Full wwPDB X-ray Structure Validation Report (i)

Nov 15, 2023 – 11:09 PM JST

PDB ID	:	6K8U
Title	:	Crystal structure of C-domain with NADP of baterial malonyl-CoA reductase
Authors	:	Kim, S.; Kim, K.-J.
Deposited on	:	2019-06-13
Resolution	:	2.00 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:

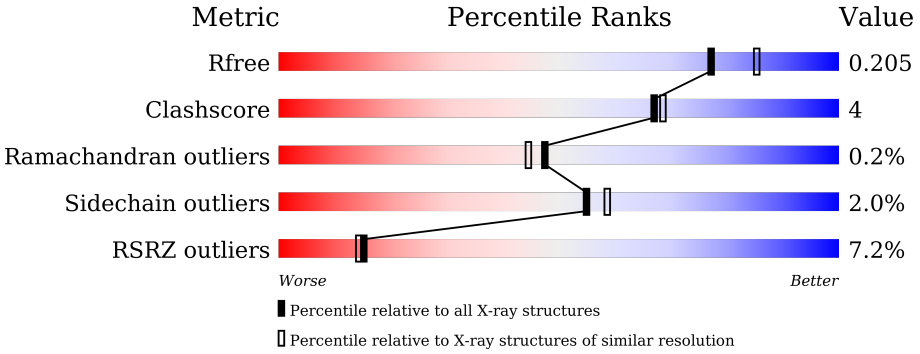
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	7% 86% 9% 5%
1	B	695	7% 87% 7% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10915 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	5095	3195	908	972	20	0	2	0
1	B	660	5091	3193	908	970	20	0	3	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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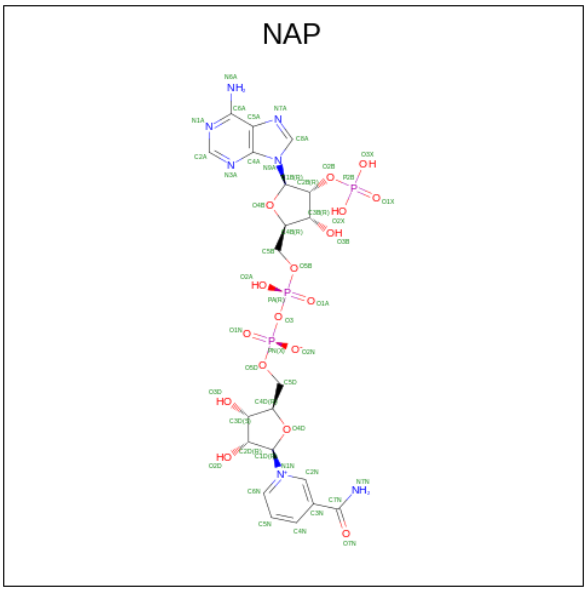
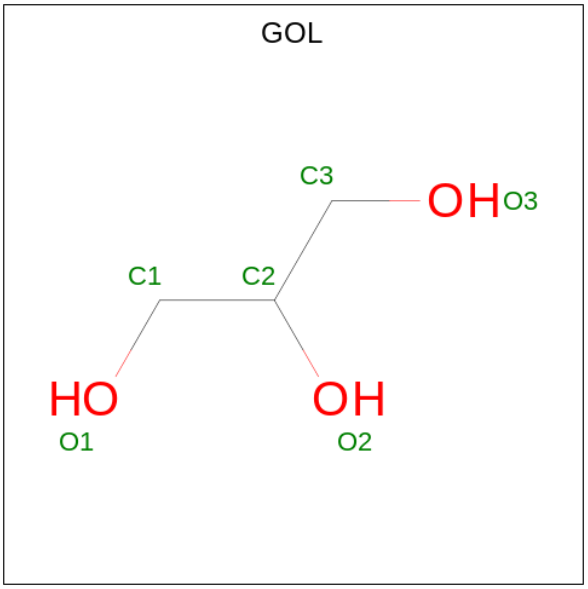
Chain	Residue	Modelled	Actual	Comment	Reference
B	539	SER	-	expression tag	UNP A0A1A7BFR5
B	540	HIS	-	expression tag	UNP A0A1A7BFR5
B	541	HIS	-	expression tag	UNP A0A1A7BFR5
B	542	HIS	-	expression tag	UNP A0A1A7BFR5
B	543	HIS	-	expression tag	UNP A0A1A7BFR5
B	544	HIS	-	expression tag	UNP A0A1A7BFR5
B	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 NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



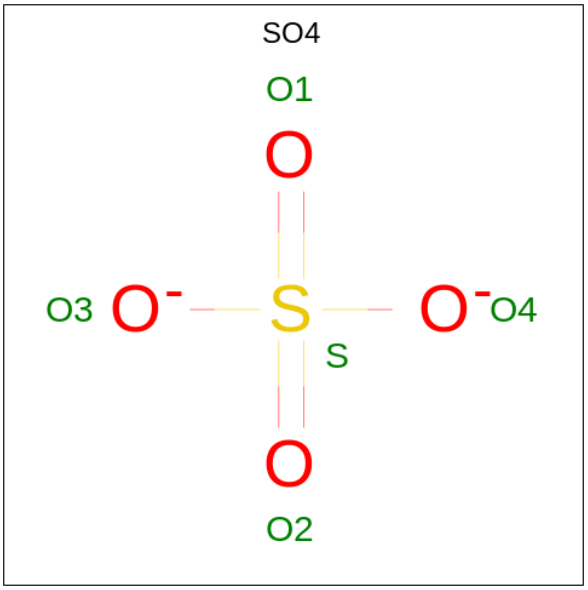
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	48	21	7	17	3	0	0
			Total	C	N	O	P		
2	B	1	48	21	7	17	3	0	0

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

- Molecule 5 is water.

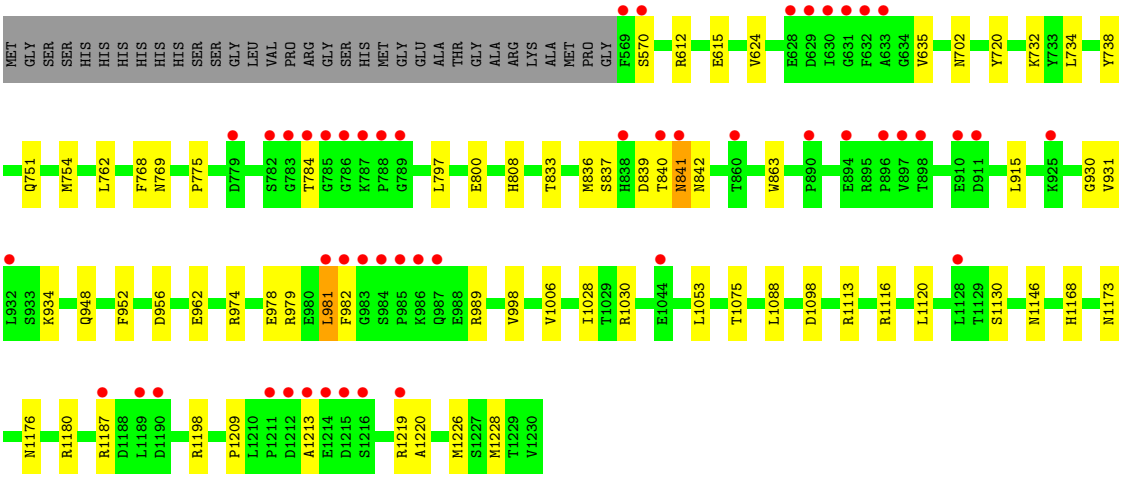
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	262	262	262	0	0
			Total	O		
5	B	284	284	284	0	0

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.

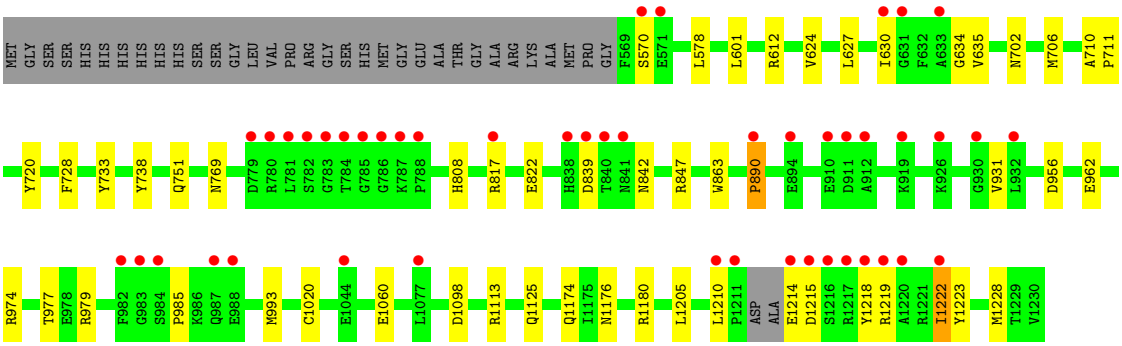
• Molecule 1: NAD-dependent epimerase/dehydratase:Short-chain dehydrogenase/reductase SDR

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	110.86Å 116.69Å 134.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.86 – 2.00 31.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (31.86-2.00) 99.0 (31.84-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	7.70 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.174 , 0.205 0.174 , 0.205	Depositor DCC
R_{free} test set	5810 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 52.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	10915	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 31.99 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0102e-03. 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: NAP, SO4, GOL

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	0.76	0/5186	0.86	0/7034
1	B	0.78	0/5181	0.86	1/7025 (0.0%)
All	All	0.77	0/10367	0.86	1/14059 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	728	PHE	CB-CA-C	5.55	121.50	110.40

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	5095	0	5068	47	0
1	B	5091	0	5065	39	0
2	A	48	0	25	0	0
2	B	48	0	25	0	0
3	A	6	0	8	0	0
3	B	6	0	8	0	0
4	A	35	0	0	1	0
4	B	40	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	262	0	0	6	0
5	B	284	0	0	3	0
All	All	10915	0	10199	81	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 (81) 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:B:612:ARG:HH11	1:B:612:ARG:HB2	1.12	1.14
1:B:1223:TYR:HB2	5:B:1410:HOH:O	1.73	0.89
1:B:612:ARG:HB2	1:B:612:ARG:NH1	1.87	0.89
1:B:702:ASN:HD21	1:B:751:GLN:HE21	1.24	0.85
1:A:981:LEU:HD12	1:A:1228:MET:SD	2.22	0.79
1:A:612:ARG:CZ	1:A:615:GLU:HG3	2.13	0.78
1:A:981:LEU:HB2	1:A:1228:MET:SD	2.23	0.78
1:A:702:ASN:HD21	1:A:751:GLN:HE21	1.28	0.78
1:B:1174:GLN:HE21	1:B:1176:ASN:HD21	1.30	0.77
1:B:612:ARG:HH11	1:B:612:ARG:CB	1.94	0.77
1:A:981:LEU:CD1	1:A:1228:MET:SD	2.74	0.76
1:A:989:ARG:HD2	1:A:1209:PRO:O	1.87	0.75
1:B:822:GLU:OE2	1:B:890:PRO:HD2	1.90	0.71
1:A:979:ARG:HA	1:B:979:ARG:CZ	2.22	0.69
1:B:1060:GLU:OE2	1:B:1113:ARG:HD3	1.94	0.67
1:B:769:ASN:HD22	1:B:962:GLU:H	1.43	0.67
1:A:769:ASN:HD22	1:A:962:GLU:H	1.42	0.64
1:A:979:ARG:HA	1:B:979:ARG:NH2	2.13	0.64
1:A:981:LEU:HB2	1:A:1228:MET:CG	2.29	0.62
4:A:1307:SO4:O1	1:B:1219:ARG:NH1	2.33	0.62
1:A:1173:ASN:HD22	1:A:1226:MET:H	1.48	0.60
1:A:612:ARG:NH1	1:A:615:GLU:HG3	2.15	0.60
1:A:808:HIS:HE1	5:A:1554:HOH:O	1.85	0.59
1:B:822:GLU:OE2	1:B:890:PRO:CD	2.50	0.58
1:A:732:LYS:HE3	5:A:1458:HOH:O	2.04	0.58
1:B:1214:GLU:O	1:B:1214:GLU:HG3	2.05	0.57
1:B:817:ARG:NH2	4:B:1309:SO4:O3	2.36	0.56
1:A:800:GLU:HG3	1:A:915:LEU:HD11	1.88	0.56
1:A:1219:ARG:HD3	4:B:1305:SO4:O1	2.05	0.56
1:B:570:SER:HB3	5:B:1588:HOH:O	2.06	0.56
1:A:981:LEU:HD23	1:A:1198:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:ASN:ND2	1:A:751:GLN:HE21	2.01	0.55
1:A:1226:MET:SD	1:A:1228:MET:HE2	2.46	0.55
1:B:769:ASN:ND2	1:B:962:GLU:H	2.05	0.54
1:A:1146:ASN:OD1	1:A:1180:ARG:HD3	2.07	0.54
1:A:1213:ALA:HA	1:A:1220:ALA:HB2	1.90	0.53
1:A:930:GLY:O	1:A:934:LYS:HG2	2.07	0.53
1:A:978:GLU:O	1:B:979:ARG:NH2	2.40	0.53
1:B:601:LEU:HD22	1:B:630:ILE:HD11	1.92	0.52
1:A:981:LEU:HD13	1:A:1228:MET:SD	2.49	0.51
1:A:769:ASN:ND2	1:A:962:GLU:H	2.07	0.51
1:A:808:HIS:HD2	5:A:1597:HOH:O	1.94	0.51
1:A:624:VAL:HG13	1:A:635:VAL:HG12	1.94	0.51
1:A:734:LEU:HD22	1:B:733:TYR:OH	2.11	0.50
1:A:1173:ASN:ND2	1:A:1226:MET:H	2.09	0.50
1:A:839:ASP:OD1	1:A:841:ASN:HB2	2.11	0.50
1:B:1205:LEU:HD23	1:B:1228:MET:HE1	1.93	0.50
1:B:702:ASN:ND2	1:B:751:GLN:HE21	2.04	0.49
1:A:1113:ARG:O	1:A:1116:ARG:HG2	2.14	0.48
1:B:570:SER:HB2	1:B:601:LEU:HD13	1.96	0.48
1:B:1214:GLU:O	1:B:1214:GLU:CG	2.62	0.47
1:B:634:GLY:HA2	4:B:1307:SO4:O3	2.13	0.47
1:A:1006:VAL:HG22	5:A:1463:HOH:O	2.15	0.46
1:A:836:MET:HA	1:A:842:ASN:ND2	2.29	0.46
1:A:570:SER:HA	1:B:578:LEU:HD22	1.97	0.46
1:B:993:MET:HB2	1:B:1020:CYS:HB3	1.99	0.45
1:A:762:LEU:HD12	1:A:768:PHE:CD2	2.51	0.45
1:B:710:ALA:N	1:B:711:PRO:CD	2.81	0.44
1:A:833:THR:O	1:A:837:SER:OG	2.29	0.44
1:A:775:PRO:HG2	1:A:931:VAL:HG11	2.00	0.44
1:A:998:VAL:HG22	1:A:1075:THR:HB	2.00	0.44
1:A:1028:ILE:HA	1:A:1053:LEU:O	2.18	0.44
1:B:1125[B]:GLN:OE1	1:B:1210:LEU:HG	2.18	0.44
1:A:982:PHE:CD1	1:A:982:PHE:O	2.71	0.44
1:B:702:ASN:O	1:B:706:MET:HG3	2.18	0.44
1:A:948:GLN:HG2	1:A:952:PHE:CE2	2.53	0.43
1:B:627:LEU:HD12	1:B:635:VAL:HG13	2.00	0.43
1:B:808:HIS:HE1	5:B:1601:HOH:O	2.01	0.43
1:B:733:TYR:O	1:B:977:THR:HG23	2.19	0.43
1:B:624:VAL:HG13	1:B:635:VAL:HG12	2.01	0.42
1:A:1130:SER:OG	1:A:1176:ASN:HA	2.20	0.42
1:B:839:ASP:HB3	1:B:842:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:601:LEU:HD22	1:B:630:ILE:CD1	2.50	0.42
1:A:1030:ARG:NH1	5:A:1416:HOH:O	2.53	0.41
1:B:1174:GLN:HE21	1:B:1176:ASN:ND2	2.07	0.41
1:B:842:ASN:O	1:B:847:ARG:NH1	2.53	0.41
1:A:754:MET:HB2	1:A:754:MET:HE2	1.93	0.41
1:A:1120:LEU:HA	1:A:1168:HIS:CD2	2.56	0.41
1:B:1218:TYR:CE1	1:B:1222:ILE:HD12	2.56	0.41
1:A:981:LEU:HA	5:A:1468:HOH:O	2.20	0.40
1:A:797:LEU:HD23	1:A:800:GLU:OE1	2.22	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	662/695 (95%)	646 (98%)	15 (2%)	1 (0%)	47	44
1	B	659/695 (95%)	646 (98%)	11 (2%)	2 (0%)	41	37
All	All	1321/1390 (95%)	1292 (98%)	26 (2%)	3 (0%)	47	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	985	PRO
1	A	1088	LEU
1	B	890	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	531/553 (96%)	520 (98%)	11 (2%)	53	57
1	B	531/553 (96%)	521 (98%)	10 (2%)	57	61
All	All	1062/1106 (96%)	1041 (98%)	21 (2%)	55	58

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	720	TYR
1	A	738	TYR
1	A	784	THR
1	A	840	THR
1	A	841	ASN
1	A	863	TRP
1	A	956	ASP
1	A	974	ARG
1	A	981	LEU
1	A	1098	ASP
1	A	1187	ARG
1	B	720	TYR
1	B	738	TYR
1	B	863	TRP
1	B	931	VAL
1	B	956	ASP
1	B	974	ARG
1	B	1098	ASP
1	B	1180	ARG
1	B	1215	ASP
1	B	1222	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	640	GLN
1	A	672	ASN
1	A	702	ASN
1	A	769	ASN
1	A	808	HIS
1	A	871	GLN

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Mol	Chain	Res	Type
1	A	1107	ASN
1	A	1173	ASN
1	B	672	ASN
1	B	702	ASN
1	B	767	GLN
1	B	769	ASN
1	B	808	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)

19 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	B	1303	-	4,4,4	0.98	0	6,6,6	0.07	0
4	SO4	B	1306	-	4,4,4	0.25	0	6,6,6	0.15	0
4	SO4	A	1307	-	4,4,4	0.30	0	6,6,6	0.10	0
4	SO4	A	1305	-	4,4,4	0.27	0	6,6,6	0.12	0
2	NAP	B	1301	-	45,52,52	1.34	5 (11%)	56,80,80	1.44	9 (16%)
4	SO4	B	1308	-	4,4,4	0.27	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	SO4	A	1306	-	4,4,4	0.25	0	6,6,6	0.11	0
4	SO4	A	1309	-	4,4,4	0.38	0	6,6,6	0.08	0
4	SO4	A	1308	-	4,4,4	0.30	0	6,6,6	0.19	0
4	SO4	A	1303	-	4,4,4	0.44	0	6,6,6	0.17	0
4	SO4	B	1309	-	4,4,4	0.43	0	6,6,6	0.23	0
4	SO4	B	1304	-	4,4,4	0.44	0	6,6,6	0.14	0
3	GOL	A	1302	-	5,5,5	0.24	0	5,5,5	0.41	0
3	GOL	B	1302	-	5,5,5	0.22	0	5,5,5	0.39	0
4	SO4	B	1305	-	4,4,4	0.30	0	6,6,6	0.22	0
2	NAP	A	1301	-	45,52,52	0.88	0	56,80,80	1.08	3 (5%)
4	SO4	B	1307	-	4,4,4	0.62	0	6,6,6	0.16	0
4	SO4	A	1304	-	4,4,4	0.38	0	6,6,6	0.18	0
4	SO4	B	1310	-	4,4,4	0.29	0	6,6,6	0.14	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	NAP	A	1301	-	-	11/31/67/67	0/5/5/5
3	GOL	A	1302	-	-	0/4/4/4	-
2	NAP	B	1301	-	-	6/31/67/67	0/5/5/5
3	GOL	B	1302	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	NAP	O4B-C1B	4.49	1.47	1.41
2	B	1301	NAP	C5A-C4A	2.94	1.48	1.40
2	B	1301	NAP	C2N-N1N	2.64	1.38	1.35
2	B	1301	NAP	C2N-C3N	2.39	1.42	1.39
2	B	1301	NAP	PN-O5D	2.24	1.68	1.59

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1301	NAP	O7N-C7N-C3N	4.45	124.95	119.63
2	A	1301	NAP	N3A-C2A-N1A	-3.02	123.96	128.68
2	B	1301	NAP	O2A-PA-O1A	2.98	126.95	112.24
2	B	1301	NAP	O4B-C4B-C5B	-2.79	100.19	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1301	NAP	N3A-C2A-N1A	-2.45	124.86	128.68
2	A	1301	NAP	C2A-N1A-C6A	2.32	122.73	118.75
2	B	1301	NAP	N6A-C6A-N1A	2.32	123.38	118.57
2	B	1301	NAP	C3B-C2B-C1B	-2.29	98.58	102.89
2	B	1301	NAP	O7N-C7N-N7N	-2.23	119.41	122.58
2	B	1301	NAP	C1B-N9A-C4A	-2.04	123.05	126.64
2	B	1301	NAP	O5B-PA-O1A	-2.04	101.09	109.07
2	A	1301	NAP	O7N-C7N-C3N	2.01	122.03	119.63

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1301	NAP	C5B-O5B-PA-O1A
2	A	1301	NAP	C5B-O5B-PA-O2A
2	A	1301	NAP	C3B-C4B-C5B-O5B
2	A	1301	NAP	C5D-O5D-PN-O2N
2	B	1301	NAP	C5D-O5D-PN-O2N
2	A	1301	NAP	O4B-C4B-C5B-O5B
2	A	1301	NAP	C5B-O5B-PA-O3
2	B	1301	NAP	C5D-O5D-PN-O3
2	A	1301	NAP	PN-O3-PA-O1A
2	A	1301	NAP	C5D-O5D-PN-O1N
2	B	1301	NAP	C3B-C2B-O2B-P2B
2	B	1301	NAP	O4B-C4B-C5B-O5B
2	A	1301	NAP	C1B-C2B-O2B-P2B
2	B	1301	NAP	C1B-C2B-O2B-P2B
2	A	1301	NAP	C3B-C2B-O2B-P2B
2	A	1301	NAP	C5D-O5D-PN-O3
2	B	1301	NAP	C5D-O5D-PN-O1N

There are no ring outliers.

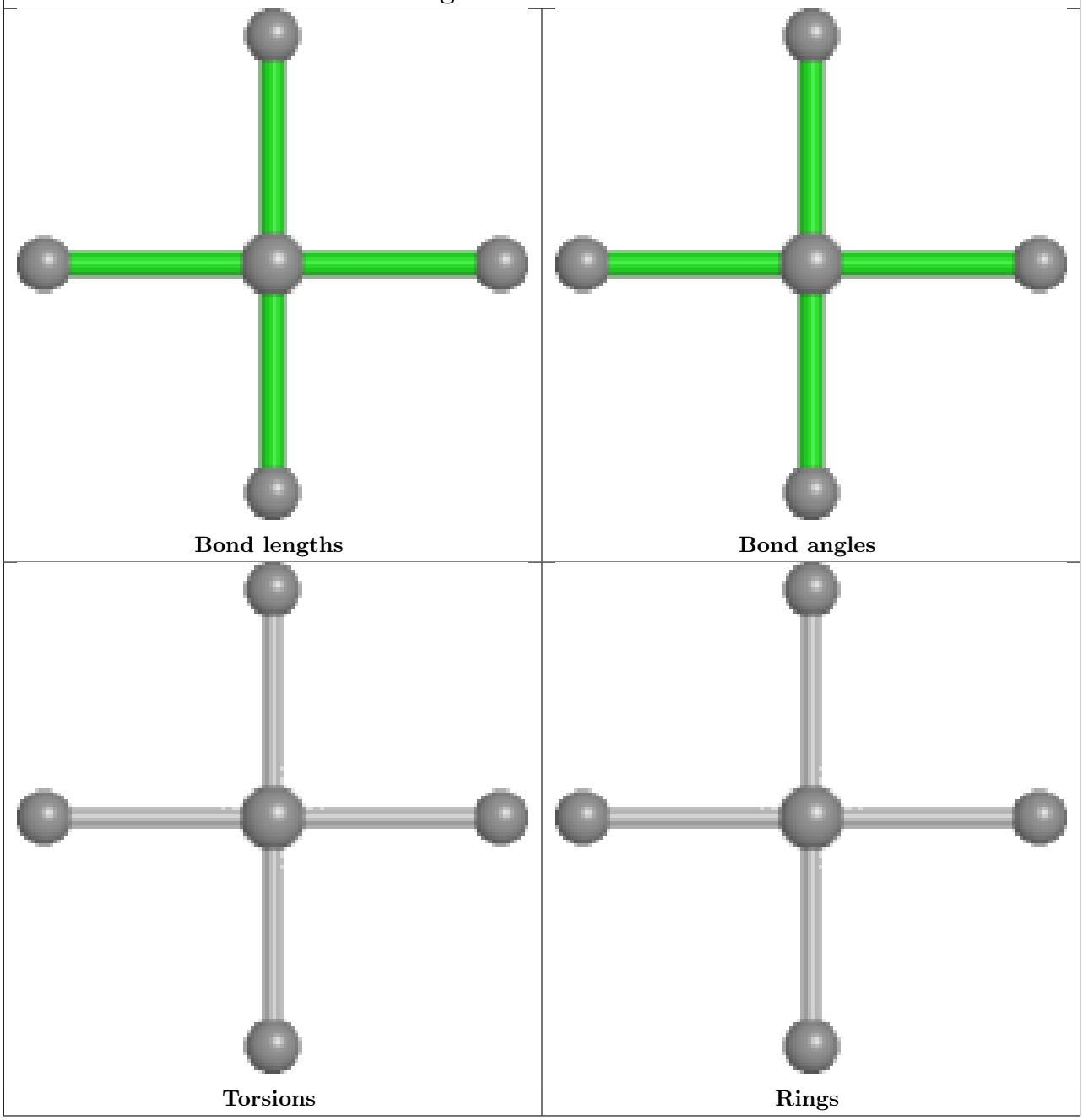
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	SO4	1	0
4	B	1309	SO4	1	0
4	B	1305	SO4	1	0
4	B	1307	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 B 1303



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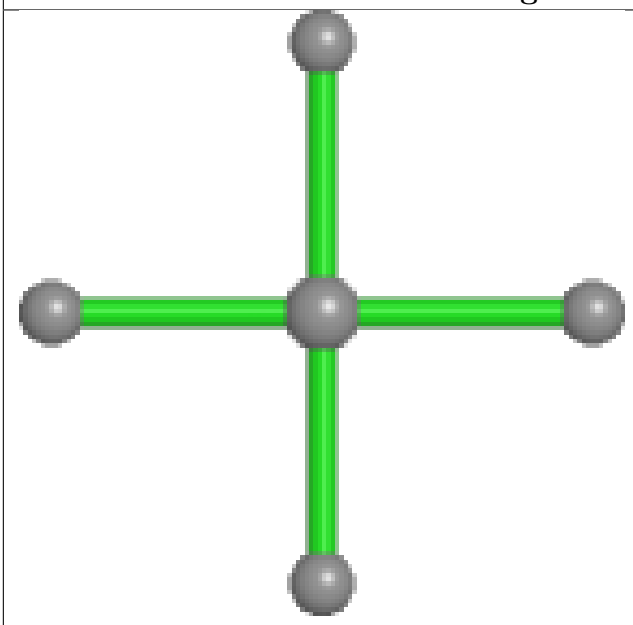
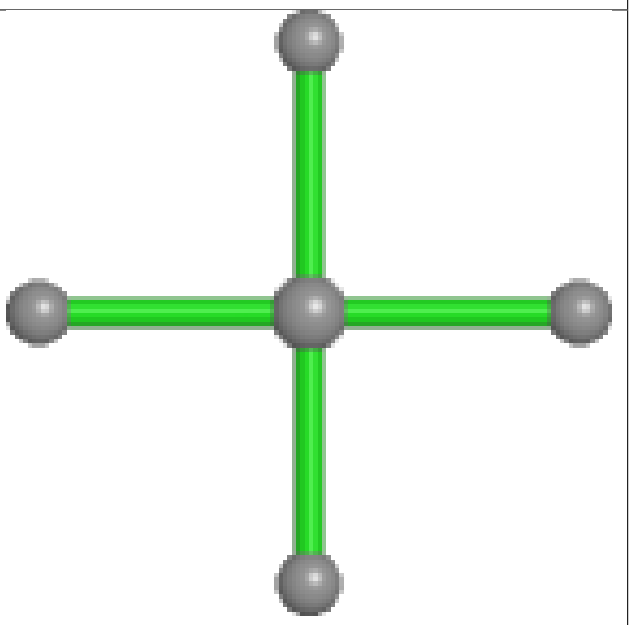
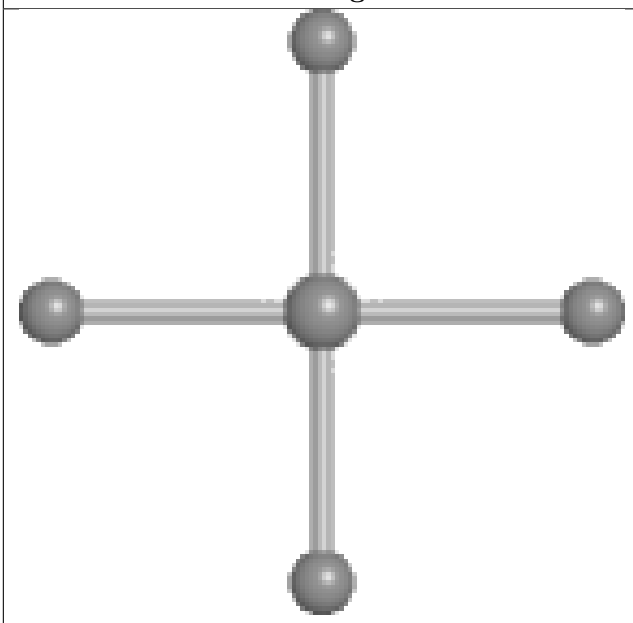


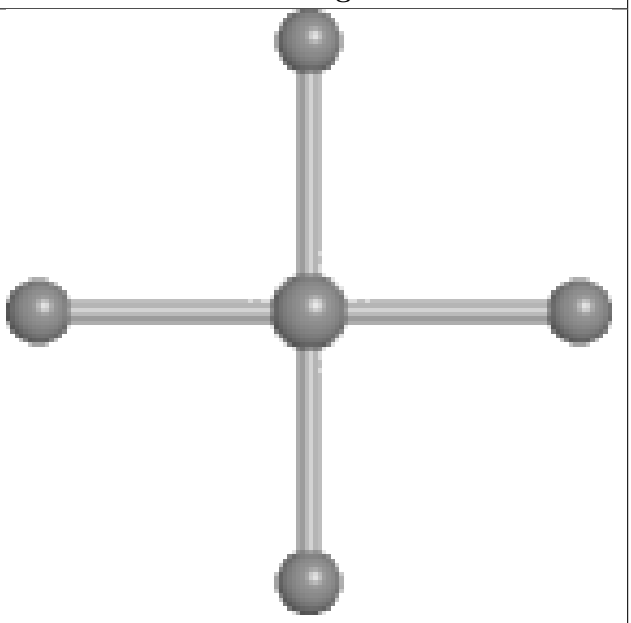
Bond lengths



Bond angles

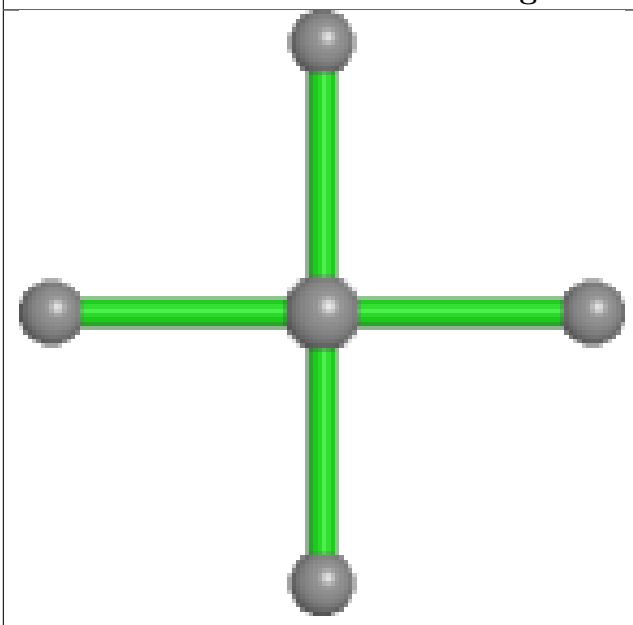


Torsions



Rings

Ligand SO4 A 1307



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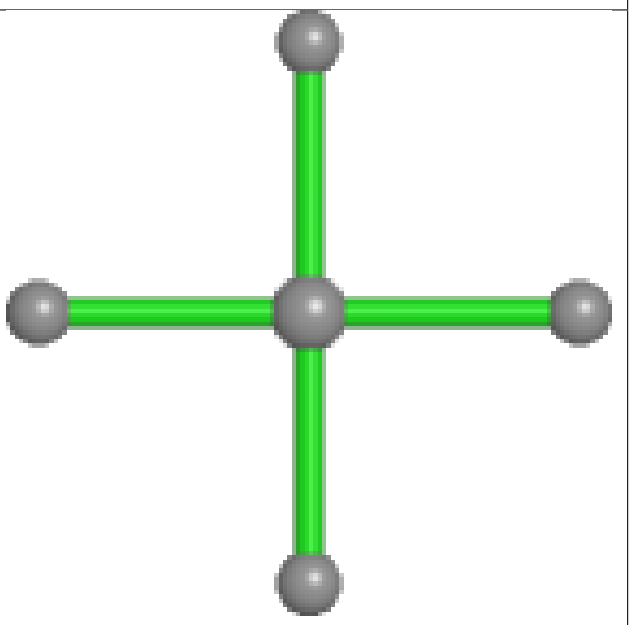

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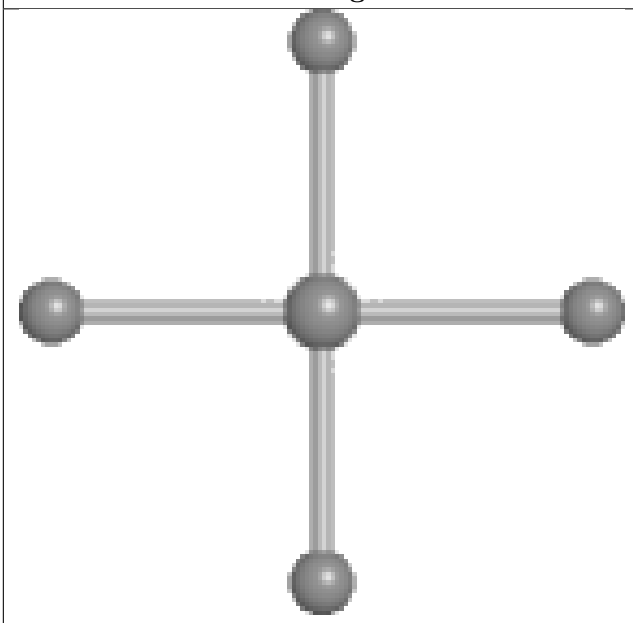

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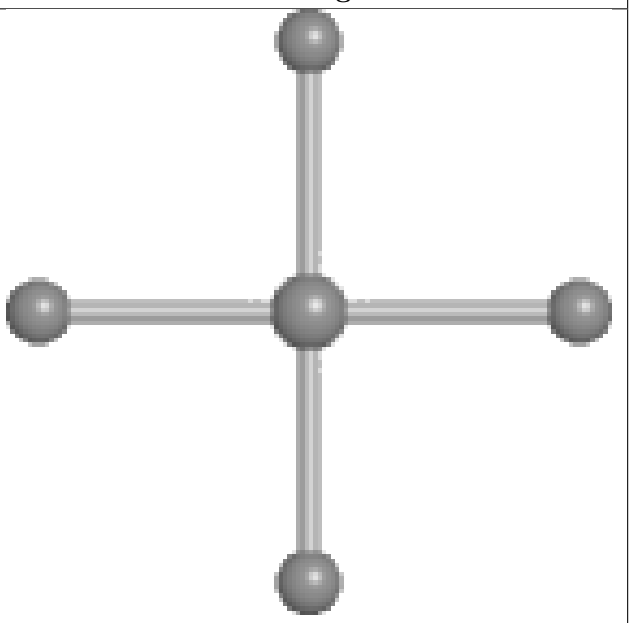
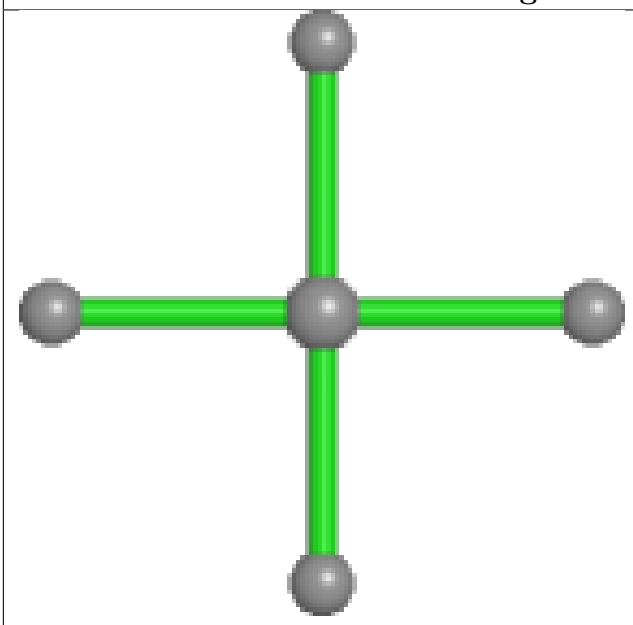


Rings

Ligand SO4 A 1305



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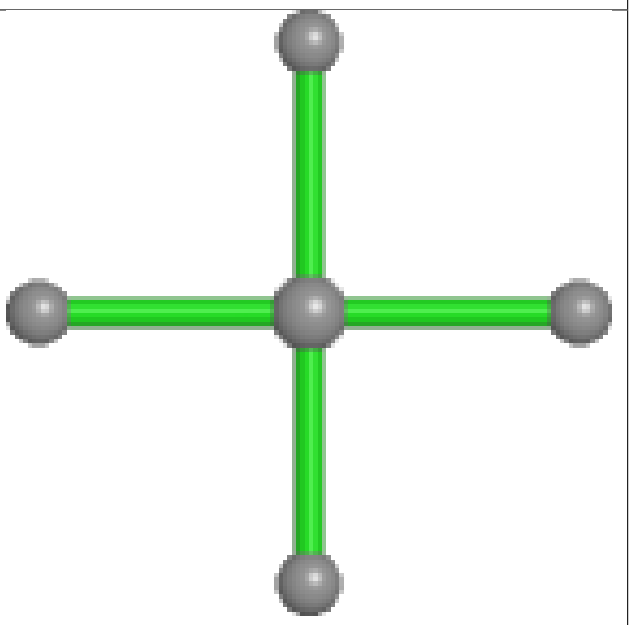
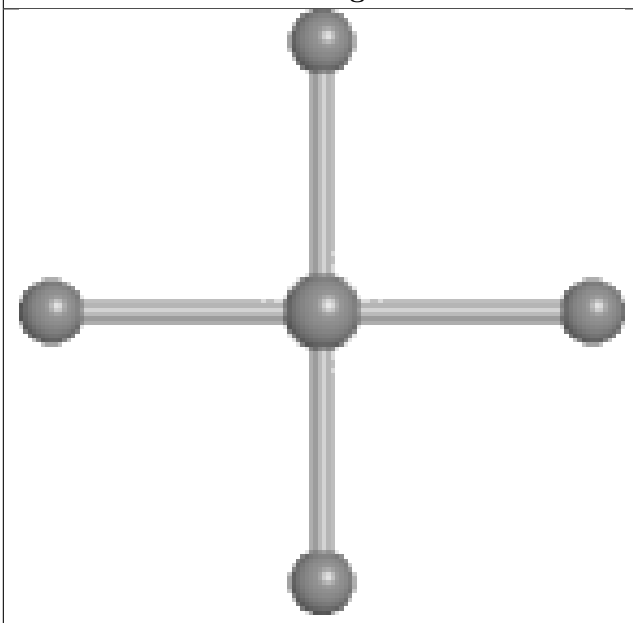


Bond angles



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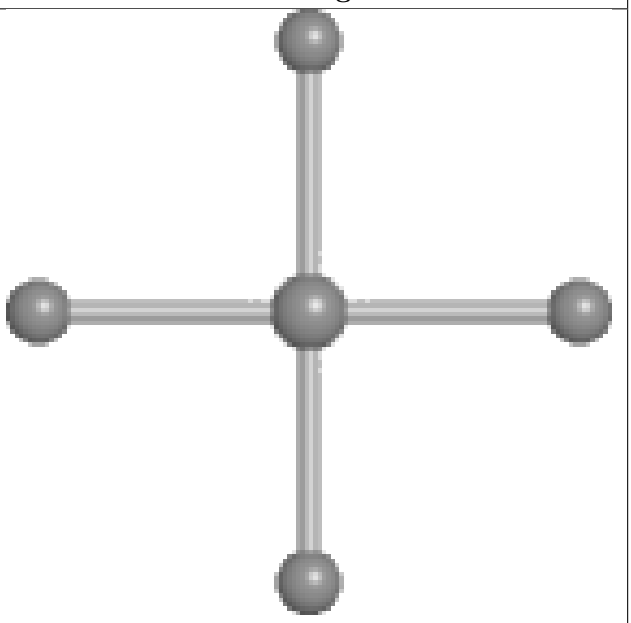
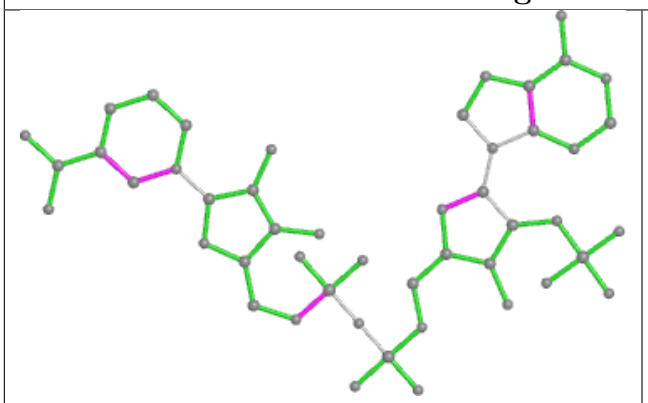


Rings

Ligand NAP B 1301



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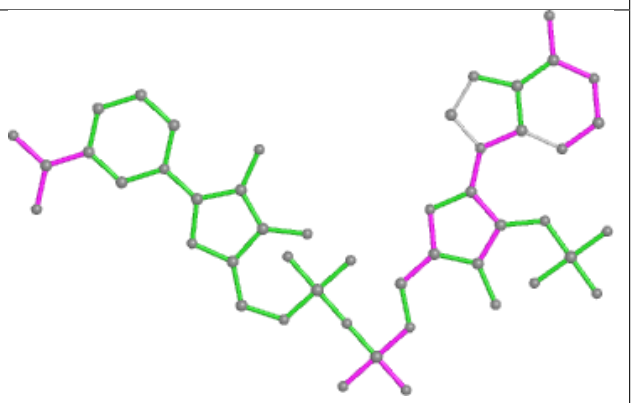
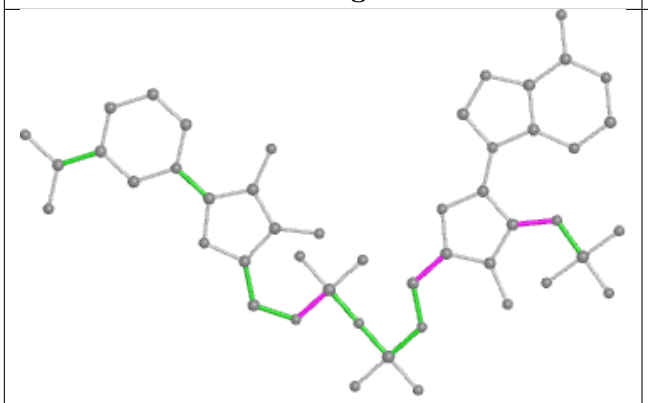
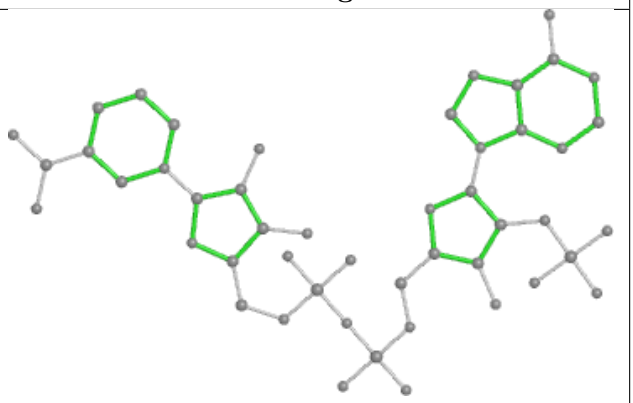


Bond angles

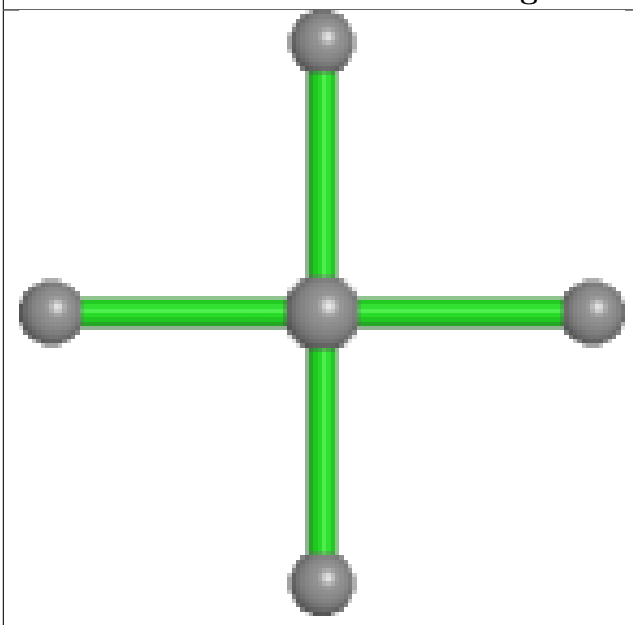


Torsions

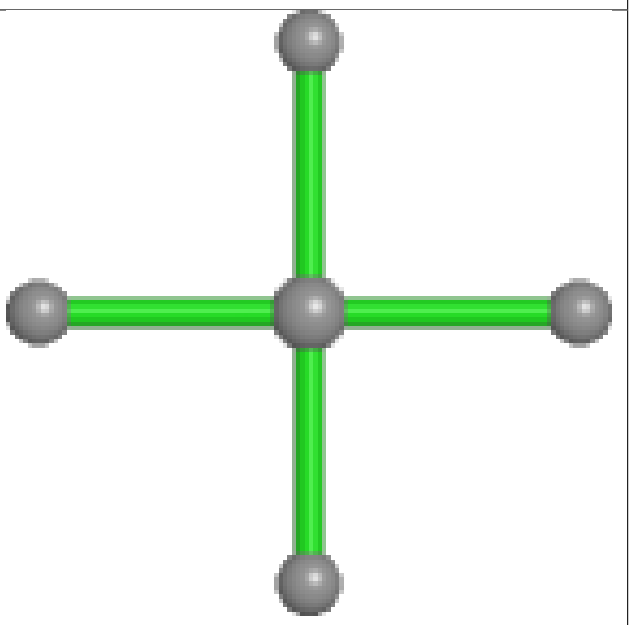


Rings

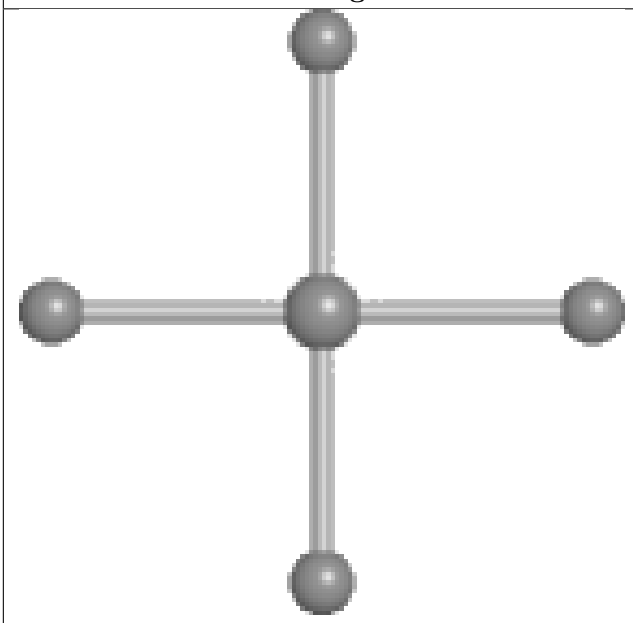
Ligand SO4 B 1308



Bond lengths



Bond angles



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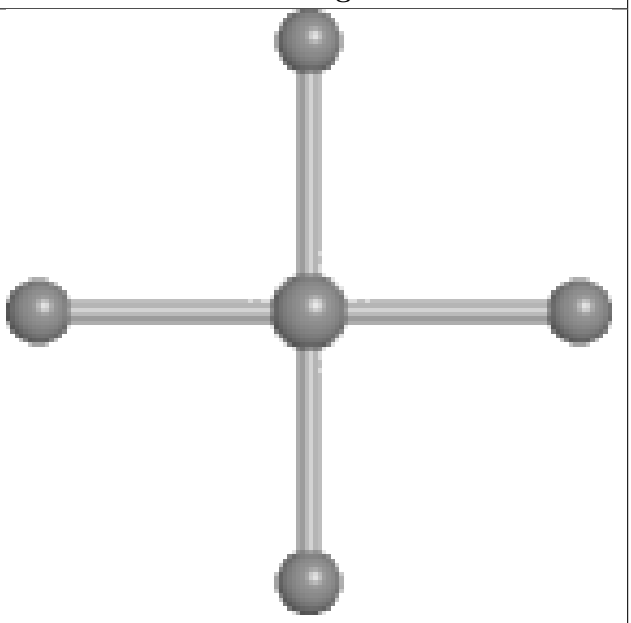
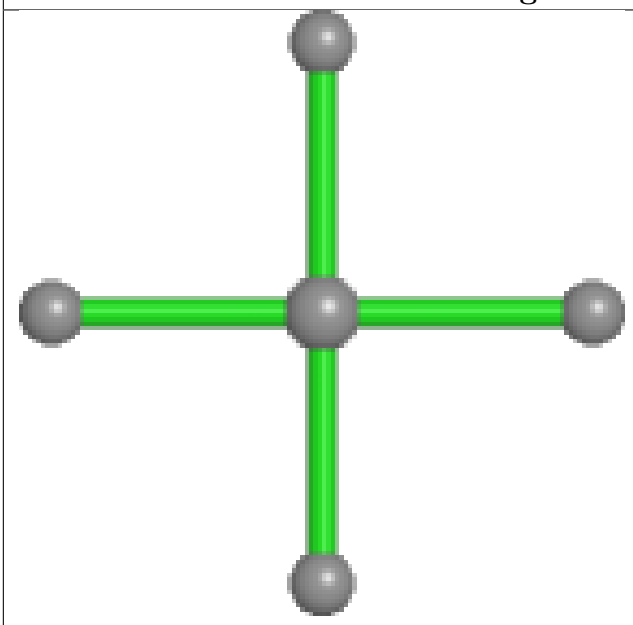


Rings

Ligand SO4 A 1306



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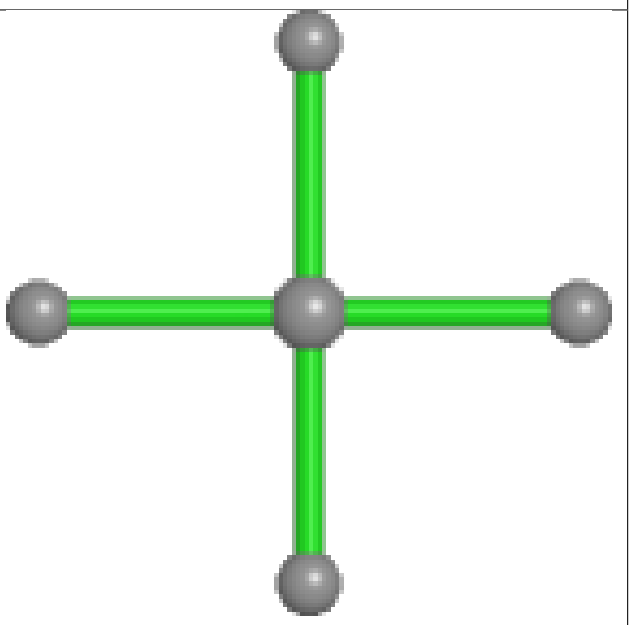
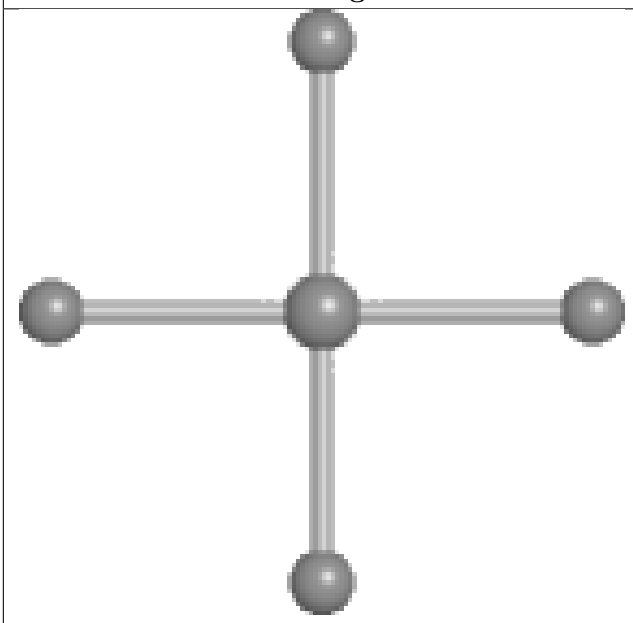


Bond angles



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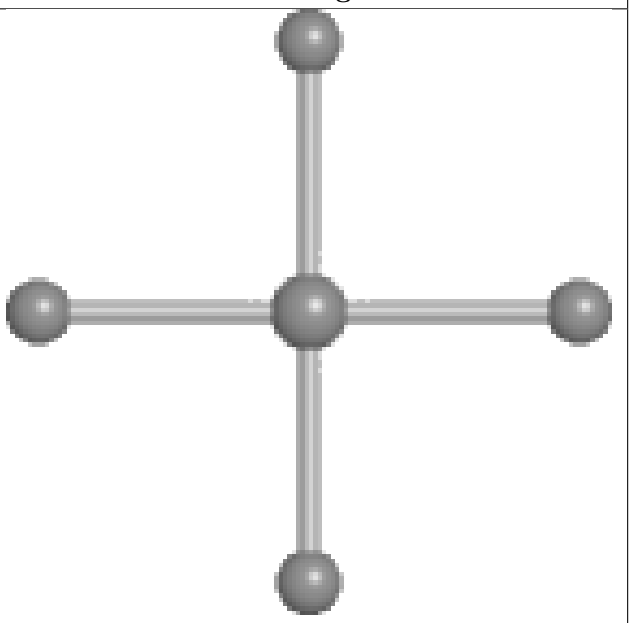
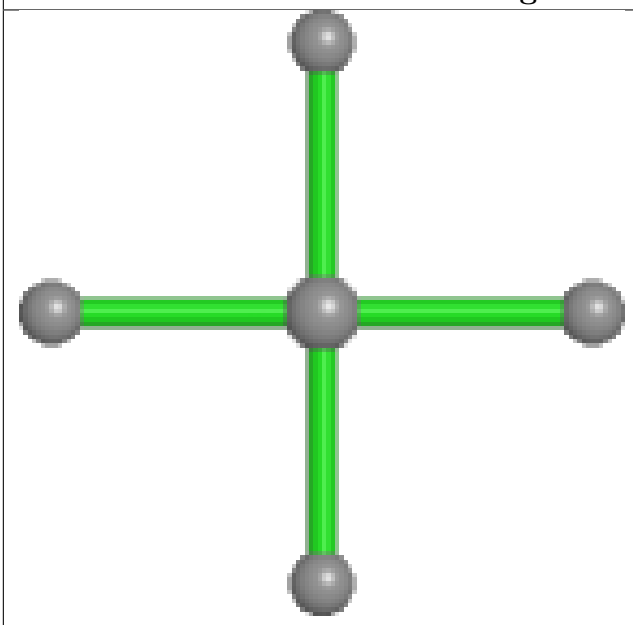
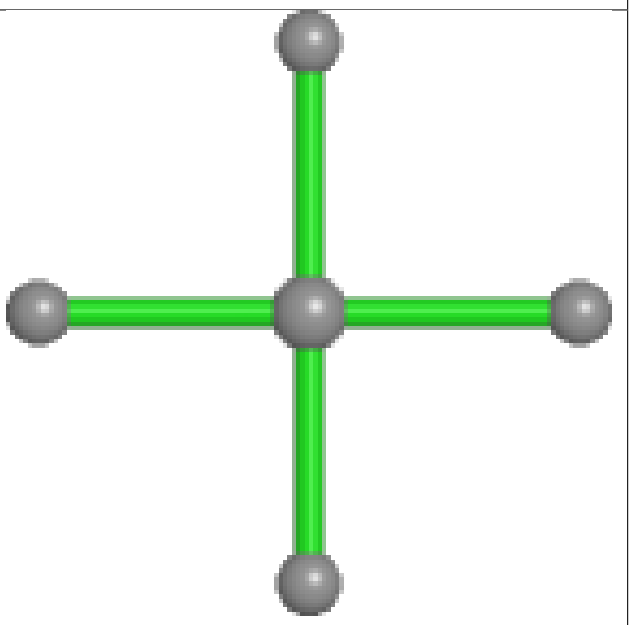


Rings

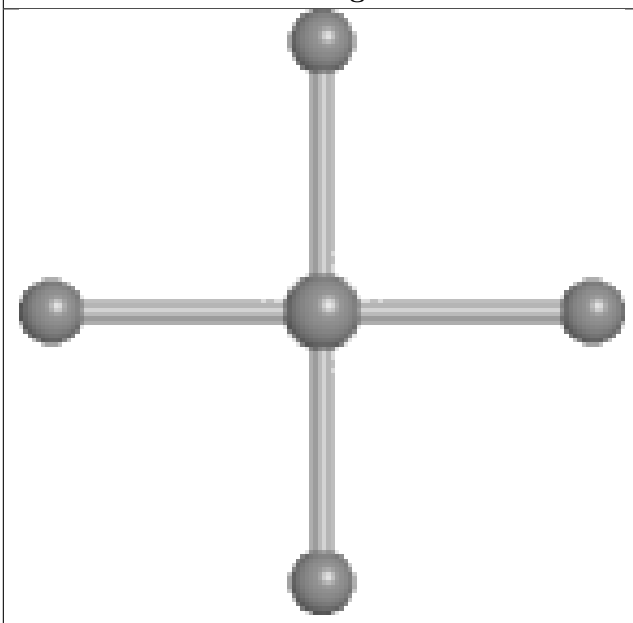
Ligand SO4 A 1309



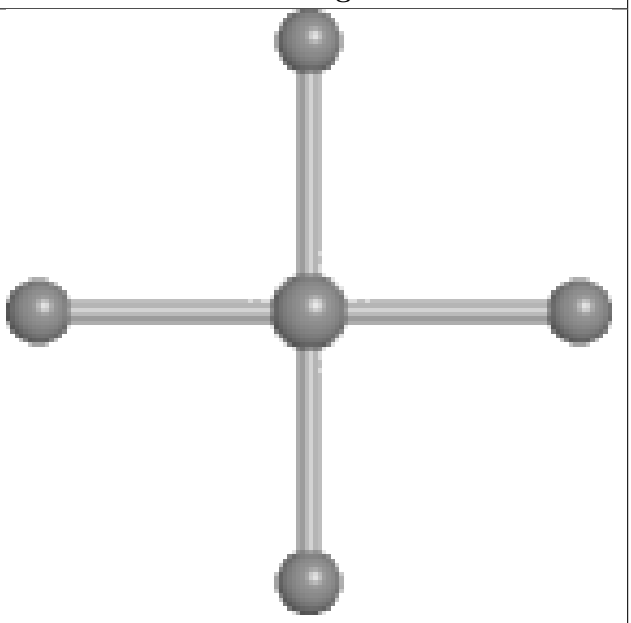
Bond lengths



Bond angles

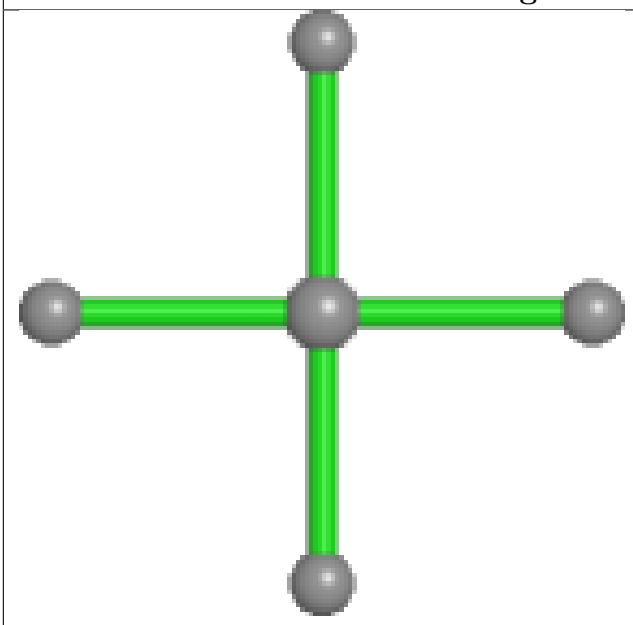


Torsions

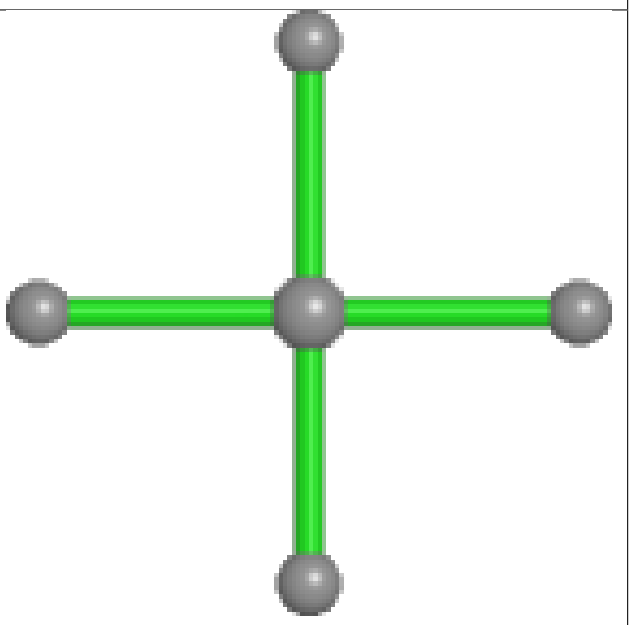


Rings

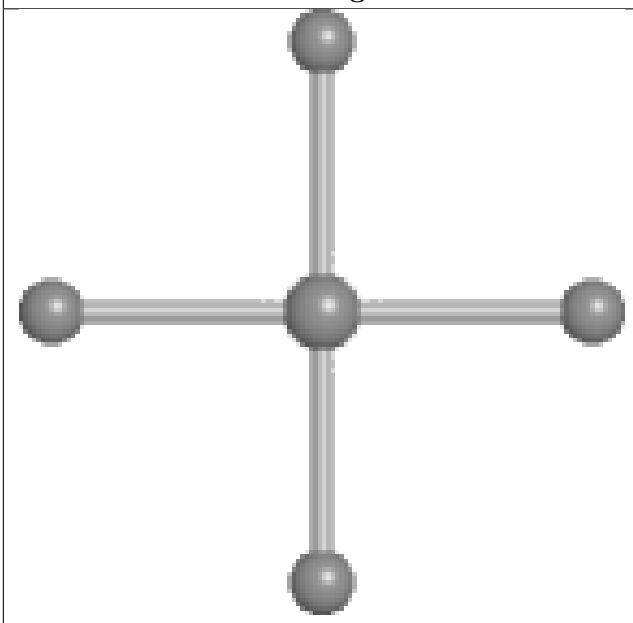
Ligand SO4 A 1308



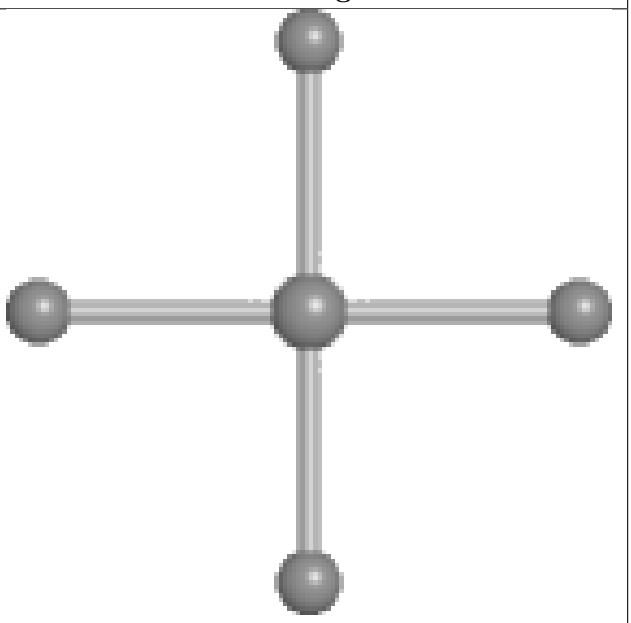
Bond lengths



Bond angles

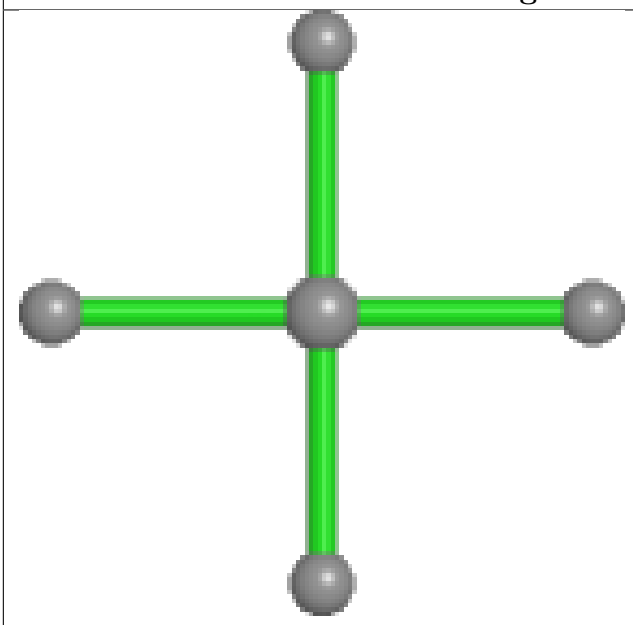


Torsions

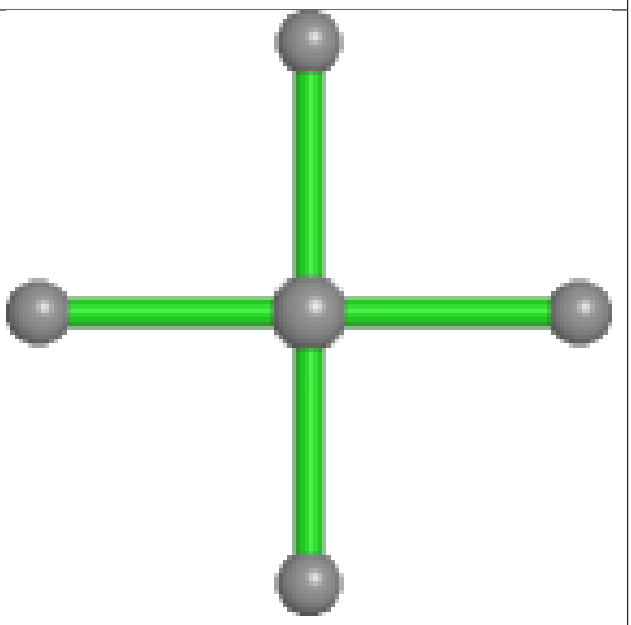


Rings

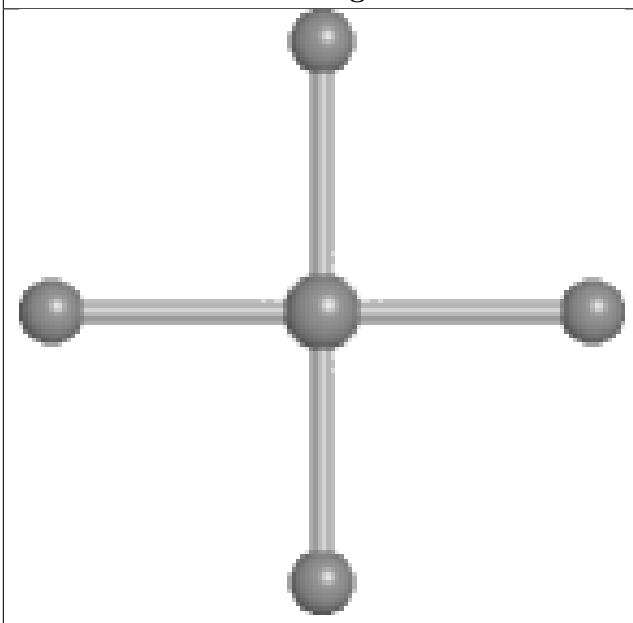
Ligand SO4 A 1303



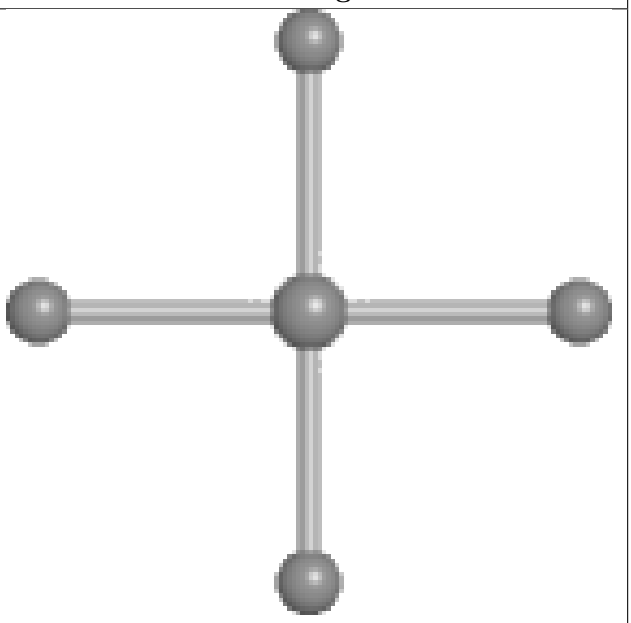
Bond lengths



Bond angles

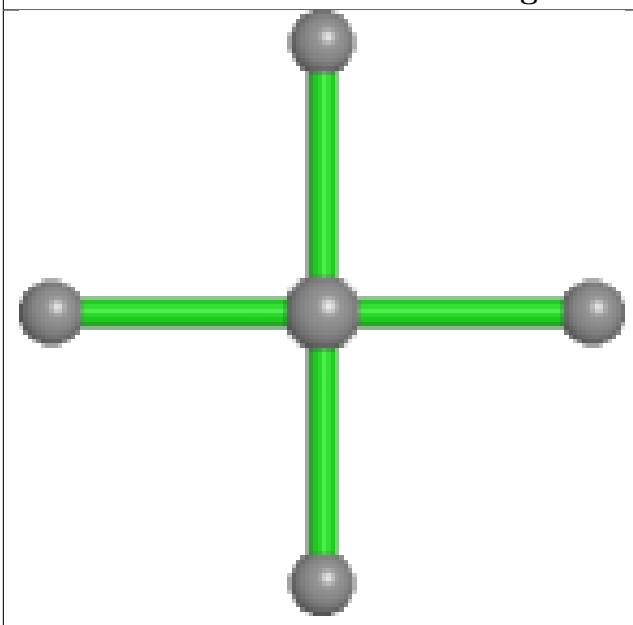


Torsions

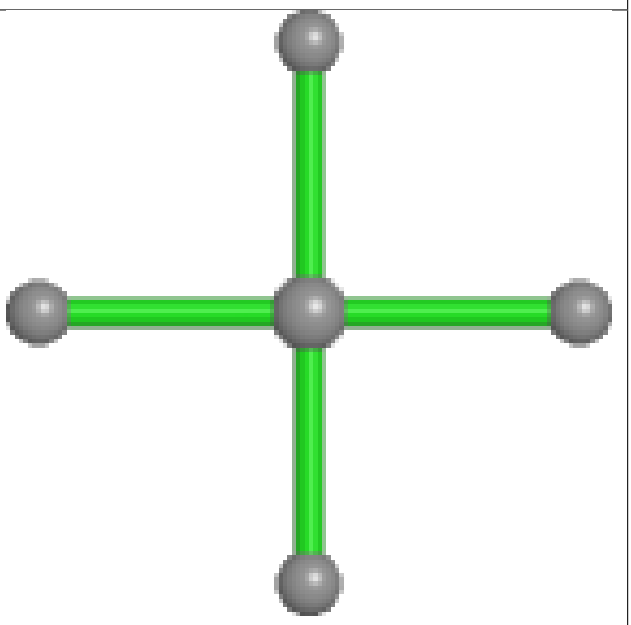


Rings

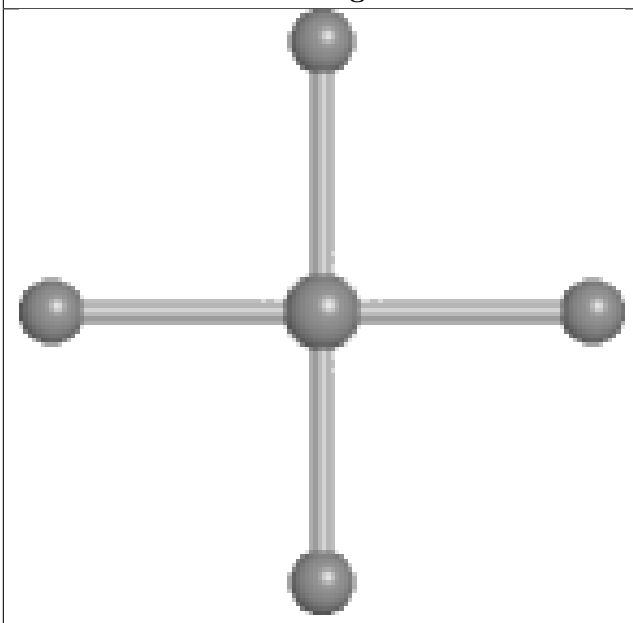
Ligand SO4 B 1309



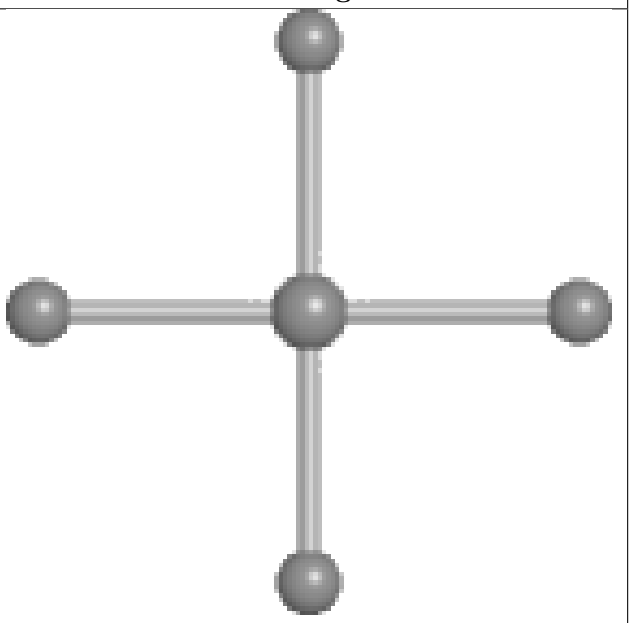
Bond lengths



Bond angles

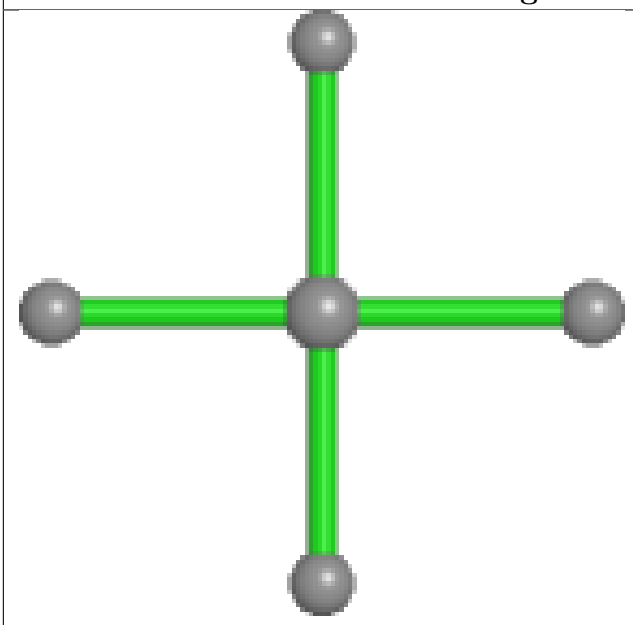


Torsions

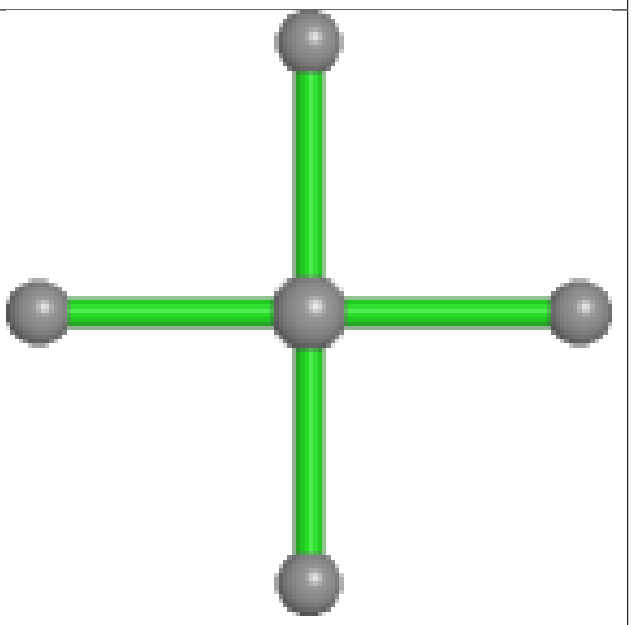


Rings

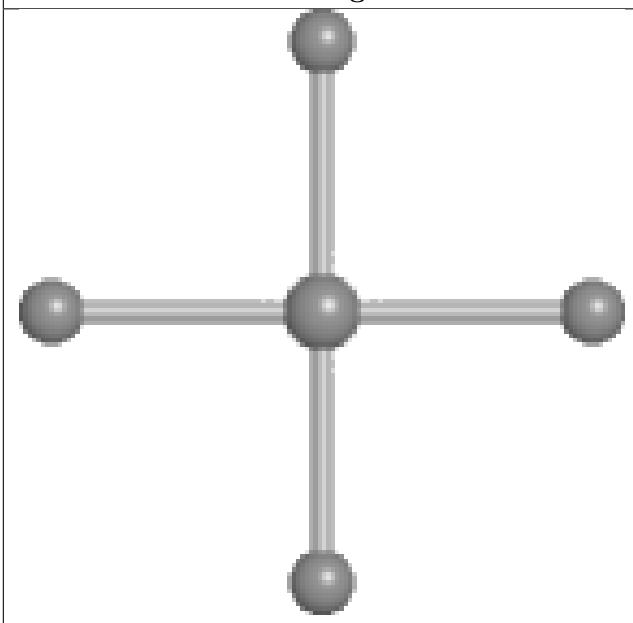
Ligand SO4 B 1304



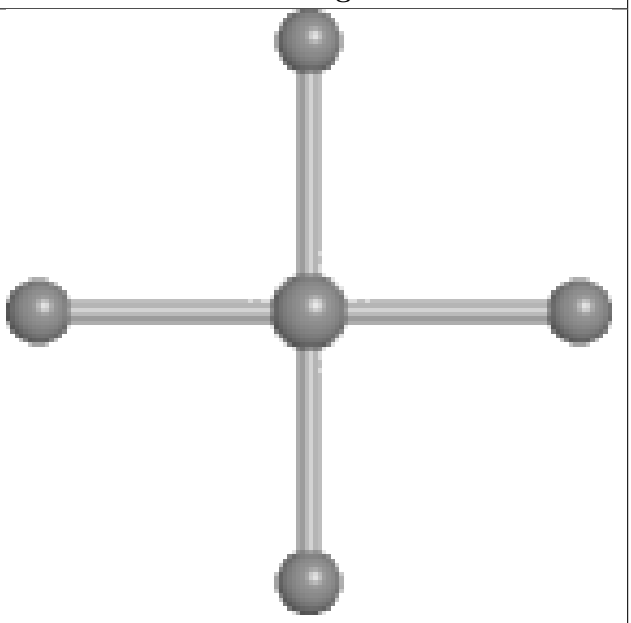
Bond lengths



Bond angles

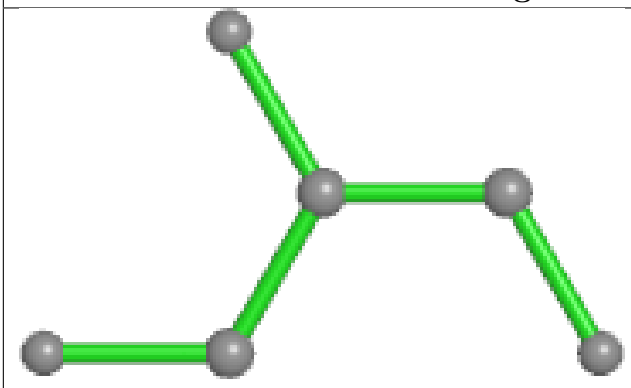


Torsions

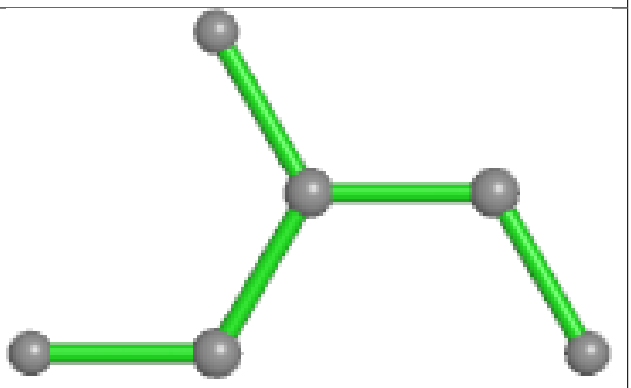


Rings

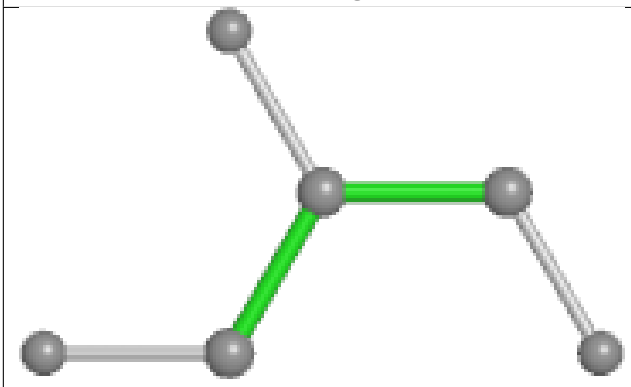
Ligand GOL A 1302



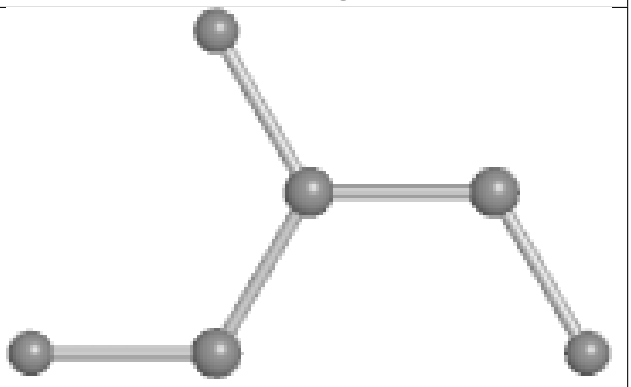
Bond lengths



Bond angles

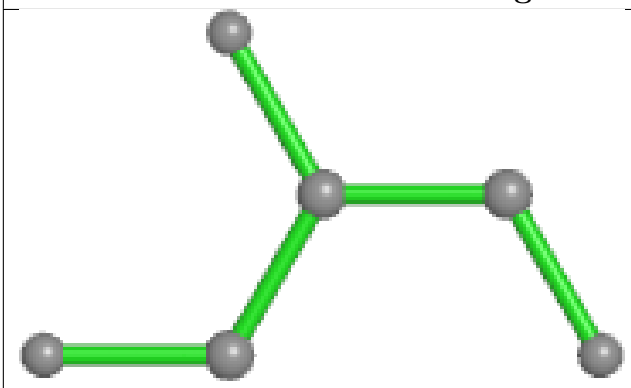


Torsions

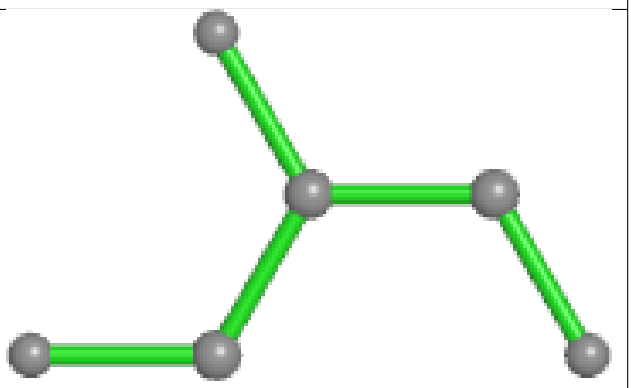


Rings

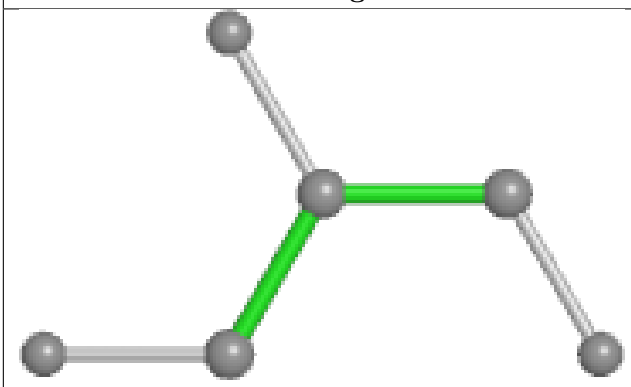
Ligand GOL B 1302



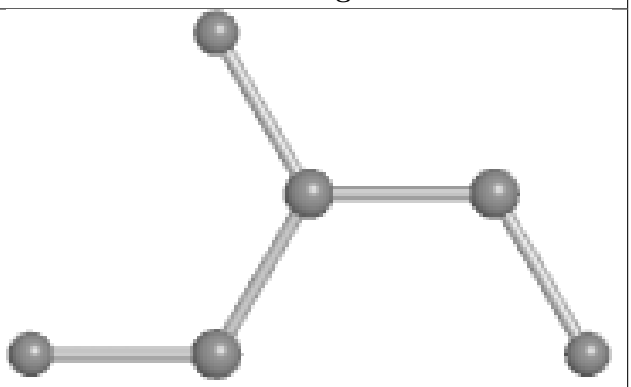
Bond lengths



Bond angles

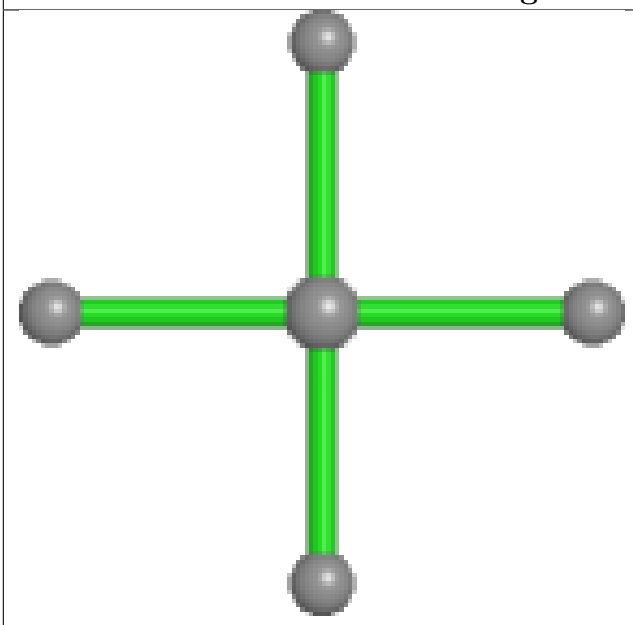


Torsions

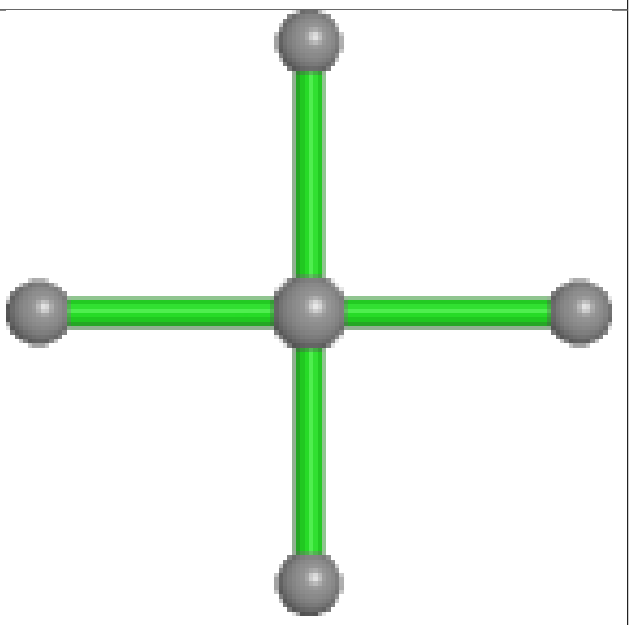


Rings

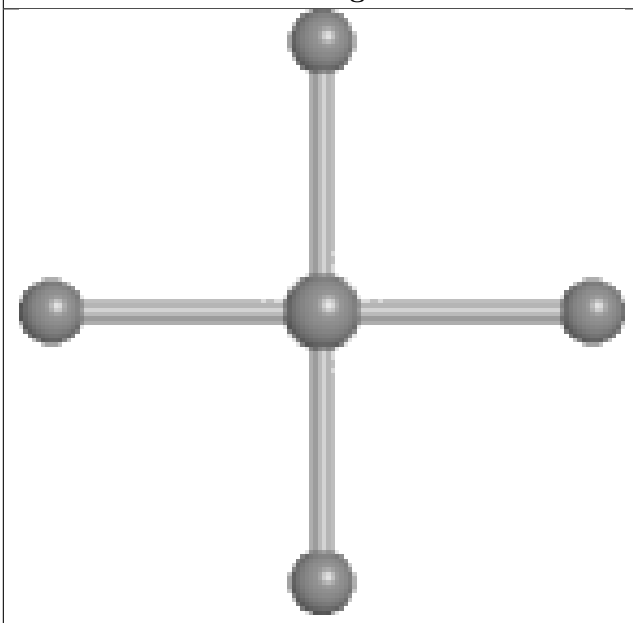
Ligand SO4 B 1305



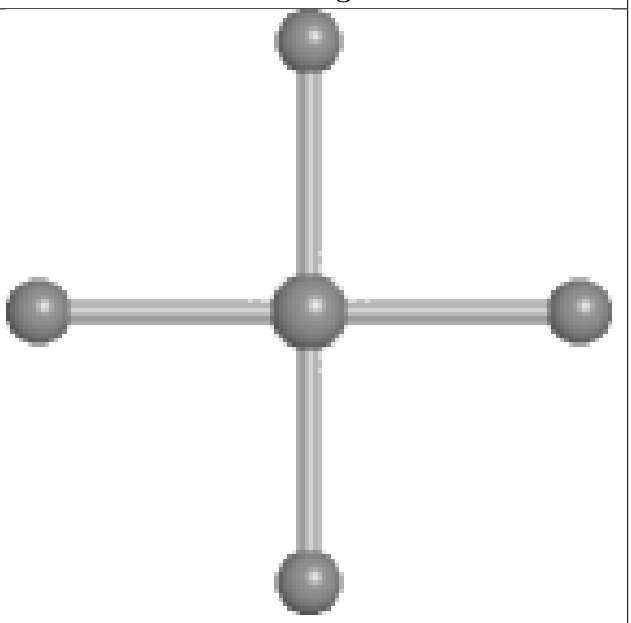
Bond lengths



Bond angles

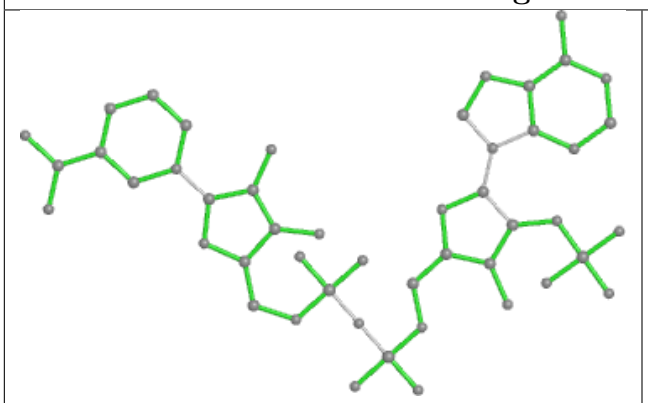


Torsions

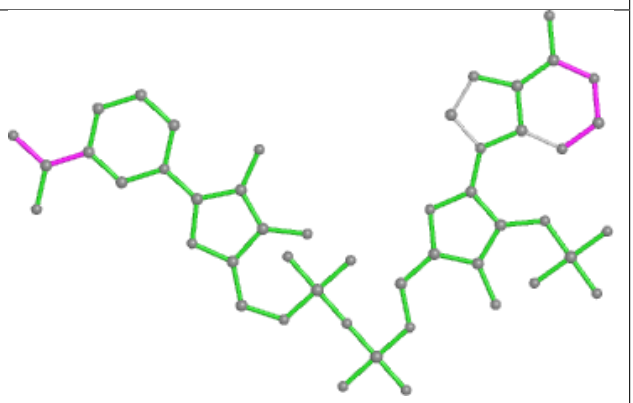


Rings

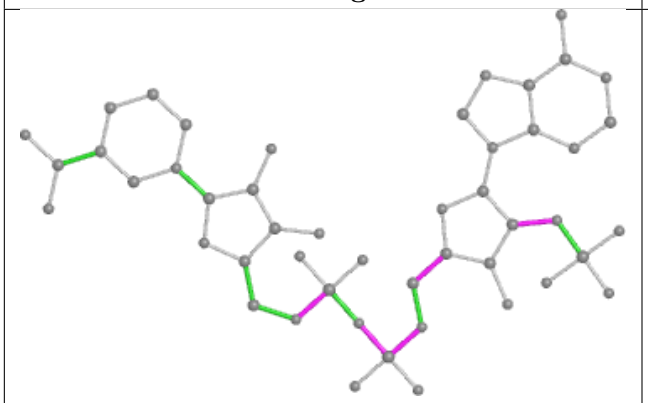
Ligand NAP A 1301



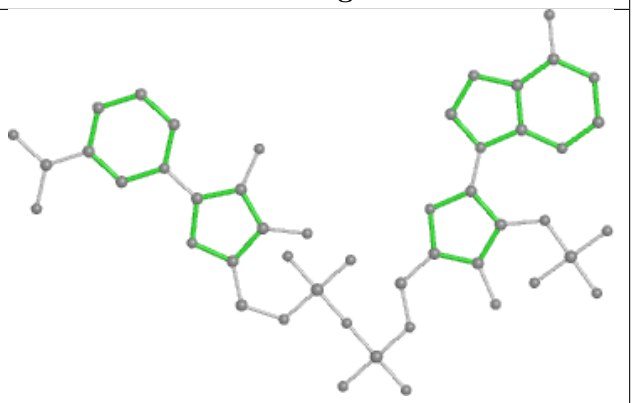
Bond lengths



Bond angles

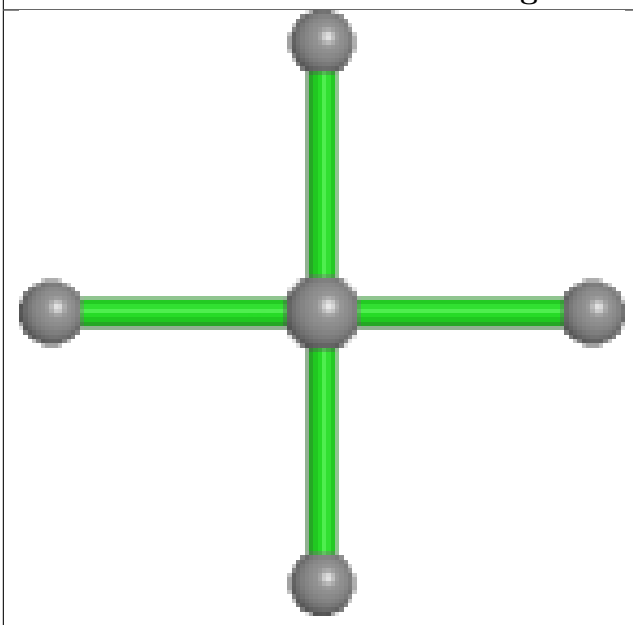


Torsions

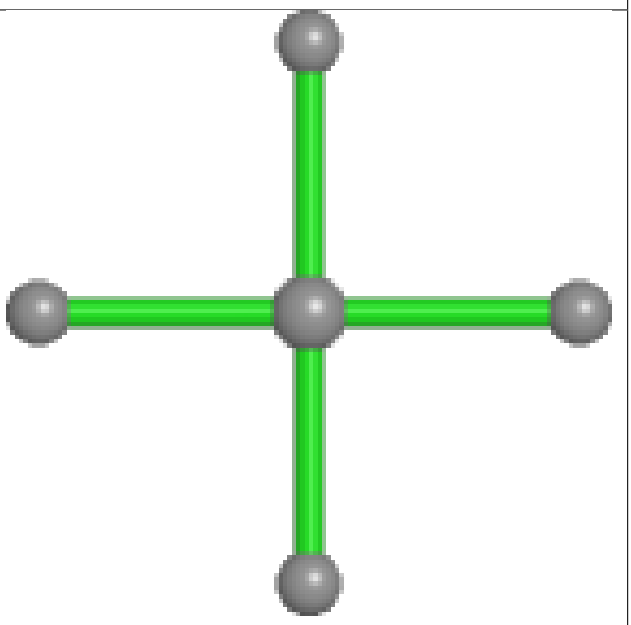


Rings

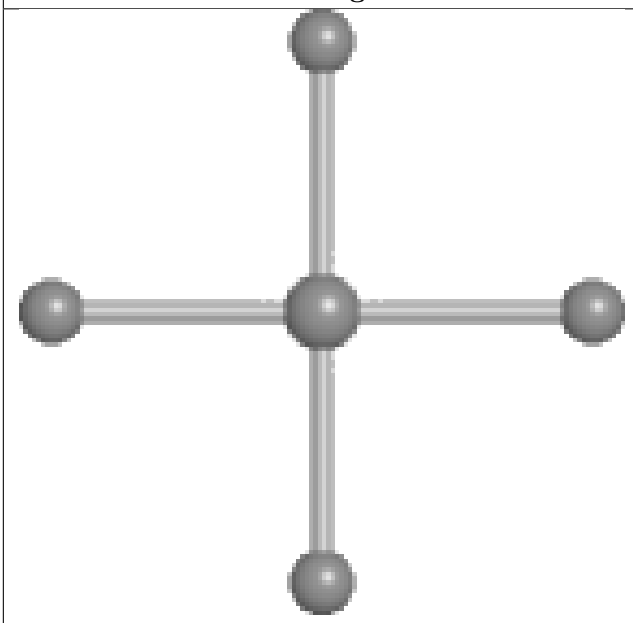
Ligand SO4 B 1307



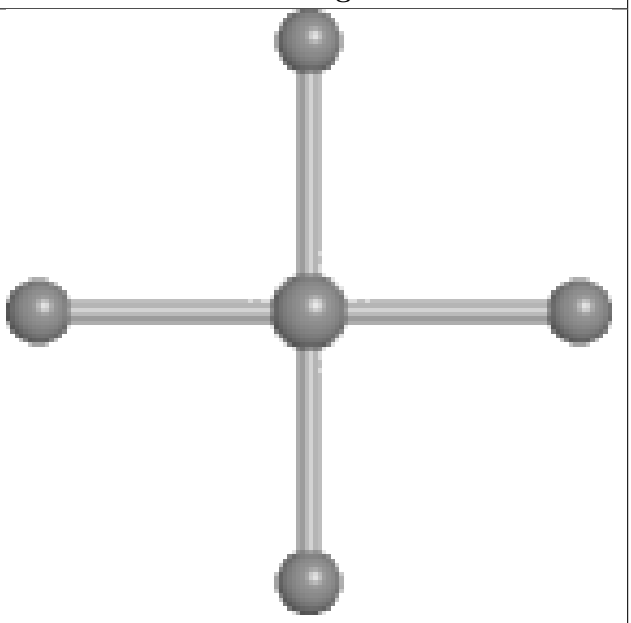
Bond lengths



Bond angles

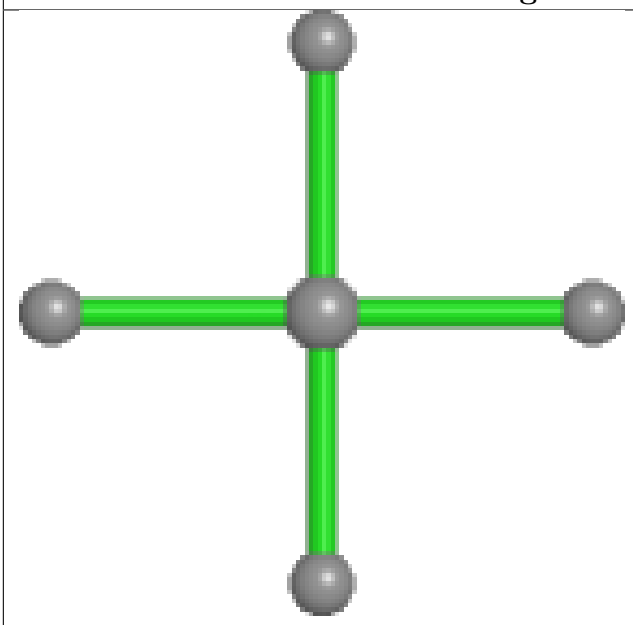


Torsions

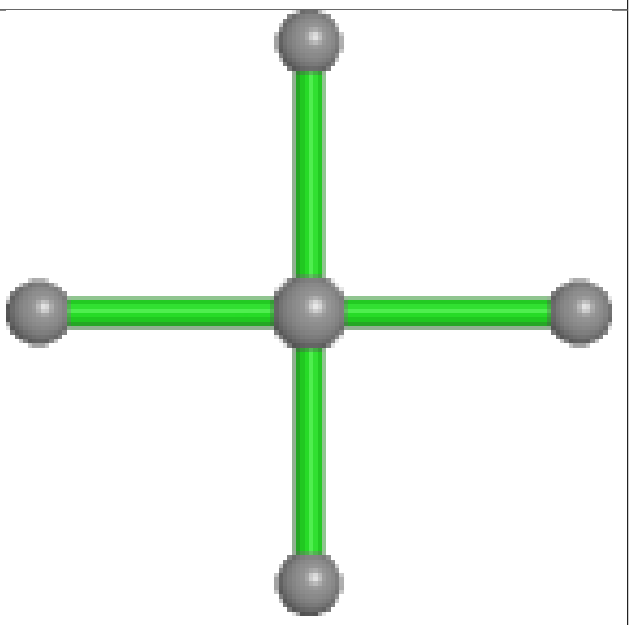


Rings

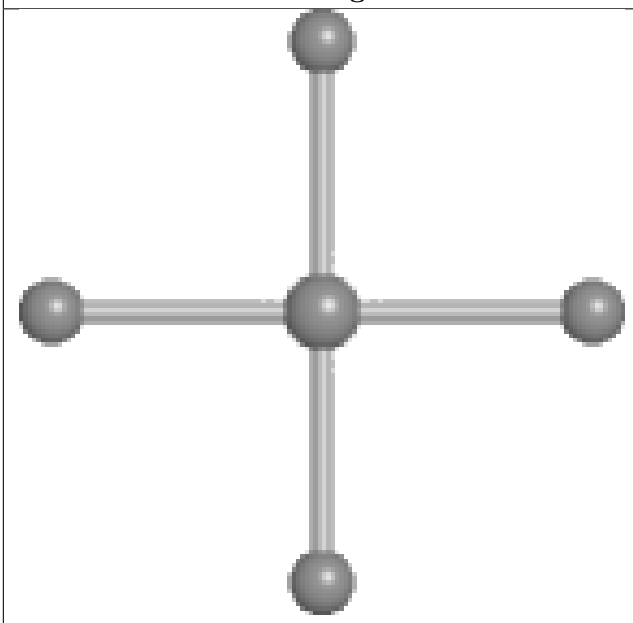
Ligand SO4 A 1304



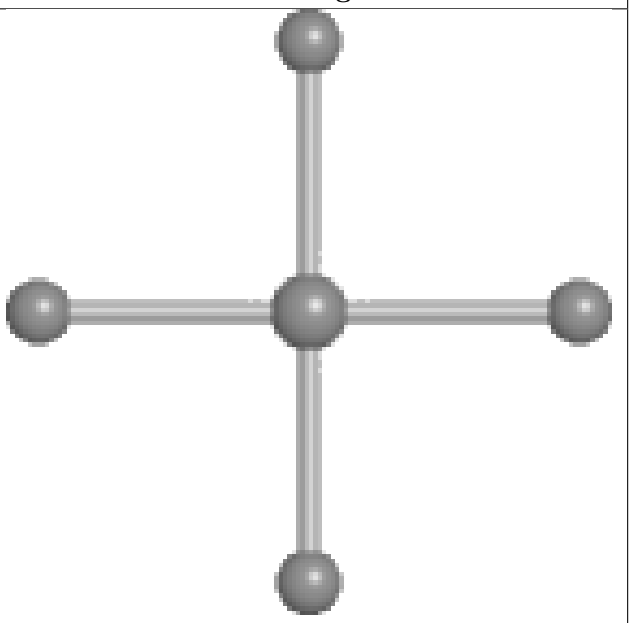
Bond lengths



Bond angles

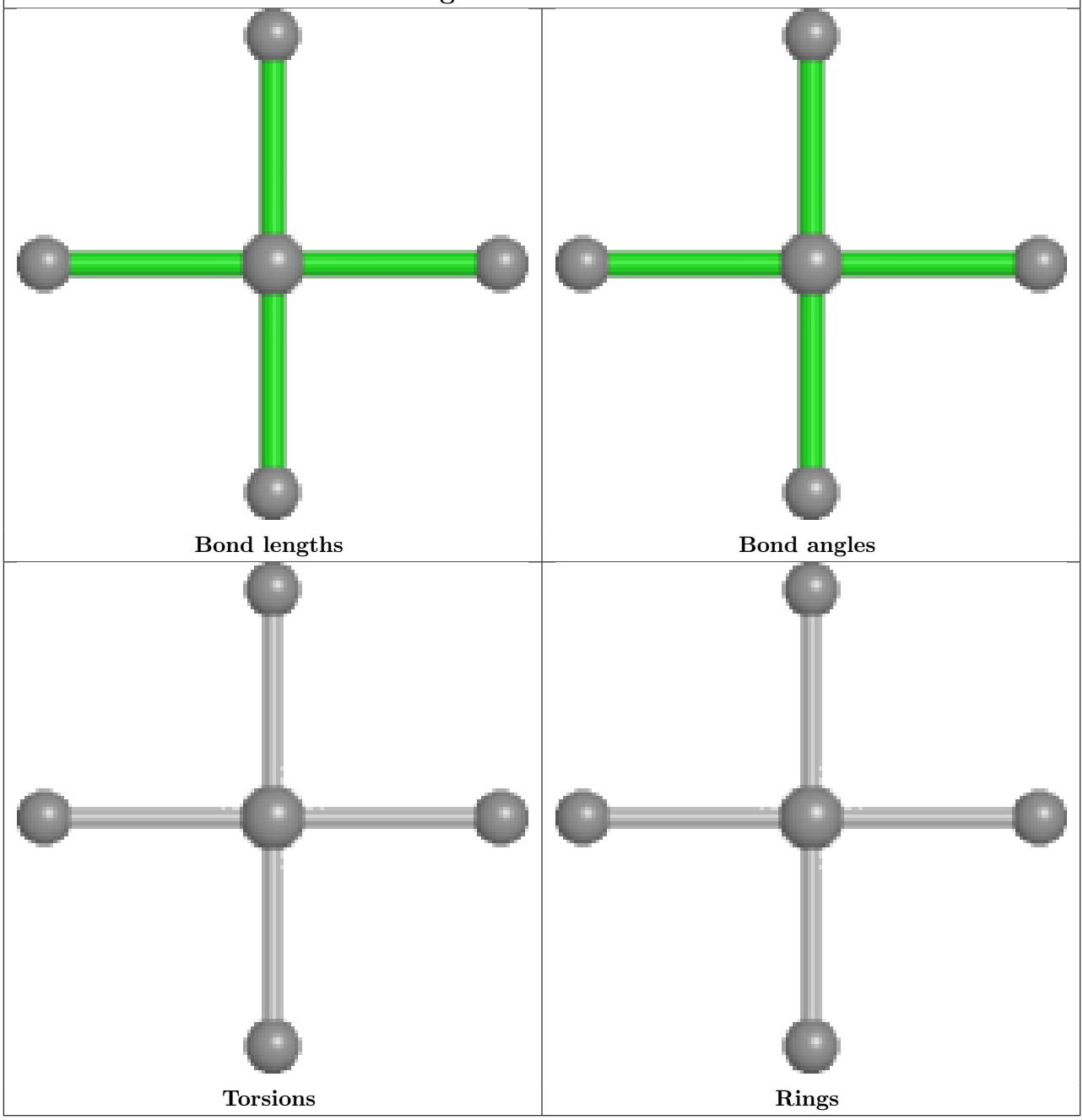


Torsions



Rings

Ligand SO4 B 1310



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%)	0.16	49 (7%)	14	13	12, 25, 62, 111	0
1	B	660/695 (94%)	0.18	46 (6%)	16	15	12, 24, 62, 111	0
All	All	1322/1390 (95%)	0.17	95 (7%)	15	14	12, 24, 62, 111	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	786	GLY	10.0
1	A	784	THR	9.5
1	B	786	GLY	8.8
1	B	784	THR	8.5
1	A	785	GLY	8.5
1	B	785	GLY	8.4
1	A	983	GLY	8.0
1	B	1216	SER	7.7
1	A	787	LYS	6.9
1	B	1215	ASP	6.7
1	B	787	LYS	6.5
1	B	782	SER	5.9
1	B	783	GLY	5.7
1	B	779	ASP	5.7
1	B	1214	GLU	5.5
1	B	984	SER	5.4
1	B	983	GLY	5.4
1	A	984	SER	5.1
1	B	911	ASP	4.9
1	A	1213	ALA	4.8
1	B	1211	PRO	4.7
1	B	840	THR	4.6
1	A	1215	ASP	4.6
1	B	1219	ARG	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	1220	ALA	4.6
1	A	1212	ASP	4.5
1	B	841	ASN	4.4
1	B	838	HIS	4.2
1	A	1214	GLU	4.1
1	A	569	PHE	4.1
1	A	838	HIS	4.1
1	A	985	PRO	4.0
1	A	630	ILE	4.0
1	A	1211	PRO	3.7
1	A	932	LEU	3.7
1	B	781	LEU	3.7
1	A	982	PHE	3.7
1	A	788	PRO	3.7
1	A	783	GLY	3.7
1	A	633	ALA	3.6
1	B	571	GLU	3.6
1	A	986	LYS	3.5
1	A	890	PRO	3.5
1	B	788	PRO	3.4
1	B	982	PHE	3.2
1	B	570	SER	3.1
1	A	782	SER	3.1
1	B	932	LEU	3.1
1	A	911	ASP	3.0
1	B	1210	LEU	3.0
1	B	630	ILE	3.0
1	B	988	GLU	3.0
1	A	840	THR	2.9
1	B	780	ARG	2.9
1	A	841	ASN	2.9
1	A	910	GLU	2.9
1	B	890	PRO	2.9
1	B	1222	ILE	2.9
1	A	981	LEU	2.8
1	B	894	GLU	2.8
1	B	910	GLU	2.8
1	A	925	LYS	2.7
1	A	779	ASP	2.6
1	B	1217	ARG	2.6
1	B	930	GLY	2.6
1	A	1190	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	926	LYS	2.5
1	B	1218	TYR	2.5
1	B	839	ASP	2.5
1	A	632	PHE	2.5
1	B	987	GLN	2.4
1	B	912	ALA	2.4
1	A	987	GLN	2.4
1	A	570	SER	2.4
1	A	896	PRO	2.4
1	A	1044	GLU	2.3
1	A	1216	SER	2.3
1	B	633	ALA	2.3
1	A	628	GLU	2.3
1	A	789	GLY	2.3
1	A	897	VAL	2.3
1	A	1219	ARG	2.2
1	B	817	ARG	2.2
1	A	1189	LEU	2.2
1	B	1077	LEU	2.2
1	A	898	THR	2.2
1	A	1128	LEU	2.1
1	A	629	ASP	2.1
1	A	860	THR	2.1
1	A	1187	ARG	2.1
1	B	1044	GLU	2.1
1	A	894	GLU	2.1
1	B	631	GLY	2.1
1	B	919	LYS	2.0
1	A	631	GLY	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)

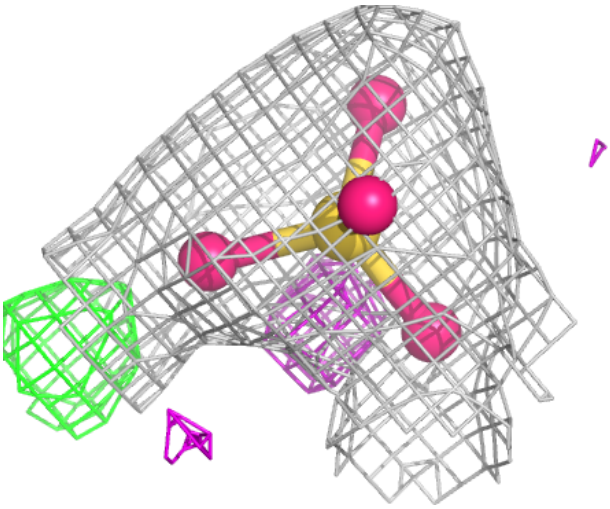
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

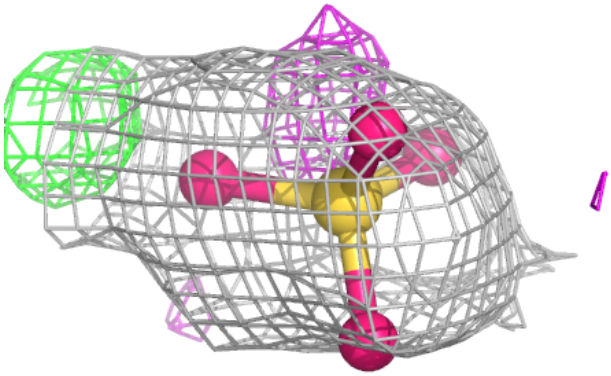
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	A	1307	5/5	0.82	0.22	90,92,100,104	0
4	SO4	B	1307	5/5	0.84	0.31	38,42,62,64	0
4	SO4	A	1309	5/5	0.86	0.28	80,86,92,98	0
4	SO4	A	1308	5/5	0.89	0.19	55,65,77,89	0
4	SO4	B	1309	5/5	0.89	0.25	65,72,76,78	0
4	SO4	B	1308	5/5	0.90	0.15	47,51,67,69	0
2	NAP	A	1301	48/48	0.90	0.15	23,39,63,69	0
4	SO4	A	1306	5/5	0.93	0.21	51,61,63,72	0
4	SO4	B	1310	5/5	0.93	0.25	59,66,76,84	0
2	NAP	B	1301	48/48	0.94	0.13	23,32,47,61	0
4	SO4	A	1304	5/5	0.94	0.16	58,59,60,79	0
4	SO4	B	1304	5/5	0.95	0.14	47,48,61,68	0
4	SO4	B	1306	5/5	0.95	0.19	50,50,57,61	0
4	SO4	A	1303	5/5	0.95	0.15	49,61,62,63	0
3	GOL	B	1302	6/6	0.96	0.11	23,28,29,30	0
4	SO4	A	1305	5/5	0.96	0.21	44,52,54,63	0
3	GOL	A	1302	6/6	0.96	0.10	25,27,30,31	0
4	SO4	B	1305	5/5	0.97	0.17	47,51,57,59	0
4	SO4	B	1303	5/5	0.97	0.12	47,50,52,59	0

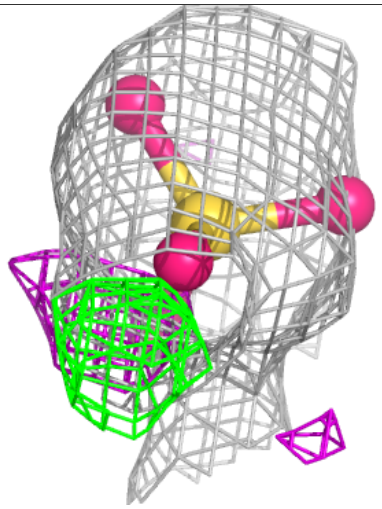
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SO4 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)

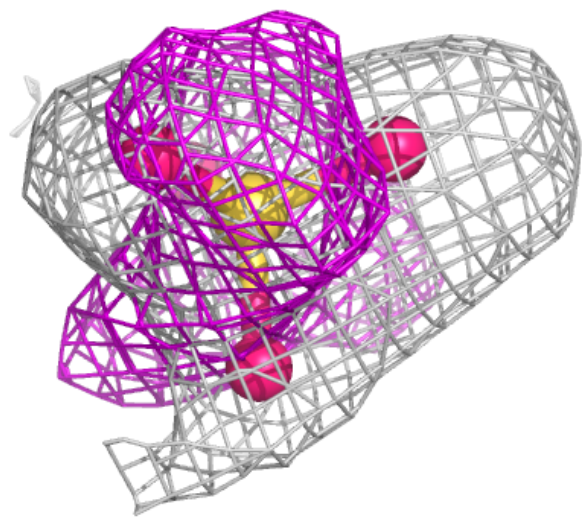


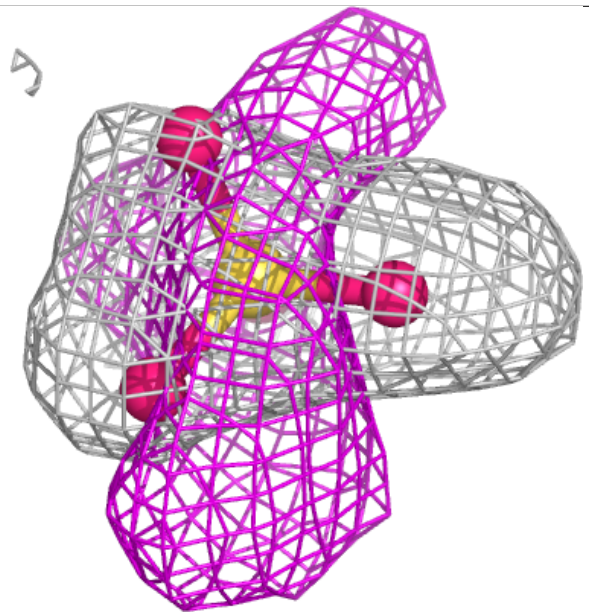


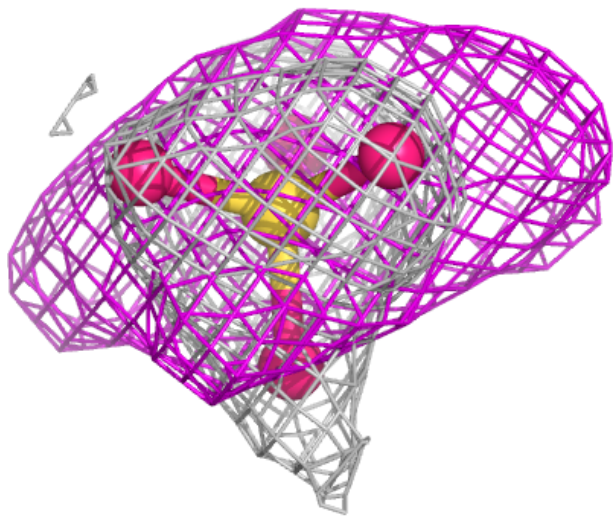


Electron density around SO4 B 1307:

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

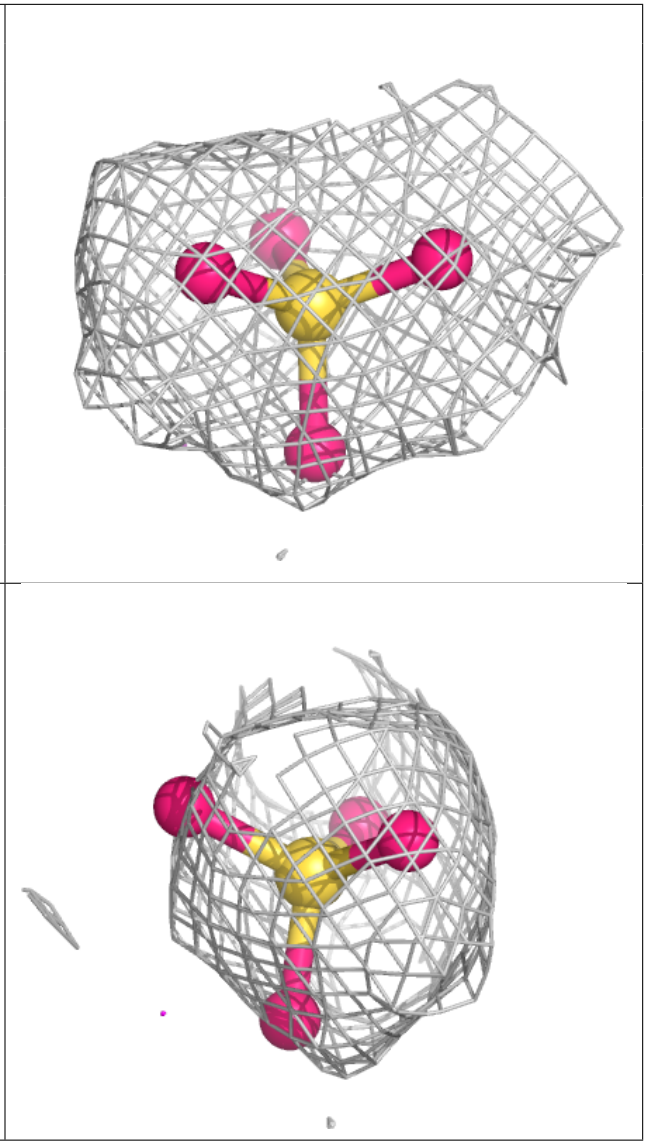






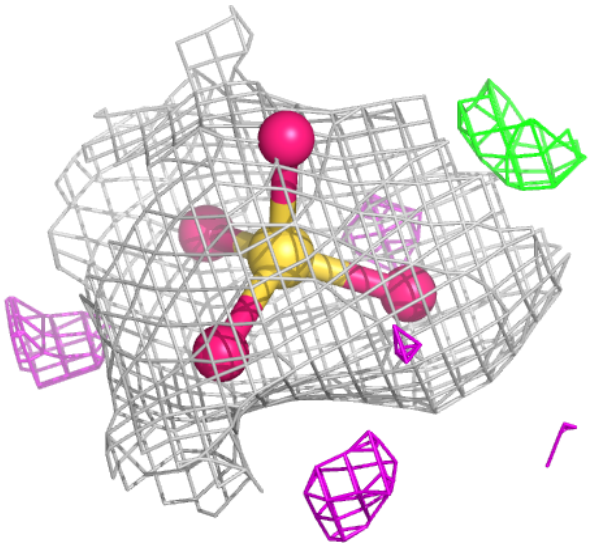
Electron density around SO4 A 1309:

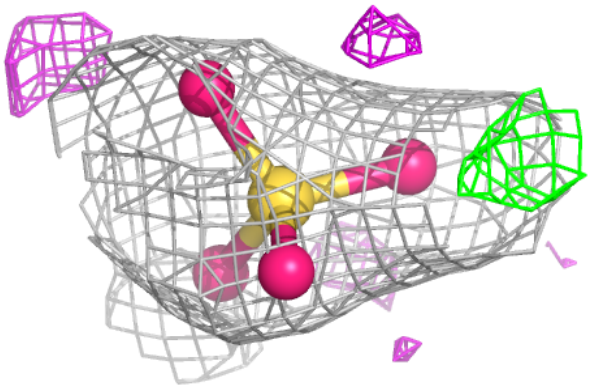
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

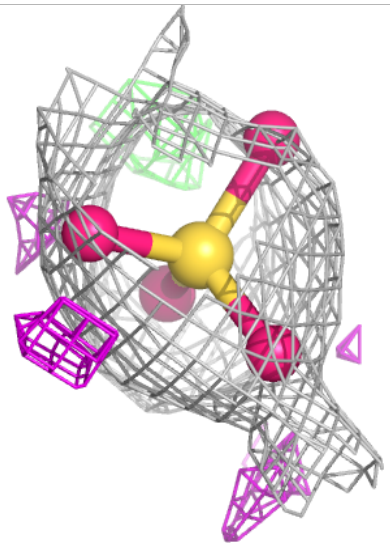


Electron density around SO4 A 1308:

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

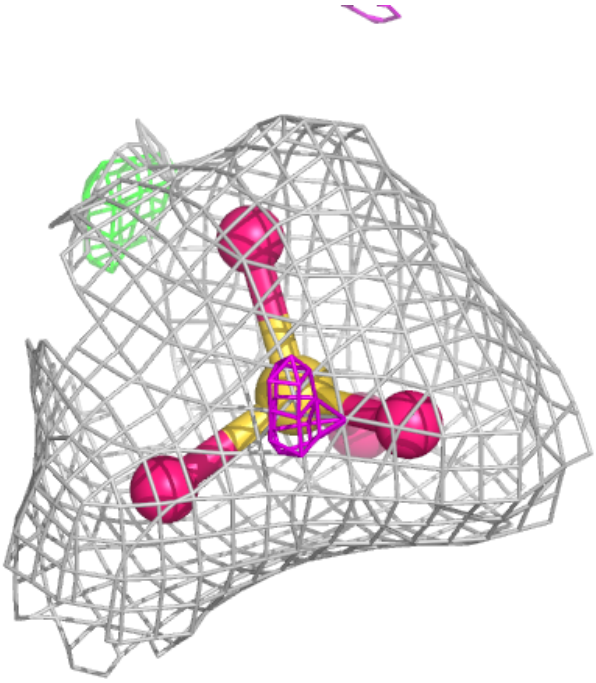


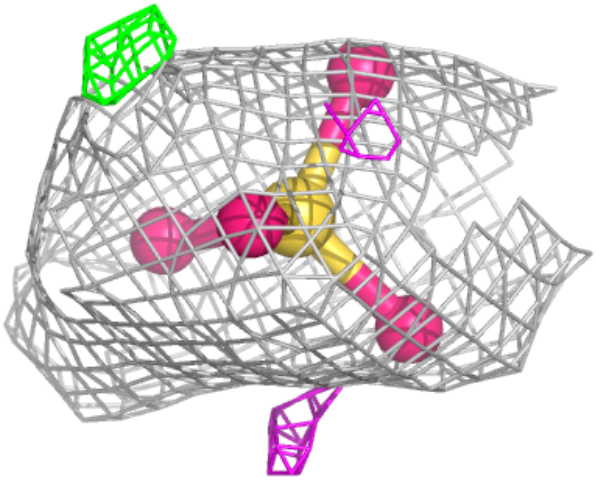


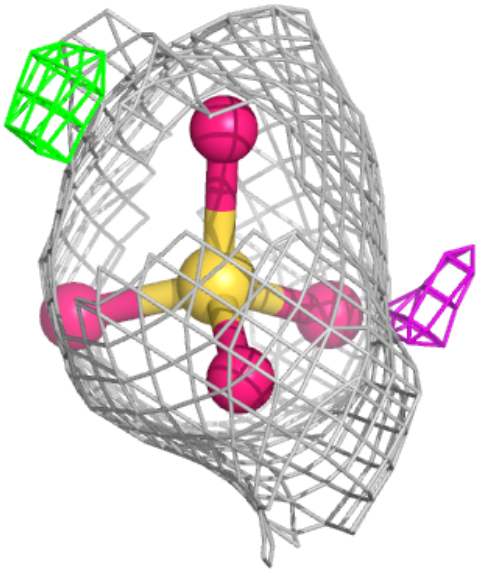


Electron density around SO4 B 1309:

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

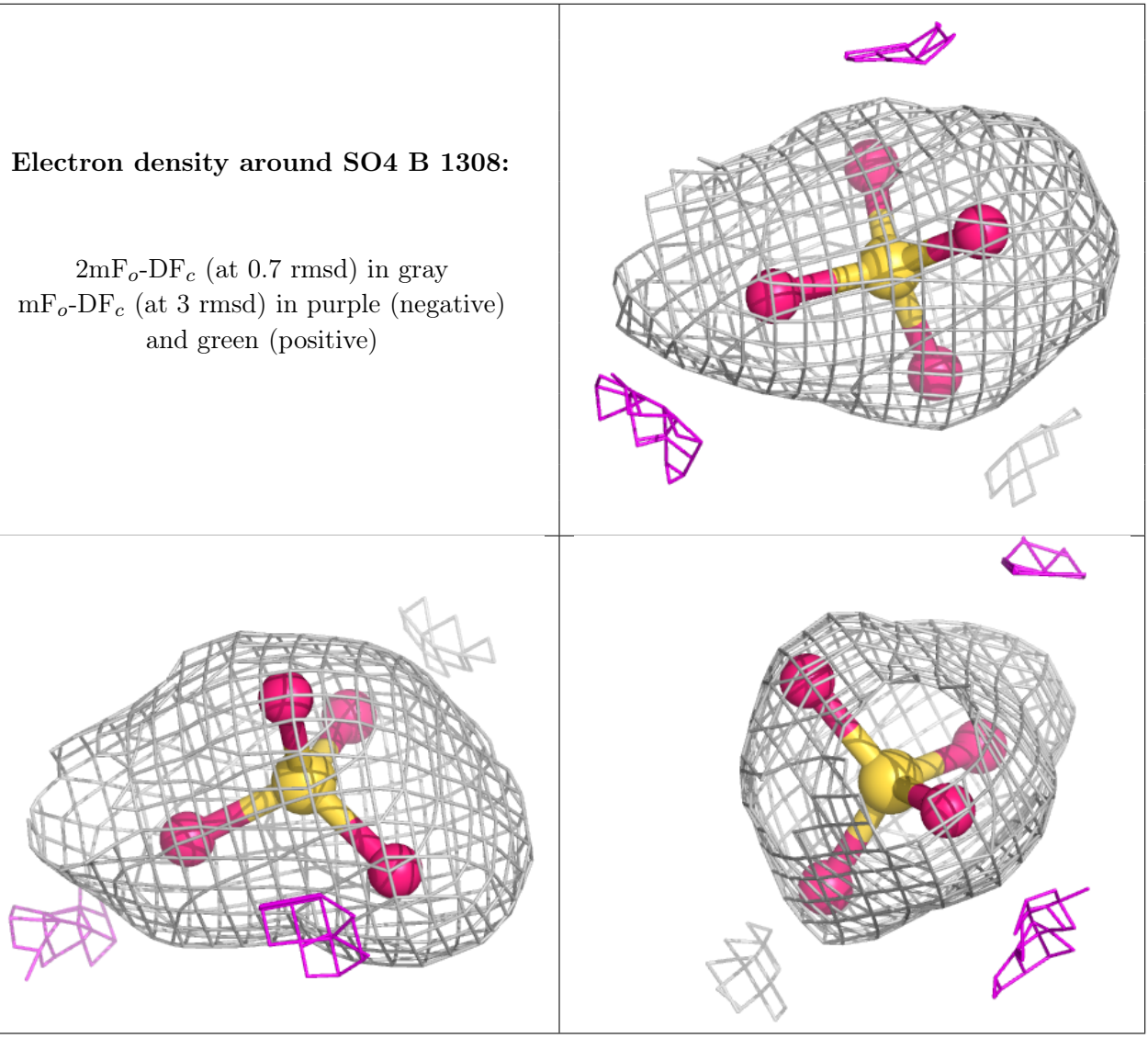






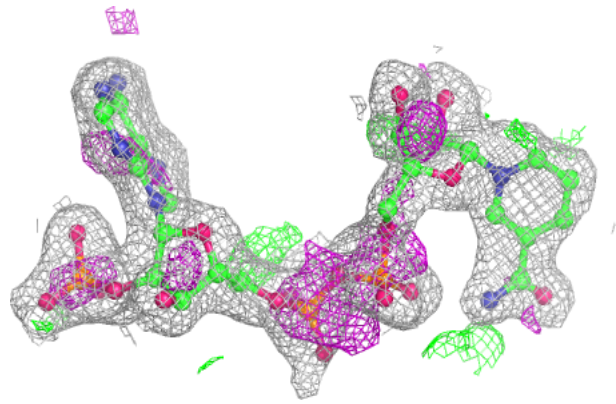
Electron density around SO4 B 1308:

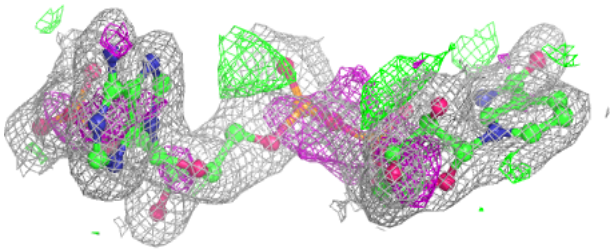
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

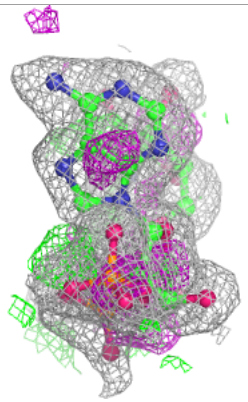


Electron density around NAP A 1301:

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

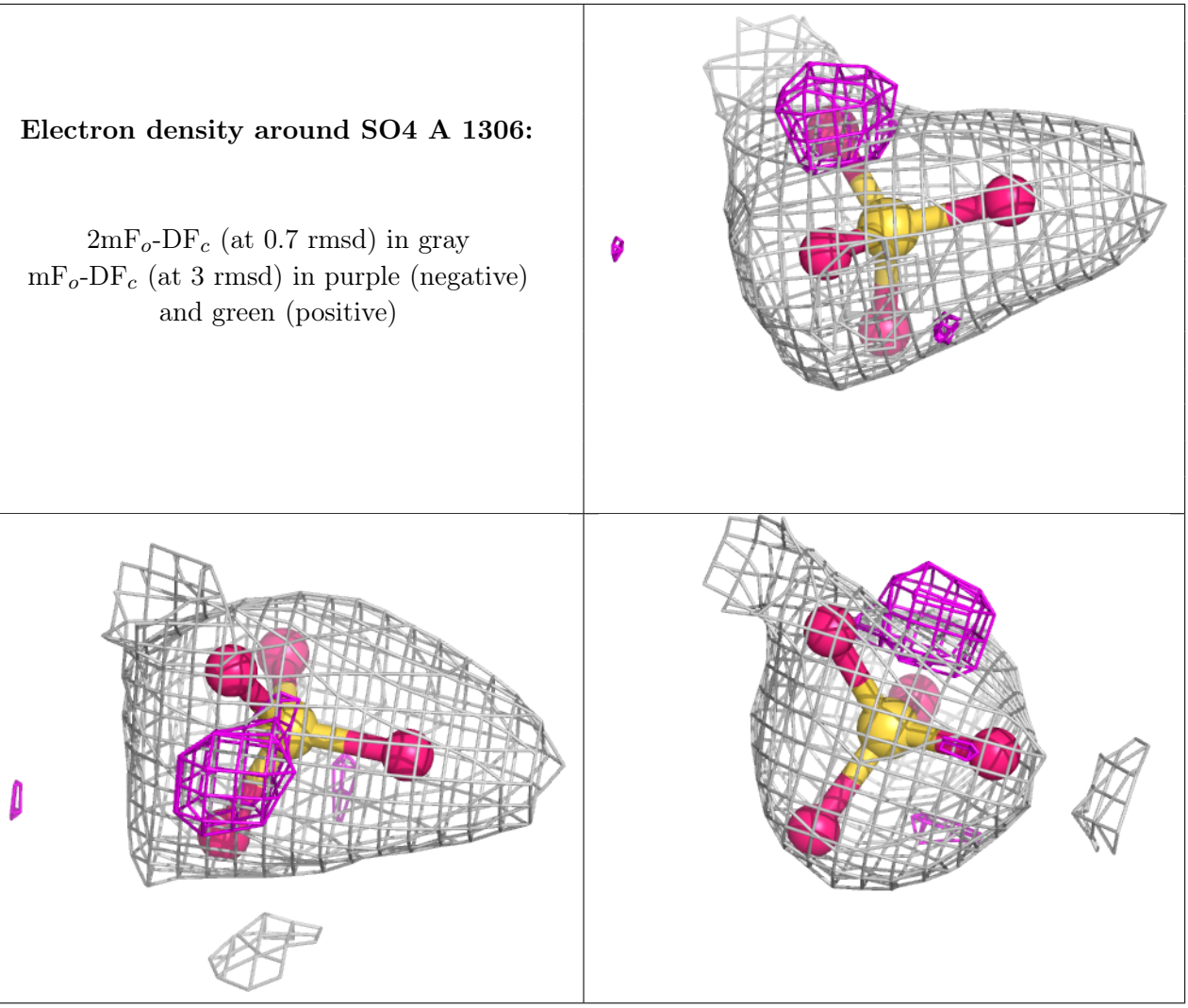






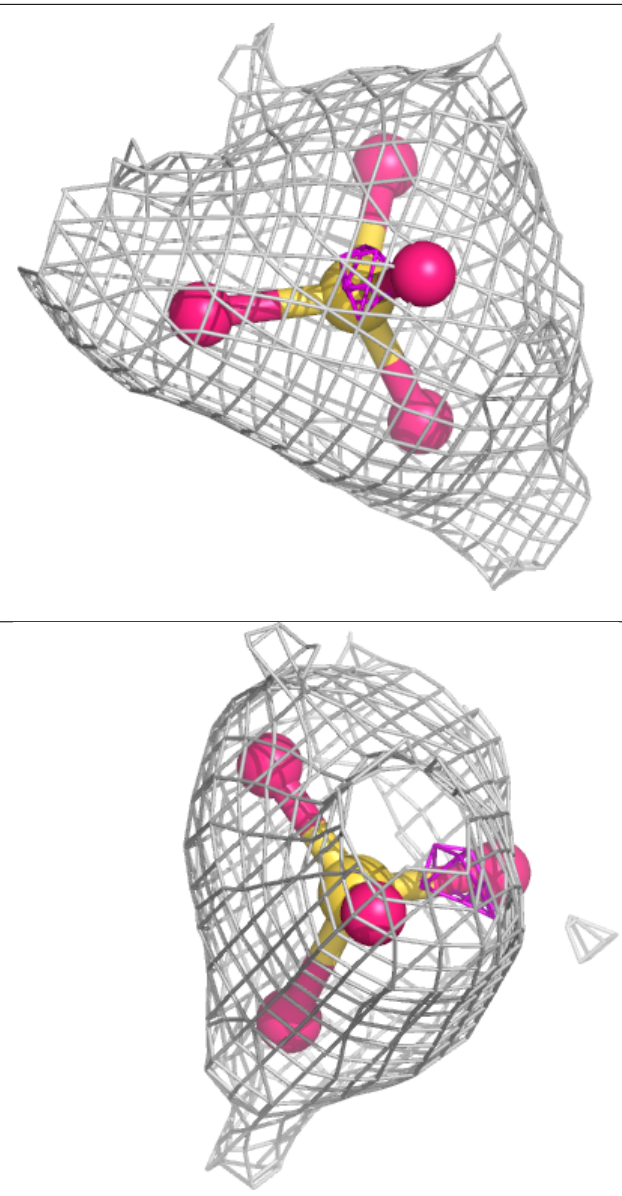
Electron density around SO4 A 1306:

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



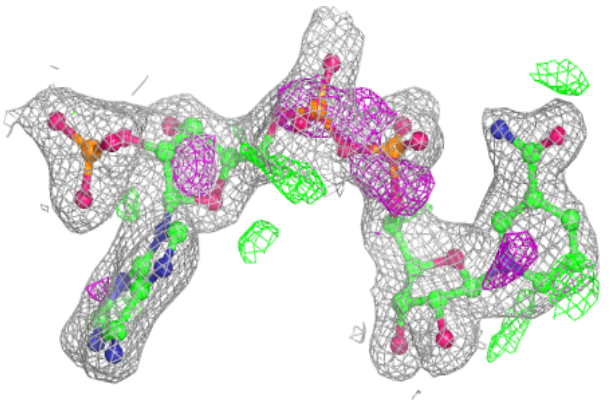
Electron density around SO4 B 1310:

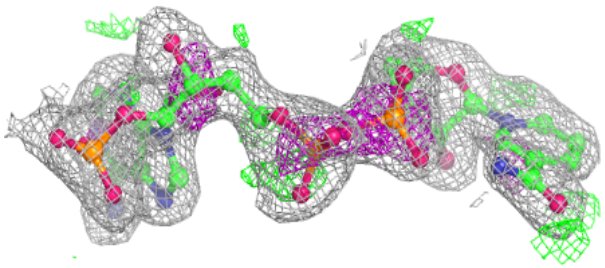
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

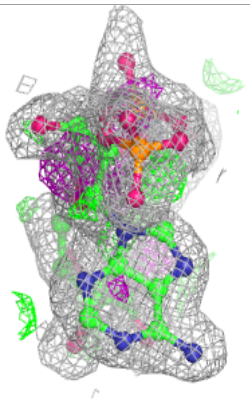


Electron density around NAP B 1301:

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

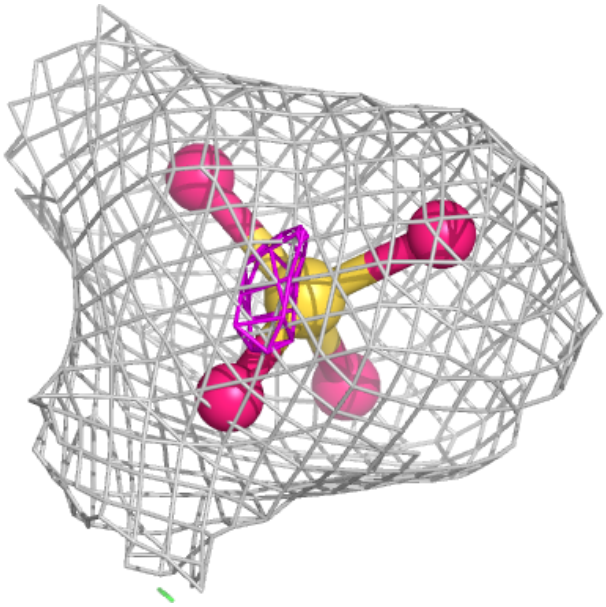


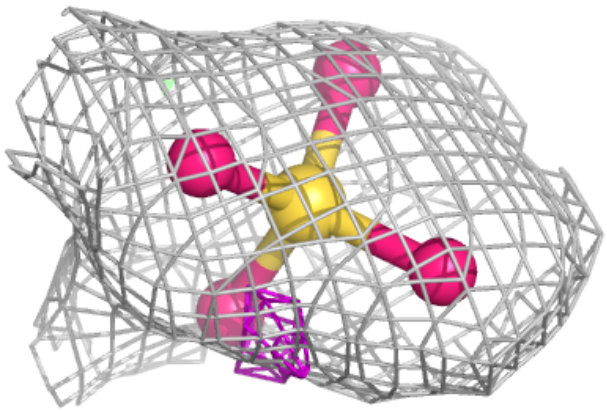


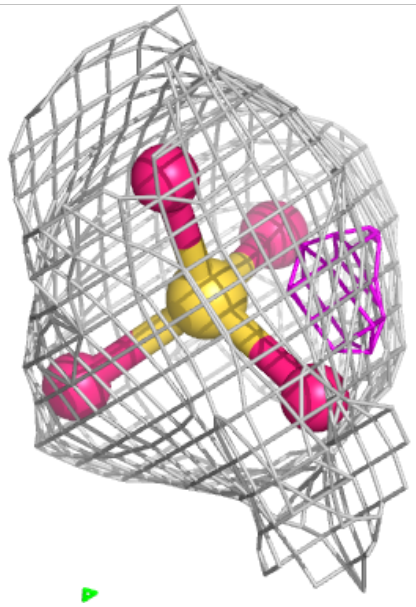


Electron density around SO4 A 1304:

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

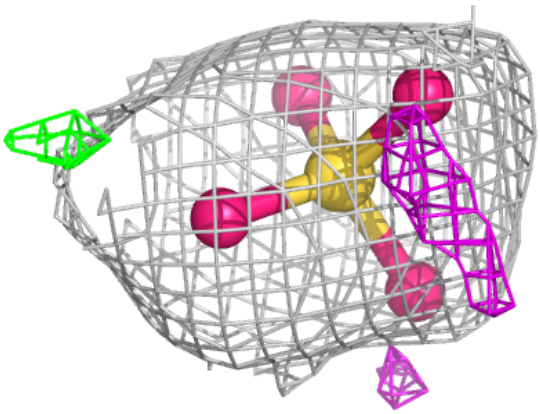


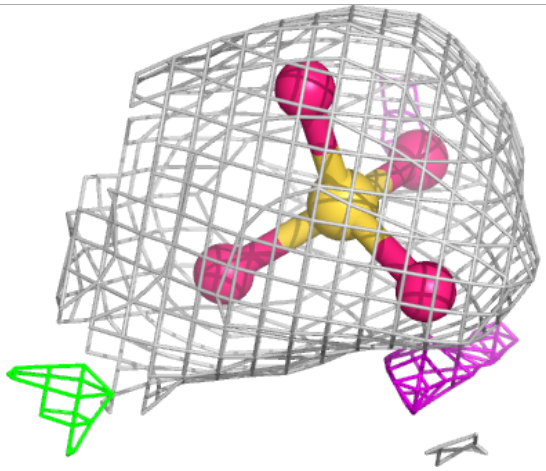


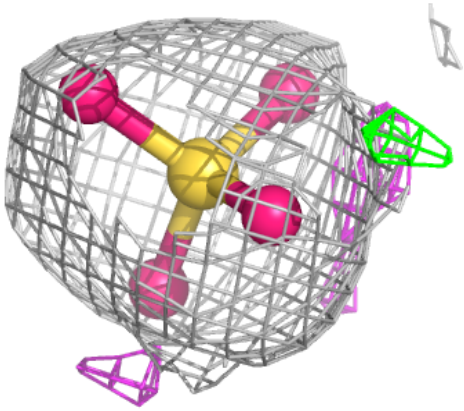


Electron density around SO4 B 1304:

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

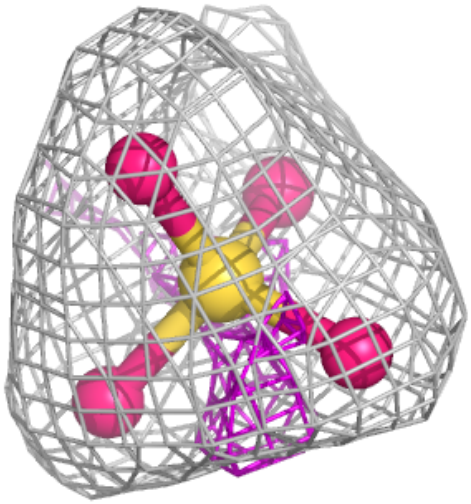


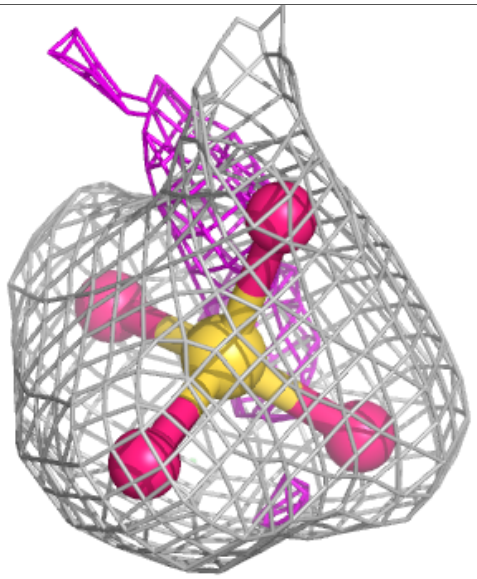


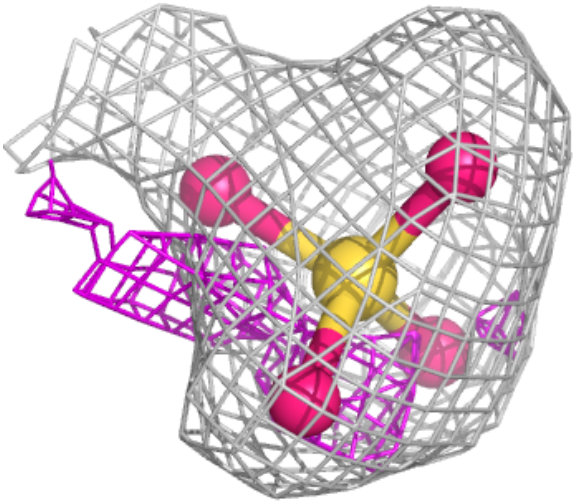


Electron density around SO4 B 1306:

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

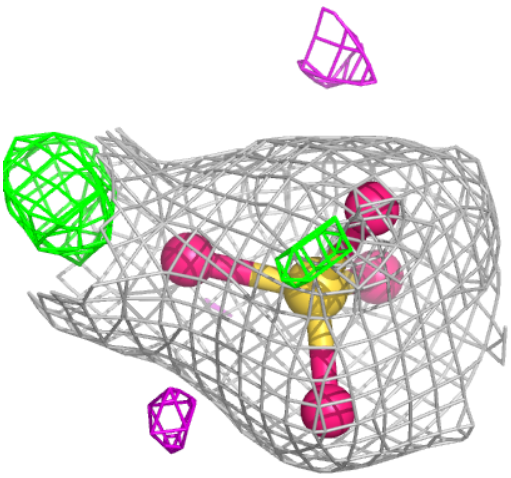


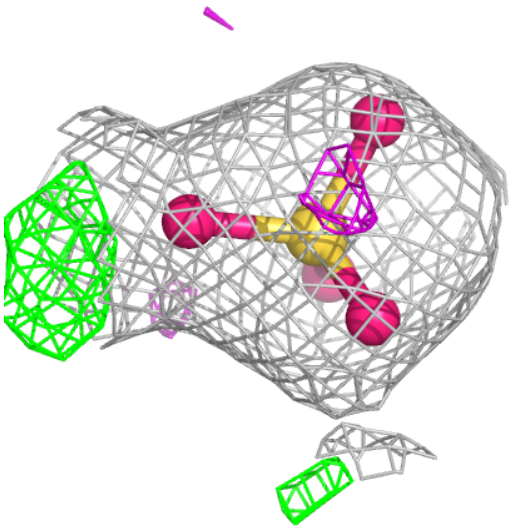


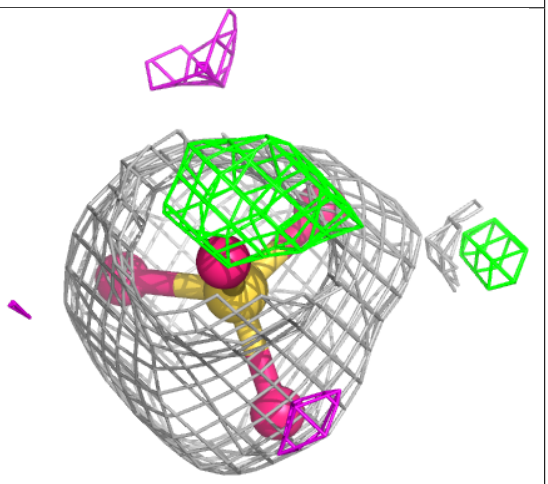


Electron density around SO4 A 1303:

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

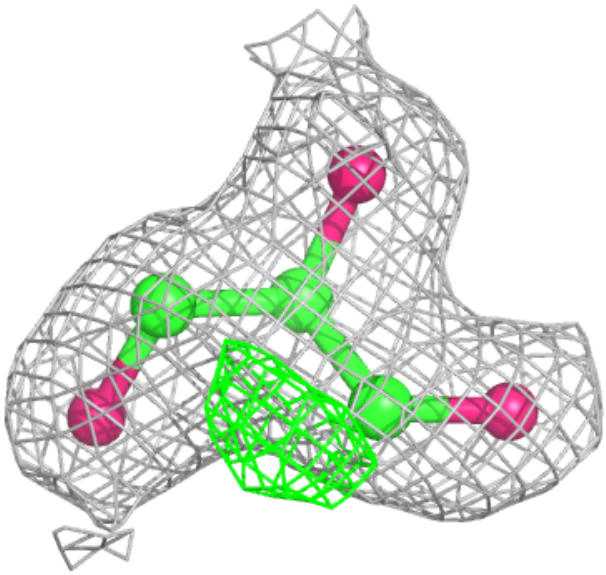


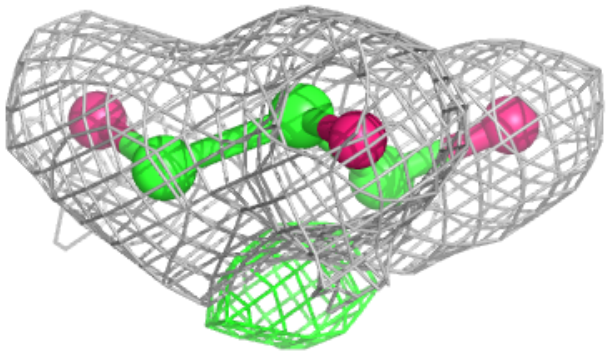


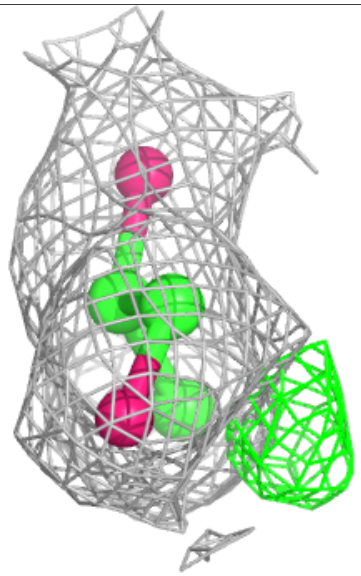


Electron density around GOL B 1302:

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

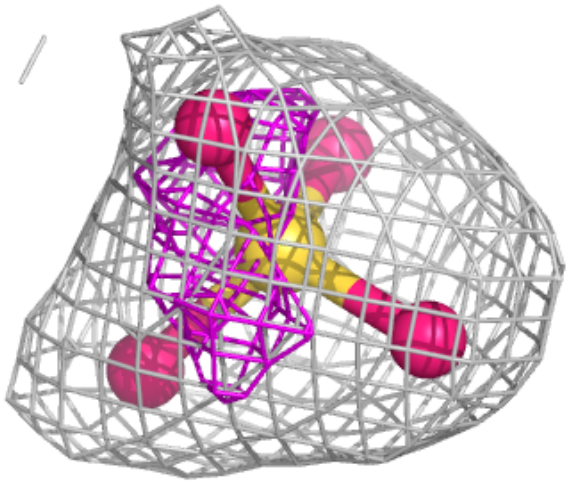


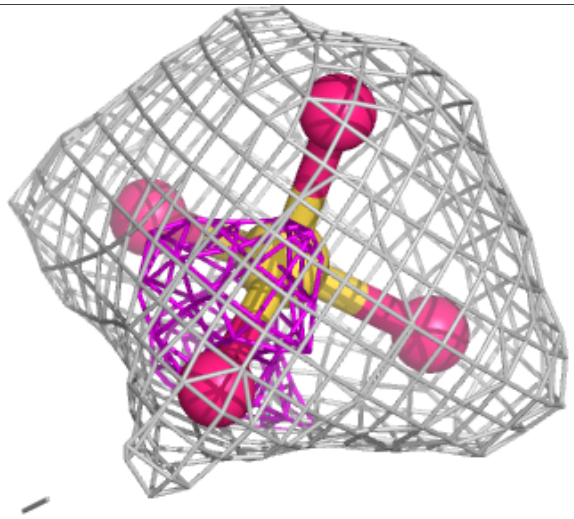


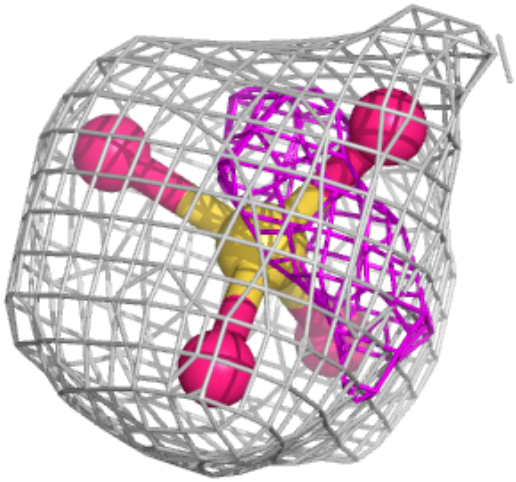


Electron density around SO4 A 1305:

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

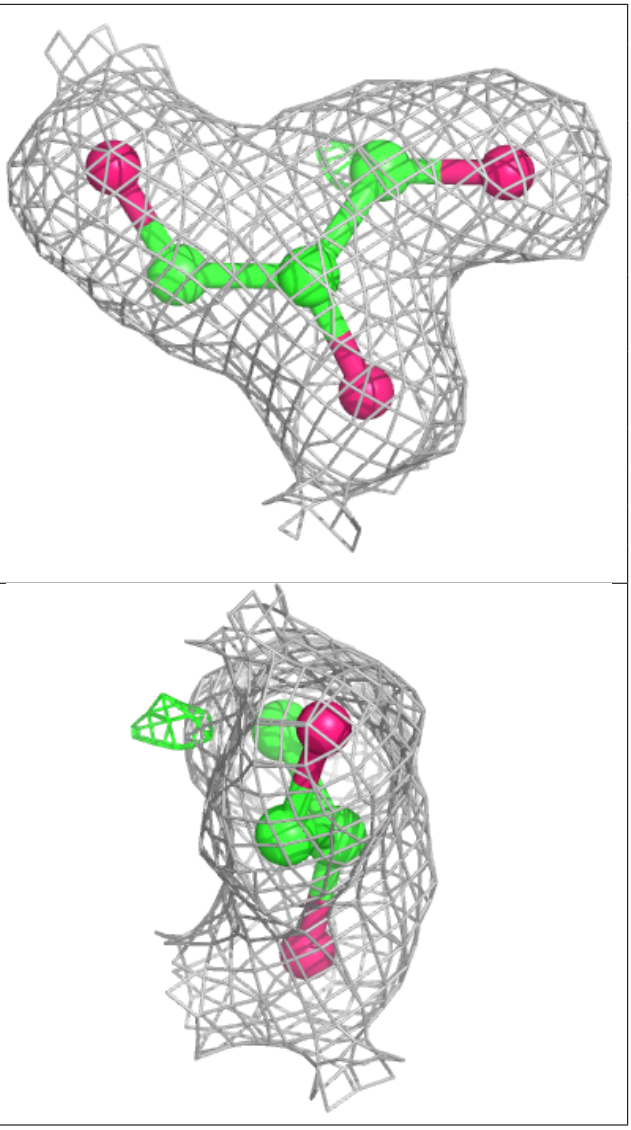






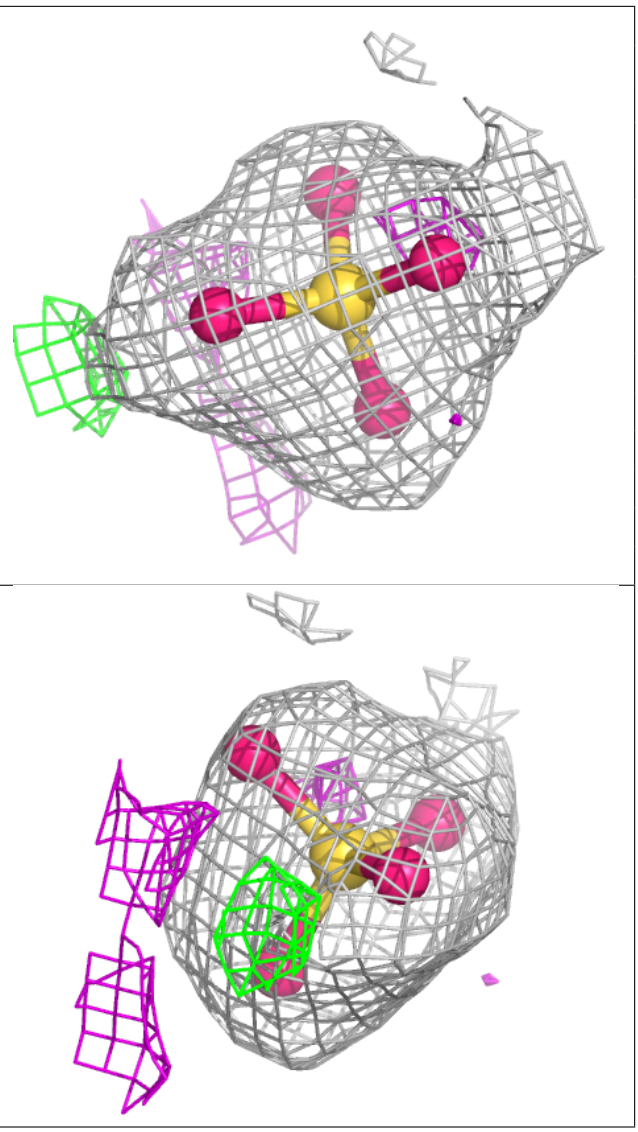
Electron density around GOL A 1302:

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



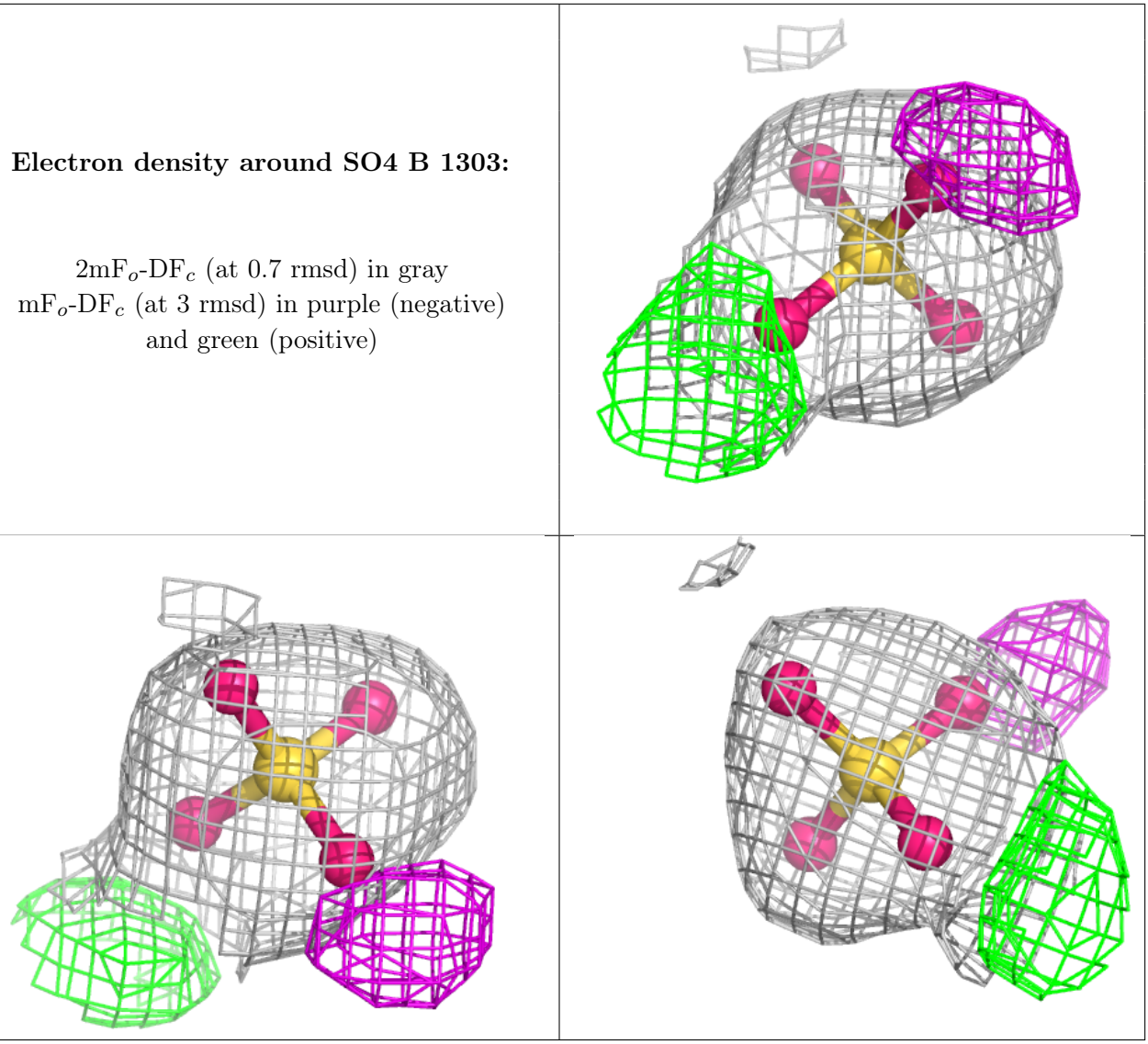
Electron density around SO4 B 1305:

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



Electron density around SO4 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)



6.5 Other polymers (i)

There are no such residues in this entry.