



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 04:58 PM UTC

PDB ID : 7AG7 / pdb_00007ag7
Title : Crystal structure of SFP aldolase YihT from Salmonella enterica in complex with sulfate bound at the active site
Authors : Sharma, M.; Davies, G.J.
Deposited on : 2020-09-21
Resolution : 1.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

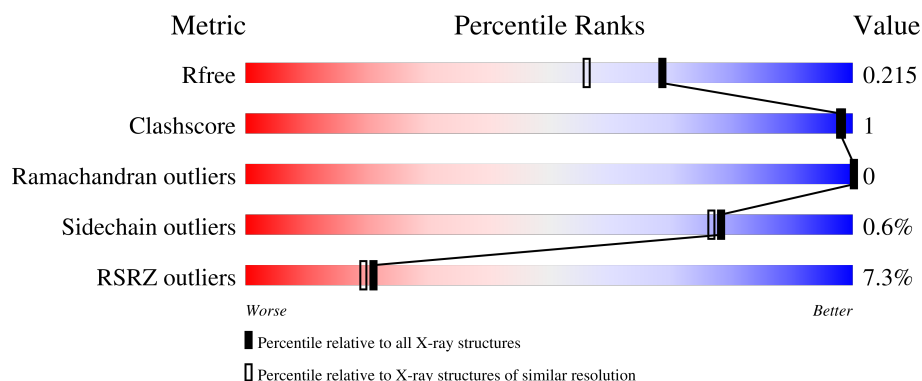
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	312	2% 91% 7%
1	B	312	5% 91% 7%
1	C	312	% 91% 7%
1	D	312	% 91% 6%
1	E	312	91% 6%

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Mol	Chain	Length	Quality of chain
1	F	312	61% 85% 12%
1	G	312	3% 91% 8%
1	H	312	4% 90% 8%
1	I	312	92% 7%
1	J	312	2% 91% 7%
1	K	312	% 91% 7%
1	L	312	2% 90% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27636 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 Sulfofructosephosphate aldolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	0	2	0
			2165	1363	378	408	16			
1	B	291	Total	C	N	O	S	0	0	0
			2152	1358	374	405	15			
1	C	290	Total	C	N	O	S	0	1	0
			2181	1372	382	411	16			
1	D	293	Total	C	N	O	S	0	2	0
			2212	1391	391	413	17			
1	E	292	Total	C	N	O	S	0	1	0
			2182	1375	383	408	16			
1	F	276	Total	C	N	O	S	0	1	0
			1895	1184	338	360	13			
1	G	288	Total	C	N	O	S	0	2	0
			2144	1353	370	405	16			
1	H	286	Total	C	N	O	S	0	1	0
			2108	1333	363	396	16			
1	I	289	Total	C	N	O	S	0	1	0
			2170	1366	380	408	16			
1	J	289	Total	C	N	O	S	0	1	0
			2148	1355	372	405	16			
1	K	289	Total	C	N	O	S	0	1	0
			2183	1375	383	409	16			
1	L	289	Total	C	N	O	S	0	2	0
			2166	1363	379	408	16			

There are 240 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q9L7R9
A	-18	GLY	-	expression tag	UNP Q9L7R9
A	-17	SER	-	expression tag	UNP Q9L7R9
A	-16	SER	-	expression tag	UNP Q9L7R9
A	-15	HIS	-	expression tag	UNP Q9L7R9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP Q9L7R9
A	-13	HIS	-	expression tag	UNP Q9L7R9
A	-12	HIS	-	expression tag	UNP Q9L7R9
A	-11	HIS	-	expression tag	UNP Q9L7R9
A	-10	HIS	-	expression tag	UNP Q9L7R9
A	-9	SER	-	expression tag	UNP Q9L7R9
A	-8	SER	-	expression tag	UNP Q9L7R9
A	-7	GLY	-	expression tag	UNP Q9L7R9
A	-6	LEU	-	expression tag	UNP Q9L7R9
A	-5	VAL	-	expression tag	UNP Q9L7R9
A	-4	PRO	-	expression tag	UNP Q9L7R9
A	-3	ARG	-	expression tag	UNP Q9L7R9
A	-2	GLY	-	expression tag	UNP Q9L7R9
A	-1	SER	-	expression tag	UNP Q9L7R9
A	0	HIS	-	expression tag	UNP Q9L7R9
B	-19	MET	-	initiating methionine	UNP Q9L7R9
B	-18	GLY	-	expression tag	UNP Q9L7R9
B	-17	SER	-	expression tag	UNP Q9L7R9
B	-16	SER	-	expression tag	UNP Q9L7R9
B	-15	HIS	-	expression tag	UNP Q9L7R9
B	-14	HIS	-	expression tag	UNP Q9L7R9
B	-13	HIS	-	expression tag	UNP Q9L7R9
B	-12	HIS	-	expression tag	UNP Q9L7R9
B	-11	HIS	-	expression tag	UNP Q9L7R9
B	-10	HIS	-	expression tag	UNP Q9L7R9
B	-9	SER	-	expression tag	UNP Q9L7R9
B	-8	SER	-	expression tag	UNP Q9L7R9
B	-7	GLY	-	expression tag	UNP Q9L7R9
B	-6	LEU	-	expression tag	UNP Q9L7R9
B	-5	VAL	-	expression tag	UNP Q9L7R9
B	-4	PRO	-	expression tag	UNP Q9L7R9
B	-3	ARG	-	expression tag	UNP Q9L7R9
B	-2	GLY	-	expression tag	UNP Q9L7R9
B	-1	SER	-	expression tag	UNP Q9L7R9
B	0	HIS	-	expression tag	UNP Q9L7R9
C	-19	MET	-	initiating methionine	UNP Q9L7R9
C	-18	GLY	-	expression tag	UNP Q9L7R9
C	-17	SER	-	expression tag	UNP Q9L7R9
C	-16	SER	-	expression tag	UNP Q9L7R9
C	-15	HIS	-	expression tag	UNP Q9L7R9
C	-14	HIS	-	expression tag	UNP Q9L7R9
C	-13	HIS	-	expression tag	UNP Q9L7R9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-12	HIS	-	expression tag	UNP Q9L7R9
C	-11	HIS	-	expression tag	UNP Q9L7R9
C	-10	HIS	-	expression tag	UNP Q9L7R9
C	-9	SER	-	expression tag	UNP Q9L7R9
C	-8	SER	-	expression tag	UNP Q9L7R9
C	-7	GLY	-	expression tag	UNP Q9L7R9
C	-6	LEU	-	expression tag	UNP Q9L7R9
C	-5	VAL	-	expression tag	UNP Q9L7R9
C	-4	PRO	-	expression tag	UNP Q9L7R9
C	-3	ARG	-	expression tag	UNP Q9L7R9
C	-2	GLY	-	expression tag	UNP Q9L7R9
C	-1	SER	-	expression tag	UNP Q9L7R9
C	0	HIS	-	expression tag	UNP Q9L7R9
D	-19	MET	-	initiating methionine	UNP Q9L7R9
D	-18	GLY	-	expression tag	UNP Q9L7R9
D	-17	SER	-	expression tag	UNP Q9L7R9
D	-16	SER	-	expression tag	UNP Q9L7R9
D	-15	HIS	-	expression tag	UNP Q9L7R9
D	-14	HIS	-	expression tag	UNP Q9L7R9
D	-13	HIS	-	expression tag	UNP Q9L7R9
D	-12	HIS	-	expression tag	UNP Q9L7R9
D	-11	HIS	-	expression tag	UNP Q9L7R9
D	-10	HIS	-	expression tag	UNP Q9L7R9
D	-9	SER	-	expression tag	UNP Q9L7R9
D	-8	SER	-	expression tag	UNP Q9L7R9
D	-7	GLY	-	expression tag	UNP Q9L7R9
D	-6	LEU	-	expression tag	UNP Q9L7R9
D	-5	VAL	-	expression tag	UNP Q9L7R9
D	-4	PRO	-	expression tag	UNP Q9L7R9
D	-3	ARG	-	expression tag	UNP Q9L7R9
D	-2	GLY	-	expression tag	UNP Q9L7R9
D	-1	SER	-	expression tag	UNP Q9L7R9
D	0	HIS	-	expression tag	UNP Q9L7R9
E	-19	MET	-	initiating methionine	UNP Q9L7R9
E	-18	GLY	-	expression tag	UNP Q9L7R9
E	-17	SER	-	expression tag	UNP Q9L7R9
E	-16	SER	-	expression tag	UNP Q9L7R9
E	-15	HIS	-	expression tag	UNP Q9L7R9
E	-14	HIS	-	expression tag	UNP Q9L7R9
E	-13	HIS	-	expression tag	UNP Q9L7R9
E	-12	HIS	-	expression tag	UNP Q9L7R9
E	-11	HIS	-	expression tag	UNP Q9L7R9

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-10	HIS	-	expression tag	UNP Q9L7R9
E	-9	SER	-	expression tag	UNP Q9L7R9
E	-8	SER	-	expression tag	UNP Q9L7R9
E	-7	GLY	-	expression tag	UNP Q9L7R9
E	-6	LEU	-	expression tag	UNP Q9L7R9
E	-5	VAL	-	expression tag	UNP Q9L7R9
E	-4	PRO	-	expression tag	UNP Q9L7R9
E	-3	ARG	-	expression tag	UNP Q9L7R9
E	-2	GLY	-	expression tag	UNP Q9L7R9
E	-1	SER	-	expression tag	UNP Q9L7R9
E	0	HIS	-	expression tag	UNP Q9L7R9
F	-19	MET	-	initiating methionine	UNP Q9L7R9
F	-18	GLY	-	expression tag	UNP Q9L7R9
F	-17	SER	-	expression tag	UNP Q9L7R9
F	-16	SER	-	expression tag	UNP Q9L7R9
F	-15	HIS	-	expression tag	UNP Q9L7R9
F	-14	HIS	-	expression tag	UNP Q9L7R9
F	-13	HIS	-	expression tag	UNP Q9L7R9
F	-12	HIS	-	expression tag	UNP Q9L7R9
F	-11	HIS	-	expression tag	UNP Q9L7R9
F	-10	HIS	-	expression tag	UNP Q9L7R9
F	-9	SER	-	expression tag	UNP Q9L7R9
F	-8	SER	-	expression tag	UNP Q9L7R9
F	-7	GLY	-	expression tag	UNP Q9L7R9
F	-6	LEU	-	expression tag	UNP Q9L7R9
F	-5	VAL	-	expression tag	UNP Q9L7R9
F	-4	PRO	-	expression tag	UNP Q9L7R9
F	-3	ARG	-	expression tag	UNP Q9L7R9
F	-2	GLY	-	expression tag	UNP Q9L7R9
F	-1	SER	-	expression tag	UNP Q9L7R9
F	0	HIS	-	expression tag	UNP Q9L7R9
G	-19	MET	-	initiating methionine	UNP Q9L7R9
G	-18	GLY	-	expression tag	UNP Q9L7R9
G	-17	SER	-	expression tag	UNP Q9L7R9
G	-16	SER	-	expression tag	UNP Q9L7R9
G	-15	HIS	-	expression tag	UNP Q9L7R9
G	-14	HIS	-	expression tag	UNP Q9L7R9
G	-13	HIS	-	expression tag	UNP Q9L7R9
G	-12	HIS	-	expression tag	UNP Q9L7R9
G	-11	HIS	-	expression tag	UNP Q9L7R9
G	-10	HIS	-	expression tag	UNP Q9L7R9
G	-9	SER	-	expression tag	UNP Q9L7R9

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-8	SER	-	expression tag	UNP Q9L7R9
G	-7	GLY	-	expression tag	UNP Q9L7R9
G	-6	LEU	-	expression tag	UNP Q9L7R9
G	-5	VAL	-	expression tag	UNP Q9L7R9
G	-4	PRO	-	expression tag	UNP Q9L7R9
G	-3	ARG	-	expression tag	UNP Q9L7R9
G	-2	GLY	-	expression tag	UNP Q9L7R9
G	-1	SER	-	expression tag	UNP Q9L7R9
G	0	HIS	-	expression tag	UNP Q9L7R9
H	-19	MET	-	initiating methionine	UNP Q9L7R9
H	-18	GLY	-	expression tag	UNP Q9L7R9
H	-17	SER	-	expression tag	UNP Q9L7R9
H	-16	SER	-	expression tag	UNP Q9L7R9
H	-15	HIS	-	expression tag	UNP Q9L7R9
H	-14	HIS	-	expression tag	UNP Q9L7R9
H	-13	HIS	-	expression tag	UNP Q9L7R9
H	-12	HIS	-	expression tag	UNP Q9L7R9
H	-11	HIS	-	expression tag	UNP Q9L7R9
H	-10	HIS	-	expression tag	UNP Q9L7R9
H	-9	SER	-	expression tag	UNP Q9L7R9
H	-8	SER	-	expression tag	UNP Q9L7R9
H	-7	GLY	-	expression tag	UNP Q9L7R9
H	-6	LEU	-	expression tag	UNP Q9L7R9
H	-5	VAL	-	expression tag	UNP Q9L7R9
H	-4	PRO	-	expression tag	UNP Q9L7R9
H	-3	ARG	-	expression tag	UNP Q9L7R9
H	-2	GLY	-	expression tag	UNP Q9L7R9
H	-1	SER	-	expression tag	UNP Q9L7R9
H	0	HIS	-	expression tag	UNP Q9L7R9
I	-19	MET	-	initiating methionine	UNP Q9L7R9
I	-18	GLY	-	expression tag	UNP Q9L7R9
I	-17	SER	-	expression tag	UNP Q9L7R9
I	-16	SER	-	expression tag	UNP Q9L7R9
I	-15	HIS	-	expression tag	UNP Q9L7R9
I	-14	HIS	-	expression tag	UNP Q9L7R9
I	-13	HIS	-	expression tag	UNP Q9L7R9
I	-12	HIS	-	expression tag	UNP Q9L7R9
I	-11	HIS	-	expression tag	UNP Q9L7R9
I	-10	HIS	-	expression tag	UNP Q9L7R9
I	-9	SER	-	expression tag	UNP Q9L7R9
I	-8	SER	-	expression tag	UNP Q9L7R9
I	-7	GLY	-	expression tag	UNP Q9L7R9

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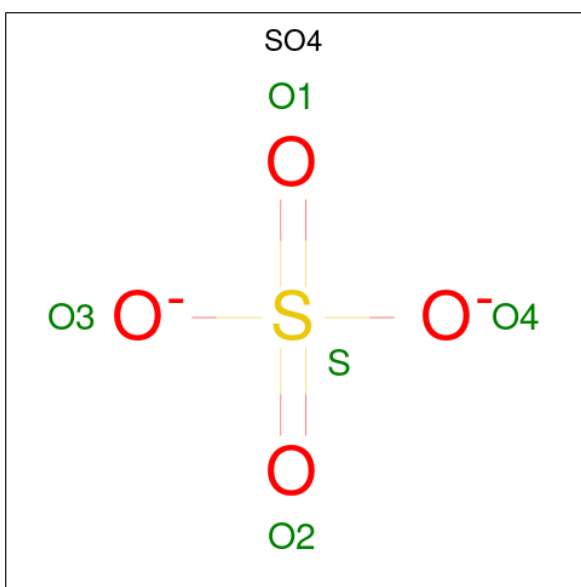
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP Q9L7R9
I	-5	VAL	-	expression tag	UNP Q9L7R9
I	-4	PRO	-	expression tag	UNP Q9L7R9
I	-3	ARG	-	expression tag	UNP Q9L7R9
I	-2	GLY	-	expression tag	UNP Q9L7R9
I	-1	SER	-	expression tag	UNP Q9L7R9
I	0	HIS	-	expression tag	UNP Q9L7R9
J	-19	MET	-	initiating methionine	UNP Q9L7R9
J	-18	GLY	-	expression tag	UNP Q9L7R9
J	-17	SER	-	expression tag	UNP Q9L7R9
J	-16	SER	-	expression tag	UNP Q9L7R9
J	-15	HIS	-	expression tag	UNP Q9L7R9
J	-14	HIS	-	expression tag	UNP Q9L7R9
J	-13	HIS	-	expression tag	UNP Q9L7R9
J	-12	HIS	-	expression tag	UNP Q9L7R9
J	-11	HIS	-	expression tag	UNP Q9L7R9
J	-10	HIS	-	expression tag	UNP Q9L7R9
J	-9	SER	-	expression tag	UNP Q9L7R9
J	-8	SER	-	expression tag	UNP Q9L7R9
J	-7	GLY	-	expression tag	UNP Q9L7R9
J	-6	LEU	-	expression tag	UNP Q9L7R9
J	-5	VAL	-	expression tag	UNP Q9L7R9
J	-4	PRO	-	expression tag	UNP Q9L7R9
J	-3	ARG	-	expression tag	UNP Q9L7R9
J	-2	GLY	-	expression tag	UNP Q9L7R9
J	-1	SER	-	expression tag	UNP Q9L7R9
J	0	HIS	-	expression tag	UNP Q9L7R9
K	-19	MET	-	initiating methionine	UNP Q9L7R9
K	-18	GLY	-	expression tag	UNP Q9L7R9
K	-17	SER	-	expression tag	UNP Q9L7R9
K	-16	SER	-	expression tag	UNP Q9L7R9
K	-15	HIS	-	expression tag	UNP Q9L7R9
K	-14	HIS	-	expression tag	UNP Q9L7R9
K	-13	HIS	-	expression tag	UNP Q9L7R9
K	-12	HIS	-	expression tag	UNP Q9L7R9
K	-11	HIS	-	expression tag	UNP Q9L7R9
K	-10	HIS	-	expression tag	UNP Q9L7R9
K	-9	SER	-	expression tag	UNP Q9L7R9
K	-8	SER	-	expression tag	UNP Q9L7R9
K	-7	GLY	-	expression tag	UNP Q9L7R9
K	-6	LEU	-	expression tag	UNP Q9L7R9
K	-5	VAL	-	expression tag	UNP Q9L7R9

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Chain	Residue	Modelled	Actual	Comment	Reference
K	-4	PRO	-	expression tag	UNP Q9L7R9
K	-3	ARG	-	expression tag	UNP Q9L7R9
K	-2	GLY	-	expression tag	UNP Q9L7R9
K	-1	SER	-	expression tag	UNP Q9L7R9
K	0	HIS	-	expression tag	UNP Q9L7R9
L	-19	MET	-	initiating methionine	UNP Q9L7R9
L	-18	GLY	-	expression tag	UNP Q9L7R9
L	-17	SER	-	expression tag	UNP Q9L7R9
L	-16	SER	-	expression tag	UNP Q9L7R9
L	-15	HIS	-	expression tag	UNP Q9L7R9
L	-14	HIS	-	expression tag	UNP Q9L7R9
L	-13	HIS	-	expression tag	UNP Q9L7R9
L	-12	HIS	-	expression tag	UNP Q9L7R9
L	-11	HIS	-	expression tag	UNP Q9L7R9
L	-10	HIS	-	expression tag	UNP Q9L7R9
L	-9	SER	-	expression tag	UNP Q9L7R9
L	-8	SER	-	expression tag	UNP Q9L7R9
L	-7	GLY	-	expression tag	UNP Q9L7R9
L	-6	LEU	-	expression tag	UNP Q9L7R9
L	-5	VAL	-	expression tag	UNP Q9L7R9
L	-4	PRO	-	expression tag	UNP Q9L7R9
L	-3	ARG	-	expression tag	UNP Q9L7R9
L	-2	GLY	-	expression tag	UNP Q9L7R9
L	-1	SER	-	expression tag	UNP Q9L7R9
L	0	HIS	-	expression tag	UNP Q9L7R9

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		

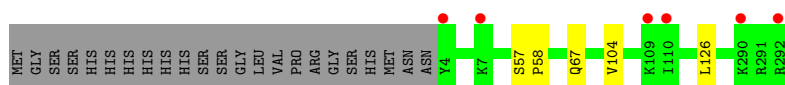
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total 146	O 146	0	0
3	B	77	Total 77	O 77	0	0
3	C	173	Total 173	O 173	0	0
3	D	279	Total 279	O 279	0	0
3	E	192	Total 192	O 192	0	0
3	F	12	Total 12	O 12	0	0
3	G	131	Total 131	O 131	0	0
3	H	53	Total 53	O 53	0	0
3	I	248	Total 248	O 248	0	0
3	J	121	Total 121	O 121	0	0
3	K	210	Total 210	O 210	0	0
3	L	228	Total 228	O 228	0	0

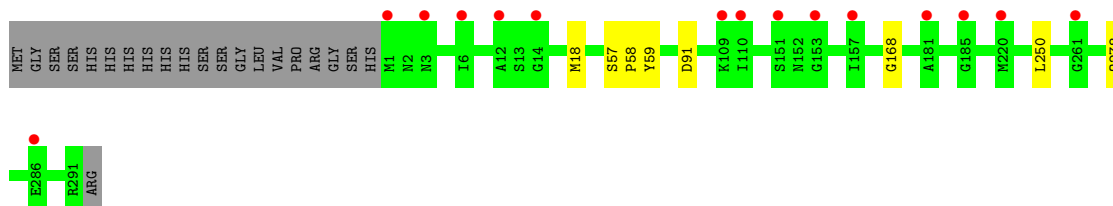
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

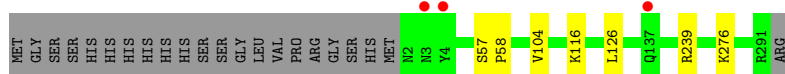
- Molecule 1: Sulfofructosephosphate aldolase



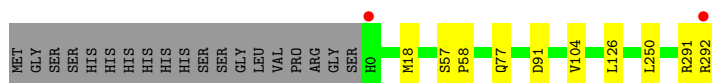
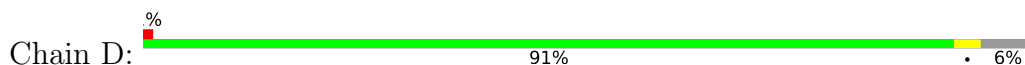
- Molecule 1: Sulfofructosephosphate aldolase



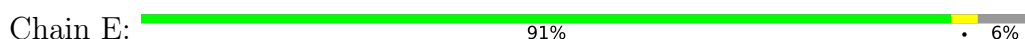
- Molecule 1: Sulfofructosephosphate aldolase



- Molecule 1: Sulfofructosephosphate aldolase

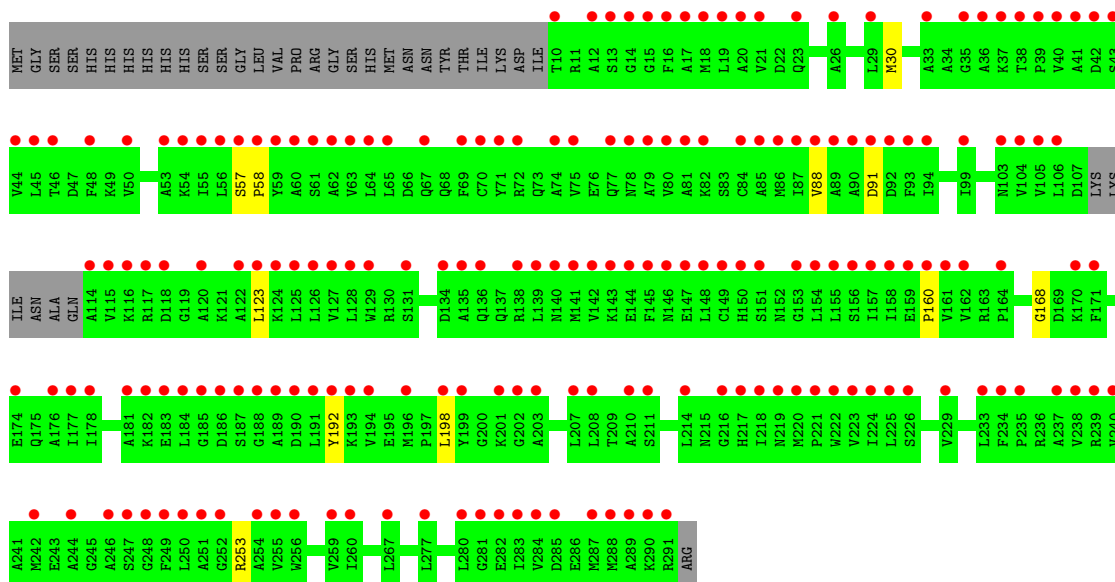
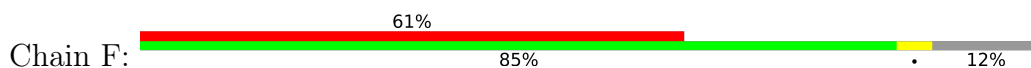


- Molecule 1: Sulfofructosephosphate aldolase

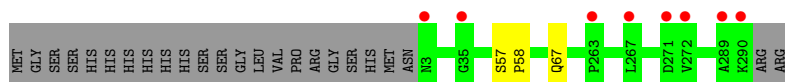




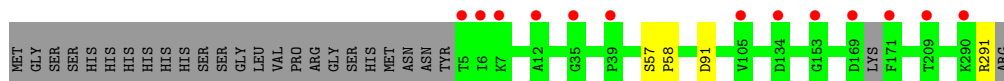
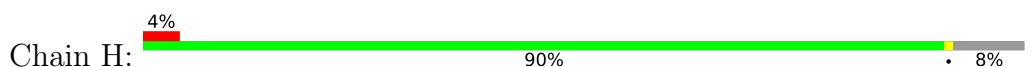
• Molecule 1: Sulfofructosephosphate aldolase



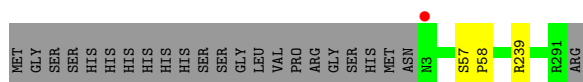
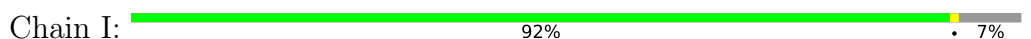
• Molecule 1: Sulfofructosephosphate aldolase



• Molecule 1: Sulfofructosephosphate aldolase

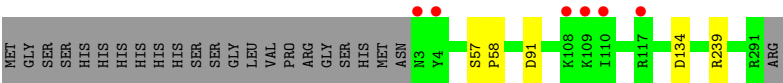


• Molecule 1: Sulfofructosephosphate aldolase

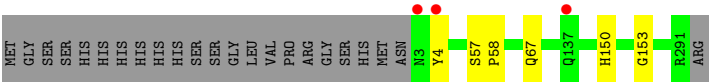
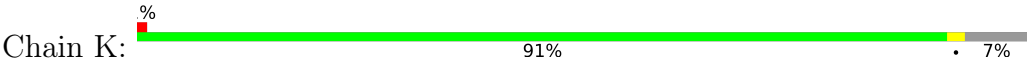


• Molecule 1: Sulfofructosephosphate aldolase

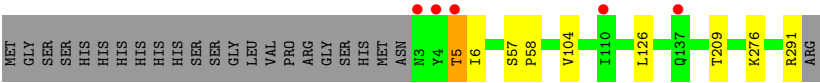
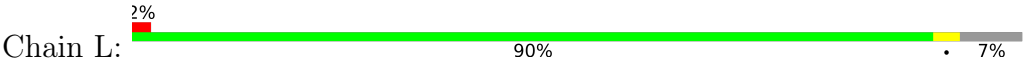




● Molecule 1: Sulfofructosephosphate aldolase



● Molecule 1: Sulfofructosephosphate aldolase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.21Å 107.23Å 126.86Å 107.42° 95.93° 110.55°	Depositor
Resolution (Å)	53.01 – 1.80 53.01 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (53.01-1.80) 97.5 (53.01-1.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0266	Depositor
R, R_{free}	0.193 , 0.207 0.200 , 0.215	Depositor DCC
R_{free} test set	17504 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	27636	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.02	0/2203	1.14	0/2985
1	B	1.00	0/2185	1.16	1/2964 (0.0%)
1	C	1.01	0/2217	1.14	0/3003
1	D	1.06	0/2252	1.18	2/3049 (0.1%)
1	E	1.04	0/2219	1.15	1/3007 (0.0%)
1	F	1.03	0/1923	1.16	1/2620 (0.0%)
1	G	1.02	0/2183	1.17	0/2961
1	H	0.99	0/2142	1.13	0/2905
1	I	1.05	0/2206	1.15	0/2988
1	J	1.00	0/2184	1.14	0/2962
1	K	1.03	1/2219 (0.0%)	1.15	0/3002
1	L	1.04	0/2204	1.18	2/2985 (0.1%)
All	All	1.02	1/26137 (0.0%)	1.15	7/35431 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	150	HIS	CE1-NE2	5.00	1.37	1.32

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	GLY	CA-C-O	-5.57	118.44	122.45
1	E	168	GLY	CA-C-O	-5.56	118.45	122.45
1	L	5	THR	OG1-CB-CG2	-5.54	98.21	109.30
1	F	168	GLY	CA-C-O	-5.26	118.66	122.45
1	L	209	THR	CA-CB-OG1	-5.22	101.77	109.60

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2165	0	2161	2	0
1	B	2152	0	2125	3	0
1	C	2181	0	2175	4	0
1	D	2212	0	2220	4	0
1	E	2182	0	2169	5	0
1	F	1895	0	1736	7	0
1	G	2144	0	2121	1	0
1	H	2108	0	2080	1	0
1	I	2170	0	2168	2	0
1	J	2148	0	2125	3	0
1	K	2183	0	2198	2	0
1	L	2166	0	2163	3	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
3	A	146	0	0	0	0
3	B	77	0	0	0	0
3	C	173	0	0	2	0
3	D	279	0	0	1	0
3	E	192	0	0	1	0
3	F	12	0	0	0	0
3	G	131	0	0	0	0
3	H	53	0	0	0	0
3	I	248	0	0	1	0
3	J	121	0	0	2	0
3	K	210	0	0	0	0
3	L	228	0	0	1	0
All	All	27636	0	25441	37	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 1.

The worst 5 of 37 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:D:104[B]:VAL:HG21	1:D:126:LEU:HD23	1.62	0.81
1:L:104:VAL:HG11	1:L:126:LEU:HD23	1.65	0.79
1:C:104:VAL:HG21	1:C:126:LEU:HD23	1.74	0.68
1:F:30:MET:HE1	1:F:253:ARG:NE	2.11	0.65
1:B:59:TYR:CD1	1:B:278:GLN:HG2	2.31	0.64

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	289/312 (93%)	282 (98%)	7 (2%)	0	100	100
1	B	289/312 (93%)	282 (98%)	7 (2%)	0	100	100
1	C	289/312 (93%)	282 (98%)	7 (2%)	0	100	100
1	D	293/312 (94%)	286 (98%)	7 (2%)	0	100	100
1	E	291/312 (93%)	284 (98%)	7 (2%)	0	100	100
1	F	273/312 (88%)	266 (97%)	7 (3%)	0	100	100
1	G	288/312 (92%)	281 (98%)	7 (2%)	0	100	100
1	H	283/312 (91%)	276 (98%)	7 (2%)	0	100	100
1	I	288/312 (92%)	281 (98%)	7 (2%)	0	100	100
1	J	288/312 (92%)	281 (98%)	7 (2%)	0	100	100
1	K	288/312 (92%)	281 (98%)	7 (2%)	0	100	100
1	L	289/312 (93%)	283 (98%)	6 (2%)	0	100	100
All	All	3448/3744 (92%)	3365 (98%)	83 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	222/252 (88%)	221 (100%)	1 (0%)	81	80
1	B	215/252 (85%)	214 (100%)	1 (0%)	81	80
1	C	224/252 (89%)	223 (100%)	1 (0%)	84	83
1	D	229/252 (91%)	228 (100%)	1 (0%)	84	83
1	E	221/252 (88%)	220 (100%)	1 (0%)	81	80
1	F	164/252 (65%)	162 (99%)	2 (1%)	63	57
1	G	217/252 (86%)	216 (100%)	1 (0%)	81	80
1	H	210/252 (83%)	208 (99%)	2 (1%)	68	64
1	I	223/252 (88%)	223 (100%)	0	100	100
1	J	217/252 (86%)	216 (100%)	1 (0%)	81	80
1	K	226/252 (90%)	225 (100%)	1 (0%)	84	83
1	L	222/252 (88%)	219 (99%)	3 (1%)	59	52
All	All	2590/3024 (86%)	2575 (99%)	15 (1%)	78	77

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	67	GLN
1	L	6	ILE
1	H	91	ASP
1	L	291	ARG
1	K	67	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 41 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	77	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	68	GLN
1	I	68	GLN
1	J	77	GLN
1	K	136	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	H	301	-	4,4,4	0.32	0	6,6,6	0.37	0
2	SO4	G	301	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	I	301	-	4,4,4	0.44	0	6,6,6	0.31	0
2	SO4	C	301	-	4,4,4	0.40	0	6,6,6	0.44	0
2	SO4	K	301	-	4,4,4	0.21	0	6,6,6	0.26	0
2	SO4	J	301	-	4,4,4	0.42	0	6,6,6	0.30	0
2	SO4	E	301	-	4,4,4	0.47	0	6,6,6	0.18	0
2	SO4	L	301	-	4,4,4	0.48	0	6,6,6	0.20	0
2	SO4	A	301	-	4,4,4	0.40	0	6,6,6	0.29	0
2	SO4	F	301	-	4,4,4	0.31	0	6,6,6	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	D	301	-	4,4,4	0.33	0	6,6,6	0.21	0
2	SO4	B	301	-	4,4,4	0.50	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

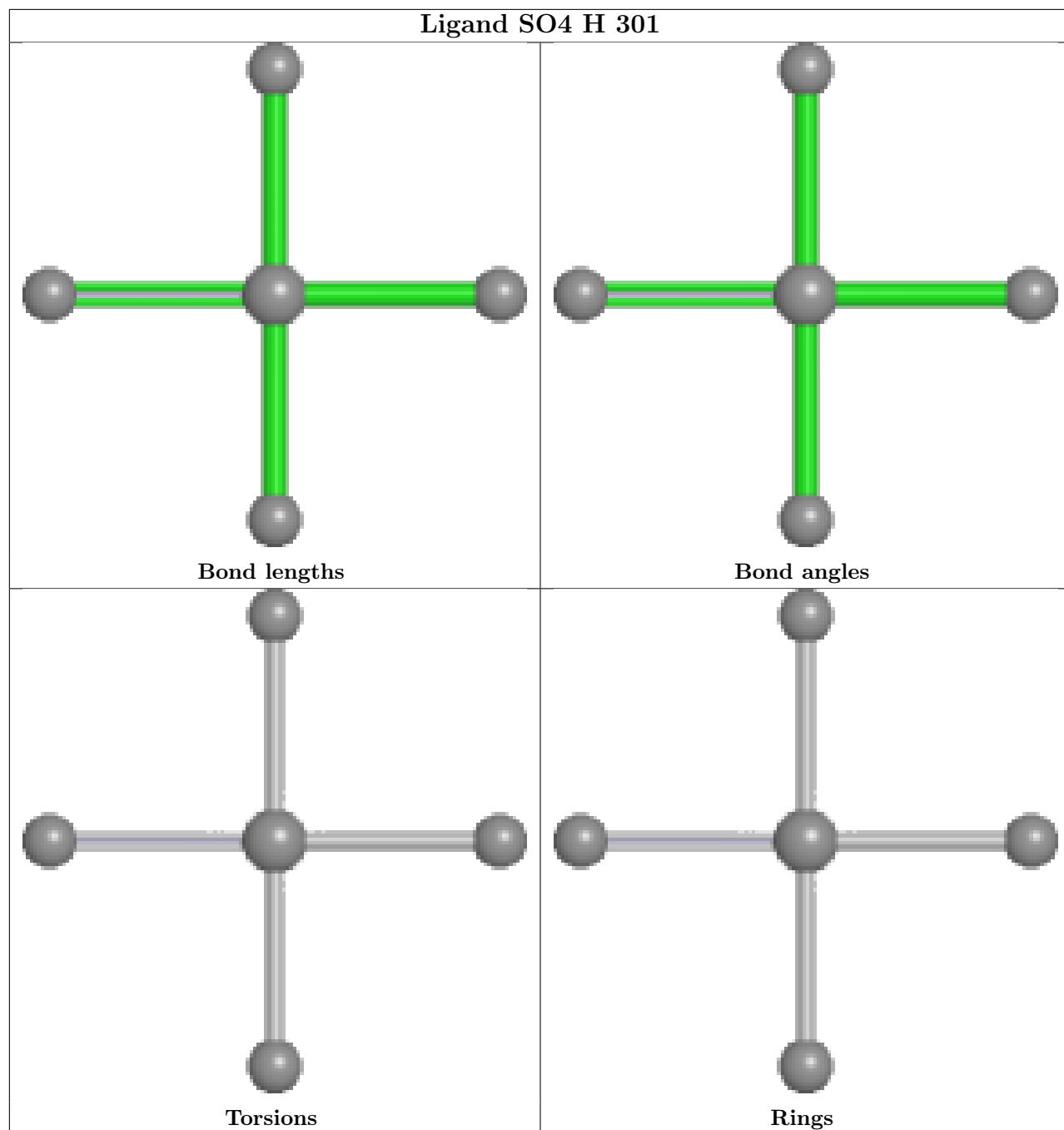
There are no chirality outliers.

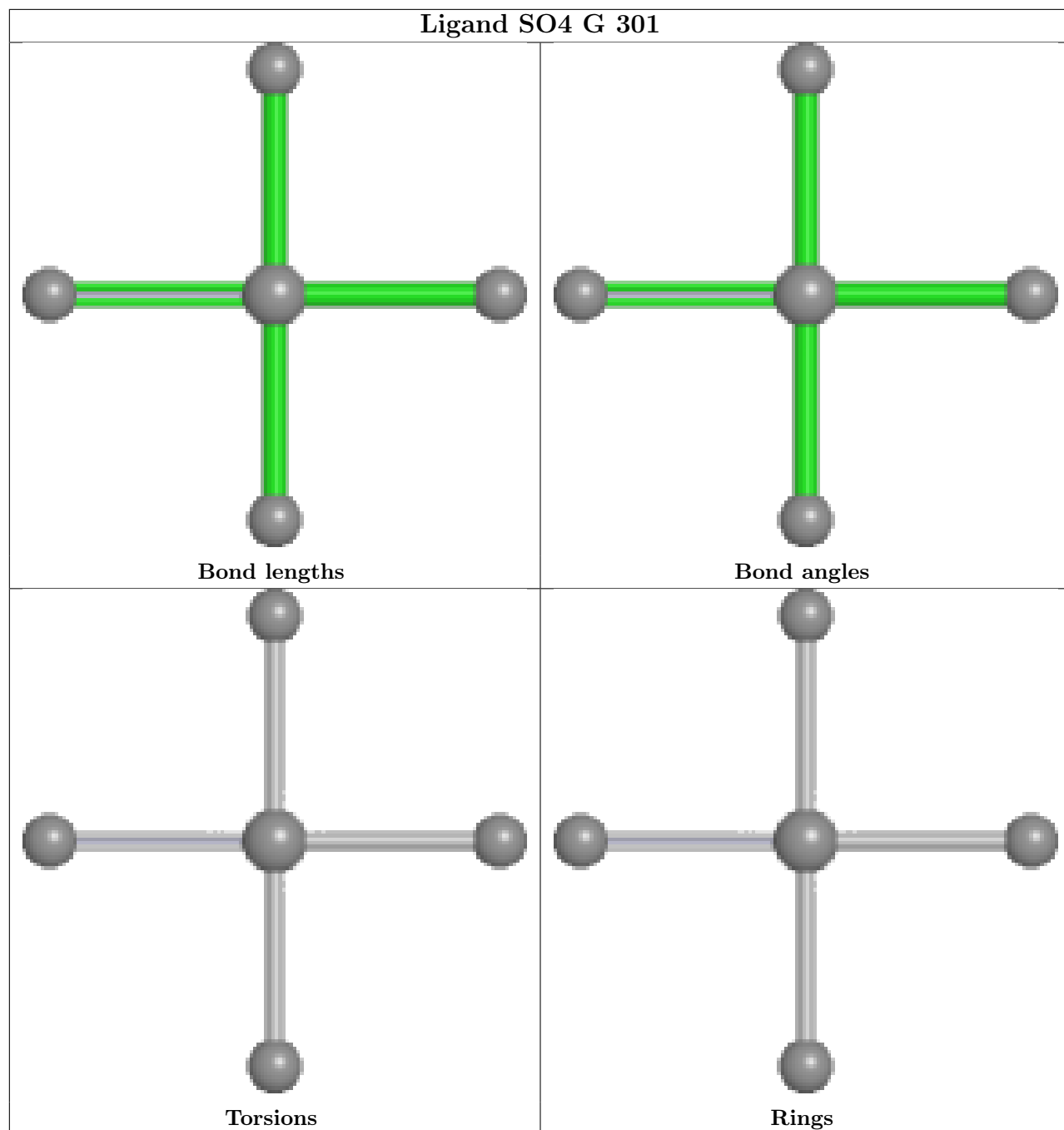
There are no torsion outliers.

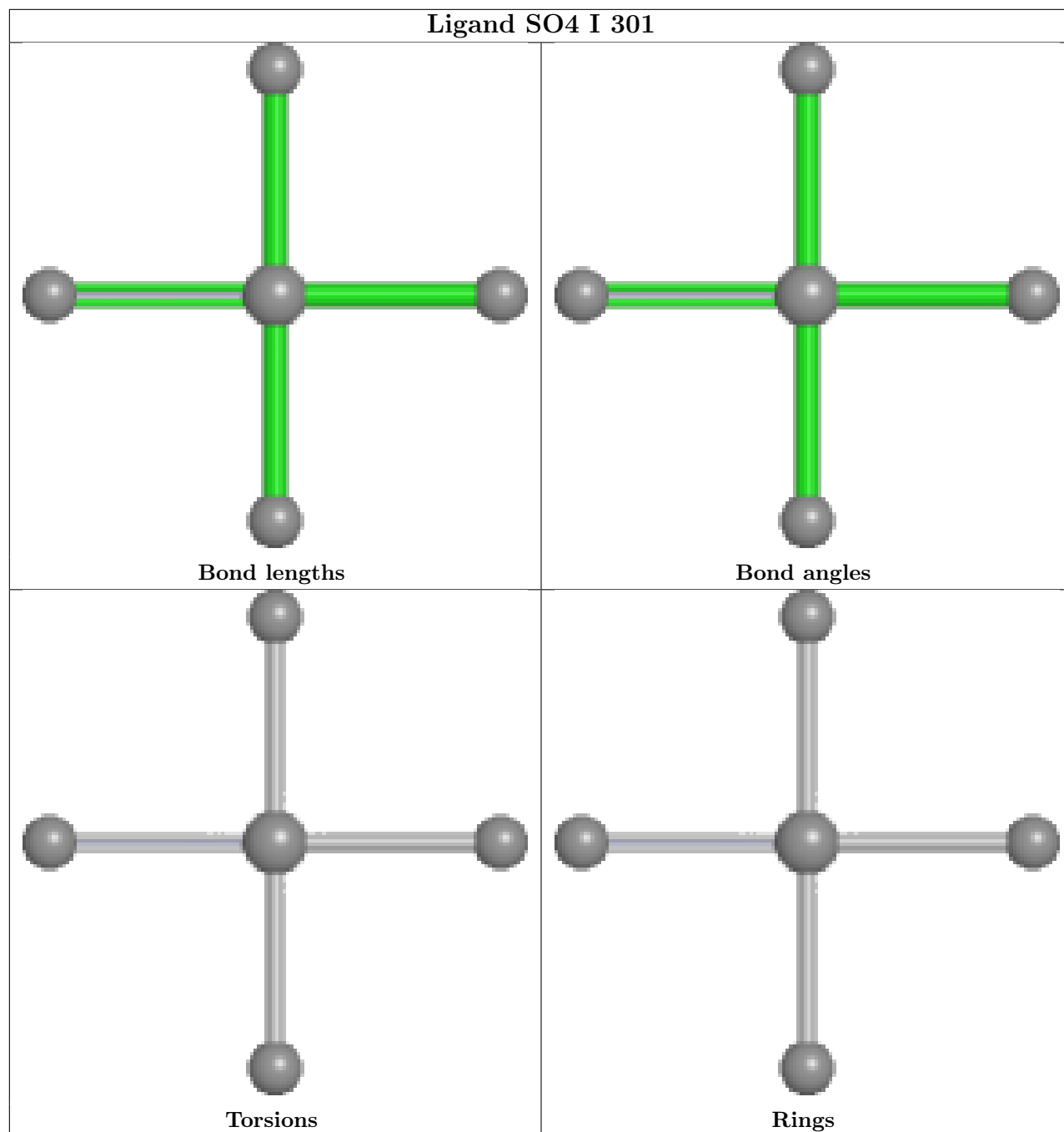
There are no ring outliers.

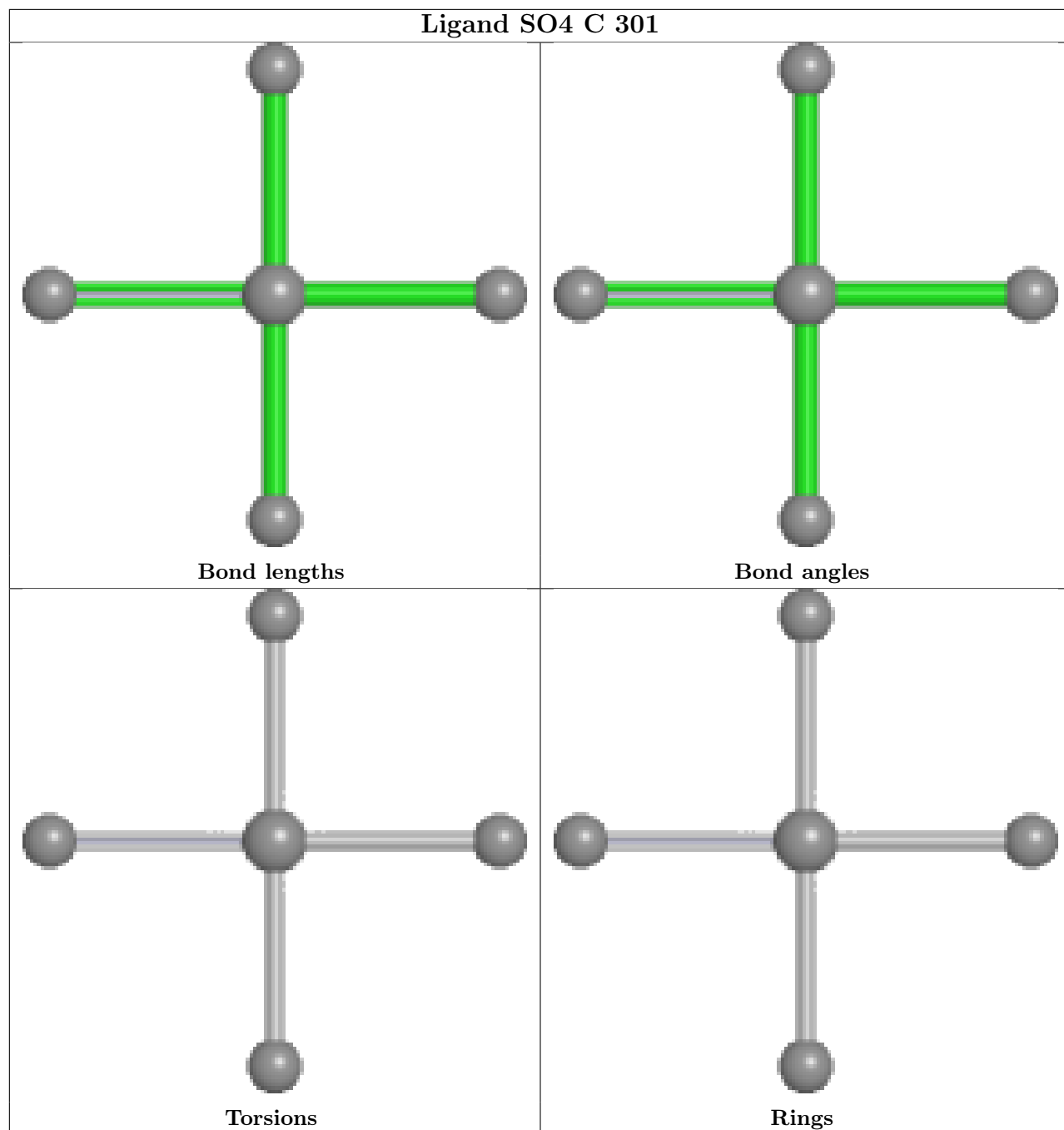
No monomer is involved in short contacts.

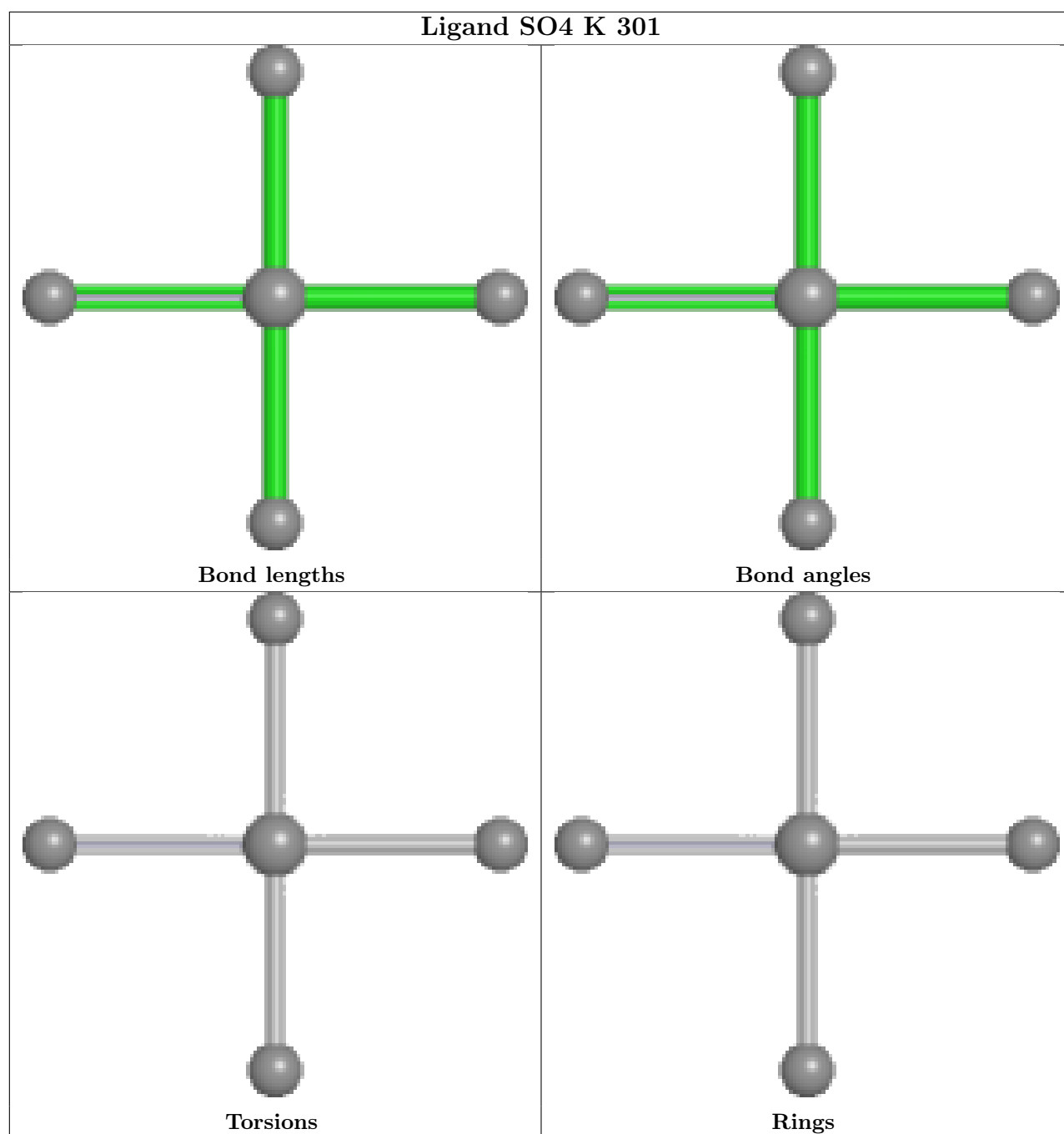
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

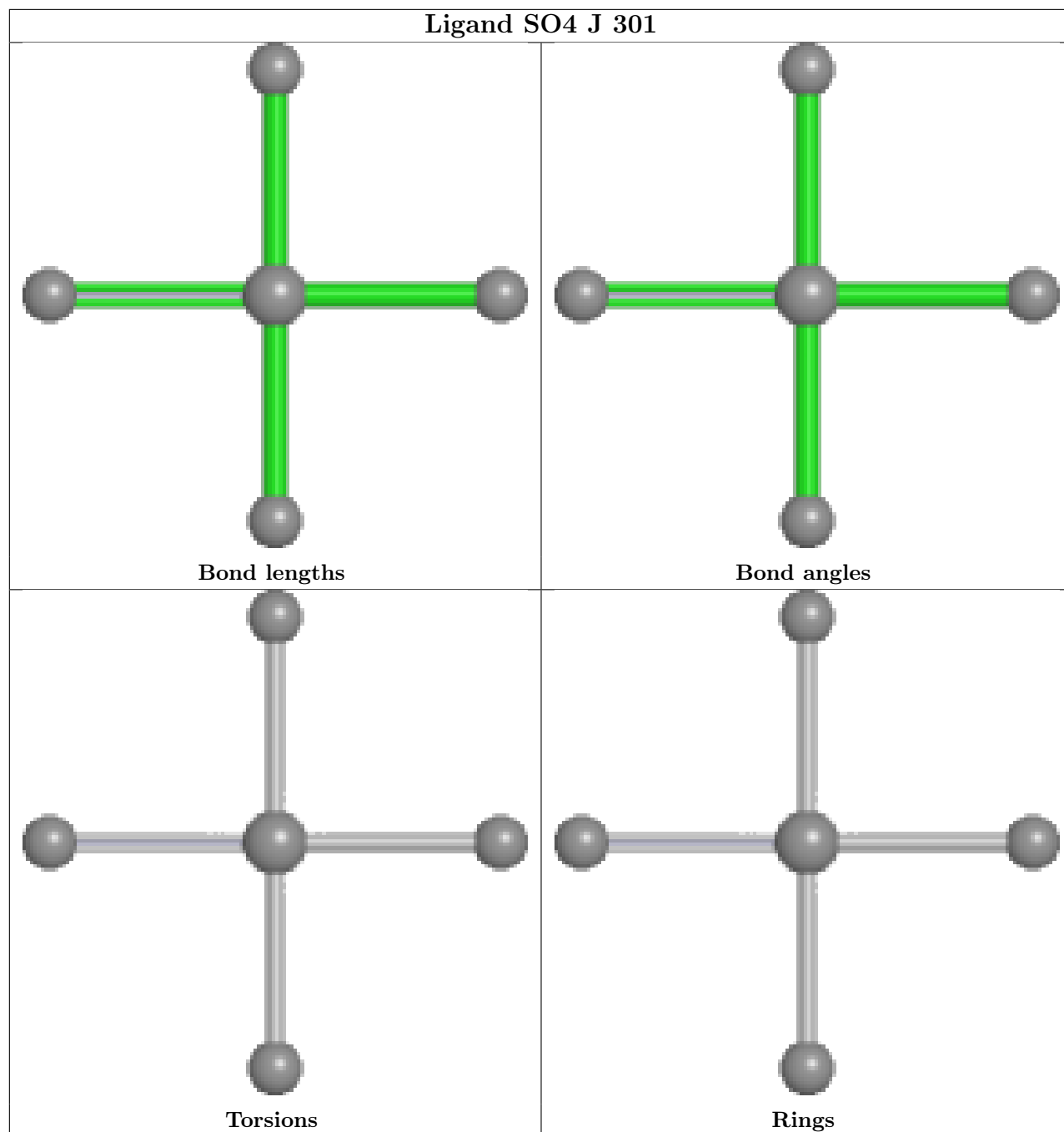


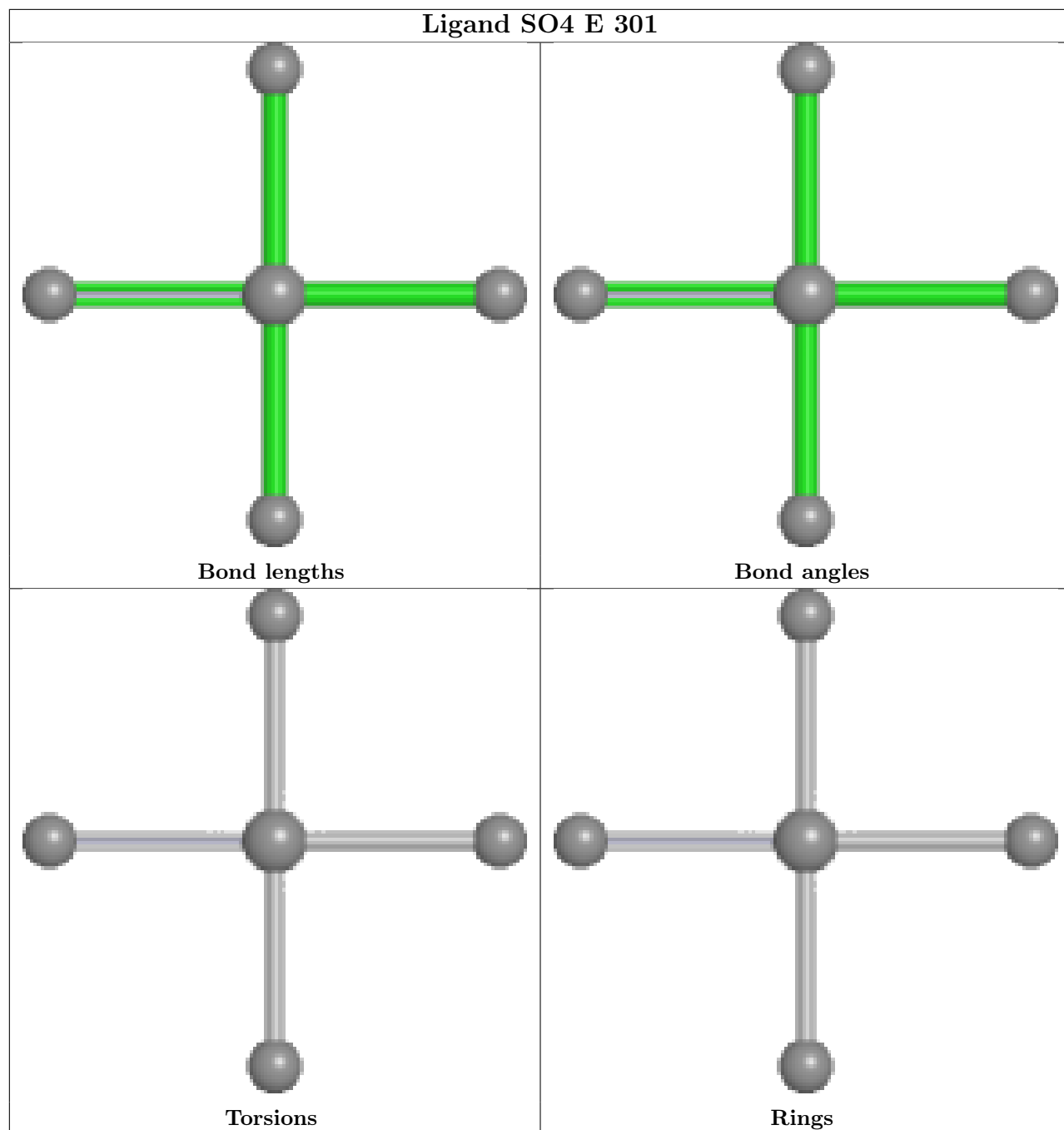


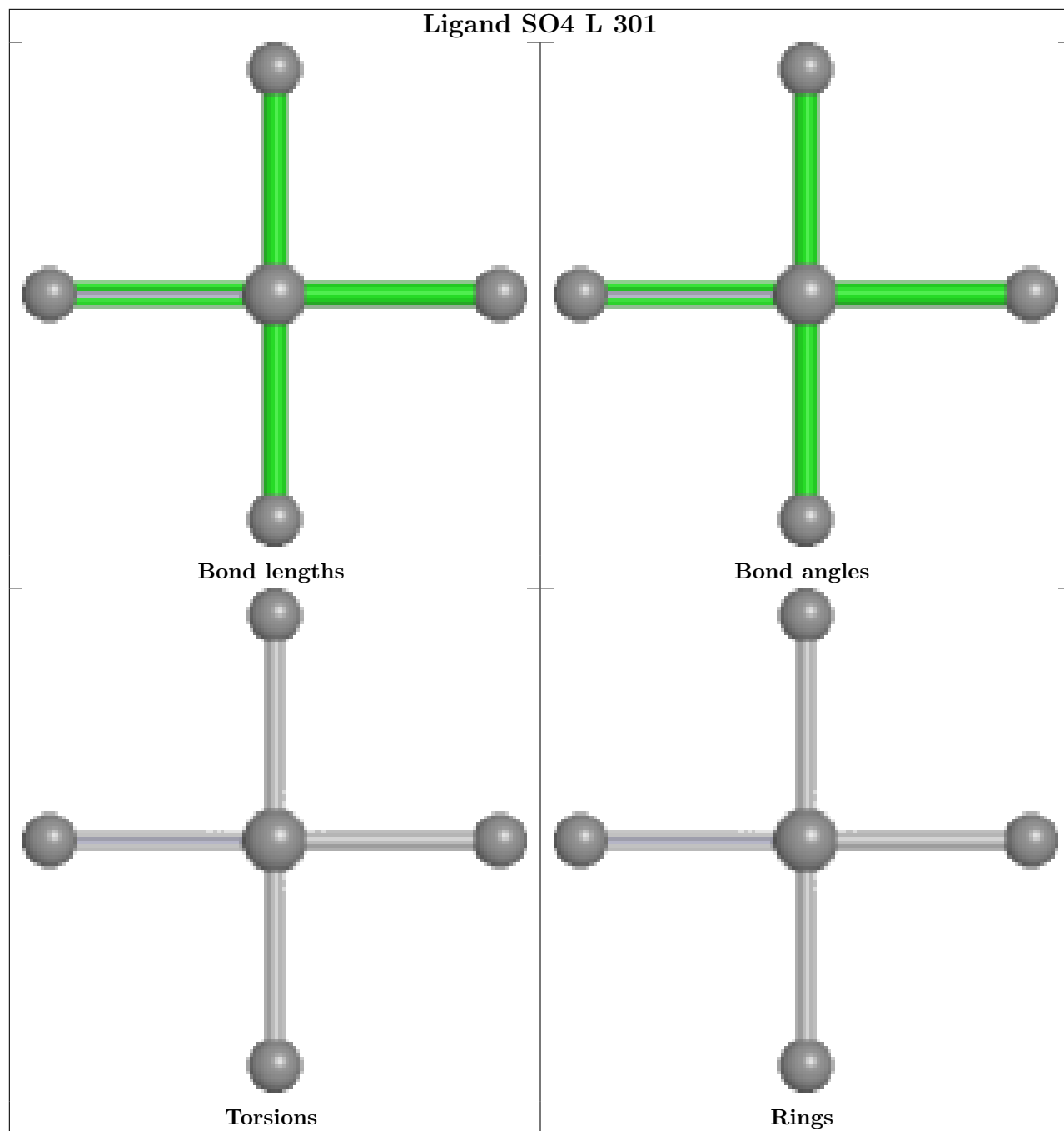


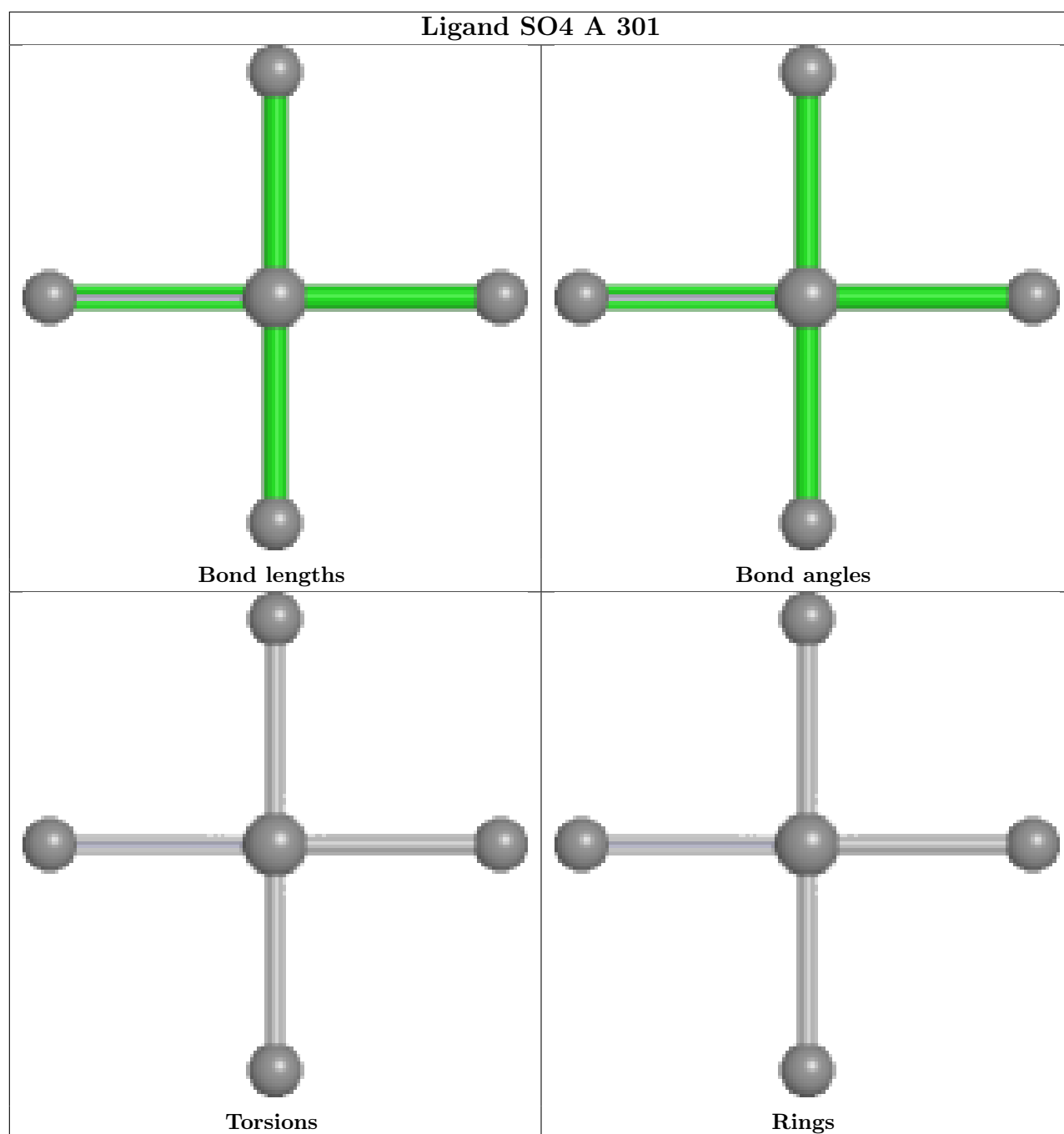


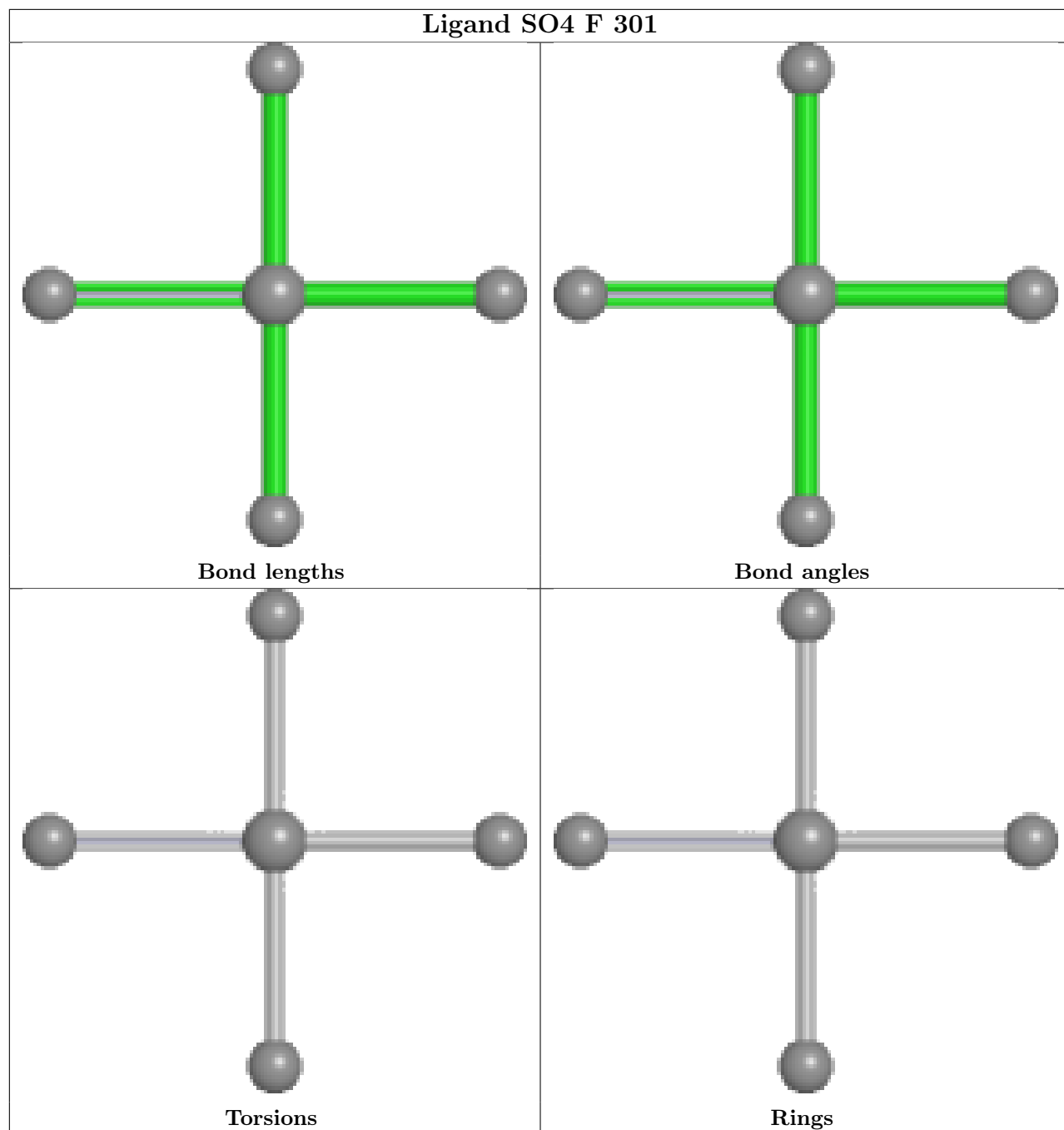


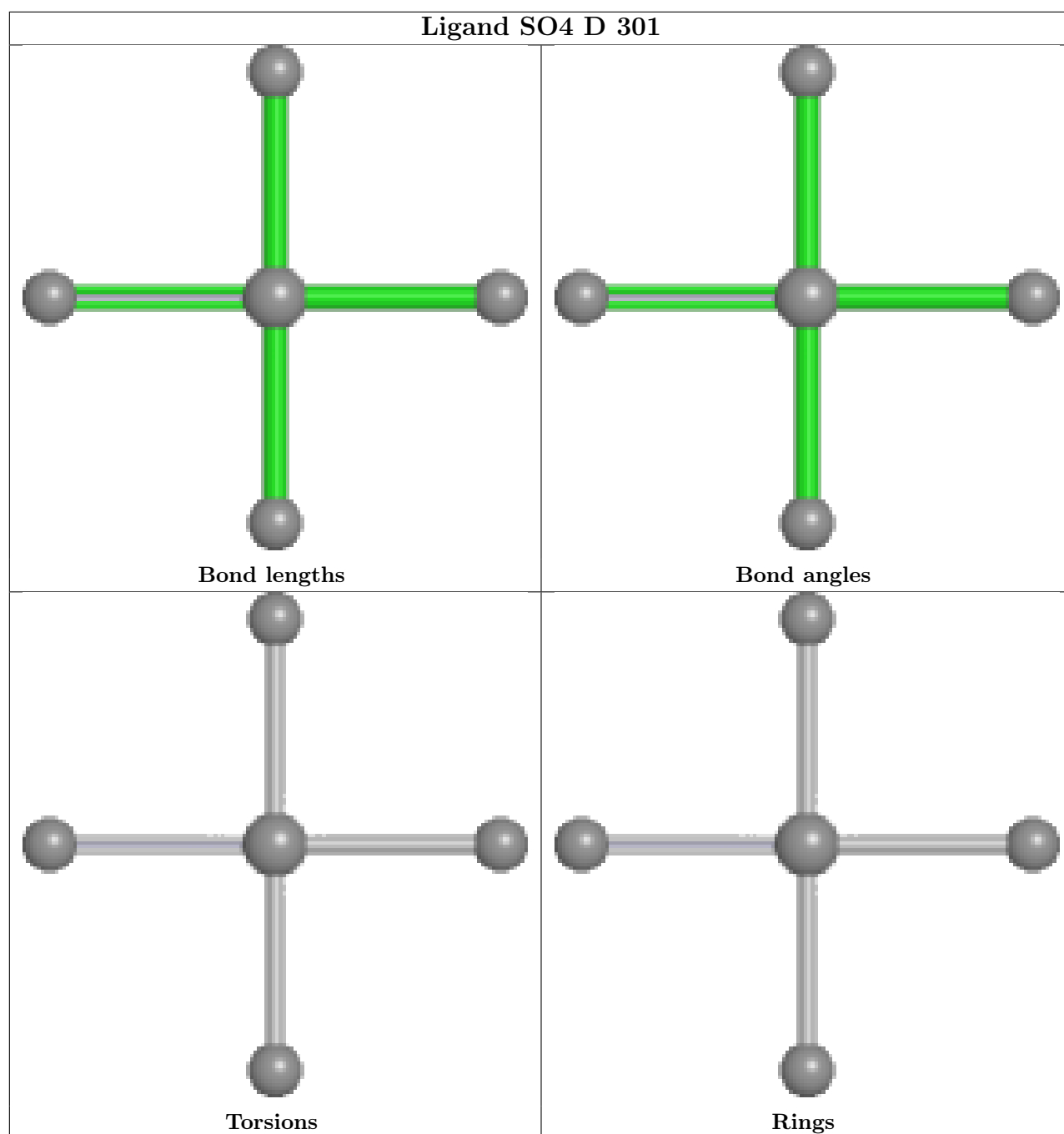


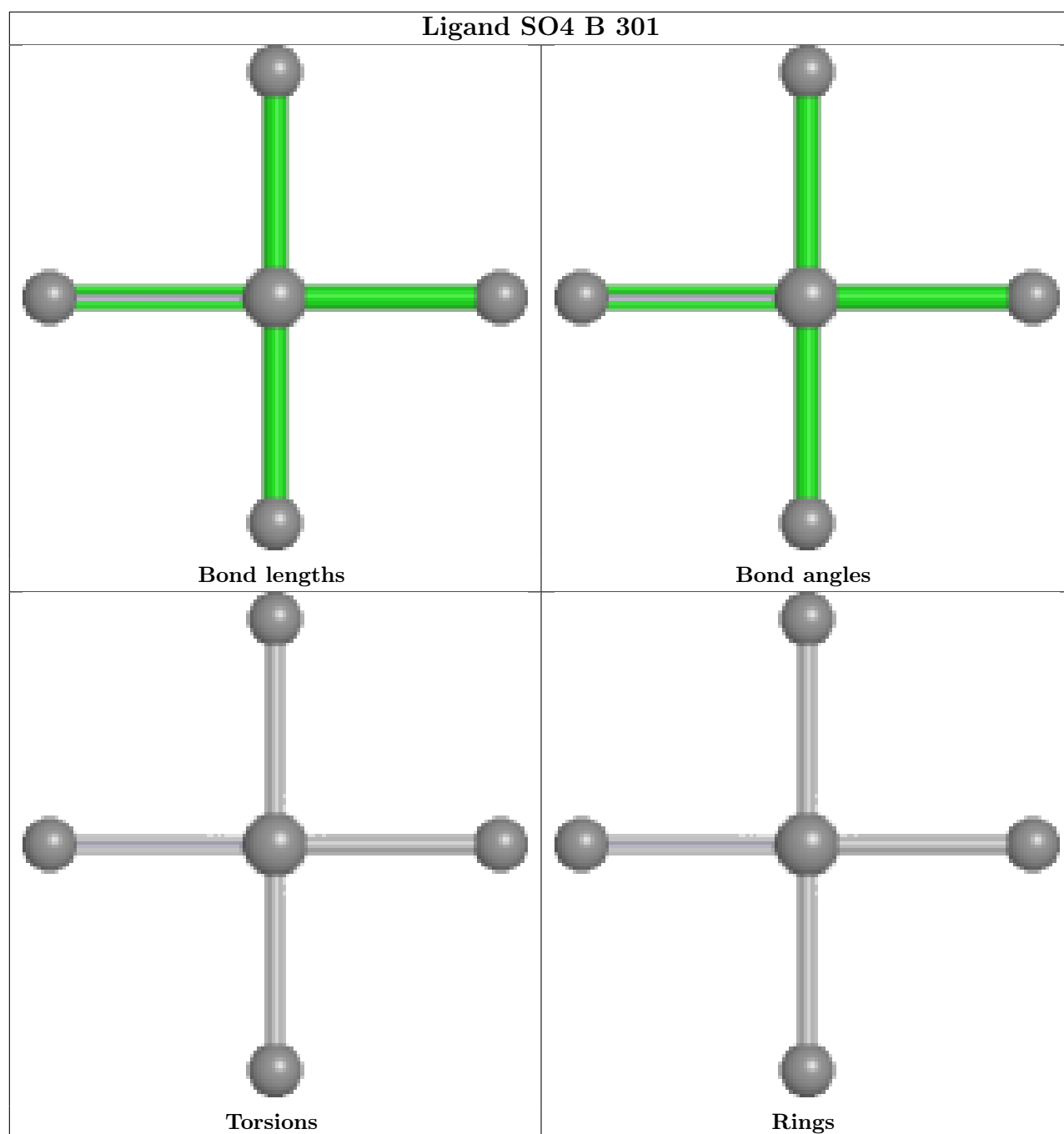












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	289/312 (92%)	0.13	6 (2%) 63 64	14, 26, 40, 72	2 (0%)
1	B	291/312 (93%)	0.83	15 (5%) 33 31	25, 34, 47, 70	0
1	C	290/312 (92%)	-0.02	3 (1%) 79 80	17, 24, 38, 58	1 (0%)
1	D	293/312 (93%)	-0.33	2 (0%) 84 85	11, 19, 32, 52	2 (0%)
1	E	292/312 (93%)	-0.08	1 (0%) 90 90	15, 23, 37, 60	1 (0%)
1	F	276/312 (88%)	2.69	191 (69%) 0 0	29, 51, 68, 80	1 (0%)
1	G	288/312 (92%)	0.34	8 (2%) 55 55	15, 28, 45, 58	2 (0%)
1	H	286/312 (91%)	0.82	13 (4%) 38 37	26, 36, 50, 64	1 (0%)
1	I	289/312 (92%)	-0.33	1 (0%) 90 90	14, 19, 31, 46	1 (0%)
1	J	289/312 (92%)	0.29	6 (2%) 63 64	21, 28, 46, 62	1 (0%)
1	K	289/312 (92%)	-0.17	3 (1%) 79 80	15, 21, 35, 56	1 (0%)
1	L	289/312 (92%)	-0.28	5 (1%) 69 69	11, 20, 35, 62	2 (0%)
All	All	3461/3744 (92%)	0.31	254 (7%) 21 19	11, 26, 52, 80	15 (0%)

The worst 5 of 254 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	149	CYS	6.2
1	F	85	ALA	5.8
1	L	4	TYR	5.5
1	F	19	LEU	5.4
1	F	86	MET	5.4

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

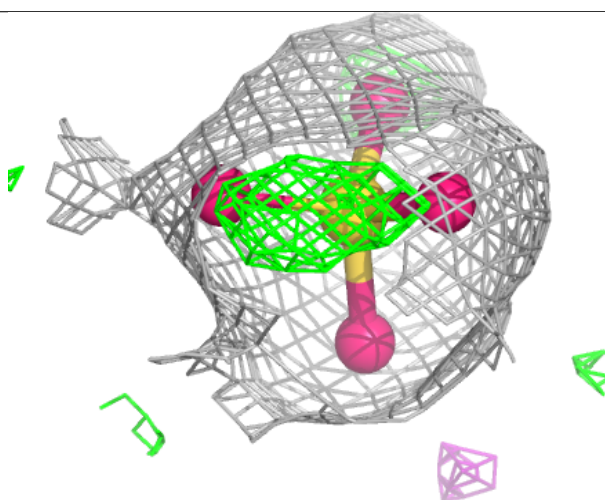
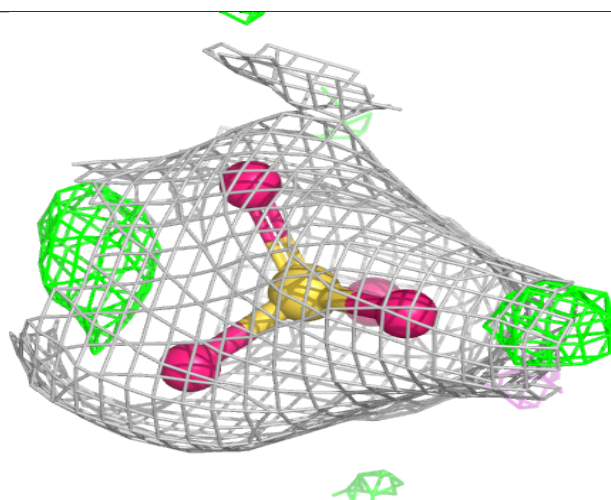
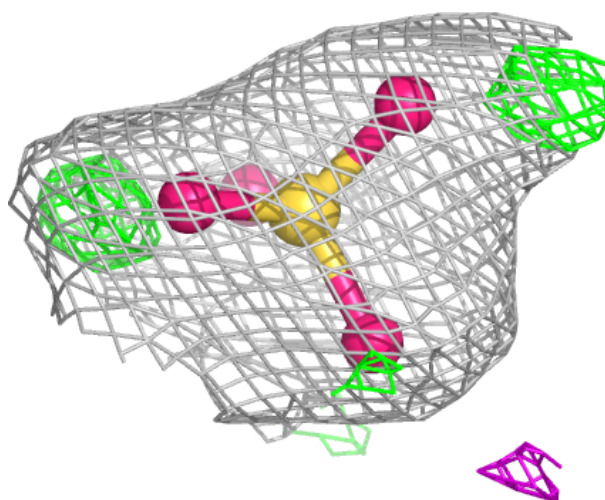
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	F	301	5/5	0.85	0.13	46,52,55,55	0
2	SO4	B	301	5/5	0.97	0.06	28,28,30,32	0
2	SO4	H	301	5/5	0.98	0.08	26,29,31,32	0
2	SO4	E	301	5/5	0.99	0.06	18,20,22,22	0
2	SO4	A	301	5/5	0.99	0.04	21,22,24,25	0
2	SO4	G	301	5/5	0.99	0.05	23,24,24,25	0
2	SO4	C	301	5/5	0.99	0.03	20,21,22,23	0
2	SO4	I	301	5/5	0.99	0.03	16,16,18,19	0
2	SO4	J	301	5/5	0.99	0.05	23,24,25,26	0
2	SO4	L	301	5/5	0.99	0.04	15,17,18,18	0
2	SO4	K	301	5/5	1.00	0.04	18,18,20,20	0
2	SO4	D	301	5/5	1.00	0.04	16,16,17,19	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.

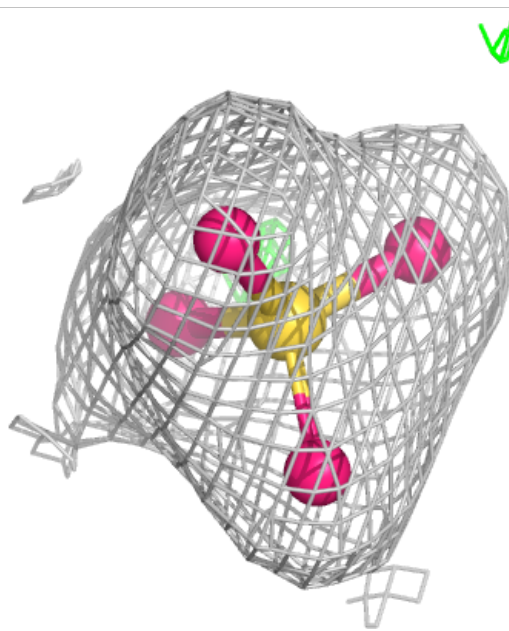
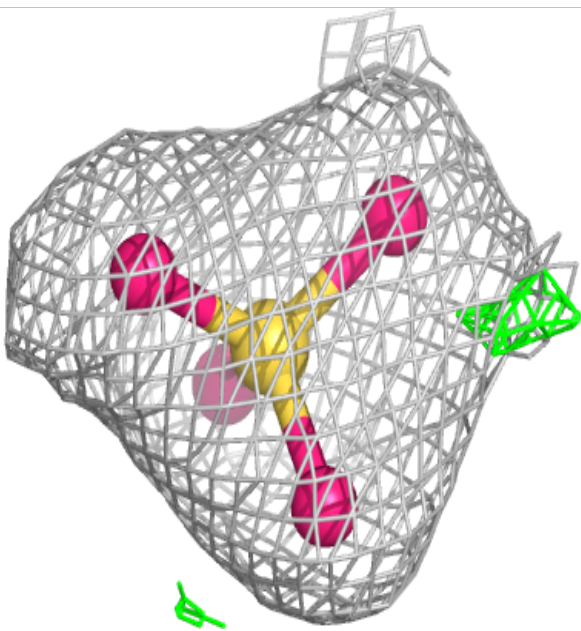
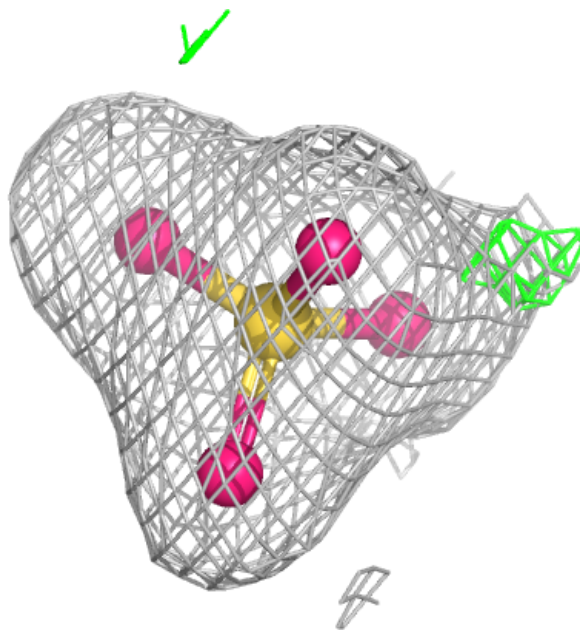
Electron density around SO4 F 301:

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



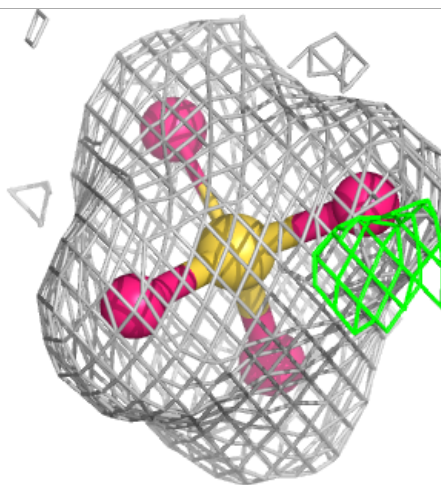
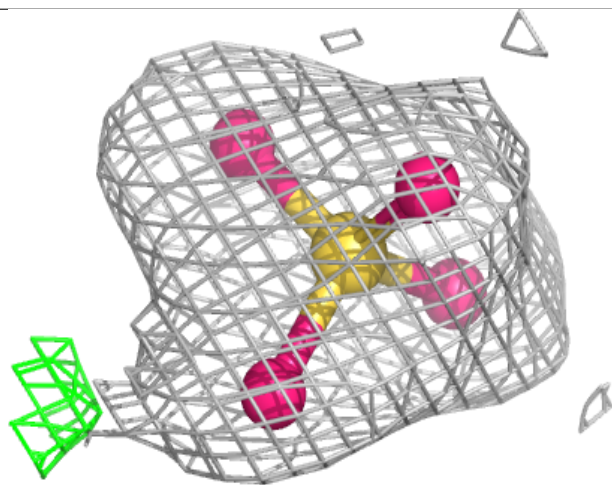
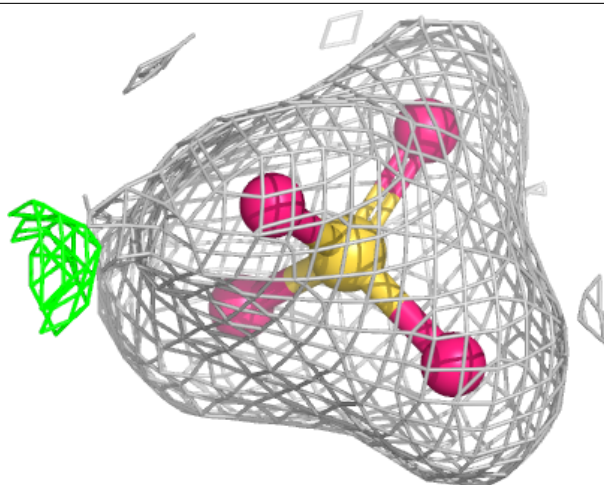
Electron density around SO4 B 301:

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



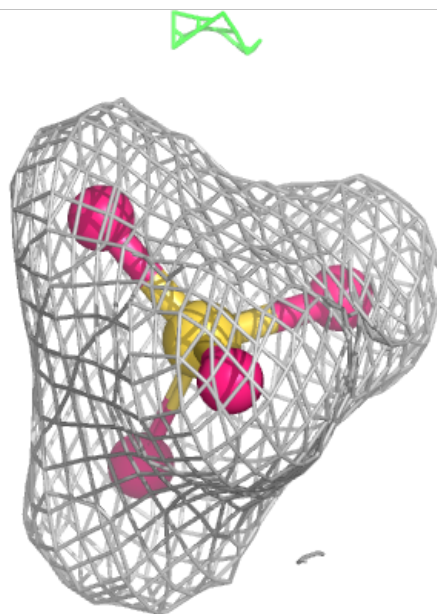
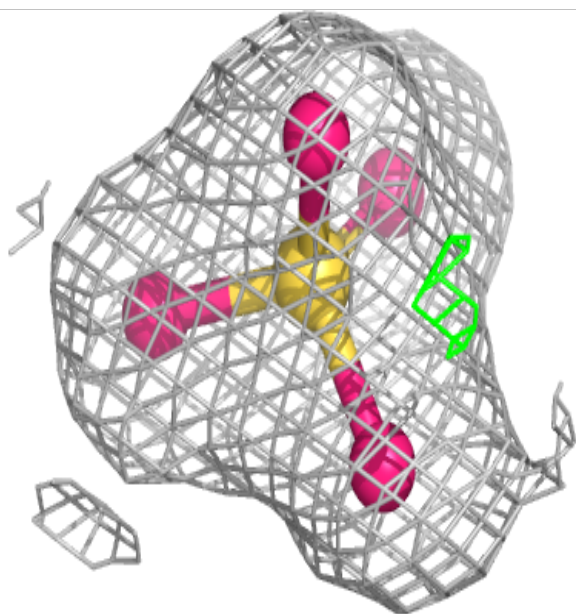
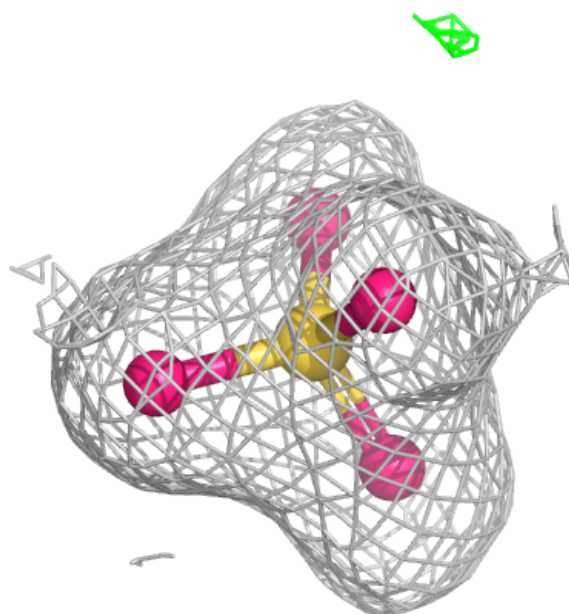
Electron density around SO4 H 301:

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



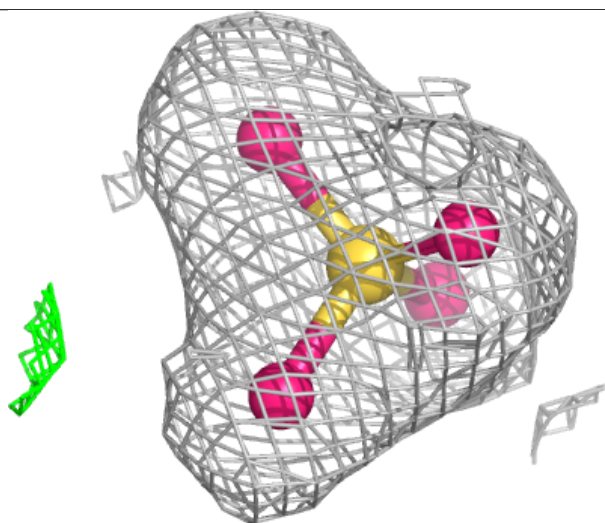
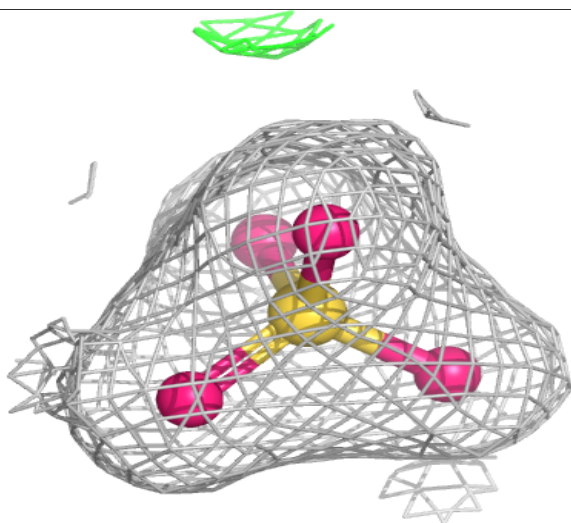
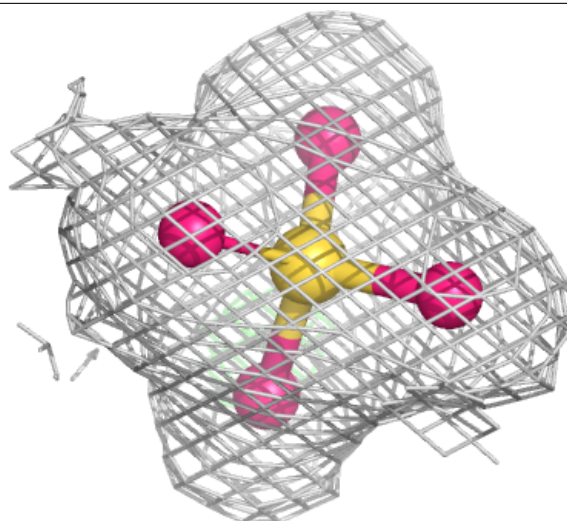
Electron density around SO4 E 301:

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



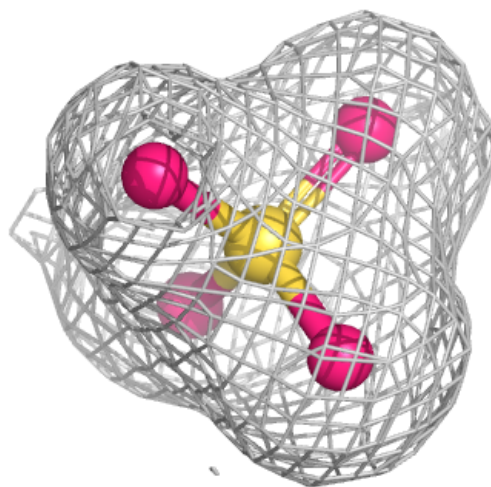
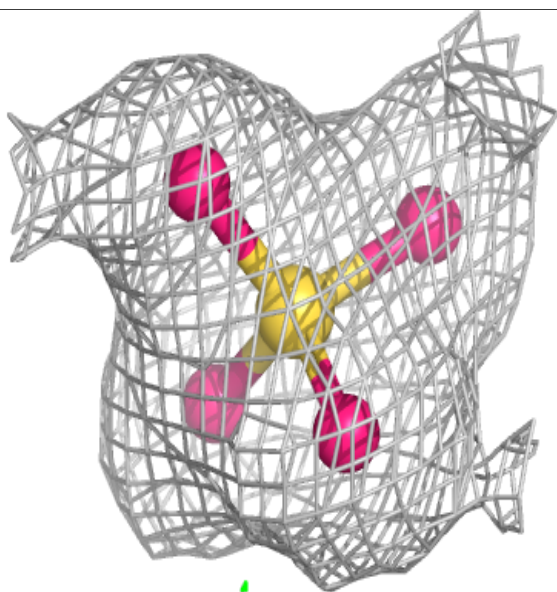
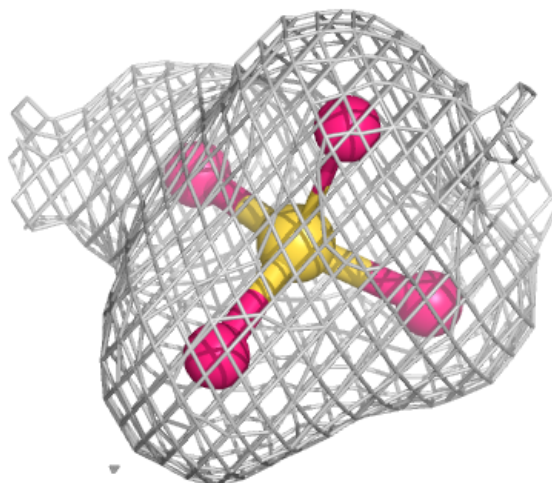
Electron density around SO4 A 301:

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



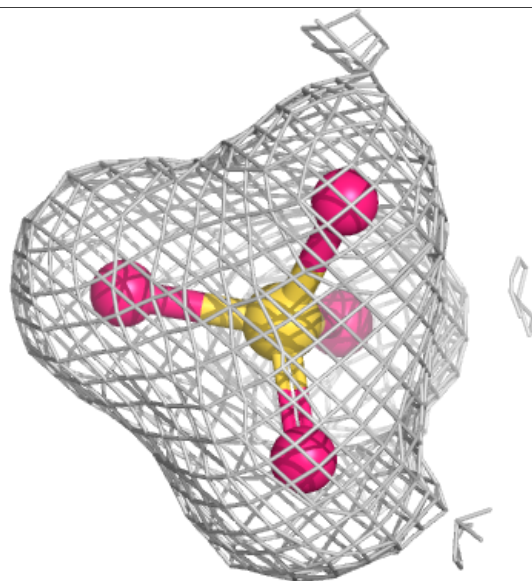
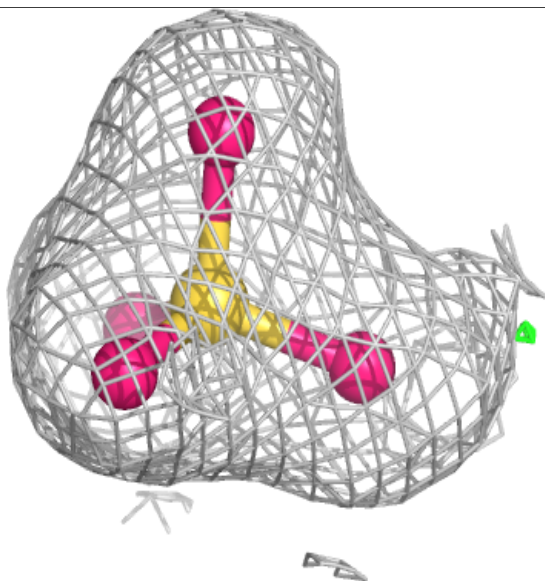
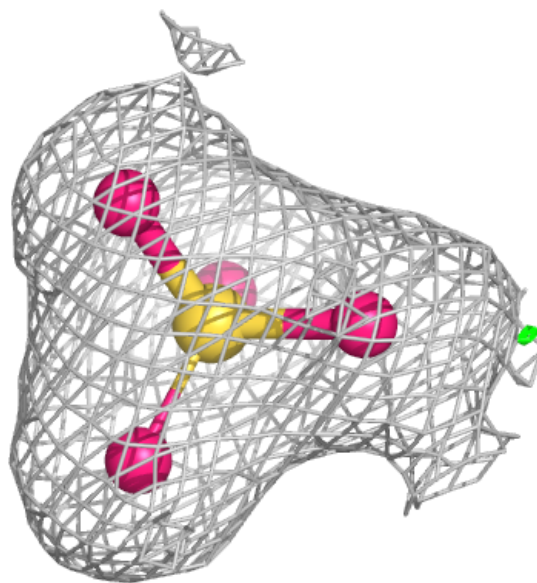
Electron density around SO4 G 301:

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



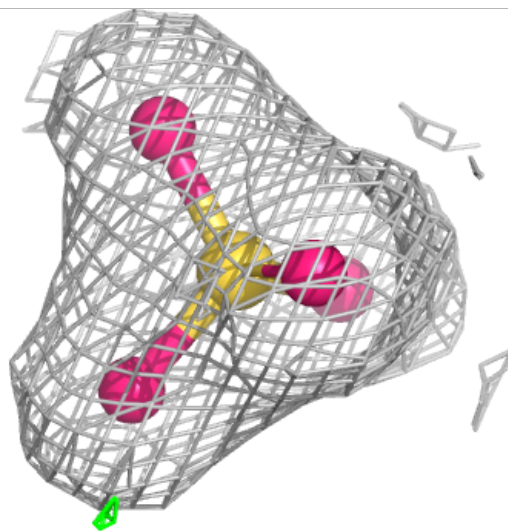
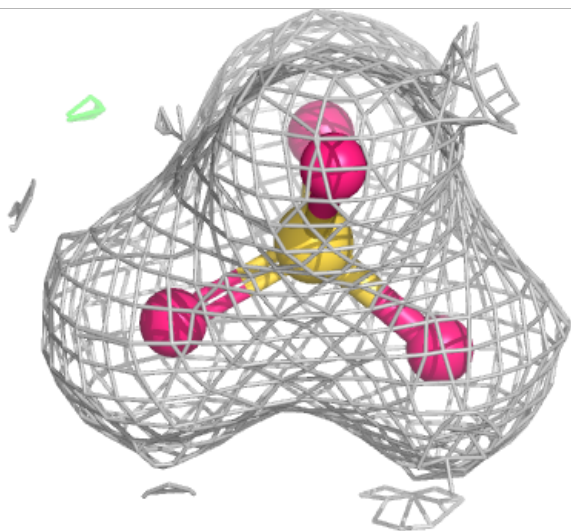
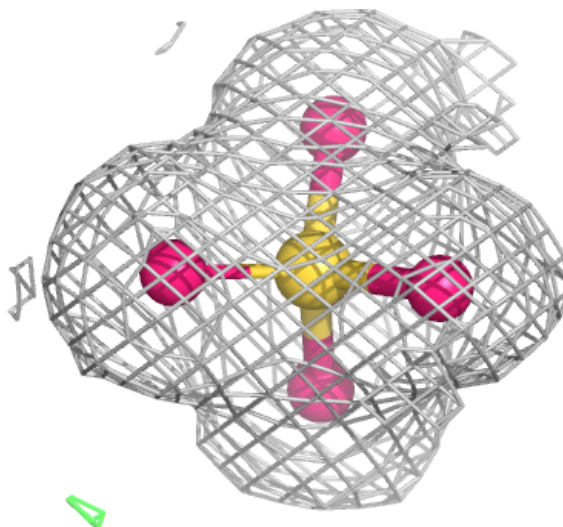
Electron density around SO4 C 301:

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



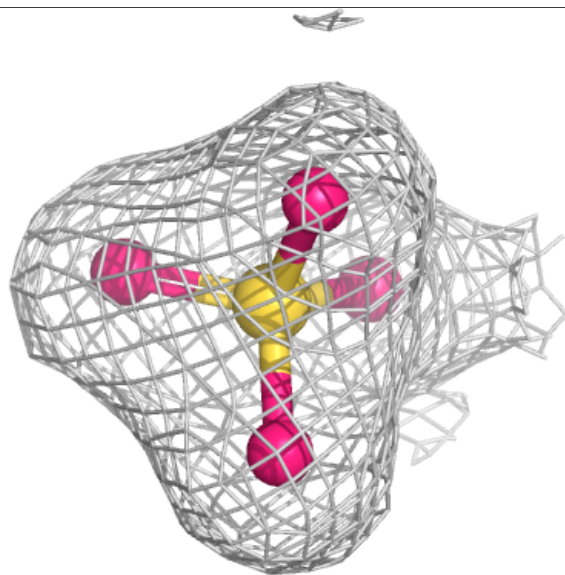
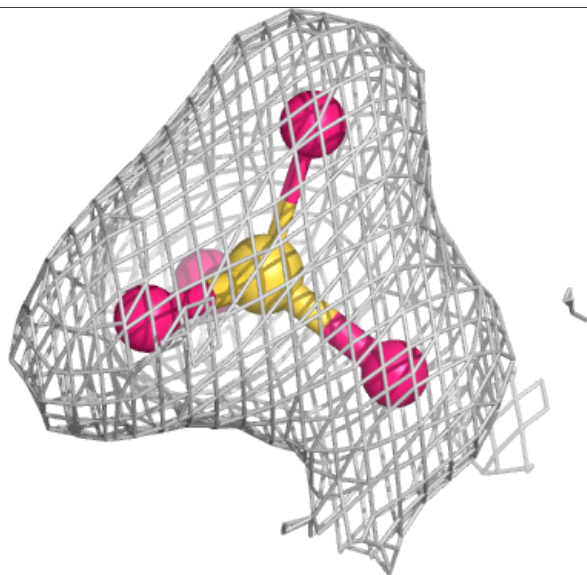
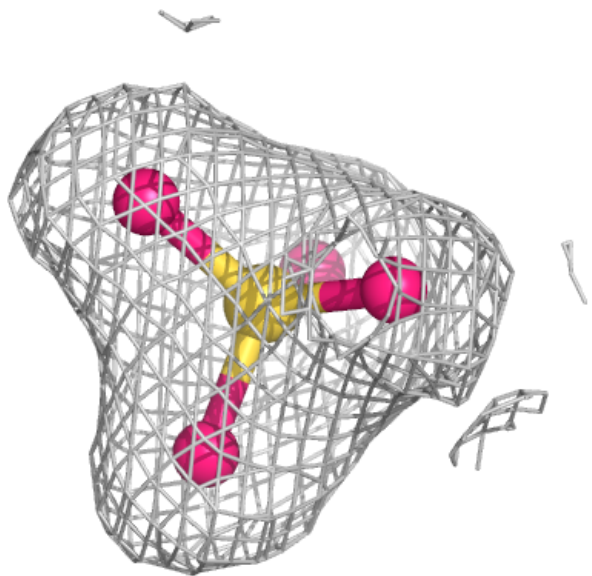
Electron density around SO4 I 301:

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



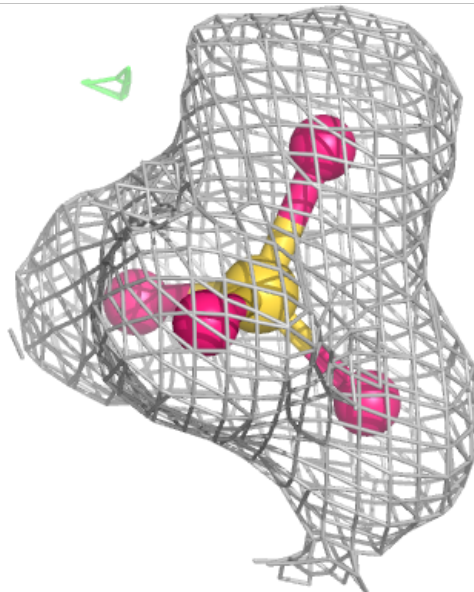
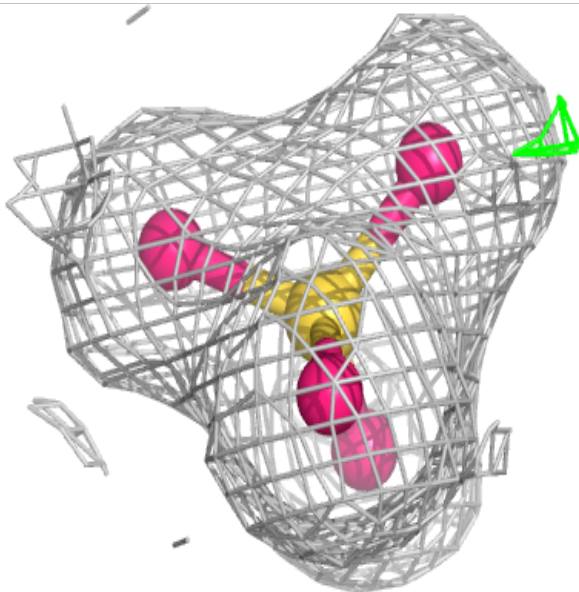
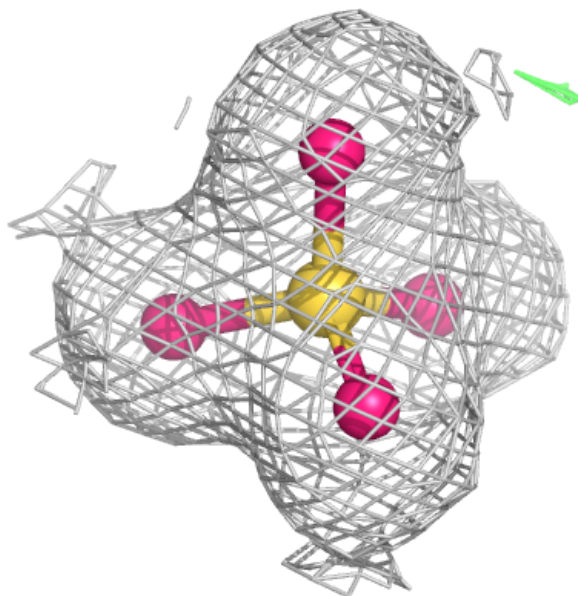
Electron density around SO4 J 301:

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



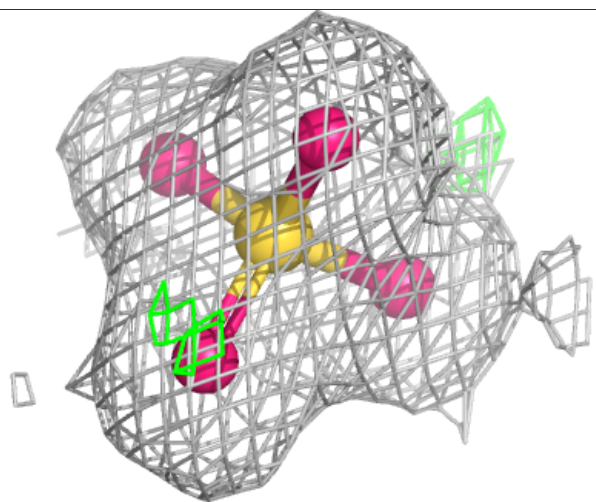
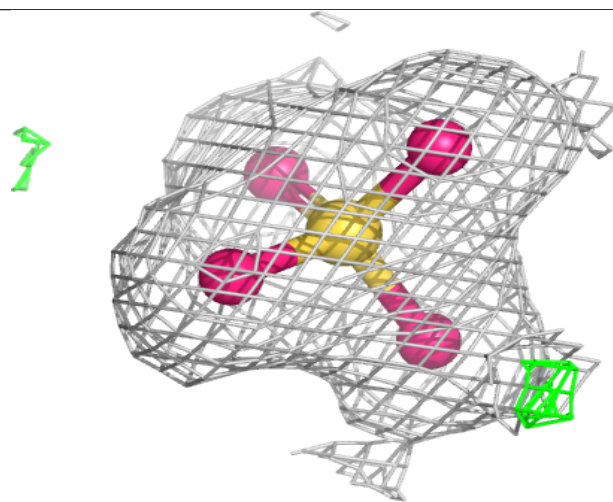
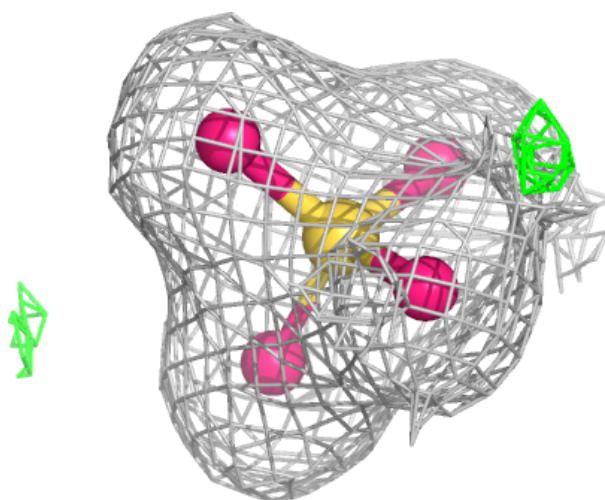
Electron density around SO4 L 301:

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



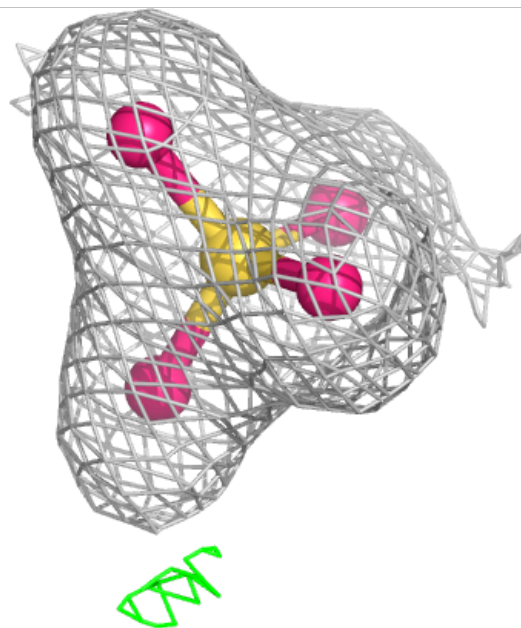
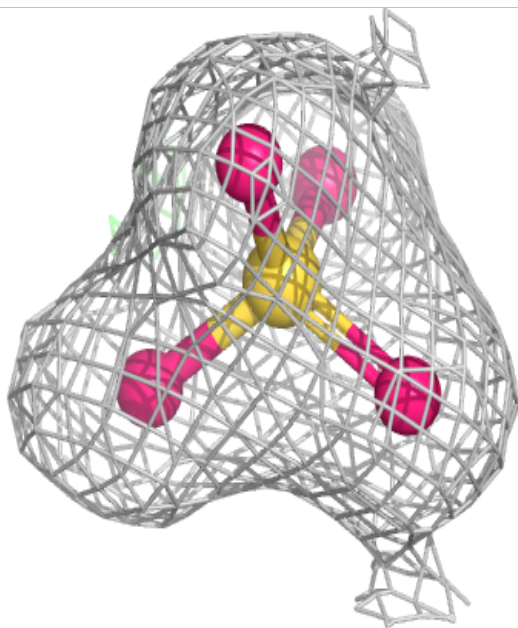
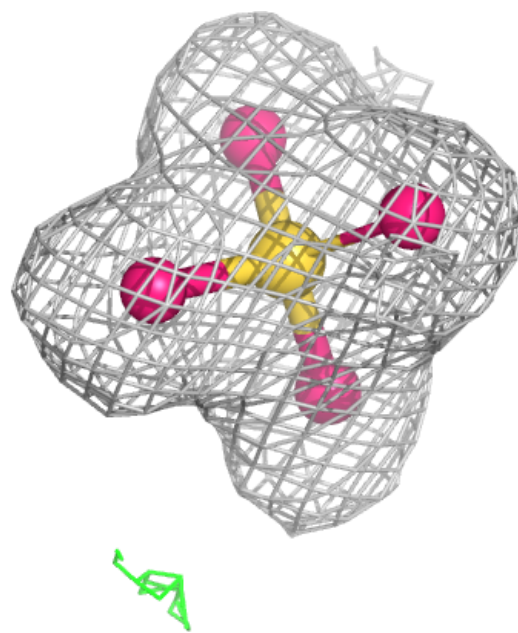
Electron density around SO4 K 301:

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



Electron density around SO4 D 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.