



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 7, 2020 – 11:18 PM BST

PDB ID : 6K7Q
Title : Crystal structure of thymidylate synthase from shrimp
Authors : Ma, Q.; Zang, K.; Liu, C.
Deposited on : 2019-06-08
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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 : 2.13.1
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) : 2.13.1

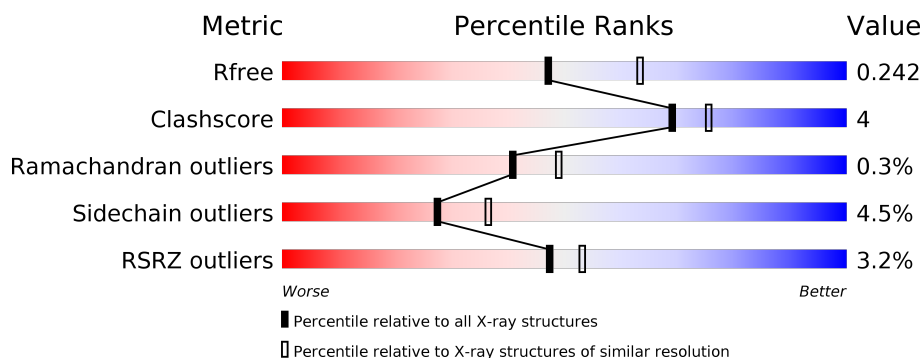
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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 on 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	292	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>15%</div> <div>7%</div> </div> </div>
1	B	292	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>10%</div> </div> </div>
1	C	292	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>9%</div> </div> </div>
1	D	292	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>11%</div> </div> </div>
1	E	292	<div> <div>3%</div> <div> <div></div> <div>76%</div> <div>12%</div> <div>11%</div> </div> </div>
1	F	292	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>9%</div> <div>10%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	292	<div><div><div></div><div></div><div></div></div><div>3%</div><div>77%</div><div>9%</div><div>•</div><div>13%</div></div>
1	H	292	<div><div><div></div><div></div><div></div></div><div>%</div><div>82%</div><div>9%</div><div>•</div><div>9%</div></div>
1	I	292	<div><div><div></div><div></div><div></div></div><div>3%</div><div>79%</div><div>12%</div><div>•</div><div>9%</div></div>
1	J	292	<div><div><div></div><div></div><div></div></div><div>3%</div><div>78%</div><div>12%</div><div>•</div><div>8%</div></div>
1	K	292	<div><div><div></div><div></div><div></div></div><div>7%</div><div>75%</div><div>13%</div><div>•</div><div>11%</div></div>
1	L	292	<div><div><div></div><div></div><div></div></div><div>2%</div><div>79%</div><div>9%</div><div>•</div><div>10%</div></div>
1	M	292	<div><div><div></div><div></div><div></div></div><div>3%</div><div>79%</div><div>10%</div><div>•</div><div>10%</div></div>
1	N	292	<div><div><div></div><div></div><div></div></div><div>%</div><div>84%</div><div>6%</div><div>•</div><div>10%</div></div>
1	O	292	<div><div><div></div><div></div><div></div></div><div>5%</div><div>81%</div><div>8%</div><div>•</div><div>10%</div></div>
1	P	292	<div><div><div></div><div></div><div></div></div><div>2%</div><div>79%</div><div>9%</div><div>•</div><div>11%</div></div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35306 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2212	1406	388	402	16			
1	B	264	Total	C	N	O	S	0	0	0
			2153	1374	374	390	15			
1	C	267	Total	C	N	O	S	0	0	0
			2178	1388	380	394	16			
1	D	261	Total	C	N	O	S	0	0	0
			2122	1353	369	385	15			
1	E	260	Total	C	N	O	S	0	0	0
			2124	1354	371	385	14			
1	F	263	Total	C	N	O	S	0	0	0
			2149	1372	373	389	15			
1	G	255	Total	C	N	O	S	0	0	0
			2089	1336	364	375	14			
1	H	266	Total	C	N	O	S	0	0	0
			2173	1385	381	392	15			
1	I	267	Total	C	N	O	S	0	1	0
			2183	1392	380	394	17			
1	J	268	Total	C	N	O	S	0	0	0
			2180	1389	378	397	16			
1	K	261	Total	C	N	O	S	0	0	0
			2128	1359	367	387	15			
1	L	262	Total	C	N	O	S	0	0	0
			2138	1366	372	385	15			
1	M	263	Total	C	N	O	S	0	0	0
			2145	1368	375	388	14			
1	N	263	Total	C	N	O	S	0	0	0
			2148	1372	373	387	16			
1	O	262	Total	C	N	O	S	0	0	0
			2138	1363	374	386	15			
1	P	261	Total	C	N	O	S	0	0	0
			2131	1361	370	385	15			

There are 48 discrepancies between the modelled and reference sequences:

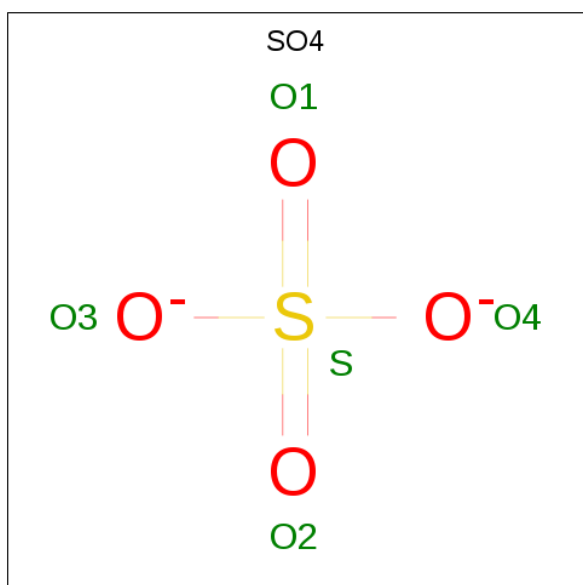
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP C6GJB8
A	-1	ASN	-	expression tag	UNP C6GJB8
A	0	ALA	-	expression tag	UNP C6GJB8
B	-2	SER	-	expression tag	UNP C6GJB8
B	-1	ASN	-	expression tag	UNP C6GJB8
B	0	ALA	-	expression tag	UNP C6GJB8
C	-2	SER	-	expression tag	UNP C6GJB8
C	-1	ASN	-	expression tag	UNP C6GJB8
C	0	ALA	-	expression tag	UNP C6GJB8
D	-2	SER	-	expression tag	UNP C6GJB8
D	-1	ASN	-	expression tag	UNP C6GJB8
D	0	ALA	-	expression tag	UNP C6GJB8
E	-2	SER	-	expression tag	UNP C6GJB8
E	-1	ASN	-	expression tag	UNP C6GJB8
E	0	ALA	-	expression tag	UNP C6GJB8
F	-2	SER	-	expression tag	UNP C6GJB8
F	-1	ASN	-	expression tag	UNP C6GJB8
F	0	ALA	-	expression tag	UNP C6GJB8
G	-2	SER	-	expression tag	UNP C6GJB8
G	-1	ASN	-	expression tag	UNP C6GJB8
G	0	ALA	-	expression tag	UNP C6GJB8
H	-2	SER	-	expression tag	UNP C6GJB8
H	-1	ASN	-	expression tag	UNP C6GJB8
H	0	ALA	-	expression tag	UNP C6GJB8
I	-2	SER	-	expression tag	UNP C6GJB8
I	-1	ASN	-	expression tag	UNP C6GJB8
I	0	ALA	-	expression tag	UNP C6GJB8
J	-2	SER	-	expression tag	UNP C6GJB8
J	-1	ASN	-	expression tag	UNP C6GJB8
J	0	ALA	-	expression tag	UNP C6GJB8
K	-2	SER	-	expression tag	UNP C6GJB8
K	-1	ASN	-	expression tag	UNP C6GJB8
K	0	ALA	-	expression tag	UNP C6GJB8
L	-2	SER	-	expression tag	UNP C6GJB8
L	-1	ASN	-	expression tag	UNP C6GJB8
L	0	ALA	-	expression tag	UNP C6GJB8
M	-2	SER	-	expression tag	UNP C6GJB8
M	-1	ASN	-	expression tag	UNP C6GJB8
M	0	ALA	-	expression tag	UNP C6GJB8
N	-2	SER	-	expression tag	UNP C6GJB8
N	-1	ASN	-	expression tag	UNP C6GJB8
N	0	ALA	-	expression tag	UNP C6GJB8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP C6GJB8
O	-1	ASN	-	expression tag	UNP C6GJB8
O	0	ALA	-	expression tag	UNP C6GJB8
P	-2	SER	-	expression tag	UNP C6GJB8
P	-1	ASN	-	expression tag	UNP C6GJB8
P	0	ALA	-	expression tag	UNP C6GJB8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by author).



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	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	E	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	76	Total	O	0	0
			76	76		
3	C	60	Total	O	0	0
			60	60		
3	D	50	Total	O	0	0
			50	50		
3	E	34	Total	O	0	0
			34	34		
3	F	60	Total	O	0	0
			60	60		
3	G	35	Total	O	0	0
			35	35		
3	H	44	Total	O	0	0
			44	44		
3	I	49	Total	O	0	0
			49	49		

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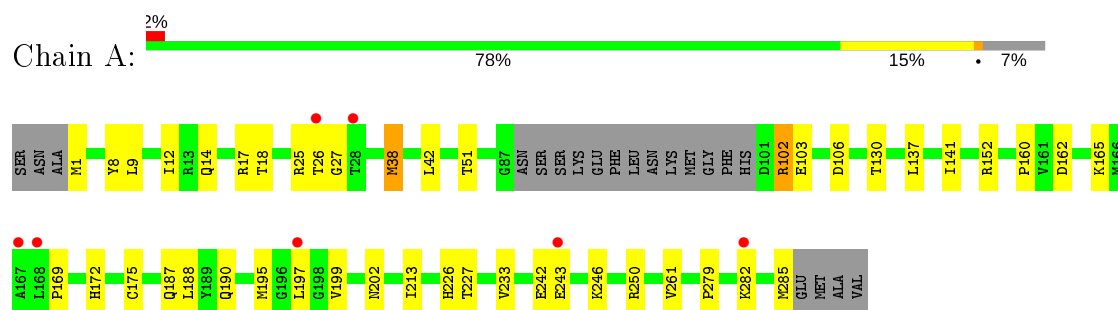
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	69	Total 69	O 69	0	0
3	K	39	Total 39	O 39	0	0
3	L	53	Total 53	O 53	0	0
3	M	47	Total 47	O 47	0	0
3	N	41	Total 41	O 41	0	0
3	O	59	Total 59	O 59	0	0
3	P	54	Total 54	O 54	0	0

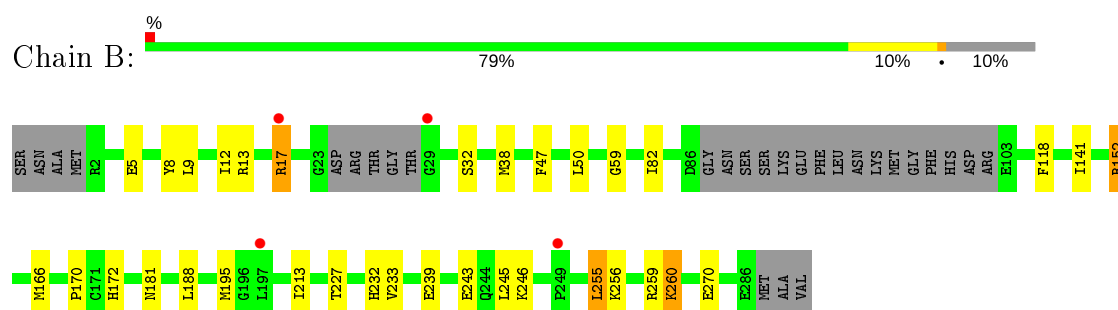
3 Residue-property plots [i](#)

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.

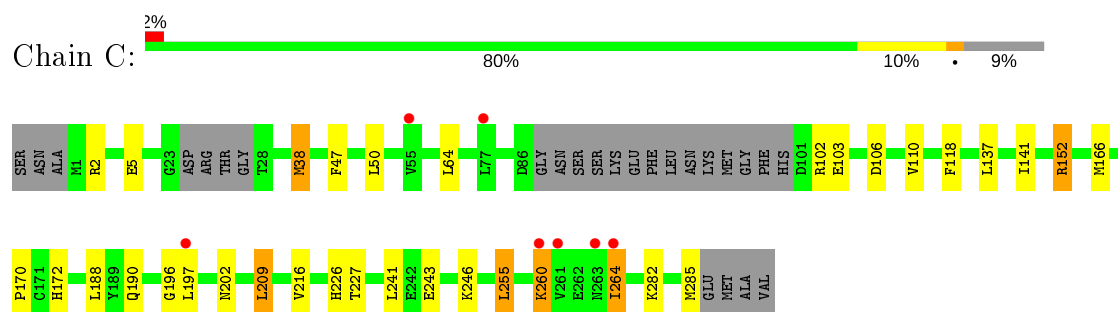
- Molecule 1: Thymidylate synthase



- Molecule 1: Thymidylate synthase

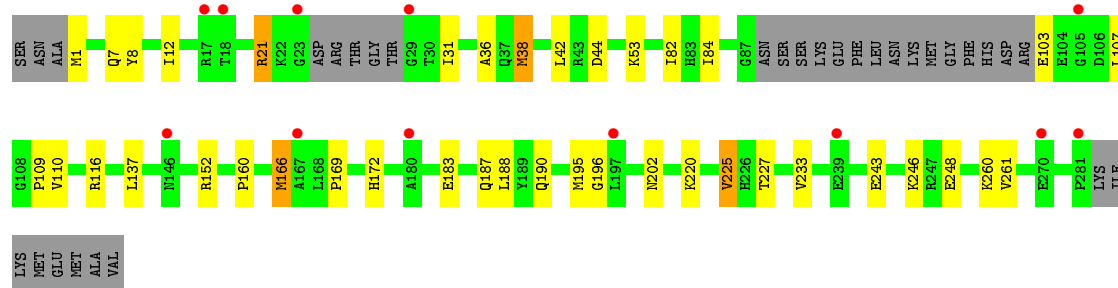


- Molecule 1: Thymidylate synthase

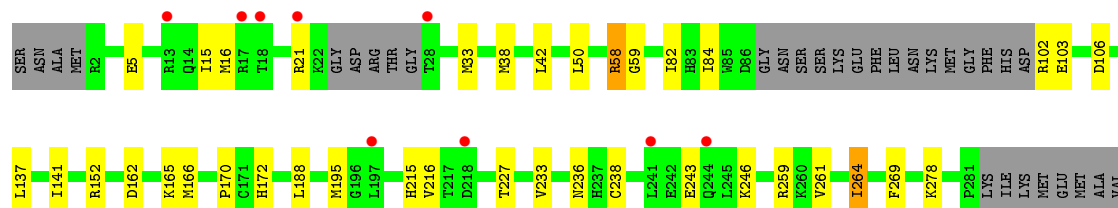
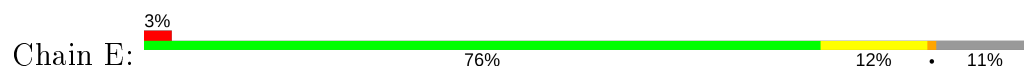


- Molecule 1: Thymidylate synthase

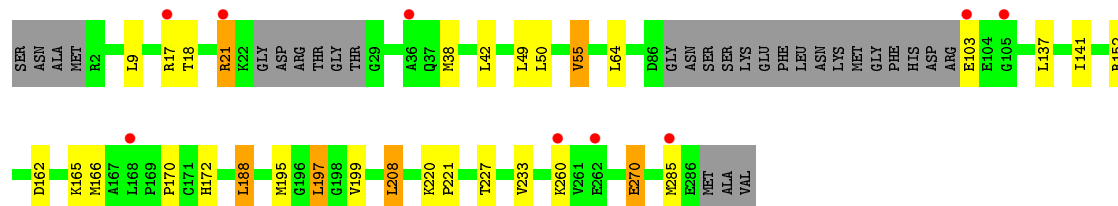
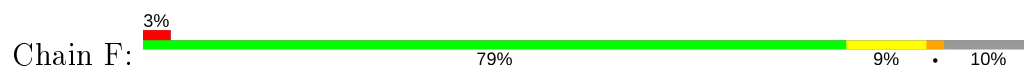




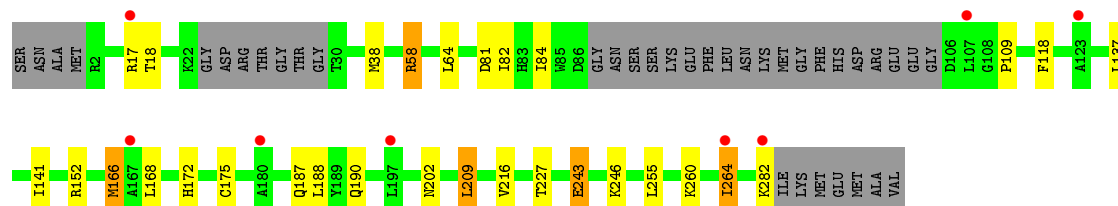
- Molecule 1: Thymidylate synthase



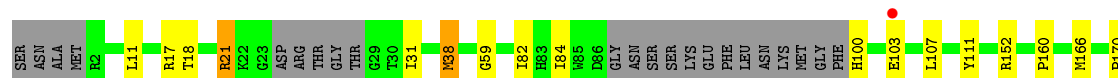
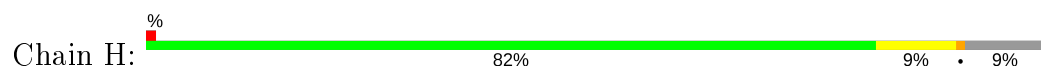
- Molecule 1: Thymidylate synthase

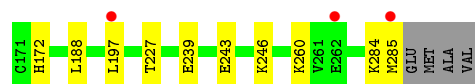


- Molecule 1: Thymidylate synthase

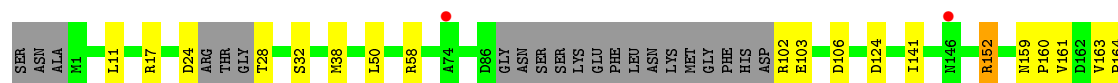
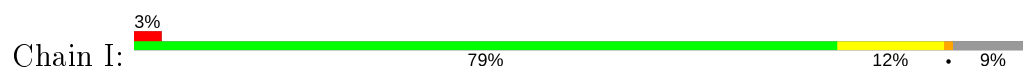


- Molecule 1: Thymidylate synthase

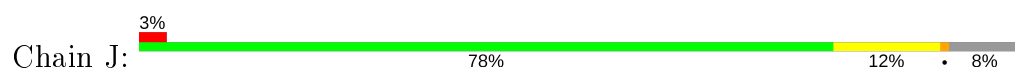




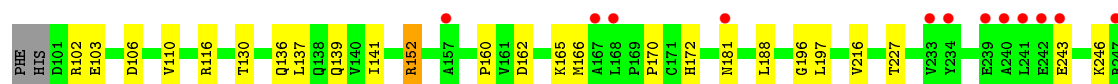
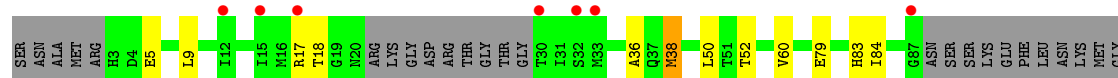
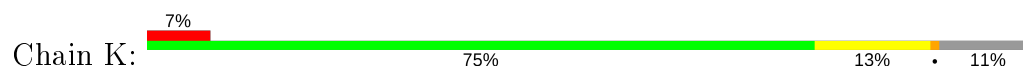
• Molecule 1: Thymidylate synthase



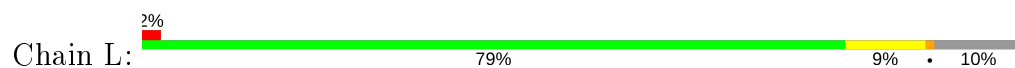
• Molecule 1: Thymidylate synthase




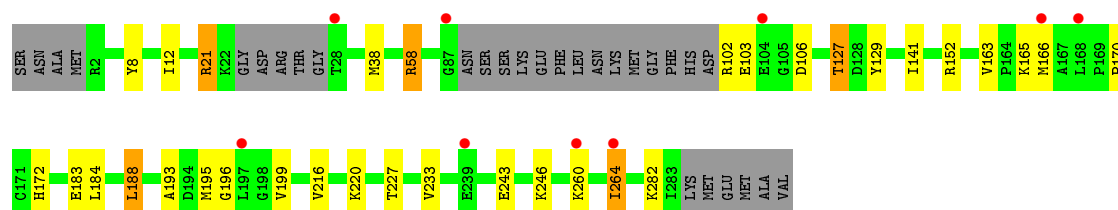
• Molecule 1: Thymidylate synthase




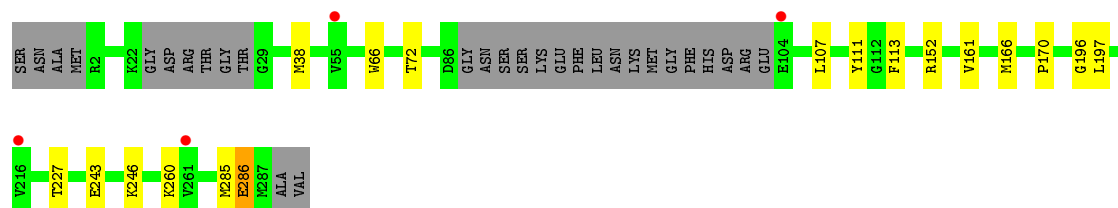
• Molecule 1: Thymidylate synthase




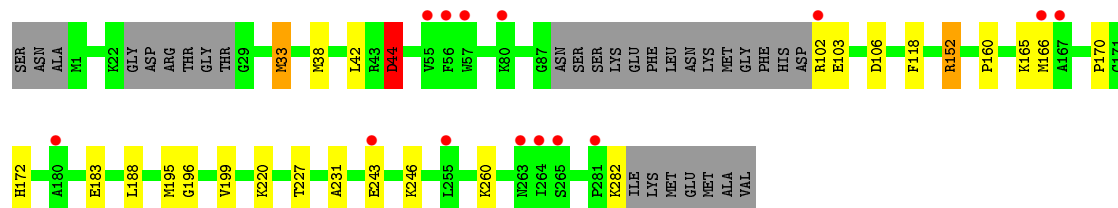
• Molecule 1: Thymidylate synthase

Chain M:  3% 79% 10% 10%


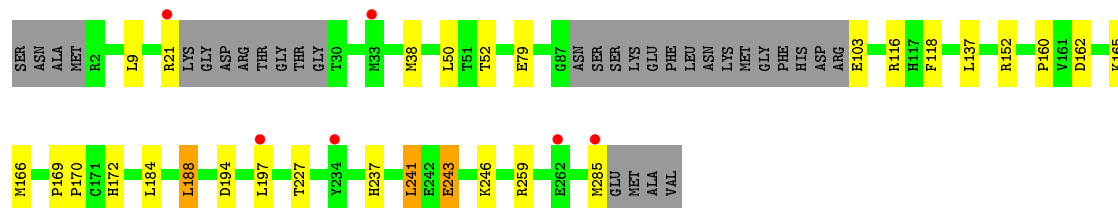
• Molecule 1: Thymidylate synthase

Chain N:  % 84% 6% 10%

• Molecule 1: Thymidylate synthase

Chain O:  5% 81% 8% 10%

• Molecule 1: Thymidylate synthase

Chain P:  2% 79% 9% 11%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.27Å 103.46Å 125.77Å 77.40° 84.81° 61.43°	Depositor
Resolution (Å)	89.03 – 2.27 89.03 – 2.27	Depositor EDS
% Data completeness (in resolution range)	96.2 (89.03-2.27) 88.7 (89.03-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.218 , 0.236 0.228 , 0.242	Depositor DCC
R_{free} test set	10707 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 27.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.128 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	35306	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4313e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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 [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	0.51	0/2270	0.71	0/3068
1	B	0.54	0/2210	0.70	0/2987
1	C	0.51	0/2235	0.69	0/3020
1	D	0.51	0/2179	0.71	0/2947
1	E	0.50	0/2181	0.71	0/2951
1	F	0.51	0/2206	0.69	0/2982
1	G	0.49	0/2146	0.70	0/2904
1	H	0.48	0/2231	0.68	0/3015
1	I	0.51	0/2243	0.70	0/3030
1	J	0.52	0/2237	0.71	0/3023
1	K	0.50	0/2185	0.68	0/2956
1	L	0.50	0/2195	0.69	0/2968
1	M	0.48	0/2202	0.70	0/2978
1	N	0.50	0/2205	0.68	0/2980
1	O	0.50	0/2195	0.69	1/2967 (0.0%)
1	P	0.52	0/2188	0.70	0/2959
All	All	0.50	0/35308	0.70	1/47735 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	44	ASP	CA-CB-CG	6.24	127.13	113.40

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	2212	0	2149	25	0
1	B	2153	0	2088	17	0
1	C	2178	0	2118	19	0
1	D	2122	0	2051	22	0
1	E	2124	0	2053	20	0
1	F	2149	0	2085	19	0
1	G	2089	0	2028	17	0
1	H	2173	0	2106	11	0
1	I	2183	0	2127	19	0
1	J	2180	0	2111	20	0
1	K	2128	0	2057	24	0
1	L	2138	0	2080	12	0
1	M	2145	0	2080	23	0
1	N	2148	0	2088	10	0
1	O	2138	0	2074	16	0
1	P	2131	0	2066	14	0
2	A	10	0	0	0	0
2	C	10	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
3	A	55	0	0	1	0
3	B	76	0	0	0	0
3	C	60	0	0	0	0
3	D	50	0	0	0	0
3	E	34	0	0	1	0
3	F	60	0	0	0	0
3	G	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	44	0	0	0	0
3	I	49	0	0	0	0
3	J	69	0	0	0	0
3	K	39	0	0	0	0
3	L	53	0	0	0	0
3	M	47	0	0	1	0
3	N	41	0	0	0	0
3	O	59	0	0	0	0
3	P	54	0	0	1	0
All	All	35306	0	33361	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 253 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:F:220:LYS:HD3	1:O:44:ASP:CB	1.68	1.23
1:F:220:LYS:CD	1:O:44:ASP:HB3	1.73	1.19
1:A:51:THR:HG21	1:A:250:ARG:HB2	1.20	1.14
1:B:260:LYS:HD2	1:K:130:THR:HG23	1.53	0.89
1:A:130:THR:O	1:J:260:LYS:HG2	1.74	0.85

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	268/292 (92%)	258 (96%)	9 (3%)	1 (0%)	34 40
1	B	258/292 (88%)	249 (96%)	9 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	261/292 (89%)	251 (96%)	8 (3%)	2 (1%)	19	22
1	D	255/292 (87%)	247 (97%)	7 (3%)	1 (0%)	34	40
1	E	254/292 (87%)	244 (96%)	9 (4%)	1 (0%)	34	40
1	F	257/292 (88%)	247 (96%)	10 (4%)	0	100	100
1	G	249/292 (85%)	238 (96%)	11 (4%)	0	100	100
1	H	260/292 (89%)	251 (96%)	8 (3%)	1 (0%)	34	40
1	I	262/292 (90%)	251 (96%)	10 (4%)	1 (0%)	34	40
1	J	262/292 (90%)	254 (97%)	8 (3%)	0	100	100
1	K	255/292 (87%)	248 (97%)	5 (2%)	2 (1%)	19	22
1	L	256/292 (88%)	246 (96%)	10 (4%)	0	100	100
1	M	257/292 (88%)	248 (96%)	8 (3%)	1 (0%)	34	40
1	N	257/292 (88%)	248 (96%)	7 (3%)	2 (1%)	19	22
1	O	256/292 (88%)	248 (97%)	7 (3%)	1 (0%)	34	40
1	P	255/292 (87%)	248 (97%)	7 (3%)	0	100	100
All	All	4122/4672 (88%)	3976 (96%)	133 (3%)	13 (0%)	41	49

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	196	GLY
1	N	111	TYR
1	H	111	TYR
1	E	238	CYS
1	A	27	GLY

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	237/254 (93%)	225 (95%)	12 (5%)	24	31
1	B	231/254 (91%)	221 (96%)	10 (4%)	29	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	234/254 (92%)	224 (96%)	10 (4%)	29	38
1	D	227/254 (89%)	213 (94%)	14 (6%)	18	23
1	E	228/254 (90%)	219 (96%)	9 (4%)	32	43
1	F	231/254 (91%)	218 (94%)	13 (6%)	21	27
1	G	225/254 (89%)	214 (95%)	11 (5%)	25	33
1	H	233/254 (92%)	224 (96%)	9 (4%)	32	43
1	I	235/254 (92%)	224 (95%)	11 (5%)	26	34
1	J	234/254 (92%)	223 (95%)	11 (5%)	26	34
1	K	229/254 (90%)	219 (96%)	10 (4%)	28	37
1	L	230/254 (91%)	218 (95%)	12 (5%)	23	30
1	M	230/254 (91%)	218 (95%)	12 (5%)	23	30
1	N	231/254 (91%)	226 (98%)	5 (2%)	52	66
1	O	229/254 (90%)	221 (96%)	8 (4%)	36	48
1	P	229/254 (90%)	219 (96%)	10 (4%)	28	37
All	All	3693/4064 (91%)	3526 (96%)	167 (4%)	27	36

5 of 167 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	255	LEU
1	I	152	ARG
1	O	152	ARG
1	G	264	ILE
1	H	152	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	244	GLN
1	I	244	GLN
1	P	117	HIS
1	I	138	GLN
1	I	181	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

18 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	A	301	-	4,4,4	0.25	0	6,6,6	0.27	0
2	SO4	D	301	-	4,4,4	0.40	0	6,6,6	0.23	0
2	SO4	F	301	-	4,4,4	0.27	0	6,6,6	0.09	0
2	SO4	E	301	-	4,4,4	0.25	0	6,6,6	0.15	0
2	SO4	C	302	-	4,4,4	0.25	0	6,6,6	0.39	0
2	SO4	J	302	-	4,4,4	0.24	0	6,6,6	0.51	0
2	SO4	A	302	-	4,4,4	0.27	0	6,6,6	0.44	0
2	SO4	I	301	-	4,4,4	0.20	0	6,6,6	0.24	0
2	SO4	G	302	-	4,4,4	0.25	0	6,6,6	0.35	0
2	SO4	C	301	-	4,4,4	0.18	0	6,6,6	0.36	0
2	SO4	N	301	-	4,4,4	0.20	0	6,6,6	0.18	0
2	SO4	M	301	-	4,4,4	0.43	0	6,6,6	0.26	0
2	SO4	P	301	-	4,4,4	0.21	0	6,6,6	0.18	0
2	SO4	J	301	-	4,4,4	0.37	0	6,6,6	0.73	0
2	SO4	K	301	-	4,4,4	0.25	0	6,6,6	0.32	0
2	SO4	O	301	-	4,4,4	0.24	0	6,6,6	0.24	0
2	SO4	L	301	-	4,4,4	0.24	0	6,6,6	0.27	0
2	SO4	G	301	-	4,4,4	0.16	0	6,6,6	0.19	0

There are no bond length outliers.

There are no bond angle outliers.

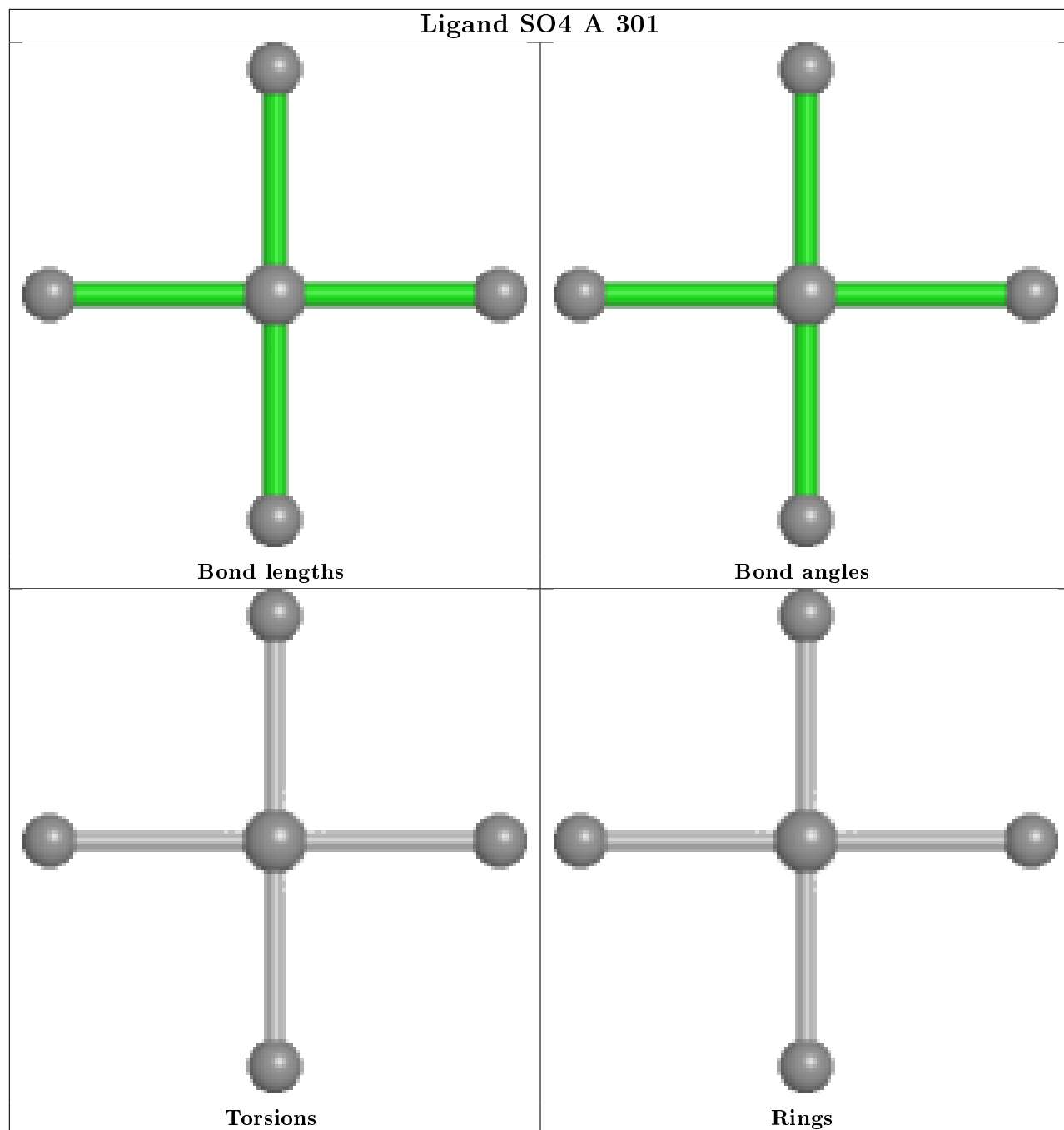
There are no chirality outliers.

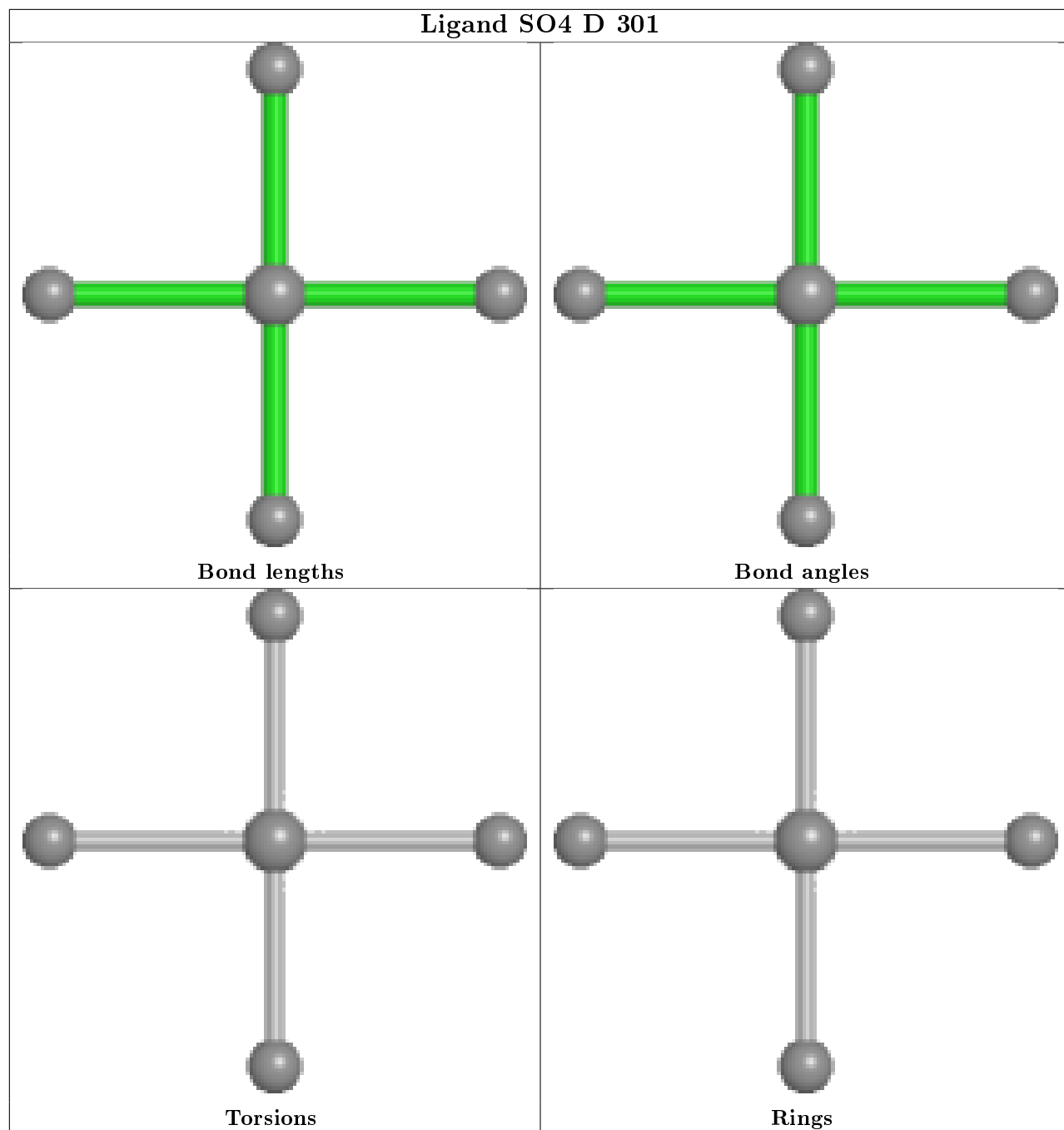
There are no torsion outliers.

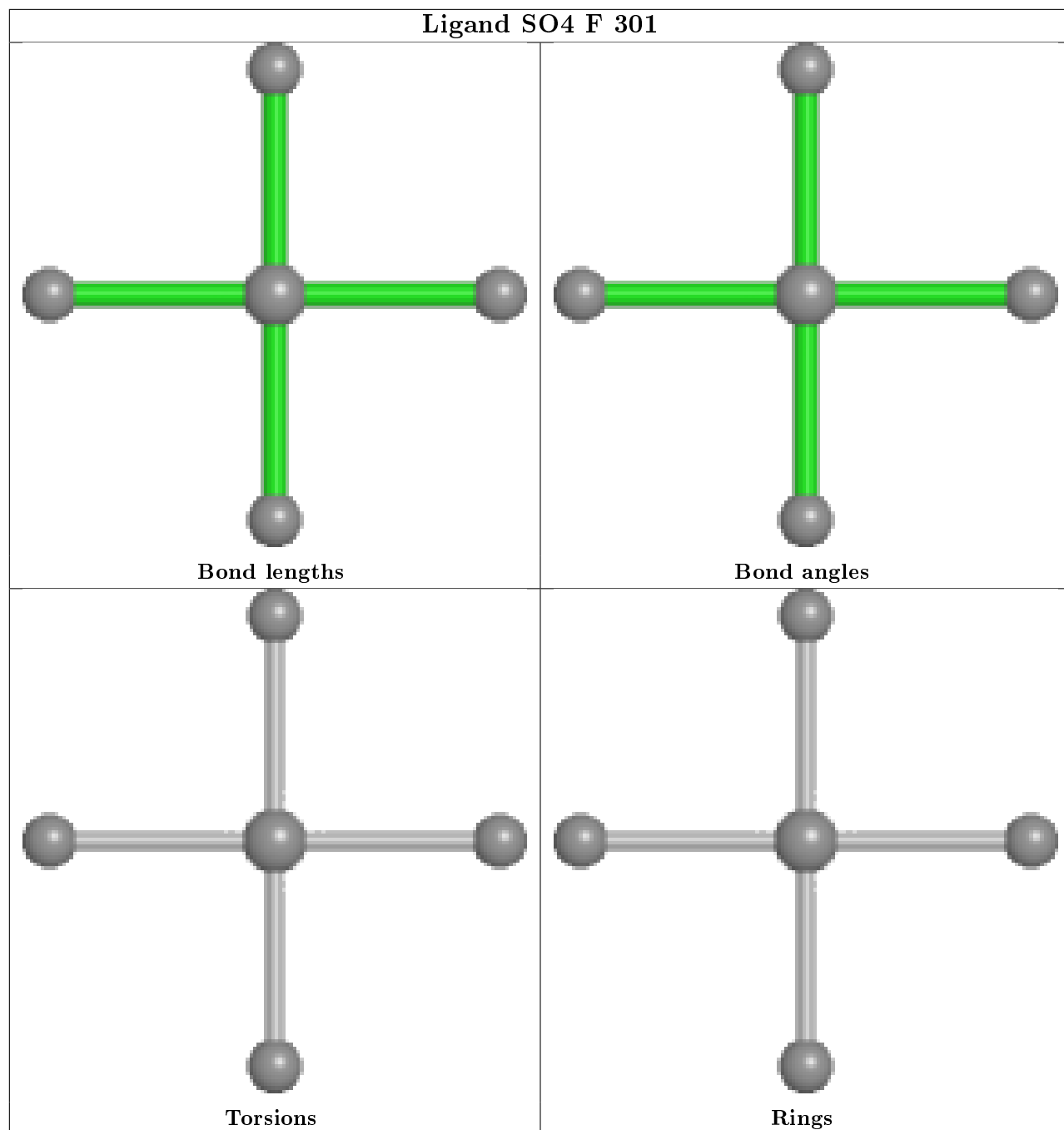
There are no ring outliers.

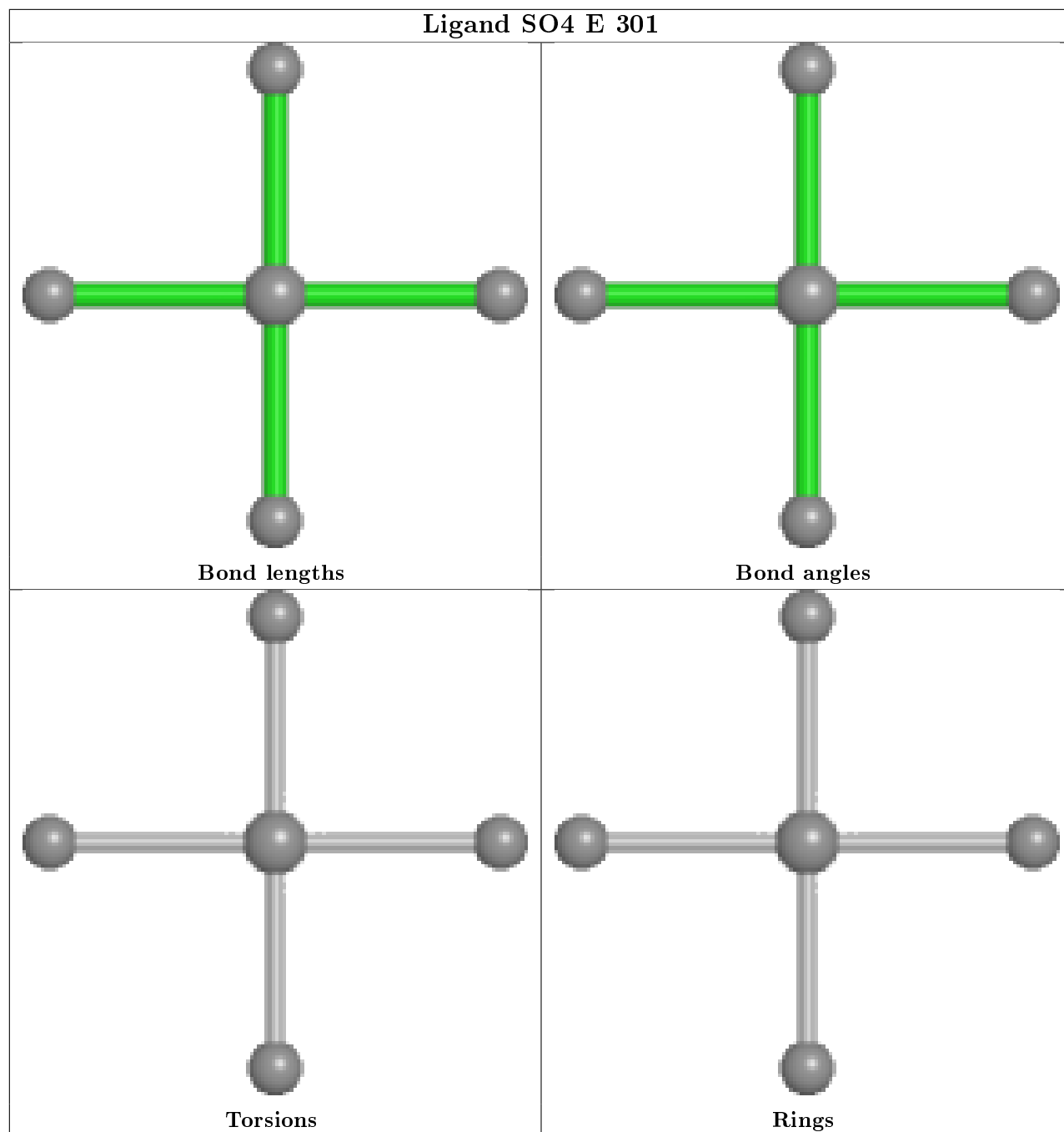
No monomer is involved in short contacts.

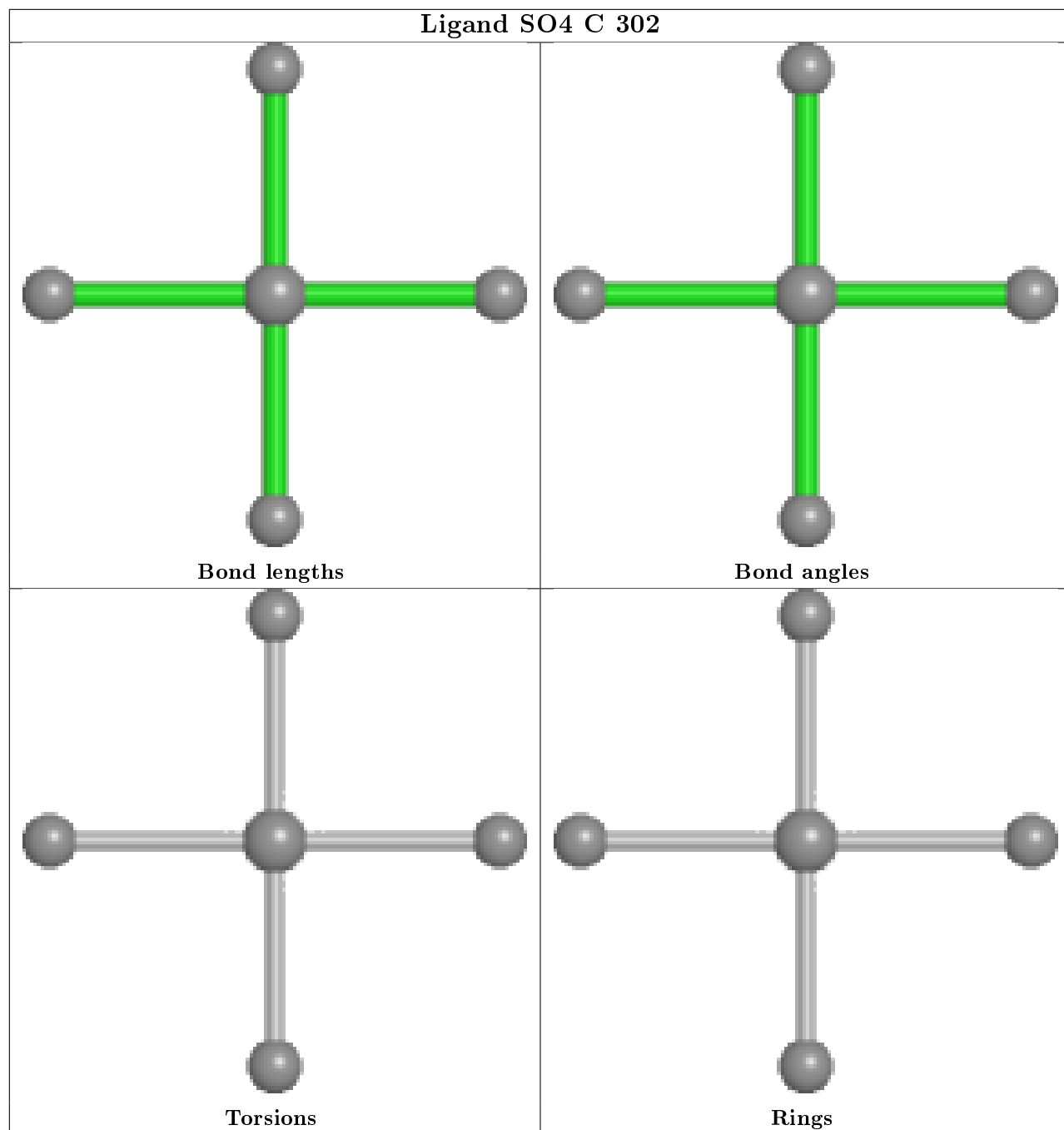
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

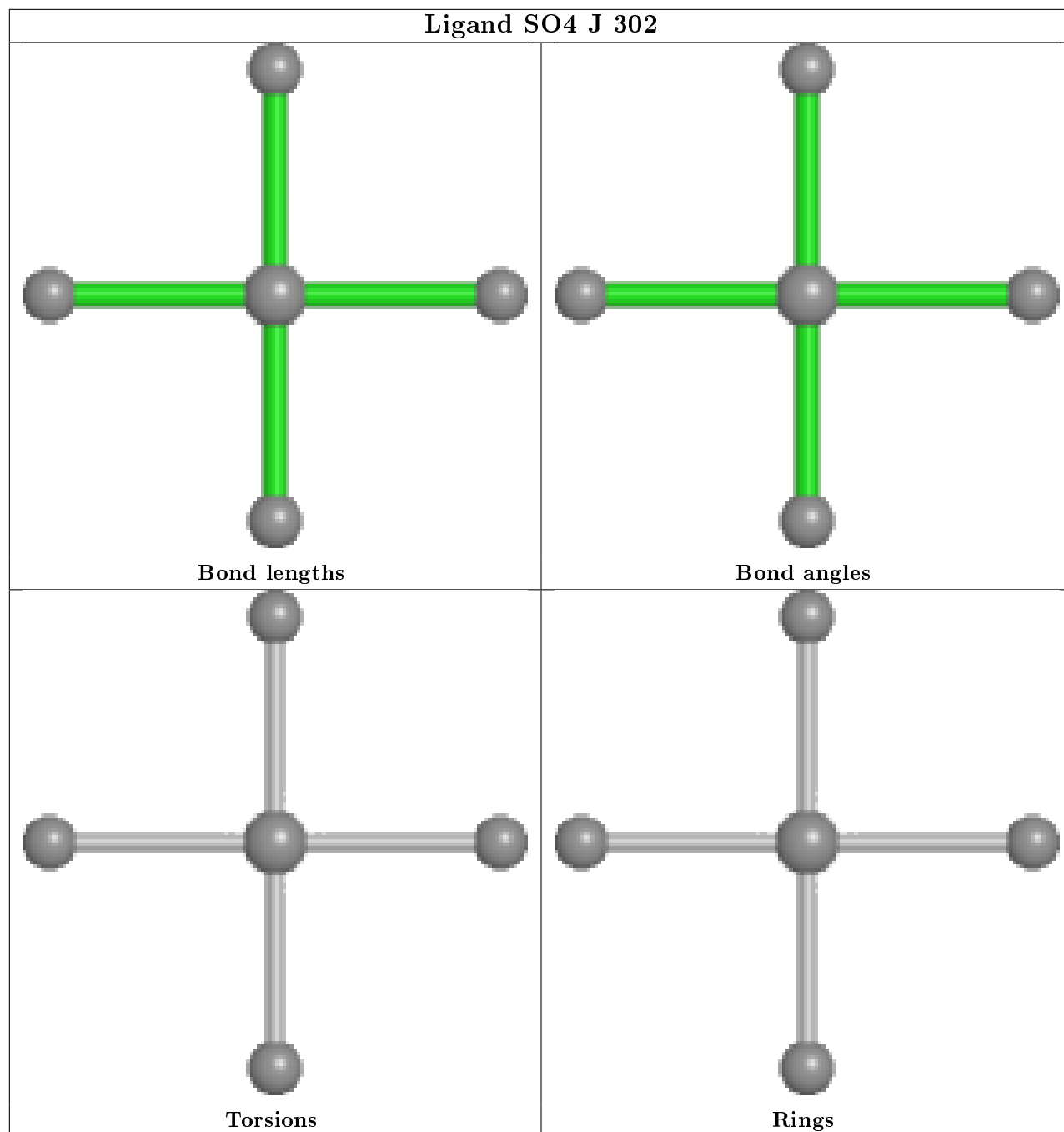


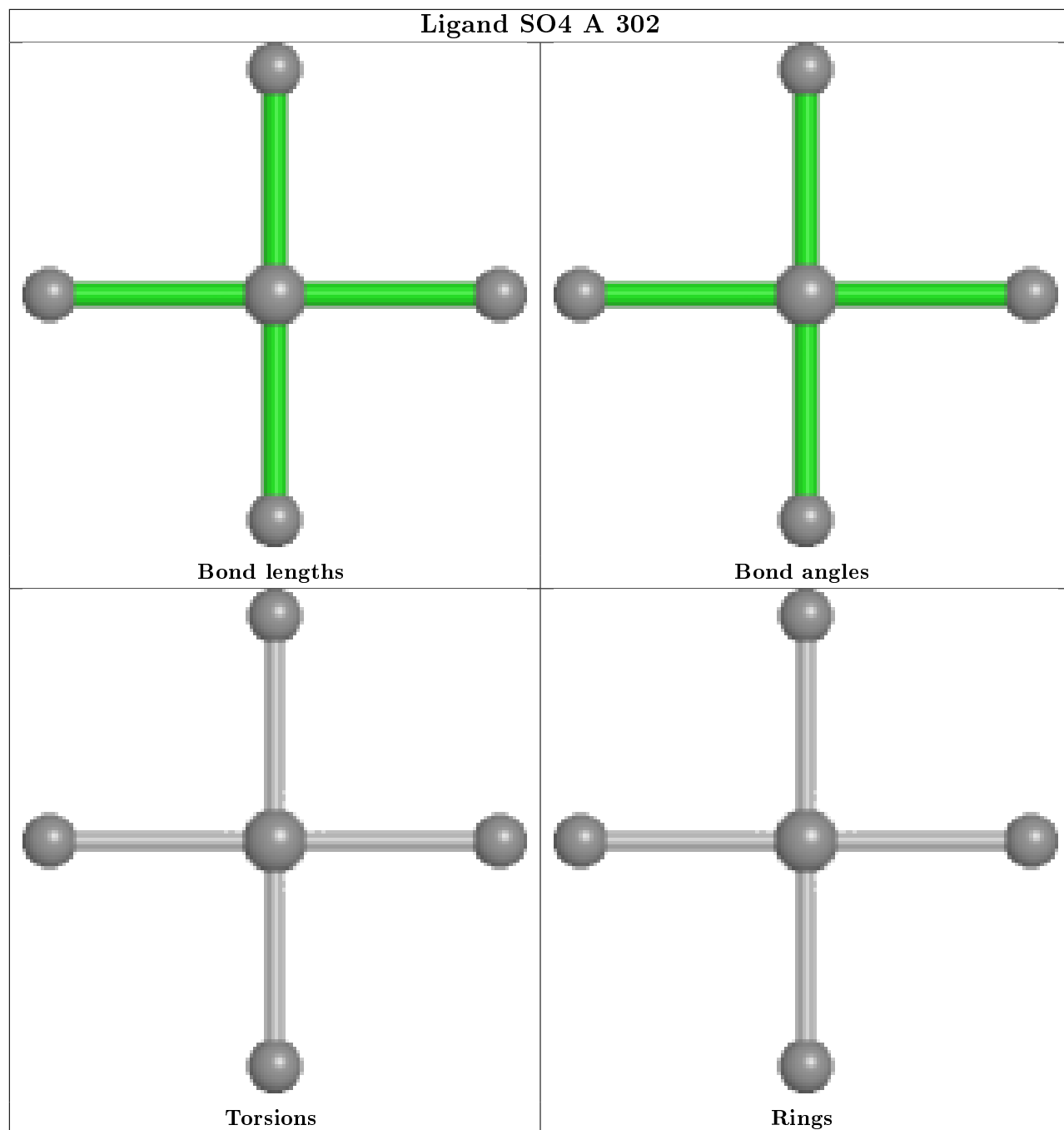


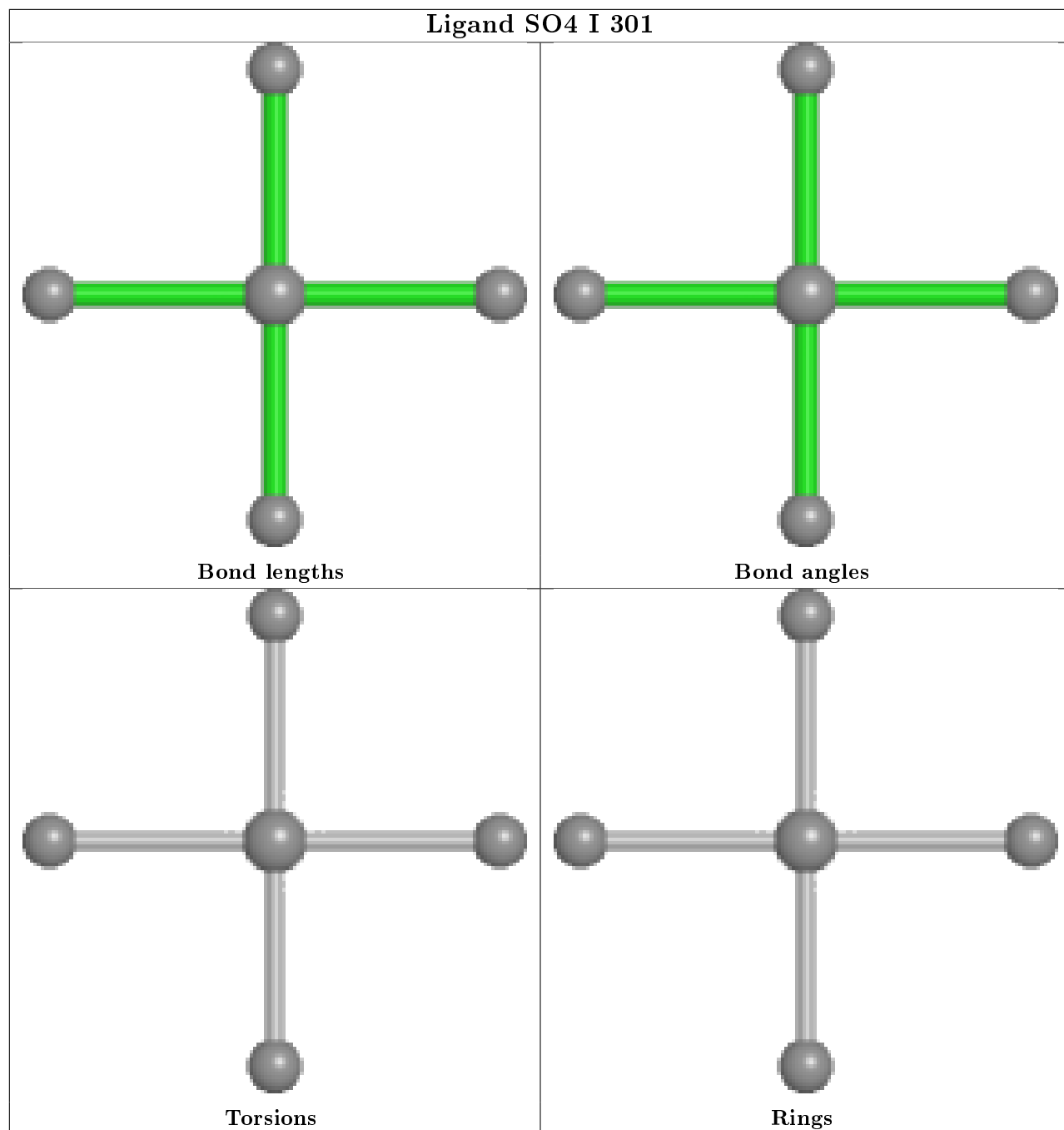


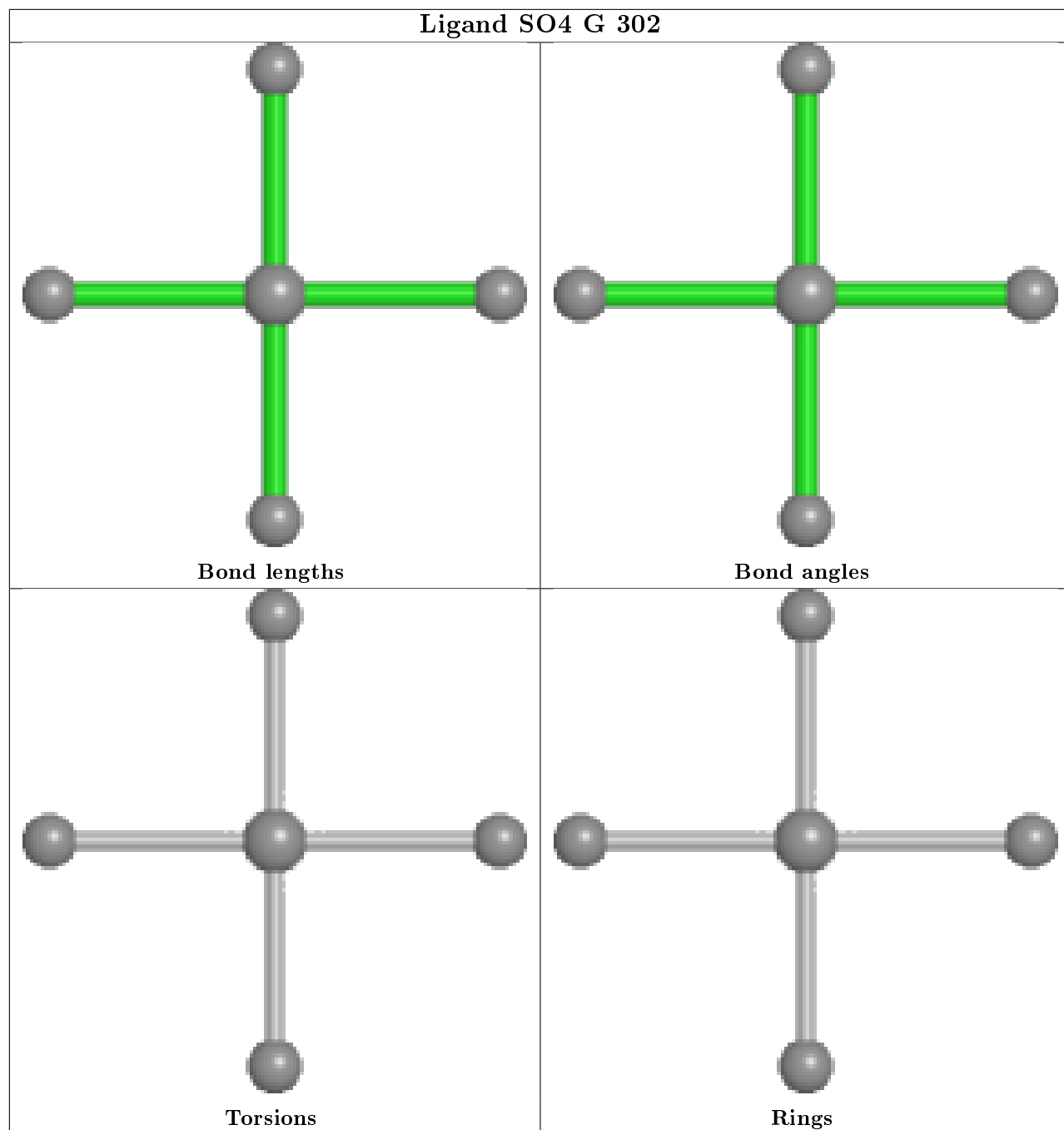


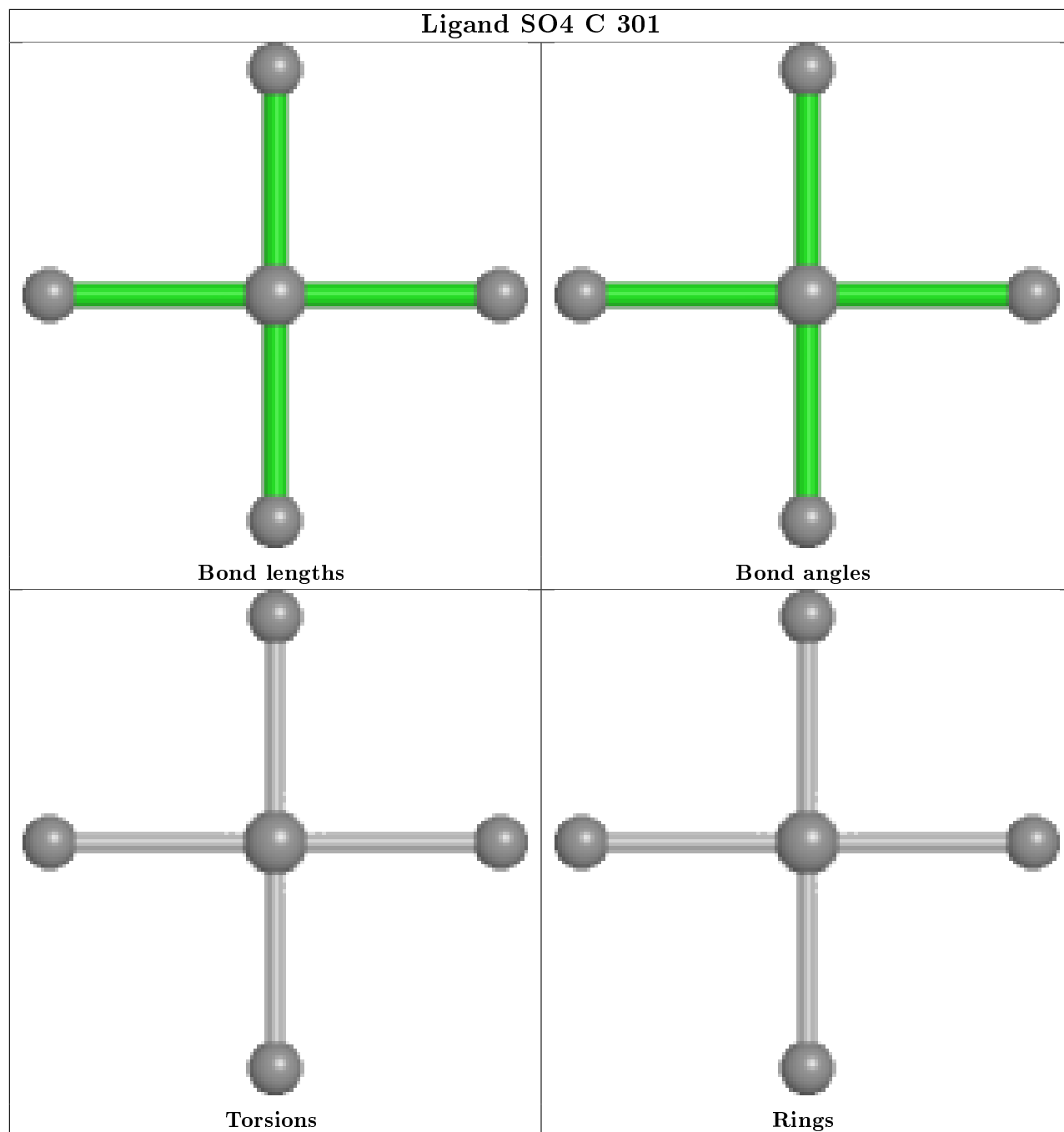


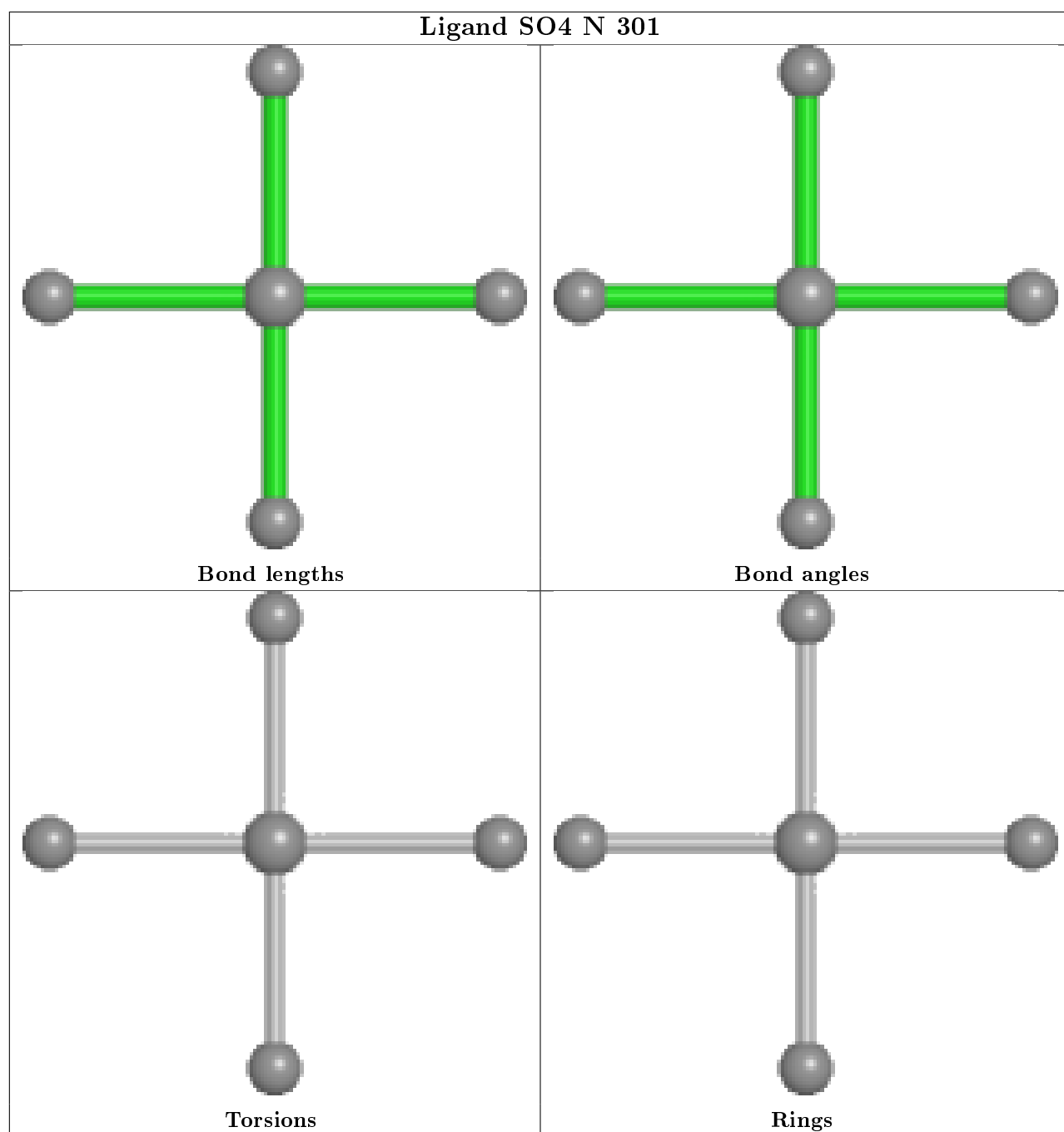


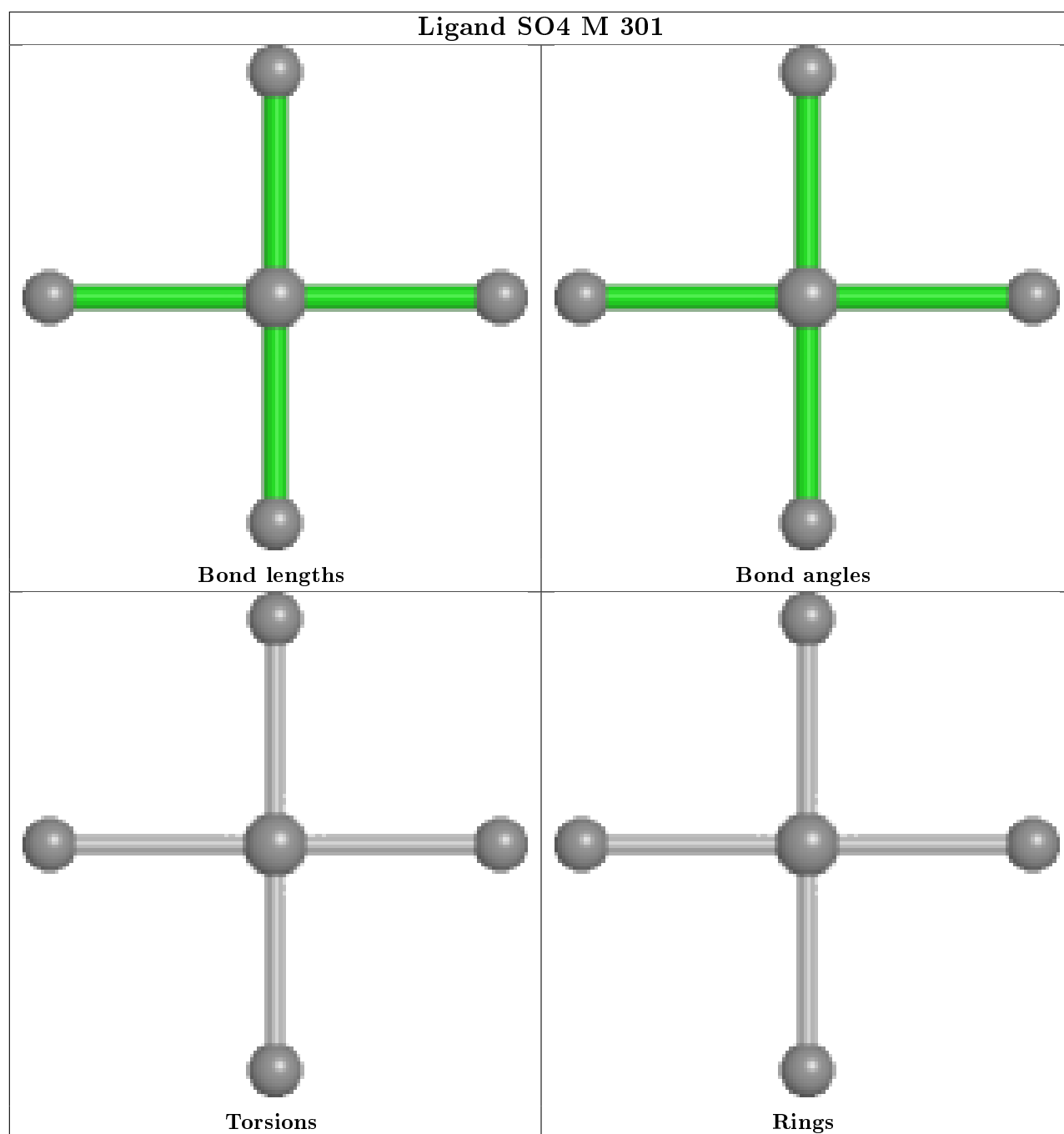


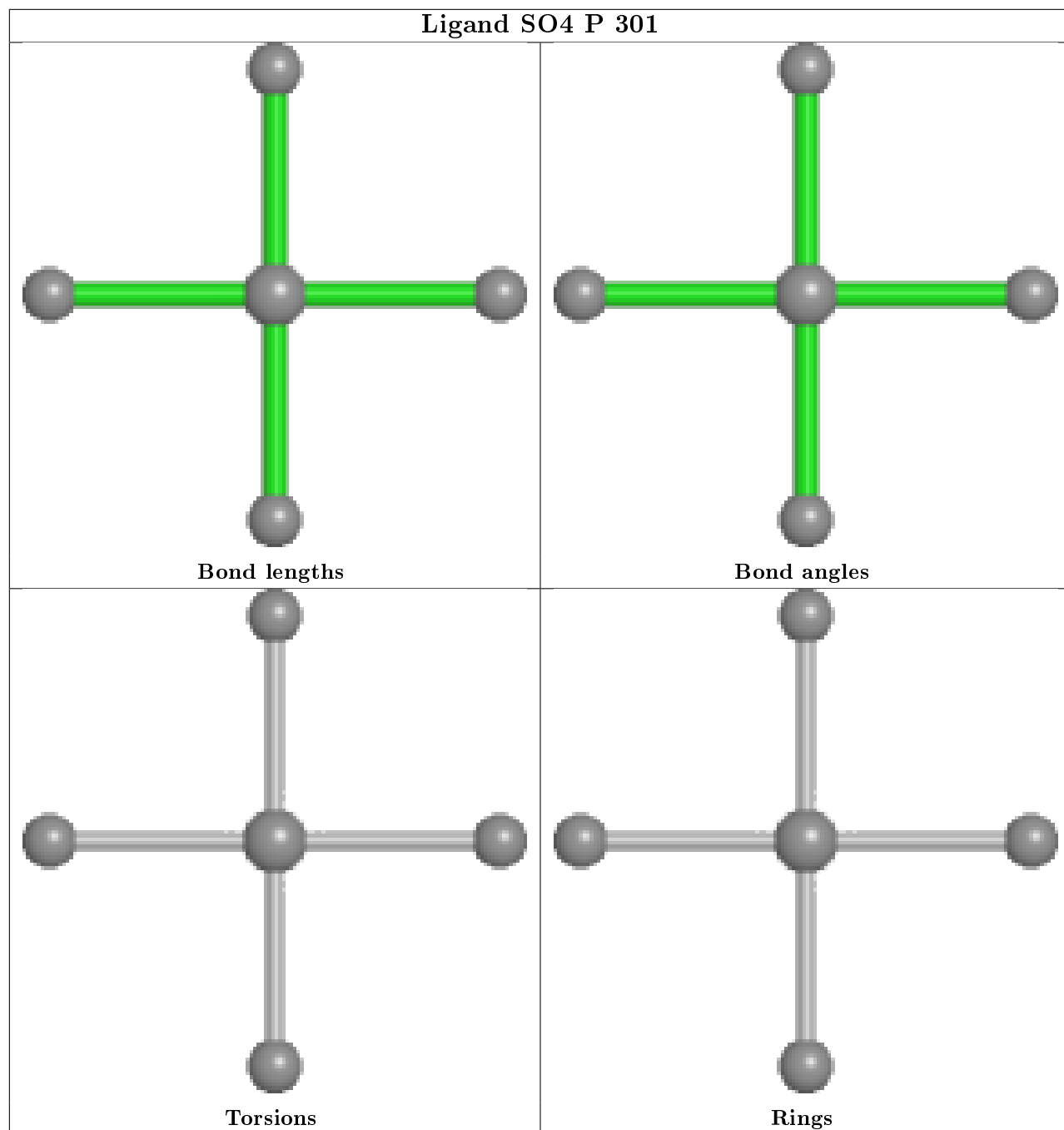


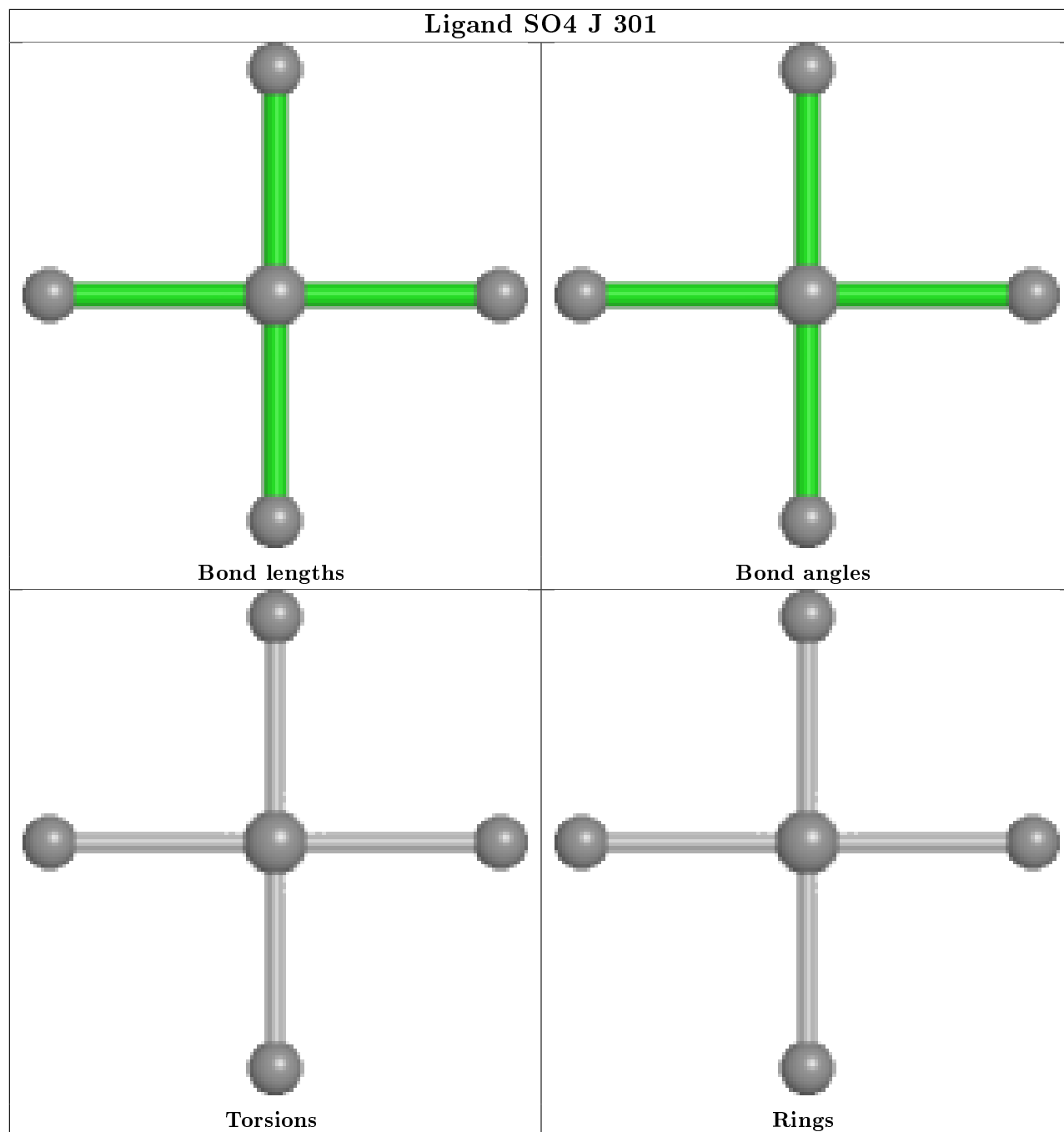


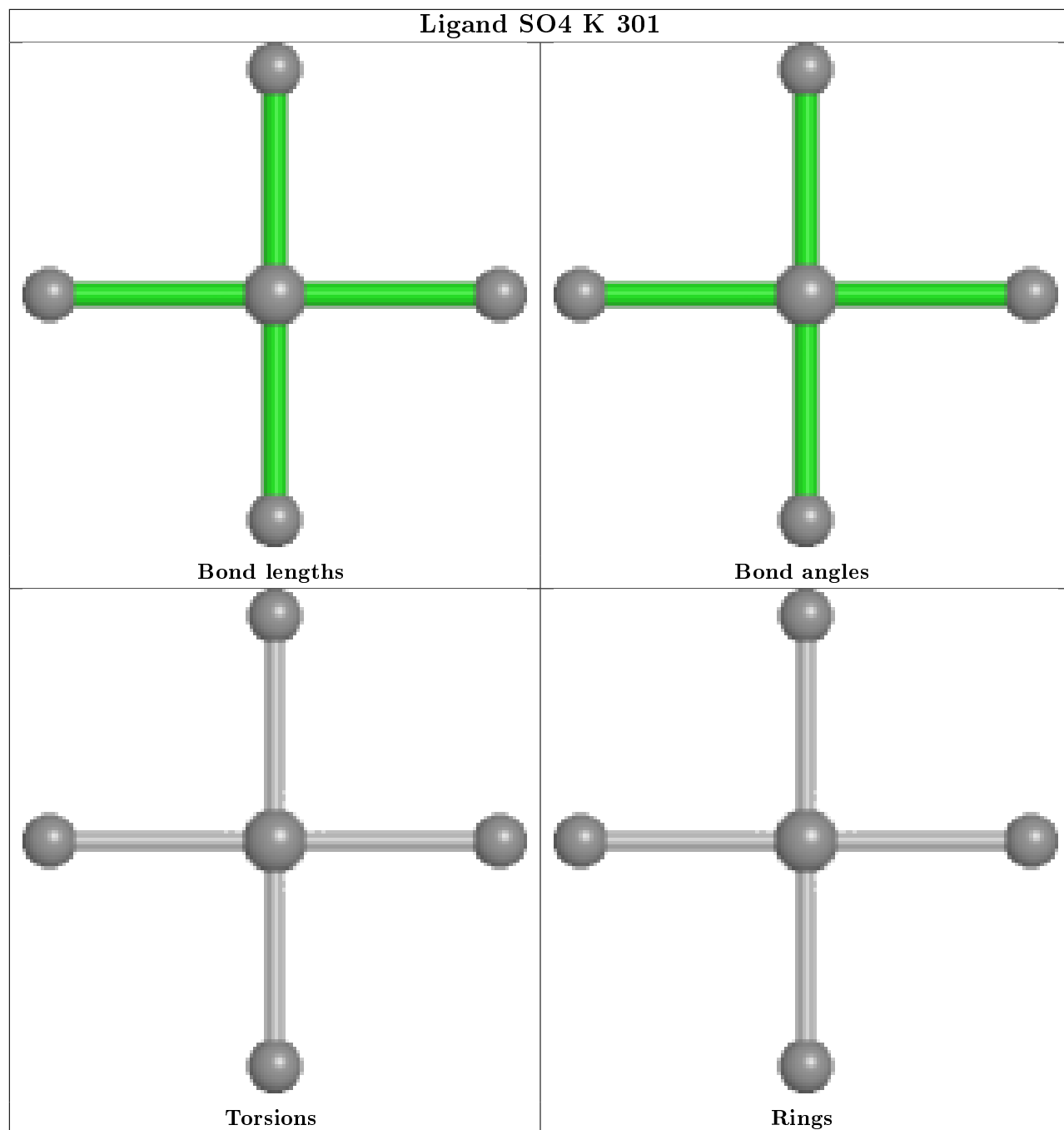


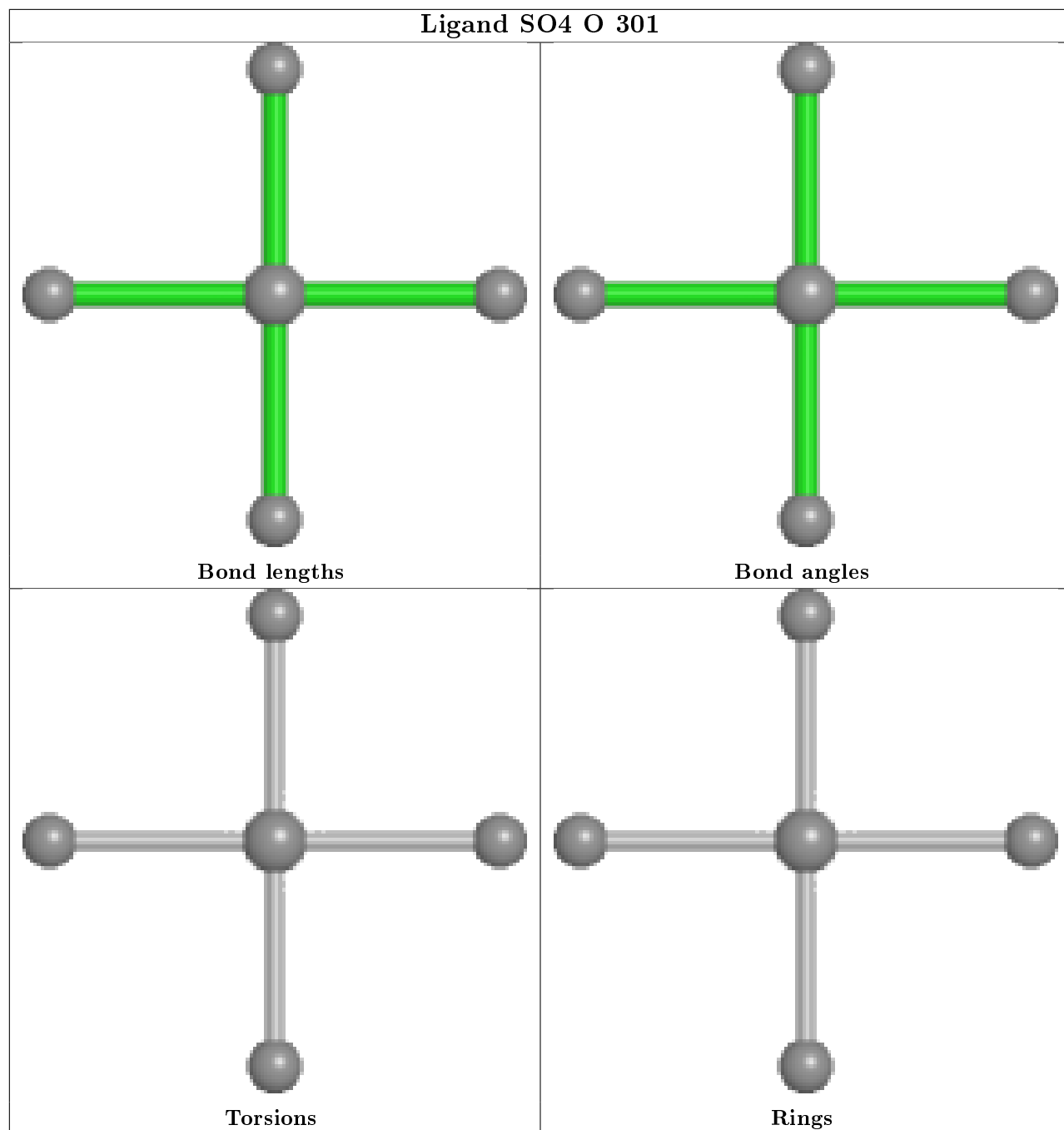


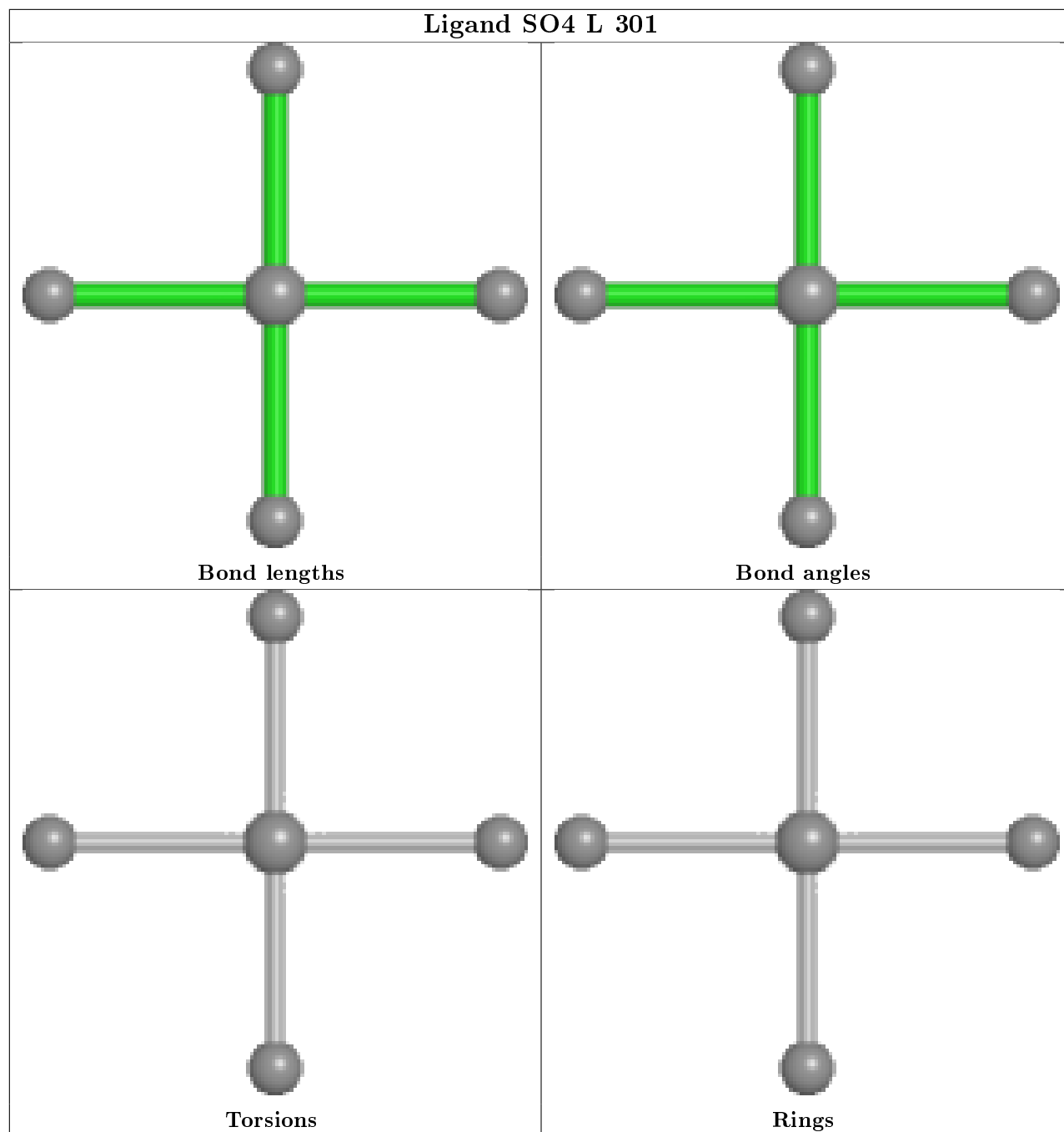


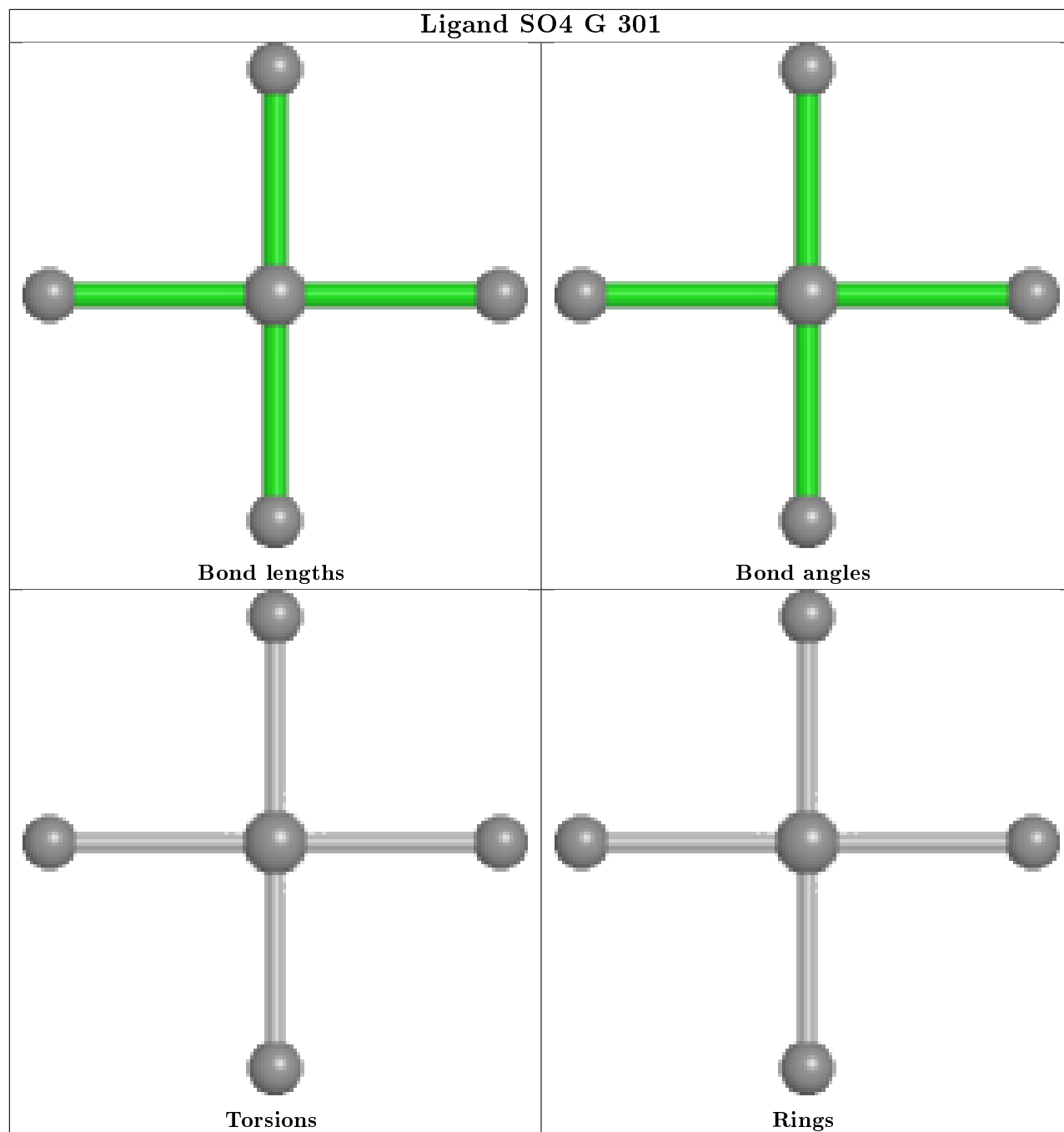












5.7 Other polymers [i](#)

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	272/292 (93%)	0.17	7 (2%) 56 62	13, 35, 63, 81	0
1	B	264/292 (90%)	0.11	4 (1%) 73 78	16, 32, 55, 85	0
1	C	267/292 (91%)	0.24	7 (2%) 56 62	20, 37, 71, 97	0
1	D	261/292 (89%)	0.32	12 (4%) 32 38	17, 40, 73, 91	0
1	E	260/292 (89%)	0.40	9 (3%) 44 49	22, 45, 78, 117	0
1	F	263/292 (90%)	0.20	9 (3%) 45 50	18, 36, 63, 89	0
1	G	255/292 (87%)	0.34	8 (3%) 49 54	19, 41, 69, 84	0
1	H	266/292 (91%)	0.14	4 (1%) 73 78	18, 36, 60, 78	0
1	I	267/292 (91%)	0.31	9 (3%) 45 50	20, 38, 65, 85	0
1	J	268/292 (91%)	0.07	8 (2%) 50 56	16, 31, 56, 80	0
1	K	261/292 (89%)	0.54	21 (8%) 12 15	18, 41, 79, 105	0
1	L	262/292 (89%)	0.27	5 (1%) 66 72	20, 41, 65, 88	0
1	M	263/292 (90%)	0.31	9 (3%) 45 50	19, 39, 67, 93	0
1	N	263/292 (90%)	0.22	4 (1%) 73 78	20, 37, 60, 79	0
1	O	262/292 (89%)	0.38	14 (5%) 26 31	20, 40, 67, 87	0
1	P	261/292 (89%)	0.17	6 (2%) 60 66	17, 34, 62, 84	0
All	All	4215/4672 (90%)	0.26	136 (3%) 47 53	13, 38, 68, 117	0

The worst 5 of 136 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	17	ARG	6.6
1	D	197	LEU	5.6
1	M	197	LEU	5.0
1	K	30	THR	5.0
1	L	241	LEU	4.8

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](#)

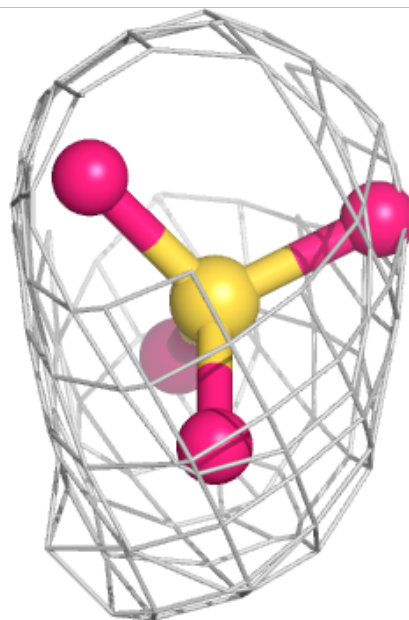
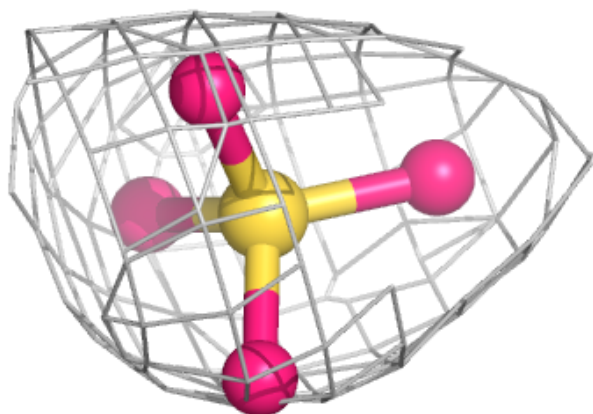
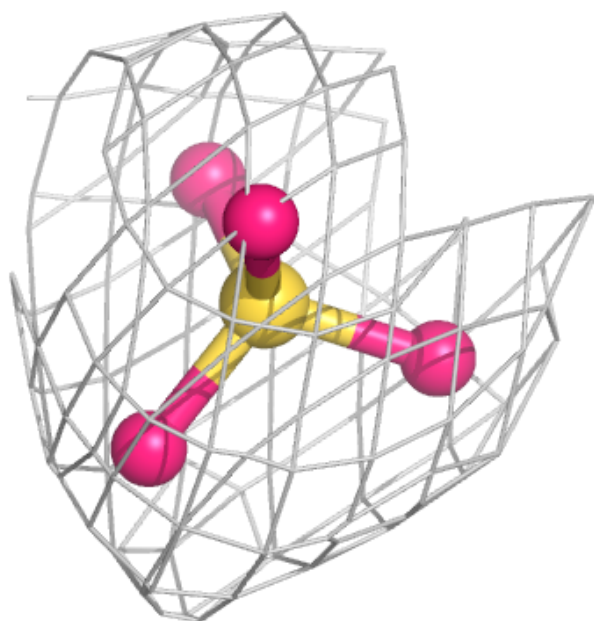
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	N	301	5/5	0.92	0.14	71,71,73,74	0
2	SO4	F	301	5/5	0.93	0.14	64,65,65,67	0
2	SO4	O	301	5/5	0.93	0.13	56,56,57,60	0
2	SO4	L	301	5/5	0.93	0.12	57,57,58,61	0
2	SO4	J	301	5/5	0.94	0.11	31,34,39,39	0
2	SO4	D	301	5/5	0.95	0.16	41,42,44,45	0
2	SO4	C	302	5/5	0.96	0.13	40,42,46,48	0
2	SO4	M	301	5/5	0.96	0.11	33,35,39,44	0
2	SO4	P	301	5/5	0.96	0.12	39,43,44,46	0
2	SO4	I	301	5/5	0.97	0.09	34,38,39,42	0
2	SO4	G	302	5/5	0.97	0.11	40,41,43,45	0
2	SO4	C	301	5/5	0.97	0.10	32,32,34,37	0
2	SO4	A	301	5/5	0.98	0.10	43,44,46,48	0
2	SO4	K	301	5/5	0.98	0.13	40,41,41,43	0
2	SO4	J	302	5/5	0.98	0.11	34,35,38,42	0
2	SO4	A	302	5/5	0.98	0.10	41,42,42,43	0
2	SO4	G	301	5/5	0.98	0.10	46,46,47,48	0
2	SO4	E	301	5/5	0.99	0.08	36,36,38,42	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.

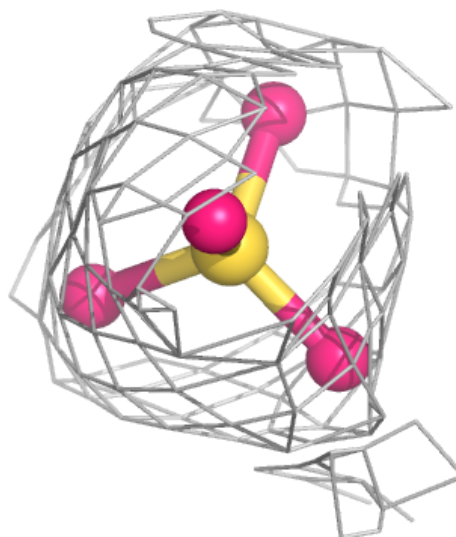
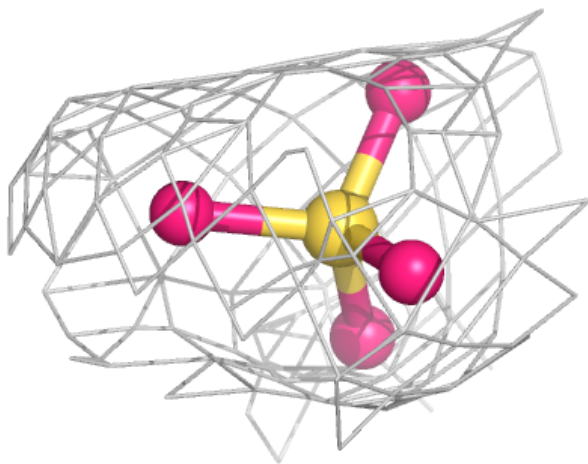
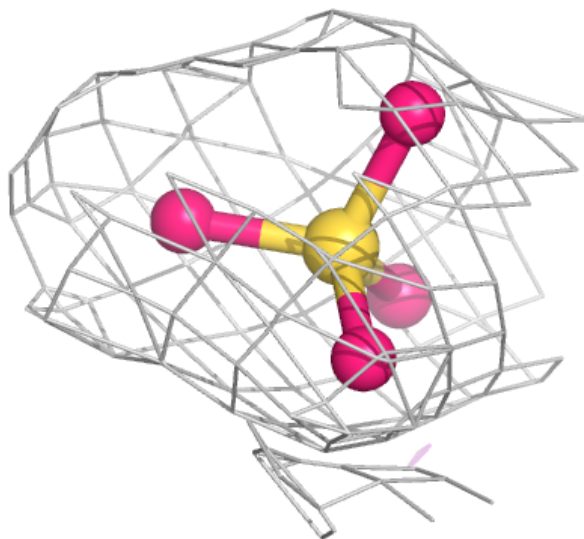
Electron density around SO4 N 301:

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



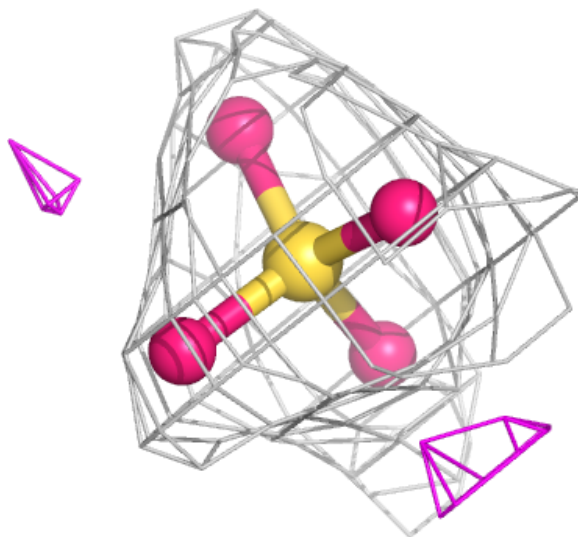
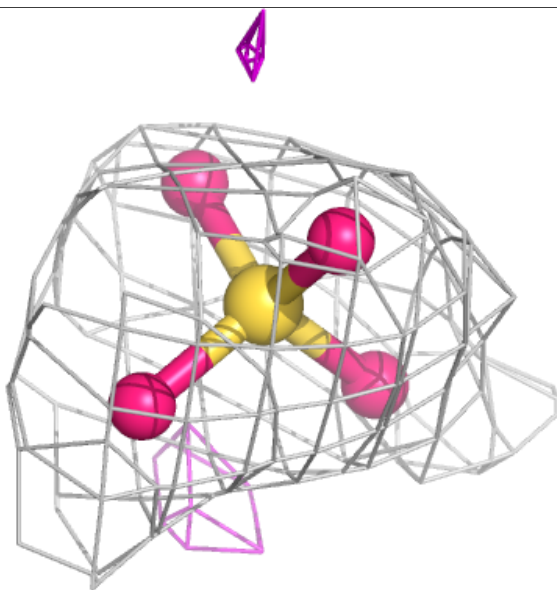
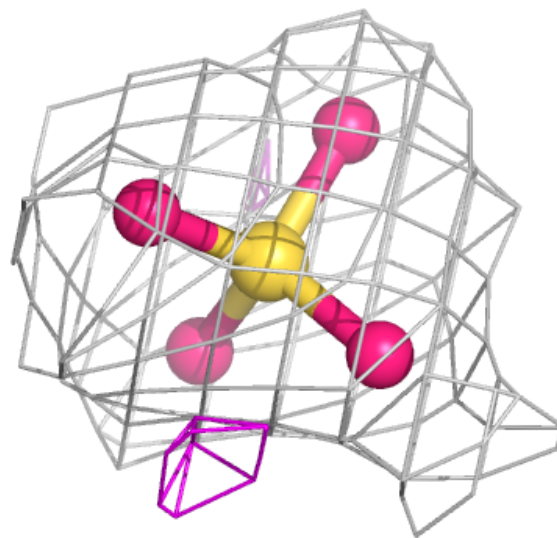
Electron density around SO4 F 301:

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



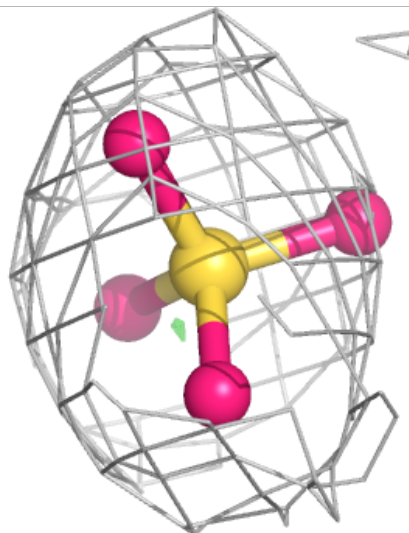
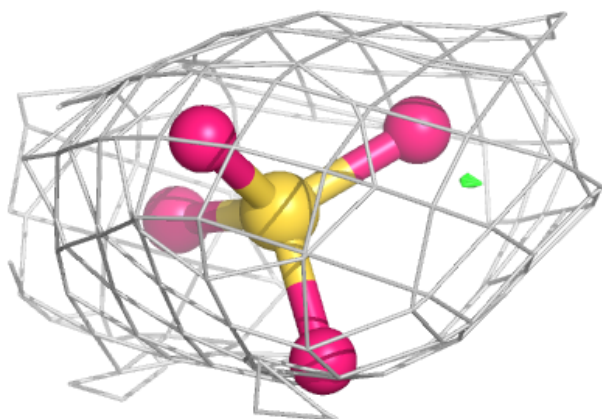
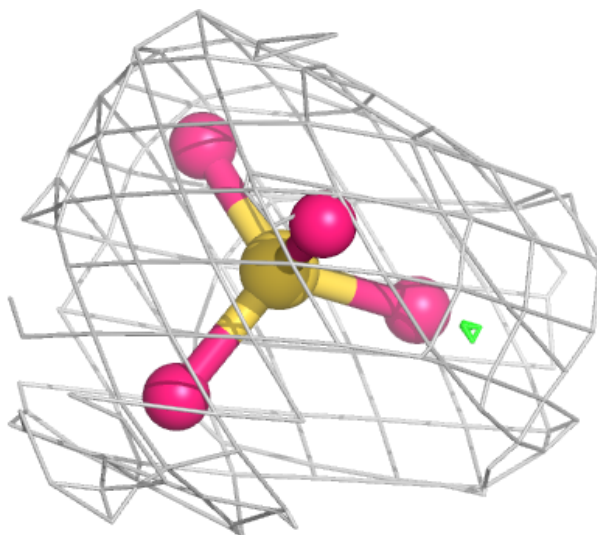
Electron density around SO4 O 301:

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



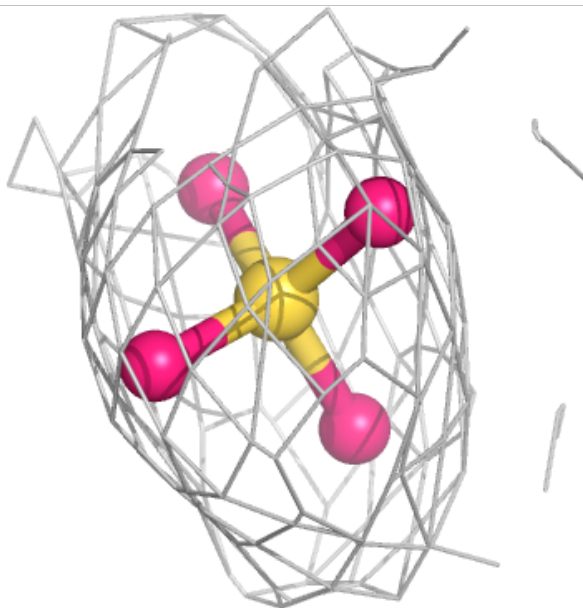
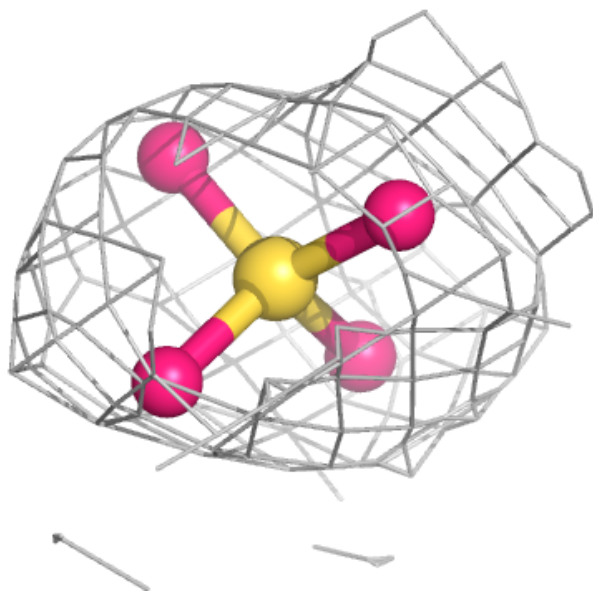
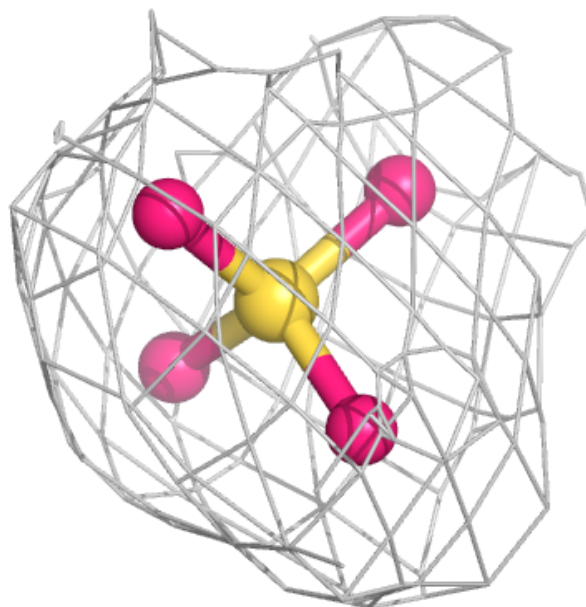
Electron density around SO4 L 301:

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



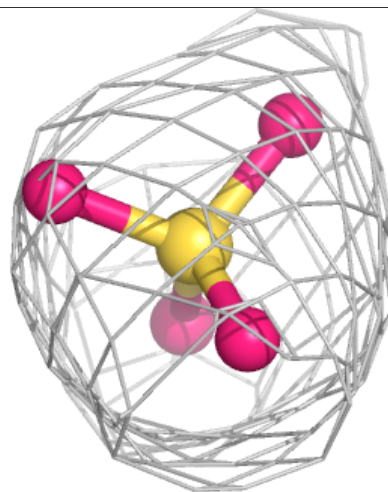
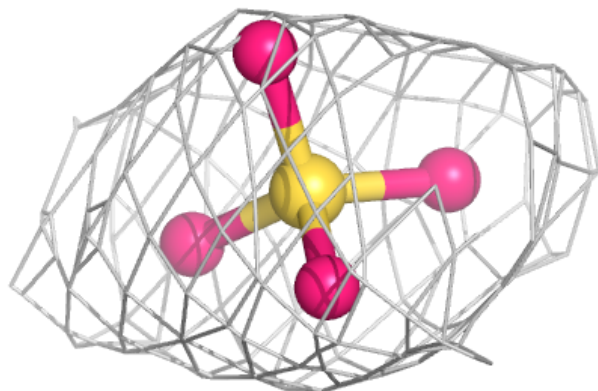
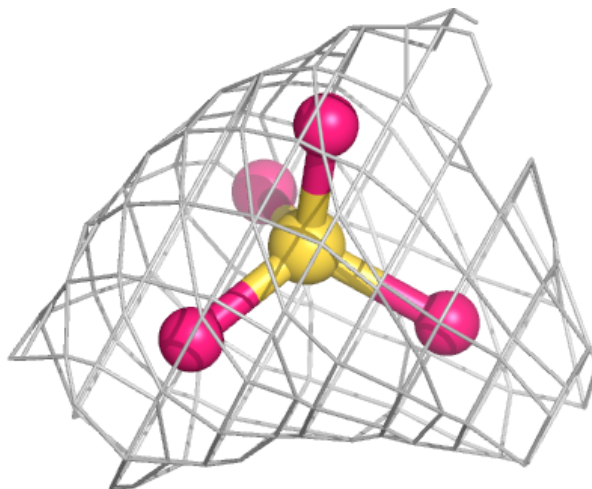
Electron density around SO4 J 301:

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



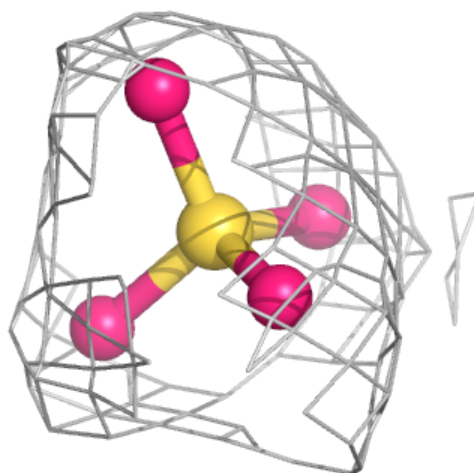
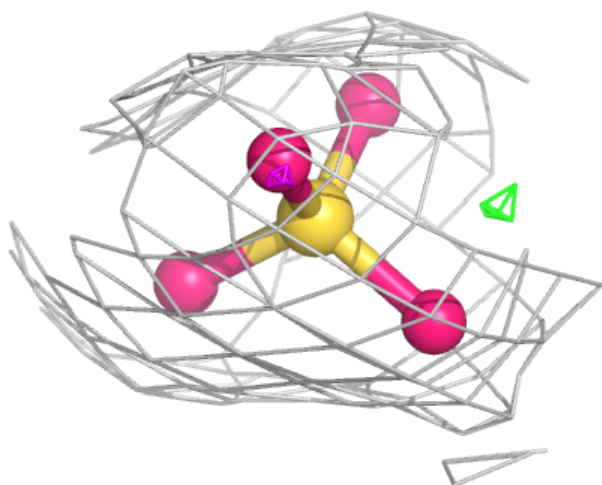
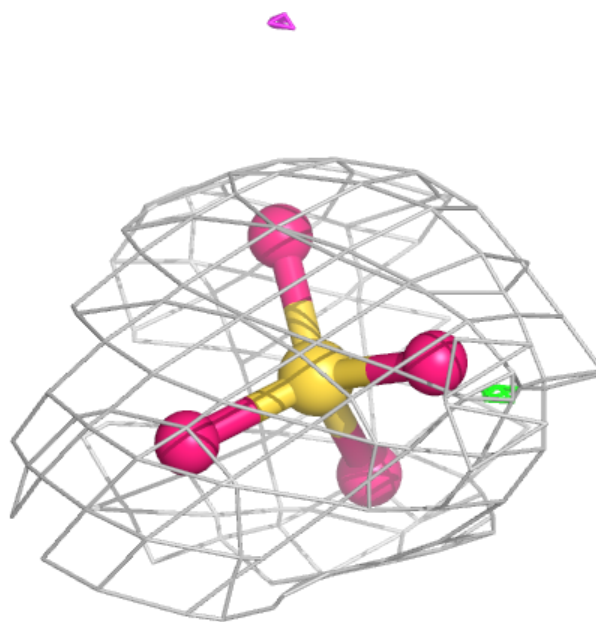
Electron density around SO4 D 301:

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



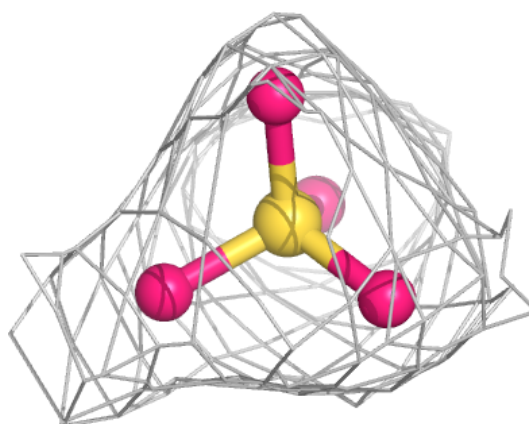
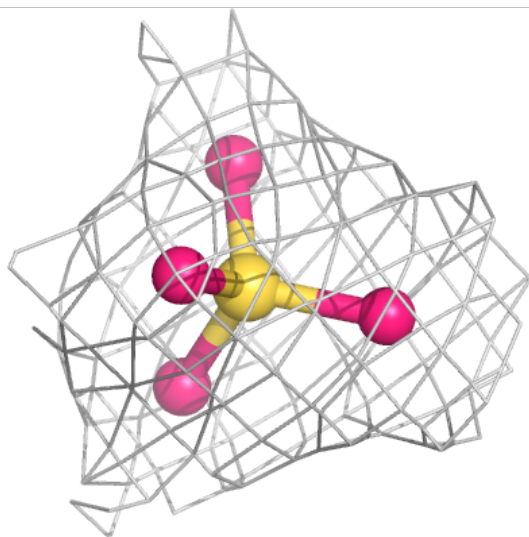
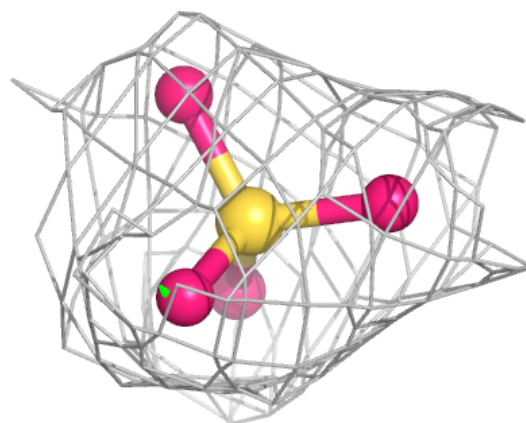
Electron density around SO4 C 302:

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



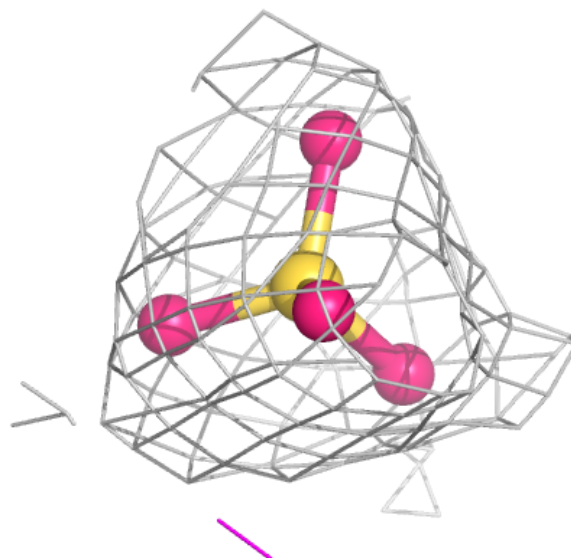
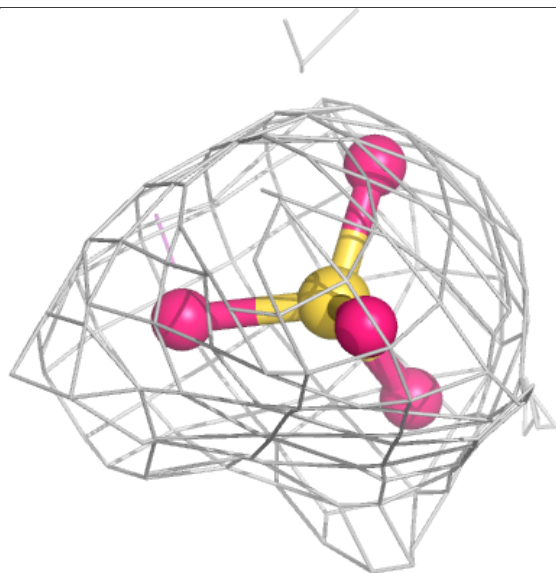
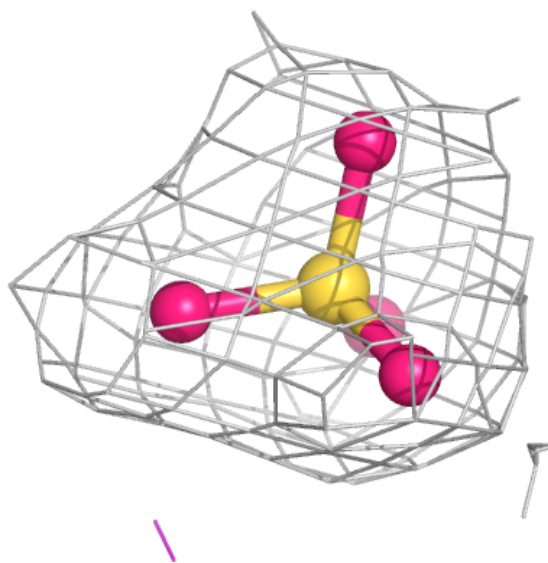
Electron density around SO4 M 301:

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



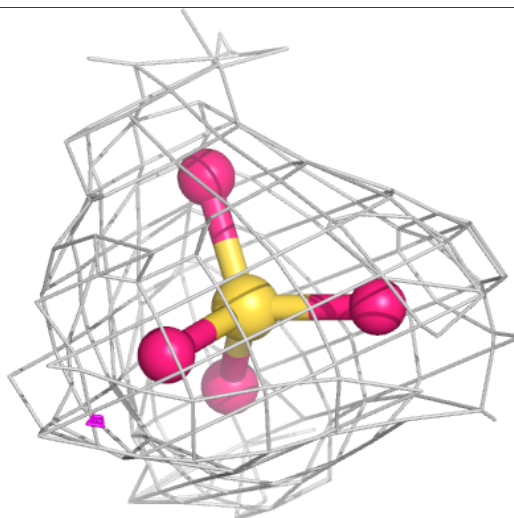
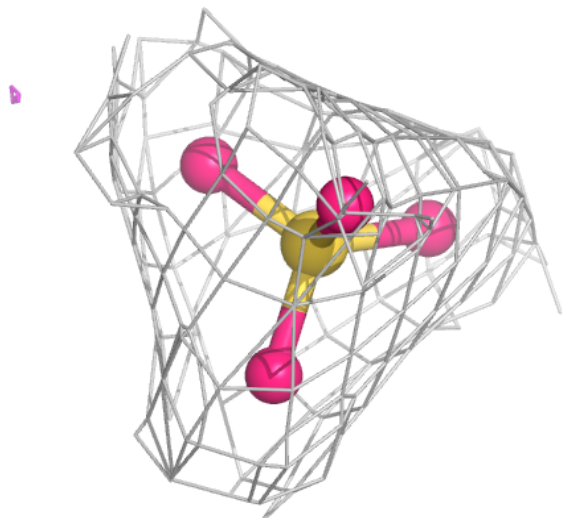
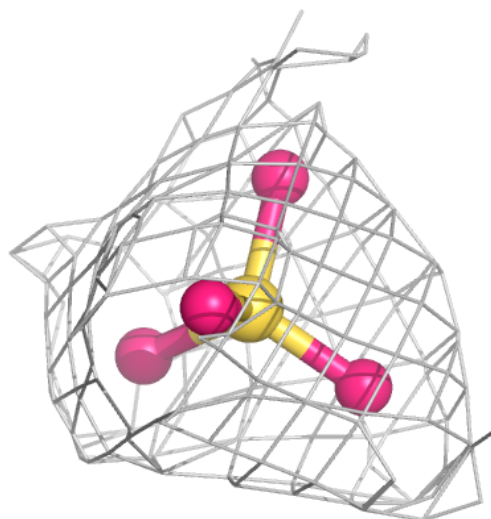
Electron density around SO4 P 301:

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



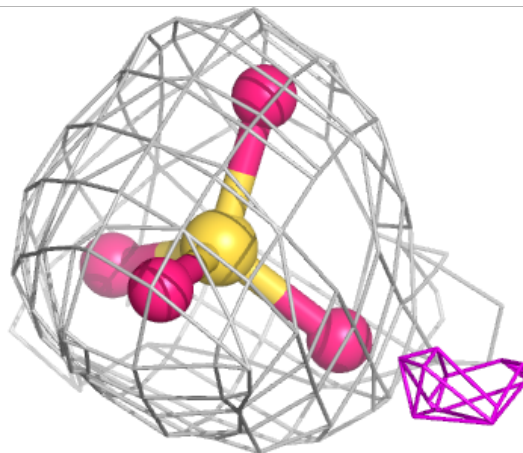
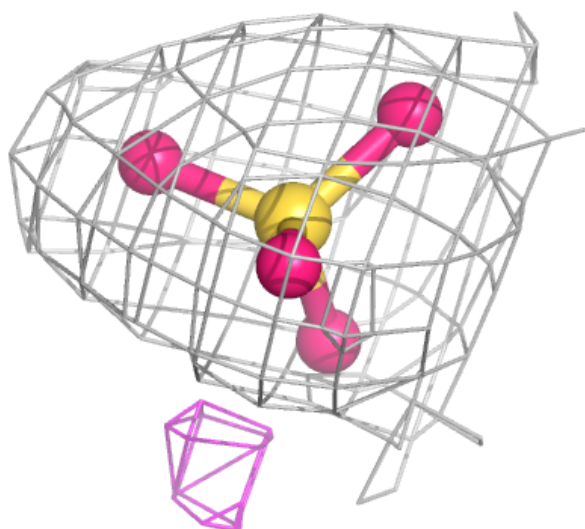
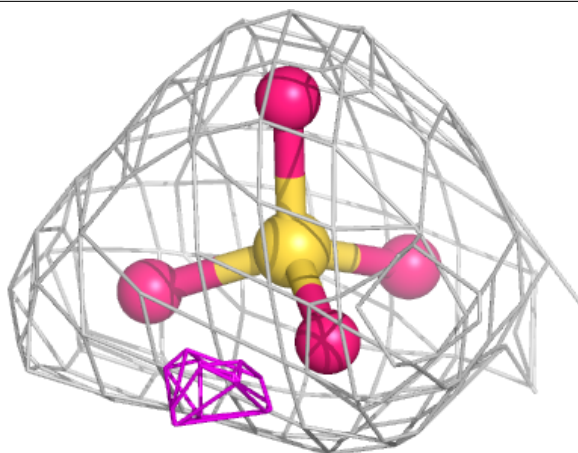
Electron density around SO4 I 301:

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



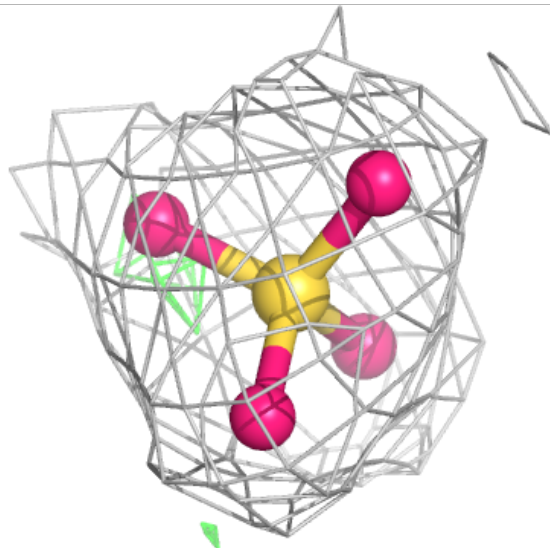
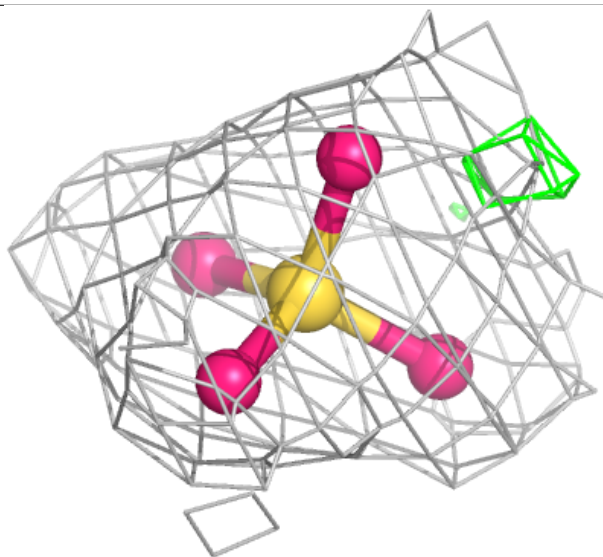
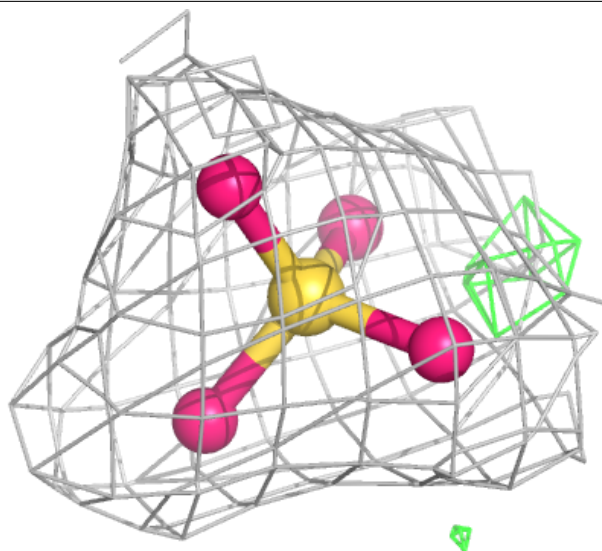
Electron density around SO4 G 302:

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



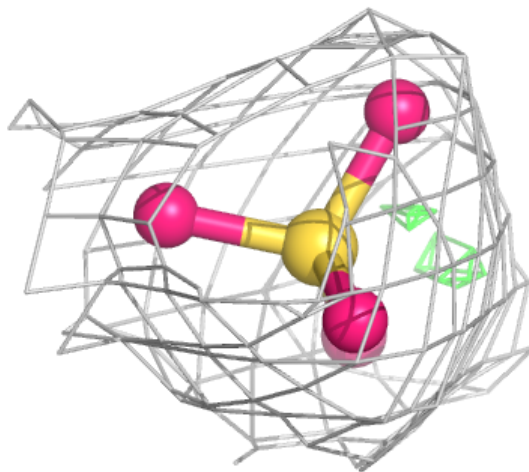
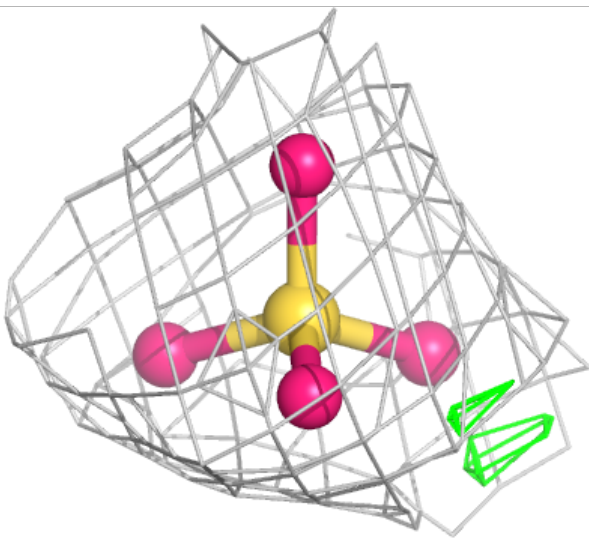
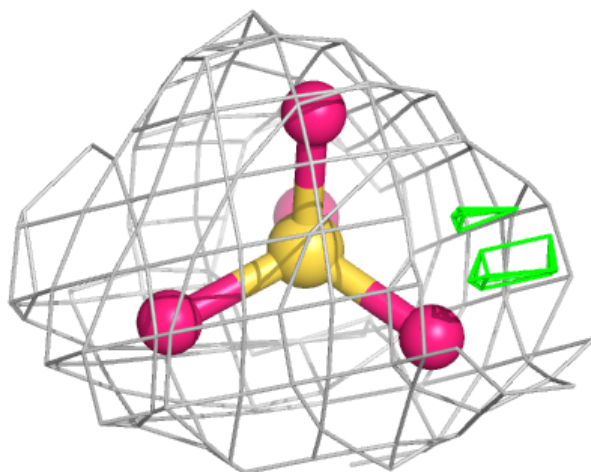
Electron density around SO4 C 301:

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



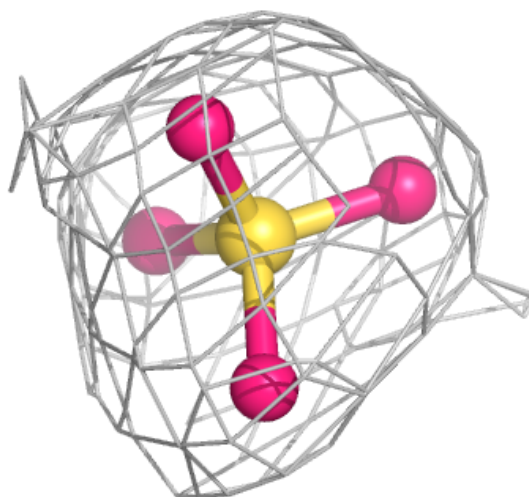
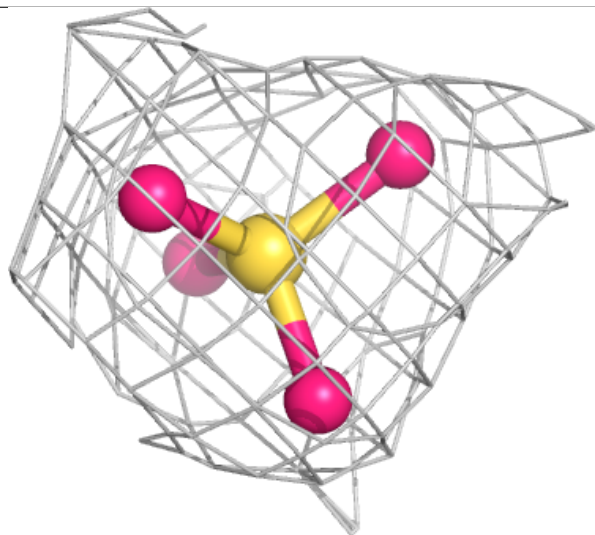
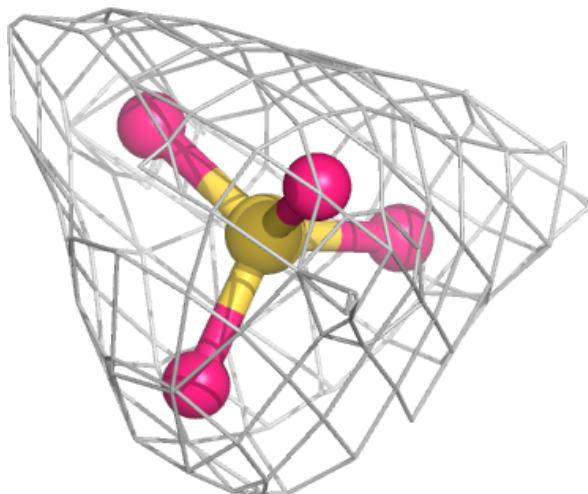
Electron density around SO4 A 301:

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



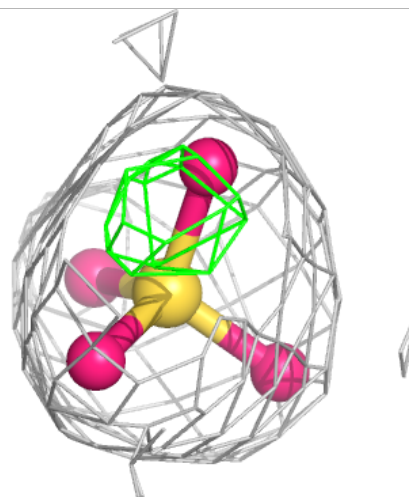
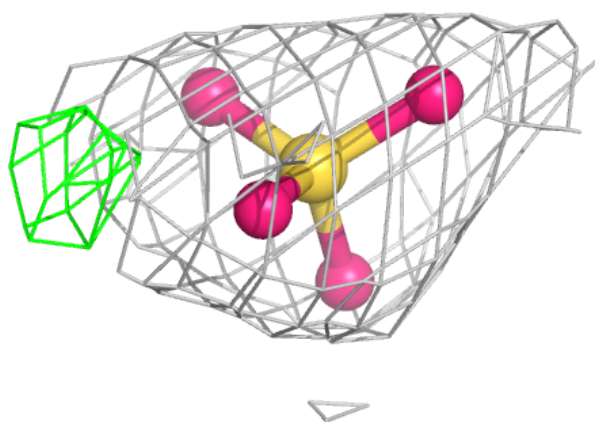
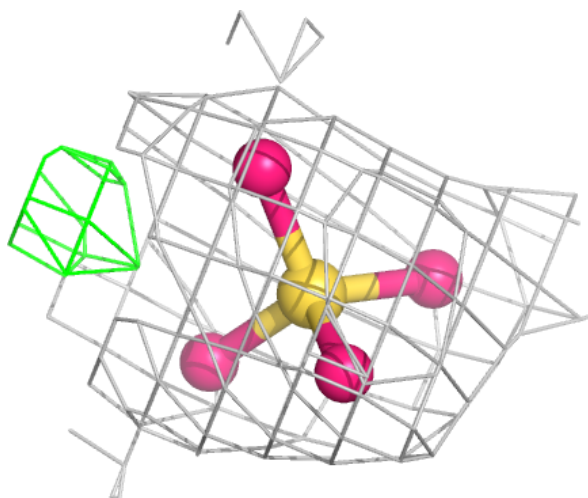
Electron density around SO4 K 301:

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



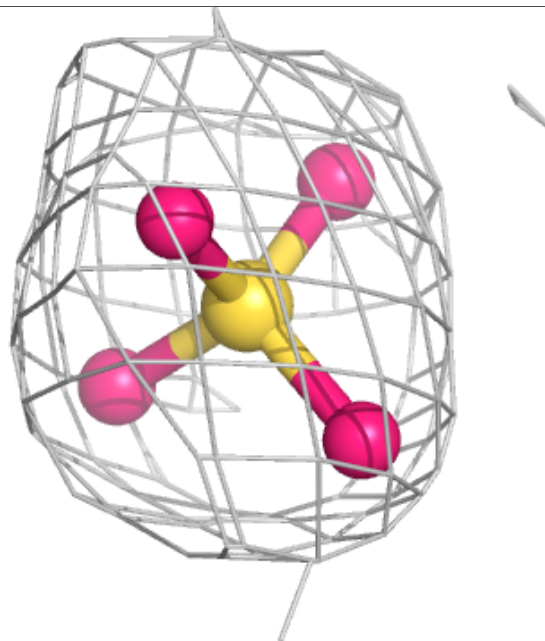
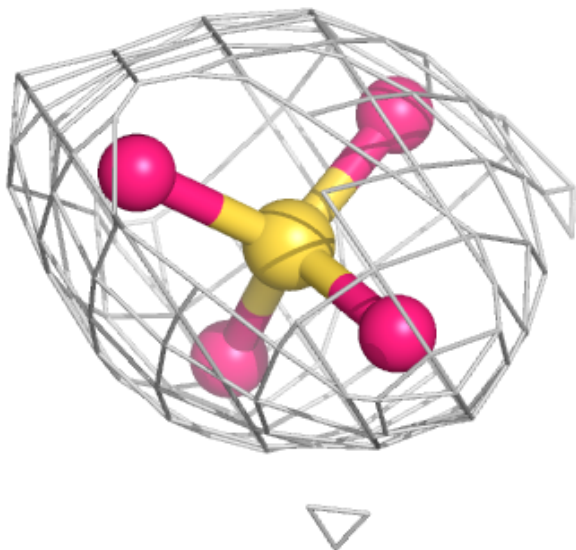
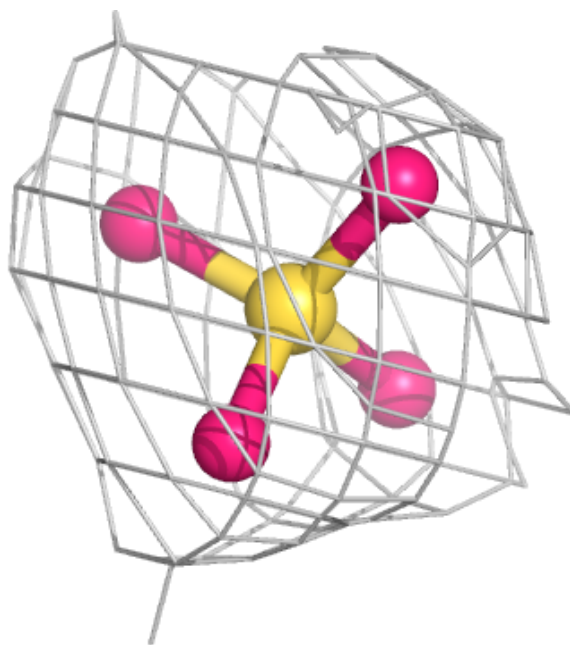
Electron density around SO4 J 302:

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



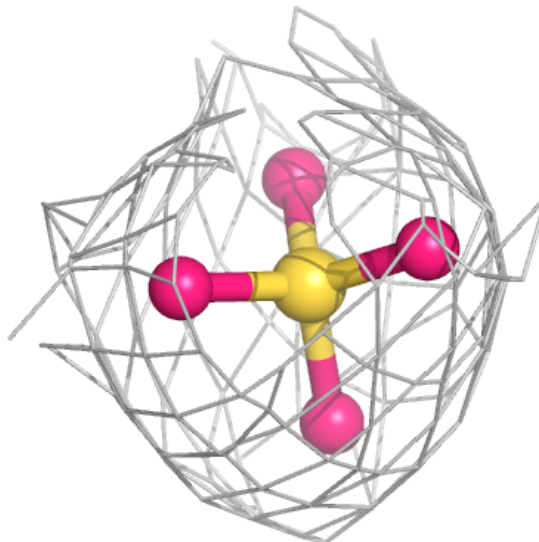
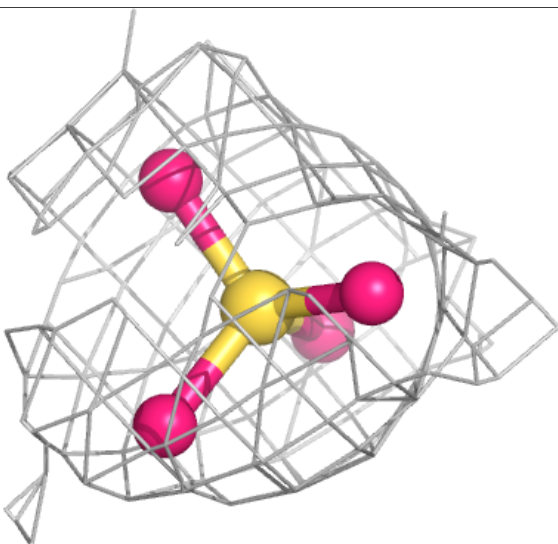
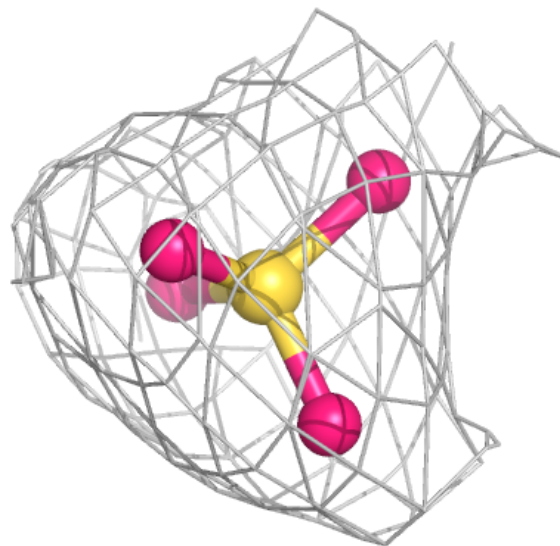
Electron density around SO4 A 302:

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



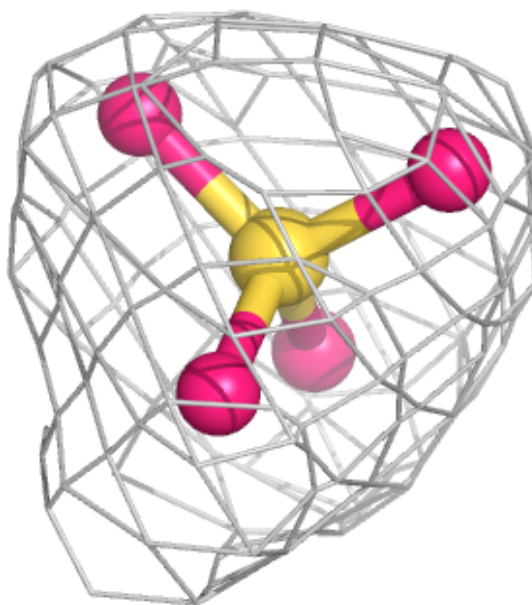
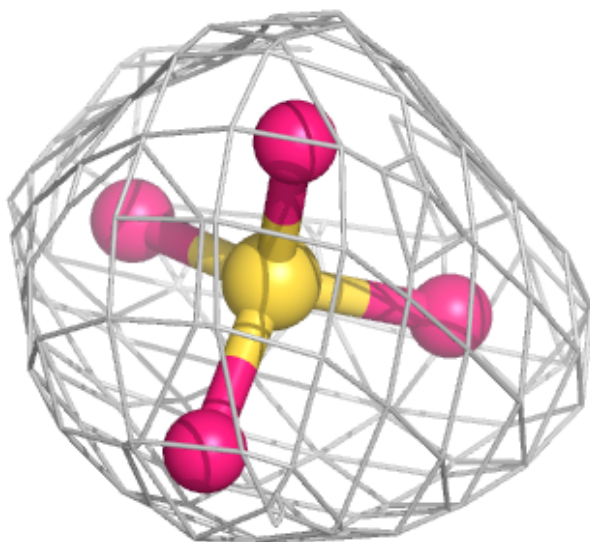
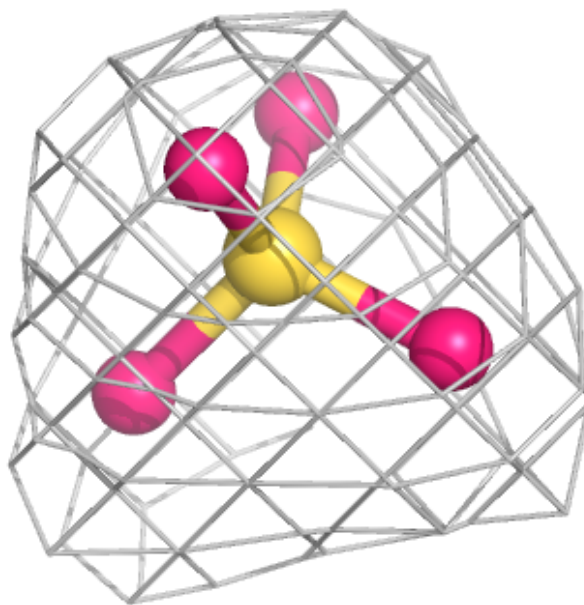
Electron density around SO4 G 301:

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



Electron density around SO4 E 301:

$2mF_o-DF_c$ (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.