



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:45 PM UTC

PDB ID : 7U1Z / pdb_00007u1z
Title : Crystal structure of the DRBD and CROPs of TcdA
Authors : Baohua, C.; Peng, C.; Kay, P.; Rongsheng, J.
Deposited on : 2022-02-22
Resolution : 3.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

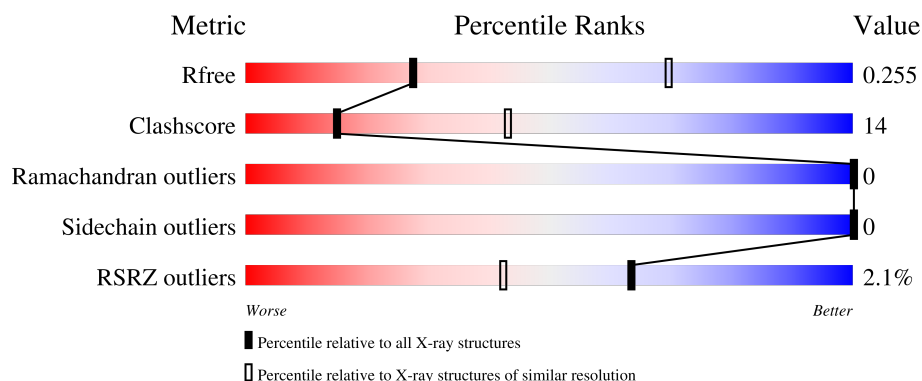
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.18 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

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

Mol	Chain	Length	Quality of chain
1	A	1640	71% 28% .
1	B	1640	3% 70% 28% .

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
2	SO4	A	2502	-	-	X	-

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25621 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

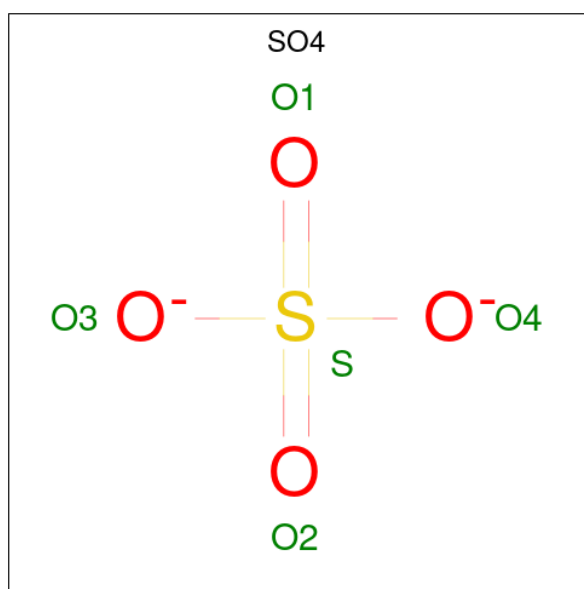
- Molecule 1 is a protein called Toxin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1612	Total	C	N	O	S	14	0	0
			12649	8130	2021	2480	18			
1	A	1620	Total	C	N	O	S	4	0	0
			12792	8213	2050	2511	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	842	SER	-	expression tag	UNP P16154
A	842	SER	-	expression tag	UNP P16154

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		

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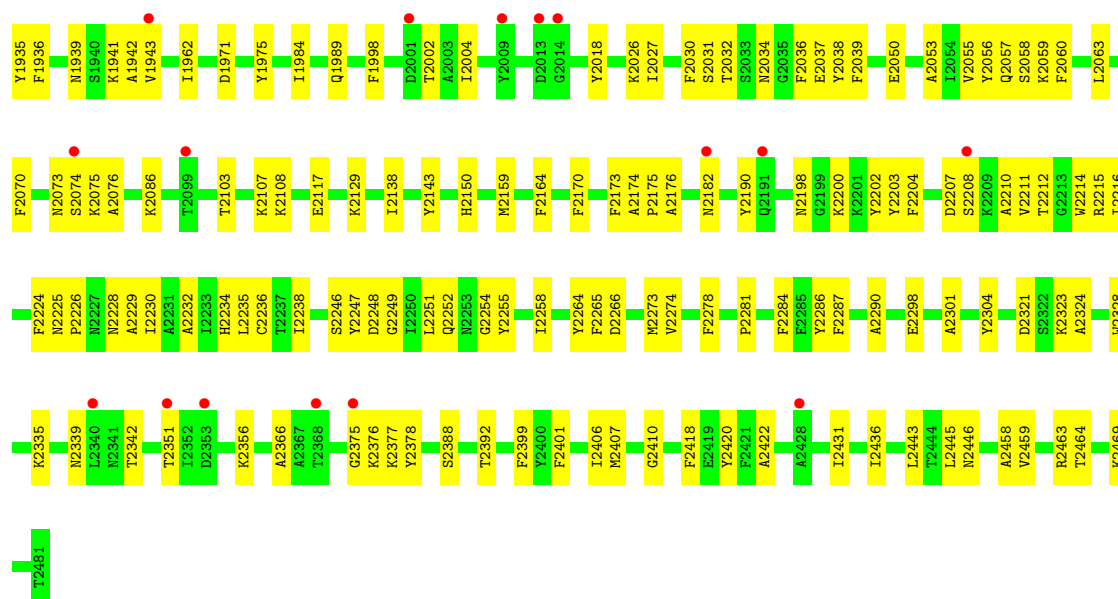
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

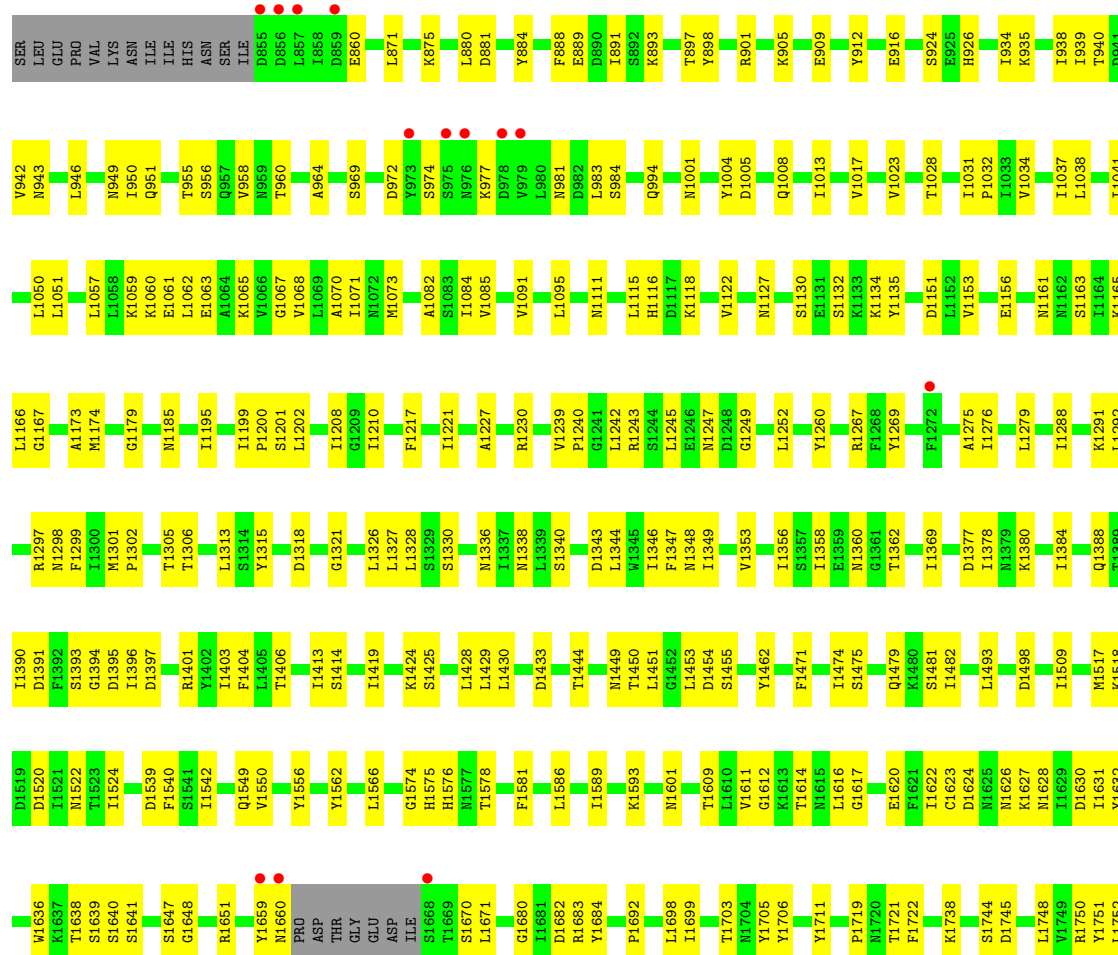
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		



• Molecule 1: Toxin A



F2399	A2290	K2107	Y1976	K1881	L1760
N2402	N2291	K2128	F1977	H1882	L1764
Q2408	N2295	F2132	N1978	F1883	I1765
I2409	N2296	F2132	T1981	I1765	K1766
G2410	I2297	T2138	A1982	A1892	G1767
V2411	E2298	A2139	I1983	L1893	I1768
A2422	I2302	S2140	W1988	K1897	M1778
P2423	V2303	T2141	Q1989	T1990	S1779
A2424	Y2304	T2144	V1991	F1902	L1788
N2430	K2307	F2153	S1994	F1903	L1788
I2431	T2310	N2154	R1995	Y1904	Y1792
E2432	K2314	T2155	F1998	P1907	I1793
G2433	K2315	I2158	T2002	T1910	N1796
Q2434	Y2316	N2159	A2003	Q1911	F1797
A2435	Y2317	Q2160	I2004	I1915	K1798
I2436	N2320	G2162	A2005	E1916	S1799
L2443	D2321	V2163	F2006	G1917	L1806
T2444	S2322	N2192	N2007	Q1918	L1806
L2445	V2325	T2196	K2010	V1921	H1810
Y2450	W2328	L2197	F2019	Y1922	L1811
T2464	Q2329	K2201	D2020	Q1923	I1815
K2469	T2330	Y2202	V2024	S1924	I1816
N2473	K2334	V2203	V2025	L1927	D1817
T2476	F2338	F2204	K2026	T1928	T1820
V2478	A2345	N2225	A2040	L1929	D1824
T2481	I2352	N2228	I2054	Y1935	E1825
	F2359	A2229	V2055	F1936	D1826
	E2365	I2230	Y2056	D1937	S1827
	T2368	L2235	Q2057	N1938	K1828
	G2369	Y2243	S2058	N1939	K1831
	W2370	S2246	T2062	S1940	Q1832
	Q2371	D2247	N2064	K1941	L1833
	T2372	D2248	G2065	A1942	L1833
	K2377	L2251	F2070	V1943	L1840
	Y2378	Q2252	S2074	T1944	F1841
	Y2379	N2253	K2075	T1949	Y1842
	F2385	F2285	A2076	E1952	K1848
	S2388	S2271	L2080	K1953	N1849
	I2394	K2272	T2092	F1956	L1850
	N2395	N2273	I2104	N1957	V1851
		V2277		P1958	T1852
				A1963	K1860
				L1967	F1864
				N1973	D1865
					I1866
					A1871

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	379.51Å 187.64Å 95.32Å 90.00° 101.30° 90.00°	Depositor
Resolution (Å)	186.08 – 3.18 186.08 – 3.18	Depositor EDS
% Data completeness (in resolution range)	98.8 (186.08-3.18) 99.1 (186.08-3.18)	Depositor EDS
R_{merge}	0.28	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.254 0.208 , 0.255	Depositor DCC
R_{free} test set	5514 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25621	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.47	0/13082	0.71	0/17780
1	B	0.47	0/12936	0.72	2/17588 (0.0%)
All	All	0.47	0/26018	0.71	2/35368 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1780	ILE	CA-C-N	-5.19	114.32	122.73
1	B	1780	ILE	C-N-CA	-5.19	114.32	122.73

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12792	0	12186	342	0
1	B	12649	0	11970	346	0
2	A	80	0	0	7	0
2	B	100	0	0	3	0
All	All	25621	0	24156	681	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 14.

The worst 5 of 681 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ILE:HG13	1:A:949:ASN:HB2	1.42	0.99
1:A:1624:ASP:HB3	1:A:1626:ASN:H	1.39	0.88
1:A:951:GLN:HE22	1:A:960:THR:HG21	1.37	0.87
1:B:1781:ASP:HB2	1:B:1786:LYS:HA	1.57	0.86
1:B:1428:LEU:HD22	1:B:1455:SER:HB2	1.57	0.85

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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1616/1640 (98%)	1492 (92%)	124 (8%)	0	100	100
1	B	1606/1640 (98%)	1483 (92%)	123 (8%)	0	100	100
All	All	3222/3280 (98%)	2975 (92%)	247 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1379/1455 (95%)	1379 (100%)	0	100	100
1	B	1345/1455 (92%)	1345 (100%)	0	100	100
All	All	2724/2910 (94%)	2724 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 42 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1576	HIS
1	A	2007	ASN
1	A	1704	ASN
1	A	1892	GLN
1	A	2291	ASN

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](#)

36 ligands 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
2	SO4	B	2505	-	4,4,4	0.29	0	6,6,6	0.19	0
2	SO4	A	2503	-	4,4,4	0.37	0	6,6,6	0.25	0
2	SO4	A	2515	-	4,4,4	0.20	0	6,6,6	0.32	0
2	SO4	B	2509	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	B	2504	-	4,4,4	0.26	0	6,6,6	0.31	0
2	SO4	A	2507	-	4,4,4	0.35	0	6,6,6	0.16	0
2	SO4	A	2505	-	4,4,4	0.37	0	6,6,6	0.49	0
2	SO4	B	2518	-	4,4,4	0.35	0	6,6,6	0.47	0
2	SO4	B	2502	-	4,4,4	0.35	0	6,6,6	0.27	0
2	SO4	A	2510	-	4,4,4	0.30	0	6,6,6	0.13	0
2	SO4	A	2508	-	4,4,4	0.32	0	6,6,6	0.26	0
2	SO4	A	2512	-	4,4,4	0.32	0	6,6,6	0.25	0
2	SO4	B	2511	-	4,4,4	0.33	0	6,6,6	0.34	0
2	SO4	B	2519	-	4,4,4	0.35	0	6,6,6	0.24	0
2	SO4	B	2516	-	4,4,4	0.29	0	6,6,6	0.22	0
2	SO4	A	2502	-	4,4,4	0.32	0	6,6,6	0.51	0
2	SO4	B	2517	-	4,4,4	0.33	0	6,6,6	0.43	0
2	SO4	B	2514	-	4,4,4	0.24	0	6,6,6	0.16	0
2	SO4	A	2516	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	B	2512	-	4,4,4	0.20	0	6,6,6	0.43	0
2	SO4	A	2514	-	4,4,4	0.30	0	6,6,6	0.20	0
2	SO4	B	2510	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	B	2513	-	4,4,4	0.26	0	6,6,6	0.25	0
2	SO4	B	2507	-	4,4,4	0.32	0	6,6,6	0.17	0
2	SO4	A	2501	-	4,4,4	0.40	0	6,6,6	0.27	0
2	SO4	B	2520	-	4,4,4	0.30	0	6,6,6	0.51	0
2	SO4	B	2501	-	4,4,4	0.32	0	6,6,6	0.28	0
2	SO4	A	2504	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	A	2506	-	4,4,4	0.33	0	6,6,6	0.43	0
2	SO4	B	2503	-	4,4,4	0.34	0	6,6,6	0.47	0
2	SO4	B	2515	-	4,4,4	0.31	0	6,6,6	0.41	0
2	SO4	A	2513	-	4,4,4	0.32	0	6,6,6	0.37	0
2	SO4	B	2508	-	4,4,4	0.31	0	6,6,6	0.33	0
2	SO4	B	2506	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	A	2509	-	4,4,4	0.34	0	6,6,6	0.40	0
2	SO4	A	2511	-	4,4,4	0.34	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

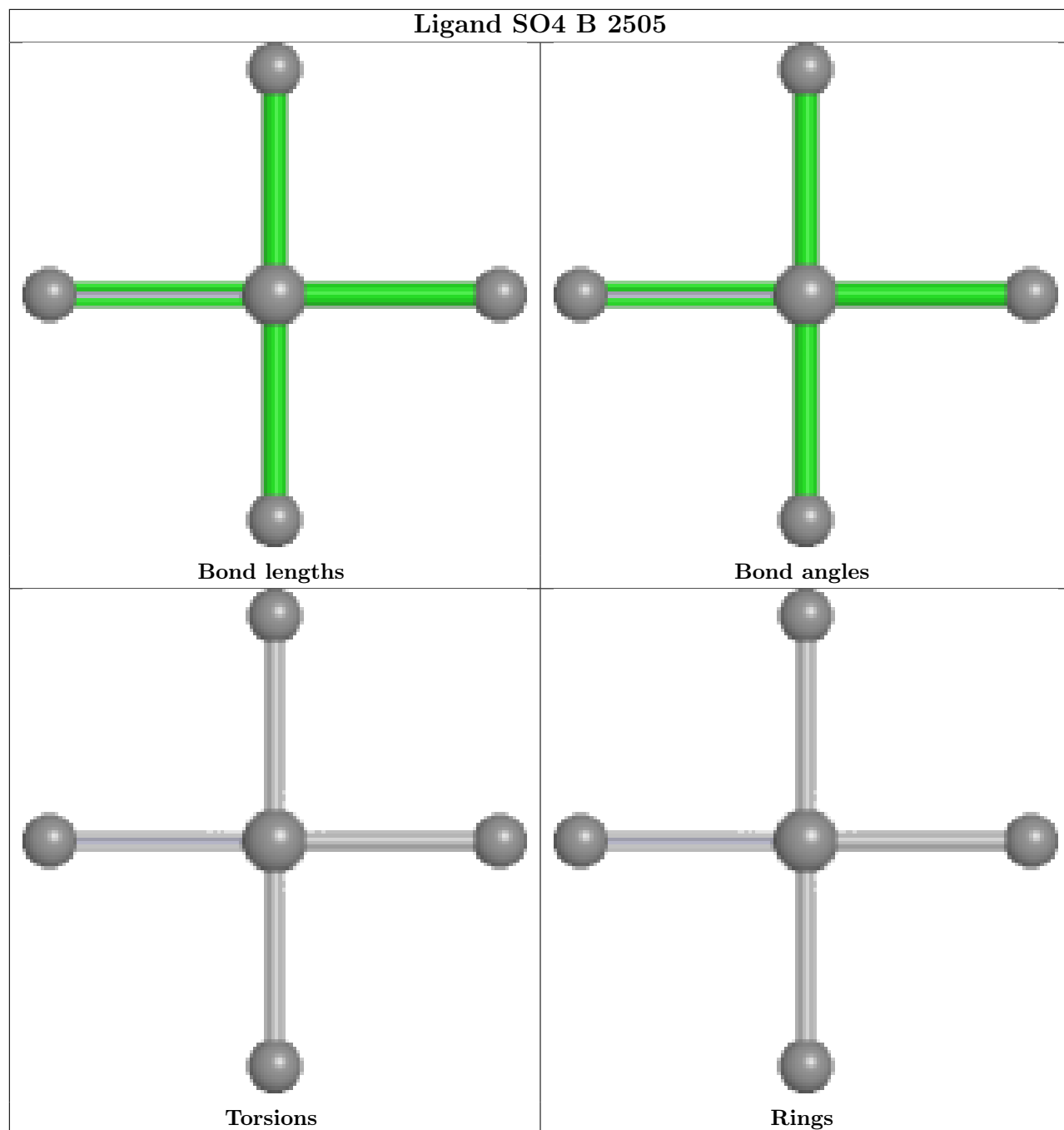
There are no torsion outliers.

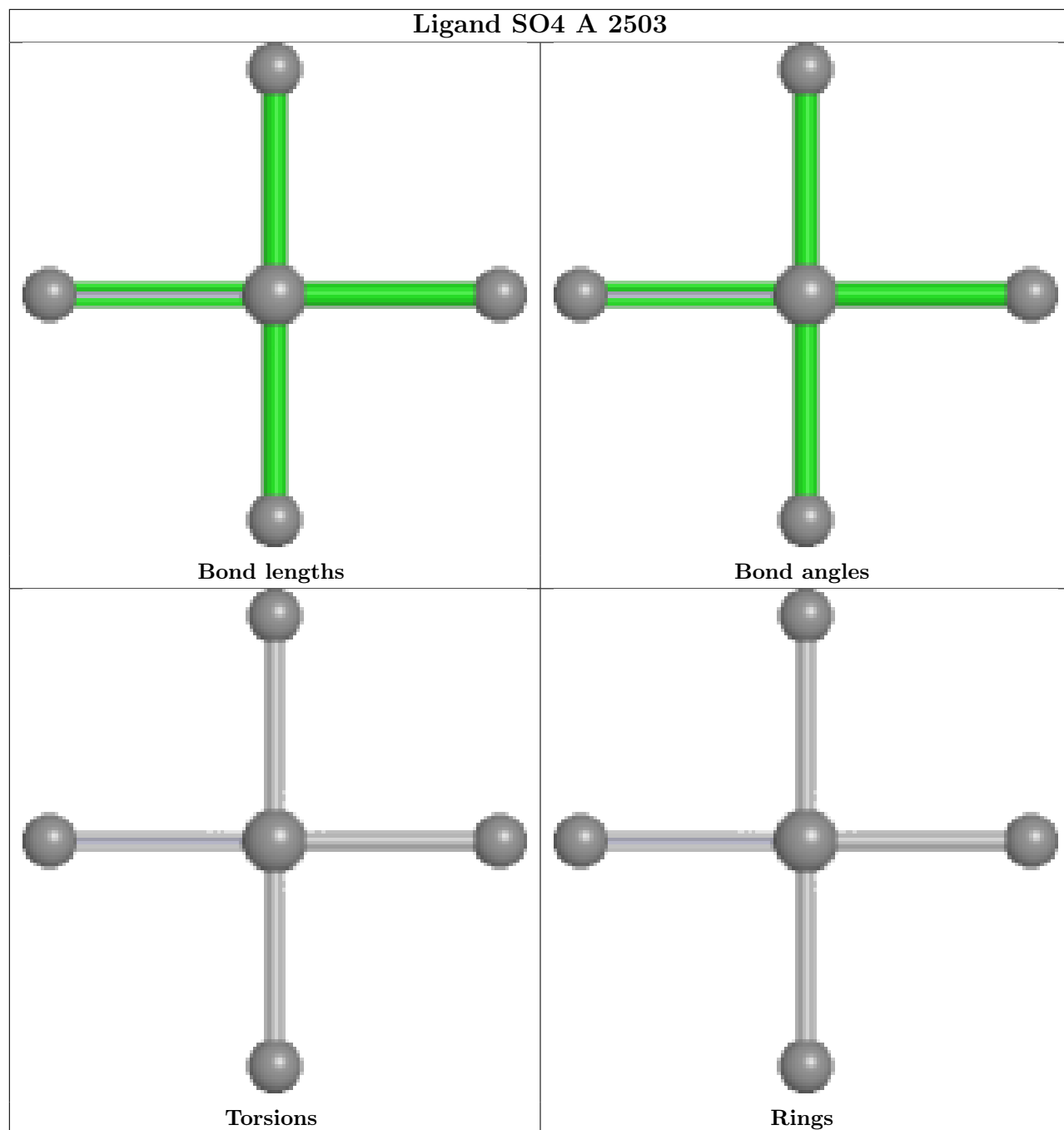
There are no ring outliers.

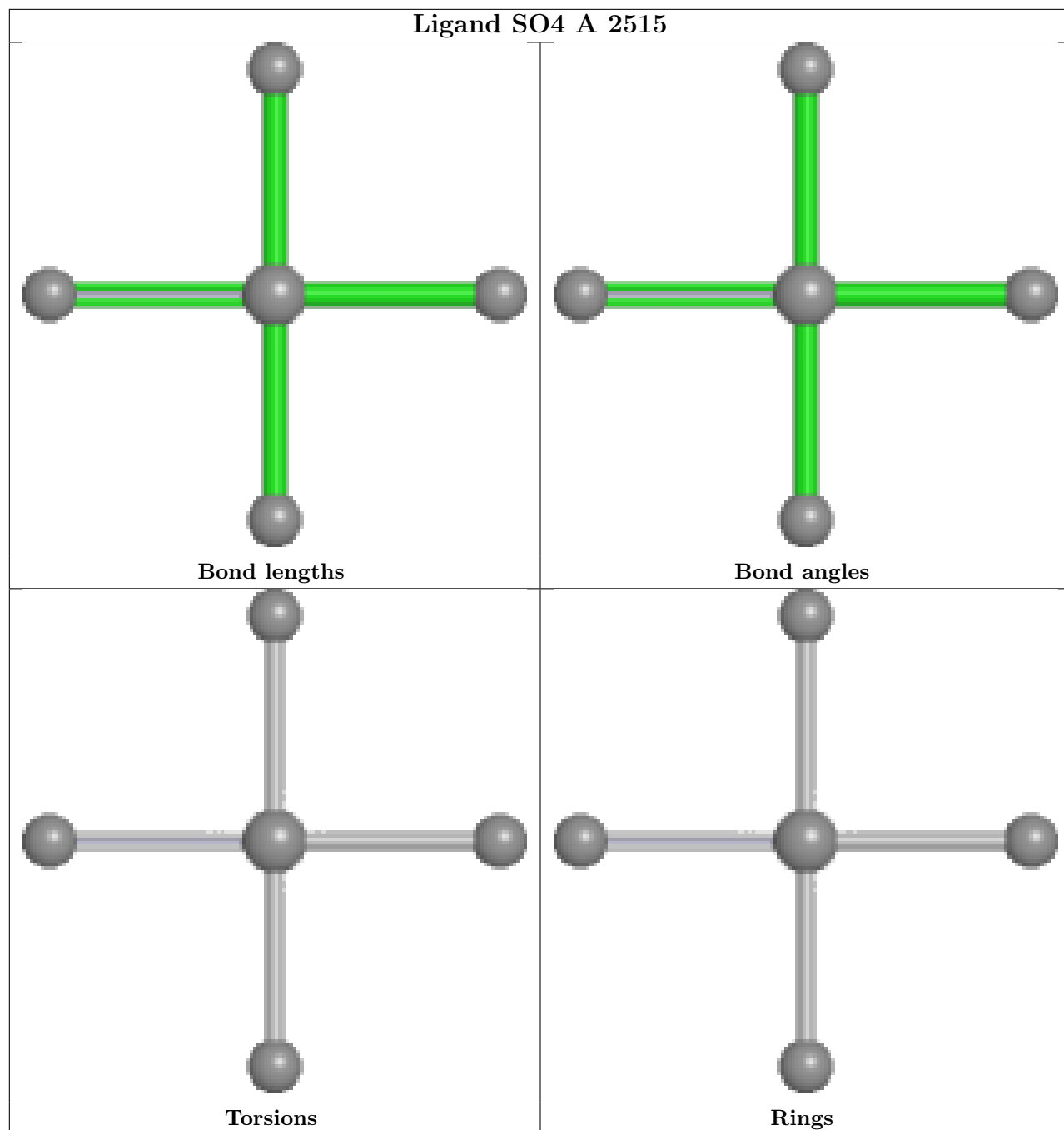
8 monomers are involved in 10 short contacts:

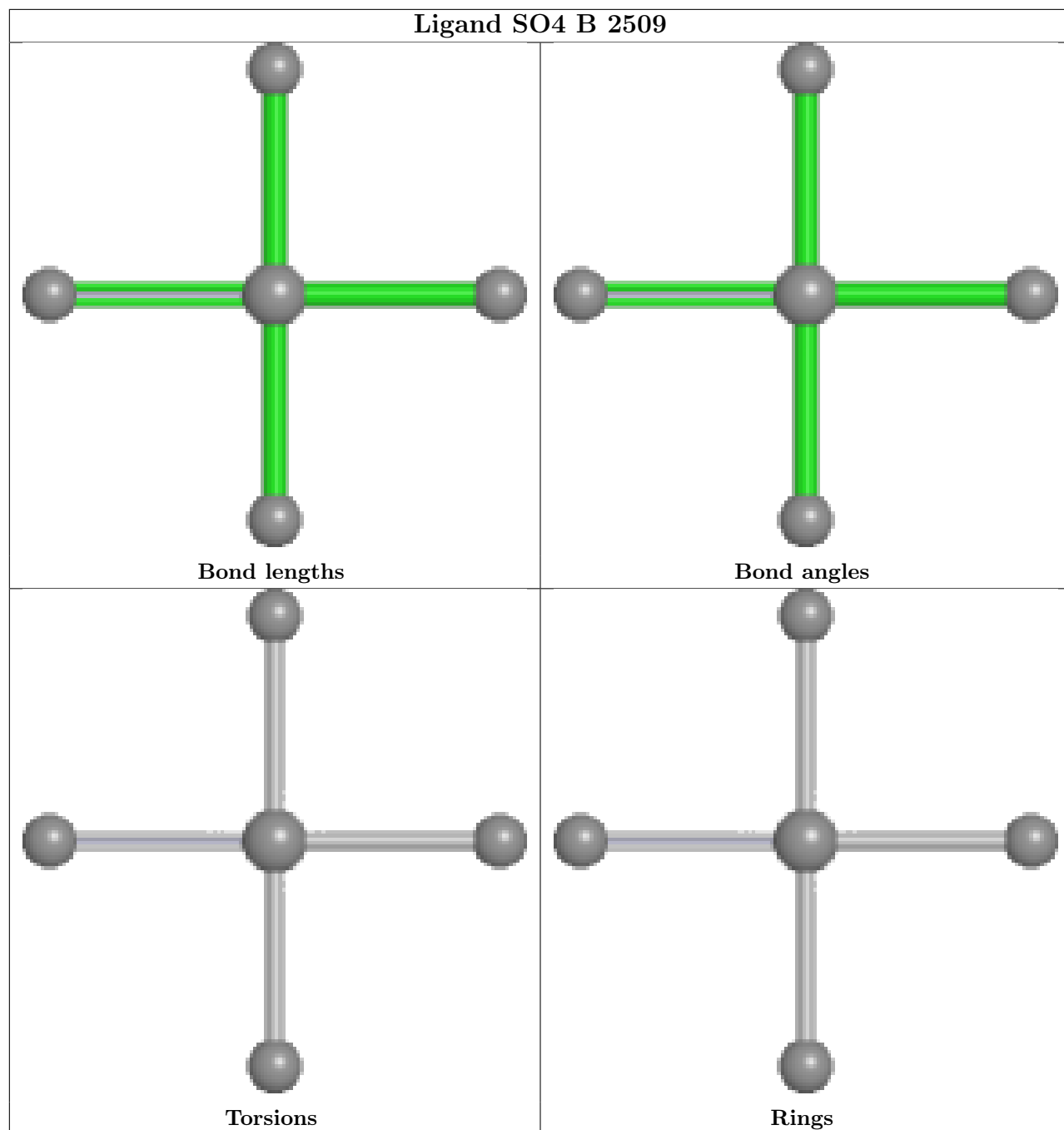
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2512	SO4	1	0
2	B	2511	SO4	1	0
2	A	2502	SO4	3	0
2	A	2501	SO4	1	0
2	A	2504	SO4	1	0
2	B	2503	SO4	1	0
2	B	2506	SO4	1	0
2	A	2509	SO4	1	0

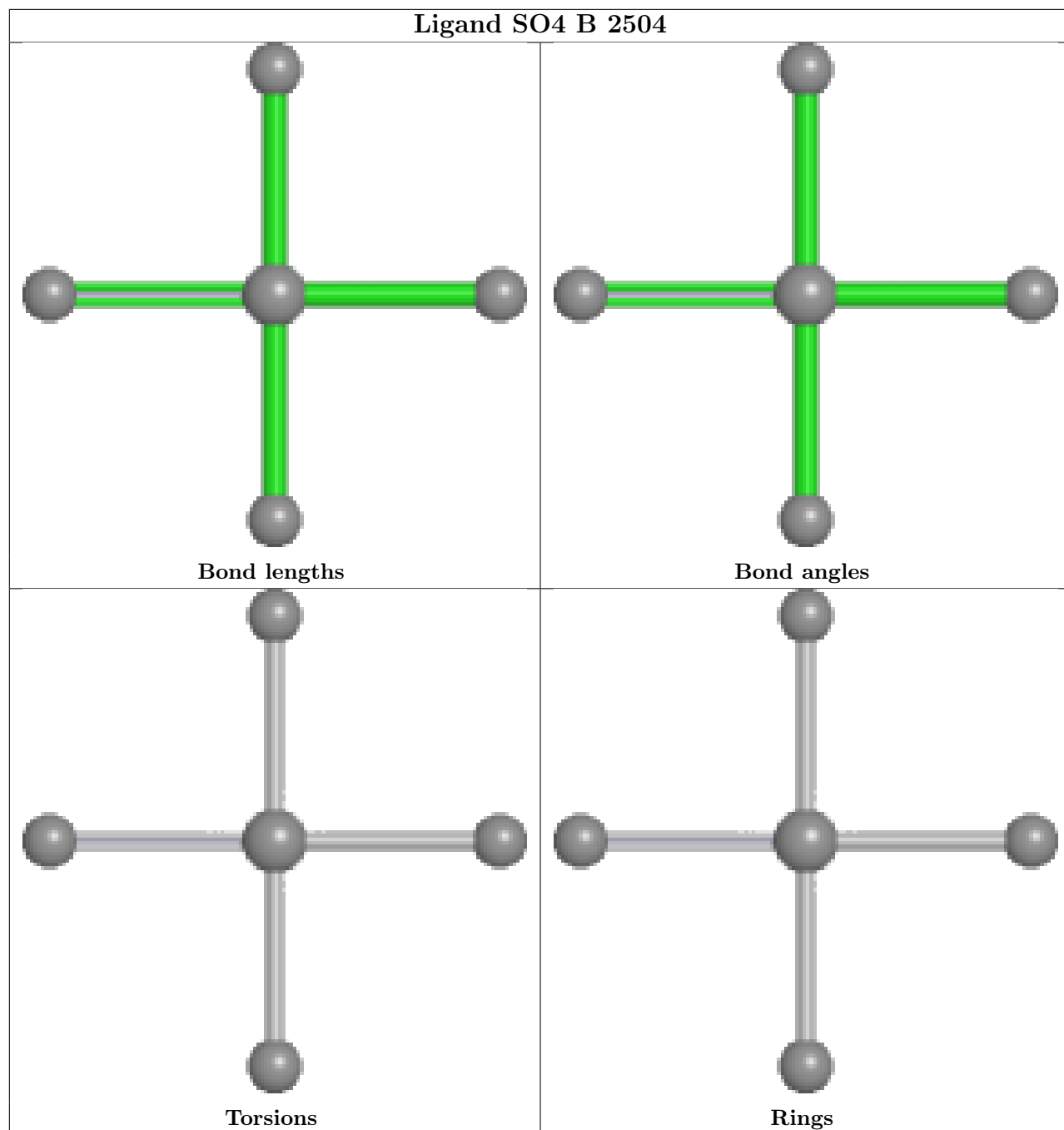
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

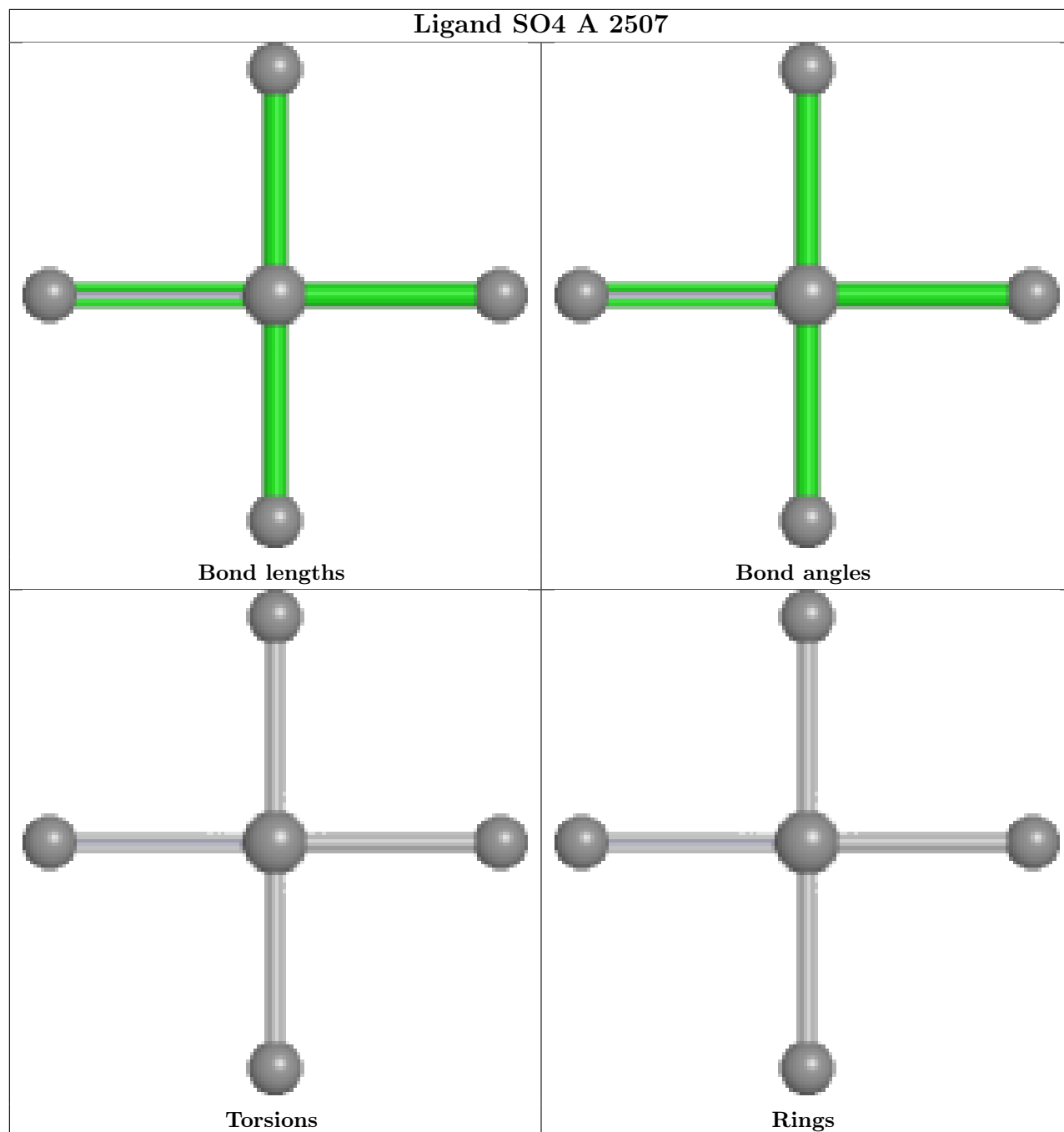


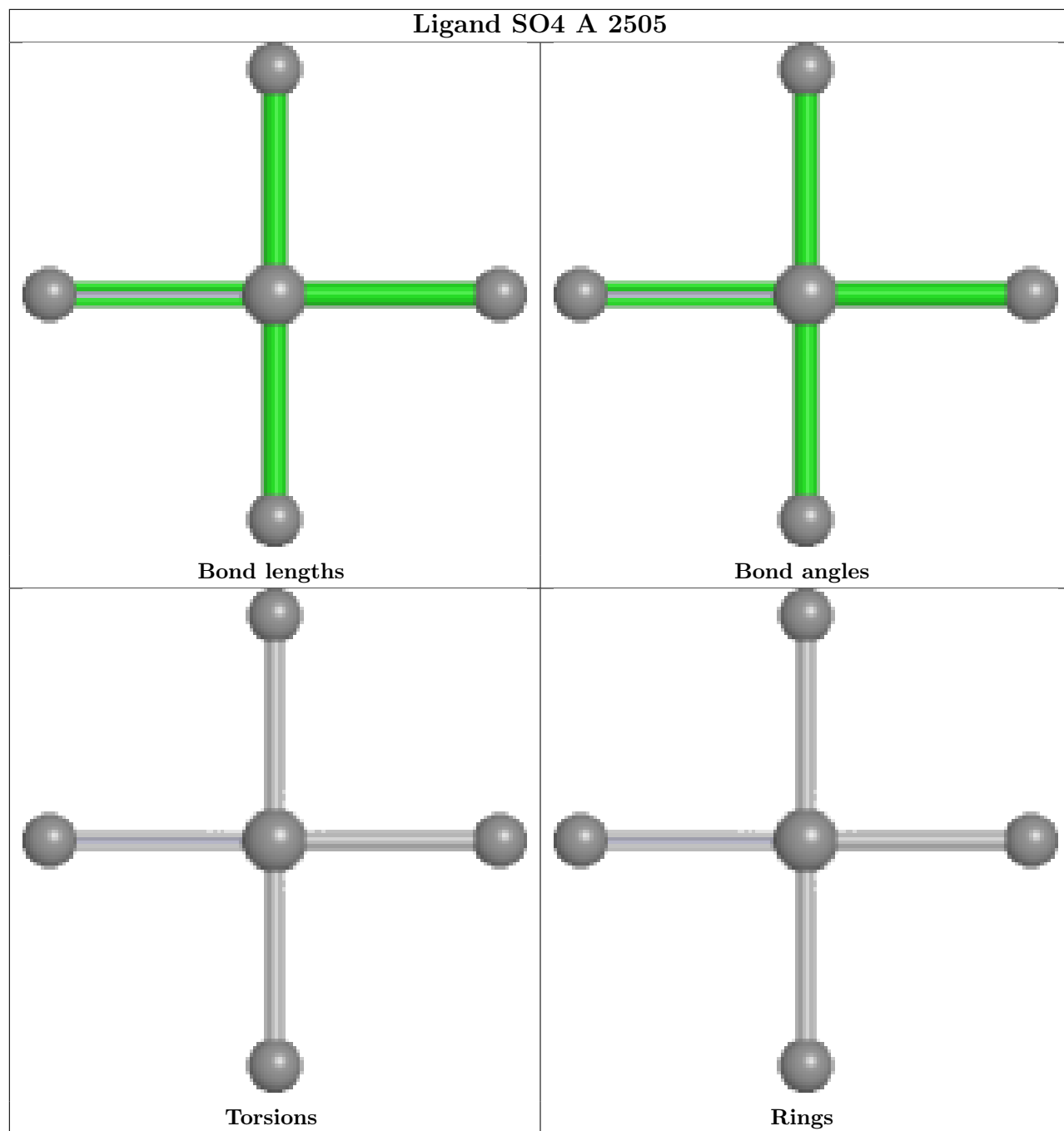


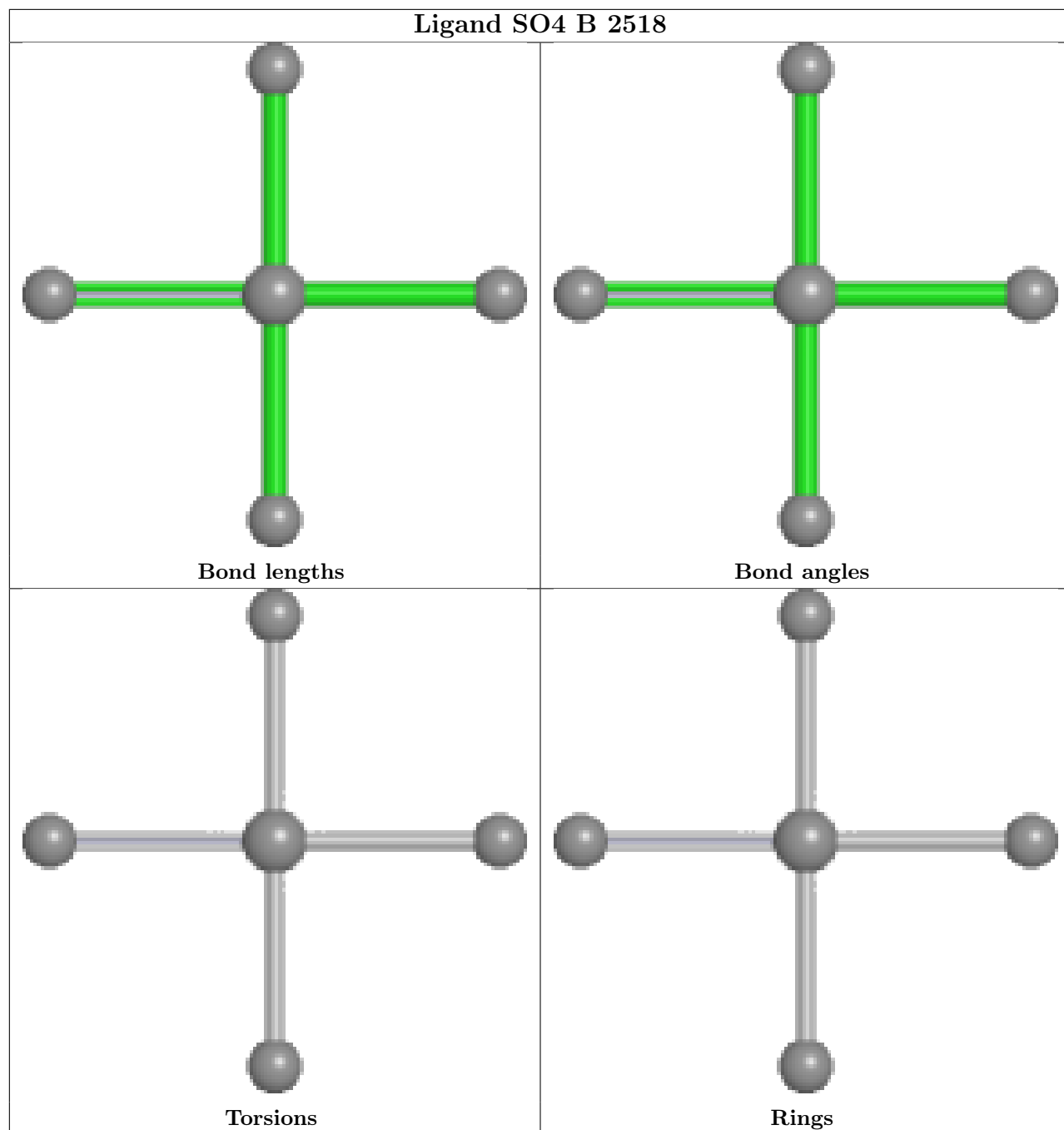


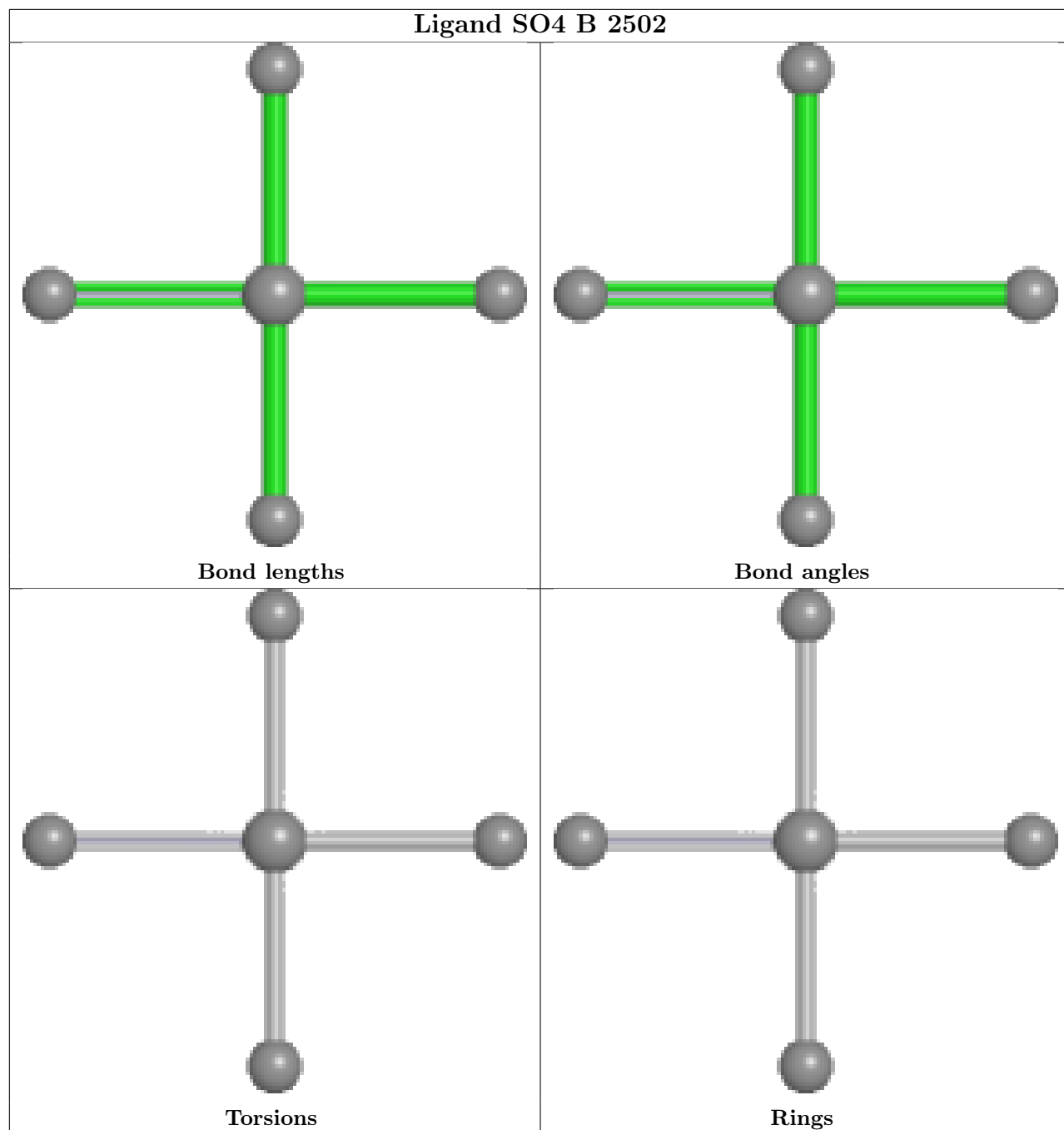


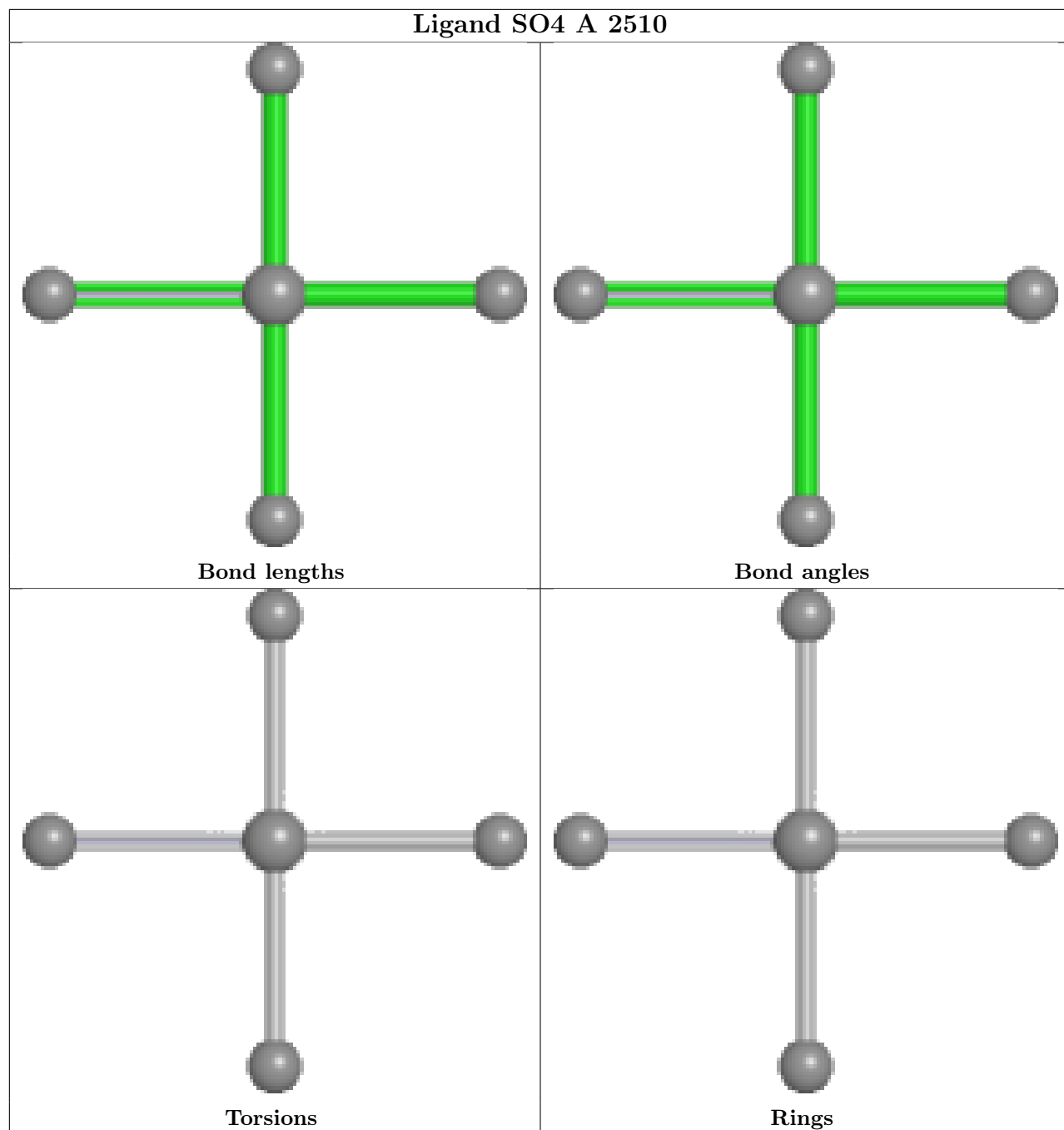


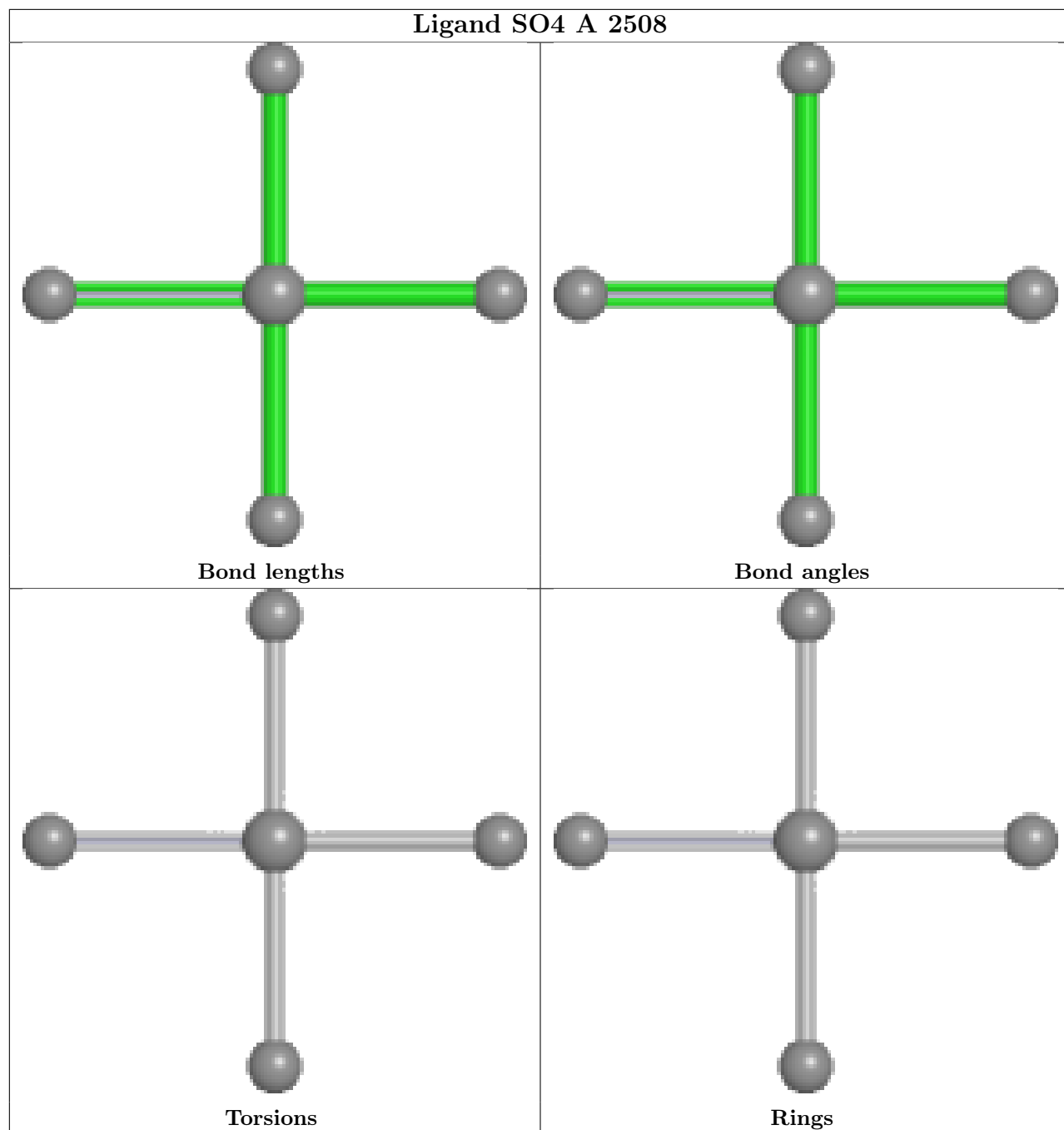


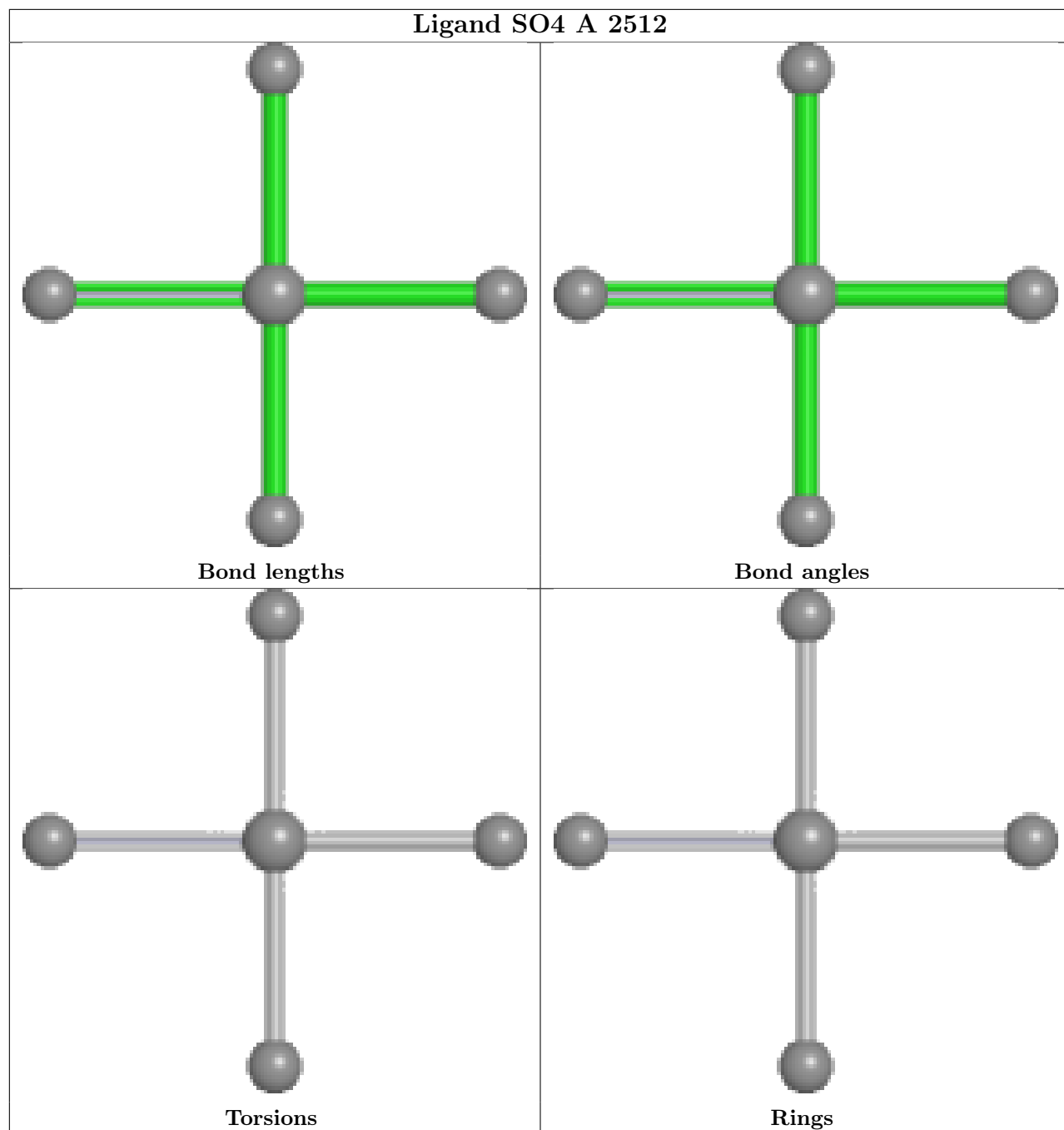


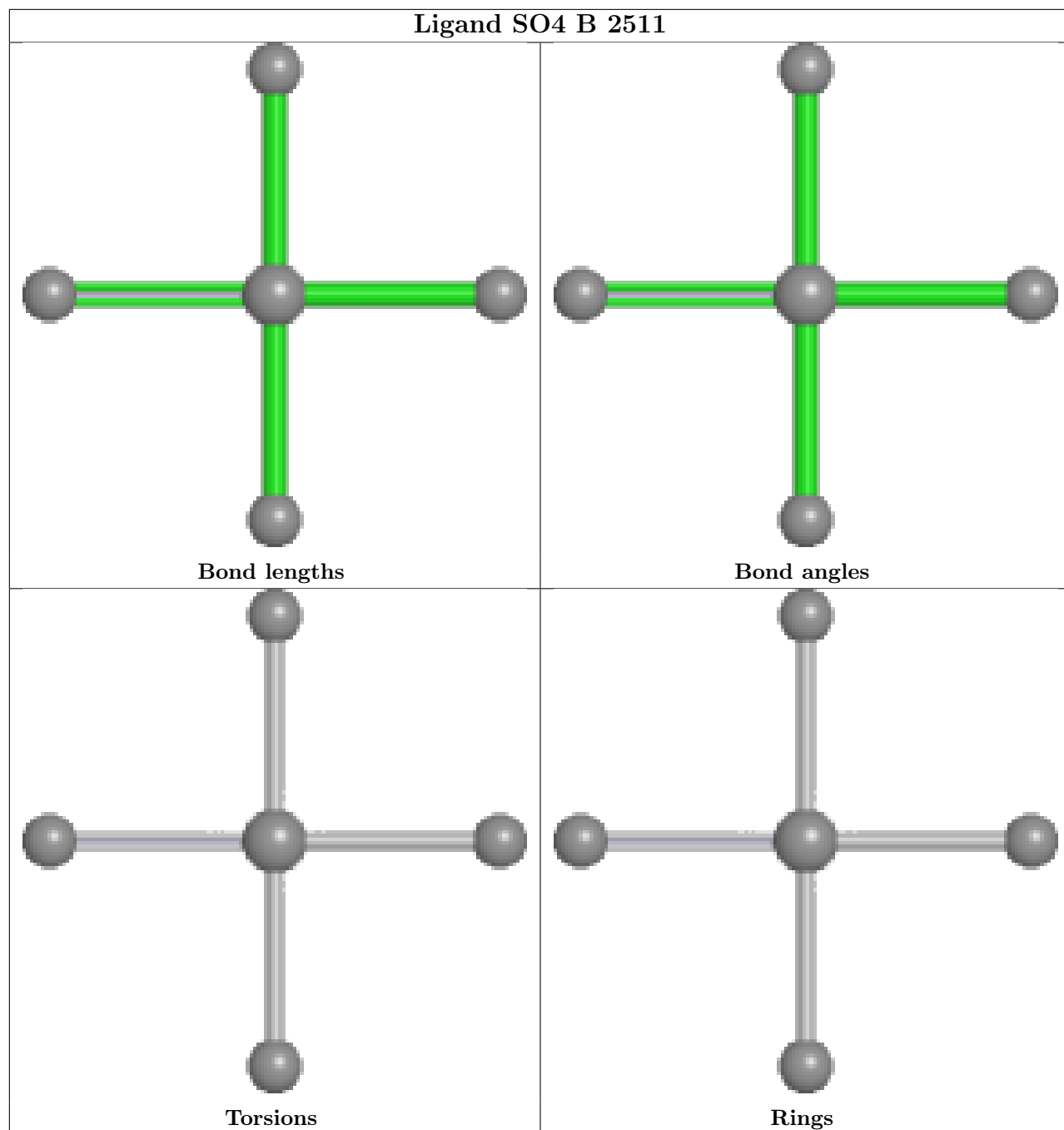


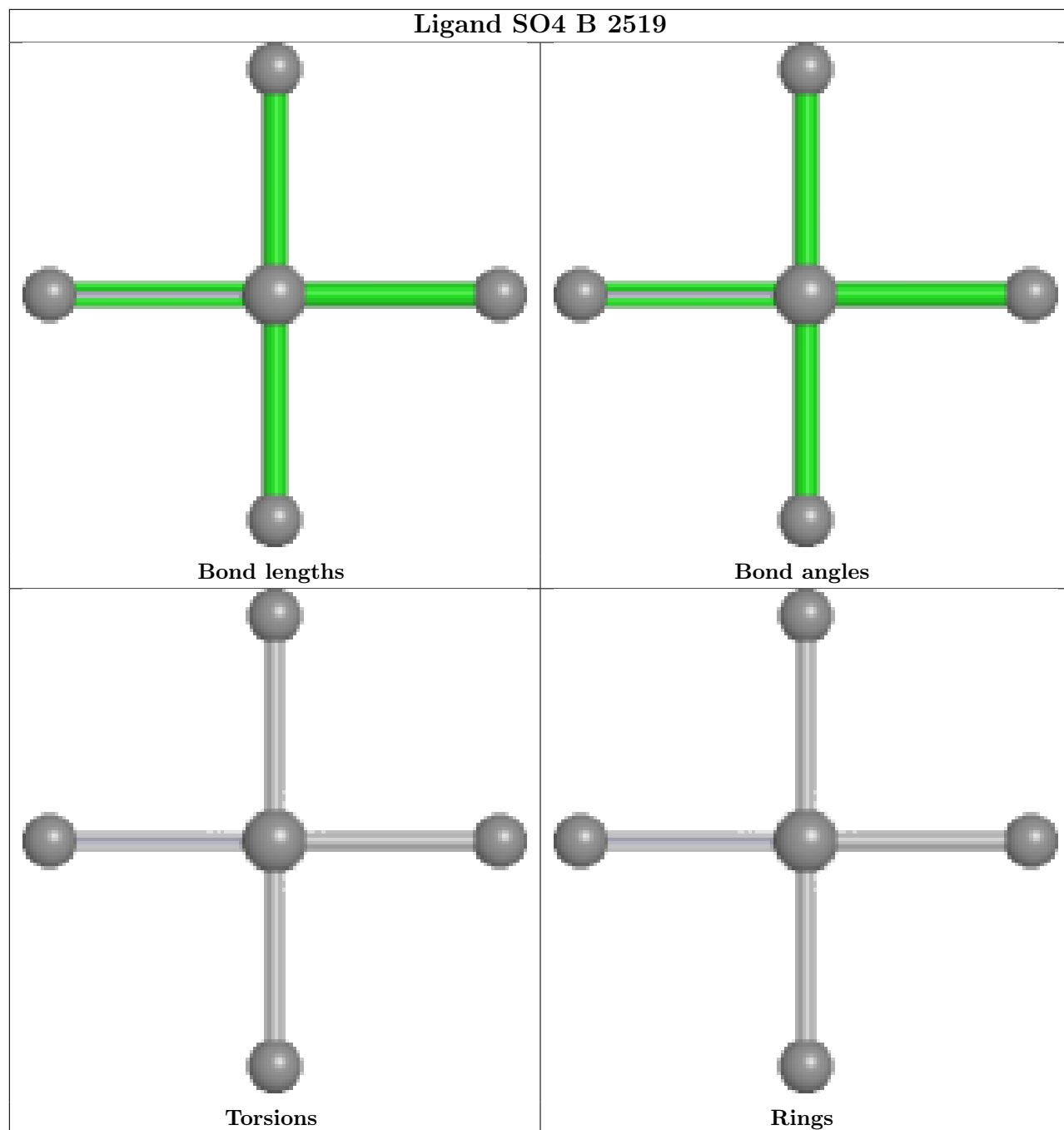


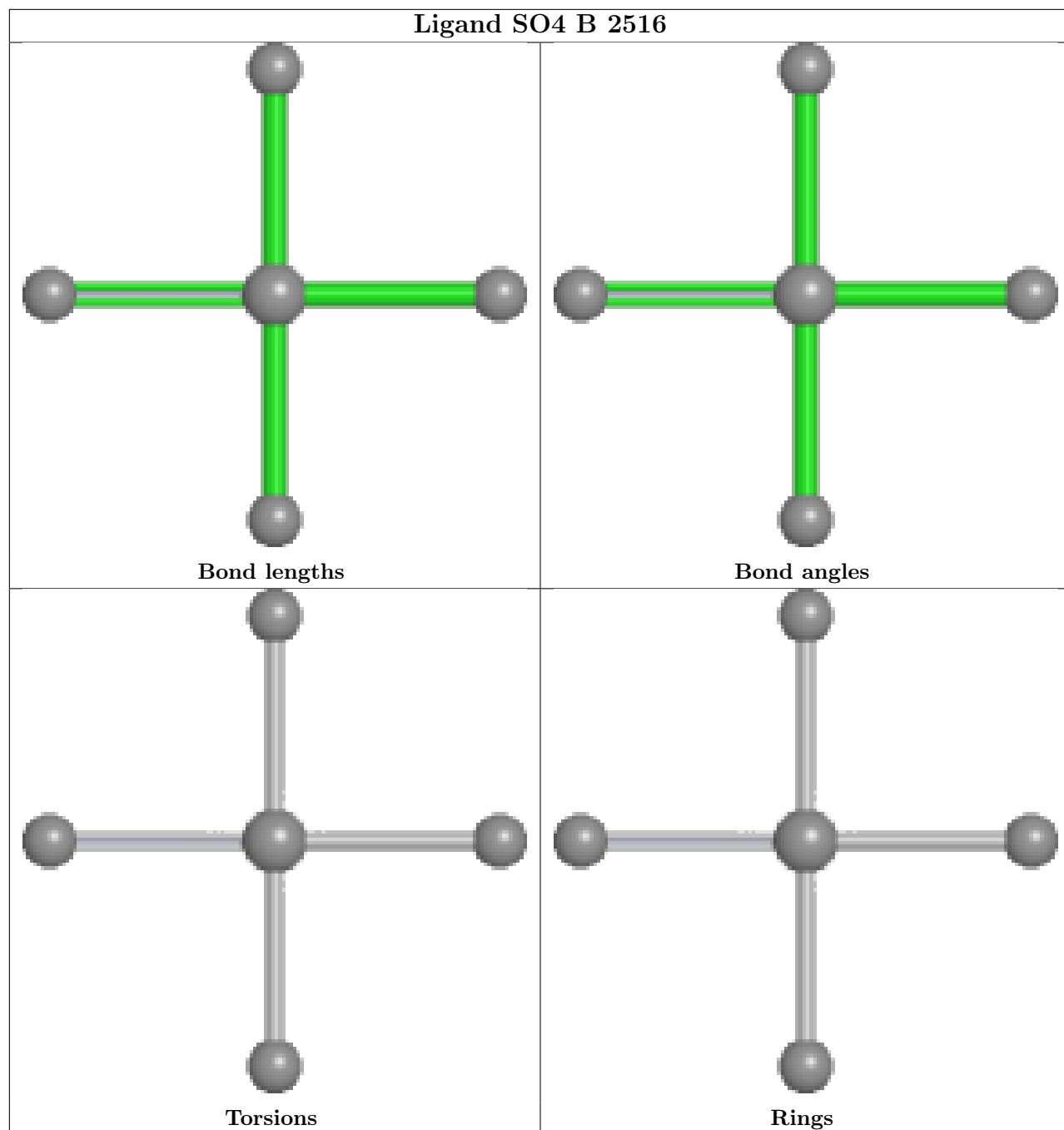


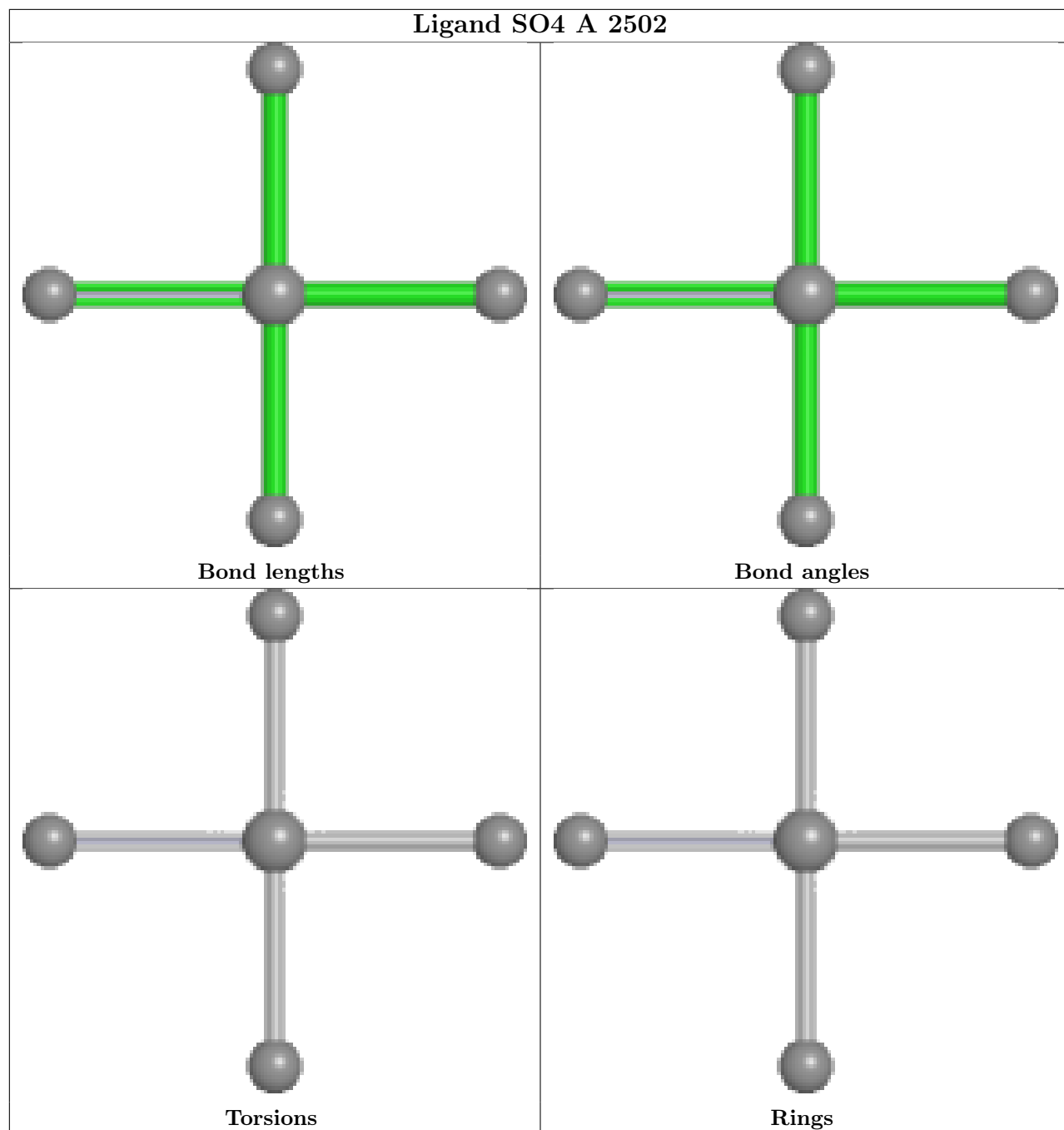


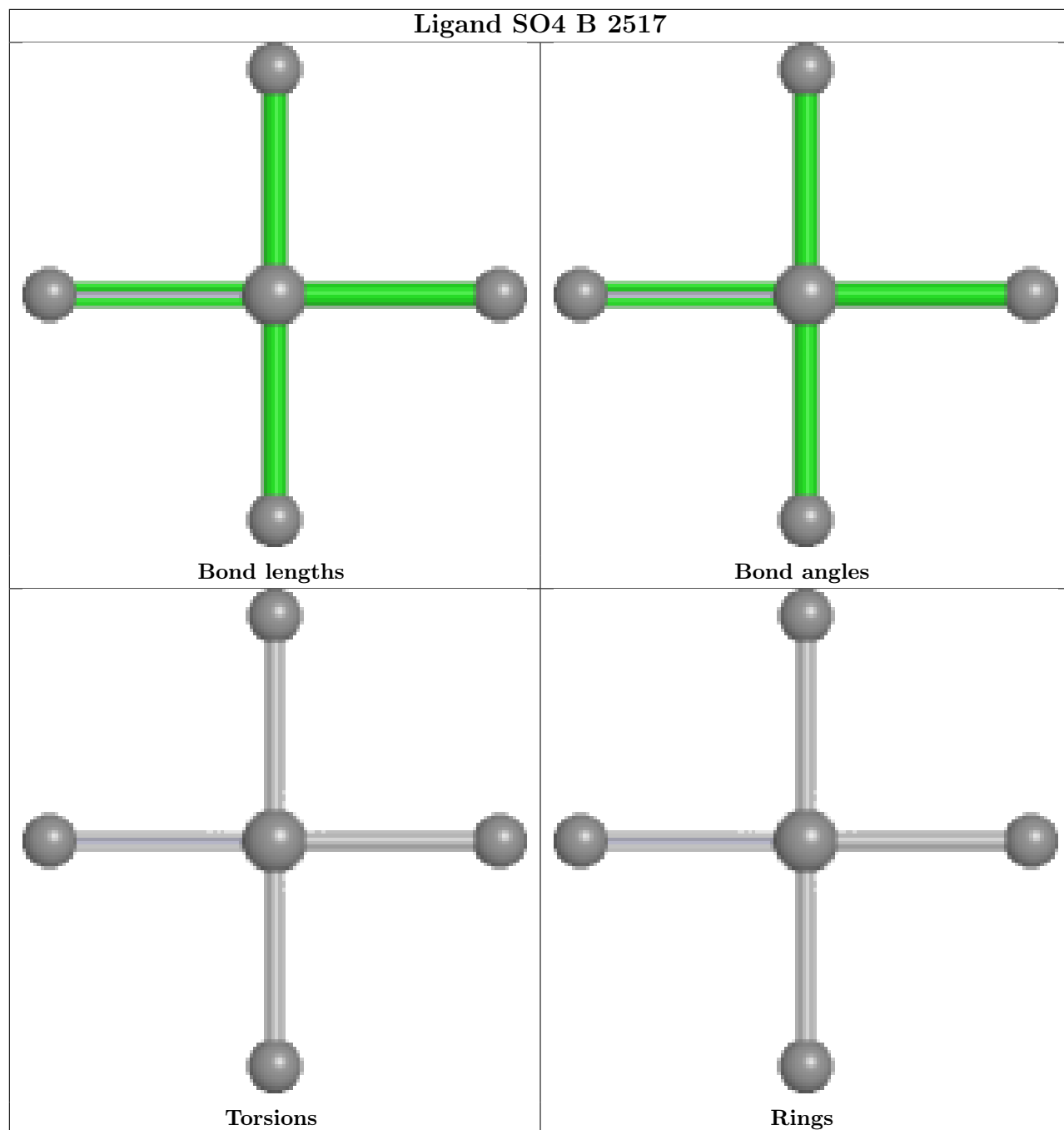


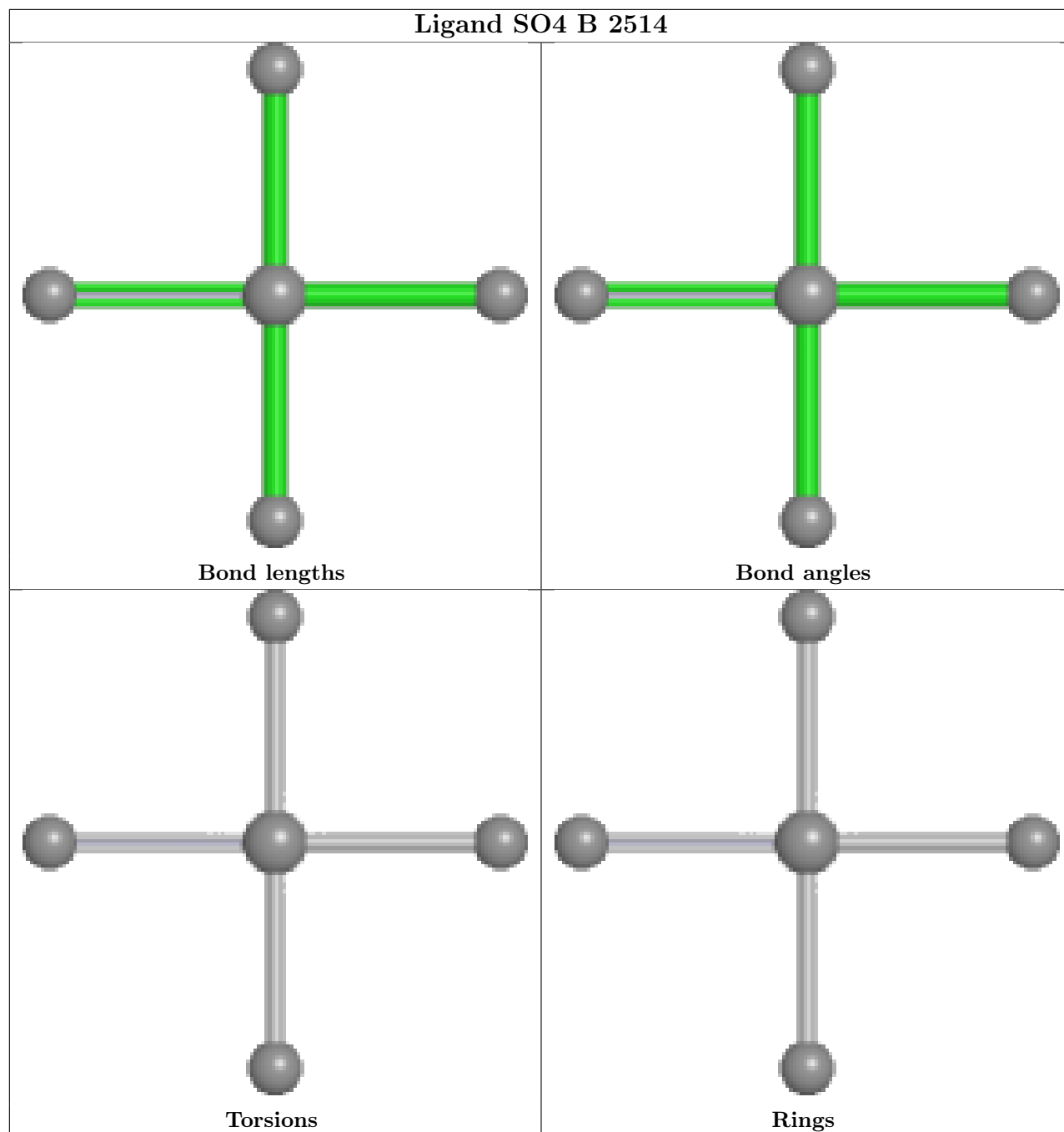


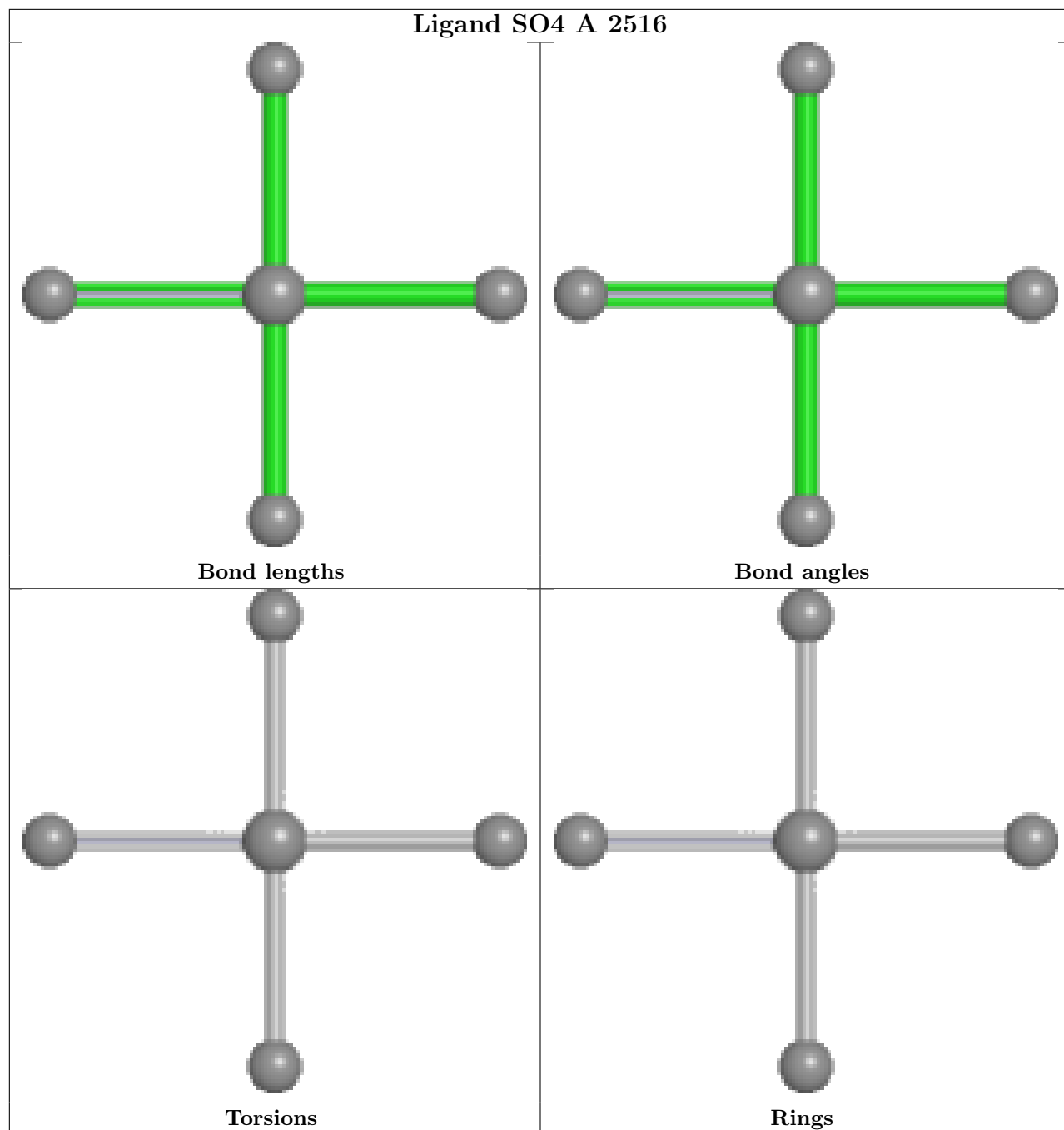


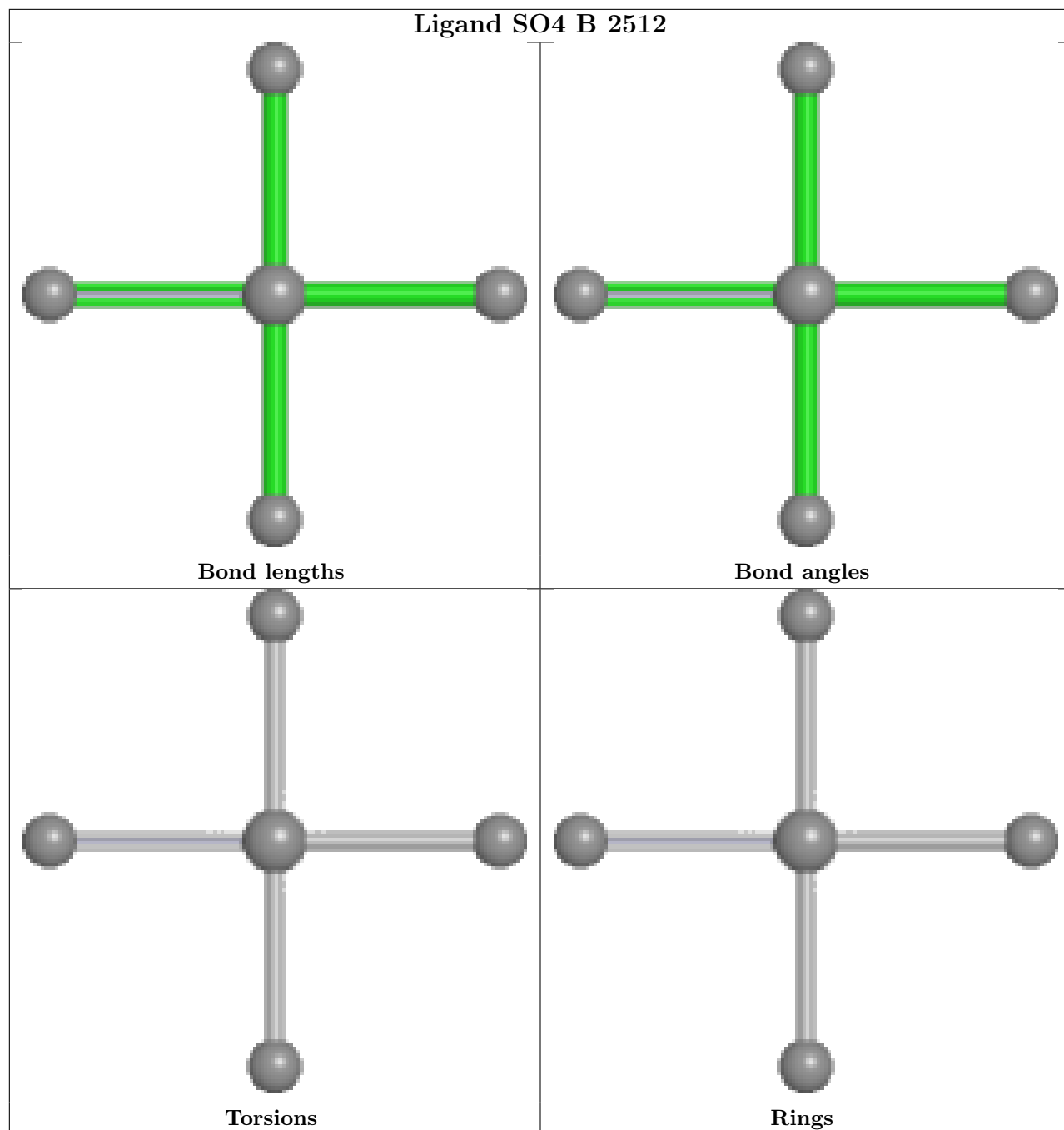


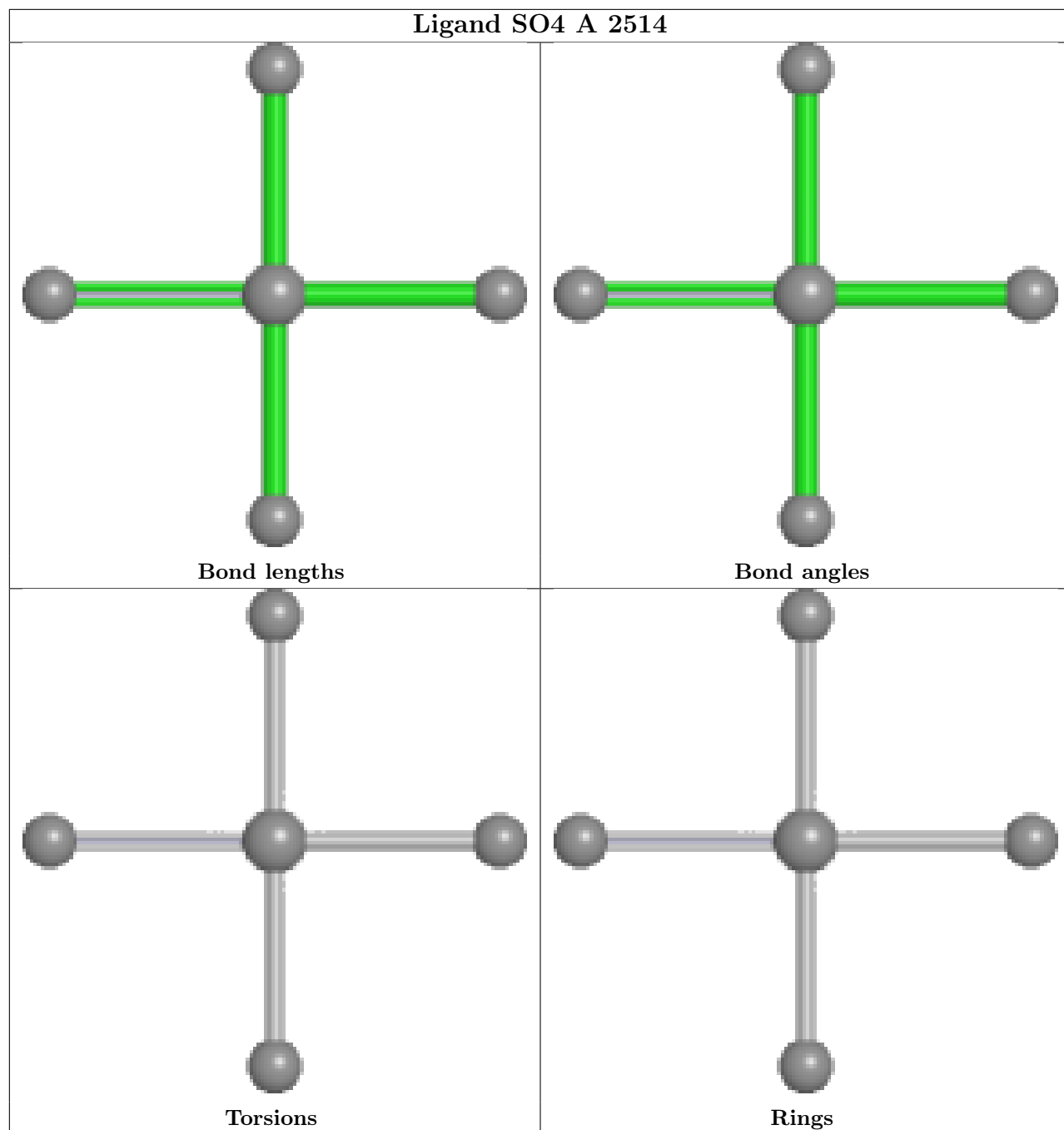


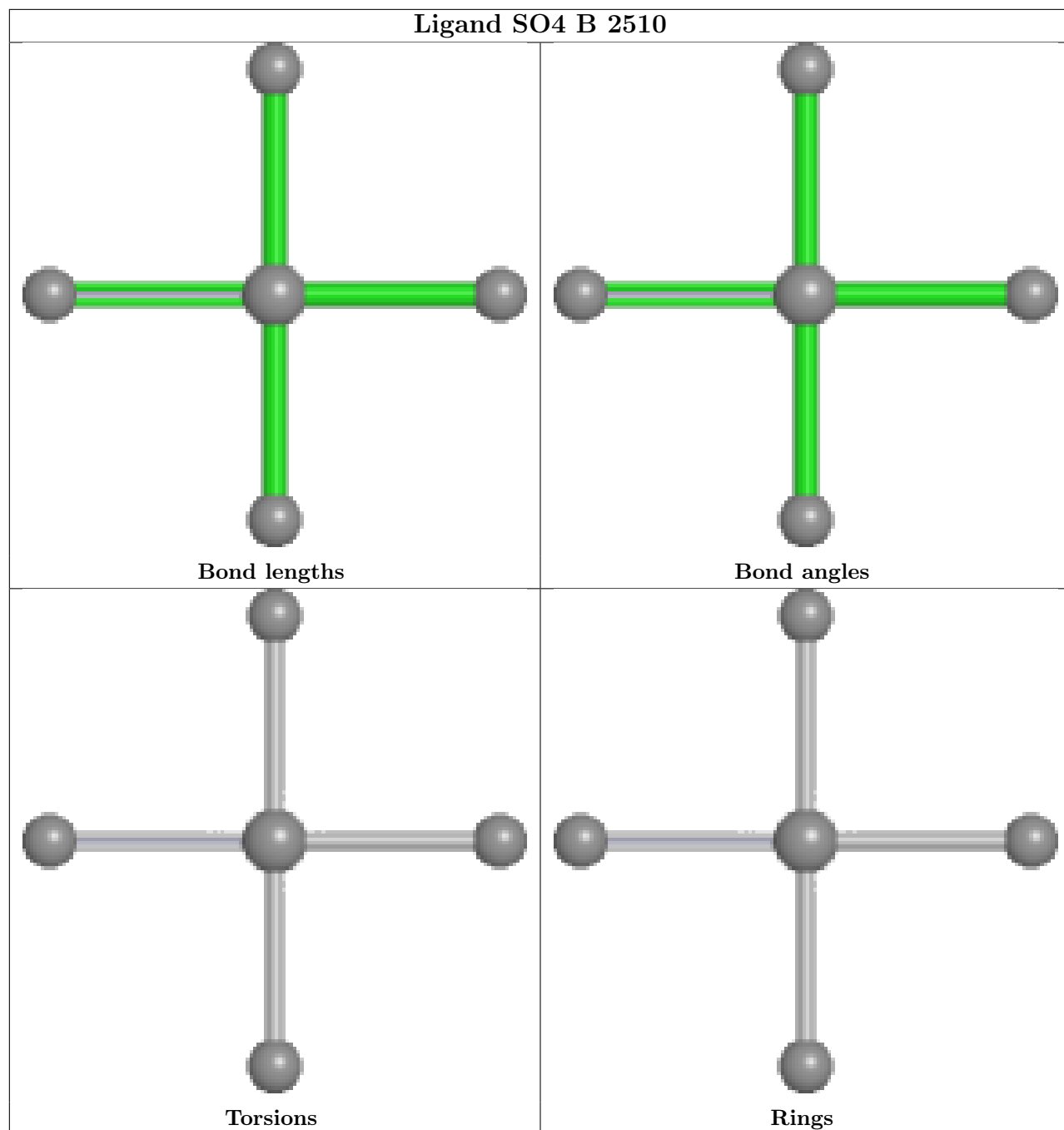


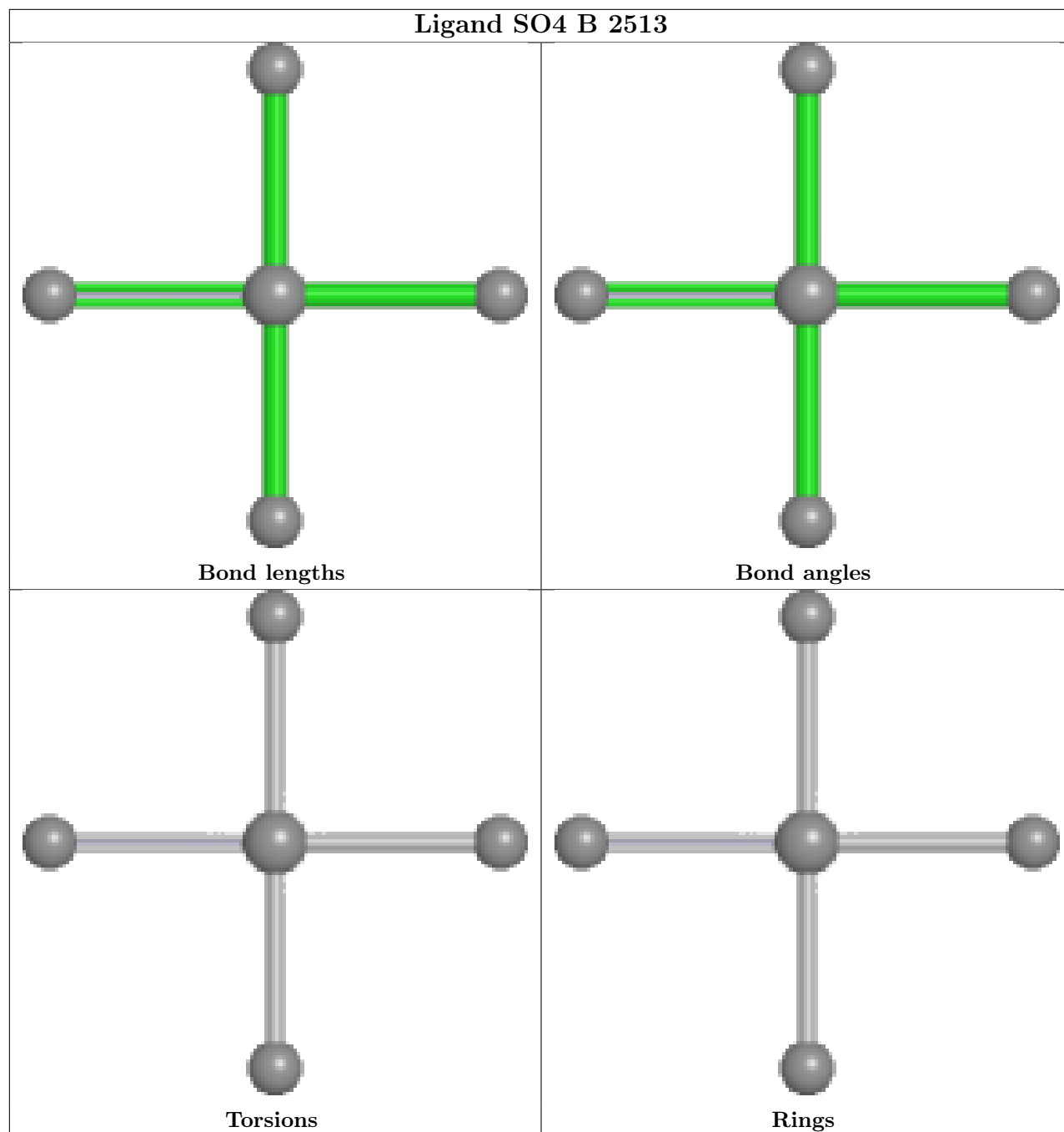


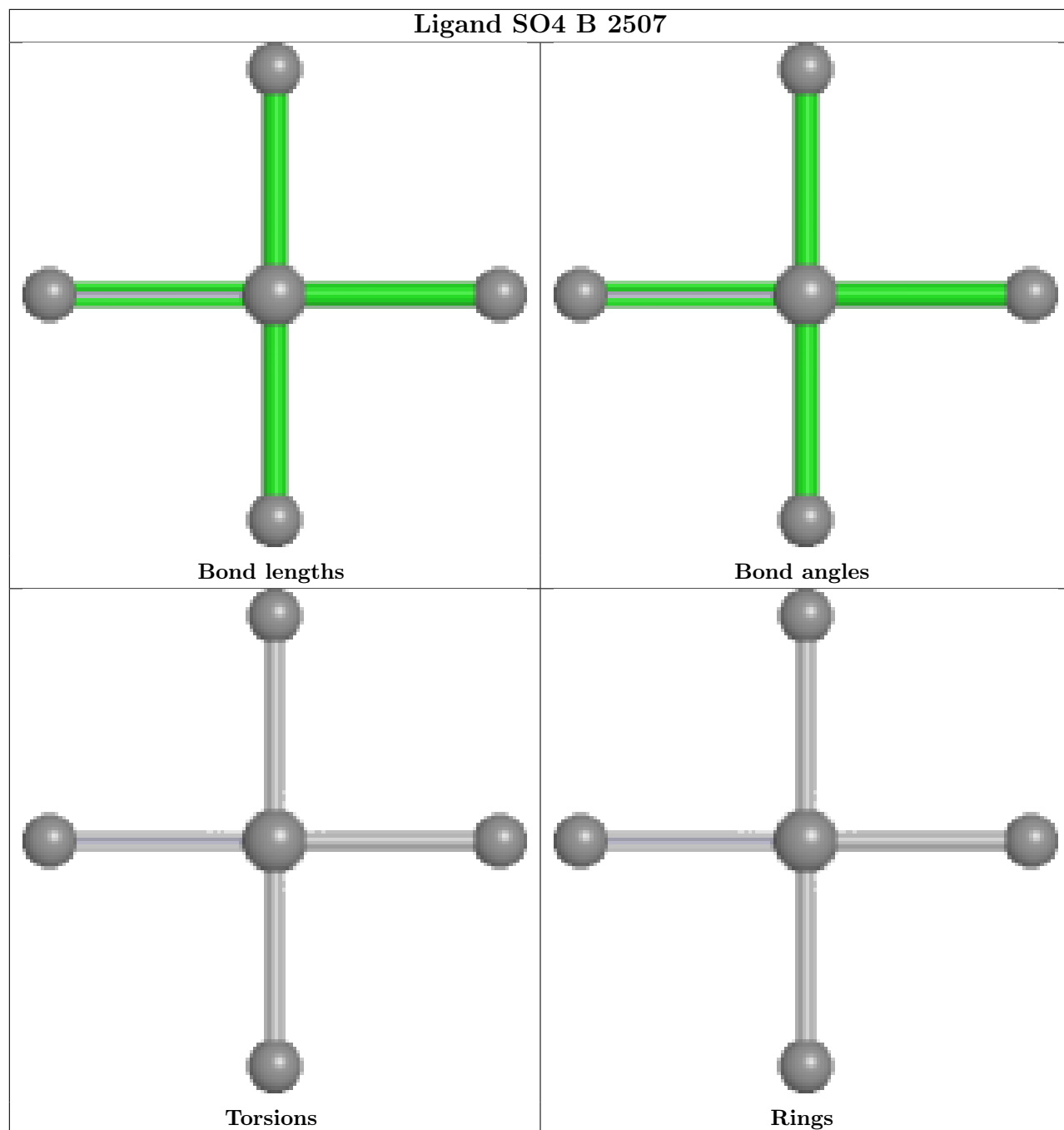


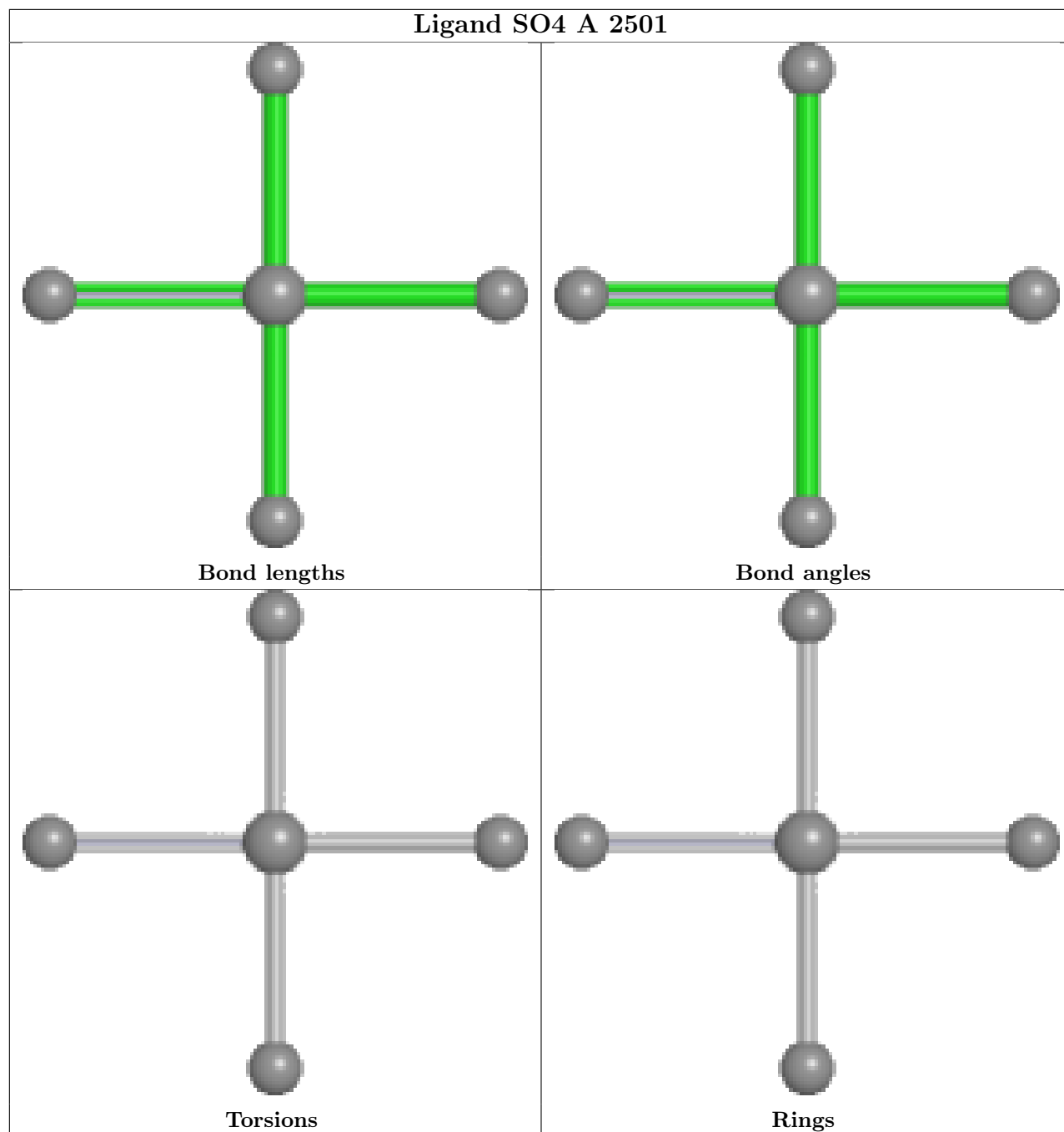


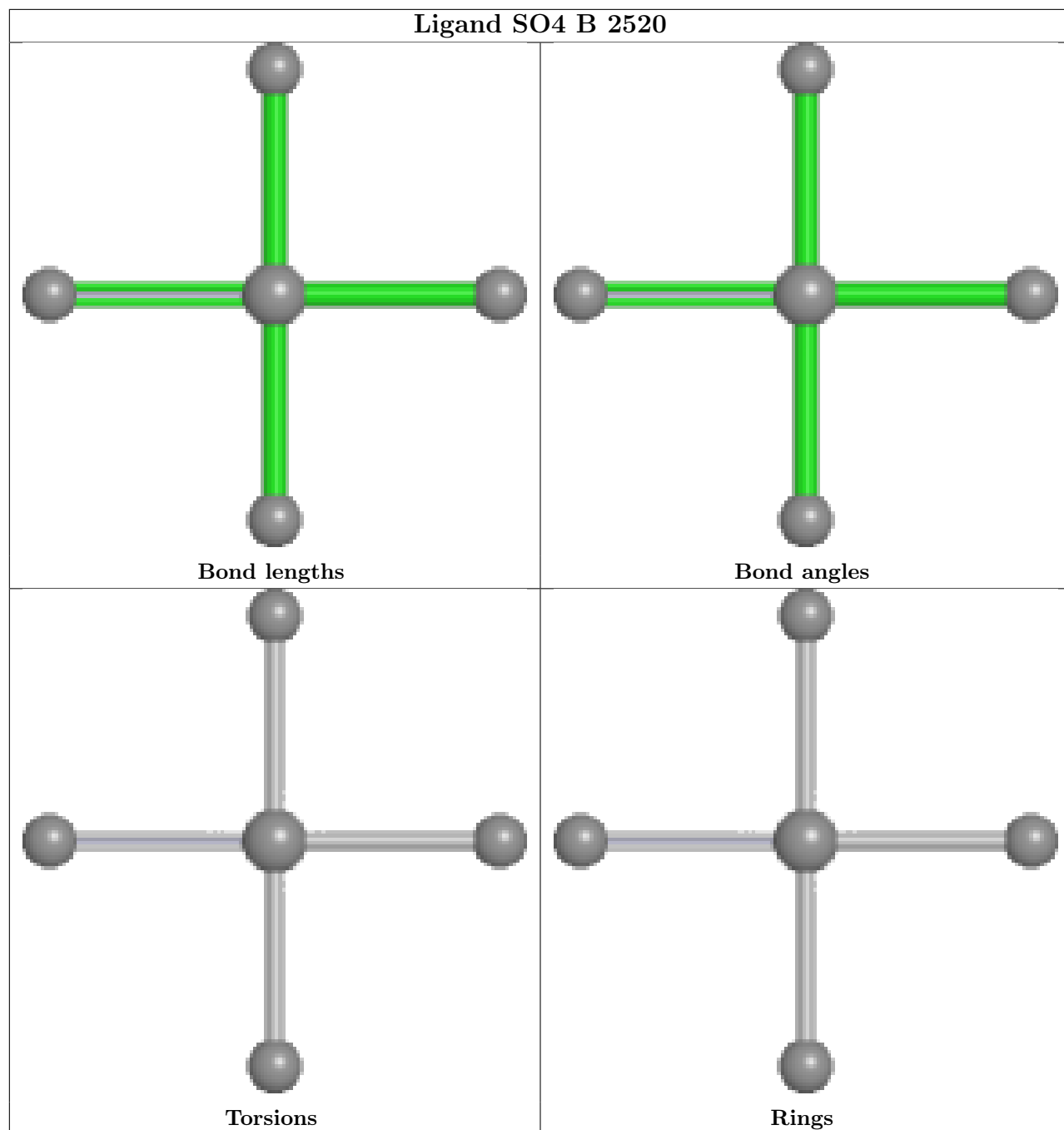


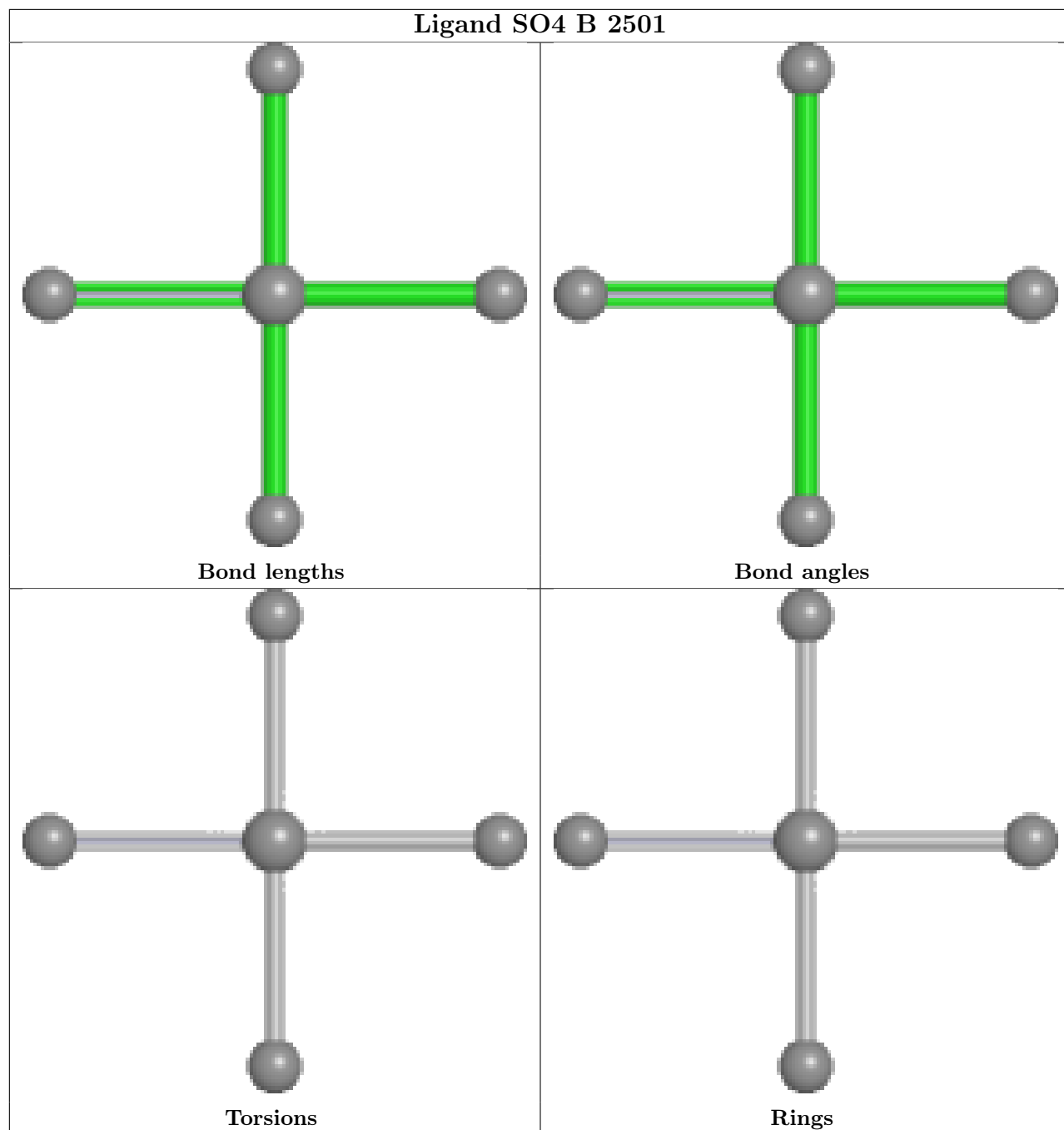


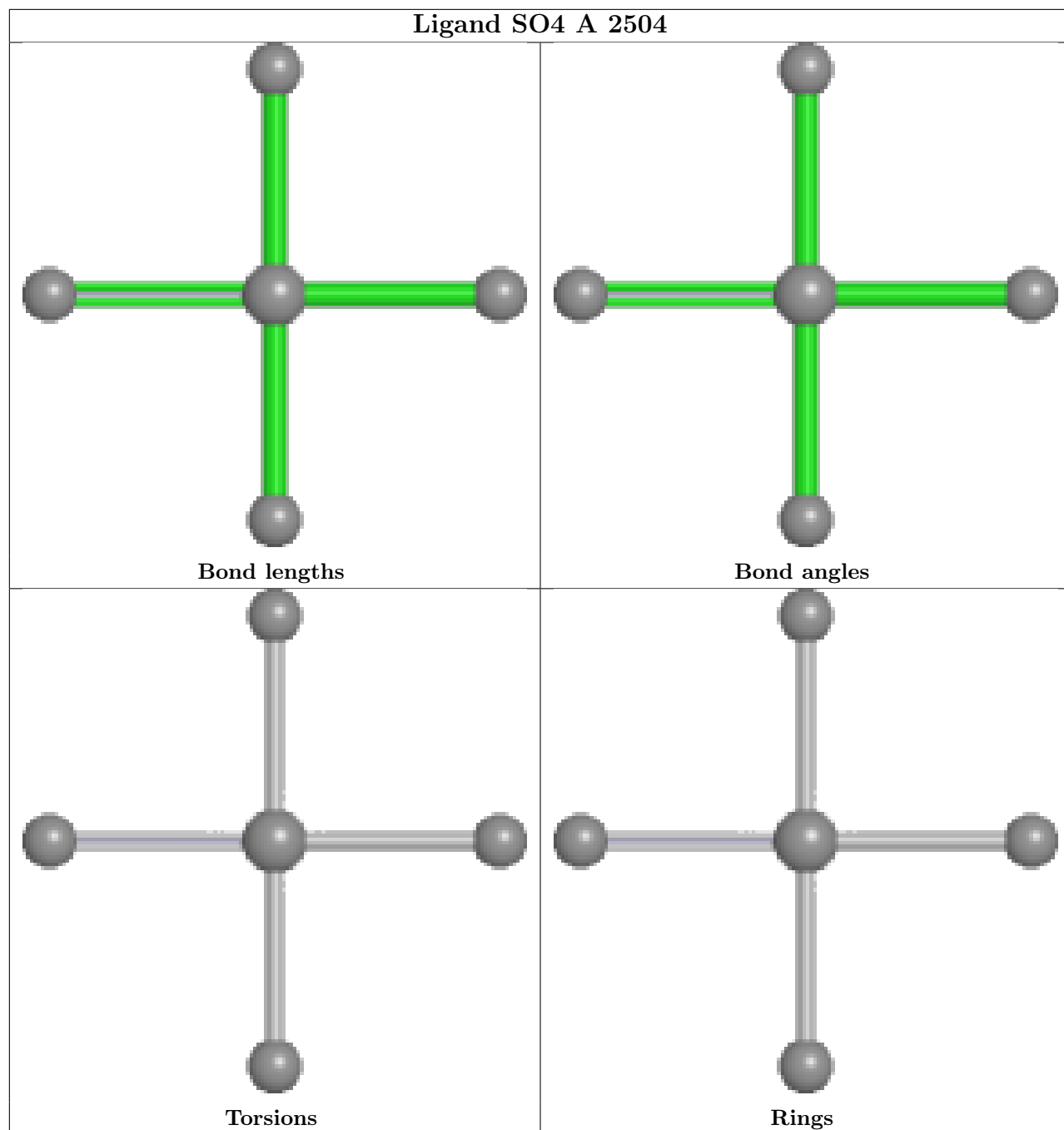


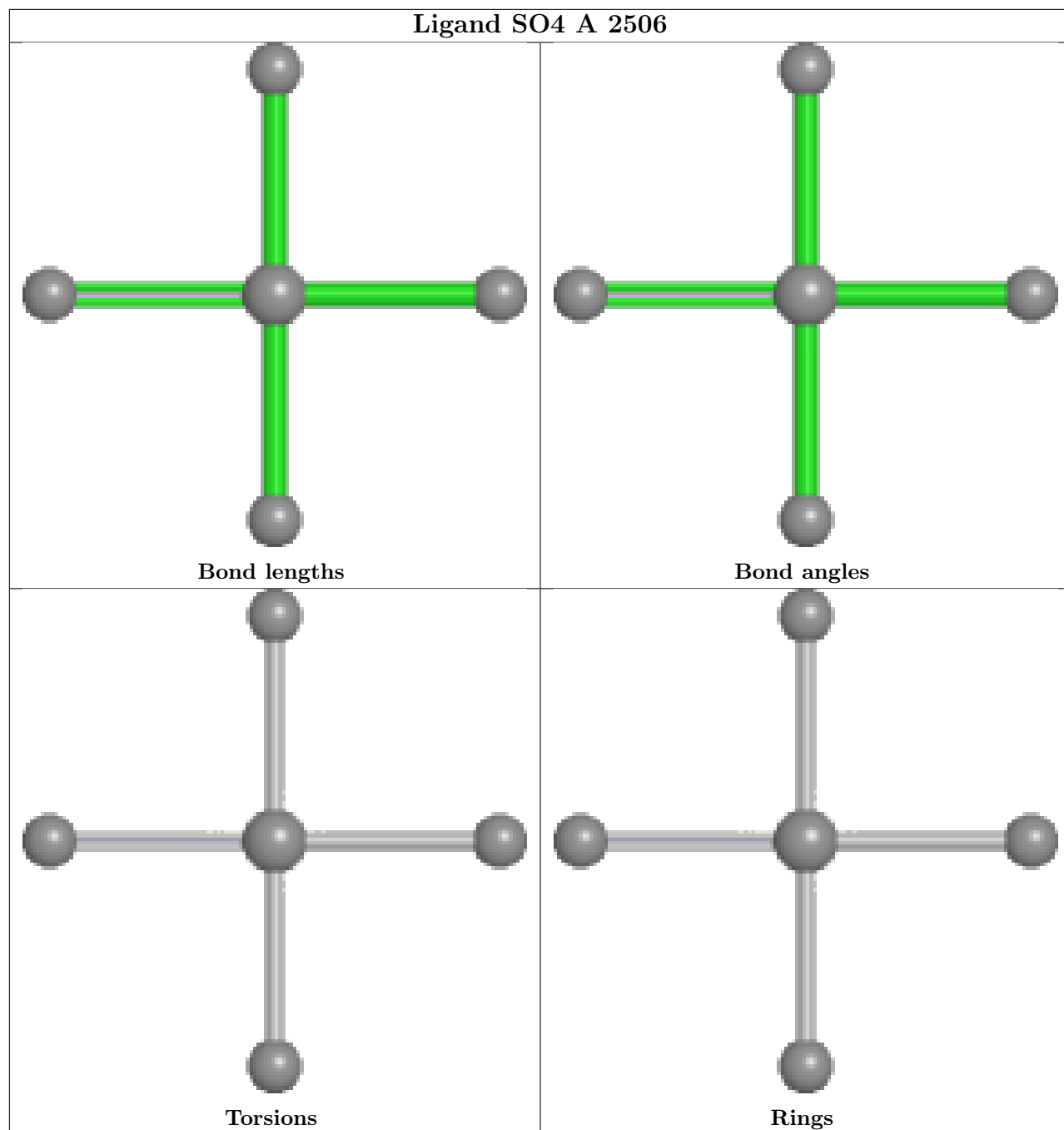


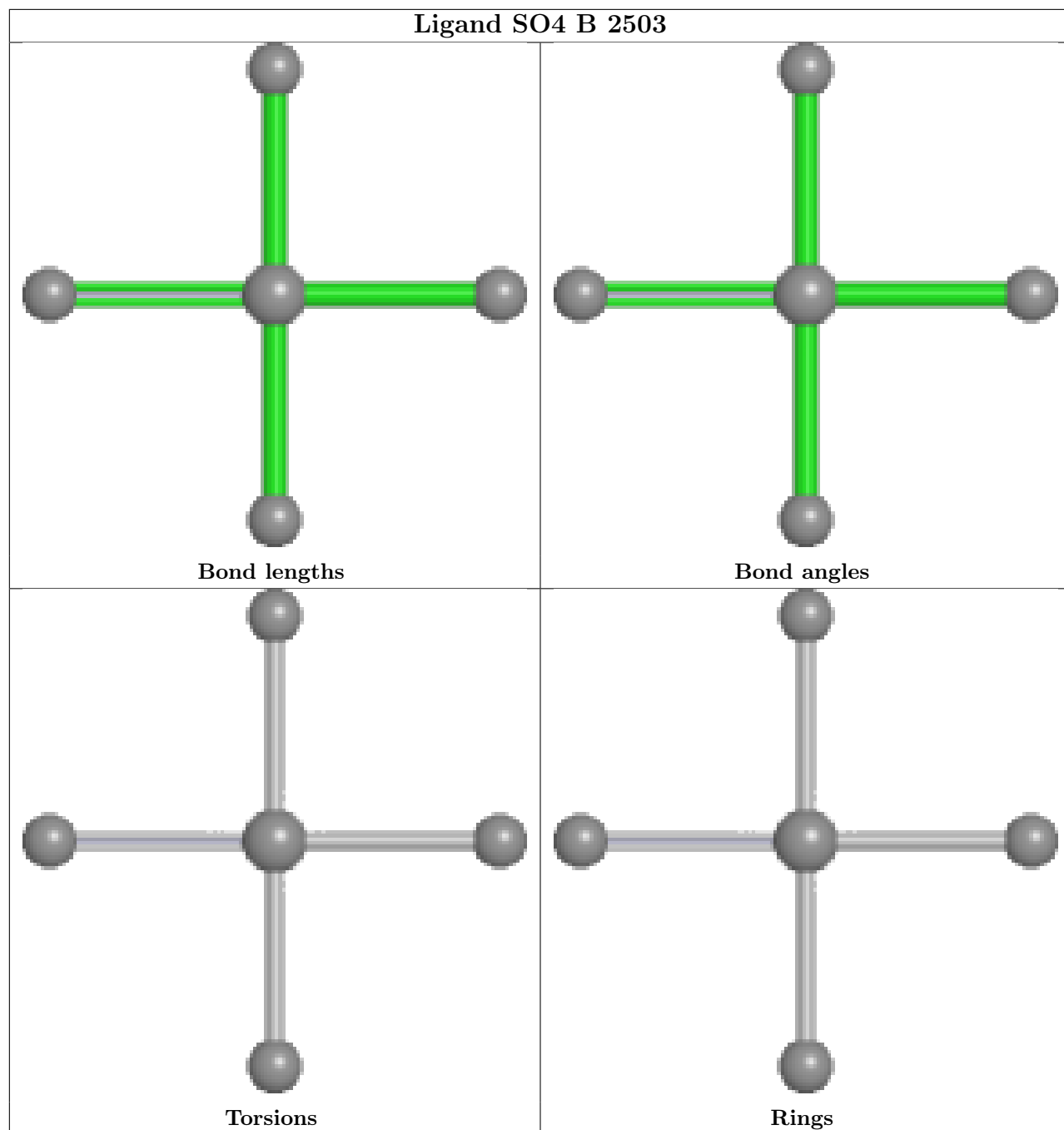


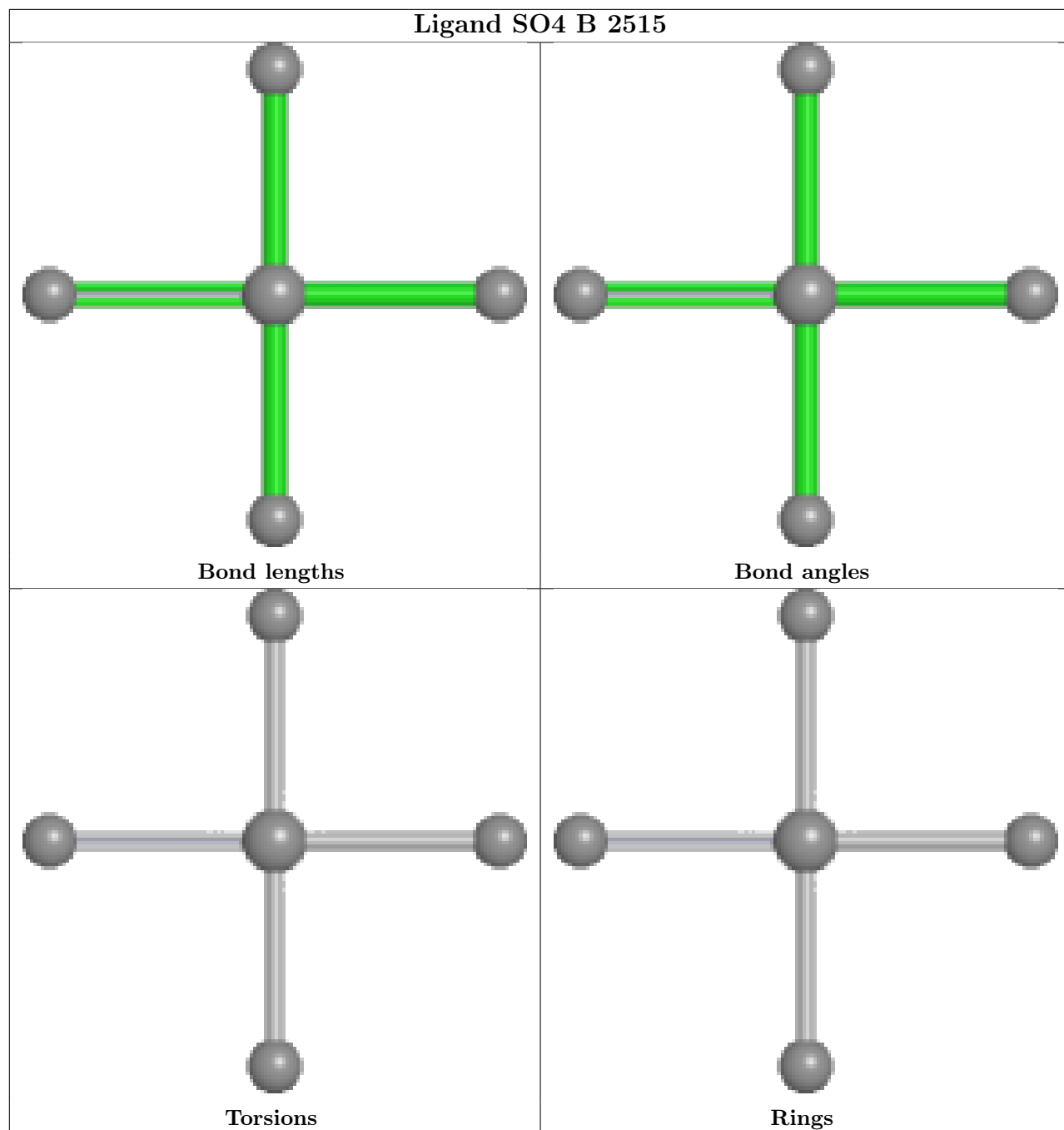


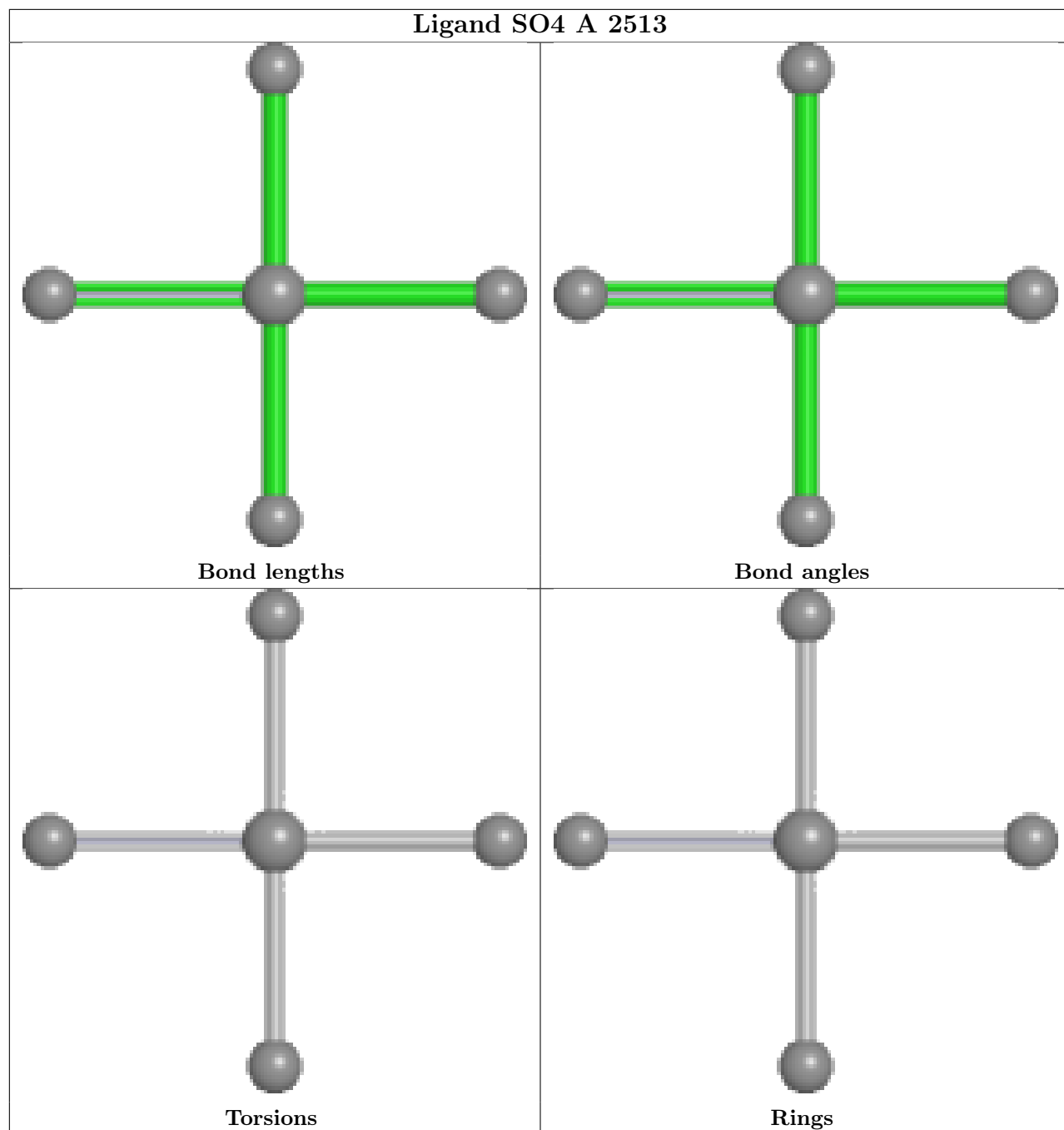


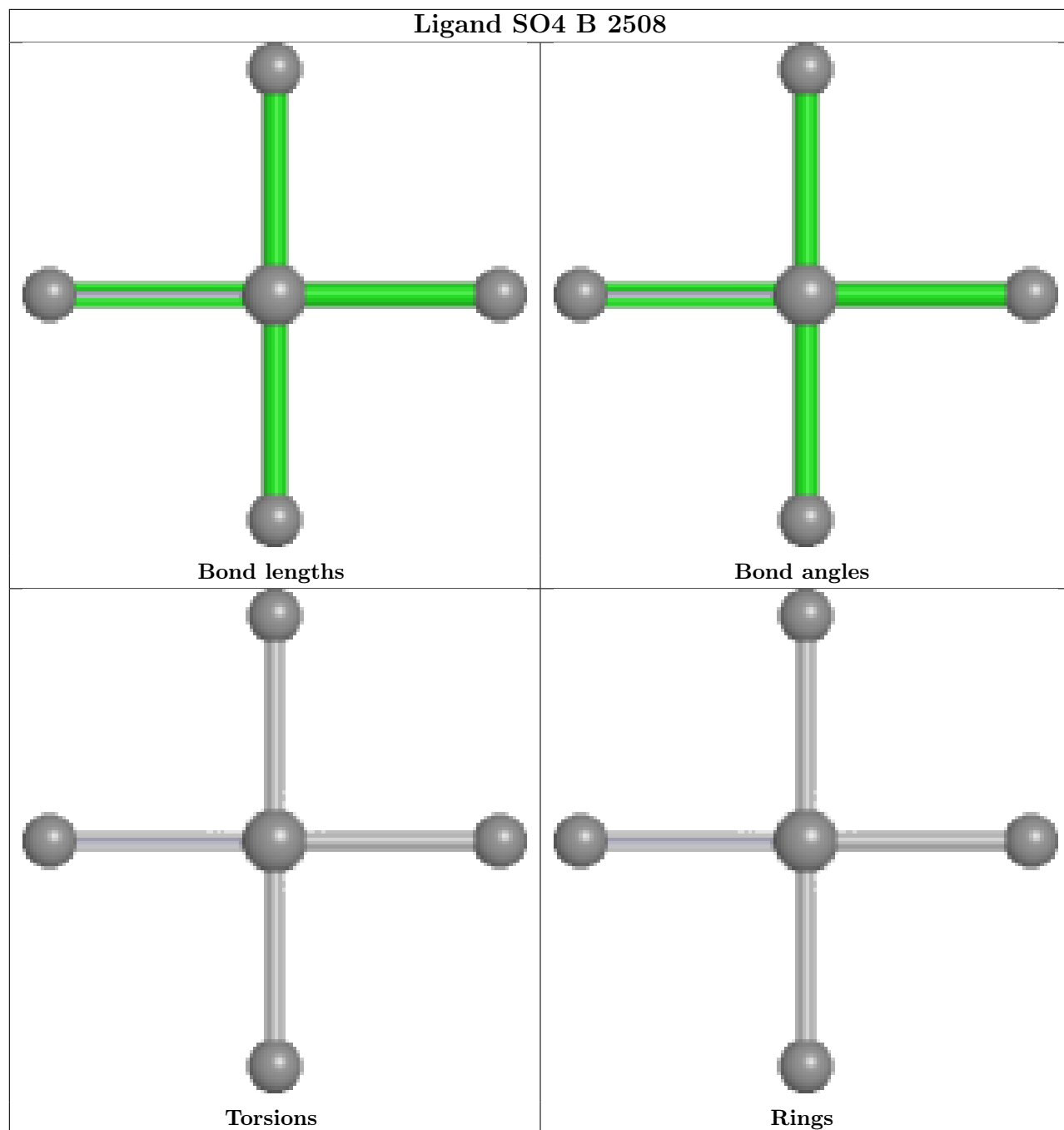


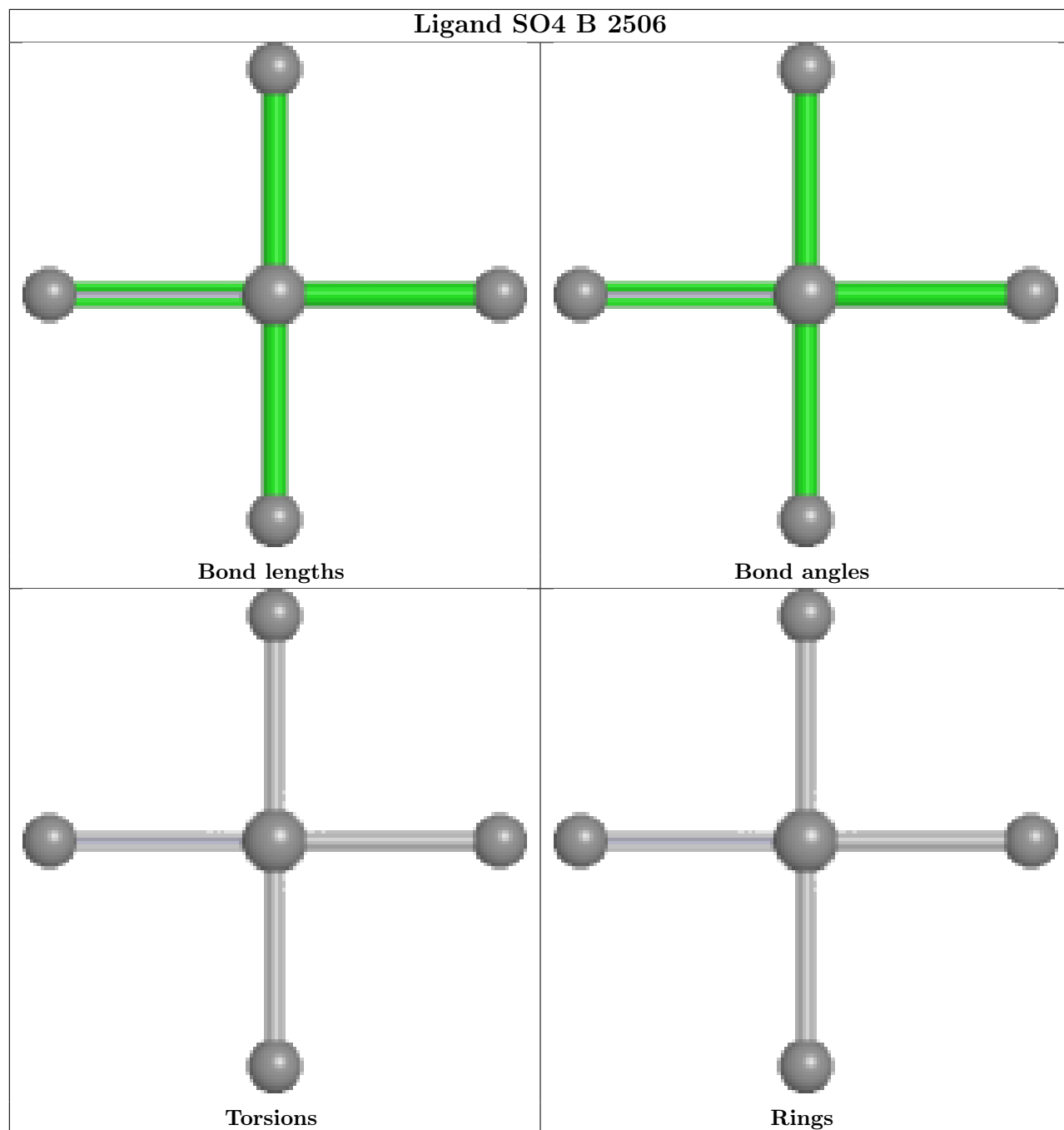


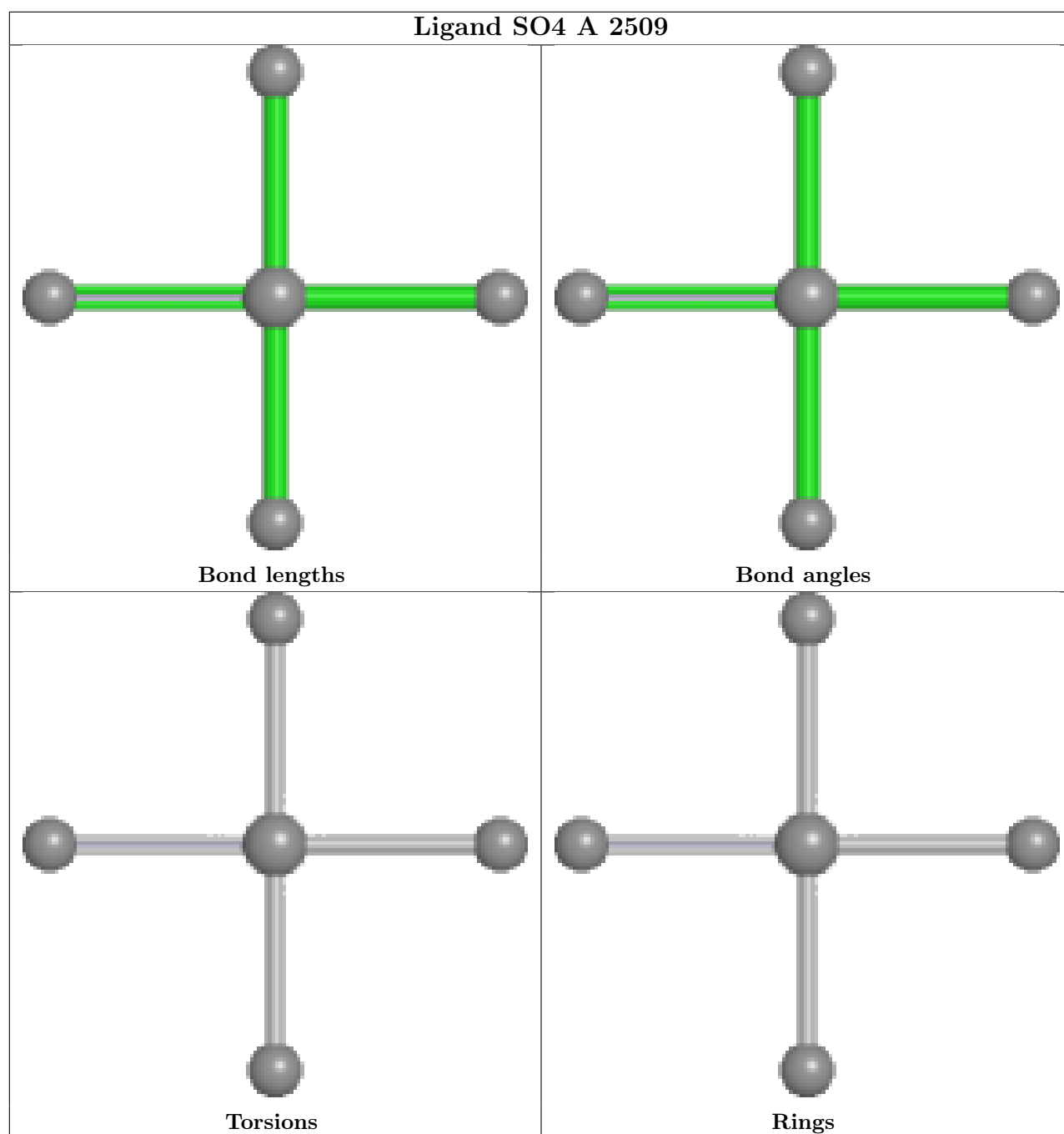


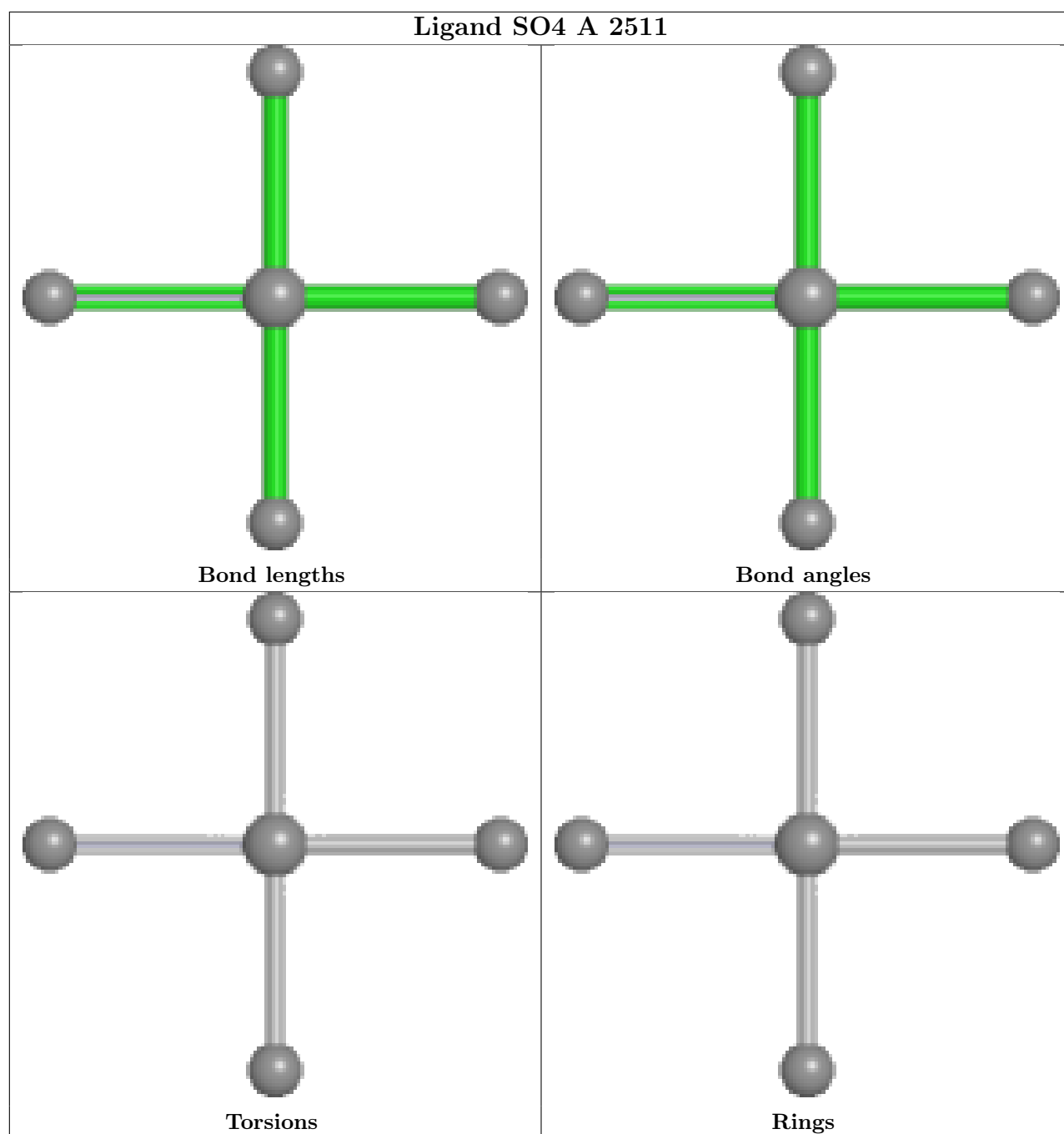












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1620/1640 (98%)	-0.13	21 (1%)	75 55	28, 48, 77, 125	3 (0%)
1	B	1612/1640 (98%)	0.09	47 (2%)	53 34	26, 52, 86, 148	10 (0%)
All	All	3232/3280 (98%)	-0.02	68 (2%)	63 42	26, 50, 83, 148	13 (0%)

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	859	ASP	5.1
1	B	1722	PHE	4.3
1	B	1723	HIS	4.0
1	A	975	SER	3.7
1	A	976	ASN	3.5

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

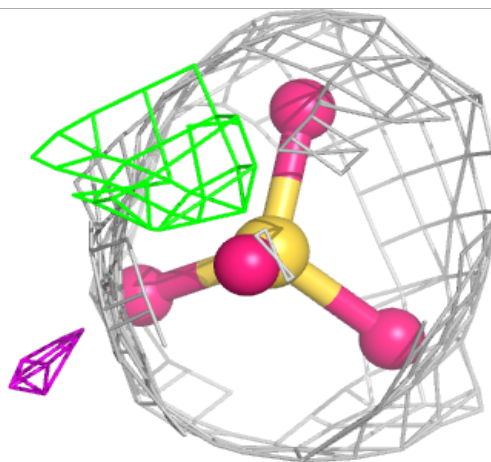
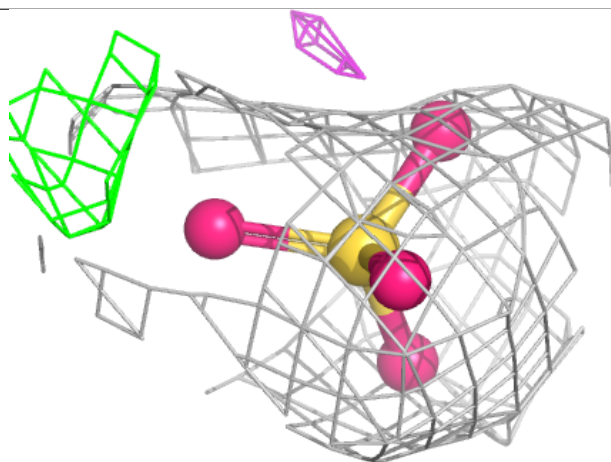
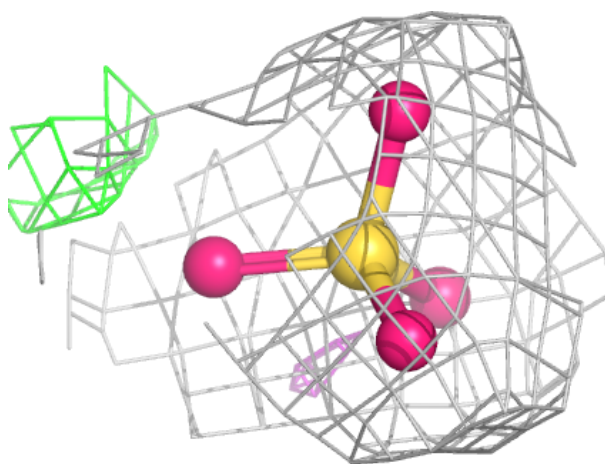
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	B	2504	5/5	0.67	0.15	90,96,113,119	0
2	SO4	A	2508	5/5	0.70	0.17	101,101,116,126	0
2	SO4	A	2507	5/5	0.77	0.14	87,88,101,119	0
2	SO4	A	2506	5/5	0.77	0.19	91,94,98,115	0
2	SO4	B	2501	5/5	0.80	0.18	78,85,90,100	0
2	SO4	B	2518	5/5	0.80	0.16	73,73,100,102	0
2	SO4	B	2519	5/5	0.80	0.15	94,95,104,118	0
2	SO4	A	2514	5/5	0.81	0.21	91,97,102,108	0
2	SO4	B	2508	5/5	0.82	0.19	83,93,102,106	0
2	SO4	B	2510	5/5	0.82	0.17	81,90,114,123	0
2	SO4	B	2509	5/5	0.83	0.18	84,90,103,108	0
2	SO4	B	2506	5/5	0.83	0.23	84,84,95,100	0
2	SO4	A	2501	5/5	0.83	0.14	80,87,98,111	0
2	SO4	A	2503	5/5	0.83	0.21	72,74,88,90	0
2	SO4	B	2517	5/5	0.84	0.16	81,91,103,117	0
2	SO4	A	2515	5/5	0.84	0.19	77,82,93,97	0
2	SO4	B	2515	5/5	0.85	0.12	75,76,86,95	0
2	SO4	A	2516	5/5	0.85	0.17	90,91,95,106	0
2	SO4	B	2503	5/5	0.86	0.16	77,79,95,104	0
2	SO4	B	2514	5/5	0.86	0.13	101,108,114,117	0
2	SO4	A	2504	5/5	0.86	0.16	70,70,96,100	0
2	SO4	B	2502	5/5	0.87	0.14	81,91,96,103	0
2	SO4	B	2505	5/5	0.89	0.17	79,88,92,102	0
2	SO4	B	2507	5/5	0.89	0.14	77,81,90,102	0
2	SO4	A	2509	5/5	0.89	0.13	57,64,79,89	0
2	SO4	A	2511	5/5	0.90	0.14	61,82,98,99	0
2	SO4	A	2512	5/5	0.90	0.12	65,67,80,90	0
2	SO4	A	2502	5/5	0.90	0.11	78,81,88,95	0
2	SO4	A	2505	5/5	0.90	0.20	59,70,94,94	0
2	SO4	B	2516	5/5	0.90	0.16	74,76,80,89	0
2	SO4	A	2513	5/5	0.91	0.12	63,77,96,98	0
2	SO4	A	2510	5/5	0.91	0.14	66,67,74,81	0
2	SO4	B	2520	5/5	0.91	0.15	62,65,78,83	0
2	SO4	B	2512	5/5	0.91	0.12	75,76,88,102	0
2	SO4	B	2513	5/5	0.92	0.16	60,66,71,84	0
2	SO4	B	2511	5/5	0.92	0.17	61,61,71,78	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

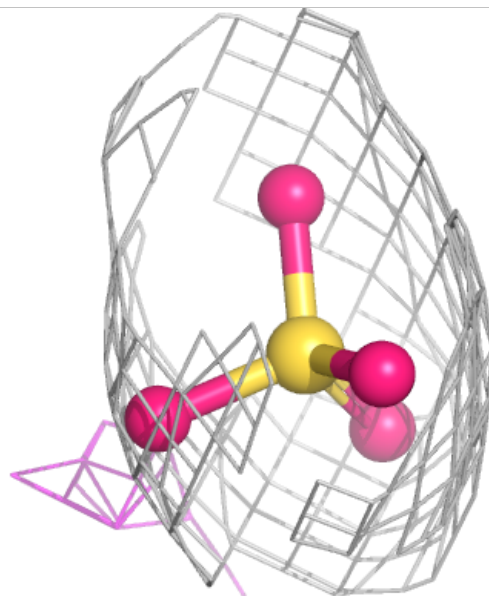
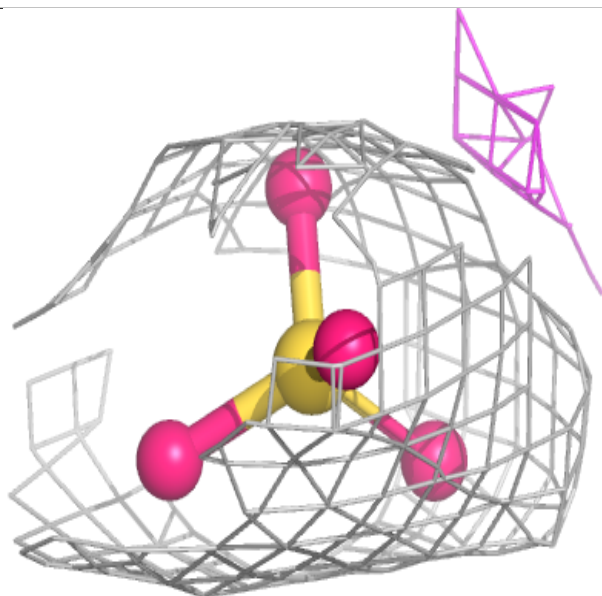
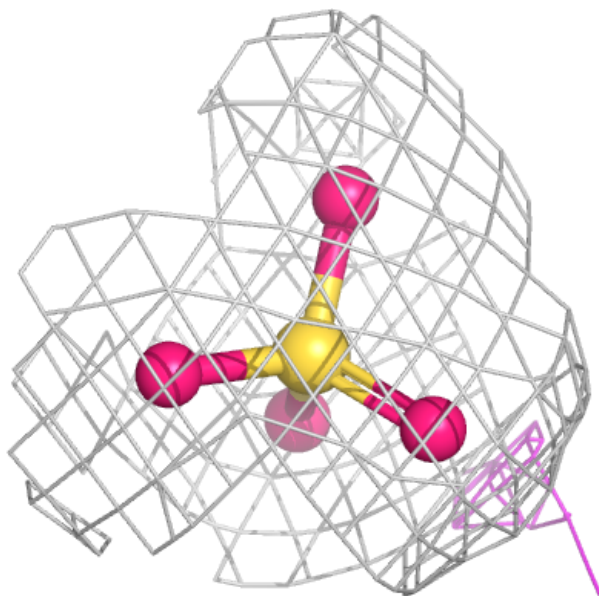
Electron density around SO4 B 2504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



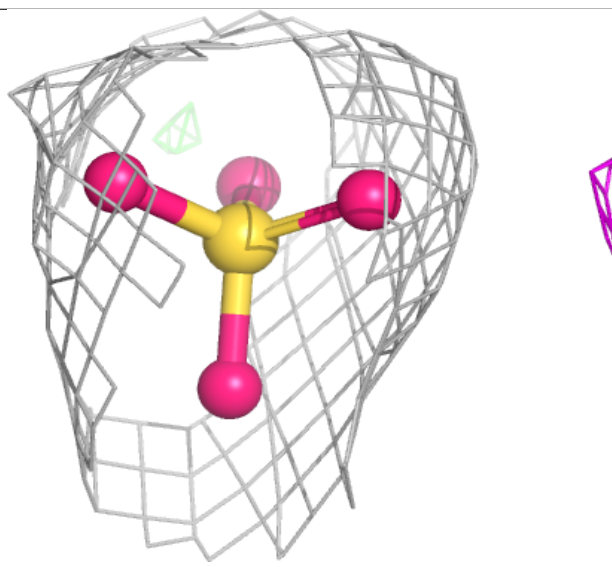
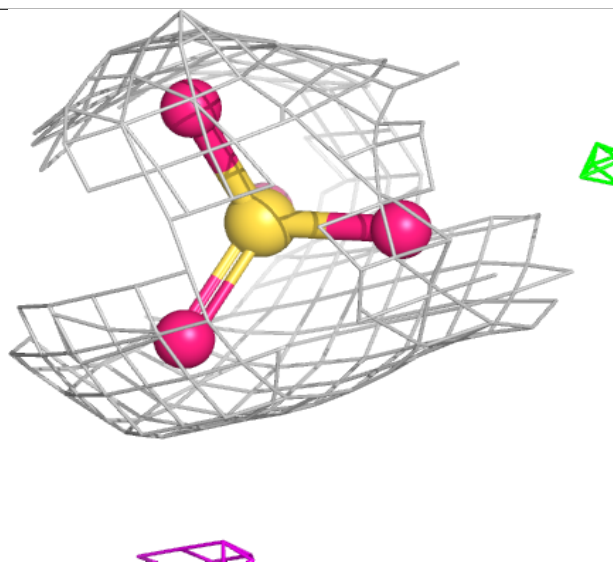
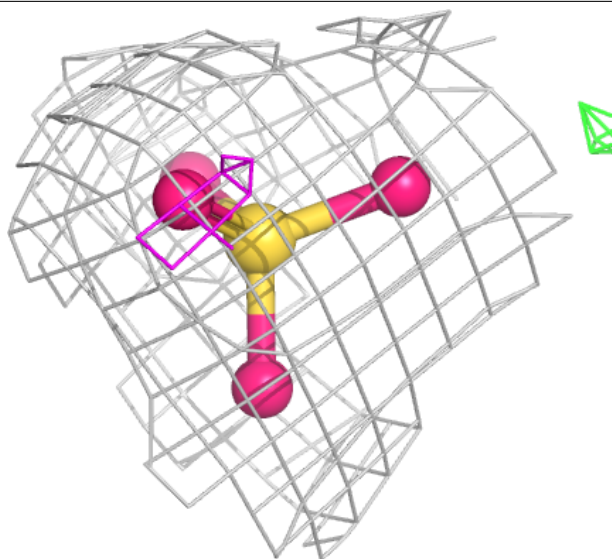
Electron density around SO4 A 2508:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



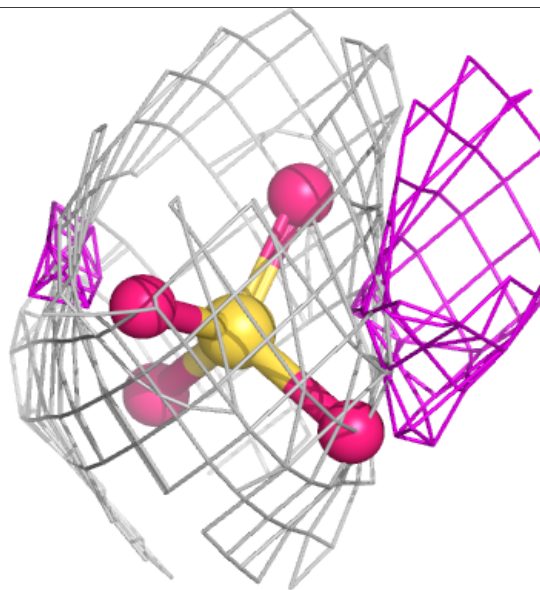
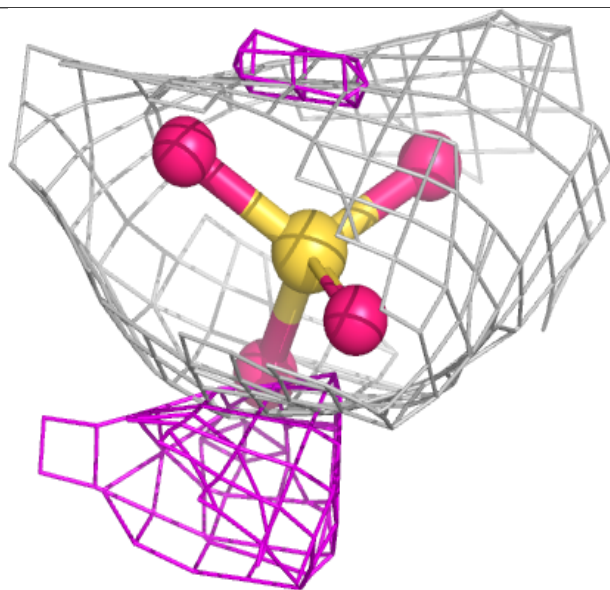
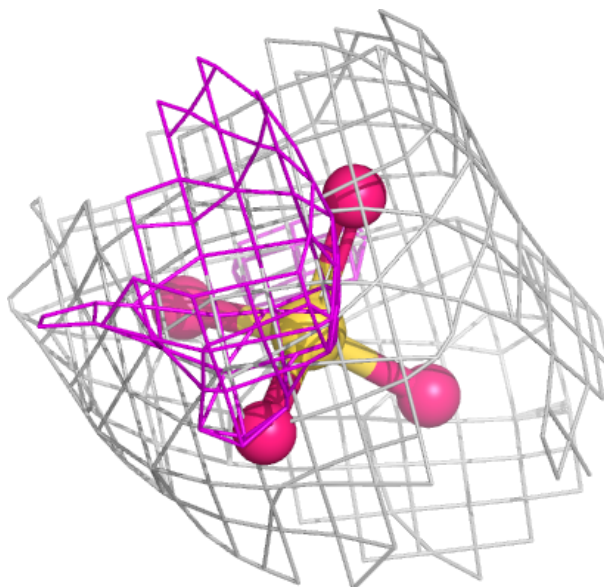
Electron density around SO4 A 2507:

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and green (positive)



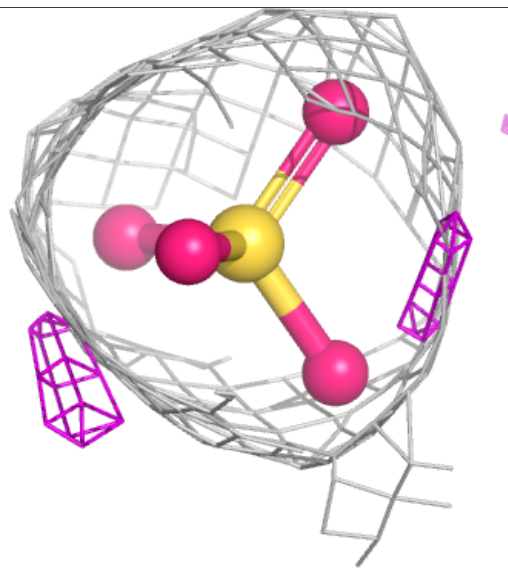
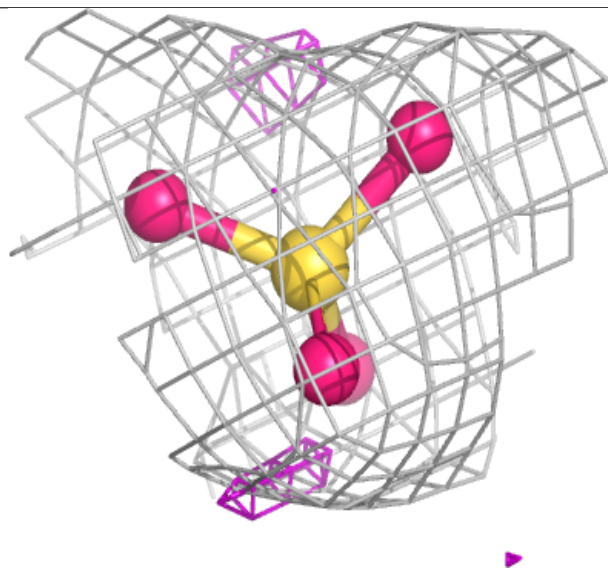
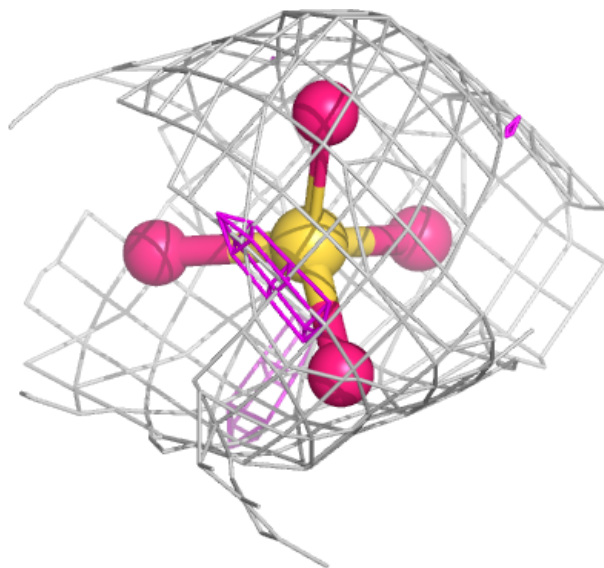
Electron density around SO4 A 2506:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



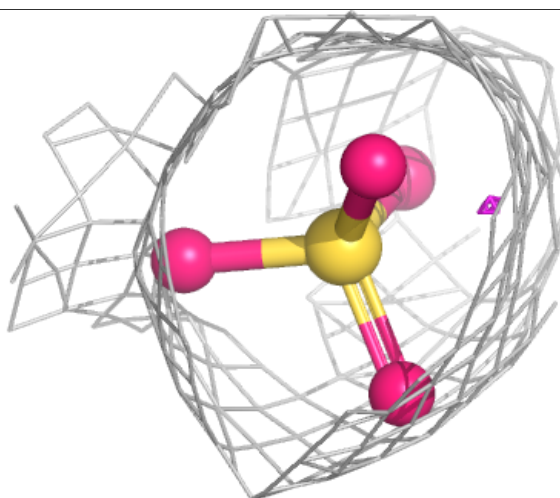
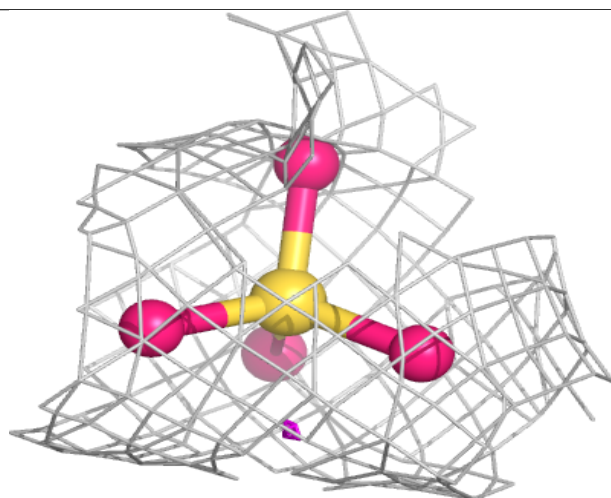
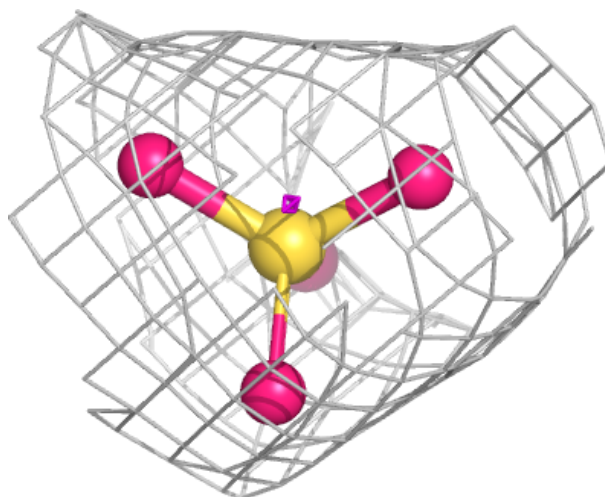
Electron density around SO4 B 2501:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



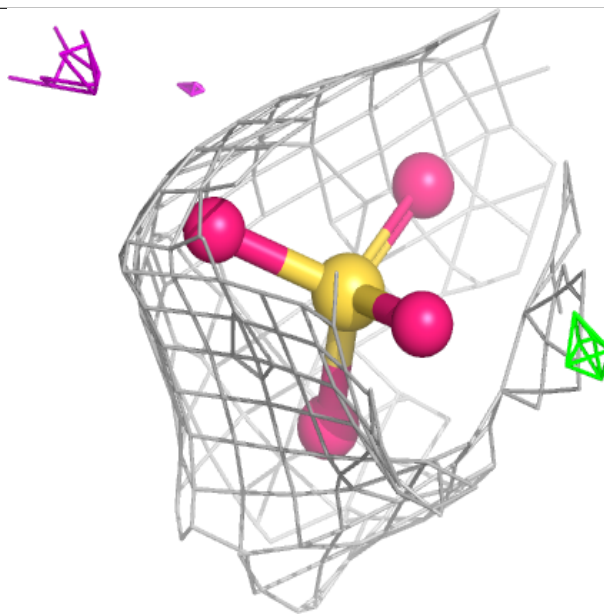
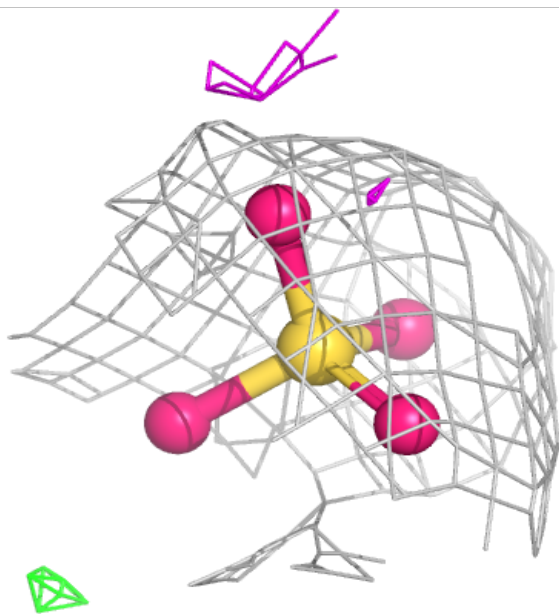
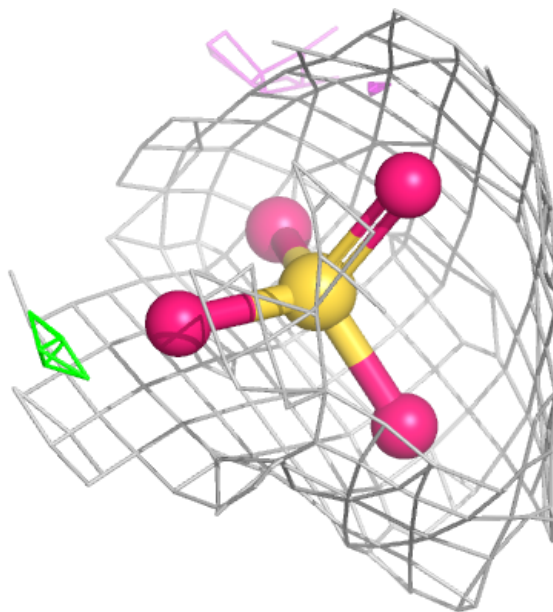
Electron density around SO4 B 2518:

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and green (positive)



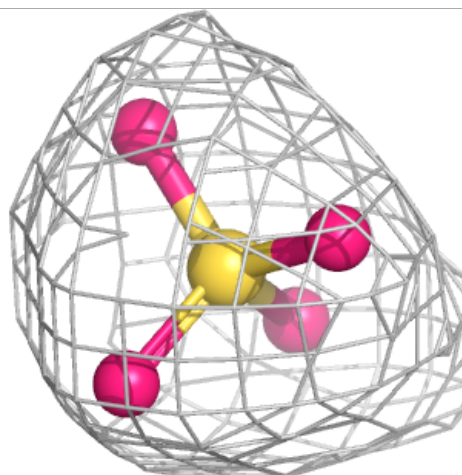
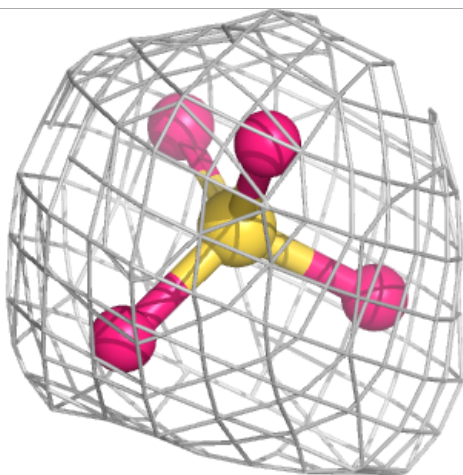
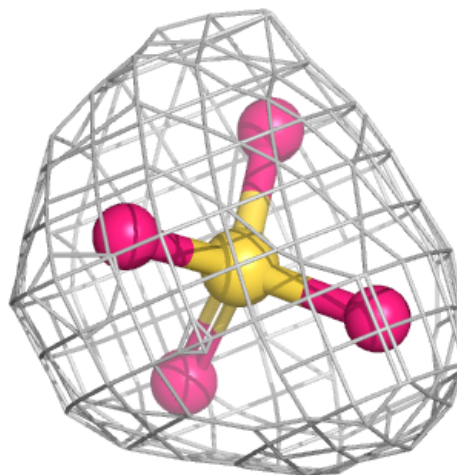
Electron density around SO4 B 2519:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



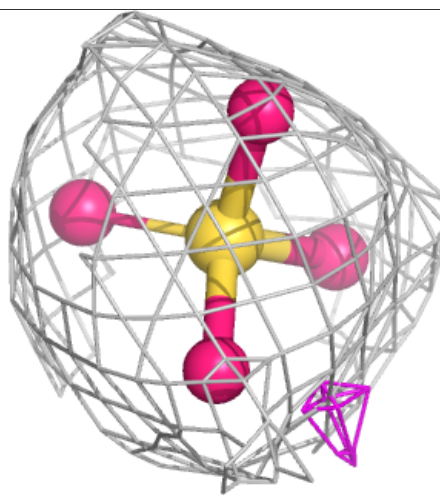
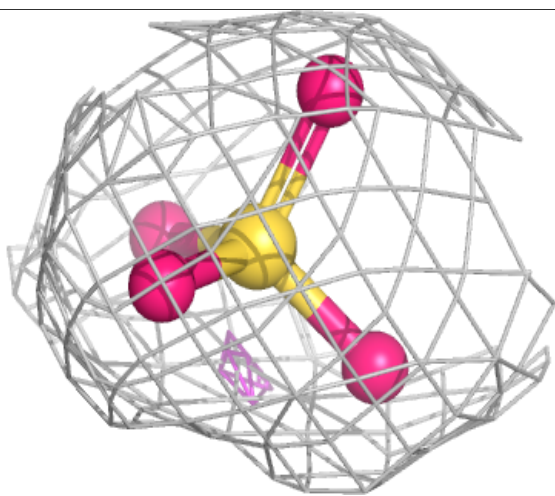
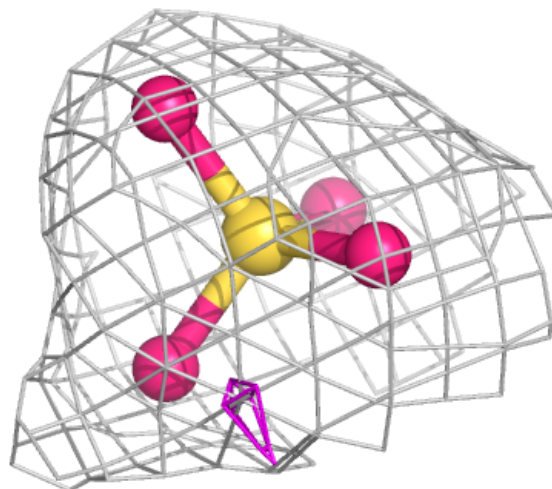
Electron density around SO4 A 2514:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



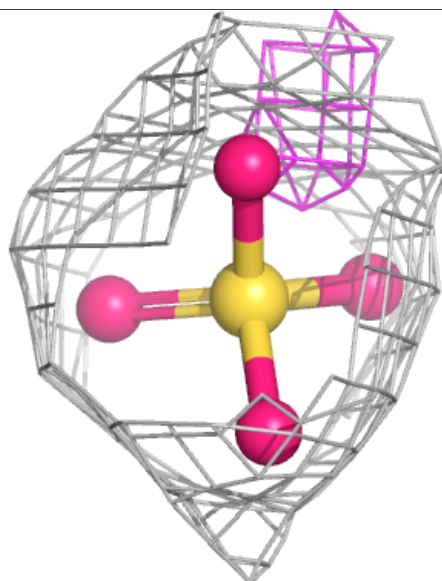
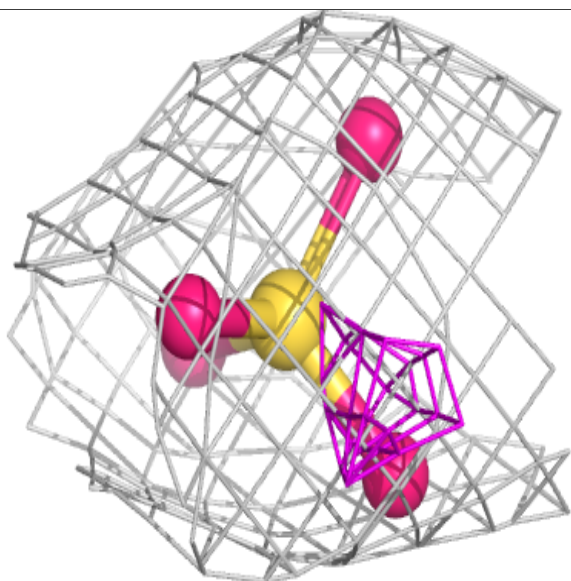
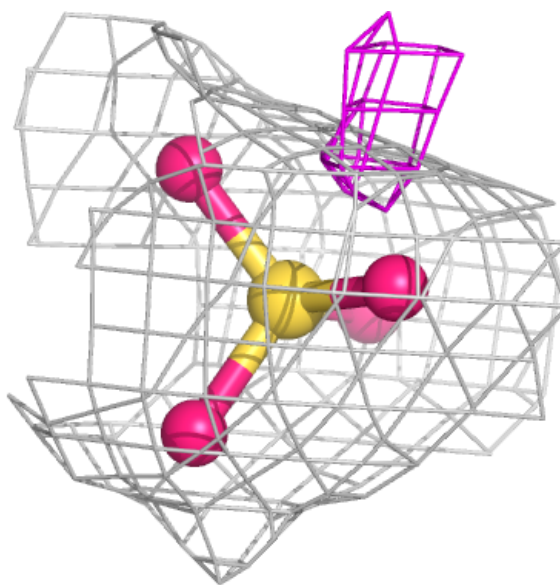
Electron density around SO4 B 2508:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



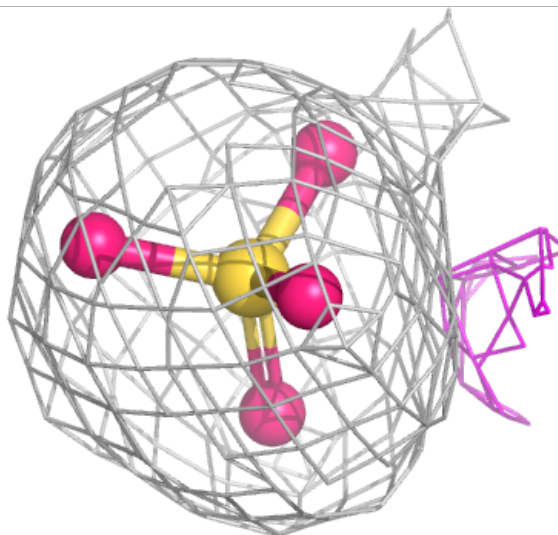
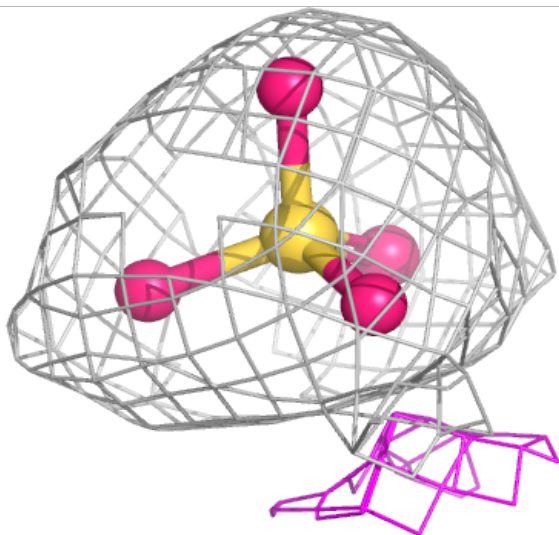
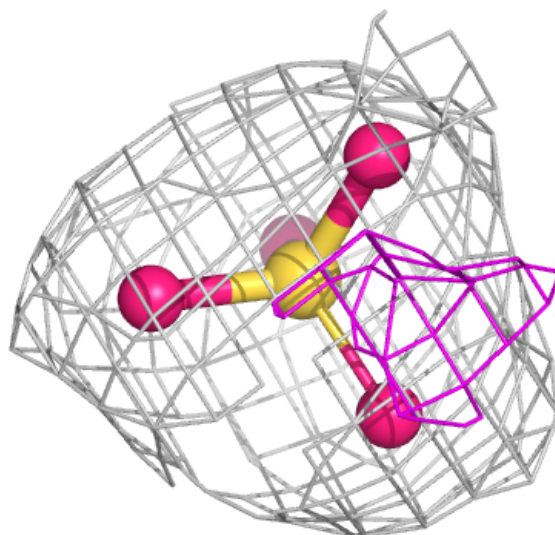
Electron density around SO4 B 2510:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



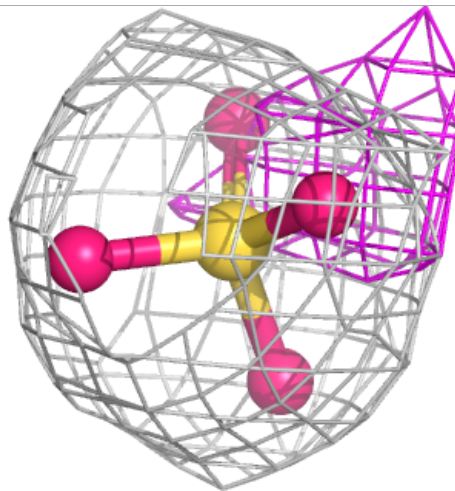
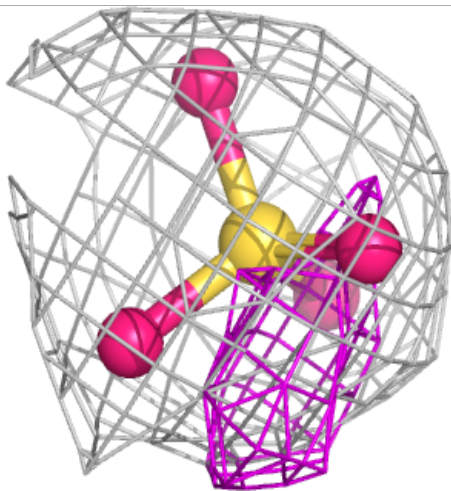
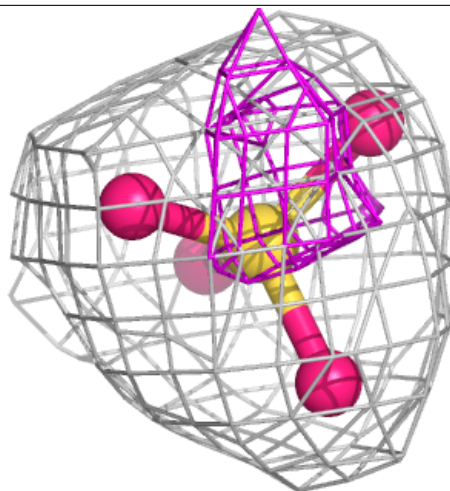
Electron density around SO4 B 2509:

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and green (positive)



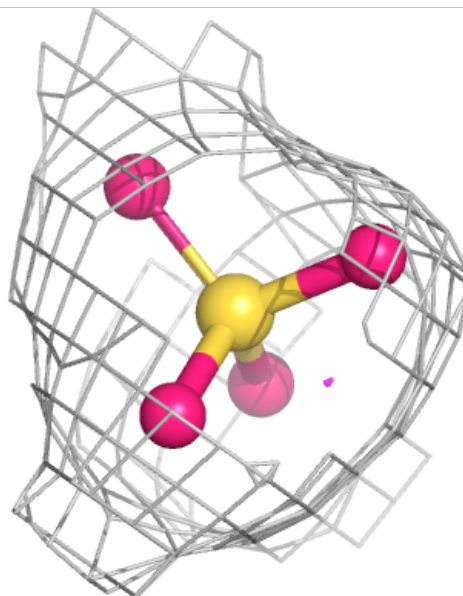
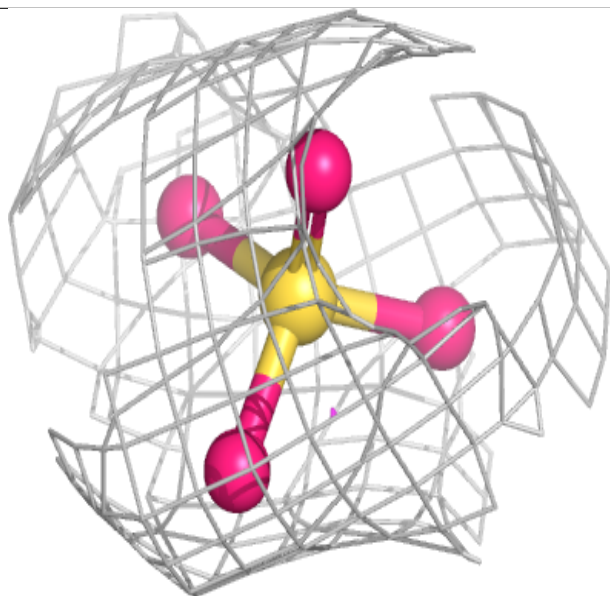
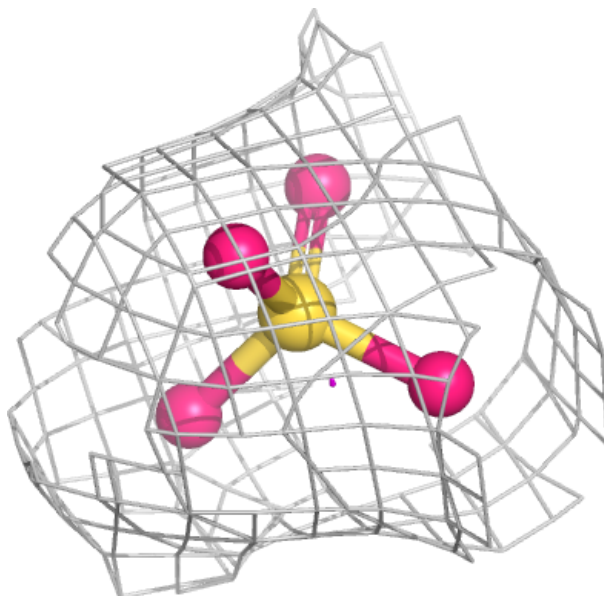
Electron density around SO4 B 2506:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



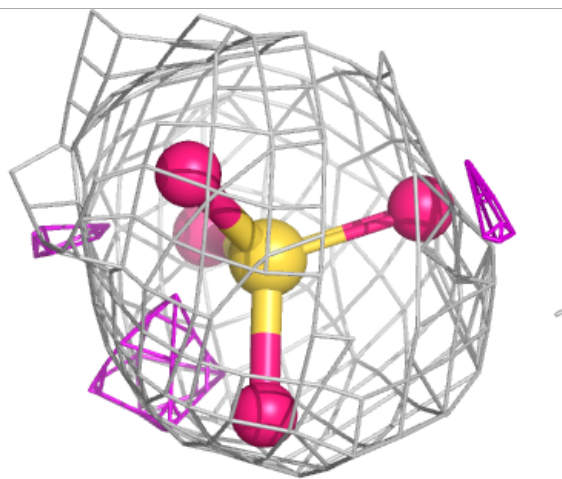
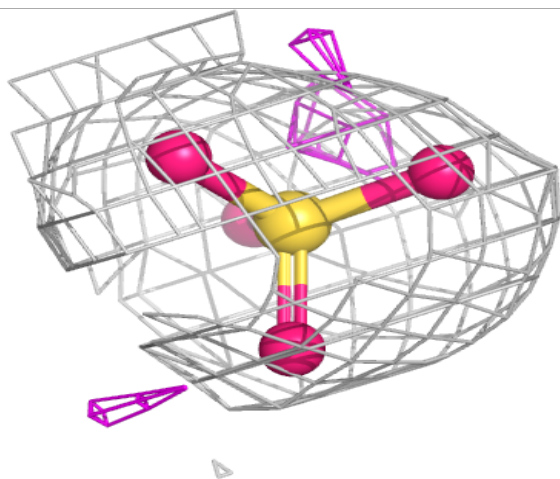
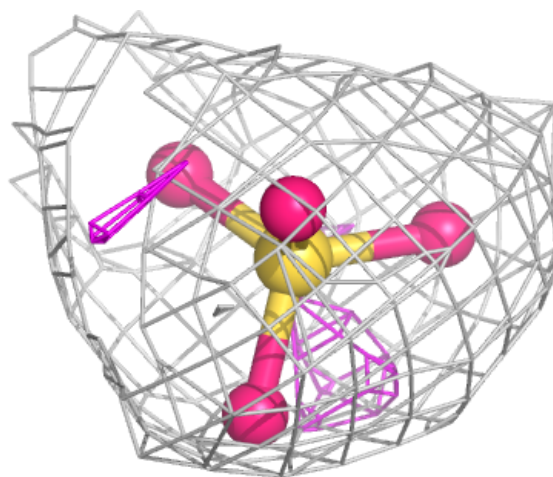
Electron density around SO4 A 2501:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



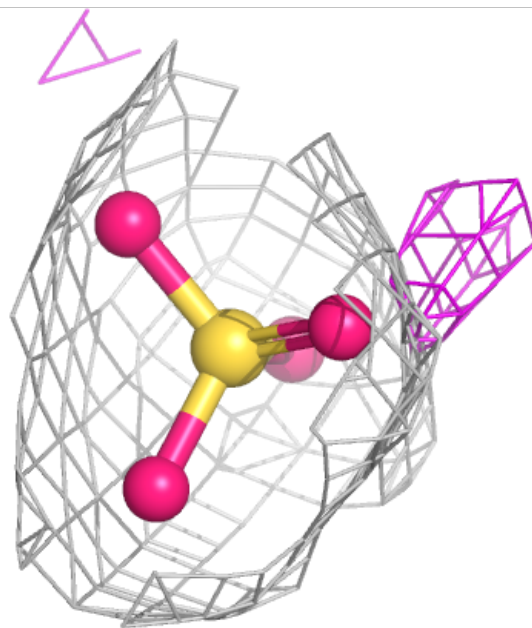
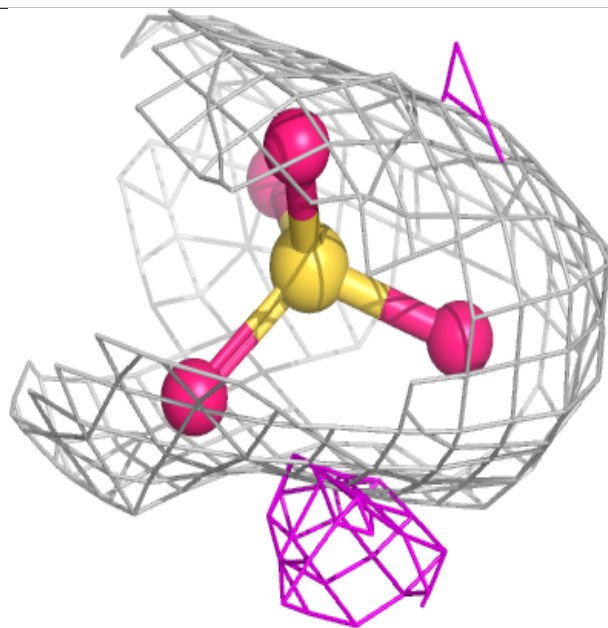
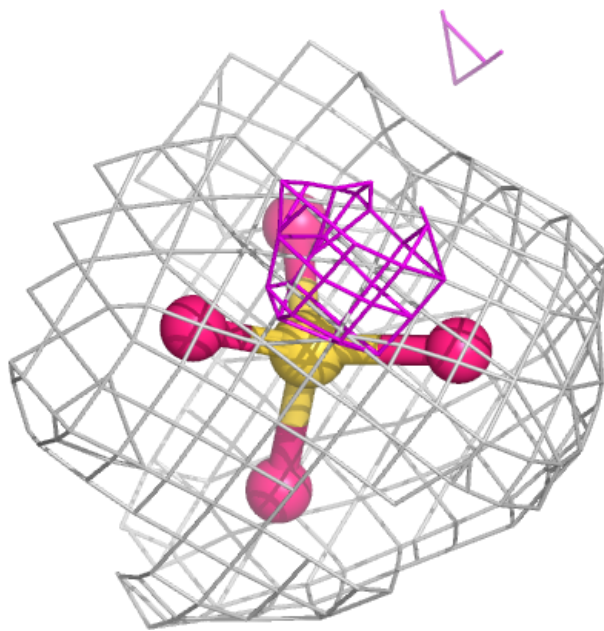
Electron density around SO4 A 2503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



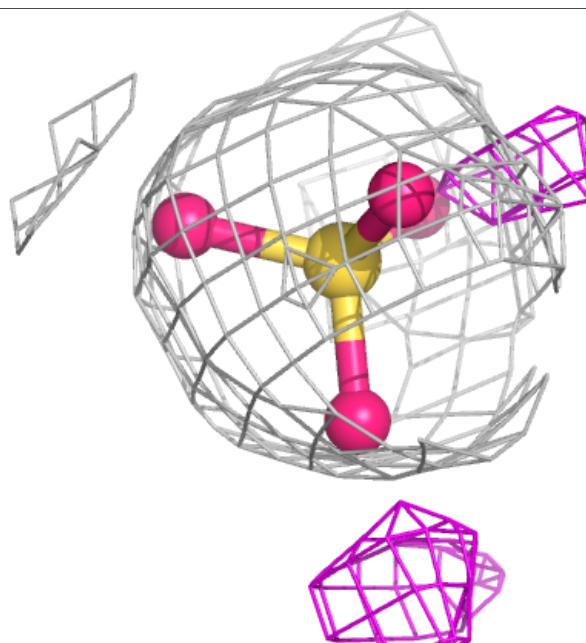
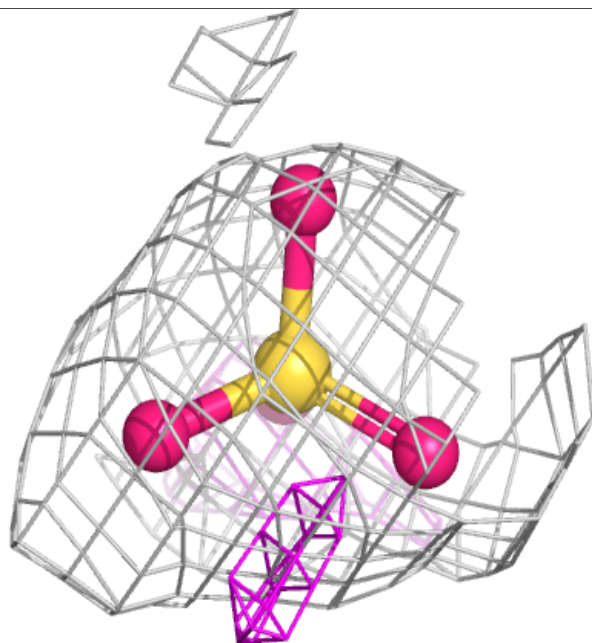
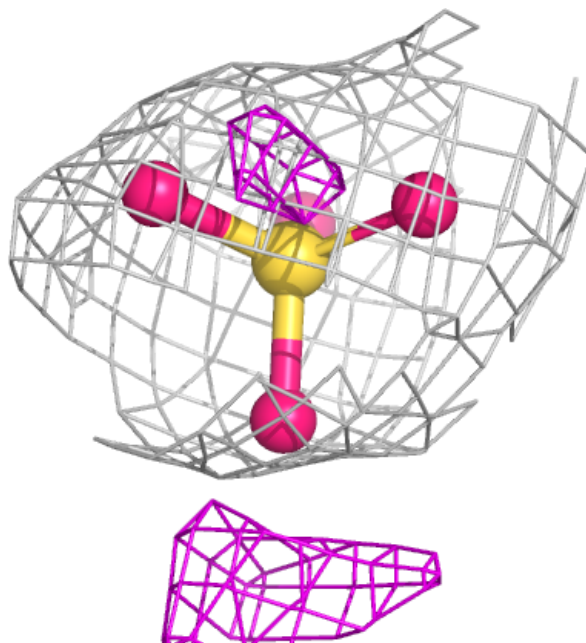
Electron density around SO4 B 2517:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



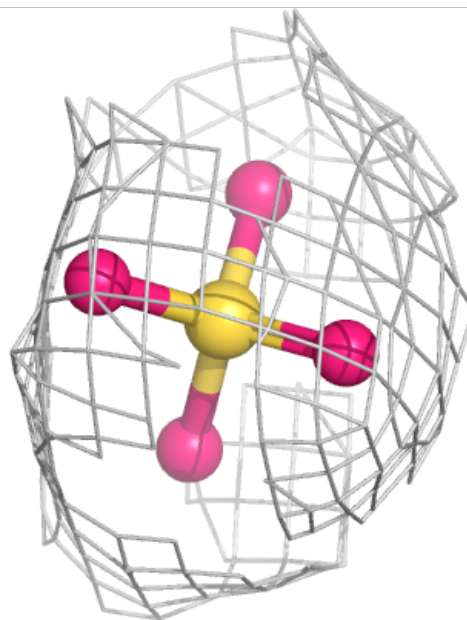
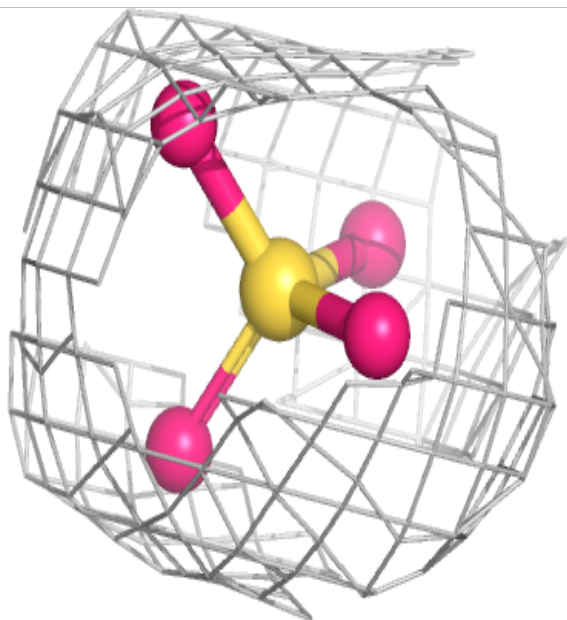
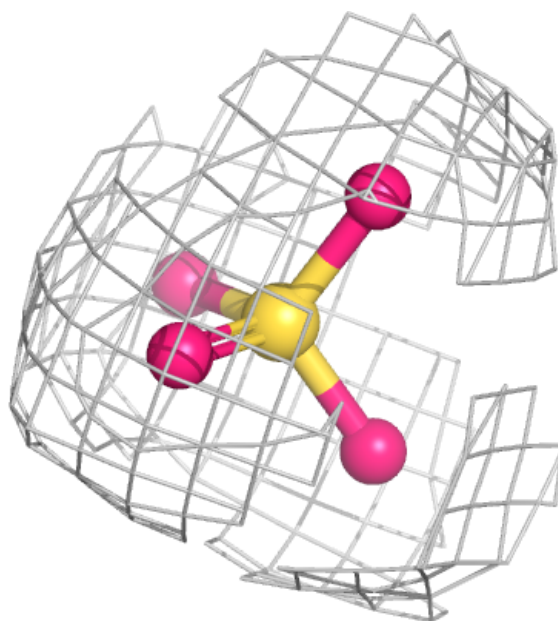
Electron density around SO4 A 2515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



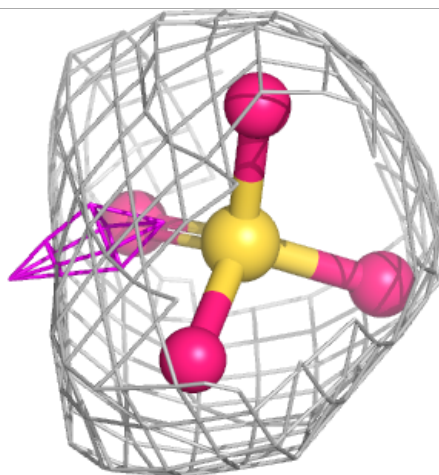
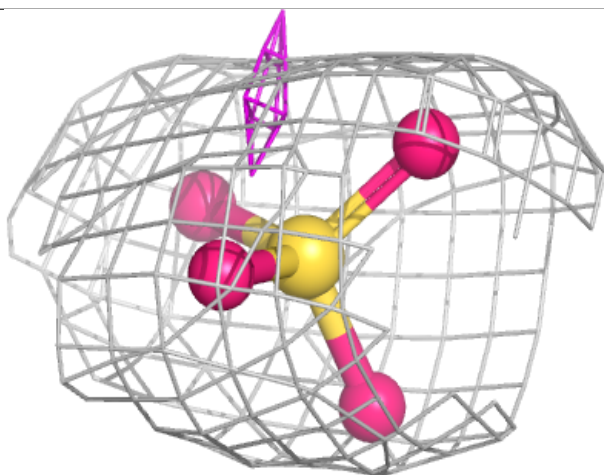
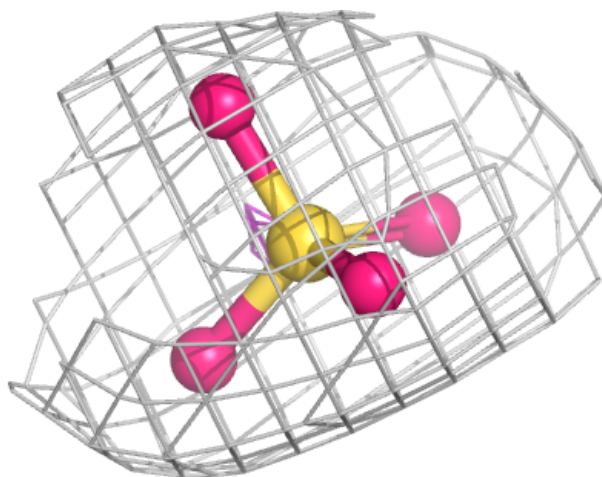
Electron density around SO4 B 2515:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



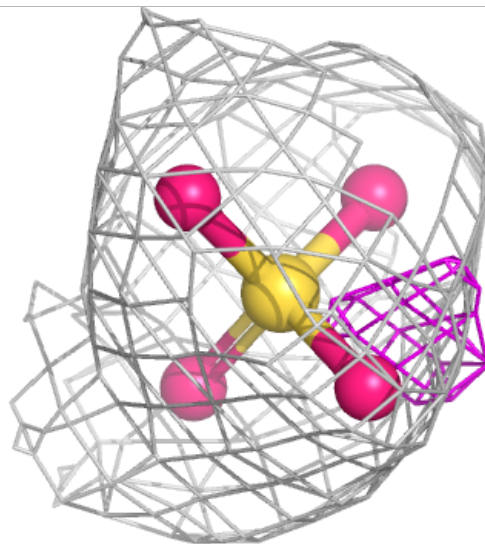
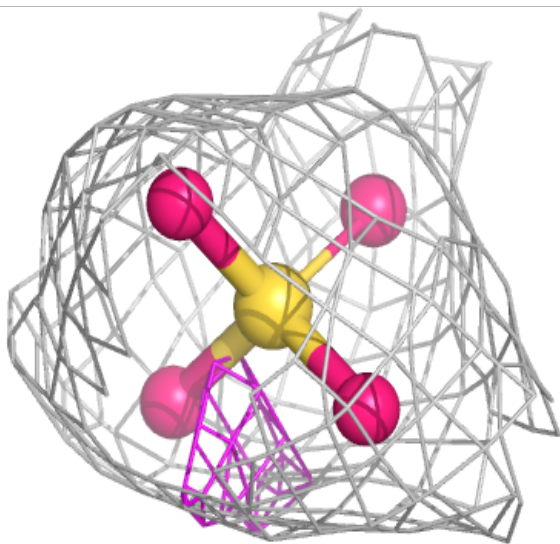
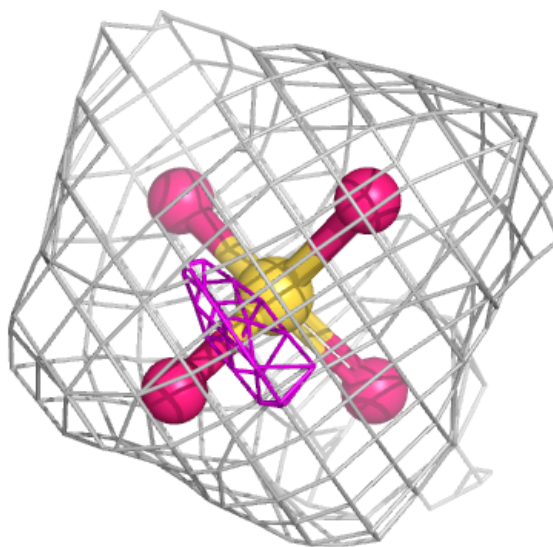
Electron density around SO4 A 2516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



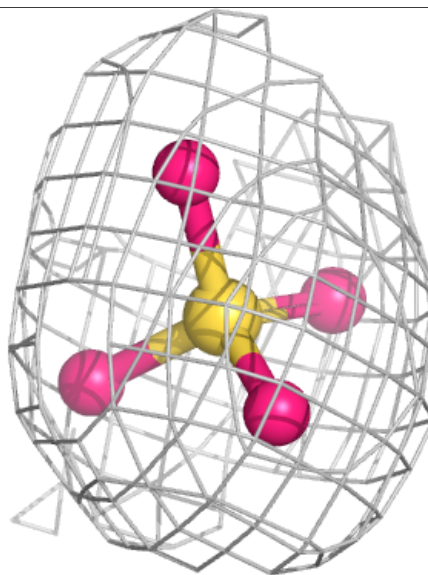
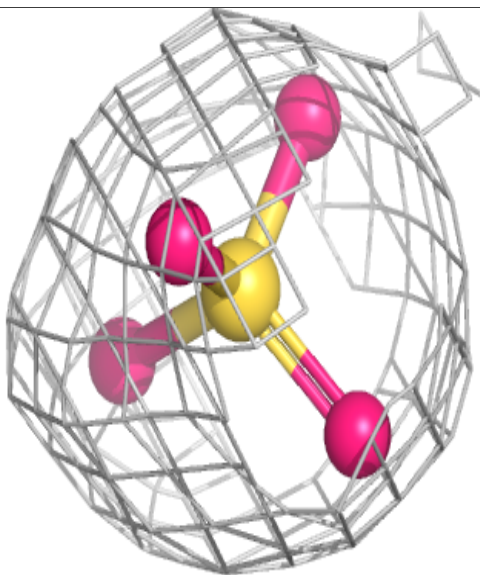
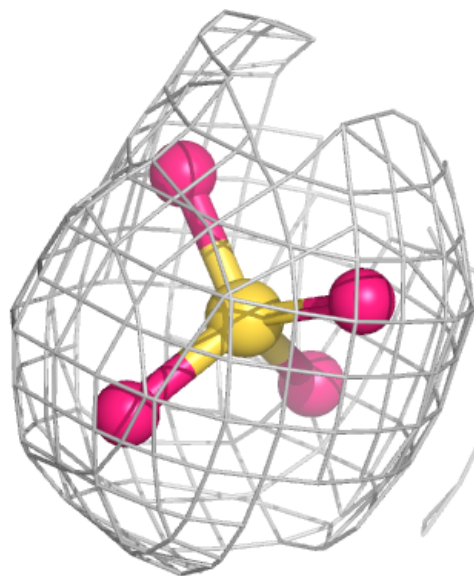
Electron density around SO4 B 2503:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



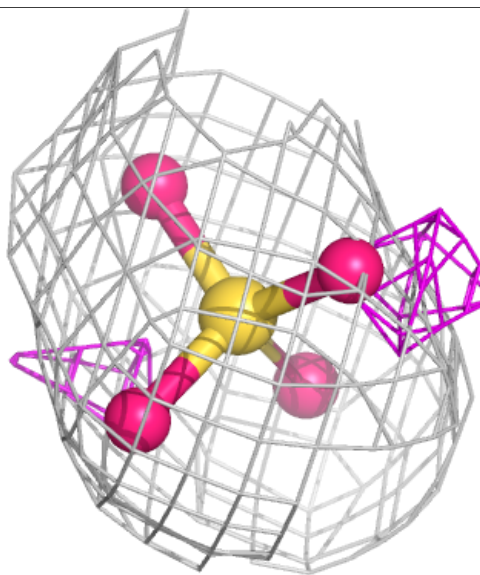
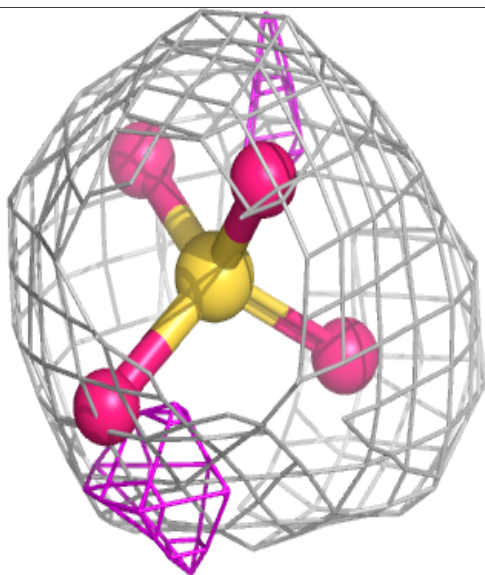
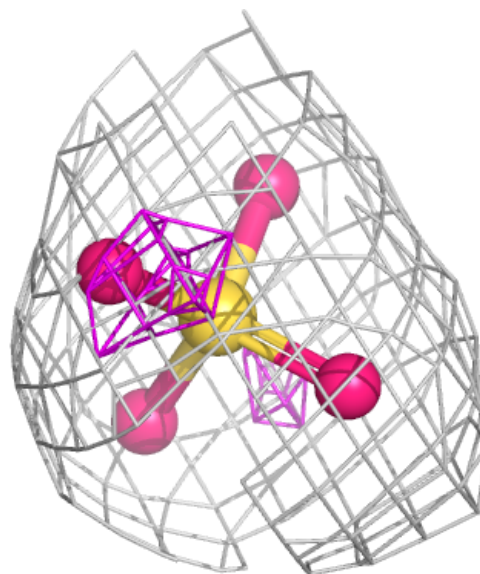
Electron density around SO4 B 2514:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



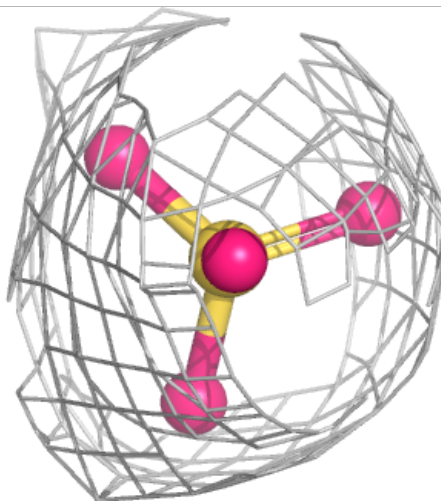
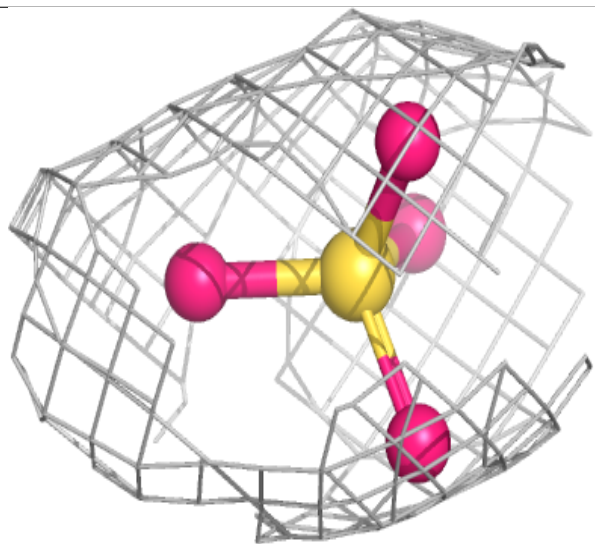
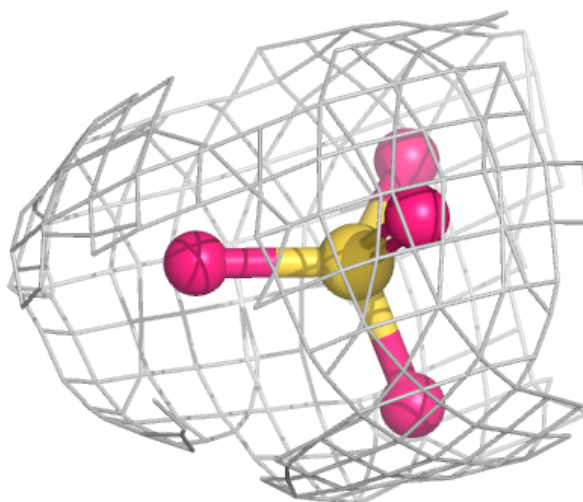
Electron density around SO4 A 2504:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



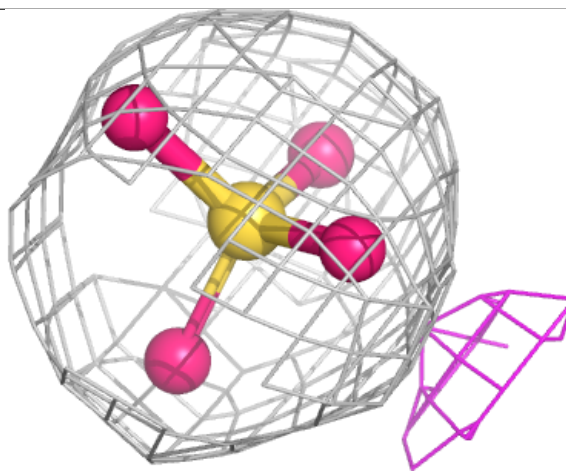
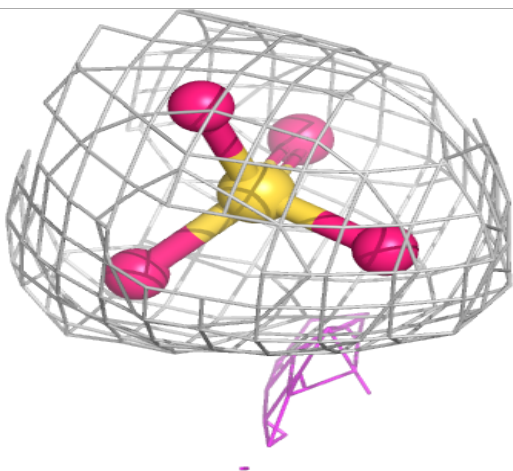
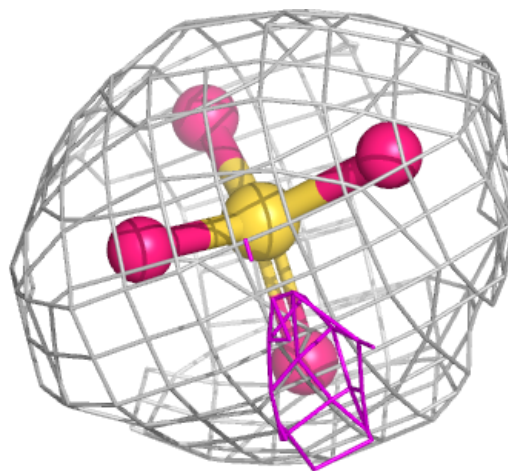
Electron density around SO4 B 2502:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



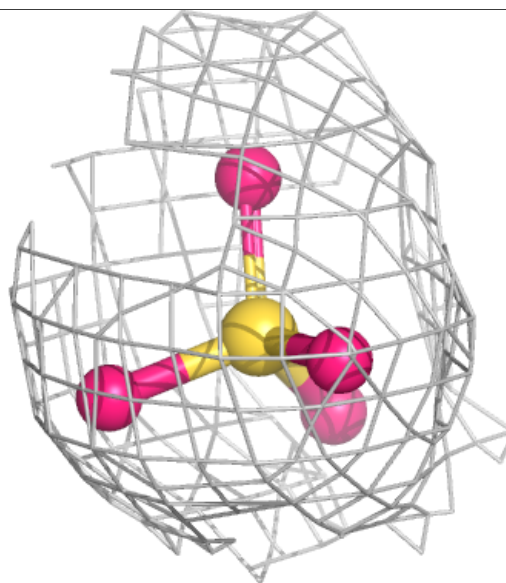
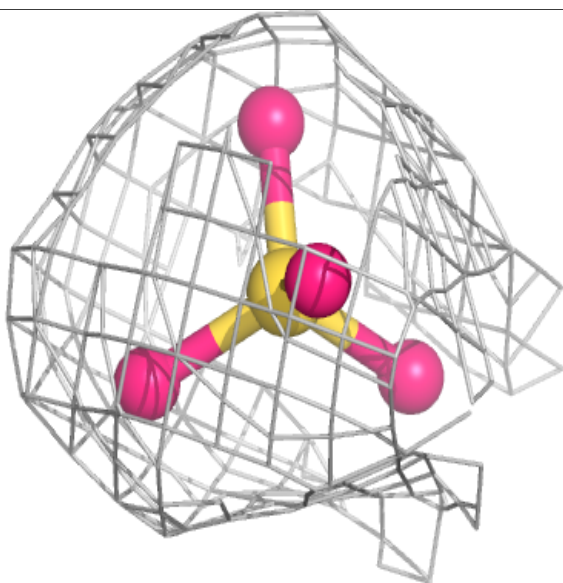
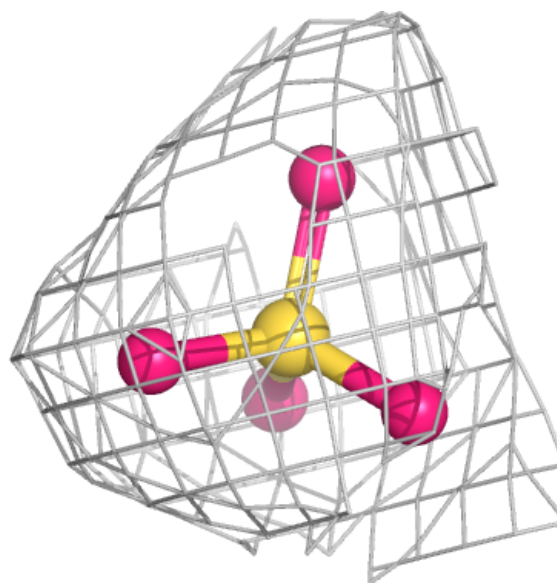
Electron density around SO4 B 2505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



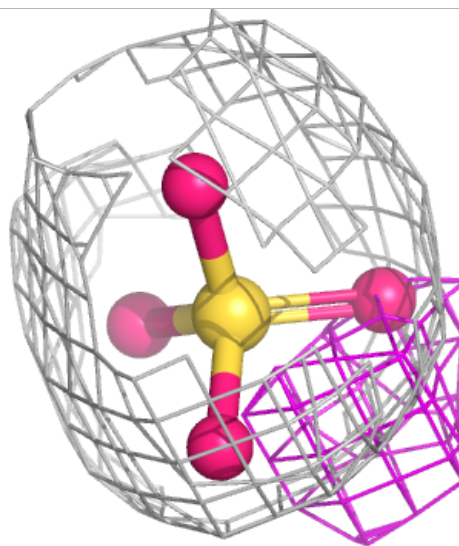
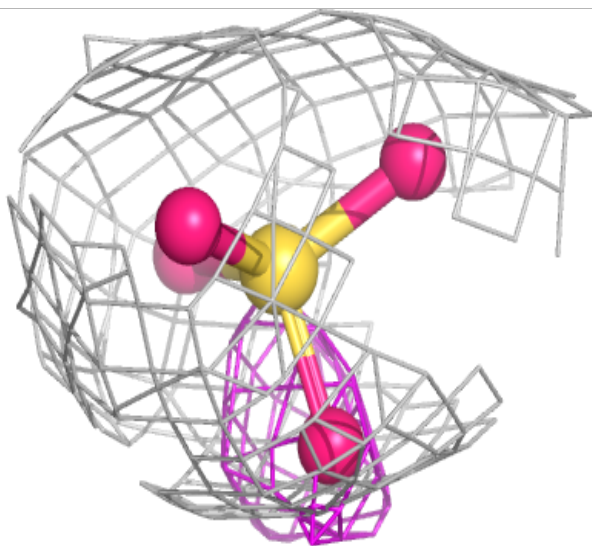
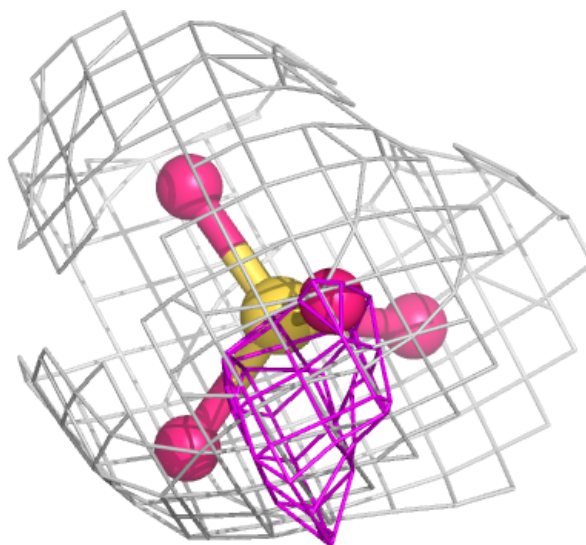
Electron density around SO4 B 2507:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



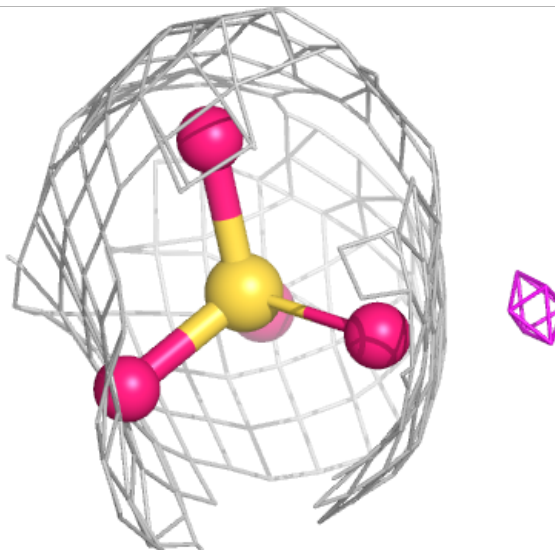
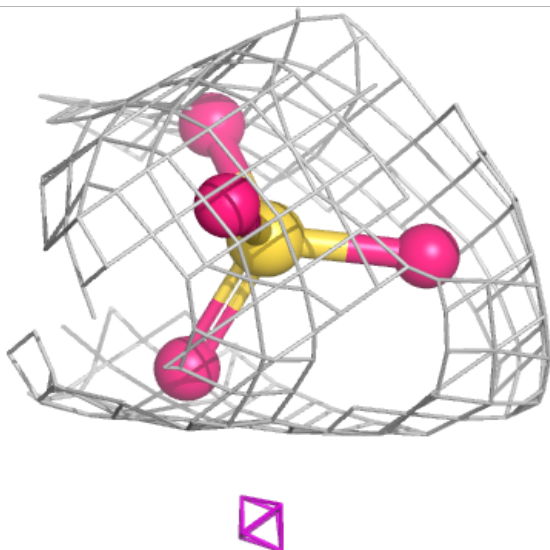
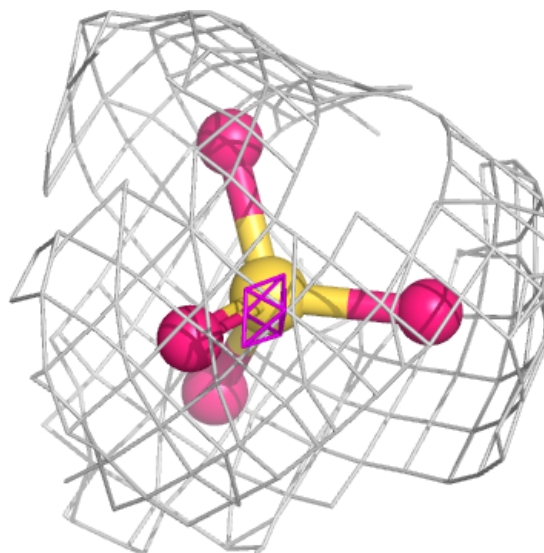
Electron density around SO4 A 2509:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



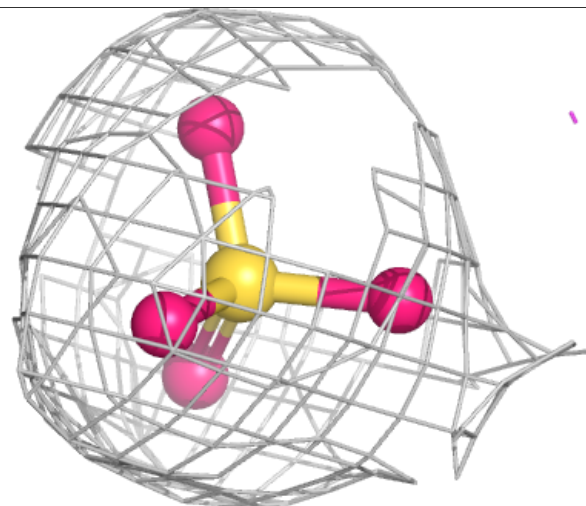
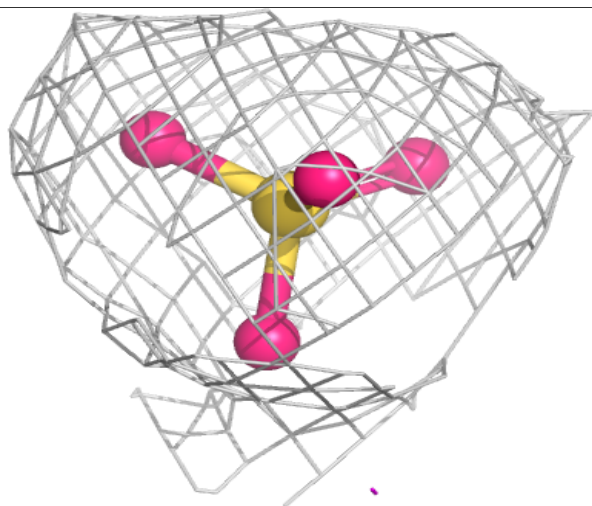
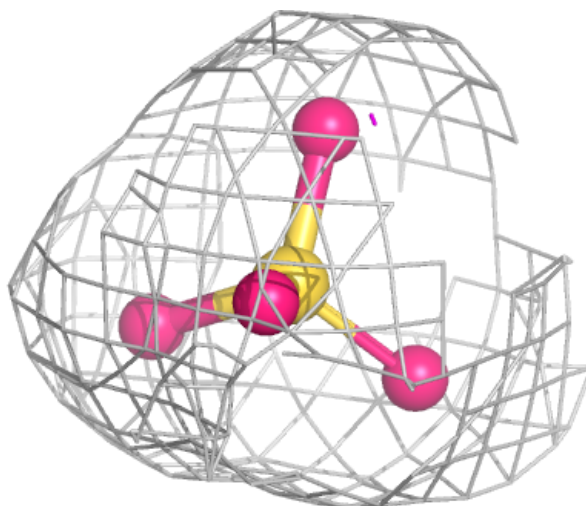
Electron density around SO4 A 2511:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



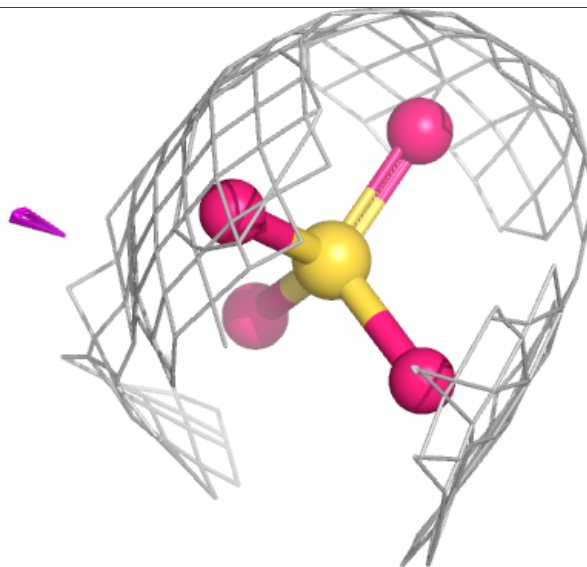
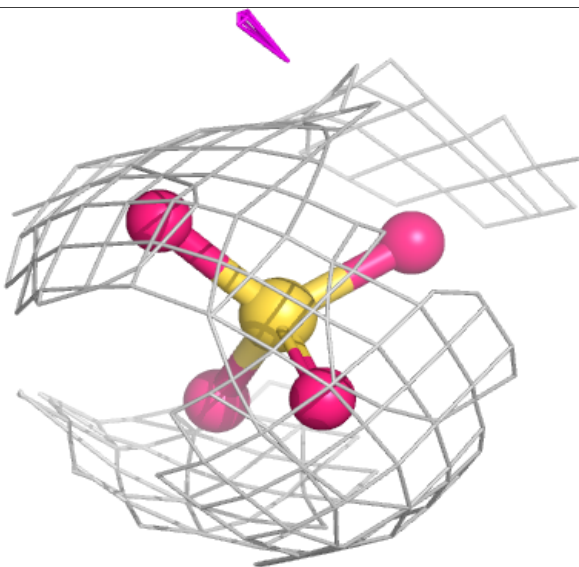
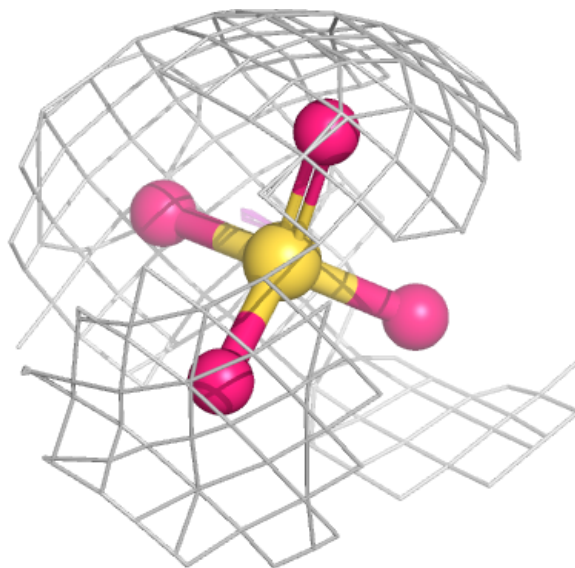
Electron density around SO4 A 2512:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



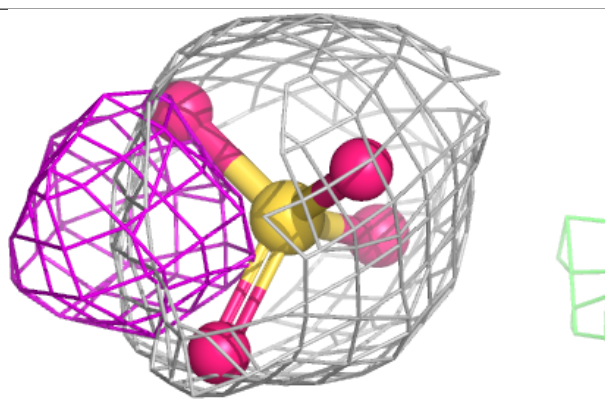
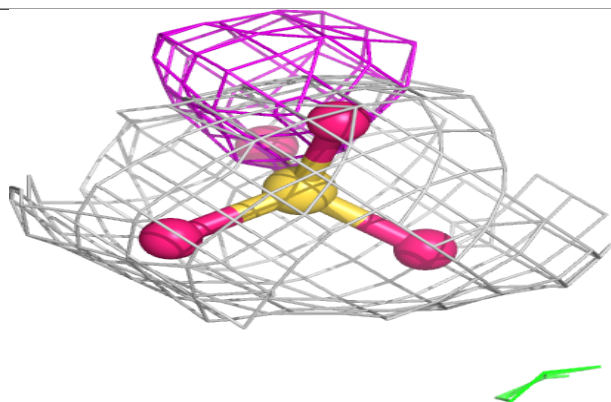
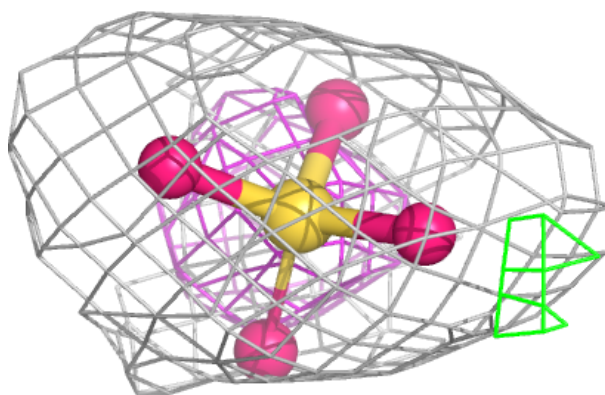
Electron density around SO4 A 2502:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



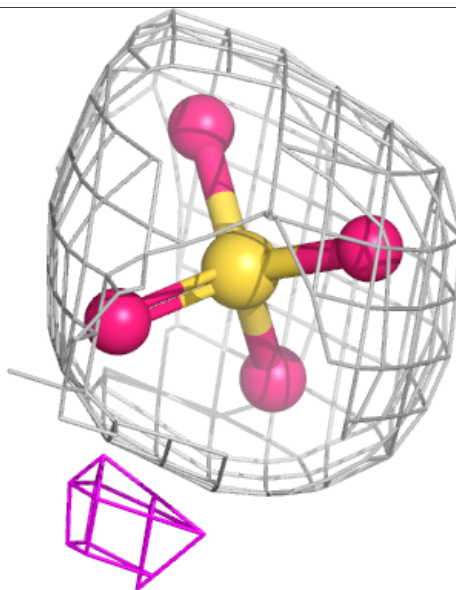
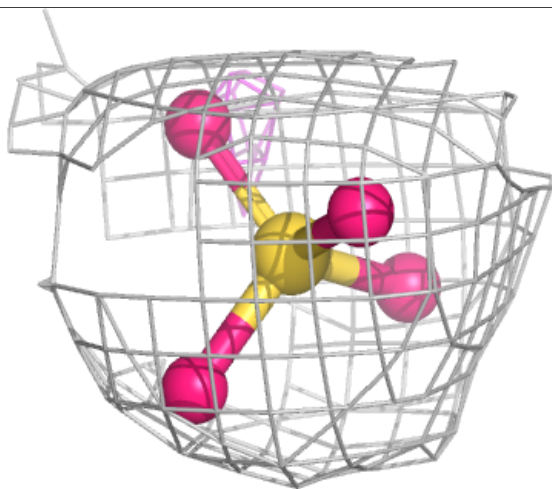
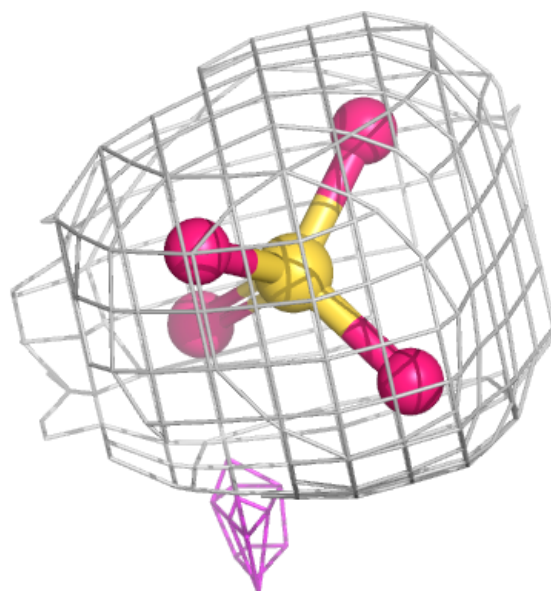
Electron density around SO4 A 2505:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



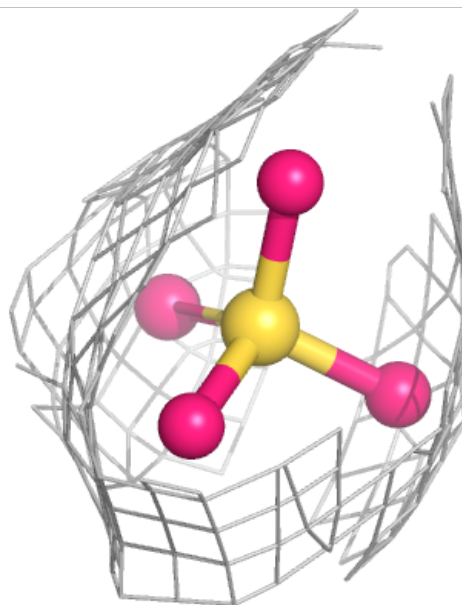
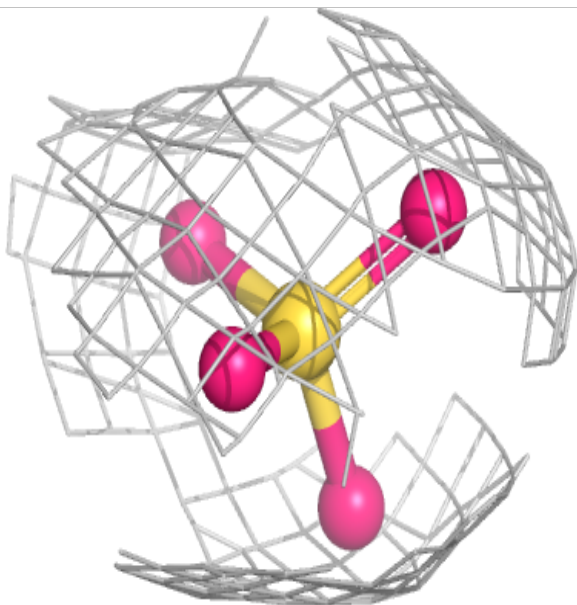
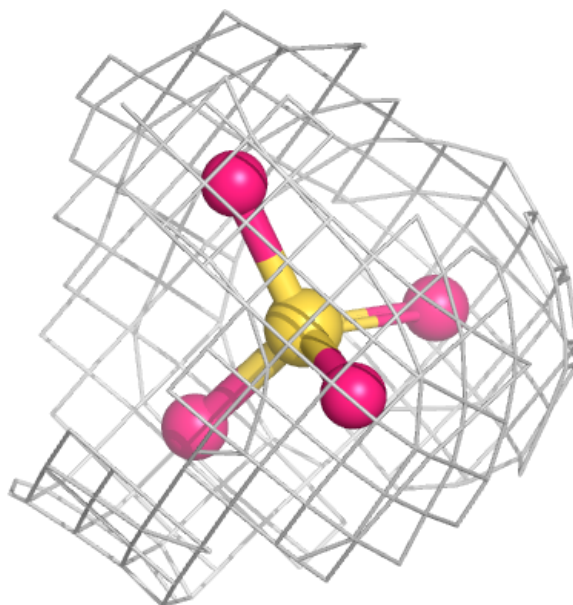
Electron density around SO4 B 2516:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



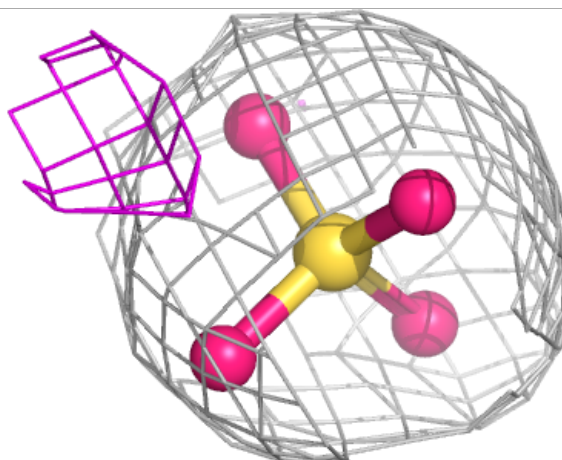
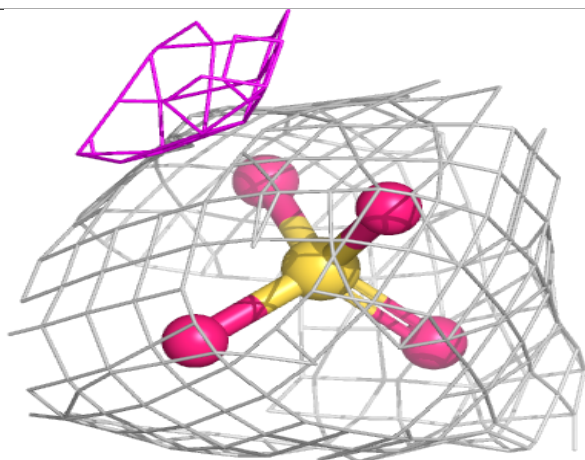
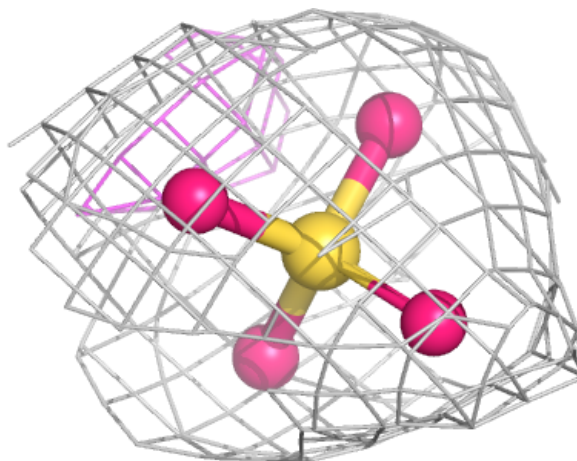
Electron density around SO4 A 2513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 A 2510:

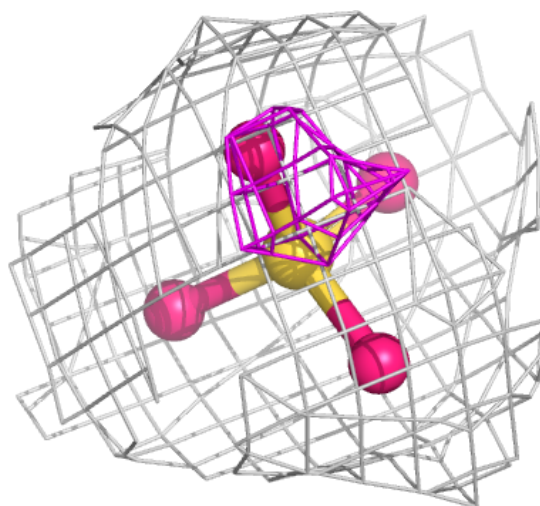
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



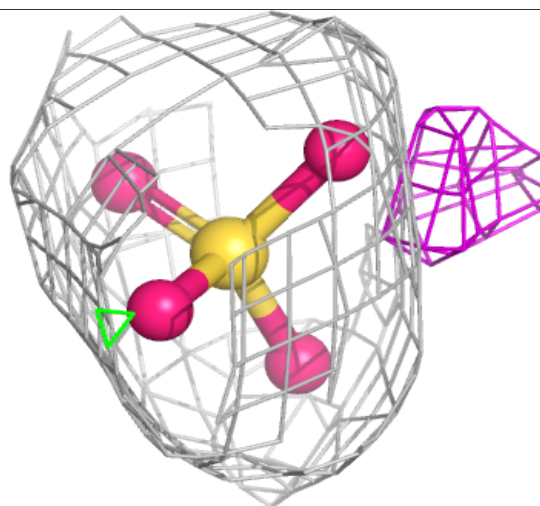
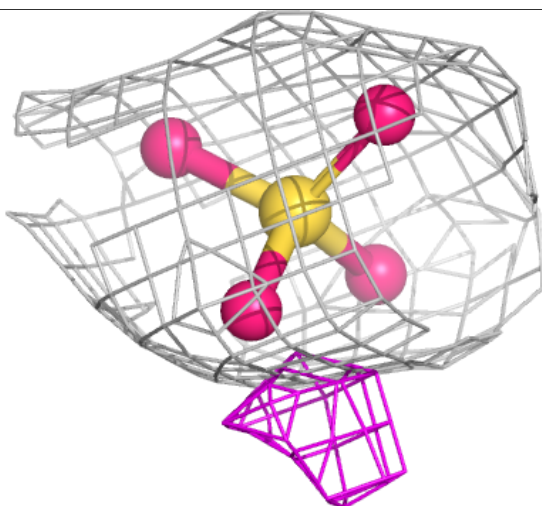
Electron density around SO4 B 2520:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

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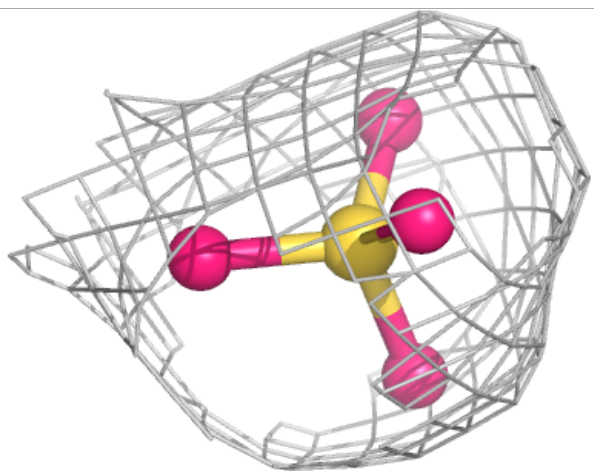
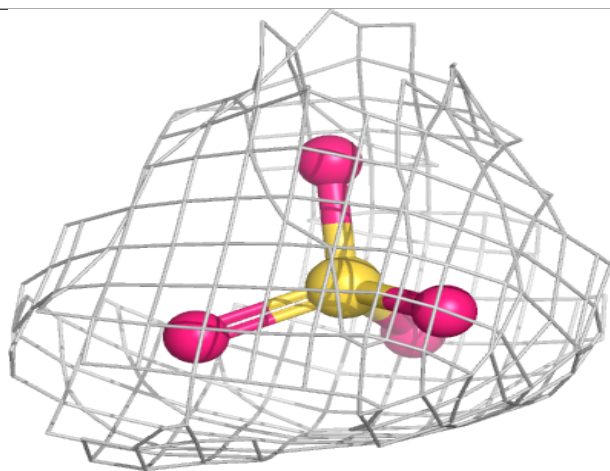
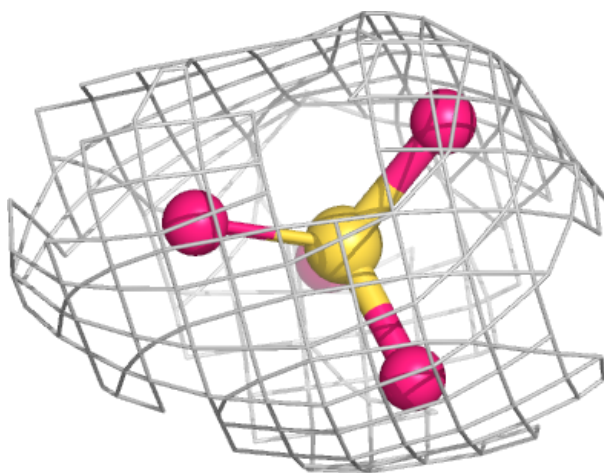


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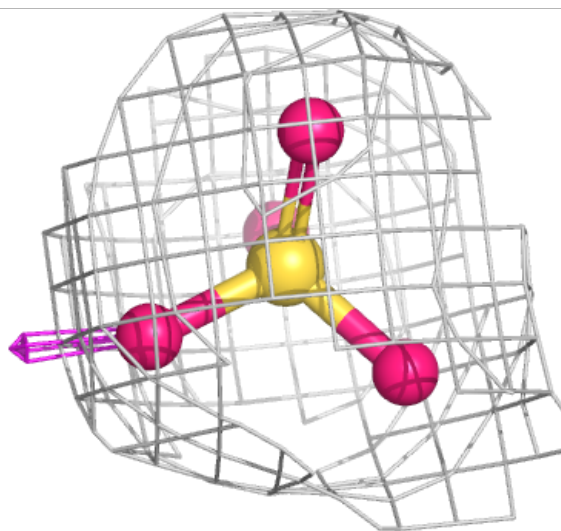
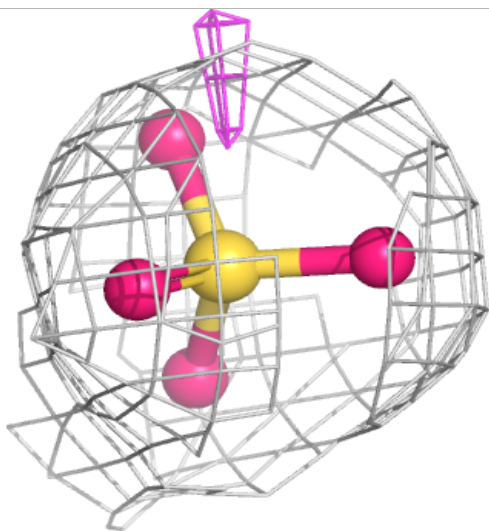
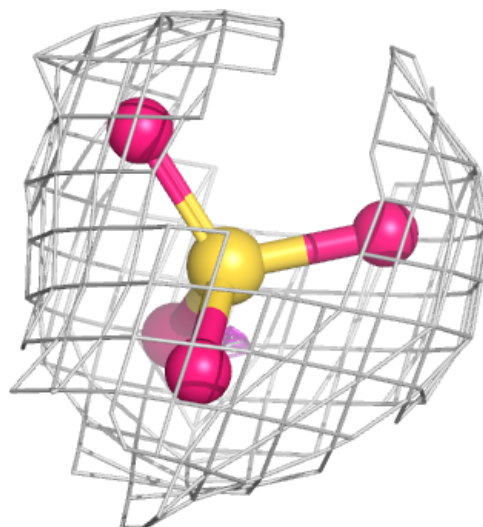
Electron density around SO4 B 2512:

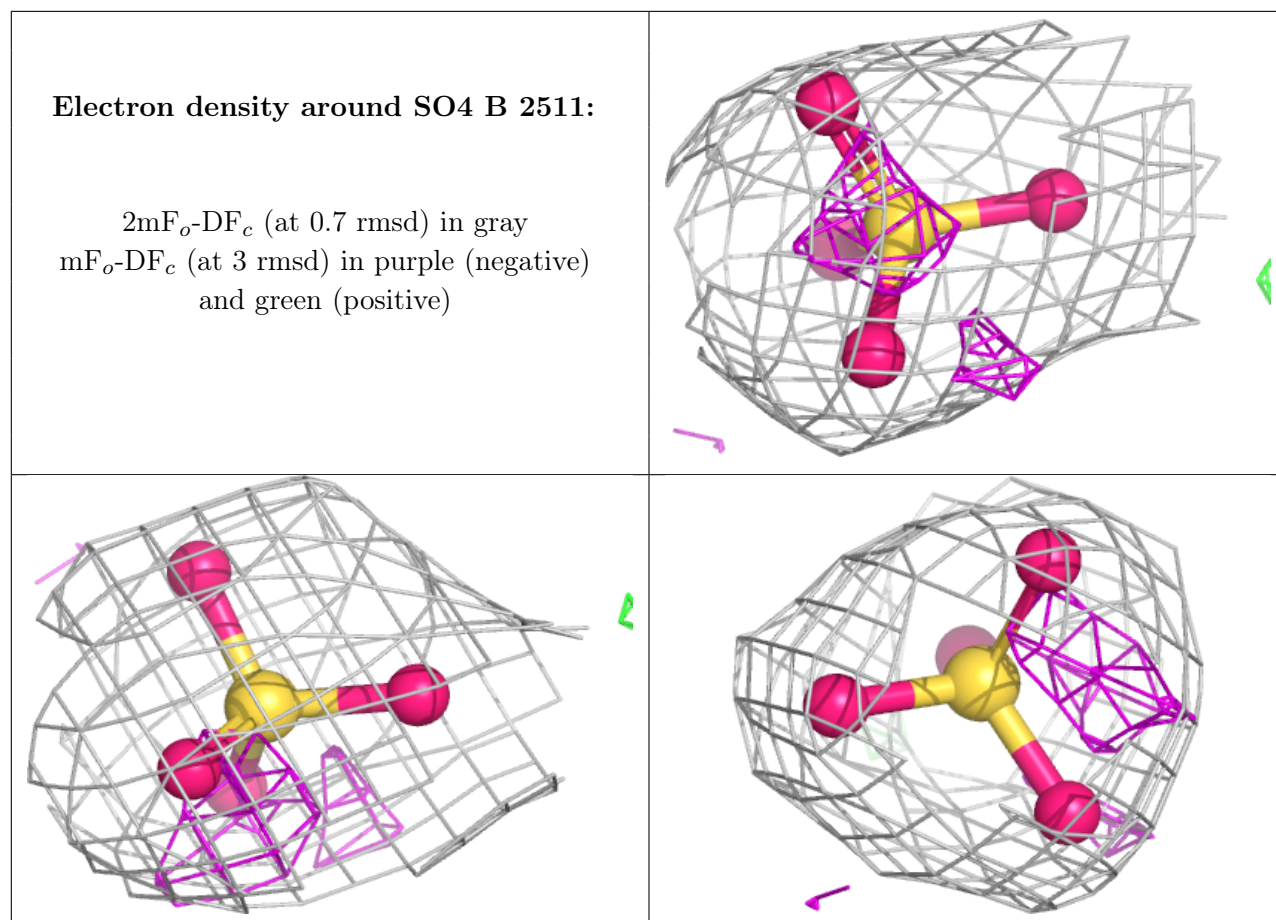
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around SO4 B 2513:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers ⓘ

There are no such residues in this entry.