



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:26 PM UTC

PDB ID : 6K7Q / pdb_00006k7q
Title : Crystal structure of thymidylate synthase from shrimp
Authors : Ma, Q.; Zang, K.; Liu, C.
Deposited on : 2019-06-08
Resolution : 2.27 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

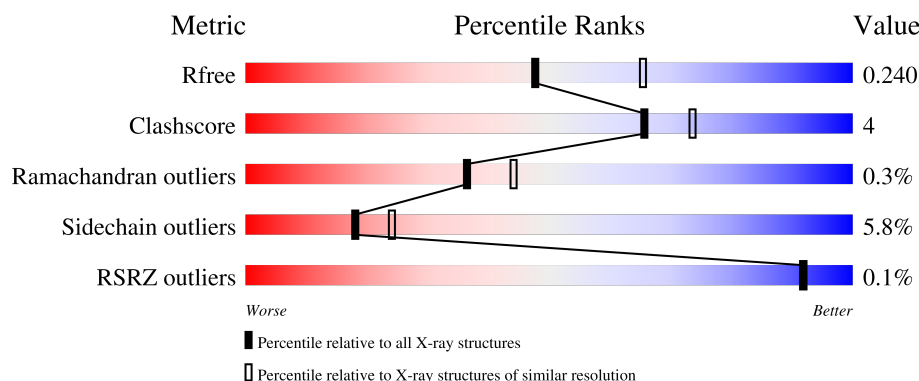
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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.



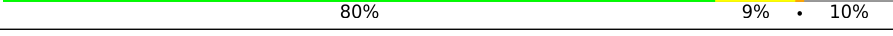
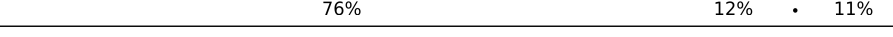
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (2.30-2.26)

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	292	 74% 17% • 7%
1	B	292	 76% 12% • 10%
1	C	292	 77% 11% • 9%
1	D	292	 74% 12% • 11%
1	E	292	 72% 15% • 11%

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Mol	Chain	Length	Quality of chain
1	F	292	 76% 12% • 10%
1	G	292	 74% 11% • 13%
1	H	292	 78% 12% • 9%
1	I	292	 76% 14% • 9%
1	J	292	 76% 14% • 8%
1	K	292	 72% 15% • 11%
1	L	292	 78% 10% • 10%
1	M	292	 76% 11% • 10%
1	N	292	 80% 9% • 10%
1	O	292	 77% 11% • 10%
1	P	292	 76% 12% • 11%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 35306 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 Thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	272	Total	C	N	O	S	0	0	0
			2212	1406	388	402	16			
1	B	264	Total	C	N	O	S	0	0	0
			2153	1374	374	390	15			
1	C	267	Total	C	N	O	S	0	0	0
			2178	1388	380	394	16			
1	D	261	Total	C	N	O	S	0	0	0
			2122	1353	369	385	15			
1	E	260	Total	C	N	O	S	0	0	0
			2124	1354	371	385	14			
1	F	263	Total	C	N	O	S	0	0	0
			2149	1372	373	389	15			
1	G	255	Total	C	N	O	S	0	0	0
			2089	1336	364	375	14			
1	H	266	Total	C	N	O	S	0	0	0
			2173	1385	381	392	15			
1	I	267	Total	C	N	O	S	0	1	0
			2183	1392	380	394	17			
1	J	268	Total	C	N	O	S	0	0	0
			2180	1389	378	397	16			
1	K	261	Total	C	N	O	S	0	0	0
			2128	1359	367	387	15			
1	L	262	Total	C	N	O	S	0	0	0
			2138	1366	372	385	15			
1	M	263	Total	C	N	O	S	0	0	0
			2145	1368	375	388	14			
1	N	263	Total	C	N	O	S	0	0	0
			2148	1372	373	387	16			
1	O	262	Total	C	N	O	S	0	0	0
			2138	1363	374	386	15			
1	P	261	Total	C	N	O	S	0	0	0
			2131	1361	370	385	15			

There are 48 discrepancies between the modelled and reference sequences:

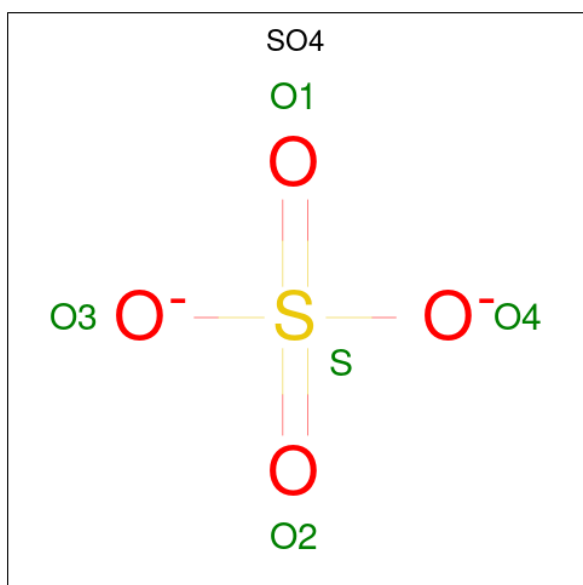
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP C6GJB8
A	-1	ASN	-	expression tag	UNP C6GJB8
A	0	ALA	-	expression tag	UNP C6GJB8
B	-2	SER	-	expression tag	UNP C6GJB8
B	-1	ASN	-	expression tag	UNP C6GJB8
B	0	ALA	-	expression tag	UNP C6GJB8
C	-2	SER	-	expression tag	UNP C6GJB8
C	-1	ASN	-	expression tag	UNP C6GJB8
C	0	ALA	-	expression tag	UNP C6GJB8
D	-2	SER	-	expression tag	UNP C6GJB8
D	-1	ASN	-	expression tag	UNP C6GJB8
D	0	ALA	-	expression tag	UNP C6GJB8
E	-2	SER	-	expression tag	UNP C6GJB8
E	-1	ASN	-	expression tag	UNP C6GJB8
E	0	ALA	-	expression tag	UNP C6GJB8
F	-2	SER	-	expression tag	UNP C6GJB8
F	-1	ASN	-	expression tag	UNP C6GJB8
F	0	ALA	-	expression tag	UNP C6GJB8
G	-2	SER	-	expression tag	UNP C6GJB8
G	-1	ASN	-	expression tag	UNP C6GJB8
G	0	ALA	-	expression tag	UNP C6GJB8
H	-2	SER	-	expression tag	UNP C6GJB8
H	-1	ASN	-	expression tag	UNP C6GJB8
H	0	ALA	-	expression tag	UNP C6GJB8
I	-2	SER	-	expression tag	UNP C6GJB8
I	-1	ASN	-	expression tag	UNP C6GJB8
I	0	ALA	-	expression tag	UNP C6GJB8
J	-2	SER	-	expression tag	UNP C6GJB8
J	-1	ASN	-	expression tag	UNP C6GJB8
J	0	ALA	-	expression tag	UNP C6GJB8
K	-2	SER	-	expression tag	UNP C6GJB8
K	-1	ASN	-	expression tag	UNP C6GJB8
K	0	ALA	-	expression tag	UNP C6GJB8
L	-2	SER	-	expression tag	UNP C6GJB8
L	-1	ASN	-	expression tag	UNP C6GJB8
L	0	ALA	-	expression tag	UNP C6GJB8
M	-2	SER	-	expression tag	UNP C6GJB8
M	-1	ASN	-	expression tag	UNP C6GJB8
M	0	ALA	-	expression tag	UNP C6GJB8
N	-2	SER	-	expression tag	UNP C6GJB8
N	-1	ASN	-	expression tag	UNP C6GJB8
N	0	ALA	-	expression tag	UNP C6GJB8

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Chain	Residue	Modelled	Actual	Comment	Reference
O	-2	SER	-	expression tag	UNP C6GJB8
O	-1	ASN	-	expression tag	UNP C6GJB8
O	0	ALA	-	expression tag	UNP C6GJB8
P	-2	SER	-	expression tag	UNP C6GJB8
P	-1	ASN	-	expression tag	UNP C6GJB8
P	0	ALA	-	expression tag	UNP C6GJB8

- 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	A	1	Total	O	S	0	0
			5	4	1		
2	C	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		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	G	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	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		
2	M	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total	O	0	0
			55	55		
3	B	76	Total	O	0	0
			76	76		
3	C	60	Total	O	0	0
			60	60		
3	D	50	Total	O	0	0
			50	50		
3	E	34	Total	O	0	0
			34	34		
3	F	60	Total	O	0	0
			60	60		
3	G	35	Total	O	0	0
			35	35		
3	H	44	Total	O	0	0
			44	44		
3	I	49	Total	O	0	0
			49	49		

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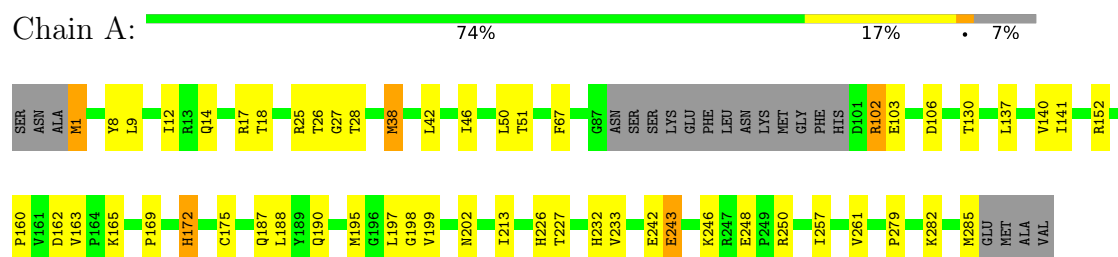
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	J	69	Total 69	O 69	0	0
3	K	39	Total 39	O 39	0	0
3	L	53	Total 53	O 53	0	0
3	M	47	Total 47	O 47	0	0
3	N	41	Total 41	O 41	0	0
3	O	59	Total 59	O 59	0	0
3	P	54	Total 54	O 54	0	0

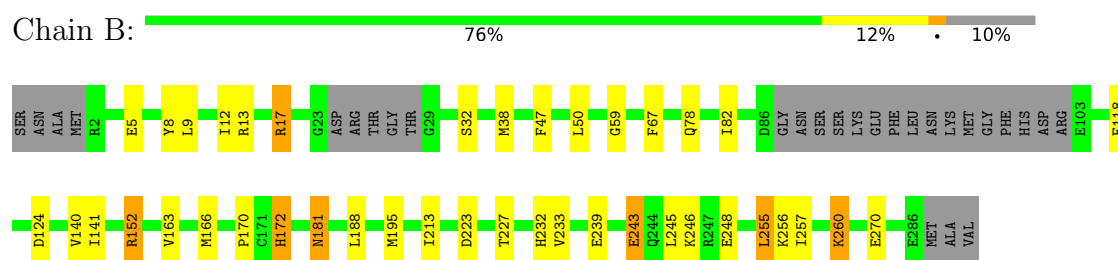
3 Residue-property plots [i](#)

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.

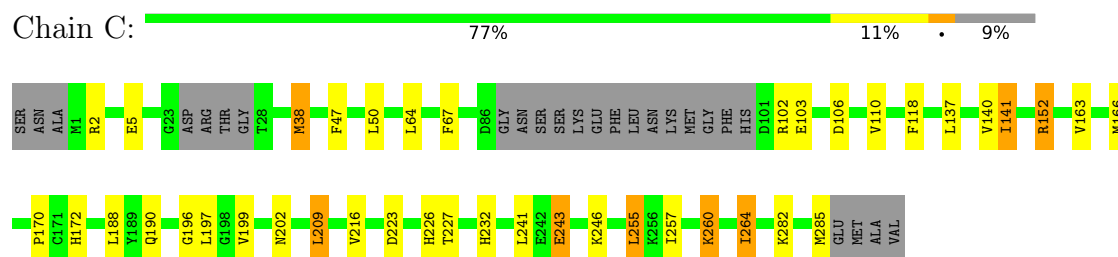
- Molecule 1: Thymidylate synthase



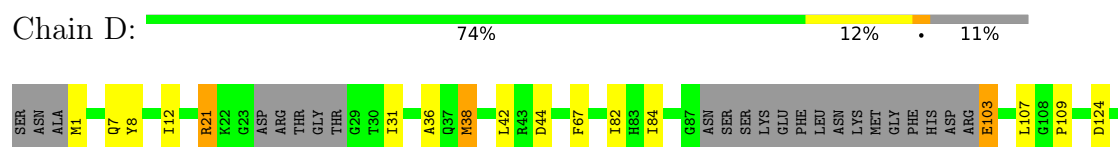
- Molecule 1: Thymidylate synthase

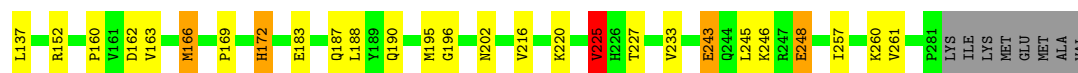


- Molecule 1: Thymidylate synthase



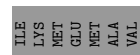
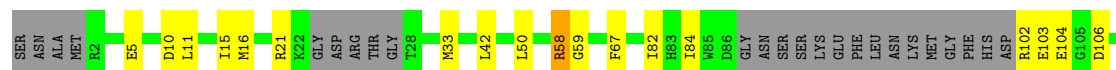
- Molecule 1: Thymidylate synthase





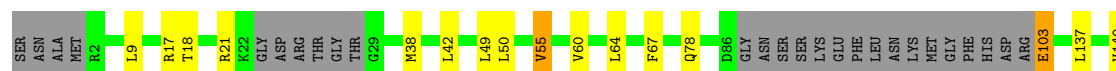
• Molecule 1: Thymidylate synthase

Chain E: 72% 15% 11%



• Molecule 1: Thymidylate synthase

Chain F: 76% 12% 10%



• Molecule 1: Thymidylate synthase

Chain G: 74% 11% 13%



• Molecule 1: Thymidylate synthase

Chain H: 78% 12% 9%



• Molecule 1: Thymidylate synthase

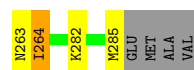
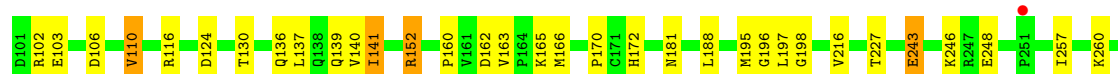
Chain I: 76% 14% 9%



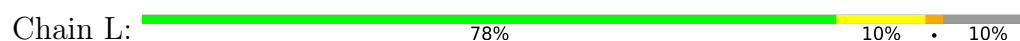
• Molecule 1: Thymidylate synthase



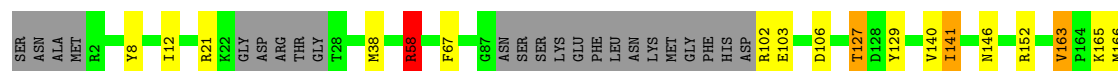
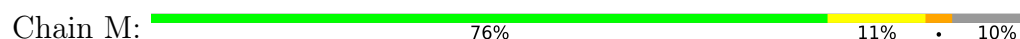
• Molecule 1: Thymidylate synthase



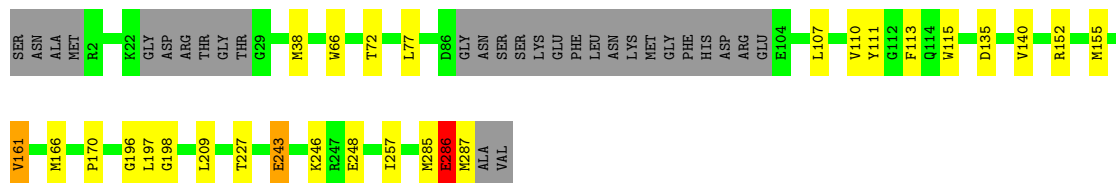
• Molecule 1: Thymidylate synthase



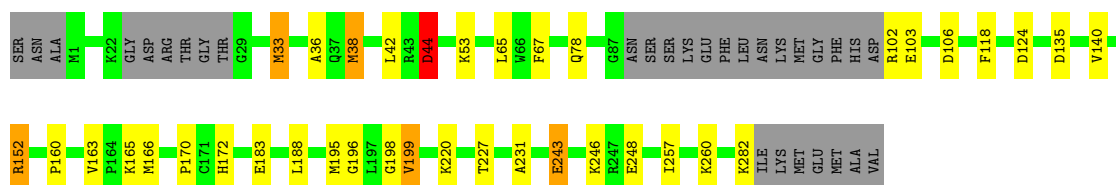
• Molecule 1: Thymidylate synthase



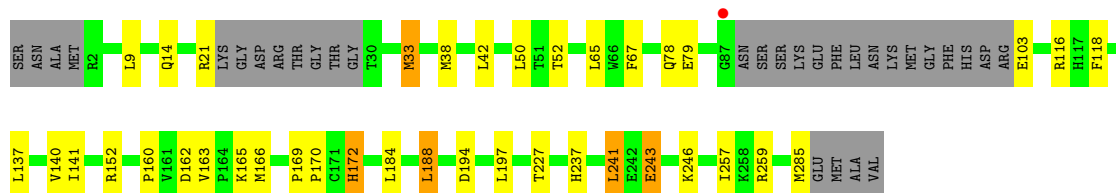
● Molecule 1: Thymidylate synthase

Chain N:  80% 9% 10%

● Molecule 1: Thymidylate synthase

Chain O:  77% 11% 10%

● Molecule 1: Thymidylate synthase

Chain P:  76% 12% 11%

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.27Å 103.46Å 125.77Å 77.40° 84.81° 61.43°	Depositor
Resolution (Å)	89.03 – 2.27 89.03 – 2.27	Depositor EDS
% Data completeness (in resolution range)	96.2 (89.03-2.27) 88.7 (89.03-2.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.27Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.218 , 0.236 0.227 , 0.240	Depositor DCC
R_{free} test set	10707 reflections (5.22%)	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.660	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.128 for h-k,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	35306	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.24 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4313e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

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	0.88	1/2270 (0.0%)	1.38	16/3068 (0.5%)
1	B	0.90	1/2210 (0.0%)	1.33	14/2987 (0.5%)
1	C	0.87	2/2235 (0.1%)	1.32	6/3020 (0.2%)
1	D	0.88	2/2179 (0.1%)	1.36	11/2947 (0.4%)
1	E	0.89	3/2181 (0.1%)	1.40	18/2951 (0.6%)
1	F	0.84	0/2206	1.31	13/2982 (0.4%)
1	G	0.84	1/2146 (0.0%)	1.36	13/2904 (0.4%)
1	H	0.83	0/2231	1.35	10/3015 (0.3%)
1	I	0.87	1/2243 (0.0%)	1.35	10/3030 (0.3%)
1	J	0.88	0/2237	1.36	13/3023 (0.4%)
1	K	0.87	2/2185 (0.1%)	1.34	15/2956 (0.5%)
1	L	0.85	0/2195	1.34	7/2968 (0.2%)
1	M	0.83	2/2202 (0.1%)	1.34	8/2978 (0.3%)
1	N	0.86	1/2205 (0.0%)	1.33	12/2980 (0.4%)
1	O	0.87	2/2195 (0.1%)	1.37	14/2967 (0.5%)
1	P	0.88	1/2188 (0.0%)	1.30	10/2959 (0.3%)
All	All	0.87	19/35308 (0.1%)	1.35	190/47735 (0.4%)

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	123	ALA	CA-C	10.22	1.57	1.52
1	D	163	VAL	CA-C	6.64	1.58	1.52
1	P	163	VAL	CA-C	6.37	1.58	1.52
1	M	163	VAL	CA-CB	5.84	1.57	1.54
1	M	199	VAL	CA-C	5.75	1.58	1.52
1	A	163	VAL	CA-C	5.74	1.57	1.52
1	I	163	VAL	CA-C	5.71	1.57	1.52
1	N	161	VAL	CA-C	5.71	1.60	1.52
1	C	163	VAL	CA-C	5.60	1.57	1.52
1	O	199	VAL	CA-CB	5.59	1.56	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	VAL	CA-C	5.55	1.57	1.52
1	K	163	VAL	CA-C	5.42	1.57	1.52
1	E	163	VAL	CA-CB	5.41	1.57	1.53
1	D	163	VAL	CA-CB	5.25	1.57	1.53
1	C	199	VAL	CA-C	5.23	1.58	1.52
1	K	110	VAL	CA-C	5.22	1.59	1.52
1	G	163	VAL	CA-C	5.10	1.56	1.52
1	O	163	VAL	CA-C	5.07	1.56	1.52
1	E	11	LEU	C-N	5.05	1.40	1.33

All (190) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	44	ASP	CA-CB-CG	14.53	127.13	112.60
1	E	163	VAL	N-CA-CB	12.28	118.24	110.50
1	J	163	VAL	N-CA-CB	11.49	117.74	110.50
1	H	198	GLY	CA-C-N	11.19	127.29	120.24
1	H	198	GLY	C-N-CA	11.19	127.29	120.24
1	B	181	ASN	CA-CB-CG	11.12	123.72	112.60
1	I	163	VAL	N-CA-CB	11.06	117.47	110.50
1	C	163	VAL	N-CA-CB	10.85	117.34	110.50
1	O	163	VAL	N-CA-CB	10.72	117.25	110.50
1	A	163	VAL	N-CA-CB	10.63	117.20	110.50
1	G	163	VAL	N-CA-CB	10.26	116.96	110.50
1	K	163	VAL	N-CA-CB	9.98	116.79	110.50
1	L	146	ASN	CA-CB-CG	9.80	122.41	112.60
1	E	198	GLY	CA-C-N	9.20	126.03	120.24
1	E	198	GLY	C-N-CA	9.20	126.03	120.24
1	E	124	ASP	CA-CB-CG	8.75	121.35	112.60
1	O	198	GLY	CA-C-N	8.14	128.25	120.43
1	O	198	GLY	C-N-CA	8.14	128.25	120.43
1	F	103	GLU	CB-CG-CD	7.92	126.06	112.60
1	B	163	VAL	N-CA-CB	7.88	115.47	110.50
1	A	198	GLY	CA-C-N	7.67	127.79	120.43
1	A	198	GLY	C-N-CA	7.67	127.79	120.43
1	G	124	ASP	CA-CB-CG	7.51	120.11	112.60
1	E	67	PHE	CA-CB-CG	7.45	121.25	113.80
1	H	67	PHE	CA-CB-CG	7.36	121.16	113.80
1	P	67	PHE	CA-CB-CG	7.22	121.02	113.80
1	A	67	PHE	CA-CB-CG	7.21	121.01	113.80
1	M	67	PHE	CA-CB-CG	7.20	121.00	113.80
1	I	67	PHE	CA-CB-CG	7.13	120.93	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	67	PHE	CA-CB-CG	7.07	120.87	113.80
1	C	67	PHE	CA-CB-CG	7.06	120.86	113.80
1	G	67	PHE	CA-CB-CG	6.97	120.77	113.80
1	K	67	PHE	CA-CB-CG	6.95	120.75	113.80
1	O	67	PHE	CA-CB-CG	6.91	120.70	113.80
1	M	200	PRO	CA-C-N	6.77	129.91	120.29
1	M	200	PRO	C-N-CA	6.77	129.91	120.29
1	D	67	PHE	CA-CB-CG	6.73	120.53	113.80
1	B	67	PHE	CA-CB-CG	6.67	120.47	113.80
1	L	163	VAL	N-CA-CB	6.58	114.65	110.50
1	F	163	VAL	N-CA-CB	6.55	114.63	110.50
1	F	67	PHE	CA-CB-CG	6.51	120.31	113.80
1	A	1	MET	CA-C-N	6.49	132.75	122.62
1	A	1	MET	C-N-CA	6.49	132.75	122.62
1	H	163	VAL	N-CA-CB	6.48	114.58	110.50
1	J	67	PHE	CA-CB-CG	6.48	120.28	113.80
1	P	163	VAL	N-CA-CB	6.44	114.56	110.50
1	G	145	LYS	CG-CD-CE	6.40	126.02	111.30
1	E	248	GLU	CB-CG-CD	6.34	123.38	112.60
1	J	198	GLY	CA-C-N	6.25	126.43	120.43
1	J	198	GLY	C-N-CA	6.25	126.43	120.43
1	K	60	VAL	N-CA-CB	6.23	119.02	110.54
1	D	103	GLU	CB-CG-CD	6.21	123.15	112.60
1	P	257	ILE	CA-C-N	6.16	128.82	120.38
1	P	257	ILE	C-N-CA	6.16	128.82	120.38
1	M	257	ILE	CA-C-N	6.16	128.81	120.38
1	M	257	ILE	C-N-CA	6.16	128.81	120.38
1	C	257	ILE	CA-C-N	6.11	128.75	120.38
1	C	257	ILE	C-N-CA	6.11	128.75	120.38
1	M	146	ASN	CA-CB-CG	6.11	118.71	112.60
1	N	198	GLY	CA-C-N	6.11	126.29	120.43
1	N	198	GLY	C-N-CA	6.11	126.29	120.43
1	J	257	ILE	CA-C-N	6.10	128.74	120.38
1	J	257	ILE	C-N-CA	6.10	128.74	120.38
1	K	198	GLY	CA-C-N	6.08	126.26	120.43
1	K	198	GLY	C-N-CA	6.08	126.26	120.43
1	E	257	ILE	CA-C-N	6.02	128.62	120.38
1	E	257	ILE	C-N-CA	6.02	128.62	120.38
1	J	31	ILE	N-CA-C	-5.99	99.72	108.11
1	A	257	ILE	CA-C-N	5.99	128.59	120.38
1	A	257	ILE	C-N-CA	5.99	128.59	120.38
1	G	78	GLN	CA-C-N	5.98	128.29	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	78	GLN	C-N-CA	5.98	128.29	120.28
1	N	286	GLU	CA-C-N	5.96	132.43	121.70
1	N	286	GLU	C-N-CA	5.96	132.43	121.70
1	O	65	LEU	CA-C-N	5.95	128.53	120.44
1	O	65	LEU	C-N-CA	5.95	128.53	120.44
1	I	59	GLY	CA-C-N	5.92	128.53	120.77
1	I	59	GLY	C-N-CA	5.92	128.53	120.77
1	L	257	ILE	CA-C-N	5.92	128.49	120.38
1	L	257	ILE	C-N-CA	5.92	128.49	120.38
1	I	257	ILE	CA-C-N	5.90	128.47	120.38
1	I	257	ILE	C-N-CA	5.90	128.47	120.38
1	G	194	ASP	CA-CB-CG	5.89	118.49	112.60
1	G	257	ILE	CA-C-N	5.88	128.43	120.38
1	G	257	ILE	C-N-CA	5.88	128.43	120.38
1	O	257	ILE	CA-C-N	5.87	128.42	120.38
1	O	257	ILE	C-N-CA	5.87	128.42	120.38
1	D	162	ASP	CA-C-N	5.87	123.94	120.24
1	D	162	ASP	C-N-CA	5.87	123.94	120.24
1	F	257	ILE	CA-C-N	5.84	128.39	120.38
1	F	257	ILE	C-N-CA	5.84	128.39	120.38
1	K	257	ILE	CA-C-N	5.82	128.35	120.38
1	K	257	ILE	C-N-CA	5.82	128.35	120.38
1	D	257	ILE	CA-C-N	5.80	128.85	120.38
1	D	257	ILE	C-N-CA	5.80	128.85	120.38
1	E	122	TYR	CA-C-N	5.79	129.80	121.98
1	E	122	TYR	C-N-CA	5.79	129.80	121.98
1	B	257	ILE	CA-C-N	5.78	128.30	120.38
1	B	257	ILE	C-N-CA	5.78	128.30	120.38
1	B	124	ASP	CA-CB-CG	5.77	118.37	112.60
1	A	46	ILE	N-CA-CB	5.70	117.76	110.13
1	A	140	VAL	CA-C-N	5.69	127.73	120.56
1	A	140	VAL	C-N-CA	5.69	127.73	120.56
1	F	232	HIS	N-CA-C	5.67	117.42	108.96
1	C	223	ASP	CA-CB-CG	5.66	118.26	112.60
1	H	257	ILE	CA-C-N	5.65	128.13	120.38
1	H	257	ILE	C-N-CA	5.65	128.13	120.38
1	D	225	VAL	N-CA-CB	5.64	117.81	111.21
1	N	257	ILE	CA-C-N	5.64	128.10	120.38
1	N	257	ILE	C-N-CA	5.64	128.10	120.38
1	H	232	HIS	N-CA-C	5.61	117.72	109.24
1	B	78	GLN	CA-C-N	5.58	128.31	120.28
1	B	78	GLN	C-N-CA	5.58	128.31	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	172	HIS	CA-C-N	5.57	127.68	120.44
1	D	172	HIS	C-N-CA	5.57	127.68	120.44
1	B	172	HIS	CA-C-N	5.55	127.66	120.44
1	B	172	HIS	C-N-CA	5.55	127.66	120.44
1	G	198	GLY	CA-C-N	5.55	125.76	120.43
1	G	198	GLY	C-N-CA	5.55	125.76	120.43
1	D	163	VAL	N-CA-CB	5.55	114.00	110.50
1	E	202	ASN	CA-C-N	5.52	127.72	120.60
1	E	202	ASN	C-N-CA	5.52	127.72	120.60
1	E	104	GLU	CB-CG-CD	5.52	121.98	112.60
1	H	124	ASP	CA-CB-CG	5.51	118.11	112.60
1	N	77	LEU	CA-C-N	5.49	127.64	120.28
1	N	77	LEU	C-N-CA	5.49	127.64	120.28
1	K	124	ASP	CA-CB-CG	5.47	118.07	112.60
1	L	202	ASN	CA-C-N	5.41	127.38	120.56
1	L	202	ASN	C-N-CA	5.41	127.38	120.56
1	E	162	ASP	CA-C-N	5.39	123.64	120.24
1	E	162	ASP	C-N-CA	5.39	123.64	120.24
1	A	172	HIS	CA-C-N	5.39	127.76	120.65
1	A	172	HIS	C-N-CA	5.39	127.76	120.65
1	I	223	ASP	CA-CB-CG	5.34	117.94	112.60
1	K	65	LEU	CA-C-N	5.32	128.40	120.31
1	K	65	LEU	C-N-CA	5.32	128.40	120.31
1	A	232	HIS	N-CA-C	5.32	117.47	109.23
1	C	232	HIS	N-CA-C	5.32	117.27	109.24
1	O	124	ASP	CA-CB-CG	5.31	117.91	112.60
1	G	172	HIS	CA-C-N	5.28	127.31	120.44
1	G	172	HIS	C-N-CA	5.28	127.31	120.44
1	O	78	GLN	CA-C-N	5.27	127.61	120.38
1	O	78	GLN	C-N-CA	5.27	127.61	120.38
1	N	135	ASP	CA-C-N	5.26	127.33	120.28
1	N	135	ASP	C-N-CA	5.26	127.33	120.28
1	E	10	ASP	CA-CB-CG	5.25	117.85	112.60
1	E	172	HIS	CA-C-N	5.21	127.53	120.65
1	E	172	HIS	C-N-CA	5.21	127.53	120.65
1	I	31	ILE	N-CA-C	-5.20	100.08	107.77
1	B	223	ASP	CA-CB-CG	5.19	117.79	112.60
1	M	58	ARG	CA-C-N	5.19	125.74	119.98
1	M	58	ARG	C-N-CA	5.19	125.74	119.98
1	O	135	ASP	CA-C-N	5.18	127.22	120.28
1	O	135	ASP	C-N-CA	5.18	127.22	120.28
1	F	214	ALA	CA-C-N	5.18	127.17	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	214	ALA	C-N-CA	5.18	127.17	120.44
1	F	199	VAL	N-CA-CB	5.17	118.45	111.21
1	F	200	PRO	CA-C-N	5.17	127.21	120.28
1	F	200	PRO	C-N-CA	5.17	127.21	120.28
1	K	78	GLN	CA-C-N	5.15	127.44	120.38
1	K	78	GLN	C-N-CA	5.15	127.44	120.38
1	B	140	VAL	N-CA-CB	5.14	117.53	110.54
1	K	84	ILE	N-CA-CB	5.10	117.47	110.54
1	P	78	GLN	CA-C-N	5.10	127.11	120.28
1	P	78	GLN	C-N-CA	5.10	127.11	120.28
1	D	124	ASP	CA-CB-CG	5.10	117.70	112.60
1	K	110	VAL	CA-C-N	5.08	127.41	120.54
1	K	110	VAL	C-N-CA	5.08	127.41	120.54
1	H	78	GLN	CA-C-N	5.05	127.05	120.28
1	H	78	GLN	C-N-CA	5.05	127.05	120.28
1	J	286	GLU	CA-C-N	5.04	130.76	121.70
1	J	286	GLU	C-N-CA	5.04	130.76	121.70
1	I	66	TRP	CA-C-N	5.03	127.29	120.44
1	I	66	TRP	C-N-CA	5.03	127.29	120.44
1	J	135	ASP	CA-C-N	5.03	127.02	120.28
1	J	135	ASP	C-N-CA	5.03	127.02	120.28
1	B	140	VAL	CA-C-N	5.03	126.90	120.56
1	B	140	VAL	C-N-CA	5.03	126.90	120.56
1	N	110	VAL	CA-C-N	5.03	131.14	121.54
1	N	110	VAL	C-N-CA	5.03	131.14	121.54
1	F	78	GLN	CA-C-N	5.02	127.01	120.28
1	F	78	GLN	C-N-CA	5.02	127.01	120.28
1	J	232	HIS	CA-C-N	5.02	129.71	123.14
1	J	232	HIS	C-N-CA	5.02	129.71	123.14
1	P	65	LEU	CA-C-N	5.02	127.41	120.29
1	P	65	LEU	C-N-CA	5.02	127.41	120.29
1	P	172	HIS	CA-C-N	5.01	126.95	120.44
1	P	172	HIS	C-N-CA	5.01	126.95	120.44
1	A	28	THR	CA-C-N	5.00	124.85	120.10
1	A	28	THR	C-N-CA	5.00	124.85	120.10

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	2212	0	2149	25	0
1	B	2153	0	2088	17	0
1	C	2178	0	2118	19	0
1	D	2122	0	2051	21	0
1	E	2124	0	2053	20	0
1	F	2149	0	2085	20	0
1	G	2089	0	2028	17	0
1	H	2173	0	2106	11	0
1	I	2183	0	2127	19	0
1	J	2180	0	2111	20	0
1	K	2128	0	2057	24	0
1	L	2138	0	2080	13	0
1	M	2145	0	2080	23	0
1	N	2148	0	2088	12	0
1	O	2138	0	2074	18	0
1	P	2131	0	2066	15	0
2	A	10	0	0	0	0
2	C	10	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	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	0	0
2	K	5	0	0	0	0
2	L	5	0	0	0	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
3	A	55	0	0	1	0
3	B	76	0	0	0	0
3	C	60	0	0	0	0
3	D	50	0	0	0	0
3	E	34	0	0	1	0
3	F	60	0	0	0	0
3	G	35	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	H	44	0	0	0	0
3	I	49	0	0	0	0
3	J	69	0	0	0	0
3	K	39	0	0	0	0
3	L	53	0	0	0	0
3	M	47	0	0	1	0
3	N	41	0	0	0	0
3	O	59	0	0	0	0
3	P	54	0	0	1	0
All	All	35306	0	33361	258	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (258) 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:F:220:LYS:HD3	1:O:44:ASP:CB	1.68	1.23
1:F:220:LYS:CD	1:O:44:ASP:HB3	1.73	1.19
1:A:51:THR:HG21	1:A:250:ARG:HB2	1.20	1.14
1:B:260:LYS:HD2	1:K:130:THR:HG23	1.53	0.89
1:A:130:THR:O	1:J:260:LYS:HG2	1.74	0.85
1:F:220:LYS:HD3	1:O:44:ASP:HB3	0.88	0.85
1:I:11:LEU:HD22	1:I:38[B]:MET:HE1	1.61	0.82
1:A:51:THR:CG2	1:A:250:ARG:HB2	2.10	0.78
1:J:64:LEU:O	1:J:68:VAL:HG12	1.86	0.76
1:A:51:THR:HG23	1:A:279:PRO:HA	1.70	0.73
1:B:9:LEU:HD12	1:B:245:LEU:HD23	1.71	0.73
1:D:31:ILE:HG23	1:D:233:VAL:HG22	1.69	0.73
1:E:264:ILE:HD13	1:E:264:ILE:H	1.54	0.71
1:G:227:THR:HG21	1:H:227:THR:HG21	1.73	0.71
1:M:264:ILE:H	1:M:264:ILE:HD13	1.54	0.71
1:F:49:LEU:HD11	1:F:55:VAL:HG22	1.72	0.70
1:A:227:THR:HG21	1:B:227:THR:HG21	1.75	0.69
1:C:227:THR:HG21	1:D:227:THR:HG21	1.76	0.67
1:A:162:ASP:HA	1:A:165:LYS:HE3	1.75	0.67
1:C:5:GLU:HG3	1:C:50:LEU:HD22	1.76	0.67
1:G:264:ILE:HD13	1:G:264:ILE:H	1.58	0.67
1:C:216:VAL:HG21	1:C:264:ILE:HG23	1.75	0.67
1:C:264:ILE:HD13	1:C:264:ILE:H	1.59	0.67
1:I:227:THR:HG21	1:J:227:THR:HG21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ARG:O	1:B:17:ARG:HG2	1.94	0.67
1:K:264:ILE:HD13	1:K:264:ILE:H	1.61	0.66
1:G:216:VAL:HG21	1:G:264:ILE:HG23	1.78	0.66
1:E:216:VAL:HG21	1:E:264:ILE:HG23	1.78	0.65
1:K:227:THR:HG21	1:L:227:THR:HG21	1.78	0.65
1:L:5:GLU:HG3	1:L:50:LEU:HD22	1.79	0.65
1:M:227:THR:HG21	1:N:227:THR:HG21	1.79	0.64
1:J:197:LEU:HD11	1:J:285:MET:O	1.97	0.64
1:M:216:VAL:HG21	1:M:264:ILE:HG23	1.80	0.64
1:F:49:LEU:HD11	1:F:55:VAL:CG2	2.27	0.64
1:O:227:THR:HG21	1:P:227:THR:HG21	1.80	0.63
1:E:243:GLU:HA	1:E:246:LYS:HE3	1.80	0.63
1:L:243:GLU:HA	1:L:246:LYS:HE3	1.81	0.63
1:I:243:GLU:HA	1:I:246:LYS:HE3	1.81	0.63
1:C:243:GLU:HA	1:C:246:LYS:HE3	1.81	0.63
1:K:243:GLU:HA	1:K:246:LYS:HE3	1.82	0.62
1:D:31:ILE:CG2	1:D:233:VAL:CG2	2.77	0.62
1:J:243:GLU:HA	1:J:246:LYS:HE3	1.82	0.62
1:B:243:GLU:HA	1:B:246:LYS:HE2	1.81	0.62
1:G:58:ARG:HD2	1:G:82:ILE:HD11	1.82	0.62
1:N:243:GLU:HA	1:N:246:LYS:HE3	1.82	0.62
1:O:243:GLU:HA	1:O:246:LYS:HE3	1.81	0.62
1:D:109:PRO:O	1:D:166:MET:HE3	2.00	0.61
1:H:243:GLU:HA	1:H:246:LYS:HE3	1.83	0.61
1:M:243:GLU:HA	1:M:246:LYS:HE3	1.82	0.61
1:G:243:GLU:HA	1:G:246:LYS:HE2	1.82	0.61
1:O:152:ARG:HD2	1:P:169:PRO:HG2	1.83	0.60
1:K:216:VAL:HG21	1:K:264:ILE:HG23	1.84	0.60
1:B:59:GLY:HA2	1:B:82:ILE:HD12	1.83	0.60
1:F:64:LEU:HD23	1:F:208:LEU:HD13	1.82	0.60
1:A:243:GLU:HA	1:A:246:LYS:HE3	1.82	0.60
1:D:31:ILE:CG2	1:D:233:VAL:HG22	2.33	0.59
1:E:227:THR:HG21	1:F:227:THR:HG21	1.85	0.59
1:H:21:ARG:HD2	1:H:31:ILE:HG12	1.85	0.59
1:M:58:ARG:HG2	1:M:58:ARG:HH21	1.67	0.58
1:N:66:TRP:HH2	1:N:107:LEU:CD1	2.16	0.58
1:H:59:GLY:HA2	1:H:82:ILE:HD12	1.84	0.58
1:D:172:HIS:HB3	1:D:188:LEU:HD11	1.85	0.58
1:P:172:HIS:HB3	1:P:188:LEU:HD21	1.86	0.58
1:D:243:GLU:HA	1:D:246:LYS:HE2	1.86	0.57
1:G:58:ARG:HH12	1:G:81:ASP:HB2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:166:MET:SD	1:M:170:PRO:HD3	2.45	0.56
1:P:166:MET:SD	1:P:170:PRO:HD3	2.46	0.56
1:M:264:ILE:H	1:M:264:ILE:CD1	2.18	0.56
1:O:166:MET:SD	1:O:170:PRO:HD3	2.46	0.56
1:N:155:MET:HE1	1:N:209:LEU:HD21	1.88	0.56
1:D:187:GLN:HG3	1:D:225:VAL:HG22	1.86	0.55
1:E:5:GLU:HG3	1:E:50:LEU:HD22	1.88	0.55
1:L:166:MET:SD	1:L:170:PRO:HD3	2.47	0.55
1:A:102:ARG:HG3	1:A:106:ASP:HB3	1.89	0.55
1:B:47:PHE:HB2	1:B:255:LEU:HB2	1.89	0.55
1:I:166:MET:SD	1:I:170:PRO:HD3	2.46	0.55
1:E:162:ASP:HA	1:E:165:LYS:HD3	1.89	0.54
1:E:264:ILE:H	1:E:264:ILE:CD1	2.20	0.54
1:F:166:MET:SD	1:F:170:PRO:HD3	2.47	0.54
1:A:165:LYS:HD3	1:D:248:GLU:OE2	2.07	0.54
1:B:5:GLU:HG3	1:B:50:LEU:HD22	1.89	0.54
1:K:136:GLN:HA	1:K:139:GLN:HG2	1.89	0.54
1:G:172:HIS:HB3	1:G:188:LEU:HD11	1.90	0.53
1:H:166:MET:SD	1:H:170:PRO:HD3	2.49	0.53
1:N:166:MET:SD	1:N:170:PRO:HD3	2.49	0.53
1:B:8:TYR:HD2	1:B:9:LEU:HD22	1.74	0.53
1:N:66:TRP:HH2	1:N:107:LEU:HD12	1.74	0.53
1:K:166:MET:SD	1:K:170:PRO:HD3	2.49	0.53
1:M:102:ARG:HG2	1:M:106:ASP:HB3	1.90	0.53
1:K:141:ILE:HD13	1:K:264:ILE:HD12	1.91	0.53
1:F:220:LYS:CG	1:O:44:ASP:HB3	2.38	0.52
1:G:190:GLN:HE22	1:G:202:ASN:ND2	2.07	0.52
1:B:166:MET:SD	1:B:170:PRO:HD3	2.49	0.52
1:A:137:LEU:O	1:A:141:ILE:HG12	2.09	0.52
1:C:118:PHE:CE1	1:D:160:PRO:HD2	2.45	0.52
1:I:102:ARG:HG2	1:I:106:ASP:HB3	1.90	0.52
1:J:65:LEU:HA	1:J:68:VAL:HG13	1.91	0.52
1:E:58:ARG:HG3	1:E:269:PHE:CZ	2.44	0.52
1:G:264:ILE:H	1:G:264:ILE:CD1	2.22	0.52
1:E:278:LYS:HA	3:E:412:HOH:O	2.09	0.52
1:K:264:ILE:H	1:K:264:ILE:CD1	2.23	0.51
1:G:114:GLN:HE21	1:G:166:MET:HE3	1.75	0.51
1:K:102:ARG:HG2	1:K:106:ASP:HB3	1.91	0.51
1:O:102:ARG:HG2	1:O:106:ASP:HB3	1.92	0.51
1:E:166:MET:SD	1:E:170:PRO:HD3	2.51	0.51
1:D:44:ASP:HA	1:J:220:LYS:HZ3	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:159:ASN:OD1	1:I:161:VAL:HG22	2.12	0.51
1:C:102:ARG:HG2	1:C:106:ASP:HB3	1.93	0.50
1:C:264:ILE:H	1:C:264:ILE:CD1	2.23	0.50
1:P:14:GLN:HG2	1:P:33:MET:HE1	1.94	0.50
1:C:47:PHE:HB2	1:C:255:LEU:HB2	1.94	0.50
1:F:21:ARG:HD3	1:M:21:ARG:NH1	2.25	0.50
1:E:102:ARG:HG2	1:E:106:ASP:HB3	1.93	0.50
1:I:11:LEU:HD22	1:I:38[B]:MET:CE	2.36	0.50
1:O:172:HIS:HB3	1:O:188:LEU:HD11	1.93	0.49
1:A:162:ASP:O	1:A:165:LYS:HG2	2.13	0.49
1:N:286:GLU:CD	1:N:286:GLU:H	2.19	0.49
1:O:33:MET:HE3	1:O:231:ALA:HB3	1.94	0.49
1:A:195:MET:HB2	1:A:233:VAL:HG12	1.93	0.49
1:M:58:ARG:HH21	1:M:58:ARG:CG	2.26	0.49
1:A:172:HIS:HB3	1:A:188:LEU:HD11	1.94	0.48
1:I:197:LEU:HD21	1:I:285:MET:HB2	1.95	0.48
1:M:193:ALA:HB1	1:M:199:VAL:CG2	2.43	0.48
1:P:116:ARG:HH21	1:P:137:LEU:HB3	1.79	0.48
1:C:38:MET:HG2	1:C:226:HIS:HB3	1.95	0.48
1:C:166:MET:SD	1:C:170:PRO:HD3	2.54	0.48
1:C:172:HIS:HB3	1:C:188:LEU:HD11	1.96	0.48
1:P:9:LEU:HD11	1:P:52:THR:HG21	1.96	0.48
1:B:32:SER:HB3	1:B:232:HIS:HB3	1.96	0.47
1:L:183:GLU:HA	1:L:220:LYS:O	2.14	0.47
1:A:38:MET:HG3	3:A:405:HOH:O	2.12	0.47
1:I:152:ARG:HD2	1:J:169:PRO:HG2	1.96	0.47
1:E:141:ILE:HD13	1:E:264:ILE:HD12	1.96	0.47
1:I:172:HIS:HB3	1:I:188:LEU:HD11	1.96	0.47
1:J:54:ARG:HB3	1:J:282:LYS:HG3	1.97	0.47
1:J:233:VAL:HG13	1:J:241:LEU:CD1	2.45	0.47
1:F:172:HIS:HB3	1:F:188:LEU:HD11	1.96	0.46
1:I:58:ARG:CZ	1:M:58:ARG:HD3	2.45	0.46
1:K:137:LEU:O	1:K:141:ILE:HD12	2.16	0.46
1:K:197:LEU:HD21	1:K:285:MET:HB2	1.97	0.46
1:E:172:HIS:HB3	1:E:188:LEU:HD11	1.97	0.46
1:K:172:HIS:HB3	1:K:188:LEU:HD11	1.95	0.46
1:N:66:TRP:CH2	1:N:107:LEU:HD12	2.50	0.46
1:M:141:ILE:HD13	1:M:264:ILE:HD12	1.96	0.46
1:H:172:HIS:HB3	1:H:188:LEU:HD11	1.97	0.46
1:K:160:PRO:HD2	1:L:118:PHE:CE1	2.50	0.46
1:C:141:ILE:HD13	1:C:264:ILE:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:ILE:HG22	1:D:233:VAL:HG23	1.97	0.46
1:J:236:ASN:HD21	1:J:287:MET:HB2	1.81	0.46
1:P:197:LEU:HD21	1:P:285:MET:HB2	1.98	0.45
1:E:137:LEU:O	1:E:141:ILE:HD12	2.17	0.45
1:M:127:THR:HB	1:M:129:TYR:CZ	2.51	0.45
1:F:21:ARG:HD3	1:M:21:ARG:CZ	2.46	0.45
1:A:190:GLN:HE22	1:A:202:ASN:ND2	2.15	0.45
1:I:216:VAL:HG21	1:I:264:ILE:HG23	1.98	0.45
1:K:162:ASP:HA	1:K:165:LYS:HD3	1.99	0.45
1:A:169:PRO:HG2	1:B:152:ARG:CZ	2.46	0.45
1:J:65:LEU:HA	1:J:68:VAL:CG1	2.46	0.45
1:C:190:GLN:HE22	1:C:202:ASN:ND2	2.14	0.45
1:K:11:LEU:HD23	1:K:195:MET:HE2	1.98	0.45
1:C:197:LEU:HD21	1:C:285:MET:HB2	1.99	0.44
1:K:152:ARG:HD2	1:L:169:PRO:HG2	1.99	0.44
1:A:8:TYR:CZ	1:A:12:ILE:HD11	2.52	0.44
1:F:220:LYS:HD3	1:O:44:ASP:CG	2.38	0.44
1:I:141:ILE:HD13	1:I:264:ILE:HD12	1.99	0.44
1:K:116:ARG:NH1	1:K:137:LEU:HD23	2.32	0.44
1:G:64:LEU:HD11	1:G:209:LEU:HG	1.99	0.44
1:N:197:LEU:HD21	1:N:285:MET:HB2	1.99	0.44
1:J:172:HIS:HB3	1:J:188:LEU:HD11	1.99	0.44
1:B:172:HIS:HB3	1:B:188:LEU:HD11	1.99	0.44
1:L:184:LEU:HD13	1:L:210:THR:HG22	1.99	0.44
1:F:162:ASP:HA	1:F:165:LYS:HD3	1.99	0.44
1:N:72:THR:CG2	1:N:113:PHE:HB2	2.47	0.44
1:J:162:ASP:HA	1:J:165:LYS:HD3	2.00	0.43
1:G:141:ILE:HD13	1:G:264:ILE:HD12	1.99	0.43
1:K:17:ARG:HG2	1:K:18:THR:HG23	2.00	0.43
1:I:160:PRO:HD2	1:J:118:PHE:CE1	2.54	0.43
1:K:264:ILE:HD13	1:K:264:ILE:N	2.31	0.43
1:O:118:PHE:CE1	1:P:160:PRO:HD2	2.53	0.43
1:D:21:ARG:HH11	1:K:181:ASN:H	1.66	0.43
1:I:12:ILE:HG22	1:I:16:MET:HE2	2.00	0.43
1:M:172:HIS:HB3	1:M:188:LEU:HD21	2.00	0.43
1:N:115:TRP:CE2	1:N:155:MET:HE3	2.53	0.43
1:C:260:LYS:H	1:C:260:LYS:HG3	1.59	0.43
1:D:82:ILE:HG22	1:D:84:ILE:HG12	2.01	0.43
1:P:162:ASP:HA	1:P:165:LYS:HD3	2.00	0.43
1:B:195:MET:HB2	1:B:233:VAL:HG12	2.01	0.43
1:C:152:ARG:HD2	1:D:169:PRO:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:17:ARG:HG2	1:F:18:THR:HG23	2.01	0.43
1:H:17:ARG:HG2	1:H:18:THR:HG23	2.01	0.43
1:L:72:THR:CG2	1:L:113:PHE:HB2	2.48	0.43
1:M:8:TYR:CZ	1:M:12:ILE:HD11	2.54	0.43
1:G:118:PHE:CE1	1:H:160:PRO:HD2	2.54	0.43
1:D:195:MET:HB2	1:D:233:VAL:HG12	2.00	0.42
1:H:82:ILE:HG22	1:H:84:ILE:HG12	2.00	0.42
1:I:58:ARG:NH2	1:M:58:ARG:HD3	2.34	0.42
1:K:5:GLU:HG3	1:K:50:LEU:HD22	2.01	0.42
1:P:243:GLU:HA	1:P:246:LYS:HE3	2.00	0.42
1:F:270:GLU:H	1:F:270:GLU:HG3	1.67	0.42
1:E:21:ARG:HE	1:P:21:ARG:HB2	1.83	0.42
1:F:195:MET:HB2	1:F:233:VAL:HG12	2.01	0.42
1:G:137:LEU:O	1:G:141:ILE:HD12	2.20	0.42
1:K:9:LEU:HD11	1:K:52:THR:HG21	2.01	0.42
1:P:259:ARG:HB2	3:P:439:HOH:O	2.18	0.42
1:J:17:ARG:HG2	1:J:18:THR:HG23	2.01	0.42
1:A:38:MET:HG2	1:A:226:HIS:HB3	2.02	0.42
1:C:137:LEU:O	1:C:141:ILE:HD12	2.20	0.42
1:D:183:GLU:HA	1:D:220:LYS:O	2.20	0.42
1:L:197:LEU:HD21	1:L:285:MET:HB2	2.02	0.42
1:D:190:GLN:HE22	1:D:202:ASN:ND2	2.17	0.42
1:H:36:ALA:HB1	1:H:38:MET:HE1	2.01	0.42
1:L:172:HIS:HB3	1:L:188:LEU:HD21	2.01	0.42
1:L:239:GLU:CD	1:L:239:GLU:H	2.27	0.42
1:A:141:ILE:HD13	1:A:213:ILE:HG23	2.02	0.41
1:B:141:ILE:HG12	1:B:213:ILE:HG23	2.01	0.41
1:E:59:GLY:HA2	1:E:82:ILE:HD12	2.02	0.41
1:F:197:LEU:HD21	1:F:285:MET:HB2	2.02	0.41
1:O:195:MET:SD	1:O:199:VAL:HG21	2.60	0.41
1:A:14:GLN:HG3	1:A:17:ARG:NH2	2.35	0.41
1:C:64:LEU:HD11	1:C:209:LEU:HG	2.02	0.41
1:M:282:LYS:HD3	3:M:419:HOH:O	2.18	0.41
1:A:160:PRO:HD2	1:B:118:PHE:CE1	2.55	0.41
1:G:175:CYS:HA	1:G:187:GLN:O	2.21	0.41
1:H:197:LEU:HD21	1:H:285:MET:HB2	2.01	0.41
1:M:264:ILE:HD13	1:M:264:ILE:N	2.28	0.41
1:D:7:GLN:HB3	1:D:38:MET:HG3	2.03	0.41
1:M:183:GLU:HA	1:M:220:LYS:O	2.20	0.41
1:O:36:ALA:HB1	1:O:38:MET:HE1	2.03	0.41
1:O:160:PRO:HD2	1:P:118:PHE:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:MET:SD	1:A:199:VAL:HG21	2.60	0.41
1:D:8:TYR:CZ	1:D:12:ILE:HD11	2.55	0.41
1:J:73:ASN:OD1	1:J:75:LYS:HB2	2.20	0.41
1:E:15:ILE:HG12	1:E:33:MET:HG2	2.03	0.41
1:A:197:LEU:HD21	1:A:285:MET:HB2	2.02	0.41
1:E:195:MET:HB2	1:E:233:VAL:HG12	2.02	0.41
1:F:137:LEU:O	1:F:141:ILE:HD12	2.21	0.41
1:I:32:SER:HB3	1:I:232:HIS:HB3	2.03	0.41
1:I:163:VAL:HG23	1:I:164:PRO:HD3	2.03	0.41
1:J:7:GLN:HB3	1:J:38:MET:HG3	2.02	0.41
1:N:66:TRP:CH2	1:N:107:LEU:CD1	3.00	0.41
1:P:237:HIS:O	1:P:241:LEU:HD22	2.21	0.41
1:I:50:LEU:HD12	1:I:200:PRO:HG3	2.02	0.41
1:J:12:ILE:HD13	1:J:241:LEU:HD22	2.03	0.40
1:M:193:ALA:HB1	1:M:199:VAL:HG22	2.02	0.40
1:M:195:MET:HB2	1:M:233:VAL:HG12	2.03	0.40
1:E:215:HIS:CE1	1:E:261:VAL:H	2.39	0.40
1:F:42:LEU:HB2	1:F:221:PRO:HB2	2.04	0.40
1:G:17:ARG:HG2	1:G:18:THR:HG23	2.03	0.40
1:D:36:ALA:HB1	1:D:38:MET:HE1	2.02	0.40
1:A:14:GLN:O	1:A:18:THR:HG22	2.22	0.40
1:G:82:ILE:HG22	1:G:84:ILE:HG12	2.02	0.40
1:K:83:HIS:CE1	1:O:282:LYS:HE2	2.57	0.40
1:O:183:GLU:HA	1:O:220:LYS:O	2.22	0.40
1:A:175:CYS:HA	1:A:187:GLN:O	2.22	0.40
1:B:9:LEU:HD13	1:B:12:ILE:HD12	2.04	0.40
1:E:82:ILE:HG22	1:E:84:ILE:HG12	2.03	0.40
1:J:163:VAL:HG23	1:J:164:PRO:HD3	2.04	0.40
1:L:17:ARG:HG2	1:L:18:THR:HG23	2.03	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	268/292 (92%)	258 (96%)	9 (3%)	1 (0%)	30	36
1	B	258/292 (88%)	249 (96%)	9 (4%)	0	100	100
1	C	261/292 (89%)	251 (96%)	8 (3%)	2 (1%)	16	18
1	D	255/292 (87%)	247 (97%)	7 (3%)	1 (0%)	30	36
1	E	254/292 (87%)	244 (96%)	9 (4%)	1 (0%)	30	36
1	F	257/292 (88%)	247 (96%)	10 (4%)	0	100	100
1	G	249/292 (85%)	238 (96%)	11 (4%)	0	100	100
1	H	260/292 (89%)	251 (96%)	8 (3%)	1 (0%)	30	36
1	I	262/292 (90%)	251 (96%)	10 (4%)	1 (0%)	30	36
1	J	262/292 (90%)	254 (97%)	8 (3%)	0	100	100
1	K	255/292 (87%)	248 (97%)	5 (2%)	2 (1%)	16	18
1	L	256/292 (88%)	246 (96%)	10 (4%)	0	100	100
1	M	257/292 (88%)	248 (96%)	8 (3%)	1 (0%)	30	36
1	N	257/292 (88%)	248 (96%)	7 (3%)	2 (1%)	16	18
1	O	256/292 (88%)	248 (97%)	7 (3%)	1 (0%)	30	36
1	P	255/292 (87%)	248 (97%)	7 (3%)	0	100	100
All	All	4122/4672 (88%)	3976 (96%)	133 (3%)	13 (0%)	36	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	196	GLY
1	N	111	TYR
1	H	111	TYR
1	E	238	CYS
1	A	27	GLY
1	O	196	GLY
1	M	196	GLY
1	C	196	GLY
1	I	196	GLY
1	K	110	VAL
1	K	196	GLY
1	C	110	VAL
1	N	196	GLY

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	237/254 (93%)	222 (94%)	15 (6%)	16	21
1	B	231/254 (91%)	220 (95%)	11 (5%)	23	32
1	C	234/254 (92%)	221 (94%)	13 (6%)	19	25
1	D	227/254 (89%)	211 (93%)	16 (7%)	14	17
1	E	228/254 (90%)	217 (95%)	11 (5%)	23	32
1	F	231/254 (91%)	215 (93%)	16 (7%)	14	18
1	G	225/254 (89%)	211 (94%)	14 (6%)	16	21
1	H	233/254 (92%)	219 (94%)	14 (6%)	17	23
1	I	235/254 (92%)	222 (94%)	13 (6%)	19	26
1	J	234/254 (92%)	222 (95%)	12 (5%)	21	29
1	K	229/254 (90%)	215 (94%)	14 (6%)	17	22
1	L	230/254 (91%)	217 (94%)	13 (6%)	18	25
1	M	230/254 (91%)	213 (93%)	17 (7%)	13	15
1	N	231/254 (91%)	223 (96%)	8 (4%)	32	45
1	O	229/254 (90%)	217 (95%)	12 (5%)	21	28
1	P	229/254 (90%)	215 (94%)	14 (6%)	17	22
All	All	3693/4064 (91%)	3480 (94%)	213 (6%)	18	24

All (213) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	9	LEU
1	A	25	ARG
1	A	26	THR
1	A	38	MET
1	A	42	LEU
1	A	50	LEU
1	A	102	ARG

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Mol	Chain	Res	Type
1	A	103	GLU
1	A	152	ARG
1	A	242	GLU
1	A	243	GLU
1	A	248	GLU
1	A	261	VAL
1	A	282	LYS
1	B	17	ARG
1	B	38	MET
1	B	152	ARG
1	B	181	ASN
1	B	239	GLU
1	B	243	GLU
1	B	248	GLU
1	B	255	LEU
1	B	256	LYS
1	B	260	LYS
1	B	270	GLU
1	C	2	ARG
1	C	38	MET
1	C	103	GLU
1	C	140	VAL
1	C	141	ILE
1	C	152	ARG
1	C	209	LEU
1	C	241	LEU
1	C	243	GLU
1	C	255	LEU
1	C	260	LYS
1	C	264	ILE
1	C	282	LYS
1	D	1	MET
1	D	21	ARG
1	D	38	MET
1	D	42	LEU
1	D	103	GLU
1	D	107	LEU
1	D	137	LEU
1	D	152	ARG
1	D	166	MET
1	D	216	VAL
1	D	225	VAL

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Mol	Chain	Res	Type
1	D	243	GLU
1	D	245	LEU
1	D	248	GLU
1	D	260	LYS
1	D	261	VAL
1	E	16	MET
1	E	42	LEU
1	E	58	ARG
1	E	103	GLU
1	E	140	VAL
1	E	141	ILE
1	E	152	ARG
1	E	236	ASN
1	E	243	GLU
1	E	259	ARG
1	E	264	ILE
1	F	9	LEU
1	F	38	MET
1	F	50	LEU
1	F	55	VAL
1	F	60	VAL
1	F	103	GLU
1	F	140	VAL
1	F	152	ARG
1	F	188	LEU
1	F	197	LEU
1	F	199	VAL
1	F	208	LEU
1	F	243	GLU
1	F	248	GLU
1	F	260	LYS
1	F	270	GLU
1	G	53	LYS
1	G	58	ARG
1	G	140	VAL
1	G	141	ILE
1	G	152	ARG
1	G	166	MET
1	G	168	LEU
1	G	209	LEU
1	G	243	GLU
1	G	248	GLU

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Mol	Chain	Res	Type
1	G	255	LEU
1	G	260	LYS
1	G	264	ILE
1	G	282	LYS
1	H	21	ARG
1	H	38	MET
1	H	53	LYS
1	H	100	HIS
1	H	103	GLU
1	H	107	LEU
1	H	140	VAL
1	H	152	ARG
1	H	239	GLU
1	H	243	GLU
1	H	248	GLU
1	H	255	LEU
1	H	260	LYS
1	H	284	LYS
1	I	17	ARG
1	I	24	ASP
1	I	28	THR
1	I	53	LYS
1	I	103	GLU
1	I	124	ASP
1	I	140	VAL
1	I	152	ARG
1	I	243	GLU
1	I	260	LYS
1	I	264	ILE
1	I	268	LYS
1	I	282	LYS
1	J	24	ASP
1	J	28	THR
1	J	38	MET
1	J	68	VAL
1	J	103	GLU
1	J	107	LEU
1	J	140	VAL
1	J	152	ARG
1	J	195	MET
1	J	243	GLU
1	J	260	LYS

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Mol	Chain	Res	Type
1	J	270	GLU
1	K	38	MET
1	K	60	VAL
1	K	79	GLU
1	K	84	ILE
1	K	103	GLU
1	K	140	VAL
1	K	141	ILE
1	K	152	ARG
1	K	243	GLU
1	K	248	GLU
1	K	260	LYS
1	K	263	ASN
1	K	264	ILE
1	K	282	LYS
1	L	46	ILE
1	L	49	LEU
1	L	53	LYS
1	L	77	LEU
1	L	140	VAL
1	L	146	ASN
1	L	152	ARG
1	L	184	LEU
1	L	188	LEU
1	L	210	THR
1	L	239	GLU
1	L	243	GLU
1	L	260	LYS
1	M	38	MET
1	M	58	ARG
1	M	103	GLU
1	M	127	THR
1	M	140	VAL
1	M	141	ILE
1	M	152	ARG
1	M	163	VAL
1	M	165	LYS
1	M	184	LEU
1	M	188	LEU
1	M	219	LEU
1	M	243	GLU
1	M	248	GLU

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Mol	Chain	Res	Type
1	M	260	LYS
1	M	264	ILE
1	M	282	LYS
1	N	38	MET
1	N	140	VAL
1	N	152	ARG
1	N	161	VAL
1	N	243	GLU
1	N	248	GLU
1	N	286	GLU
1	N	287	MET
1	O	33	MET
1	O	38	MET
1	O	42	LEU
1	O	44	ASP
1	O	53	LYS
1	O	103	GLU
1	O	140	VAL
1	O	152	ARG
1	O	165	LYS
1	O	243	GLU
1	O	248	GLU
1	O	260	LYS
1	P	33	MET
1	P	38	MET
1	P	42	LEU
1	P	50	LEU
1	P	79	GLU
1	P	103	GLU
1	P	140	VAL
1	P	141	ILE
1	P	152	ARG
1	P	184	LEU
1	P	188	LEU
1	P	194	ASP
1	P	241	LEU
1	P	243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	GLN

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Mol	Chain	Res	Type
1	A	187	GLN
1	A	202	ASN
1	A	236	ASN
1	A	244	GLN
1	B	114	GLN
1	B	146	ASN
1	B	159	ASN
1	B	236	ASN
1	B	244	GLN
1	C	37	GLN
1	C	78	GLN
1	C	187	GLN
1	C	202	ASN
1	C	236	ASN
1	C	263	ASN
1	D	78	GLN
1	D	138	GLN
1	D	146	ASN
1	D	202	ASN
1	E	78	GLN
1	E	181	ASN
1	E	232	HIS
1	F	37	GLN
1	F	114	GLN
1	F	146	ASN
1	F	159	ASN
1	F	181	ASN
1	F	187	GLN
1	F	232	HIS
1	F	244	GLN
1	G	117	HIS
1	G	138	GLN
1	G	202	ASN
1	G	232	HIS
1	H	78	GLN
1	H	114	GLN
1	H	146	ASN
1	H	159	ASN
1	H	181	ASN
1	I	138	GLN
1	I	187	GLN
1	I	263	ASN

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Mol	Chain	Res	Type
1	J	37	GLN
1	J	181	ASN
1	J	187	GLN
1	K	114	GLN
1	K	139	GLN
1	K	146	ASN
1	K	159	ASN
1	K	232	HIS
1	K	244	GLN
1	L	37	GLN
1	L	187	GLN
1	M	37	GLN
1	M	187	GLN
1	N	20	ASN
1	N	146	ASN
1	O	37	GLN
1	O	78	GLN
1	O	146	ASN
1	O	187	GLN
1	O	232	HIS
1	O	236	ASN
1	O	263	ASN
1	P	132	GLN
1	P	236	ASN
1	P	244	GLN
1	P	263	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 oligosaccharides in this entry.

5.6 Ligand geometry

18 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	A	301	-	4,4,4	0.29	0	6,6,6	0.27	0
2	SO4	F	301	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	E	301	-	4,4,4	0.26	0	6,6,6	0.14	0
2	SO4	G	301	-	4,4,4	0.22	0	6,6,6	0.14	0
2	SO4	G	302	-	4,4,4	0.27	0	6,6,6	0.34	0
2	SO4	I	301	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	C	301	-	4,4,4	0.20	0	6,6,6	0.35	0
2	SO4	M	301	-	4,4,4	0.52	0	6,6,6	0.26	0
2	SO4	O	301	-	4,4,4	0.35	0	6,6,6	0.28	0
2	SO4	L	301	-	4,4,4	0.32	0	6,6,6	0.30	0
2	SO4	D	301	-	4,4,4	0.48	0	6,6,6	0.25	0
2	SO4	J	302	-	4,4,4	0.26	0	6,6,6	0.50	0
2	SO4	C	302	-	4,4,4	0.35	0	6,6,6	0.42	0
2	SO4	P	301	-	4,4,4	0.19	0	6,6,6	0.16	0
2	SO4	J	301	-	4,4,4	0.43	0	6,6,6	0.71	0
2	SO4	N	301	-	4,4,4	0.25	0	6,6,6	0.19	0
2	SO4	A	302	-	4,4,4	0.30	0	6,6,6	0.39	0
2	SO4	K	301	-	4,4,4	0.24	0	6,6,6	0.33	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

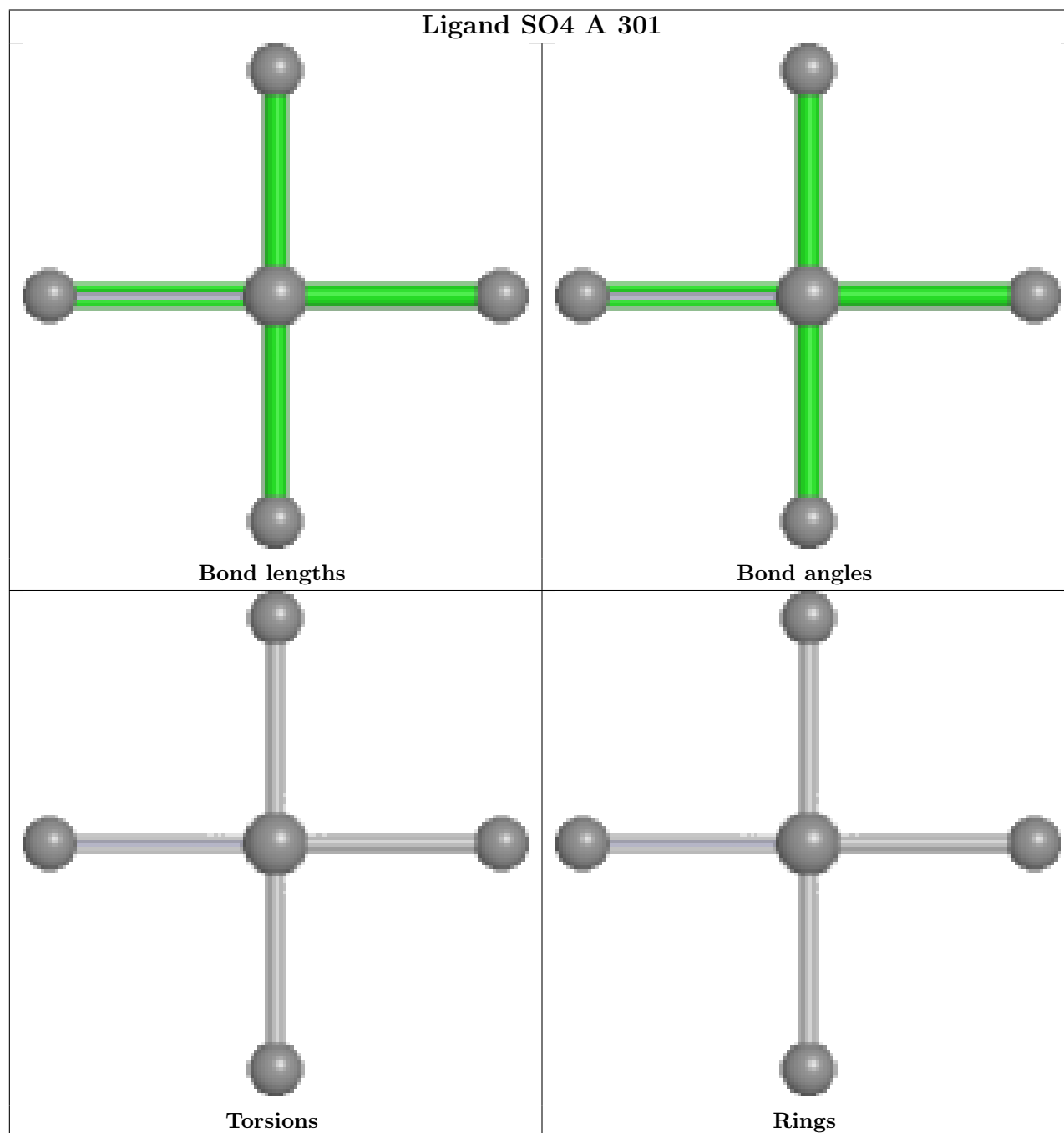
There are no torsion outliers.

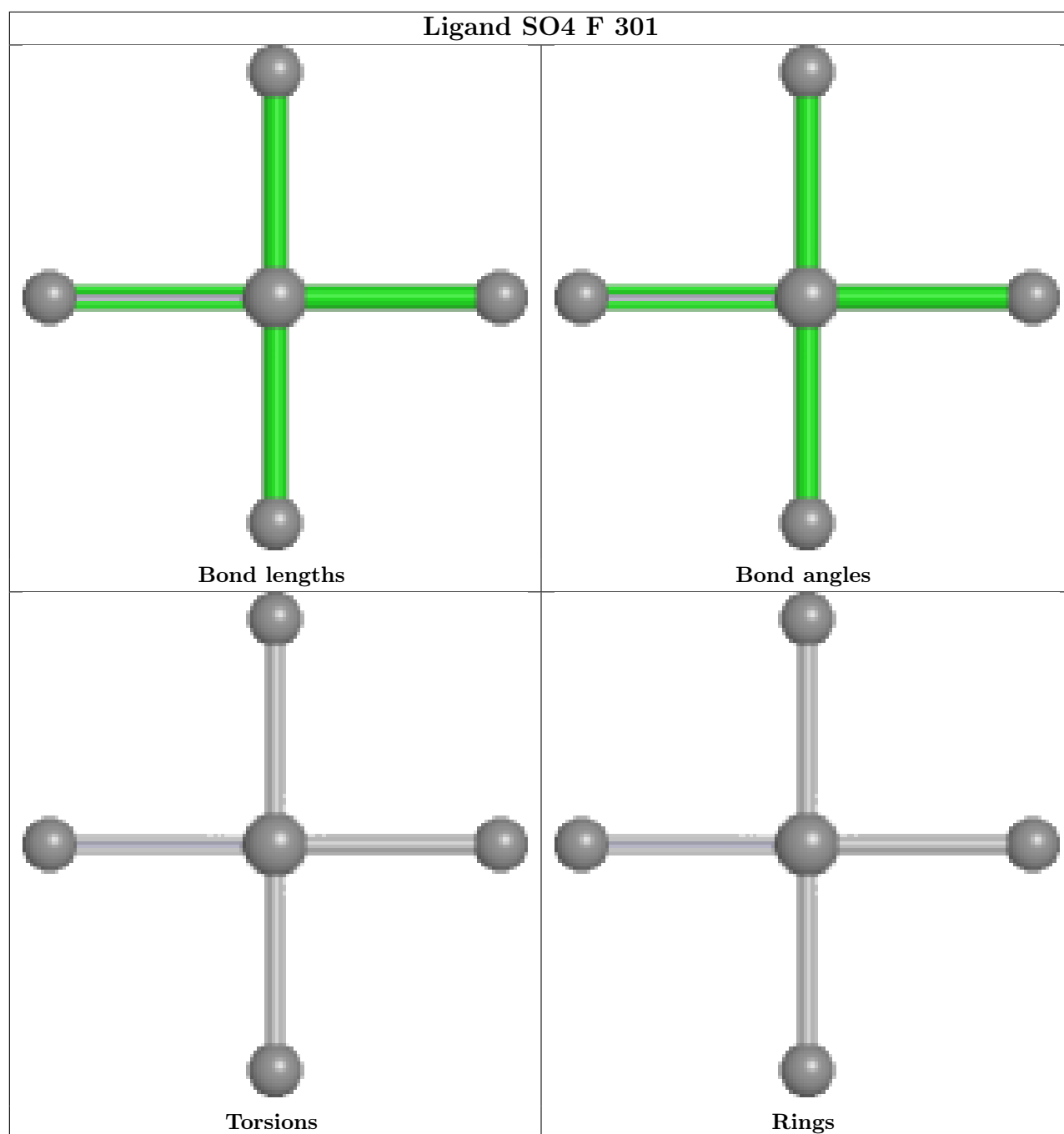
There are no ring outliers.

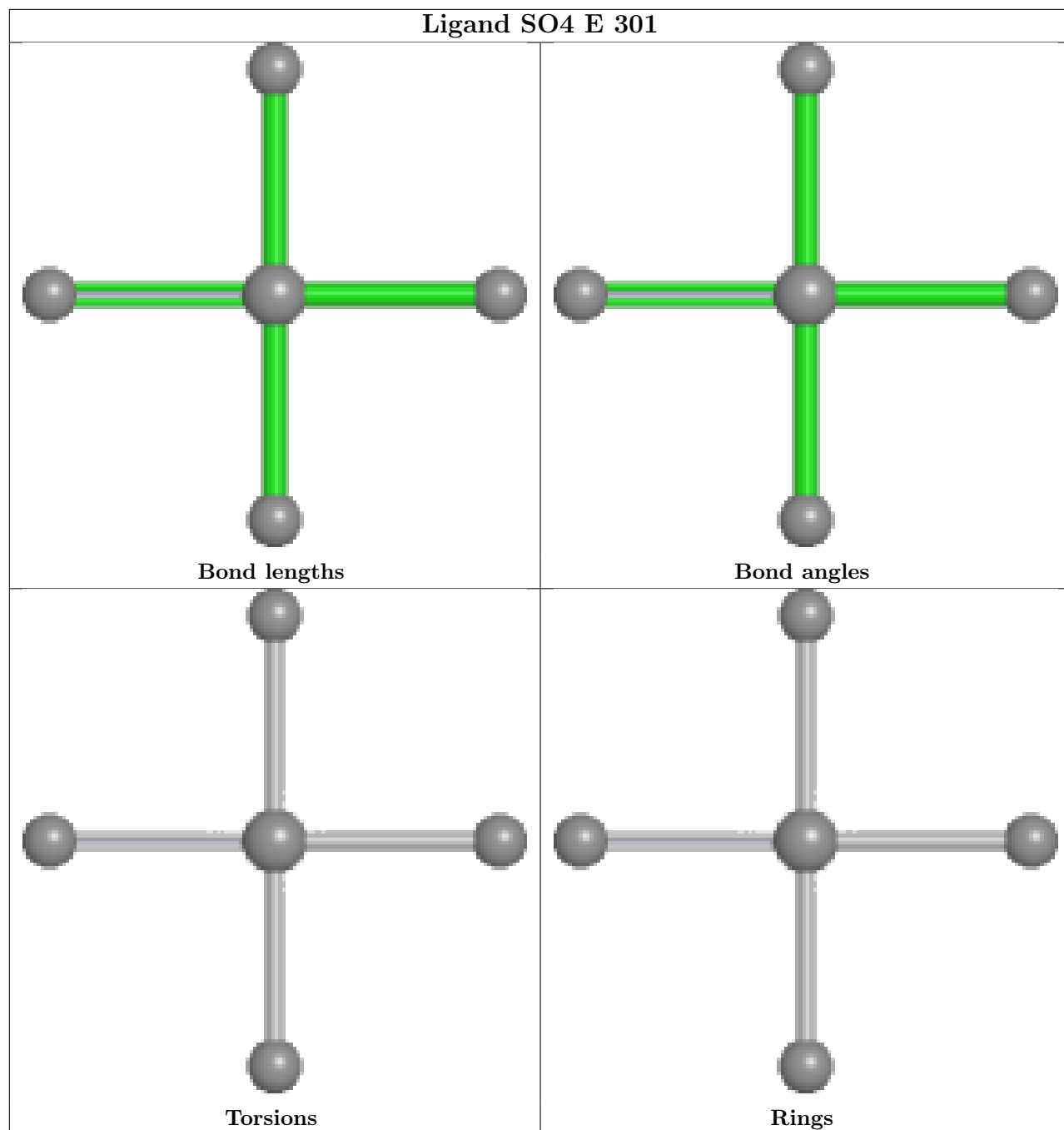
No monomer is involved in short contacts.

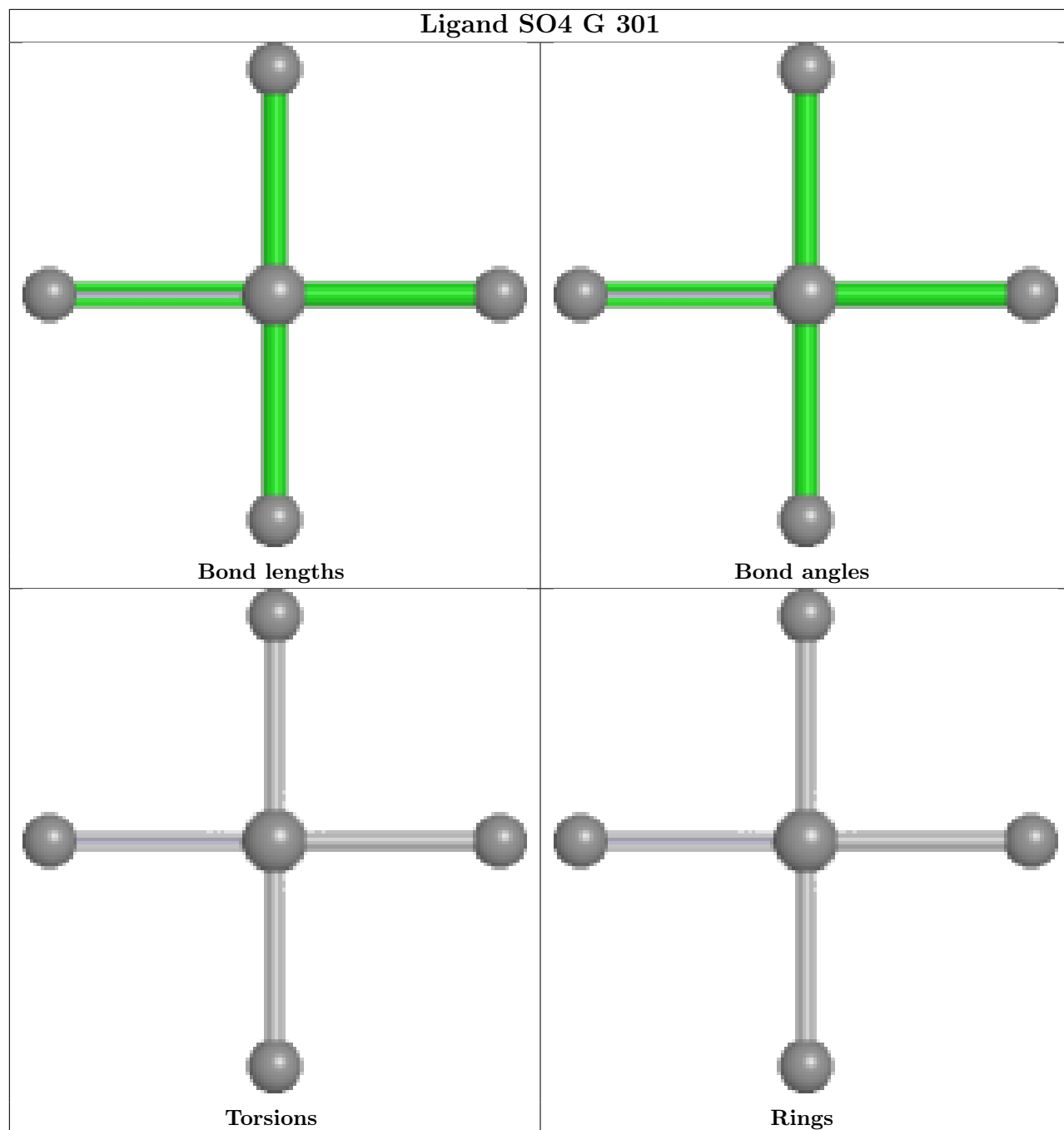
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is

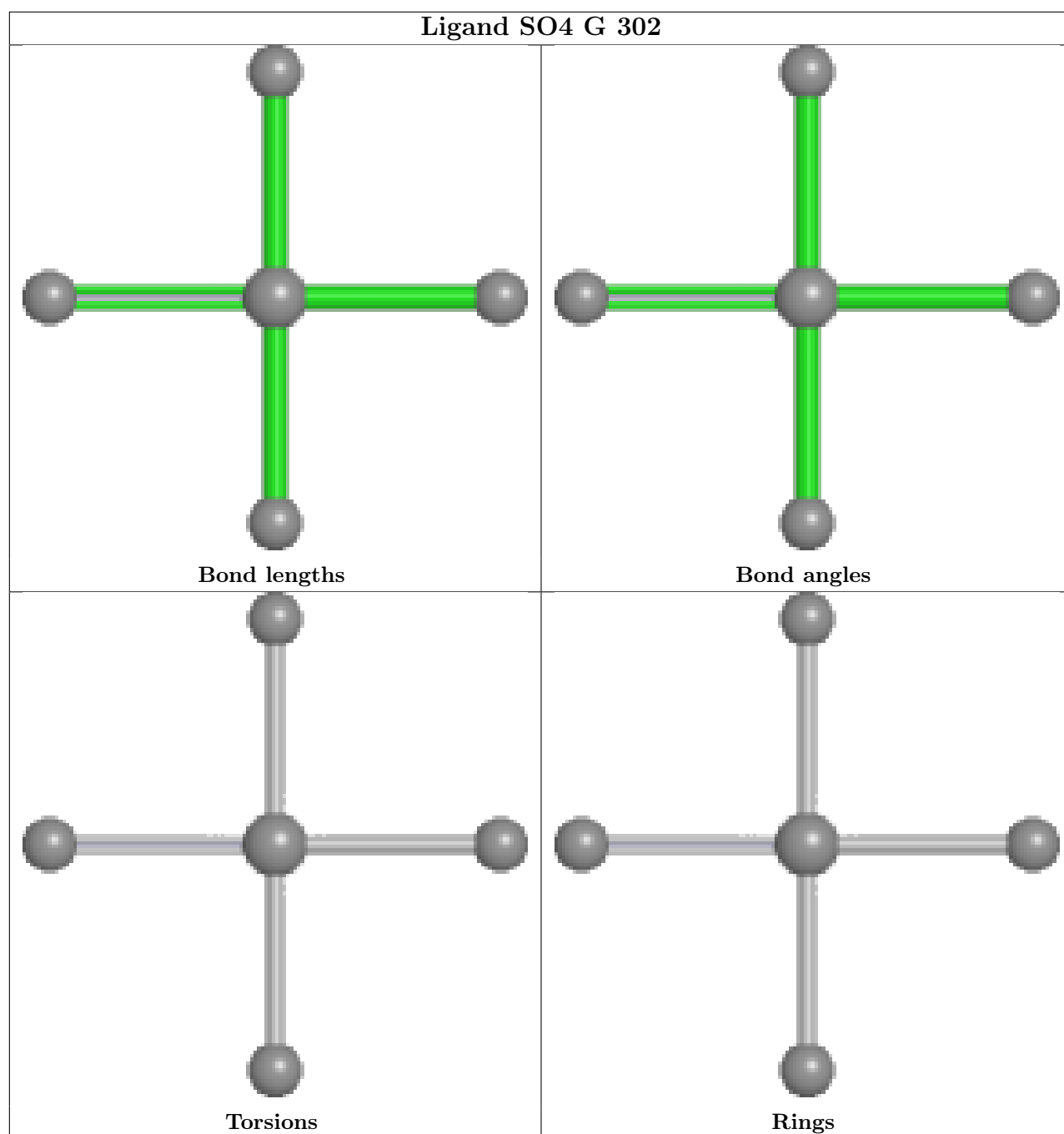
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

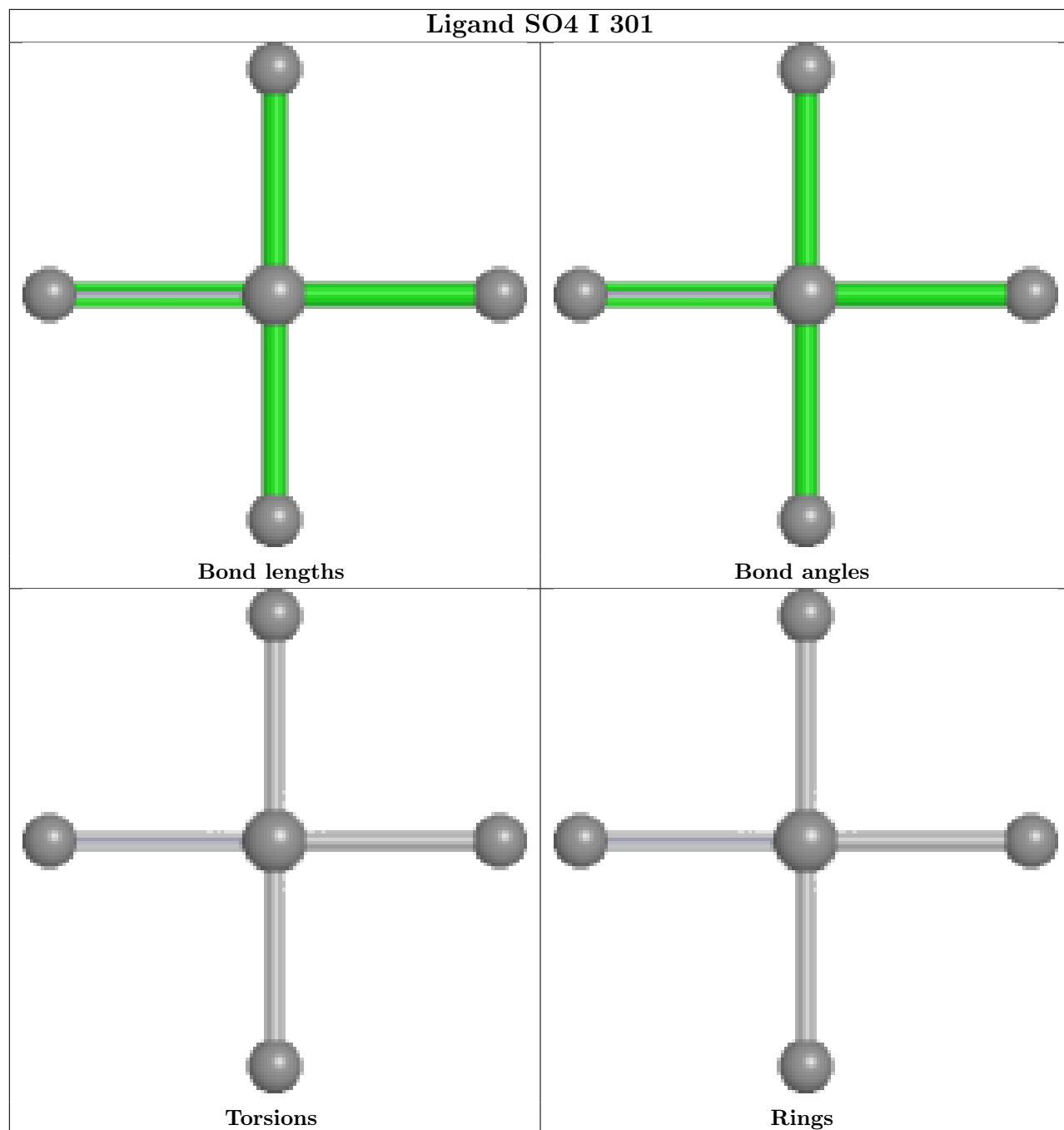


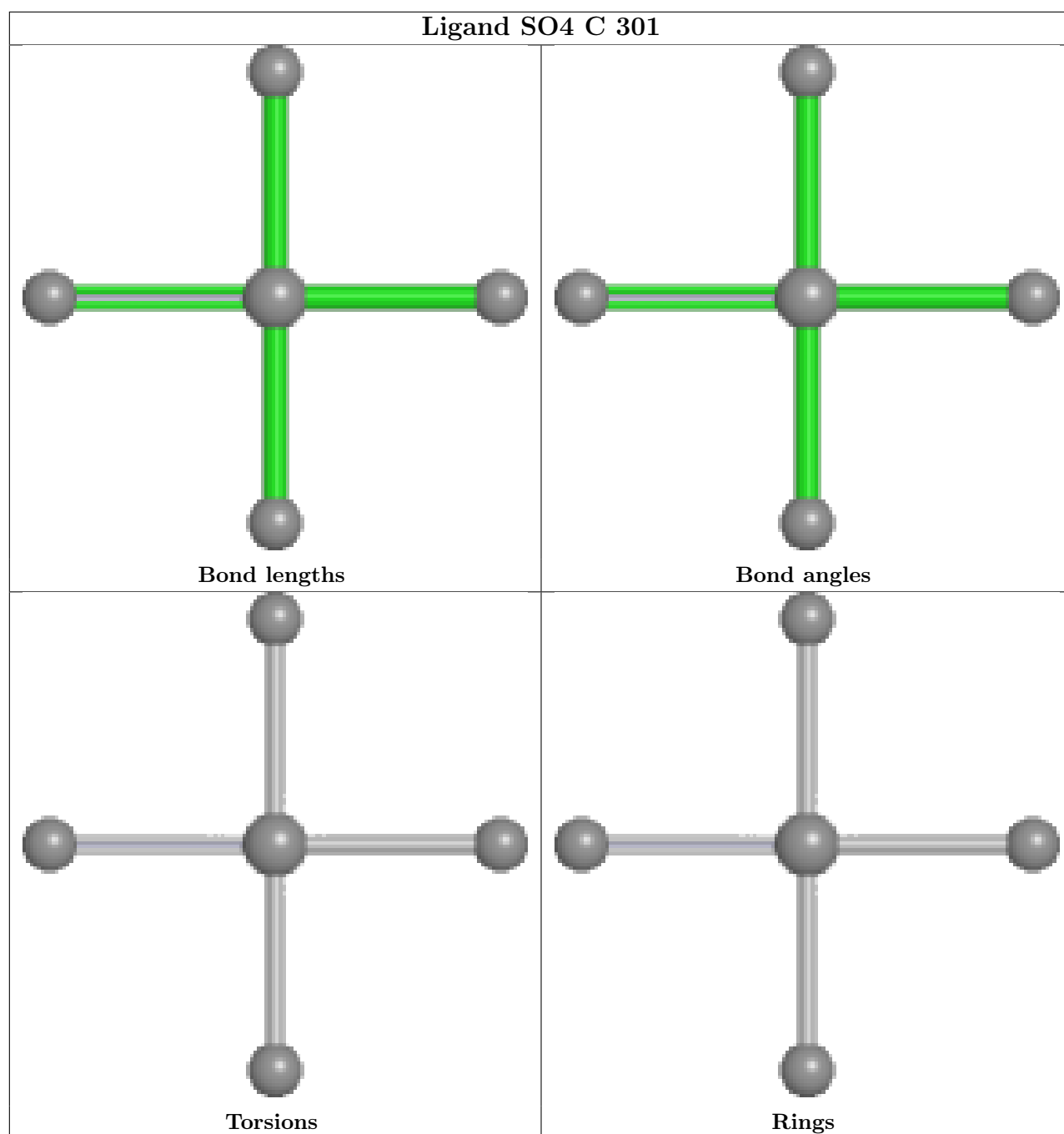


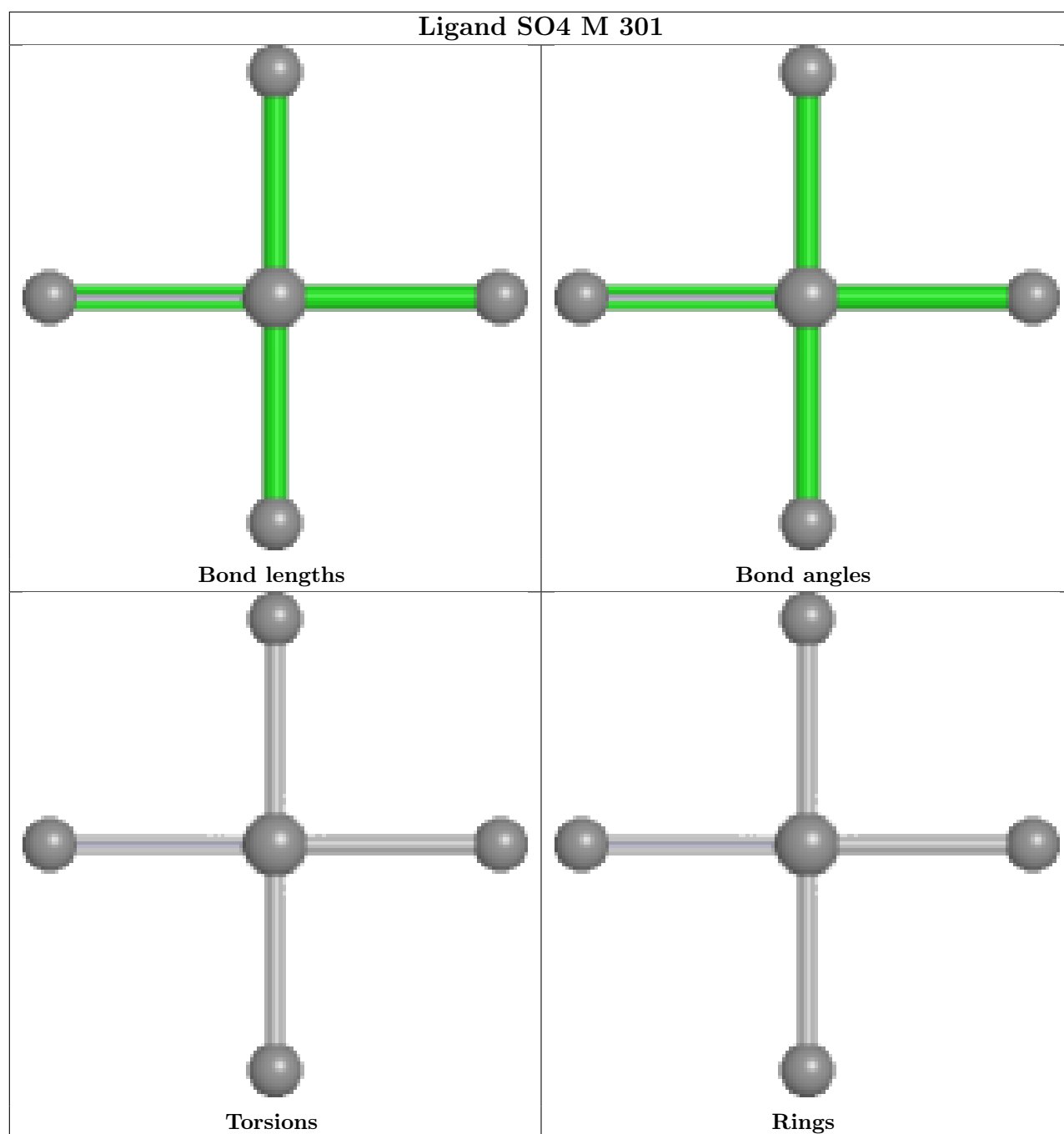


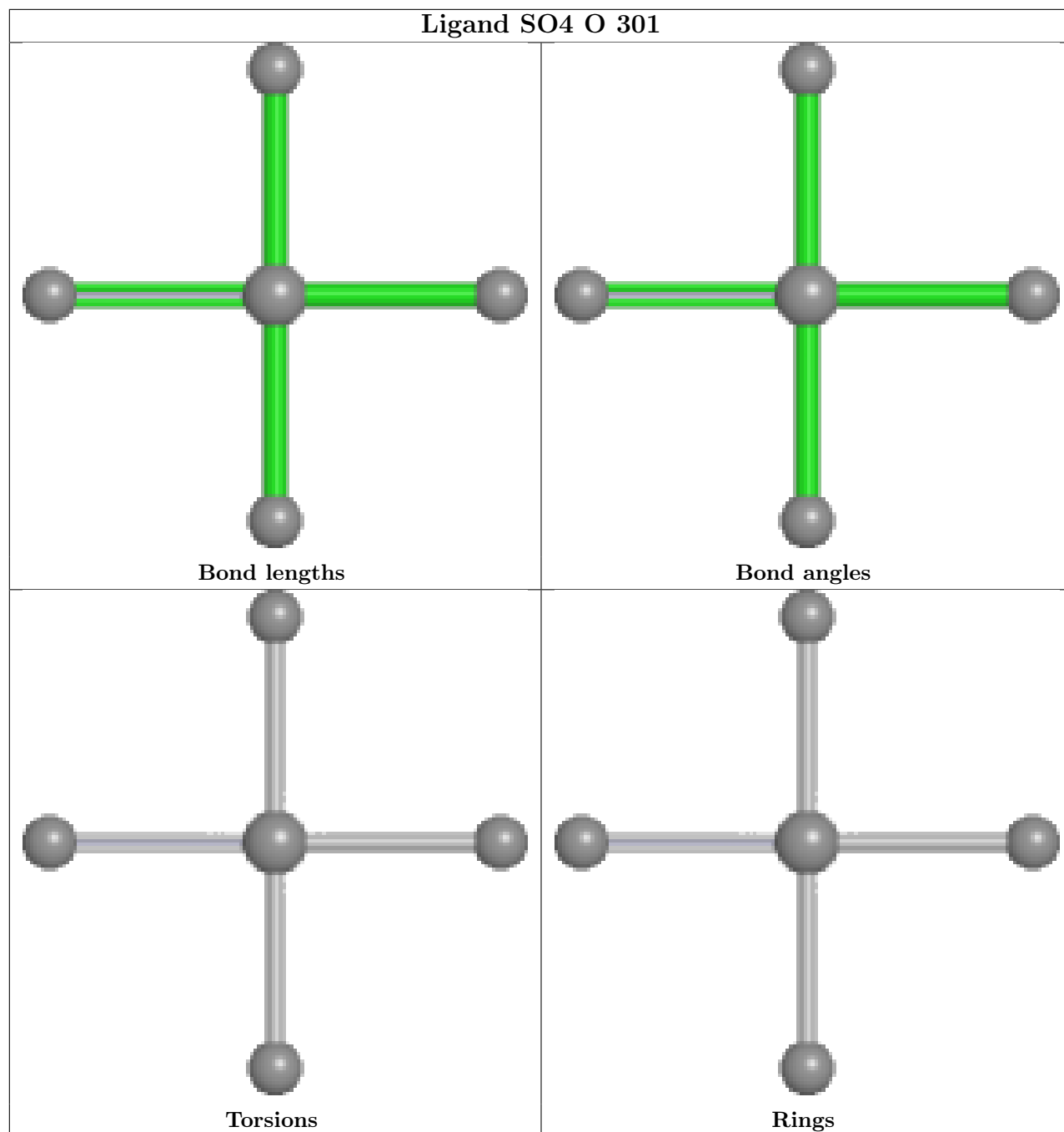


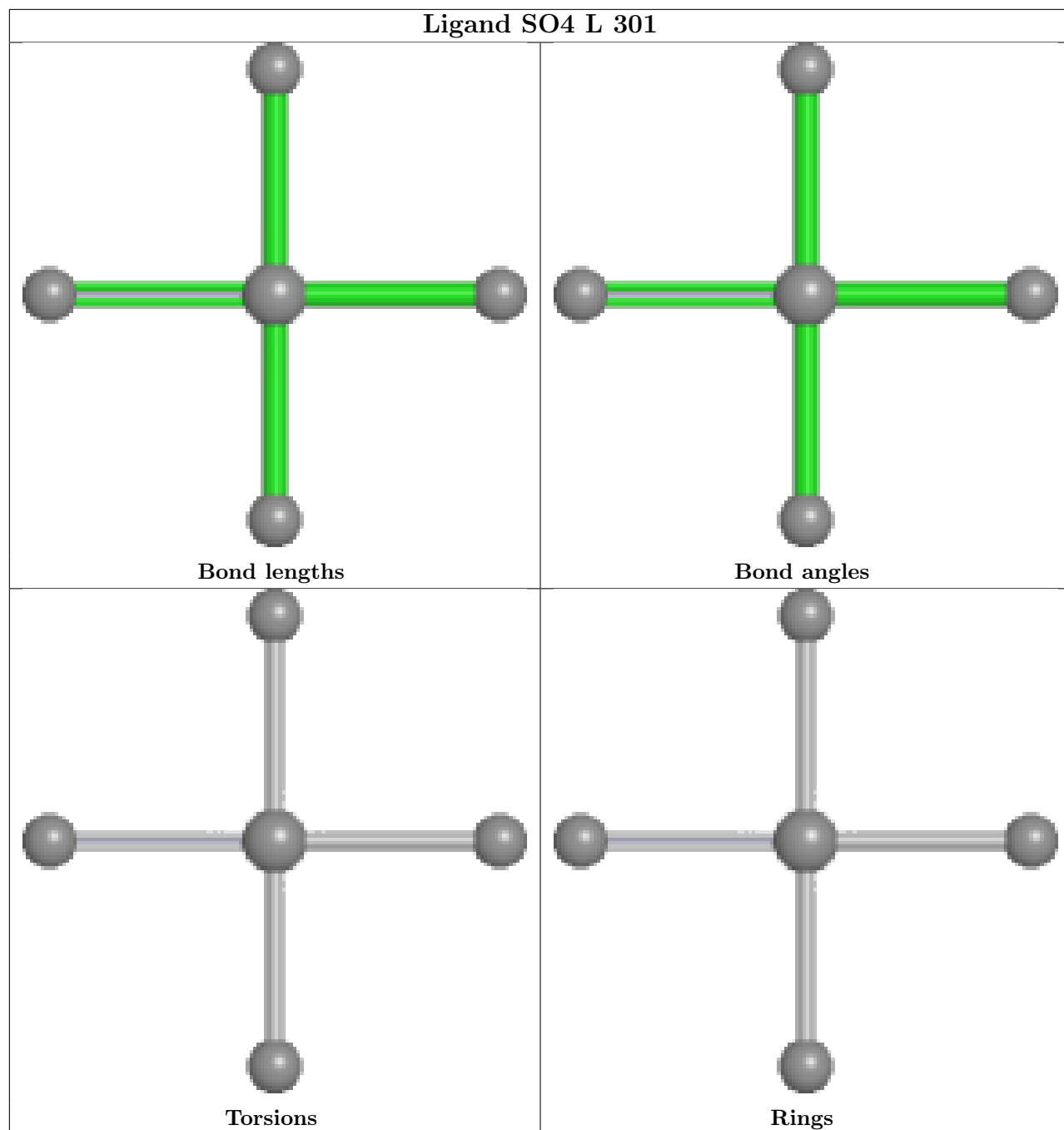


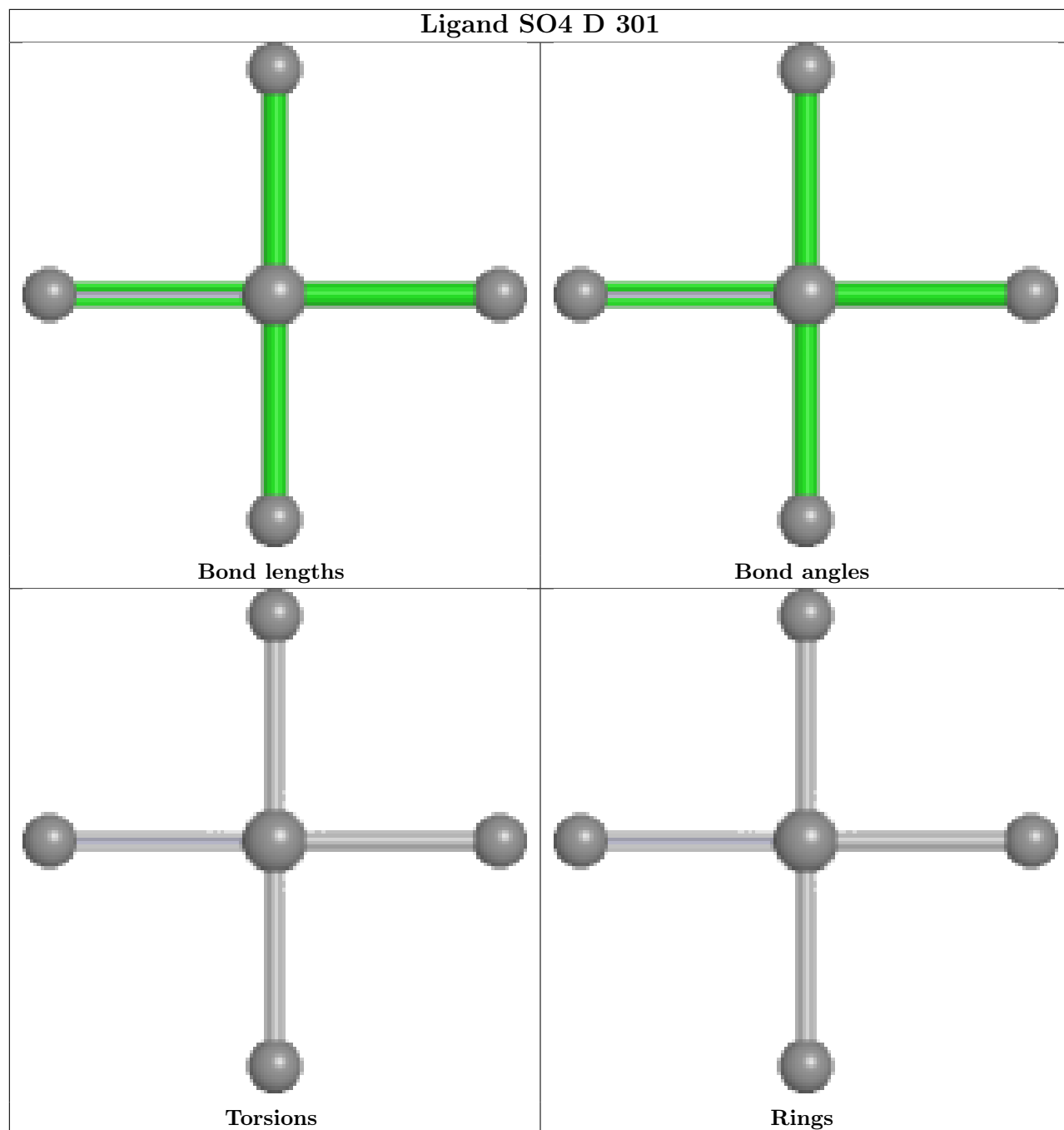


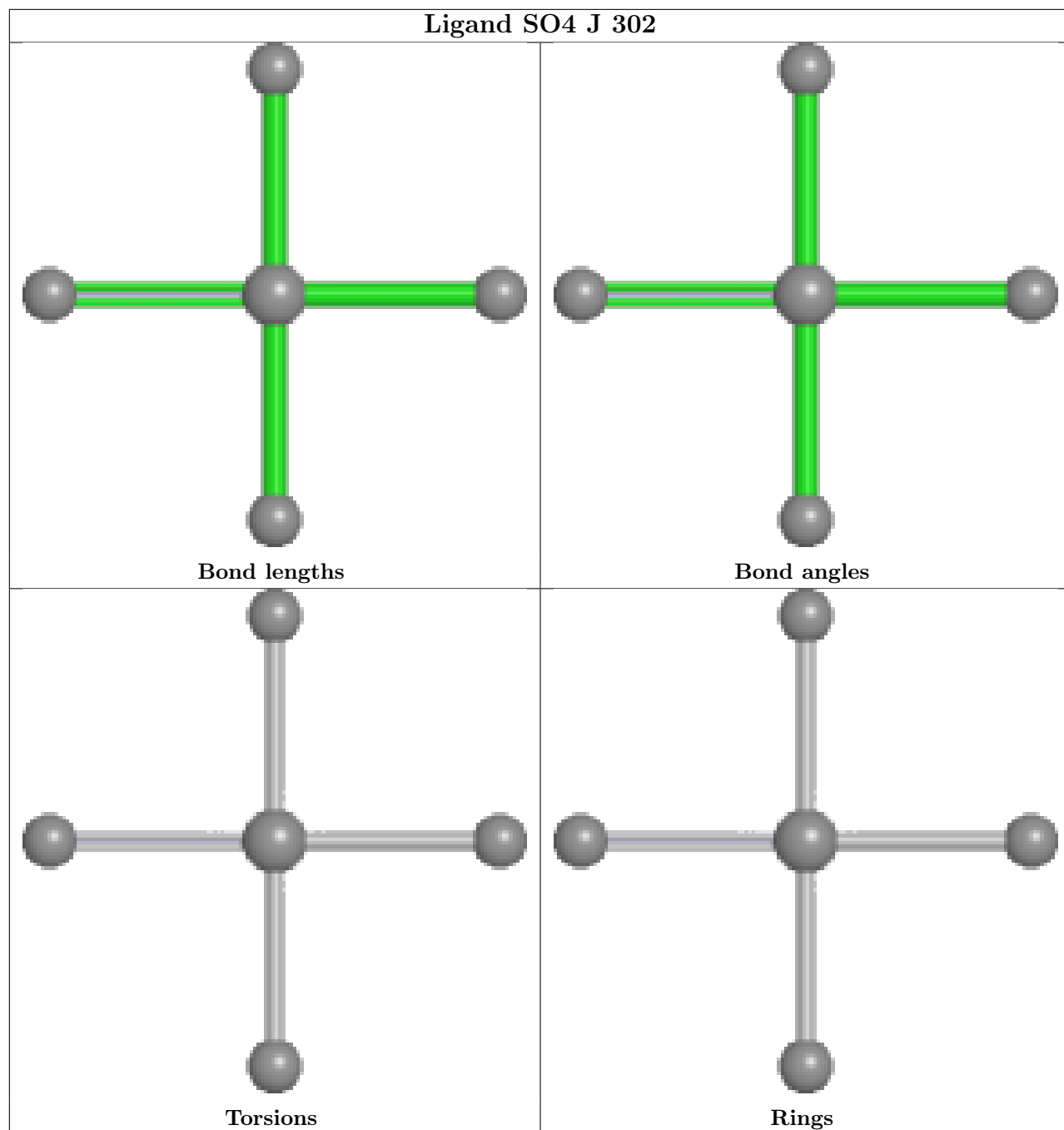


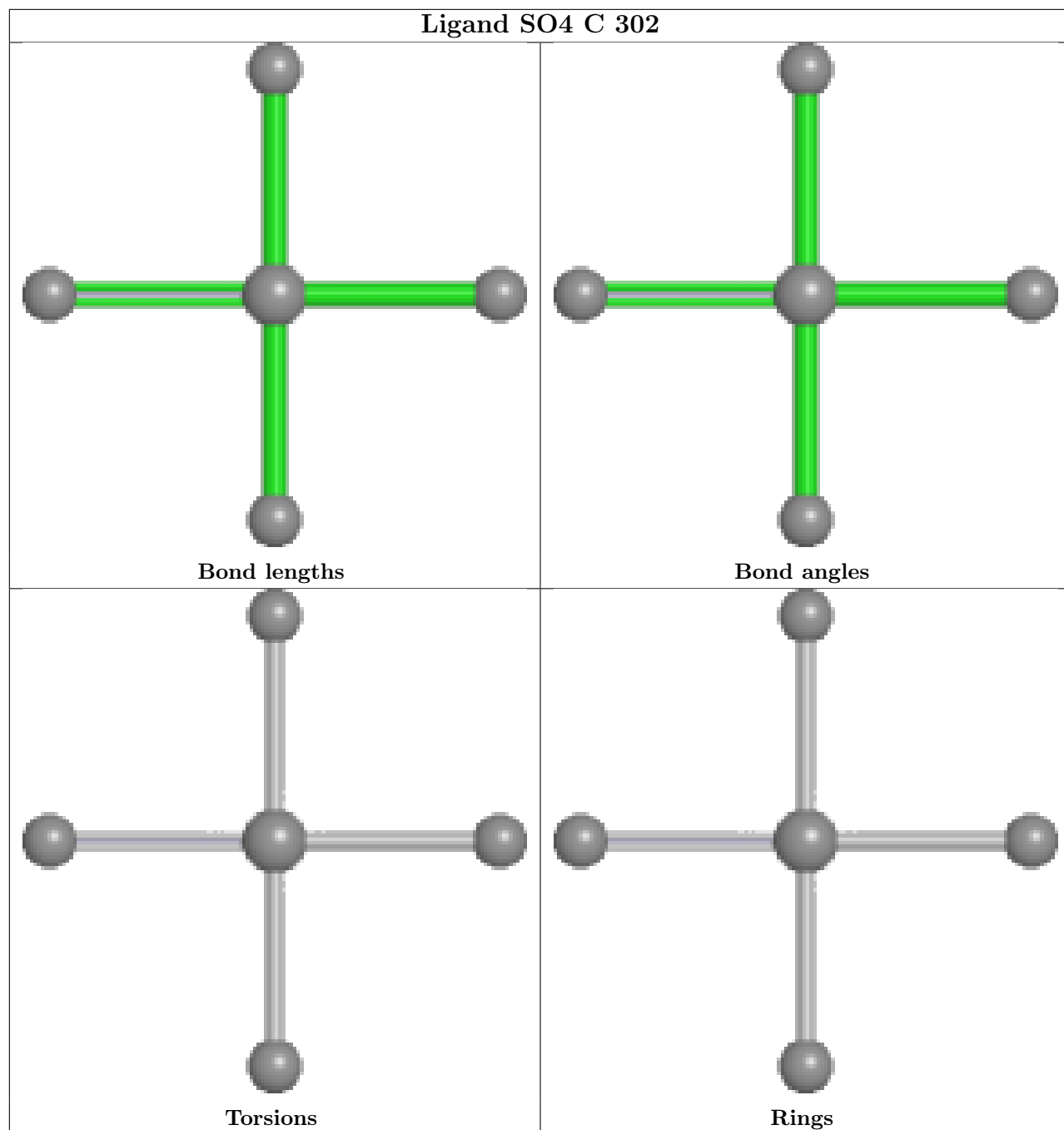


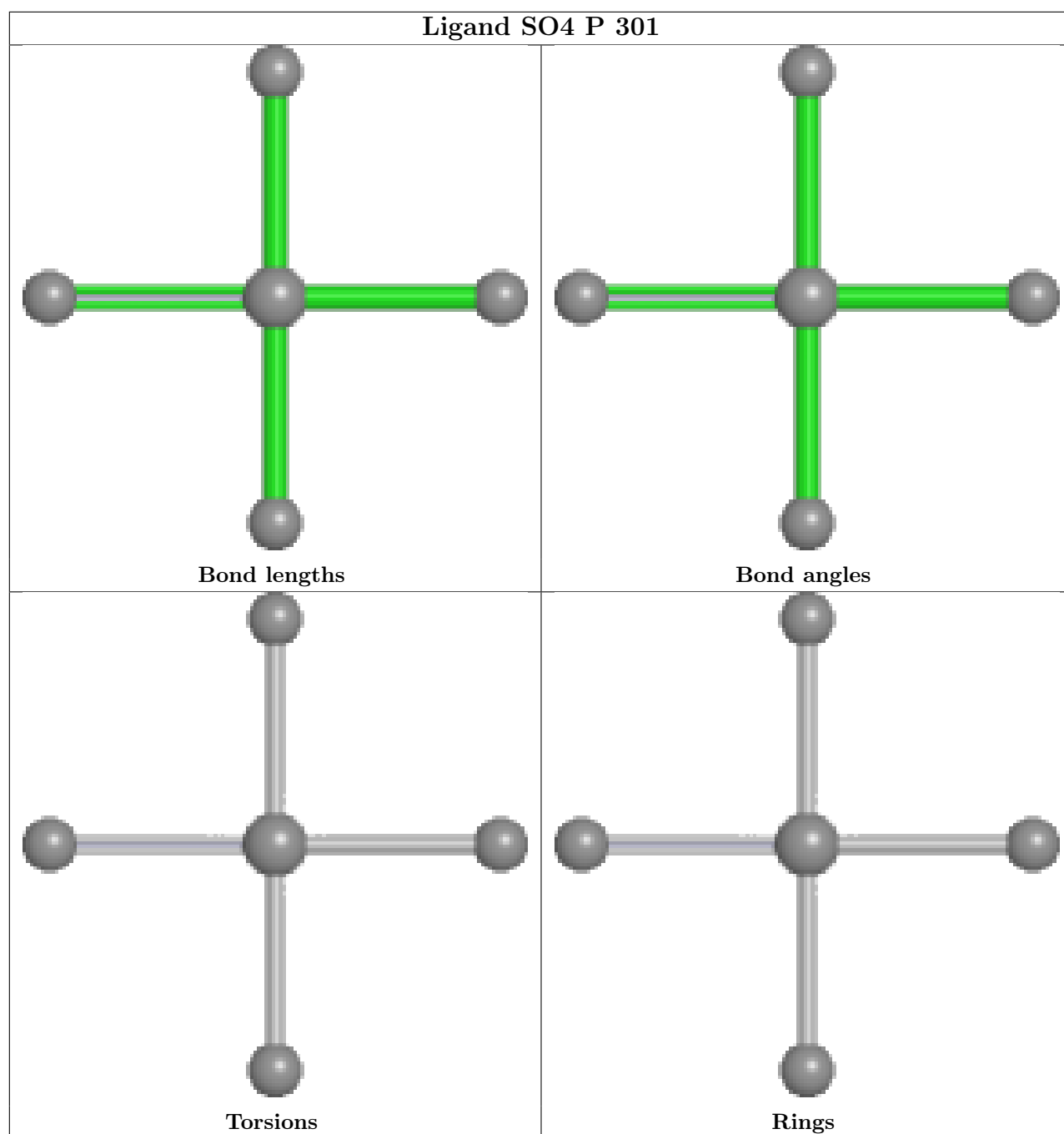


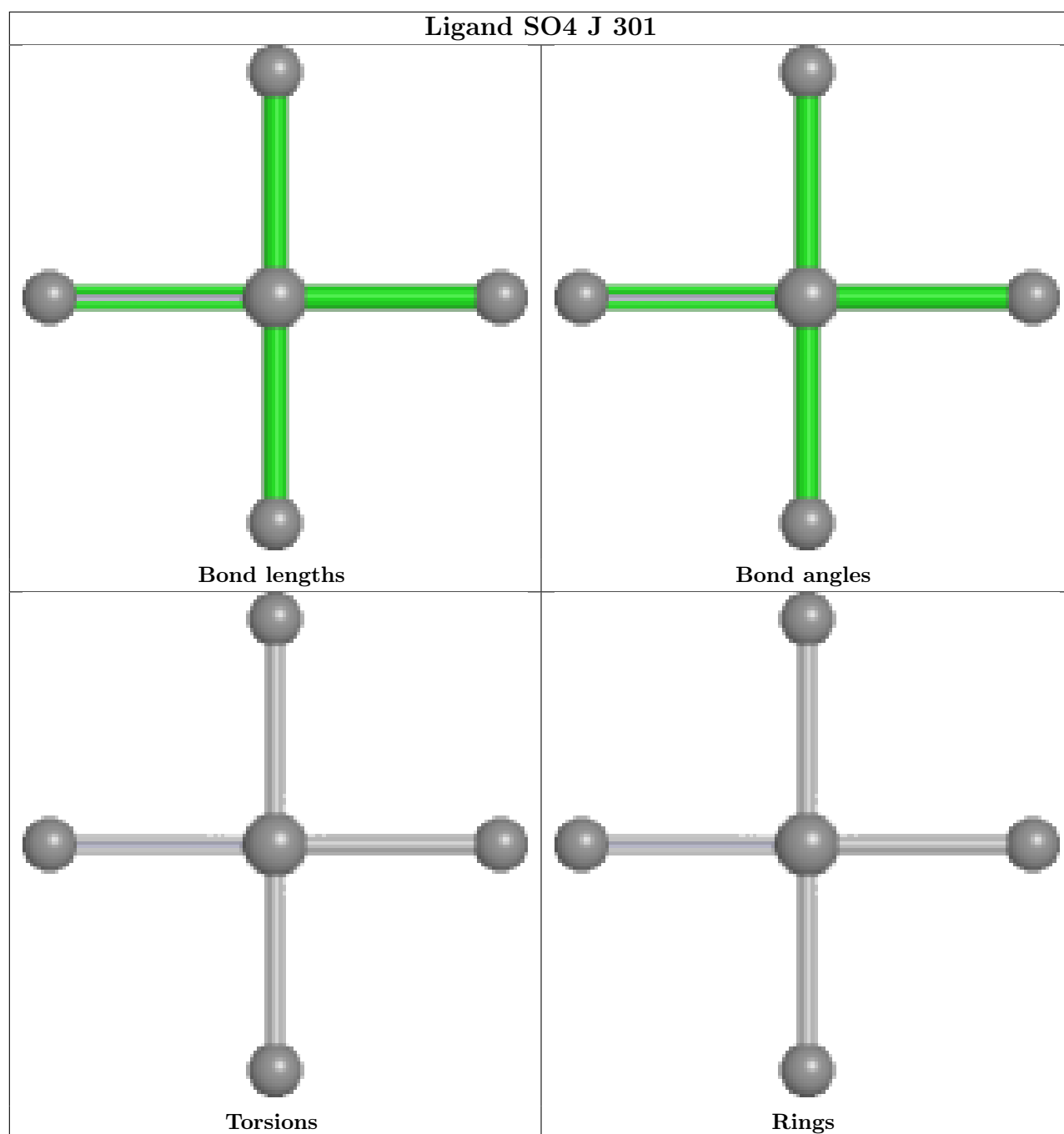


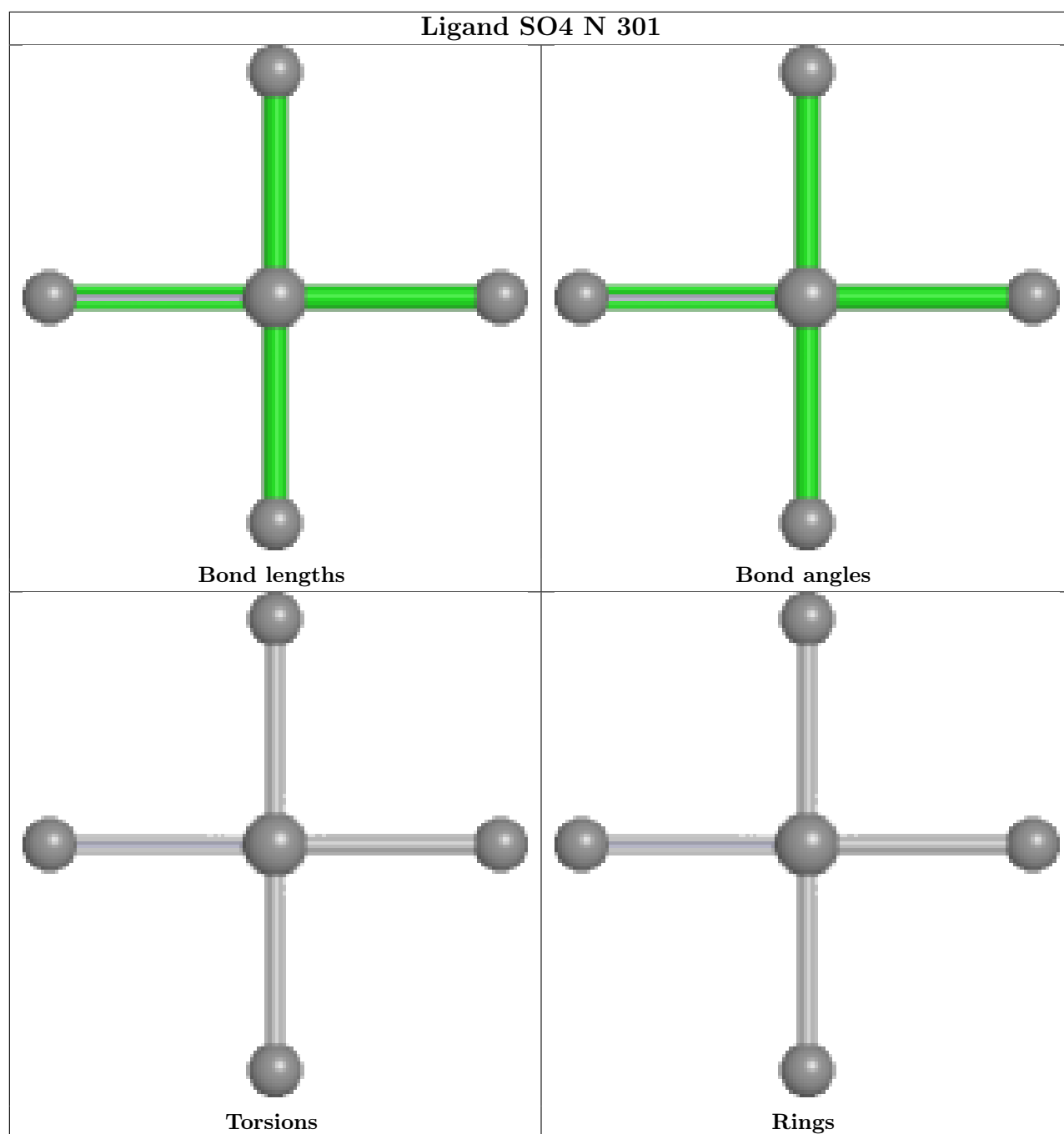


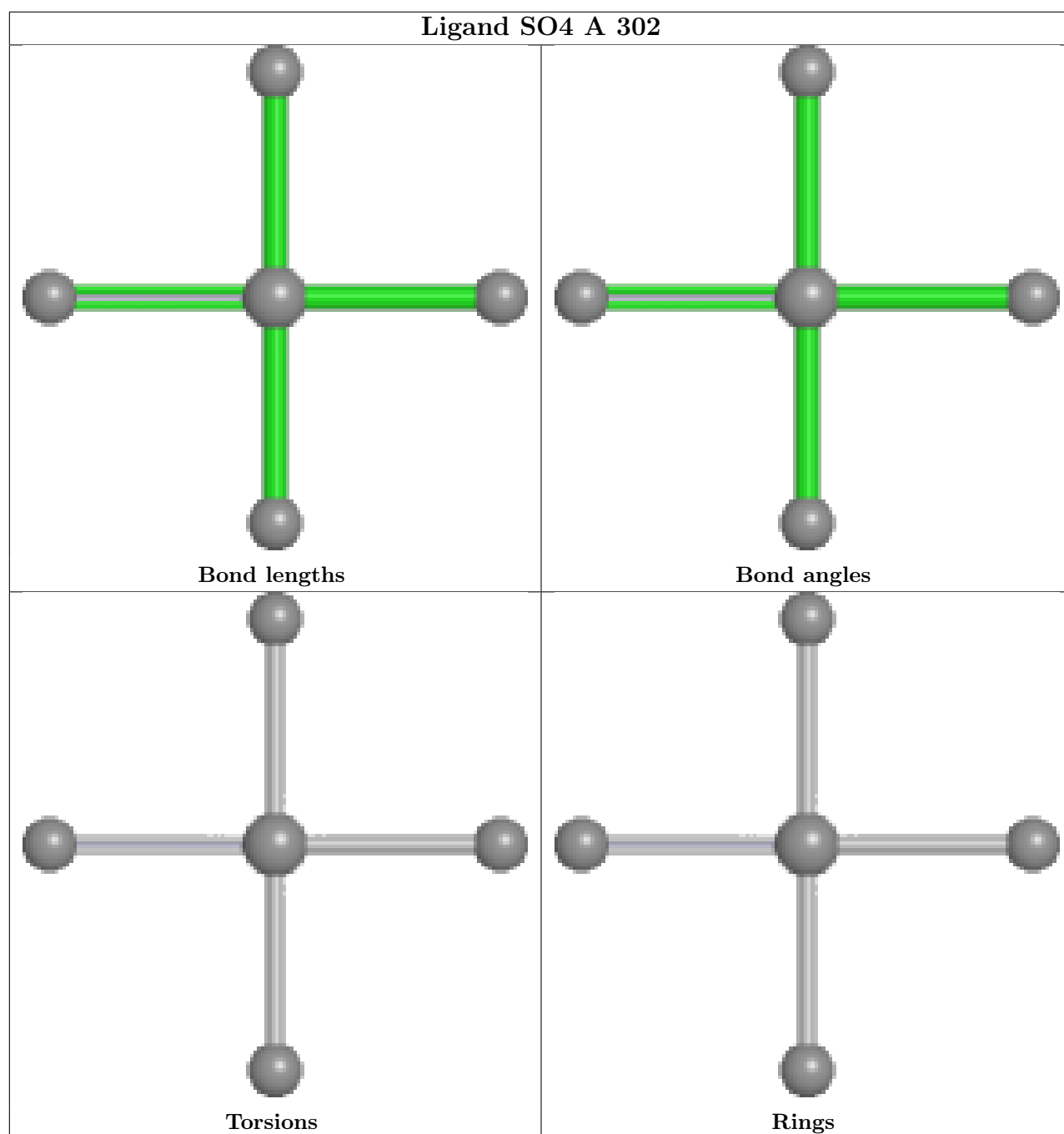


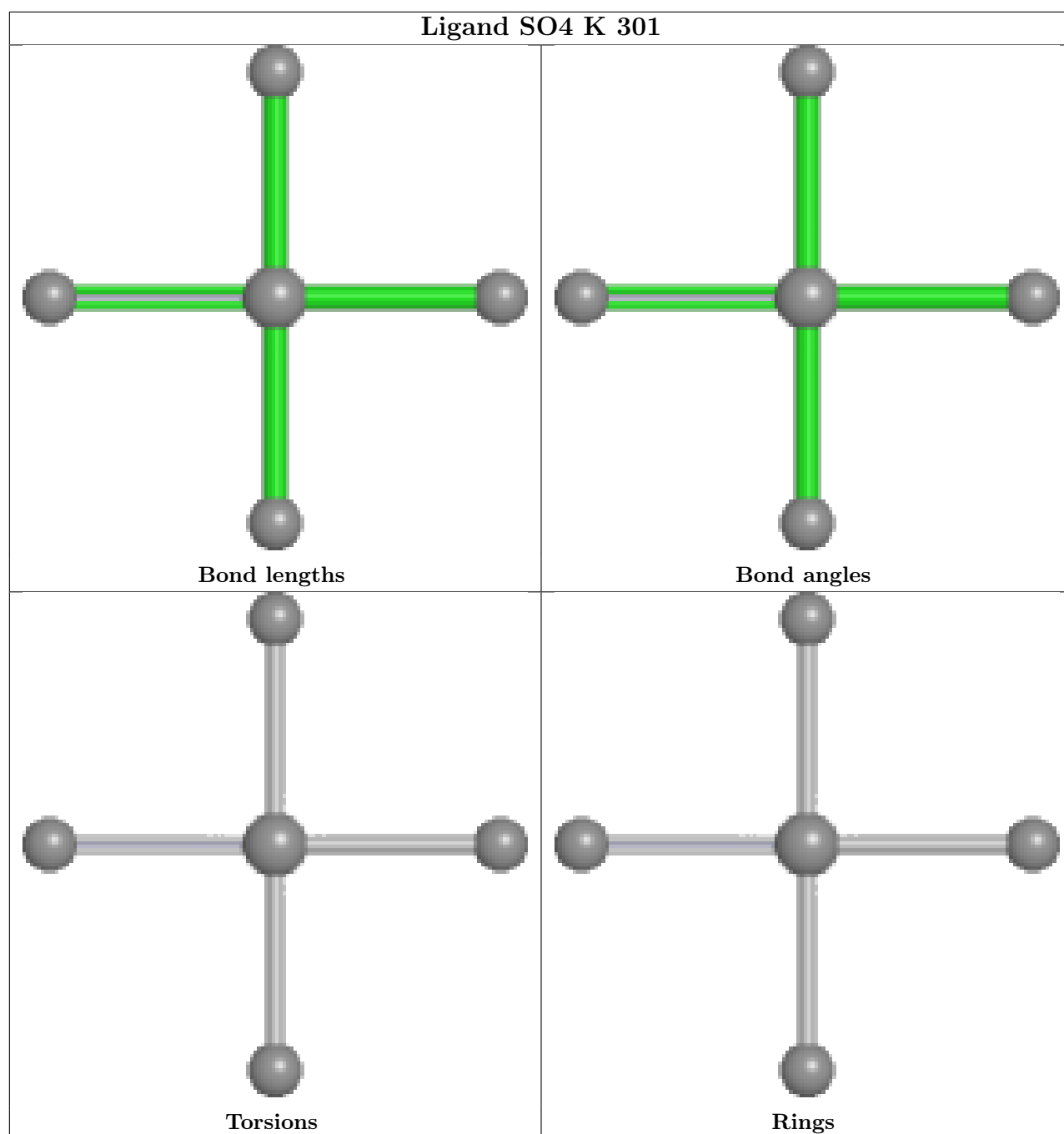












5.7 Other polymers [i](#)

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	272/292 (93%)	-0.76	0	100	100	13, 35, 63, 81	0
1	B	264/292 (90%)	-0.86	0	100	100	16, 32, 55, 85	0
1	C	267/292 (91%)	-0.67	0	100	100	20, 37, 71, 97	0
1	D	261/292 (89%)	-0.62	0	100	100	17, 40, 73, 91	0
1	E	260/292 (89%)	-0.40	0	100	100	22, 45, 78, 117	0
1	F	263/292 (90%)	-0.77	0	100	100	18, 36, 63, 89	0
1	G	255/292 (87%)	-0.67	0	100	100	19, 41, 69, 84	0
1	H	266/292 (91%)	-0.83	0	100	100	18, 36, 60, 78	0
1	I	267/292 (91%)	-0.73	1 (0%)	88	89	18, 38, 65, 85	1 (0%)
1	J	268/292 (91%)	-0.90	0	100	100	16, 31, 56, 80	0
1	K	261/292 (89%)	-0.56	1 (0%)	88	89	18, 41, 79, 105	0
1	L	262/292 (89%)	-0.69	0	100	100	20, 41, 65, 88	0
1	M	263/292 (90%)	-0.76	0	100	100	19, 39, 67, 93	0
1	N	263/292 (90%)	-0.83	0	100	100	20, 37, 60, 79	0
1	O	262/292 (89%)	-0.70	0	100	100	20, 40, 67, 87	0
1	P	261/292 (89%)	-0.81	1 (0%)	88	89	17, 34, 62, 84	0
All	All	4215/4672 (90%)	-0.72	3 (0%)	92	92	13, 38, 68, 117	1 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	P	87	GLY	2.4
1	I	240	ALA	2.3
1	K	251	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

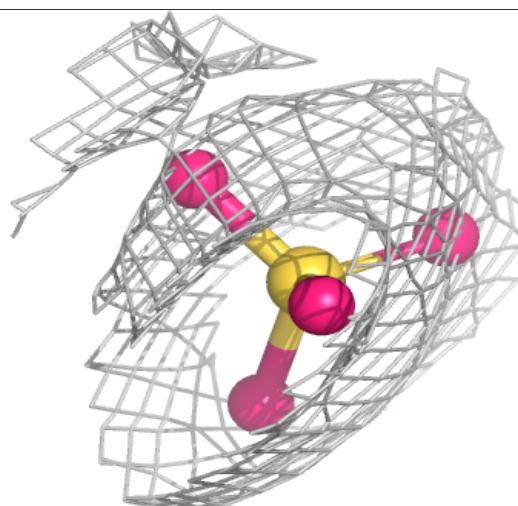
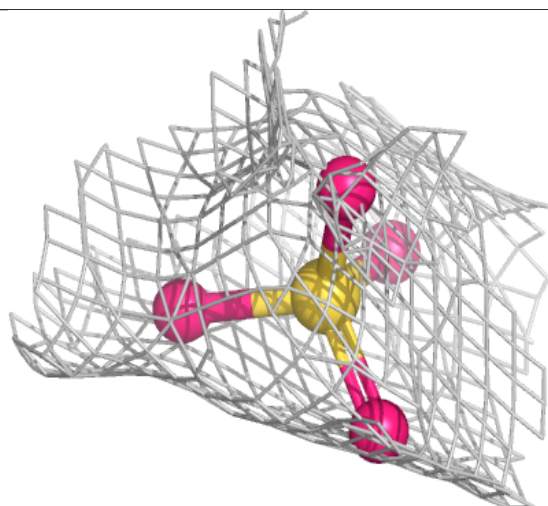
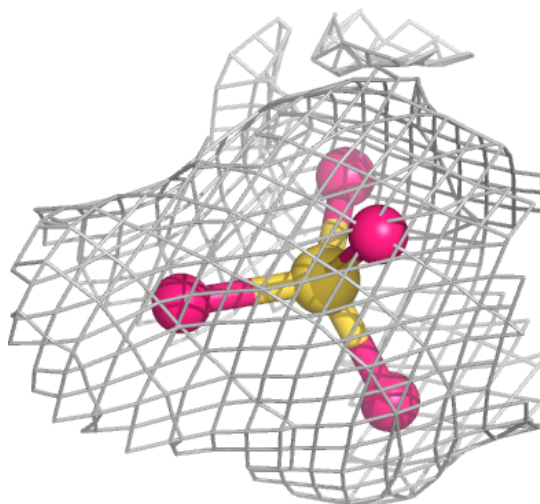
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.98	0.06	64,65,65,67	0
2	SO4	N	301	5/5	0.98	0.06	71,71,73,74	0
2	SO4	O	301	5/5	0.98	0.07	56,56,57,60	0
2	SO4	P	301	5/5	0.98	0.06	39,43,44,46	0
2	SO4	D	301	5/5	0.99	0.05	41,42,44,45	0
2	SO4	E	301	5/5	0.99	0.07	36,36,38,42	0
2	SO4	A	301	5/5	0.99	0.04	43,44,46,48	0
2	SO4	G	301	5/5	0.99	0.04	46,46,47,48	0
2	SO4	G	302	5/5	0.99	0.05	40,41,43,45	0
2	SO4	I	301	5/5	0.99	0.06	34,38,39,42	0
2	SO4	J	301	5/5	0.99	0.05	31,34,39,39	0
2	SO4	J	302	5/5	0.99	0.05	34,35,38,42	0
2	SO4	K	301	5/5	0.99	0.04	40,41,41,43	0
2	SO4	L	301	5/5	0.99	0.06	57,57,58,61	0
2	SO4	M	301	5/5	0.99	0.05	33,35,39,44	0
2	SO4	A	302	5/5	0.99	0.07	41,42,42,43	0
2	SO4	C	301	5/5	0.99	0.04	32,32,34,37	0
2	SO4	C	302	5/5	0.99	0.05	40,42,46,48	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.

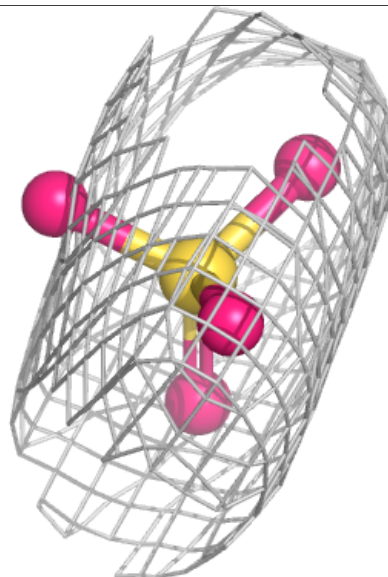
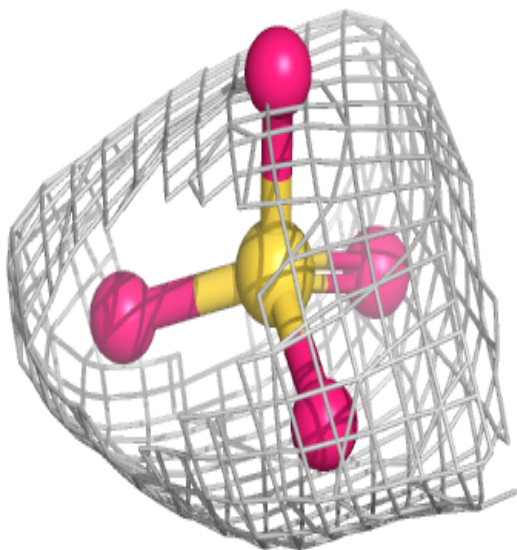
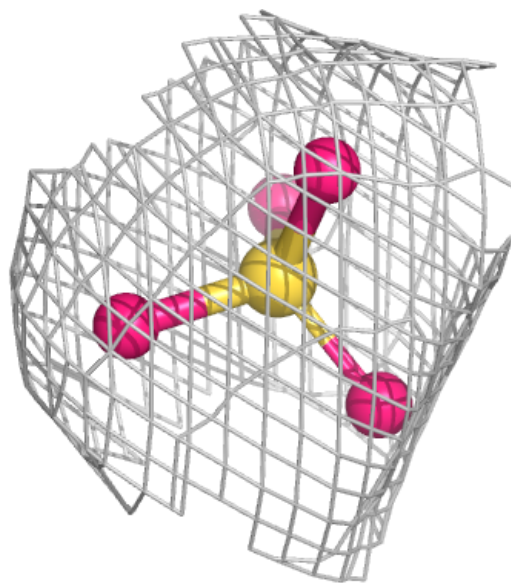
Electron density around SO4 F 301:

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



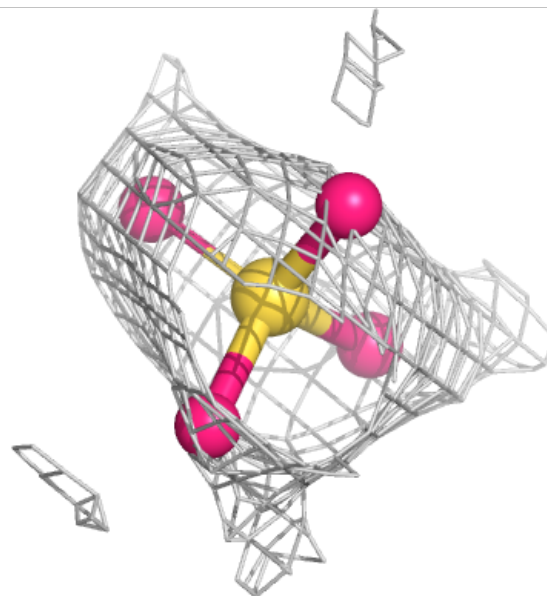
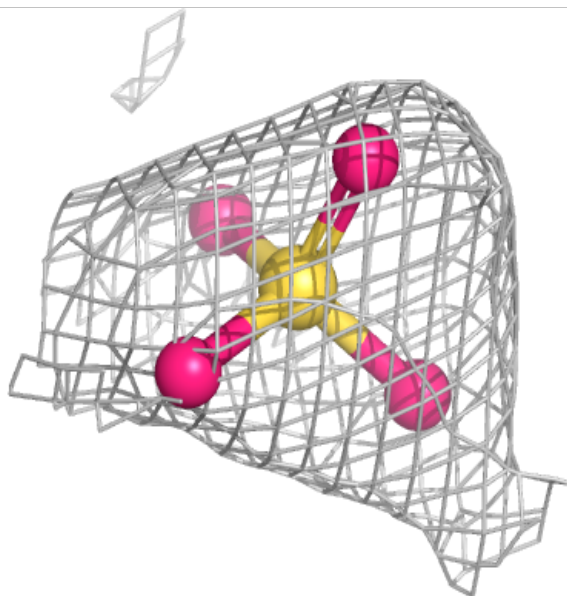
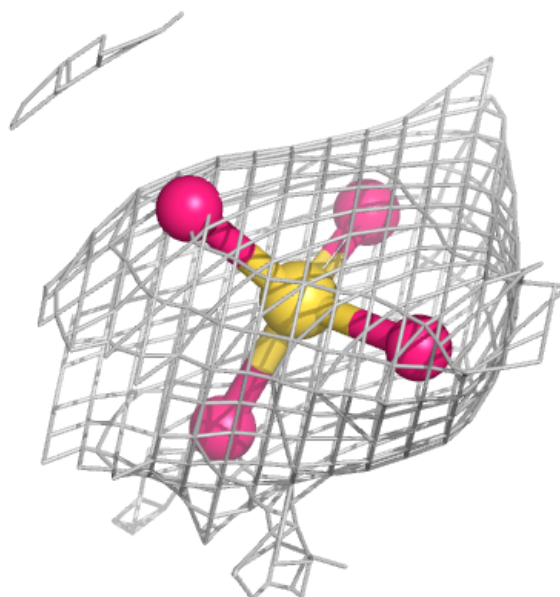
Electron density around SO4 N 301:

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



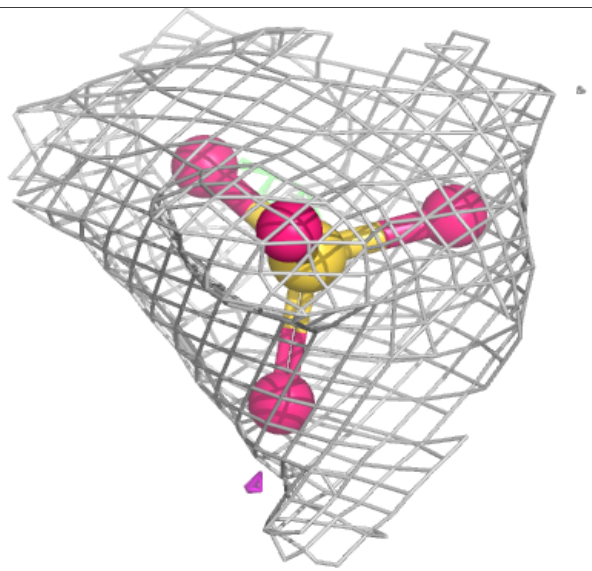
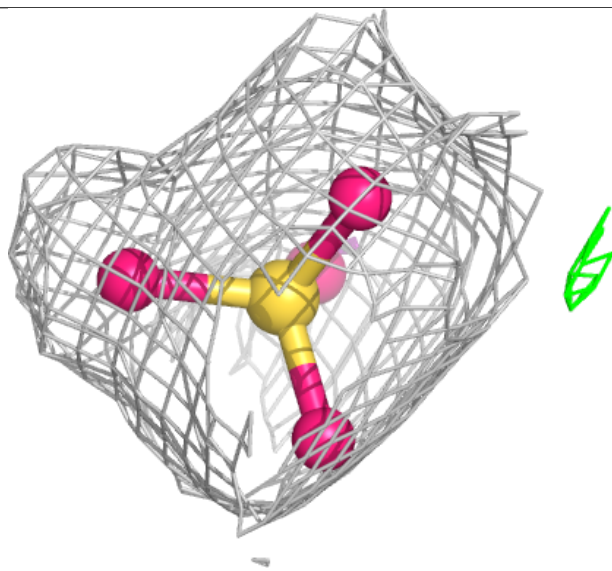
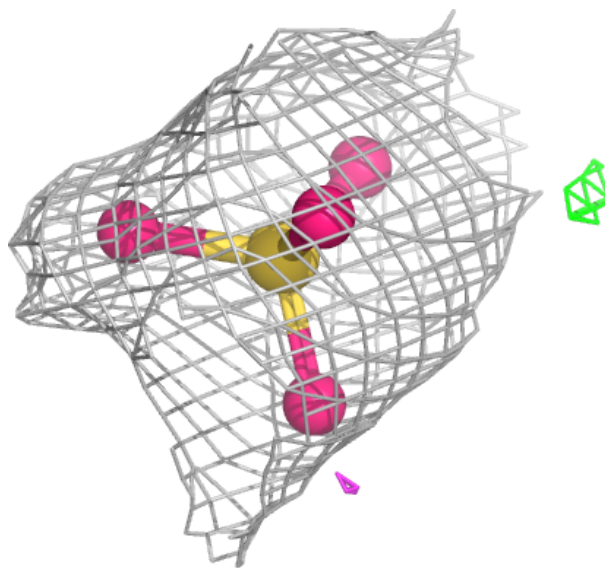
Electron density around SO4 O 301:

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



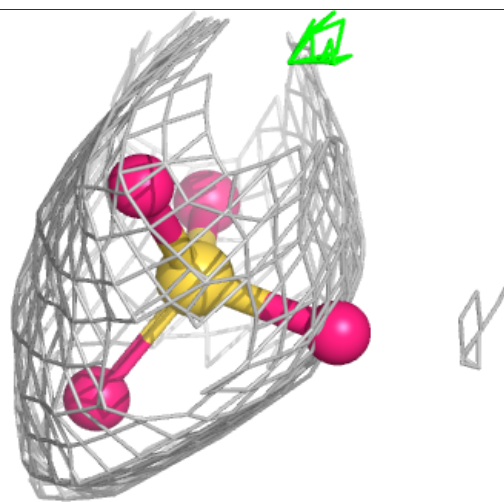
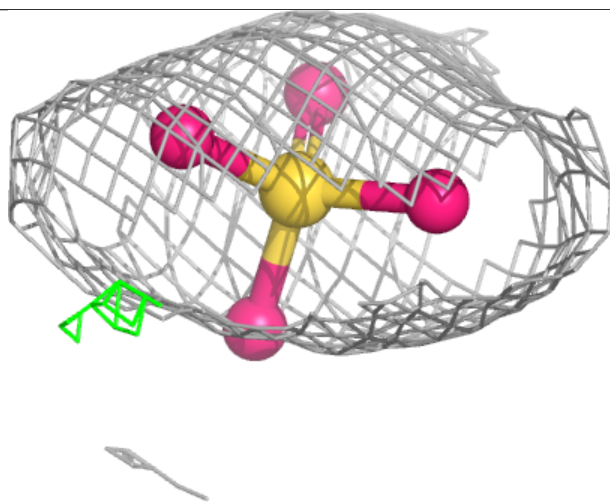
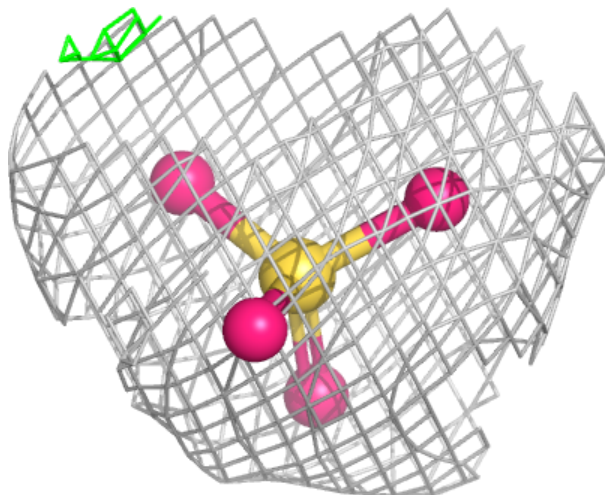
Electron density around SO4 P 301:

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



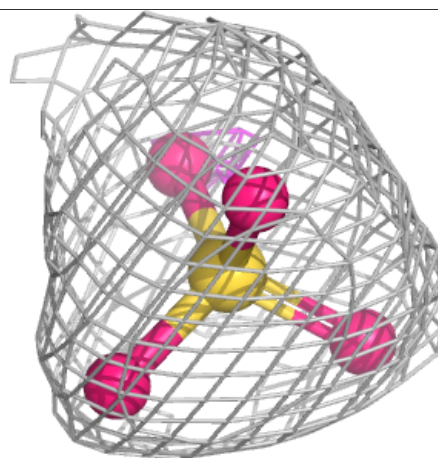
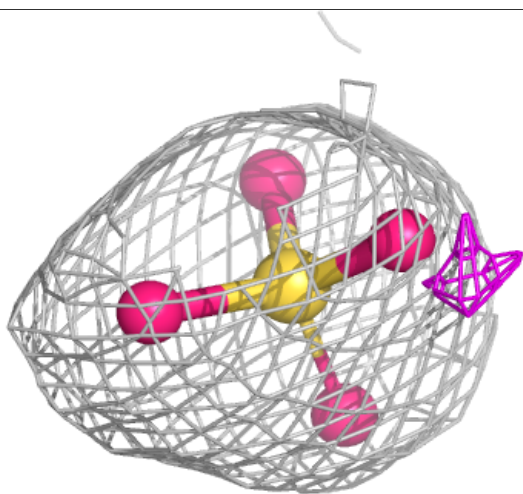
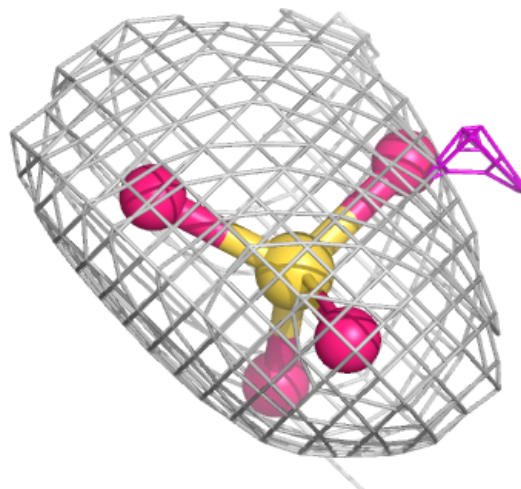
Electron density around SO4 D 301:

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



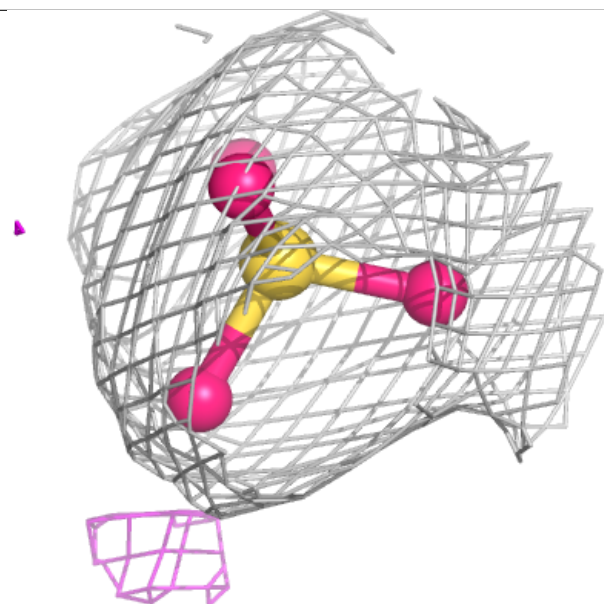
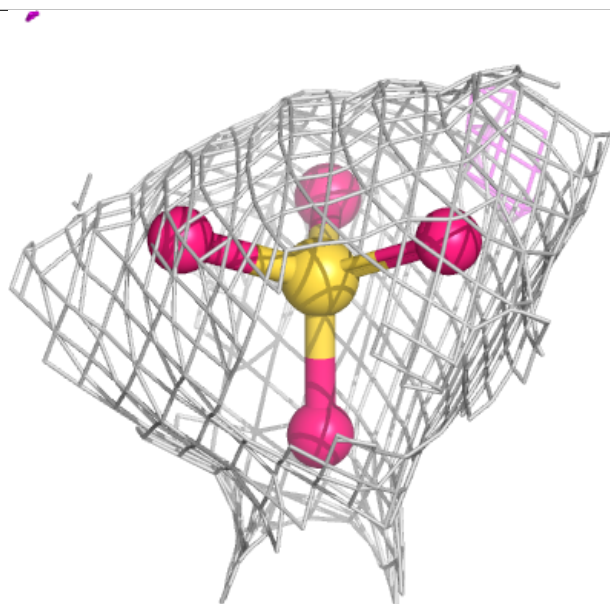
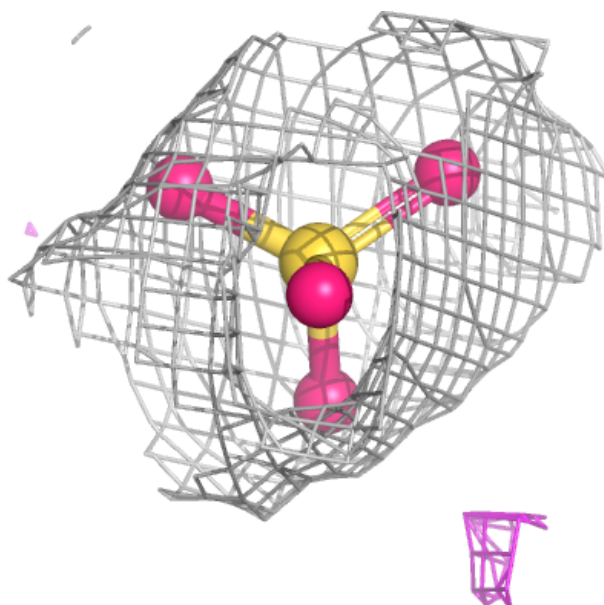
Electron density around SO4 E 301:

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



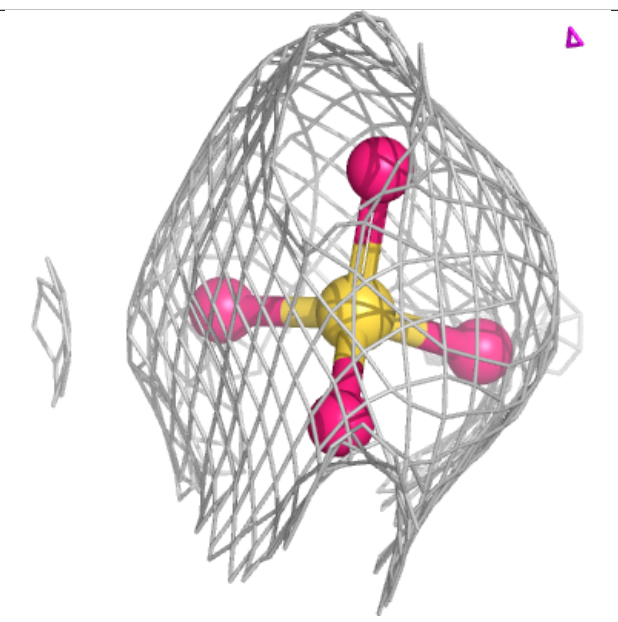
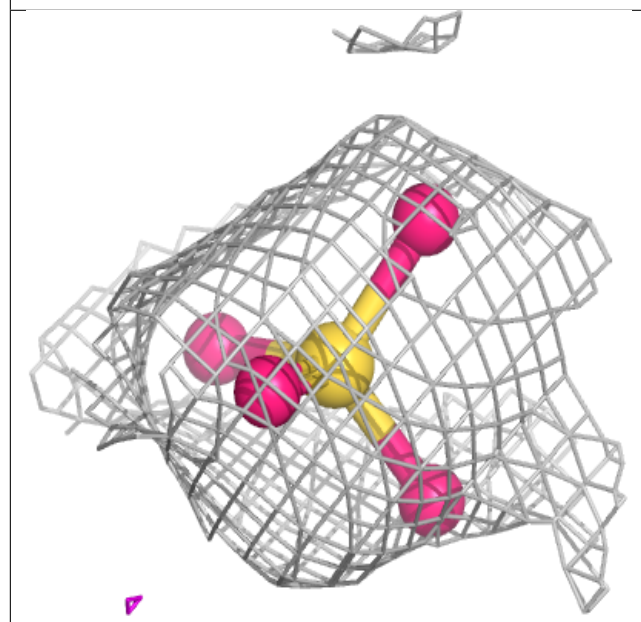
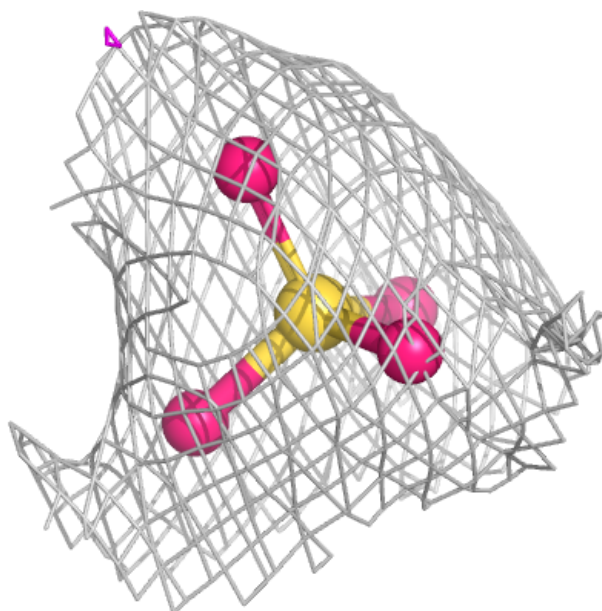
Electron density around SO4 A 301:

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



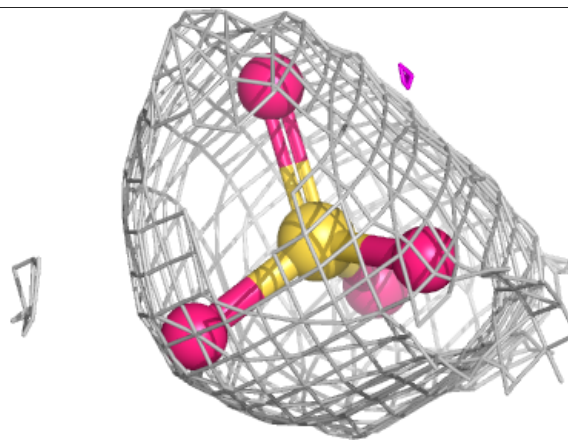
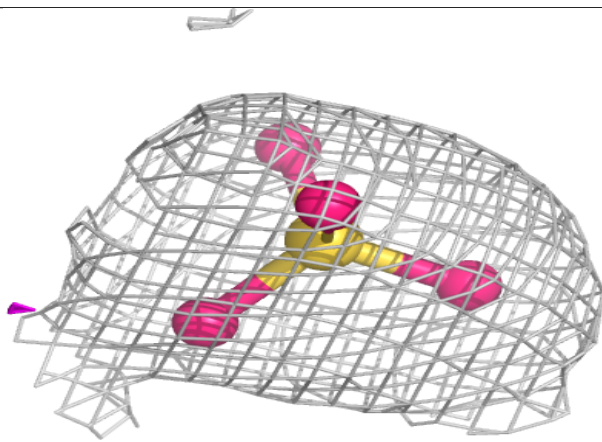
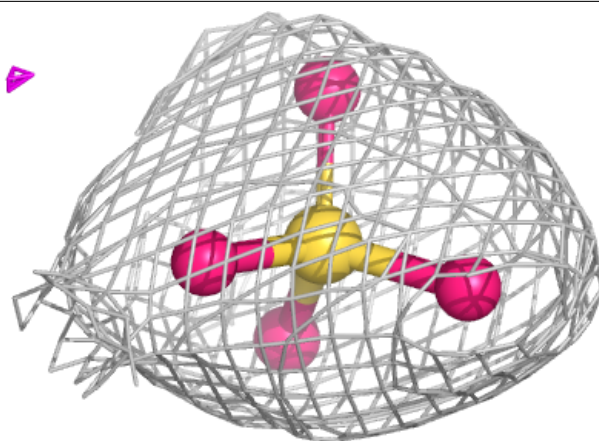
Electron density around SO4 G 301:

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



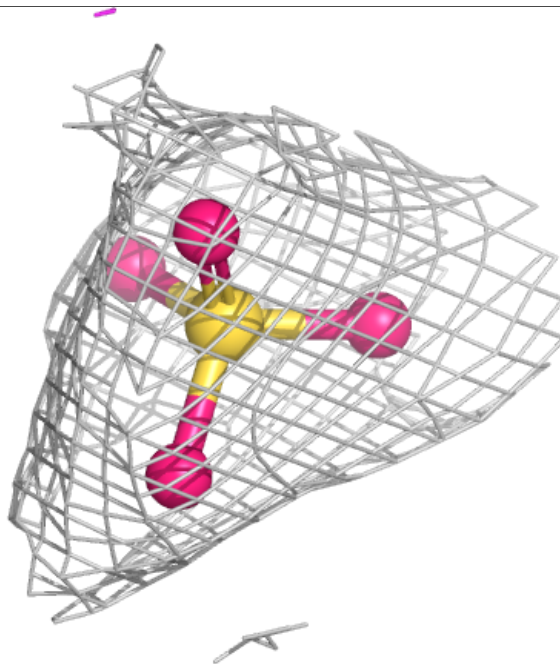
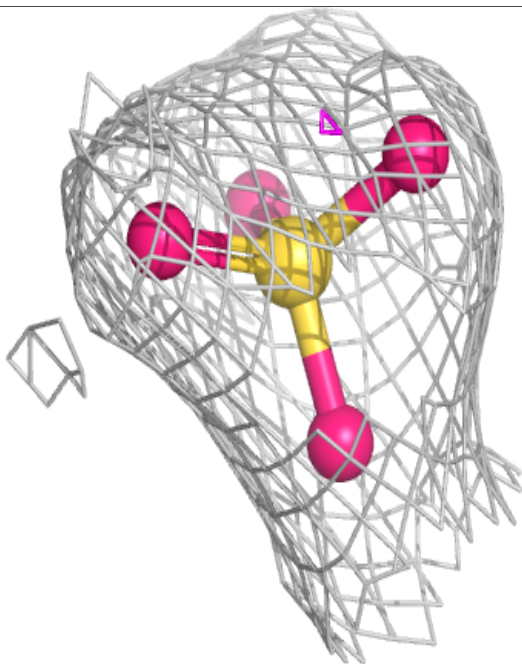
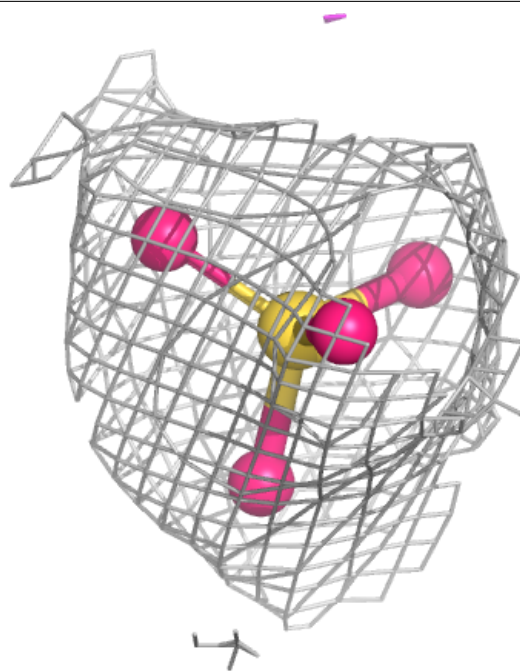
Electron density around SO4 G 302:

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



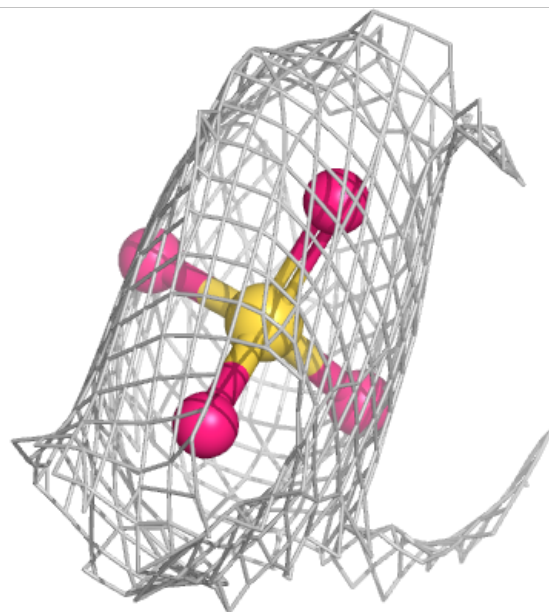
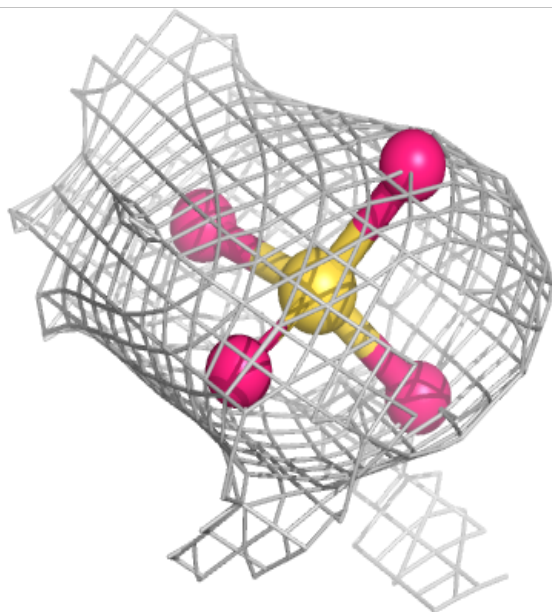
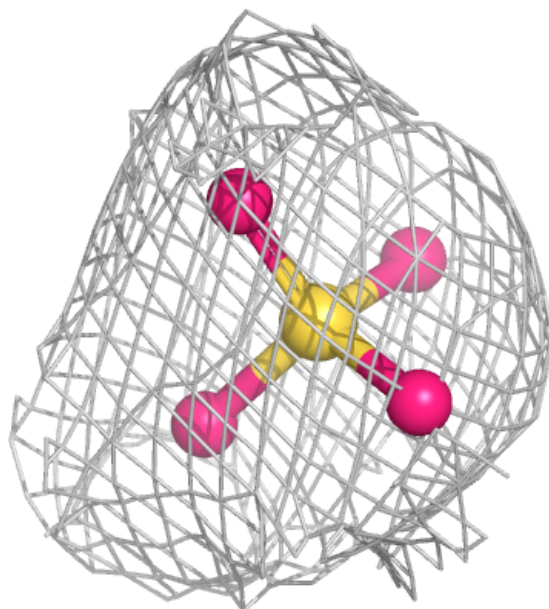
Electron density around SO4 I 301:

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



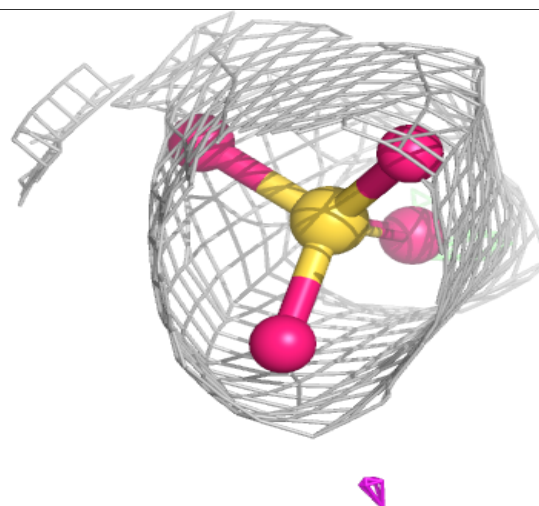
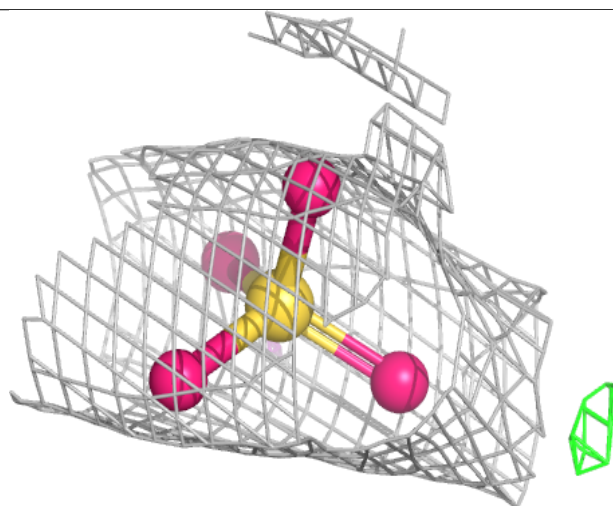
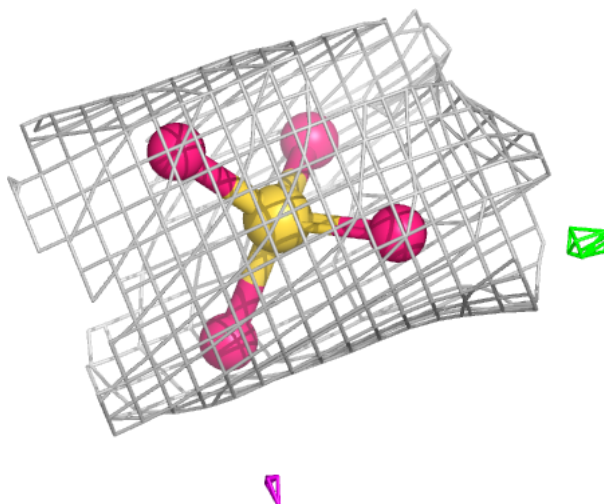
Electron density around SO4 J 301:

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



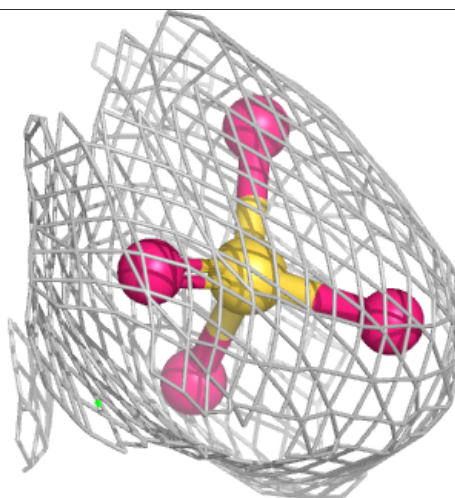
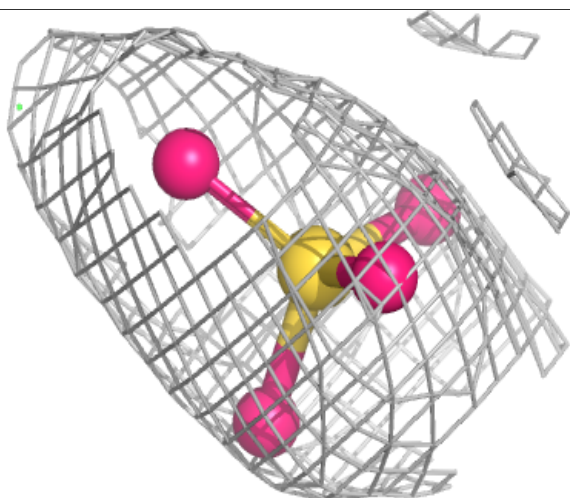
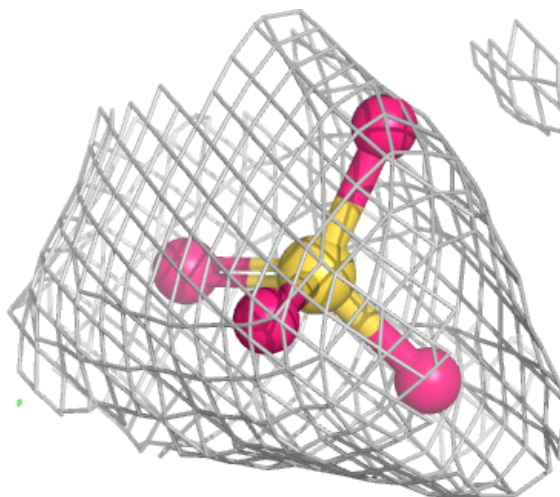
Electron density around SO4 J 302:

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



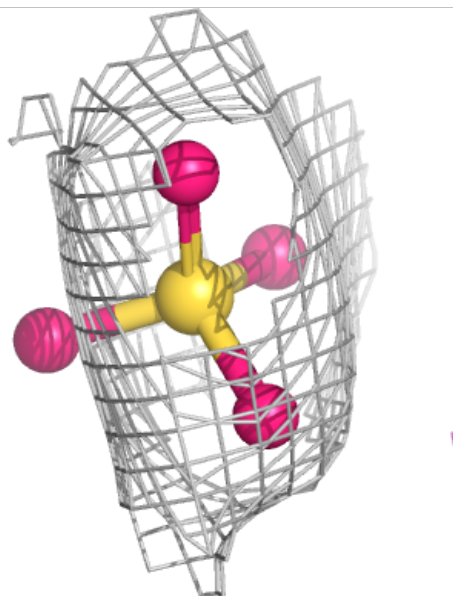
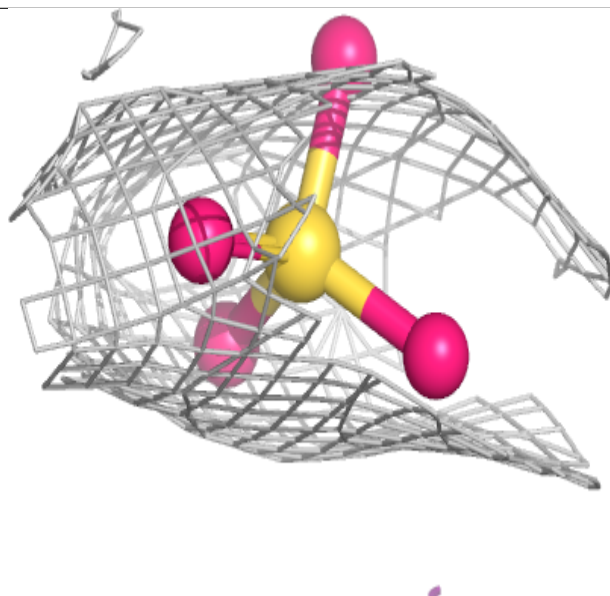
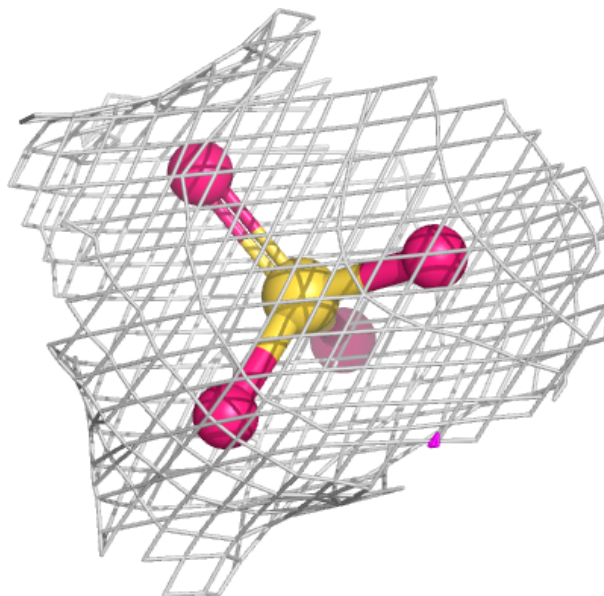
Electron density around SO4 K 301:

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



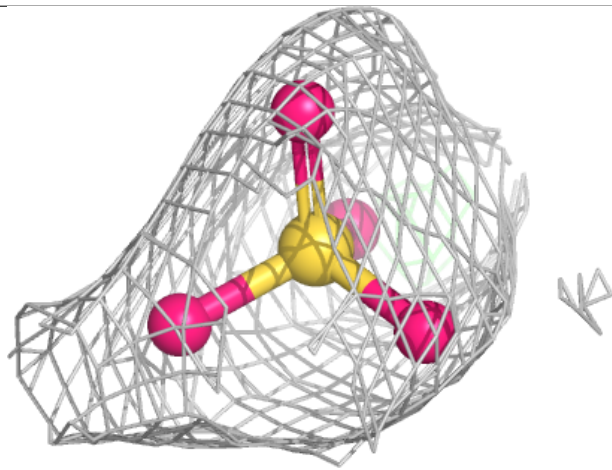
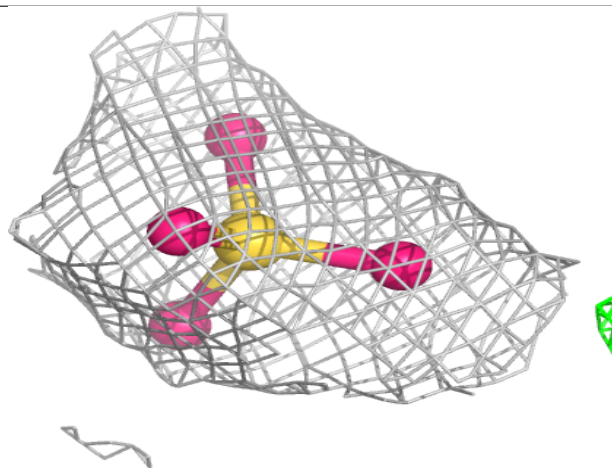
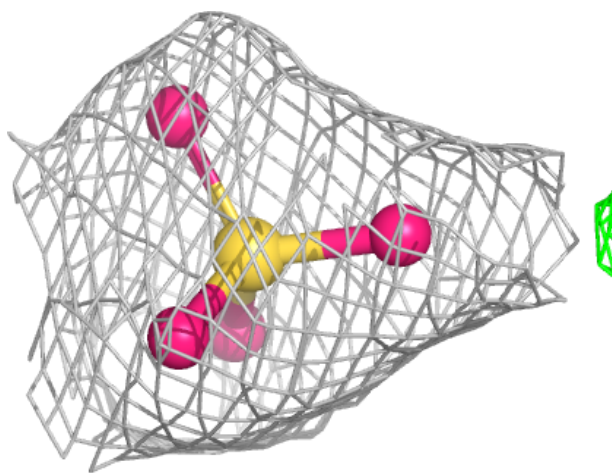
Electron density around SO4 L 301:

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



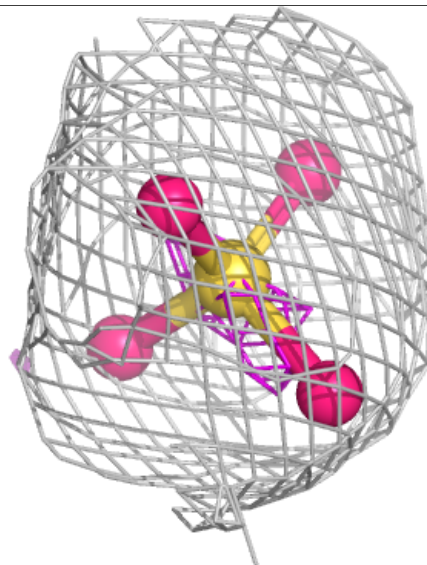
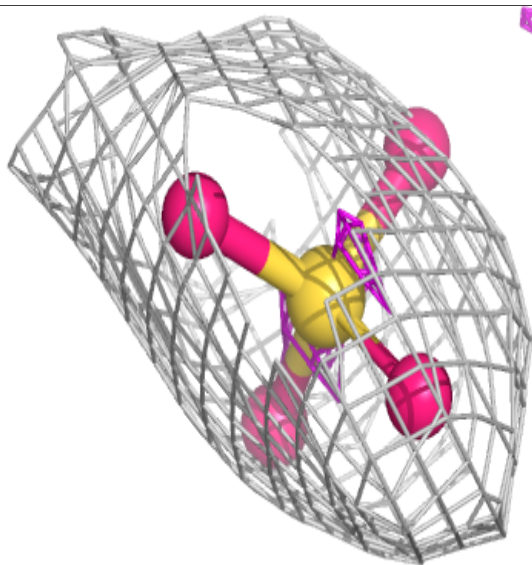
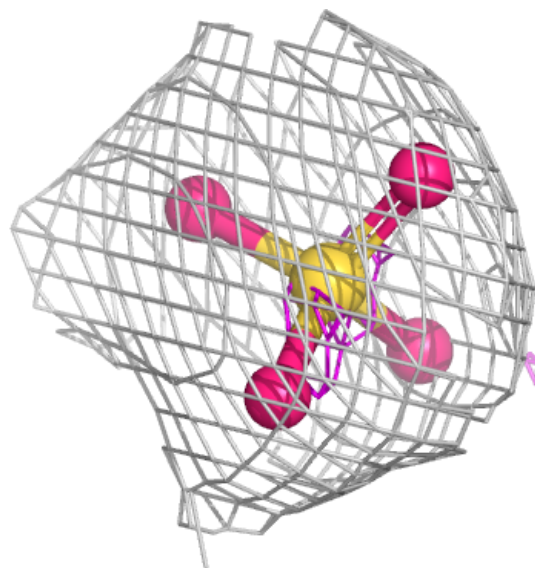
Electron density around SO4 M 301:

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



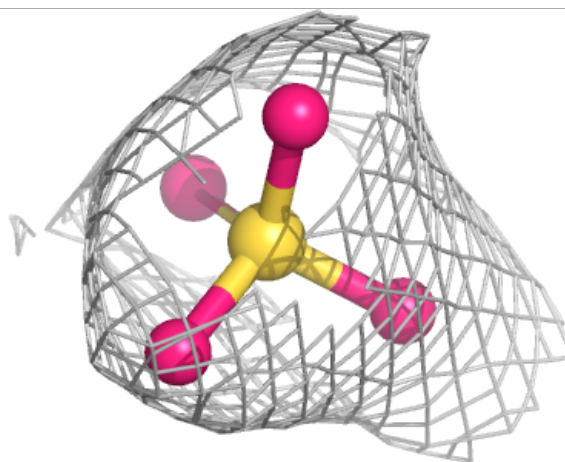
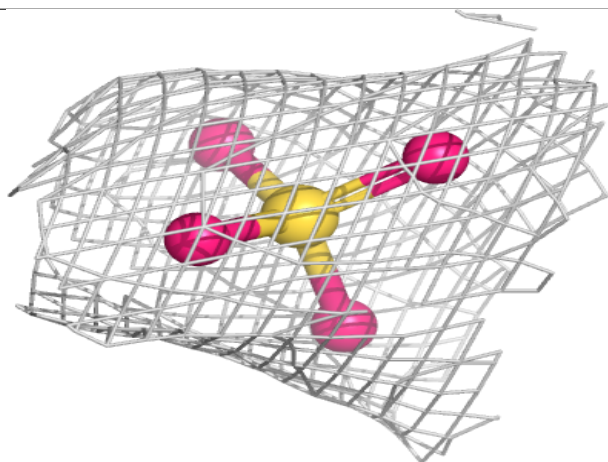
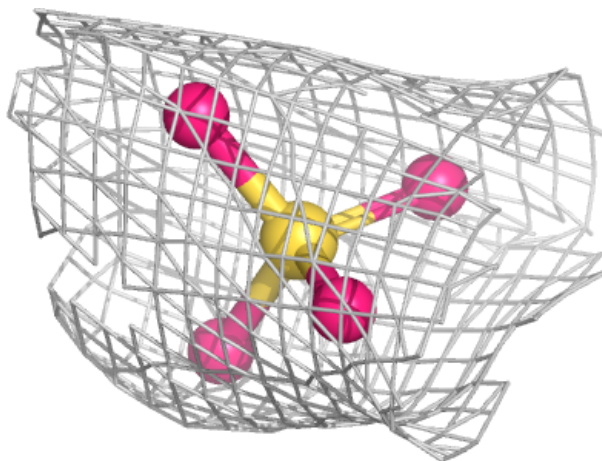
Electron density around SO4 A 302:

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



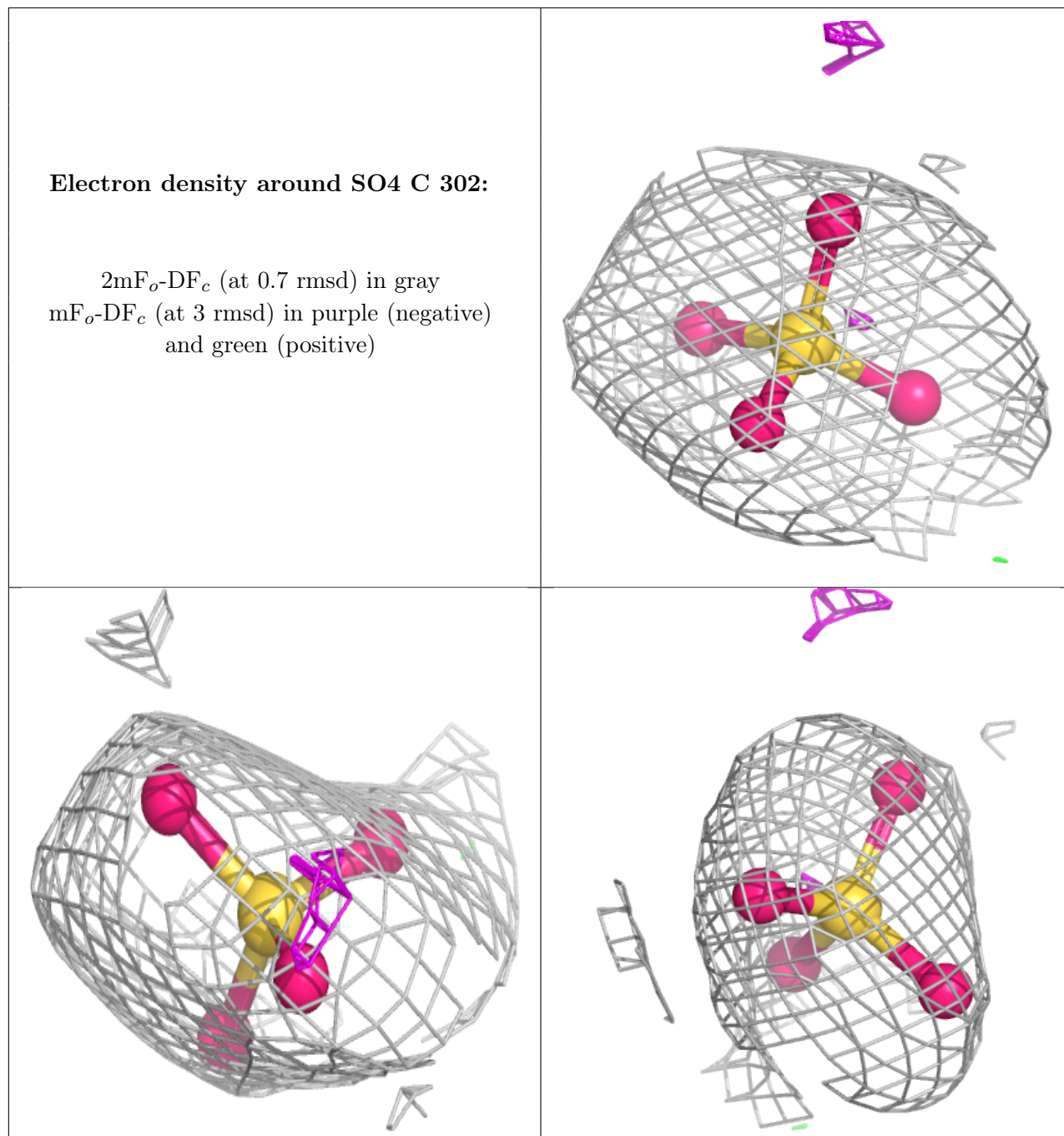
Electron density around SO4 C 301:

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



Electron density around SO4 C 302:

$2mF_o-DF_c$ (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.