



Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2022 – 06:09 PM JST

PDB ID : 7X8K
Title : Arabidopsis GDP-D-mannose pyrophosphorylase (VTC1) structure (product-bound)
Authors : Zhao, S.; Zhang, C.; Liu, L.
Deposited on : 2022-03-13
Resolution : 3.00 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 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 : 2.28.1
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) : 2.28.1

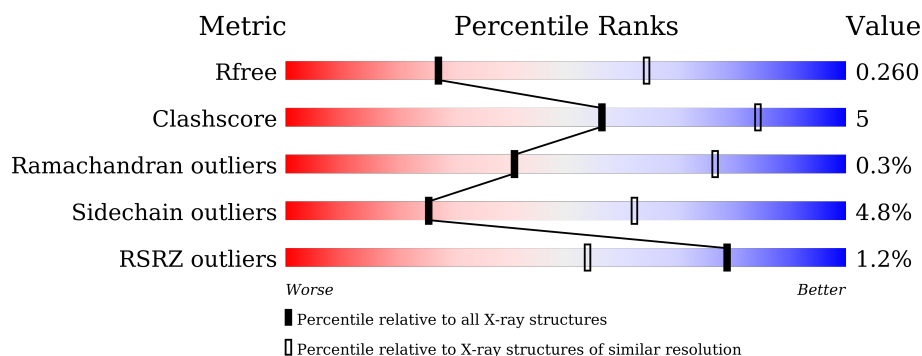
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	376	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 84%; background-color: green;"></div> <div style="width: 13%; background-color: yellow;"></div> <div style="width: 1%; background-color: orange;"></div> <div style="width: 0%; background-color: grey;"></div> </div> <p>2% 84% 13% ..</p>
1	B	376	<div> <div style="width: 0%; background-color: red;"></div> <div style="width: 82%; background-color: green;"></div> <div style="width: 14%; background-color: yellow;"></div> <div style="width: 2%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <p>82% 14% ..</p>
1	C	376	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 77%; background-color: green;"></div> <div style="width: 16%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <p>2% 77% 16% • 6%</p>
1	D	376	<div> <div style="width: 2%; background-color: red;"></div> <div style="width: 81%; background-color: green;"></div> <div style="width: 12%; background-color: yellow;"></div> <div style="width: 3%; background-color: orange;"></div> <div style="width: 2%; background-color: grey;"></div> </div> <p>2% 81% 12% • 6%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	C	405	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11191 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 Mannose-1-phosphate guanylyltransferase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2783	1788	466	513	16			
1	B	367	Total	C	N	O	S	0	0	0
			2805	1802	470	517	16			
1	C	355	Total	C	N	O	S	0	0	0
			2717	1746	456	500	15			
1	D	355	Total	C	N	O	S	0	0	0
			2697	1728	455	499	15			

There are 60 discrepancies between the modelled and reference sequences:

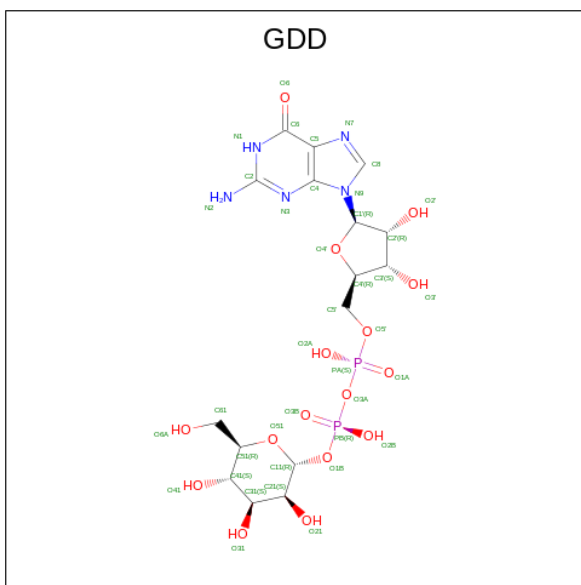
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	initiating methionine	UNP O22287
A	0	GLY	-	expression tag	UNP O22287
A	362	LYS	-	expression tag	UNP O22287
A	363	LEU	-	expression tag	UNP O22287
A	364	ALA	-	expression tag	UNP O22287
A	365	ALA	-	expression tag	UNP O22287
A	366	ALA	-	expression tag	UNP O22287
A	367	LEU	-	expression tag	UNP O22287
A	368	GLU	-	expression tag	UNP O22287
A	369	HIS	-	expression tag	UNP O22287
A	370	HIS	-	expression tag	UNP O22287
A	371	HIS	-	expression tag	UNP O22287
A	372	HIS	-	expression tag	UNP O22287
A	373	HIS	-	expression tag	UNP O22287
A	374	HIS	-	expression tag	UNP O22287
B	-1	MET	-	initiating methionine	UNP O22287
B	0	GLY	-	expression tag	UNP O22287
B	362	LYS	-	expression tag	UNP O22287
B	363	LEU	-	expression tag	UNP O22287
B	364	ALA	-	expression tag	UNP O22287
B	365	ALA	-	expression tag	UNP O22287

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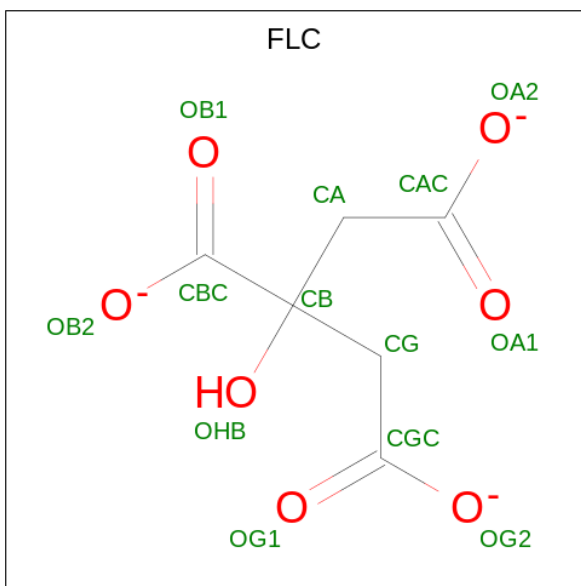
Chain	Residue	Modelled	Actual	Comment	Reference
B	366	ALA	-	expression tag	UNP O22287
B	367	LEU	-	expression tag	UNP O22287
B	368	GLU	-	expression tag	UNP O22287
B	369	HIS	-	expression tag	UNP O22287
B	370	HIS	-	expression tag	UNP O22287
B	371	HIS	-	expression tag	UNP O22287
B	372	HIS	-	expression tag	UNP O22287
B	373	HIS	-	expression tag	UNP O22287
B	374	HIS	-	expression tag	UNP O22287
C	-1	MET	-	initiating methionine	UNP O22287
C	0	GLY	-	expression tag	UNP O22287
C	362	LYS	-	expression tag	UNP O22287
C	363	LEU	-	expression tag	UNP O22287
C	364	ALA	-	expression tag	UNP O22287
C	365	ALA	-	expression tag	UNP O22287
C	366	ALA	-	expression tag	UNP O22287
C	367	LEU	-	expression tag	UNP O22287
C	368	GLU	-	expression tag	UNP O22287
C	369	HIS	-	expression tag	UNP O22287
C	370	HIS	-	expression tag	UNP O22287
C	371	HIS	-	expression tag	UNP O22287
C	372	HIS	-	expression tag	UNP O22287
C	373	HIS	-	expression tag	UNP O22287
C	374	HIS	-	expression tag	UNP O22287
D	-1	MET	-	initiating methionine	UNP O22287
D	0	GLY	-	expression tag	UNP O22287
D	362	LYS	-	expression tag	UNP O22287
D	363	LEU	-	expression tag	UNP O22287
D	364	ALA	-	expression tag	UNP O22287
D	365	ALA	-	expression tag	UNP O22287
D	366	ALA	-	expression tag	UNP O22287
D	367	LEU	-	expression tag	UNP O22287
D	368	GLU	-	expression tag	UNP O22287
D	369	HIS	-	expression tag	UNP O22287
D	370	HIS	-	expression tag	UNP O22287
D	371	HIS	-	expression tag	UNP O22287
D	372	HIS	-	expression tag	UNP O22287
D	373	HIS	-	expression tag	UNP O22287
D	374	HIS	-	expression tag	UNP O22287

- Molecule 2 is GUANOSINE-5'-DIPHOSPHATE-ALPHA-D-MANNOSE (three-letter code: GDD) (formula: C₁₆H₂₅N₅O₁₆P₂) (labeled as "Ligand of Interest" by depositor).



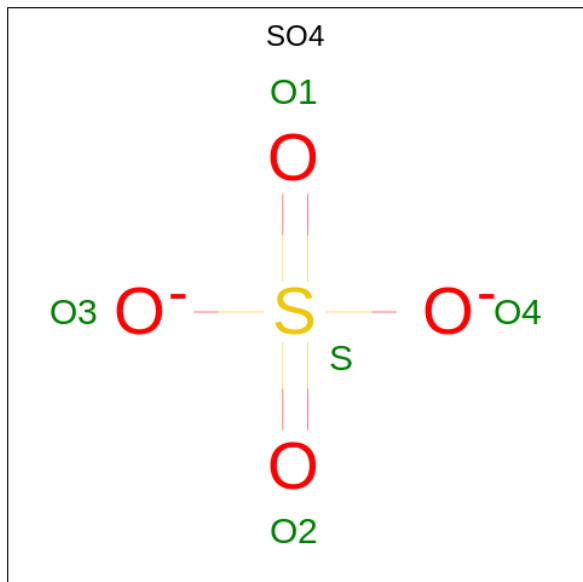
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	A	1	Total 39	C 16	N 5	O 16	P 2	0	0

- Molecule 3 is CITRATE ANION (three-letter code: FLC) (formula: $\text{C}_6\text{H}_5\text{O}_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 13 6 7	0	0
3	C	1	Total C O 13 6 7	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



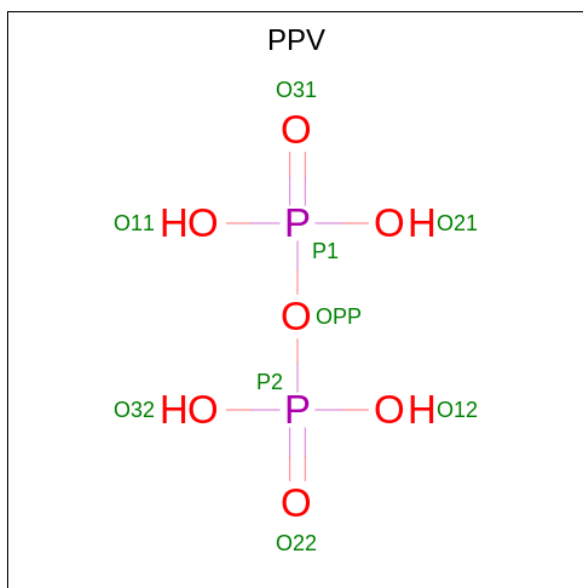
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		

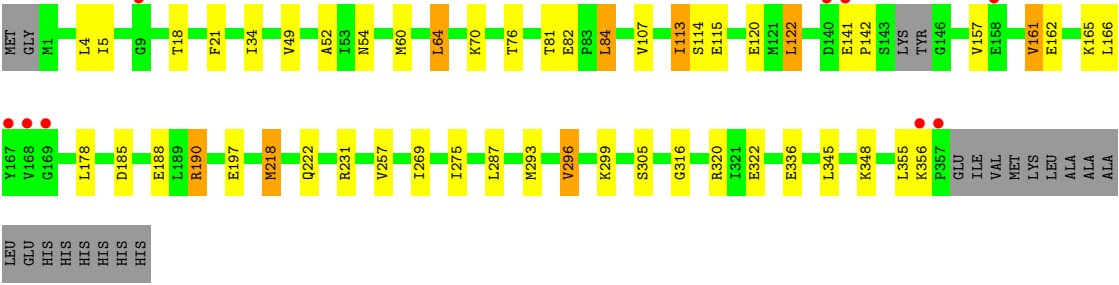
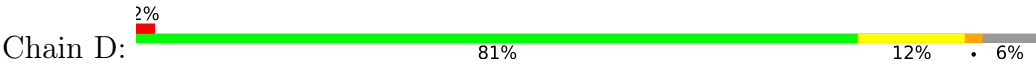
- Molecule 5 is PYROPHOSPHATE (three-letter code: PPV) (formula: $\text{H}_4\text{O}_7\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	D	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is water.

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



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	185.11Å 185.11Å 371.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.82 – 3.00 30.82 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.82-3.00) 99.2 (30.82-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.234 , 0.260 0.233 , 0.260	Depositor DCC
R_{free} test set	2443 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.094	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11191	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FLC, GDD, SO4, PPV

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	0.25	0/2836	0.46	0/3842
1	B	0.25	0/2859	0.44	0/3872
1	C	0.25	0/2770	0.47	0/3751
1	D	0.25	0/2748	0.48	0/3723
All	All	0.25	0/11213	0.46	0/15188

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2783	0	2877	27	0
1	B	2805	0	2908	31	0
1	C	2717	0	2812	38	0
1	D	2697	0	2778	24	0
2	A	39	0	23	1	0
3	A	13	0	5	1	0
3	C	13	0	5	3	0
4	A	30	0	0	0	0
4	B	25	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	20	0	0	1	0
4	D	20	0	0	1	0
5	B	9	0	0	0	0
5	D	9	0	0	0	0
6	A	6	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	D	2	0	0	0	0
All	All	11191	0	11408	113	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 5.

All (113) 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)
2:A:401:GDD:O4'	2:A:401:GDD:C1'	1.63	1.23
1:C:11:GLY:HA2	3:C:401:FLC:HG1	1.52	0.90
1:A:301:HIS:HD2	1:B:301:HIS:HD2	1.28	0.81
1:A:11:GLY:HA2	3:A:402:FLC:HG1	1.67	0.76
1:C:156:ARG:HH12	1:C:206:GLN:HB3	1.54	0.72
1:A:84:LEU:HB3	1:A:88:GLY:HA3	1.70	0.71
1:B:84:LEU:HB3	1:B:88:GLY:HA3	1.71	0.70
1:B:143:SER:HA	1:B:164:PRO:HD2	1.73	0.70
1:A:70:LYS:NZ	1:C:349:GLU:OE2	2.25	0.68
1:C:13:ARG:HD2	1:C:222:GLN:HG2	1.76	0.67
1:A:140:ASP:OD1	1:A:140:ASP:N	2.21	0.65
1:D:113:ILE:HD11	1:D:218:MET:HB3	1.78	0.65
1:C:269:ILE:HG23	1:C:287:LEU:HB2	1.79	0.64
1:C:341:GLY:HA3	1:C:357:PRO:HA	1.80	0.63
1:C:161:VAL:HG21	1:C:168:VAL:HG21	1.79	0.63
1:D:188:GLU:HB2	1:D:190:ARG:HG2	1.80	0.63
1:B:356:LYS:HE3	1:B:358:GLU:HG3	1.83	0.61
1:D:5:ILE:HG21	1:D:34:ILE:HD11	1.84	0.60
1:C:84:LEU:HB3	1:C:88:GLY:HA3	1.84	0.58
1:A:13:ARG:HD2	1:A:222:GLN:HG2	1.84	0.58
1:A:282:GLU:OE2	1:A:297:ARG:NH1	2.37	0.57
1:C:12:THR:H	3:C:401:FLC:HA1	1.69	0.57
1:C:336:GLU:O	1:D:320:ARG:NH2	2.37	0.57
1:D:122:LEU:HD13	1:D:178:LEU:HD21	1.86	0.56
1:C:320:ARG:NH2	1:D:336:GLU:O	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:SER:OG	1:D:115:GLU:N	2.39	0.56
1:B:54:ASN:ND2	1:B:80:GLU:OE1	2.39	0.55
1:B:42:LYS:NZ	1:B:71:LEU:O	2.38	0.54
1:D:82:GLU:O	1:D:84:LEU:HD22	2.08	0.54
1:C:5:ILE:HG21	1:C:34:ILE:HD11	1.90	0.53
1:B:11:GLY:H	1:B:23:LYS:HB2	1.74	0.53
1:B:299:LYS:HD2	1:B:316:GLY:HA2	1.91	0.53
1:A:94:ARG:HG3	1:A:184:LEU:HD13	1.91	0.52
1:A:188:GLU:HB2	1:A:190:ARG:HG2	1.90	0.52
1:D:190:ARG:NH2	1:D:197:GLU:OE1	2.42	0.52
1:A:32:PRO:HD2	1:A:35:LEU:HD12	1.91	0.51
1:D:299:LYS:HD2	1:D:316:GLY:HA2	1.93	0.51
1:C:257:VAL:HG22	1:C:275:ILE:HD12	1.92	0.51
1:C:332:HIS:HB2	1:C:349:GLU:HG2	1.92	0.51
1:C:263:ILE:HD11	1:C:275:ILE:HD13	1.91	0.51
1:B:5:ILE:HG21	1:B:34:ILE:HD11	1.92	0.50
1:C:120:GLU:N	1:C:120:GLU:OE1	2.43	0.50
1:C:122:LEU:HD13	1:C:178:LEU:HD21	1.94	0.50
1:D:142:PRO:HB3	1:D:165:LYS:HD3	1.92	0.50
1:D:257:VAL:HG22	1:D:275:ILE:HD12	1.92	0.50
1:D:345:LEU:H	1:D:348:LYS:HZ1	1.58	0.49
1:D:269:ILE:HD12	1:D:287:LEU:HD12	1.95	0.49
1:C:17:LEU:HD11	1:C:308:ILE:HG21	1.95	0.48
1:C:139:VAL:HG22	1:C:140:ASP:H	1.77	0.48
1:C:107:VAL:HB	1:C:177:TYR:HB2	1.95	0.48
1:B:269:ILE:HG23	1:B:287:LEU:HB2	1.96	0.48
1:A:336:GLU:O	1:B:320:ARG:NH2	2.47	0.47
1:B:32:PRO:HD2	1:B:35:LEU:HD12	1.96	0.47
1:D:4:LEU:HD11	1:D:52:ALA:HB2	1.95	0.47
1:A:355:LEU:C	1:A:357:PRO:HD3	2.34	0.47
1:C:10:PHE:HZ	1:C:15:ARG:HE	1.63	0.47
1:A:286:ARG:HB2	1:B:318:TRP:CE2	2.50	0.47
1:C:138:LYS:HE2	1:C:138:LYS:HB2	1.60	0.47
1:A:305:SER:O	1:A:322:GLU:HA	2.15	0.46
1:B:136:VAL:HG12	1:B:212:VAL:HA	1.96	0.46
1:B:292:VAL:HG13	1:B:296:VAL:HG22	1.97	0.46
1:A:257:VAL:HG22	1:A:275:ILE:HD12	1.97	0.46
1:D:120:GLU:OE1	1:D:120:GLU:N	2.46	0.46
1:B:350:ILE:HD12	1:B:354:ILE:HD11	1.98	0.46
1:C:9:GLY:H	3:C:401:FLC:CBC	2.29	0.45
1:D:269:ILE:HG23	1:D:287:LEU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:MET:O	1:C:296:VAL:HG13	2.16	0.45
1:C:305:SER:O	1:C:322:GLU:HA	2.16	0.44
1:C:23:LYS:HB3	1:C:23:LYS:HE3	1.77	0.44
1:D:231:ARG:NE	4:D:501:SO4:O4	2.39	0.44
1:C:14:LEU:HD12	1:C:23:LYS:HG2	2.00	0.43
1:B:257:VAL:HG22	1:B:275:ILE:HD12	2.01	0.43
1:D:305:SER:O	1:D:322:GLU:HA	2.19	0.43
1:A:87:ALA:HB2	1:A:194:ILE:HB	2.00	0.43
1:B:356:LYS:O	1:B:360:VAL:HG23	2.18	0.43
1:A:355:LEU:HB3	1:B:363:LEU:HD13	2.00	0.43
1:A:301:HIS:HD2	1:B:301:HIS:CD2	2.20	0.43
1:B:132:ALA:HB1	1:B:179:LEU:HD12	2.01	0.43
1:C:154:THR:HB	1:C:156:ARG:HG3	2.01	0.43
1:C:238:ARG:HE	1:C:245:LEU:HD12	1.84	0.43
1:A:293:MET:O	1:A:296:VAL:HG13	2.18	0.43
1:C:142:PRO:HB2	1:C:164:PRO:HG2	2.00	0.43
1:A:107:VAL:HB	1:A:177:TYR:HB2	2.01	0.43
1:B:226:TYR:HB2	1:B:308:ILE:HD11	2.01	0.42
1:C:292:VAL:HG13	1:C:296:VAL:HG22	2.00	0.42
1:C:18:THR:HA	1:C:21:PHE:O	2.19	0.42
1:B:293:MET:O	1:B:296:VAL:HG13	2.19	0.42
1:C:4:LEU:HD11	1:C:52:ALA:HB2	2.02	0.42
1:B:35:LEU:HD21	1:B:67:PHE:CG	2.54	0.42
1:D:70:LYS:HE3	1:D:70:LYS:HB2	1.83	0.42
1:D:293:MET:O	1:D:296:VAL:HG13	2.20	0.42
1:A:309:ILE:HG23	1:A:313:SER:HB2	2.02	0.42
1:B:358:GLU:H	1:B:358:GLU:HG2	1.36	0.42
1:A:141:GLU:O	1:A:143:SER:N	2.51	0.41
1:C:179:LEU:HB3	1:C:183:VAL:HG21	2.01	0.41
1:D:18:THR:HA	1:D:21:PHE:O	2.20	0.41
1:A:122:LEU:HD12	1:A:178:LEU:HD21	2.02	0.41
1:B:119:LYS:HE3	1:B:119:LYS:HB3	1.88	0.41
1:B:107:VAL:HB	1:B:177:TYR:HB2	2.01	0.41
1:D:165:LYS:HG3	1:D:166:LEU:H	1.86	0.41
1:A:238:ARG:O	1:A:242:PRO:HG3	2.21	0.41
1:B:252:VAL:O	1:B:270:GLY:HA3	2.21	0.41
1:D:60:MET:O	1:D:64:LEU:HD22	2.21	0.41
1:A:84:LEU:HB2	1:A:89:PRO:HD3	2.01	0.40
1:A:131:GLU:OE1	1:A:186:LYS:NZ	2.46	0.40
1:B:4:LEU:HD23	1:B:90:LEU:HD22	2.03	0.40
1:B:224:ARG:HG3	1:B:324:MET:SD	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:ARG:NE	4:C:402:SO4:O2	2.54	0.40
1:C:240:LYS:HE2	1:C:240:LYS:HB3	1.91	0.40
1:A:224:ARG:HD3	1:A:324:MET:HG3	2.04	0.40
1:B:87:ALA:O	1:B:90:LEU:HB2	2.21	0.40
1:C:87:ALA:HB2	1:C:194:ILE:HB	2.02	0.40
1:C:16:PRO:HD3	1:C:343:VAL:HG13	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	361/376 (96%)	343 (95%)	16 (4%)	2 (1%)	25	64
1	B	365/376 (97%)	349 (96%)	15 (4%)	1 (0%)	41	76
1	C	351/376 (93%)	336 (96%)	15 (4%)	0	100	100
1	D	351/376 (93%)	329 (94%)	21 (6%)	1 (0%)	41	76
All	All	1428/1504 (95%)	1357 (95%)	67 (5%)	4 (0%)	41	76

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	161	VAL
1	B	11	GLY
1	A	167	TYR
1	A	142	PRO

5.3.2 Protein sidechains [i](#)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/321 (96%)	298 (97%)	9 (3%)	42	76
1	B	310/321 (97%)	295 (95%)	15 (5%)	25	62
1	C	302/321 (94%)	287 (95%)	15 (5%)	24	60
1	D	298/321 (93%)	278 (93%)	20 (7%)	16	49
All	All	1217/1284 (95%)	1158 (95%)	59 (5%)	25	62

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	69	THR
1	A	140	ASP
1	A	150	MET
1	A	158	GLU
1	A	161	VAL
1	A	163	LYS
1	A	179	LEU
1	A	296	VAL
1	B	63	PHE
1	B	119	LYS
1	B	122	LEU
1	B	136	VAL
1	B	139	VAL
1	B	153	SER
1	B	158	GLU
1	B	161	VAL
1	B	166	LEU
1	B	179	LEU
1	B	198	THR
1	B	228	THR
1	B	246	THR
1	B	296	VAL
1	B	358	GLU
1	C	13	ARG
1	C	23	LYS
1	C	62	ASN
1	C	122	LEU

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Mol	Chain	Res	Type
1	C	136	VAL
1	C	138	LYS
1	C	140	ASP
1	C	154	THR
1	C	171	LYS
1	C	179	LEU
1	C	195	GLU
1	C	246	THR
1	C	252	VAL
1	C	262	THR
1	C	296	VAL
1	D	49	VAL
1	D	54	ASN
1	D	64	LEU
1	D	76	THR
1	D	81	THR
1	D	84	LEU
1	D	107	VAL
1	D	113	ILE
1	D	122	LEU
1	D	141	GLU
1	D	157	VAL
1	D	161	VAL
1	D	162	GLU
1	D	185	ASP
1	D	190	ARG
1	D	218	MET
1	D	222	GLN
1	D	296	VAL
1	D	355	LEU
1	D	356	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
1	B	301	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	504	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	503	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	C	405	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	C	404	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.05	0
4	SO4	A	407	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	B	501	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	C	403	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	405	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	D	502	-	4,4,4	0.13	0	6,6,6	0.04	0
4	SO4	A	403	-	4,4,4	0.14	0	6,6,6	0.05	0
3	FLC	A	402	-	3,12,12	1.27	0	3,17,17	1.67	1 (33%)
4	SO4	B	502	-	4,4,4	0.14	0	6,6,6	0.06	0
5	PPV	D	505	-	6,8,8	0.81	0	13,13,13	1.25	2 (15%)
2	GDD	A	401	-	35,42,42	4.86	18 (51%)	47,65,65	1.53	8 (17%)
3	FLC	C	401	-	3,12,12	2.12	2 (66%)	3,17,17	2.98	1 (33%)
4	SO4	A	406	-	4,4,4	0.44	0	6,6,6	0.05	0
4	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.07	0
5	PPV	B	506	-	6,8,8	0.74	0	13,13,13	1.10	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	402	-	4,4,4	0.14	0	6,6,6	0.06	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
3	FLC	C	401	-	-	3/6/16/16	-
5	PPV	D	505	-	-	0/6/6/6	-
5	PPV	B	506	-	-	1/6/6/6	-
2	GDD	A	401	-	-	5/19/59/59	0/4/4/4
3	FLC	A	402	-	-	3/6/16/16	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GDD	O4'-C1'	16.38	1.63	1.41
2	A	401	GDD	C2'-C1'	-13.29	1.33	1.53
2	A	401	GDD	C4-N3	8.79	1.49	1.35
2	A	401	GDD	C2-N2	6.97	1.47	1.33
2	A	401	GDD	C5-C6	6.93	1.53	1.41
2	A	401	GDD	C2-N1	6.54	1.47	1.35
2	A	401	GDD	O4'-C4'	-6.22	1.31	1.45
2	A	401	GDD	C6-N1	6.07	1.43	1.33
2	A	401	GDD	PB-O1B	4.09	1.71	1.60
2	A	401	GDD	O2'-C2'	3.41	1.51	1.43
2	A	401	GDD	O31-C31	2.97	1.50	1.43
3	C	401	FLC	CG-CB	-2.54	1.51	1.54
2	A	401	GDD	C41-C31	-2.42	1.46	1.52
2	A	401	GDD	PA-O5'	2.26	1.68	1.59
2	A	401	GDD	C2-N3	2.24	1.45	1.34
2	A	401	GDD	O3'-C3'	-2.23	1.37	1.43
2	A	401	GDD	O51-C11	2.17	1.47	1.41
2	A	401	GDD	O41-C41	2.12	1.48	1.43
3	C	401	FLC	OHB-CB	-2.11	1.39	1.43
2	A	401	GDD	O6-C6	-2.02	1.19	1.24

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	GDD	N3-C2-N1	-5.41	120.01	127.22
3	C	401	FLC	CB-CG-CGC	-4.83	107.25	114.98
2	A	401	GDD	C2-N3-C4	4.20	120.15	115.36
2	A	401	GDD	O3A-PB-O1B	3.27	109.09	102.48
5	D	505	PPV	P2-OPP-P1	-3.15	122.00	132.83
5	B	506	PPV	P2-OPP-P1	-2.70	123.56	132.83
2	A	401	GDD	C5-C6-N1	-2.68	119.77	123.43
2	A	401	GDD	PB-O3A-PA	-2.67	123.65	132.83
2	A	401	GDD	C2-N1-C6	2.43	119.78	115.93
2	A	401	GDD	O51-C11-O1B	-2.14	108.57	111.36
3	A	402	FLC	CB-CA-CAC	-2.12	111.58	114.98
5	D	505	PPV	O21-P1-OPP	2.10	111.68	104.64
2	A	401	GDD	C3'-C2'-C1'	2.05	104.06	100.98

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	GDD	C11-O1B-PB-O3A
3	A	402	FLC	CA-CB-CG-CGC
3	A	402	FLC	CBC-CB-CG-CGC
3	A	402	FLC	OHB-CB-CG-CGC
3	C	401	FLC	CA-CB-CG-CGC
3	C	401	FLC	CBC-CB-CG-CGC
3	C	401	FLC	OHB-CB-CG-CGC
2	A	401	GDD	C3'-C4'-C5'-O5'
2	A	401	GDD	O4'-C4'-C5'-O5'
5	B	506	PPV	P2-OPP-P1-O11
2	A	401	GDD	C41-C51-C61-O6A
2	A	401	GDD	O51-C51-C61-O6A

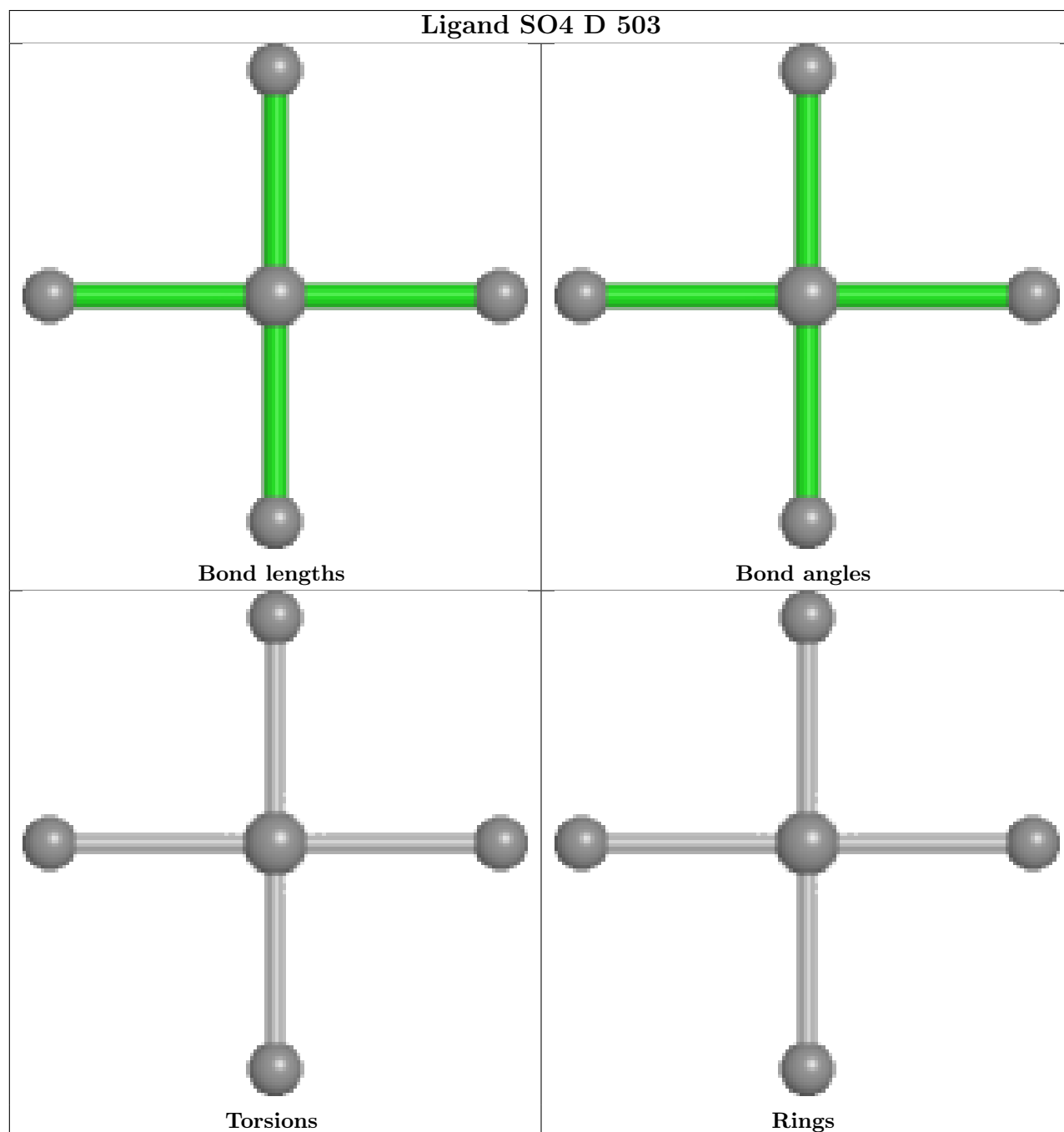
There are no ring outliers.

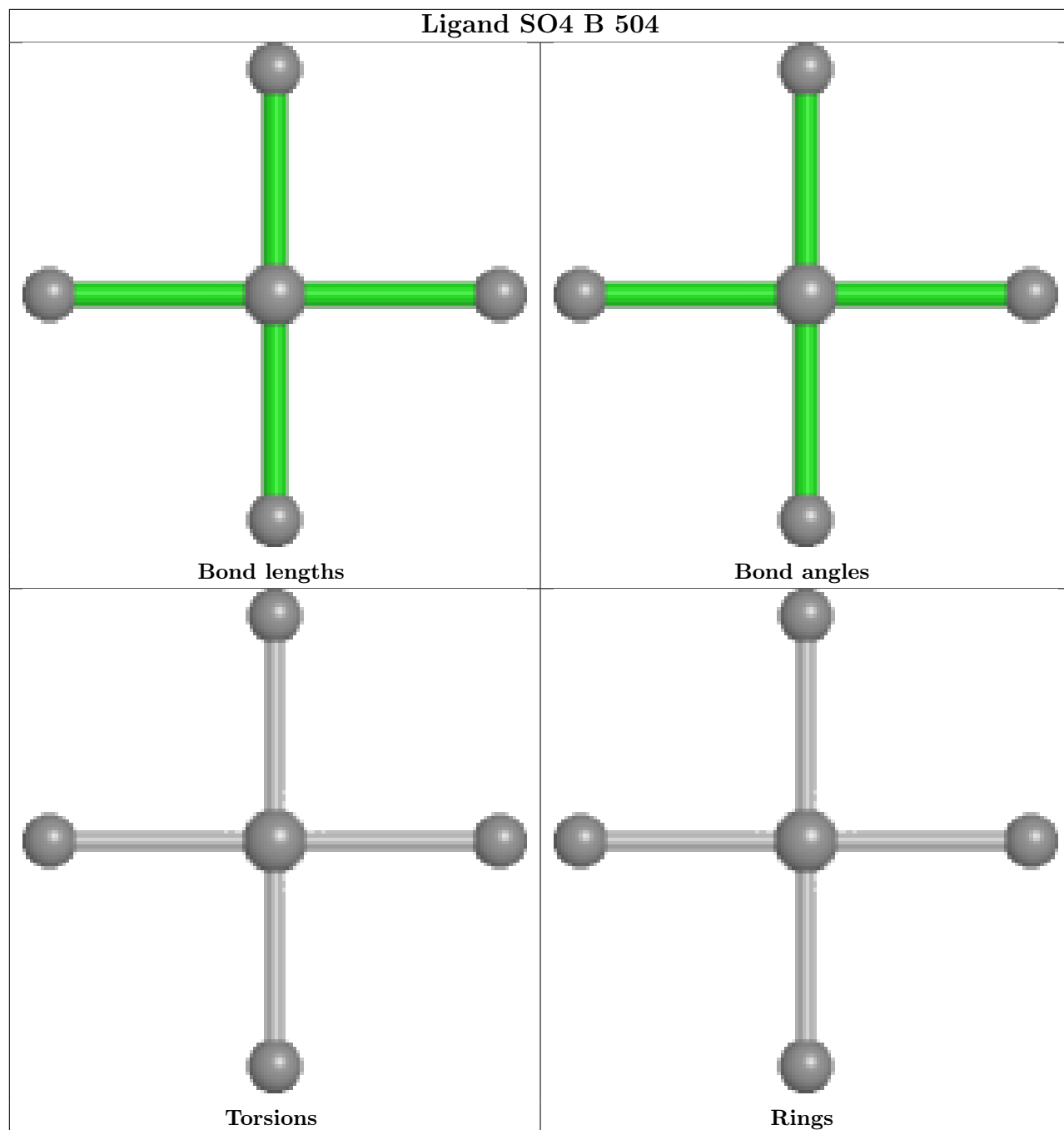
5 monomers are involved in 7 short contacts:

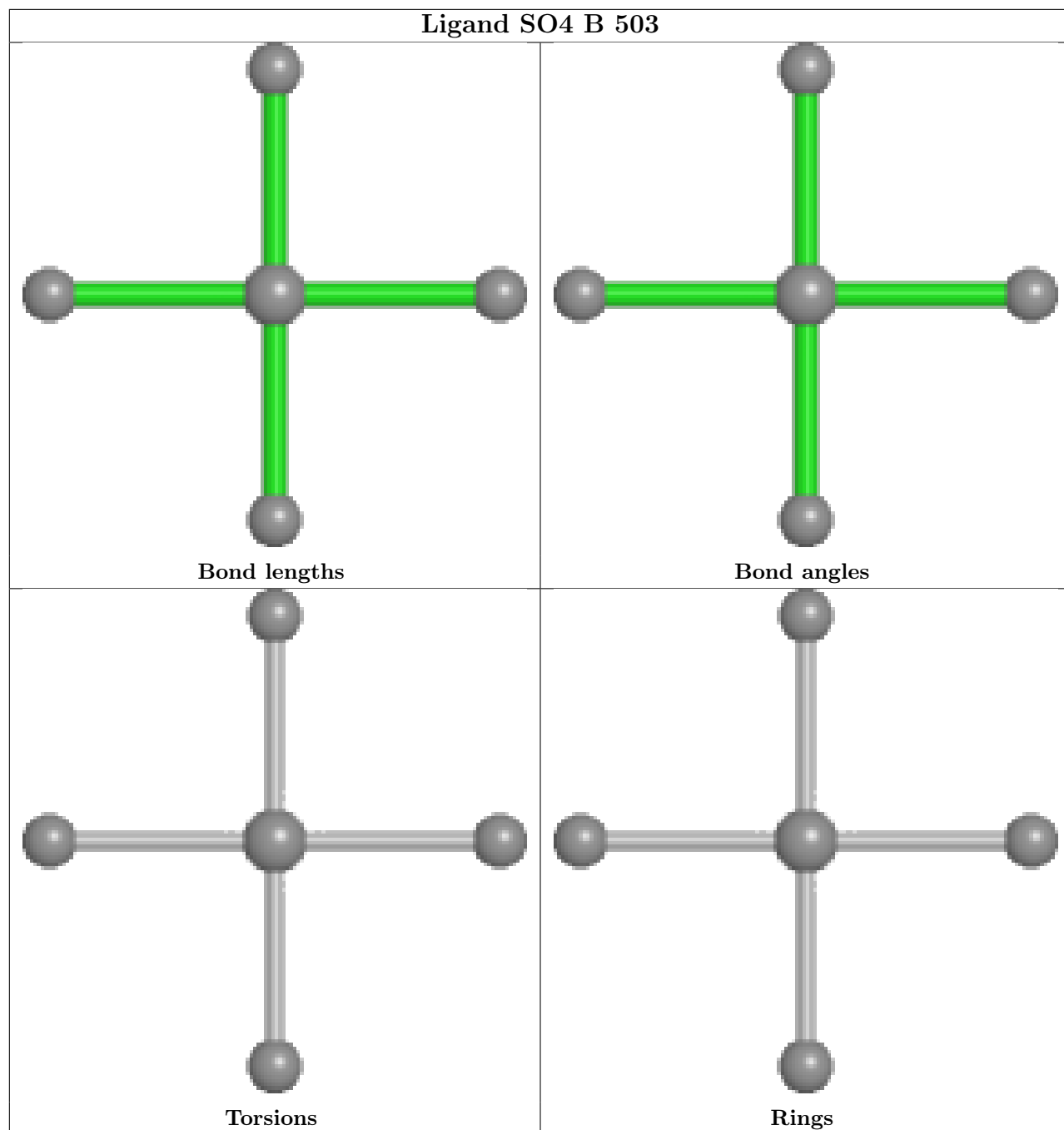
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	FLC	1	0
2	A	401	GDD	1	0
3	C	401	FLC	3	0
4	D	501	SO4	1	0
4	C	402	SO4	1	0

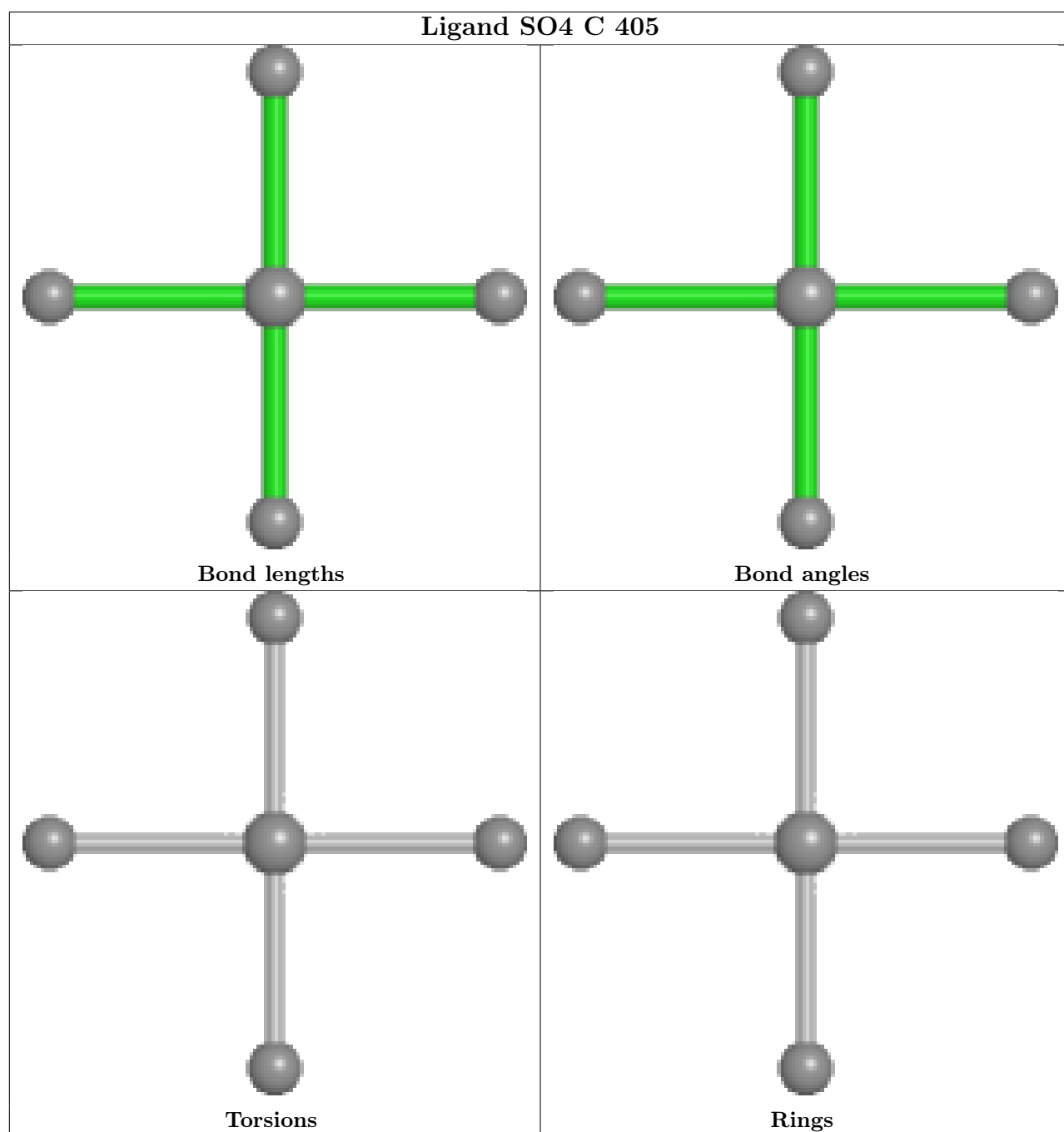
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

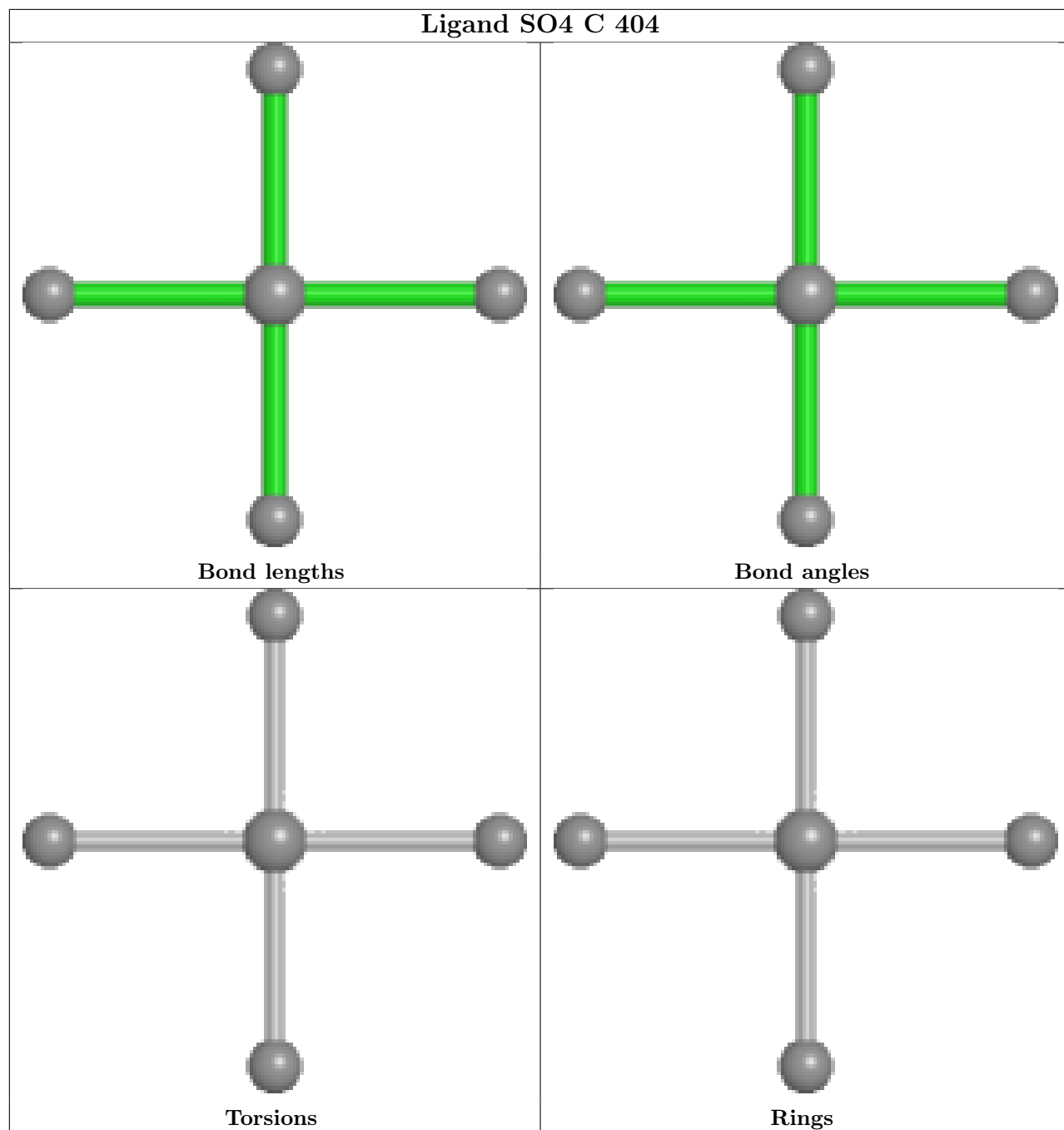
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within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

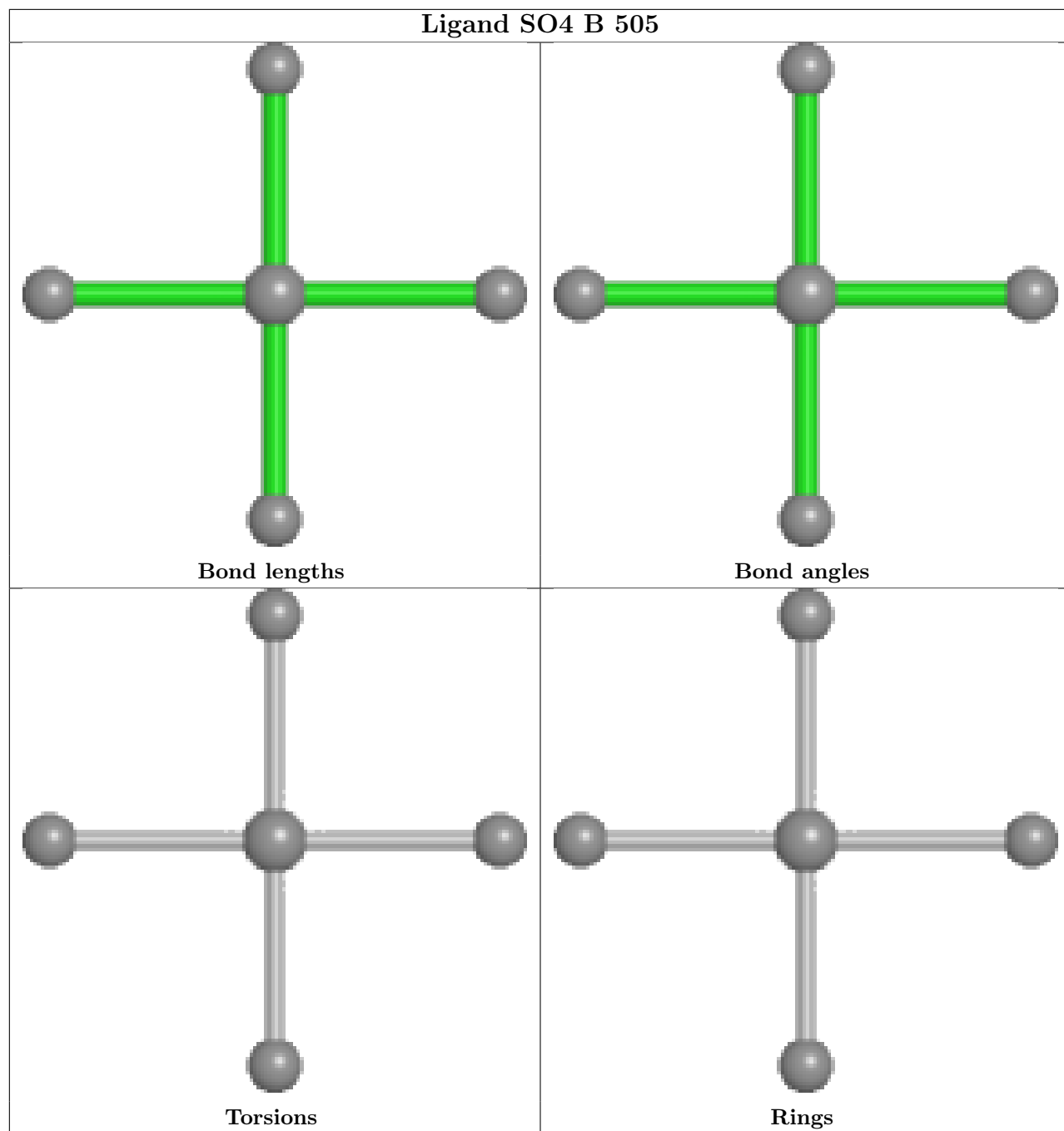


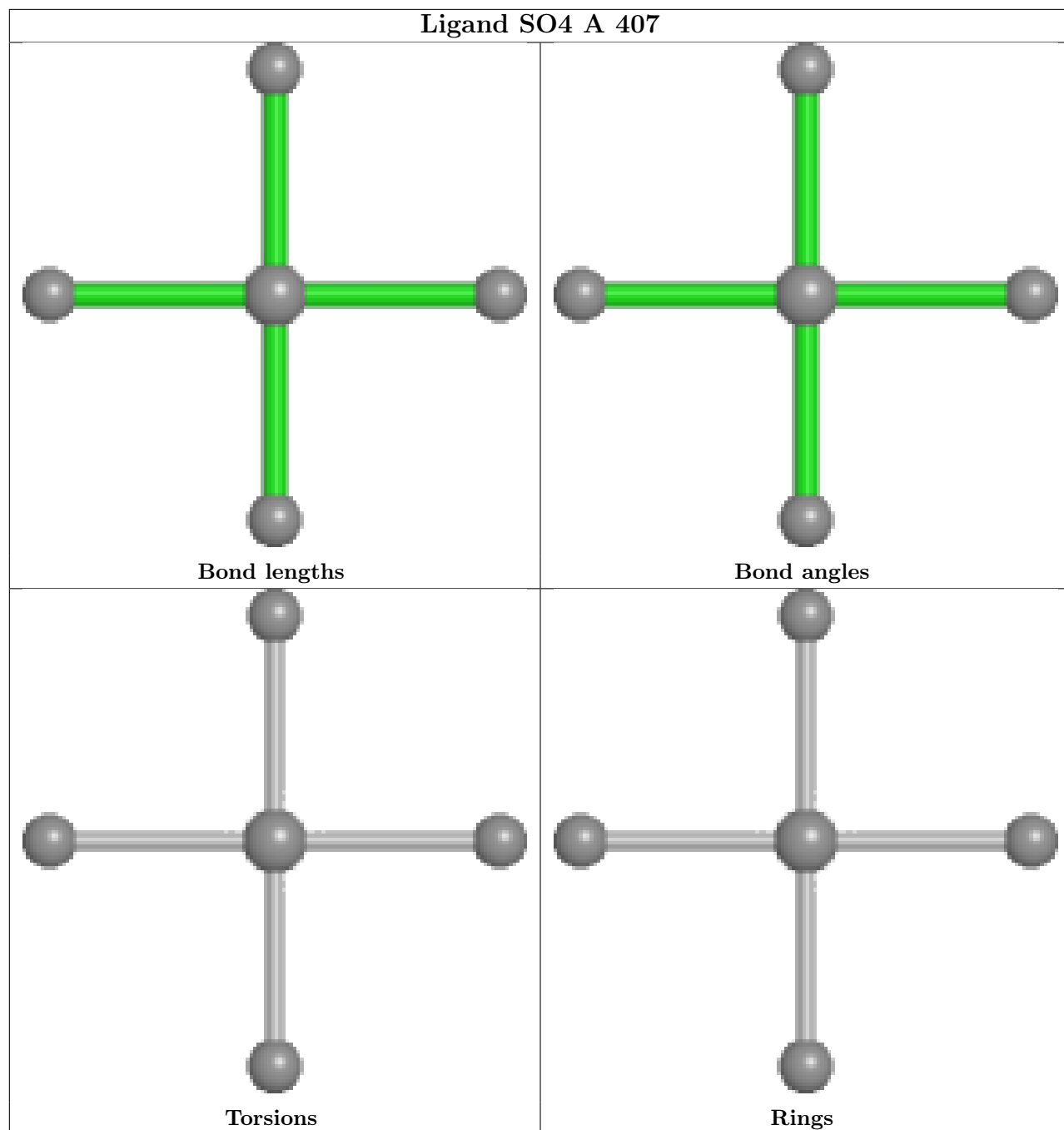


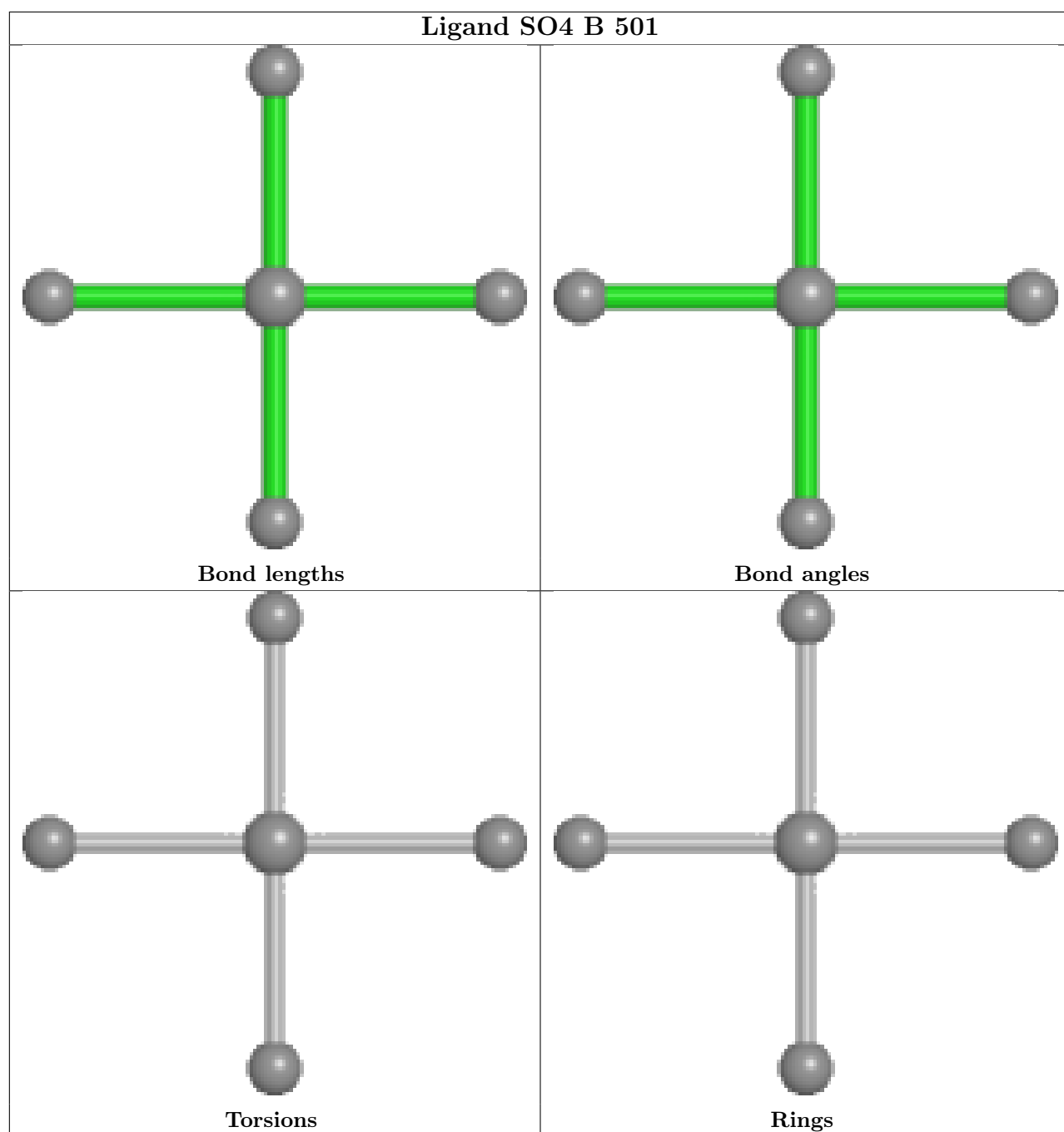


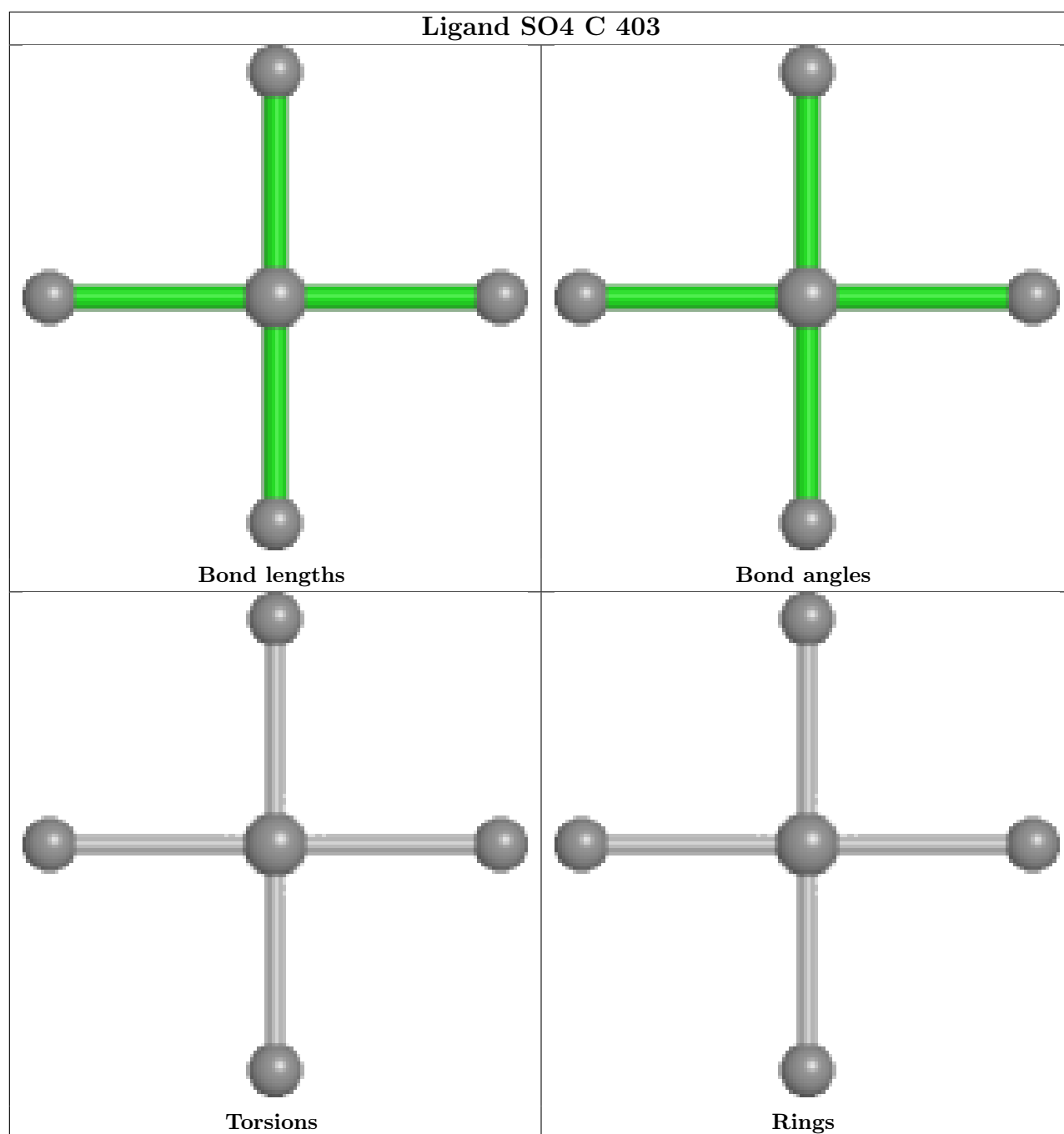


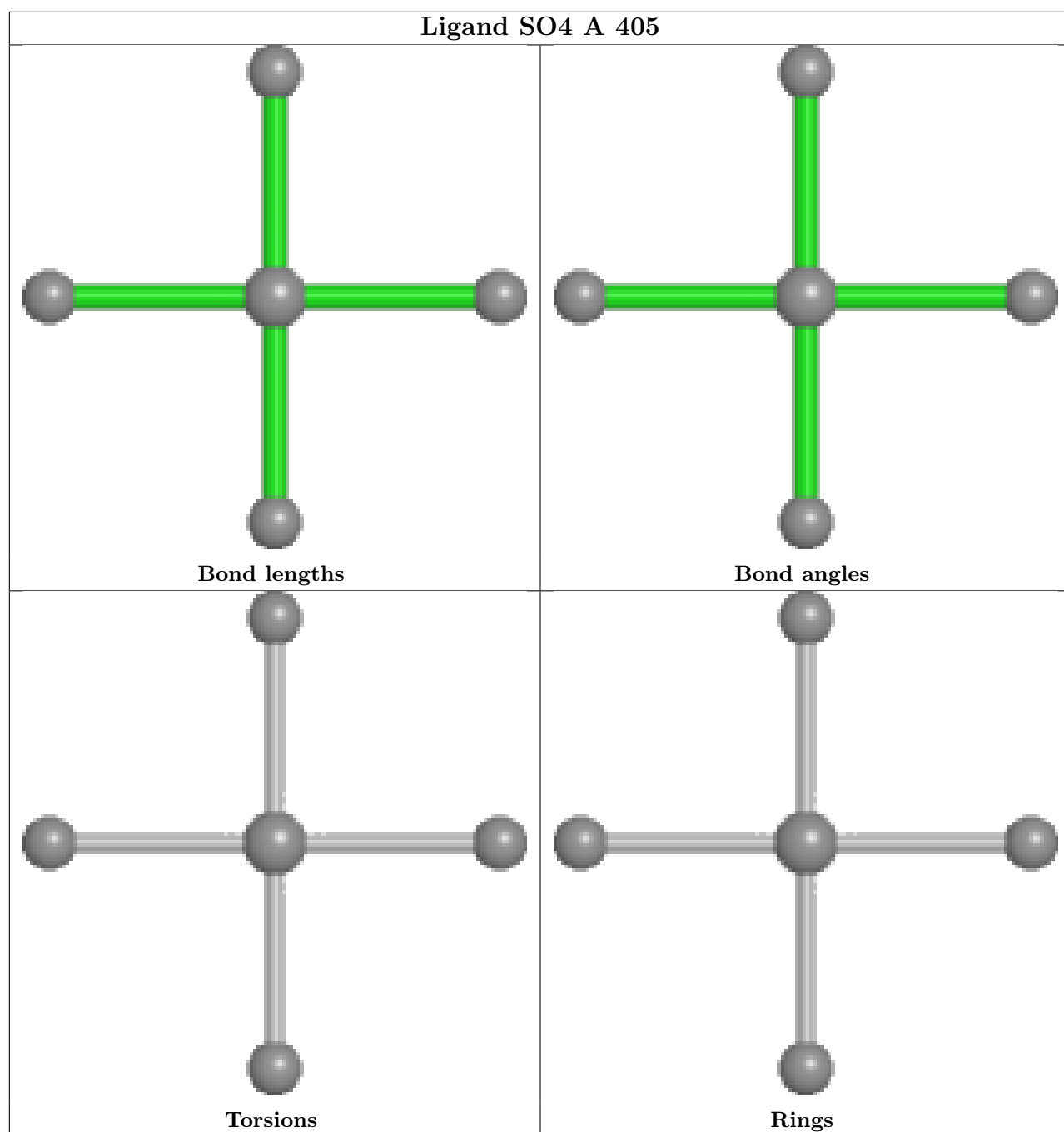


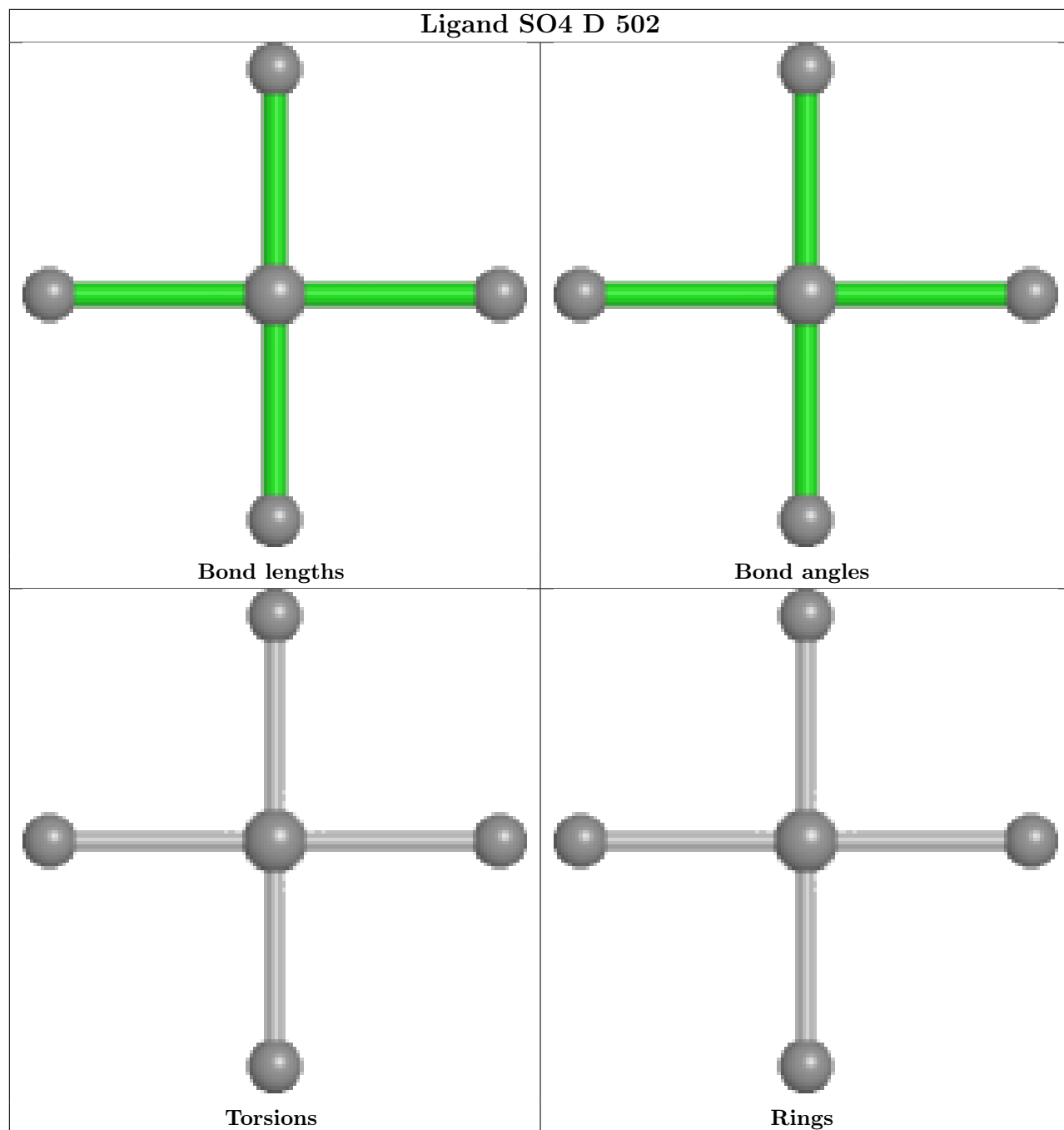


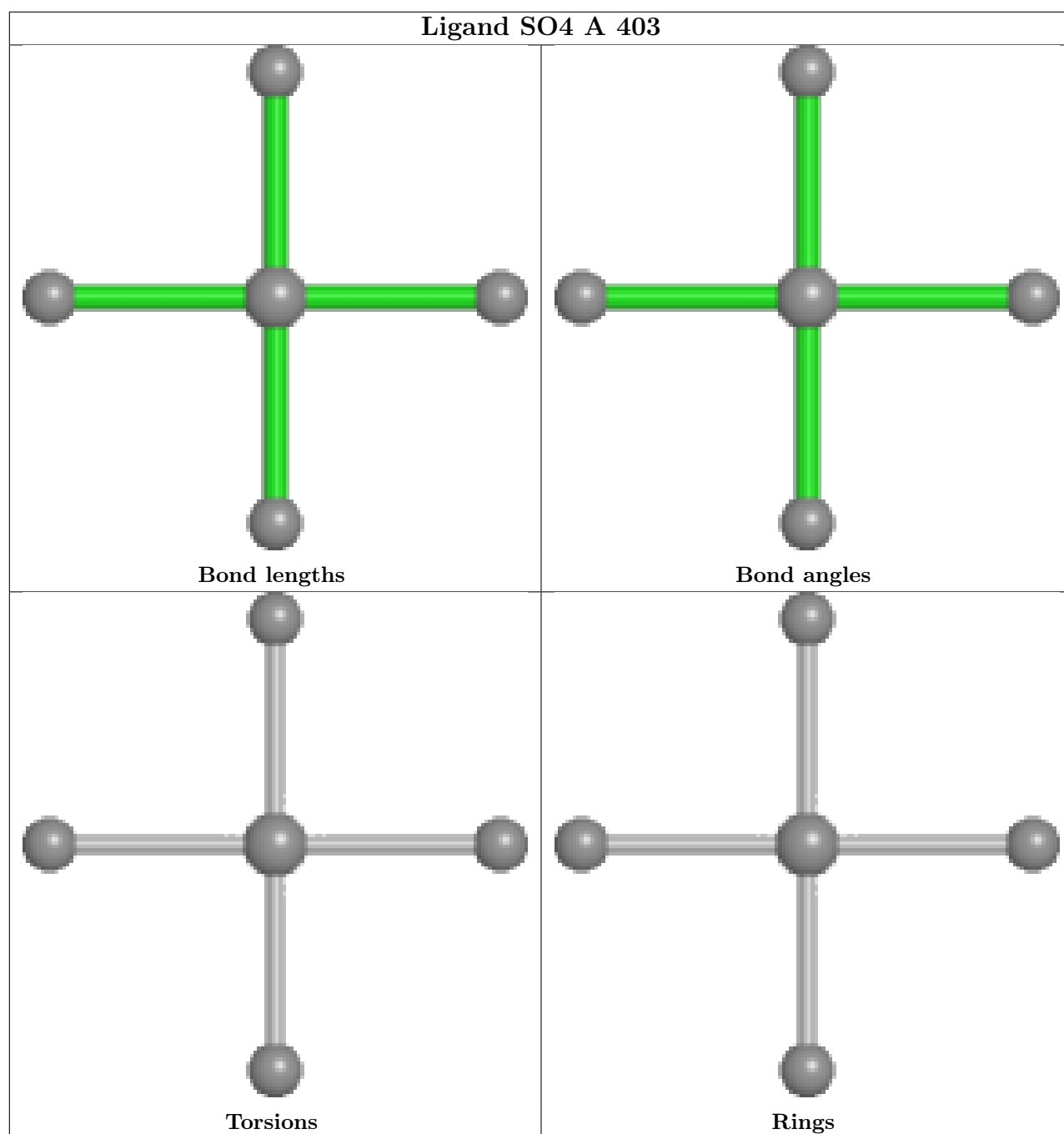


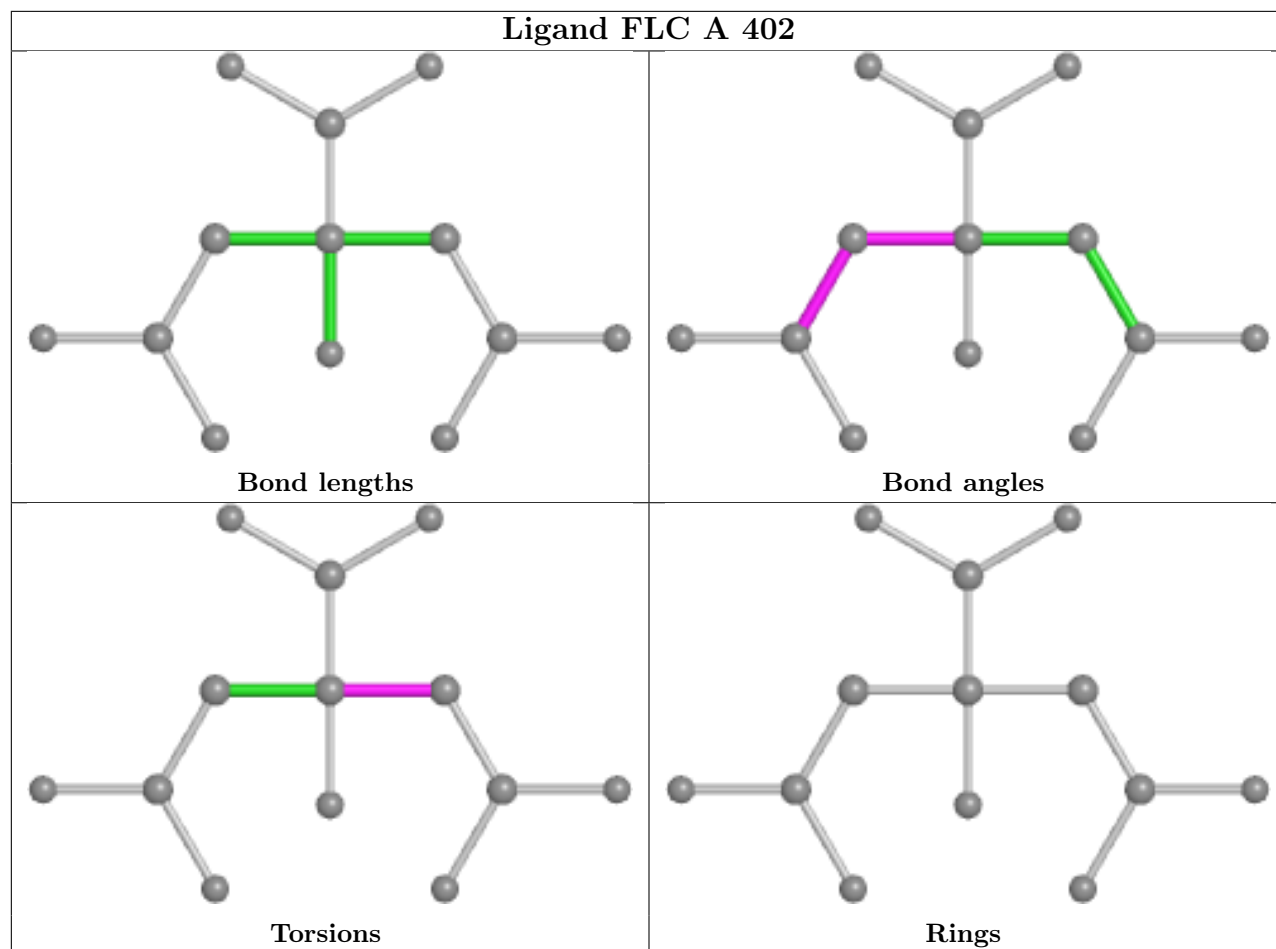


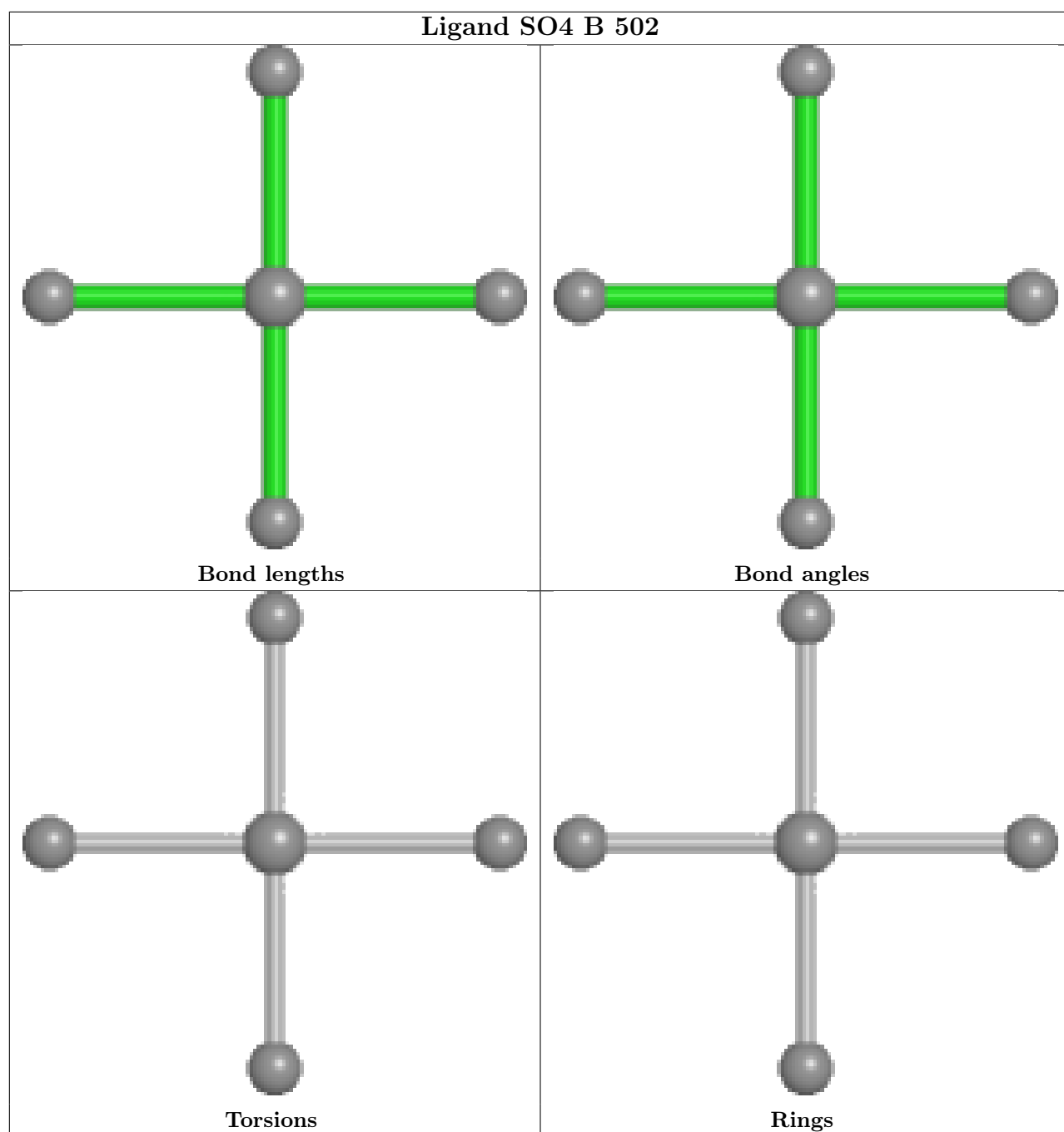


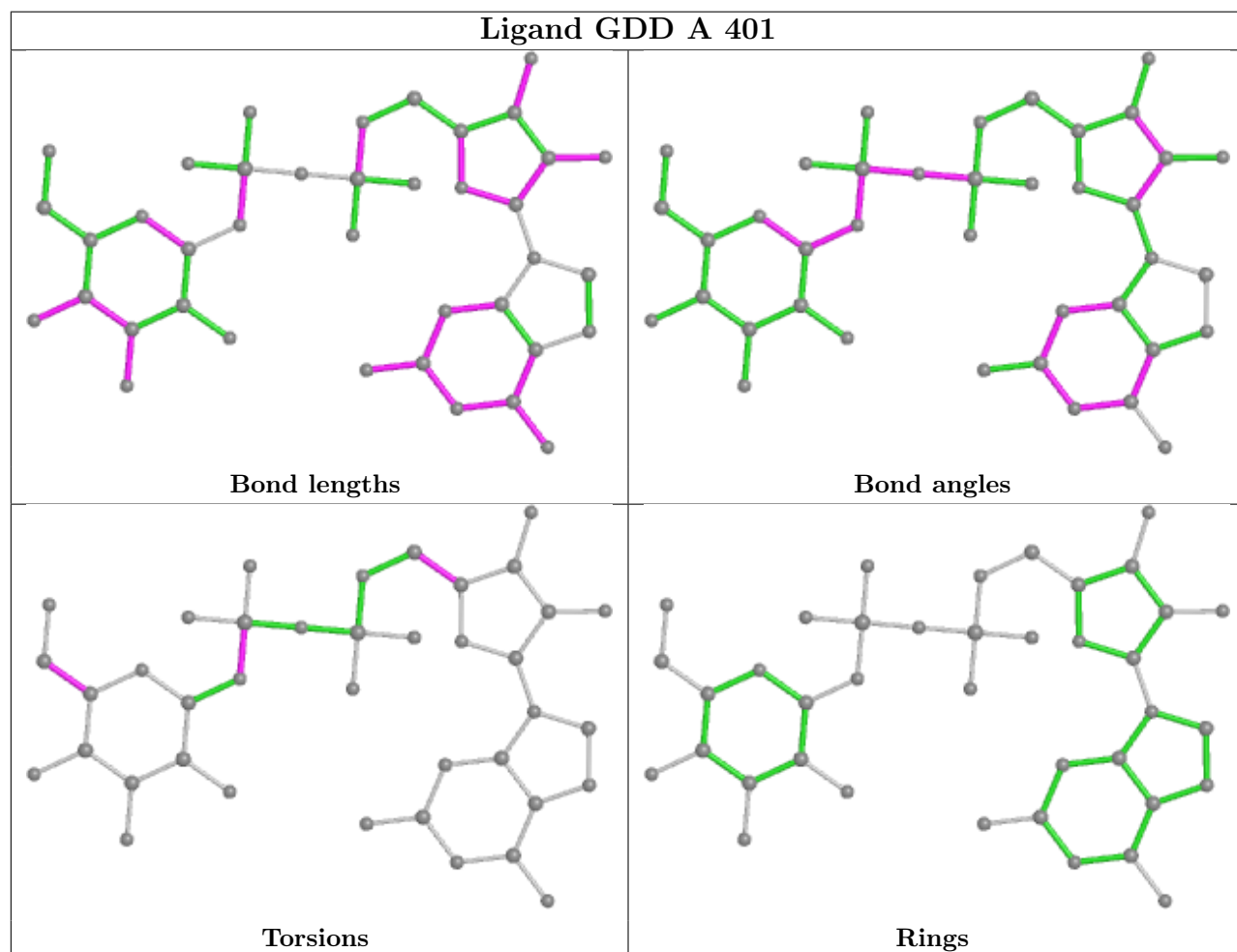
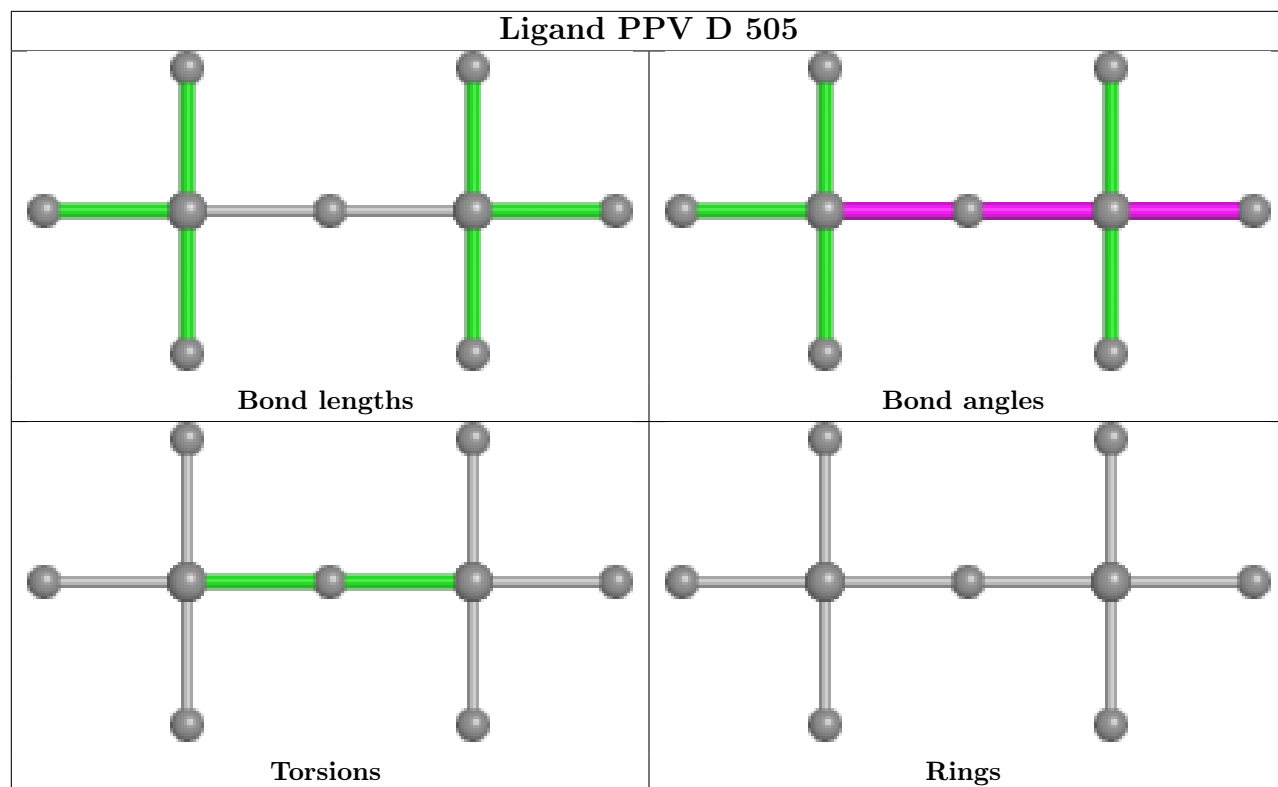


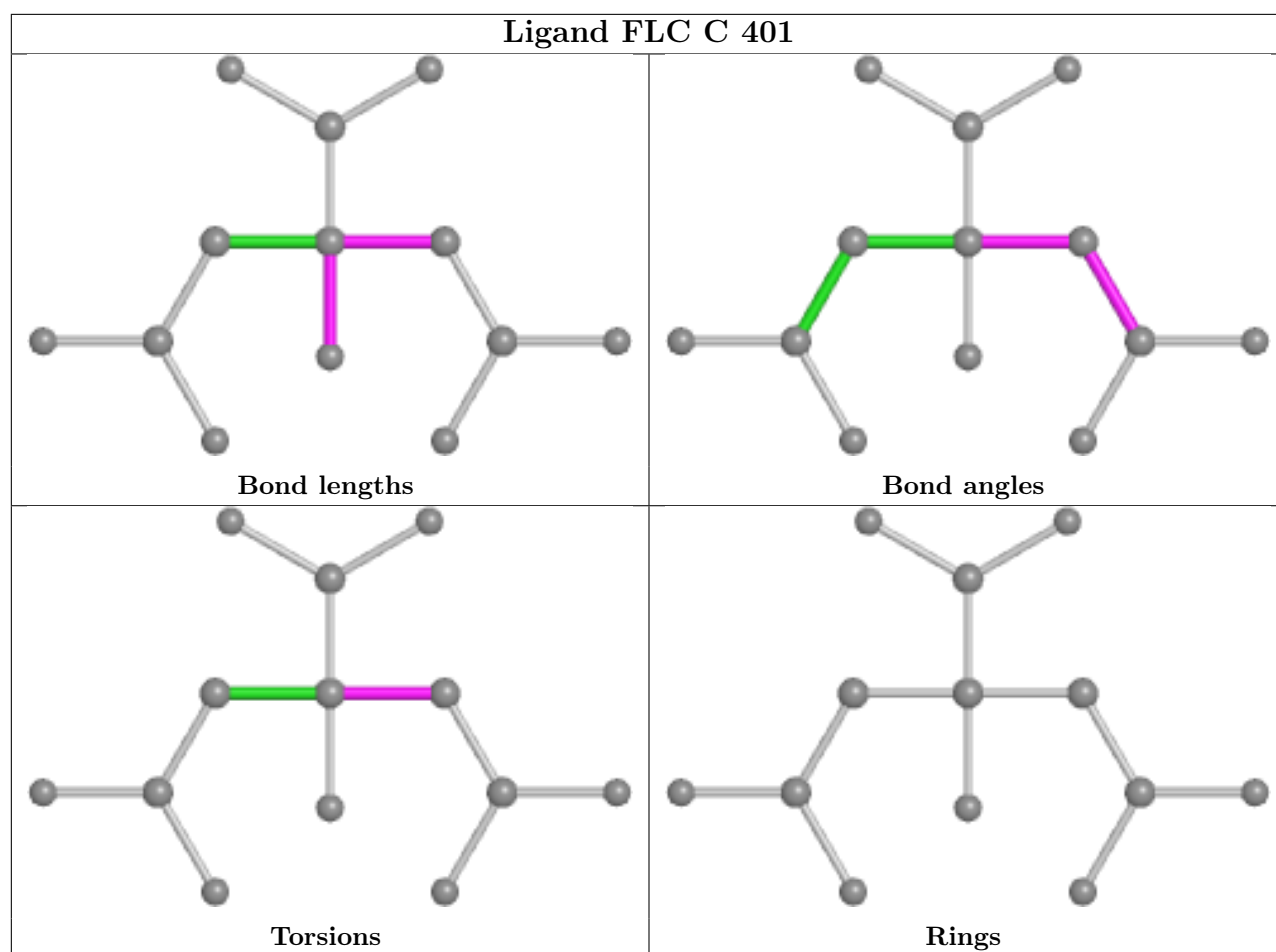


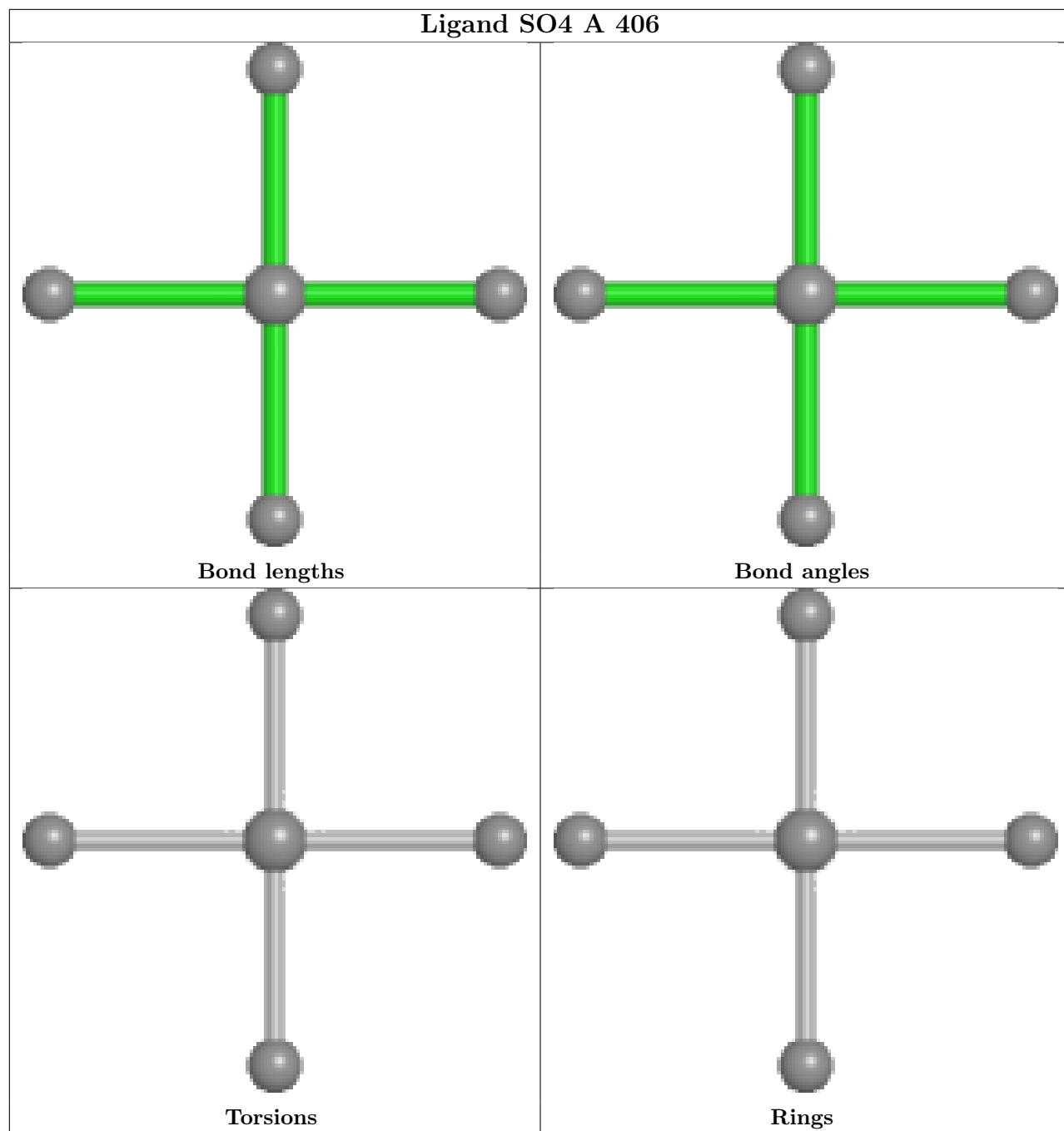


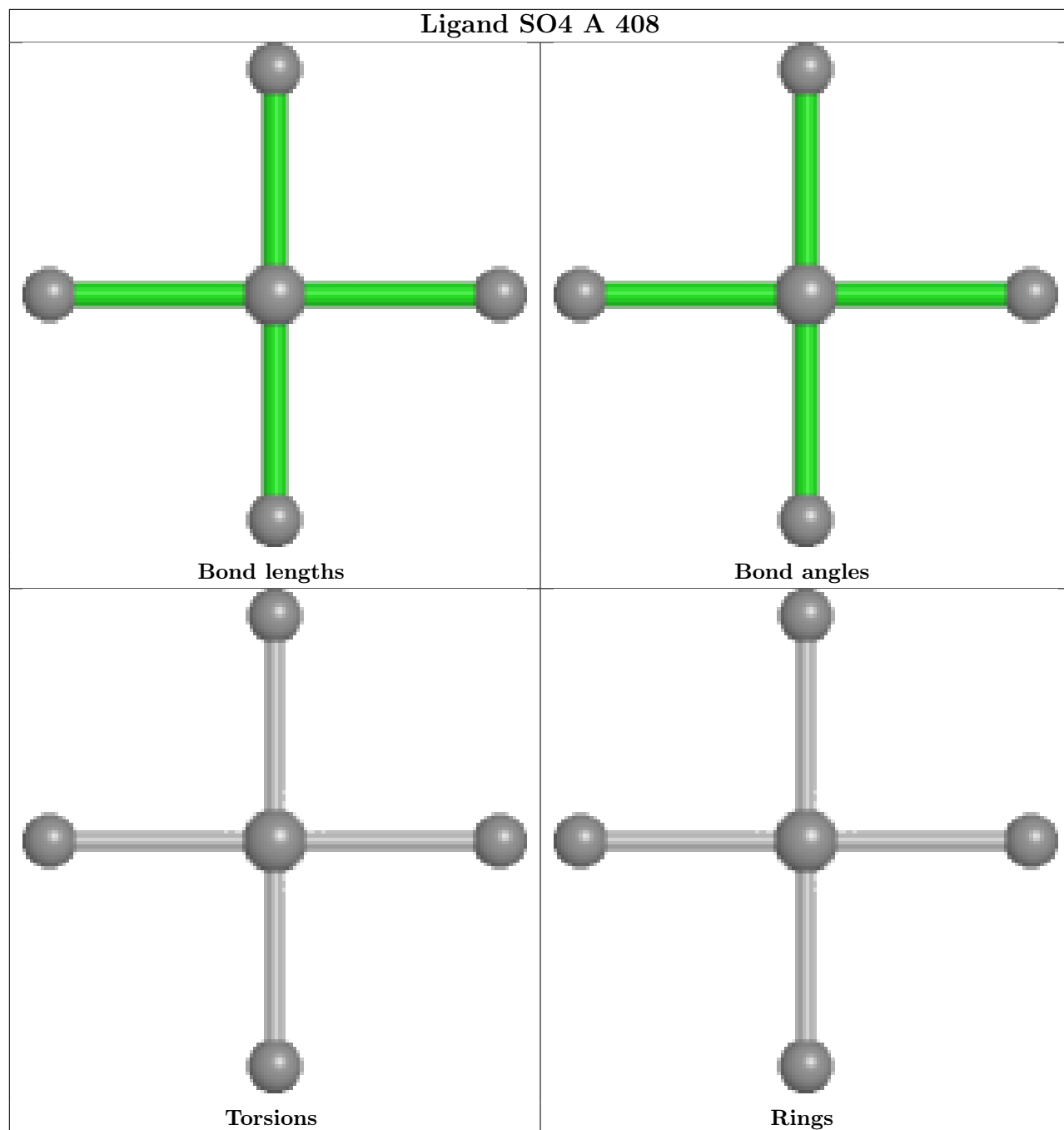


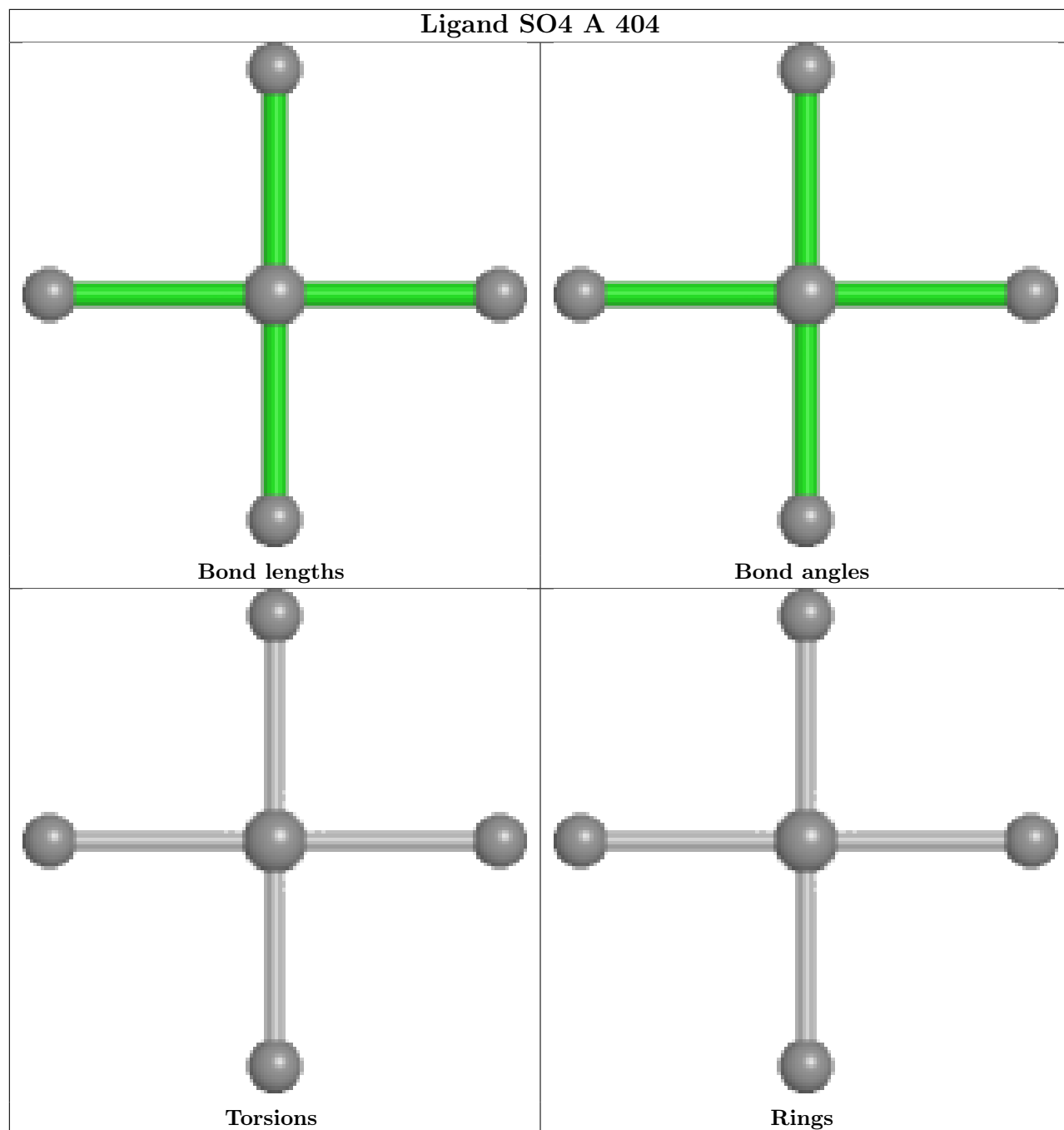


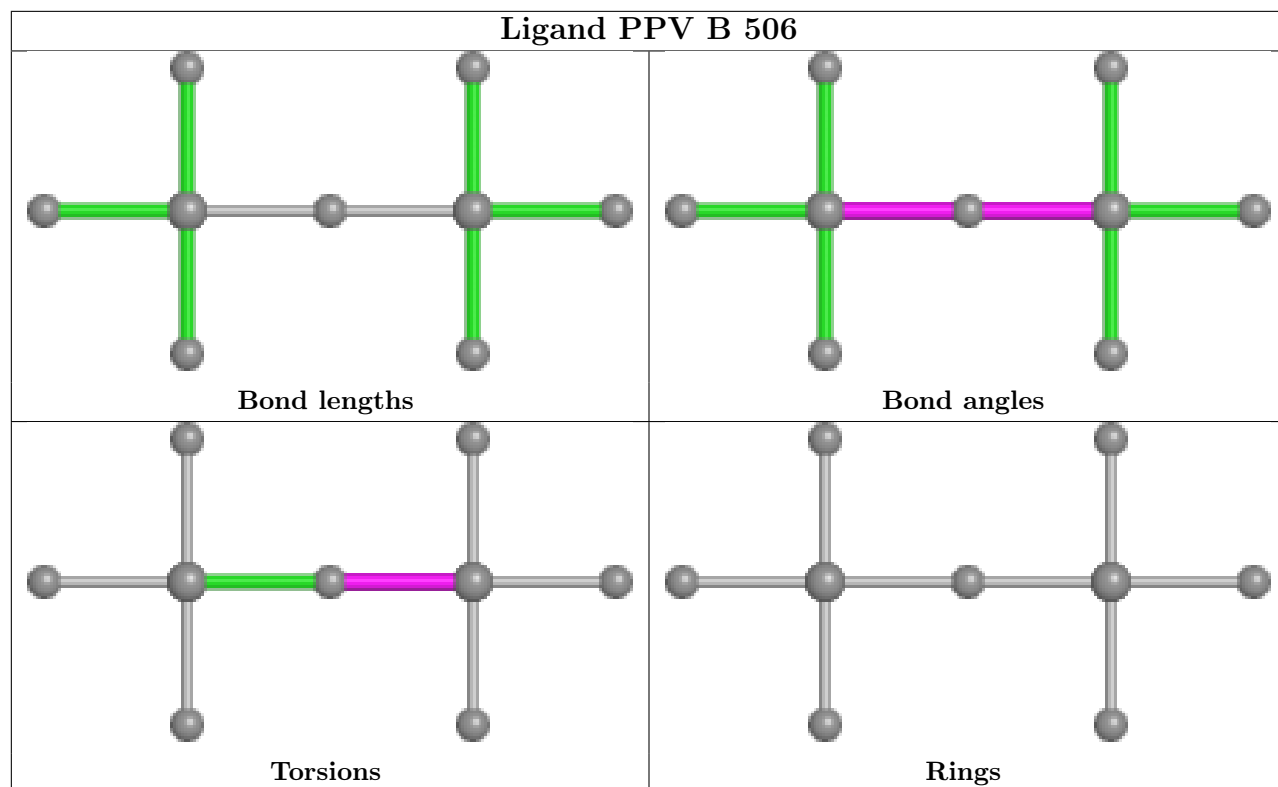


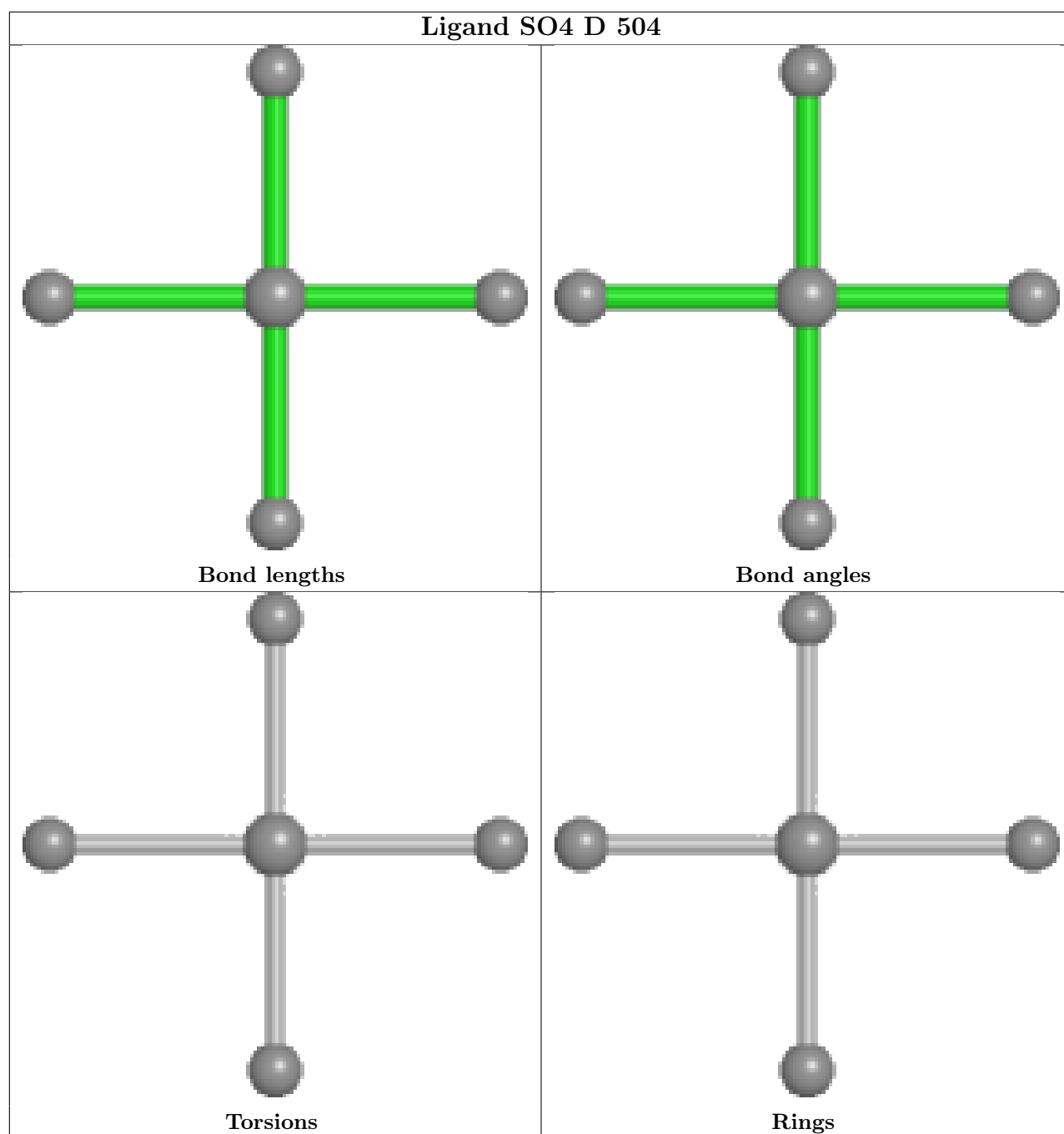


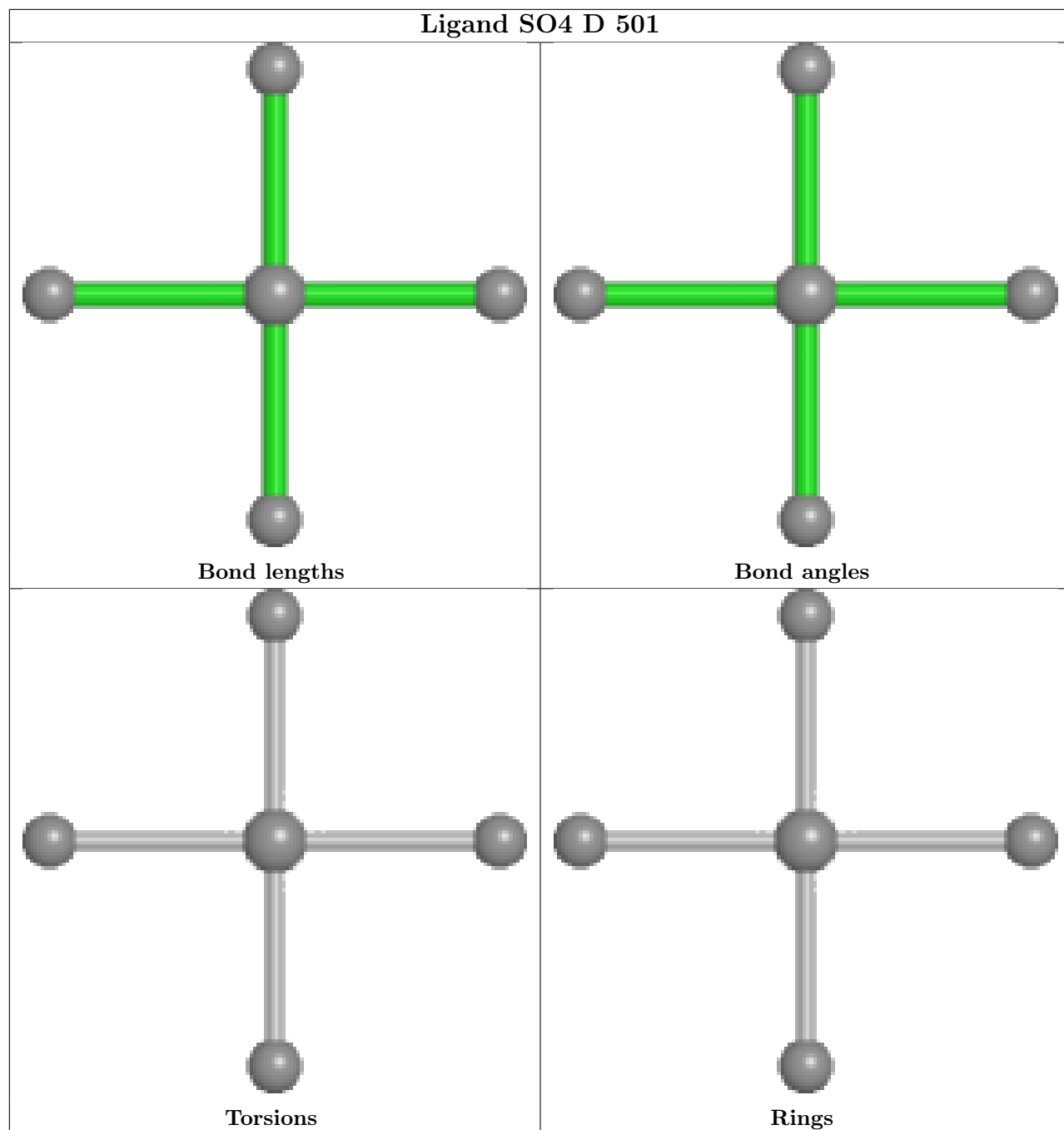


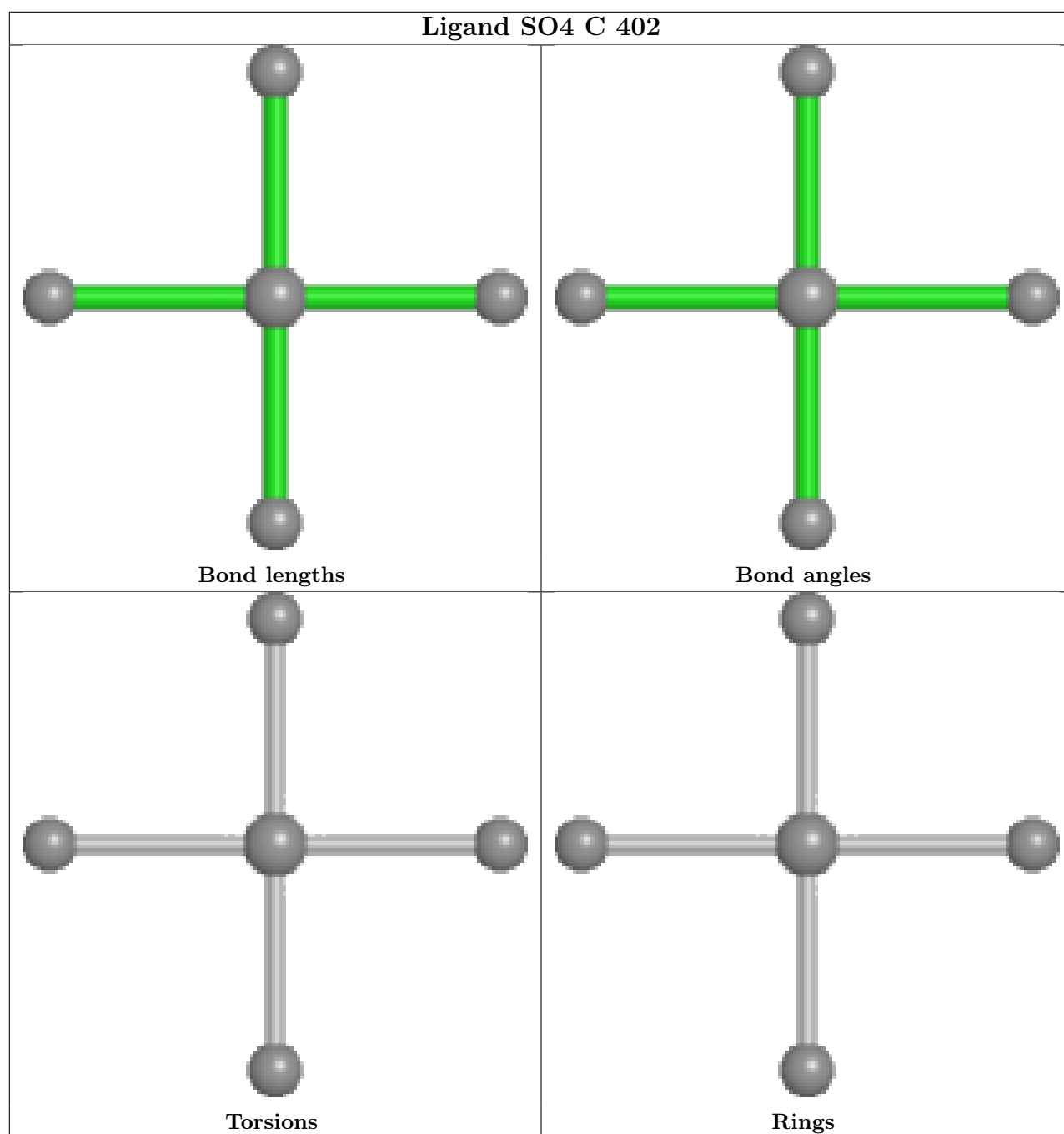












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	365/376 (97%)	-0.23	3 (0%) 86 65	28, 48, 86, 120	0
1	B	367/376 (97%)	-0.28	0 100 100	30, 54, 88, 119	0
1	C	355/376 (94%)	-0.17	6 (1%) 70 41	27, 54, 110, 150	0
1	D	355/376 (94%)	-0.13	9 (2%) 57 29	30, 63, 111, 128	0
All	All	1442/1504 (95%)	-0.21	18 (1%) 79 54	27, 55, 96, 150	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	165	LYS	4.8
1	D	357	PRO	4.4
1	C	141	GLU	4.3
1	C	140	ASP	4.2
1	D	168	VAL	4.1
1	C	168	VAL	3.1
1	A	169	GLY	2.7
1	D	356	LYS	2.6
1	A	144	LYS	2.5
1	C	169	GLY	2.4
1	D	167	TYR	2.4
1	D	140	ASP	2.3
1	D	158	GLU	2.3
1	D	169	GLY	2.3
1	A	153	SER	2.2
1	C	163	LYS	2.1
1	D	9	GLY	2.1
1	D	141	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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.

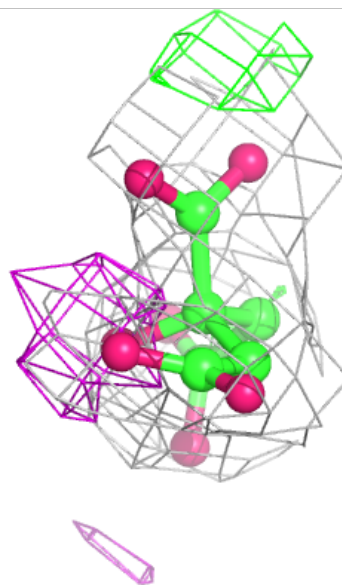
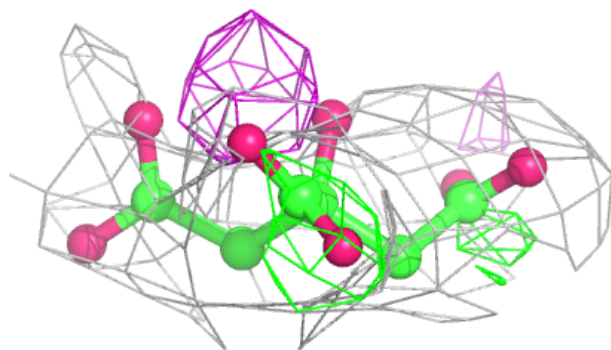
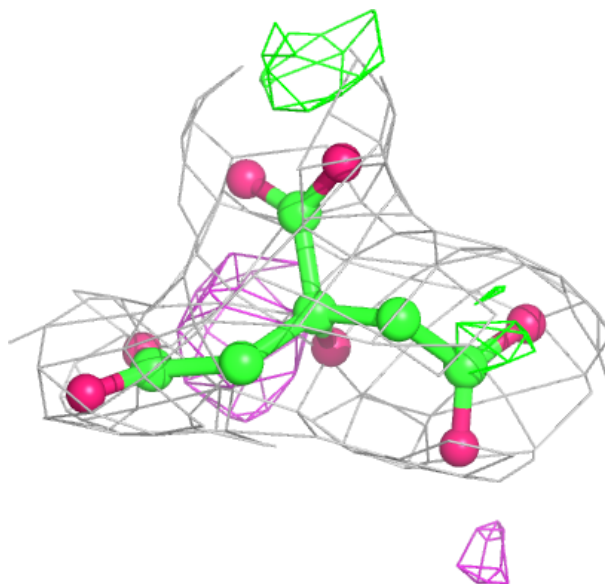
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	FLC	C	401	13/13	0.69	0.30	81,84,94,94	0
3	FLC	A	402	13/13	0.79	0.24	85,88,96,100	0
4	SO4	C	405	5/5	0.79	0.44	71,72,83,86	5
5	PPV	D	505	9/9	0.79	0.28	85,88,92,93	9
4	SO4	D	504	5/5	0.80	0.42	111,119,136,139	0
4	SO4	A	407	5/5	0.83	0.20	97,99,104,111	0
5	PPV	B	506	9/9	0.83	0.26	82,89,91,93	9
2	GDD	A	401	39/39	0.83	0.30	59,75,90,93	39
4	SO4	B	505	5/5	0.85	0.28	60,61,63,66	5
4	SO4	A	406	5/5	0.86	0.35	75,75,76,80	5
4	SO4	A	404	5/5	0.89	0.23	60,60,62,65	5
4	SO4	C	404	5/5	0.90	0.25	59,60,71,74	5
4	SO4	B	503	5/5	0.93	0.21	56,58,65,67	5
4	SO4	A	405	5/5	0.94	0.20	55,57,58,61	5
4	SO4	D	502	5/5	0.94	0.21	49,49,54,56	5
4	SO4	D	503	5/5	0.94	0.27	93,93,100,108	0
4	SO4	D	501	5/5	0.95	0.20	56,59,71,72	0
4	SO4	C	403	5/5	0.95	0.14	49,55,60,62	5
4	SO4	A	403	5/5	0.96	0.23	56,57,66,73	0
4	SO4	B	504	5/5	0.96	0.10	49,56,60,62	5
4	SO4	B	502	5/5	0.97	0.16	32,33,36,39	5
4	SO4	A	408	5/5	0.97	0.23	52,52,59,62	5
4	SO4	C	402	5/5	0.97	0.15	56,57,66,71	0
4	SO4	B	501	5/5	0.98	0.09	33,34,37,41	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.

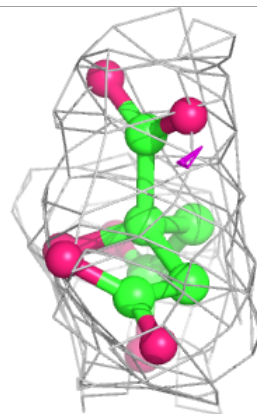
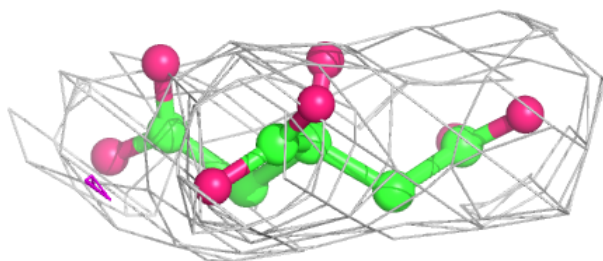
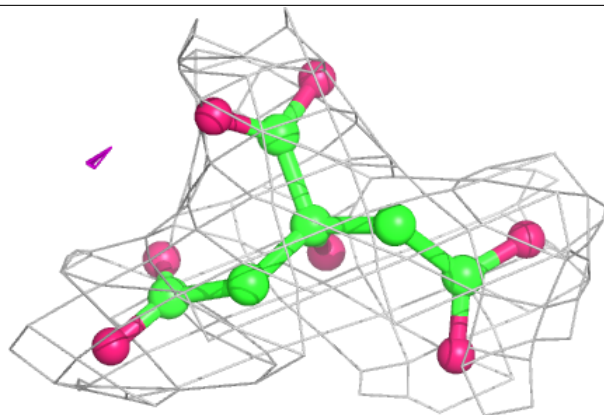
Electron density around FLC C 401:

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



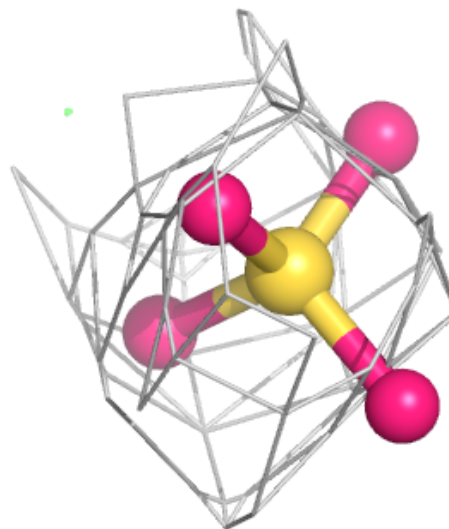
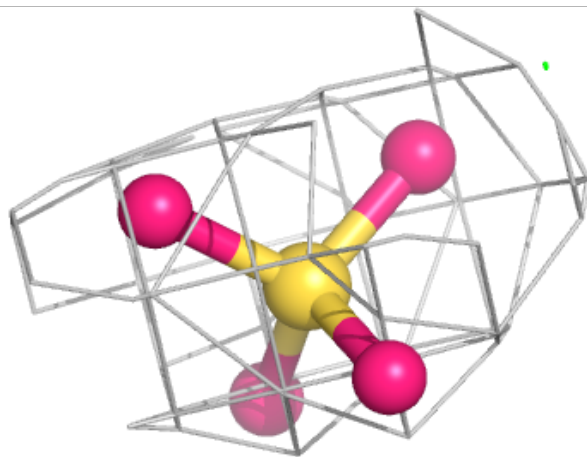
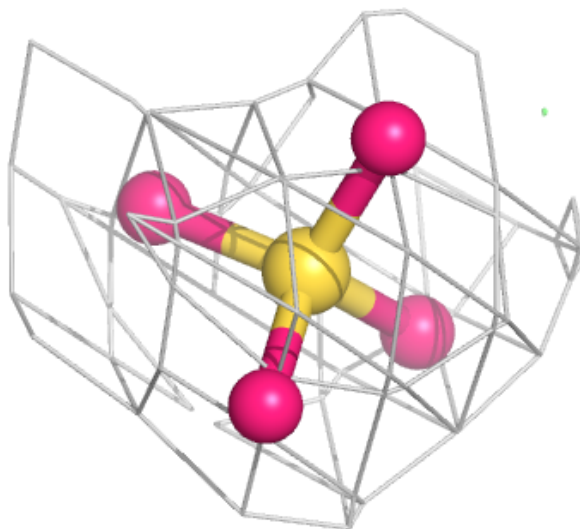
Electron density around FLC A 402:

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



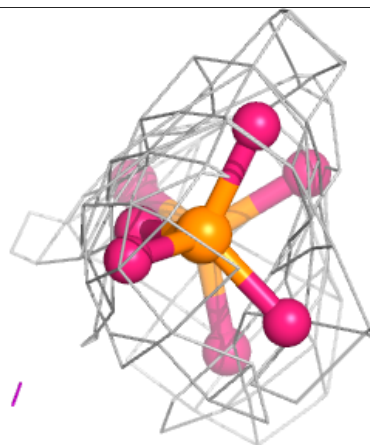
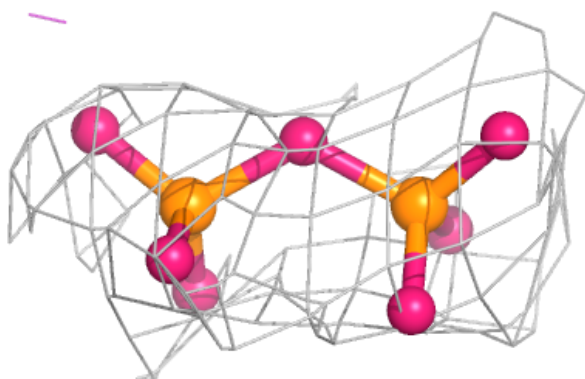
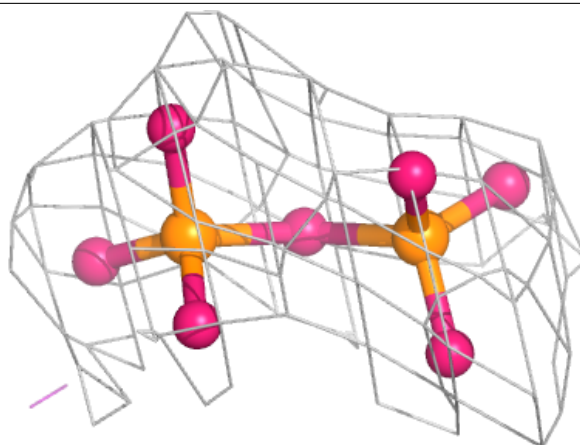
Electron density around SO4 C 405:

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



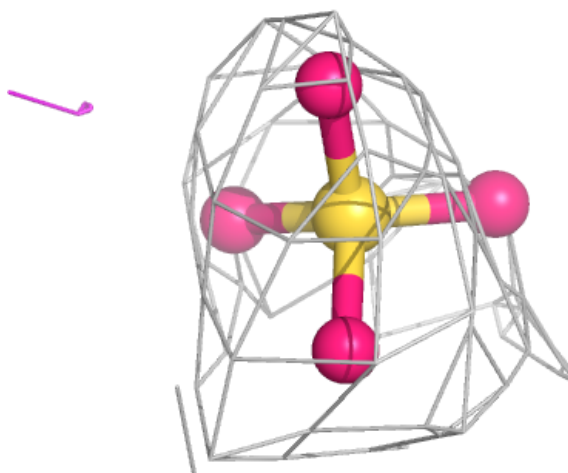
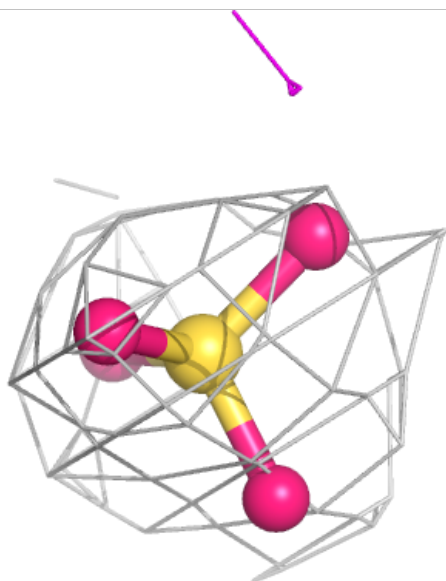
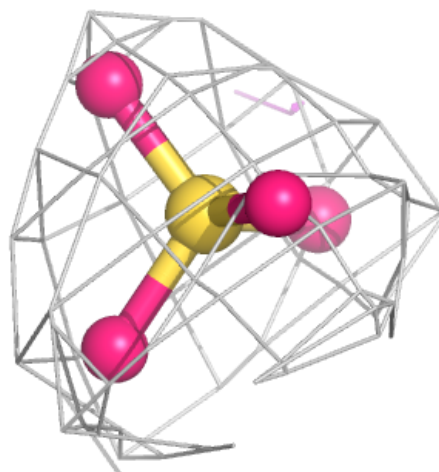
Electron density around PPV D 505:

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



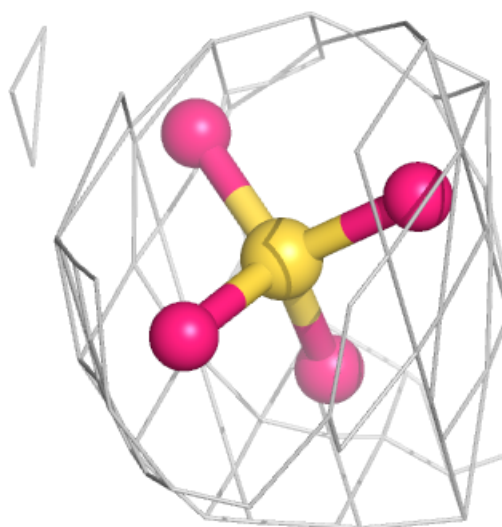
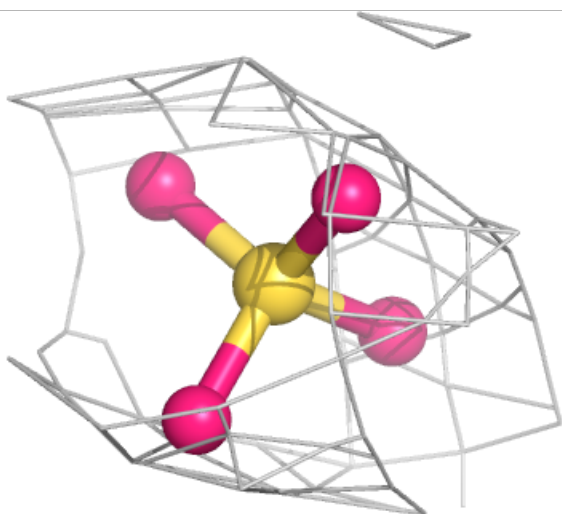
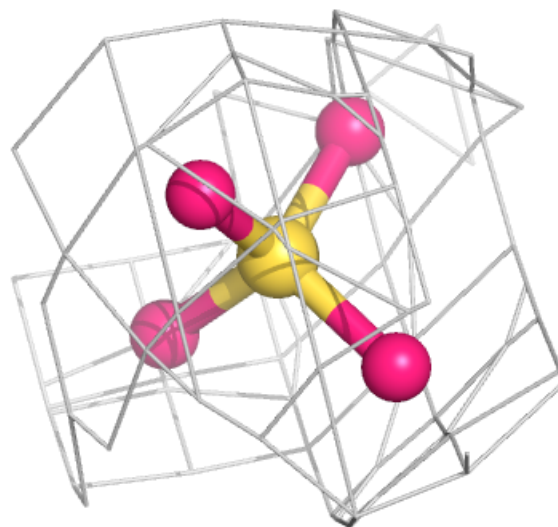
Electron density around SO4 D 504:

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and green (positive)



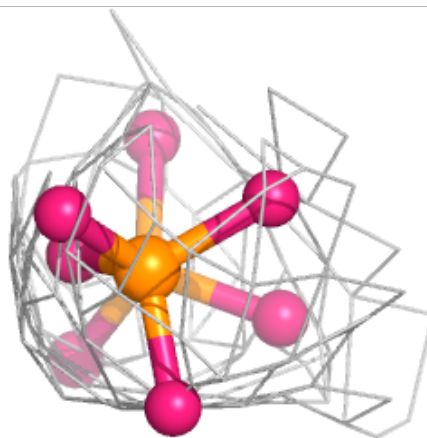
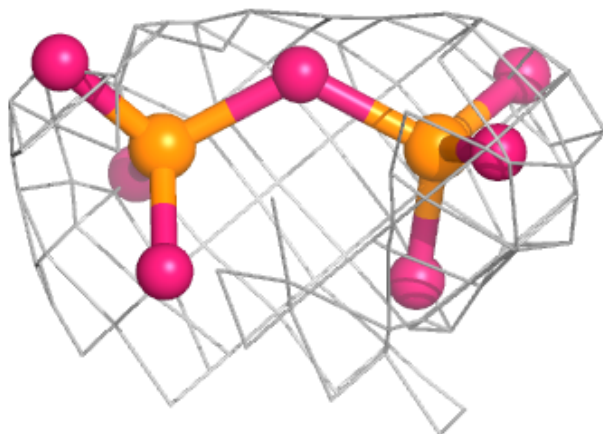
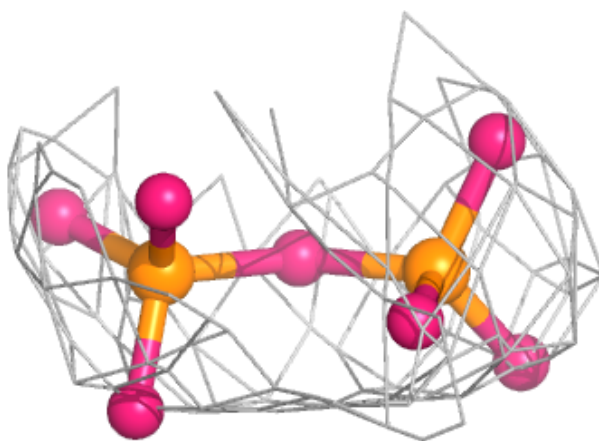
Electron density around SO4 A 407:

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



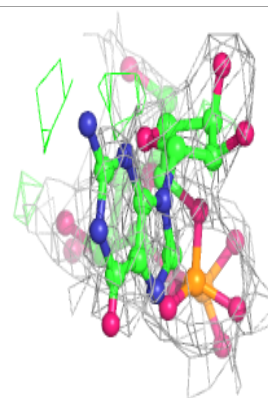
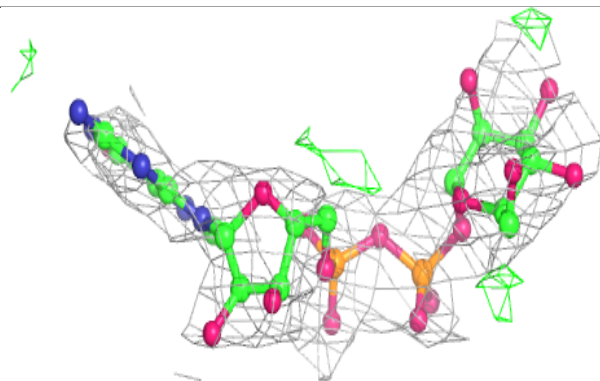
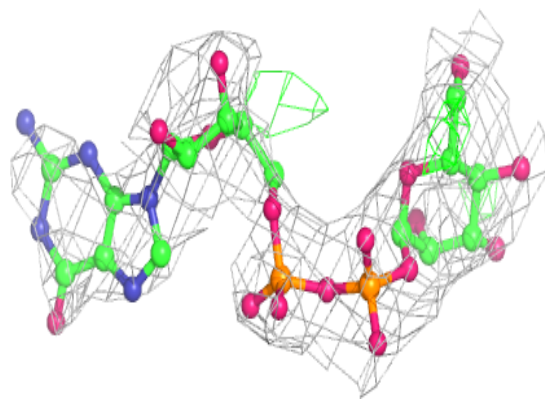
Electron density around PPV B 506:

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



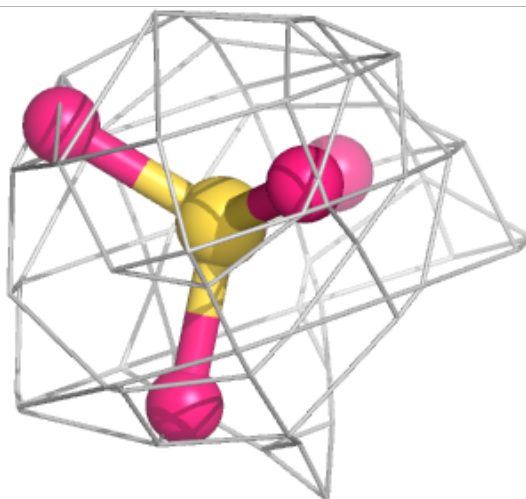
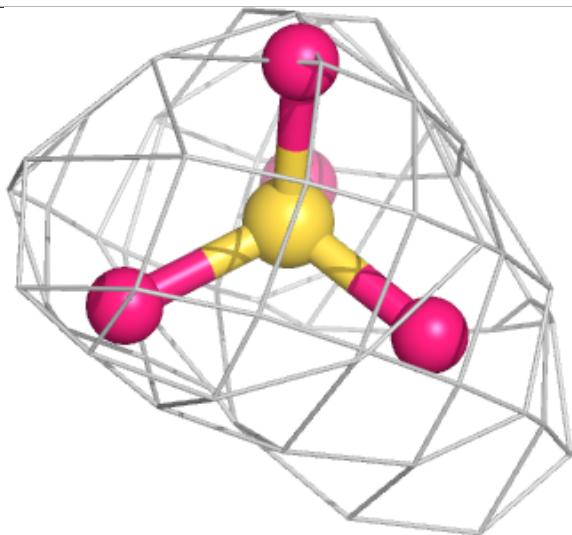
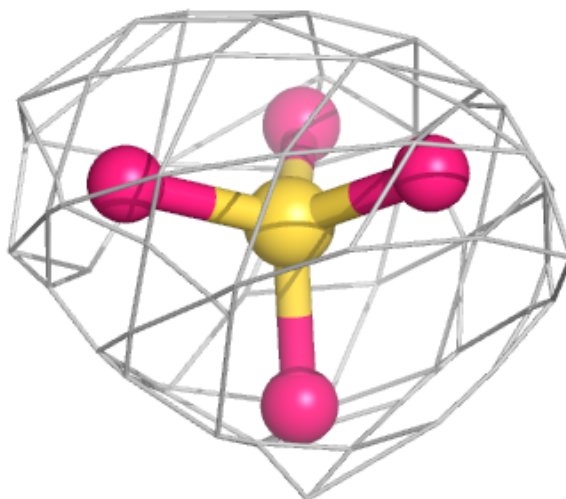
Electron density around GDD A 401:

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and green (positive)



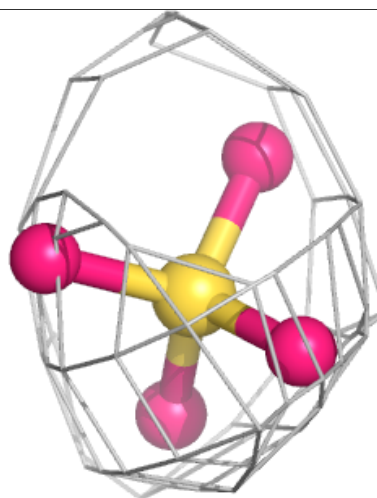
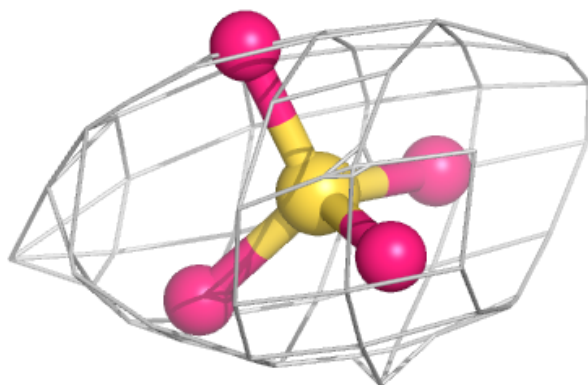
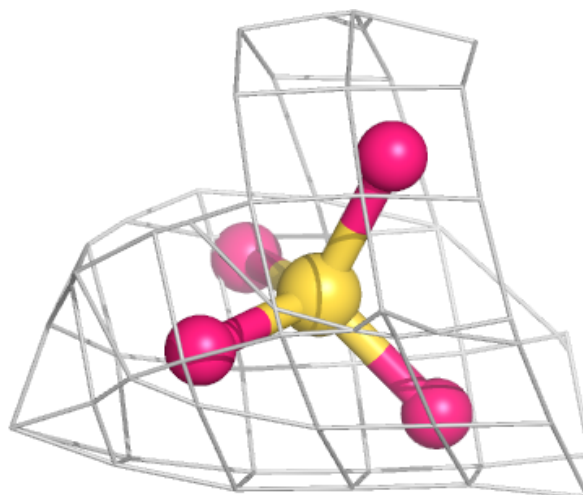
Electron density around SO4 B 505:

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



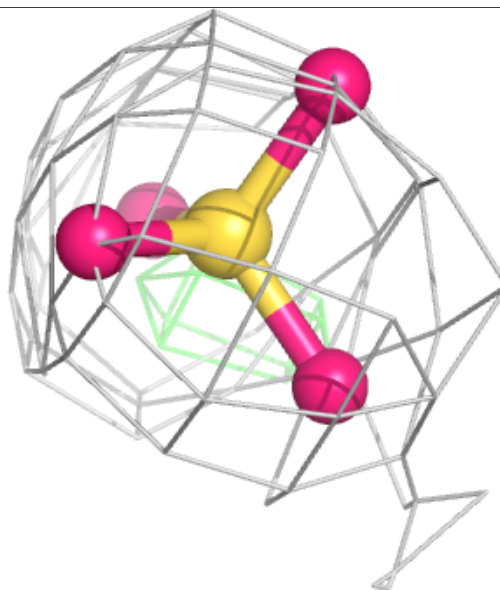
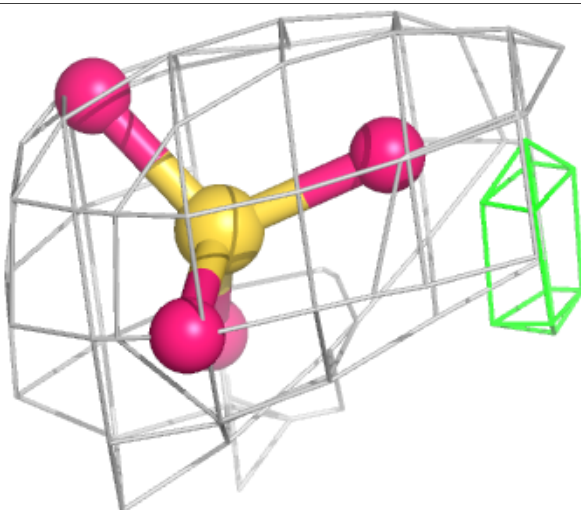
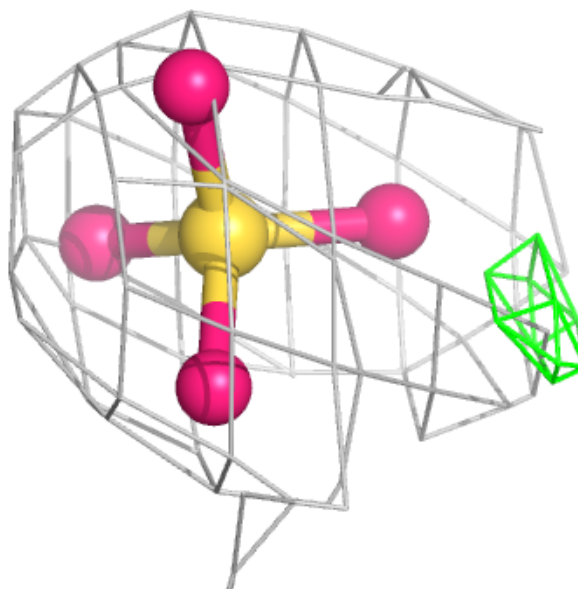
Electron density around SO4 A 406:

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



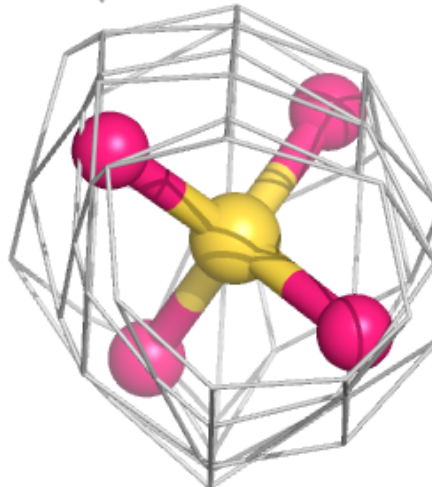
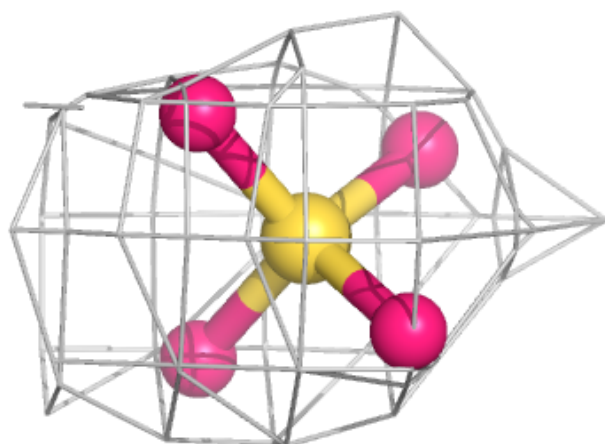
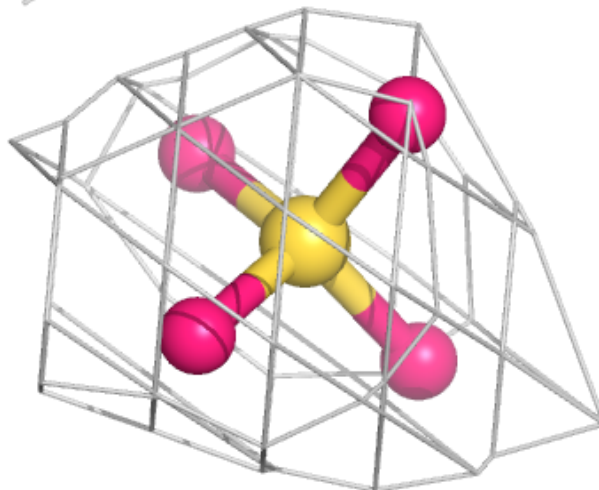
Electron density around SO4 A 404:

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



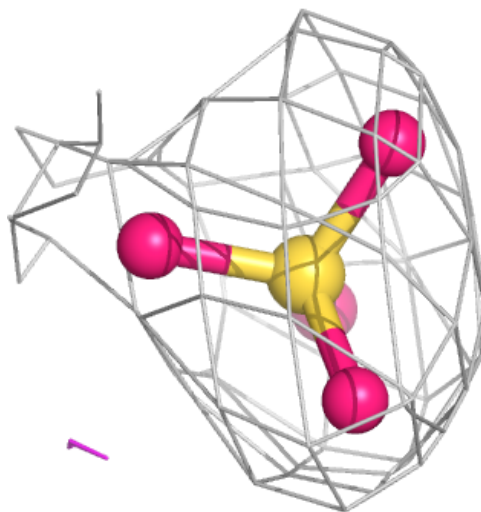
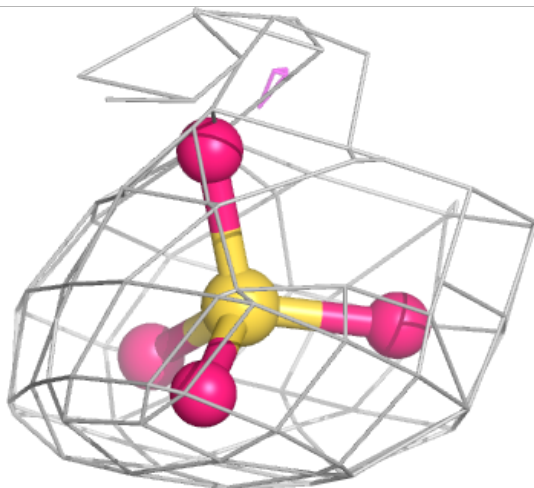
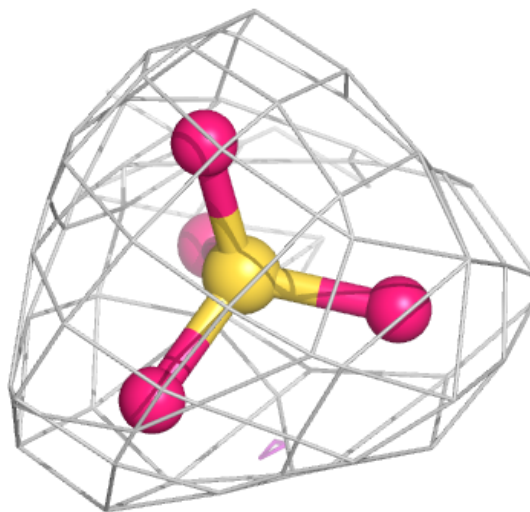
Electron density around SO4 C 404:

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



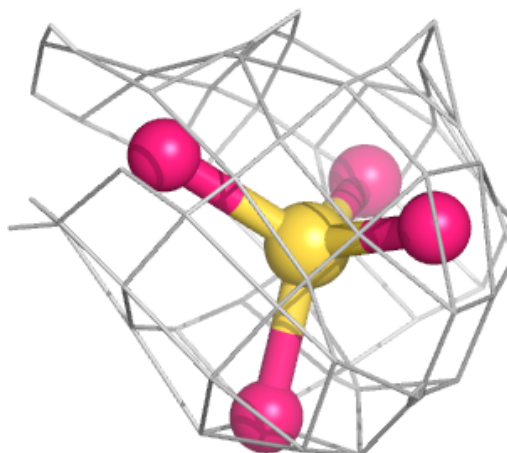
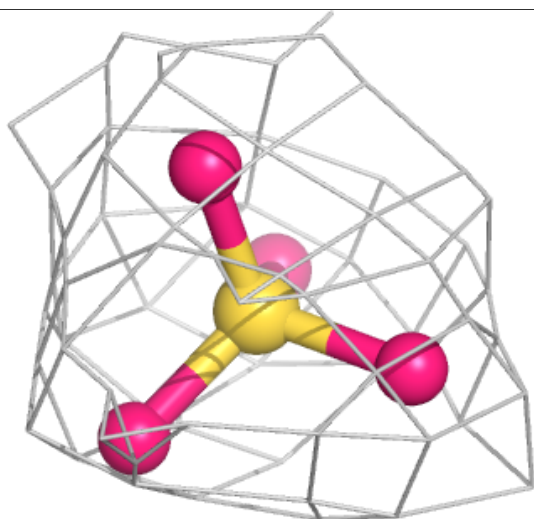
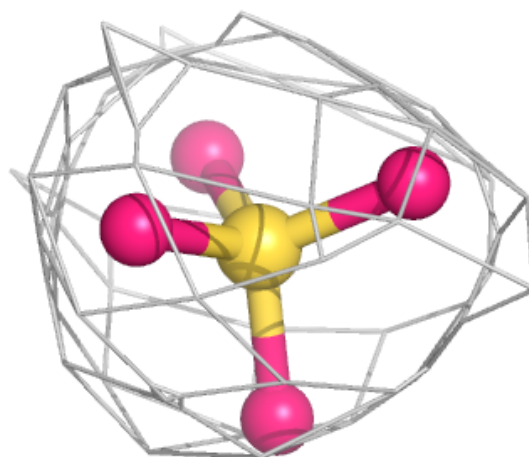
Electron density around SO4 B 503:

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



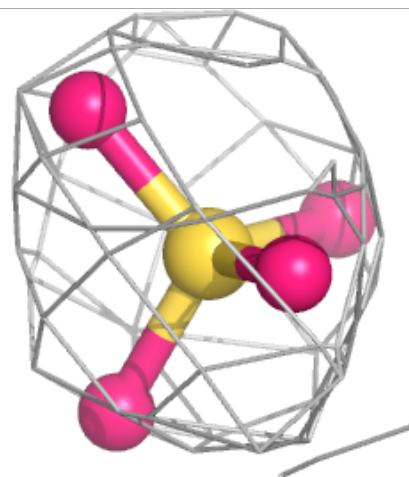
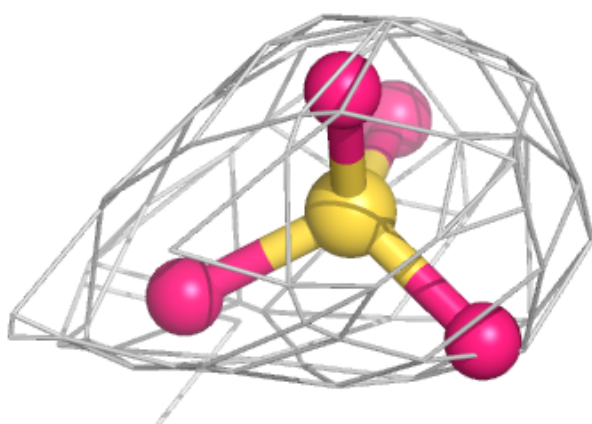
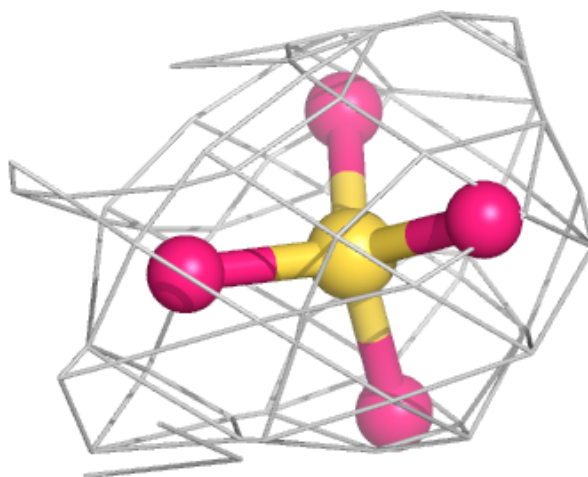
Electron density around SO4 A 405:

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



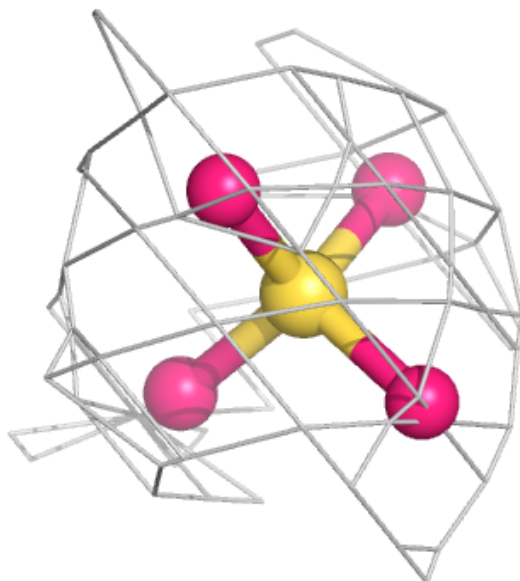
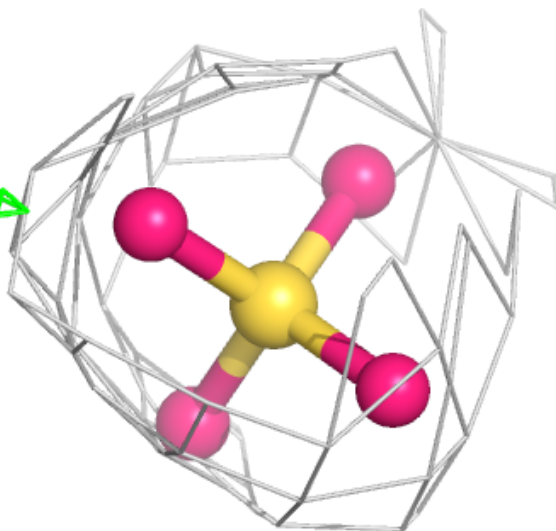
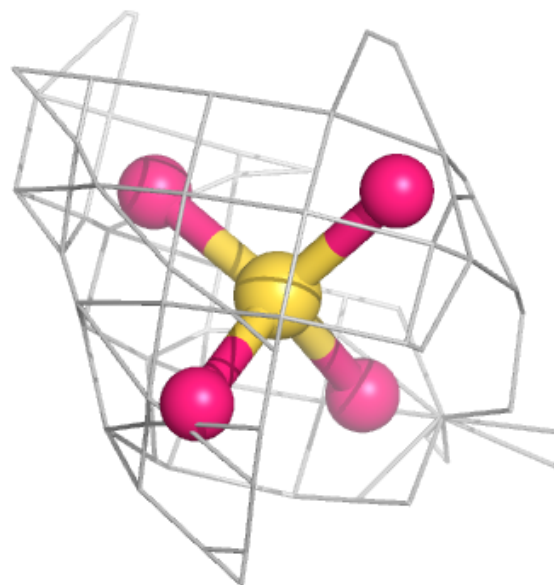
Electron density around SO4 D 502:

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and green (positive)



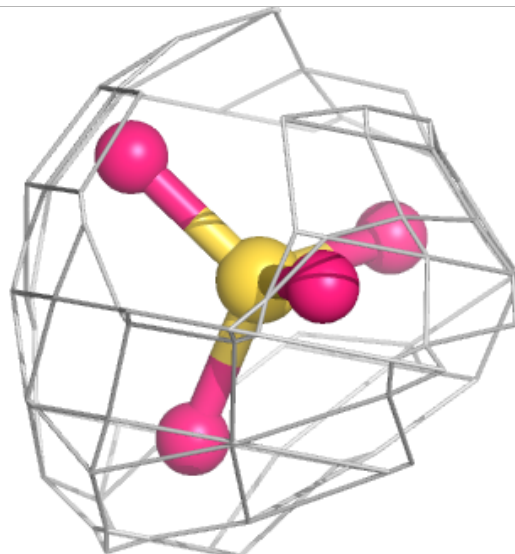
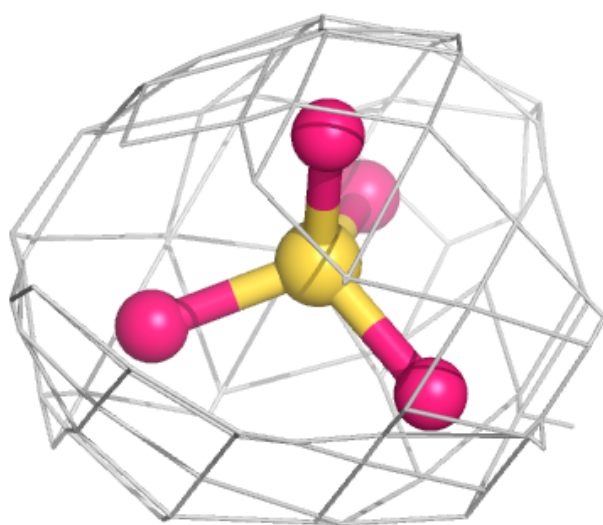
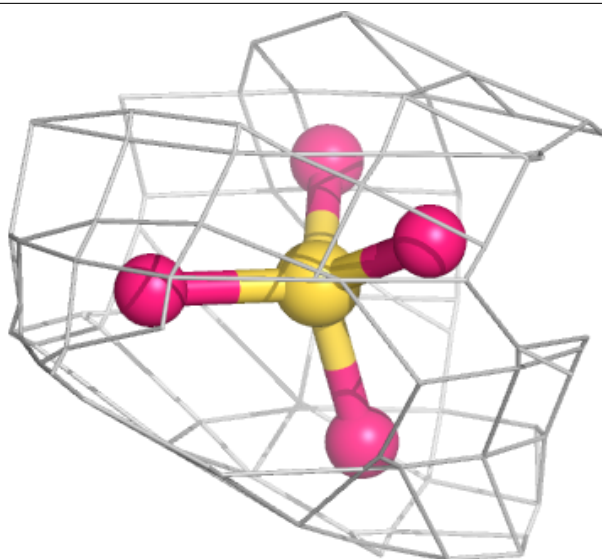
Electron density around SO4 D 503:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
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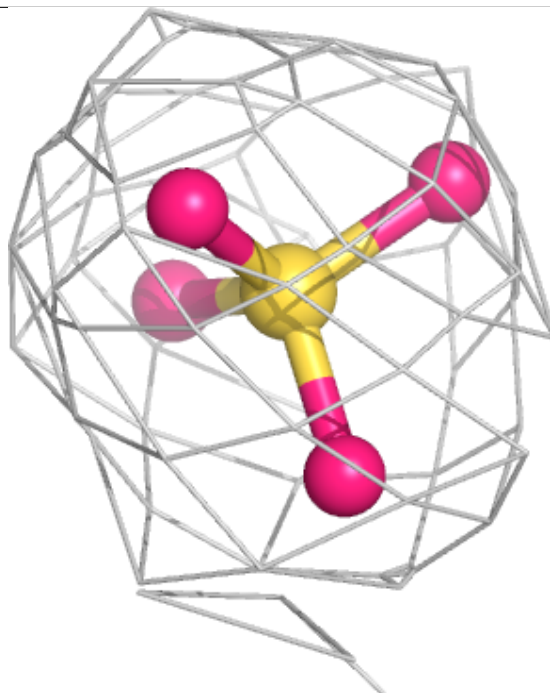
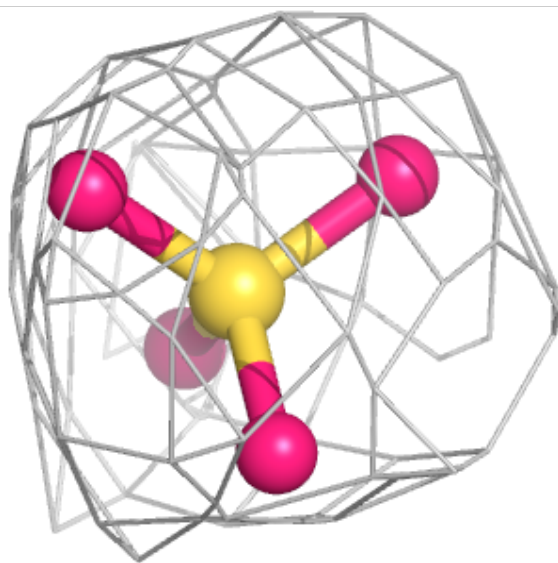
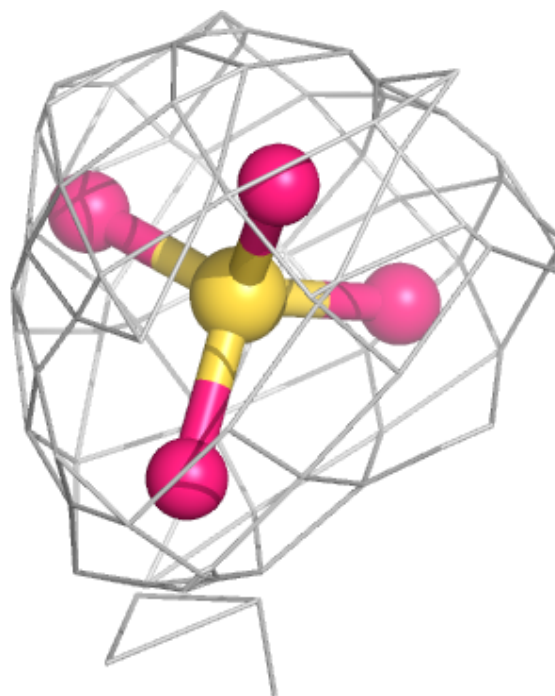
Electron density around SO4 D 501:

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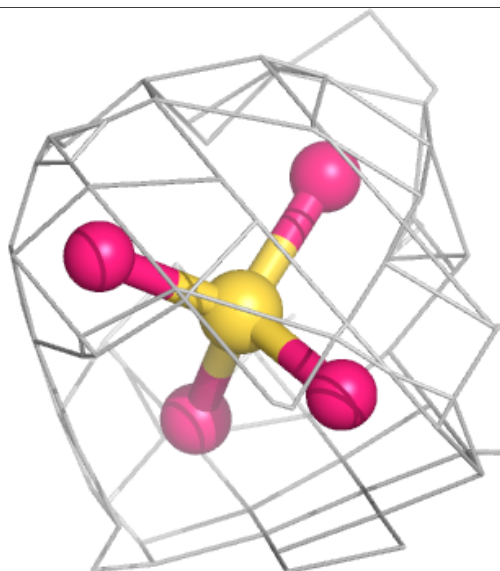
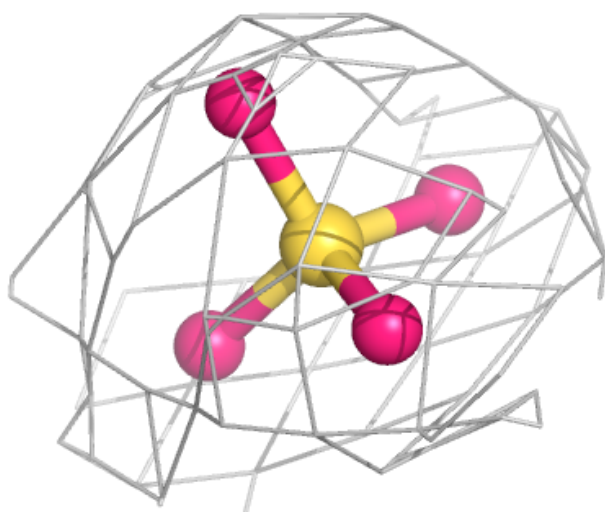
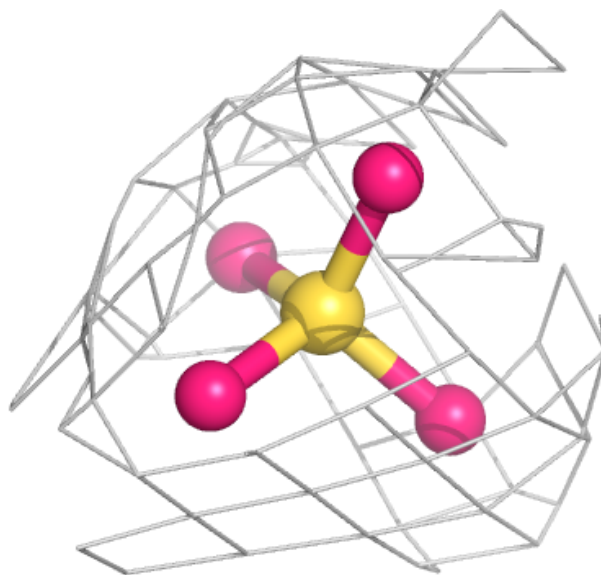
Electron density around SO4 C 403:

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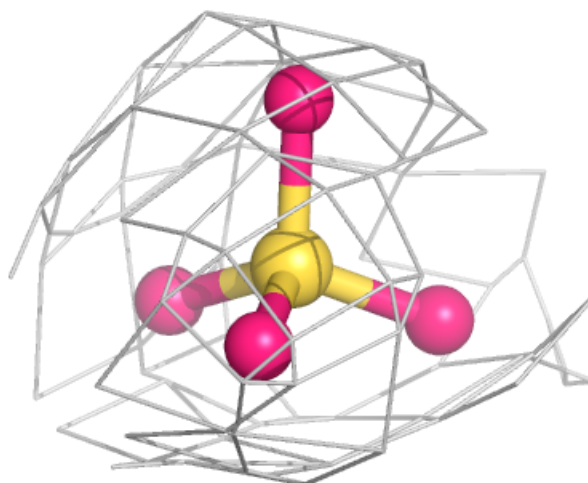
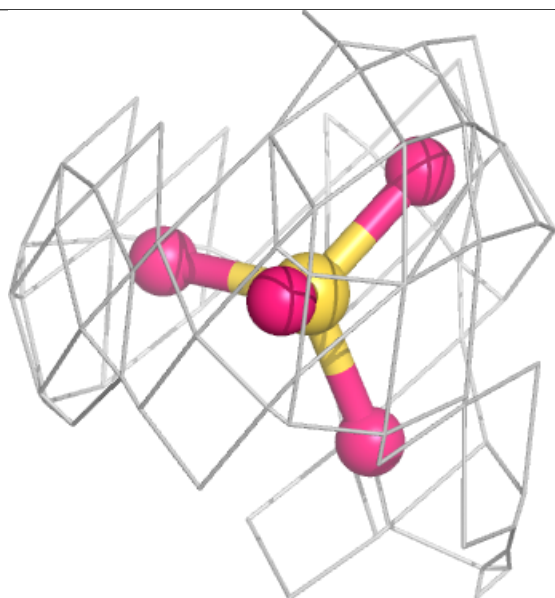
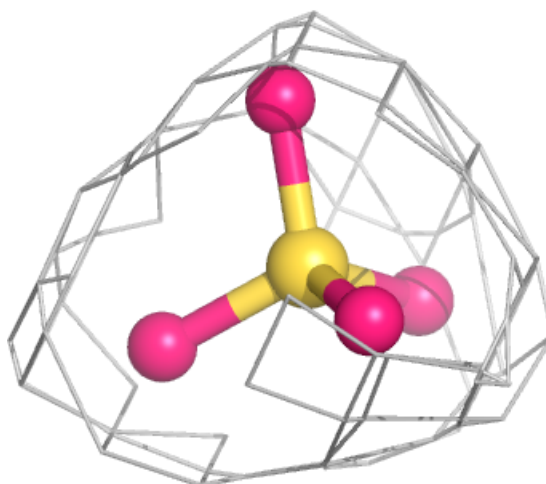
Electron density around SO4 A 403:

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



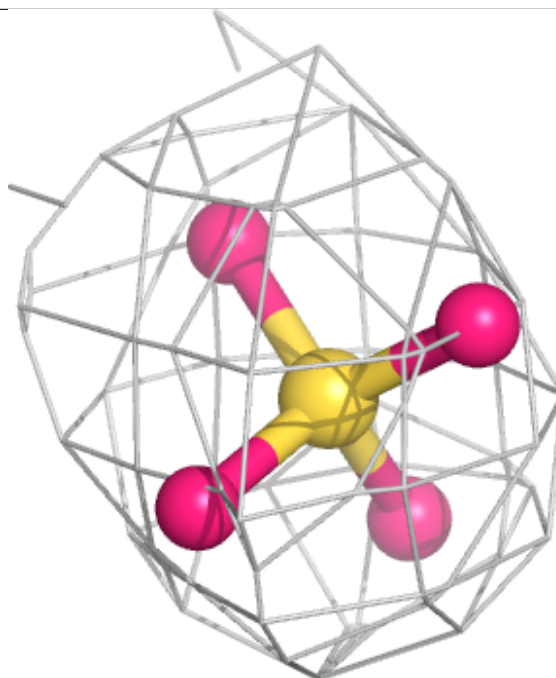
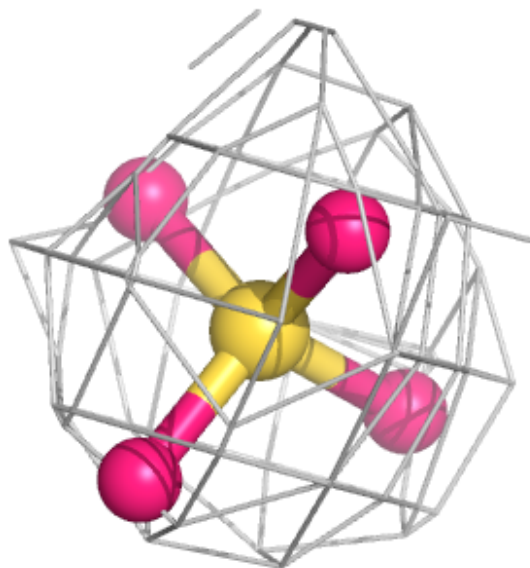
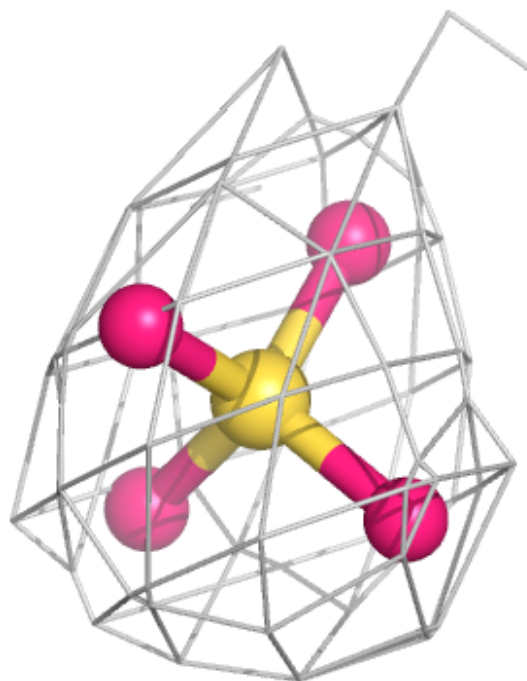
Electron density around SO4 B 504:

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and green (positive)



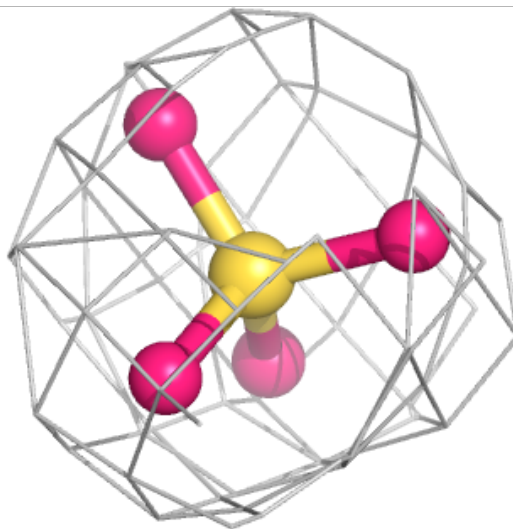
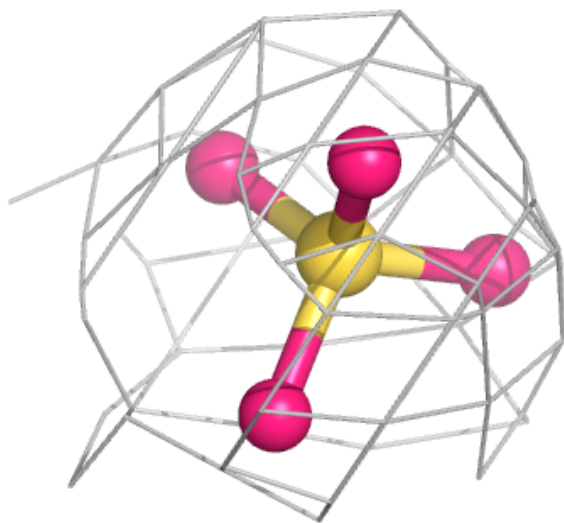
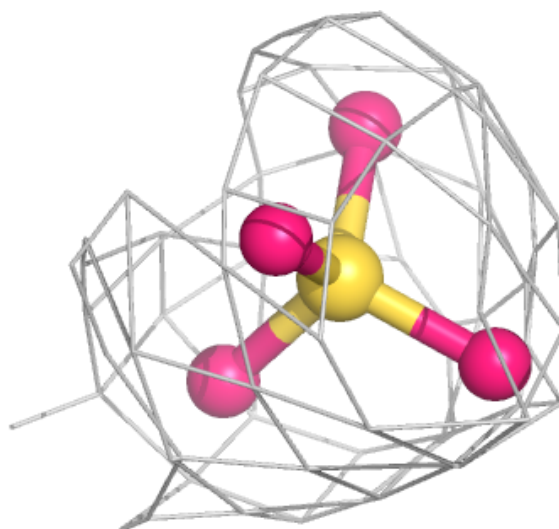
Electron density around SO4 B 502:

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



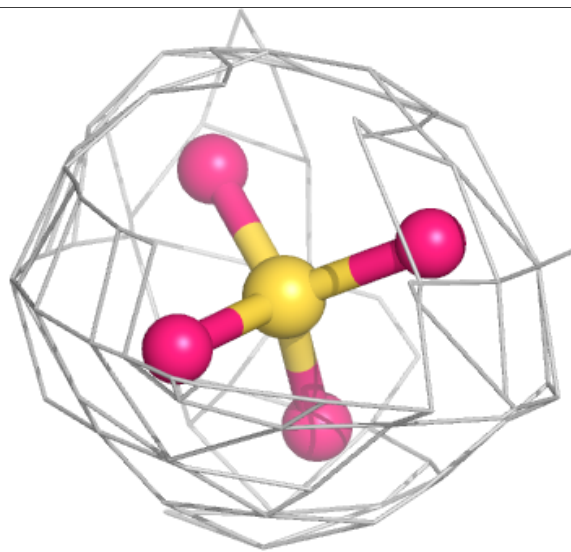
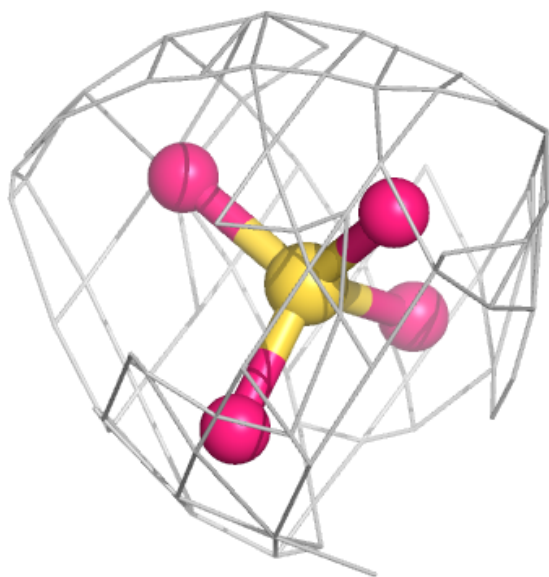
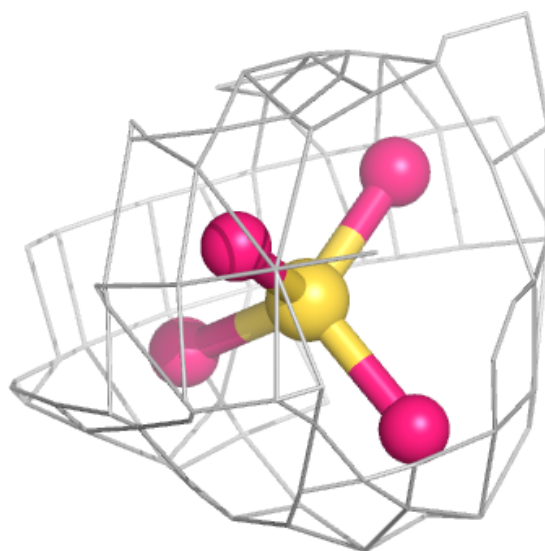
Electron density around SO4 A 408:

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



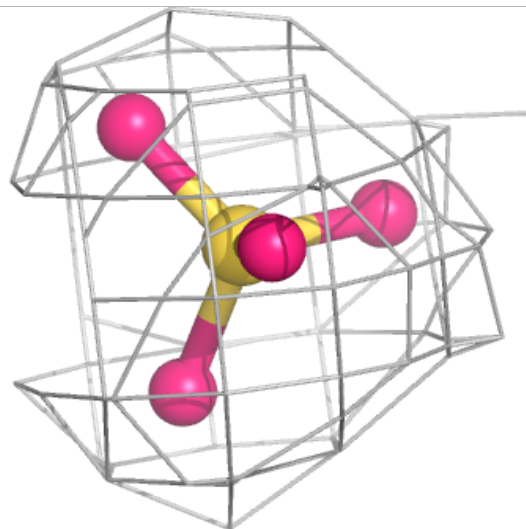
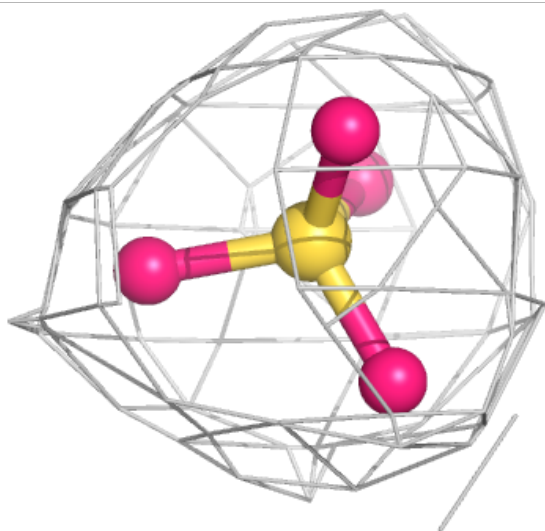
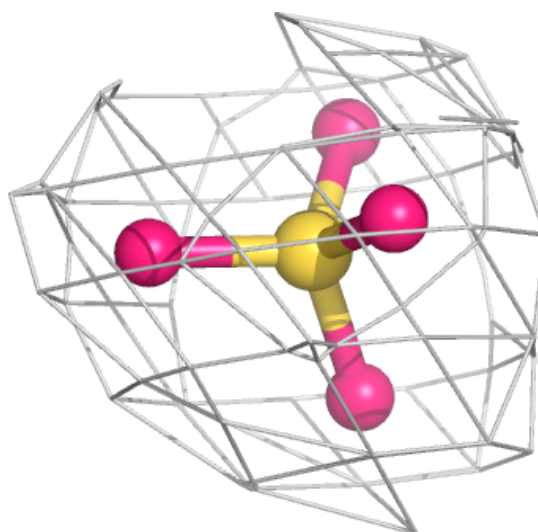
Electron density around SO4 C 402:

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



Electron density around SO4 B 501:

$2mF_o-DF_c$ (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.