Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 11:27 PM JST

PDB ID	:	6K8T
Title	:	Crystal structure of C-domain with CoA of baterial malonyl-CoA reductase
Authors	:	Kim, S.; Kim, K.-J.
Deposited on	:	2019-06-13
Resolution	:	1.90 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 (i) 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 (i)) were used in the production of this report:

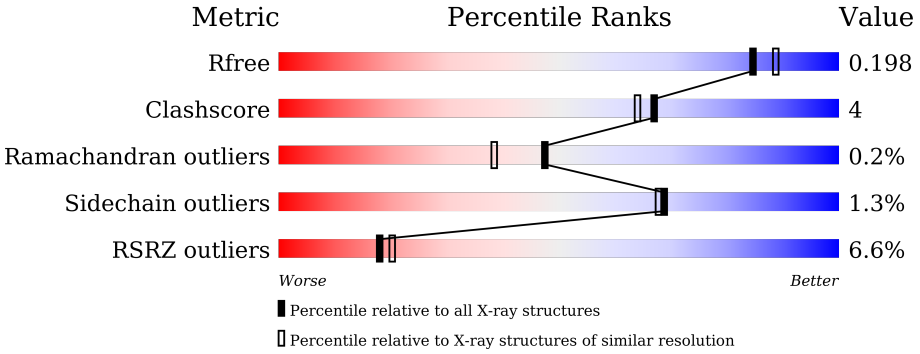
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	695	6% 87% 8% 5%
1	B	695	6% 86% 9% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10892 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 NAD-dependent epimerase/dehydratase:Short-chain dehydro genase/reductase SDR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	662	5079	3187	905	967	20	0	0	0
1	B	662	5079	3187	905	967	20	0	0	0

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	536	MET	-	initiating methionine	UNP A0A1A7BFR5
A	537	GLY	-	expression tag	UNP A0A1A7BFR5
A	538	SER	-	expression tag	UNP A0A1A7BFR5
A	539	SER	-	expression tag	UNP A0A1A7BFR5
A	540	HIS	-	expression tag	UNP A0A1A7BFR5
A	541	HIS	-	expression tag	UNP A0A1A7BFR5
A	542	HIS	-	expression tag	UNP A0A1A7BFR5
A	543	HIS	-	expression tag	UNP A0A1A7BFR5
A	544	HIS	-	expression tag	UNP A0A1A7BFR5
A	545	HIS	-	expression tag	UNP A0A1A7BFR5
A	546	SER	-	expression tag	UNP A0A1A7BFR5
A	547	SER	-	expression tag	UNP A0A1A7BFR5
A	548	GLY	-	expression tag	UNP A0A1A7BFR5
A	549	LEU	-	expression tag	UNP A0A1A7BFR5
A	550	VAL	-	expression tag	UNP A0A1A7BFR5
A	551	PRO	-	expression tag	UNP A0A1A7BFR5
A	552	ARG	-	expression tag	UNP A0A1A7BFR5
A	553	GLY	-	expression tag	UNP A0A1A7BFR5
A	554	SER	-	expression tag	UNP A0A1A7BFR5
A	555	HIS	-	expression tag	UNP A0A1A7BFR5
A	556	MET	-	expression tag	UNP A0A1A7BFR5
B	536	MET	-	initiating methionine	UNP A0A1A7BFR5
B	537	GLY	-	expression tag	UNP A0A1A7BFR5
B	538	SER	-	expression tag	UNP A0A1A7BFR5

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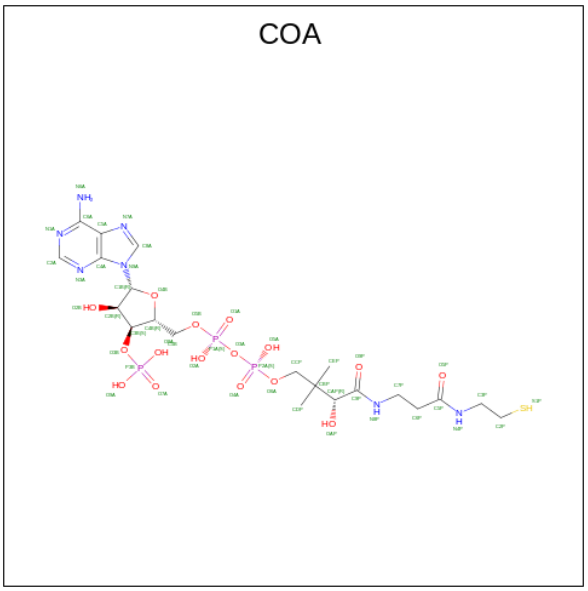
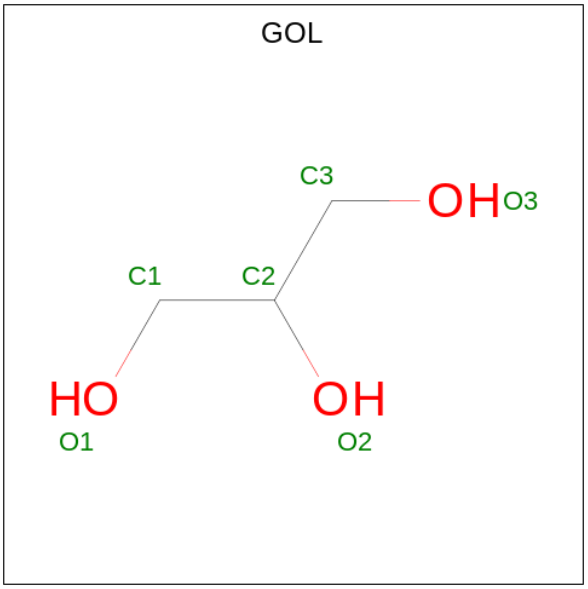
Chain	Residue	Modelled	Actual	Comment	Reference
B	539	SER	-	expression tag	UNP A0A1A7BFR5
B	540	HIS	-	expression tag	UNP A0A1A7BFR5
B	541	HIS	-	expression tag	UNP A0A1A7BFR5
B	542	HIS	-	expression tag	UNP A0A1A7BFR5
B	543	HIS	-	expression tag	UNP A0A1A7BFR5
B	544	HIS	-	expression tag	UNP A0A1A7BFR5
B	545	HIS	-	expression tag	UNP A0A1A7BFR5
B	546	SER	-	expression tag	UNP A0A1A7BFR5
B	547	SER	-	expression tag	UNP A0A1A7BFR5
B	548	GLY	-	expression tag	UNP A0A1A7BFR5
B	549	LEU	-	expression tag	UNP A0A1A7BFR5
B	550	VAL	-	expression tag	UNP A0A1A7BFR5
B	551	PRO	-	expression tag	UNP A0A1A7BFR5
B	552	ARG	-	expression tag	UNP A0A1A7BFR5
B	553	GLY	-	expression tag	UNP A0A1A7BFR5
B	554	SER	-	expression tag	UNP A0A1A7BFR5
B	555	HIS	-	expression tag	UNP A0A1A7BFR5
B	556	MET	-	expression tag	UNP A0A1A7BFR5

- Molecule 2 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$) (labeled as "Ligand of Interest" by depositor).



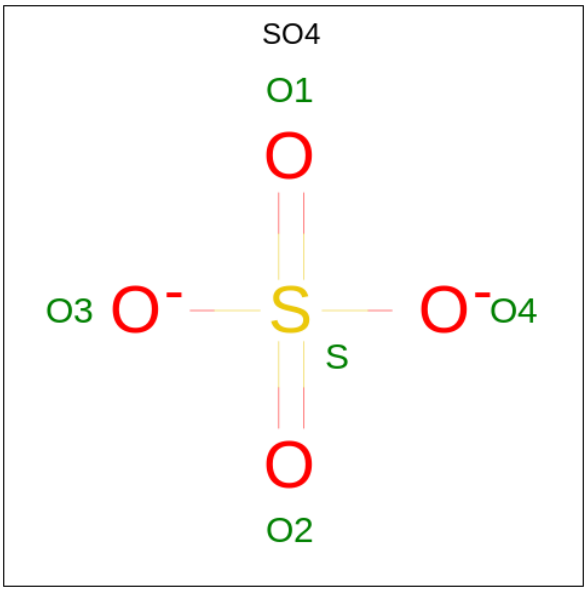
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	A	1	48	21	7	16	3	1	0	0
			Total	C	N	O	P	S		
2	B	1	48	21	7	16	3	1	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	A	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0
			Total	C	O		
3	B	1	6	3	3	0	0

- 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 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is water.

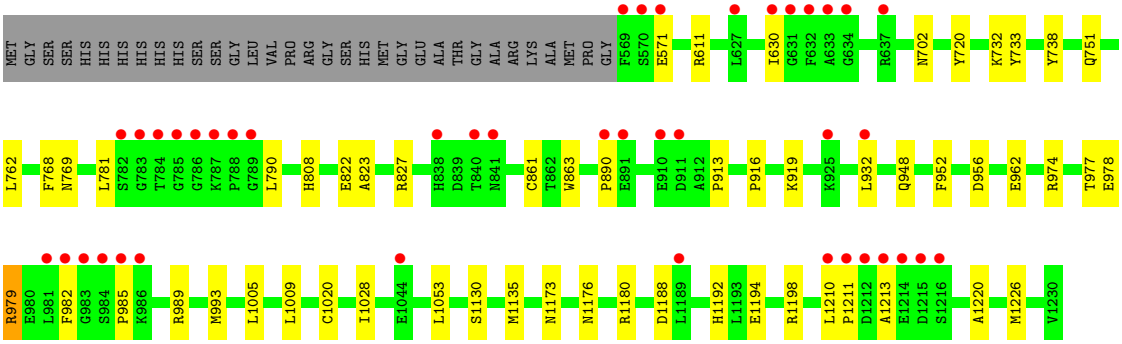
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	268	Total O 268 268	0	0
5	B	296	Total O 296 296	0	0

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.

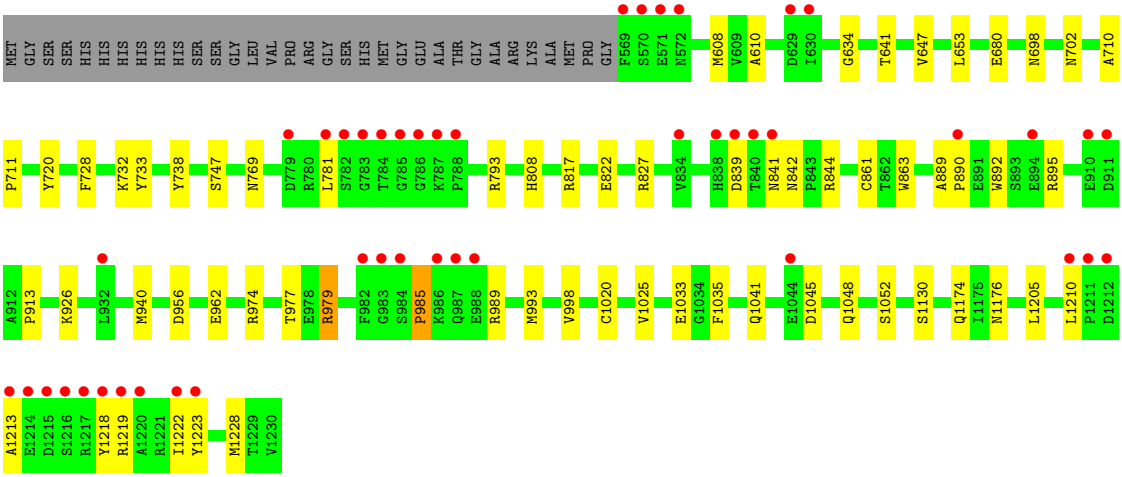
• Molecule 1: NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR

Chain A:



• Molecule 1: NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	110.47Å 116.24Å 134.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.89 – 1.90 30.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.3 (30.89-1.90) 99.4 (30.87-1.90)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.24 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.176 , 0.198 0.176 , 0.198	Depositor DCC
R_{free} test set	6643 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 50.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10892	wwPDB-VP
Average B, all atoms (Å^2)	27.0	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 39.92 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.9541e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.79	0/5170	0.88	0/7012
1	B	0.78	0/5170	0.87	0/7012
All	All	0.79	0/10340	0.87	0/14024

There are no bond length outliers.

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	5079	0	5060	36	0
1	B	5079	0	5060	46	0
2	A	48	0	32	0	0
2	B	48	0	32	3	0
3	A	12	0	16	2	0
3	B	12	0	16	1	0
4	A	20	0	0	0	0
4	B	30	0	0	1	0
5	A	268	0	0	2	0
5	B	296	0	0	7	0
All	All	10892	0	10216	80	0

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

All (80) 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:1301:COA:S1P	5:B:1662:HOH:O	2.37	0.82
1:B:1045:ASP:O	1:B:1048:GLN:HG2	1.81	0.81
1:B:1174:GLN:HE21	1:B:1176:ASN:HD21	1.29	0.79
1:A:702:ASN:HD21	1:A:751:GLN:HE21	1.29	0.78
1:A:611:ARG:H	3:A:1303:GOL:H12	1.51	0.74
1:A:769:ASN:HD22	1:A:962:GLU:H	1.37	0.71
1:B:769:ASN:HD22	1:B:962:GLU:H	1.37	0.70
1:A:733:TYR:O	1:A:977:THR:HA	1.93	0.69
1:A:822:GLU:OE1	1:A:890:PRO:HD2	1.92	0.68
1:A:702:ASN:ND2	1:A:751:GLN:HE21	1.93	0.67
1:A:1213:ALA:HA	1:A:1220:ALA:HB2	1.77	0.65
1:B:822:GLU:OE1	1:B:890:PRO:HD3	1.96	0.64
1:B:827:ARG:HH22	1:B:841:ASN:ND2	1.95	0.64
1:B:822:GLU:OE1	1:B:890:PRO:CD	2.47	0.63
1:A:611:ARG:HB2	3:A:1303:GOL:H32	1.82	0.61
1:A:1173:ASN:HD22	1:A:1226:MET:H	1.50	0.58
1:A:979:ARG:HA	1:B:979:ARG:NH1	2.21	0.56
1:B:781:LEU:CD2	1:B:940:MET:SD	2.95	0.55
1:B:1041:GLN:HG3	5:B:1525:HOH:O	2.06	0.55
1:B:733:TYR:O	1:B:977:THR:HG23	2.07	0.55
1:A:948:GLN:HG2	1:A:952:PHE:CE2	2.41	0.55
1:A:1135:MET:HE1	1:A:1188:ASP:O	2.07	0.54
1:B:1218:TYR:CE2	1:B:1222:ILE:HD11	2.44	0.54
1:B:769:ASN:ND2	1:B:962:GLU:H	2.06	0.53
1:A:1173:ASN:ND2	1:A:1226:MET:H	2.07	0.52
1:B:892:TRP:CE3	1:B:895:ARG:HD2	2.45	0.52
1:B:1033:GLU:HG2	5:B:1641:HOH:O	2.10	0.51
1:B:610:ALA:HB1	3:B:1303:GOL:H2	1.93	0.51
1:A:808:HIS:HE1	5:A:1554:HOH:O	1.93	0.51
1:A:989:ARG:NH2	1:A:1210:LEU:HD23	2.26	0.51
1:A:979:ARG:HA	1:B:979:ARG:CZ	2.40	0.50
1:B:827:ARG:HH22	1:B:841:ASN:HD21	1.60	0.49
1:A:1210:LEU:HD22	1:A:1211:PRO:HD2	1.95	0.49
1:B:680:GLU:OE1	1:B:793:ARG:NH2	2.44	0.49
1:B:1205:LEU:HD23	1:B:1228:MET:HE1	1.95	0.48
1:A:978:GLU:O	1:B:979:ARG:NH1	2.46	0.48
1:A:762:LEU:HD12	1:A:768:PHE:CD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:647:VAL:HG12	1:B:653:LEU:HD21	1.95	0.47
1:B:1213:ALA:HB1	1:B:1219:ARG:CB	2.44	0.47
1:B:998:VAL:CG2	1:B:1025:VAL:HG22	2.45	0.47
1:A:1194:GLU:OE2	1:A:1198:ARG:NH2	2.45	0.47
1:B:1213:ALA:HB1	1:B:1219:ARG:HB3	1.97	0.47
1:B:839:ASP:HB3	1:B:842:ASN:ND2	2.30	0.46
1:A:1028:ILE:HA	1:A:1053:LEU:O	2.16	0.46
1:B:808:HIS:HE1	5:B:1602:HOH:O	1.97	0.46
1:B:1041:GLN:CG	5:B:1525:HOH:O	2.64	0.46
1:A:916:PRO:HG2	1:A:919:LYS:HB2	1.98	0.45
1:B:732:LYS:HE3	5:B:1510:HOH:O	2.16	0.45
1:B:926:LYS:HE3	2:B:1301:COA:O9A	2.17	0.45
1:A:571:GLU:OE2	1:A:630:ILE:HD11	2.16	0.45
1:B:817:ARG:HH21	1:B:844:ARG:HG2	1.82	0.45
1:B:822:GLU:OE1	1:B:890:PRO:HD2	2.16	0.45
1:A:982:PHE:CD2	1:A:982:PHE:O	2.70	0.44
1:B:808:HIS:HD2	5:B:1613:HOH:O	1.99	0.44
1:B:993:MET:HB2	1:B:1020:CYS:HB3	1.99	0.44
1:A:769:ASN:ND2	1:A:962:GLU:H	2.09	0.44
1:A:993:MET:HB2	1:A:1020:CYS:HB3	1.99	0.44
1:A:1135:MET:HE3	1:A:1192:HIS:HB2	1.99	0.44
1:B:608:MET:O	1:B:641:THR:HA	2.18	0.44
1:B:1174:GLN:HE21	1:B:1176:ASN:ND2	2.05	0.44
1:A:823:ALA:O	1:A:827:ARG:HG2	2.17	0.44
1:B:1130:SER:OG	1:B:1176:ASN:HA	2.17	0.44
1:B:1035:PHE:CD1	1:B:1052:SER:HB2	2.53	0.43
1:A:861:CYS:HA	1:A:913:PRO:O	2.19	0.43
1:B:728:PHE:CZ	2:B:1301:COA:H62	2.54	0.43
1:A:732:LYS:HG2	1:A:733:TYR:CE2	2.53	0.42
1:B:822:GLU:OE1	1:B:889:ALA:HA	2.19	0.42
1:B:634:GLY:HA2	4:B:1308:SO4:O3	2.19	0.42
1:B:861:CYS:HA	1:B:913:PRO:O	2.19	0.42
1:A:1005:LEU:O	1:A:1009:LEU:HG	2.20	0.42
1:B:827:ARG:NH2	1:B:841:ASN:ND2	2.66	0.42
1:A:808:HIS:HD2	5:A:1597:HOH:O	2.03	0.41
1:B:710:ALA:HB3	1:B:711:PRO:HD3	2.02	0.41
1:A:978:GLU:OE1	1:A:1180:ARG:NH2	2.44	0.41
1:A:1130:SER:OG	1:A:1176:ASN:HA	2.21	0.41
1:A:781:LEU:HA	1:A:790:LEU:HG	2.03	0.40
1:B:1210:LEU:HD21	1:B:1223:TYR:HB3	2.03	0.40
1:B:985:PRO:HB3	1:B:989:ARG:HH11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:PHE:O	1:A:982:PHE:CG	2.74	0.40
1:B:698:ASN:HB2	1:B:747:SER:HB2	2.04	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	660/695 (95%)	647 (98%)	12 (2%)	1 (0%)	47	38
1	B	660/695 (95%)	647 (98%)	12 (2%)	1 (0%)	47	38
All	All	1320/1390 (95%)	1294 (98%)	24 (2%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	985	PRO
1	B	985	PRO

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	529/553 (96%)	522 (99%)	7 (1%)	69	68
1	B	529/553 (96%)	522 (99%)	7 (1%)	69	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1058/1106 (96%)	1044 (99%)	14 (1%)	69 68

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	TYR
1	A	738	TYR
1	A	863	TRP
1	A	932	LEU
1	A	956	ASP
1	A	974	ARG
1	A	979	ARG
1	B	702	ASN
1	B	720	TYR
1	B	738	TYR
1	B	863	TRP
1	B	956	ASP
1	B	974	ARG
1	B	979	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	672	ASN
1	A	702	ASN
1	A	769	ASN
1	A	808	HIS
1	A	842	ASN
1	A	1107	ASN
1	A	1173	ASN
1	A	1182	GLN
1	B	594	GLN
1	B	640	GLN
1	B	672	ASN
1	B	767	GLN
1	B	769	ASN
1	B	808	HIS
1	B	944	HIS
1	B	1176	ASN

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)

16 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	A	1305	-	4,4,4	0.31	0	6,6,6	0.13	0
4	SO4	B	1308	-	4,4,4	0.33	0	6,6,6	0.25	0
4	SO4	B	1304	-	4,4,4	0.53	0	6,6,6	0.16	0
4	SO4	A	1307	-	4,4,4	0.20	0	6,6,6	0.33	0
2	COA	A	1301	-	41,50,50	0.74	1 (2%)	52,75,75	1.02	4 (7%)
4	SO4	B	1305	-	4,4,4	0.28	0	6,6,6	0.12	0
3	GOL	A	1303	-	5,5,5	0.11	0	5,5,5	0.57	0
2	COA	B	1301	-	41,50,50	0.65	0	52,75,75	1.23	3 (5%)
4	SO4	A	1304	-	4,4,4	0.21	0	6,6,6	0.17	0
3	GOL	A	1302	-	5,5,5	0.34	0	5,5,5	0.39	0
4	SO4	B	1307	-	4,4,4	0.35	0	6,6,6	0.28	0
3	GOL	B	1303	-	5,5,5	0.30	0	5,5,5	0.76	0
4	SO4	A	1306	-	4,4,4	0.52	0	6,6,6	0.20	0
4	SO4	B	1309	-	4,4,4	0.29	0	6,6,6	0.11	0
4	SO4	B	1306	-	4,4,4	0.24	0	6,6,6	0.14	0
3	GOL	B	1302	-	5,5,5	0.11	0	5,5,5	0.95	0

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
2	COA	A	1301	-	-	8/44/64/64	0/3/3/3
3	GOL	A	1303	-	-	2/4/4/4	-
2	COA	B	1301	-	-	10/44/64/64	0/3/3/3
3	GOL	A	1302	-	-	0/4/4/4	-
3	GOL	B	1303	-	-	2/4/4/4	-
3	GOL	B	1302	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	COA	P3B-O3B	2.22	1.63	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1301	COA	O3B-P3B-O7A	-4.19	93.23	109.39
2	B	1301	COA	C3P-N4P-C5P	3.29	128.95	122.84
2	A	1301	COA	O6A-CCP-CBP	-3.10	105.57	110.55
2	B	1301	COA	CEP-CBP-CAP	2.73	113.55	108.82
2	A	1301	COA	C5A-C6A-N6A	2.23	123.74	120.35
2	A	1301	COA	O8A-P3B-O3B	-2.18	96.24	105.99
2	A	1301	COA	O9A-P3B-O8A	2.08	115.59	107.64

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	COA	C5B-O5B-P1A-O3A
2	A	1301	COA	O9P-C9P-CAP-OAP
2	A	1301	COA	N8P-C9P-CAP-OAP
2	B	1301	COA	C3B-O3B-P3B-O7A
2	B	1301	COA	C5B-O5B-P1A-O2A
2	B	1301	COA	C5B-O5B-P1A-O3A
2	B	1301	COA	O9P-C9P-CAP-OAP
2	B	1301	COA	N8P-C9P-CAP-OAP
3	B	1302	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	B	1303	GOL	C1-C2-C3-O3
3	B	1303	GOL	O2-C2-C3-O3
3	B	1302	GOL	O2-C2-C3-O3
3	A	1303	GOL	C1-C2-C3-O3
3	A	1303	GOL	O2-C2-C3-O3
2	A	1301	COA	P2A-O3A-P1A-O1A
2	A	1301	COA	O5P-C5P-N4P-C3P
2	A	1301	COA	C6P-C5P-N4P-C3P
2	B	1301	COA	C3B-O3B-P3B-O8A
3	B	1302	GOL	O1-C1-C2-O2
2	A	1301	COA	P2A-O3A-P1A-O2A
2	B	1301	COA	O5P-C5P-N4P-C3P
2	A	1301	COA	C5B-O5B-P1A-O2A
2	B	1301	COA	P2A-O3A-P1A-O1A
2	B	1301	COA	P2A-O3A-P1A-O2A
2	B	1301	COA	C2P-C3P-N4P-C5P

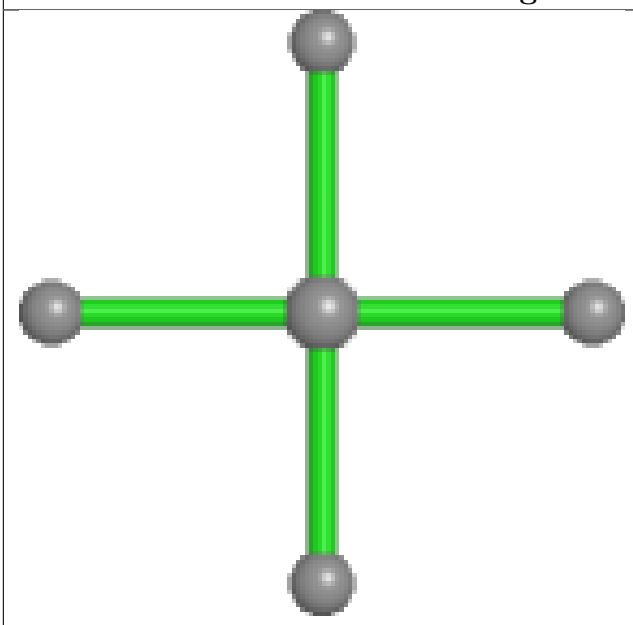
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1308	SO4	1	0
3	A	1303	GOL	2	0
2	B	1301	COA	3	0
3	B	1303	GOL	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 A 1305



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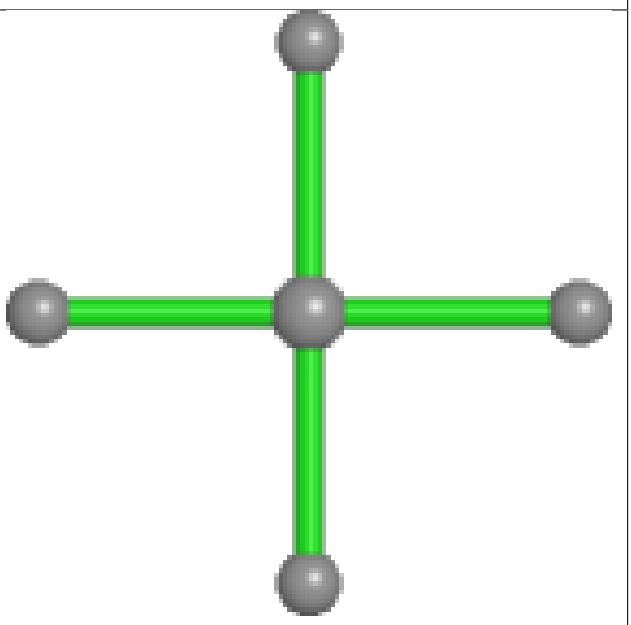

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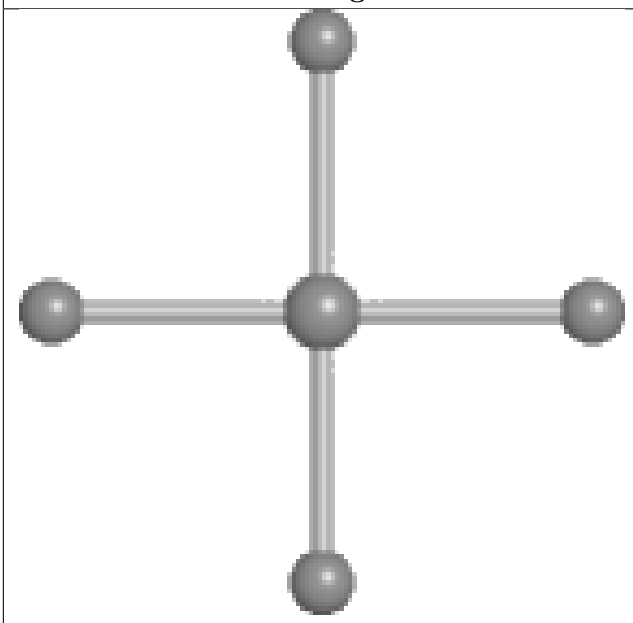
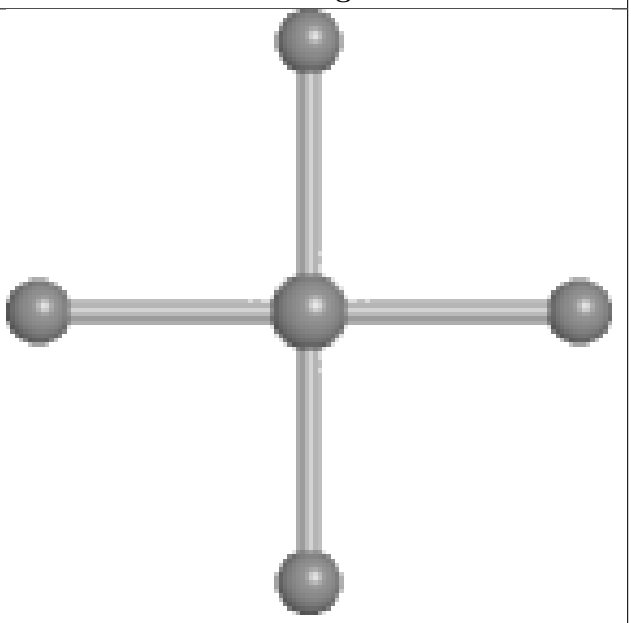
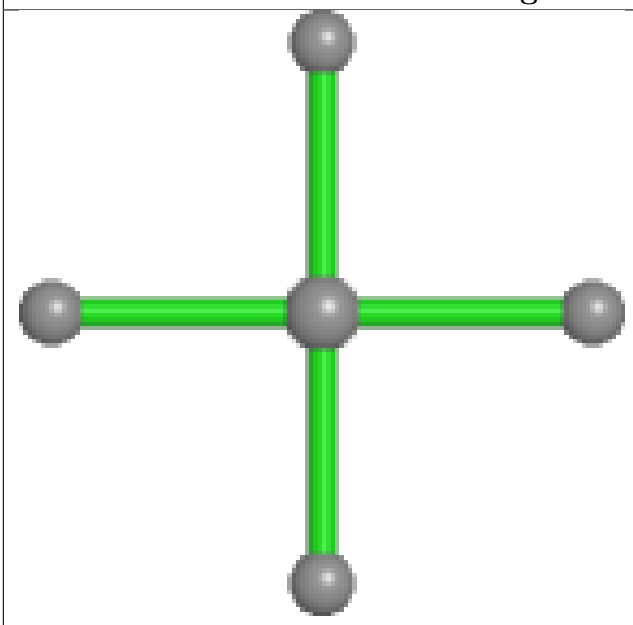


Torsions



Rings

Ligand SO4 B 1308



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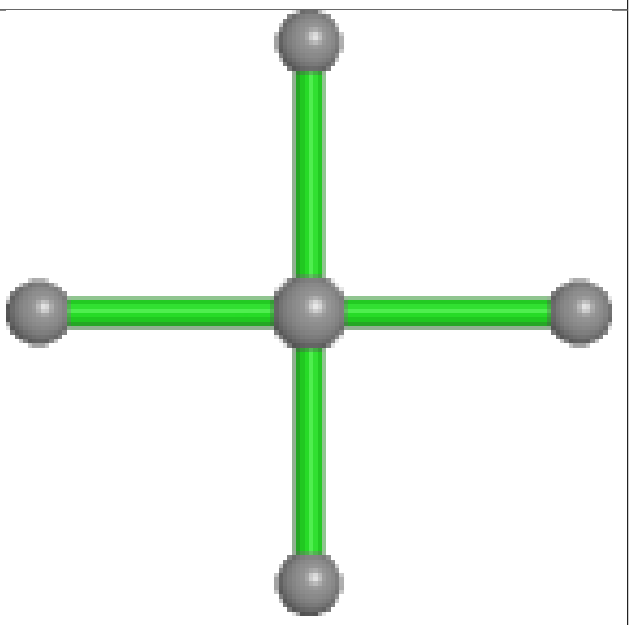

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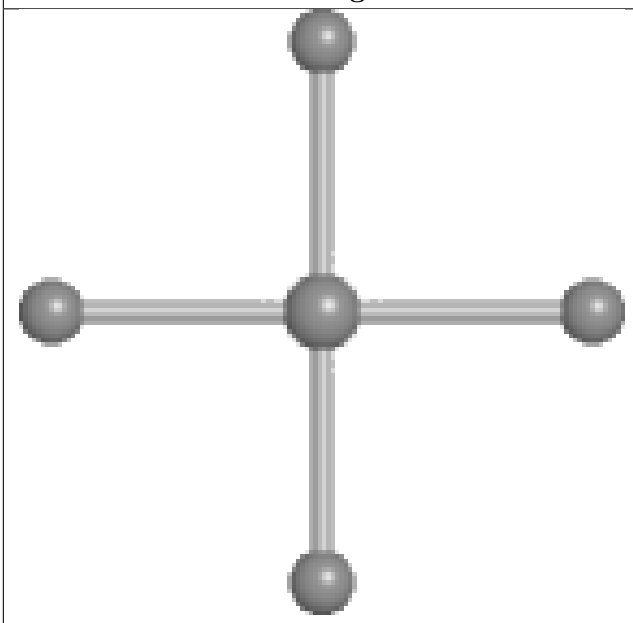

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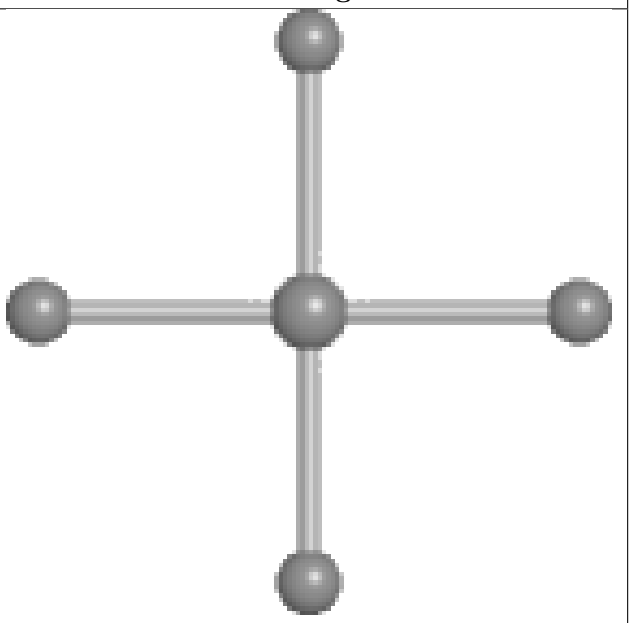
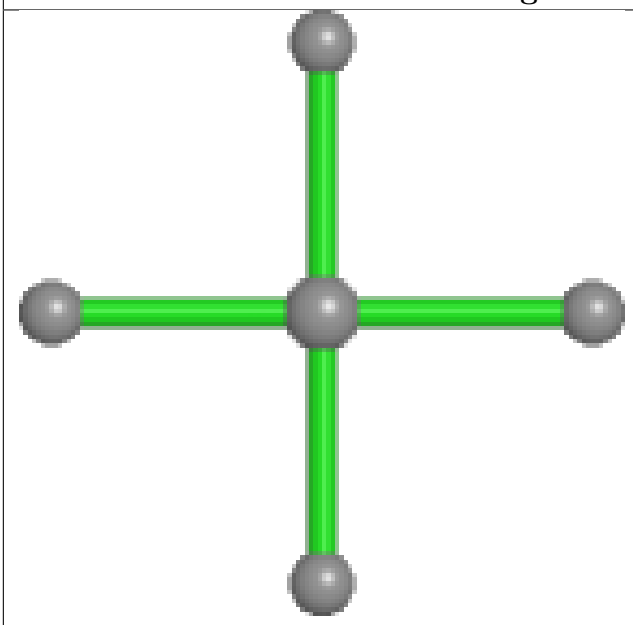


Rings

Ligand SO4 B 1304



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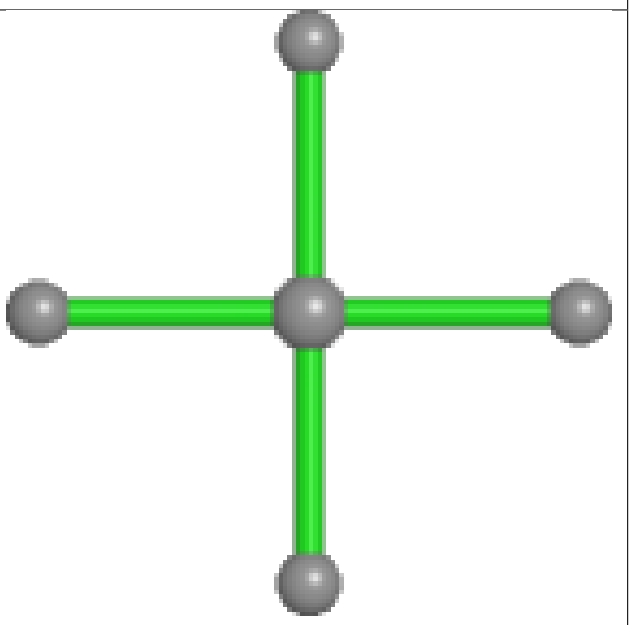

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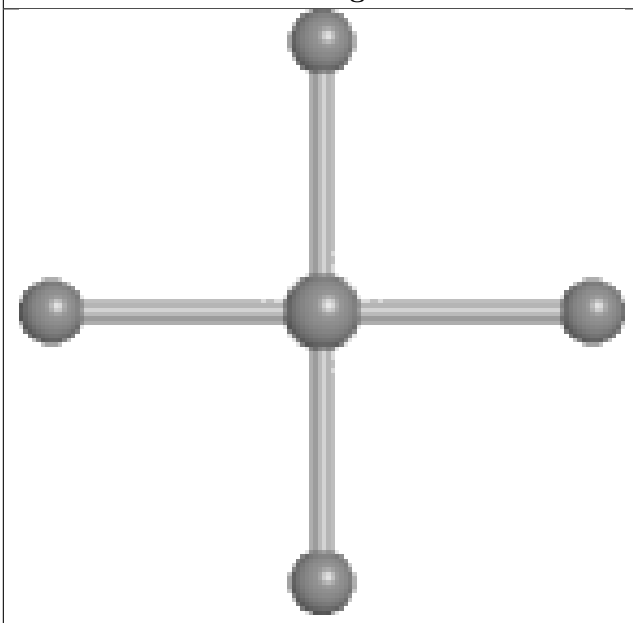

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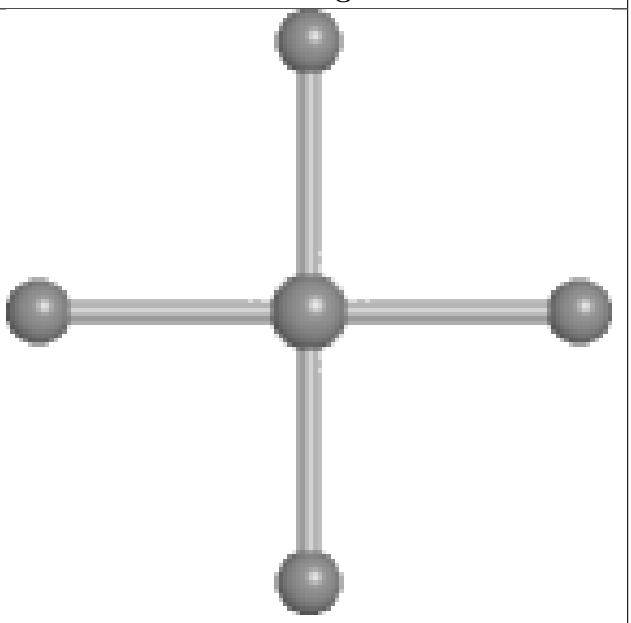
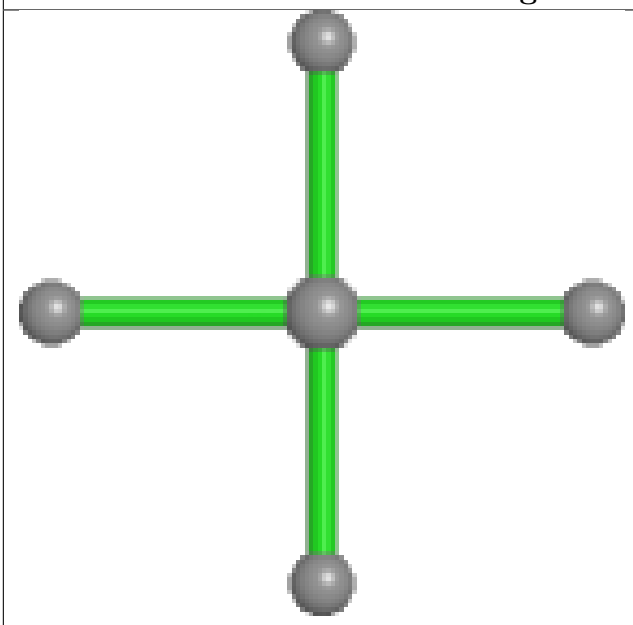


Rings

Ligand SO4 A 1307



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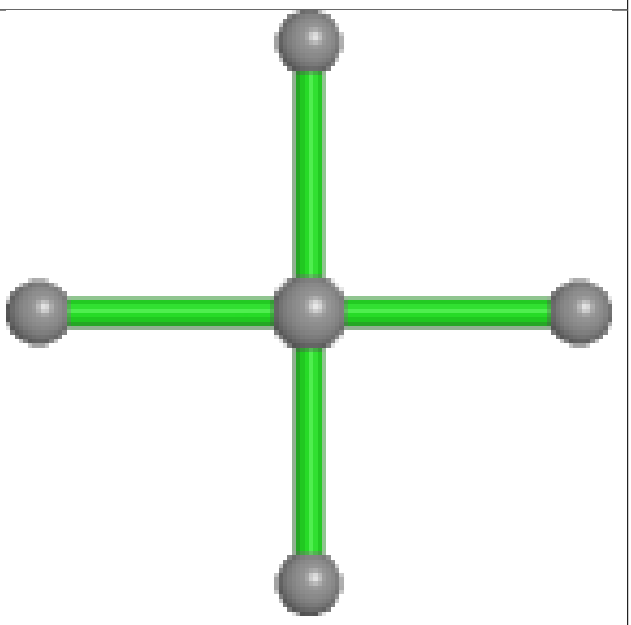

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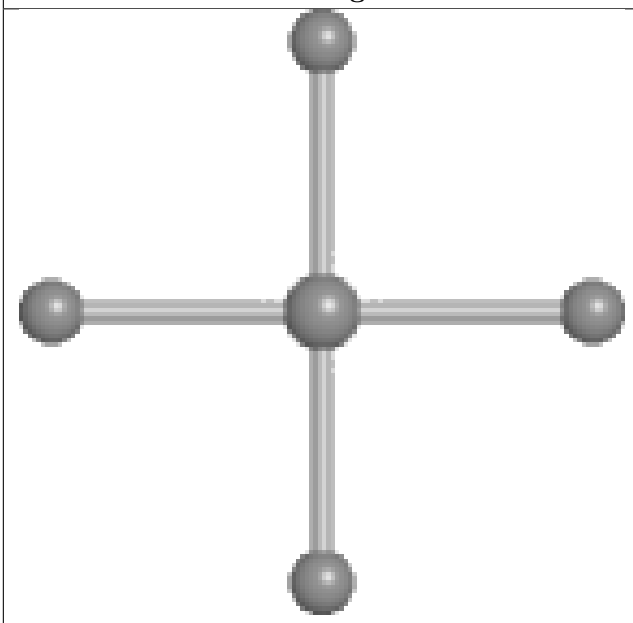

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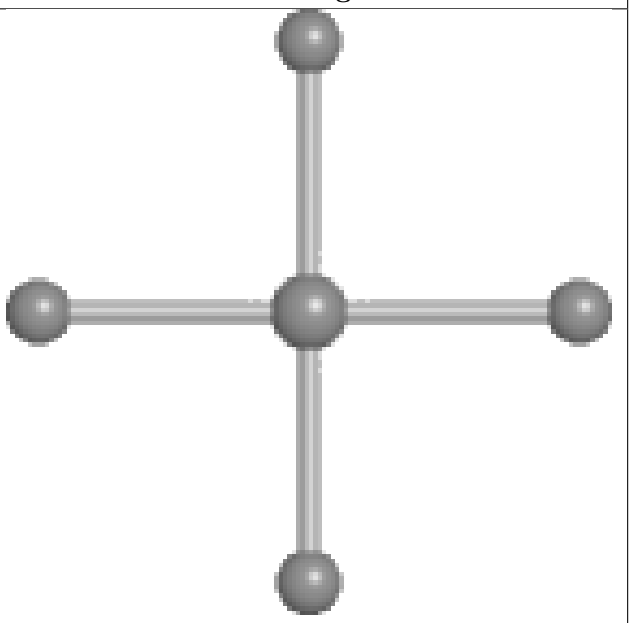
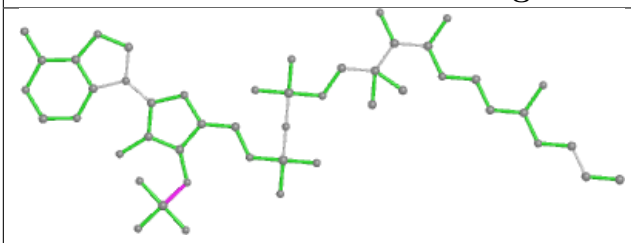


Rings

Ligand COA A 1301



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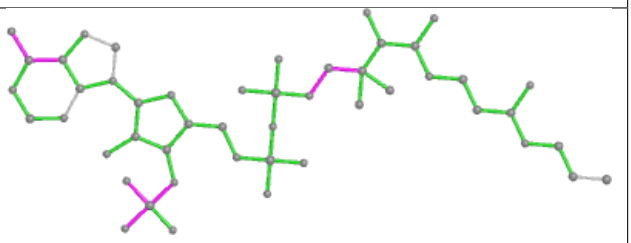

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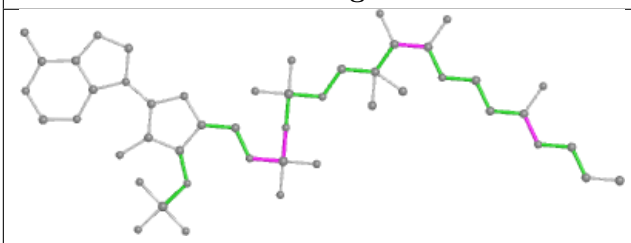

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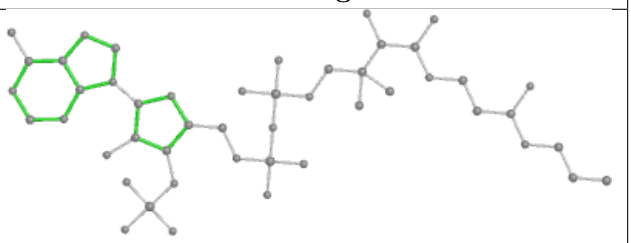
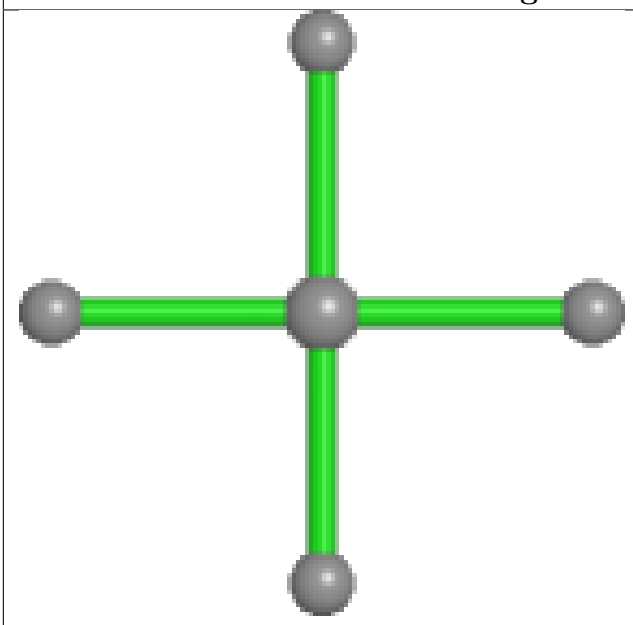


Rings

Ligand SO4 B 1305



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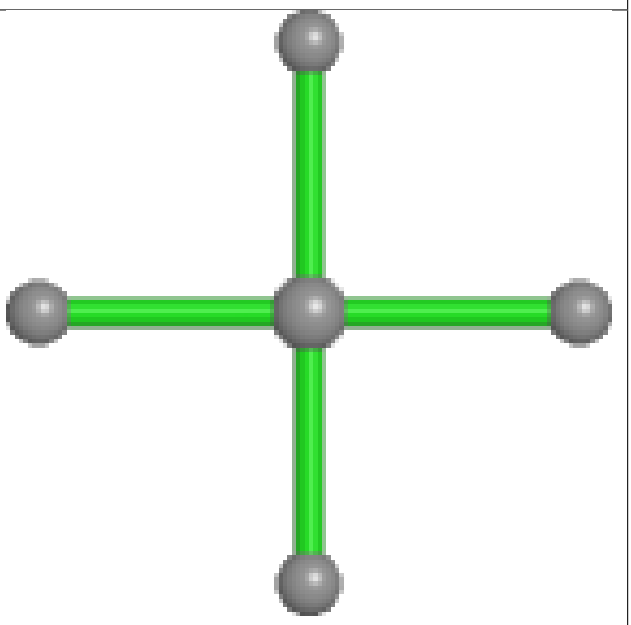

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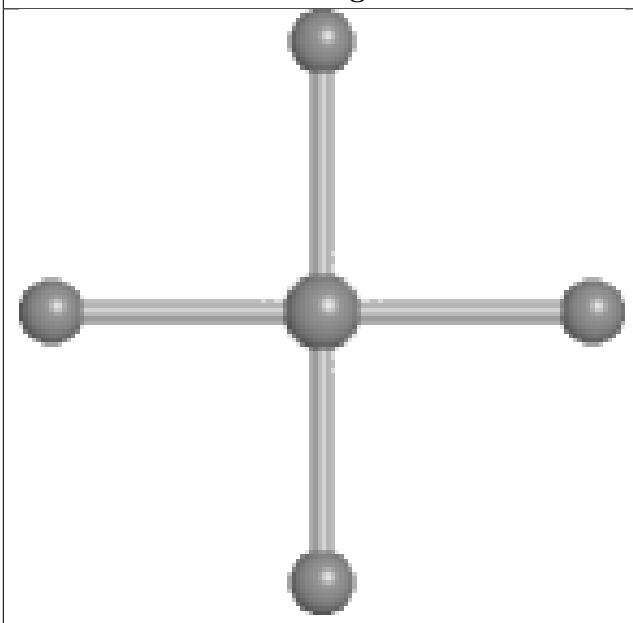

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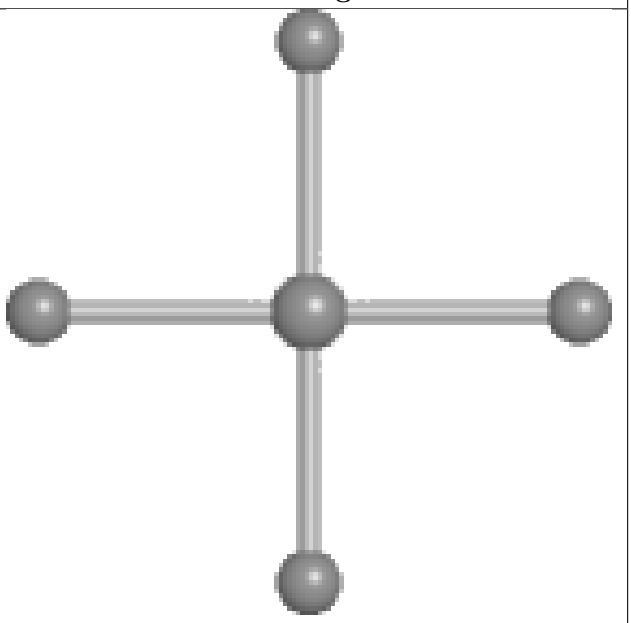
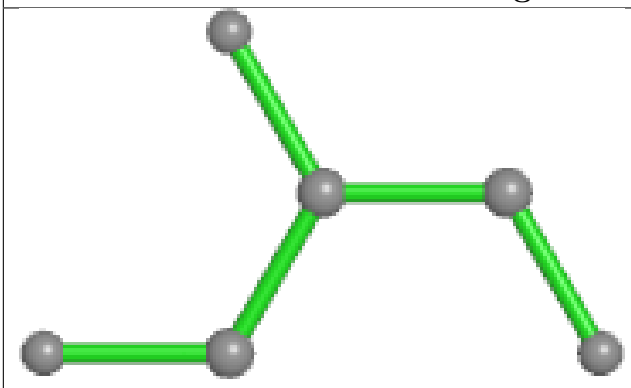


Rings

Ligand GOL A 1303



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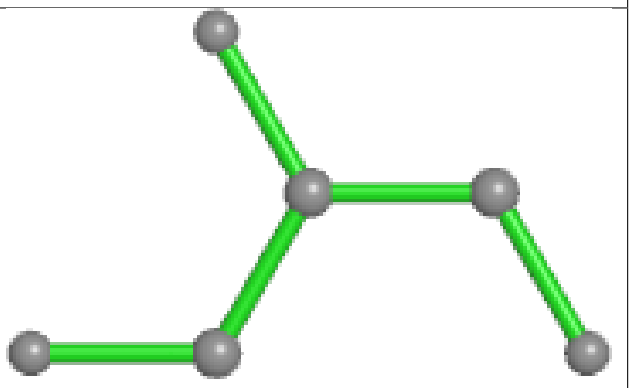

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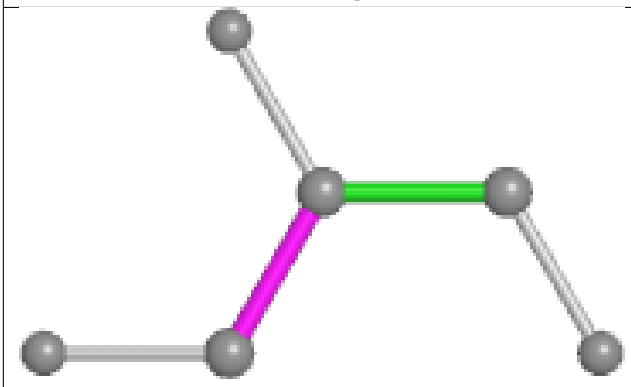

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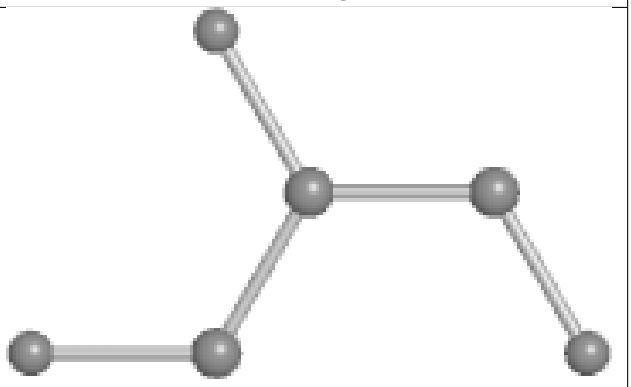
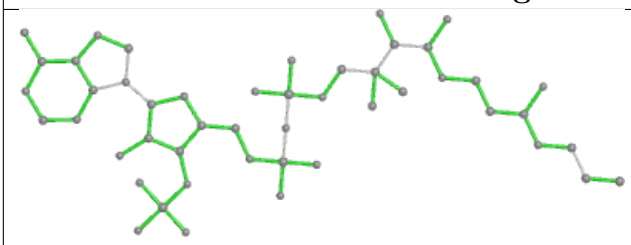
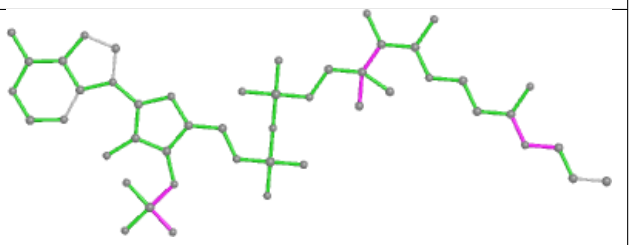


Rings

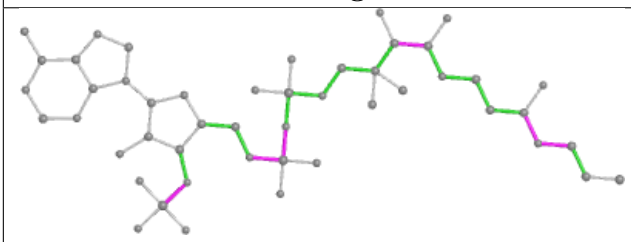
Ligand COA B 1301



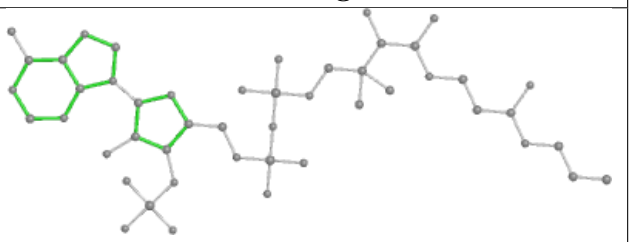
Bond lengths



Bond angles

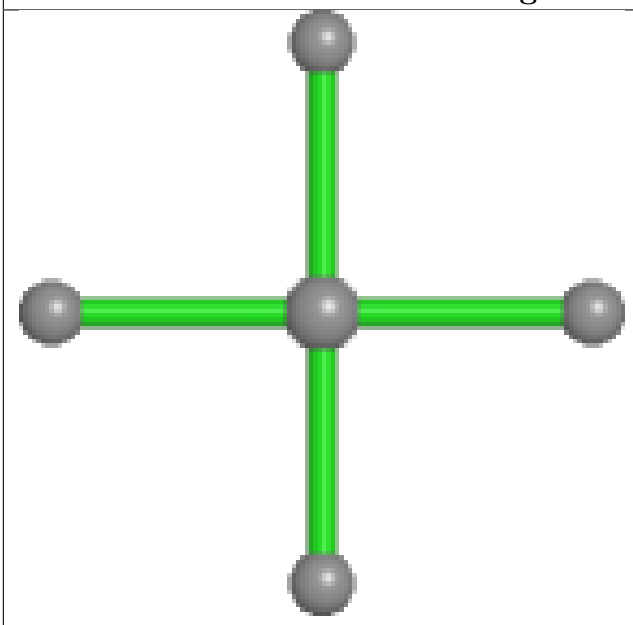


Torsions

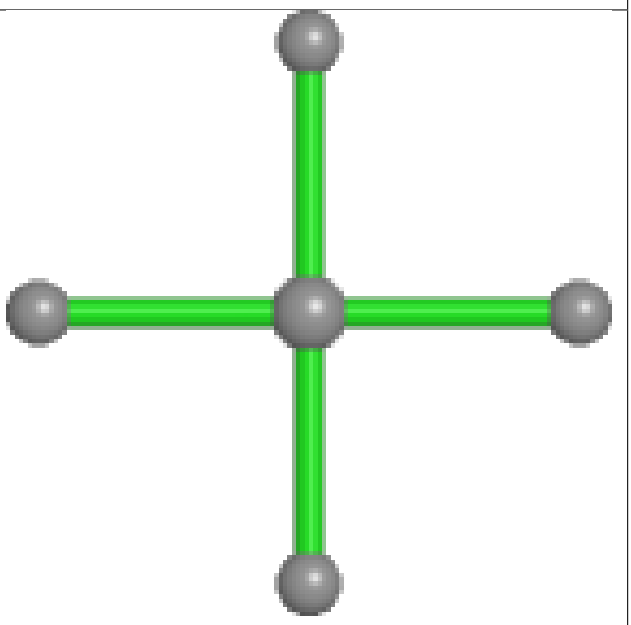


Rings

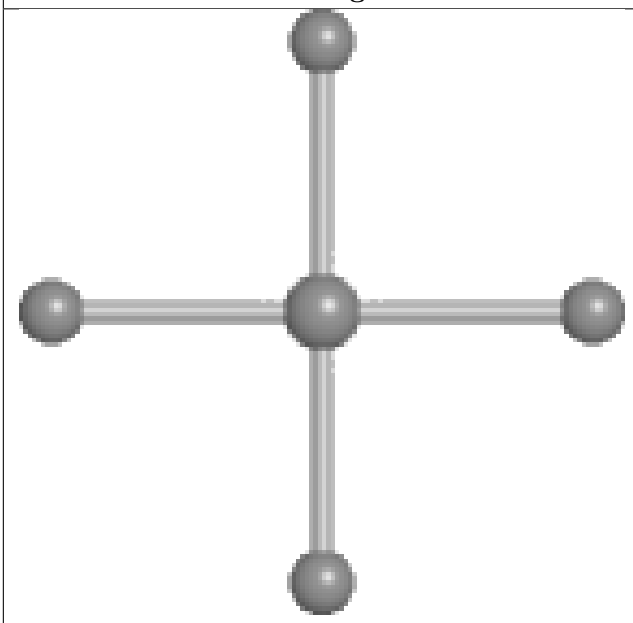
Ligand SO4 A 1304



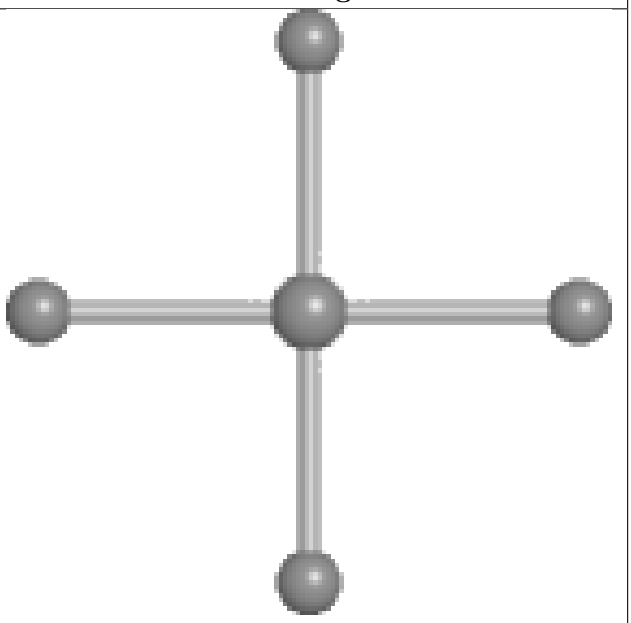
Bond lengths



Bond angles

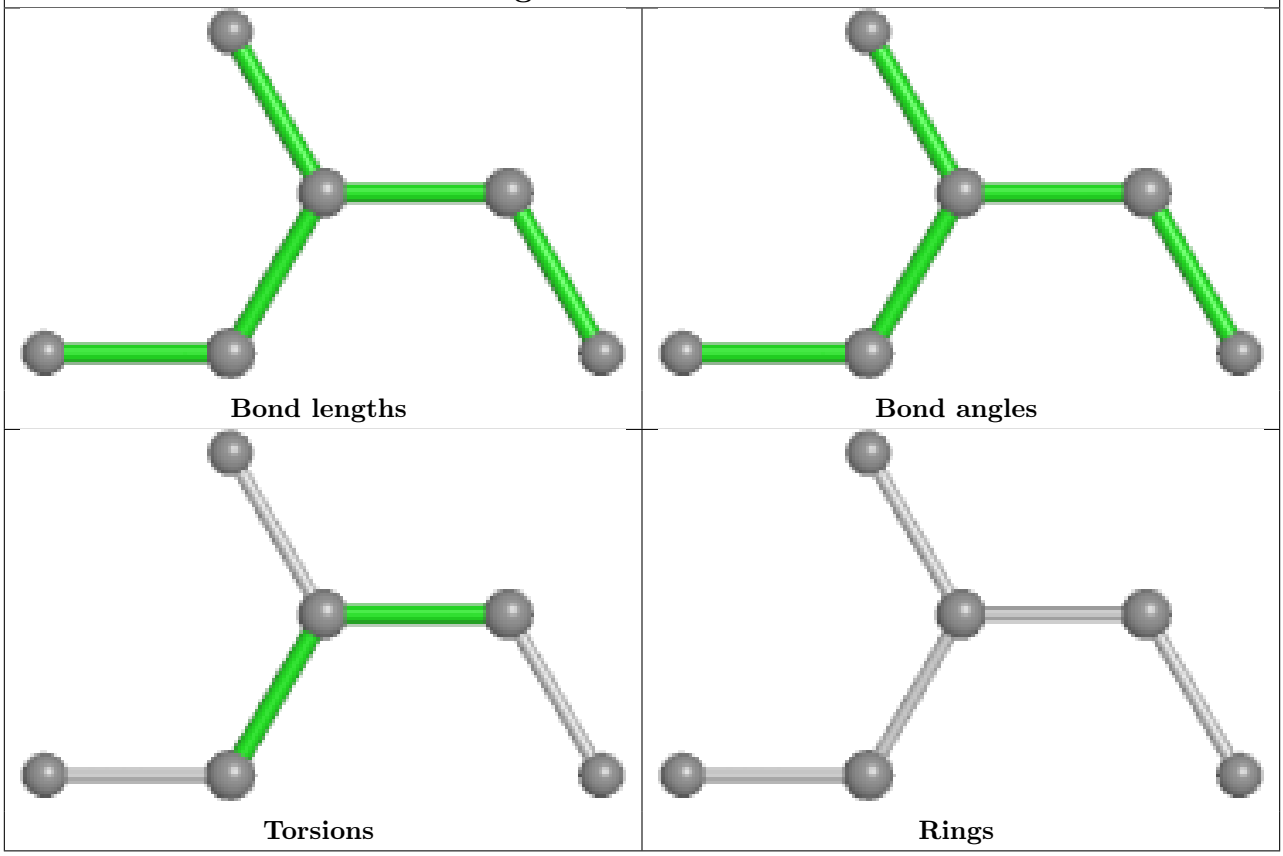


Torsions

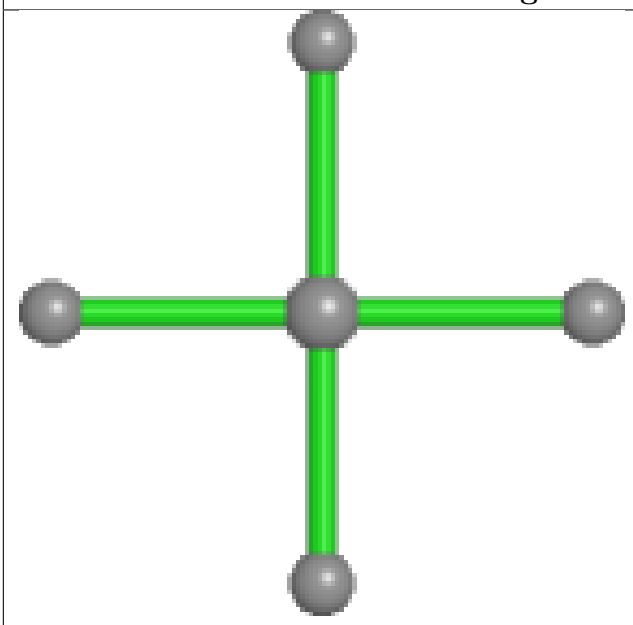


Rings

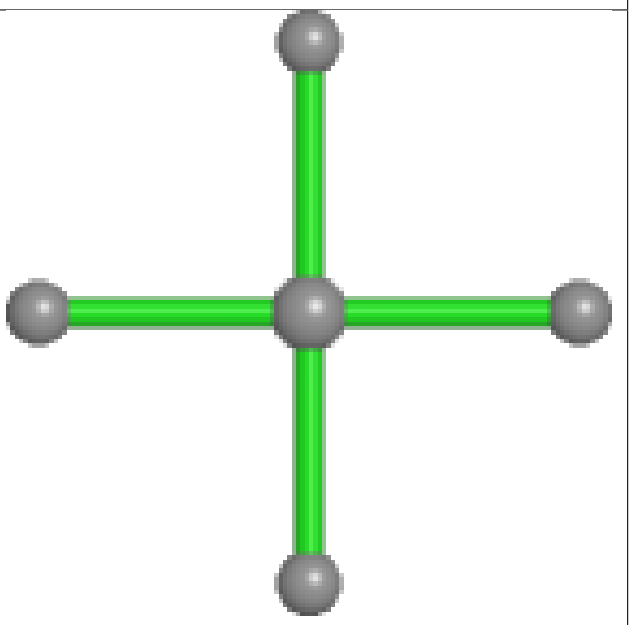
Ligand GOL A 1302



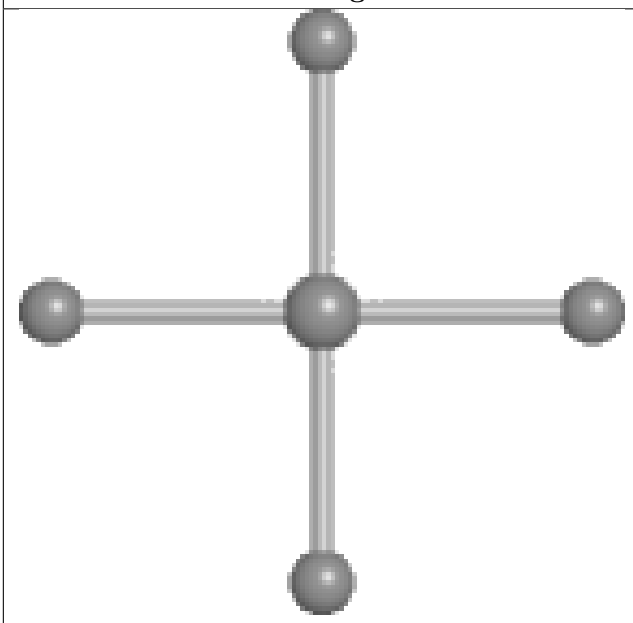
Ligand SO4 B 1307



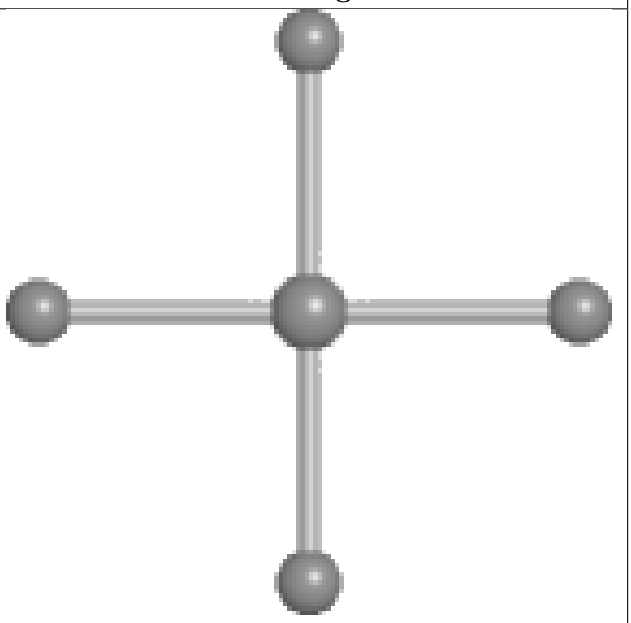
Bond lengths



Bond angles

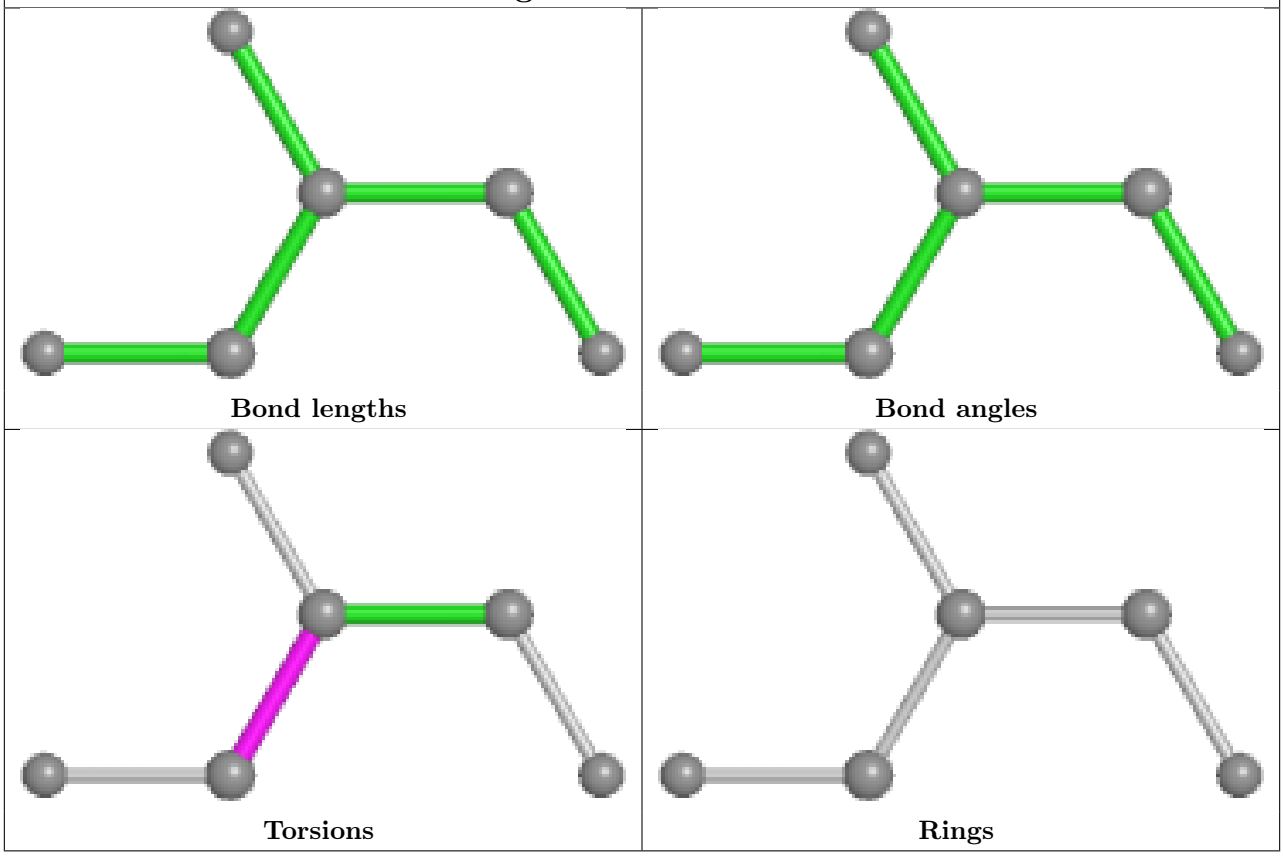


Torsions

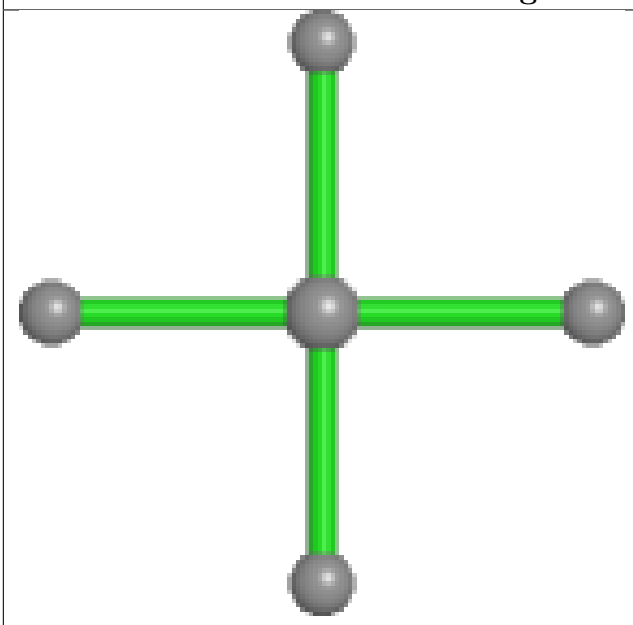


Rings

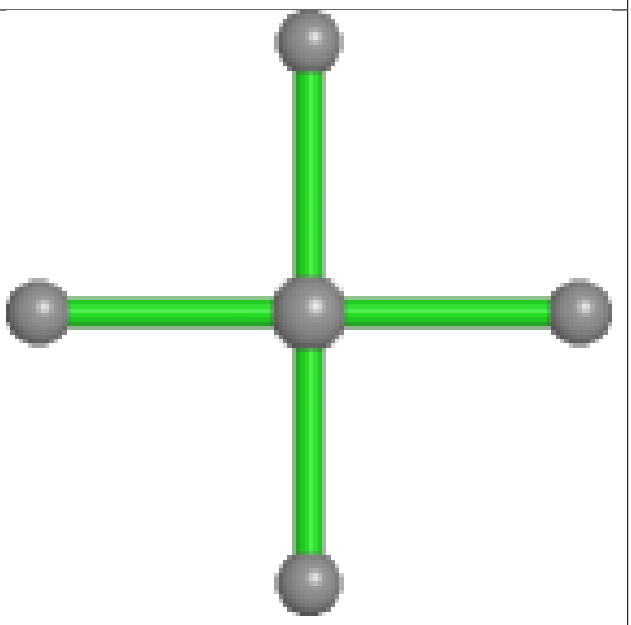
Ligand GOL B 1303



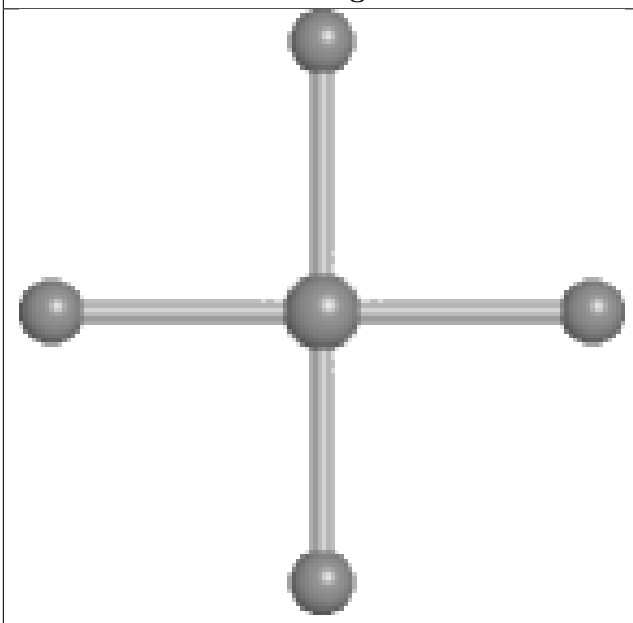
Ligand SO4 A 1306



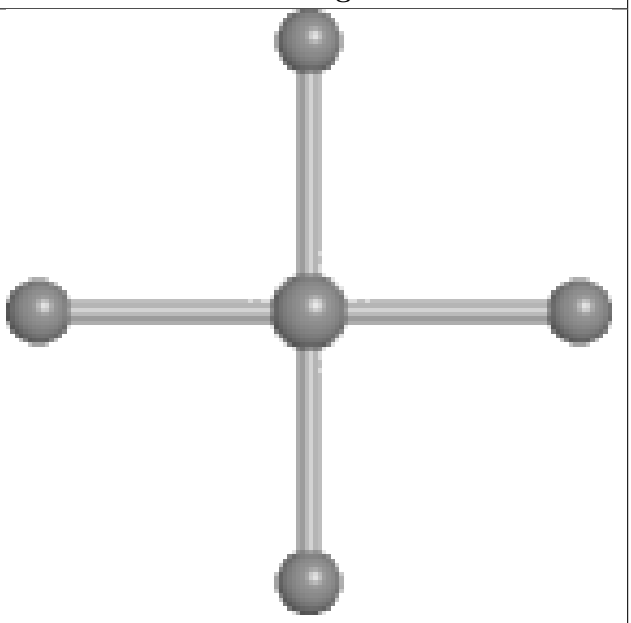
Bond lengths



Bond angles

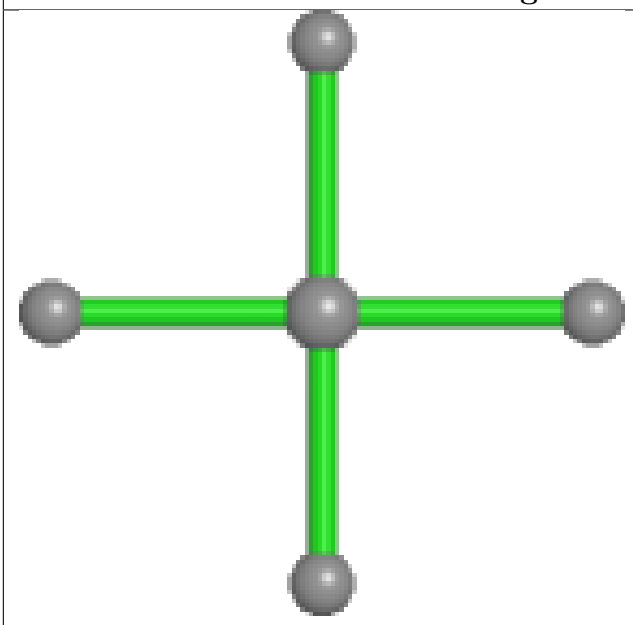


Torsions

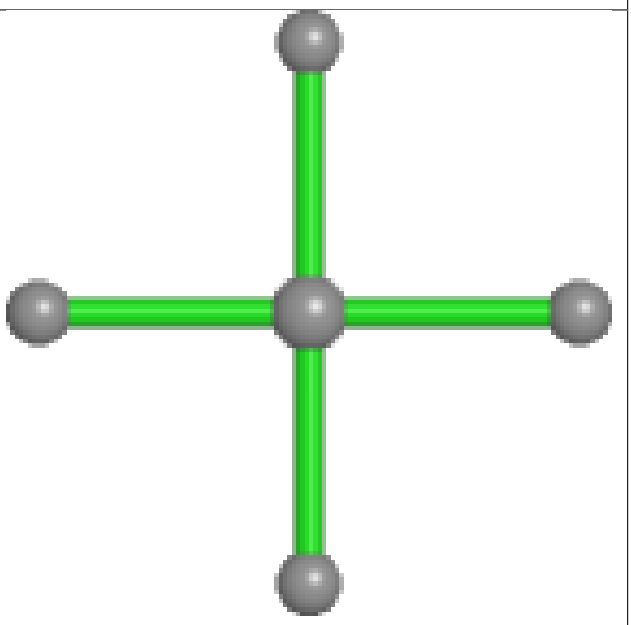


Rings

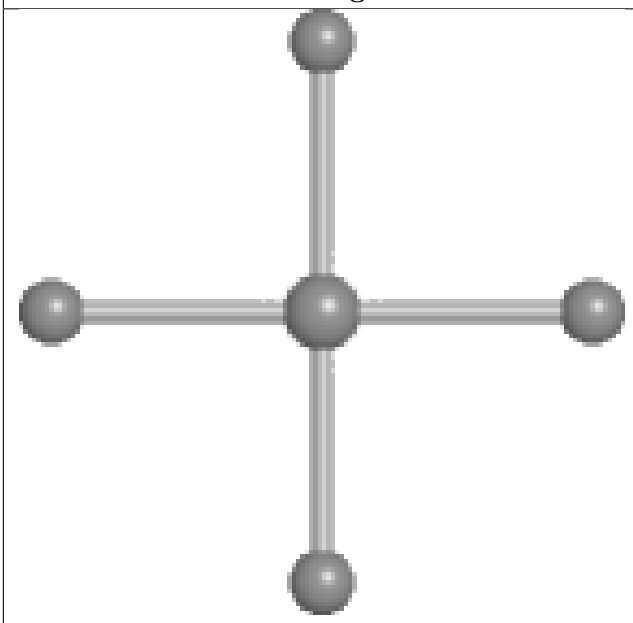
Ligand SO4 B 1309



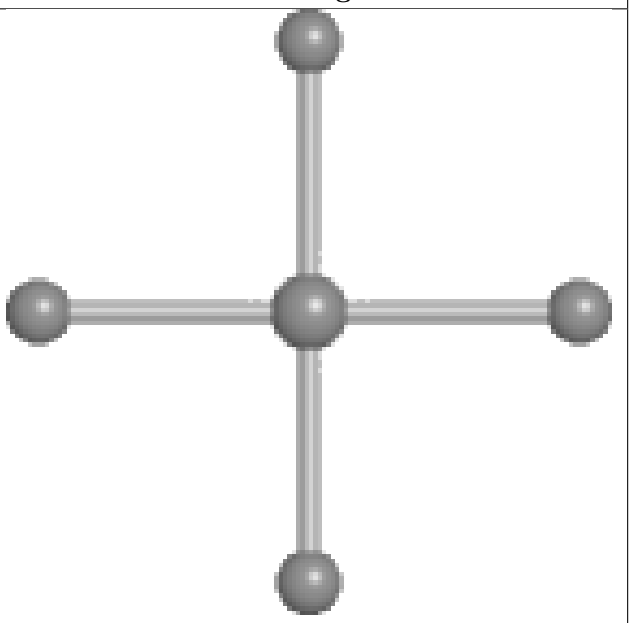
Bond lengths



Bond angles

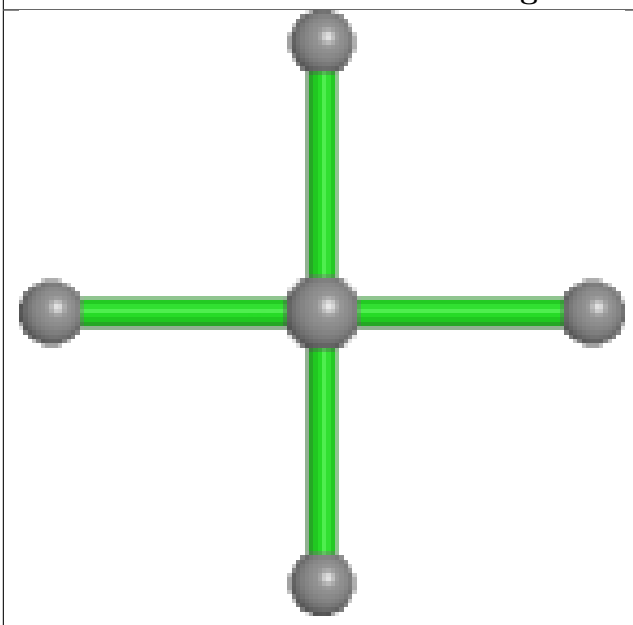


Torsions

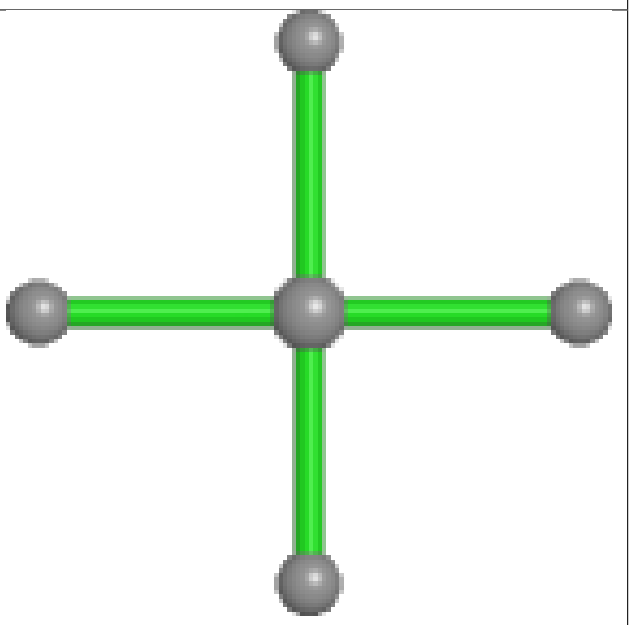


Rings

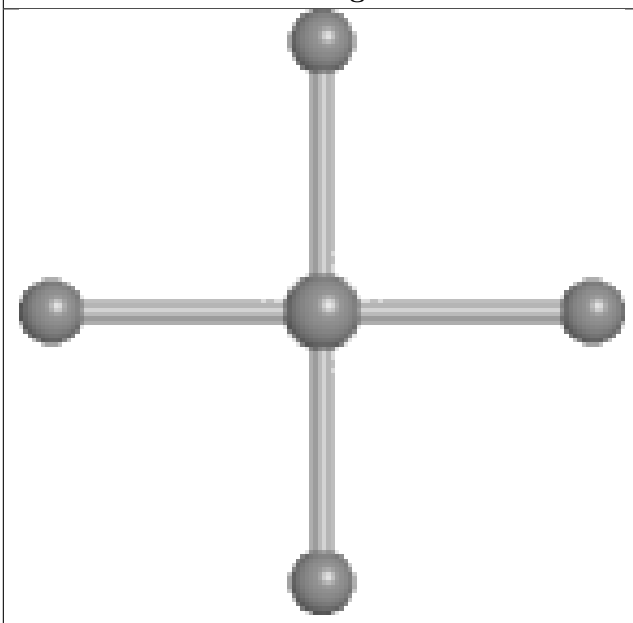
Ligand SO4 B 1306



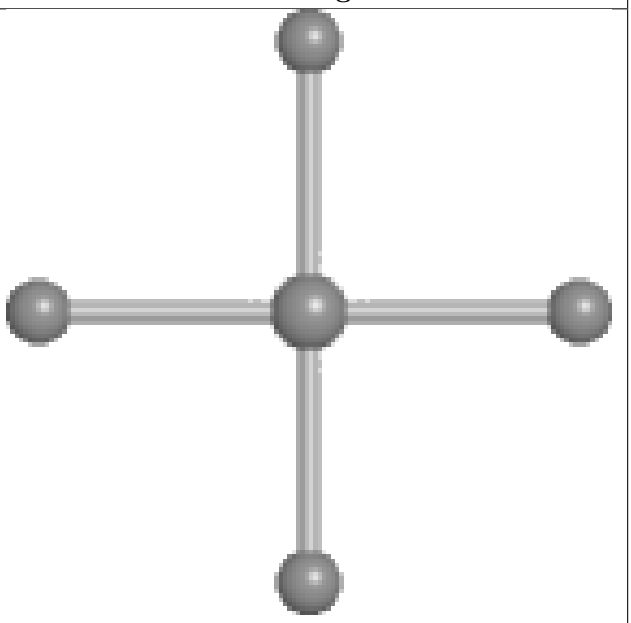
Bond lengths



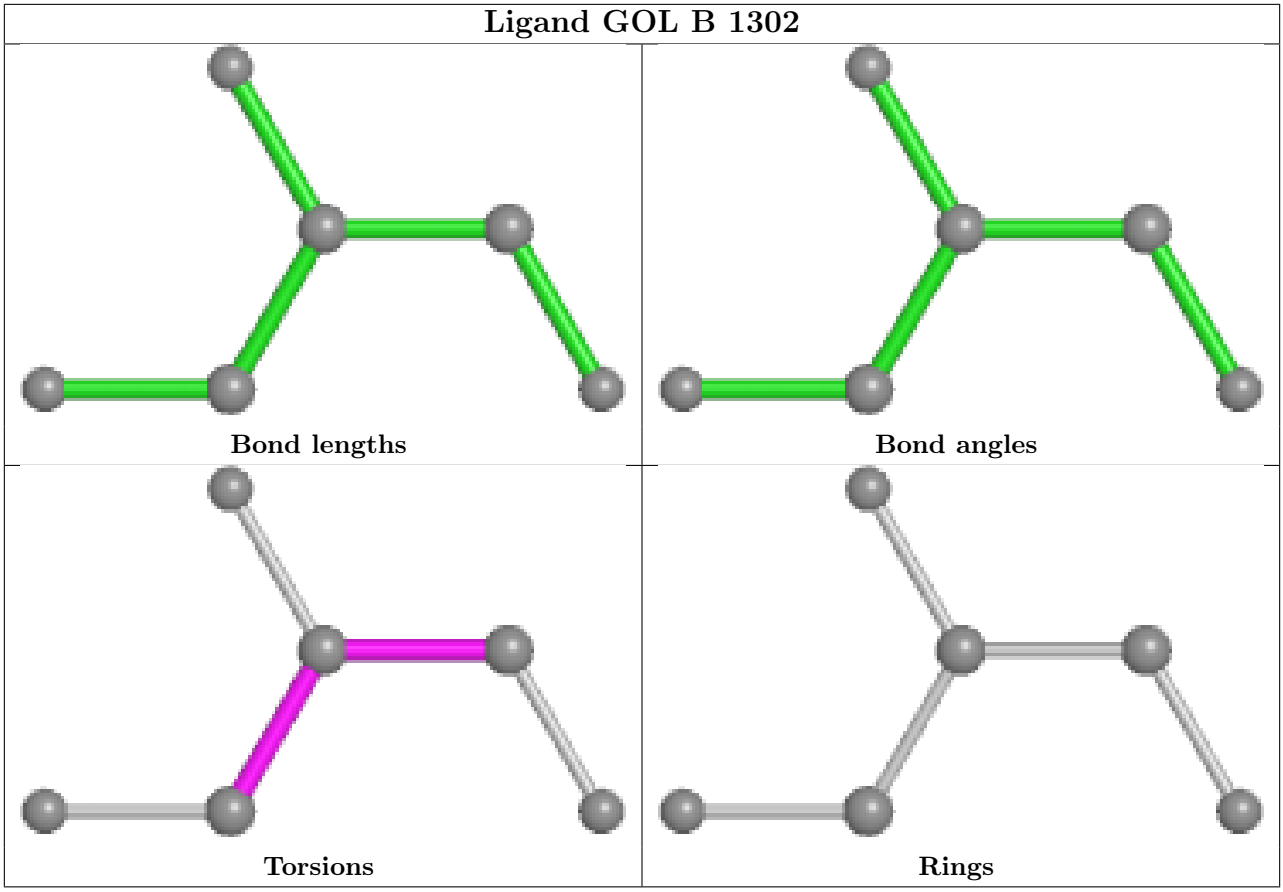
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	662/695 (95%)	0.19	42 (6%)	20	22	11, 22, 61, 109	0
1	B	662/695 (95%)	0.24	45 (6%)	17	19	10, 21, 55, 119	0
All	All	1324/1390 (95%)	0.22	87 (6%)	18	20	10, 22, 58, 119	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1213	ALA	12.7
1	B	785	GLY	10.6
1	B	784	THR	10.3
1	B	1212	ASP	10.1
1	A	983	GLY	9.1
1	A	785	GLY	8.8
1	B	786	GLY	8.3
1	A	784	THR	7.6
1	B	984	SER	7.3
1	B	1211	PRO	7.3
1	B	1214	GLU	7.2
1	A	787	LYS	7.2
1	A	982	PHE	6.8
1	A	786	GLY	6.8
1	B	1215	ASP	6.7
1	B	1220	ALA	6.5
1	A	1214	GLU	6.4
1	A	1215	ASP	6.2
1	B	983	GLY	6.1
1	A	630	ILE	5.9
1	A	569	PHE	5.8
1	B	840	THR	5.8
1	B	787	LYS	5.7
1	A	1213	ALA	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	1211	PRO	5.4
1	B	1210	LEU	5.4
1	A	1212	ASP	5.3
1	B	783	GLY	5.2
1	B	1216	SER	5.1
1	B	782	SER	4.9
1	B	838	HIS	4.8
1	A	789	GLY	4.7
1	B	841	ASN	4.5
1	A	788	PRO	4.5
1	B	911	ASP	4.1
1	A	634	GLY	4.0
1	B	571	GLU	4.0
1	B	982	PHE	4.0
1	B	1222	ILE	3.9
1	A	631	GLY	3.9
1	A	1210	LEU	3.9
1	B	890	PRO	3.9
1	A	633	ALA	3.9
1	A	911	ASP	3.8
1	A	783	GLY	3.8
1	B	570	SER	3.7
1	A	986	LYS	3.7
1	B	1223	TYR	3.6
1	A	841	ASN	3.6
1	B	988	GLU	3.5
1	B	779	ASP	3.4
1	A	984	SER	3.4
1	A	910	GLU	3.4
1	A	1189	LEU	3.4
1	B	910	GLU	3.3
1	B	788	PRO	3.3
1	A	890	PRO	3.3
1	B	1219	ARG	3.2
1	A	637	ARG	3.1
1	A	840	THR	3.1
1	B	630	ILE	3.0
1	B	781	LEU	2.9
1	B	987	GLN	2.8
1	A	925	LYS	2.7
1	A	981	LEU	2.7
1	A	782	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	570	SER	2.6
1	B	569	PHE	2.6
1	A	838	HIS	2.6
1	A	632	PHE	2.6
1	B	932	LEU	2.5
1	B	839	ASP	2.5
1	A	571	GLU	2.4
1	A	1044	GLU	2.4
1	B	986	LYS	2.4
1	A	627	LEU	2.3
1	B	834	VAL	2.3
1	A	985	PRO	2.2
1	B	572	ASN	2.1
1	B	1044	GLU	2.1
1	A	1216	SER	2.1
1	B	1218	TYR	2.1
1	A	891	GLU	2.1
1	B	894	GLU	2.0
1	B	629	ASP	2.0
1	A	932	LEU	2.0
1	B	1217	ARG	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, 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
3	GOL	B	1303	6/6	0.83	0.19	33,33,45,46	0
4	SO4	B	1309	5/5	0.85	0.22	61,69,82,88	0

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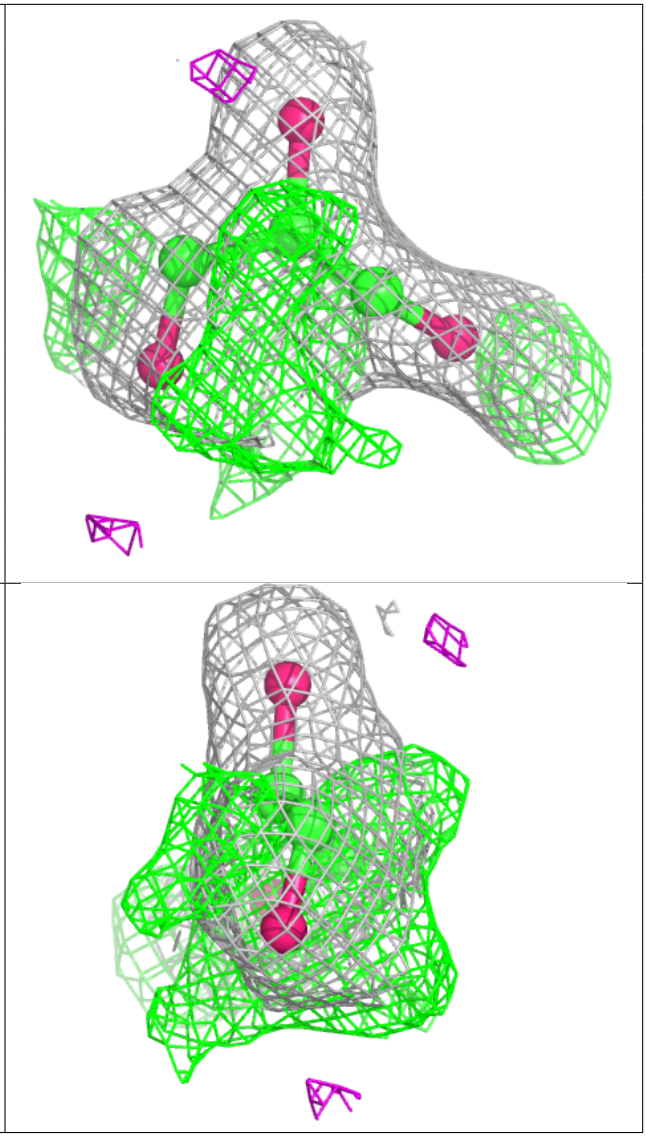
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1303	6/6	0.86	0.16	33,35,38,43	0
4	SO4	A	1307	5/5	0.89	0.11	52,62,67,85	0
4	SO4	B	1308	5/5	0.90	0.26	36,36,55,57	0
2	COA	B	1301	48/48	0.92	0.15	20,33,59,66	0
4	SO4	A	1305	5/5	0.94	0.13	55,56,58,67	0
2	COA	A	1301	48/48	0.94	0.13	19,31,53,63	0
3	GOL	B	1302	6/6	0.95	0.12	22,25,29,30	0
4	SO4	B	1306	5/5	0.95	0.19	39,48,49,51	0
4	SO4	B	1307	5/5	0.96	0.18	51,52,54,63	0
4	SO4	A	1304	5/5	0.97	0.24	36,44,49,49	0
4	SO4	B	1305	5/5	0.97	0.13	50,50,52,53	0
3	GOL	A	1302	6/6	0.97	0.07	18,20,22,22	0
4	SO4	B	1304	5/5	0.98	0.10	49,53,55,58	0
4	SO4	A	1306	5/5	0.98	0.08	47,50,57,62	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.

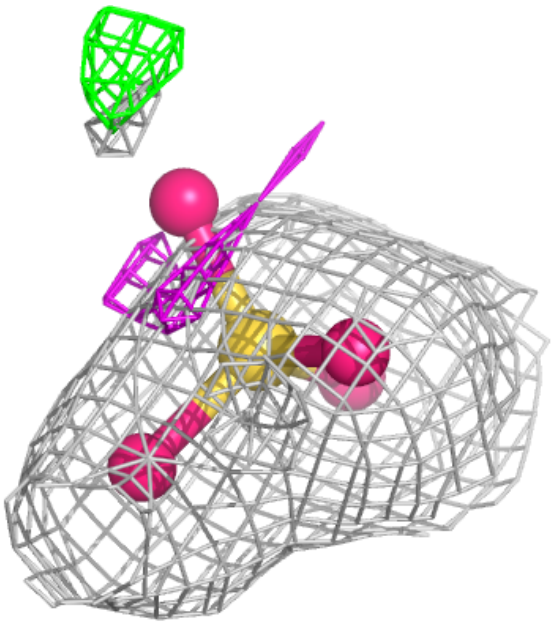
Electron density around GOL B 1303:

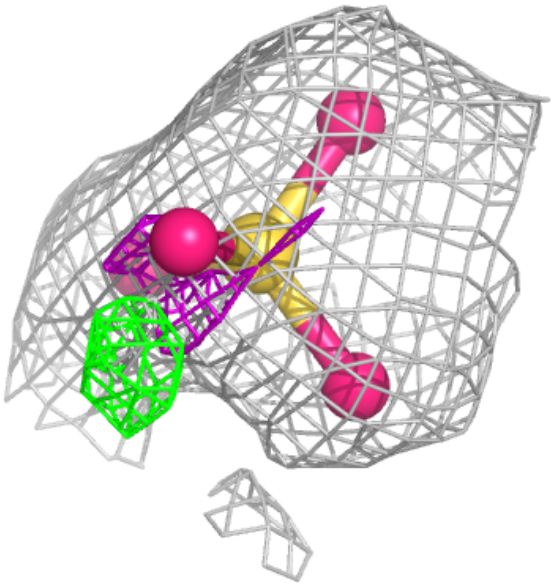
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

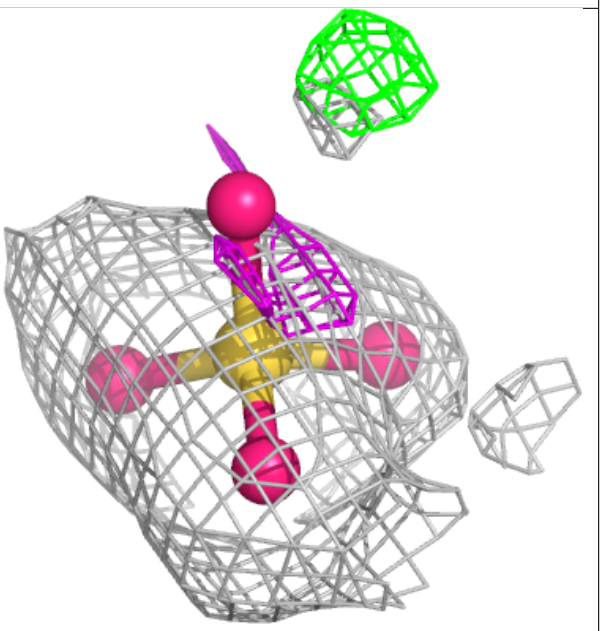


Electron density around SO4 B 1309:

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

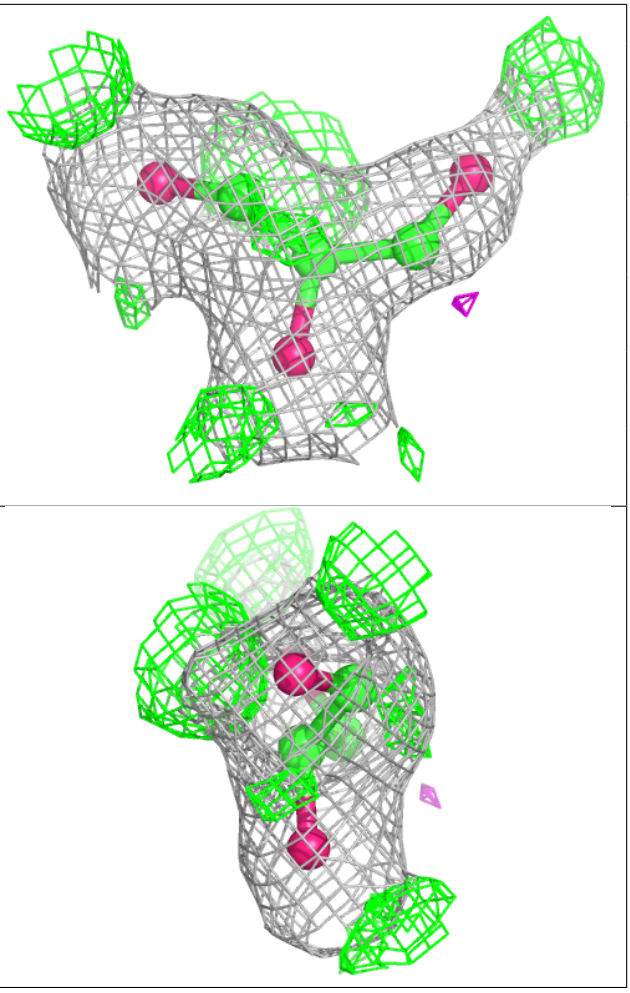






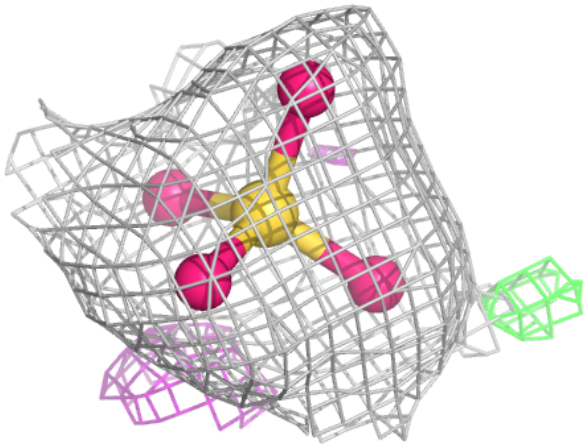
Electron density around GOL A 1303:

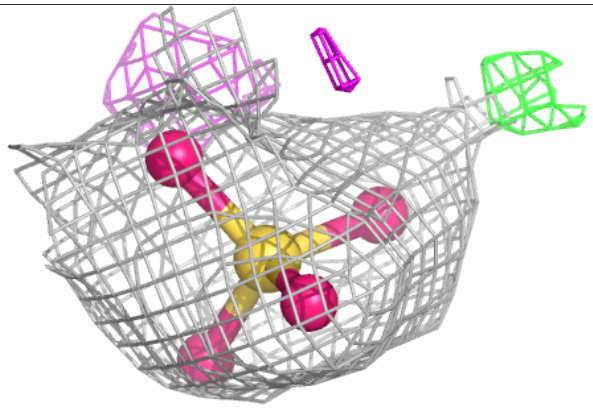
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

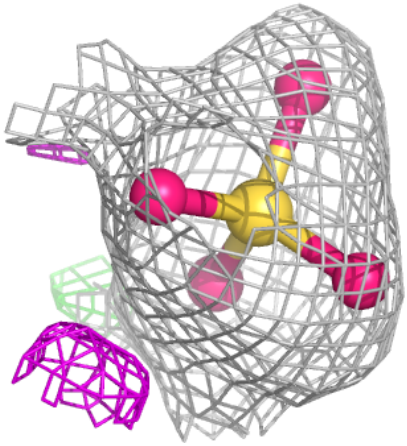


Electron density around SO4 A 1307:

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

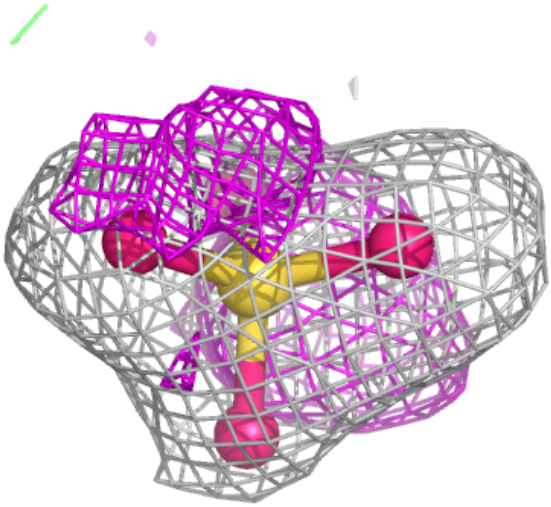


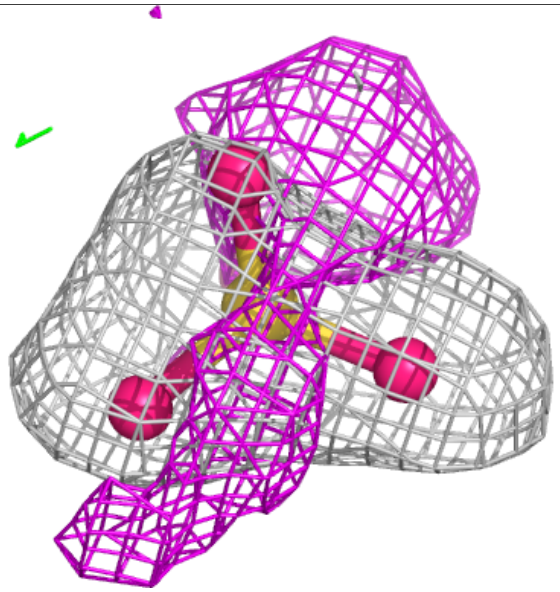


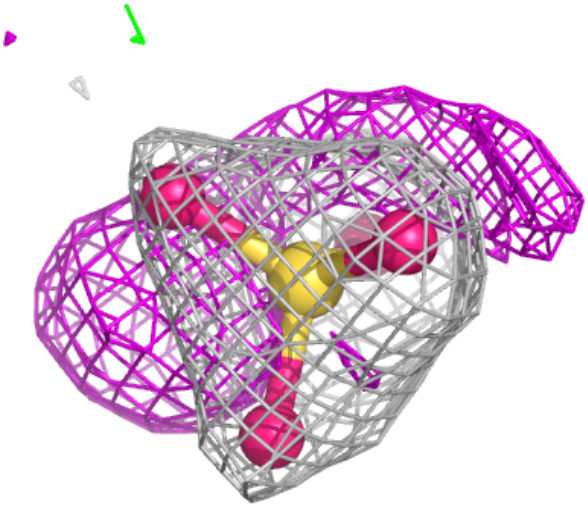


Electron density around SO4 B 1308:

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

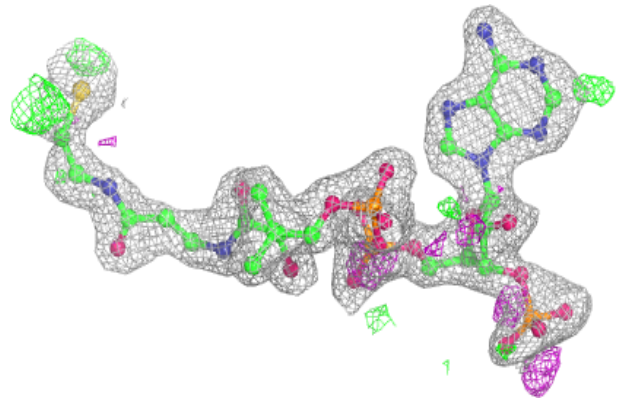


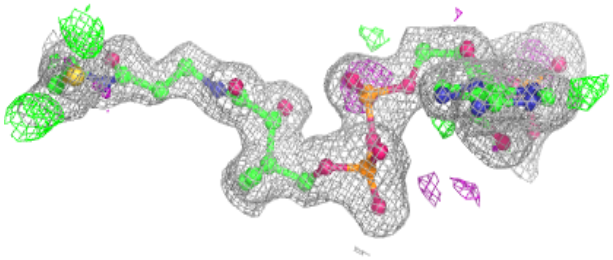


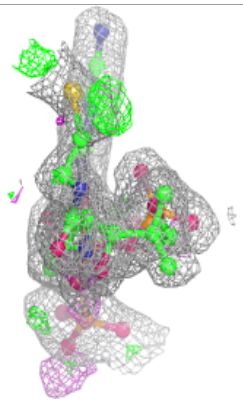


Electron density around COA B 1301:

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

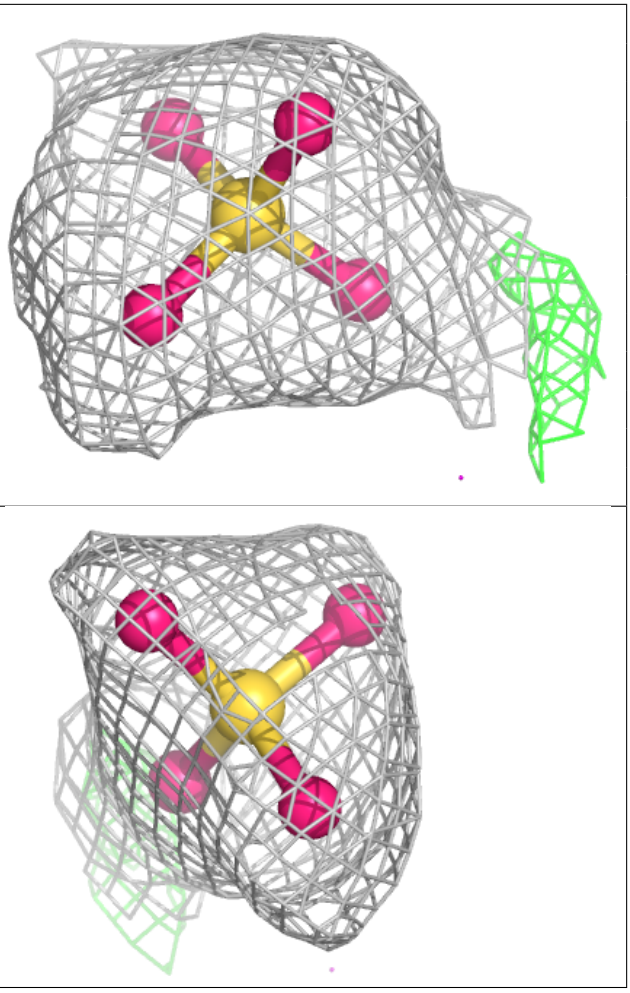






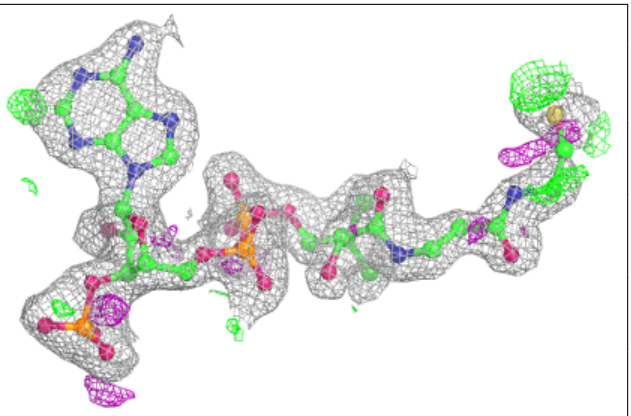
Electron density around SO4 A 1305:

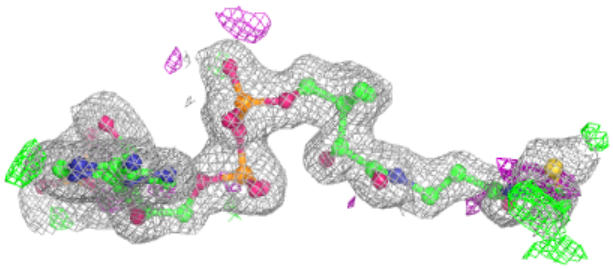
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around COA A 1301:

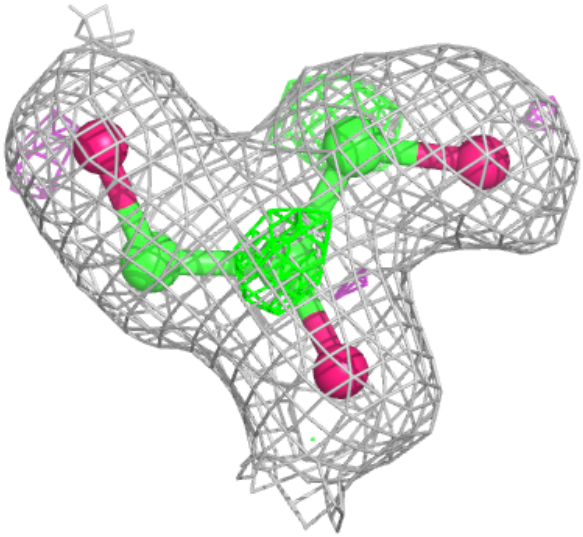
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

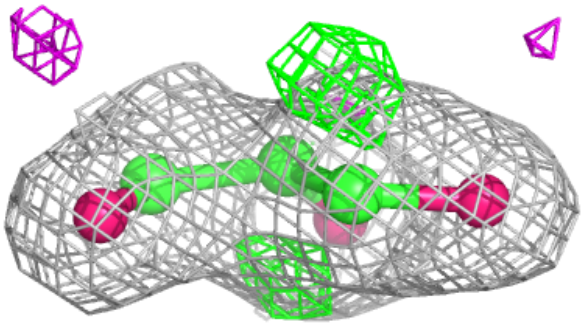


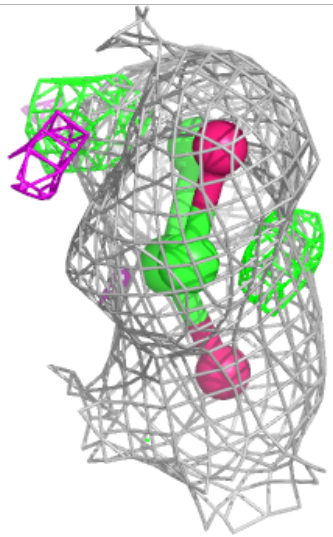


Electron density around GOL B 1302:

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

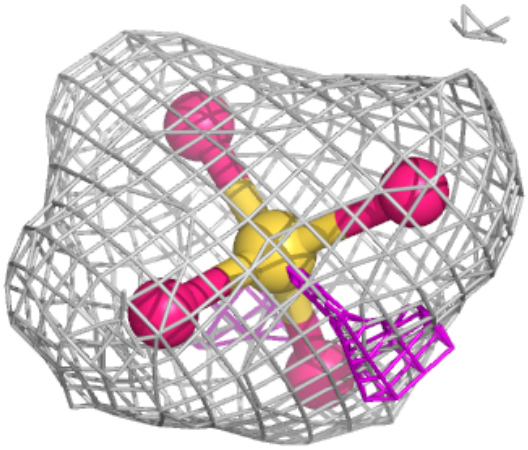


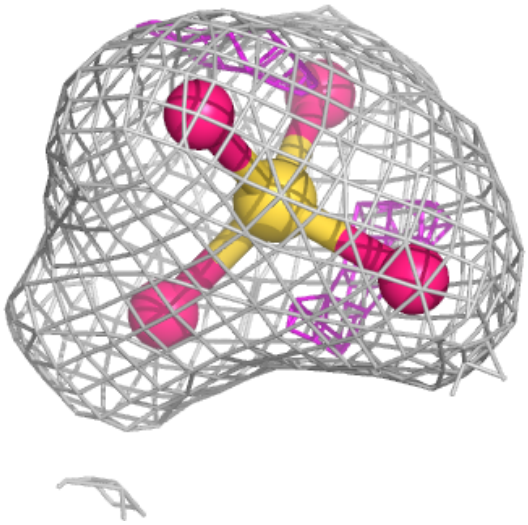


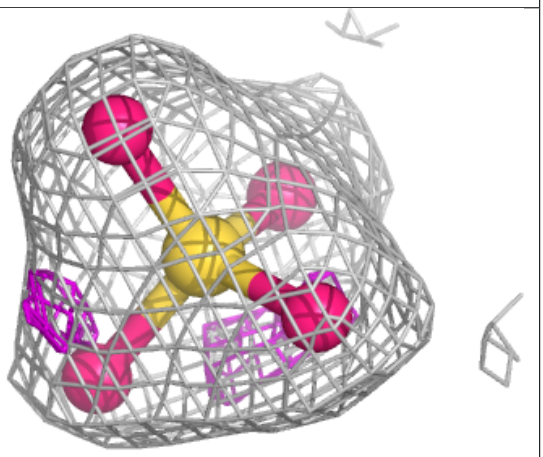


Electron density around SO4 B 1306:

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

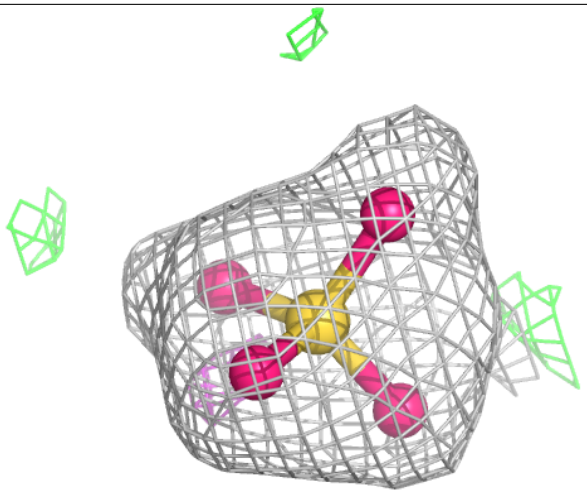


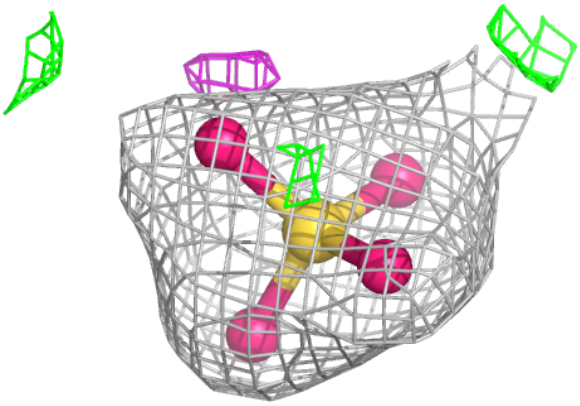


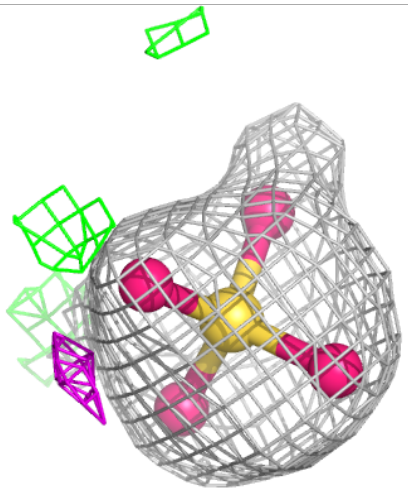


Electron density around SO4 B 1307:

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

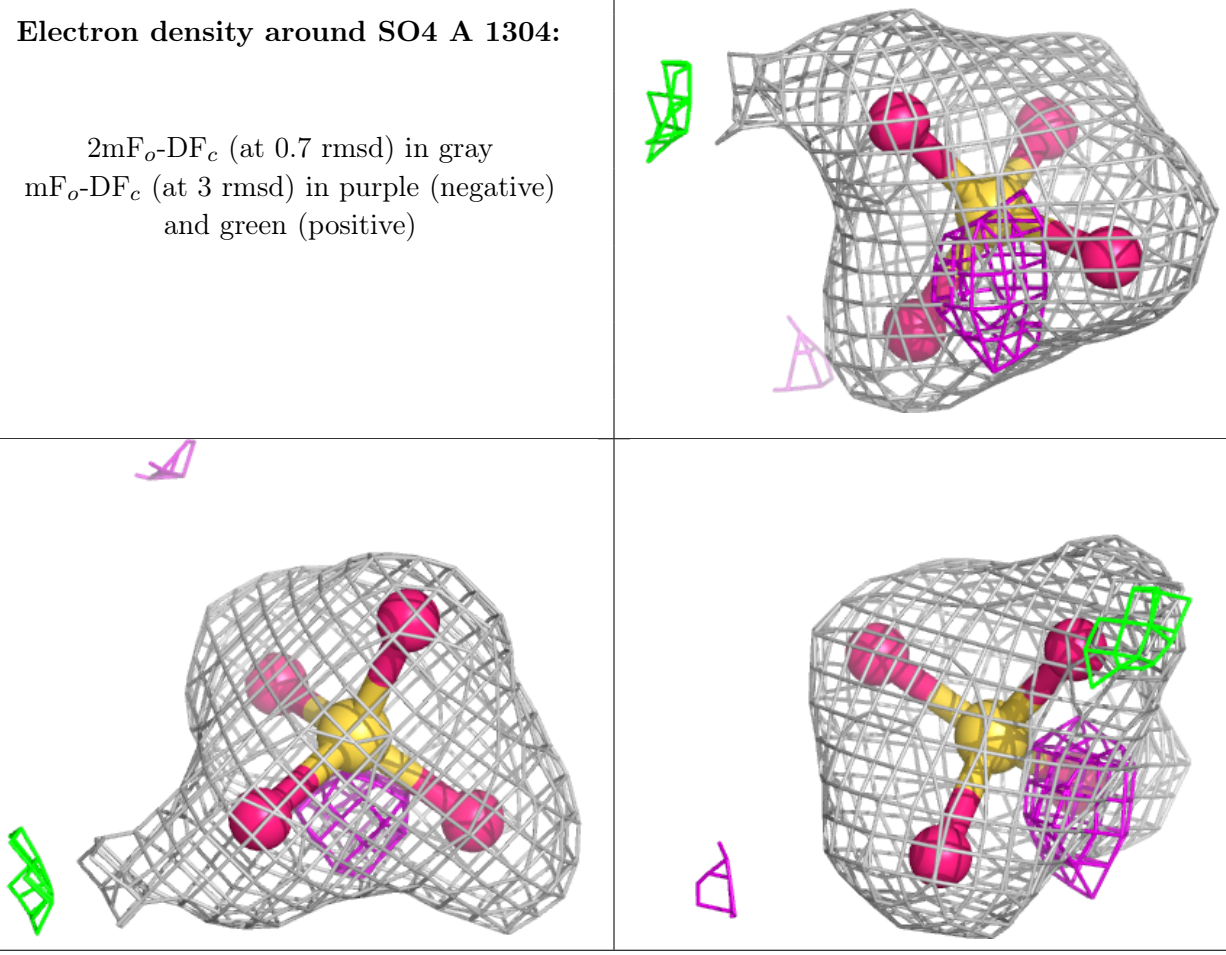






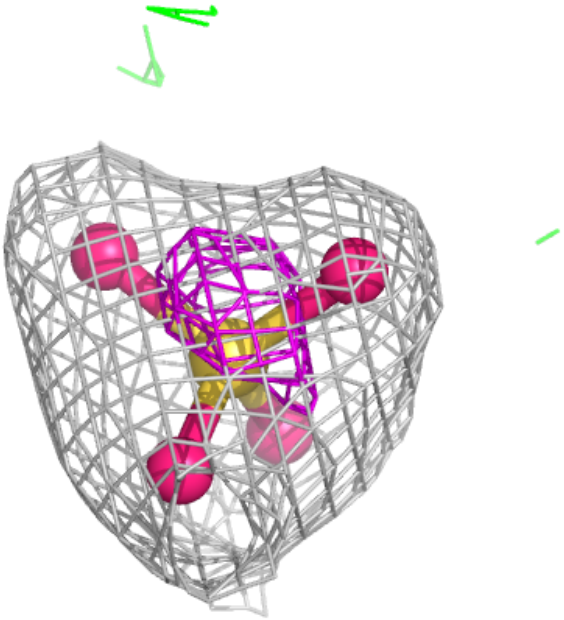
Electron density around SO4 A 1304:

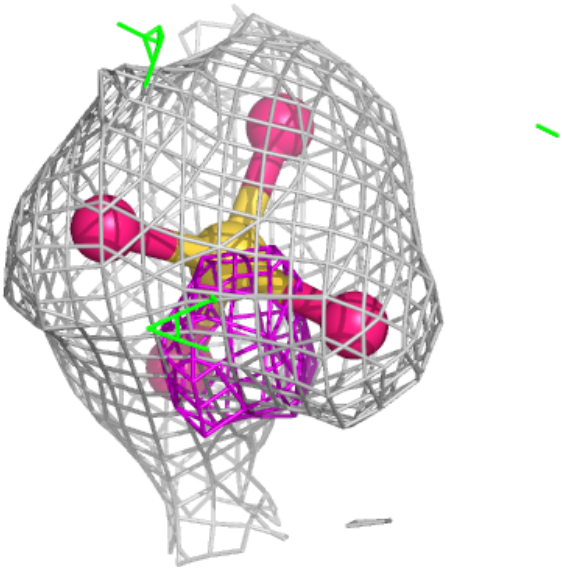
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

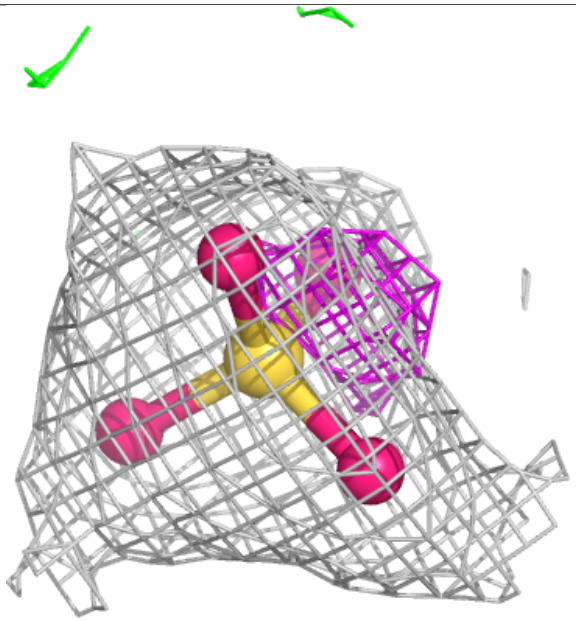


Electron density around SO4 B 1305:

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

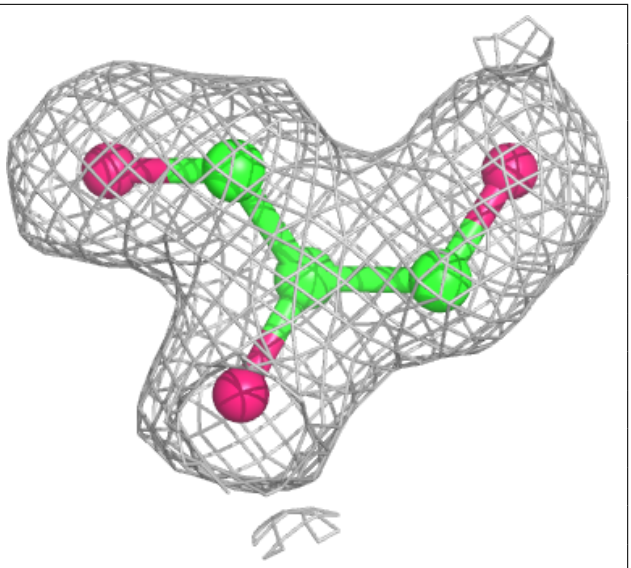


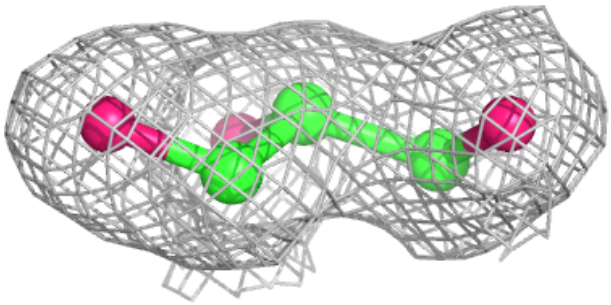


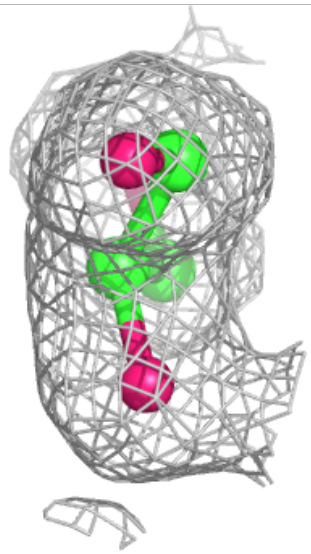


Electron density around GOL A 1302:

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

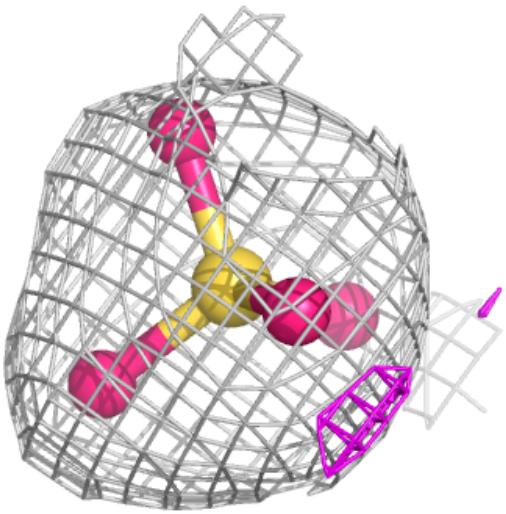


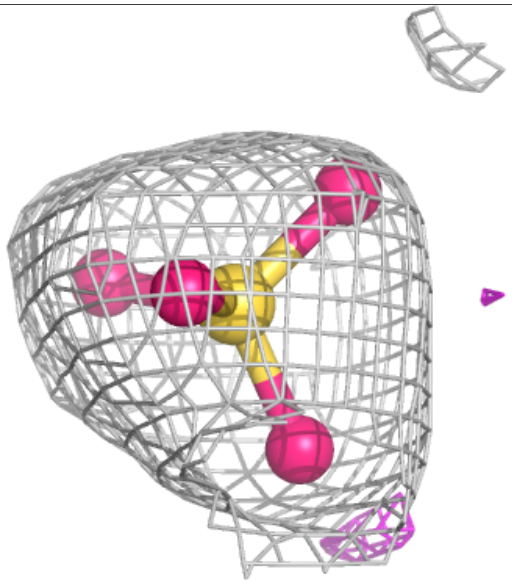


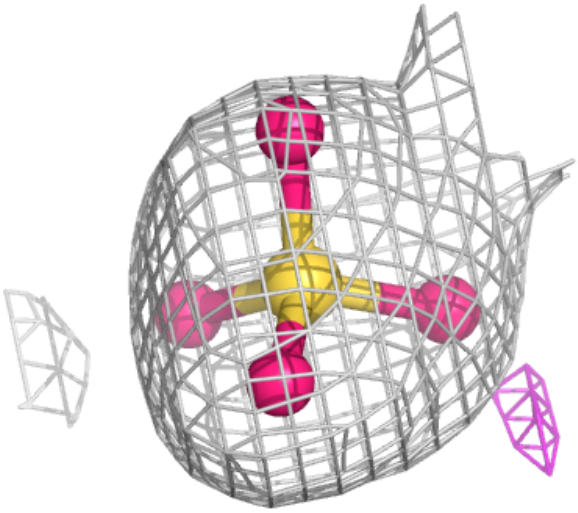


Electron density around SO4 B 1304:

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

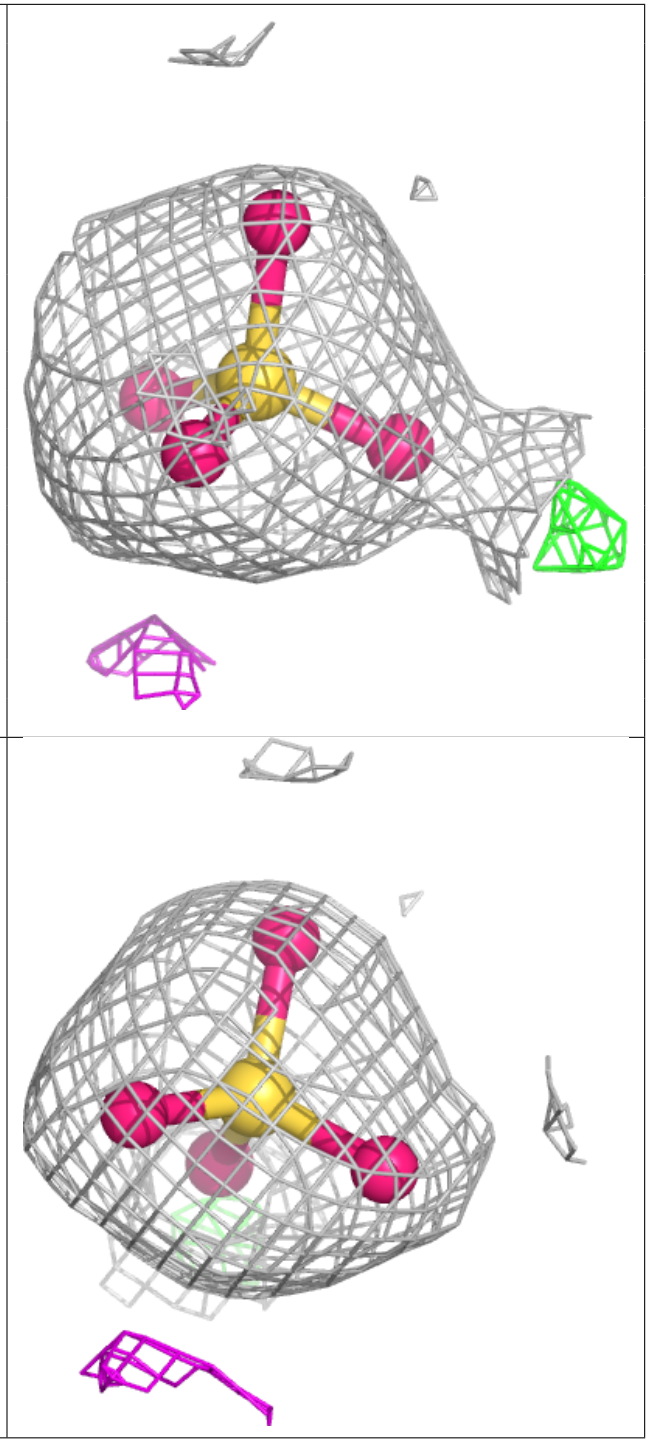






Electron density around SO4 A 1306:

$2mF_o$-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.