



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2022 – 04:51 PM EST

PDB ID : 7U1Z  
Title : Crystal structure of the DRBD and CROPs of TcdA  
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Deposited on : 2022-02-22  
Resolution : 3.18 Å(reported)

This is a Full wwPDB X-ray Structure 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/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.27  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

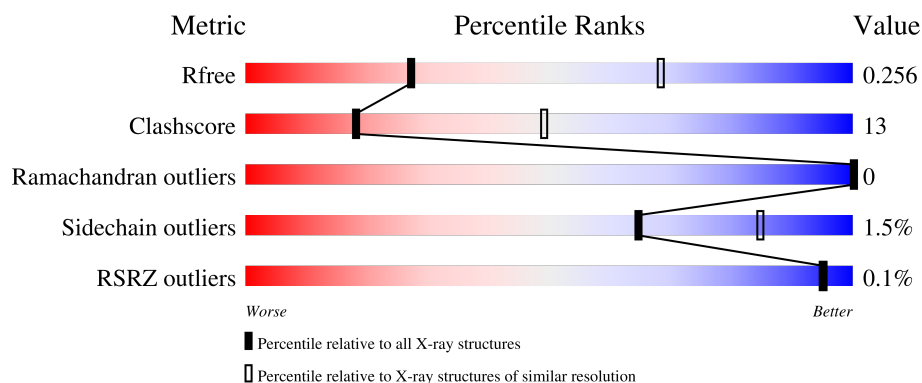
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1640	 70% 28% .
1	B	1640	 70% 27% ..

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.

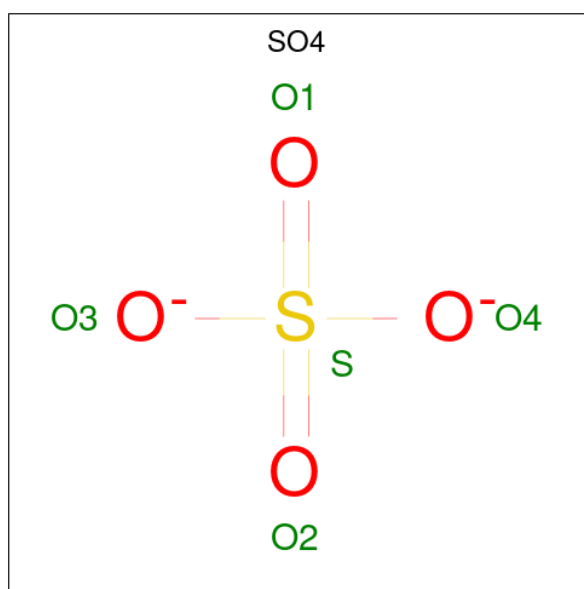
- Molecule 1 is a protein called Toxin A.

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 (three-letter code: SO4) (formula: O<sub>4</sub>S) (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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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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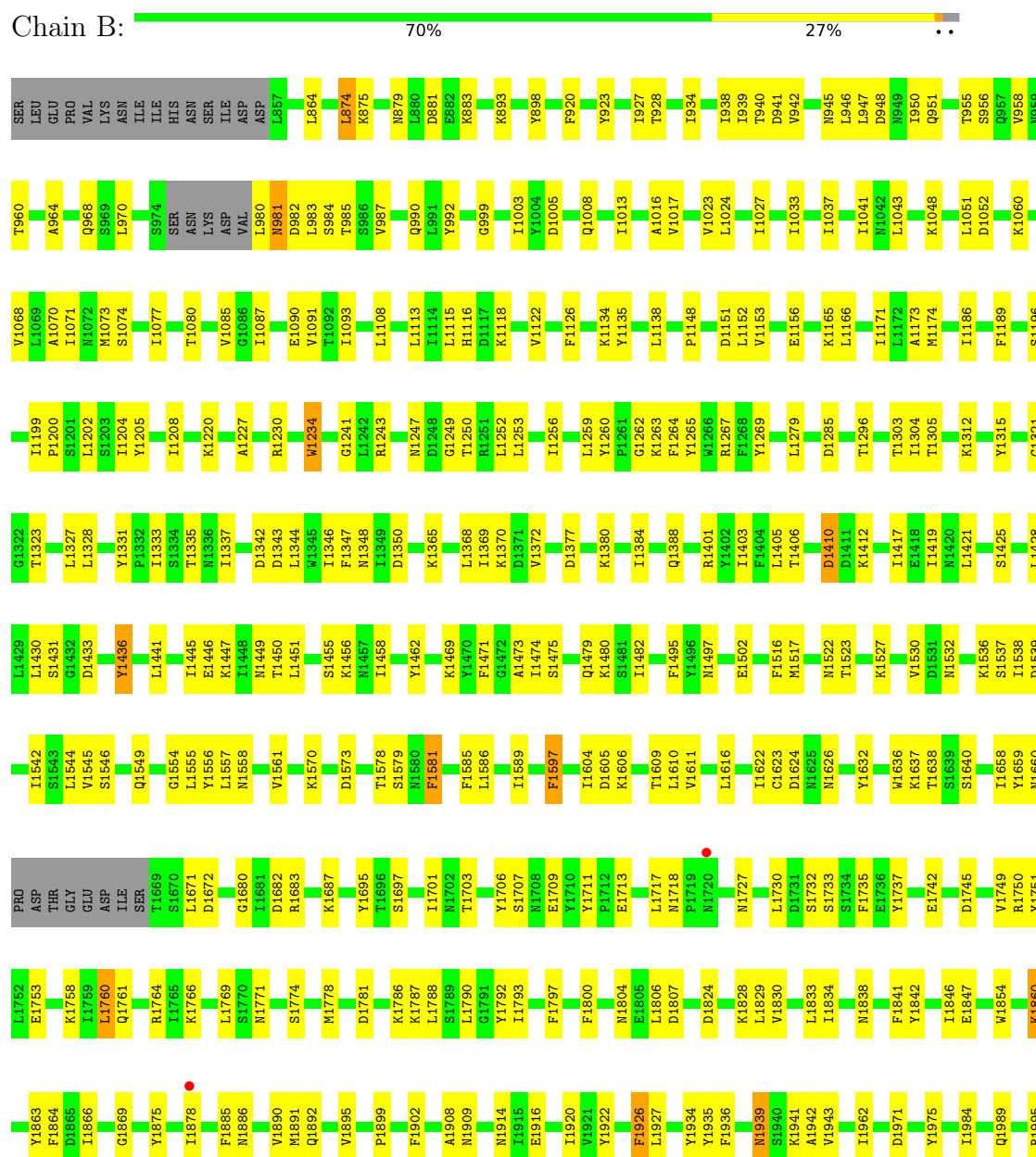
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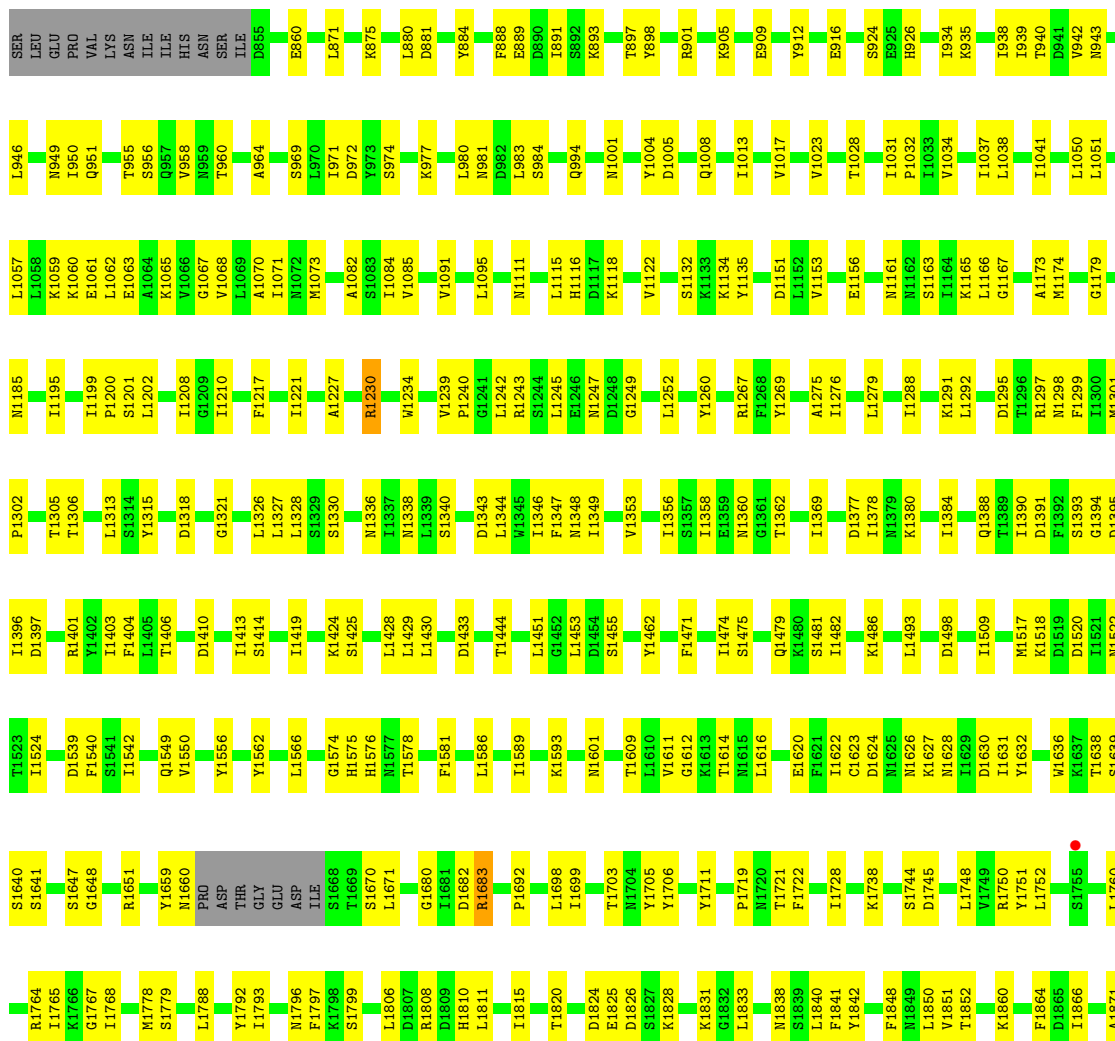
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	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		

### 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 electron 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 dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). 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: Toxin A







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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) 98.8 (186.08-3.18)	Depositor EDS
$R_{merge}$	0.28	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.30 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.207 , 0.254 0.208 , 0.256	Depositor DCC
$R_{free}$ test set	5513 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 53.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.53	0/13082	0.69	0/17780
1	B	0.52	0/12936	0.70	0/17588
All	All	0.52	0/26018	0.70	0/35368

There are no bond length outliers.

There are no bond angle outliers.

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	12792	0	12186	335	0
1	B	12649	0	11970	337	0
2	A	80	0	0	7	0
2	B	100	0	0	3	0
All	All	25621	0	24156	665	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 13.

All (665) 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
1:B:1895:VAL:HG21	1:B:1934:TYR:CE2	2.14	0.83
1:B:1846:ILE:HG13	1:B:1847:GLU:HG2	1.63	0.80
1:B:2376:LYS:HB3	1:B:2406:ILE:HG23	1.65	0.79
1:B:1914:ASN:HD22	1:B:1920:ILE:HG21	1.48	0.78
1:A:1692:PRO:HG3	1:A:1699:ILE:HD11	1.64	0.77
1:B:1530:VAL:HG21	1:B:1589:ILE:HG13	1.66	0.76
1:B:1241:GLY:H	1:B:1243:ARG:HH12	1.33	0.76
1:B:2190:TYR:H	1:B:2208:SER:HB2	1.50	0.76
1:A:2411:VAL:HG21	1:A:2450:TYR:CE2	2.21	0.76
1:A:1659:TYR:O	1:A:1660:ASN:ND2	2.19	0.75
1:A:897:THR:HG22	1:A:916:GLU:OE2	1.87	0.75
1:B:2103:THR:HG22	1:B:2108:LYS:HG3	1.69	0.75
1:B:2290:ALA:HB2	1:B:2298:GLU:HG2	1.70	0.73
1:A:1240:PRO:HB2	1:A:2252:GLN:HG2	1.70	0.73
1:B:1369:ILE:HG23	1:B:1372:VAL:HG21	1.68	0.72
1:B:955:THR:HA	1:B:958:VAL:HG12	1.72	0.72
1:B:2215:ARG:HE	1:B:2216:ILE:H	1.36	0.71
1:B:2170:PHE:HB2	1:B:2210:ALA:HB3	1.73	0.71
1:B:2418:PHE:HB2	1:B:2458:ALA:HB3	1.72	0.71
1:A:1517:MET:HE1	1:A:1520:ASP:HA	1.73	0.71
1:A:1624:ASP:HB2	1:A:1628:ASN:H	1.53	0.71
1:B:1579:SER:HB2	1:B:1604:ILE:HG22	1.71	0.71
1:A:1071:ILE:HD11	1:A:1073:MET:HE3	1.72	0.71
1:A:1122:VAL:HG13	1:A:1279:LEU:HD22	1.73	0.70
1:B:1545:VAL:HG23	1:B:1549:GLN:HG2	1.72	0.70
1:B:2200:LYS:HG2	1:B:2230:ILE:HD11	1.73	0.70
1:B:1886:ASN:ND2	1:B:1890:VAL:HG12	2.06	0.70
1:B:1134:LYS:HG2	1:B:1135:TYR:CE1	2.26	0.70
1:B:2410:GLY:HA2	1:B:2445:LEU:HD21	1.73	0.70
1:B:1638:THR:HG23	1:B:1640:SER:H	1.57	0.70
1:A:1156:GLU:HB3	1:A:1165:LYS:HB2	1.71	0.70
1:B:2286:TYR:HD2	1:B:2304:TYR:HD2	1.38	0.70
1:B:927:ILE:HD11	1:B:987:VAL:HG13	1.72	0.69
1:B:1475:SER:HB3	1:B:1517:MET:HE1	1.72	0.69
1:A:1988:TRP:HE1	1:A:1995:ARG:HG2	1.55	0.69
1:A:1630:ASP:OD1	1:A:1631:ILE:N	2.25	0.69
1:A:1095:LEU:HD11	1:A:1362:THR:HB	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2002:THR:HG23	1:A:2004:ILE:HG22	1.76	0.68
1:B:1908:ALA:HB2	1:B:1916:GLU:HG2	1.75	0.68
1:B:2264:TYR:HB2	1:B:2287:PHE:CE2	2.28	0.68
1:A:2026:LYS:NZ	2:A:2502:SO4:O2	2.28	0.67
1:B:1939:ASN:O	1:B:1939:ASN:ND2	2.28	0.67
1:A:2476:THR:OG1	1:A:2478:VAL:HG12	1.95	0.66
1:A:950:ILE:HG13	1:A:1037:ILE:HD13	1.76	0.66
1:A:1614:THR:HG23	1:A:1616:LEU:H	1.60	0.66
1:A:2370:TRP:HB2	1:A:2378:TYR:O	1.95	0.66
1:A:1395:ASP:OD2	1:A:1401:ARG:NH2	2.29	0.65
1:B:2214:TRP:CZ2	1:B:2238:ILE:HD11	2.32	0.65
1:B:1091:VAL:HG12	1:B:1327:LEU:HD22	1.78	0.65
1:A:1616:LEU:HD12	1:A:1636:TRP:HB2	1.76	0.65
1:A:1428:LEU:HD22	1:A:1455:SER:HB2	1.78	0.65
1:B:1173:ALA:HB3	1:B:1199:ILE:HG23	1.77	0.65
1:A:2290:ALA:HB2	1:A:2298:GLU:HB2	1.79	0.65
1:B:1545:VAL:CG2	1:B:1549:GLN:HG2	2.27	0.65
1:B:2164:PHE:HB2	1:B:2173:PHE:CE2	2.32	0.65
1:B:1370:LYS:HE3	1:B:1450:THR:HG23	1.79	0.64
1:A:2370:TRP:HB3	1:A:2379:TYR:HA	1.79	0.64
1:A:1068:VAL:HG12	1:A:1518:LYS:HB2	1.80	0.64
1:B:1609:THR:HG22	1:B:1622:ILE:HG13	1.80	0.64
1:A:1115:LEU:O	1:A:1116:HIS:ND1	2.30	0.64
1:B:1202:LEU:HD12	1:B:1260:TYR:CG	2.32	0.64
1:B:1557:LEU:HD11	1:B:1610:LEU:HD11	1.81	0.63
1:A:974:SER:HB3	1:A:984:SER:OG	1.98	0.63
1:B:1202:LEU:HD12	1:B:1260:TYR:CD2	2.33	0.63
1:B:1751:TYR:CE2	1:B:1753:GLU:HB3	2.34	0.63
1:B:1605:ASP:OD1	1:B:1606:LYS:N	2.32	0.62
1:B:2056:TYR:HD2	1:B:2070:PHE:CD2	2.16	0.62
1:A:1911:GLN:HG2	1:A:1921:VAL:HG23	1.81	0.62
1:B:1073:MET:HG2	1:B:1471:PHE:CG	2.33	0.62
1:A:2056:TYR:H	1:A:2074:SER:HB3	1.63	0.62
1:B:1885:PHE:CE1	1:B:1891:MET:HG3	2.35	0.62
1:A:1034:VAL:HG22	1:A:1539:ASP:HB3	1.81	0.62
1:B:1071:ILE:HG21	1:B:1473:ALA:HB2	1.82	0.62
1:B:1886:ASN:HD21	1:B:1890:VAL:HG12	1.62	0.62
1:A:860:GLU:OE2	1:A:926:HIS:NE2	2.32	0.62
1:A:1611:VAL:HG12	1:A:1620:GLU:HA	1.81	0.62
1:A:1824:ASP:HB3	1:A:1826:ASP:H	1.65	0.62
1:B:2399:PHE:HZ	1:B:2431:ILE:HD11	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2006:PHE:CD2	1:A:2010:LYS:HG2	2.34	0.62
1:B:1804:ASN:HB3	1:B:1807:ASP:HB3	1.81	0.62
1:A:1199:ILE:HG13	1:A:1200:PRO:HD2	1.82	0.62
1:A:2291:ASN:ND2	1:A:2295:ASN:OD1	2.33	0.61
1:B:1441:LEU:HD11	1:B:1474:ILE:HD13	1.82	0.61
1:B:1683:ARG:NH2	1:B:1709:GLU:OE1	2.32	0.61
1:B:1606:LYS:HA	1:B:1623:CYS:HB3	1.82	0.61
1:A:1380:LYS:HG2	1:A:1396:ILE:HD12	1.81	0.61
1:B:950:ILE:HG13	1:B:1037:ILE:HD13	1.81	0.61
1:B:1546:SER:HB3	1:B:1549:GLN:HB3	1.83	0.61
1:A:2160:GLN:O	1:A:2161:ILE:HD12	2.00	0.61
1:A:2368:THR:HB	1:A:2385:PHE:HE1	1.64	0.61
1:B:2235:LEU:HD22	1:B:2258:ILE:HD13	1.83	0.60
1:A:1330:SER:OG	1:A:1356:ILE:HG13	2.01	0.60
1:B:1446:GLU:HA	1:B:1449:ASN:HD22	1.67	0.60
1:B:2246:SER:HB3	1:B:2252:GLN:HE21	1.66	0.60
1:A:2253:ASN:HB3	1:A:2271:SER:HB3	1.82	0.60
1:A:1060:LYS:HD2	1:A:1425:SER:HB3	1.81	0.60
1:A:1474:ILE:HG12	1:A:1481:SER:HB3	1.84	0.60
1:A:1240:PRO:CB	1:A:2252:GLN:HG2	2.31	0.59
1:B:1742:GLU:OE1	1:B:1764:ARG:NH1	2.30	0.59
1:B:1538:ILE:HG13	1:B:1557:LEU:HD23	1.84	0.59
1:B:2388:SER:HB2	1:B:2392:THR:HG21	1.85	0.59
1:B:2031:SER:HB3	1:B:2036:PHE:CE1	2.38	0.59
1:A:893:LYS:HD2	1:A:898:TYR:CE1	2.38	0.59
1:A:1831:LYS:HD3	1:A:1848:PHE:HE1	1.67	0.59
1:B:1108:LEU:HD13	1:B:1113:LEU:HD12	1.83	0.59
1:A:871:LEU:O	1:A:875:LYS:HG3	2.02	0.59
1:A:1850:LEU:HD12	1:A:1851:VAL:H	1.67	0.58
1:A:1852:THR:HB	1:A:1866:ILE:HA	1.84	0.58
1:B:2215:ARG:HE	1:B:2216:ILE:N	2.00	0.58
1:A:1967:LEU:CD2	1:A:1991:VAL:HG11	2.33	0.58
1:A:2402:ASN:ND2	1:A:2408:GLN:OE1	2.36	0.58
1:B:1051:LEU:HD21	1:B:1070:ALA:HB1	1.84	0.58
1:B:2225:ASN:OD1	1:B:2226:PRO:HD2	2.03	0.58
1:B:2286:TYR:CD2	1:B:2304:TYR:HD2	2.21	0.58
1:B:1033:ILE:HG21	1:B:1048:LYS:HD2	1.84	0.58
1:A:1850:LEU:HD12	1:A:1851:VAL:N	2.19	0.58
1:B:951:GLN:OE1	1:B:960:THR:HG21	2.02	0.58
1:B:1090:GLU:O	1:B:1093:ILE:HG22	2.02	0.58
1:A:1682:ASP:OD1	1:A:1683:ARG:NH1	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2394:ILE:HG13	1:A:2394:ILE:O	2.04	0.58
1:B:864:LEU:HD11	1:B:970:LEU:HG	1.84	0.58
1:B:1315:TYR:HD2	1:B:1335:THR:HG22	1.69	0.58
1:A:1967:LEU:HD23	1:A:1991:VAL:HG11	1.85	0.57
1:A:1482:ILE:HD11	1:A:1524:ILE:HD11	1.85	0.57
1:A:1540:PHE:CD2	1:A:1542:ILE:HD12	2.39	0.57
1:A:939:ILE:CD1	1:A:1041:ILE:HG12	2.34	0.57
1:B:1368:LEU:HB2	2:B:2511:SO4:O2	2.05	0.57
1:A:1578:THR:O	1:A:1581:PHE:HB3	2.04	0.57
1:A:1091:VAL:HG12	1:A:1327:LEU:HD22	1.86	0.57
1:A:1493:LEU:HD21	1:A:1524:ILE:HD13	1.87	0.57
1:B:881:ASP:HB3	1:B:883:LYS:HG2	1.86	0.57
1:A:934:ILE:HD11	1:A:964:ALA:HA	1.85	0.56
1:A:938:ILE:HG21	1:A:946:LEU:HD22	1.88	0.56
1:A:1377:ASP:HB3	1:A:1384:ILE:HB	1.88	0.56
1:B:1241:GLY:H	1:B:1243:ARG:NH1	2.03	0.56
1:A:1227:ALA:HB1	1:A:1230:ARG:HH12	1.71	0.56
1:A:1831:LYS:HB3	1:A:1848:PHE:HD1	1.71	0.56
1:B:1241:GLY:N	1:B:1243:ARG:HH12	2.03	0.56
1:B:1866:ILE:HD12	1:B:1866:ILE:H	1.71	0.56
1:B:2164:PHE:HB2	1:B:2173:PHE:HE2	1.69	0.56
1:A:958:VAL:HG23	1:A:1648:GLY:O	2.06	0.56
1:B:1682:ASP:OD1	1:B:1683:ARG:NH1	2.38	0.56
1:B:2264:TYR:HB2	1:B:2287:PHE:CD2	2.41	0.56
1:A:1937:ASP:OD1	1:A:1939:ASN:N	2.36	0.56
1:A:1166:LEU:HD21	1:A:1210:ILE:HG13	1.87	0.56
1:A:1353:VAL:O	1:A:1369:ILE:HG22	2.05	0.56
1:A:1638:THR:HG22	1:A:1641:SER:H	1.71	0.56
1:B:1909:ASN:N	1:B:1914:ASN:OD1	2.39	0.56
1:B:2328:TRP:CD1	1:B:2335:LYS:HE2	2.41	0.56
1:A:1632:TYR:HA	1:A:1647:SER:OG	2.05	0.56
1:B:893:LYS:HB2	1:B:898:TYR:CE1	2.41	0.56
1:B:1935:TYR:O	1:B:1943:VAL:HG12	2.06	0.56
1:A:2370:TRP:CB	1:A:2379:TYR:HA	2.36	0.56
1:B:2060:PHE:HB2	2:B:2506:SO4:O2	2.06	0.55
1:A:2328:TRP:CZ2	1:A:2352:ILE:HD11	2.40	0.55
1:B:1005:ASP:HB3	1:B:1008:GLN:HB3	1.88	0.55
1:B:874:LEU:HD13	1:B:920:PHE:CE2	2.42	0.55
1:B:1788:LEU:HD22	1:B:1792:TYR:CG	2.41	0.55
1:B:1806:LEU:HD13	1:B:1829:LEU:HD21	1.89	0.55
1:B:1824:ASP:OD2	1:B:1828:LYS:HE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:ILE:HG22	1:A:940:THR:HG22	1.87	0.55
1:A:1034:VAL:CG2	1:A:1539:ASP:HB3	2.36	0.55
1:B:2328:TRP:HE1	1:B:2335:LYS:HG2	1.71	0.55
1:A:2372:THR:HG22	1:A:2377:LYS:HD3	1.88	0.55
1:B:1570:LYS:NZ	1:B:1707:SER:O	2.39	0.54
1:A:1927:LEU:HD11	1:A:1929:LEU:HD13	1.89	0.54
1:A:2080:LEU:HD13	1:A:2104:ILE:HD11	1.89	0.54
1:A:1179:GLY:N	2:A:2501:SO4:O4	2.35	0.54
1:B:1115:LEU:O	1:B:1116:HIS:ND1	2.40	0.54
1:B:2203:TYR:O	1:B:2211:VAL:HG12	2.08	0.54
1:A:1833:LEU:HD11	1:A:1840:LEU:HG	1.90	0.54
1:B:1495:PHE:HB2	1:B:1544:LEU:HD23	1.90	0.54
1:B:1482:ILE:HG13	1:B:1522:ASN:HB2	1.88	0.54
1:B:2056:TYR:CE1	1:B:2059:LYS:HD2	2.43	0.54
1:B:980:LEU:HD12	1:B:982:ASP:H	1.73	0.54
1:B:1703:THR:OG1	1:B:1732:SER:OG	2.25	0.54
1:A:2277:VAL:HG21	1:A:2316:TYR:CE2	2.43	0.54
1:B:1043:LEU:HD22	1:B:1068:VAL:HG21	1.89	0.53
1:B:1733:SER:HB3	1:B:1735:PHE:CE2	2.43	0.53
1:A:1005:ASP:HB3	1:A:1008:GLN:HB3	1.89	0.53
1:A:1475:SER:HB3	1:A:1517:MET:HE1	1.90	0.53
1:B:893:LYS:HB2	1:B:898:TYR:CD1	2.43	0.53
1:A:1542:ILE:HG23	1:A:1550:VAL:HG13	1.91	0.53
1:A:1956:PHE:CE1	1:A:1963:ALA:HB2	2.44	0.53
1:A:1247:ASN:HB3	1:A:1249:GLY:H	1.74	0.53
1:A:2128:LYS:HE3	1:A:2158:ILE:HD13	1.90	0.53
1:B:1204:ILE:HG23	1:B:1256:ILE:HD11	1.91	0.53
1:A:2040:ALA:HB2	1:A:2054:ILE:HD13	1.90	0.53
1:B:1156:GLU:HB3	1:B:1165:LYS:HB2	1.91	0.53
1:B:1532:ASN:ND2	1:B:1532:ASN:O	2.41	0.53
1:B:2321:ASP:O	1:B:2323:LYS:HG3	2.08	0.53
1:A:1288:ILE:HD12	1:A:1315:TYR:CE1	2.44	0.53
1:B:2238:ILE:HG13	1:B:2238:ILE:O	2.09	0.53
1:A:2201:LYS:NZ	1:A:2248:ASP:O	2.40	0.53
1:B:2445:LEU:HD12	1:B:2446:ASN:HB2	1.91	0.53
1:B:1208:ILE:HG12	1:B:1252:LEU:HD11	1.91	0.52
1:B:1368:LEU:HG	1:B:1451:LEU:HD11	1.91	0.52
1:B:956:SER:O	1:B:960:THR:HG23	2.09	0.52
1:B:1060:LYS:HD2	1:B:1425:SER:HB3	1.91	0.52
1:B:1303:THR:HG23	1:B:1331:TYR:HD2	1.73	0.52
1:B:1749:VAL:HG21	1:B:1800:PHE:CZ	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2056:TYR:HD2	1:B:2070:PHE:HD2	1.55	0.52
1:B:2058:SER:HA	1:B:2070:PHE:O	2.08	0.52
1:B:2246:SER:OG	1:B:2248:ASP:OD1	2.28	0.52
1:A:1132:SER:HB2	1:A:1210:ILE:HD12	1.92	0.52
1:B:1027:ILE:HG13	1:B:1632:TYR:CE2	2.44	0.52
1:B:1186:ILE:HD11	1:B:1243:ARG:HB2	1.92	0.52
1:B:2284:PHE:CB	1:B:2324:ALA:HB3	2.39	0.52
1:B:934:ILE:HD11	1:B:964:ALA:HA	1.91	0.52
1:A:1327:LEU:HA	1:A:1348:ASN:HB2	1.90	0.52
1:A:2368:THR:HB	1:A:2385:PHE:CE1	2.45	0.52
1:A:2399:PHE:HZ	1:A:2431:ILE:HD11	1.73	0.52
1:A:880:LEU:HD22	1:A:884:TYR:CG	2.45	0.52
1:A:1728:ILE:HG13	1:A:1778:MET:HE3	1.92	0.52
1:A:1566:LEU:HD22	1:A:1680:GLY:HA3	1.92	0.52
1:B:2264:TYR:HE1	1:B:2266:ASP:HA	1.75	0.51
1:B:2225:ASN:HB3	1:B:2228:ASN:OD1	2.10	0.51
1:B:1989:GLN:HB2	1:B:1998:PHE:HE2	1.76	0.51
1:A:1062:LEU:HD22	1:A:1068:VAL:HG21	1.93	0.51
1:B:1151:ASP:HA	1:B:1227:ALA:HB2	1.93	0.51
1:B:2422:ALA:HB2	1:B:2436:ILE:HD13	1.92	0.51
1:A:2020:ASP:HB2	2:A:2502:SO4:O3	2.10	0.51
1:B:1247:ASN:HB3	1:B:1249:GLY:H	1.75	0.51
1:B:2032:THR:HG23	1:B:2034:ASN:H	1.76	0.51
1:A:1793:ILE:HG23	1:A:1797:PHE:CG	2.46	0.51
1:A:1935:TYR:CD1	1:A:1949:ILE:HD13	2.45	0.51
1:A:1556:TYR:HD1	1:A:1611:VAL:HG23	1.76	0.51
1:A:1842:TYR:HB2	1:A:1864:PHE:CZ	2.45	0.51
1:B:2212:THR:HB	1:B:2226:PRO:HA	1.93	0.51
1:B:2190:TYR:H	1:B:2208:SER:CB	2.23	0.51
1:B:2287:PHE:HE1	1:B:2301:ALA:HB2	1.75	0.51
1:A:1050:LEU:HD11	1:A:1059:LYS:HB2	1.93	0.51
1:A:1517:MET:CE	1:A:1520:ASP:HA	2.40	0.51
1:A:1922:TYR:O	1:A:1940:SER:HA	2.11	0.51
1:B:939:ILE:HG13	1:B:1041:ILE:HG23	1.93	0.51
1:B:1530:VAL:CG2	1:B:1589:ILE:HG13	2.40	0.51
1:B:2266:ASP:HB2	1:B:2274:VAL:HG21	1.92	0.51
1:A:2228:ASN:HD22	1:A:2230:ILE:HD12	1.76	0.51
1:B:875:LYS:NZ	1:B:982:ASP:OD2	2.43	0.50
1:B:1305:THR:HG23	1:A:1004:TYR:CE2	2.46	0.50
1:B:1616:LEU:HB3	1:B:1636:TRP:HB2	1.93	0.50
1:A:1240:PRO:CG	1:A:2252:GLN:HG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1706:TYR:CE1	1:A:1752:LEU:HD11	2.46	0.50
1:B:1377:ASP:HB2	1:B:1384:ILE:HB	1.93	0.50
1:B:1863:TYR:CZ	1:B:1878:ILE:HD12	2.46	0.50
1:A:1994:SER:HB3	1:A:2024:VAL:HG21	1.92	0.50
1:B:1445:ILE:O	1:B:1449:ASN:ND2	2.45	0.50
1:A:1641:SER:HB3	1:A:1671:LEU:HD23	1.94	0.50
1:A:1902:PHE:HB3	1:A:1942:ALA:HB3	1.93	0.50
1:B:1328:LEU:HG	1:B:1388:GLN:HG3	1.92	0.50
1:A:2196:THR:O	1:A:2197:LEU:HD23	2.12	0.50
1:B:879:ASN:HB3	1:A:2297:ILE:HD12	1.94	0.50
1:B:1886:ASN:HD22	1:B:1892:GLN:HE21	1.59	0.50
1:B:2251:LEU:HD12	1:B:2252:GLN:H	1.77	0.50
1:A:1651:ARG:HD2	1:A:1826:ASP:OD2	2.12	0.50
1:A:2056:TYR:H	1:A:2074:SER:CB	2.24	0.50
1:B:2376:LYS:HB2	1:B:2378:TYR:CE1	2.47	0.50
1:A:2007:ASN:HA	1:A:2019:PHE:HB2	1.93	0.50
1:B:1527:LYS:HD3	1:B:1537:SER:HB2	1.93	0.50
1:B:1556:TYR:HD1	1:B:1611:VAL:HG13	1.77	0.50
1:A:889:GLU:HB2	1:A:1001:ASN:HB3	1.94	0.50
1:B:1247:ASN:HB2	1:B:1250:THR:H	1.76	0.50
1:B:1927:LEU:HD23	1:B:1936:PHE:HE2	1.76	0.50
1:A:888:PHE:HB3	1:A:924:SER:HB2	1.93	0.50
1:B:1751:TYR:CD1	1:B:1760:LEU:HD12	2.47	0.49
1:B:1793:ILE:HG23	1:B:1797:PHE:CG	2.47	0.49
1:B:1864:PHE:HB3	1:B:1869:GLY:O	2.13	0.49
1:A:1185:ASN:ND2	1:A:1185:ASN:O	2.46	0.49
1:A:1201:SER:OG	2:A:2512:SO4:O1	2.30	0.49
1:B:1687:LYS:HD3	1:B:1713:GLU:HB3	1.93	0.49
1:B:1971:ASP:OD2	1:A:1897:LYS:HE2	2.12	0.49
1:A:2320:ASN:C	1:A:2322:SER:H	2.16	0.49
1:A:1976:TYR:HB2	1:A:1998:PHE:CZ	2.47	0.49
1:A:1013:ILE:O	1:A:1017:VAL:HG23	2.12	0.49
1:A:1122:VAL:HG11	1:A:1276:ILE:HG12	1.95	0.49
1:A:1556:TYR:CD1	1:A:1611:VAL:HG23	2.47	0.49
1:A:1831:LYS:HB3	1:A:1848:PHE:CD1	2.48	0.49
1:A:2062:THR:HA	1:A:2066:LYS:O	2.13	0.49
1:B:1152:LEU:HD12	1:B:1205:TYR:CZ	2.48	0.49
1:B:1530:VAL:CG1	1:B:1536:LYS:HB3	2.42	0.49
1:B:1640:SER:OG	1:B:1672:ASP:OD2	2.26	0.49
1:A:1217:PHE:HB3	1:A:1297:ARG:HH12	1.77	0.49
1:A:2243:TYR:CE2	1:A:2272:LYS:HB3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1899:PRO:O	1:A:1953:LYS:NZ	2.42	0.49
1:B:2464:THR:OG1	1:B:2469:LYS:NZ	2.45	0.49
1:A:881:ASP:OD1	1:A:881:ASP:N	2.37	0.49
1:A:2228:ASN:HD22	1:A:2230:ILE:CD1	2.26	0.49
1:B:981:ASN:O	1:B:985:THR:HG23	2.12	0.49
1:A:1073:MET:HA	1:A:1471:PHE:CE1	2.48	0.49
1:A:1118:LYS:O	1:A:1122:VAL:HG23	2.13	0.49
1:B:1156:GLU:OE1	1:B:1165:LYS:HD3	2.13	0.48
1:B:1497:ASN:HB2	1:B:1502:GLU:HG3	1.95	0.48
1:A:1347:PHE:CE1	1:A:1390:ILE:HD13	2.47	0.48
1:A:1833:LEU:HD12	1:A:1841:PHE:O	2.13	0.48
1:B:1342:ASP:OD1	1:B:1342:ASP:N	2.39	0.48
1:B:2420:TYR:CD2	1:B:2443:LEU:HD22	2.49	0.48
1:B:2286:TYR:CD2	1:B:2304:TYR:CD2	3.01	0.48
1:A:2330:THR:HA	1:A:2334:LYS:O	2.13	0.48
1:B:940:THR:OG1	1:B:941:ASP:N	2.46	0.48
1:B:1259:LEU:HD22	1:B:1260:TYR:CZ	2.49	0.48
1:B:1885:PHE:HE1	1:B:1891:MET:HG3	1.77	0.48
1:B:2055:VAL:HG22	1:B:2057:GLN:HG3	1.94	0.48
1:B:968:GLN:HG2	1:B:1024:LEU:HD11	1.96	0.48
1:B:1122:VAL:HG13	1:B:1279:LEU:HD22	1.95	0.48
1:A:2328:TRP:CE2	1:A:2352:ILE:HD11	2.49	0.48
1:B:1108:LEU:HD23	1:A:909:GLU:OE1	2.13	0.48
1:B:1126:PHE:HD2	1:B:1252:LEU:HD22	1.78	0.48
1:B:1926:PHE:CD1	1:B:1935:TYR:HD1	2.32	0.48
1:B:1074:SER:HB3	1:B:1077:ILE:HD13	1.95	0.48
1:B:2328:TRP:HD1	1:B:2335:LYS:HE2	1.77	0.48
1:A:888:PHE:O	1:A:891:ILE:HG13	2.13	0.48
1:A:943:ASN:ND2	1:A:1057:LEU:HD23	2.29	0.48
1:A:1061:GLU:HB3	1:A:1065:LYS:HD2	1.94	0.48
1:A:1380:LYS:HB2	2:A:2504:SO4:O1	2.13	0.48
1:A:1744:SER:HB2	1:A:1767:GLY:HA2	1.95	0.48
1:A:955:THR:O	1:A:958:VAL:HG12	2.14	0.48
1:A:1403:ILE:HG22	1:A:1419:ILE:O	2.14	0.48
1:A:1479:GLN:NE2	1:A:1498:ASP:OD1	2.43	0.48
1:B:1369:ILE:O	1:B:1372:VAL:HG23	2.14	0.48
1:B:1405:LEU:HB2	1:B:1417:ILE:HB	1.95	0.48
1:A:1562:TYR:CD1	1:A:1612:GLY:HA3	2.49	0.48
1:A:1840:LEU:HB3	1:A:1871:ALA:HB3	1.96	0.48
1:B:1262:GLY:HA2	1:B:1265:TYR:CE2	2.49	0.47
1:A:1199:ILE:CG1	1:A:1200:PRO:HD2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1321:GLY:HA2	1:A:1343:ASP:HB3	1.96	0.47
1:B:1126:PHE:CE2	1:B:1204:ILE:HD13	2.49	0.47
1:B:1671:LEU:HD23	1:B:1671:LEU:HA	1.69	0.47
1:B:1936:PHE:CE1	1:B:1942:ALA:HB2	2.49	0.47
1:A:1517:MET:HG2	1:A:1522:ASN:HA	1.96	0.47
1:B:2036:PHE:HB3	1:B:2076:ALA:HB3	1.96	0.47
1:A:1242:LEU:O	1:A:1267:ARG:NH1	2.45	0.47
1:A:1670:SER:HB3	1:A:1698:LEU:HD23	1.96	0.47
1:B:1753:GLU:O	1:B:1758:LYS:NZ	2.39	0.47
1:B:2018:TYR:HB3	1:B:2026:LYS:HB2	1.95	0.47
1:B:1118:LYS:HD3	1:B:2234:HIS:CD2	2.50	0.47
1:A:1788:LEU:HD22	1:A:1792:TYR:CD1	2.49	0.47
1:A:1998:PHE:HB3	1:A:2003:ALA:O	2.15	0.47
1:B:1433:ASP:HA	1:B:1462:TYR:CE2	2.50	0.47
1:A:2225:ASN:ND2	1:A:2228:ASN:OD1	2.47	0.47
1:B:1186:ILE:CD1	1:B:1243:ARG:HB2	2.45	0.47
1:B:1227:ALA:HB1	1:B:1230:ARG:HH12	1.79	0.47
1:B:2202:TYR:HD1	1:B:2229:ALA:O	1.96	0.47
1:A:956:SER:O	1:A:960:THR:HG23	2.15	0.47
1:A:1336:ASN:HA	1:A:1391:ASP:O	2.15	0.47
1:B:2232:ALA:O	1:B:2249:GLY:HA2	2.15	0.47
1:B:1793:ILE:HG23	1:B:1797:PHE:CD2	2.49	0.47
1:A:1745:ASP:OD2	1:A:1764:ARG:HD3	2.15	0.47
1:A:1824:ASP:HB3	1:A:1826:ASP:N	2.29	0.47
1:A:1230:ARG:O	1:A:1230:ARG:HG2	2.14	0.46
1:A:1623:CYS:SG	1:A:1627:LYS:HA	2.55	0.46
1:B:1405:LEU:HD13	1:B:1419:ILE:HD12	1.97	0.46
1:B:2037:GLU:HG2	1:B:2075:LYS:HE3	1.97	0.46
1:A:1719:PRO:HG2	1:A:1721:THR:HG23	1.96	0.46
1:A:2338:PHE:CE1	1:A:2345:ALA:HB2	2.50	0.46
1:A:1433:ASP:HA	1:A:1462:TYR:CE2	2.50	0.46
1:A:1952:GLU:HG2	1:A:1983:ILE:HG21	1.97	0.46
1:B:1984:ILE:HD12	1:B:1984:ILE:O	2.16	0.46
1:B:2287:PHE:CE1	1:B:2301:ALA:HB2	2.50	0.46
1:A:1084:ILE:HG12	1:A:1346:ILE:HG12	1.98	0.46
1:B:2284:PHE:HB3	1:B:2324:ALA:HB3	1.97	0.46
1:A:1034:VAL:HG22	1:A:1539:ASP:CB	2.43	0.46
1:B:1321:GLY:H	1:B:1343:ASP:HB3	1.81	0.46
1:B:1886:ASN:ND2	1:B:1892:GLN:HE21	2.14	0.46
1:A:1881:LYS:HB2	1:A:1883:PHE:CE1	2.51	0.46
1:A:1988:TRP:NE1	1:A:1995:ARG:HG2	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1348:ASN:HA	1:B:1406:THR:O	2.16	0.46
1:B:2459:VAL:HG11	1:B:2463:ARG:HG3	1.96	0.46
1:A:1153:VAL:CG1	1:A:1167:GLY:HA3	2.45	0.46
1:B:1410:ASP:OD1	1:B:1447:LYS:NZ	2.49	0.46
1:B:1751:TYR:HD1	1:B:1760:LEU:HD12	1.81	0.46
1:A:888:PHE:HB3	1:A:924:SER:CB	2.46	0.46
1:A:2443:LEU:HD11	1:A:2445:LEU:HD21	1.98	0.46
1:B:1138:LEU:HD23	1:B:1148:PRO:HA	1.98	0.45
1:B:1703:THR:HB	1:B:1761:GLN:OE1	2.16	0.45
1:A:1279:LEU:HA	1:A:1279:LEU:HD12	1.73	0.45
1:A:1806:LEU:HD23	1:A:1806:LEU:HA	1.74	0.45
1:B:1118:LYS:HD3	1:B:2234:HIS:NE2	2.31	0.45
1:B:1202:LEU:CD1	1:B:1260:TYR:CG	2.98	0.45
1:B:1262:GLY:HA2	1:B:1265:TYR:HE2	1.81	0.45
1:B:1347:PHE:HE2	1:B:1403:ILE:HD11	1.81	0.45
1:B:1697:SER:O	1:B:1727:ASN:ND2	2.49	0.45
1:B:1860:LYS:HB3	1:B:1890:VAL:HG23	1.97	0.45
1:B:2278:PHE:O	1:B:2284:PHE:HA	2.17	0.45
1:A:1208:ILE:HG12	1:A:1252:LEU:HD13	1.97	0.45
1:A:1243:ARG:HH21	1:A:1269:TYR:HD2	1.64	0.45
1:A:1824:ASP:HB2	1:A:1828:LYS:H	1.81	0.45
1:B:1085:VAL:HG11	1:B:1431:SER:HB3	1.99	0.45
1:A:1202:LEU:HG	1:A:1260:TYR:CG	2.51	0.45
1:A:2370:TRP:HE3	1:A:2379:TYR:HB2	1.81	0.45
1:B:923:TYR:O	1:B:927:ILE:HG22	2.16	0.45
1:B:1350:ASP:HB3	1:B:1365:LYS:HD3	1.99	0.45
1:B:1863:TYR:OH	1:B:1866:ILE:HD11	2.16	0.45
1:A:1151:ASP:OD1	1:A:1230:ARG:NH2	2.48	0.45
1:A:1153:VAL:HG12	1:A:1167:GLY:HA3	1.98	0.45
1:A:1349:ILE:HG12	1:A:1406:THR:O	2.17	0.45
1:A:1944:THR:CG2	1:A:1958:PRO:HA	2.47	0.45
1:A:1990:THR:OG1	1:A:1995:ARG:NH1	2.49	0.45
1:B:2286:TYR:HD2	1:B:2304:TYR:CD2	2.25	0.45
1:A:1883:PHE:HZ	1:A:1915:ILE:HD11	1.80	0.45
1:A:1981:THR:OG1	1:A:1983:ILE:HG12	2.16	0.45
1:B:1624:ASP:CB	1:B:1626:ASN:H	2.30	0.45
1:B:1771:ASN:HB3	1:B:1774:SER:HB2	1.99	0.45
1:B:1875:TYR:CE2	1:B:1899:PRO:HD2	2.50	0.45
1:A:983:LEU:HD12	1:A:983:LEU:O	2.16	0.45
1:B:1412:LYS:HB2	1:B:1436:TYR:CE2	2.51	0.45
1:B:1737:TYR:CE2	1:B:1750:ARG:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1134:LYS:HG2	1:B:1135:TYR:CD1	2.52	0.45
1:B:1368:LEU:HG	1:B:1451:LEU:CD1	2.47	0.45
1:B:2038:TYR:HB2	1:B:2070:PHE:CZ	2.51	0.45
1:A:1305:THR:HG22	1:A:1306:THR:N	2.32	0.45
1:A:2317:TYR:O	1:A:2325:VAL:HG22	2.17	0.45
1:A:2409:ILE:CD1	1:A:2433:GLY:HA2	2.47	0.45
1:B:2200:LYS:CG	1:B:2230:ILE:HD11	2.44	0.45
1:A:1353:VAL:C	1:A:1369:ILE:HG22	2.37	0.45
1:A:1638:THR:HG23	1:A:1639:SER:N	2.32	0.45
1:A:2423:PRO:O	1:A:2430:ASN:ND2	2.47	0.45
1:B:938:ILE:HG21	1:B:946:LEU:HD22	1.99	0.45
1:B:1846:ILE:CG1	1:B:1847:GLU:HG2	2.43	0.45
1:A:1429:LEU:HD12	1:A:1430:LEU:N	2.32	0.45
1:A:1705:TYR:O	1:A:1711:TYR:OH	2.23	0.45
1:A:2070:PHE:HA	1:A:2076:ALA:HA	1.99	0.45
1:A:2251:LEU:HD23	1:A:2252:GLN:N	2.31	0.45
1:B:1267:ARG:O	1:B:1267:ARG:HG2	2.17	0.44
1:B:1902:PHE:O	1:B:1941:LYS:HA	2.17	0.44
1:A:1944:THR:HG21	1:A:1958:PRO:HA	1.99	0.44
1:A:2132:PHE:CE2	1:A:2139:ALA:HB2	2.52	0.44
1:B:1578:THR:O	1:B:1581:PHE:HB3	2.18	0.44
1:A:1174:MET:CG	1:A:1195:ILE:HG22	2.47	0.44
1:A:1291:LYS:HA	1:A:1318:ASP:HB2	1.99	0.44
1:A:1340:SER:HB3	1:A:1343:ASP:OD2	2.17	0.44
1:A:1574:GLY:HA2	1:A:1576:HIS:CD2	2.53	0.44
1:B:1305:THR:HG23	1:A:1004:TYR:CD2	2.52	0.44
1:B:1542:ILE:HD13	1:B:1542:ILE:HA	1.77	0.44
1:B:1554:GLY:HA2	1:B:1609:THR:O	2.18	0.44
1:B:2339:ASN:HB3	1:B:2342:THR:H	1.82	0.44
1:A:1071:ILE:HG21	1:A:1071:ILE:HD13	1.72	0.44
1:A:1831:LYS:HD3	1:A:1848:PHE:CE1	2.51	0.44
1:B:1323:THR:HG23	1:B:1344:LEU:HD13	2.00	0.44
1:B:1539:ASP:O	1:B:1555:LEU:HA	2.17	0.44
1:B:1558:ASN:OD1	1:B:1561:VAL:HG23	2.17	0.44
1:B:1934:TYR:CE2	1:B:1962:ILE:HG12	2.53	0.44
1:A:1082:ALA:O	1:A:1085:VAL:HG12	2.18	0.44
1:A:1638:THR:HG23	1:A:1640:SER:H	1.82	0.44
1:B:1253:LEU:HD23	1:B:1253:LEU:HA	1.82	0.44
1:A:1292:LEU:HB2	1:A:1318:ASP:O	2.18	0.44
1:A:1338:ASN:HA	1:A:1393:SER:O	2.17	0.44
1:B:1151:ASP:OD1	1:B:1230:ARG:NH2	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1189:PHE:N	1:B:1269:TYR:O	2.47	0.44
1:B:1285:ASP:HA	1:B:1312:LYS:HB3	2.00	0.44
1:B:1421:LEU:HD23	1:B:1421:LEU:HA	1.70	0.44
1:B:1445:ILE:CD1	1:B:1479:GLN:HG2	2.48	0.44
1:B:1659:TYR:O	1:B:1660:ASN:HB3	2.18	0.44
1:A:1358:ILE:HG22	1:A:1360:ASN:O	2.17	0.44
1:B:999:GLY:O	1:B:1003:ILE:HG12	2.17	0.44
1:B:1585:PHE:O	1:B:1589:ILE:HG22	2.17	0.44
1:B:1745:ASP:OD1	1:B:1766:LYS:HD2	2.18	0.44
1:A:2074:SER:O	1:A:2075:LYS:HG3	2.17	0.44
1:A:2163:VAL:HG21	1:A:2202:TYR:CD1	2.53	0.44
1:A:2228:ASN:HD22	1:A:2230:ILE:CG1	2.31	0.44
1:A:2430:ASN:HB2	1:A:2434:GLN:HG2	1.99	0.44
1:A:934:ILE:HD13	1:A:1023:VAL:HG21	2.00	0.44
1:A:1063:GLU:O	1:A:1067:GLY:HA2	2.18	0.44
1:B:1220:LYS:HD2	1:B:1296:THR:O	2.18	0.44
1:A:1683:ARG:HH11	1:A:1683:ARG:HG2	1.83	0.44
1:A:1939:ASN:O	1:A:1941:LYS:HG2	2.18	0.44
1:B:1516:PHE:CZ	1:B:1523:THR:HB	2.53	0.43
1:B:2265:PHE:CE2	1:B:2273:MET:HB2	2.52	0.43
1:B:2459:VAL:CG1	1:B:2463:ARG:HG3	2.48	0.43
1:A:1134:LYS:HG2	1:A:1135:TYR:CE1	2.52	0.43
1:A:1221:ILE:HA	1:A:1298:ASN:O	2.17	0.43
1:A:1380:LYS:HD2	1:A:1397:ASP:OD1	2.17	0.43
1:A:2144:THR:HB	1:A:2153:PHE:HE1	1.83	0.43
1:A:2265:PHE:CE2	1:A:2273:MET:HB3	2.53	0.43
1:A:2430:ASN:CB	1:A:2434:GLN:HE21	2.32	0.43
1:B:1456:LYS:HB3	1:B:1456:LYS:HE2	1.79	0.43
1:B:1555:LEU:HD11	1:B:1586:LEU:HD21	1.98	0.43
1:B:2232:ALA:HB1	1:B:2236:CYS:SG	2.58	0.43
1:A:1062:LEU:HB3	1:A:1068:VAL:CG2	2.48	0.43
1:A:1575:HIS:CD2	1:A:1833:LEU:HD23	2.53	0.43
1:B:1037:ILE:HA	1:B:1041:ILE:O	2.18	0.43
1:B:2198:ASN:OD1	1:B:2198:ASN:O	2.36	0.43
1:A:1313:LEU:HD23	1:A:1313:LEU:HA	1.69	0.43
1:B:1073:MET:HG2	1:B:1471:PHE:CD2	2.53	0.43
1:B:1717:LEU:HA	1:B:1717:LEU:HD23	1.72	0.43
1:B:2377:LYS:HB3	1:B:2377:LYS:HE3	1.76	0.43
1:A:2141:THR:HA	1:A:2153:PHE:HB2	1.99	0.43
1:B:928:THR:HG22	1:B:990:GLN:OE1	2.19	0.43
1:B:941:ASP:HA	1:B:945:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1156:GLU:HB3	1:B:1165:LYS:CB	2.49	0.43
1:B:1975:TYR:CE2	1:B:2004:ILE:HD13	2.52	0.43
1:A:1031:ILE:HA	1:A:1032:PRO:HD3	1.70	0.43
1:A:1095:LEU:CD1	1:A:1362:THR:HB	2.47	0.43
1:A:1240:PRO:HB2	1:A:2252:GLN:CG	2.45	0.43
1:A:1517:MET:HE2	1:A:1517:MET:HB3	1.77	0.43
1:A:1860:LYS:HA	1:A:1860:LYS:HD3	1.84	0.43
1:A:1907:PRO:HG2	1:A:1910:THR:HG23	1.99	0.43
1:A:2379:TYR:O	1:A:2388:SER:HB2	2.18	0.43
1:B:1830:VAL:HG21	1:B:1834:ILE:HD13	2.01	0.43
1:B:1833:LEU:HD12	1:B:1841:PHE:O	2.18	0.43
1:B:2375:GLY:O	1:B:2376:LYS:HD3	2.19	0.43
1:A:1161:ASN:HB3	1:A:1163:SER:OG	2.17	0.43
1:A:1509:ILE:HD11	1:A:1593:LYS:O	2.19	0.43
1:A:2104:ILE:O	1:A:2104:ILE:HG13	2.17	0.43
1:A:2424:ALA:HB2	1:A:2432:GLU:HB2	2.00	0.43
1:A:1239:VAL:CG1	1:A:1275:ALA:HB3	2.49	0.43
1:A:1353:VAL:HG22	1:A:1451:LEU:HD11	2.00	0.43
1:A:2394:ILE:HG12	1:A:2399:PHE:CE1	2.54	0.43
1:B:1305:THR:CG2	1:A:1004:TYR:CZ	3.01	0.43
1:A:1151:ASP:HA	1:A:1227:ALA:HB2	2.00	0.43
1:A:1556:TYR:HD1	1:A:1611:VAL:CG2	2.32	0.43
1:B:1080:THR:HG23	1:B:1344:LEU:HD11	1.99	0.43
1:B:2073:ASN:O	1:B:2075:LYS:HG3	2.19	0.43
1:B:2255:TYR:CD2	1:B:2281:PRO:HD2	2.53	0.43
1:A:1413:ILE:HD12	1:A:1444:THR:HG21	2.00	0.43
1:A:1973:ASN:HB3	1:A:2004:ILE:HD12	2.01	0.43
1:A:2372:THR:O	1:A:2372:THR:OG1	2.35	0.43
1:A:1031:ILE:HD13	1:A:1031:ILE:HG21	1.73	0.43
1:A:1085:VAL:HG23	1:A:1414:SER:CB	2.49	0.43
1:B:942:VAL:HG22	1:B:947:LEU:CD1	2.49	0.42
1:B:1013:ILE:O	1:B:1017:VAL:HG22	2.19	0.42
1:B:1778:MET:HG2	1:B:1790:LEU:HD21	2.01	0.42
1:B:2204:PHE:CE1	1:B:2210:ALA:HB2	2.54	0.42
1:B:2284:PHE:HB2	1:B:2324:ALA:HB3	2.01	0.42
1:B:2351:THR:HB	1:B:2356:LYS:HG2	2.00	0.42
1:A:2464:THR:HA	1:A:2469:LYS:HA	2.01	0.42
1:B:2129:LYS:HB3	1:B:2159:MET:HE2	2.00	0.42
1:A:939:ILE:HD12	1:A:1041:ILE:HG23	2.01	0.42
1:A:1174:MET:HG2	1:A:1195:ILE:HG22	2.00	0.42
1:A:1299:PHE:O	1:A:1326:LEU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1328:LEU:HG	1:A:1388:GLN:HG3	2.00	0.42
1:A:1796:ASN:OD1	1:A:1796:ASN:N	2.51	0.42
1:A:2296:ASN:ND2	1:A:2302:ILE:HG21	2.34	0.42
1:B:1279:LEU:HD12	1:B:1279:LEU:HA	1.82	0.42
1:B:1337:ILE:CD1	1:B:1347:PHE:HZ	2.32	0.42
1:B:1380:LYS:HB2	2:B:2503:SO4:O4	2.19	0.42
1:B:1480:LYS:HG2	1:B:1497:ASN:OD1	2.18	0.42
1:B:1842:TYR:HB2	1:B:1864:PHE:CZ	2.54	0.42
1:B:2027:ILE:HD11	1:B:2050:GLU:HG2	2.00	0.42
1:B:2039:PHE:CE1	1:B:2053:ALA:HB2	2.54	0.42
1:A:977:LYS:HA	1:A:981:ASN:HD22	1.84	0.42
1:B:1048:LYS:HE3	1:B:1052:ASP:OD2	2.20	0.42
1:B:1166:LEU:HD23	1:B:1205:TYR:CD2	2.54	0.42
1:A:1904:TYR:HB2	1:A:1936:PHE:CZ	2.54	0.42
1:A:2370:TRP:CE3	1:A:2379:TYR:HB2	2.54	0.42
1:A:969:SER:HA	1:A:972:ASP:HB2	2.02	0.42
1:A:1153:VAL:HG22	1:A:1230:ARG:HH11	1.84	0.42
1:A:2310:THR:HA	1:A:2314:LYS:O	2.19	0.42
1:A:1245:LEU:HD12	1:A:1245:LEU:HA	1.80	0.42
1:A:1451:LEU:HD12	1:A:1451:LEU:HA	1.82	0.42
1:A:2192:ASN:N	1:A:2204:PHE:O	2.52	0.42
1:B:983:LEU:O	1:B:987:VAL:HG23	2.19	0.42
1:B:1303:THR:HG23	1:B:1331:TYR:CD2	2.54	0.42
1:B:1469:LYS:HB3	1:B:1471:PHE:CZ	2.55	0.42
1:B:2176:ALA:HA	1:B:2182:ASN:O	2.20	0.42
1:A:1586:LEU:HD23	1:A:1586:LEU:HA	1.91	0.42
1:A:1893:LEU:CD2	1:A:1917:GLY:HA2	2.50	0.42
1:A:2304:TYR:CZ	1:A:2307:LYS:HD2	2.55	0.42
1:B:1196:SER:HB3	1:B:1199:ILE:HG22	2.02	0.42
1:B:2224:PHE:N	1:B:2224:PHE:CD1	2.87	0.42
1:A:1703:THR:O	1:A:1750:ARG:NH1	2.53	0.42
1:A:1765:ILE:HG22	1:A:1768:ILE:HB	2.01	0.42
1:B:2247:TYR:CD1	1:B:2247:TYR:C	2.92	0.42
1:A:1549:GLN:HG2	1:A:1601:ASN:OD1	2.20	0.42
1:A:1566:LEU:HD23	1:A:1566:LEU:HA	1.82	0.42
1:A:1882:HIS:O	1:A:1918:GLN:HA	2.19	0.42
1:A:2228:ASN:OD1	1:A:2228:ASN:N	2.52	0.42
1:B:1087:ILE:HD12	1:B:1346:ILE:HD12	2.02	0.42
1:B:1171:ILE:HD13	1:B:1264:PHE:CE1	2.55	0.42
1:B:2056:TYR:H	1:B:2074:SER:CB	2.33	0.42
1:A:2107:LYS:HB3	1:A:2138:ILE:CG2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1027:ILE:HG13	1:B:1632:TYR:CD2	2.55	0.41
1:A:1071:ILE:CD1	1:A:1073:MET:HE3	2.45	0.41
1:A:1301:MET:HG3	1:A:1302:PRO:HD2	2.01	0.41
1:A:1576:HIS:CD2	1:A:1683:ARG:HD3	2.54	0.41
1:A:2422:ALA:CB	1:A:2436:ILE:HD13	2.49	0.41
1:B:1071:ILE:HG21	1:B:1071:ILE:HD13	1.76	0.41
1:B:2070:PHE:HD1	1:B:2075:LYS:C	2.23	0.41
1:A:1028:THR:O	1:A:1031:ILE:HG12	2.19	0.41
1:A:1111:ASN:O	1:A:1111:ASN:ND2	2.54	0.41
1:A:1239:VAL:HA	1:A:1240:PRO:HD2	1.89	0.41
1:A:1778:MET:HG3	1:A:1779:SER:N	2.36	0.41
1:A:1793:ILE:O	1:A:1797:PHE:HB2	2.20	0.41
1:A:1978:ASN:ND2	1:A:1981:THR:OG1	2.53	0.41
1:A:2026:LYS:NZ	2:A:2502:SO4:S	2.94	0.41
1:A:2248:ASP:OD1	1:A:2248:ASP:N	2.50	0.41
1:B:934:ILE:HD13	1:B:1023:VAL:HG21	2.02	0.41
1:B:1706:TYR:HA	1:B:1711:TYR:OH	2.20	0.41
1:A:2228:ASN:HD22	1:A:2230:ILE:HG13	1.86	0.41
1:B:1234:TRP:CD1	1:B:1234:TRP:N	2.89	0.41
1:B:1412:LYS:HB2	1:B:1436:TYR:CD2	2.55	0.41
1:B:2246:SER:HB3	1:B:2252:GLN:NE2	2.32	0.41
1:A:901:ARG:HB2	1:A:912:TYR:CD2	2.55	0.41
1:A:935:LYS:HD2	1:A:994:GLN:HG3	2.02	0.41
1:A:1378:ILE:HG22	1:A:1424:LYS:HA	2.02	0.41
1:A:1394:GLY:O	1:A:1396:ILE:N	2.53	0.41
1:A:1683:ARG:NH1	1:A:1683:ARG:HG2	2.36	0.41
1:B:2002:THR:OG1	1:B:2004:ILE:HG12	2.20	0.41
1:B:2335:LYS:HB3	1:B:2366:ALA:HB3	2.03	0.41
1:A:942:VAL:HG23	1:A:942:VAL:O	2.21	0.41
1:A:1751:TYR:CD1	1:A:1760:LEU:HD12	2.56	0.41
1:B:1430:LEU:HG	1:B:1458:ILE:HG21	2.03	0.41
1:A:1051:LEU:HD21	1:A:1070:ALA:HB1	2.02	0.41
1:A:1793:ILE:HG23	1:A:1797:PHE:CD1	2.56	0.41
1:B:1854:TRP:HE1	1:B:1878:ILE:HG21	1.85	0.41
1:B:2254:GLY:O	1:B:2264:TYR:HA	2.21	0.41
1:A:1721:THR:OG1	1:A:1722:PHE:N	2.53	0.41
1:A:2132:PHE:CD2	1:A:2139:ALA:HB2	2.56	0.41
1:B:1828:LYS:HE2	1:B:1828:LYS:HB2	1.73	0.41
1:B:2264:TYR:CE1	1:B:2266:ASP:HA	2.55	0.41
1:A:1132:SER:CB	1:A:1210:ILE:HD12	2.51	0.41
1:A:1173:ALA:HB3	1:A:1199:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1815:ILE:HG13	1:A:1820:THR:HG22	2.02	0.41
1:A:2359:PHE:HA	1:A:2365:GLU:O	2.21	0.41
1:B:970:LEU:O	1:B:984:SER:HB2	2.21	0.41
1:B:1597:PHE:CD1	1:B:1597:PHE:N	2.89	0.41
1:B:1701:ILE:HB	1:B:1730:LEU:HD23	2.03	0.41
1:B:2174:ALA:HB1	1:B:2175:PRO:HD2	2.03	0.41
1:B:2207:ASP:OD1	1:B:2207:ASP:N	2.54	0.41
1:B:2422:ALA:CB	1:B:2436:ILE:HD13	2.50	0.41
1:A:905:LYS:HB2	1:A:905:LYS:HE2	1.81	0.41
1:A:1738:LYS:HD3	1:A:1799:SER:O	2.20	0.41
1:A:1810:HIS:CG	1:A:1811:LEU:H	2.39	0.41
1:B:864:LEU:HD13	1:B:983:LEU:HD21	2.03	0.41
1:B:1153:VAL:HG13	1:B:1227:ALA:O	2.20	0.41
1:B:2107:LYS:CB	1:B:2138:ILE:HD11	2.51	0.41
1:B:2401:PHE:CD1	1:B:2407:MET:HA	2.55	0.41
1:A:1403:ILE:HD13	1:A:1403:ILE:HG21	1.66	0.41
1:A:1589:ILE:HG21	1:A:1589:ILE:HD13	1.72	0.41
1:A:1815:ILE:HA	1:A:1820:THR:HA	2.03	0.41
1:A:2235:LEU:HD23	1:A:2235:LEU:HA	1.73	0.41
1:B:1769:LEU:HA	1:B:1769:LEU:HD23	1.78	0.40
1:B:1792:TYR:CD1	1:B:1792:TYR:C	2.94	0.40
1:B:2143:TYR:OH	1:B:2150:HIS:ND1	2.41	0.40
1:A:1609:THR:HG23	1:A:1622:ILE:HG13	2.04	0.40
1:A:2295:ASN:ND2	1:A:2295:ASN:O	2.53	0.40
1:B:992:TYR:CD2	1:B:1016:ALA:HA	2.56	0.40
1:B:1174:MET:N	1:B:1263:LYS:O	2.52	0.40
1:B:1199:ILE:HG13	1:B:1200:PRO:HD2	2.03	0.40
1:A:1195:ILE:HG21	1:A:1195:ILE:HD13	1.87	0.40
1:A:2455:ASP:N	1:A:2455:ASP:OD1	2.53	0.40
1:B:1304:ILE:HD12	1:B:1333:ILE:HD11	2.03	0.40
1:B:1482:ILE:HD12	1:B:1482:ILE:HG23	1.75	0.40
1:B:1637:LYS:HD3	1:B:1658:ILE:HD12	2.03	0.40
1:B:2030:PHE:HD2	1:B:2039:PHE:HD2	1.70	0.40
1:B:2063:LEU:HD23	1:B:2063:LEU:HA	1.77	0.40
1:A:1453:LEU:HD23	1:A:1453:LEU:HA	1.87	0.40
1:A:1748:LEU:HD23	1:A:1748:LEU:HA	1.91	0.40
1:A:2409:ILE:HD11	1:A:2433:GLY:HA2	2.03	0.40
1:B:927:ILE:HG21	1:B:927:ILE:HD13	1.87	0.40
1:B:1680:GLY:O	1:B:1683:ARG:HD2	2.21	0.40
1:B:1781:ASP:CB	1:B:1787:LYS:H	2.34	0.40
1:B:2401:PHE:CE1	1:B:2407:MET:HG3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1750:ARG:O	1:A:1750:ARG:HG2	2.22	0.40
1:A:1825:GLU:H	1:A:1825:GLU:HG3	1.52	0.40
1:A:1924:SER:OG	2:A:2509:SO4:O1	2.34	0.40
1:B:2230:ILE:HG21	1:B:2230:ILE:HD13	1.77	0.40
1:A:971:ILE:O	1:A:974:SER:OG	2.33	0.40
1:A:1038:LEU:HD23	1:A:1518:LYS:HB3	2.02	0.40
1:A:1344:LEU:HD11	1:A:1404:PHE:HE2	1.87	0.40
1:A:2409:ILE:HA	1:A:2409:ILE:HD13	1.77	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 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%)	1362 (99%)	17 (1%)	71	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1345/1455 (92%)	1320 (98%)	25 (2%)	57 80
All	All	2724/2910 (94%)	2682 (98%)	42 (2%)	65 85

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	874	LEU
1	B	948	ASP
1	B	981	ASN
1	B	1234	TRP
1	B	1401	ARG
1	B	1410	ASP
1	B	1436	TYR
1	B	1573	ASP
1	B	1581	PHE
1	B	1597	PHE
1	B	1695	TYR
1	B	1718	ASN
1	B	1760	LEU
1	B	1838	ASN
1	B	1860	LYS
1	B	1922	TYR
1	B	1926	PHE
1	B	1939	ASN
1	B	1995	ARG
1	B	2018	TYR
1	B	2045	TYR
1	B	2126	ASP
1	B	2129	LYS
1	B	2304	TYR
1	B	2335	LYS
1	A	980	LEU
1	A	1230	ARG
1	A	1234	TRP
1	A	1295	ASP
1	A	1410	ASP
1	A	1486	LYS
1	A	1683	ARG
1	A	1808	ARG
1	A	1838	ASN
1	A	1951	ASN
1	A	1988	TRP

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Mol	Chain	Res	Type
1	A	2126	ASP
1	A	2149	LYS
1	A	2215	ARG
1	A	2357	TYR
1	A	2370	TRP
1	A	2427	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	990	GLN
1	B	1892	GLN
1	B	1939	ASN
1	A	943	ASN
1	A	951	GLN
1	A	981	ASN
1	A	1484	HIS
1	A	1978	ASN
1	A	2291	ASN
1	A	2434	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	2511	-	4,4,4	0.24	0	6,6,6	0.32	0
2	SO4	B	2515	-	4,4,4	0.20	0	6,6,6	0.40	0
2	SO4	A	2511	-	4,4,4	0.23	0	6,6,6	0.34	0
2	SO4	B	2504	-	4,4,4	0.14	0	6,6,6	0.32	0
2	SO4	B	2507	-	4,4,4	0.21	0	6,6,6	0.17	0
2	SO4	B	2503	-	4,4,4	0.23	0	6,6,6	0.46	0
2	SO4	B	2508	-	4,4,4	0.20	0	6,6,6	0.31	0
2	SO4	A	2503	-	4,4,4	0.26	0	6,6,6	0.22	0
2	SO4	B	2519	-	4,4,4	0.23	0	6,6,6	0.22	0
2	SO4	B	2512	-	4,4,4	0.10	0	6,6,6	0.46	0
2	SO4	B	2501	-	4,4,4	0.21	0	6,6,6	0.29	0
2	SO4	A	2508	-	4,4,4	0.21	0	6,6,6	0.27	0
2	SO4	A	2504	-	4,4,4	0.17	0	6,6,6	0.20	0
2	SO4	B	2517	-	4,4,4	0.23	0	6,6,6	0.46	0
2	SO4	B	2513	-	4,4,4	0.14	0	6,6,6	0.26	0
2	SO4	A	2507	-	4,4,4	0.24	0	6,6,6	0.14	0
2	SO4	B	2509	-	4,4,4	0.18	0	6,6,6	0.21	0
2	SO4	B	2502	-	4,4,4	0.24	0	6,6,6	0.31	0
2	SO4	A	2505	-	4,4,4	0.26	0	6,6,6	0.50	0
2	SO4	B	2506	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	A	2514	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	A	2512	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	B	2516	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	A	2513	-	4,4,4	0.21	0	6,6,6	0.37	0
2	SO4	A	2506	-	4,4,4	0.22	0	6,6,6	0.40	0
2	SO4	B	2520	-	4,4,4	0.19	0	6,6,6	0.52	0
2	SO4	B	2510	-	4,4,4	0.20	0	6,6,6	0.21	0
2	SO4	A	2515	-	4,4,4	0.08	0	6,6,6	0.34	0
2	SO4	A	2516	-	4,4,4	0.19	0	6,6,6	0.28	0
2	SO4	A	2502	-	4,4,4	0.21	0	6,6,6	0.55	0
2	SO4	B	2518	-	4,4,4	0.26	0	6,6,6	0.47	0
2	SO4	B	2505	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	B	2514	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	A	2510	-	4,4,4	0.19	0	6,6,6	0.17	0
2	SO4	A	2501	-	4,4,4	0.29	0	6,6,6	0.30	0
2	SO4	A	2509	-	4,4,4	0.24	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

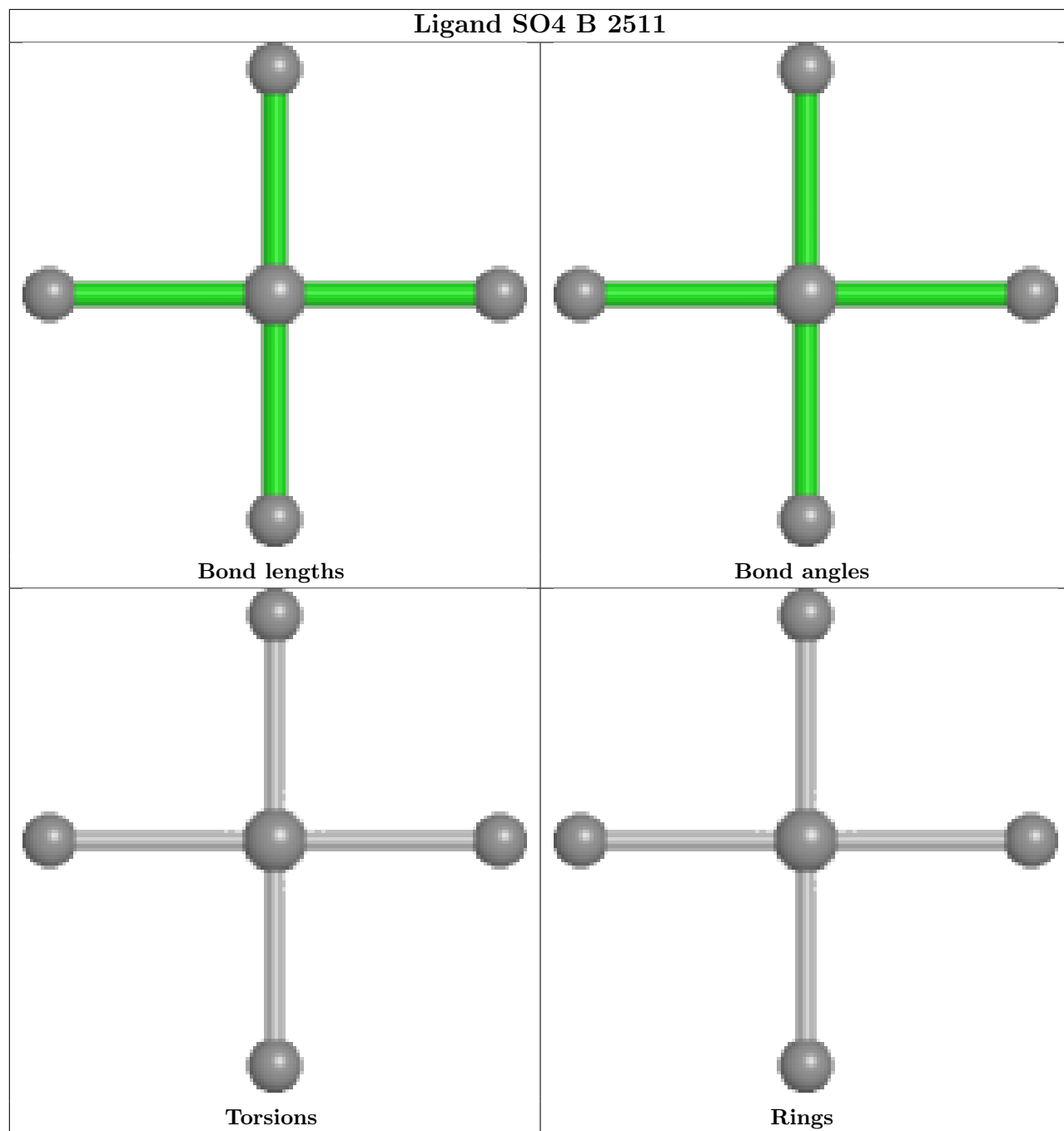
There are no torsion outliers.

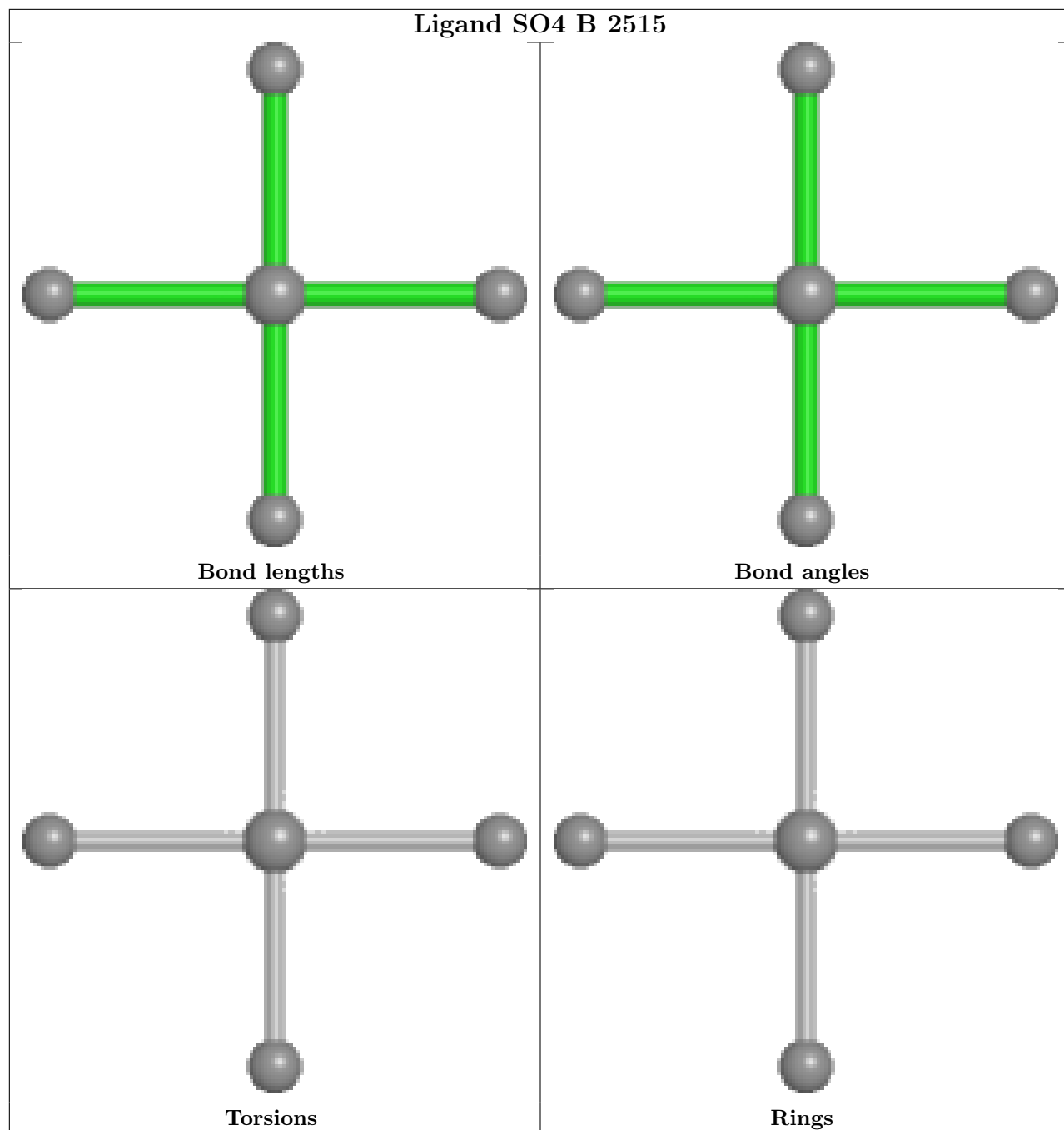
There are no ring outliers.

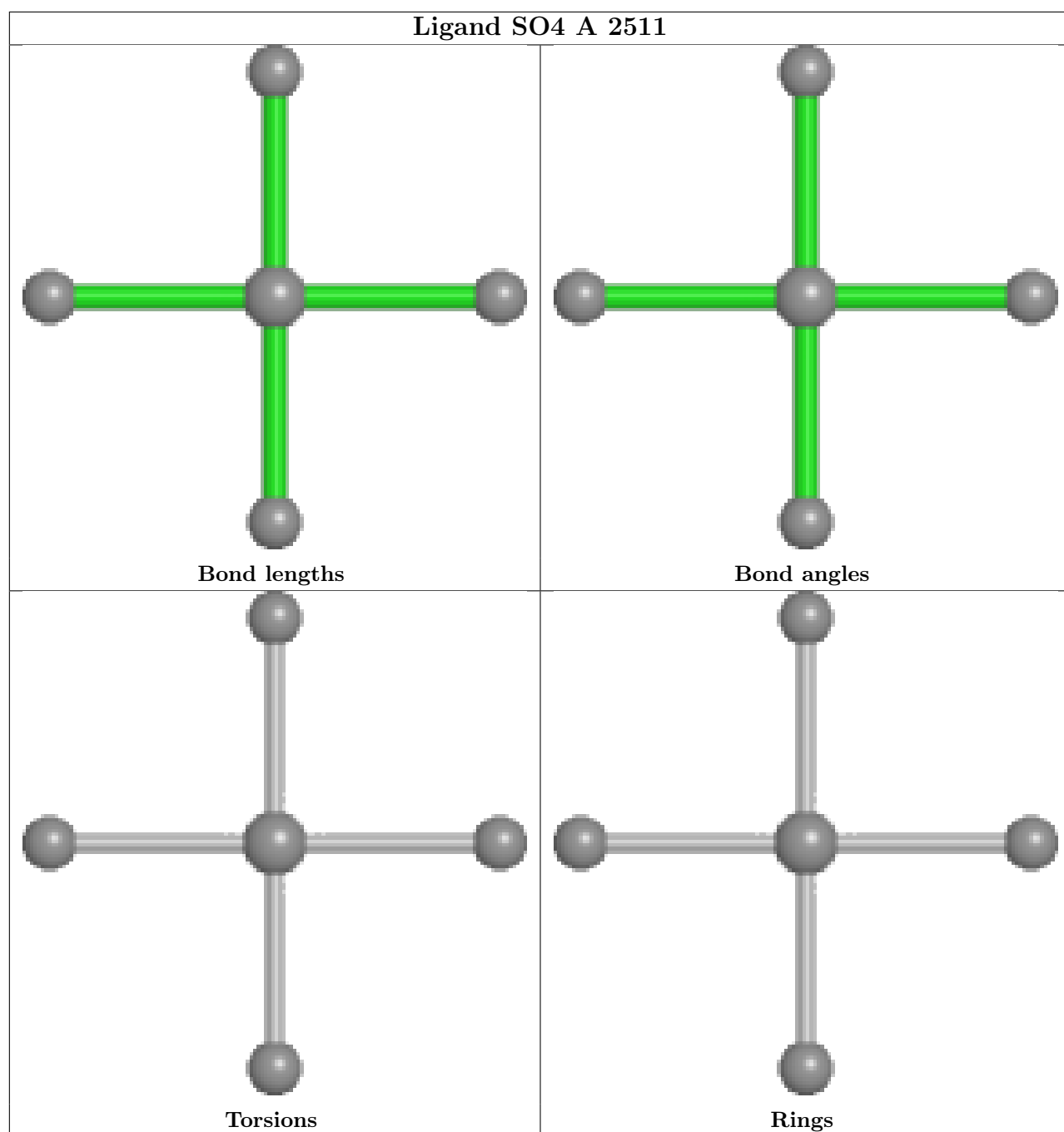
8 monomers are involved in 10 short contacts:

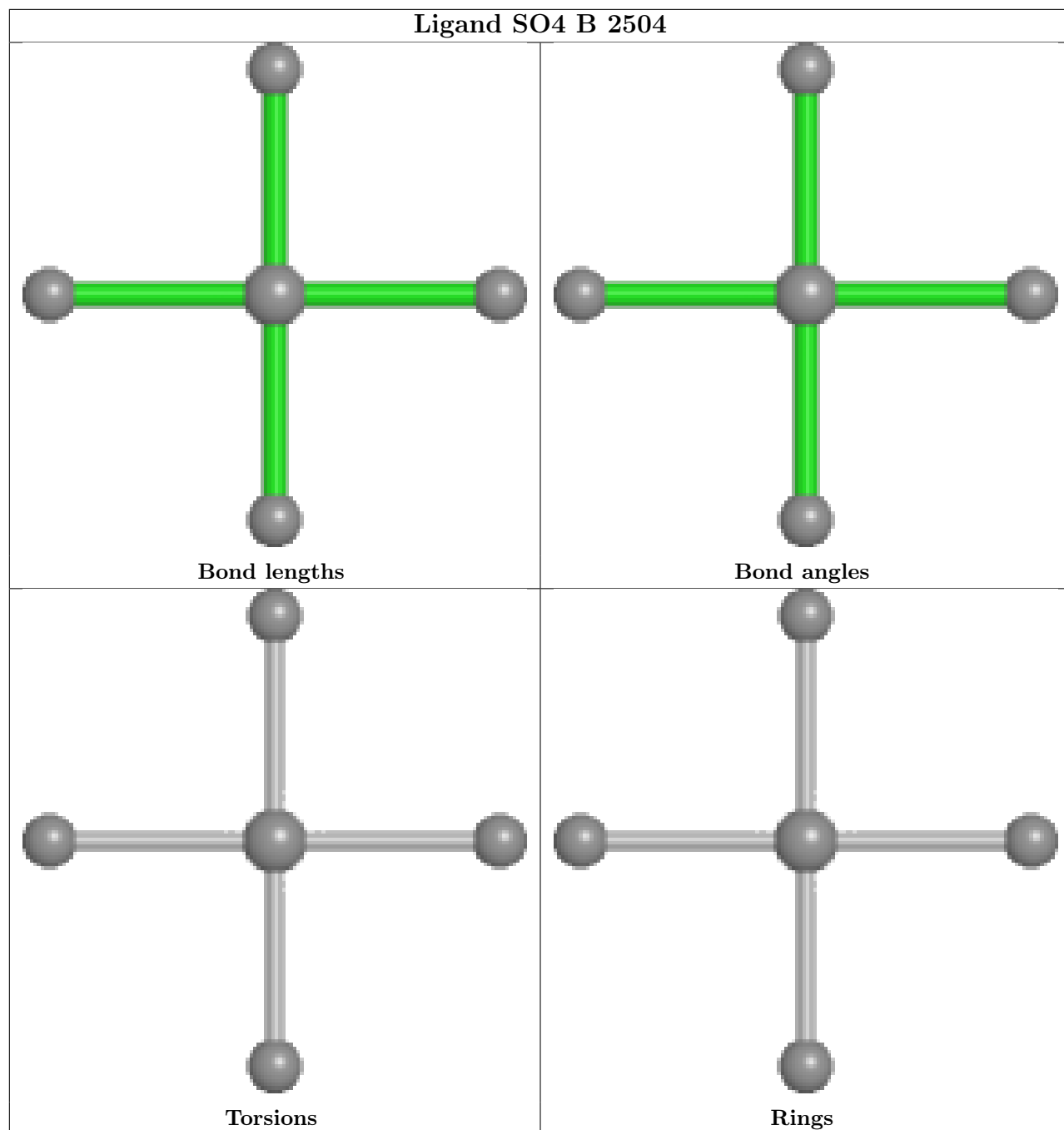
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2511	SO4	1	0
2	B	2503	SO4	1	0
2	A	2504	SO4	1	0
2	B	2506	SO4	1	0
2	A	2512	SO4	1	0
2	A	2502	SO4	3	0
2	A	2501	SO4	1	0
2	A	2509	SO4	1	0

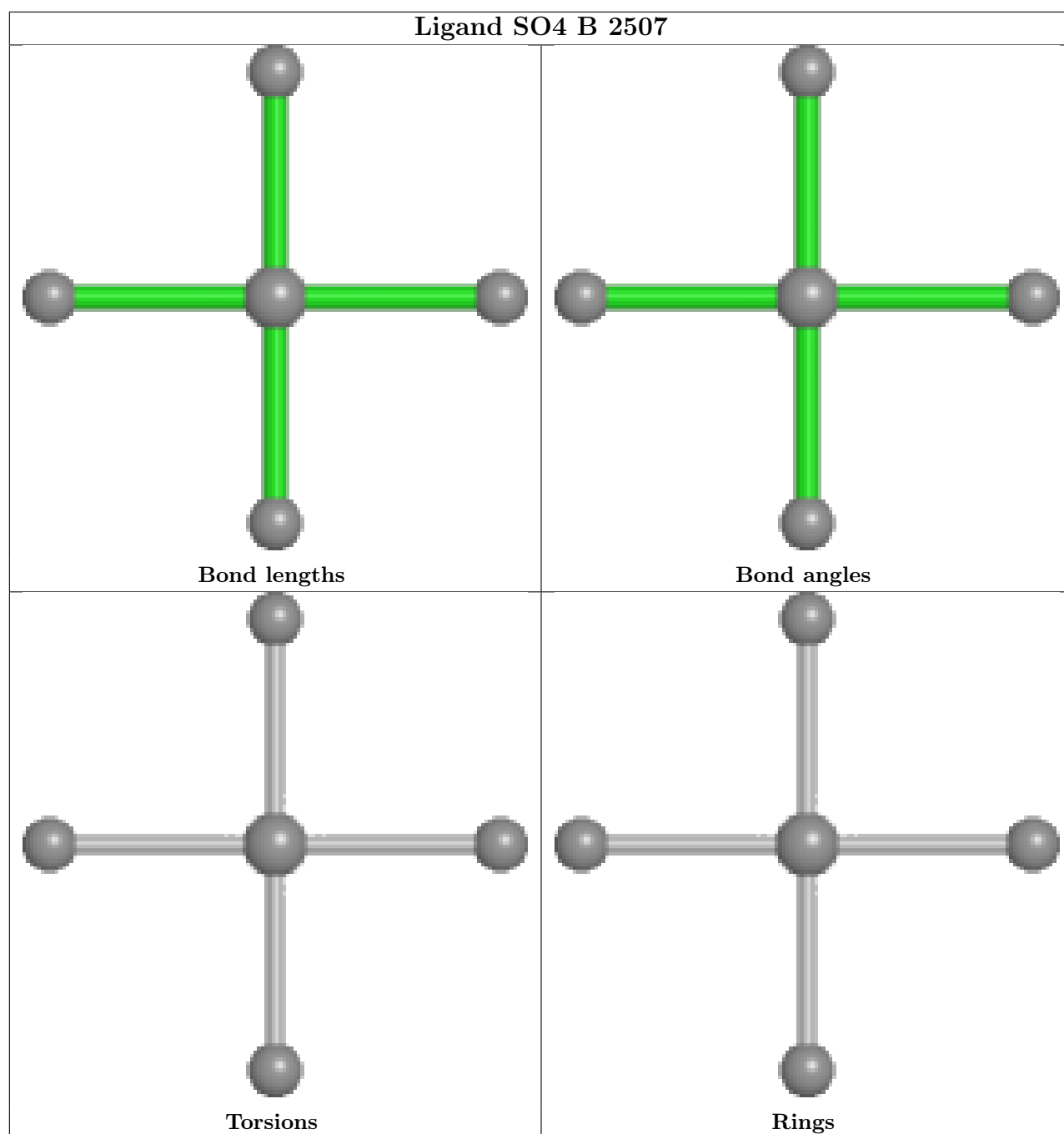
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

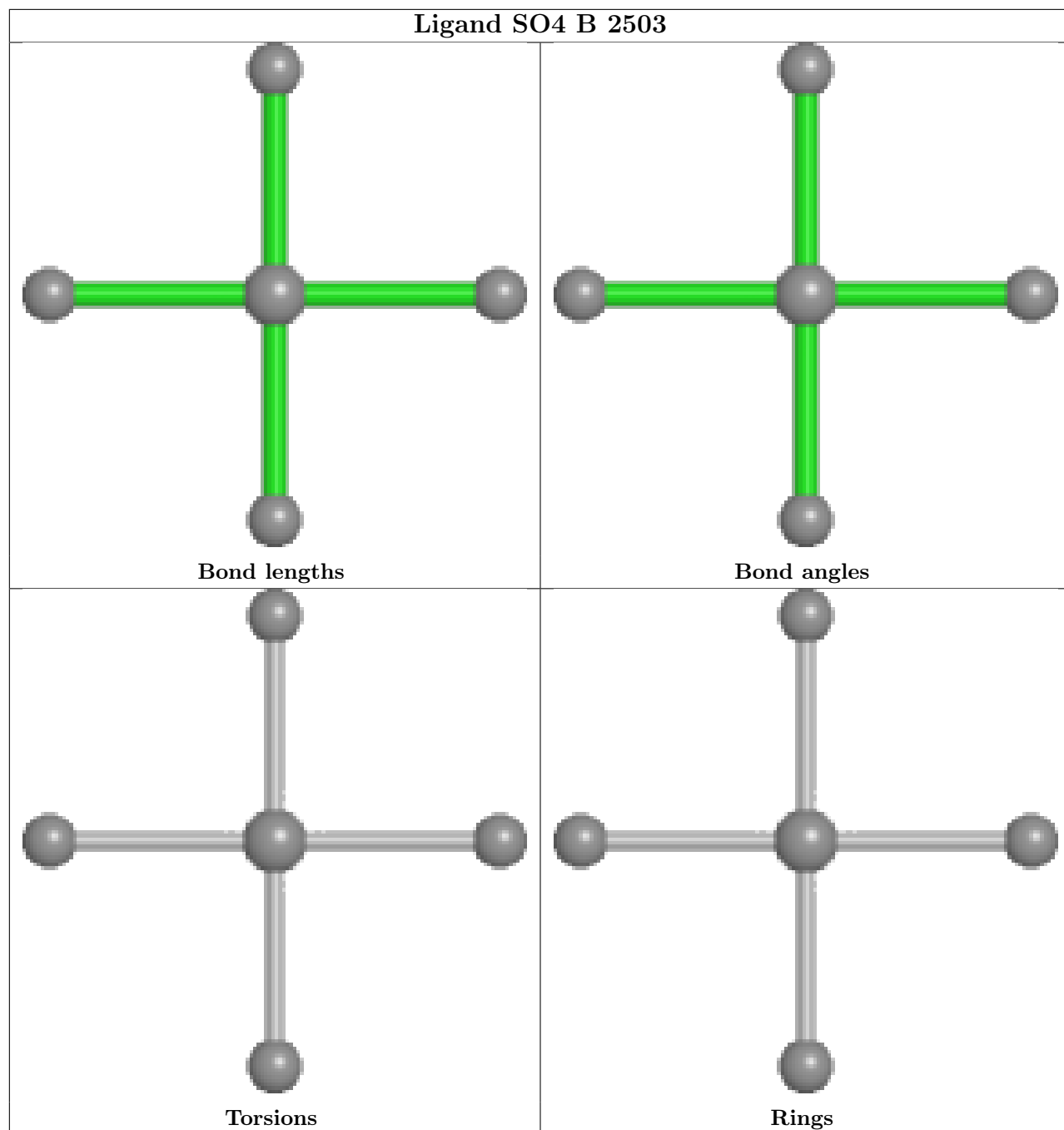


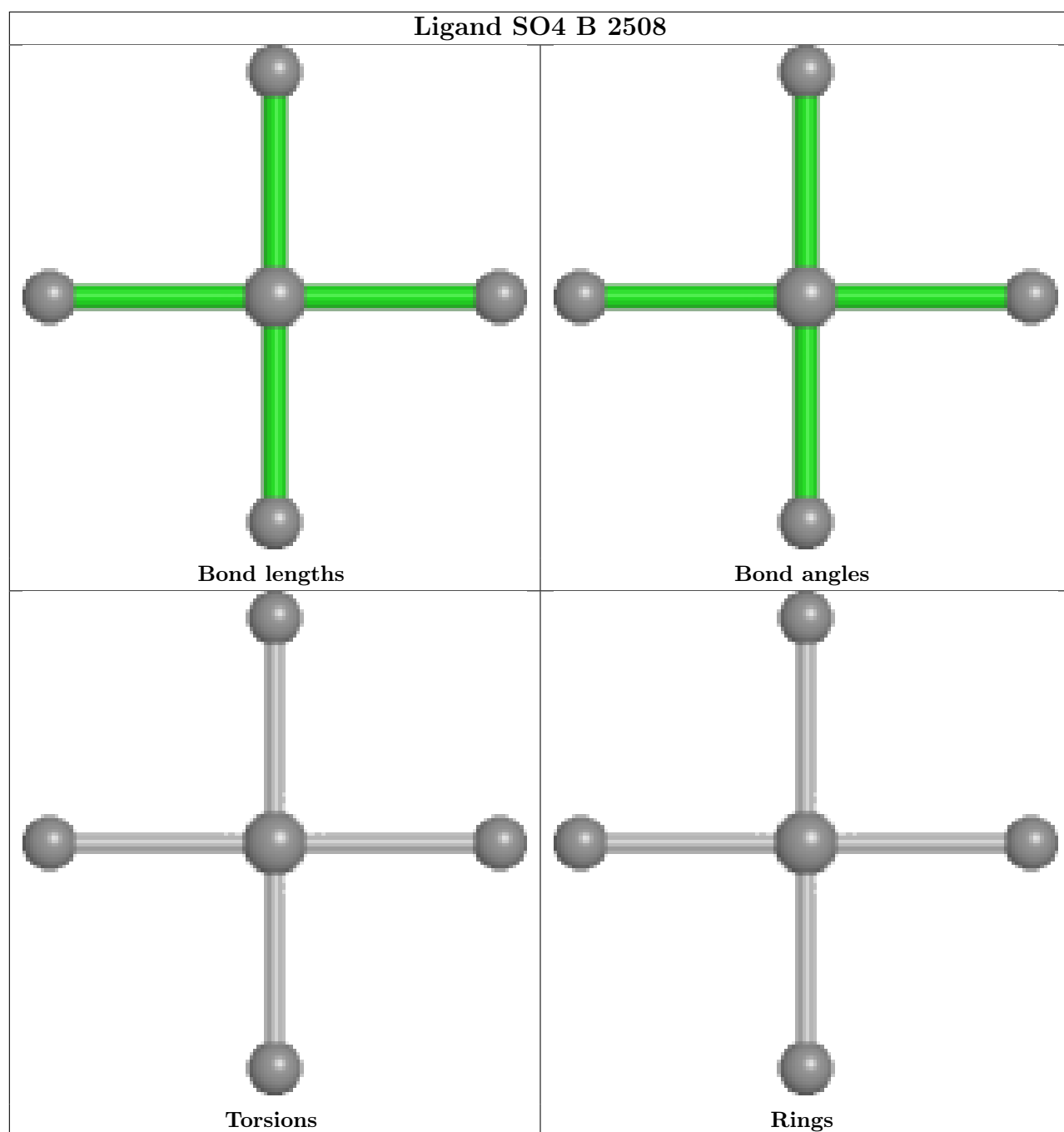


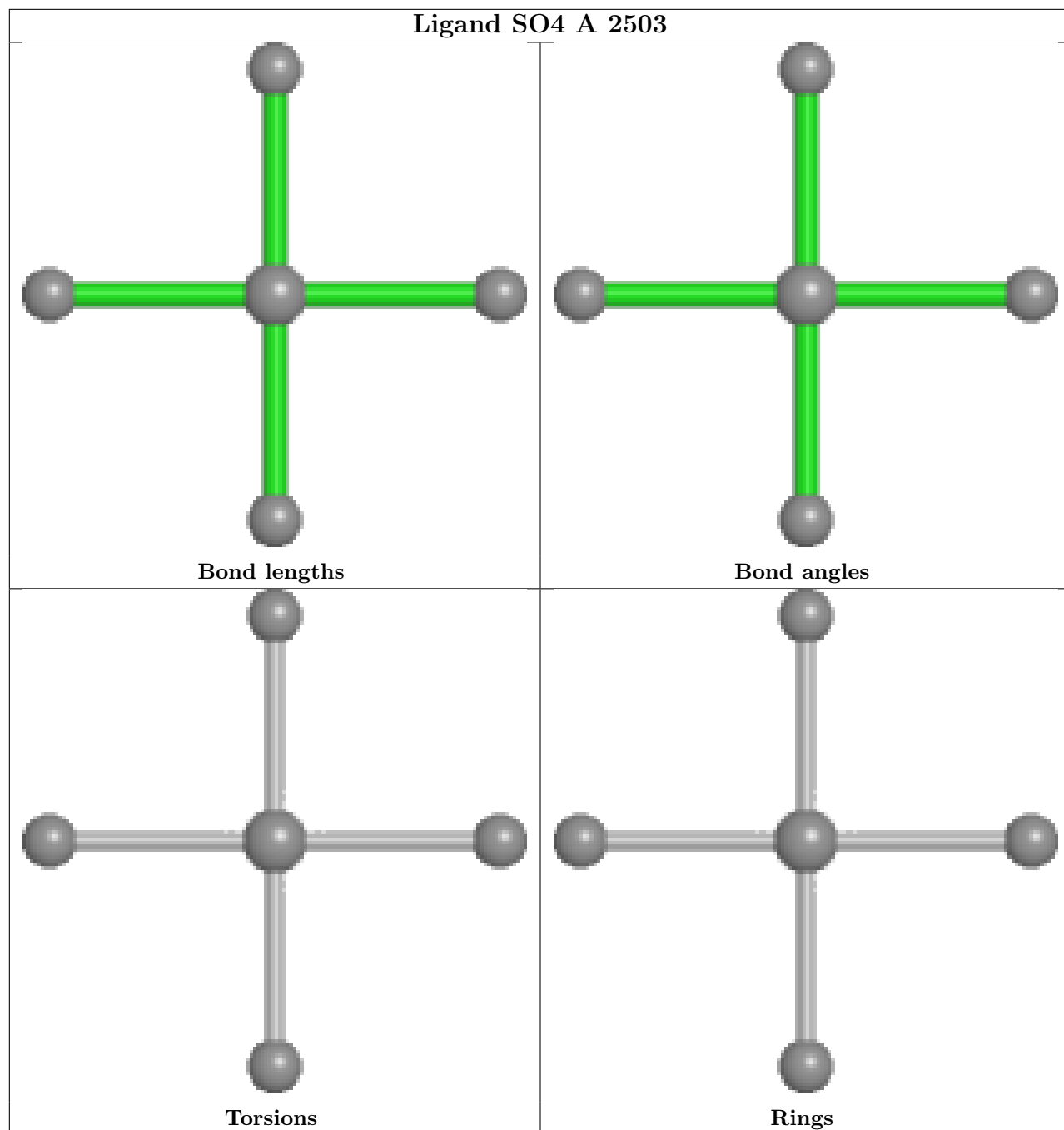


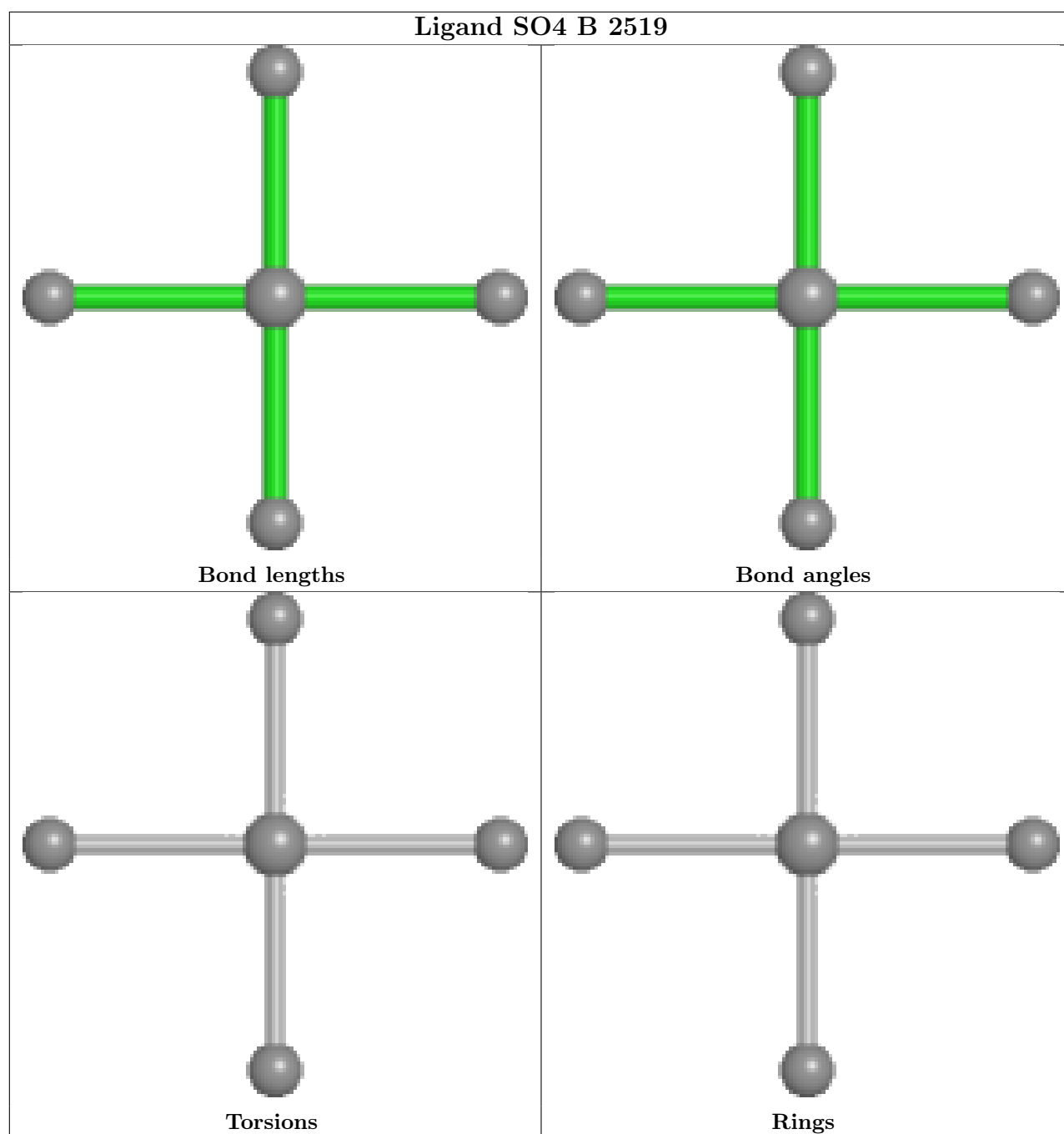


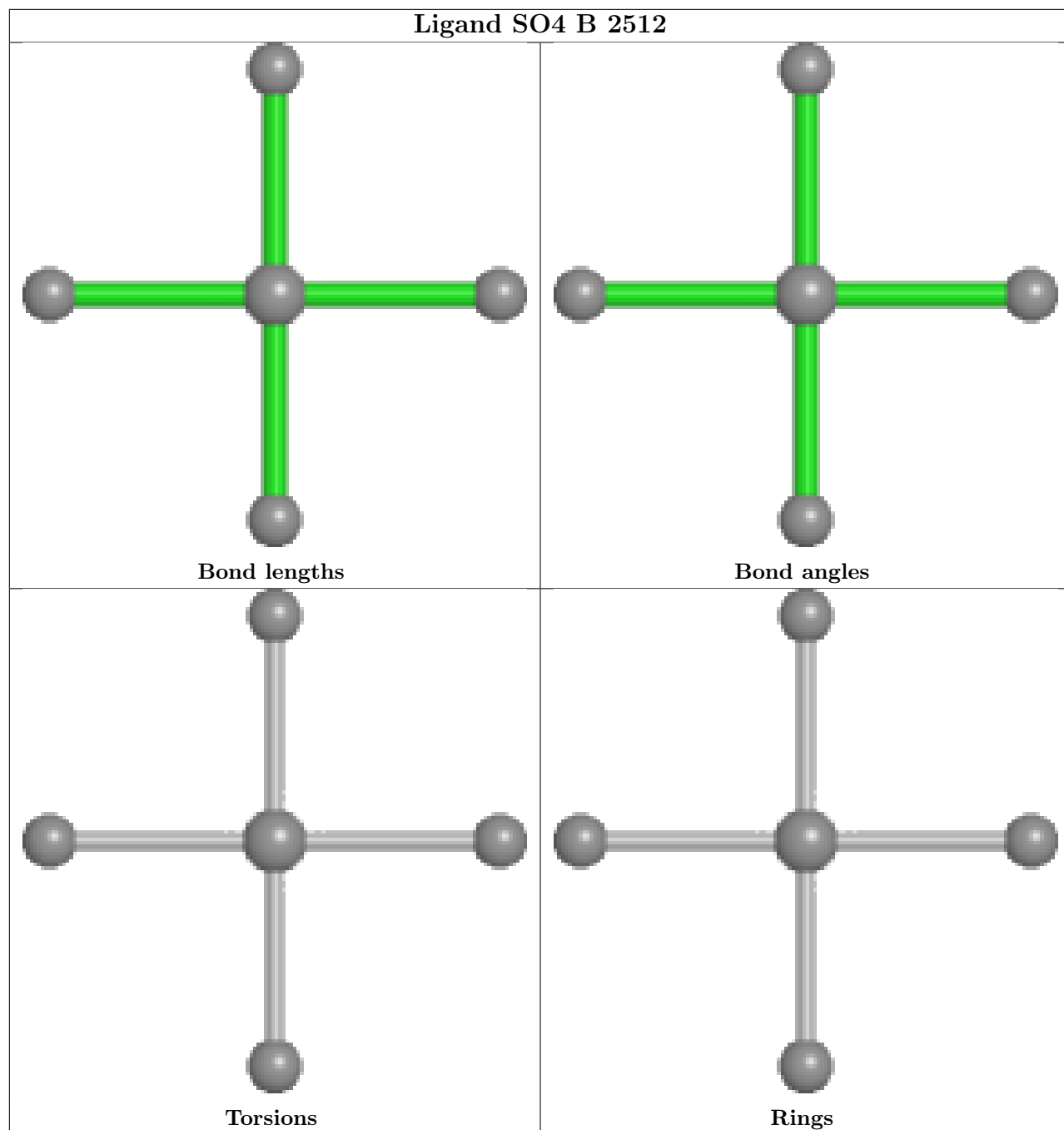


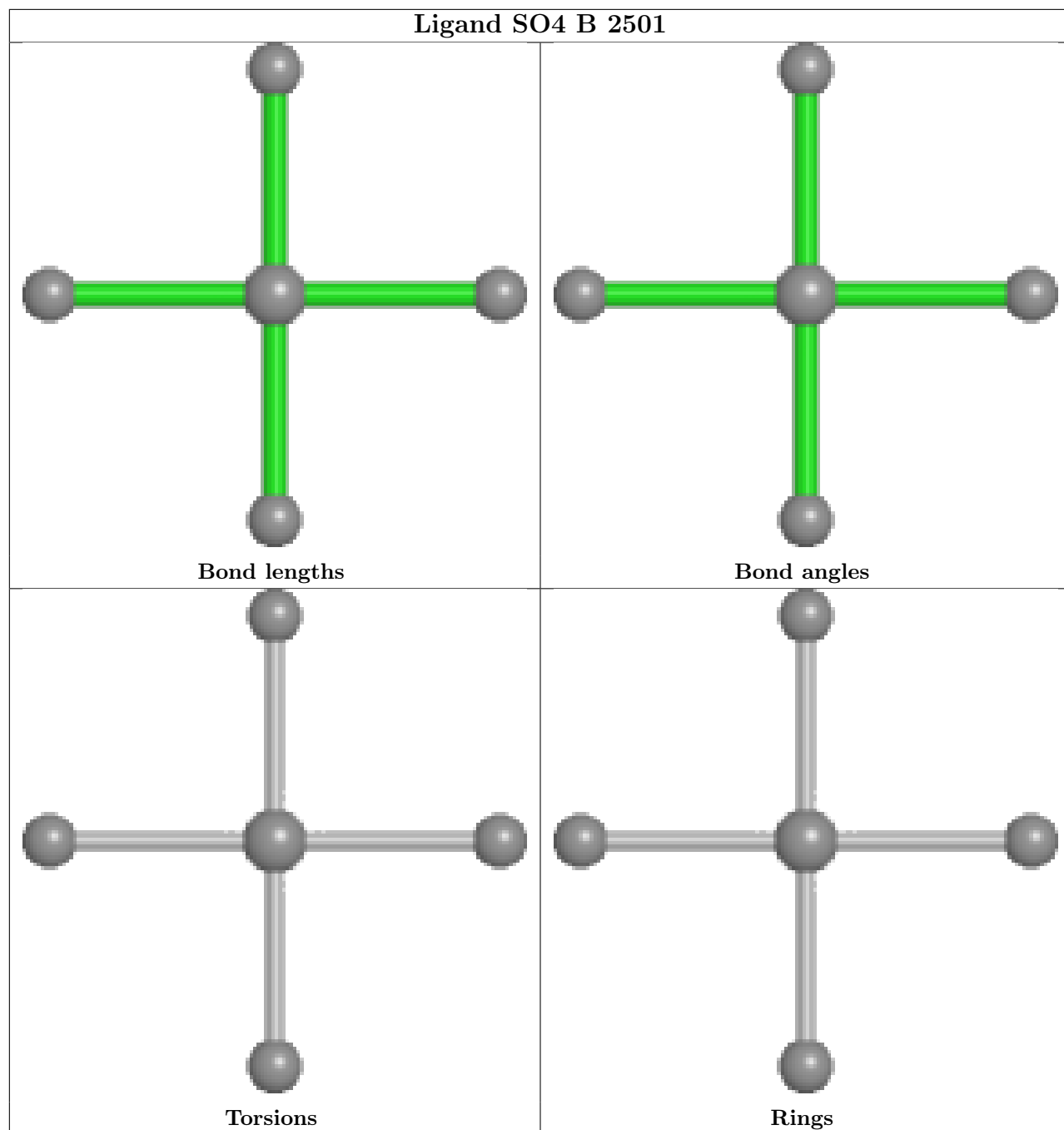


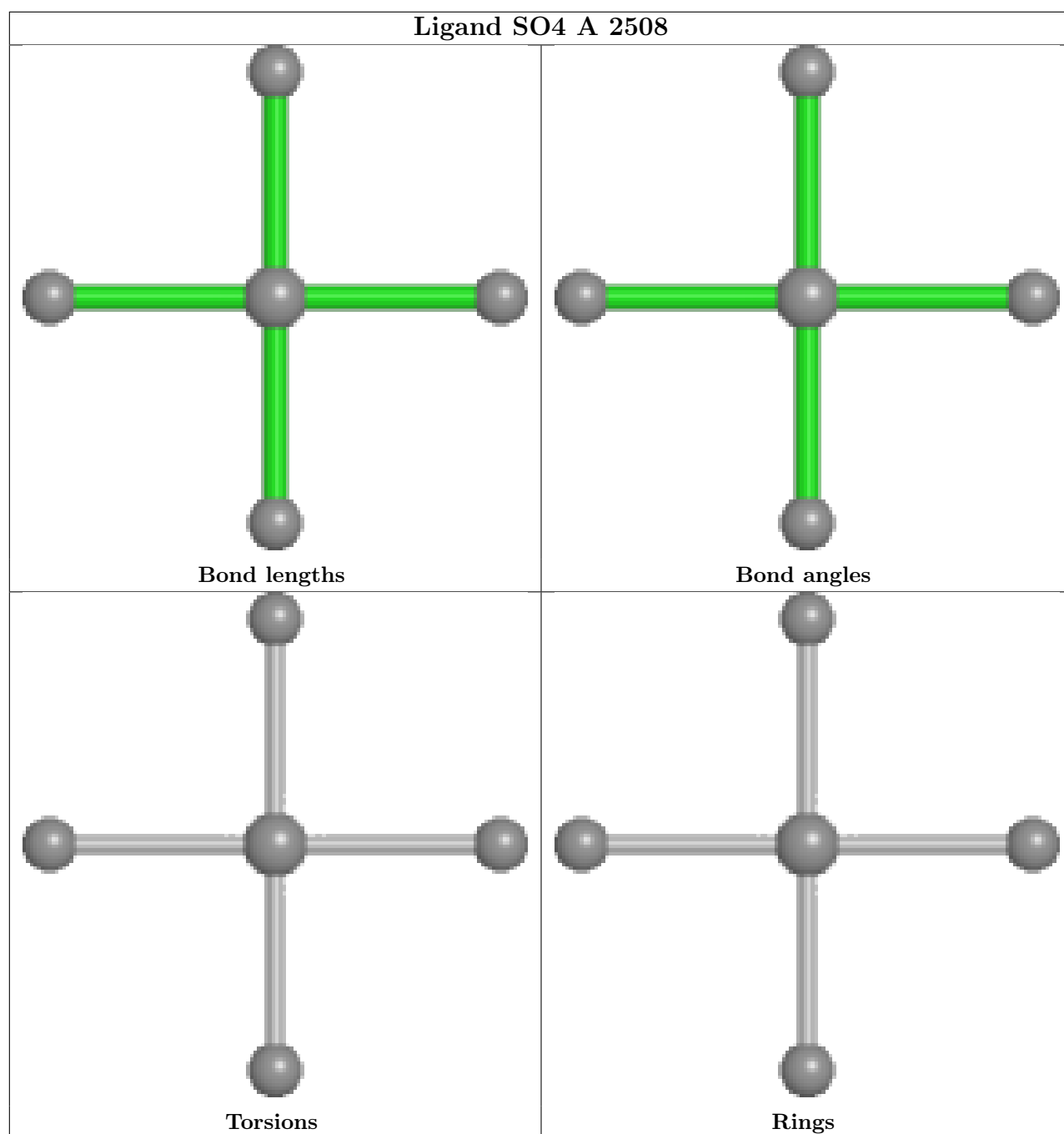


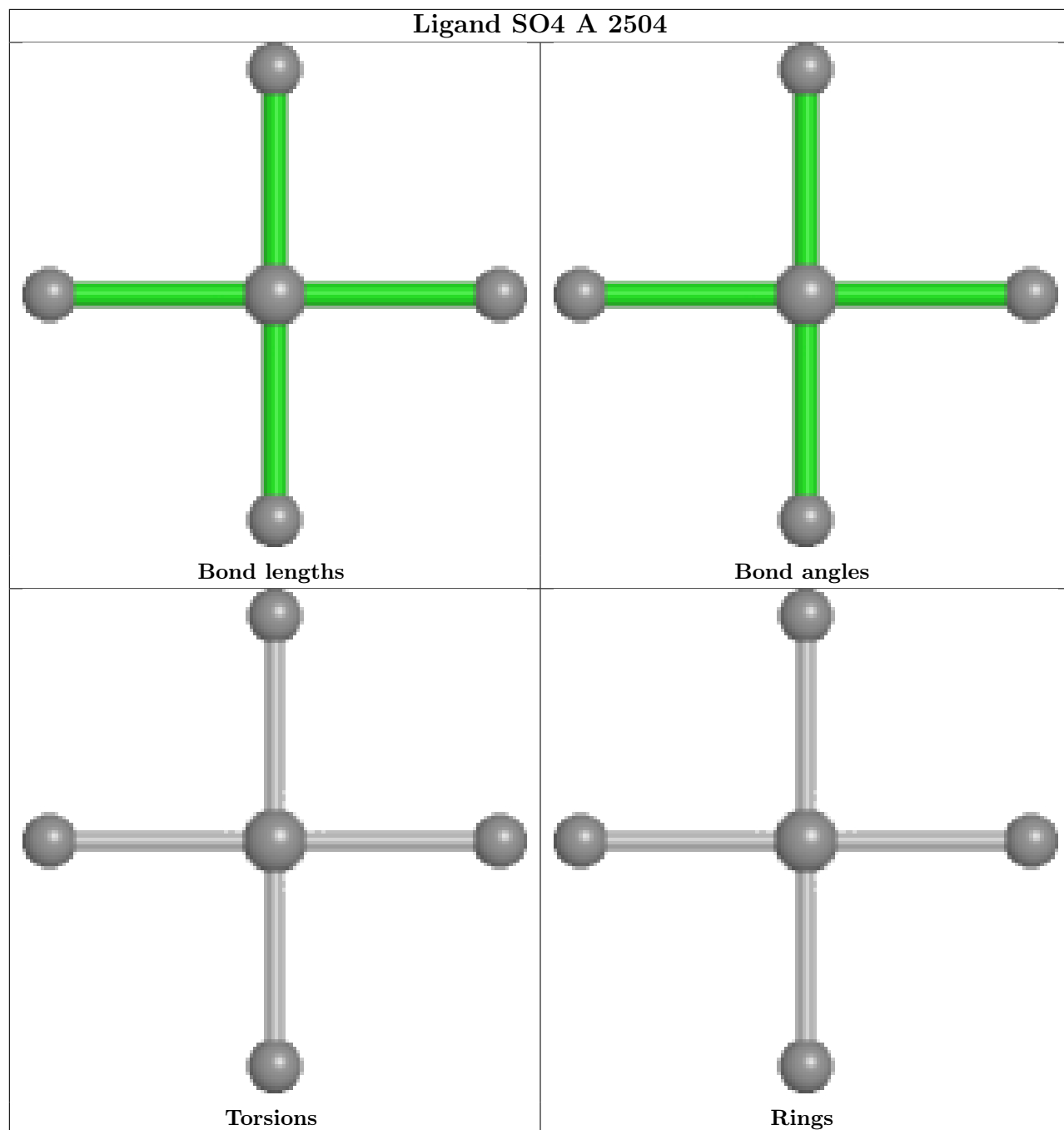


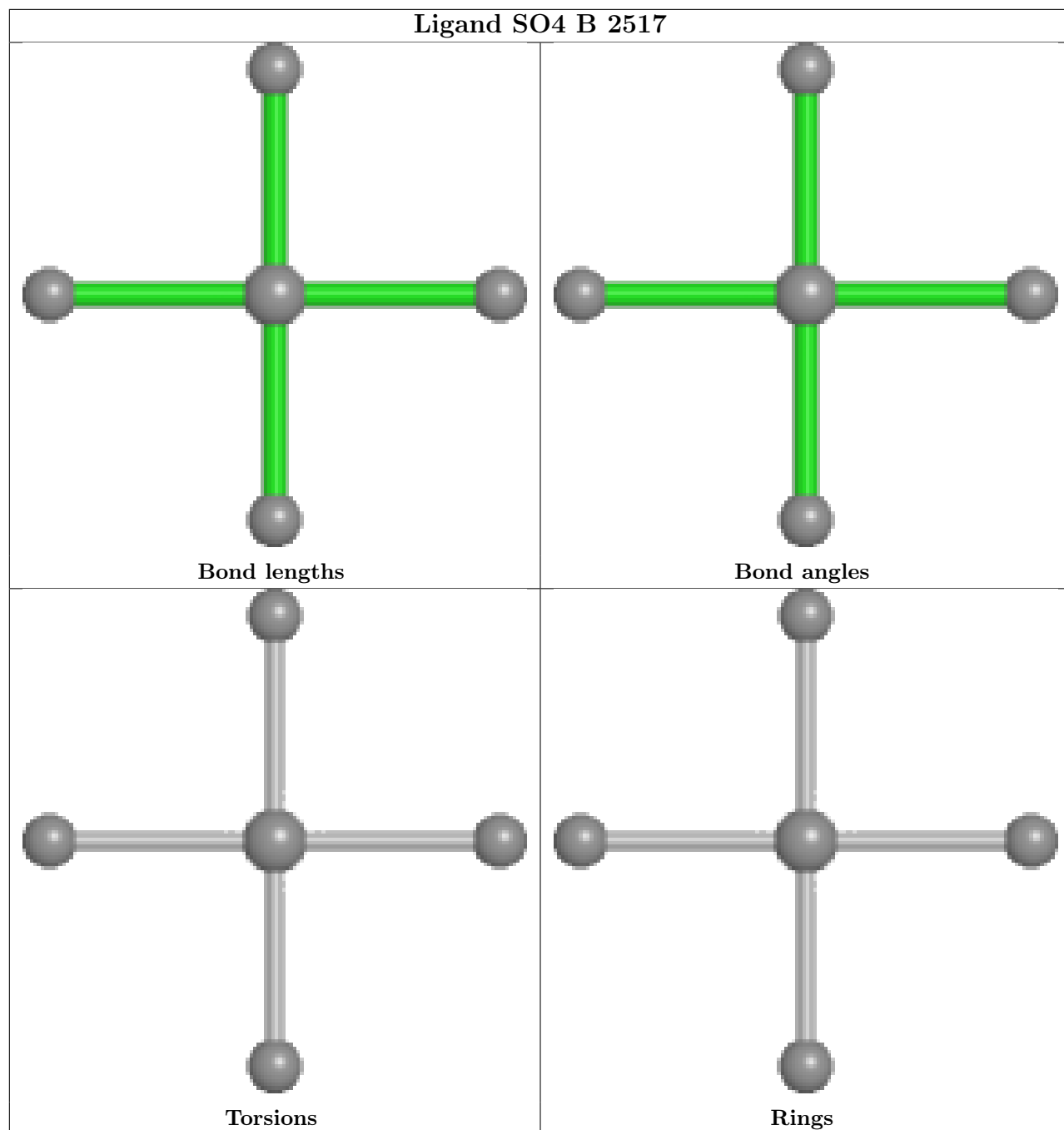


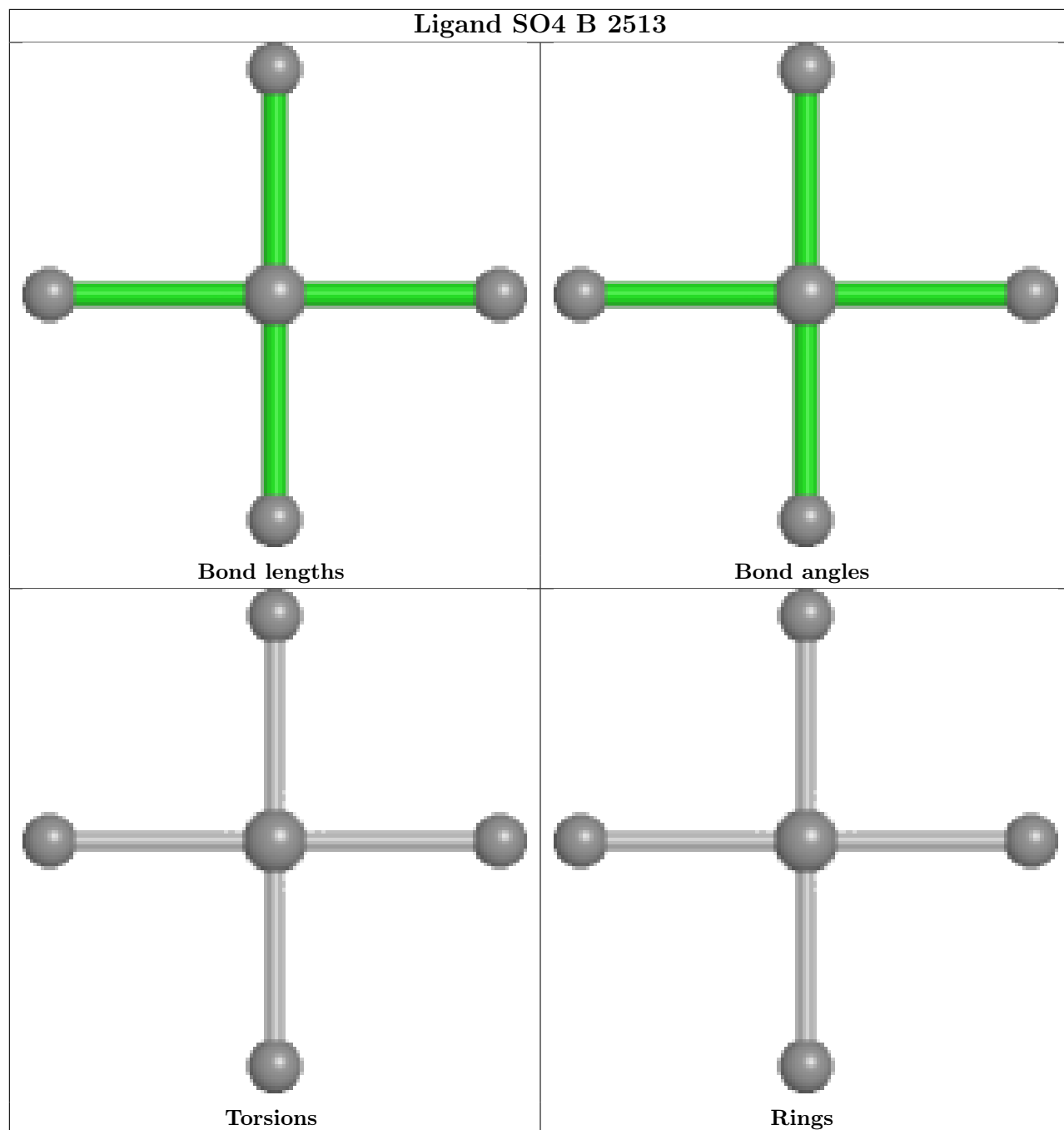


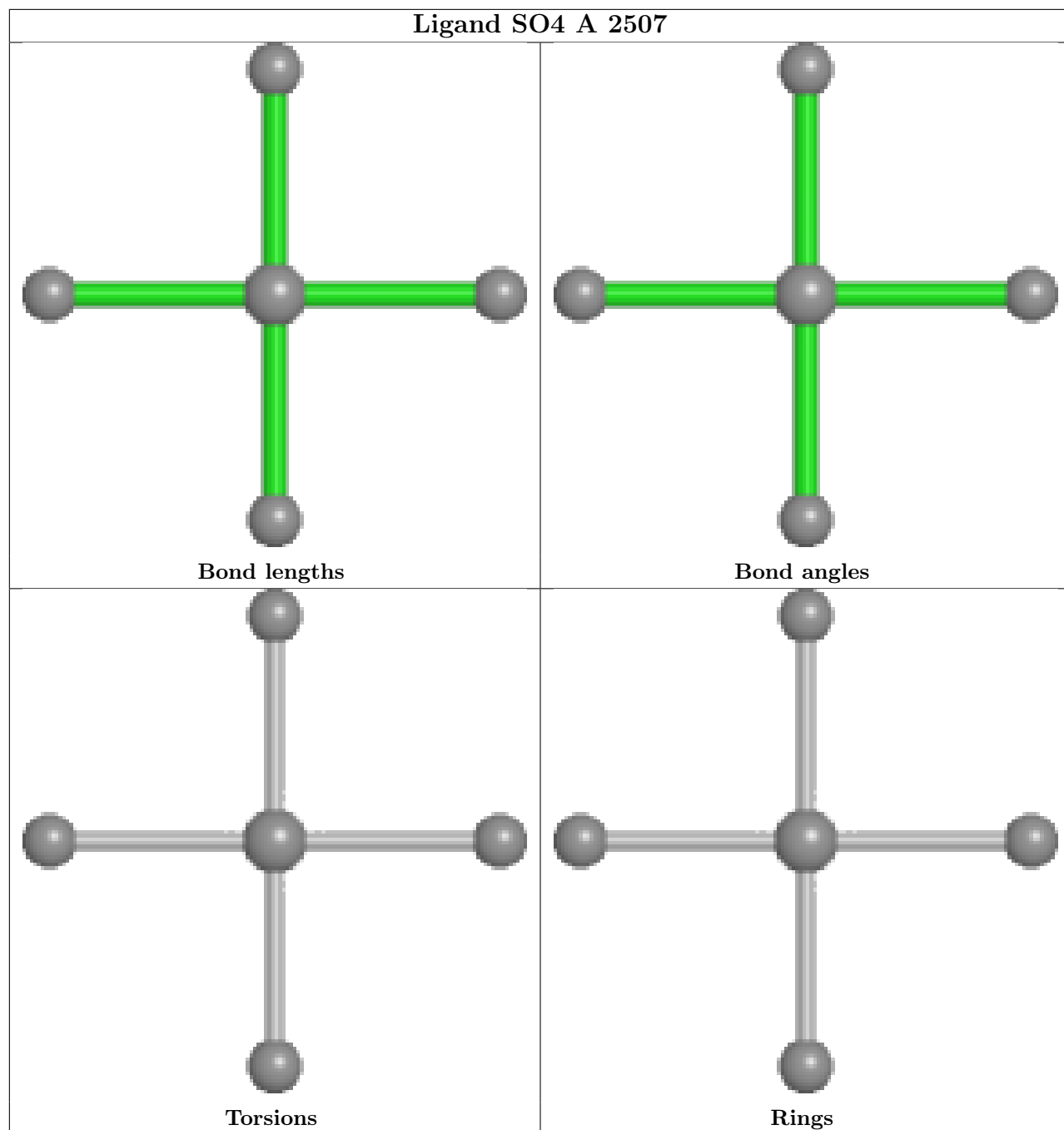


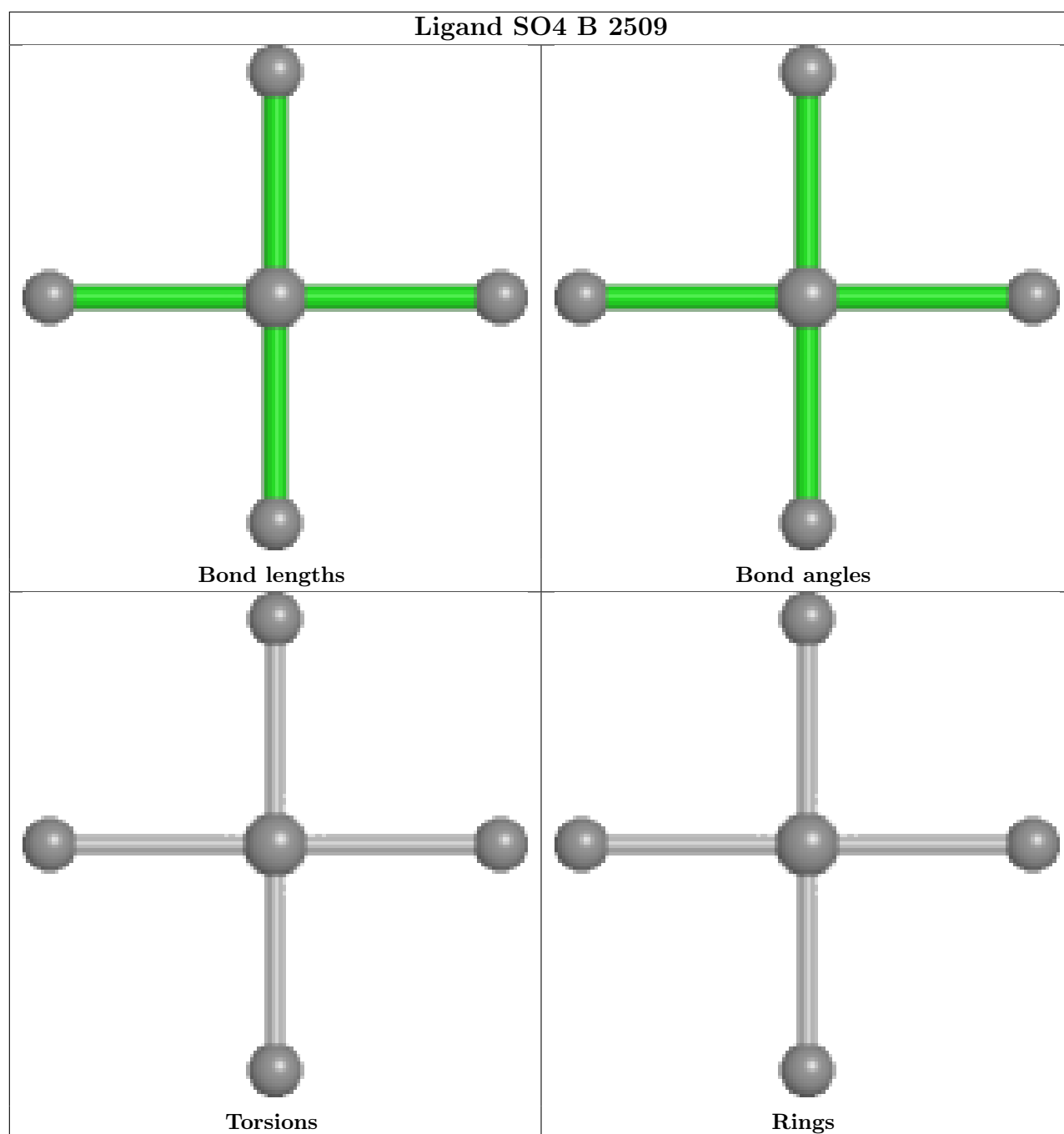


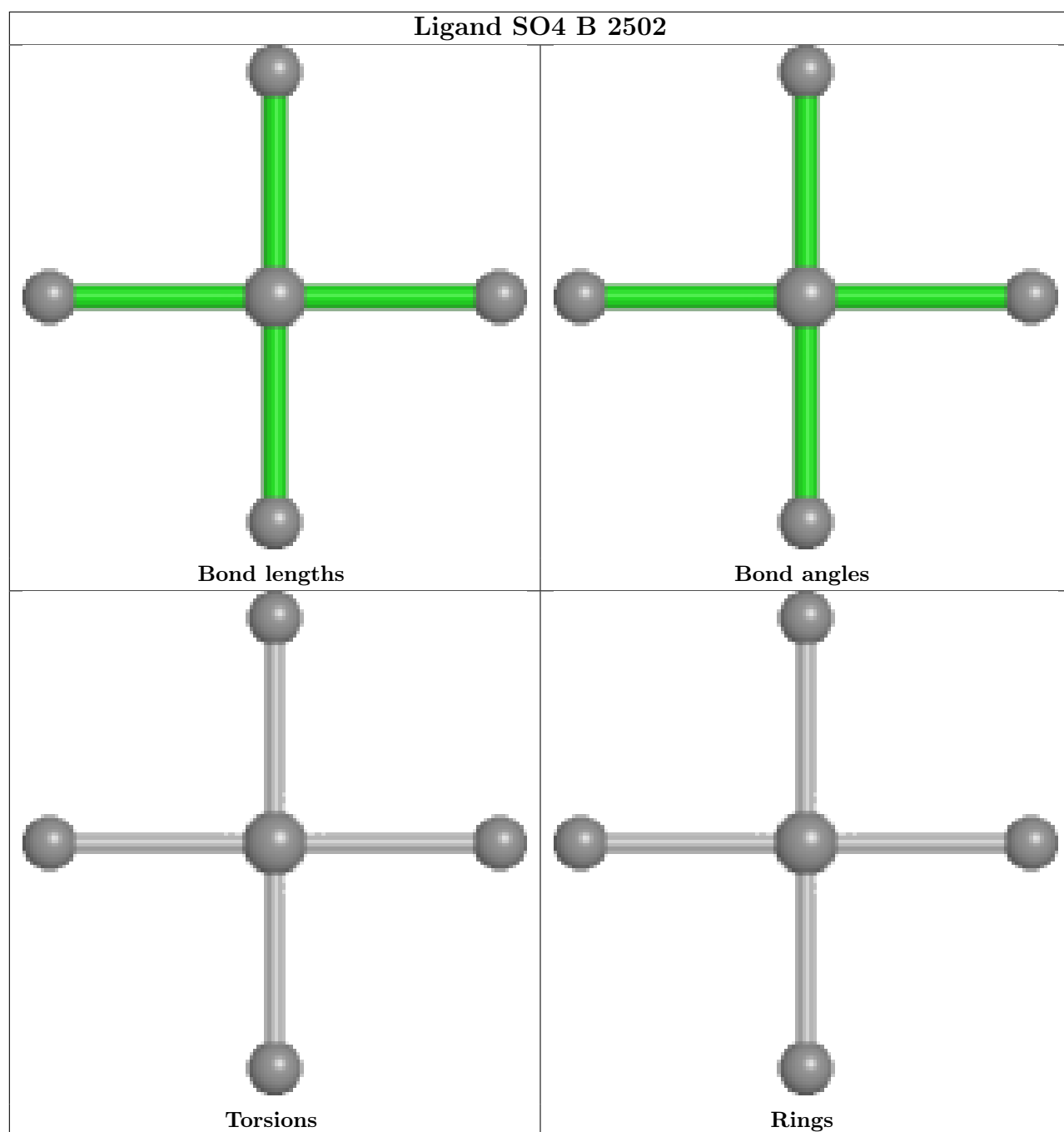


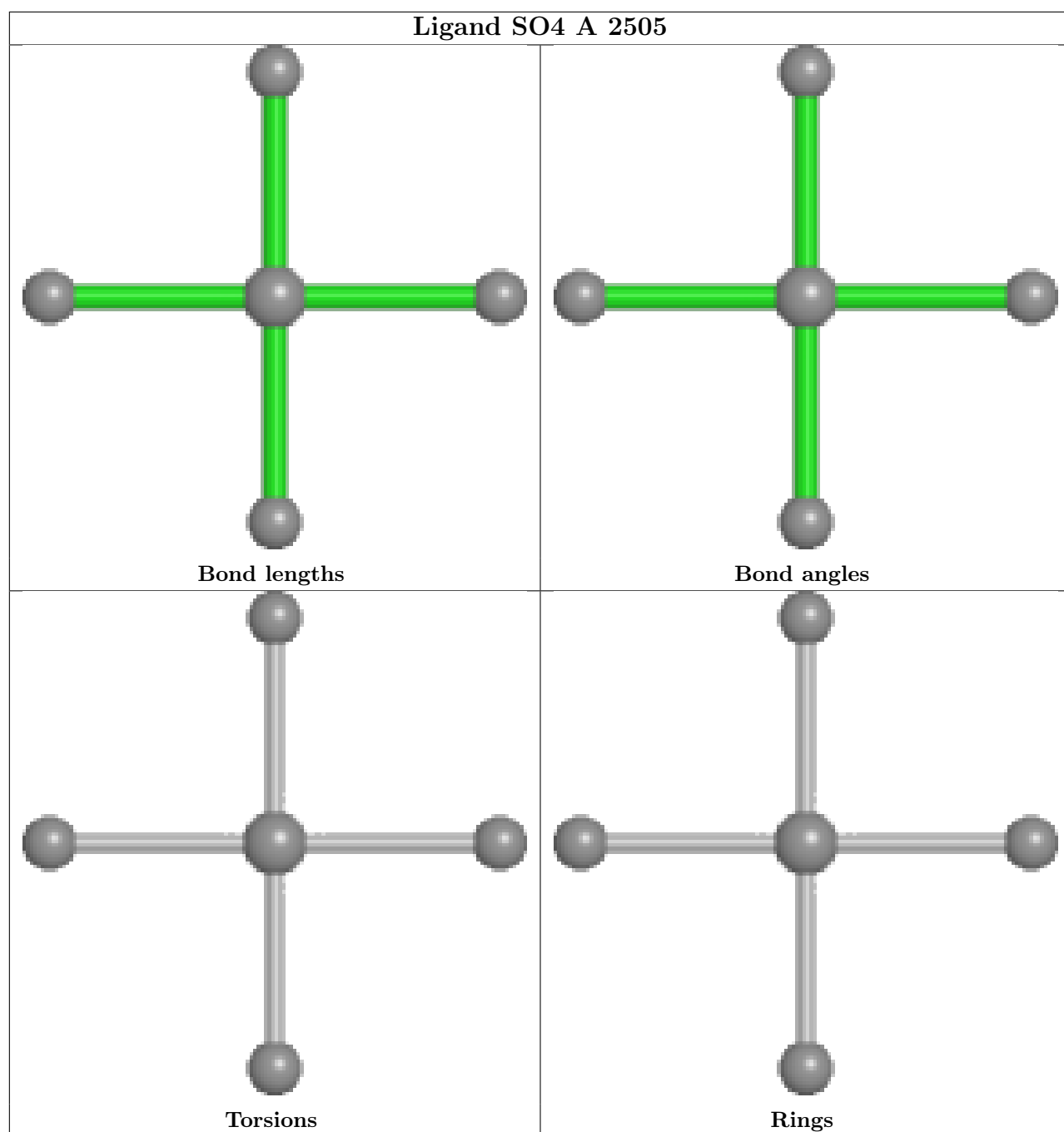


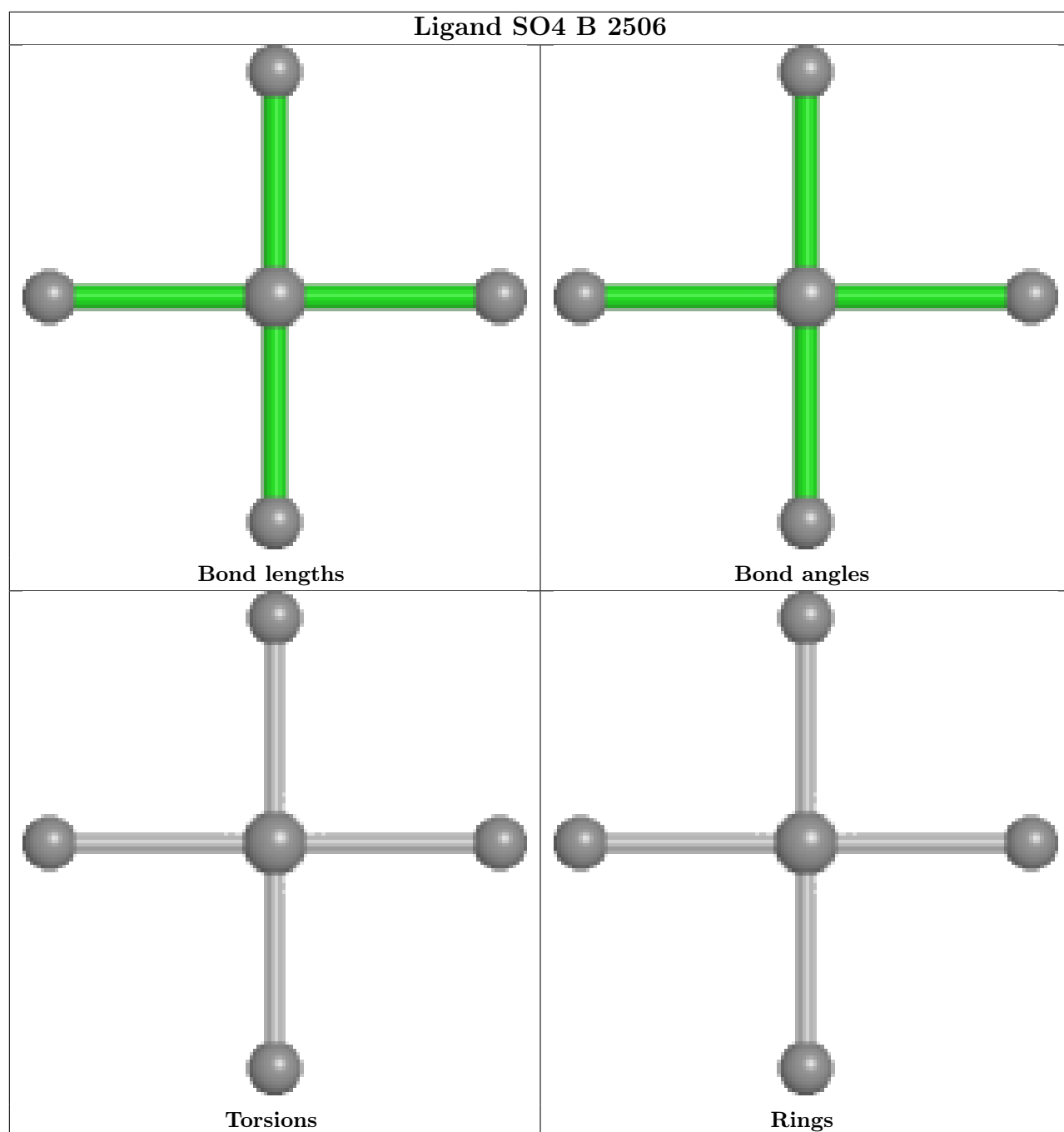


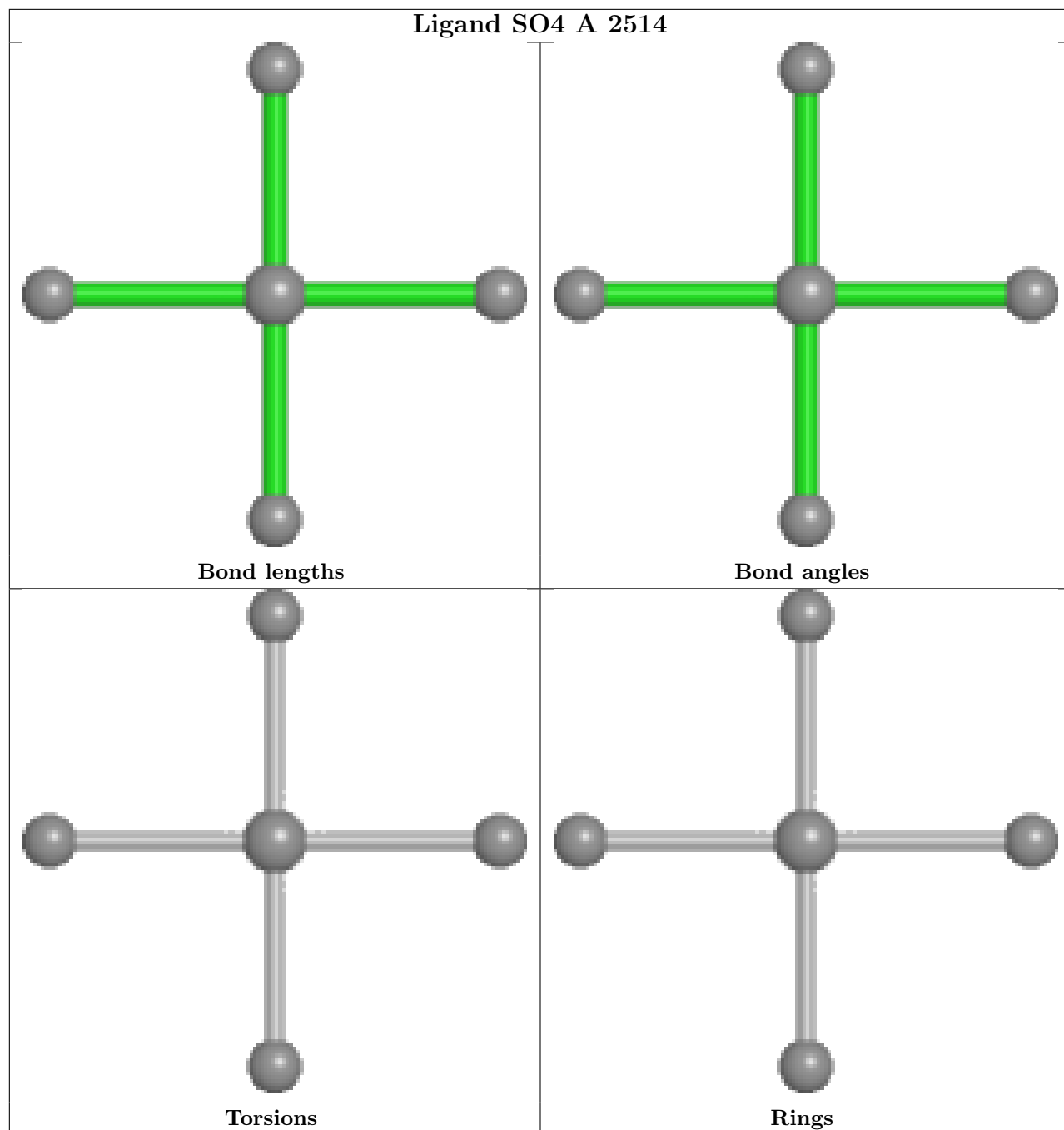


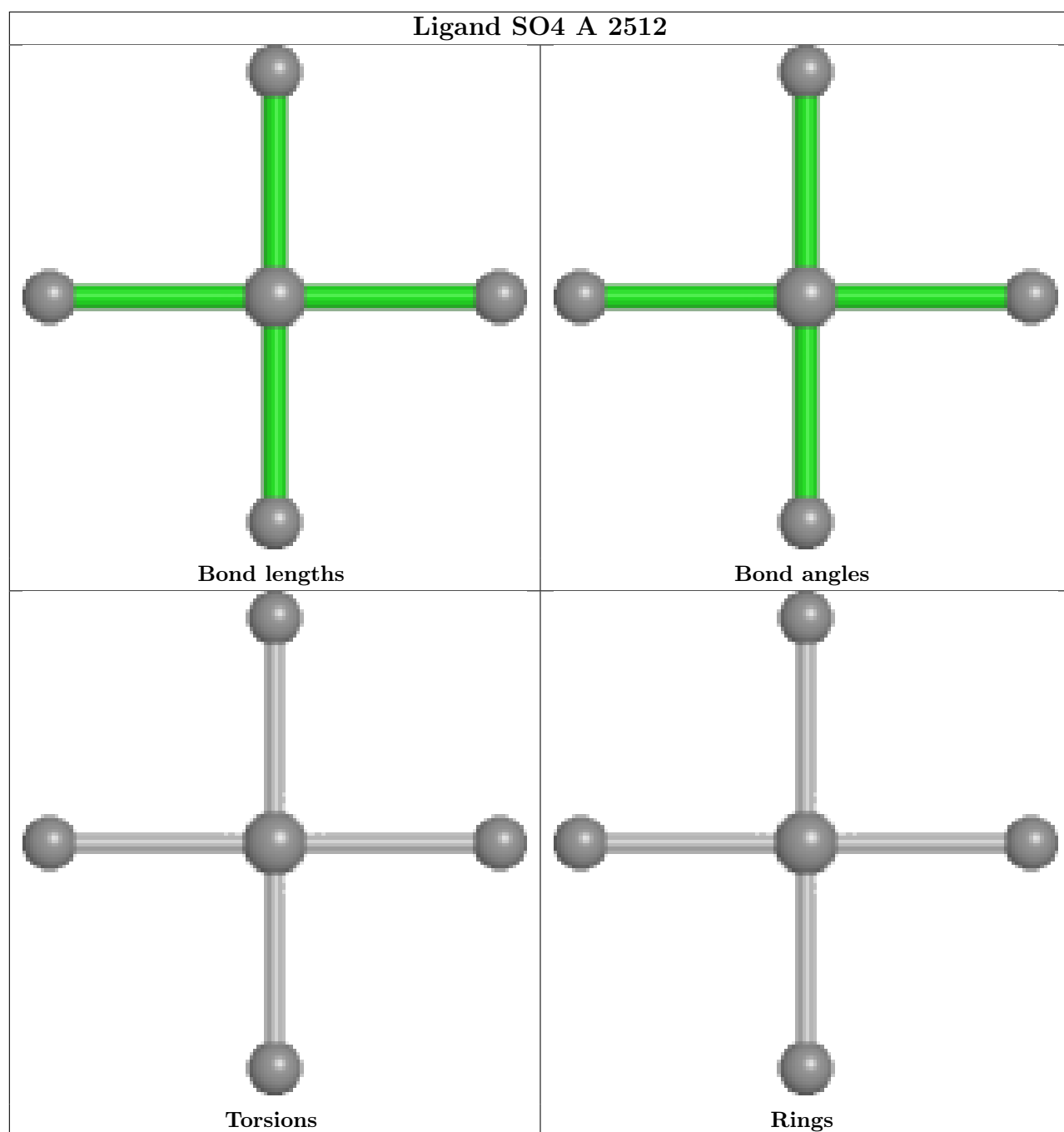


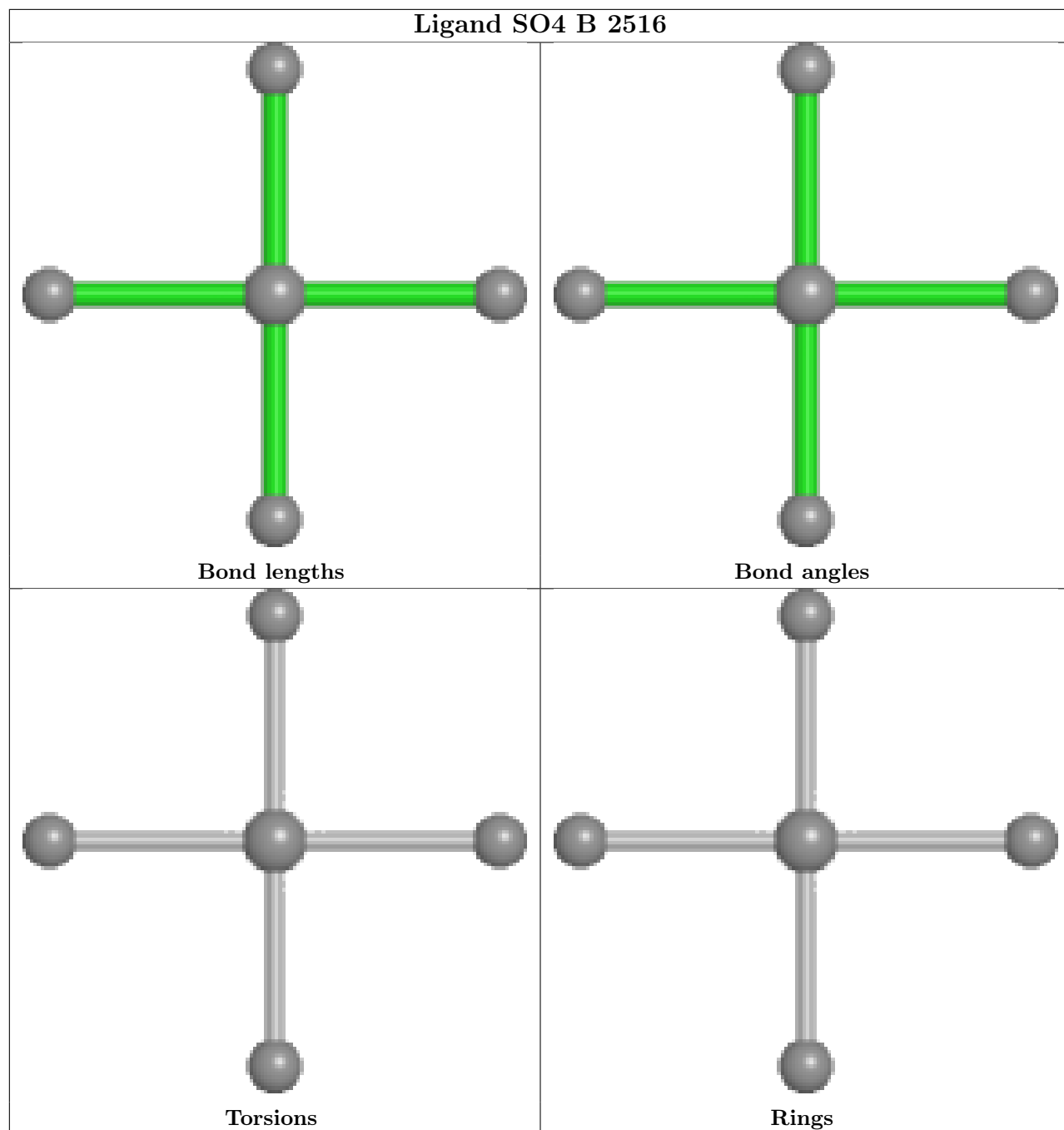


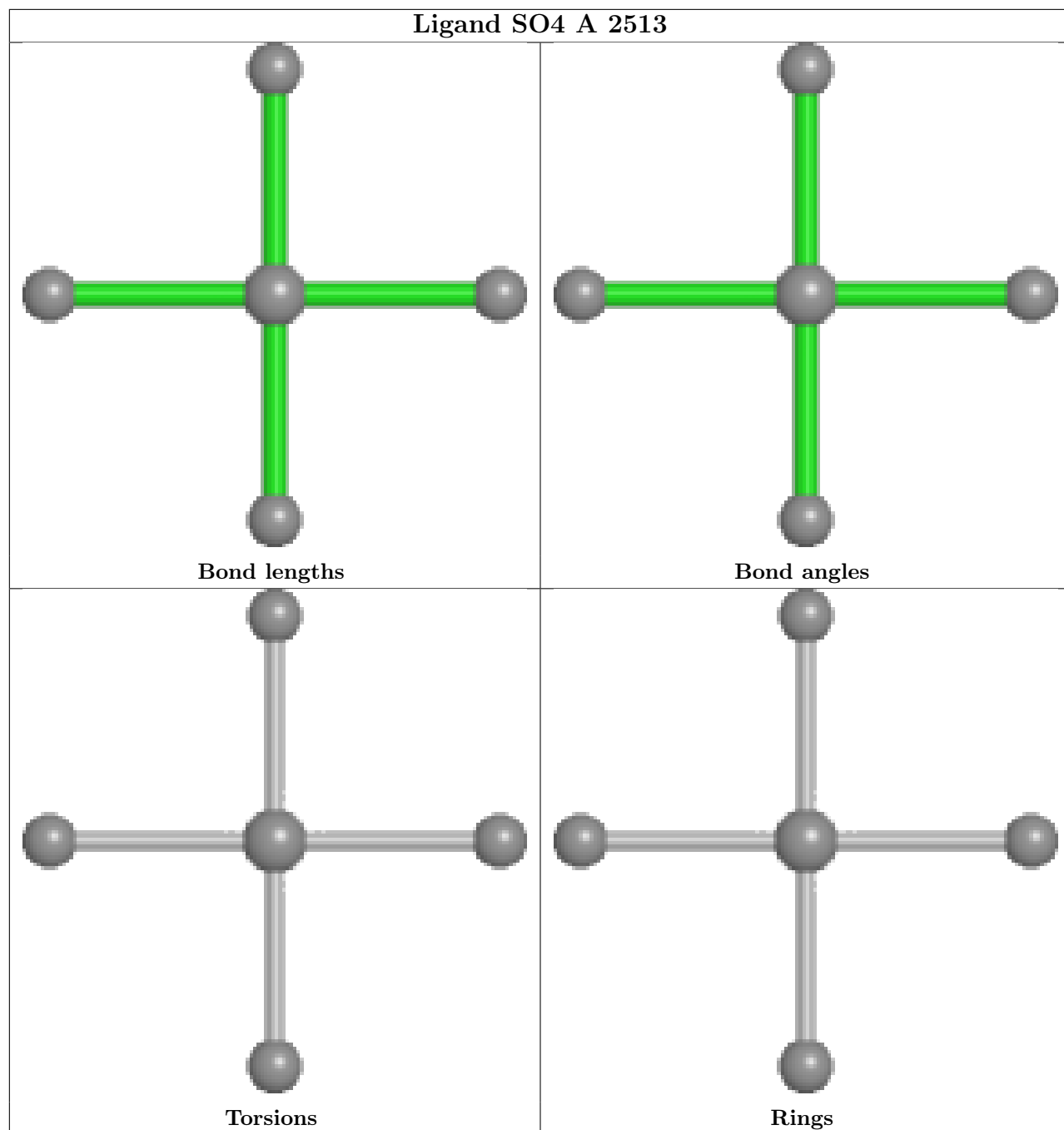


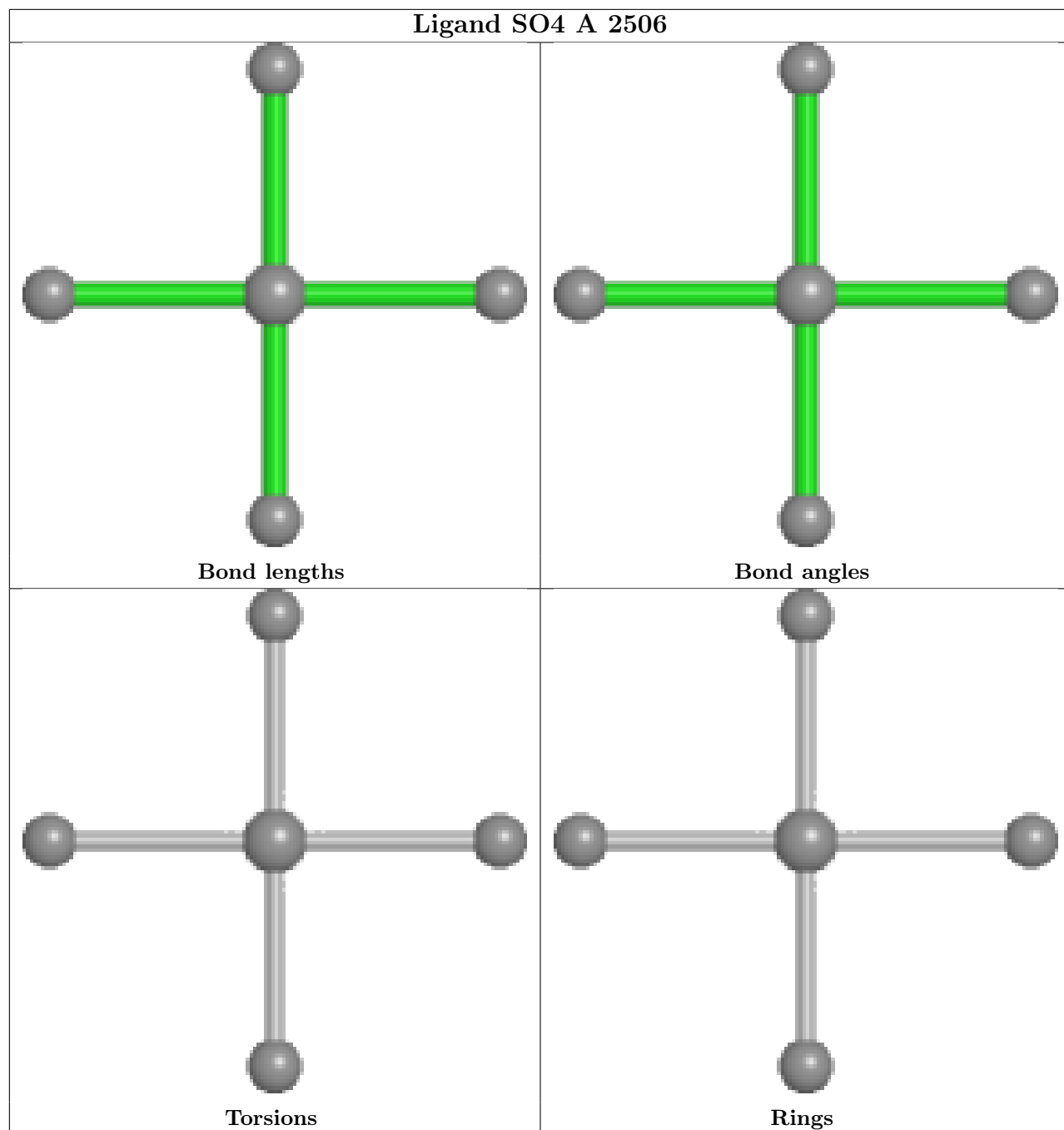


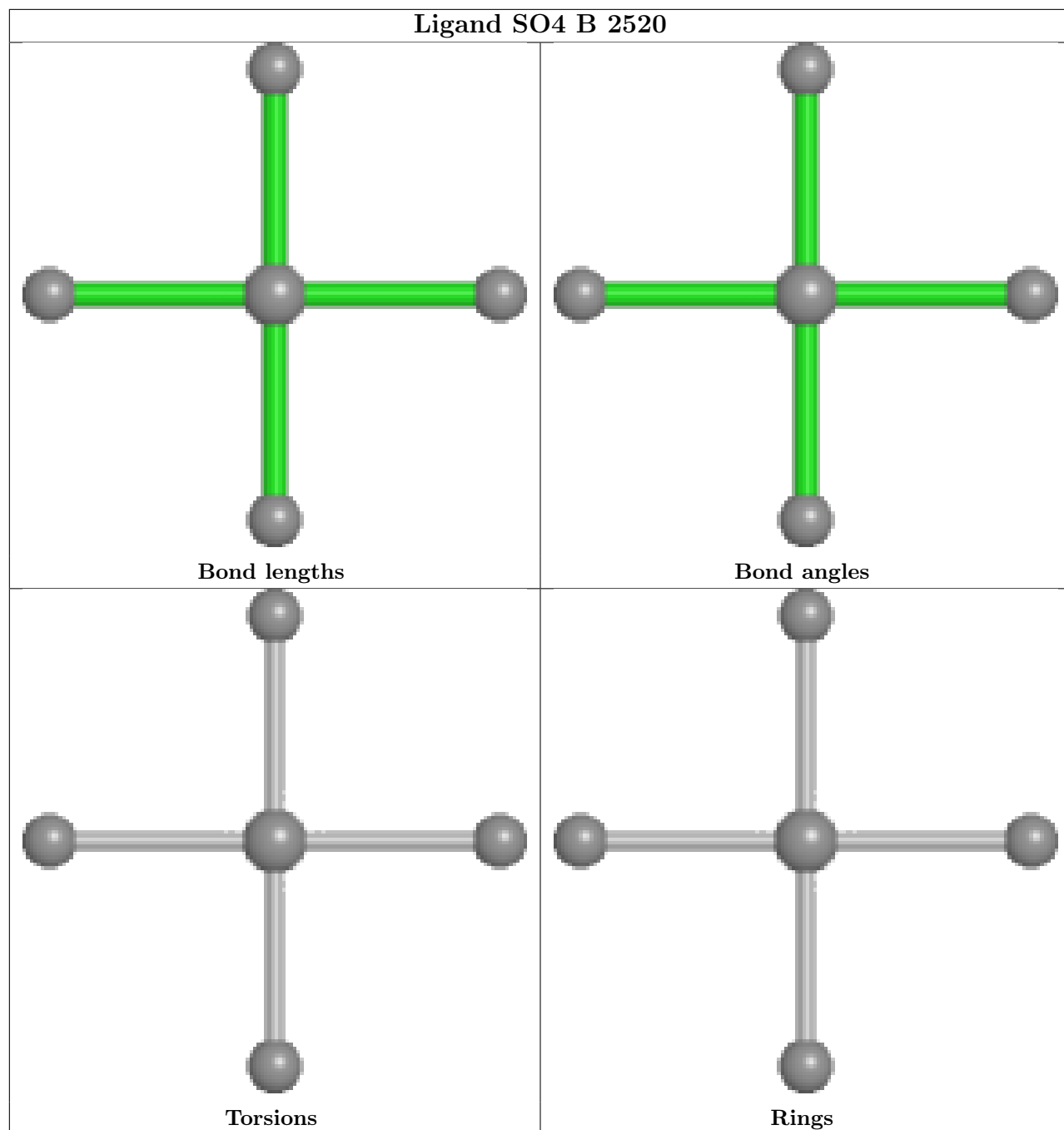


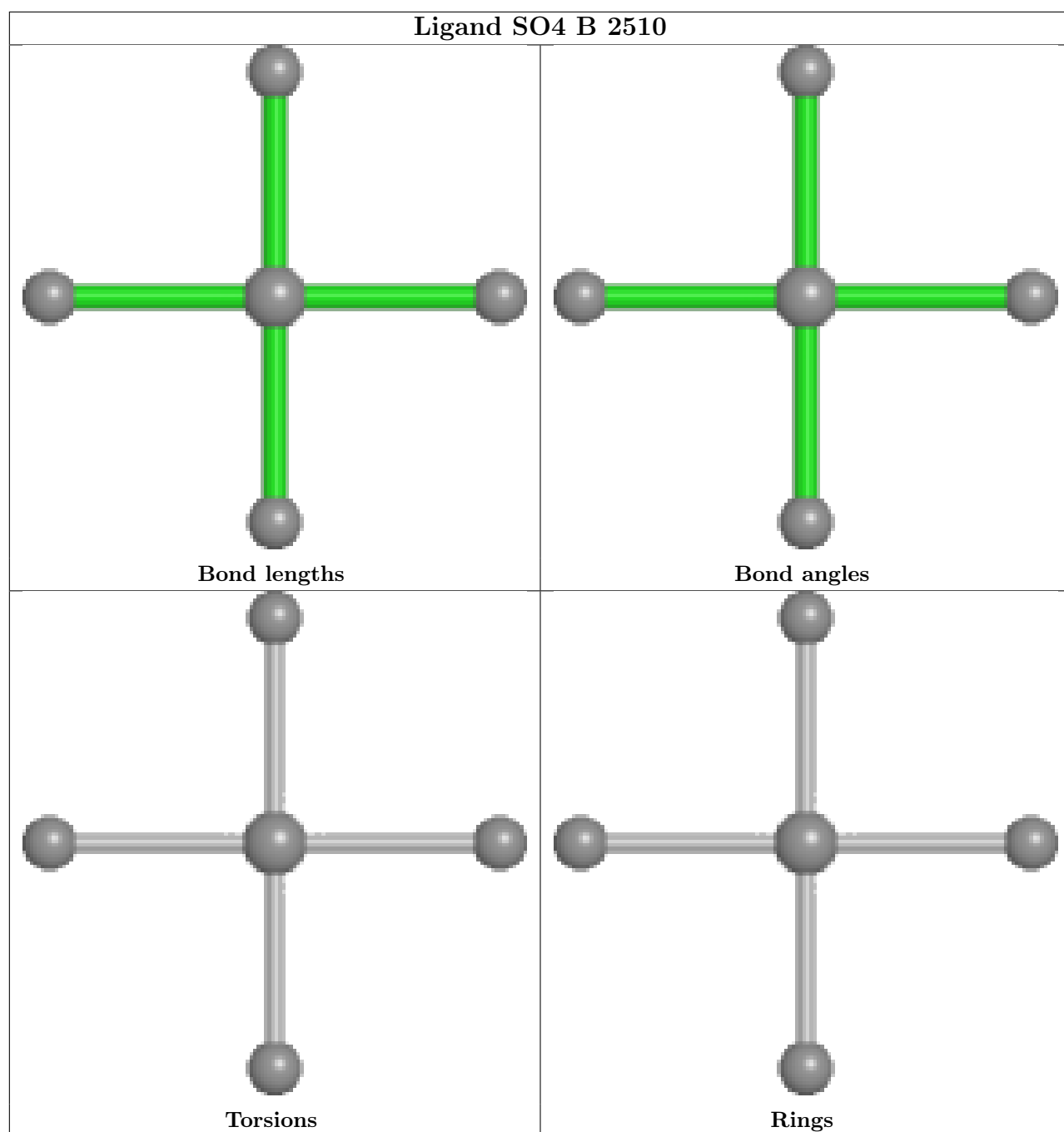


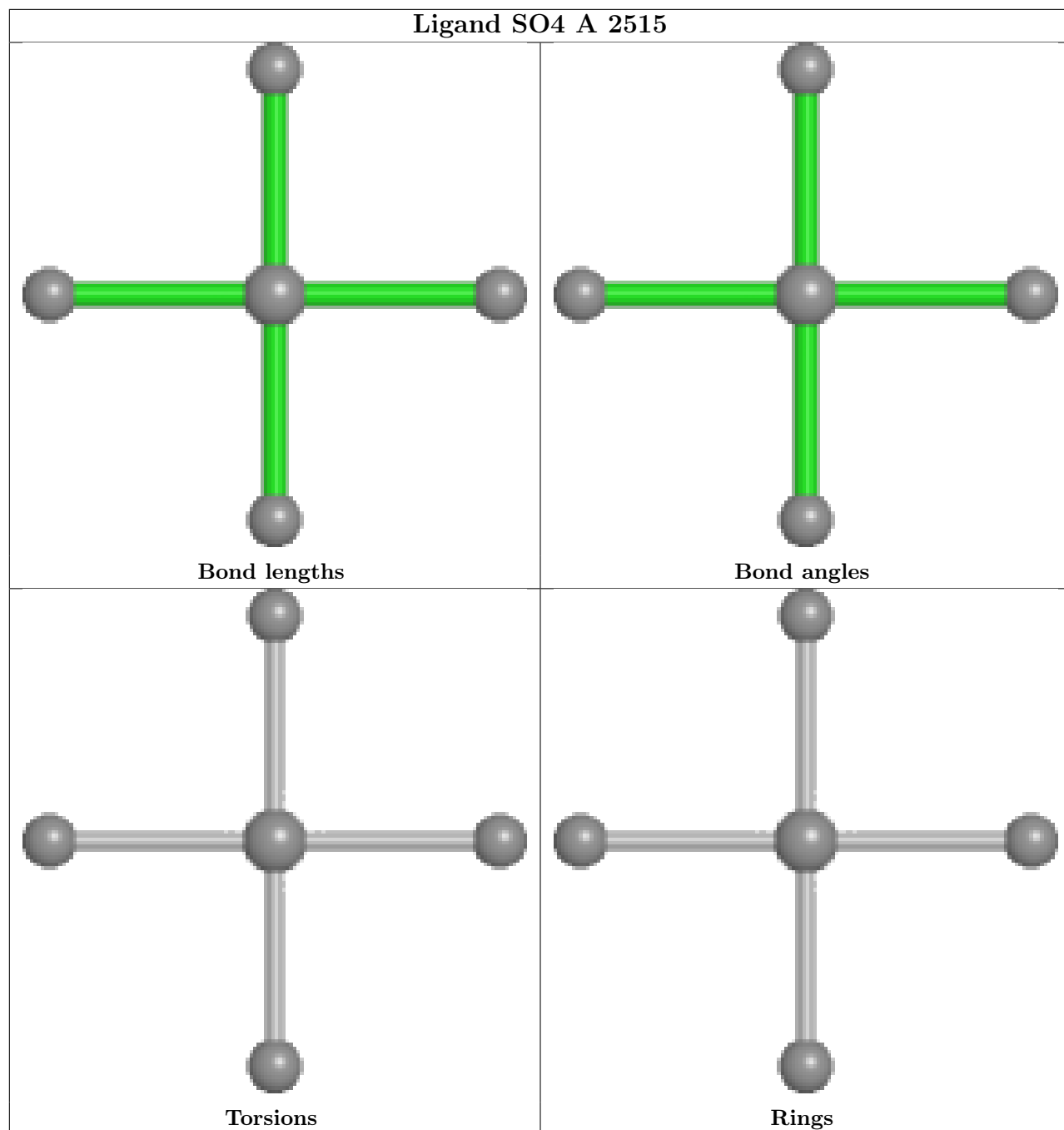


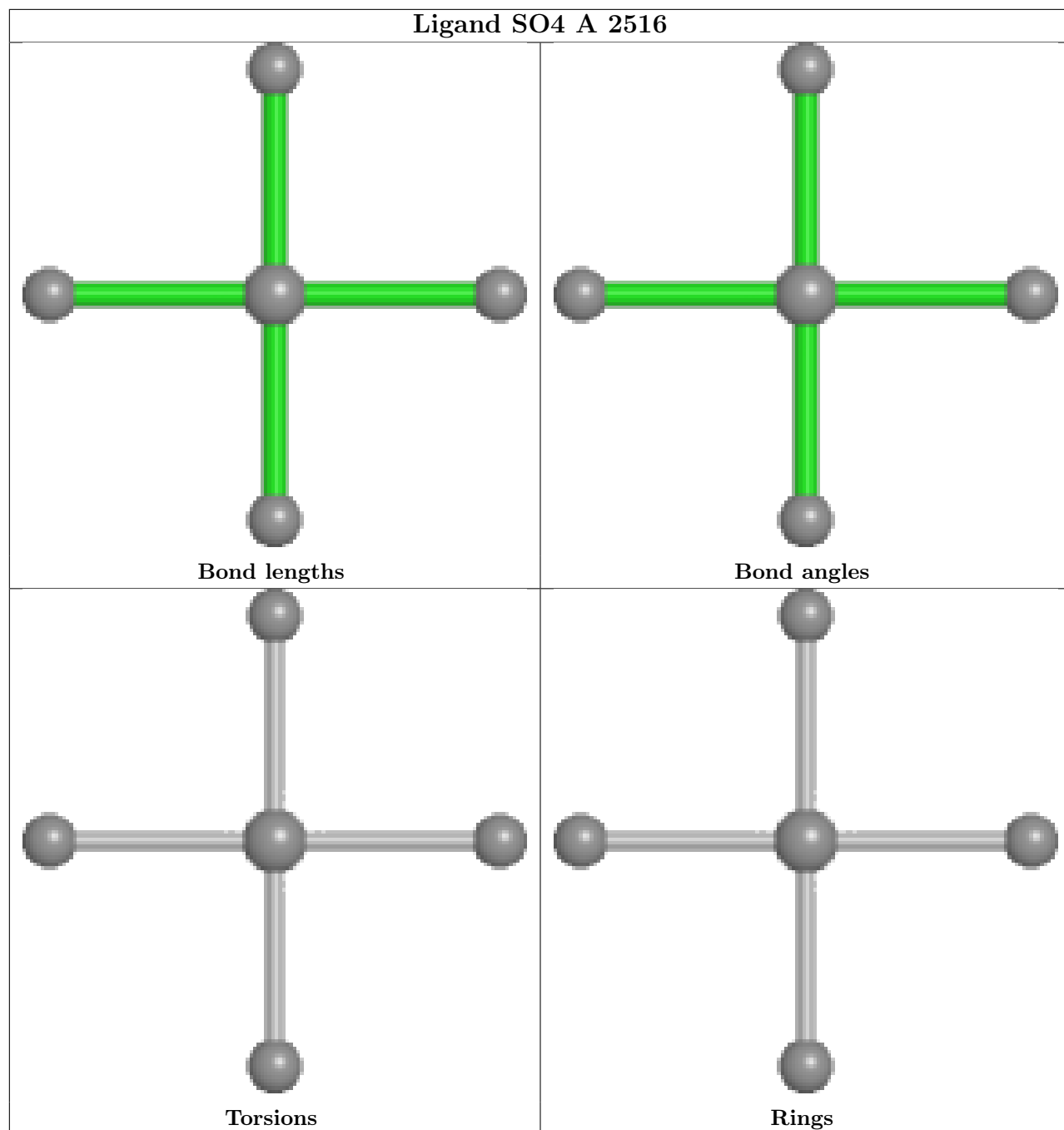


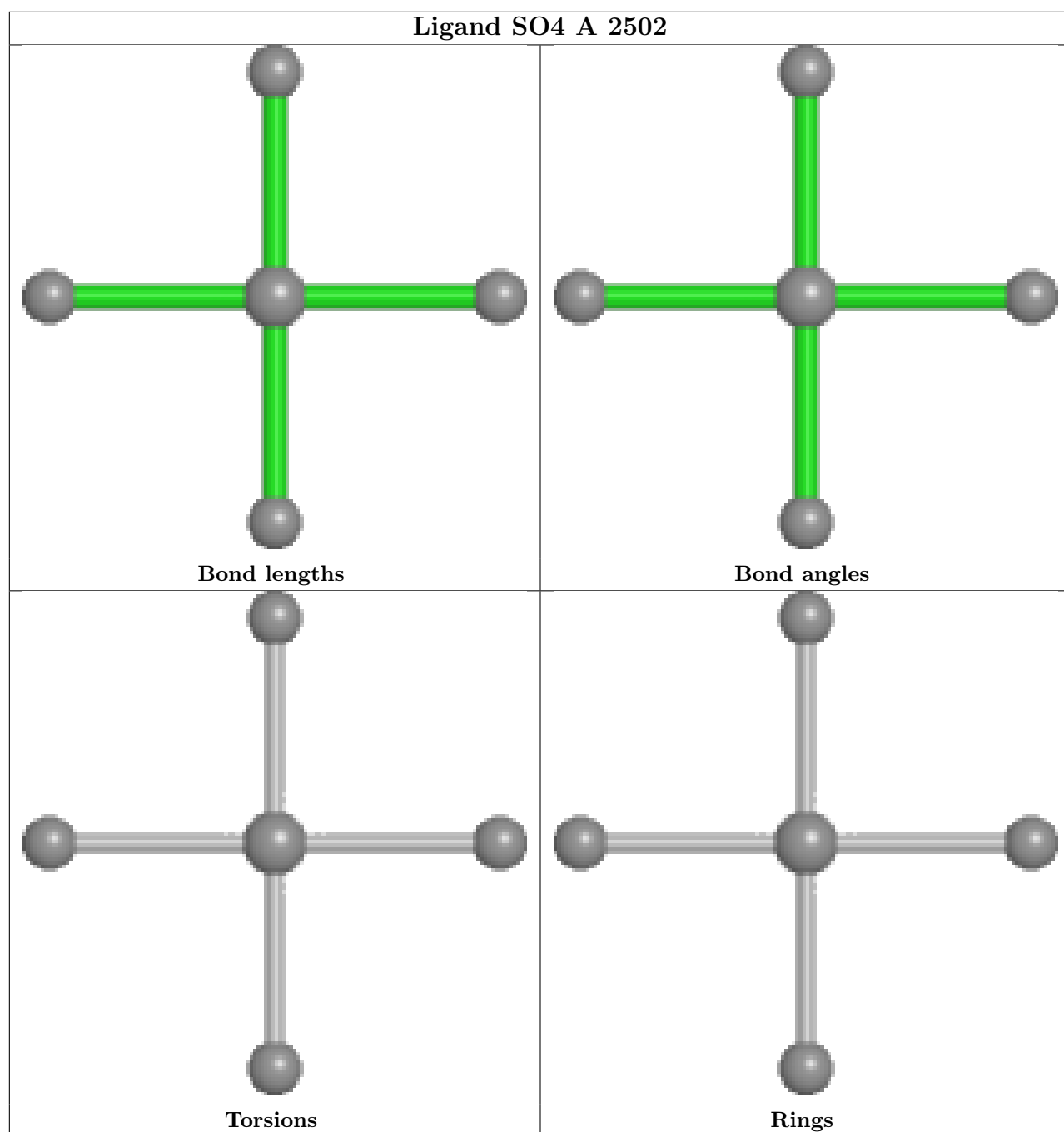


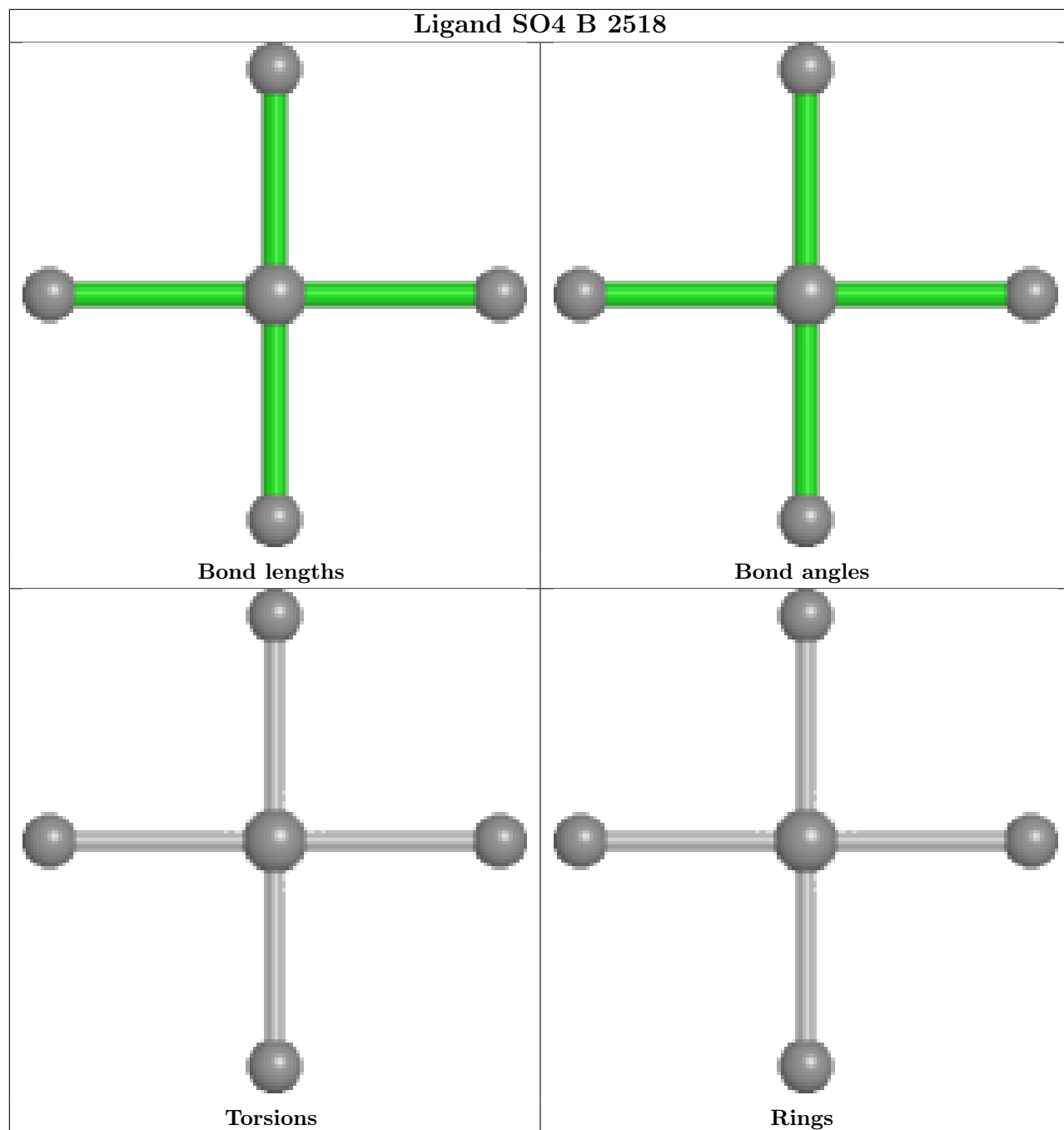


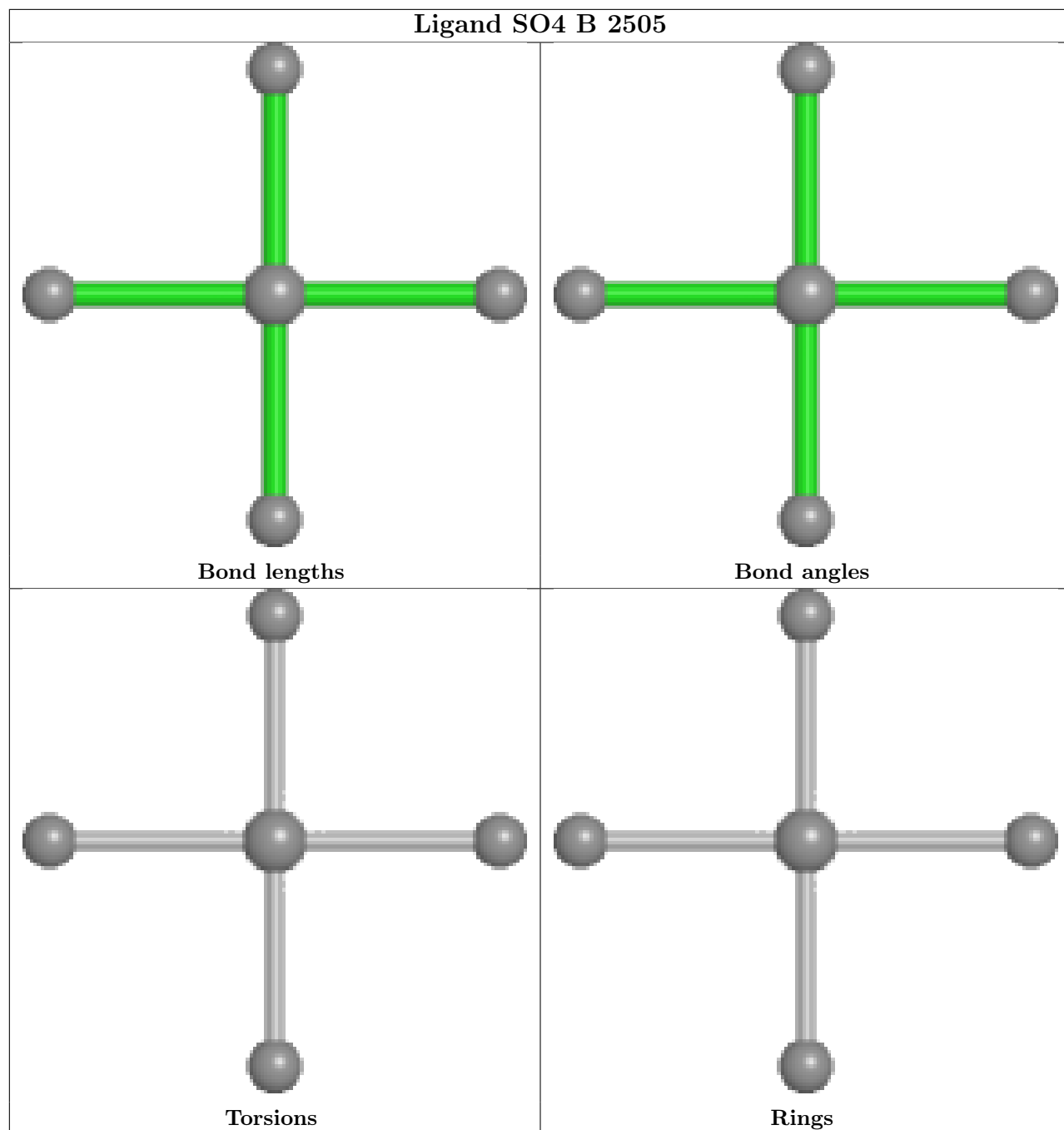


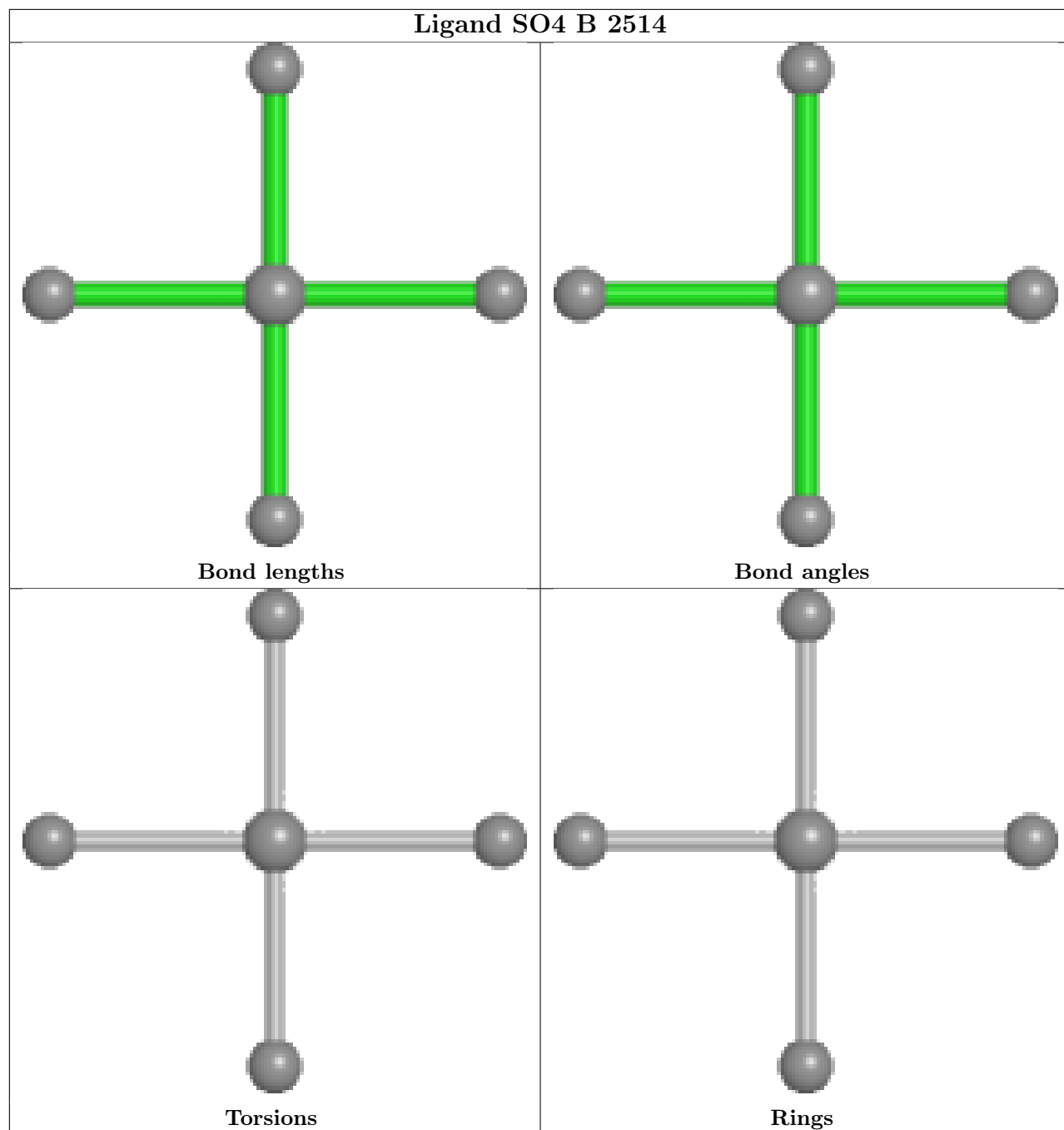


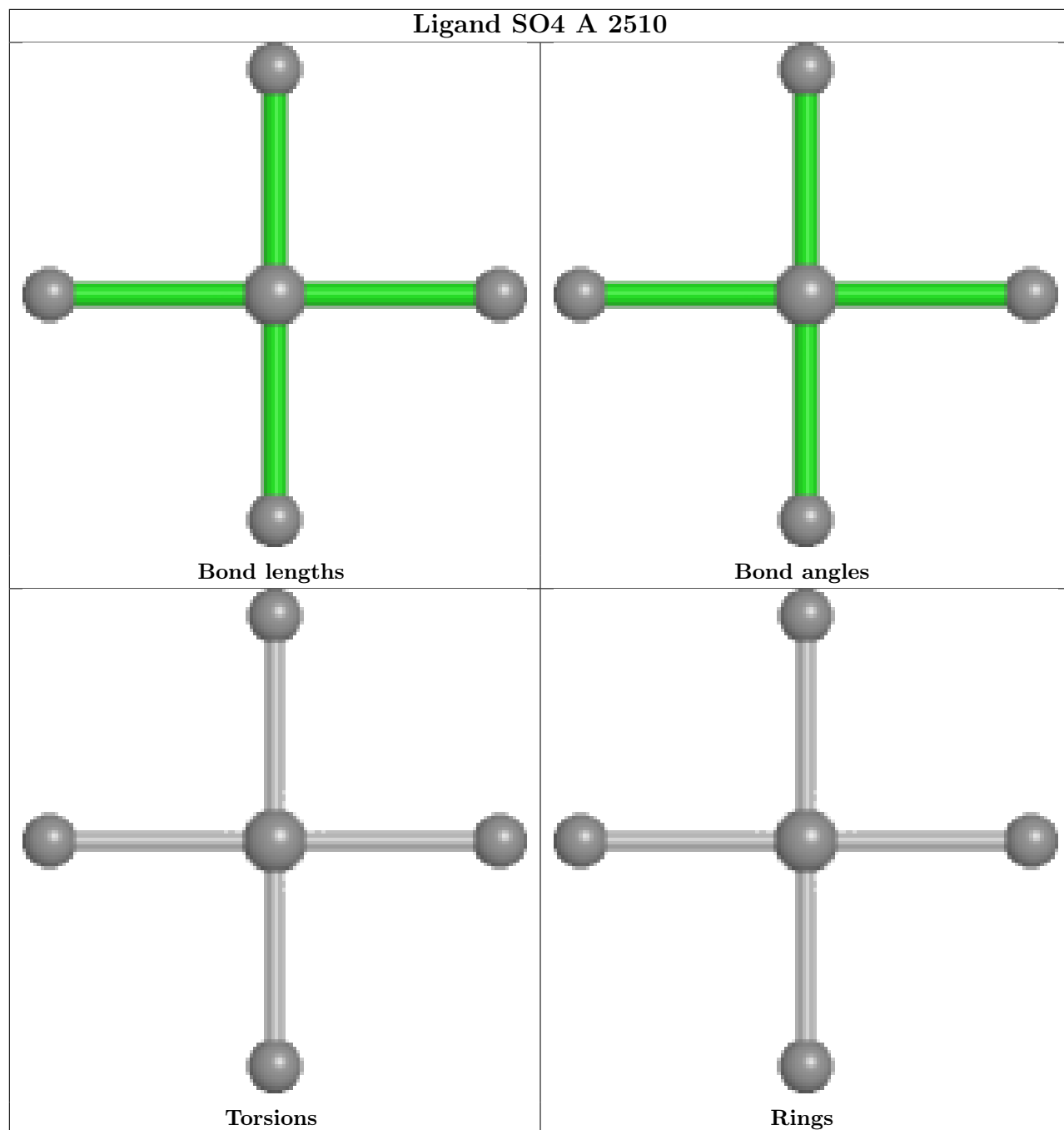


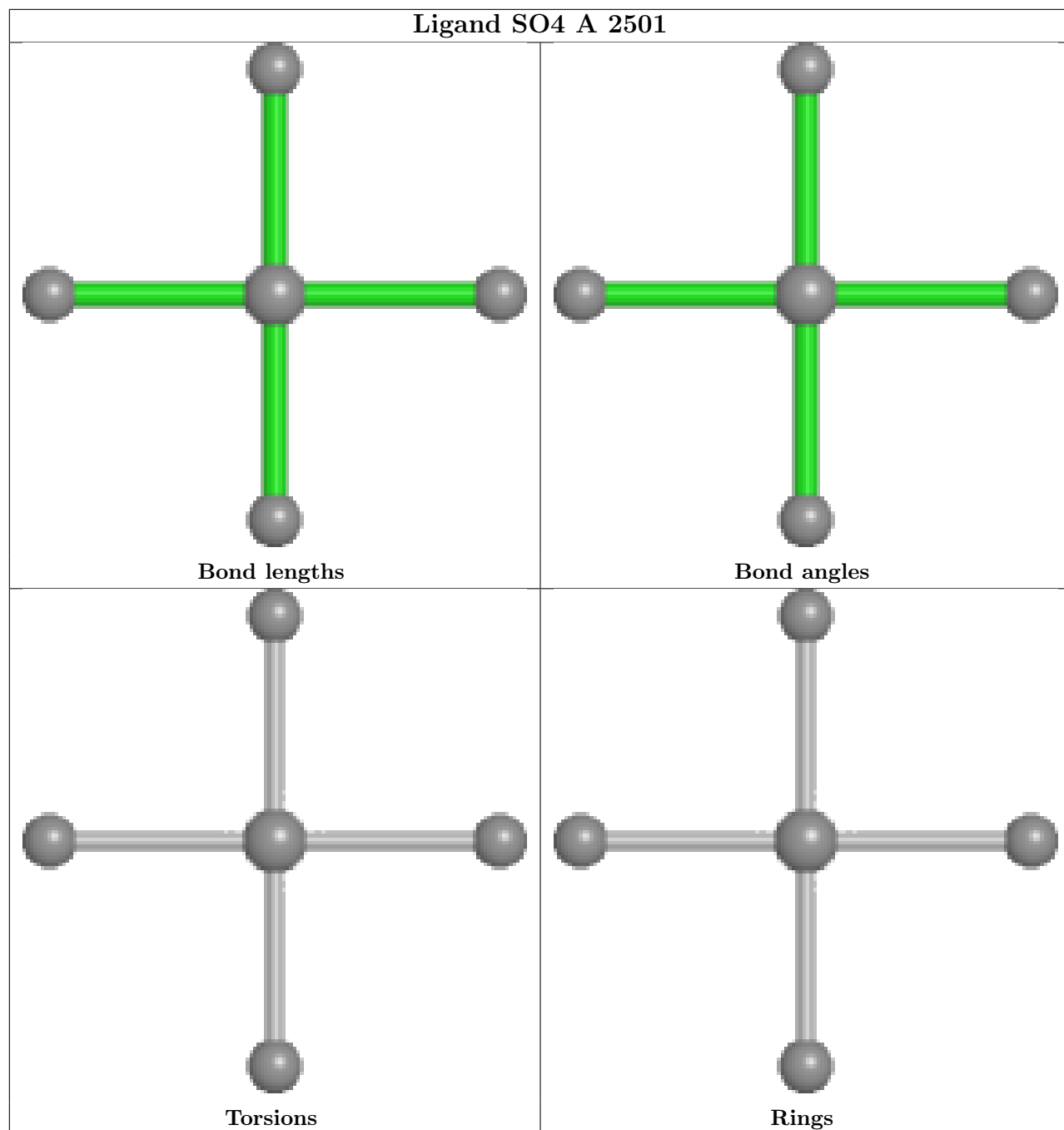


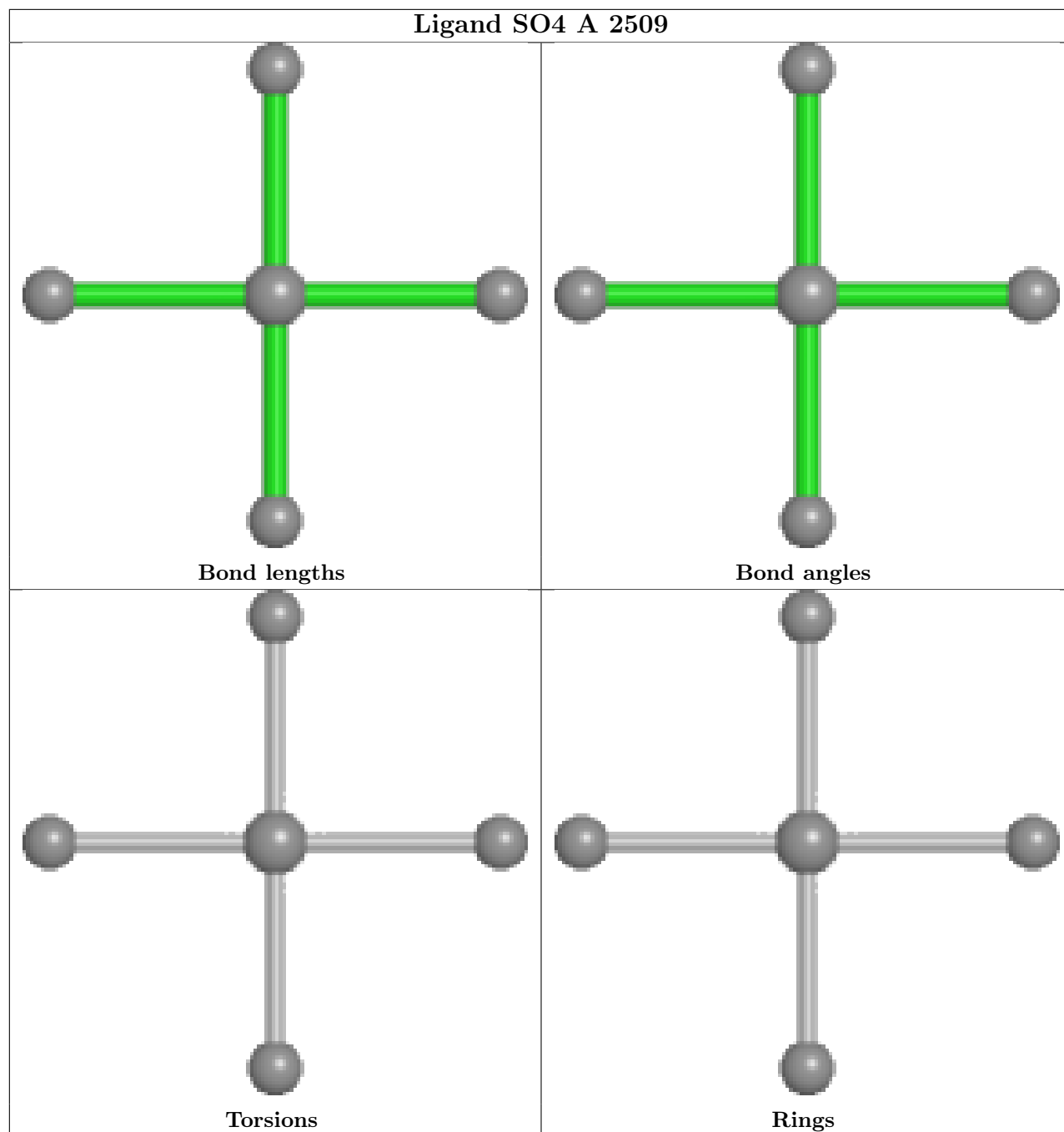












## 5.7 Other polymers [i](#)

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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	1620/1640 (98%)	0.12	1 (0%) 95 95	28, 48, 77, 125	3 (0%)
1	B	1612/1640 (98%)	0.14	3 (0%) 95 94	26, 52, 86, 148	10 (0%)
All	All	3232/3280 (98%)	0.13	4 (0%) 95 95	26, 50, 84, 148	13 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1878	ILE	3.0
1	A	1755	SER	2.5
1	B	1720	ASN	2.3
1	B	2368	THR	2.0

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	B	2504	5/5	0.79	0.19	90,96,113,119	0

*Continued on next page...*

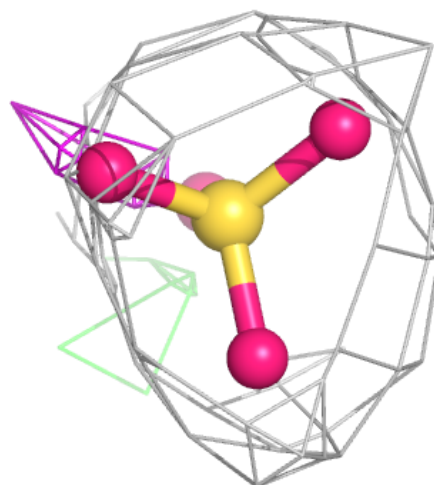
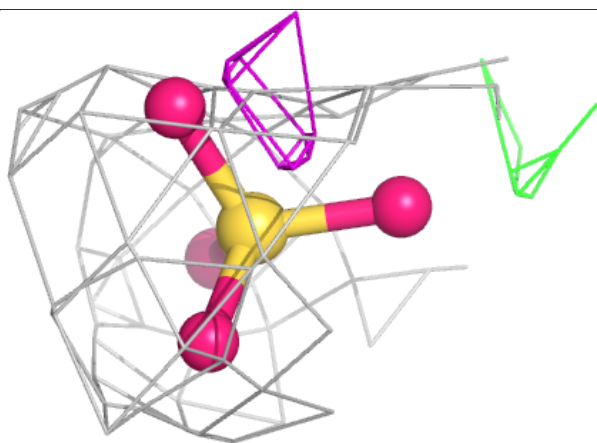
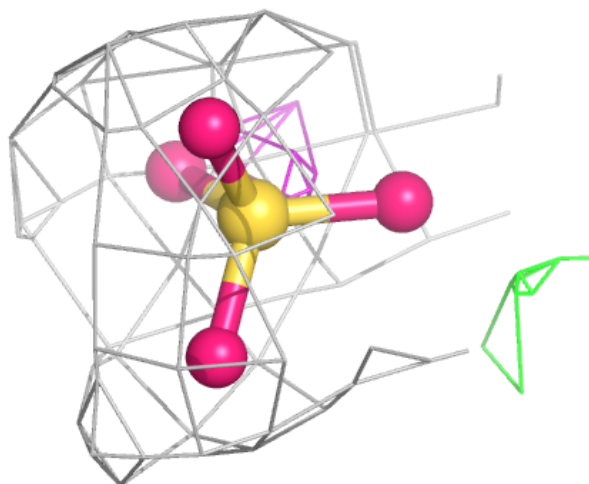
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	2519	5/5	0.81	0.23	94,95,104,118	0
2	SO4	B	2510	5/5	0.82	0.19	81,90,114,123	0
2	SO4	A	2506	5/5	0.82	0.22	91,94,98,115	0
2	SO4	B	2518	5/5	0.85	0.17	73,73,100,102	0
2	SO4	A	2507	5/5	0.85	0.13	87,88,101,119	0
2	SO4	A	2516	5/5	0.86	0.21	90,91,95,106	0
2	SO4	B	2517	5/5	0.87	0.16	81,91,103,117	0
2	SO4	A	2508	5/5	0.88	0.14	101,101,116,126	0
2	SO4	B	2501	5/5	0.89	0.18	78,85,90,100	0
2	SO4	A	2501	5/5	0.89	0.13	80,87,98,111	0
2	SO4	B	2520	5/5	0.90	0.18	62,65,78,83	0
2	SO4	B	2503	5/5	0.90	0.18	77,79,95,104	0
2	SO4	A	2511	5/5	0.91	0.18	61,82,98,99	0
2	SO4	A	2513	5/5	0.91	0.16	63,77,96,98	0
2	SO4	B	2512	5/5	0.91	0.16	75,76,88,102	0
2	SO4	B	2507	5/5	0.92	0.14	77,81,90,102	0
2	SO4	B	2515	5/5	0.92	0.14	75,76,86,95	0
2	SO4	B	2508	5/5	0.92	0.25	83,93,102,106	0
2	SO4	A	2505	5/5	0.92	0.23	59,70,94,94	0
2	SO4	B	2502	5/5	0.92	0.16	81,91,96,103	0
2	SO4	A	2514	5/5	0.93	0.22	91,97,102,108	0
2	SO4	A	2504	5/5	0.93	0.17	70,70,96,100	0
2	SO4	B	2514	5/5	0.94	0.22	101,108,114,117	0
2	SO4	A	2510	5/5	0.94	0.17	66,67,74,81	0
2	SO4	A	2502	5/5	0.94	0.12	78,81,88,95	0
2	SO4	B	2505	5/5	0.95	0.14	79,88,92,102	0
2	SO4	B	2511	5/5	0.95	0.20	61,61,71,78	0
2	SO4	A	2515	5/5	0.95	0.25	77,82,93,97	0
2	SO4	B	2509	5/5	0.95	0.13	84,90,103,108	0
2	SO4	A	2509	5/5	0.96	0.18	57,64,79,89	0
2	SO4	A	2503	5/5	0.96	0.14	72,74,88,90	0
2	SO4	B	2516	5/5	0.96	0.18	74,76,80,89	0
2	SO4	A	2512	5/5	0.96	0.13	65,67,80,90	0
2	SO4	B	2506	5/5	0.97	0.20	84,84,95,100	0
2	SO4	B	2513	5/5	0.98	0.12	60,66,71,84	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.

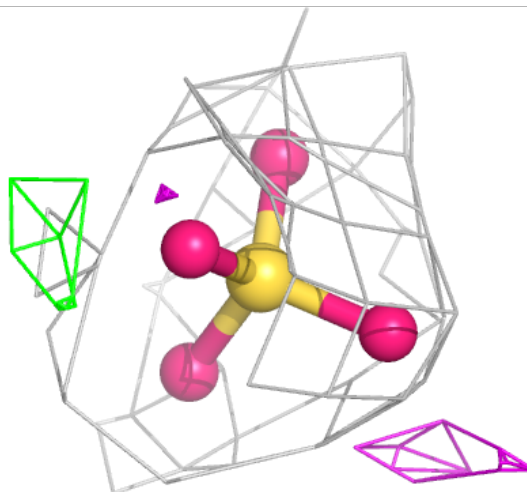
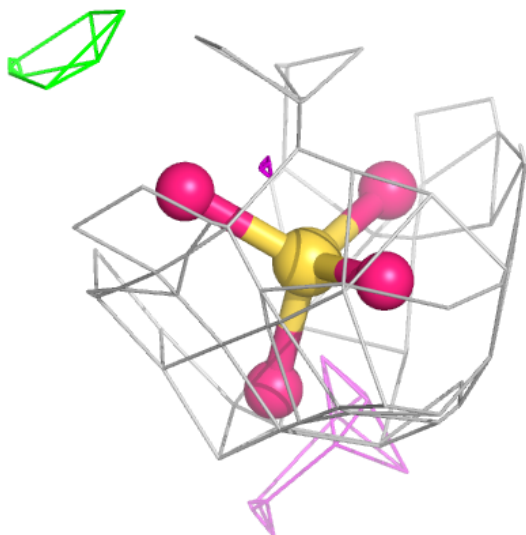
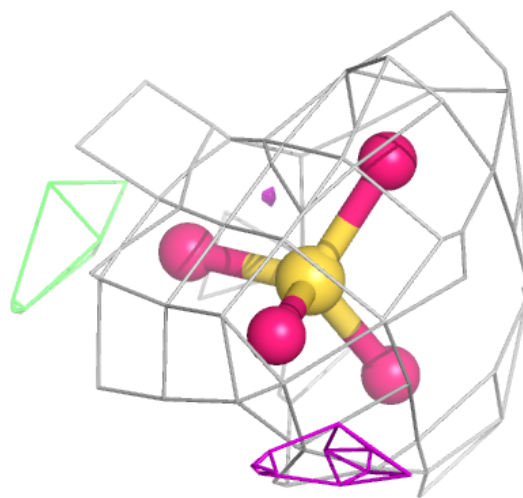
**Electron density around SO4 B 2504:**

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



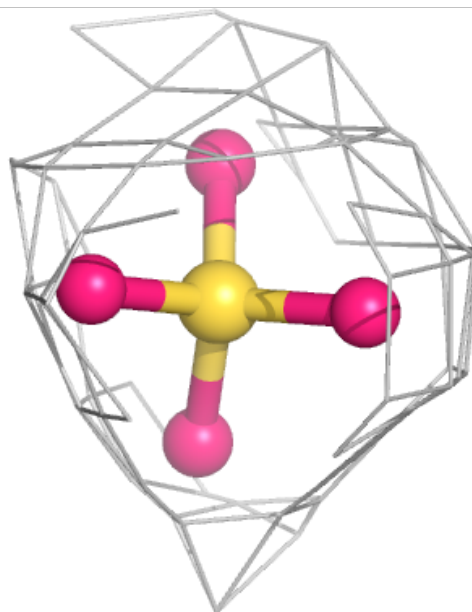
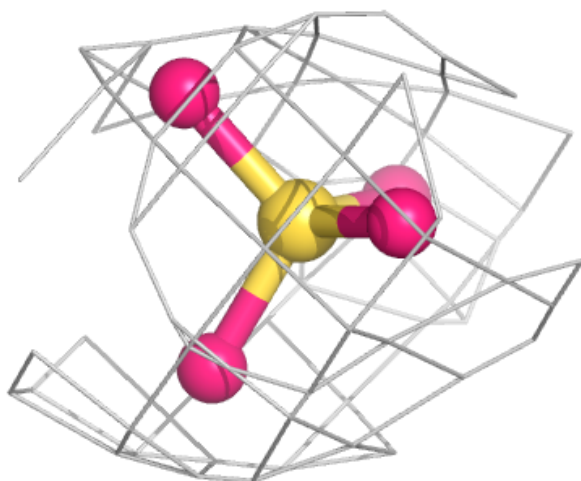
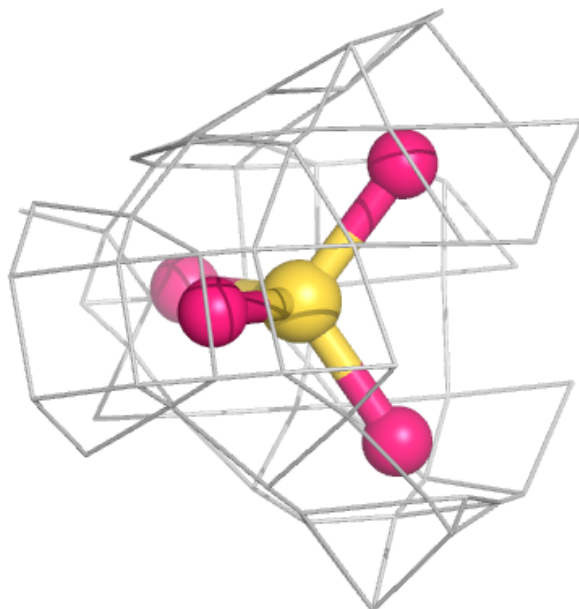
**Electron density around SO4 B 2519:**

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



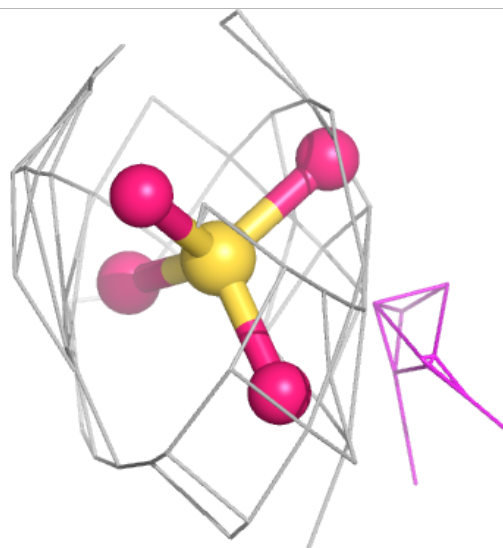
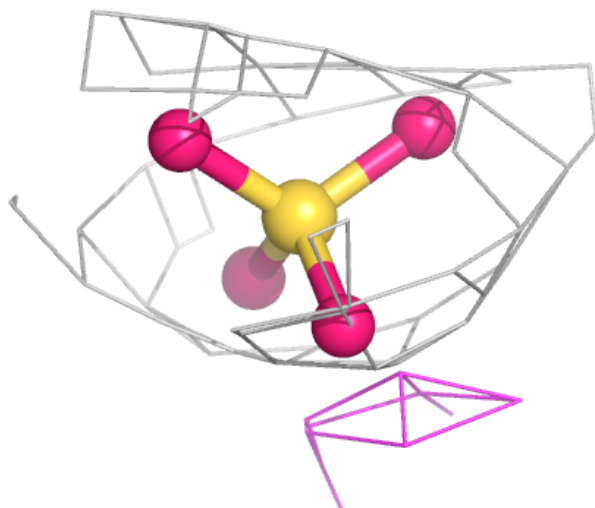
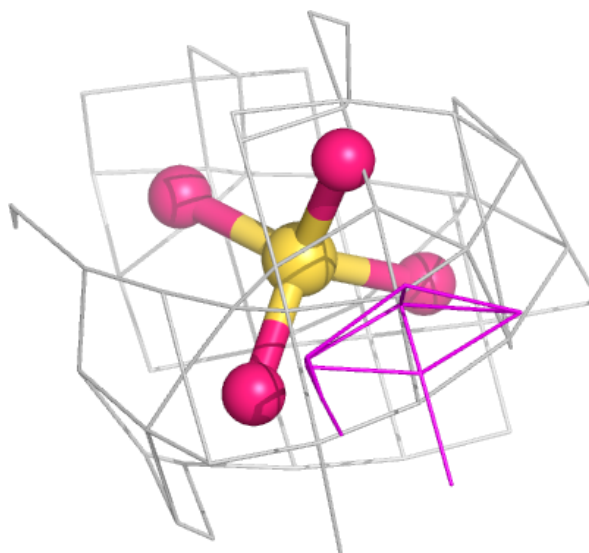
**Electron density around SO4 B 2510:**

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and green (positive)



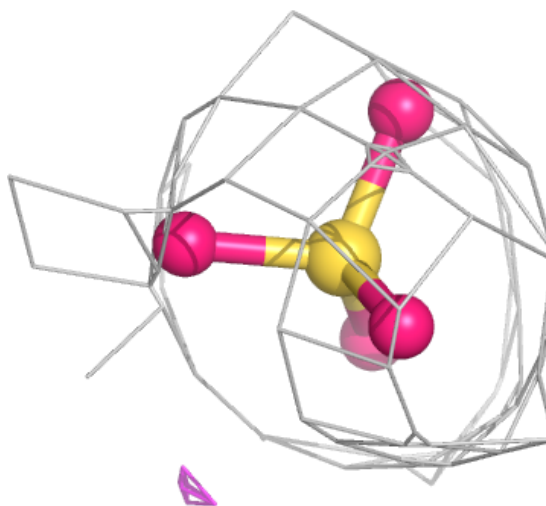
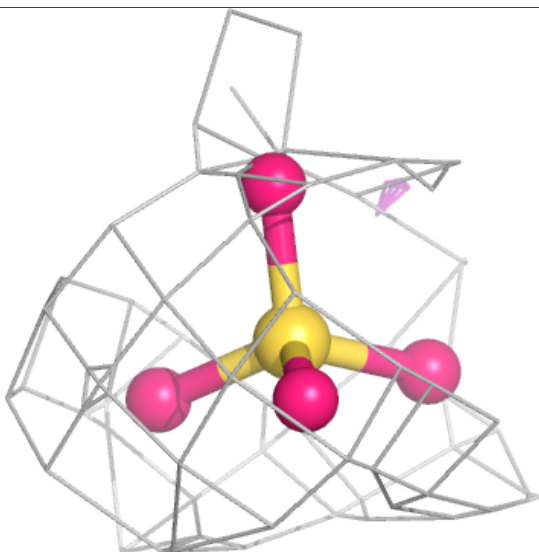
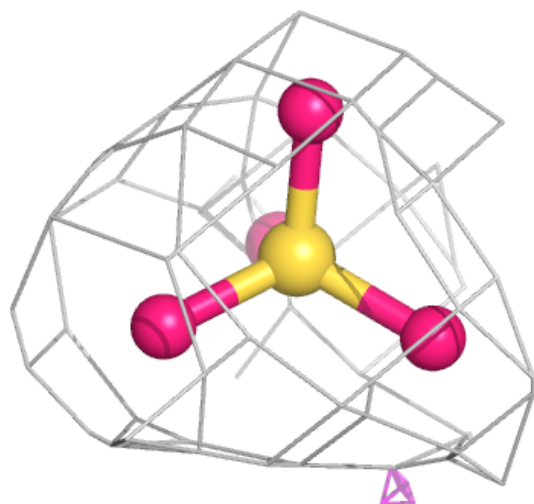
**Electron density around SO4 A 2506:**

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



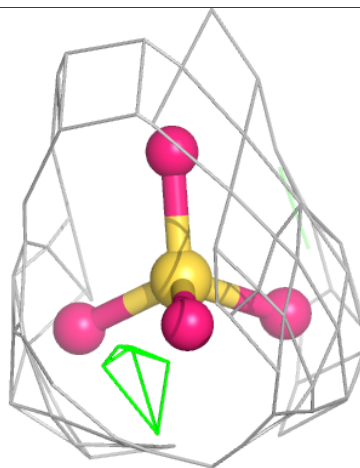
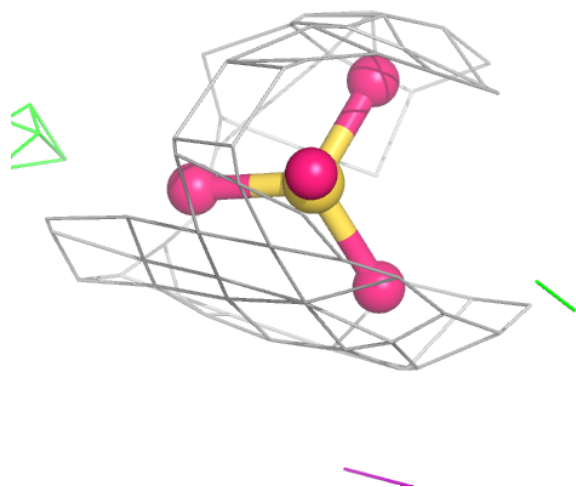
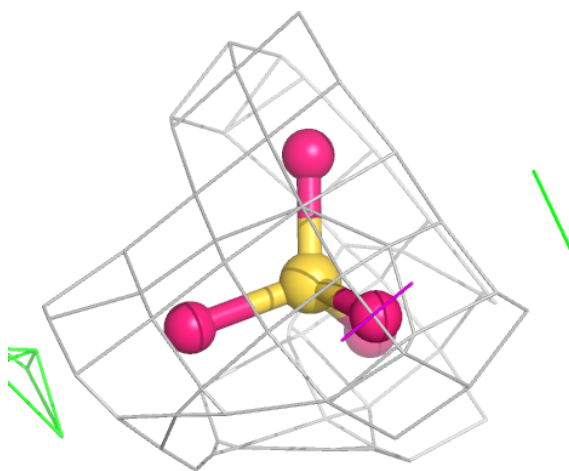
**Electron density around SO4 B 2518:**

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



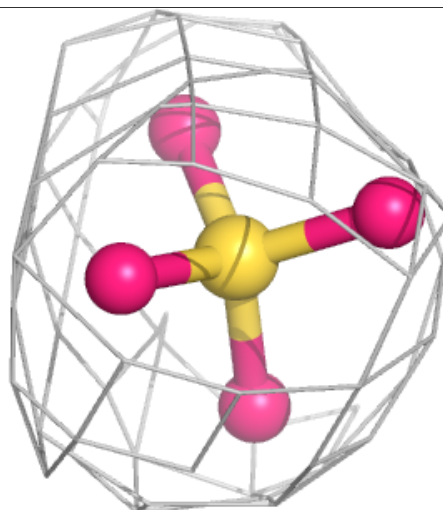
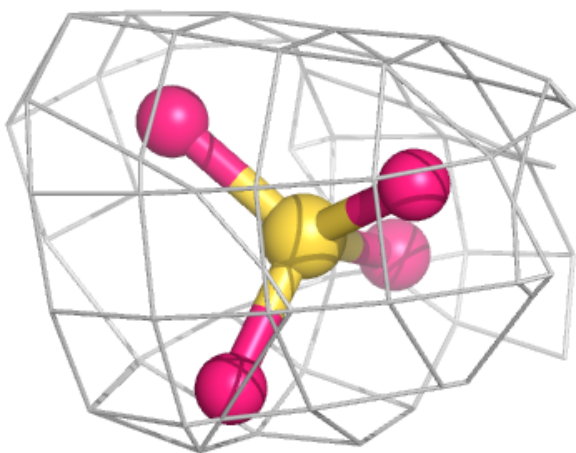
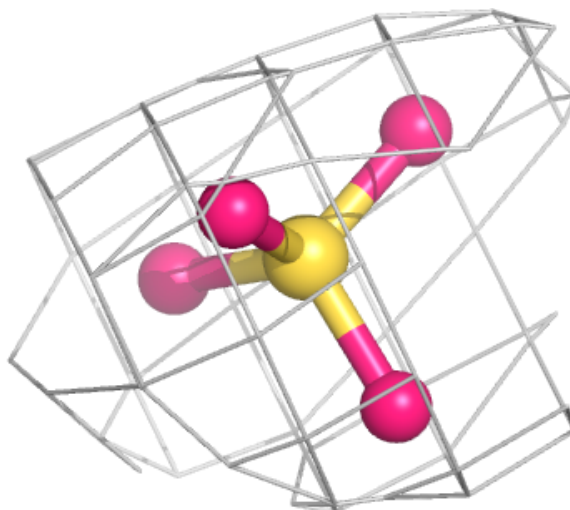
**Electron density around SO4 A 2507:**

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and green (positive)



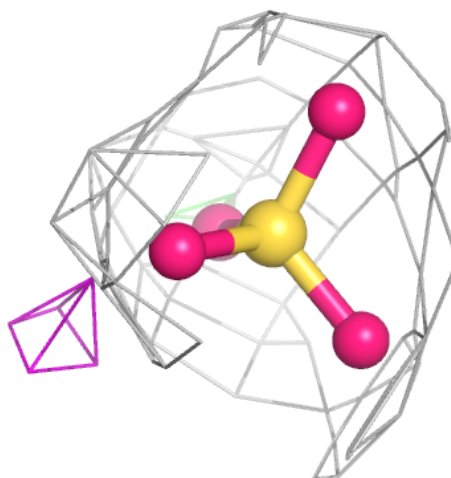
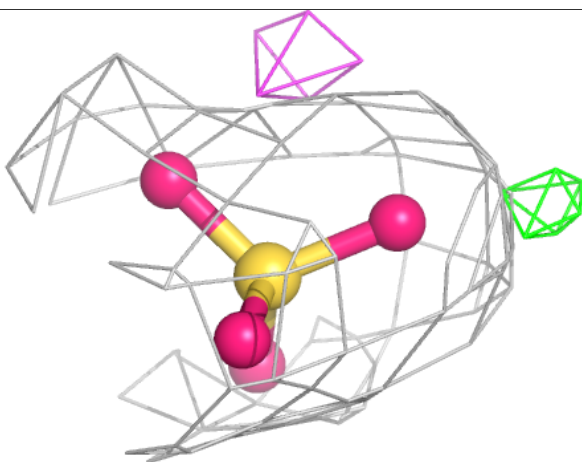
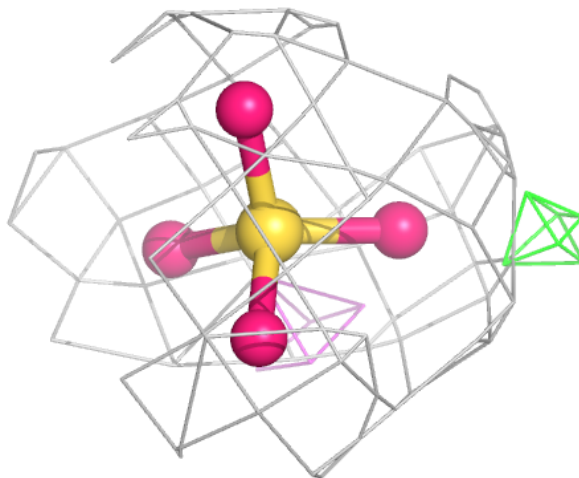
**Electron density around SO4 A 2516:**

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and green (positive)



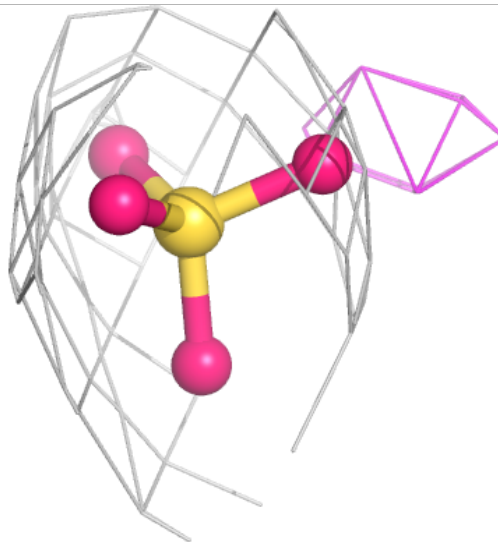
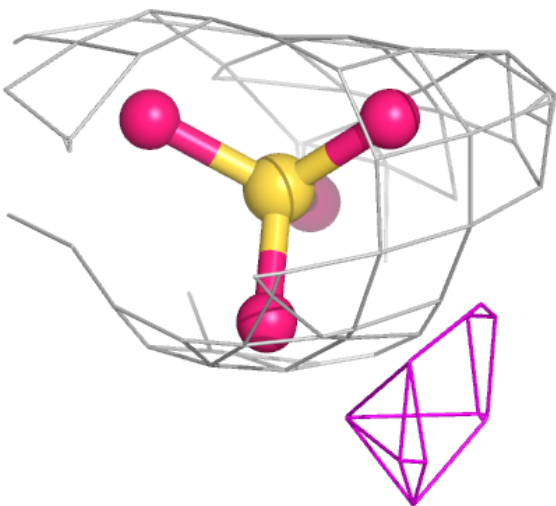
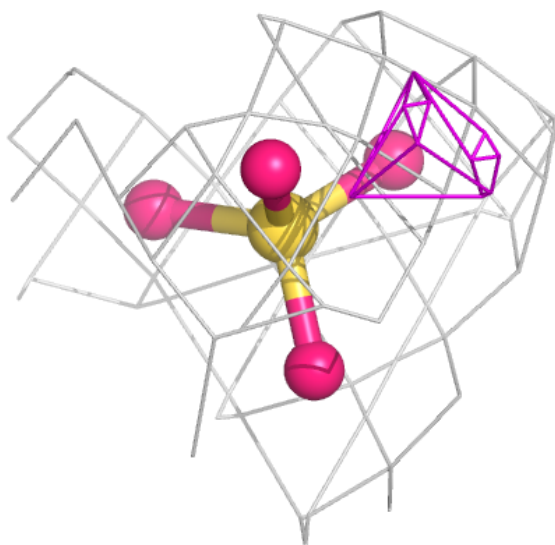
**Electron density around SO4 B 2517:**

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and green (positive)



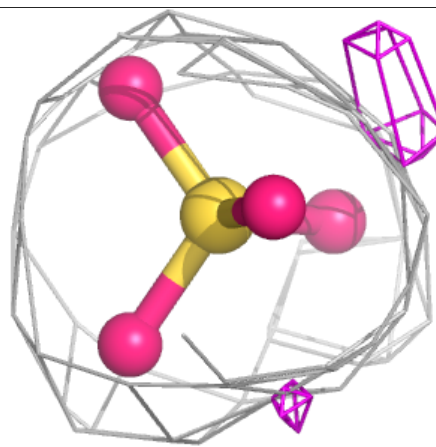
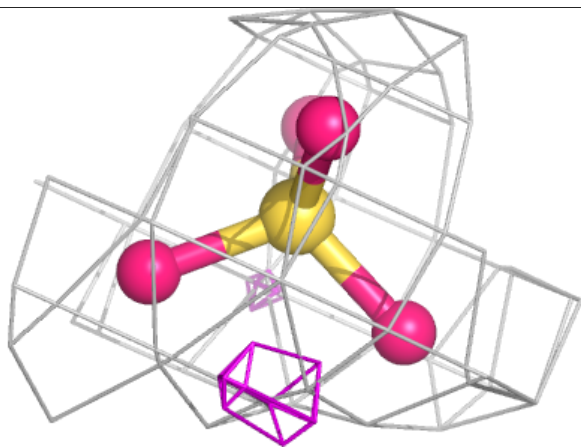
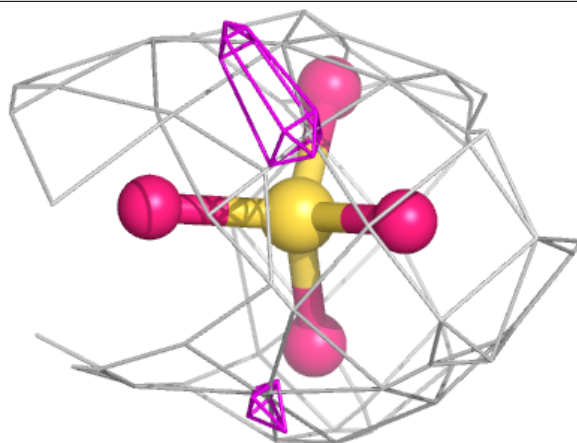
**Electron density around SO4 A 2508:**

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and green (positive)



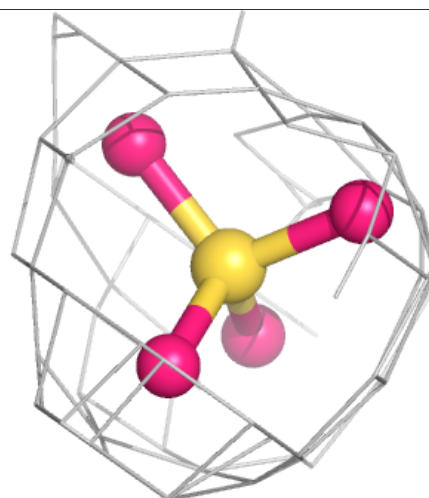
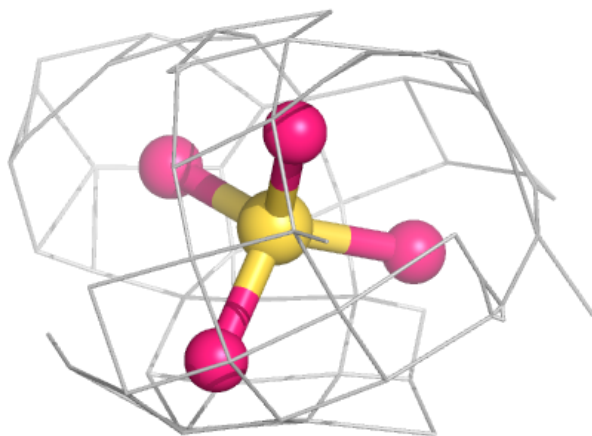
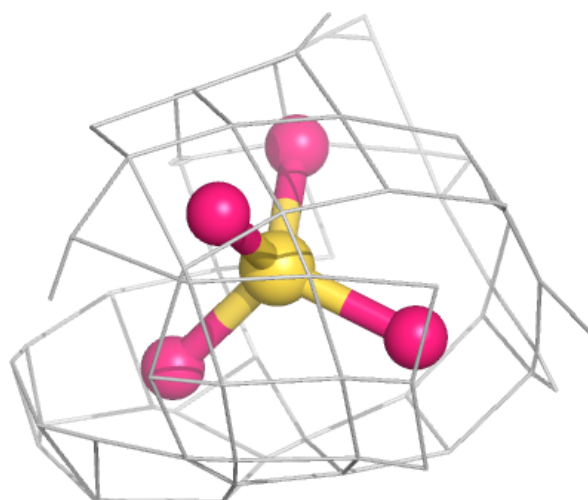
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and green (positive)



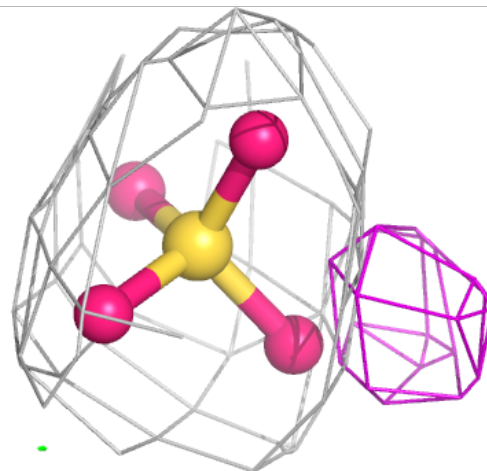
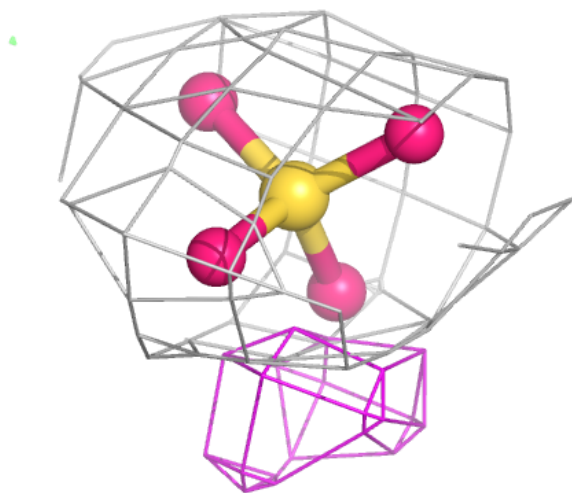
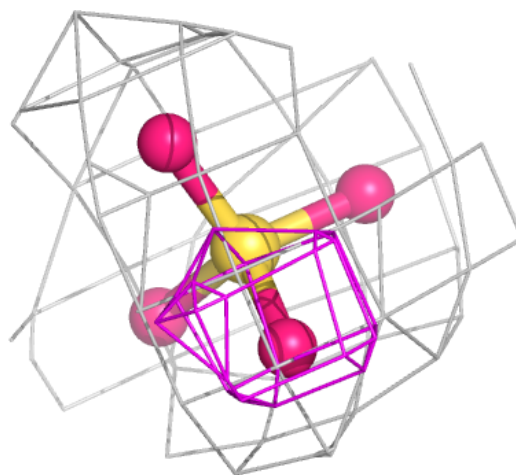
**Electron density around SO4 A 2501:**

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and green (positive)



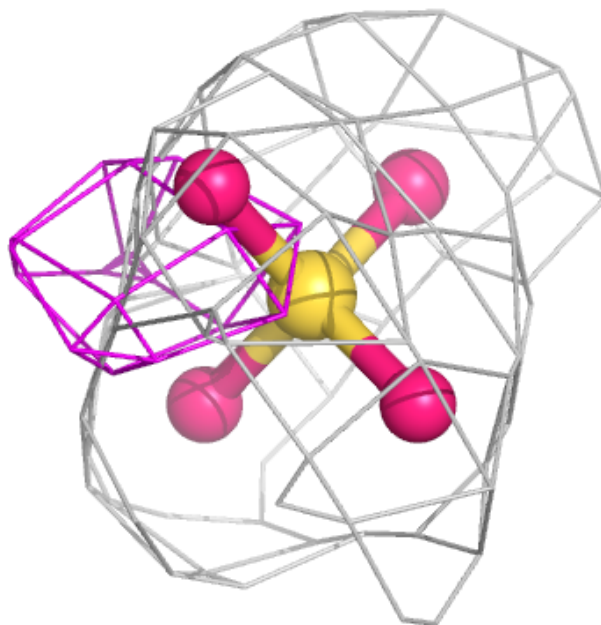
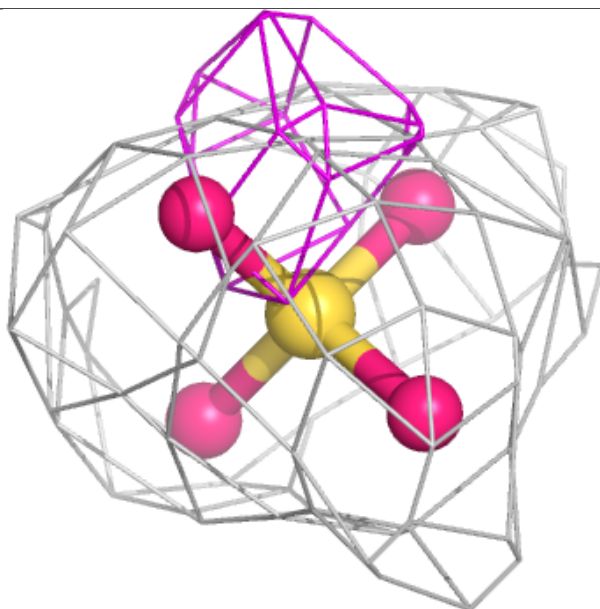
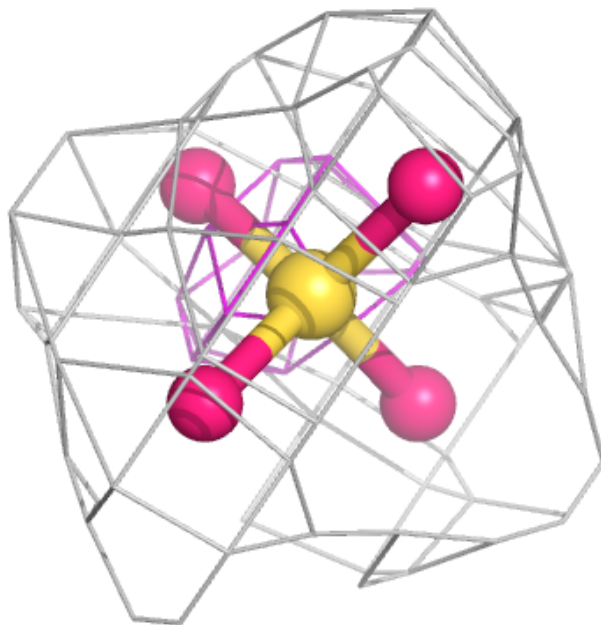
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and green (positive)



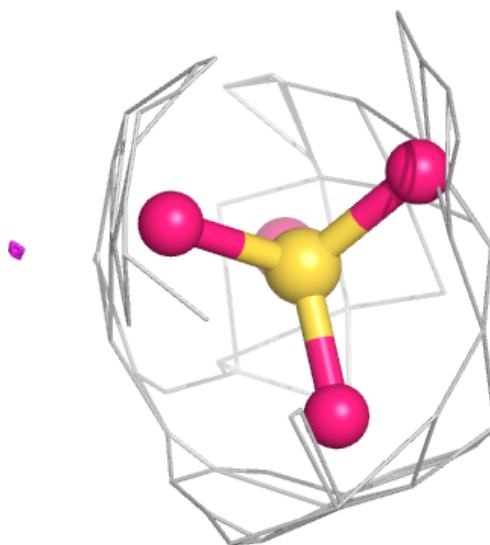
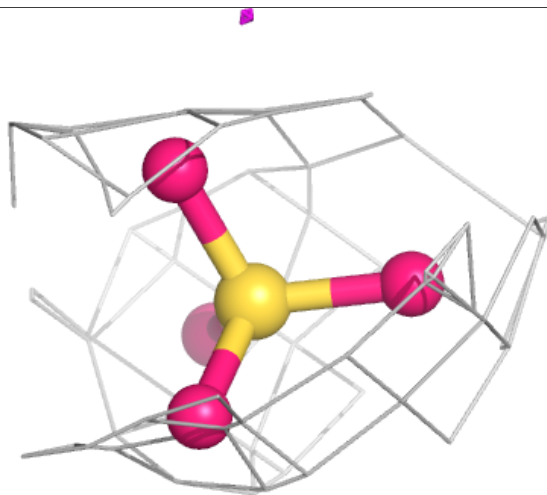
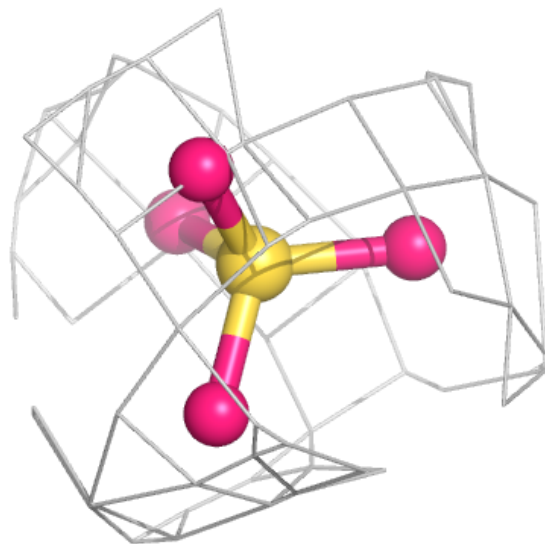
**Electron density around SO4 B 2503:**

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and green (positive)



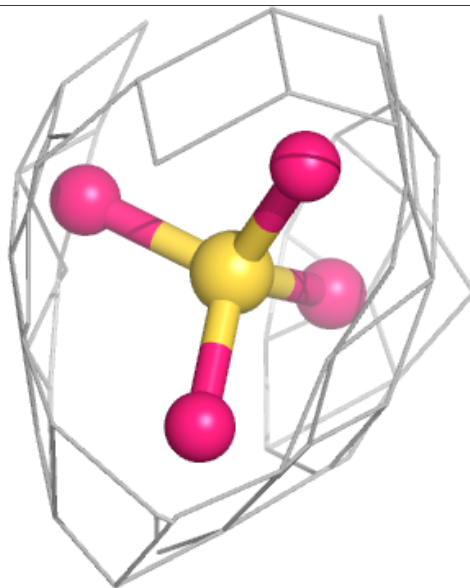
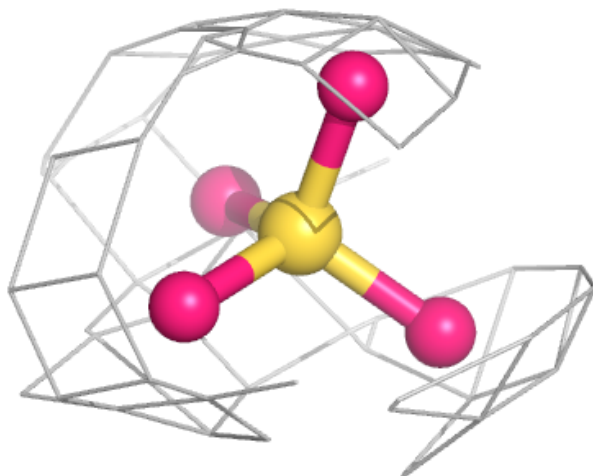
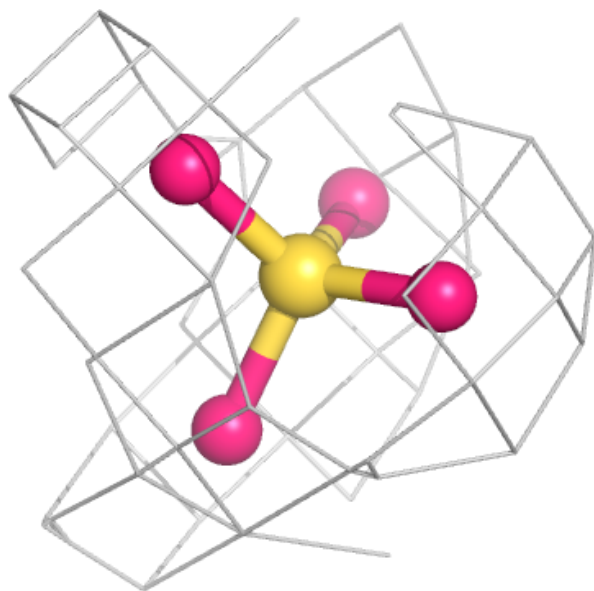
**Electron density around SO4 A 2511:**

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and green (positive)



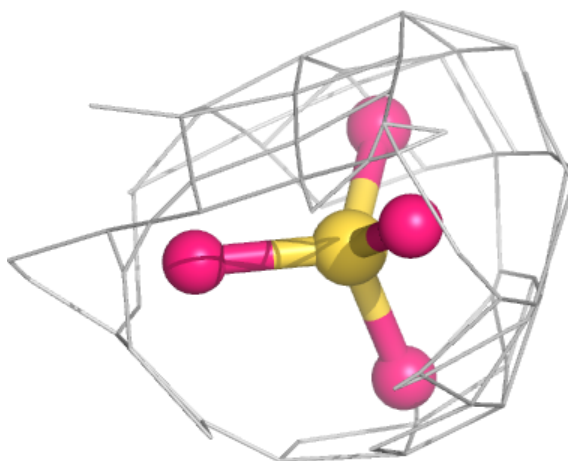
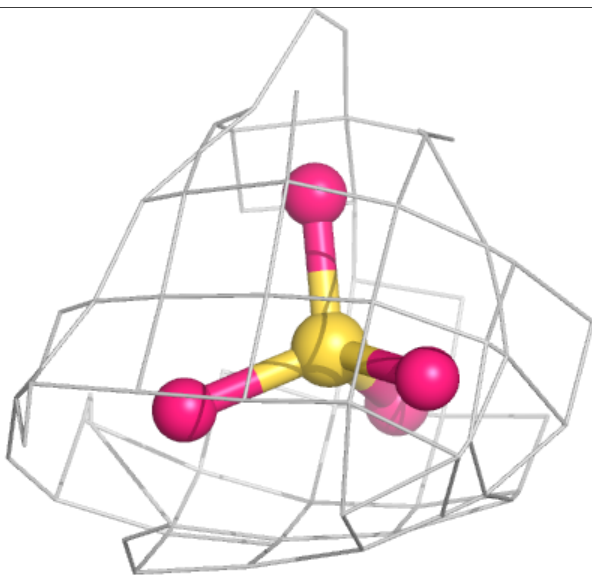
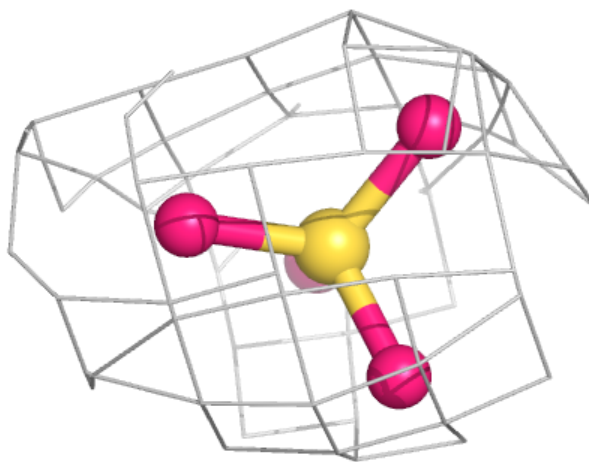
**Electron density around SO4 A 2513:**

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and green (positive)



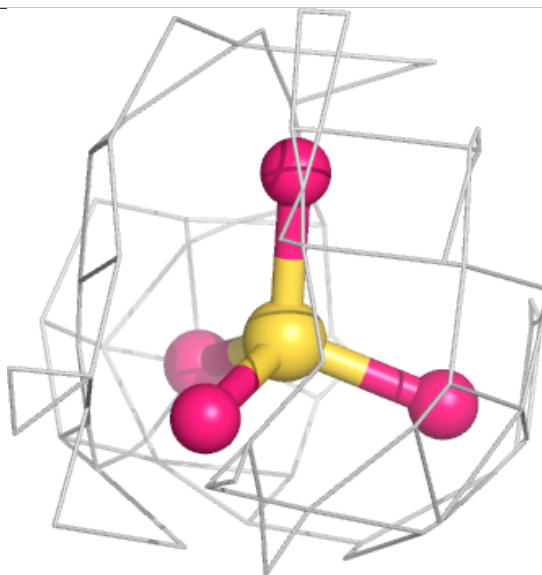
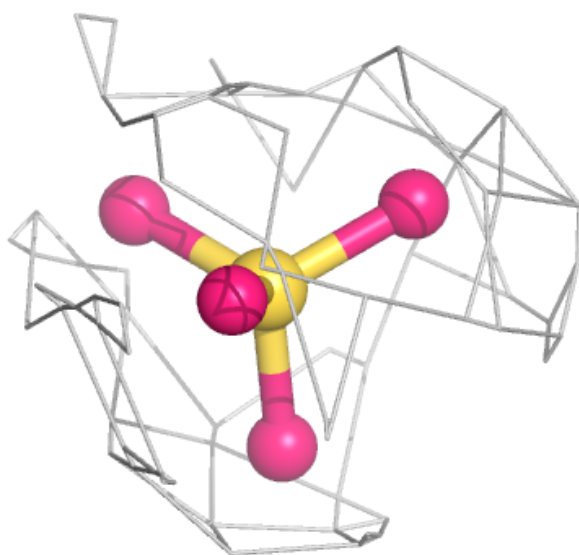
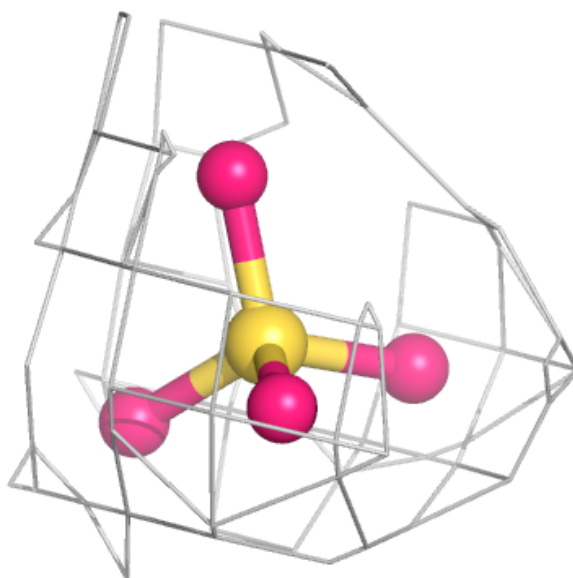
**Electron density around SO4 B 2512:**

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and green (positive)



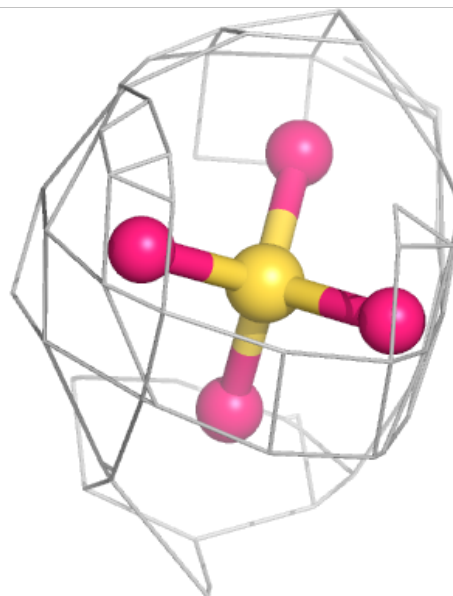
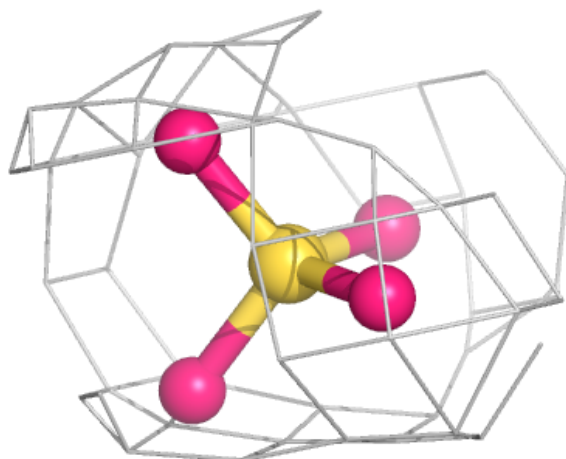
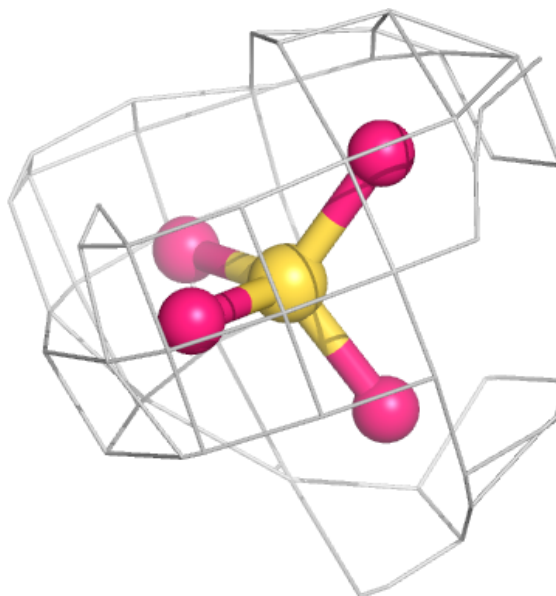
**Electron density around SO4 B 2507:**

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



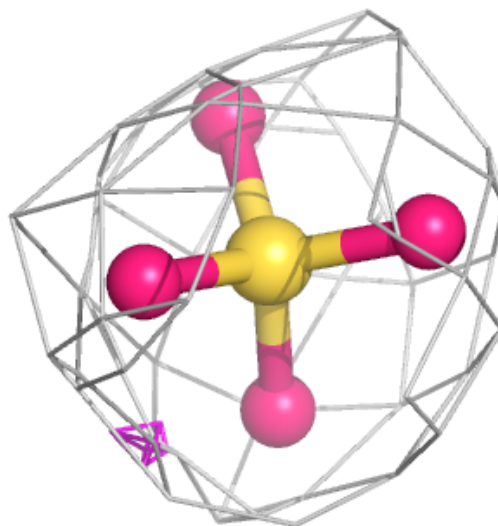
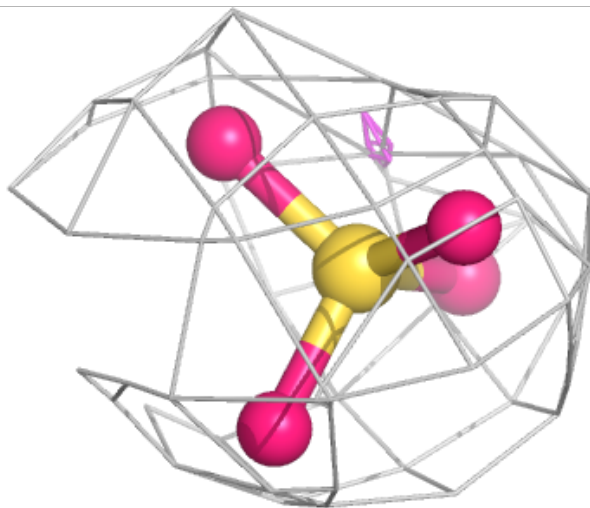
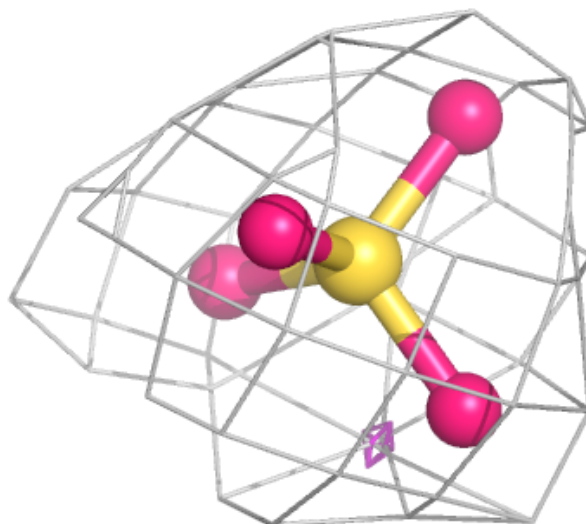
**Electron density around SO4 B 2515:**

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



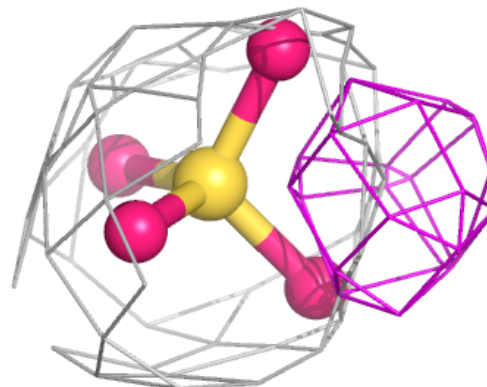
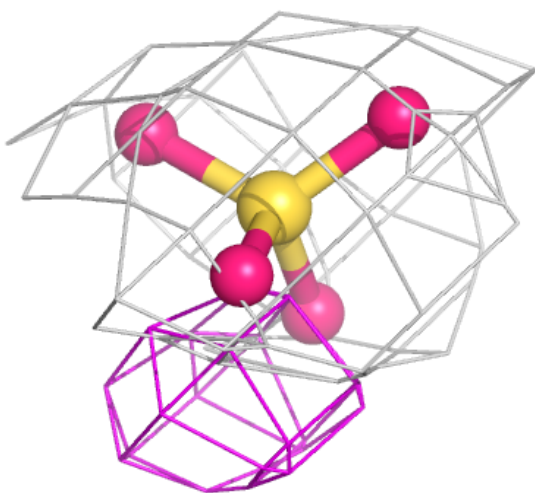
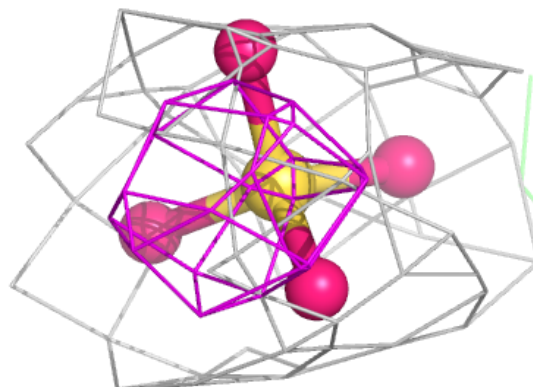
**Electron density around SO4 B 2508:**

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



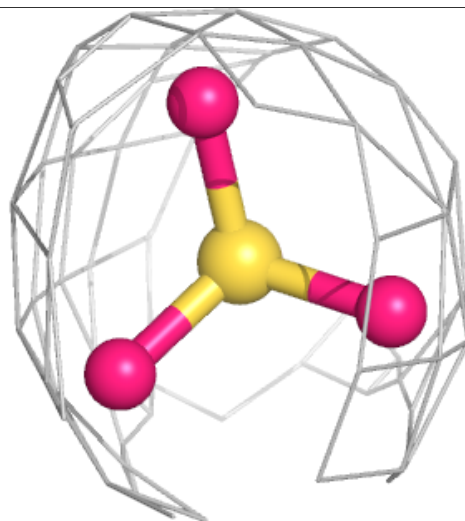
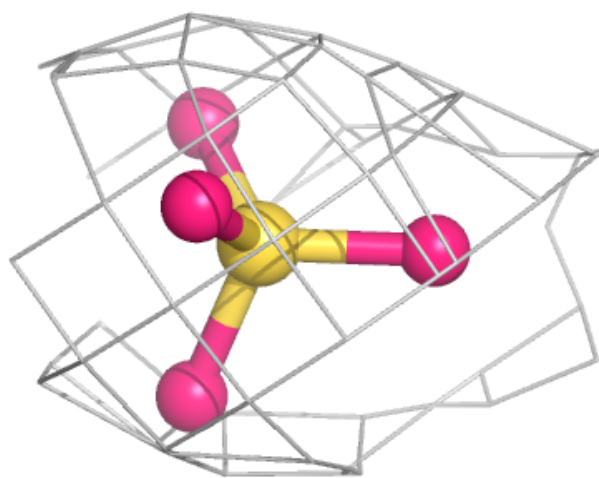
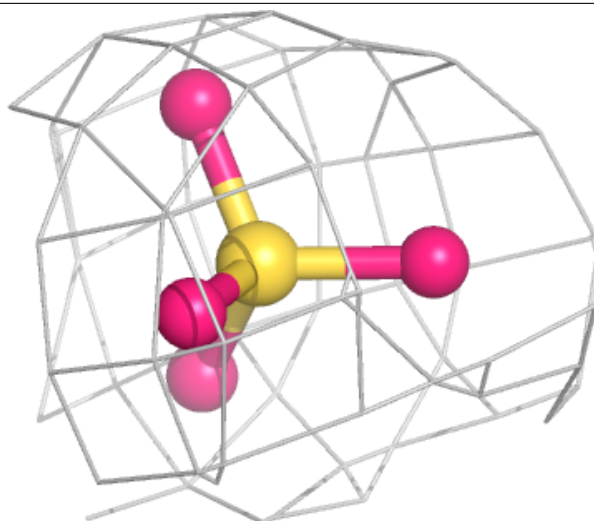
**Electron density around SO4 A 2505:**

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



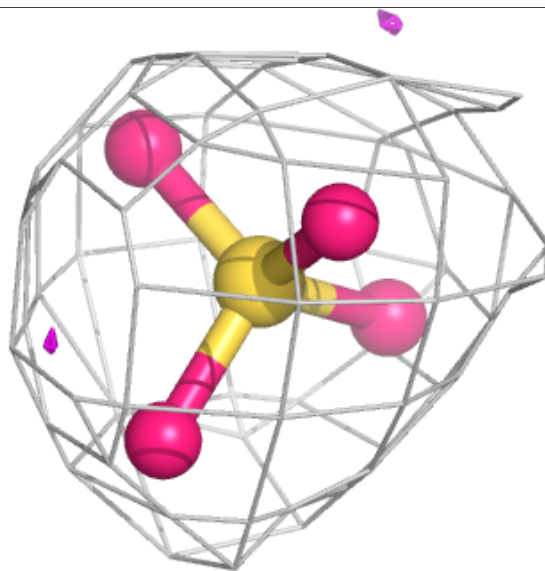
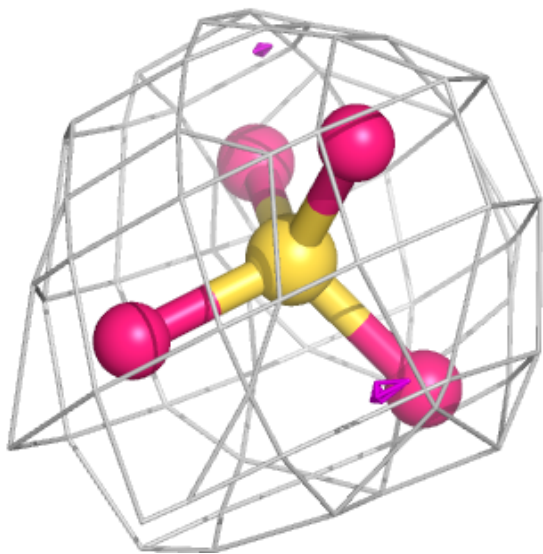
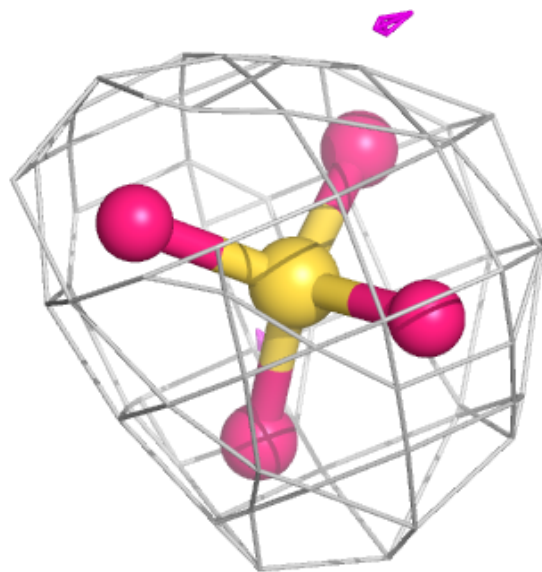
**Electron density around SO4 B 2502:**

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



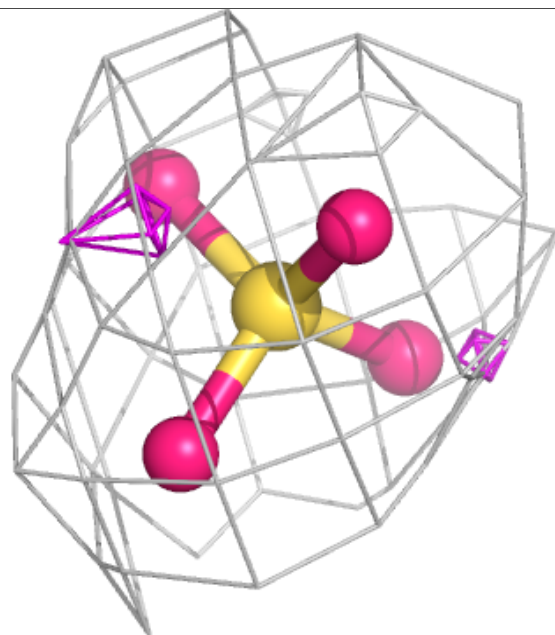
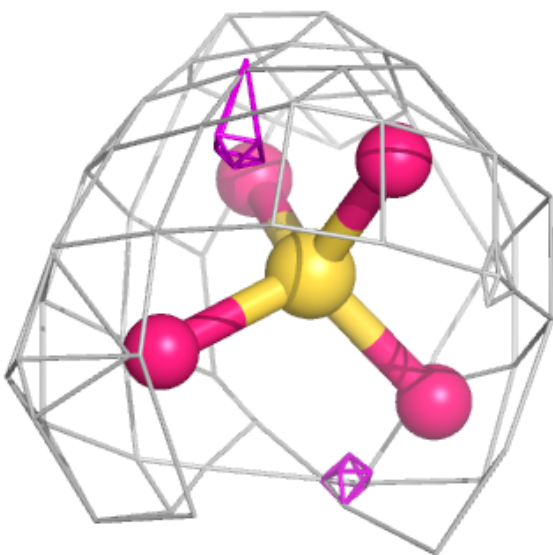
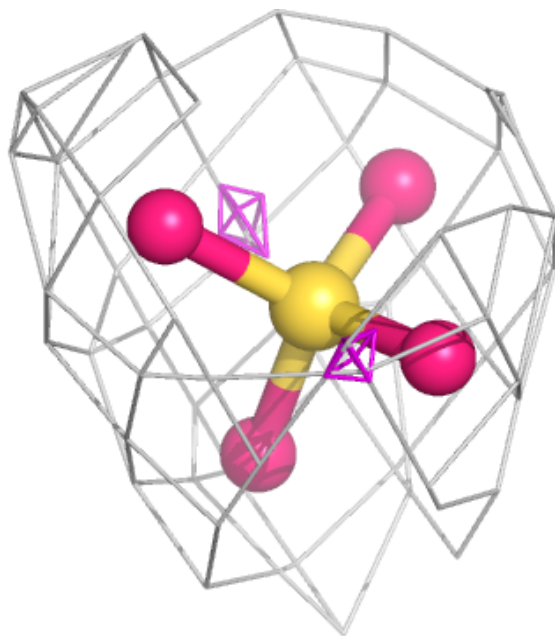
**Electron density around SO4 A 2514:**

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



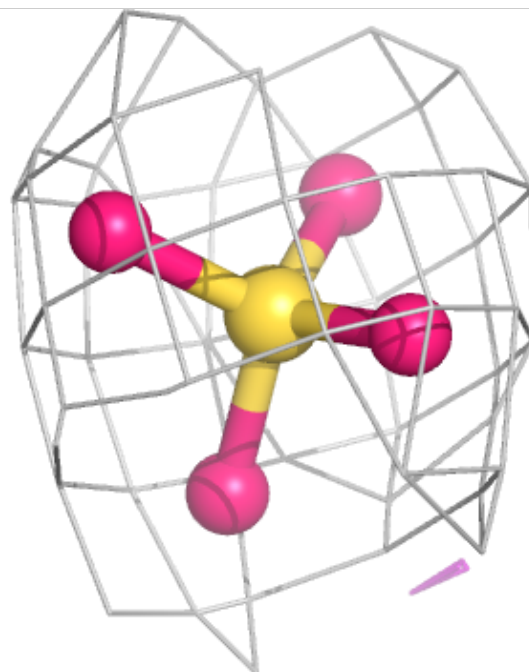
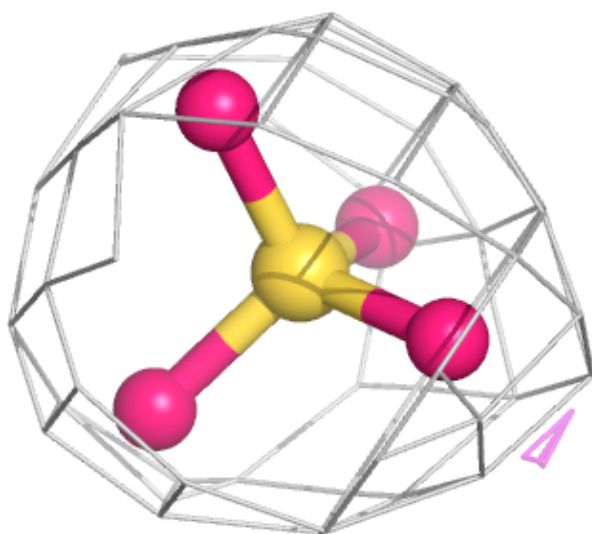
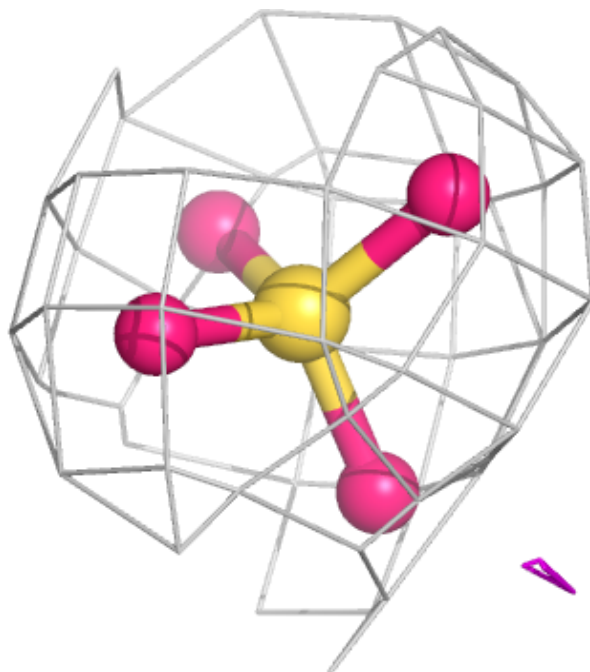
**Electron density around SO4 A 2504:**

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



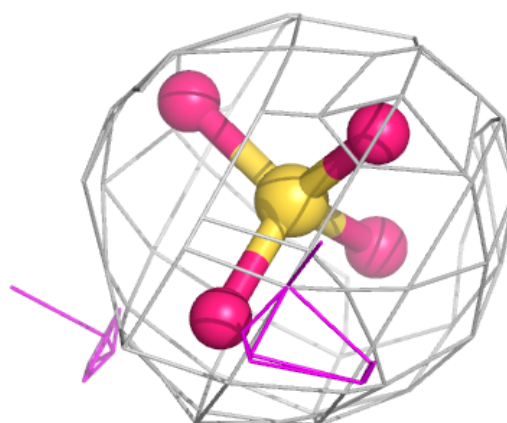
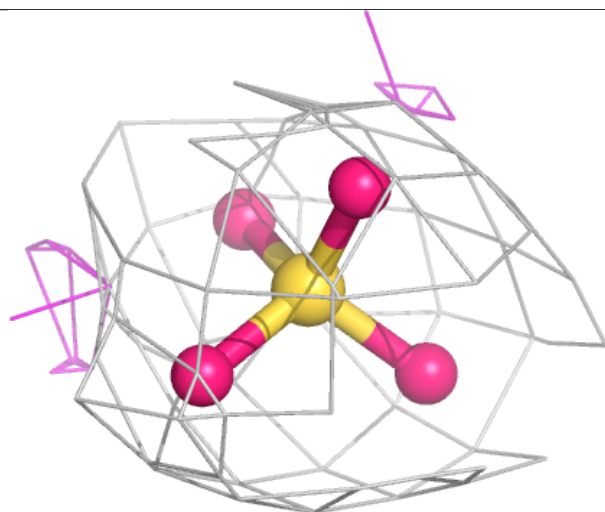
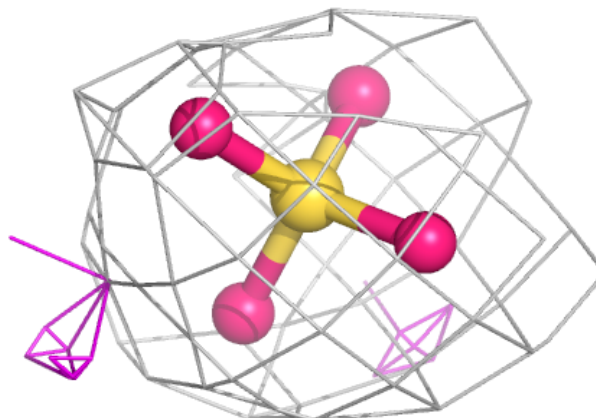
**Electron density around SO4 B 2514:**

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



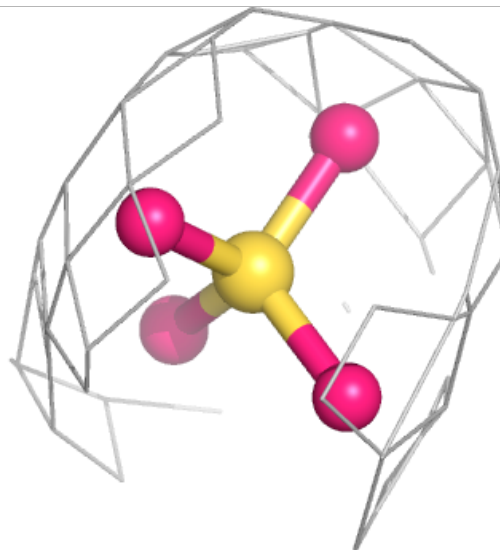
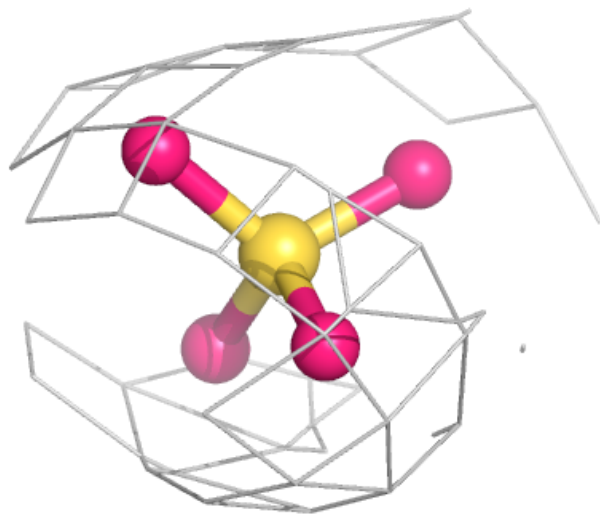
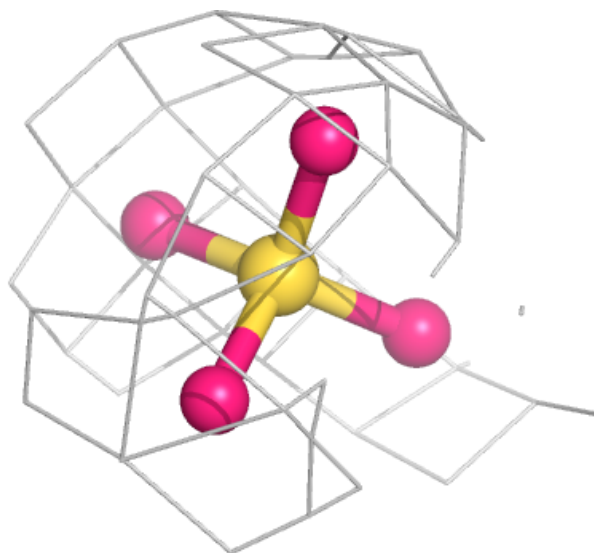
**Electron density around SO4 A 2510:**

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



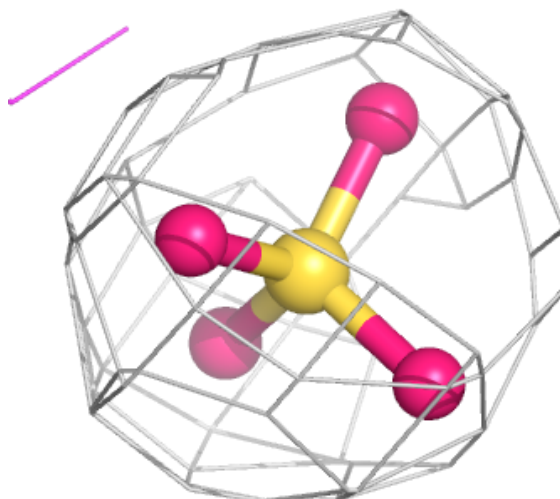
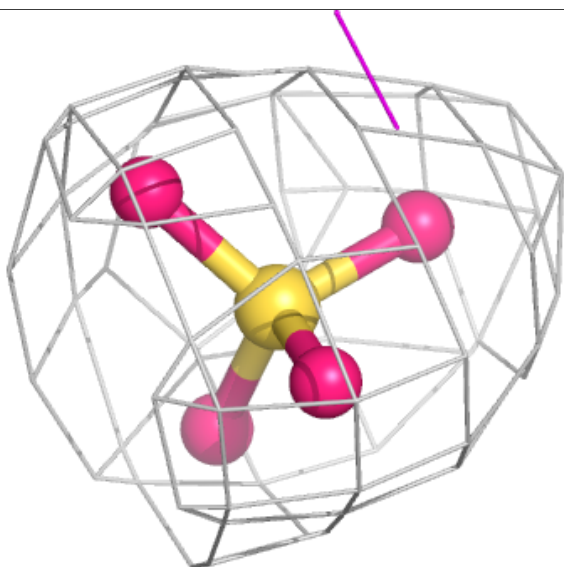
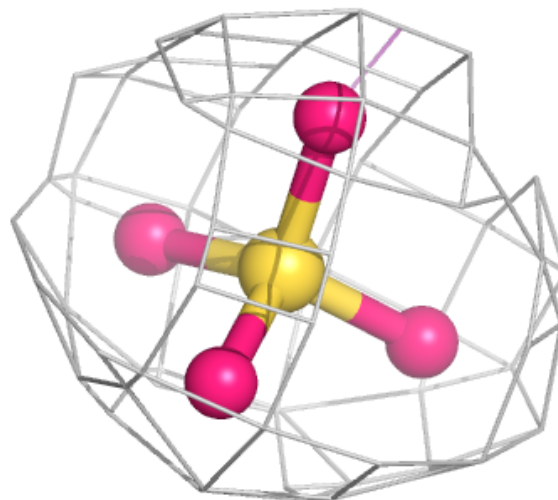
**Electron density around SO4 A 2502:**

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



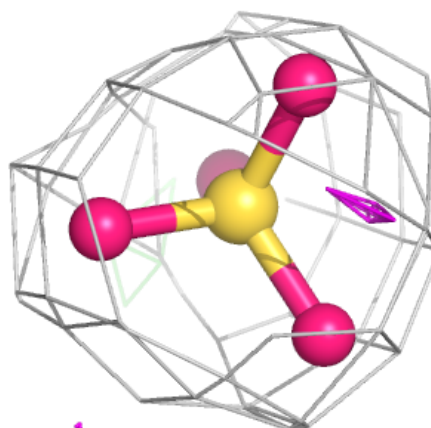
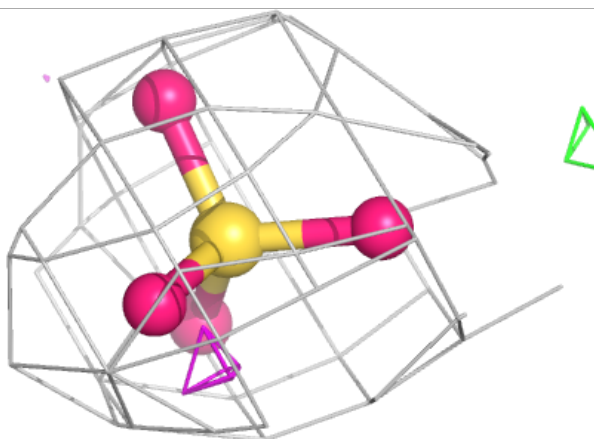
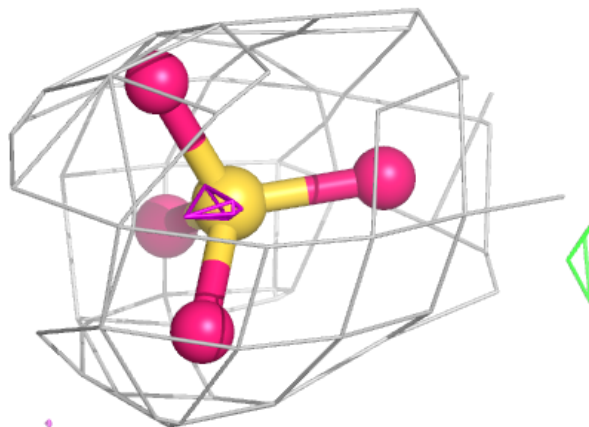
**Electron density around SO4 B 2505:**

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



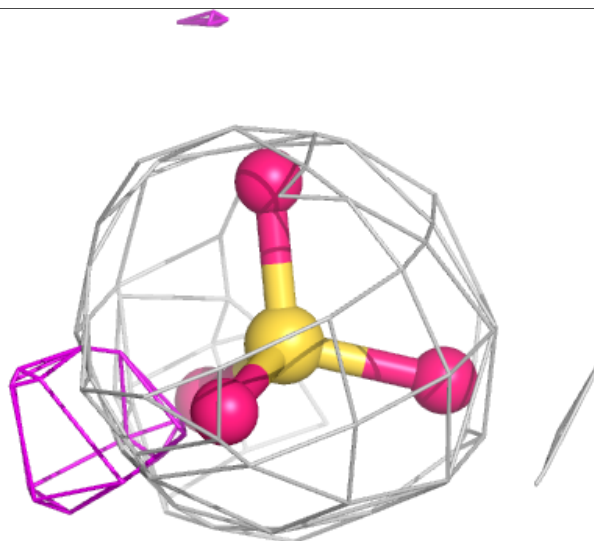
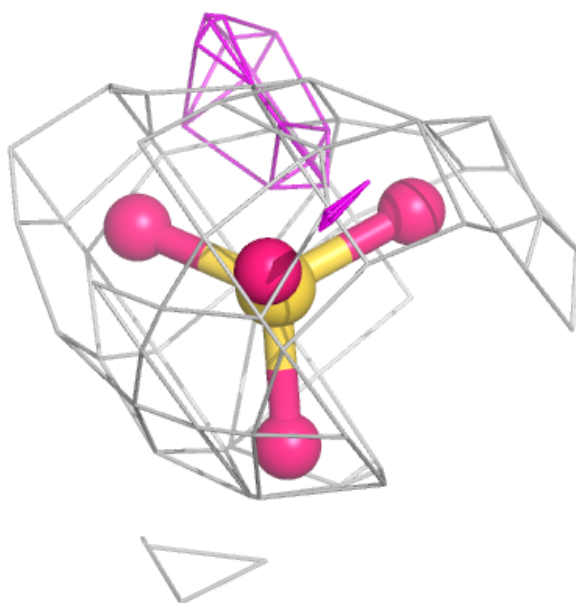
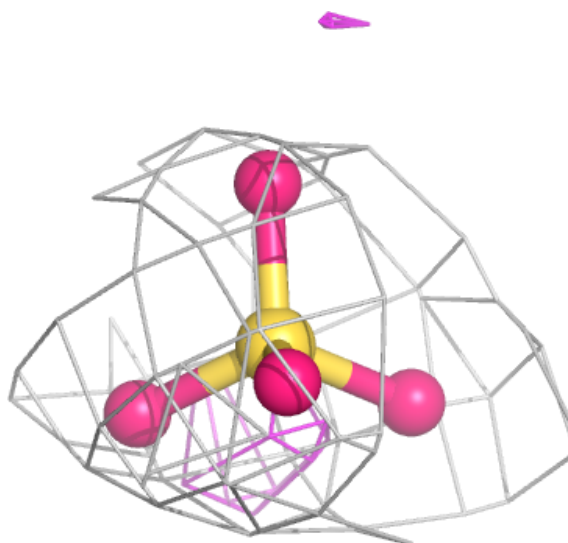
**Electron density around SO4 B 2511:**

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



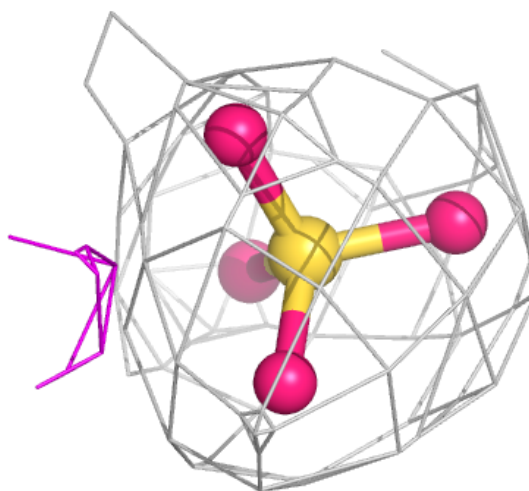
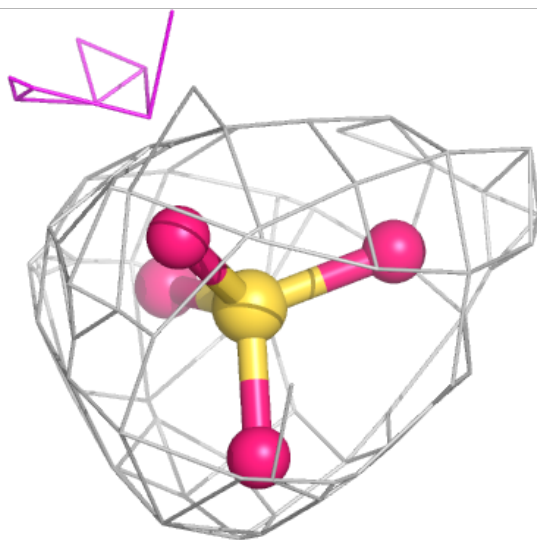
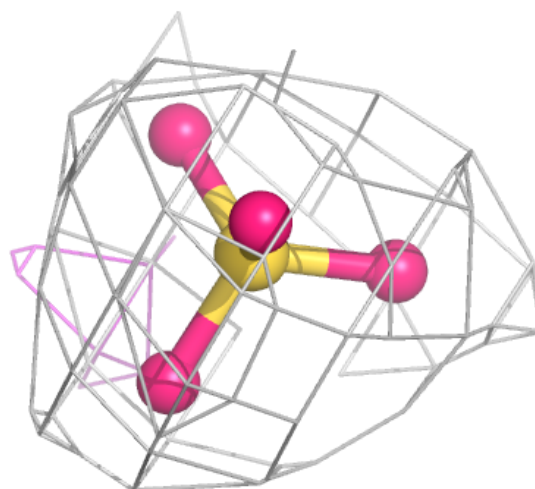
**Electron density around SO4 A 2515:**

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



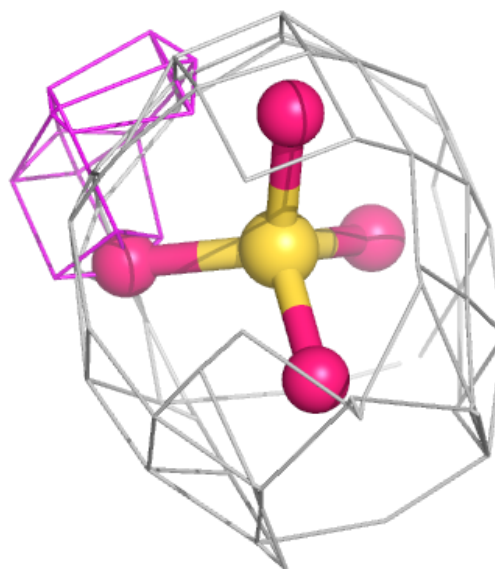
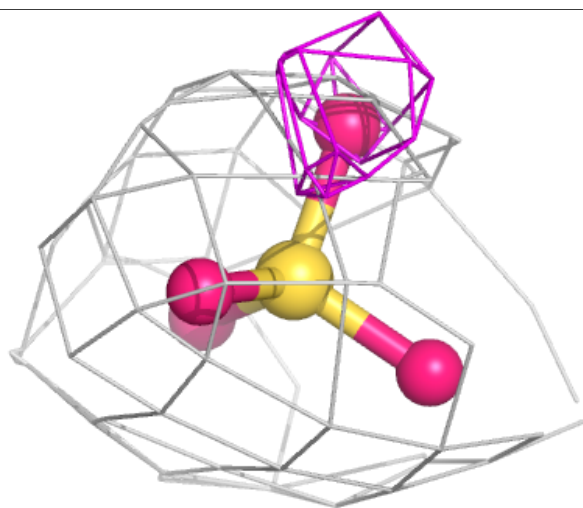
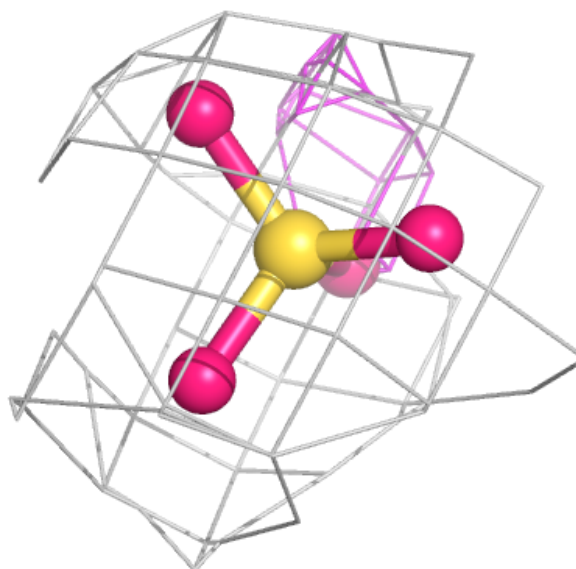
**Electron density around SO4 B 2509:**

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



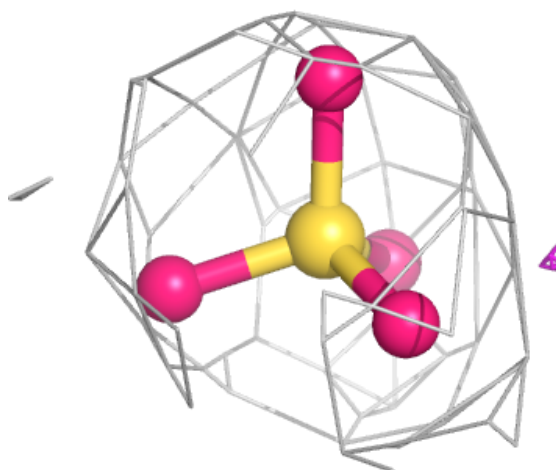
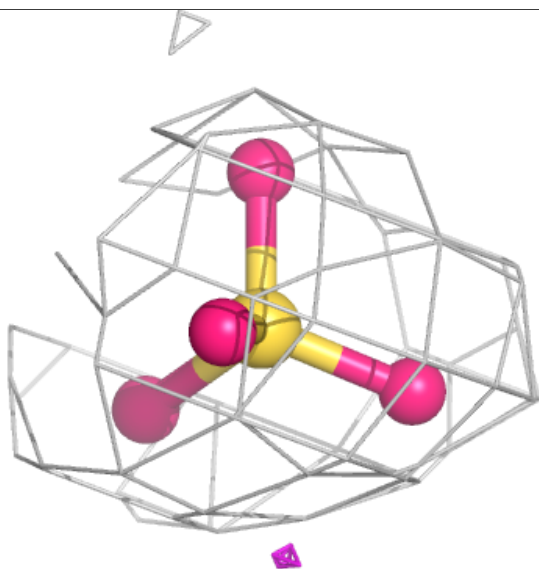
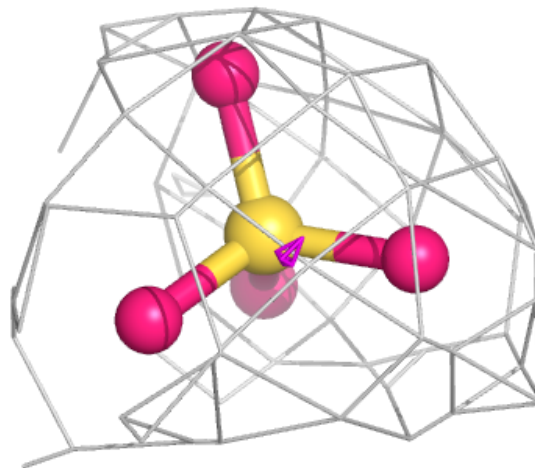
**Electron density around SO4 A 2509:**

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



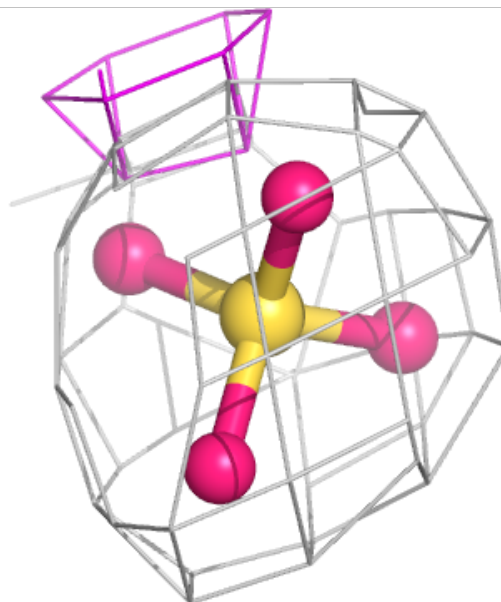
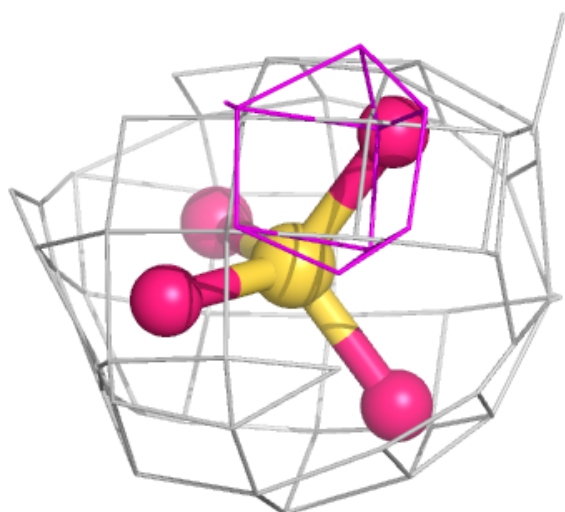
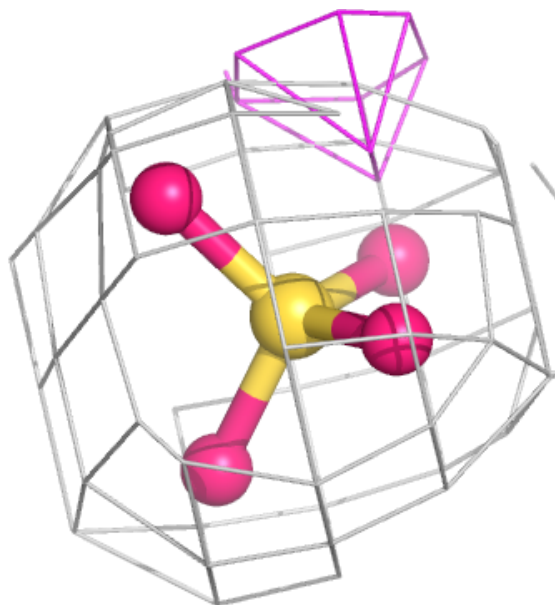
**Electron density around SO4 A 2503:**

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



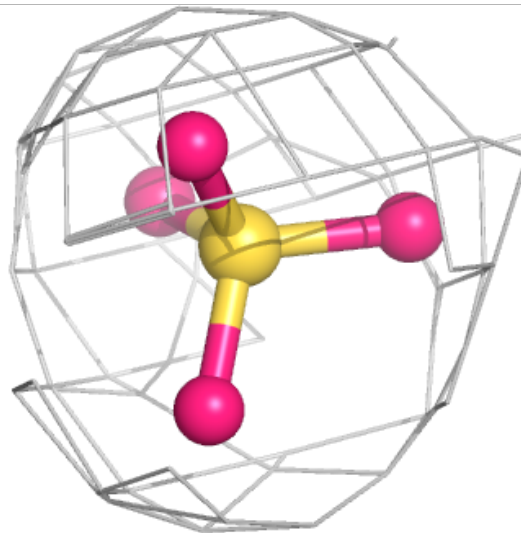
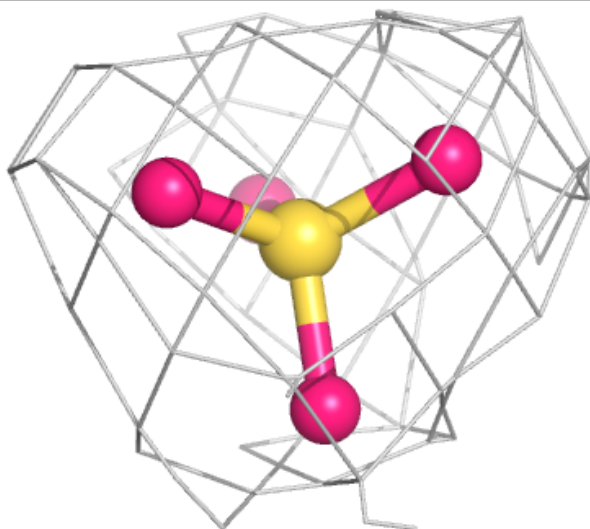
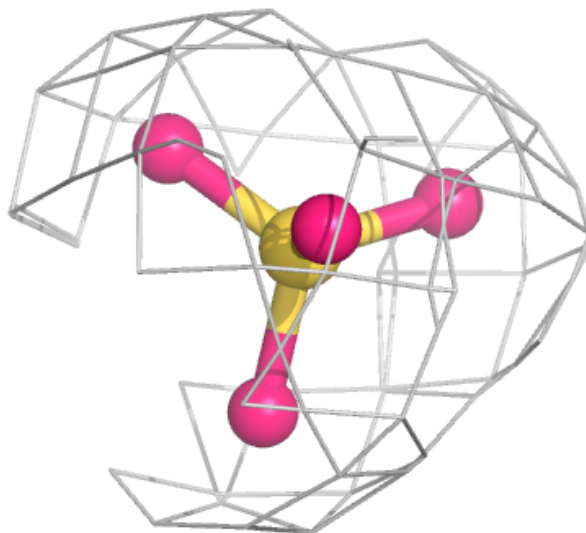
**Electron density around SO4 B 2516:**

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



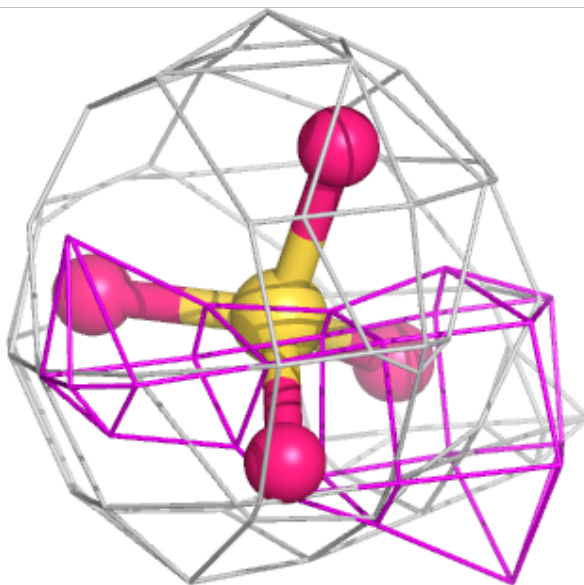
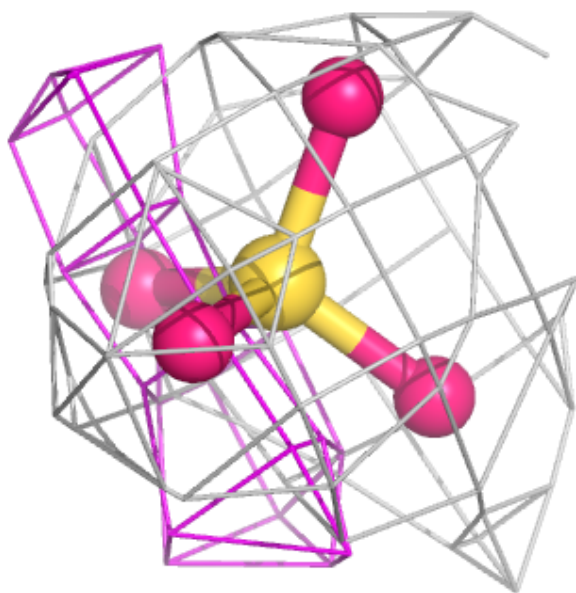
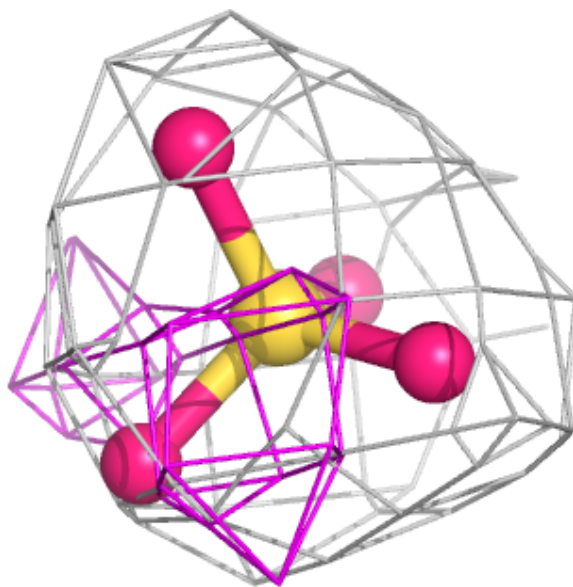
**Electron density around SO4 A 2512:**

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



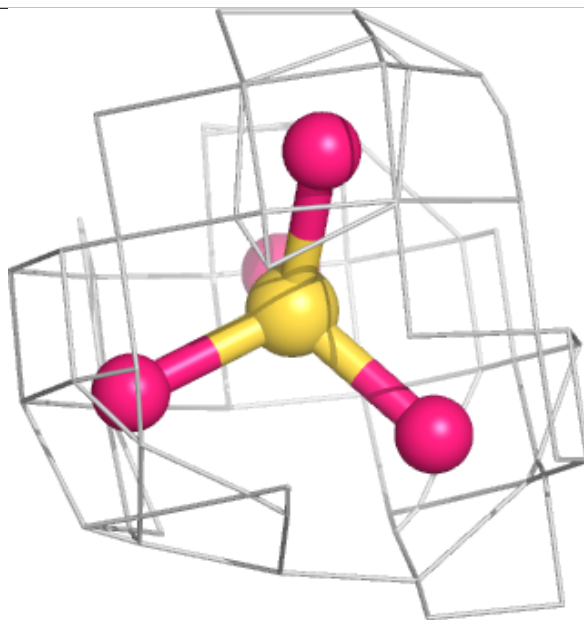
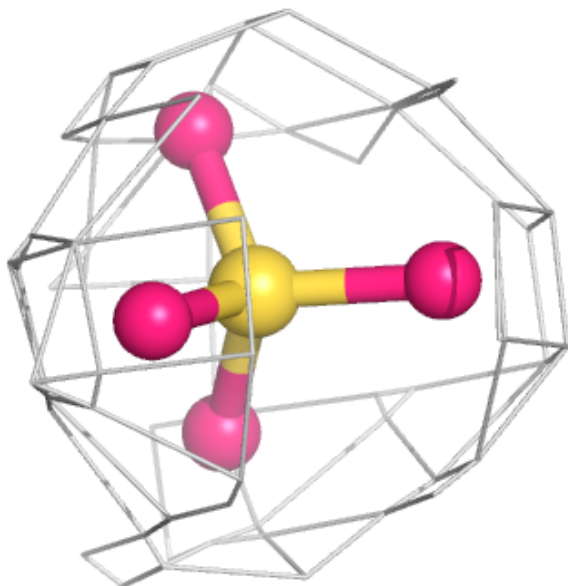
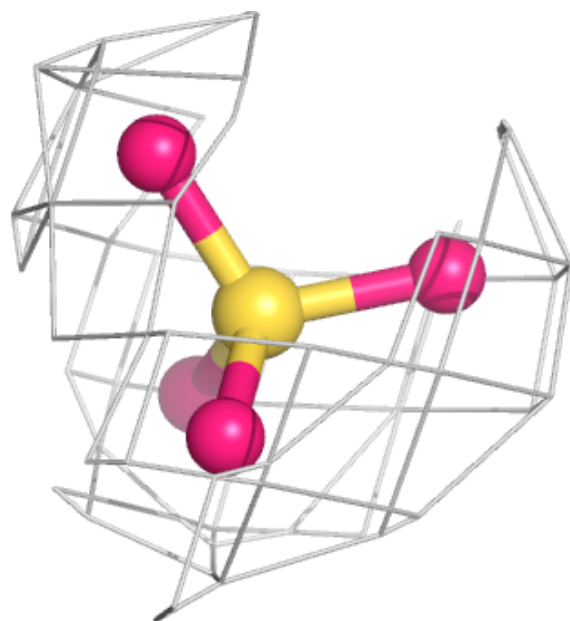
**Electron density around SO4 B 2506:**

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



**Electron density around SO4 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.