



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:11 AM UTC

PDB ID : 6K8U / pdb_00006k8u
Title : Crystal structure of C-domain with NADP of bacterial malonyl-CoA reductase
Authors : Kim, S.; Kim, K.-J.
Deposited on : 2019-06-13
Resolution : 2.00 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

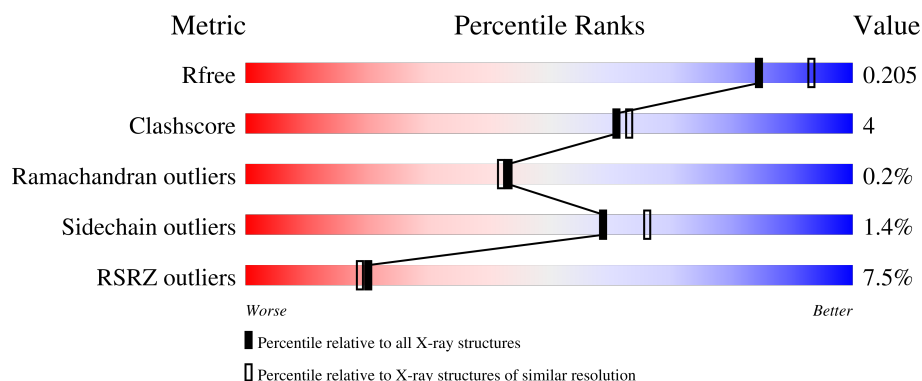
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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% 85% 10% 5%
1	B	695	8% 85% 9% 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10915 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	2	0
			5095	3195	908	972	20			
1	B	660	Total	C	N	O	S	0	3	0
			5091	3193	908	970	20			

There are 42 discrepancies between the modelled and reference sequences:

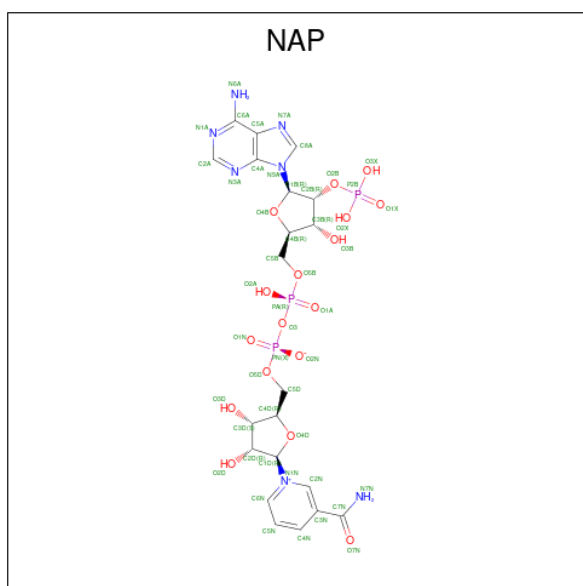
Chain	Residue	Modelled	Actual	Comment	Reference
A	536	MET	-	initiating methionine	UNP A0A1A7BFR5
A	537	GLY	-	expression tag	UNP A0A1A7BFR5
A	538	SER	-	expression tag	UNP A0A1A7BFR5
A	539	SER	-	expression tag	UNP A0A1A7BFR5
A	540	HIS	-	expression tag	UNP A0A1A7BFR5
A	541	HIS	-	expression tag	UNP A0A1A7BFR5
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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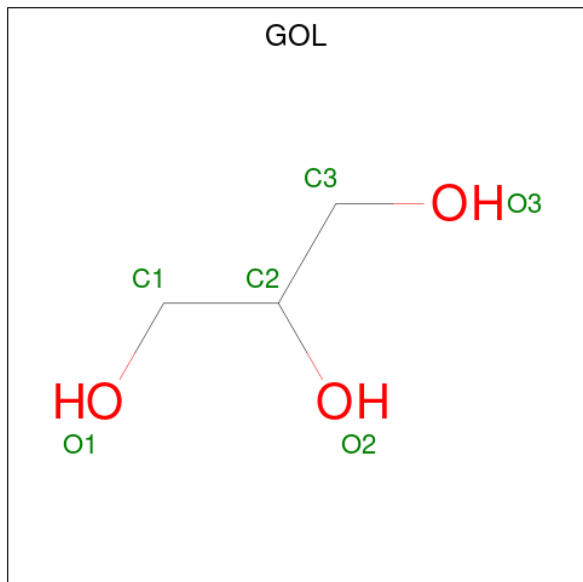
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Chain	Residue	Modelled	Actual	Comment	Reference
B	539	SER	-	expression tag	UNP A0A1A7BFR5
B	540	HIS	-	expression tag	UNP A0A1A7BFR5
B	541	HIS	-	expression tag	UNP A0A1A7BFR5
B	542	HIS	-	expression tag	UNP A0A1A7BFR5
B	543	HIS	-	expression tag	UNP A0A1A7BFR5
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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

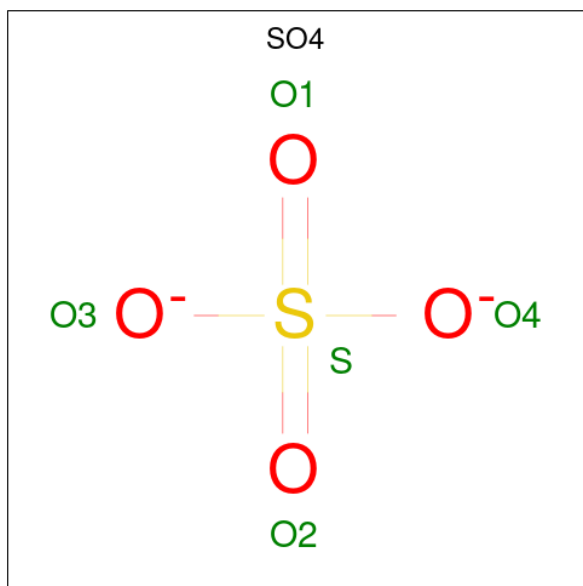


- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

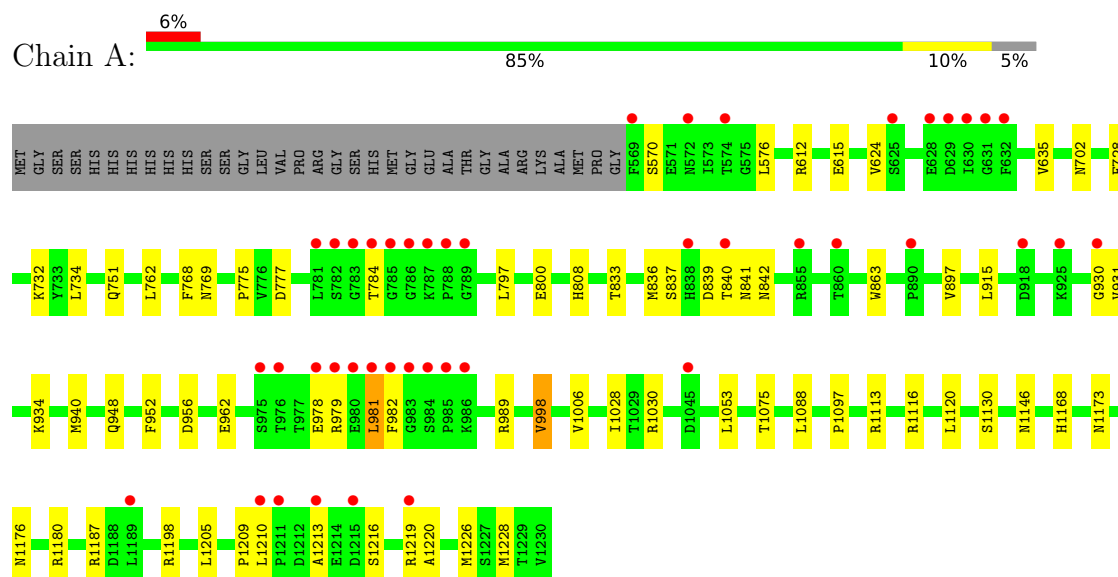
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	262	Total O 262 262	0	0
5	B	284	Total O 284 284	0	0

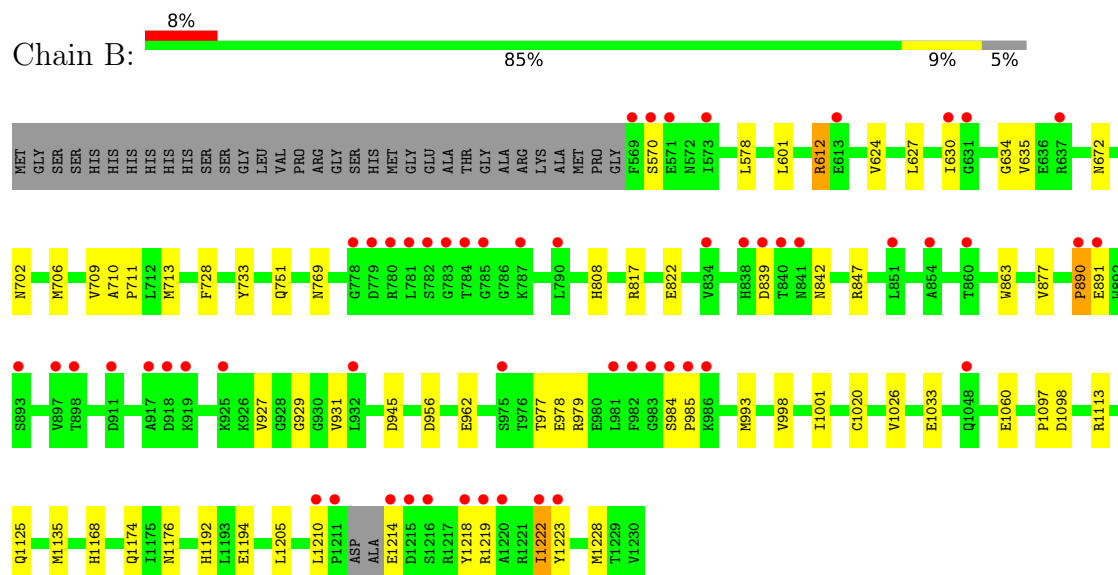
3 Residue-property plots [i](#)

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: NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR



- Molecule 1: NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	110.86Å 116.69Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.86 – 2.00 31.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.86-2.00) 98.9 (31.86-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.174 , 0.205 0.175 , 0.205	Depositor DCC
R_{free} test set	5810 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	22.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 41.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10915	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 31.99 % 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 1.0102e-03. 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: SO4, NAP, GOL

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	1.11	1/5186 (0.0%)	1.38	4/7034 (0.1%)
1	B	1.15	7/5181 (0.1%)	1.37	10/7025 (0.1%)
All	All	1.13	8/10367 (0.1%)	1.37	14/14059 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1026	VAL	C-O	6.04	1.30	1.23
1	B	1168	HIS	CE1-NE2	5.92	1.38	1.32
1	B	984	SER	N-CA	5.80	1.51	1.46
1	B	998	VAL	C-O	5.72	1.29	1.24
1	B	1097	PRO	C-O	-5.49	1.17	1.24
1	A	1097	PRO	C-O	-5.47	1.17	1.24
1	B	1001	ILE	C-O	5.07	1.29	1.24
1	B	672	ASN	C-O	5.00	1.29	1.23

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	945	ASP	CA-CB-CG	6.10	118.70	112.60
1	A	897	VAL	CA-C-N	5.89	128.97	120.38
1	A	897	VAL	C-N-CA	5.89	128.97	120.38
1	B	728	PHE	CB-CA-C	5.80	121.50	109.95
1	B	978	GLU	CA-C-O	-5.59	115.63	120.88
1	B	891	GLU	CB-CG-CD	5.38	121.75	112.60
1	B	927	VAL	CA-C-N	5.38	125.92	119.94
1	B	927	VAL	C-N-CA	5.38	125.92	119.94
1	B	984	SER	N-CA-C	5.30	114.23	108.14
1	B	929	GLY	CA-C-N	5.25	125.77	119.94
1	B	929	GLY	C-N-CA	5.25	125.77	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1033	GLU	CB-CG-CD	5.21	121.47	112.60
1	A	728	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	576	LEU	CA-C-O	-5.16	115.41	120.82

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	5095	0	5068	49	0
1	B	5091	0	5065	44	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	35	0	0	1	0
4	B	40	0	0	3	0
5	A	262	0	0	6	0
5	B	284	0	0	3	0
All	All	10915	0	10199	87	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 (87) 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:612:ARG:HH11	1:B:612:ARG:HB2	1.12	1.14
1:B:1223:TYR:HB2	5:B:1410:HOH:O	1.73	0.89
1:B:612:ARG:HB2	1:B:612:ARG:NH1	1.87	0.89
1:B:702:ASN:HD21	1:B:751:GLN:HE21	1.24	0.85
1:A:981:LEU:HD12	1:A:1228:MET:SD	2.22	0.79
1:A:612:ARG:CZ	1:A:615:GLU:HG3	2.13	0.78
1:A:981:LEU:HB2	1:A:1228:MET:SD	2.23	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ASN:HD21	1:A:751:GLN:HE21	1.28	0.78
1:B:1174:GLN:HE21	1:B:1176:ASN:HD21	1.30	0.77
1:B:612:ARG:HH11	1:B:612:ARG:CB	1.94	0.77
1:A:981:LEU:CD1	1:A:1228:MET:SD	2.74	0.76
1:A:989:ARG:HD2	1:A:1209:PRO:O	1.87	0.75
1:B:822:GLU:OE2	1:B:890:PRO:HD2	1.90	0.71
1:A:979:ARG:HA	1:B:979:ARG:CZ	2.22	0.69
1:B:1060:GLU:OE2	1:B:1113:ARG:HD3	1.94	0.67
1:B:769:ASN:HD22	1:B:962:GLU:H	1.43	0.67
1:A:769:ASN:HD22	1:A:962:GLU:H	1.42	0.64
1:A:979:ARG:HA	1:B:979:ARG:NH2	2.13	0.64
1:A:981:LEU:HB2	1:A:1228:MET:CG	2.29	0.62
4:A:1307:SO4:O1	1:B:1219:ARG:NH1	2.33	0.62
1:A:1173:ASN:HD22	1:A:1226:MET:H	1.48	0.60
1:A:612:ARG:NH1	1:A:615:GLU:HG3	2.15	0.60
1:A:808:HIS:HE1	5:A:1554:HOH:O	1.85	0.59
1:B:822:GLU:OE2	1:B:890:PRO:CD	2.50	0.58
1:A:732:LYS:HE3	5:A:1458:HOH:O	2.04	0.58
1:B:1214:GLU:O	1:B:1214:GLU:HG3	2.05	0.57
1:B:817:ARG:NH2	4:B:1309:SO4:O3	2.36	0.56
1:A:800:GLU:HG3	1:A:915:LEU:HD11	1.88	0.56
1:A:1219:ARG:HD3	4:B:1305:SO4:O1	2.05	0.56
1:B:570:SER:HB3	5:B:1588:HOH:O	2.06	0.56
1:A:981:LEU:HD23	1:A:1198:ARG:HD3	1.87	0.55
1:A:702:ASN:ND2	1:A:751:GLN:HE21	2.01	0.55
1:B:769:ASN:ND2	1:B:962:GLU:H	2.05	0.54
1:A:1146:ASN:OD1	1:A:1180:ARG:HD3	2.07	0.54
1:A:1213:ALA:HA	1:A:1220:ALA:HB2	1.90	0.53
1:A:930:GLY:O	1:A:934:LYS:HG2	2.07	0.53
1:A:978:GLU:O	1:B:979:ARG:NH2	2.40	0.53
1:B:601:LEU:HD22	1:B:630:ILE:HD11	1.92	0.52
1:A:981:LEU:HD13	1:A:1228:MET:SD	2.49	0.51
1:A:769:ASN:ND2	1:A:962:GLU:H	2.07	0.51
1:A:808:HIS:HD2	5:A:1597:HOH:O	1.94	0.51
1:A:624:VAL:HG13	1:A:635:VAL:HG12	1.94	0.51
1:A:734:LEU:HD22	1:B:733:TYR:OH	2.11	0.50
1:A:1173:ASN:ND2	1:A:1226:MET:H	2.09	0.50
1:A:833:THR:O	1:A:837:SER:OG	2.29	0.50
1:A:839:ASP:OD1	1:A:841:ASN:HB2	2.11	0.50
1:A:1226:MET:SD	1:A:1228:MET:HE2	2.52	0.49
1:B:702:ASN:ND2	1:B:751:GLN:HE21	2.04	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1113:ARG:O	1:A:1116:ARG:HG2	2.14	0.48
1:B:570:SER:HB2	1:B:601:LEU:HD13	1.96	0.48
1:B:1214:GLU:O	1:B:1214:GLU:CG	2.62	0.47
1:B:634:GLY:HA2	4:B:1307:SO4:O3	2.13	0.47
1:B:1205:LEU:HD23	1:B:1228:MET:HE1	1.95	0.47
1:A:1006:VAL:HG22	5:A:1463:HOH:O	2.15	0.46
1:A:836:MET:HA	1:A:842:ASN:ND2	2.29	0.46
1:A:570:SER:HA	1:B:578:LEU:HD22	1.97	0.46
1:B:993:MET:HB2	1:B:1020:CYS:HB3	1.99	0.45
1:A:762:LEU:HD12	1:A:768:PHE:CD2	2.51	0.45
1:B:710:ALA:N	1:B:711:PRO:CD	2.81	0.44
1:A:775:PRO:HG2	1:A:931:VAL:HG11	2.00	0.44
1:A:998:VAL:HG22	1:A:1075:THR:HB	2.00	0.44
1:A:1028:ILE:HA	1:A:1053:LEU:O	2.18	0.44
1:A:1216:SER:OG	1:B:1194:GLU:OE1	2.34	0.44
1:B:1125[B]:GLN:OE1	1:B:1210:LEU:HG	2.18	0.44
1:A:982:PHE:CD1	1:A:982:PHE:O	2.71	0.44
1:B:702:ASN:O	1:B:706:MET:HG3	2.18	0.44
1:B:709:VAL:CG1	1:B:713:MET:HE3	2.48	0.44
1:B:1135:MET:HE3	1:B:1135:MET:HB2	1.91	0.43
1:A:948:GLN:HG2	1:A:952:PHE:CE2	2.53	0.43
1:B:627:LEU:HD12	1:B:635:VAL:HG13	2.00	0.43
1:B:808:HIS:HE1	5:B:1601:HOH:O	2.01	0.43
1:B:733:TYR:O	1:B:977:THR:HG23	2.19	0.43
1:B:624:VAL:HG13	1:B:635:VAL:HG12	2.01	0.42
1:A:1130:SER:OG	1:A:1176:ASN:HA	2.20	0.42
1:B:839:ASP:HB3	1:B:842:ASN:ND2	2.35	0.42
1:B:601:LEU:HD22	1:B:630:ILE:CD1	2.50	0.42
1:A:1030:ARG:NH1	5:A:1416:HOH:O	2.53	0.41
1:A:1205:LEU:HD23	1:A:1228:MET:HE1	2.02	0.41
1:B:1174:GLN:HE21	1:B:1176:ASN:ND2	2.07	0.41
1:A:777:ASP:HB2	1:A:940:MET:HE2	2.02	0.41
1:B:842:ASN:O	1:B:847:ARG:NH1	2.53	0.41
1:B:1135:MET:HE1	1:B:1192:HIS:HB2	2.02	0.41
1:A:1120:LEU:HA	1:A:1168:HIS:CD2	2.56	0.41
1:B:1218:TYR:CE1	1:B:1222:ILE:HD12	2.56	0.41
1:A:981:LEU:HA	5:A:1468:HOH:O	2.20	0.40
1:B:1060:GLU:CD	1:B:1113:ARG:HD3	2.46	0.40
1:A:797:LEU:HD23	1:A:800:GLU:OE1	2.22	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	662/695 (95%)	646 (98%)	15 (2%)	1 (0%)	43	42
1	B	659/695 (95%)	646 (98%)	11 (2%)	2 (0%)	36	35
All	All	1321/1390 (95%)	1292 (98%)	26 (2%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	985	PRO
1	A	1088	LEU
1	B	890	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	531/553 (96%)	523 (98%)	8 (2%)	57	64
1	B	531/553 (96%)	524 (99%)	7 (1%)	61	68
All	All	1062/1106 (96%)	1047 (99%)	15 (1%)	59	66

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	784	THR
1	A	840	THR
1	A	863	TRP

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Mol	Chain	Res	Type
1	A	956	ASP
1	A	981	LEU
1	A	998	VAL
1	A	1187	ARG
1	A	1210	LEU
1	B	612	ARG
1	B	863	TRP
1	B	877	VAL
1	B	931	VAL
1	B	956	ASP
1	B	1098	ASP
1	B	1222	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	640	GLN
1	A	644	ASN
1	A	702	ASN
1	A	769	ASN
1	A	808	HIS
1	A	871	GLN
1	A	1004	HIS
1	A	1125	GLN
1	A	1173	ASN
1	B	640	GLN
1	B	702	ASN
1	B	767	GLN
1	B	769	ASN
1	B	801	ASN
1	B	808	HIS
1	B	1004	HIS
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 [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](#)

19 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	$\# Z > 2$
4	SO4	A	1305	-	4,4,4	0.28	0	6,6,6	0.11	0
4	SO4	A	1309	-	4,4,4	0.35	0	6,6,6	0.12	0
3	GOL	B	1302	-	5,5,5	0.23	0	5,5,5	0.41	0
4	SO4	B	1303	-	4,4,4	0.86	0	6,6,6	0.10	0
4	SO4	B	1306	-	4,4,4	0.26	0	6,6,6	0.17	0
4	SO4	B	1307	-	4,4,4	0.54	0	6,6,6	0.18	0
2	NAP	A	1301	-	50,52,52	1.21	5 (10%)	71,80,80	1.55	9 (12%)
4	SO4	B	1308	-	4,4,4	0.29	0	6,6,6	0.27	0
4	SO4	A	1306	-	4,4,4	0.25	0	6,6,6	0.15	0
4	SO4	B	1310	-	4,4,4	0.26	0	6,6,6	0.14	0
4	SO4	B	1305	-	4,4,4	0.24	0	6,6,6	0.19	0
4	SO4	B	1309	-	4,4,4	0.38	0	6,6,6	0.25	0
2	NAP	B	1301	-	50,52,52	1.81	11 (22%)	71,80,80	1.67	15 (21%)
4	SO4	A	1304	-	4,4,4	0.37	0	6,6,6	0.17	0
4	SO4	A	1303	-	4,4,4	0.37	0	6,6,6	0.19	0
3	GOL	A	1302	-	5,5,5	0.24	0	5,5,5	0.42	0
4	SO4	A	1308	-	4,4,4	0.29	0	6,6,6	0.23	0
4	SO4	A	1307	-	4,4,4	0.26	0	6,6,6	0.12	0
4	SO4	B	1304	-	4,4,4	0.38	0	6,6,6	0.17	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	NAP	A	1301	-	-	13/35/67/67	0/5/5/5
2	NAP	B	1301	-	-	6/35/67/67	0/5/5/5
3	GOL	A	1302	-	-	0/4/4/4	-
3	GOL	B	1302	-	-	0/4/4/4	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	NAP	PN-O3	5.73	1.65	1.59
2	B	1301	NAP	C5A-C4A	5.40	1.48	1.39
2	B	1301	NAP	PA-O3	4.67	1.64	1.59
2	A	1301	NAP	C5A-C4A	3.92	1.46	1.39
2	A	1301	NAP	C5A-N7A	-3.22	1.33	1.39
2	B	1301	NAP	C4A-N9A	-3.02	1.31	1.37
2	B	1301	NAP	C2N-N1N	2.90	1.38	1.35
2	A	1301	NAP	C4A-N9A	-2.80	1.31	1.37
2	B	1301	NAP	C5A-C6A	2.62	1.48	1.41
2	A	1301	NAP	C8A-N9A	-2.57	1.33	1.37
2	B	1301	NAP	C2N-C3N	2.34	1.42	1.39
2	B	1301	NAP	O4B-C1B	2.31	1.47	1.42
2	B	1301	NAP	PN-O5D	2.29	1.68	1.59
2	B	1301	NAP	C8A-N7A	2.17	1.35	1.31
2	A	1301	NAP	C5A-C6A	2.08	1.46	1.41
2	B	1301	NAP	C5A-N7A	-2.07	1.35	1.39

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1301	NAP	C5A-C4A-N3A	-5.17	119.60	126.72
2	A	1301	NAP	N3A-C4A-N9A	4.59	134.97	127.17
2	B	1301	NAP	O7N-C7N-C3N	4.38	124.95	119.60
2	B	1301	NAP	C4A-N9A-C8A	4.32	110.27	105.74
2	A	1301	NAP	O2N-PN-O3	4.28	118.85	107.27
2	B	1301	NAP	N3A-C4A-N9A	3.68	133.43	127.17
2	B	1301	NAP	C5A-C4A-N3A	-3.62	121.73	126.72
2	B	1301	NAP	O2A-PA-O1A	3.12	126.95	112.44
2	A	1301	NAP	C2A-N3A-C4A	3.09	119.38	111.83
2	A	1301	NAP	C4A-N9A-C8A	3.07	108.96	105.74
2	A	1301	NAP	N3A-C2A-N1A	-3.05	123.96	128.58
2	B	1301	NAP	N9A-C8A-N7A	-2.93	109.77	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	NAP	O4B-C4B-C5B	-2.86	100.19	109.33
2	B	1301	NAP	C2A-N3A-C4A	2.67	118.36	111.83
2	A	1301	NAP	C4A-C5A-N7A	-2.63	107.58	110.58
2	B	1301	NAP	N3A-C2A-N1A	-2.46	124.86	128.58
2	A	1301	NAP	C2A-N1A-C6A	2.43	122.73	118.73
2	B	1301	NAP	C5A-N7A-C8A	2.26	107.00	103.45
2	B	1301	NAP	O2N-PN-O3	2.25	113.35	107.27
2	B	1301	NAP	N6A-C6A-N1A	2.25	123.38	118.38
2	B	1301	NAP	C4A-C5A-N7A	-2.23	108.03	110.58
2	B	1301	NAP	O7N-C7N-N7N	-2.22	119.41	122.62
2	B	1301	NAP	C3B-C2B-C1B	-2.21	98.58	102.81
2	A	1301	NAP	C5B-C4B-C3B	-2.00	108.00	115.21

There are no chirality outliers.

All (19) torsion outliers are listed below:

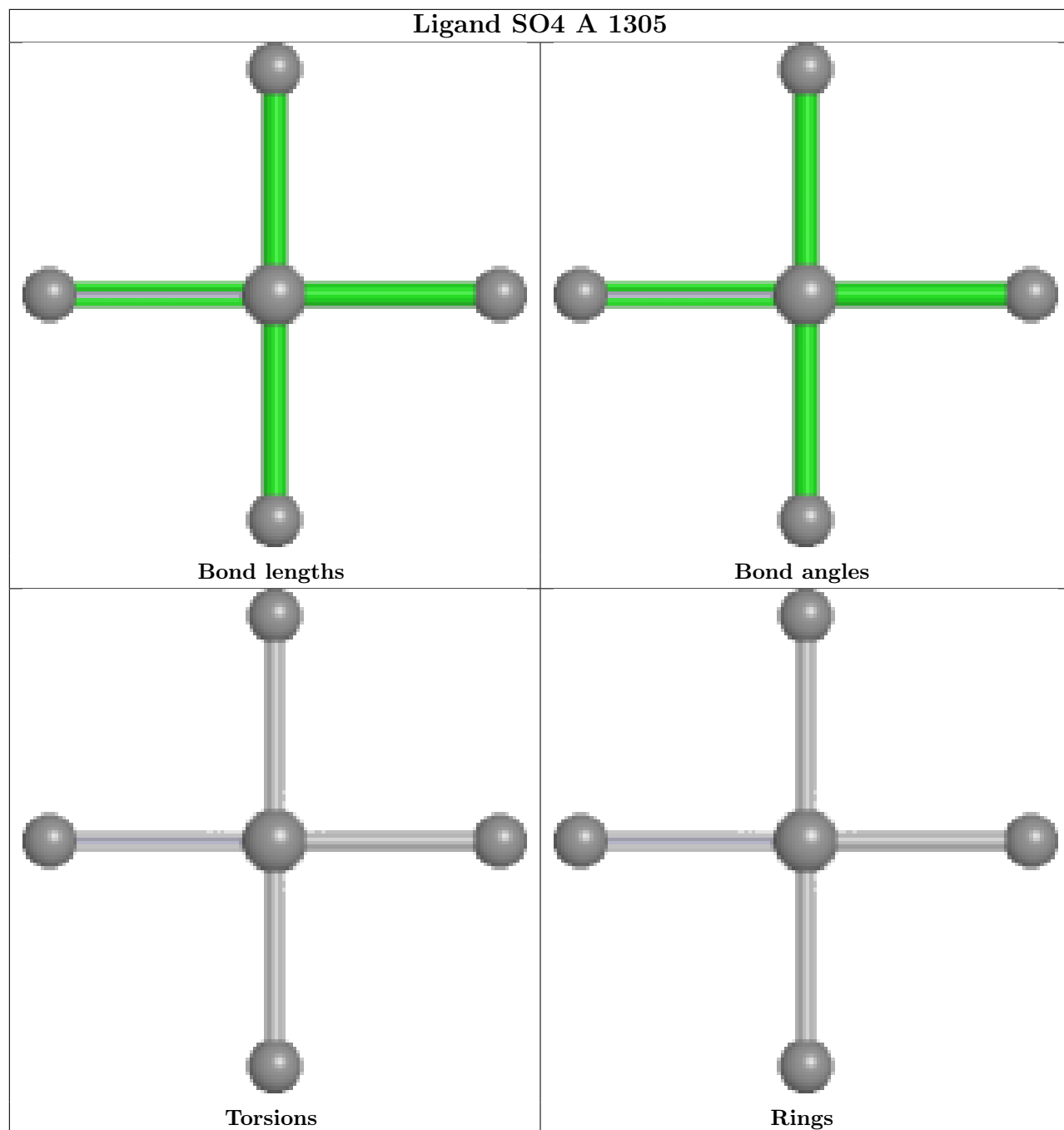
Mol	Chain	Res	Type	Atoms
2	A	1301	NAP	C5B-O5B-PA-O1A
2	A	1301	NAP	C5B-O5B-PA-O2A
2	A	1301	NAP	C5B-O5B-PA-O3
2	A	1301	NAP	C5D-O5D-PN-O3
2	A	1301	NAP	C5D-O5D-PN-O2N
2	B	1301	NAP	C5D-O5D-PN-O2N
2	A	1301	NAP	C3B-C4B-C5B-O5B
2	A	1301	NAP	O4B-C4B-C5B-O5B
2	A	1301	NAP	PN-O3-PA-O1A
2	A	1301	NAP	C5D-O5D-PN-O1N
2	B	1301	NAP	C5D-O5D-PN-O3
2	B	1301	NAP	C3B-C2B-O2B-P2B
2	A	1301	NAP	O4D-C1D-N1N-C6N
2	A	1301	NAP	C1B-C2B-O2B-P2B
2	B	1301	NAP	C1B-C2B-O2B-P2B
2	A	1301	NAP	C3B-C2B-O2B-P2B
2	A	1301	NAP	PN-O3-PA-O2A
2	B	1301	NAP	PN-O3-PA-O2A
2	B	1301	NAP	O4B-C4B-C5B-O5B

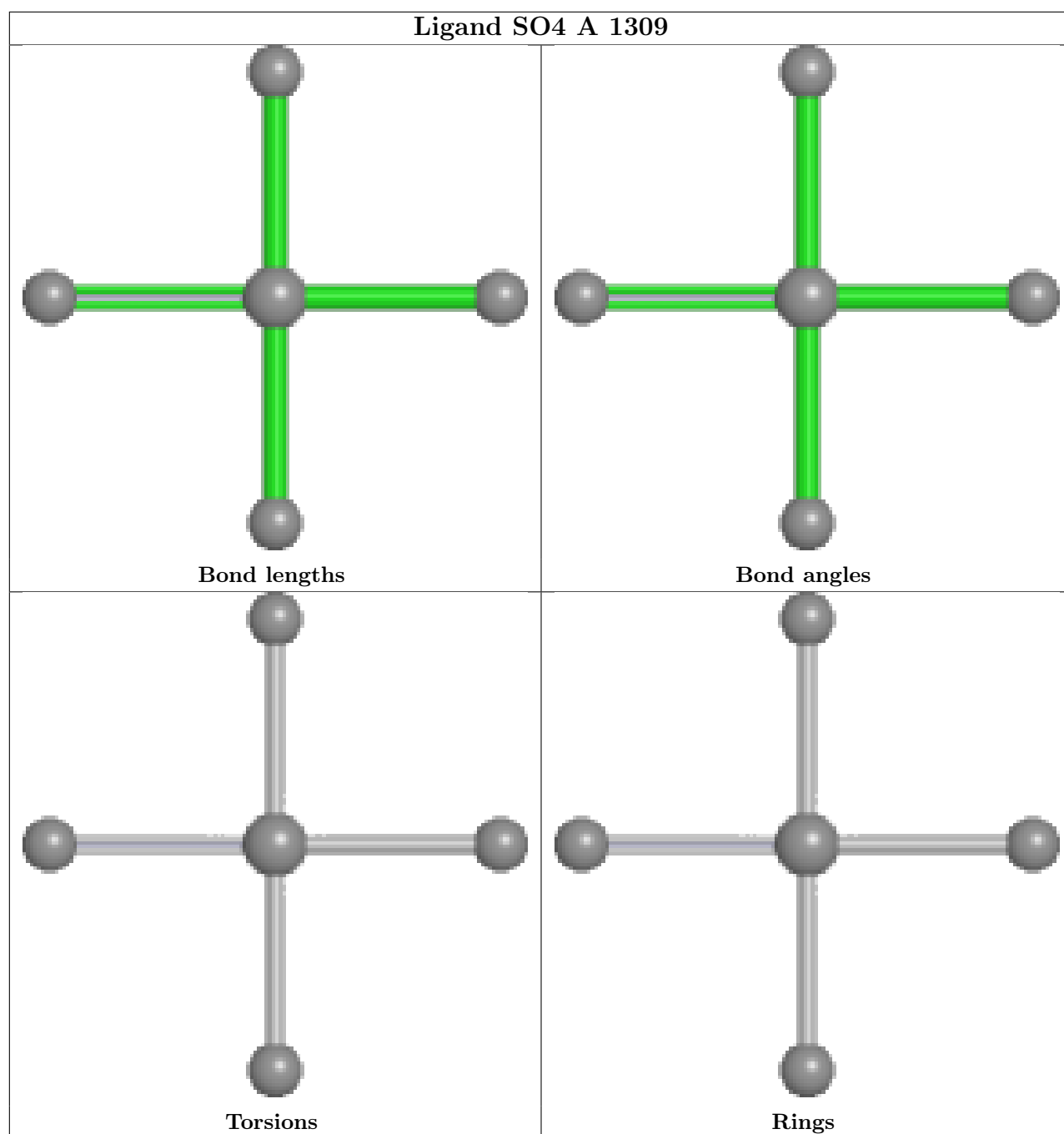
There are no ring outliers.

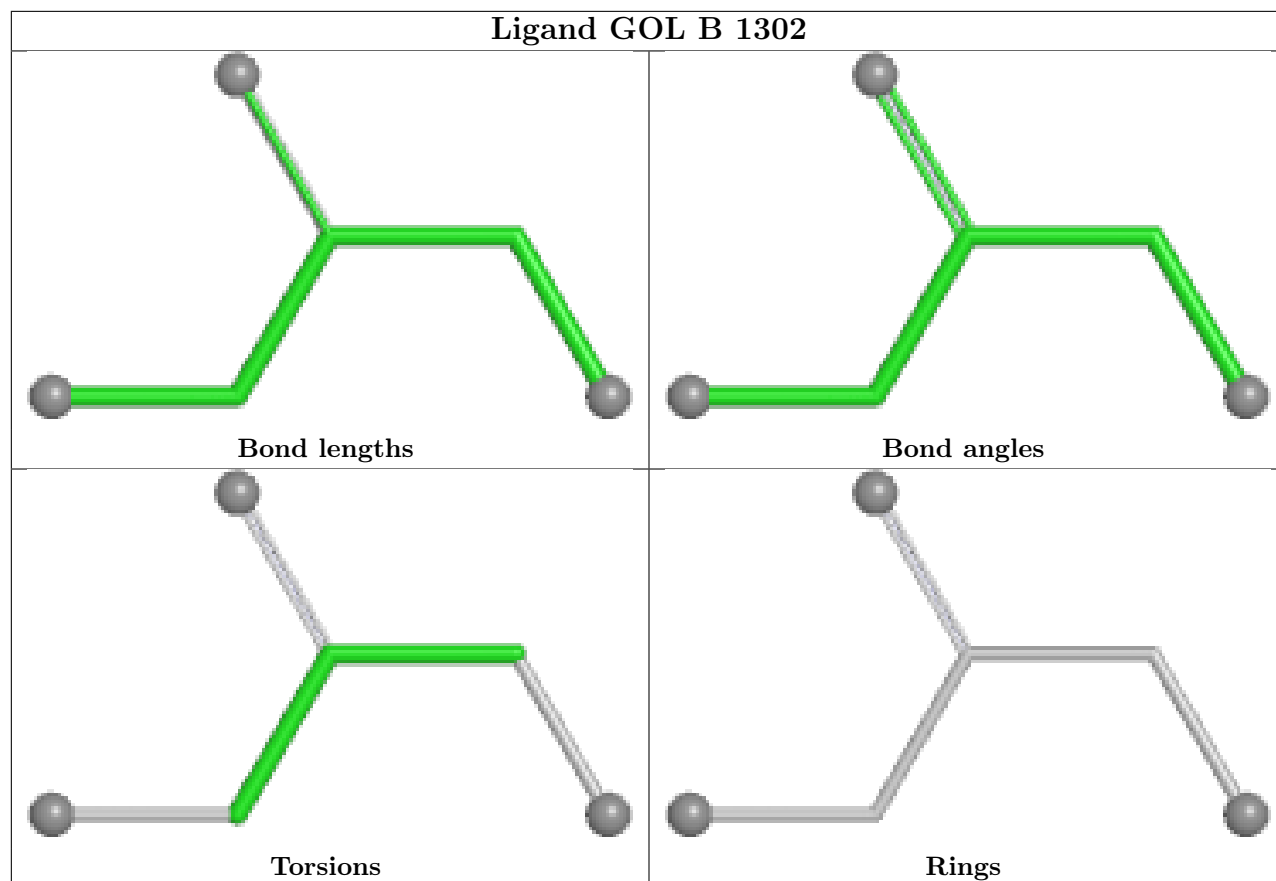
4 monomers are involved in 4 short contacts:

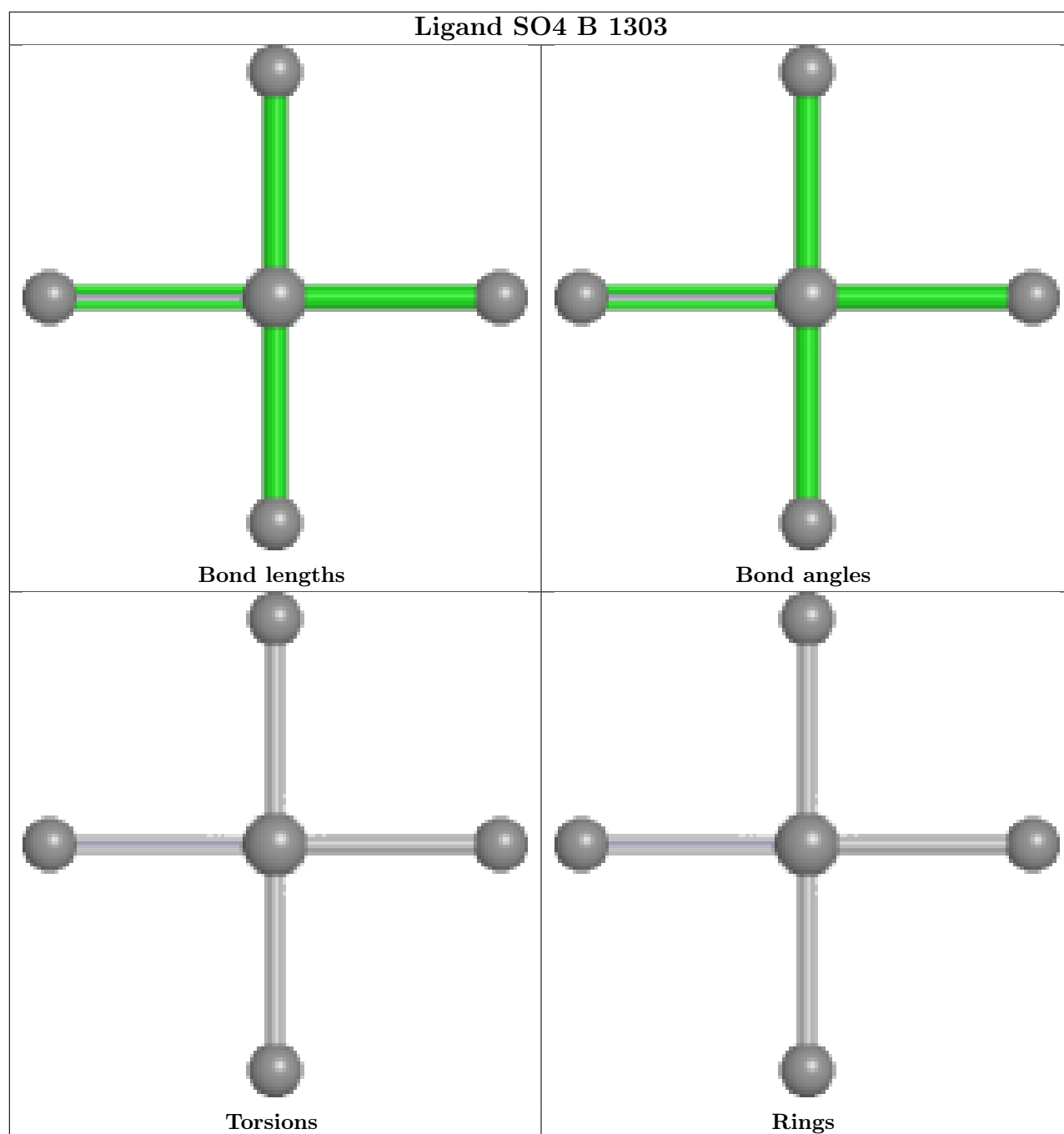
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1307	SO4	1	0
4	B	1305	SO4	1	0
4	B	1309	SO4	1	0
4	A	1307	SO4	1	0

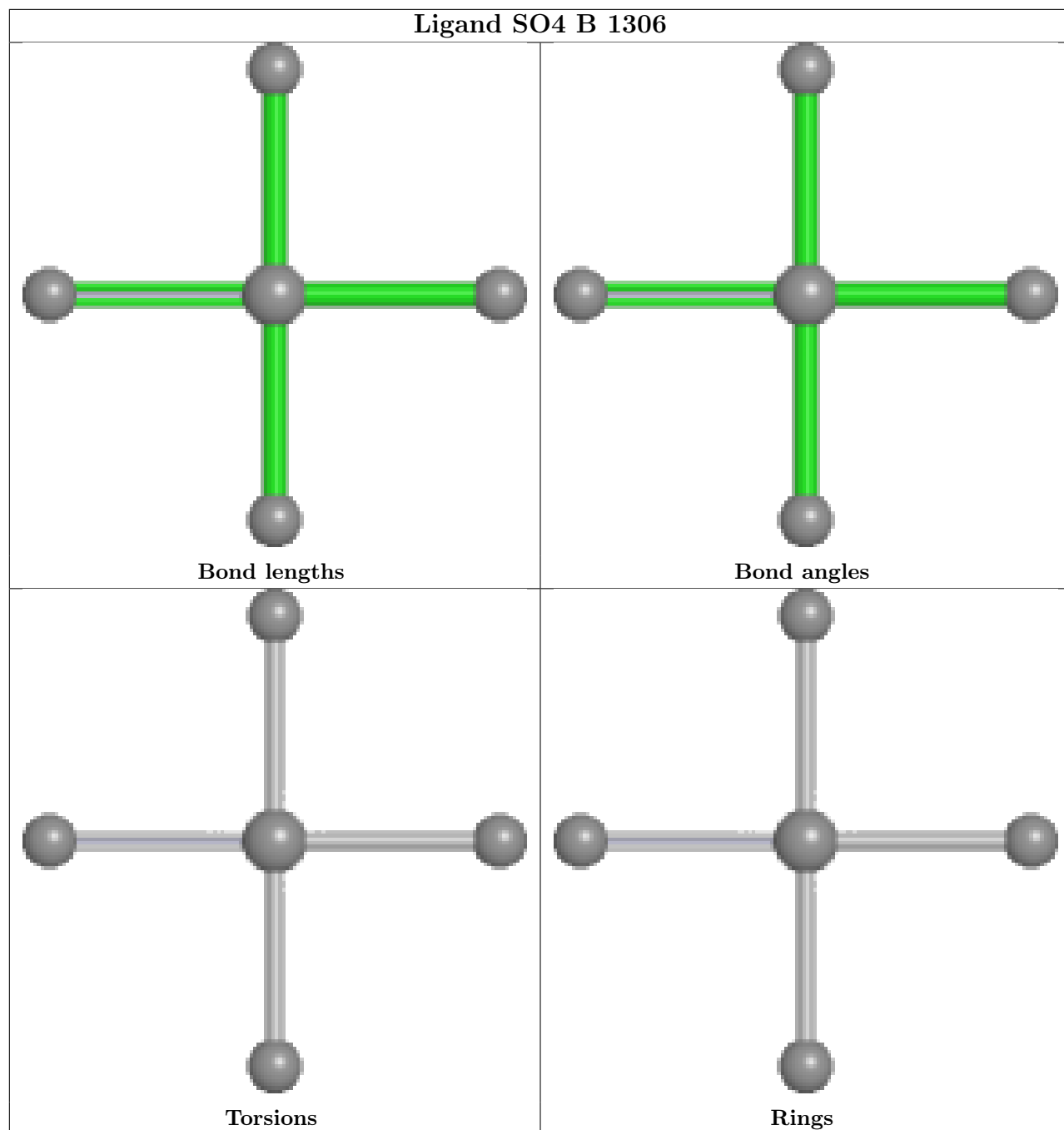
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

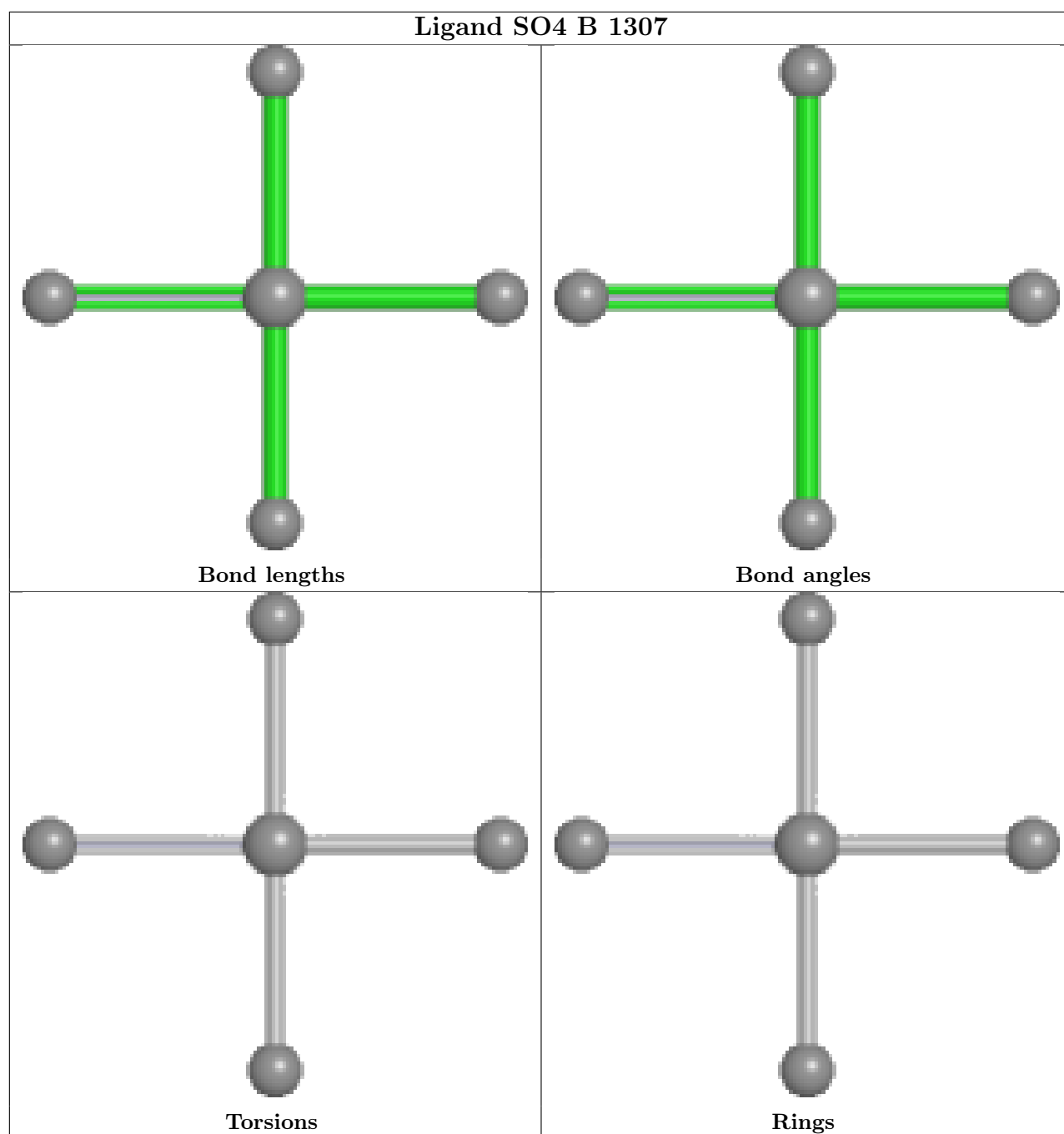


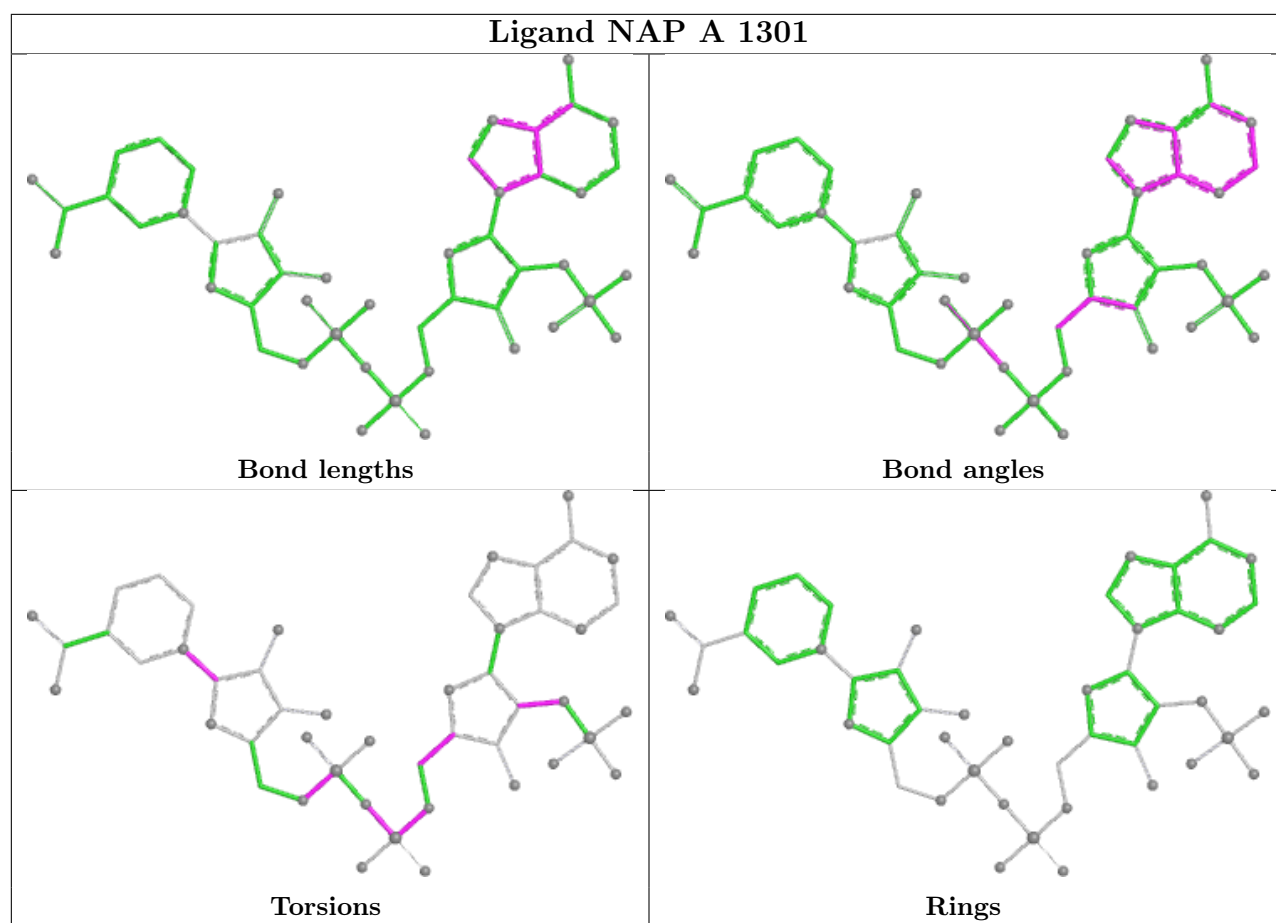


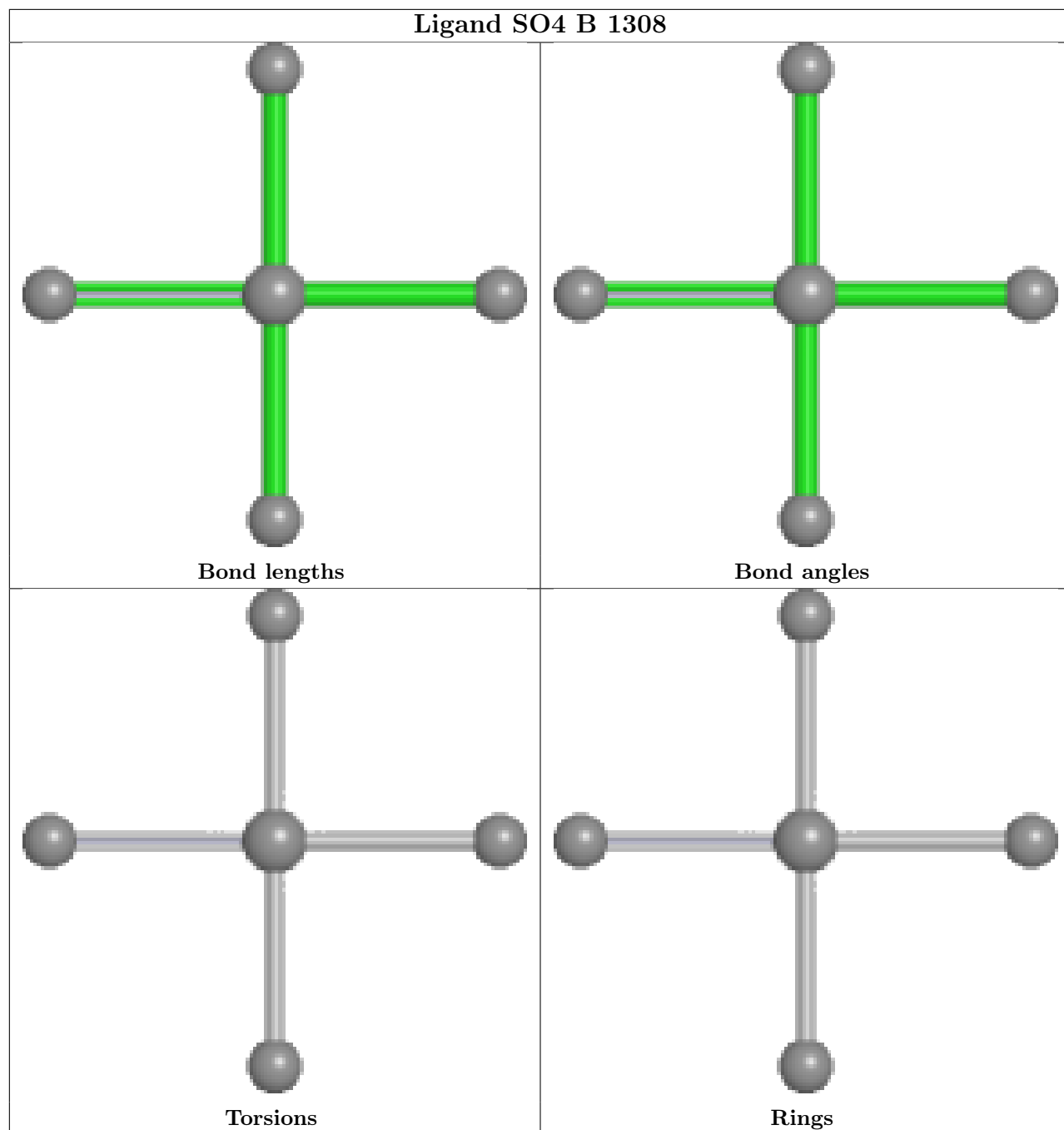


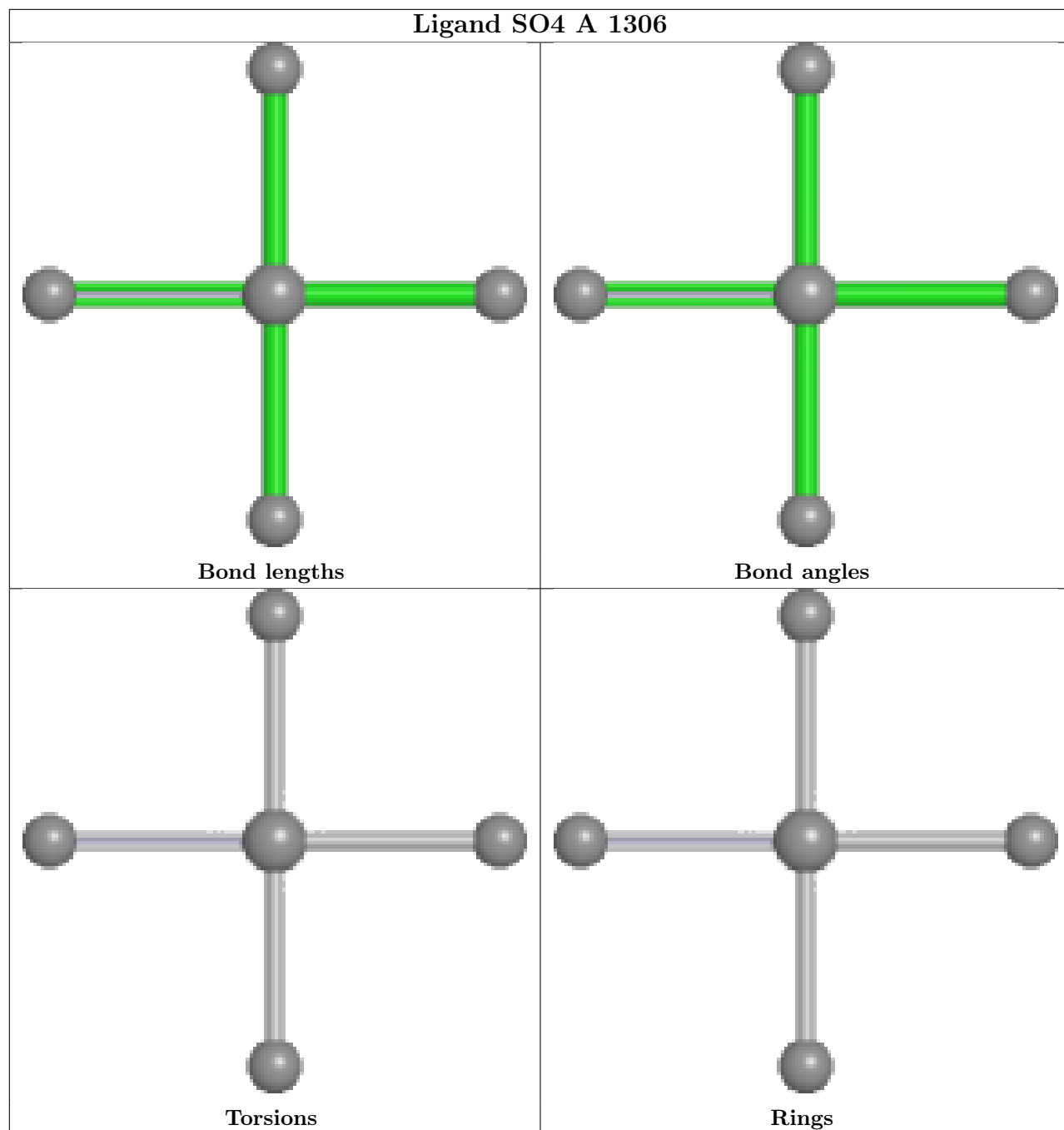


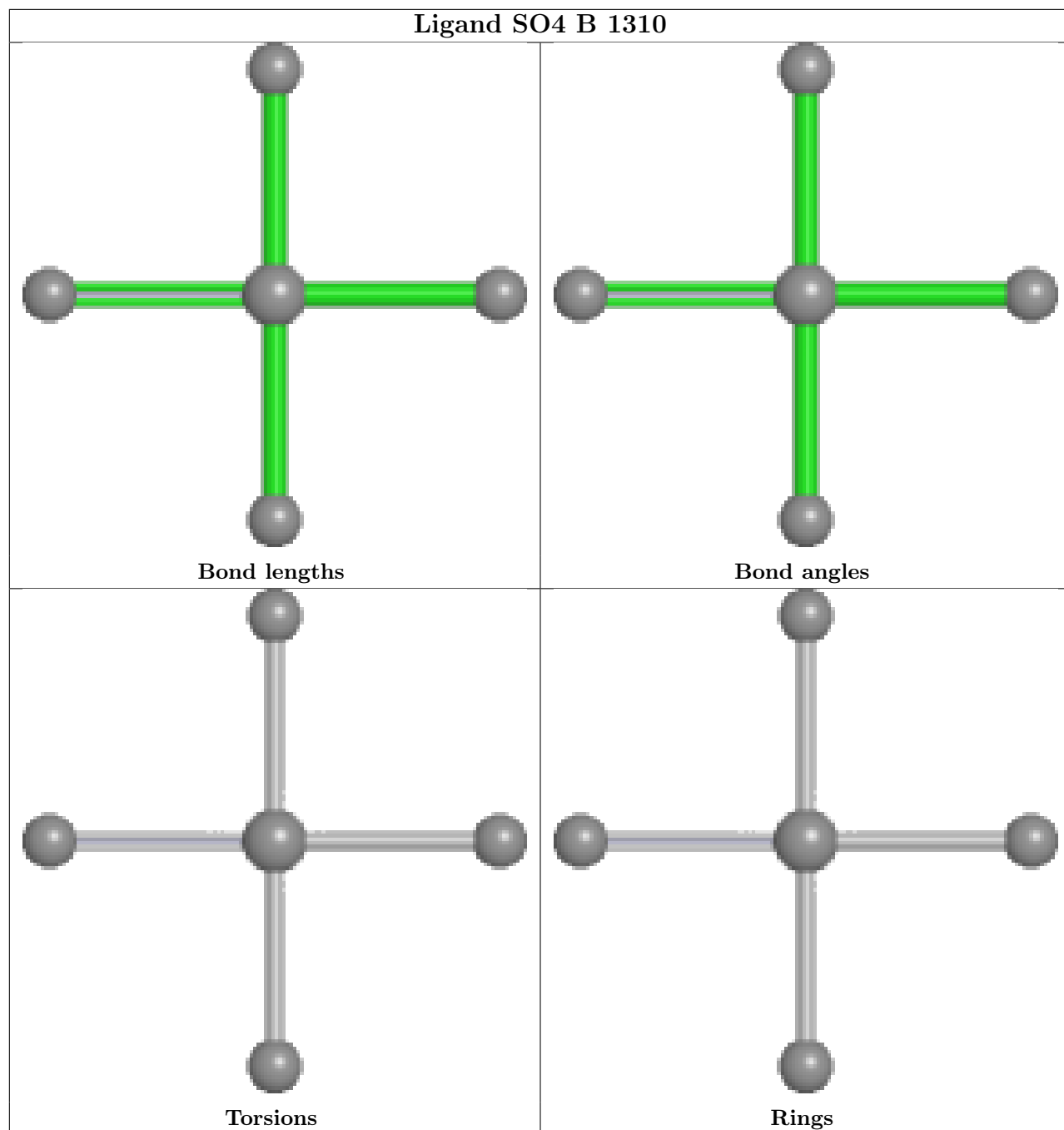


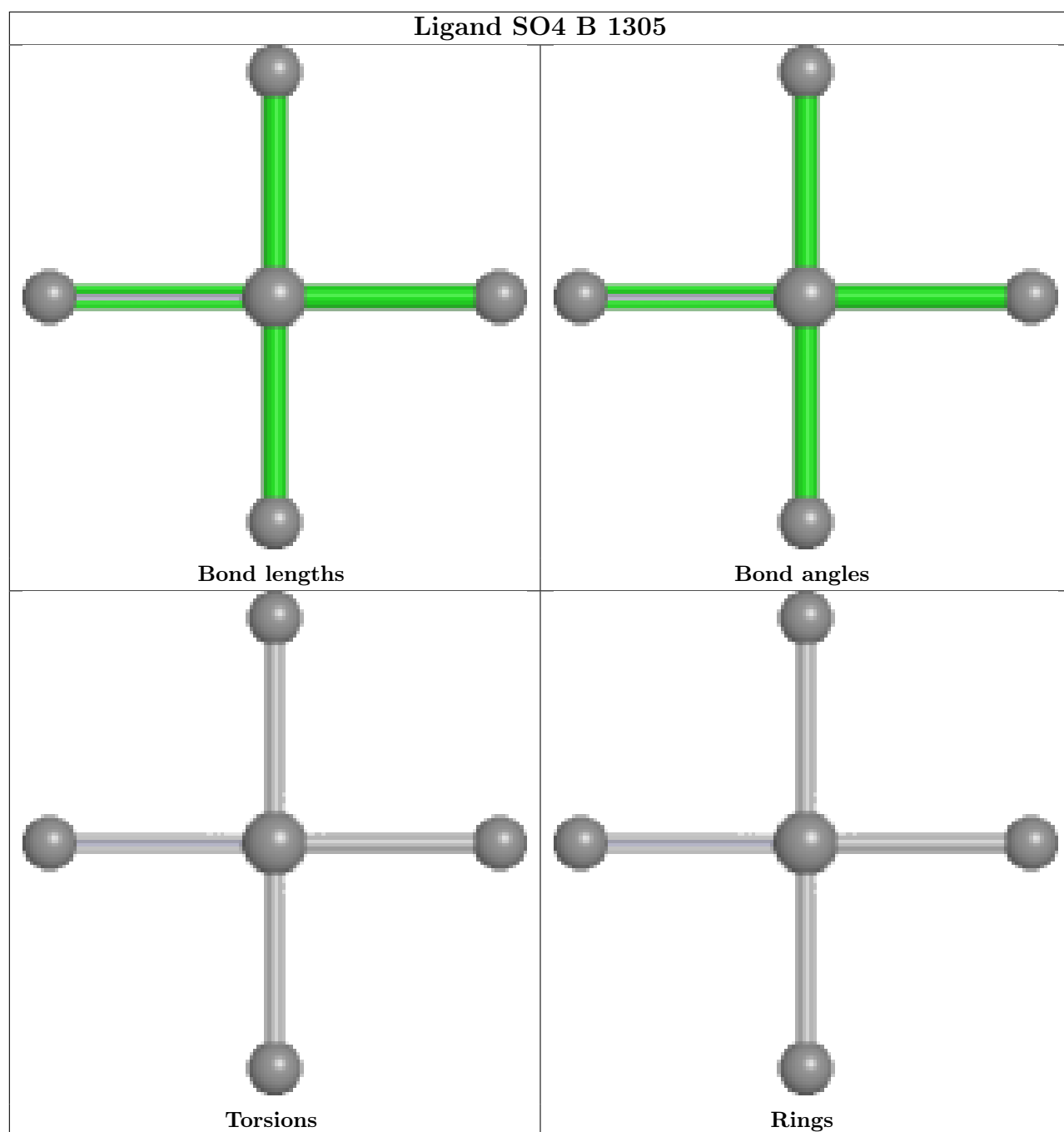


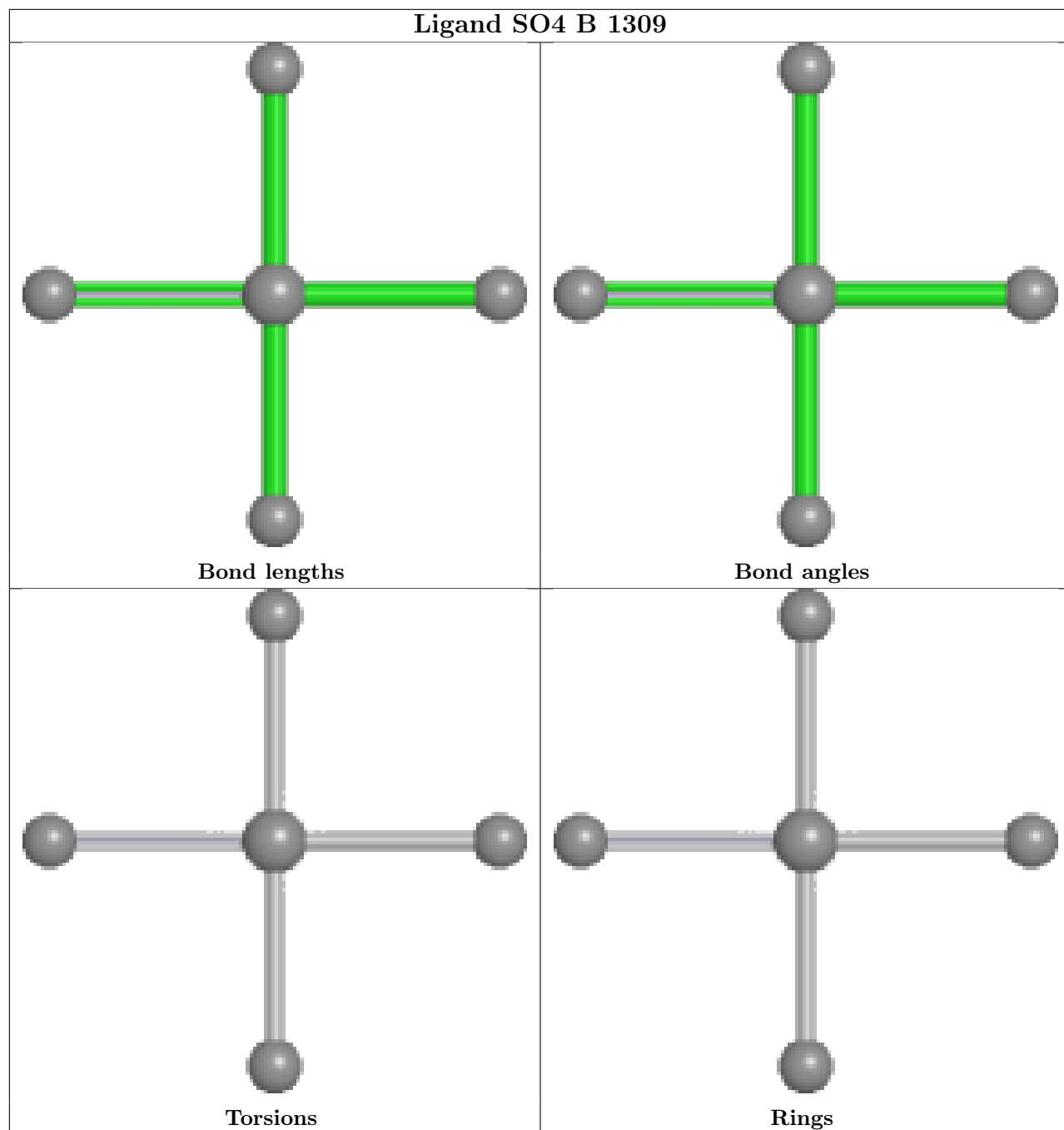


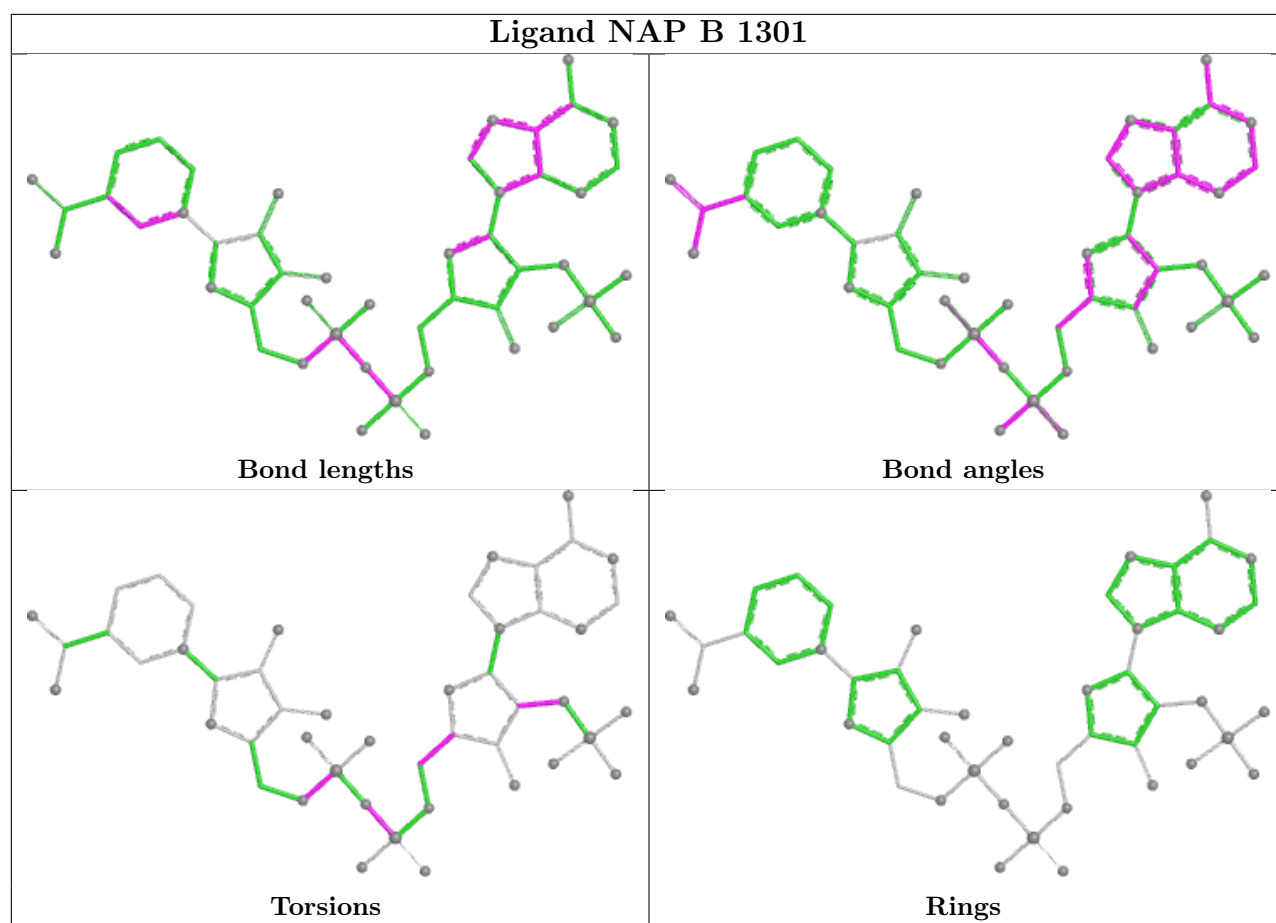


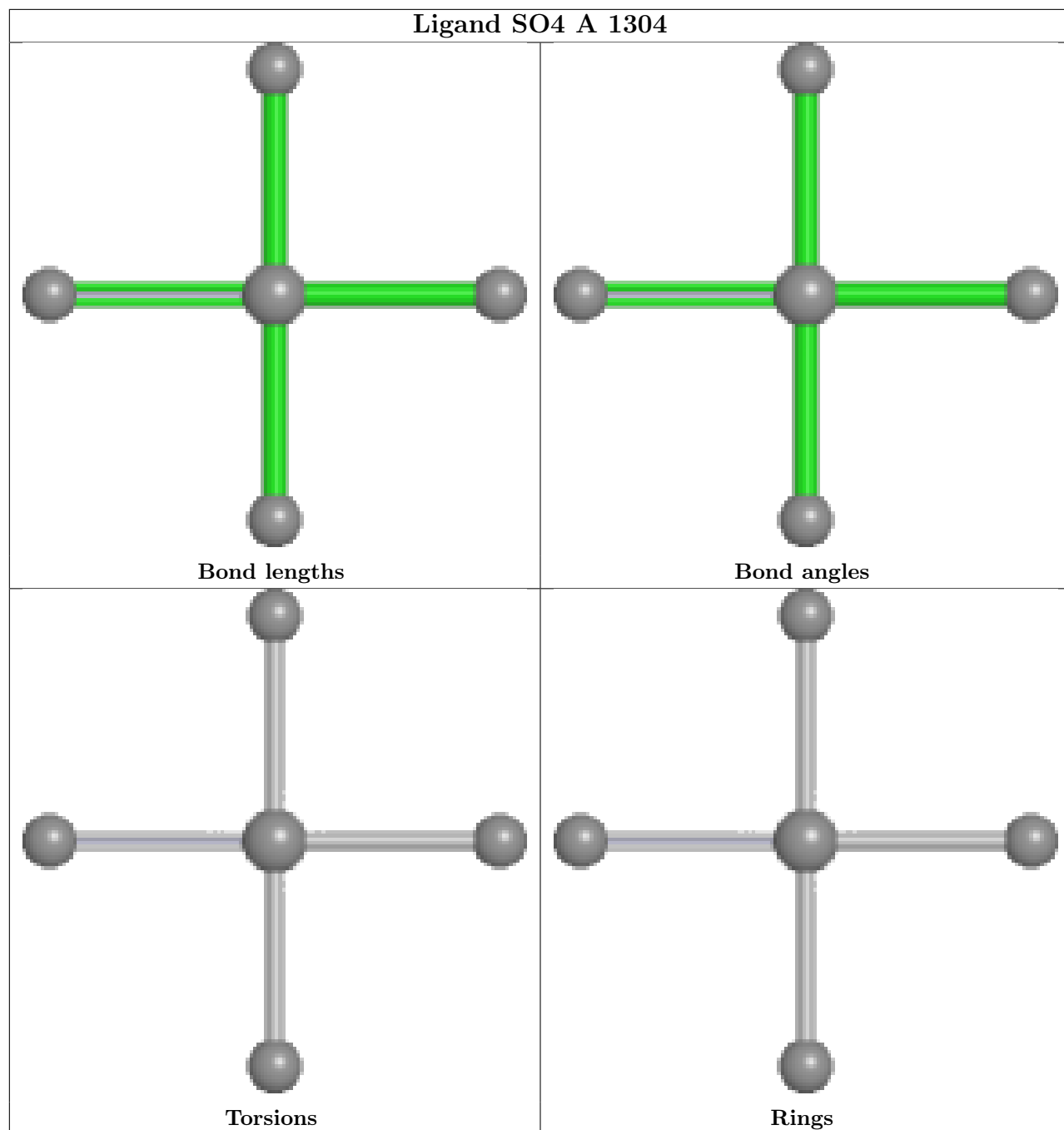


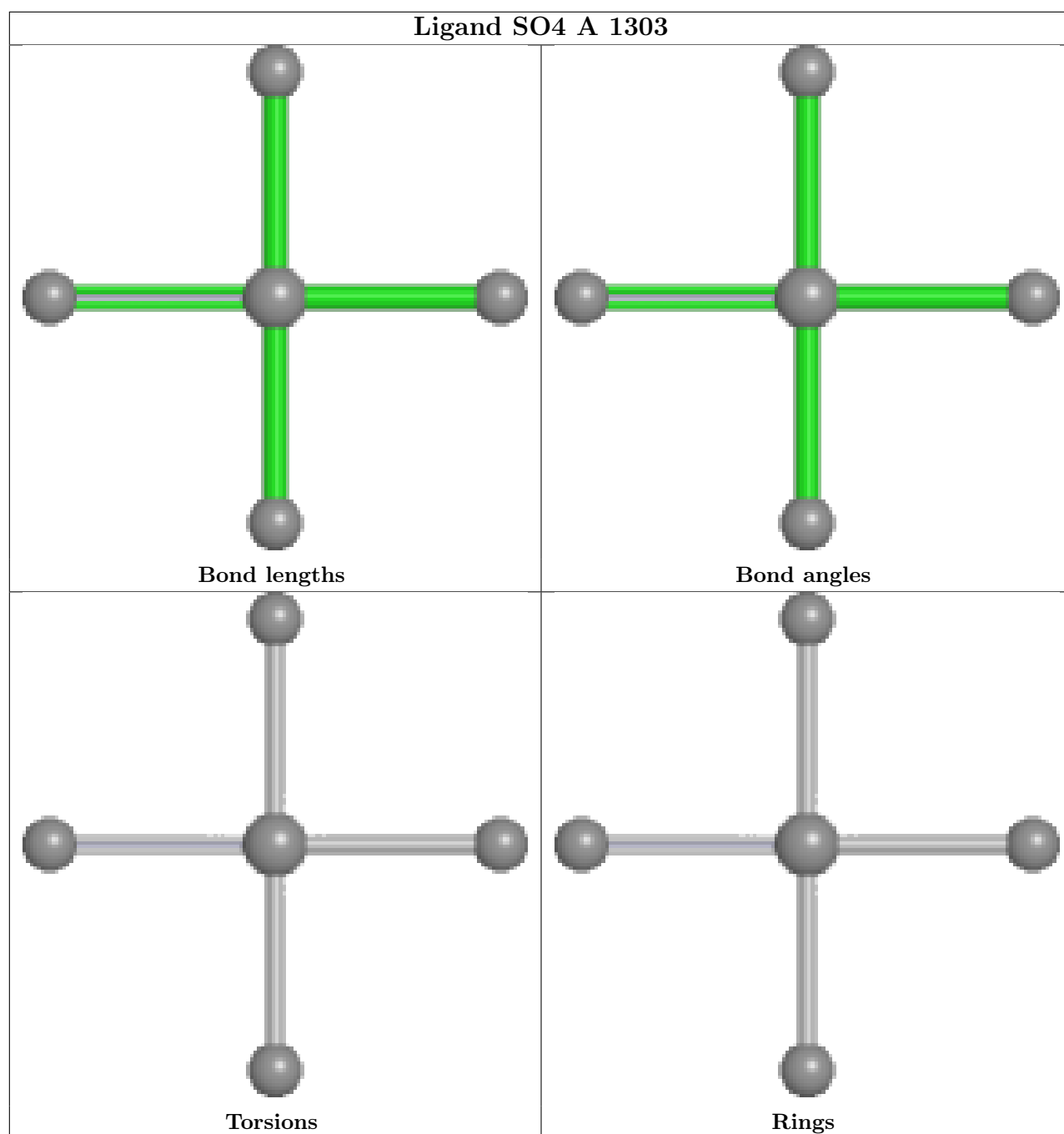


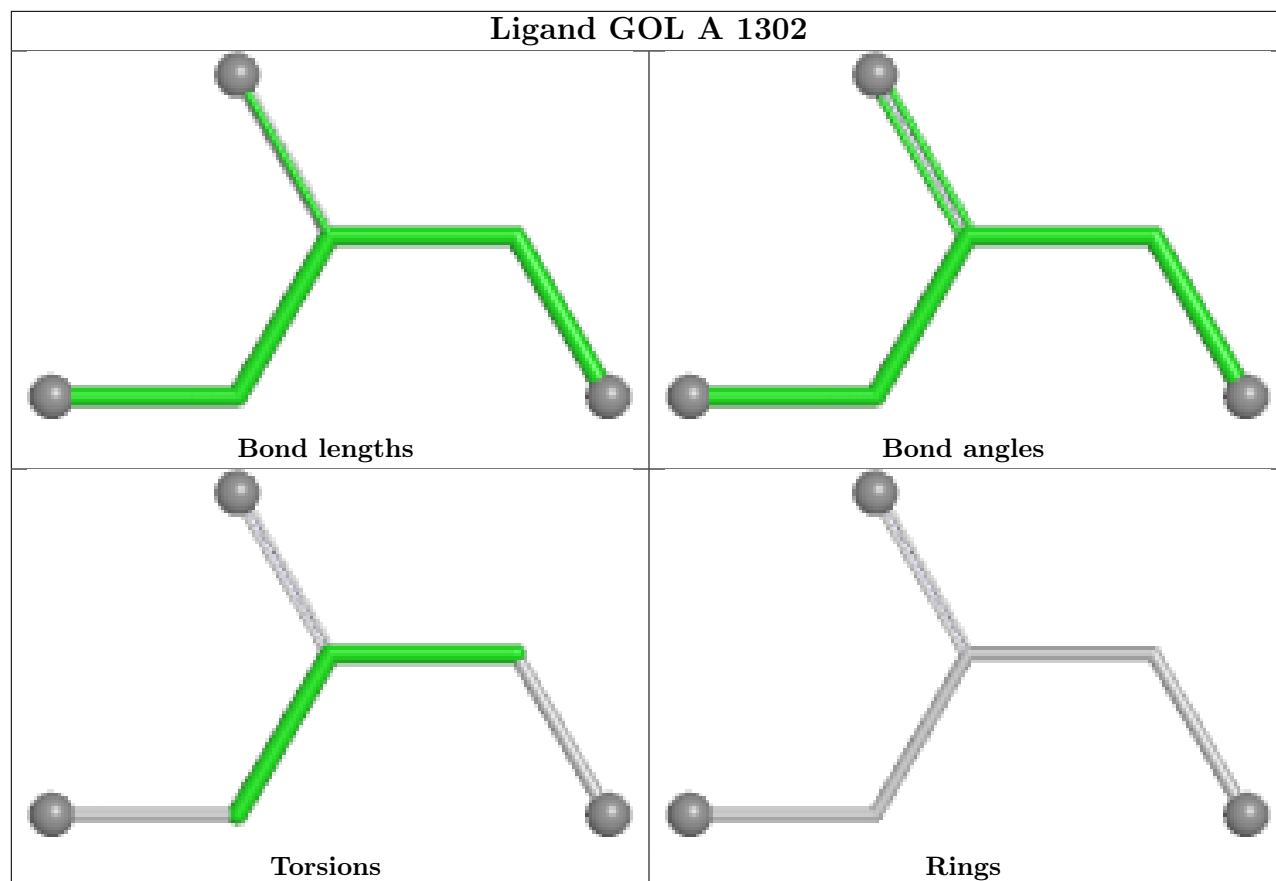


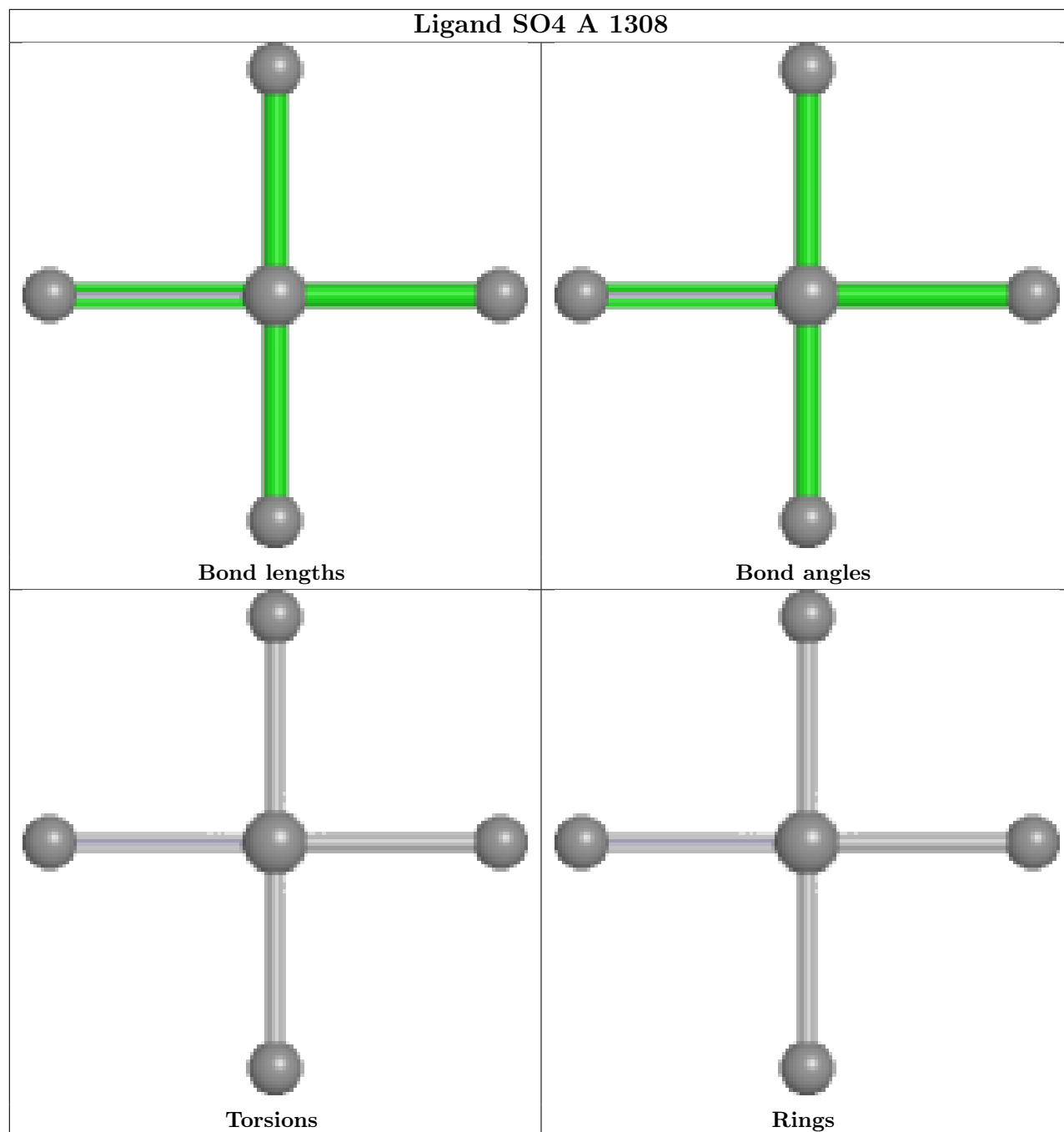


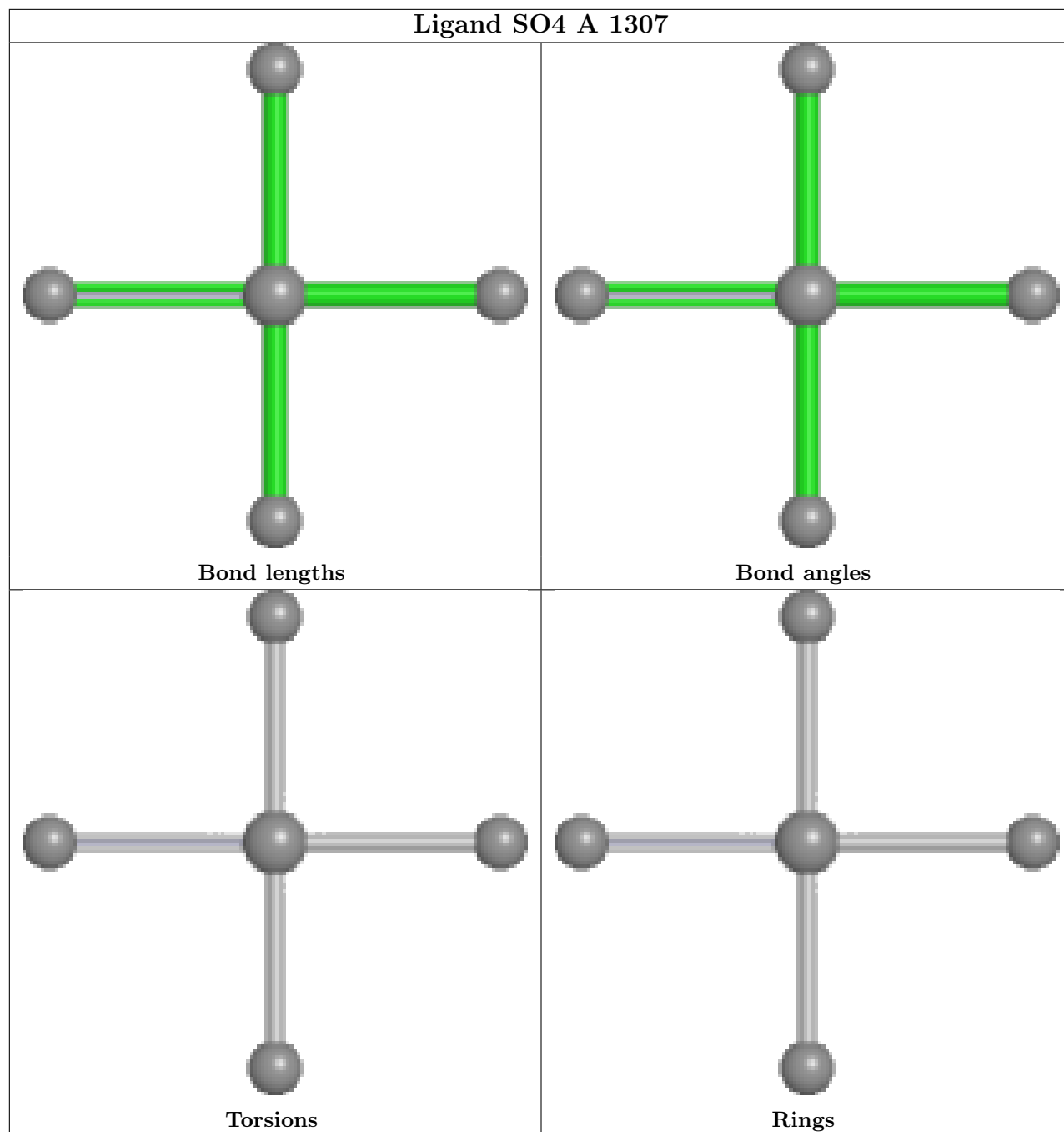


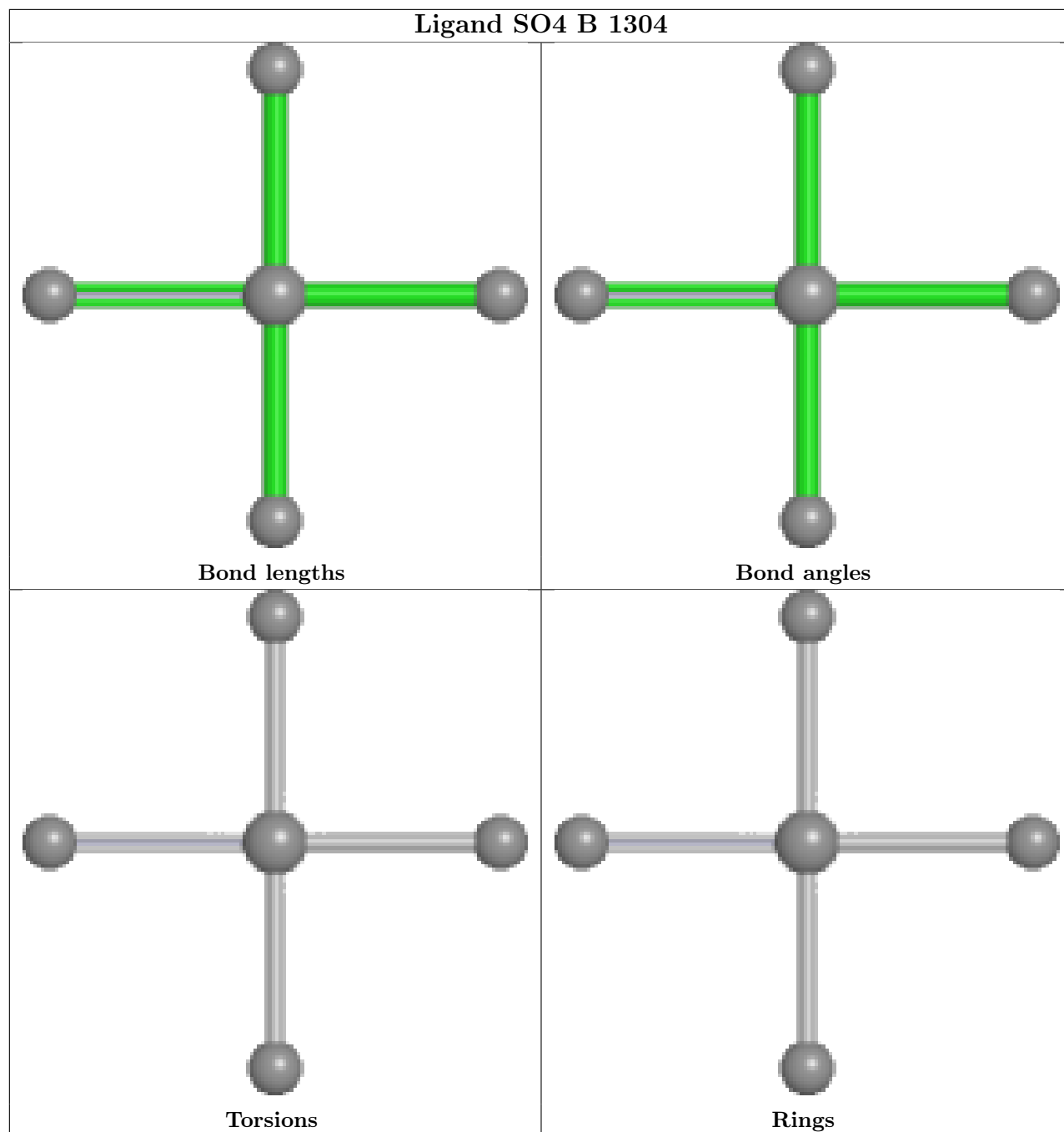












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	662/695 (95%)	0.08	44 (6%)	24 23	9, 25, 62, 111	2 (0%)
1	B	660/695 (94%)	0.07	55 (8%)	17 16	9, 24, 62, 111	3 (0%)
All	All	1322/1390 (95%)	0.07	99 (7%)	20 19	9, 24, 62, 111	5 (0%)

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	983	GLY	7.5
1	A	982	PHE	6.6
1	A	784	THR	5.5
1	B	784	THR	5.4
1	A	630	ILE	5.4
1	A	890	PRO	5.4
1	B	1216	SER	4.8
1	B	983	GLY	4.7
1	B	1220	ALA	4.7
1	A	838	HIS	4.7
1	B	982	PHE	4.6
1	A	787	LYS	4.1
1	B	838	HIS	4.1
1	A	1211	PRO	4.1
1	B	1222	ILE	4.0
1	A	981	LEU	3.9
1	A	986	LYS	3.9
1	A	785	GLY	3.9
1	A	569	PHE	3.8
1	A	840	THR	3.8
1	A	985	PRO	3.8
1	B	1219	ARG	3.7
1	B	1210	LEU	3.6
1	A	984	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	630	ILE	3.6
1	B	890	PRO	3.6
1	B	911	ASP	3.5
1	B	840	THR	3.5
1	B	790	LEU	3.5
1	A	918	ASP	3.5
1	A	1189	LEU	3.4
1	A	979	ARG	3.3
1	B	839	ASP	3.3
1	B	834	VAL	3.3
1	B	1223	TYR	3.3
1	B	984	SER	3.3
1	A	786	GLY	3.2
1	B	785	GLY	3.2
1	A	1210	LEU	3.2
1	B	779	ASP	3.1
1	B	1211	PRO	3.1
1	B	781	LEU	3.1
1	A	978	GLU	3.0
1	B	860	THR	3.0
1	A	631	GLY	2.9
1	B	783	GLY	2.9
1	A	628	GLU	2.8
1	B	986	LYS	2.8
1	A	860	THR	2.8
1	A	975	SER	2.8
1	B	932	LEU	2.8
1	A	632	PHE	2.7
1	B	613	GLU	2.7
1	B	975	SER	2.7
1	A	930	GLY	2.7
1	B	1214	GLU	2.6
1	A	1215	ASP	2.6
1	B	782	SER	2.6
1	B	893	SER	2.6
1	A	980	GLU	2.5
1	B	897	VAL	2.5
1	B	1218	TYR	2.5
1	B	854	ALA	2.5
1	B	898	THR	2.5
1	B	570	SER	2.4
1	A	788	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	981	LEU	2.4
1	B	919	LYS	2.4
1	A	1045	ASP	2.4
1	B	780	ARG	2.4
1	B	891	GLU	2.3
1	B	569	PHE	2.3
1	B	917	ALA	2.3
1	B	985	PRO	2.3
1	B	1048	GLN	2.3
1	A	781	LEU	2.3
1	A	976	THR	2.2
1	B	851	LEU	2.2
1	A	1219	ARG	2.2
1	B	841	ASN	2.2
1	A	925	LYS	2.2
1	A	625	SER	2.1
1	A	629	ASP	2.1
1	B	573	ILE	2.1
1	A	855	ARG	2.1
1	A	572	ASN	2.1
1	B	571	GLU	2.1
1	B	918	ASP	2.1
1	B	637	ARG	2.1
1	B	778	GLY	2.1
1	B	1215	ASP	2.1
1	A	574	THR	2.1
1	A	789	GLY	2.1
1	B	631	GLY	2.1
1	B	787	LYS	2.1
1	A	783	GLY	2.0
1	A	782	SER	2.0
1	A	1213	ALA	2.0
1	B	925	LYS	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 ⓘ

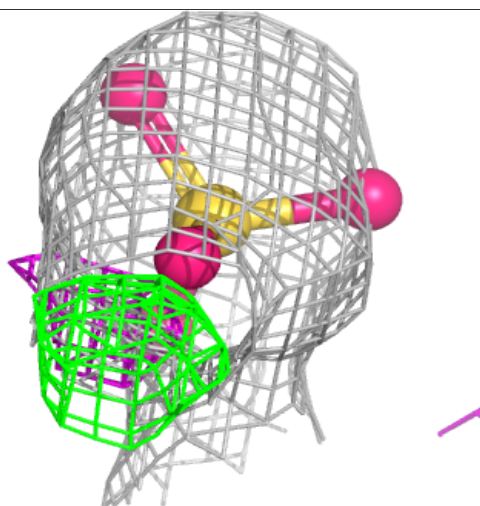
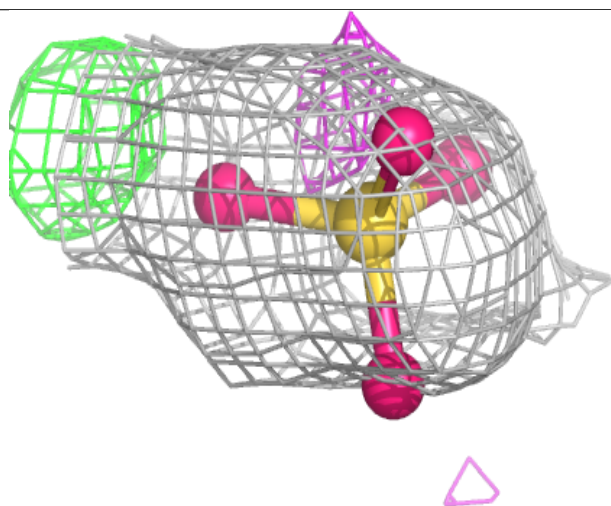
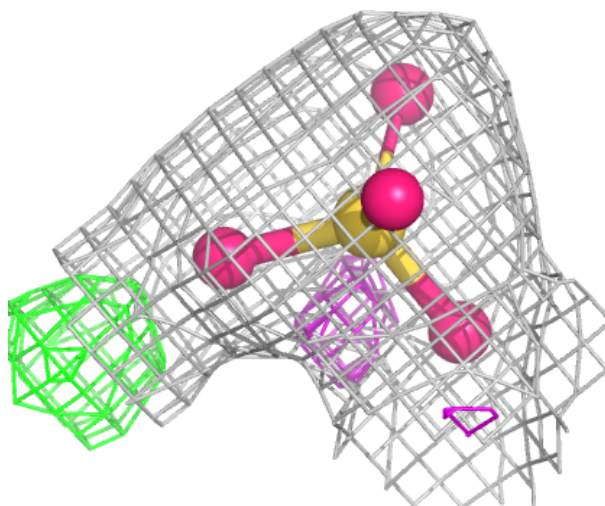
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	A	1307	5/5	0.65	0.15	90,92,100,104	0
4	SO4	B	1309	5/5	0.78	0.17	65,72,76,78	0
4	SO4	A	1309	5/5	0.81	0.15	80,86,92,98	0
4	SO4	B	1310	5/5	0.81	0.11	59,66,76,84	0
4	SO4	A	1308	5/5	0.83	0.16	55,65,77,89	0
4	SO4	B	1307	5/5	0.85	0.25	38,42,62,64	0
4	SO4	A	1304	5/5	0.87	0.12	58,59,60,79	0
2	NAP	A	1301	48/48	0.88	0.14	23,39,63,69	0
4	SO4	A	1306	5/5	0.88	0.10	51,61,63,72	0
4	SO4	B	1308	5/5	0.90	0.09	47,51,67,69	0
4	SO4	B	1303	5/5	0.90	0.12	47,50,52,59	0
4	SO4	A	1303	5/5	0.90	0.11	49,61,62,63	0
2	NAP	B	1301	48/48	0.92	0.09	23,32,47,61	0
4	SO4	B	1305	5/5	0.92	0.14	47,51,57,59	0
4	SO4	B	1304	5/5	0.93	0.08	47,48,61,68	0
3	GOL	B	1302	6/6	0.94	0.07	23,28,29,30	0
4	SO4	B	1306	5/5	0.94	0.15	50,50,57,61	0
4	SO4	A	1305	5/5	0.94	0.17	44,52,54,63	0
3	GOL	A	1302	6/6	0.95	0.07	25,27,30,31	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.

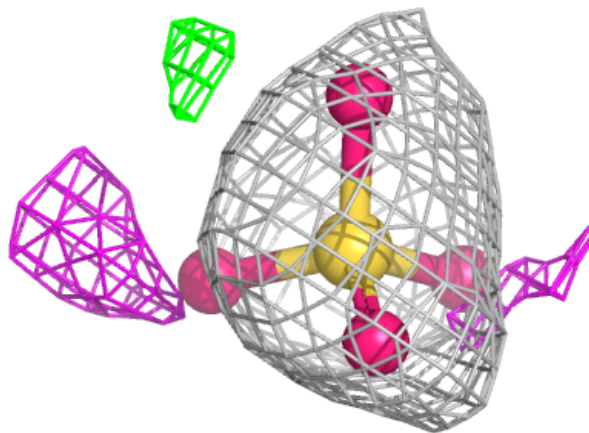
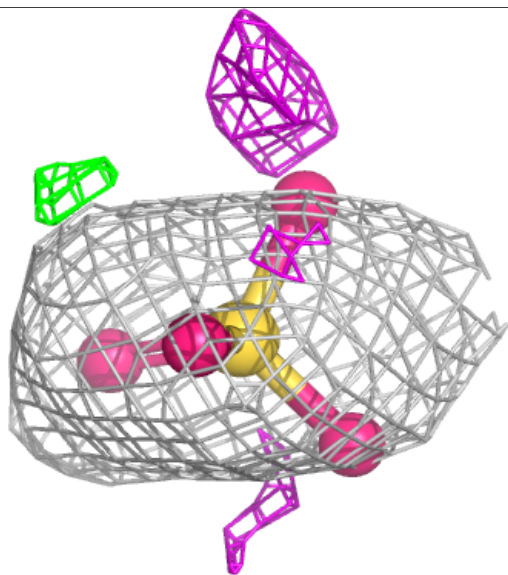
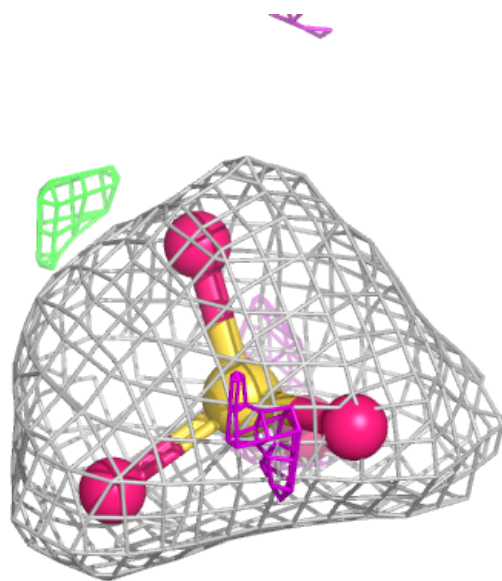
Electron density around SO4 A 1307:

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



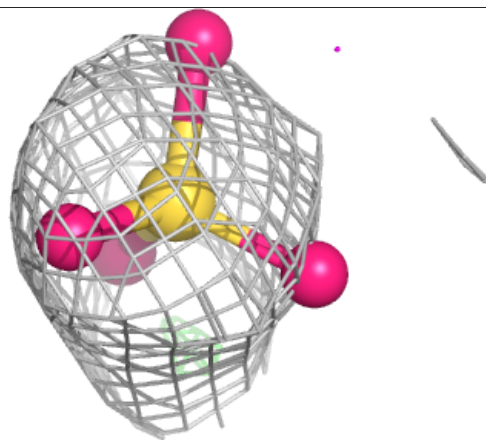
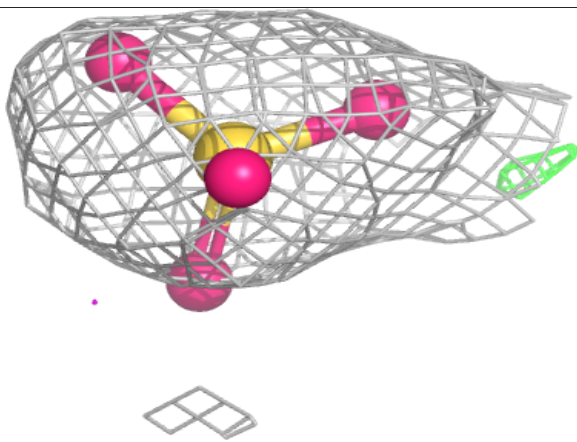
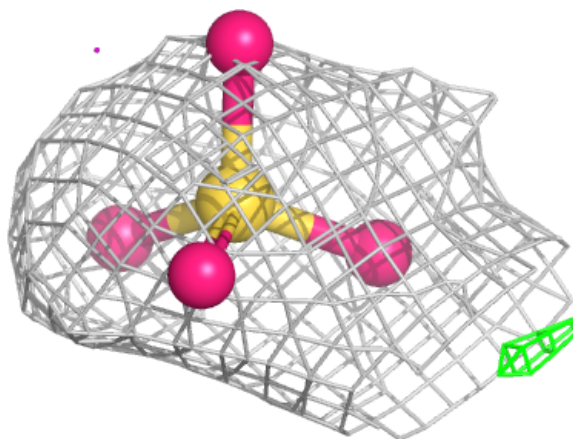
Electron density around SO4 B 1309:

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and green (positive)



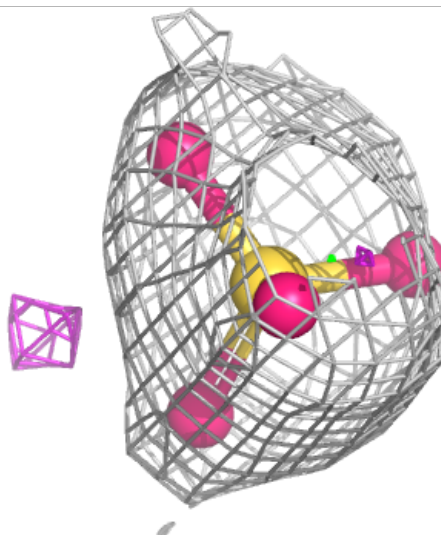
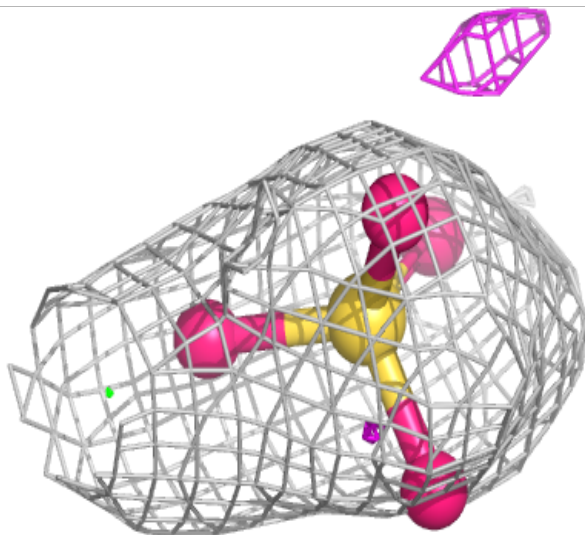
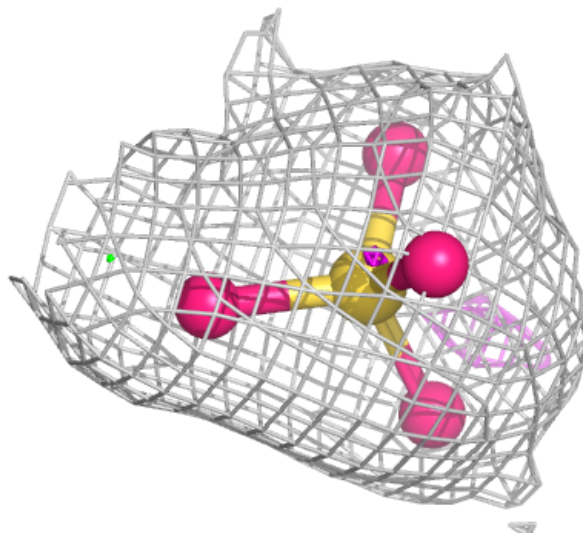
Electron density around SO4 A 1309:

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and green (positive)



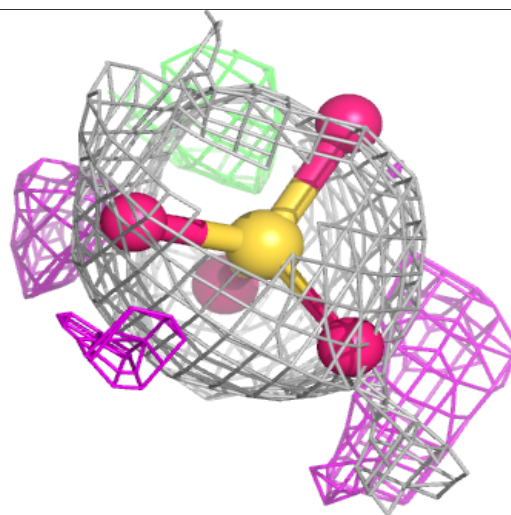
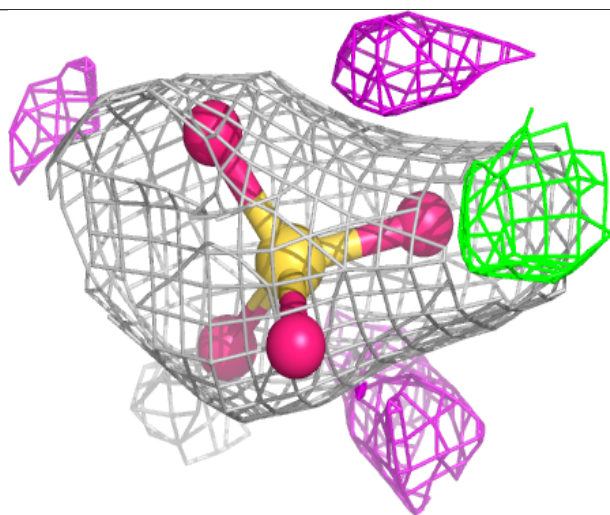
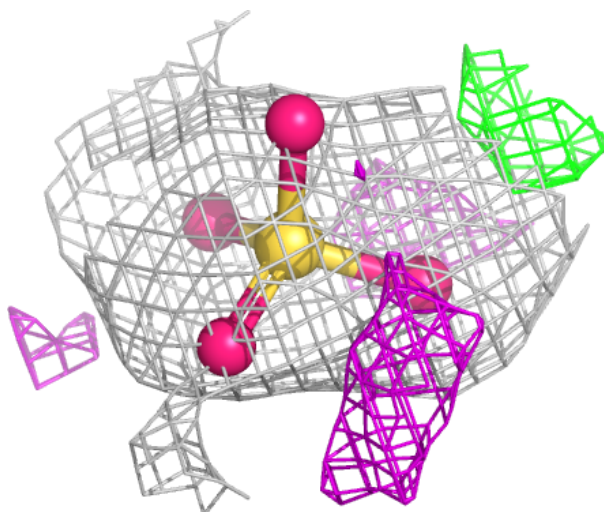
Electron density around SO4 B 1310:

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and green (positive)



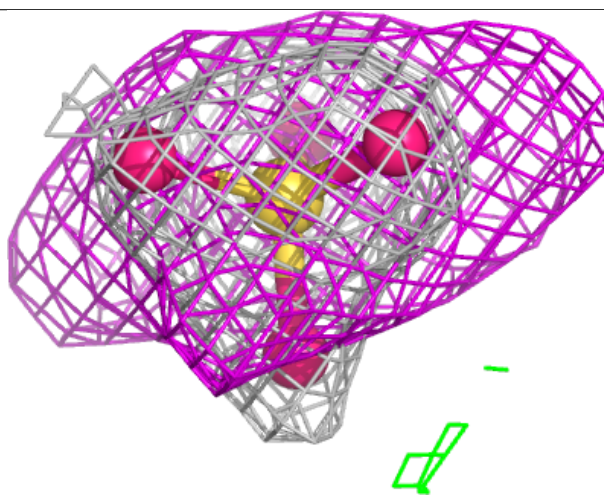
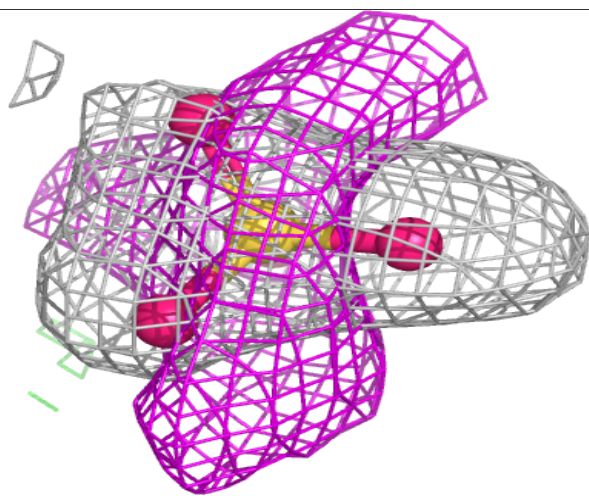
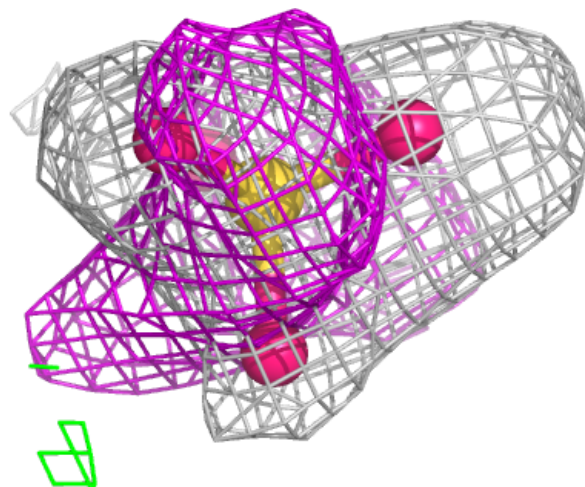
Electron density around SO4 A 1308:

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and green (positive)



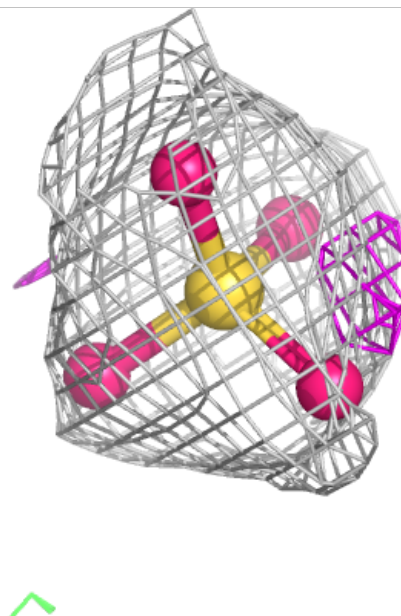
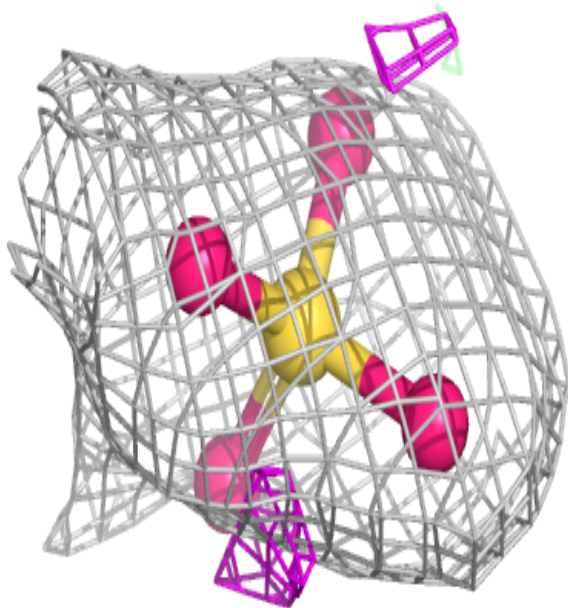
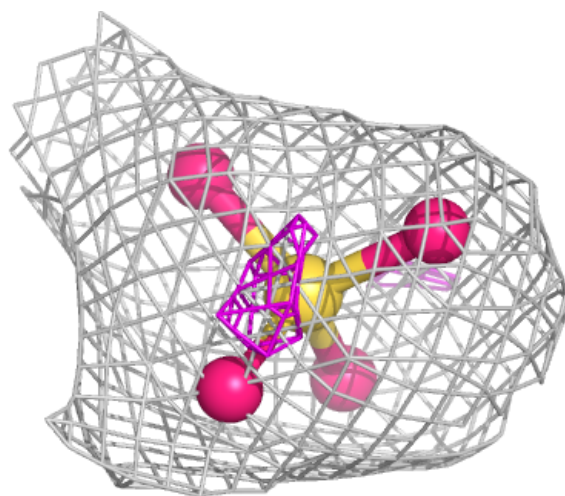
Electron density around SO4 B 1307:

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



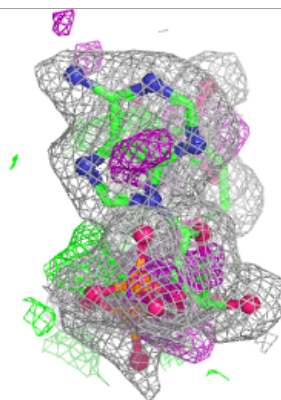
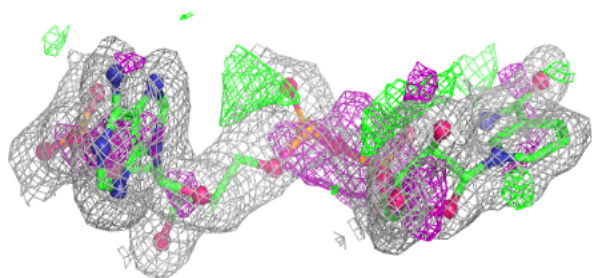
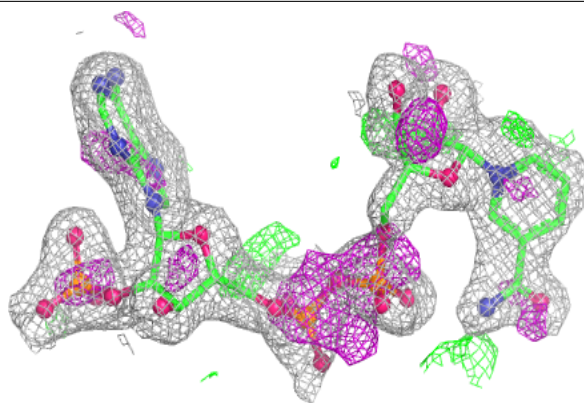
Electron density around SO4 A 1304:

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and green (positive)

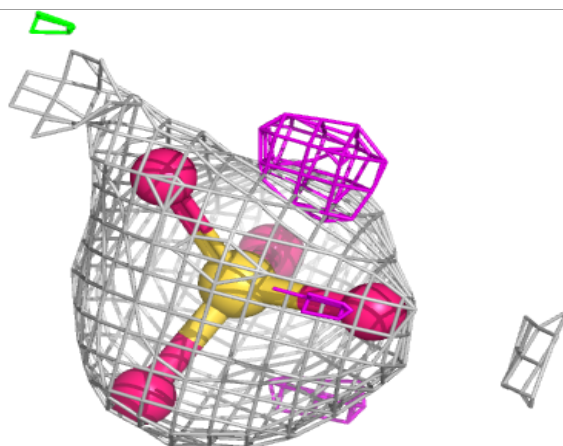
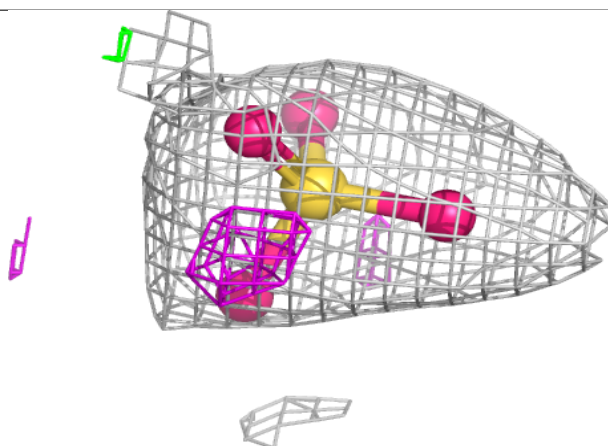
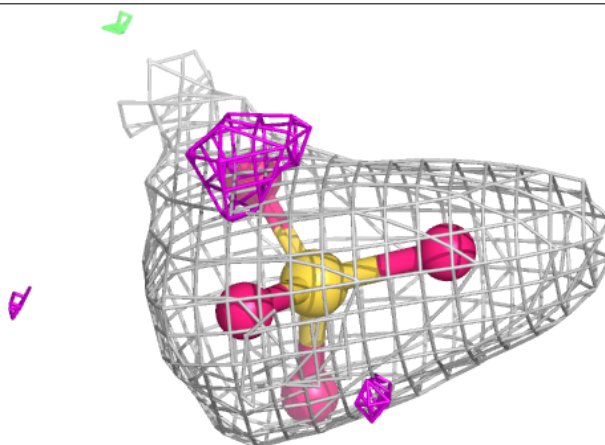


Electron density around NAP A 1301:

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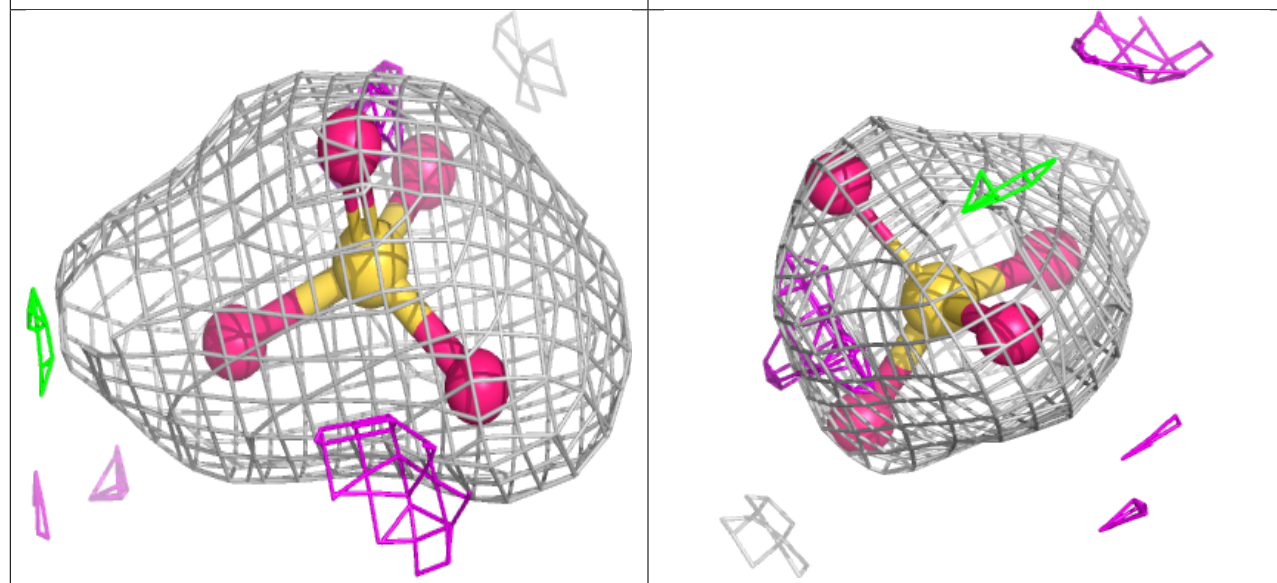
**Electron density around SO4 A 1306:**

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and green (positive)



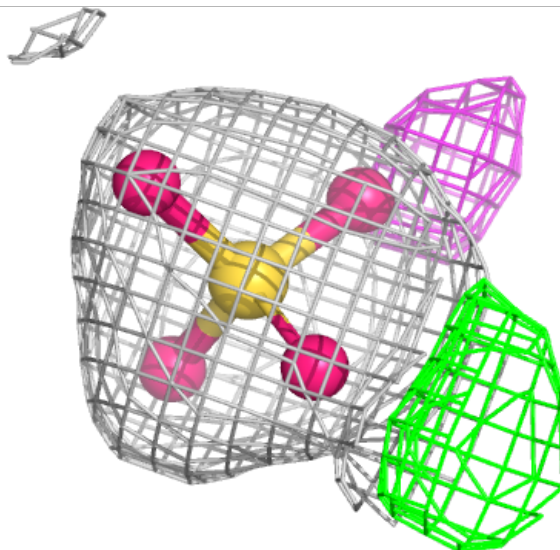
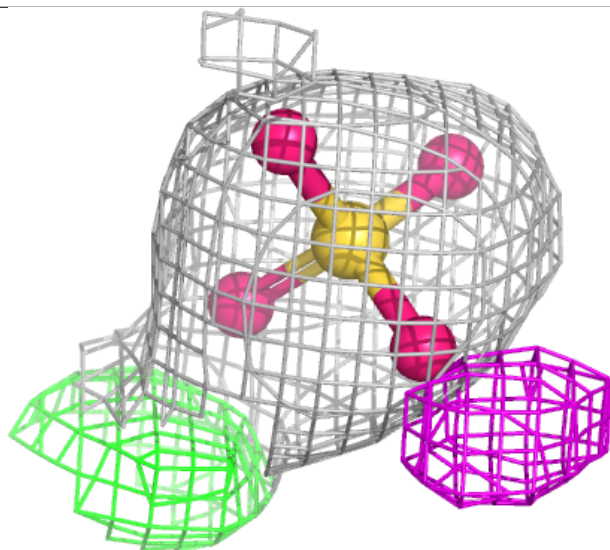
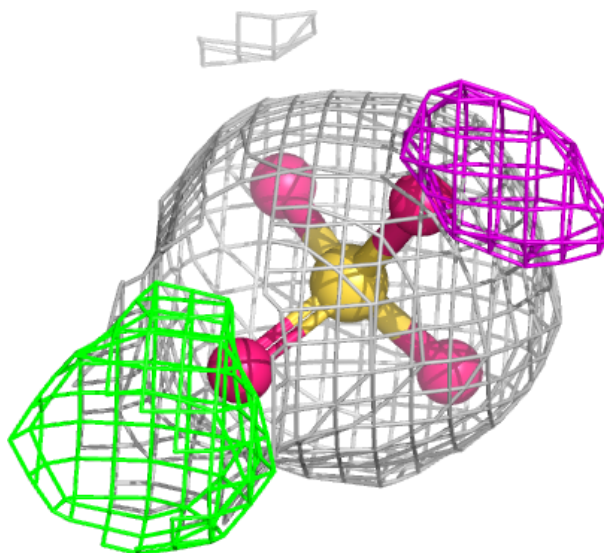
Electron density around SO4 B 1308:

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and green (positive)



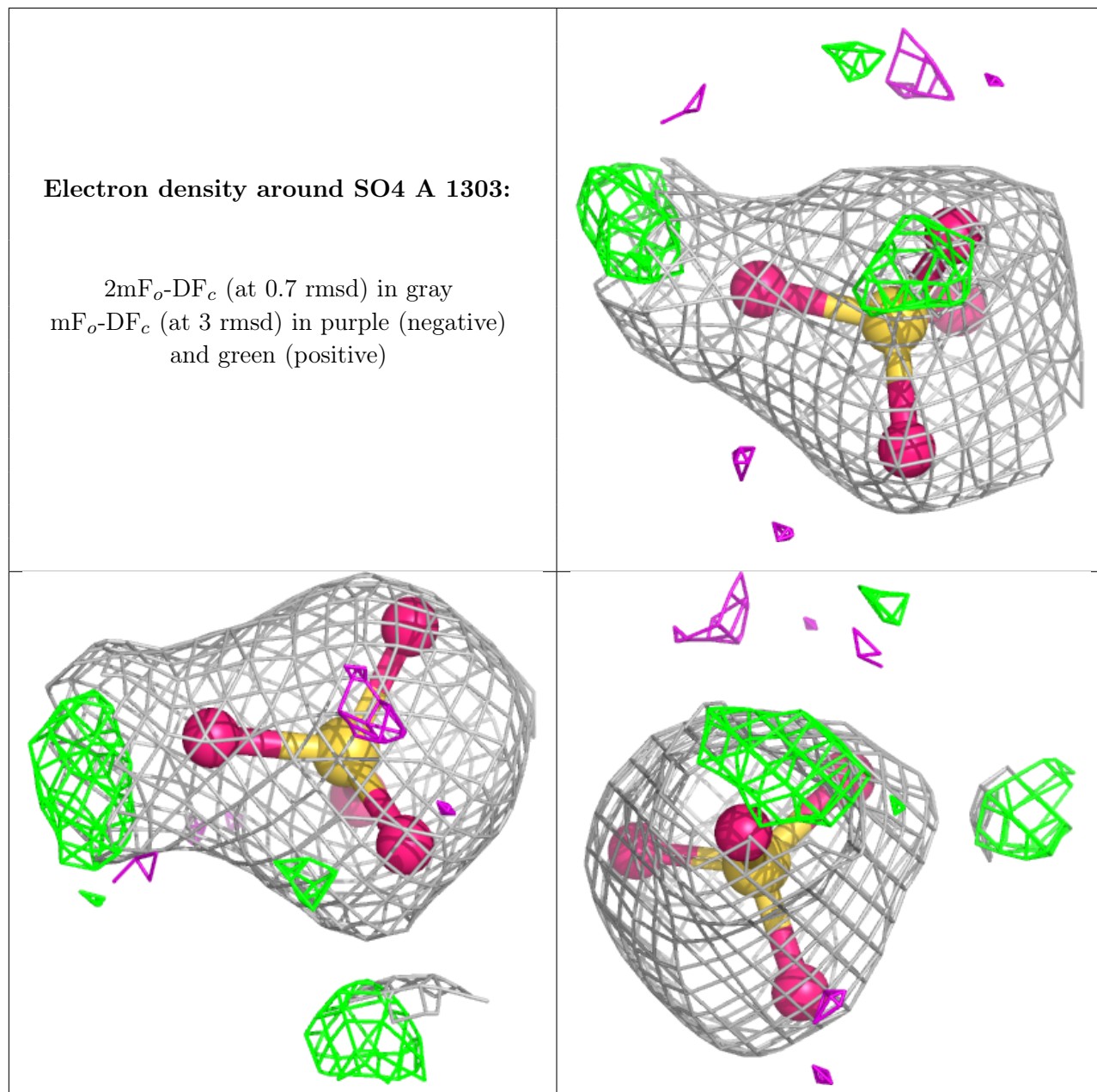
Electron density around SO4 B 1303:

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and green (positive)



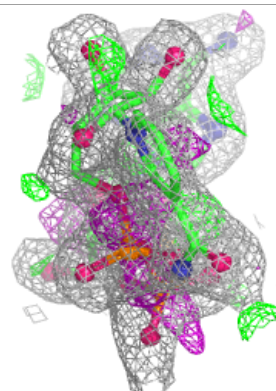
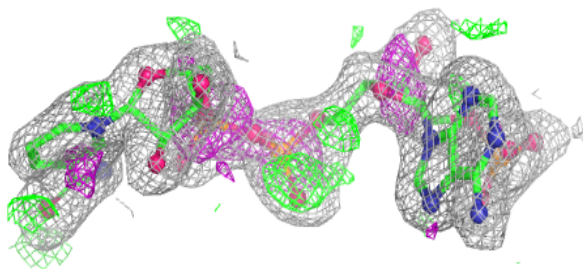
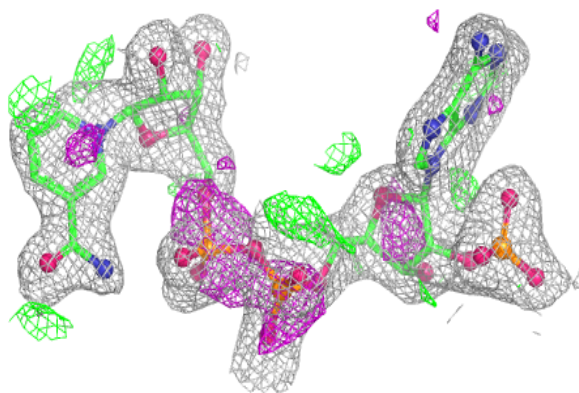
Electron density around SO4 A 1303:

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and green (positive)



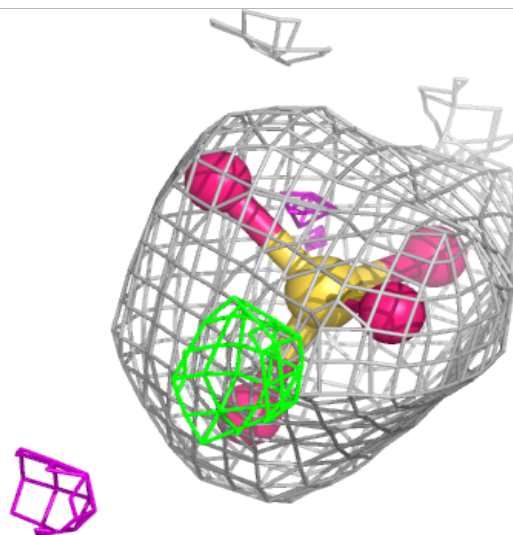
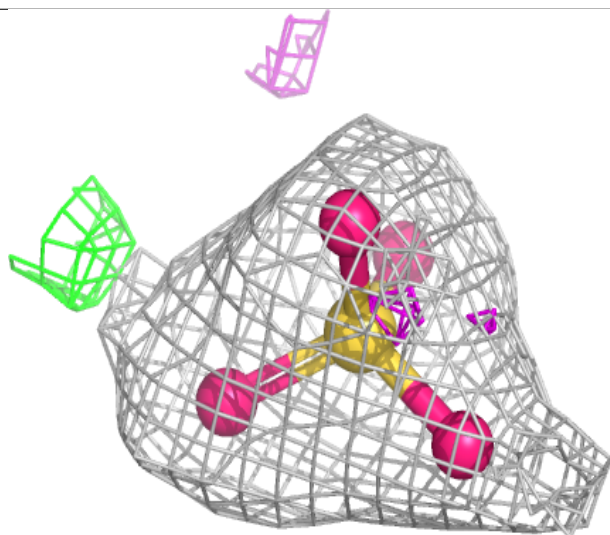
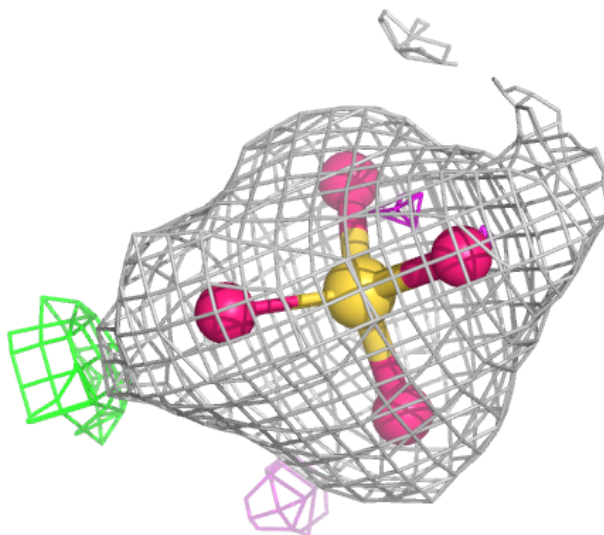
Electron density around NAP B 1301:

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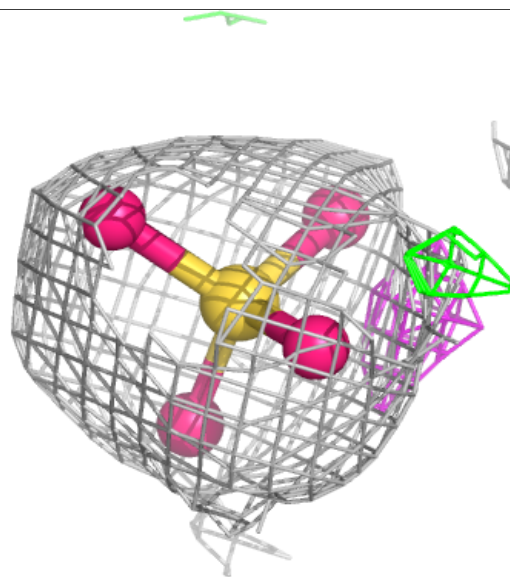
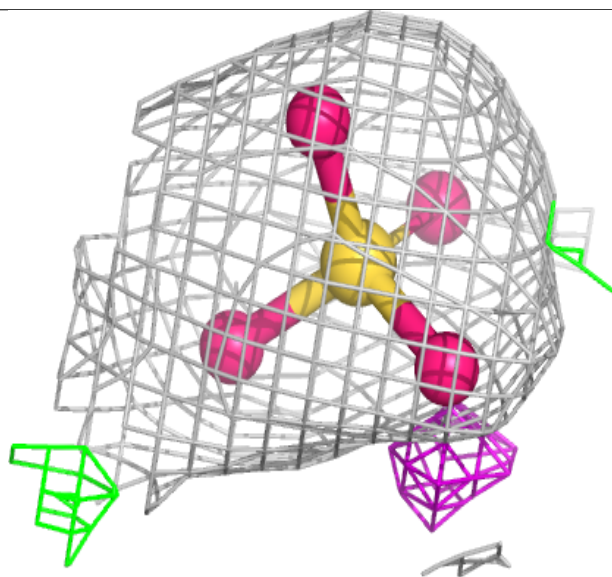
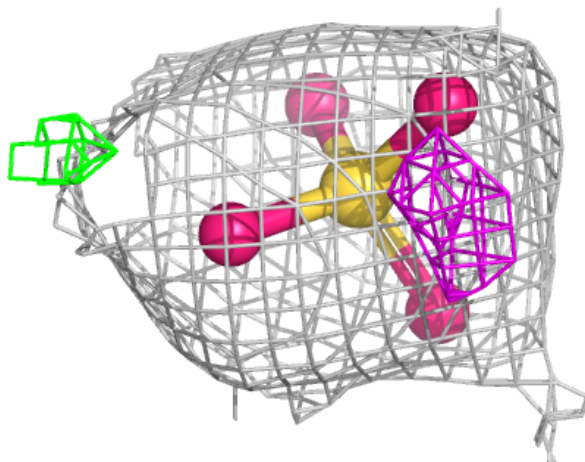
Electron density around SO4 B 1305:

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and green (positive)



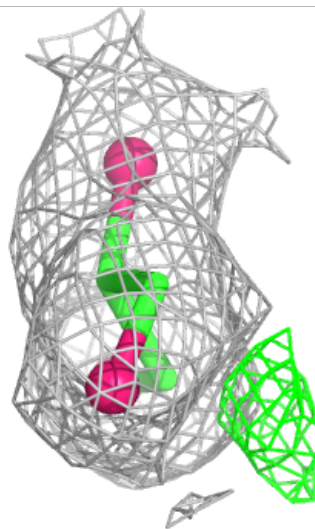
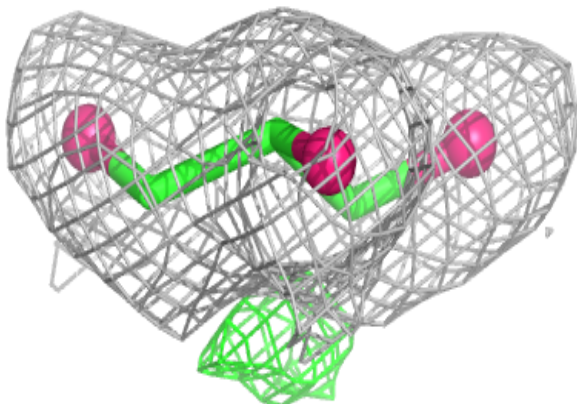
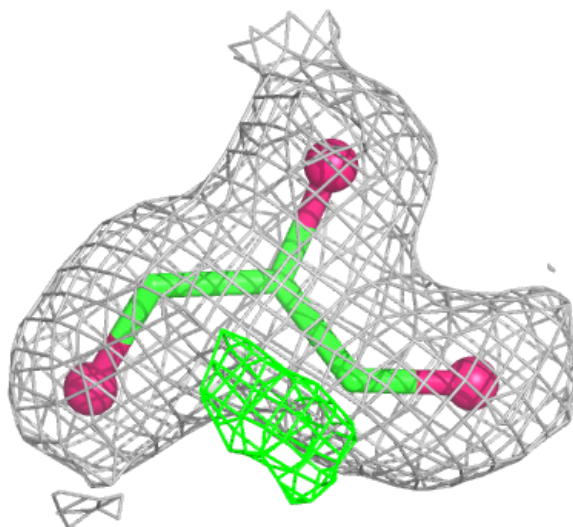
Electron density around SO4 B 1304:

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and green (positive)



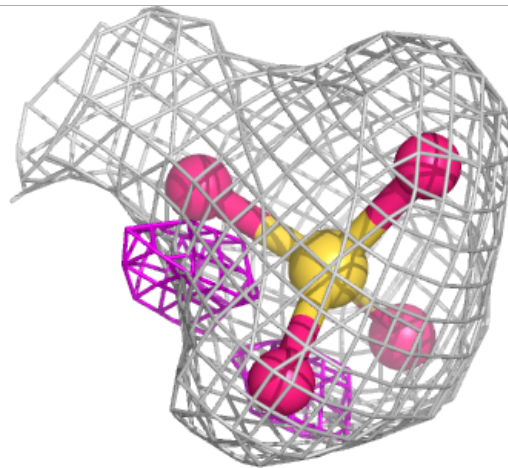
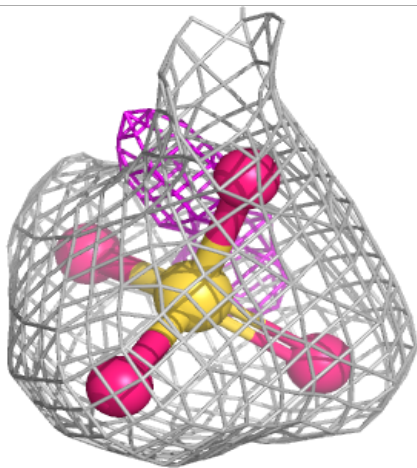
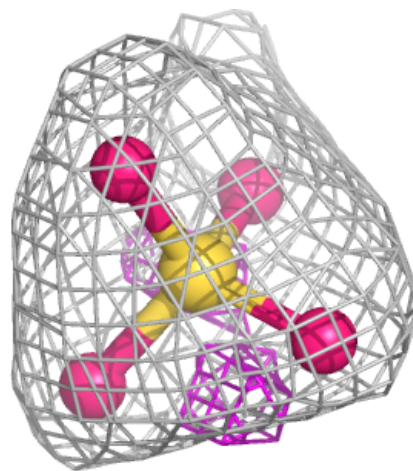
Electron density around GOL B 1302:

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



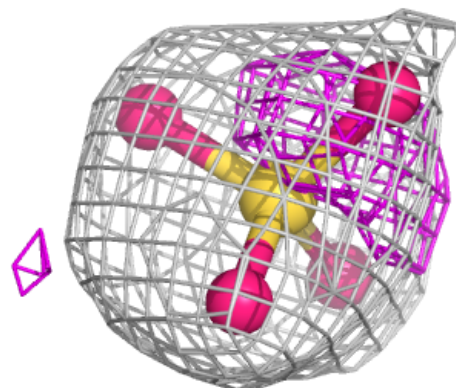
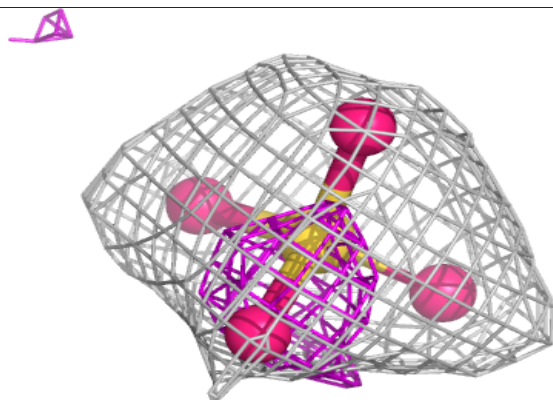
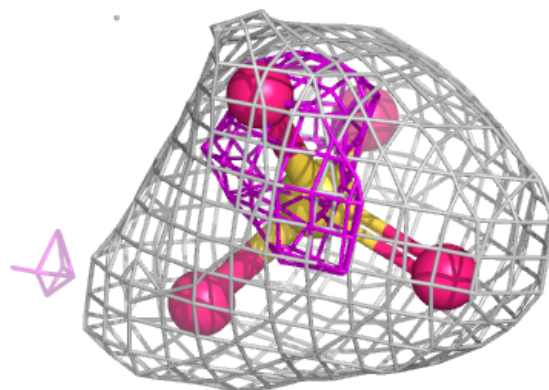
Electron density around SO4 B 1306:

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and green (positive)



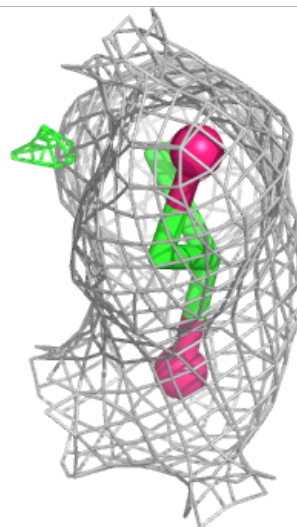
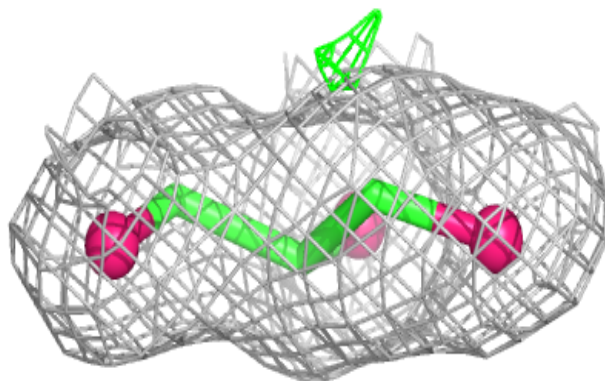
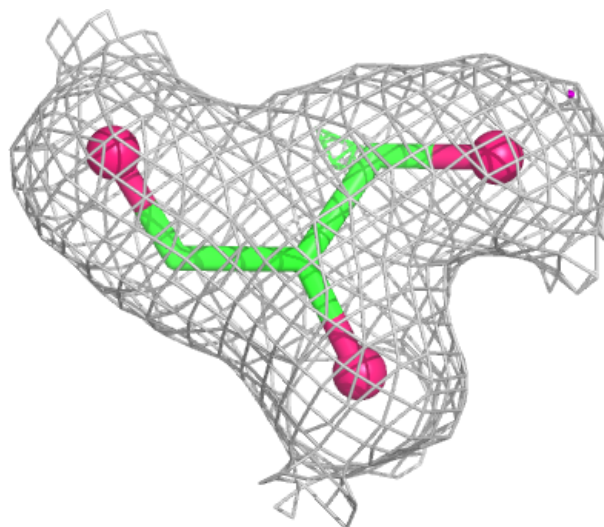
Electron density around SO4 A 1305:

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and green (positive)



Electron density around GOL 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.