



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:24 AM UTC

PDB ID : 7DO5 / pdb_00007do5
Title : Crystal structure of Azotobacter vinelandii L-rhamnose 1-dehydrogenase(apo-form)
Authors : Yoshiwara, K.; Watanabe, Y.; Watanabe, S.
Deposited on : 2020-12-12
Resolution : 1.84 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

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

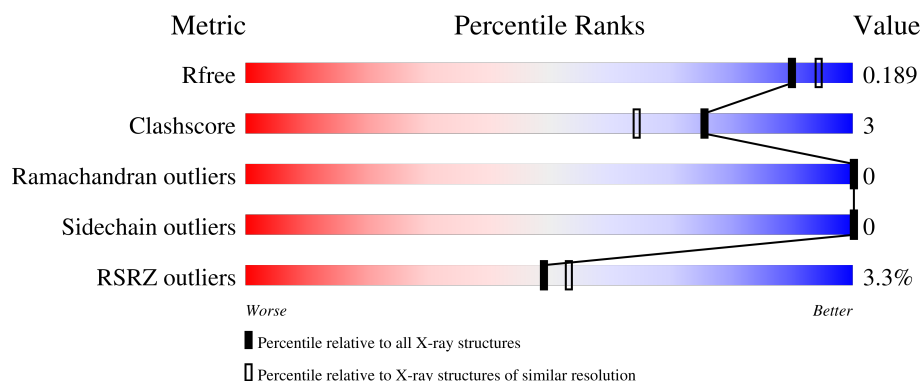
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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.



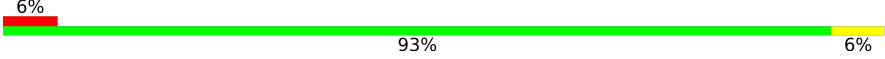
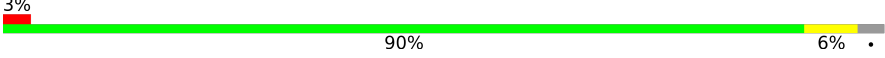
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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	267	2% 88% 8% .
1	B	267	4% 89% 9% .
1	C	267	% 89% 7% .
1	D	267	3% 91% 5% .
1	E	267	% 89% 7% .

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Mol	Chain	Length	Quality of chain
1	F	267	 3% 88% 8% •
1	G	267	 6% 93% 6%
1	H	267	 3% 90% 6% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16027 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 Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	256	Total	C	N	O	S	0	0	0
			1813	1133	327	343	10			
1	B	261	Total	C	N	O	S	0	0	0
			1838	1146	337	345	10			
1	C	256	Total	C	N	O	S	0	0	0
			1803	1124	326	343	10			
1	D	257	Total	C	N	O	S	0	0	0
			1799	1126	323	340	10			
1	E	248	Total	C	N	O	S	0	0	0
			1736	1086	314	326	10			
1	F	257	Total	C	N	O	S	0	0	0
			1791	1118	324	339	10			
1	G	266	Total	C	N	O	S	0	0	0
			1874	1168	346	350	10			
1	H	258	Total	C	N	O	S	0	0	0
			1811	1130	329	342	10			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP C1DMX5
A	-9	ARG	-	expression tag	UNP C1DMX5
A	-8	GLY	-	expression tag	UNP C1DMX5
A	-7	SER	-	expression tag	UNP C1DMX5
A	-6	HIS	-	expression tag	UNP C1DMX5
A	-5	HIS	-	expression tag	UNP C1DMX5
A	-4	HIS	-	expression tag	UNP C1DMX5
A	-3	HIS	-	expression tag	UNP C1DMX5
A	-2	HIS	-	expression tag	UNP C1DMX5
A	-1	HIS	-	expression tag	UNP C1DMX5
A	0	GLY	-	expression tag	UNP C1DMX5
A	1	SER	-	expression tag	UNP C1DMX5
B	-10	MET	-	initiating methionine	UNP C1DMX5

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	ARG	-	expression tag	UNP C1DMX5
B	-8	GLY	-	expression tag	UNP C1DMX5
B	-7	SER	-	expression tag	UNP C1DMX5
B	-6	HIS	-	expression tag	UNP C1DMX5
B	-5	HIS	-	expression tag	UNP C1DMX5
B	-4	HIS	-	expression tag	UNP C1DMX5
B	-3	HIS	-	expression tag	UNP C1DMX5
B	-2	HIS	-	expression tag	UNP C1DMX5
B	-1	HIS	-	expression tag	UNP C1DMX5
B	0	GLY	-	expression tag	UNP C1DMX5
B	1	SER	-	expression tag	UNP C1DMX5
C	-10	MET	-	initiating methionine	UNP C1DMX5
C	-9	ARG	-	expression tag	UNP C1DMX5
C	-8	GLY	-	expression tag	UNP C1DMX5
C	-7	SER	-	expression tag	UNP C1DMX5
C	-6	HIS	-	expression tag	UNP C1DMX5
C	-5	HIS	-	expression tag	UNP C1DMX5
C	-4	HIS	-	expression tag	UNP C1DMX5
C	-3	HIS	-	expression tag	UNP C1DMX5
C	-2	HIS	-	expression tag	UNP C1DMX5
C	-1	HIS	-	expression tag	UNP C1DMX5
C	0	GLY	-	expression tag	UNP C1DMX5
C	1	SER	-	expression tag	UNP C1DMX5
D	-10	MET	-	initiating methionine	UNP C1DMX5
D	-9	ARG	-	expression tag	UNP C1DMX5
D	-8	GLY	-	expression tag	UNP C1DMX5
D	-7	SER	-	expression tag	UNP C1DMX5
D	-6	HIS	-	expression tag	UNP C1DMX5
D	-5	HIS	-	expression tag	UNP C1DMX5
D	-4	HIS	-	expression tag	UNP C1DMX5
D	-3	HIS	-	expression tag	UNP C1DMX5
D	-2	HIS	-	expression tag	UNP C1DMX5
D	-1	HIS	-	expression tag	UNP C1DMX5
D	0	GLY	-	expression tag	UNP C1DMX5
D	1	SER	-	expression tag	UNP C1DMX5
E	-10	MET	-	initiating methionine	UNP C1DMX5
E	-9	ARG	-	expression tag	UNP C1DMX5
E	-8	GLY	-	expression tag	UNP C1DMX5
E	-7	SER	-	expression tag	UNP C1DMX5
E	-6	HIS	-	expression tag	UNP C1DMX5
E	-5	HIS	-	expression tag	UNP C1DMX5
E	-4	HIS	-	expression tag	UNP C1DMX5

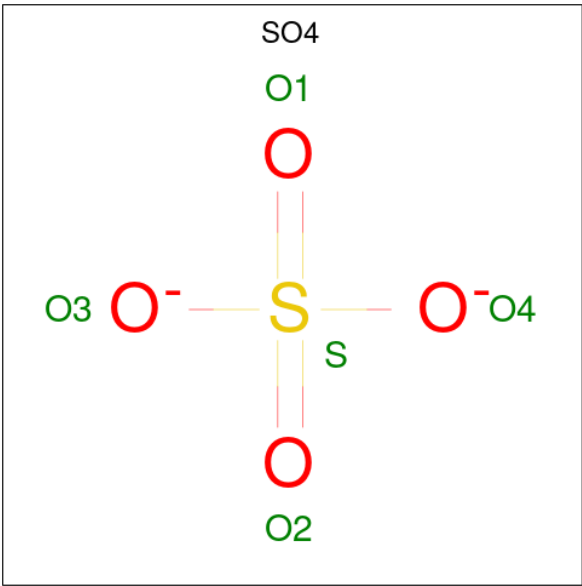
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-3	HIS	-	expression tag	UNP C1DMX5
E	-2	HIS	-	expression tag	UNP C1DMX5
E	-1	HIS	-	expression tag	UNP C1DMX5
E	0	GLY	-	expression tag	UNP C1DMX5
E	1	SER	-	expression tag	UNP C1DMX5
F	-10	MET	-	initiating methionine	UNP C1DMX5
F	-9	ARG	-	expression tag	UNP C1DMX5
F	-8	GLY	-	expression tag	UNP C1DMX5
F	-7	SER	-	expression tag	UNP C1DMX5
F	-6	HIS	-	expression tag	UNP C1DMX5
F	-5	HIS	-	expression tag	UNP C1DMX5
F	-4	HIS	-	expression tag	UNP C1DMX5
F	-3	HIS	-	expression tag	UNP C1DMX5
F	-2	HIS	-	expression tag	UNP C1DMX5
F	-1	HIS	-	expression tag	UNP C1DMX5
F	0	GLY	-	expression tag	UNP C1DMX5
F	1	SER	-	expression tag	UNP C1DMX5
G	-10	MET	-	initiating methionine	UNP C1DMX5
G	-9	ARG	-	expression tag	UNP C1DMX5
G	-8	GLY	-	expression tag	UNP C1DMX5
G	-7	SER	-	expression tag	UNP C1DMX5
G	-6	HIS	-	expression tag	UNP C1DMX5
G	-5	HIS	-	expression tag	UNP C1DMX5
G	-4	HIS	-	expression tag	UNP C1DMX5
G	-3	HIS	-	expression tag	UNP C1DMX5
G	-2	HIS	-	expression tag	UNP C1DMX5
G	-1	HIS	-	expression tag	UNP C1DMX5
G	0	GLY	-	expression tag	UNP C1DMX5
G	1	SER	-	expression tag	UNP C1DMX5
H	-10	MET	-	initiating methionine	UNP C1DMX5
H	-9	ARG	-	expression tag	UNP C1DMX5
H	-8	GLY	-	expression tag	UNP C1DMX5
H	-7	SER	-	expression tag	UNP C1DMX5
H	-6	HIS	-	expression tag	UNP C1DMX5
H	-5	HIS	-	expression tag	UNP C1DMX5
H	-4	HIS	-	expression tag	UNP C1DMX5
H	-3	HIS	-	expression tag	UNP C1DMX5
H	-2	HIS	-	expression tag	UNP C1DMX5
H	-1	HIS	-	expression tag	UNP C1DMX5
H	0	GLY	-	expression tag	UNP C1DMX5
H	1	SER	-	expression tag	UNP C1DMX5

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

by depositor).



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	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	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

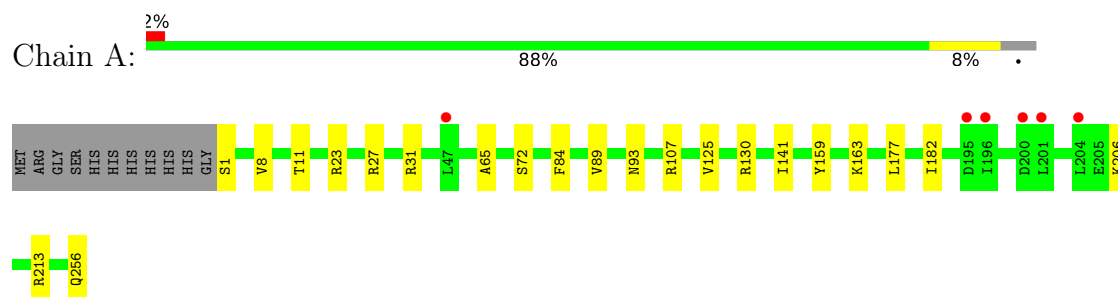
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	161	Total	O	0	0
			161	161		
3	B	194	Total	O	0	0
			194	194		
3	C	205	Total	O	0	0
			205	205		
3	D	163	Total	O	0	0
			163	163		
3	E	175	Total	O	0	0
			175	175		
3	F	169	Total	O	0	0
			169	169		
3	G	191	Total	O	0	0
			191	191		
3	H	184	Total	O	0	0
			184	184		

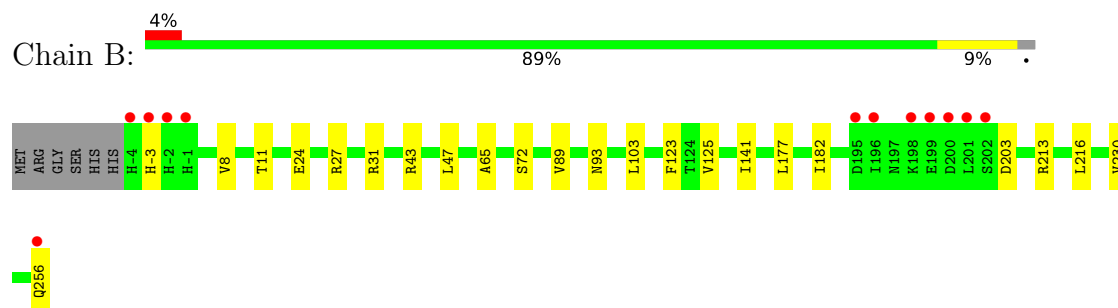
3 Residue-property plots [i](#)

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

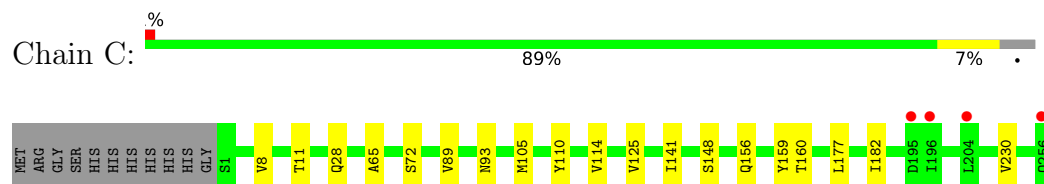
- Molecule 1: Short-chain dehydrogenase/reductase SDR



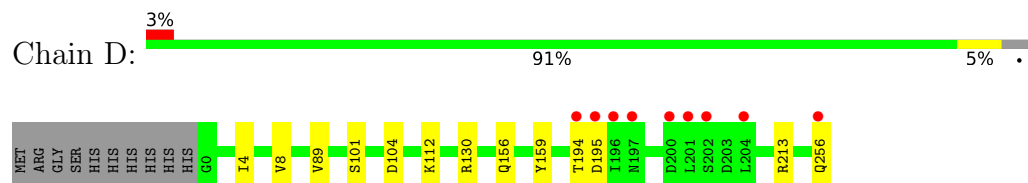
- Molecule 1: Short-chain dehydrogenase/reductase SDR



- Molecule 1: Short-chain dehydrogenase/reductase SDR



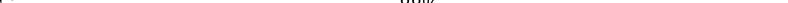
- Molecule 1: Short-chain dehydrogenase/reductase SDR

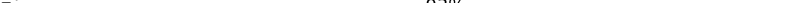


- Molecule 1: Short-chain dehydrogenase/reductase SDR

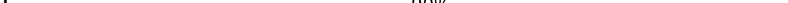
Number of amino acids

NET ARG GLY SER HIS HIS HIS HIS HIS HIS GO I4 V8 A55 D71 V89 R107 Y110 V114 K133 A193 THR ASP ILE ASN LYS GLU ASP LEU SER D203 L204 R213 Q256

- Chain F:  3% 88% 8%

- Chain G:  6% 93% 6%

Category	Gene Count	p-value < 0.05
MET	1	Yes
G-8	1	Yes
G-3	1	Yes
S-7	1	Yes
H-6	1	Yes
H-5	1	Yes
H-4	1	Yes
H-3	1	Yes
V8	1	No
T11	1	No
R27	1	No
V89	1	No
N93	1	No
K112	1	No
V125	1	No
I141	1	No
S148	1	No
A154	1	No
T160	1	No
I175	1	No
T194	1	Yes
D195	1	Yes
I196	1	Yes
M197	1	Yes
K198	1	Yes
E199	1	Yes
D200	1	Yes
L201	1	Yes
L202	1	Yes
D203	1	Yes
S202	1	Yes
L204	1	Yes
R213	1	No
M236	1	No
D245	1	Yes

- Chain H:  3% 90% 6%

MET	ARG	GLY	SER	HIS	HIS	HIS	HIS	HIS	HIS	H-1	GO	V8	T11	E52	K75	V89	N93	H100	M105	V125	I141	A154	I175	A176	L177	I182	T194	D195	I196	N197	K198	E199	D200	L201	S202	L255	L256
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	75.37Å 81.58Å 91.18Å 80.45° 74.55° 75.20°	Depositor
Resolution (Å)	47.59 – 1.84 47.59 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.4 (47.59-1.84) 96.4 (47.59-1.84)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 1.83Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.160 , 0.188 0.160 , 0.189	Depositor DCC
R_{free} test set	8540 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.242	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	16027	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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	0.27	0/1835	0.45	0/2485
1	B	0.30	0/1863	0.48	0/2525
1	C	0.31	0/1825	0.49	0/2473
1	D	0.28	0/1821	0.46	0/2470
1	E	0.29	0/1757	0.47	0/2379
1	F	0.27	0/1813	0.45	0/2458
1	G	0.29	0/1901	0.48	0/2576
1	H	0.29	0/1834	0.47	0/2487
All	All	0.29	0/14649	0.47	0/19853

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 [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	1813	0	1835	17	0
1	B	1838	0	1827	15	0
1	C	1803	0	1806	10	0
1	D	1799	0	1808	8	0
1	E	1736	0	1748	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1791	0	1785	15	0
1	G	1874	0	1855	12	0
1	H	1811	0	1807	12	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	15	0	0	0	0
2	E	15	0	0	0	0
2	F	15	0	0	1	0
2	G	15	0	0	0	0
2	H	15	0	0	1	0
3	A	161	0	0	6	0
3	B	194	0	0	4	2
3	C	205	0	0	1	1
3	D	163	0	0	1	0
3	E	175	0	0	1	0
3	F	169	0	0	3	0
3	G	191	0	0	3	2
3	H	184	0	0	5	1
All	All	16027	0	14471	88	3

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 3.

All (88) 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:23:ARG:NH2	3:A:401:HOH:O	1.85	1.09
1:H:52:GLU:OE1	3:H:401:HOH:O	1.88	0.90
1:G:198:LYS:O	3:G:402:HOH:O	1.91	0.89
1:B:27:ARG:NH1	3:B:401:HOH:O	1.95	0.87
1:F:199:GLU:N	3:F:401:HOH:O	2.09	0.84
1:H:256:GLN:O	3:H:402:HOH:O	2.08	0.70
1:B:203:ASP:OD2	3:B:402:HOH:O	2.12	0.67
1:G:27:ARG:NH1	3:G:401:HOH:O	1.85	0.67
1:H:194:THR:OG1	3:H:403:HOH:O	2.16	0.61
1:A:107:ARG:NH1	3:A:406:HOH:O	2.34	0.60
1:D:4:ILE:HG21	1:E:4:ILE:HG21	1.84	0.60
1:E:71:ASP:OD1	1:F:107:ARG:NH1	2.28	0.58
1:A:130:ARG:HG3	1:B:103:LEU:HD22	1.86	0.58
1:B:8:VAL:HG22	1:B:89:VAL:HB	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:148:SER:HB3	1:F:160:THR:HG22	1.88	0.56
1:A:256:GLN:NE2	3:A:410:HOH:O	2.39	0.55
1:F:213:ARG:NH1	3:F:404:HOH:O	2.28	0.54
1:B:31:ARG:HD2	3:B:404:HOH:O	2.08	0.54
1:H:75:LYS:NZ	3:H:405:HOH:O	2.40	0.54
1:D:130:ARG:NH1	3:D:404:HOH:O	2.41	0.53
1:A:8:VAL:HG22	1:A:89:VAL:HB	1.91	0.53
1:F:11:THR:O	1:F:93:ASN:HB3	2.09	0.52
2:H:302:SO4:O3	3:H:404:HOH:O	2.18	0.52
1:C:8:VAL:HG22	1:C:89:VAL:HB	1.91	0.52
1:D:194:THR:HG22	1:D:195:ASP:H	1.75	0.51
1:C:28:GLN:HG3	1:C:230:VAL:HG11	1.93	0.50
1:F:27:ARG:HB3	1:G:-4:HIS:HB3	1.94	0.50
1:A:125:VAL:HG13	1:A:141:ILE:HD13	1.93	0.50
1:A:11:THR:O	1:A:93:ASN:HB3	2.12	0.49
1:A:213:ARG:HD2	3:C:548:HOH:O	2.13	0.49
1:G:125:VAL:HG13	1:G:141:ILE:HD13	1.94	0.48
1:B:125:VAL:HG13	1:B:141:ILE:HD13	1.95	0.48
1:D:8:VAL:HG22	1:D:89:VAL:HB	1.96	0.48
1:C:125:VAL:HG13	1:C:141:ILE:HD13	1.95	0.48
1:D:101:SER:OG	1:D:104:ASP:OD1	2.29	0.47
1:A:31:ARG:NH2	3:A:412:HOH:O	2.47	0.47
1:F:177:LEU:HB3	1:F:182:ILE:HB	1.97	0.47
1:G:112:LYS:NZ	3:G:404:HOH:O	2.43	0.47
1:C:11:THR:O	1:C:93:ASN:HB3	2.15	0.47
1:G:-3:HIS:CG	1:G:236:MET:HG2	2.50	0.47
1:G:154:ALA:HB2	1:H:175:ILE:HG22	1.97	0.47
1:H:8:VAL:HG22	1:H:89:VAL:HB	1.97	0.47
1:G:148:SER:HB3	1:G:160:THR:HG22	1.97	0.46
1:B:65:ALA:HB1	1:B:72:SER:HB3	1.96	0.46
1:F:197:ASN:C	3:F:401:HOH:O	2.57	0.46
1:H:125:VAL:HG13	1:H:141:ILE:HD13	1.97	0.45
1:D:112:LYS:HB3	1:D:112:LYS:HE2	1.73	0.45
1:D:213:ARG:NH2	1:D:256:GLN:HG3	2.31	0.45
1:H:100:HIS:HB3	1:H:105:MET:HE1	1.98	0.45
1:G:175:ILE:HG22	1:H:154:ALA:HB2	1.99	0.45
1:C:148:SER:HB3	1:C:160:THR:HG22	1.99	0.44
1:H:11:THR:O	1:H:93:ASN:HB3	2.17	0.44
1:A:31:ARG:HG2	1:A:84:PHE:CD1	2.53	0.44
1:B:-3:HIS:HB3	3:B:401:HOH:O	2.17	0.44
1:B:24:GLU:HG3	1:B:230:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:8:VAL:HG22	1:E:89:VAL:HB	1.99	0.44
1:F:28:GLN:HG3	1:F:230:VAL:HG11	2.00	0.44
1:D:156:GLN:HB3	1:D:159:TYR:HB3	2.00	0.43
1:B:213:ARG:HG2	1:B:256:GLN:OE1	2.18	0.43
1:G:8:VAL:HG22	1:G:89:VAL:HB	2.00	0.43
1:E:110:TYR:CZ	1:E:114:VAL:HG21	2.53	0.43
1:E:256:GLN:HB3	1:G:213:ARG:CZ	2.49	0.42
1:H:177:LEU:HB3	1:H:182:ILE:HB	2.02	0.42
1:E:133:LYS:NZ	3:E:401:HOH:O	2.04	0.42
1:E:213:ARG:NH1	1:E:256:GLN:HG3	2.35	0.42
1:A:27:ARG:NE	3:A:402:HOH:O	2.22	0.41
1:C:156:GLN:HB3	1:C:159:TYR:HB3	2.01	0.41
1:A:206:LYS:NZ	2:A:303:SO4:O3	2.52	0.41
1:F:43:ARG:NH1	2:F:302:SO4:O3	2.41	0.41
1:C:177:LEU:HB3	1:C:182:ILE:HB	2.02	0.41
1:B:11:THR:O	1:B:93:ASN:HB3	2.19	0.41
1:B:177:LEU:HB3	1:B:182:ILE:HB	2.02	0.41
1:F:151:VAL:HG21	1:H:255:LEU:HB2	2.02	0.41
1:G:11:THR:O	1:G:93:ASN:HB3	2.21	0.41
1:F:8:VAL:HG22	1:F:89:VAL:HB	2.03	0.41
1:F:125:VAL:HG13	1:F:141:ILE:HD13	2.01	0.41
1:A:1:SER:N	3:A:408:HOH:O	2.35	0.41
1:A:65:ALA:HB1	1:A:72:SER:HB3	2.03	0.41
1:A:107:ARG:HG2	1:B:123:PHE:CZ	2.56	0.41
1:A:159:TYR:CE1	1:A:163:LYS:HD3	2.56	0.41
1:B:43:ARG:O	1:B:47:LEU:HG	2.21	0.41
1:C:65:ALA:HB1	1:C:72:SER:HB3	2.03	0.41
1:C:110:TYR:CZ	1:C:114:VAL:HG21	2.56	0.41
1:A:177:LEU:HB3	1:A:182:ILE:HB	2.03	0.40
1:F:156:GLN:HB3	1:F:159:TYR:HB3	2.03	0.40
1:C:105:MET:HE2	1:C:105:MET:HB2	1.99	0.40
1:E:107:ARG:HA	1:F:123:PHE:CZ	2.56	0.40
1:B:216:LEU:HD23	1:B:216:LEU:HA	1.88	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:525:HOH:O	3:G:541:HOH:O[1_466]	1.64	0.56
3:C:556:HOH:O	3:H:532:HOH:O[1_465]	1.67	0.53
3:B:406:HOH:O	3:G:530:HOH:O[1_466]	1.82	0.38

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	254/267 (95%)	245 (96%)	9 (4%)	0	100	100
1	B	259/267 (97%)	252 (97%)	7 (3%)	0	100	100
1	C	254/267 (95%)	246 (97%)	8 (3%)	0	100	100
1	D	255/267 (96%)	250 (98%)	5 (2%)	0	100	100
1	E	244/267 (91%)	236 (97%)	8 (3%)	0	100	100
1	F	255/267 (96%)	250 (98%)	5 (2%)	0	100	100
1	G	264/267 (99%)	255 (97%)	9 (3%)	0	100	100
1	H	256/267 (96%)	248 (97%)	8 (3%)	0	100	100
All	All	2041/2136 (96%)	1982 (97%)	59 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	178/196 (91%)	178 (100%)	0	100	100
1	B	176/196 (90%)	176 (100%)	0	100	100
1	C	175/196 (89%)	175 (100%)	0	100	100
1	D	174/196 (89%)	174 (100%)	0	100	100
1	E	167/196 (85%)	167 (100%)	0	100	100
1	F	171/196 (87%)	171 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	179/196 (91%)	179 (100%)	0	100	100
1	H	174/196 (89%)	174 (100%)	0	100	100
All	All	1394/1568 (89%)	1394 (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. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	93	ASN
1	E	256	GLN
1	G	256	GLN
1	H	93	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](#)

24 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	D	303	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	C	301	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	A	303	-	4,4,4	0.26	0	6,6,6	0.06	0
2	SO4	C	303	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	B	302	-	4,4,4	0.28	0	6,6,6	0.32	0
2	SO4	C	302	-	4,4,4	0.25	0	6,6,6	0.08	0
2	SO4	H	303	-	4,4,4	0.25	0	6,6,6	0.12	0
2	SO4	D	302	-	4,4,4	0.26	0	6,6,6	0.10	0
2	SO4	B	303	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	F	301	-	4,4,4	0.18	0	6,6,6	0.09	0
2	SO4	H	302	-	4,4,4	0.24	0	6,6,6	0.10	0
2	SO4	G	302	-	4,4,4	0.22	0	6,6,6	0.17	0
2	SO4	D	301	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	E	303	-	4,4,4	0.25	0	6,6,6	0.09	0
2	SO4	F	303	-	4,4,4	0.23	0	6,6,6	0.06	0
2	SO4	A	301	-	4,4,4	0.28	0	6,6,6	0.18	0
2	SO4	G	301	-	4,4,4	0.19	0	6,6,6	0.21	0
2	SO4	H	301	-	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	B	301	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	E	302	-	4,4,4	0.26	0	6,6,6	0.35	0
2	SO4	A	302	-	4,4,4	0.21	0	6,6,6	0.19	0
2	SO4	G	303	-	4,4,4	0.26	0	6,6,6	0.07	0
2	SO4	F	302	-	4,4,4	0.20	0	6,6,6	0.24	0
2	SO4	E	301	-	4,4,4	0.29	0	6,6,6	0.16	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

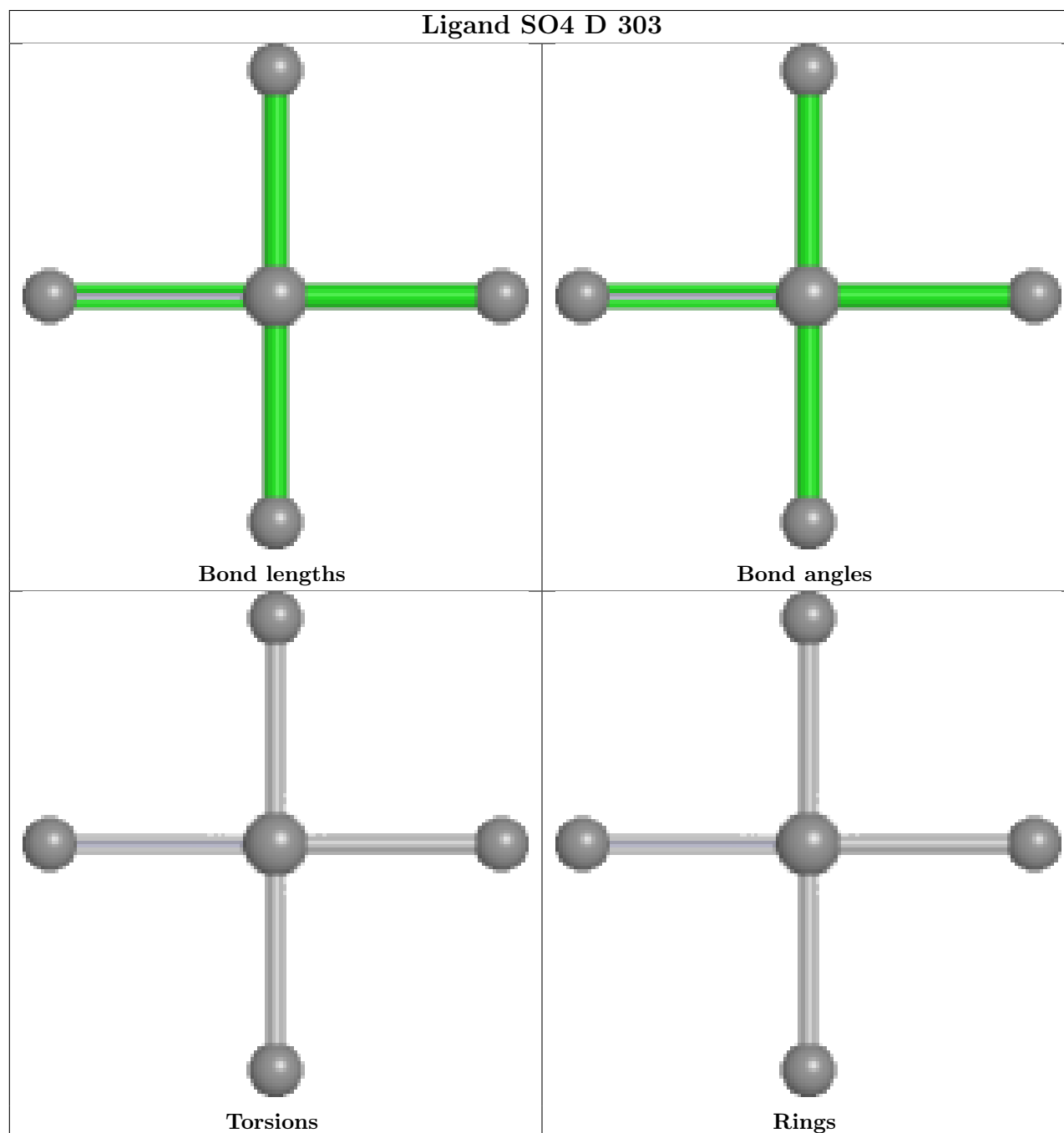
There are no ring outliers.

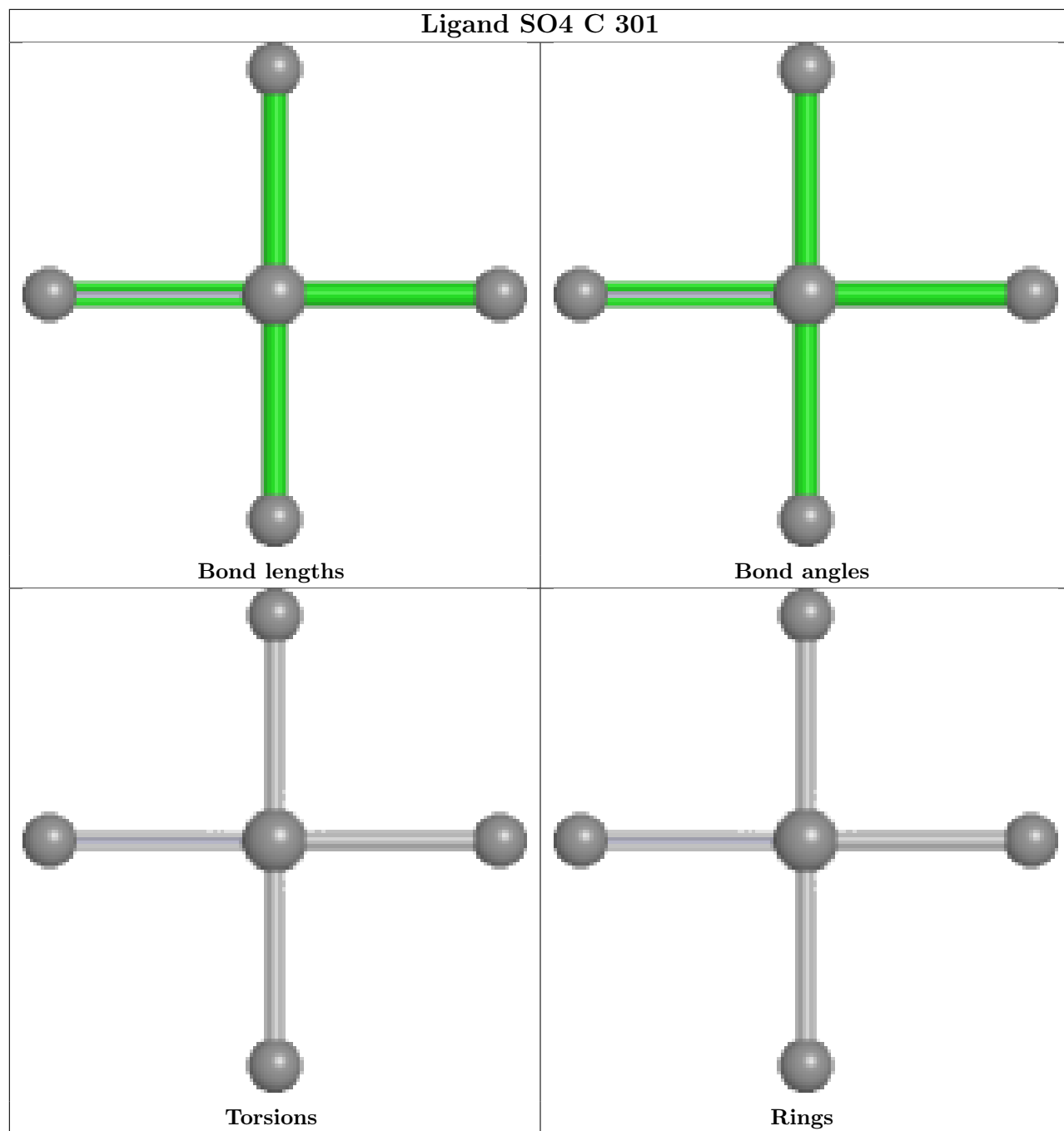
3 monomers are involved in 3 short contacts:

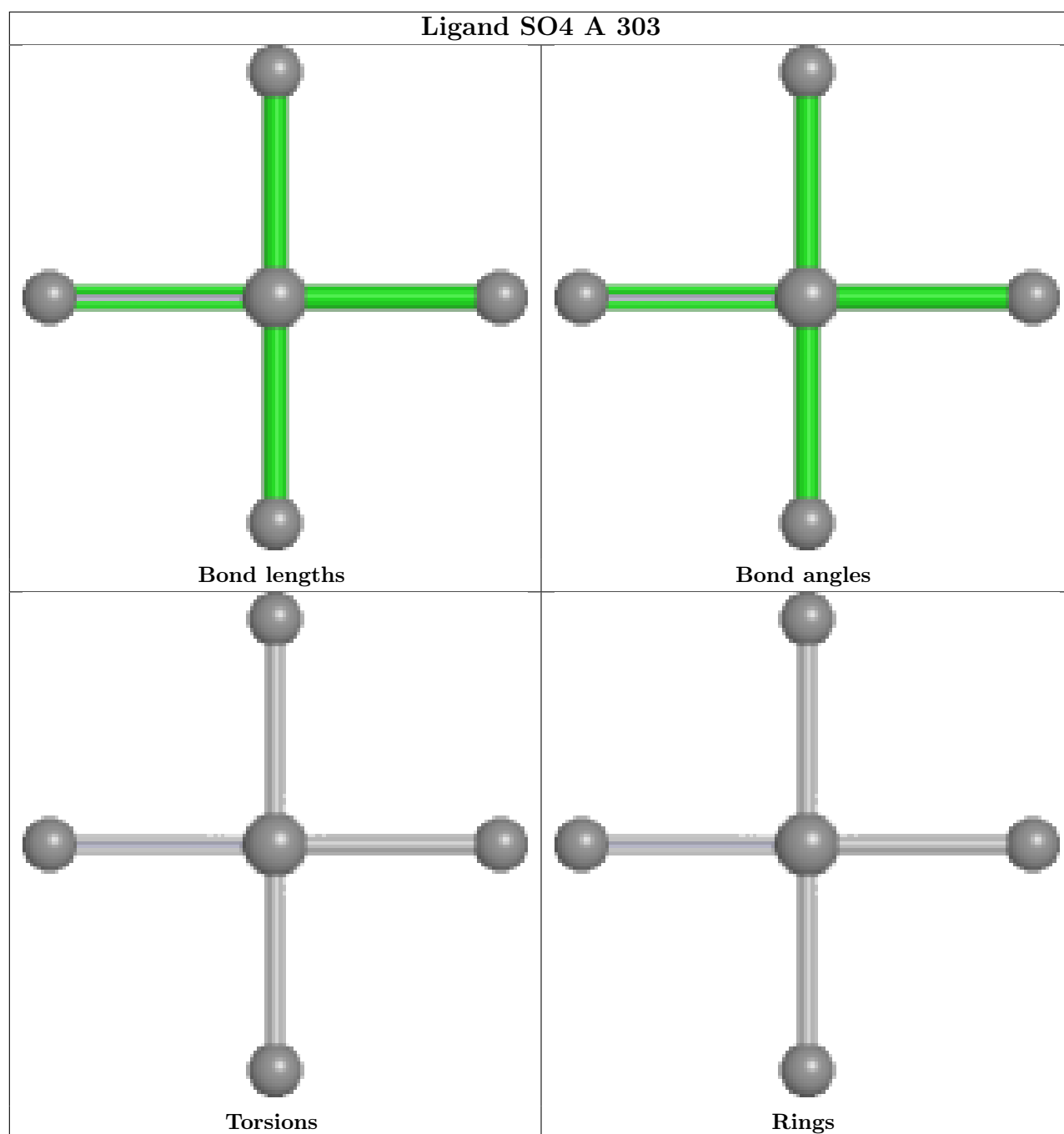
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	303	SO4	1	0
2	H	302	SO4	1	0
2	F	302	SO4	1	0

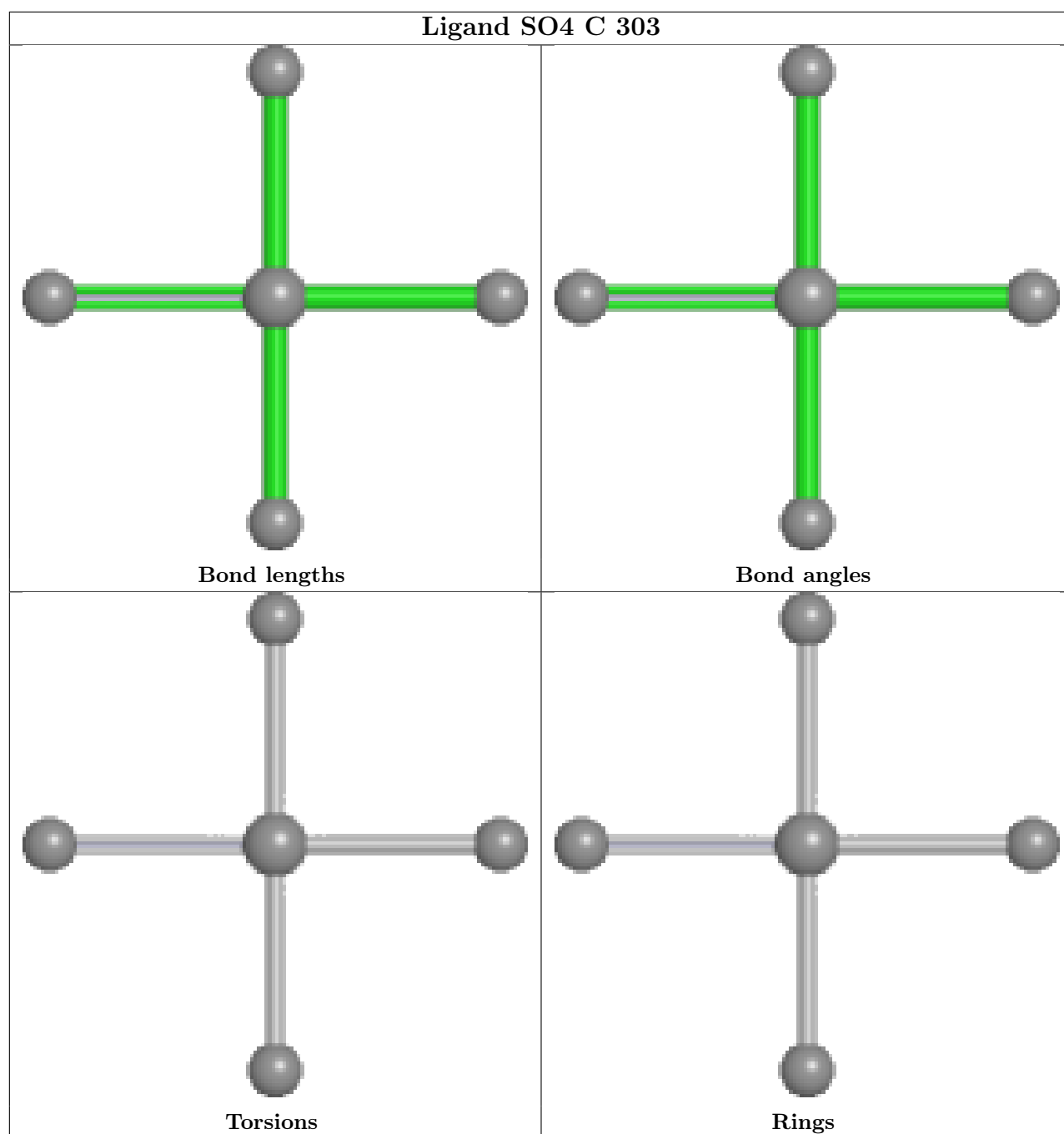
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

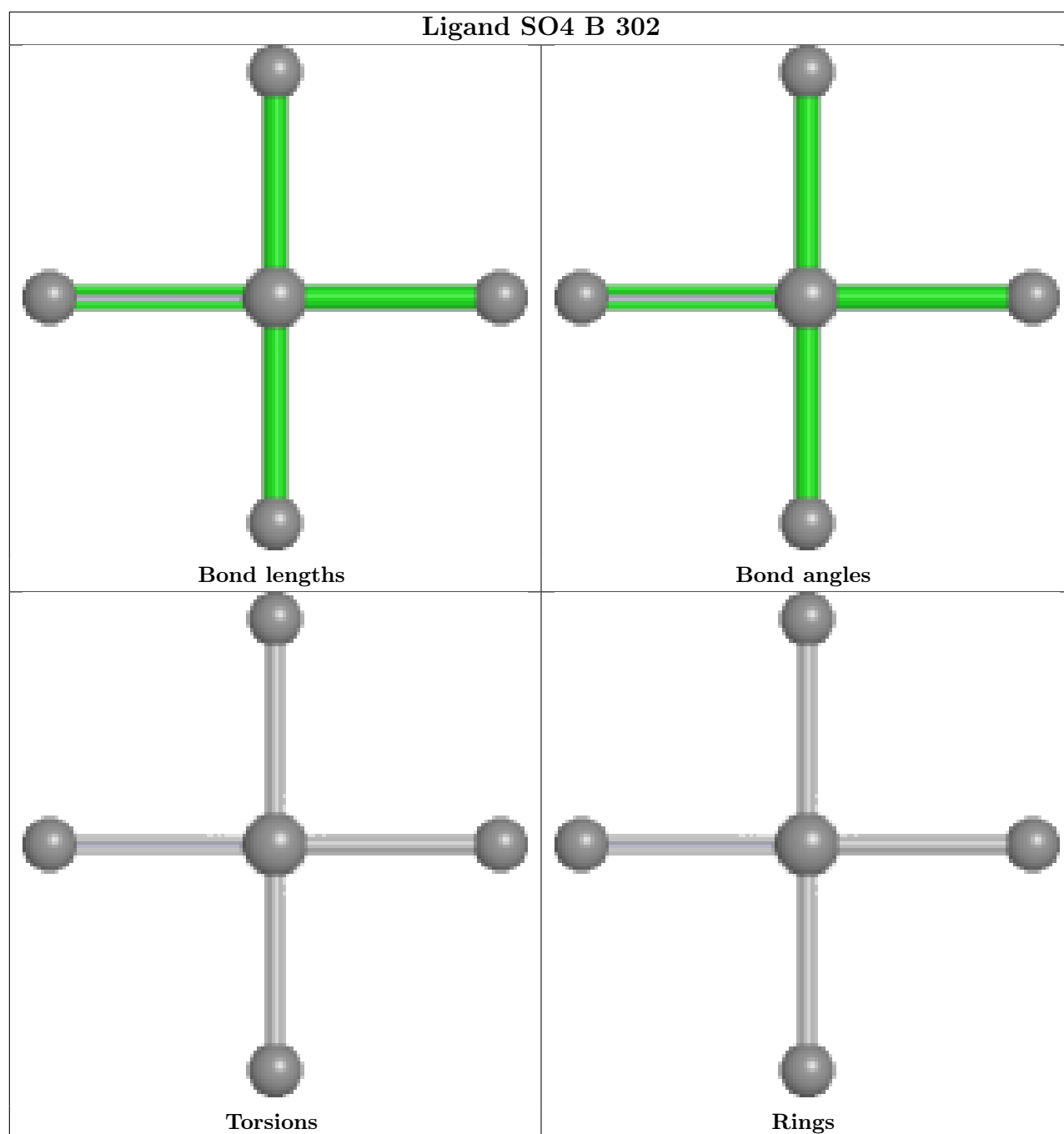
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

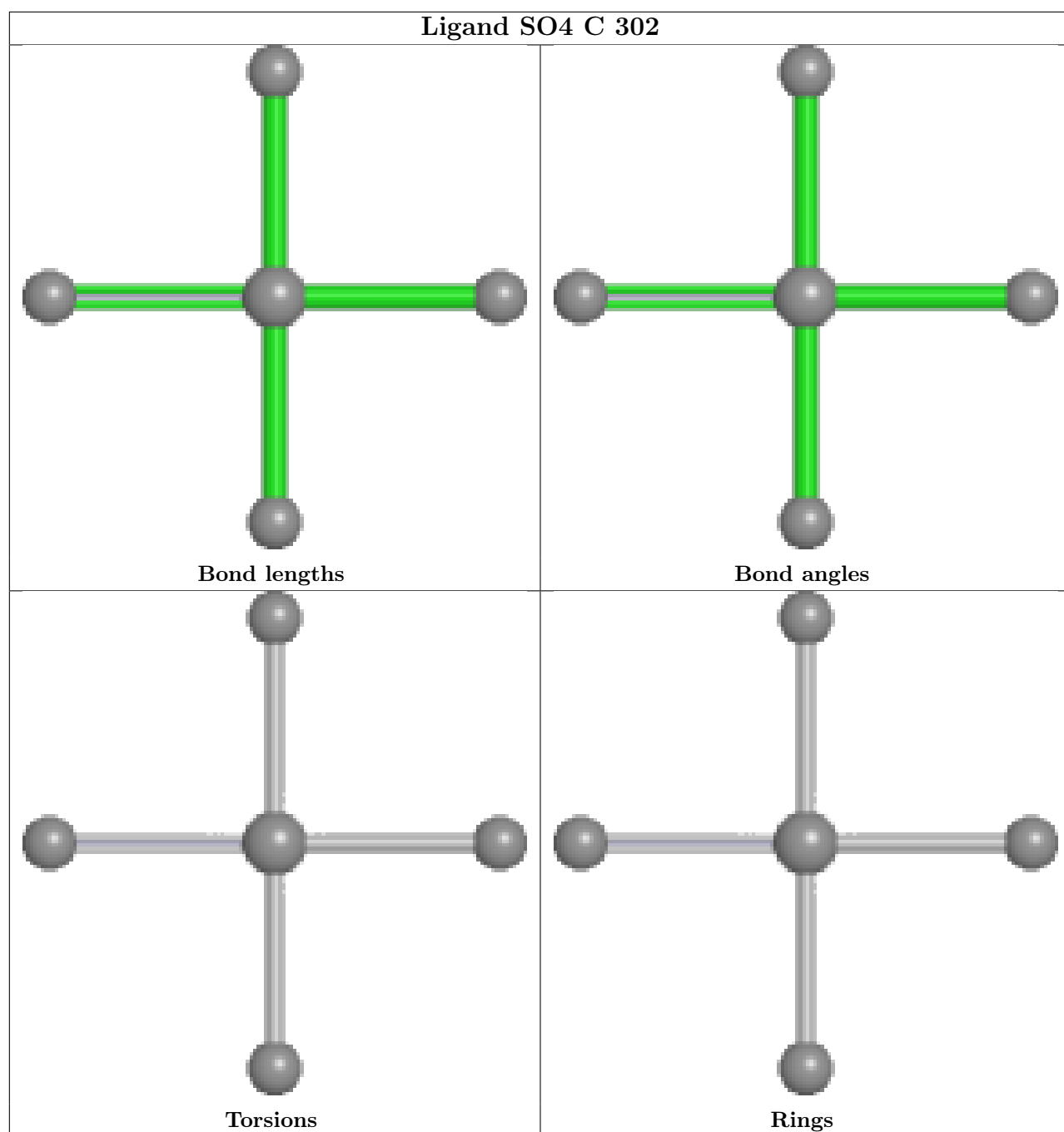


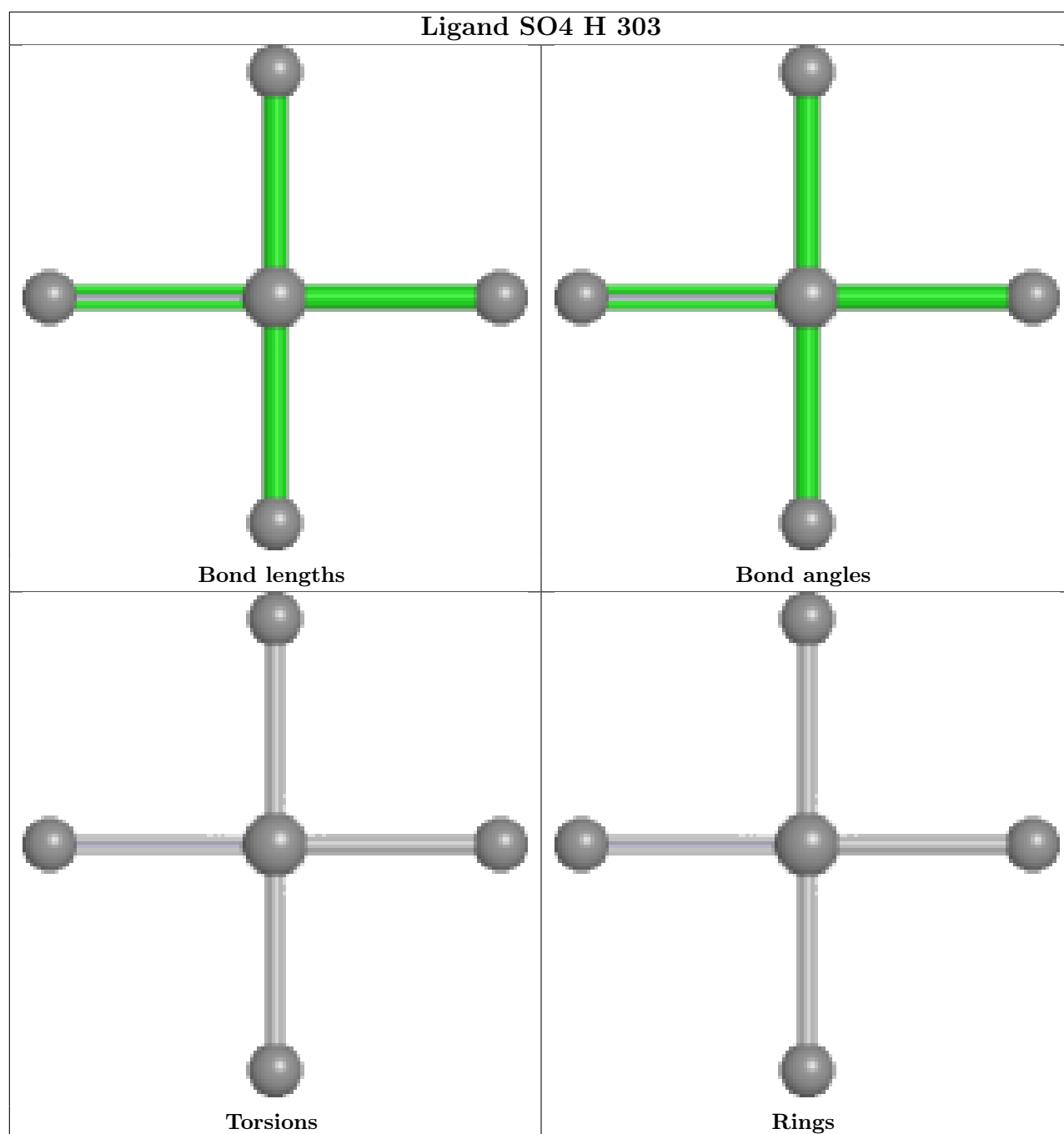


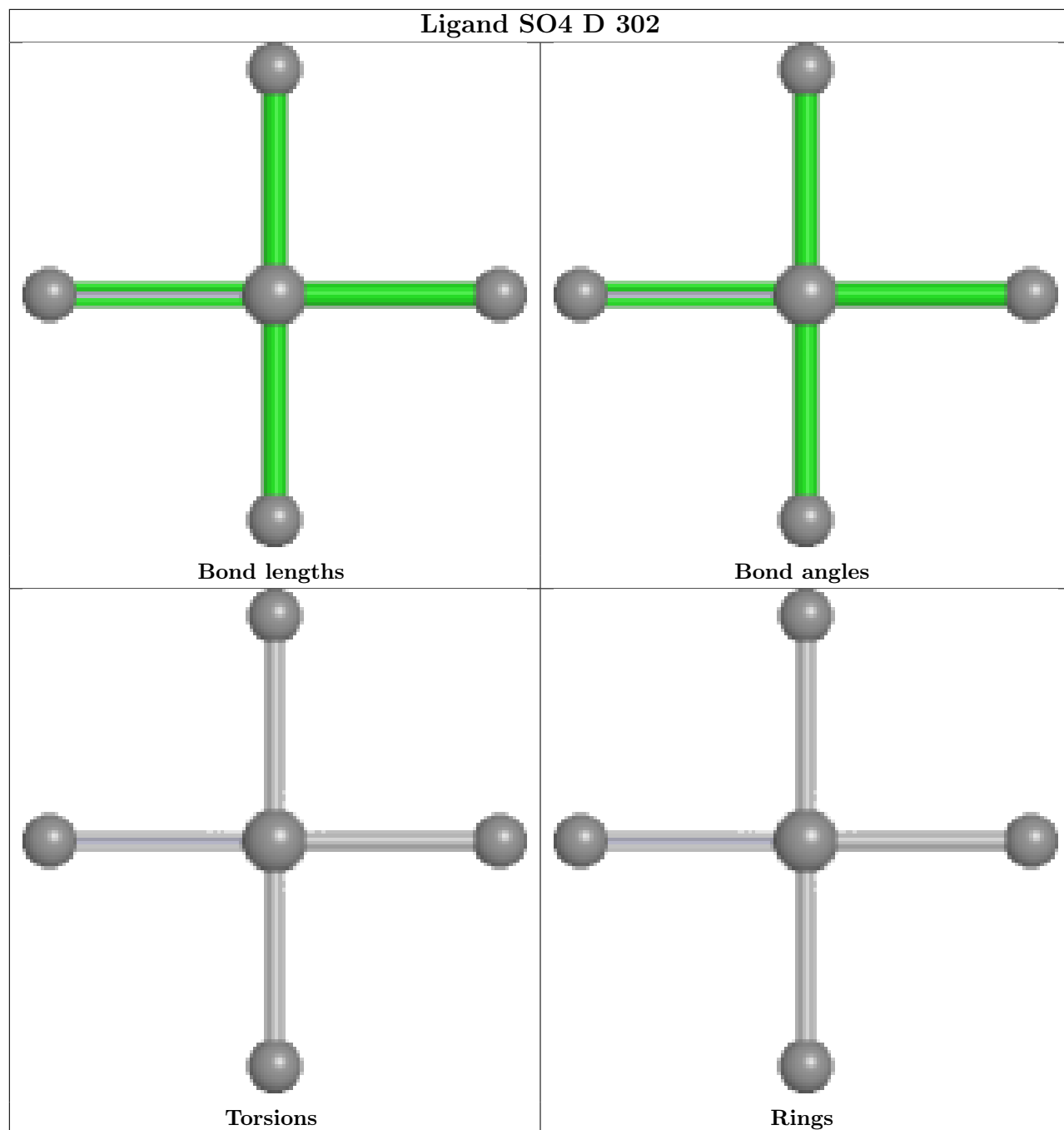


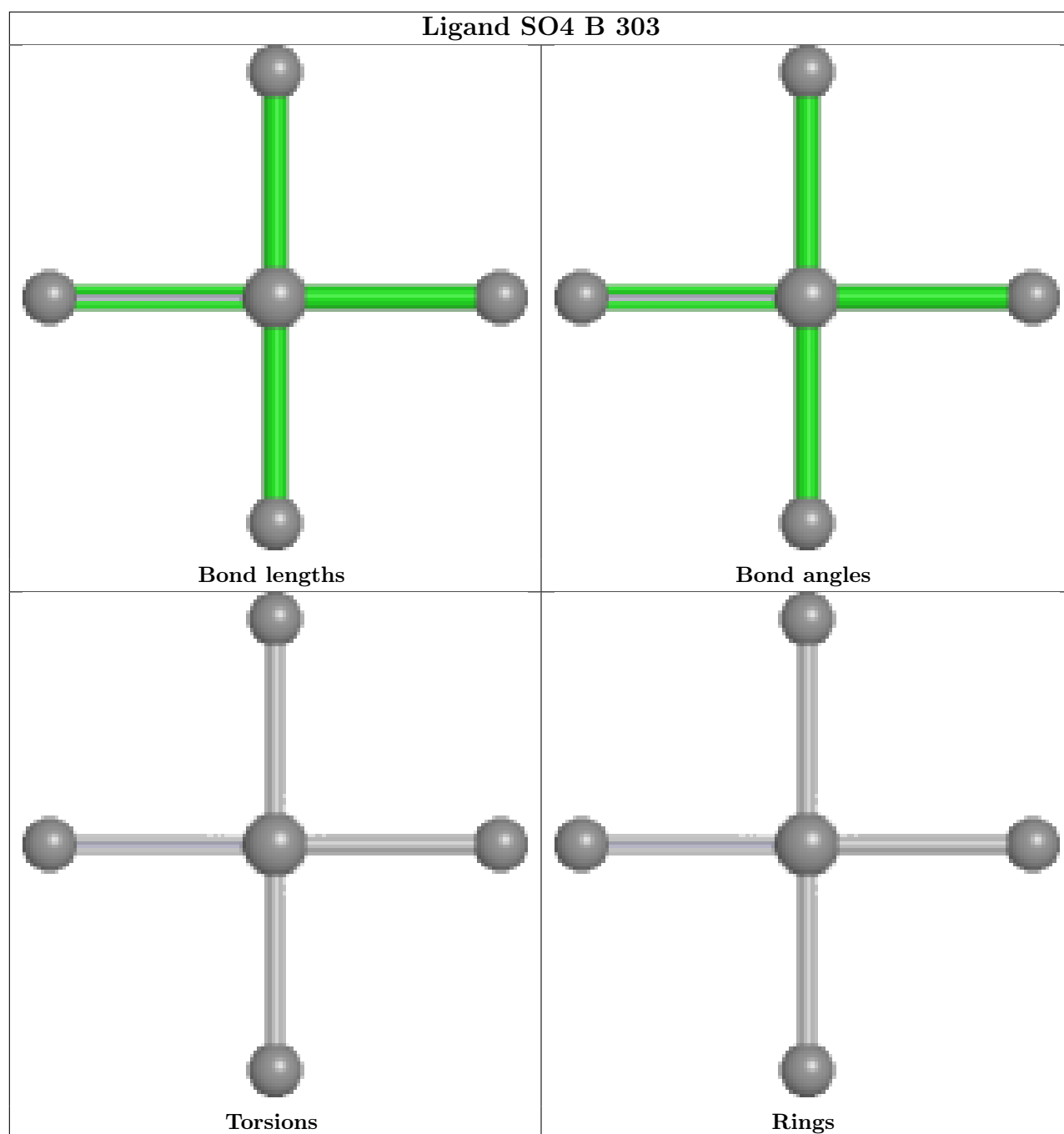


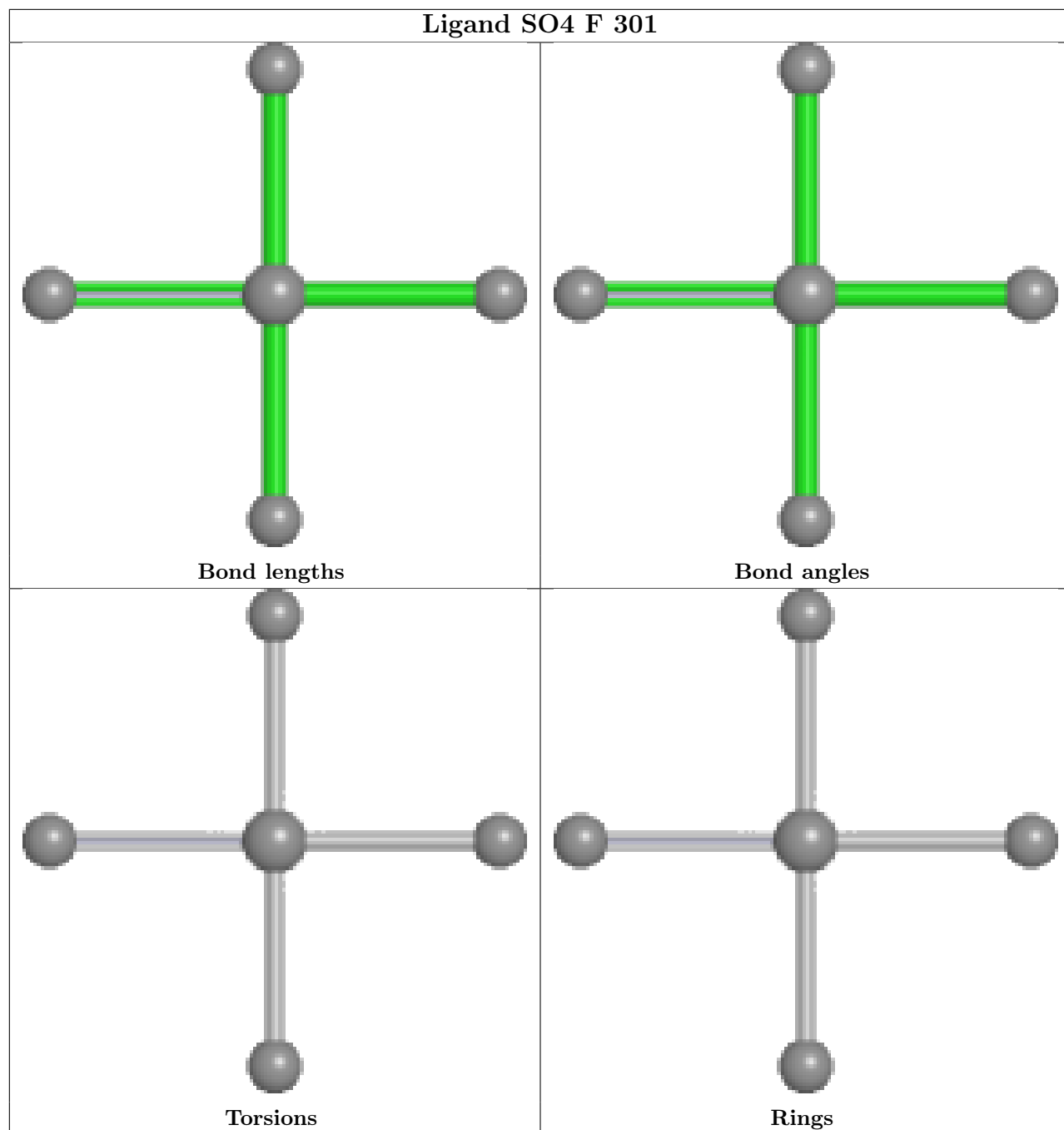


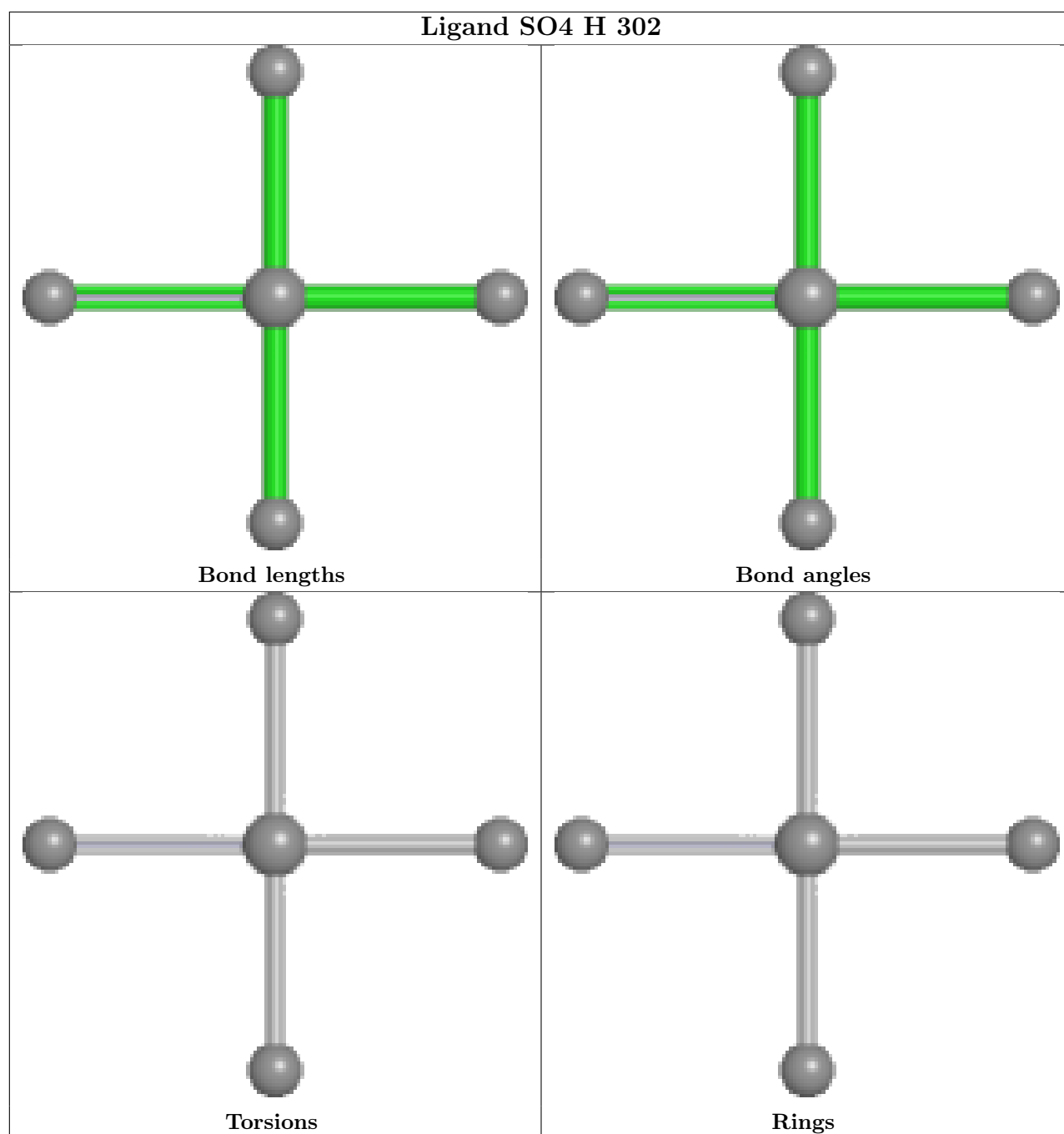


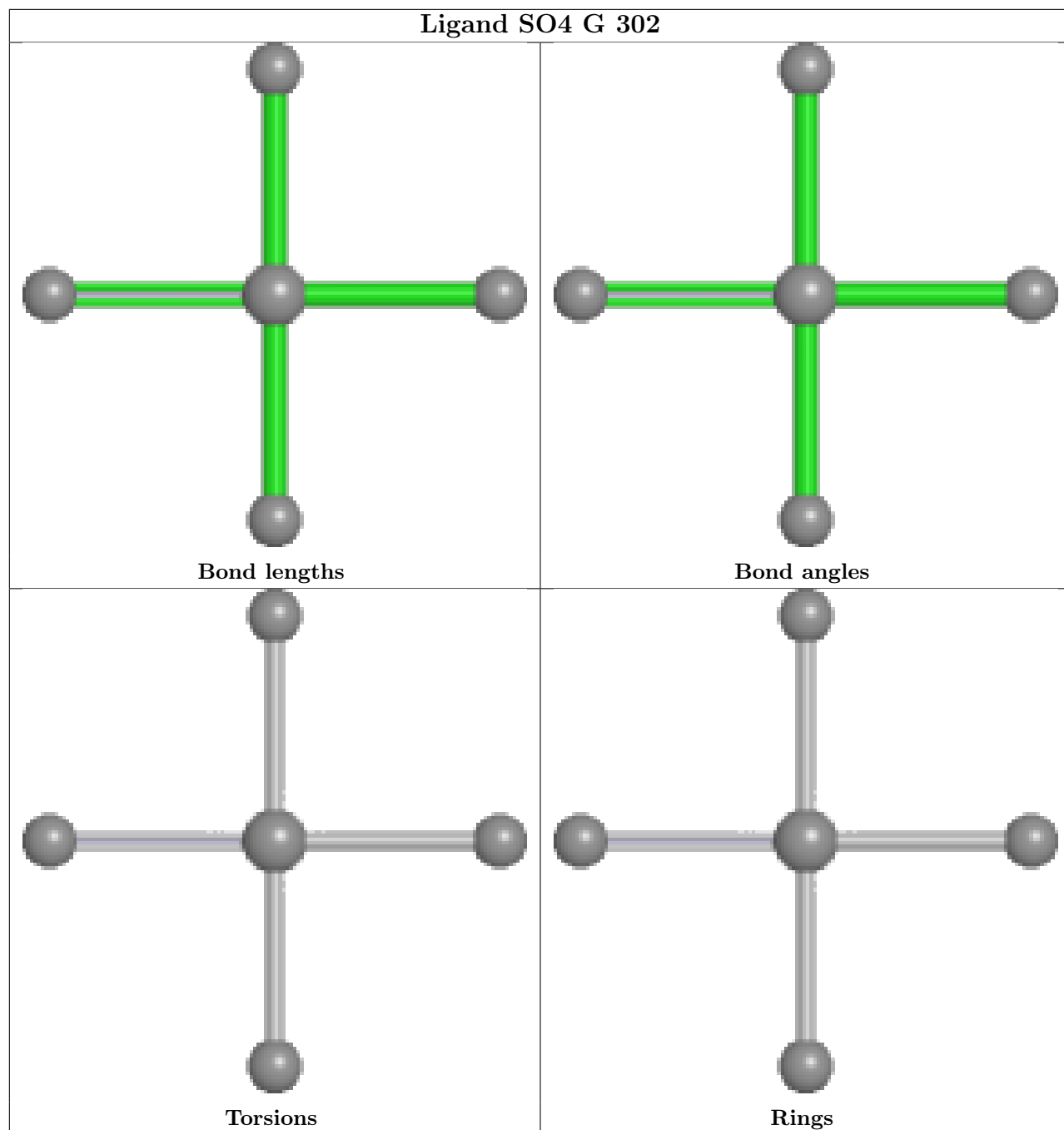


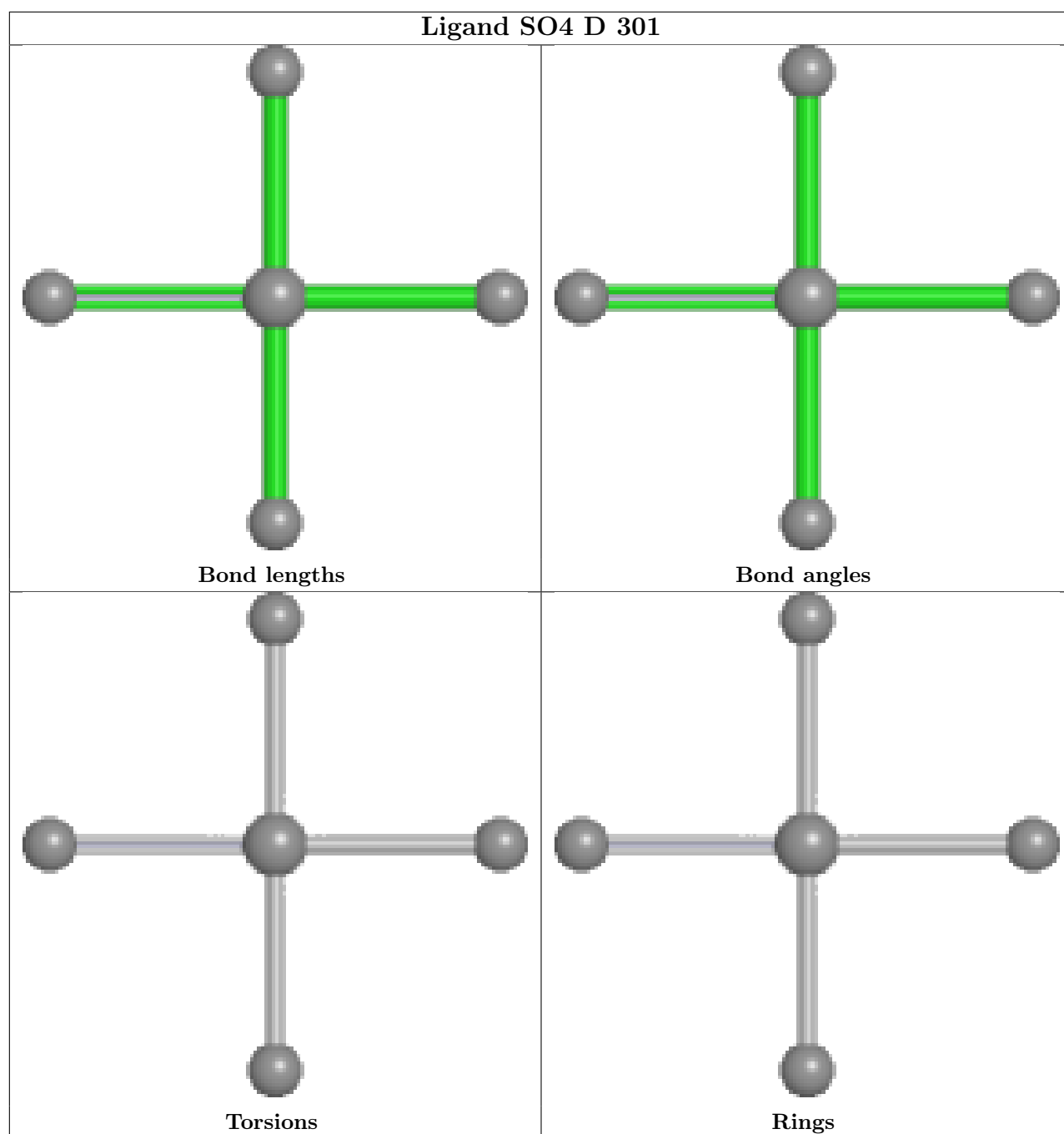


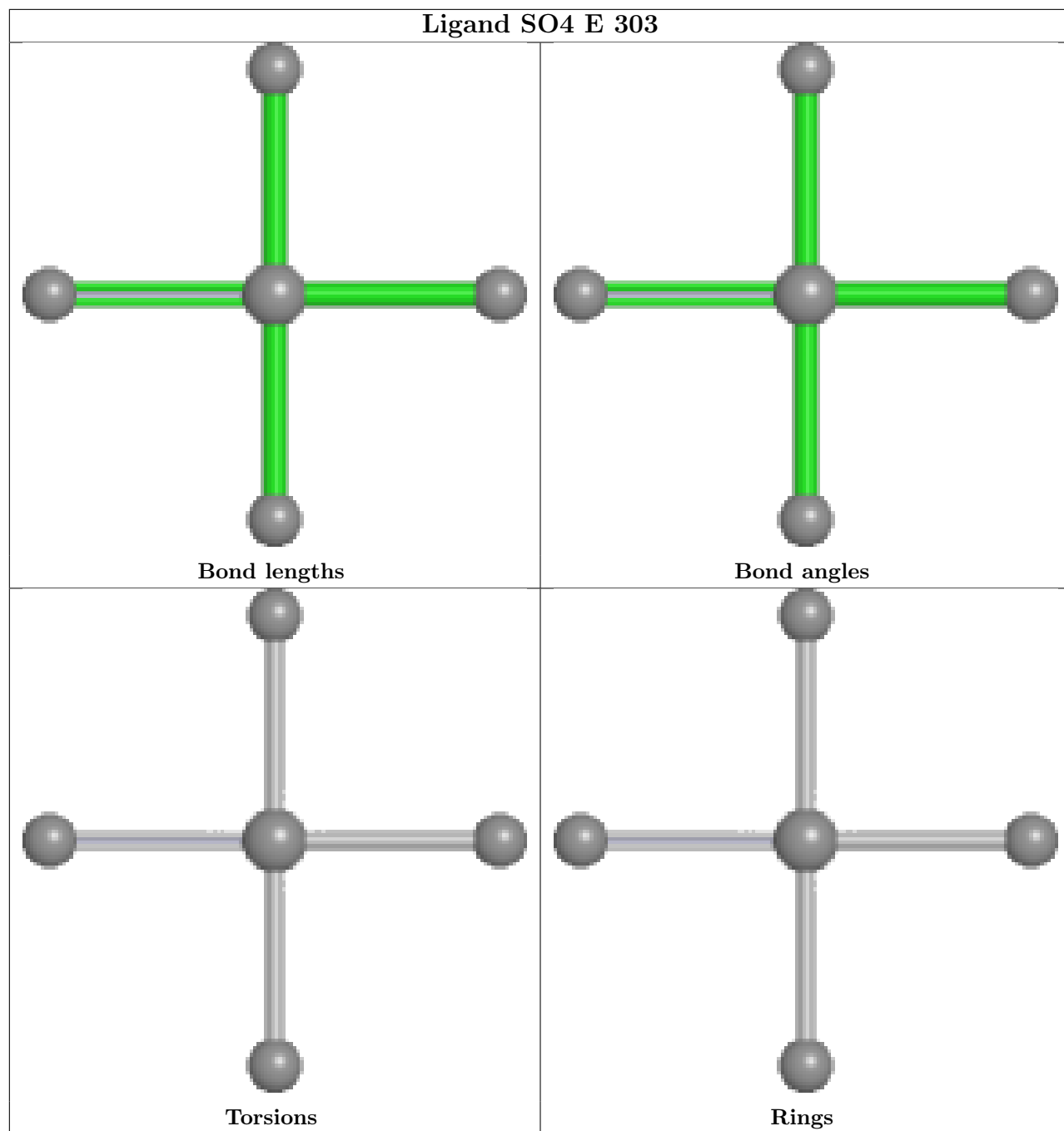


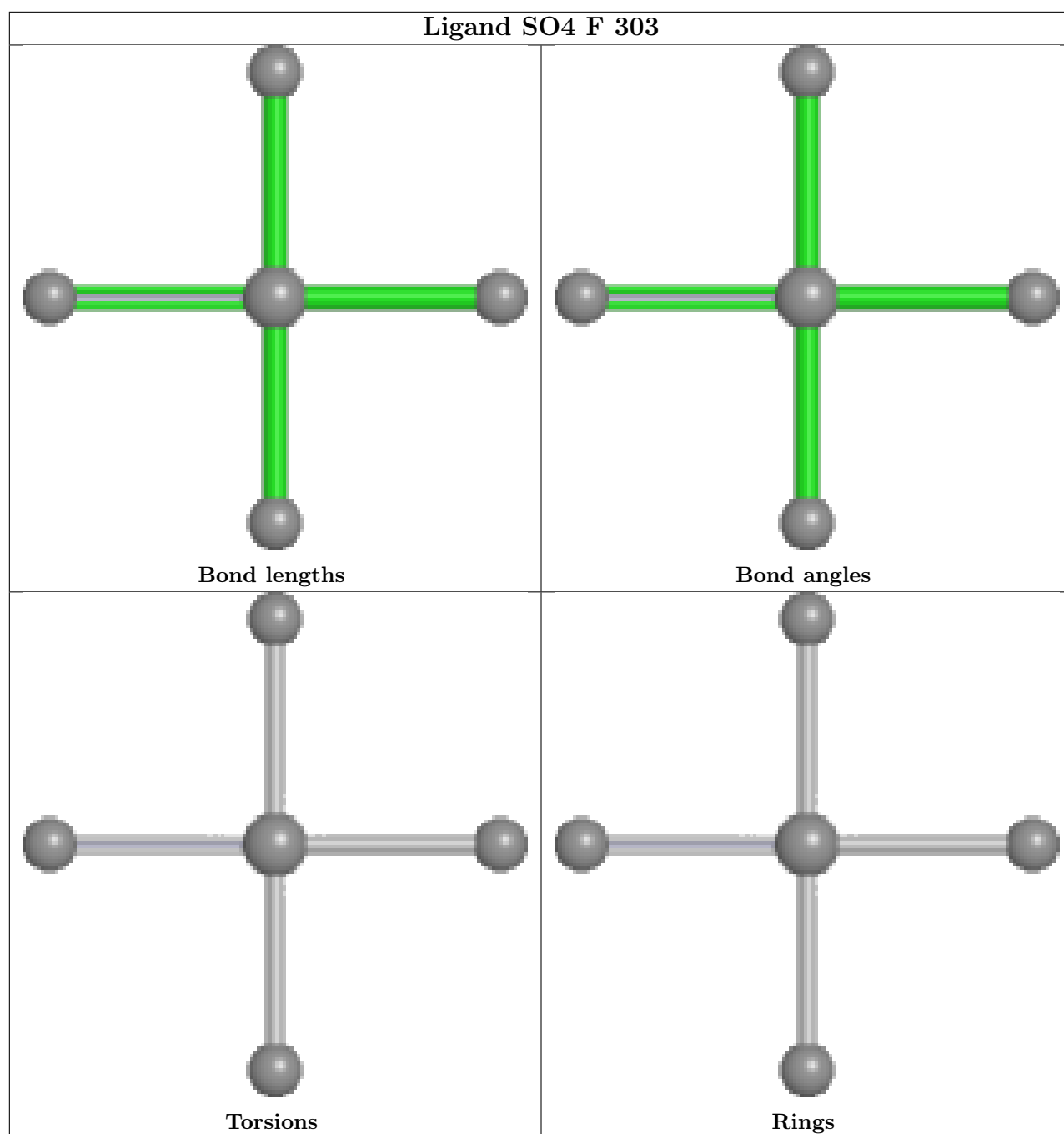


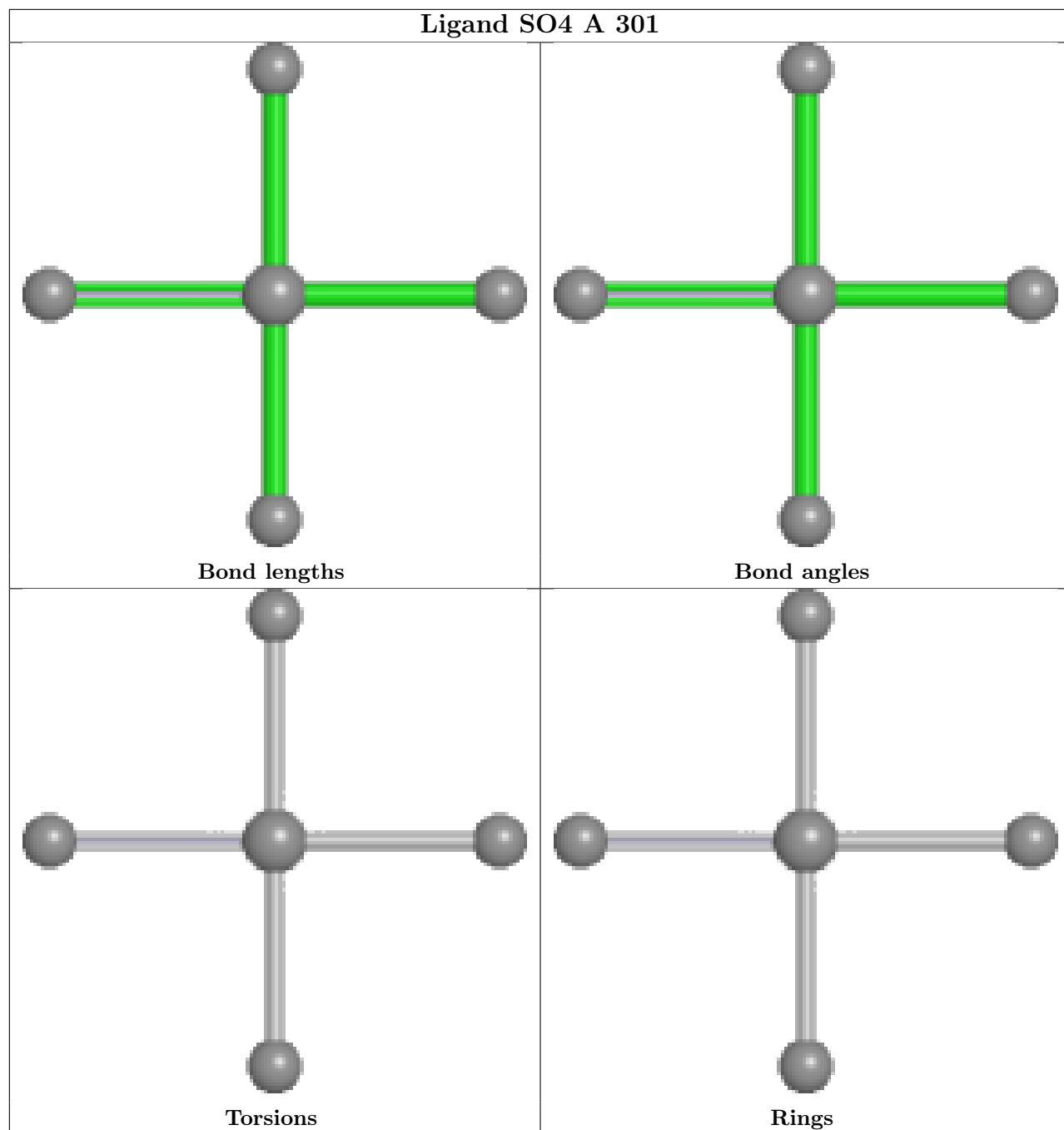


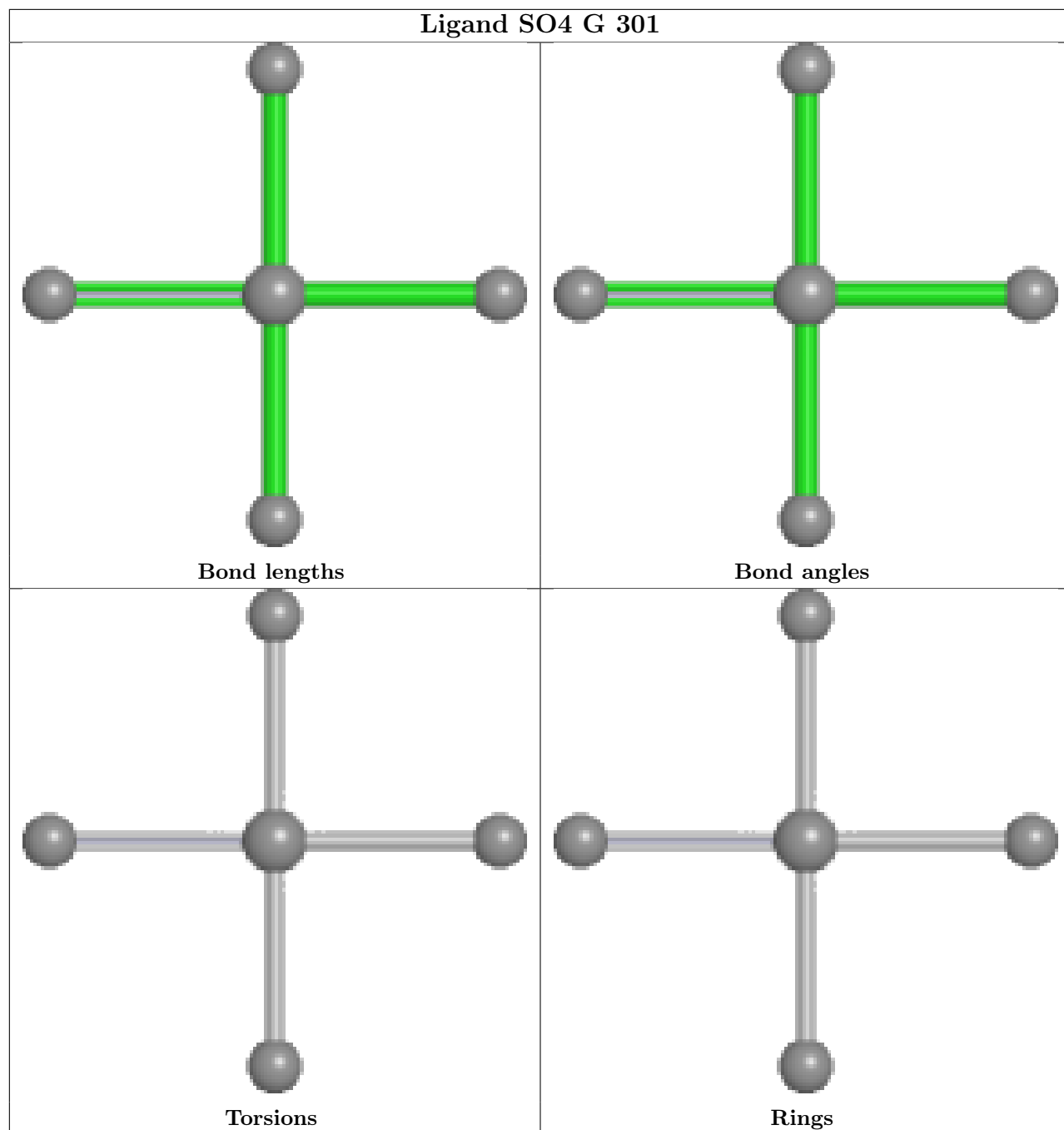


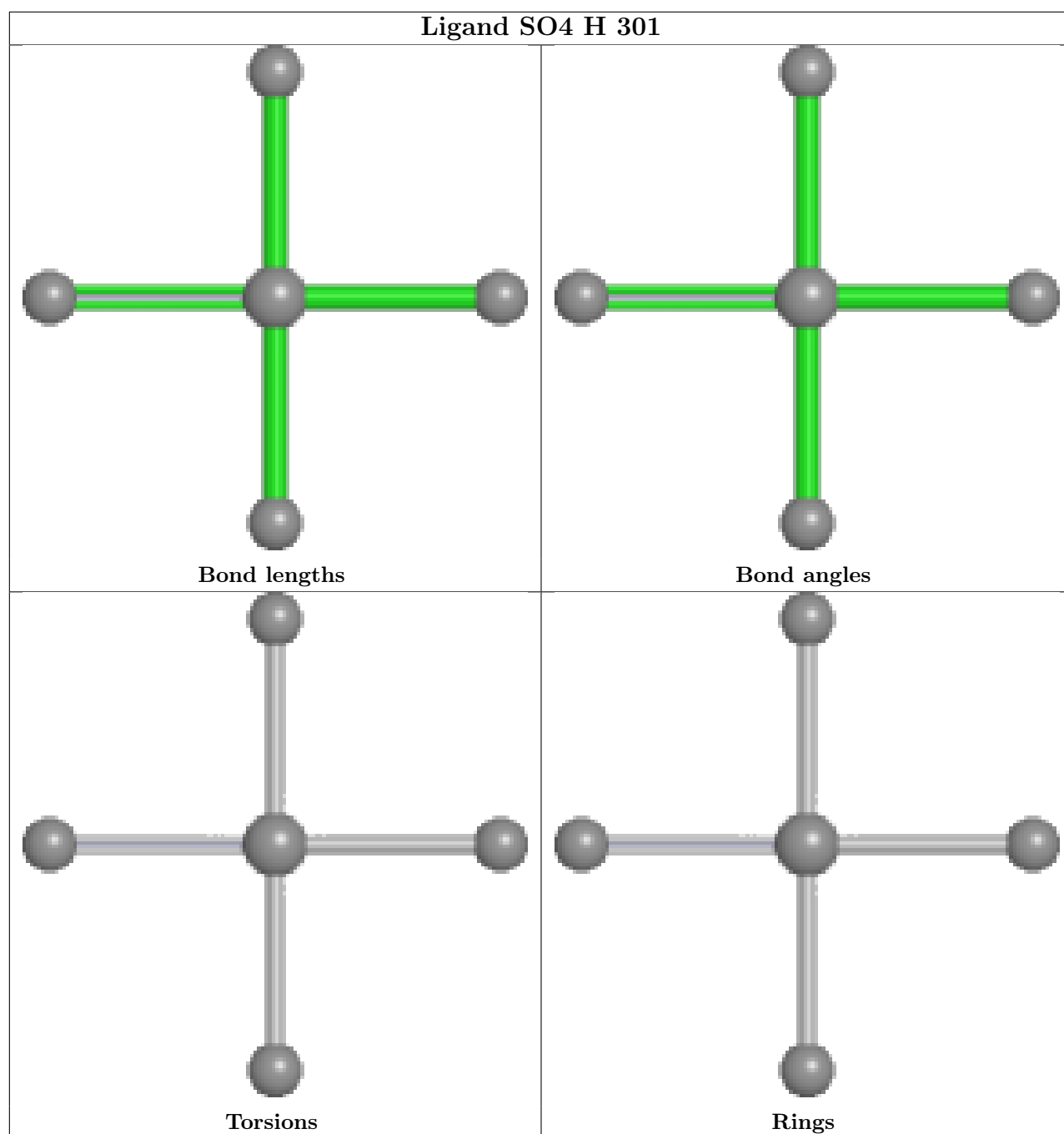


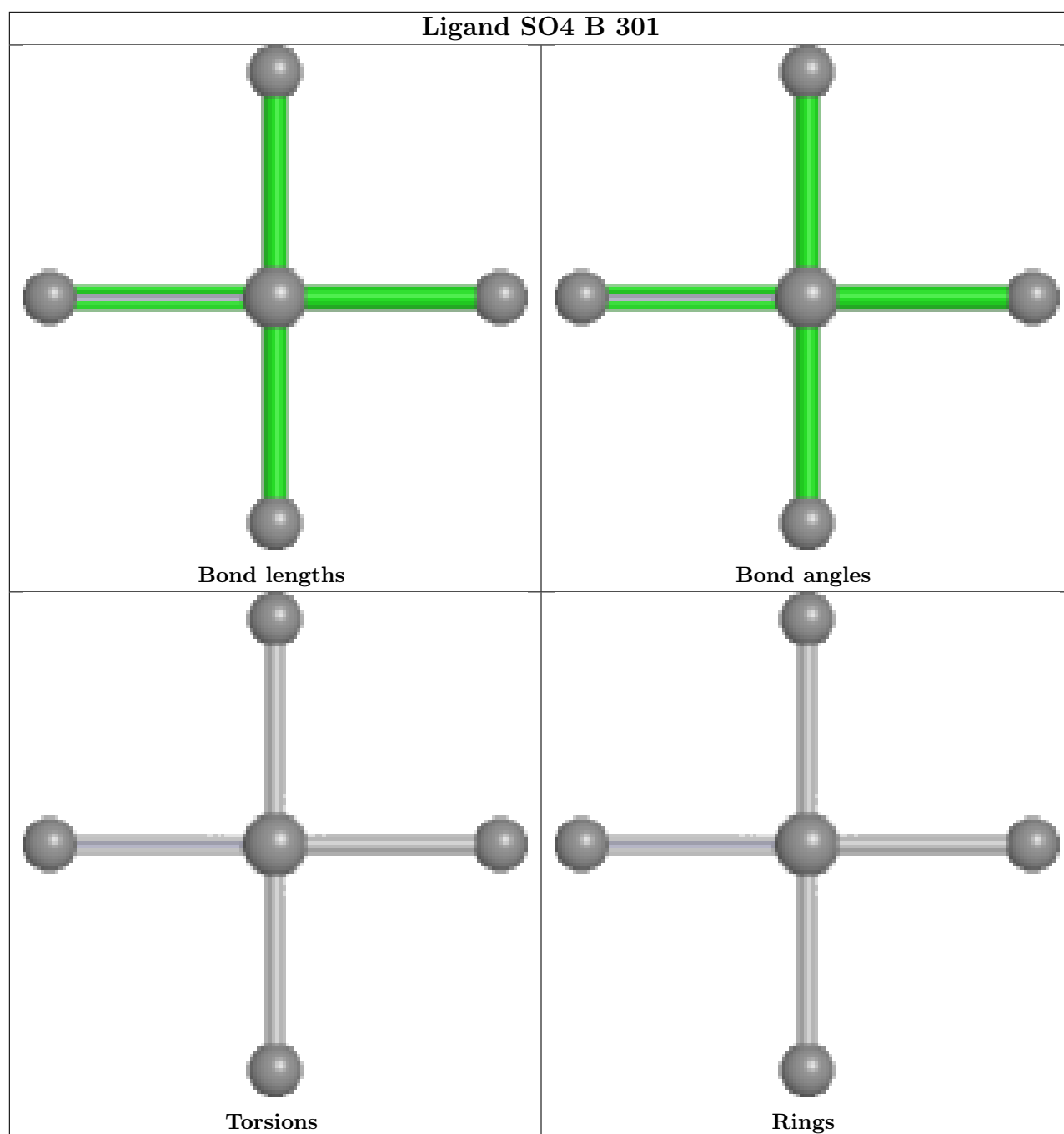


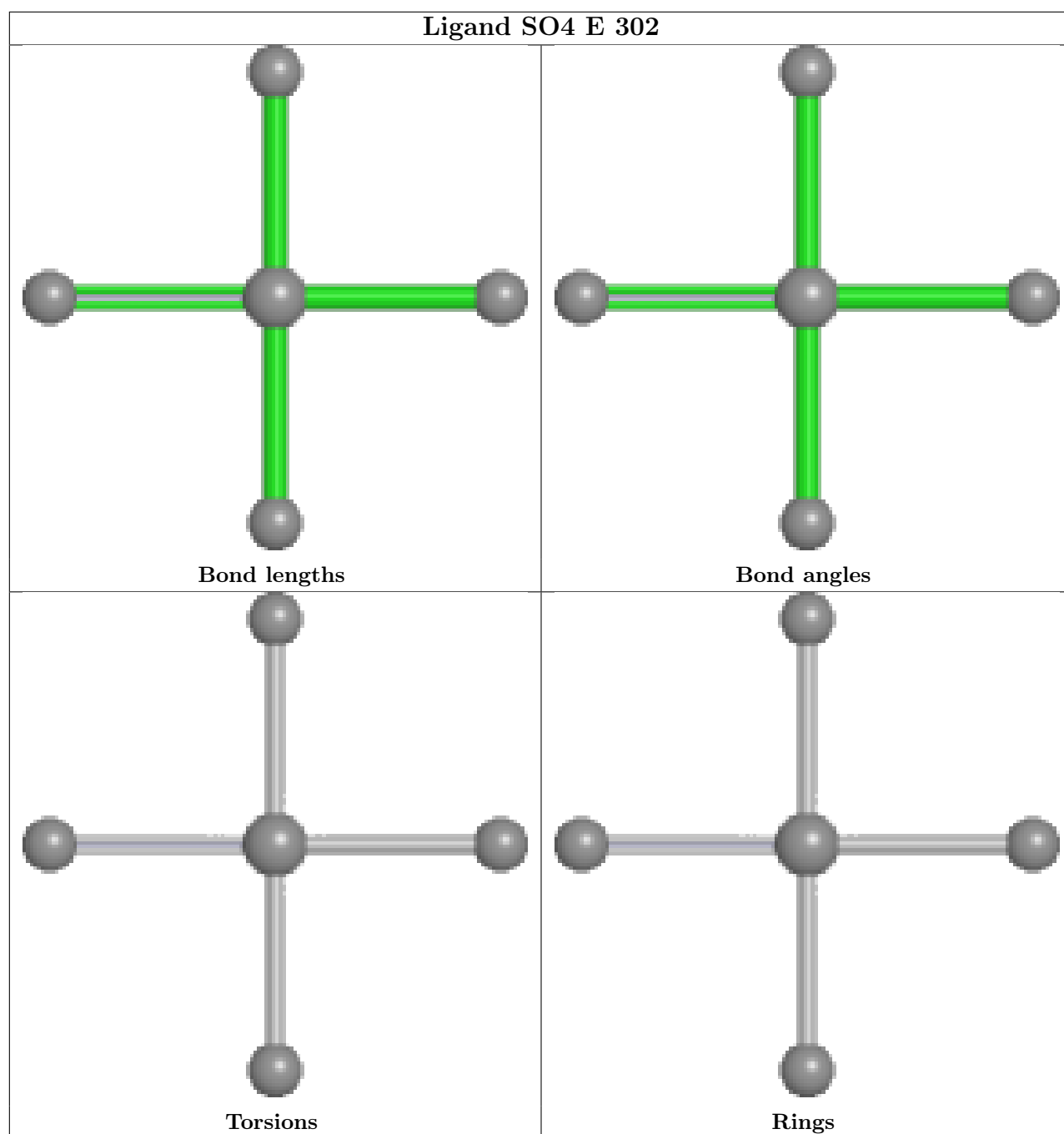


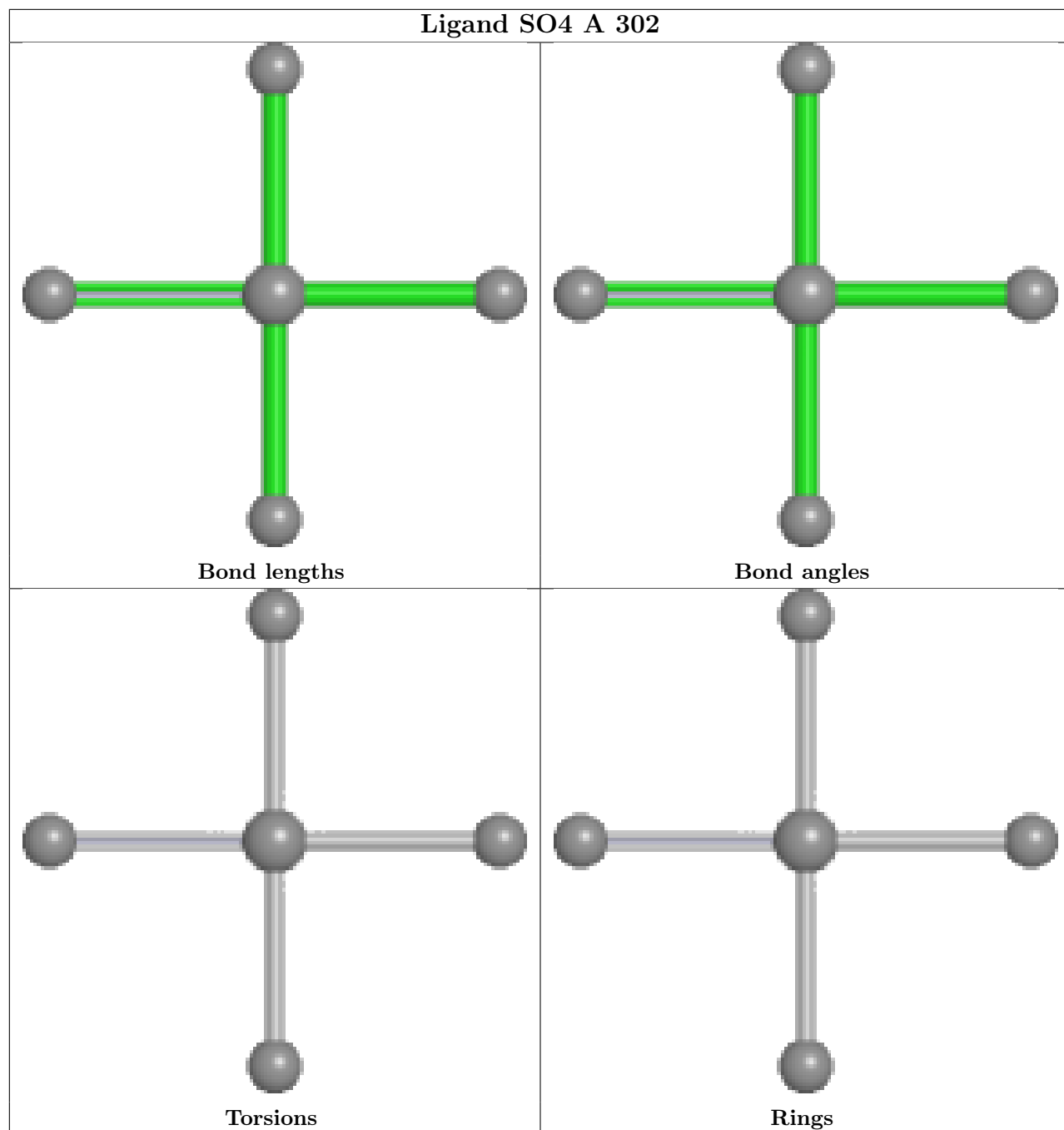


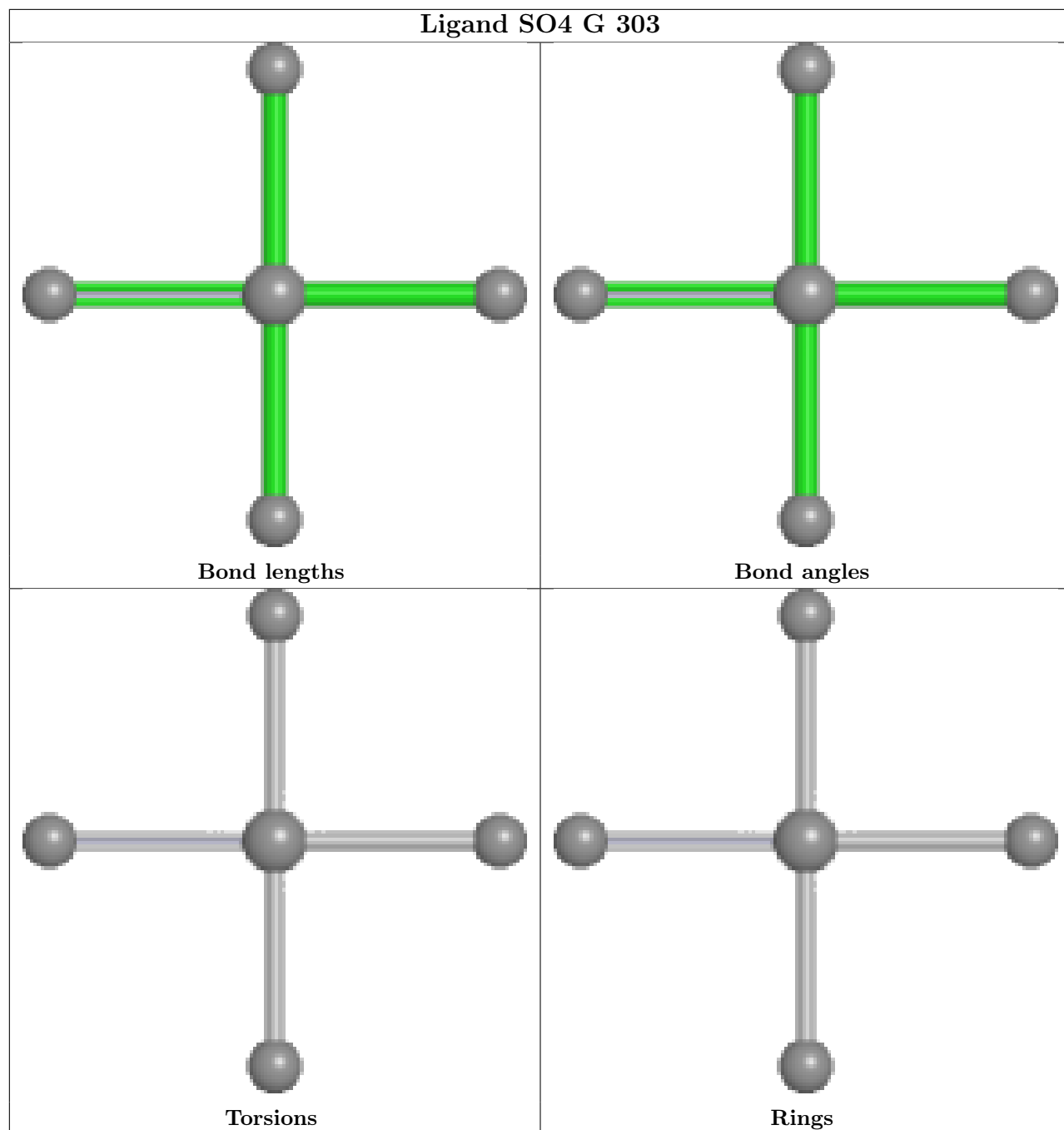


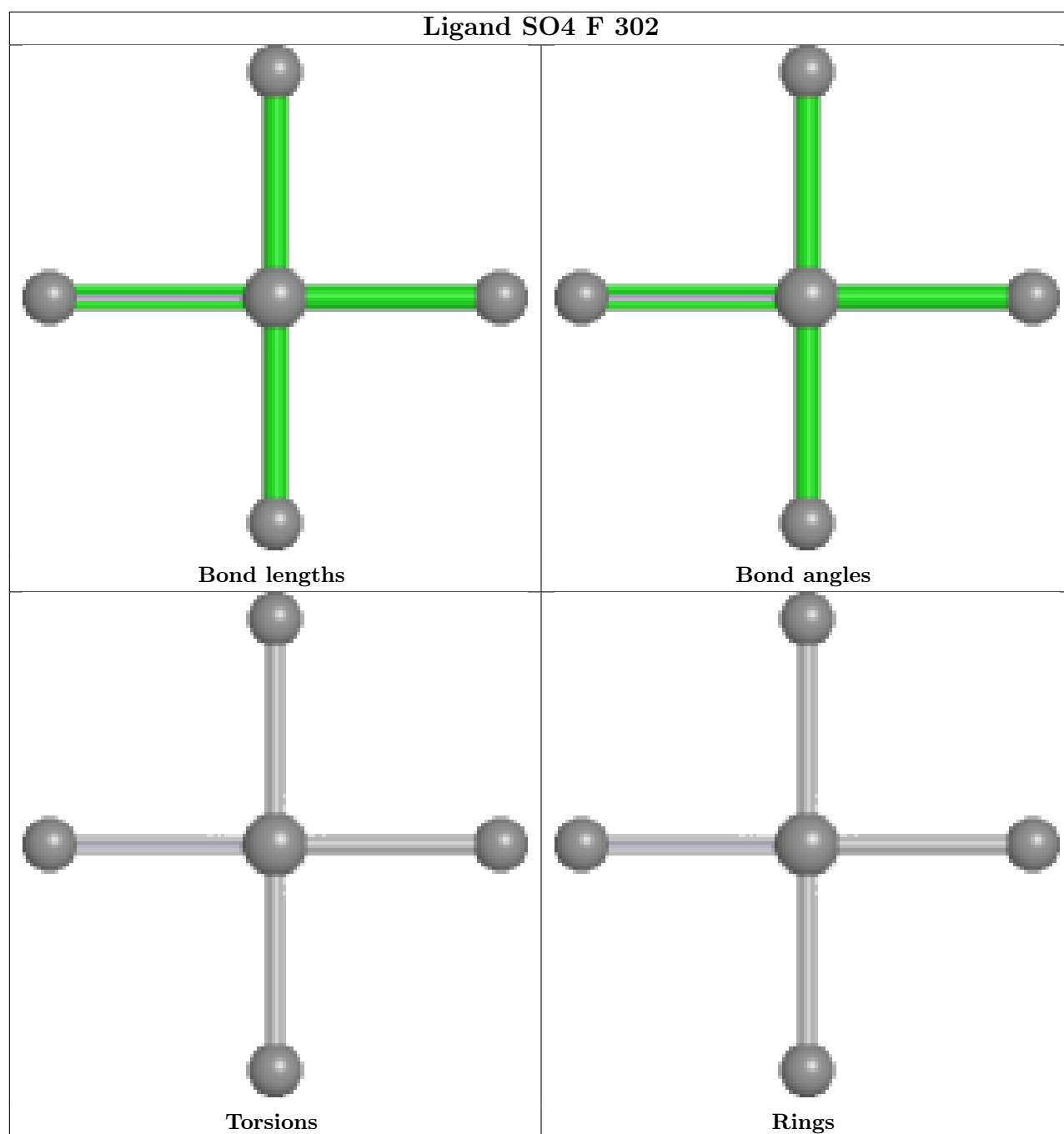


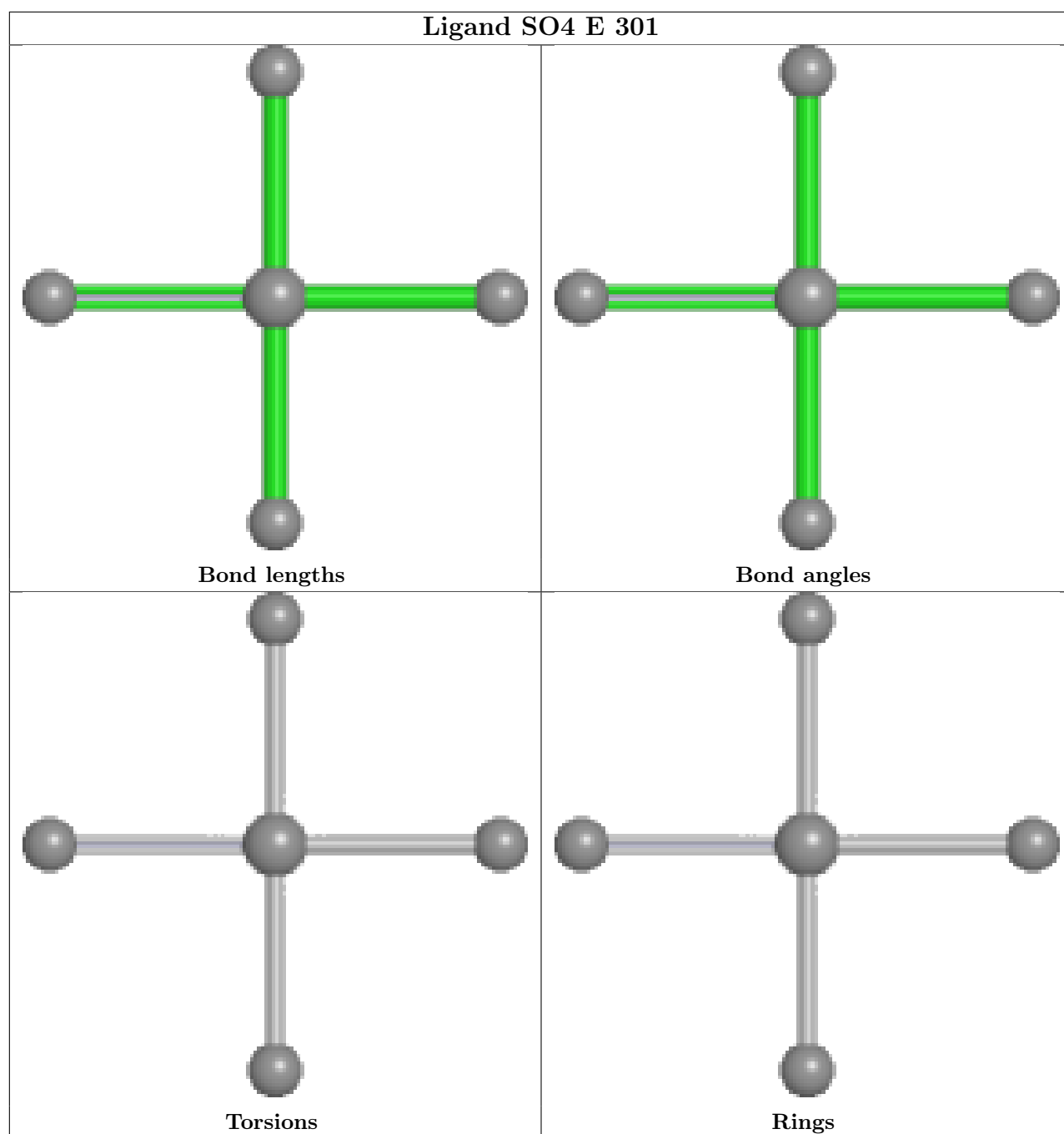












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	256/267 (95%)	-0.06	6 (2%) 61 67	20, 28, 50, 63	0
1	B	261/267 (97%)	-0.14	12 (4%) 37 39	18, 24, 52, 69	0
1	C	256/267 (95%)	-0.25	4 (1%) 70 78	16, 24, 50, 65	0
1	D	257/267 (96%)	-0.12	9 (3%) 47 51	20, 26, 52, 61	0
1	E	248/267 (92%)	-0.22	3 (1%) 76 82	19, 26, 42, 60	0
1	F	257/267 (96%)	-0.07	8 (3%) 51 56	20, 27, 53, 72	0
1	G	266/267 (99%)	-0.15	16 (6%) 27 29	18, 24, 54, 70	0
1	H	258/267 (96%)	-0.22	9 (3%) 47 51	19, 25, 48, 64	0
All	All	2059/2136 (96%)	-0.15	67 (3%) 49 53	16, 26, 51, 72	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	195	ASP	5.6
1	G	196	ILE	5.2
1	B	196	ILE	5.0
1	F	195	ASP	5.0
1	G	-5	HIS	4.4
1	H	196	ILE	4.4
1	A	196	ILE	4.1
1	D	194	THR	4.0
1	F	196	ILE	4.0
1	B	201	LEU	3.9
1	G	195	ASP	3.6
1	G	-9	ARG	3.6
1	H	-1	HIS	3.6
1	D	204	LEU	3.6
1	A	195	ASP	3.5
1	H	201	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	F	201	LEU	3.4
1	D	195	ASP	3.4
1	G	194	THR	3.4
1	F	194	THR	3.3
1	C	204	LEU	3.3
1	A	204	LEU	3.3
1	G	202	SER	3.3
1	C	196	ILE	3.2
1	G	-8	GLY	3.2
1	B	-1	HIS	3.1
1	B	200	ASP	3.1
1	B	-3	HIS	3.1
1	C	256	GLN	3.0
1	H	256	GLN	3.0
1	B	-4	HIS	3.0
1	B	202	SER	3.0
1	H	200	ASP	3.0
1	D	201	LEU	2.9
1	G	200	ASP	2.9
1	C	195	ASP	2.8
1	G	256	GLN	2.8
1	B	198	LYS	2.7
1	H	195	ASP	2.7
1	G	-7	SER	2.7
1	B	-2	HIS	2.7
1	D	256	GLN	2.6
1	E	204	LEU	2.6
1	G	-6	HIS	2.6
1	B	256	GLN	2.6
1	G	204	LEU	2.6
1	F	200	ASP	2.5
1	B	199	GLU	2.4
1	G	199	GLU	2.4
1	G	-3	HIS	2.4
1	A	201	LEU	2.4
1	F	198	LYS	2.4
1	G	197	ASN	2.4
1	H	202	SER	2.4
1	A	47	LEU	2.3
1	F	204	LEU	2.3
1	G	201	LEU	2.3
1	A	200	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	200	ASP	2.2
1	D	196	ILE	2.2
1	D	197	ASN	2.2
1	H	198	LYS	2.2
1	D	202	SER	2.1
1	H	0	GLY	2.1
1	E	55	ALA	2.1
1	E	0	GLY	2.1
1	F	256	GLN	2.1

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(Å ²)	Q<0.9
2	SO4	D	303	5/5	0.60	0.13	69,72,77,81	0
2	SO4	C	303	5/5	0.77	0.11	61,62,68,71	0
2	SO4	D	302	5/5	0.80	0.11	43,51,60,61	0
2	SO4	G	303	5/5	0.84	0.10	62,63,64,70	0
2	SO4	B	302	5/5	0.85	0.11	41,49,58,58	0
2	SO4	C	302	5/5	0.85	0.10	45,55,61,64	0
2	SO4	E	302	5/5	0.86	0.10	46,52,59,59	0
2	SO4	E	303	5/5	0.87	0.08	57,64,69,73	0
2	SO4	A	301	5/5	0.87	0.10	45,50,56,59	0
2	SO4	F	303	5/5	0.90	0.08	65,69,70,71	0
2	SO4	G	302	5/5	0.90	0.09	40,47,51,54	0
2	SO4	B	303	5/5	0.90	0.07	56,59,63,68	0
2	SO4	F	302	5/5	0.91	0.08	44,45,55,56	0
2	SO4	H	303	5/5	0.92	0.07	51,57,60,62	0

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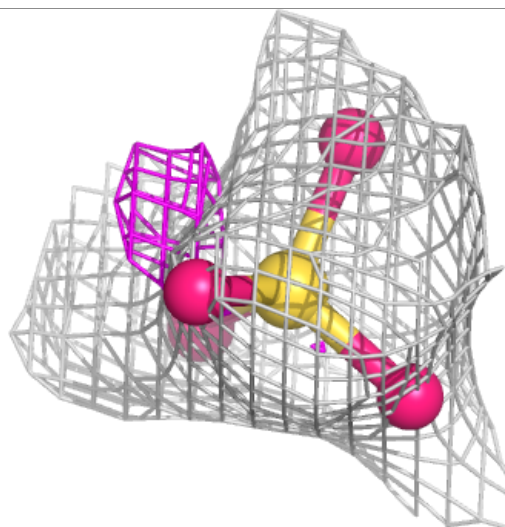
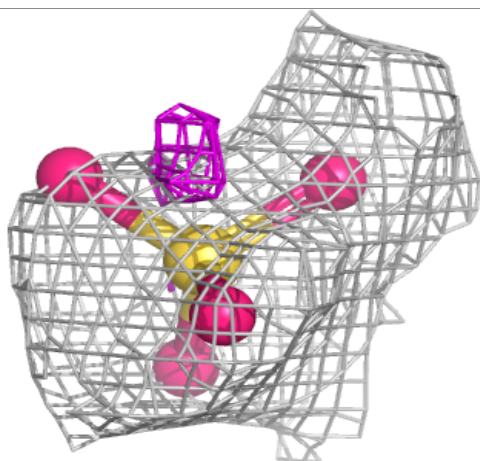
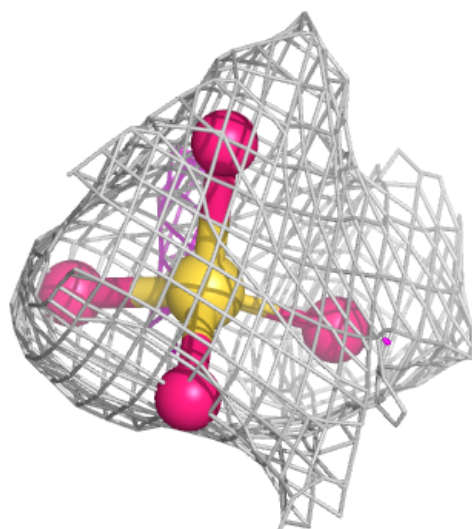
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	H	302	5/5	0.93	0.07	45,47,53,56	0
2	SO4	A	303	5/5	0.93	0.07	59,59,63,64	0
2	SO4	D	301	5/5	0.97	0.06	32,38,41,44	0
2	SO4	F	301	5/5	0.97	0.08	34,39,40,41	0
2	SO4	E	301	5/5	0.97	0.10	36,40,42,46	0
2	SO4	C	301	5/5	0.97	0.07	32,35,39,41	0
2	SO4	B	301	5/5	0.98	0.10	31,31,38,39	0
2	SO4	H	301	5/5	0.98	0.08	30,34,38,38	0
2	SO4	G	301	5/5	0.98	0.07	30,32,33,39	0
2	SO4	A	302	5/5	0.98	0.07	38,39,39,45	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.

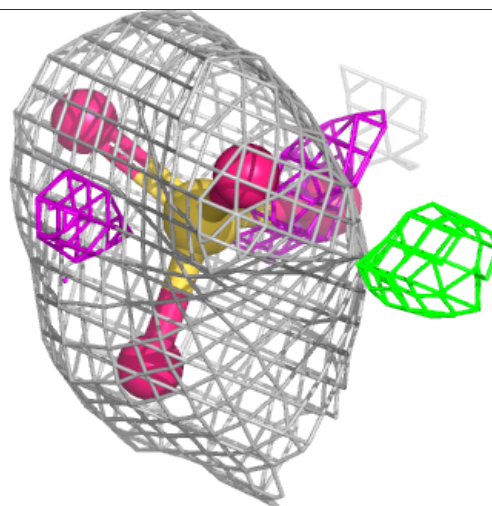
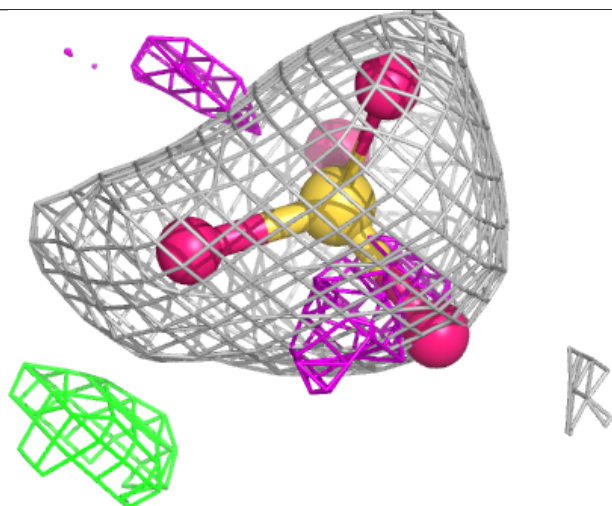
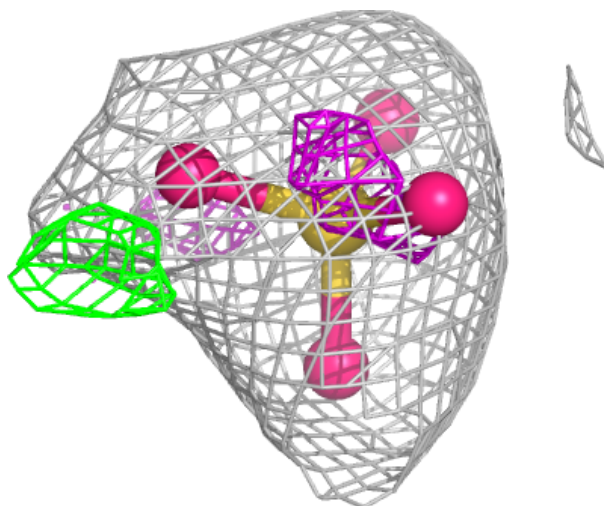
Electron density around SO4 D 303:

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



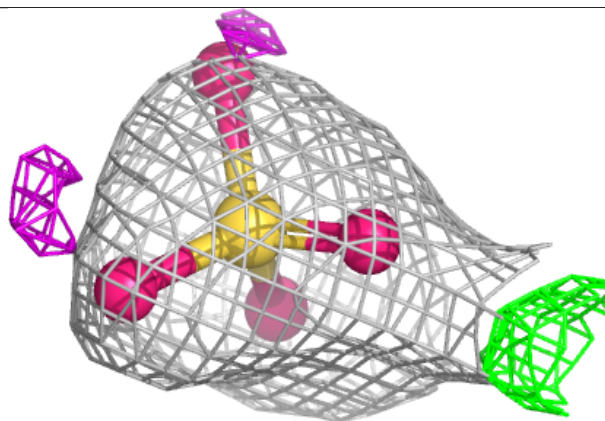
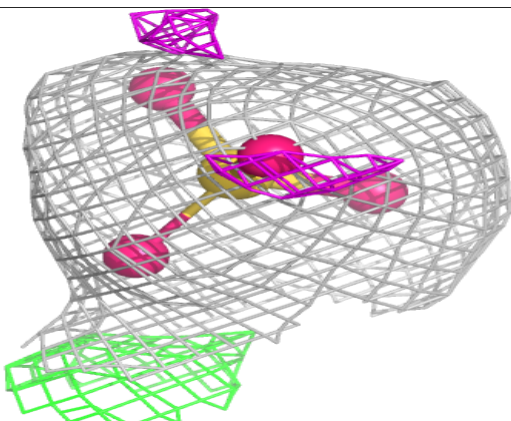
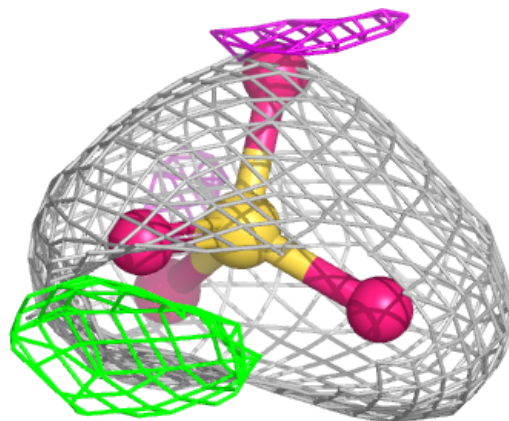
Electron density around SO4 C 303:

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and green (positive)



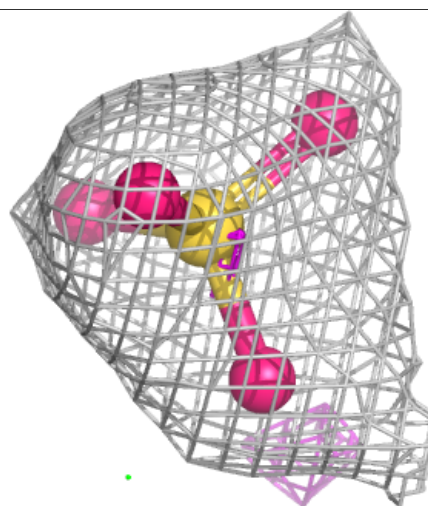
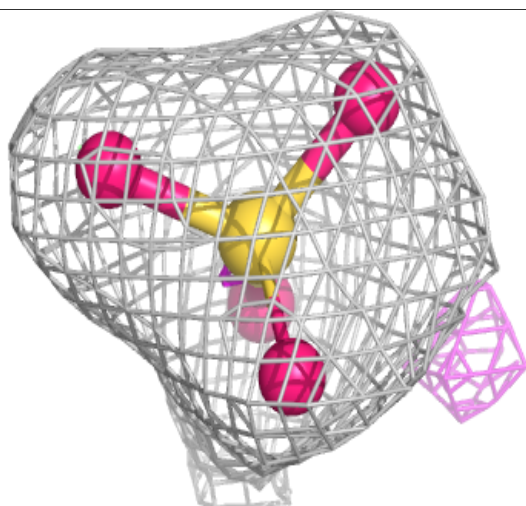
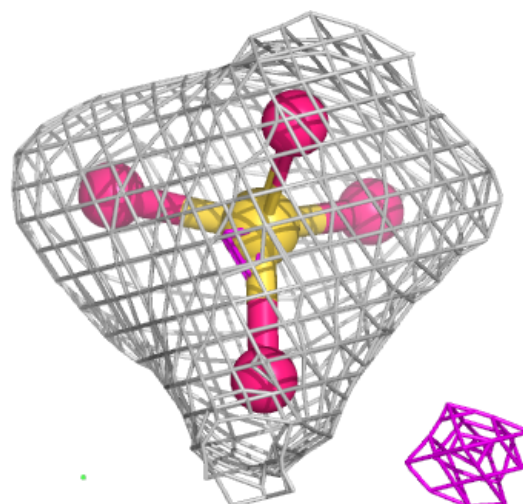
Electron density around SO4 D 302:

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and green (positive)



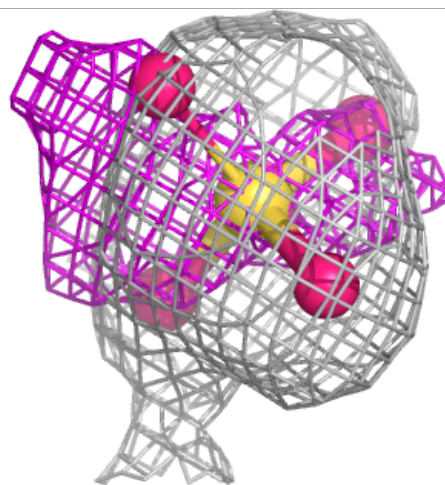
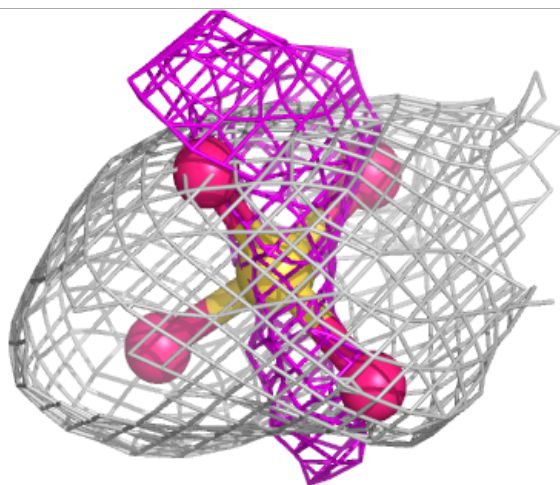
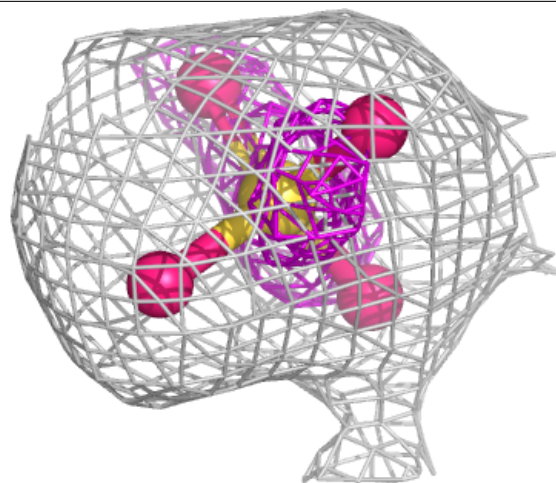
Electron density around SO4 G 303:

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and green (positive)



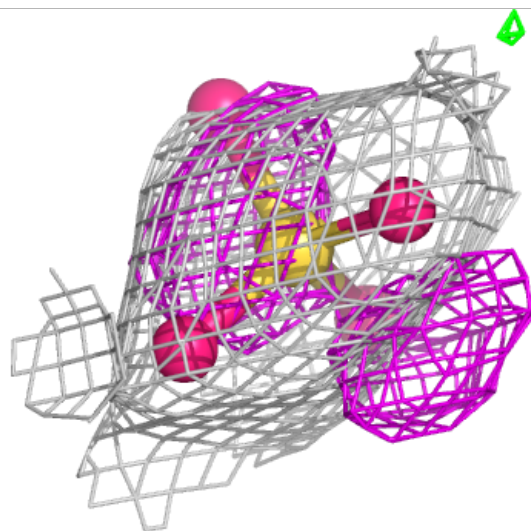
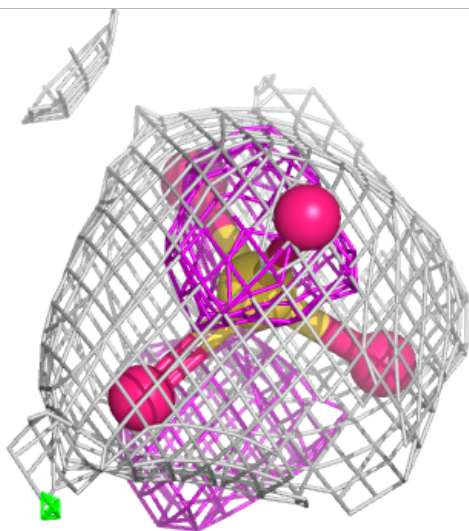
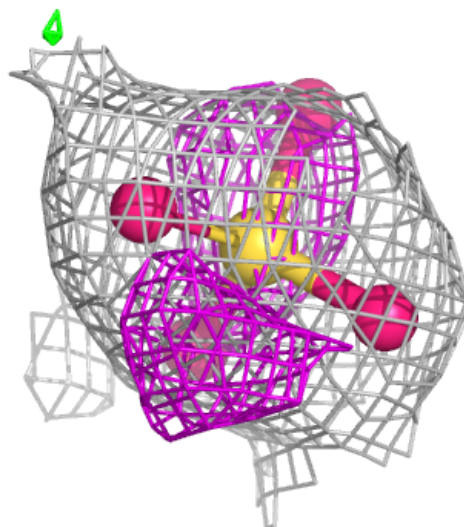
Electron density around SO4 B 302:

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and green (positive)



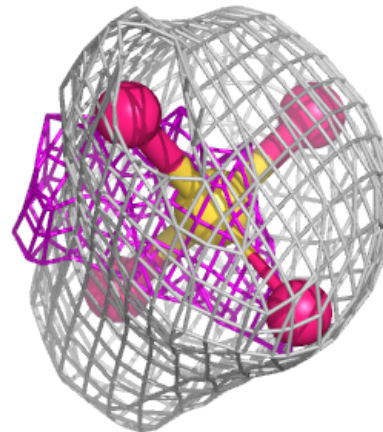
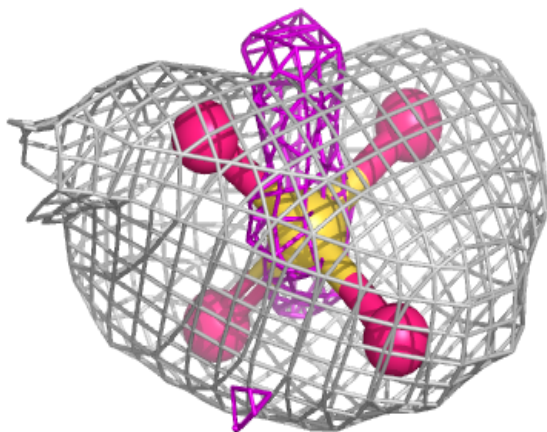
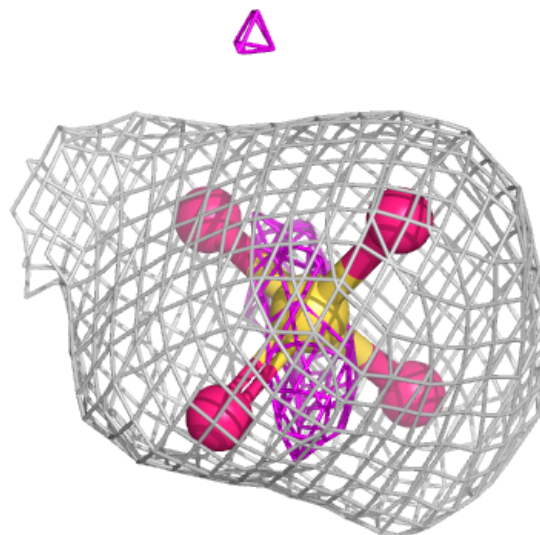
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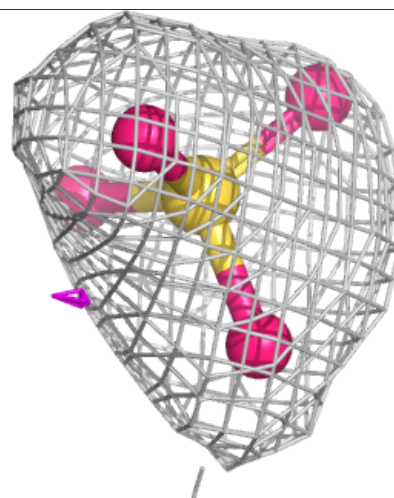
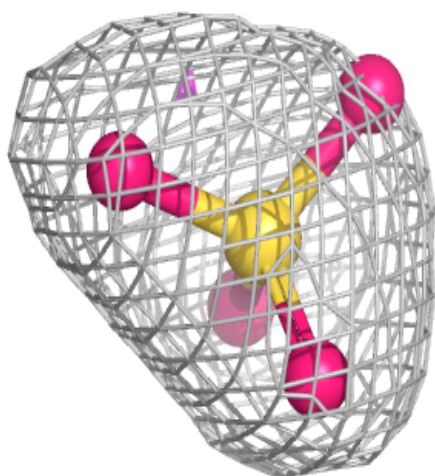
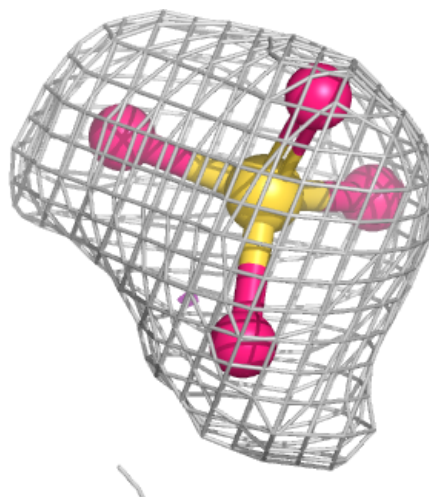
Electron density around SO4 E 302:

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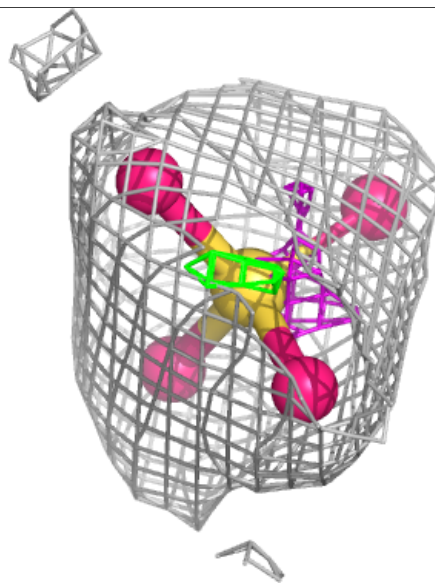
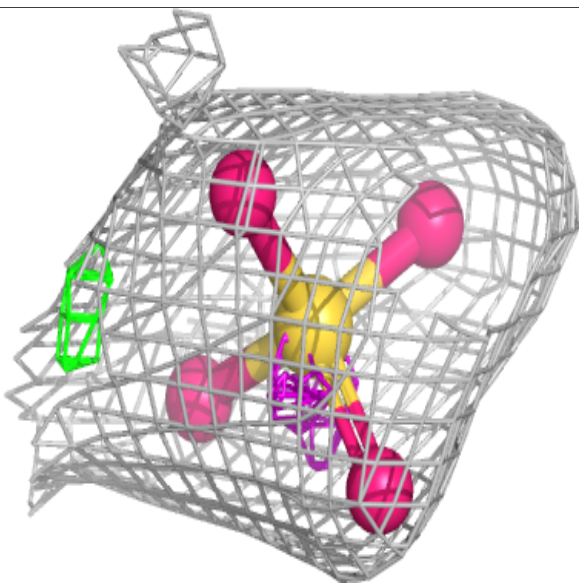
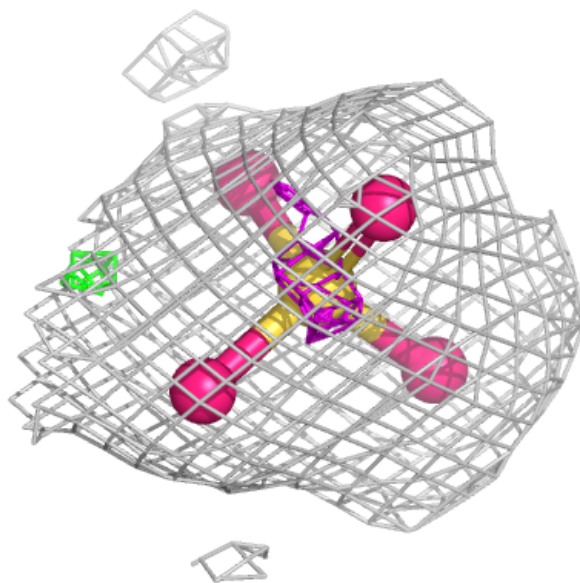
Electron density around SO4 E 303:

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and green (positive)



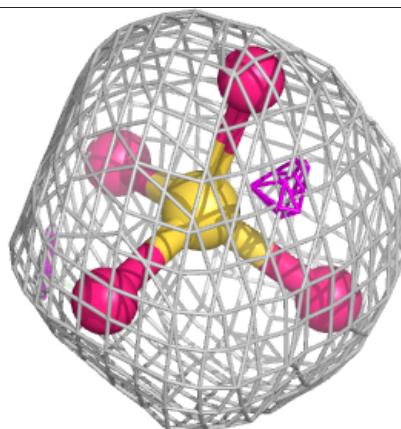
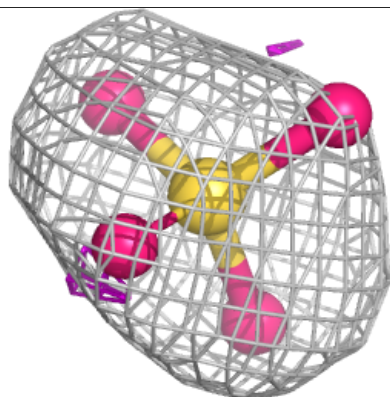
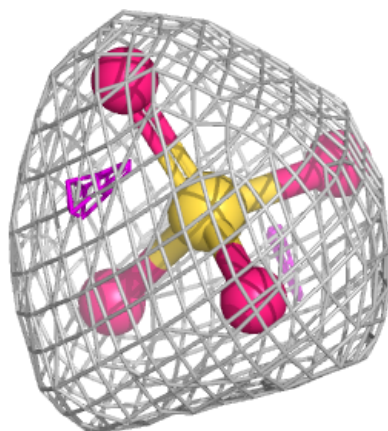
Electron density around SO4 A 301:

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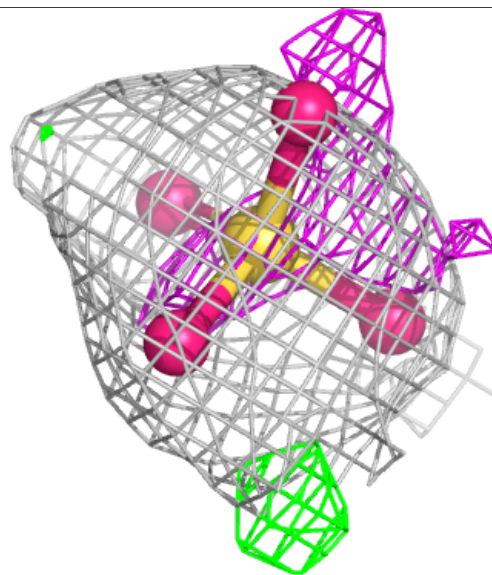
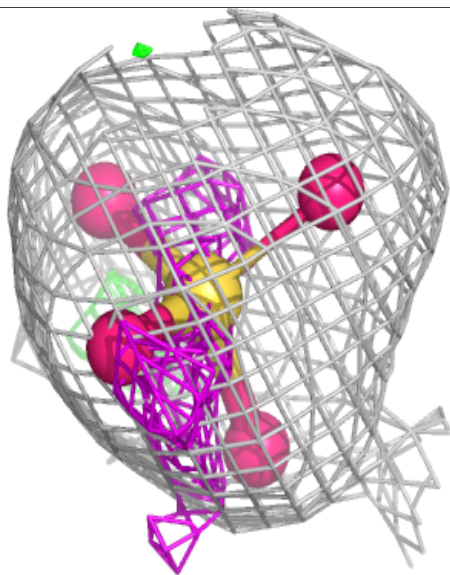
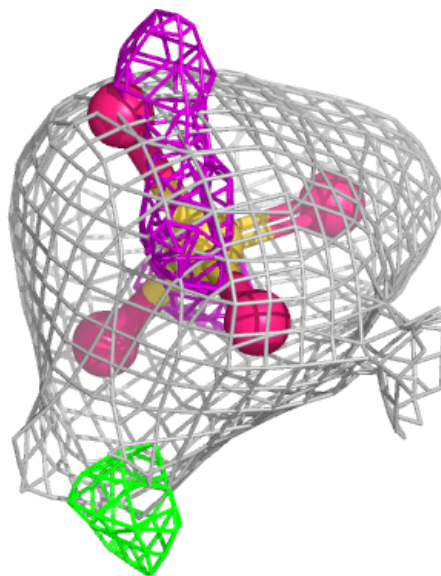
Electron density around SO4 F 303:

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and green (positive)



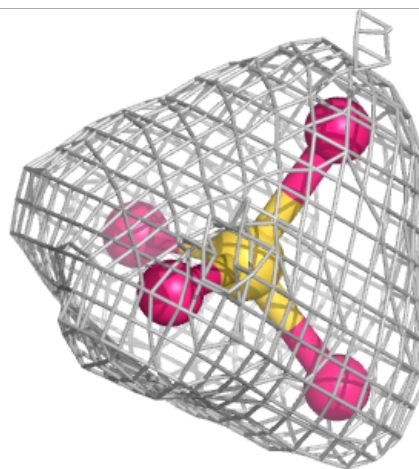
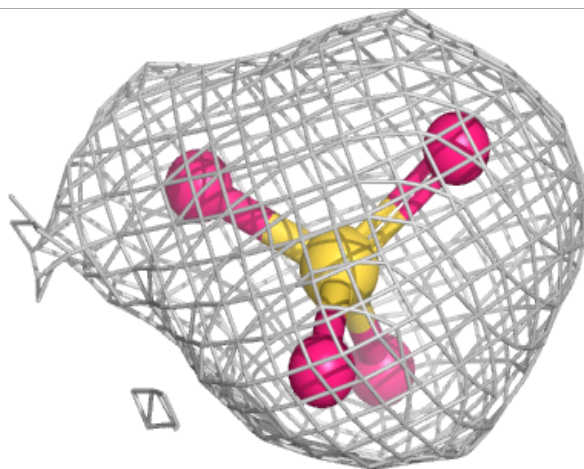
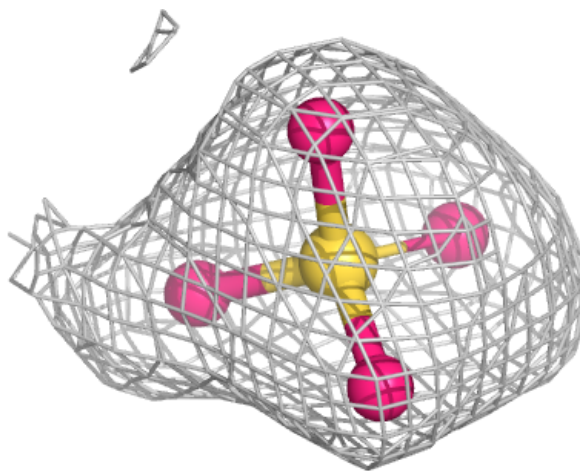
Electron density around SO4 G 302:

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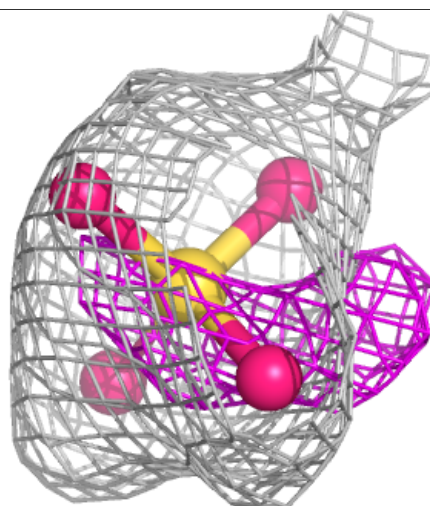
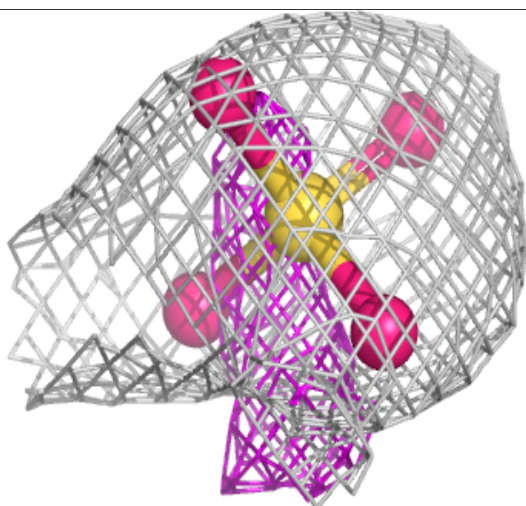
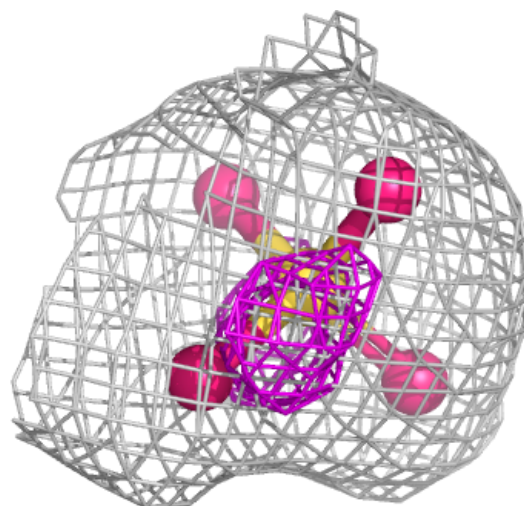
Electron density around SO4 B 303:

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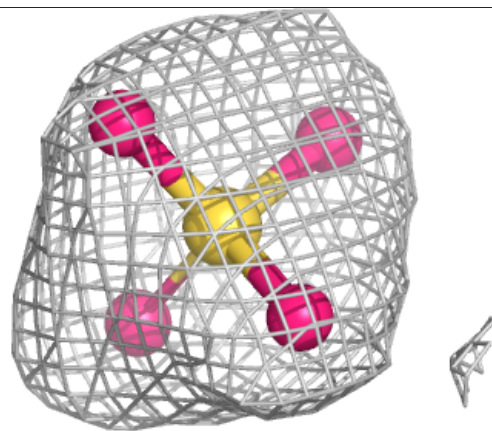
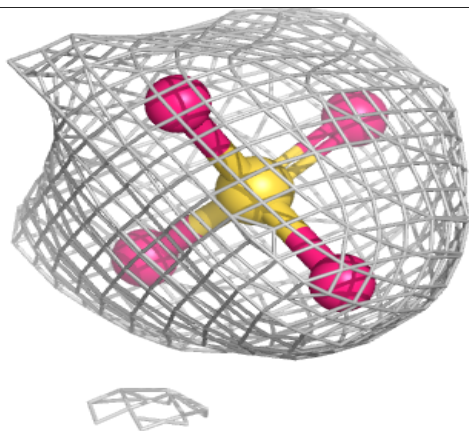
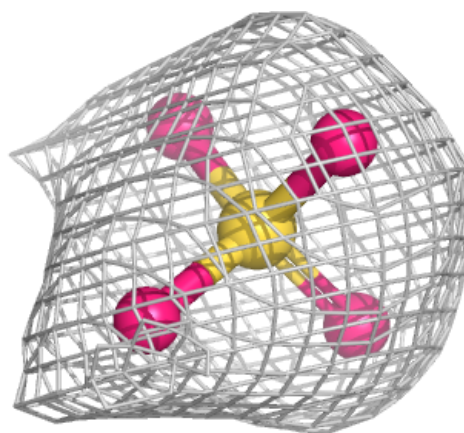
Electron density around SO4 F 302:

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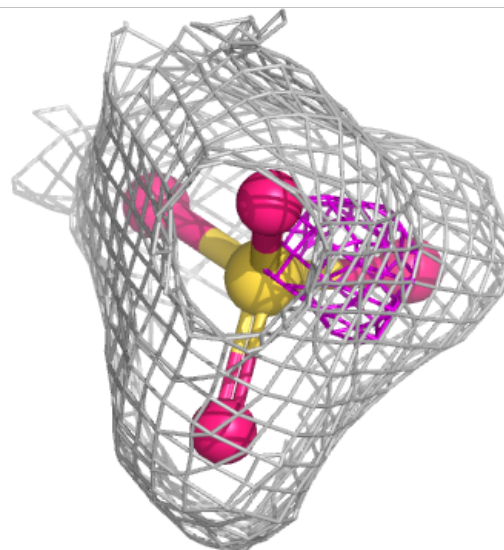
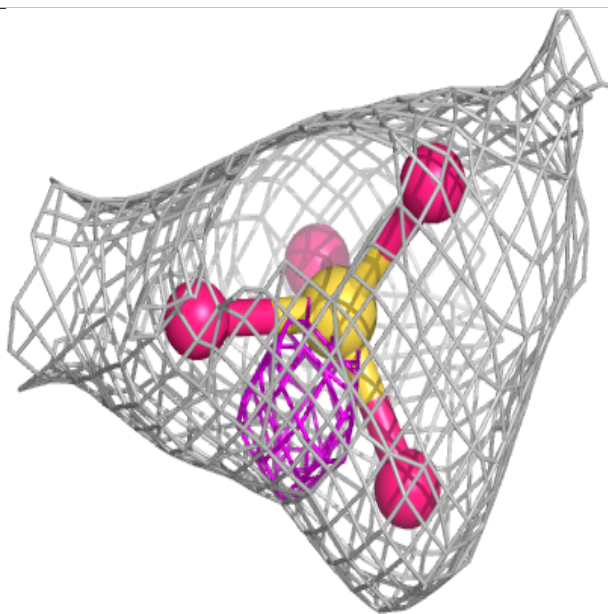
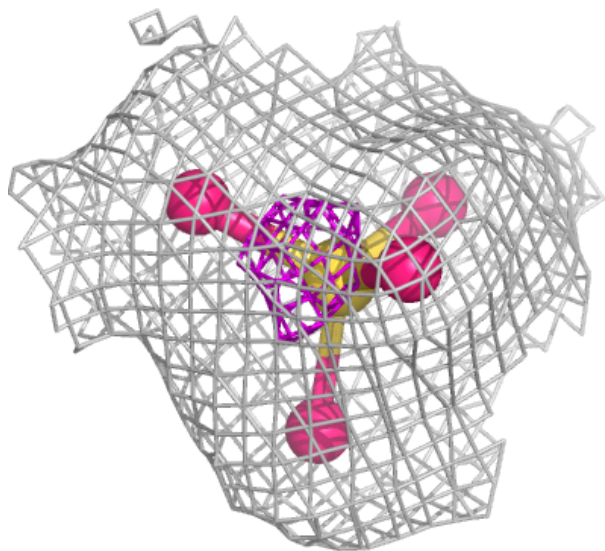
Electron density around SO4 H 303:

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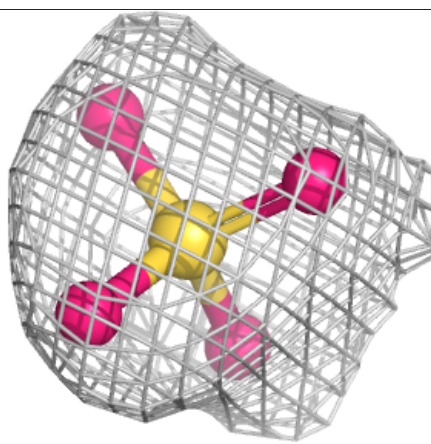
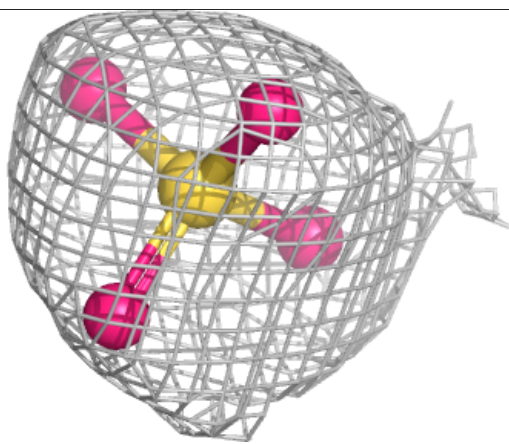
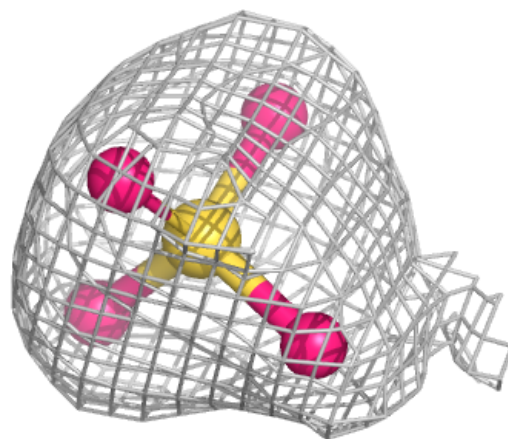
Electron density around SO4 H 302:

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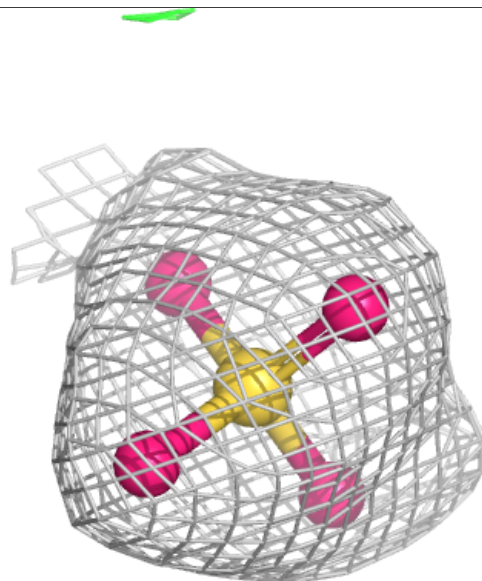
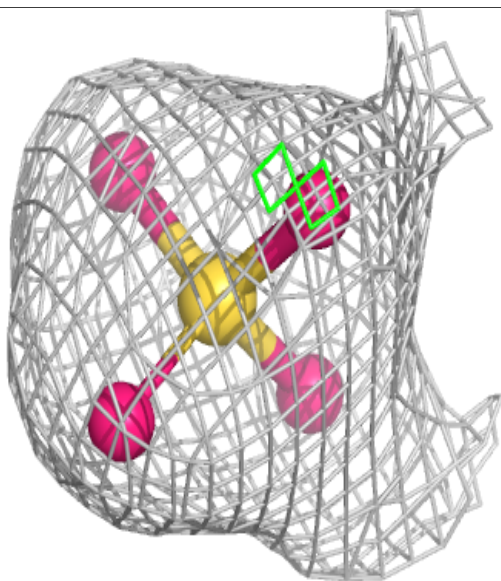
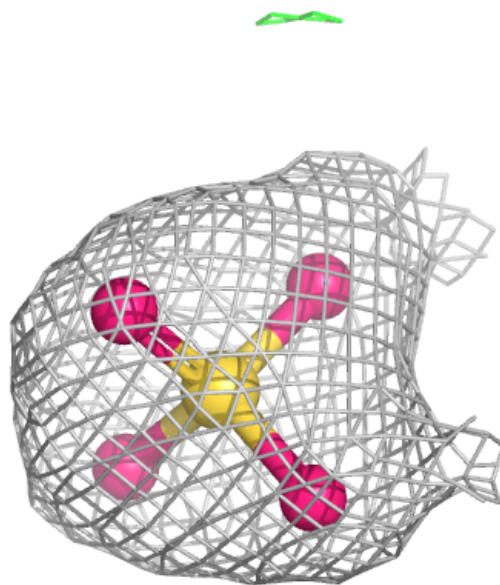
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and green (positive)



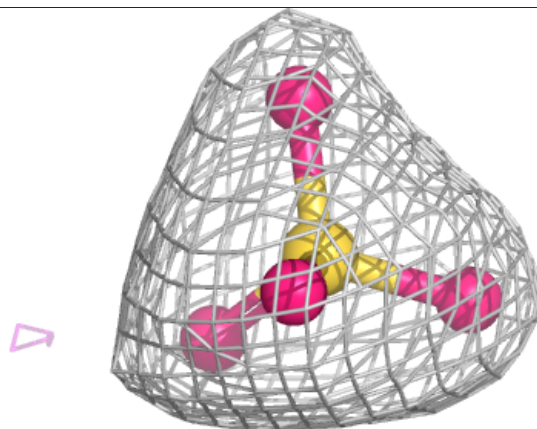
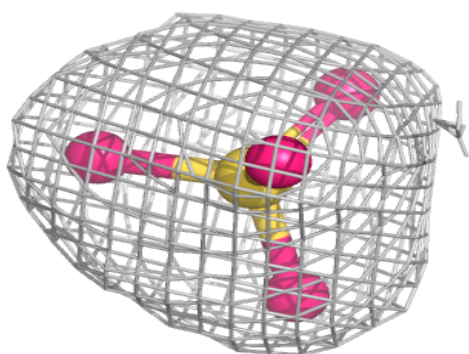
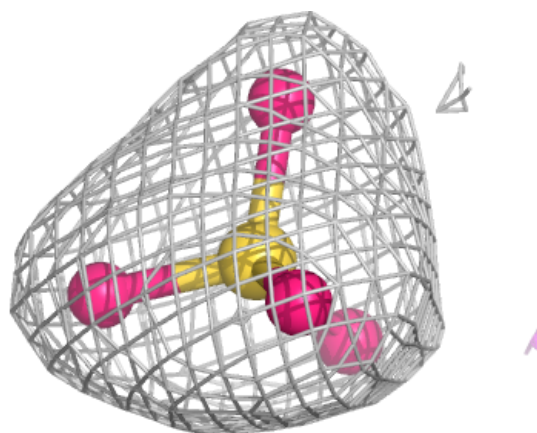
Electron density around SO4 D 301:

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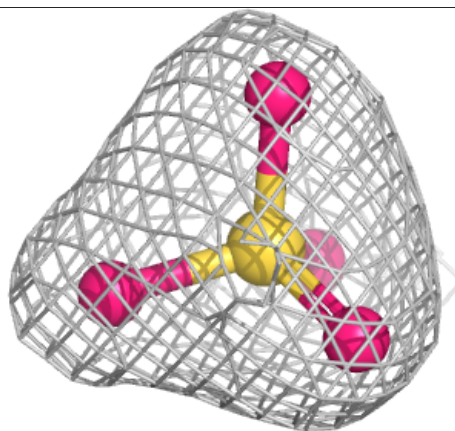
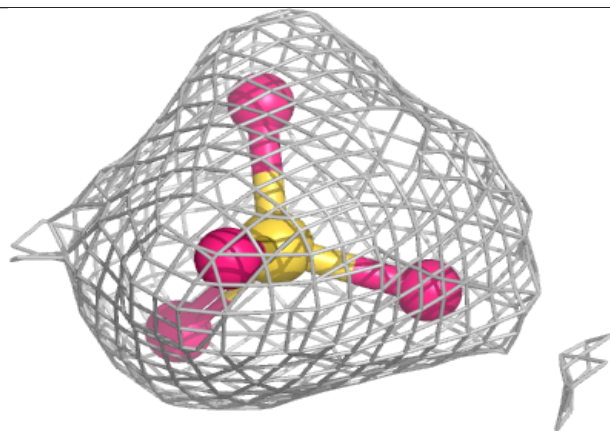
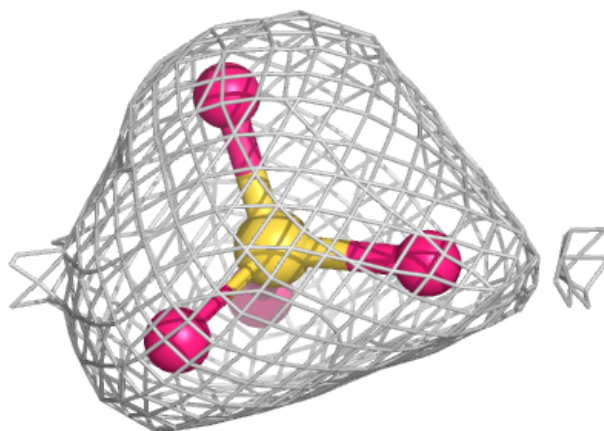
Electron density around SO4 F 301:

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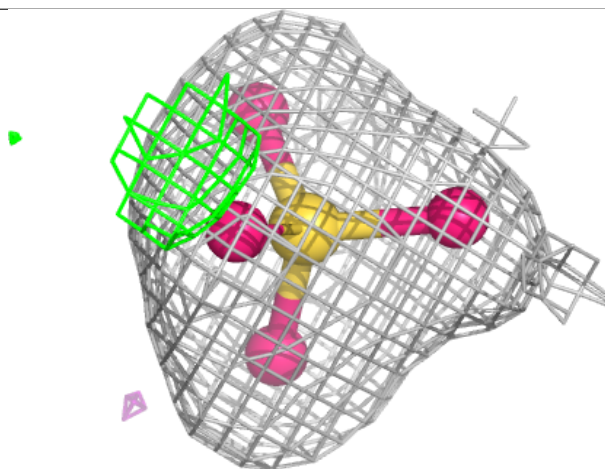
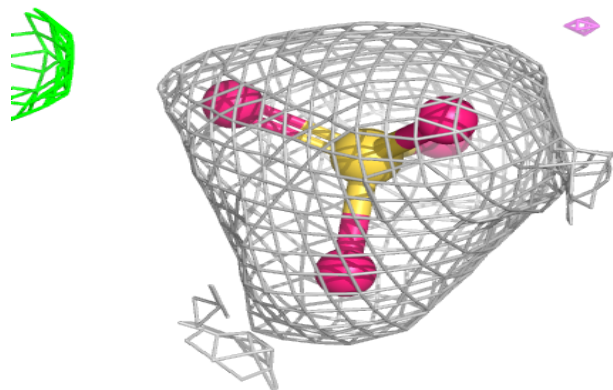
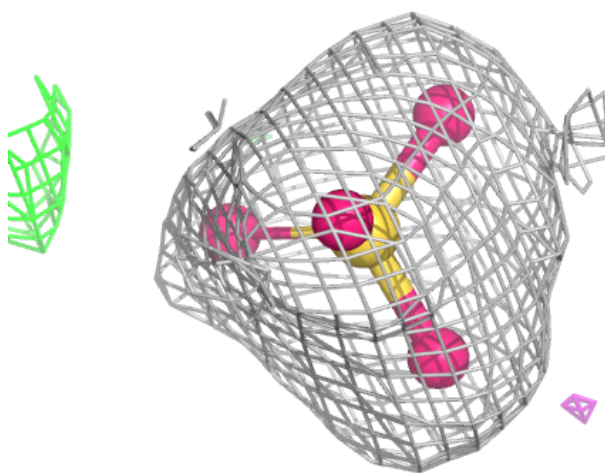
Electron density around SO4 E 301:

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and green (positive)



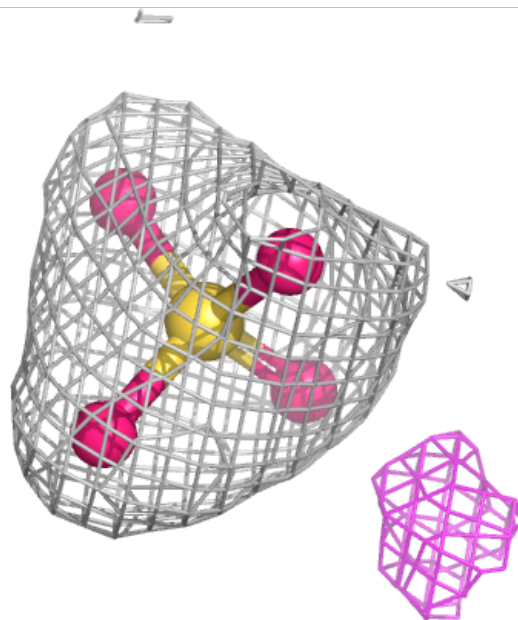
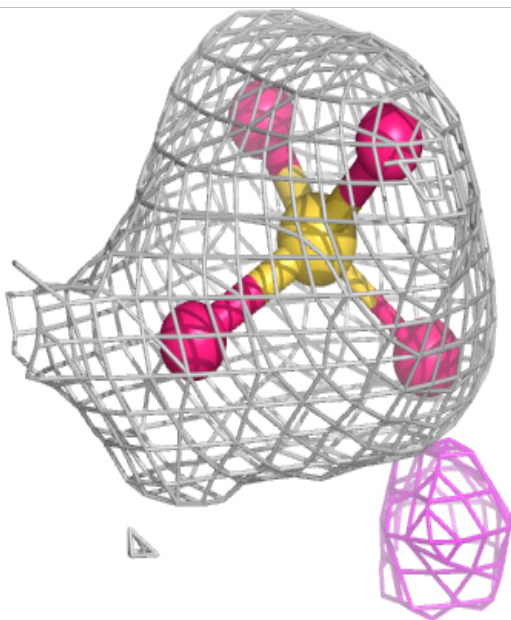
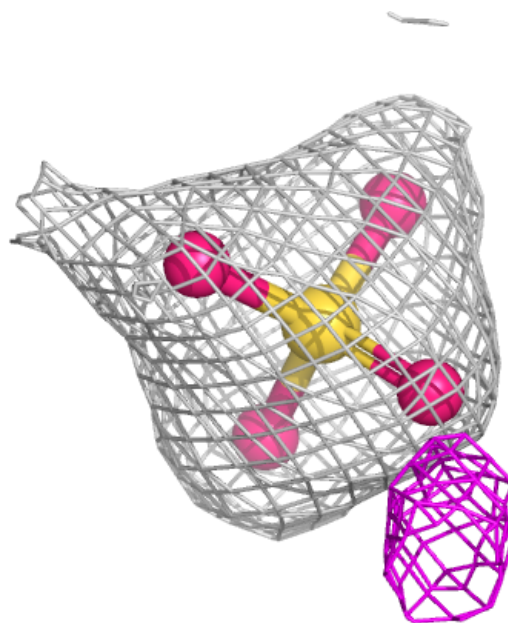
Electron density around SO4 C 301:

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



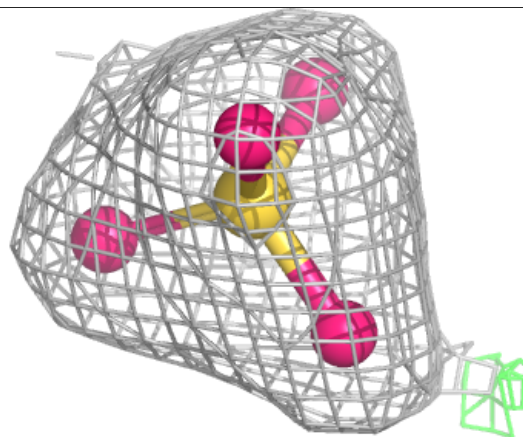
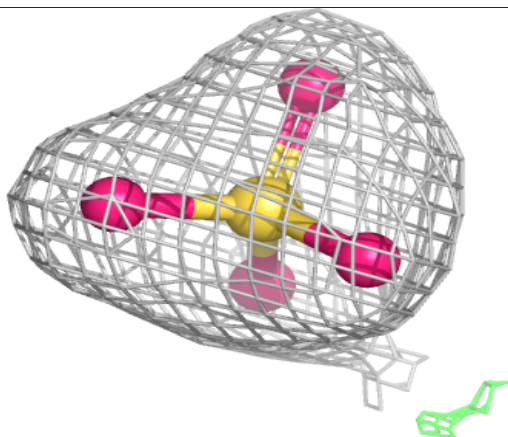
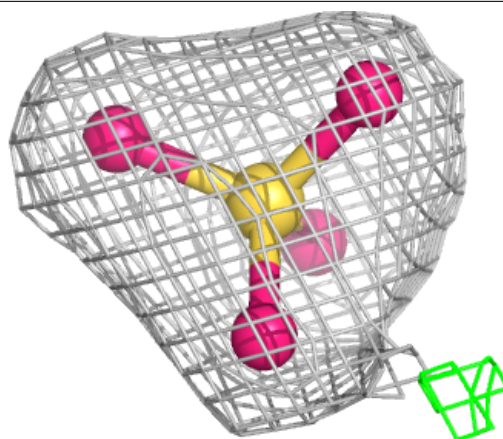
Electron density around SO4 B 301:

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



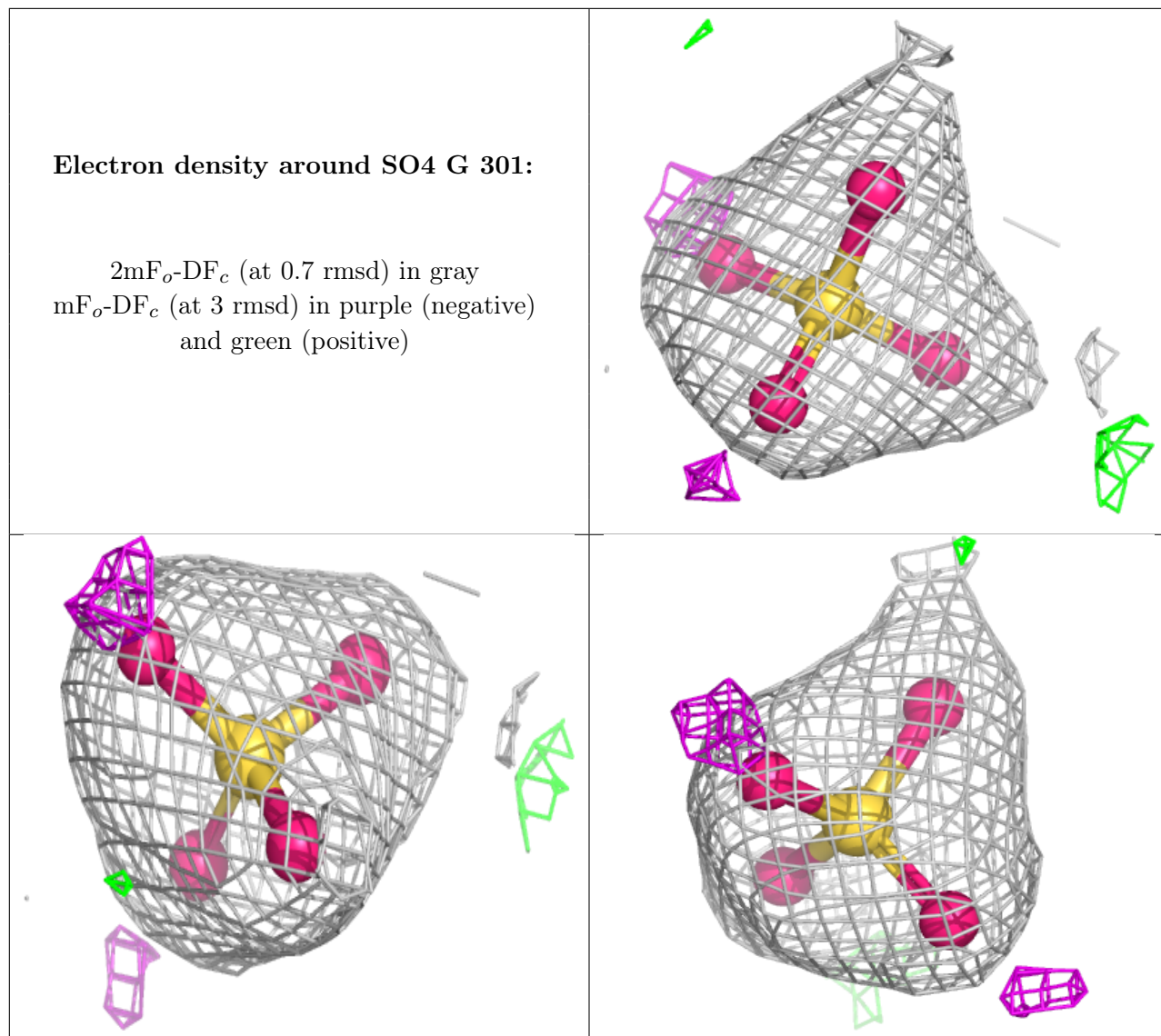
Electron density around SO4 H 301:

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



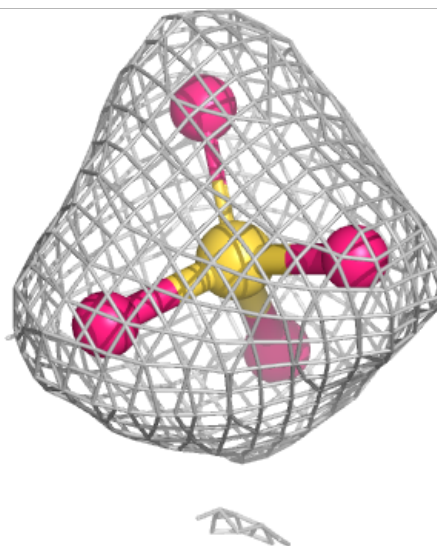
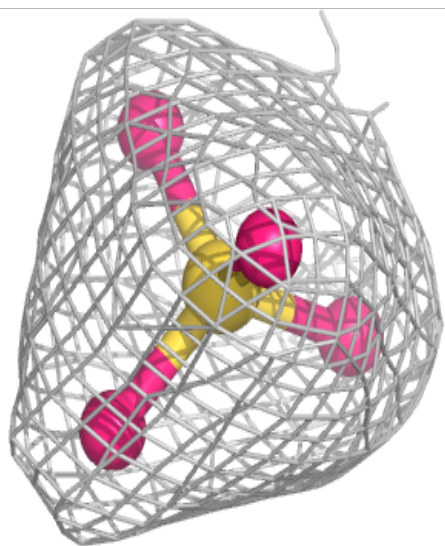
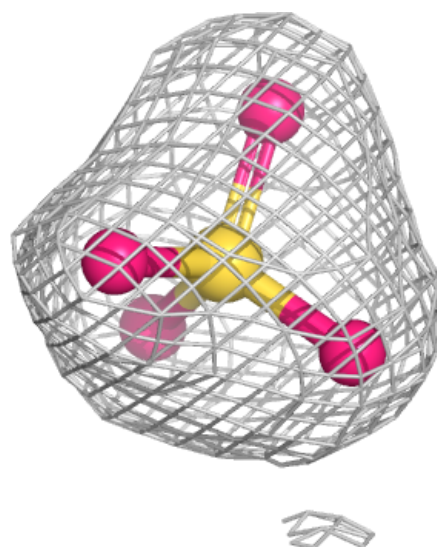
Electron density around SO4 G 301:

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



Electron density around SO4 A 302:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.