wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 10:51 PM EDT

PDB ID	:	6VVT
Title	:	Crystal structure of a Mycobacterium smegmatis transcription initiation complex with Rifampicin-resistant RNA polymerase and antibiotic Sorangicin
Authors	:	Lilic, M.; Darst, S.A.; Campbell, E.A.
Deposited on	:	2020-02-18
Resolution	:	2.90 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (1)) were used in the production of this report:

MolProbity	:	FAILED
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 23757 atoms, of which 10 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 RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	J	84	Total	C	N	O	S	0	0	0
			672	421	122	127	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	222	Total	C	N	O	S	0	0	0
			1641	1040	277	321	3			
2	B	225	Total	C	N	O	S	0	0	0
			1616	1018	283	313	2			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	883	Total	C	N	O	S	0	0	0
			6474	4060	1130	1255	29			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	447	LEU	SER	variant	UNP P60281

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	1200	Total	C	N	O	S	0	0	0
			9053	5669	1623	1722	39			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	82	Total	C	N	O	0	0	0
			613	388	106	119			

- Molecule 6 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	303	Total	C	N	O	S	0	0	0
			2393	1501	433	452	7			

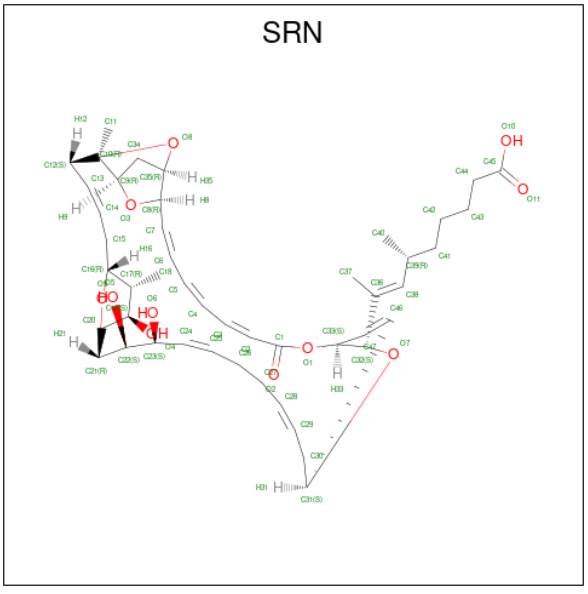
- Molecule 7 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	O	31	Total	C	N	O	P	0	0	0
			635	306	114	185	30			

- Molecule 8 is a DNA chain called DNA (26-MER).

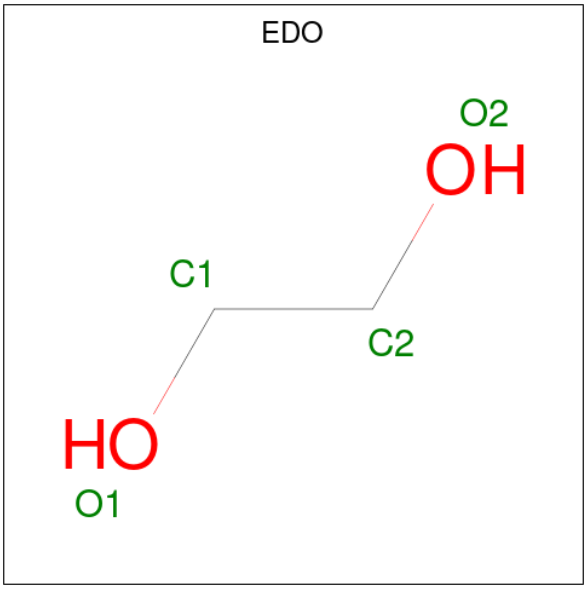
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	P	26	Total	C	N	O	P	0	0	0
			526	254	94	153	25			

- Molecule 9 is SORANGICIN A (three-letter code: SRN) (formula: $C_{47}H_{66}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			58	47	11		

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).

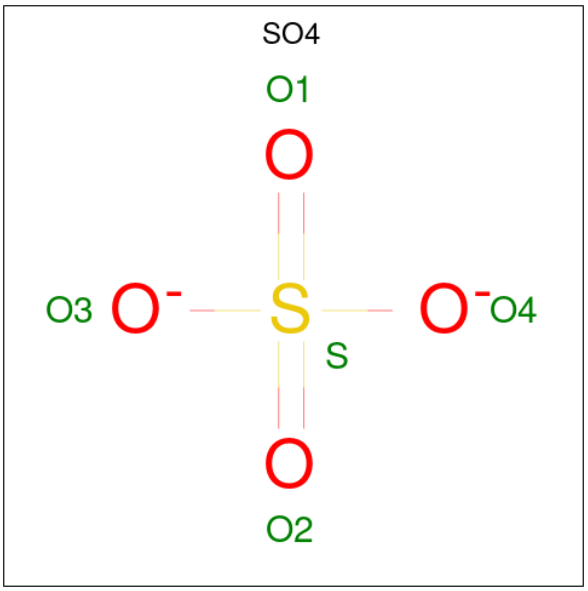


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

- Molecule 12 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	D	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0
12	F	1	Total O S 5 4 1	0	0

- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	J	1	Total O 1 1	0	0
13	B	1	Total O 1 1	0	0
13	C	2	Total H O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	D	8	Total H O 10 2 8	0	0
13	F	1	Total O 1 1	0	0
13	O	1	Total O 1 1	0	0
13	P	1	Total O 1 1	0	0

MolProbity and EDS failed to run properly - this section is therefore empty.

3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	129.22Å 162.21Å 136.29Å 90.00° 111.36° 90.00°	Depositor
Resolution (Å)	49.75 – 2.90	Depositor
% Data completeness (in resolution range)	82.6 (49.75-2.90)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.99 (at 2.91Å)	Xtriage
Refinement program	PHENIX v0	Depositor
R, R_{free}	0.240 , 0.275	Depositor
Wilson B-factor (Å^2)	101.7	Xtriage
Anisotropy	0.176	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	23757	wwPDB-VP
Average B, all atoms (Å^2)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

4 Model quality

4.1 Standard geometry

MolProbity failed to run properly - this section is therefore empty.

4.2 Too-close contacts

MolProbity failed to run properly - this section is therefore empty.

4.3 Torsion angles

4.3.1 Protein backbone

MolProbity failed to run properly - this section is therefore empty.

4.3.2 Protein sidechains

MolProbity failed to run properly - this section is therefore empty.

4.3.3 RNA

MolProbity failed to run properly - this section is therefore empty.

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
12	SO4	D	2007	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	F	502	-	4,4,4	0.14	0	6,6,6	0.05	0
9	SRN	C	1201	-	60,62,62	5.11	31 (51%)	62,84,84	1.60	11 (17%)
12	SO4	F	501	-	4,4,4	0.13	0	6,6,6	0.09	0
12	SO4	D	2003	-	4,4,4	0.13	0	6,6,6	0.09	0
10	EDO	C	1202	-	3,3,3	0.45	0	2,2,2	0.31	0
12	SO4	D	2004	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	F	504	-	4,4,4	0.13	0	6,6,6	0.05	0
12	SO4	D	2005	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	D	2006	-	4,4,4	0.14	0	6,6,6	0.05	0
12	SO4	F	503	-	4,4,4	0.14	0	6,6,6	0.06	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
10	EDO	C	1202	-	-	0/1/1/1	-
9	SRN	C	1201	-	-	8/52/105/105	0/4/5/5

The worst 5 of 31 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1201	SRN	O3-C8	19.93	1.80	1.44
9	C	1201	SRN	O3-C9	16.27	1.81	1.45
9	C	1201	SRN	C34-C9	-11.11	1.28	1.52
9	C	1201	SRN	C3-C2	9.61	1.59	1.34
9	C	1201	SRN	C34-C35	-8.87	1.33	1.52

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	C	1201	SRN	O9-C21-C20	4.37	114.47	109.94
9	C	1201	SRN	C8-C7-C6	-4.01	117.75	125.61
9	C	1201	SRN	C6-C5-C4	-3.30	117.46	124.81
9	C	1201	SRN	C9-C34-C35	3.17	112.89	103.73
9	C	1201	SRN	C37-C36-C32	2.84	120.58	115.68

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

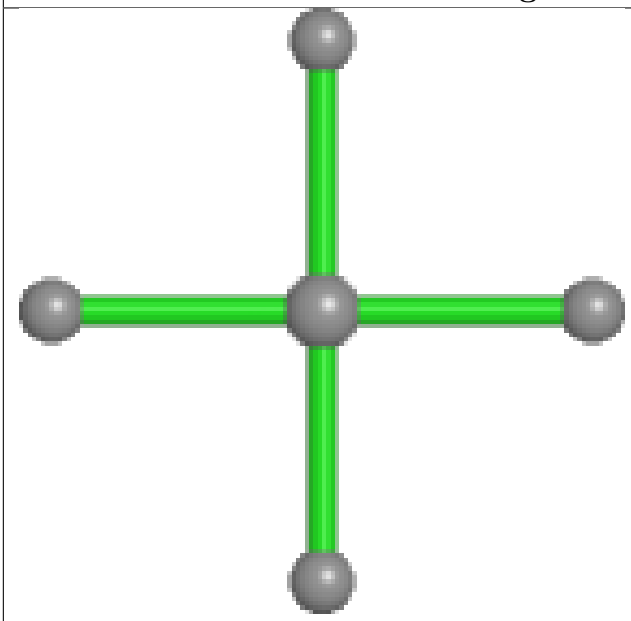
Mol	Chain	Res	Type	Atoms
9	C	1201	SRN	C25-C26-C27-C28
9	C	1201	SRN	C14-C15-C16-O9
9	C	1201	SRN	C42-C43-C44-C45
9	C	1201	SRN	C39-C41-C42-C43
9	C	1201	SRN	C14-C15-C16-C17

There are no ring outliers.

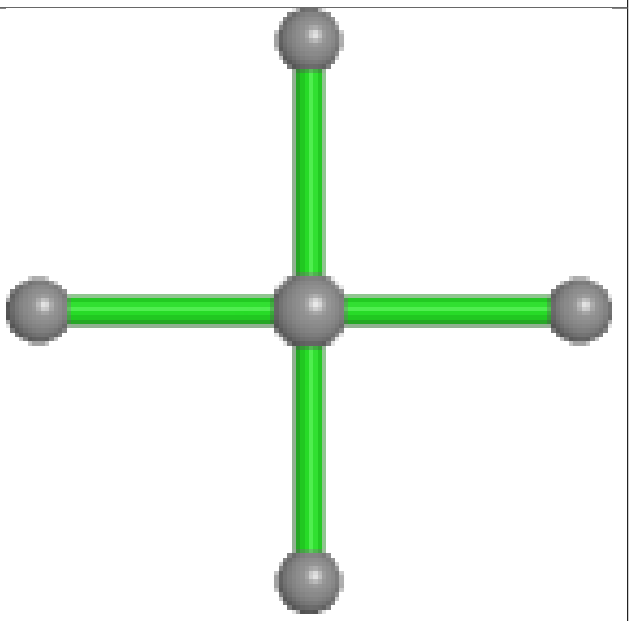
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

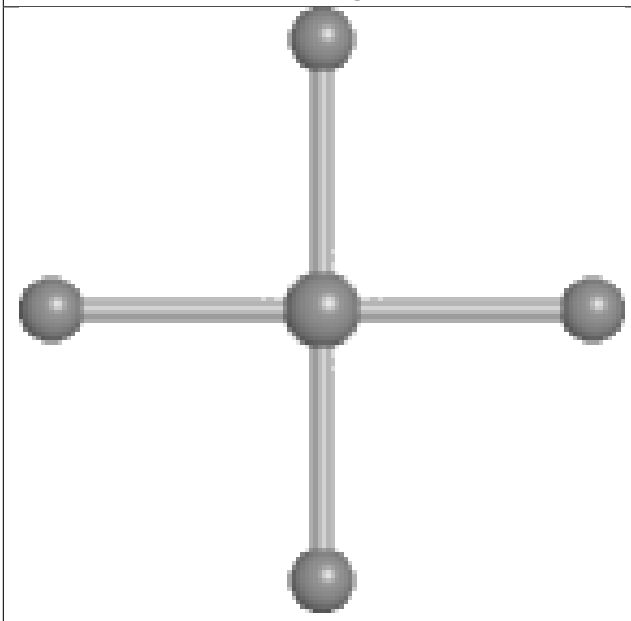
Ligand SO4 D 2007



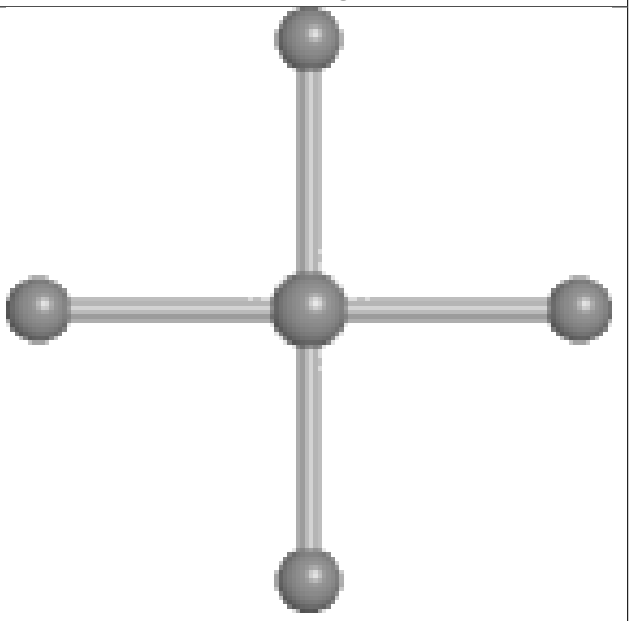
Bond lengths



Bond angles

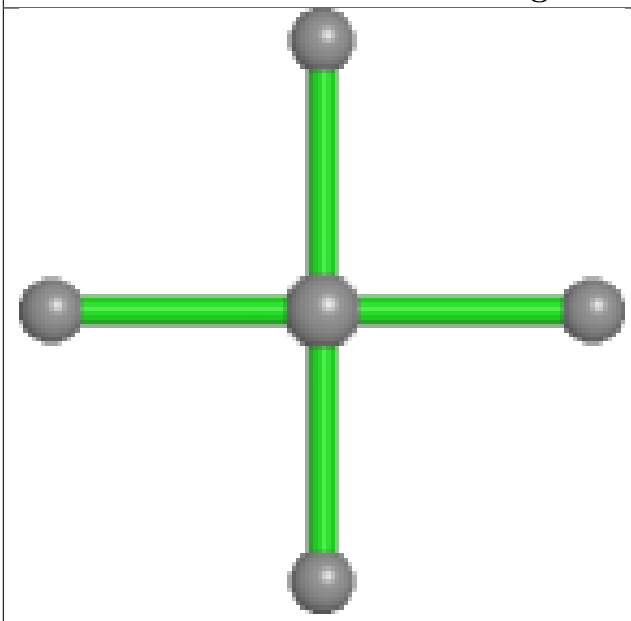


Torsions



Rings

Ligand SO4 F 502



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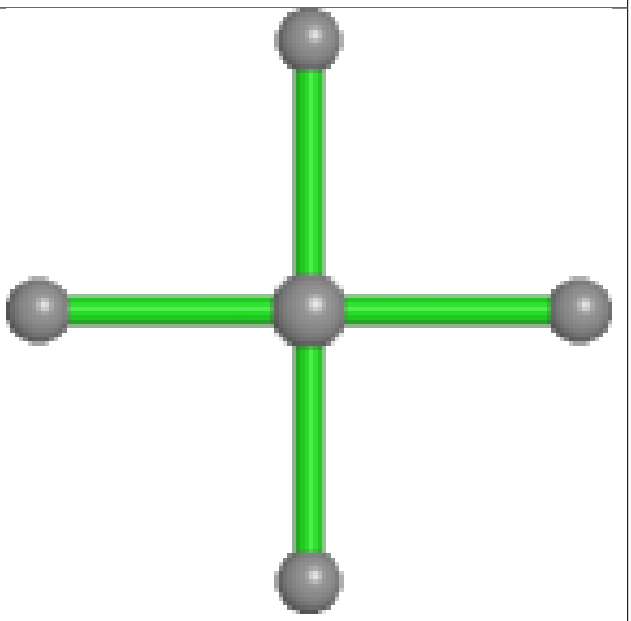
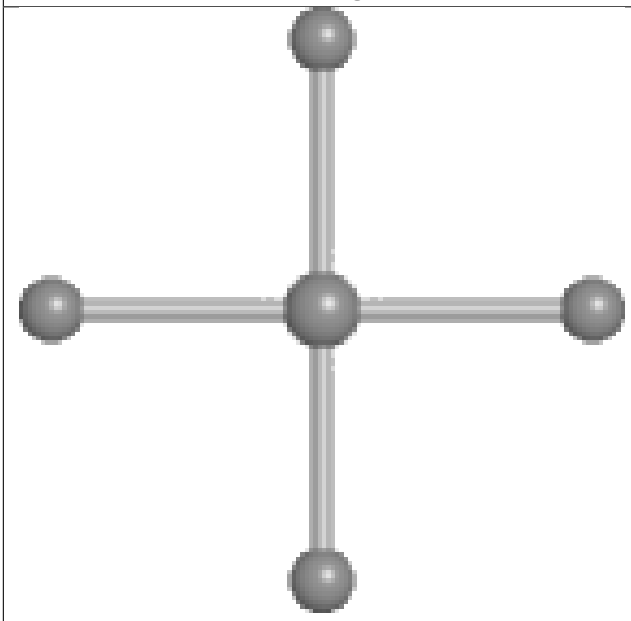
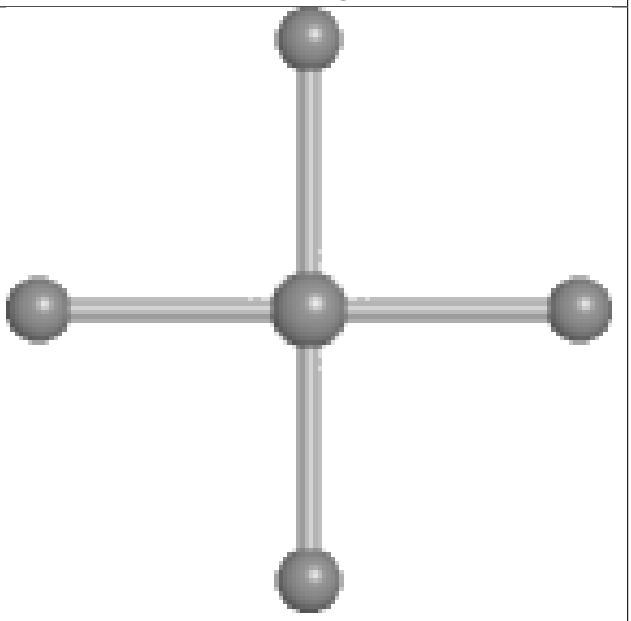


Bond angles

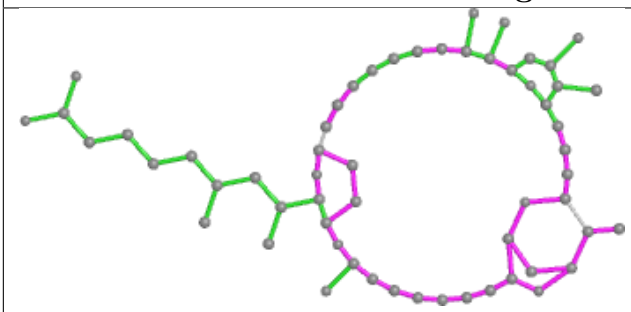


Torsions

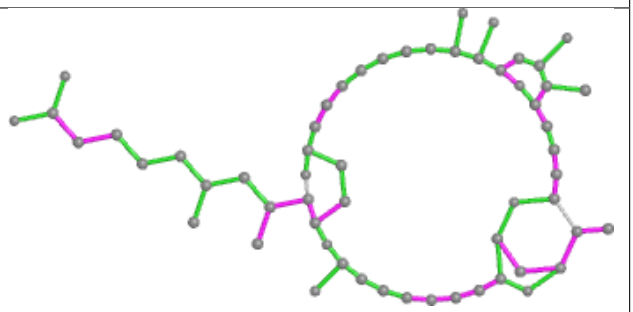


Rings

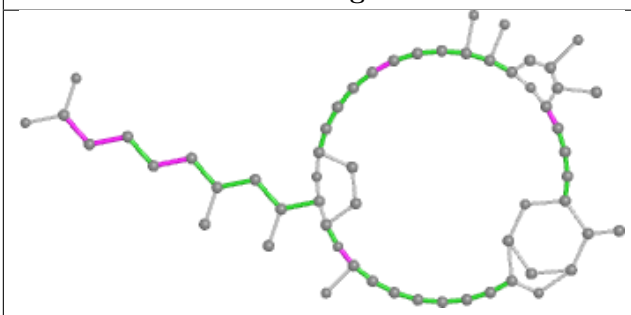
Ligand SRN C 1201



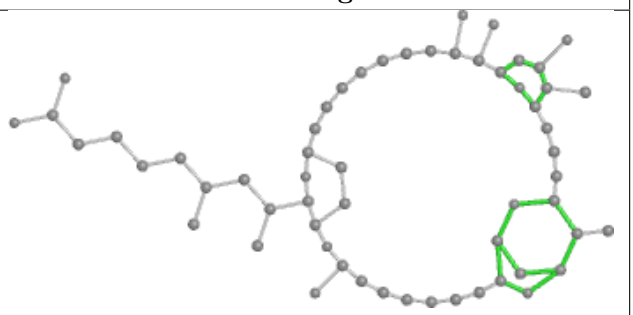
Bond lengths



Bond angles

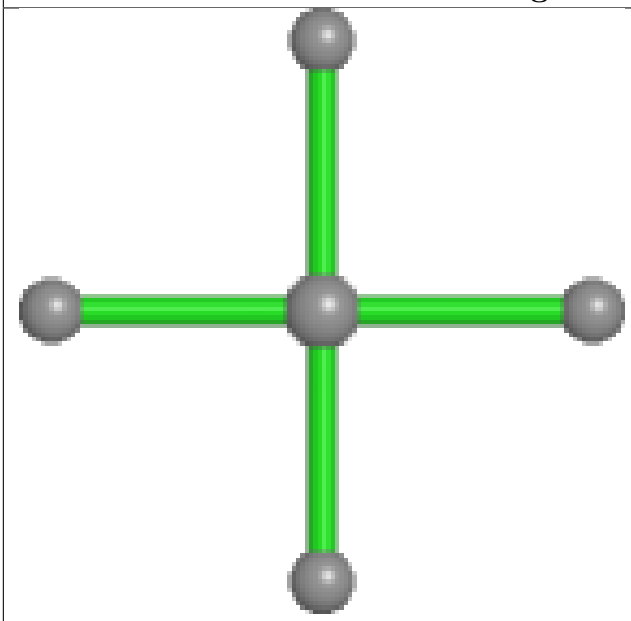


Torsions

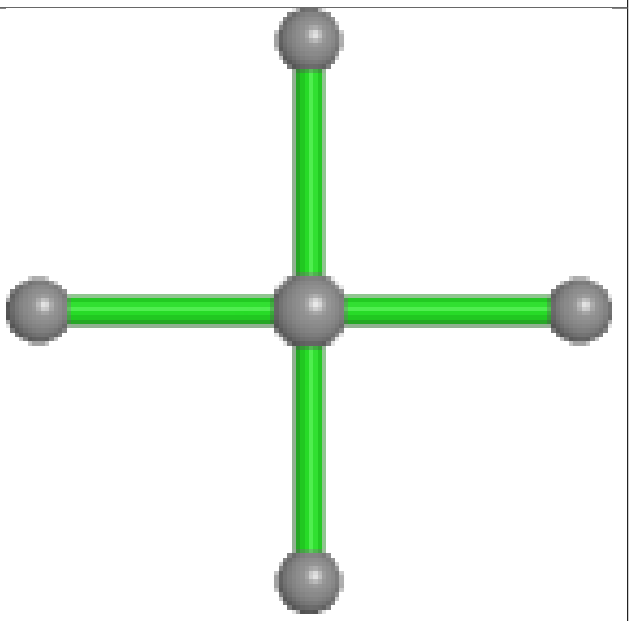


Rings

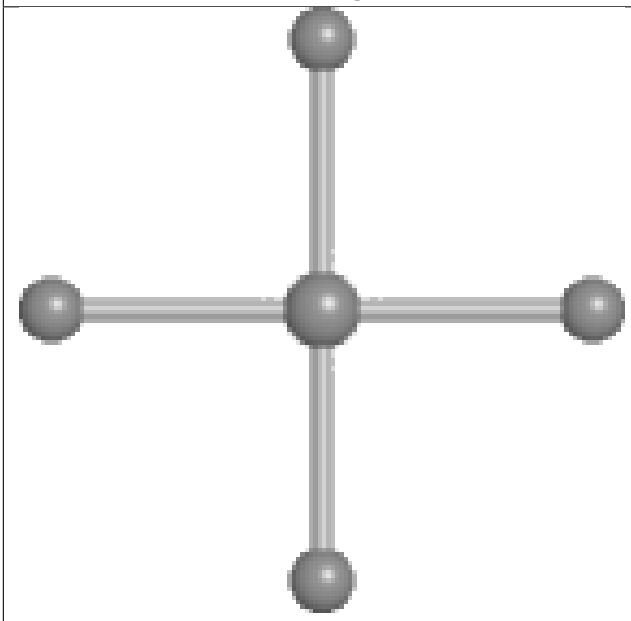
Ligand SO4 F 501



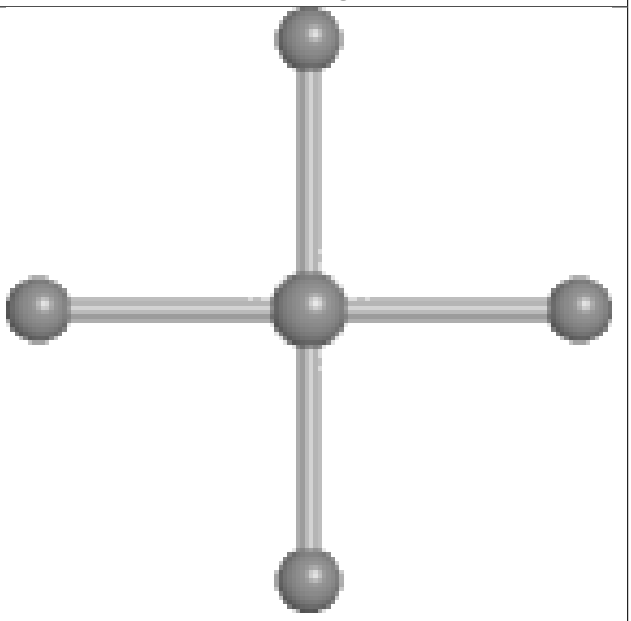
Bond lengths



Bond angles

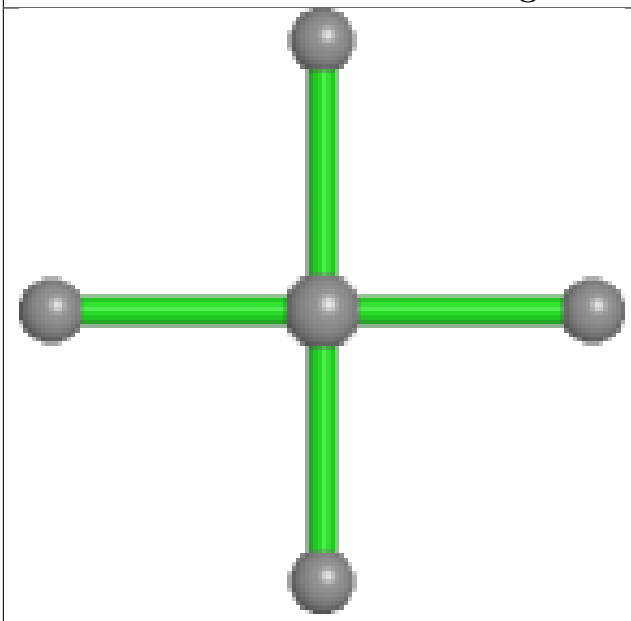


Torsions

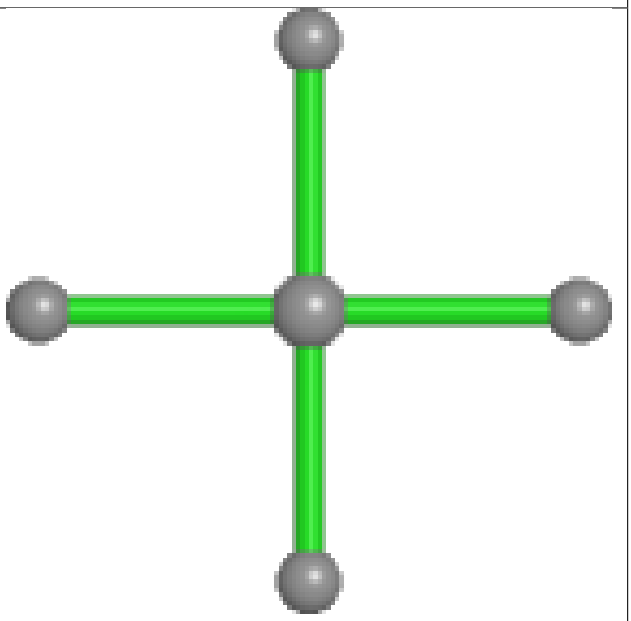


Rings

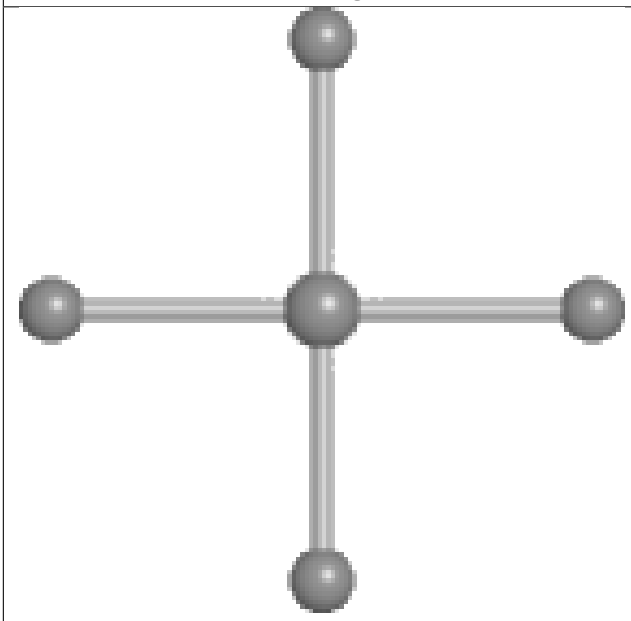
Ligand SO4 D 2003



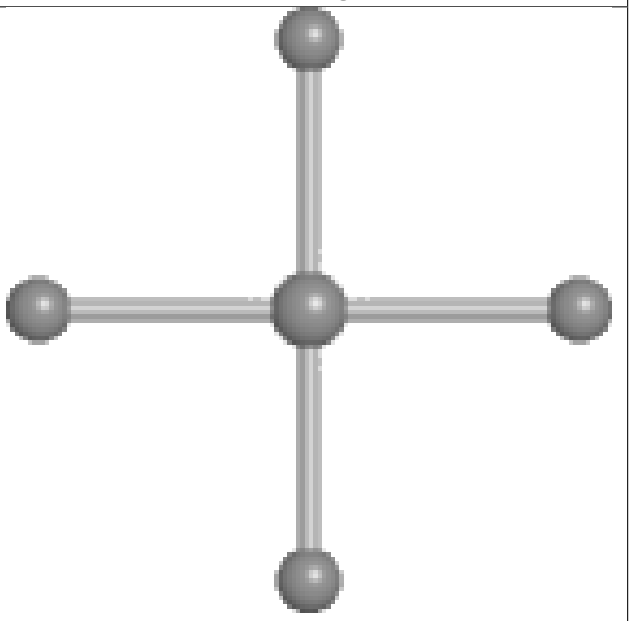
Bond lengths



Bond angles

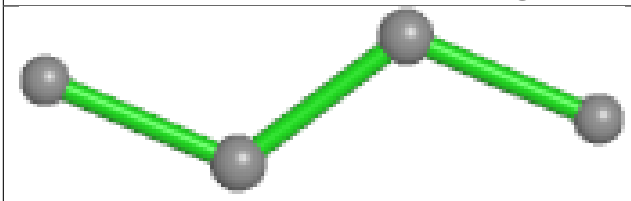


Torsions

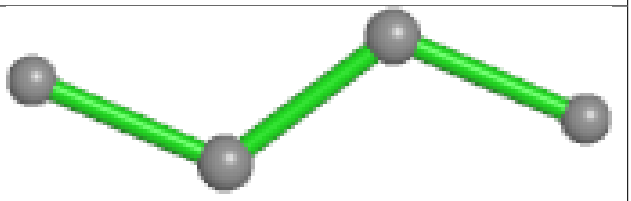


Rings

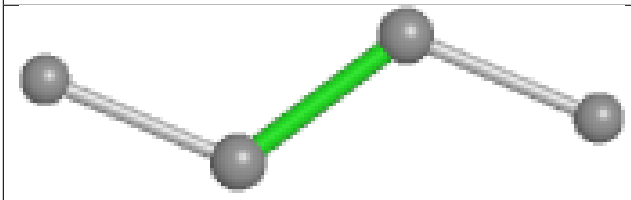
Ligand EDO C 1202



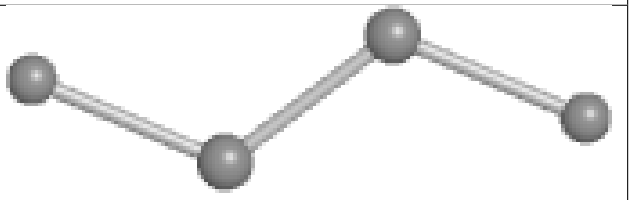
Bond lengths



Bond angles

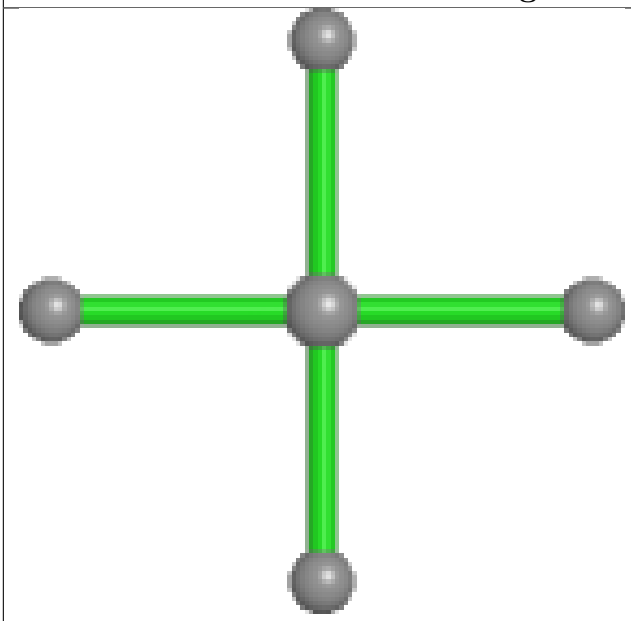


Torsions

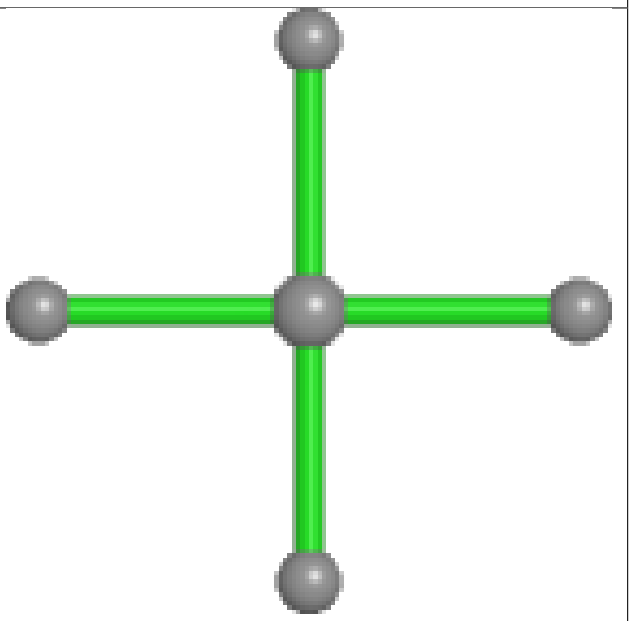


Rings

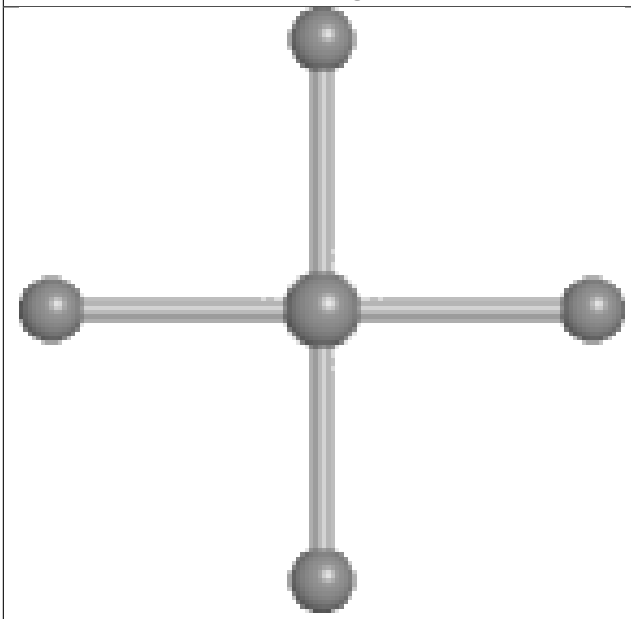
Ligand SO4 D 2004



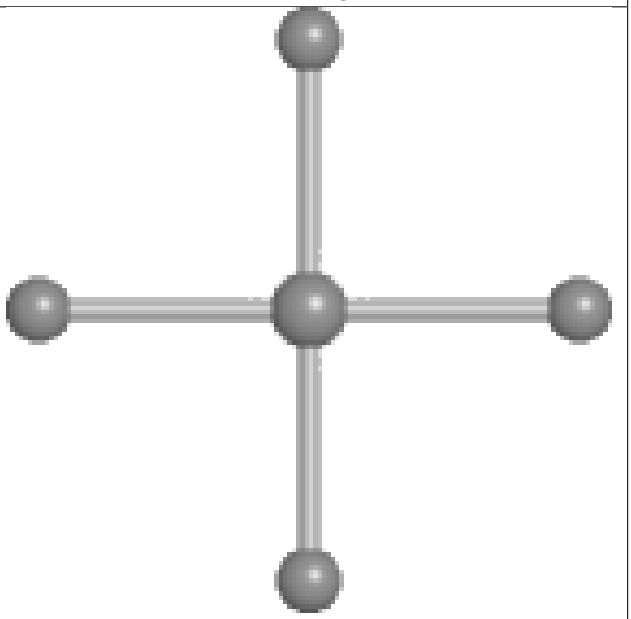
Bond lengths



Bond angles

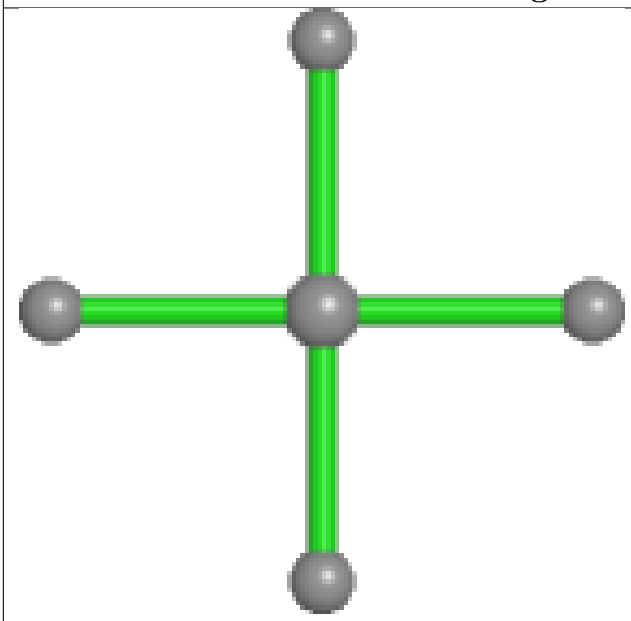


Torsions

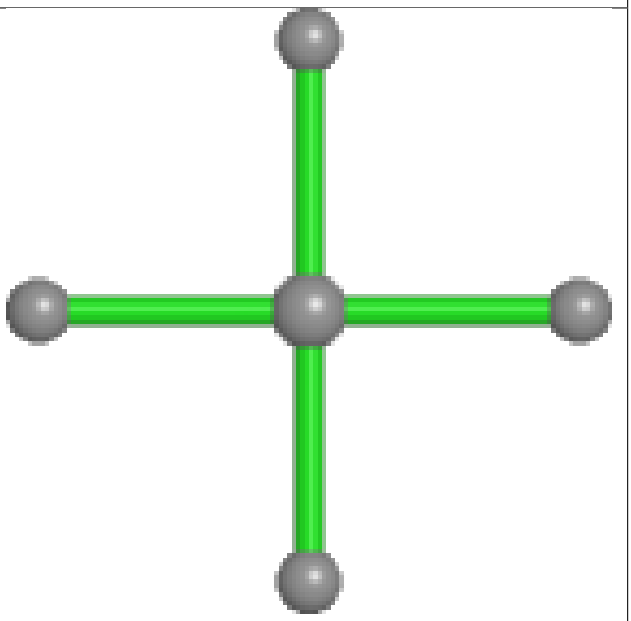


Rings

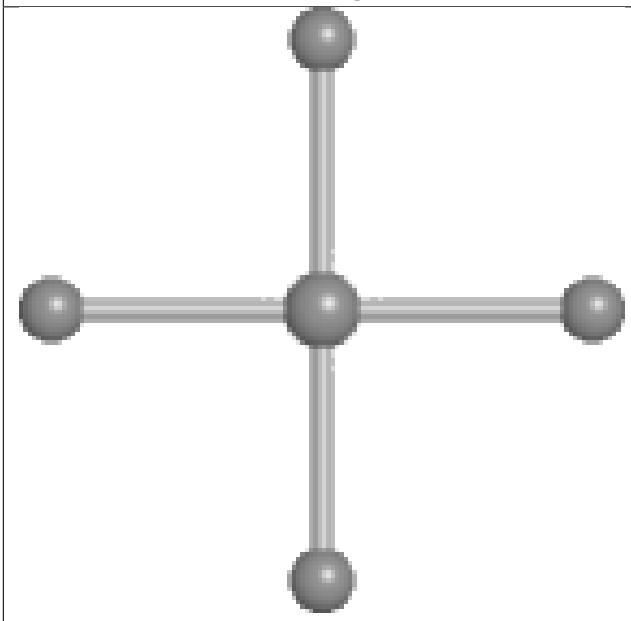
Ligand SO4 F 504



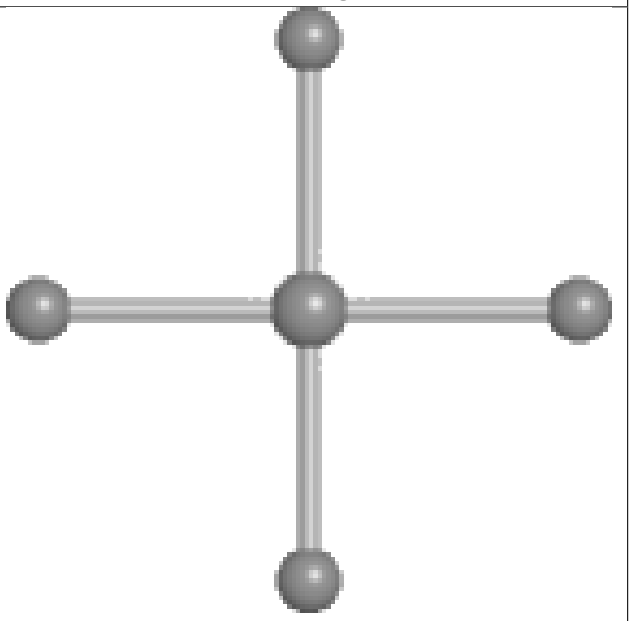
Bond lengths



Bond angles

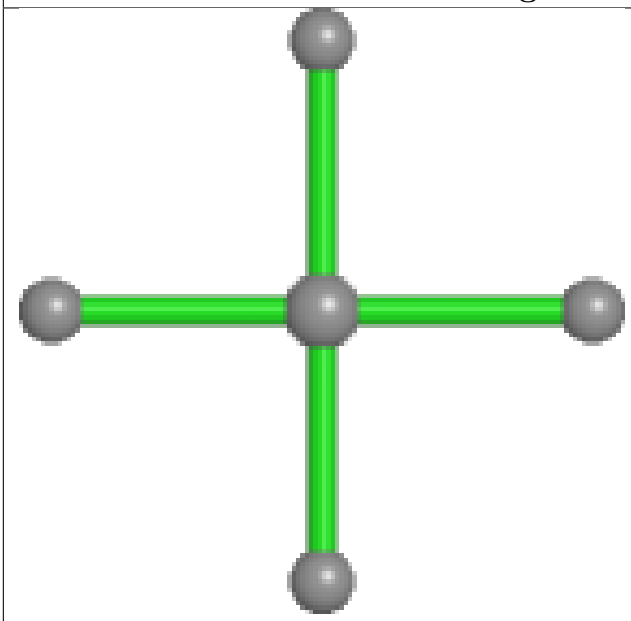


Torsions

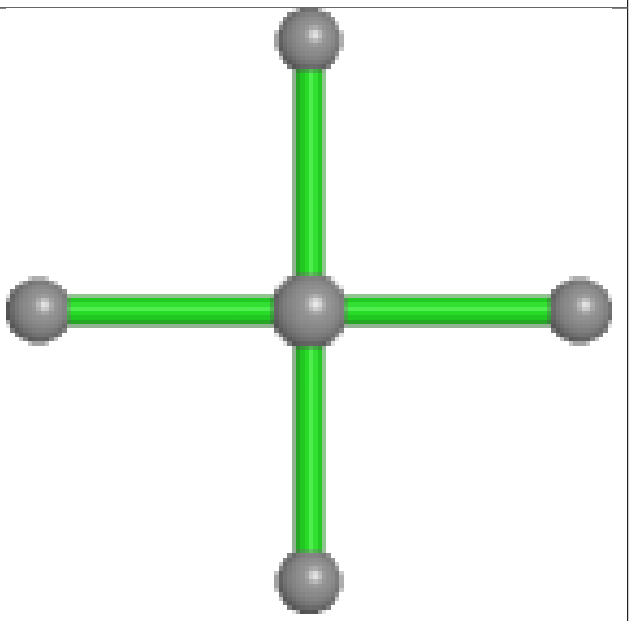


Rings

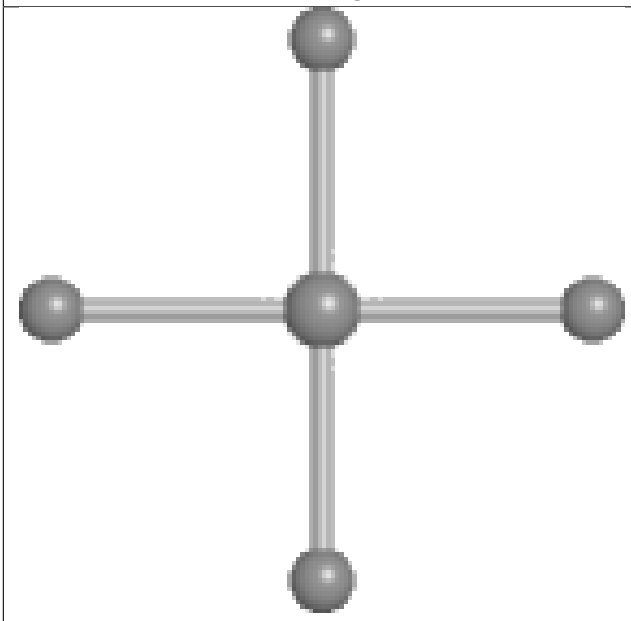
Ligand SO4 D 2005



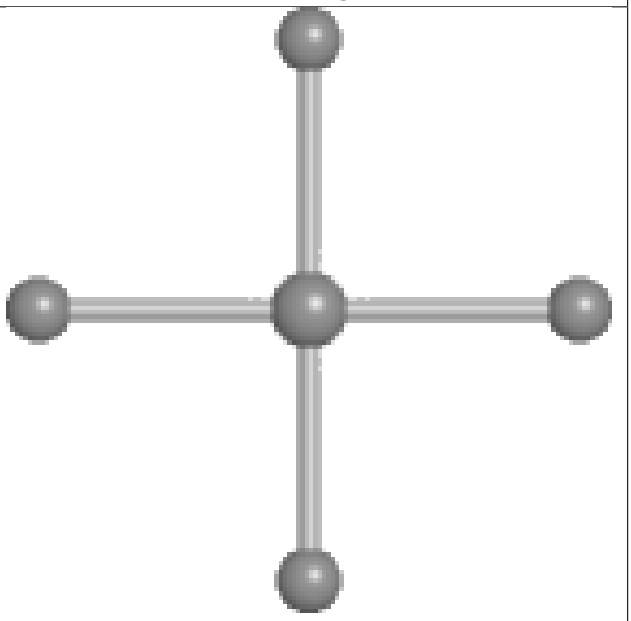
Bond lengths



Bond angles

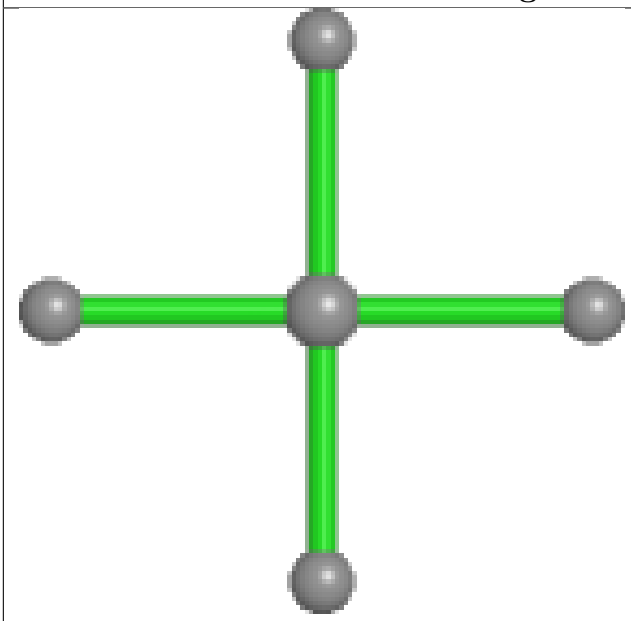


Torsions

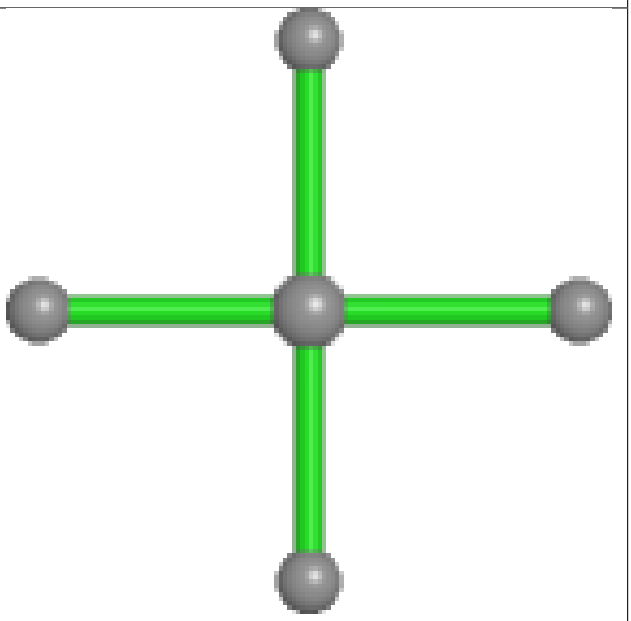


Rings

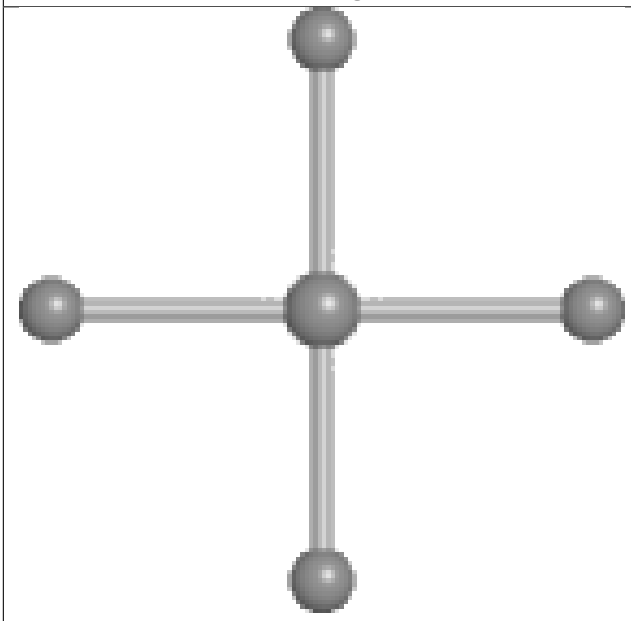
Ligand SO4 D 2006



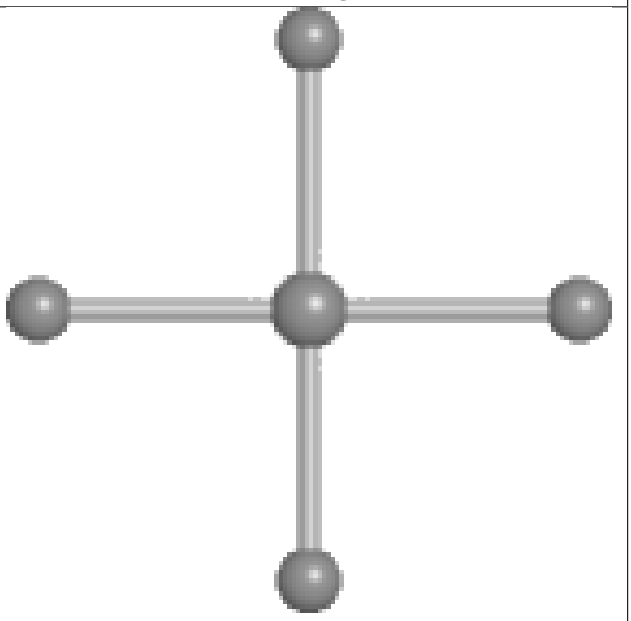
Bond lengths



Bond angles

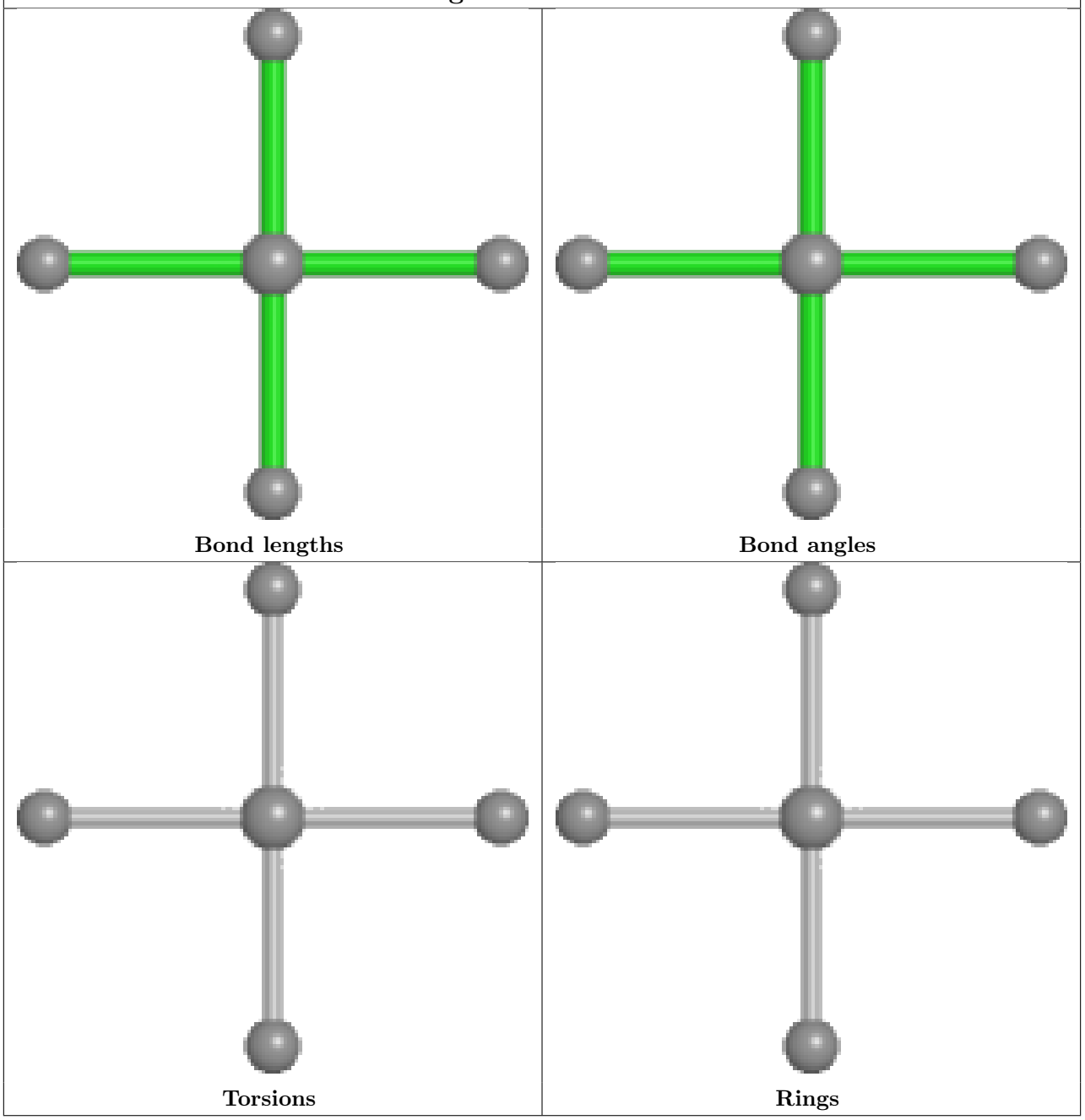


Torsions



Rings

Ligand SO4 F 503



4.7 Other polymers (i)

There are no such residues in this entry.

4.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

5 Fit of model and data

5.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

5.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

5.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

5.4 Ligands

EDS failed to run properly - this section is therefore empty.

5.5 Other polymers

EDS failed to run properly - this section is therefore empty.