



wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 13, 2020 – 12:32 PM EDT

PDB ID : 6VVV
Title : Crystal structure of a Mycobacterium smegmatis transcription initiation complex with Rifampicin-resistant RNA polymerase
Authors : Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on : 2020-02-18
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

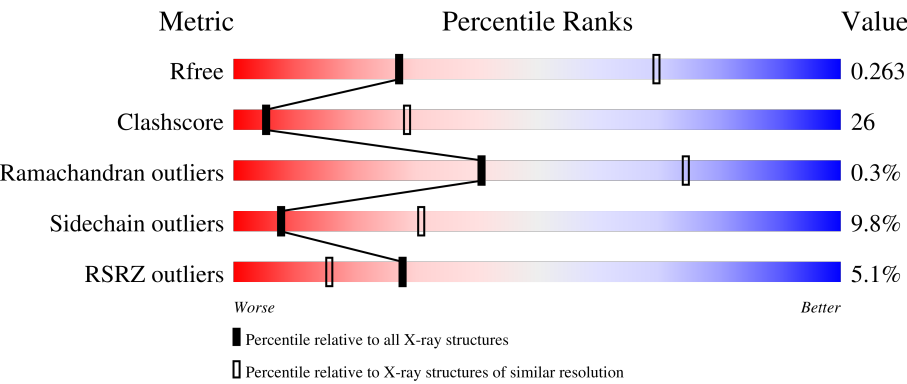
MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.14.6
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.14.6

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	J	114	
2	A	350	
2	B	350	
2	T	350	
3	C	1169	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	D	1317	
5	E	107	
6	F	466	
7	O	31	
8	P	26	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	SO4	D	1403	-	-	X	-
9	SO4	D	1405	-	-	X	-
9	SO4	D	1406	-	-	X	-
9	SO4	F	1201	-	-	X	-
9	SO4	F	1204	-	-	X	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 22970 atoms, of which 16 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 RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	88	Total	C	N	O	S	0	0	0
			678	425	122	129	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	223	Total	C	N	O	S	0	0	0
			1645	1038	284	320	3			
2	B	235	Total	C	N	O	S	0	0	0
			1643	1037	293	312	1			
2	T	53	Total	C	N	O	S	0	0	0
			374	236	65	72	1			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	790	Total	C	N	O	S	0	0	0
			5774	3620	1008	1121	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	447	LEU	SER	conflict	UNP P60281

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1174	Total	C	N	O	S	0	0	0
			8679	5438	1548	1654	39			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	77	Total	C	N	O	0	0	0
			586	372	100	114			

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	302	Total	C	N	O	S	0	0	0
			2349	1474	423	445	7			

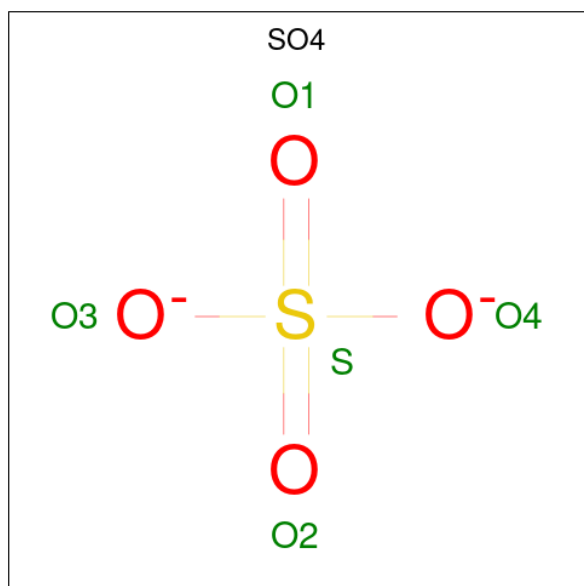
- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	31	Total	C	N	O	P	0	0	0
			635	306	114	185	30			

- Molecule 8 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is SULFATE ION (three-letter code: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	D	1	Total	O	0	0
			3	3		

Continued on next page...

Continued from previous page...

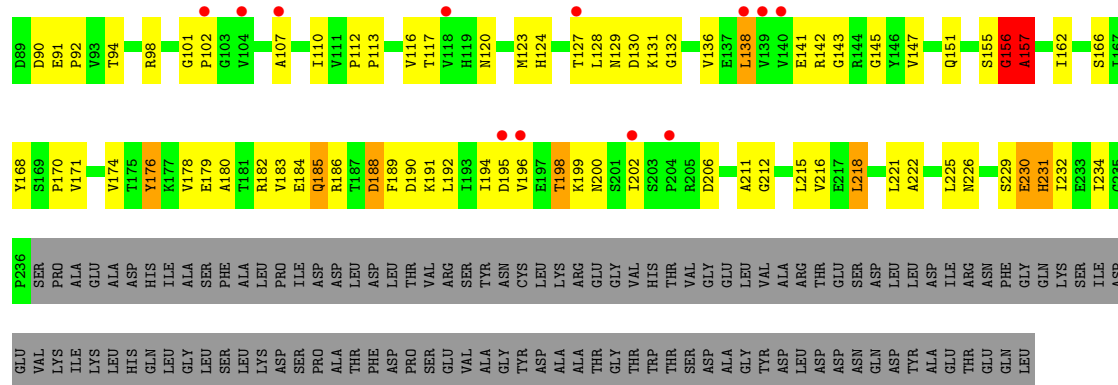
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	D	1	Total	O	S	0	0
			2	1	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	D	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		
9	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by author).

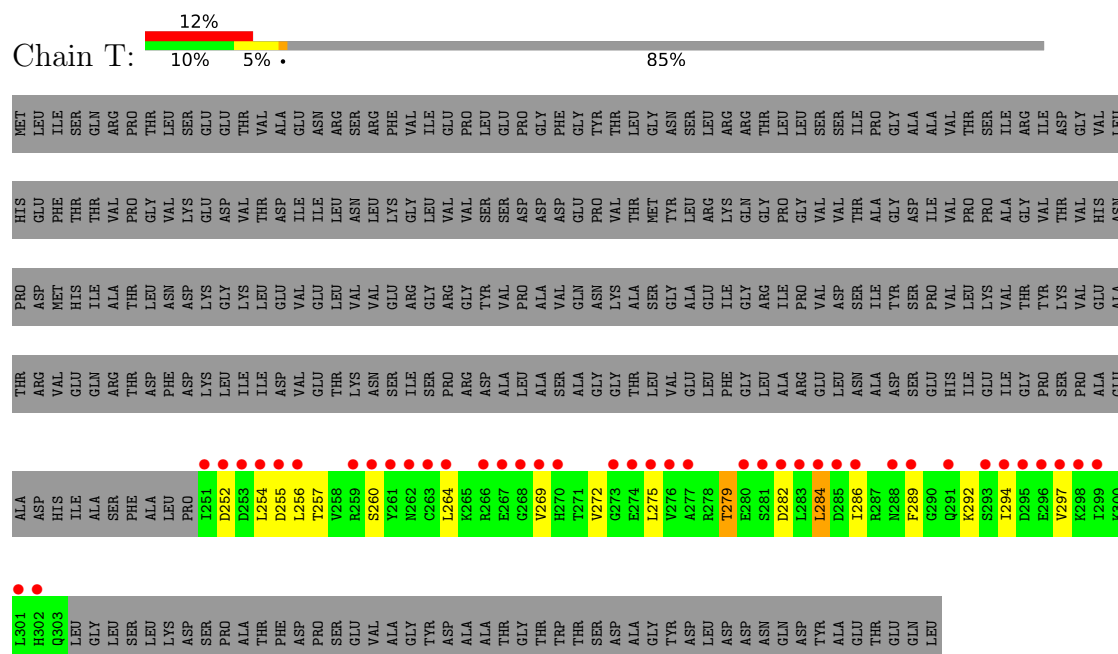
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	2	Total	Zn	0	0
			2	2		

- Molecule 11 is water.

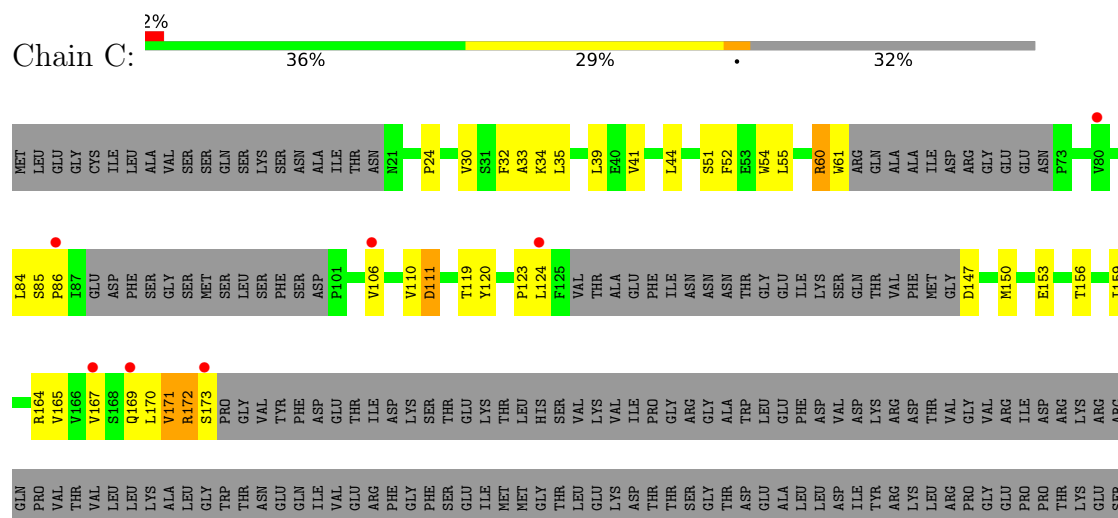
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	H	O	0	0
			3	2	1		
11	D	3	Total	H	O	0	0
			9	6	3		
11	F	3	Total	H	O	0	0
			9	6	3		
11	P	1	Total	H	O	0	0
			3	2	1		

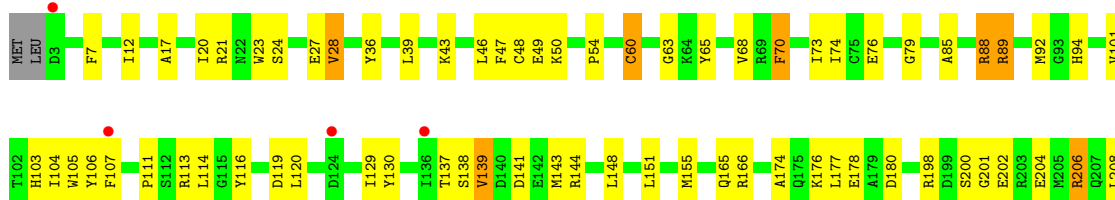


• Molecule 2: DNA-directed RNA polymerase subunit alpha

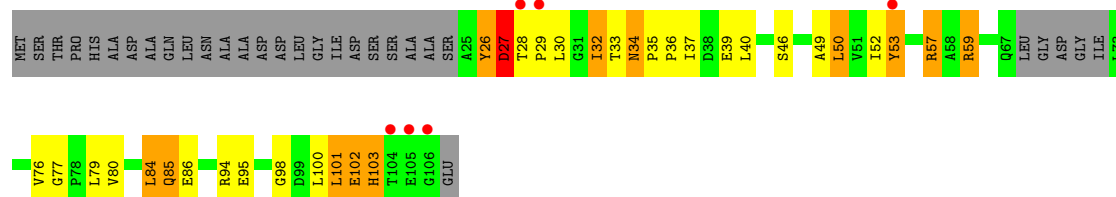


• Molecule 3: DNA-directed RNA polymerase subunit beta

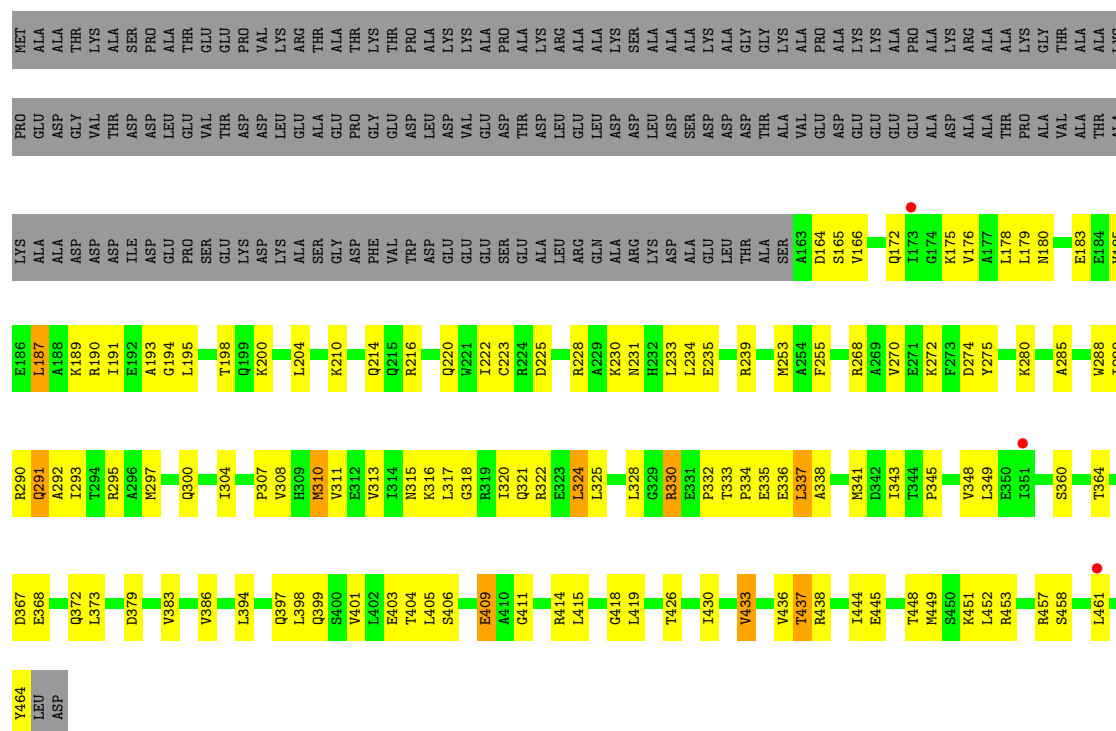




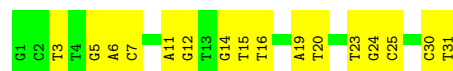




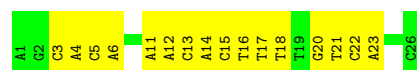
• Molecule 6: RNA polymerase sigma factor SigA



• Molecule 7: DNA (31-MER)



• Molecule 8: DNA (26-MER)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	129.75Å 162.34Å 137.16Å 90.00° 111.27° 90.00°	Depositor
Resolution (Å)	49.83 – 3.20 49.83 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.5 (49.83-3.20) 95.4 (49.83-3.20)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.03 (at 3.19Å)	Xtriage
Refinement program	PHENIX v0	Depositor
R, R_{free}	0.234 , 0.262 0.236 , 0.263	Depositor DCC
R_{free} test set	1957 reflections (2.36%)	wwPDB-VP
Wilson B-factor (Å ²)	119.1	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 78.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	22970	wwPDB-VP
Average B, all atoms (Å ²)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	J	0.24	0/692	0.43	0/940
2	A	0.24	0/1671	0.46	0/2279
2	B	0.24	0/1670	0.47	1/2292 (0.0%)
2	T	0.22	0/376	0.35	0/511
3	C	0.25	0/5870	0.44	1/7988 (0.0%)
4	D	0.24	0/8815	0.42	2/11982 (0.0%)
5	E	0.24	0/597	0.40	0/814
6	F	0.22	0/2379	0.38	0/3218
7	O	0.51	0/712	0.94	0/1098
8	P	0.51	0/589	0.91	0/906
All	All	0.26	0/23371	0.48	4/32028 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	1
2	B	0	2
3	C	0	5
4	D	0	1
5	E	0	1
All	All	0	10

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	984	LEU	CA-CB-CG	5.86	128.77	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	579	LEU	CA-CB-CG	5.78	128.59	115.30
2	B	206	ASP	CB-CG-OD2	5.21	122.99	118.30
4	D	405	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	156	GLY	Peptide
2	B	157	ALA	Peptide
3	C	171	VAL	Peptide
3	C	398	GLN	Peptide
1	J	109	ARG	Peptide

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	J	678	0	642	36	0
2	A	1645	0	1656	109	0
2	B	1643	0	1583	115	0
2	T	374	0	344	13	0
3	C	5774	0	5503	374	0
4	D	8679	0	8318	457	1
5	E	586	0	567	41	0
6	F	2349	0	2346	110	0
7	O	635	0	354	30	0
8	P	526	0	296	18	0
9	D	35	0	0	9	0
9	F	20	0	0	9	1
10	D	2	0	0	0	0
11	C	1	2	0	1	0
11	D	3	6	0	2	0
11	F	3	6	0	2	0
11	P	1	2	0	0	0
All	All	22954	16	21609	1170	1

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 26.

The worst 5 of 1170 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:J:68:ASP:HA	1:J:69:VAL:HG22	1.28	1.09
2:B:90:ASP:HA	2:B:142:ARG:HG3	1.35	1.09
3:C:758:GLU:HG2	3:C:798:THR:HG22	1.33	1.08
3:C:937:ILE:HD11	3:C:955:TYR:HB3	1.31	1.06
3:C:937:ILE:HD13	3:C:939:VAL:HG12	1.35	1.06

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:628:SER:OG	9:F:1201:SO4:O4[1_554]	1.88	0.32

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	J	86/114 (75%)	80 (93%)	6 (7%)	0	100	100
2	A	221/350 (63%)	208 (94%)	11 (5%)	2 (1%)	17	56
2	B	233/350 (67%)	213 (91%)	16 (7%)	4 (2%)	9	42
2	T	51/350 (15%)	50 (98%)	1 (2%)	0	100	100
3	C	774/1169 (66%)	720 (93%)	52 (7%)	2 (0%)	41	74
4	D	1160/1317 (88%)	1118 (96%)	41 (4%)	1 (0%)	51	83
5	E	73/107 (68%)	69 (94%)	3 (4%)	1 (1%)	11	46
6	F	300/466 (64%)	296 (99%)	4 (1%)	0	100	100
All	All	2898/4223 (69%)	2754 (95%)	134 (5%)	10 (0%)	41	74

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1169	ILE
5	E	27	ASP
2	A	158	GLU
3	C	172	ARG
2	B	157	ALA

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	J	68/98 (69%)	57 (84%)	11 (16%)	2	11
2	A	178/297 (60%)	158 (89%)	20 (11%)	6	25
2	B	162/297 (54%)	148 (91%)	14 (9%)	10	38
2	T	35/297 (12%)	31 (89%)	4 (11%)	5	24
3	C	579/984 (59%)	520 (90%)	59 (10%)	7	29
4	D	853/1095 (78%)	779 (91%)	74 (9%)	10	37
5	E	60/86 (70%)	46 (77%)	14 (23%)	1	3
6	F	241/379 (64%)	224 (93%)	17 (7%)	14	47
All	All	2176/3533 (62%)	1963 (90%)	213 (10%)	8	31

5 of 213 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	1008	GLU
4	D	206	ARG
6	F	291	GLN
3	C	1045	GLN
4	D	70	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	165	GLN
4	D	410	GLN
6	F	326	GLN
4	D	245	GLN
4	D	267	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
9	SO4	F	1201	-	4,4,4	0.15	0	6,6,6	0.06	0
9	SO4	D	1403	-	4,4,4	0.15	0	6,6,6	0.07	0
9	SO4	D	1404	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	D	1406	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	F	1204	-	4,4,4	0.13	0	6,6,6	0.09	0
9	SO4	D	1402	-	0,1,4	0.00	-	-		
9	SO4	D	1405	-	4,4,4	0.14	0	6,6,6	0.06	0
9	SO4	F	1203	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SO4	F	1202	-	4,4,4	0.14	0	6,6,6	0.04	0
9	SO4	D	1407	-	4,4,4	0.15	0	6,6,6	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	SO4	D	1408	-	4,4,4	0.14	0	6,6,6	0.07	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

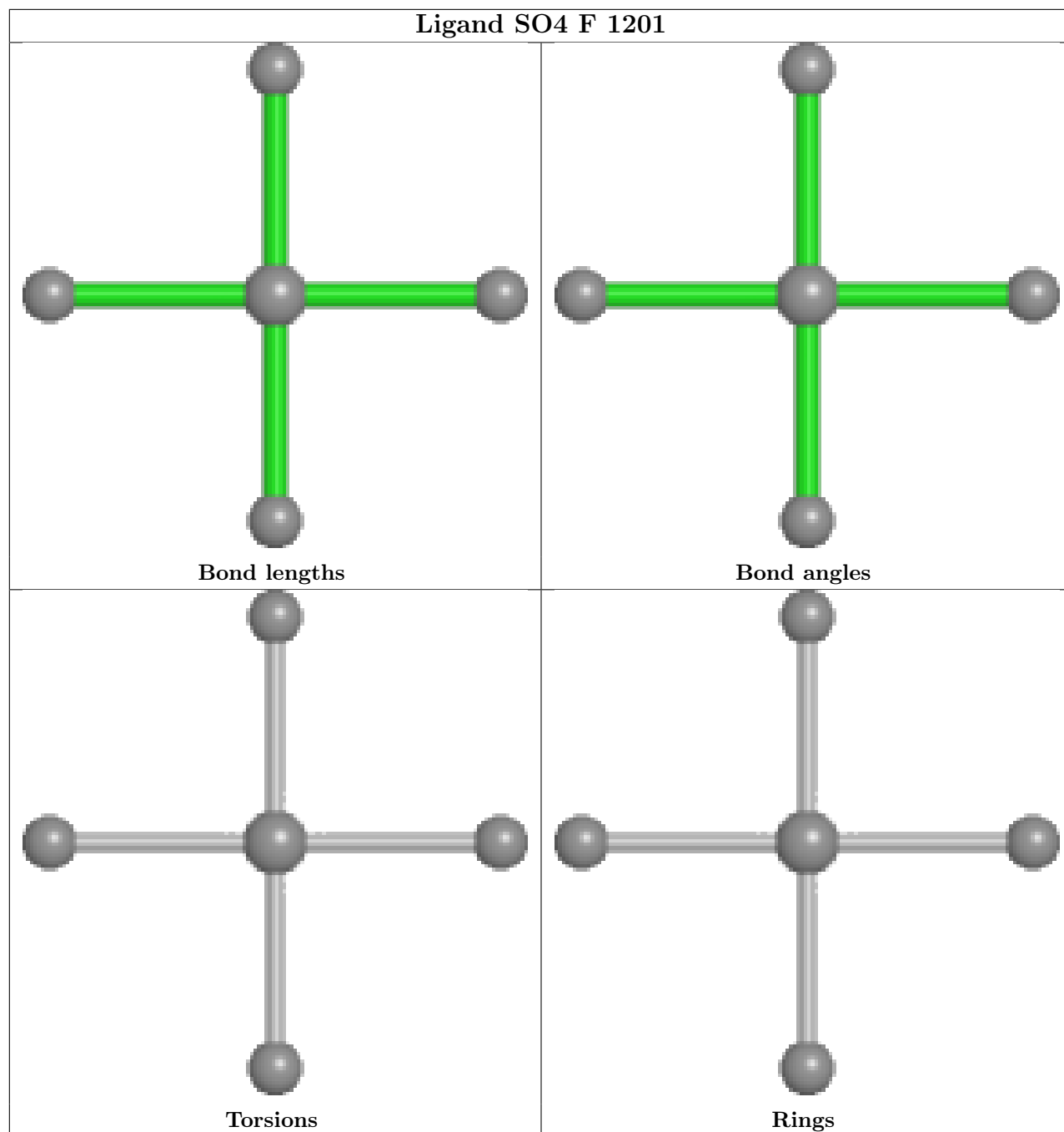
There are no torsion outliers.

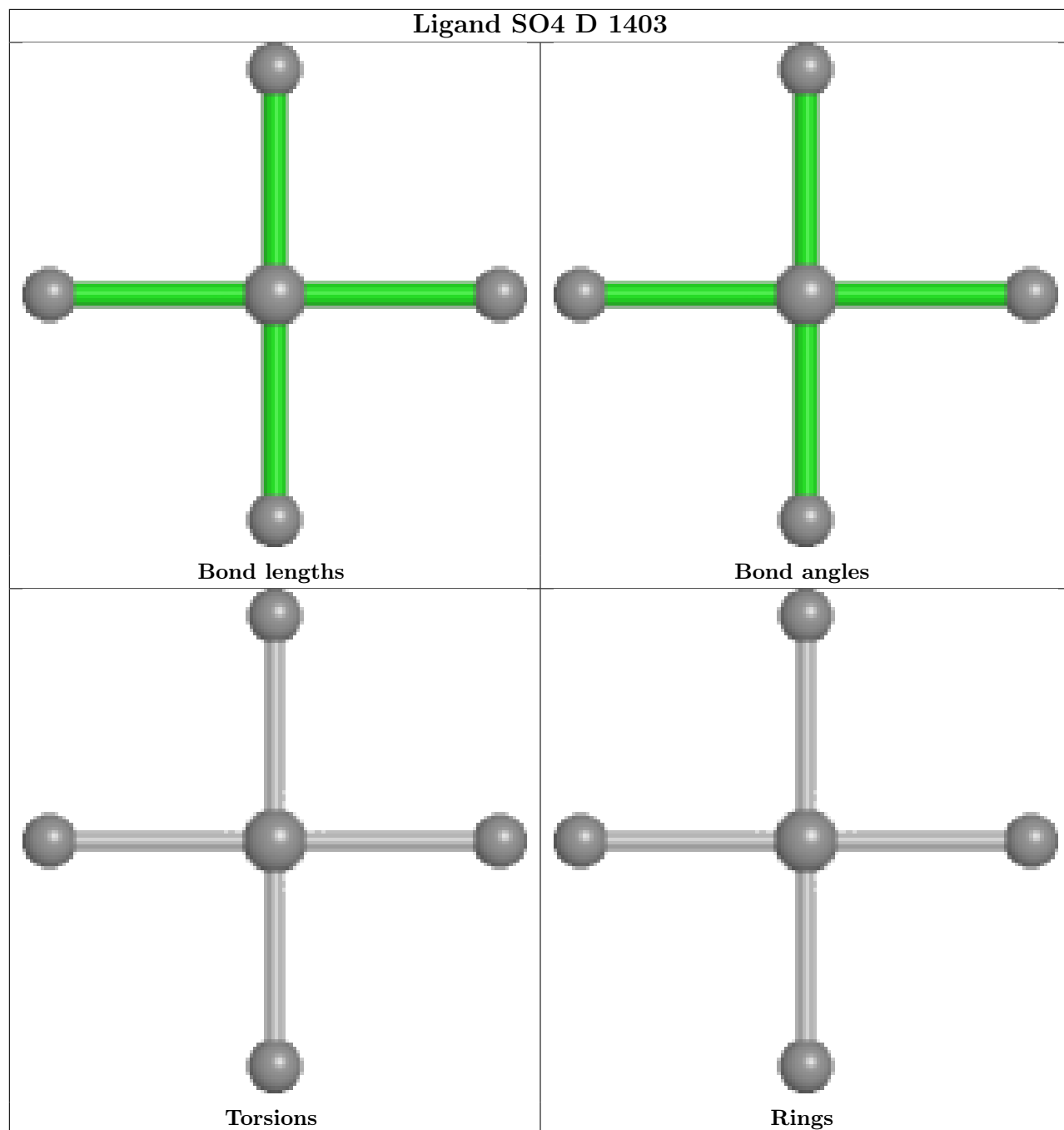
There are no ring outliers.

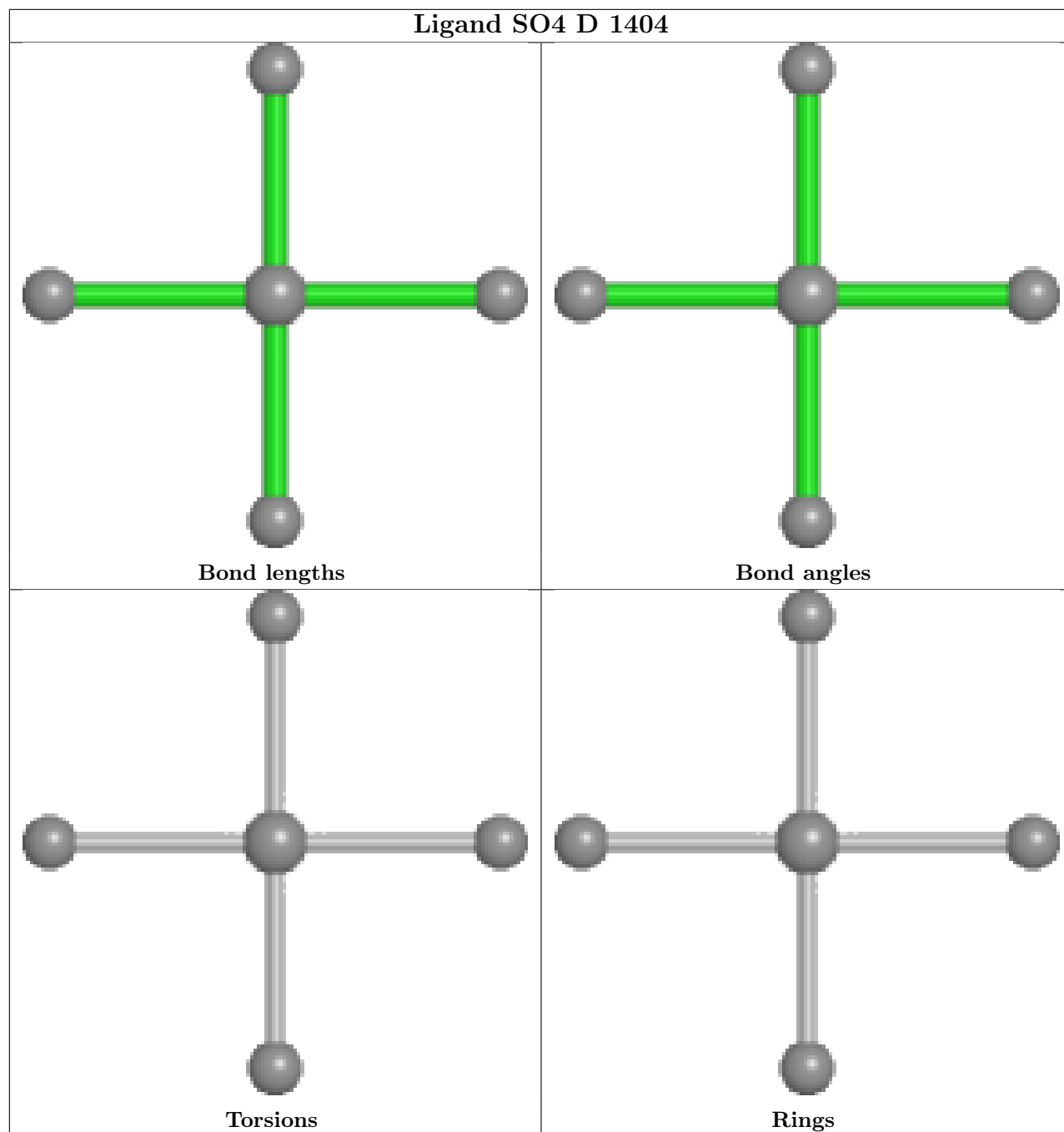
10 monomers are involved in 19 short contacts:

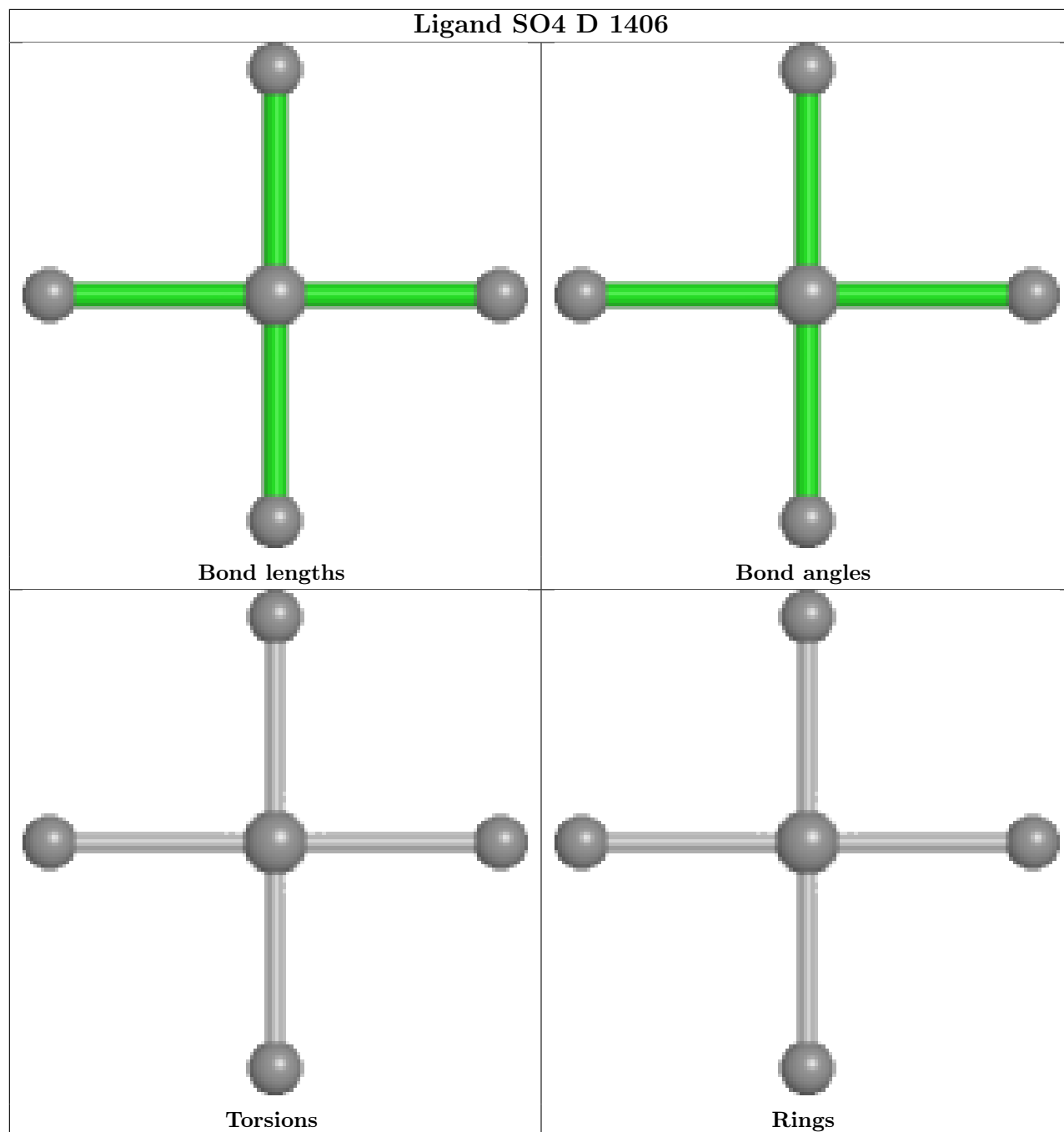
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	1201	SO4	3	1
9	D	1403	SO4	2	0
9	D	1404	SO4	1	0
9	D	1406	SO4	2	0
9	F	1204	SO4	4	0
9	D	1405	SO4	2	0
9	F	1203	SO4	1	0
9	F	1202	SO4	1	0
9	D	1407	SO4	1	0
9	D	1408	SO4	1	0

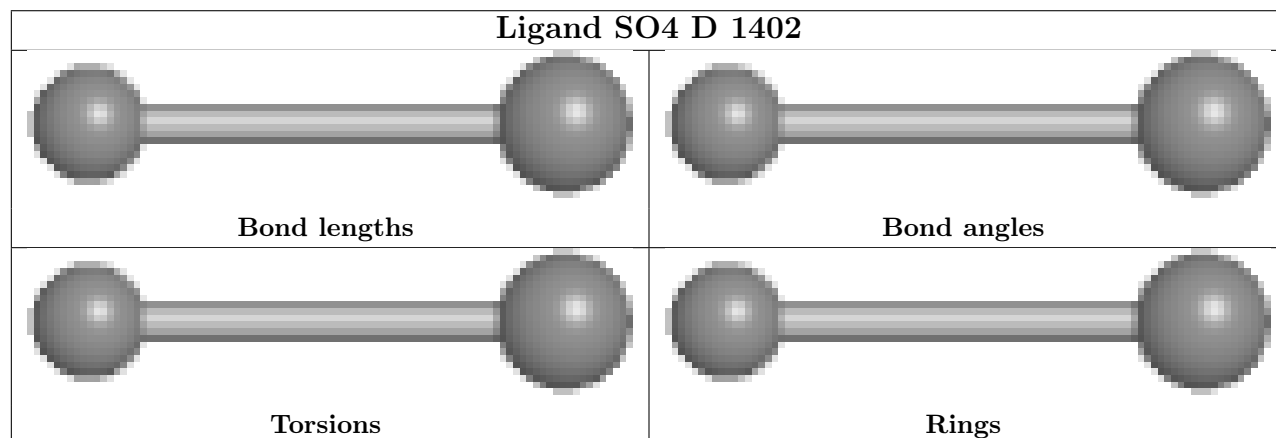
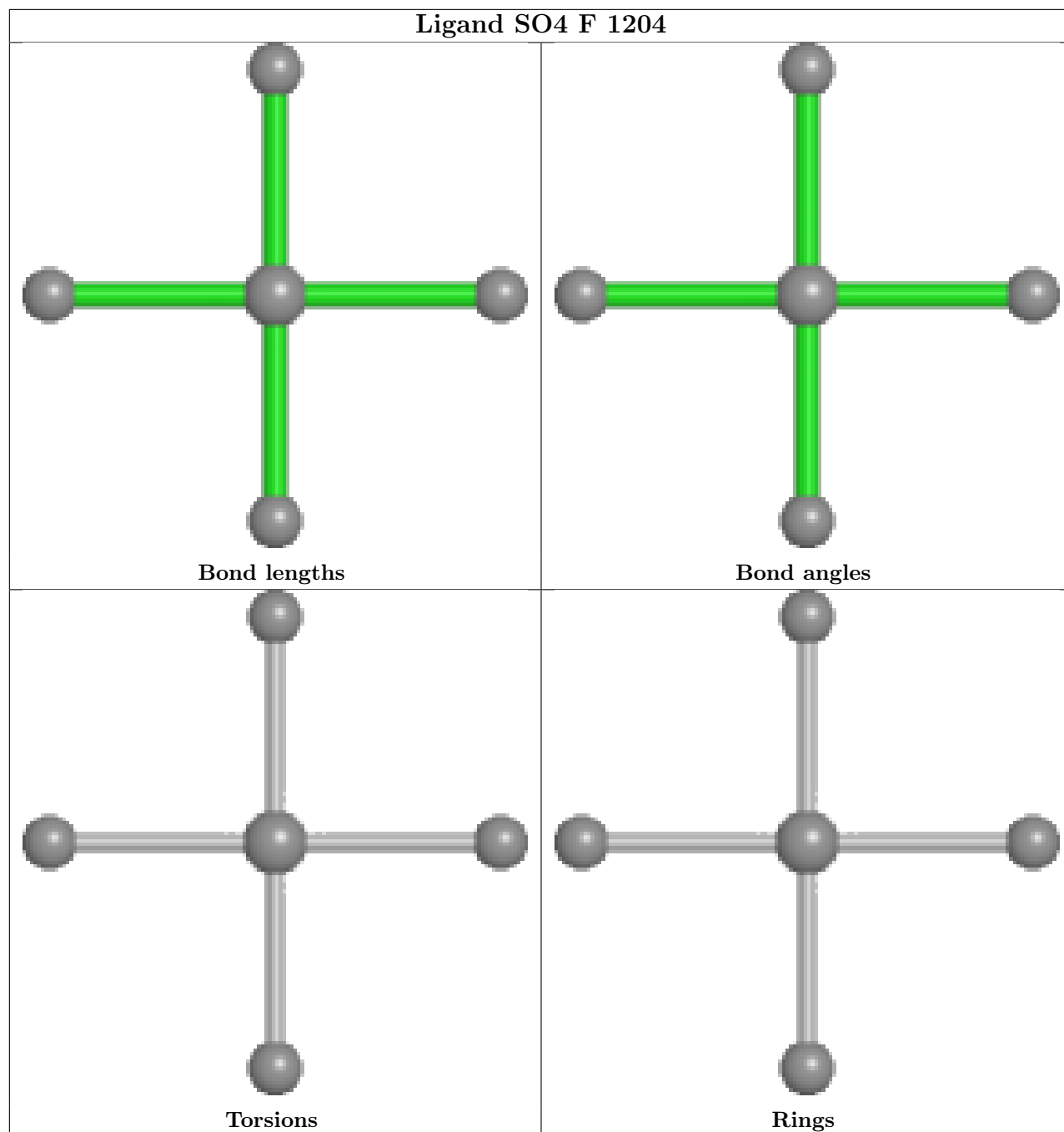
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

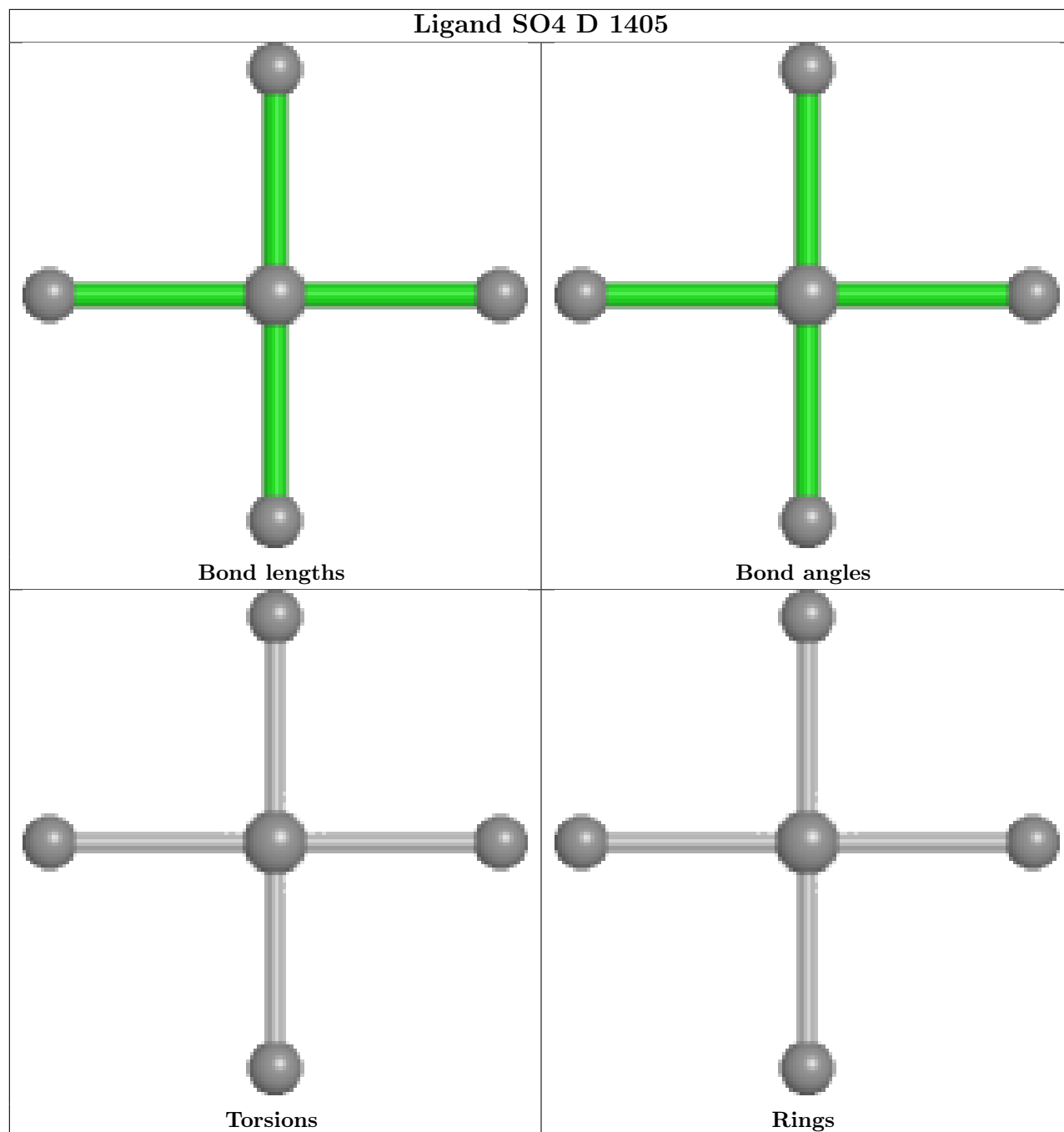


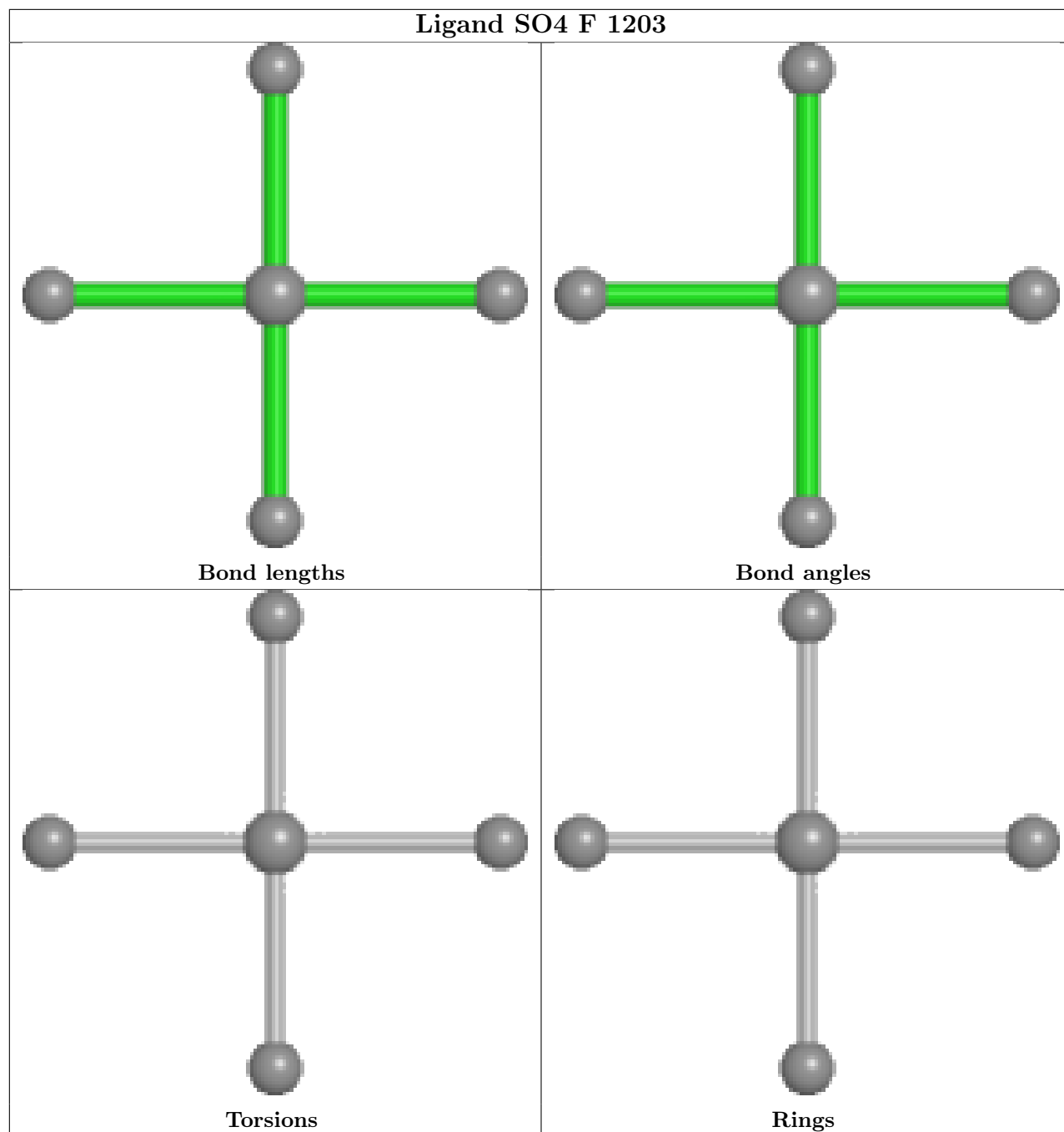


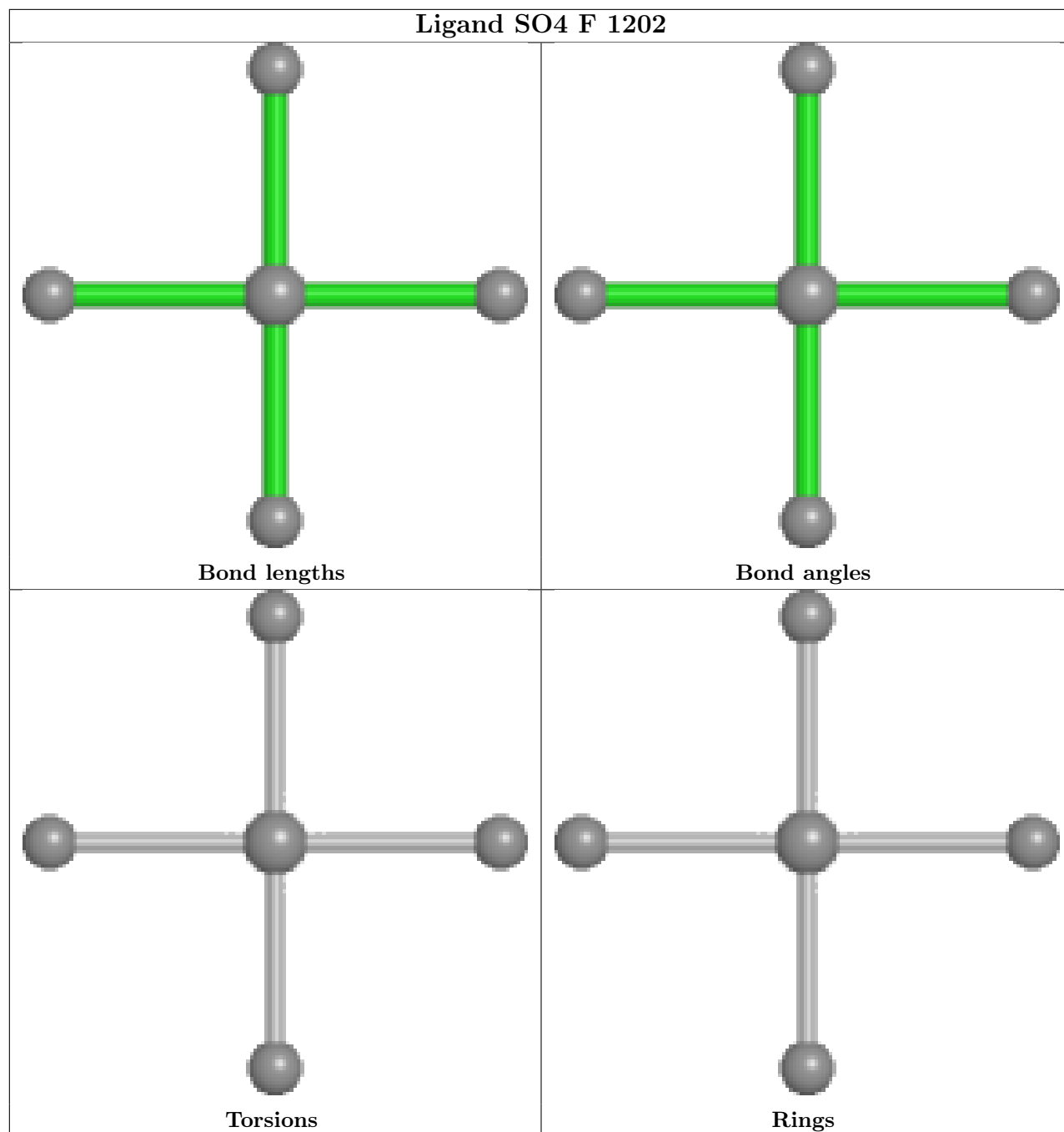


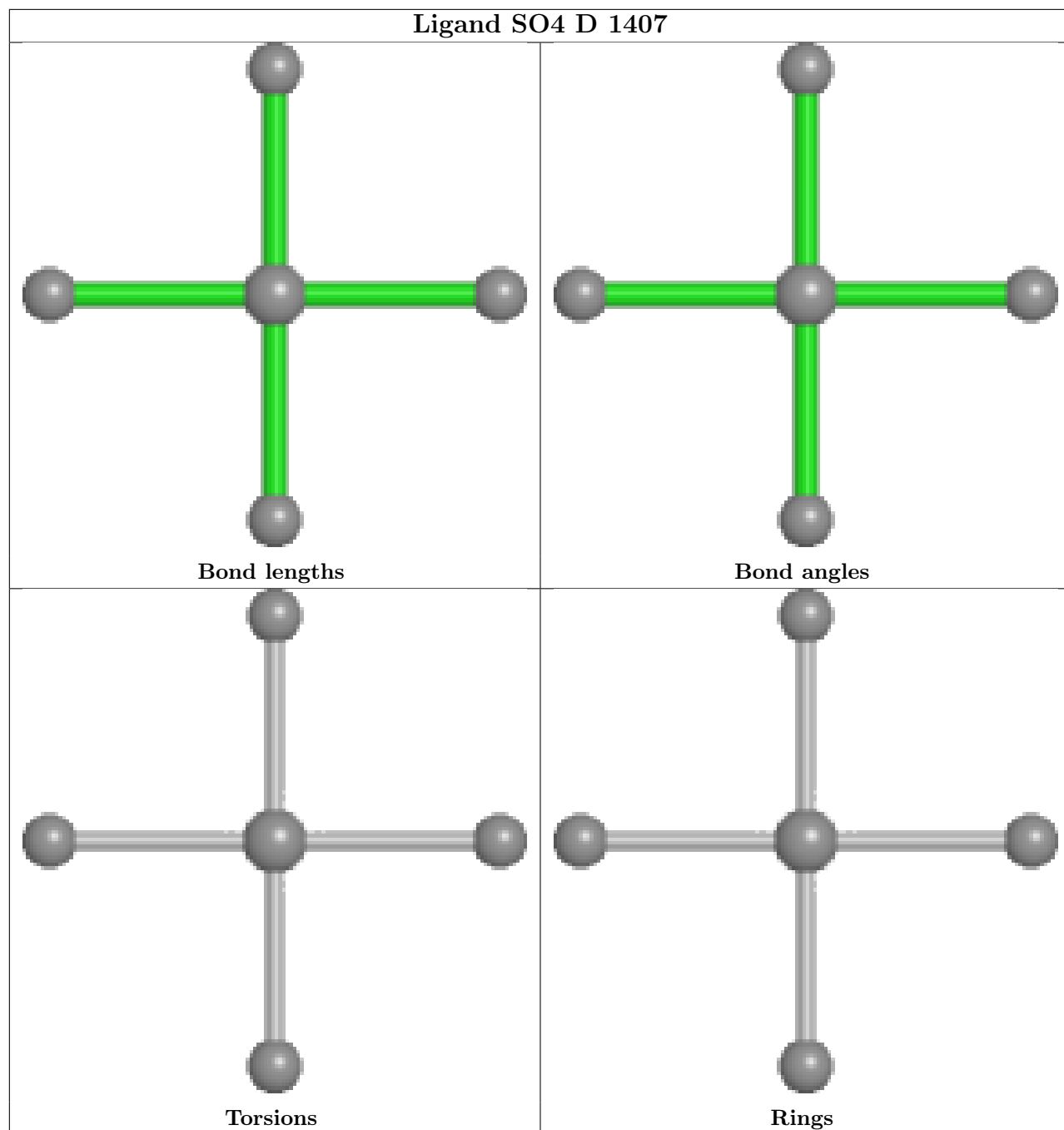


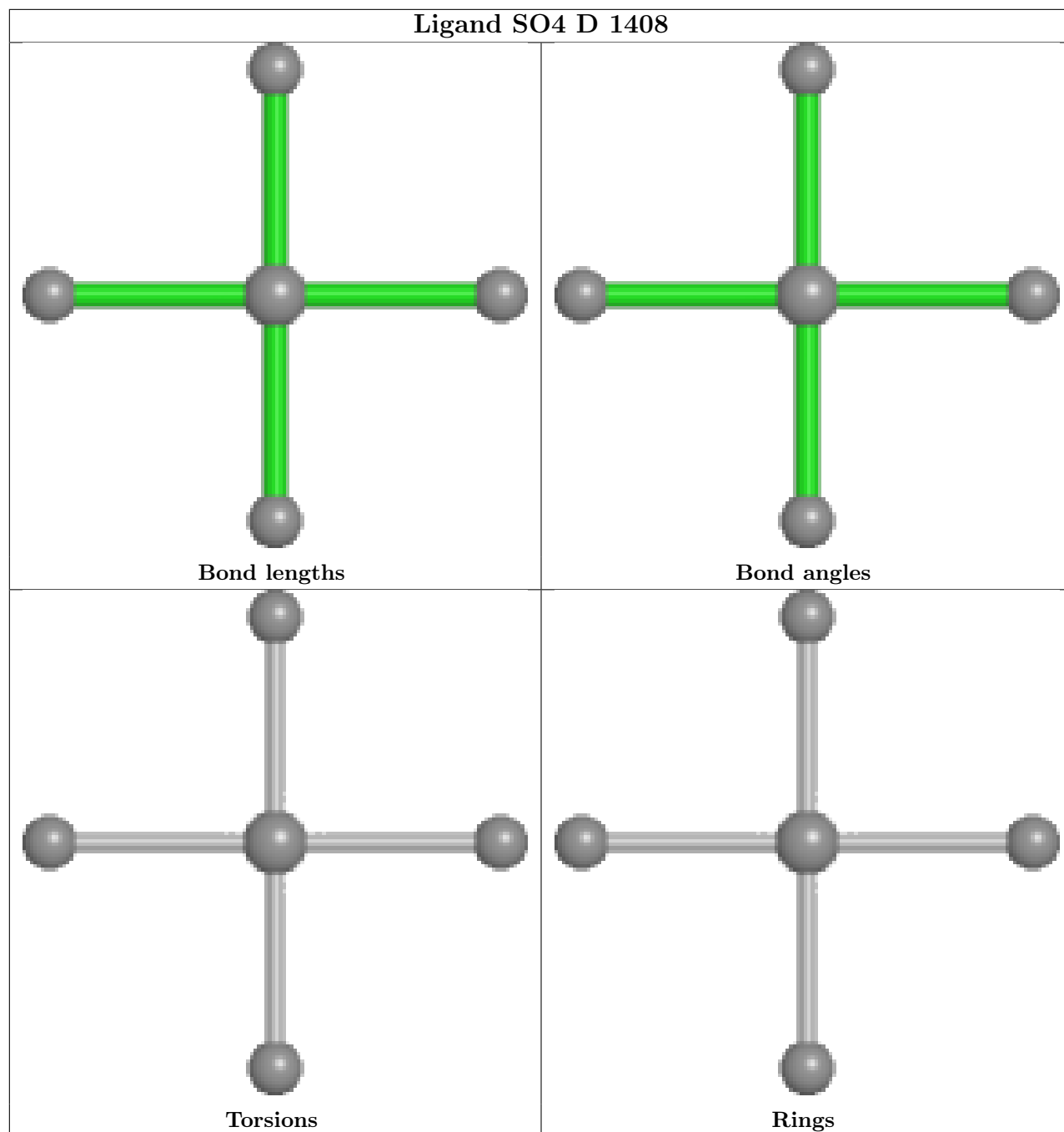


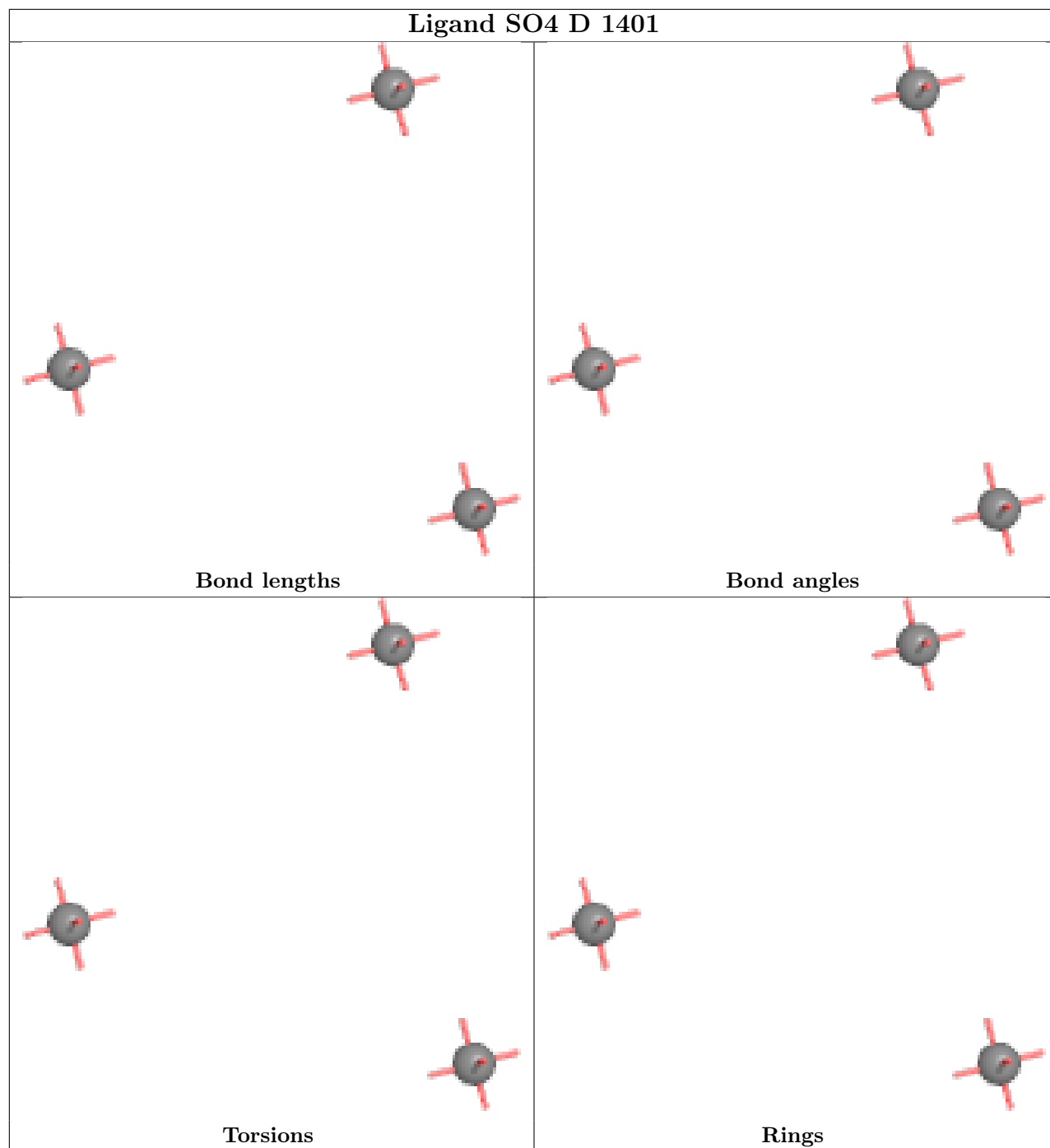












5.7 Other polymers [i](#)

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	J	88/114 (77%)	-0.17	1 (1%) 80 69	76, 128, 174, 187	0
2	A	223/350 (63%)	-0.04	1 (0%) 92 89	82, 115, 150, 177	0
2	B	235/350 (67%)	0.18	15 (6%) 19 11	86, 136, 167, 206	0
2	T	53/350 (15%)	3.61	41 (77%) 0 0	170, 212, 225, 234	0
3	C	790/1169 (67%)	0.19	27 (3%) 45 29	63, 116, 174, 201	0
4	D	1174/1317 (89%)	0.22	59 (5%) 28 16	53, 107, 180, 215	0
5	E	77/107 (71%)	0.42	6 (7%) 13 7	80, 112, 164, 184	0
6	F	302/466 (64%)	0.01	3 (0%) 82 72	64, 104, 146, 189	0
7	O	31/31 (100%)	-0.79	0 100 100	81, 107, 150, 162	0
8	P	26/26 (100%)	-0.74	0 100 100	95, 107, 150, 162	0
All	All	2999/4280 (70%)	0.20	153 (5%) 28 16	53, 115, 179, 234	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	T	289	PHE	8.6
5	E	106	GLY	7.5
4	D	766	HIS	7.1
2	T	283	LEU	7.0
4	D	739	PRO	6.5

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](#)

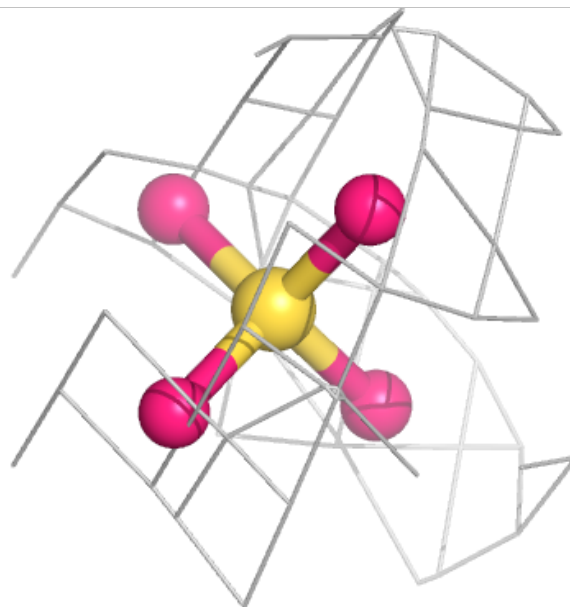
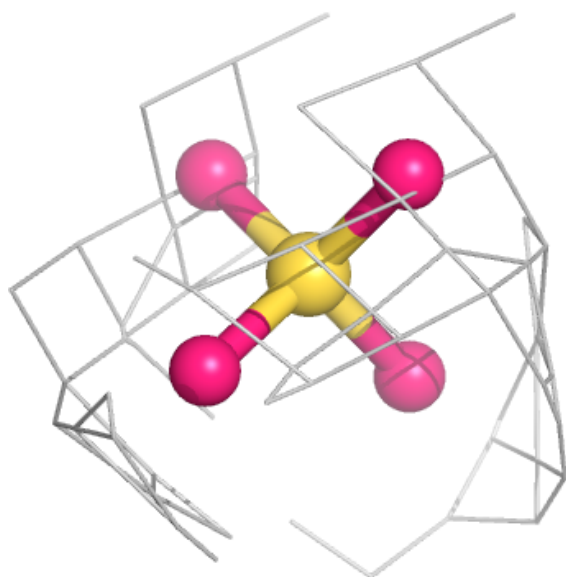
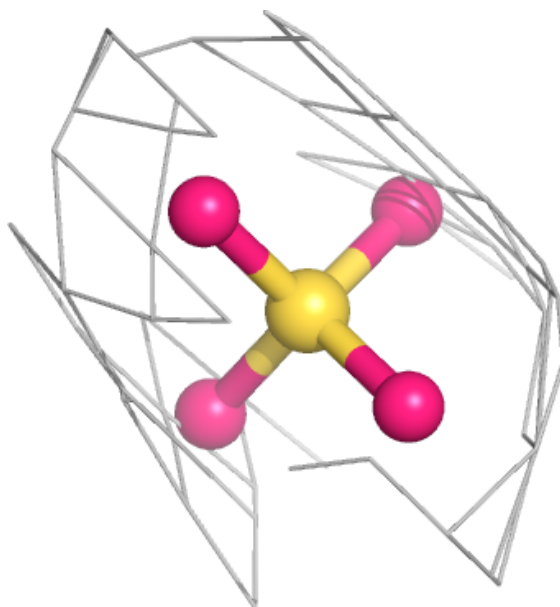
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	SO4	D	1408	5/5	0.54	0.31	197,200,219,408	0
9	SO4	D	1405	5/5	0.77	0.27	129,140,169,242	0
9	SO4	F	1204	5/5	0.79	0.65	181,184,229,383	0
9	SO4	F	1203	5/5	0.86	0.24	114,121,134,176	0
9	SO4	D	1406	5/5	0.86	0.23	145,154,158,235	0
9	SO4	D	1407	5/5	0.87	0.18	132,144,164,224	0
9	SO4	D	1404	5/5	0.89	0.30	134,138,153,204	0
9	SO4	D	1403	5/5	0.90	0.13	154,154,189,244	0
9	SO4	F	1201	5/5	0.91	0.20	94,96,132,149	0
9	SO4	F	1202	5/5	0.91	0.12	113,115,129,138	0
9	SO4	D	1401	3/5	0.93	0.21	107,107,111,117	0
9	SO4	D	1402	2/5	0.96	0.15	131,131,131,153	0
10	ZN	D	1409	1/1	0.98	0.33	161,161,161,161	0
10	ZN	D	1410	1/1	0.99	0.23	149,149,149,149	0

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

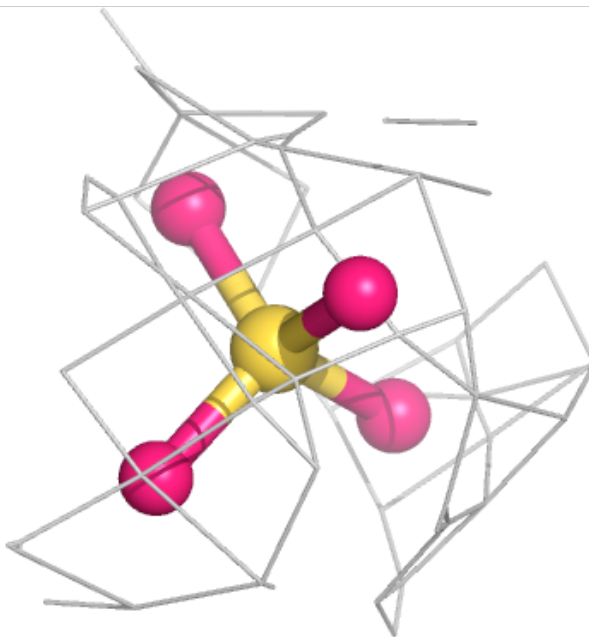
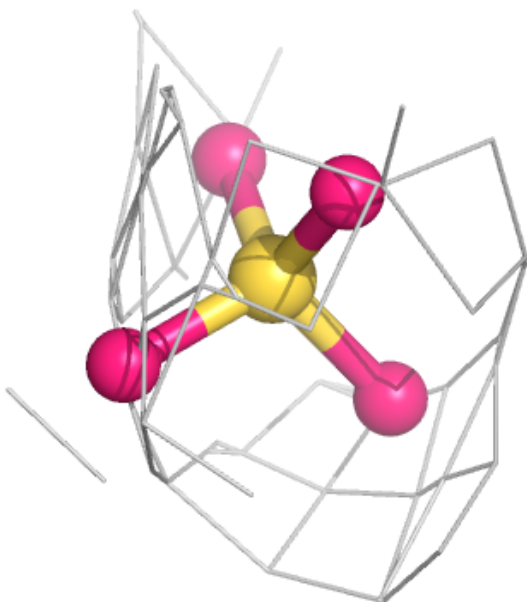
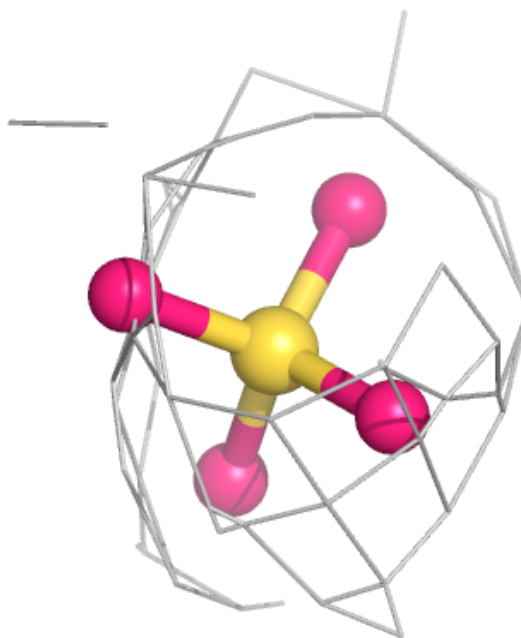
Electron density around SO4 D 1408:

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



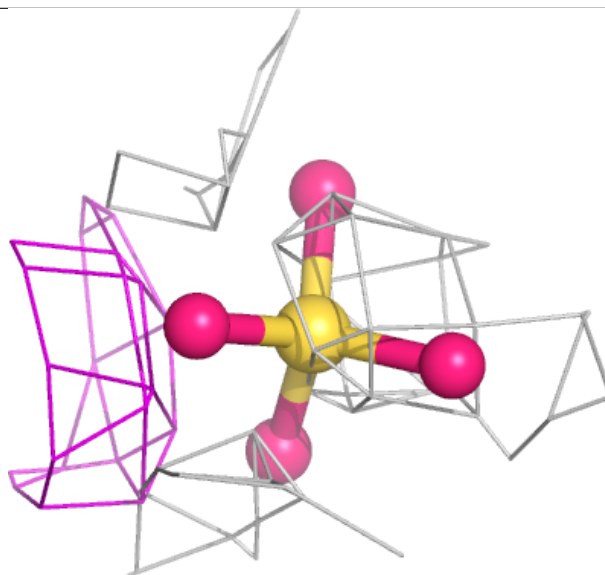
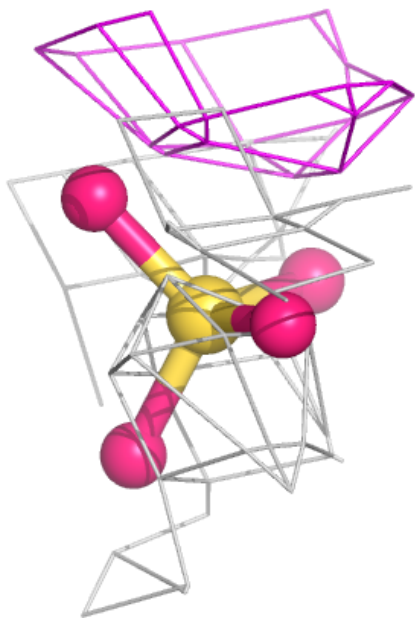
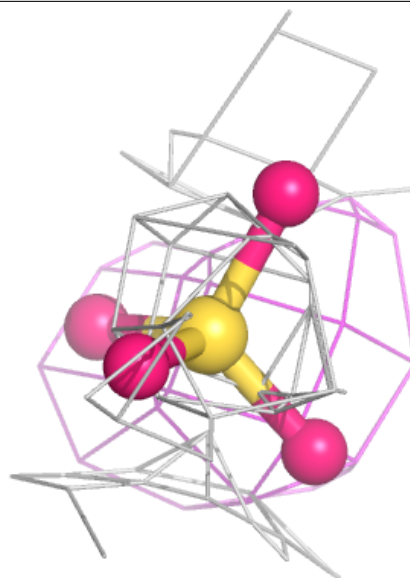
Electron density around SO4 D 1405:

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



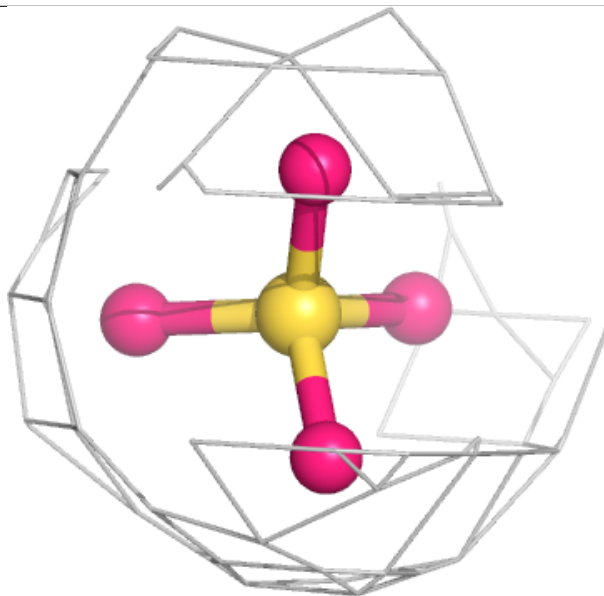
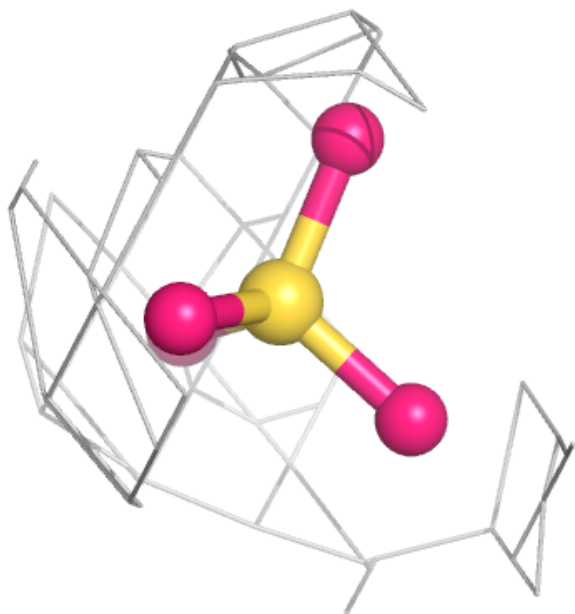
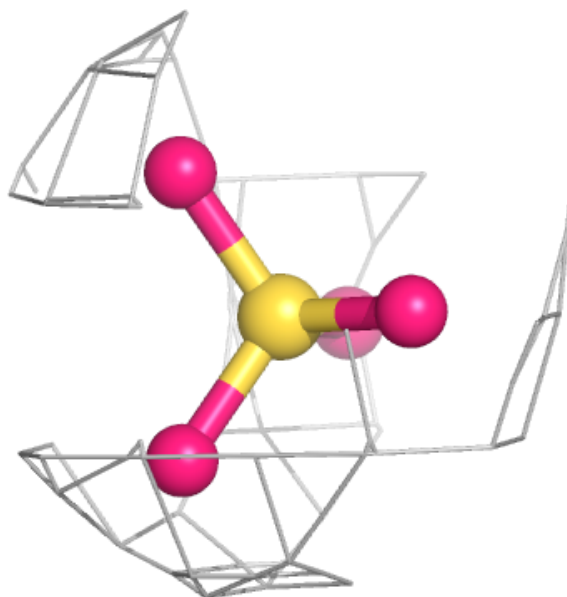
Electron density around SO4 F 1204:

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



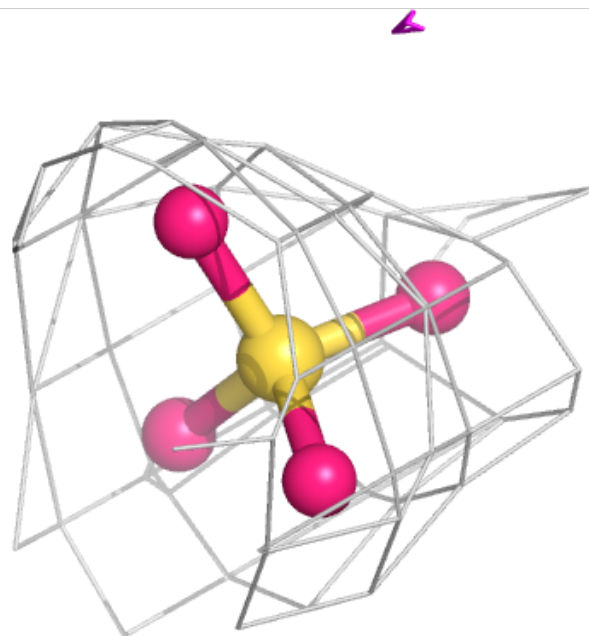
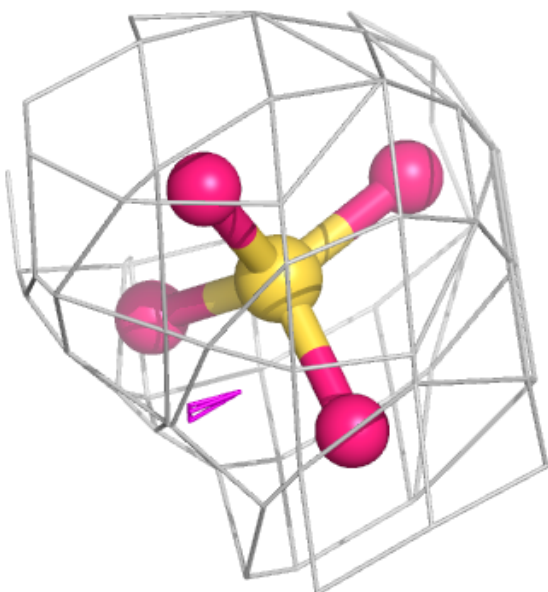
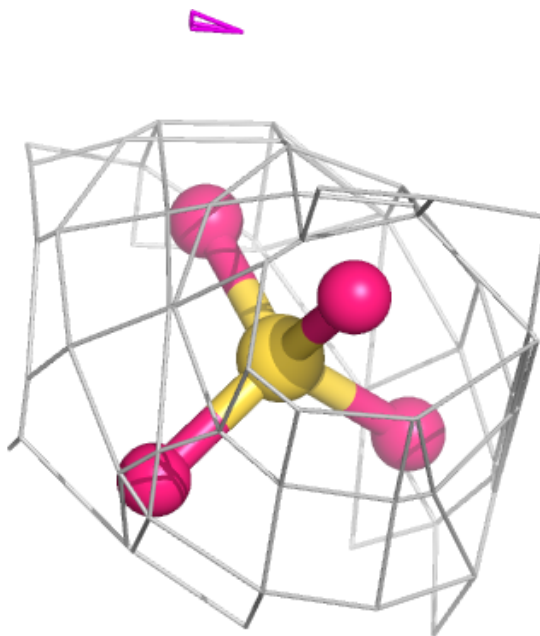
Electron density around SO4 F 1203:

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



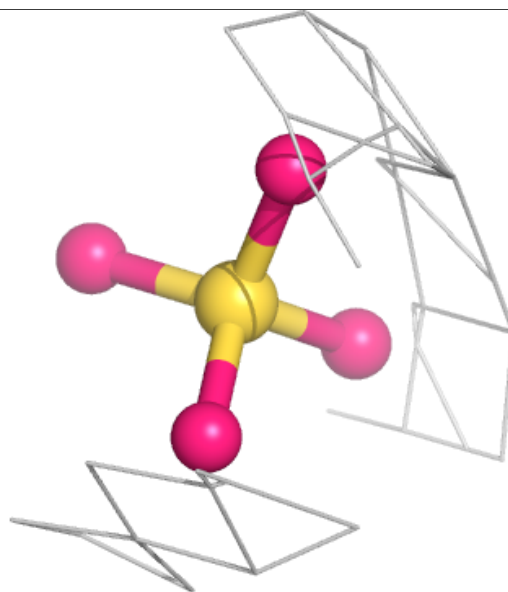
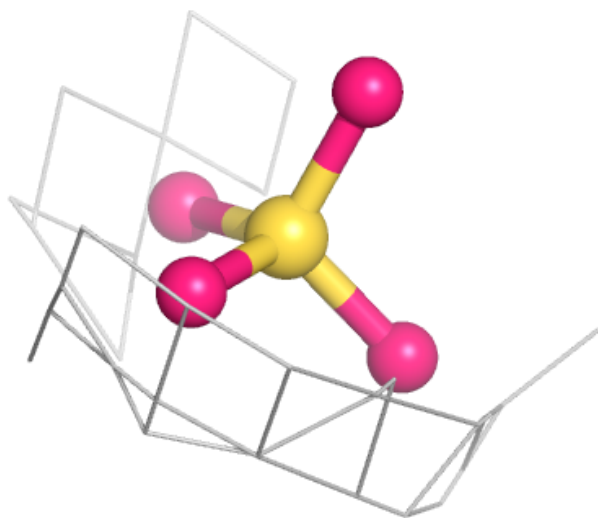
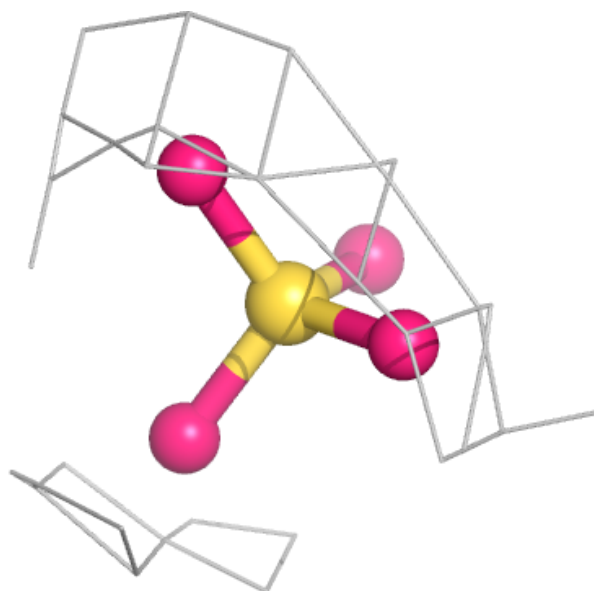
Electron density around SO4 D 1406:

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



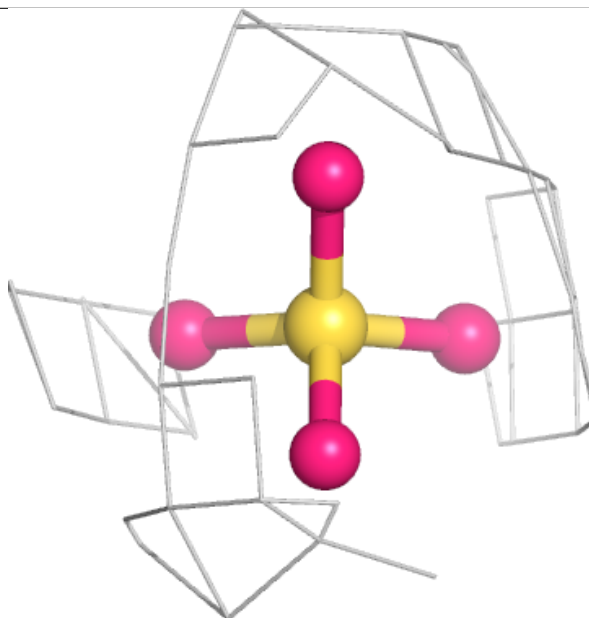
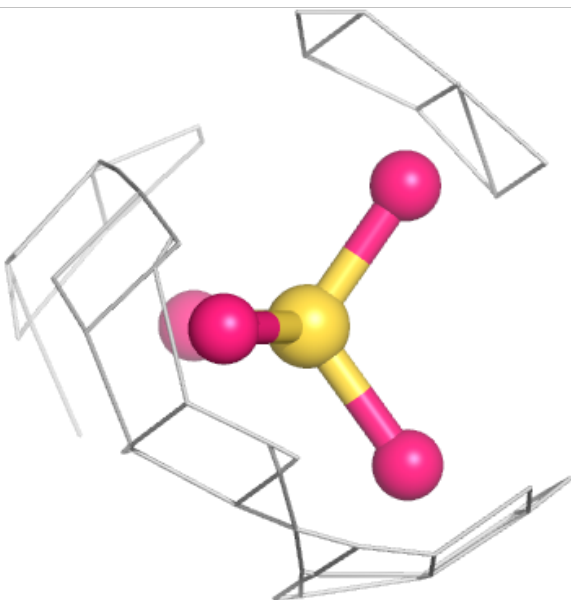
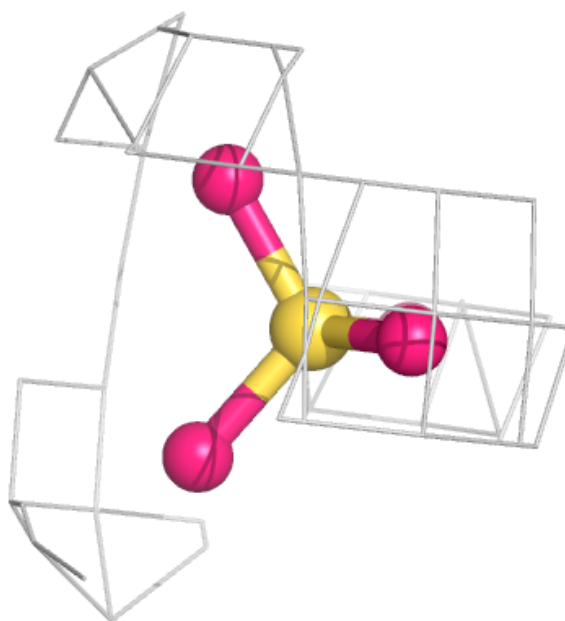
Electron density around SO4 D 1407:

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



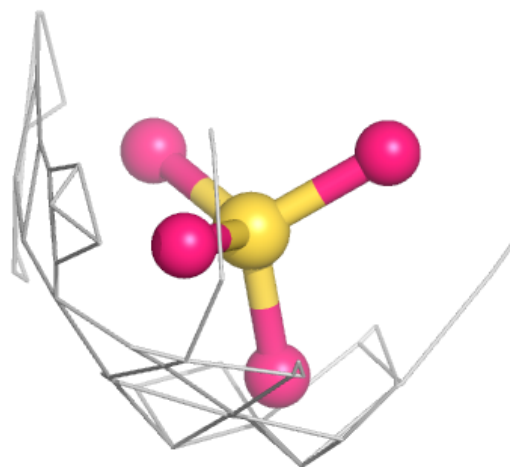
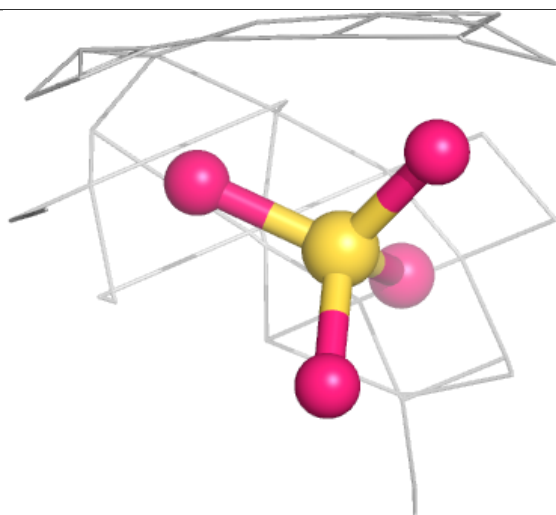
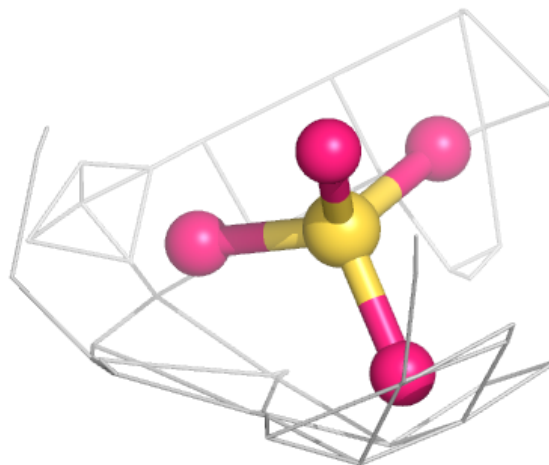
Electron density around SO4 D 1404:

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



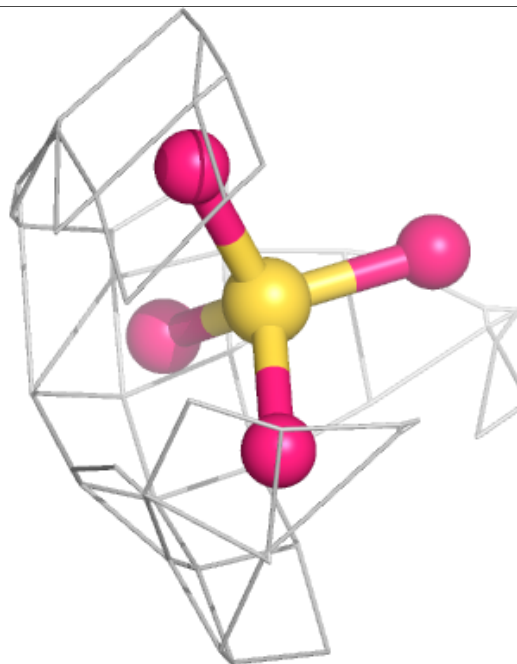
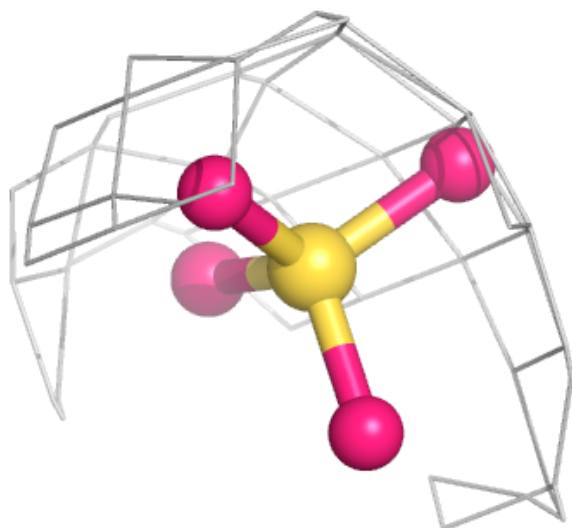
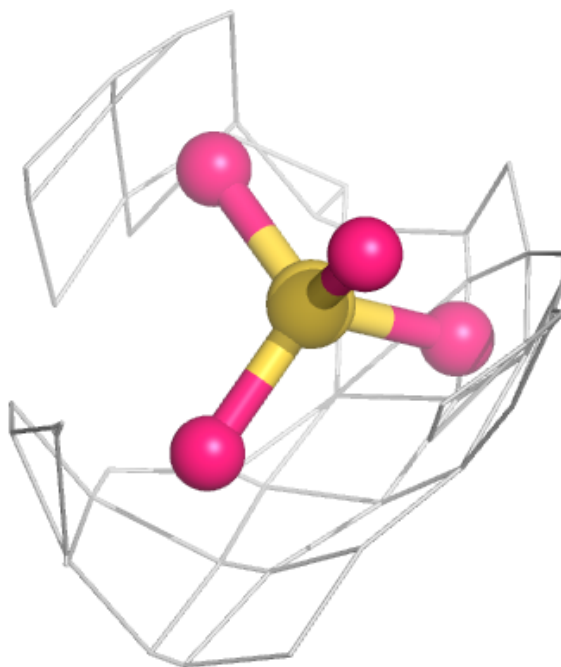
Electron density around SO4 D 1403:

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



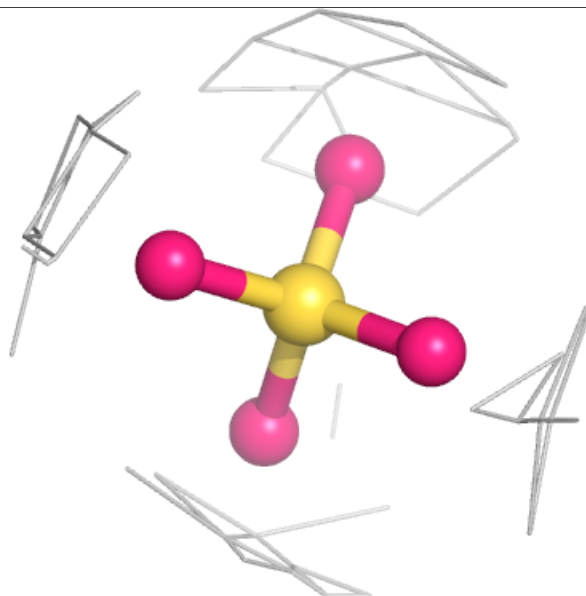
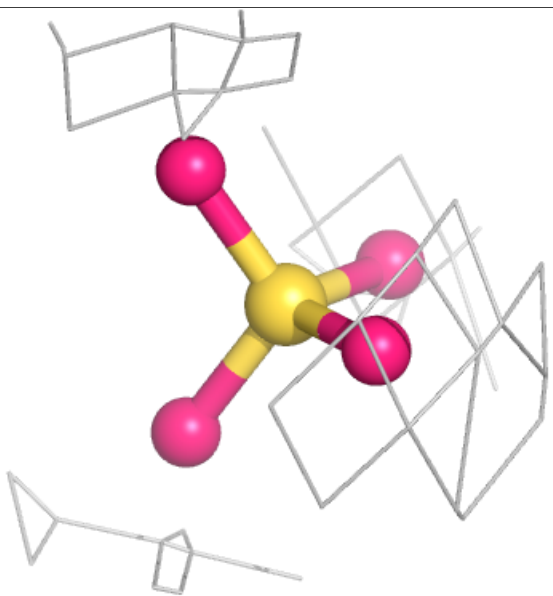
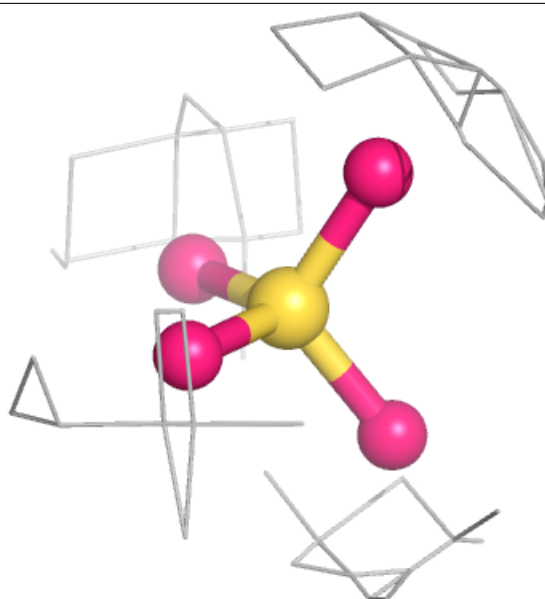
Electron density around SO4 F 1201:

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



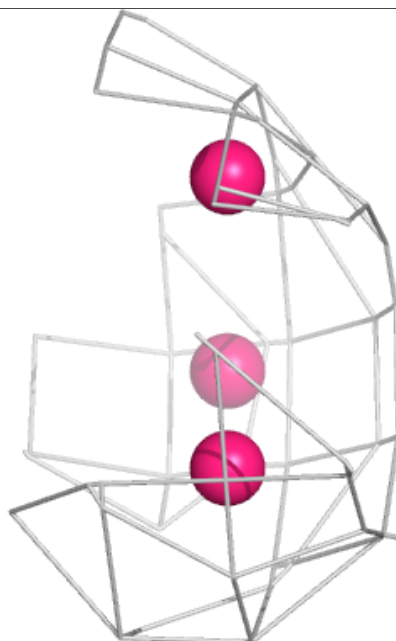
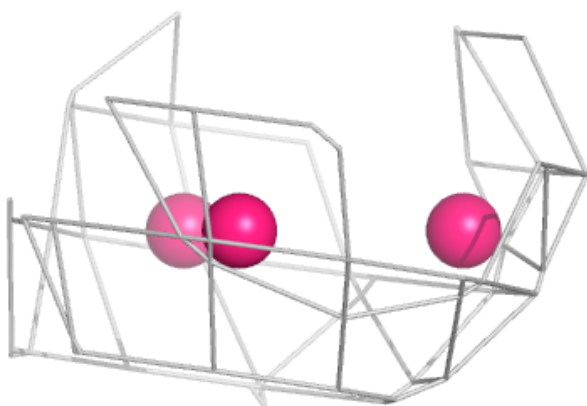
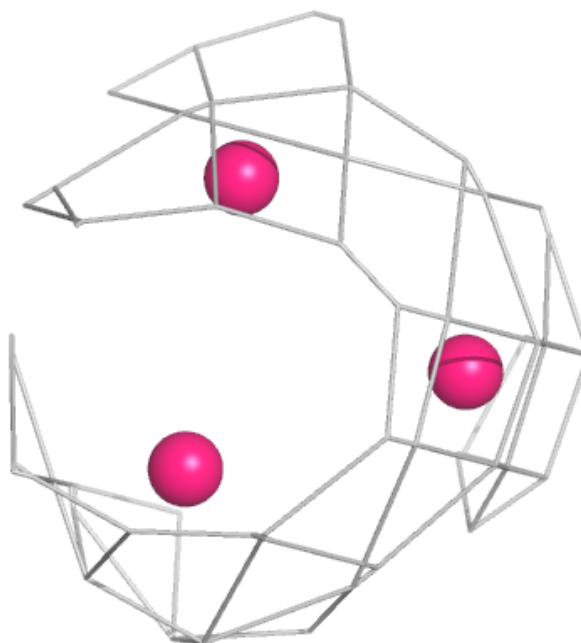
Electron density around SO4 F 1202:

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



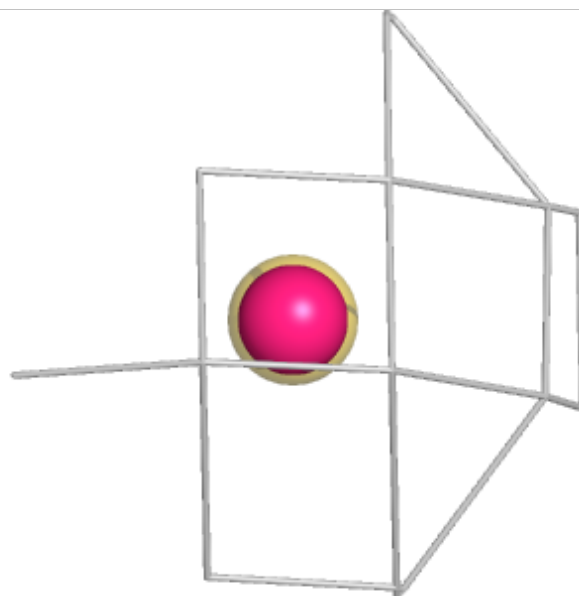
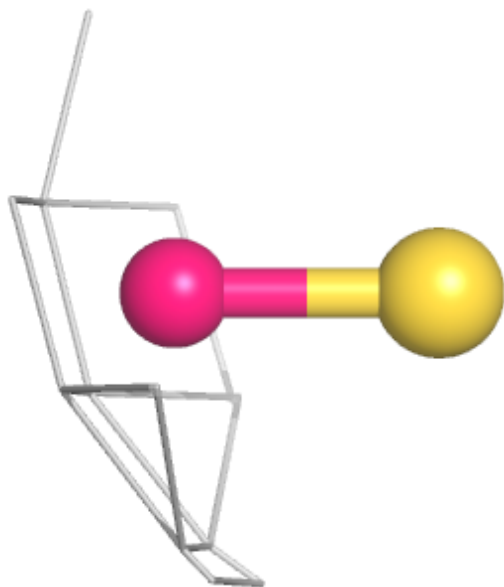
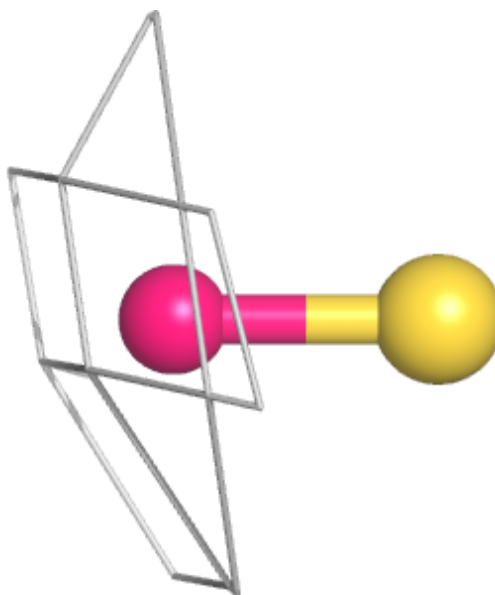
Electron density around SO4 D 1401:

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



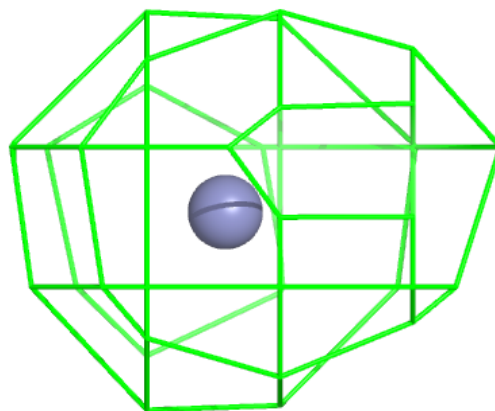
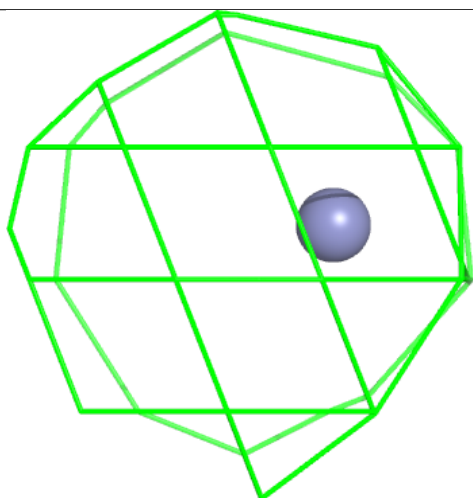
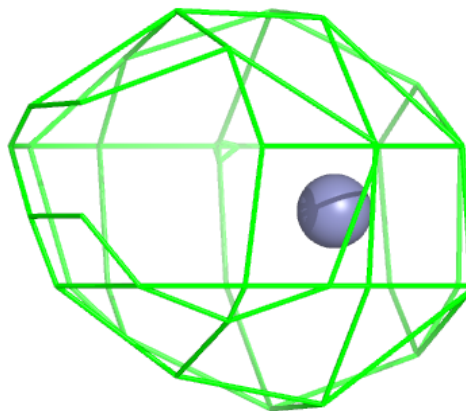
Electron density around SO4 D 1402:

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



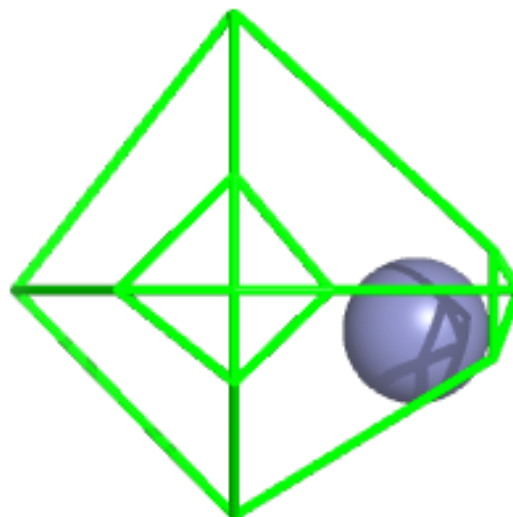
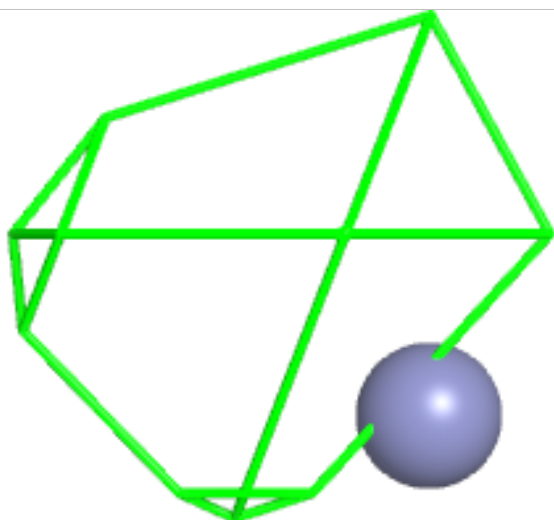
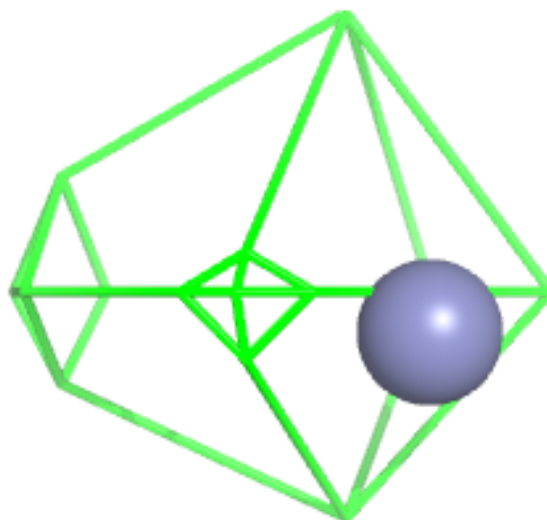
Electron density around ZN D 1409:

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



Electron density around ZN D 1410:

$2mF_o-DF_c$ (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.