



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 01:45 PM EDT

PDB ID : 7AG7
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 Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

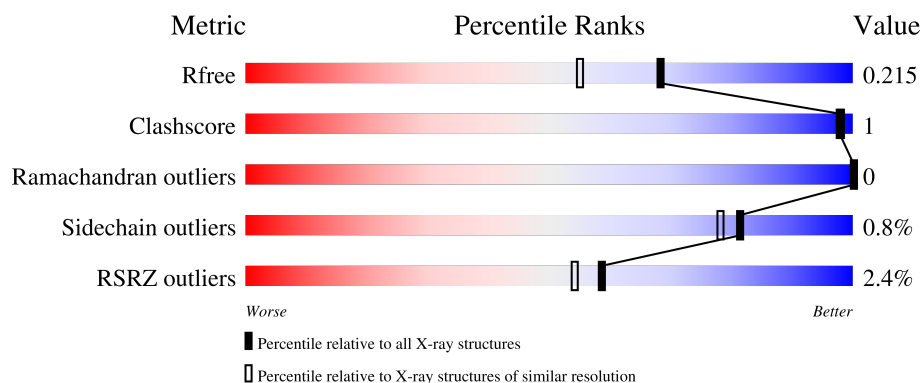
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 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}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (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	
1	B	312	
1	C	312	
1	D	312	
1	E	312	

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Mol	Chain	Length	Quality of chain
1	F	312	<div><div></div><div>26%</div><div>85%</div><div>12%</div></div>
1	G	312	<div><div></div><div>91%</div><div>8%</div></div>
1	H	312	<div><div>%</div><div>90%</div><div>8%</div></div>
1	I	312	<div><div></div><div>90%</div><div>7%</div></div>
1	J	312	<div><div></div><div>90%</div><div>7%</div></div>
1	K	312	<div><div></div><div>90%</div><div>7%</div></div>
1	L	312	<div><div></div><div>90%</div><div>7%</div></div>

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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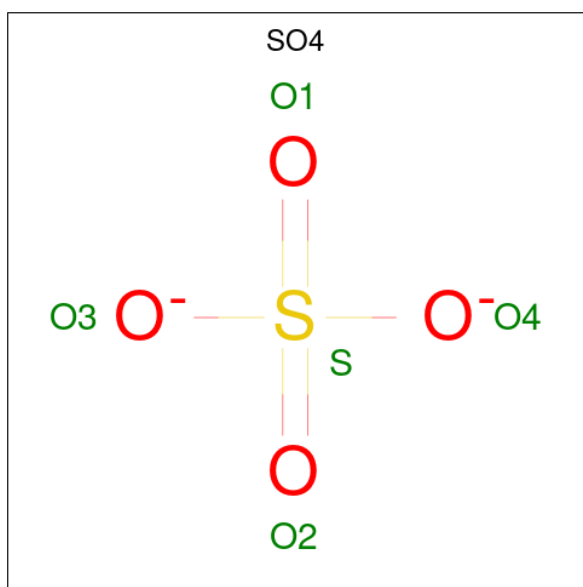
Chain	Residue	Modelled	Actual	Comment	Reference
I	-6	LEU	-	expression tag	UNP Q9L7R9
I	-5	VAL	-	expression tag	UNP Q9L7R9
I	-4	PRO	-	expression tag	UNP Q9L7R9
I	-3	ARG	-	expression tag	UNP Q9L7R9
I	-2	GLY	-	expression tag	UNP Q9L7R9
I	-1	SER	-	expression tag	UNP Q9L7R9
I	0	HIS	-	expression tag	UNP Q9L7R9
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 (three-letter code: 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.

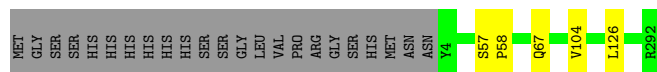
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	146	Total 146	O 146	0	0
3	B	77	Total 77	O 77	0	0
3	C	173	Total 173	O 173	0	0
3	D	279	Total 279	O 279	0	0
3	E	192	Total 192	O 192	0	0
3	F	12	Total 12	O 12	0	0
3	G	131	Total 131	O 131	0	0
3	H	53	Total 53	O 53	0	0
3	I	248	Total 248	O 248	0	0
3	J	121	Total 121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

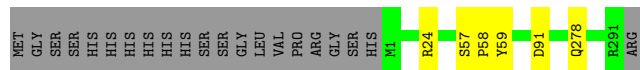
- Molecule 1: Sulfofructosephosphate aldolase

Chain A:  91% 7%



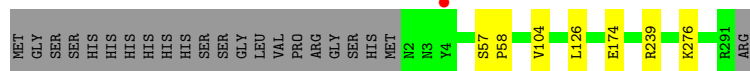
- Molecule 1: Sulfofructosephosphate aldolase

Chain B:  91% 7%



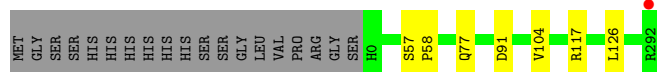
- Molecule 1: Sulfofructosephosphate aldolase

Chain C:  91% 7%




- Molecule 1: Sulfofructosephosphate aldolase

Chain D:  92% 6%

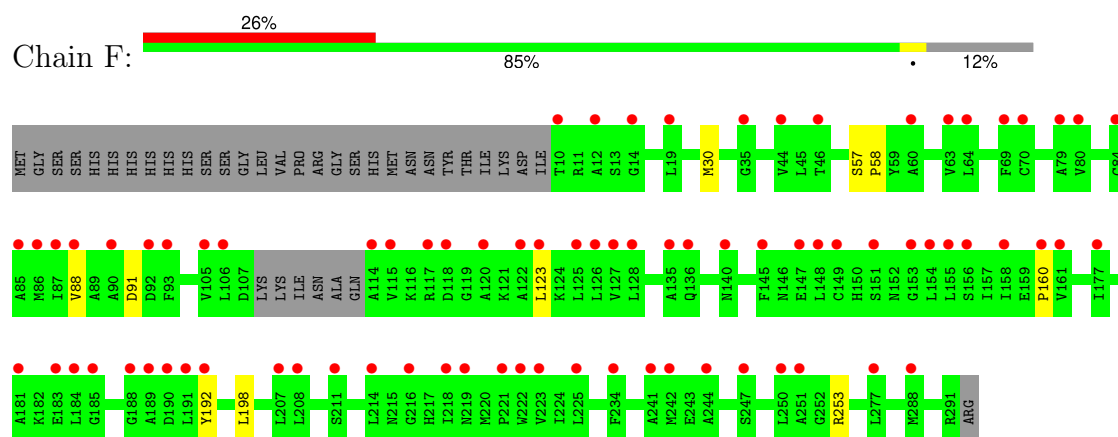


- Molecule 1: Sulfofructosephosphate aldolase

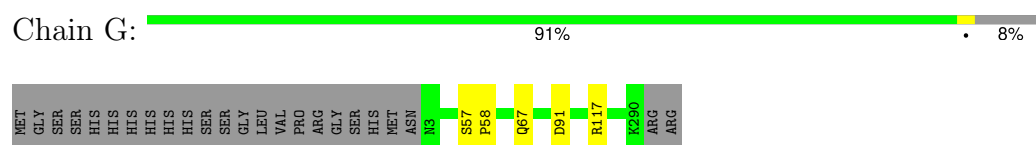
Chain E:  90% 6%



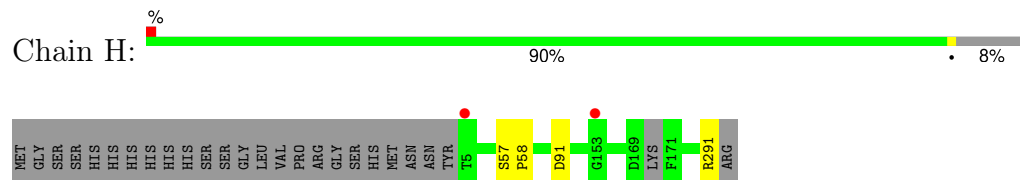
- Molecule 1: Sulfofructosephosphate aldolase



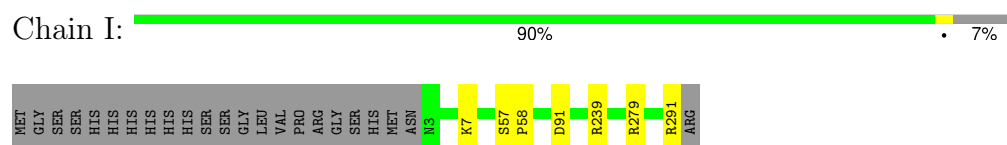
- Molecule 1: Sulfofructosephosphate aldolase



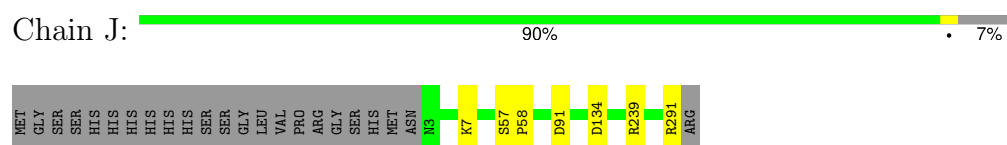
- Molecule 1: Sulfofructosephosphate aldolase



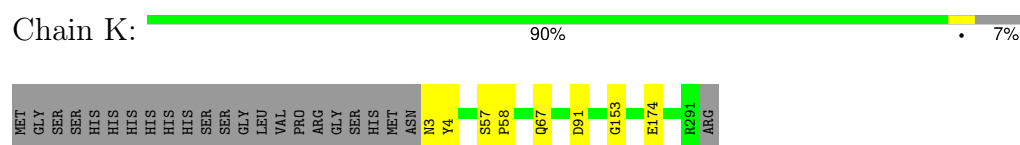
- Molecule 1: Sulfofructosephosphate aldolase




- Molecule 1: Sulfofructosephosphate aldolase



- Molecule 1: Sulfofructosephosphate aldolase



- Molecule 1: Sulfofructosephosphate aldolase

Chain L: 

MET	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	SER	SER	GLY	LEU	VAL	PRO	ARG	GLY	SER	HIS	MET	ASN	N3	Y4	T5	S57	P58	V104	L126	K276	R291	ARG
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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 53.71 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (53.01-1.80) 97.5 (53.71-1.80)	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	17503 reflections (4.97%)	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)	0.32 , 37.8	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

5.1 Standard geometry

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	0.71	0/2203	0.75	0/2985
1	B	0.68	0/2185	0.79	2/2964 (0.1%)
1	C	0.71	1/2217 (0.0%)	0.76	0/3003
1	D	0.76	0/2252	0.83	1/3049 (0.0%)
1	E	0.71	0/2219	0.78	1/3007 (0.0%)
1	F	0.70	0/1923	0.73	0/2620
1	G	0.71	0/2183	0.78	1/2961 (0.0%)
1	H	0.66	0/2142	0.75	0/2905
1	I	0.74	0/2206	0.81	2/2988 (0.1%)
1	J	0.68	0/2184	0.75	1/2962 (0.0%)
1	K	0.72	1/2219 (0.0%)	0.80	0/3002
1	L	0.73	0/2204	0.82	3/2985 (0.1%)
All	All	0.71	2/26137 (0.0%)	0.78	11/35431 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	174	GLU	CD-OE1	-6.69	1.18	1.25
1	C	174	GLU	CD-OE1	-5.35	1.19	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	24	ARG	NE-CZ-NH2	-10.60	115.00	120.30
1	I	291	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	E	117	ARG	NE-CZ-NH1	7.15	123.87	120.30
1	B	24	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	117	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	J	291	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	G	117	ARG	NE-CZ-NH2	5.30	122.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	291	ARG	NE-CZ-NH1	-5.29	117.65	120.30
1	L	5	THR	OG1-CB-CG2	-5.12	98.21	110.00
1	I	279	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	L	104	VAL	CG1-CB-CG2	-5.11	102.72	110.90

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	2	0
1	C	2181	0	2175	4	0
1	D	2212	0	2220	3	0
1	E	2182	0	2169	5	0
1	F	1895	0	1736	8	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	36	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.

All (36) 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:B:59:TYR:CD1	1:B:278:GLN:HG2	2.31	0.64
1:J:239:ARG:NH2	3:J:402:HOH:O	2.31	0.60
1:A:104[B]:VAL:HG21	1:A:126:LEU:HD23	1.84	0.60
1:E:113:GLN:HE21	1:E:152:ASN:HD21	1.50	0.59
1:I:239:ARG:NH1	3:I:401:HOH:O	2.28	0.53
1:F:30:MET:HE2	1:F:253:ARG:HE	1.76	0.51
1:C:239:ARG:NH2	3:C:401:HOH:O	2.28	0.50
1:J:134:ASP:OD1	3:J:401:HOH:O	2.20	0.49
1:E:113:GLN:HE21	1:E:152:ASN:ND2	2.11	0.49
1:F:30:MET:CE	1:F:253:ARG:NE	2.76	0.49
1:F:30:MET:CE	1:F:253:ARG:HE	2.26	0.48
1:K:4:TYR:HB3	1:K:153:GLY:O	2.15	0.47
1:C:276:LYS:NZ	3:C:405:HOH:O	2.47	0.46
1:L:276:LYS:NZ	3:L:403:HOH:O	2.48	0.46
1:F:30:MET:HE1	1:F:253:ARG:NE	2.30	0.46
1:F:30:MET:HE1	1:F:253:ARG:CZ	2.47	0.44
1:I:57:SER:N	1:I:58:PRO:CD	2.82	0.42
1:B:57:SER:N	1:B:58:PRO:CD	2.82	0.42
1:G:57:SER:N	1:G:58:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:SER:N	1:H:58:PRO:CD	2.83	0.42
1:F:57:SER:N	1:F:58:PRO:CD	2.83	0.41
1:C:57:SER:N	1:C:58:PRO:CD	2.84	0.41
1:D:57:SER:N	1:D:58:PRO:CD	2.83	0.41
1:J:57:SER:N	1:J:58:PRO:CD	2.82	0.41
1:F:160:PRO:HG2	1:F:192:TYR:CZ	2.56	0.41
1:F:88:VAL:O	1:F:123:LEU:HA	2.21	0.41
1:E:88:VAL:O	1:E:123:LEU:HA	2.21	0.41
1:A:57:SER:N	1:A:58:PRO:CD	2.84	0.41
1:E:57:SER:N	1:E:58:PRO:CD	2.84	0.40
1:K:57:SER:N	1:K:58:PRO:CD	2.84	0.40
1:D:77:GLN:NE2	3:D:404:HOH:O	2.49	0.40
1:L:57:SER:N	1:L:58:PRO:CD	2.84	0.40
1:E:10:THR:O	3:E:401:HOH:O	2.22	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	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	88	87
1	B	215/252 (85%)	214 (100%)	1 (0%)	88	87
1	C	224/252 (89%)	224 (100%)	0	100	100
1	D	229/252 (91%)	228 (100%)	1 (0%)	91	89
1	E	221/252 (88%)	219 (99%)	2 (1%)	78	75
1	F	164/252 (65%)	162 (99%)	2 (1%)	71	65
1	G	217/252 (86%)	215 (99%)	2 (1%)	78	75
1	H	210/252 (83%)	208 (99%)	2 (1%)	76	71
1	I	223/252 (88%)	221 (99%)	2 (1%)	78	75
1	J	217/252 (86%)	215 (99%)	2 (1%)	78	75
1	K	226/252 (90%)	223 (99%)	3 (1%)	69	62
1	L	222/252 (88%)	220 (99%)	2 (1%)	78	75
All	All	2590/3024 (86%)	2570 (99%)	20 (1%)	81	78

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	B	91	ASP

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Mol	Chain	Res	Type
1	D	91	ASP
1	E	91	ASP
1	E	291	ARG
1	F	91	ASP
1	F	198	LEU
1	G	67	GLN
1	G	91	ASP
1	H	91	ASP
1	H	291	ARG
1	I	7	LYS
1	I	91	ASP
1	J	7	LYS
1	J	91	ASP
1	K	3	ASN
1	K	67	GLN
1	K	91	ASP
1	L	5	THR
1	L	291	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	GLN
1	A	212	GLN
1	D	77	GLN
1	D	103	ASN
1	D	212	GLN
1	E	2	ASN
1	E	3	ASN
1	E	77	GLN
1	E	152	ASN
1	F	140	ASN
1	G	103	ASN
1	G	212	GLN
1	H	77	GLN
1	H	212	GLN
1	J	77	GLN
1	J	212	GLN
1	K	67	GLN
1	K	77	GLN
1	L	219	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	E	301	-	4,4,4	0.47	0	6,6,6	0.18	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	A	301	-	4,4,4	0.40	0	6,6,6	0.29	0
2	SO4	D	301	-	4,4,4	0.33	0	6,6,6	0.21	0
2	SO4	G	301	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	L	301	-	4,4,4	0.48	0	6,6,6	0.20	0
2	SO4	I	301	-	4,4,4	0.44	0	6,6,6	0.31	0
2	SO4	B	301	-	4,4,4	0.50	0	6,6,6	0.33	0
2	SO4	C	301	-	4,4,4	0.40	0	6,6,6	0.44	0
2	SO4	H	301	-	4,4,4	0.32	0	6,6,6	0.37	0
2	SO4	F	301	-	4,4,4	0.31	0	6,6,6	0.29	0

There are no bond length outliers.

There are no bond angle outliers.

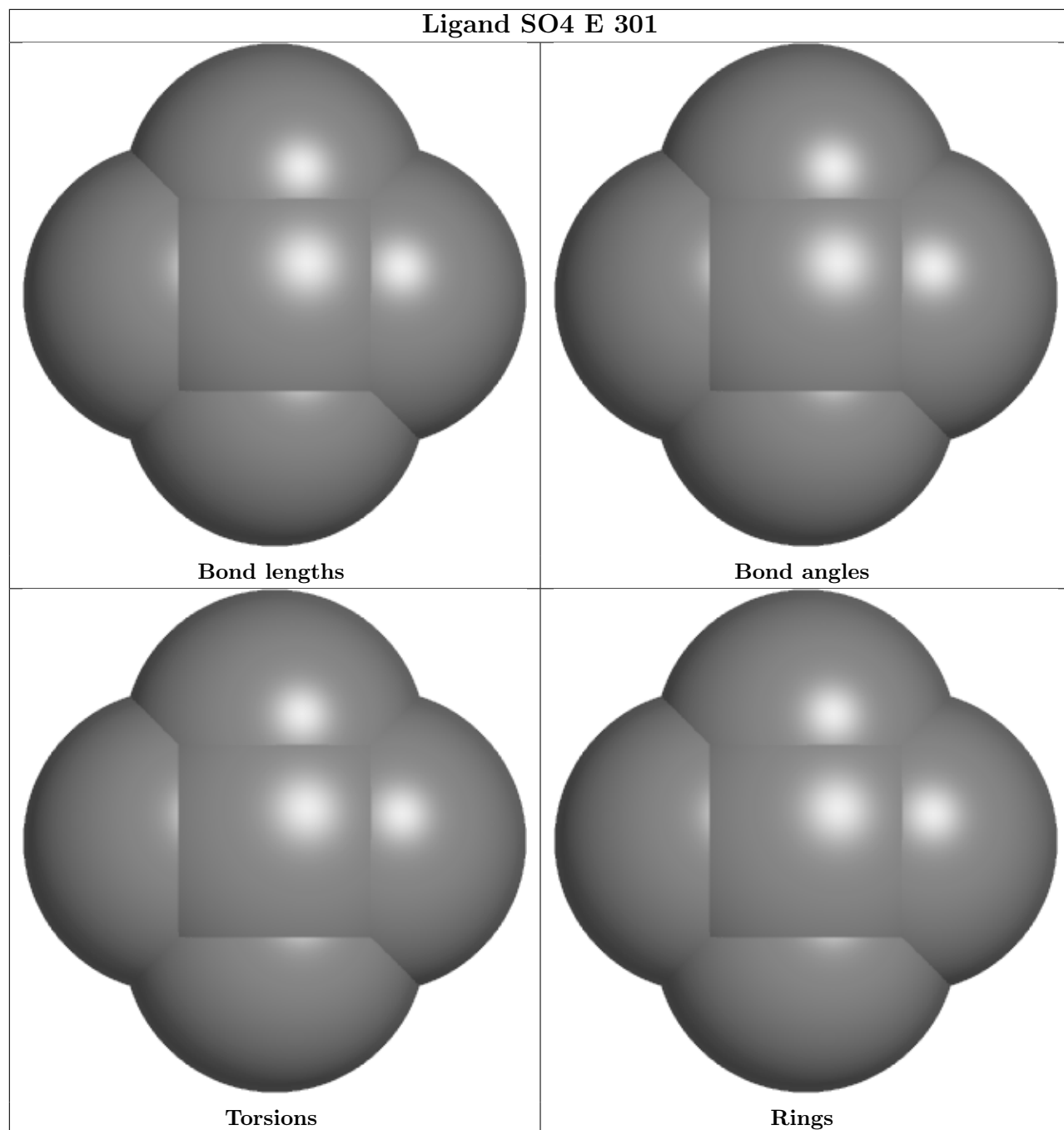
There are no chirality outliers.

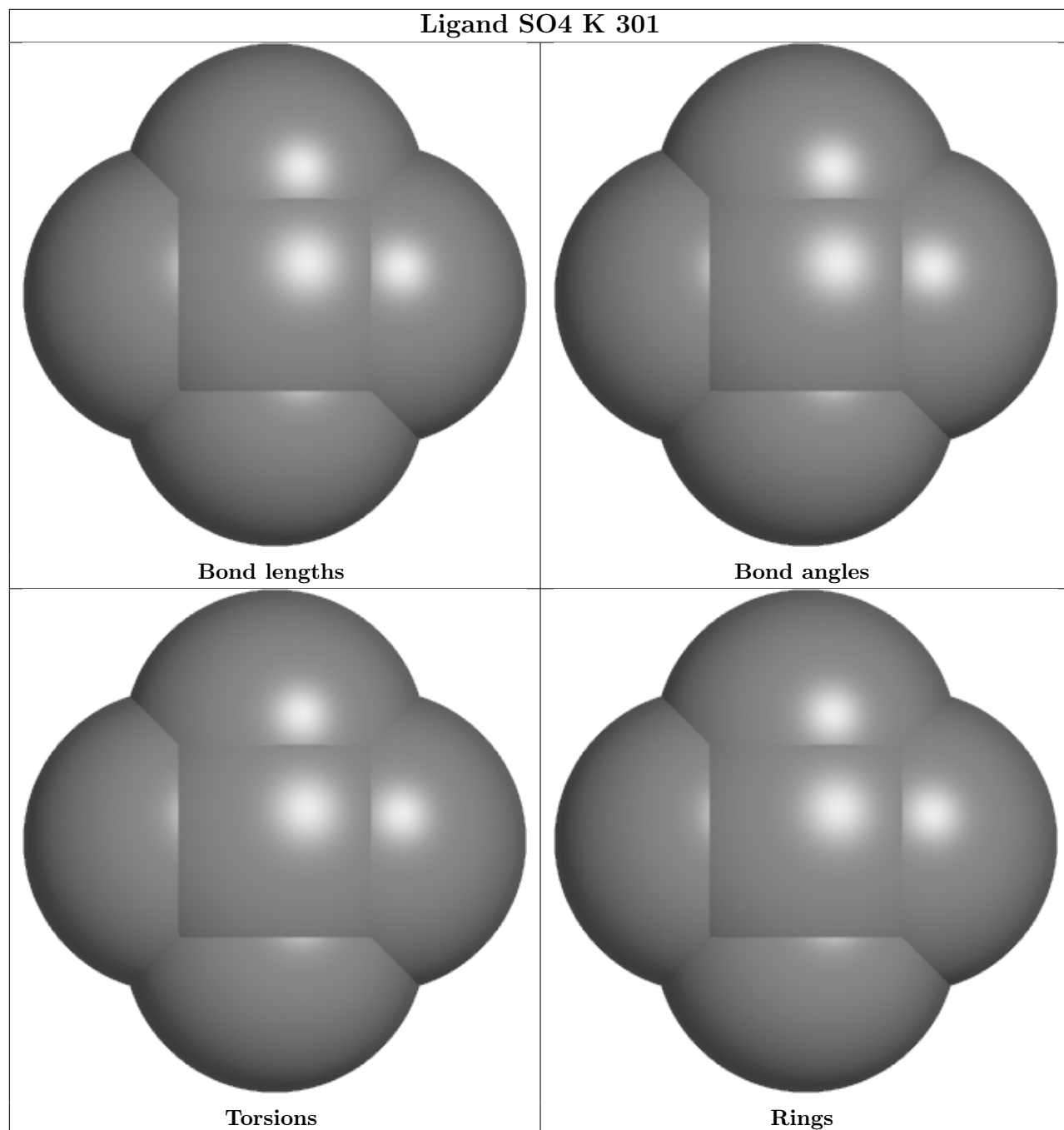
There are no torsion outliers.

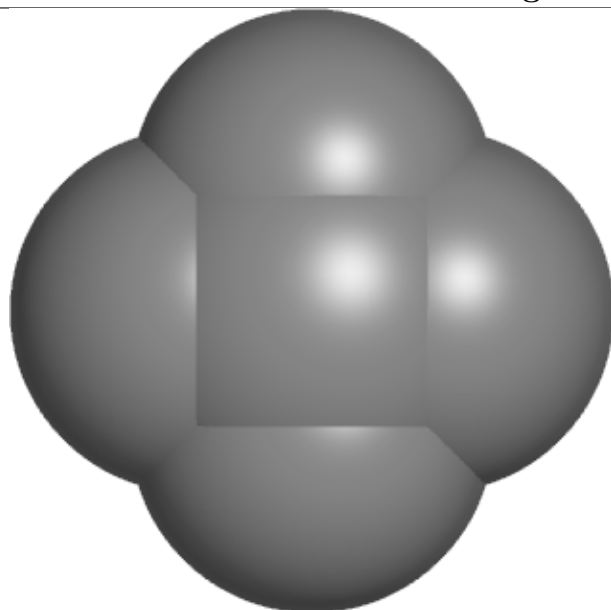
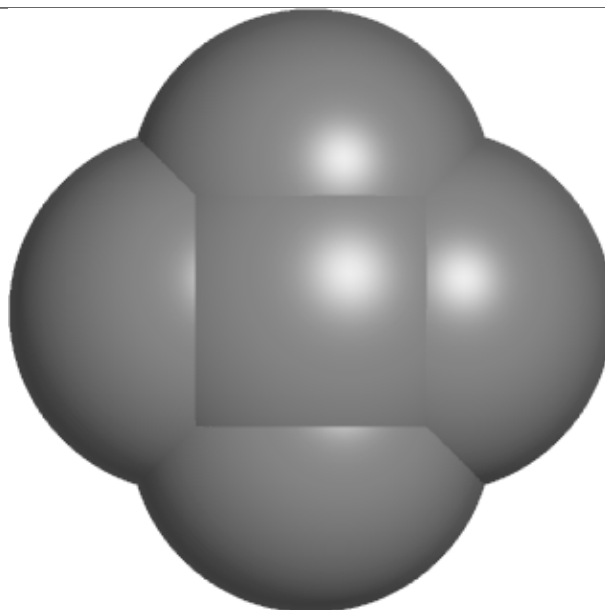
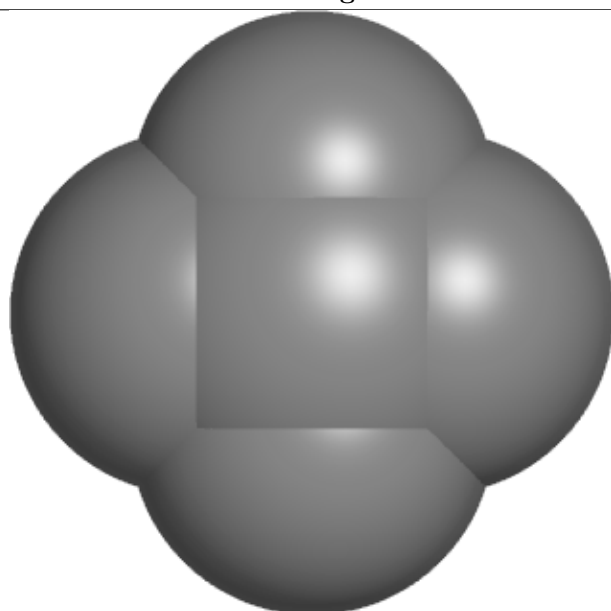
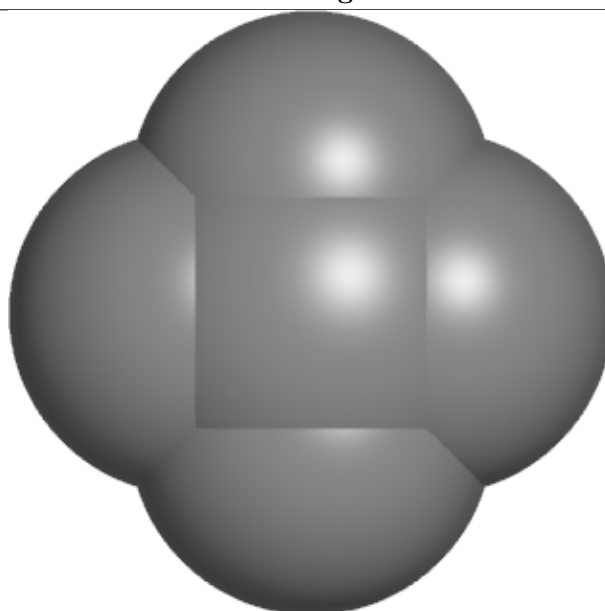
There are no ring outliers.

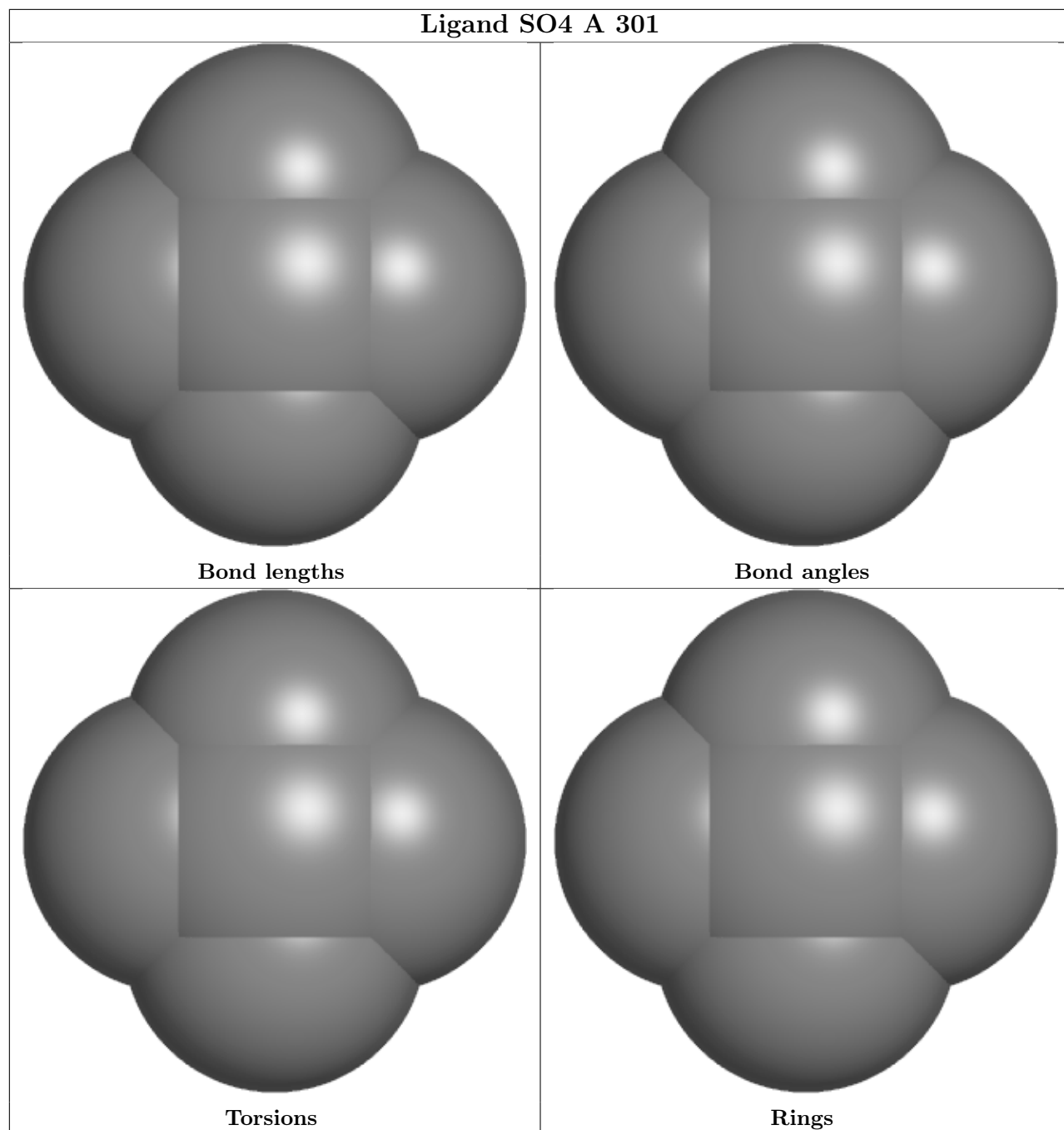
No monomer is involved in short contacts.

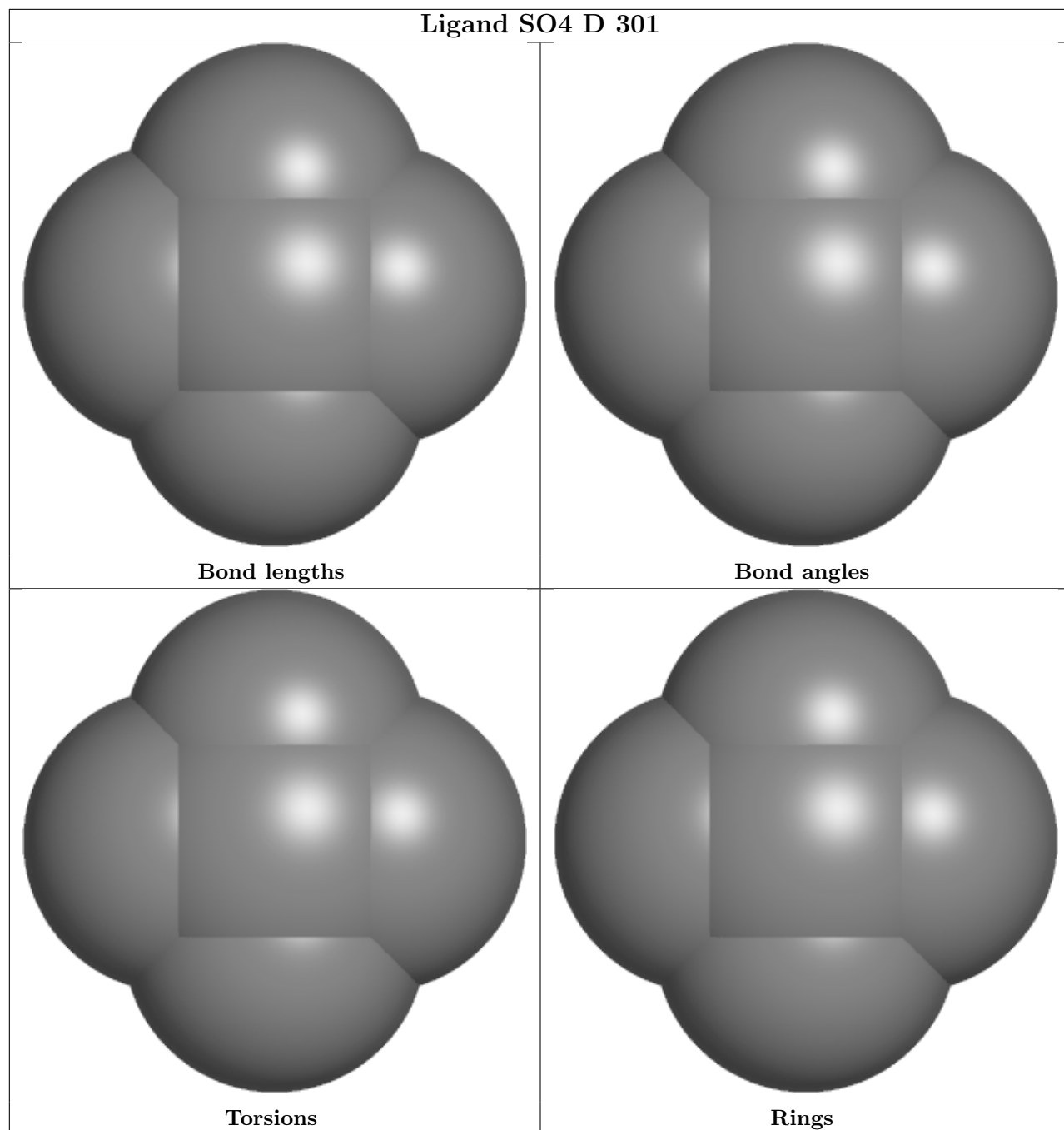
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

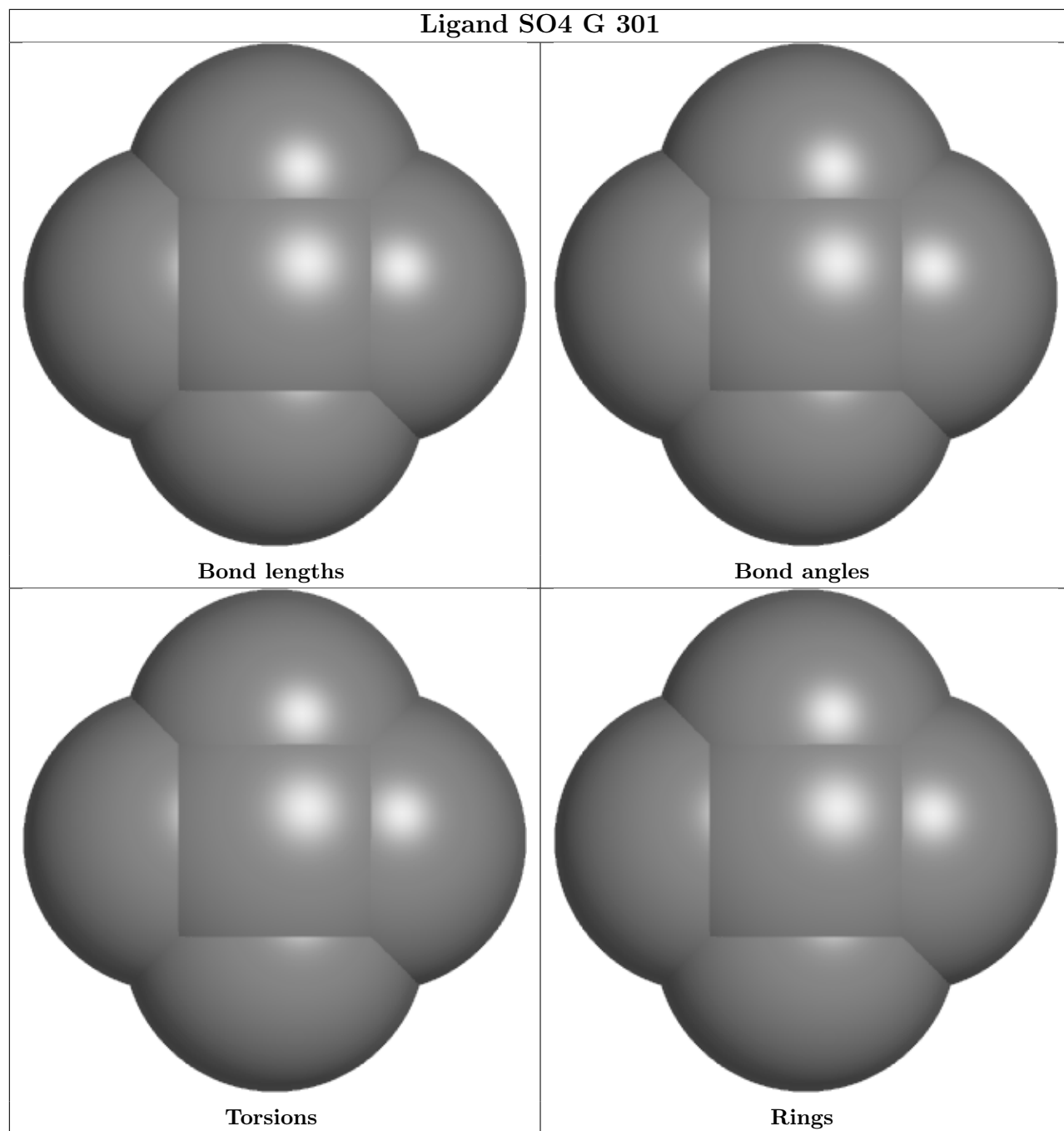


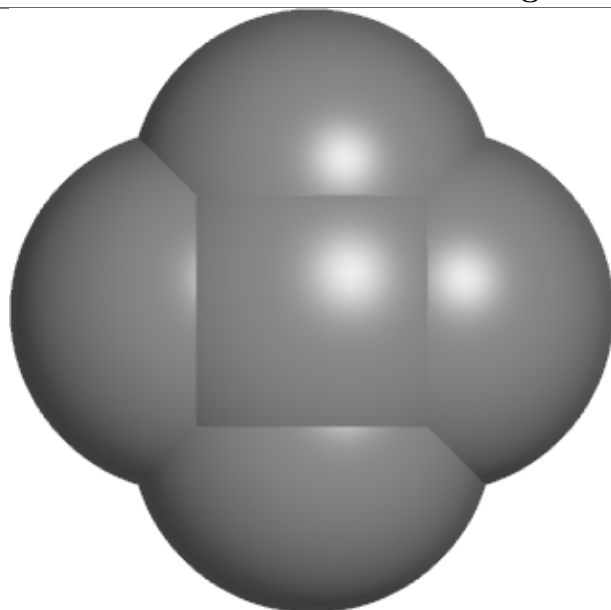
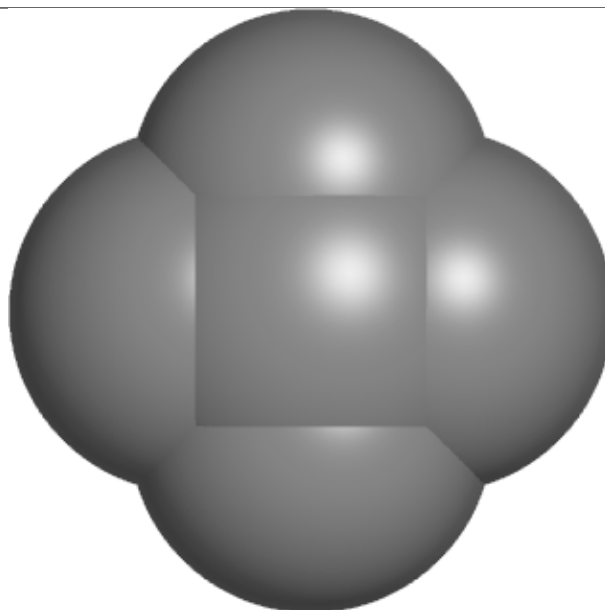
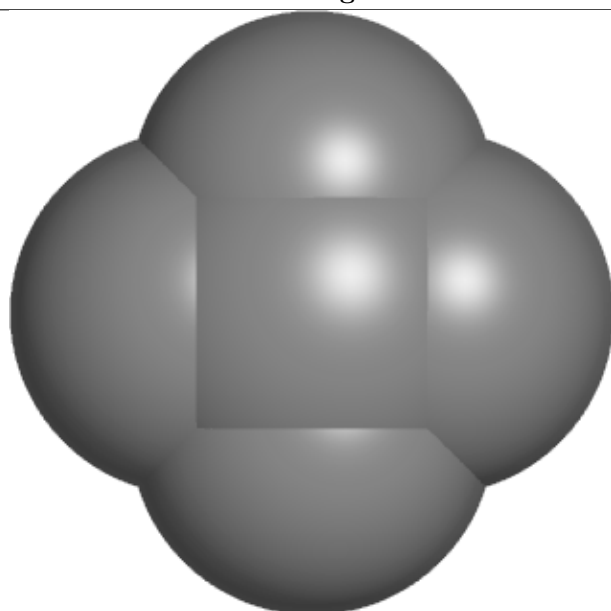
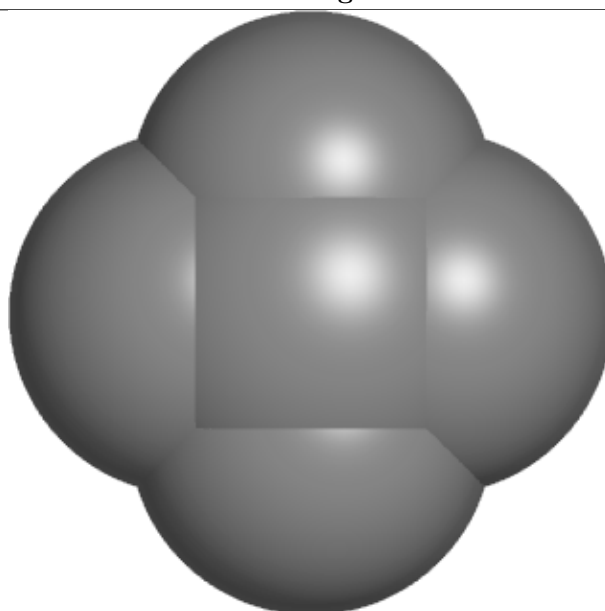


Ligand SO4 J 301**Bond lengths****Bond angles****Torsions****Rings**

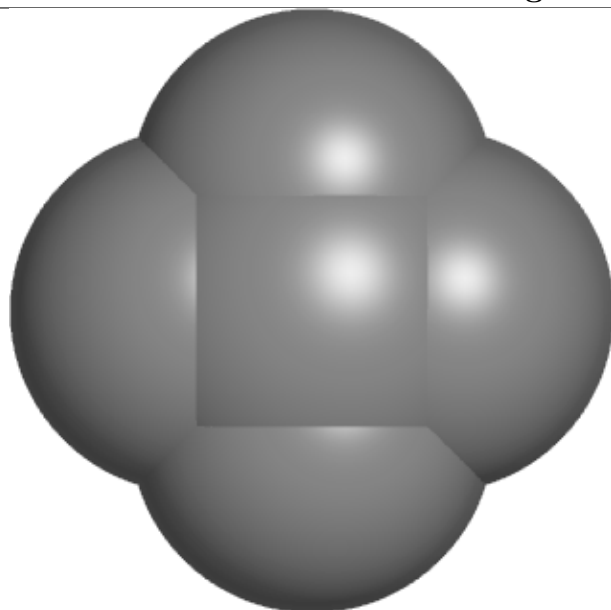




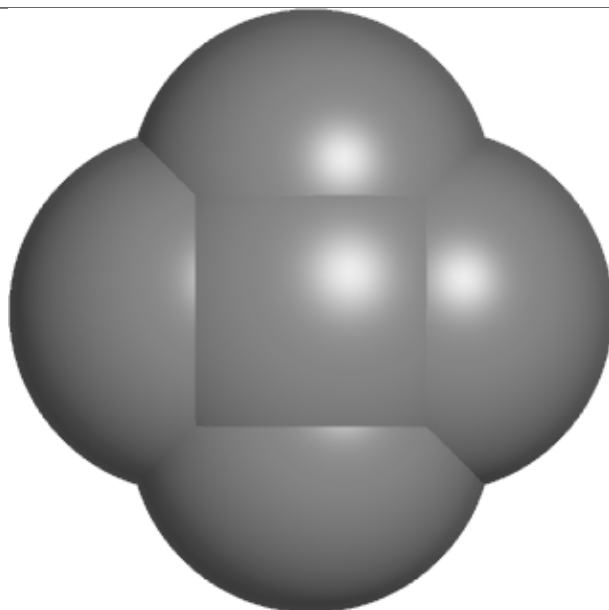


Ligand SO4 L 301**Bond lengths****Bond angles****Torsions****Rings**

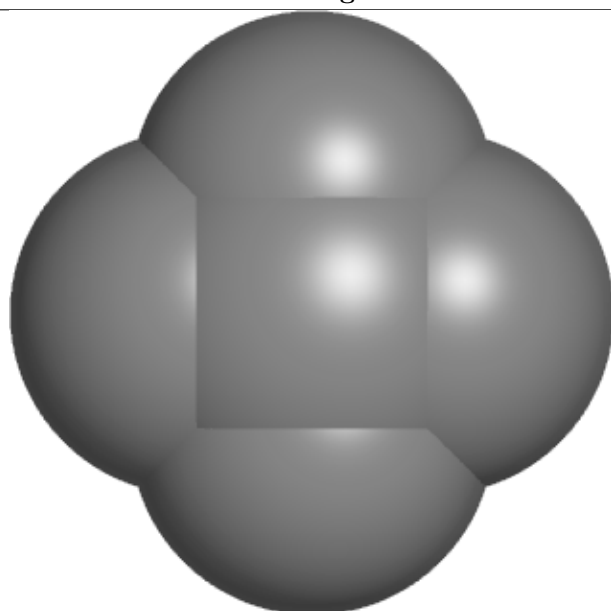
Ligand SO4 I 301



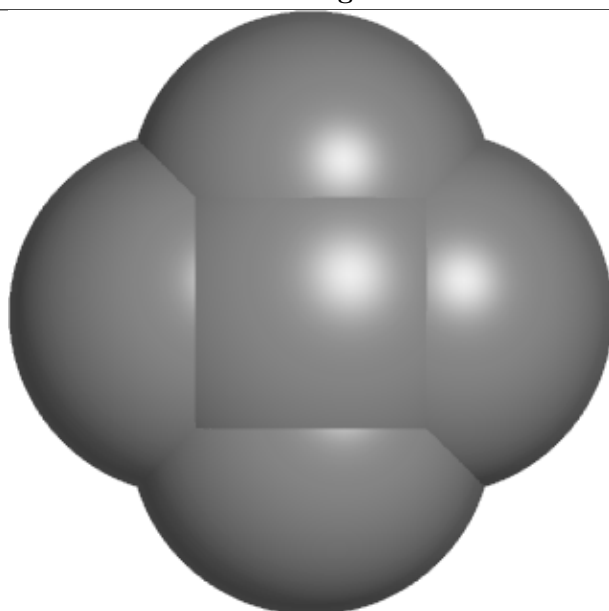
Bond lengths



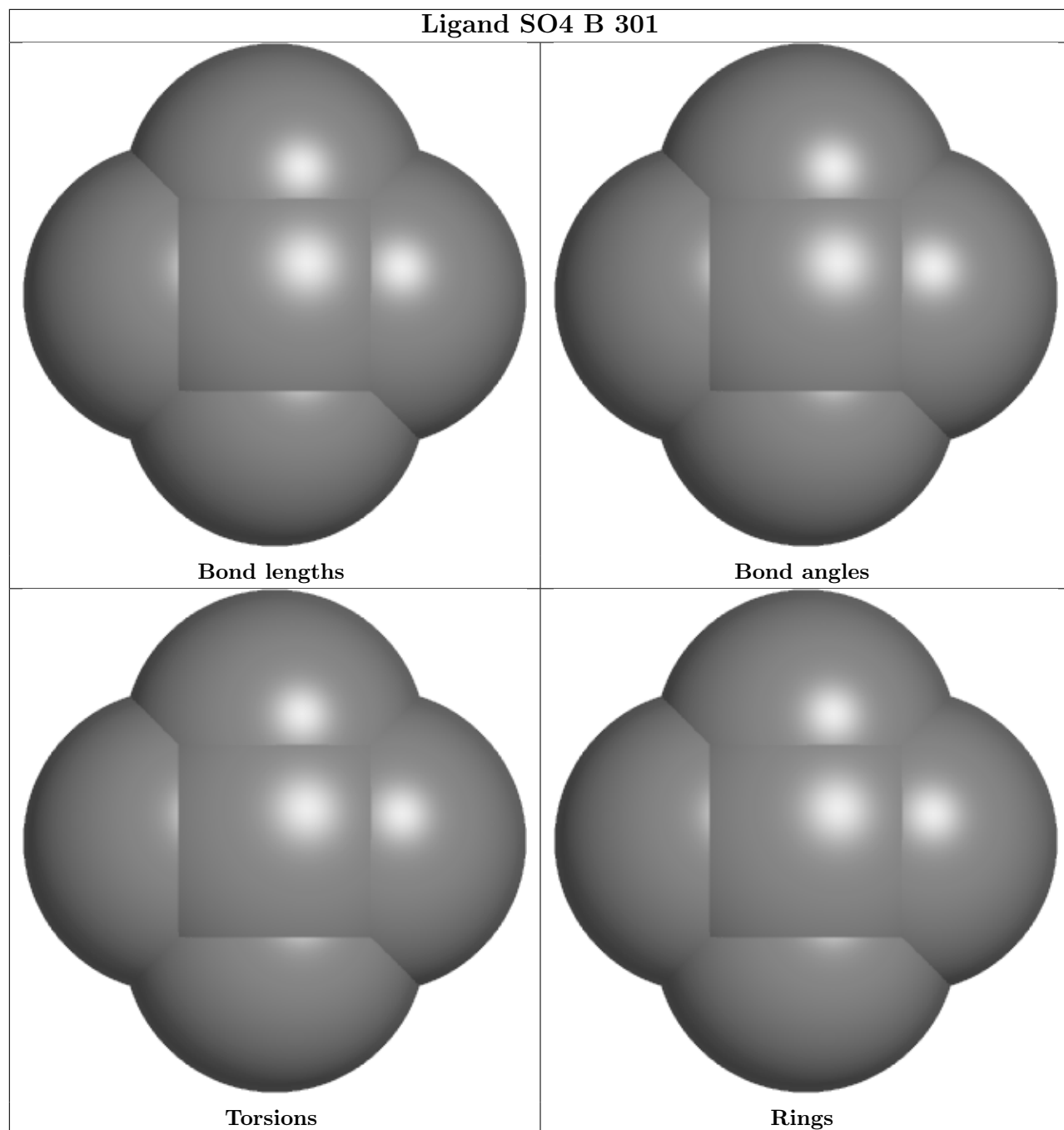
Bond angles

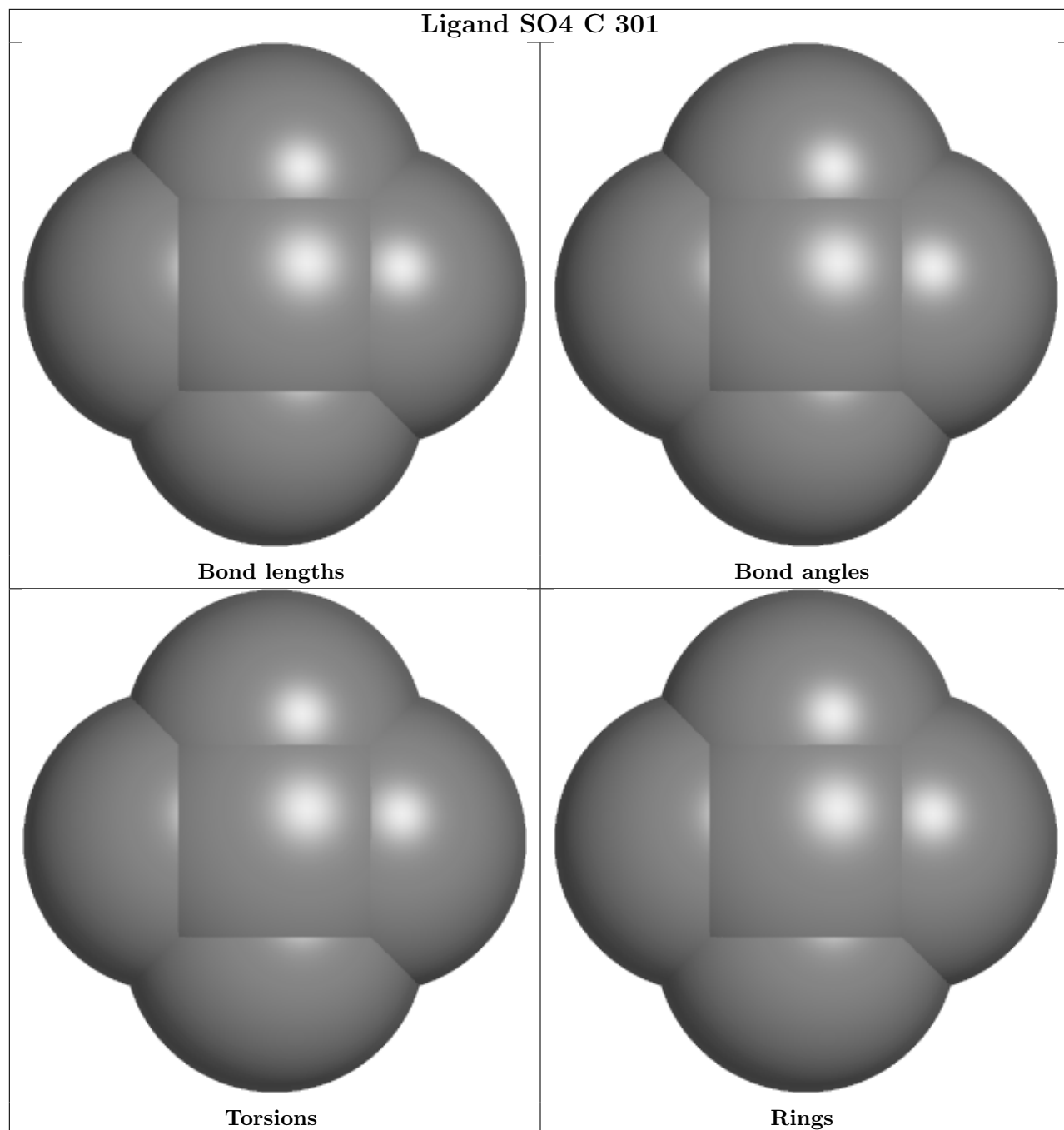


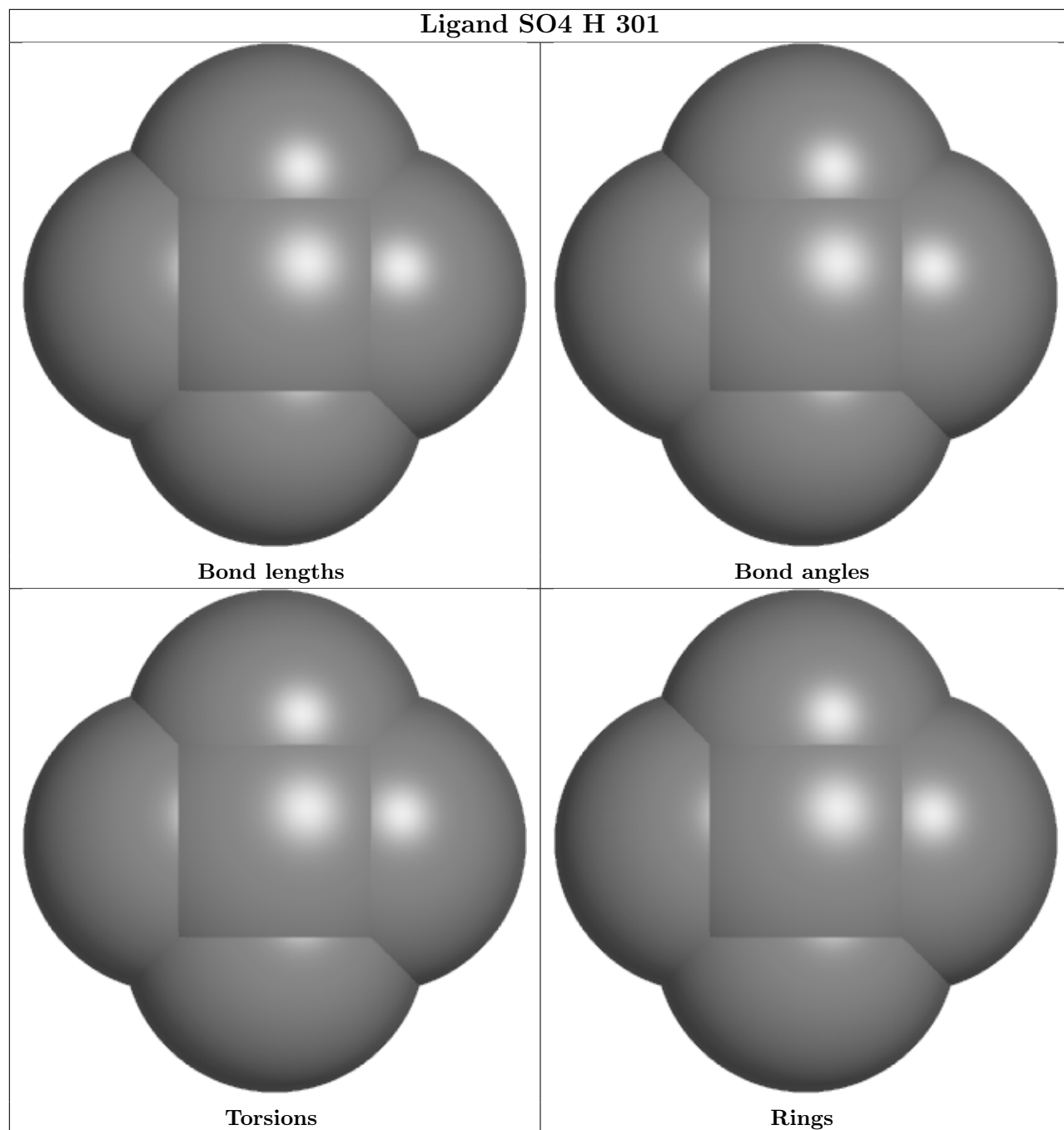
Torsions

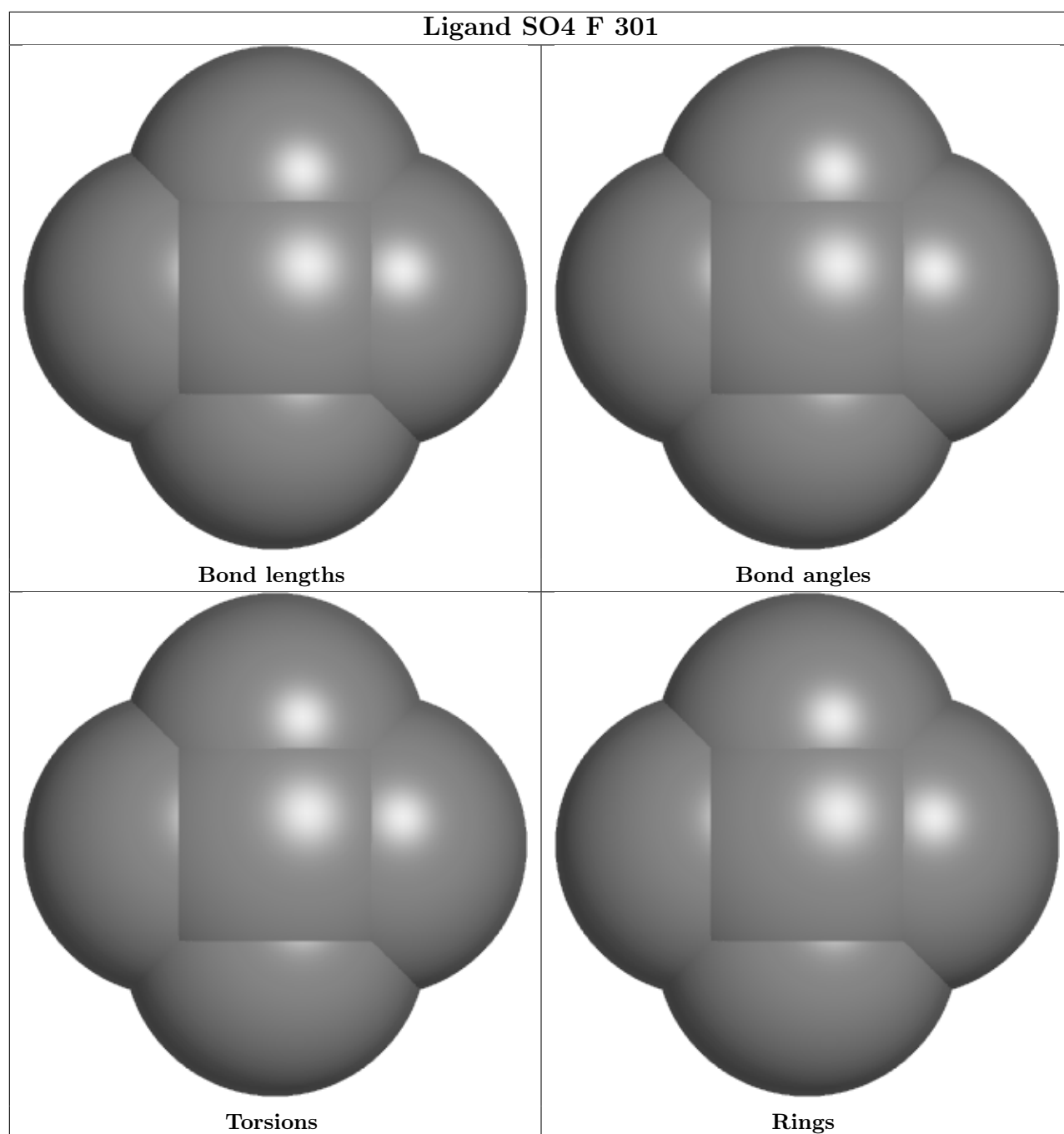


Rings









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%)	-0.44	0 100 100	19, 26, 40, 72	0
1	B	291/312 (93%)	-0.16	0 100 100	25, 34, 47, 70	0
1	C	290/312 (92%)	-0.47	1 (0%) 94 92	17, 24, 38, 58	0
1	D	293/312 (93%)	-0.32	1 (0%) 94 92	14, 19, 32, 52	0
1	E	292/312 (93%)	-0.46	0 100 100	15, 23, 37, 60	0
1	F	276/312 (88%)	1.47	80 (28%) 0 0	37, 51, 68, 80	0
1	G	288/312 (92%)	-0.32	0 100 100	17, 28, 45, 58	0
1	H	286/312 (91%)	-0.09	2 (0%) 87 86	26, 36, 50, 64	0
1	I	289/312 (92%)	-0.34	0 100 100	14, 19, 31, 46	0
1	J	289/312 (92%)	-0.42	0 100 100	21, 28, 46, 62	0
1	K	289/312 (92%)	-0.44	0 100 100	15, 21, 35, 56	0
1	L	289/312 (92%)	-0.40	0 100 100	14, 20, 35, 62	0
All	All	3461/3744 (92%)	-0.21	84 (2%) 59 54	14, 26, 52, 80	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	149	CYS	8.5
1	F	145	PHE	6.3
1	F	79	ALA	5.5
1	F	85	ALA	5.2
1	F	153	GLY	4.7
1	F	115	VAL	4.5
1	F	117	ARG	4.3
1	F	192	TYR	4.1
1	F	221	PRO	4.1
1	F	216	GLY	4.0
1	F	125	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
1	F	244	ALA	3.9
1	F	12	ALA	3.9
1	F	219	ASN	3.8
1	F	120	ALA	3.7
1	F	64	LEU	3.7
1	F	223	VAL	3.7
1	F	122	ALA	3.6
1	F	189	ALA	3.6
1	F	46	THR	3.5
1	F	184	LEU	3.5
1	F	86	MET	3.5
1	F	14	GLY	3.4
1	F	218	ILE	3.4
1	C	4	TYR	3.4
1	F	88	VAL	3.4
1	F	148	LEU	3.4
1	F	211	SER	3.4
1	F	214	LEU	3.3
1	F	147	GLU	3.3
1	F	222	TRP	3.2
1	F	63	VAL	3.2
1	F	80	VAL	3.2
1	F	105	VAL	3.2
1	F	128	LEU	3.2
1	F	188	GLY	3.1
1	F	19	LEU	3.1
1	F	151	SER	3.0
1	F	92	ASP	3.0
1	F	84	CYS	3.0
1	F	126	LEU	2.9
1	F	155	LEU	2.9
1	F	177	ILE	2.9
1	F	90	ALA	2.9
1	F	123	LEU	2.9
1	F	87	ILE	2.9
1	F	234	PHE	2.8
1	F	140	ASN	2.8
1	F	208	LEU	2.7
1	F	161	VAL	2.7
1	F	242	MET	2.7
1	F	154	LEU	2.7
1	F	191	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	69	PHE	2.7
1	F	114	ALA	2.6
1	F	181	ALA	2.6
1	F	183	GLU	2.6
1	F	70	CYS	2.6
1	F	250	LEU	2.6
1	F	93	PHE	2.6
1	F	207	LEU	2.6
1	F	35	GLY	2.6
1	F	158	ILE	2.5
1	F	251	ALA	2.5
1	F	60	ALA	2.4
1	F	156	SER	2.4
1	F	106	LEU	2.4
1	F	135	ALA	2.4
1	F	241	ALA	2.3
1	F	225	LEU	2.3
1	F	118	ASP	2.3
1	D	292	ARG	2.2
1	F	127	VAL	2.2
1	F	277	LEU	2.2
1	H	5	THR	2.2
1	H	153	GLY	2.2
1	F	185	GLY	2.1
1	F	44	VAL	2.1
1	F	160	PRO	2.1
1	F	10	THR	2.1
1	F	247	SER	2.1
1	F	190	ASP	2.1
1	F	288	MET	2.0
1	F	136	GLN	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

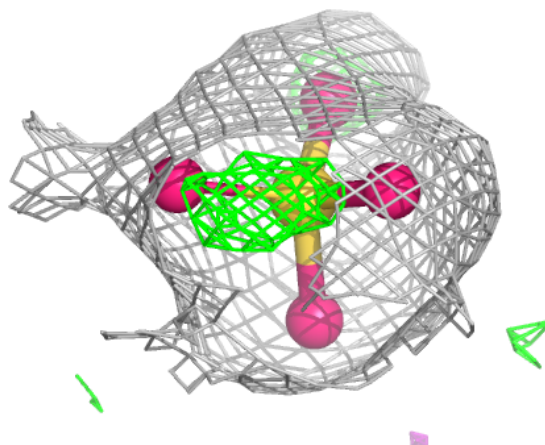
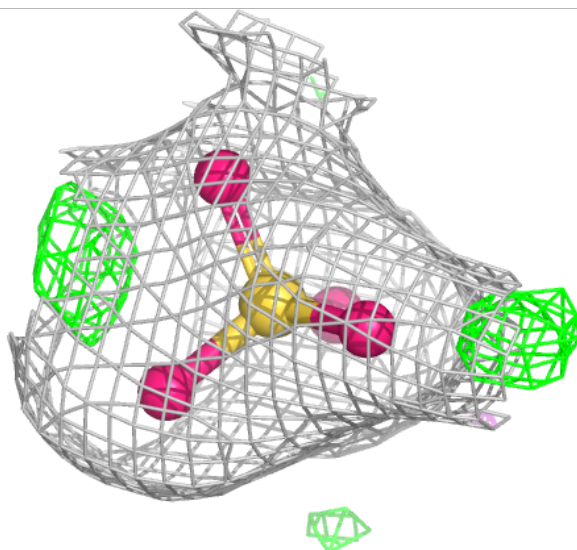
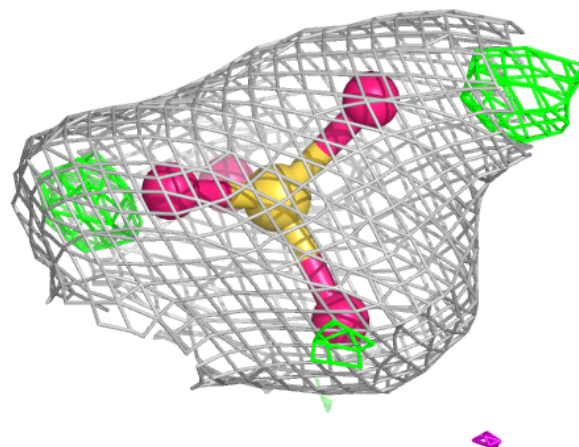
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	F	301	5/5	0.95	0.10	46,52,55,55	0
2	SO4	B	301	5/5	0.99	0.07	28,28,30,32	0
2	SO4	C	301	5/5	0.99	0.07	20,21,22,23	0
2	SO4	E	301	5/5	0.99	0.07	18,20,22,22	0
2	SO4	A	301	5/5	0.99	0.08	21,22,24,25	0
2	SO4	G	301	5/5	0.99	0.06	23,24,24,25	0
2	SO4	H	301	5/5	0.99	0.07	26,29,31,32	0
2	SO4	I	301	5/5	0.99	0.09	16,16,18,19	0
2	SO4	J	301	5/5	0.99	0.07	23,24,25,26	0
2	SO4	K	301	5/5	0.99	0.05	18,18,20,20	0
2	SO4	L	301	5/5	0.99	0.07	15,17,18,18	0
2	SO4	D	301	5/5	1.00	0.07	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.

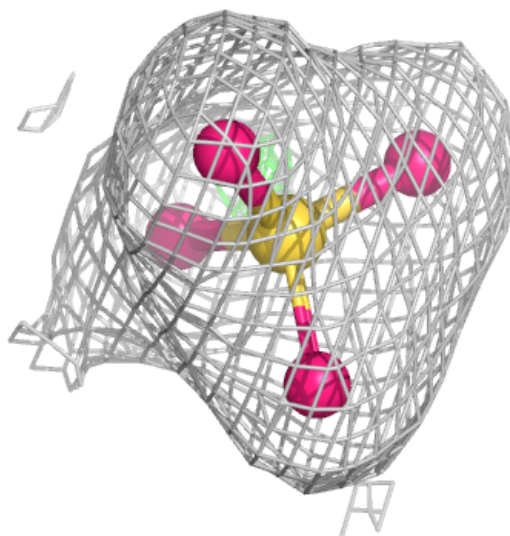
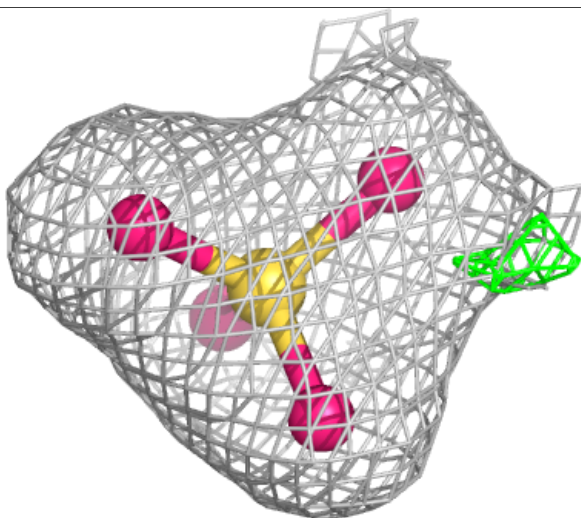
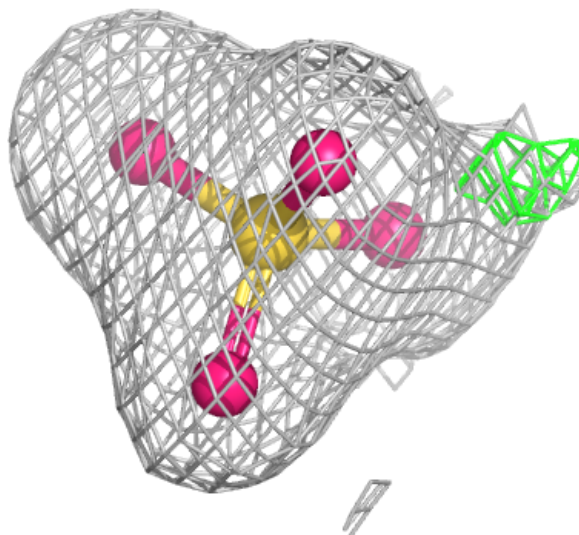
Electron density around SO4 F 301:

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



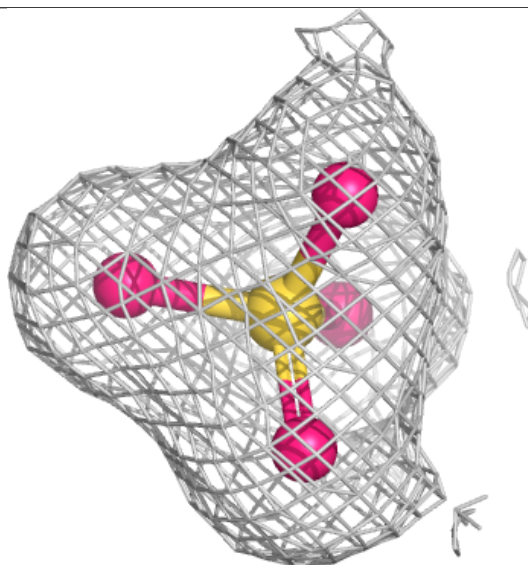
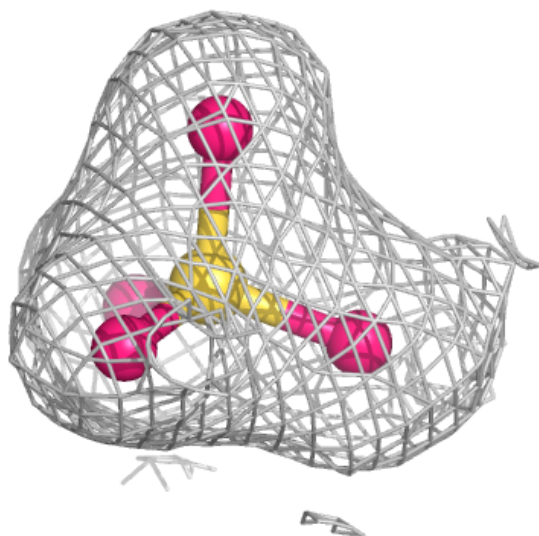
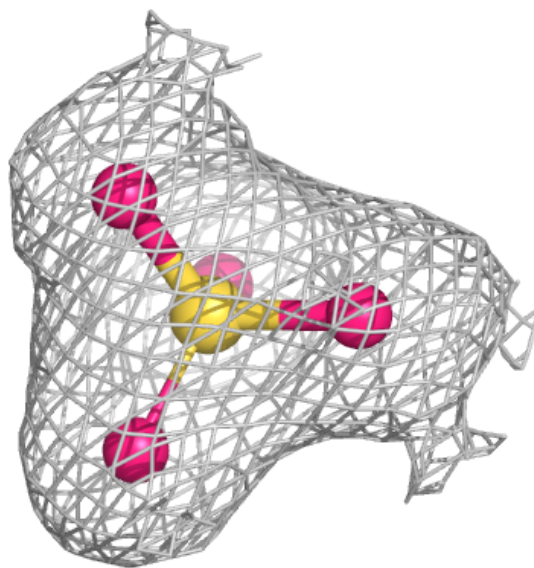
Electron density around SO4 B 301:

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



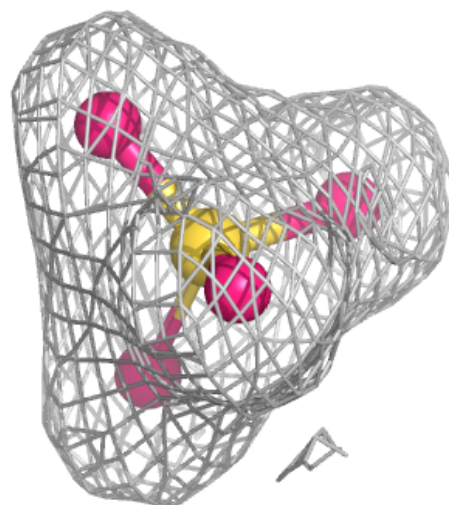
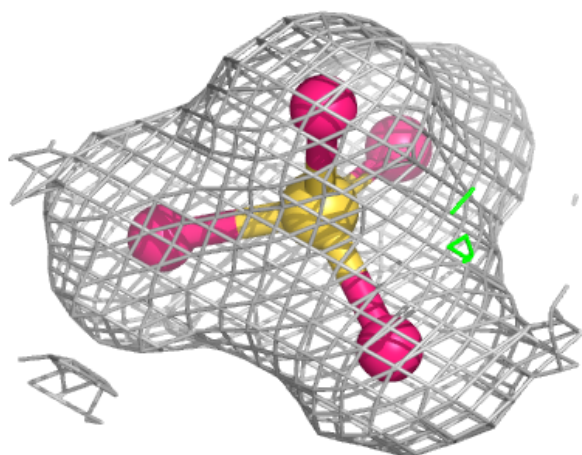
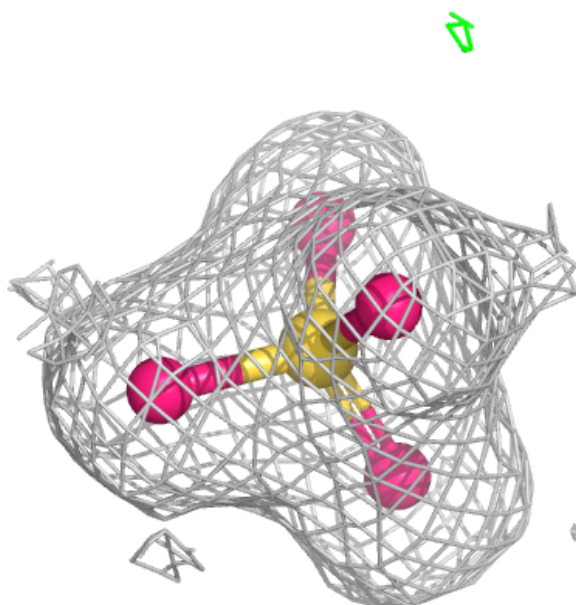
Electron density around SO4 C 301:

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



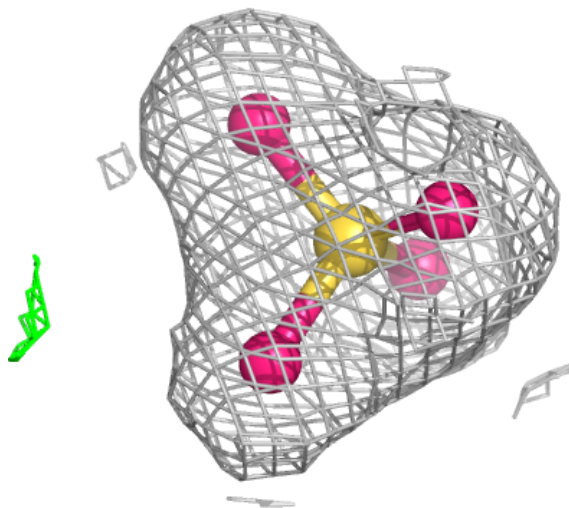
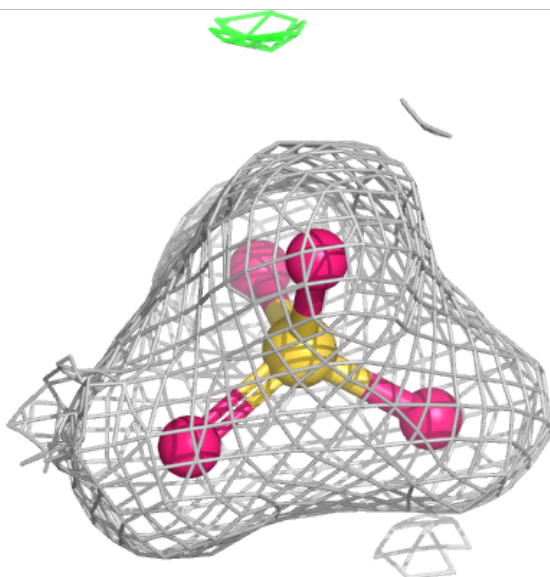
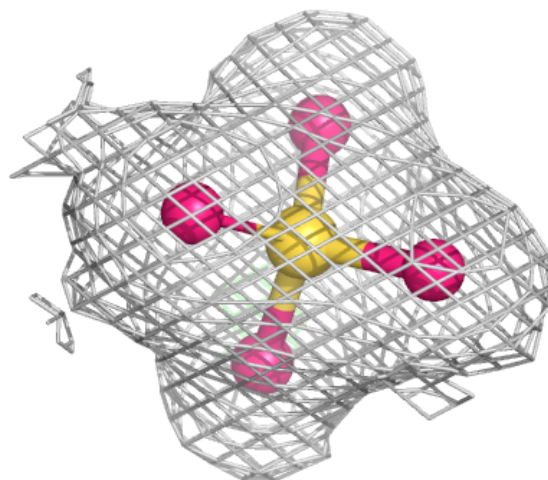
Electron density around SO4 E 301:

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and green (positive)



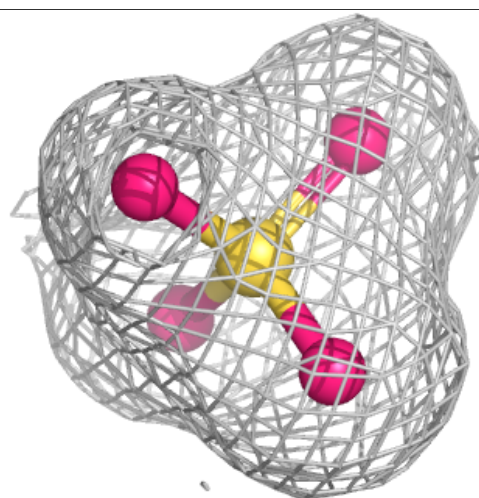
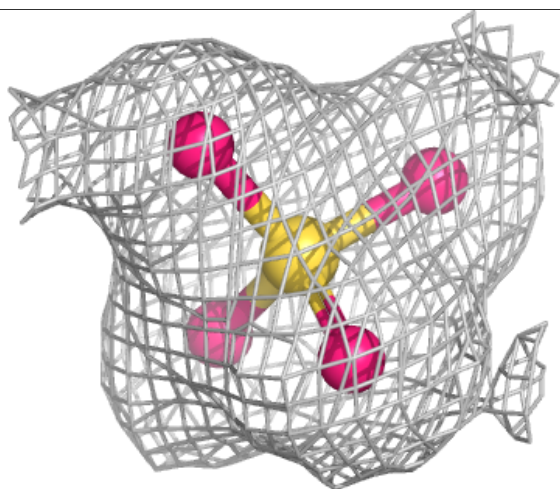
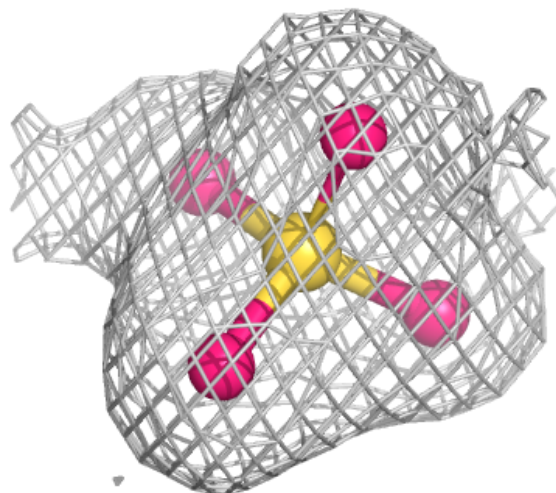
Electron density around SO4 A 301:

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and green (positive)



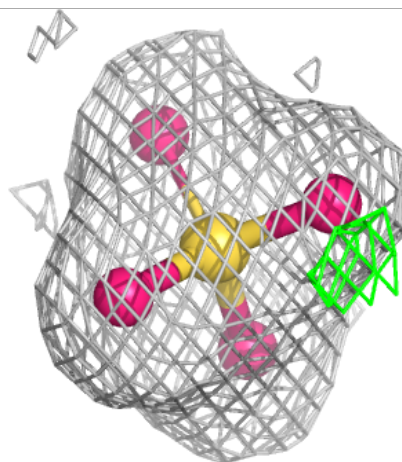
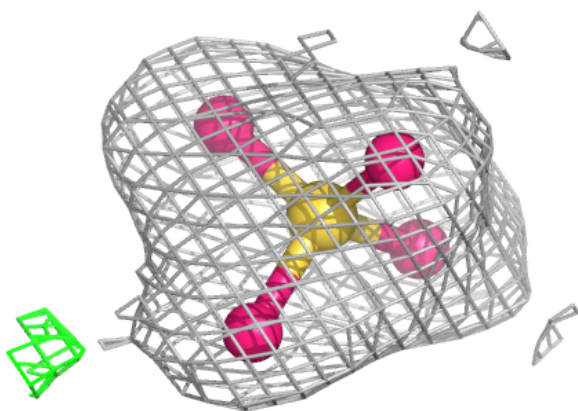
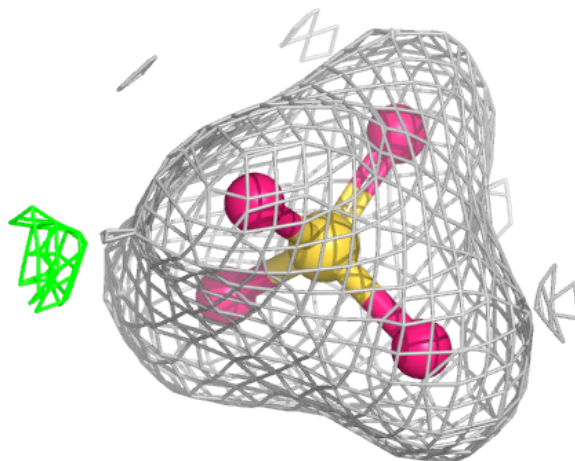
Electron density around SO4 G 301:

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



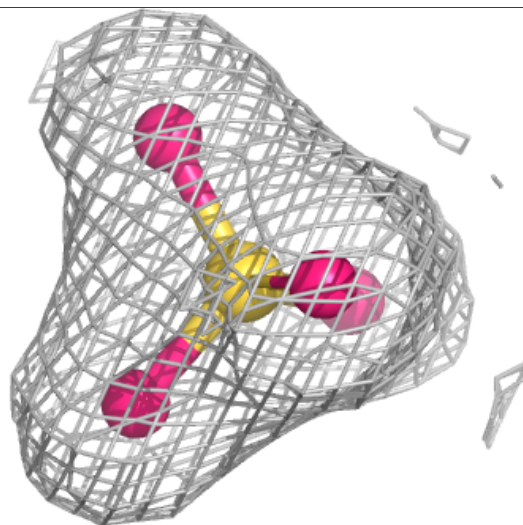
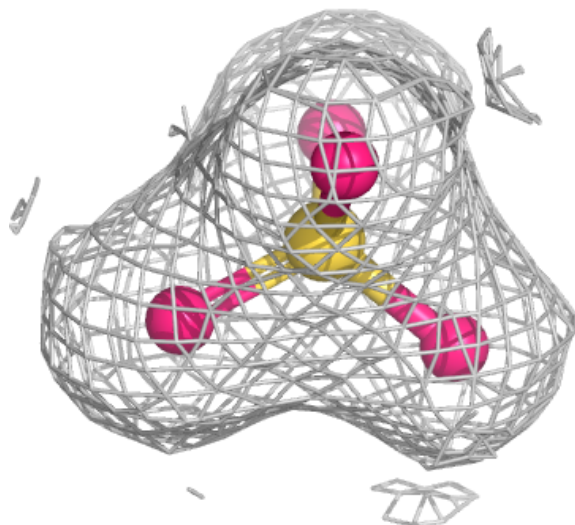
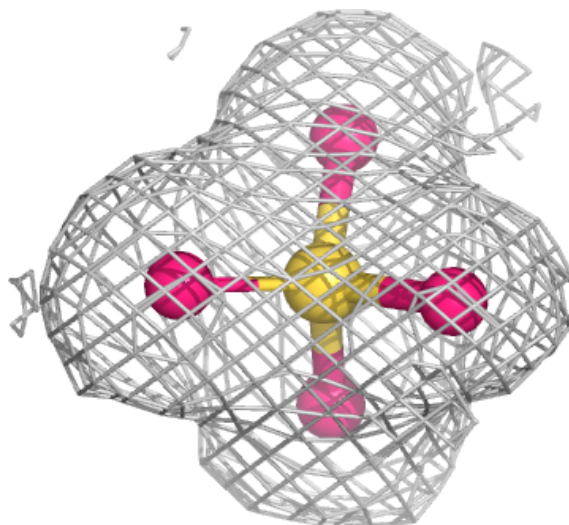
Electron density around SO4 H 301:

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



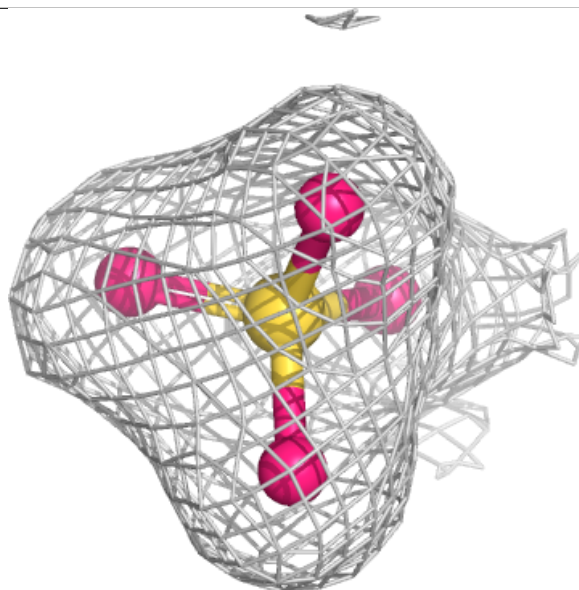
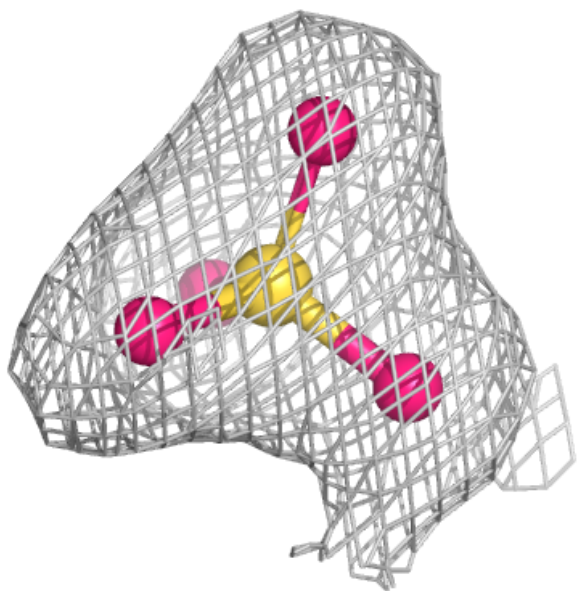
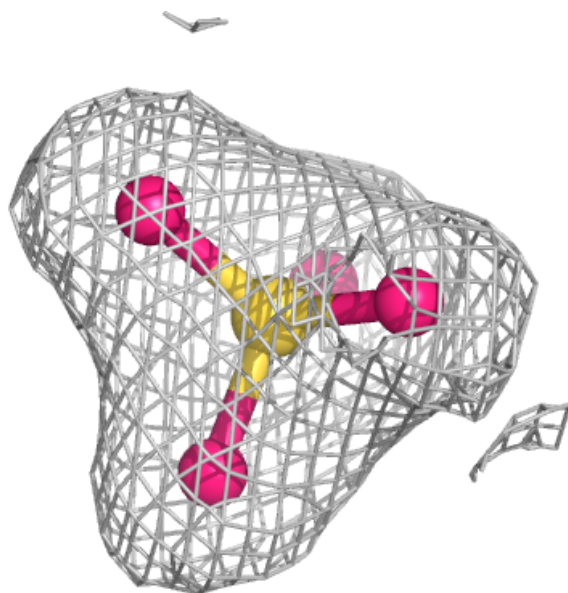
Electron density around SO4 I 301:

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



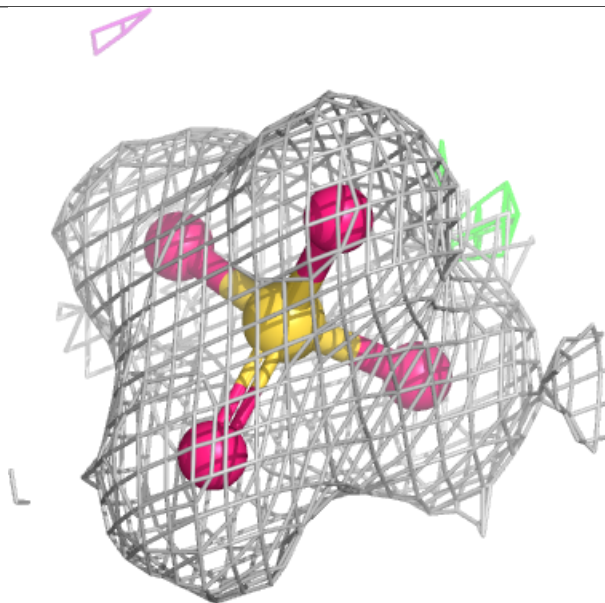
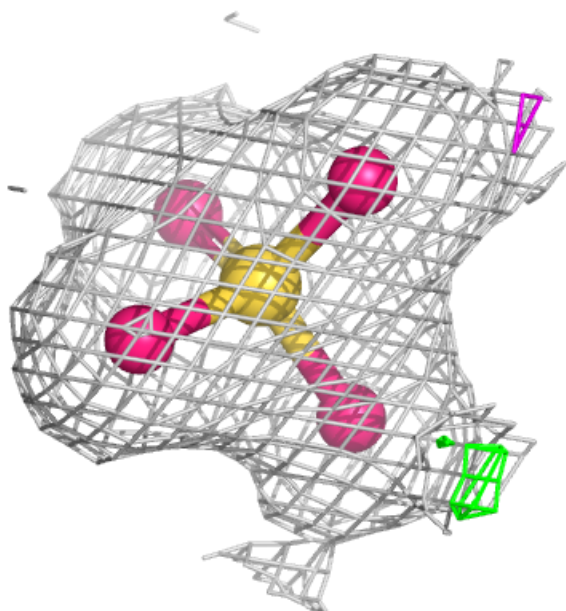
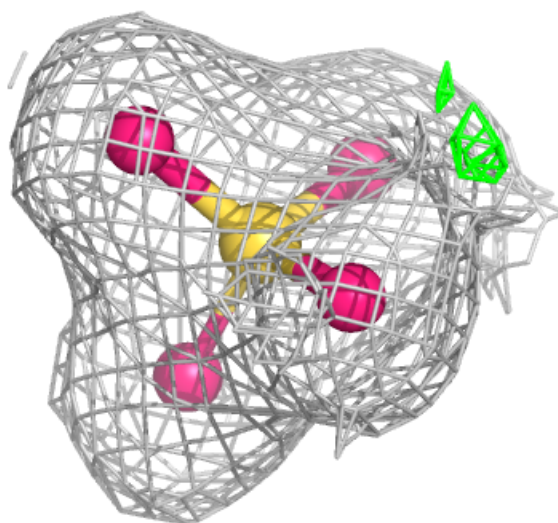
Electron density around SO4 J 301:

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and green (positive)



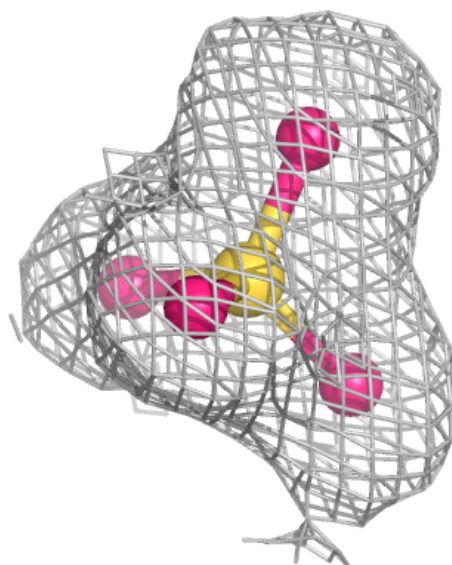
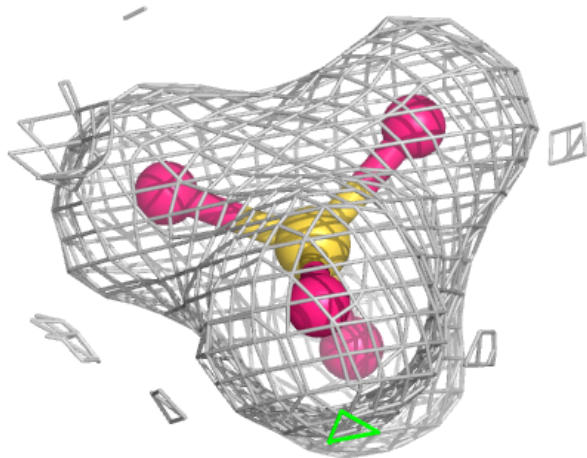
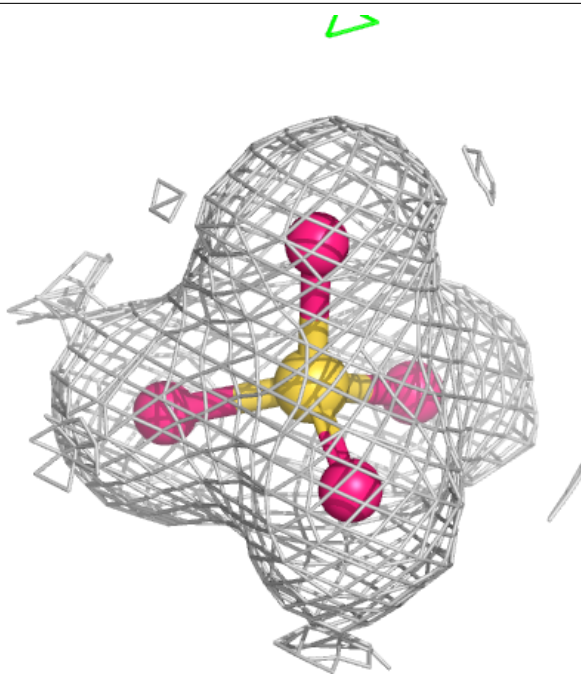
Electron density around SO4 K 301:

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and green (positive)



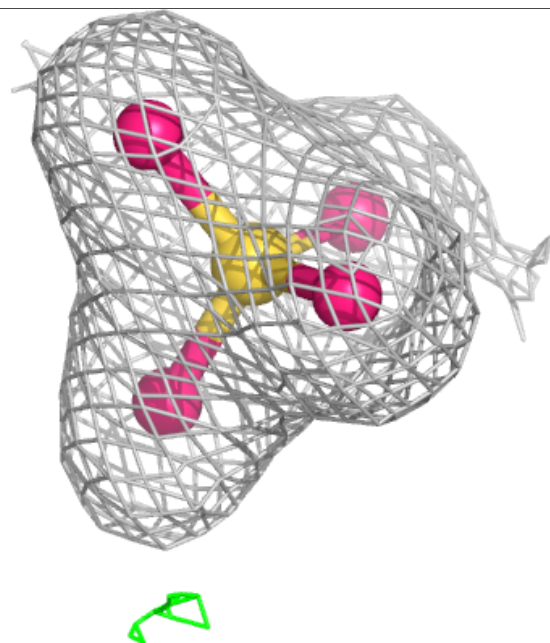
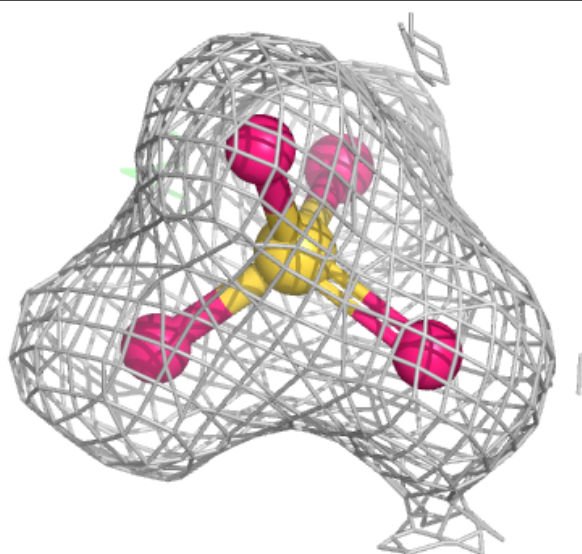
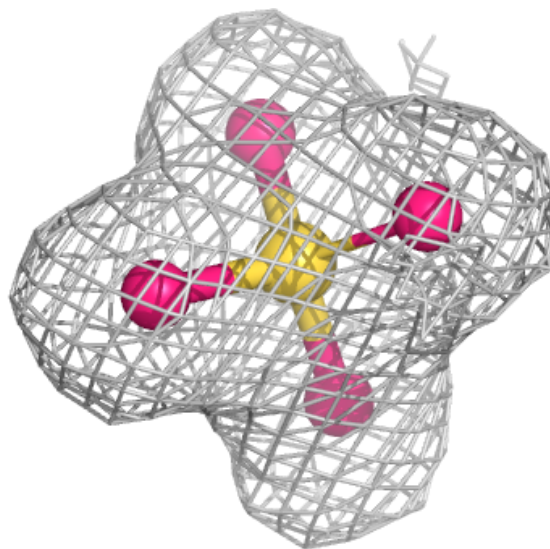
Electron density around SO4 L 301:

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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 [i](#)

There are no such residues in this entry.