Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2024 – 12:13 pm GMT

PDB ID	:	8QA9
Title	:	Crystal structure of the RK2 plasmid encoded co-complex of the C-terminally truncated transcriptional repressor protein KorB complexed with the partner repressor protein KorA bound to OA-DNA
Authors	:	McLean, T.C.; Mundy, J.E.A.; Lawson, D.M.; Le, T.B.K.
Deposited on	:	2023-08-22
Resolution	:	2.70 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:

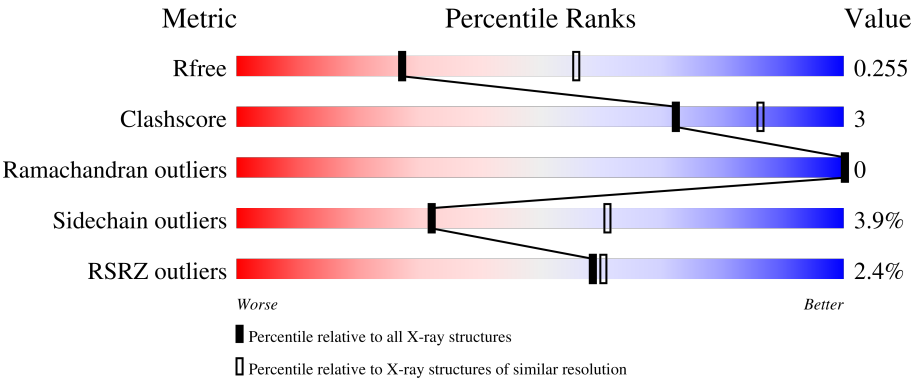
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 <=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	237	2% 79% 8% • 12%
1	B	237	3% 77% 9% • 12%
2	C	114	% 82% 12% 6%
2	D	114	3% 82% 11% • 6%

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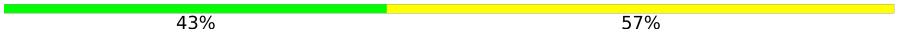
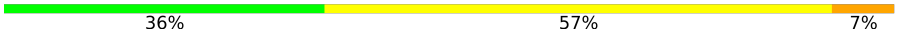
Mol	Chain	Length	Quality of chain
3	E	14	
3	F	14	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5584 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 Transcriptional repressor protein KorB.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	208	Total 1655	C 1035	N 298	O 322	0	1	0
1	B	209	Total 1651	C 1031	N 295	O 325	0	1	0

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	30	MET	-	initiating methionine	UNP P07674
A	254	LYS	-	expression tag	UNP P07674
A	255	LEU	-	expression tag	UNP P07674
A	256	ALA	-	expression tag	UNP P07674
A	257	ALA	-	expression tag	UNP P07674
A	258	ALA	-	expression tag	UNP P07674
A	259	LEU	-	expression tag	UNP P07674
A	260	GLU	-	expression tag	UNP P07674
A	261	HIS	-	expression tag	UNP P07674
A	262	HIS	-	expression tag	UNP P07674
A	263	HIS	-	expression tag	UNP P07674
A	264	HIS	-	expression tag	UNP P07674
A	265	HIS	-	expression tag	UNP P07674
A	266	HIS	-	expression tag	UNP P07674
B	30	MET	-	initiating methionine	UNP P07674
B	254	LYS	-	expression tag	UNP P07674
B	255	LEU	-	expression tag	UNP P07674
B	256	ALA	-	expression tag	UNP P07674
B	257	ALA	-	expression tag	UNP P07674
B	258	ALA	-	expression tag	UNP P07674
B	259	LEU	-	expression tag	UNP P07674
B	260	GLU	-	expression tag	UNP P07674
B	261	HIS	-	expression tag	UNP P07674
B	262	HIS	-	expression tag	UNP P07674
B	263	HIS	-	expression tag	UNP P07674

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Chain	Residue	Modelled	Actual	Comment	Reference
B	264	HIS	-	expression tag	UNP P07674
B	265	HIS	-	expression tag	UNP P07674
B	266	HIS	-	expression tag	UNP P07674

- Molecule 2 is a protein called TrfB transcriptional repressor protein.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	107	Total	C	N	O	0	1	0
			836	527	155	154			
2	D	107	Total	C	N	O	0	0	0
			830	523	152	155			

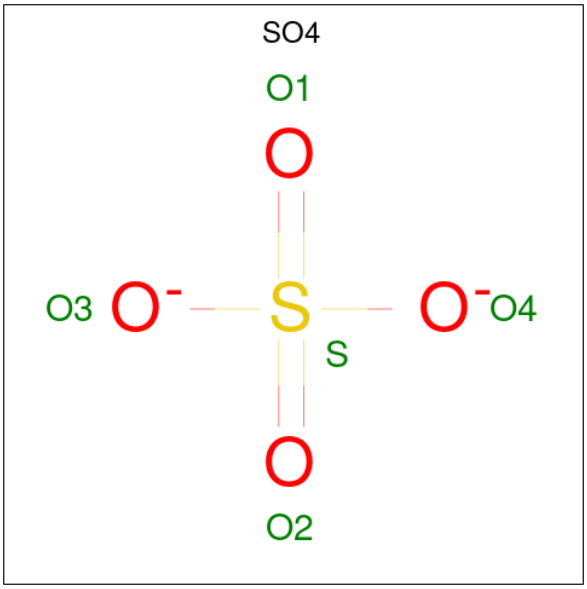
There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	102	LYS	-	expression tag	UNP P03052
C	103	LEU	-	expression tag	UNP P03052
C	104	ALA	-	expression tag	UNP P03052
C	105	ALA	-	expression tag	UNP P03052
C	106	ALA	-	expression tag	UNP P03052
C	107	LEU	-	expression tag	UNP P03052
C	108	GLU	-	expression tag	UNP P03052
C	109	HIS	-	expression tag	UNP P03052
C	110	HIS	-	expression tag	UNP P03052
C	111	HIS	-	expression tag	UNP P03052
C	112	HIS	-	expression tag	UNP P03052
C	113	HIS	-	expression tag	UNP P03052
C	114	HIS	-	expression tag	UNP P03052
D	102	LYS	-	expression tag	UNP P03052
D	103	LEU	-	expression tag	UNP P03052
D	104	ALA	-	expression tag	UNP P03052
D	105	ALA	-	expression tag	UNP P03052
D	106	ALA	-	expression tag	UNP P03052
D	107	LEU	-	expression tag	UNP P03052
D	108	GLU	-	expression tag	UNP P03052
D	109	HIS	-	expression tag	UNP P03052
D	110	HIS	-	expression tag	UNP P03052
D	111	HIS	-	expression tag	UNP P03052
D	112	HIS	-	expression tag	UNP P03052
D	113	HIS	-	expression tag	UNP P03052
D	114	HIS	-	expression tag	UNP P03052

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*GP*TP*TP*TP*AP*GP*CP*TP*AP*AP*AP*CP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	14	Total	C	N	O	P	0	0	0
			284	138	51	82	13			
3	F	14	Total	C	N	O	P	0	0	0
			284	138	51	82	13			

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	9	Total	O	0	0
			9	9		

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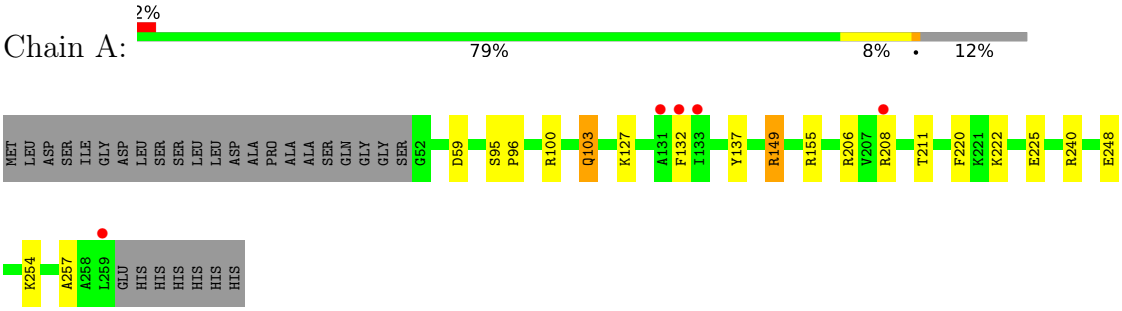
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	4	Total O 4 4	0	0
5	C	2	Total O 2 2	0	0
5	D	1	Total O 1 1	0	0
5	F	3	Total O 3 3	0	0

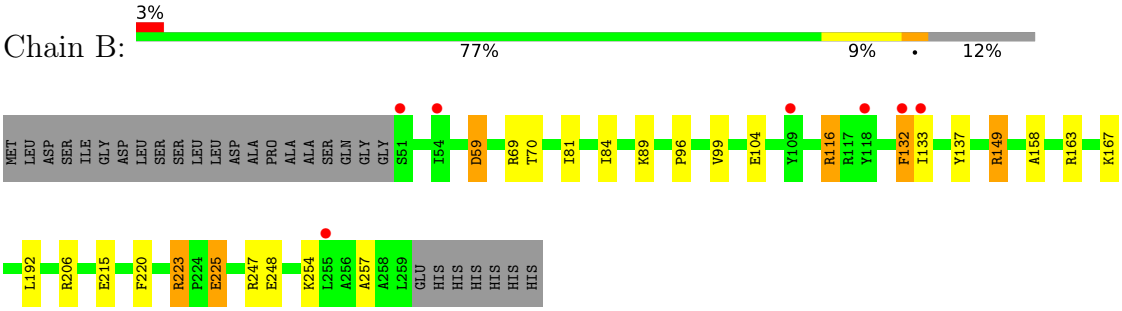
3 Residue-property plots (i)

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.

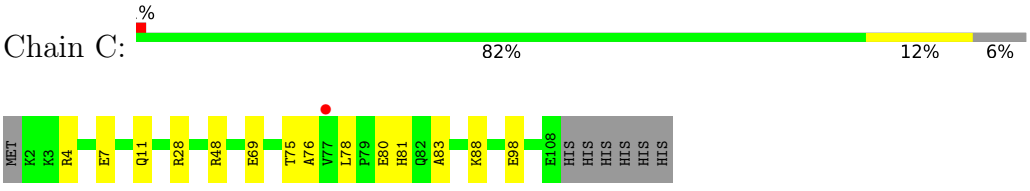
• Molecule 1: Transcriptional repressor protein KorB



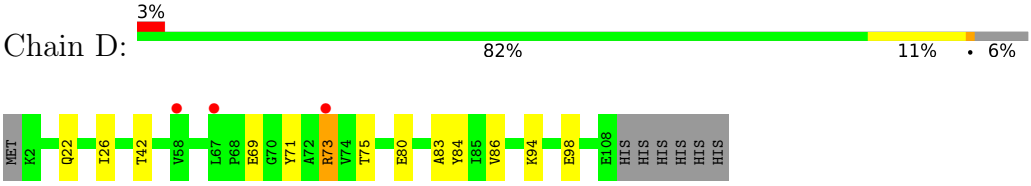
• Molecule 1: Transcriptional repressor protein KorB



• Molecule 2: TrfB transcriptional repressor protein

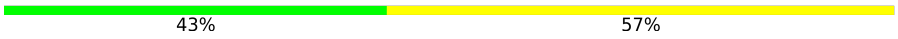


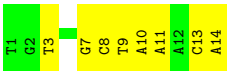
• Molecule 2: TrfB transcriptional repressor protein



• Molecule 3: DNA (5'-D(*TP*GP*TP*TP*TP*AP*GP*CP*TP*AP*AP*AP*CP*A)-3')

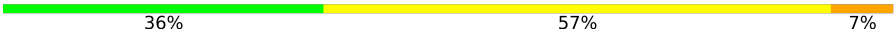
Chain E:

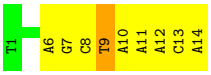




• Molecule 3: DNA (5'-D(*TP*GP*TP*TP*TP*AP*GP*CP*TP*AP*AP*AP*CP*A)-3')

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	173.25Å 77.09Å 84.61Å 90.00° 107.42° 90.00°	Depositor
Resolution (Å)	82.65 – 2.70 82.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (82.65-2.70) 100.0 (82.65-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.25 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.191 , 0.252 0.197 , 0.255	Depositor DCC
R_{free} test set	1444 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	71.6	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5584	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.47	0/1683	0.80	0/2273
1	B	0.46	0/1679	0.82	4/2271 (0.2%)
2	C	0.42	0/850	0.85	2/1149 (0.2%)
2	D	0.58	1/843 (0.1%)	0.86	0/1139
3	E	0.83	0/318	1.85	14/489 (2.9%)
3	F	0.88	0/318	1.75	9/489 (1.8%)
All	All	0.53	1/5691 (0.0%)	1.00	29/7810 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	98	GLU	CD-OE1	5.28	1.31	1.25

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	10	DA	O5'-P-OP2	-10.61	96.15	105.70
3	F	6	DA	O5'-P-OP1	10.02	122.73	110.70
3	F	11	DA	O4'-C1'-N9	8.44	113.91	108.00
3	E	13	DC	P-O3'-C3'	-8.16	109.90	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	7	DG	P-O3'-C3'	-6.55	111.84	119.70
3	E	14	DA	O4'-C1'-N9	6.39	112.48	108.00
3	E	3	DT	OP1-P-OP2	6.30	129.06	119.60
3	E	9	DT	OP2-P-O3'	6.06	118.53	105.20
1	B	163	ARG	NE-CZ-NH1	6.04	123.32	120.30
3	E	11	DA	O4'-C1'-N9	5.96	112.17	108.00
1	B	70	THR	CA-CB-OG1	5.89	121.36	109.00
3	F	9	DT	P-O3'-C3'	-5.85	112.68	119.70
3	E	14	DA	O4'-C4'-C3'	5.67	109.40	106.00
1	B	69	ARG	NE-CZ-NH1	-5.62	117.49	120.30
3	E	13	DC	OP2-P-O3'	5.61	117.55	105.20
3	E	7	DG	C8-N9-C1'	5.50	134.15	127.00
3	E	9	DT	P-O3'-C3'	-5.46	113.15	119.70
3	F	13	DC	P-O3'-C3'	-5.46	113.15	119.70
1	B	163	ARG	NE-CZ-NH2	-5.43	117.58	120.30
2	C	81[A]	HIS	CA-CB-CG	5.37	122.73	113.60
2	C	81[B]	HIS	CA-CB-CG	5.37	122.73	113.60
3	E	11	DA	OP1-P-OP2	5.28	127.51	119.60
3	F	7	DG	C8-N9-C1'	5.26	133.84	127.00
3	F	12	DA	P-O3'-C3'	-5.20	113.46	119.70
3	F	10	DA	O5'-P-OP2	-5.15	101.06	105.70
3	F	14	DA	OP1-P-OP2	5.15	127.33	119.60
3	E	8	DC	O4'-C4'-C3'	-5.10	102.46	104.50
3	F	6	DA	O5'-P-OP2	-5.05	101.15	105.70
3	E	7	DG	OP2-P-O3'	5.05	116.31	105.20

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	ARG	Sidechain
1	A	155[A]	ARG	Sidechain
1	A	206	ARG	Sidechain
1	A	208	ARG	Sidechain
1	B	116	ARG	Sidechain
1	B	149	ARG	Sidechain
1	B	206	ARG	Sidechain
1	B	223	ARG	Sidechain

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	1655	0	1654	13	0
1	B	1651	0	1632	17	0
2	C	836	0	839	11	0
2	D	830	0	837	8	0
3	E	284	0	161	0	0
3	F	284	0	161	1	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
5	A	9	0	0	1	0
5	B	4	0	0	1	0
5	C	2	0	0	0	0
5	D	1	0	0	0	0
5	F	3	0	0	0	0
All	All	5584	0	5284	37	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (37) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:75:THR:HG1	2:D:75:THR:HG1	1.21	0.79
1:B:248:GLU:OE1	2:C:88:LYS:NZ	2.31	0.64
2:C:48:ARG:HB2	2:C:48:ARG:HH11	1.67	0.59
1:B:225:GLU:HG3	5:B:401:HOH:O	2.03	0.59
1:A:132:PHE:HZ	1:B:96:PRO:HD2	1.68	0.58
1:A:149:ARG:HH11	1:B:149:ARG:HH11	1.57	0.53
1:A:96:PRO:HD2	1:B:132:PHE:CZ	2.43	0.53
1:A:211:THR:HG21	1:A:240:ARG:HH22	1.73	0.52
2:C:48:ARG:HH11	2:C:48:ARG:CB	2.23	0.52
2:C:80:GLU:O	2:C:83:ALA:HB3	2.11	0.51
2:D:80:GLU:O	2:D:83:ALA:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:LYS:O	1:A:257:ALA:HB3	2.11	0.50
2:C:4:ARG:HH21	2:C:4:ARG:HB3	1.77	0.50
2:C:7:GLU:OE2	2:C:28:ARG:NH2	2.45	0.49
2:D:22:GLN:O	2:D:26:ILE:HG13	2.12	0.49
1:A:103:GLN:HE21	1:A:103:GLN:HA	1.78	0.47
1:B:220:PHE:CD2	1:B:220:PHE:C	2.87	0.47
1:A:220:PHE:C	1:A:220:PHE:CD2	2.88	0.47
2:C:76:ALA:O	2:D:73:ARG:HA	2.15	0.47
1:A:59:ASP:OD1	1:A:59:ASP:N	2.46	0.46
1:B:59:ASP:OD1	1:B:59:ASP:N	2.49	0.45
1:A:132:PHE:CZ	1:B:96:PRO:HG2	2.51	0.45
2:C:75:THR:OG1	2:D:75:THR:OG1	2.03	0.45
1:B:223:ARG:HE	1:B:254:LYS:HG3	1.81	0.45
1:B:116:ARG:HB2	4:B:301:SO4:S	2.57	0.45
1:A:149:ARG:HH11	1:B:149:ARG:NH1	2.15	0.45
2:C:78:LEU:HD11	2:D:86:VAL:HG13	1.99	0.44
1:B:215:GLU:OE2	1:B:247:ARG:NH1	2.34	0.43
1:B:99:VAL:O	1:B:133:ILE:HA	2.19	0.43
3:F:8:DC:H2"	3:F:9:DT:H5'	2.01	0.43
1:A:132:PHE:CZ	1:B:96:PRO:HD2	2.51	0.42
1:A:225:GLU:HB2	5:A:408:HOH:O	2.18	0.42
1:B:254:LYS:O	1:B:257:ALA:HB3	2.19	0.42
2:C:78:LEU:O	2:D:71:TYR:HA	2.20	0.42
1:B:158:ALA:O	1:B:192:LEU:HD21	2.20	0.41
1:B:81:ILE:HA	1:B:84:ILE:HG22	2.02	0.41
1:A:248:GLU:HB3	2:D:84:TYR:OH	2.20	0.41

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	207/237 (87%)	199 (96%)	8 (4%)	0	100	100
1	B	208/237 (88%)	203 (98%)	5 (2%)	0	100	100
2	C	106/114 (93%)	106 (100%)	0	0	100	100
2	D	105/114 (92%)	104 (99%)	1 (1%)	0	100	100
All	All	626/702 (89%)	612 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	176/199 (88%)	170 (97%)	6 (3%)	37	66
1	B	175/199 (88%)	168 (96%)	7 (4%)	31	60
2	C	82/91 (90%)	79 (96%)	3 (4%)	34	63
2	D	82/91 (90%)	78 (95%)	4 (5%)	25	52
All	All	515/580 (89%)	495 (96%)	20 (4%)	32	61

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

Mol	Chain	Res	Type
1	A	95	SER
1	A	103	GLN
1	A	127	LYS
1	A	137	TYR
1	A	149	ARG
1	A	222	LYS
1	B	59	ASP
1	B	89	LYS
1	B	104	GLU
1	B	132	PHE
1	B	137	TYR
1	B	167	LYS
1	B	225	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	11	GLN
2	C	69	GLU
2	C	98	GLU
2	D	42	THR
2	D	69	GLU
2	D	73	ARG
2	D	94	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	103	GLN
1	A	105	GLN
1	B	103	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\|>2$
4	SO4	E	101	-	4,4,4	0.28	0	6,6,6	0.12	0
4	SO4	B	301	-	4,4,4	0.35	0	6,6,6	0.45	0
4	SO4	D	201	-	4,4,4	0.30	0	6,6,6	0.22	0
4	SO4	C	201	-	4,4,4	0.26	0	6,6,6	0.22	0
4	SO4	A	301	-	4,4,4	0.39	0	6,6,6	0.32	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

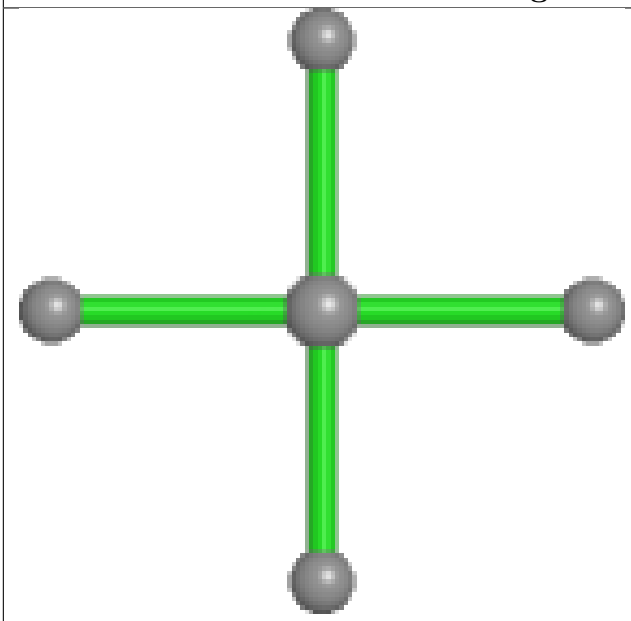
There are no ring outliers.

1 monomer is involved in 1 short contact:

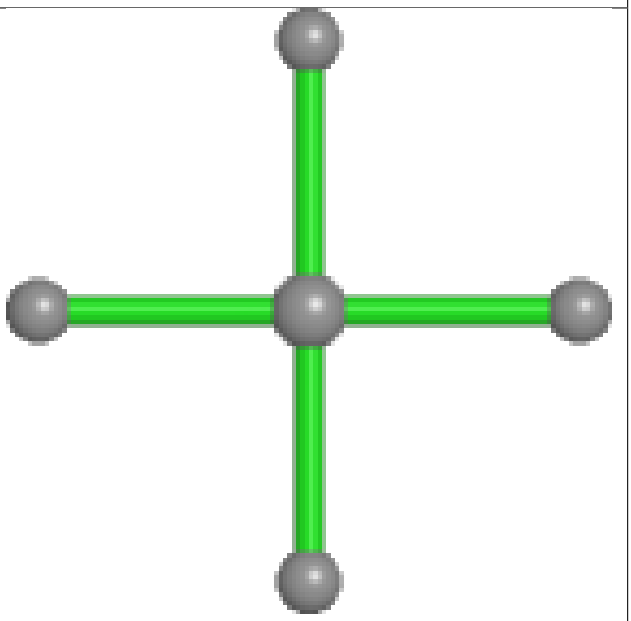
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	301	SO4	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

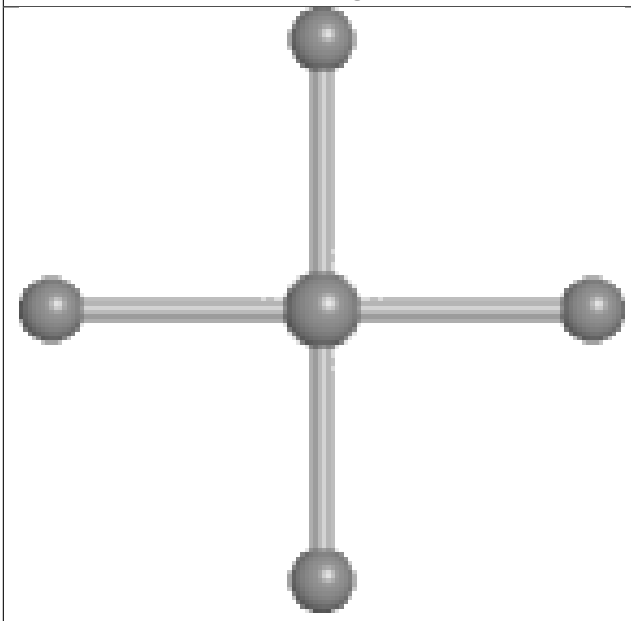
Ligand SO4 E 101



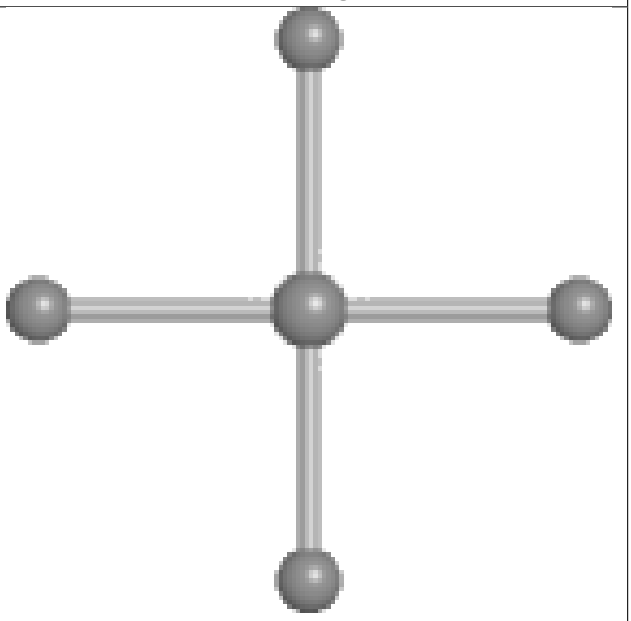
Bond lengths



Bond angles

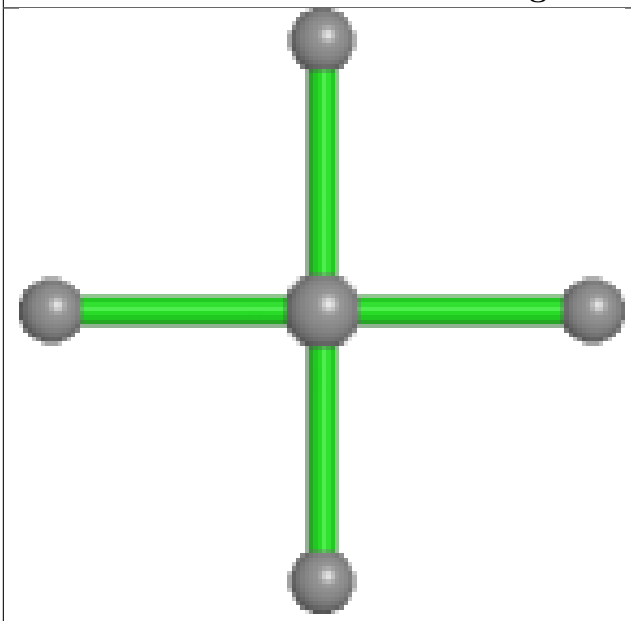


Torsions

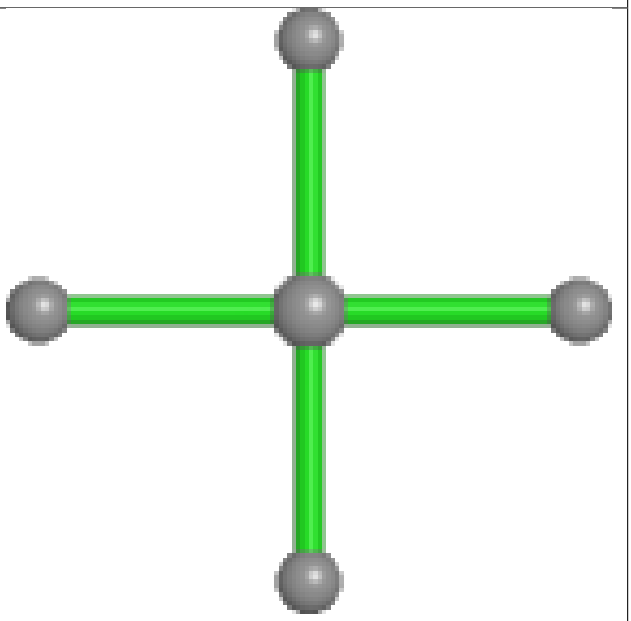


Rings

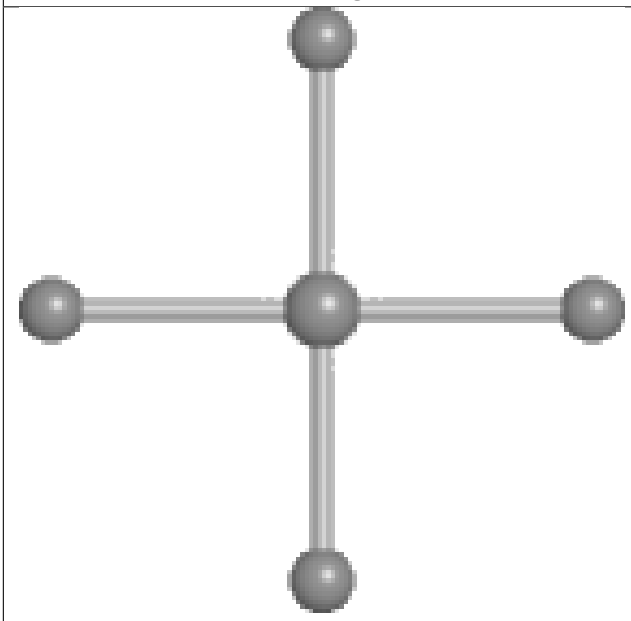
Ligand SO4 B 301



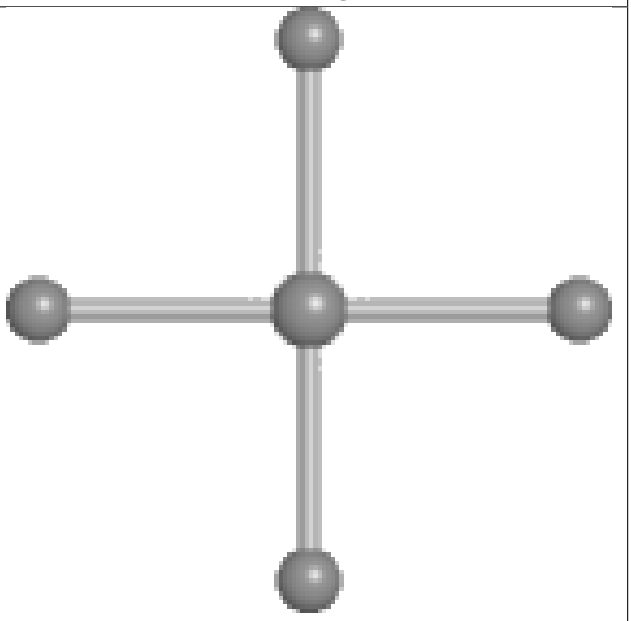
Bond lengths



Bond angles

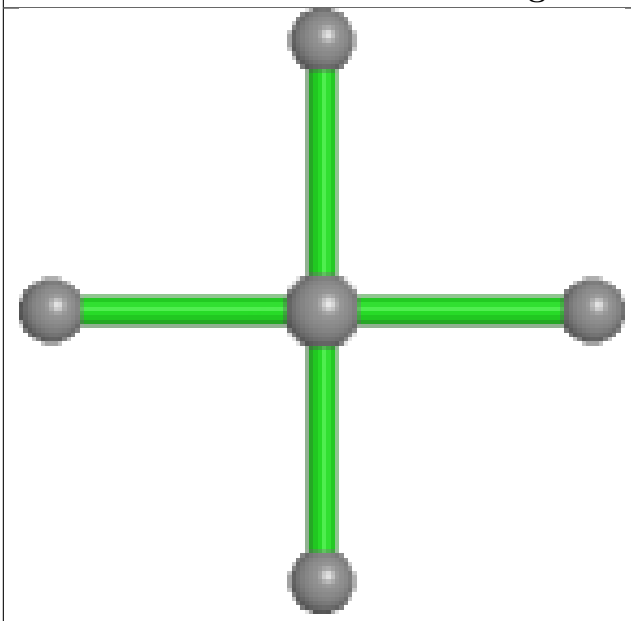


Torsions

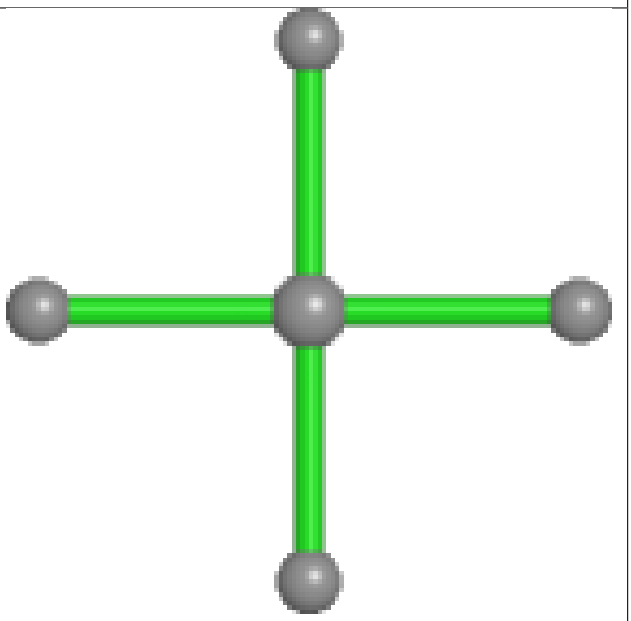


Rings

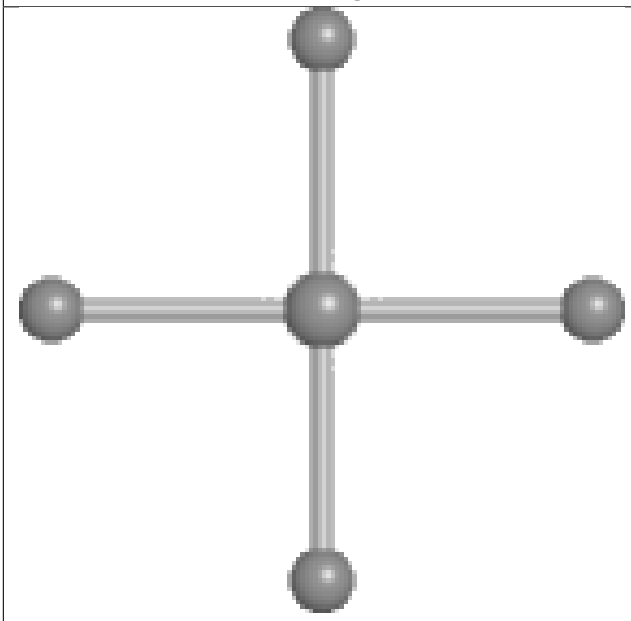
Ligand SO4 D 201



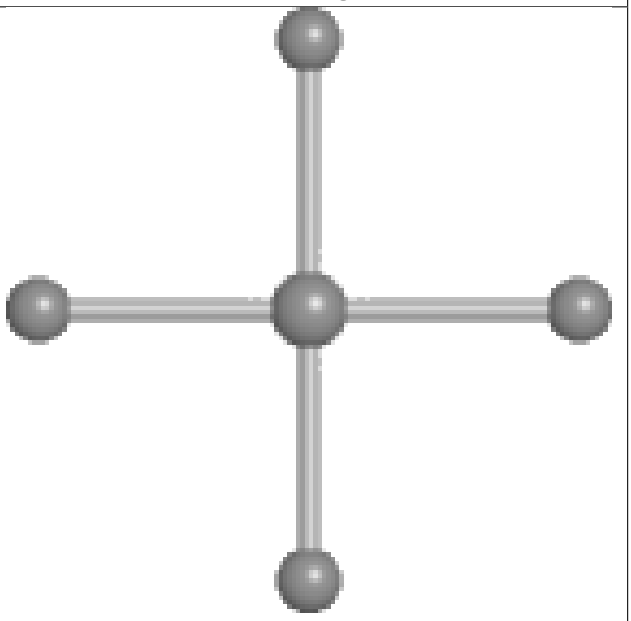
Bond lengths



Bond angles

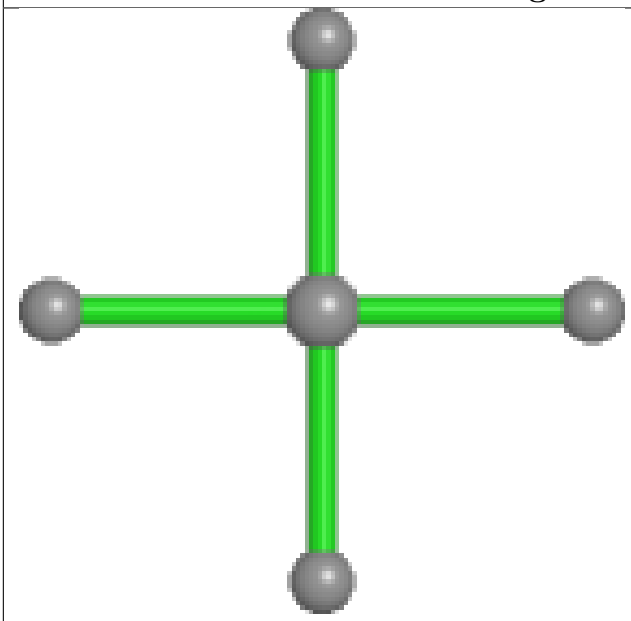


Torsions

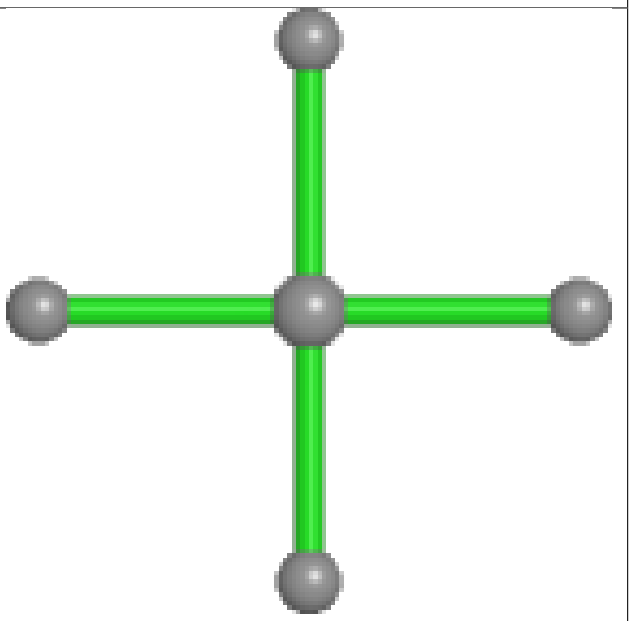


Rings

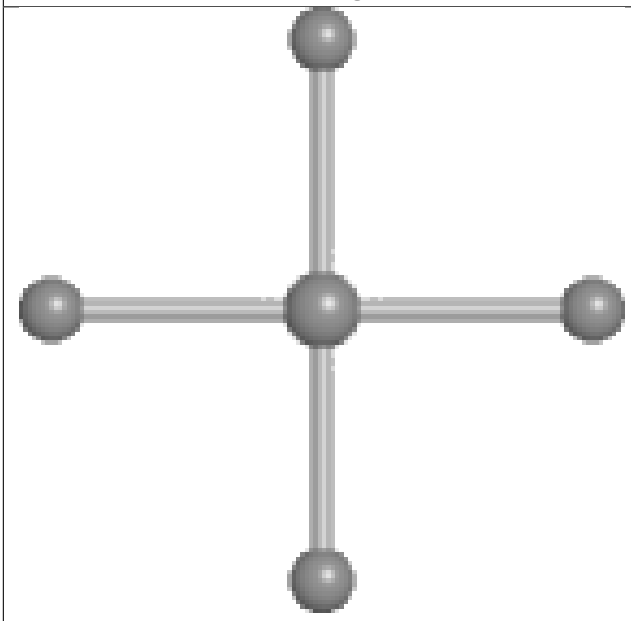
Ligand SO4 C 201



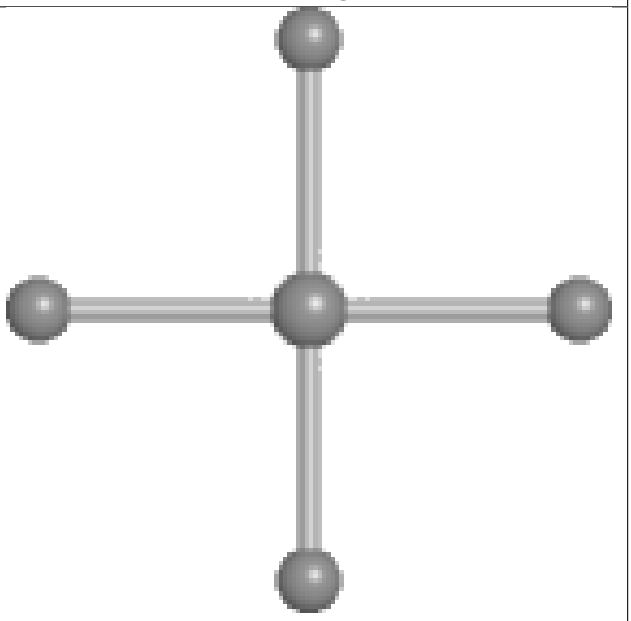
Bond lengths



Bond angles

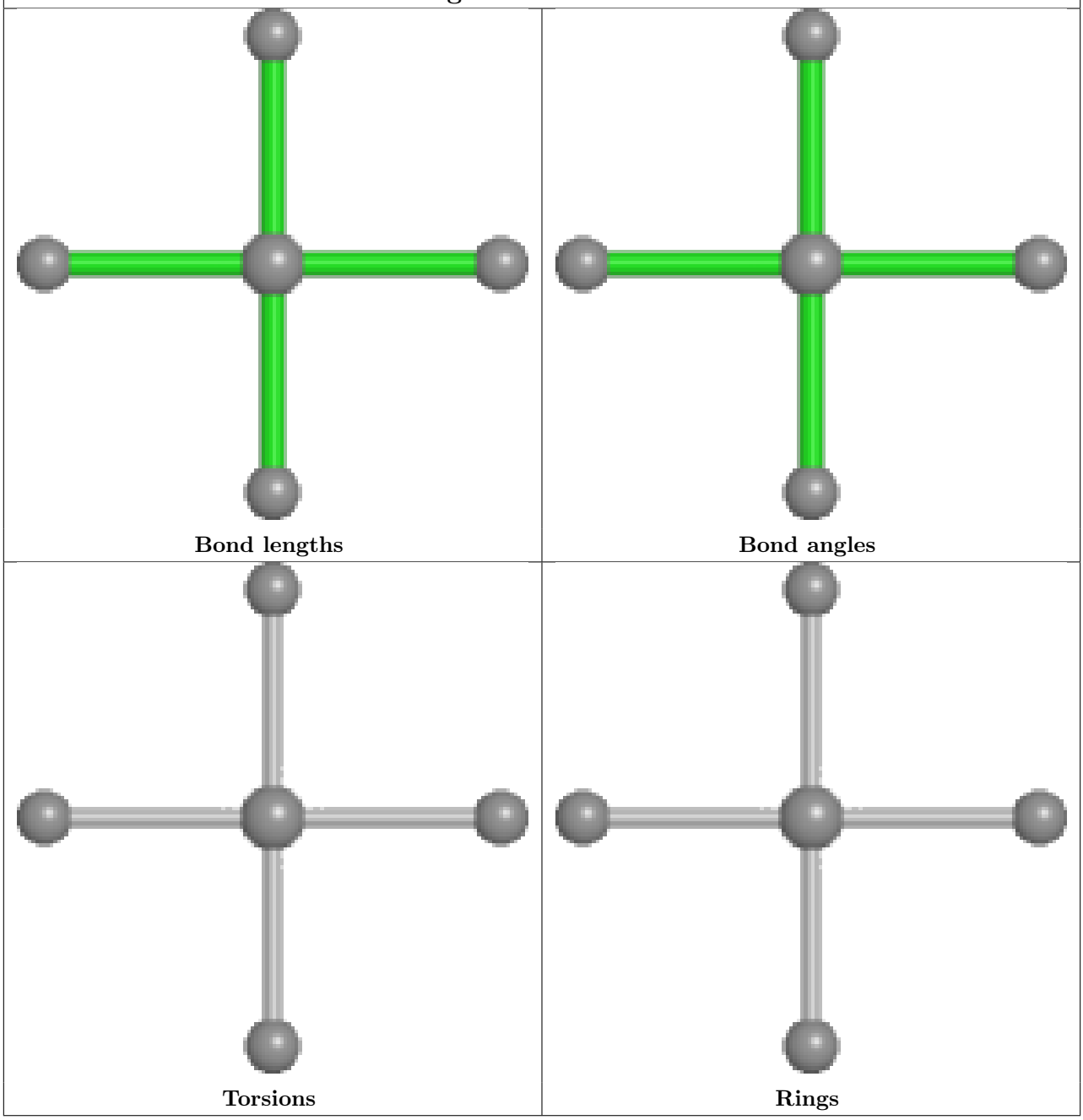


Torsions



Rings

Ligand SO4 A 301



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, 95^{th} 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	208/237 (87%)	0.33	5 (2%) 59 60	50, 73, 112, 154	0
1	B	209/237 (88%)	0.27	7 (3%) 46 46	53, 76, 115, 140	0
2	C	107/114 (93%)	0.21	1 (0%) 84 85	55, 81, 115, 148	0
2	D	107/114 (93%)	0.53	3 (2%) 53 54	52, 69, 95, 111	0
3	E	14/14 (100%)	0.26	0 100 100	59, 66, 81, 82	0
3	F	14/14 (100%)	0.23	0 100 100	56, 63, 91, 102	0
All	All	659/730 (90%)	0.32	16 (2%) 59 60	50, 75, 113, 154	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	132	PHE	5.3
1	B	132	PHE	4.9
1	B	51	SER	4.5
2	D	73	ARG	3.6
1	A	133	ILE	3.4
1	B	133	ILE	3.0
1	A	259	LEU	2.8
1	A	208	ARG	2.7
1	A	131	ALA	2.6
2	D	58	VAL	2.6
2	C	77	VAL	2.3
1	B	255	LEU	2.3
1	B	118	TYR	2.2
1	B	54	ILE	2.1
1	B	109	TYR	2.1
2	D	67	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

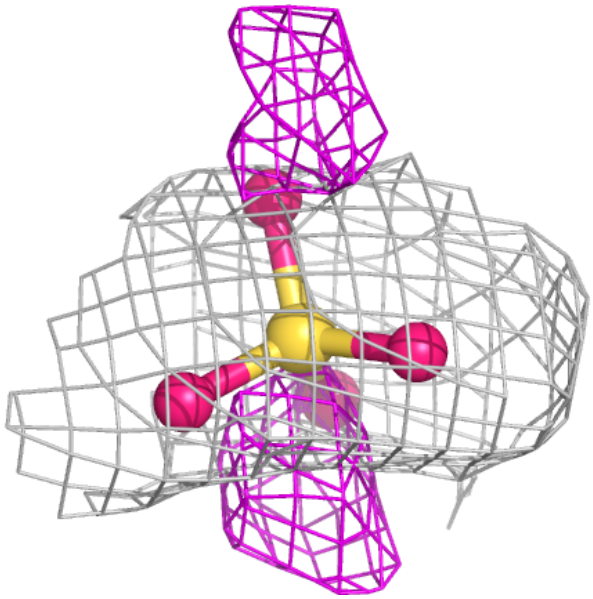
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

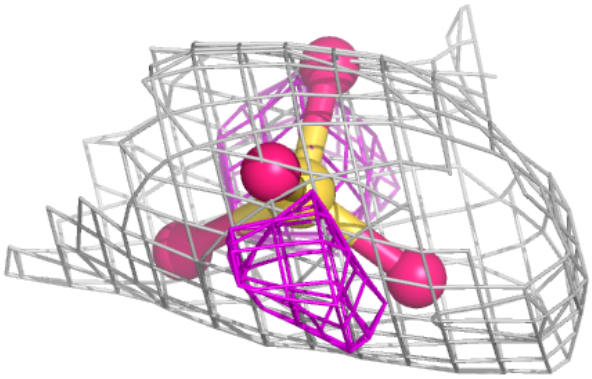
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	D	201	5/5	0.75	0.26	88,104,131,154	0
4	SO4	E	101	5/5	0.87	0.28	102,114,146,155	0
4	SO4	C	201	5/5	0.92	0.33	104,108,119,123	0
4	SO4	B	301	5/5	0.99	0.17	49,63,69,79	0
4	SO4	A	301	5/5	0.99	0.20	55,57,65,67	0

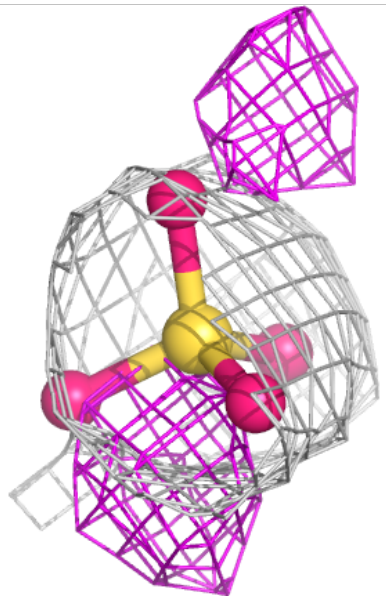
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SO4 D 201:

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

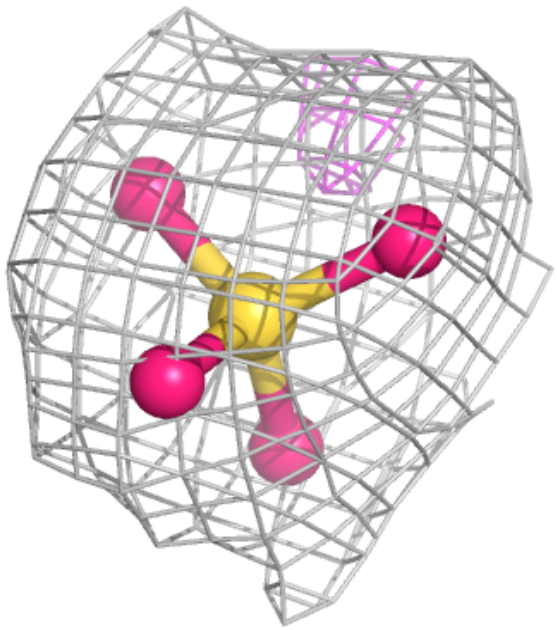


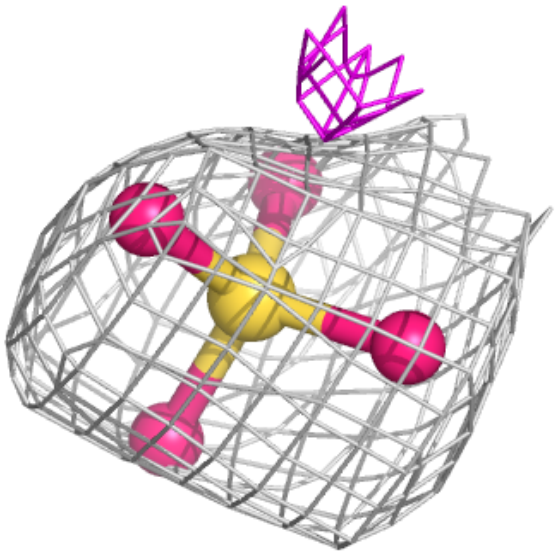


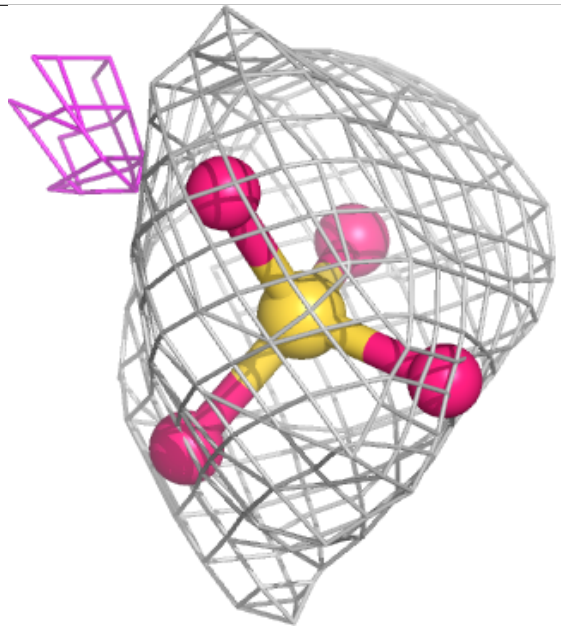


Electron density around SO4 E 101:

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

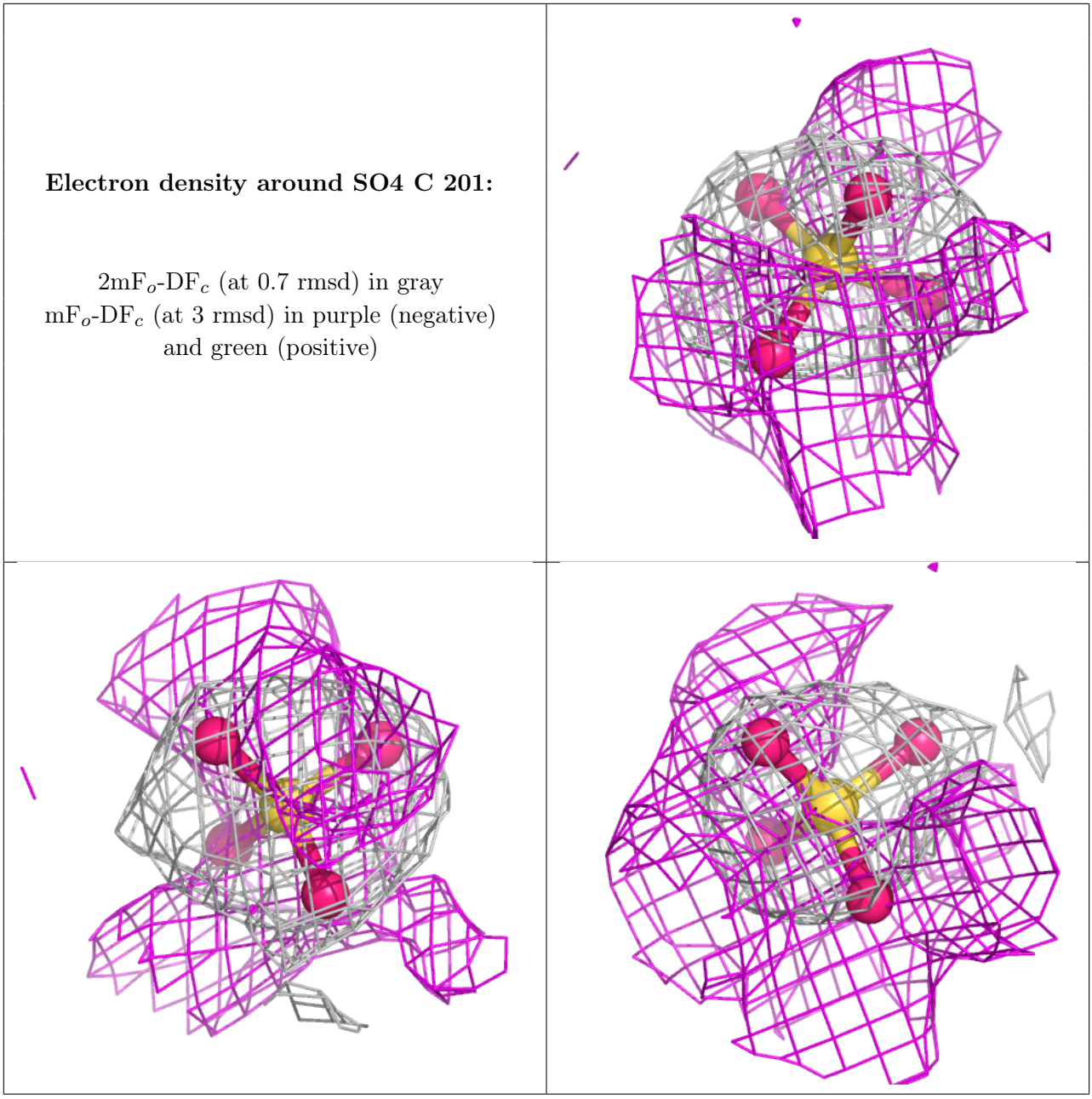






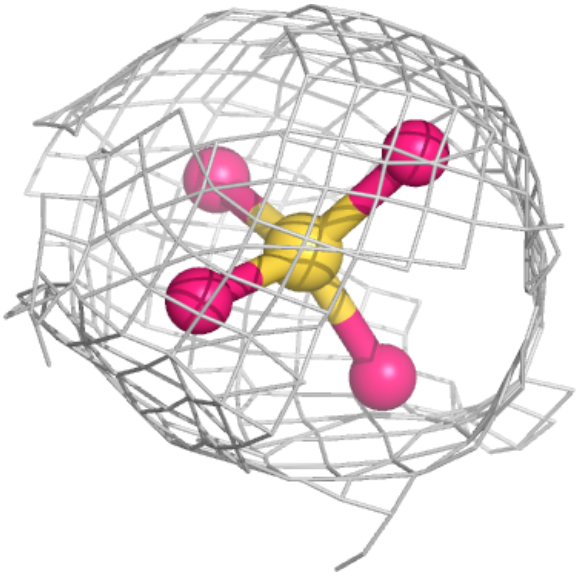
Electron density around SO4 C 201:

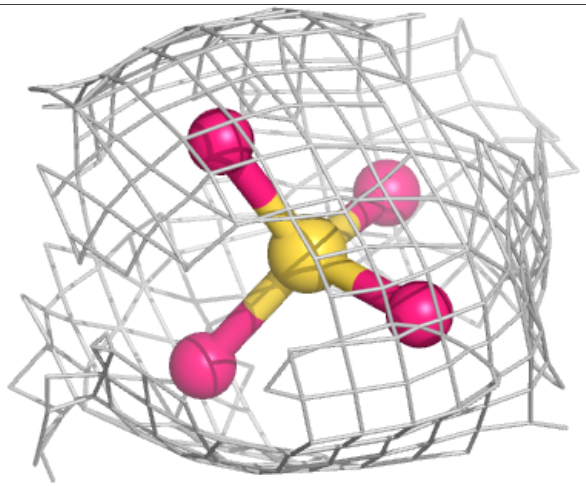
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

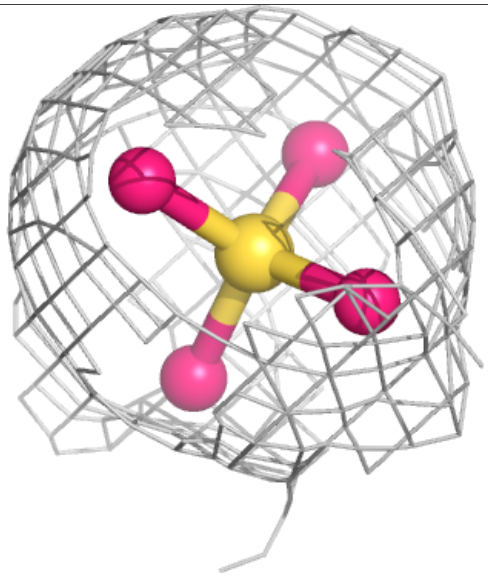


Electron density around SO4 B 301:

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

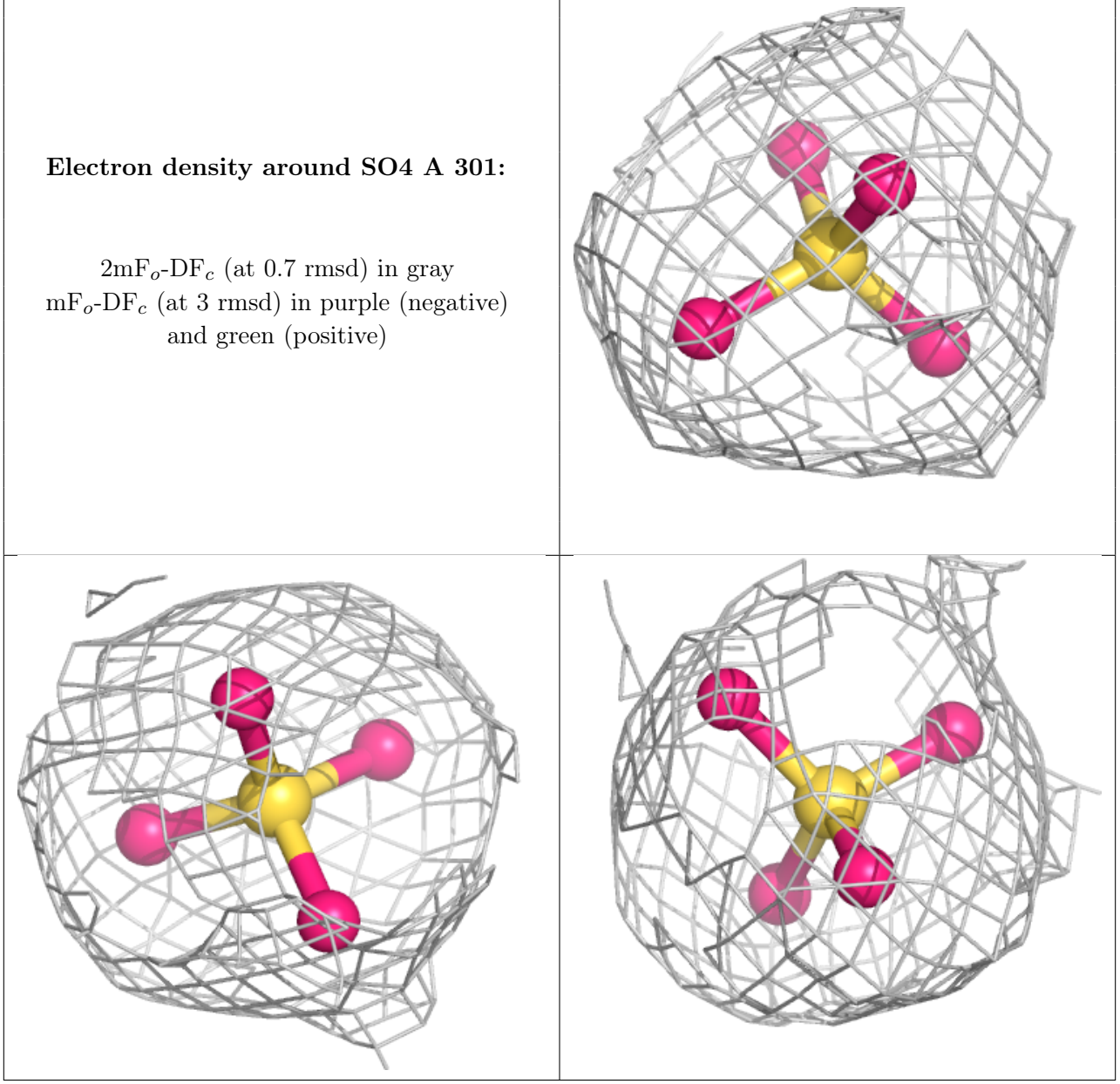






Electron density around SO4 A 301:

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



6.5 Other polymers

There are no such residues in this entry.