



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 05:45 PM BST

PDB ID : 6KTR
Title : Crystal structure of fibroblast growth factor 19 in complex with Fab
Authors : Liu, H.; Zheng, S.; Hou, X.; Liu, X.; Lv, X.; Li, Y.; Li, W.; Sui, J.
Deposited on : 2019-08-28
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
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) : 2.13.1

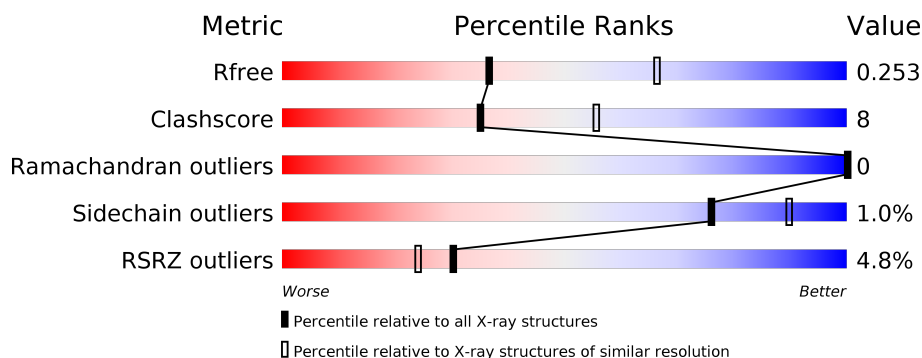
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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

Mol	Chain	Length	Quality of chain
1	A	233	
1	F	233	
2	B	216	
2	G	216	
3	C	218	
3	D	218	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8740 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 G1A8-Fab-HC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	211	Total	C	N	O	S	0	0	0
			1580	1001	261	312	6			
1	F	210	Total	C	N	O	S	0	0	0
			1573	997	260	310	6			

- Molecule 2 is a protein called G1A8-Fab-LC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	213	Total	C	N	O	S	0	0	0
			1570	977	263	325	5			
2	G	212	Total	C	N	O	S	0	0	0
			1561	971	261	324	5			

- Molecule 3 is a protein called Fibroblast growth factor 19.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	136	Total	C	N	O	S	0	0	0
			1067	673	197	189	8			
3	D	136	Total	C	N	O	S	0	0	0
			1071	676	198	189	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	217	SER	-	expression tag	UNP O95750
C	218	GLY	-	expression tag	UNP O95750
C	219	GLY	-	expression tag	UNP O95750
C	220	GLY	-	expression tag	UNP O95750
C	221	HIS	-	expression tag	UNP O95750
C	222	HIS	-	expression tag	UNP O95750
C	223	HIS	-	expression tag	UNP O95750
C	224	HIS	-	expression tag	UNP O95750

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Chain	Residue	Modelled	Actual	Comment	Reference
C	225	HIS	-	expression tag	UNP O95750
C	226	HIS	-	expression tag	UNP O95750
C	227	LEU	-	expression tag	UNP O95750
C	228	ASN	-	expression tag	UNP O95750
C	229	ASP	-	expression tag	UNP O95750
C	230	ILE	-	expression tag	UNP O95750
C	231	PHE	-	expression tag	UNP O95750
C	232	GLU	-	expression tag	UNP O95750
C	233	ALA	-	expression tag	UNP O95750
C	234	GLN	-	expression tag	UNP O95750
C	235	LYS	-	expression tag	UNP O95750
C	236	ILE	-	expression tag	UNP O95750
C	237	GLU	-	expression tag	UNP O95750
C	238	TRP	-	expression tag	UNP O95750
C	239	HIS	-	expression tag	UNP O95750
C	240	GLU	-	expression tag	UNP O95750
D	217	SER	-	expression tag	UNP O95750
D	218	GLY	-	expression tag	UNP O95750
D	219	GLY	-	expression tag	UNP O95750
D	220	GLY	-	expression tag	UNP O95750
D	221	HIS	-	expression tag	UNP O95750
D	222	HIS	-	expression tag	UNP O95750
D	223	HIS	-	expression tag	UNP O95750
D	224	HIS	-	expression tag	UNP O95750
D	225	HIS	-	expression tag	UNP O95750
D	226	HIS	-	expression tag	UNP O95750
D	227	LEU	-	expression tag	UNP O95750
D	228	ASN	-	expression tag	UNP O95750
D	229	ASP	-	expression tag	UNP O95750
D	230	ILE	-	expression tag	UNP O95750
D	231	PHE	-	expression tag	UNP O95750
D	232	GLU	-	expression tag	UNP O95750
D	233	ALA	-	expression tag	UNP O95750
D	234	GLN	-	expression tag	UNP O95750
D	235	LYS	-	expression tag	UNP O95750
D	236	ILE	-	expression tag	UNP O95750
D	237	GLU	-	expression tag	UNP O95750
D	238	TRP	-	expression tag	UNP O95750
D	239	HIS	-	expression tag	UNP O95750
D	240	GLU	-	expression tag	UNP O95750

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



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

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	G	1	Total	Na	0	0
			1	1		

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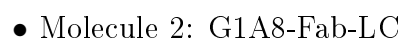
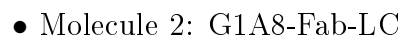
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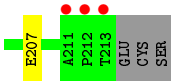
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	2	Total	Na	0	0
			2	2		

- Molecule 6 is water.

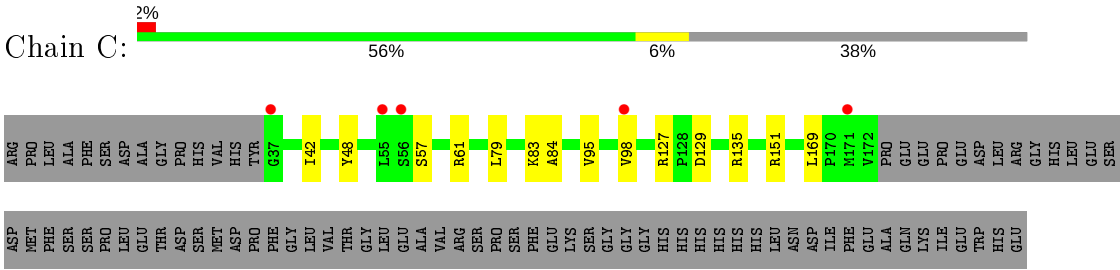
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total	O	0	0
			25	25		
6	B	50	Total	O	0	0
			50	50		
6	C	35	Total	O	0	0
			35	35		
6	D	42	Total	O	0	0
			42	42		
6	F	53	Total	O	0	0
			53	53		
6	G	60	Total	O	0	0
			60	60		

- Molecule 1: G1A8-Fab-HC

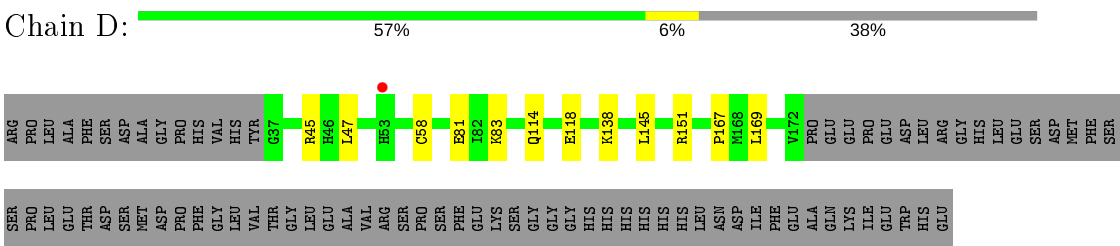




● Molecule 3: Fibroblast growth factor 19



● Molecule 3: Fibroblast growth factor 19



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.97Å 104.12Å 165.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.72 – 2.60 48.72 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.72-2.60) 99.7 (48.72-2.60)	Depositor EDS
R_{merge}	0.02	Depositor
R_{sym}	0.02	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.12 _2829	Depositor
R, R_{free}	0.202 , 0.253 0.202 , 0.253	Depositor DCC
R_{free} test set	2000 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	58.1	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 46.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8740	wwPDB-VP
Average B, all atoms (Å ²)	64.0	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 30.11 % 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 1.3820e-03. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, 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	0.27	0/1618	0.49	0/2205
1	F	0.26	0/1611	0.48	0/2195
2	B	0.29	0/1608	0.49	1/2195 (0.0%)
2	G	0.26	0/1599	0.44	0/2184
3	C	0.26	0/1091	0.45	0/1471
3	D	0.25	0/1095	0.43	0/1475
All	All	0.26	0/8622	0.47	1/11725 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	129	LEU	CA-CB-CG	-5.65	102.31	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1580	0	1539	33	0
1	F	1573	0	1532	25	0
2	B	1570	0	1508	43	0
2	G	1561	0	1492	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1067	0	1061	19	0
3	D	1071	0	1072	7	0
4	B	5	0	0	0	0
4	C	20	0	0	2	0
4	D	20	0	0	1	0
4	G	5	0	0	0	0
5	F	2	0	0	0	0
5	G	1	0	0	0	0
6	A	25	0	0	3	0
6	B	50	0	0	1	0
6	C	35	0	0	1	0
6	D	42	0	0	0	0
6	F	53	0	0	1	0
6	G	60	0	0	0	0
All	All	8740	0	8204	137	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 8.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:LYS:NZ	2:B:176:TYR:HE2	1.36	1.22
2:B:137:VAL:HG12	2:B:139:LEU:HD11	1.25	1.13
2:B:170:LYS:NZ	2:B:176:TYR:CE2	2.17	1.11
2:B:170:LYS:CE	2:B:176:TYR:HE2	1.64	1.10
2:B:170:LYS:CD	2:B:176:TYR:CE2	2.46	0.98
2:B:170:LYS:CE	2:B:176:TYR:CE2	2.51	0.94
2:B:170:LYS:HD2	2:B:176:TYR:CE2	2.03	0.93
1:A:141:THR:N	1:A:192:SER:HG	1.67	0.92
3:C:42:ILE:CD1	3:C:83:LYS:HD3	1.99	0.92
3:C:42:ILE:HD13	3:C:83:LYS:HD3	1.54	0.88
2:B:170:LYS:CD	2:B:176:TYR:CD2	2.57	0.86
2:B:152:TRP:HE1	2:B:180:SER:HG	1.16	0.86
2:B:137:VAL:HG12	2:B:139:LEU:CD1	2.06	0.86
2:B:170:LYS:CD	2:B:176:TYR:HE2	1.89	0.83
2:B:170:LYS:HD3	2:B:176:TYR:HD2	1.44	0.81
2:B:170:LYS:HD3	2:B:176:TYR:CD2	2.15	0.80
2:B:137:VAL:CG1	2:B:139:LEU:HD11	2.10	0.80
1:F:73:ASP:OD2	1:F:76:LYS:NZ	2.18	0.73
2:B:138:CYS:HB3	2:B:180:SER:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:72:ARG:HE	1:F:74:ASN:HD21	1.37	0.71
1:A:62:ASP:OD1	1:A:65:LYS:NZ	2.21	0.70
2:B:170:LYS:HD2	2:B:176:TYR:CD2	2.24	0.70
1:F:200:TYR:H	1:F:216:LYS:HZ1	1.40	0.69
3:C:42:ILE:HD13	3:C:83:LYS:CD	2.23	0.68
1:F:9:GLY:HA2	1:F:18:LEU:HD21	1.75	0.68
2:G:185:THR:H	2:G:188:GLN:HE21	1.42	0.68
2:B:166:THR:HG22	2:B:179:SER:H	1.59	0.67
3:C:127:ARG:NH1	3:C:129:ASP:OD2	2.29	0.66
3:C:42:ILE:HD12	3:C:83:LYS:HD3	1.78	0.65
3:C:135:ARG:NH2	6:C:401:HOH:O	2.29	0.65
1:A:70:ILE:HD11	1:A:79:LEU:HD11	1.78	0.64
1:A:100:ASN:HA	1:A:107:ASP:OD1	1.97	0.64
1:A:216:LYS:HD3	1:A:218:GLU:OE2	1.97	0.64
1:F:161:ASN:ND2	1:F:201:ILE:H	1.97	0.62
1:F:175:VAL:HG21	2:G:164:GLU:HB3	1.82	0.62
1:A:169:VAL:HG22	1:A:188:VAL:HG12	1.82	0.61
1:F:161:ASN:HD21	1:F:201:ILE:H	1.50	0.60
1:F:200:TYR:H	1:F:216:LYS:NZ	1.99	0.59
2:B:187:GLU:HG3	2:B:190:LYS:NZ	2.18	0.59
1:F:161:ASN:HD21	1:F:200:TYR:HA	1.67	0.59
1:F:142:ALA:N	1:F:192:SER:HG	2.01	0.58
3:C:151:ARG:NH1	4:C:302:SO4:O2	2.31	0.58
2:B:128:GLU:OE2	6:B:401:HOH:O	2.17	0.57
1:A:73:ASP:OD2	1:A:76:LYS:HG2	2.04	0.57
2:G:151:ALA:HB1	2:G:153:LYS:HZ3	1.69	0.56
3:C:42:ILE:HD11	3:C:83:LYS:NZ	2.20	0.56
2:B:200:THR:HG22	2:B:205:THR:HB	1.86	0.56
1:F:199:THR:HB	1:F:216:LYS:HE2	1.87	0.56
2:B:117:PRO:HB3	2:B:143:PHE:HB3	1.88	0.55
2:B:187:GLU:HG3	2:B:190:LYS:HZ3	1.73	0.54
1:A:102:GLN:NE2	6:A:301:HOH:O	2.38	0.54
1:A:60:TYR:CZ	1:A:70:ILE:HG22	2.43	0.53
3:C:48:TYR:CE2	3:C:57:SER:HB2	2.44	0.53
2:B:139:LEU:N	2:B:139:LEU:HD12	2.24	0.53
2:B:170:LYS:NZ	2:B:176:TYR:OH	2.42	0.53
1:A:1:GLU:HG3	1:A:2:VAL:H	1.75	0.52
1:F:190:VAL:HG21	1:F:200:TYR:CZ	2.45	0.52
2:B:155:ASP:OD2	2:B:193:ARG:N	2.43	0.52
3:C:42:ILE:CD1	3:C:83:LYS:NZ	2.74	0.51
2:G:198:GLN:HG2	2:G:207:GLU:HG3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:SER:HB2	2:B:99:LEU:HD11	1.91	0.51
2:G:153:LYS:HZ1	2:G:158:PRO:HB3	1.76	0.51
1:F:72:ARG:NE	1:F:74:ASN:HD21	2.07	0.51
2:G:117:PRO:HB3	2:G:143:PHE:HB3	1.92	0.50
2:B:18:ILE:HD11	2:B:77:ILE:HD12	1.93	0.50
2:B:155:ASP:OD1	2:B:194:SER:N	2.42	0.50
3:D:169:LEU:HD12	2:G:57:PRO:HB3	1.93	0.50
1:A:51:ILE:HD11	1:A:55:GLY:HA2	1.93	0.50
1:A:107:ASP:HB3	1:A:108:TYR:CD2	2.47	0.49
2:G:126:SER:O	2:G:130:GLN:HG3	2.11	0.49
1:A:71:SER:OG	1:A:80:TYR:HB2	2.12	0.49
1:A:73:ASP:OD2	1:A:76:LYS:HE3	2.13	0.49
2:B:57:PRO:HB3	3:C:169:LEU:HD12	1.93	0.49
2:G:171:GLN:HG3	2:G:173:ASN:OD1	2.13	0.49
1:F:177:GLN:HG2	2:G:164:GLU:HG3	1.95	0.48
1:A:52:SER:O	6:A:301:HOH:O	2.20	0.48
1:A:149:LYS:NZ	2:B:128:GLU:OE1	2.42	0.48
1:F:14:PRO:HD2	1:F:119:SER:HB3	1.94	0.48
2:B:163:VAL:HG22	2:B:182:LEU:HD13	1.96	0.48
2:B:129:LEU:HA	2:B:129:LEU:HD23	1.35	0.48
2:B:144:TYR:CD2	2:B:176:TYR:CE1	3.02	0.47
1:A:203:ASN:HD21	1:A:212:LYS:HE2	1.79	0.47
3:D:81:GLU:OE2	3:D:83:LYS:HE2	2.14	0.47
2:G:122:PHE:HB2	2:G:137:VAL:HB	1.97	0.47
2:G:18:ILE:HD11	2:G:77:ILE:HD12	1.96	0.47
2:B:155:ASP:OD2	2:B:192:HIS:HB3	2.15	0.47
1:A:144:LEU:HD12	1:A:188:VAL:HG23	1.96	0.47
1:A:206:HIS:CD2	1:A:208:PRO:HD2	2.50	0.47
1:A:51:ILE:CG1	1:A:72:ARG:HD2	2.45	0.47
1:A:1:GLU:CG	1:A:2:VAL:H	2.29	0.46
1:F:91:THR:HG23	1:F:116:THR:HA	1.97	0.46
2:G:151:ALA:HB1	2:G:153:LYS:NZ	2.30	0.46
1:A:216:LYS:NZ	6:A:304:HOH:O	2.49	0.46
3:C:135:ARG:HG2	3:C:135:ARG:HH11	1.79	0.46
1:A:192:SER:HA	1:A:195:LEU:HD11	1.98	0.46
2:B:143:PHE:O	2:B:176:TYR:HD1	1.99	0.45
1:F:201:ILE:HG22	1:F:216:LYS:HA	1.97	0.45
1:F:170:HIS:HE1	2:G:177:ALA:HB3	1.82	0.45
1:A:5:LEU:HB2	1:A:23:ALA:HB3	1.98	0.45
3:C:42:ILE:HD11	3:C:83:LYS:HZ3	1.82	0.45
1:F:8:GLY:O	1:F:113:THR:HG21	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLN:HB3	3:C:42:ILE:CG1	2.47	0.45
1:A:51:ILE:HB	1:A:70:ILE:HG12	1.98	0.45
3:D:58:CYS:SG	3:D:145:LEU:HD13	2.57	0.45
2:B:138:CYS:O	2:B:180:SER:N	2.46	0.44
3:D:118:GLU:HG3	3:D:138:LYS:HD2	2.00	0.44
2:G:155:ASP:OD1	2:G:193:ARG:HB2	2.16	0.44
2:B:144:TYR:CD2	2:B:176:TYR:HE1	2.35	0.44
1:F:14:PRO:HG2	1:F:119:SER:HB3	1.99	0.44
1:A:125:PRO:HB3	1:A:151:TYR:HB3	1.98	0.44
1:A:51:ILE:HG12	1:A:72:ARG:HD2	1.99	0.44
1:A:195:LEU:N	1:A:195:LEU:HD12	2.32	0.44
2:G:52:ASP:HB2	2:G:55:ASN:HD22	1.83	0.43
2:B:145:PRO:HA	2:B:176:TYR:HE1	1.84	0.43
2:B:193:ARG:NE	2:B:193:ARG:HA	2.33	0.43
3:C:42:ILE:CD1	3:C:83:LYS:HZ3	2.32	0.43
1:A:1:GLU:HG3	1:A:2:VAL:N	2.33	0.43
1:F:192:SER:OG	6:F:401:HOH:O	2.21	0.43
1:A:67:ARG:HD3	1:A:87:ARG:HH21	1.83	0.42
1:A:177:GLN:HA	2:B:164:GLU:HG3	2.00	0.42
2:B:184:LEU:HB3	2:B:188:GLN:HG3	2.00	0.42
1:F:12:VAL:O	1:F:117:VAL:HA	2.19	0.42
1:F:100:ASN:HA	1:F:107:ASP:OD2	2.19	0.42
1:A:149:LYS:HG2	1:A:150:ASP:OD2	2.20	0.42
3:C:61:ARG:NH2	4:C:304:SO4:O4	2.53	0.42
2:G:185:THR:H	2:G:188:GLN:NE2	2.14	0.41
3:D:45:ARG:HD2	3:D:167:PRO:HB2	2.02	0.41
2:B:196:SER:HB2	2:B:209:THR:HG22	2.03	0.41
2:B:37:TRP:HB2	2:B:50:ILE:HB	2.02	0.41
1:F:175:VAL:HB	2:G:166:THR:HG22	2.02	0.41
3:C:79:LEU:HD23	3:C:95:VAL:HG21	2.02	0.41
2:G:32:TYR:HB3	2:G:34:TYR:CD2	2.55	0.41
3:C:98:VAL:HG22	3:C:98:VAL:O	2.21	0.40
1:F:72:ARG:HE	1:F:74:ASN:ND2	2.11	0.40
3:D:151:ARG:NH1	4:D:302:SO4:O2	2.41	0.40
3:D:47:LEU:HA	3:D:47:LEU:HD23	1.89	0.40
3:C:83:LYS:HG3	3:C:84:ALA:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	207/233 (89%)	199 (96%)	8 (4%)	0	100	100
1	F	206/233 (88%)	199 (97%)	7 (3%)	0	100	100
2	B	211/216 (98%)	201 (95%)	10 (5%)	0	100	100
2	G	210/216 (97%)	199 (95%)	11 (5%)	0	100	100
3	C	134/218 (62%)	131 (98%)	3 (2%)	0	100	100
3	D	134/218 (62%)	133 (99%)	1 (1%)	0	100	100
All	All	1102/1334 (83%)	1062 (96%)	40 (4%)	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	175/195 (90%)	173 (99%)	2 (1%)	73	88
1	F	174/195 (89%)	171 (98%)	3 (2%)	60	81
2	B	176/180 (98%)	174 (99%)	2 (1%)	73	88
2	G	175/180 (97%)	174 (99%)	1 (1%)	86	95
3	C	114/186 (61%)	114 (100%)	0	100	100
3	D	115/186 (62%)	114 (99%)	1 (1%)	78	91
All	All	929/1122 (83%)	920 (99%)	9 (1%)	76	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	TYR
1	A	119	SER
2	B	28	ASP
2	B	170	LYS
3	D	114	GLN
1	F	3	GLN
1	F	59	TYR
1	F	83	MET
2	G	28	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	ASN
1	A	177	GLN
1	A	203	ASN
1	A	205	ASN
2	B	55	ASN
2	B	132	ASN
3	D	77	HIS
3	D	96	HIS
1	F	13	GLN
1	F	74	ASN
1	F	77	ASN
1	F	82	GLN
1	F	84	ASN
1	F	100	ASN
1	F	161	ASN
1	F	170	HIS
1	F	177	GLN
2	G	55	ASN
2	G	171	GLN
2	G	174	ASN
2	G	188	GLN
2	G	198	GLN

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 ⓘ

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	G	301	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	C	302	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	D	303	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	D	304	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	C	304	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	303	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	D	302	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.06	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.

3 monomers are involved in 3 short contacts:

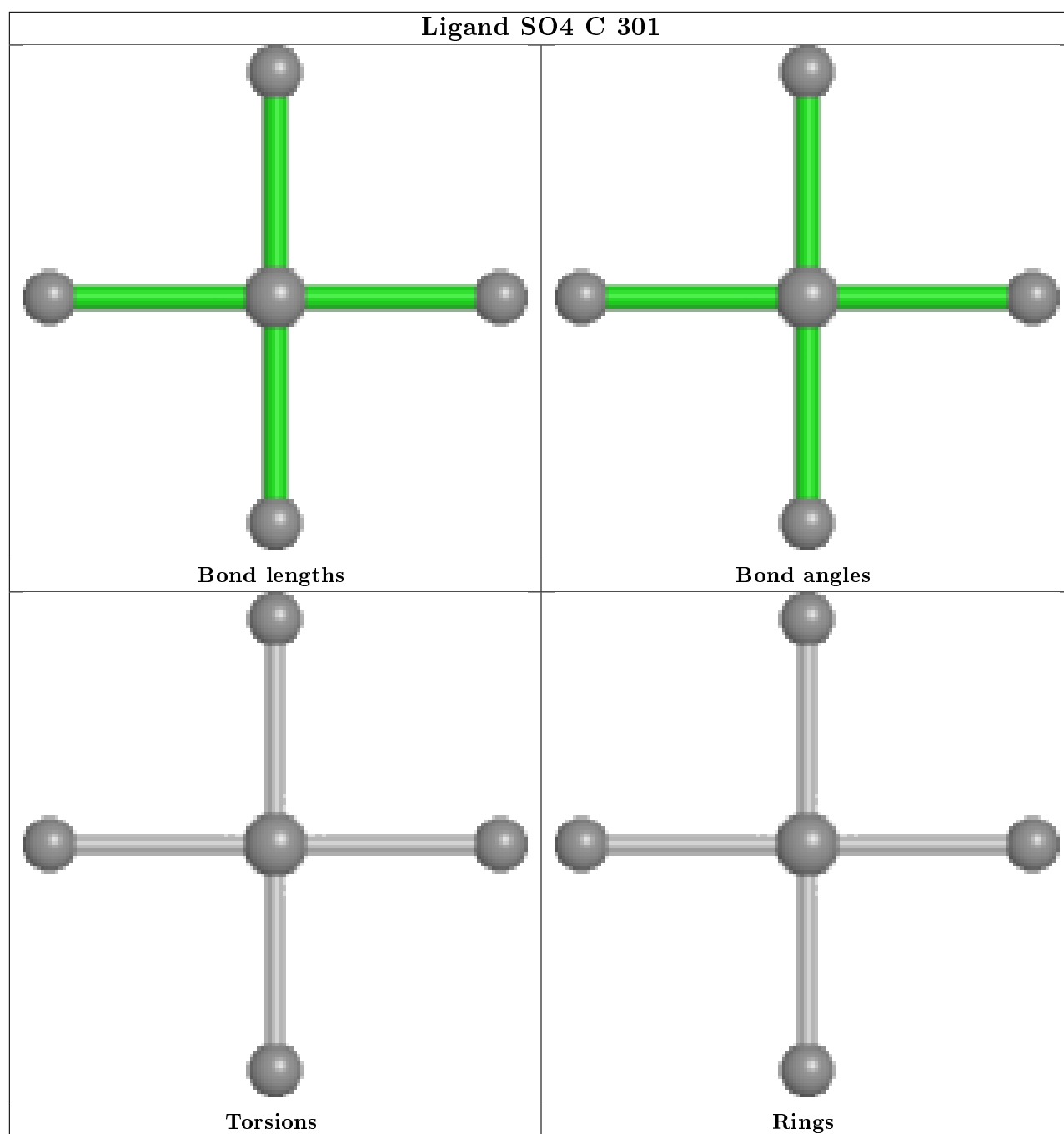
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	302	SO4	1	0

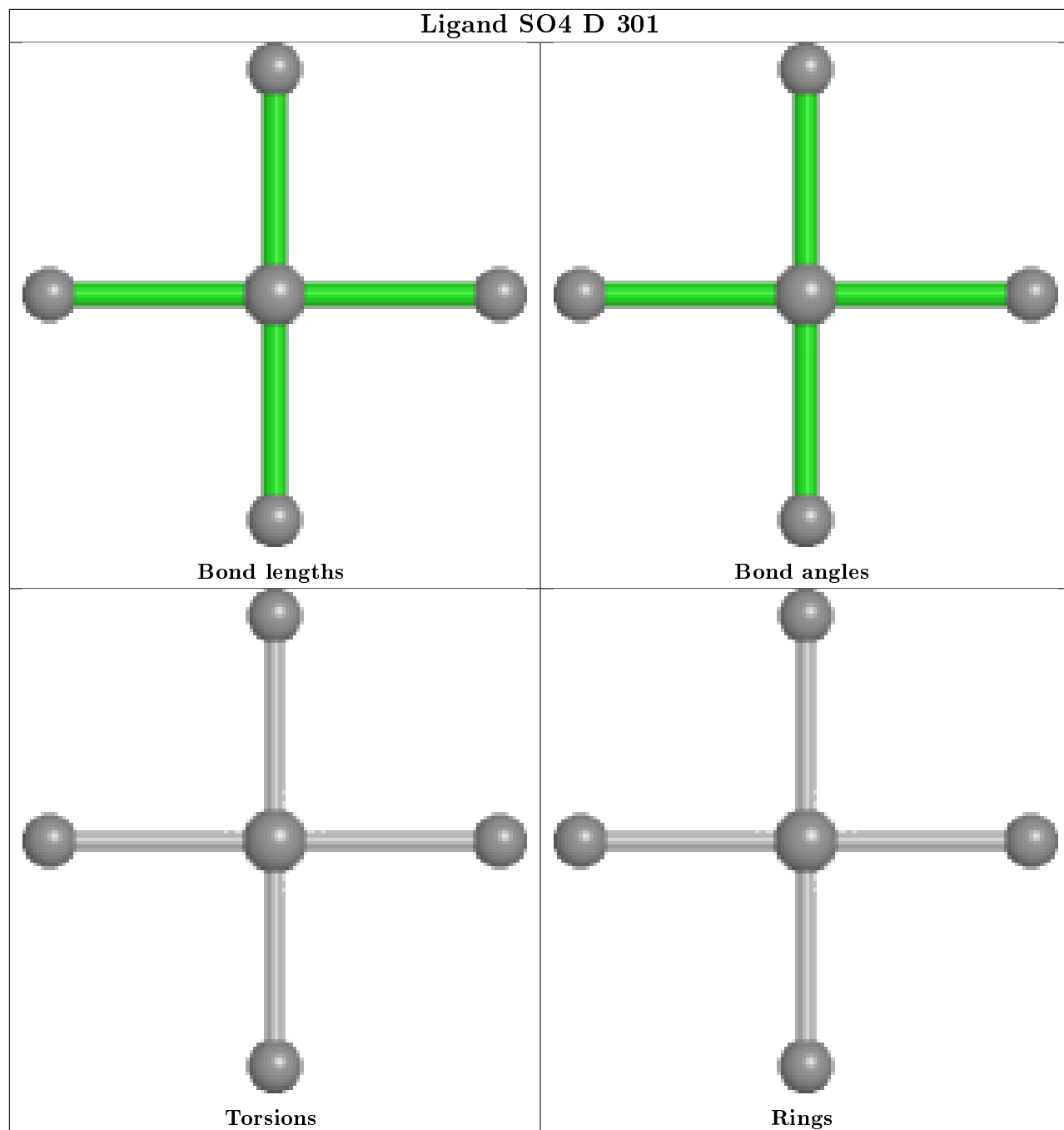
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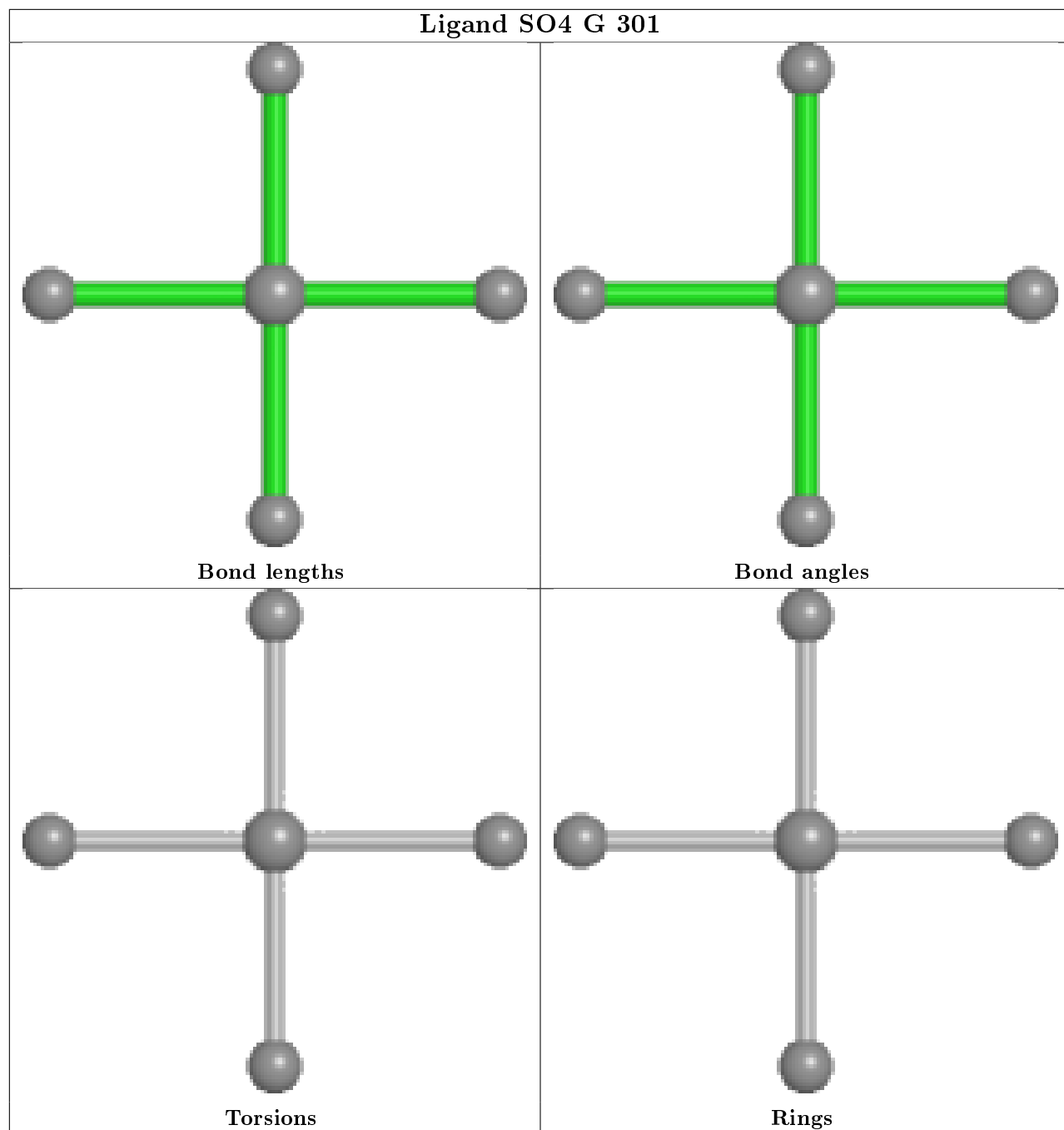
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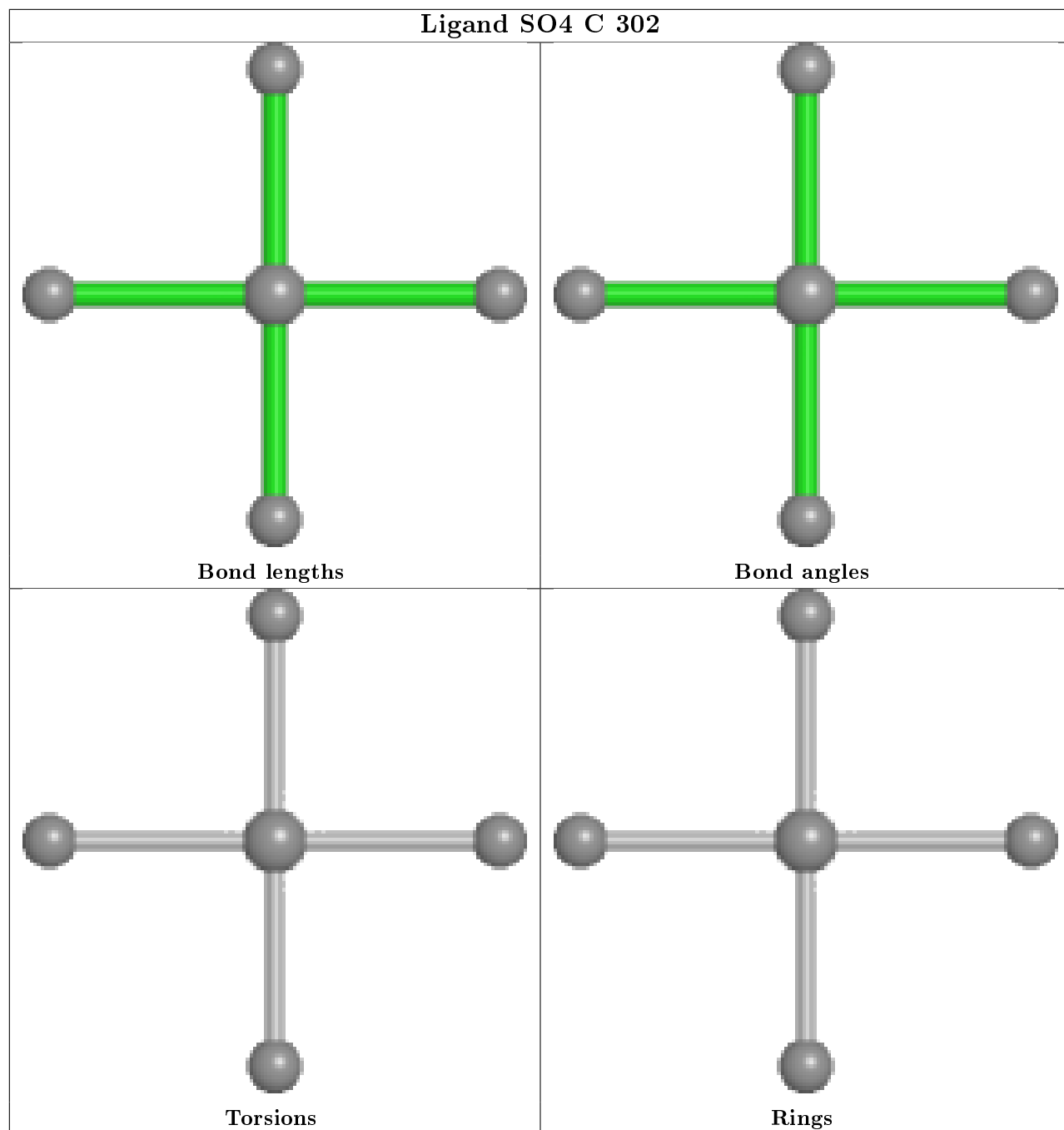
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	304	SO4	1	0
4	D	302	SO4	1	0

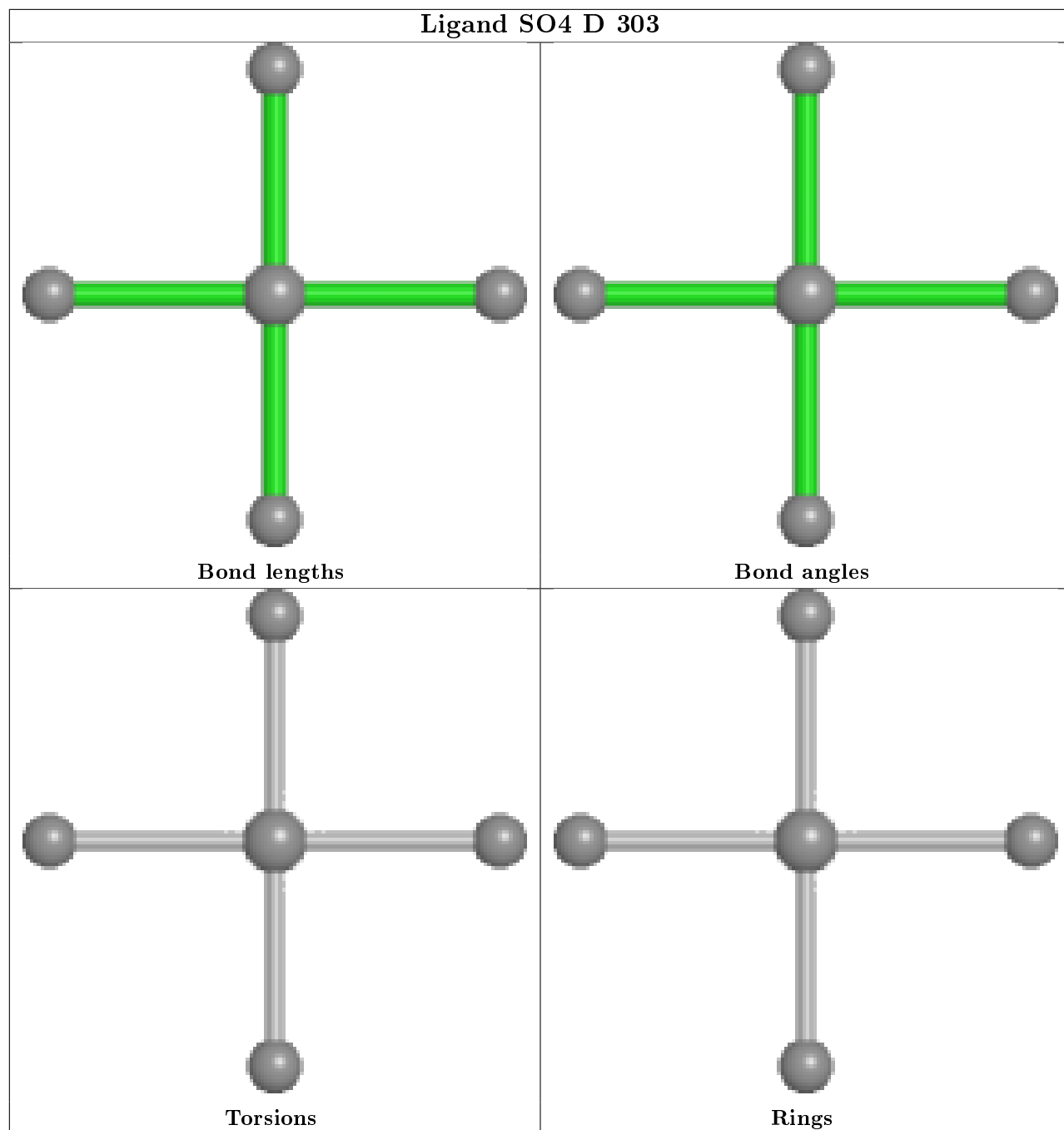
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

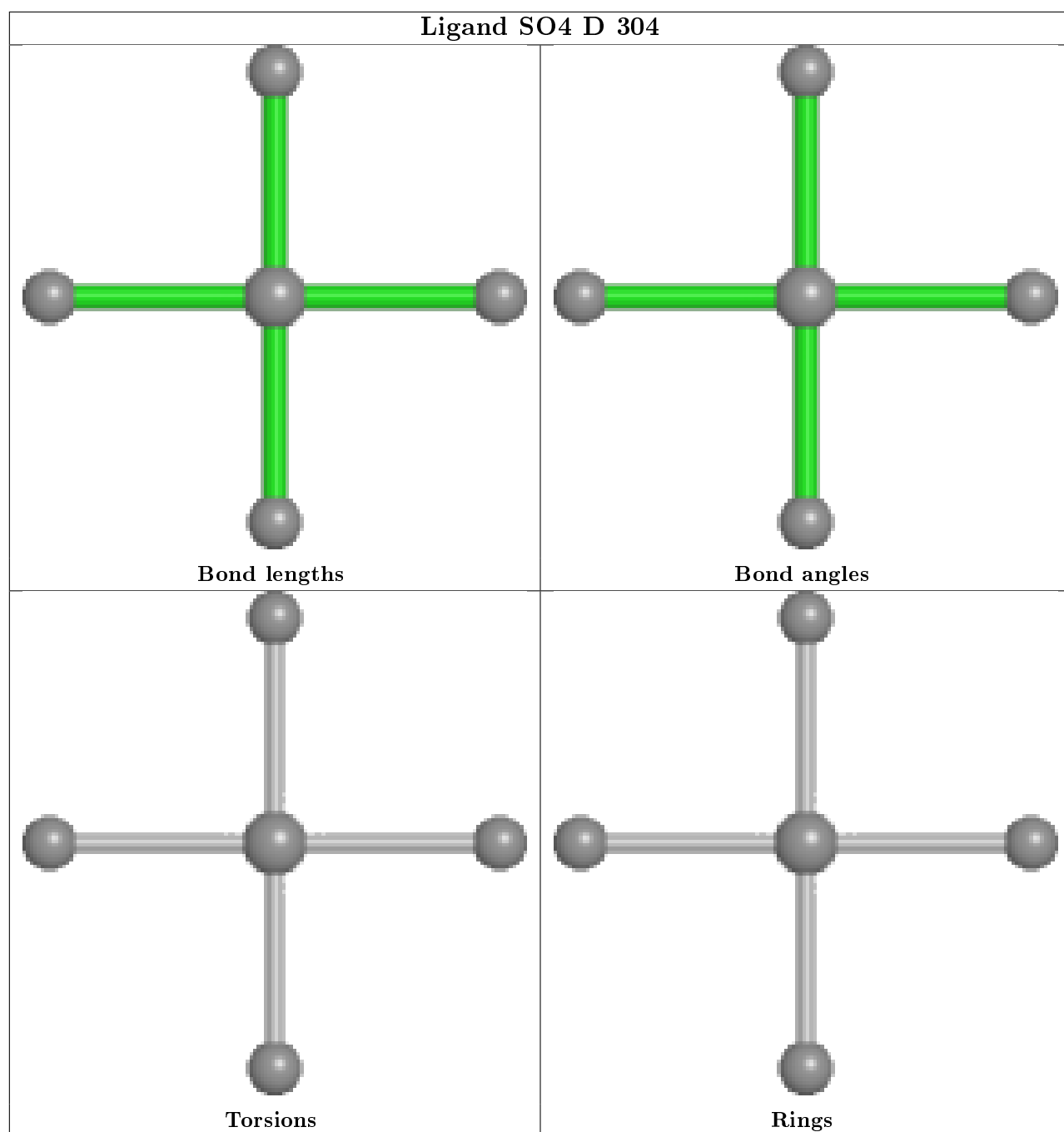


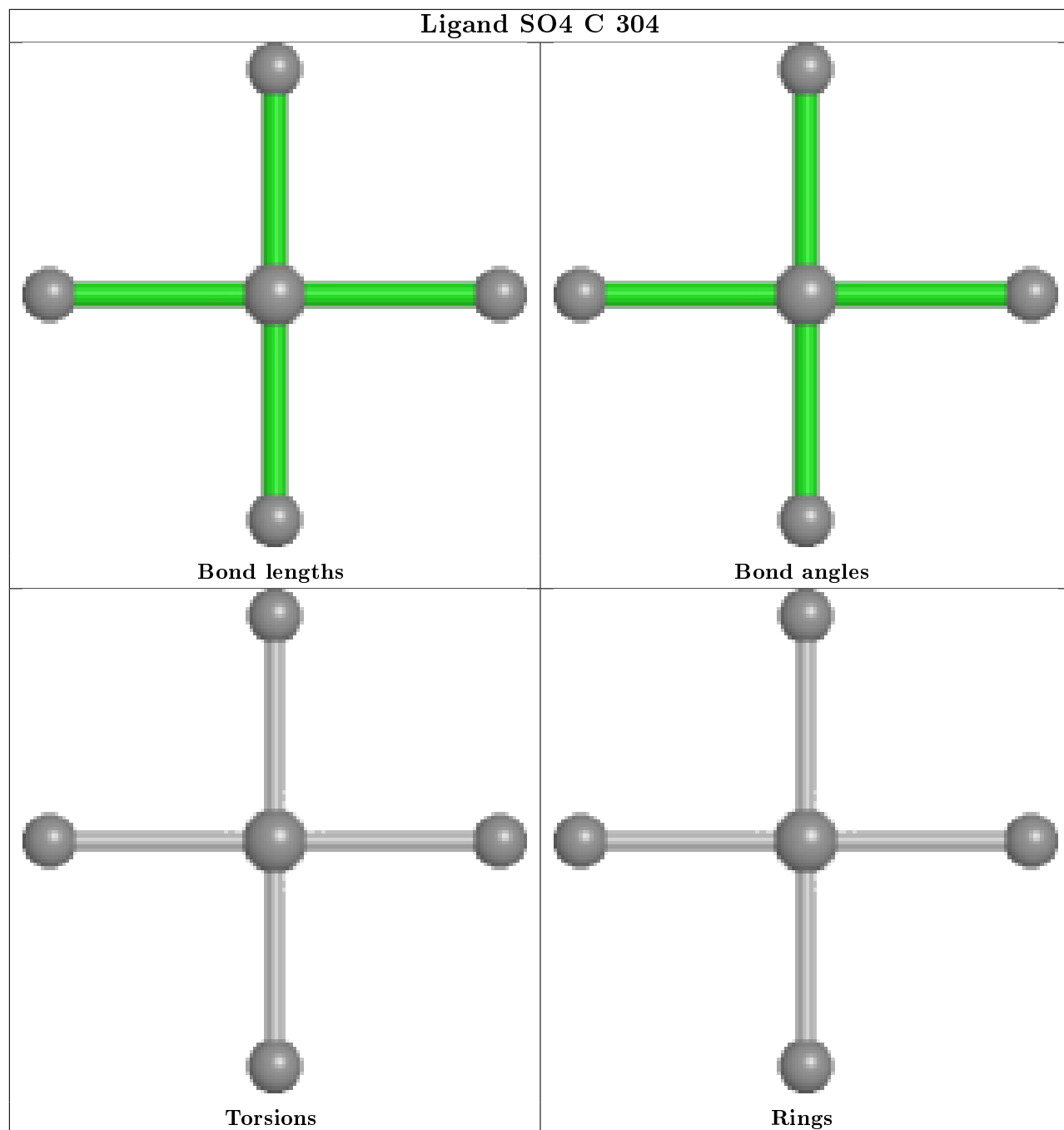


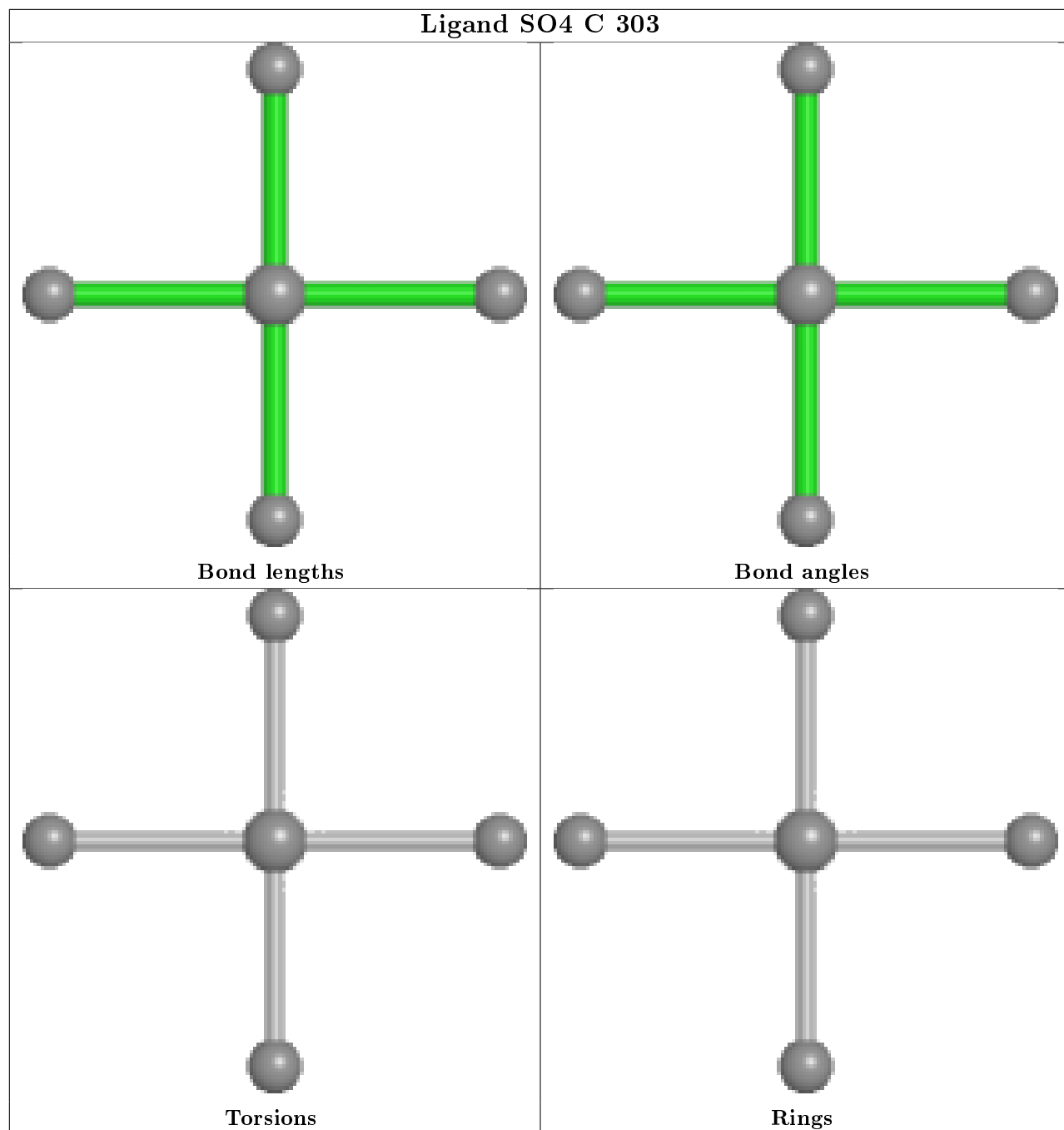


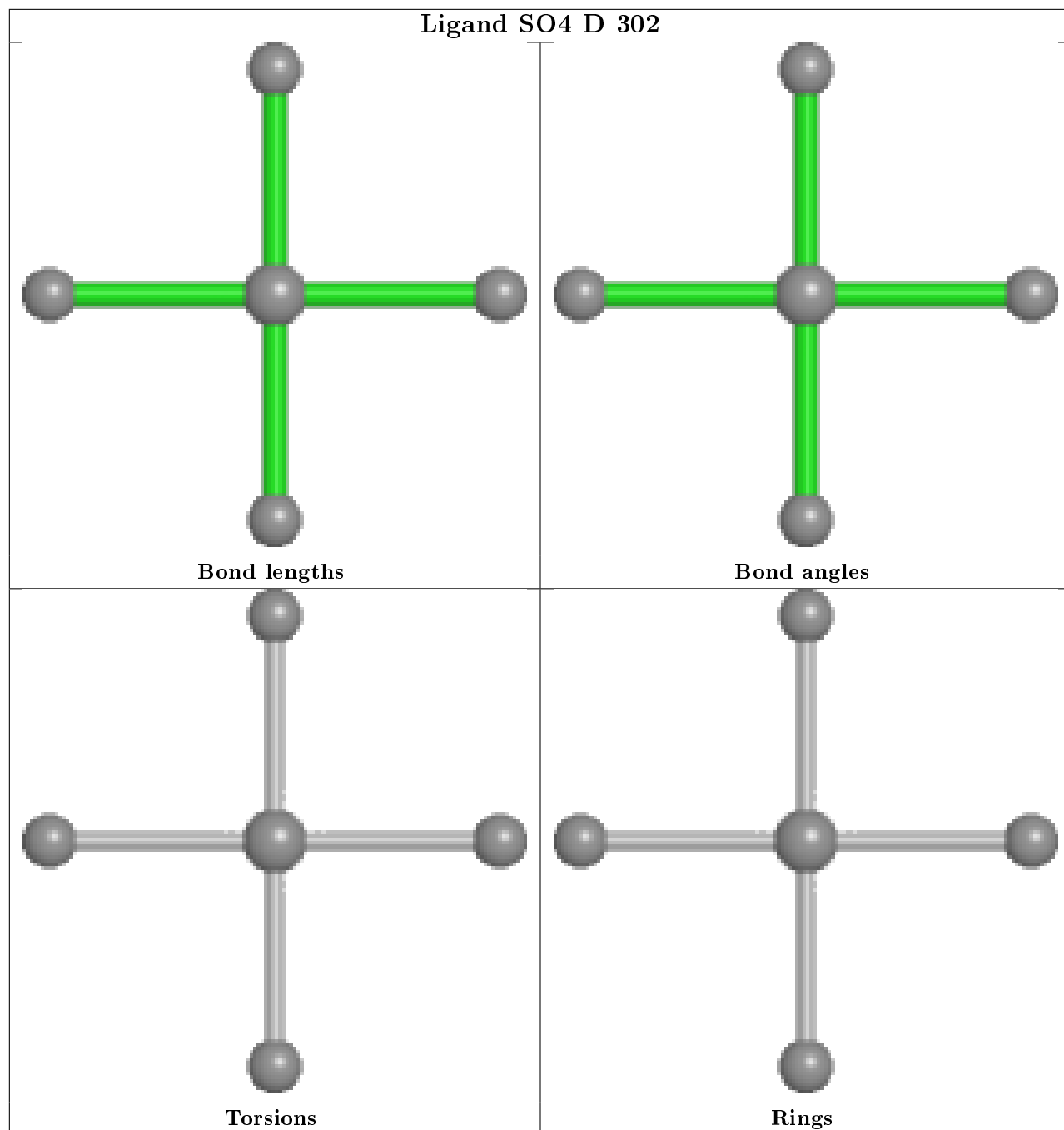


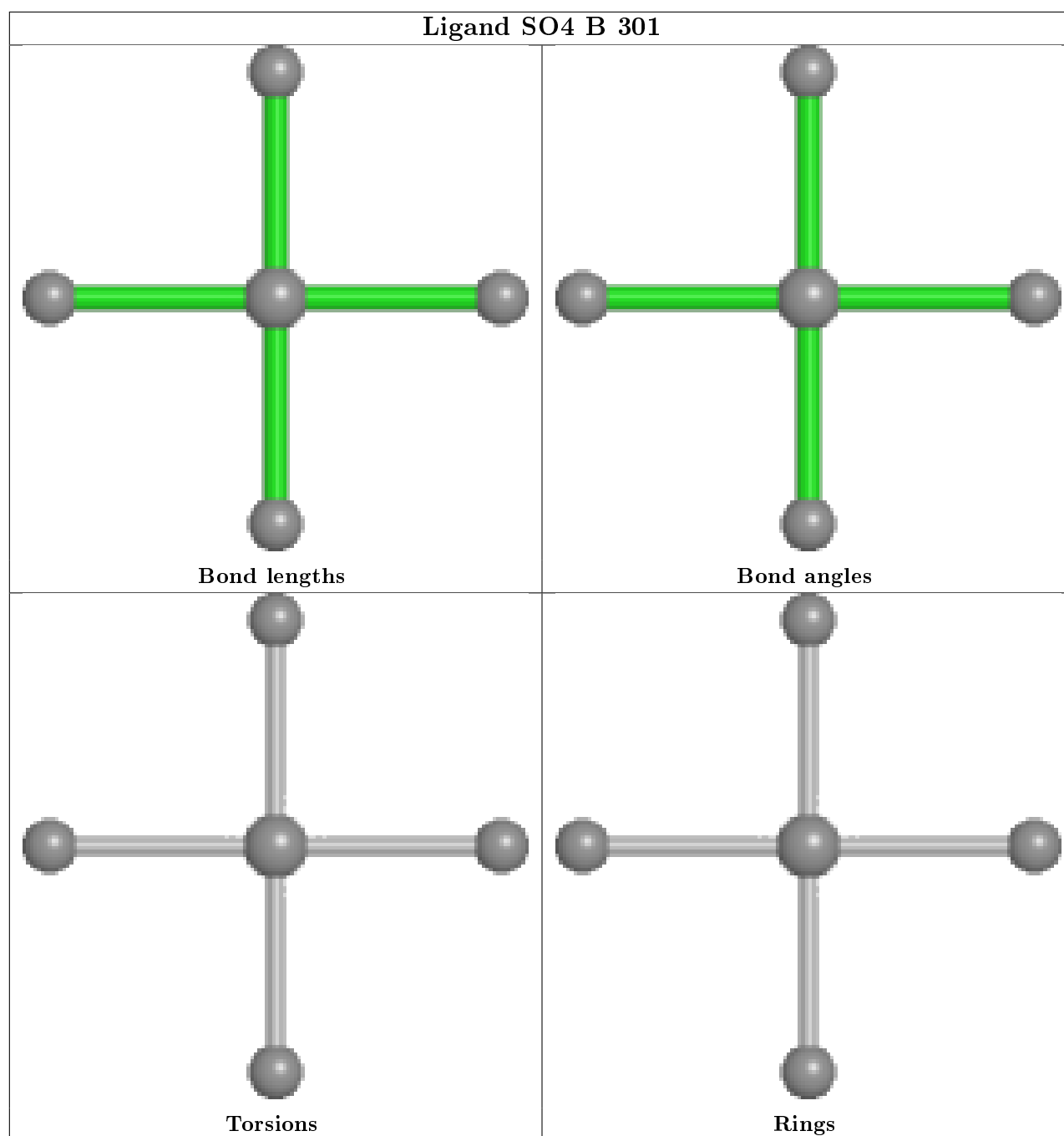












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	211/233 (90%)	0.51	15 (7%)	16	11	44, 72, 113, 126	0
1	F	210/233 (90%)	0.35	7 (3%)	46	39	35, 61, 105, 131	0
2	B	213/216 (98%)	0.56	18 (8%)	10	7	35, 65, 115, 132	0
2	G	212/216 (98%)	0.33	8 (3%)	40	33	32, 60, 101, 109	0
3	C	136/218 (62%)	0.32	5 (3%)	41	34	38, 59, 90, 109	2 (1%)
3	D	136/218 (62%)	0.15	1 (0%)	87	86	32, 50, 78, 114	2 (1%)
All	All	1118/1334 (83%)	0.39	54 (4%)	30	24	32, 62, 106, 132	4 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	55	LEU	5.1
1	A	192	SER	5.0
1	A	165	LEU	4.5
2	B	190	LYS	4.4
1	A	190	VAL	4.1
2	B	186	PRO	4.0
1	F	165	LEU	3.8
2	B	187	GLU	3.8
2	G	131	ALA	3.7
1	A	193	SER	3.7
2	B	193	ARG	3.6
1	A	142	ALA	3.5
2	B	191	SER	3.5
2	B	197	CYS	3.4
2	B	176	TYR	3.4
1	A	1	GLU	3.3
2	G	189	TRP	3.3
1	F	195	LEU	3.3
2	B	192	HIS	3.3

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Mol	Chain	Res	Type	RSRZ
3	C	56	SER	3.3
1	A	167	SER	3.1
1	A	131	ALA	3.1
1	A	143	ALA	3.0
1	A	195	LEU	3.0
2	B	1	GLN	3.0
2	B	154	ALA	2.9
2	G	211	ALA	2.9
2	B	213	THR	2.9
2	B	194	SER	2.8
1	F	162	SER	2.7
2	G	193	ARG	2.6
3	C	171	MET	2.6
1	A	168	GLY	2.6
2	G	154	ALA	2.5
1	F	200	TYR	2.5
1	F	198	GLN	2.5
2	B	161	ALA	2.4
2	G	191	SER	2.4
1	A	76	LYS	2.4
3	C	37	GLY	2.4
1	A	132	PRO	2.3
1	A	164	ALA	2.3
3	D	53	HIS	2.3
1	F	132	PRO	2.2
2	B	140	ILE	2.2
2	B	156	GLY	2.2
3	C	98	VAL	2.2
1	A	65	LYS	2.1
2	B	129	LEU	2.1
1	F	1	GLU	2.1
2	B	139	LEU	2.1
2	B	189	TRP	2.0
2	G	213	THR	2.0
2	G	212	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

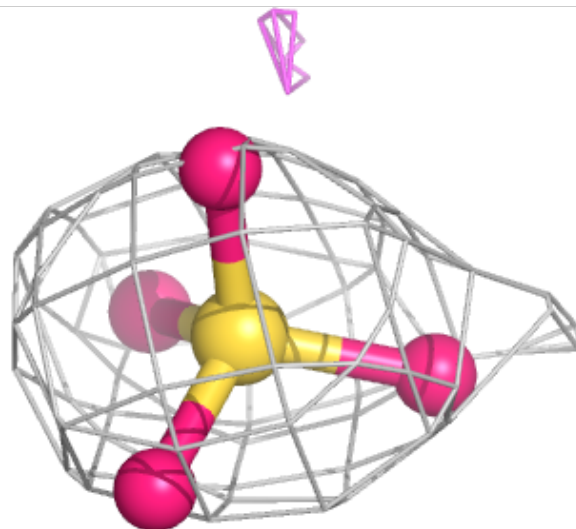
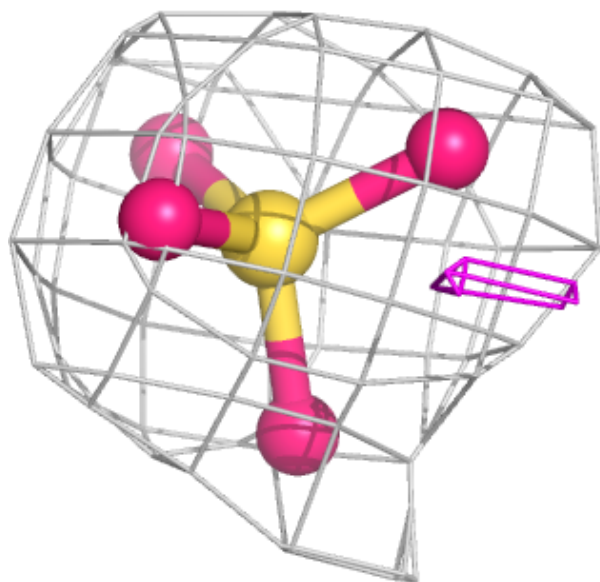
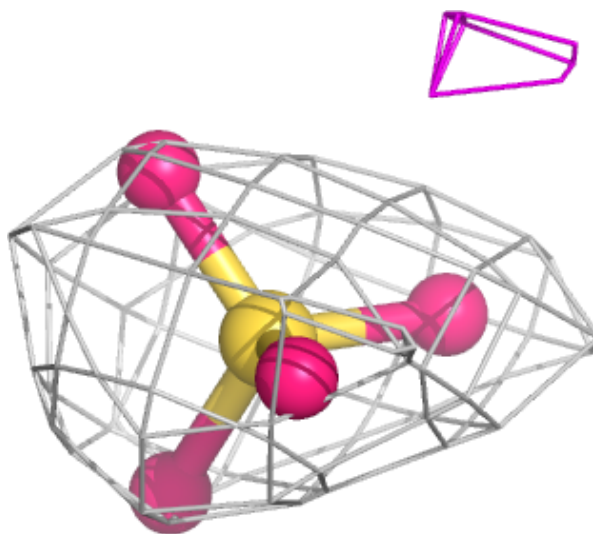
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	SO4	C	304	5/5	0.86	0.35	114,114,136,137	0
4	SO4	C	303	5/5	0.86	0.32	99,102,128,139	0
4	SO4	C	302	5/5	0.88	0.28	96,106,117,117	0
4	SO4	D	302	5/5	0.89	0.27	82,88,112,116	0
4	SO4	D	304	5/5	0.91	0.28	104,105,127,138	0
4	SO4	C	301	5/5	0.92	0.31	86,94,129,140	0
4	SO4	B	301	5/5	0.93	0.19	90,94,113,114	0
4	SO4	G	301	5/5	0.94	0.17	73,78,101,107	0
4	SO4	D	303	5/5	0.95	0.16	88,95,114,117	0
5	NA	F	302	1/1	0.95	0.25	46,46,46,46	0
5	NA	G	302	1/1	0.97	0.21	48,48,48,48	0
5	NA	F	301	1/1	0.98	0.14	46,46,46,46	0
4	SO4	D	301	5/5	0.98	0.12	40,42,58,62	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.

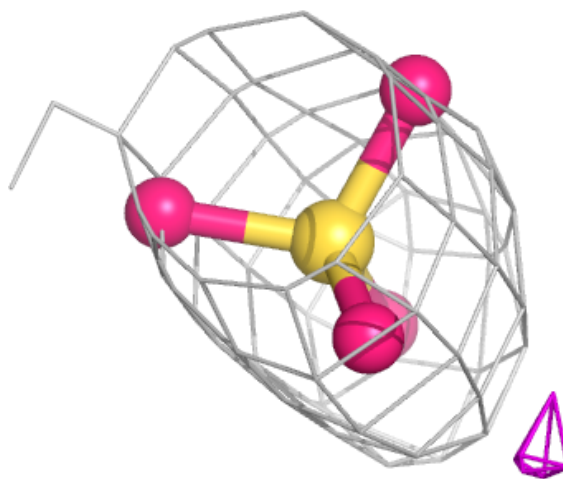
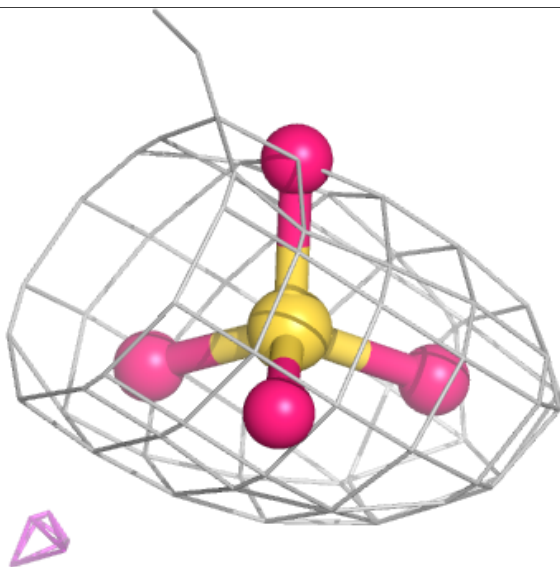
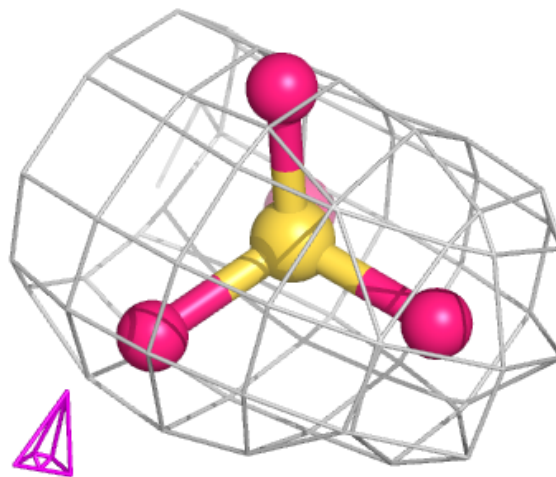
Electron density around SO4 C 304:

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



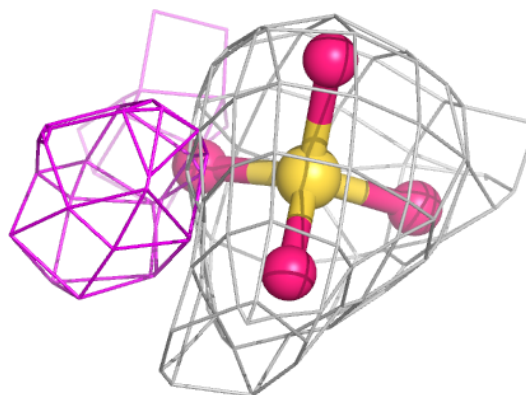
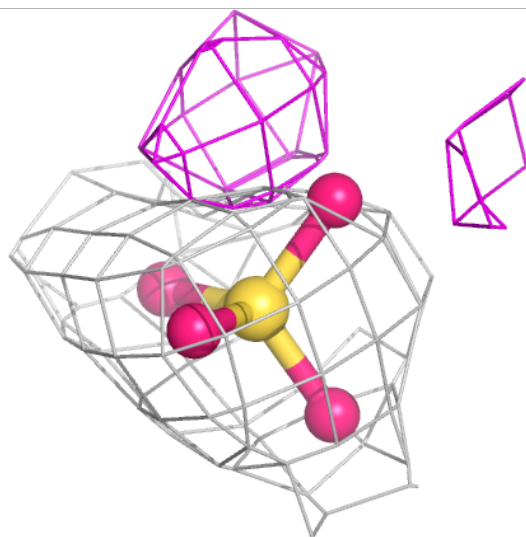
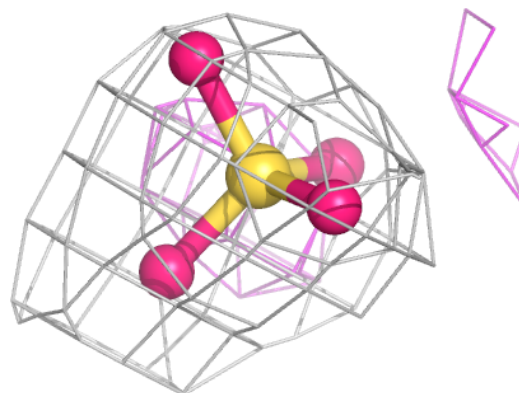
Electron density around SO4 C 303:

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



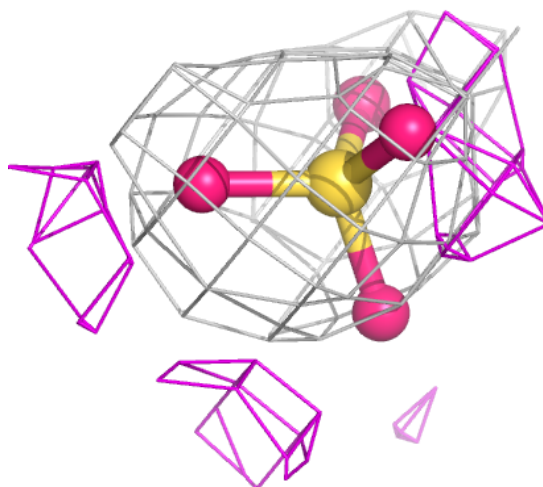
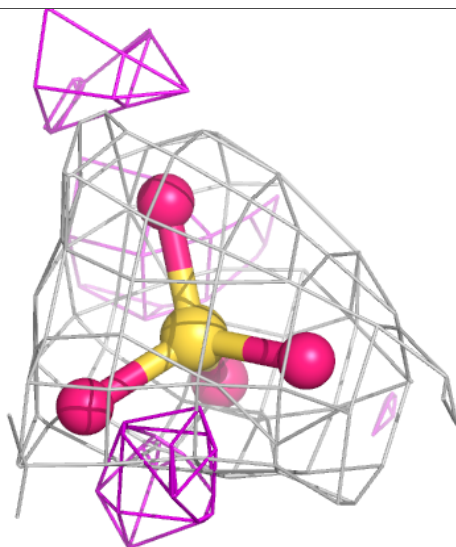
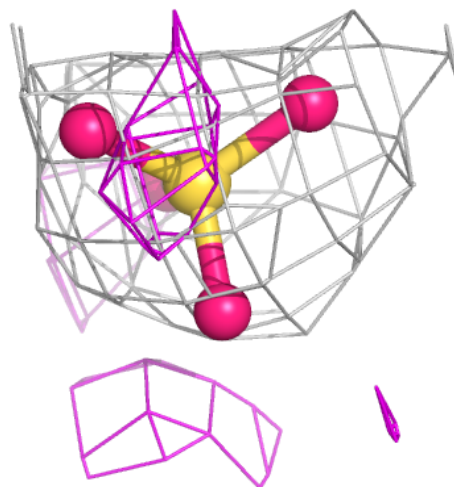
Electron density around SO4 C 302:

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



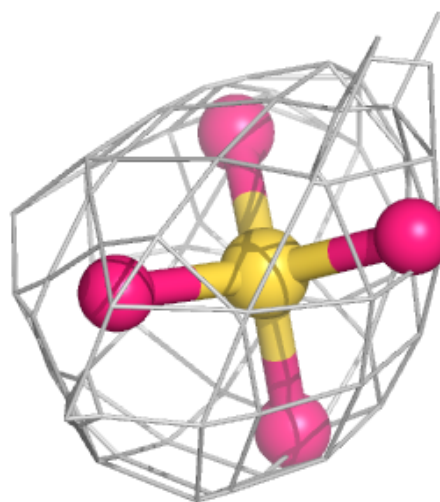
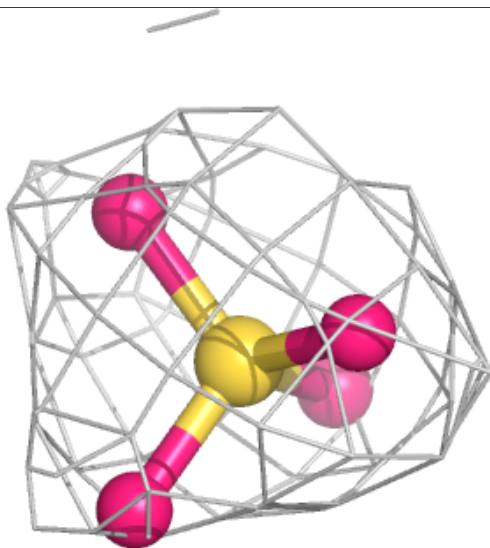
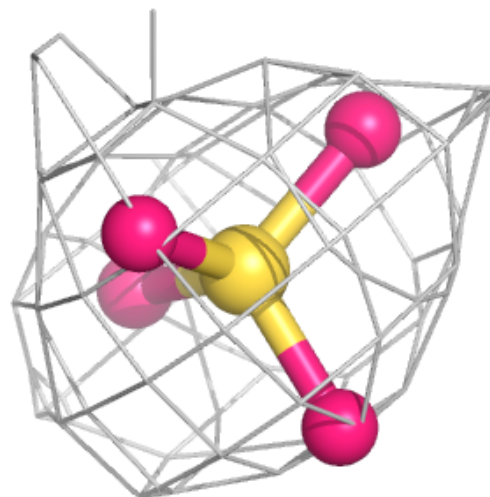
Electron density around SO4 D 302:

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



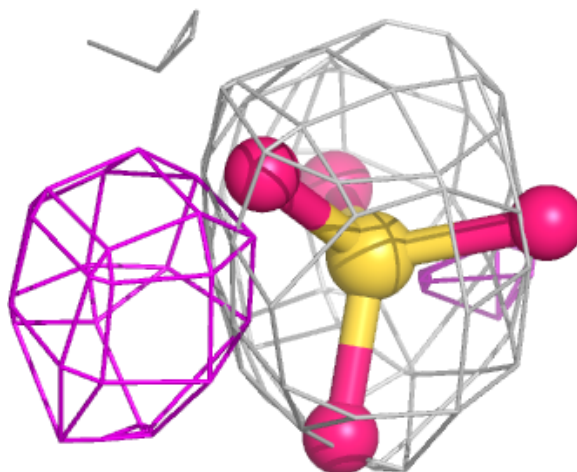
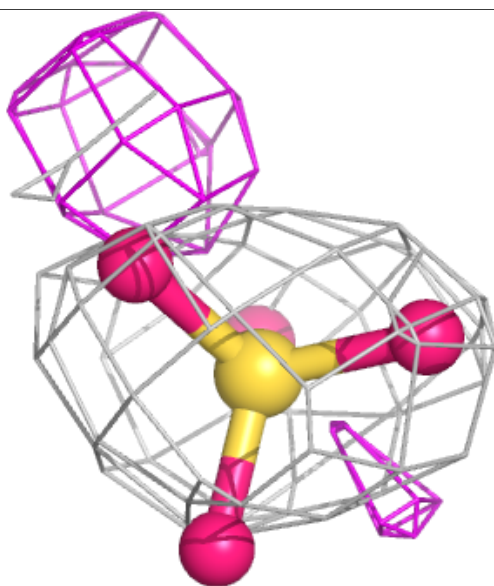
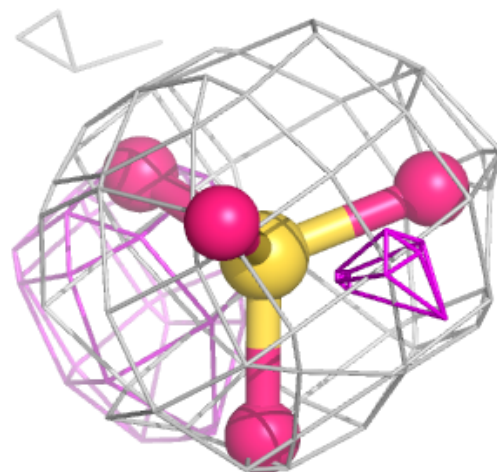
Electron density around SO4 D 304:

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



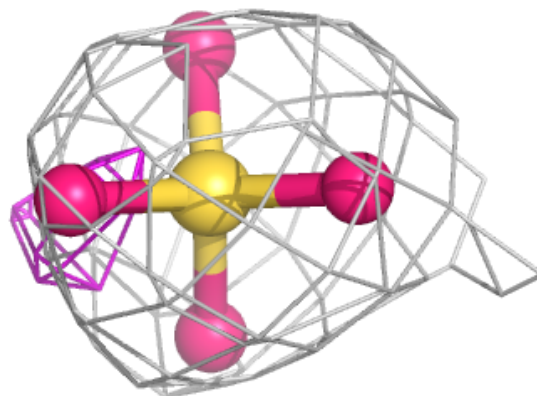
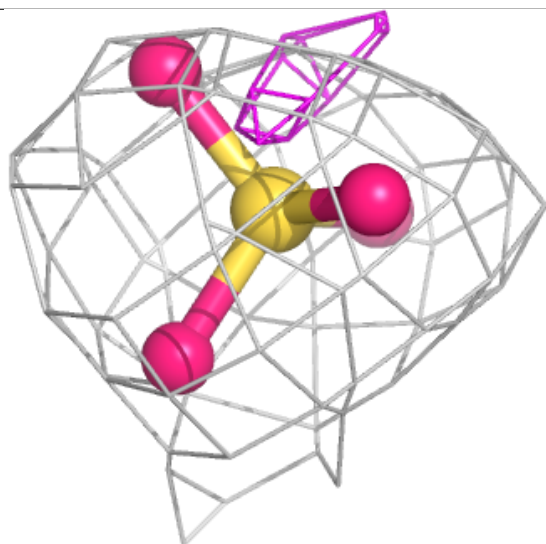
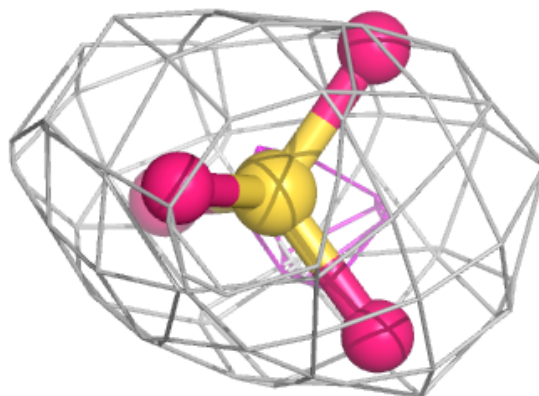
Electron density around SO4 C 301:

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



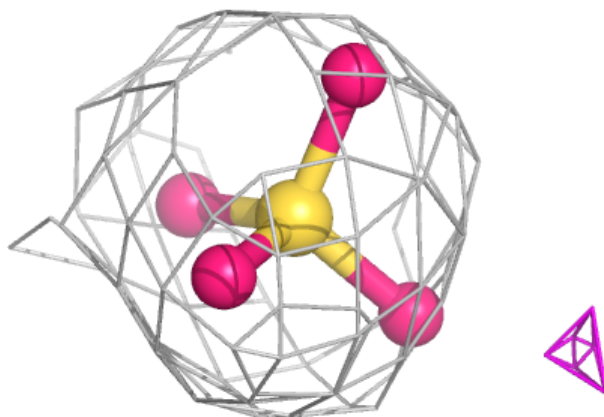
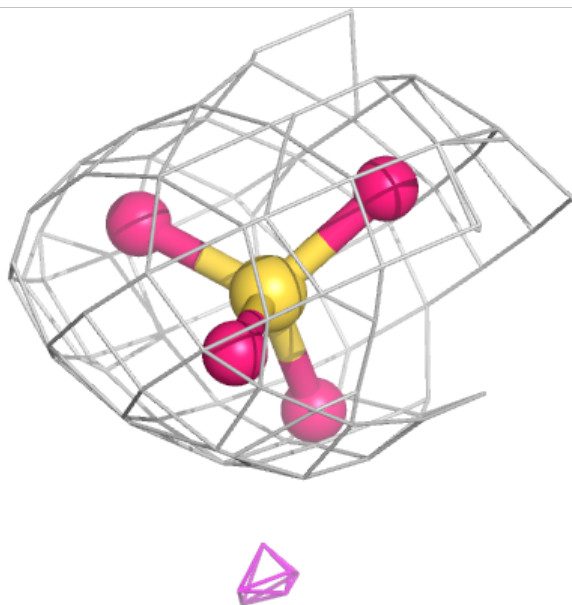
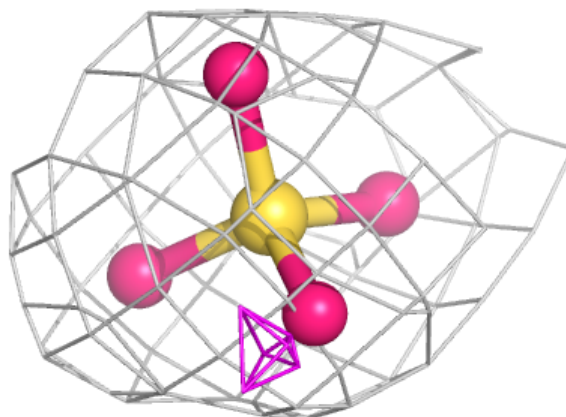
Electron density around SO4 B 301:

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



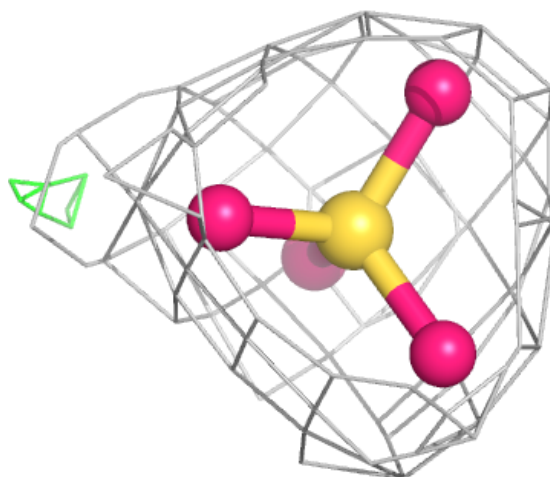
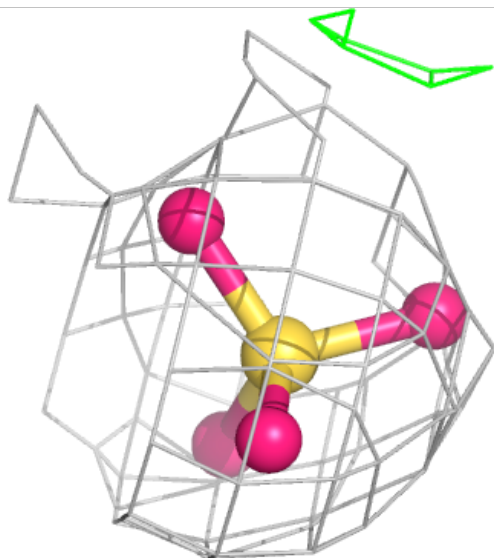
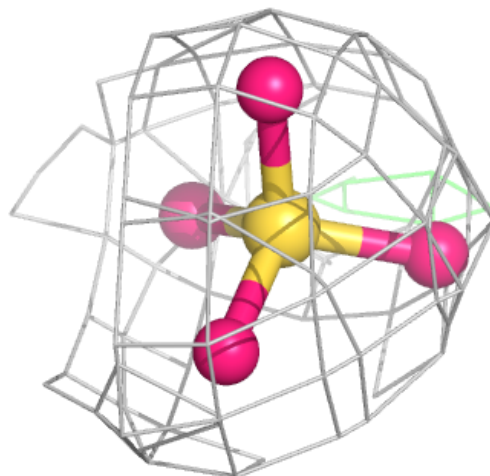
Electron density around SO4 G 301:

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



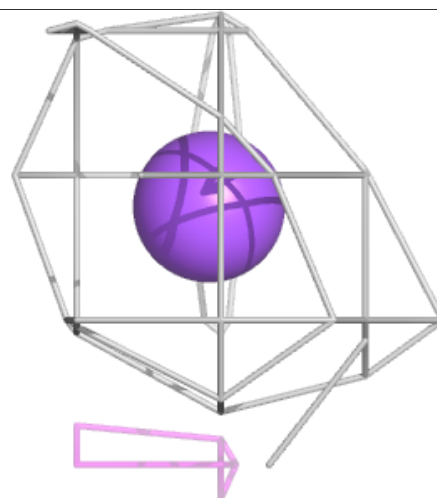
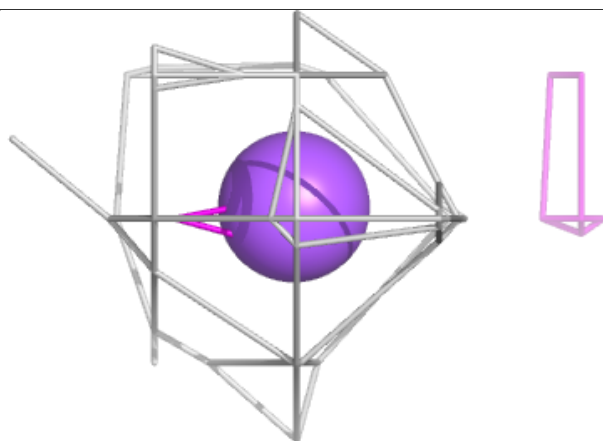
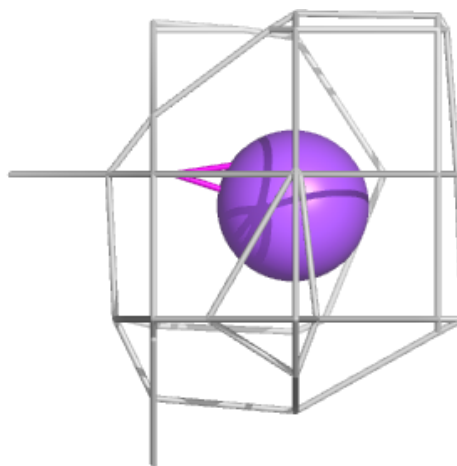
Electron density around SO4 D 303:

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



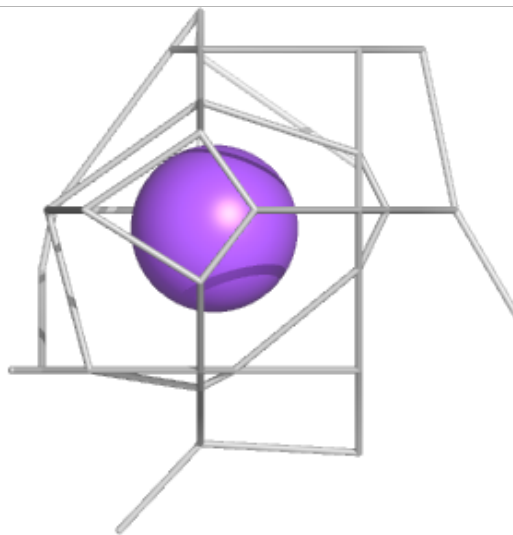
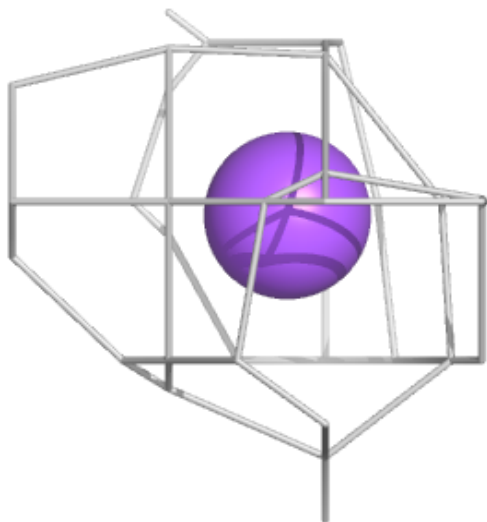
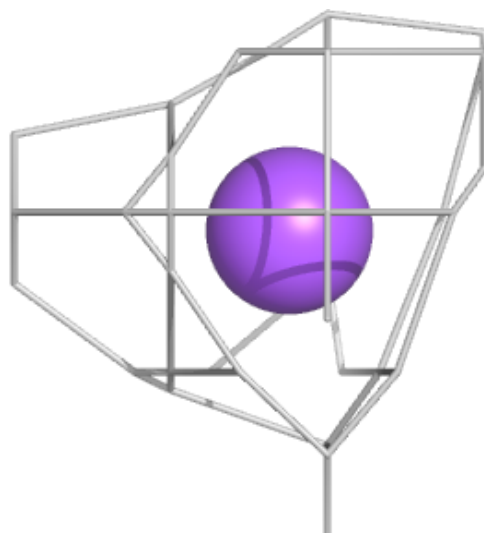
Electron density around NA F 302:

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



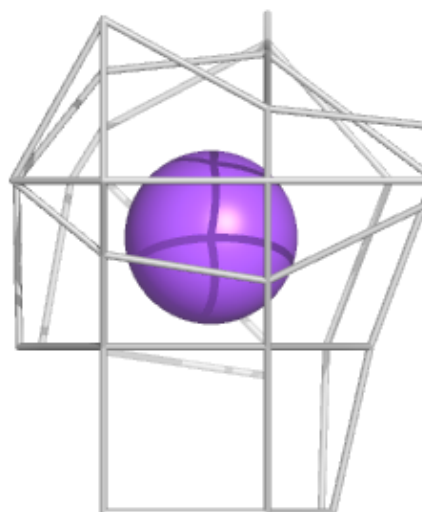
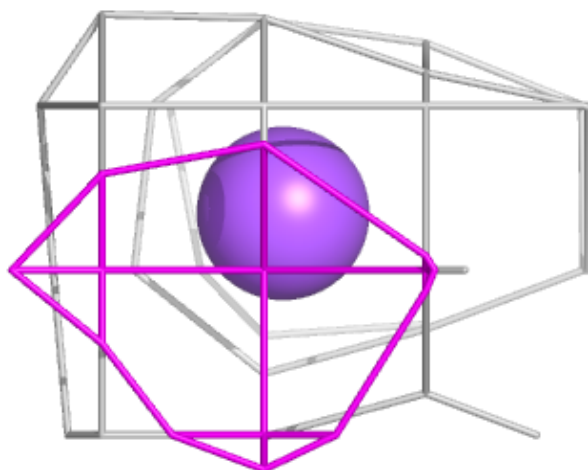
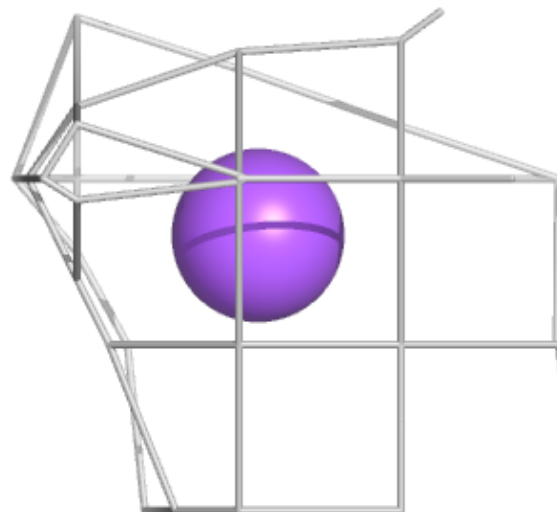
Electron density around NA G 302:

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



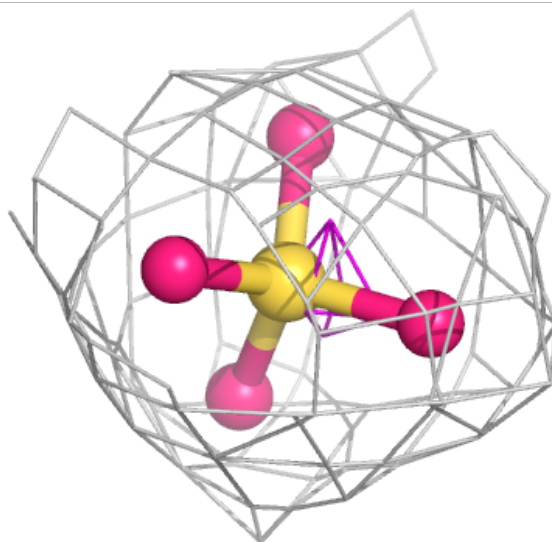
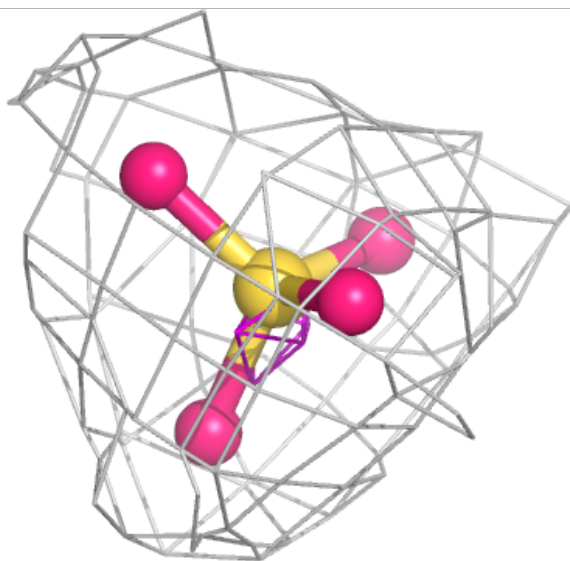
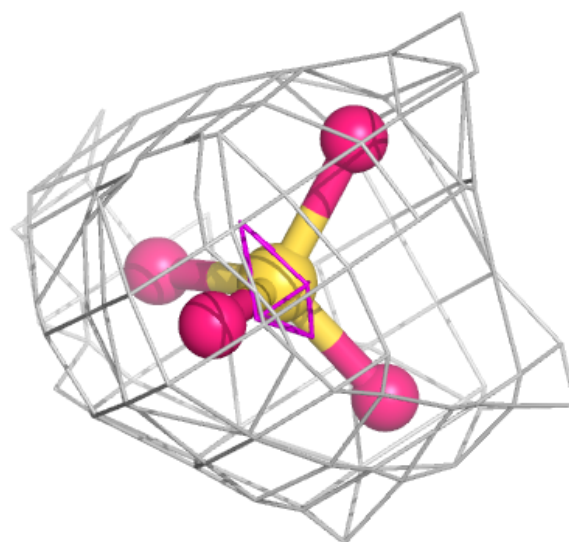
Electron density around NA F 301:

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



Electron density around SO4 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.