Full wwPDB X-ray Structure Validation Report (i)

Nov 21, 2023 – 03:20 PM JST

PDB ID	:	7VG9
Title	:	Crystal structure of phosphotransbutyrylase from Clostridium acetobutylicum
Authors	:	Kim, S.; Kim, K.-J.
Deposited on	:	2021-09-15
Resolution	:	2.91 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:

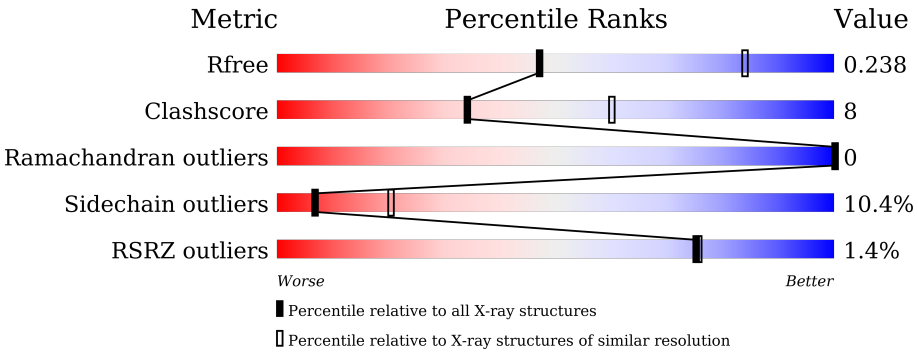
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.91 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	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	321	2% 69% 22% • 6%
1	B	321	2% 74% 18% • 7%
1	C	321	% 76% 17% • 5%
1	D	321	% 74% 17% • 7%
1	E	321	% 75% 17% • 6%
1	F	321	% 69% 22% • 6%

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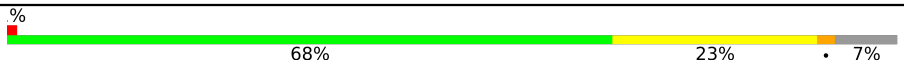
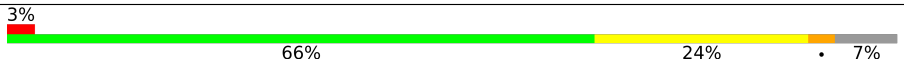
Mol	Chain	Length	Quality of chain
1	G	321	
1	H	321	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	F	401	-	-	X	-
2	SO4	F	404	-	-	X	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18432 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 Phosphate butyryltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	0	0
			2253	1424	380	434	15			
1	B	300	Total	C	N	O	S	0	0	0
			2243	1418	378	432	15			
1	C	306	Total	C	N	O	S	0	0	0
			2288	1445	389	439	15			
1	D	300	Total	C	N	O	S	0	0	0
			2243	1418	378	432	15			
1	E	301	Total	C	N	O	S	0	0	0
			2253	1424	380	434	15			
1	F	303	Total	C	N	O	S	0	0	0
			2269	1433	384	437	15			
1	G	300	Total	C	N	O	S	0	0	0
			2243	1418	378	432	15			
1	H	300	Total	C	N	O	S	0	0	0
			2243	1418	378	432	15			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
A	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
A	-17	SER	-	expression tag	UNP A0A7Y9ABB0
A	-16	SER	-	expression tag	UNP A0A7Y9ABB0
A	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
A	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
A	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
A	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
A	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
A	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
A	-9	SER	-	expression tag	UNP A0A7Y9ABB0
A	-8	SER	-	expression tag	UNP A0A7Y9ABB0
A	-7	GLY	-	expression tag	UNP A0A7Y9ABB0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
A	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
A	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
A	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
A	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
A	-1	SER	-	expression tag	UNP A0A7Y9ABB0
A	0	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
B	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
B	-17	SER	-	expression tag	UNP A0A7Y9ABB0
B	-16	SER	-	expression tag	UNP A0A7Y9ABB0
B	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
B	-9	SER	-	expression tag	UNP A0A7Y9ABB0
B	-8	SER	-	expression tag	UNP A0A7Y9ABB0
B	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
B	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
B	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
B	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
B	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
B	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
B	-1	SER	-	expression tag	UNP A0A7Y9ABB0
B	0	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
C	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
C	-17	SER	-	expression tag	UNP A0A7Y9ABB0
C	-16	SER	-	expression tag	UNP A0A7Y9ABB0
C	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
C	-9	SER	-	expression tag	UNP A0A7Y9ABB0
C	-8	SER	-	expression tag	UNP A0A7Y9ABB0
C	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
C	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
C	-5	VAL	-	expression tag	UNP A0A7Y9ABB0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
C	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
C	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
C	-1	SER	-	expression tag	UNP A0A7Y9ABB0
C	0	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
D	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
D	-17	SER	-	expression tag	UNP A0A7Y9ABB0
D	-16	SER	-	expression tag	UNP A0A7Y9ABB0
D	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
D	-9	SER	-	expression tag	UNP A0A7Y9ABB0
D	-8	SER	-	expression tag	UNP A0A7Y9ABB0
D	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
D	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
D	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
D	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
D	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
D	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
D	-1	SER	-	expression tag	UNP A0A7Y9ABB0
D	0	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
E	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
E	-17	SER	-	expression tag	UNP A0A7Y9ABB0
E	-16	SER	-	expression tag	UNP A0A7Y9ABB0
E	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
E	-9	SER	-	expression tag	UNP A0A7Y9ABB0
E	-8	SER	-	expression tag	UNP A0A7Y9ABB0
E	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
E	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
E	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
E	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
E	-3	ARG	-	expression tag	UNP A0A7Y9ABB0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
E	-1	SER	-	expression tag	UNP A0A7Y9ABB0
E	0	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
F	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
F	-17	SER	-	expression tag	UNP A0A7Y9ABB0
F	-16	SER	-	expression tag	UNP A0A7Y9ABB0
F	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
F	-9	SER	-	expression tag	UNP A0A7Y9ABB0
F	-8	SER	-	expression tag	UNP A0A7Y9ABB0
F	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
F	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
F	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
F	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
F	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
F	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
F	-1	SER	-	expression tag	UNP A0A7Y9ABB0
F	0	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
G	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
G	-17	SER	-	expression tag	UNP A0A7Y9ABB0
G	-16	SER	-	expression tag	UNP A0A7Y9ABB0
G	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
G	-9	SER	-	expression tag	UNP A0A7Y9ABB0
G	-8	SER	-	expression tag	UNP A0A7Y9ABB0
G	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
G	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
G	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
G	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
G	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
G	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
G	-1	SER	-	expression tag	UNP A0A7Y9ABB0

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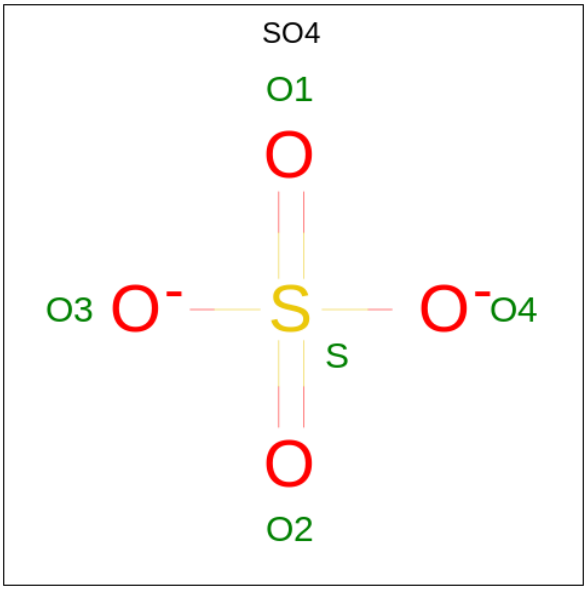
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-19	MET	-	initiating methionine	UNP A0A7Y9ABB0
H	-18	GLY	-	expression tag	UNP A0A7Y9ABB0
H	-17	SER	-	expression tag	UNP A0A7Y9ABB0
H	-16	SER	-	expression tag	UNP A0A7Y9ABB0
H	-15	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-14	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-13	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-12	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-11	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-10	HIS	-	expression tag	UNP A0A7Y9ABB0
H	-9	SER	-	expression tag	UNP A0A7Y9ABB0
H	-8	SER	-	expression tag	UNP A0A7Y9ABB0
H	-7	GLY	-	expression tag	UNP A0A7Y9ABB0
H	-6	LEU	-	expression tag	UNP A0A7Y9ABB0
H	-5	VAL	-	expression tag	UNP A0A7Y9ABB0
H	-4	PRO	-	expression tag	UNP A0A7Y9ABB0
H	-3	ARG	-	expression tag	UNP A0A7Y9ABB0
H	-2	GLY	-	expression tag	UNP A0A7Y9ABB0
H	-1	SER	-	expression tag	UNP A0A7Y9ABB0
H	0	HIS	-	expression tag	UNP A0A7Y9ABB0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	E	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0

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

- Molecule 3 is water.

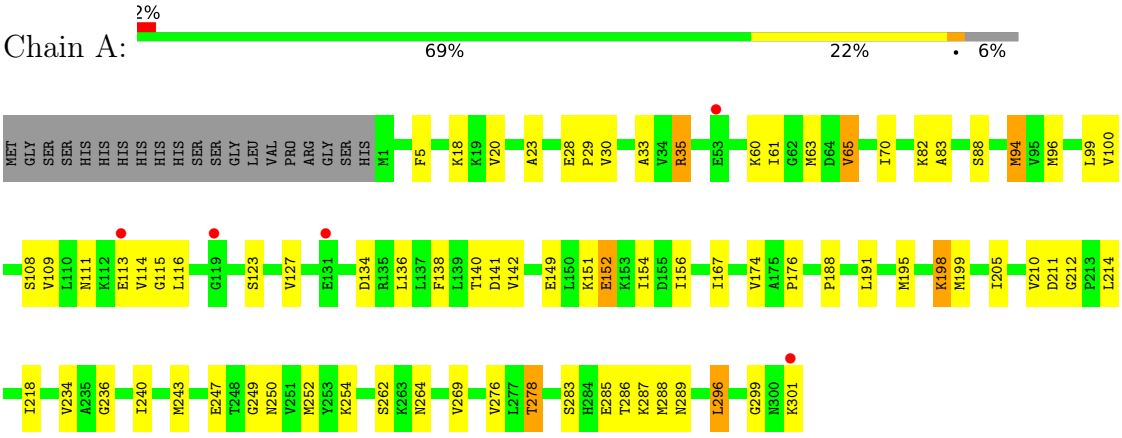
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	12	Total O 12 12	0	0
3	B	15	Total O 15 15	0	0
3	C	27	Total O 27 27	0	0
3	D	20	Total O 20 20	0	0
3	E	28	Total O 28 28	0	0
3	F	23	Total O 23 23	0	0
3	G	15	Total O 15 15	0	0
3	H	17	Total O 17 17	0	0

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.

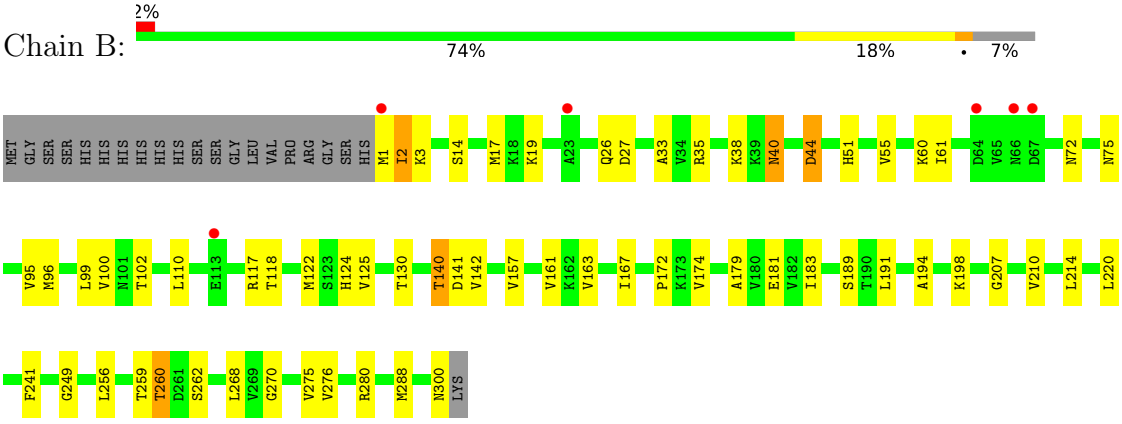
• Molecule 1: Phosphate butyryltransferase

Chain A:



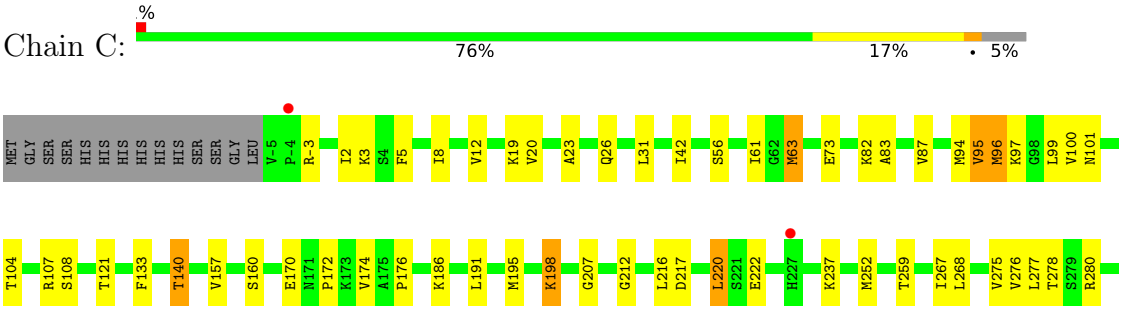
• Molecule 1: Phosphate butyryltransferase

Chain B:



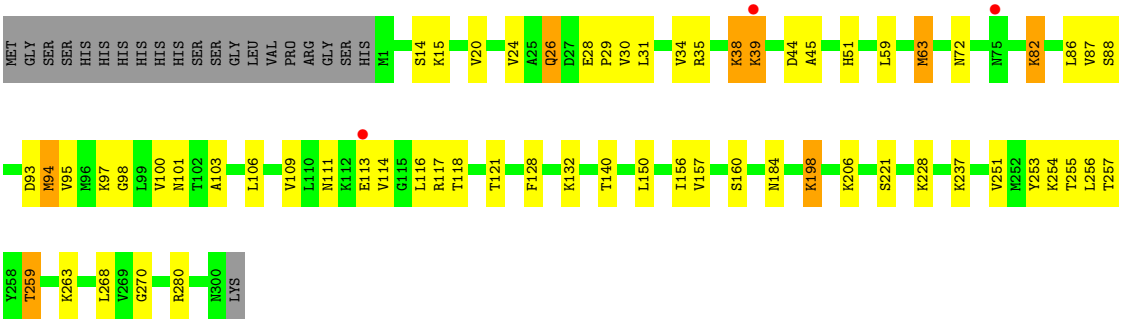
• Molecule 1: Phosphate butyryltransferase

Chain C:



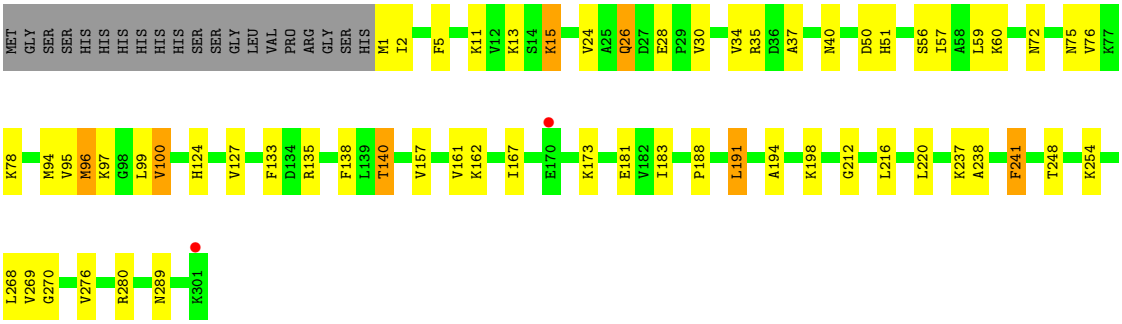
• Molecule 1: Phosphate butyryltransferase

Chain D:



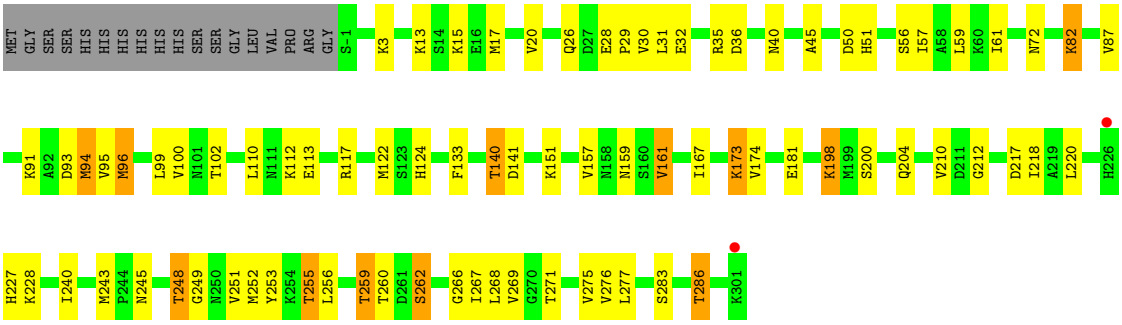
• Molecule 1: Phosphate butyryltransferase

Chain E:



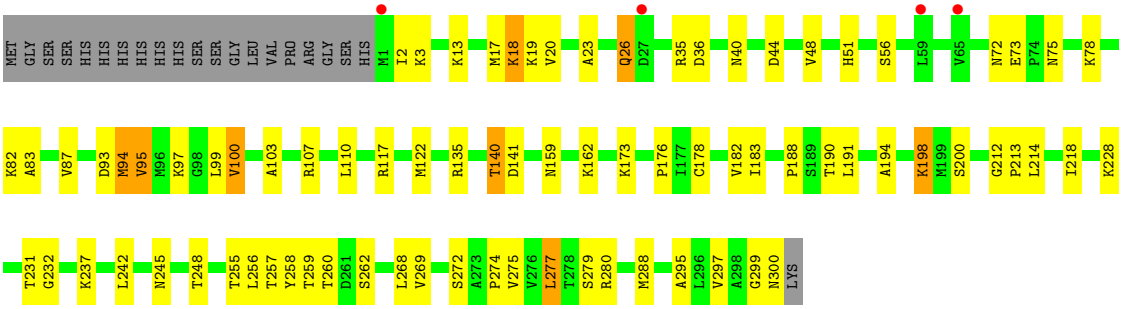
• Molecule 1: Phosphate butyryltransferase

Chain F:

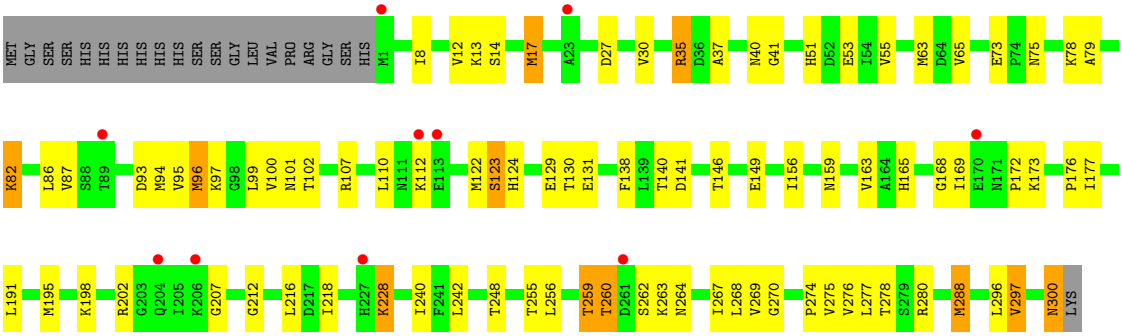


• Molecule 1: Phosphate butyryltransferase

Chain G:



• Molecule 1: Phosphate butyryltransferase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.69Å 143.41Å 113.28Å 90.00° 93.99° 90.00°	Depositor
Resolution (Å)	30.29 – 2.91 30.27 – 2.91	Depositor EDS
% Data completeness (in resolution range)	95.2 (30.29-2.91) 95.3 (30.27-2.91)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.53 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.172 , 0.239 0.177 , 0.238	Depositor DCC
R_{free} test set	3125 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	40.2	Xtriage
Anisotropy	0.582	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18432	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.71	0/2279	0.90	0/3077
1	B	0.71	0/2269	0.91	0/3066
1	C	0.72	0/2316	0.92	0/3130
1	D	0.72	0/2269	0.92	0/3066
1	E	0.72	0/2279	0.91	0/3077
1	F	0.73	0/2296	0.91	0/3100
1	G	0.69	0/2269	0.88	0/3066
1	H	0.71	0/2269	0.89	0/3066
All	All	0.71	0/18246	0.91	0/24648

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	140	THR	Peptide
1	D	140	THR	Peptide

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	2253	0	2356	46	0
1	B	2243	0	2343	29	0
1	C	2288	0	2387	32	0
1	D	2243	0	2343	31	0
1	E	2253	0	2356	33	0
1	F	2269	0	2368	65	0
1	G	2243	0	2343	46	0
1	H	2243	0	2343	48	0
2	A	30	0	0	0	0
2	B	25	0	0	0	0
2	C	25	0	0	2	0
2	D	15	0	0	0	0
2	E	65	0	0	0	0
2	F	35	0	0	6	0
2	G	20	0	0	1	0
2	H	25	0	0	0	0
3	A	12	0	0	0	0
3	B	15	0	0	0	0
3	C	27	0	0	0	0
3	D	20	0	0	0	0
3	E	28	0	0	0	0
3	F	23	0	0	0	0
3	G	15	0	0	0	0
3	H	17	0	0	0	0
All	All	18432	0	18839	311	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (311) 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:H:255:THR:O	1:H:259:THR:HB	1.74	0.88
1:G:122:MET:SD	1:G:268:LEU:HD13	2.19	0.82
1:G:255:THR:O	1:G:259:THR:HB	1.79	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:THR:HG21	1:B:270:GLY:O	1.80	0.82
1:H:96:MET:HG2	1:H:276:VAL:HB	1.63	0.80
1:F:96:MET:HG2	1:F:276:VAL:HB	1.65	0.78
1:D:30:VAL:O	1:D:34:VAL:HG23	1.86	0.75
1:D:118:THR:HG21	1:D:270:GLY:O	1.87	0.75
1:B:191:LEU:HD22	1:C:195:MET:SD	2.27	0.74
1:D:31:LEU:HB3	1:D:63:MET:HE1	1.70	0.73
1:F:198:LYS:HD3	1:G:212:GLY:O	1.88	0.73
1:F:260:THR:CG2	1:F:262:SER:OG	2.37	0.72
1:F:260:THR:HG22	1:F:262:SER:OG	1.90	0.72
1:F:30:VAL:HG13	1:F:96:MET:CE	2.20	0.71
1:F:30:VAL:HG13	1:F:96:MET:HE1	1.73	0.71
1:B:2:ILE:HG13	1:B:167:ILE:O	1.92	0.70
1:G:159:ASN:HB3	1:G:269:VAL:HG23	1.74	0.69
1:B:174:VAL:HB	1:B:210:VAL:HG22	1.73	0.68
1:C:87:VAL:HG21	1:C:95:VAL:HG22	1.76	0.67
1:E:13:LYS:HE3	1:E:40:ASN:O	1.94	0.67
1:B:181:GLU:OE1	1:B:181:GLU:N	2.22	0.67
1:B:183:ILE:HD11	1:B:194:ALA:HB2	1.76	0.66
1:A:152:GLU:O	1:A:156:ILE:HG13	1.95	0.66
1:F:159:ASN:HB3	1:F:269:VAL:HG23	1.78	0.66
1:G:18:LYS:HB3	1:G:94:MET:HE3	1.78	0.66
1:A:111:ASN:O	1:A:115:GLY:HA3	1.97	0.65
1:H:268:LEU:HB2	1:H:275:VAL:HB	1.78	0.65
1:A:195:MET:SD	1:H:191:LEU:HD22	2.37	0.65
1:F:245:ASN:OD1	1:F:248:THR:HG23	1.96	0.65
1:H:87:VAL:HG21	1:H:95:VAL:HG22	1.79	0.64
1:H:8:ILE:O	1:H:12:VAL:HG23	1.98	0.63
1:A:250:ASN:HD21	1:A:254:LYS:HZ2	1.47	0.63
1:A:250:ASN:HD21	1:A:254:LYS:NZ	1.96	0.63
1:C:20:VAL:HG13	1:C:94:MET:HG3	1.82	0.62
1:F:122:MET:HG3	1:F:271:THR:HG23	1.82	0.61
1:B:172:PRO:HD2	1:B:207:GLY:O	2.01	0.61
1:F:251:VAL:O	1:F:255:THR:HG22	2.00	0.61
1:C:61:ILE:HD11	1:C:63:MET:HE2	1.82	0.60
1:F:51:HIS:H	1:F:72:ASN:HD22	1.48	0.60
1:H:124:HIS:O	1:H:140:THR:HG23	2.01	0.60
1:B:19:LYS:HG3	1:B:44:ASP:HB3	1.85	0.59
1:G:299:GLY:O	1:G:300:ASN:HB2	2.02	0.59
1:D:38:LYS:CE	1:D:44:ASP:OD1	2.51	0.59
1:C:252:MET:HE2	1:D:251:VAL:HG13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:ALA:HA	1:A:83:ALA:HB2	1.85	0.58
1:A:33:ALA:HA	1:A:288:MET:HE3	1.84	0.58
1:F:15:LYS:HA	2:F:404:SO4:O2	2.04	0.58
1:F:124:HIS:O	1:F:140:THR:HG22	2.03	0.57
1:A:154:ILE:HG23	1:A:205:ILE:CD1	2.34	0.57
1:E:11:LYS:O	1:E:15:LYS:HG3	2.04	0.57
1:E:13:LYS:CE	1:E:40:ASN:O	2.52	0.57
1:F:31:LEU:HD12	1:F:57:ILE:CG2	2.35	0.57
1:F:110:LEU:HD21	1:F:122:MET:HE2	1.85	0.57
1:C:216:LEU:HG	1:C:220:LEU:HD21	1.86	0.57
1:H:218:ILE:HD11	1:H:228:LYS:HD2	1.87	0.57
1:B:124:HIS:O	1:B:140:THR:HG23	2.04	0.56
1:C:133:PHE:CZ	1:C:220:LEU:HD12	2.40	0.56
1:D:87:VAL:HG21	1:D:95:VAL:HG22	1.88	0.56
1:E:124:HIS:O	1:E:140:THR:HG23	2.05	0.56
1:C:284:HIS:O	1:C:288:MET:HG2	2.06	0.56
1:E:24:VAL:HG21	1:E:76:VAL:HG13	1.87	0.56
1:B:142:VAL:HG22	1:B:249:GLY:O	2.06	0.56
1:H:165:HIS:O	1:H:168:GLY:N	2.33	0.56
1:A:65:VAL:CG1	1:A:70:ILE:HD11	2.36	0.56
1:F:268:LEU:HB2	1:F:275:VAL:HB	1.88	0.56
1:F:251:VAL:O	1:F:255:THR:CG2	2.55	0.55
1:G:183:ILE:HD11	1:G:194:ALA:HB2	1.88	0.55
1:E:2:ILE:HB	1:E:167:ILE:HG22	1.88	0.55
1:H:82:LYS:O	1:H:86:LEU:HG	2.05	0.55
1:E:30:VAL:HG13	1:E:96:MET:CE	2.37	0.55
1:A:278:THR:HG23	1:A:287:LYS:HE3	1.88	0.55
1:F:15:LYS:CB	2:F:404:SO4:O2	2.55	0.55
1:G:97:LYS:HD3	1:G:100:VAL:O	2.07	0.55
1:G:256:LEU:O	1:G:260:THR:HB	2.07	0.54
1:C:96:MET:CE	1:C:291:ILE:HD11	2.37	0.54
1:D:109:VAL:HG13	1:D:116:LEU:HD12	1.90	0.54
1:F:157:VAL:O	1:F:161:VAL:HG13	2.07	0.54
1:D:38:LYS:HE3	1:D:44:ASP:OD1	2.06	0.54
1:E:51:HIS:HB2	1:E:72:ASN:HB2	1.90	0.54
1:F:255:THR:O	1:F:259:THR:HB	2.07	0.54
1:F:15:LYS:HB3	2:F:404:SO4:O2	2.08	0.53
1:F:217:ASP:N	1:F:217:ASP:OD1	2.41	0.53
1:F:256:LEU:O	1:F:260:THR:HB	2.07	0.53
1:G:190:THR:HB	1:G:213:PRO:HG3	1.90	0.53
1:B:96:MET:HG2	1:B:276:VAL:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:111:ASN:HD22	1:D:114:VAL:H	1.56	0.53
1:H:172:PRO:HD2	1:H:207:GLY:O	2.08	0.53
1:G:274:PRO:HG3	1:G:297:VAL:HG12	1.91	0.53
1:H:163:VAL:CG2	1:H:269:VAL:HG21	2.39	0.53
1:B:110:LEU:HD21	1:B:122:MET:HE3	1.89	0.53
1:F:96:MET:HG2	1:F:276:VAL:CB	2.35	0.53
1:F:198:LYS:HE3	1:F:198:LYS:HA	1.90	0.52
1:G:248:THR:HG22	1:H:248:THR:OG1	2.10	0.52
1:G:18:LYS:HB3	1:G:94:MET:CE	2.39	0.52
1:G:274:PRO:HG3	1:G:297:VAL:CG1	2.39	0.52
1:B:40:ASN:OD1	1:B:40:ASN:N	2.40	0.52
1:B:163:VAL:O	1:B:167:ILE:HD13	2.09	0.52
1:B:241:PHE:CD1	1:B:241:PHE:N	2.78	0.52
1:A:65:VAL:HG12	1:A:70:ILE:HD11	1.92	0.52
1:B:157:VAL:O	1:B:161:VAL:HG13	2.10	0.52
1:G:2:ILE:HD12	1:G:2:ILE:N	2.25	0.52
1:H:110:LEU:HD21	1:H:122:MET:HE3	1.92	0.51
1:H:123:SER:HB3	1:H:159:ASN:HD22	1.74	0.51
1:C:96:MET:HG2	1:C:276:VAL:HB	1.92	0.51
1:F:31:LEU:HD12	1:F:57:ILE:HG21	1.91	0.51
1:H:96:MET:CG	1:H:276:VAL:HB	2.39	0.51
1:E:183:ILE:HD11	1:E:194:ALA:HB2	1.91	0.51
1:F:102:THR:HG23	1:F:277:LEU:HD11	1.92	0.51
1:E:96:MET:HG2	1:E:276:VAL:HB	1.92	0.51
1:E:135:ARG:NH1	1:E:238:ALA:O	2.41	0.51
1:C:252:MET:CE	1:D:251:VAL:HG13	2.40	0.51
1:E:26:GLN:HE22	1:E:50:ASP:H	1.59	0.51
1:F:174:VAL:HG22	1:F:240:ILE:HB	1.93	0.51
1:F:51:HIS:H	1:F:72:ASN:ND2	2.08	0.51
1:H:110:LEU:HD21	1:H:122:MET:CE	2.40	0.51
1:A:33:ALA:CA	1:A:288:MET:HE3	2.41	0.51
1:H:260:THR:HG23	1:H:262:SER:OG	2.11	0.51
1:E:241:PHE:N	1:E:241:PHE:CD1	2.78	0.50
1:G:159:ASN:HB3	1:G:269:VAL:CG2	2.41	0.50
1:F:212:GLY:O	1:G:198:LYS:HD3	2.11	0.50
1:A:176:PRO:HD2	1:A:212:GLY:HA3	1.92	0.50
1:F:30:VAL:HG13	1:F:96:MET:HE3	1.91	0.50
1:C:12:VAL:HG11	1:C:42:ILE:HG23	1.94	0.50
1:C:157:VAL:O	1:C:160:SER:HB2	2.12	0.50
1:E:127:VAL:HG22	1:E:138:PHE:CD2	2.46	0.50
1:A:151:LYS:HE2	1:A:152:GLU:OE2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:35:ARG:HB2	1:D:63:MET:HG3	1.93	0.50
1:D:24:VAL:O	1:D:98:GLY:HA3	2.11	0.50
1:D:113:GLU:HG3	1:D:114:VAL:HG13	1.94	0.50
1:F:15:LYS:CA	2:F:404:SO4:O2	2.60	0.49
1:F:260:THR:HG22	1:F:262:SER:H	1.77	0.49
1:A:167:ILE:HD13	1:A:296:LEU:HD13	1.93	0.49
1:D:128:PHE:CD2	1:D:256:LEU:HD13	2.47	0.49
1:E:30:VAL:HG13	1:E:96:MET:HE3	1.93	0.49
1:A:211:ASP:HB3	1:A:234:VAL:HG21	1.95	0.49
1:F:110:LEU:O	1:F:117:ARG:NH2	2.46	0.49
1:H:107:ARG:HH11	1:H:107:ARG:CG	2.25	0.49
1:H:140:THR:CG2	1:H:156:ILE:HG23	2.42	0.49
1:F:173:LYS:N	1:F:173:LYS:HD2	2.27	0.49
1:B:61:ILE:HG22	1:B:61:ILE:O	2.12	0.49
1:F:260:THR:HG22	1:F:262:SER:N	2.28	0.49
1:D:24:VAL:HG12	1:D:26:GLN:HG2	1.95	0.49
1:D:198:LYS:HD3	1:E:212:GLY:O	2.12	0.49
1:F:204:GLN:HE22	1:G:183:ILE:H	1.60	0.49
1:C:268:LEU:HB2	1:C:275:VAL:HB	1.95	0.49
1:E:97:LYS:HE3	1:E:100:VAL:O	2.13	0.49
1:B:51:HIS:HB2	1:B:72:ASN:HB2	1.96	0.48
1:D:28:GLU:N	1:D:29:PRO:CD	2.76	0.48
1:F:32:GLU:HG2	1:F:35:ARG:NH2	2.29	0.48
1:F:266:GLY:O	1:F:267:ILE:HG23	2.13	0.48
1:E:248:THR:HA	1:F:248:THR:HB	1.95	0.48
1:F:251:VAL:O	1:F:252:MET:C	2.51	0.48
1:H:177:ILE:HD12	1:H:216:LEU:HA	1.96	0.48
1:A:198:LYS:HD3	1:H:212:GLY:O	2.13	0.48
1:A:283:SER:OG	1:A:286:THR:HG23	2.14	0.48
1:A:5:PHE:CE1	1:A:289:ASN:HB3	2.49	0.48
1:A:278:THR:CG2	1:A:287:LYS:HG2	2.43	0.48
1:G:110:LEU:O	1:G:117:ARG:NE	2.46	0.48
1:C:268:LEU:HD11	1:C:277:LEU:HD12	1.95	0.48
1:F:87:VAL:HG21	1:F:95:VAL:HG22	1.96	0.48
1:G:51:HIS:H	1:G:72:ASN:HD22	1.62	0.48
1:B:268:LEU:HB2	1:B:275:VAL:HB	1.96	0.47
1:C:267:ILE:CD1	1:C:297:VAL:HG21	2.43	0.47
1:E:28:GLU:HG2	1:E:57:ILE:HD13	1.95	0.47
1:E:157:VAL:O	1:E:161:VAL:HG23	2.14	0.47
1:F:260:THR:HG21	1:F:262:SER:OG	2.14	0.47
1:G:87:VAL:HG21	1:G:95:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:GLU:HB3	1:H:79:ALA:HB2	1.96	0.47
1:E:269:VAL:HG12	1:E:270:GLY:N	2.29	0.47
1:F:283:SER:HB3	2:F:401:SO4:O4	2.14	0.47
1:H:37:ALA:HB2	1:H:288:MET:HE1	1.96	0.47
1:H:274:PRO:HG3	1:H:297:VAL:CG2	2.44	0.47
1:E:51:HIS:H	1:E:72:ASN:HD22	1.62	0.47
1:F:20:VAL:O	1:F:45:ALA:HA	2.14	0.47
1:C:217:ASP:HB3	1:D:254:LYS:HD2	1.97	0.47
1:F:28:GLU:N	1:F:29:PRO:CD	2.78	0.47
1:F:167:ILE:N	1:F:167:ILE:HD13	2.28	0.47
1:F:200:SER:HB2	1:F:210:VAL:HB	1.97	0.47
1:D:93:ASP:C	1:D:94:MET:HG3	2.34	0.47
1:D:255:THR:O	1:D:259:THR:HB	2.14	0.47
1:E:26:GLN:H	1:E:26:GLN:HE21	1.63	0.47
1:G:140:THR:HA	1:G:141:ASP:HA	1.70	0.47
1:H:140:THR:HG22	1:H:156:ILE:HG23	1.96	0.47
1:G:23:ALA:HA	1:G:83:ALA:HB2	1.96	0.47
1:G:13:LYS:HE3	1:G:40:ASN:O	2.14	0.47
1:A:111:ASN:HD22	1:A:114:VAL:H	1.63	0.46
1:C:198:LYS:HD3	1:C:198:LYS:HA	1.49	0.46
1:B:33:ALA:HA	1:B:288:MET:HE2	1.97	0.46
1:E:5:PHE:CE1	1:E:289:ASN:HB3	2.50	0.46
1:G:277:LEU:HD12	1:G:277:LEU:C	2.36	0.46
1:G:103:ALA:HB1	1:G:107:ARG:NH1	2.31	0.46
1:A:18:LYS:HE2	1:A:299:GLY:HA2	1.98	0.46
1:B:124:HIS:O	1:B:140:THR:CG2	2.63	0.46
1:E:248:THR:CG2	1:F:251:VAL:HG21	2.46	0.46
1:G:26:GLN:HE21	1:G:26:GLN:HB2	1.49	0.46
1:G:260:THR:HG22	1:G:262:SER:OG	2.16	0.46
1:A:218:ILE:O	1:A:236:GLY:N	2.49	0.46
1:C:300:ASN:HD22	1:C:300:ASN:HA	1.58	0.46
1:H:87:VAL:HG21	1:H:95:VAL:CG2	2.44	0.46
1:B:110:LEU:HD21	1:B:122:MET:CE	2.46	0.46
1:C:5:PHE:HA	1:C:8:ILE:HB	1.97	0.45
1:D:51:HIS:HB2	1:D:72:ASN:HD22	1.81	0.45
1:C:216:LEU:HD13	1:C:252:MET:HE1	1.98	0.45
1:A:278:THR:HG21	1:A:287:LYS:HG2	1.98	0.45
1:A:247:GLU:HG2	1:B:179:ALA:HB2	1.97	0.45
1:D:101:ASN:OD1	1:D:103:ALA:HB3	2.16	0.45
1:A:28:GLU:N	1:A:29:PRO:HD2	2.31	0.45
1:A:243:MET:HE3	1:A:249:GLY:HA2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:176:PRO:HA	1:G:242:LEU:HB3	1.98	0.45
1:A:127:VAL:O	1:A:264:ASN:HA	2.17	0.45
1:E:75:ASN:ND2	1:E:78:LYS:HG3	2.31	0.45
1:G:48:VAL:HG11	1:G:82:LYS:HB2	1.99	0.45
1:E:34:VAL:O	1:E:37:ALA:HB3	2.17	0.45
1:H:138:PHE:HB2	1:H:240:ILE:HA	1.98	0.45
1:G:35:ARG:HG3	1:G:36:ASP:N	2.31	0.44
1:D:253:TYR:O	1:D:257:THR:HG23	2.17	0.44
1:G:257:THR:HG22	1:G:258:TYR:CD1	2.52	0.44
1:A:20:VAL:HG22	1:A:94:MET:CE	2.46	0.44
1:A:191:LEU:HG	1:H:195:MET:CE	2.47	0.44
1:G:268:LEU:HB2	1:G:275:VAL:HB	1.99	0.44
1:G:231:THR:CG2	1:G:232:GLY:N	2.81	0.44
1:A:211:ASP:HB3	1:A:234:VAL:CG2	2.48	0.44
1:A:243:MET:HE1	1:A:252:MET:SD	2.58	0.44
1:B:35:ARG:HH21	1:B:61:ILE:CG2	2.31	0.44
1:H:260:THR:CG2	1:H:262:SER:OG	2.66	0.44
1:F:218:ILE:HD11	1:F:228:LYS:HD3	1.98	0.44
1:H:35:ARG:HB2	1:H:63:MET:HG2	1.98	0.44
1:A:188:PRO:HA	1:A:191:LEU:HD22	2.00	0.44
1:E:188:PRO:HA	1:E:191:LEU:HD22	2.00	0.44
1:G:135:ARG:NH1	2:G:401:SO4:O1	2.50	0.44
1:H:51:HIS:O	1:H:55:VAL:HG23	2.18	0.44
1:F:181:GLU:OE1	1:F:181:GLU:N	2.47	0.43
1:C:96:MET:HE1	1:C:291:ILE:HD11	1.99	0.43
1:A:109:VAL:HG13	1:A:116:LEU:HD12	2.00	0.43
1:G:75:ASN:HD22	1:G:78:LYS:HG3	1.83	0.43
1:H:140:THR:HA	1:H:141:ASP:HA	1.73	0.43
1:A:20:VAL:HG22	1:A:94:MET:HE2	2.01	0.43
1:C:172:PRO:HD2	1:C:207:GLY:O	2.18	0.43
1:H:141:ASP:OD1	1:H:141:ASP:C	2.57	0.43
1:C:31:LEU:HB3	1:C:63:MET:CE	2.49	0.43
1:A:30:VAL:O	1:A:33:ALA:HB3	2.19	0.43
1:D:39:LYS:HA	1:D:39:LYS:CE	2.49	0.43
1:G:51:HIS:H	1:G:72:ASN:ND2	2.16	0.43
1:H:202:ARG:HA	1:H:202:ARG:HD3	1.76	0.43
1:H:300:ASN:N	1:H:300:ASN:ND2	2.67	0.43
1:A:96:MET:HA	1:A:276:VAL:O	2.19	0.43
1:C:220:LEU:HD23	1:C:220:LEU:N	2.34	0.43
1:A:138:PHE:HB2	1:A:240:ILE:HD13	2.01	0.43
1:H:27:ASP:HB3	1:H:30:VAL:HB	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:THR:HA	1:A:141:ASP:HA	1.74	0.42
1:D:20:VAL:O	1:D:45:ALA:HA	2.19	0.42
1:E:248:THR:OG1	1:F:248:THR:HG22	2.19	0.42
1:H:176:PRO:HA	1:H:242:LEU:HB3	2.00	0.42
1:C:259:THR:HA	1:D:132:LYS:HG3	2.00	0.42
1:C:101:ASN:OD1	1:C:104:THR:CB	2.67	0.42
1:G:218:ILE:HD11	1:G:228:LYS:HD2	2.00	0.42
1:G:268:LEU:HD12	1:G:275:VAL:HG11	2.01	0.42
1:E:280:ARG:HD2	1:F:227:HIS:CE1	2.54	0.42
1:F:82:LYS:HD3	1:F:82:LYS:HA	1.85	0.42
1:F:93:ASP:C	1:F:94:MET:HG3	2.39	0.42
1:H:269:VAL:HG12	1:H:270:GLY:H	1.84	0.42
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.80	0.42
1:B:125:VAL:HG22	1:B:140:THR:HG23	2.01	0.42
1:D:156:ILE:O	1:D:160:SER:HB2	2.20	0.42
1:F:286:THR:HG21	2:F:401:SO4:S	2.59	0.42
1:C:23:ALA:HA	1:C:83:ALA:CB	2.50	0.42
1:G:19:LYS:HA	1:G:44:ASP:O	2.20	0.42
1:H:17:MET:CE	1:H:41:GLY:HA2	2.50	0.42
1:E:173:LYS:HD2	1:E:173:LYS:N	2.34	0.41
1:F:35:ARG:NH1	1:F:36:ASP:OD1	2.51	0.41
1:H:129:GLU:HB3	1:H:263:LYS:HB2	2.02	0.41
1:C:222:GLU:N	2:C:402:SO4:O4	2.39	0.41
1:G:94:MET:HE2	1:G:295:ALA:HA	2.03	0.41
1:H:163:VAL:HG21	1:H:269:VAL:HG21	2.03	0.41
1:A:65:VAL:HG11	1:A:70:ILE:HD11	2.03	0.41
1:C:176:PRO:HD2	1:C:212:GLY:HA3	2.01	0.41
1:A:28:GLU:CG	1:A:61:ILE:HD11	2.51	0.41
1:F:133:PHE:CZ	1:F:220:LEU:HG	2.56	0.41
1:G:23:ALA:HA	1:G:83:ALA:CB	2.51	0.41
1:G:178:CYS:SG	1:G:213:PRO:HB3	2.61	0.41
1:H:107:ARG:HH11	1:H:107:ARG:HG2	1.86	0.41
1:B:33:ALA:HA	1:B:288:MET:CE	2.51	0.41
1:B:256:LEU:O	1:B:260:THR:HB	2.20	0.41
1:A:243:MET:HG3	1:A:249:GLY:HA2	2.01	0.41
1:D:184:ASN:C	1:D:184:ASN:OD1	2.59	0.41
1:B:140:THR:HA	1:B:141:ASP:HA	1.92	0.41
1:B:260:THR:CG2	1:B:262:SER:OG	2.68	0.41
1:D:157:VAL:O	1:D:160:SER:HB3	2.21	0.41
1:F:243:MET:HG3	1:F:249:GLY:HA2	2.03	0.41
1:H:75:ASN:HD22	1:H:78:LYS:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:ARG:CG	1:H:107:ARG:NH1	2.82	0.41
1:D:39:LYS:HA	1:D:39:LYS:HE2	2.02	0.41
1:E:133:PHE:CZ	1:E:220:LEU:HG	2.56	0.41
1:H:102:THR:HG23	1:H:277:LEU:HD21	2.02	0.41
1:A:35:ARG:HG3	1:A:63:MET:HB3	2.02	0.40
1:C:170:GLU:N	2:C:401:SO4:O3	2.54	0.40
1:D:82:LYS:O	1:D:86:LEU:HG	2.21	0.40
1:F:13:LYS:HE2	1:F:40:ASN:O	2.20	0.40
1:G:73:GLU:HG3	1:G:82:LYS:HG3	2.02	0.40
1:A:174:VAL:HB	1:A:210:VAL:HG22	2.03	0.40
1:F:140:THR:HA	1:F:141:ASP:HA	1.87	0.40
1:F:200:SER:CB	1:F:210:VAL:HB	2.51	0.40
1:G:188:PRO:HA	1:G:191:LEU:HD12	2.03	0.40
1:H:123:SER:HB2	1:H:156:ILE:HG12	2.03	0.40
1:A:199:MET:HB3	1:A:205:ILE:HG12	2.04	0.40
1:C:216:LEU:O	1:C:220:LEU:HD23	2.20	0.40
1:E:254:LYS:HZ3	1:F:217:ASP:CG	2.25	0.40
1:F:96:MET:HG2	1:F:276:VAL:CG1	2.51	0.40
1:G:245:ASN:OD1	1:G:248:THR:HG23	2.22	0.40
1:H:13:LYS:HE2	1:H:40:ASN:O	2.22	0.40
1:F:253:TYR:CD1	1:F:253:TYR:C	2.94	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	299/321 (93%)	284 (95%)	15 (5%)	0	100	100
1	B	298/321 (93%)	285 (96%)	13 (4%)	0	100	100
1	C	304/321 (95%)	294 (97%)	10 (3%)	0	100	100
1	D	298/321 (93%)	282 (95%)	16 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	299/321 (93%)	289 (97%)	10 (3%)	0	100	100
1	F	301/321 (94%)	282 (94%)	19 (6%)	0	100	100
1	G	298/321 (93%)	279 (94%)	19 (6%)	0	100	100
1	H	298/321 (93%)	284 (95%)	14 (5%)	0	100	100
All	All	2395/2568 (93%)	2279 (95%)	116 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/266 (94%)	226 (91%)	23 (9%)	9	26
1	B	248/266 (93%)	220 (89%)	28 (11%)	6	17
1	C	253/266 (95%)	226 (89%)	27 (11%)	6	19
1	D	248/266 (93%)	223 (90%)	25 (10%)	7	22
1	E	249/266 (94%)	228 (92%)	21 (8%)	11	30
1	F	251/266 (94%)	226 (90%)	25 (10%)	7	22
1	G	248/266 (93%)	224 (90%)	24 (10%)	8	24
1	H	248/266 (93%)	214 (86%)	34 (14%)	3	10
All	All	1994/2128 (94%)	1787 (90%)	207 (10%)	7	20

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ARG
1	A	60	LYS
1	A	65	VAL
1	A	82	LYS
1	A	88	SER
1	A	94	MET

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Mol	Chain	Res	Type
1	A	100	VAL
1	A	108	SER
1	A	113	GLU
1	A	123	SER
1	A	134	ASP
1	A	136	LEU
1	A	142	VAL
1	A	149	GLU
1	A	152	GLU
1	A	198	LYS
1	A	214	LEU
1	A	262	SER
1	A	269	VAL
1	A	278	THR
1	A	285	GLU
1	A	296	LEU
1	A	301	LYS
1	B	1	MET
1	B	2	ILE
1	B	3	LYS
1	B	14	SER
1	B	17	MET
1	B	26	GLN
1	B	27	ASP
1	B	38	LYS
1	B	40	ASN
1	B	44	ASP
1	B	55	VAL
1	B	60	LYS
1	B	75	ASN
1	B	95	VAL
1	B	99	LEU
1	B	100	VAL
1	B	102	THR
1	B	117	ARG
1	B	130	THR
1	B	140	THR
1	B	189	SER
1	B	198	LYS
1	B	214	LEU
1	B	220	LEU
1	B	259	THR

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Mol	Chain	Res	Type
1	B	260	THR
1	B	280	ARG
1	B	300	ASN
1	C	-3	ARG
1	C	2	ILE
1	C	3	LYS
1	C	19	LYS
1	C	26	GLN
1	C	56	SER
1	C	63	MET
1	C	73	GLU
1	C	82	LYS
1	C	95	VAL
1	C	96	MET
1	C	97	LYS
1	C	99	LEU
1	C	100	VAL
1	C	107	ARG
1	C	108	SER
1	C	121	THR
1	C	140	THR
1	C	174	VAL
1	C	186	LYS
1	C	191	LEU
1	C	198	LYS
1	C	220	LEU
1	C	237	LYS
1	C	278	THR
1	C	280	ARG
1	C	300	ASN
1	D	14	SER
1	D	15	LYS
1	D	26	GLN
1	D	38	LYS
1	D	39	LYS
1	D	59	LEU
1	D	63	MET
1	D	82	LYS
1	D	88	SER
1	D	94	MET
1	D	97	LYS
1	D	100	VAL

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Mol	Chain	Res	Type
1	D	106	LEU
1	D	117	ARG
1	D	121	THR
1	D	150	LEU
1	D	198	LYS
1	D	206	LYS
1	D	221	SER
1	D	228	LYS
1	D	237	LYS
1	D	259	THR
1	D	263	LYS
1	D	268	LEU
1	D	280	ARG
1	E	1	MET
1	E	15	LYS
1	E	26	GLN
1	E	35	ARG
1	E	56	SER
1	E	59	LEU
1	E	60	LYS
1	E	94	MET
1	E	95	VAL
1	E	96	MET
1	E	99	LEU
1	E	100	VAL
1	E	140	THR
1	E	162	LYS
1	E	181	GLU
1	E	191	LEU
1	E	198	LYS
1	E	216	LEU
1	E	237	LYS
1	E	241	PHE
1	E	268	LEU
1	F	3	LYS
1	F	17	MET
1	F	26	GLN
1	F	50	ASP
1	F	56	SER
1	F	59	LEU
1	F	61	ILE
1	F	82	LYS

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Mol	Chain	Res	Type
1	F	91	LYS
1	F	94	MET
1	F	96	MET
1	F	99	LEU
1	F	100	VAL
1	F	112	LYS
1	F	113	GLU
1	F	140	THR
1	F	151	LYS
1	F	161	VAL
1	F	173	LYS
1	F	198	LYS
1	F	248	THR
1	F	255	THR
1	F	259	THR
1	F	262	SER
1	F	286	THR
1	G	3	LYS
1	G	17	MET
1	G	18	LYS
1	G	20	VAL
1	G	26	GLN
1	G	56	SER
1	G	93	ASP
1	G	94	MET
1	G	95	VAL
1	G	99	LEU
1	G	100	VAL
1	G	140	THR
1	G	162	LYS
1	G	173	LYS
1	G	182	VAL
1	G	198	LYS
1	G	200	SER
1	G	214	LEU
1	G	237	LYS
1	G	272	SER
1	G	277	LEU
1	G	279	SER
1	G	280	ARG
1	G	288	MET
1	H	14	SER

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Mol	Chain	Res	Type
1	H	17	MET
1	H	35	ARG
1	H	53	GLU
1	H	65	VAL
1	H	82	LYS
1	H	93	ASP
1	H	94	MET
1	H	96	MET
1	H	97	LYS
1	H	99	LEU
1	H	100	VAL
1	H	101	ASN
1	H	112	LYS
1	H	123	SER
1	H	130	THR
1	H	131	GLU
1	H	146	THR
1	H	149	GLU
1	H	169	ILE
1	H	173	LYS
1	H	198	LYS
1	H	228	LYS
1	H	256	LEU
1	H	259	THR
1	H	260	THR
1	H	264	ASN
1	H	267	ILE
1	H	278	THR
1	H	280	ARG
1	H	288	MET
1	H	296	LEU
1	H	297	VAL
1	H	300	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	158	ASN
1	A	250	ASN
1	A	284	HIS
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	75	ASN
1	B	124	HIS
1	B	204	GLN
1	B	300	ASN
1	C	250	ASN
1	C	300	ASN
1	D	72	ASN
1	D	75	ASN
1	D	111	ASN
1	D	204	GLN
1	D	250	ASN
1	E	26	GLN
1	E	72	ASN
1	E	124	HIS
1	E	171	ASN
1	E	250	ASN
1	F	40	ASN
1	F	72	ASN
1	F	171	ASN
1	F	204	GLN
1	F	264	ASN
1	G	72	ASN
1	G	75	ASN
1	G	250	ASN
1	G	264	ASN
1	H	75	ASN
1	H	264	ASN
1	H	300	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)

48 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	E	406	-	4,4,4	0.39	0	6,6,6	0.13	0
2	SO4	G	402	-	4,4,4	0.31	0	6,6,6	0.13	0
2	SO4	A	401	-	4,4,4	0.30	0	6,6,6	0.14	0
2	SO4	H	403	-	4,4,4	0.29	0	6,6,6	0.18	0
2	SO4	B	403	-	4,4,4	0.35	0	6,6,6	0.12	0
2	SO4	C	402	-	4,4,4	0.38	0	6,6,6	0.26	0
2	SO4	F	407	-	4,4,4	0.21	0	6,6,6	0.13	0
2	SO4	G	403	-	4,4,4	0.31	0	6,6,6	0.10	0
2	SO4	E	408	-	4,4,4	0.35	0	6,6,6	0.08	0
2	SO4	E	410	-	4,4,4	0.35	0	6,6,6	0.15	0
2	SO4	H	404	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	C	405	-	4,4,4	0.32	0	6,6,6	0.09	0
2	SO4	E	404	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	E	405	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	F	403	-	4,4,4	0.27	0	6,6,6	0.17	0
2	SO4	B	405	-	4,4,4	0.35	0	6,6,6	0.11	0
2	SO4	F	402	-	4,4,4	0.31	0	6,6,6	0.14	0
2	SO4	H	401	-	4,4,4	0.37	0	6,6,6	0.16	0
2	SO4	F	404	-	4,4,4	0.42	0	6,6,6	0.19	0
2	SO4	D	402	-	4,4,4	0.37	0	6,6,6	0.19	0
2	SO4	D	403	-	4,4,4	0.28	0	6,6,6	0.21	0
2	SO4	E	401	-	4,4,4	0.27	0	6,6,6	0.10	0
2	SO4	G	401	-	4,4,4	0.54	0	6,6,6	0.29	0
2	SO4	E	411	-	4,4,4	0.31	0	6,6,6	0.11	0
2	SO4	A	405	-	4,4,4	0.27	0	6,6,6	0.11	0
2	SO4	D	401	-	4,4,4	0.26	0	6,6,6	0.24	0
2	SO4	B	402	-	4,4,4	0.28	0	6,6,6	0.15	0
2	SO4	A	406	-	4,4,4	0.46	0	6,6,6	0.19	0
2	SO4	E	403	-	4,4,4	0.32	0	6,6,6	0.16	0
2	SO4	E	413	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	G	404	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	F	406	-	4,4,4	0.35	0	6,6,6	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.08	0
2	SO4	C	404	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	C	401	-	4,4,4	0.43	0	6,6,6	0.24	0
2	SO4	A	403	-	4,4,4	0.36	0	6,6,6	0.11	0
2	SO4	E	407	-	4,4,4	0.31	0	6,6,6	0.14	0
2	SO4	F	401	-	4,4,4	0.37	0	6,6,6	0.17	0
2	SO4	H	405	-	4,4,4	0.31	0	6,6,6	0.28	0
2	SO4	H	402	-	4,4,4	0.34	0	6,6,6	0.12	0
2	SO4	E	409	-	4,4,4	0.33	0	6,6,6	0.10	0
2	SO4	A	404	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	B	404	-	4,4,4	0.37	0	6,6,6	0.07	0
2	SO4	B	401	-	4,4,4	0.31	0	6,6,6	0.12	0
2	SO4	E	412	-	4,4,4	0.34	0	6,6,6	0.08	0
2	SO4	C	403	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	E	402	-	4,4,4	0.37	0	6,6,6	0.15	0
2	SO4	F	405	-	4,4,4	0.39	0	6,6,6	0.11	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

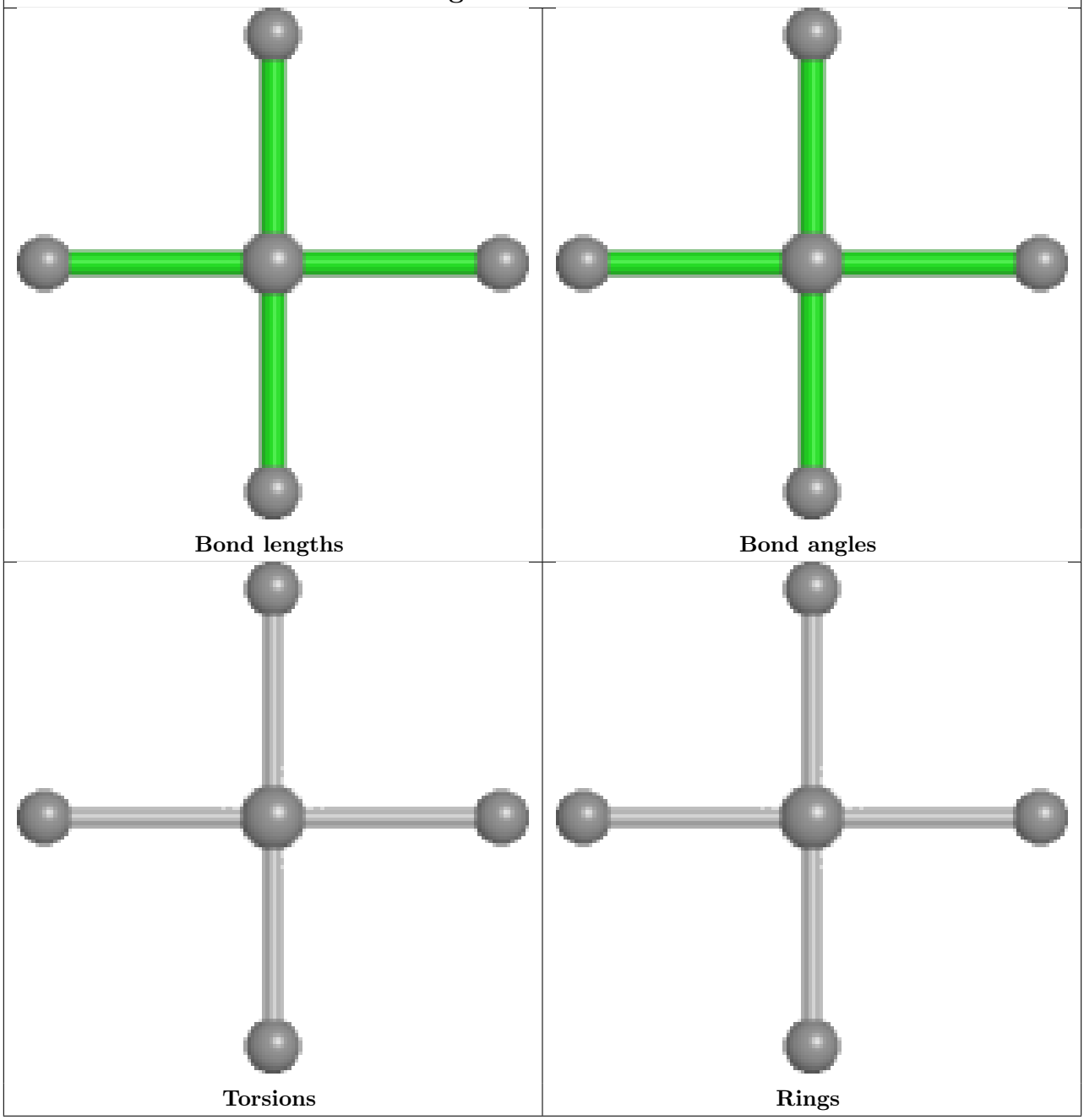
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	402	SO4	1	0
2	F	404	SO4	4	0
2	G	401	SO4	1	0
2	C	401	SO4	1	0
2	F	401	SO4	2	0

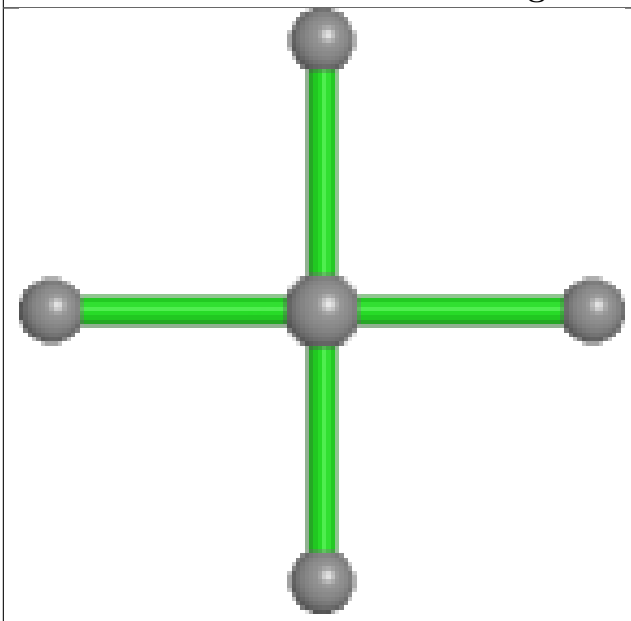
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

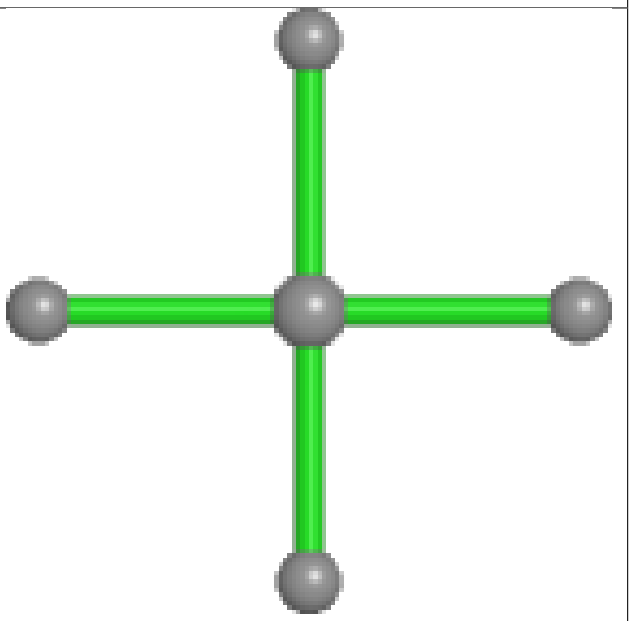
Ligand SO4 E 406



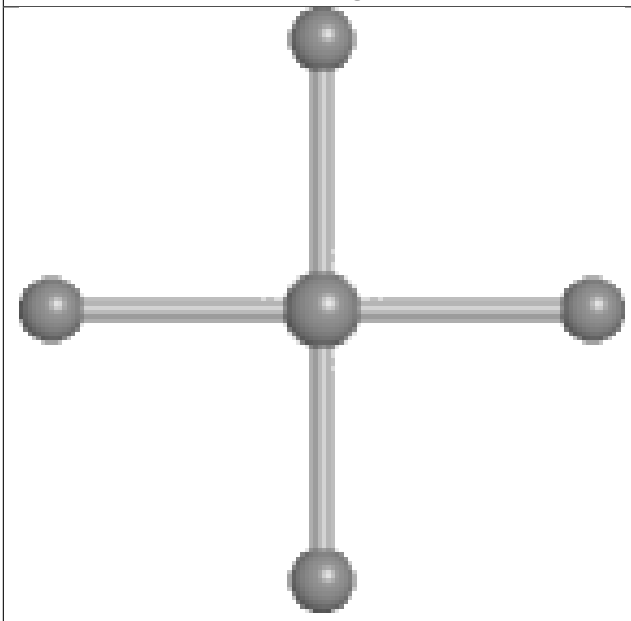
Ligand SO4 G 402



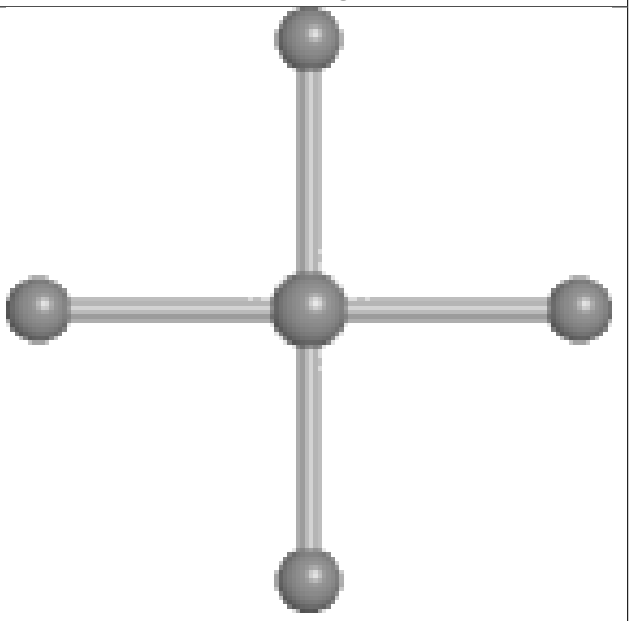
Bond lengths



Bond angles

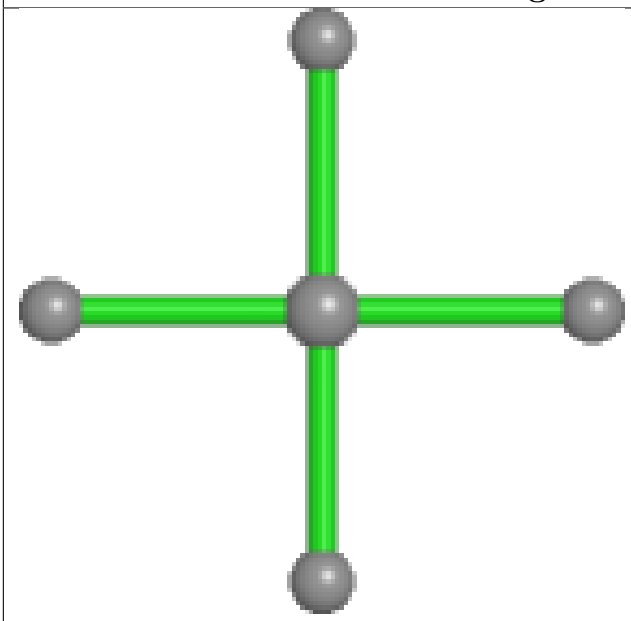


Torsions

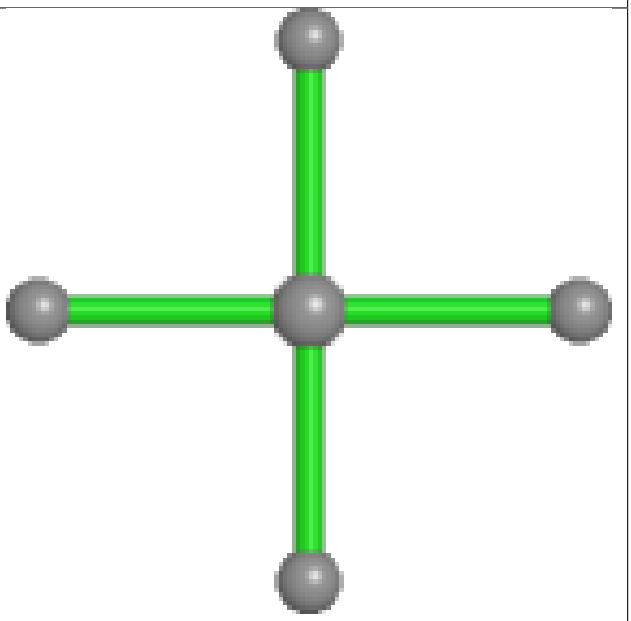


Rings

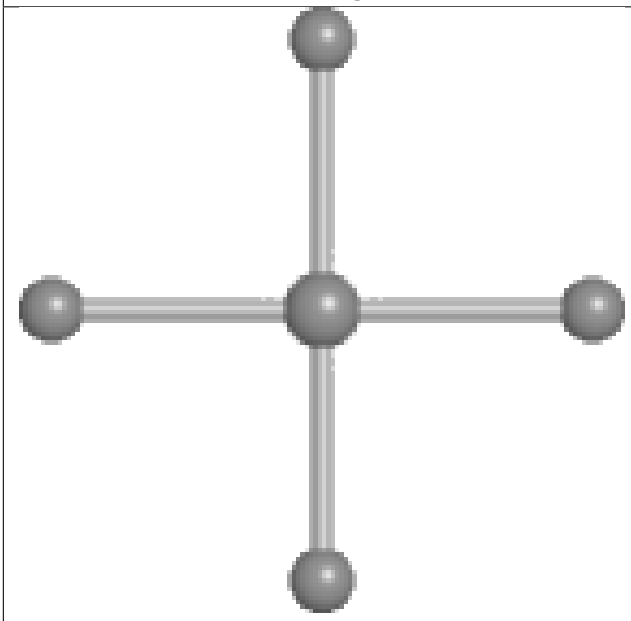
Ligand SO4 A 401



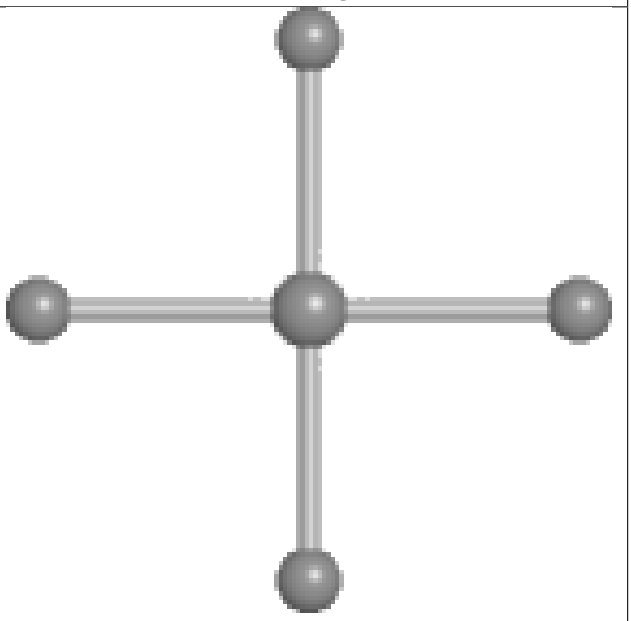
Bond lengths



Bond angles

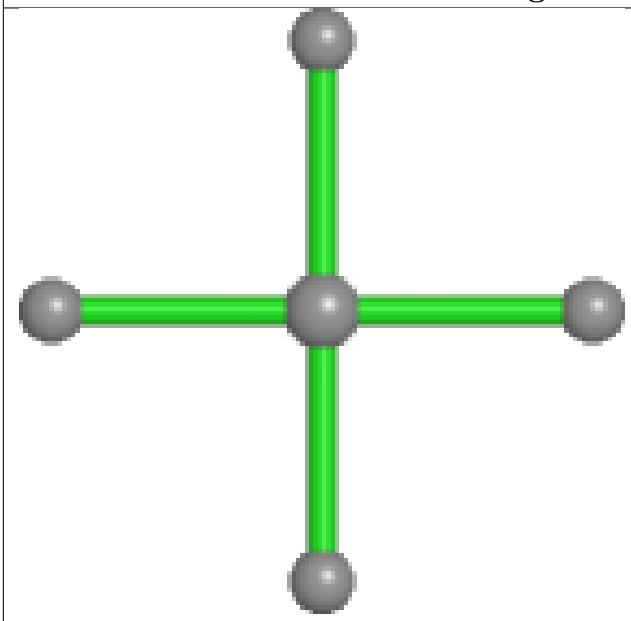


Torsions

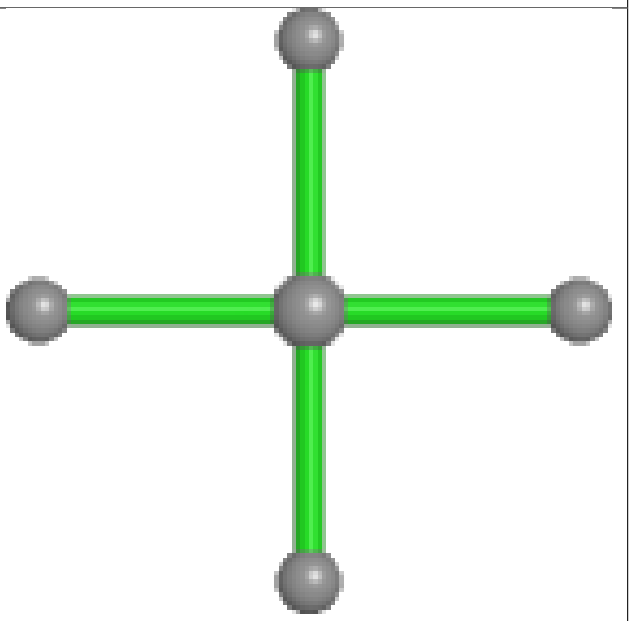


Rings

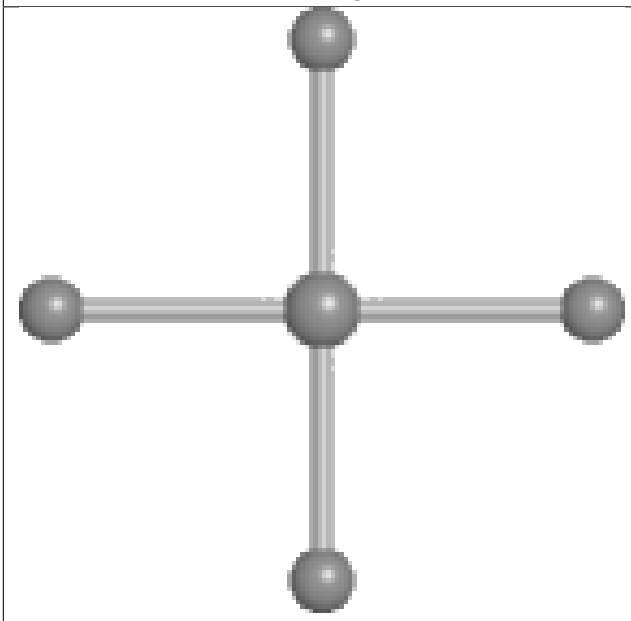
Ligand SO4 H 403



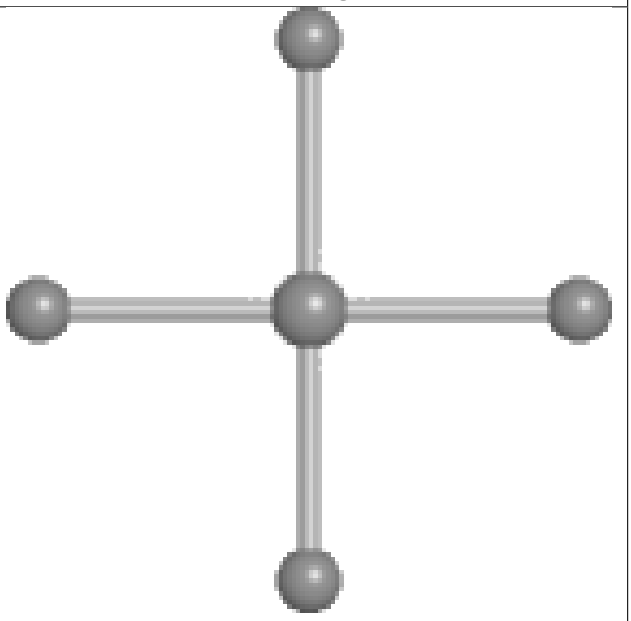
Bond lengths



Bond angles

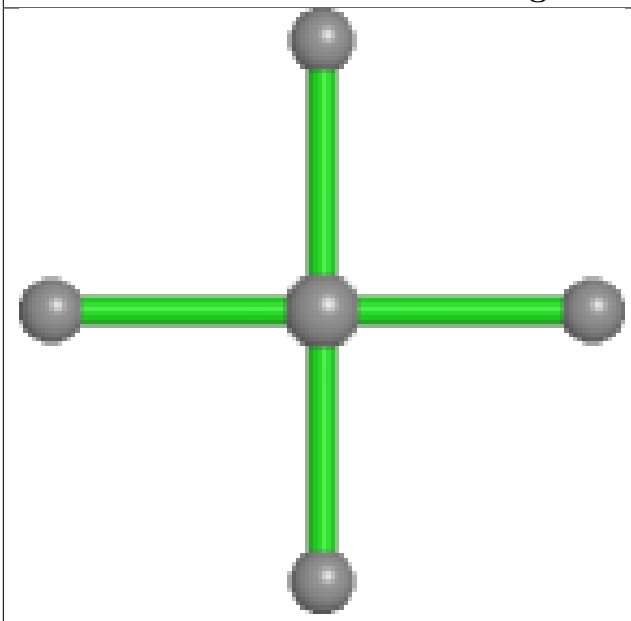


Torsions

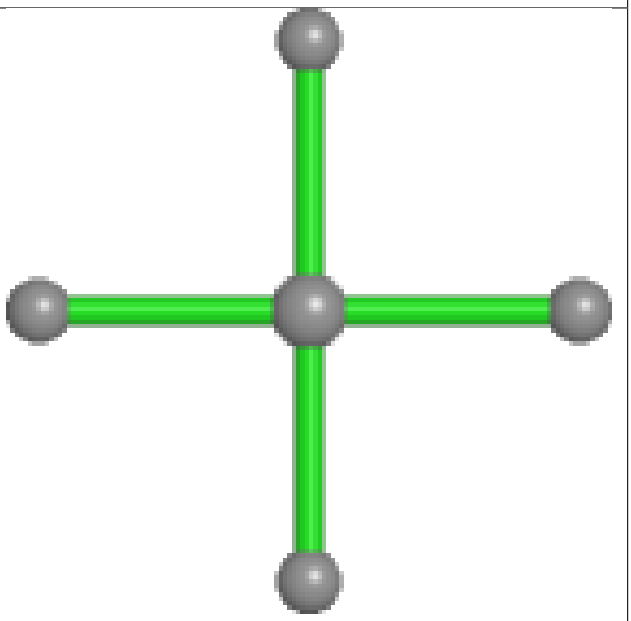


Rings

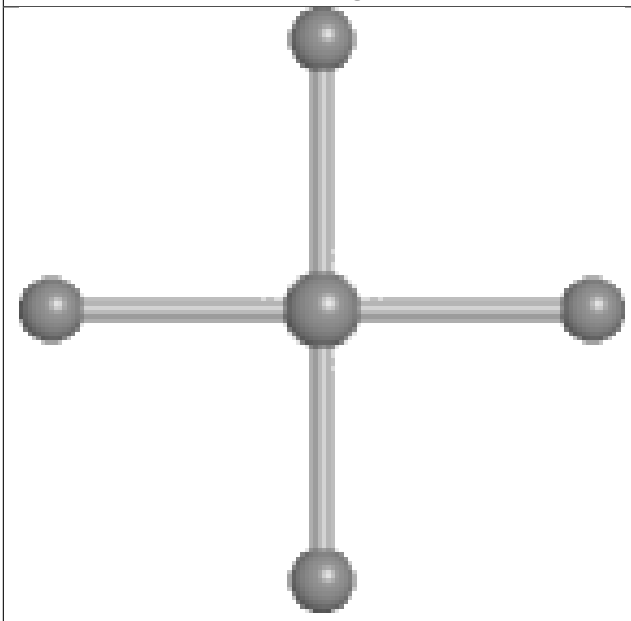
Ligand SO4 B 403



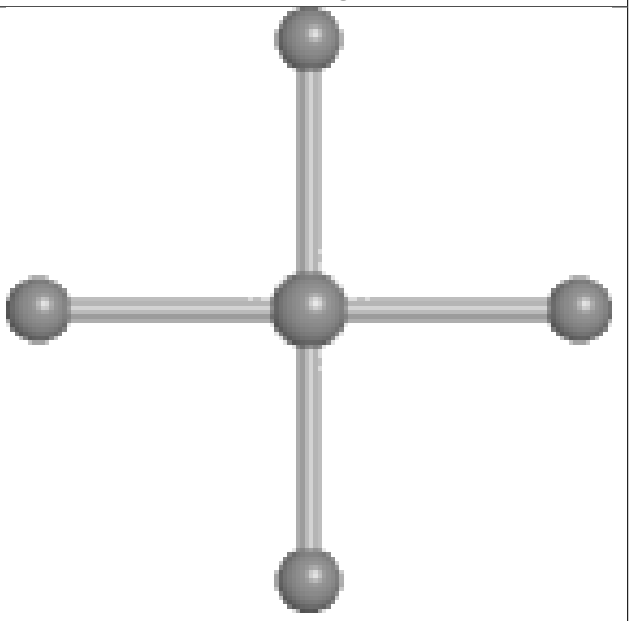
Bond lengths



Bond angles

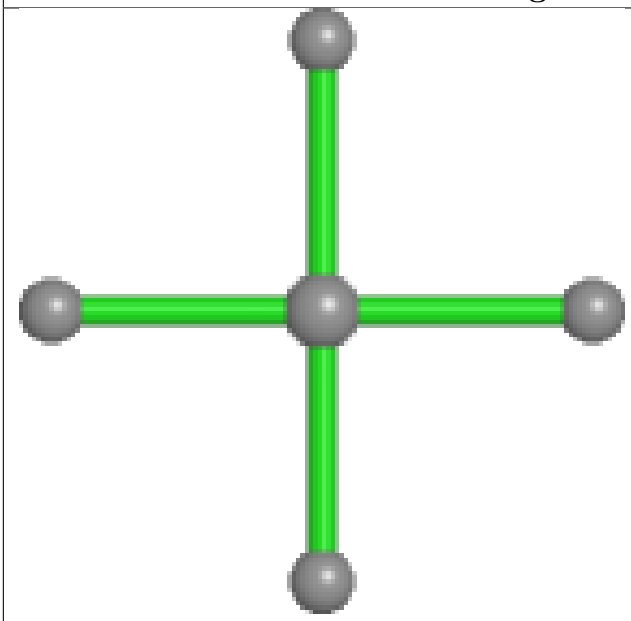


Torsions

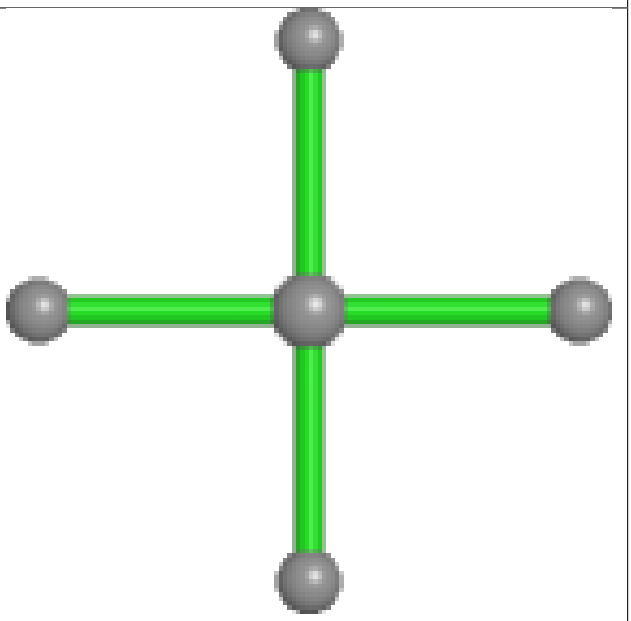


Rings

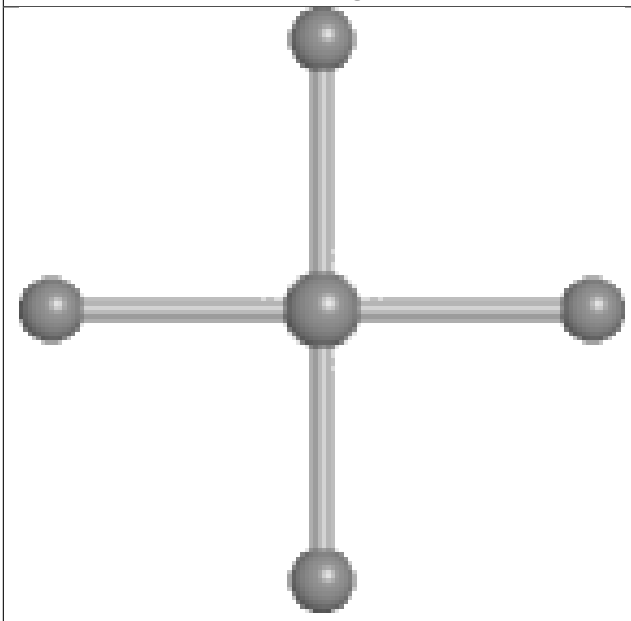
Ligand SO4 C 402



Bond lengths



Bond angles



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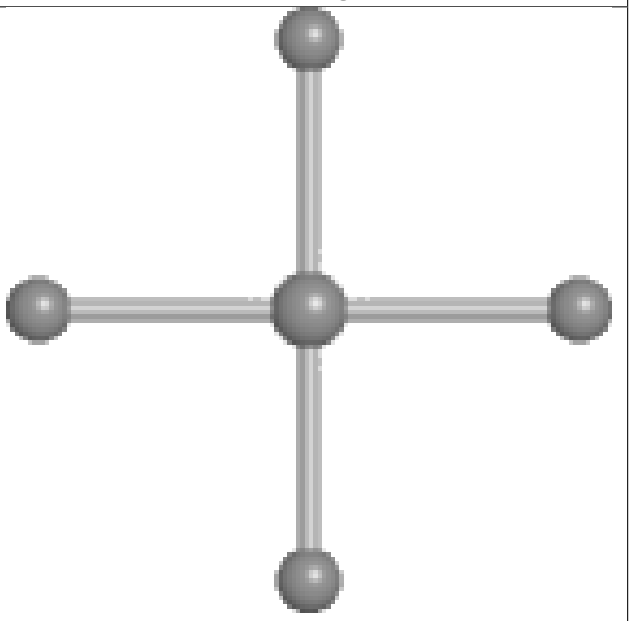
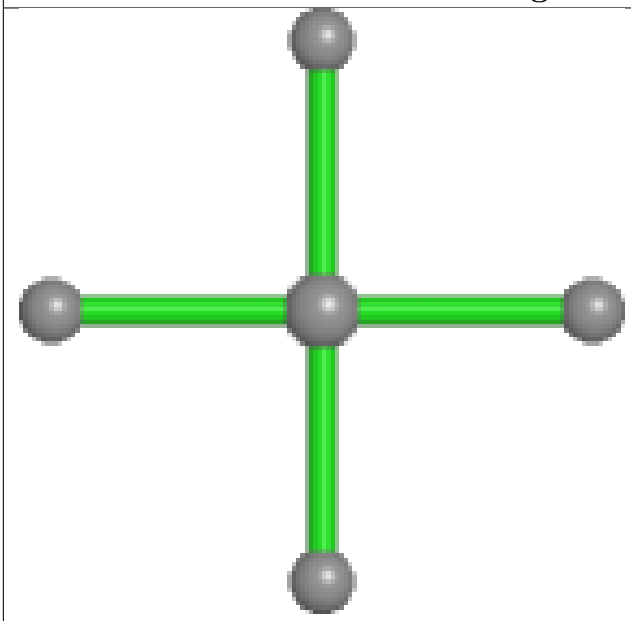
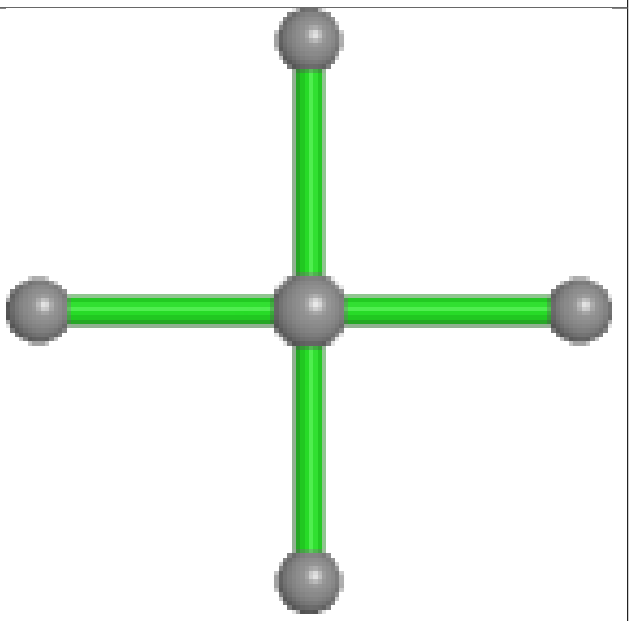


Rings

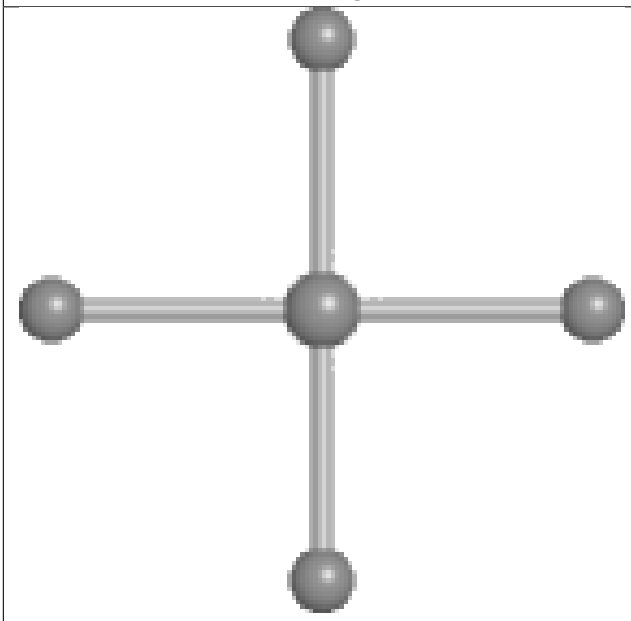
Ligand SO4 F 407



Bond lengths



Bond angles



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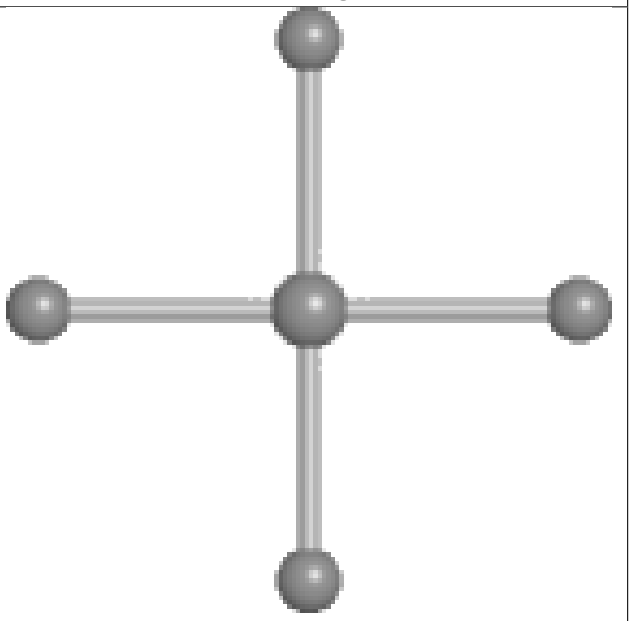
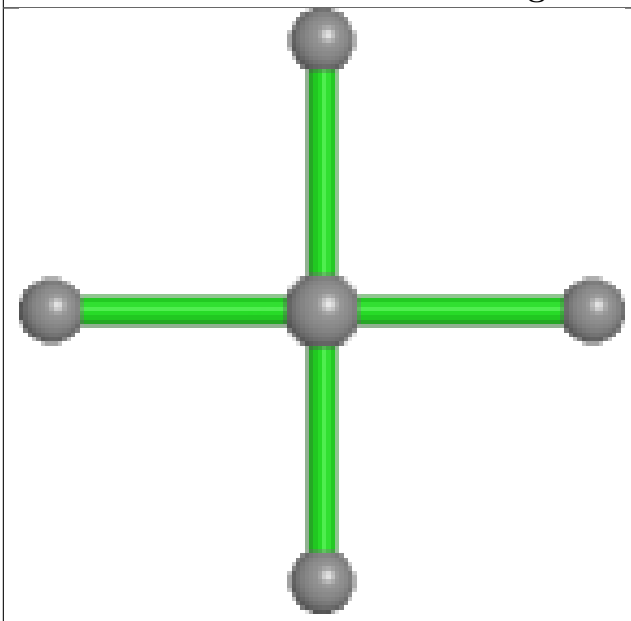
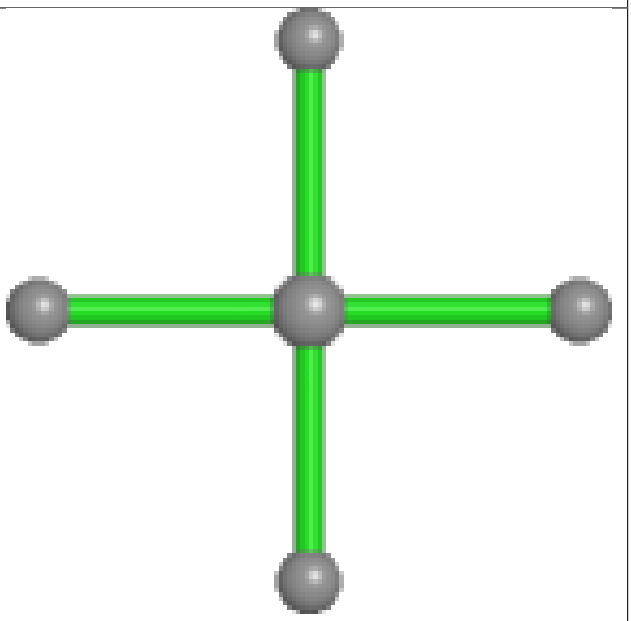


Rings

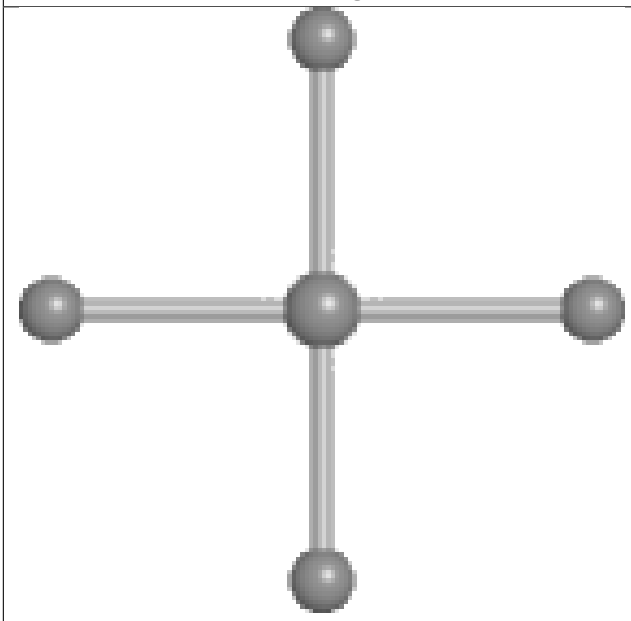
Ligand SO4 G 403



Bond lengths



Bond angles



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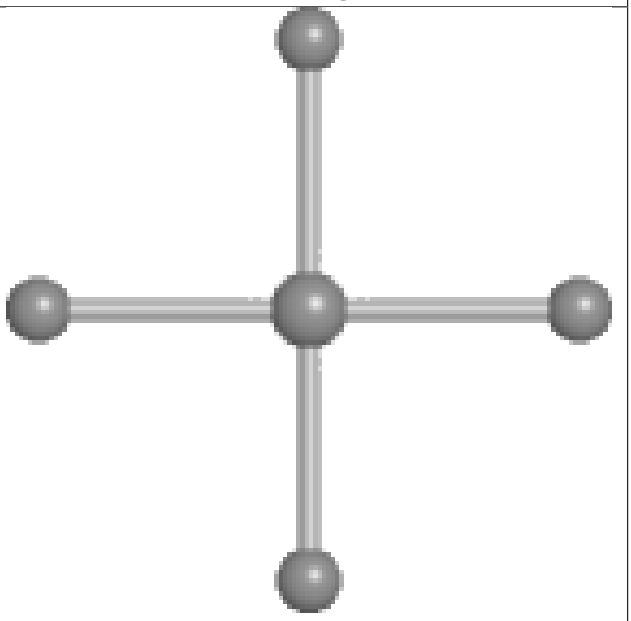
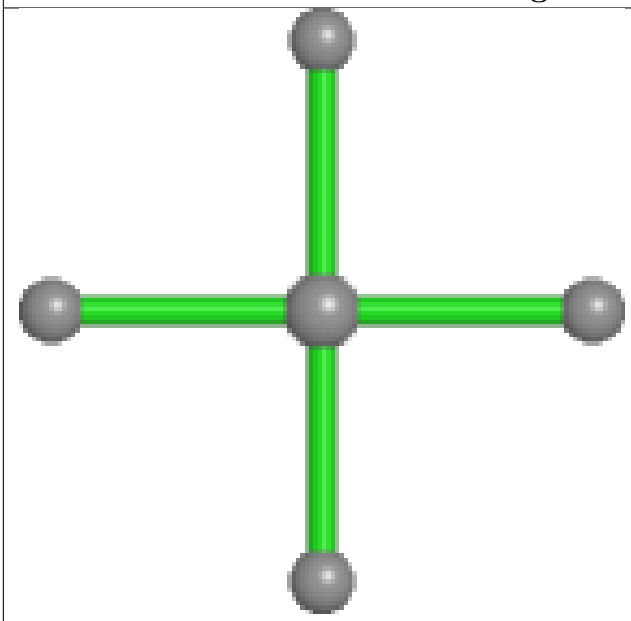
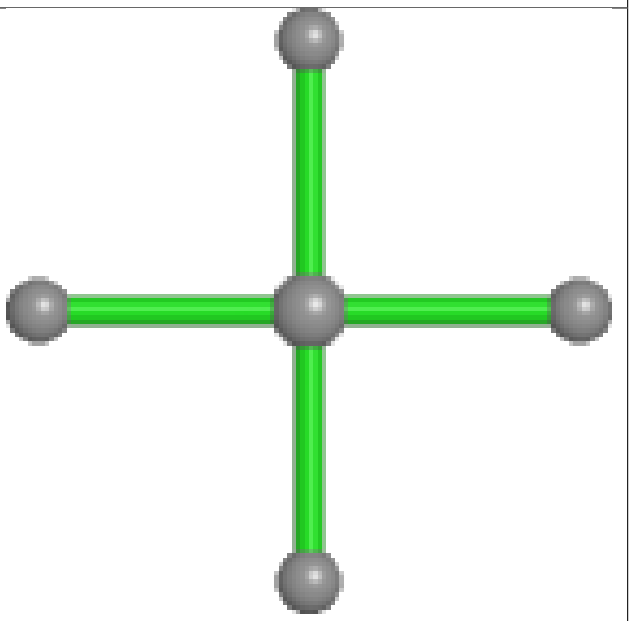


Rings

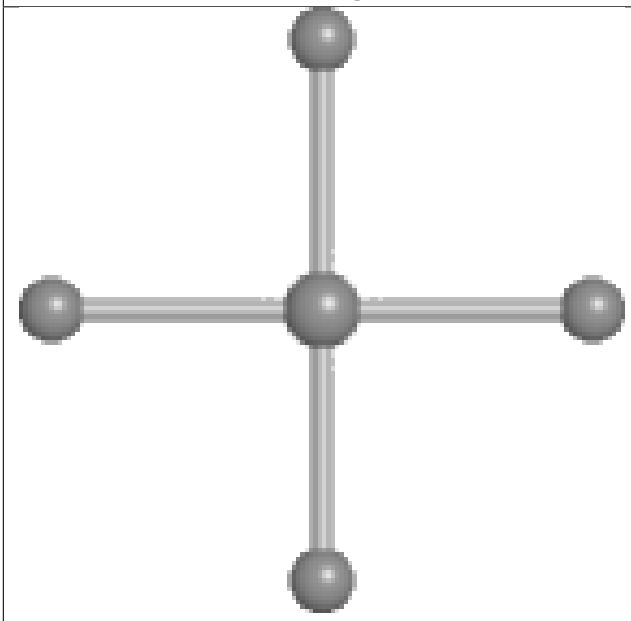
Ligand SO4 E 408



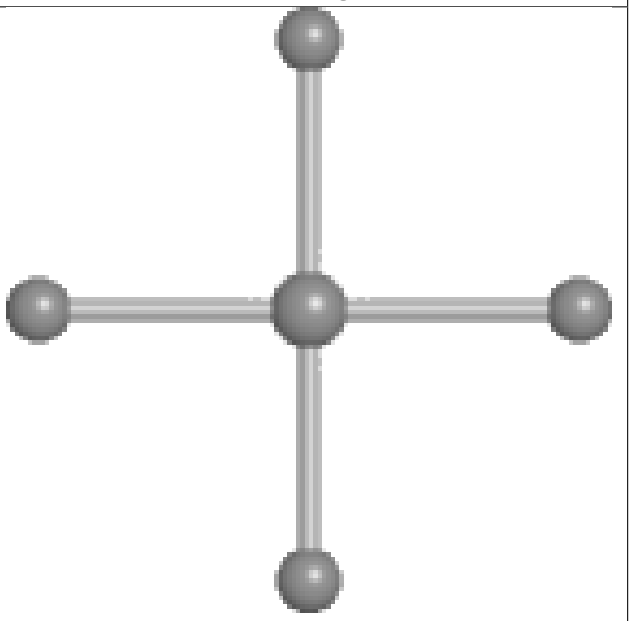
Bond lengths



Bond angles

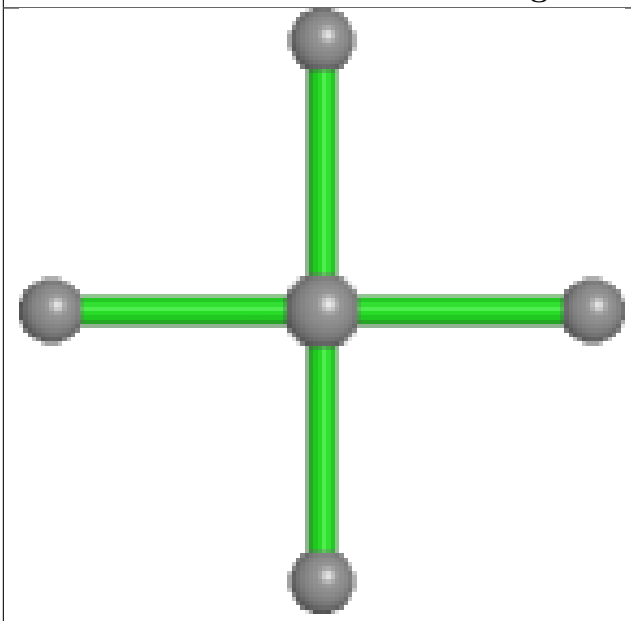


Torsions

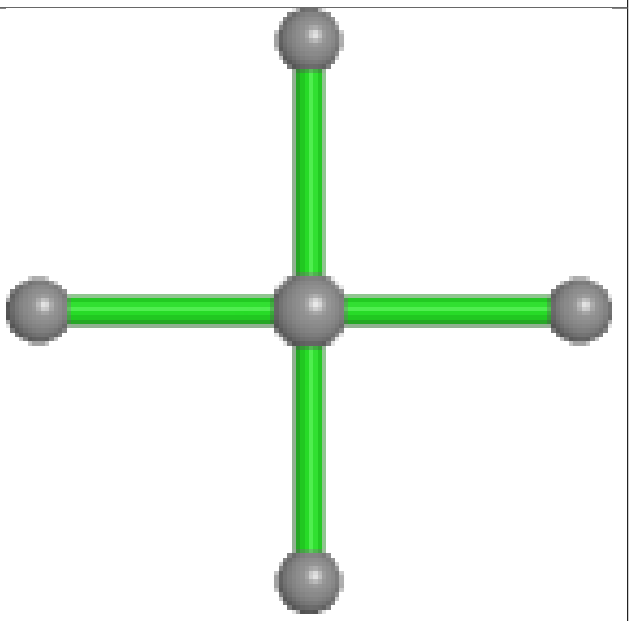


Rings

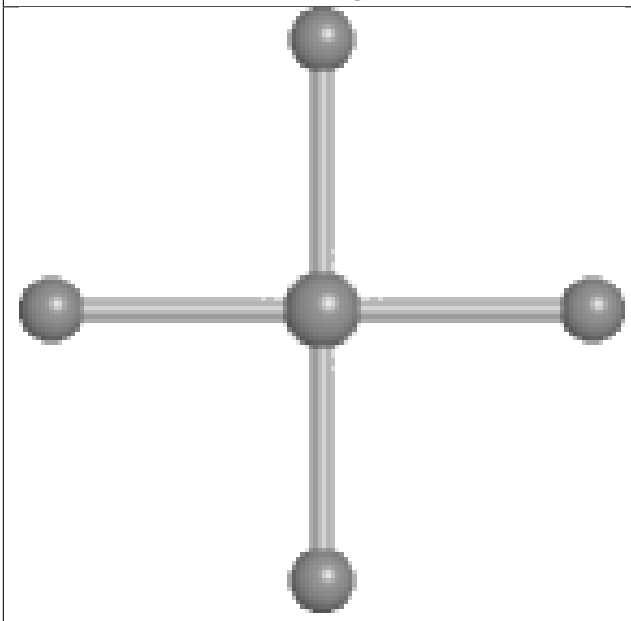
Ligand SO4 E 410



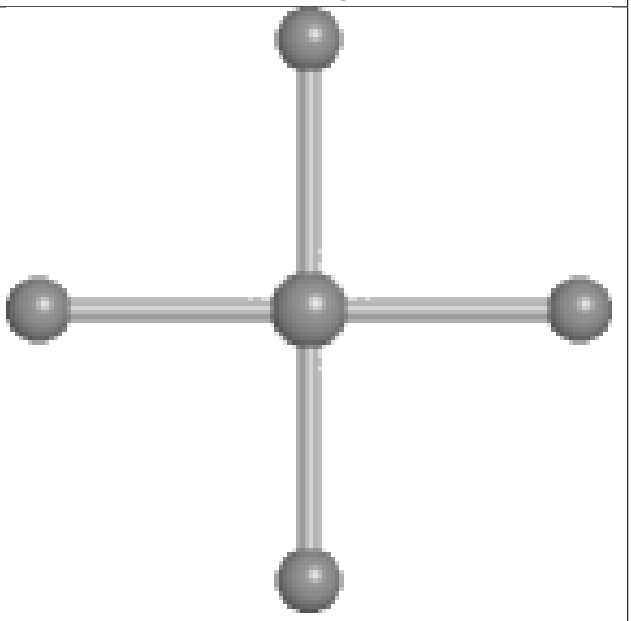
Bond lengths



Bond angles

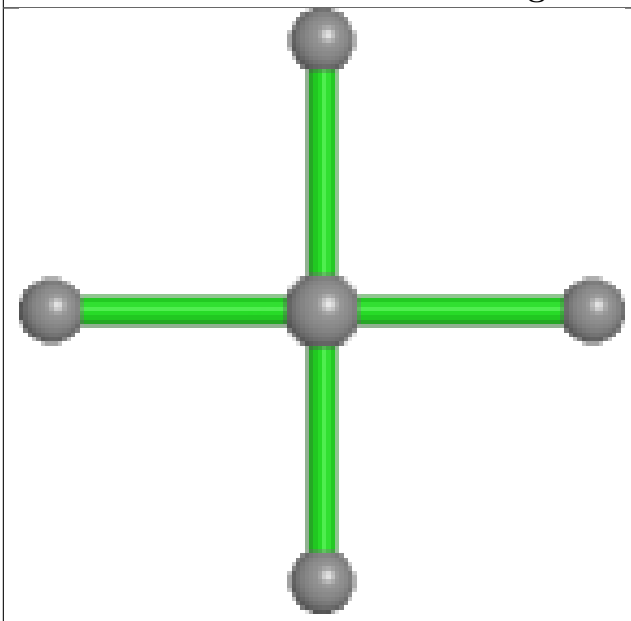


Torsions

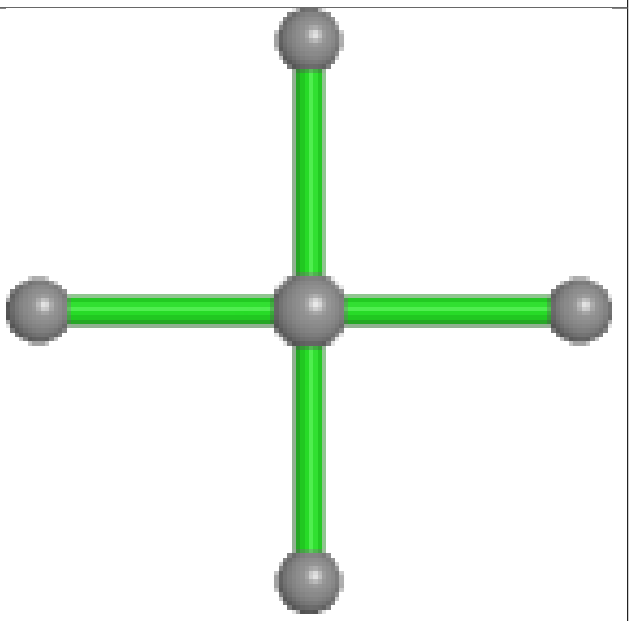


Rings

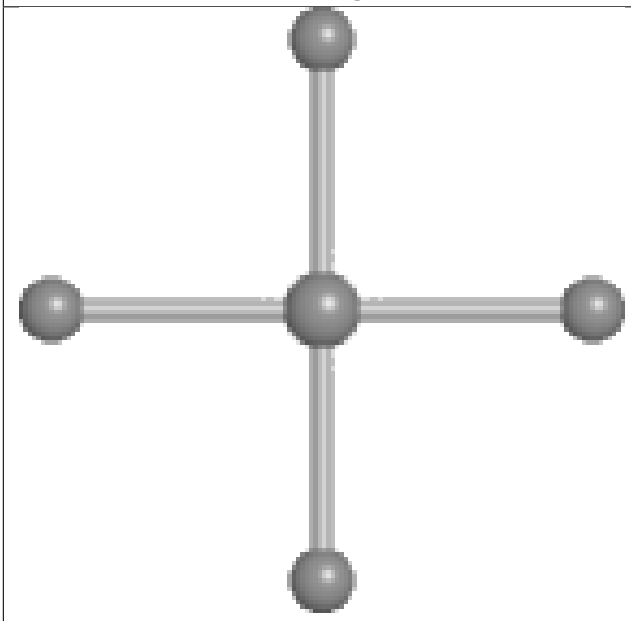
Ligand SO4 H 404



Bond lengths



Bond angles



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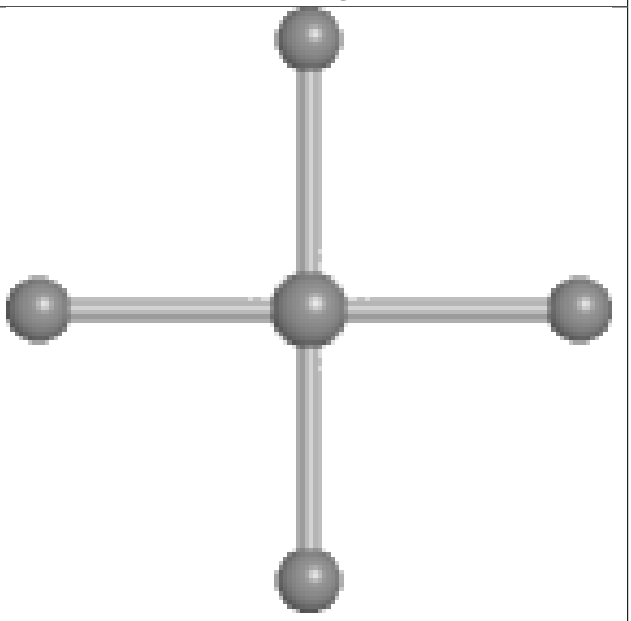
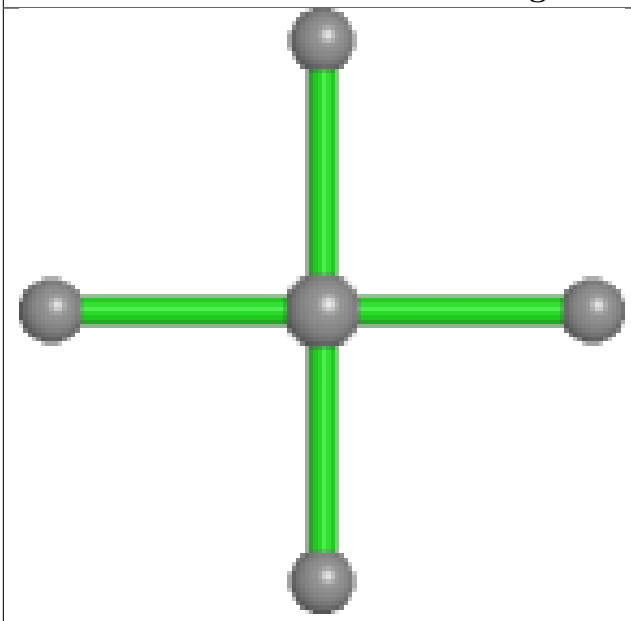


Rings

Ligand SO4 C 405



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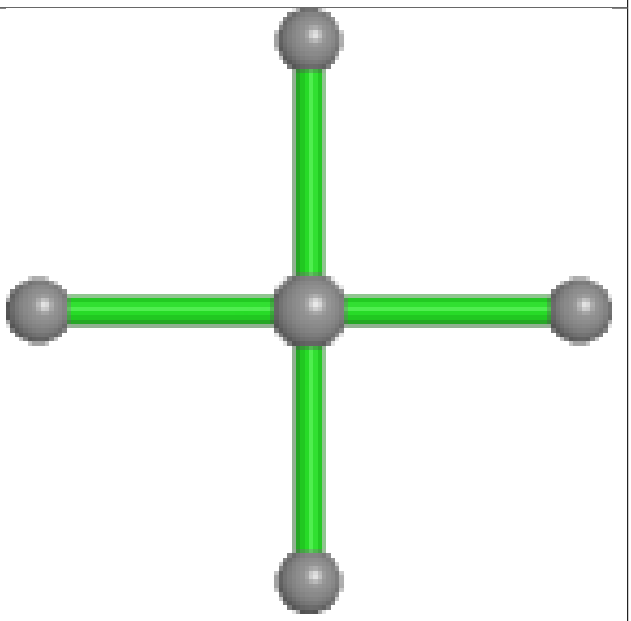
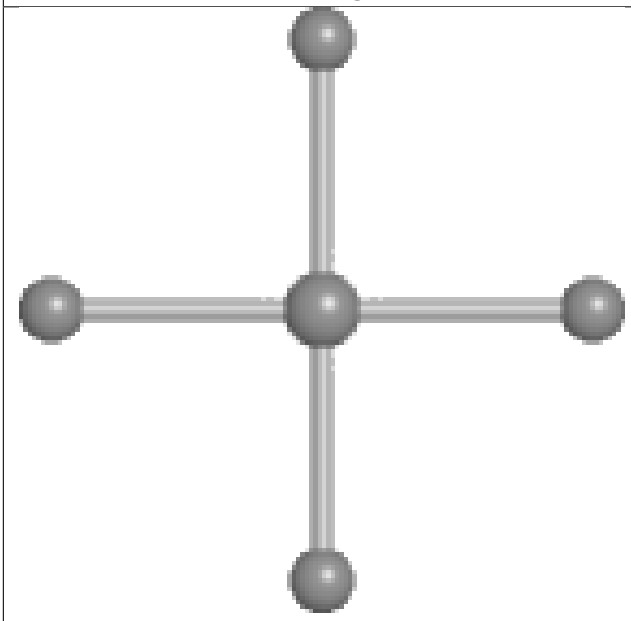
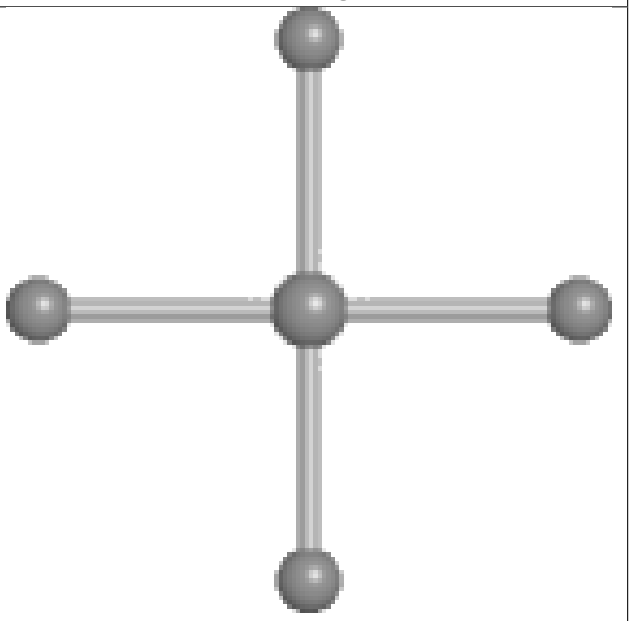


Bond angles

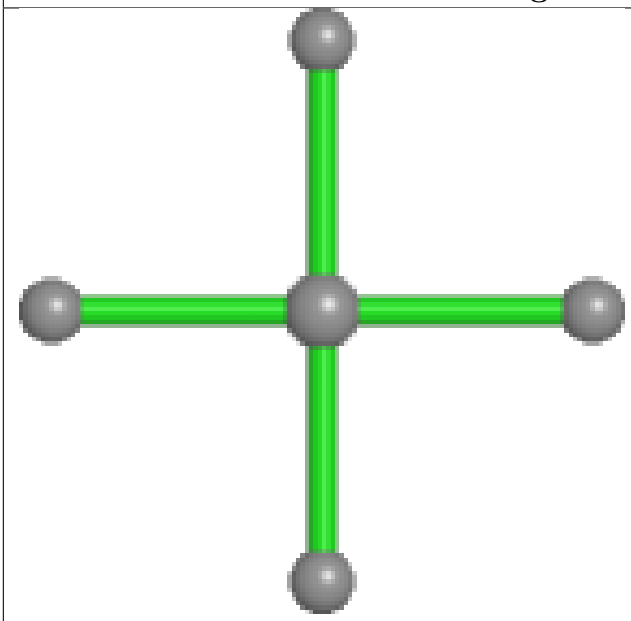


Torsions



Rings

Ligand SO4 E 404



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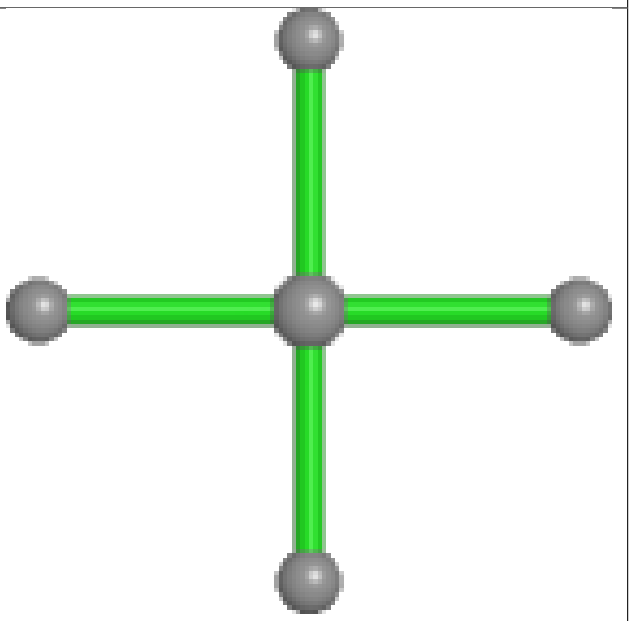

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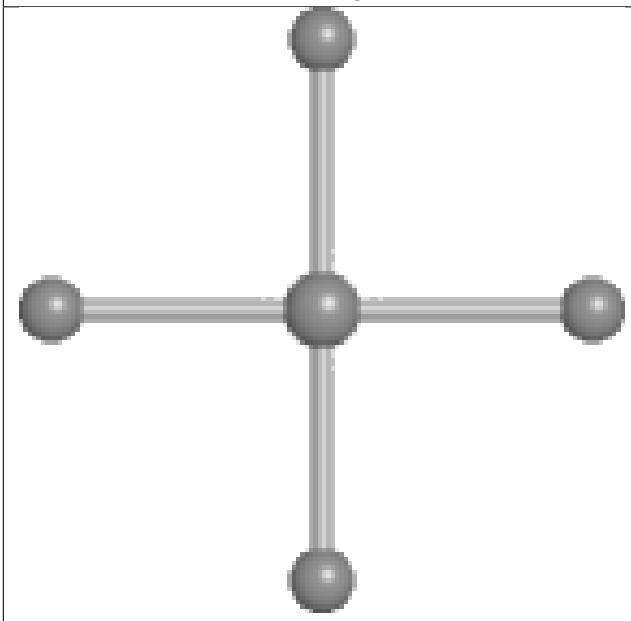

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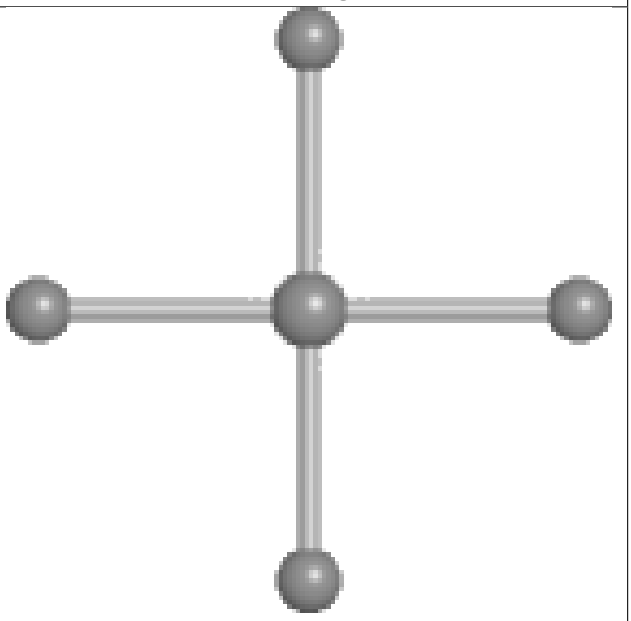
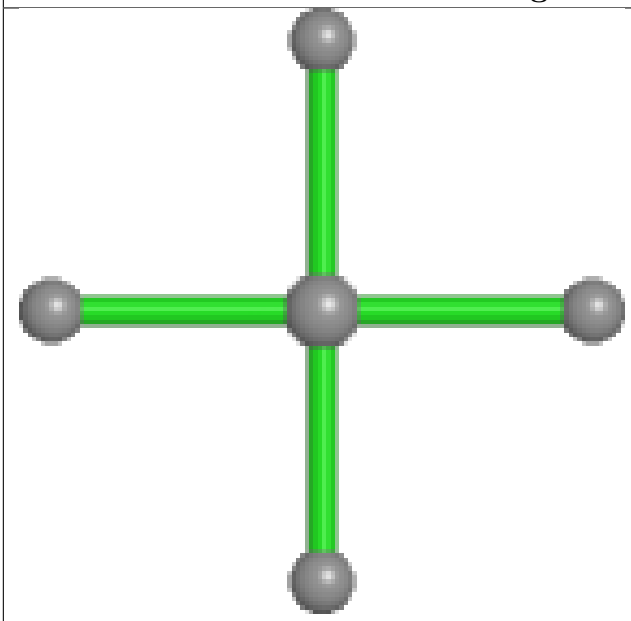


Rings

Ligand SO4 E 405



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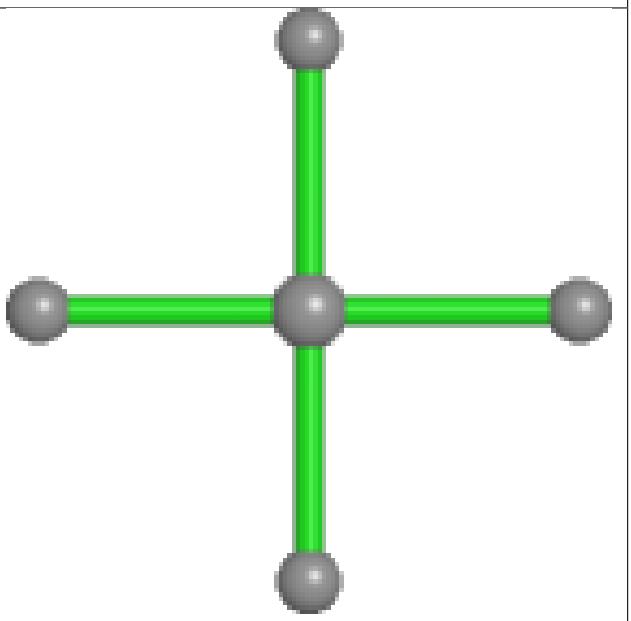

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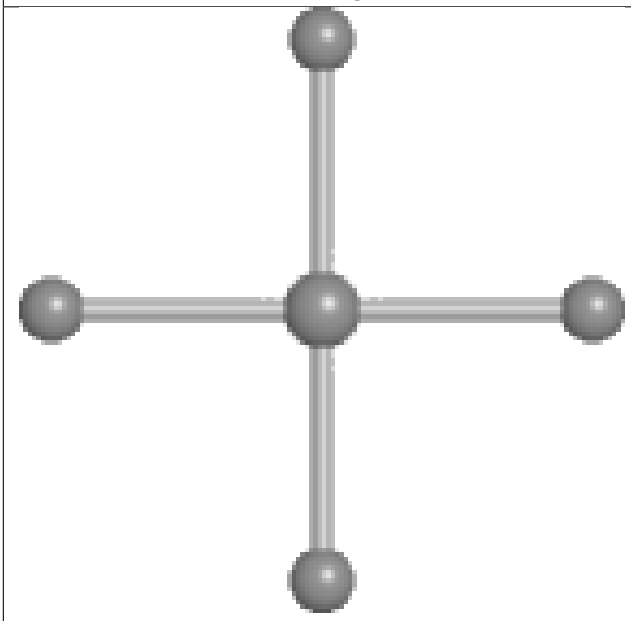

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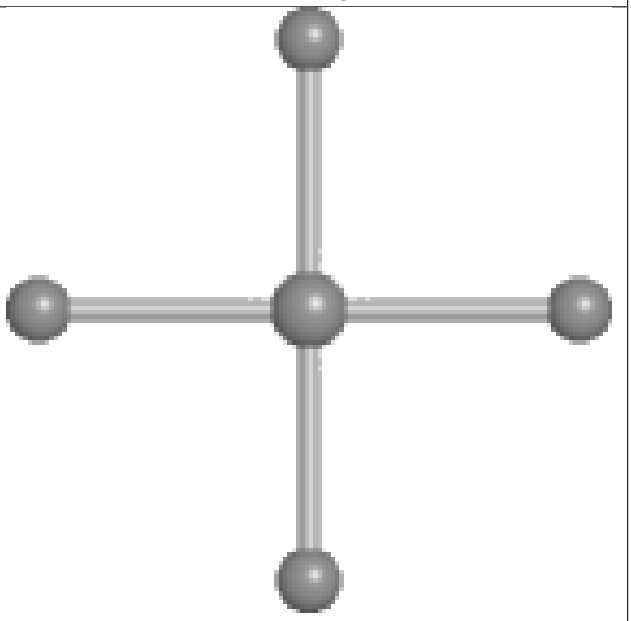
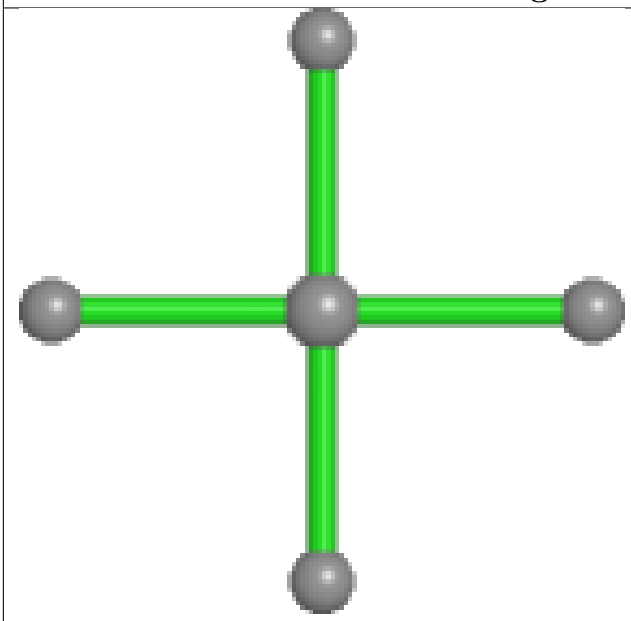


Rings

Ligand SO4 F 403



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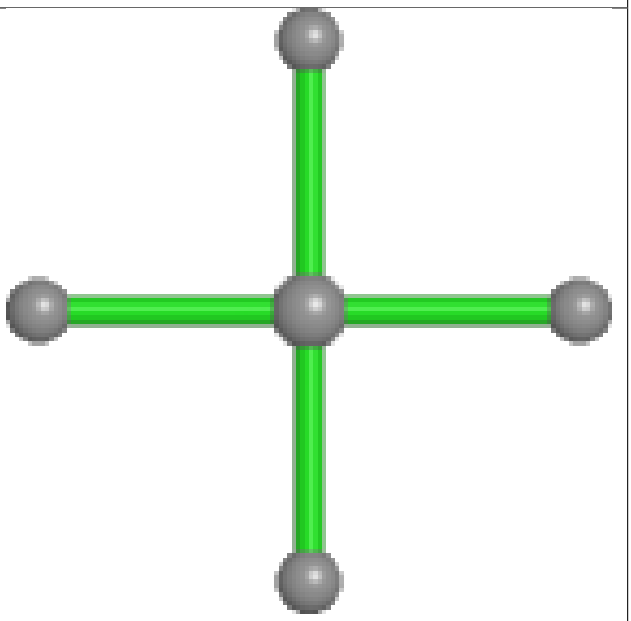

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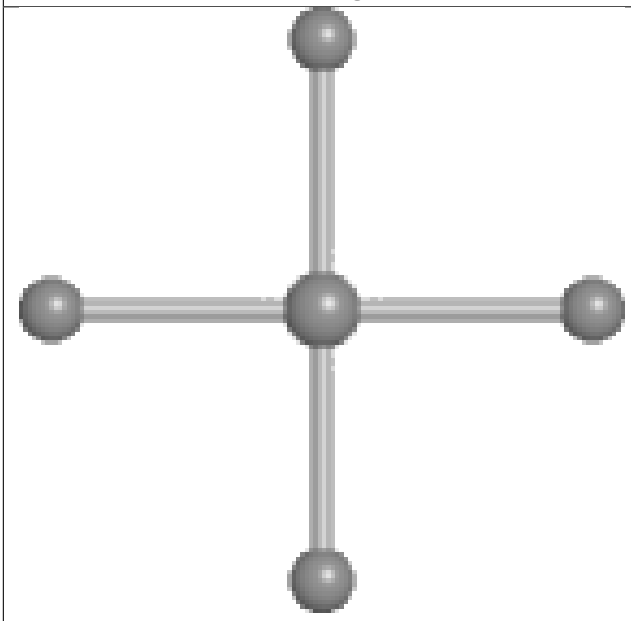

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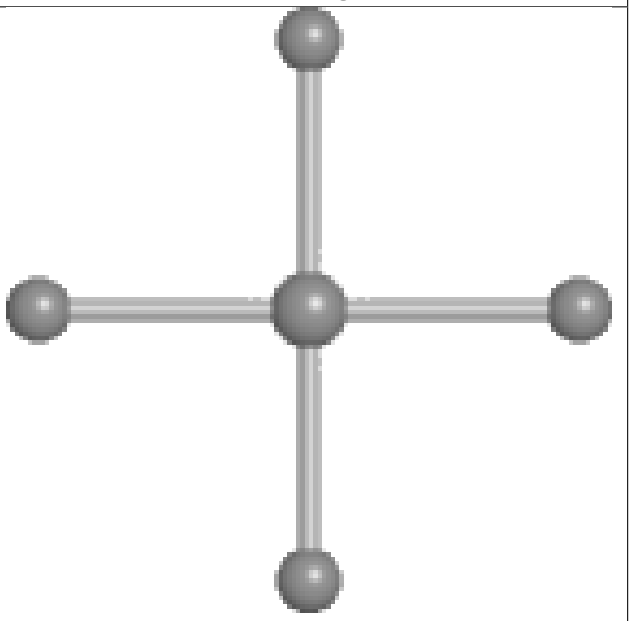
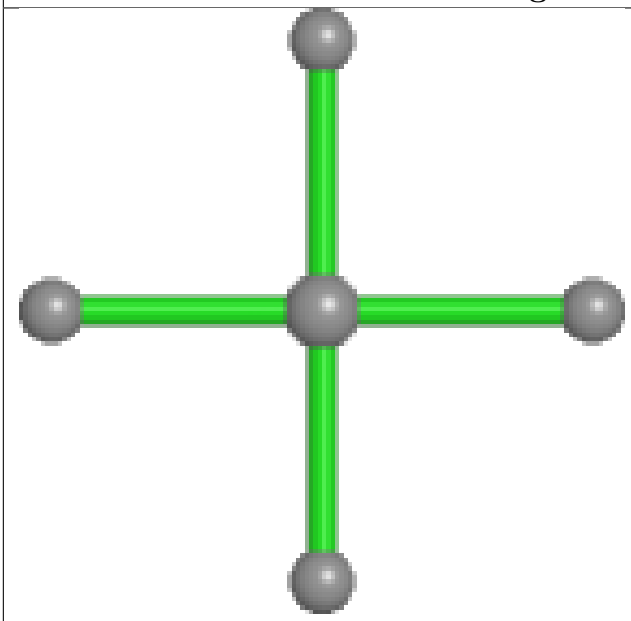


Rings

Ligand SO4 B 405



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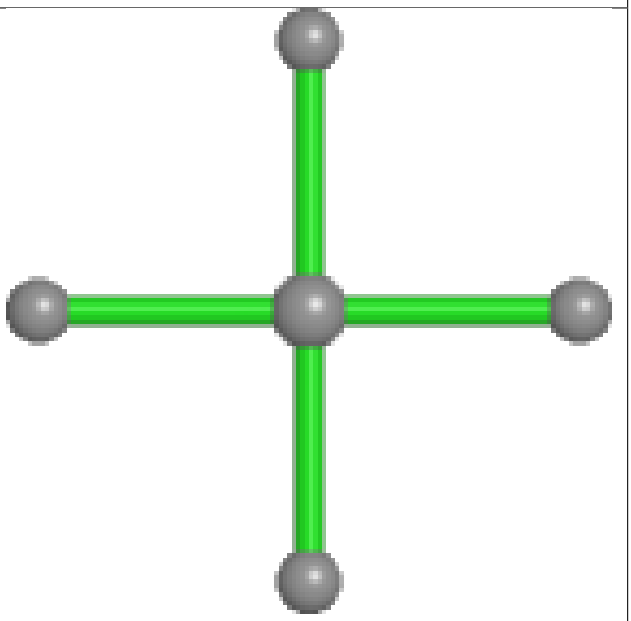

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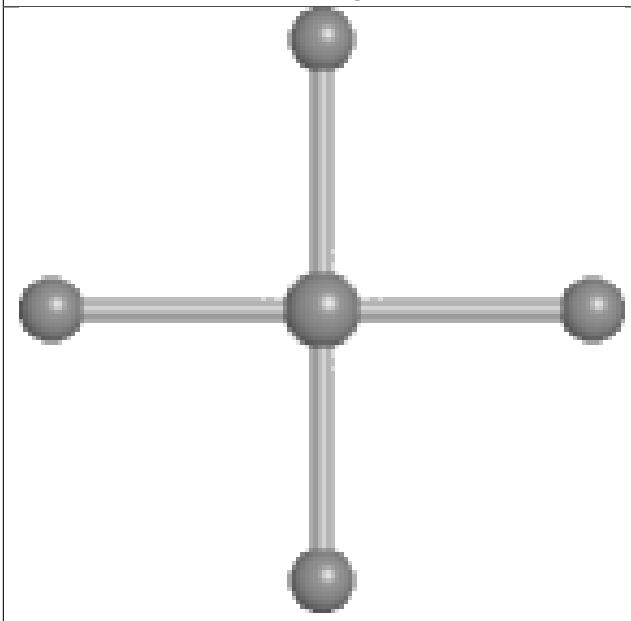

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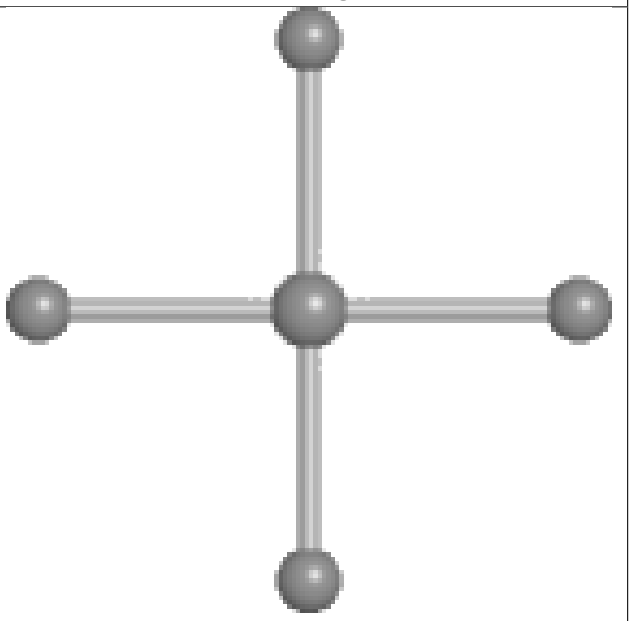
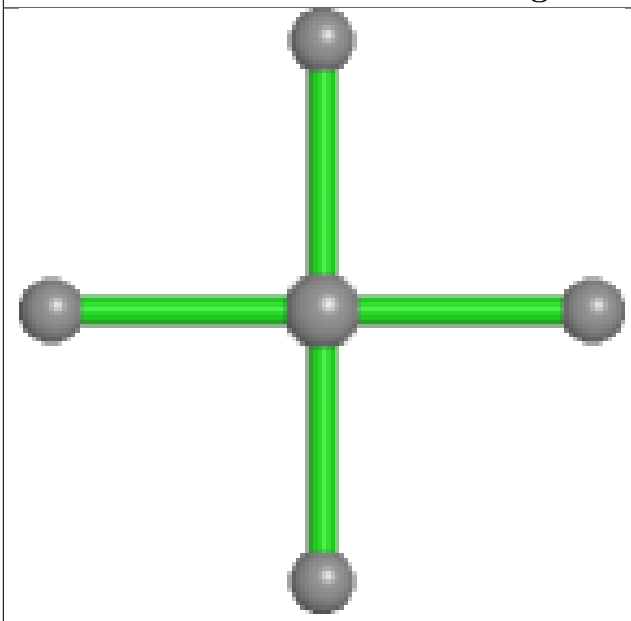


Rings

Ligand SO4 F 402



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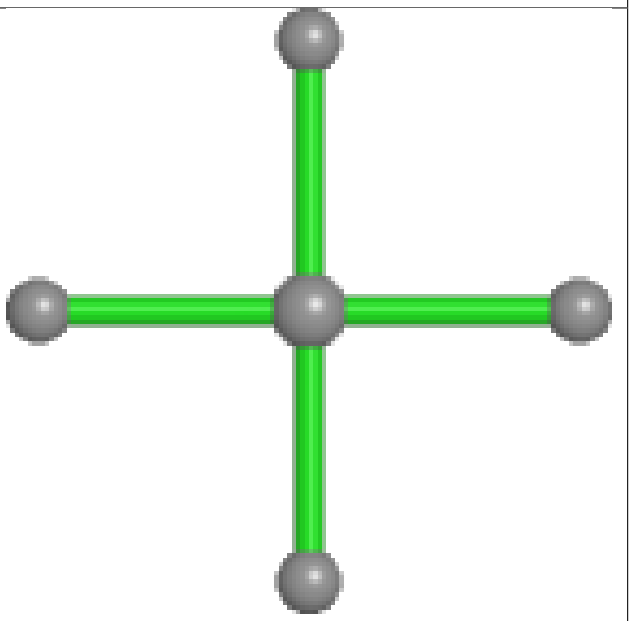

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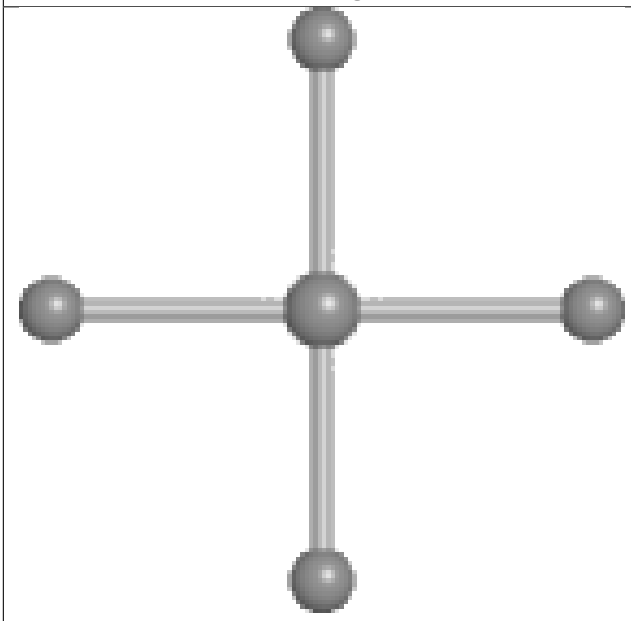

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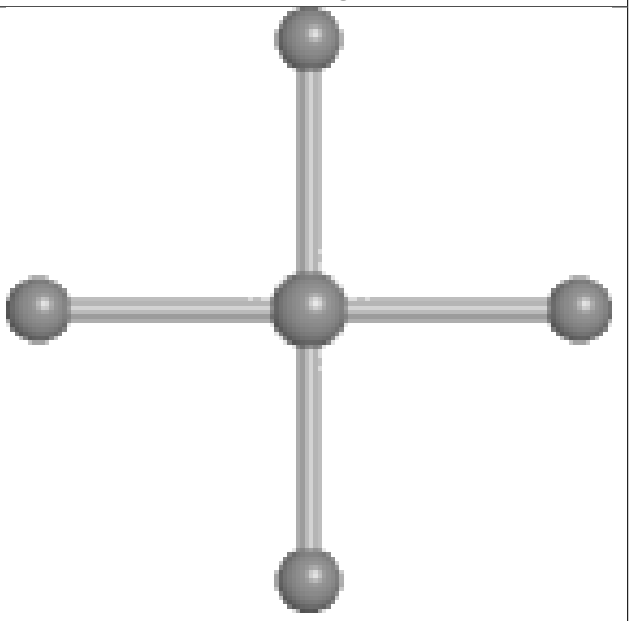
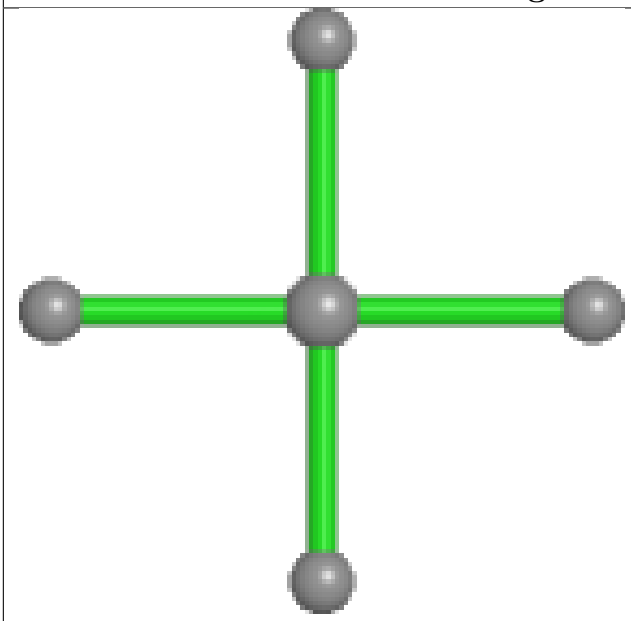


Rings

Ligand SO4 H 401



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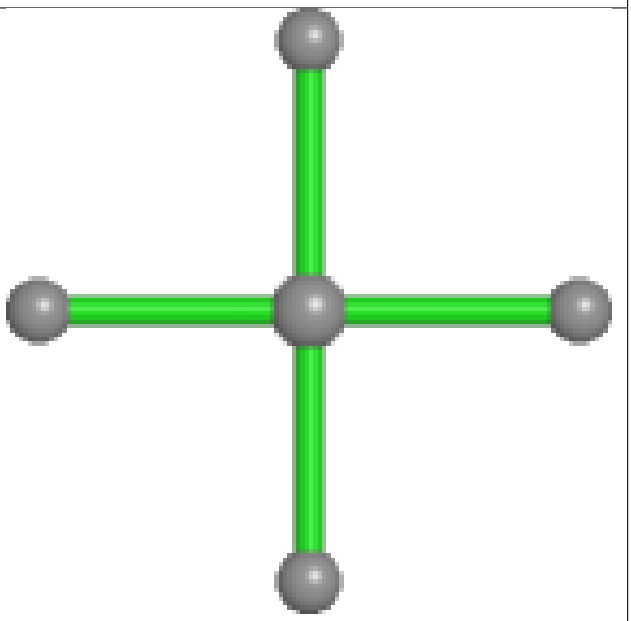

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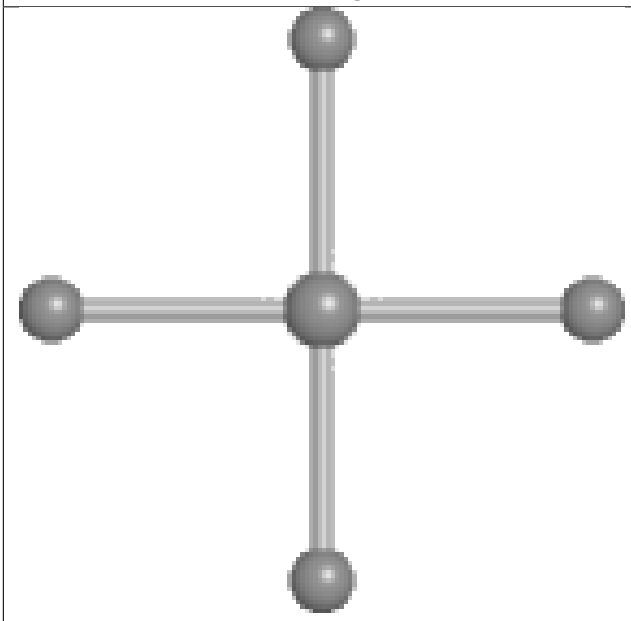

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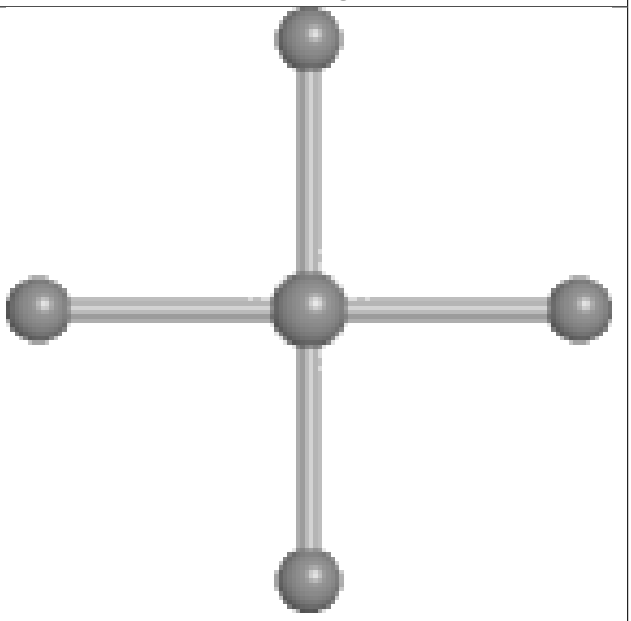
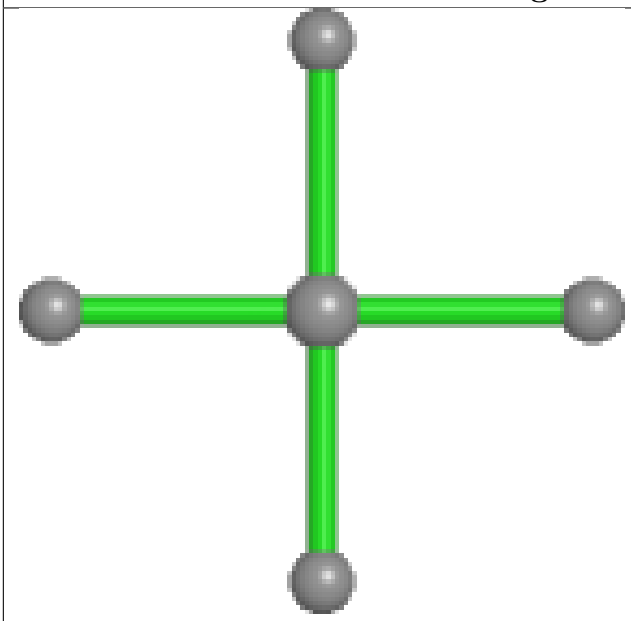


Rings

Ligand SO4 F 404



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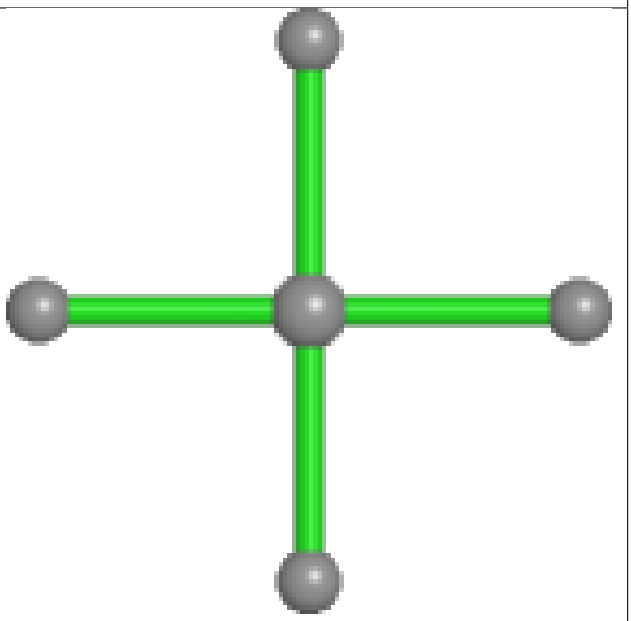

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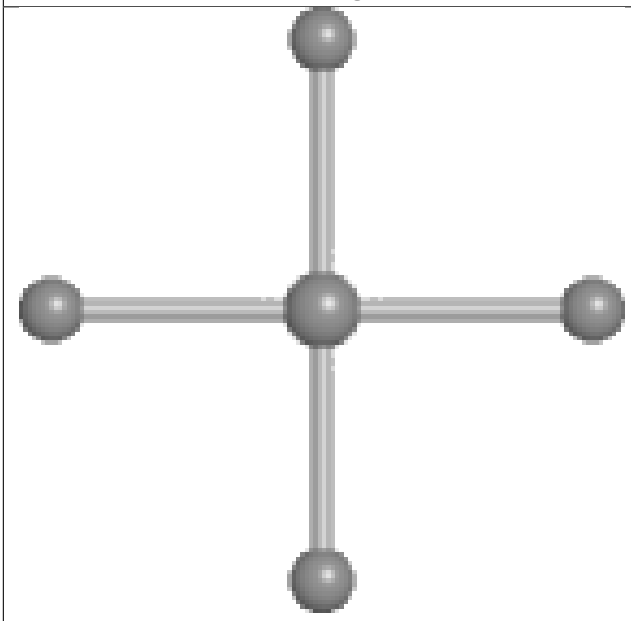

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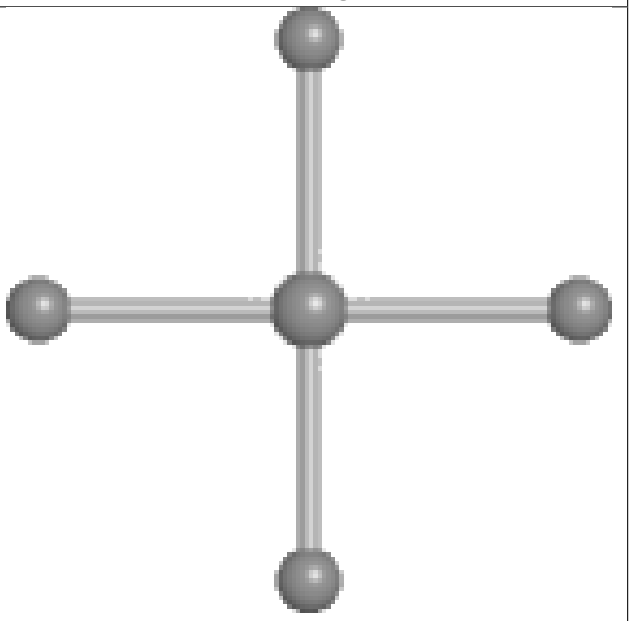
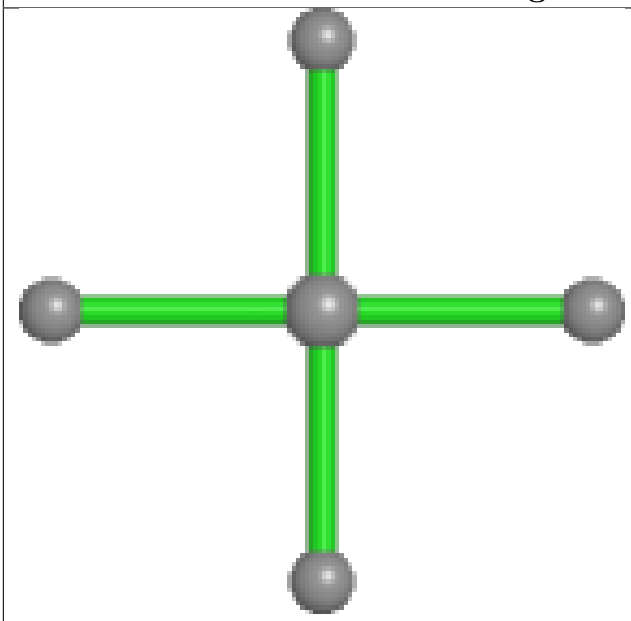


Rings

Ligand SO4 D 402



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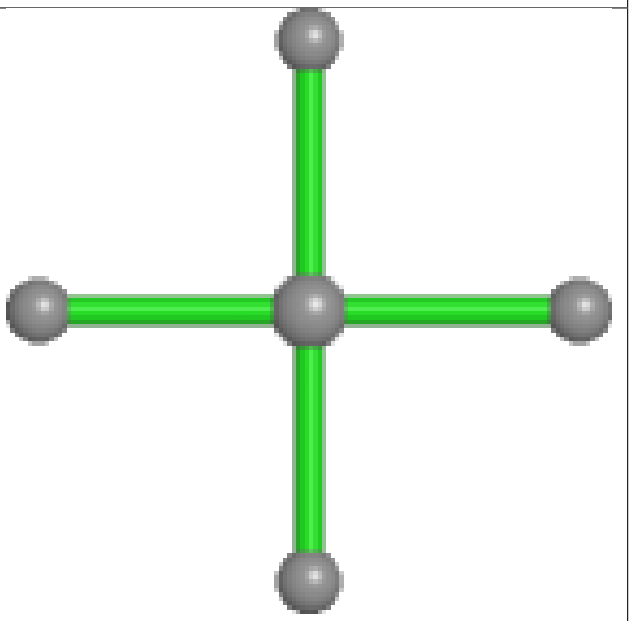
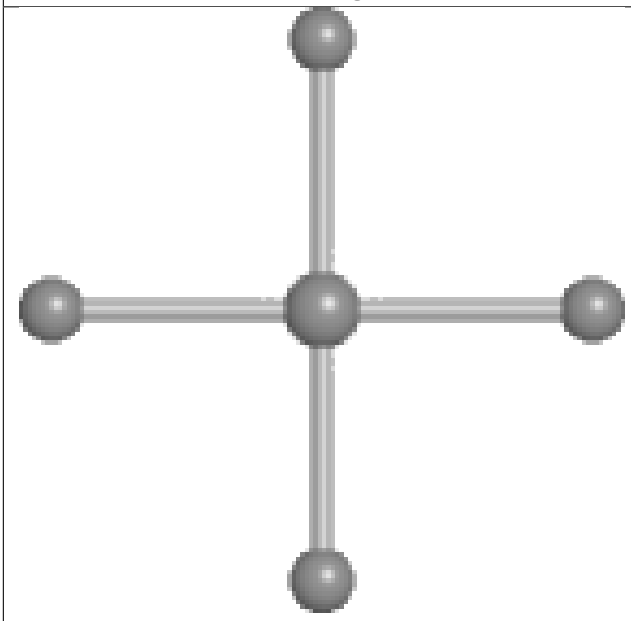


Bond angles



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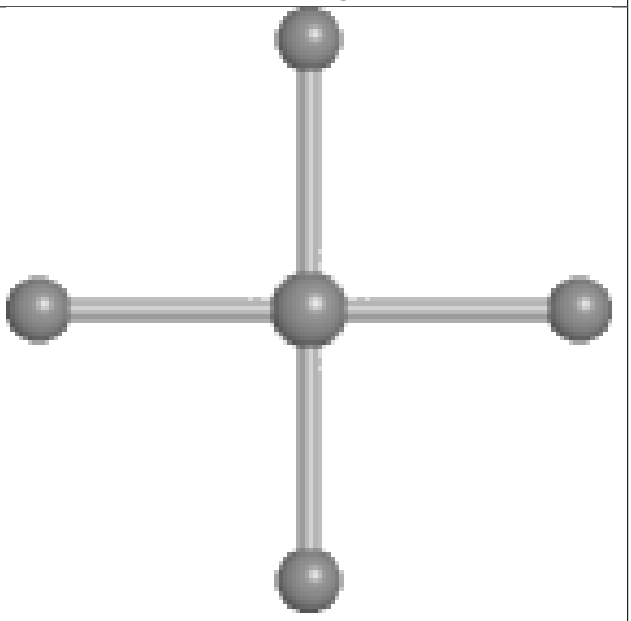
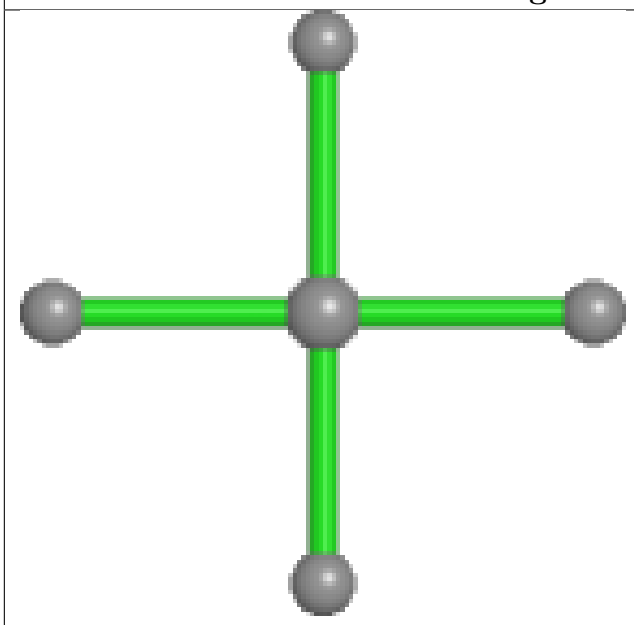


Rings

Ligand SO4 D 403



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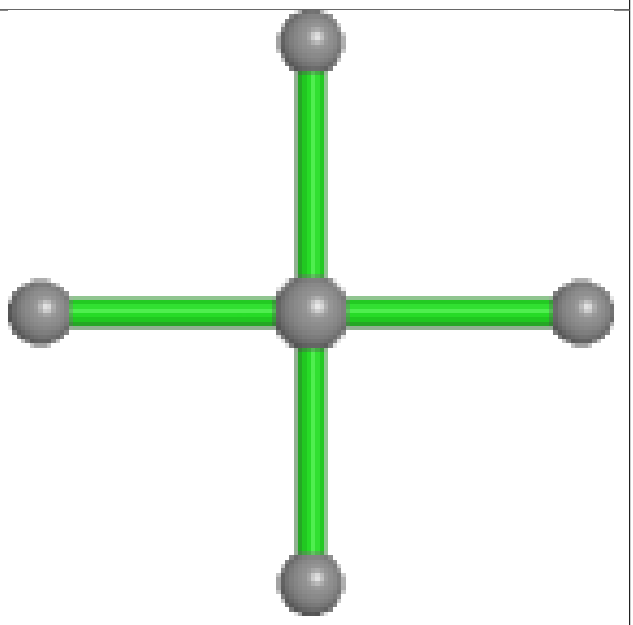

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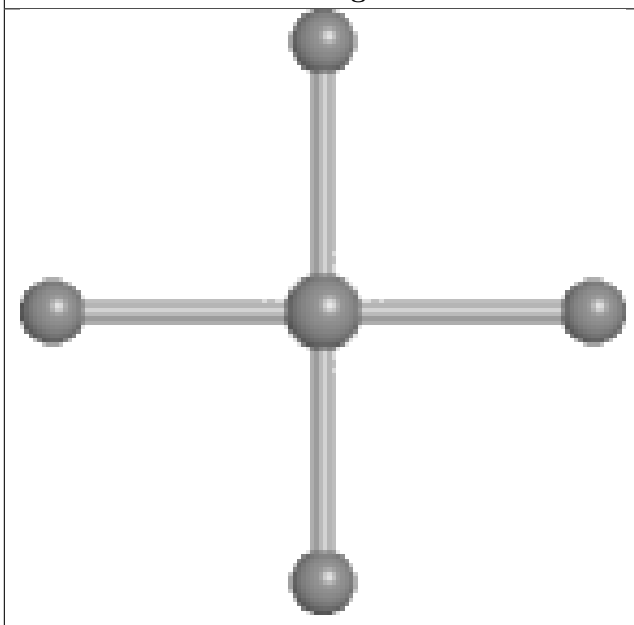
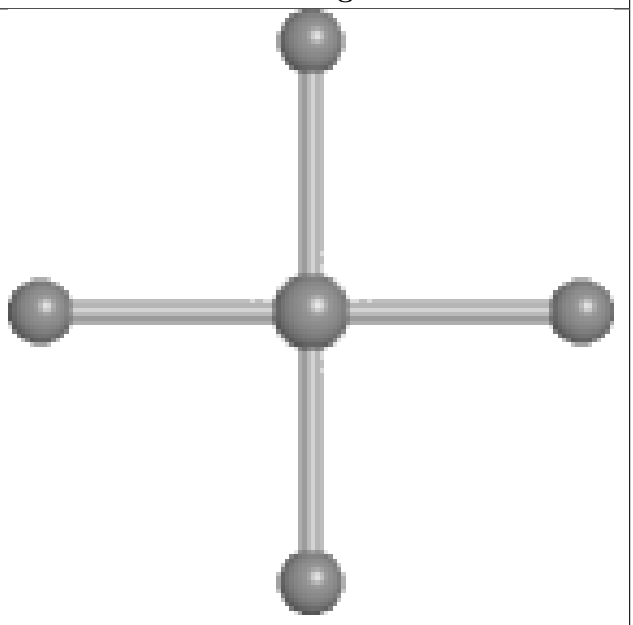
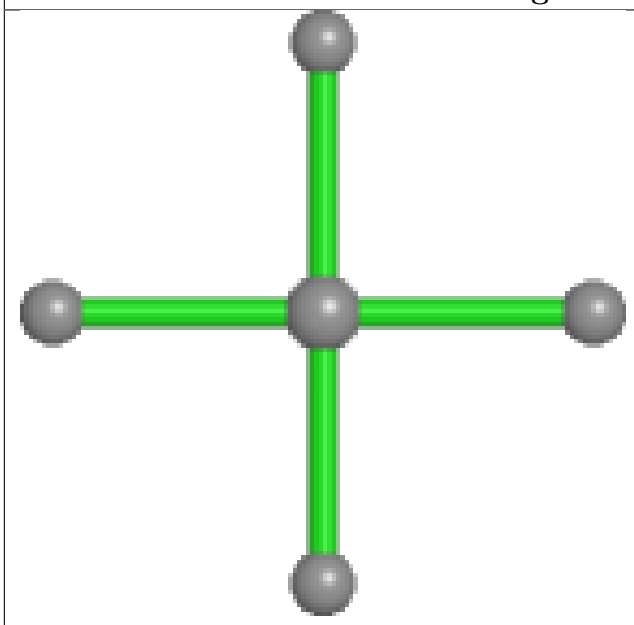


Torsions



Rings

Ligand SO4 E 401



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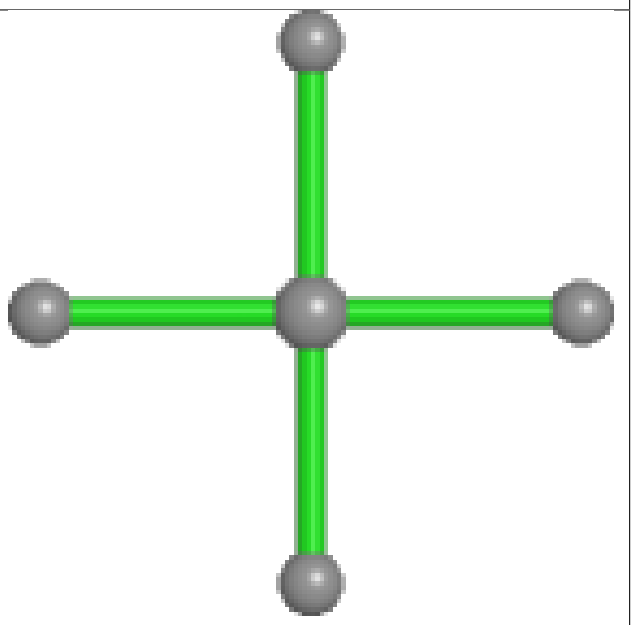

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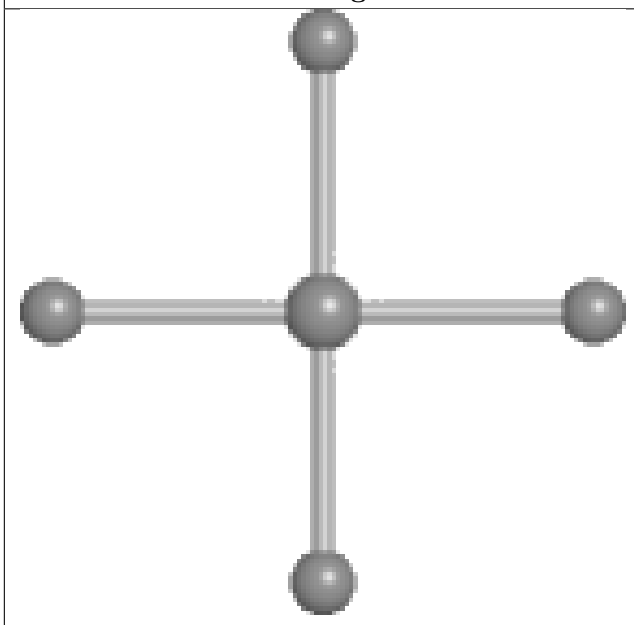

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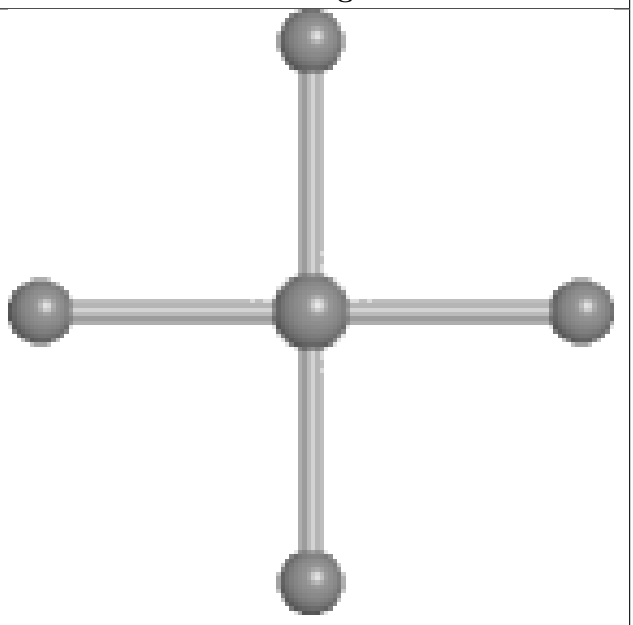
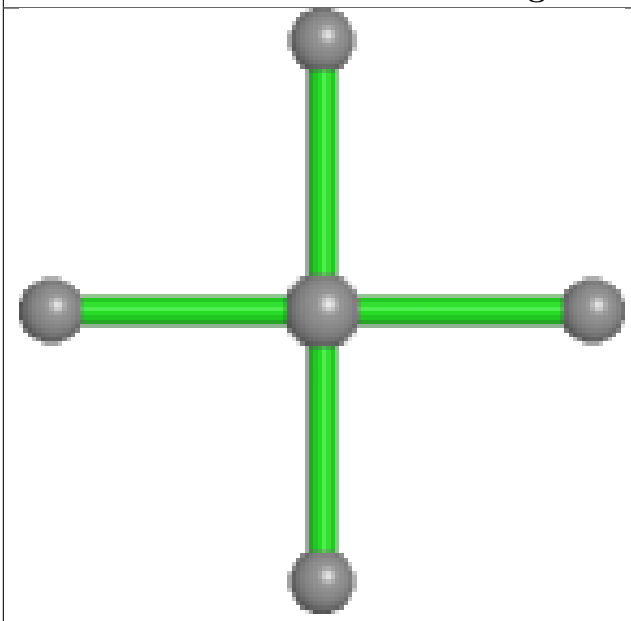


Rings

Ligand SO4 G 401



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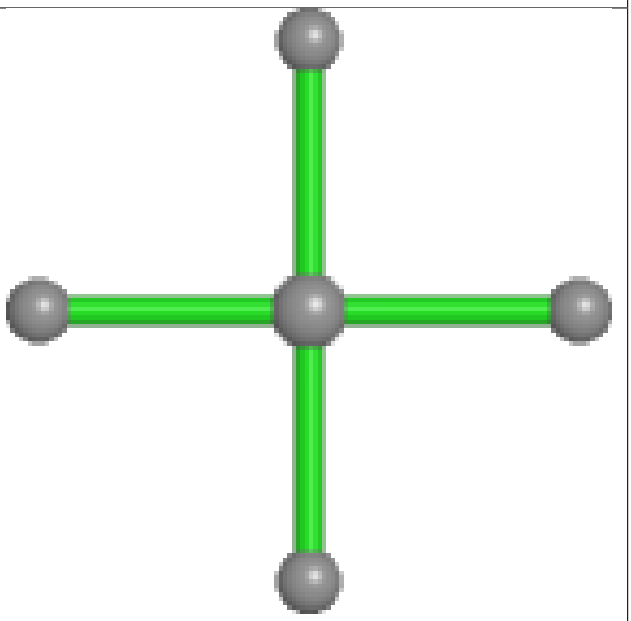

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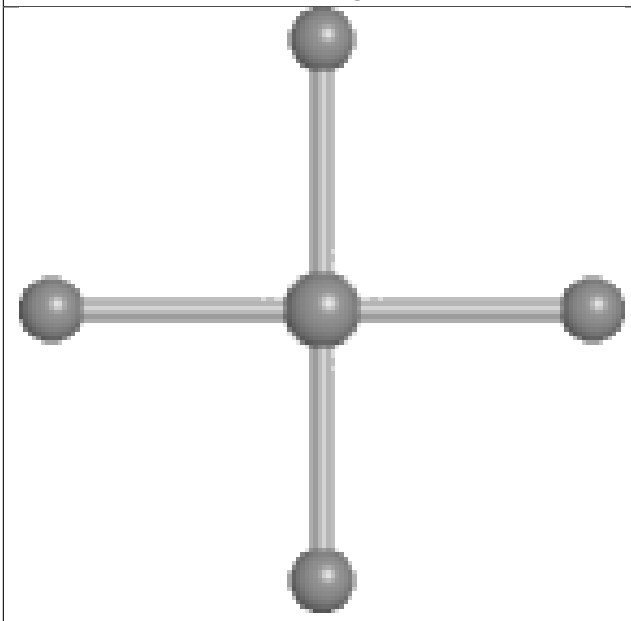

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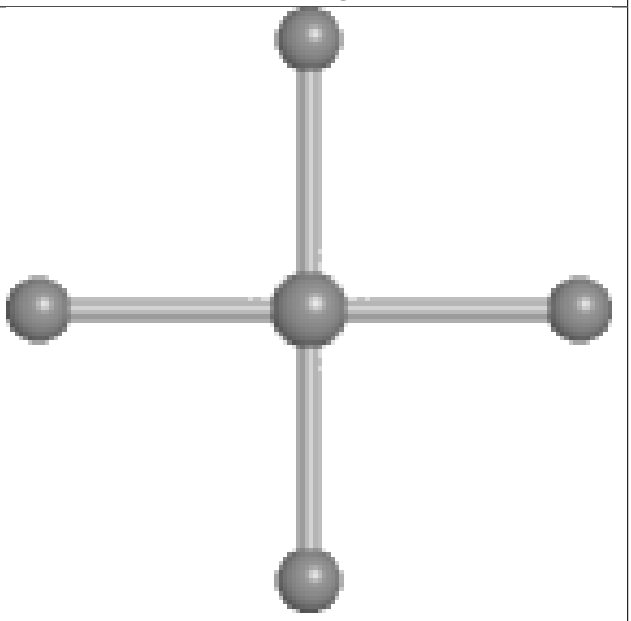
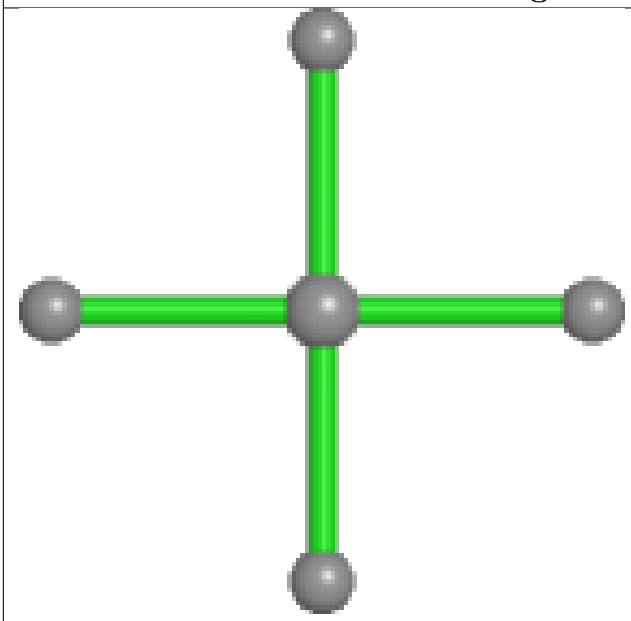


Rings

Ligand SO4 E 411



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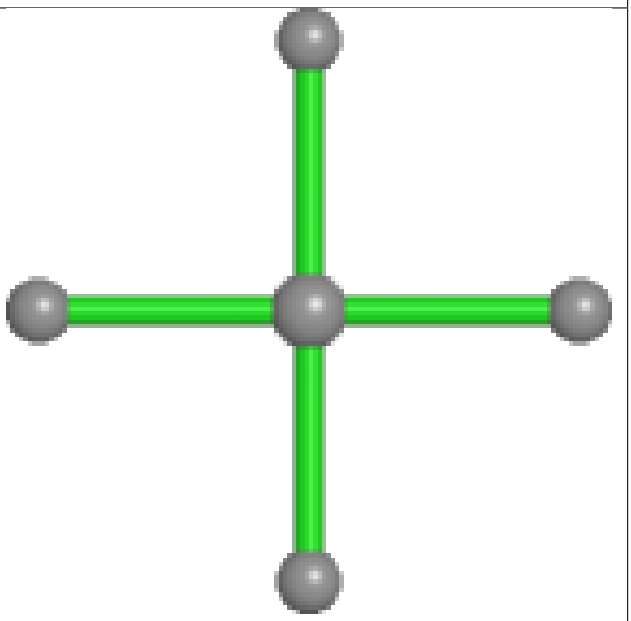

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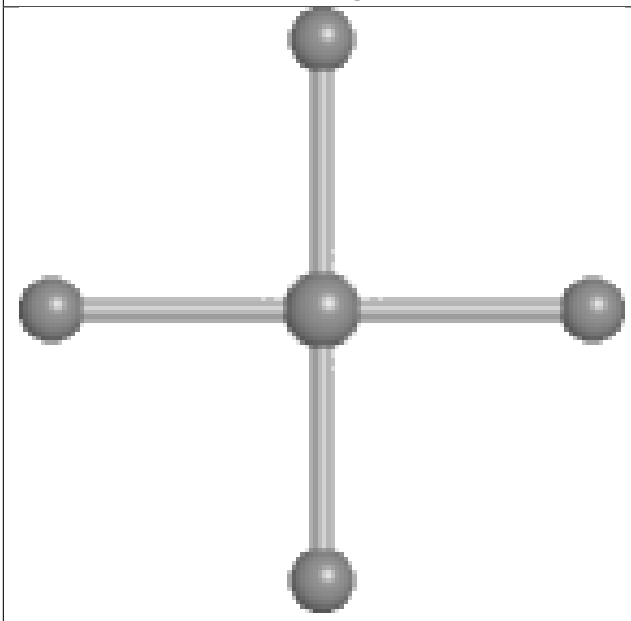

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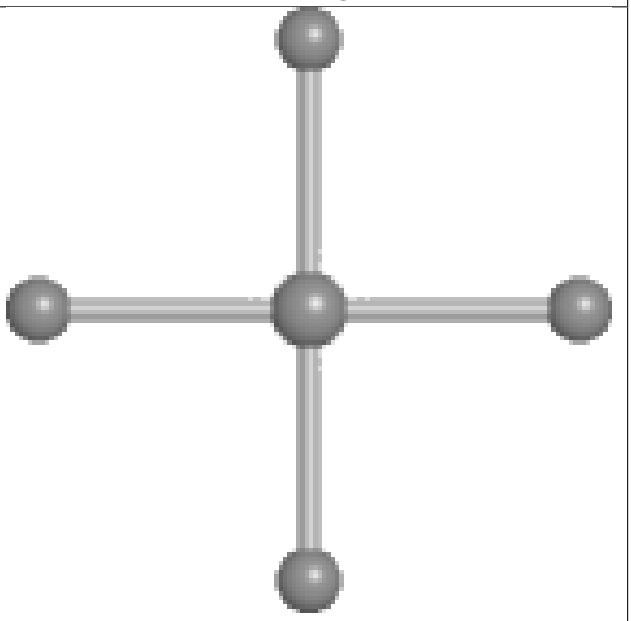
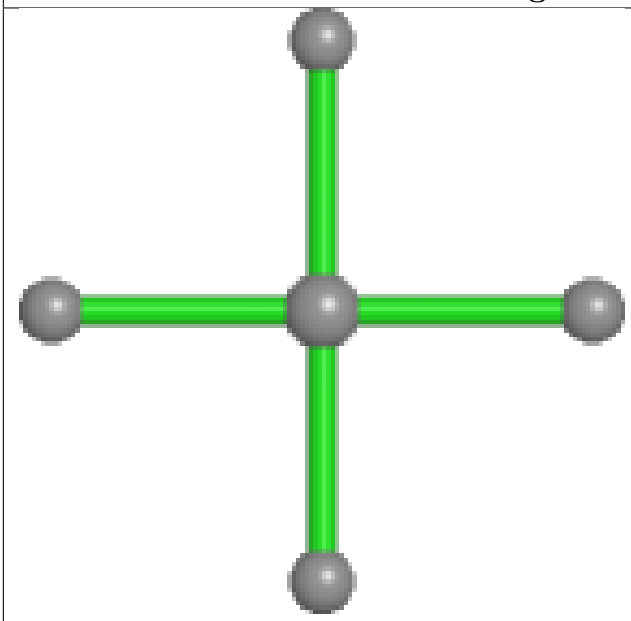


Rings

Ligand SO4 A 405



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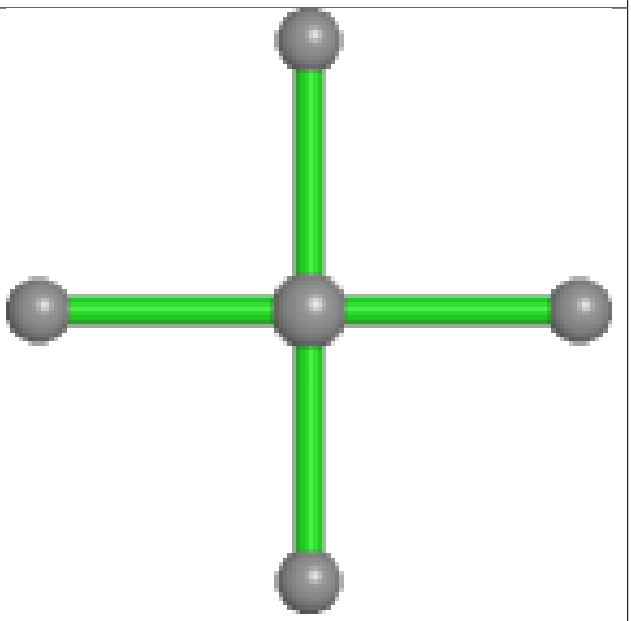
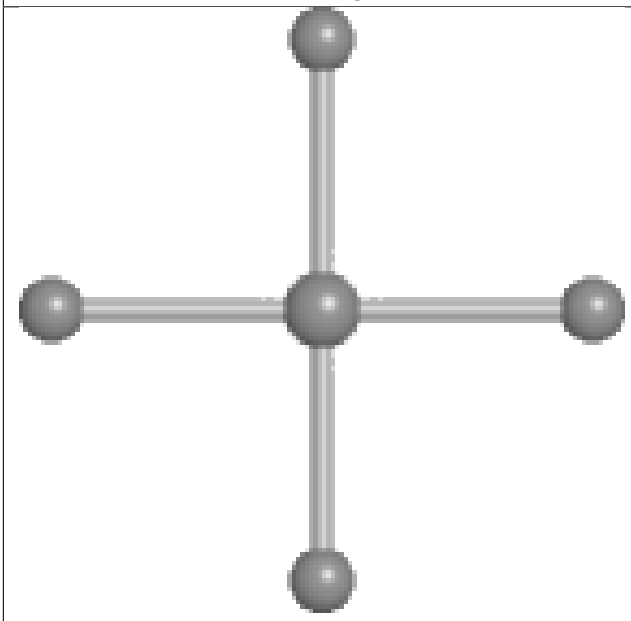


Bond angles



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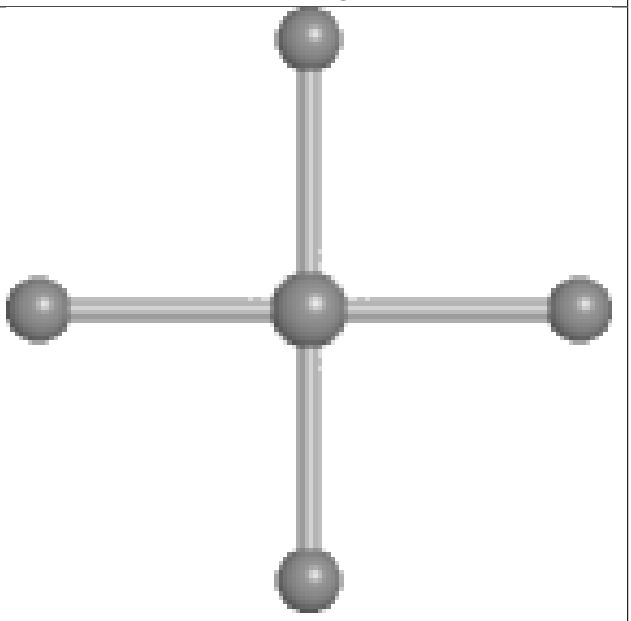
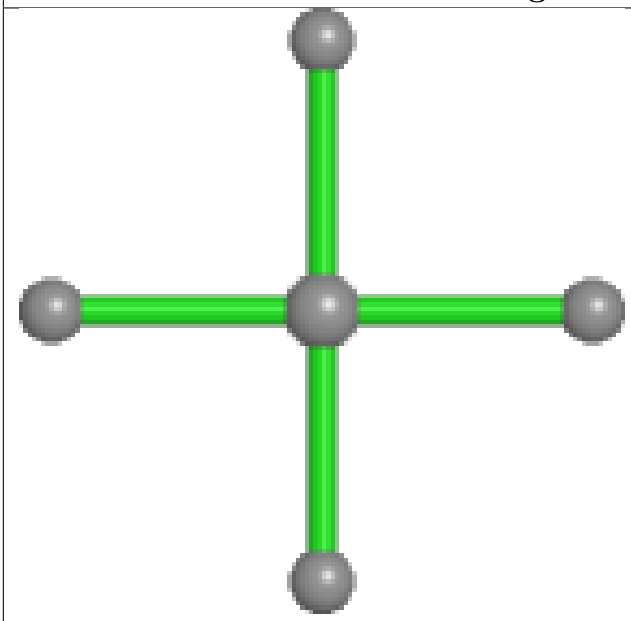


Rings

Ligand SO4 D 401



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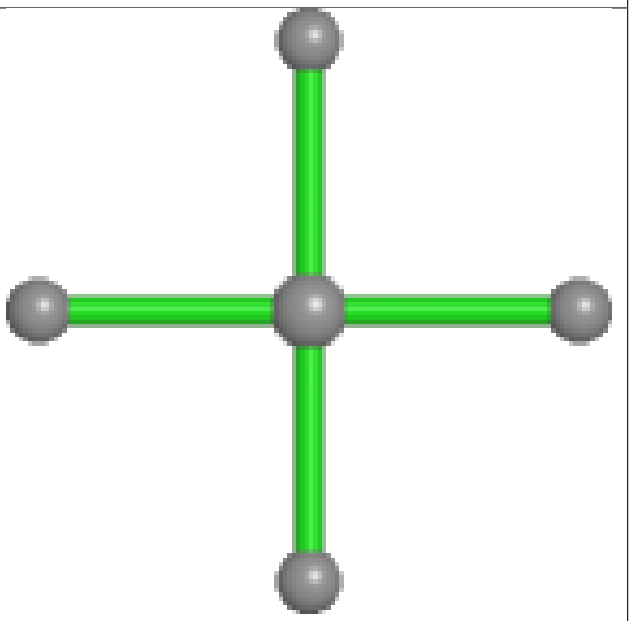

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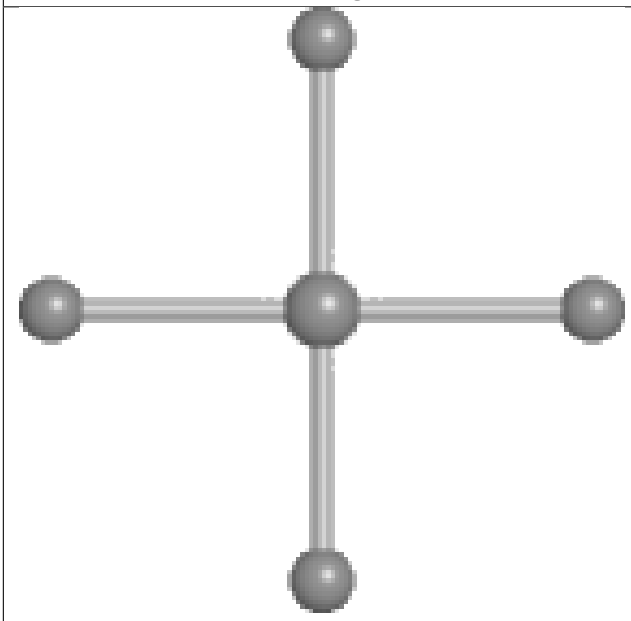
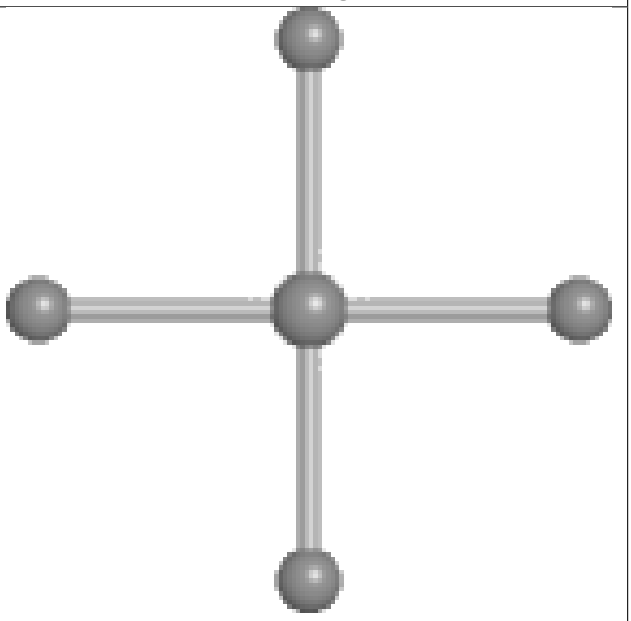
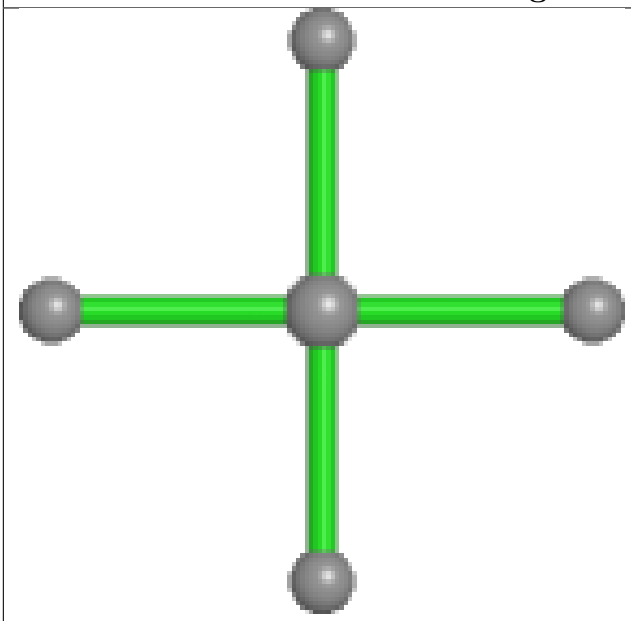


Torsions

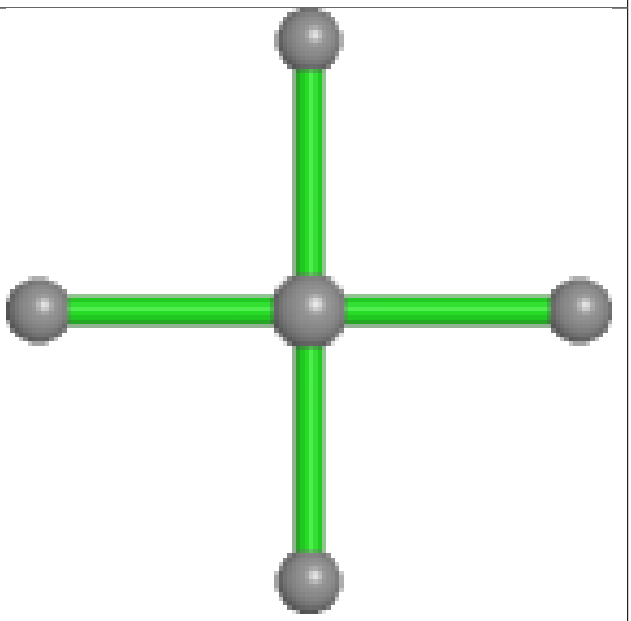


Rings

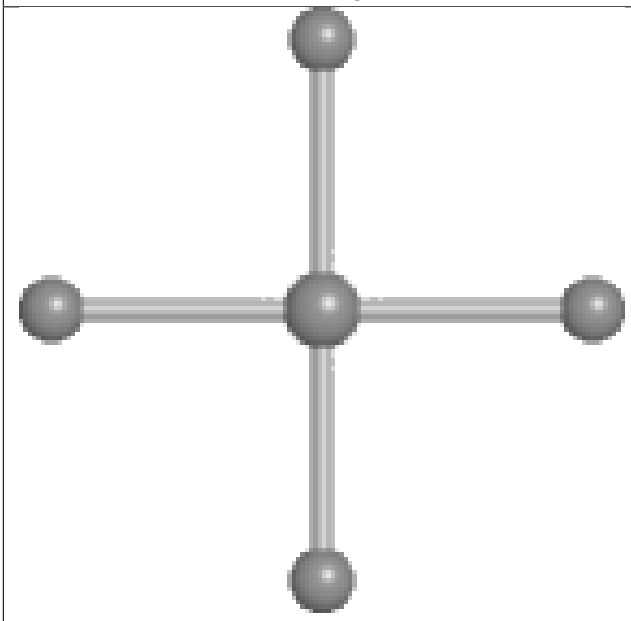
Ligand SO4 B 402



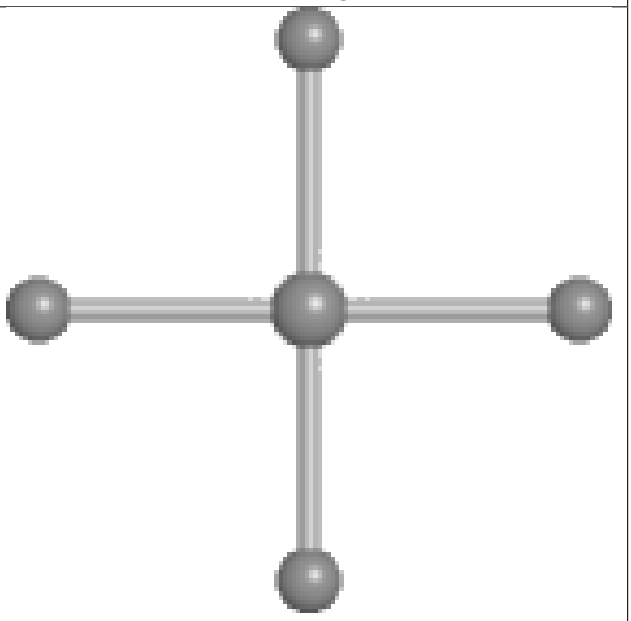
Bond lengths



Bond angles

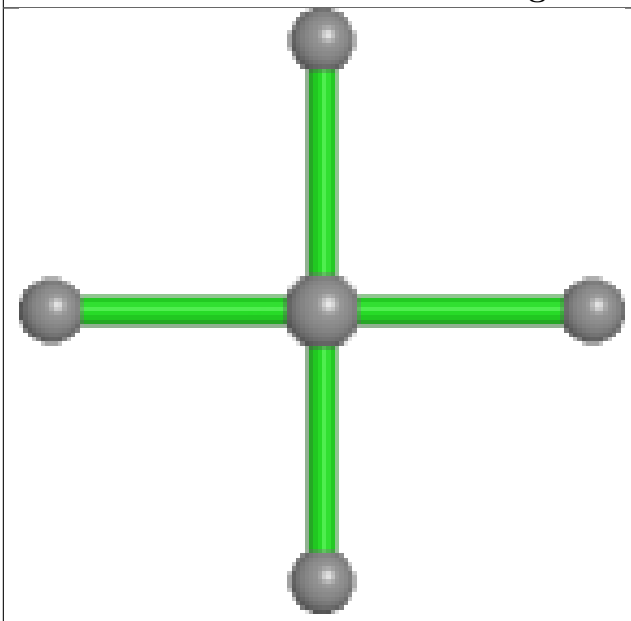


Torsions



Rings

Ligand SO4 A 406



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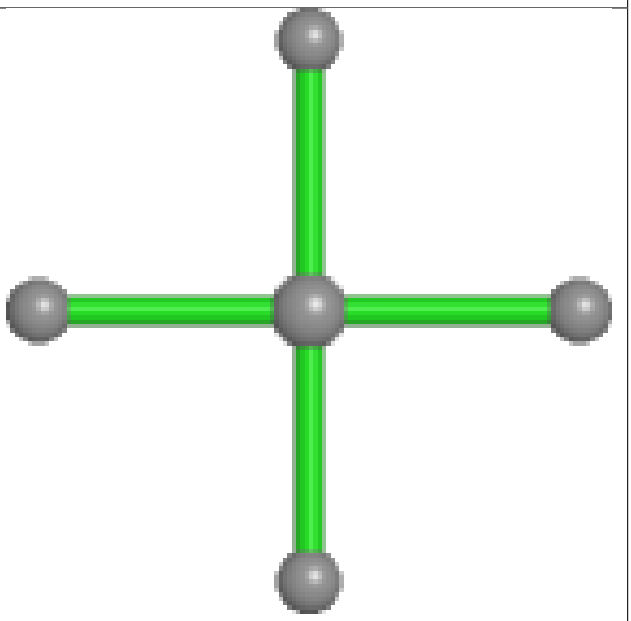

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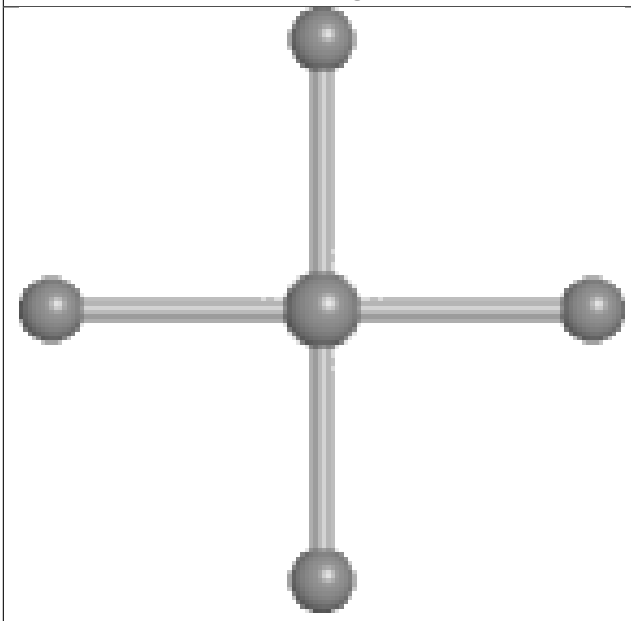

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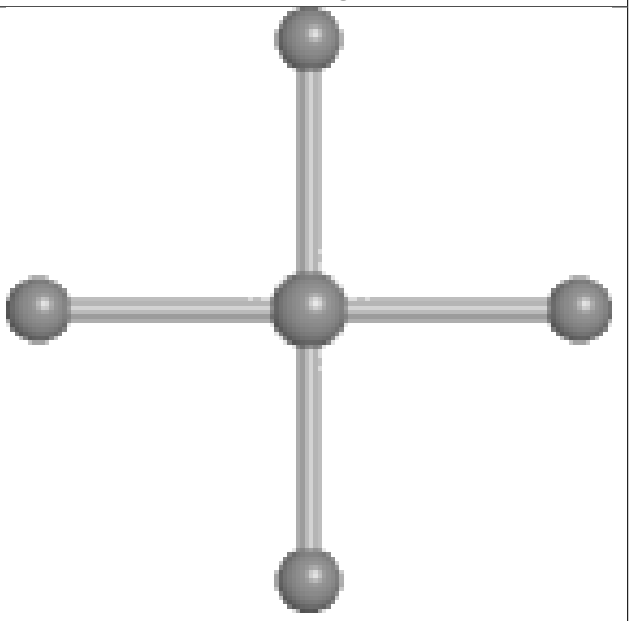
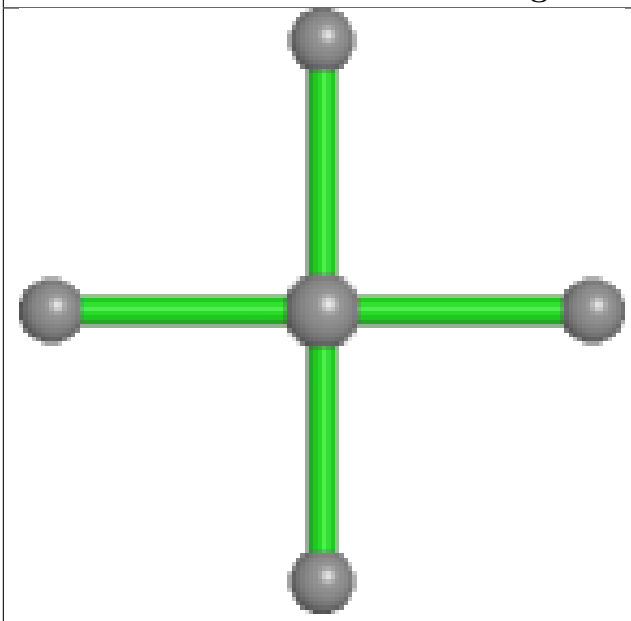


Rings

Ligand SO4 E 403



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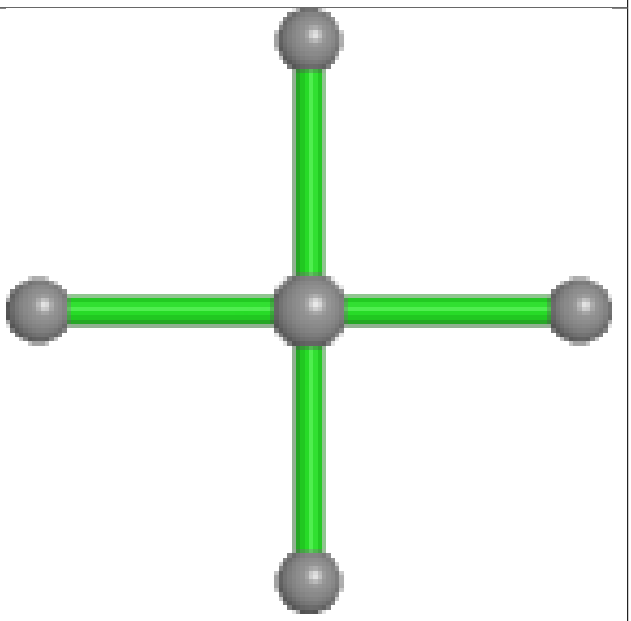

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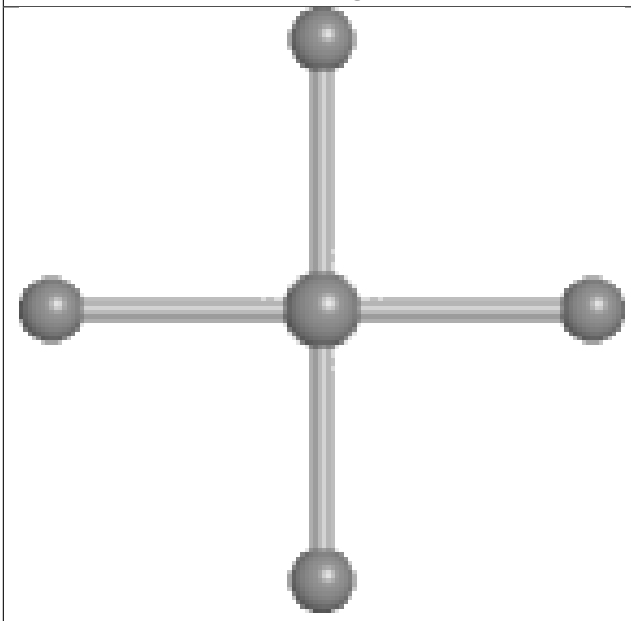

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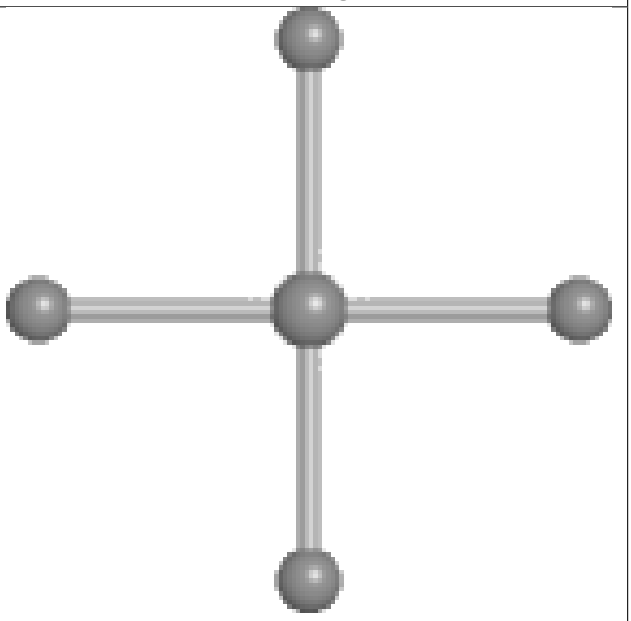
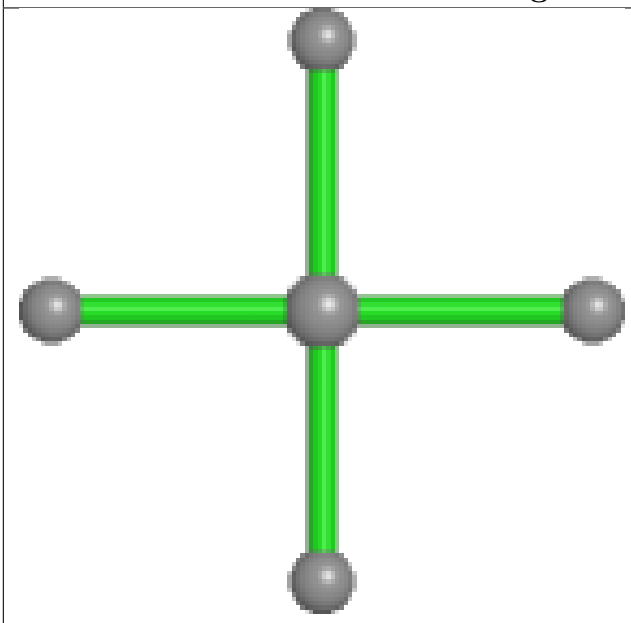


Rings

Ligand SO4 E 413



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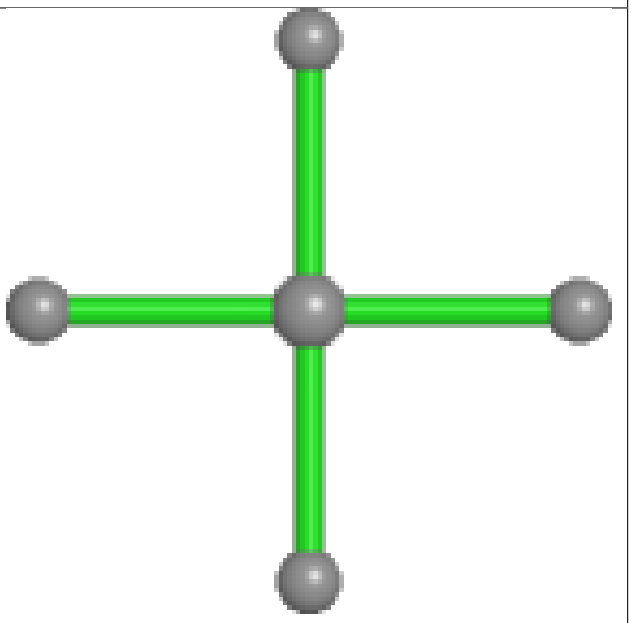

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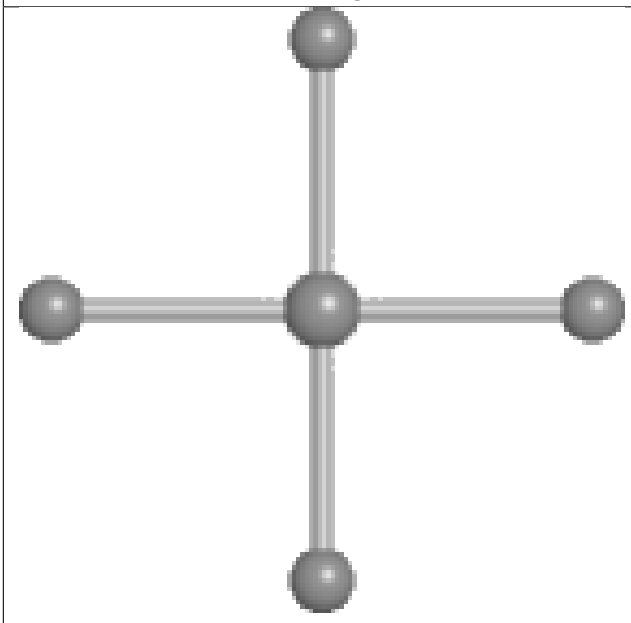

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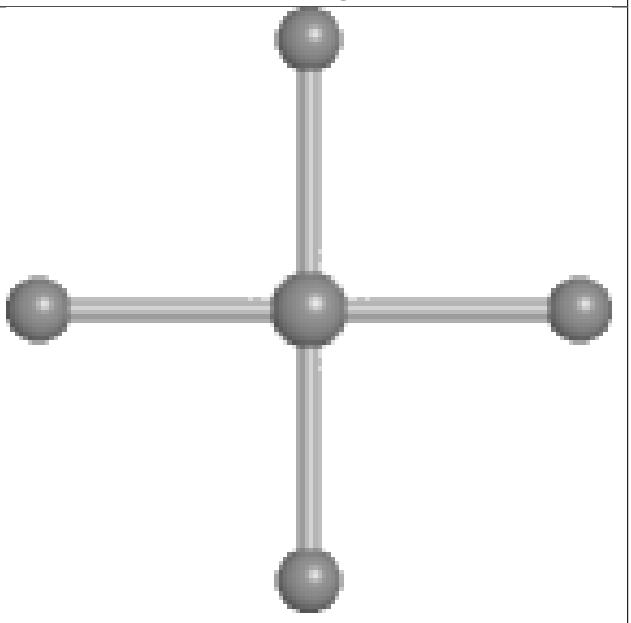
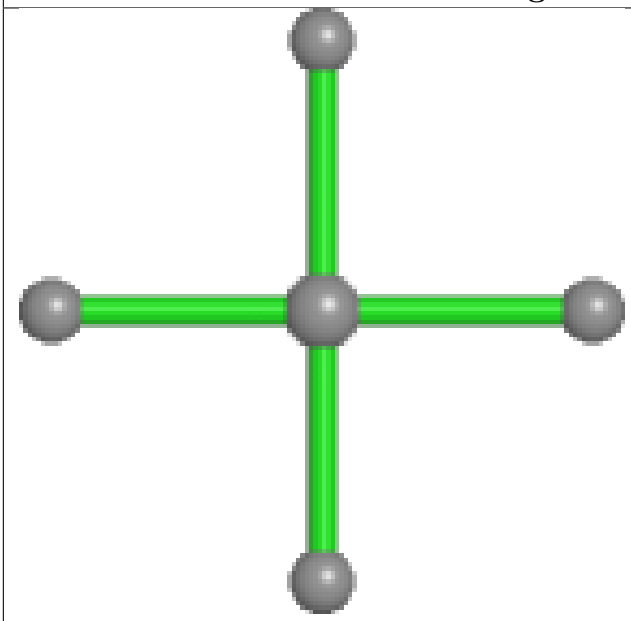


Rings

Ligand SO4 G 404



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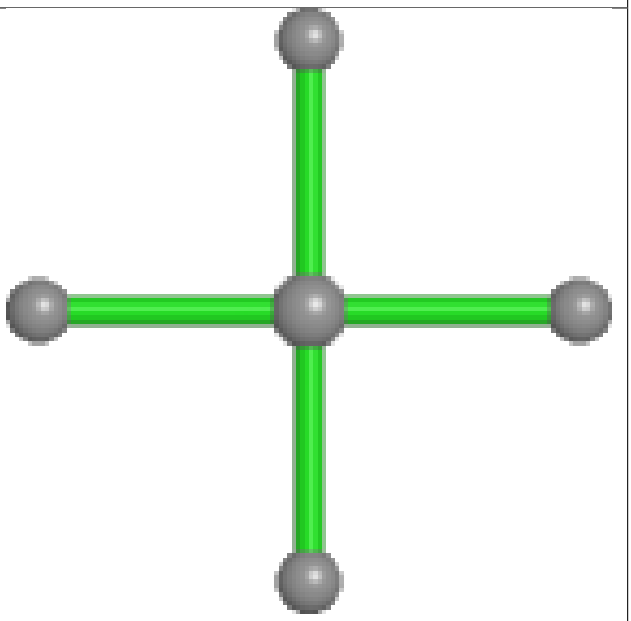
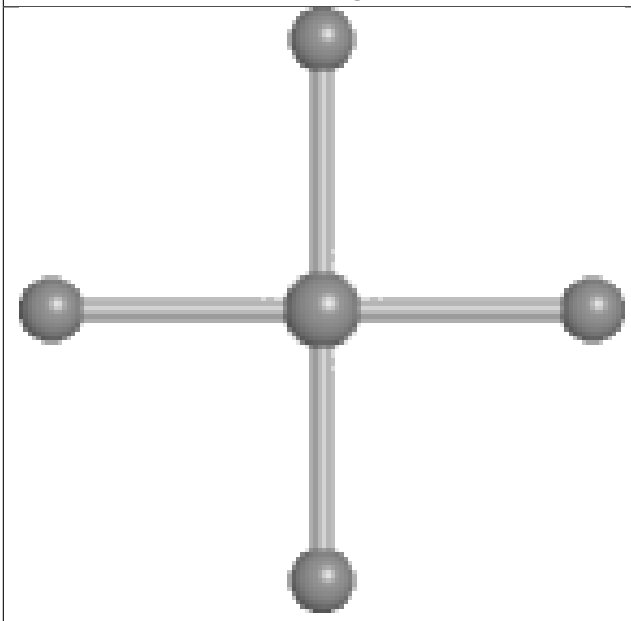


Bond angles



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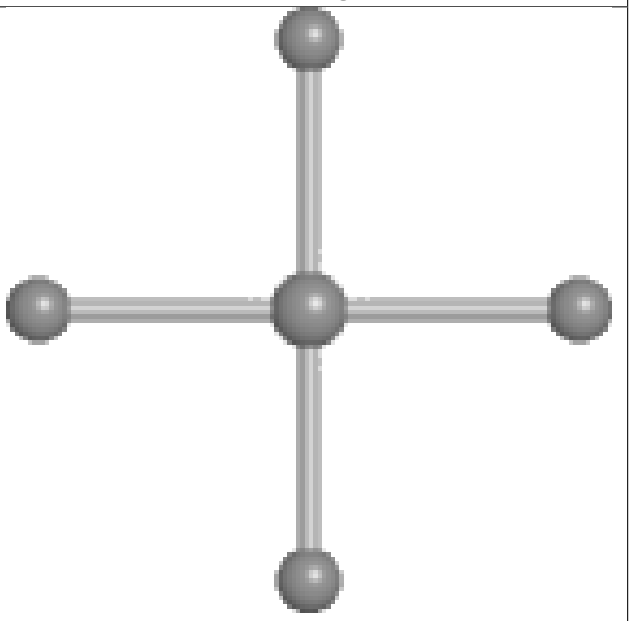
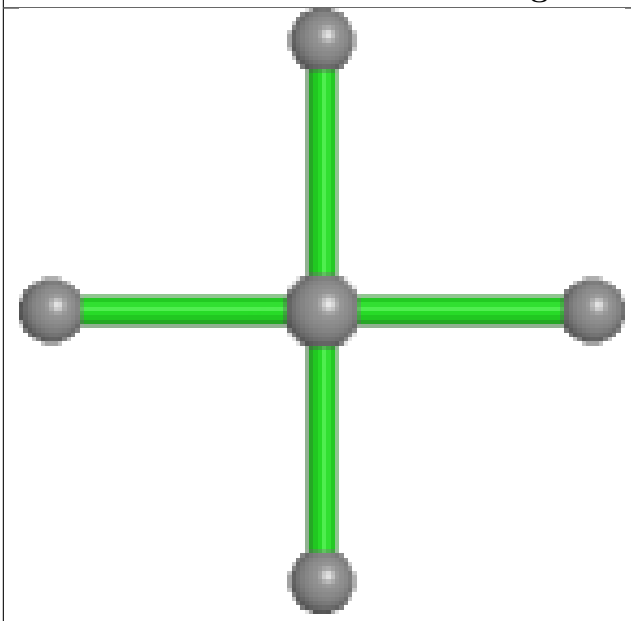


Rings

Ligand SO4 F 406



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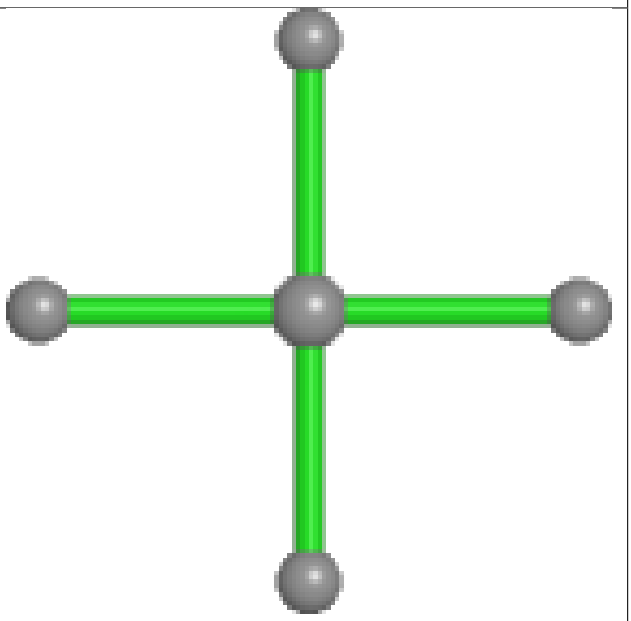
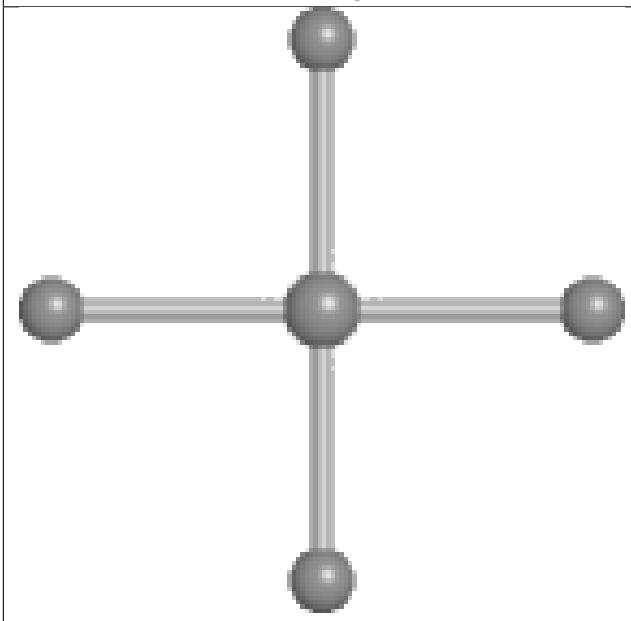


Bond angles



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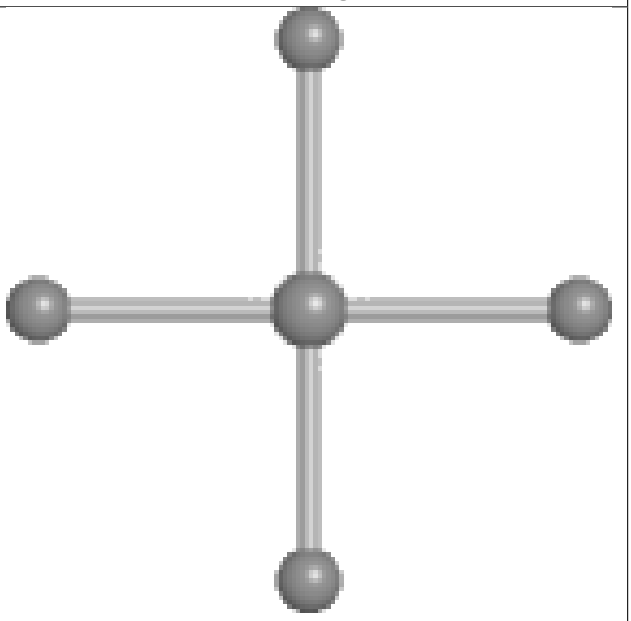
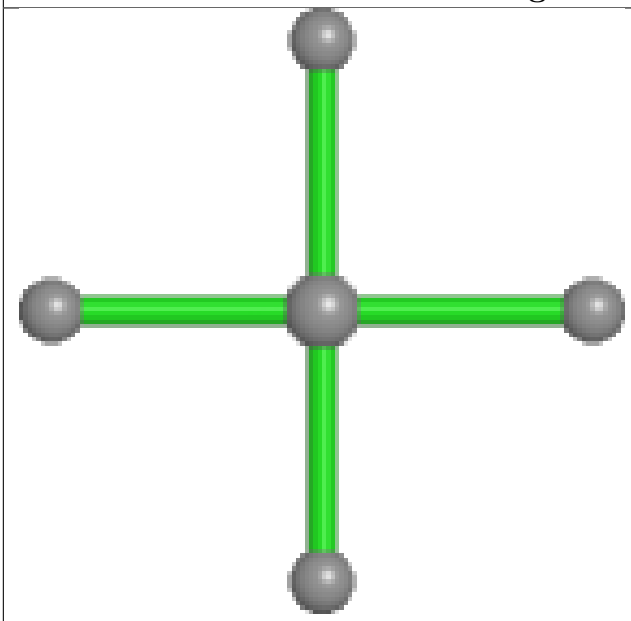


Rings

Ligand SO4 A 402



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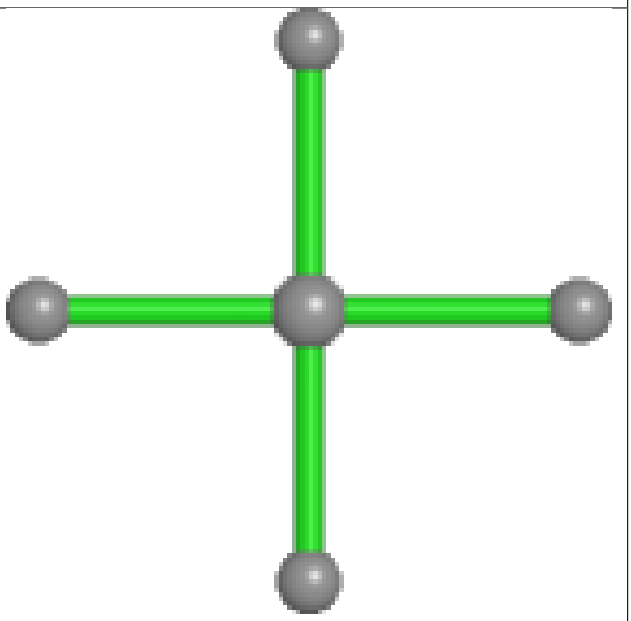
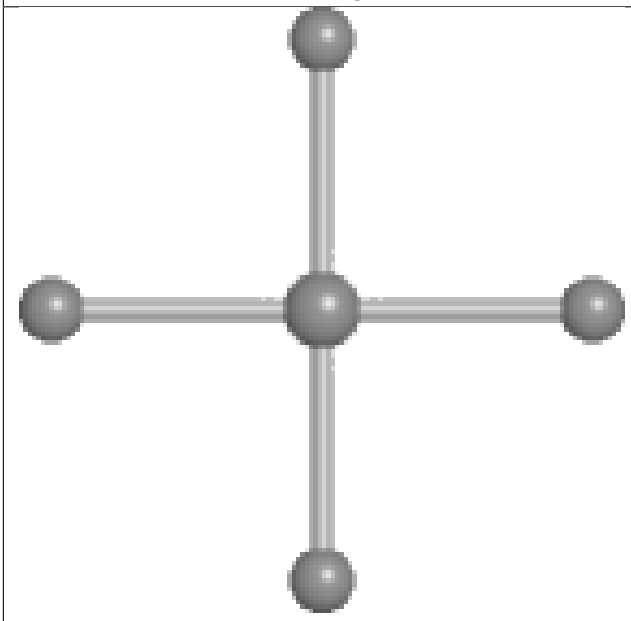


Bond angles



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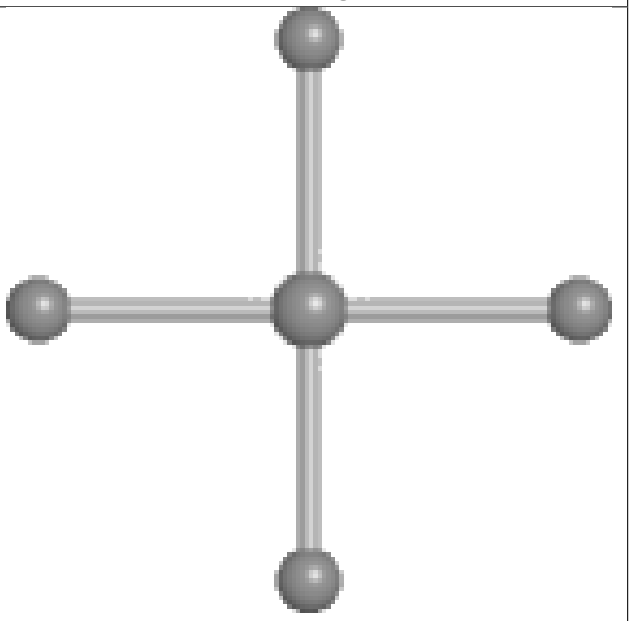
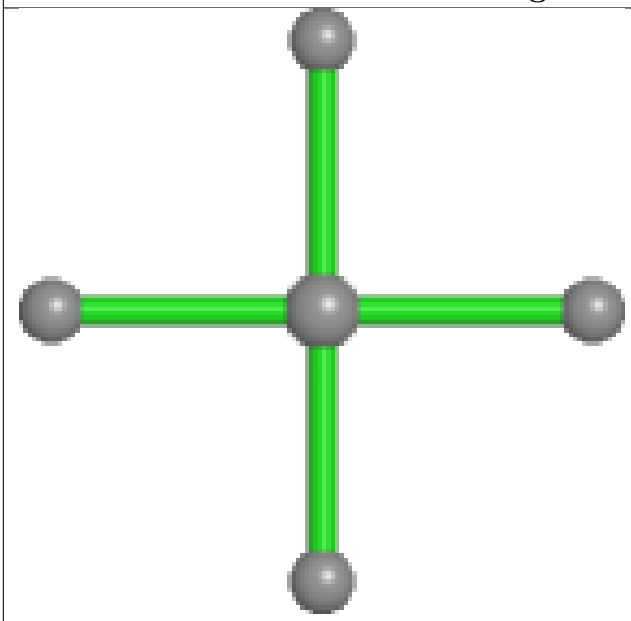


Rings

Ligand SO4 C 404



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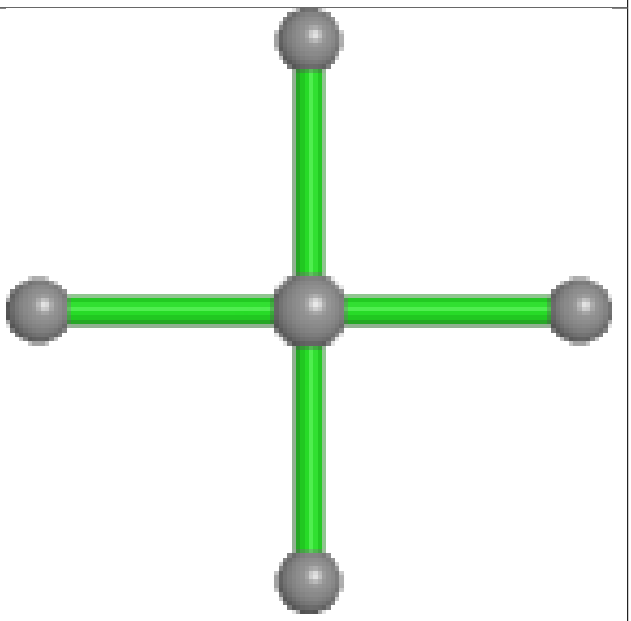
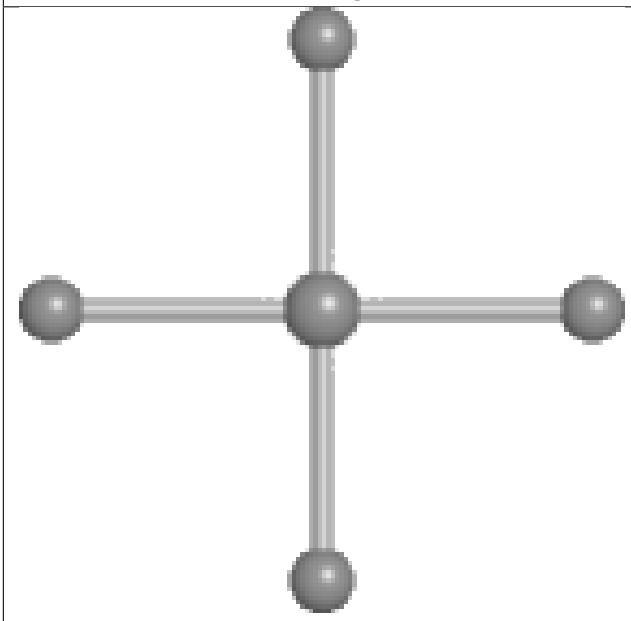


Bond angles



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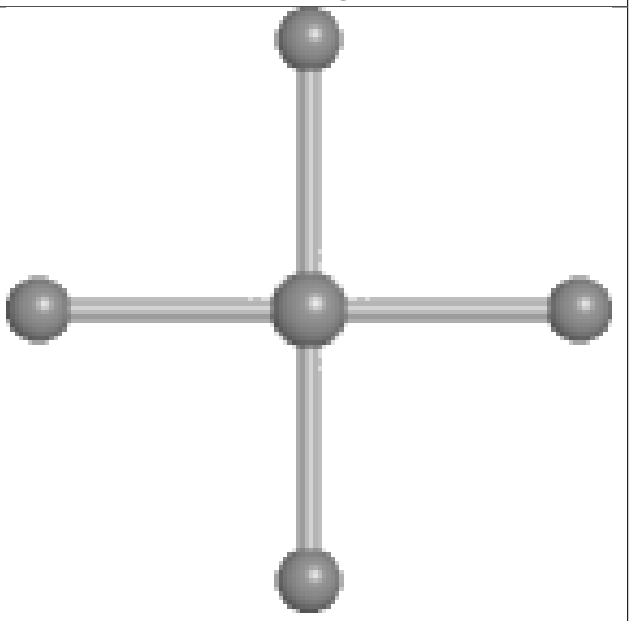
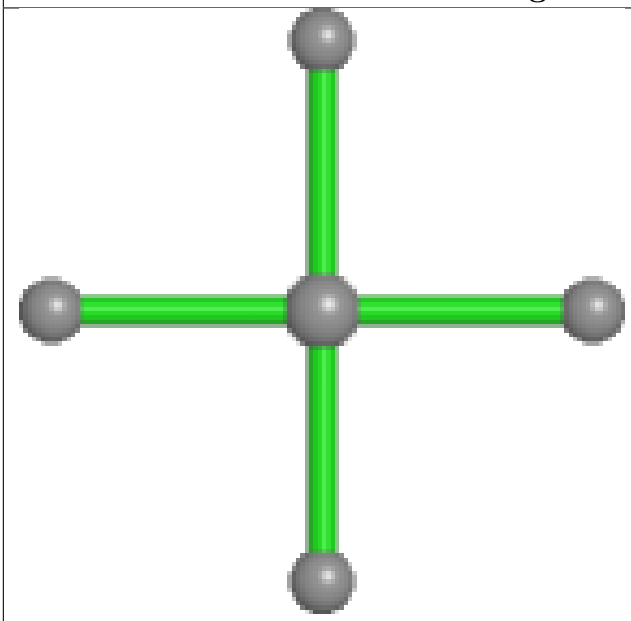


Rings

Ligand SO4 C 401



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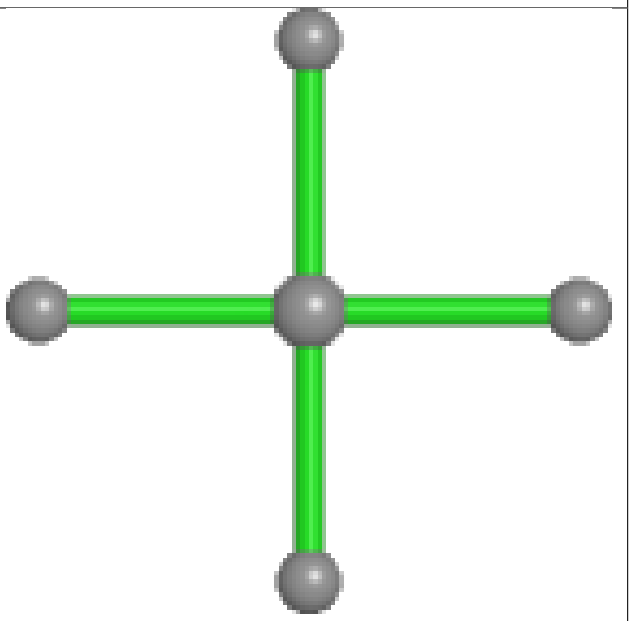

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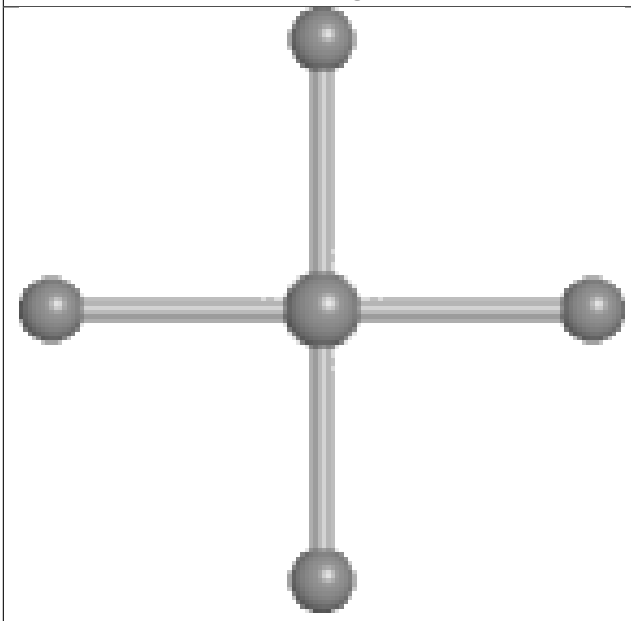
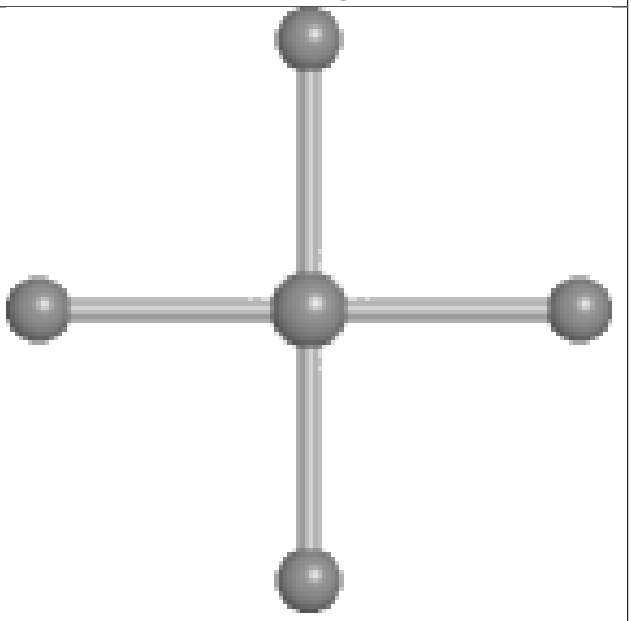
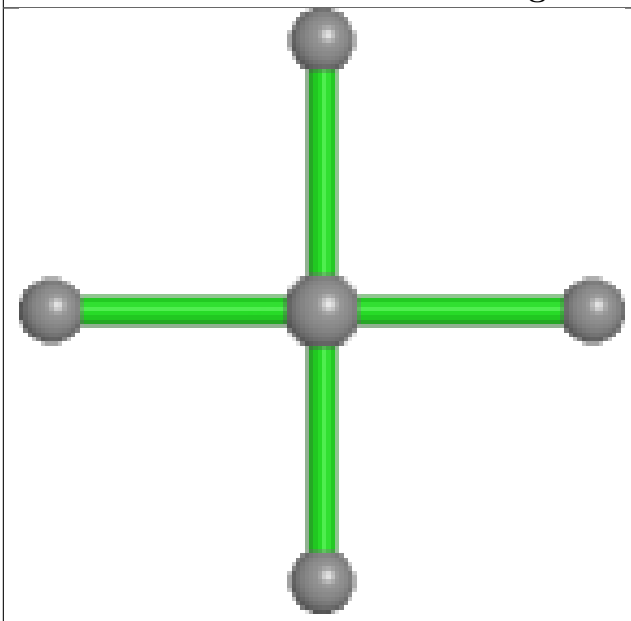


Torsions

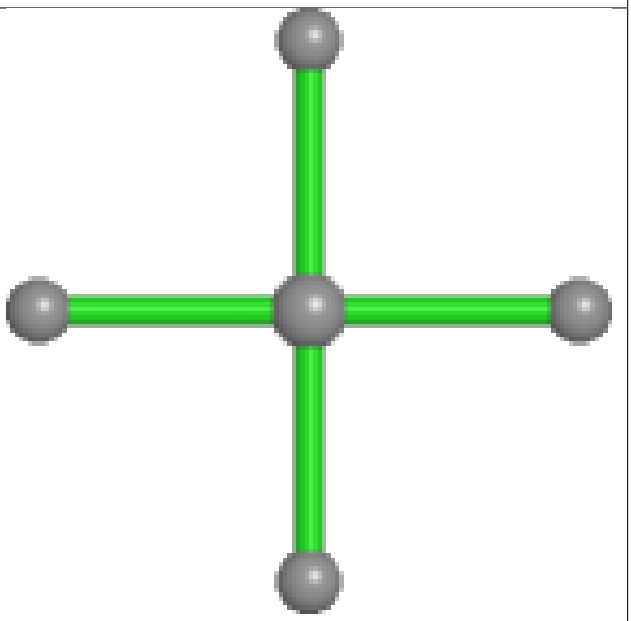


Rings

Ligand SO4 A 403



Bond lengths



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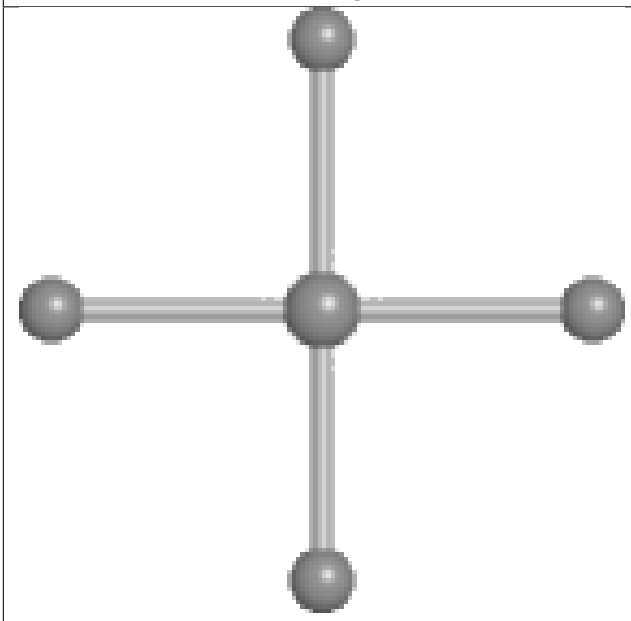

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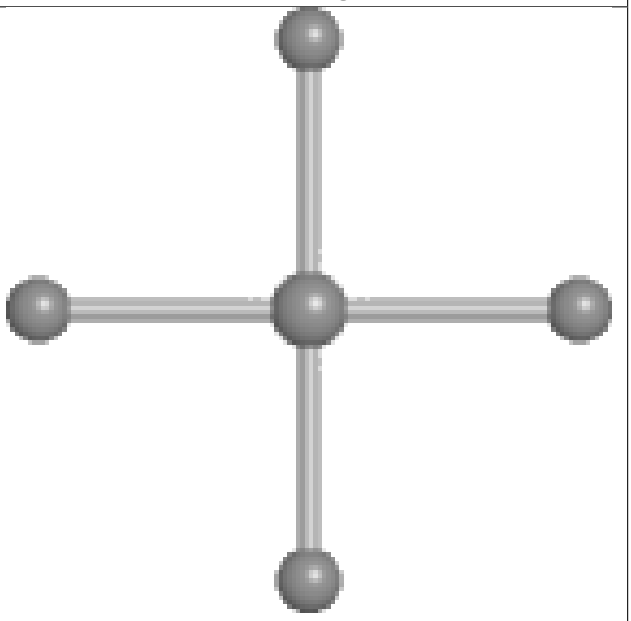
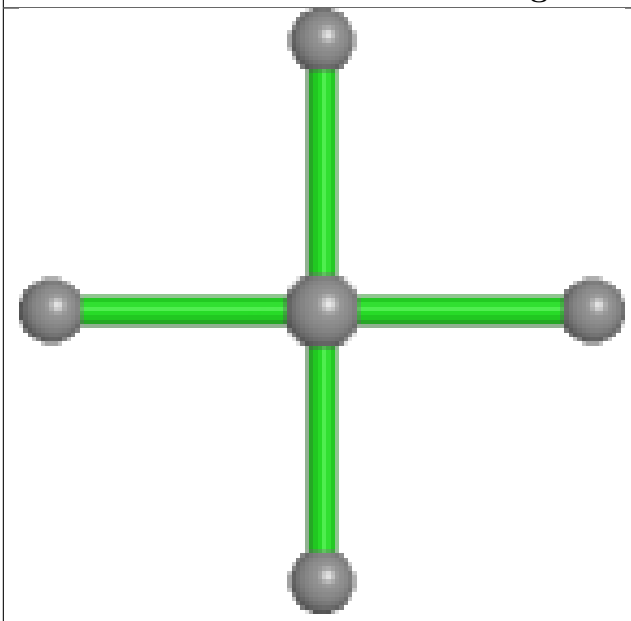


Rings

Ligand SO4 E 407



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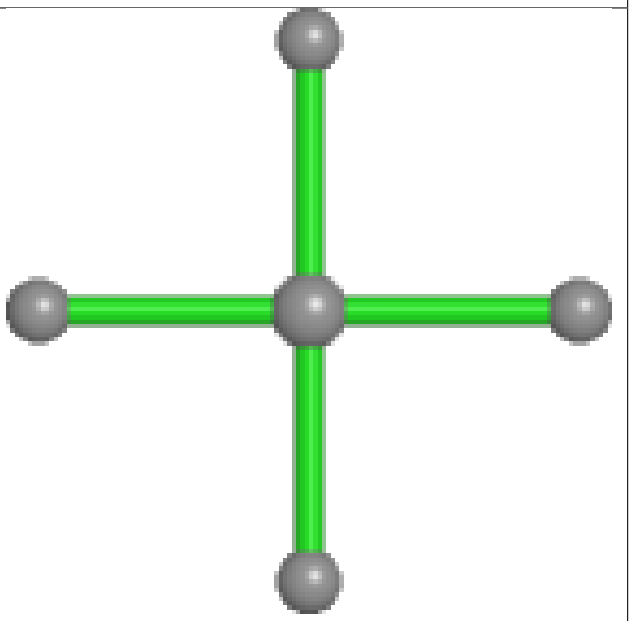

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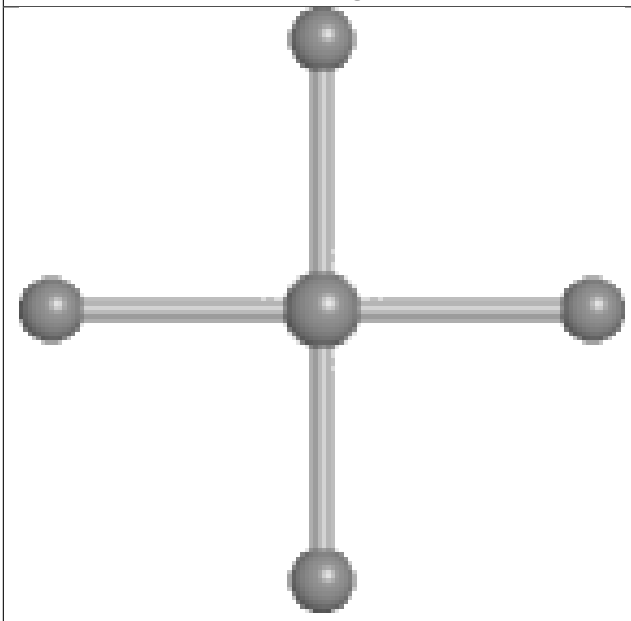

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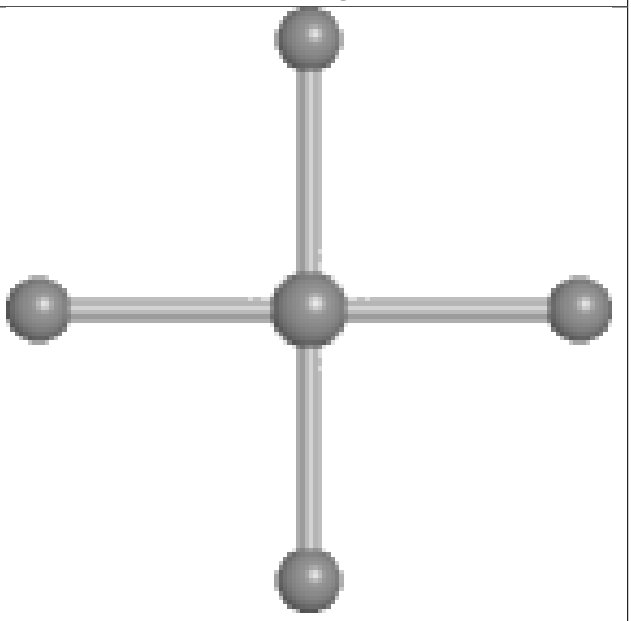
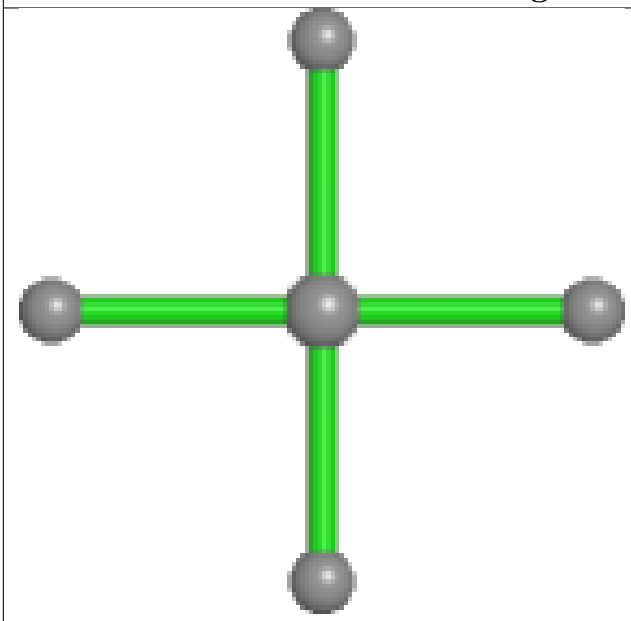


Rings

Ligand SO4 F 401



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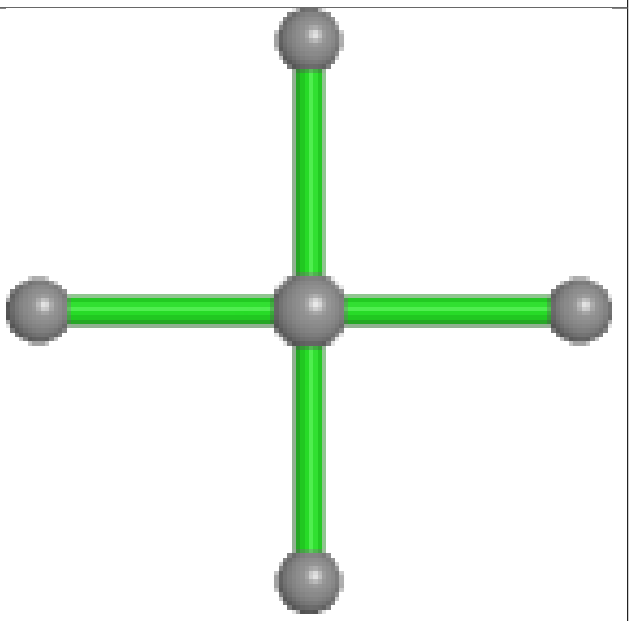
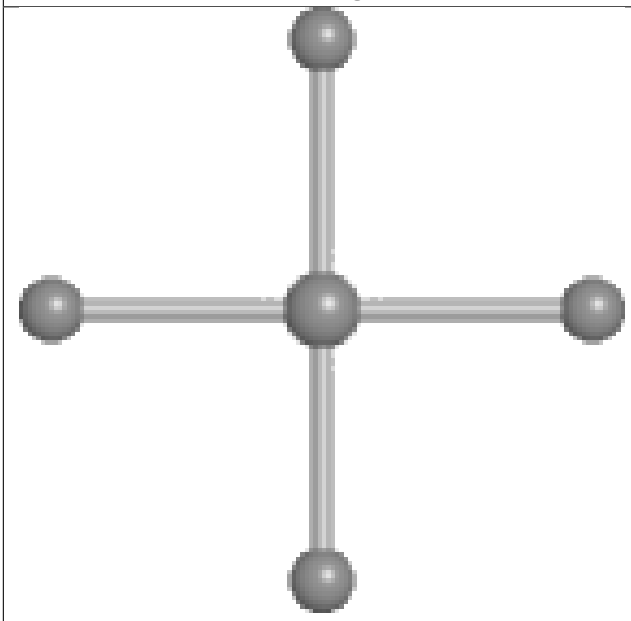


Bond angles



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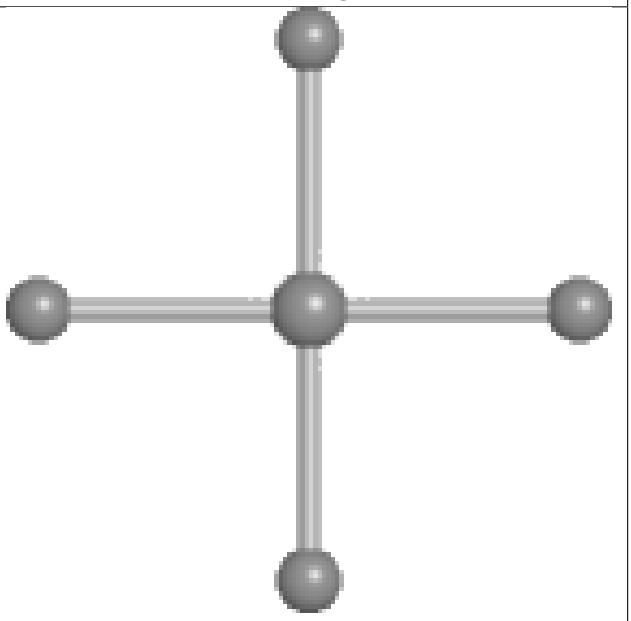
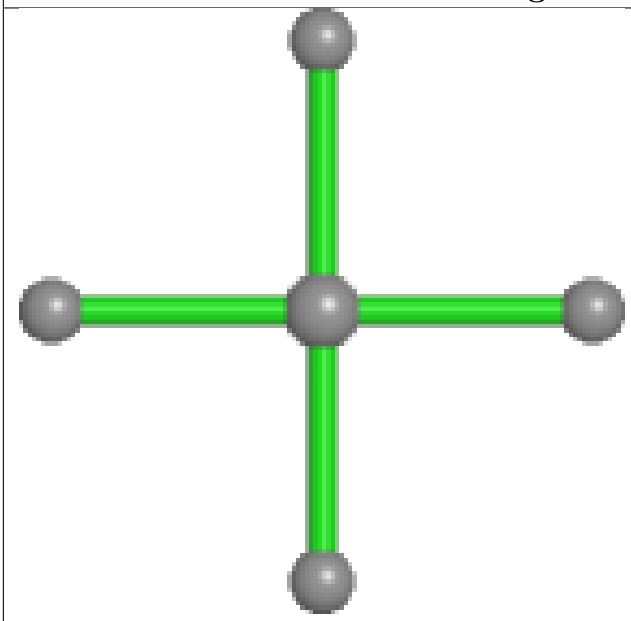


Rings

Ligand SO4 H 405



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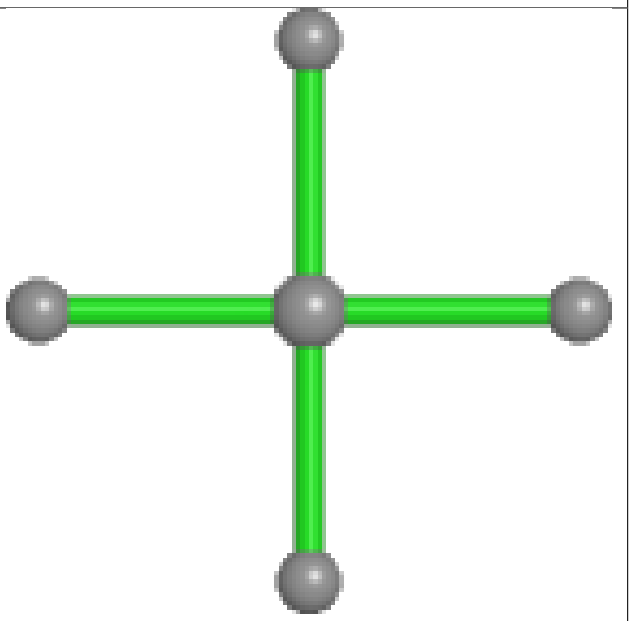
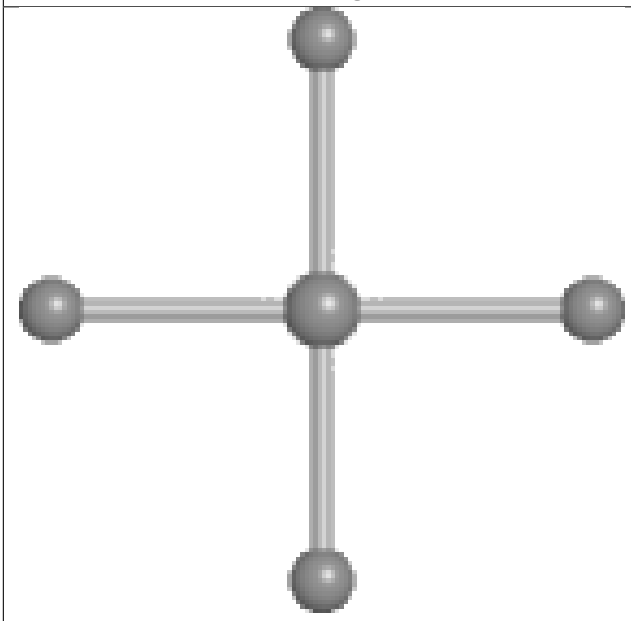
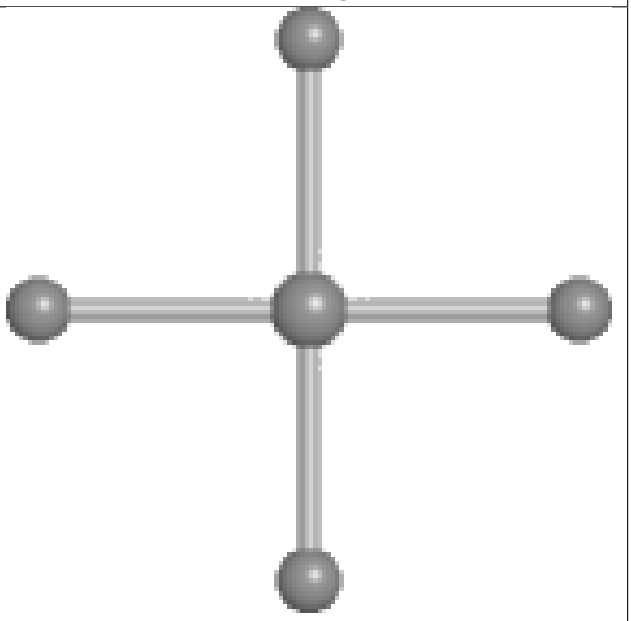


Bond angles

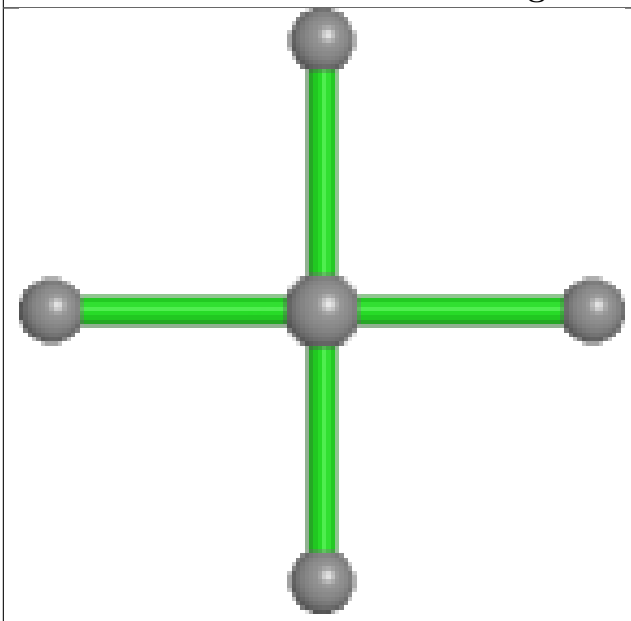


Torsions



Rings

Ligand SO4 H 402



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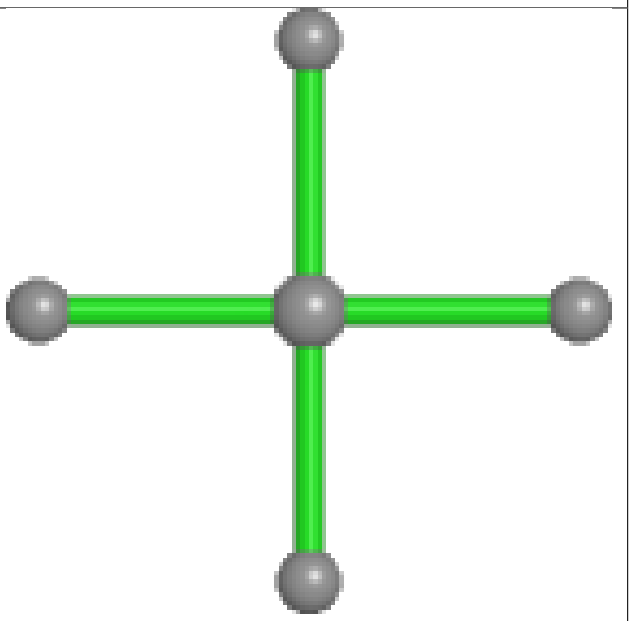
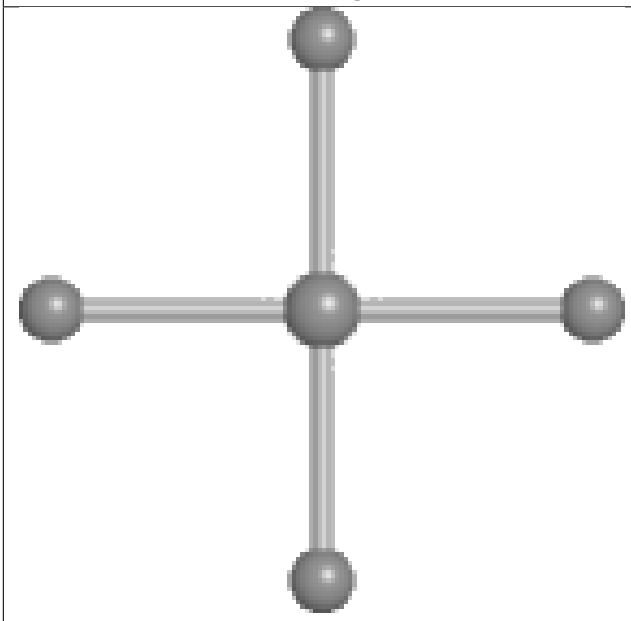


Bond angles



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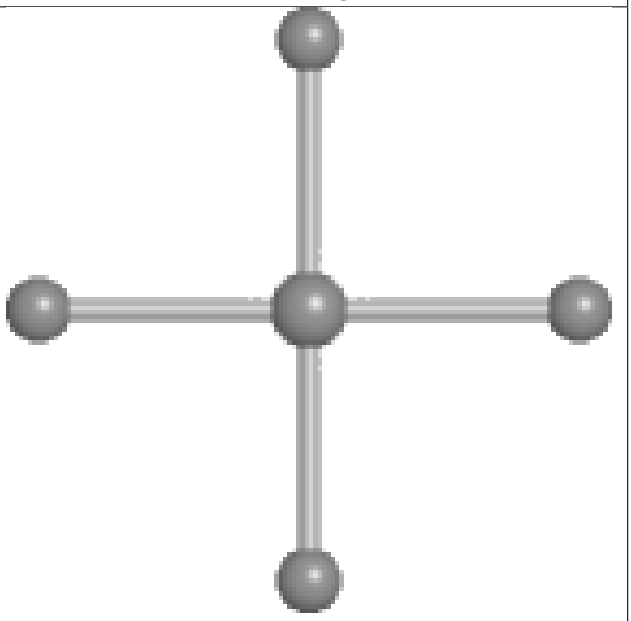
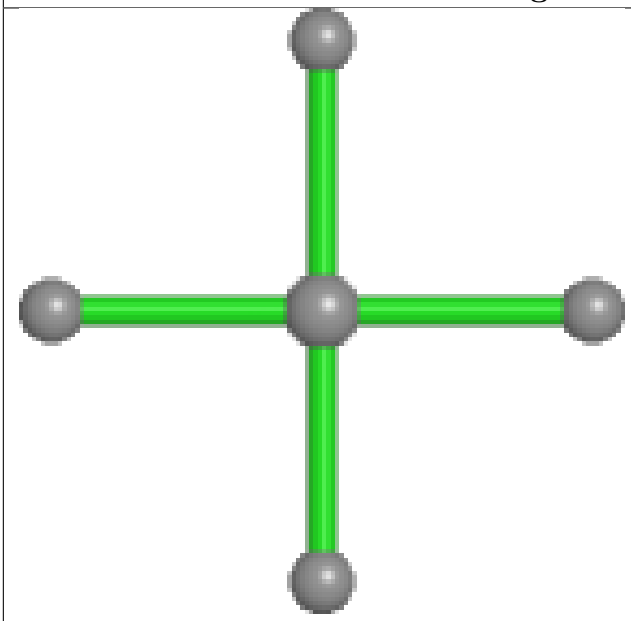
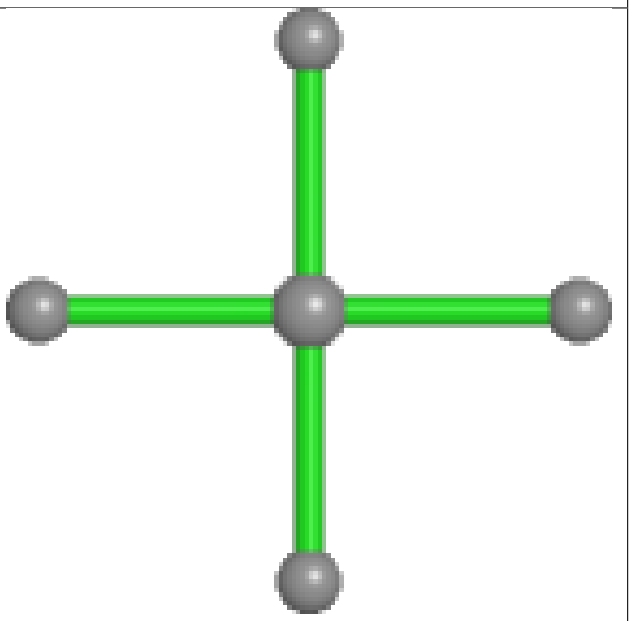


Rings

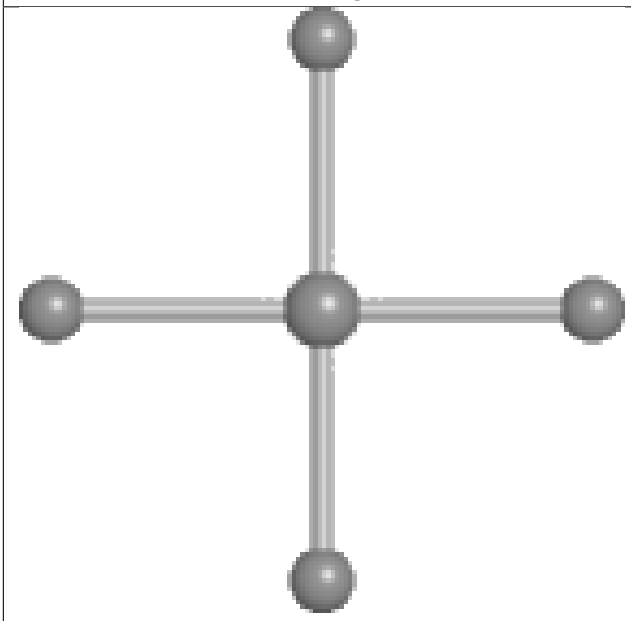
Ligand SO4 E 409



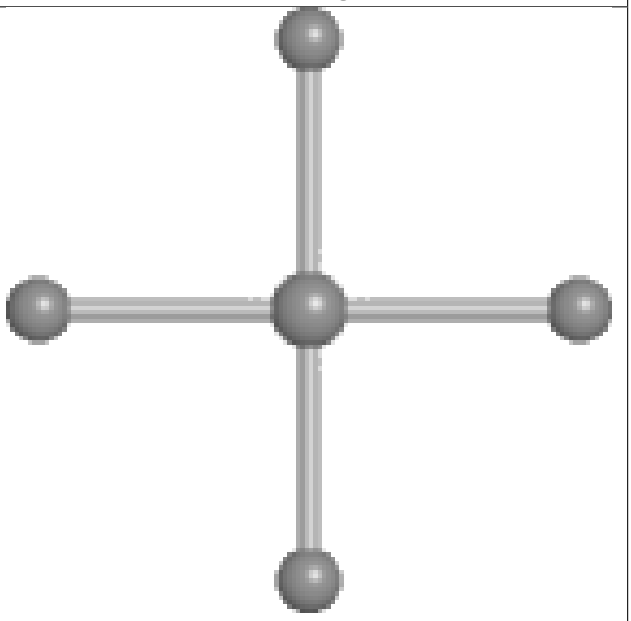
Bond lengths



Bond angles

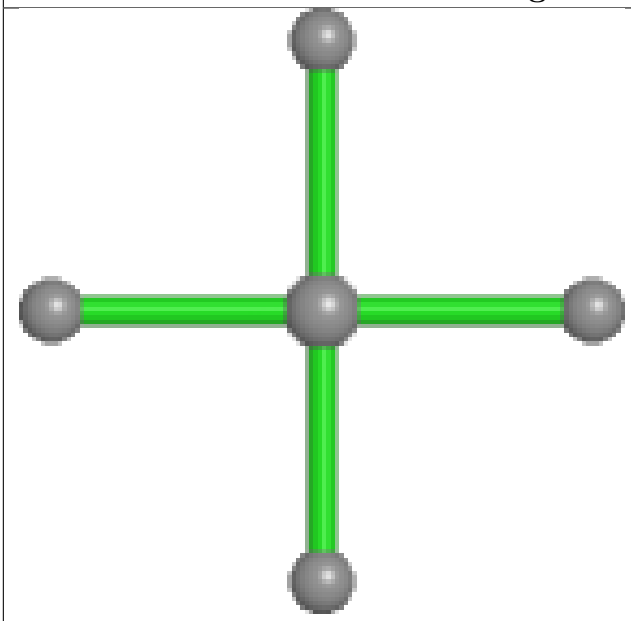


Torsions

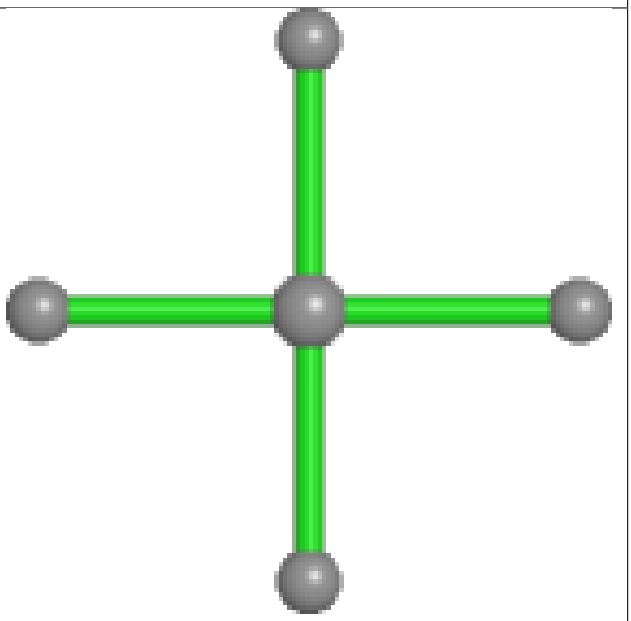


Rings

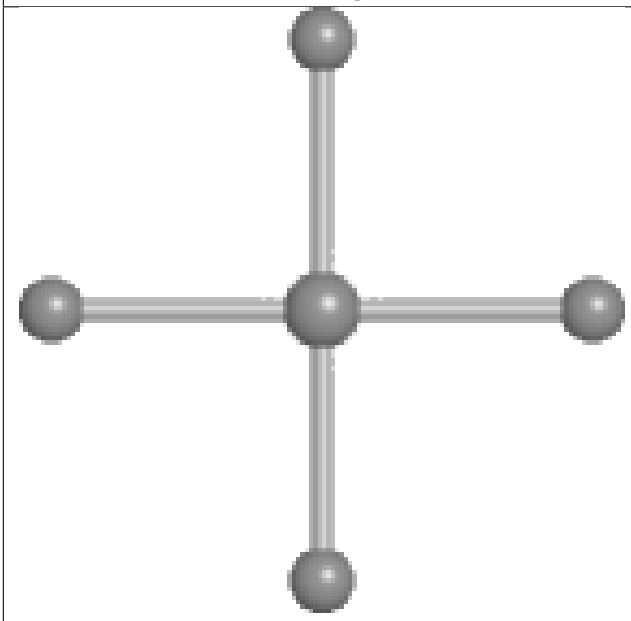
Ligand SO4 A 404



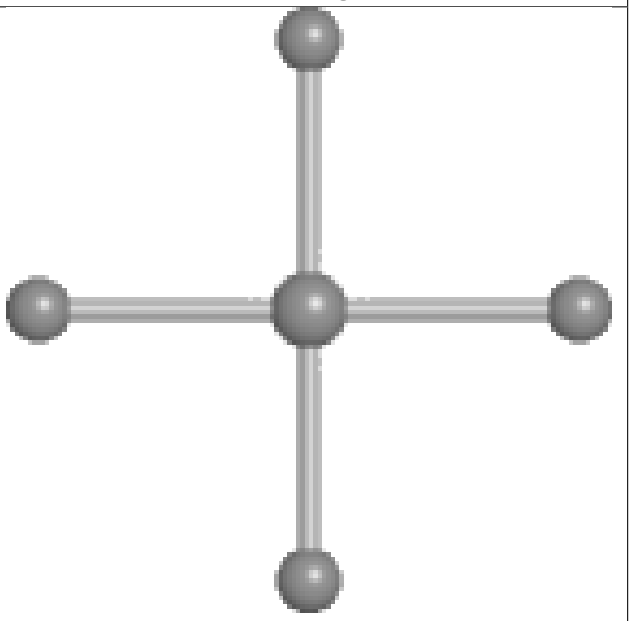
Bond lengths



Bond angles

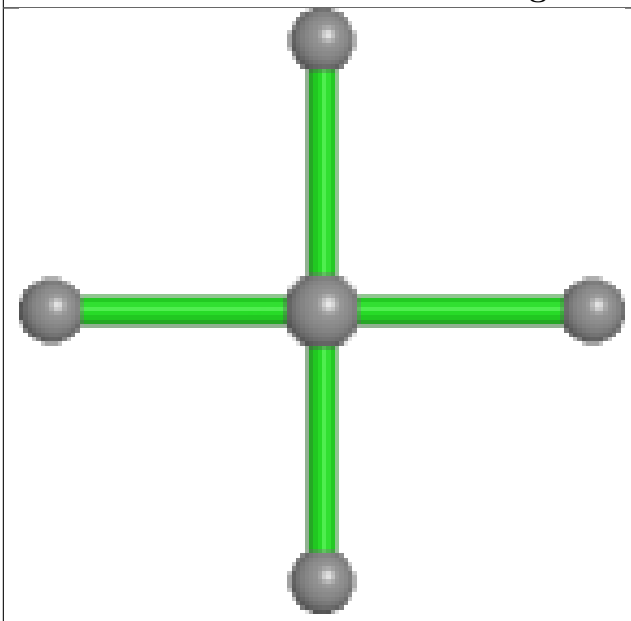


Torsions

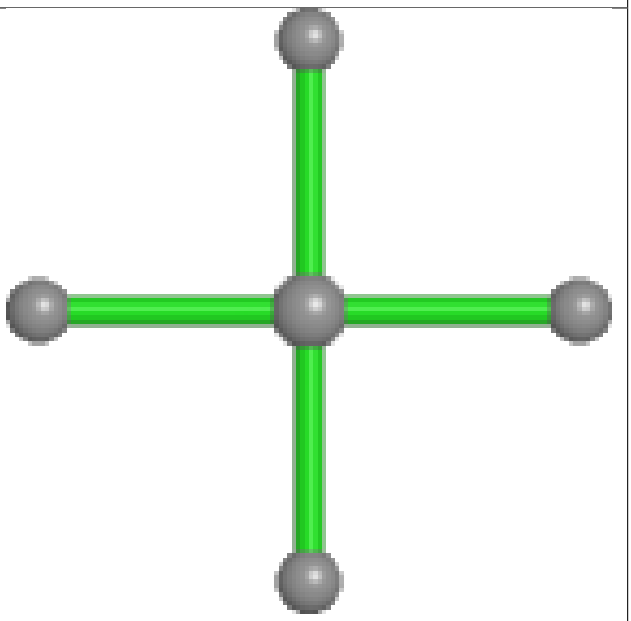


Rings

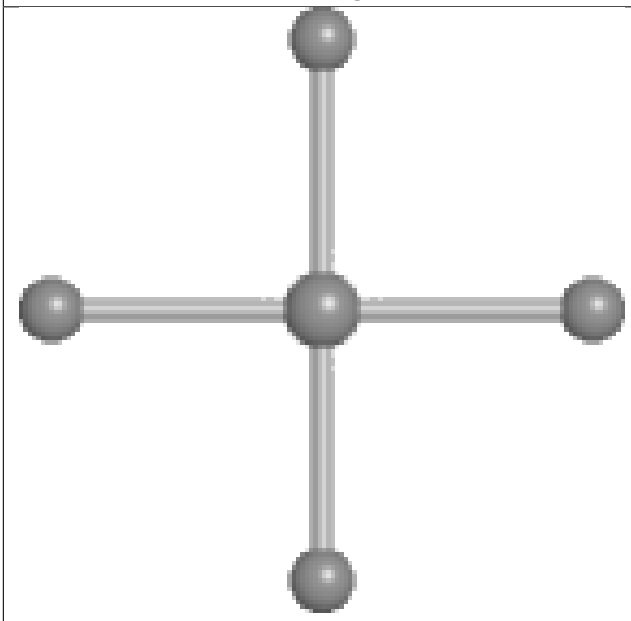
Ligand SO4 B 404



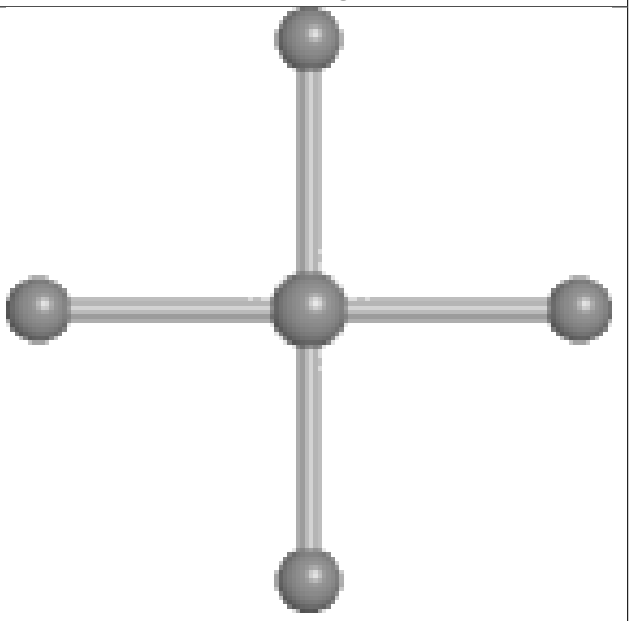
Bond lengths



Bond angles

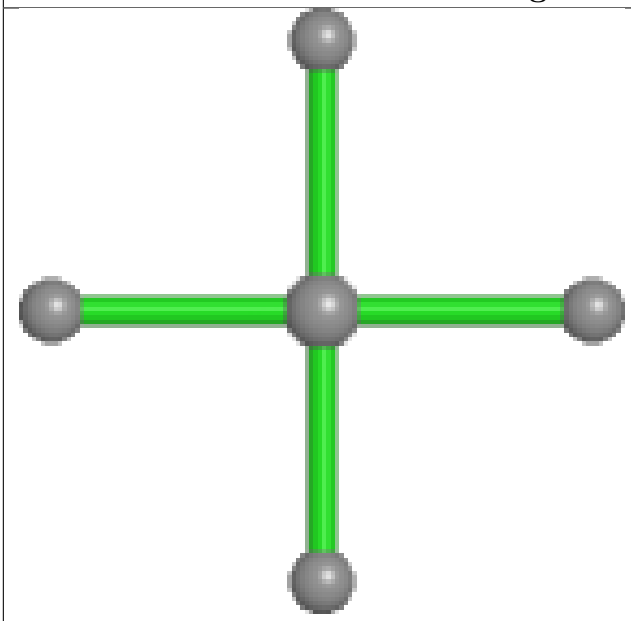


Torsions

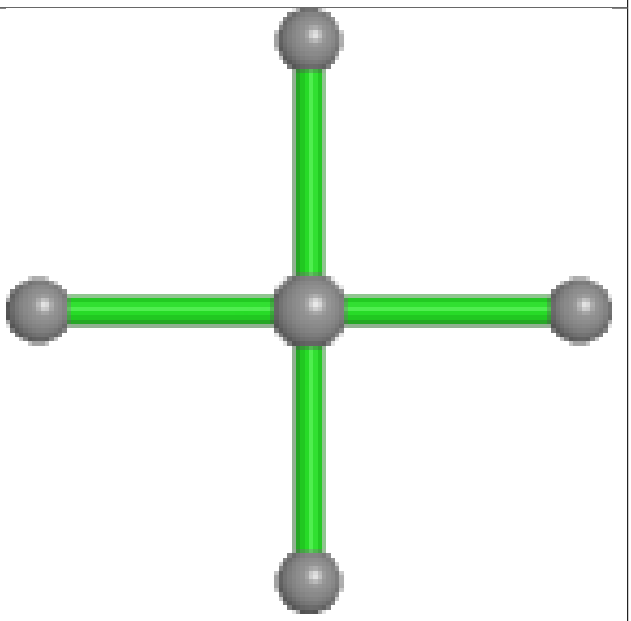


Rings

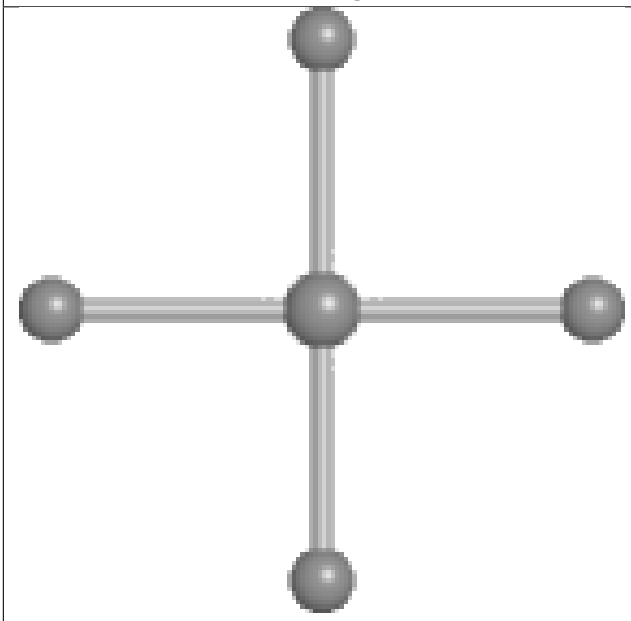
Ligand SO4 B 401



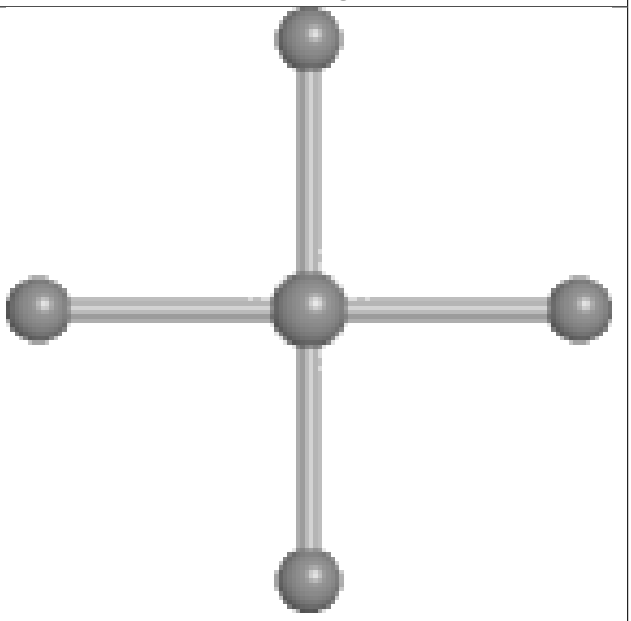
Bond lengths



Bond angles

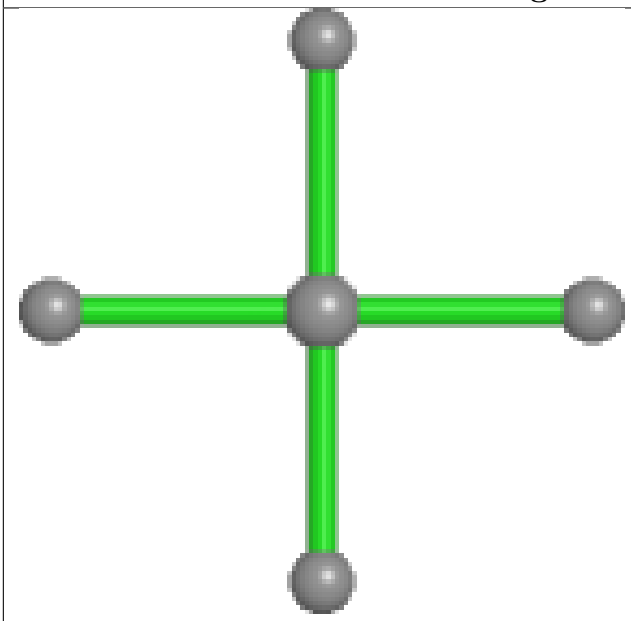


Torsions

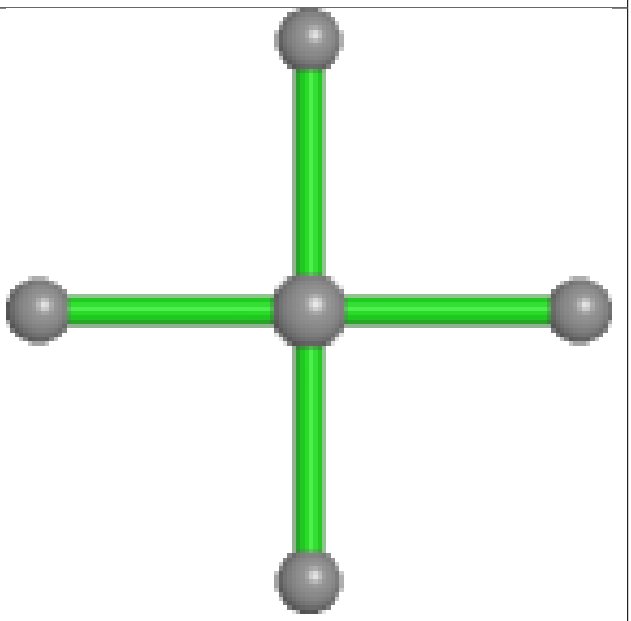


Rings

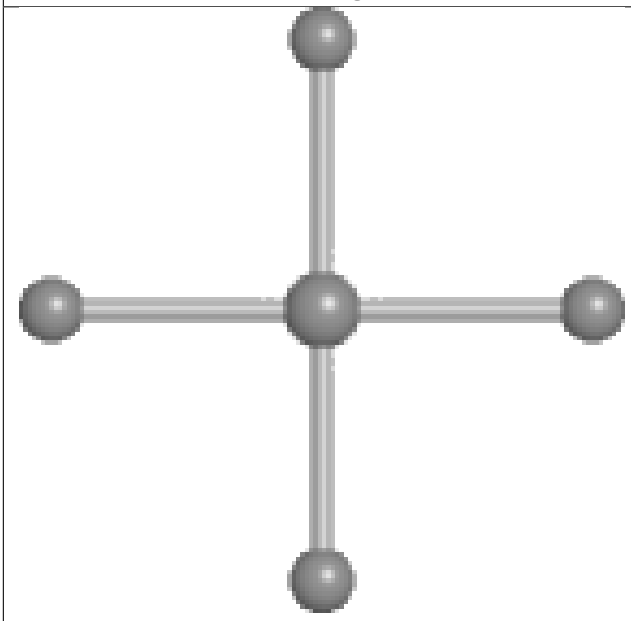
Ligand SO4 E 412



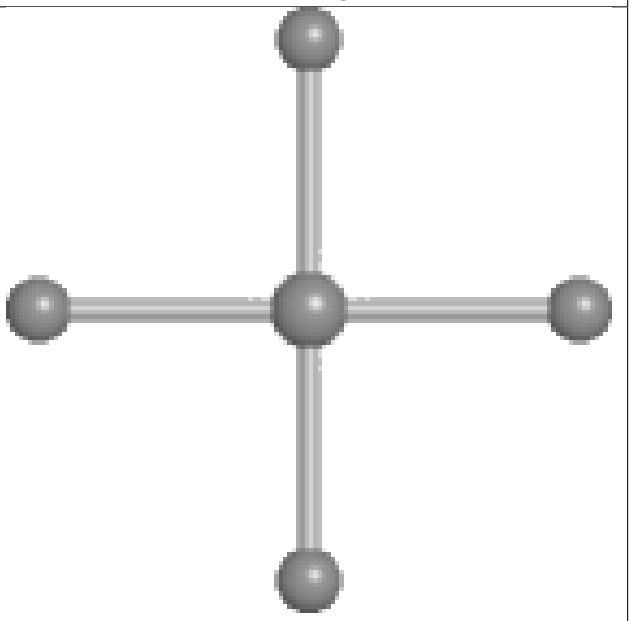
Bond lengths



Bond angles

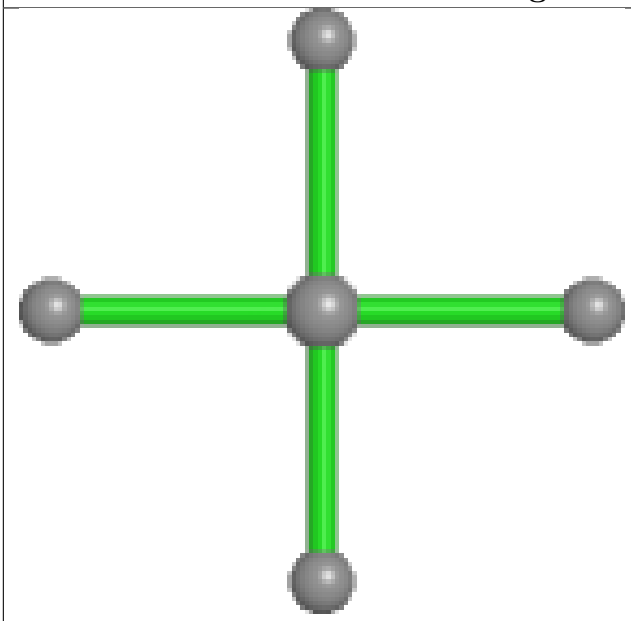


Torsions

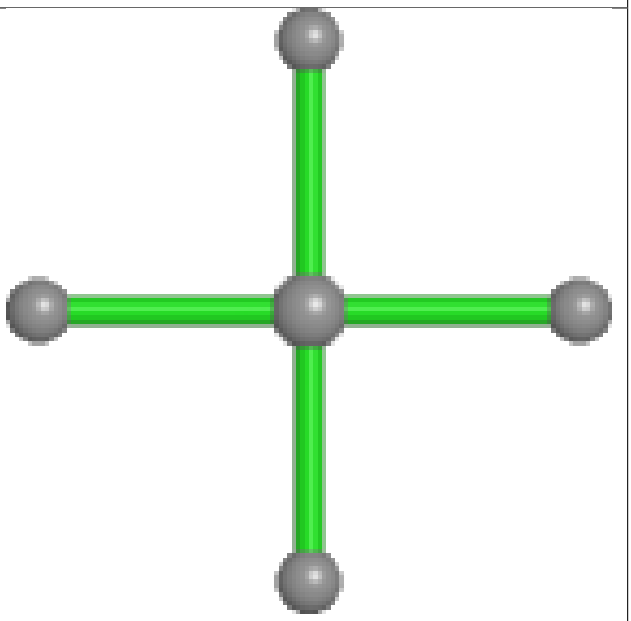


Rings

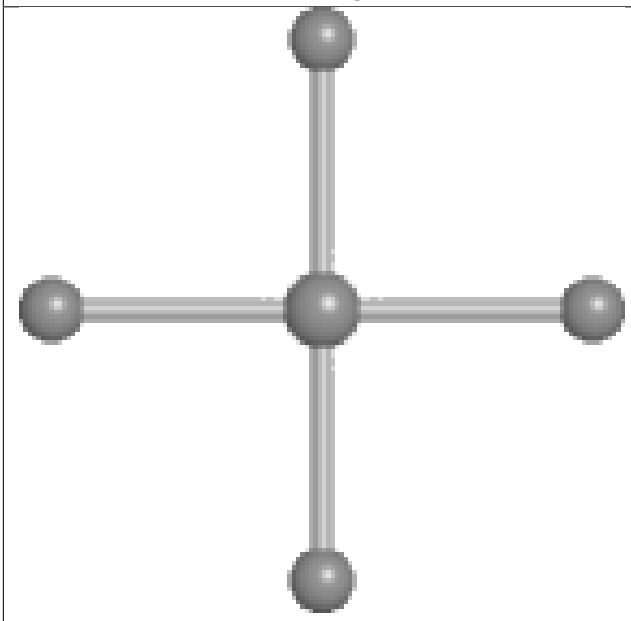
Ligand SO4 C 403



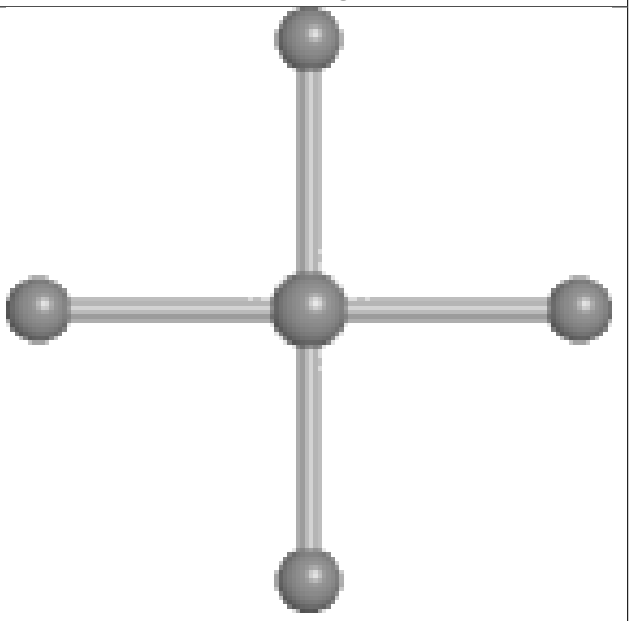
Bond lengths



Bond angles

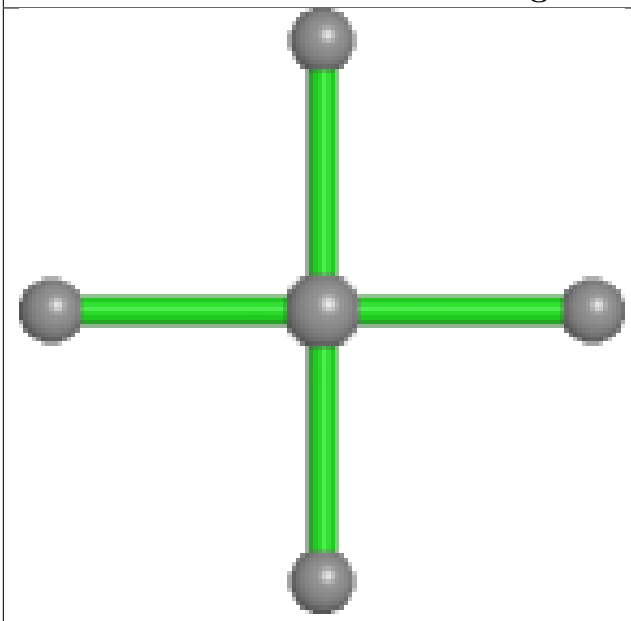


Torsions

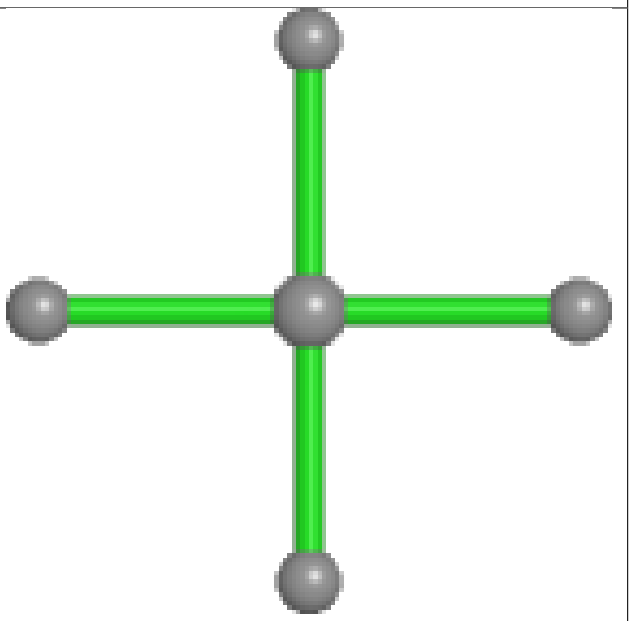


Rings

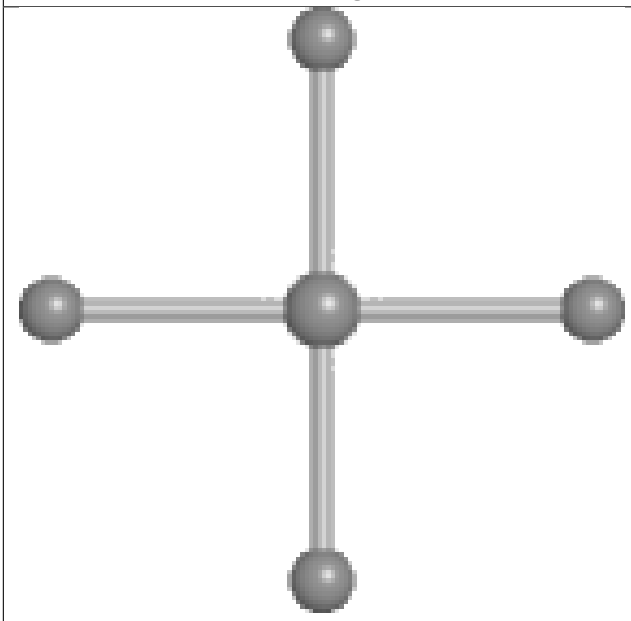
Ligand SO4 E 402



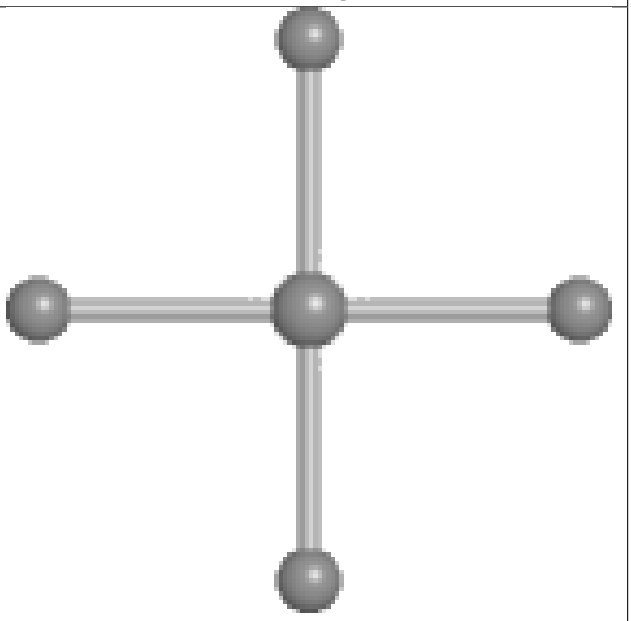
Bond lengths



Bond angles

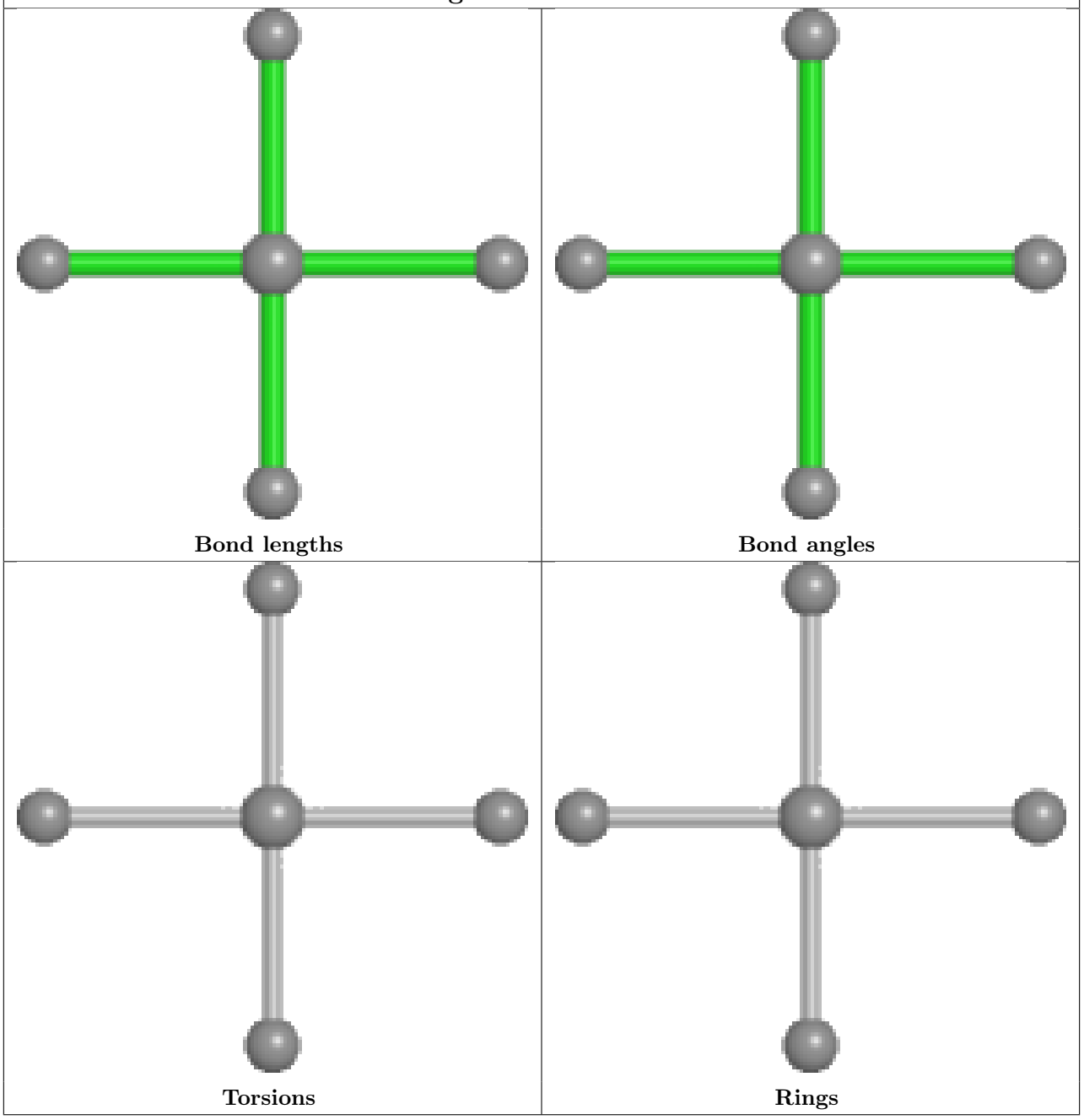


Torsions



Rings

Ligand SO4 F 405



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	301/321 (93%)	-0.13	5 (1%)	70	70	24, 44, 66, 87	0
1	B	300/321 (93%)	-0.14	6 (2%)	65	64	24, 40, 67, 86	0
1	C	306/321 (95%)	-0.36	2 (0%)	87	88	18, 32, 55, 84	0
1	D	300/321 (93%)	-0.28	3 (1%)	82	82	20, 35, 59, 72	0
1	E	301/321 (93%)	-0.30	2 (0%)	87	88	19, 33, 57, 89	0
1	F	303/321 (94%)	-0.34	2 (0%)	87	88	20, 32, 52, 63	0
1	G	300/321 (93%)	-0.21	4 (1%)	77	77	23, 41, 62, 87	0
1	H	300/321 (93%)	-0.02	10 (3%)	46	42	23, 45, 71, 84	0
All	All	2411/2568 (93%)	-0.22	34 (1%)	75	76	18, 38, 63, 89	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	67	ASP	4.2
1	F	301	LYS	3.4
1	G	1	MET	3.4
1	B	113	GLU	3.3
1	H	112	LYS	3.3
1	B	66	ASN	3.2
1	F	226	HIS	3.1
1	E	301	LYS	3.1
1	H	113	GLU	2.9
1	B	23	ALA	2.9
1	D	75	ASN	2.9
1	H	261	ASP	2.8
1	H	23	ALA	2.8
1	B	1	MET	2.6
1	G	65	VAL	2.6
1	E	170	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	G	27	ASP	2.4
1	C	-4	PRO	2.4
1	G	59	LEU	2.4
1	H	89	THR	2.3
1	A	113	GLU	2.3
1	D	39	LYS	2.3
1	H	170	GLU	2.2
1	H	204	GLN	2.2
1	D	113	GLU	2.2
1	A	301	LYS	2.2
1	A	131	GLU	2.2
1	H	206	LYS	2.1
1	H	227	HIS	2.0
1	B	64	ASP	2.0
1	A	53	GLU	2.0
1	H	1	MET	2.0
1	A	119	GLY	2.0
1	C	227	HIS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	411	5/5	0.81	0.27	88,98,104,106	0
2	SO4	C	405	5/5	0.82	0.27	96,96,108,109	0
2	SO4	A	404	5/5	0.82	0.24	66,67,82,92	0
2	SO4	E	412	5/5	0.83	0.51	105,108,114,119	0
2	SO4	H	404	5/5	0.83	0.36	87,88,97,104	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	E	410	5/5	0.84	0.26	83,90,93,96	0
2	SO4	B	404	5/5	0.87	0.39	85,90,97,97	0
2	SO4	E	409	5/5	0.87	0.51	104,108,112,116	0
2	SO4	F	404	5/5	0.88	0.37	67,79,87,87	0
2	SO4	E	404	5/5	0.88	0.31	78,85,86,90	0
2	SO4	F	406	5/5	0.89	0.37	80,88,91,91	0
2	SO4	B	405	5/5	0.90	0.23	96,99,102,105	0
2	SO4	E	413	5/5	0.91	0.52	96,99,104,107	0
2	SO4	H	403	5/5	0.91	0.18	69,72,77,84	0
2	SO4	E	405	5/5	0.91	0.30	86,87,89,91	0
2	SO4	H	402	5/5	0.92	0.28	59,71,74,77	0
2	SO4	E	407	5/5	0.92	0.30	82,84,88,91	0
2	SO4	E	403	5/5	0.92	0.25	54,56,69,74	0
2	SO4	H	405	5/5	0.92	0.22	68,73,77,80	0
2	SO4	F	403	5/5	0.93	0.40	66,67,71,84	0
2	SO4	A	403	5/5	0.93	0.52	93,105,117,117	0
2	SO4	F	405	5/5	0.93	0.35	99,101,103,104	0
2	SO4	D	401	5/5	0.93	0.20	46,48,51,53	0
2	SO4	E	406	5/5	0.93	0.20	110,111,114,114	0
2	SO4	C	404	5/5	0.93	0.31	74,76,79,84	0
2	SO4	E	408	5/5	0.93	0.37	95,95,105,107	0
2	SO4	F	402	5/5	0.93	0.20	54,57,64,68	0
2	SO4	A	402	5/5	0.94	0.36	73,75,81,83	0
2	SO4	A	405	5/5	0.94	0.30	67,73,82,87	0
2	SO4	B	403	5/5	0.94	0.20	86,90,97,101	0
2	SO4	A	401	5/5	0.94	0.27	62,66,72,83	0
2	SO4	G	404	5/5	0.95	0.20	72,74,77,78	0
2	SO4	H	401	5/5	0.95	0.15	62,68,72,78	0
2	SO4	A	406	5/5	0.95	0.15	56,58,67,73	0
2	SO4	C	402	5/5	0.95	0.20	64,64,66,68	0
2	SO4	B	402	5/5	0.95	0.23	58,63,68,71	0
2	SO4	F	407	5/5	0.95	0.28	42,44,46,47	0
2	SO4	D	402	5/5	0.96	0.19	51,55,63,71	0
2	SO4	D	403	5/5	0.96	0.24	60,60,65,73	0
2	SO4	E	401	5/5	0.96	0.19	48,53,56,59	0
2	SO4	C	401	5/5	0.96	0.12	51,53,61,69	0
2	SO4	G	401	5/5	0.96	0.14	47,48,57,59	0
2	SO4	G	402	5/5	0.96	0.12	47,50,58,60	0
2	SO4	C	403	5/5	0.97	0.22	68,71,74,75	0
2	SO4	G	403	5/5	0.97	0.20	57,63,71,72	0
2	SO4	F	401	5/5	0.97	0.17	58,59,61,64	0
2	SO4	E	402	5/5	0.97	0.13	60,61,71,73	0

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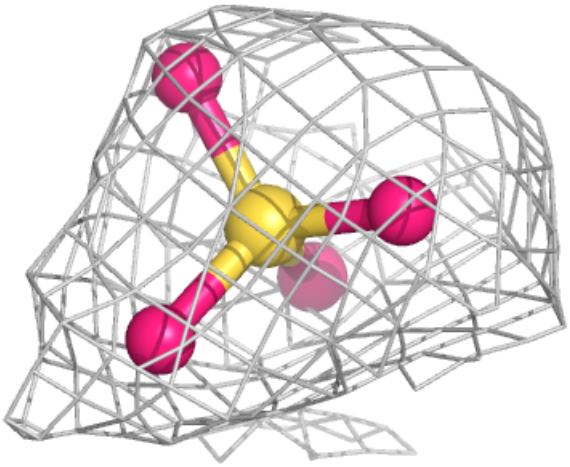
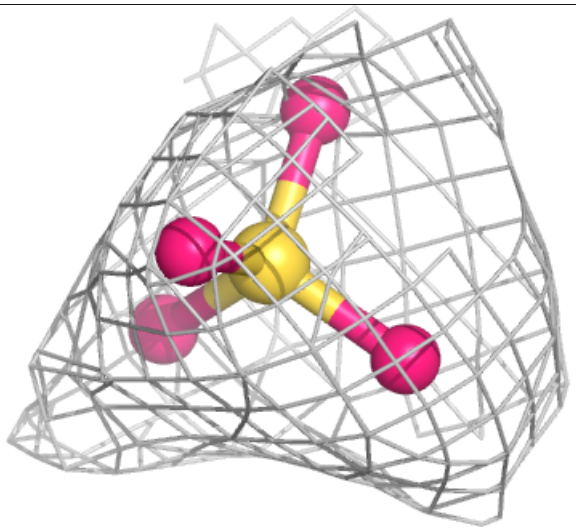
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	B	401	5/5	0.99	0.08	33,33,35,37	0

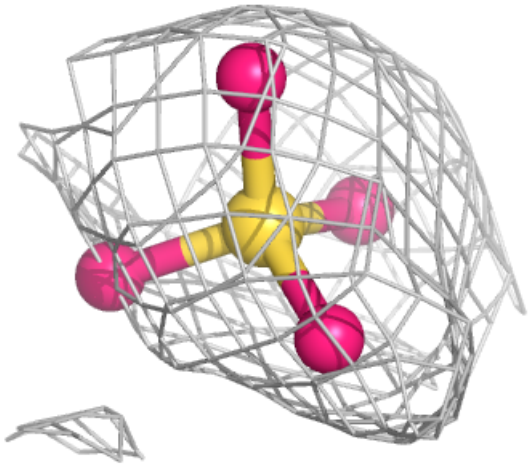
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SO4 E 411:

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

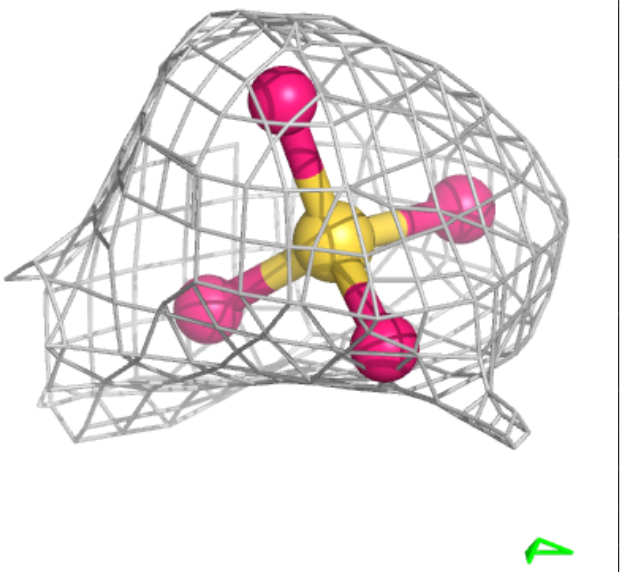


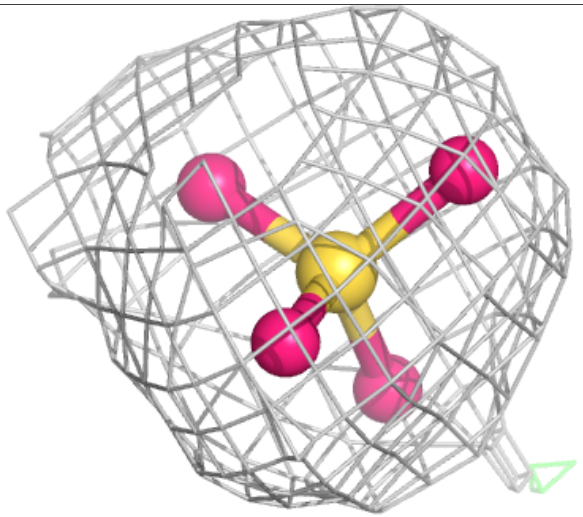


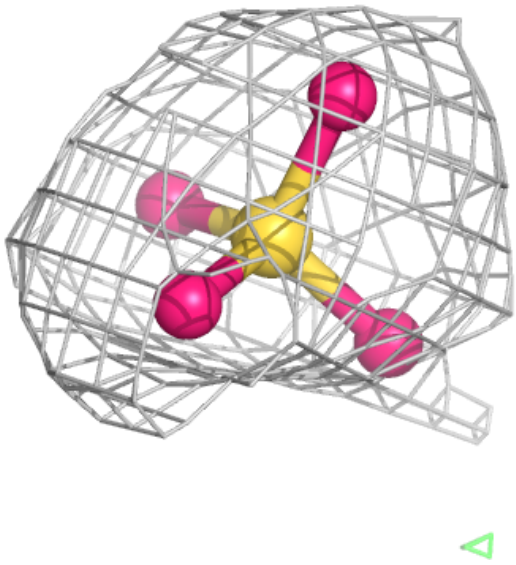


Electron density around SO4 C 405:

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

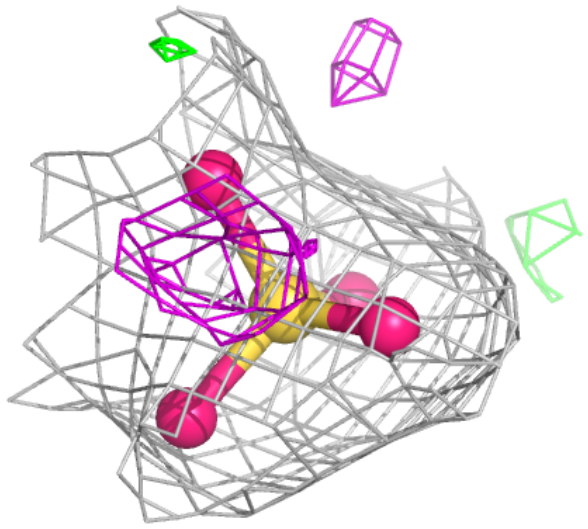


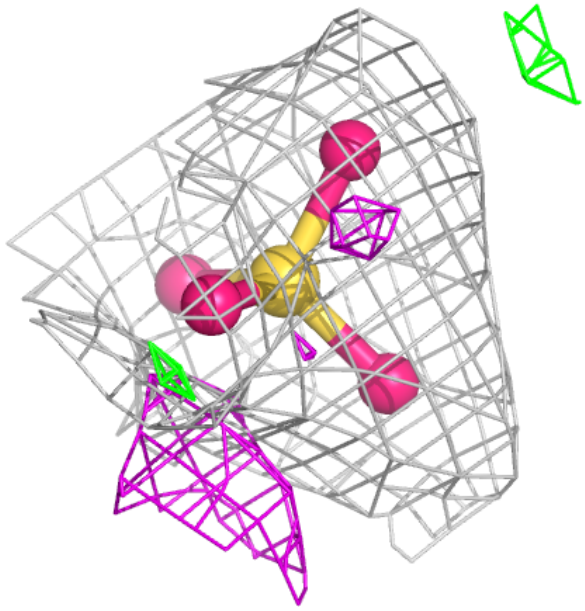


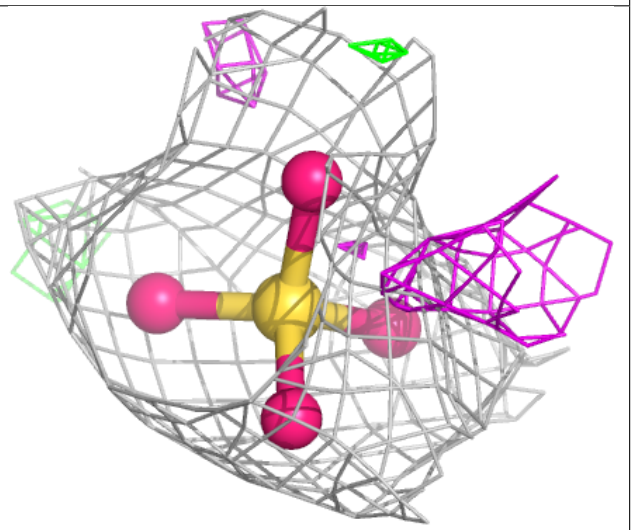


Electron density around SO4 A 404:

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

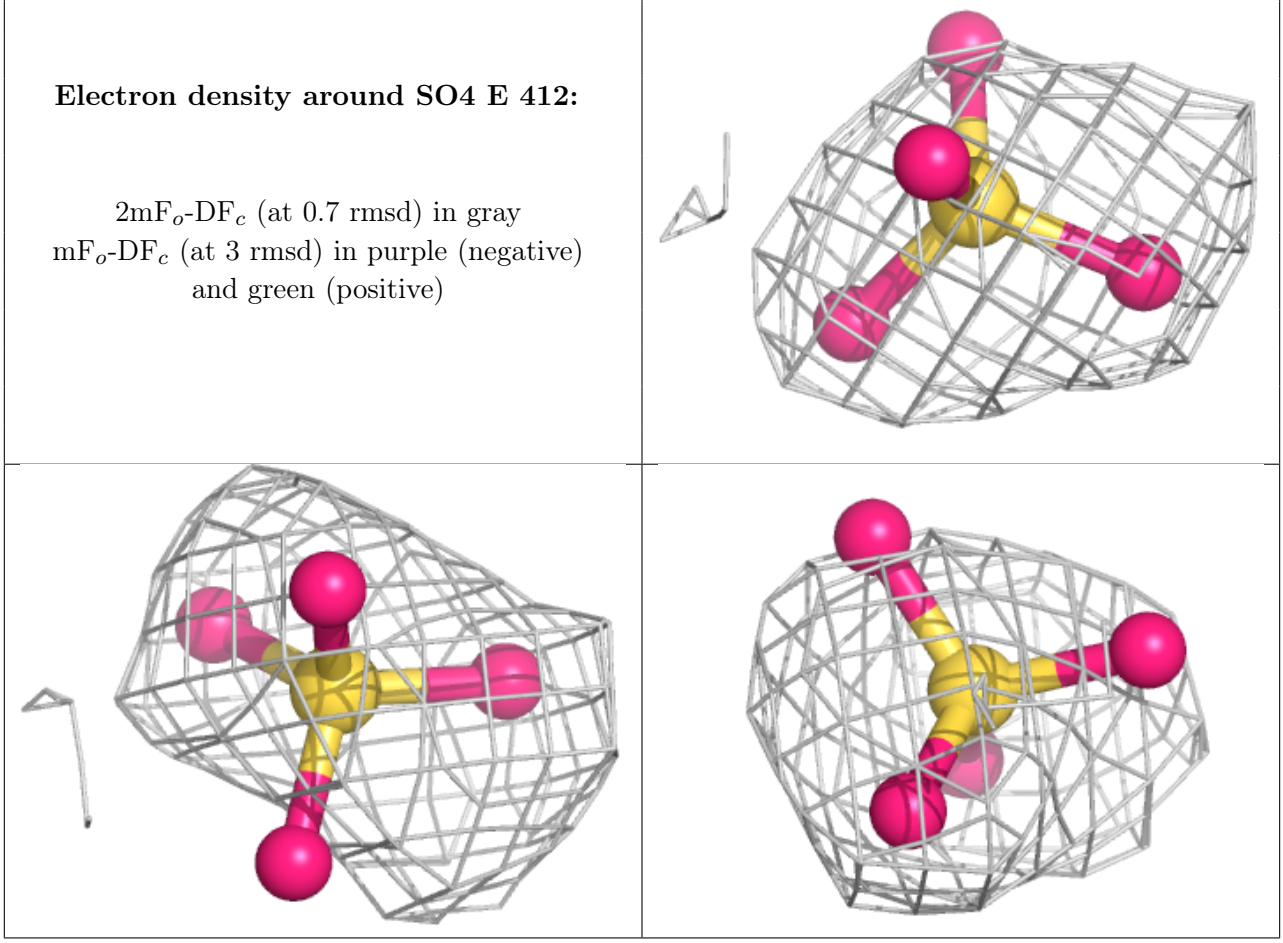






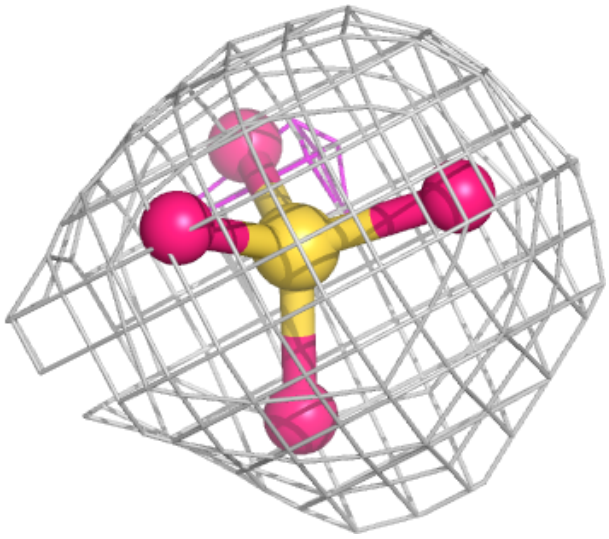
Electron density around SO4 E 412:

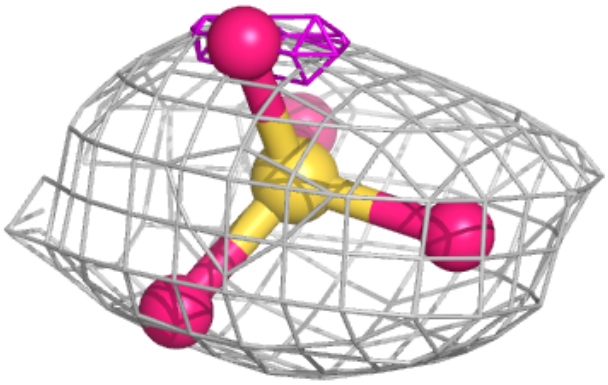
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

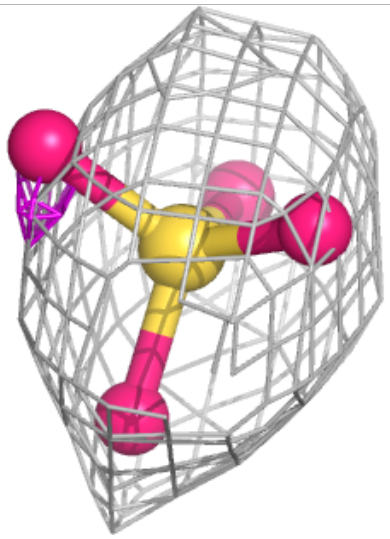


Electron density around SO4 H 404:

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

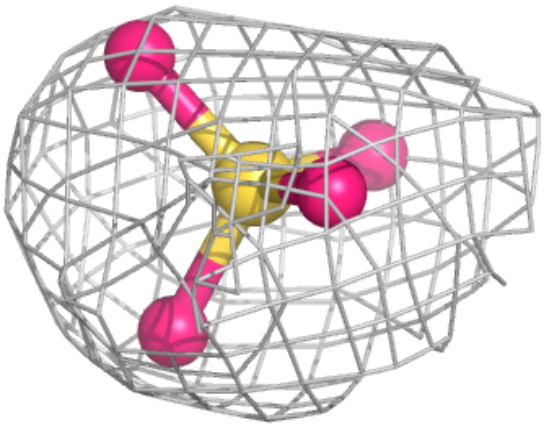


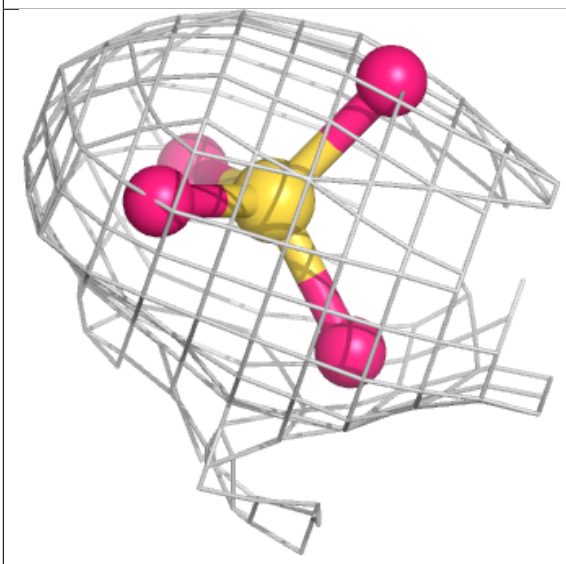


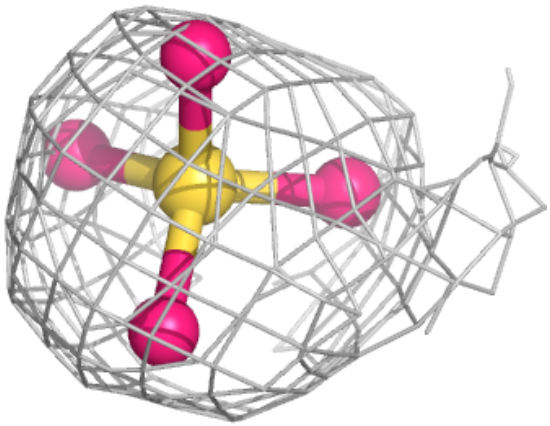


Electron density around SO4 E 410:

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

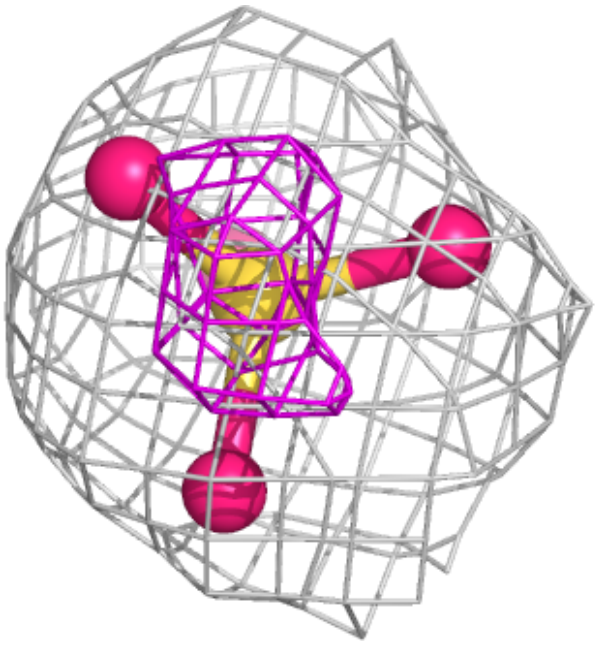


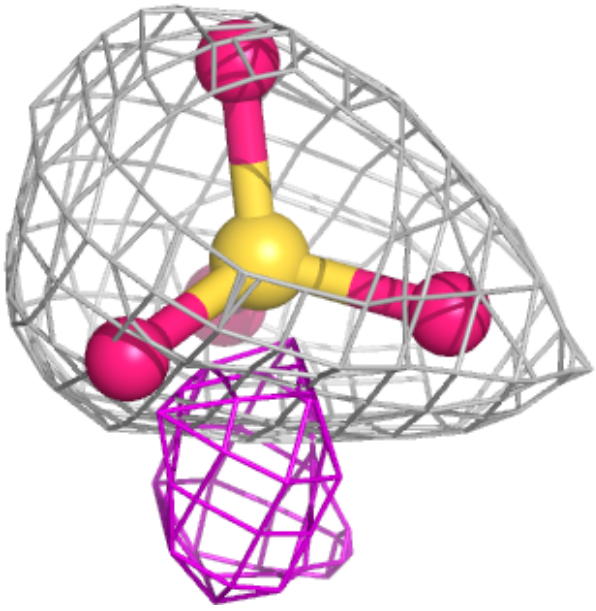


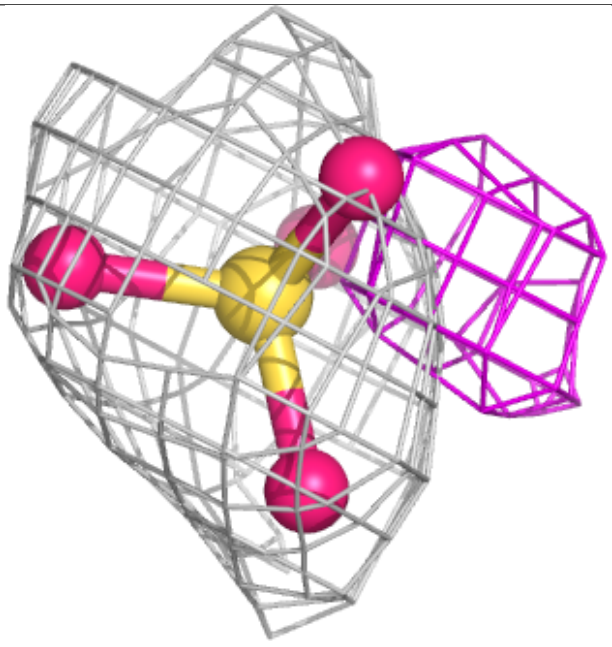


Electron density around SO4 B 404:

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

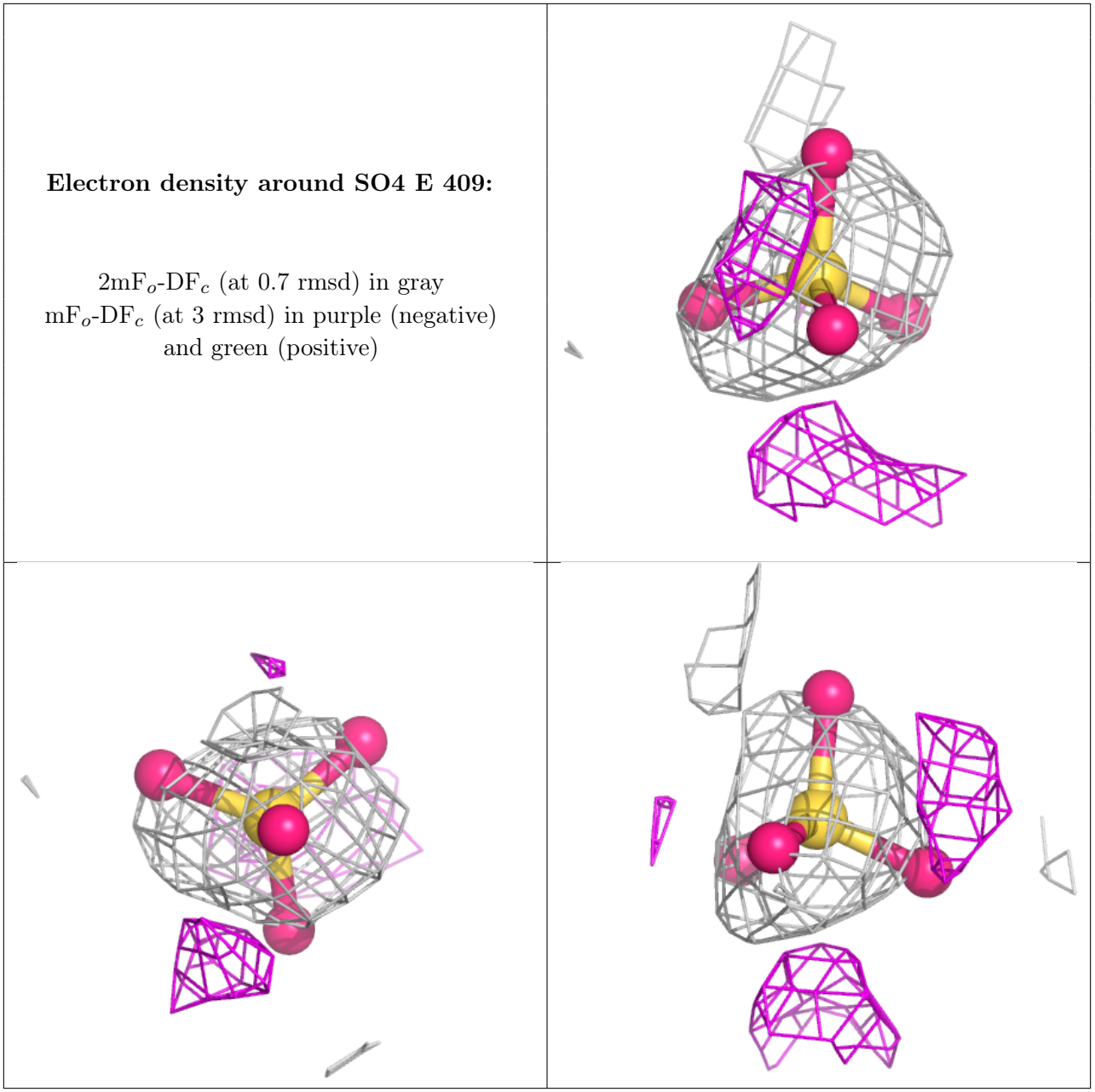






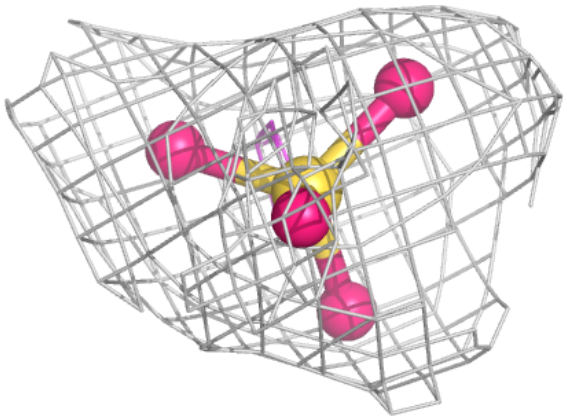
Electron density around SO4 E 409:

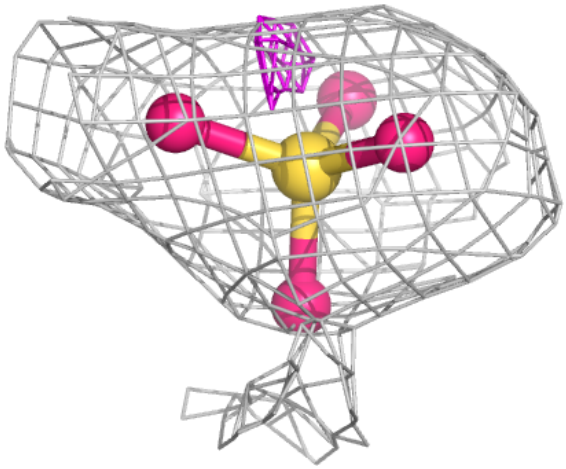
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

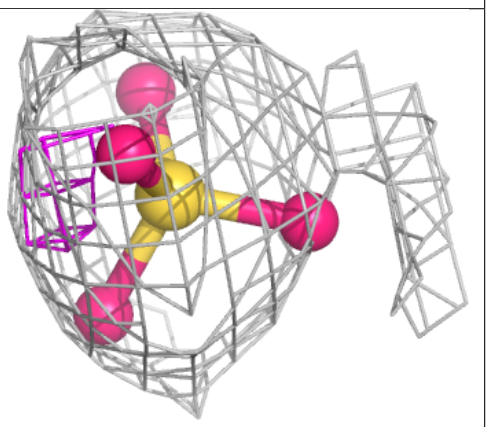


Electron density around SO4 F 404:

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

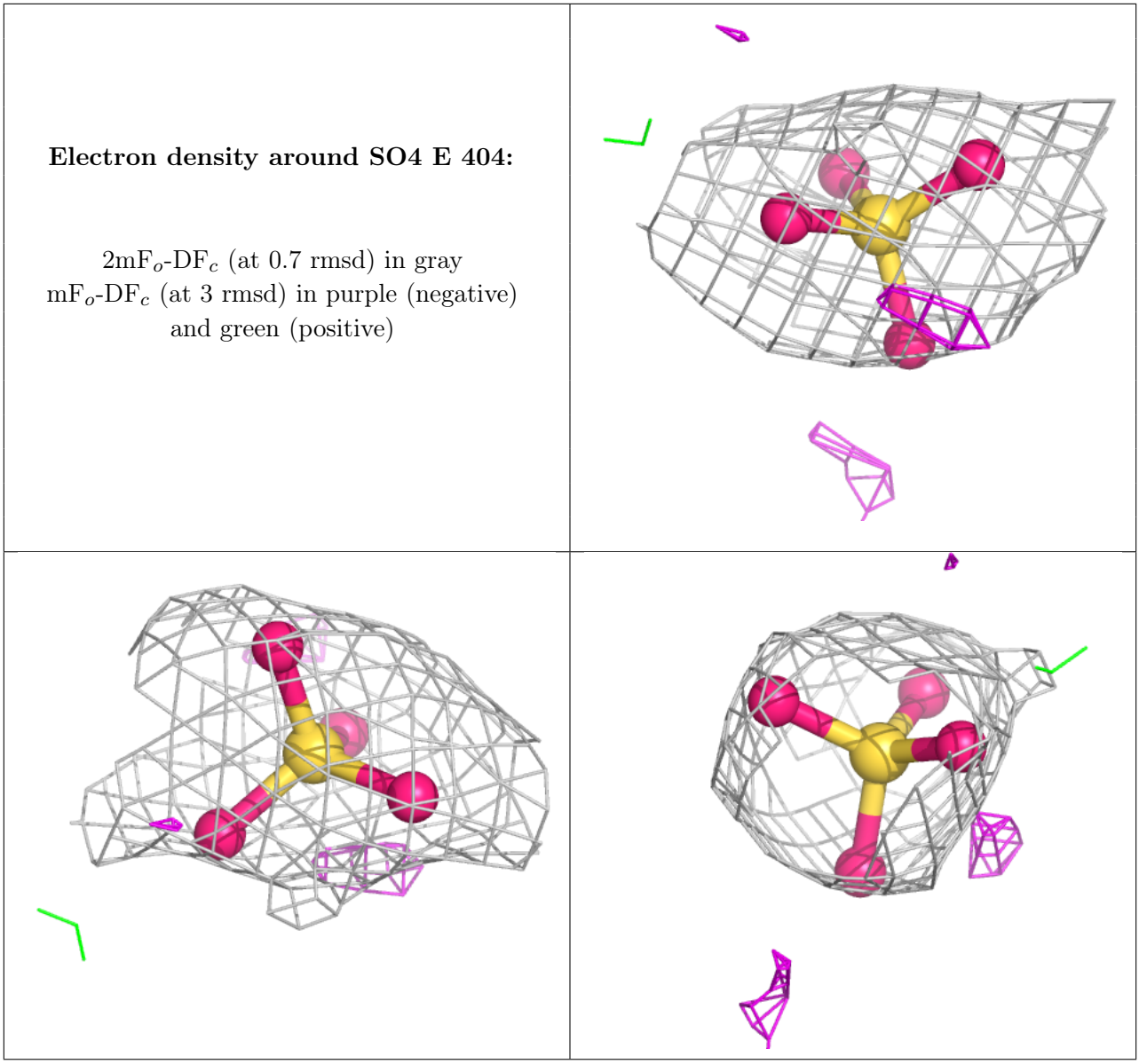






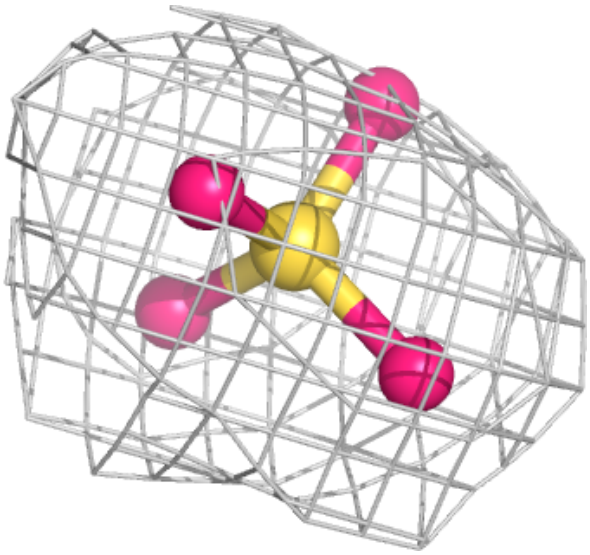
Electron density around SO4 E 404:

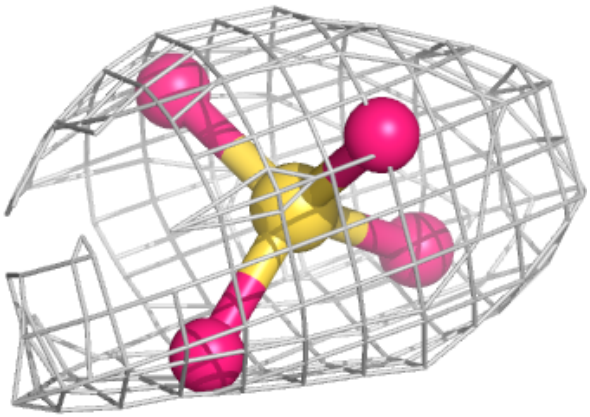
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

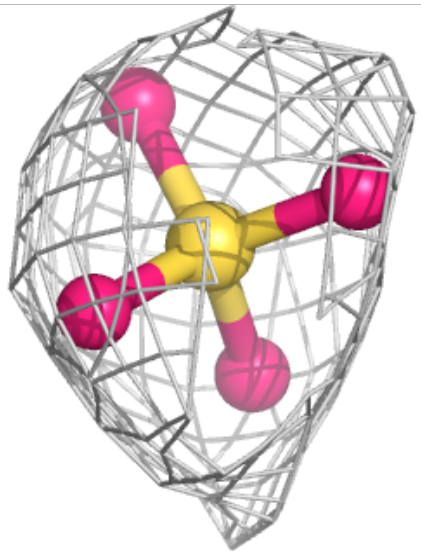


Electron density around SO4 F 406:

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

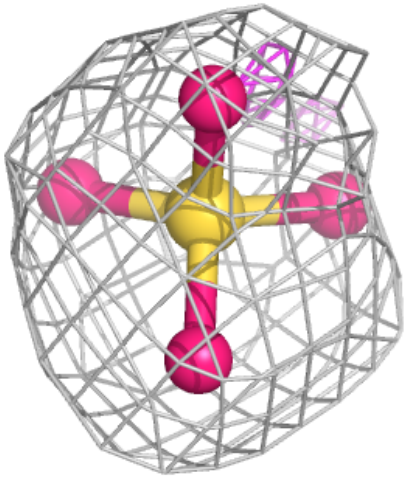


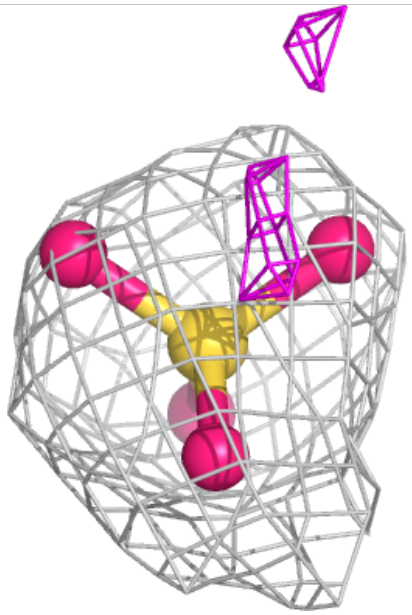


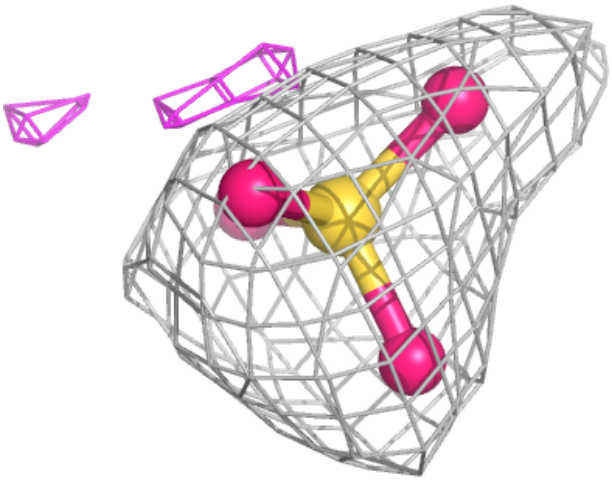


Electron density around SO4 B 405:

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

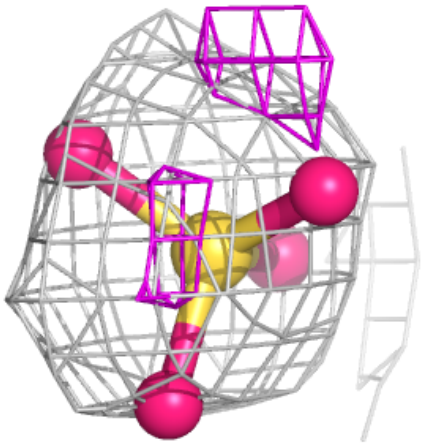


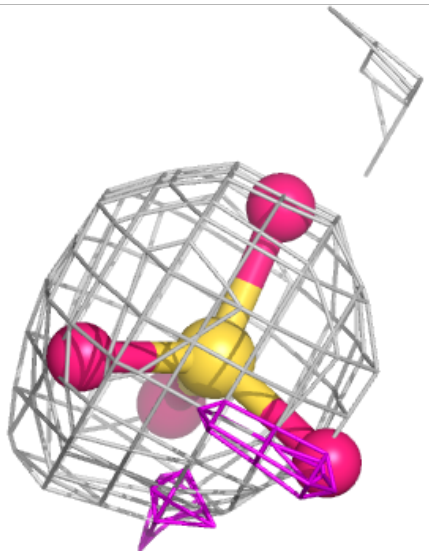


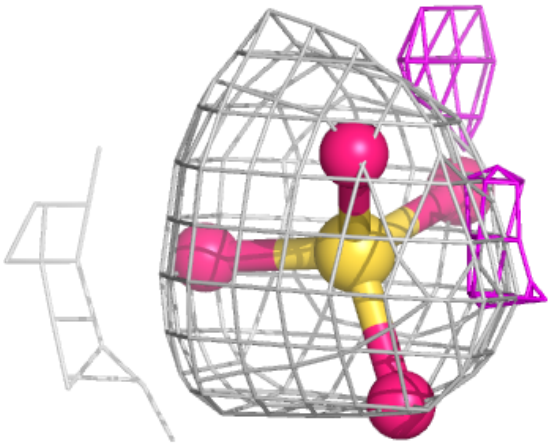


Electron density around SO4 E 413:

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

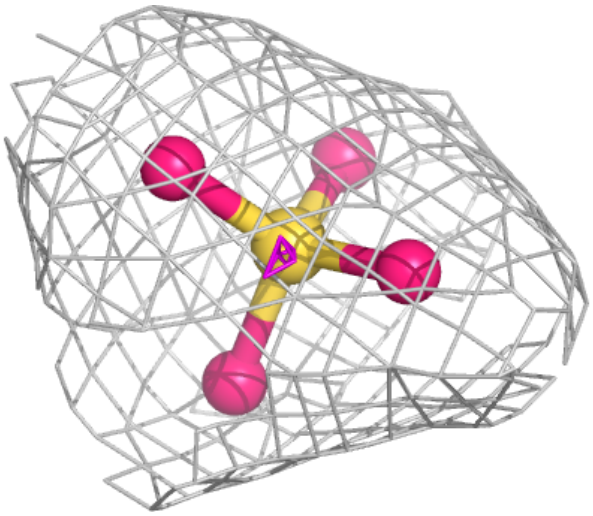


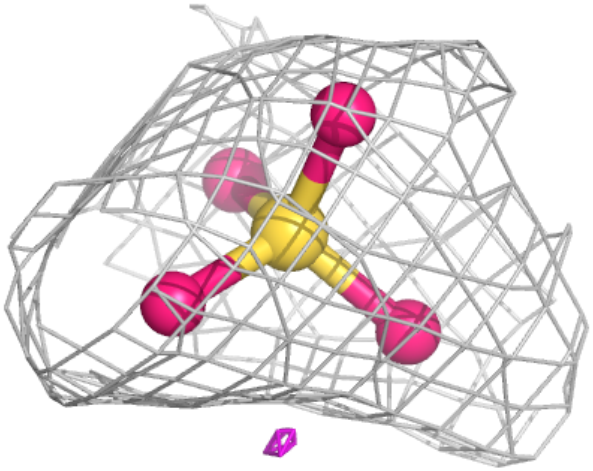


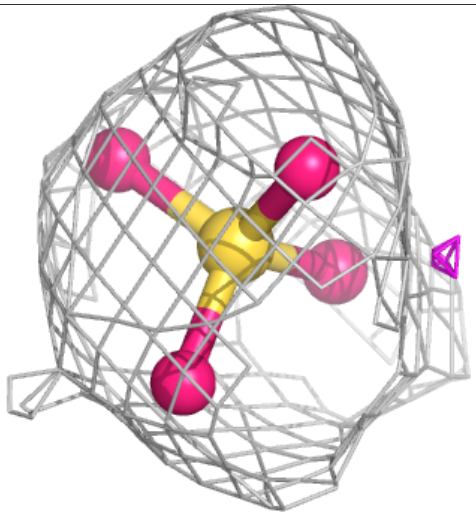


Electron density around SO4 H 403:

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

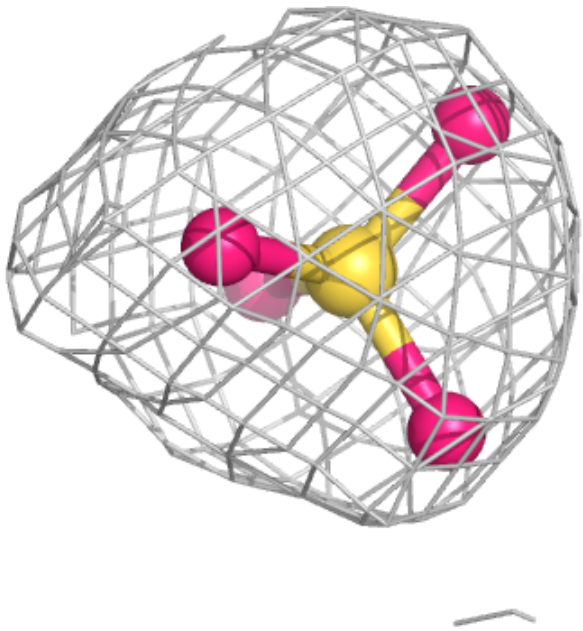


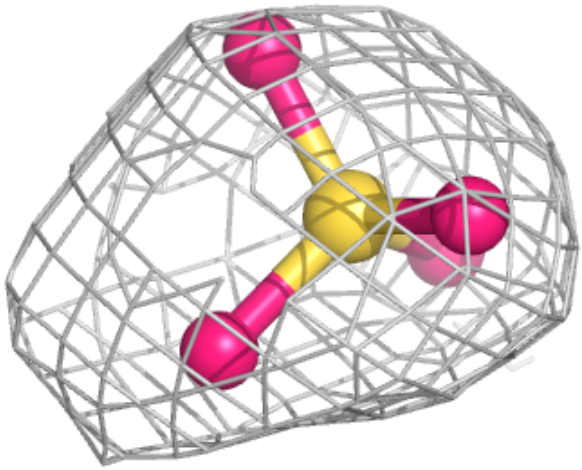


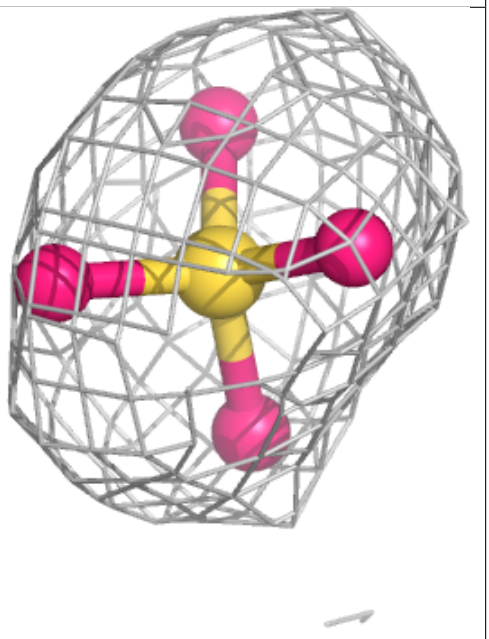


Electron density around SO4 E 405:

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

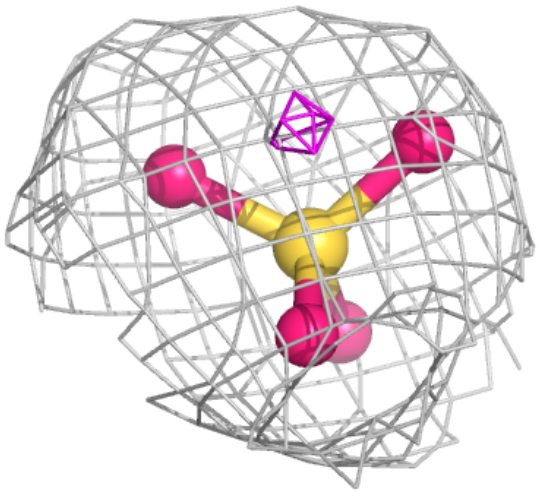


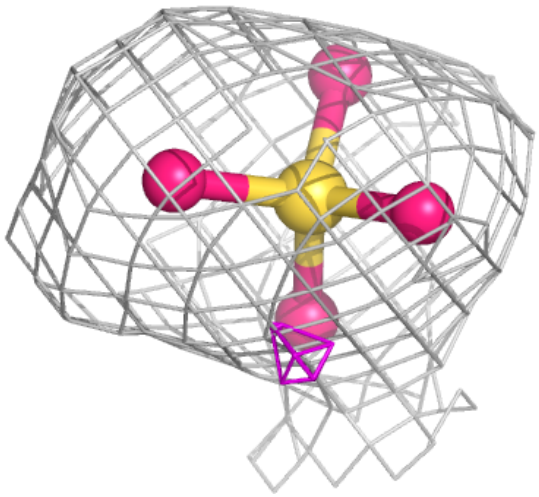


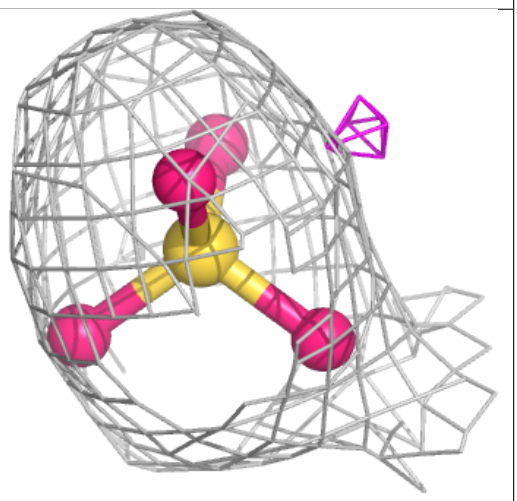


Electron density around SO4 H 402:

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

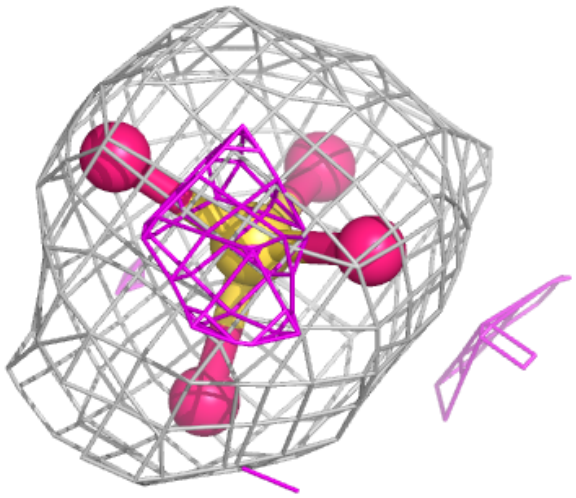


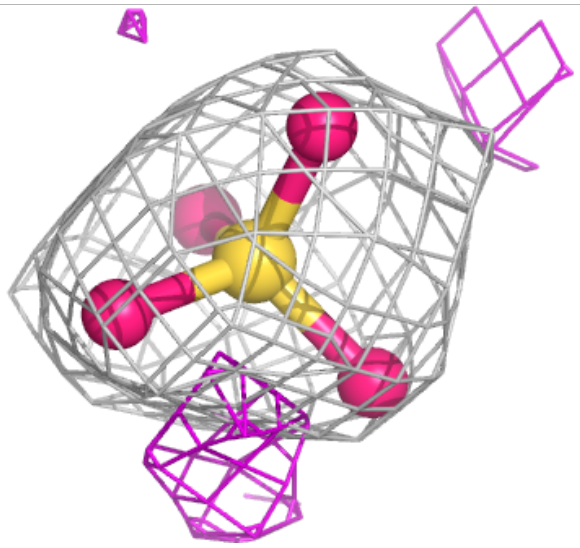


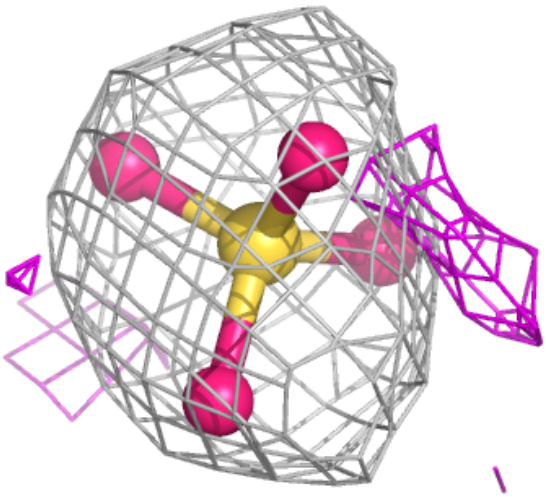


Electron density around SO4 E 407:

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

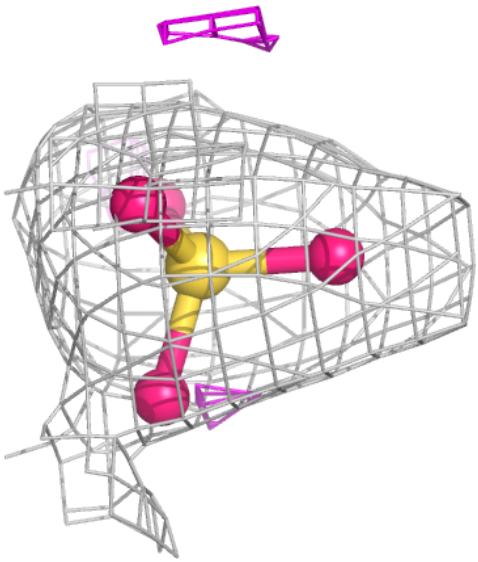


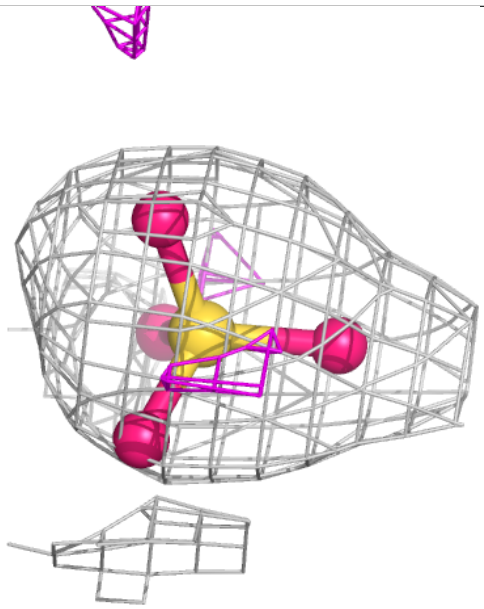


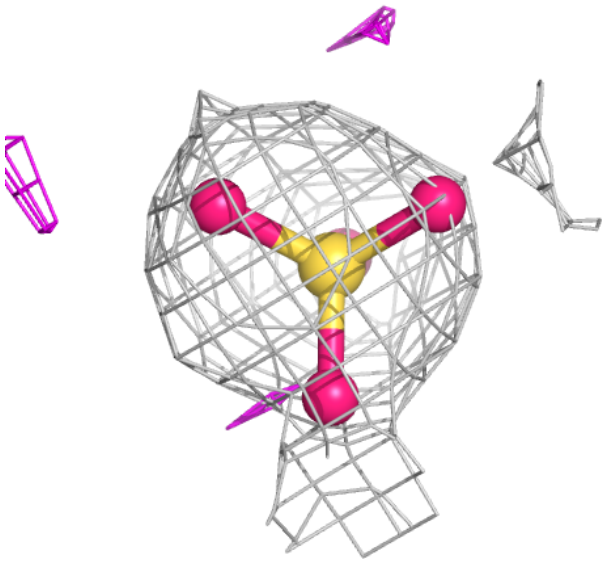


Electron density around SO4 E 403:

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

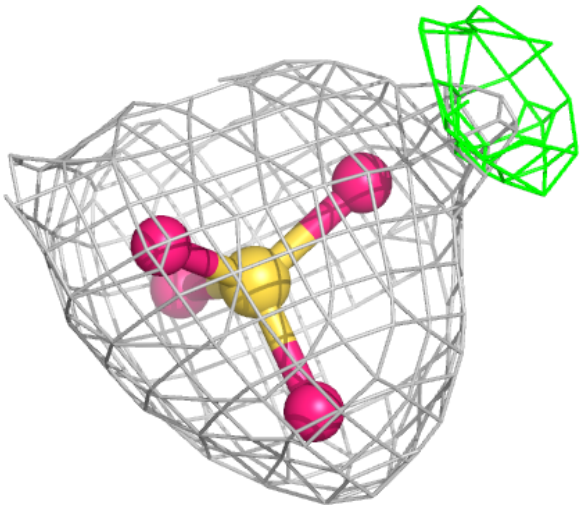


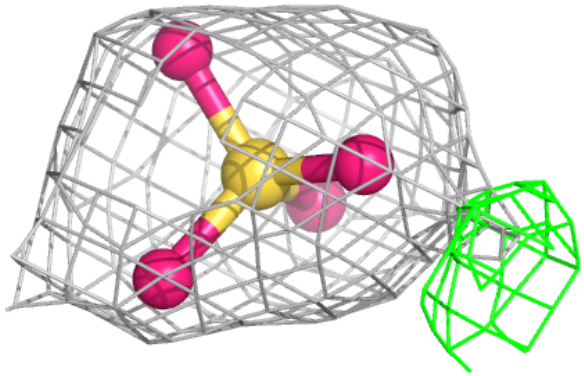


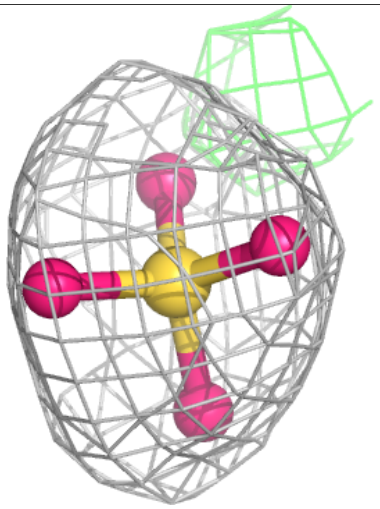


Electron density around SO4 H 405:

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

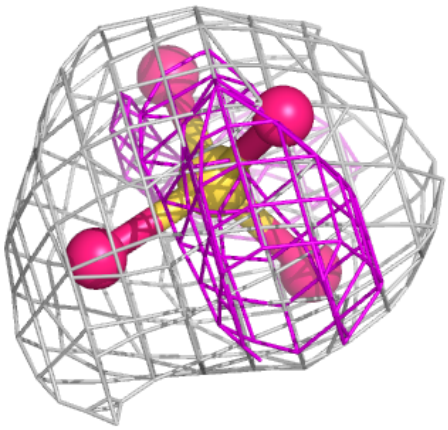


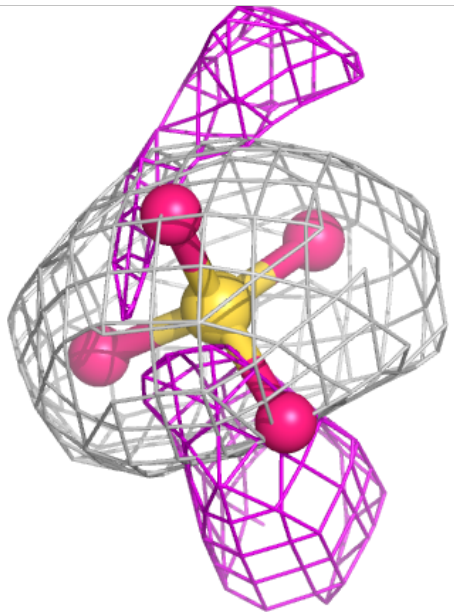


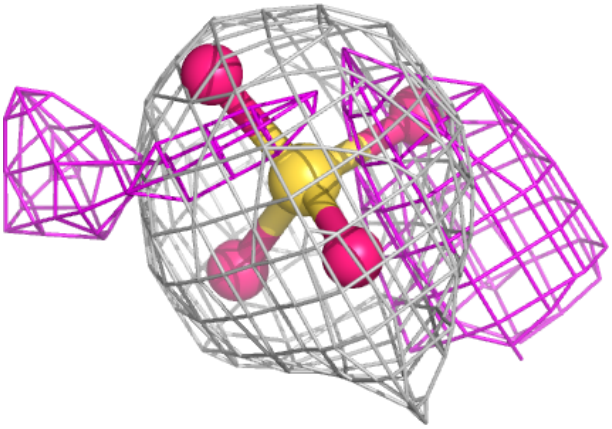


Electron density around SO4 F 403:

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

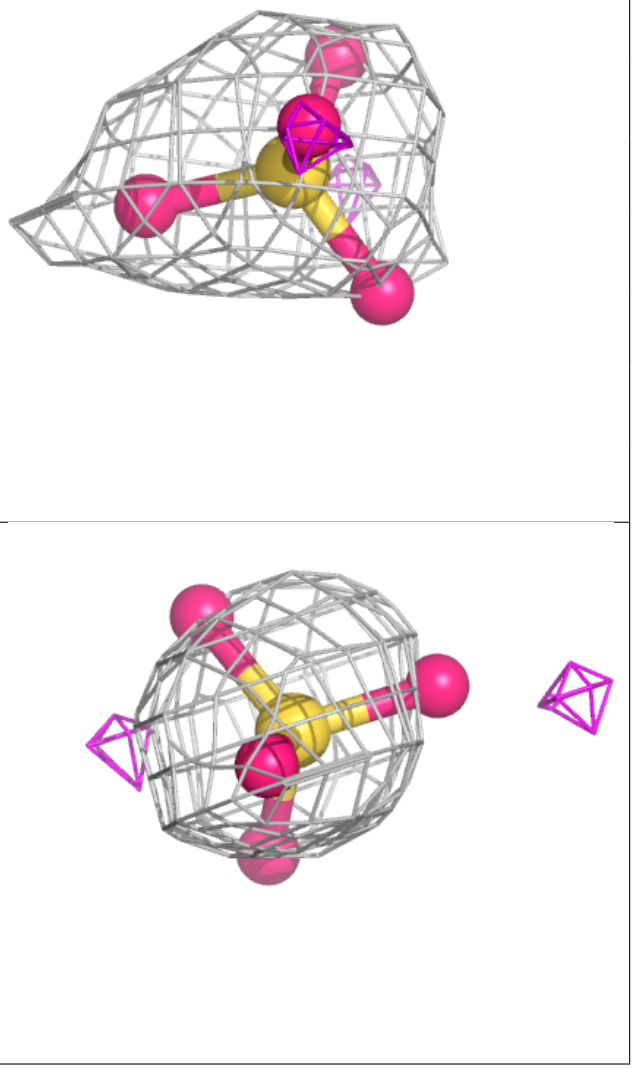






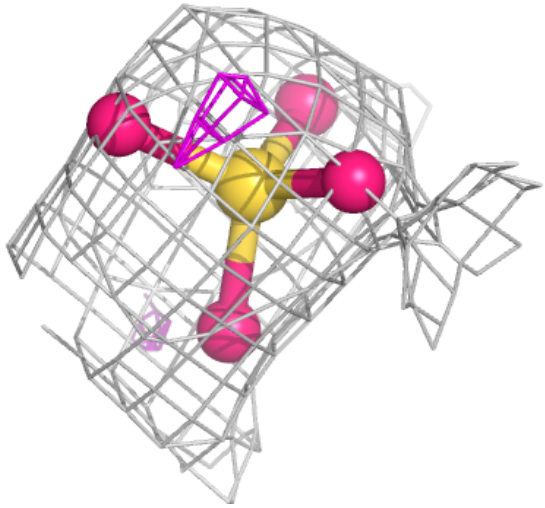
Electron density around SO4 A 403:

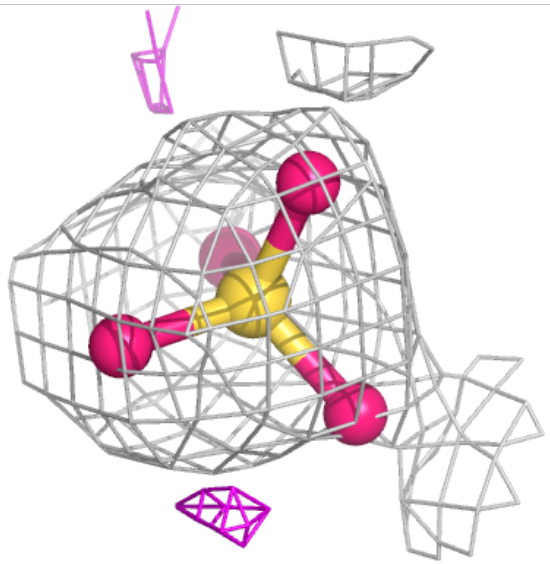
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

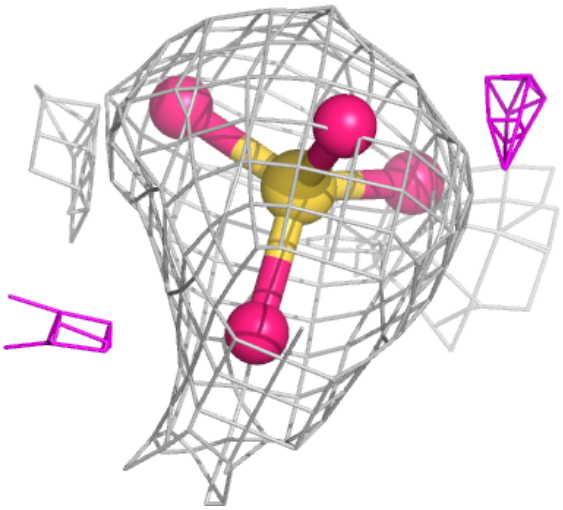


Electron density around SO4 F 405:

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

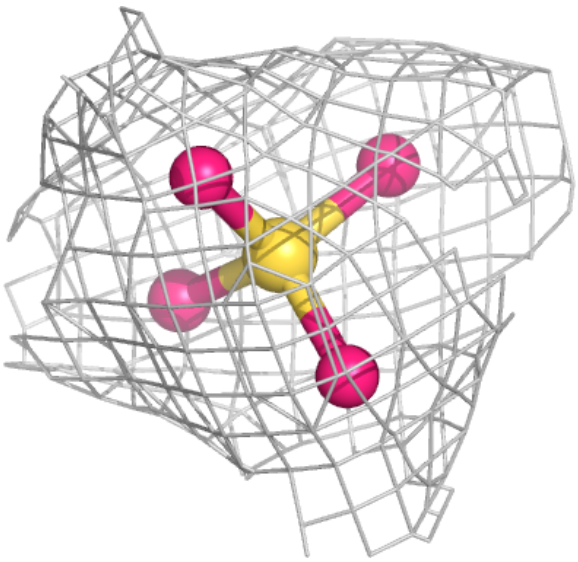


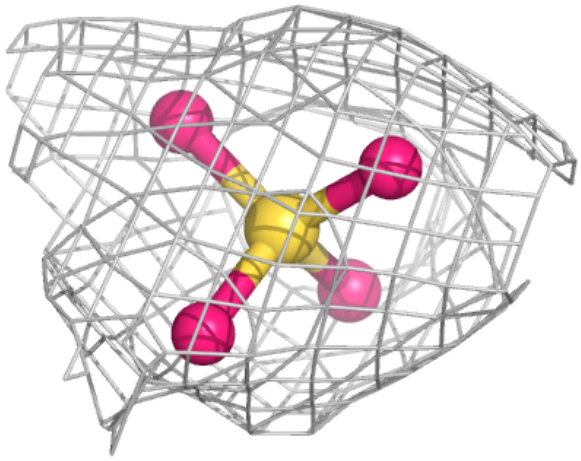


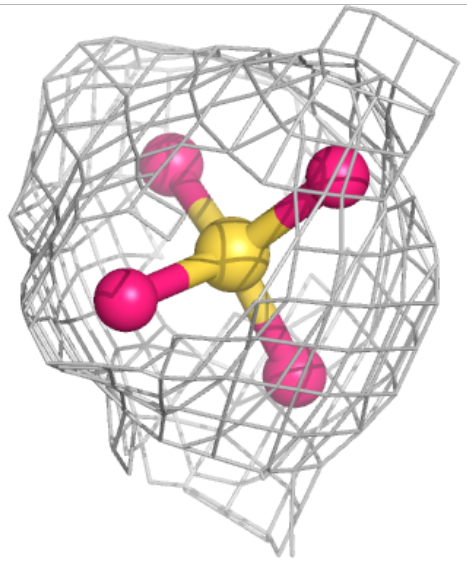


Electron density around SO4 D 401:

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

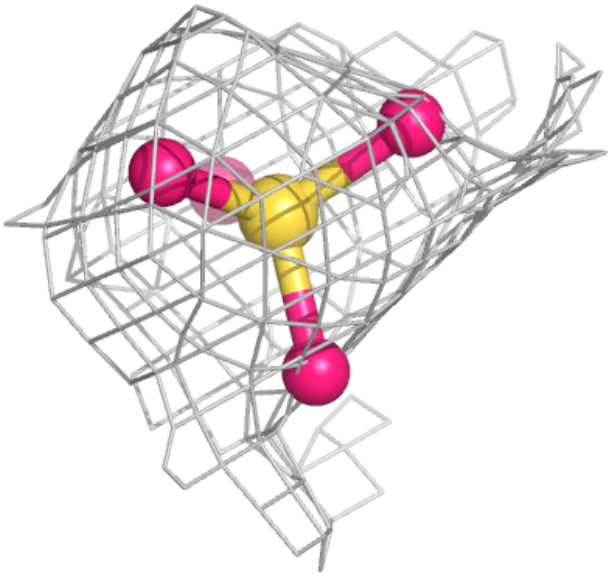


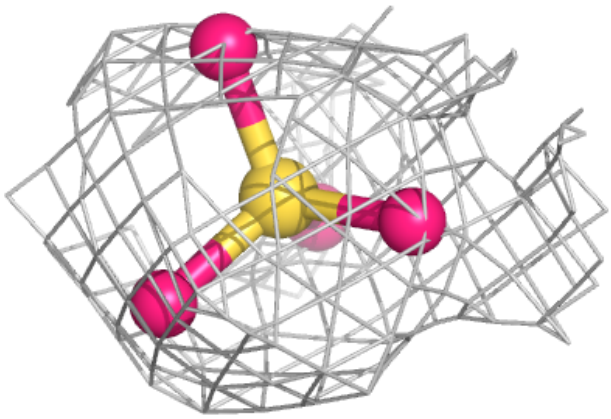


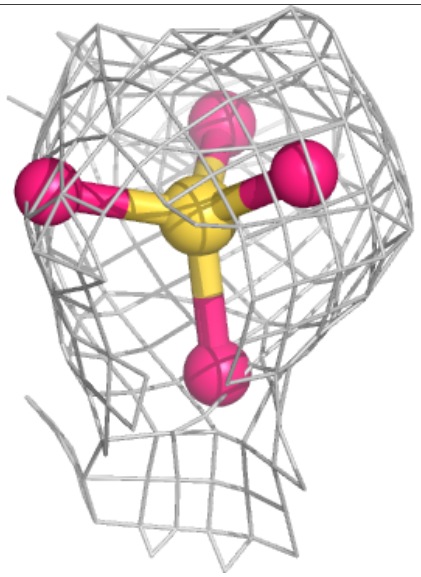


Electron density around SO4 E 406:

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

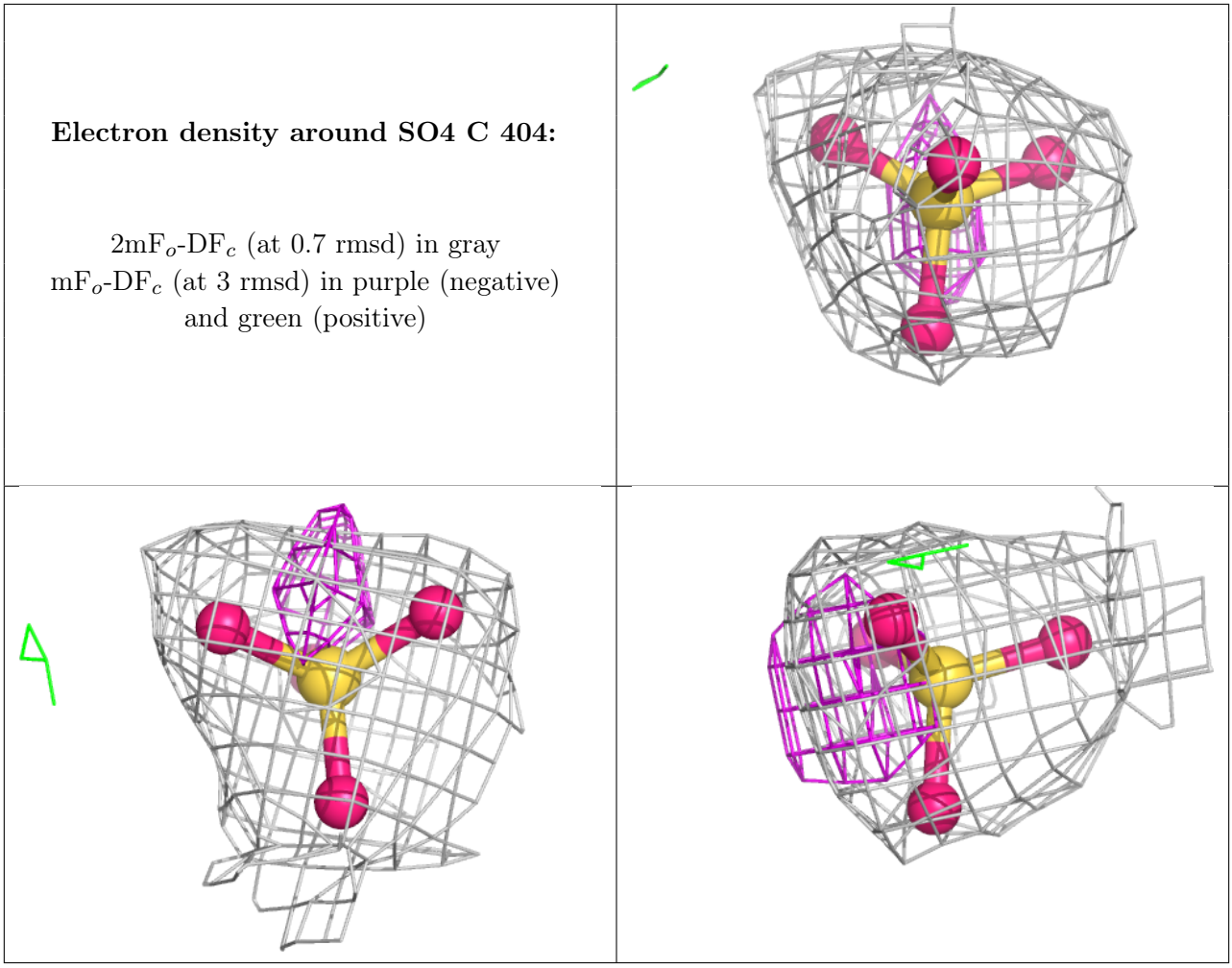






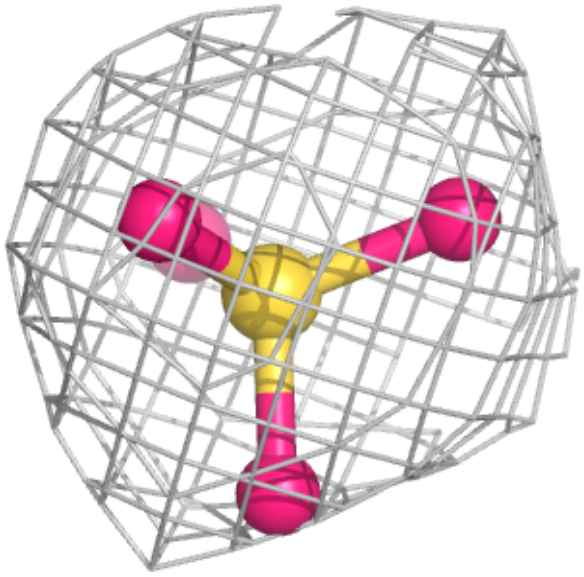
Electron density around SO4 C 404:

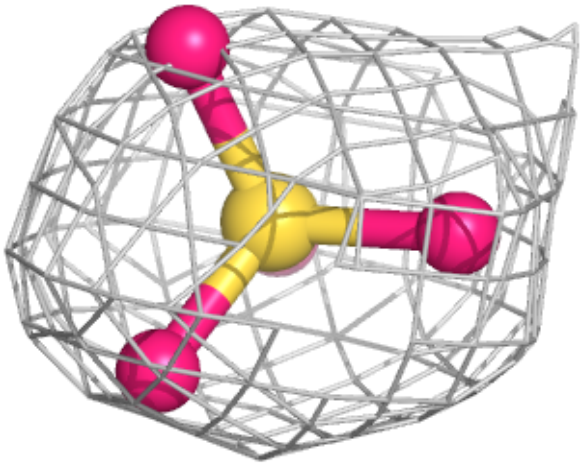
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

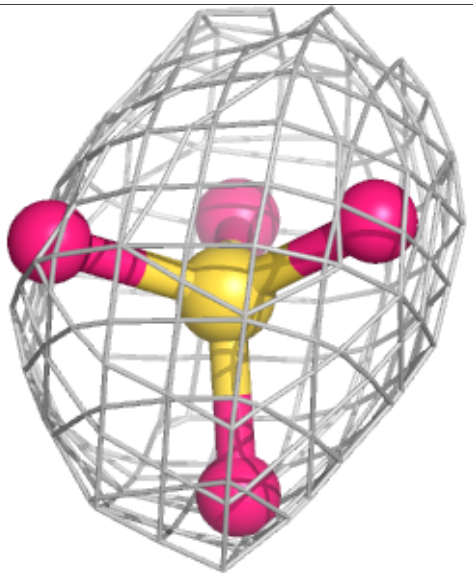


Electron density around SO4 E 408:

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

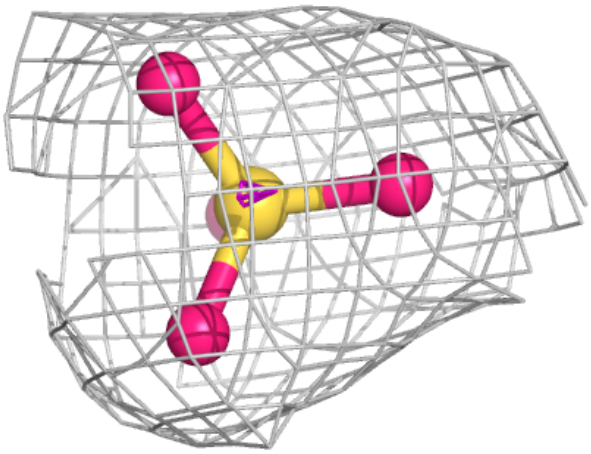


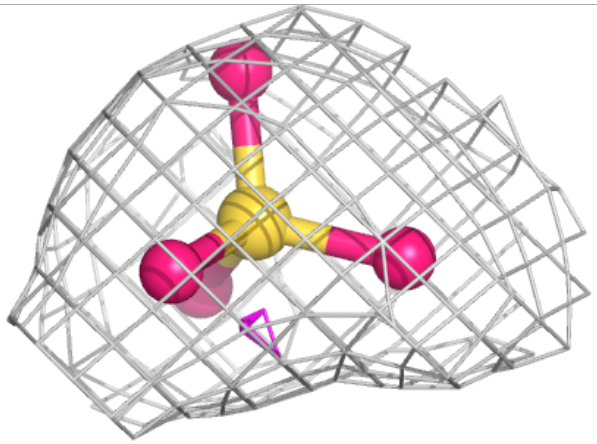


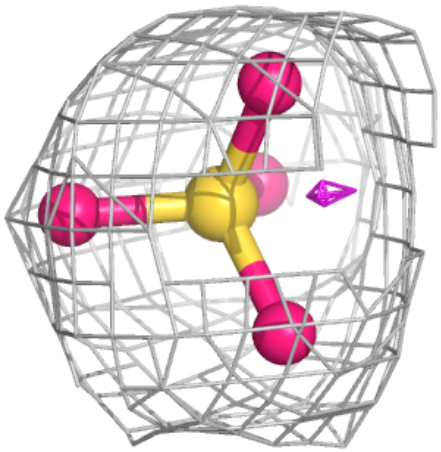


Electron density around SO4 F 402:

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

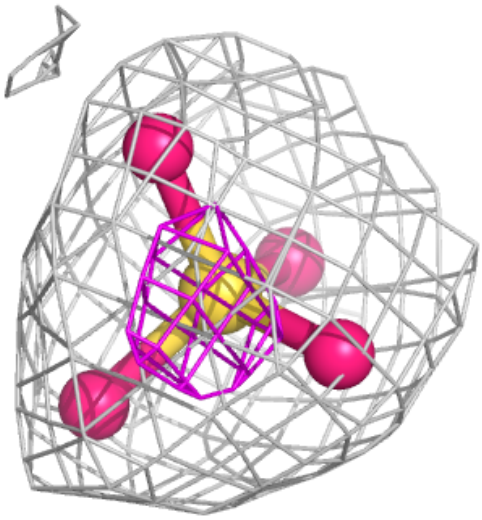


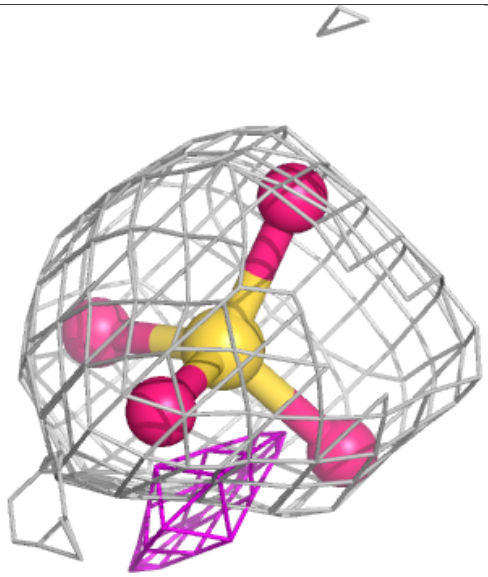


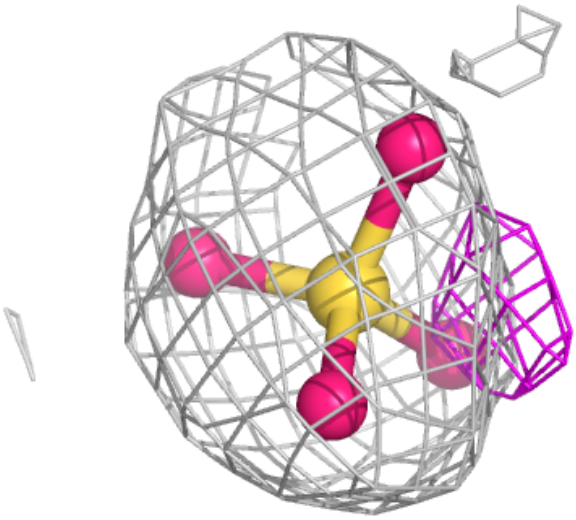


Electron density around SO4 A 402:

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

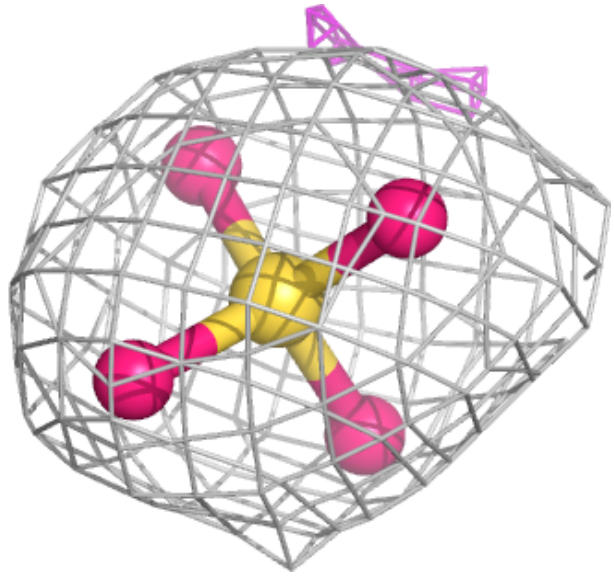


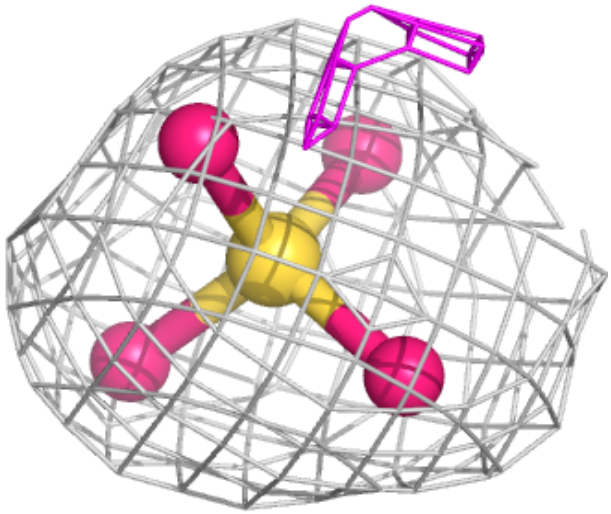


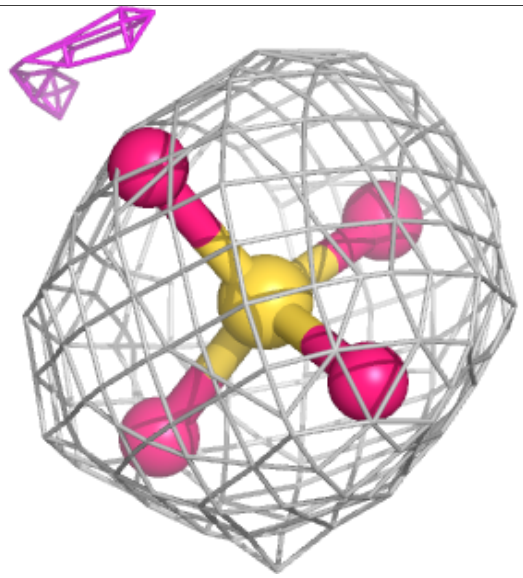


Electron density around SO4 A 405:

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

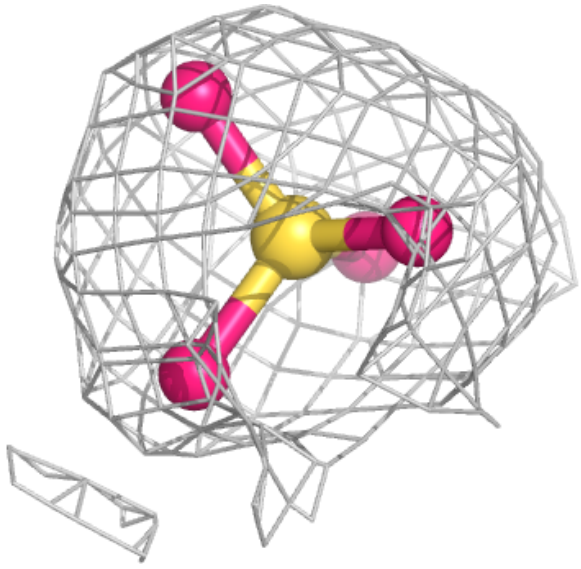


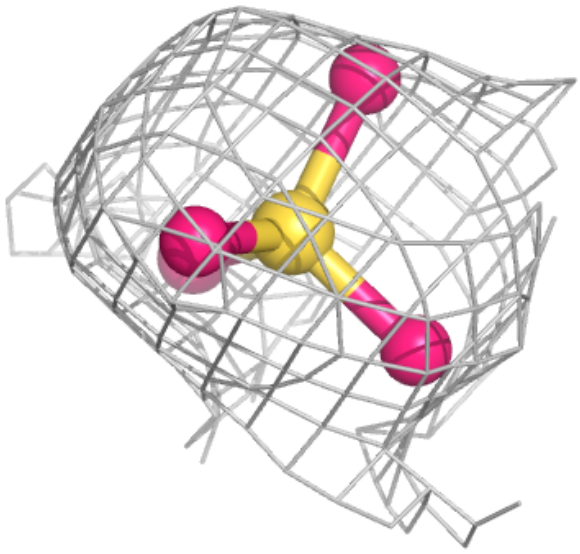


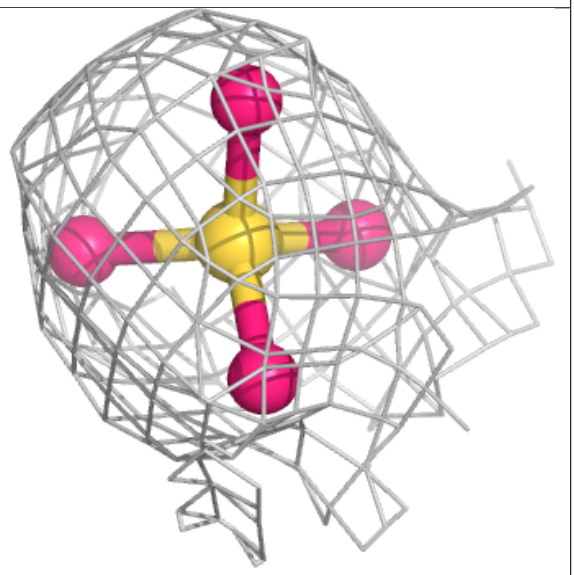


Electron density around SO4 B 403:

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

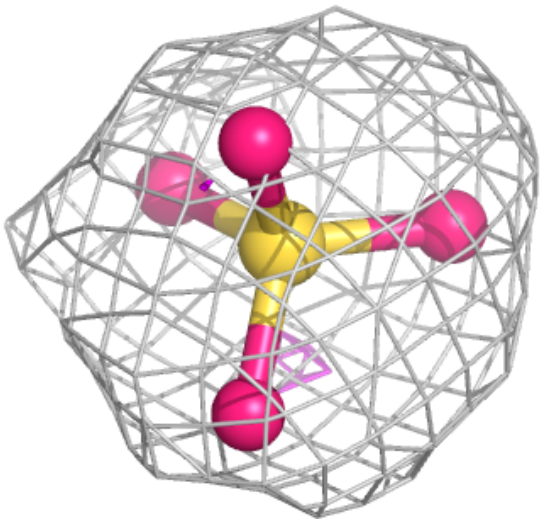


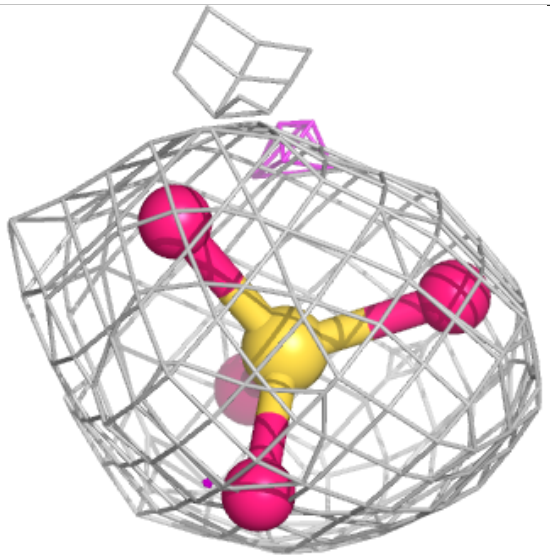


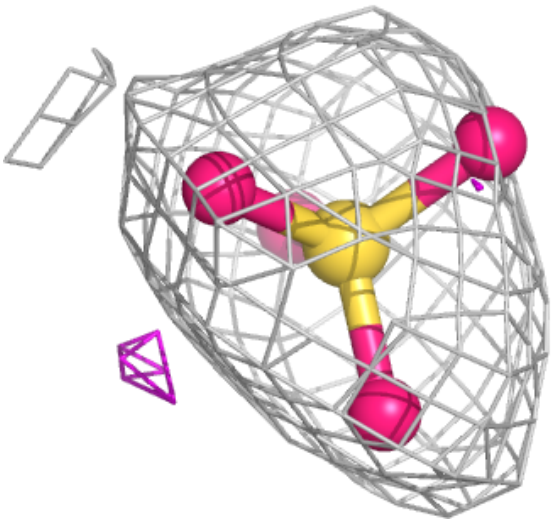


Electron density around SO4 A 401:

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

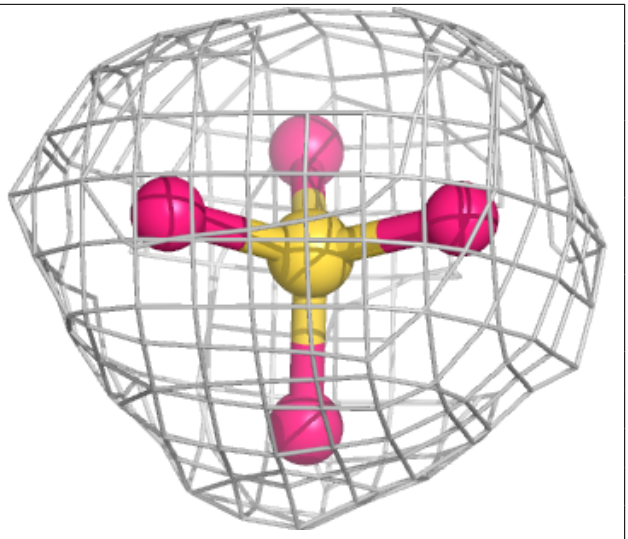


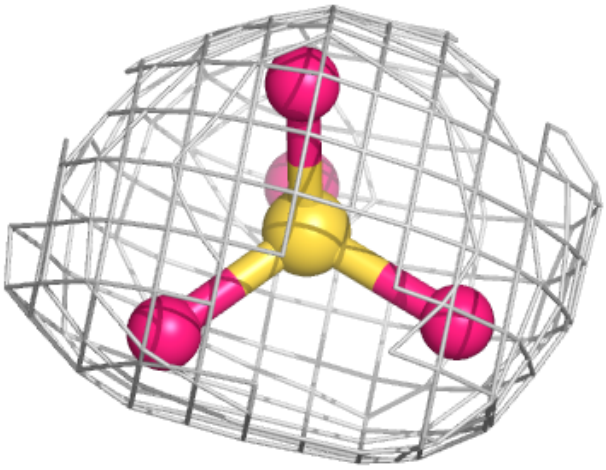


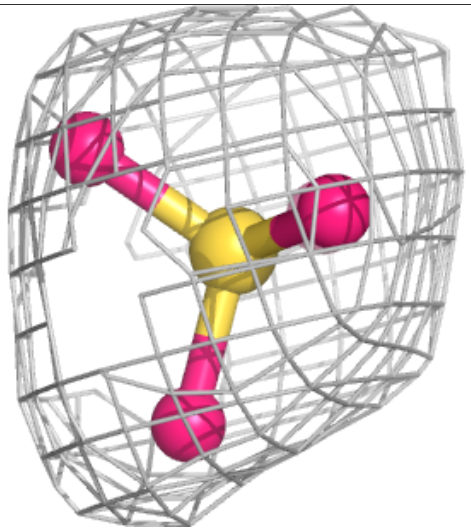


Electron density around SO4 G 404:

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

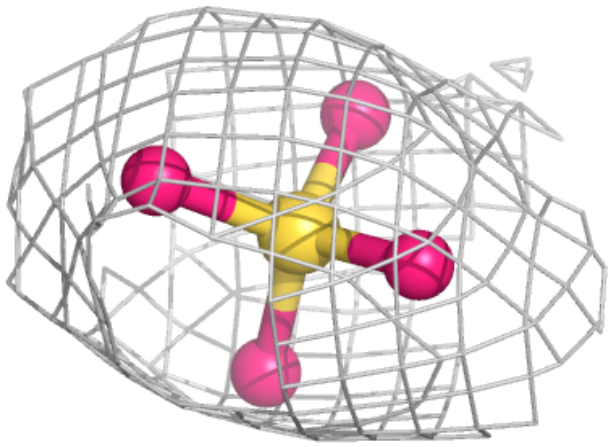


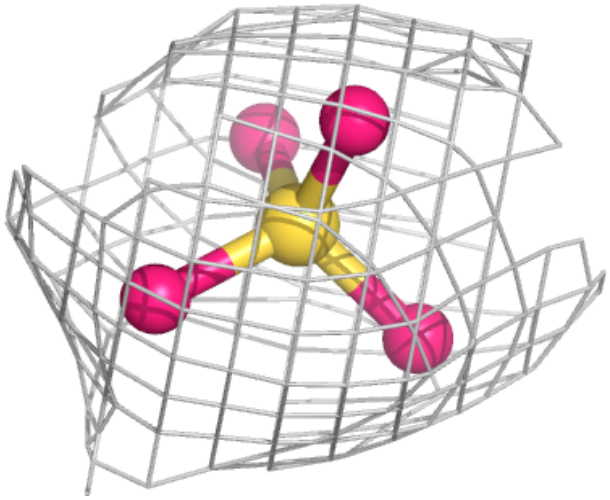


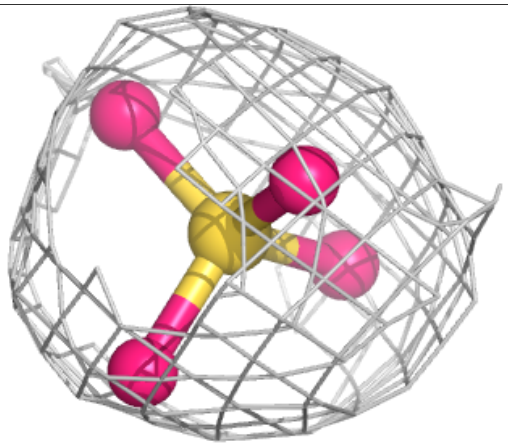


Electron density around SO4 H 401:

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

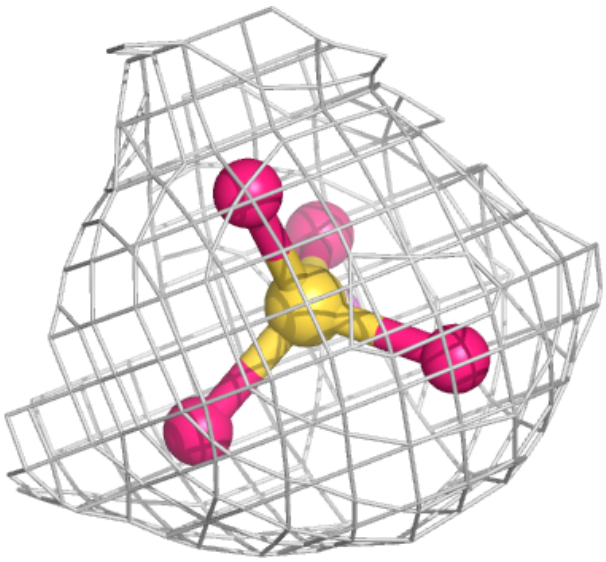


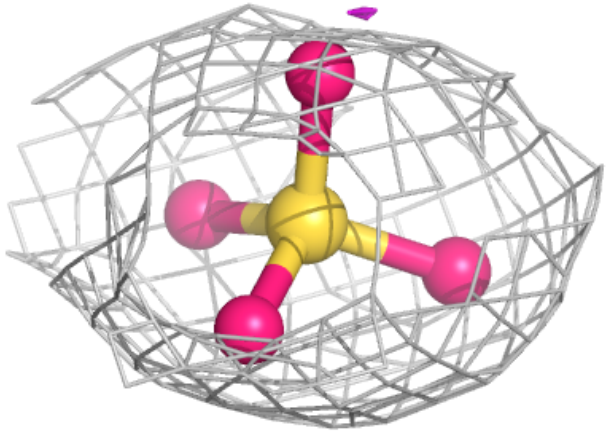


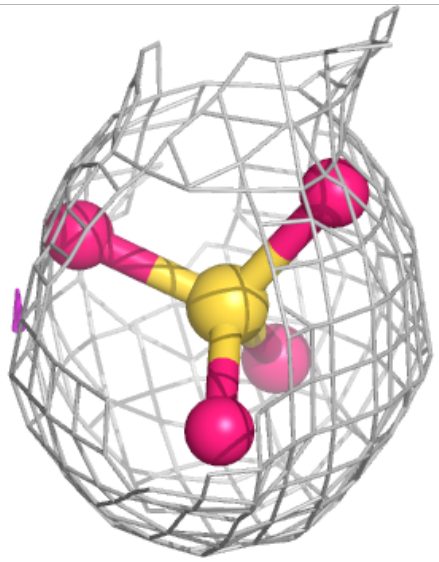


Electron density around SO4 A 406:

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

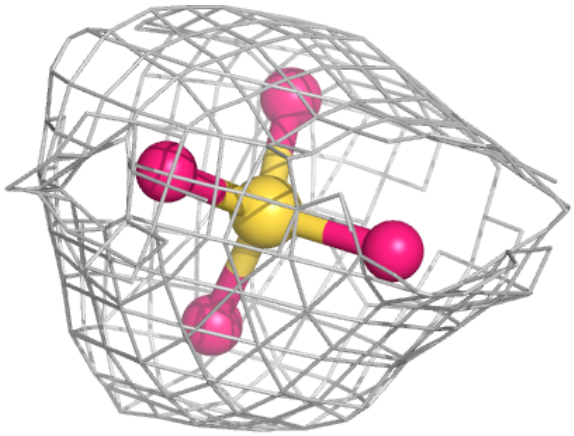


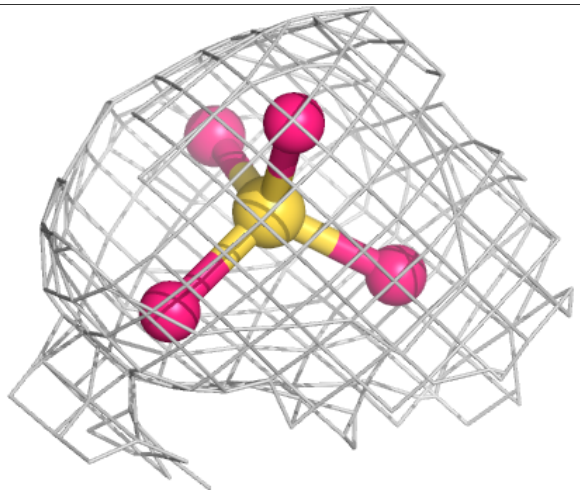


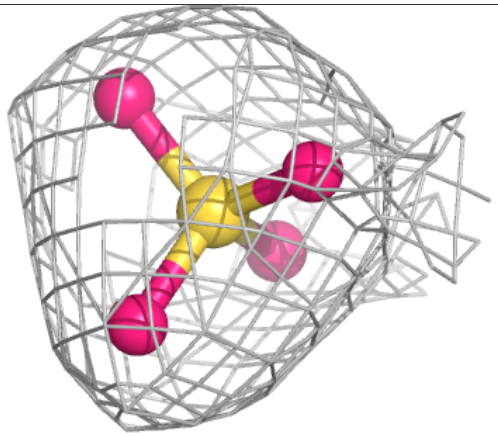


Electron density around SO4 C 402:

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

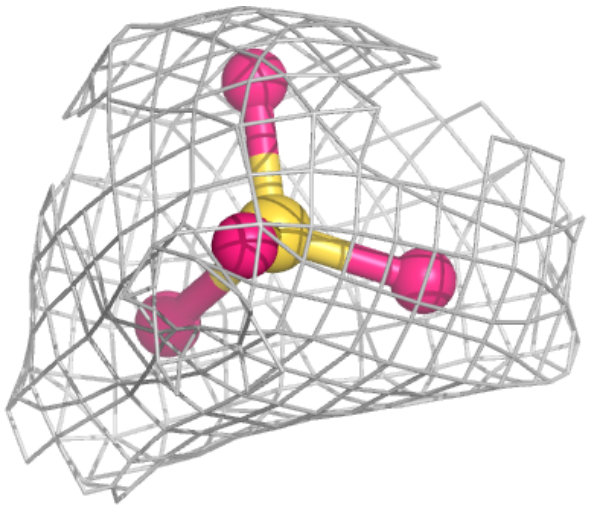


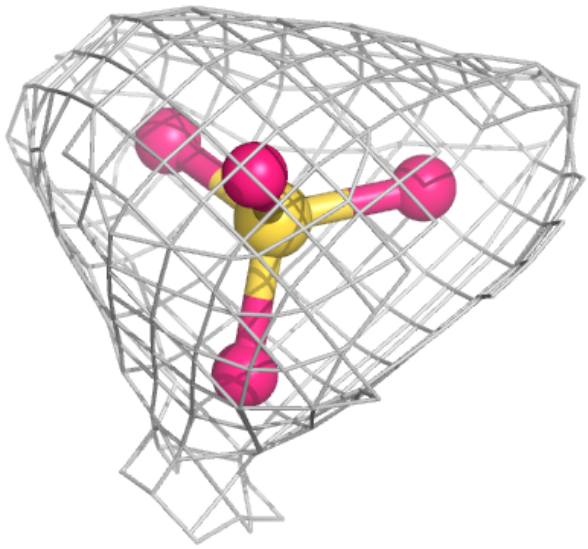


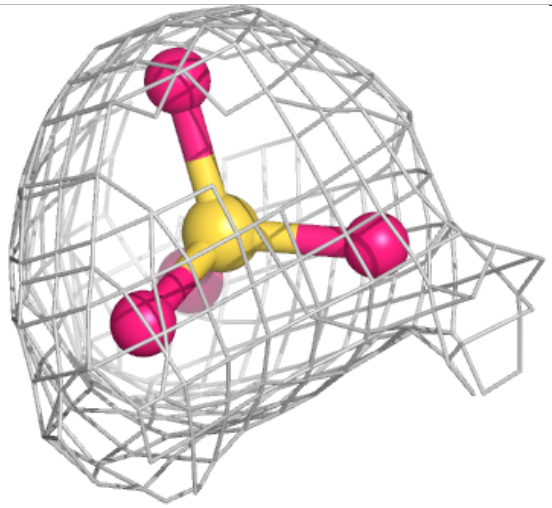


Electron density around SO4 B 402:

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

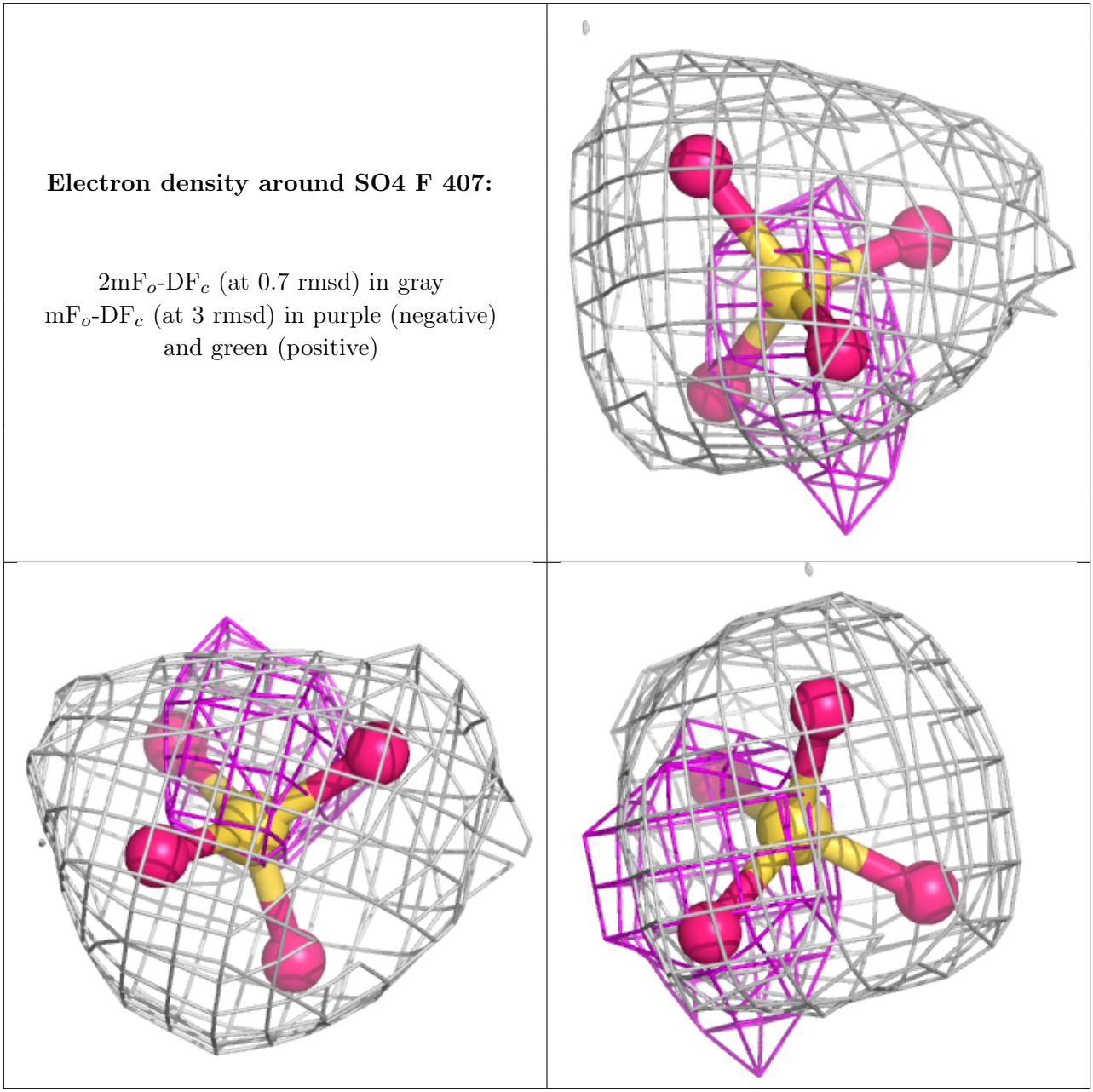






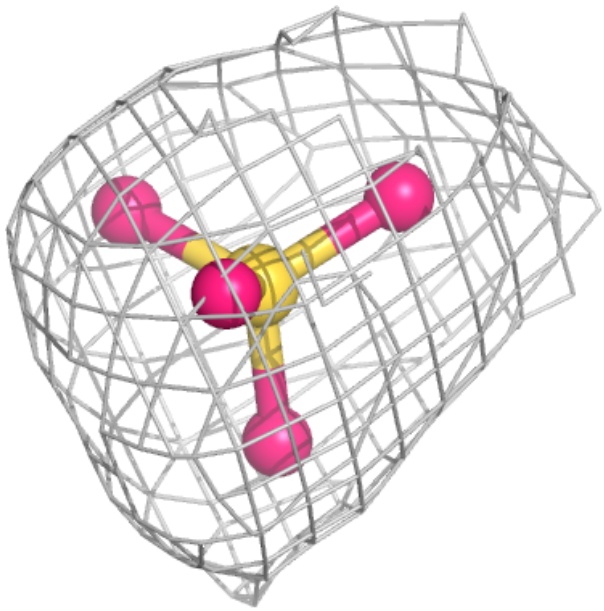
Electron density around SO4 F 407:

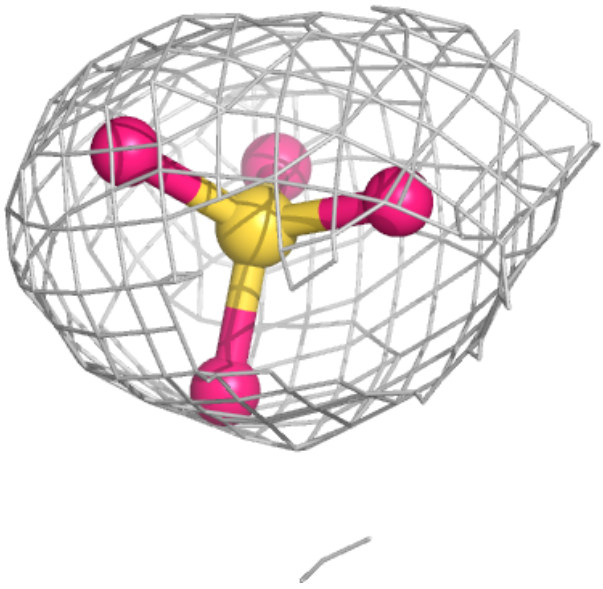
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

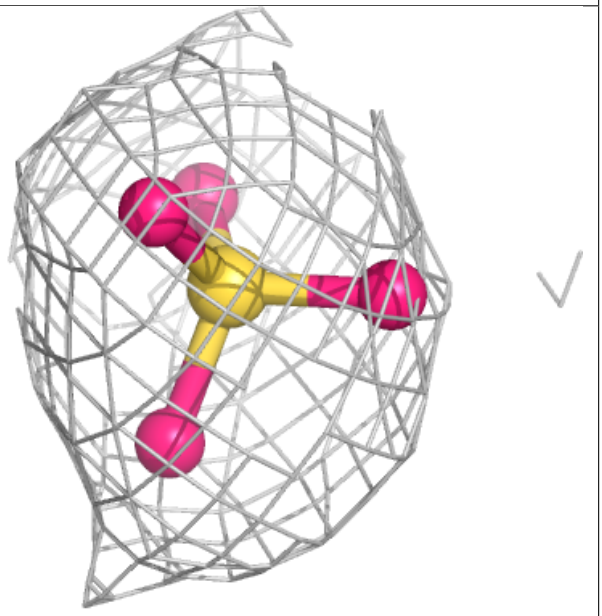


Electron density around SO4 D 402:

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

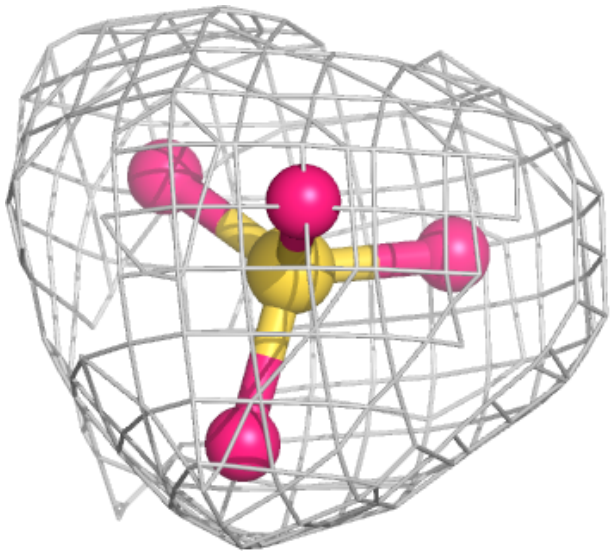


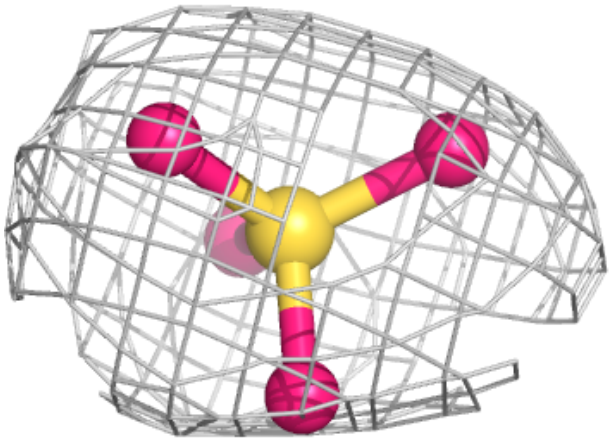


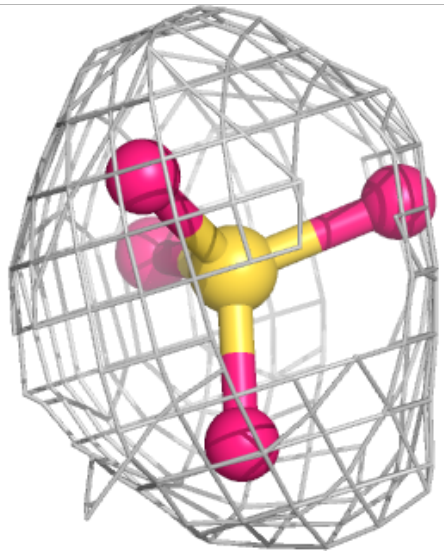


Electron density around SO4 D 403:

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

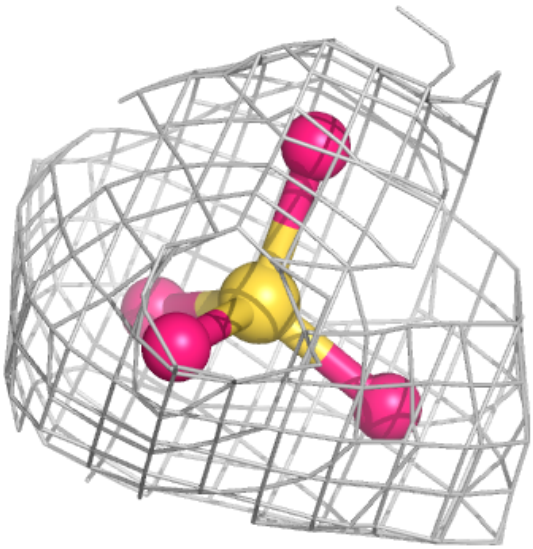


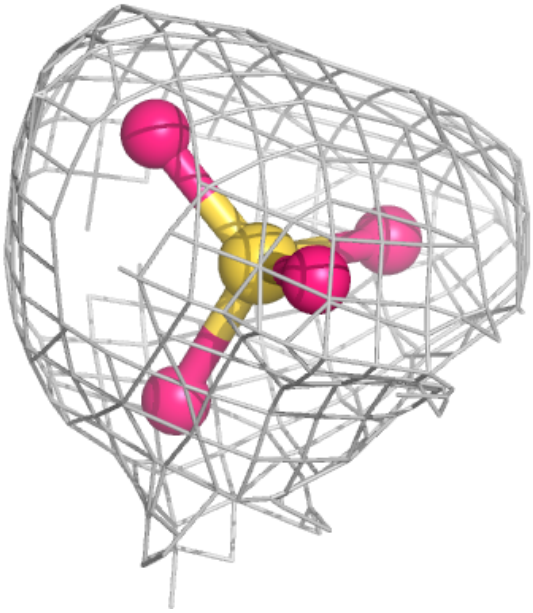


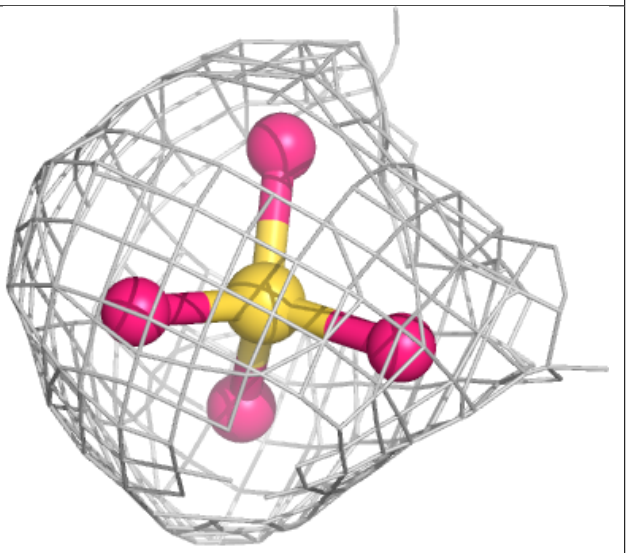


Electron density around SO4 E 401:

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

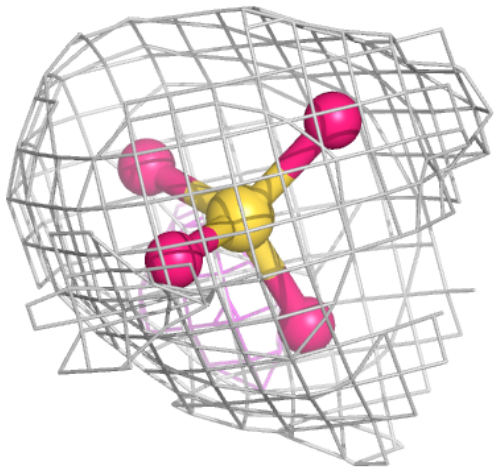


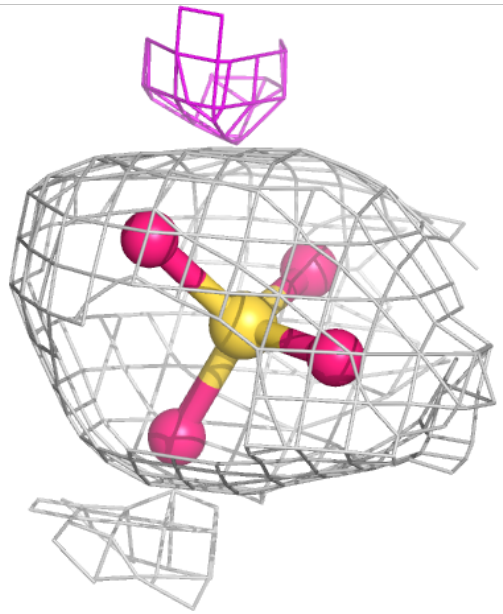


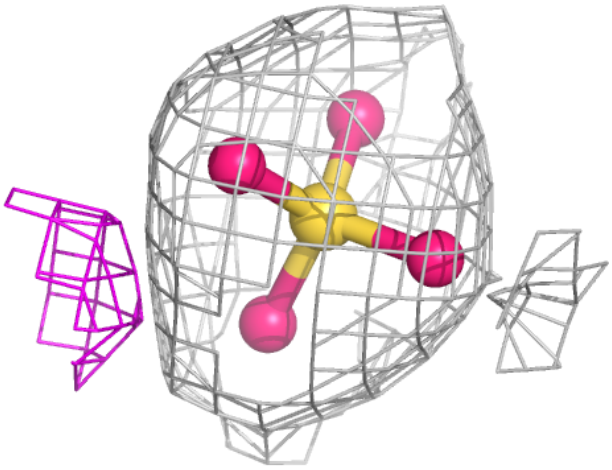


Electron density around SO4 C 401:

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

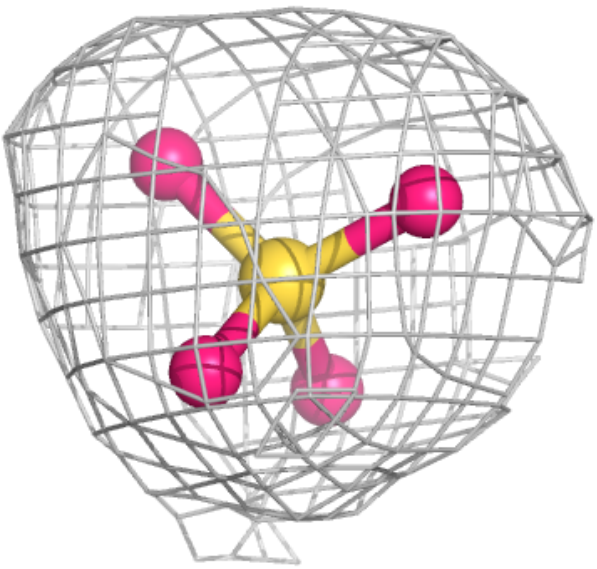


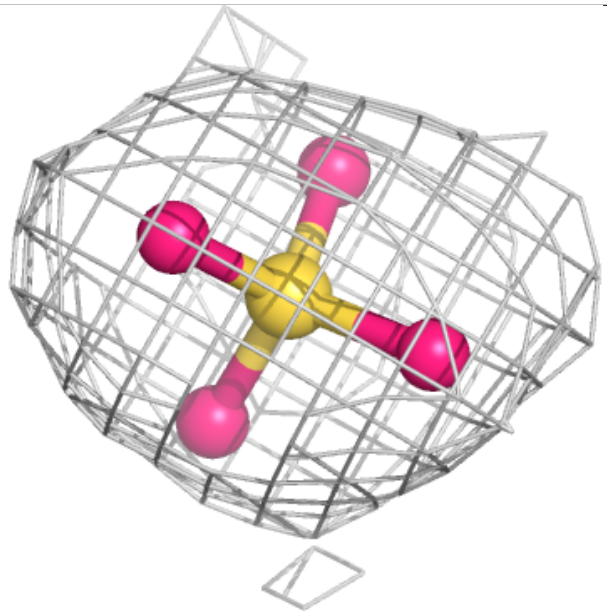


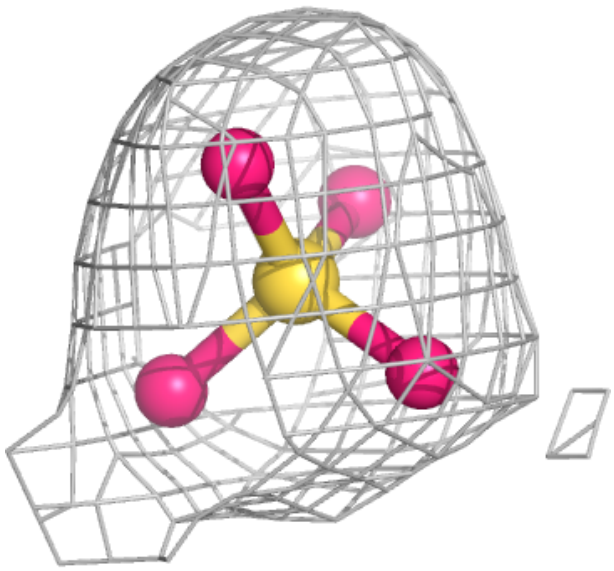


Electron density around SO4 G 401:

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

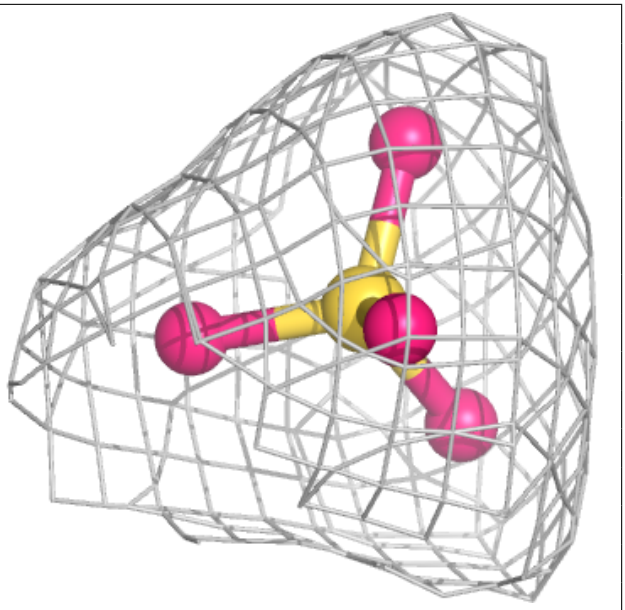


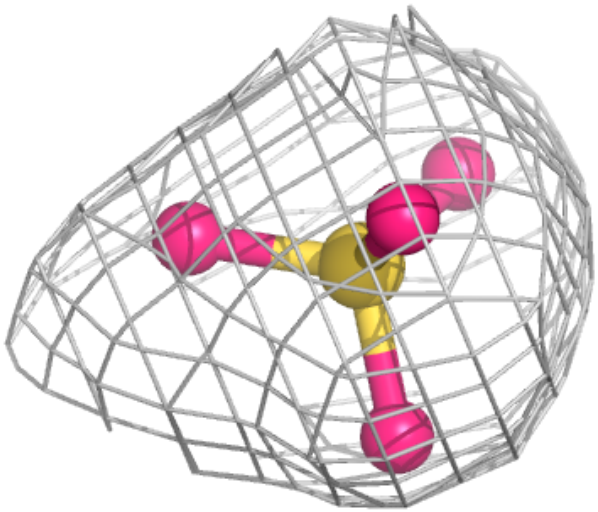


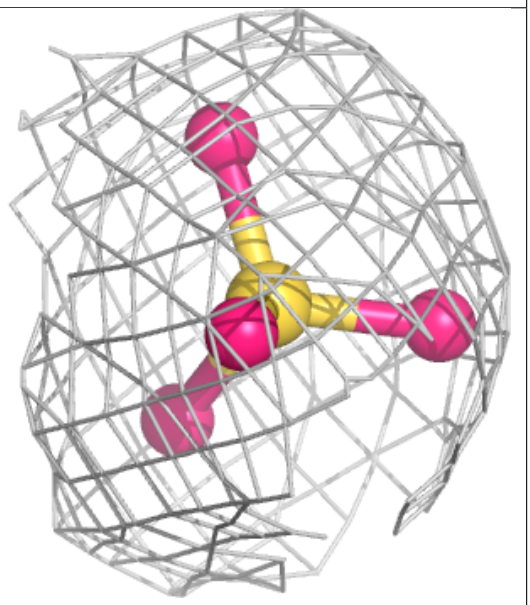


Electron density around SO4 G 402:

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

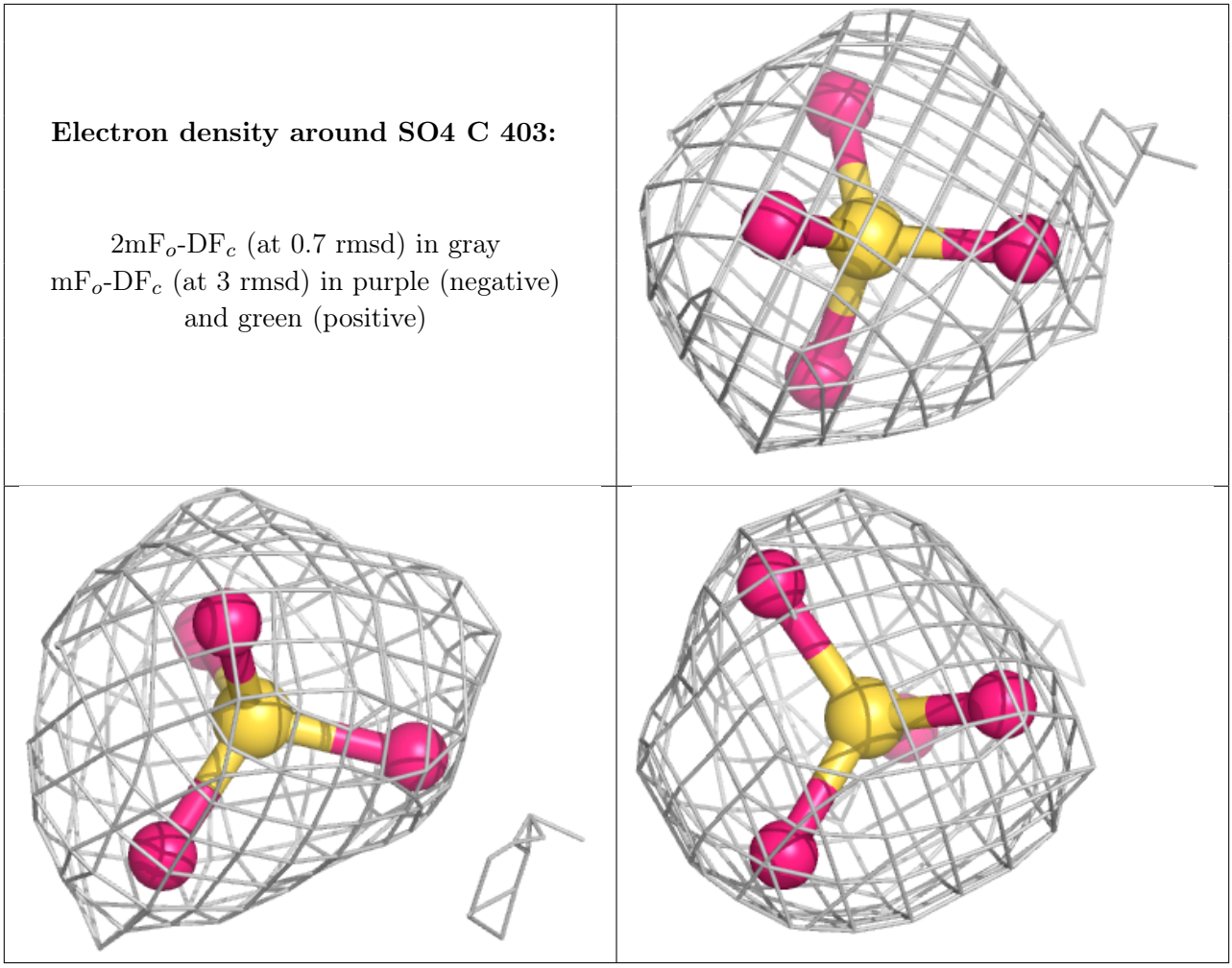






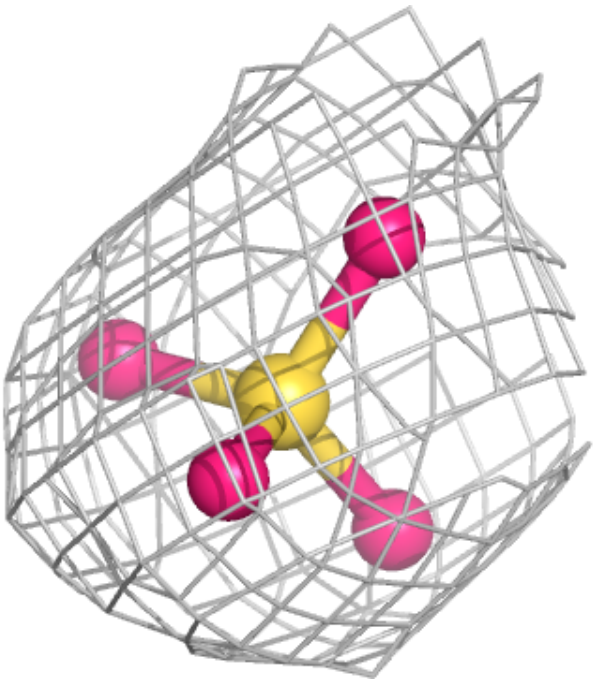
Electron density around SO4 C 403:

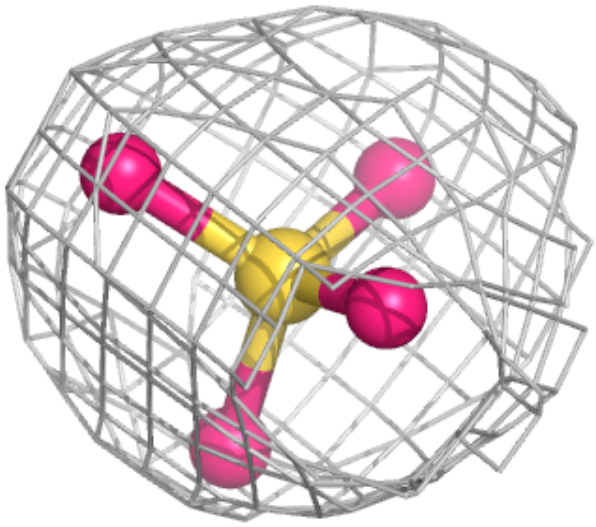
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

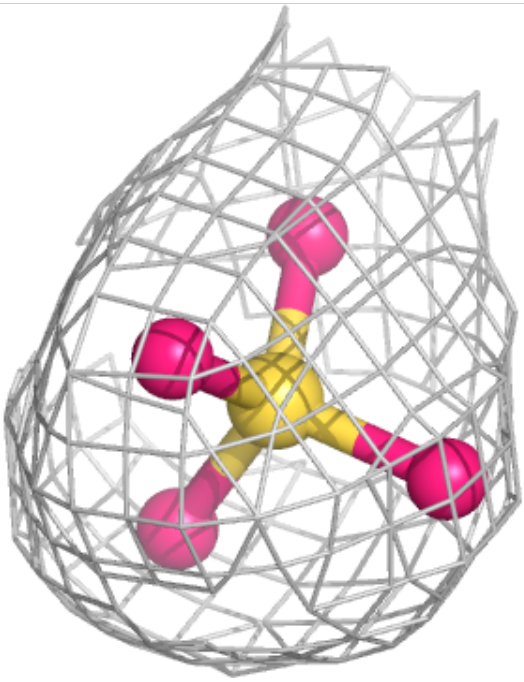


Electron density around SO4 G 403:

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

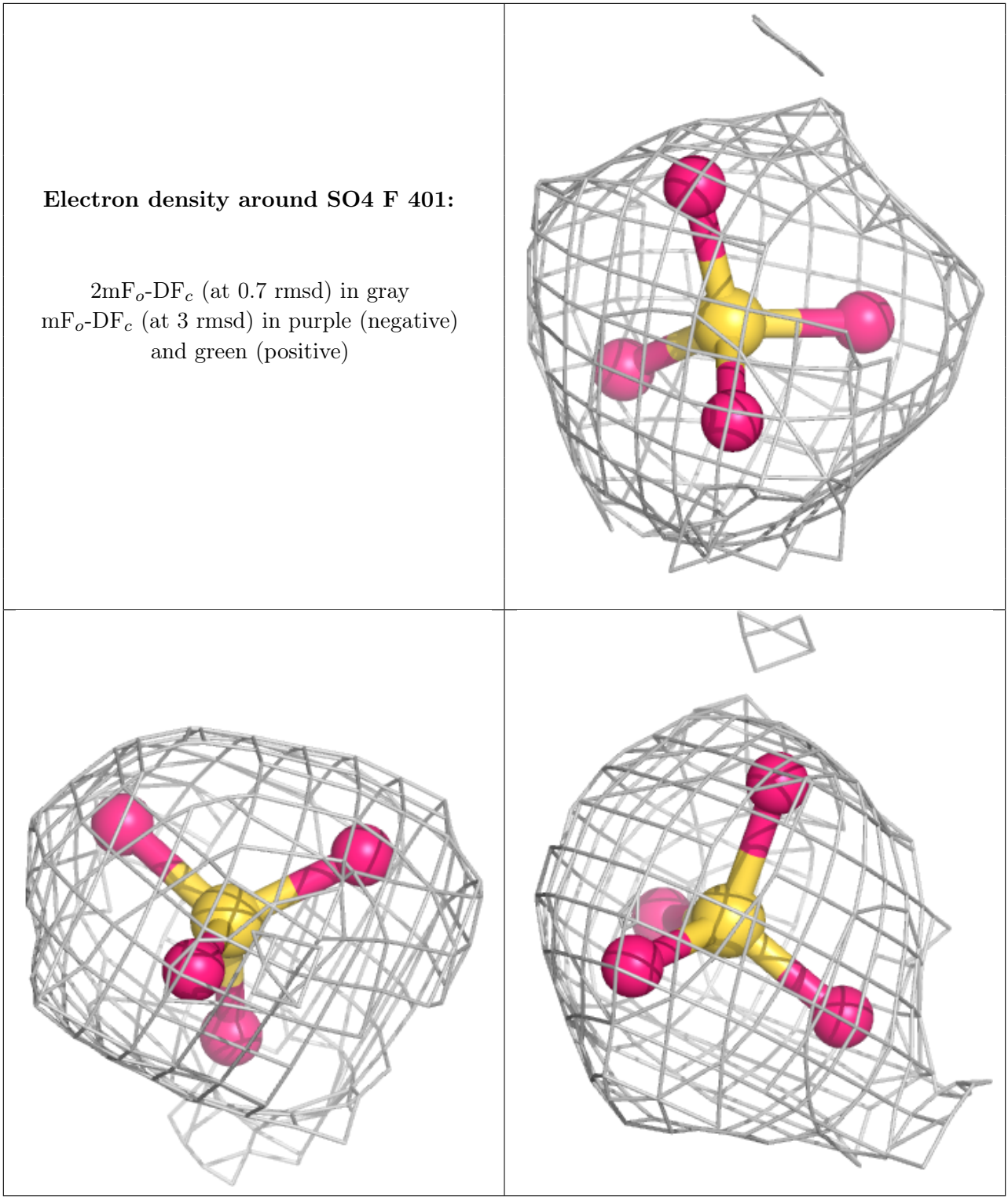






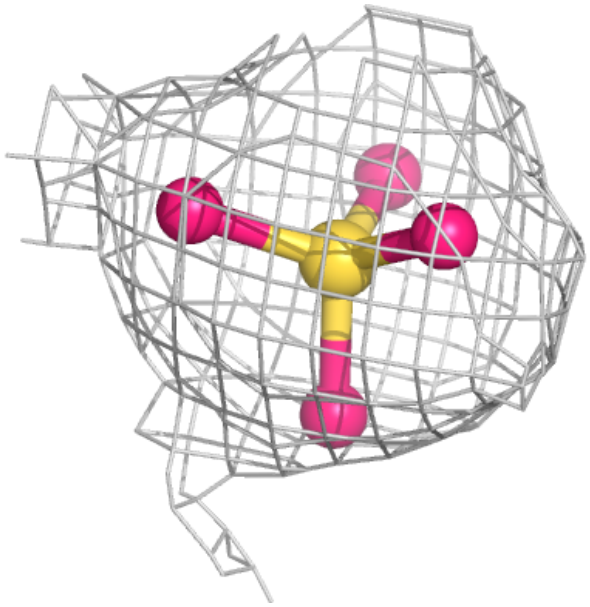
Electron density around SO4 F 401:

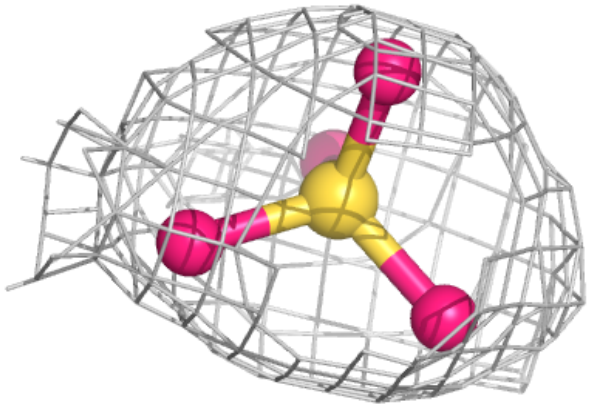
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

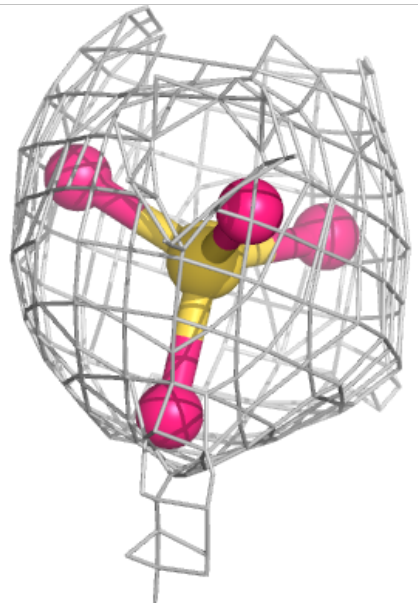


Electron density around SO4 E 402:

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

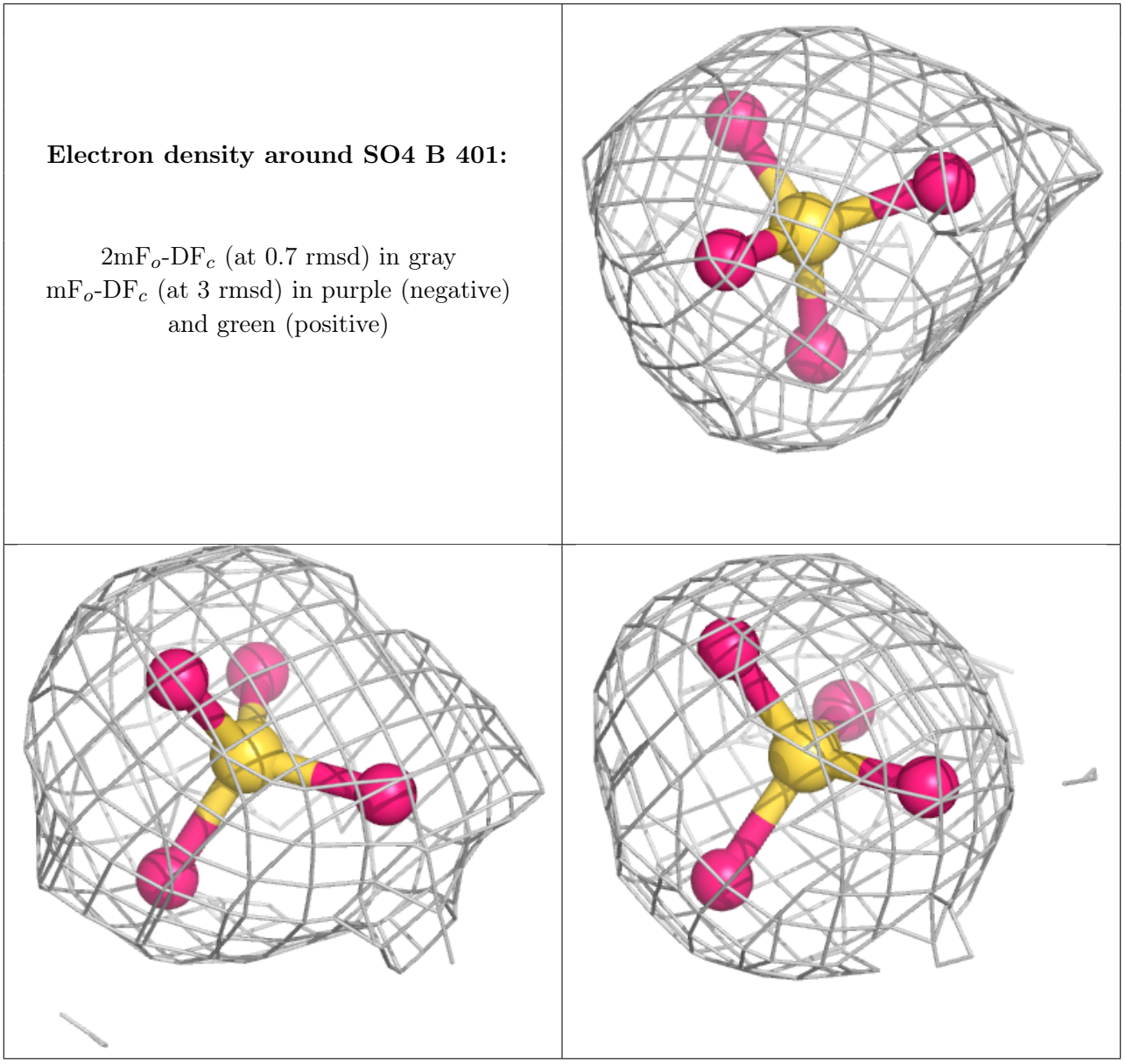






Electron density around SO4 B 401:

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



6.5 Other polymers

There are no such residues in this entry.