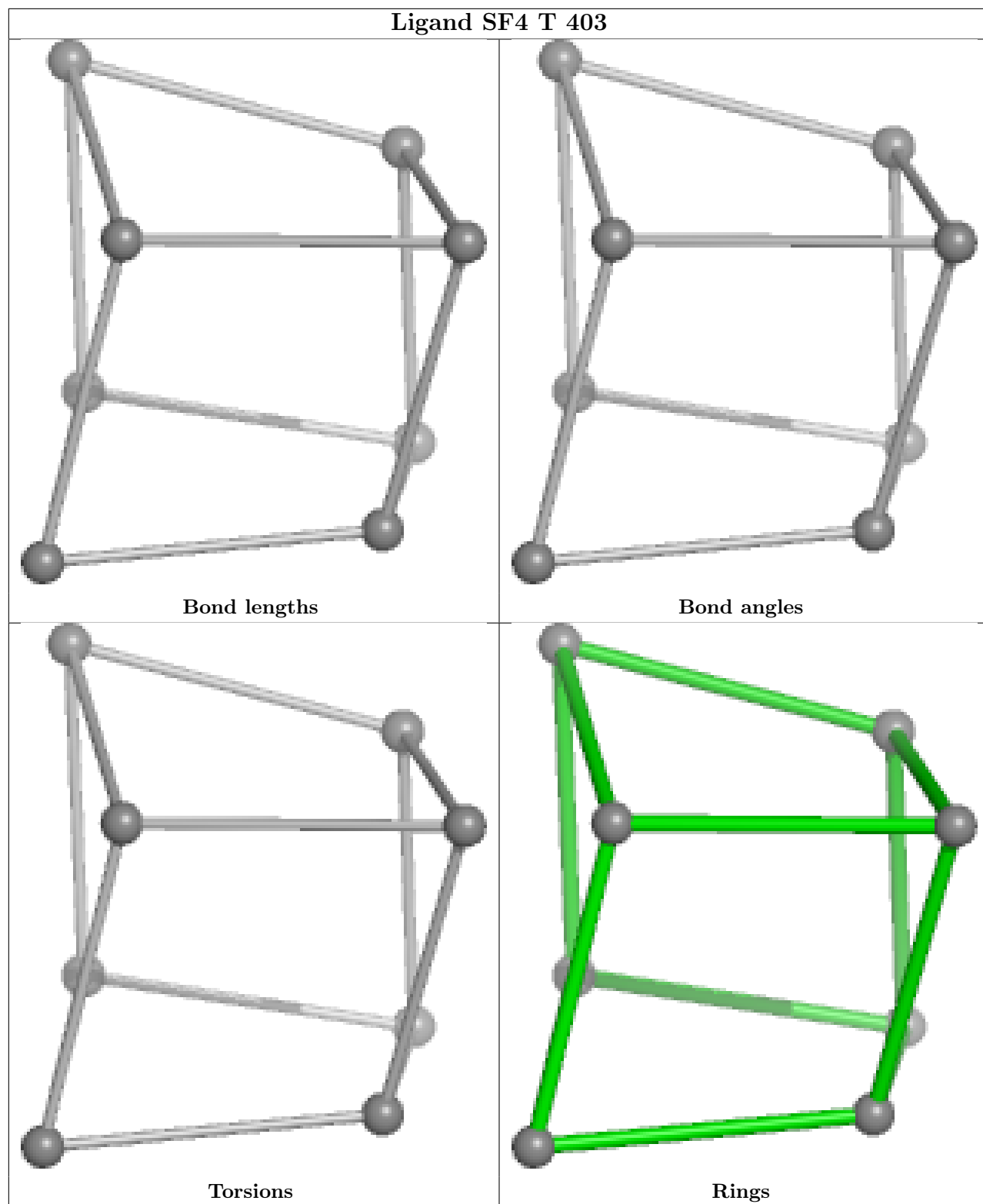


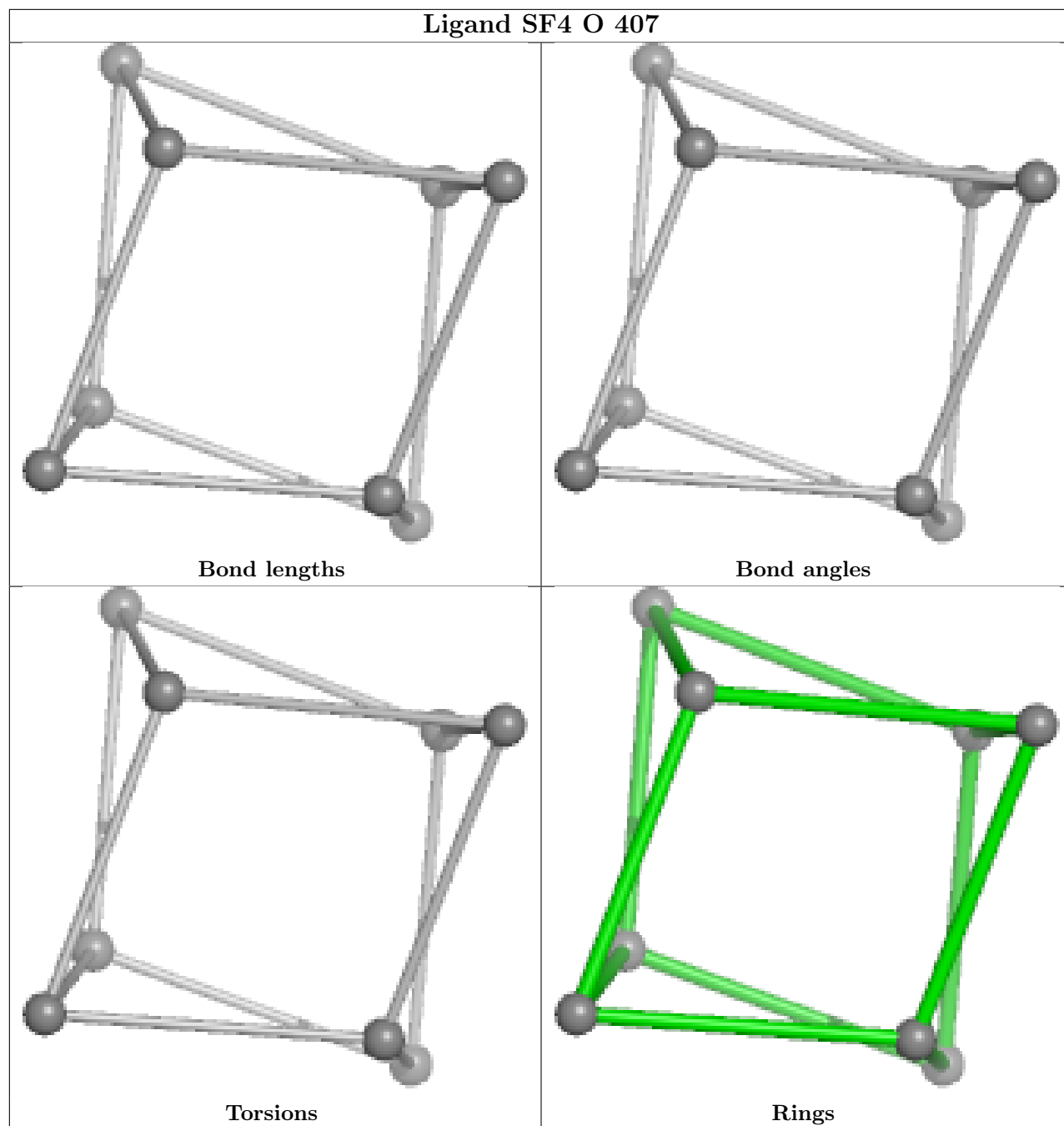


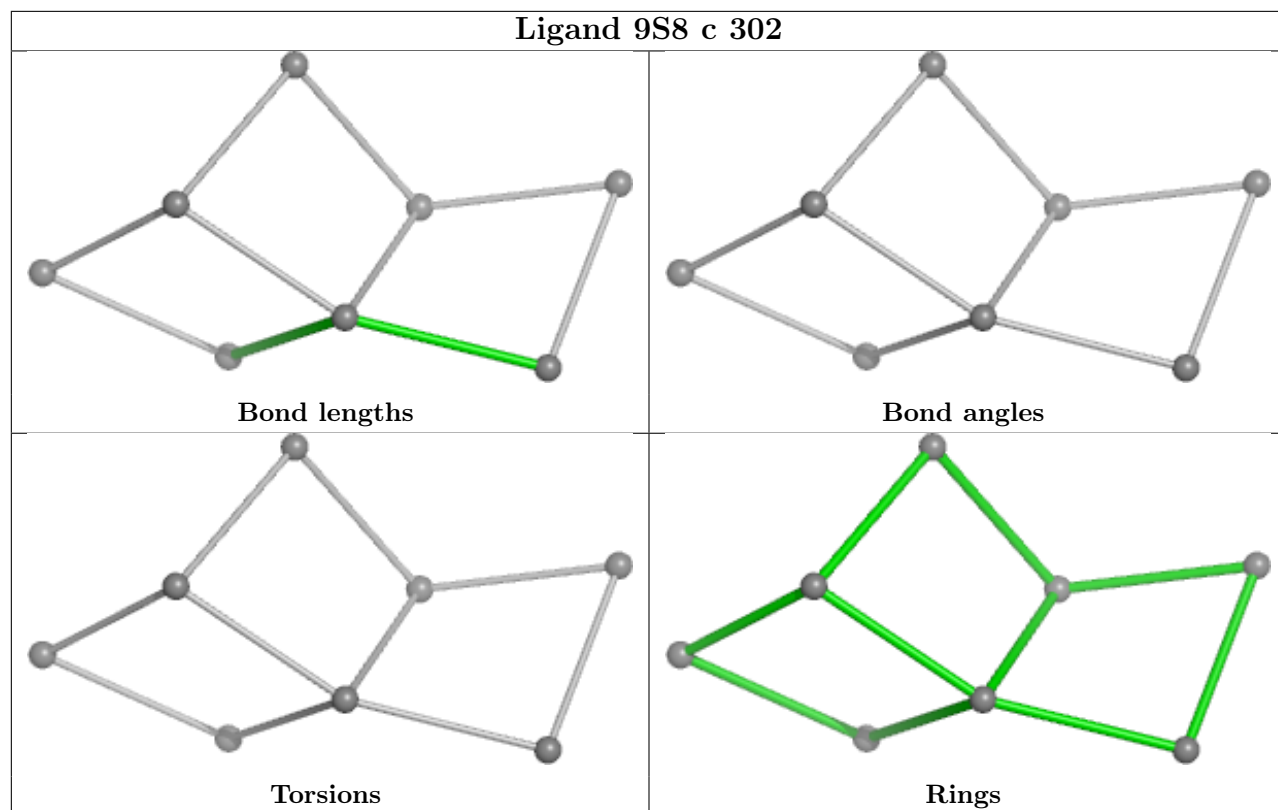


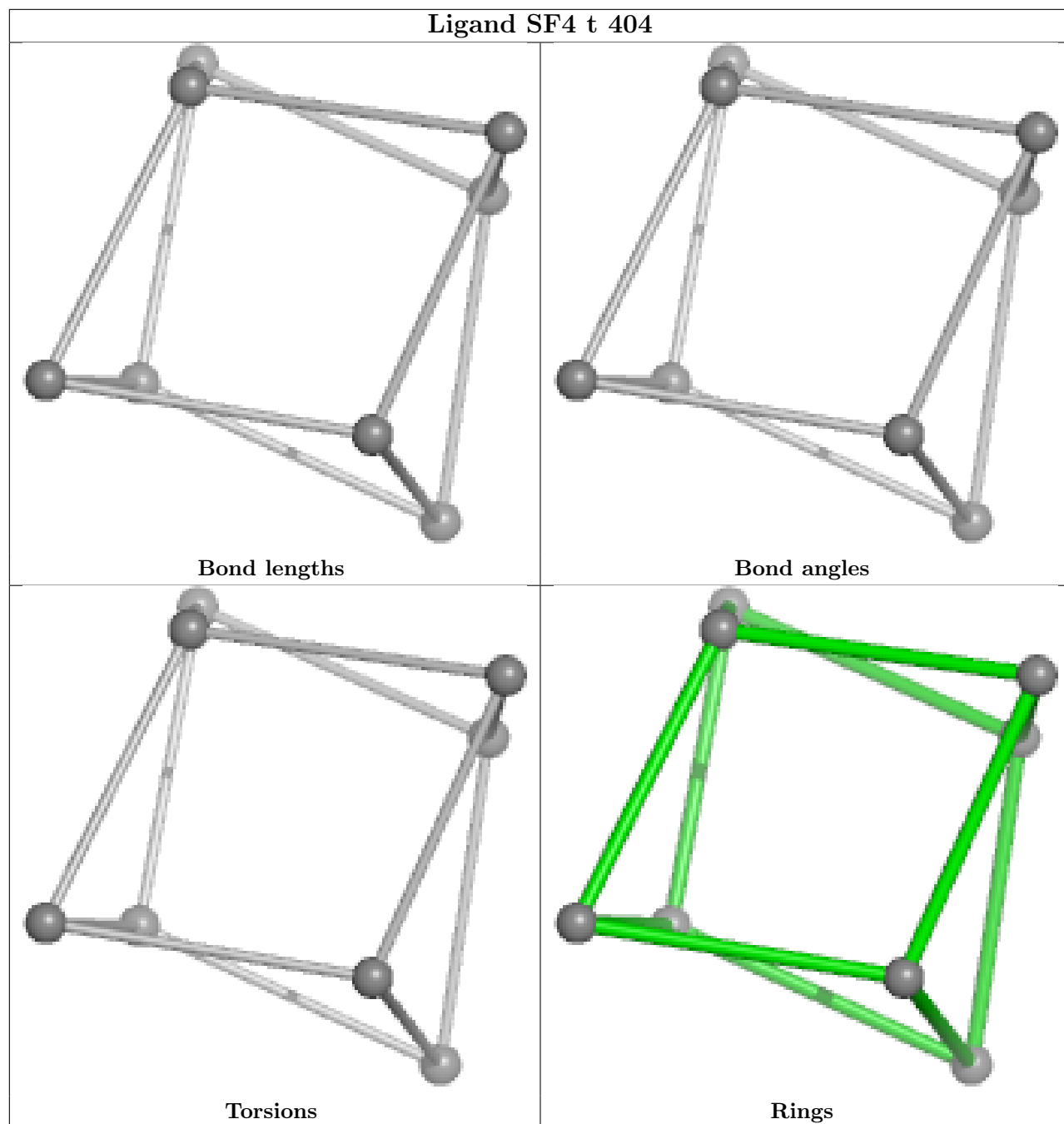


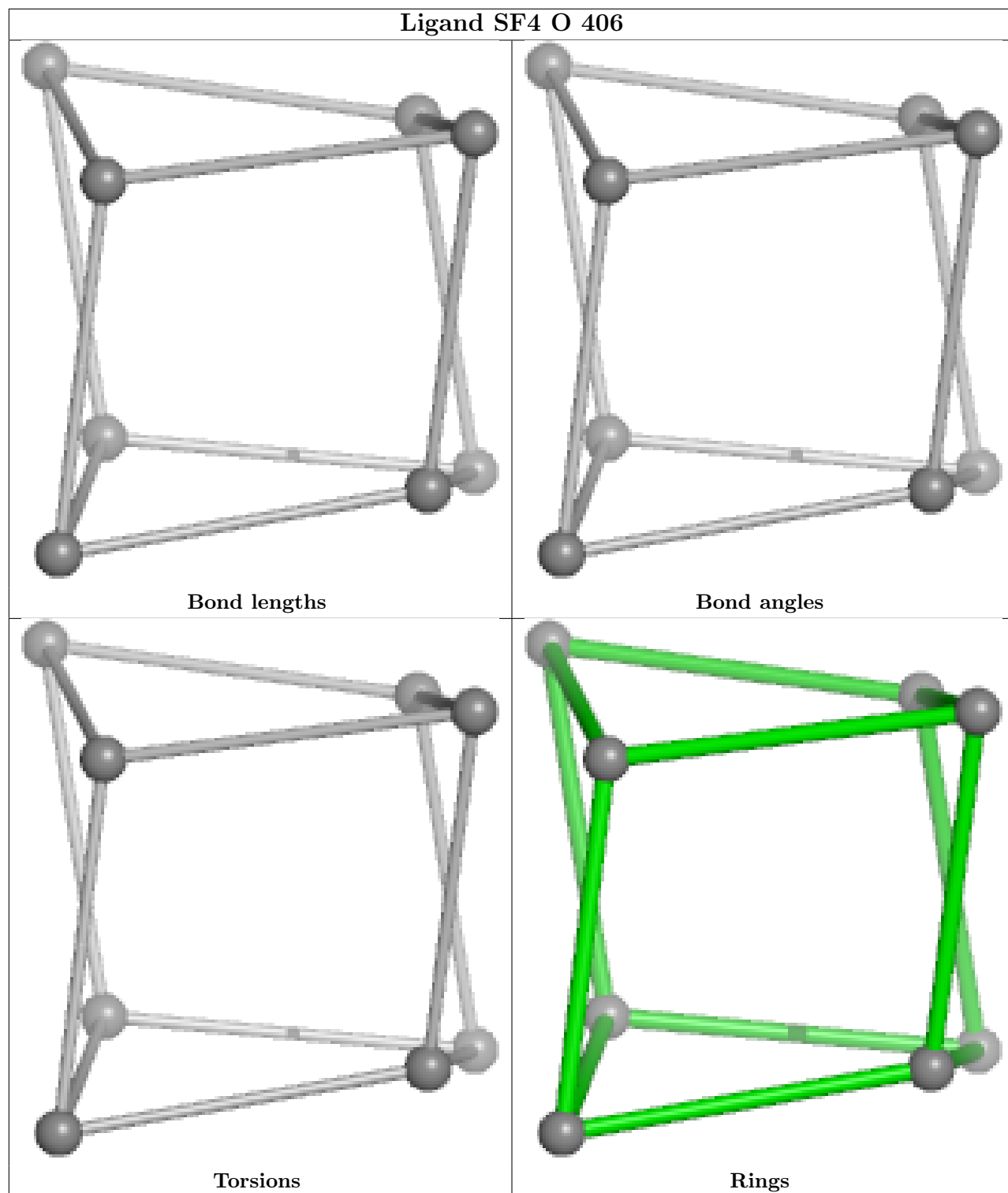


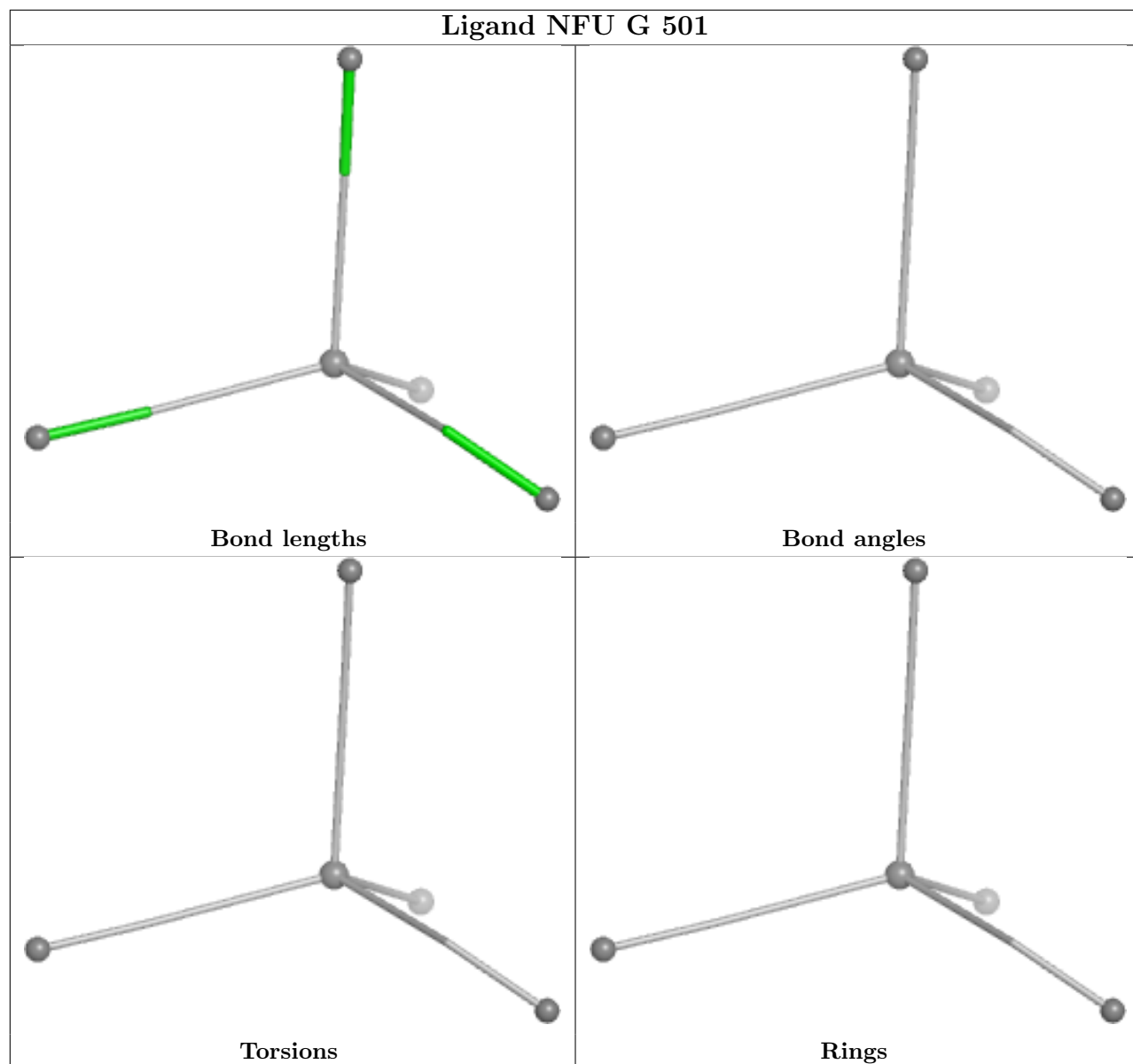


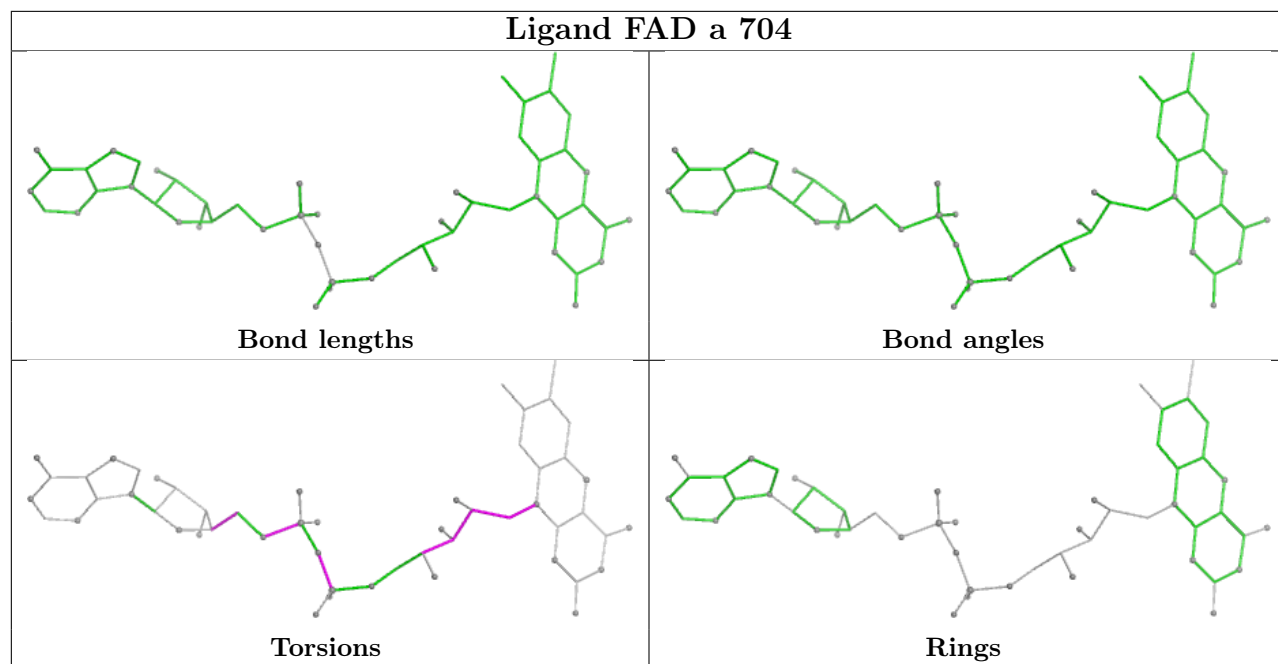


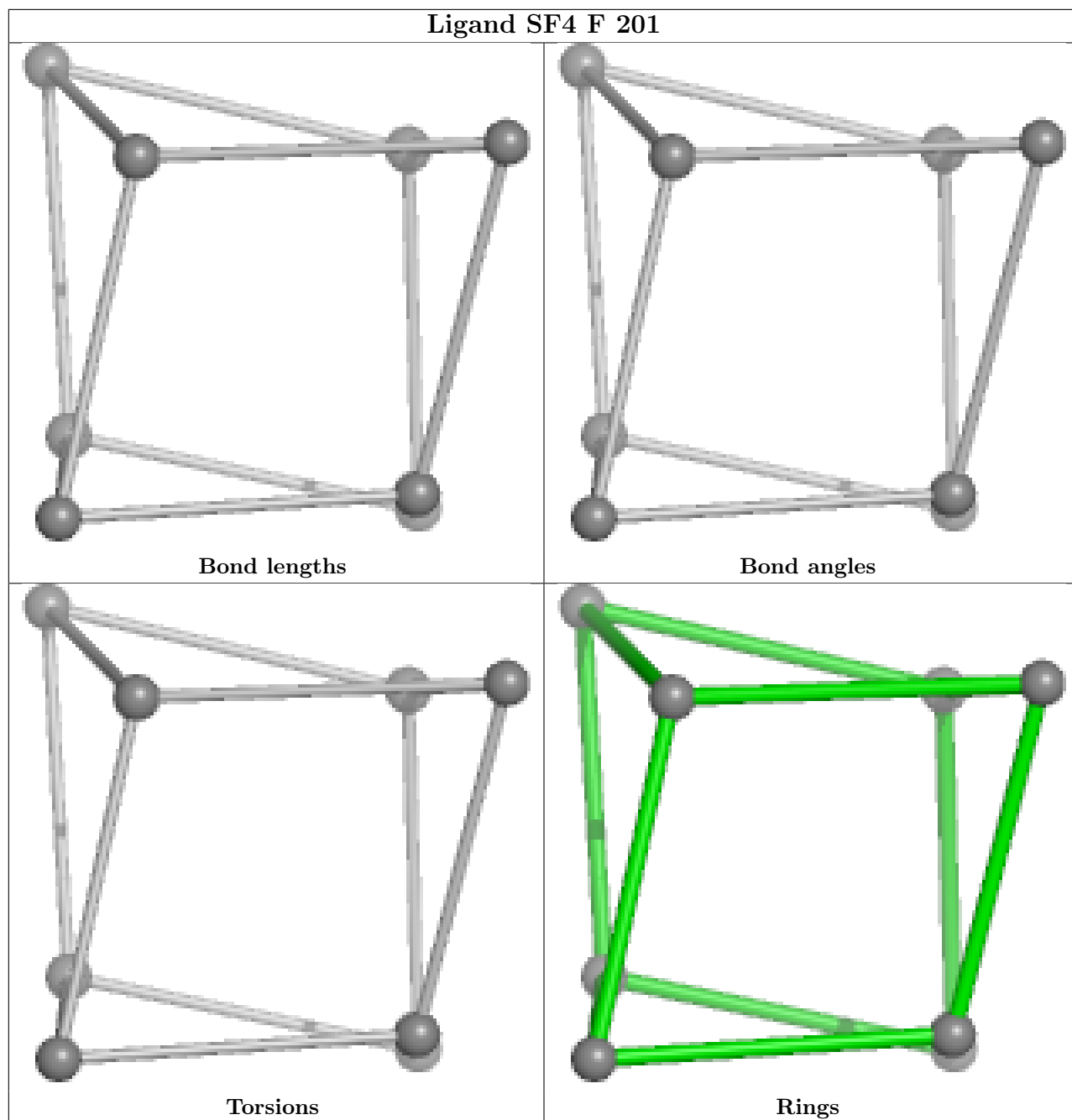


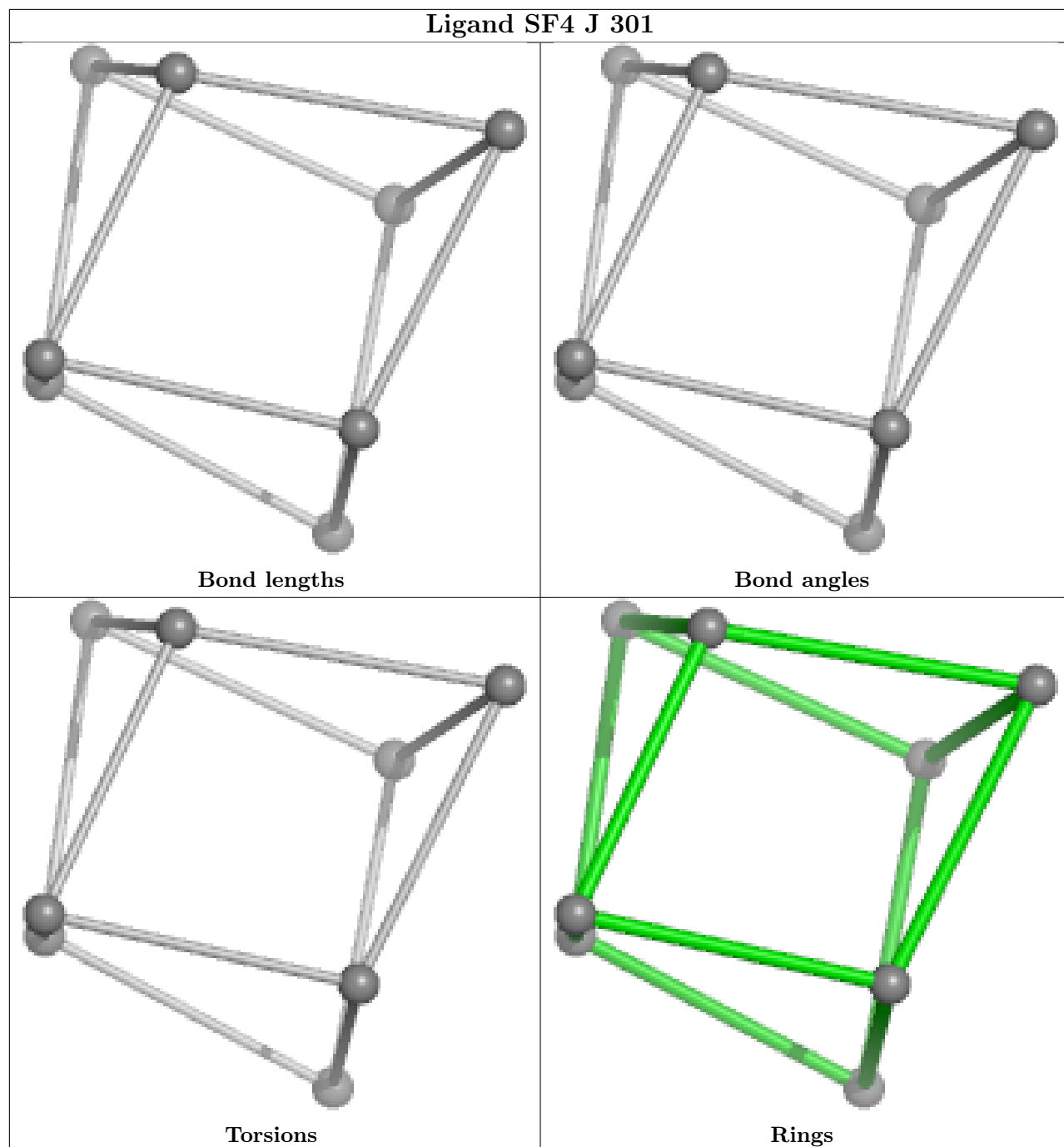


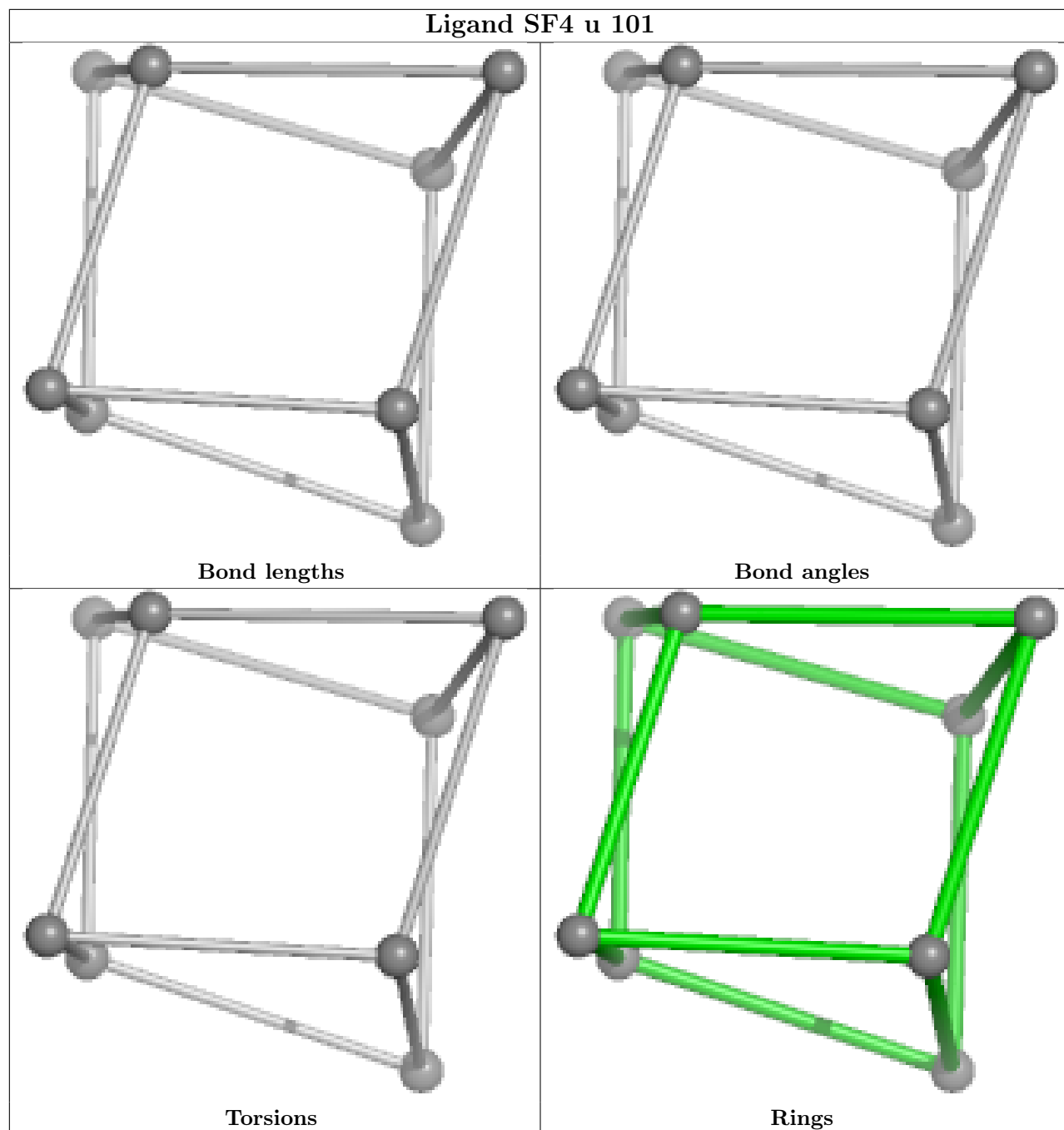


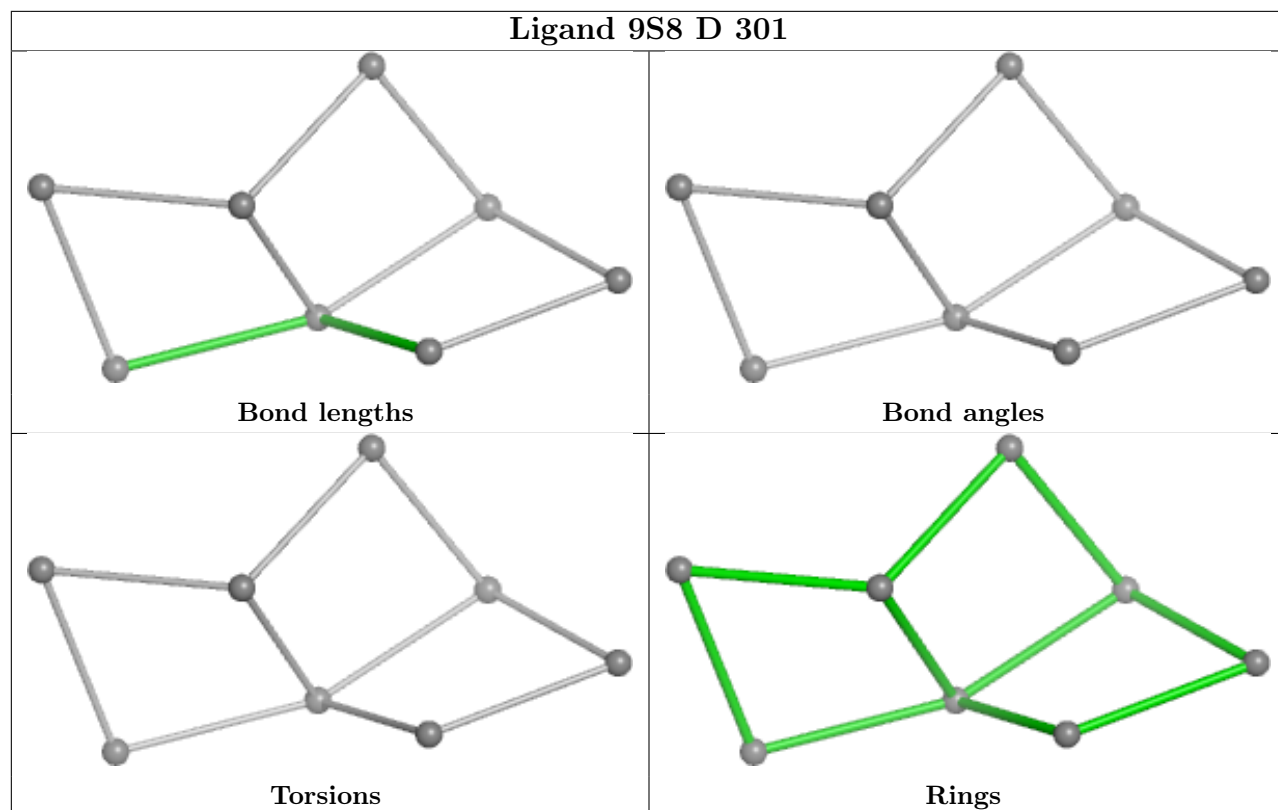


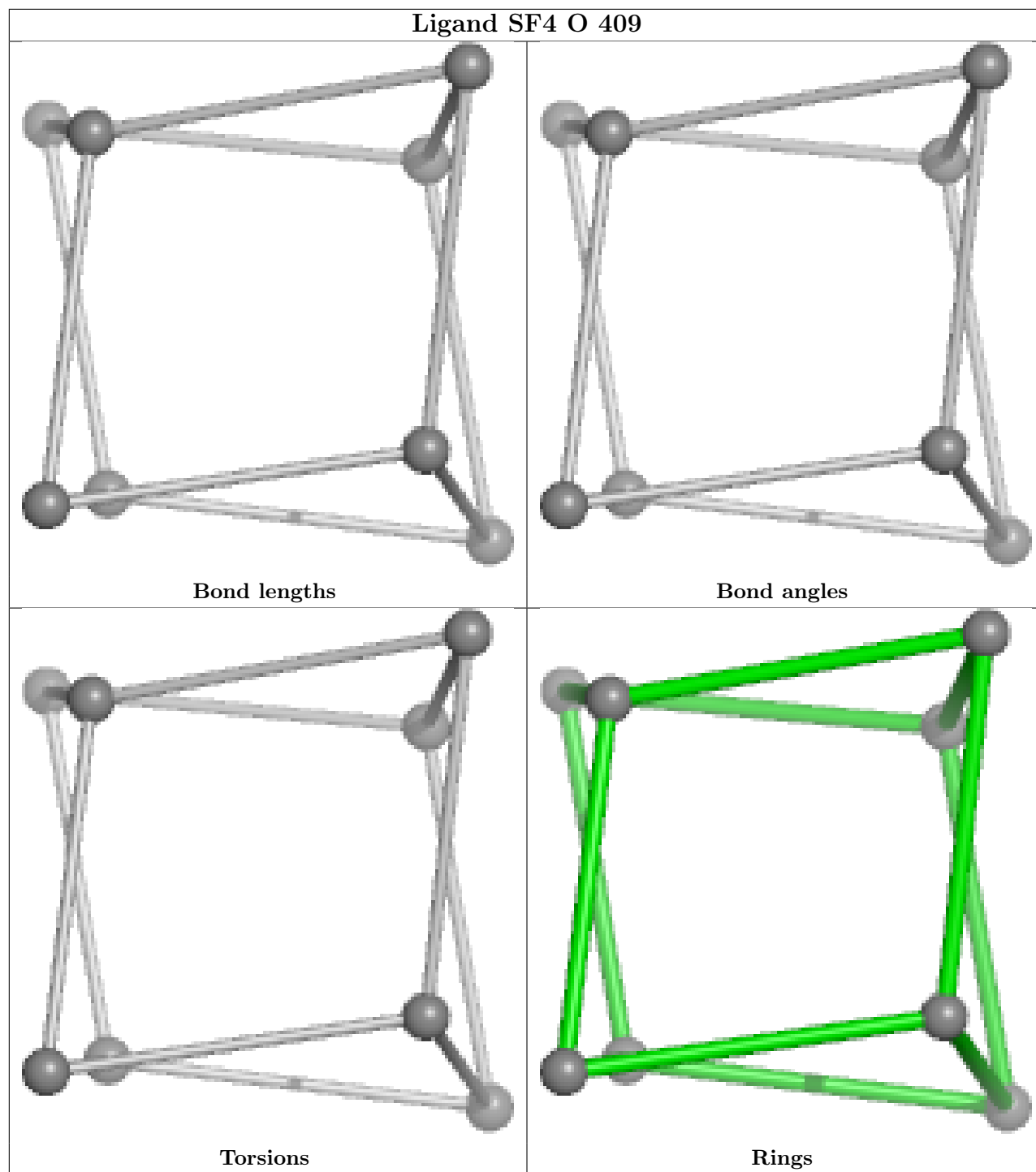


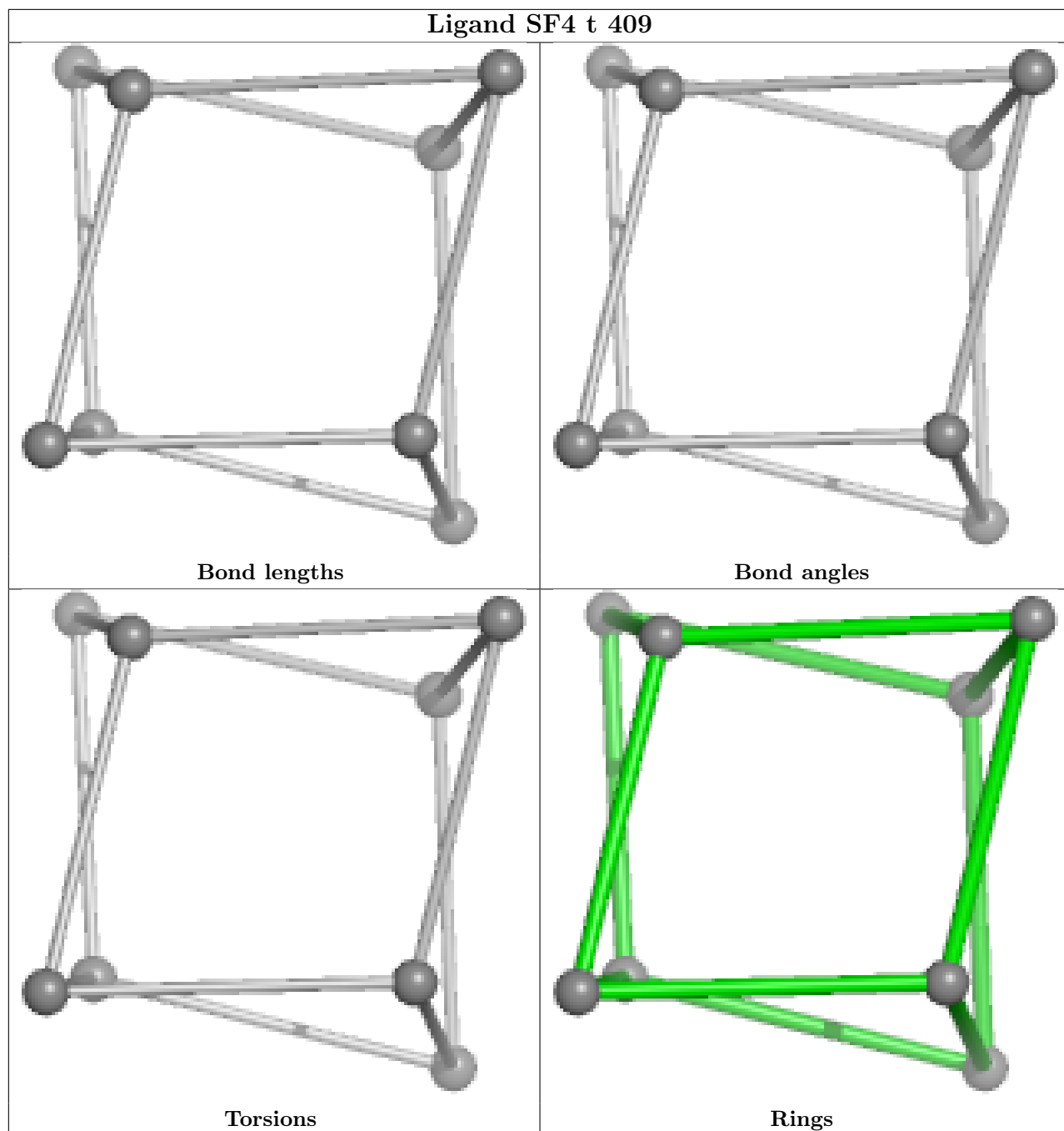


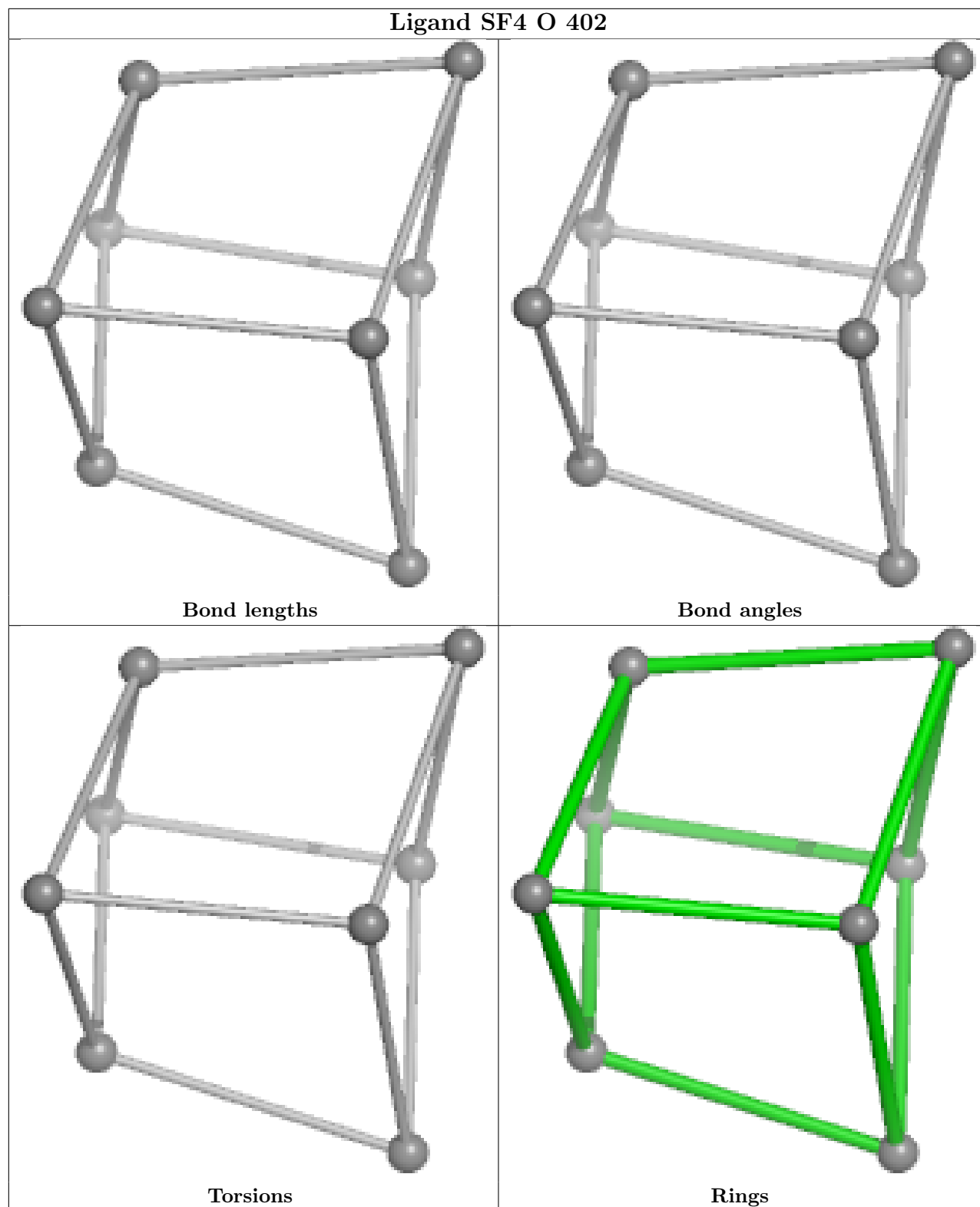


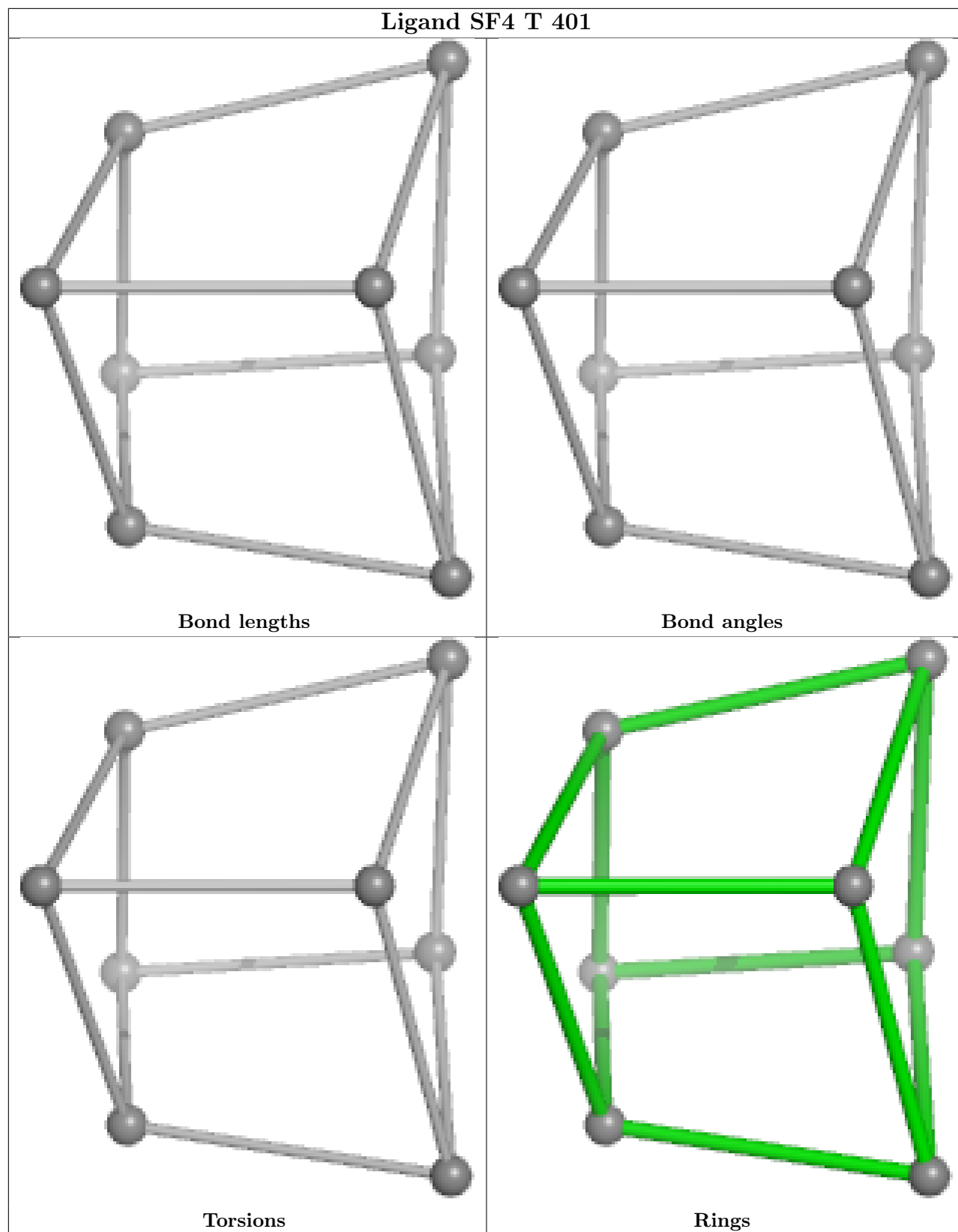


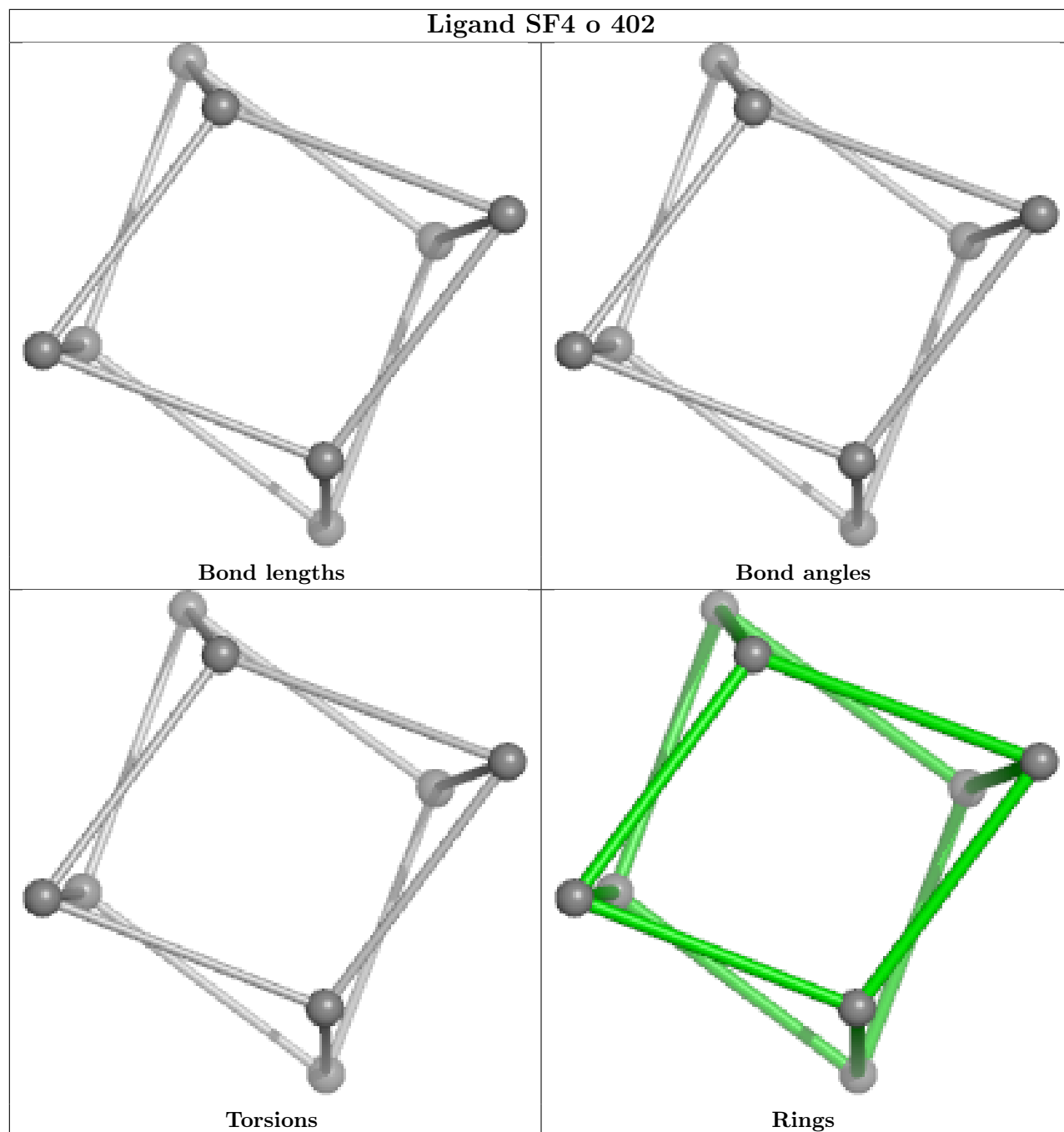


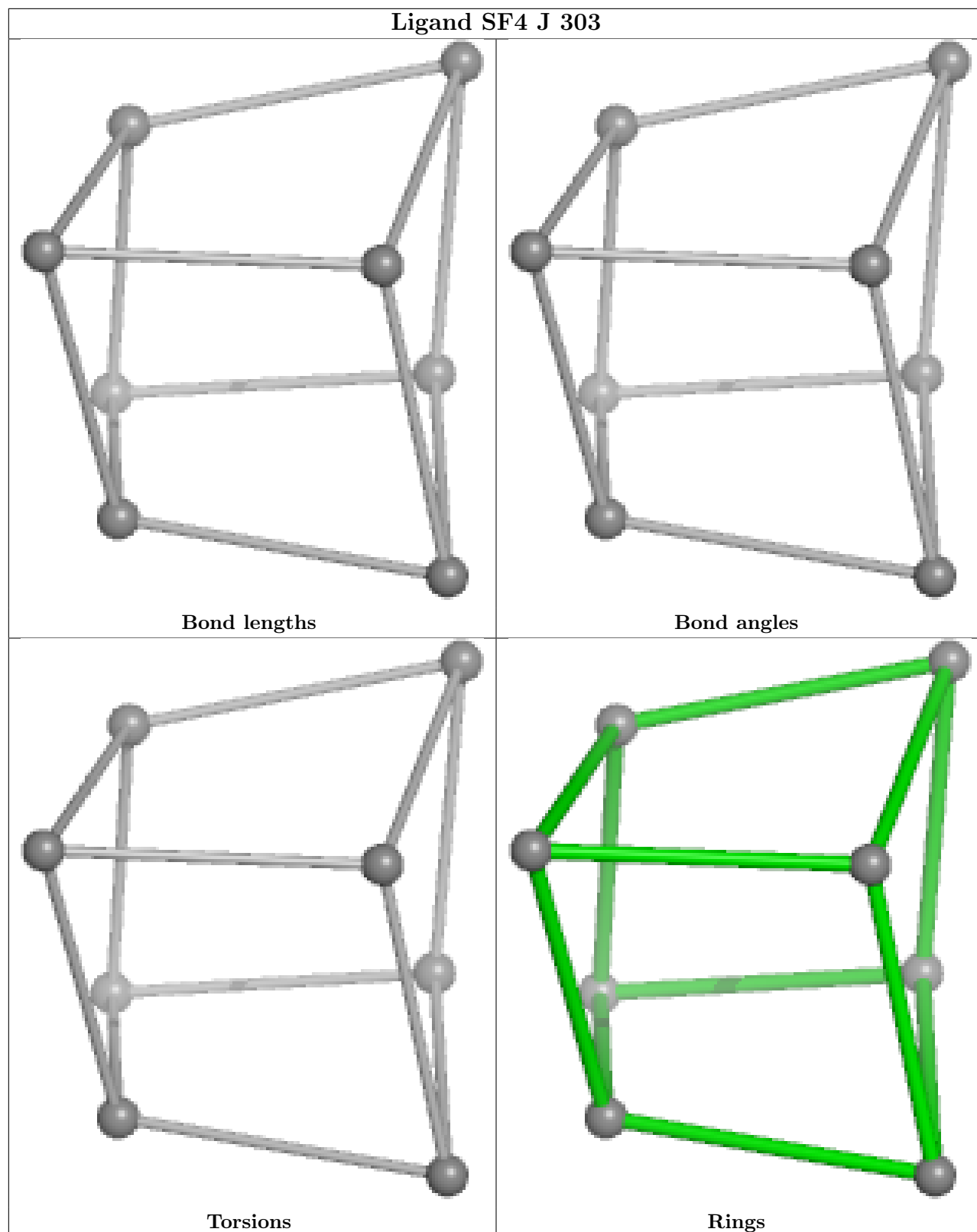


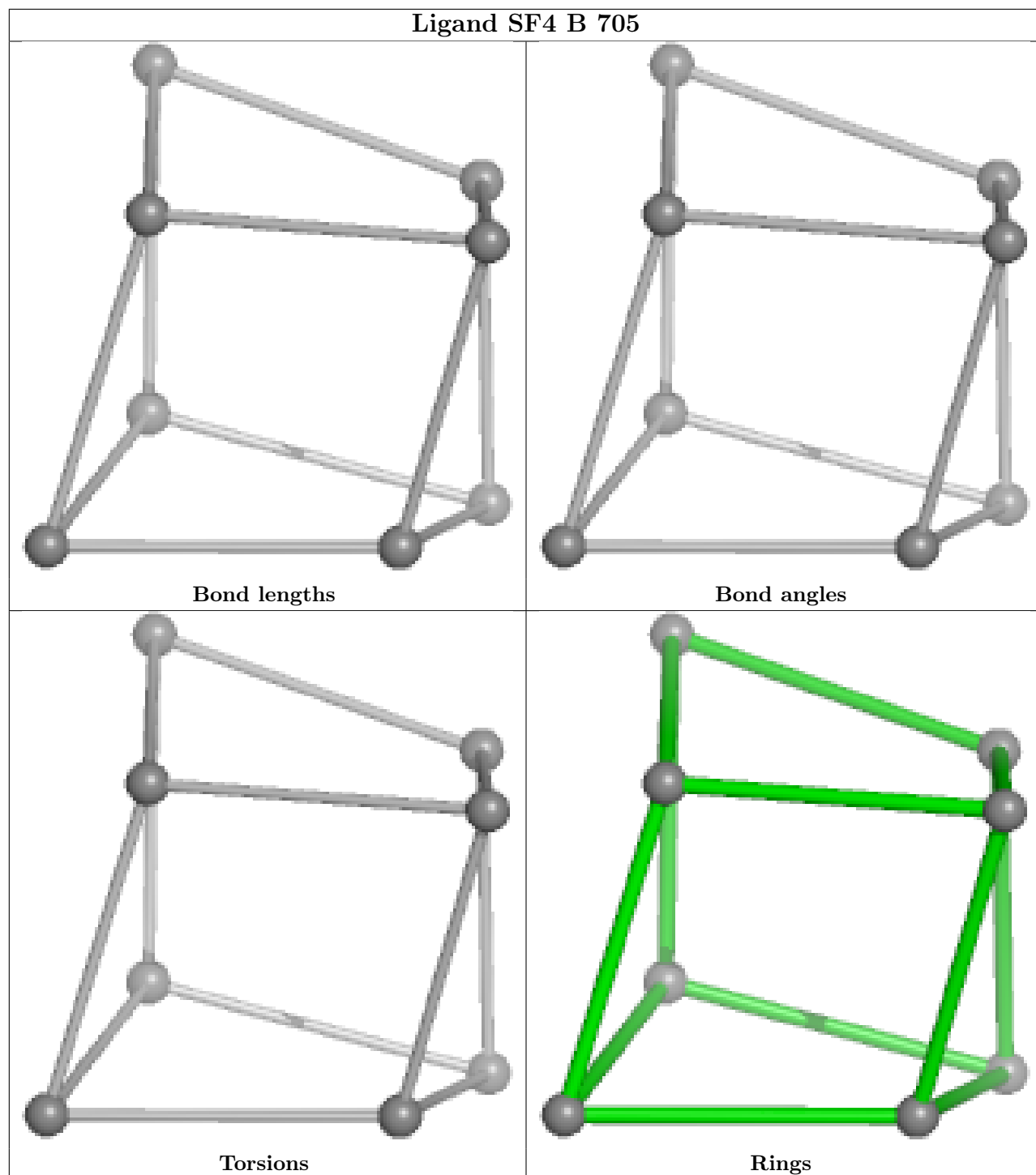


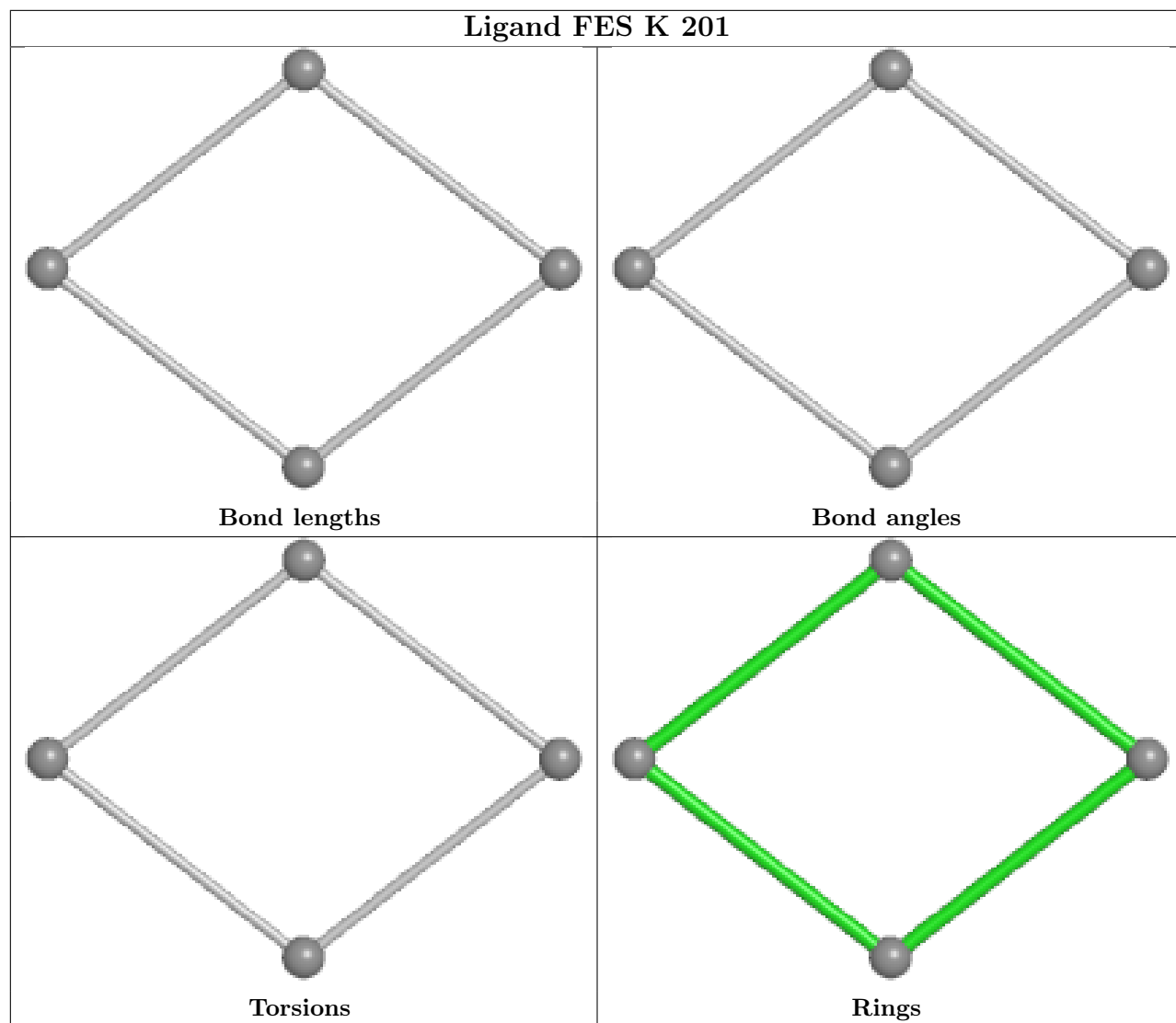


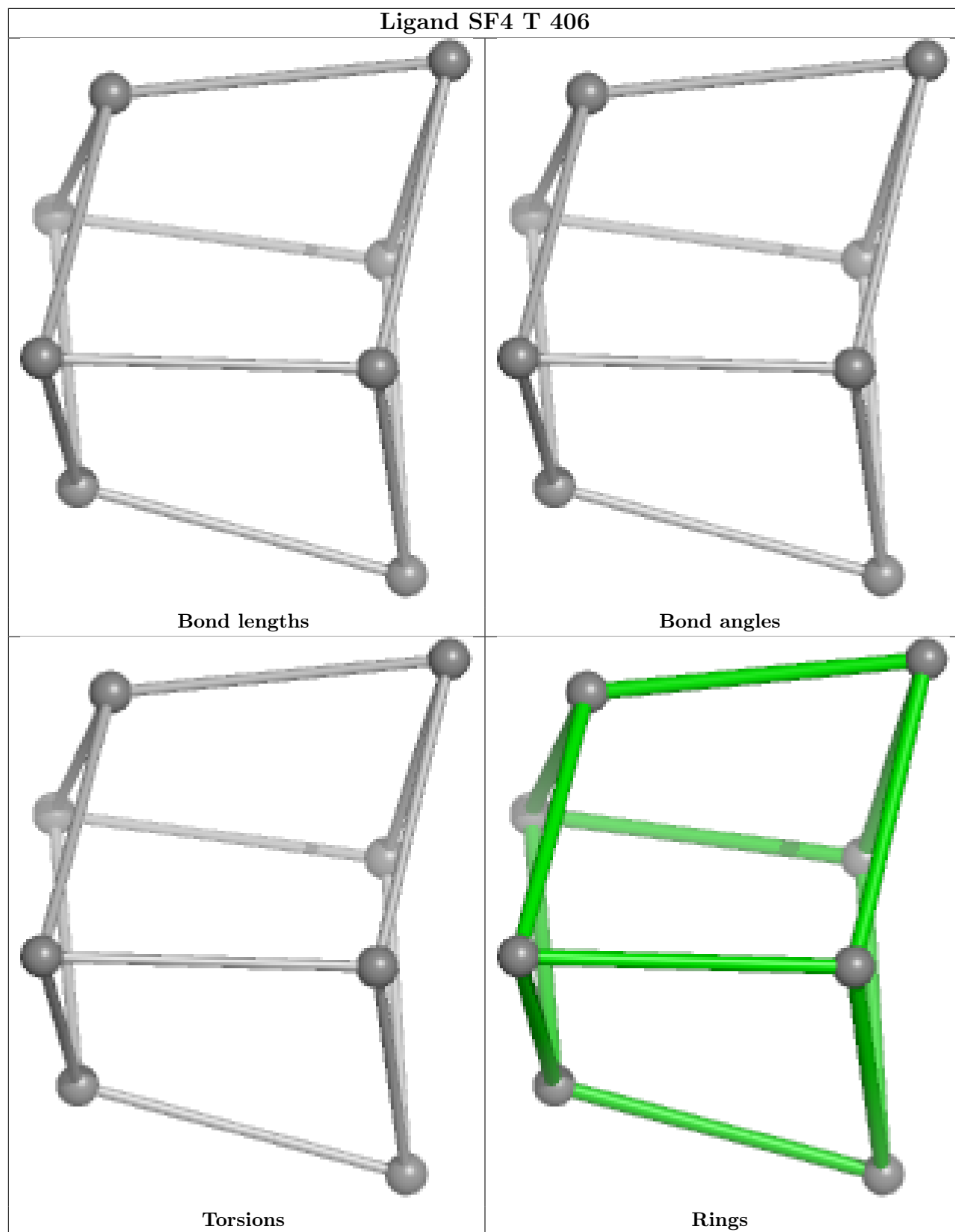


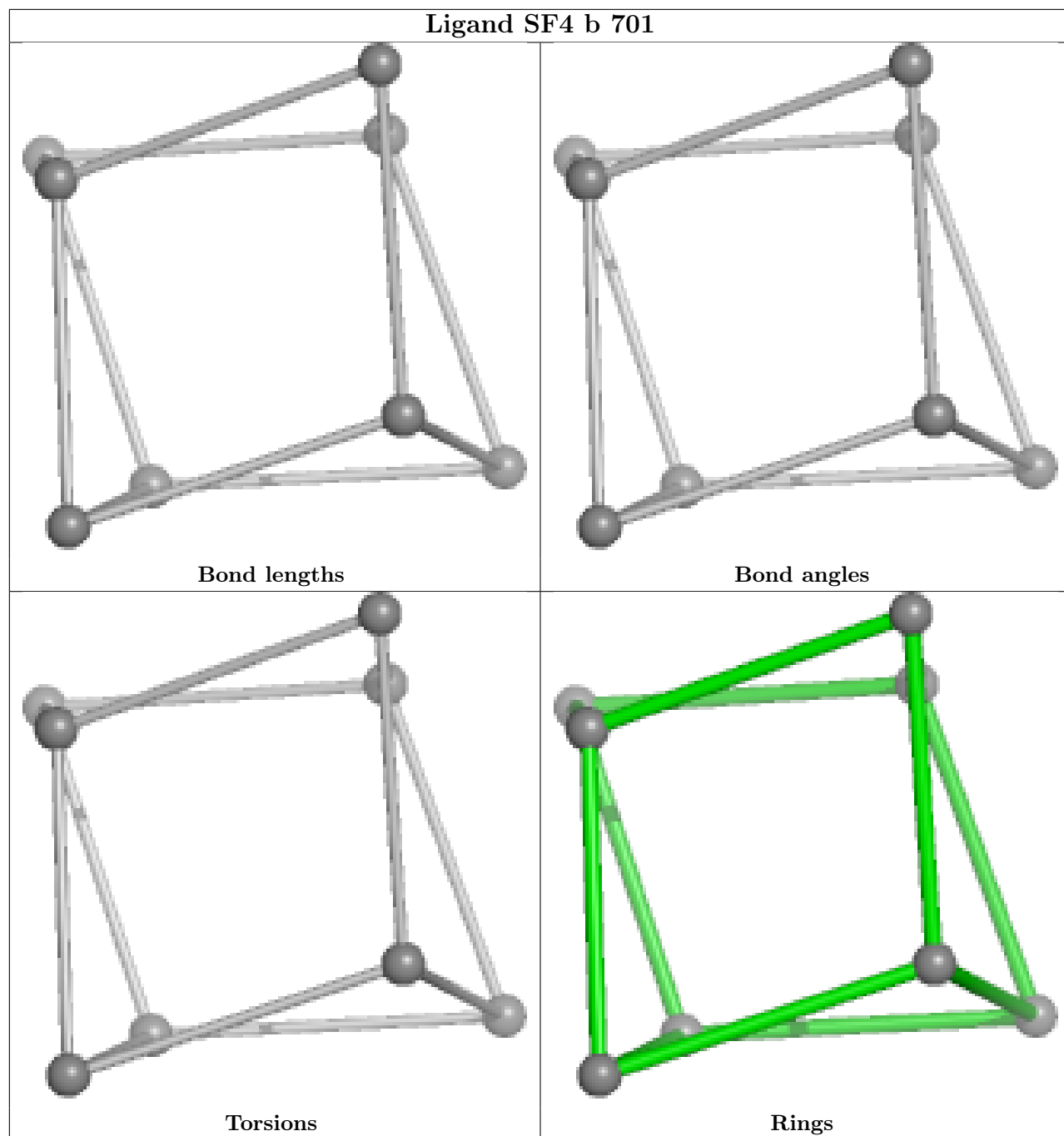


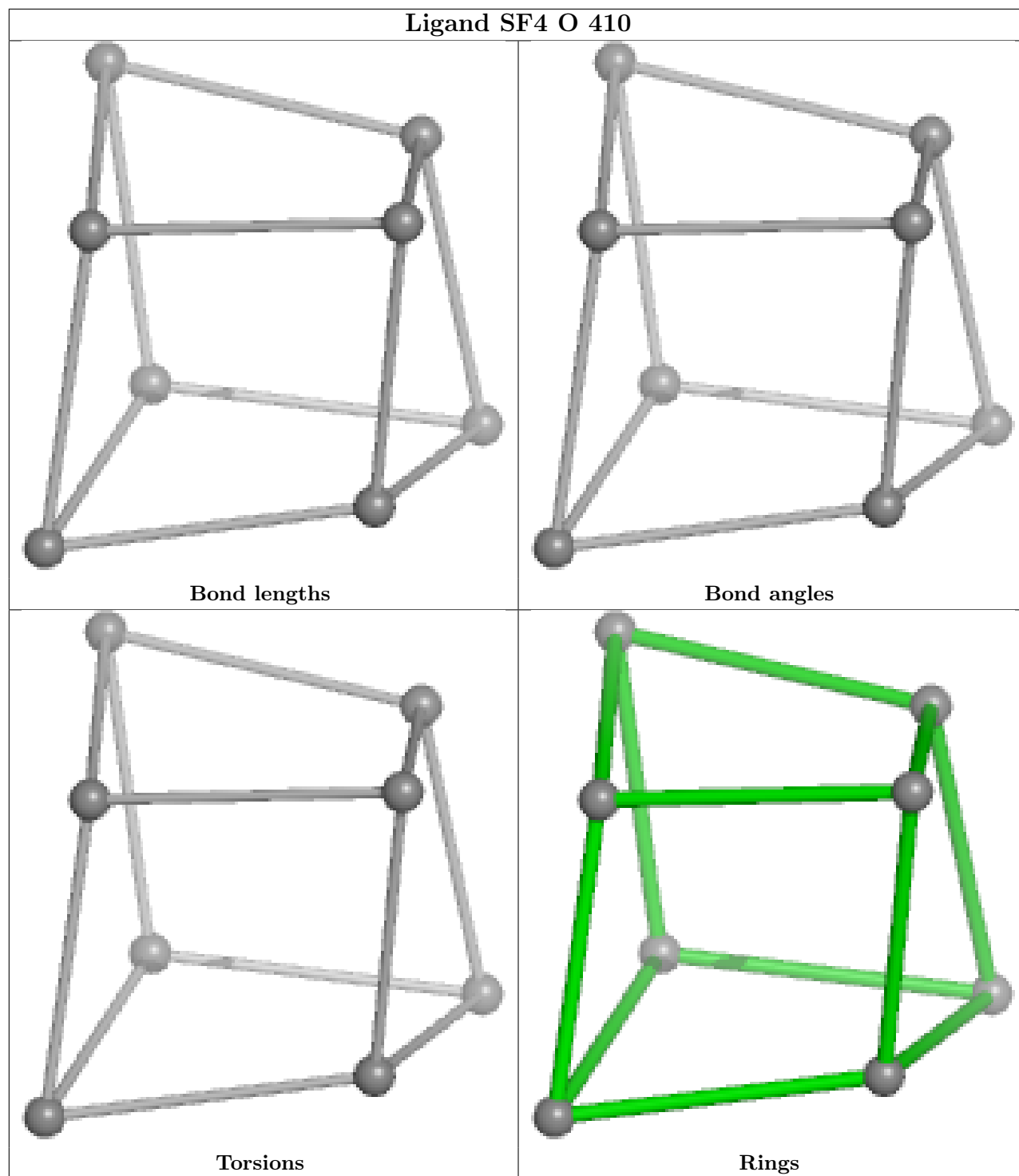


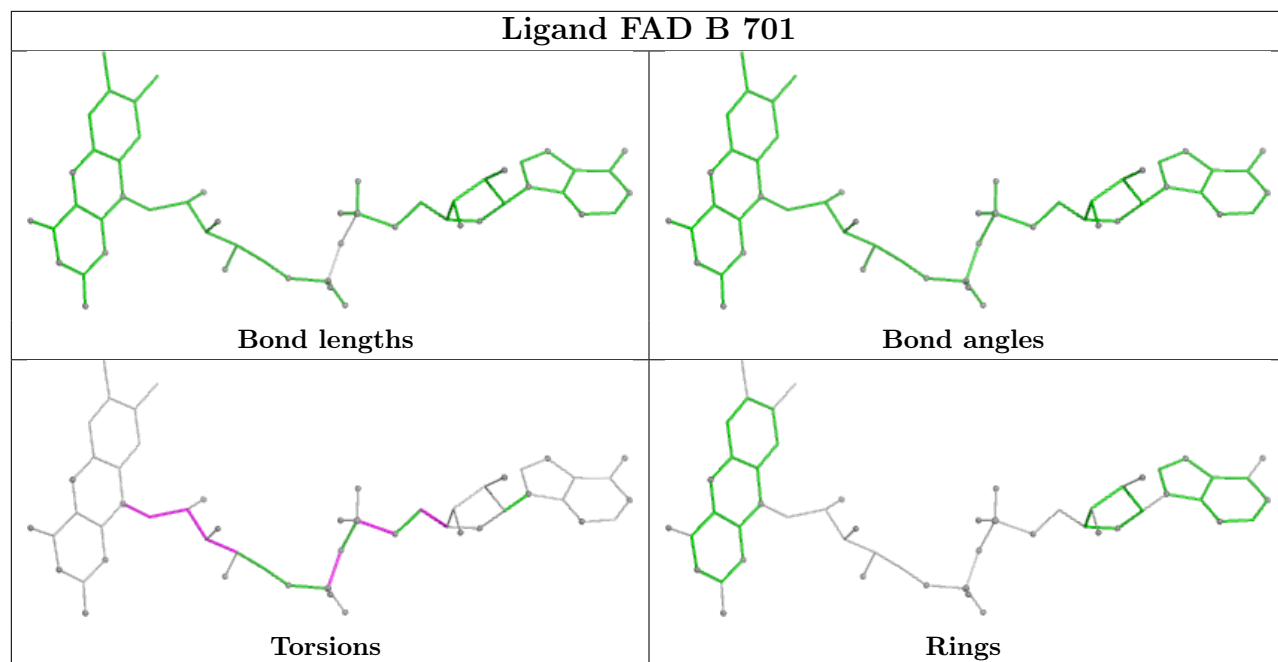


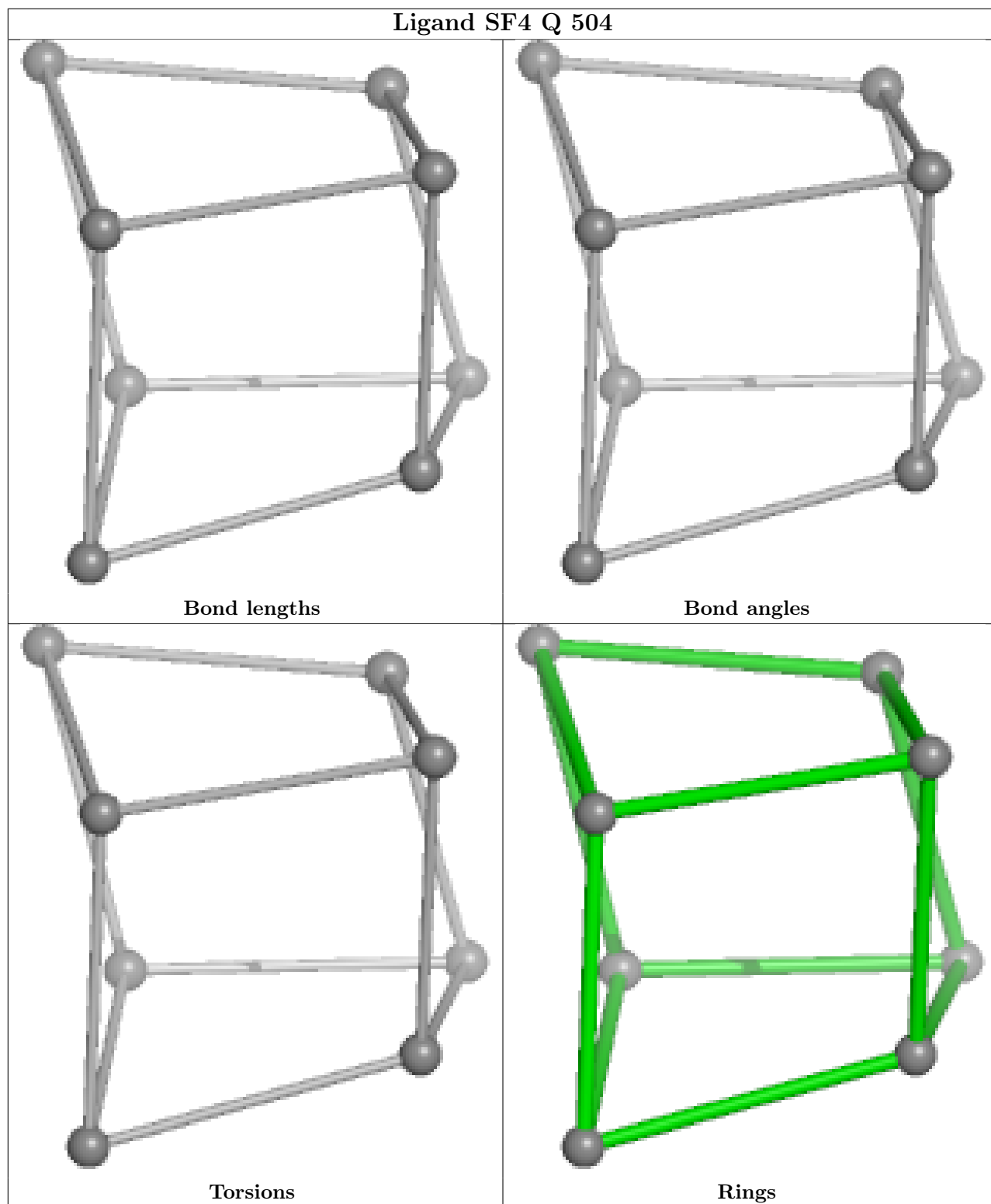


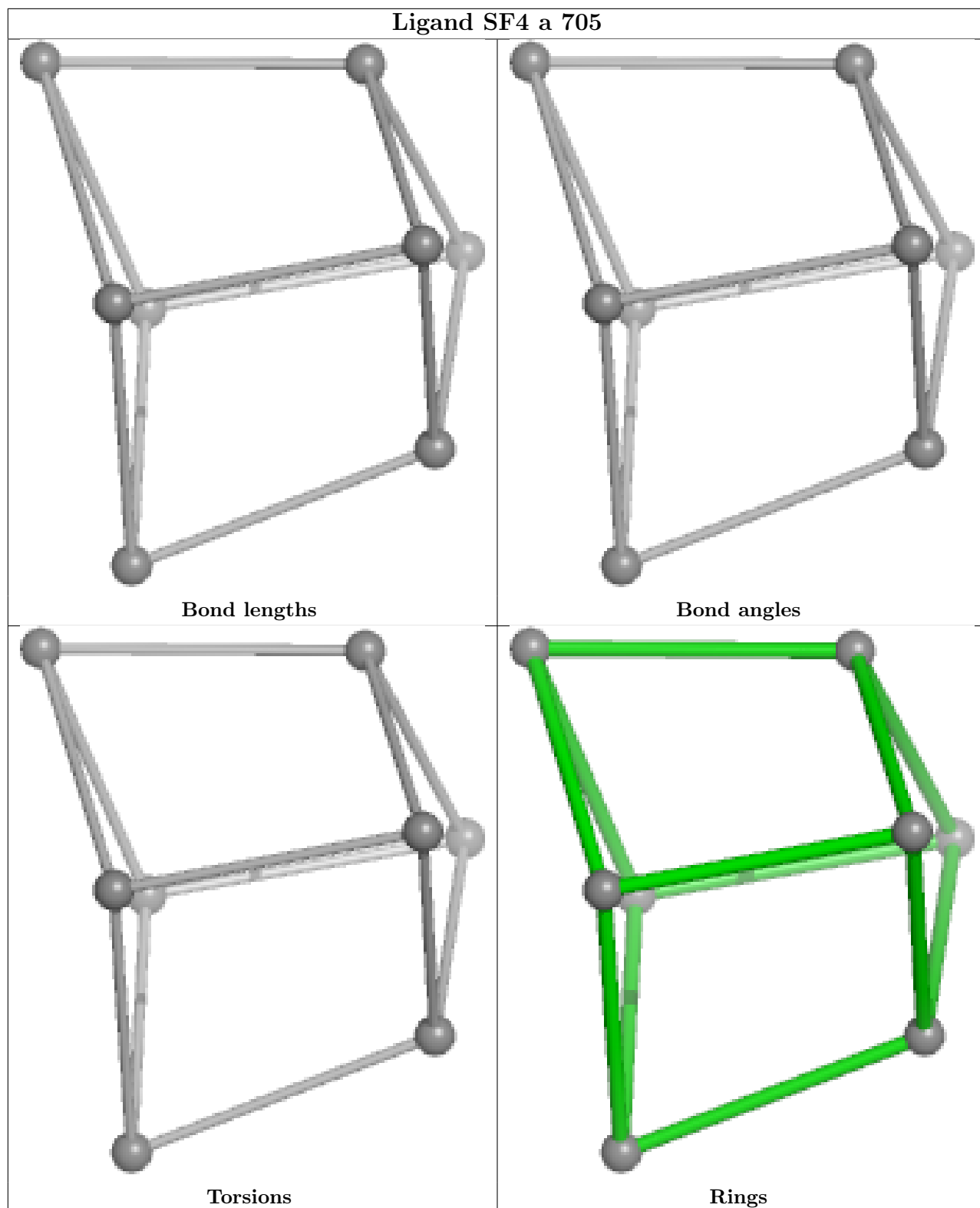


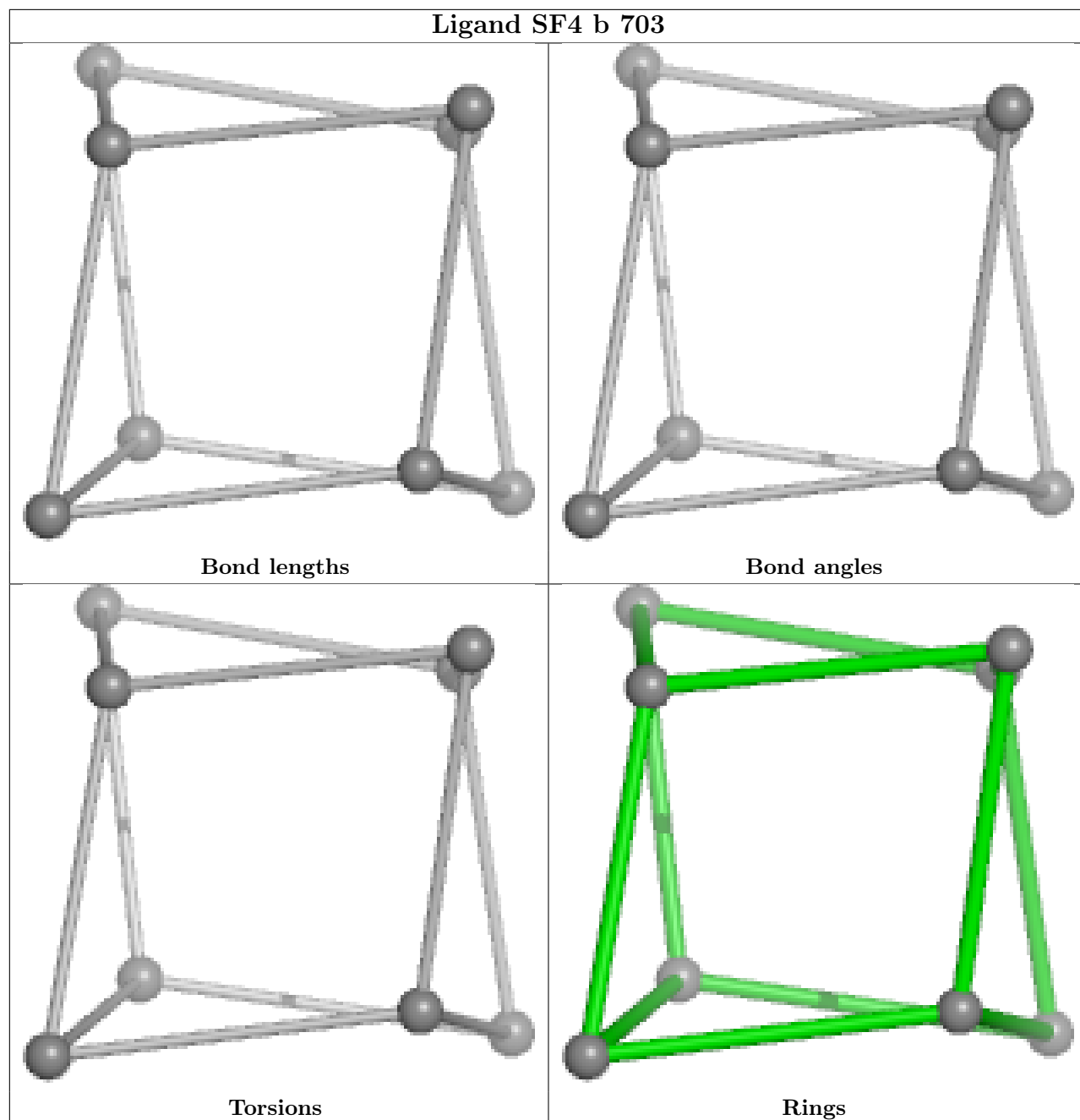


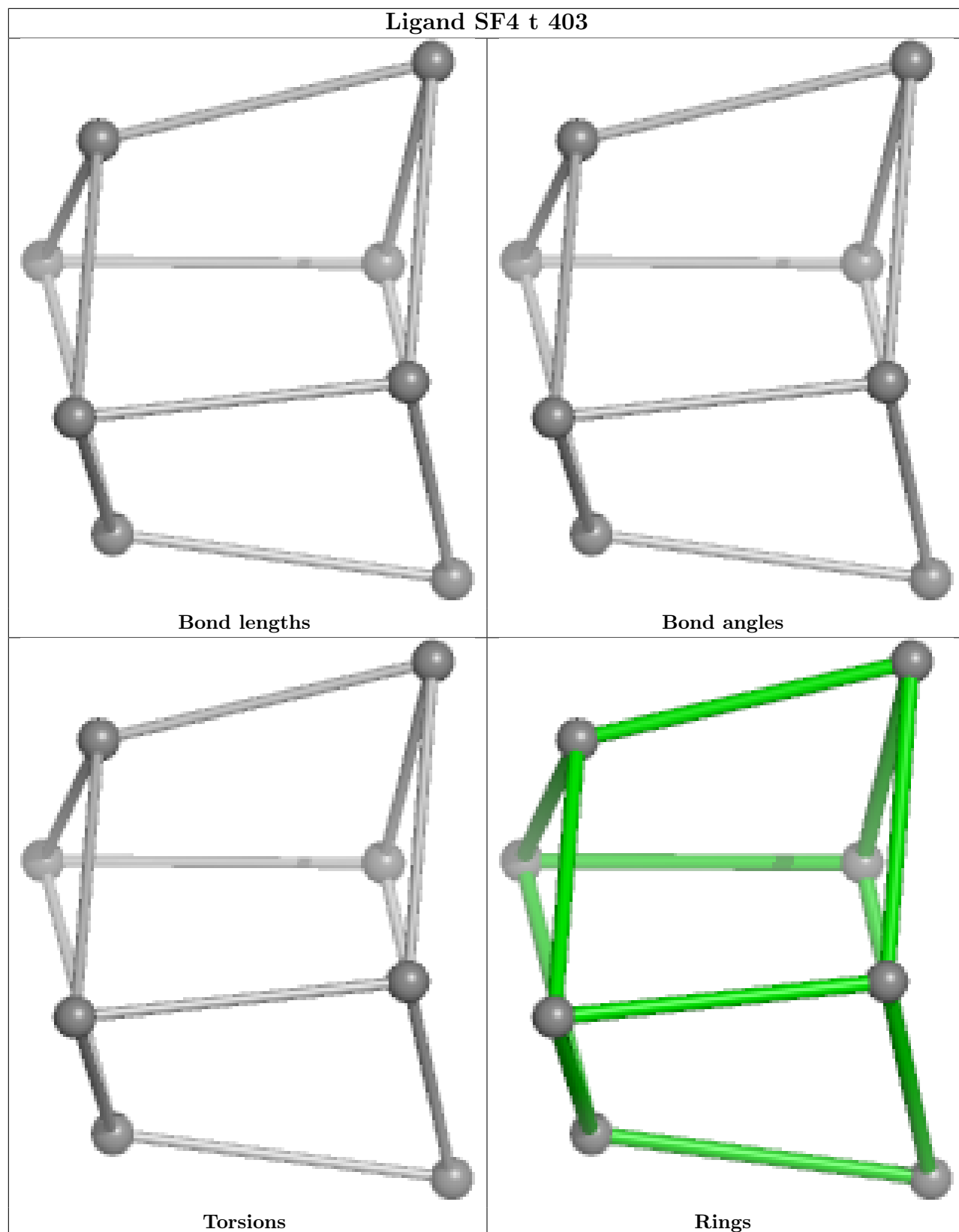


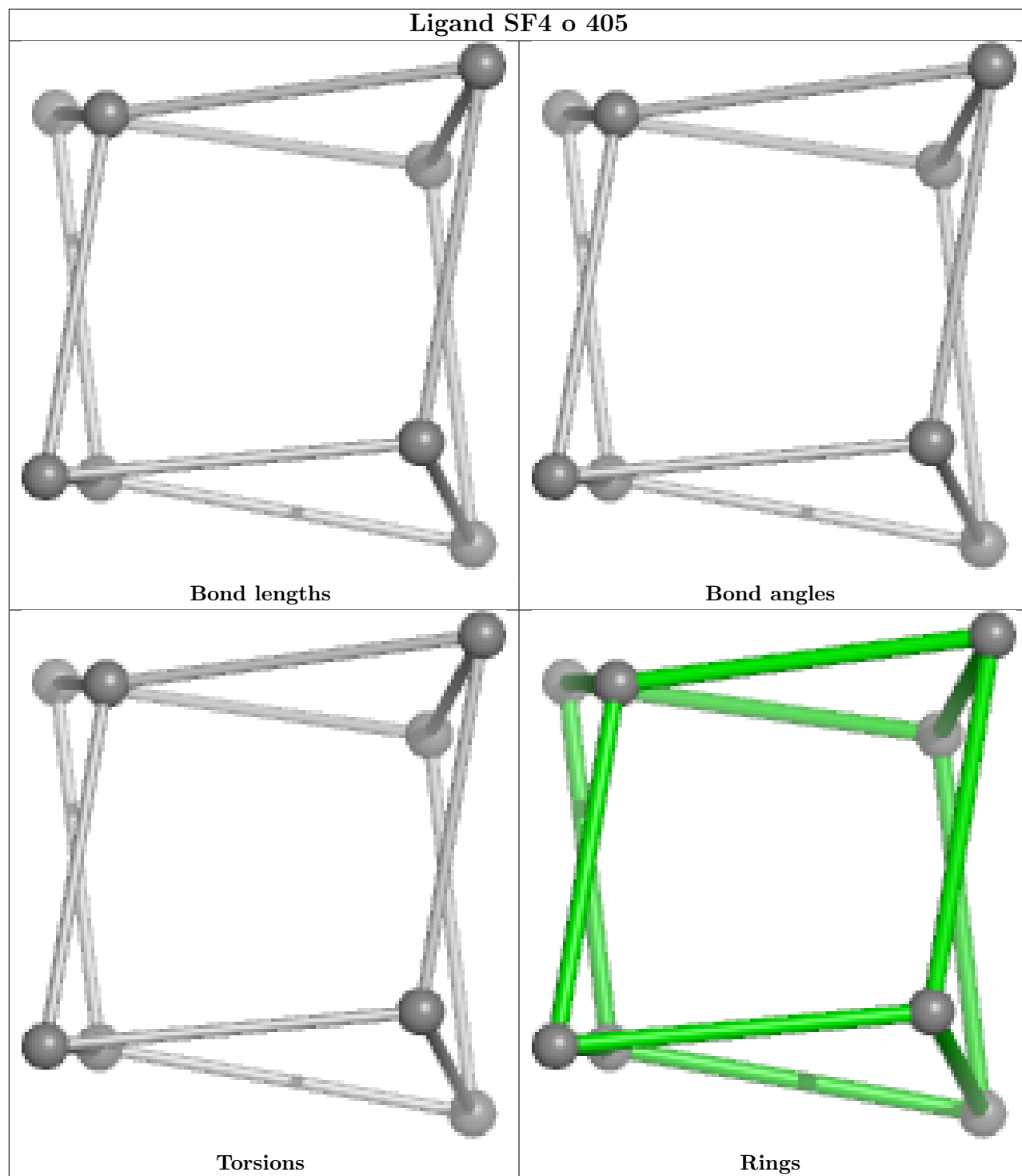


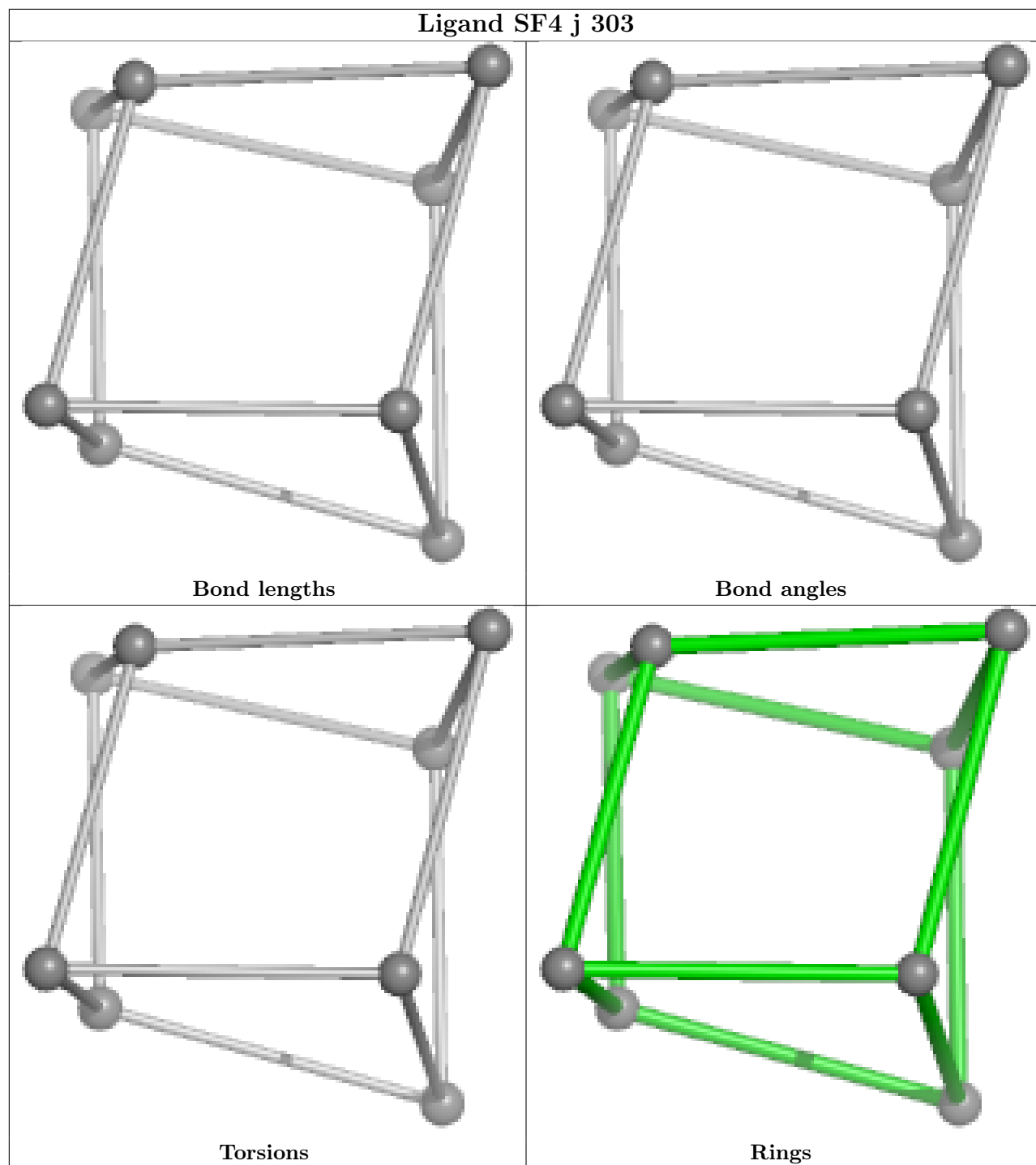


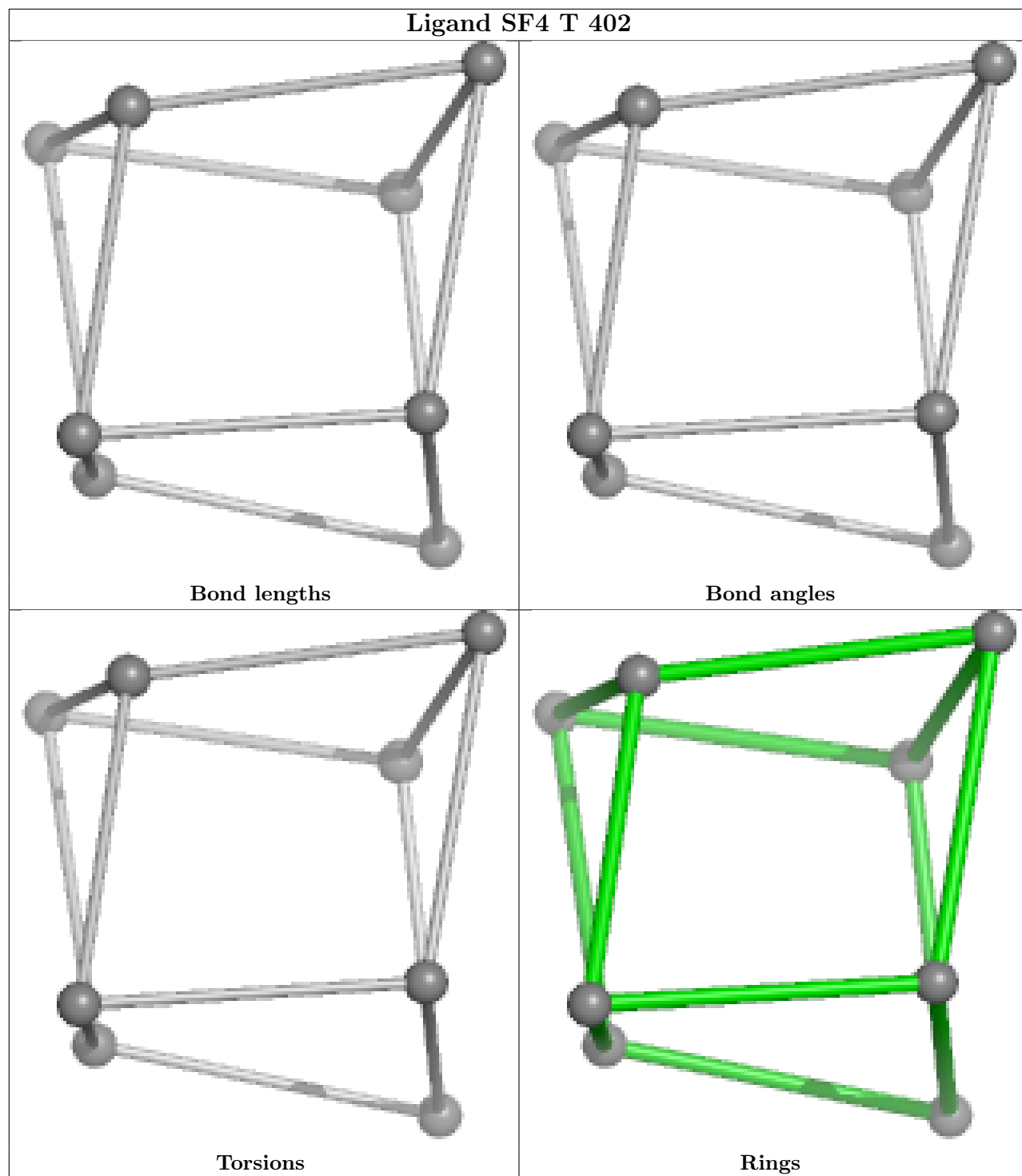


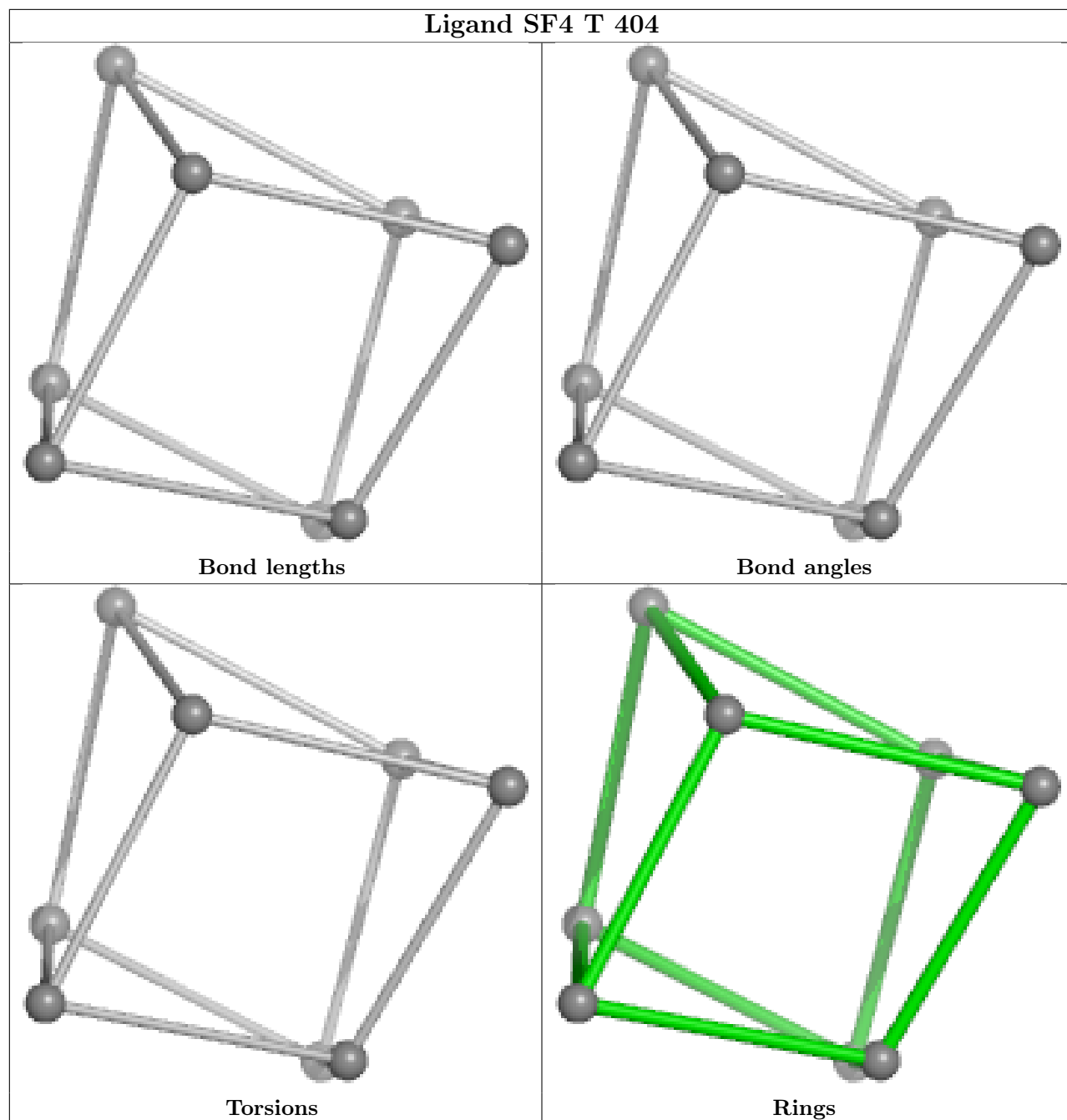


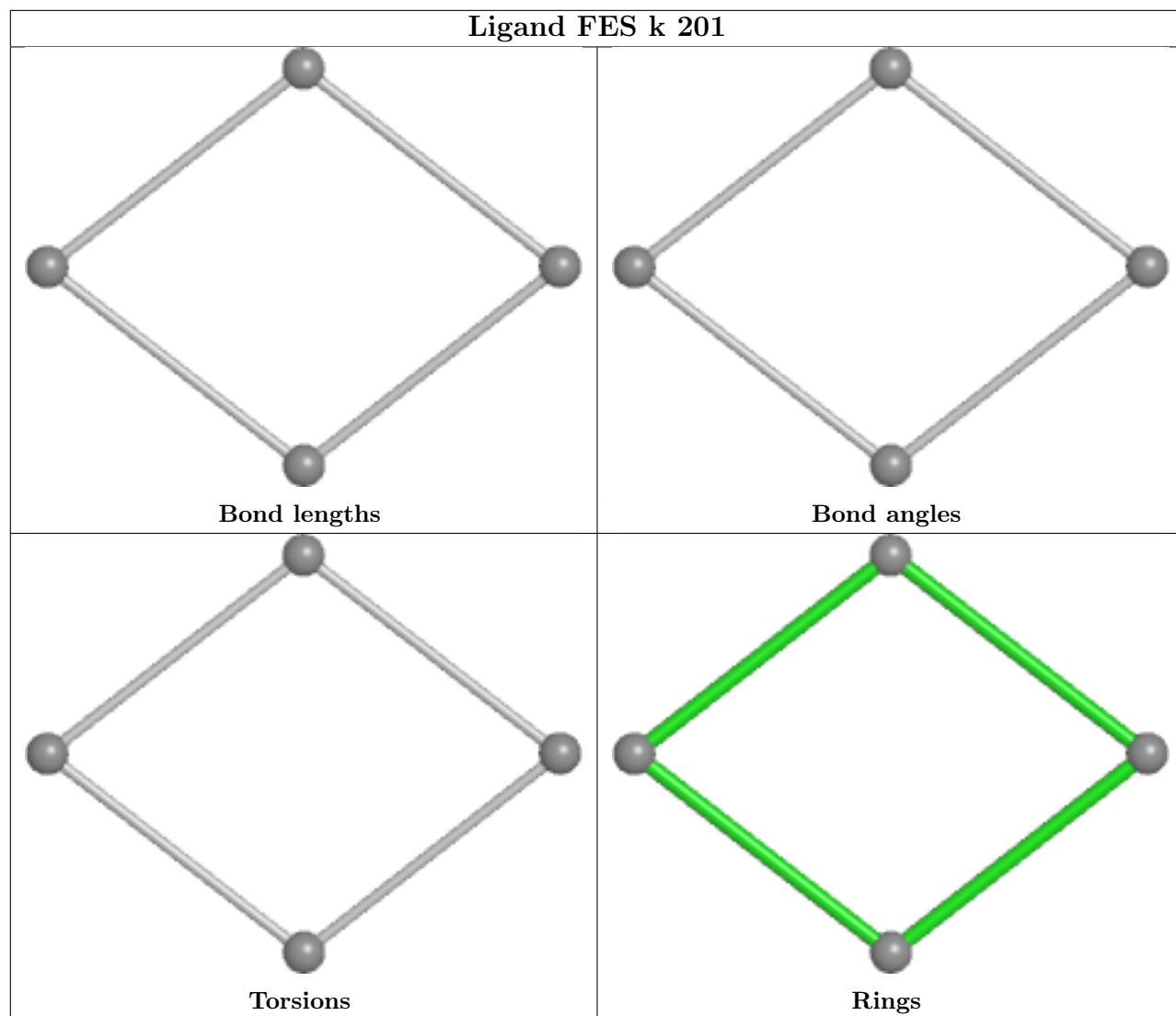


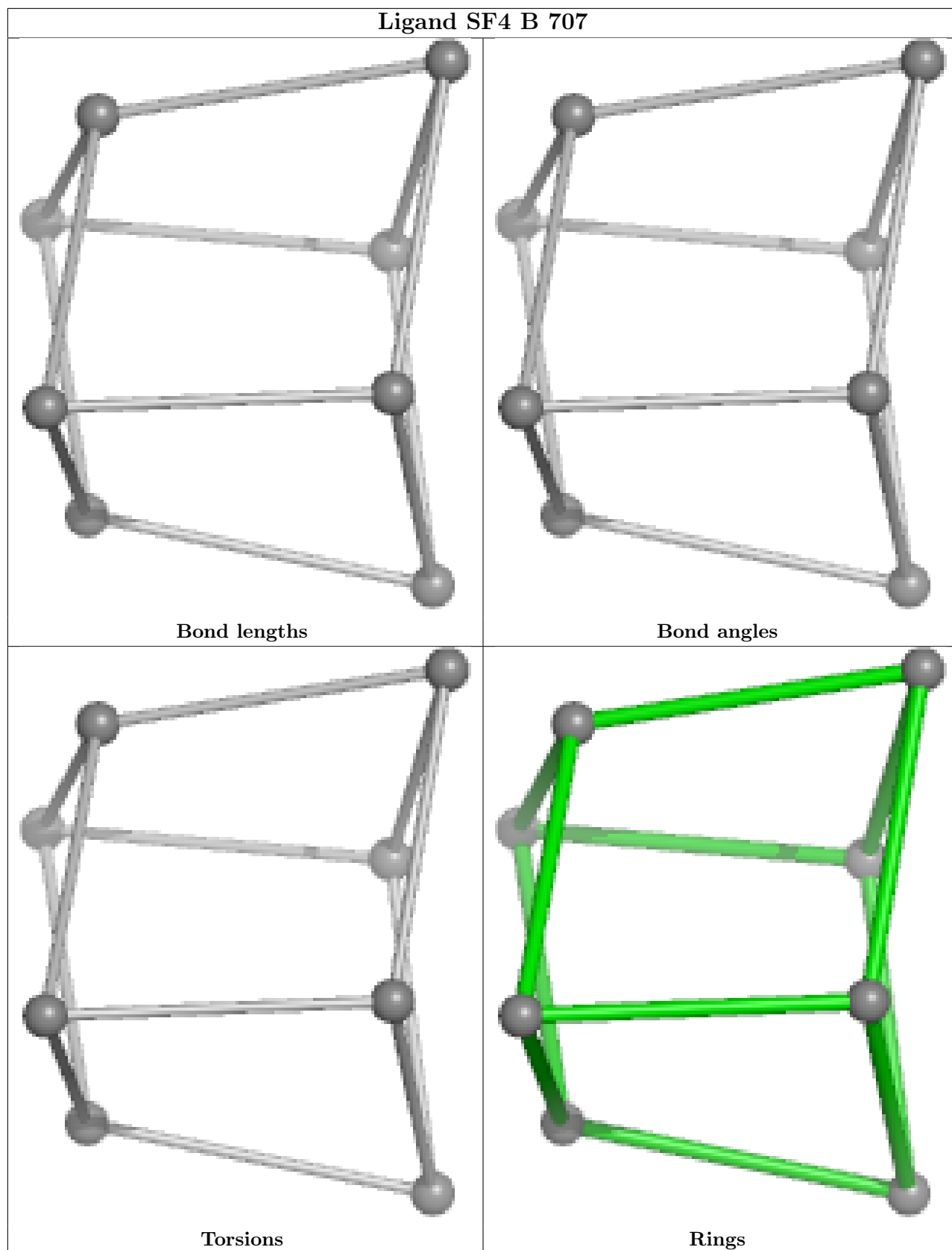


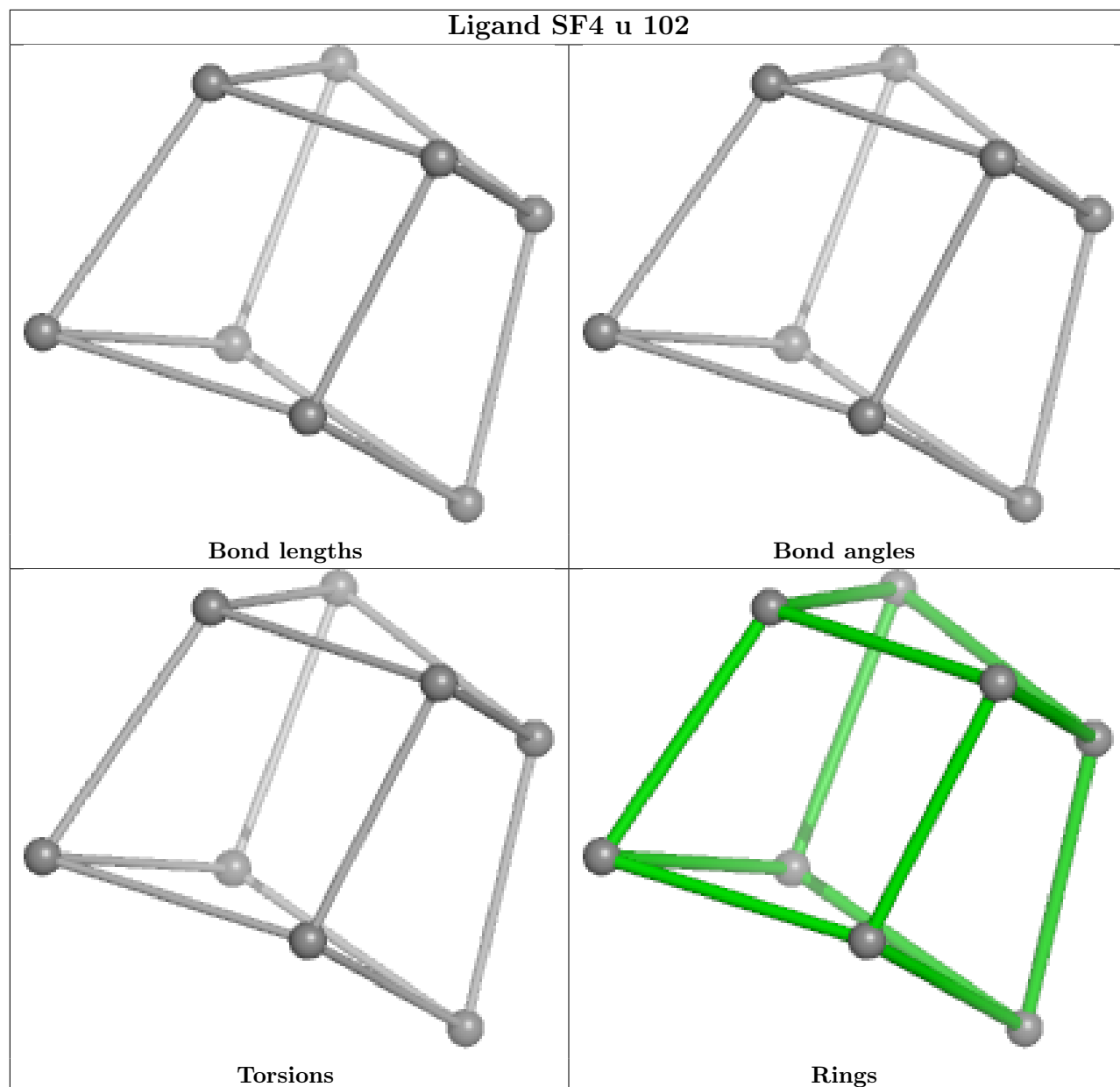


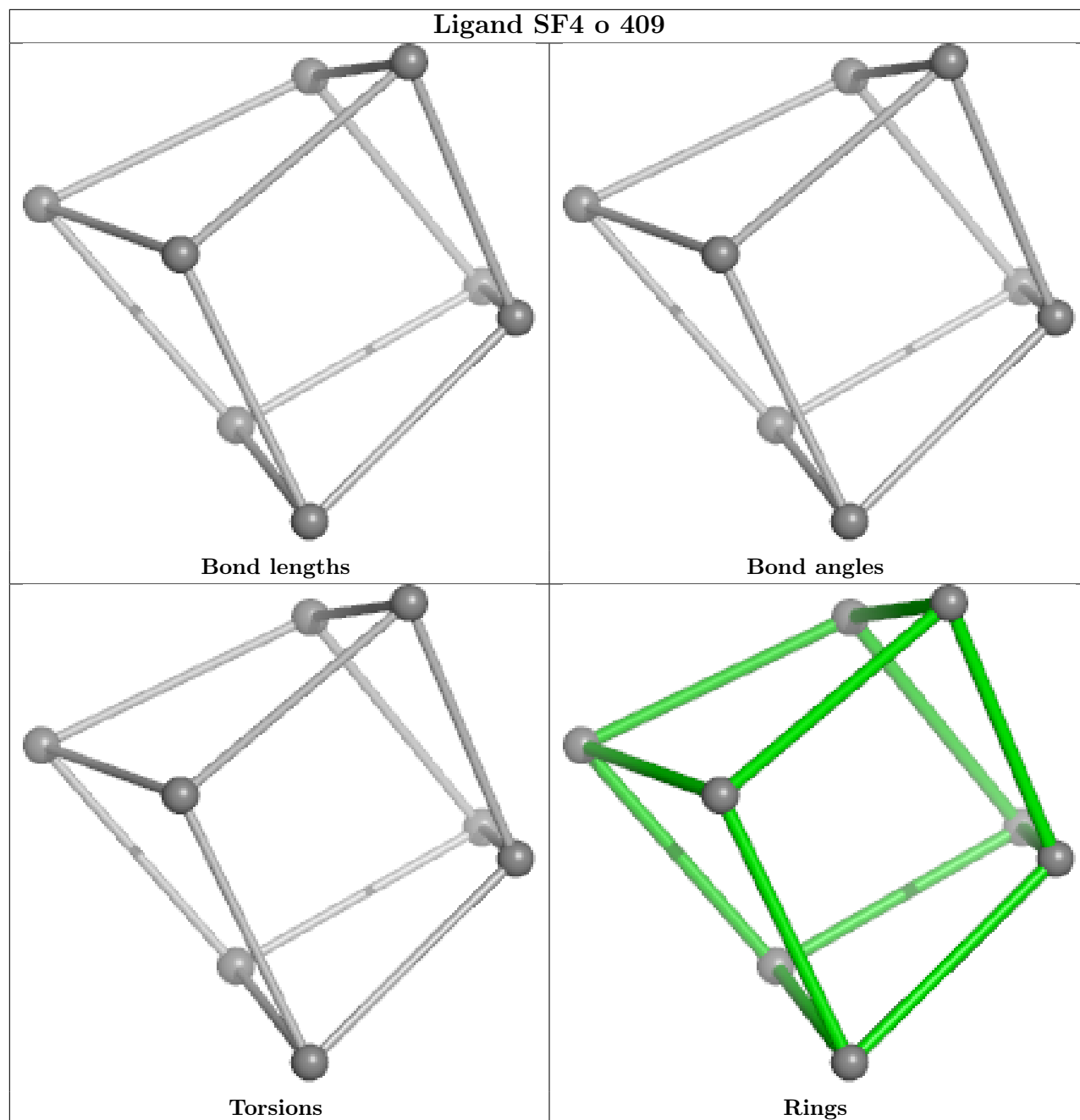


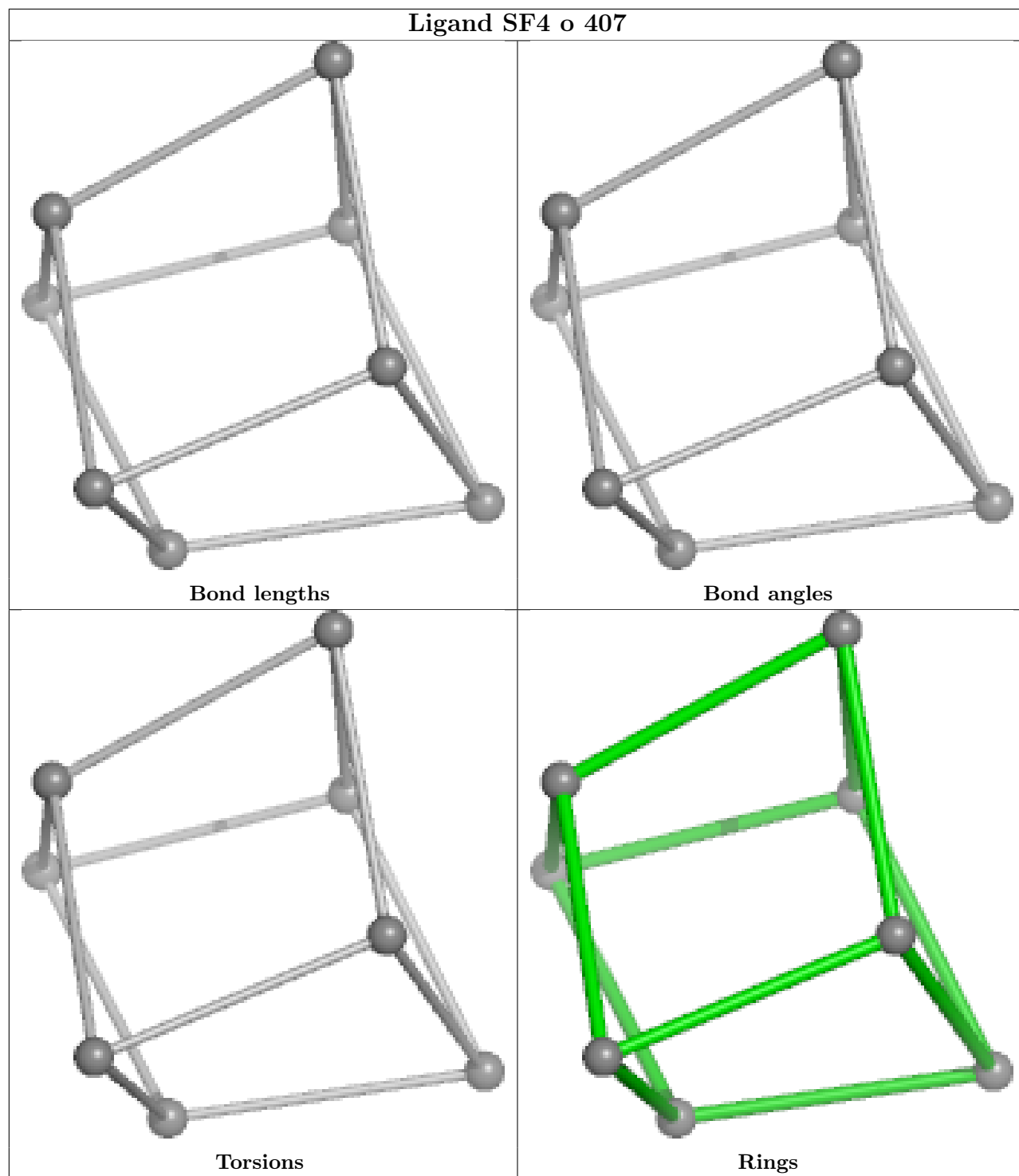




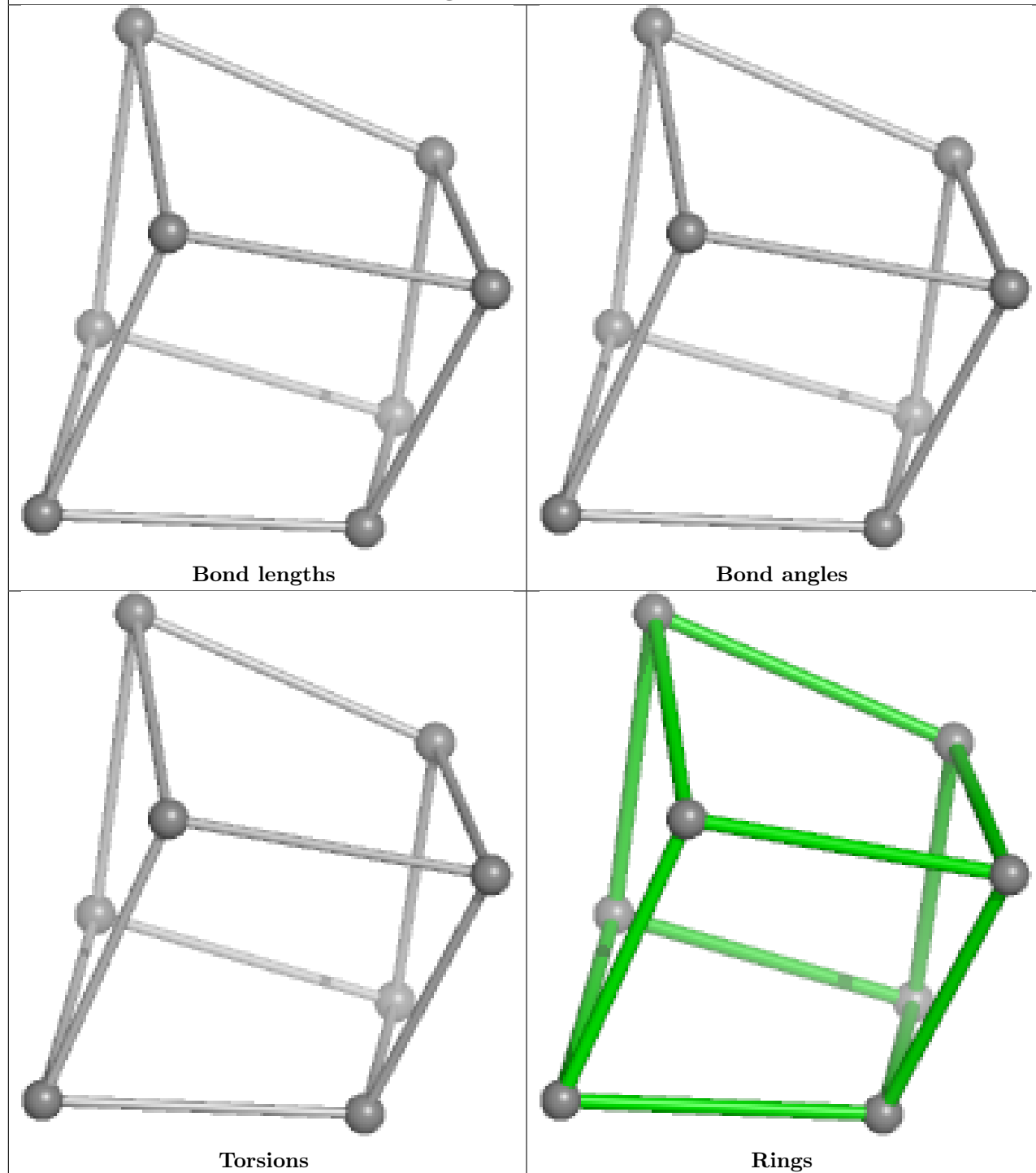


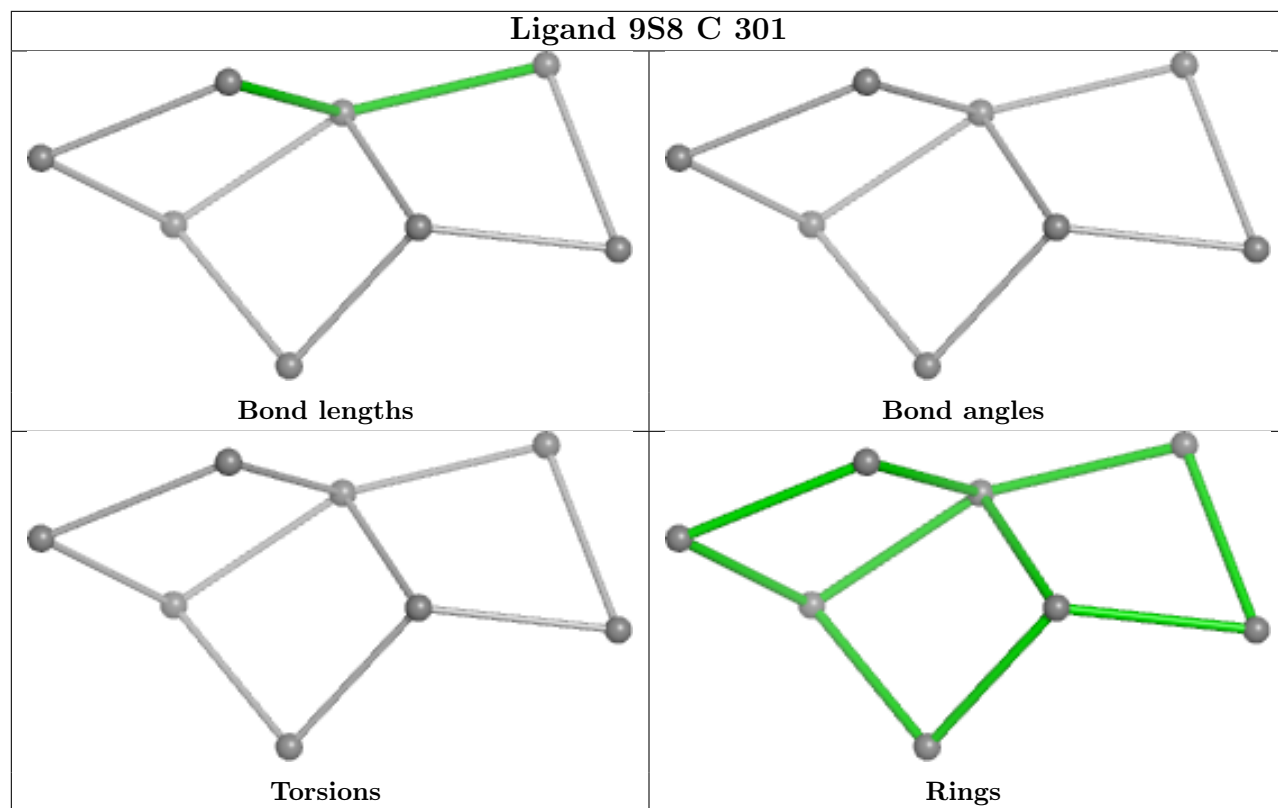


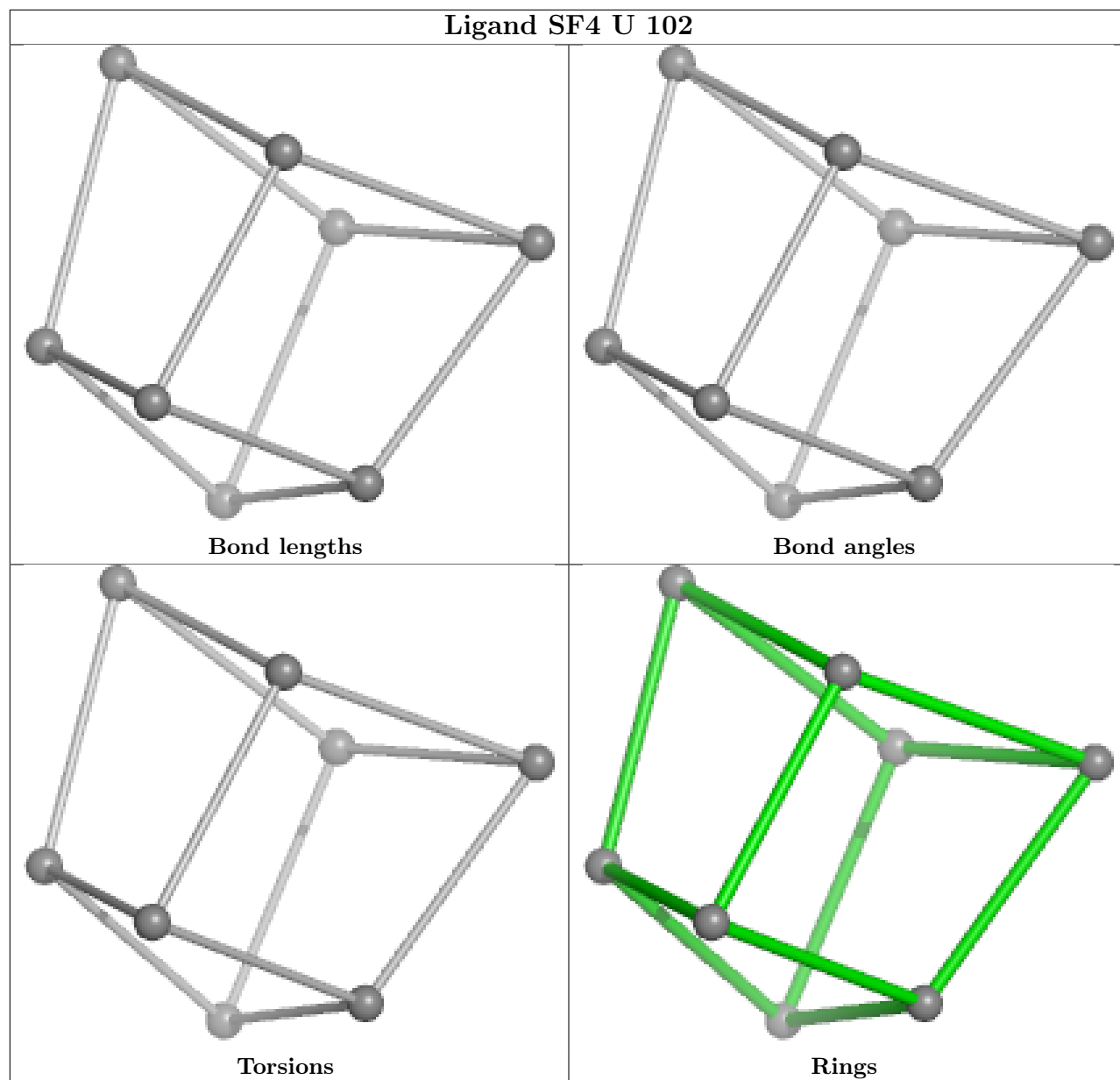


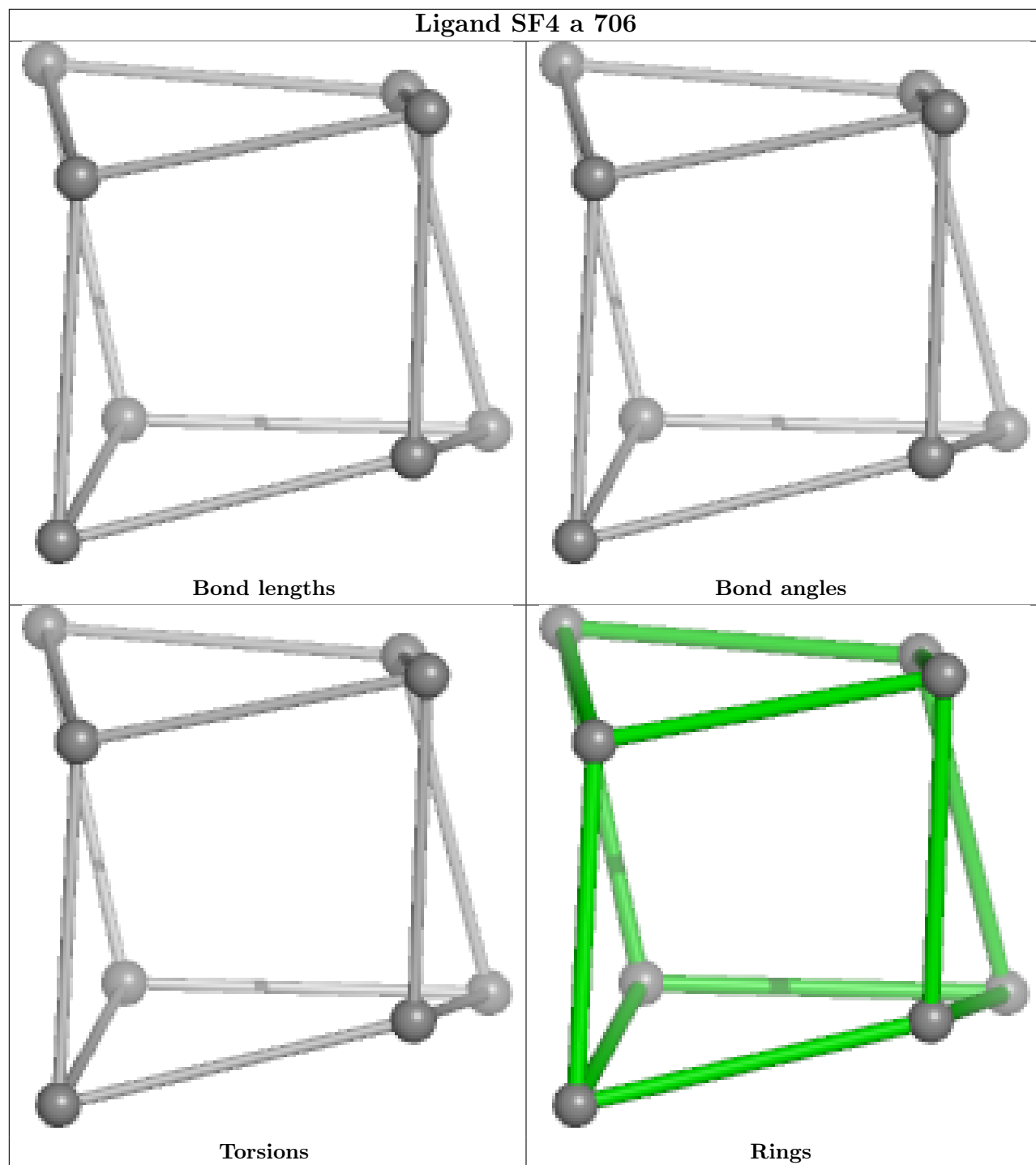


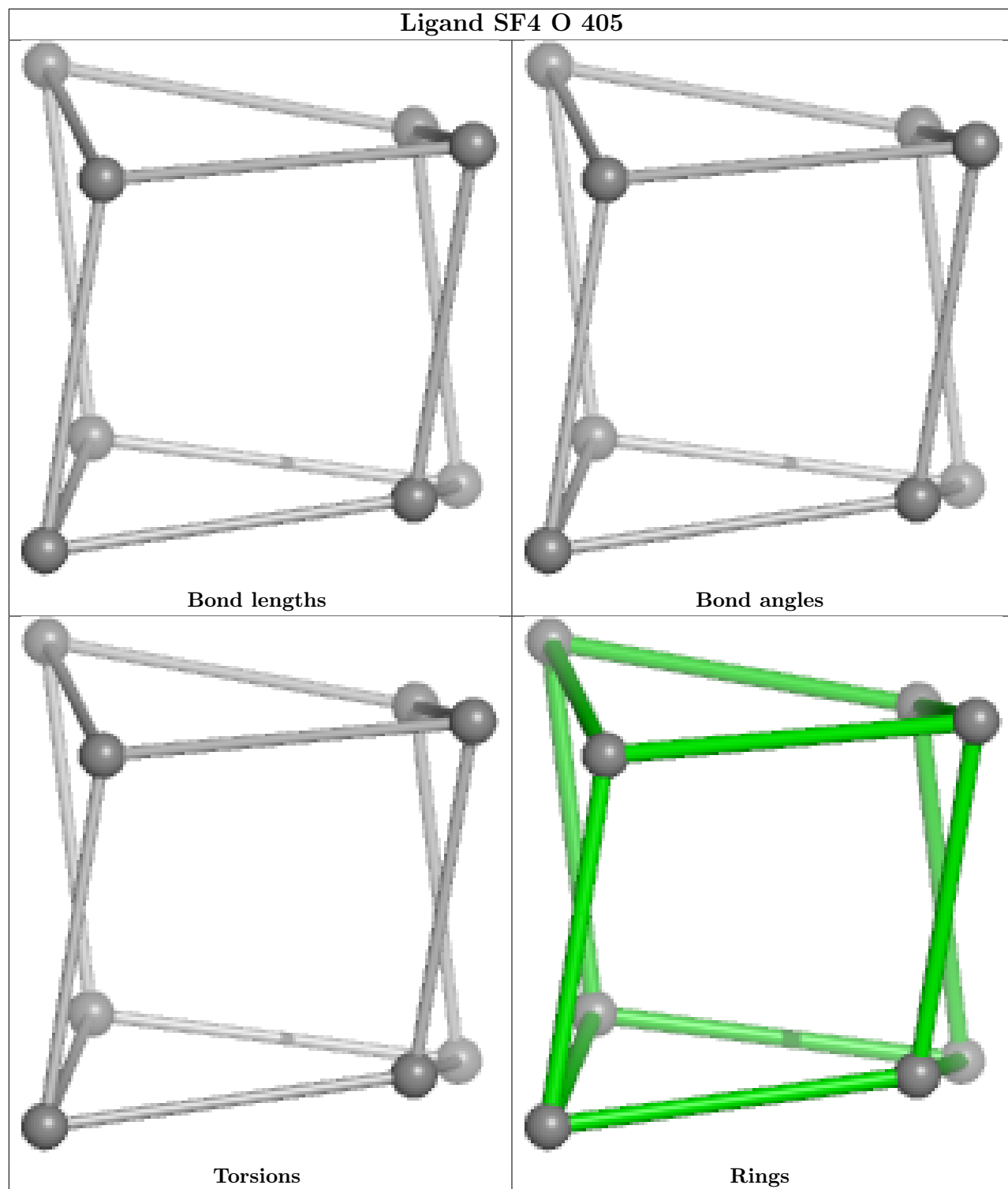
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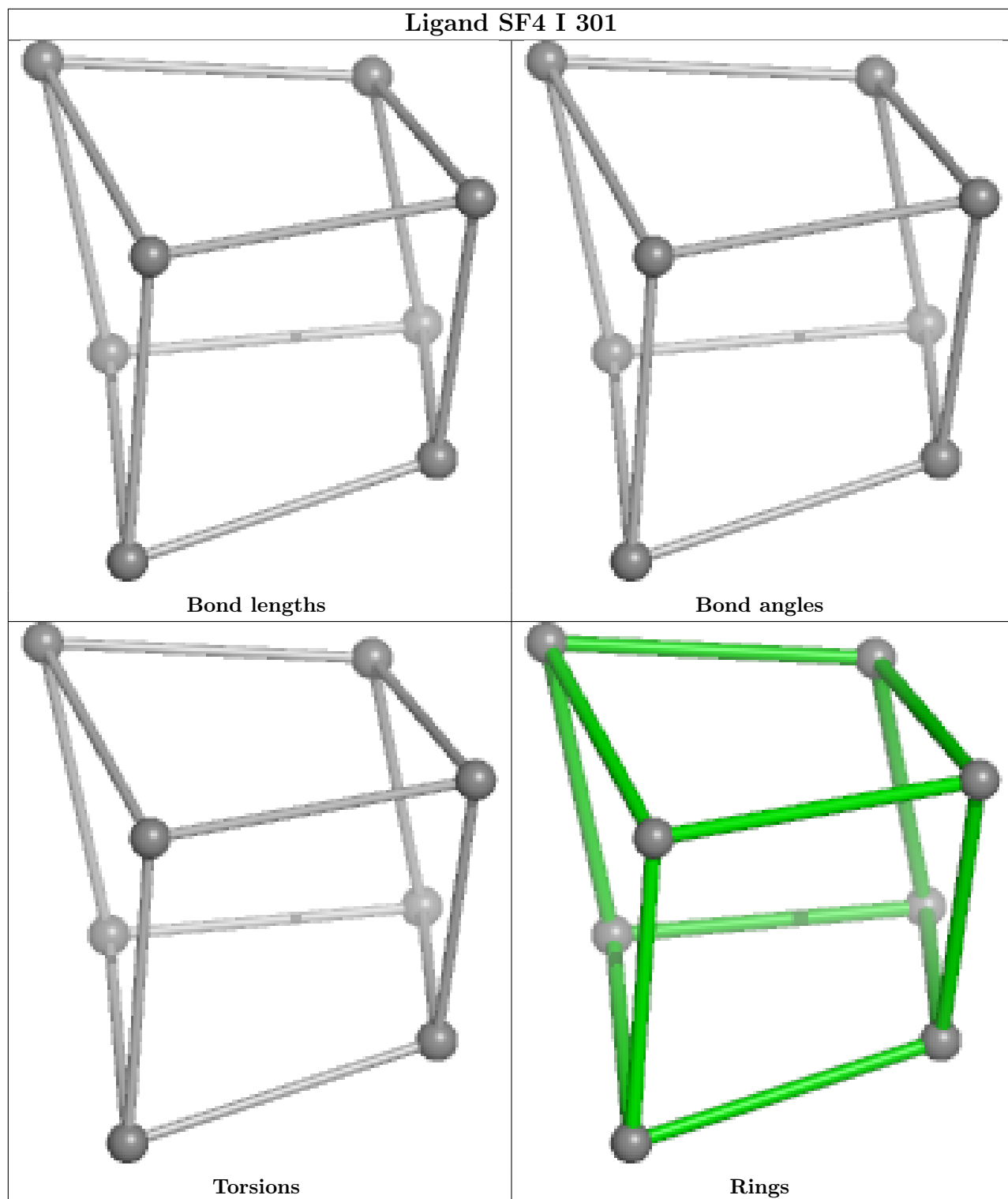


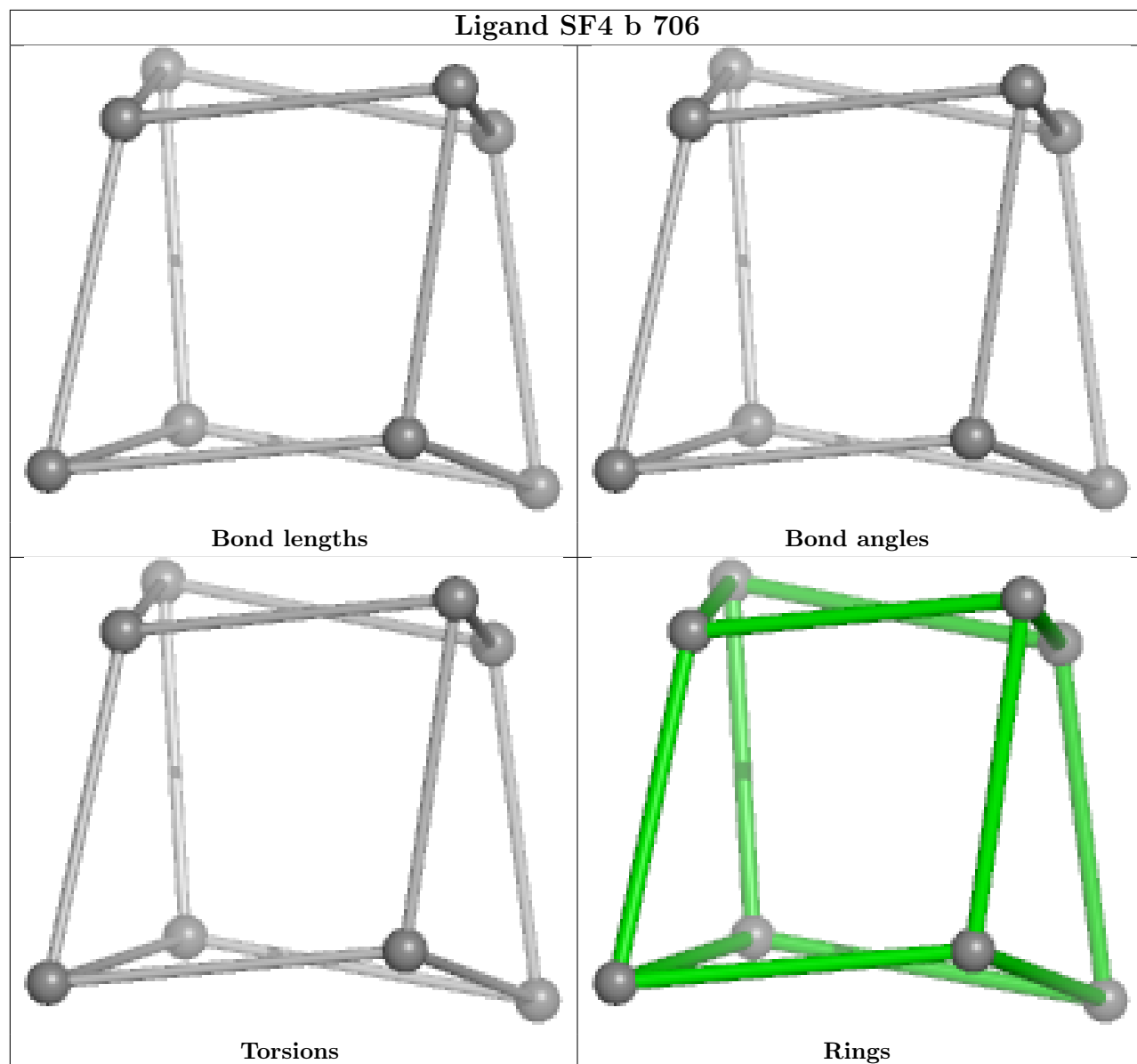


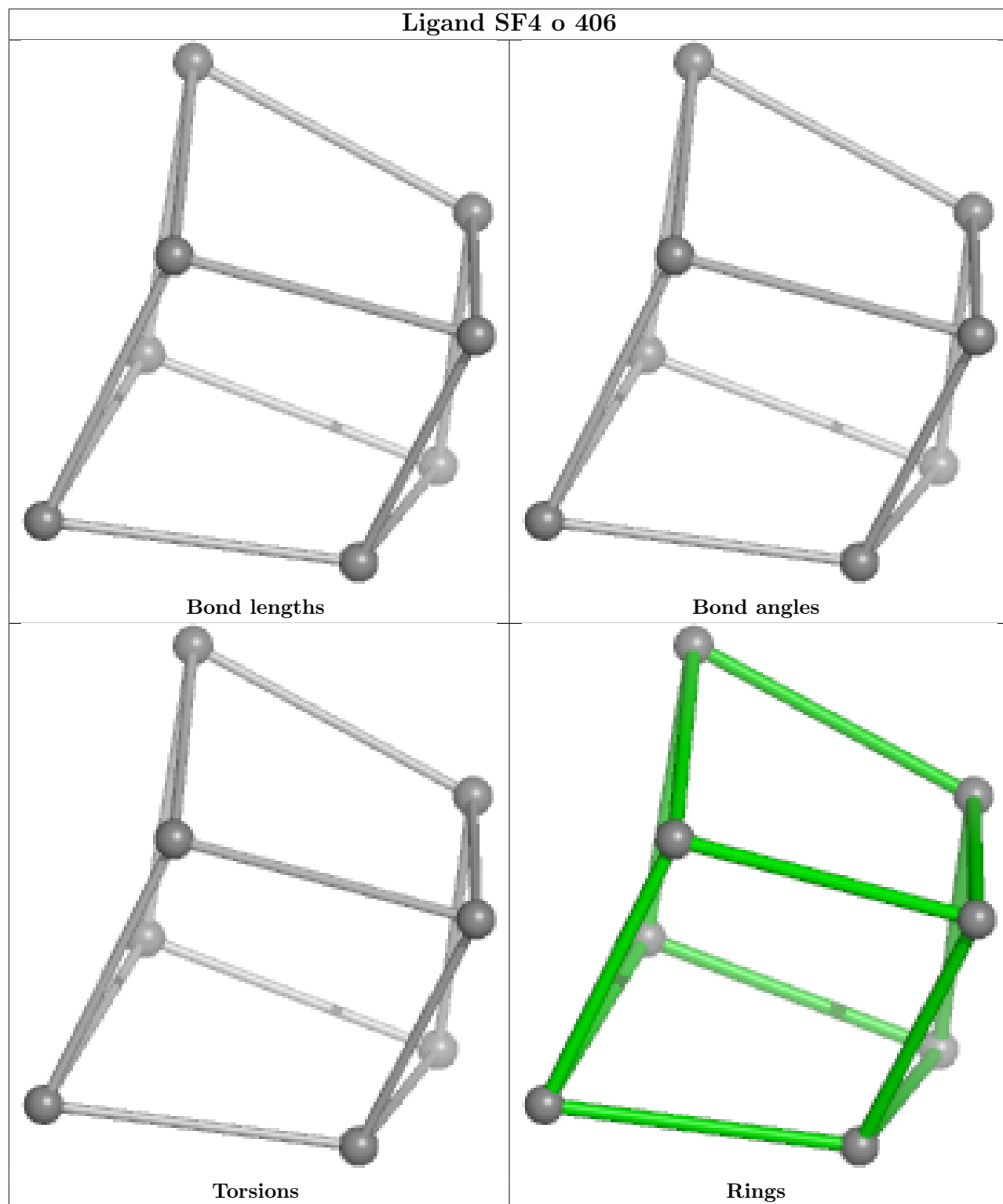


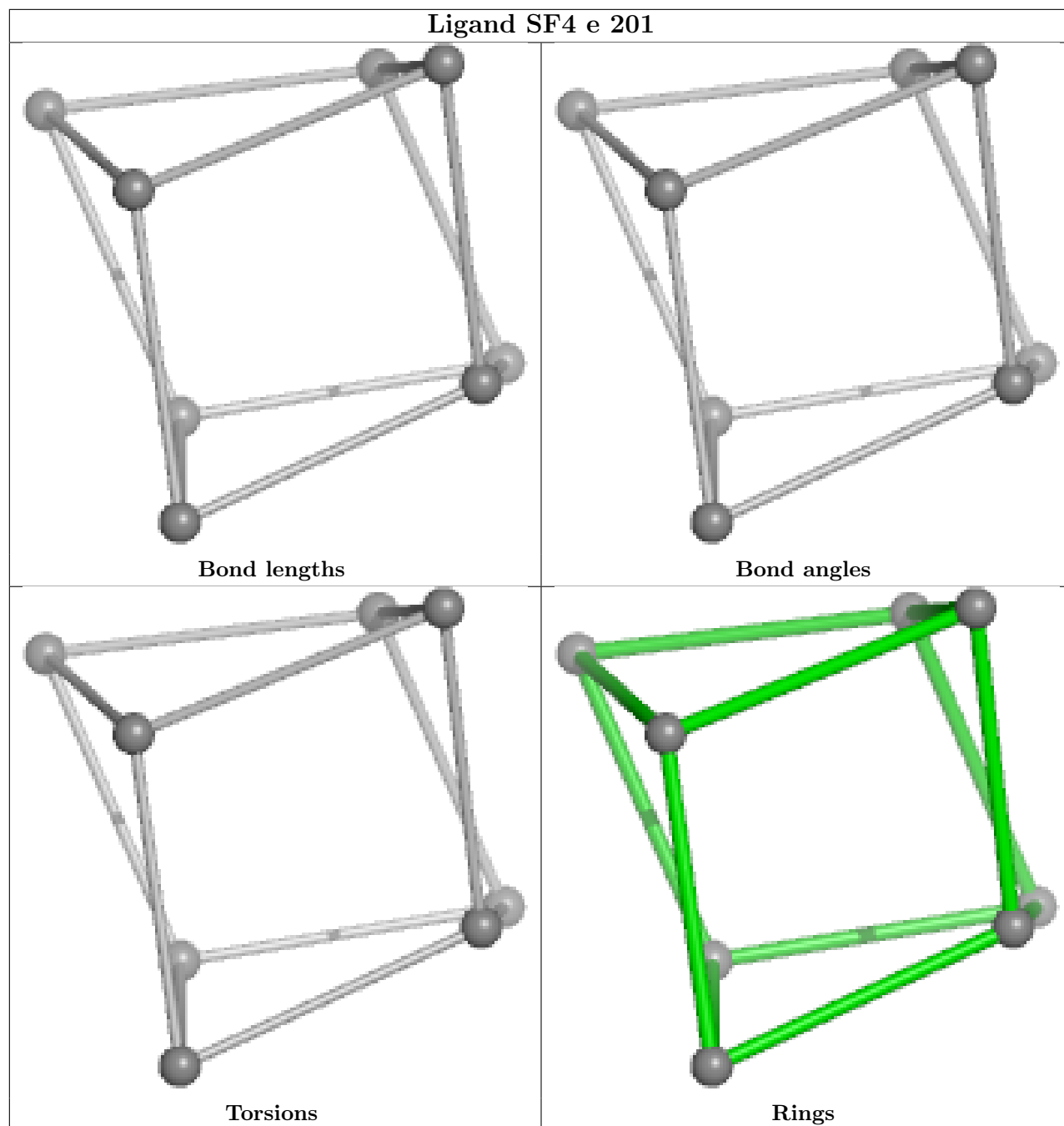


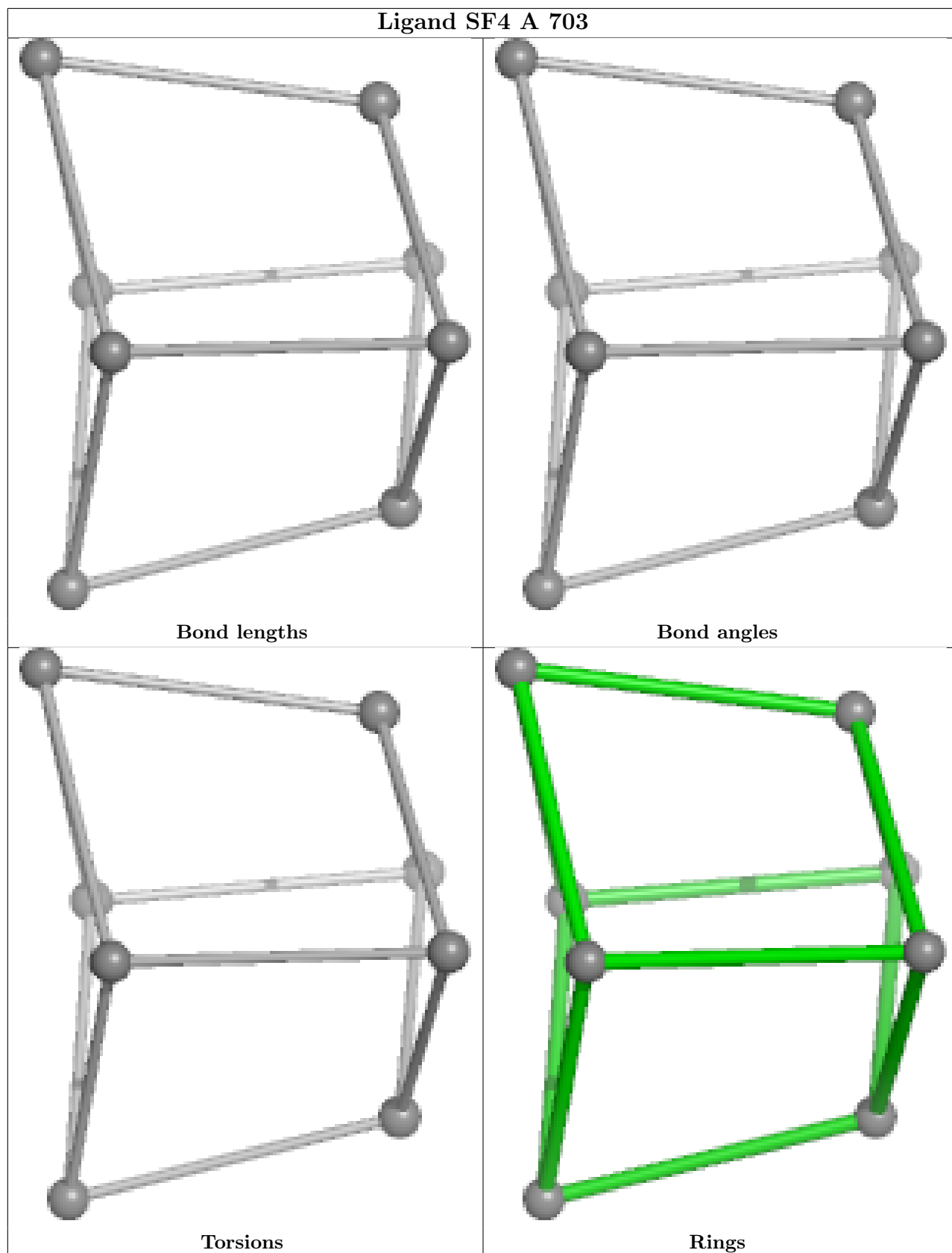


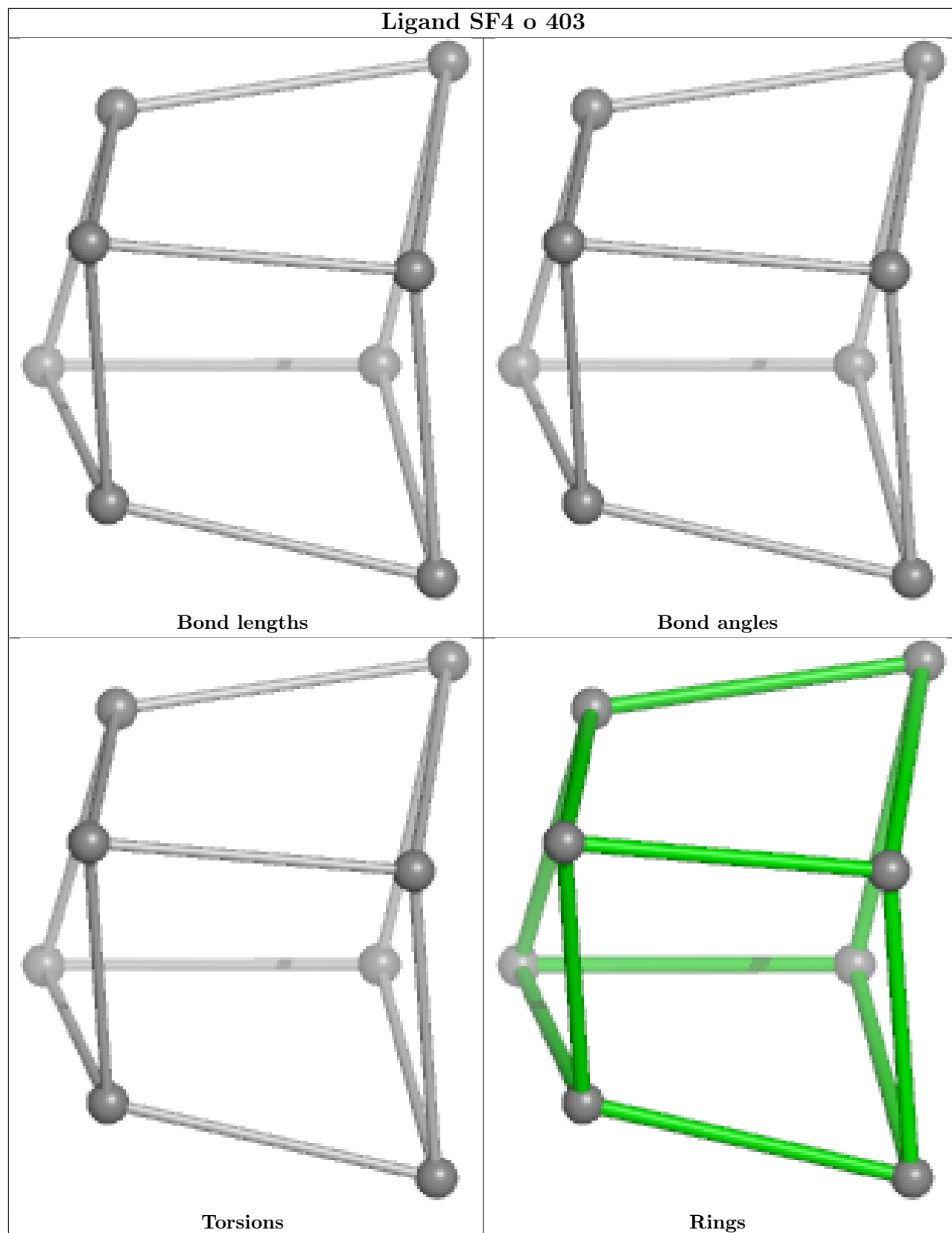


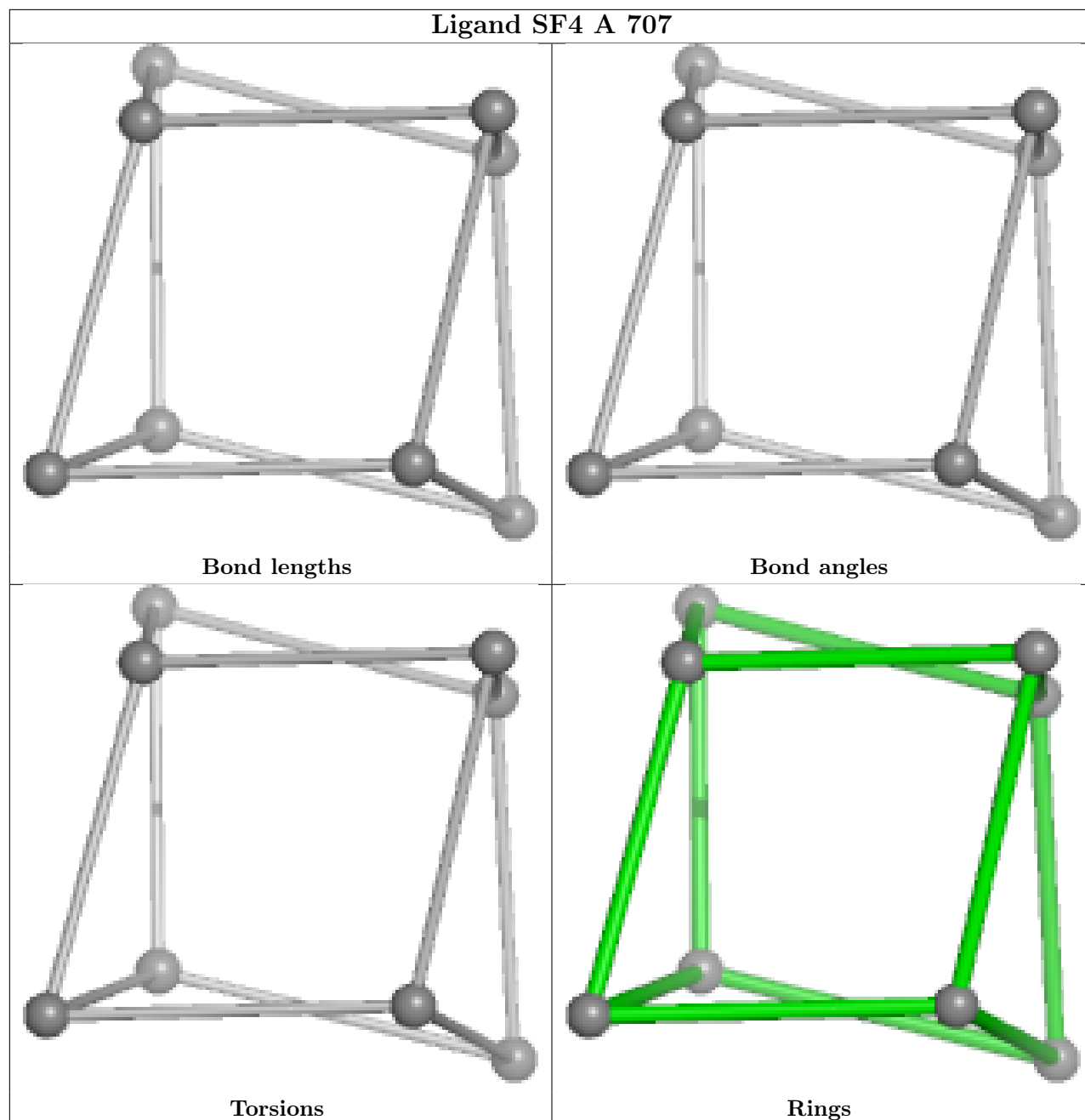


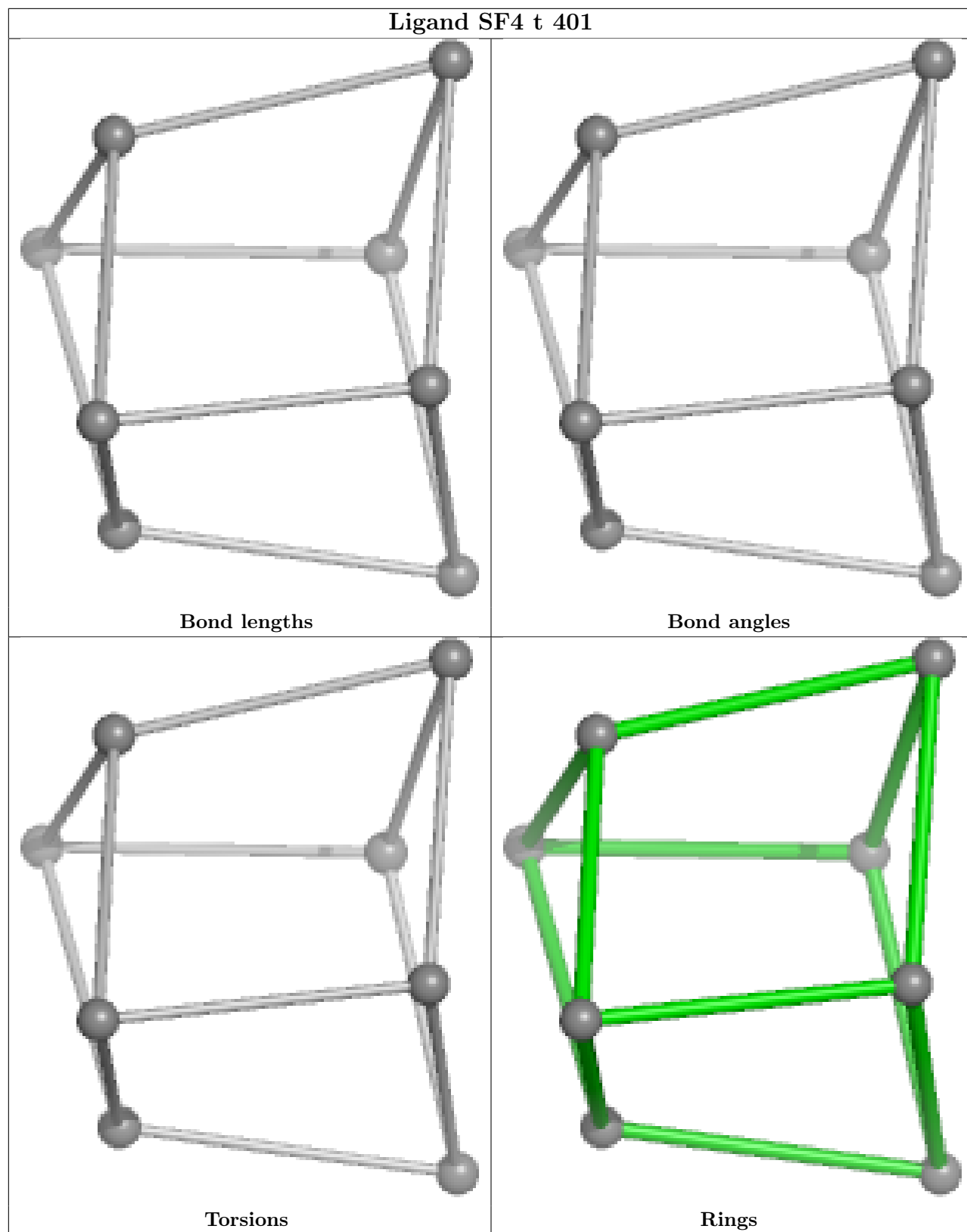


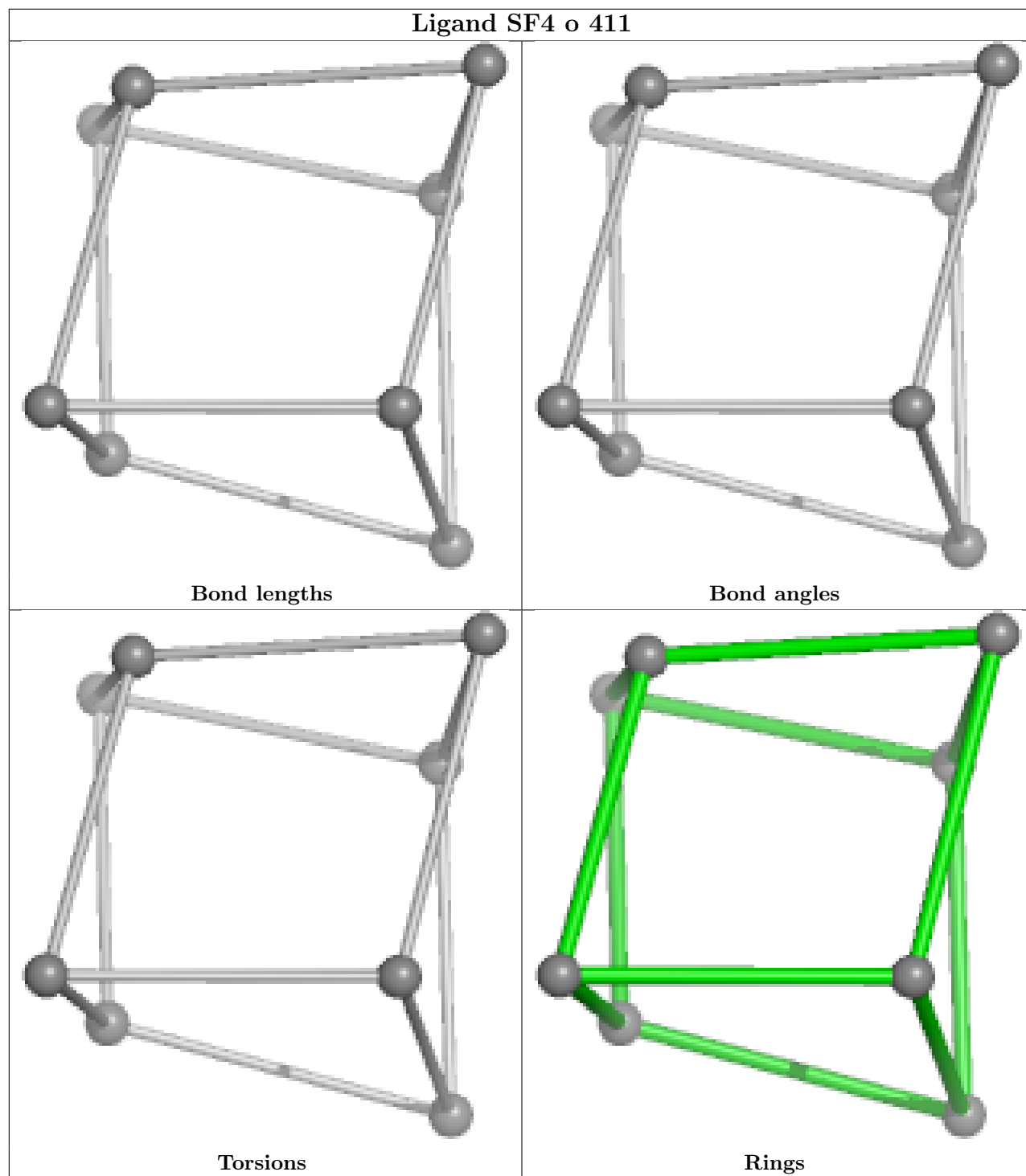


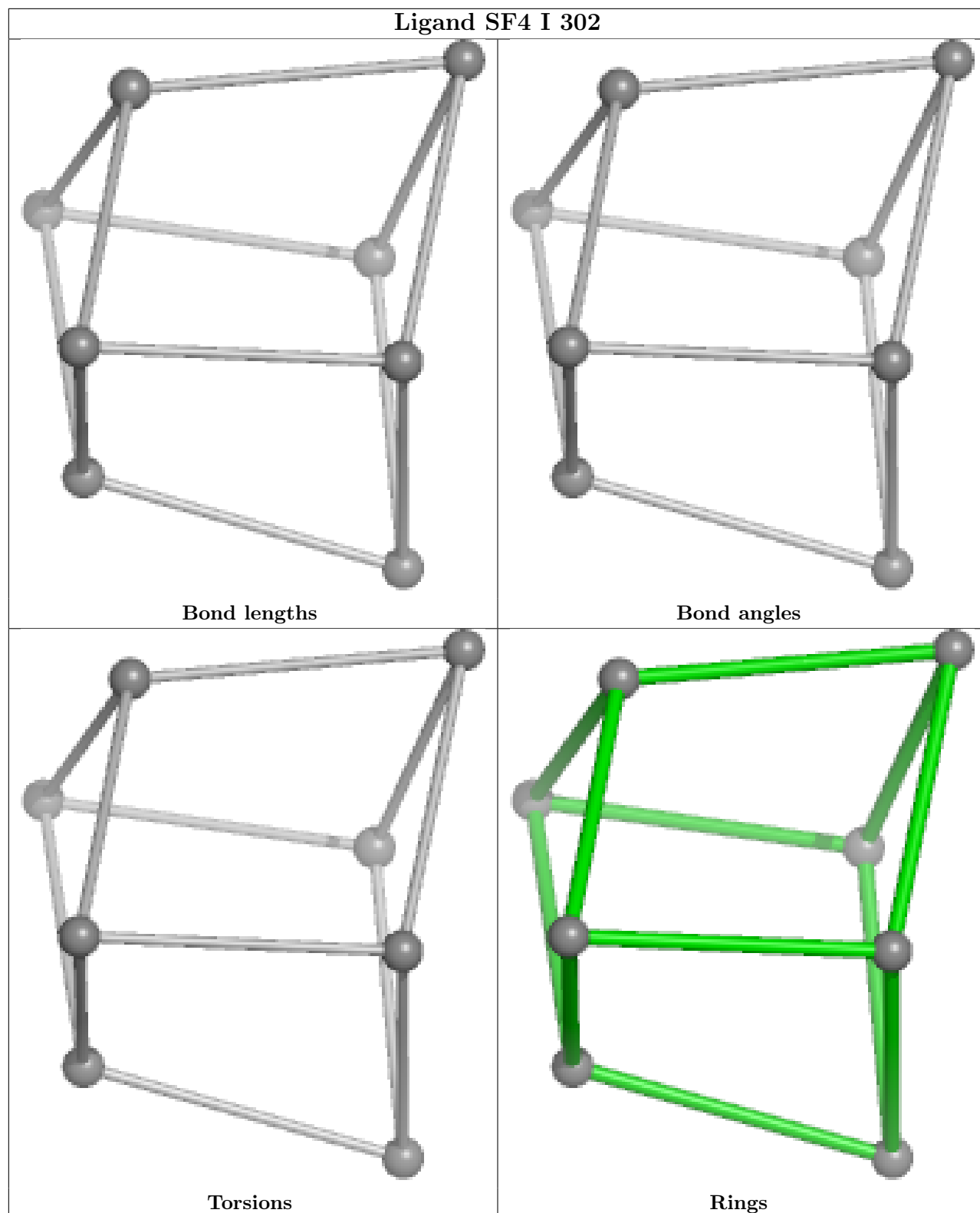


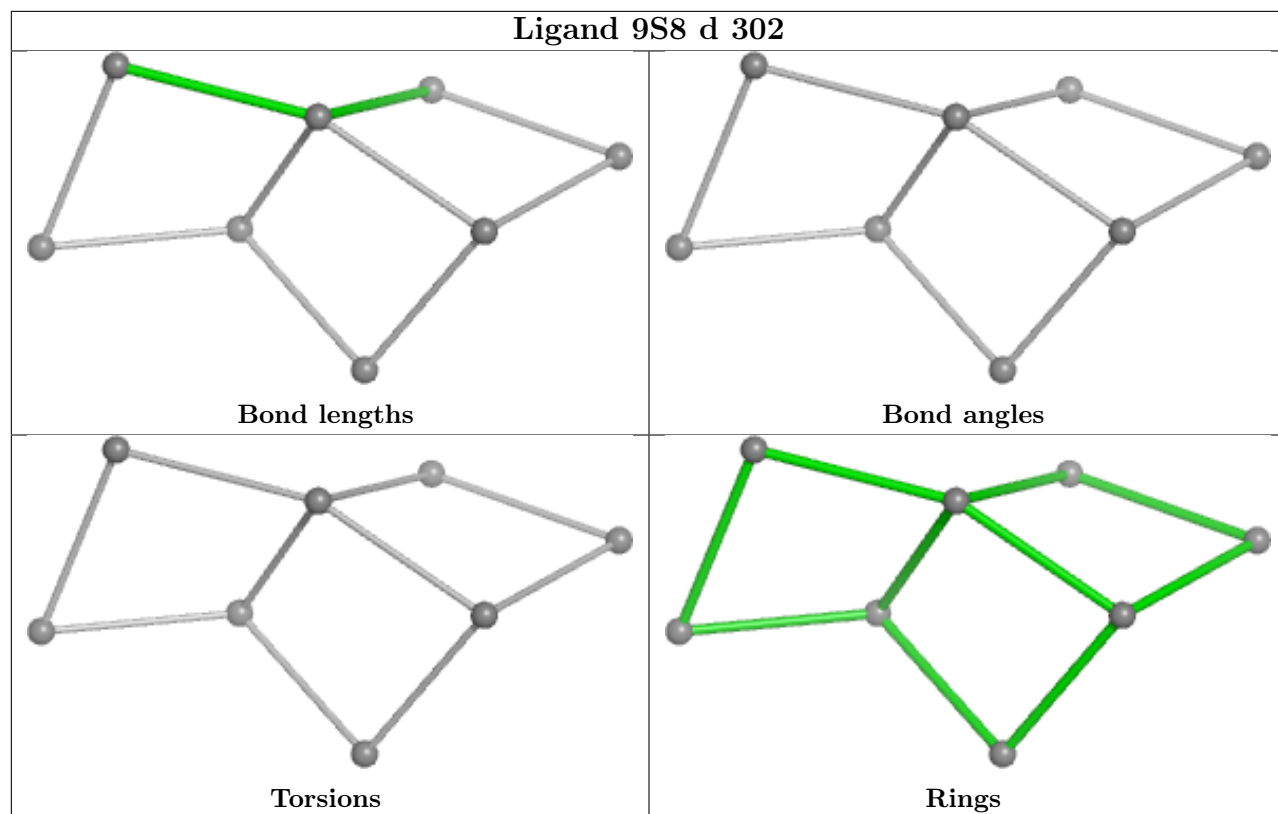


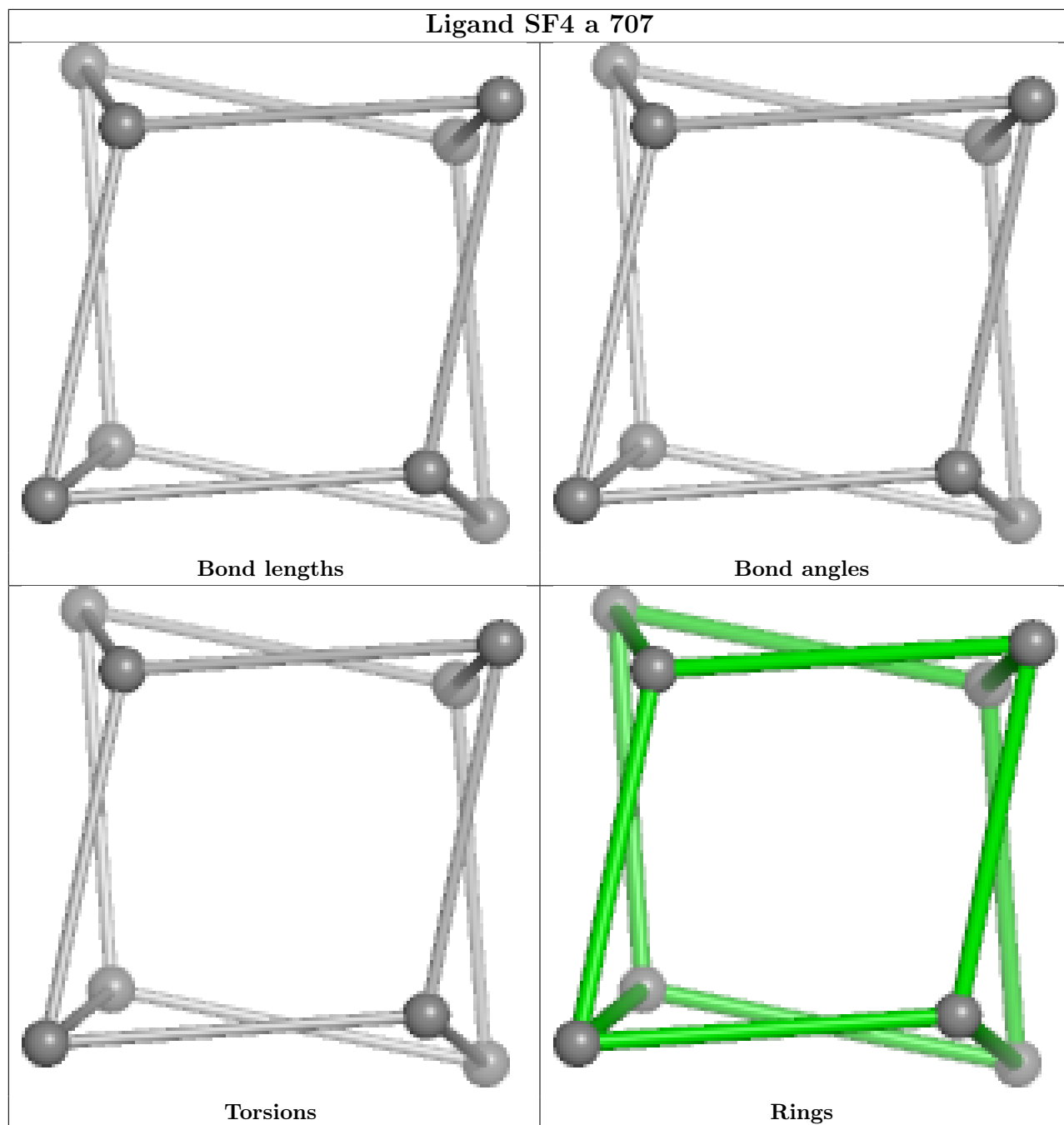


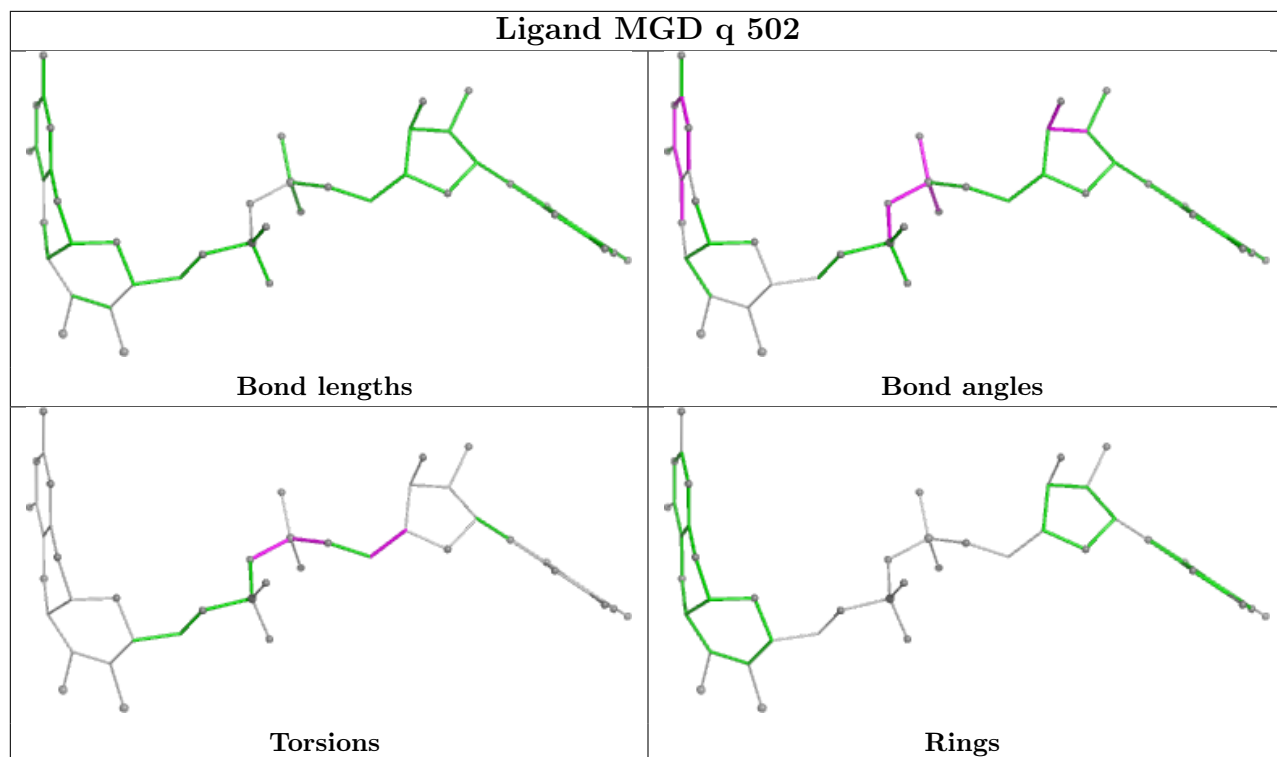




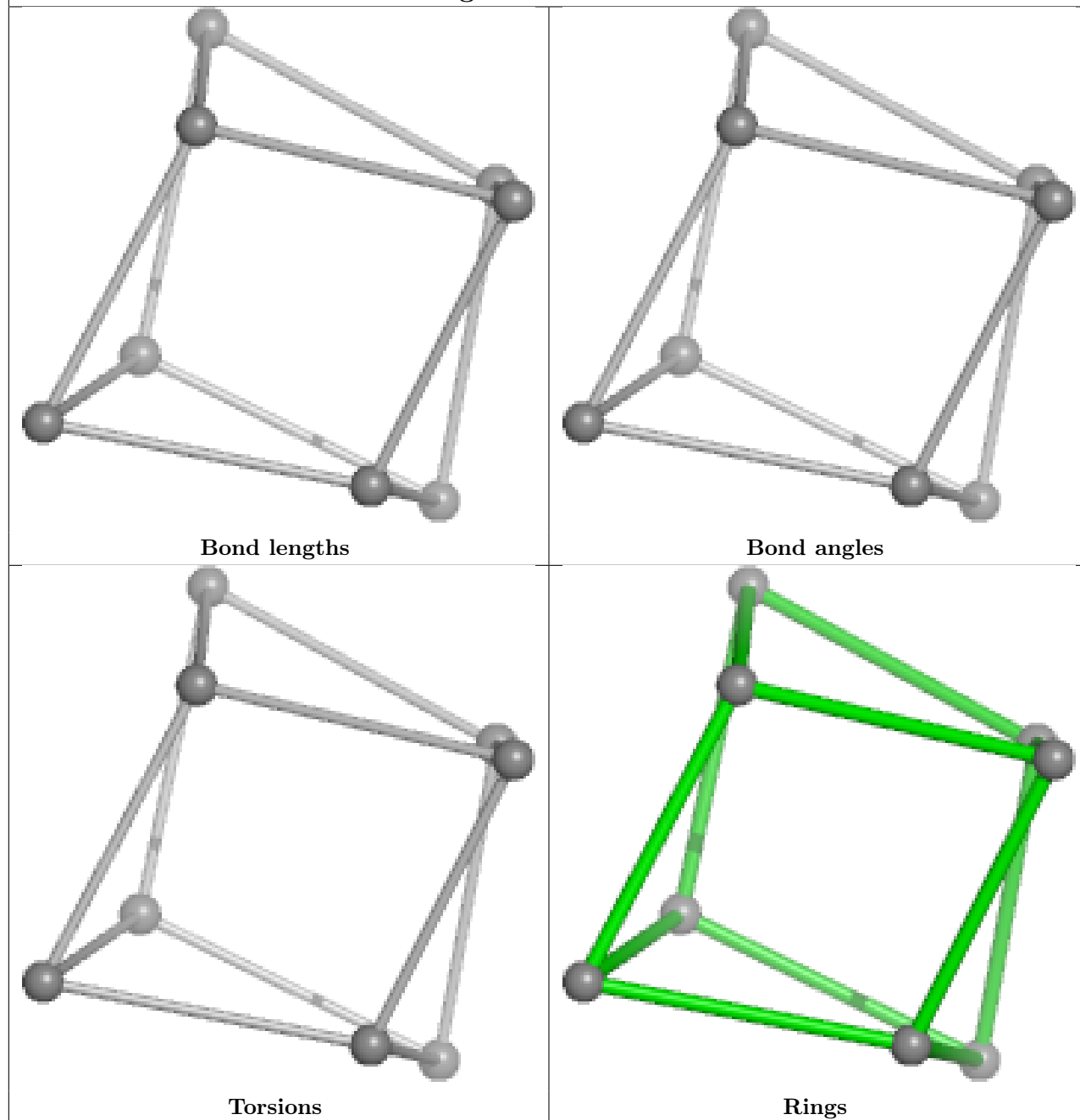


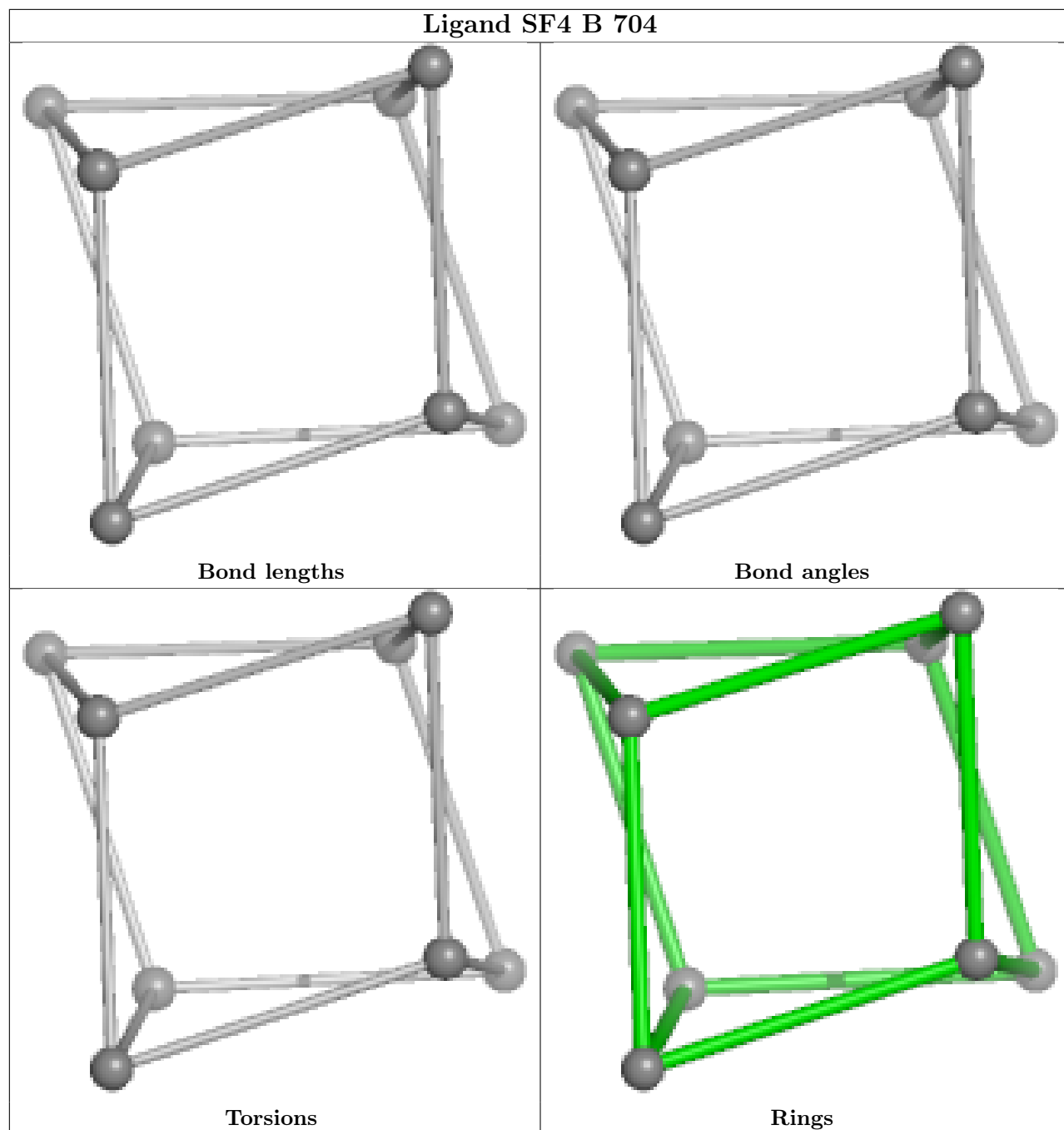


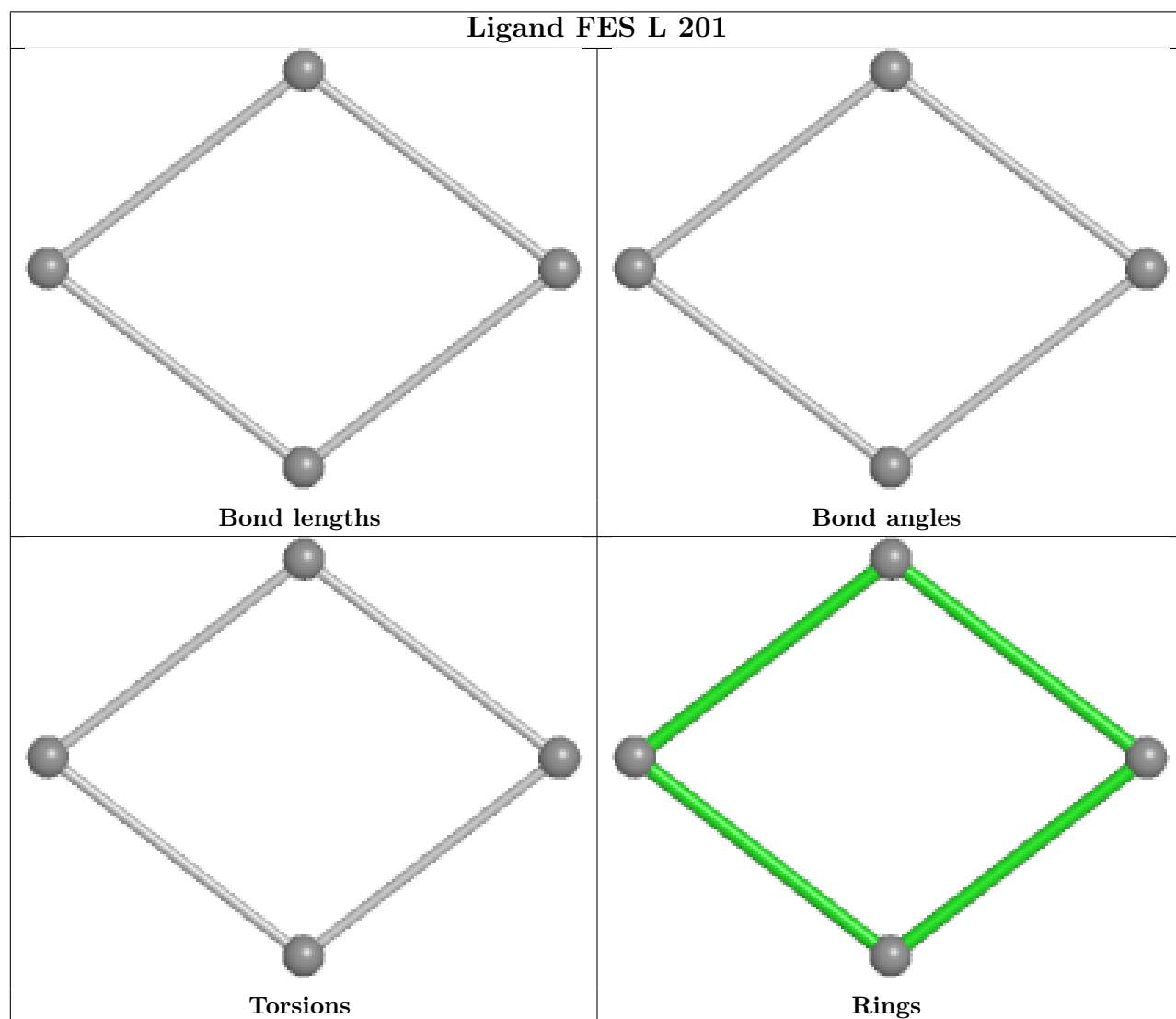
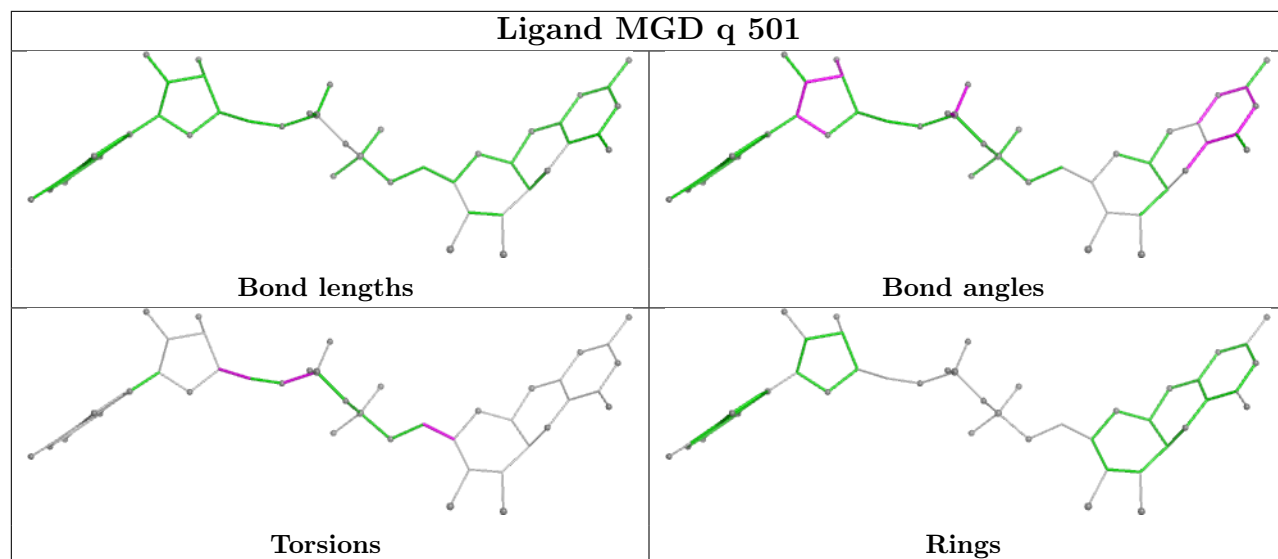


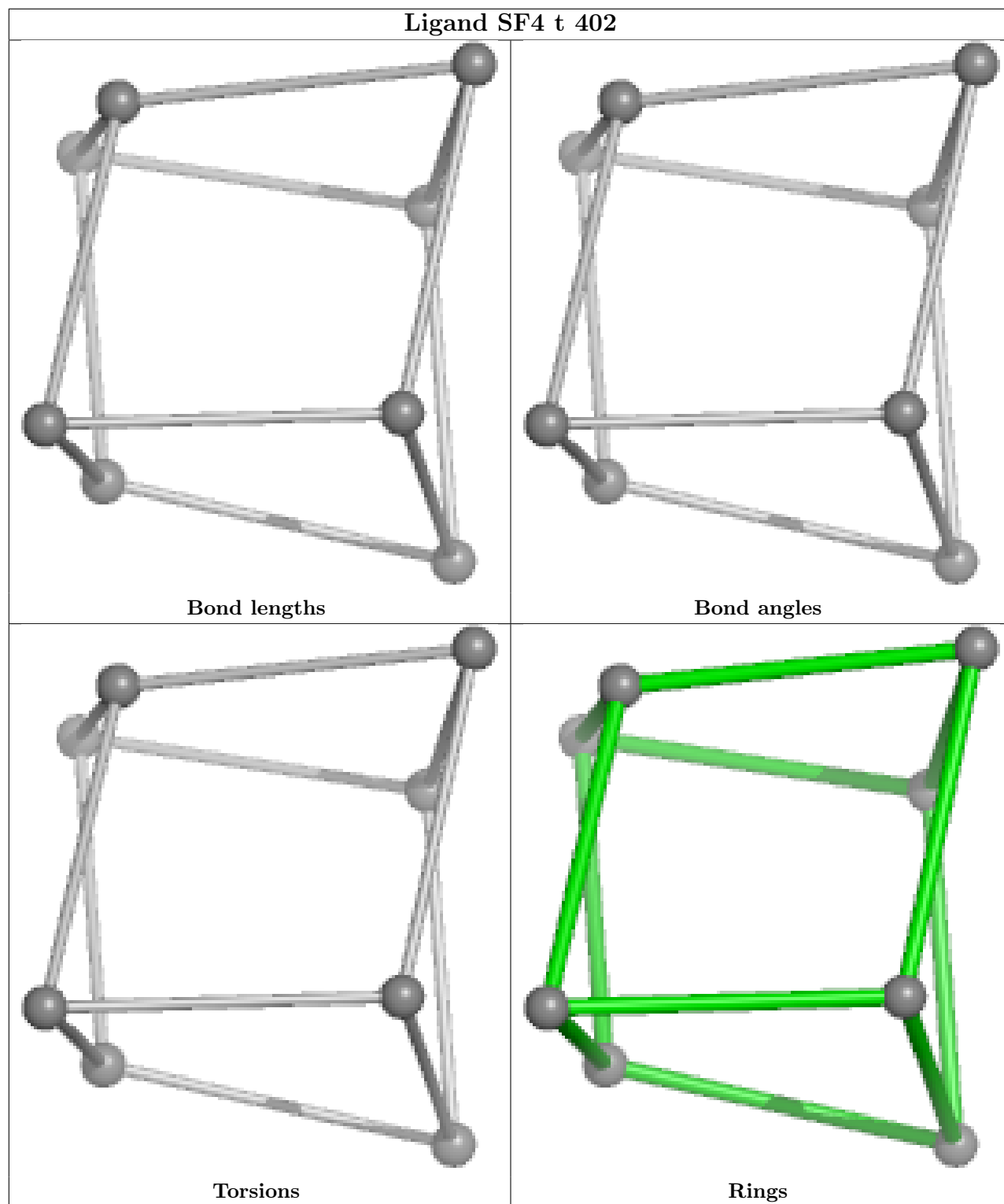


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5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

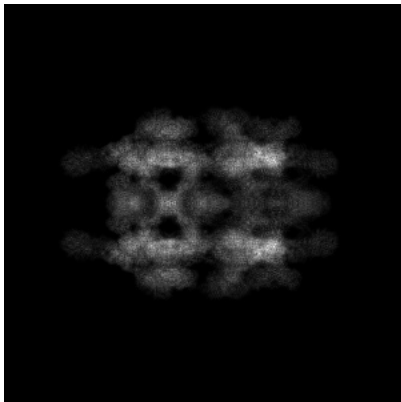
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54825. These allow visual inspection of the internal detail of the map and identification of artifacts.

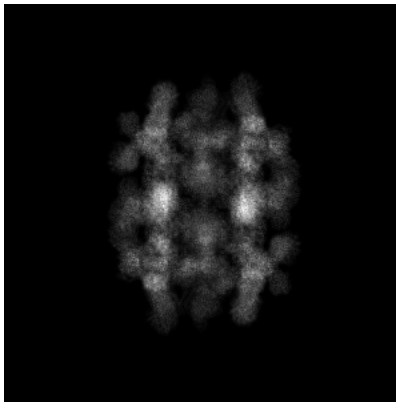
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

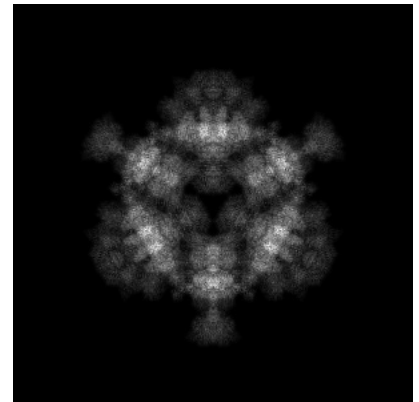
6.1.1 Primary map



X



Y

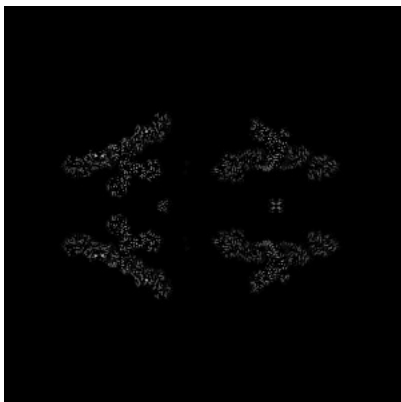


Z

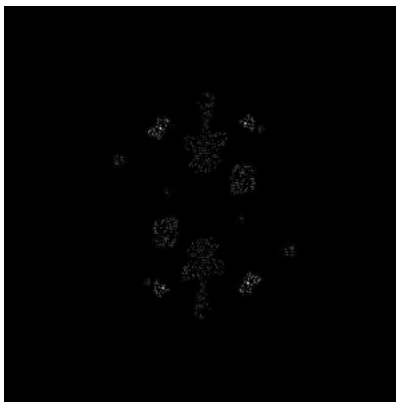
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 400



Y Index: 400

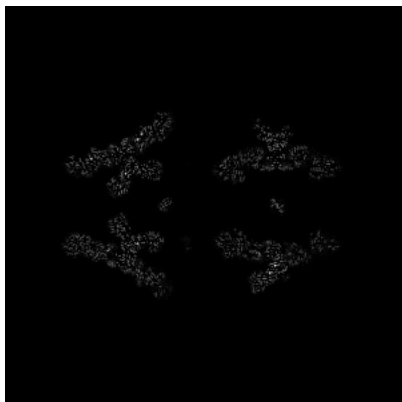


Z Index: 400

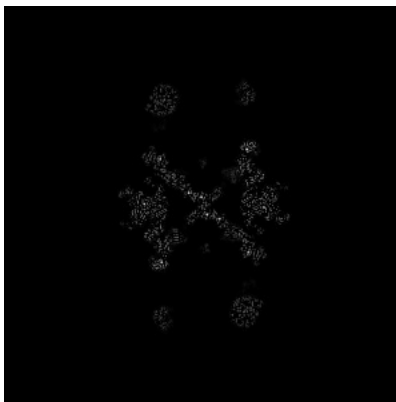
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

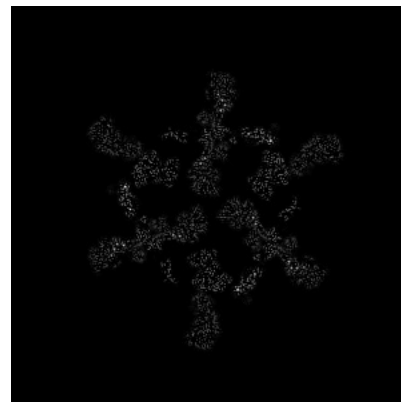
6.3.1 Primary map



X Index: 403



Y Index: 539

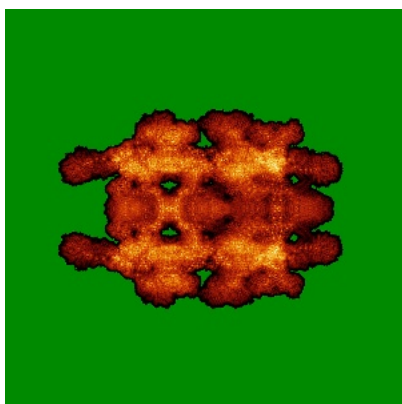


Z Index: 478

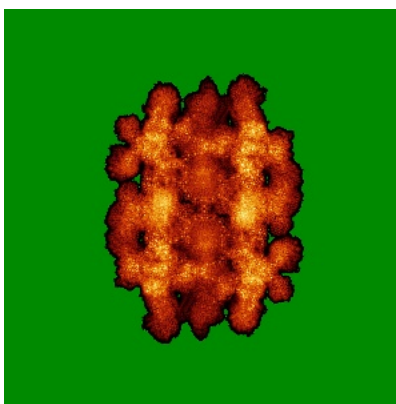
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

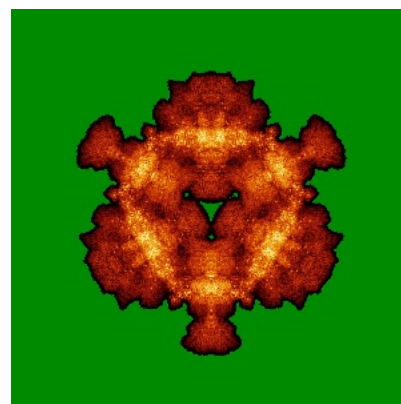
6.4.1 Primary map



X



Y

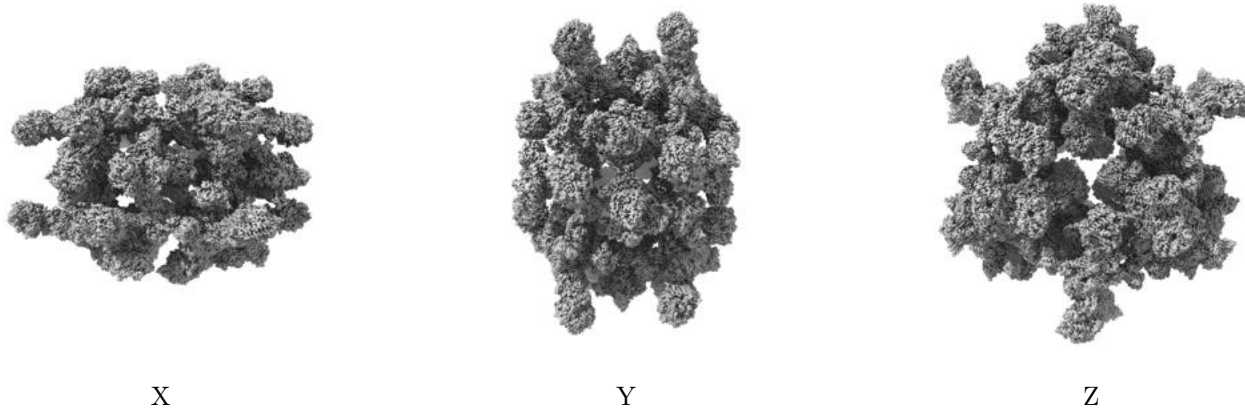


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.084. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

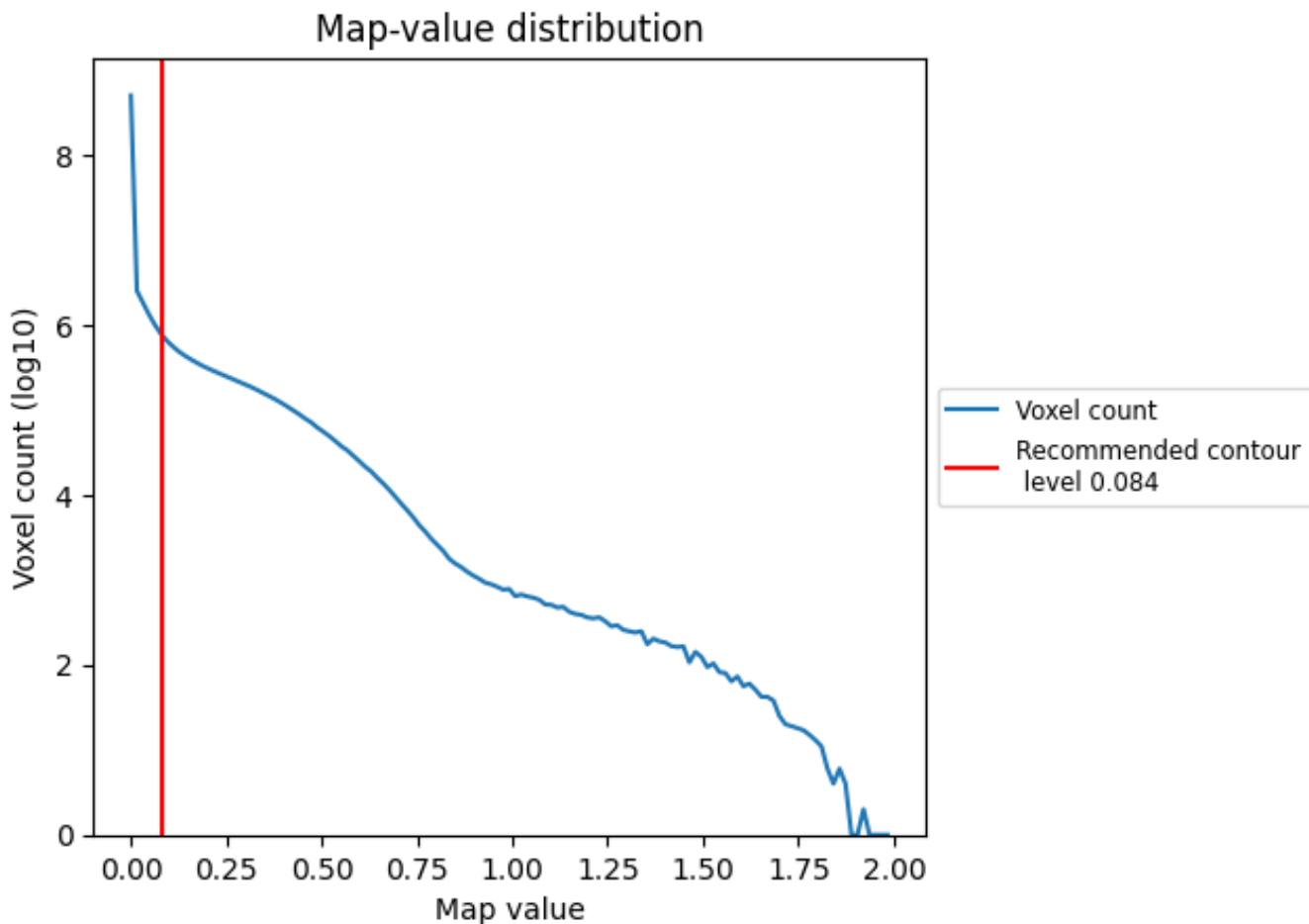
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

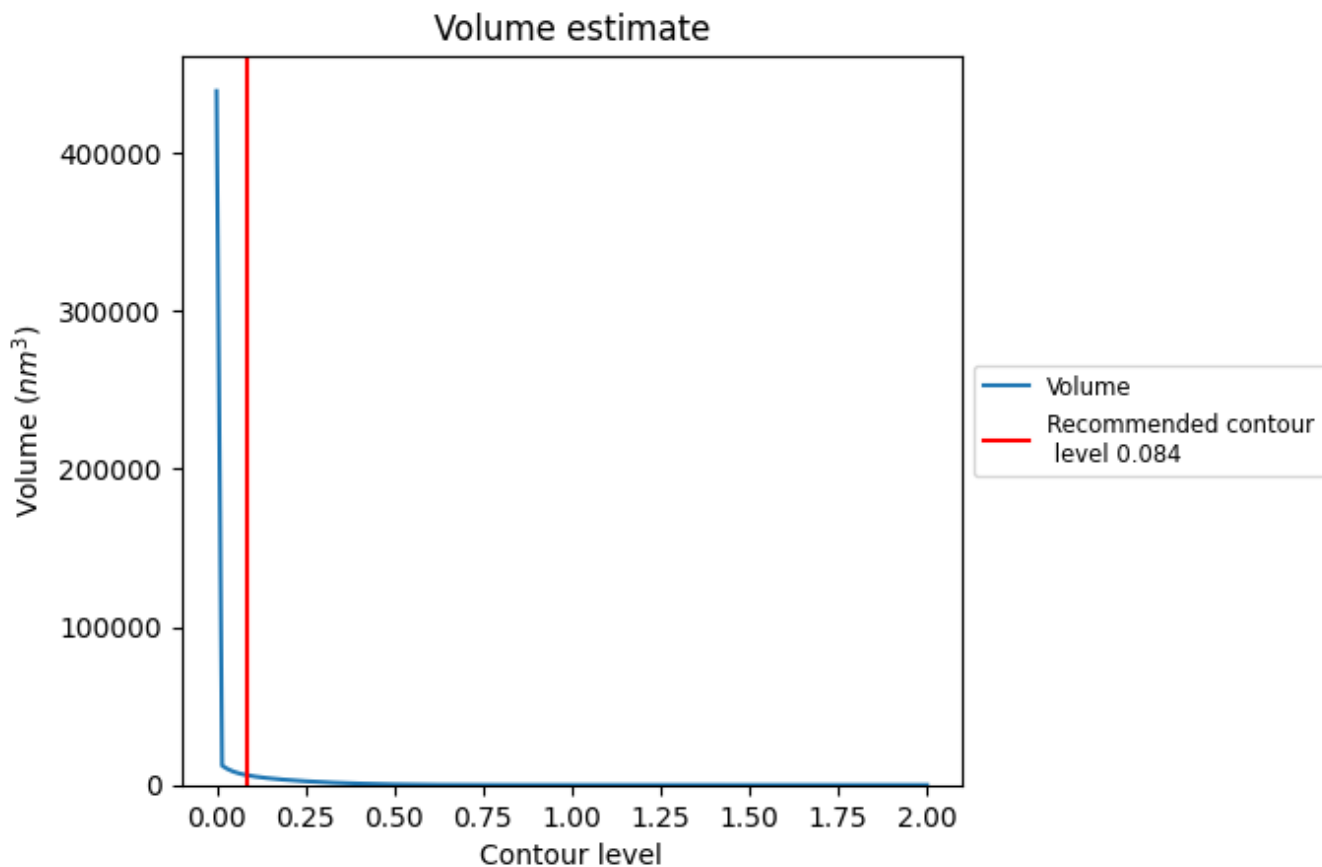
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

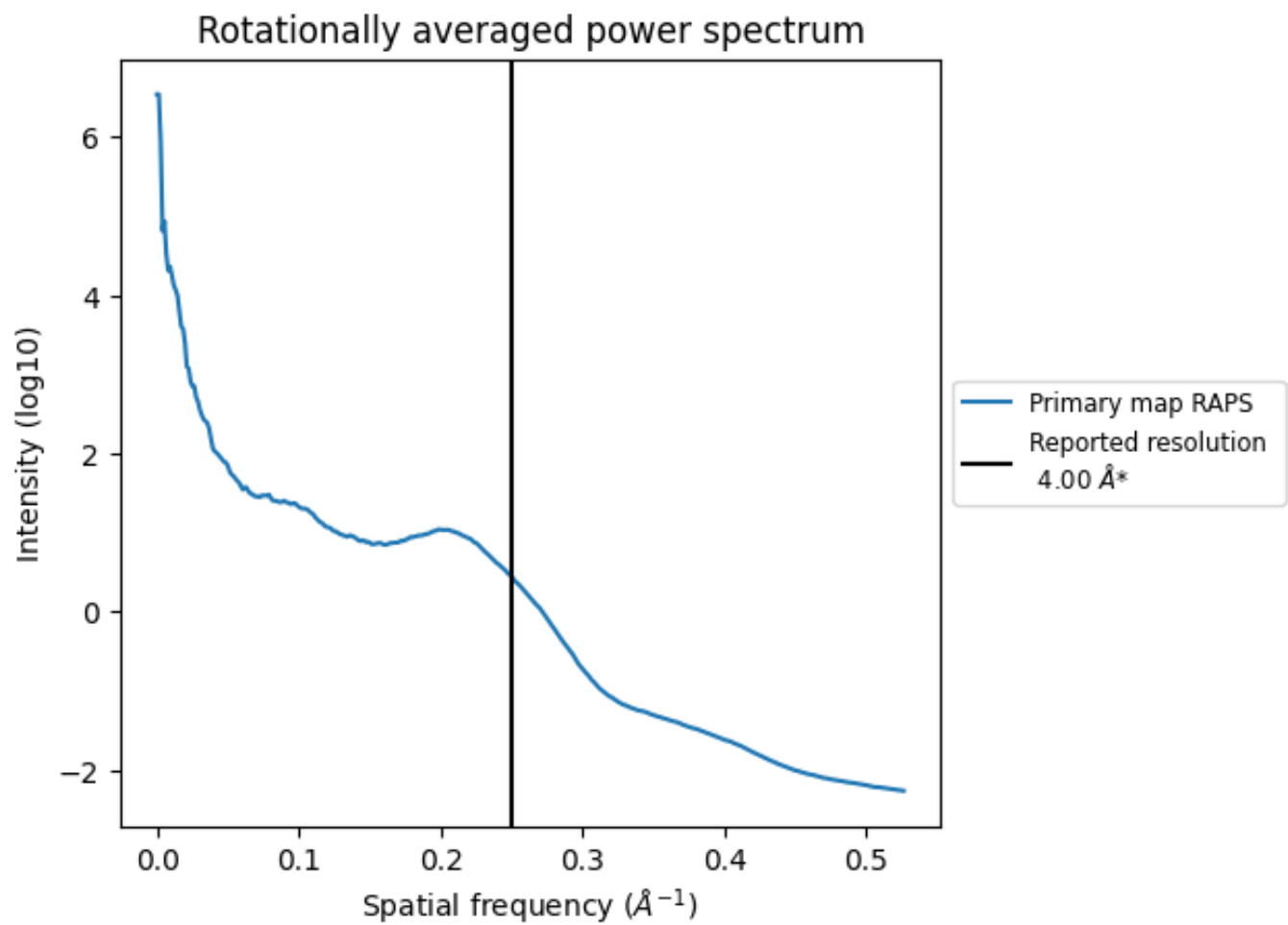
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 6257 nm^3 ; this corresponds to an approximate mass of 5652 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

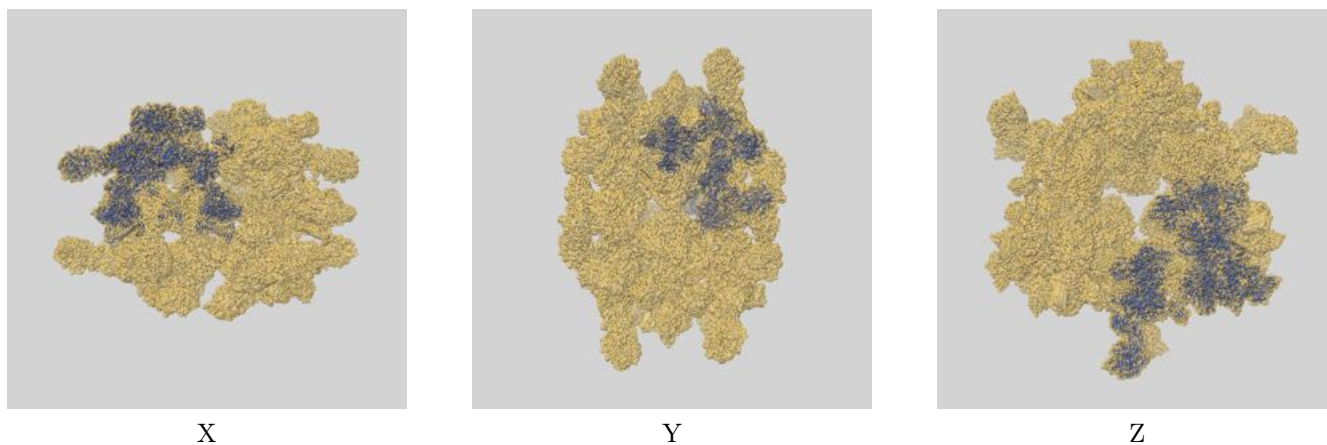
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

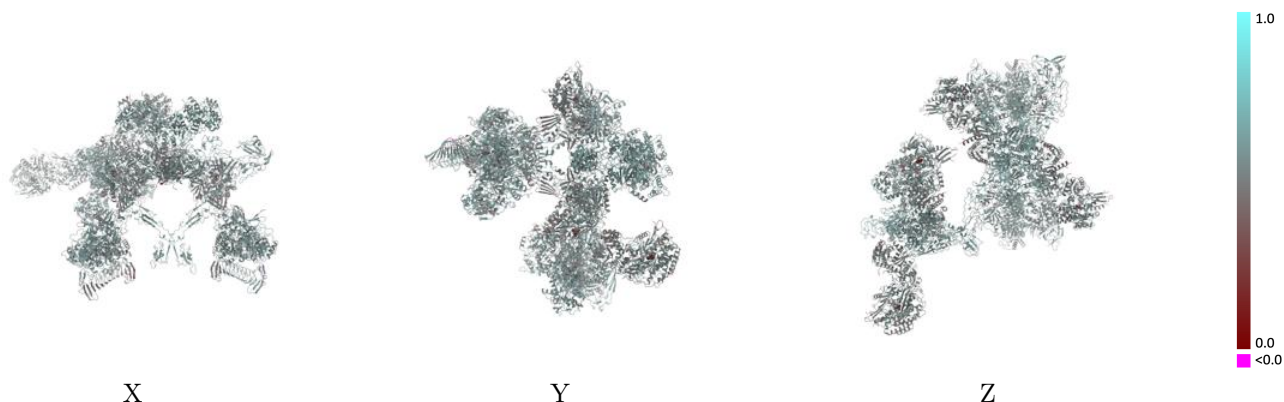
This section contains information regarding the fit between EMDB map EMD-54825 and PDB model 9SFI. Per-residue inclusion information can be found in section 3 on page 18.

9.1 Map-model overlay [i](#)



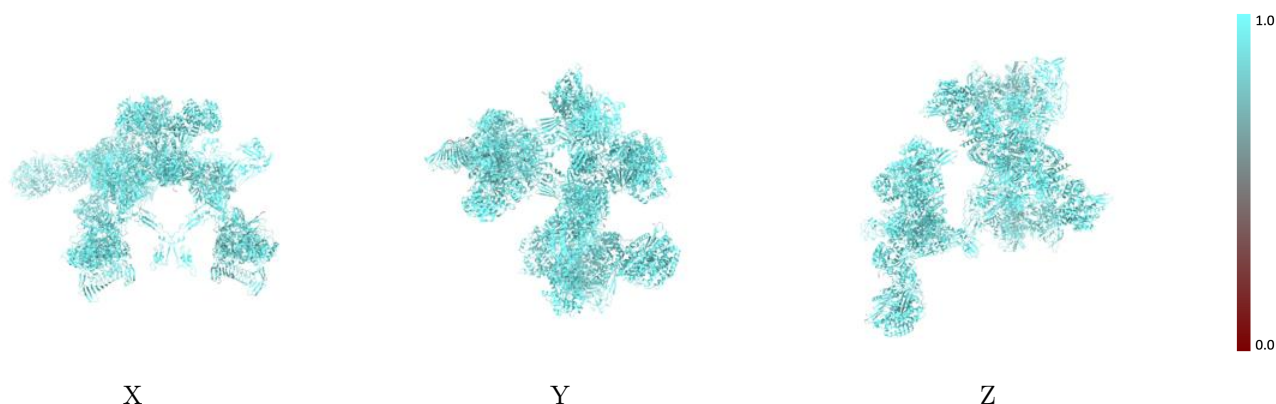
The images above show the 3D surface view of the map at the recommended contour level 0.084 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



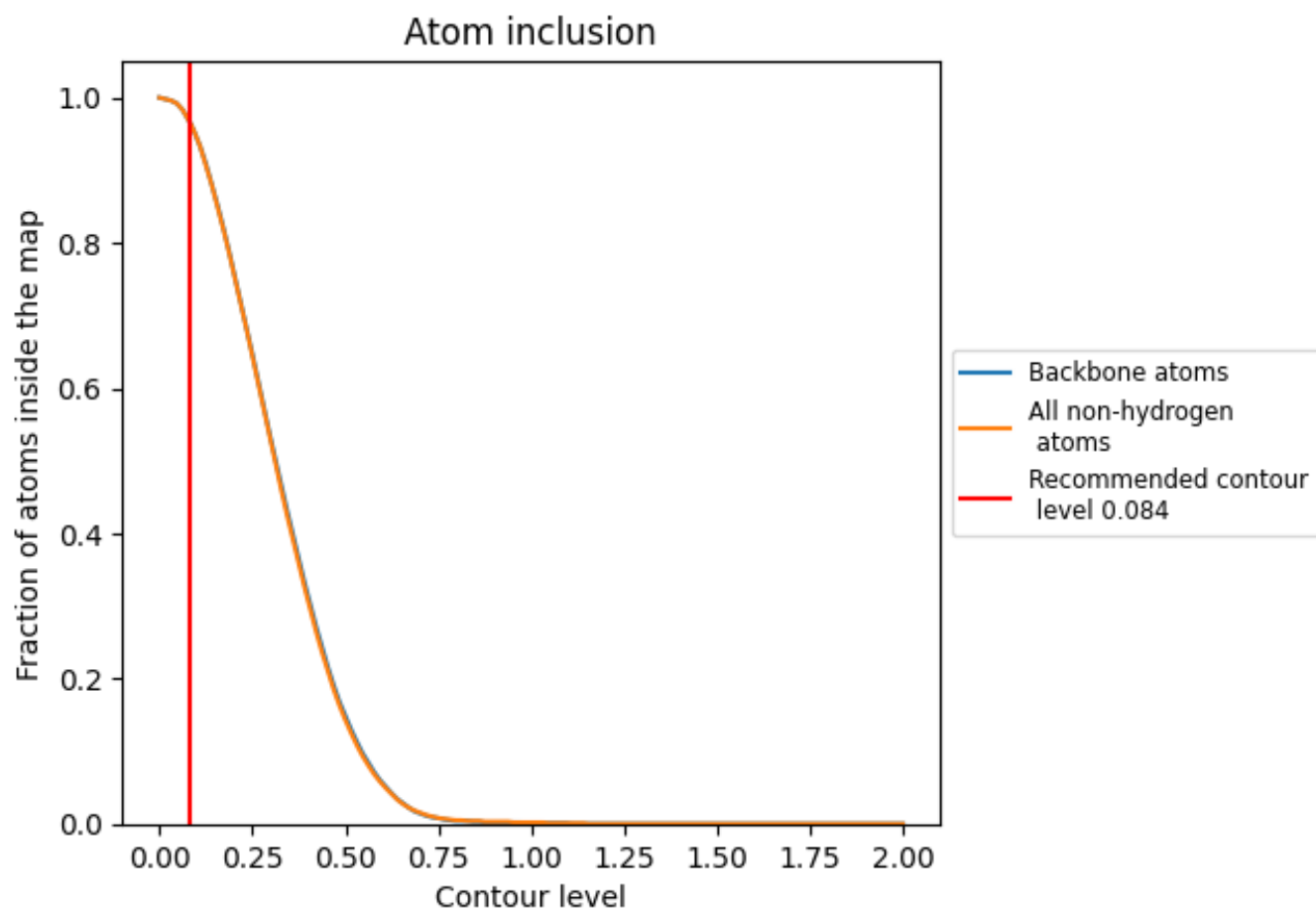
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.084).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 96% of all backbone atoms, 96% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

















The table lists the average atom inclusion at the recommended contour level (0.084) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9640	 0.5350
A	 0.9830	 0.5480
B	 0.9870	 0.5490
C	 0.9870	 0.5630
D	 0.9870	 0.5670
E	 0.9820	 0.5610
F	 0.9860	 0.5660
G	 0.9710	 0.5170
H	 0.9710	 0.5140
I	 0.9630	 0.5080
J	 0.9660	 0.5070
K	 0.9660	 0.5010
L	 0.9580	 0.4960
M	 0.9470	 0.4920
N	 0.9320	 0.4790
O	 0.9910	 0.5480
P	 0.9520	 0.5460
Q	 0.9510	 0.5370
R	 0.8800	 0.4790
S	 0.9190	 0.5160
T	 0.9710	 0.5170
U	 0.9640	 0.5300
a	 0.9880	 0.5510
b	 0.9840	 0.5510
c	 0.9860	 0.5670
d	 0.9860	 0.5640
e	 0.9820	 0.5690
f	 0.9800	 0.5630
g	 0.9710	 0.5150
h	 0.9710	 0.5150
i	 0.9660	 0.5070
j	 0.9610	 0.5090
k	 0.9610	 0.4970
l	 0.9610	 0.5010
m	 0.9470	 0.4870



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Chain	Atom inclusion	Q-score
n	 0.9180	 0.4660
o	 0.9780	 0.5240
p	 0.9210	 0.5520
q	 0.9100	 0.5460
r	 0.8580	 0.5270
s	 0.8970	 0.5390
t	 0.9730	 0.5220
u	 0.9160	 0.5390