



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 21, 2023 – 04:11 PM JST

PDB ID : 7VRX
Title : Pad-1 in the absence of substrate
Authors : Choi, M.; Rhee, S.
Deposited on : 2021-10-25
Resolution : 1.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

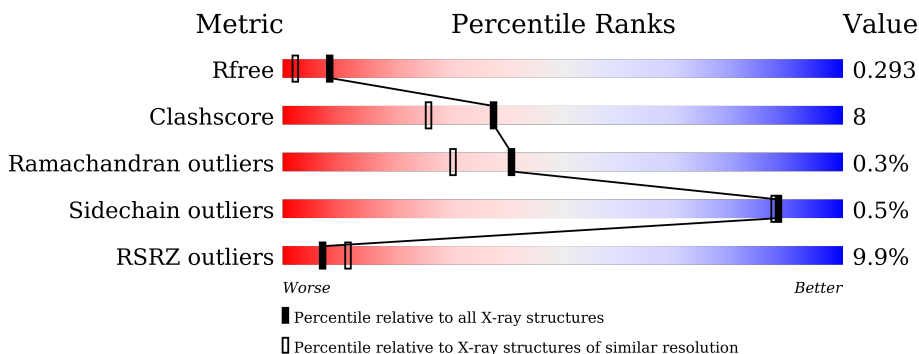
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	404	
1	B	404	
1	C	404	
1	D	404	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 11513 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 Aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	359	2794	1795	463	515	1	20	0	0	0
1	B	352	2740	1760	450	510	1	19	0	0	0
1	C	363	2833	1817	472	523	1	20	0	0	0
1	D	357	2782	1787	461	513	1	20	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

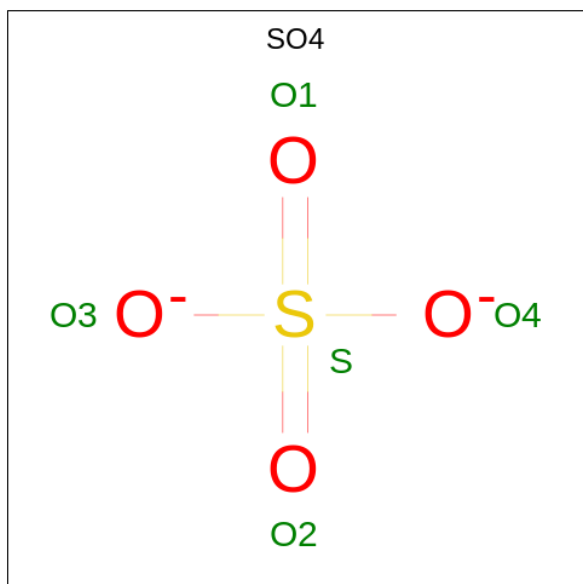
Chain	Residue	Modelled	Actual	Comment	Reference
A	395	LEU	-	expression tag	UNP A0A6J4AG16
A	396	GLU	-	expression tag	UNP A0A6J4AG16
A	397	HIS	-	expression tag	UNP A0A6J4AG16
A	398	HIS	-	expression tag	UNP A0A6J4AG16
A	399	HIS	-	expression tag	UNP A0A6J4AG16
A	400	HIS	-	expression tag	UNP A0A6J4AG16
A	401	HIS	-	expression tag	UNP A0A6J4AG16
A	402	HIS	-	expression tag	UNP A0A6J4AG16
A	403	HIS	-	expression tag	UNP A0A6J4AG16
A	404	HIS	-	expression tag	UNP A0A6J4AG16
B	395	LEU	-	expression tag	UNP A0A6J4AG16
B	396	GLU	-	expression tag	UNP A0A6J4AG16
B	397	HIS	-	expression tag	UNP A0A6J4AG16
B	398	HIS	-	expression tag	UNP A0A6J4AG16
B	399	HIS	-	expression tag	UNP A0A6J4AG16
B	400	HIS	-	expression tag	UNP A0A6J4AG16
B	401	HIS	-	expression tag	UNP A0A6J4AG16
B	402	HIS	-	expression tag	UNP A0A6J4AG16
B	403	HIS	-	expression tag	UNP A0A6J4AG16
B	404	HIS	-	expression tag	UNP A0A6J4AG16
C	395	LEU	-	expression tag	UNP A0A6J4AG16

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Chain	Residue	Modelled	Actual	Comment	Reference
C	396	GLU	-	expression tag	UNP A0A6J4AG16
C	397	HIS	-	expression tag	UNP A0A6J4AG16
C	398	HIS	-	expression tag	UNP A0A6J4AG16
C	399	HIS	-	expression tag	UNP A0A6J4AG16
C	400	HIS	-	expression tag	UNP A0A6J4AG16
C	401	HIS	-	expression tag	UNP A0A6J4AG16
C	402	HIS	-	expression tag	UNP A0A6J4AG16
C	403	HIS	-	expression tag	UNP A0A6J4AG16
C	404	HIS	-	expression tag	UNP A0A6J4AG16
D	395	LEU	-	expression tag	UNP A0A6J4AG16
D	396	GLU	-	expression tag	UNP A0A6J4AG16
D	397	HIS	-	expression tag	UNP A0A6J4AG16
D	398	HIS	-	expression tag	UNP A0A6J4AG16
D	399	HIS	-	expression tag	UNP A0A6J4AG16
D	400	HIS	-	expression tag	UNP A0A6J4AG16
D	401	HIS	-	expression tag	UNP A0A6J4AG16
D	402	HIS	-	expression tag	UNP A0A6J4AG16
D	403	HIS	-	expression tag	UNP A0A6J4AG16
D	404	HIS	-	expression tag	UNP A0A6J4AG16

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	114	Total	O	0	0
			114	114		
3	B	90	Total	O	0	0
			90	90		
3	C	69	Total	O	0	0
			69	69		
3	D	71	Total	O	0	0
			71	71		

4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	96.16Å 96.16Å 407.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.86 – 1.97 33.86 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.86-1.97) 93.8 (33.86-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.01 (at 1.97Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.253 , 0.291 0.259 , 0.293	Depositor DCC
R_{free} test set	1986 reflections (1.33%)	wwPDB-VP
Wilson B-factor (Å ²)	35.9	Xtrriage
Anisotropy	0.124	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 45.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	0.114 for h,-h-k,-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11513	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.34	0/2834	0.54	0/3852
1	B	0.34	0/2780	0.54	0/3781
1	C	0.30	0/2873	0.52	0/3903
1	D	0.34	1/2822 (0.0%)	0.52	0/3835
All	All	0.33	1/11309 (0.0%)	0.53	0/15371

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	327	LEU	C-N	8.09	1.49	1.34

There are no bond angle outliers.

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	2794	0	2796	37	0
1	B	2740	0	2723	48	0
1	C	2833	0	2833	64	0
1	D	2782	0	2781	43	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	114	0	0	2	0
3	B	90	0	0	2	0
3	C	69	0	0	1	0
3	D	71	0	0	1	0
All	All	11513	0	11133	172	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 (172) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:PRO:HA	1:D:20:VAL:HG23	1.32	1.06
1:C:23:GLN:HE22	1:D:260:LYS:HA	1.22	1.03
1:D:17:PRO:HA	1:D:20:VAL:CG2	1.95	0.97
1:A:118:MET:SD	3:A:684:HOH:O	2.36	0.82
1:C:33:ILE:HD11	1:C:374:ARG:CZ	2.12	0.79
1:C:33:ILE:HD11	1:C:374:ARG:NE	1.97	0.79
1:D:17:PRO:CA	1:D:20:VAL:HG23	2.14	0.76
1:C:33:ILE:HD11	1:C:374:ARG:NH2	2.01	0.76
1:C:33:ILE:CD1	1:C:374:ARG:HE	1.99	0.75
1:C:23:GLN:HE21	1:D:263:ASP:HB3	1.53	0.72
1:B:16:THR:HG23	1:B:17:PRO:HD3	1.74	0.70
1:B:311:LYS:NZ	3:B:601:HOH:O	2.27	0.67
1:A:233:LLP:OP1	1:A:241:ARG:NH2	2.24	0.66
1:D:20:VAL:HG13	1:D:131:GLN:HB2	1.77	0.66
1:C:98:ALA:HB2	1:C:230:SER:HB2	1.79	0.65
1:A:302:LEU:HD23	1:A:376:ALA:HB2	1.78	0.65
1:A:260:LYS:HD3	1:B:20:VAL:HG23	1.79	0.64
1:A:16:THR:O	1:A:20:VAL:HG23	1.99	0.63
1:A:275:ARG:NH1	3:A:602:HOH:O	2.31	0.63
1:B:23:GLN:OE1	1:B:23:GLN:N	2.31	0.62
1:B:312:GLY:O	1:B:315:LYS:NZ	2.32	0.62
1:A:14:THR:HG21	1:B:110:CYS:C	2.20	0.62
1:B:335:PHE:CE2	1:B:353:SER:OG	2.50	0.62
1:C:33:ILE:CD1	1:C:374:ARG:NE	2.59	0.61
1:B:41:TYR:CG	1:B:369:ILE:CG2	2.84	0.61
1:C:23:GLN:HA	1:C:124:PHE:HE2	1.65	0.61
1:A:260:LYS:HA	1:B:23:GLN:NE2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD22	1:D:221:GLU:HB3	1.83	0.60
1:B:328:PRO:HG2	1:B:331:TYR:HD2	1.67	0.59
1:C:20:VAL:CG2	1:D:260:LYS:HD3	2.32	0.59
1:C:23:GLN:NE2	1:D:263:ASP:HB3	2.18	0.58
1:C:117:VAL:HB	1:C:169:VAL:HG22	1.84	0.58
1:B:233:LLP:OP1	1:B:241:ARG:NH2	2.34	0.57
1:B:41:TYR:CD1	1:B:369:ILE:CG2	2.87	0.57
1:A:87:LEU:HD22	1:A:221:GLU:HB3	1.85	0.57
1:B:369:ILE:O	1:B:369:ILE:HG13	2.04	0.57
1:C:23:GLN:N	1:C:23:GLN:OE1	2.38	0.57
1:C:188:LYS:NZ	3:C:602:HOH:O	2.37	0.56
1:A:260:LYS:HD3	1:B:20:VAL:CG2	2.34	0.56
1:B:16:THR:O	1:B:20:VAL:HG13	2.04	0.56
1:B:17:PRO:HA	1:B:20:VAL:HG13	1.87	0.56
1:D:98:ALA:HB2	1:D:230:SER:HB2	1.88	0.56
1:A:334:ASP:OD1	1:A:359:GLY:N	2.38	0.55
1:C:33:ILE:HD11	1:C:374:ARG:HH21	1.71	0.55
1:B:41:TYR:CG	1:B:369:ILE:HG23	2.42	0.55
1:C:17:PRO:HG3	1:D:108:THR:HA	1.89	0.55
1:D:334:ASP:OD1	1:D:334:ASP:N	2.39	0.54
1:A:49:LEU:HD12	1:C:332:MET:HE1	1.90	0.54
1:A:302:LEU:HD12	1:A:365:PHE:HB3	1.88	0.54
1:C:23:GLN:NE2	1:D:260:LYS:HA	2.06	0.54
1:C:214:ASN:OD1	1:C:216:LYS:NZ	2.41	0.53
1:A:312:GLY:O	1:A:315:LYS:NZ	2.43	0.52
1:B:117:VAL:HB	1:B:169:VAL:HG22	1.92	0.52
1:A:114:ASP:OD2	1:A:167:LYS:HG3	2.09	0.52
1:D:262:GLN:O	1:D:266:PRO:HD2	2.09	0.52
1:B:51:LYS:O	1:B:54:GLU:HG2	2.10	0.51
1:C:23:GLN:HB2	1:C:25:LEU:HG	1.92	0.51
1:C:192:ASP:O	1:C:196:LYS:HG2	2.11	0.51
1:D:16:THR:O	1:D:20:VAL:CG2	2.58	0.51
1:D:332:MET:HA	1:D:359:GLY:HA2	1.92	0.51
1:D:231:PHE:HE2	1:D:281:MET:HG3	1.76	0.51
1:A:108:THR:HA	1:B:17:PRO:HG3	1.94	0.50
1:B:87:LEU:HD22	1:B:221:GLU:HB3	1.92	0.50
1:D:17:PRO:HA	1:D:20:VAL:HG21	1.90	0.50
1:B:20:VAL:HG12	1:B:131:GLN:HB3	1.94	0.50
1:C:262:GLN:O	1:C:266:PRO:HD2	2.12	0.50
1:C:349:LEU:HD22	1:C:363:VAL:HG22	1.93	0.50
1:C:87:LEU:HD22	1:C:221:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:PRO:HG2	1:B:331:TYR:CD2	2.47	0.49
1:D:109:LEU:HD13	1:D:200:TRP:CG	2.47	0.49
1:D:329:ASP:O	1:D:332:MET:SD	2.71	0.49
1:A:260:LYS:HA	1:B:23:GLN:HE22	1.77	0.49
1:D:253:GLY:O	1:D:257:GLN:HG2	2.13	0.49
1:C:20:VAL:HG23	1:D:260:LYS:HD3	1.95	0.49
1:C:23:GLN:HA	1:C:124:PHE:CE2	2.46	0.49
1:A:347:VAL:HG23	1:A:378:GLU:HB2	1.94	0.48
1:C:302:LEU:HD12	1:C:365:PHE:HB3	1.94	0.48
1:D:168:LEU:CB	1:D:200:TRP:HB2	2.43	0.48
1:C:295:LEU:HD22	1:C:366:GLY:HA2	1.94	0.48
1:B:23:GLN:HA	1:B:124:PHE:CZ	2.49	0.48
1:D:328:PRO:HB2	1:D:331:TYR:HD1	1.79	0.48
1:B:23:GLN:HA	1:B:124:PHE:CE2	2.48	0.48
1:C:35:LEU:HD13	1:C:363:VAL:HG13	1.95	0.48
1:C:14:THR:HG23	1:D:111:ASP:CG	2.35	0.47
1:A:349:LEU:HD22	1:A:363:VAL:HG22	1.96	0.47
1:B:286:GLU:H	1:B:286:GLU:CD	2.19	0.46
1:C:379:ARG:HD3	1:C:379:ARG:HA	1.61	0.46
1:C:23:GLN:HG3	1:C:128:MET:SD	2.56	0.46
1:A:14:THR:O	1:A:17:PRO:HD2	2.15	0.46
1:A:262:GLN:O	1:A:266:PRO:HD2	2.14	0.46
1:C:253:GLY:O	1:C:257:GLN:HG2	2.15	0.46
1:C:286:GLU:H	1:C:286:GLU:CD	2.19	0.46
1:A:12:VAL:HB	1:A:13:LEU:H	1.59	0.46
1:D:168:LEU:HB3	1:D:200:TRP:HB2	1.98	0.46
1:C:326:LYS:HG2	1:C:327:LEU:O	2.16	0.46
1:C:14:THR:O	1:C:17:PRO:HD2	2.15	0.46
1:B:41:TYR:CD1	1:B:369:ILE:HG22	2.51	0.45
1:B:17:PRO:O	1:B:20:VAL:HG22	2.16	0.45
1:C:36:ALA:O	1:C:362:ARG:NH2	2.44	0.45
1:A:104:ASN:HA	1:A:261:VAL:HG11	1.99	0.45
1:B:270:SER:HB2	1:B:273:SER:HB2	1.97	0.45
1:C:299:ARG:NH1	1:C:317:GLY:O	2.48	0.45
1:A:233:LLP:P	1:A:241:ARG:HH22	2.37	0.45
1:A:168:LEU:HD11	1:A:202:VAL:HG21	1.99	0.45
1:A:250:GLU:H	1:A:250:GLU:CD	2.19	0.45
1:C:84:GLU:OE1	1:C:209:TYR:OH	2.28	0.45
1:A:33:ILE:HG21	1:A:375:ALA:HB2	1.99	0.44
1:A:265:ILE:HB	1:A:266:PRO:HD3	1.98	0.44
1:C:184:GLU:O	1:C:188:LYS:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:VAL:HB	1:D:169:VAL:HG22	1.99	0.44
1:C:38:GLY:HA3	1:C:322:TYR:OH	2.18	0.44
1:B:311:LYS:HD2	1:B:312:GLY:H	1.83	0.44
1:C:326:LYS:HB2	1:C:360:TYR:CE2	2.53	0.44
1:B:349:LEU:HD22	1:B:363:VAL:HG22	2.00	0.44
1:C:23:GLN:HG2	1:D:263:ASP:OD2	2.18	0.44
1:B:41:TYR:CB	1:B:369:ILE:HG23	2.48	0.43
1:B:232:SER:O	1:B:238:MET:HG3	2.18	0.43
1:C:20:VAL:HG12	1:C:131:GLN:CB	2.49	0.43
1:C:272:ILE:HD13	1:D:272:ILE:HD13	2.00	0.43
1:D:13:LEU:N	3:D:610:HOH:O	2.50	0.43
1:B:181:TYR:CE1	1:B:215:ARG:HD3	2.54	0.43
1:C:128:MET:HB3	1:C:128:MET:HE2	1.66	0.43
1:C:181:TYR:CE2	1:C:215:ARG:HD3	2.53	0.43
1:C:349:LEU:HD11	1:C:378:GLU:OE2	2.17	0.43
1:B:22:ILE:O	1:B:124:PHE:HZ	2.01	0.43
1:D:286:GLU:H	1:D:286:GLU:CD	2.22	0.43
1:B:20:VAL:HG11	1:B:132:MET:HA	2.01	0.43
1:C:296:VAL:O	1:C:300:GLU:HG2	2.18	0.43
1:B:233:LLP:P	1:B:241:ARG:HH22	2.41	0.42
1:C:265:ILE:HG12	1:D:103:VAL:HG21	2.01	0.42
1:B:98:ALA:HB2	1:B:230:SER:HB2	2.02	0.42
1:C:376:ALA:C	1:C:378:GLU:H	2.23	0.42
1:C:16:THR:O	1:C:20:VAL:HG13	2.19	0.42
1:A:265:ILE:HB	1:A:266:PRO:CD	2.49	0.42
1:D:16:THR:O	1:D:20:VAL:HG23	2.20	0.42
1:A:341:LEU:HB3	1:A:347:VAL:O	2.19	0.42
1:C:33:ILE:CD1	1:C:374:ARG:HH21	2.32	0.42
1:C:104:ASN:HA	1:C:261:VAL:HG11	2.00	0.42
1:A:22:ILE:H	1:A:22:ILE:HD12	1.83	0.42
1:B:14:THR:HB	1:B:17:PRO:HD2	2.02	0.42
1:D:104:ASN:HA	1:D:261:VAL:HG11	2.02	0.42
1:D:302:LEU:HD12	1:D:365:PHE:HB3	2.01	0.42
1:A:286:GLU:H	1:A:286:GLU:CD	2.23	0.42
1:B:73:LEU:HD23	1:B:94:VAL:HG21	2.02	0.42
1:D:242:VAL:CG2	1:D:273:SER:HB3	2.49	0.42
1:B:167:LYS:NZ	3:B:607:HOH:O	2.37	0.42
1:C:20:VAL:HG22	1:D:260:LYS:HD3	2.00	0.42
1:D:148:LEU:HD11	1:D:324:TRP:HD1	1.84	0.42
1:C:265:ILE:HB	1:C:266:PRO:HD3	2.02	0.41
1:C:311:LYS:HB3	1:C:311:LYS:HE2	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:369:ILE:C	1:D:371:LYS:H	2.23	0.41
1:B:130:PHE:HZ	1:B:168:LEU:HD11	1.84	0.41
1:C:142:PRO:HD2	1:C:154:TRP:CG	2.55	0.41
1:C:144:ASP:HA	1:C:145:PRO:HD3	1.91	0.41
1:D:59:PRO:O	1:D:63:ARG:HG3	2.20	0.41
1:C:17:PRO:O	1:C:20:VAL:HG22	2.20	0.41
1:A:58:GLU:HA	1:A:59:PRO:HD3	1.98	0.41
1:C:20:VAL:HG12	1:C:131:GLN:HB3	2.01	0.41
1:C:236:GLY:HA2	1:C:238:MET:HE3	2.02	0.41
1:A:17:PRO:HA	1:A:20:VAL:HG23	2.03	0.41
1:A:47:GLN:O	1:A:51:LYS:HG3	2.20	0.41
1:B:265:ILE:HB	1:B:266:PRO:HD3	2.02	0.41
1:D:148:LEU:HD11	1:D:324:TRP:CD1	2.56	0.41
1:A:241:ARG:NH2	1:B:64:TYR:HE1	2.19	0.41
1:B:148:LEU:HD11	1:B:324:TRP:CD1	2.56	0.41
1:C:85:ASN:HB3	1:C:219:CYS:HB2	2.03	0.41
1:D:123:TYR:CZ	1:D:125:ASN:HB2	2.56	0.41
1:A:118:MET:HE2	1:A:138:ILE:HG21	2.04	0.40
1:B:335:PHE:CZ	1:B:353:SER:OG	2.74	0.40
1:D:265:ILE:HB	1:D:266:PRO:HD3	2.02	0.40
1:B:262:GLN:O	1:B:266:PRO:HD2	2.22	0.40
1:C:350:ILE:HA	1:C:351:PRO:HD2	1.93	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	352/404 (87%)	337 (96%)	14 (4%)	1 (0%)	41 30
1	B	345/404 (85%)	331 (96%)	13 (4%)	1 (0%)	41 30
1	C	356/404 (88%)	335 (94%)	20 (6%)	1 (0%)	41 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	350/404 (87%)	333 (95%)	16 (5%)	1 (0%)	41	30
All	All	1403/1616 (87%)	1336 (95%)	63 (4%)	4 (0%)	41	30

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	265	ILE
1	A	265	ILE
1	B	265	ILE
1	C	265	ILE

5.3.2 Protein sidechains [i](#)

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	302/339 (89%)	301 (100%)	1 (0%)	92	92
1	B	296/339 (87%)	296 (100%)	0	100	100
1	C	306/339 (90%)	303 (99%)	3 (1%)	76	74
1	D	301/339 (89%)	299 (99%)	2 (1%)	84	82
All	All	1205/1356 (89%)	1199 (100%)	6 (0%)	88	88

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	THR
1	C	56	ILE
1	C	185	SER
1	C	241	ARG
1	D	241	ARG
1	D	334	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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
1	LLP	C	233	1	23,24,25	2.28	6 (26%)	25,32,34	1.30	2 (8%)
1	LLP	A	233	1	23,24,25	2.31	5 (21%)	25,32,34	1.36	3 (12%)
1	LLP	B	233	1	23,24,25	2.37	6 (26%)	25,32,34	1.28	3 (12%)
1	LLP	D	233	1	23,24,25	2.30	5 (21%)	25,32,34	1.15	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	233	1	-	6/16/17/19	0/1/1/1
1	LLP	A	233	1	-	6/16/17/19	0/1/1/1
1	LLP	B	233	1	-	7/16/17/19	0/1/1/1
1	LLP	D	233	1	-	5/16/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	LLP	C4-C4'	6.50	1.59	1.46
1	D	233	LLP	C4-C4'	6.49	1.59	1.46
1	A	233	LLP	C4-C4'	6.40	1.58	1.46
1	C	233	LLP	C4'-NZ	6.10	1.47	1.27
1	C	233	LLP	C4-C4'	6.07	1.58	1.46
1	D	233	LLP	C4'-NZ	5.86	1.46	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	233	LLP	C4'-NZ	5.82	1.46	1.27
1	A	233	LLP	C4'-NZ	5.80	1.46	1.27
1	B	233	LLP	C4-C5	-3.75	1.37	1.42
1	A	233	LLP	C4-C5	-3.69	1.37	1.42
1	D	233	LLP	C4-C5	-3.22	1.37	1.42
1	B	233	LLP	C2-N1	3.09	1.39	1.33
1	C	233	LLP	C2-N1	2.99	1.39	1.33
1	C	233	LLP	C4-C5	-2.84	1.38	1.42
1	A	233	LLP	C2-N1	2.77	1.39	1.33
1	D	233	LLP	C2-N1	2.61	1.38	1.33
1	B	233	LLP	C2'-C2	2.34	1.54	1.50
1	A	233	LLP	O3-C3	2.17	1.42	1.37
1	D	233	LLP	C2'-C2	2.11	1.53	1.50
1	C	233	LLP	O3-C3	2.09	1.41	1.37
1	C	233	LLP	C2'-C2	2.07	1.53	1.50
1	B	233	LLP	C6-C5	2.04	1.42	1.37

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	LLP	C4-C4'-NZ	-4.08	105.59	124.31
1	A	233	LLP	C4-C4'-NZ	-3.63	107.65	124.31
1	B	233	LLP	C4-C4'-NZ	-3.40	108.72	124.31
1	D	233	LLP	C4-C4'-NZ	-3.15	109.84	124.31
1	A	233	LLP	C5-C6-N1	-2.47	119.71	123.82
1	D	233	LLP	CE-NZ-C4'	-2.29	111.85	118.90
1	A	233	LLP	CE-NZ-C4'	-2.29	111.86	118.90
1	D	233	LLP	C5-C6-N1	-2.27	120.03	123.82
1	B	233	LLP	CE-NZ-C4'	-2.22	112.08	118.90
1	B	233	LLP	C5-C6-N1	-2.14	120.26	123.82
1	C	233	LLP	C5-C6-N1	-2.04	120.42	123.82

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	233	LLP	C5'-OP4-P-OP2
1	A	233	LLP	C5'-OP4-P-OP3
1	B	233	LLP	C5'-OP4-P-OP1
1	B	233	LLP	C5'-OP4-P-OP2
1	B	233	LLP	C5'-OP4-P-OP3
1	D	233	LLP	CG-CD-CE-NZ

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Mol	Chain	Res	Type	Atoms
1	D	233	LLP	C4-C4'-NZ-CE
1	C	233	LLP	C4-C4'-NZ-CE
1	A	233	LLP	CG-CD-CE-NZ
1	A	233	LLP	C3-C4-C4'-NZ
1	B	233	LLP	C3-C4-C4'-NZ
1	D	233	LLP	CA-CB-CG-CD
1	B	233	LLP	CG-CD-CE-NZ
1	A	233	LLP	C5-C4-C4'-NZ
1	C	233	LLP	C3-C4-C4'-NZ
1	C	233	LLP	CD-CE-NZ-C4'
1	D	233	LLP	C-CA-CB-CG
1	A	233	LLP	CD-CE-NZ-C4'
1	D	233	LLP	C3-C4-C4'-NZ
1	C	233	LLP	CA-CB-CG-CD
1	B	233	LLP	CD-CE-NZ-C4'
1	B	233	LLP	CA-CB-CG-CD
1	C	233	LLP	C5-C4-C4'-NZ
1	C	233	LLP	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	233	LLP	2	0
1	B	233	LLP	2	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	C	501	-	4,4,4	0.15	0	6,6,6	0.11	0
2	SO4	A	501	-	4,4,4	0.14	0	6,6,6	0.13	0
2	SO4	B	501	-	4,4,4	0.15	0	6,6,6	0.14	0
2	SO4	D	501	-	4,4,4	0.16	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

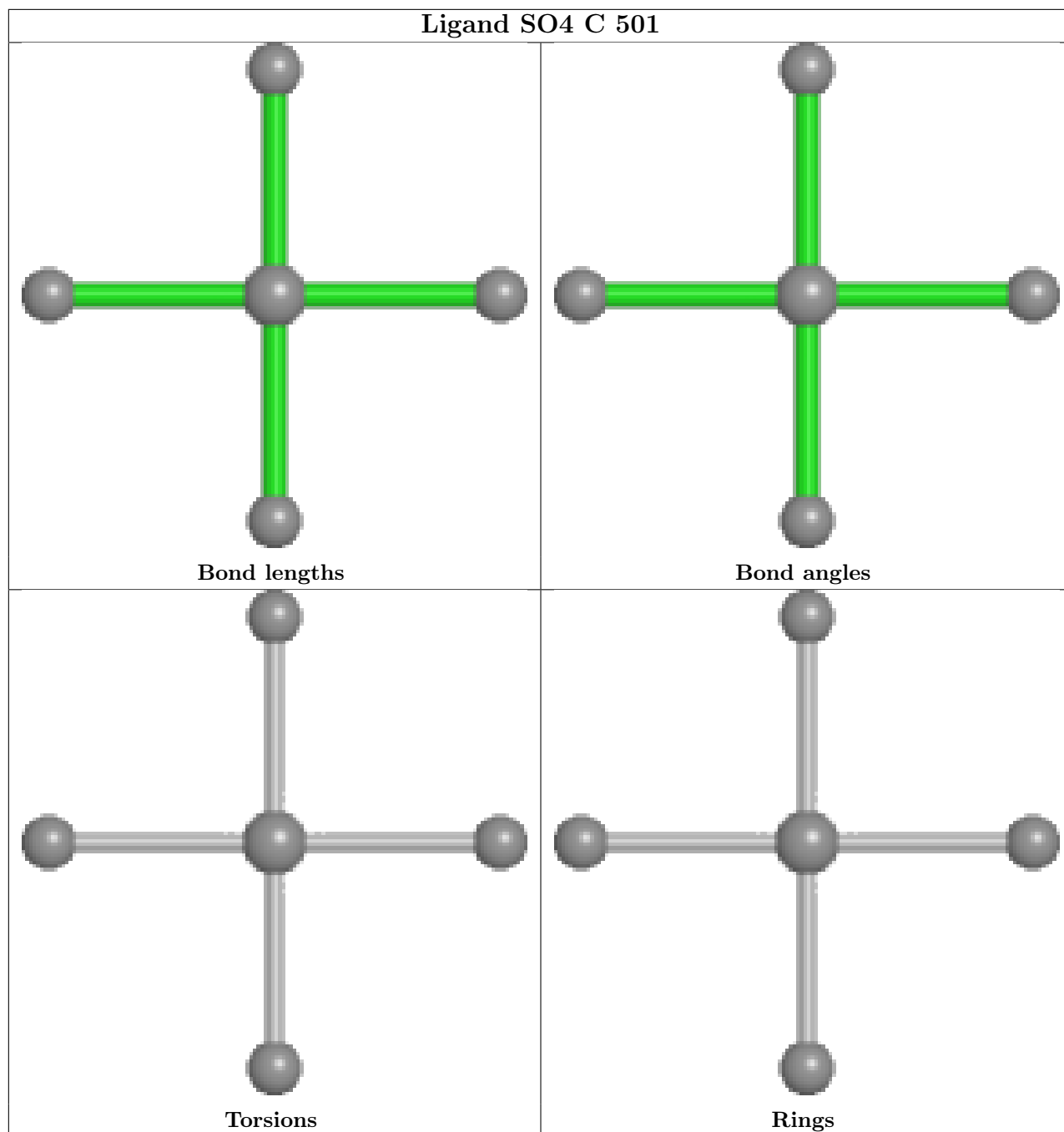
There are no chirality outliers.

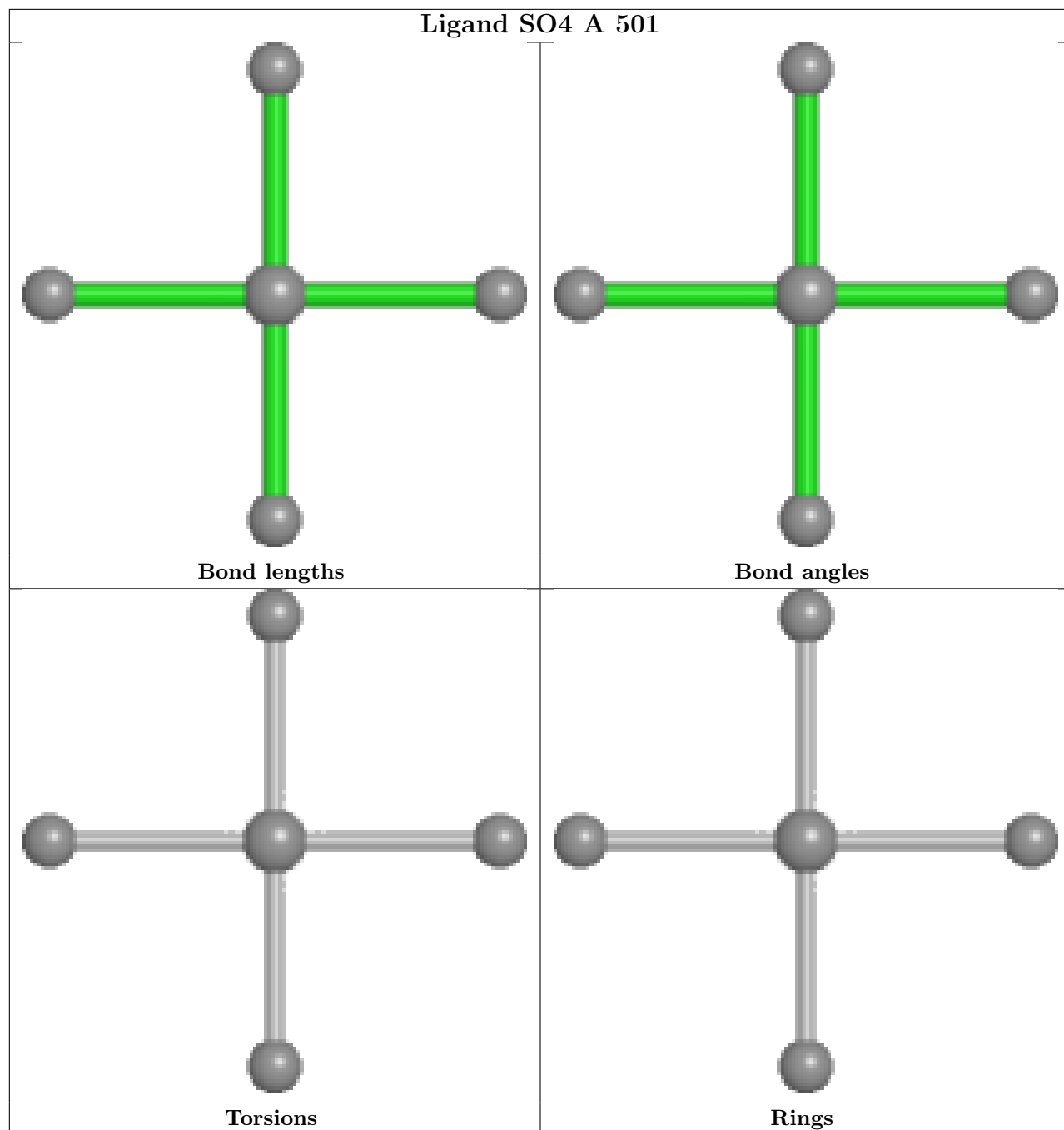
There are no torsion outliers.

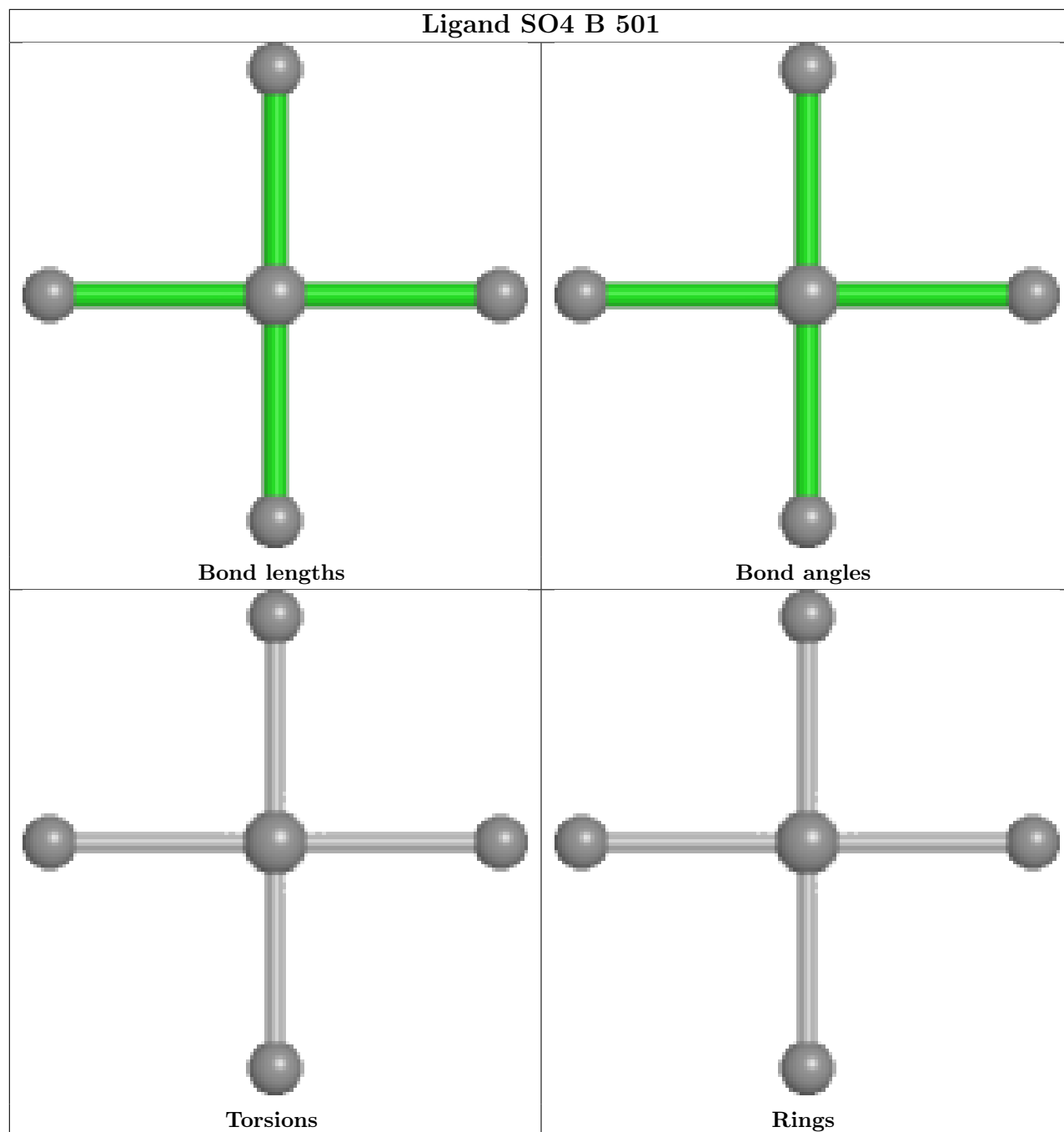
There are no ring outliers.

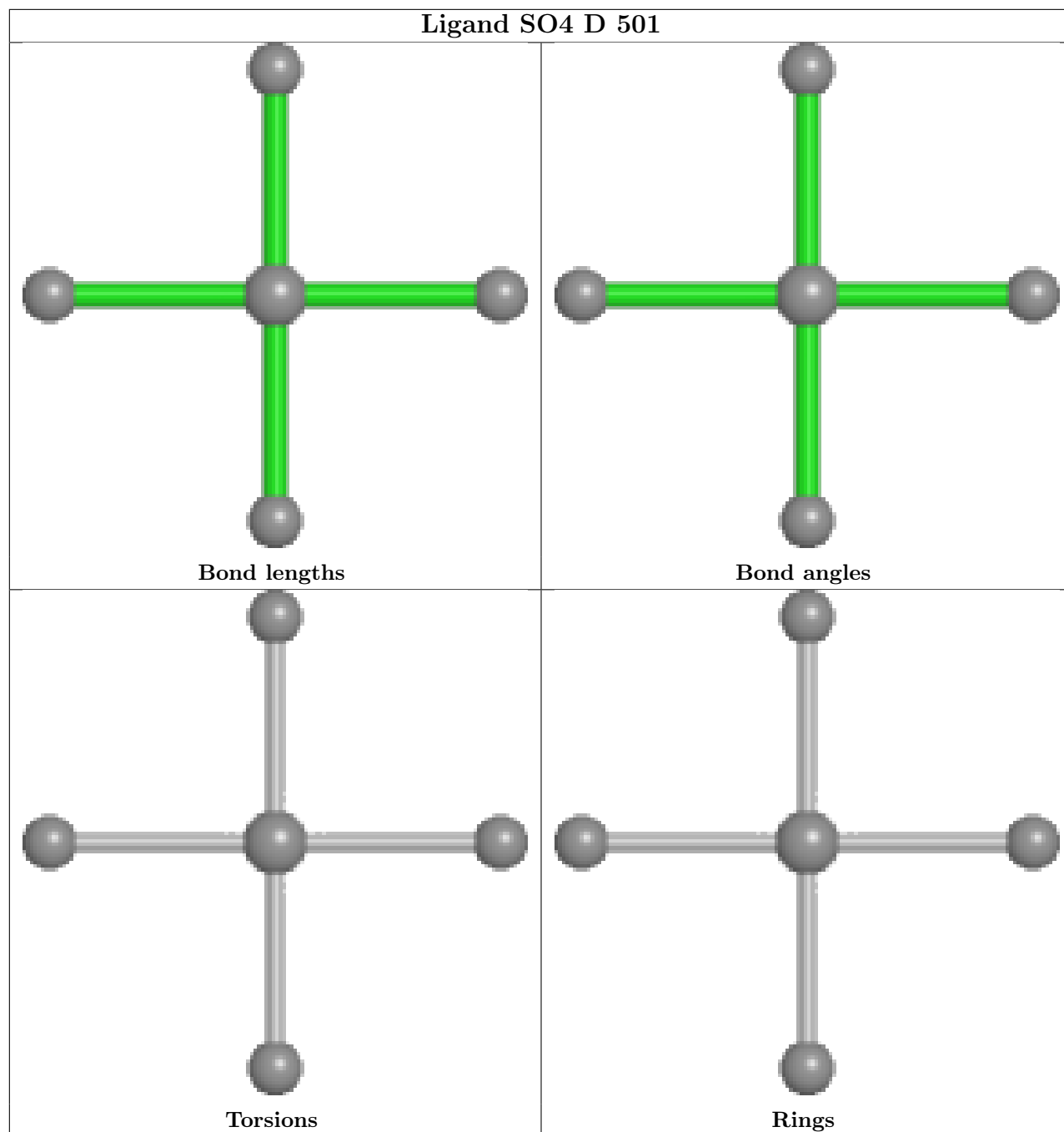
No monomer is involved in short contacts.

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	358/404 (88%)	0.76	32 (8%) 9 15	26, 40, 78, 88	0
1	B	351/404 (86%)	0.82	21 (5%) 21 30	28, 44, 74, 86	0
1	C	362/404 (89%)	0.81	36 (9%) 7 12	32, 49, 69, 84	0
1	D	356/404 (88%)	1.05	52 (14%) 2 3	30, 55, 78, 86	0
All	All	1427/1616 (88%)	0.86	141 (9%) 7 12	26, 47, 75, 88	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	359	GLY	7.4
1	D	335	PHE	7.4
1	B	369	ILE	6.3
1	D	20	VAL	5.7
1	B	335	PHE	5.3
1	B	311	LYS	5.2
1	A	380	LEU	5.0
1	B	373	CYS	4.9
1	D	309	LEU	4.7
1	D	17	PRO	4.7
1	D	159	LEU	4.6
1	D	19	MET	4.6
1	D	13	LEU	4.6
1	A	32	CYS	4.5
1	A	332	MET	4.4
1	D	340	TRP	4.3
1	A	340	TRP	4.3
1	C	33	ILE	4.3
1	D	341	LEU	4.1
1	C	376	ALA	4.1
1	D	336	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	331	TYR	4.0
1	C	380	LEU	3.9
1	A	373	CYS	3.8
1	B	375	ALA	3.8
1	B	330	LYS	3.7
1	D	374	ARG	3.7
1	D	328	PRO	3.6
1	D	381	ARG	3.6
1	C	163	VAL	3.5
1	D	32	CYS	3.5
1	B	212	TYR	3.4
1	D	141	GLY	3.4
1	D	154	TRP	3.4
1	B	12	VAL	3.4
1	D	87	LEU	3.4
1	D	33	ILE	3.4
1	A	369	ILE	3.4
1	D	163	VAL	3.3
1	C	311	LYS	3.3
1	A	335	PHE	3.2
1	C	23	GLN	3.2
1	D	330	LYS	3.2
1	B	374	ARG	3.1
1	D	142	PRO	3.1
1	A	336	LYS	3.1
1	D	153	ASP	3.1
1	C	369	ILE	3.1
1	D	331	TYR	3.1
1	B	347	VAL	3.0
1	C	22	ILE	3.0
1	D	369	ILE	3.0
1	D	197	ALA	3.0
1	D	222	ALA	2.9
1	A	377	ALA	2.9
1	A	342	ALA	2.9
1	D	311	LYS	2.8
1	A	379	ARG	2.8
1	C	307	SER	2.8
1	D	327	LEU	2.8
1	B	359	GLY	2.8
1	C	374	ARG	2.8
1	C	32	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	339	HIS	2.7
1	A	311	LYS	2.7
1	D	155	LEU	2.7
1	C	296	VAL	2.7
1	A	328	PRO	2.7
1	A	341	LEU	2.7
1	C	344	ARG	2.7
1	D	165	THR	2.6
1	C	373	CYS	2.6
1	D	181	TYR	2.6
1	A	381	ARG	2.6
1	D	86	ASN	2.6
1	C	70	LEU	2.5
1	C	26	ILE	2.5
1	A	305	ALA	2.5
1	A	214	ASN	2.5
1	C	16	THR	2.5
1	C	301	VAL	2.5
1	D	220	ILE	2.5
1	A	17	PRO	2.4
1	C	340	TRP	2.4
1	D	302	LEU	2.4
1	D	161	ASN	2.4
1	A	301	VAL	2.4
1	C	343	LYS	2.4
1	A	331	TYR	2.4
1	A	309	LEU	2.3
1	B	341	LEU	2.3
1	D	196	LYS	2.3
1	A	22	ILE	2.3
1	C	190	ILE	2.3
1	D	373	CYS	2.3
1	C	342	ALA	2.3
1	D	116	VAL	2.3
1	D	14	THR	2.3
1	A	326	LYS	2.3
1	A	339	HIS	2.3
1	A	310	GLY	2.3
1	D	83	HIS	2.3
1	D	382	LYS	2.2
1	D	185	SER	2.2
1	C	379	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	352	GLY	2.2
1	B	316	GLY	2.2
1	C	264	ASN	2.2
1	D	347	VAL	2.2
1	B	214	ASN	2.2
1	B	297	LYS	2.2
1	D	339	HIS	2.2
1	A	15	ASP	2.2
1	A	382	LYS	2.2
1	D	194	CYS	2.2
1	C	339	HIS	2.1
1	A	371	LYS	2.1
1	A	39	VAL	2.1
1	A	304	GLU	2.1
1	C	282	GLU	2.1
1	D	140	VAL	2.1
1	B	249	SER	2.1
1	C	146	LYS	2.1
1	C	124	PHE	2.1
1	B	22	ILE	2.1
1	C	13	LEU	2.1
1	C	25	LEU	2.1
1	D	157	SER	2.1
1	C	310	GLY	2.1
1	D	89	LYS	2.1
1	C	112	ALA	2.1
1	C	197	ALA	2.1
1	D	377	ALA	2.1
1	A	55	ILE	2.1
1	C	300	GLU	2.0
1	C	160	LYS	2.0
1	B	327	LEU	2.0
1	C	35	LEU	2.0
1	D	303	LEU	2.0
1	D	376	ALA	2.0
1	B	13	LEU	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column

labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
1	LLP	C	233	24/25	0.95	0.14	34,41,45,49	0
1	LLP	D	233	24/25	0.95	0.14	35,44,50,52	0
1	LLP	A	233	24/25	0.96	0.16	26,42,45,48	0
1	LLP	B	233	24/25	0.96	0.13	28,38,46,48	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

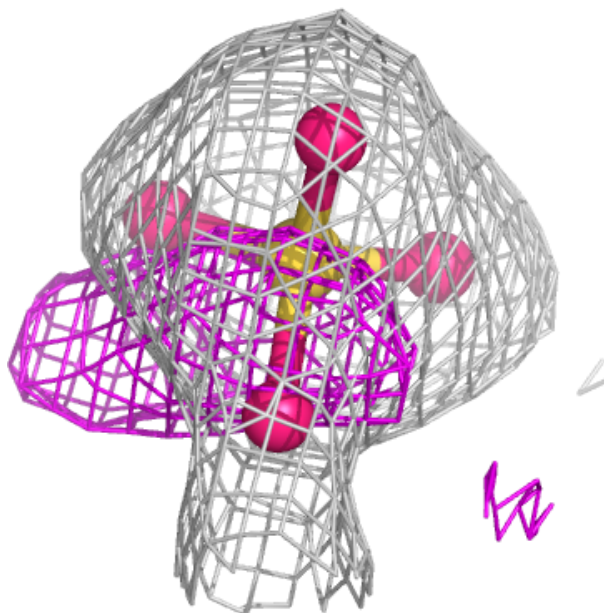
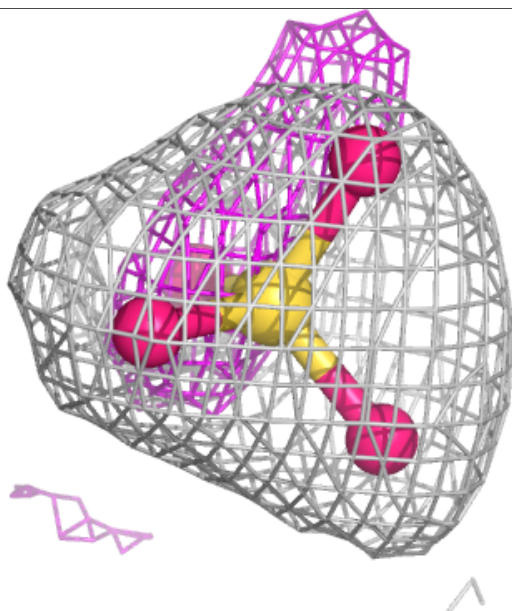
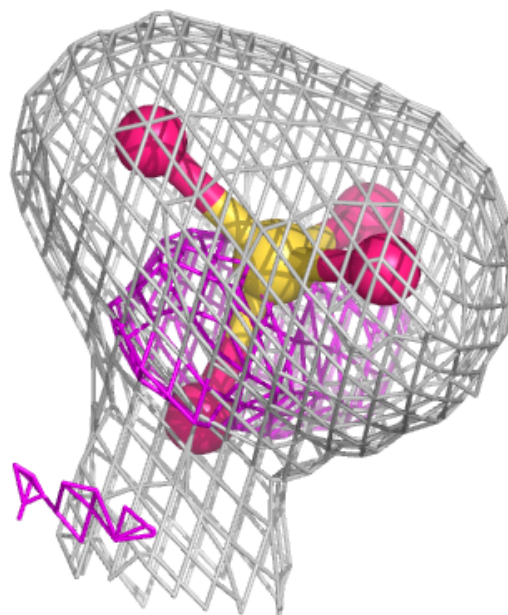
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	C	501	5/5	0.94	0.14	51,54,68,71	0
2	SO4	A	501	5/5	0.96	0.11	54,55,57,60	0
2	SO4	B	501	5/5	0.97	0.09	44,48,55,55	0
2	SO4	D	501	5/5	0.97	0.09	57,60,65,70	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.

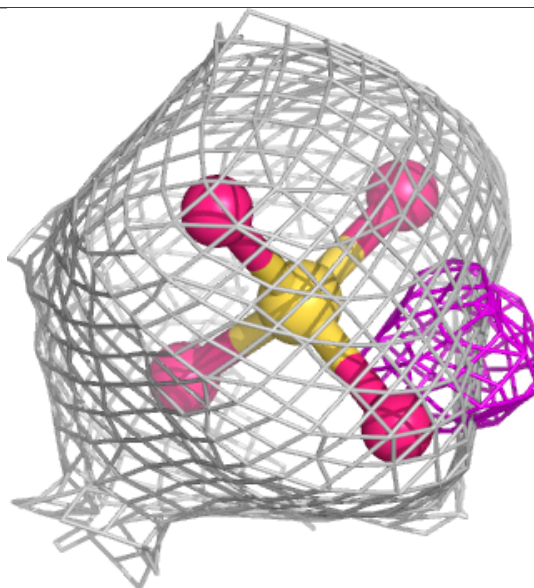
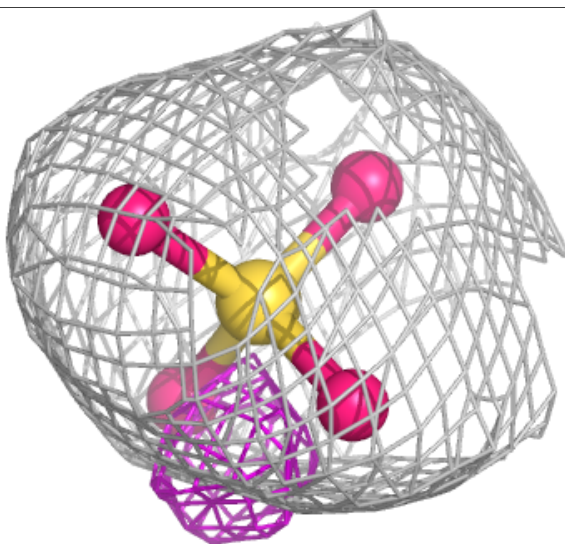
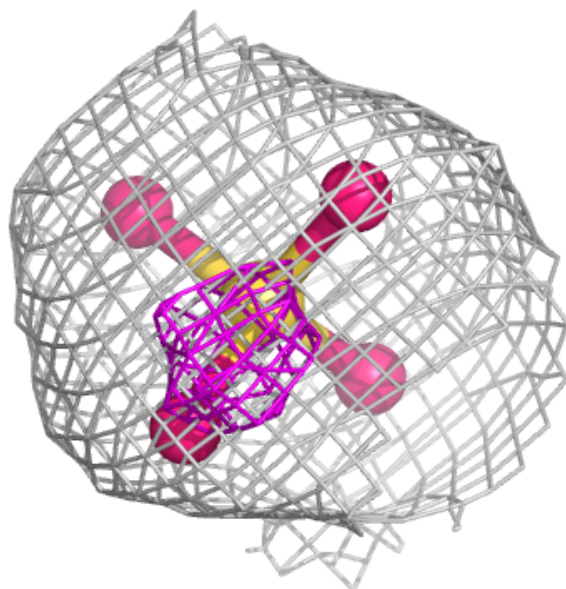
Electron density around SO4 C 501:

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



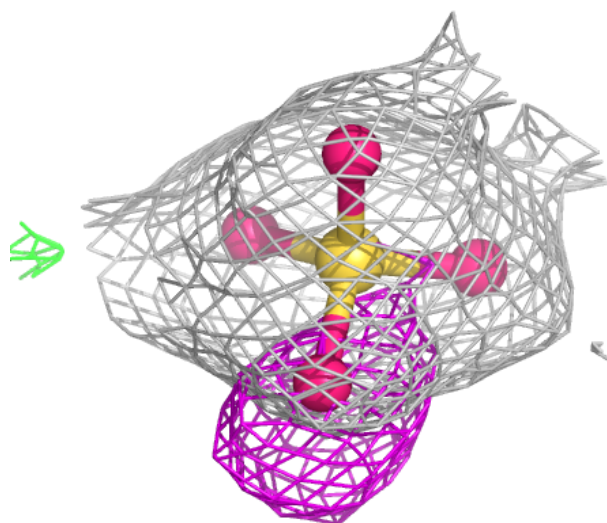
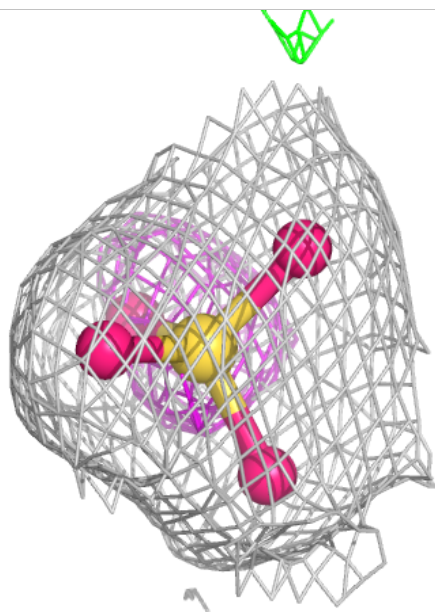
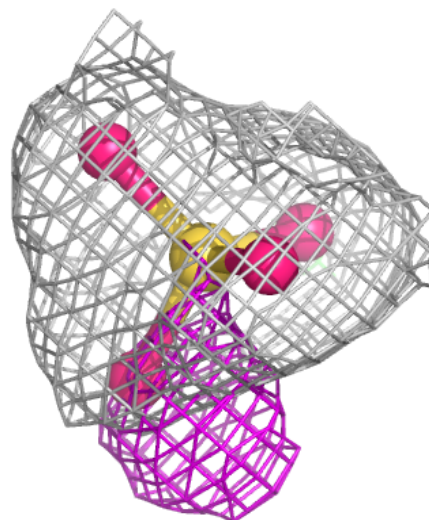
Electron density around SO4 A 501:

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



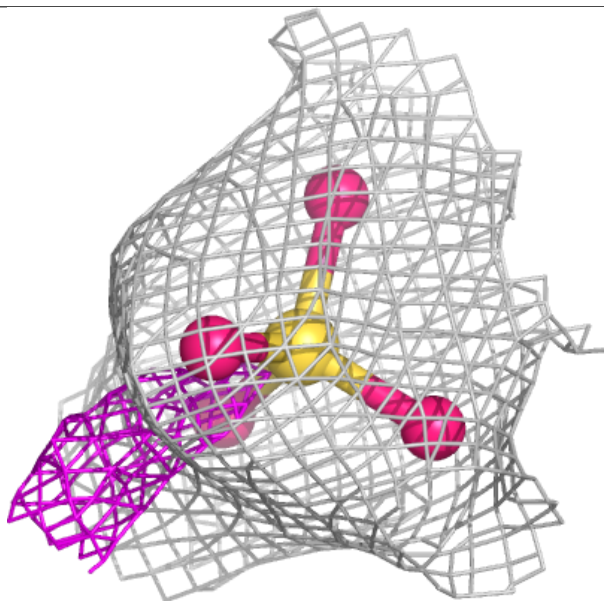
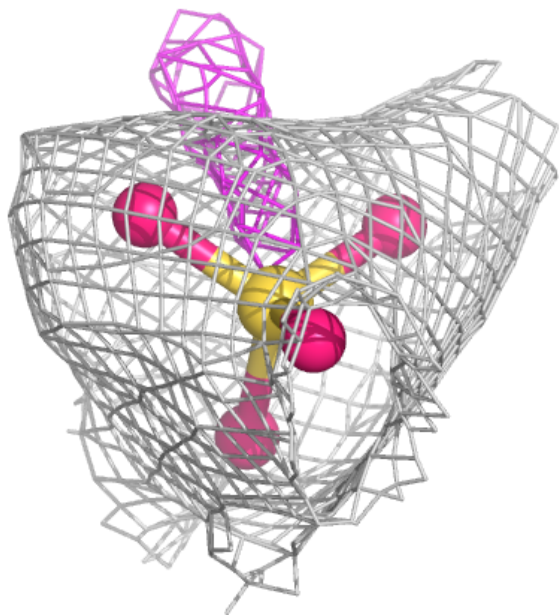
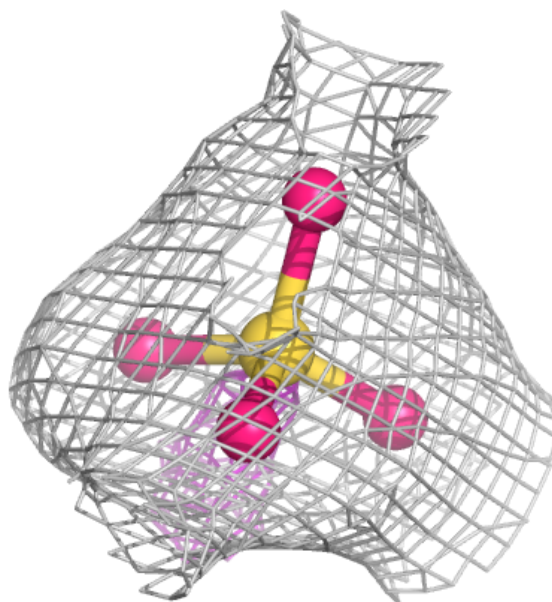
Electron density around SO4 B 501:

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



Electron density around SO4 D 501:

$2mF_o-DF_c$ (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.