



## Full wwPDB EM Validation Report ⓘ

Apr 20, 2026 – 08:06 pm BST

PDB ID : 9SW6 / pdb\_00009sw6  
EMDB ID : EMD-55299  
Title : Structure of the Mvh-Hdr-Fmd complex of Methanothermobacter marburgensis (composite structure)  
Authors : San Segundo-Acosta, P.; Murphy, B.J.  
Deposited on : 2025-10-04  
Resolution : 2.70 Å(reported)  
Based on initial model : .

This is a Full wwPDB EM Validation 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/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>.

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

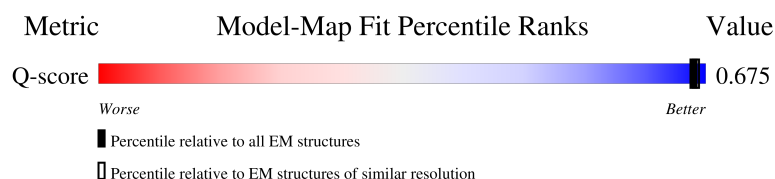
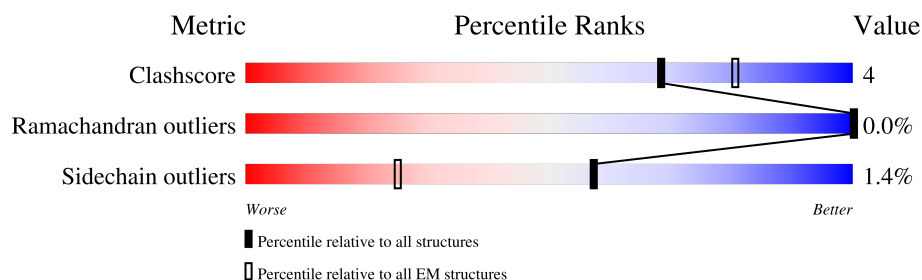
EMDB validation analysis : 0.0.1.dev132  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using 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) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 2.70 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.




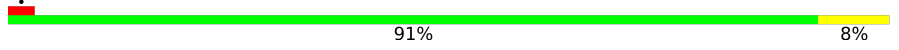
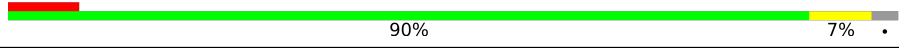
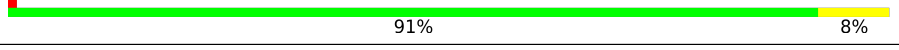
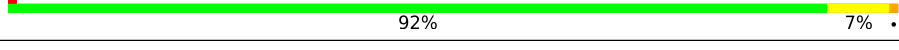


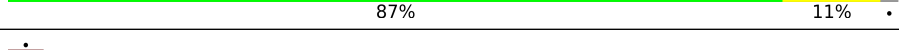
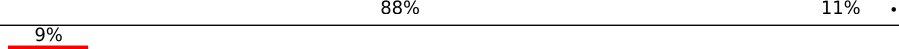
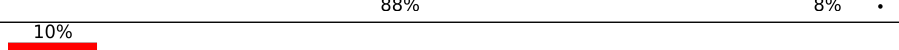

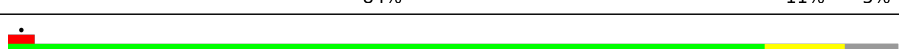
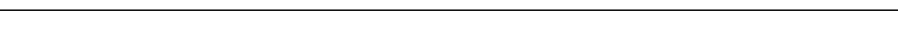
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 ( 2.20 - 3.20 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	659	
2	B	302	
3	C	185	
4	D	141	

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Mol	Chain	Length	Quality of chain
5	E	308	
6	H	349	
6	h	349	
7	I	569	
7	i	569	
8	J	436	
8	j	436	
9	L	82	
9	l	82	
10	K	400	
10	k	400	
11	G	412	
12	F	472	

## 2 Entry composition [i](#)

There are 23 unique types of molecules in this entry. The entry contains 92174 atoms, of which 45185 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 H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	647	Total	C	H	N	O	S	0	0
			9834	3114	4894	822	956	48		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	286	Total	C	H	N	O	S	0	0
			4365	1396	2152	366	430	21		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	184	Total	C	H	N	O	S	0	0
			2854	893	1432	253	265	11		

- Molecule 4 is a protein called F420-non-reducing hydrogenase iron-sulfur subunit D.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	136	Total	C	H	N	O	S	0	0
			2139	675	1063	198	191	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E	301	Total	C	H	N	O	S	0	0
			4555	1462	2250	365	458	20		

- Molecule 6 is a protein called Tungsten formylmethanofuran dehydrogenase, subunit F.

Mol	Chain	Residues	Atoms						AltConf	Trace
6	H	348	Total	C	H	N	O	S	0	0
			5111	1615	2508	428	518	42		
6	h	339	Total	C	H	N	O	S	0	0
			5025	1585	2465	420	513	42		

- Molecule 7 is a protein called Tungsten formylmethanofuran dehydrogenase, subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I	568	Total	C	H	N	O	S	0	0
			8706	2814	4280	742	848	22		
7	i	567	Total	C	H	N	O	S	0	0
			8687	2809	4269	741	847	21		

- Molecule 8 is a protein called formylmethanofuran dehydrogenase subunit B.

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J	434	Total	C	H	N	O	S	0	0
			6633	2097	3292	579	640	25		
8	j	434	Total	C	H	N	O	S	0	0
			6633	2097	3292	579	640	25		

- Molecule 9 is a protein called Tungsten formylmethanofuran dehydrogenase, subunit G.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	L	80	Total	C	H	N	O	S	0	0
			1125	354	553	96	113	9		
9	l	81	Total	C	H	N	O	S	0	0
			1150	359	569	97	116	9		

- Molecule 10 is a protein called Molybdenum-containing formylmethanofuran dehydrogenase 1 subunit C.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	K	386	Total	C	H	N	O	S	0	0
			5827	1838	2911	500	560	18		
10	k	386	Total	C	H	N	O	S	0	0
			5837	1840	2917	501	561	18		

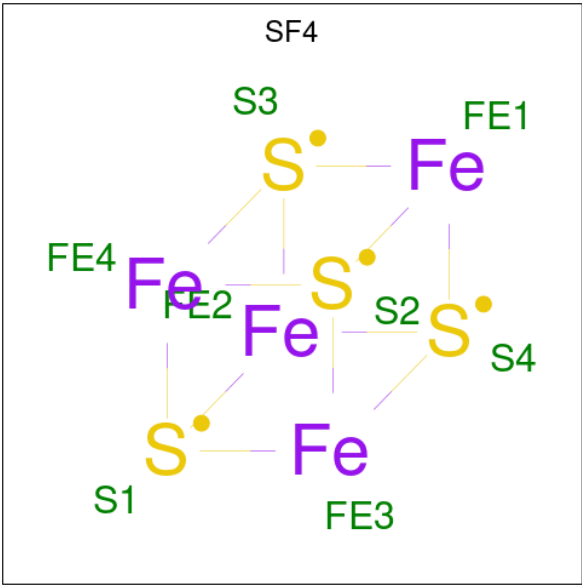
- Molecule 11 is a protein called Polyferredoxin protein MvhB.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	G	393	Total	C	H	N	O	S	0	0
			5665	1784	2800	467	560	54		

- Molecule 12 is a protein called F420-non-reducing hydrogenase subunit A.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
12	F	445	6917	2227	3414	600	658	18	0	0

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
13	A	1	8	4	4	0
13	A	1	8	4	4	0
13	A	1	8	4	4	0
13	A	1	8	4	4	0
13	A	1	8	4	4	0
13	A	1	8	4	4	0
13	C	1	8	4	4	0
13	C	1	8	4	4	0
13	E	1	8	4	4	0

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Mol	Chain	Residues	Atoms			AltConf
13	E	1	Total 8	Fe 4	S 4	0
13	E	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	H	1	Total 8	Fe 4	S 4	0
13	J	1	Total 8	Fe 4	S 4	0
13	L	1	Total 8	Fe 4	S 4	0
13	L	1	Total 8	Fe 4	S 4	0
13	l	1	Total 8	Fe 4	S 4	0
13	l	1	Total 8	Fe 4	S 4	0
13	j	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0

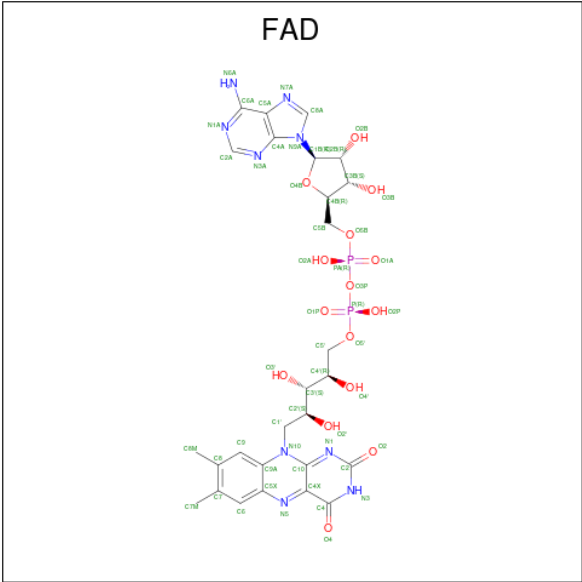
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Mol	Chain	Residues	Atoms			AltConf
13	h	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0
13	h	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0
13	G	1	Total 8	Fe 4	S 4	0

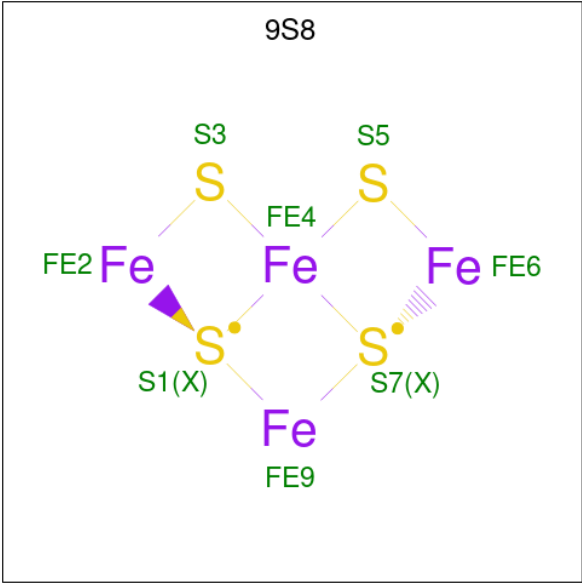
- Molecule 14 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula:  $C_{27}H_{33}N_9O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).





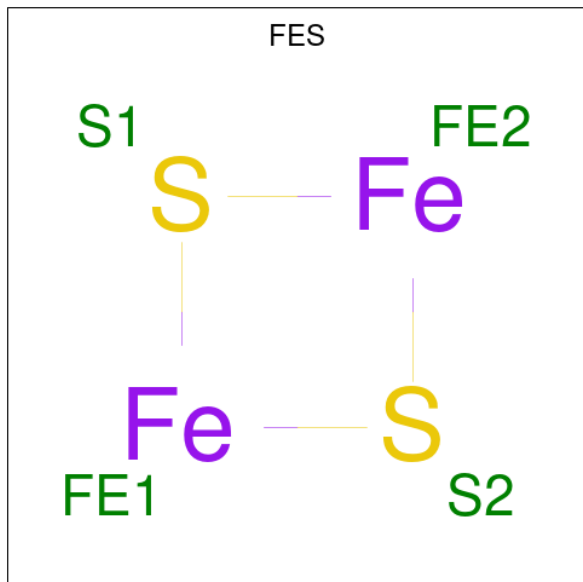
Mol	Chain	Residues	Atoms						AltConf
14	A	1	Total	C	H	N	O	P	0
			84	27	31	9	15	2	

- Molecule 15 is Non-cubane [4Fe-4S]-cluster (CCD ID: 9S8) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula:  $\text{Fe}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

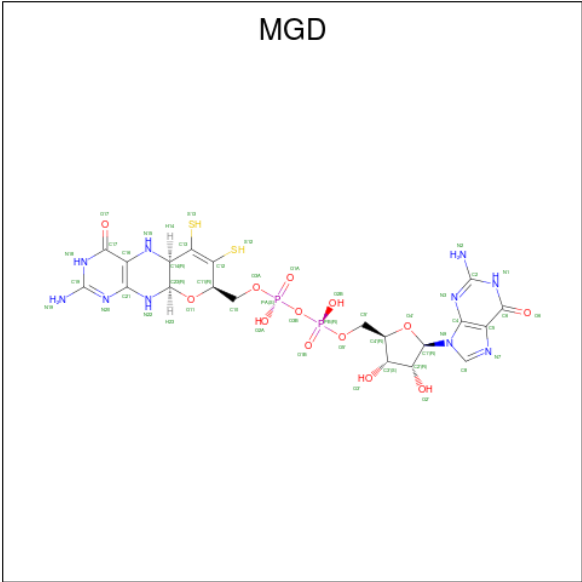


Mol	Chain	Residues	Atoms			AltConf
16	D	1	Total	Fe	S	0
			4	2	2	

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
17	I	2	Total	Zn	0
			2	2	
17	i	2	Total	Zn	0
			2	2	

- Molecule 18 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:  $\text{C}_{20}\text{H}_{26}\text{N}_{10}\text{O}_{13}\text{P}_2\text{S}_2$ ) (labeled as "Ligand of Interest" by depositor).

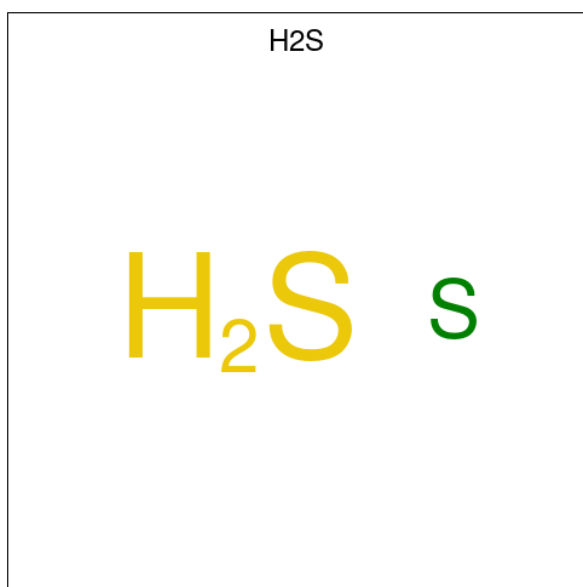


Mol	Chain	Residues	Atoms							AltConf
18	J	1	Total	C	H	N	O	P	S	0
			69	20	22	10	13	2	2	
18	J	1	Total	C	H	N	O	P	S	0
			69	20	22	10	13	2	2	
18	j	1	Total	C	H	N	O	P	S	0
			69	20	22	10	13	2	2	
18	j	1	Total	C	H	N	O	P	S	0
			69	20	22	10	13	2	2	

- Molecule 19 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo) (labeled as "Ligand of Interest" by depositor).

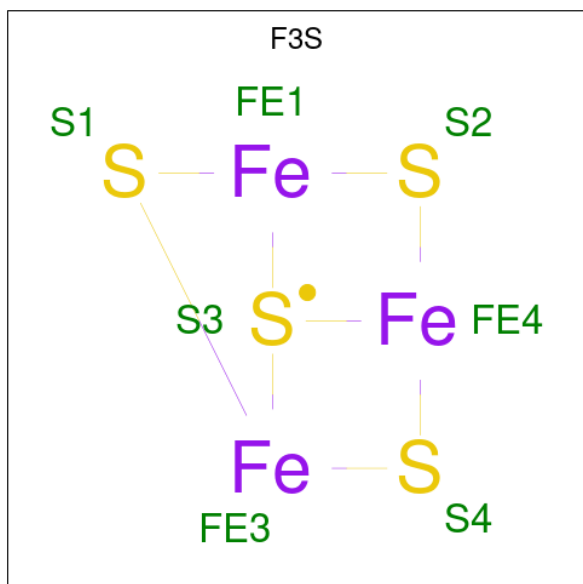
Mol	Chain	Residues	Atoms		AltConf
19	J	1	Total	Mo	0
			1	1	
19	j	1	Total	Mo	0
			1	1	

- Molecule 20 is HYDROSULFURIC ACID (CCD ID: H2S) (formula: H<sub>2</sub>S) (labeled as "Ligand of Interest" by depositor).



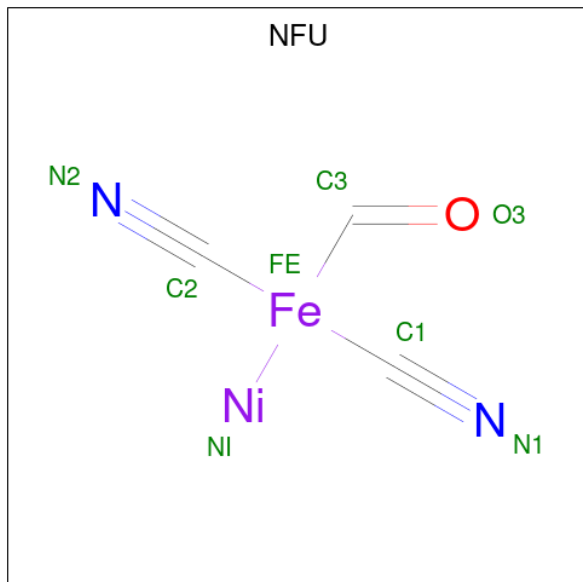
Mol	Chain	Residues	Atoms			AltConf
20	J	1	Total	H	S	0
			3	2	1	
20	j	1	Total	H	S	0
			3	2	1	

- Molecule 21 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe<sub>3</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
21	G	1	Total	Fe	S	0
			7	3	4	

- Molecule 22 is formyl[bis(hydrocyanato-1kappaC)]ironnickel(Fe-Ni) (CCD ID: NFU) (formula:  $\text{C}_3\text{HFeN}_2\text{NiO}$ ) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 23 is water.

Mol	Chain	Residues	Atoms		AltConf
23	A	27	Total	O	0
			27	27	
23	B	1	Total	O	0
			1	1	
23	D	1	Total	O	0
			1	1	
23	E	22	Total	O	0
			22	22	
23	H	27	Total	O	0
			27	27	
23	I	50	Total	O	0
			50	50	
23	J	49	Total	O	0
			49	49	
23	L	14	Total	O	0
			14	14	
23	i	45	Total	O	0
			45	45	

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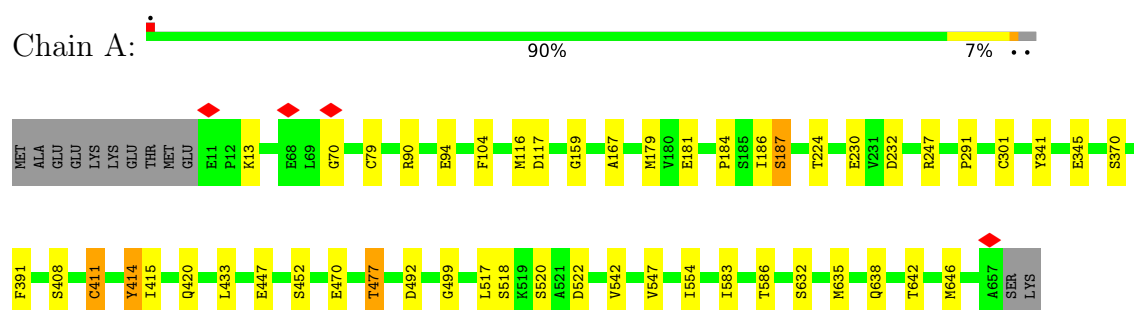
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Mol	Chain	Residues	Atoms		AltConf
23	l	6	Total 6	O 6	0
23	j	26	Total 26	O 26	0
23	K	23	Total 23	O 23	0
23	h	30	Total 30	O 30	0
23	k	5	Total 5	O 5	0
23	G	5	Total 5	O 5	0
23	F	12	Total 12	O 12	0

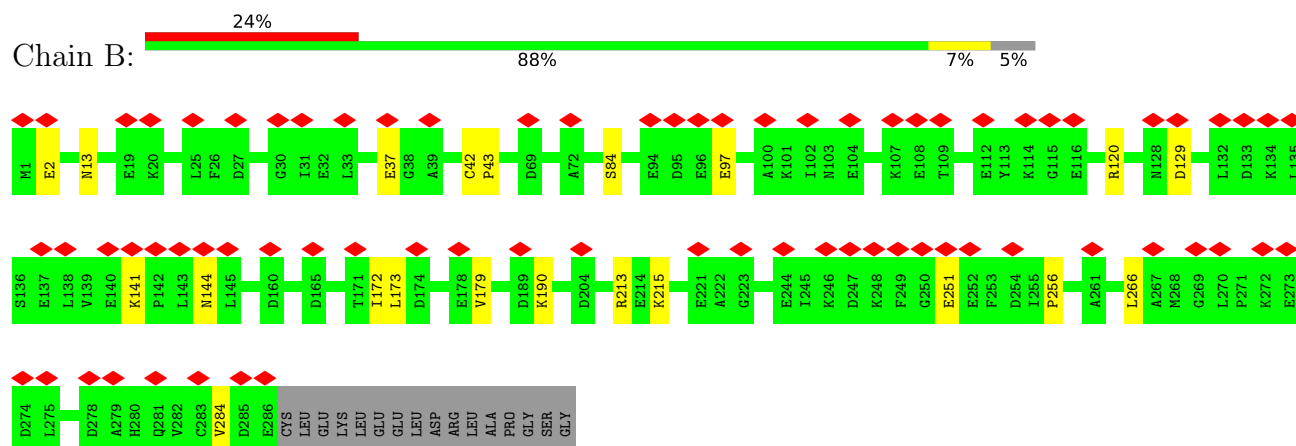
### 3 Residue-property plots

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.

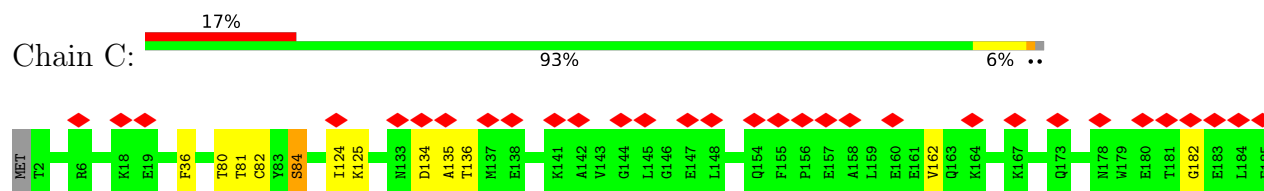
- Molecule 1: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit A



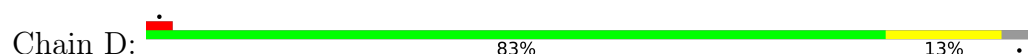
- Molecule 2: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit B

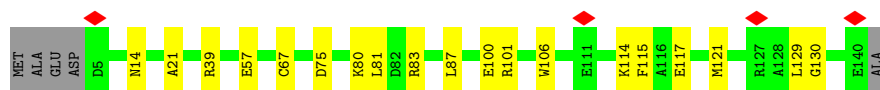


- Molecule 3: H(2):CoB-CoM heterodisulfide,ferredoxin reductase subunit C



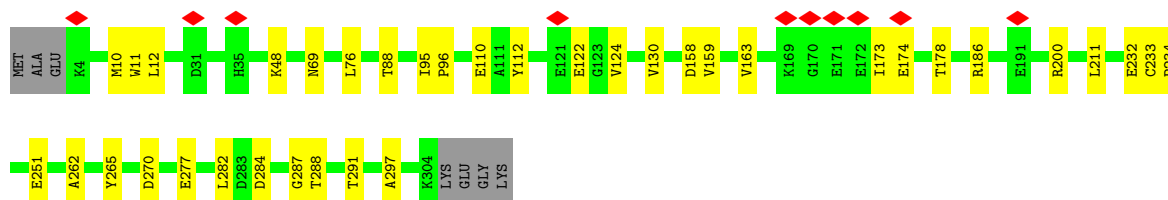
- Molecule 4: F420-non-reducing hydrogenase iron-sulfur subunit D





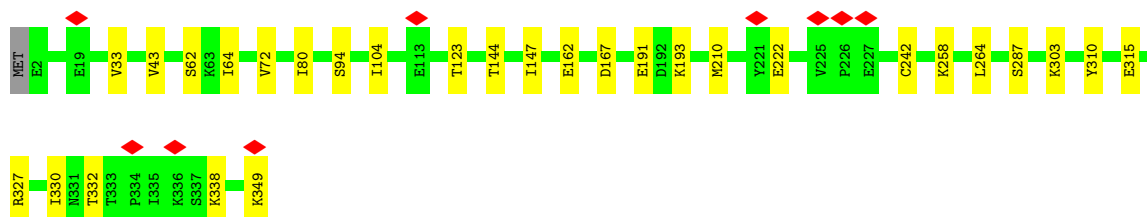
- Molecule 5: F420-non-reducing hydrogenase subunit G

Chain E: 86% 12%



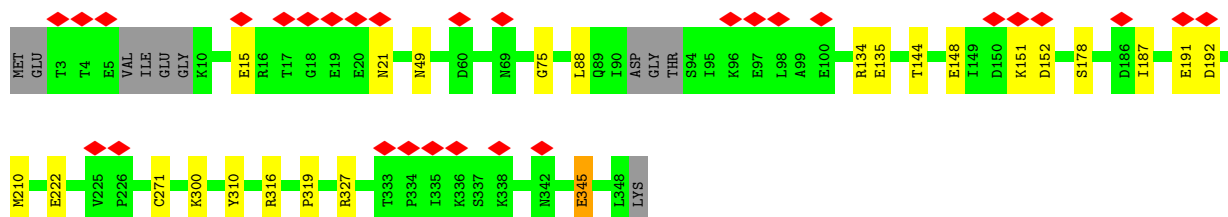
- Molecule 6: Tungsten formylmethanofuran dehydrogenase, subunit F

Chain H: 91% 8%



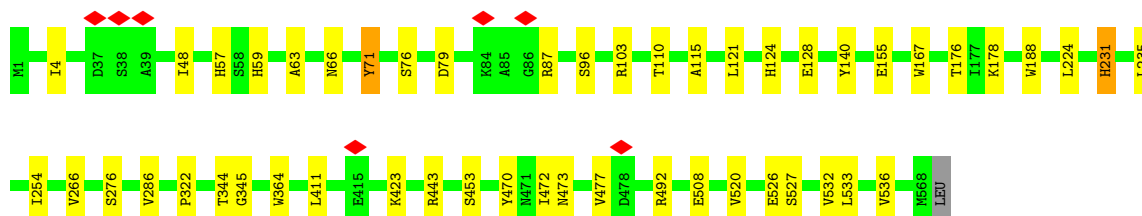
- Molecule 6: Tungsten formylmethanofuran dehydrogenase, subunit F

Chain h: 8% 90% 7%




- Molecule 7: Tungsten formylmethanofuran dehydrogenase, subunit A

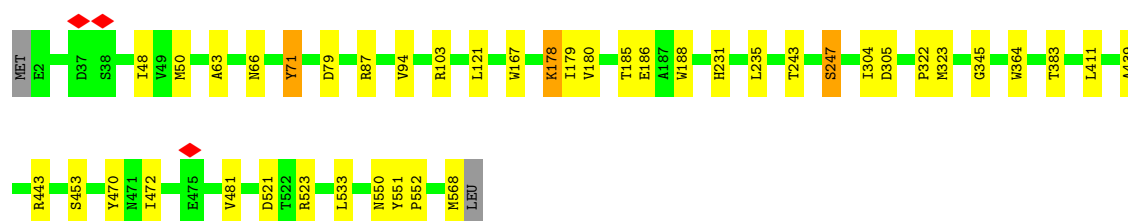
Chain I: 91% 8%




- Molecule 7: Tungsten formylmethanofuran dehydrogenase, subunit A

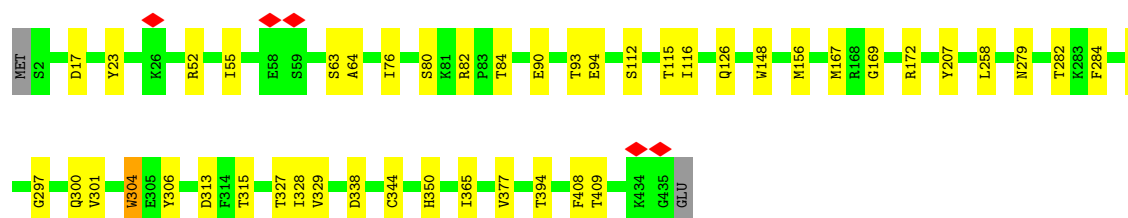


Chain i:  92% 7%




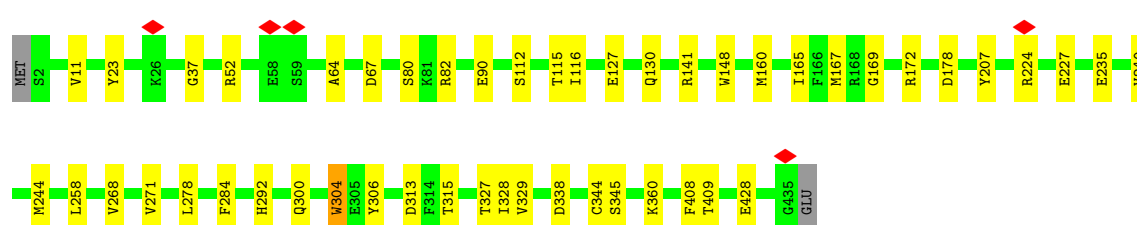
- Molecule 8: formylmethanofuran dehydrogenase subunit B

Chain J:  89% 10%




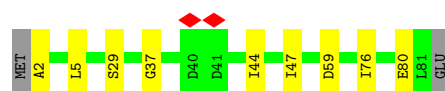
- Molecule 8: formylmethanofuran dehydrogenase subunit B

Chain j:  88% 11%




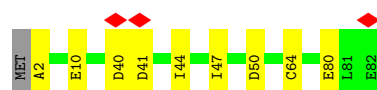
- Molecule 9: Tungsten formylmethanofuran dehydrogenase, subunit G

Chain L:  87% 11%

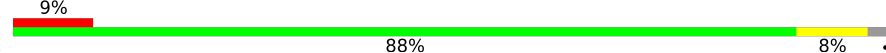


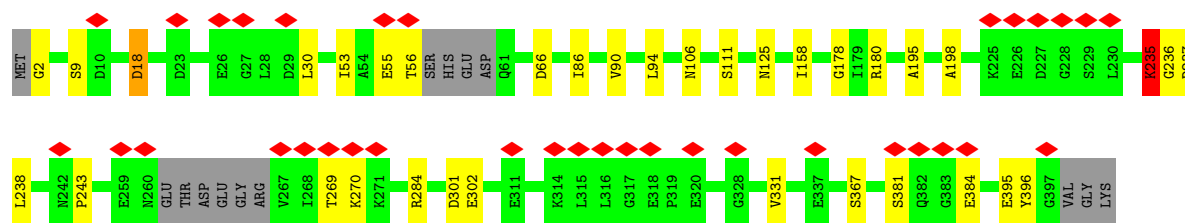
- Molecule 9: Tungsten formylmethanofuran dehydrogenase, subunit G

Chain l:  88% 11%

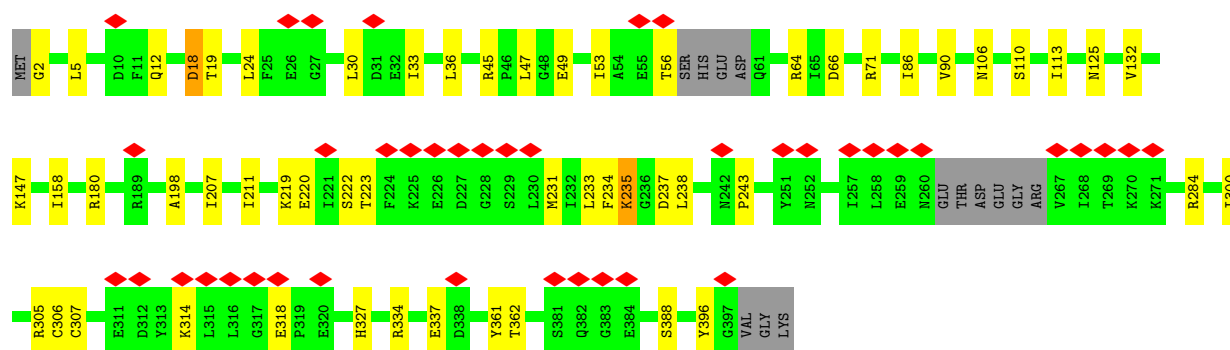
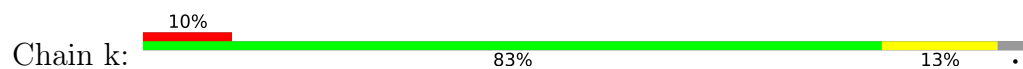


- Molecule 10: Molybdenum-containing formylmethanofuran dehydrogenase 1 subunit C

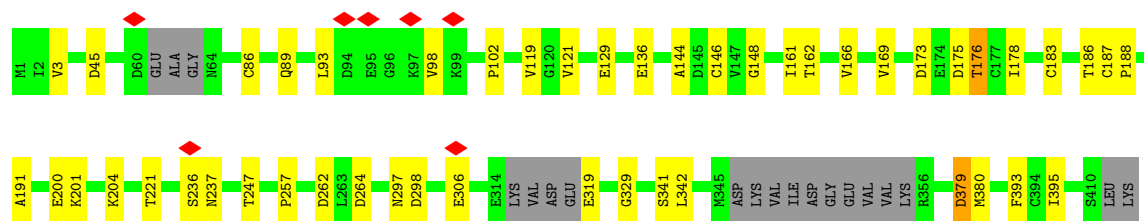
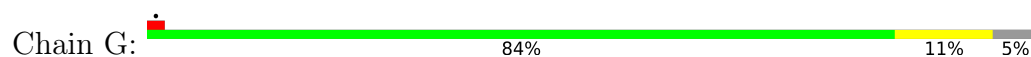
Chain K:  9% 88% 8%



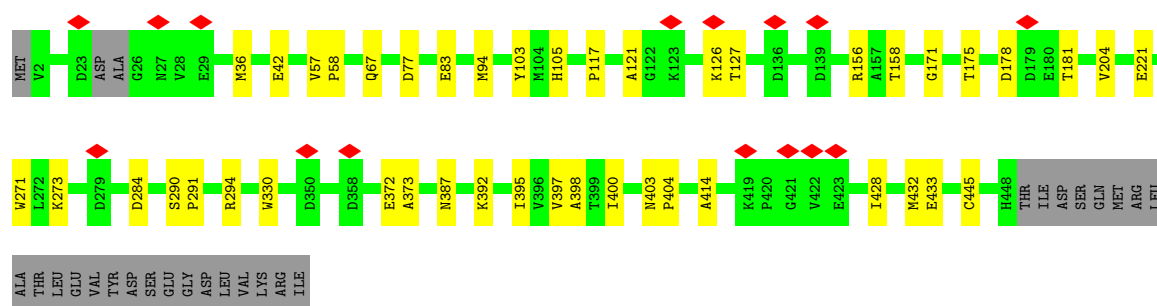
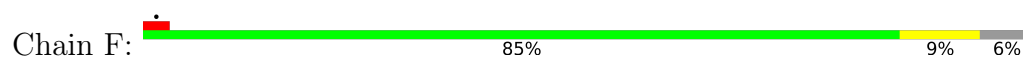
- Molecule 10: Molybdenum-containing formylmethanofuran dehydrogenase 1 subunit C



- Molecule 11: Polyferredoxin protein MvhB



- Molecule 12: F420-non-reducing hydrogenase subunit A



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	722594	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)	700	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	50.924	Depositor
Minimum map value	-28.134	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.916	Depositor
Recommended contour level	4.2	Depositor
Map size (Å)	401.1, 401.1, 401.1	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.835625, 0.835625, 0.835625	Depositor

## 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: MO, 9S8, NFU, KCX, H2S, FAD, F3S, MGD, FES, SF4, ZN

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	0.11	0/5030	0.27	0/6808
2	B	0.20	0/2250	0.32	0/3036
3	C	0.10	0/1447	0.22	0/1951
4	D	0.23	0/1098	0.47	1/1474 (0.1%)
5	E	0.11	0/2352	0.26	0/3195
6	H	0.11	0/2640	0.27	0/3582
6	h	0.10	0/2595	0.26	0/3518
7	I	0.12	0/4530	0.29	0/6169
7	i	0.11	0/4522	0.28	0/6159
8	J	0.11	0/3406	0.27	0/4610
8	j	0.11	0/3406	0.27	0/4610
9	L	0.11	0/579	0.28	0/787
9	l	0.11	0/588	0.26	0/799
10	K	0.30	2/2962 (0.1%)	0.31	1/3984 (0.0%)
10	k	0.25	1/2966 (0.0%)	0.36	1/3989 (0.0%)
11	G	0.14	0/2907	0.32	0/3944
12	F	0.11	0/3582	0.28	0/4858
All	All	0.15	3/46860 (0.0%)	0.29	3/63473 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	K	236	GLY	C-O	-10.95	1.12	1.23
10	K	235	LYS	C-O	-5.93	1.16	1.24
10	k	237	ASP	C-O	-5.22	1.13	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	75	ASP	CA-CB-CG	6.34	118.94	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	K	237	ASP	CA-C-O	-6.22	110.22	120.80
10	k	235	LYS	CB-CA-C	5.75	119.67	109.72

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4940	4894	4895	30	0
2	B	2213	2152	2171	14	0
3	C	1422	1432	1431	6	0
4	D	1076	1063	1062	12	0
5	E	2305	2250	2258	26	0
6	H	2603	2508	2511	18	0
6	h	2560	2465	2468	16	0
7	I	4426	4280	4280	30	0
7	i	4418	4269	4268	26	0
8	J	3341	3292	3291	32	0
8	j	3341	3292	3291	31	0
9	L	572	553	567	6	0
9	l	581	569	573	7	0
10	K	2916	2911	2908	21	0
10	k	2920	2917	2914	30	0
11	G	2865	2800	2797	30	0
12	F	3503	3414	3440	33	0
13	A	48	0	0	0	0
13	C	16	0	0	0	0
13	E	24	0	0	0	0
13	G	88	0	0	1	0
13	H	72	0	0	0	0
13	J	8	0	0	0	0
13	L	16	0	0	0	0
13	h	64	0	0	0	0
13	j	8	0	0	0	0
13	l	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	A	53	31	31	1	0
15	B	16	0	0	0	0
16	D	4	0	0	0	0
17	I	2	0	0	0	0
17	i	2	0	0	0	0
18	J	94	44	44	1	0
18	j	94	44	44	0	0
19	J	1	0	0	0	0
19	j	1	0	0	0	0
20	J	1	2	0	0	0
20	j	1	2	0	1	0
21	G	7	0	0	0	0
22	F	8	1	0	1	0
23	A	27	0	0	3	0
23	B	1	0	0	0	0
23	D	1	0	0	0	0
23	E	22	0	0	4	0
23	F	12	0	0	2	0
23	G	5	0	0	1	0
23	H	27	0	0	0	0
23	I	50	0	0	3	0
23	J	49	0	0	1	0
23	K	23	0	0	3	0
23	L	14	0	0	1	0
23	h	30	0	0	0	0
23	i	45	0	0	3	0
23	j	26	0	0	3	0
23	k	5	0	0	1	0
23	l	6	0	0	1	0
All	All	46989	45185	45244	342	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 4.

All (342) 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)
11:G:187:CYS:O	11:G:201:LYS:NZ	2.04	0.90
7:I:76:SER:OG	23:I:701:HOH:O	1.96	0.83
9:I:10:GLU:O	10:k:284:ARG:NH2	2.14	0.80
10:K:180:ARG:NH1	23:K:502:HOH:O	2.14	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:115:THR:HG23	8:J:116:ILE:HG23	1.65	0.79
6:h:151:LYS:NZ	6:h:187:ILE:O	2.15	0.79
4:D:106:TRP:O	4:D:114:LYS:NZ	2.17	0.78
1:A:638:GLN:O	23:A:801:HOH:O	2.02	0.78
10:k:180:ARG:NH1	23:k:501:HOH:O	2.16	0.78
11:G:204:LYS:NZ	11:G:247:THR:O	2.13	0.77
1:A:520:SER:OG	1:A:522:ASP:OD1	2.02	0.77
12:F:42:GLU:OE2	23:F:601:HOH:O	2.02	0.77
8:j:130:GLN:OE1	23:j:601:HOH:O	2.02	0.76
9:l:40:ASP:OD1	9:l:41:ASP:N	2.19	0.76
11:G:200:GLU:N	11:G:200:GLU:OE1	2.17	0.75
8:j:127:GLU:OE2	23:j:602:HOH:O	2.05	0.74
11:G:178:ILE:O	23:G:601:HOH:O	2.04	0.74
12:F:126:LYS:O	12:F:127:THR:OG1	2.05	0.73
1:A:341:TYR:OH	1:A:345:GLU:OE2	2.03	0.73
8:J:313:ASP:OD1	8:J:315:THR:HG23	1.89	0.72
8:J:207:TYR:OH	10:K:198:ALA:HB1	1.90	0.72
9:l:2:ALA:HB1	9:l:80:GLU:OE1	1.89	0.72
5:E:112:TYR:OH	12:F:271:TRP:O	2.08	0.71
8:j:244:MET:HE3	8:j:278:LEU:HD11	1.70	0.71
8:j:115:THR:HG23	8:j:116:ILE:HG23	1.72	0.71
9:L:37:GLY:O	23:L:201:HOH:O	2.08	0.71
1:A:470:GLU:OE2	23:A:802:HOH:O	2.09	0.70
5:E:232:GLU:OE1	23:E:501:HOH:O	2.10	0.70
11:G:319:GLU:OE1	11:G:319:GLU:N	2.24	0.70
7:I:79:ASP:OD2	7:I:103:ARG:NH2	2.25	0.70
12:F:83:GLU:OE1	12:F:83:GLU:N	2.24	0.69
6:H:80:ILE:HG23	6:H:80:ILE:O	1.92	0.69
7:I:492:ARG:NH2	7:I:508:GLU:OE2	2.25	0.69
1:A:291:PRO:O	23:A:803:HOH:O	2.11	0.69
4:D:100:GLU:HG2	4:D:129:LEU:HD21	1.75	0.69
8:j:178:ASP:OD2	23:j:603:HOH:O	2.11	0.69
9:l:50:ASP:O	23:l:201:HOH:O	2.10	0.68
8:J:115:THR:HG21	8:J:328:ILE:HG22	1.75	0.68
7:i:305:ASP:OD1	7:i:383:THR:OG1	2.10	0.68
4:D:100:GLU:OE1	4:D:100:GLU:N	2.23	0.68
8:J:17:ASP:OD1	23:J:602:HOH:O	2.12	0.68
8:j:80:SER:OG	8:j:338:ASP:OD1	2.11	0.67
8:j:360:LYS:NZ	10:k:396:TYR:O	2.22	0.67
11:G:173:ASP:OD2	11:G:176:THR:OG1	2.12	0.67
7:I:66:ASN:ND2	8:J:300:GLN:OE1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:313:ASP:OD1	8:j:315:THR:HG23	1.94	0.67
10:k:106:ASN:OD1	10:k:125:ASN:ND2	2.27	0.66
11:G:297:ASN:ND2	11:G:393:PHE:O	2.28	0.66
1:A:420:GLN:OE1	1:A:452:SER:OG	2.14	0.66
12:F:397:VAL:O	12:F:400:ILE:HG22	1.96	0.66
5:E:297:ALA:O	23:E:502:HOH:O	2.13	0.66
8:J:80:SER:OG	8:J:338:ASP:OD1	2.09	0.66
12:F:395:ILE:O	23:F:601:HOH:O	2.12	0.65
7:I:443:ARG:NH2	7:I:470:TYR:OH	2.29	0.65
6:H:167:ASP:O	6:H:193:LYS:NZ	2.27	0.65
7:I:167:TRP:CD1	7:I:533:LEU:HD21	2.31	0.65
8:j:207:TYR:OH	10:k:198:ALA:HB1	1.97	0.65
6:h:49:ASN:O	6:h:316:ARG:NH2	2.30	0.65
12:F:397:VAL:HG11	12:F:445:CYS:HB3	1.78	0.64
2:B:120:ARG:NH2	2:B:129:ASP:OD2	2.30	0.64
6:h:310:TYR:O	6:h:327:ARG:NH1	2.31	0.64
10:k:45:ARG:NH2	10:k:49:GLU:OE1	2.31	0.64
10:k:220:GLU:OE2	10:k:222:SER:N	2.31	0.63
10:k:64:ARG:NH1	10:k:66:ASP:OD2	2.32	0.63
2:B:2:GLU:OE1	2:B:2:GLU:N	2.30	0.62
10:K:18:ASP:OD1	10:K:18:ASP:N	2.32	0.62
6:H:264:LEU:O	6:H:303:LYS:NZ	2.31	0.62
9:L:44:ILE:HD11	9:L:47:ILE:HG22	1.81	0.62
7:i:167:TRP:CD1	7:i:533:LEU:HD21	2.35	0.62
10:K:301:ASP:OD1	10:K:302:GLU:N	2.34	0.61
10:k:2:GLY:O	10:k:56:THR:OG1	2.15	0.61
6:H:144:THR:OG1	6:H:222:GLU:OE1	2.19	0.60
8:J:52:ARG:NH2	8:J:64:ALA:O	2.34	0.60
12:F:126:LYS:HD3	12:F:127:THR:HG23	1.83	0.60
10:k:314:LYS:NZ	10:k:337:GLU:OE2	2.35	0.60
2:B:190:LYS:O	2:B:215:LYS:NZ	2.35	0.60
11:G:247:THR:OG1	13:G:508:SF4:S4	2.60	0.59
12:F:103:TYR:OH	12:F:372:GLU:O	2.09	0.59
7:I:364:TRP:CZ2	7:I:411:LEU:HD23	2.37	0.59
12:F:178:ASP:OD1	12:F:181:THR:OG1	2.10	0.59
10:K:106:ASN:OD1	10:K:125:ASN:ND2	2.35	0.59
1:A:13:LYS:NZ	1:A:70:GLY:O	2.35	0.59
8:j:82:ARG:HH12	8:j:315:THR:HG21	1.68	0.59
8:J:82:ARG:HH12	8:J:315:THR:HG21	1.68	0.58
10:k:305:ARG:NH1	10:k:307:CYS:SG	2.76	0.58
10:k:300:ILE:HD11	10:k:388:SER:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:i:79:ASP:OD2	7:i:103:ARG:NH2	2.37	0.58
6:h:135:GLU:OE1	6:h:135:GLU:N	2.36	0.58
3:C:134:ASP:OD1	3:C:135:ALA:N	2.36	0.58
2:B:37:GLU:N	2:B:37:GLU:OE1	2.35	0.58
12:F:36:MET:HA	12:F:36:MET:HE2	1.85	0.58
5:E:122:GLU:HG2	5:E:124:VAL:HG23	1.86	0.57
8:J:93:THR:HG23	8:J:301:VAL:CG2	2.33	0.57
10:K:381:SER:N	10:K:384:GLU:OE1	2.37	0.57
8:j:112:SER:O	8:j:115:THR:HG22	2.05	0.57
12:F:158:THR:O	12:F:175:THR:HG21	2.04	0.57
2:B:13:ASN:C	3:C:136:THR:HG21	2.30	0.57
5:E:287:GLY:O	5:E:291:THR:OG1	2.22	0.57
5:E:130:VAL:HG12	12:F:36:MET:HE1	1.86	0.57
7:i:443:ARG:NH2	7:i:470:TYR:OH	2.33	0.57
11:G:93:LEU:HD23	11:G:102:PRO:O	2.05	0.57
6:H:310:TYR:O	6:H:327:ARG:NH1	2.35	0.57
8:J:112:SER:O	8:J:115:THR:HG22	2.05	0.57
8:J:93:THR:HG23	8:J:301:VAL:HG21	1.86	0.56
2:B:256:PRO:HB3	2:B:284:VAL:HG23	1.87	0.56
5:E:130:VAL:HG12	12:F:36:MET:CE	2.35	0.56
10:K:2:GLY:N	10:K:56:THR:HG1	2.03	0.56
11:G:86:CYS:O	11:G:89:GLN:NE2	2.38	0.56
12:F:273:LYS:HB2	12:F:400:ILE:HD11	1.88	0.56
9:l:44:ILE:HD11	9:l:47:ILE:HG22	1.86	0.56
7:i:180:VAL:HA	7:i:231:HIS:HB3	1.88	0.56
10:k:12:GLN:O	10:k:71:ARG:NH2	2.39	0.56
11:G:146:CYS:HB3	11:G:169:VAL:HG13	1.88	0.56
3:C:125:LYS:NZ	3:C:182:GLY:O	2.37	0.56
10:K:86:ILE:HG21	10:K:90:VAL:HG22	1.87	0.56
12:F:397:VAL:HG12	12:F:398:ALA:H	1.72	0.55
6:H:315:GLU:OE1	6:H:349:LYS:NZ	2.37	0.55
12:F:294:ARG:NH1	12:F:372:GLU:OE1	2.33	0.55
8:J:156:MET:HE3	8:J:289:ILE:HG23	1.87	0.55
7:i:66:ASN:ND2	8:j:300:GLN:OE1	2.36	0.55
10:k:18:ASP:OD1	10:k:18:ASP:N	2.40	0.55
1:A:370:SER:O	1:A:370:SER:OG	2.23	0.55
6:H:72:VAL:HG11	11:G:257:PRO:HG3	1.89	0.55
7:i:87:ARG:NH1	8:j:306:TYR:OH	2.39	0.55
6:H:62:SER:OG	6:H:64:ILE:O	2.25	0.54
6:H:147:ILE:HG22	6:H:191:GLU:OE2	2.06	0.54
11:G:188:PRO:HB2	11:G:247:THR:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:F:77:ASP:OD1	12:F:171:GLY:N	2.39	0.54
6:H:104:ILE:HD13	6:H:332:THR:HG22	1.89	0.54
8:j:115:THR:HG21	8:j:328:ILE:HG22	1.88	0.54
2:B:213:ARG:NE	2:B:251:GLU:OE2	2.38	0.54
10:K:30:LEU:HD11	10:K:55:GLU:HB2	1.88	0.54
5:E:12:LEU:O	5:E:69:ASN:ND2	2.41	0.54
5:E:122:GLU:CG	5:E:124:VAL:HG23	2.38	0.54
5:E:174:GLU:OE1	5:E:174:GLU:N	2.39	0.54
7:i:48:ILE:HD12	7:i:472:ILE:HB	1.90	0.54
7:i:186:GLU:OE2	23:i:703:HOH:O	2.18	0.53
10:k:45:ARG:NH1	10:k:49:GLU:OE2	2.41	0.53
10:k:110:SER:O	10:k:113:ILE:HD11	2.08	0.53
7:I:286:VAL:HG12	7:I:423:LYS:HD2	1.91	0.53
9:l:44:ILE:HD11	9:l:47:ILE:CG2	2.37	0.53
10:k:318:GLU:N	10:k:318:GLU:OE1	2.41	0.53
23:E:501:HOH:O	12:F:156:ARG:NH1	2.35	0.53
5:E:284:ASP:O	5:E:288:THR:OG1	2.14	0.52
2:B:141:LYS:NZ	2:B:266:LEU:O	2.42	0.52
10:K:396:TYR:OH	23:K:503:HOH:O	2.16	0.52
11:G:129:GLU:N	11:G:129:GLU:OE2	2.43	0.52
8:j:292:HIS:ND1	20:j:505:H2S:S	2.82	0.52
7:I:526:GLU:CD	7:I:526:GLU:H	2.18	0.52
7:i:364:TRP:CZ2	7:i:411:LEU:HD23	2.45	0.51
8:j:160:MET:HG2	8:j:165:ILE:HD12	1.92	0.51
5:E:10:MET:HG2	5:E:76:LEU:HD11	1.92	0.51
8:j:235:GLU:C	8:j:235:GLU:OE2	2.53	0.51
4:D:14:ASN:OD1	4:D:39:ARG:NH1	2.40	0.51
7:I:57:HIS:CE1	7:I:115:ALA:HB1	2.46	0.51
8:j:67:ASP:OD2	8:j:67:ASP:N	2.38	0.51
10:K:235:LYS:CD	10:K:238:LEU:HD21	2.41	0.51
1:A:477:THR:OG1	1:A:492:ASP:OD1	2.26	0.51
9:L:59:ASP:C	9:L:59:ASP:OD2	2.54	0.51
1:A:186:ILE:O	1:A:187:SER:HB3	2.11	0.50
8:J:377:VAL:HG12	8:J:377:VAL:O	2.11	0.50
8:j:148:TRP:CD1	8:j:258:LEU:HD21	2.46	0.50
8:J:169:GLY:N	8:J:172:ARG:O	2.44	0.50
11:G:136:GLU:OE1	11:G:136:GLU:N	2.43	0.50
2:B:256:PRO:CB	2:B:284:VAL:HG23	2.41	0.50
8:j:408:PHE:CD1	8:j:409:THR:HG23	2.46	0.50
11:G:306:GLU:OE1	11:G:306:GLU:N	2.45	0.50
12:F:284:ASP:C	12:F:284:ASP:OD1	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:87:ARG:NH1	8:J:306:TYR:OH	2.45	0.50
8:J:350:HIS:ND1	18:J:503:MGD:O2A	2.43	0.50
7:i:550:ASN:O	23:i:704:HOH:O	2.20	0.50
10:K:367:SER:OG	23:K:501:HOH:O	1.99	0.50
8:j:141:ARG:O	8:j:172:ARG:NE	2.44	0.49
6:H:330:ILE:HG22	6:H:332:THR:HG23	1.94	0.49
8:J:148:TRP:CD1	8:J:258:LEU:HD21	2.46	0.49
8:J:297:GLY:O	8:J:301:VAL:HG23	2.13	0.49
8:j:23:TYR:CE2	8:j:409:THR:HG21	2.47	0.49
4:D:57:GLU:OE2	4:D:57:GLU:HA	2.13	0.49
10:K:90:VAL:HG11	10:K:94:LEU:HD13	1.94	0.49
2:B:97:GLU:OE1	2:B:97:GLU:N	2.42	0.49
9:L:2:ALA:HB1	9:L:80:GLU:OE1	2.12	0.49
1:A:415:ILE:HD11	1:A:499:GLY:HA3	1.95	0.48
4:D:101:ARG:NH2	4:D:130:GLY:O	2.46	0.48
5:E:95:ILE:N	5:E:96:PRO:CD	2.76	0.48
5:E:110:GLU:OE2	12:F:392:LYS:NZ	2.47	0.48
8:j:52:ARG:NH2	8:j:64:ALA:O	2.47	0.48
1:A:414:TYR:CD1	1:A:414:TYR:C	2.91	0.48
7:i:453:SER:OG	23:i:702:HOH:O	2.03	0.48
8:J:94:GLU:OE1	8:J:94:GLU:N	2.42	0.48
7:I:532:VAL:O	7:I:536:VAL:HG23	2.14	0.48
2:B:42:CYS:N	2:B:43:PRO:HA	2.29	0.47
6:h:75:GLY:CA	6:h:88:LEU:HD22	2.44	0.47
7:I:231:HIS:C	7:I:231:HIS:CD2	2.92	0.47
8:J:304:TRP:CD1	8:J:304:TRP:C	2.92	0.47
7:I:63:ALA:HB2	7:I:121:LEU:HD13	1.96	0.47
8:J:167:MET:SD	8:J:167:MET:N	2.87	0.47
6:h:192:ASP:OD2	6:h:192:ASP:C	2.58	0.47
8:J:84:THR:HG21	8:J:328:ILE:HD13	1.97	0.47
6:h:148:GLU:C	6:h:148:GLU:OE2	2.58	0.47
1:A:586:THR:OG1	1:A:635:MET:SD	2.71	0.47
7:i:235:LEU:HD22	7:i:323:MET:HE2	1.96	0.47
6:h:144:THR:OG1	6:h:222:GLU:OE1	2.28	0.47
4:D:83:ARG:NH1	5:E:270:ASP:OD1	2.43	0.47
7:I:344:THR:OG1	7:I:345:GLY:N	2.48	0.47
10:k:19:THR:HA	10:k:24:LEU:HD12	1.96	0.47
8:j:304:TRP:CD1	8:j:304:TRP:C	2.93	0.47
10:k:86:ILE:HG21	10:k:90:VAL:HG22	1.96	0.47
10:k:238:LEU:HD23	10:k:243:PRO:CG	2.45	0.47
12:F:57:VAL:N	12:F:58:PRO:CD	2.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:124:HIS:NE2	7:I:128:GLU:OE2	2.48	0.46
1:A:301:CYS:O	11:G:98:VAL:HG21	2.16	0.46
5:E:158:ASP:OD1	5:E:159:VAL:N	2.47	0.46
1:A:90:ARG:O	1:A:94:GLU:HG3	2.15	0.46
4:D:87:LEU:HD12	5:E:262:ALA:HB2	1.98	0.46
5:E:69:ASN:ND2	23:E:503:HOH:O	2.45	0.46
1:A:186:ILE:O	1:A:187:SER:CB	2.63	0.46
6:H:80:ILE:O	6:H:80:ILE:CG2	2.62	0.46
5:E:48:LYS:NZ	12:F:433:GLU:OE2	2.48	0.45
10:K:195:ALA:HB1	10:K:198:ALA:HB2	1.98	0.45
10:K:238:LEU:HA	10:K:243:PRO:HG2	1.98	0.45
12:F:414:ALA:HB2	12:F:432:MET:HE3	1.98	0.45
10:K:53:ILE:N	10:K:53:ILE:HD12	2.31	0.45
12:F:94:MET:HE3	12:F:175:THR:HG23	1.98	0.45
7:I:48:ILE:HD12	7:I:472:ILE:HB	1.98	0.45
11:G:264:ASP:OD1	11:G:264:ASP:C	2.60	0.45
6:H:162:GLU:OE2	6:h:134:ARG:NH1	2.50	0.45
1:A:391:PHE:HB2	1:A:433:LEU:HD22	1.98	0.45
5:E:265:TYR:OH	5:E:277:GLU:OE1	2.24	0.45
8:j:328:ILE:HG23	8:j:329:VAL:N	2.32	0.45
1:A:167:ALA:CB	1:A:179:MET:HE2	2.47	0.45
1:A:547:VAL:HG12	1:A:547:VAL:O	2.16	0.45
4:D:21:ALA:HB2	4:D:115:PHE:CE2	2.51	0.45
11:G:148:GLY:O	11:G:166:VAL:O	2.35	0.45
4:D:80:LYS:NZ	5:E:270:ASP:OD2	2.50	0.44
4:D:117:GLU:OE2	4:D:117:GLU:HA	2.16	0.44
7:I:224:LEU:HD22	7:I:520:VAL:HG11	1.99	0.44
1:A:517:LEU:HD21	1:A:542:VAL:HG11	1.98	0.44
7:I:110:THR:OG1	23:I:702:HOH:O	2.08	0.44
7:i:63:ALA:CB	7:i:121:LEU:HD13	2.47	0.44
9:l:64:CYS:HB3	6:h:319:PRO:HG3	1.98	0.44
8:j:167:MET:SD	8:j:167:MET:N	2.88	0.44
5:E:200:ARG:NH1	12:F:387:ASN:O	2.50	0.44
8:j:268:VAL:O	8:j:271:VAL:HG12	2.18	0.44
10:K:235:LYS:HD2	10:K:238:LEU:HD21	1.98	0.44
6:h:271:CYS:O	6:h:300:LYS:NZ	2.40	0.44
6:h:15:GLU:OE1	6:h:21:ASN:ND2	2.47	0.44
10:k:233:LEU:HD23	10:k:234:PHE:N	2.33	0.44
11:G:45:ASP:N	11:G:45:ASP:OD1	2.48	0.44
10:k:2:GLY:N	10:k:56:THR:OG1	2.50	0.44
11:G:380:MET:HE3	11:G:380:MET:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:144:ASN:CG	2:B:144:ASN:O	2.61	0.44
11:G:119:VAL:HG23	11:G:121:VAL:HG13	1.98	0.44
7:I:188:TRP:HB2	7:I:322:PRO:HG3	1.99	0.44
9:L:44:ILE:HD11	9:L:47:ILE:CG2	2.48	0.44
8:j:224:ARG:O	8:j:227:GLU:OE2	2.35	0.44
1:A:117:ASP:N	1:A:117:ASP:OD1	2.49	0.43
7:i:63:ALA:HB2	7:i:121:LEU:HD13	1.99	0.43
7:i:185:THR:HG21	7:i:345:GLY:N	2.33	0.43
10:K:158:ILE:O	10:K:178:GLY:N	2.48	0.43
6:H:242:CYS:O	6:H:258:LYS:NZ	2.38	0.43
10:K:395:GLU:OE1	10:K:395:GLU:C	2.62	0.43
1:A:79:CYS:O	1:A:104:PHE:CE1	2.72	0.43
2:B:172:ILE:HG23	2:B:173:LEU:N	2.34	0.42
6:H:43:VAL:HG11	11:G:257:PRO:HB2	2.00	0.42
7:i:188:TRP:HB2	7:i:322:PRO:HG3	2.00	0.42
6:H:287:SER:OG	6:h:178:SER:OG	2.36	0.42
8:J:76:ILE:CG2	8:J:365:ILE:HD11	2.49	0.42
6:H:210:MET:SD	6:H:210:MET:C	3.03	0.42
7:I:63:ALA:CB	7:I:121:LEU:HD13	2.49	0.42
7:I:254:ILE:HB	7:I:266:VAL:HG21	2.01	0.42
6:h:210:MET:SD	6:h:210:MET:C	3.02	0.42
7:I:4:ILE:O	7:I:4:ILE:HG23	2.20	0.42
12:F:204:VAL:HG13	12:F:330:TRP:CZ2	2.54	0.42
8:J:55:ILE:HD12	8:J:64:ALA:CB	2.50	0.42
8:j:169:GLY:N	8:j:172:ARG:O	2.52	0.42
10:k:235:LYS:HD3	10:k:238:LEU:HD21	2.02	0.42
11:G:144:ALA:N	11:G:191:ALA:O	2.49	0.42
7:i:523:ARG:HG2	7:i:523:ARG:HH11	1.85	0.42
1:A:554:ILE:HD12	14:A:704:FAD:C2	2.50	0.42
7:I:59:HIS:CE1	7:I:115:ALA:HB3	2.54	0.42
7:i:243:THR:O	7:i:247:SER:OG	2.34	0.42
7:I:140:TYR:CD1	7:I:176:THR:HB	2.54	0.42
10:k:361:TYR:O	10:k:362:THR:OG1	2.29	0.42
12:F:428:ILE:N	12:F:428:ILE:HD12	2.35	0.42
7:I:453:SER:OG	23:I:703:HOH:O	2.20	0.42
8:J:115:THR:HG21	8:J:328:ILE:CG2	2.46	0.42
9:L:5:LEU:HG	9:L:76:ILE:HD11	2.02	0.42
1:A:408:SER:HB2	1:A:411:CYS:SG	2.60	0.42
7:i:481:VAL:O	7:i:481:VAL:HG12	2.20	0.42
6:h:345:GLU:OE1	6:h:345:GLU:N	2.52	0.42
10:k:306:CYS:N	10:k:334:ARG:O	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:121:MET:SD	4:D:121:MET:C	3.03	0.41
8:J:23:TYR:CE2	8:J:409:THR:HG21	2.55	0.41
12:F:290:SER:CB	12:F:291:PRO:CD	2.98	0.41
1:A:642:THR:O	1:A:646:MET:HG2	2.20	0.41
3:C:80:THR:O	3:C:81:THR:OG1	2.26	0.41
5:E:163:VAL:HA	5:E:173:ILE:HD13	2.01	0.41
7:i:178:KCX:HD2	7:i:179:ILE:N	2.35	0.41
11:G:136:GLU:CD	11:G:136:GLU:O	2.63	0.41
7:I:71:TYR:HA	8:J:126:GLN:HG2	2.03	0.41
2:B:13:ASN:O	3:C:136:THR:HG21	2.19	0.41
6:h:191:GLU:OE1	6:h:191:GLU:N	2.54	0.41
10:k:132:VAL:O	10:k:158:ILE:O	2.37	0.41
11:G:379:ASP:OD1	11:G:379:ASP:N	2.51	0.41
12:F:445:CYS:CB	22:F:501:NFU:C2	2.98	0.41
5:E:233:CYS:HB2	5:E:234:PRO:HD3	2.03	0.41
7:I:155:GLU:O	7:I:155:GLU:CD	2.63	0.41
10:K:269:THR:HG22	10:K:270:LYS:H	1.84	0.41
11:G:236:SER:O	11:G:237:ASN:OD1	2.37	0.41
12:F:67:GLN:HG2	12:F:373:ALA:HA	2.03	0.41
1:A:159:GLY:N	1:A:181:GLU:OE1	2.54	0.41
3:C:82:CYS:SG	3:C:84:SER:OG	2.73	0.41
10:K:269:THR:HG22	10:K:270:LYS:N	2.35	0.41
10:k:36:LEU:O	10:k:47:LEU:N	2.52	0.41
11:G:329:GLY:HA3	11:G:342:LEU:HD11	2.02	0.41
12:F:117:PRO:HA	12:F:121:ALA:HB2	2.02	0.41
12:F:403:ASN:HB3	12:F:404:PRO:HD3	2.03	0.41
1:A:447:GLU:OE1	1:A:447:GLU:N	2.45	0.41
8:j:90:GLU:HB2	8:j:344:CYS:SG	2.61	0.41
1:A:184:PRO:O	1:A:247:ARG:NH2	2.50	0.41
1:A:230:GLU:OE2	1:A:232:ASP:OD1	2.39	0.41
1:A:583:ILE:HD12	1:A:583:ILE:C	2.45	0.41
5:E:186:ARG:NH1	5:E:211:LEU:O	2.47	0.41
8:j:11:VAL:HG21	8:j:37:GLY:HA2	2.02	0.41
10:k:5:LEU:HD22	10:k:53:ILE:HG13	2.03	0.41
11:G:161:ILE:HD11	11:G:183:CYS:HB3	2.03	0.41
8:J:328:ILE:HG23	8:J:329:VAL:N	2.35	0.41
7:i:71:TYR:CD1	7:i:71:TYR:C	2.98	0.41
8:J:408:PHE:CD1	8:J:409:THR:HG23	2.56	0.40
7:i:50:MET:HE2	7:i:439:ALA:HB2	2.04	0.40
7:i:551:TYR:HB3	7:i:552:PRO:HD3	2.03	0.40
10:k:207:ILE:HG21	10:k:211:ILE:HG22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:338:LYS:HD3	6:H:338:LYS:N	2.36	0.40
8:J:279:ASN:HA	8:J:282:THR:O	2.22	0.40
5:E:95:ILE:HG22	5:E:96:PRO:HD3	2.02	0.40
10:k:219:LYS:HE3	10:k:219:LYS:HB2	1.89	0.40
7:I:473:ASN:O	7:I:477:VAL:HG12	2.21	0.40
7:i:521:ASP:O	7:i:568:MET:HE2	2.22	0.40
7:I:231:HIS:CE1	7:I:235:LEU:HD13	2.57	0.40
8:J:90:GLU:HB2	8:J:344:CYS:SG	2.61	0.40
7:i:305:ASP:CG	7:i:383:THR:HG1	2.22	0.40
11:G:298:ASP:OD1	11:G:298:ASP:N	2.55	0.40

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	645/659 (98%)	631 (98%)	13 (2%)	1 (0%)	43	68
2	B	284/302 (94%)	276 (97%)	8 (3%)	0	100	100
3	C	182/185 (98%)	180 (99%)	2 (1%)	0	100	100
4	D	134/141 (95%)	131 (98%)	3 (2%)	0	100	100
5	E	299/308 (97%)	285 (95%)	14 (5%)	0	100	100
6	H	346/349 (99%)	337 (97%)	9 (3%)	0	100	100
6	h	333/349 (95%)	325 (98%)	8 (2%)	0	100	100
7	I	565/569 (99%)	553 (98%)	12 (2%)	0	100	100
7	i	564/569 (99%)	552 (98%)	12 (2%)	0	100	100
8	J	432/436 (99%)	417 (96%)	15 (4%)	0	100	100
8	j	432/436 (99%)	416 (96%)	16 (4%)	0	100	100
9	L	78/82 (95%)	78 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	l	79/82 (96%)	79 (100%)	0	0	100	100
10	K	380/400 (95%)	367 (97%)	13 (3%)	0	100	100
10	k	380/400 (95%)	365 (96%)	15 (4%)	0	100	100
11	G	385/412 (93%)	366 (95%)	19 (5%)	0	100	100
12	F	441/472 (93%)	425 (96%)	16 (4%)	0	100	100
All	All	5959/6151 (97%)	5783 (97%)	175 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	187	SER

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	536/547 (98%)	529 (99%)	7 (1%)	61	83
2	B	241/255 (94%)	239 (99%)	2 (1%)	73	88
3	C	153/155 (99%)	149 (97%)	4 (3%)	40	70
4	D	112/115 (97%)	110 (98%)	2 (2%)	51	78
5	E	257/262 (98%)	252 (98%)	5 (2%)	50	77
6	H	295/313 (94%)	292 (99%)	3 (1%)	68	86
6	h	294/313 (94%)	292 (99%)	2 (1%)	76	90
7	I	470/471 (100%)	465 (99%)	5 (1%)	65	85
7	i	469/471 (100%)	465 (99%)	4 (1%)	70	87
8	J	363/369 (98%)	358 (99%)	5 (1%)	59	82
8	j	363/369 (98%)	357 (98%)	6 (2%)	53	79
9	L	65/67 (97%)	64 (98%)	1 (2%)	57	81
9	l	66/67 (98%)	66 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	K	308/324 (95%)	301 (98%)	7 (2%)	44	73
10	k	309/324 (95%)	302 (98%)	7 (2%)	44	73
11	G	325/348 (93%)	315 (97%)	10 (3%)	35	65
12	F	371/396 (94%)	369 (100%)	2 (0%)	81	92
All	All	4997/5166 (97%)	4925 (99%)	72 (1%)	57	82

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	116	MET
1	A	224	THR
1	A	411	CYS
1	A	414	TYR
1	A	477	THR
1	A	518	SER
1	A	632	SER
2	B	84	SER
2	B	179	VAL
3	C	36	PHE
3	C	84	SER
3	C	124	ILE
3	C	162	VAL
4	D	67	CYS
4	D	81	LEU
5	E	11	TRP
5	E	88	THR
5	E	178	THR
5	E	251	GLU
5	E	282	LEU
6	H	33	VAL
6	H	94	SER
6	H	123	THR
7	I	71	TYR
7	I	96	SER
7	I	231	HIS
7	I	276	SER
7	I	527	SER
8	J	63	SER
8	J	284	PHE
8	J	304	TRP
8	J	327	THR

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Mol	Chain	Res	Type
8	J	394	THR
9	L	29	SER
7	i	71	TYR
7	i	94	VAL
7	i	247	SER
7	i	304	ILE
8	j	240	VAL
8	j	284	PHE
8	j	304	TRP
8	j	327	THR
8	j	345	SER
8	j	428	GLU
10	K	9	SER
10	K	18	ASP
10	K	66	ASP
10	K	111	SER
10	K	235	LYS
10	K	284	ARG
10	K	331	VAL
6	h	152	ASP
6	h	345	GLU
10	k	18	ASP
10	k	30	LEU
10	k	33	ILE
10	k	147	LYS
10	k	223	THR
10	k	231	MET
10	k	327	HIS
11	G	3	VAL
11	G	162	THR
11	G	175	ASP
11	G	176	THR
11	G	186	THR
11	G	221	THR
11	G	262	ASP
11	G	341	SER
11	G	379	ASP
11	G	395	ILE
12	F	105	HIS
12	F	221	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	84	HIS
1	A	165	GLN
1	A	237	ASN
1	A	654	ASN
4	D	34	ASN
6	H	174	GLN
6	H	272	GLN
6	H	321	ASN
7	I	106	GLN
7	i	15	ASN
7	i	473	ASN
7	i	514	HIS
8	j	48	HIS
8	j	246	ASN
8	j	281	HIS
8	j	333	GLN
10	K	93	GLN
6	h	174	GLN
6	h	246	GLN
10	k	12	GLN
10	k	342	GLN
11	G	362	ASN
12	F	67	GLN
12	F	215	ASN
12	F	329	HIS
12	F	394	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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
7	KCX	I	178	17,7	9,11,12	0.80	0	5,12,14	1.55	1 (20%)
7	KCX	i	178	17,7	9,11,12	0.77	0	5,12,14	1.59	1 (20%)

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
7	KCX	I	178	17,7	-	0/9/10/12	-
7	KCX	i	178	17,7	-	2/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	178	KCX	OQ1-CX-NZ	-3.43	119.64	124.96
7	I	178	KCX	OQ1-CX-NZ	-3.19	120.02	124.96

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	i	178	KCX	N-CA-CB-CG
7	i	178	KCX	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	i	178	KCX	1	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 63 ligands modelled in this entry, 6 are monoatomic and 2 are modelled with single atom - leaving 55 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
13	SF4	H	405	6	0,12,12	-	-	-		
13	SF4	L	102	9	0,12,12	-	-	-		
13	SF4	G	506	11	0,12,12	-	-	-		
13	SF4	H	401	6	0,12,12	-	-	-		
13	SF4	A	703	1	0,12,12	-	-	-		
15	9S8	B	401	2	2,10,10	1.05	0	-		
13	SF4	h	407	6	0,12,12	-	-	-		
13	SF4	H	407	6	0,12,12	-	-	-		
13	SF4	A	702	1	0,12,12	-	-	-		
13	SF4	E	403	5	0,12,12	-	-	-		
13	SF4	h	402	6	0,12,12	-	-	-		
13	SF4	h	408	6	0,12,12	-	-	-		
13	SF4	H	409	6	0,12,12	-	-	-		
13	SF4	G	502	11	0,12,12	-	-	-		
13	SF4	G	504	11	0,12,12	-	-	-		
14	FAD	A	704	-	56,58,58	0.63	1 (1%)	81,89,89	0.80	2 (2%)
15	9S8	B	402	2	2,10,10	1.01	0	-		
13	SF4	h	403	6	0,12,12	-	-	-		
13	SF4	A	706	1	0,12,12	-	-	-		
13	SF4	H	403	6	0,12,12	-	-	-		
13	SF4	G	503	11	0,12,12	-	-	-		
13	SF4	G	508	11	0,12,12	-	-	-		
13	SF4	G	509	11	0,12,12	-	-	-		
13	SF4	h	404	6	0,12,12	-	-	-		
13	SF4	G	510	11	0,12,12	-	-	-		
13	SF4	G	507	11	0,12,12	-	-	-		
13	SF4	H	404	6	0,12,12	-	-	-		
18	MGD	J	502	19	45,52,52	0.98	1 (2%)	54,81,81	2.25	18 (33%)
18	MGD	j	503	19	45,52,52	1.00	1 (2%)	54,81,81	2.00	14 (25%)
13	SF4	G	505	11	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
13	SF4	G	501	11	0,12,12	-	-	-		
13	SF4	C	201	3	0,12,12	-	-	-		
13	SF4	l	102	9	0,12,12	-	-	-		
13	SF4	H	406	6	0,12,12	-	-	-		
13	SF4	j	501	8	0,12,12	-	-	-		
13	SF4	h	405	6	0,12,12	-	-	-		
13	SF4	A	701	1	0,12,12	-	-	-		
13	SF4	H	408	6	0,12,12	-	-	-		
13	SF4	A	705	1	0,12,12	-	-	-		
13	SF4	h	406	6	0,12,12	-	-	-		
13	SF4	A	707	1	0,12,12	-	-	-		
16	FES	D	201	4	0,4,4	-	-	-		
13	SF4	h	401	6	0,12,12	-	-	-		
22	NFU	F	501	12	2,7,7	0.28	0	-		
13	SF4	E	401	5	0,12,12	-	-	-		
13	SF4	H	402	6	0,12,12	-	-	-		
18	MGD	j	502	19	45,52,52	0.97	1 (2%)	54,81,81	2.34	17 (31%)
13	SF4	G	511	11	0,12,12	-	-	-		
13	SF4	E	402	5	0,12,12	-	-	-		
18	MGD	J	503	19	45,52,52	1.01	3 (6%)	54,81,81	1.98	13 (24%)
13	SF4	L	101	9	0,12,12	-	-	-		
13	SF4	J	501	8	0,12,12	-	-	-		
13	SF4	l	101	9	0,12,12	-	-	-		
21	F3S	G	512	11	0,9,9	-	-	-		
13	SF4	C	202	3	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
13	SF4	H	405	6	-	-	0/6/5/5
13	SF4	L	102	9	-	-	0/6/5/5
13	SF4	G	506	11	-	-	0/6/5/5
13	SF4	H	401	6	-	-	0/6/5/5
13	SF4	A	703	1	-	-	0/6/5/5
15	9S8	B	401	2	-	-	0/3/3/3
13	SF4	h	407	6	-	-	0/6/5/5
13	SF4	H	407	6	-	-	0/6/5/5
13	SF4	A	702	1	-	-	0/6/5/5
13	SF4	E	403	5	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	h	402	6	-	-	0/6/5/5
13	SF4	h	408	6	-	-	0/6/5/5
13	SF4	H	409	6	-	-	0/6/5/5
13	SF4	G	502	11	-	-	0/6/5/5
13	SF4	G	504	11	-	-	0/6/5/5
14	FAD	A	704	-	-	2/34/50/50	0/6/6/6
15	9S8	B	402	2	-	-	0/3/3/3
13	SF4	h	403	6	-	-	0/6/5/5
13	SF4	A	706	1	-	-	0/6/5/5
13	SF4	H	403	6	-	-	0/6/5/5
13	SF4	G	503	11	-	-	0/6/5/5
13	SF4	G	508	11	-	-	0/6/5/5
13	SF4	G	509	11	-	-	0/6/5/5
13	SF4	h	404	6	-	-	0/6/5/5
13	SF4	G	510	11	-	-	0/6/5/5
13	SF4	G	507	11	-	-	0/6/5/5
18	MGD	J	502	19	-	5/22/66/66	0/6/6/6
18	MGD	j	503	19	-	10/22/66/66	0/6/6/6
13	SF4	H	404	6	-	-	0/6/5/5
13	SF4	G	505	11	-	-	0/6/5/5
13	SF4	G	501	11	-	-	0/6/5/5
13	SF4	C	201	3	-	-	0/6/5/5
13	SF4	l	102	9	-	-	0/6/5/5
13	SF4	H	406	6	-	-	0/6/5/5
13	SF4	j	501	8	-	-	0/6/5/5
13	SF4	h	405	6	-	-	0/6/5/5
13	SF4	A	701	1	-	-	0/6/5/5
13	SF4	H	408	6	-	-	0/6/5/5
13	SF4	A	705	1	-	-	0/6/5/5
13	SF4	h	406	6	-	-	0/6/5/5
13	SF4	A	707	1	-	-	0/6/5/5
16	FES	D	201	4	-	-	0/1/1/1
13	SF4	h	401	6	-	-	0/6/5/5
13	SF4	E	401	5	-	-	0/6/5/5
13	SF4	H	402	6	-	-	0/6/5/5
18	MGD	j	502	19	-	4/22/66/66	0/6/6/6
13	SF4	G	511	11	-	-	0/6/5/5
18	MGD	J	503	19	-	6/22/66/66	0/6/6/6
13	SF4	E	402	5	-	-	0/6/5/5
13	SF4	L	101	9	-	-	0/6/5/5
13	SF4	J	501	8	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	SF4	l	101	9	-	-	0/6/5/5
21	F3S	G	512	11	-	-	0/3/3/3
13	SF4	C	202	3	-	-	0/6/5/5

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	503	MGD	C21-N22	3.27	1.39	1.35
18	j	503	MGD	C21-N22	3.11	1.38	1.35
18	J	502	MGD	C21-N22	2.84	1.38	1.35
18	j	502	MGD	C21-N22	2.72	1.38	1.35
14	A	704	FAD	C10-N10	2.12	1.42	1.37
18	J	503	MGD	C17-N18	-2.02	1.35	1.38
18	J	503	MGD	C6-N1	-2.02	1.35	1.38

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	j	502	MGD	O11-C23-N22	-8.53	99.80	108.57
18	J	502	MGD	O11-C23-N22	-7.69	100.67	108.57
18	J	503	MGD	PA-O3B-PB	-6.69	109.86	132.83
18	j	503	MGD	PA-O3B-PB	-6.53	110.40	132.83
18	j	502	MGD	PA-O3B-PB	-5.59	113.65	132.83
18	j	503	MGD	C5-C4-N3	-5.49	119.56	128.46
18	J	503	MGD	C5-C4-N3	-5.42	119.67	128.46
18	J	502	MGD	C5-C4-N3	-5.39	119.71	128.46
18	J	502	MGD	PA-O3B-PB	-5.35	114.47	132.83
18	j	502	MGD	C5-C4-N3	-5.21	120.01	128.46
18	J	502	MGD	C2-N3-C4	5.00	121.20	112.30
18	j	503	MGD	C2-N3-C4	4.97	121.16	112.30
18	j	502	MGD	C2-N3-C4	4.93	121.09	112.30
18	J	503	MGD	C2-N3-C4	4.88	121.00	112.30
18	j	503	MGD	C19-N20-C21	4.40	121.38	113.43
18	j	502	MGD	C19-N20-C21	4.32	121.23	113.43
18	J	502	MGD	C19-N20-C21	4.29	121.17	113.43
18	J	503	MGD	C19-N20-C21	4.23	121.06	113.43
18	j	503	MGD	N9-C4-N3	4.04	134.06	125.94
18	J	502	MGD	N9-C4-N3	4.02	134.01	125.94
18	J	503	MGD	N9-C4-N3	3.96	133.89	125.94
18	j	502	MGD	N9-C4-N3	3.67	133.31	125.94
14	A	704	FAD	C9-C9A-N10	3.02	125.91	121.84
18	j	502	MGD	C4'-O4'-C1'	-2.97	102.92	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	j	502	MGD	C8-N7-C5	2.92	109.52	104.24
18	J	502	MGD	O17-C17-C16	-2.88	120.64	127.24
18	J	502	MGD	C4'-O4'-C1'	-2.85	103.18	109.47
18	J	503	MGD	C8-N7-C5	2.83	109.36	104.24
18	j	502	MGD	C19-N18-C17	-2.81	119.97	125.10
18	j	503	MGD	C8-N7-C5	2.81	109.32	104.24
18	j	502	MGD	O17-C17-C16	-2.79	120.86	127.24
18	J	502	MGD	C8-N7-C5	2.76	109.24	104.24
18	J	502	MGD	C19-N18-C17	-2.74	120.11	125.10
18	j	503	MGD	C19-N18-C17	-2.73	120.12	125.10
18	j	503	MGD	O17-C17-C16	-2.70	121.05	127.24
18	J	503	MGD	C19-N18-C17	-2.67	120.22	125.10
18	J	503	MGD	O17-C17-C16	-2.67	121.13	127.24
18	j	503	MGD	C2-N1-C6	-2.66	120.24	125.10
18	J	503	MGD	C2-N1-C6	-2.63	120.31	125.10
18	j	502	MGD	O4'-C1'-C2'	-2.58	101.02	106.64
18	J	502	MGD	O4'-C1'-C2'	-2.56	101.05	106.64
18	J	502	MGD	C2-N1-C6	-2.52	120.50	125.10
18	j	502	MGD	C6-C5-N7	2.49	134.88	130.25
18	j	502	MGD	C2-N1-C6	-2.48	120.58	125.10
18	j	502	MGD	C4-C5-N7	-2.47	106.81	110.72
14	A	704	FAD	C4-N3-C2	-2.37	121.26	125.64
18	J	503	MGD	C4-C5-N7	-2.33	107.03	110.72
18	j	502	MGD	PB-O5'-C5'	-2.33	108.02	121.68
18	j	503	MGD	C4-C5-N7	-2.26	107.15	110.72
18	J	502	MGD	C4-C5-N7	-2.19	107.25	110.72
18	J	503	MGD	C6-C5-N7	2.16	134.27	130.25
18	J	502	MGD	C6-C5-N7	2.13	134.20	130.25
18	j	503	MGD	C16-C17-N18	2.12	118.64	112.31
18	j	502	MGD	C16-C17-N18	2.12	118.61	112.31
18	j	503	MGD	O6-C6-C5	-2.11	121.00	126.60
18	J	502	MGD	C16-C17-N18	2.11	118.58	112.31
18	j	503	MGD	C6-C5-N7	2.10	134.16	130.25
18	J	502	MGD	O6-C6-C5	-2.09	121.05	126.60
18	j	502	MGD	PA-O3A-C10	-2.06	109.57	121.68
18	J	503	MGD	O6-C6-C5	-2.06	121.14	126.60
18	J	503	MGD	C16-C17-N18	2.04	118.39	112.31
18	j	503	MGD	C5-C6-N1	2.03	118.36	113.19
18	J	502	MGD	C5-C6-N1	2.03	118.36	113.19
18	J	502	MGD	PB-O5'-C5'	-2.03	109.76	121.68

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	J	502	MGD	C10-O3A-PA-O3B
18	J	503	MGD	O3A-C10-C11-C12
18	j	503	MGD	C5'-O5'-PB-O2B
18	j	503	MGD	O3A-C10-C11-C12
18	j	503	MGD	O4'-C4'-C5'-O5'
18	j	503	MGD	C3'-C4'-C5'-O5'
18	j	503	MGD	O3A-C10-C11-O11
18	J	503	MGD	PA-O3B-PB-O5'
18	j	503	MGD	PA-O3B-PB-O5'
18	J	502	MGD	C10-O3A-PA-O1A
18	J	503	MGD	C5'-O5'-PB-O1B
18	j	503	MGD	C5'-O5'-PB-O1B
18	J	502	MGD	PB-O3B-PA-O2A
14	A	704	FAD	O4B-C4B-C5B-O5B
18	J	503	MGD	O4'-C4'-C5'-O5'
18	J	503	MGD	O3A-C10-C11-O11
18	j	502	MGD	O3A-C10-C11-O11
14	A	704	FAD	C2B-C1B-N9A-C8A
18	J	503	MGD	C5'-O5'-PB-O3B
18	j	503	MGD	C5'-O5'-PB-O3B
18	j	503	MGD	C10-O3A-PA-O3B
18	J	502	MGD	PB-O3B-PA-O1A
18	j	502	MGD	PA-O3B-PB-O2B
18	j	502	MGD	PB-O3B-PA-O1A
18	j	503	MGD	PA-O3B-PB-O2B
18	J	502	MGD	C10-O3A-PA-O2A
18	j	502	MGD	C10-O3A-PA-O1A

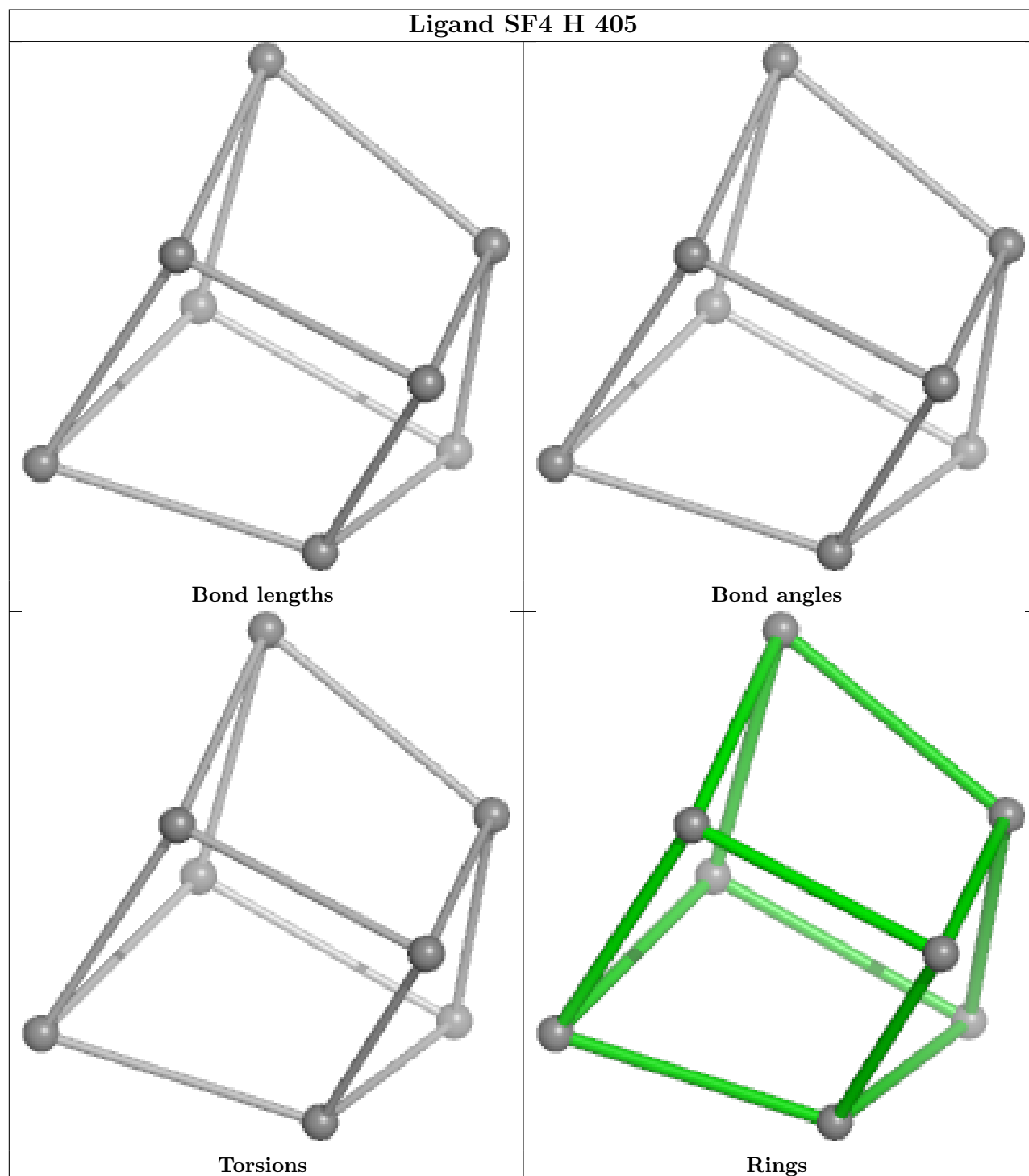
There are no ring outliers.

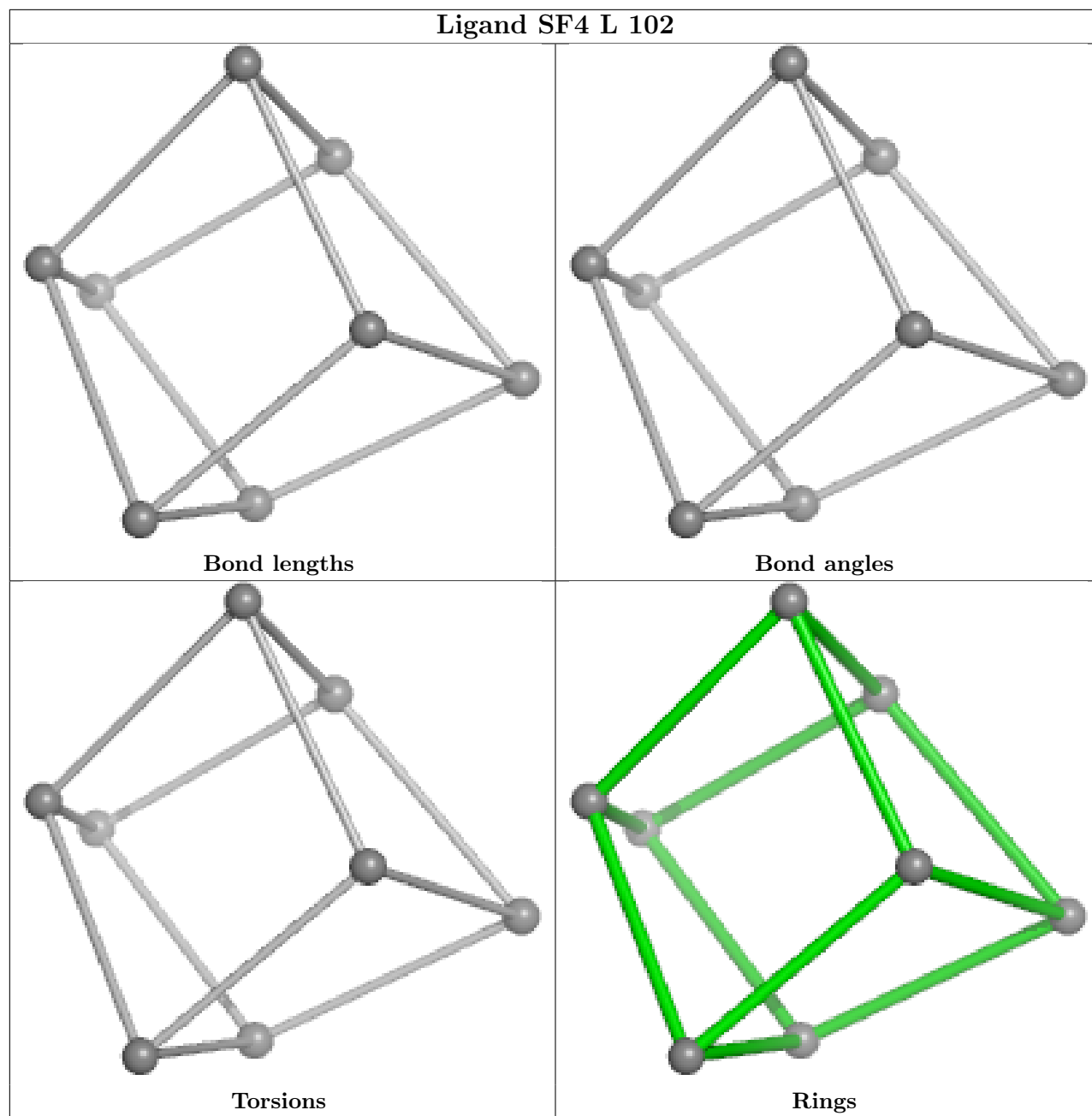
4 monomers are involved in 4 short contacts:

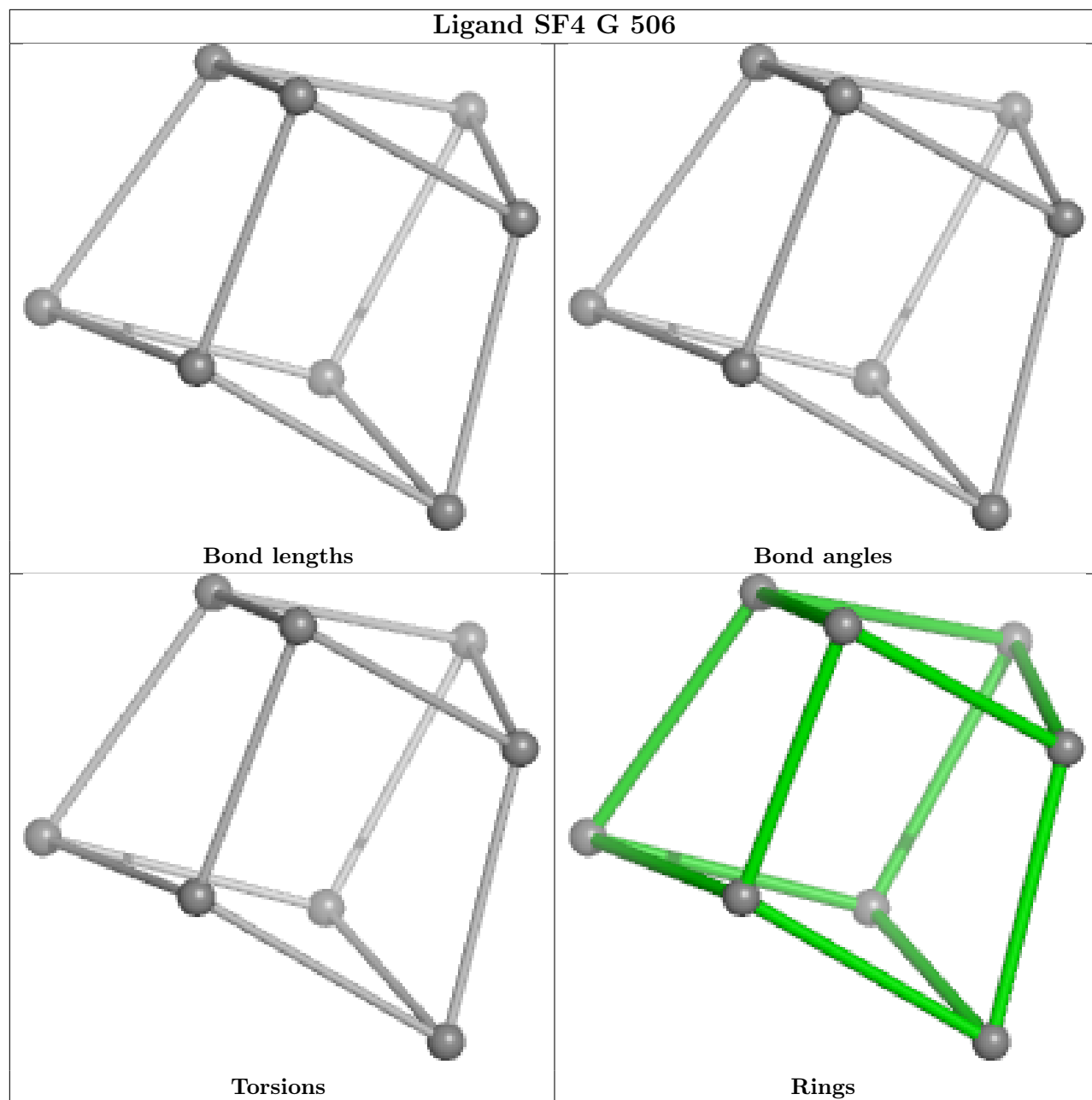
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	704	FAD	1	0
13	G	508	SF4	1	0
22	F	501	NFU	1	0
18	J	503	MGD	1	0

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

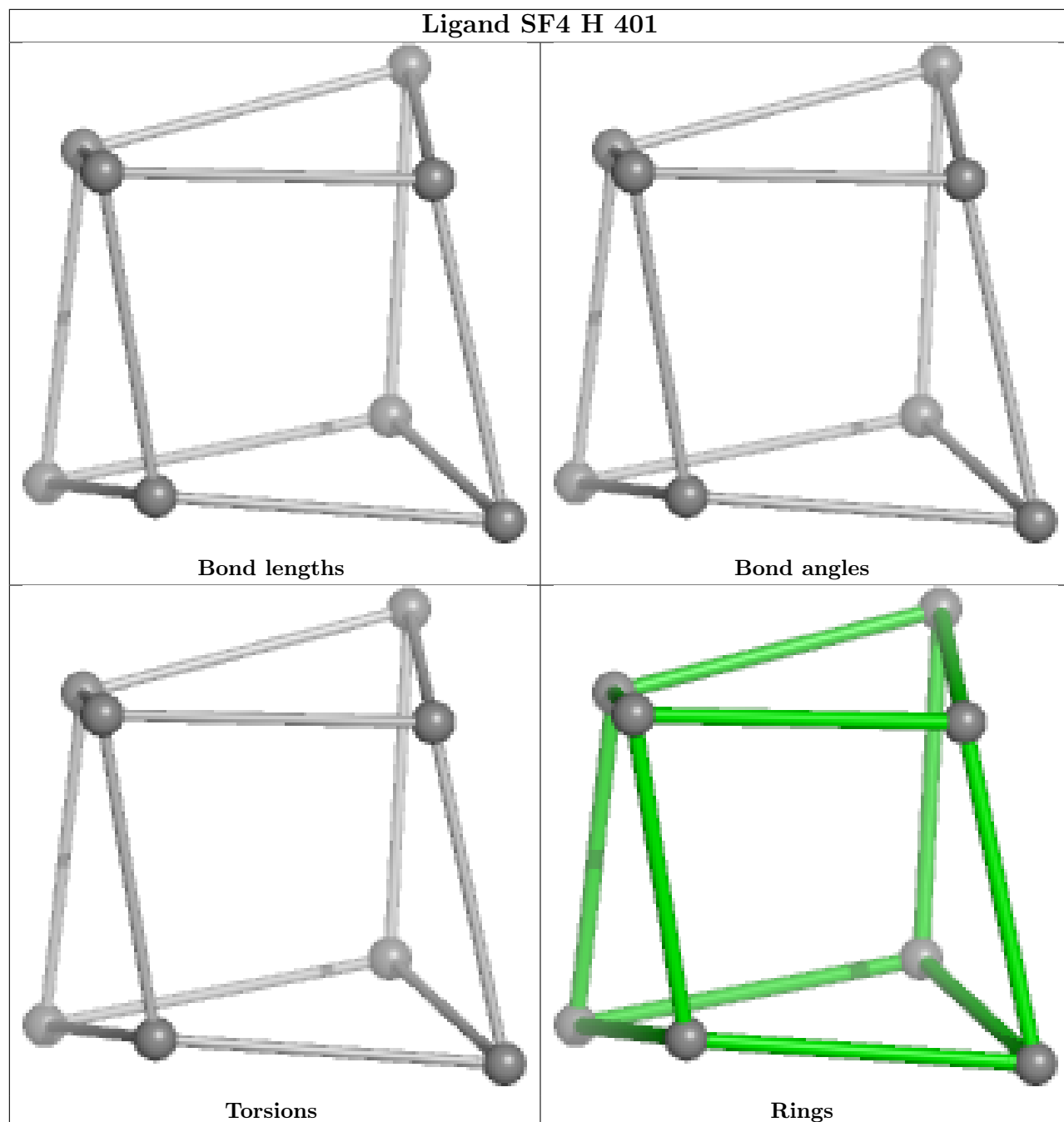
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.



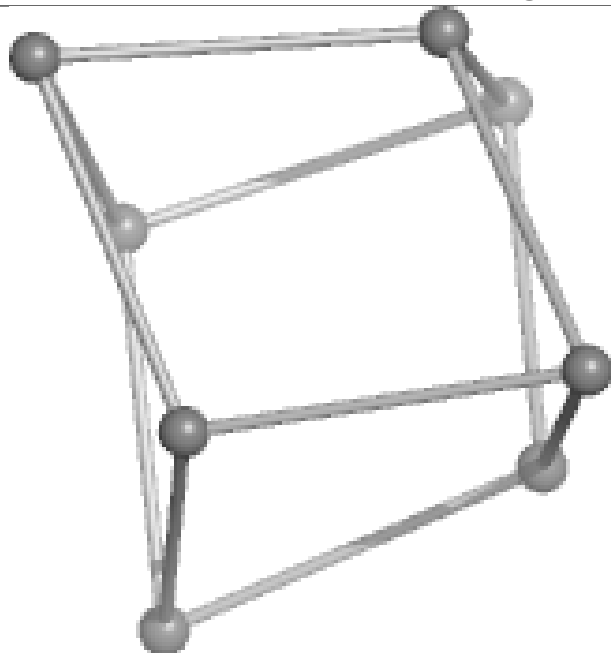




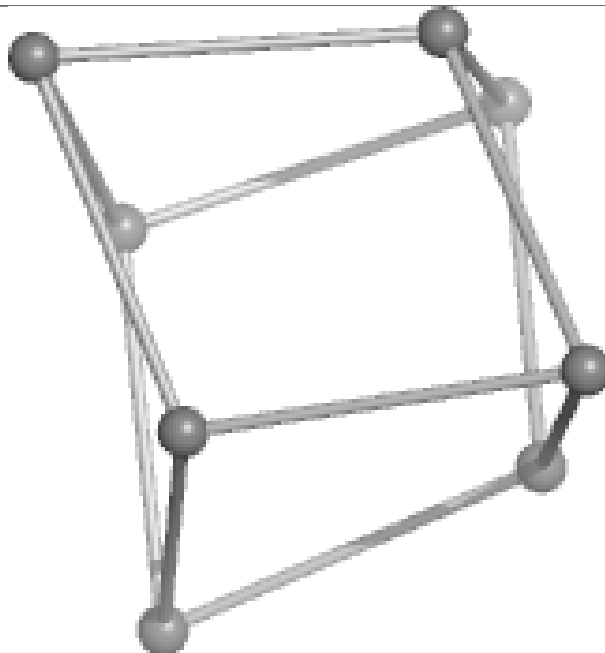
## Ligand SF4 H 401



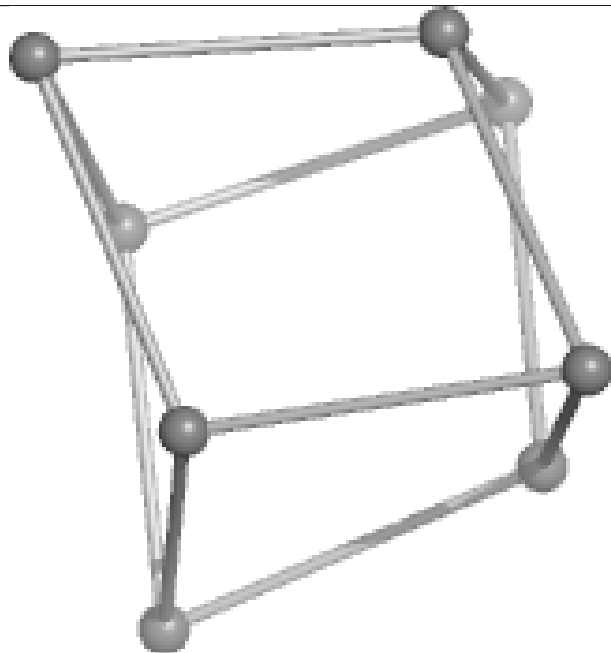
## Ligand SF4 A 703



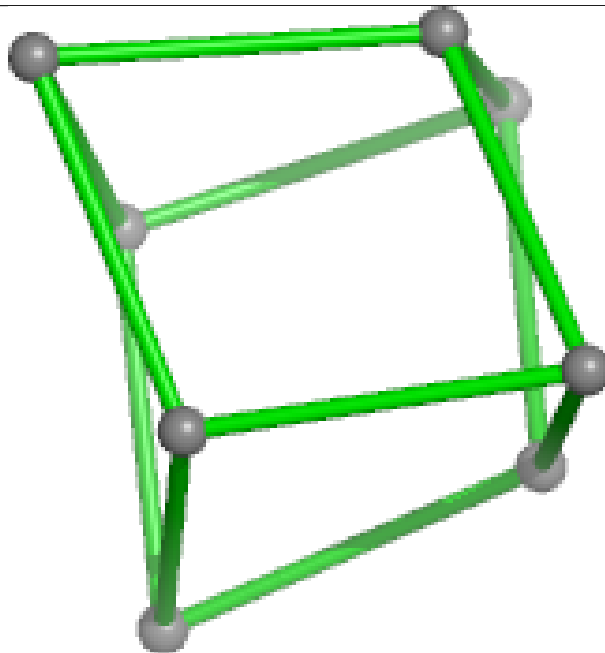
Bond lengths



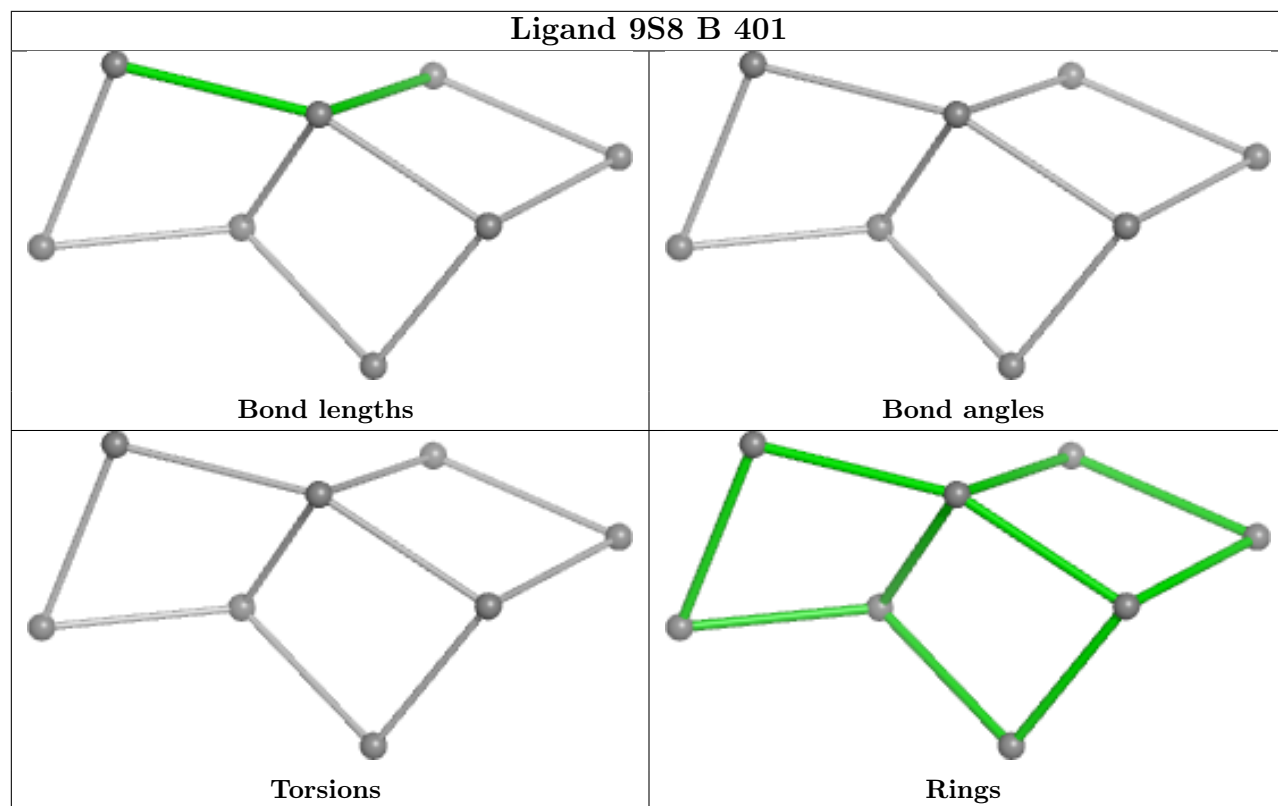
Bond angles



Torsions

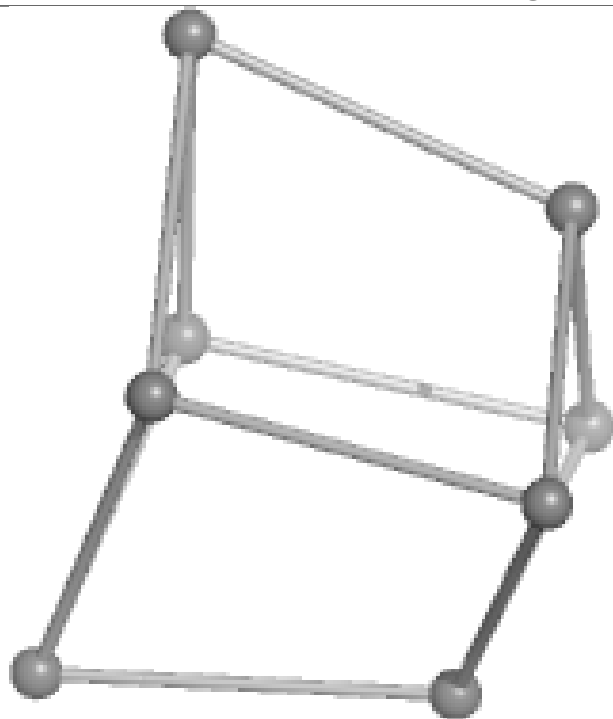


Rings

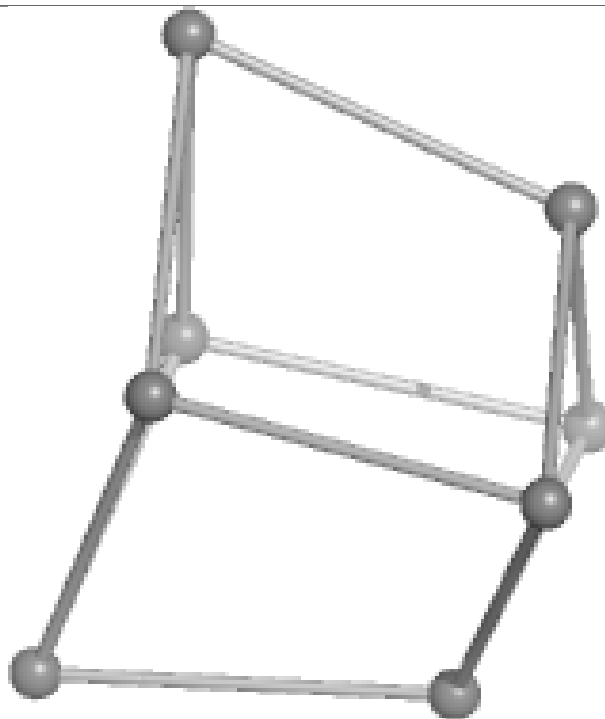




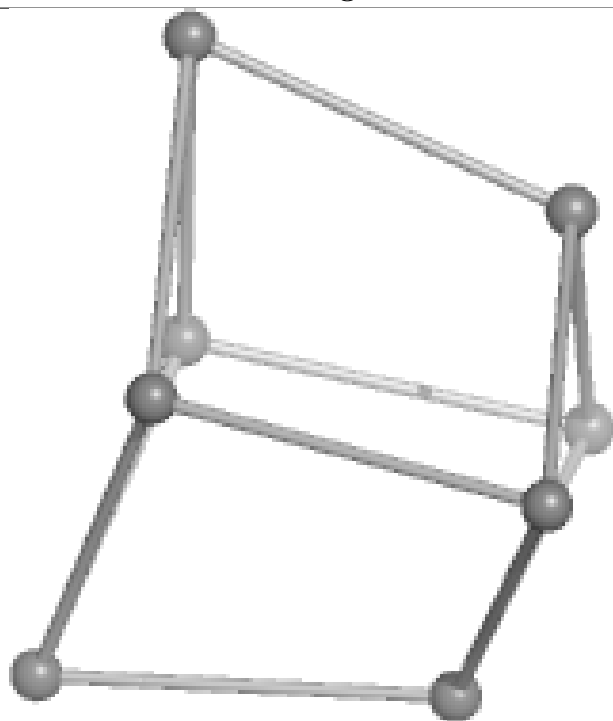
## Ligand SF4 h 407



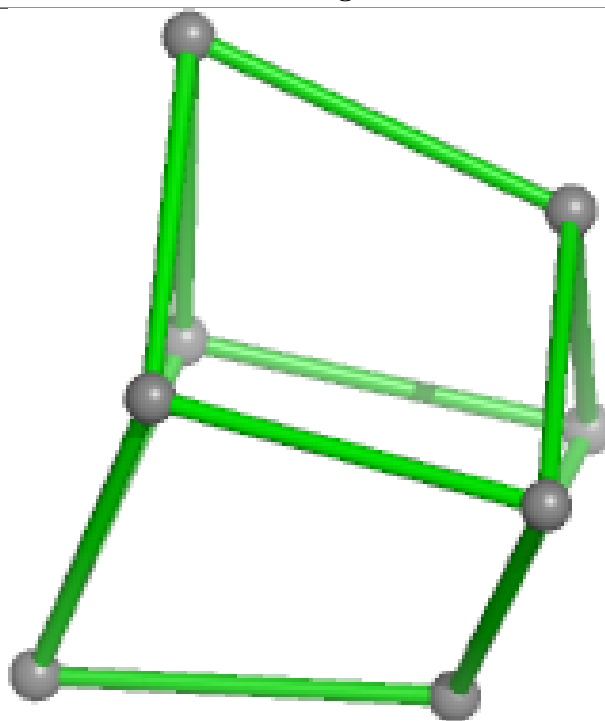
Bond lengths



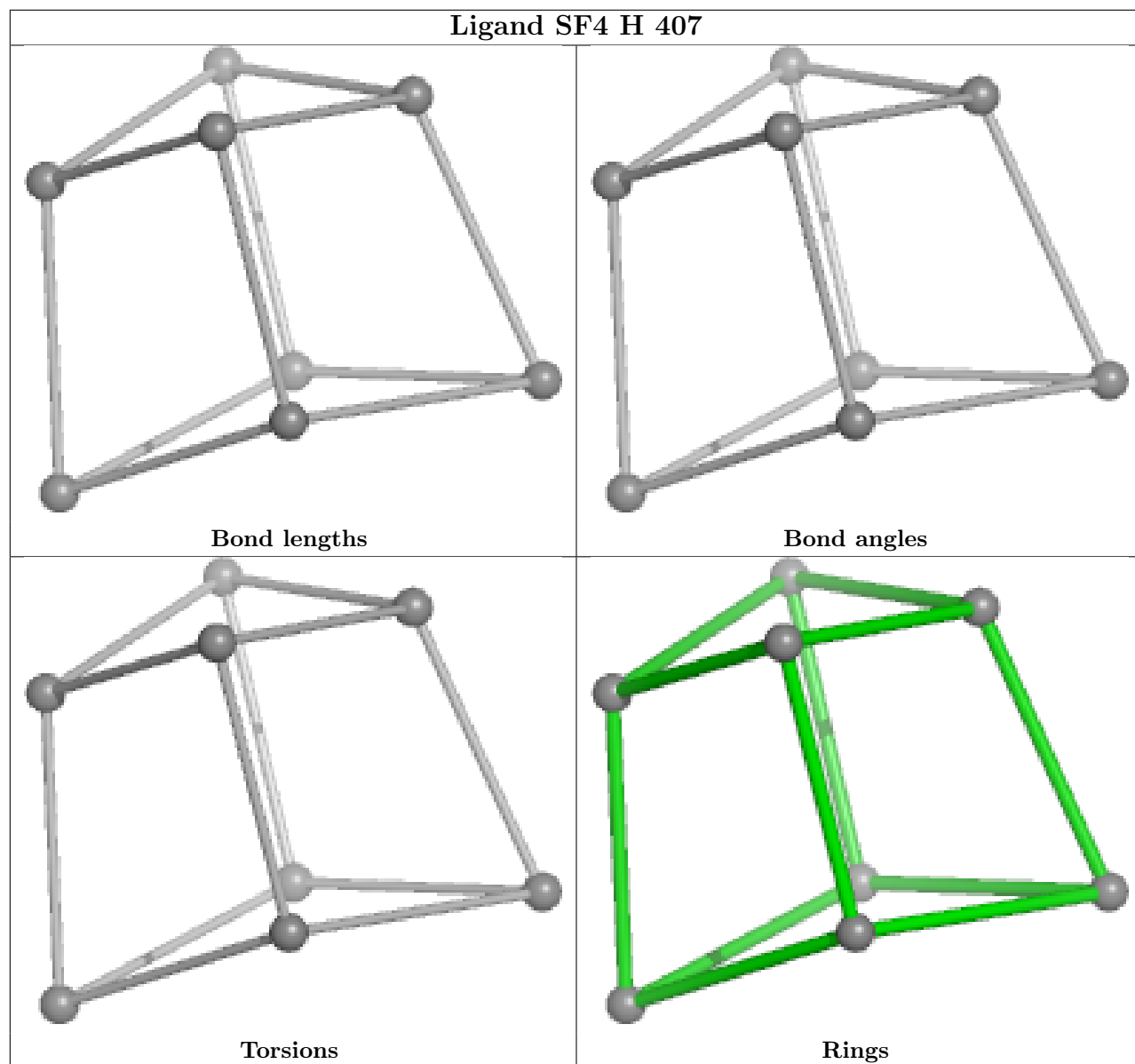
Bond angles

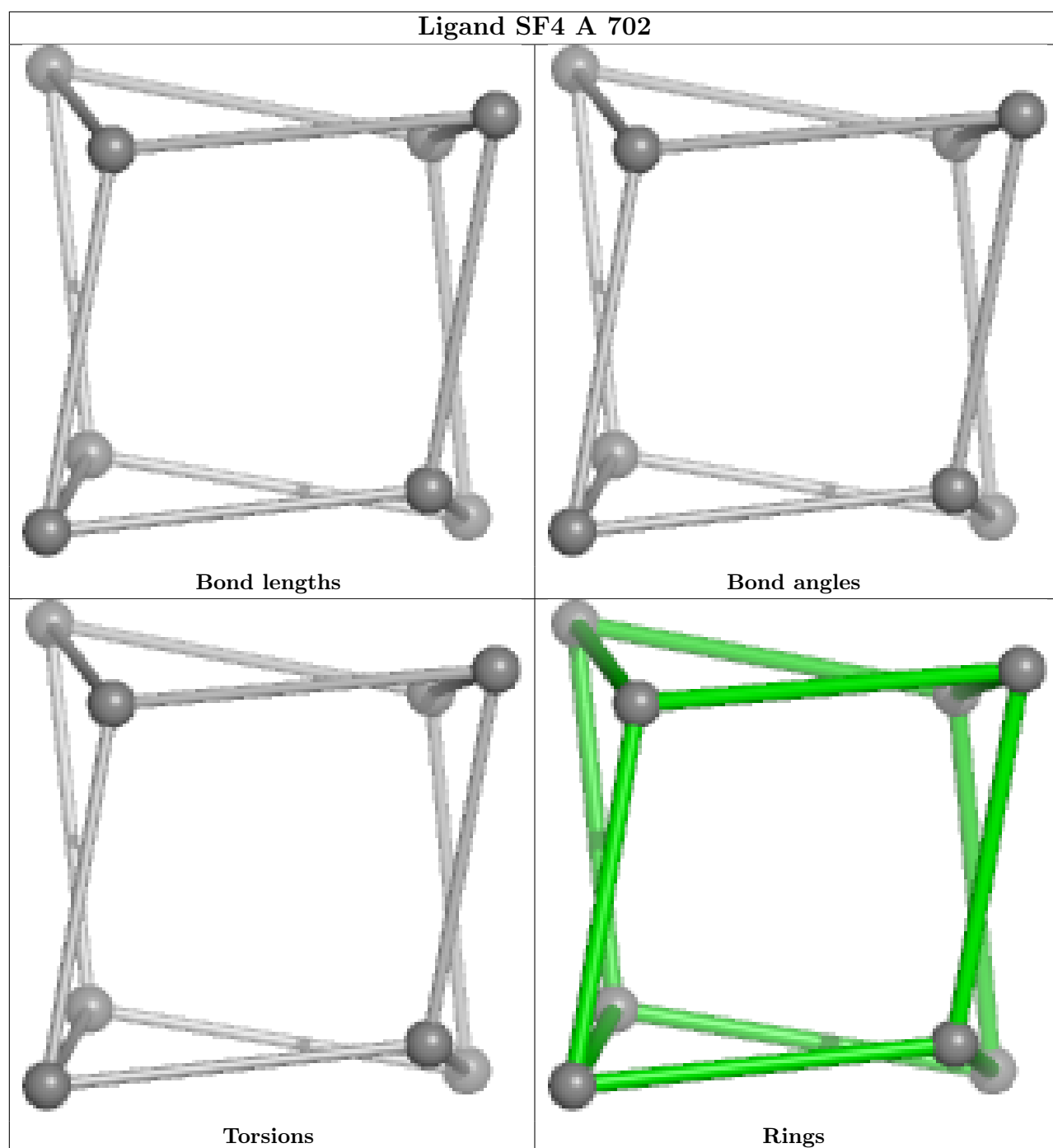


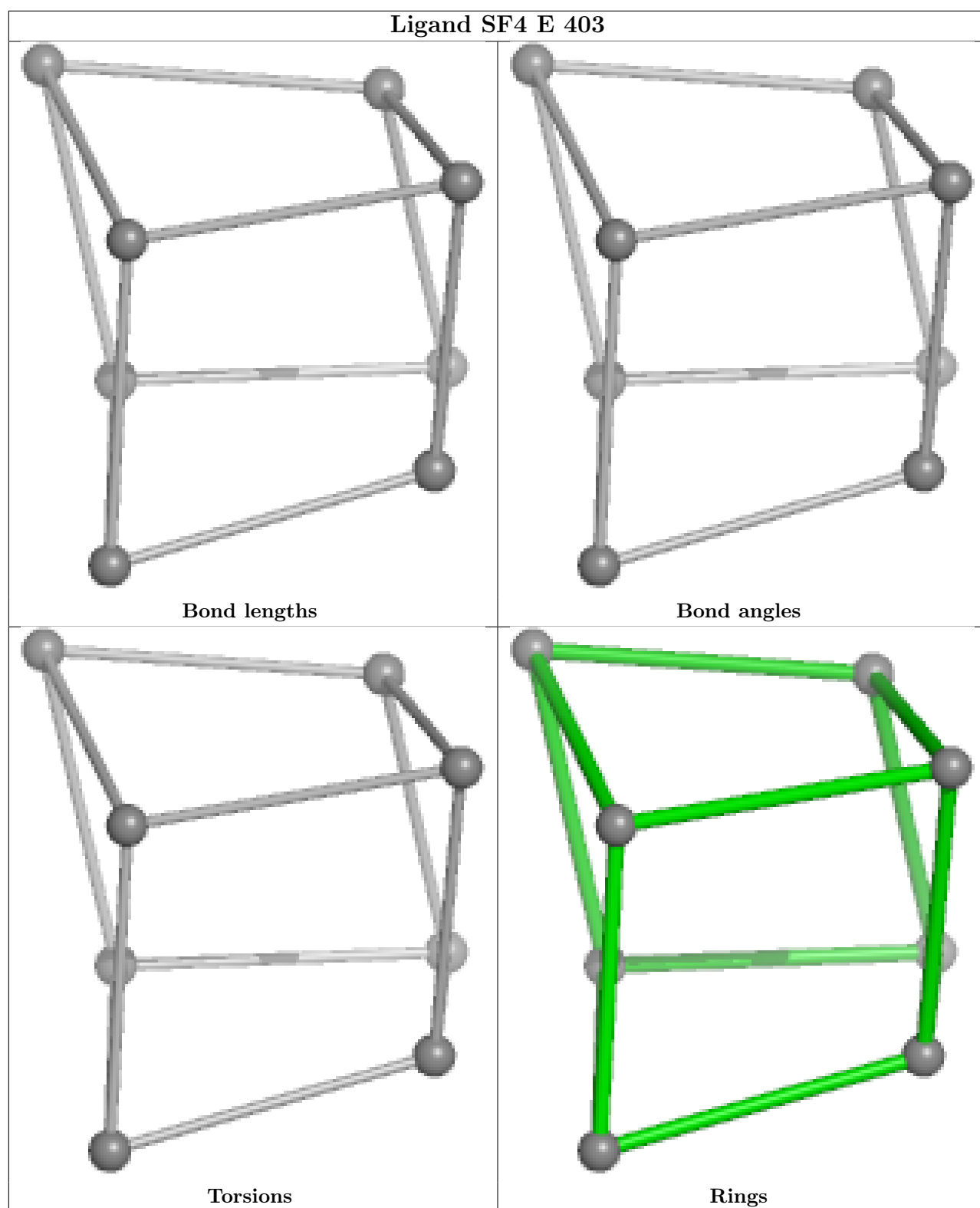
Torsions

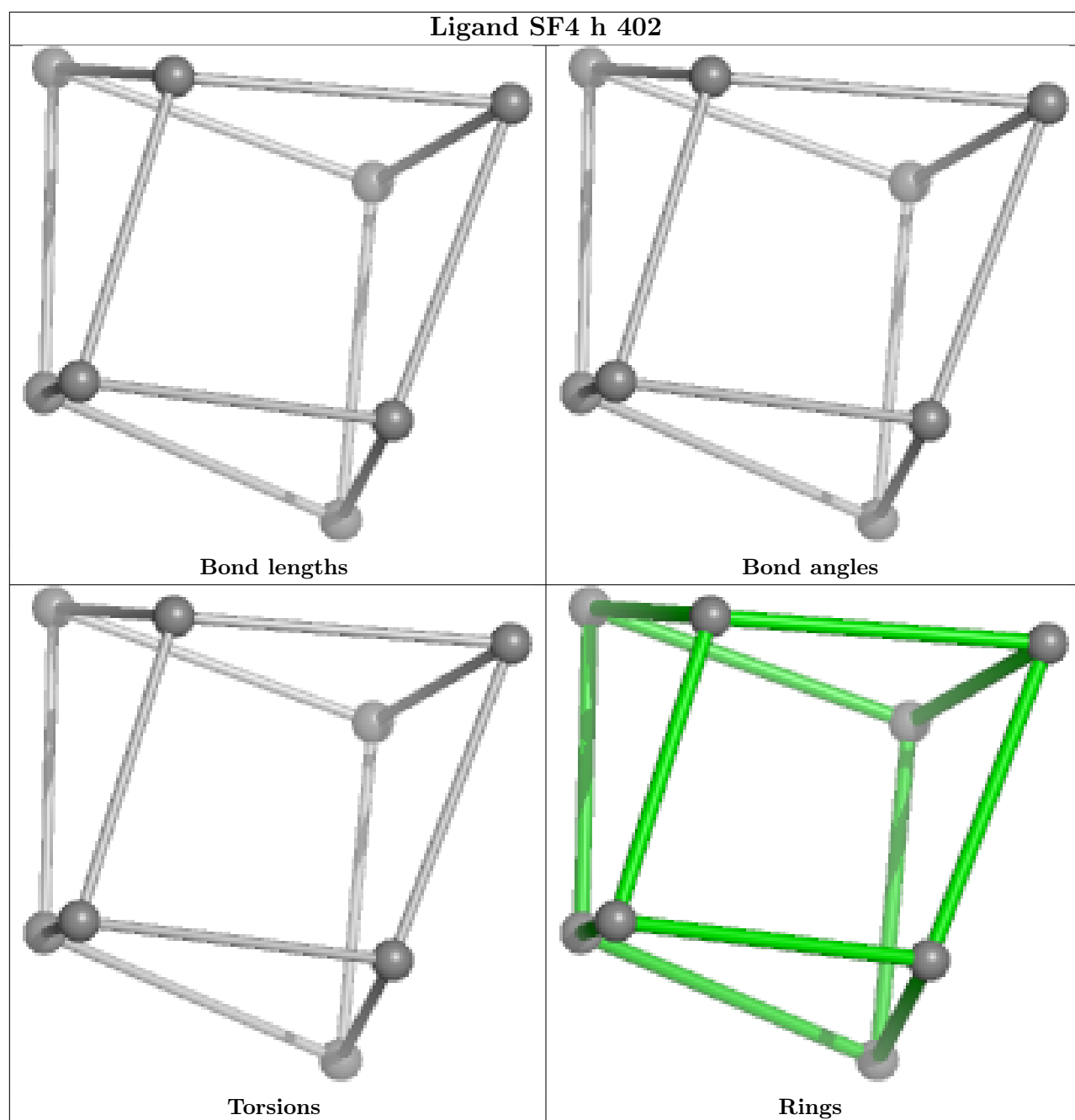


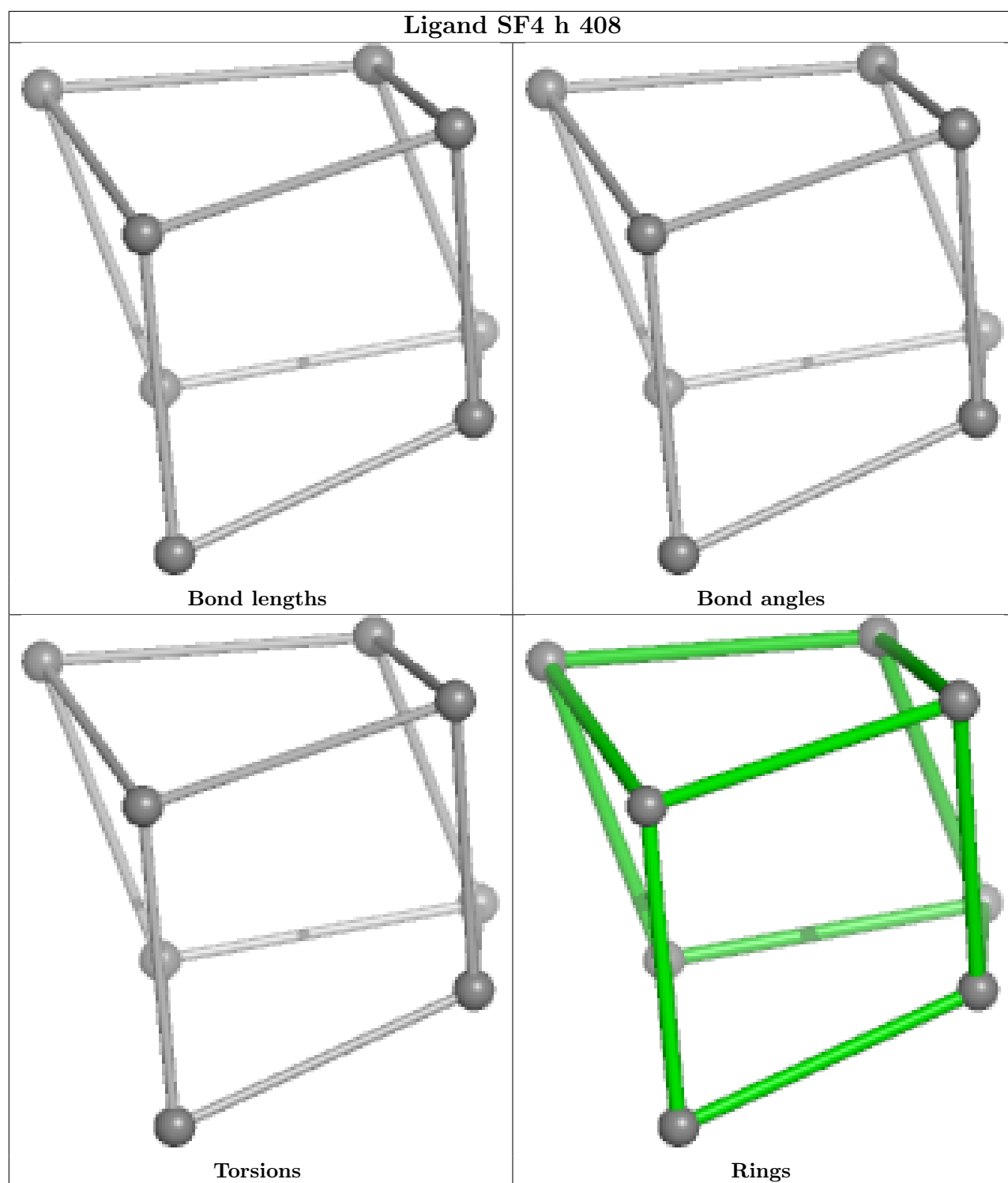
Rings



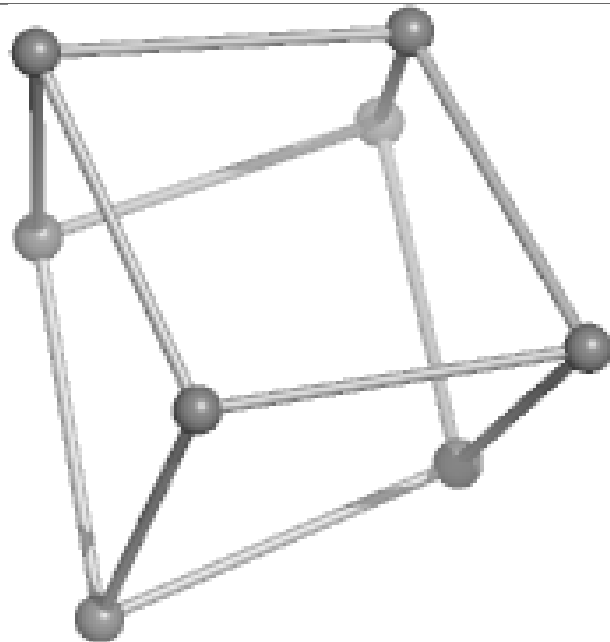




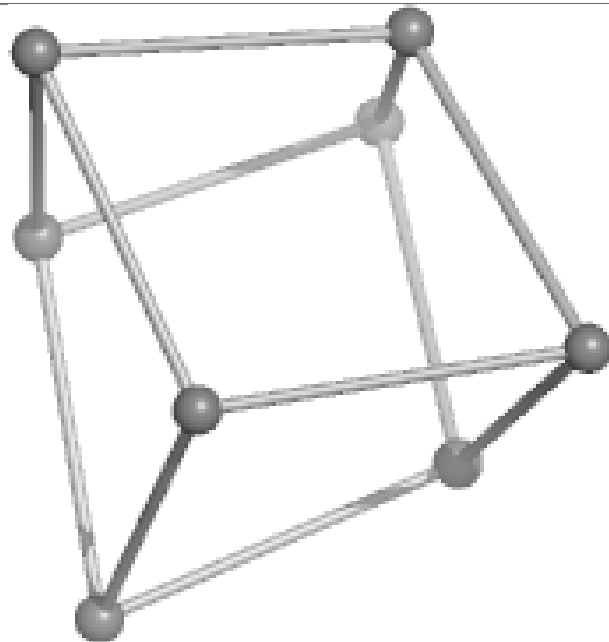




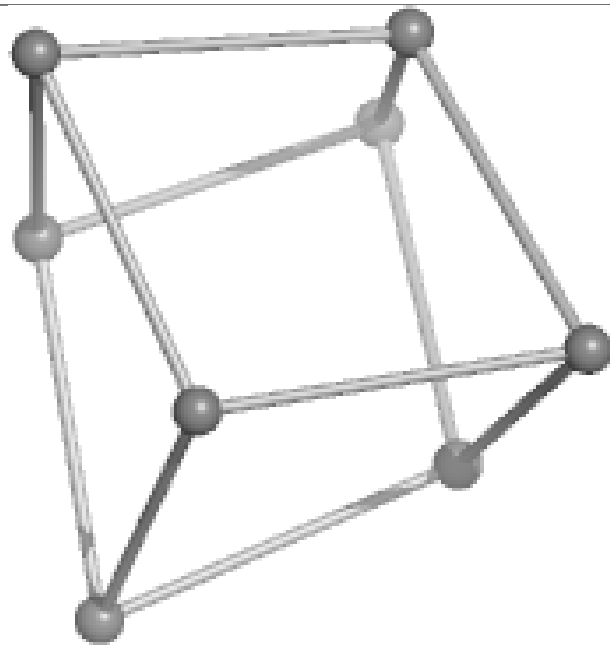
## Ligand SF4 H 409



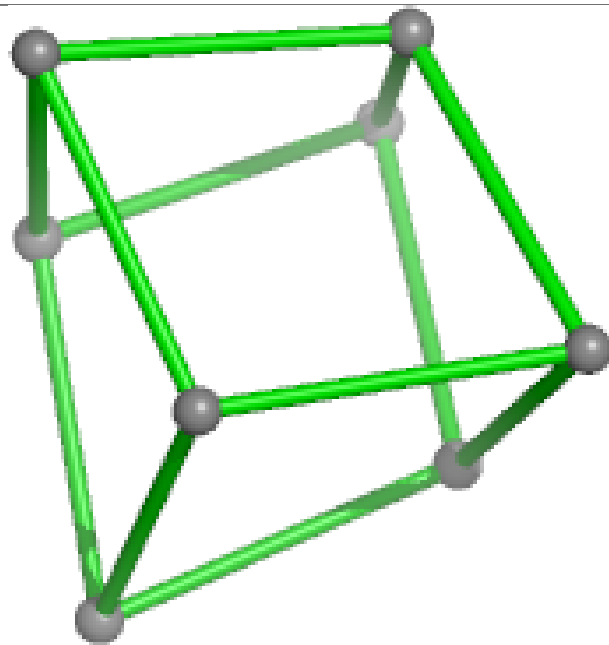
Bond lengths



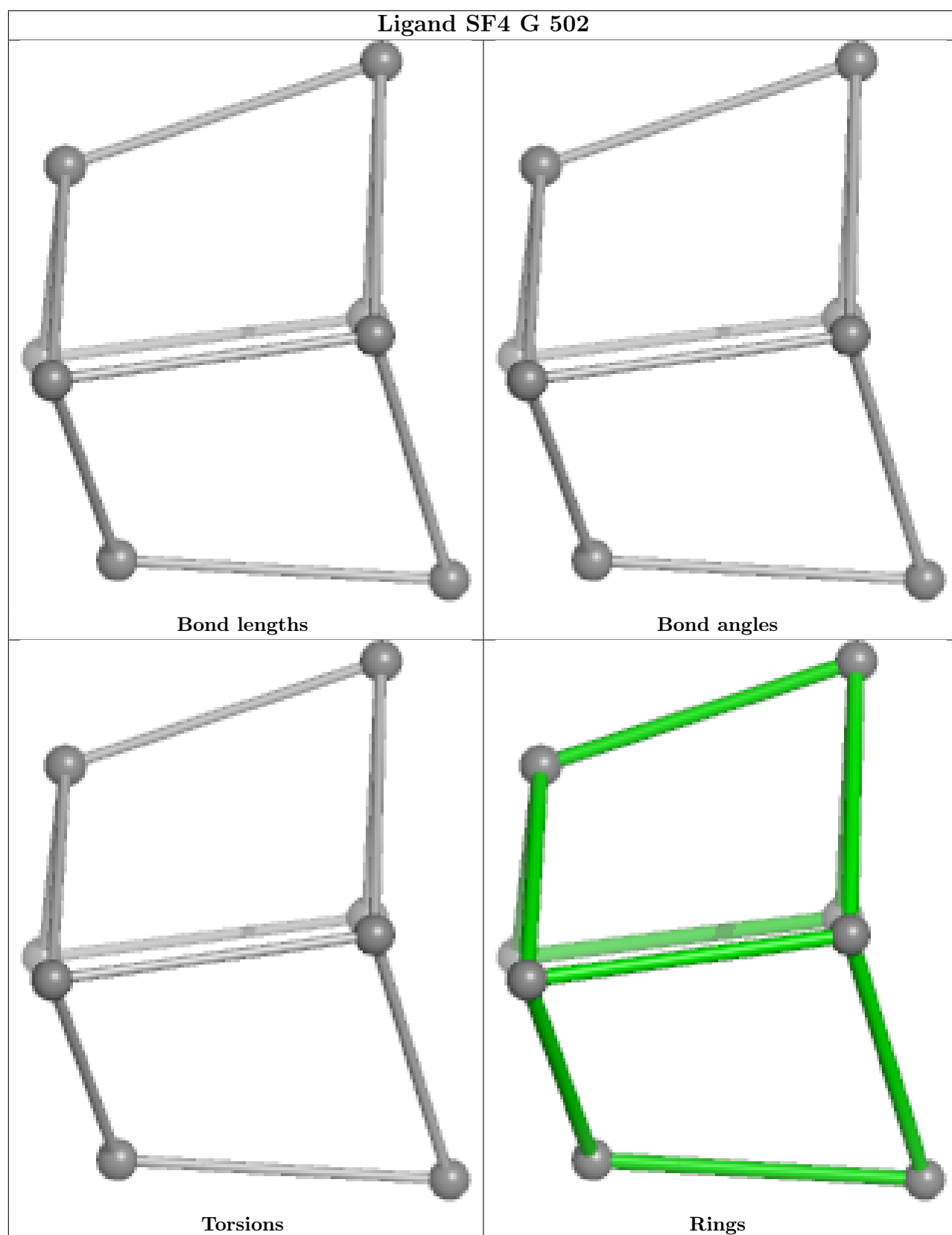
Bond angles



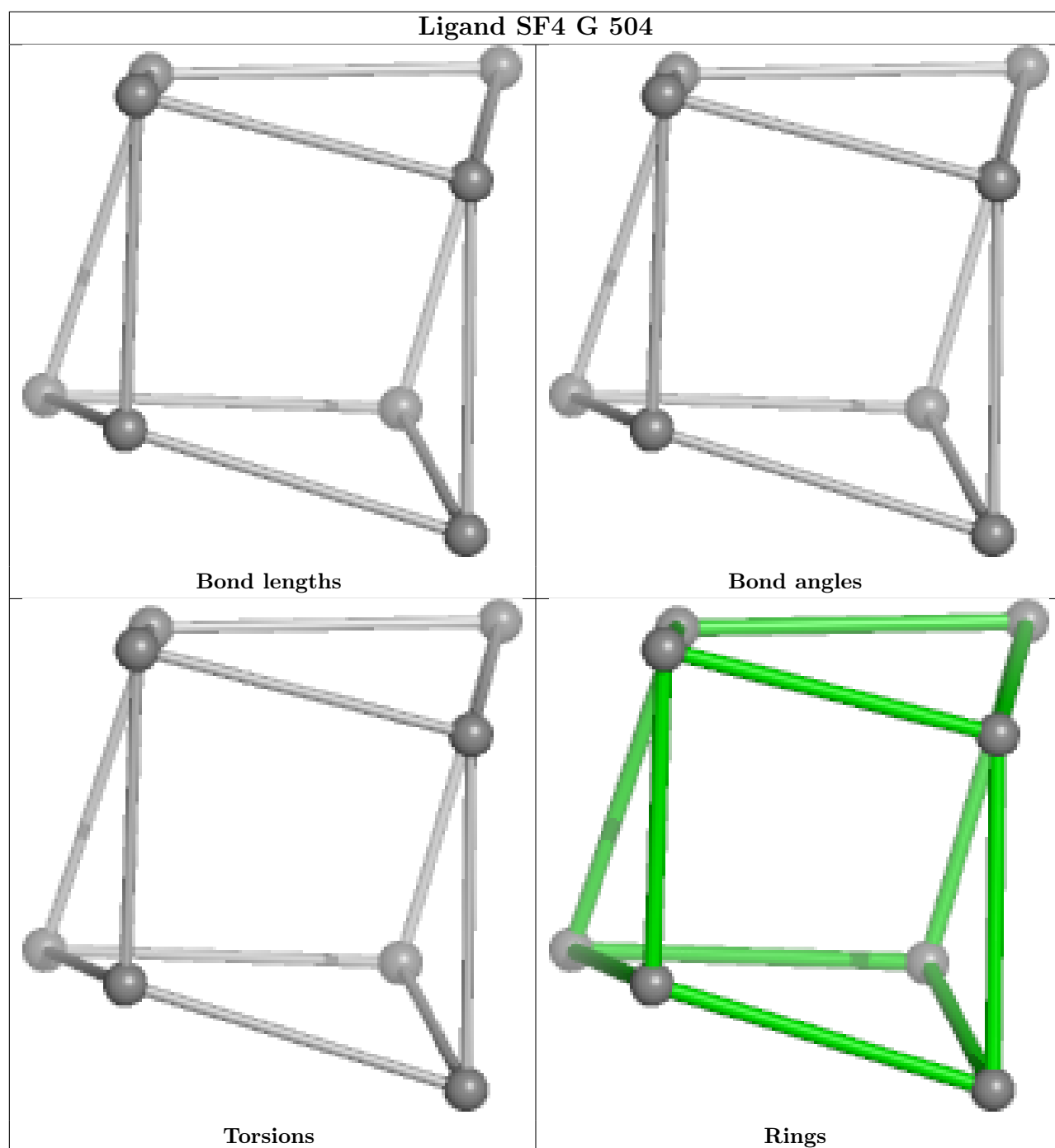
Torsions

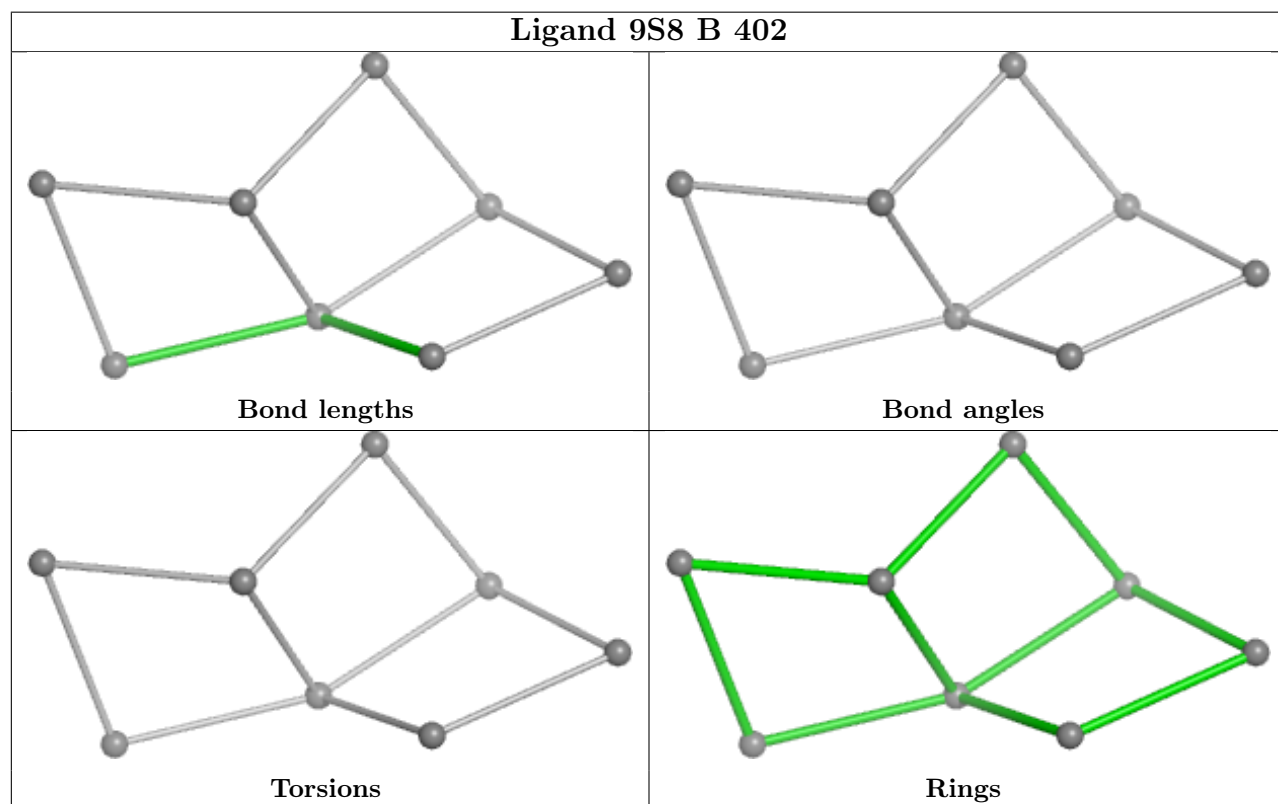
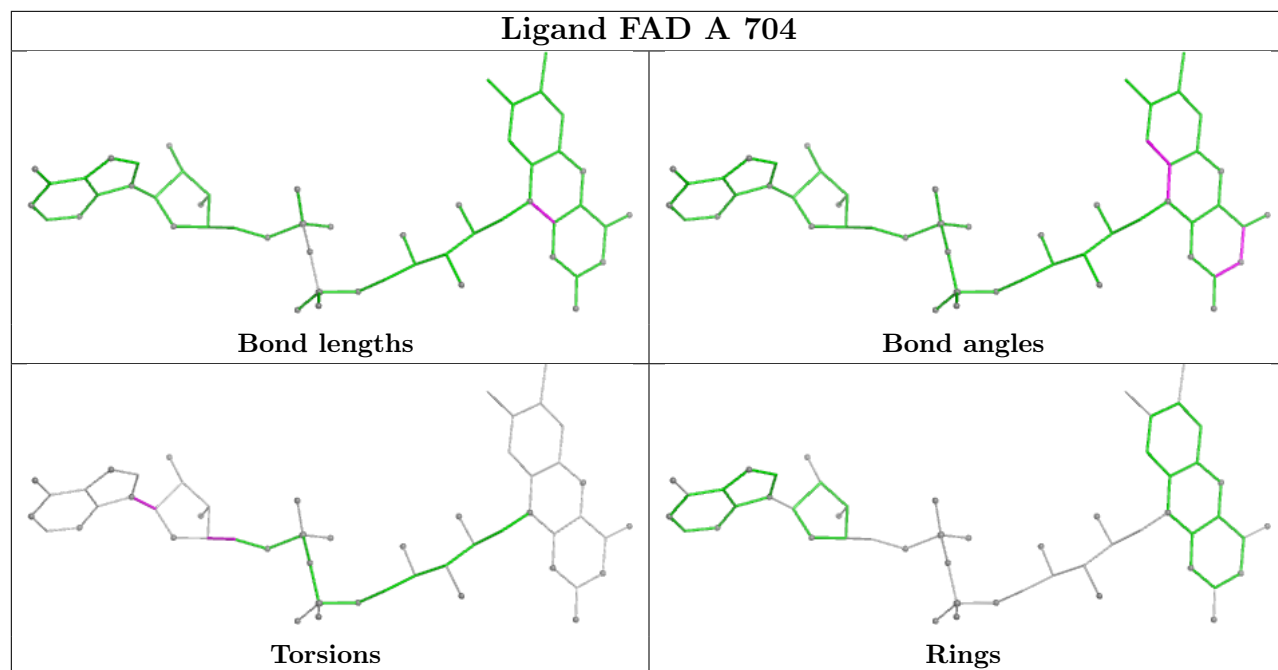


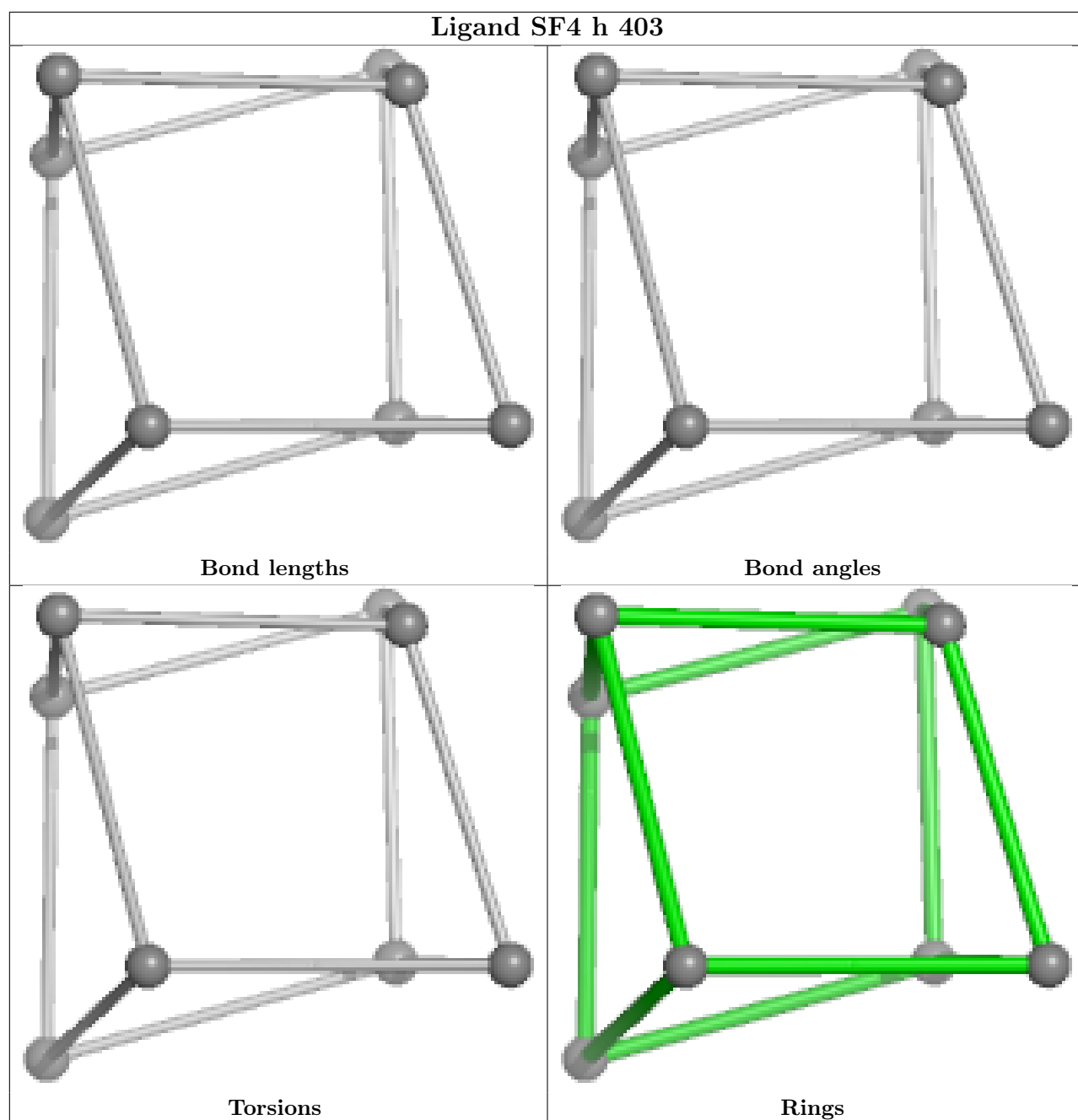
Rings



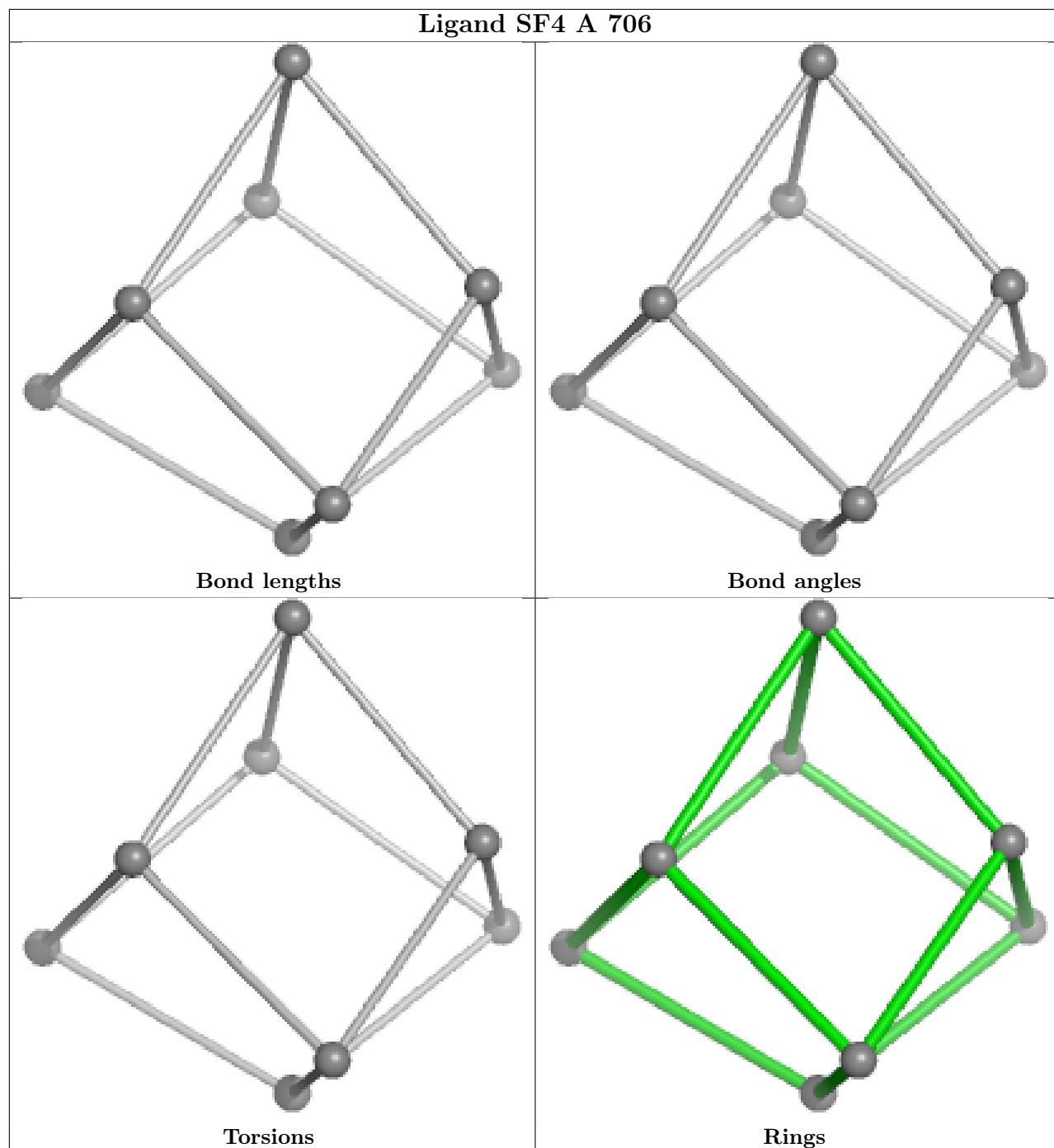




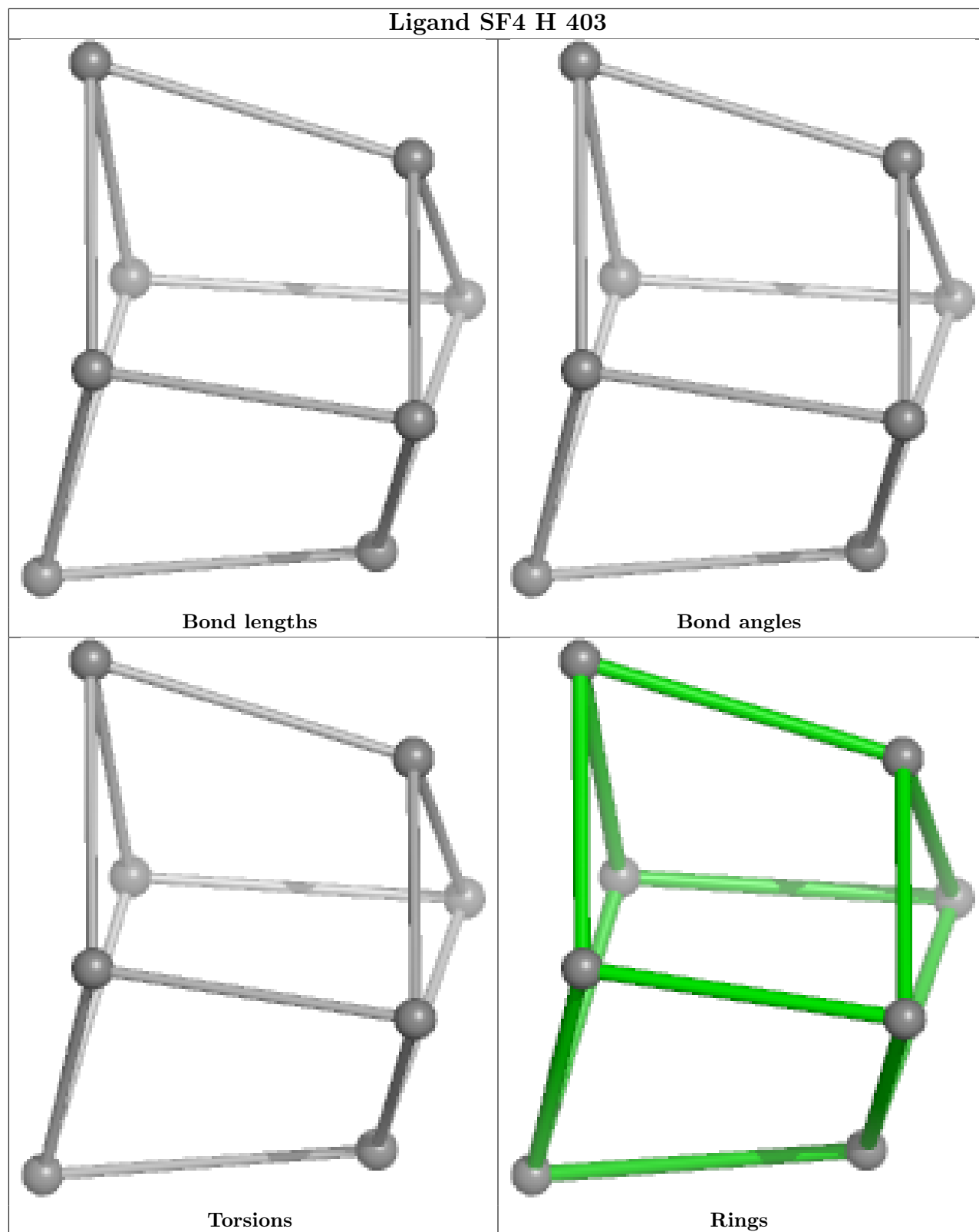


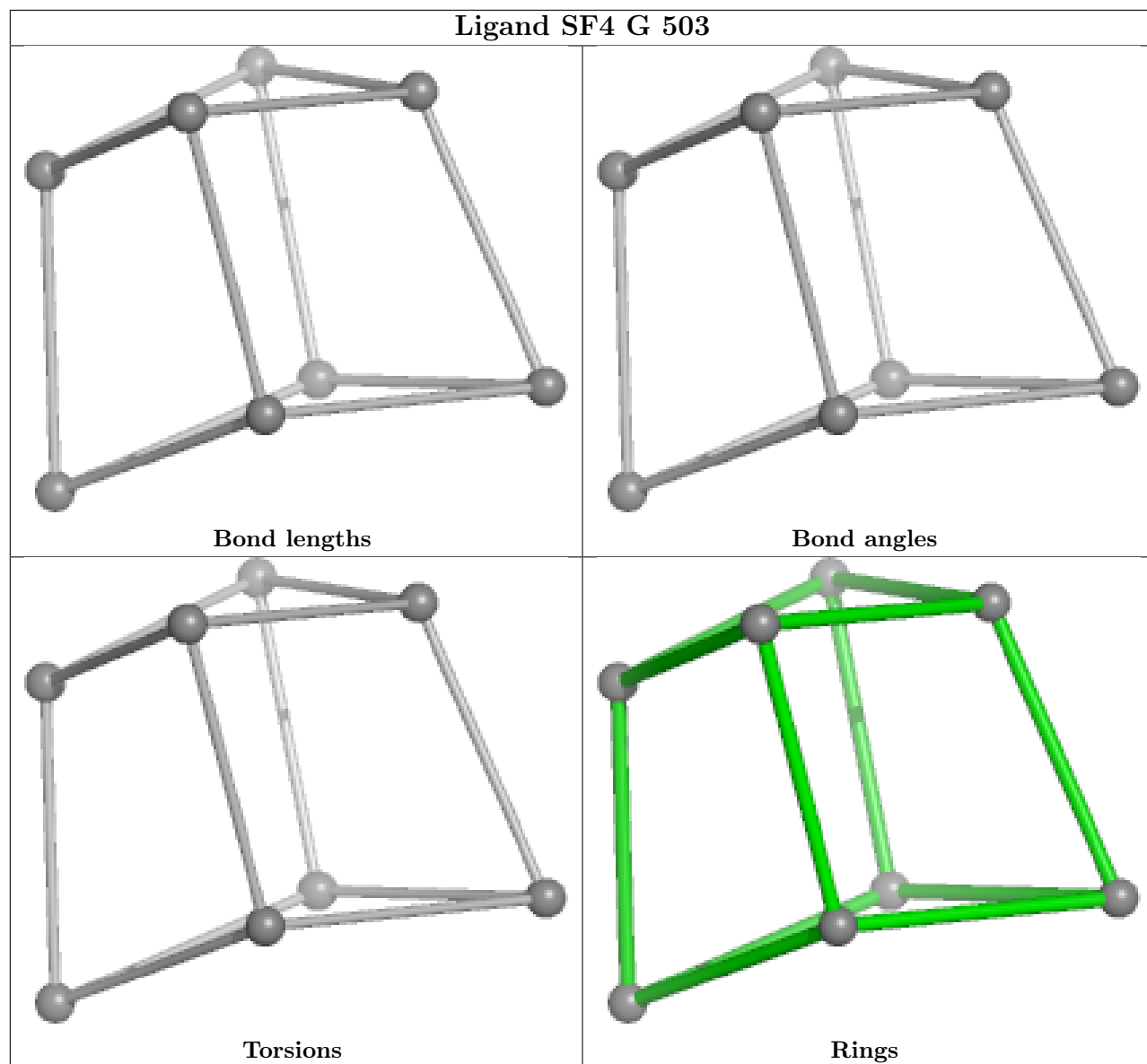


## Ligand SF4 A 706

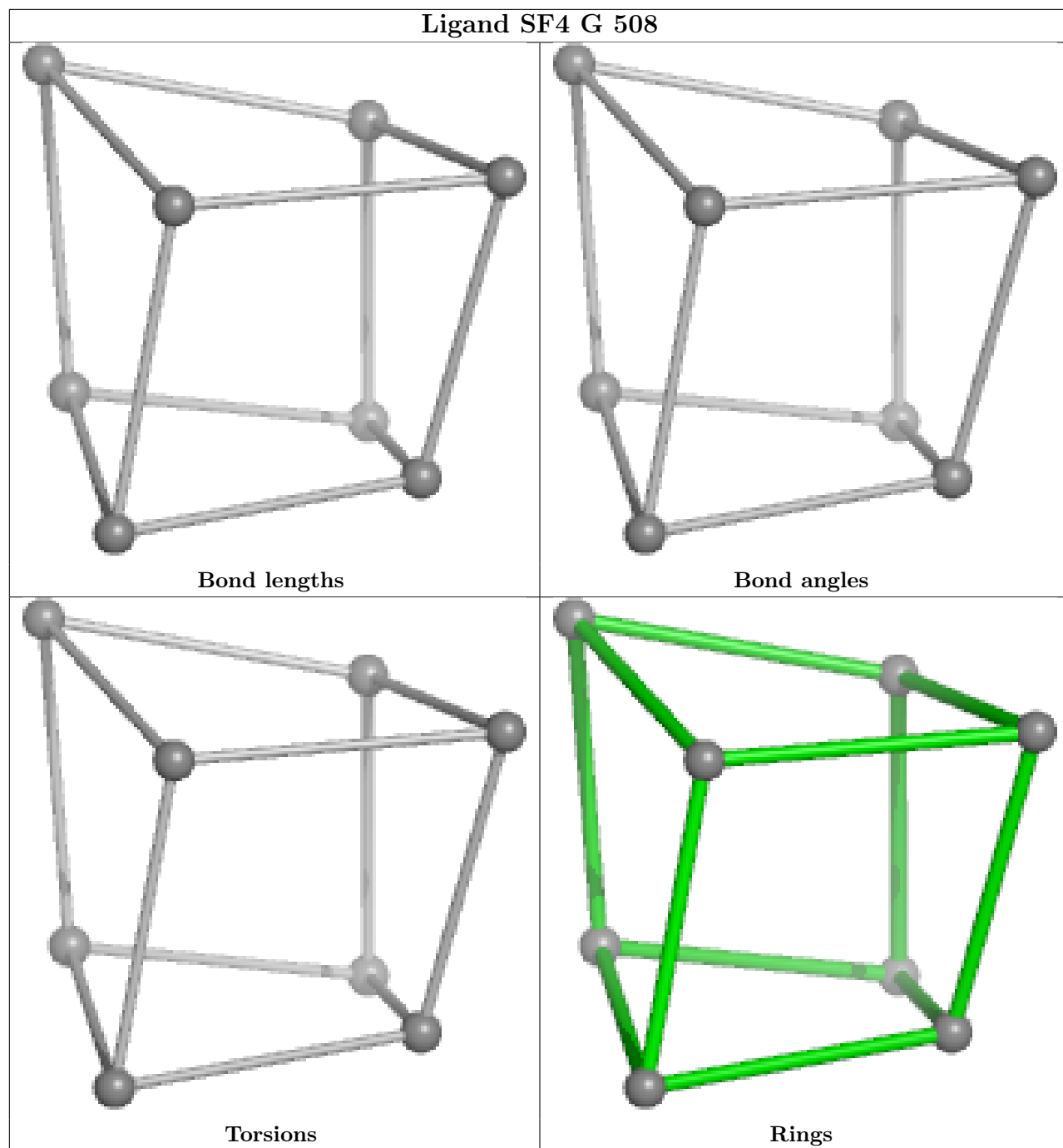


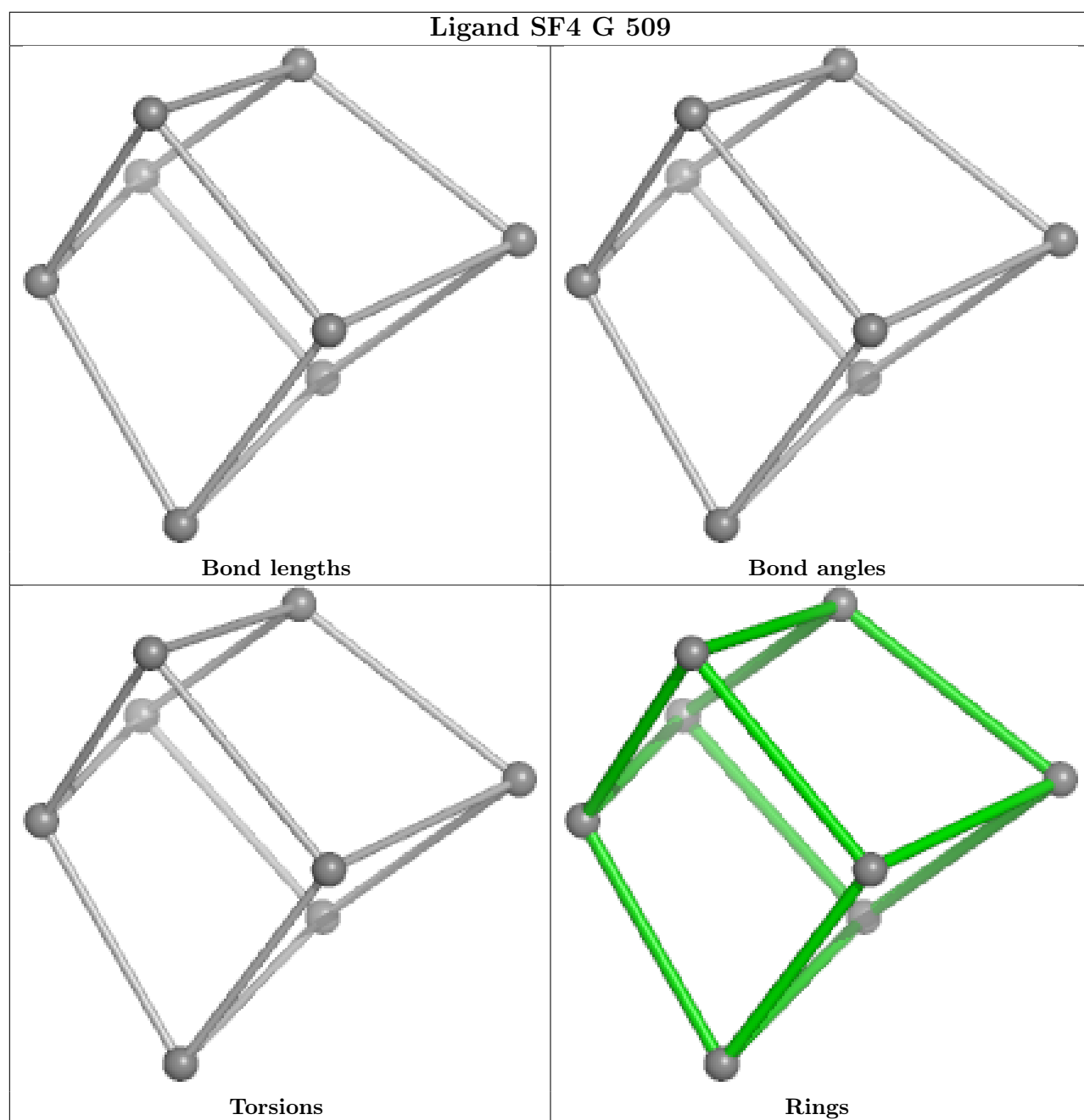
## Ligand SF4 H 403



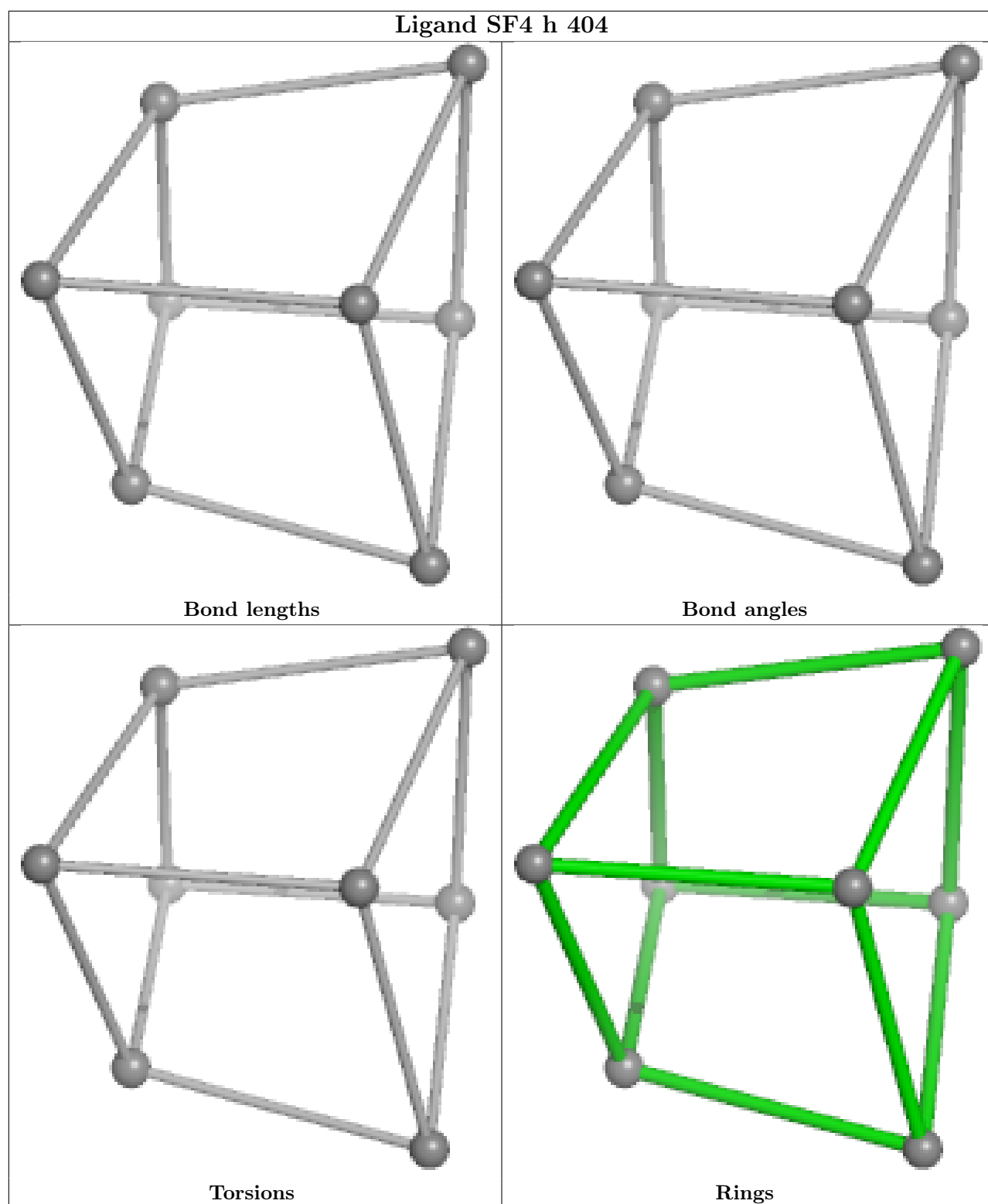


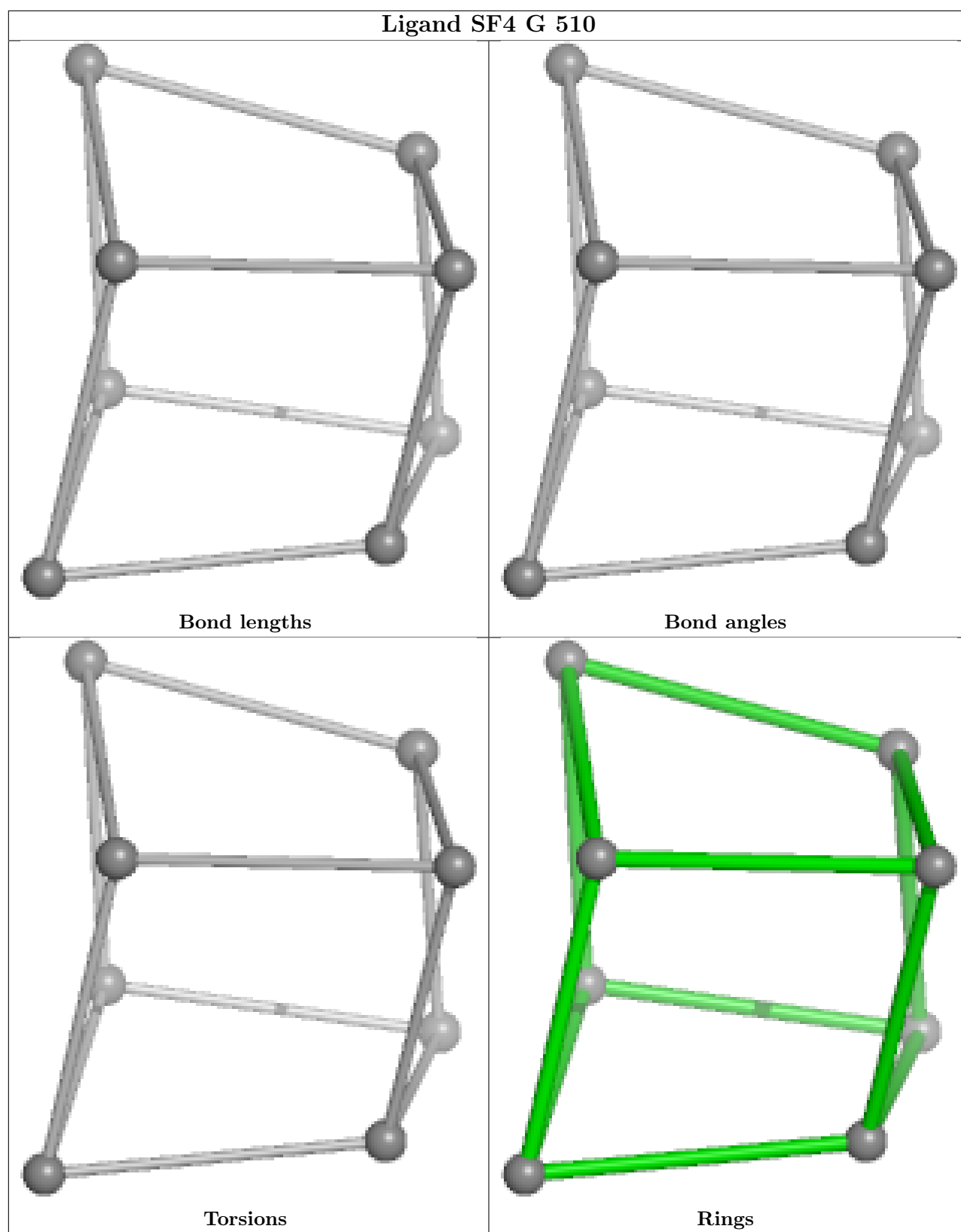
## Ligand SF4 G 508

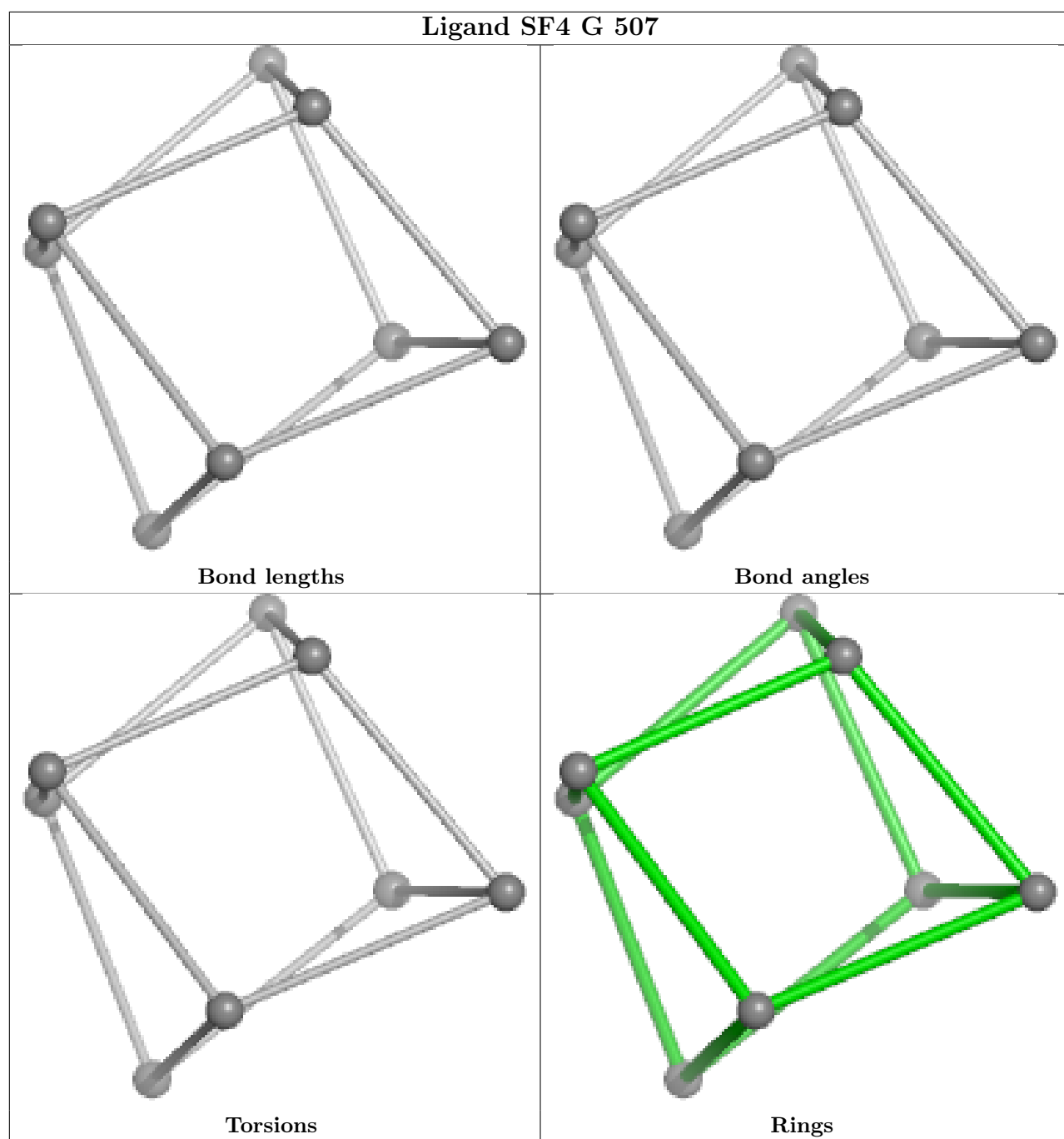


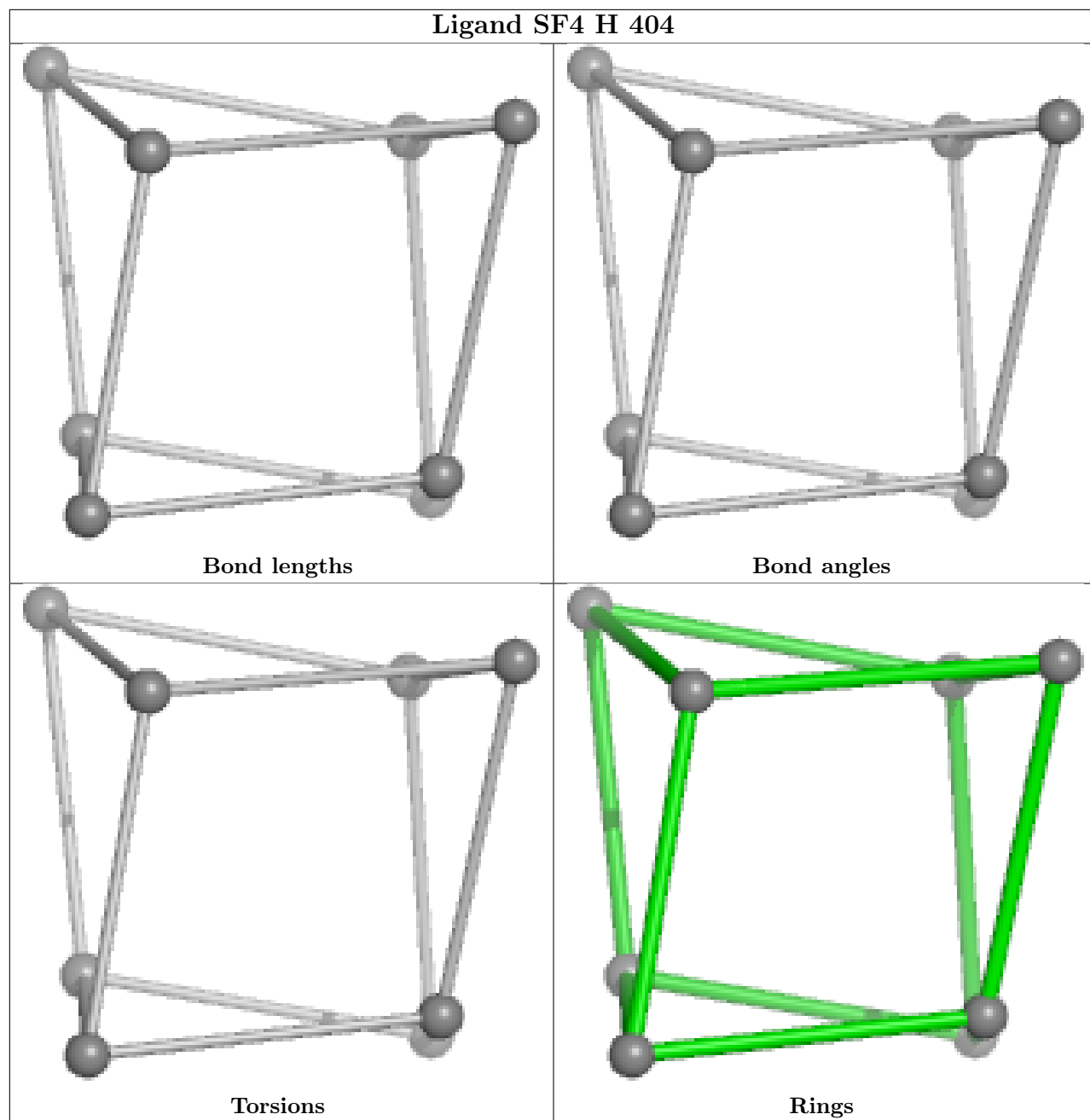


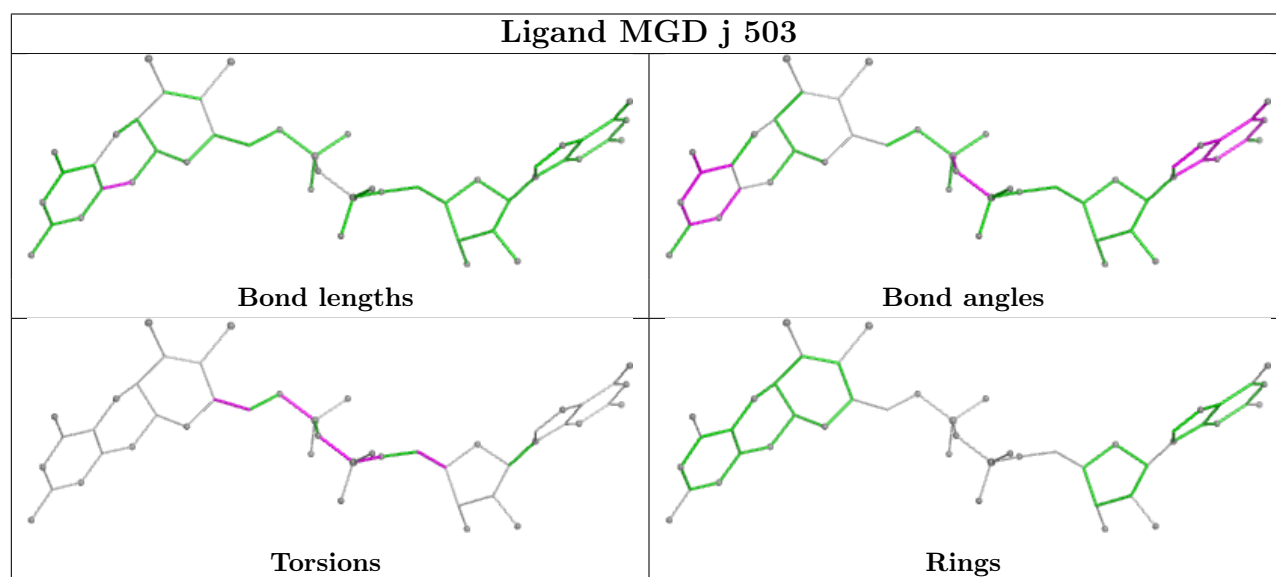
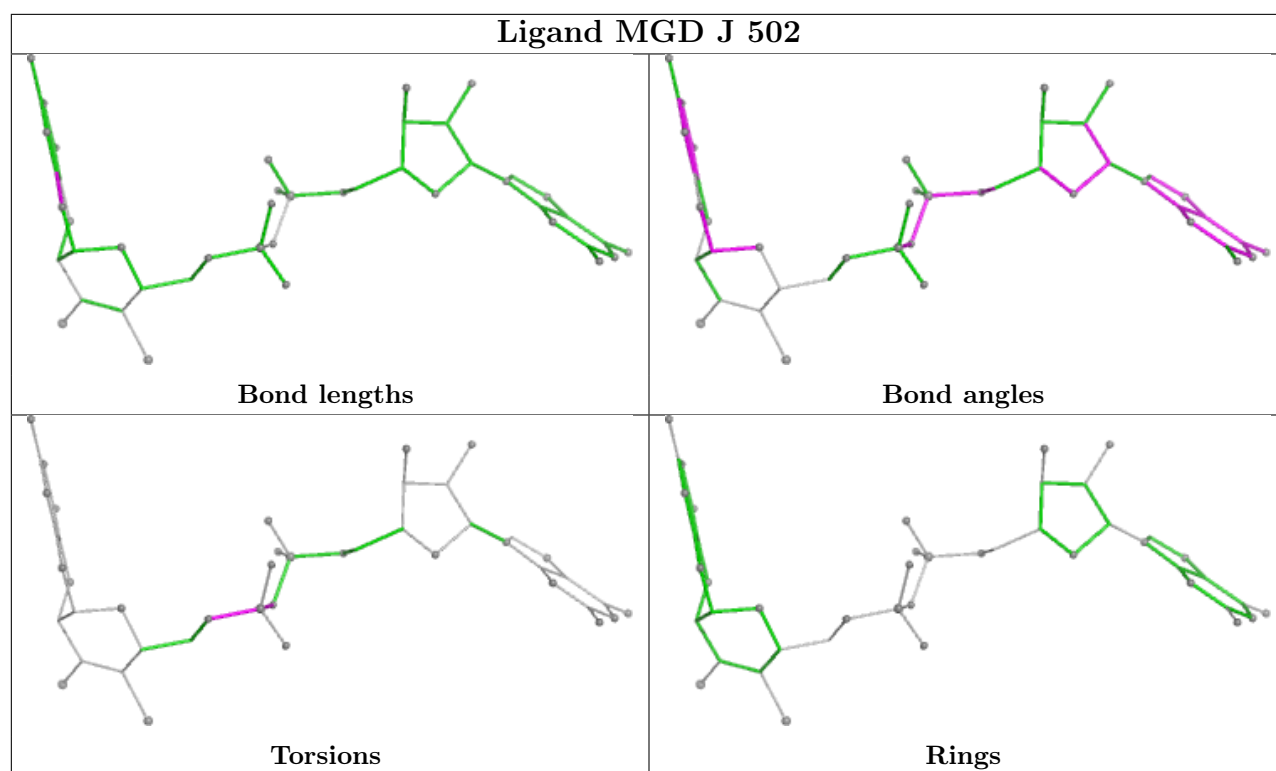




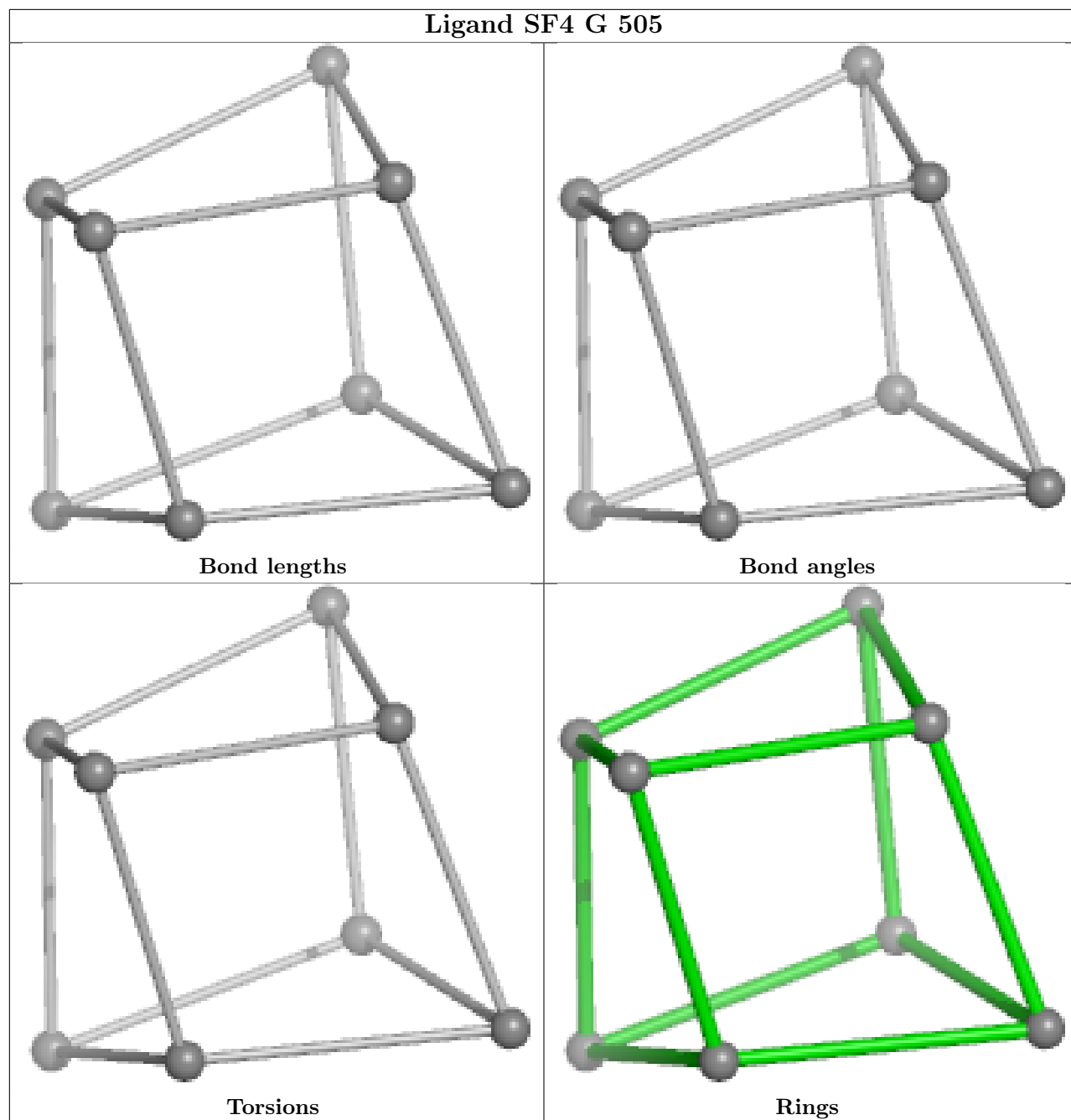


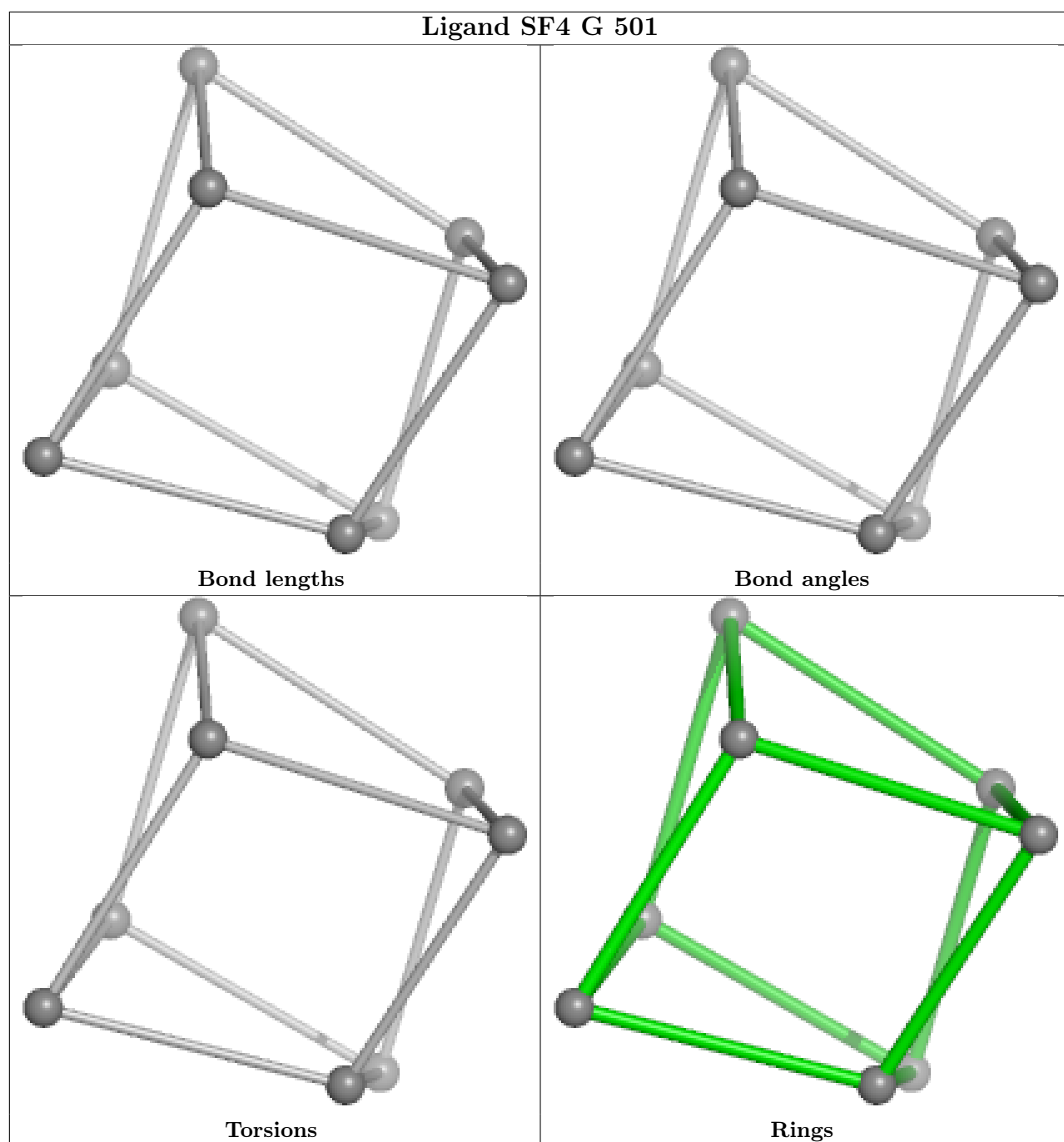


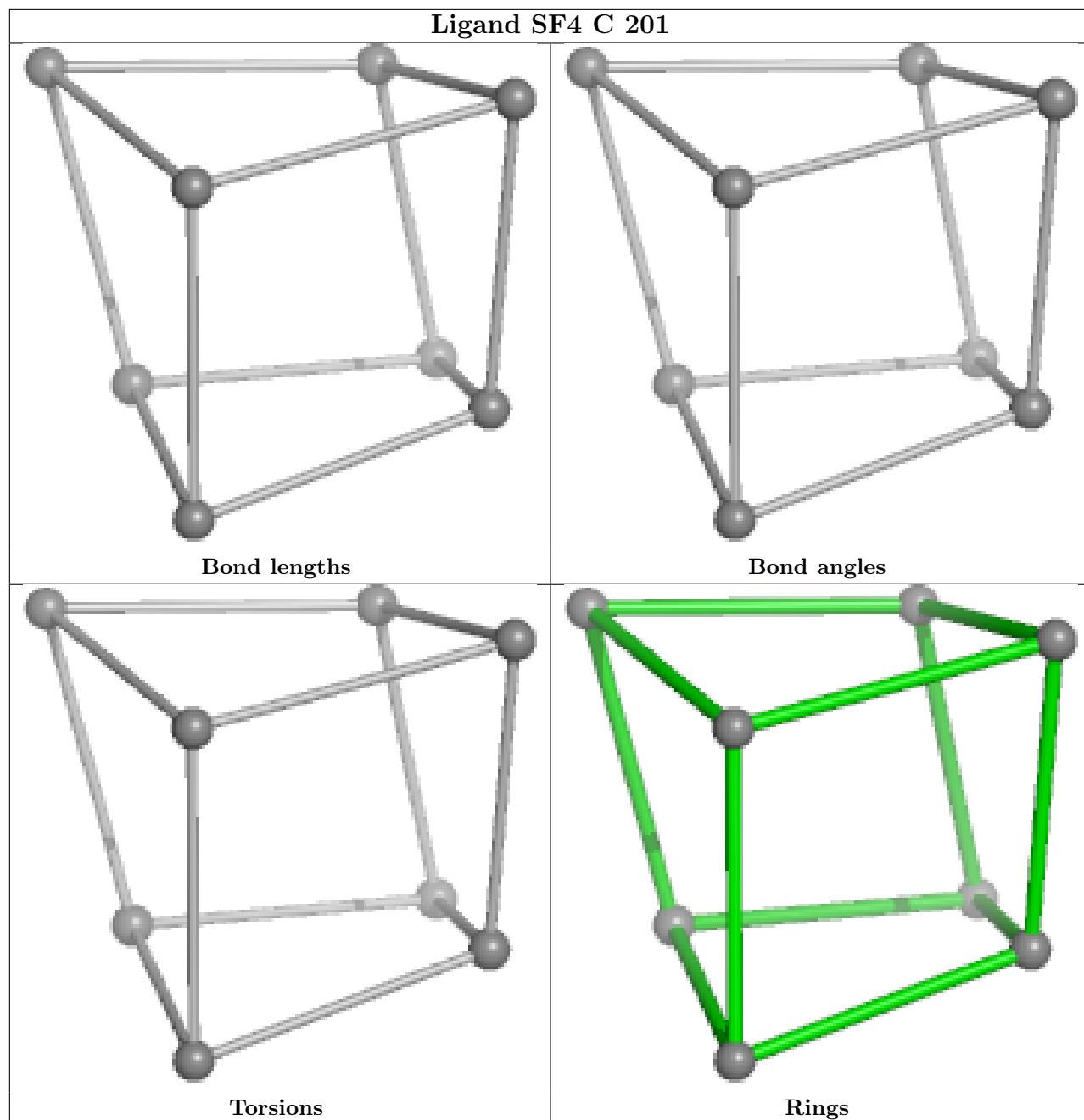




## Ligand SF4 G 505

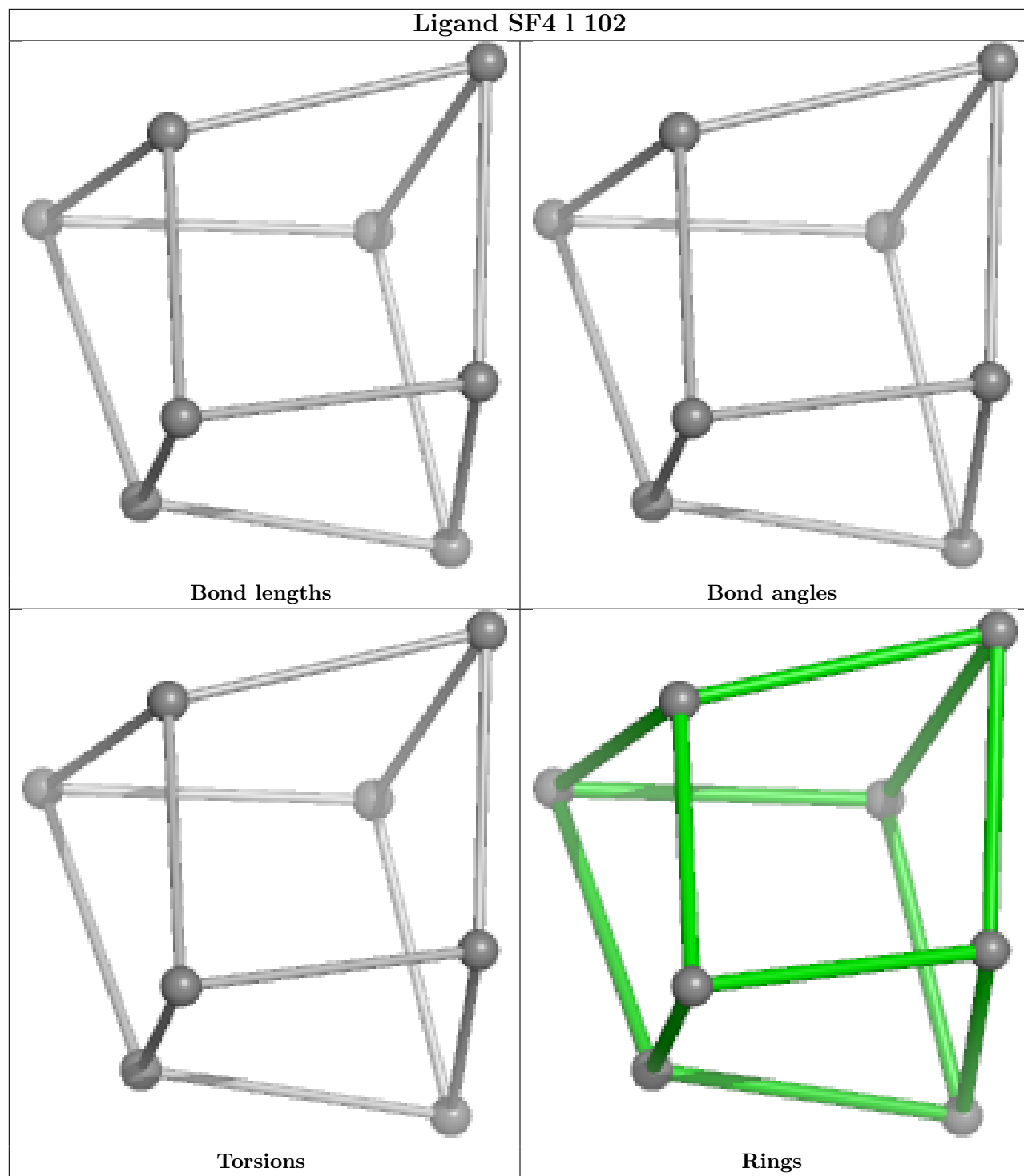


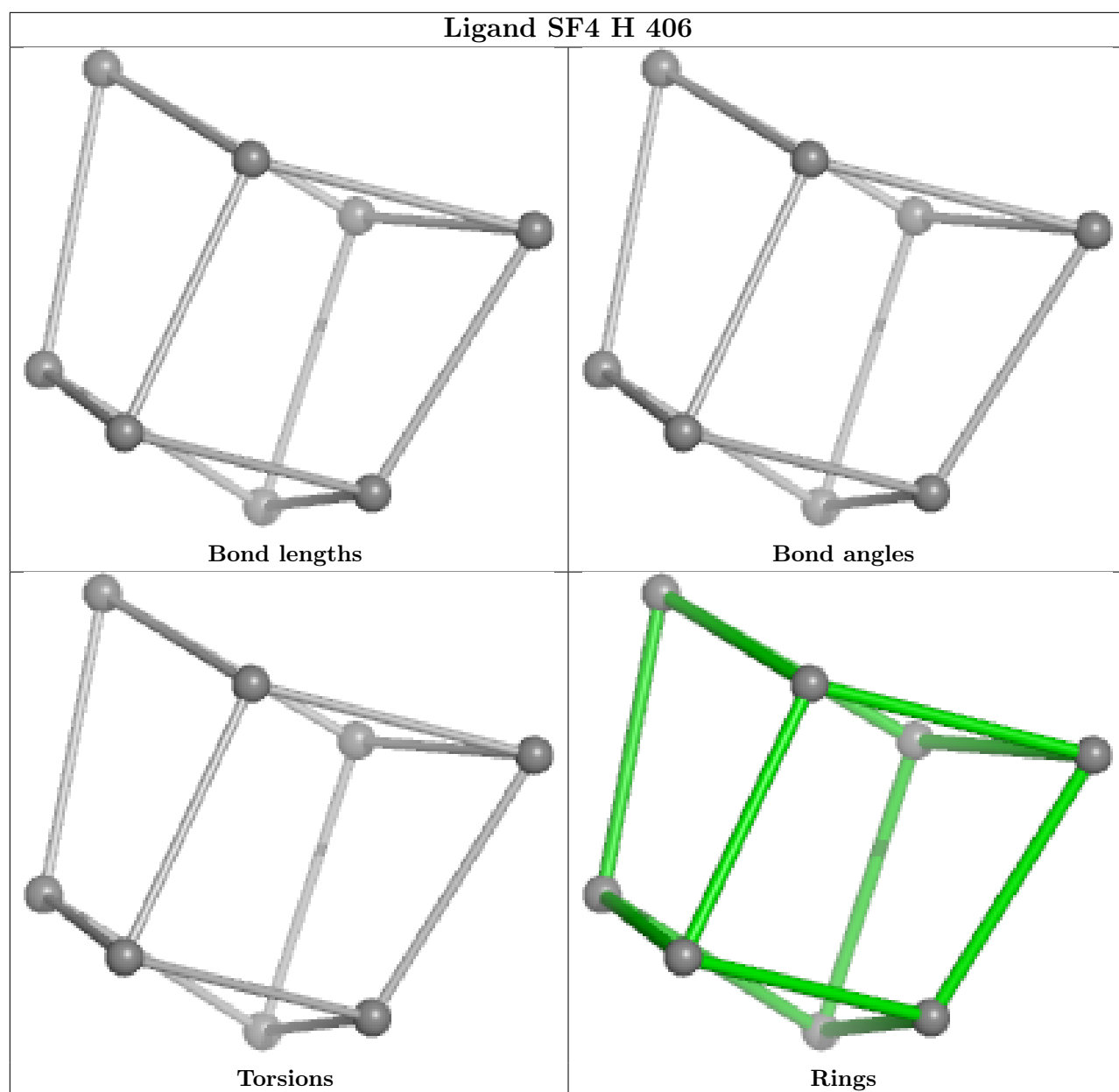


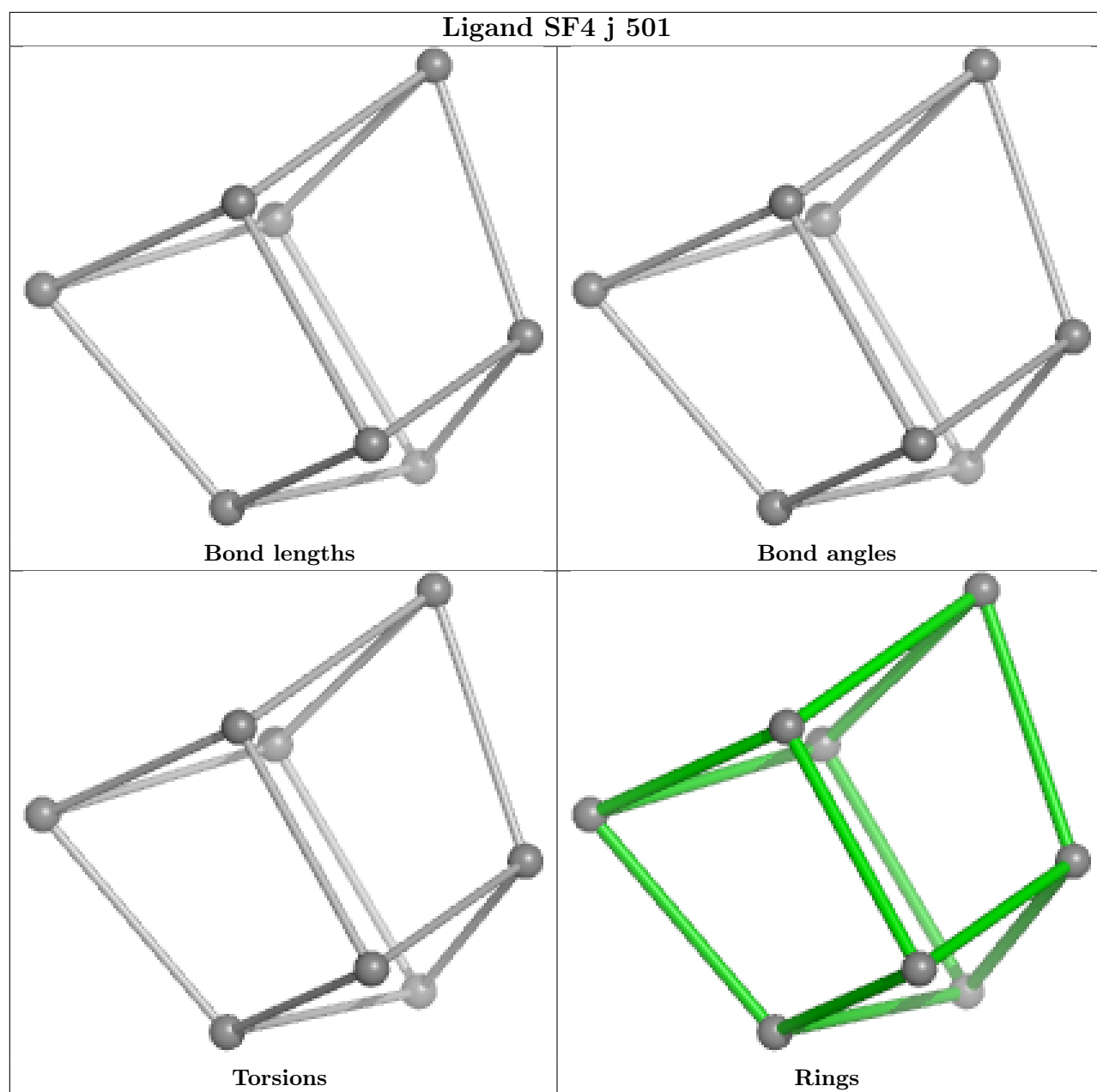


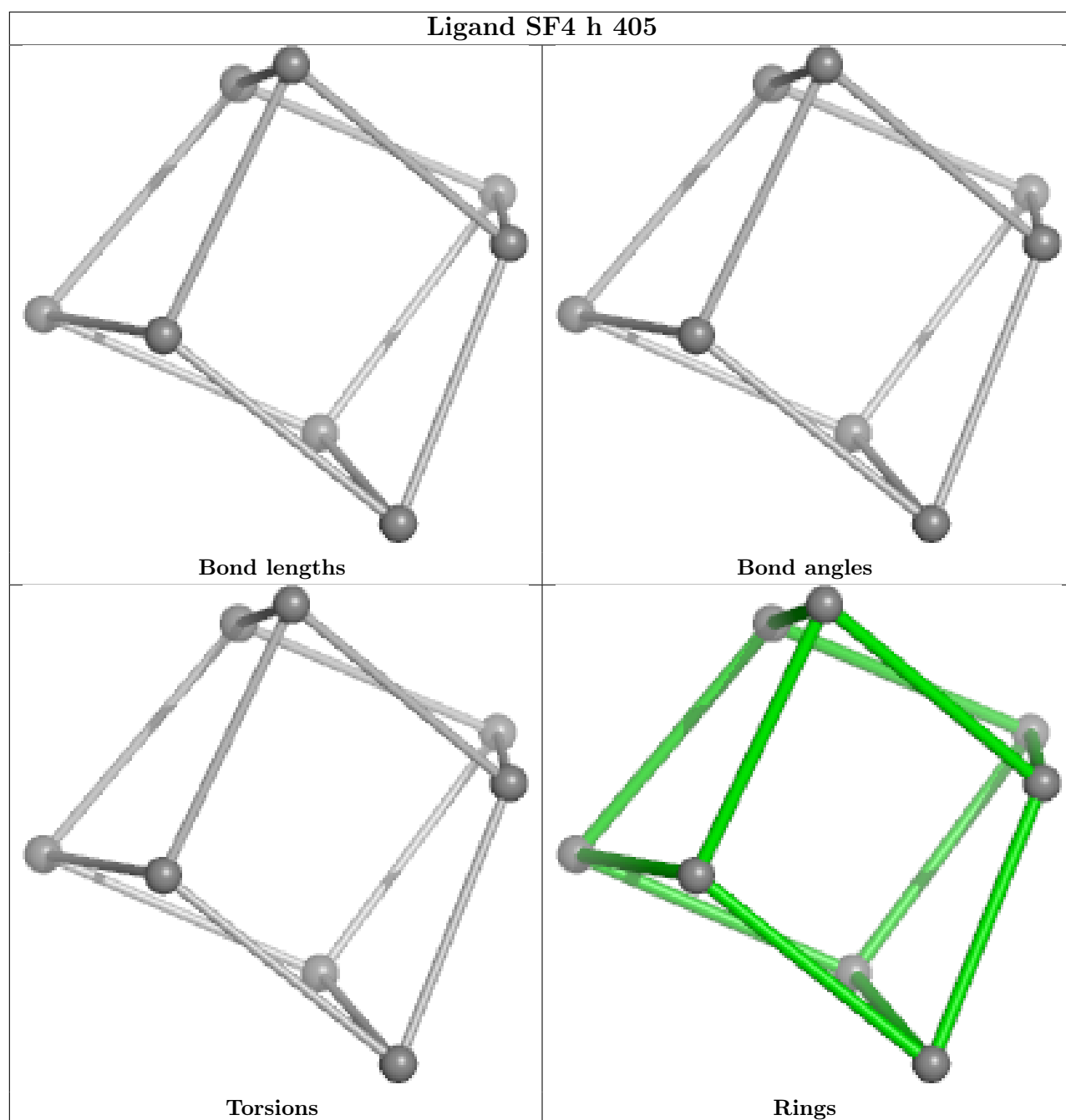


## Ligand SF4 1 102

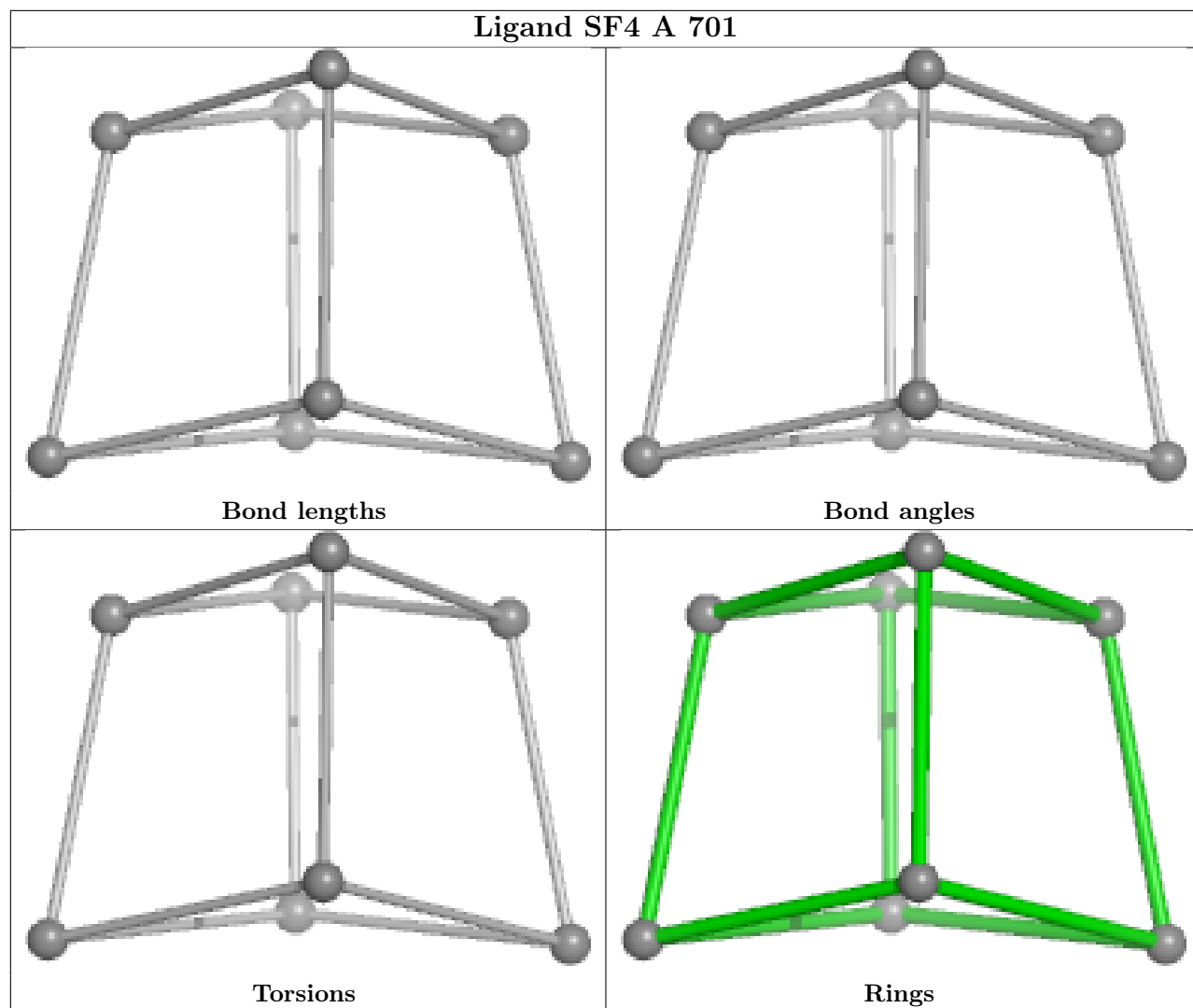


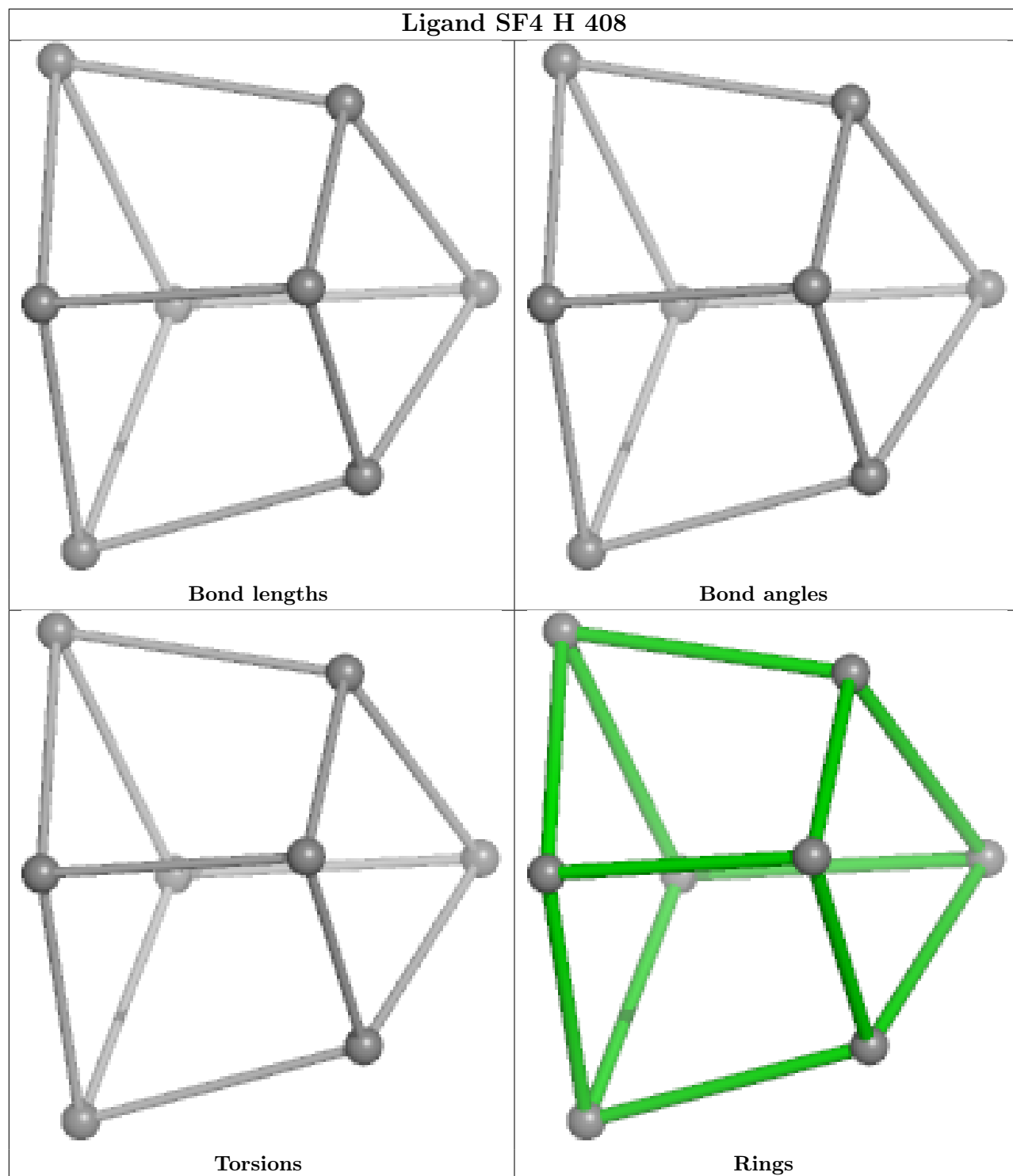


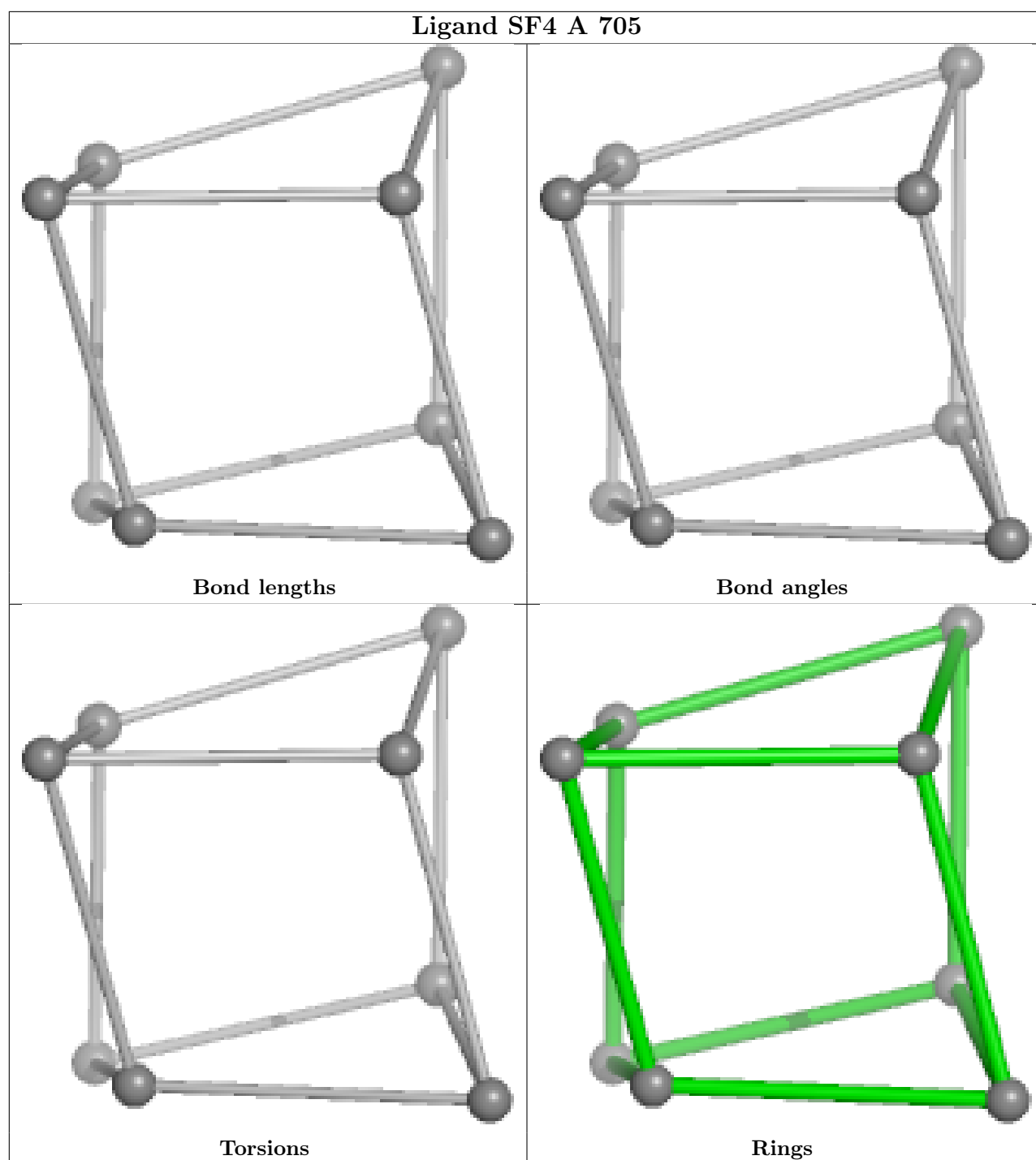


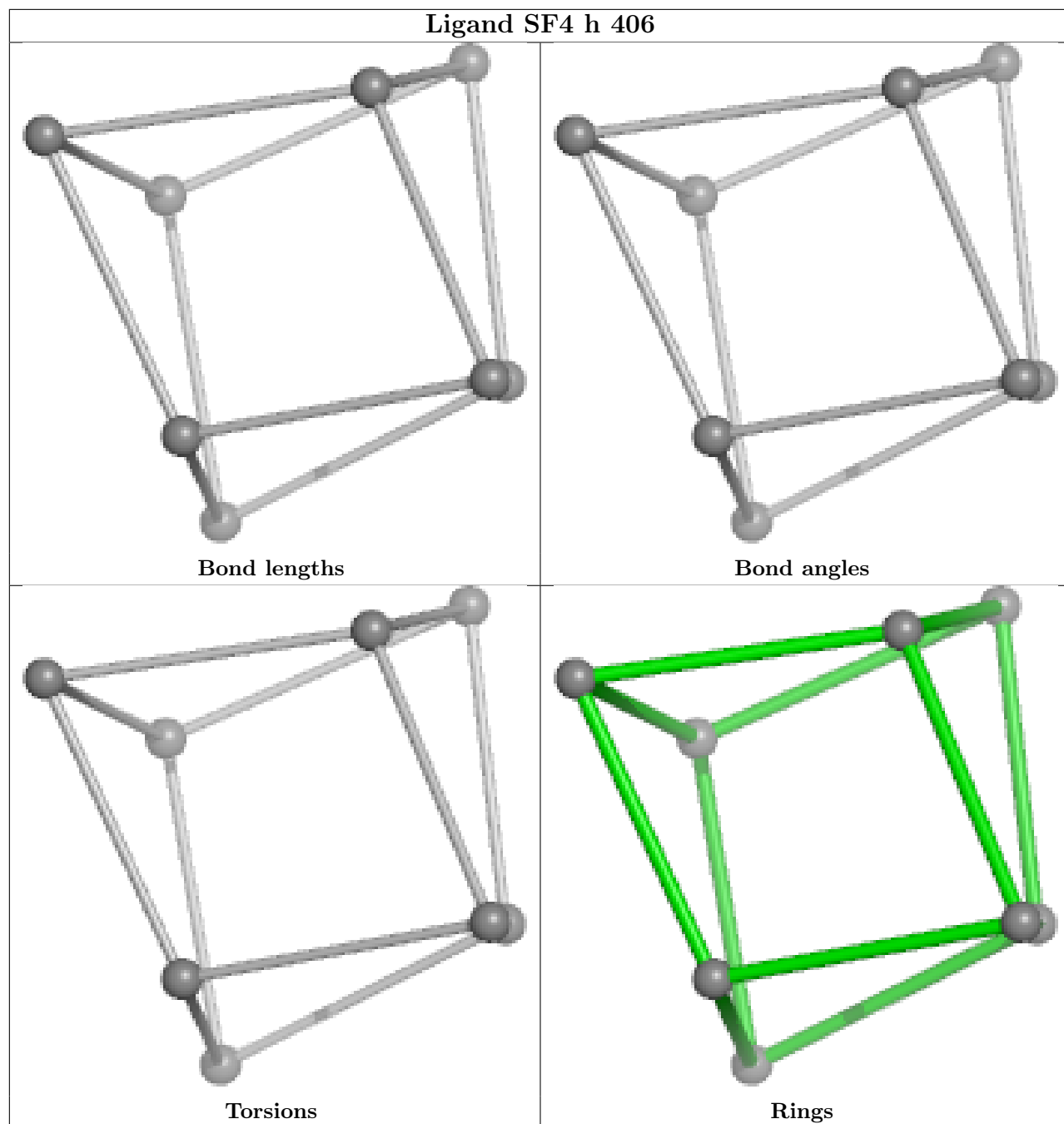


## Ligand SF4 A 701

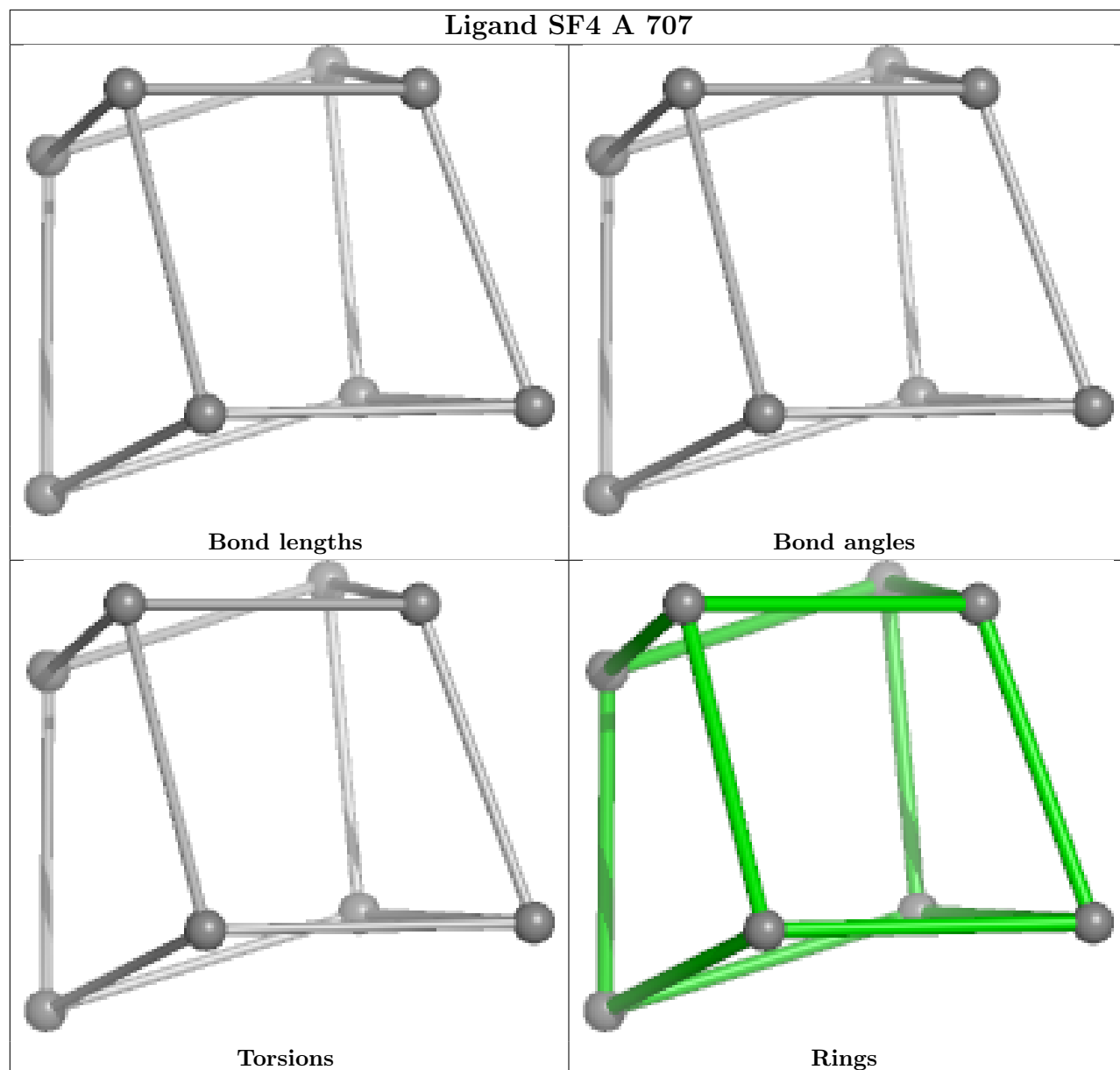


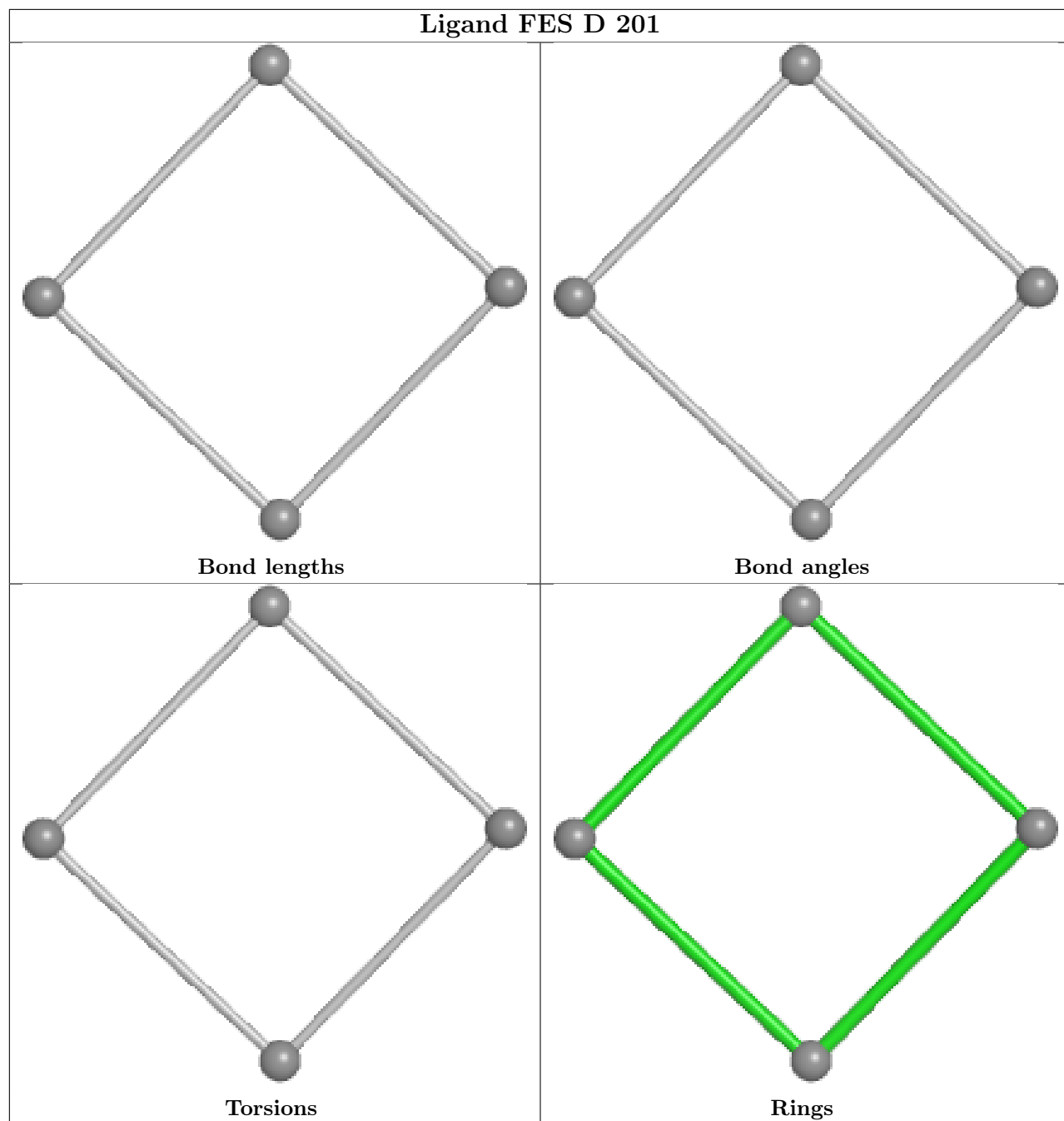


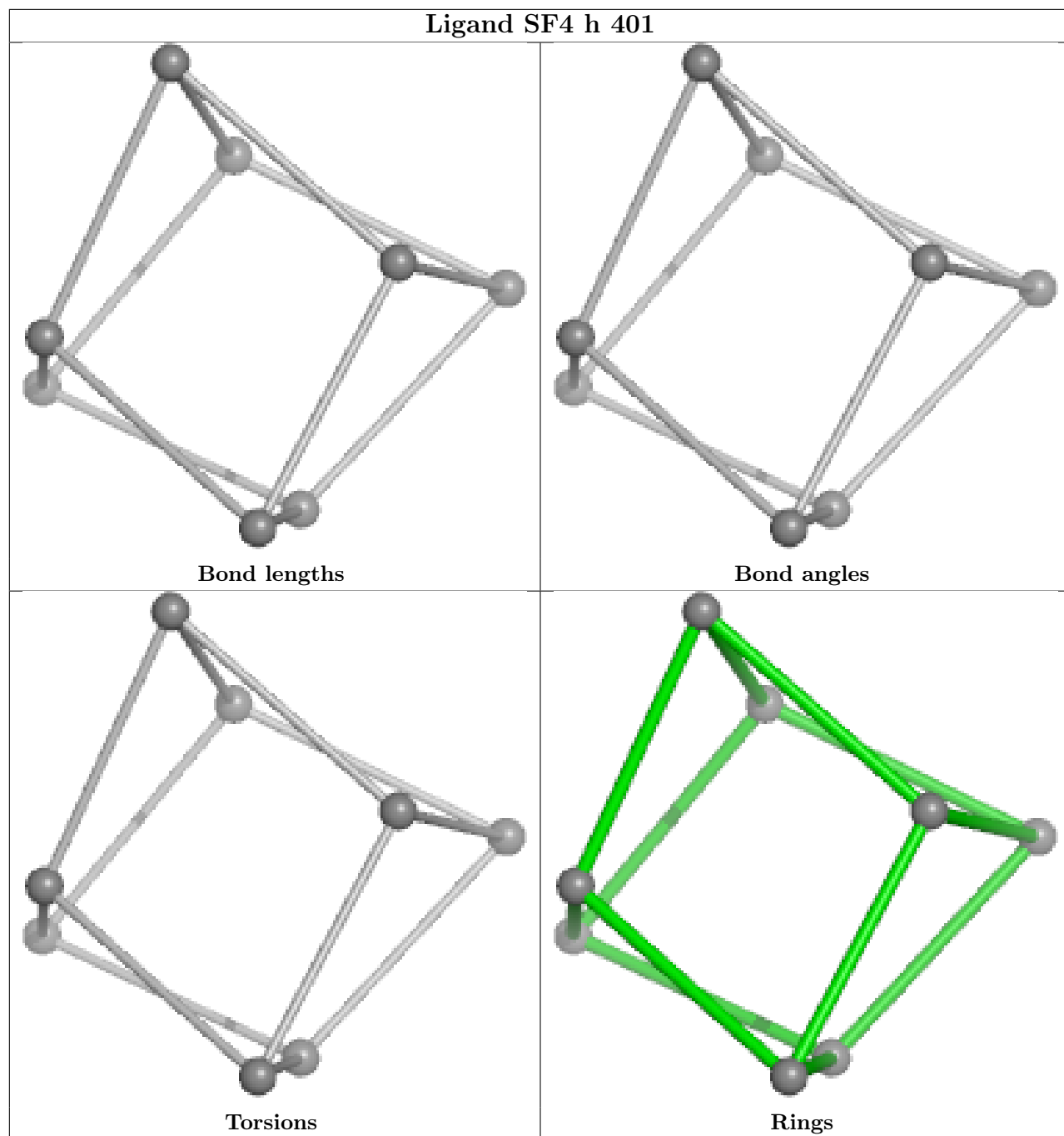


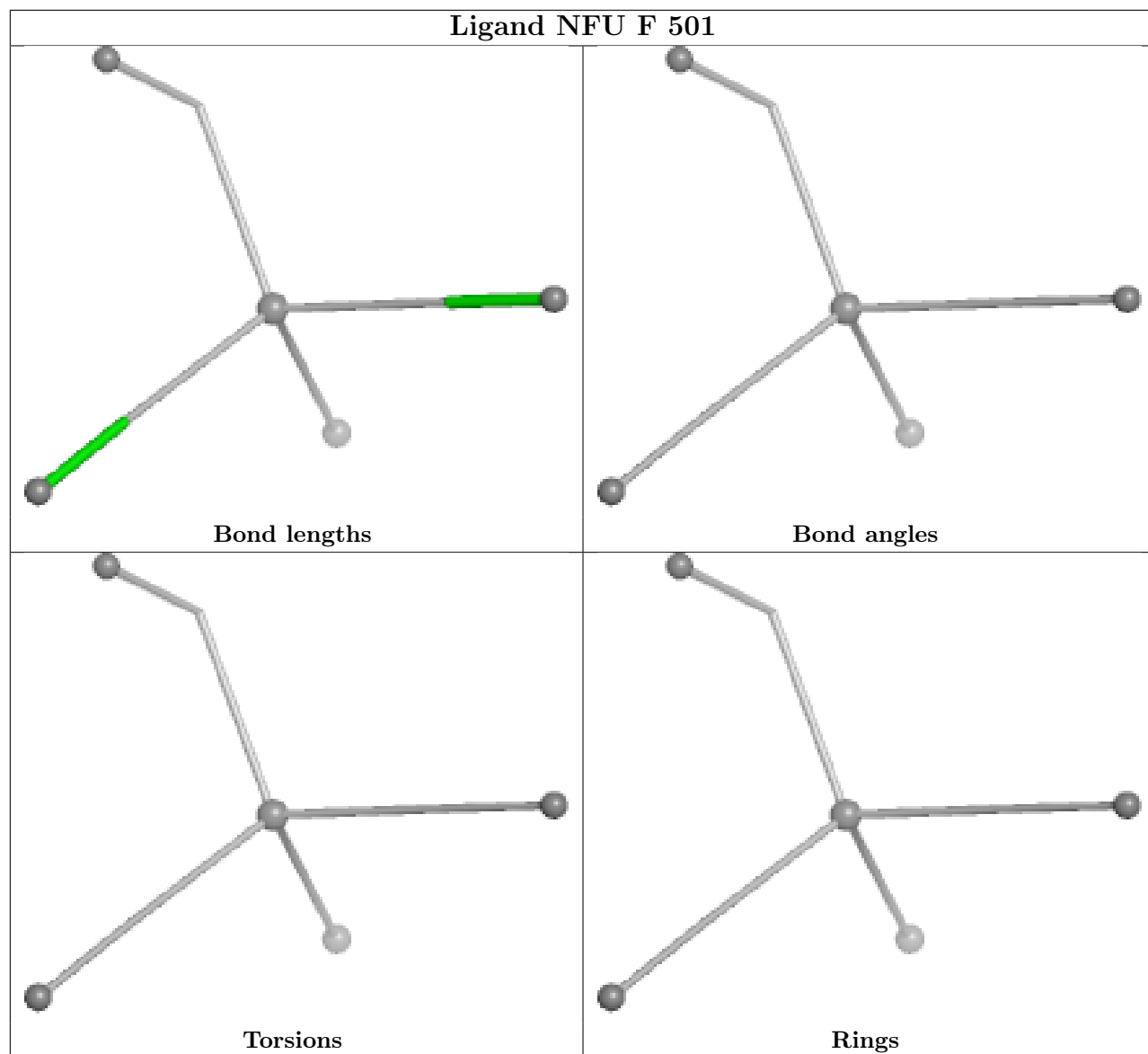


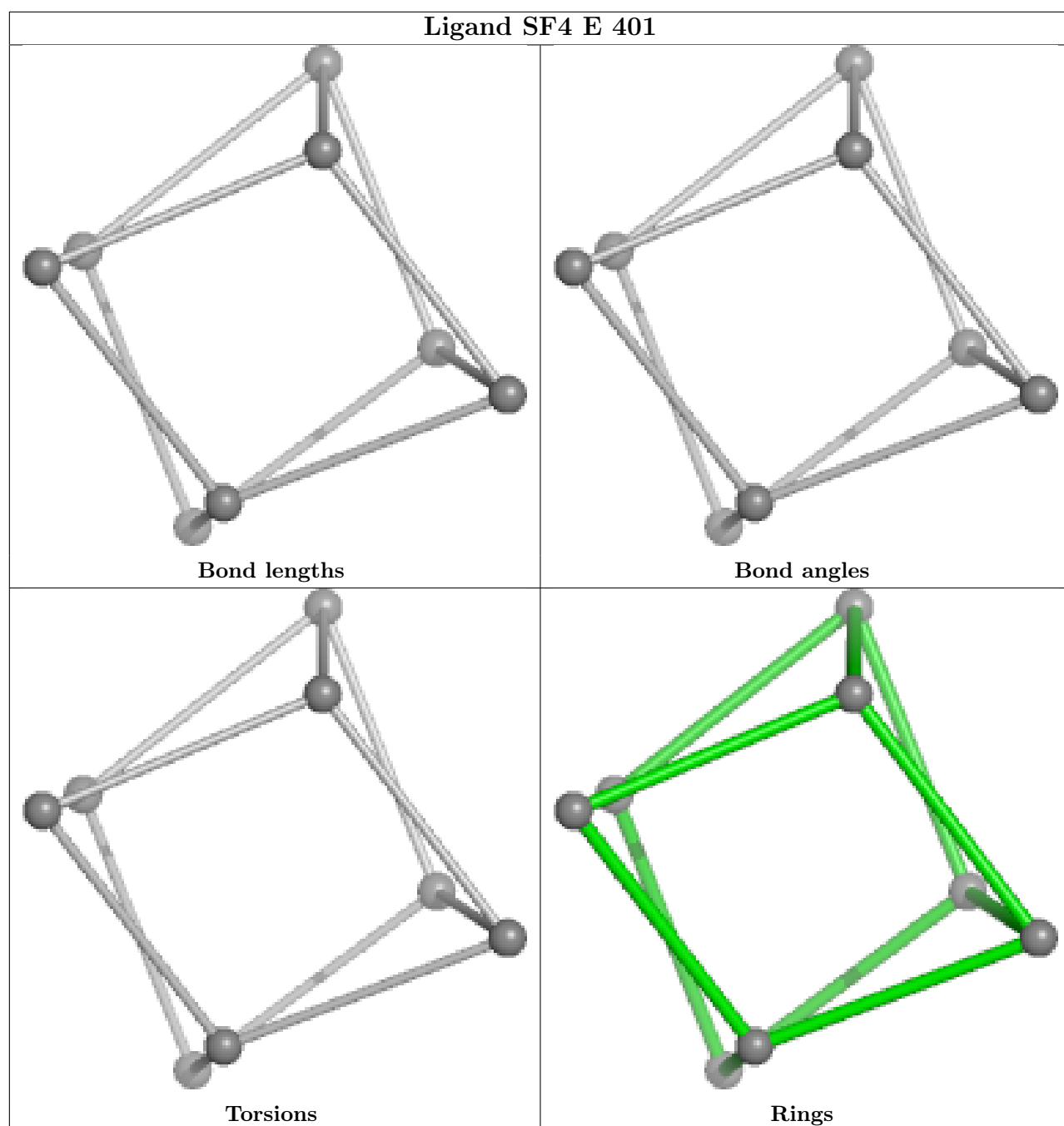


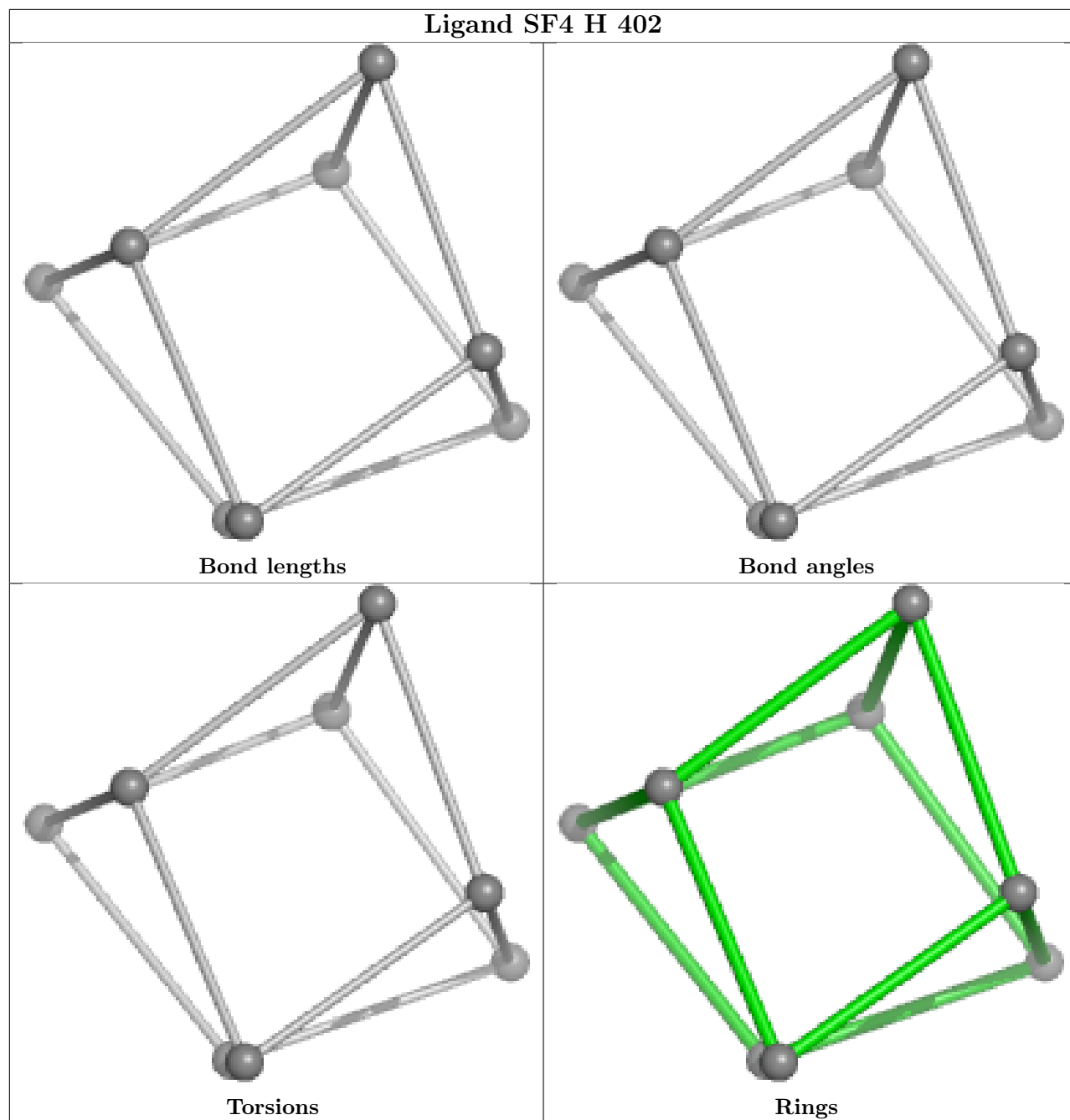


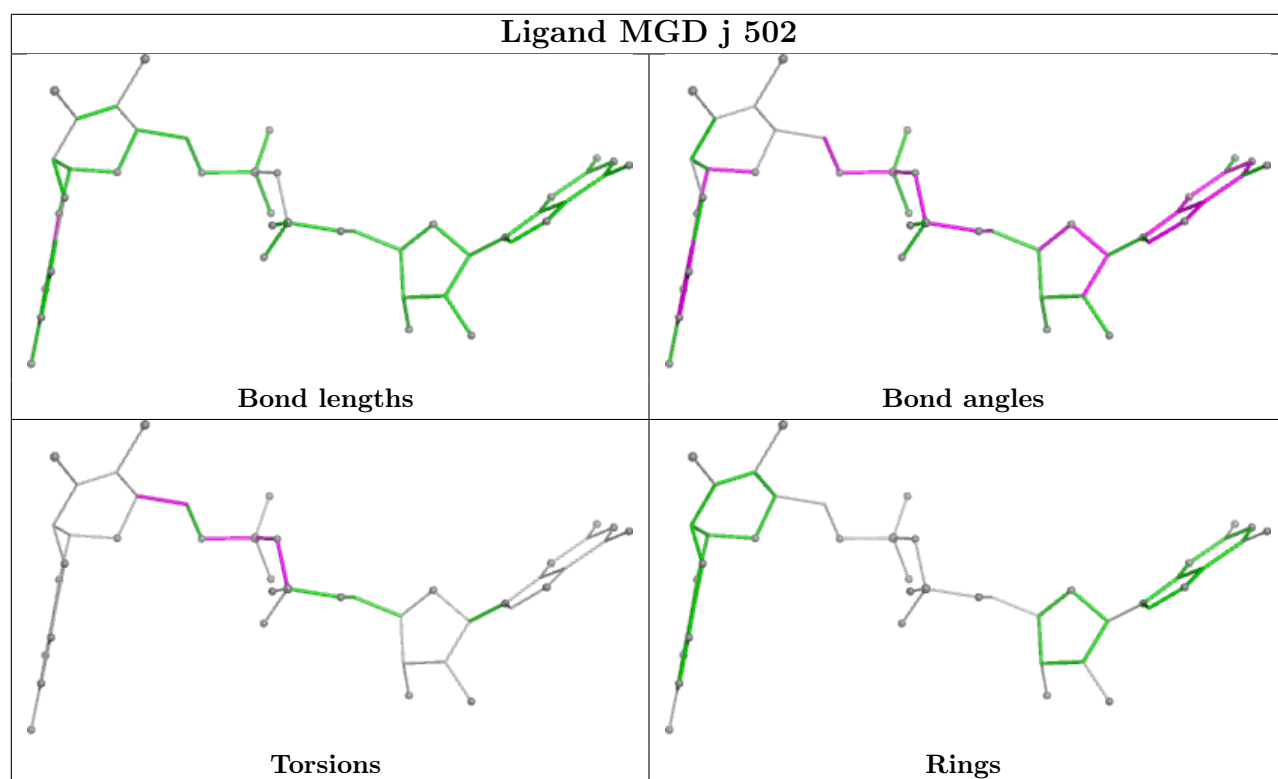


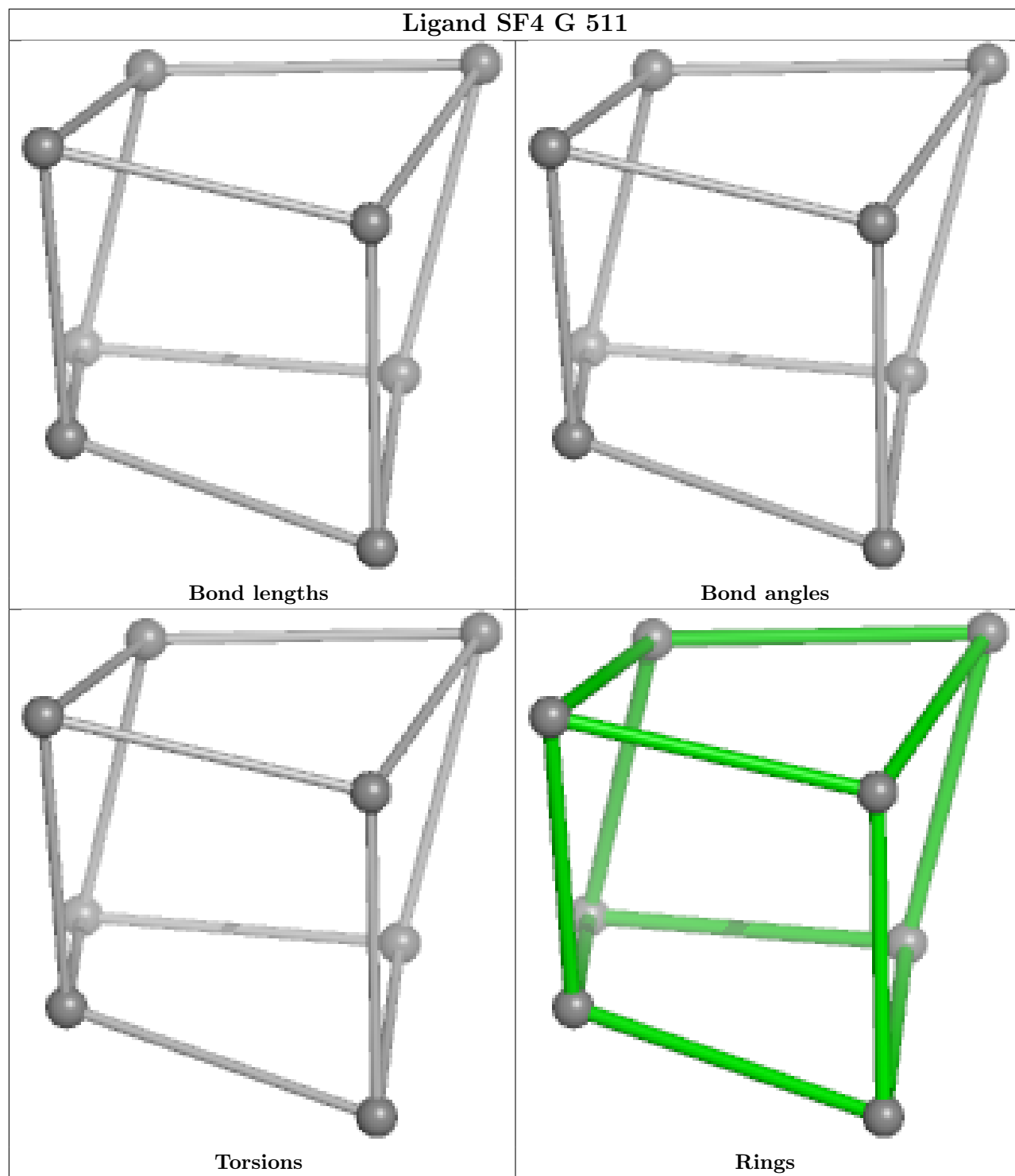




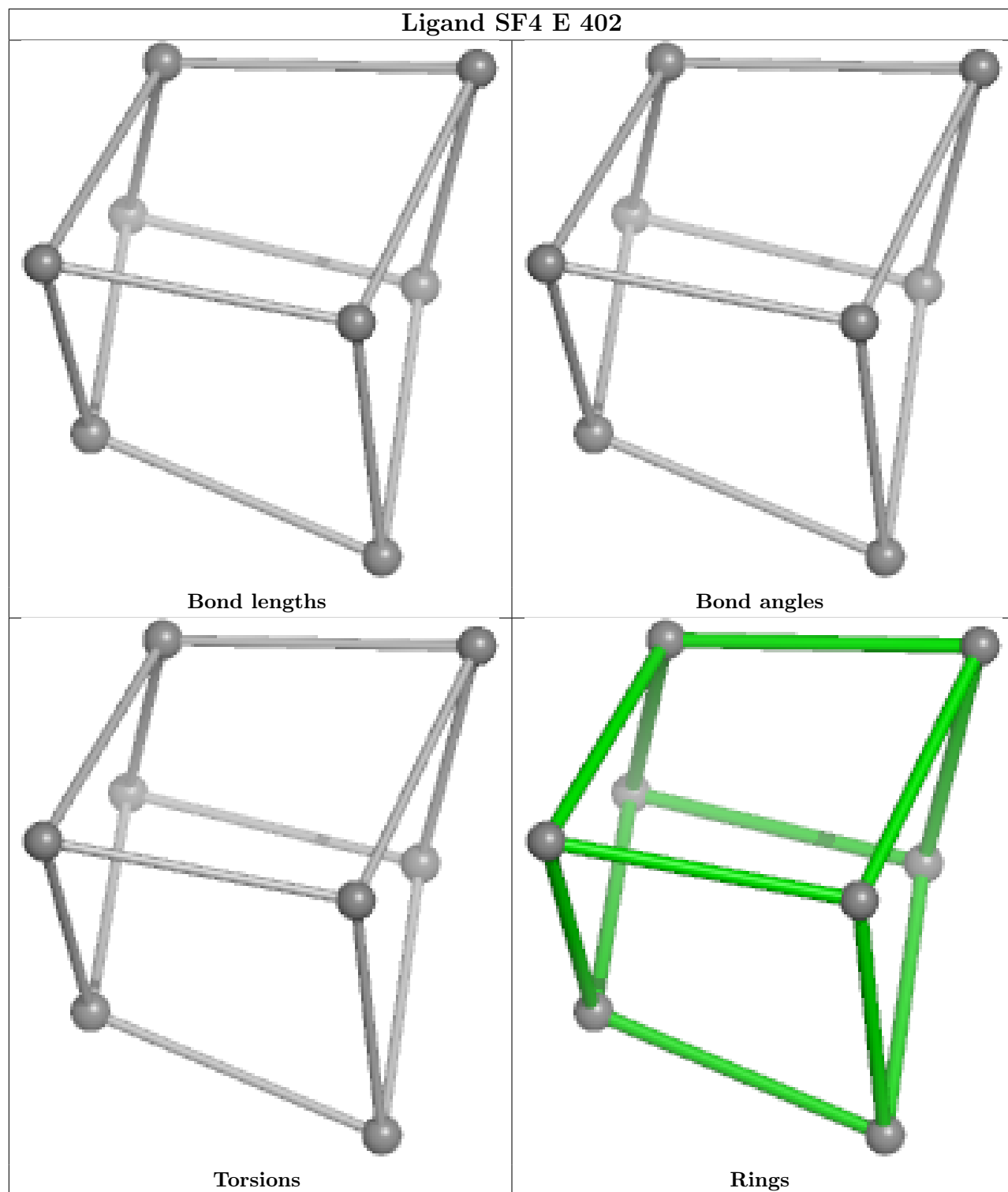


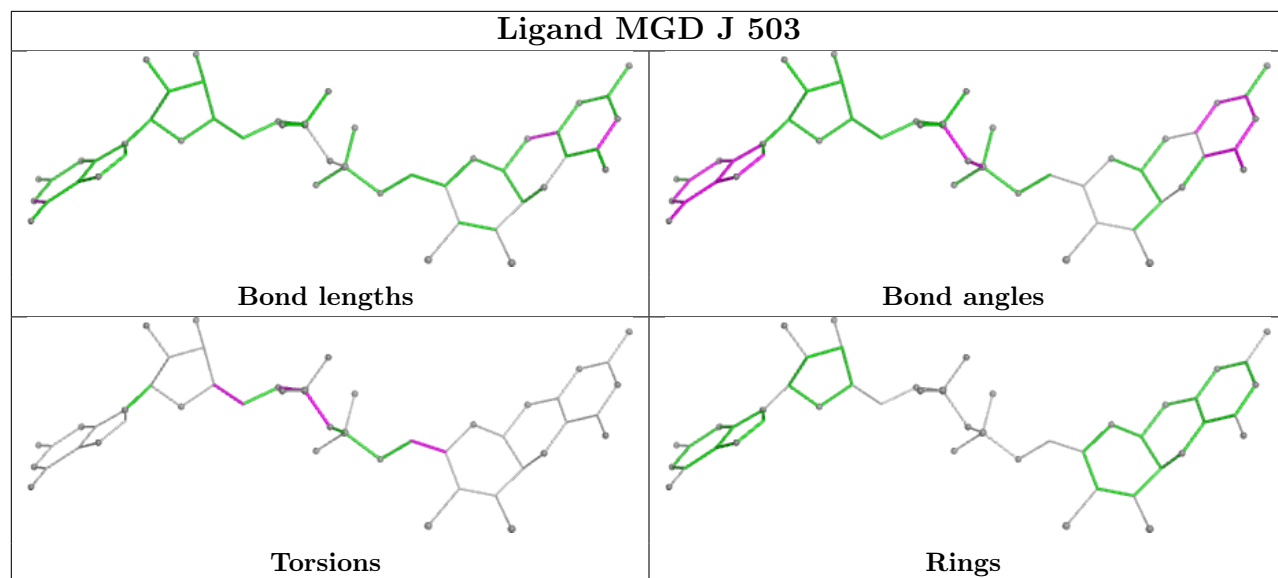


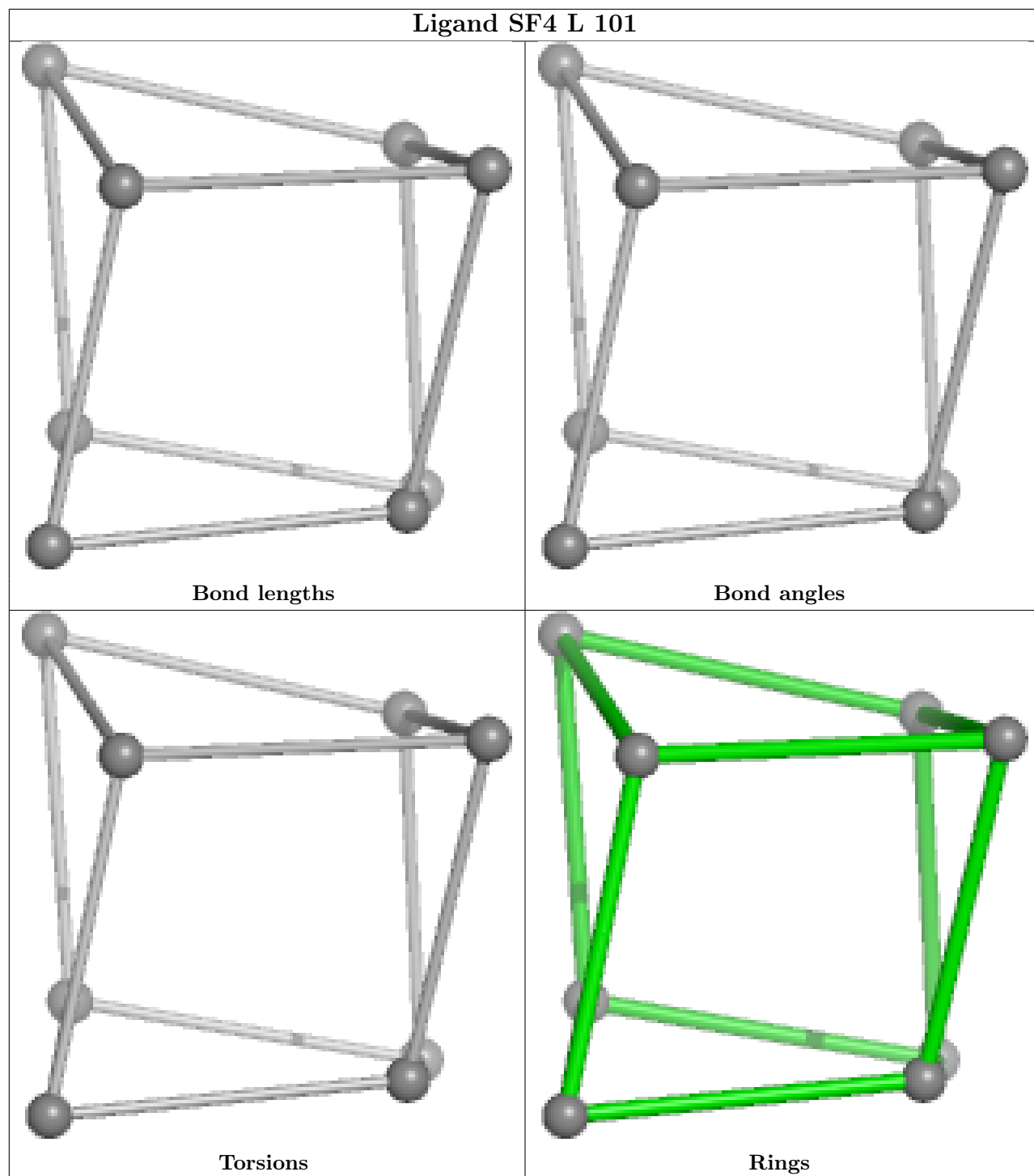




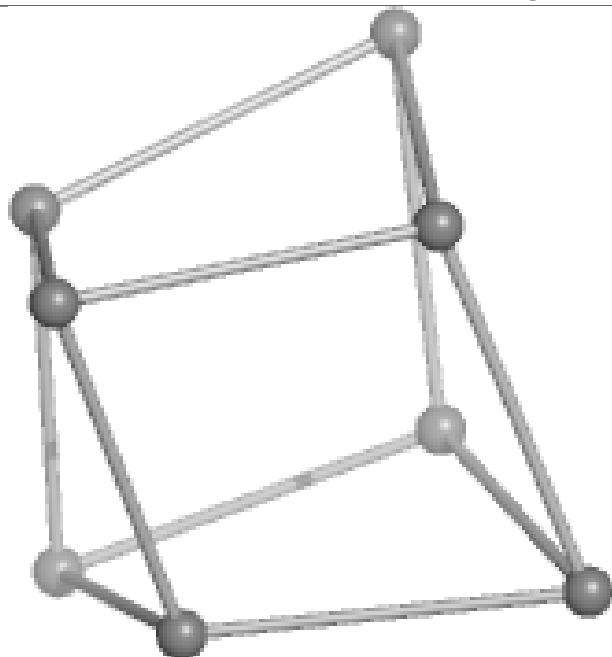




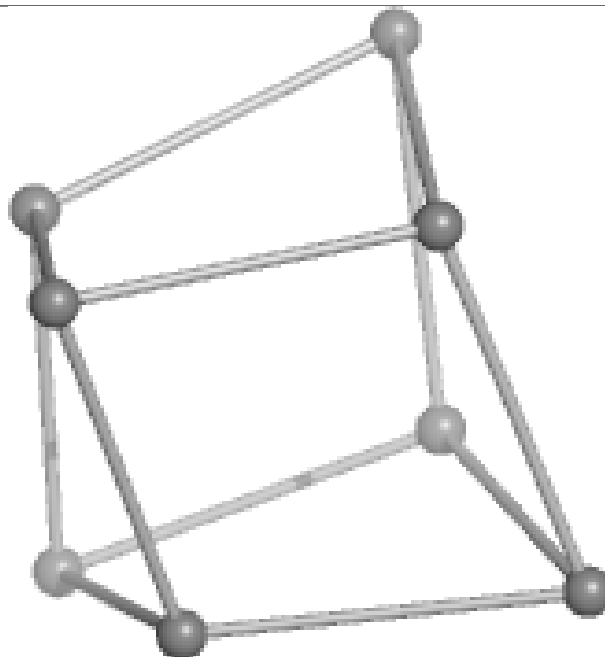




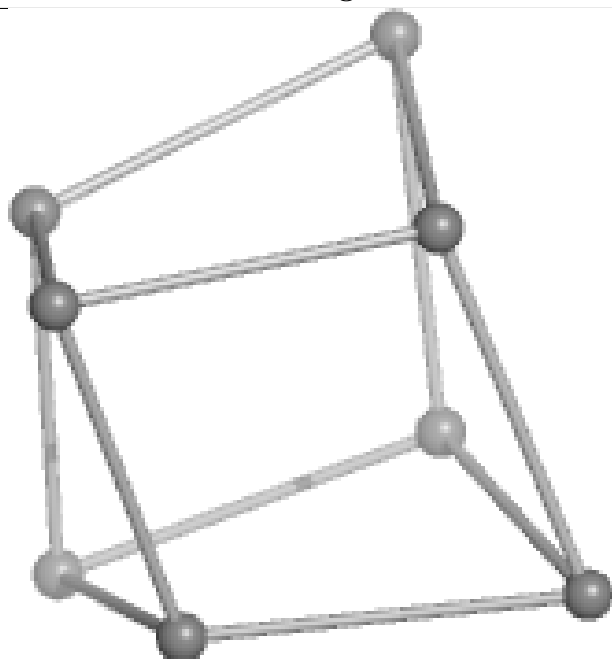
## Ligand SF4 J 501



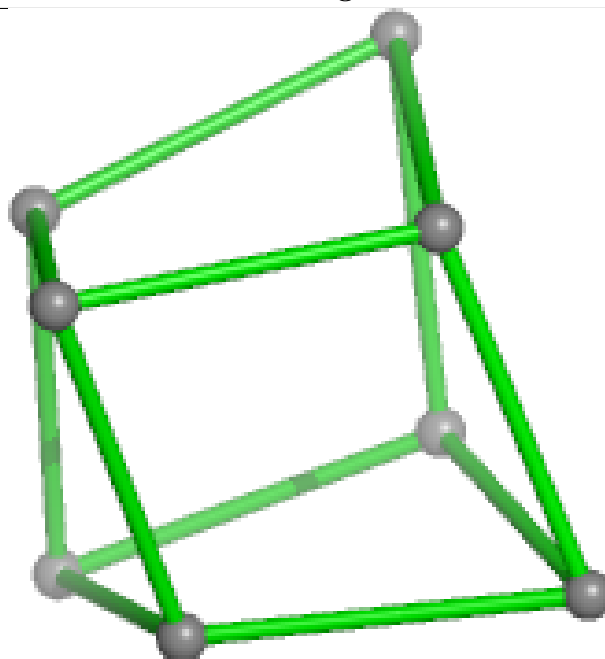
Bond lengths



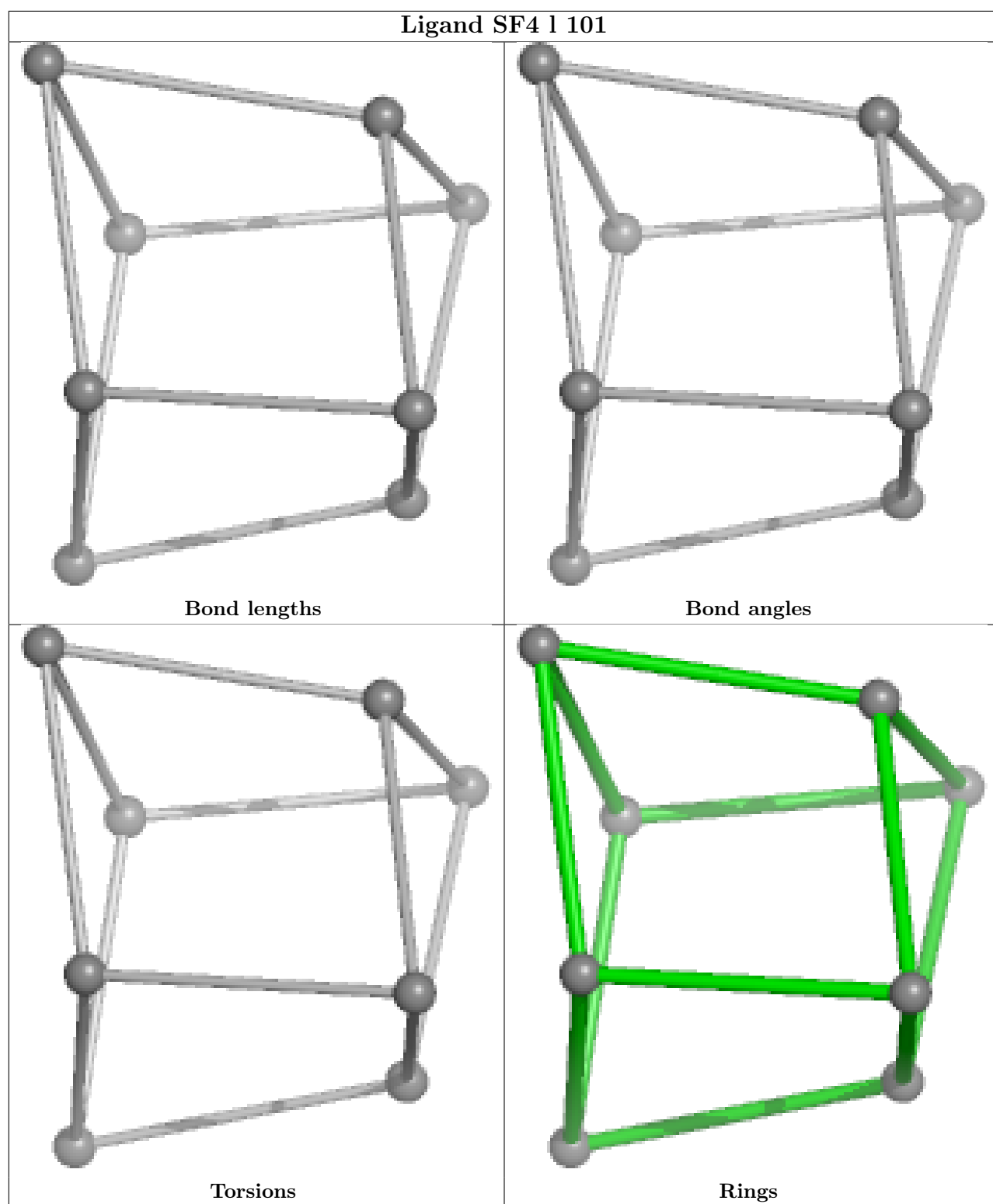
Bond angles

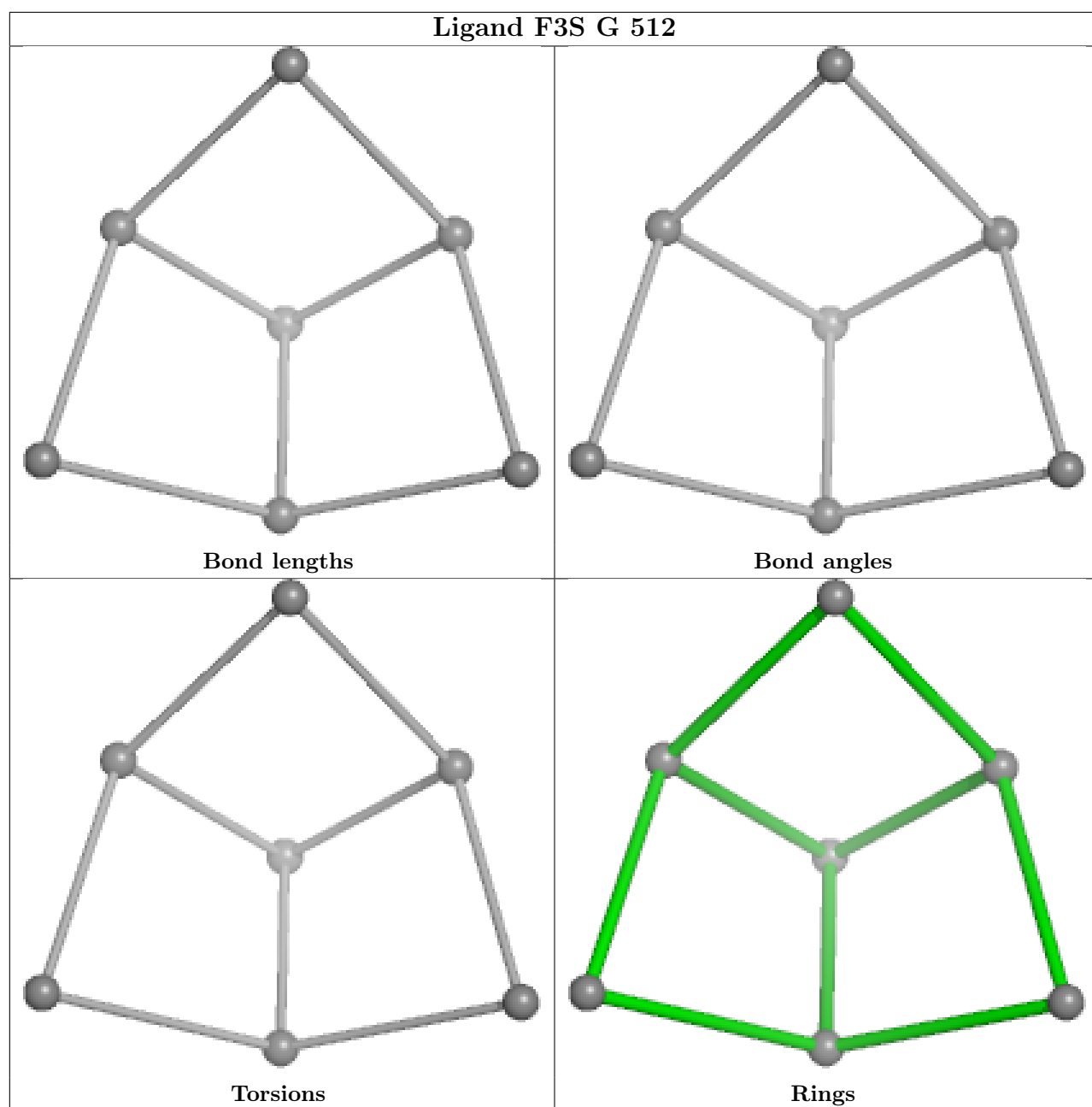


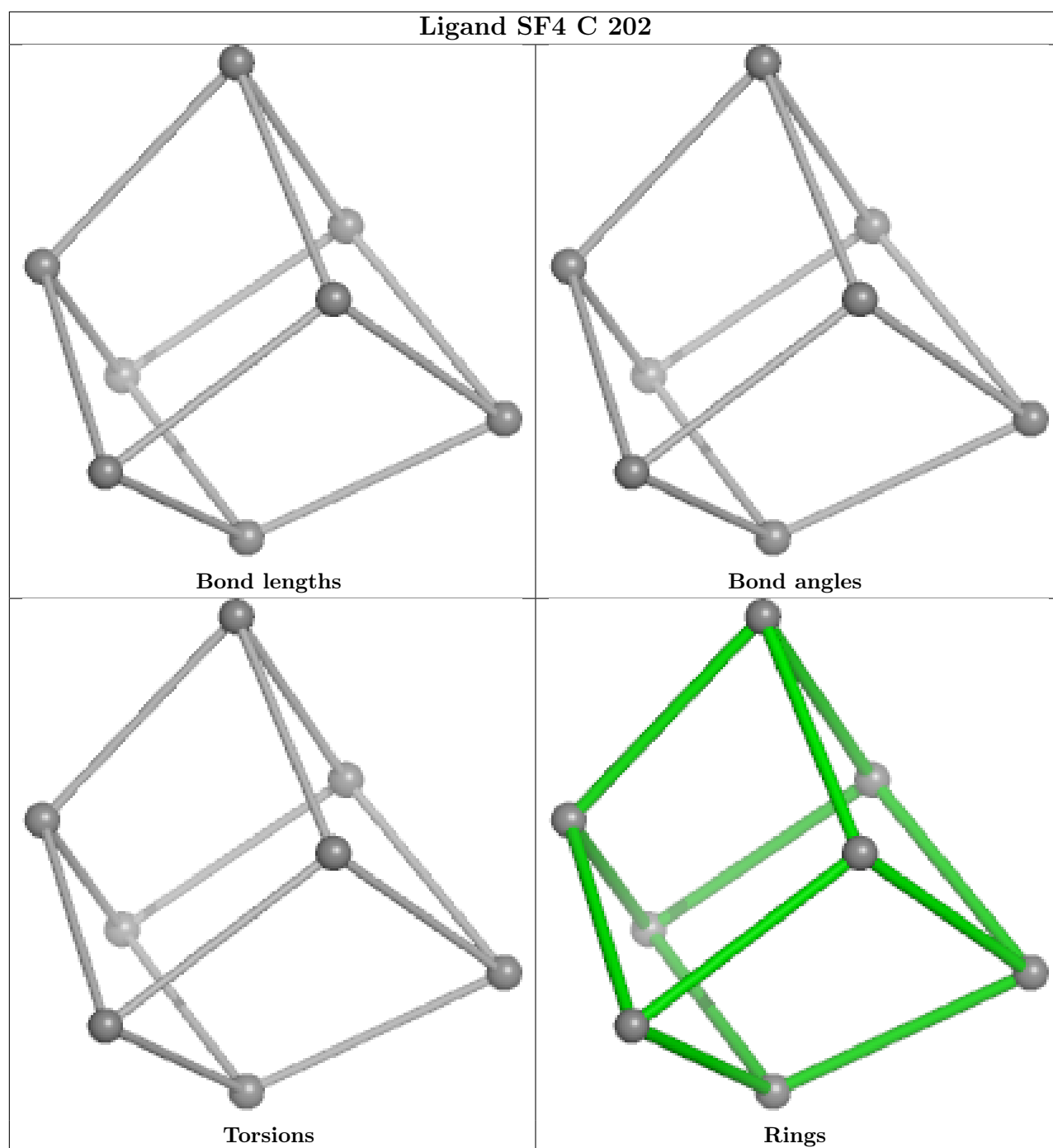
Torsions



Rings







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

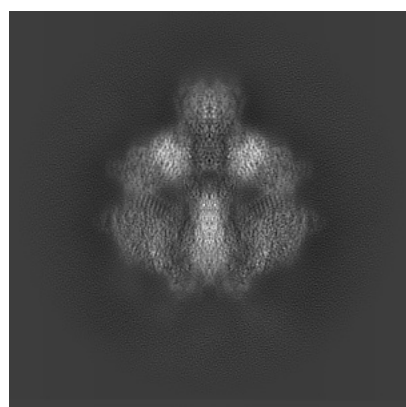
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55299. These allow visual inspection of the internal detail of the map and identification of artifacts.

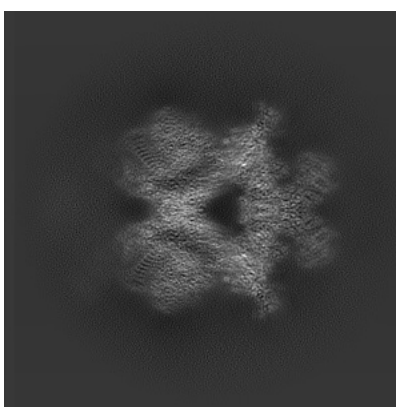
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

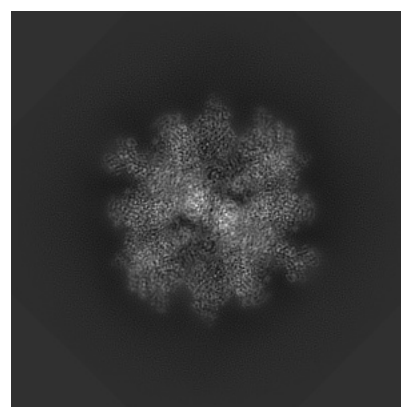
#### 6.1.1 Primary map



X



Y

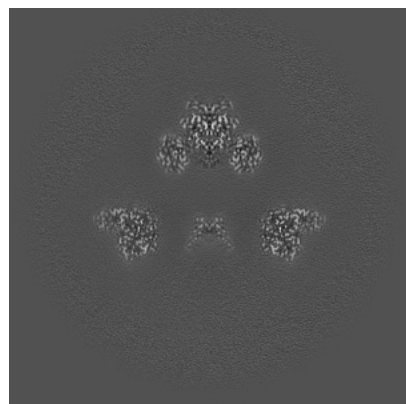


Z

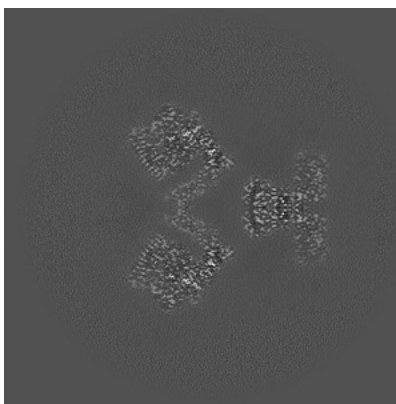
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

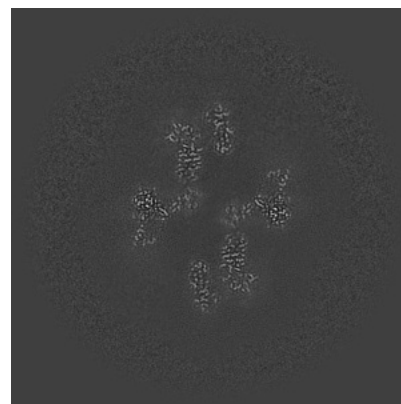
#### 6.2.1 Primary map



X Index: 240



Y Index: 240



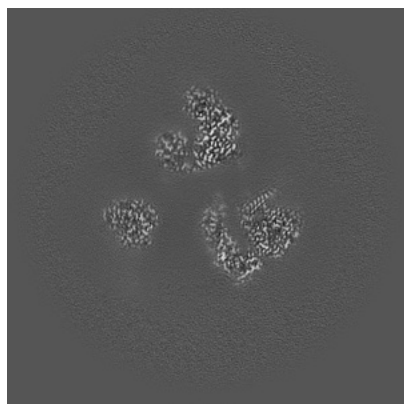
Z Index: 240



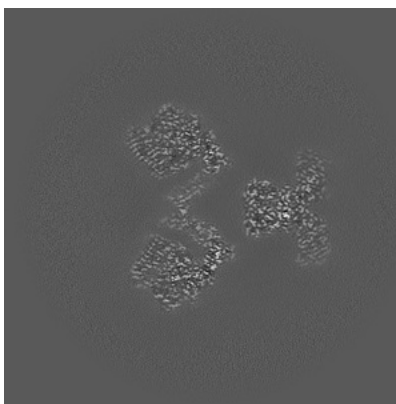
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

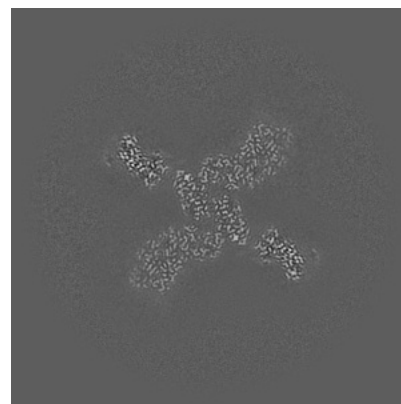
### 6.3.1 Primary map



X Index: 223



Y Index: 243

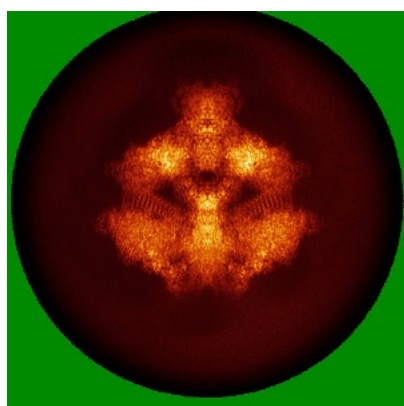


Z Index: 303

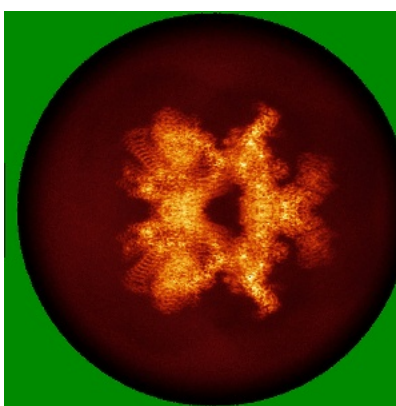
The images above show the largest variance slices of the map in three orthogonal directions.

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

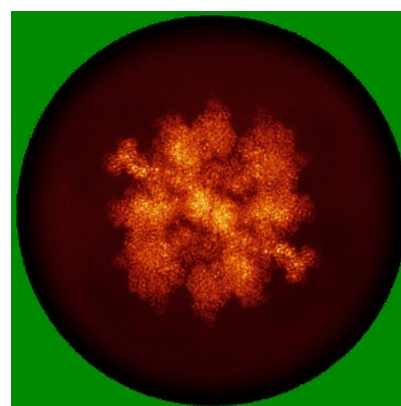
### 6.4.1 Primary map



X



Y

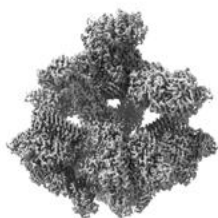


Z

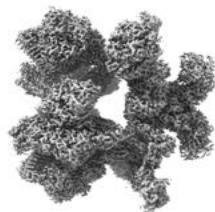
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

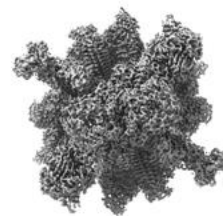
### 6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

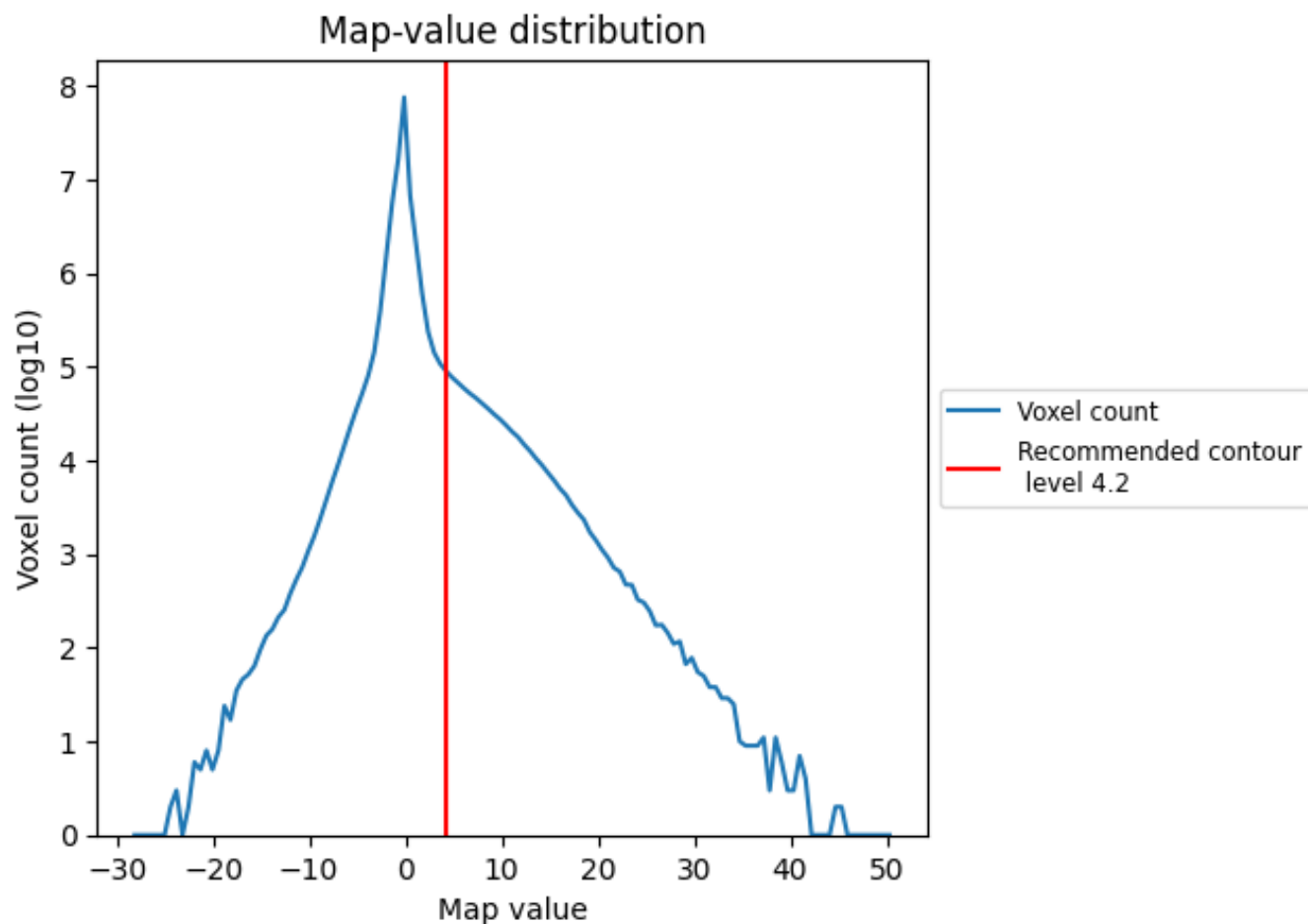
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

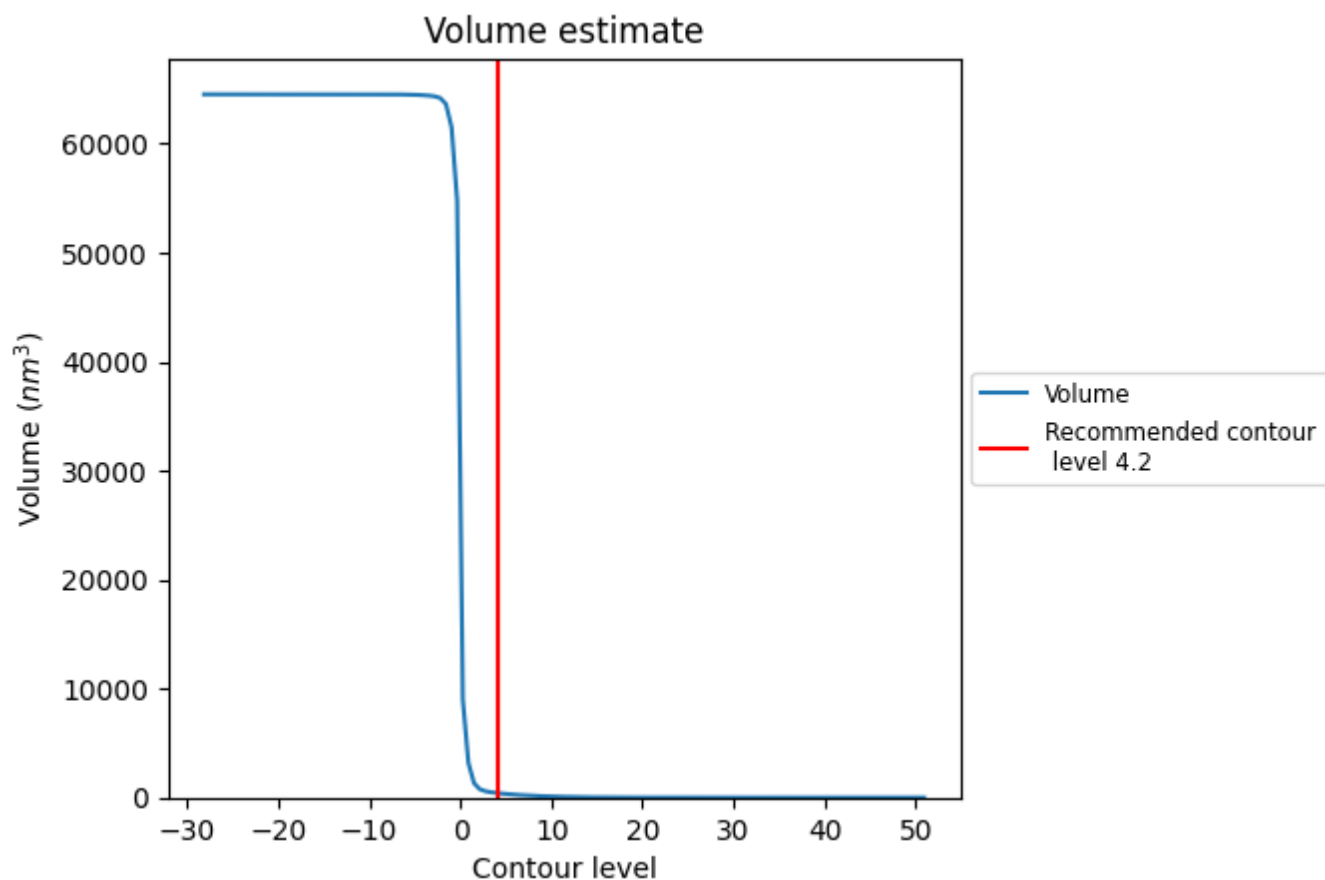
This section contains the results of statistical analysis of the map.

### 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.

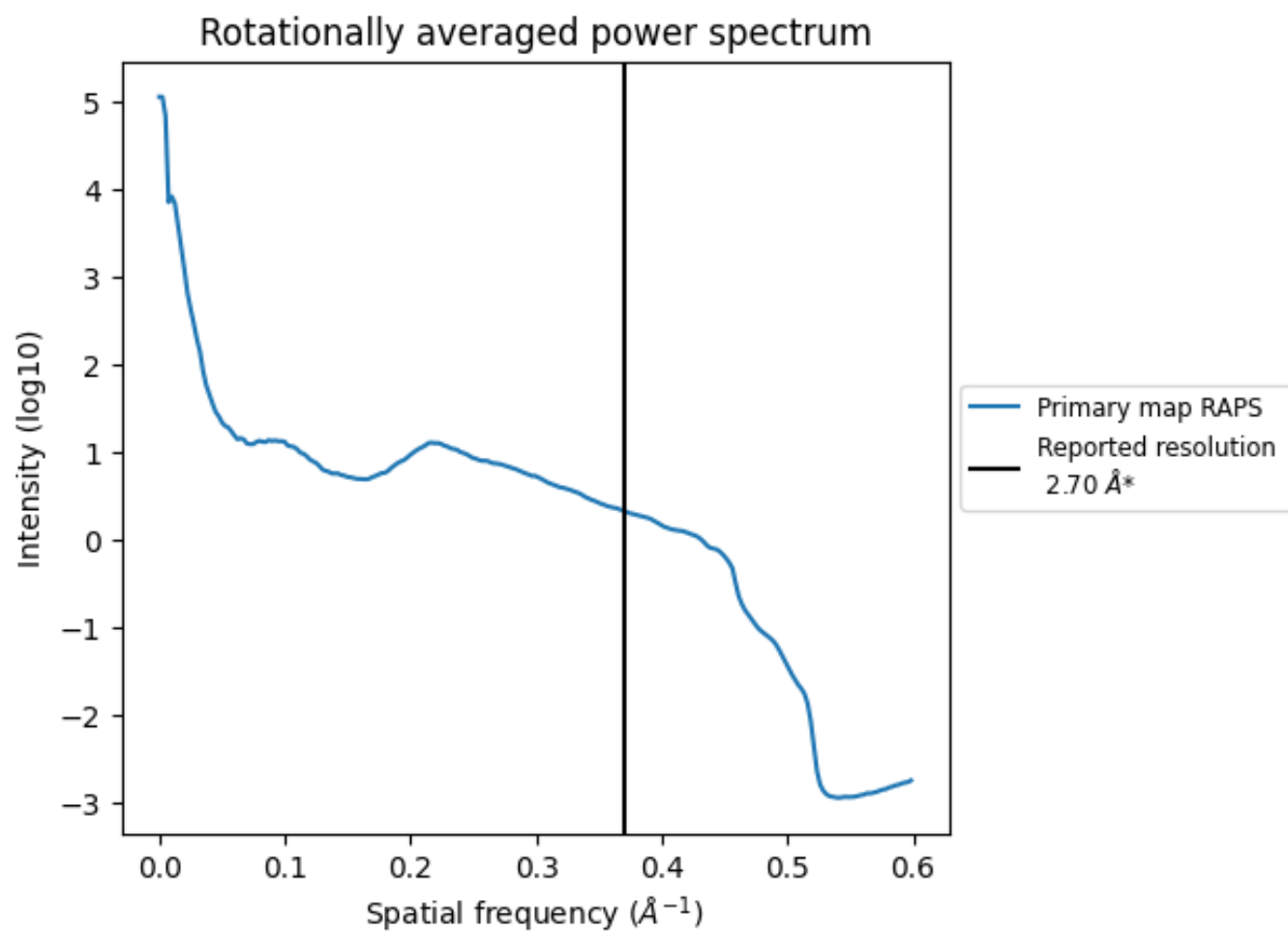
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 400 nm<sup>3</sup>; this corresponds to an approximate mass of 361 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.370 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

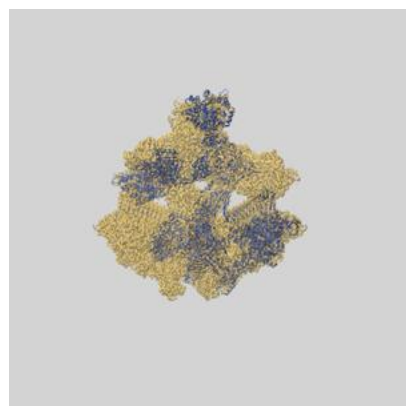
This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

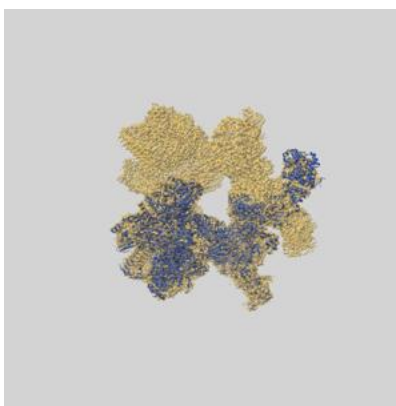
This section contains information regarding the fit between EMDB map EMD-55299 and PDB model 9SW6. Per-residue inclusion information can be found in section 3 on page 15.

### 9.1 Map-model overlays

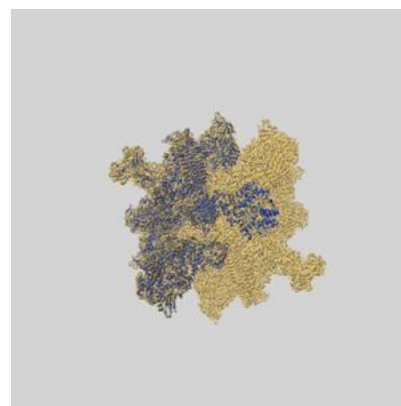
#### 9.1.1 Map-model overlay [i](#)



X

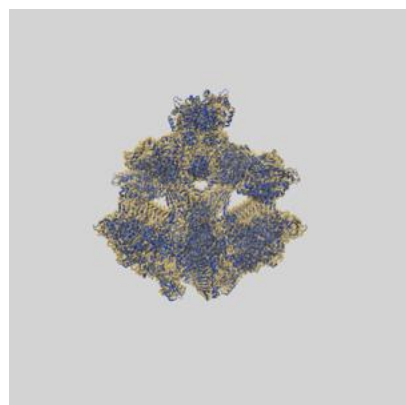


Y

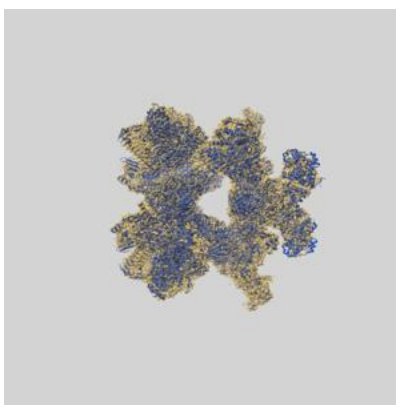


Z

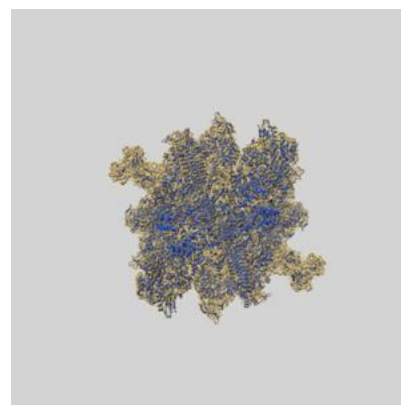
#### 9.1.2 Map-model assembly overlay [i](#)



X



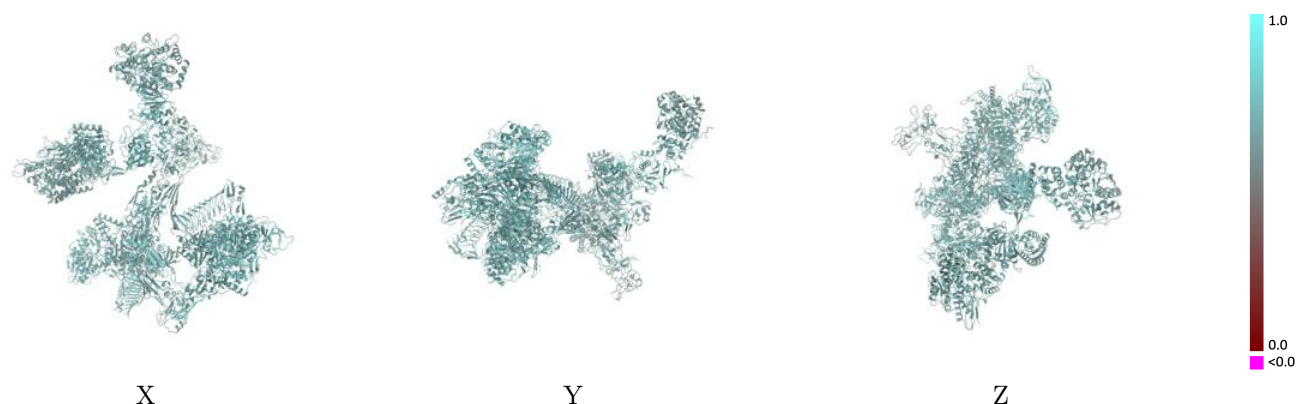
Y



Z

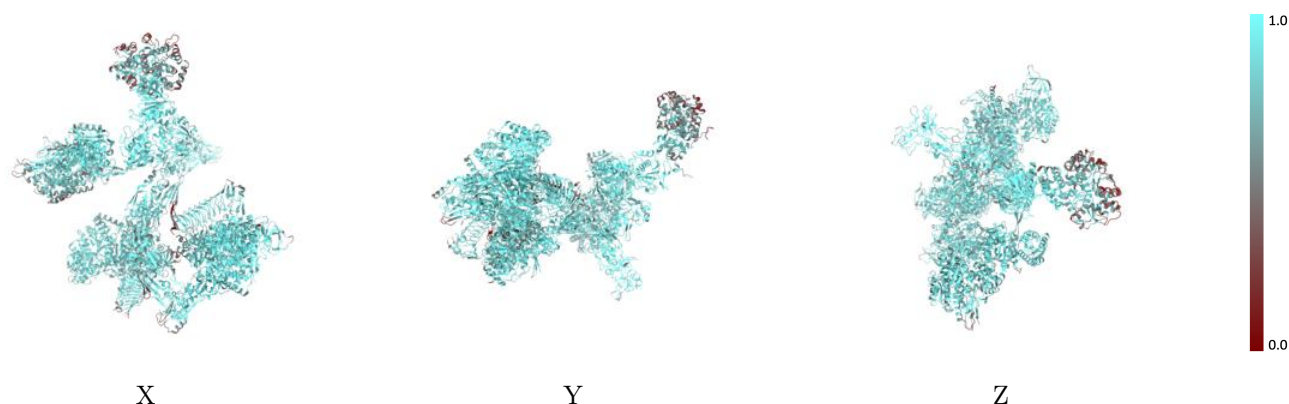
The images above show the 3D surface view of the map at the recommended contour level 4.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



The images above show the model with each residue coloured according 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.

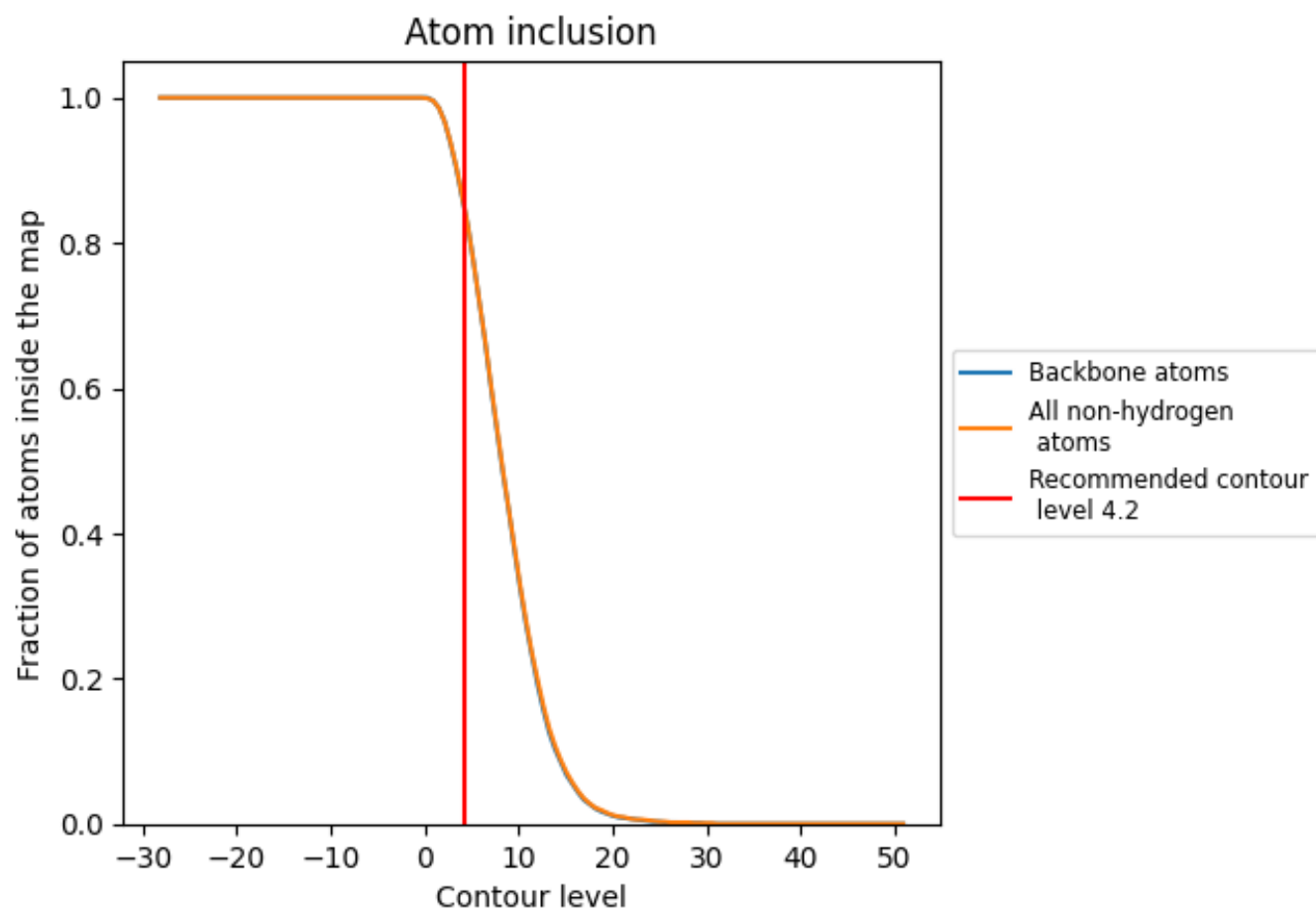
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (4.2).







































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 85% 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 (4.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.6750
A	 0.9100	 0.6790
B	 0.6190	 0.6270
C	 0.6840	 0.6450
D	 0.8610	 0.6590
E	 0.8240	 0.6530
F	 0.8210	 0.6340
G	 0.8570	 0.6050
H	 0.8720	 0.6760
I	 0.9080	 0.7210
J	 0.9200	 0.7210
K	 0.8010	 0.6790
L	 0.9310	 0.7220
h	 0.8130	 0.6530
i	 0.9190	 0.7050
j	 0.9120	 0.7010
k	 0.7840	 0.6640
l	 0.9100	 0.6950

