



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:44 PM UTC

PDB ID : 6K8S / pdb_00006k8s
Title : Crystal structure of C-domain of bacterial malonyl-CoA reductase
Authors : Kim, S.; Kim, K.-J.
Deposited on : 2019-06-13
Resolution : 1.80 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

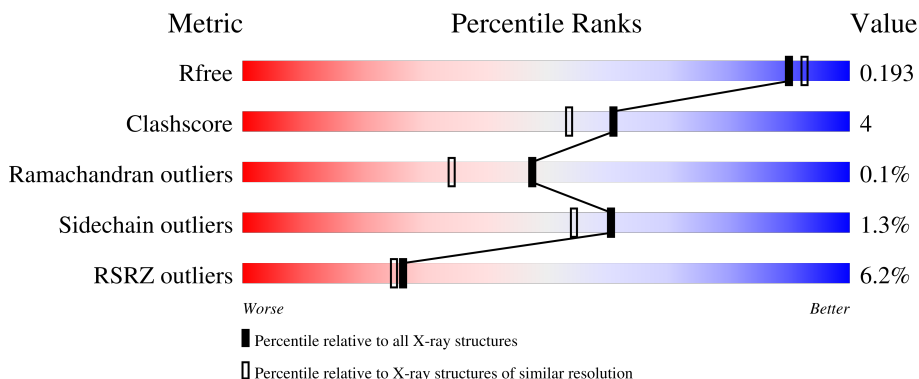
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	695	6% 86% 9% • 5%
1	B	695	5% 85% 9% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11399 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 NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	662	Total	C	N	O	S	0	6	0
			5130	3214	913	983	20			
1	B	662	Total	C	N	O	S	0	3	0
			5104	3200	909	975	20			

There are 42 discrepancies between the modelled and reference sequences:

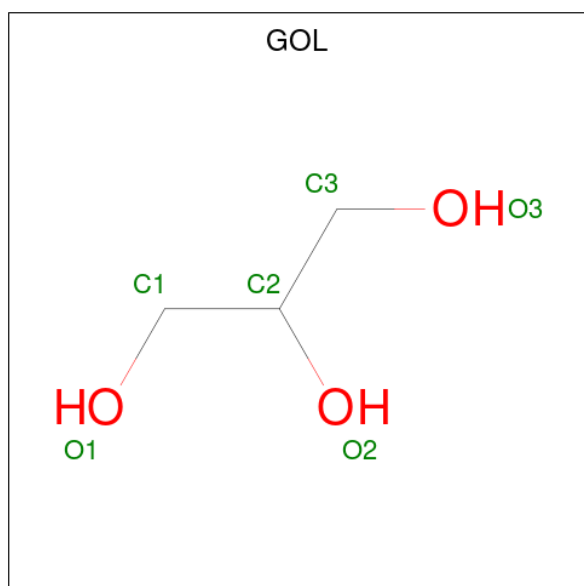
Chain	Residue	Modelled	Actual	Comment	Reference
A	536	MET	-	initiating methionine	UNP A0A1A7BFR5
A	537	GLY	-	expression tag	UNP A0A1A7BFR5
A	538	SER	-	expression tag	UNP A0A1A7BFR5
A	539	SER	-	expression tag	UNP A0A1A7BFR5
A	540	HIS	-	expression tag	UNP A0A1A7BFR5
A	541	HIS	-	expression tag	UNP A0A1A7BFR5
A	542	HIS	-	expression tag	UNP A0A1A7BFR5
A	543	HIS	-	expression tag	UNP A0A1A7BFR5
A	544	HIS	-	expression tag	UNP A0A1A7BFR5
A	545	HIS	-	expression tag	UNP A0A1A7BFR5
A	546	SER	-	expression tag	UNP A0A1A7BFR5
A	547	SER	-	expression tag	UNP A0A1A7BFR5
A	548	GLY	-	expression tag	UNP A0A1A7BFR5
A	549	LEU	-	expression tag	UNP A0A1A7BFR5
A	550	VAL	-	expression tag	UNP A0A1A7BFR5
A	551	PRO	-	expression tag	UNP A0A1A7BFR5
A	552	ARG	-	expression tag	UNP A0A1A7BFR5
A	553	GLY	-	expression tag	UNP A0A1A7BFR5
A	554	SER	-	expression tag	UNP A0A1A7BFR5
A	555	HIS	-	expression tag	UNP A0A1A7BFR5
A	556	MET	-	expression tag	UNP A0A1A7BFR5
B	536	MET	-	initiating methionine	UNP A0A1A7BFR5
B	537	GLY	-	expression tag	UNP A0A1A7BFR5
B	538	SER	-	expression tag	UNP A0A1A7BFR5

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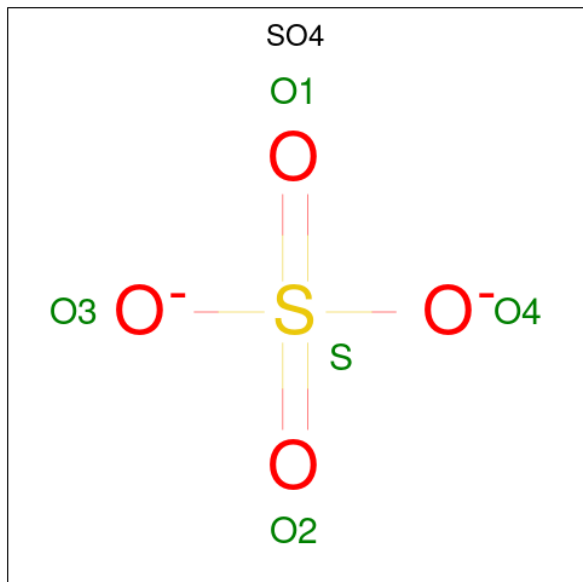
Chain	Residue	Modelled	Actual	Comment	Reference
B	539	SER	-	expression tag	UNP A0A1A7BFR5
B	540	HIS	-	expression tag	UNP A0A1A7BFR5
B	541	HIS	-	expression tag	UNP A0A1A7BFR5
B	542	HIS	-	expression tag	UNP A0A1A7BFR5
B	543	HIS	-	expression tag	UNP A0A1A7BFR5
B	544	HIS	-	expression tag	UNP A0A1A7BFR5
B	545	HIS	-	expression tag	UNP A0A1A7BFR5
B	546	SER	-	expression tag	UNP A0A1A7BFR5
B	547	SER	-	expression tag	UNP A0A1A7BFR5
B	548	GLY	-	expression tag	UNP A0A1A7BFR5
B	549	LEU	-	expression tag	UNP A0A1A7BFR5
B	550	VAL	-	expression tag	UNP A0A1A7BFR5
B	551	PRO	-	expression tag	UNP A0A1A7BFR5
B	552	ARG	-	expression tag	UNP A0A1A7BFR5
B	553	GLY	-	expression tag	UNP A0A1A7BFR5
B	554	SER	-	expression tag	UNP A0A1A7BFR5
B	555	HIS	-	expression tag	UNP A0A1A7BFR5
B	556	MET	-	expression tag	UNP A0A1A7BFR5

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	533	Total 533	O 533	0	0
4	B	560	Total 560	O 560	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.34Å 116.69Å 134.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.86 – 1.80 29.86 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.8 (29.86-1.80) 97.8 (29.86-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.03	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.88 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.174 , 0.204 (Not available) , 0.193	Depositor DCC
R_{free} test set	7789 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtrriage
Anisotropy	0.215	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11399	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.47 % 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 3.6710e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: GOL, 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	1.09	2/5221 (0.0%)	1.33	4/7081 (0.1%)
1	B	1.13	5/5195 (0.1%)	1.32	7/7046 (0.1%)
All	All	1.11	7/10416 (0.1%)	1.33	11/14127 (0.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1192	HIS	CE1-NE2	6.80	1.39	1.32
1	B	739	PRO	C-O	-6.20	1.16	1.23
1	A	1192	HIS	CE1-NE2	5.86	1.38	1.32
1	B	963	THR	C-O	5.43	1.30	1.24
1	B	672	ASN	C-O	5.39	1.29	1.23
1	B	582	ALA	C-O	5.34	1.30	1.24
1	A	719	GLY	C-O	5.15	1.29	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	976	THR	CA-CB-OG1	-6.50	99.85	109.60
1	A	982	PHE	CB-CA-C	6.43	119.17	110.94
1	A	918	ASP	CA-CB-CG	6.34	118.94	112.60
1	B	891	GLU	CB-CG-CD	6.06	122.91	112.60
1	B	982	PHE	CB-CA-C	5.74	118.55	111.43
1	B	1033	GLU	CB-CG-CD	5.46	121.89	112.60
1	B	927	VAL	CA-C-N	5.37	125.90	119.94
1	B	927	VAL	C-N-CA	5.37	125.90	119.94
1	B	624	VAL	CA-C-O	-5.28	115.46	120.95
1	A	945	ASP	CA-CB-CG	5.26	117.86	112.60
1	B	728	PHE	CA-CB-CG	-5.15	108.65	113.80

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	5130	0	5088	44	0
1	B	5104	0	5073	47	0
2	A	6	0	8	0	0
2	B	6	0	8	0	0
3	A	25	0	0	0	0
3	B	35	0	0	0	0
4	A	533	0	0	7	0
4	B	560	0	0	6	0
All	All	11399	0	10177	86	0

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

All (86) 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:B:702:ASN:HD21	1:B:751:GLN:HE21	1.26	0.83
1:A:702:ASN:HD21	1:A:751:GLN:HE21	1.29	0.81
1:B:1226:MET:SD	1:B:1228:MET:HE2	2.21	0.80
1:B:1174:GLN:HE21	1:B:1176:ASN:HD21	1.30	0.79
1:B:1045:ASP:O	1:B:1048:GLN:HG2	1.86	0.76
1:B:1212:ASP:O	1:B:1215:ASP:HB2	1.90	0.72
1:B:769:ASN:HD22	1:B:962:GLU:H	1.38	0.71
1:A:769:ASN:HD22	1:A:962:GLU:H	1.37	0.70
1:B:981:LEU:HD13	1:B:1228:MET:SD	2.33	0.68
1:A:1173:ASN:HD22	1:A:1226:MET:H	1.41	0.68
1:B:822[B]:GLU:HA	1:B:822[B]:GLU:OE1	1.92	0.67
1:A:1213:ALA:HA	1:A:1220:ALA:HB2	1.75	0.66
1:A:948:GLN:HG2	1:A:952:PHE:CE2	2.31	0.65
1:A:640:GLN:HE21	1:A:663:ALA:HB1	1.60	0.65
1:A:1173:ASN:ND2	1:A:1226:MET:H	1.97	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:SER:HA	4:A:1799:HOH:O	2.02	0.59
1:B:948:GLN:HG2	1:B:952:PHE:CZ	2.38	0.58
1:A:1006:VAL:HG22	4:A:1534:HOH:O	2.03	0.57
1:B:740[B]:ASN:ND2	1:B:801:ASN:OD1	2.38	0.57
1:A:973:GLU:HA	4:A:1649:HOH:O	2.05	0.57
1:B:987:GLN:NE2	1:B:991:ASP:OD1	2.37	0.56
1:A:1216:SER:OG	1:A:1219:ARG:HG3	2.04	0.56
1:A:702:ASN:ND2	1:A:751:GLN:HE21	2.00	0.56
1:A:981:LEU:HD13	1:A:1228:MET:CE	2.35	0.56
1:A:981:LEU:HB2	1:A:1228:MET:SD	2.45	0.56
1:A:808:HIS:HE1	4:A:1683:HOH:O	1.89	0.55
1:A:682:MET:SD	1:A:801:ASN:ND2	2.81	0.54
1:B:1222:ILE:O	1:B:1226:MET:HE2	2.08	0.54
1:B:732:LYS:HD2	1:B:733:TYR:CE2	2.43	0.53
1:A:612:ARG:NH2	4:A:1410:HOH:O	2.42	0.53
1:B:1174:GLN:HE21	1:B:1176:ASN:ND2	2.04	0.53
1:A:682:MET:HG3	1:A:801:ASN:ND2	2.24	0.53
1:B:808:HIS:HE1	4:B:1723:HOH:O	1.92	0.52
1:A:980:GLU:HG3	1:B:979:ARG:HH11	1.75	0.52
1:B:780:ARG:NH1	1:B:790:LEU:HD11	2.25	0.52
1:B:784:THR:O	1:B:787:LYS:HG2	2.09	0.51
1:B:948:GLN:HG2	1:B:952:PHE:CE2	2.45	0.51
1:B:981:LEU:HB2	1:B:1228:MET:CG	2.41	0.51
1:B:702:ASN:ND2	1:B:751:GLN:HE21	2.01	0.51
1:A:979:ARG:HB3	1:A:979:ARG:HH11	1.75	0.50
1:B:732:LYS:HE2	4:B:1601:HOH:O	2.11	0.50
1:B:611:ARG:HD3	4:B:1873:HOH:O	2.11	0.50
1:B:769:ASN:ND2	1:B:962:GLU:H	2.07	0.50
1:A:836:MET:HA	1:A:842:ASN:ND2	2.26	0.50
1:B:570:SER:HB3	4:B:1759:HOH:O	2.11	0.50
1:A:981:LEU:HB2	1:A:1228:MET:CG	2.42	0.49
1:B:570:SER:HB2	1:B:601:LEU:HD13	1.95	0.49
1:A:978:GLU:O	1:B:979:ARG:NH2	2.45	0.49
1:B:981:LEU:HB2	1:B:1228:MET:SD	2.53	0.49
1:B:723:ASN:ND2	1:B:754:MET:HE3	2.28	0.49
1:A:808:HIS:HD2	4:A:1756:HOH:O	1.96	0.48
1:B:910:GLU:O	1:B:910:GLU:HG2	2.13	0.48
1:A:576:LEU:CD2	1:B:952:PHE:CE1	2.97	0.48
1:B:830:ARG:NH2	4:B:1407:HOH:O	2.46	0.48
1:B:775:PRO:HG2	1:B:931:VAL:HG11	1.96	0.46
1:A:1028:ILE:HA	1:A:1053:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:MET:HG3	1:A:801:ASN:HD21	1.80	0.46
1:A:979:ARG:HA	1:B:979:ARG:CZ	2.46	0.46
1:B:776:VAL:HG12	1:B:943:GLU:HG3	1.98	0.46
1:B:993:MET:HB2	1:B:1020:CYS:HB3	1.98	0.46
1:A:800:GLU:HG3	1:A:915:LEU:HD11	1.98	0.46
1:B:660:THR:HG21	1:B:667:ILE:HG12	1.98	0.45
1:B:1130:SER:HB2	1:B:1131:PRO:CD	2.47	0.45
1:A:762:LEU:HD12	1:A:768:PHE:CD2	2.52	0.44
1:B:1033:GLU:H	1:B:1033:GLU:CD	2.26	0.44
1:B:630:ILE:HD11	1:B:632:PHE:HE2	1.83	0.44
1:B:723:ASN:HD21	1:B:754:MET:HE3	1.83	0.43
1:B:1041:GLN:HG3	4:B:1659:HOH:O	2.19	0.43
1:A:1210:LEU:HD22	1:A:1223:TYR:HB3	2.01	0.43
1:A:1130:SER:OG	1:A:1176:ASN:HA	2.19	0.43
1:A:798:ILE:O	1:A:802:LYS:HG2	2.19	0.42
1:B:628:GLU:HG3	1:B:635:VAL:HG21	2.01	0.42
1:A:863:TRP:HB3	1:A:914:PHE:O	2.20	0.42
1:B:1000:ILE:CG2	1:B:1009:LEU:HD22	2.49	0.42
1:A:1107:ASN:ND2	1:A:1131:PRO:HG3	2.34	0.42
1:A:732:LYS:HG2	1:A:733:TYR:CD2	2.54	0.42
1:A:769:ASN:ND2	1:A:962:GLU:H	2.11	0.42
1:A:916:PRO:HG2	1:A:919:LYS:HB2	2.02	0.41
1:A:781:LEU:HA	1:A:790:LEU:HG	2.02	0.41
1:B:630:ILE:HD11	1:B:632:PHE:CE2	2.56	0.41
1:A:576:LEU:HD21	1:B:952:PHE:CE1	2.56	0.41
1:A:1153:HIS:CE1	4:A:1682:HOH:O	2.73	0.41
1:A:993:MET:HB2	1:A:1020:CYS:HB3	2.02	0.41
1:A:1177:LEU:HD23	1:A:1177:LEU:HA	1.94	0.40
1:A:710:ALA:N	1:A:711:PRO:CD	2.84	0.40
1:B:981:LEU:HB2	1:B:1228:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

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	666/695 (96%)	650 (98%)	16 (2%)	0	100	100
1	B	663/695 (95%)	650 (98%)	12 (2%)	1 (0%)	43	31
All	All	1329/1390 (96%)	1300 (98%)	28 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	985	PRO

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	535/553 (97%)	527 (98%)	8 (2%)	57	49
1	B	532/553 (96%)	526 (99%)	6 (1%)	65	60
All	All	1067/1106 (96%)	1053 (99%)	14 (1%)	61	54

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	801	ASN
1	A	840	THR
1	A	863	TRP
1	A	934	LYS
1	A	956	ASP
1	A	979	ARG
1	A	984	SER
1	A	1210	LEU
1	B	863	TRP
1	B	932	LEU
1	B	956	ASP
1	B	976	THR

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Mol	Chain	Res	Type
1	B	985	PRO
1	B	1215	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	572	ASN
1	A	640	GLN
1	A	644	ASN
1	A	702	ASN
1	A	769	ASN
1	A	801	ASN
1	A	808	HIS
1	A	842	ASN
1	A	987	GLN
1	A	992	GLN
1	A	1004	HIS
1	A	1107	ASN
1	A	1125	GLN
1	A	1153	HIS
1	A	1173	ASN
1	B	572	ASN
1	B	640	GLN
1	B	702	ASN
1	B	723	ASN
1	B	767	GLN
1	B	769	ASN
1	B	801	ASN
1	B	808	HIS
1	B	1004	HIS
1	B	1125	GLN
1	B	1176	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

14 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	$\# Z > 2$
3	SO4	B	1304	-	4,4,4	0.36	0	6,6,6	0.32	0
3	SO4	B	1305	-	4,4,4	0.30	0	6,6,6	0.12	0
3	SO4	B	1306	-	4,4,4	0.34	0	6,6,6	0.22	0
3	SO4	A	1303	-	4,4,4	0.31	0	6,6,6	0.14	0
3	SO4	B	1303	-	4,4,4	0.38	0	6,6,6	0.26	0
3	SO4	A	1304	-	4,4,4	0.29	0	6,6,6	0.22	0
3	SO4	A	1302	-	4,4,4	0.61	0	6,6,6	0.13	0
2	GOL	B	1301	-	5,5,5	0.19	0	5,5,5	0.43	0
2	GOL	A	1301	-	5,5,5	0.33	0	5,5,5	0.39	0
3	SO4	A	1305	-	4,4,4	0.36	0	6,6,6	0.16	0
3	SO4	A	1306	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	B	1307	-	4,4,4	0.27	0	6,6,6	0.12	0
3	SO4	B	1302	-	4,4,4	0.44	0	6,6,6	0.16	0
3	SO4	B	1308	-	4,4,4	0.60	0	6,6,6	0.22	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1301	-	-	0/4/4/4	-
2	GOL	A	1301	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

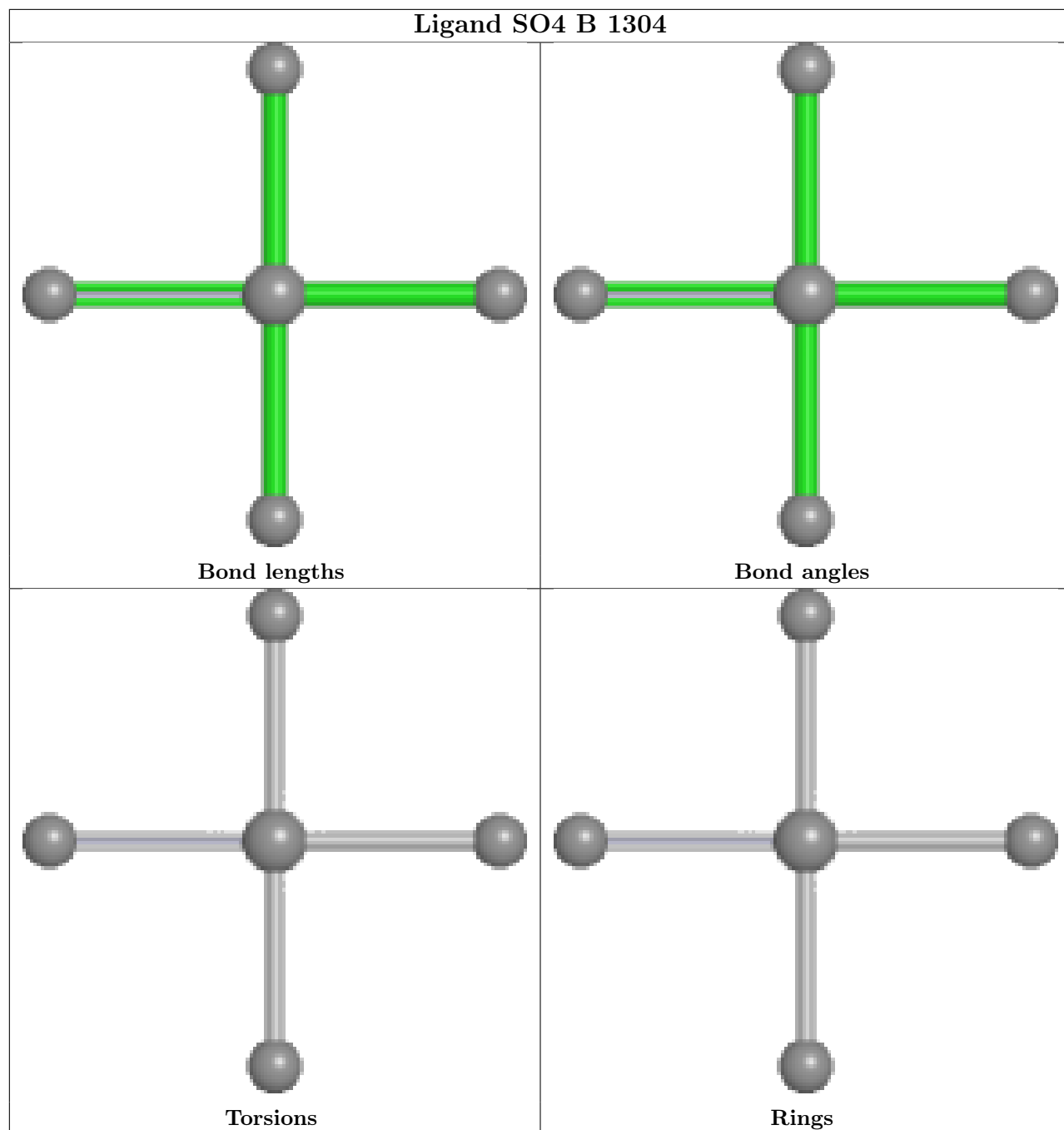
There are no chirality outliers.

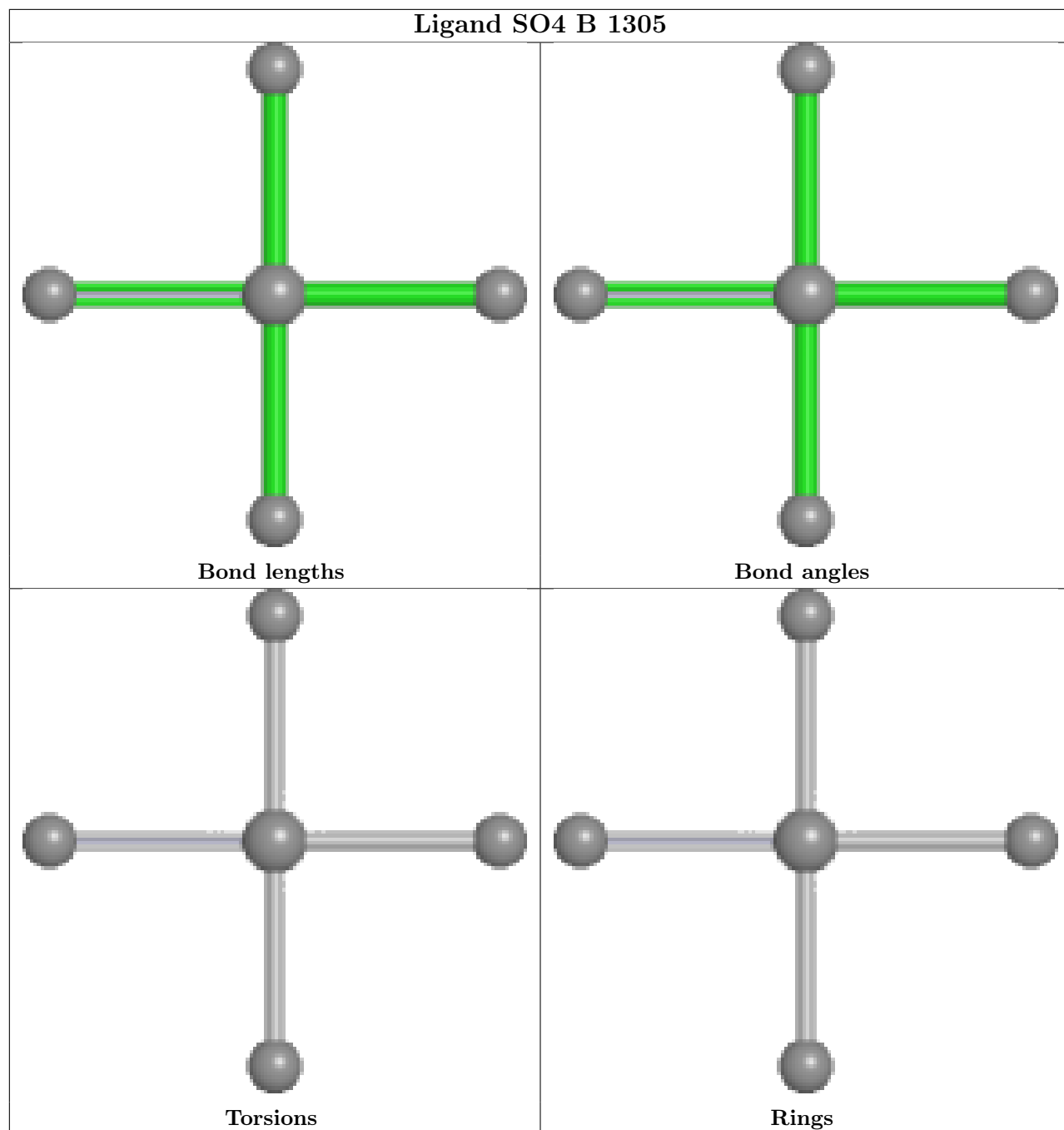
There are no torsion outliers.

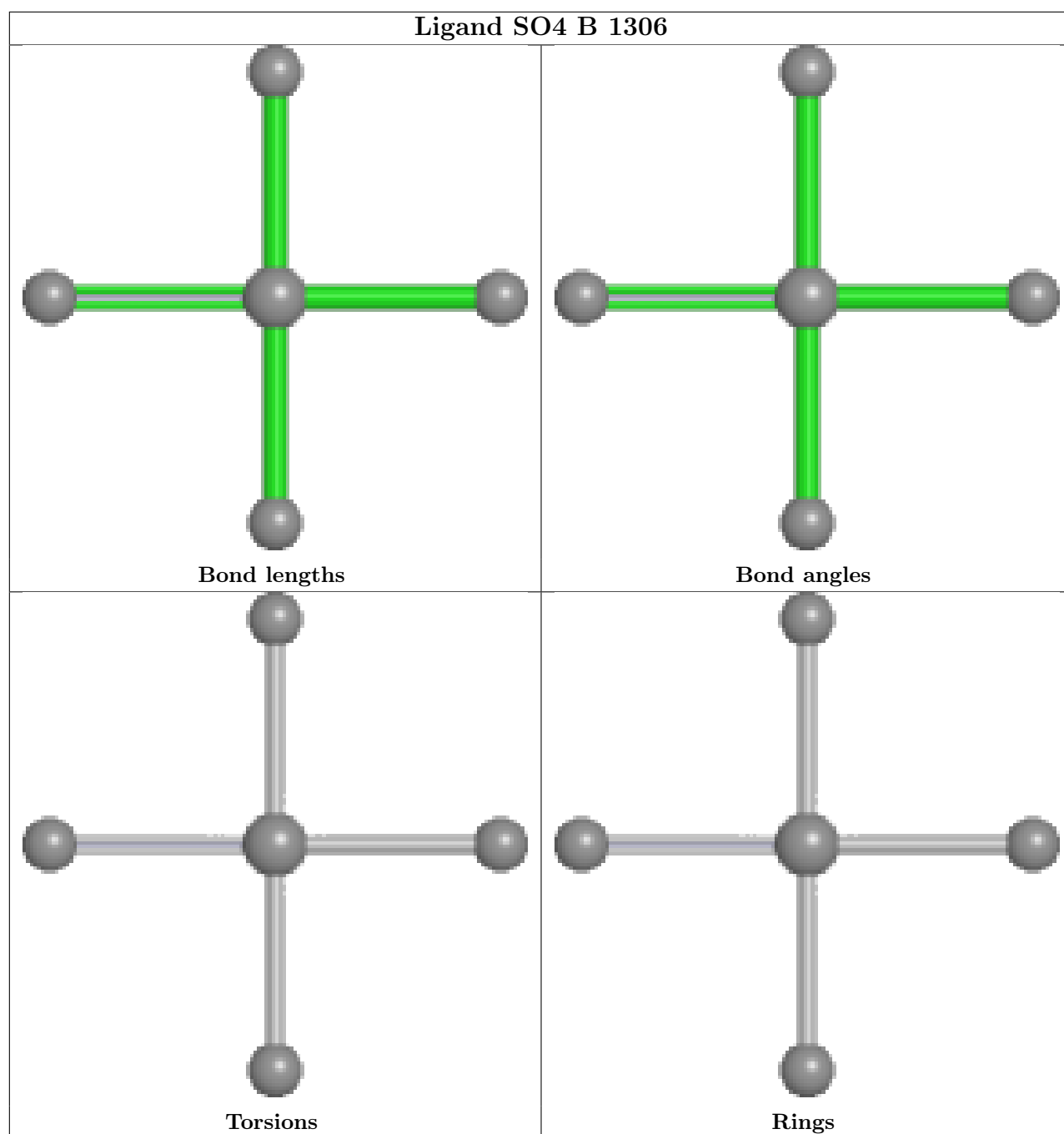
There are no ring outliers.

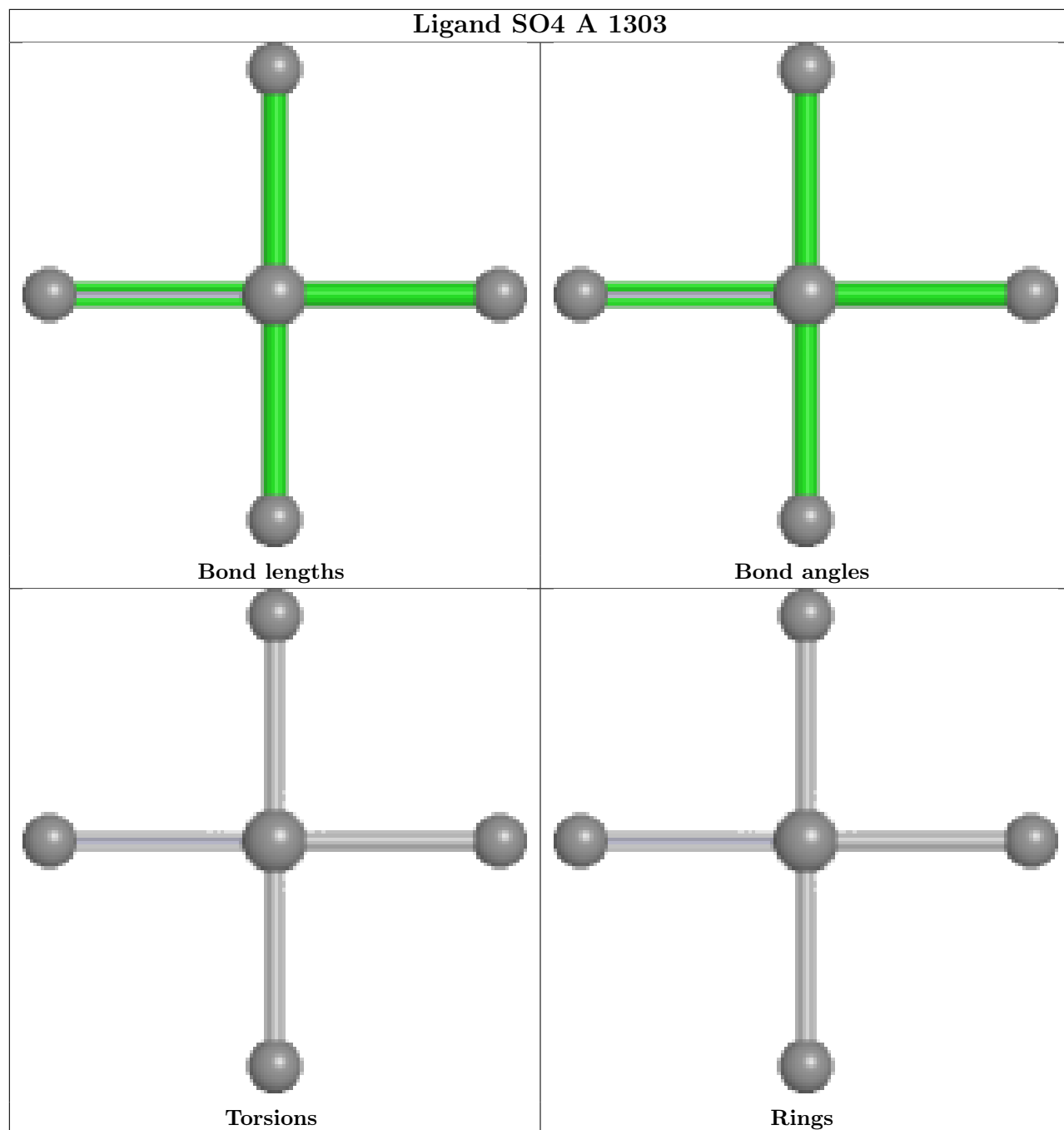
No monomer is involved in short contacts.

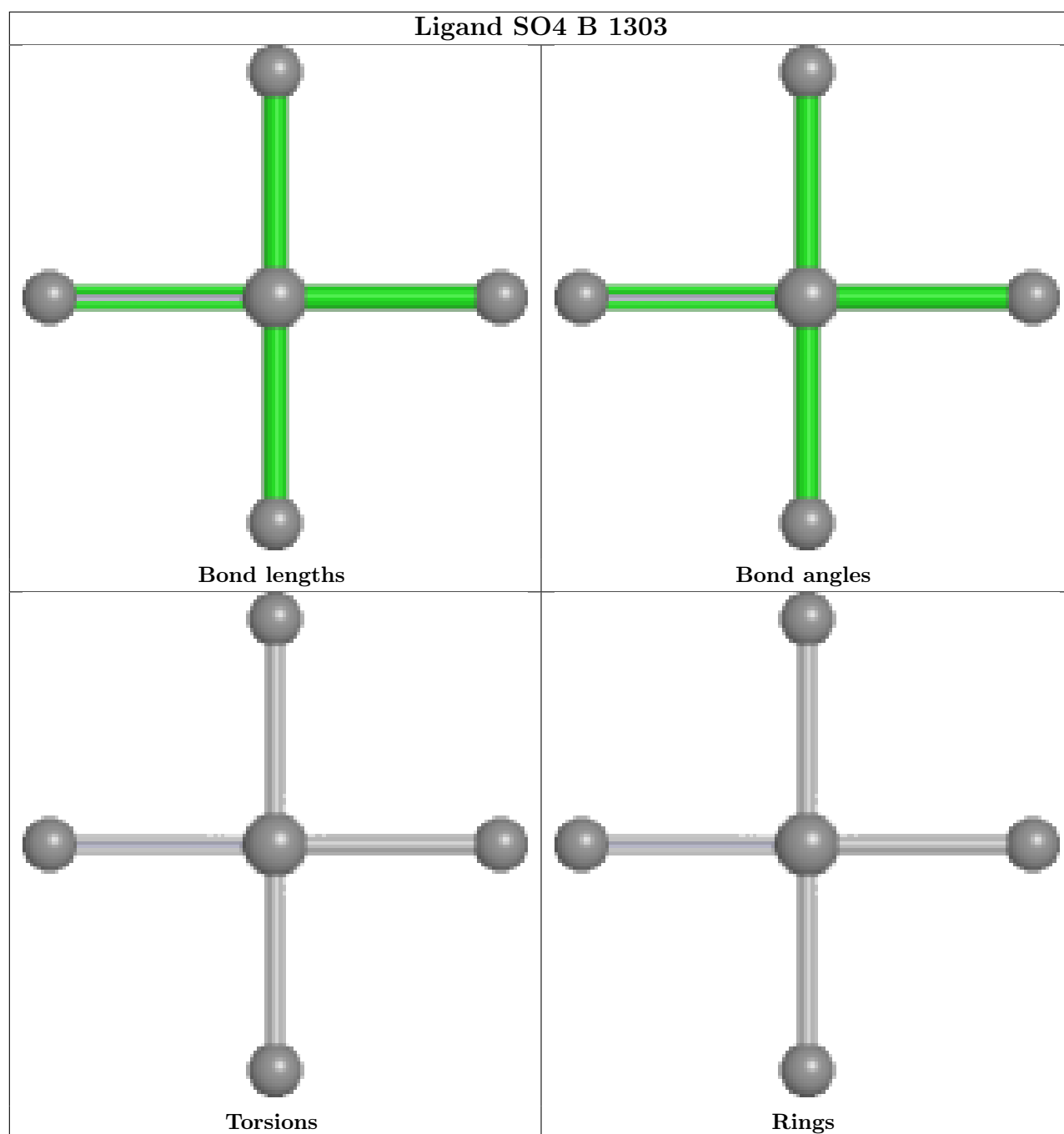
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

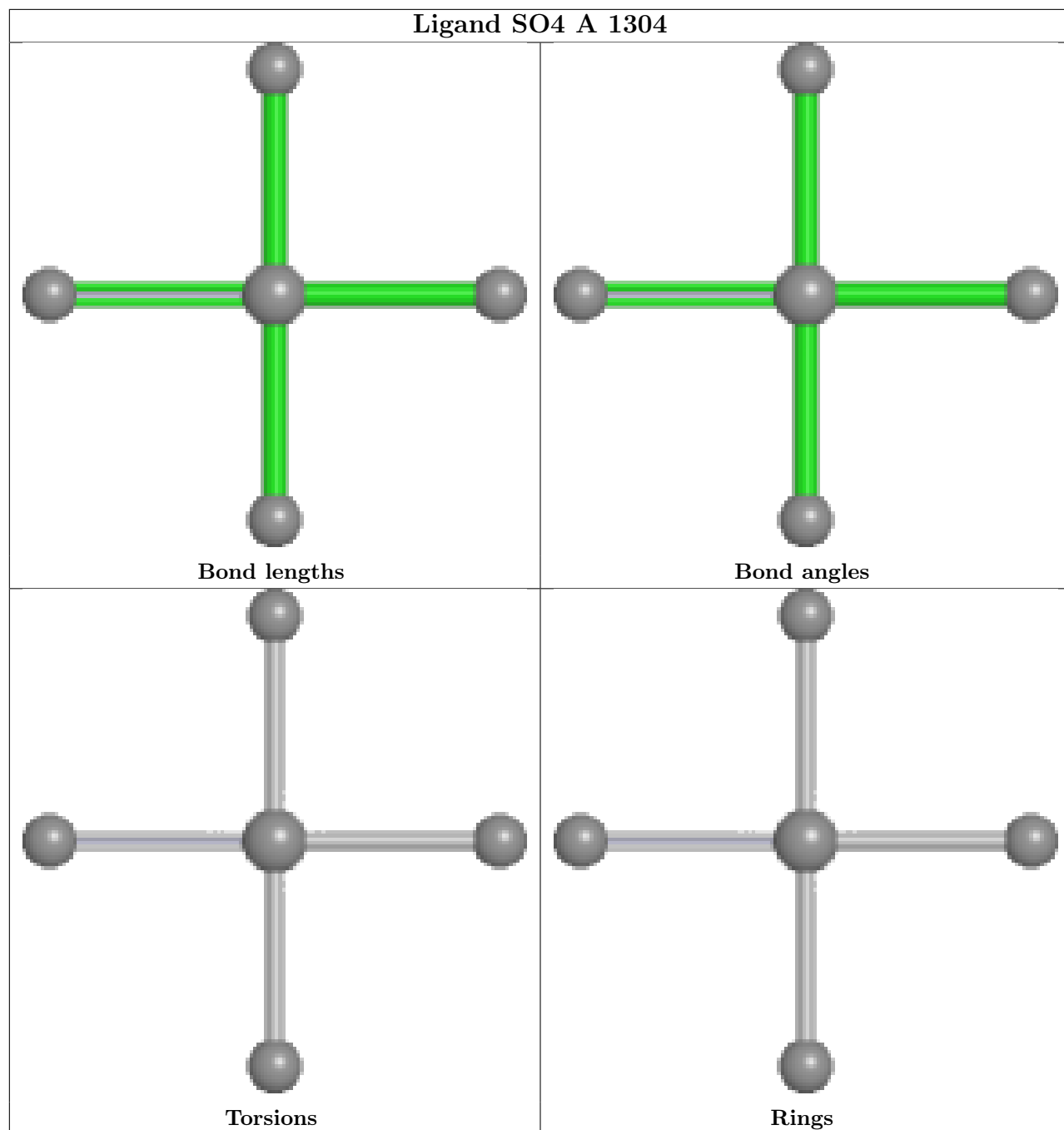


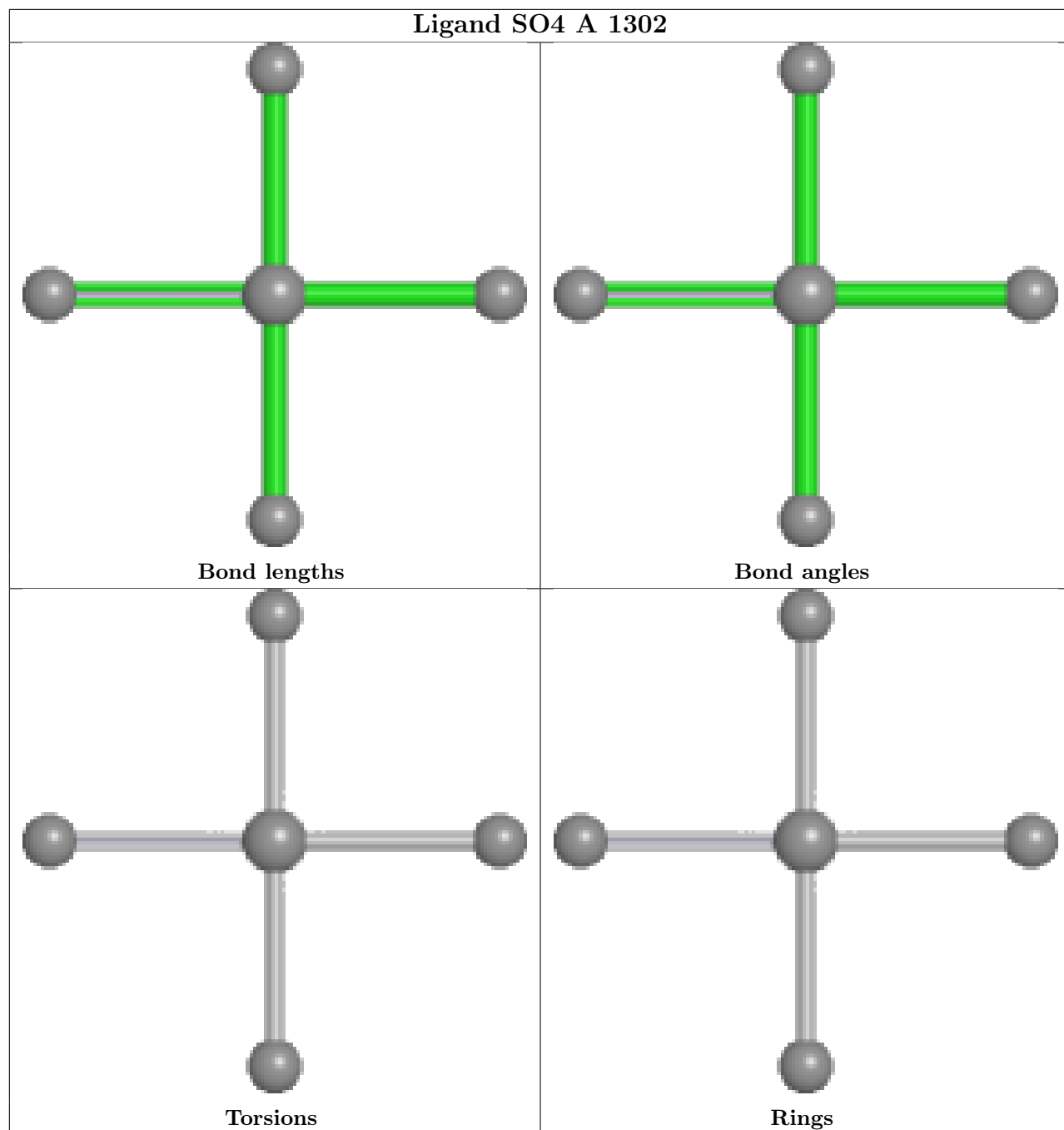


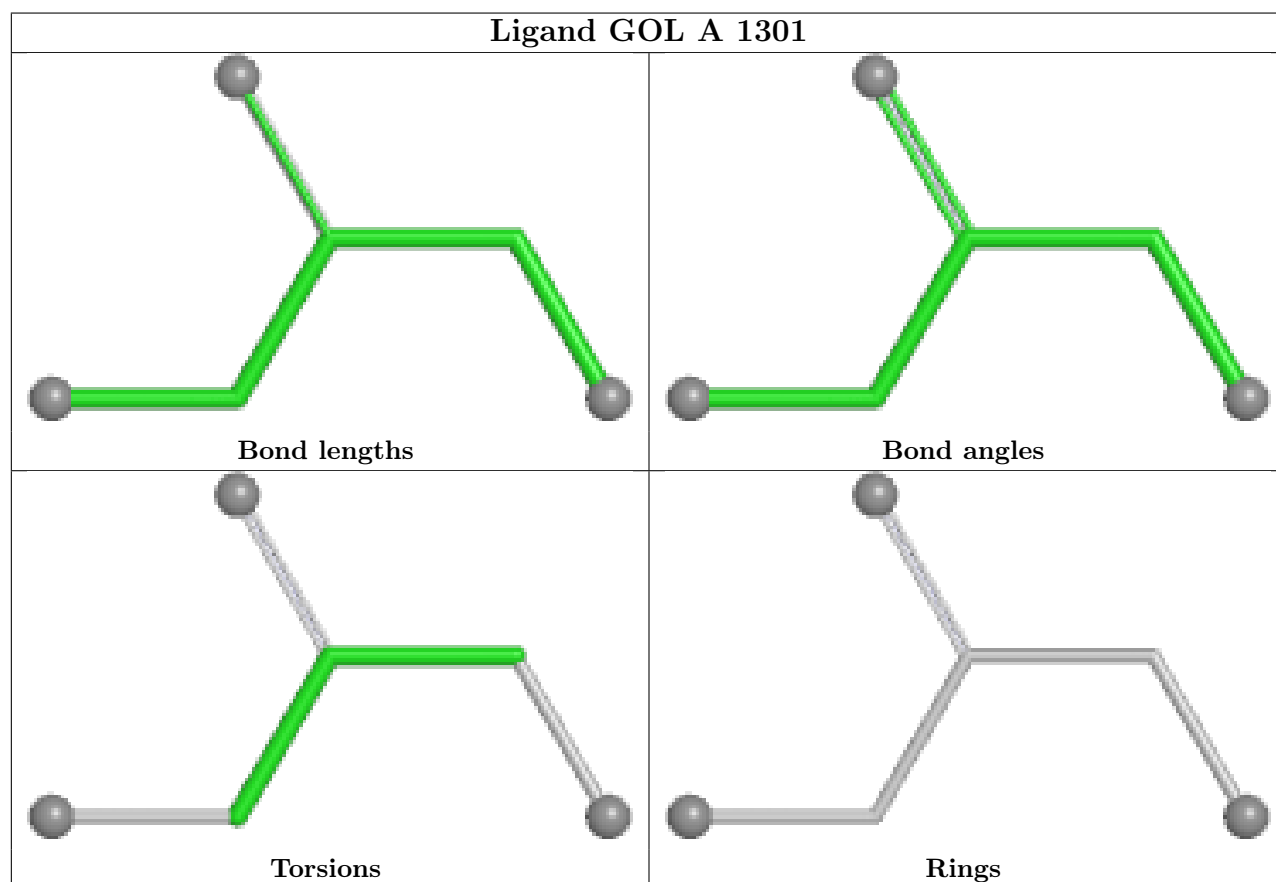
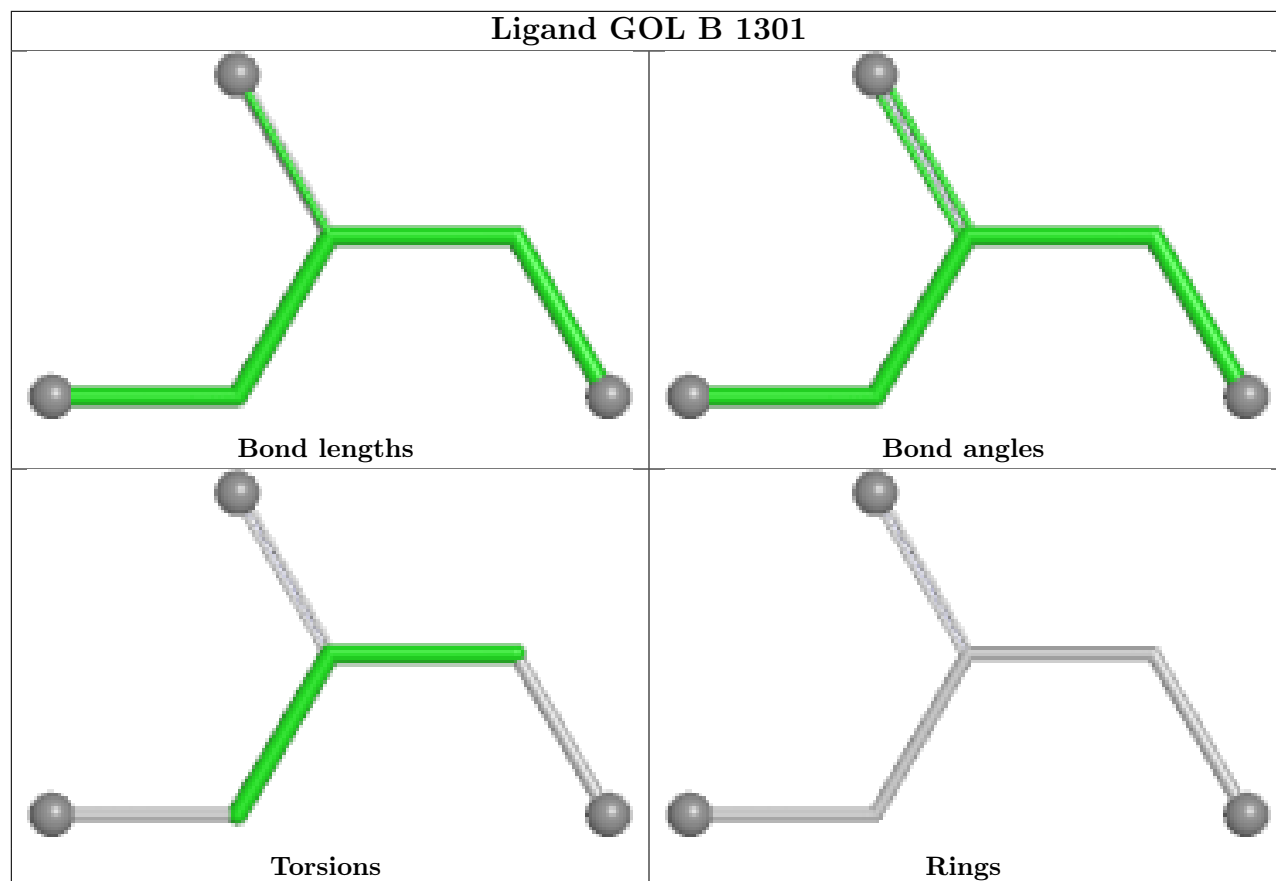


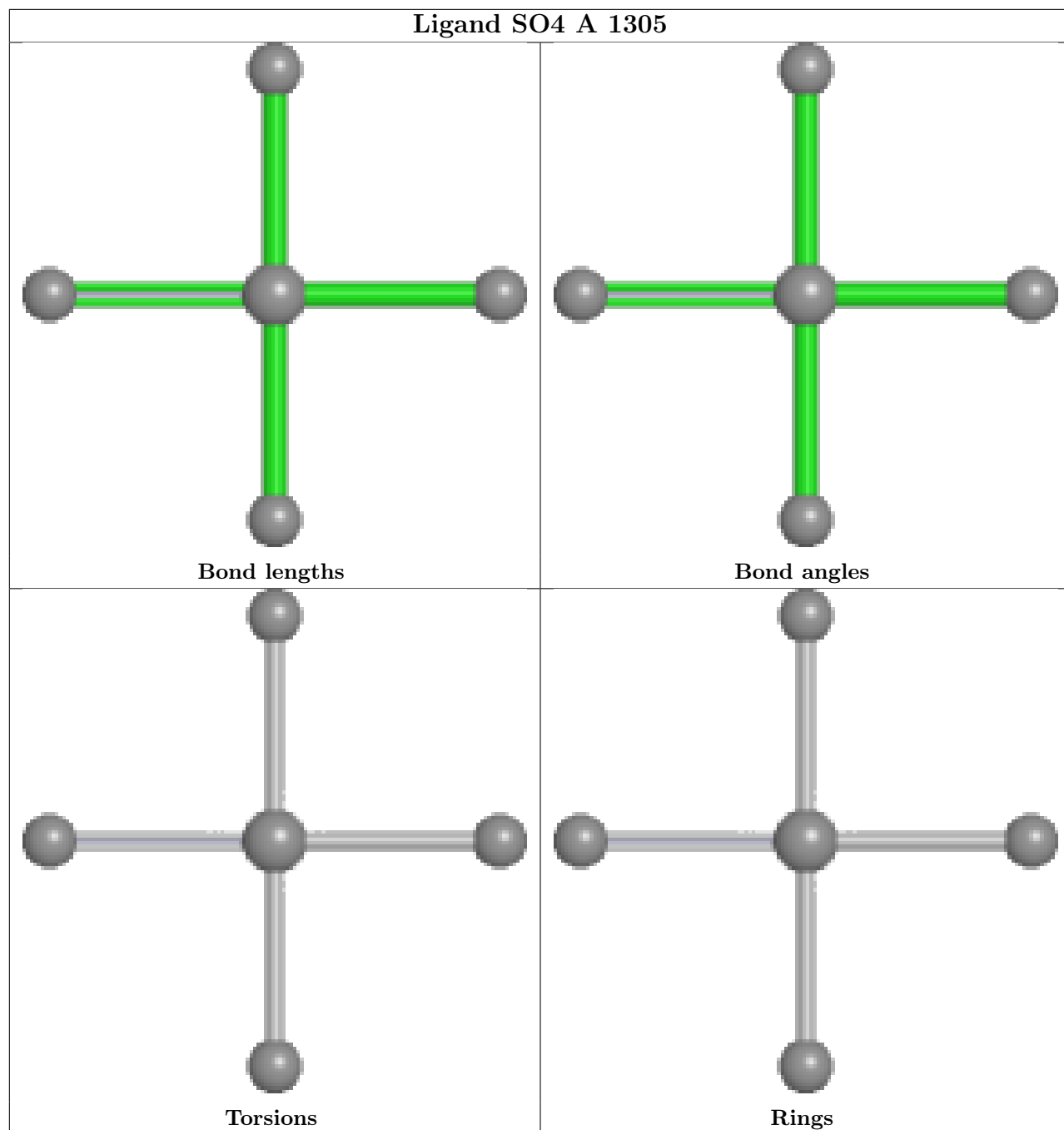


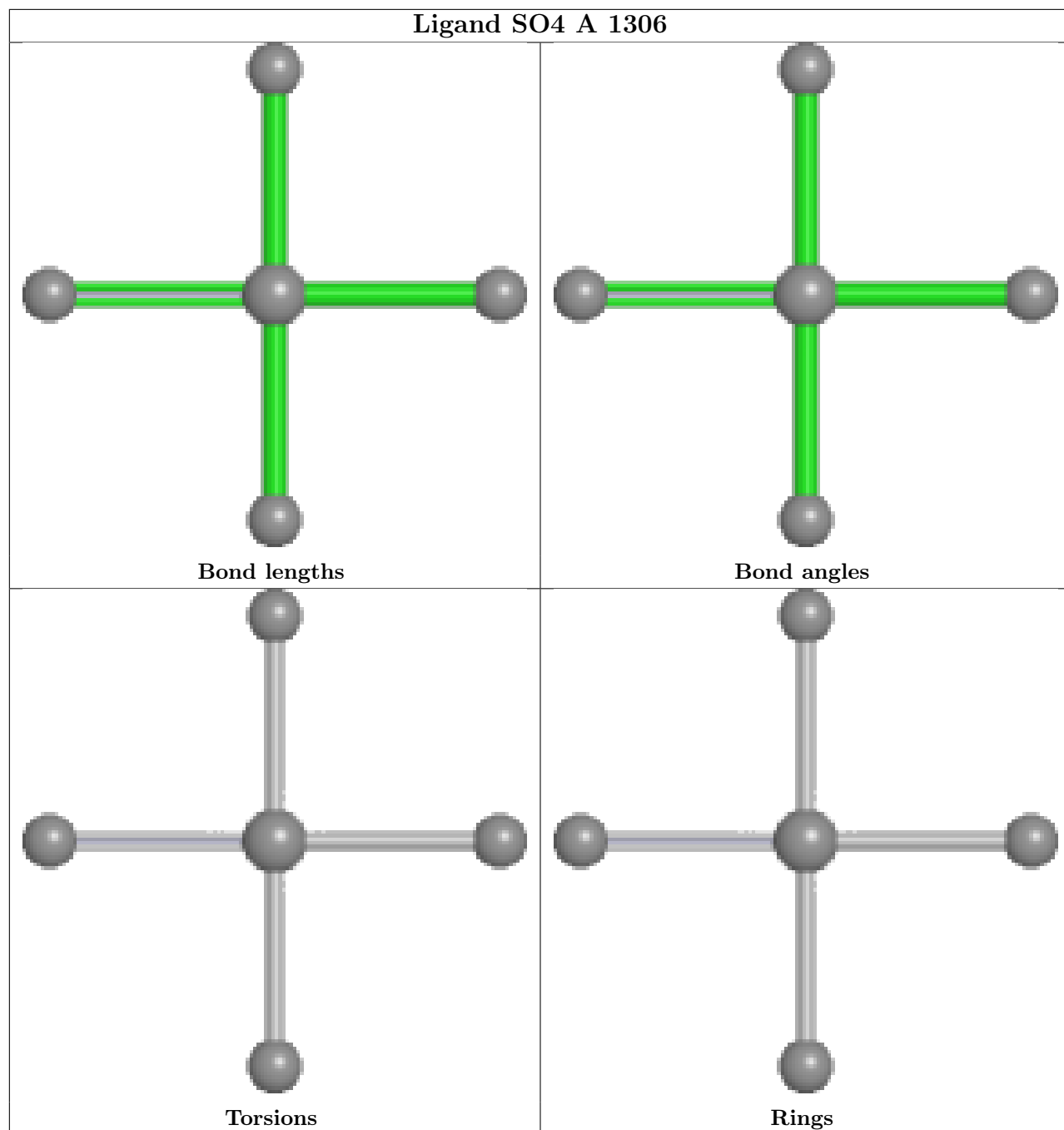


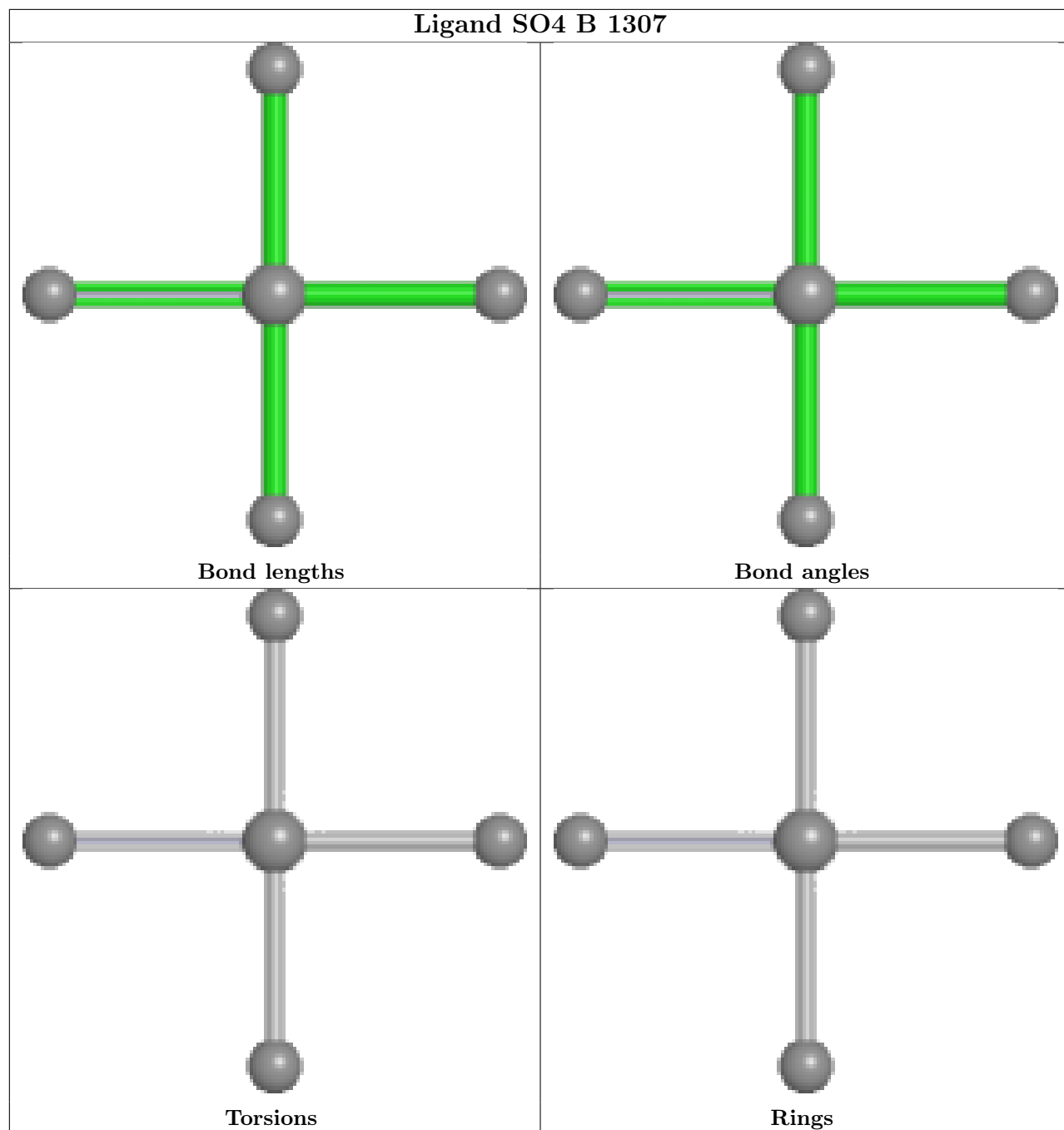


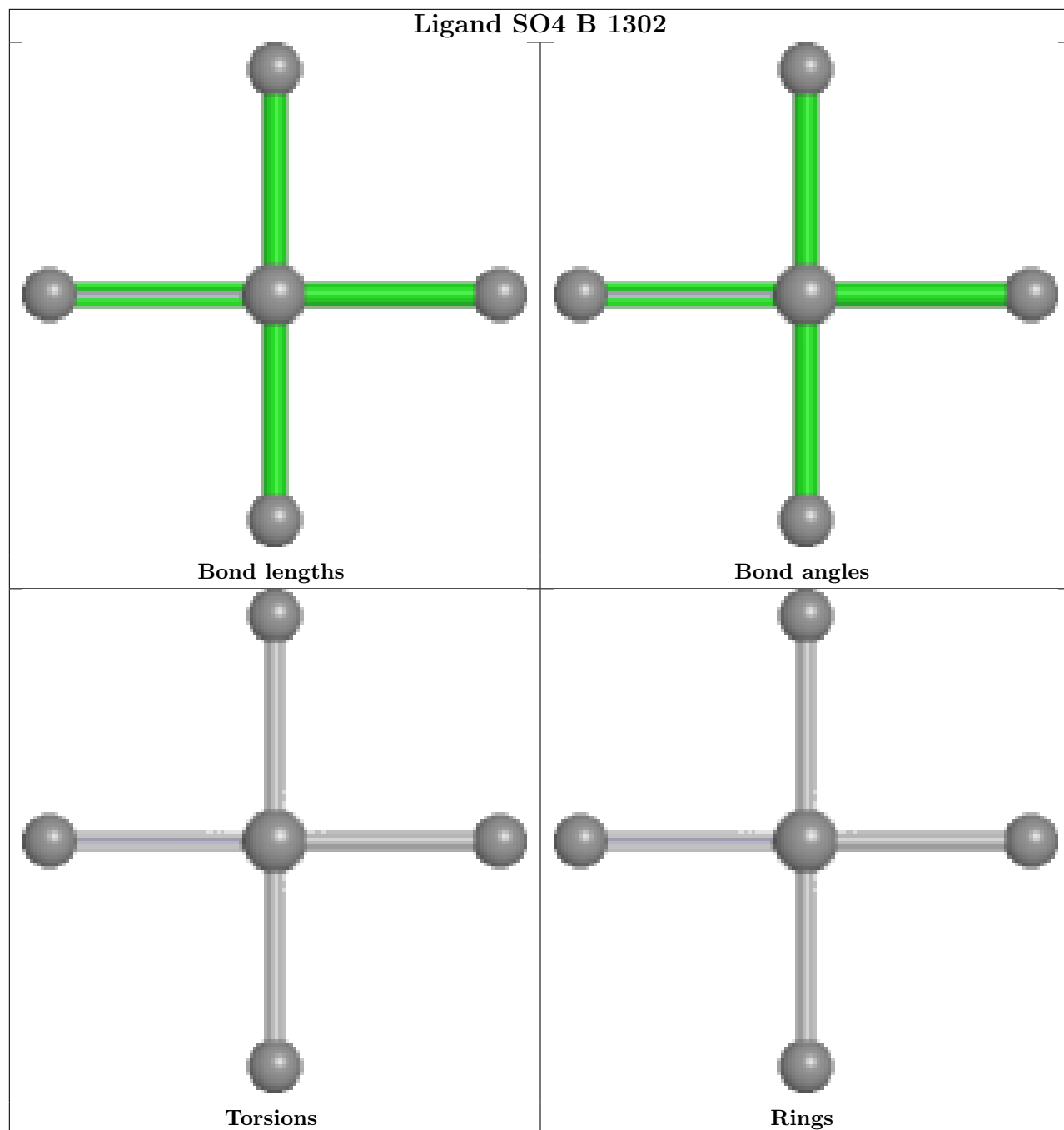


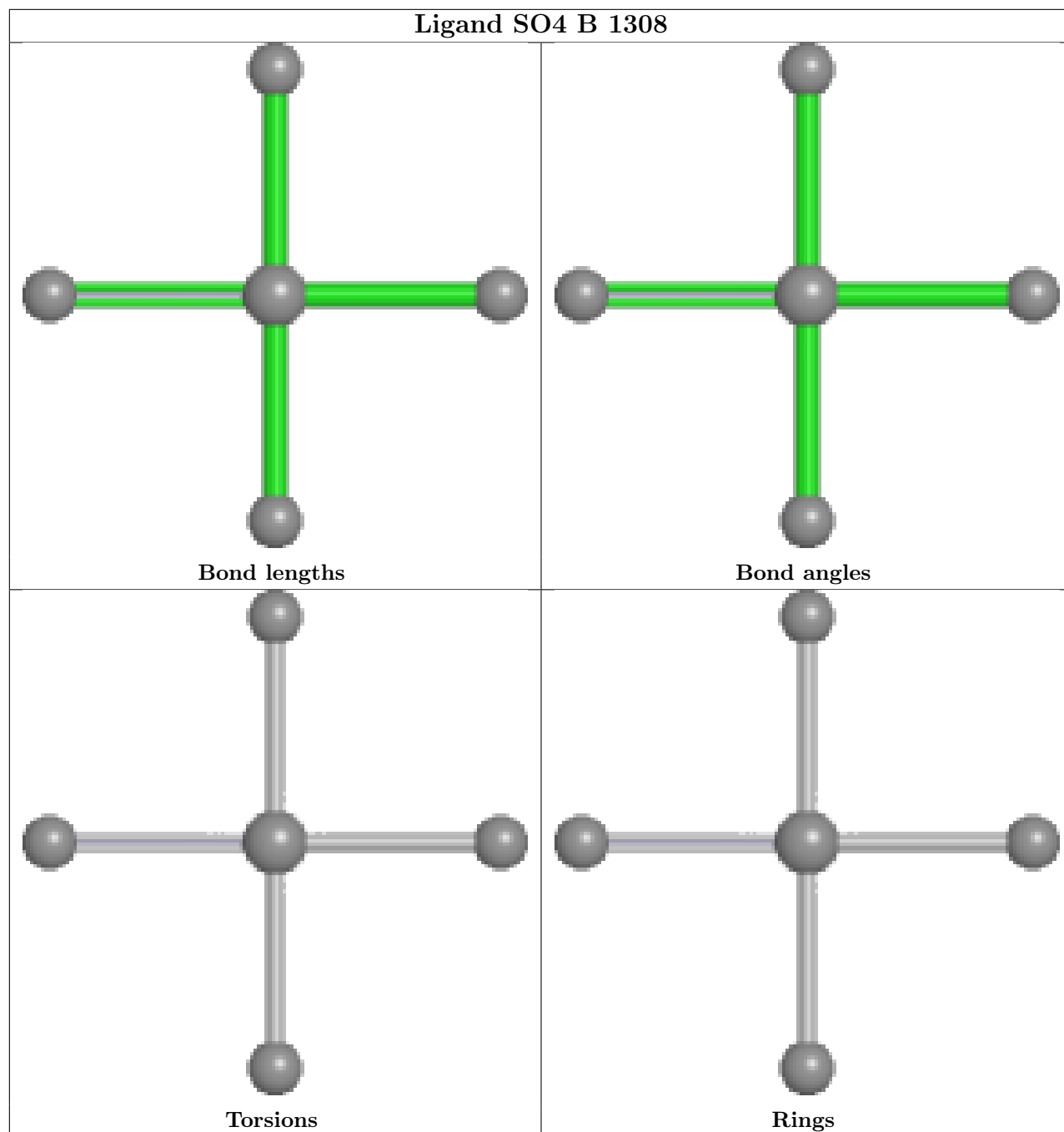












5.7 Other polymers [i](#)

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	662/695 (95%)	0.03	44 (6%) 24 23	8, 22, 58, 101	6 (0%)
1	B	662/695 (95%)	0.01	38 (5%) 29 28	8, 22, 56, 110	3 (0%)
All	All	1324/1390 (95%)	0.02	82 (6%) 26 25	8, 22, 57, 110	9 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	983	GLY	7.1
1	A	1211	PRO	6.6
1	B	983	GLY	6.3
1	A	630	ILE	6.0
1	B	1222	ILE	5.6
1	A	982	PHE	5.6
1	B	1211	PRO	5.4
1	B	1213	ALA	4.6
1	B	982	PHE	4.1
1	B	890	PRO	4.1
1	A	838	HIS	4.1
1	B	1223	TYR	4.0
1	A	979	ARG	3.9
1	B	784	THR	3.9
1	A	787	LYS	3.7
1	A	569	PHE	3.6
1	A	1210	LEU	3.6
1	A	631	GLY	3.5
1	B	984	SER	3.4
1	B	1210	LEU	3.3
1	A	984	SER	3.3
1	A	1189	LEU	3.2
1	A	784	THR	3.2
1	B	838	HIS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	893	SER	3.1
1	B	898	THR	3.0
1	A	978	GLU	3.0
1	A	1215	ASP	2.9
1	A	981	LEU	2.9
1	A	786	GLY	2.9
1	B	841	ASN	2.9
1	B	840	THR	2.8
1	A	785	GLY	2.8
1	A	573	ILE	2.8
1	A	986	LYS	2.7
1	A	840	THR	2.7
1	B	630	ILE	2.7
1	A	890	PRO	2.7
1	A	1213	ALA	2.7
1	B	1220	ALA	2.7
1	A	901	GLY	2.6
1	B	786	GLY	2.6
1	A	632	PHE	2.6
1	A	627	LEU	2.6
1	A	634	GLY	2.6
1	A	855	ARG	2.6
1	B	854	ALA	2.6
1	A	633	ALA	2.6
1	A	985	PRO	2.5
1	B	981	LEU	2.5
1	B	569	PHE	2.5
1	A	801	ASN	2.5
1	A	1222	ILE	2.5
1	B	1212	ASP	2.5
1	A	637	ARG	2.4
1	B	1218	TYR	2.4
1	A	980	GLU	2.4
1	A	976	THR	2.4
1	B	986	LYS	2.4
1	B	894	GLU	2.4
1	A	622	ARG	2.4
1	B	834	VAL	2.4
1	B	785	GLY	2.3
1	B	787	LYS	2.3
1	B	897	VAL	2.2
1	A	1223	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	985	PRO	2.2
1	B	782	SER	2.2
1	A	925	LYS	2.2
1	B	925	LYS	2.2
1	A	615	GLU	2.1
1	A	975	SER	2.1
1	B	1216	SER	2.1
1	B	631	GLY	2.1
1	A	839	ASP	2.1
1	A	918	ASP	2.1
1	B	979	ARG	2.1
1	B	891	GLU	2.1
1	B	977	THR	2.1
1	B	1214	GLU	2.0
1	B	930	GLY	2.0
1	A	794	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	1307	5/5	0.85	0.11	57,61,65,81	0
3	SO4	B	1308	5/5	0.85	0.16	28,32,45,46	0
3	SO4	A	1305	5/5	0.87	0.12	64,67,76,78	0
3	SO4	B	1306	5/5	0.87	0.13	56,62,67,74	0
3	SO4	A	1304	5/5	0.88	0.11	52,54,56,67	0
3	SO4	A	1306	5/5	0.91	0.10	42,44,48,52	0
3	SO4	B	1304	5/5	0.92	0.10	45,45,50,55	0

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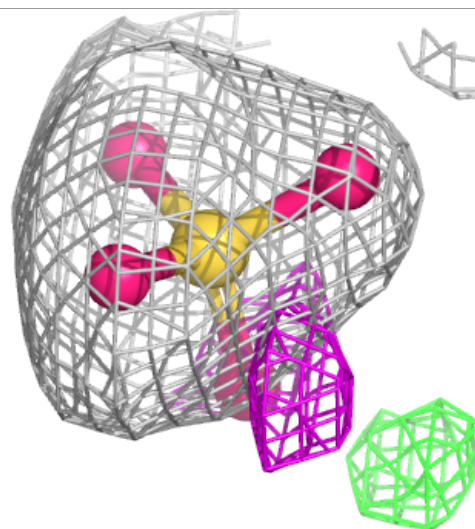
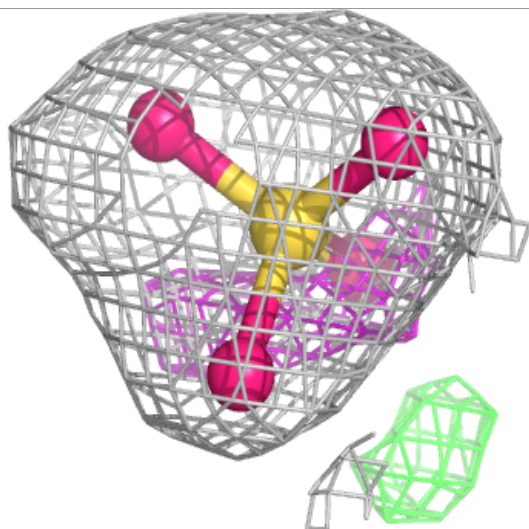
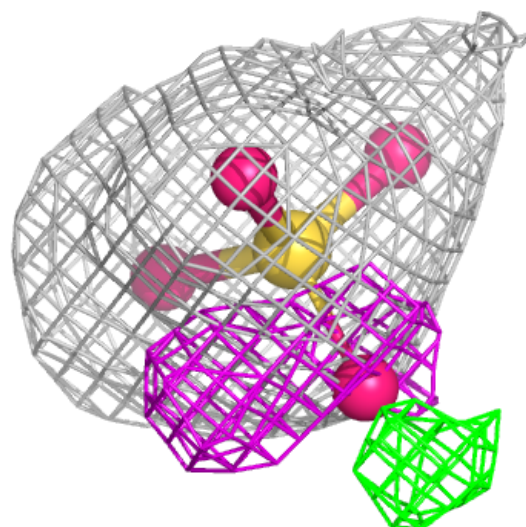
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	GOL	B	1301	6/6	0.92	0.10	25,26,29,30	0
3	SO4	B	1302	5/5	0.93	0.09	42,44,50,58	0
3	SO4	B	1303	5/5	0.93	0.09	43,43,55,57	0
3	SO4	A	1303	5/5	0.93	0.07	40,47,55,56	0
3	SO4	A	1302	5/5	0.96	0.08	43,49,50,51	0
2	GOL	A	1301	6/6	0.96	0.08	20,25,26,26	0
3	SO4	B	1305	5/5	0.96	0.06	39,46,50,50	0

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

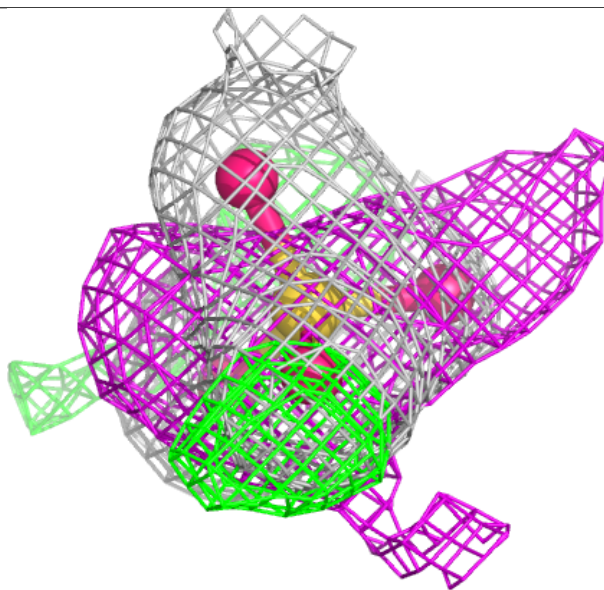
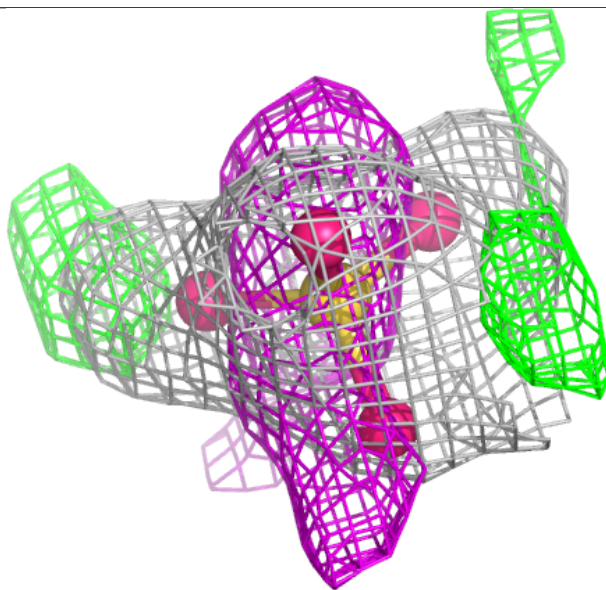
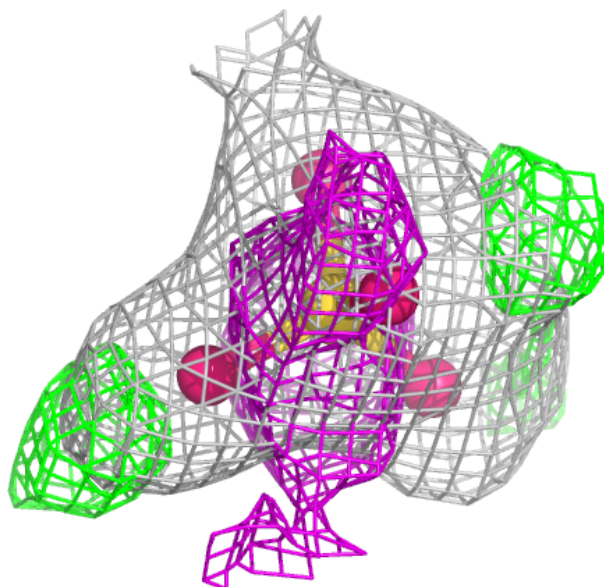
Electron density around SO4 B 1307:

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



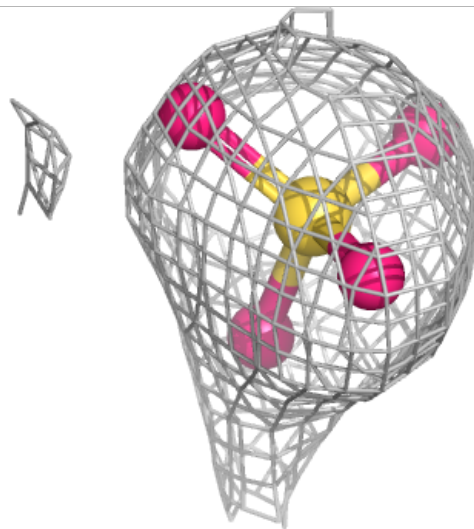
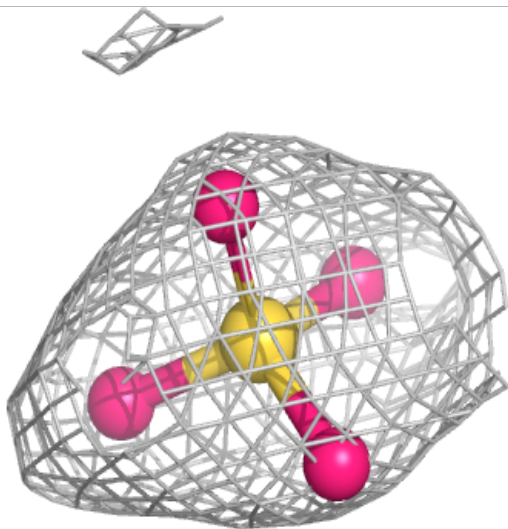
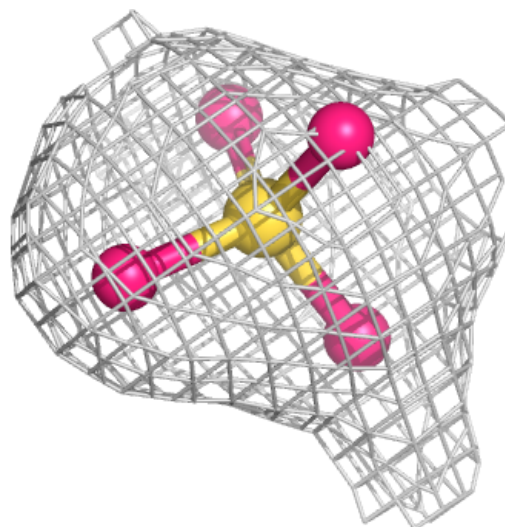
Electron density around SO4 B 1308:

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



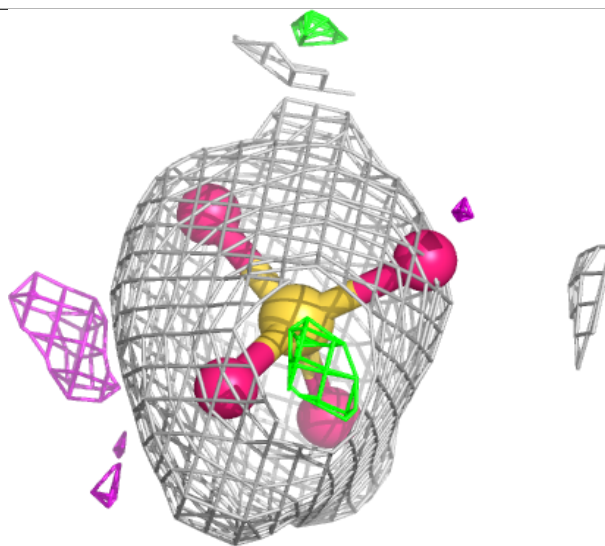
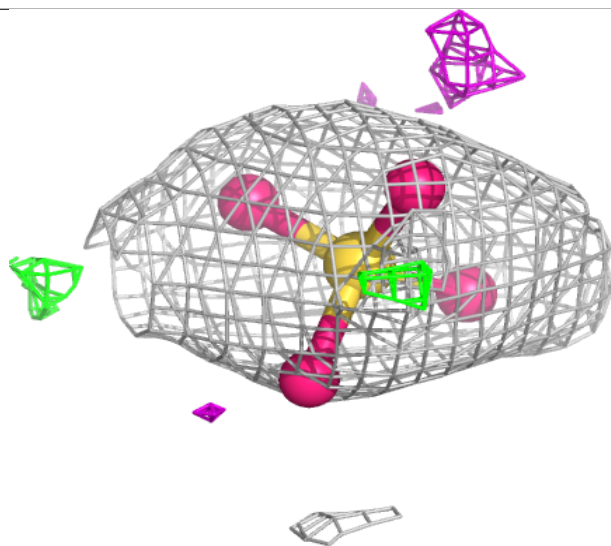
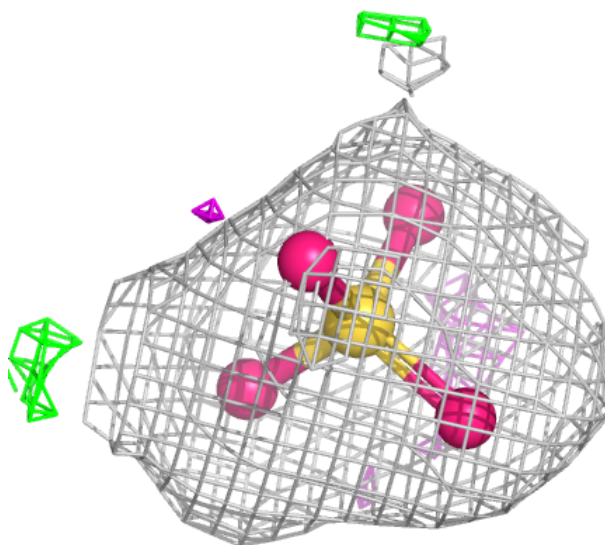
Electron density around SO4 A 1305:

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



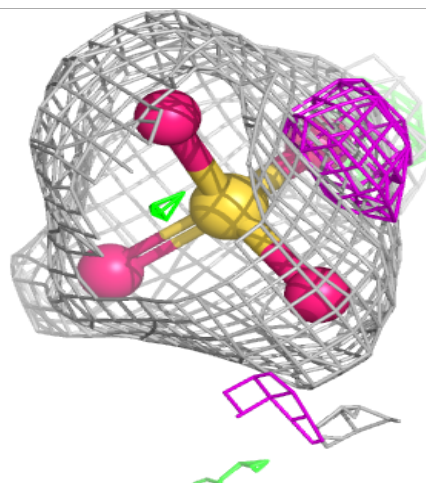
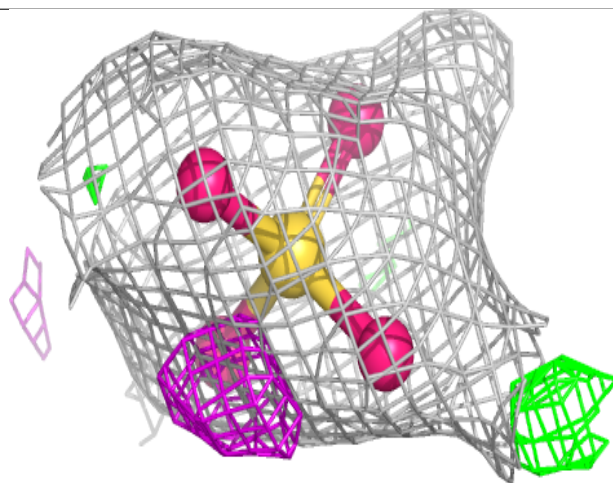
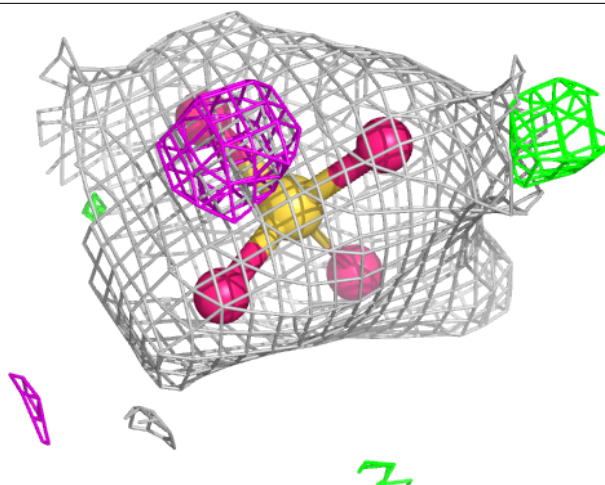
Electron density around SO4 B 1306:

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



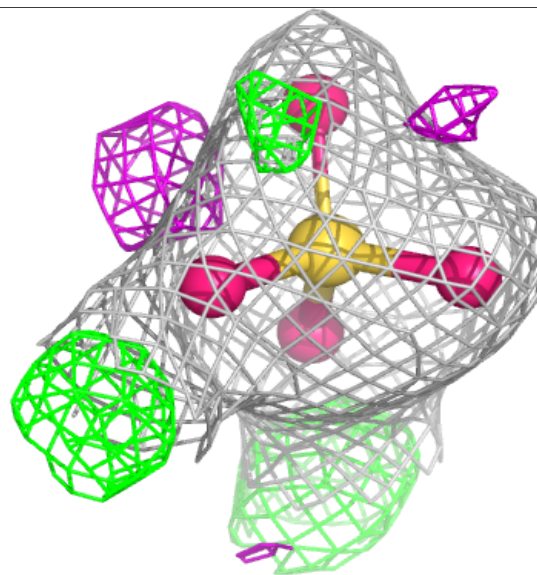
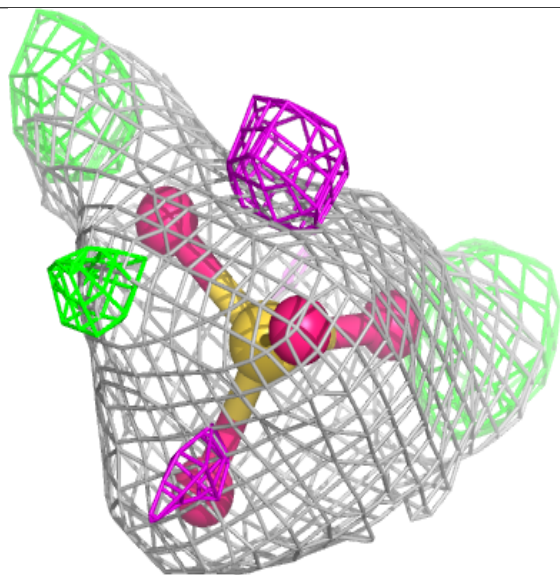
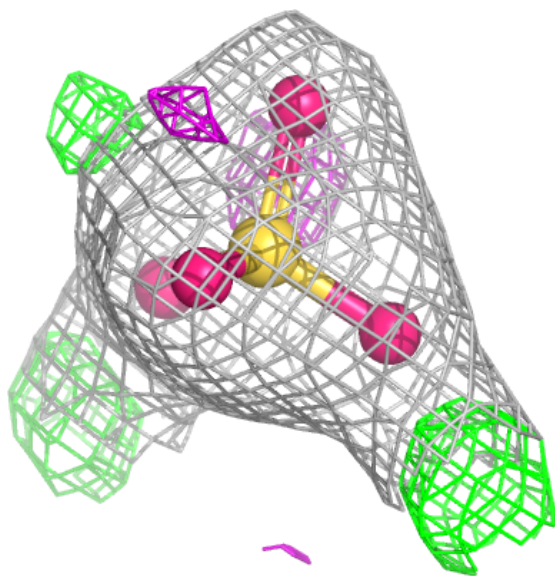
Electron density around SO4 A 1304:

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



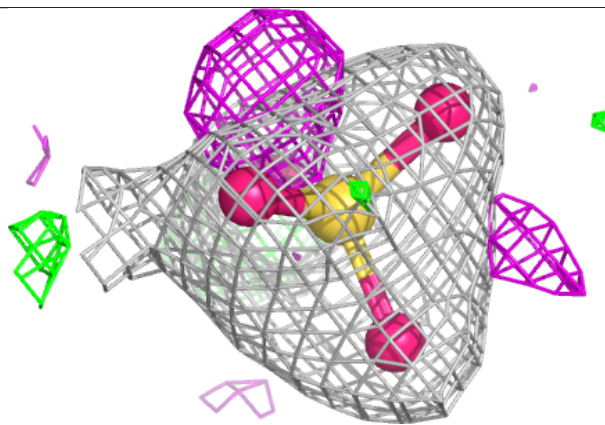
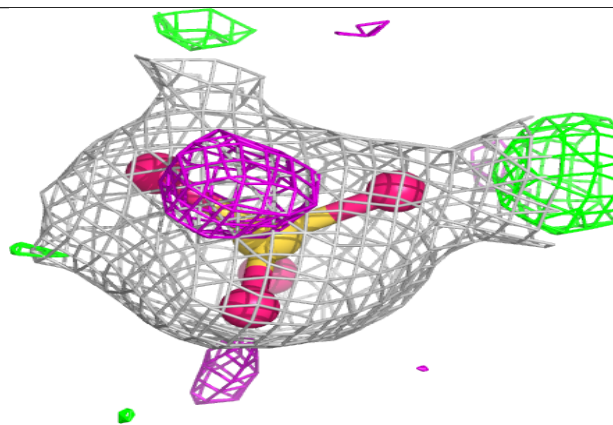
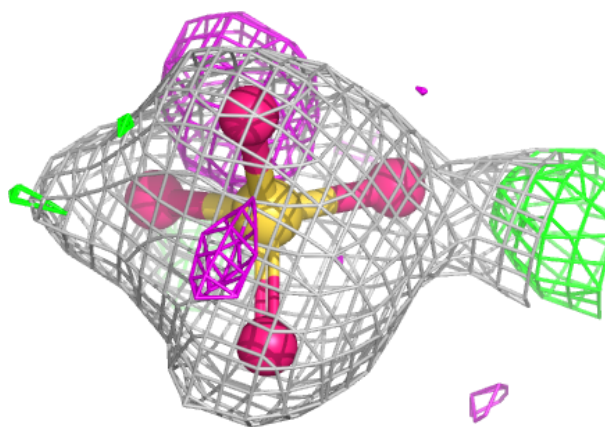
Electron density around SO4 A 1306:

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



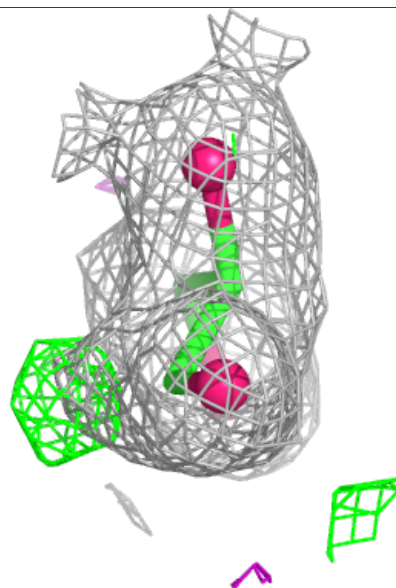
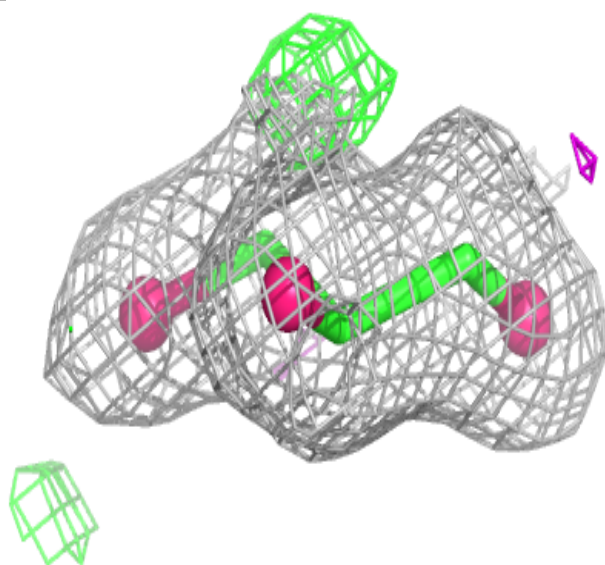
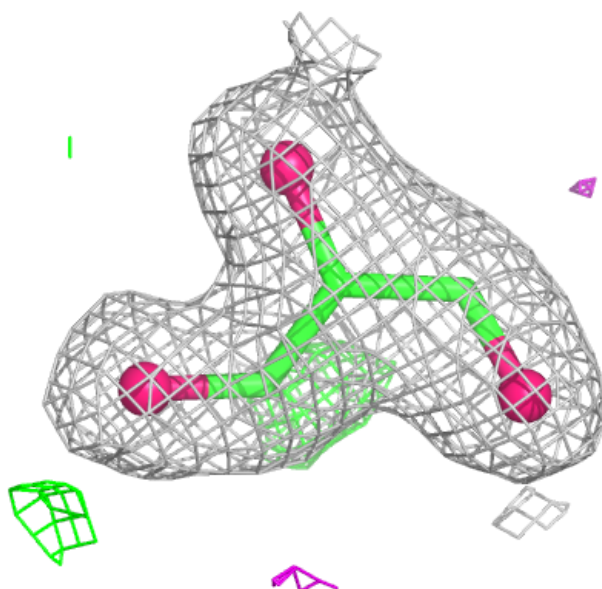
Electron density around SO4 B 1304:

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



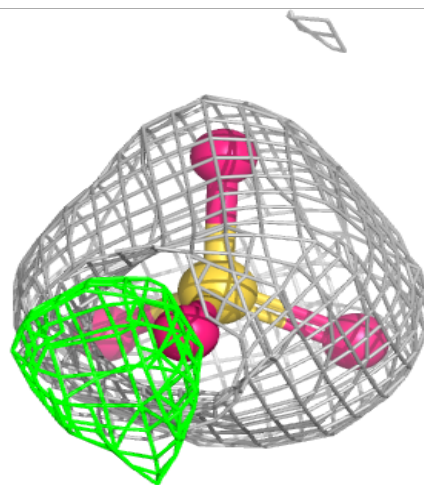
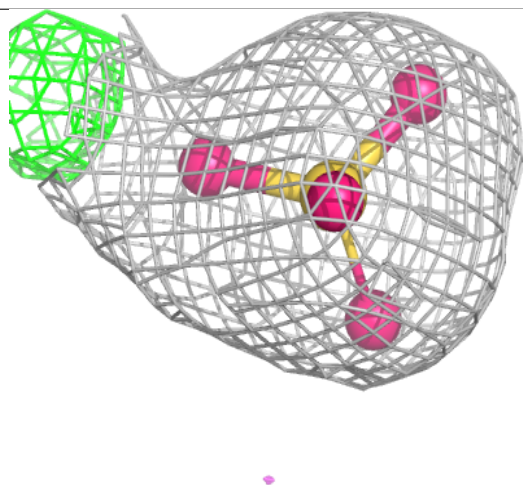
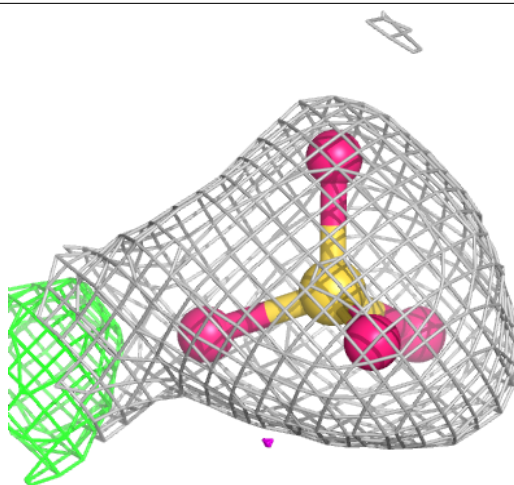
Electron density around GOL B 1301:

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



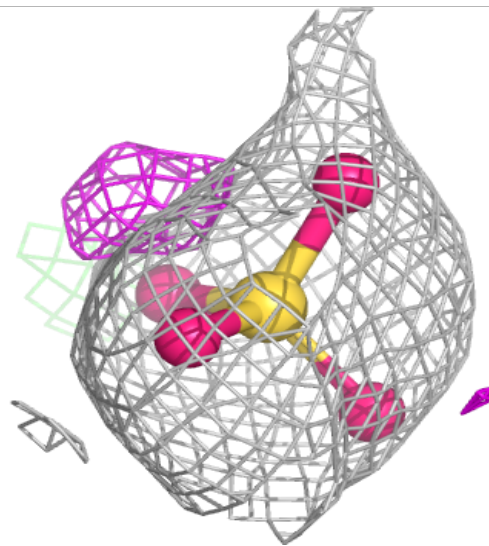
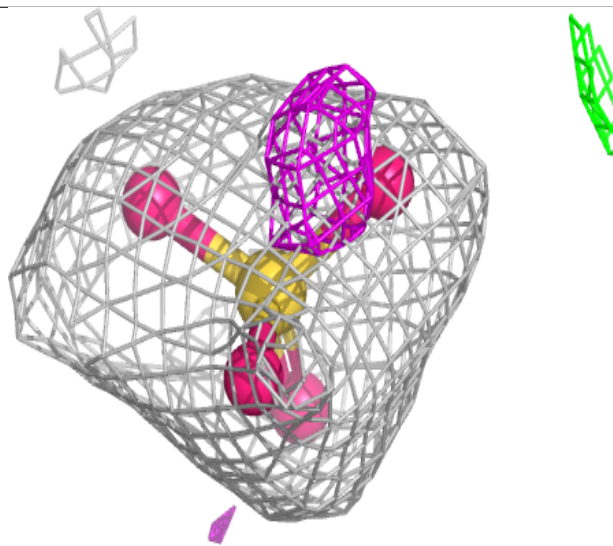
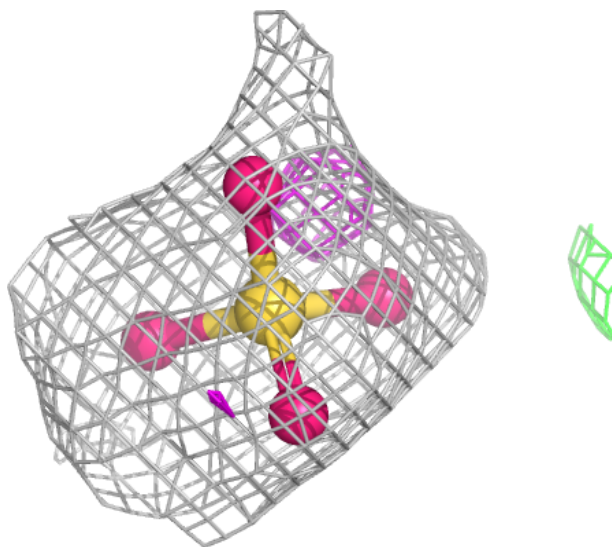
Electron density around SO4 B 1302:

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



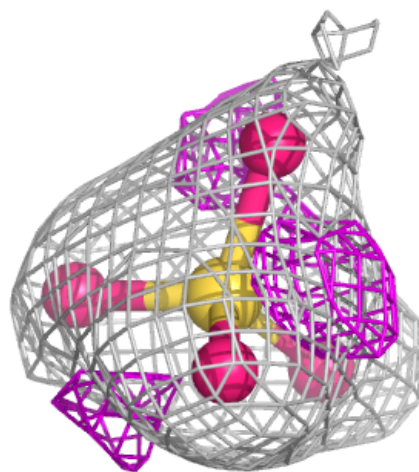
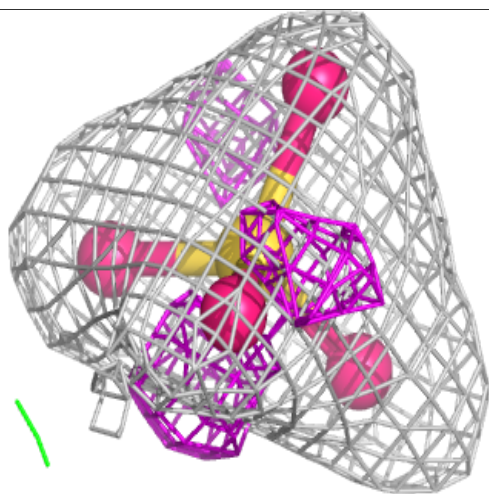
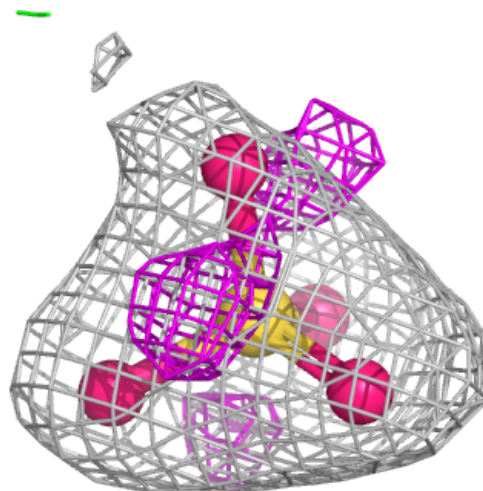
Electron density around SO4 B 1303:

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



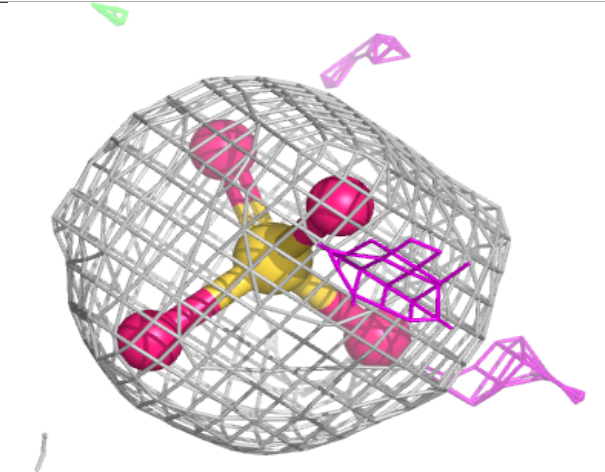
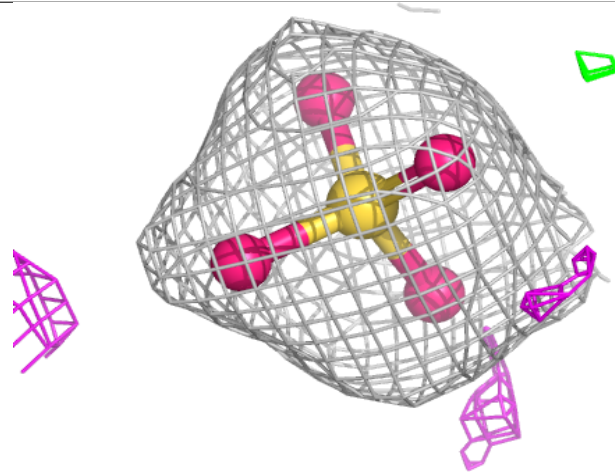
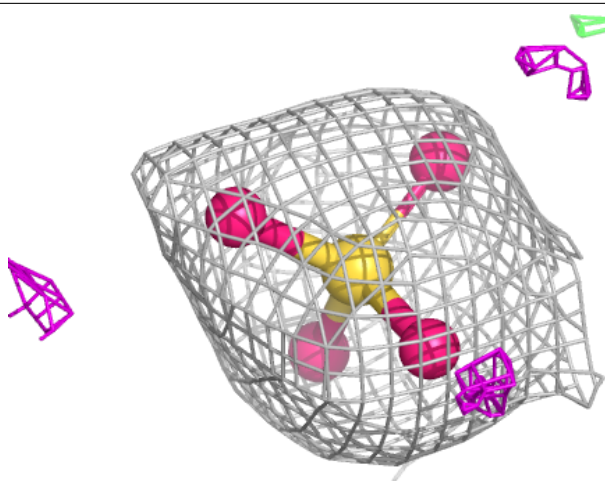
Electron density around SO4 A 1303:

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



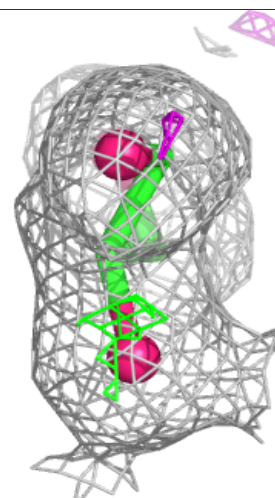
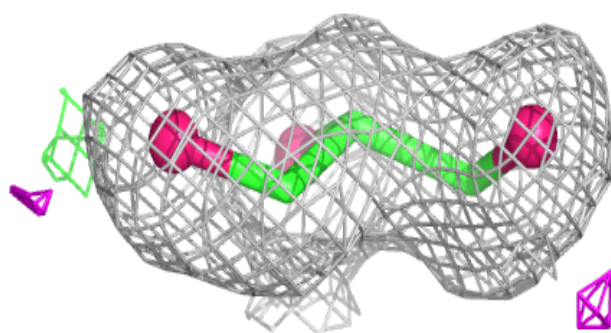
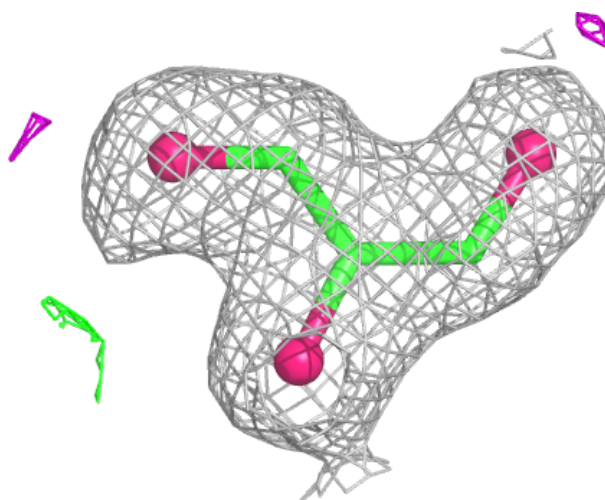
Electron density around SO4 A 1302:

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



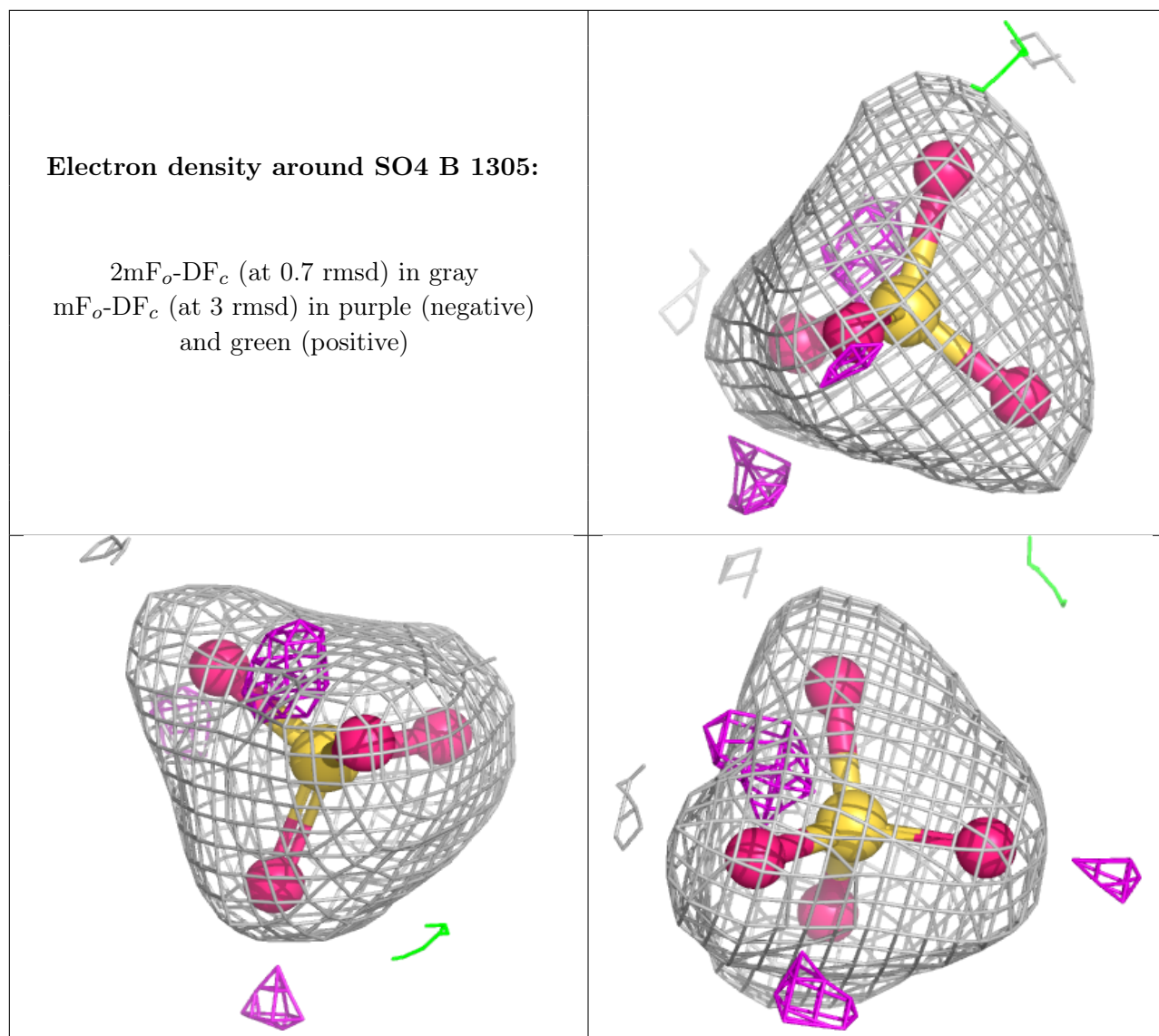
Electron density around GOL A 1301:

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



Electron density around SO4 B 1305:

$2mF_o-DF_c$ (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.