Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2023 – 01:27 am BST

PDB ID	:	6SCY
Title	:	U34-tRNA thiolase NcsA from Methanococcus maripaludis with its [4Fe-4S] cluster
Authors	:	Bimai, O.; Legrand, P.; Golinelli-Pimpaneau, B.
Deposited on	:	2019-07-25
Resolution	:	2.81 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

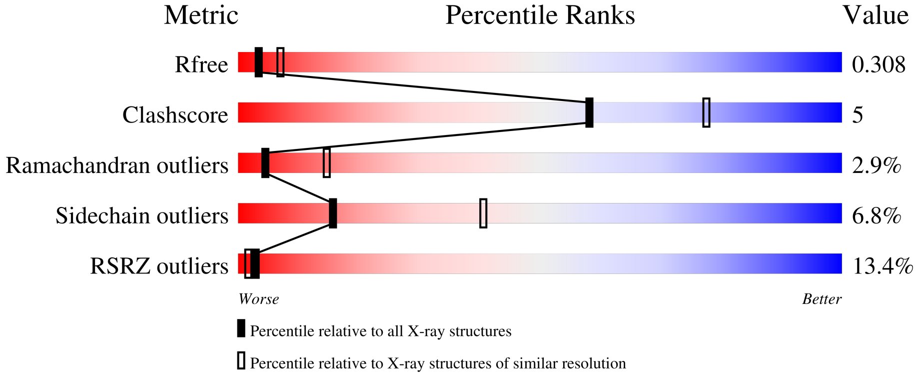
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance ⓘ

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

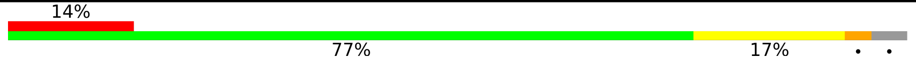
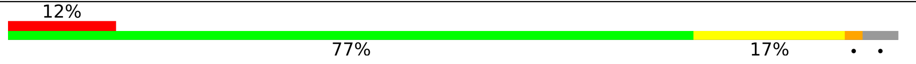
The reported resolution of this entry is 2.81 Å.

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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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	308	
2	B	311	

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
5	SO4	A	415	-	-	-	X
5	SO4	A	421	-	-	-	X
5	SO4	A	422	-	-	-	X
5	SO4	A	423	-	-	-	X
5	SO4	A	424	-	-	-	X
5	SO4	B	411	-	-	-	X
5	SO4	B	417	-	-	-	X
5	SO4	B	420	-	-	-	X
5	SO4	B	424	-	-	-	X

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 5174 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 [4Fe-4S]-dependent U34-ARNt thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total 2385	C 1521	N 406	O 435	S 23	0	2	0

- Molecule 2 is a protein called [4Fe-4S]-dependent U34-ARNt thiolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	298	Total 2365	C 1504	N 404	O 434	S 23	0	0	0

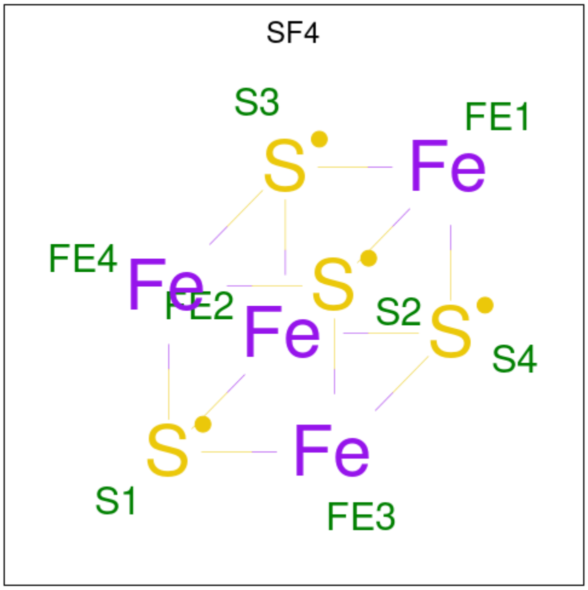
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	287	GLY	ASP	conflict	UNP Q6LXJ4
B	300	GLY	LEU	conflict	UNP Q6LXJ4

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

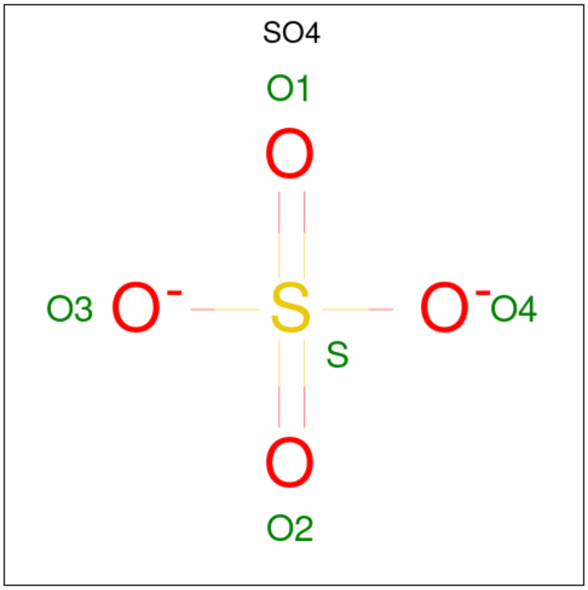
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total 2	Zn 2	0	0
3	B	2	Total 2	Zn 2	0	0

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Fe S 8 4 4	0	0
4	B	1	Total Fe S 8 4 4	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

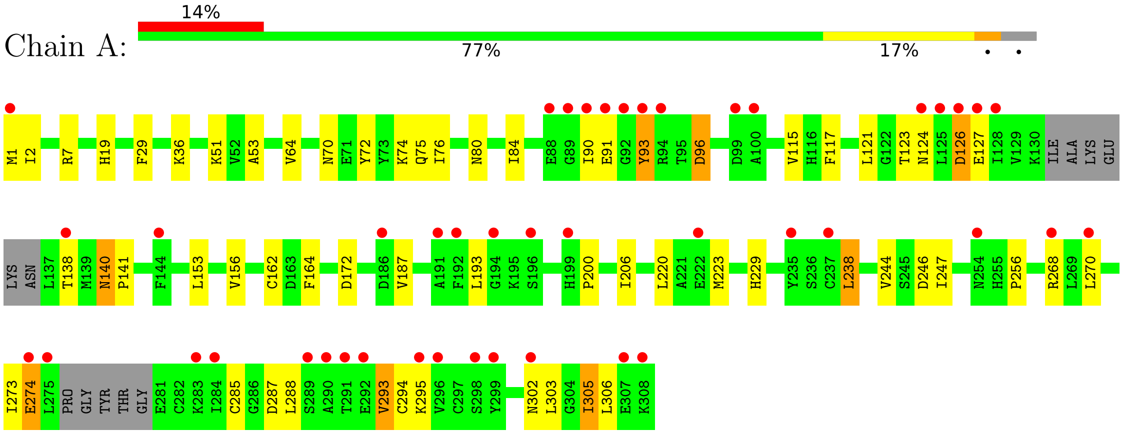
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	86	Total O 86 86	0	0
6	B	93	Total O 93 93	0	0

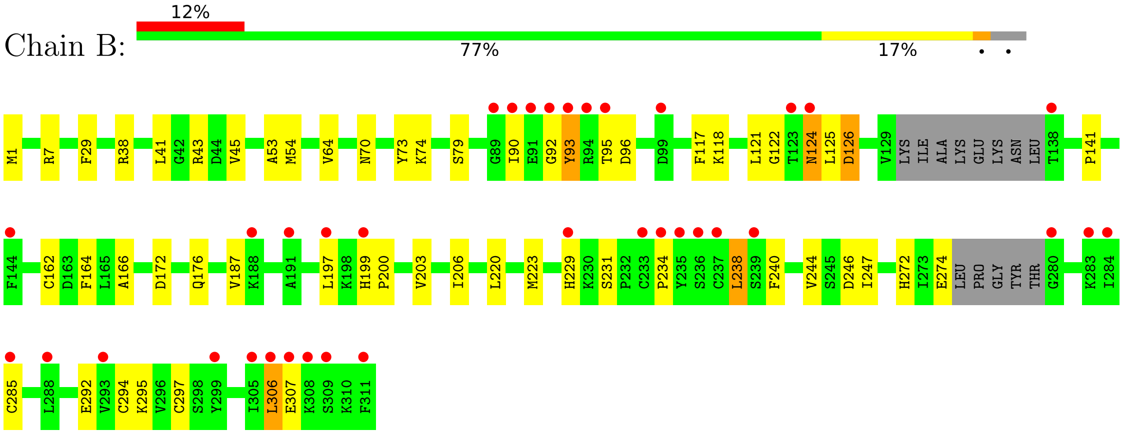
3 Residue-property plots

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: [4Fe-4S]-dependent U34-ARNt thiolase



- Molecule 2: [4Fe-4S]-dependent U34-ARNt thiolase



4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.98Å 84.48Å 145.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.85 – 2.81 31.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	76.7 (31.85-2.81) 76.5 (31.85-2.80)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.209 , 0.287 0.226 , 0.308	Depositor DCC
R_{free} test set	645 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å^2)	77.8	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 116.7	EDS
L-test for twinning[2]	$< \|L\| >= 0.49$, $< L^2 >= 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5174	wwPDB-VP
Average B, all atoms (Å^2)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.26% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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, ZN, SF4

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	0.43	0/2429	0.65	0/3253
2	B	0.42	0/2403	0.64	0/3216
All	All	0.42	0/4832	0.65	0/6469

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2385	0	2458	25	0
2	B	2365	0	2419	25	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	8	0	0	0	0
4	B	8	0	0	0	0
5	A	110	0	0	0	0
5	B	115	0	0	0	0
6	A	86	0	0	0	0
6	B	93	0	0	0	0
All	All	5174	0	4877	47	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 5.

All (47) 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:A:124:ASN:HA	1:A:127:GLU:HB2	1.58	0.85
1:A:140:ASN:HB3	1:A:141:PRO:HD3	1.66	0.77
2:B:199:HIS:HB3	2:B:200:PRO:HD2	1.68	0.74
1:A:19:HIS:HA	1:A:256:PRO:HB3	1.74	0.69
2:B:29:PHE:HD2	2:B:223:MET:HE1	1.60	0.65
1:A:29:PHE:HD2	1:A:223:MET:HE1	1.64	0.62
1:A:84:ILE:HG21	1:A:156:VAL:HG21	1.81	0.62
1:A:268:ARG:HB3	2:B:187:VAL:HG21	1.82	0.59
1:A:53:ALA:HB2	1:A:162:CYS:SG	2.50	0.52
2:B:294:CYS:HB3	2:B:297:CYS:HB2	1.92	0.52
1:A:1:MET:HG3	1:A:2:ILE:HG13	1.92	0.50
1:A:274:GLU:HB3	2:B:272:HIS:HB3	1.92	0.50
2:B:53:ALA:HB2	2:B:162:CYS:SG	2.53	0.48
2:B:70:ASN:O	2:B:74:LYS:HB2	2.13	0.48
2:B:122:GLY:H	2:B:306:LEU:HD13	1.77	0.48
1:A:84:ILE:HD13	1:A:156:VAL:HG23	1.95	0.48
1:A:193:LEU:HB3	1:A:270:LEU:HD21	1.94	0.48
2:B:93:TYR:CE1	2:B:231:SER:HA	2.49	0.48
2:B:73:TYR:CD1	2:B:79:SER:HB3	2.49	0.47
1:A:93:TYR:HD2	1:A:96:ASP:HB2	1.78	0.47
2:B:64:VAL:HG13	2:B:220:LEU:HD23	1.98	0.46
2:B:38:ARG:HG2	2:B:43:ARG:HH22	1.80	0.46
1:A:70:ASN:O	1:A:74:LYS:HB2	2.15	0.46
2:B:93:TYR:H	2:B:234:PRO:HG3	1.81	0.46
1:A:72[B]:TYR:CE2	1:A:76:ILE:HG13	2.52	0.45
2:B:90:ILE:HG22	2:B:92:GLY:H	1.80	0.45
1:A:90:ILE:HG23	1:A:126:ASP:HA	1.98	0.45
1:A:64:VAL:HG13	1:A:220:LEU:HD23	1.98	0.44
2:B:164:PHE:HB3	2:B:206:ILE:HG12	1.99	0.44
1:A:244:VAL:HA	1:A:247:ILE:HD12	2.00	0.43
2:B:199:HIS:HB3	2:B:200:PRO:CD	2.44	0.43
2:B:41:LEU:HD22	2:B:45:VAL:HG11	2.01	0.43
2:B:244:VAL:HA	2:B:247:ILE:HD12	2.00	0.43
1:A:51:LYS:HG3	1:A:80:ASN:HB3	1.99	0.43
2:B:90:ILE:HG12	2:B:125:LEU:HD23	2.00	0.43
1:A:164:PHE:HB3	1:A:206:ILE:HG12	1.99	0.43
1:A:53:ALA:HB1	1:A:84:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ARG:HE	2:B:187:VAL:HB	1.84	0.42
2:B:93:TYR:CE1	2:B:96:ASP:HB3	2.55	0.42
2:B:238:LEU:HD21	2:B:240:PHE:HB3	2.02	0.41
2:B:54:MET:HB3	2:B:166:ALA:HB3	2.01	0.41
1:A:115:VAL:HG21	1:A:156:VAL:HG11	2.02	0.41
2:B:29:PHE:HD2	2:B:223:MET:CE	2.30	0.41
1:A:138:THR:HB	1:A:238:LEU:HD11	2.02	0.41
1:A:153:LEU:HA	1:A:156:VAL:HG22	2.02	0.40
2:B:118:LYS:HB3	2:B:124:ASN:HB3	2.02	0.40
1:A:96:ASP:HB3	1:A:229:HIS:NE2	2.36	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	293/308 (95%)	252 (86%)	31 (11%)	10 (3%)	3	12
2	B	292/311 (94%)	256 (88%)	29 (10%)	7 (2%)	6	19
All	All	585/619 (94%)	508 (87%)	60 (10%)	17 (3%)	4	15

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	140	ASN
2	B	126	ASP
1	A	91	GLU
1	A	287	ASP
2	B	285	CYS
1	A	121	LEU
1	A	200	PRO
1	A	293	VAL

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Mol	Chain	Res	Type
1	A	305	ILE
2	B	197	LEU
2	B	292	GLU
2	B	307	GLU
1	A	285	CYS
1	A	295	LYS
1	A	302	ASN
2	B	141	PRO
2	B	203	VAL

5.3.2 Protein sidechains ⓘ

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	269/275 (98%)	249 (93%)	20 (7%)	13	36
2	B	265/276 (96%)	249 (94%)	16 (6%)	19	47
All	All	534/551 (97%)	498 (93%)	36 (7%)	16	41

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	36	LYS
1	A	75	GLN
1	A	93	TYR
1	A	96	ASP
1	A	117	PHE
1	A	123	THR
1	A	126	ASP
1	A	172	ASP
1	A	187	VAL
1	A	238	LEU
1	A	246	ASP
1	A	273	ILE
1	A	274	GLU

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Mol	Chain	Res	Type
1	A	288	LEU
1	A	293	VAL
1	A	294	CYS
1	A	303	LEU
1	A	305	ILE
1	A	306	LEU
2	B	1	MET
2	B	7	ARG
2	B	93	TYR
2	B	95	THR
2	B	117	PHE
2	B	121	LEU
2	B	124	ASN
2	B	126	ASP
2	B	172	ASP
2	B	176	GLN
2	B	229	HIS
2	B	238	LEU
2	B	246	ASP
2	B	274	GLU
2	B	295	LYS
2	B	306	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 51 ligands modelled in this entry, 4 are monoatomic - leaving 47 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	SO4	A	416	-	4,4,4	0.16	0	6,6,6	0.05	0
5	SO4	B	415	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	406	-	4,4,4	0.16	0	6,6,6	0.10	0
5	SO4	B	421	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	408	-	4,4,4	0.20	0	6,6,6	0.11	0
5	SO4	A	424	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	B	404	-	4,4,4	0.12	0	6,6,6	0.08	0
5	SO4	A	411	-	4,4,4	0.12	0	6,6,6	0.09	0
5	SO4	A	415	-	4,4,4	0.15	0	6,6,6	0.08	0
5	SO4	A	414	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	420	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	A	418	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	A	419	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	A	422	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	410	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	421	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	405	4	4,4,4	0.16	0	6,6,6	0.07	0
5	SO4	B	409	-	4,4,4	0.13	0	6,6,6	0.10	0
5	SO4	B	417	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	B	425	-	4,4,4	0.14	0	6,6,6	0.07	0
5	SO4	B	416	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	412	-	4,4,4	0.11	0	6,6,6	0.14	0
5	SO4	B	424	-	4,4,4	0.14	0	6,6,6	0.05	0
5	SO4	A	413	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	B	423	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	A	407	-	4,4,4	0.12	0	6,6,6	0.07	0
5	SO4	B	411	-	4,4,4	0.15	0	6,6,6	0.07	0
5	SO4	A	408	-	4,4,4	0.14	0	6,6,6	0.09	0
5	SO4	B	420	-	4,4,4	0.13	0	6,6,6	0.06	0
5	SO4	B	426	-	4,4,4	0.15	0	6,6,6	0.06	0
5	SO4	A	410	-	4,4,4	0.14	0	6,6,6	0.12	0
5	SO4	B	406	-	4,4,4	0.14	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$\|Z\|>2$	Counts	RMSZ	#$\|Z\|>2$
5	SO4	B	407	4	4,4,4	0.16	0	6,6,6	0.06	0
5	SO4	B	413	-	4,4,4	0.14	0	6,6,6	0.15	0
5	SO4	B	412	-	4,4,4	0.14	0	6,6,6	0.04	0
5	SO4	A	404	-	4,4,4	0.14	0	6,6,6	0.12	0
4	SF4	B	403	5,2	0,12,12	-	-	-		
5	SO4	A	417	-	4,4,4	0.14	0	6,6,6	0.06	0
5	SO4	B	414	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	A	425	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	B	422	-	4,4,4	0.13	0	6,6,6	0.07	0
5	SO4	A	423	-	4,4,4	0.15	0	6,6,6	0.05	0
5	SO4	B	405	-	4,4,4	0.15	0	6,6,6	0.16	0
5	SO4	B	419	-	4,4,4	0.12	0	6,6,6	0.08	0
5	SO4	A	409	-	4,4,4	0.13	0	6,6,6	0.05	0
4	SF4	A	403	1,5	0,12,12	-	-	-		
5	SO4	B	418	-	4,4,4	0.13	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	B	403	5,2	-	-	0/6/5/5
4	SF4	A	403	1,5	-	-	0/6/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

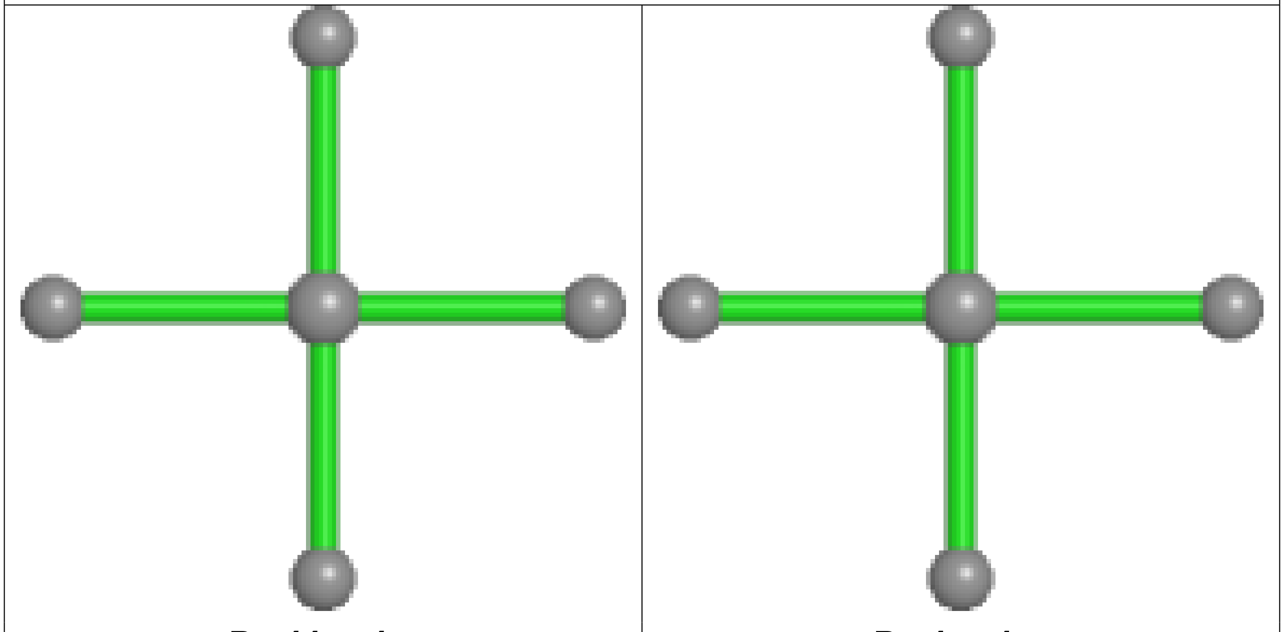
There are no torsion outliers.

There are no ring outliers.

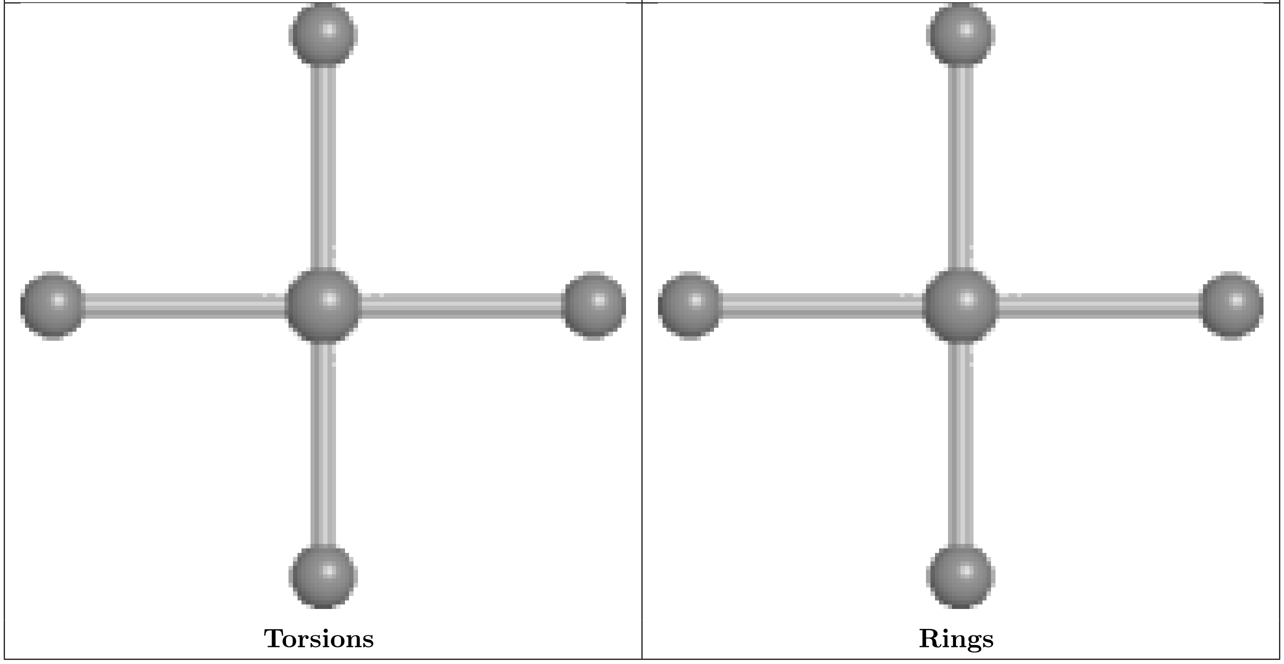
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand SO4 A 416

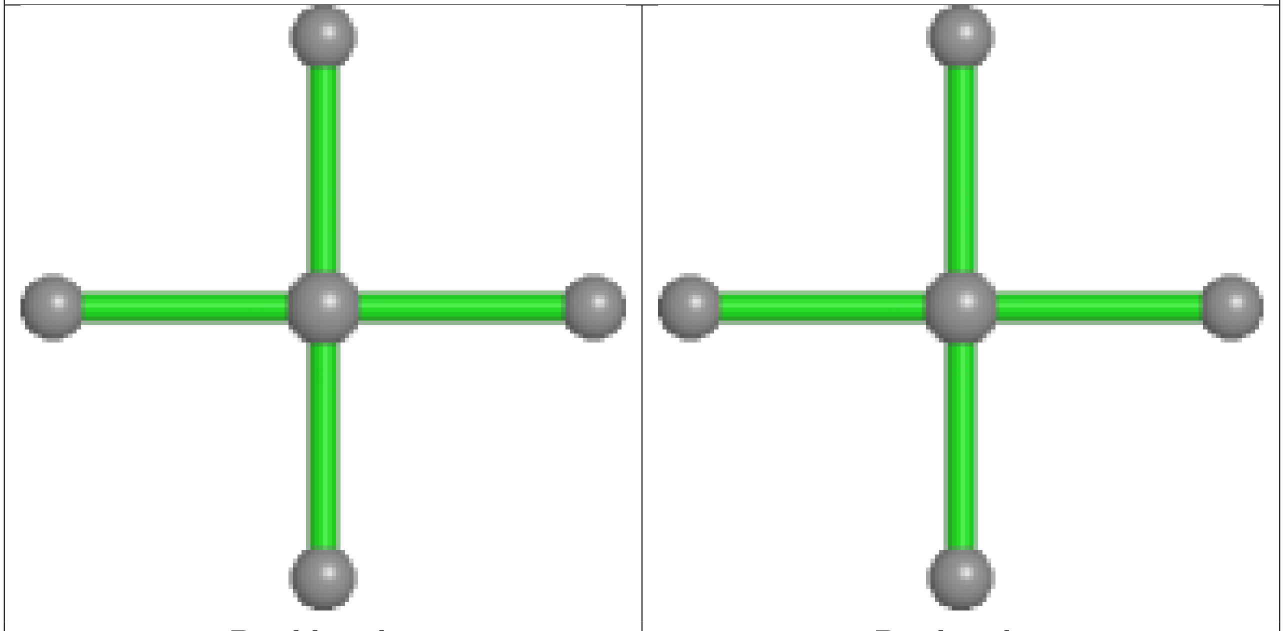


Bond lengths **Bond angles**



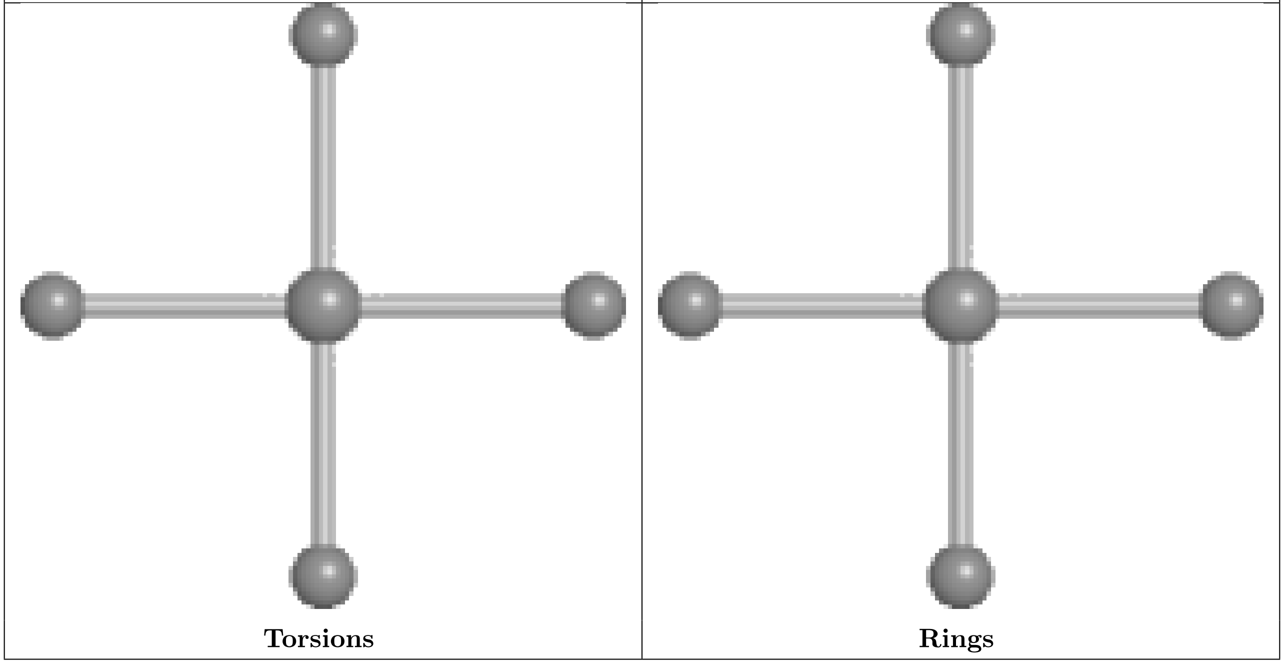
Torsions **Rings**

Ligand SO4 B 415



Bond lengths

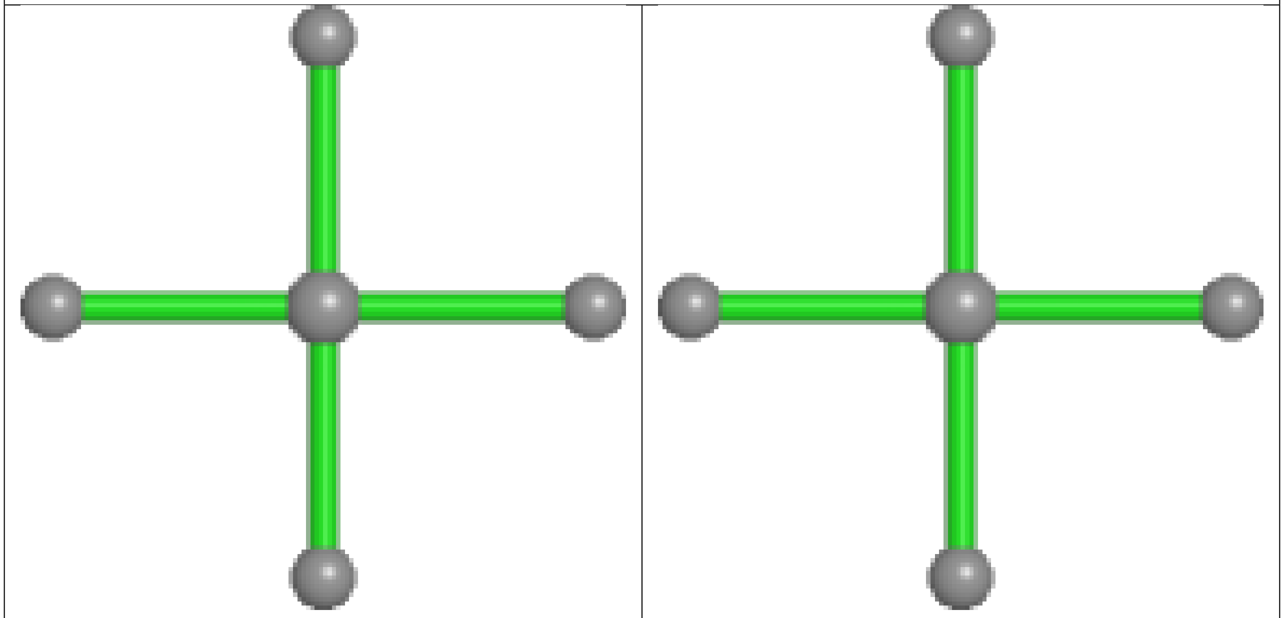
Bond angles



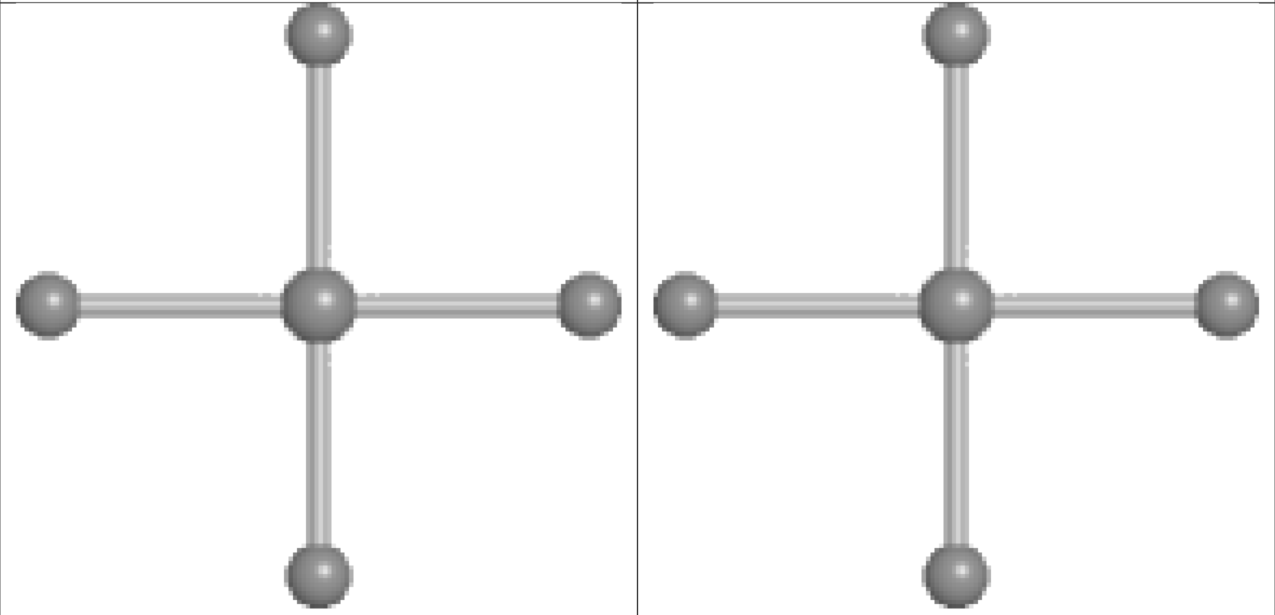
Torsions

Rings

Ligand SO4 A 406

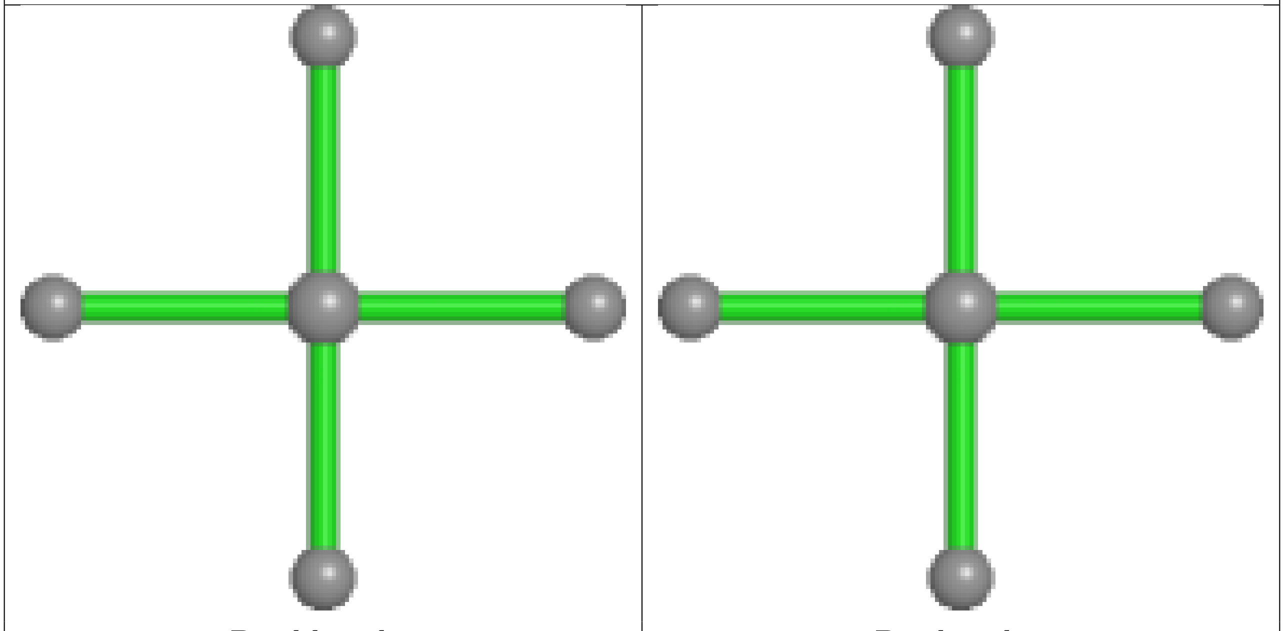


Bond lengths **Bond angles**

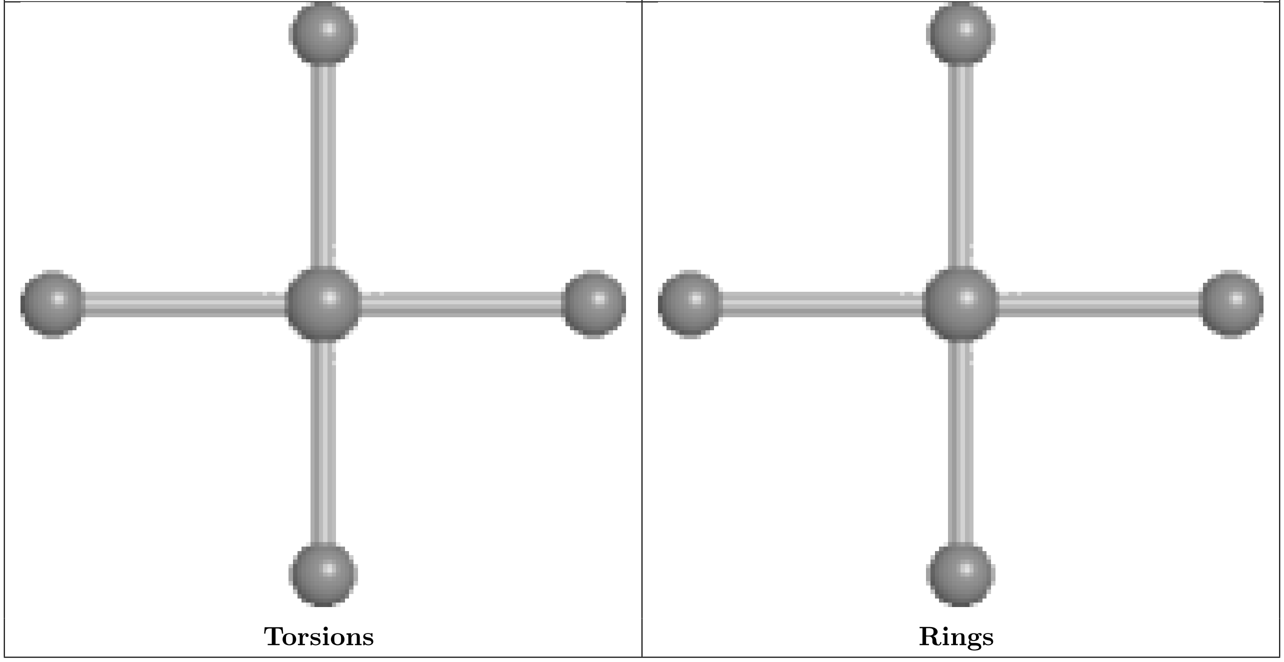


Torsions **Rings**

Ligand SO4 B 421

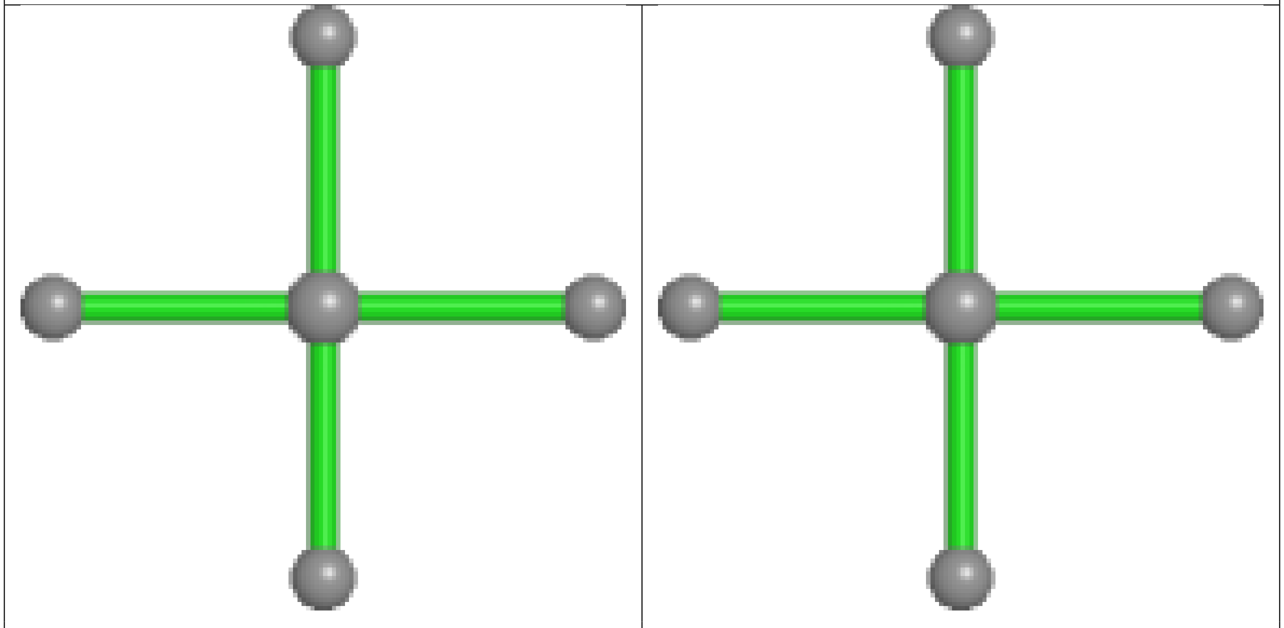


Bond lengths Bond angles

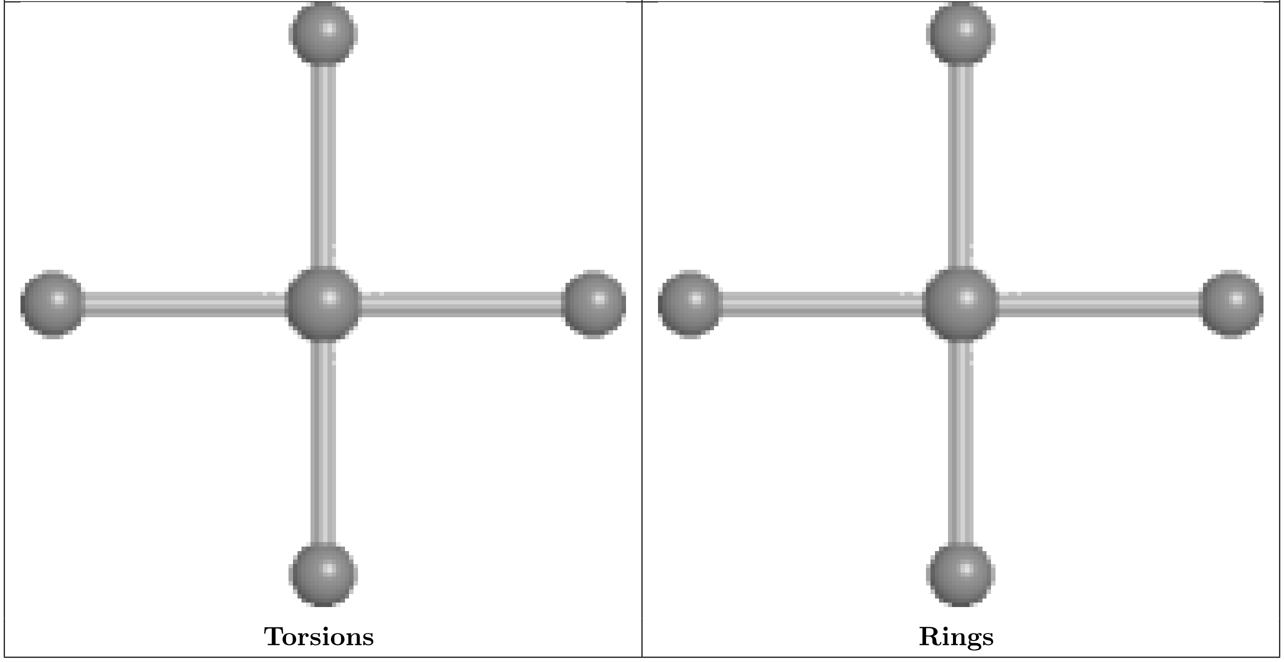


Torsions Rings

Ligand SO4 B 408

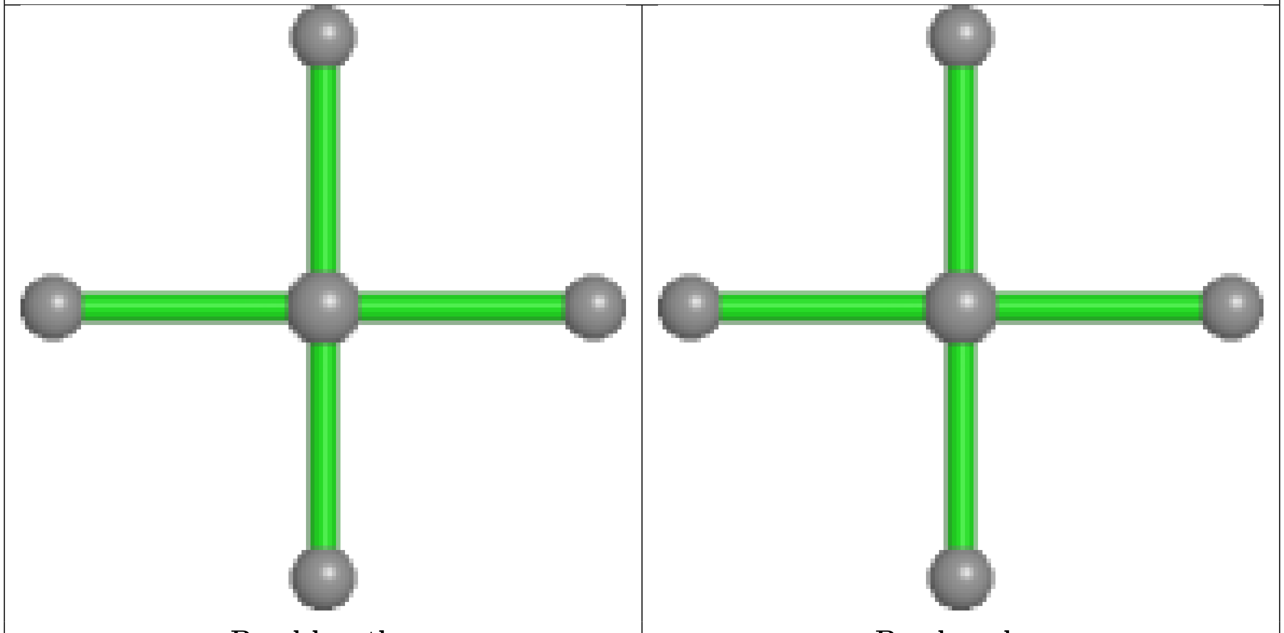


Bond lengths **Bond angles**

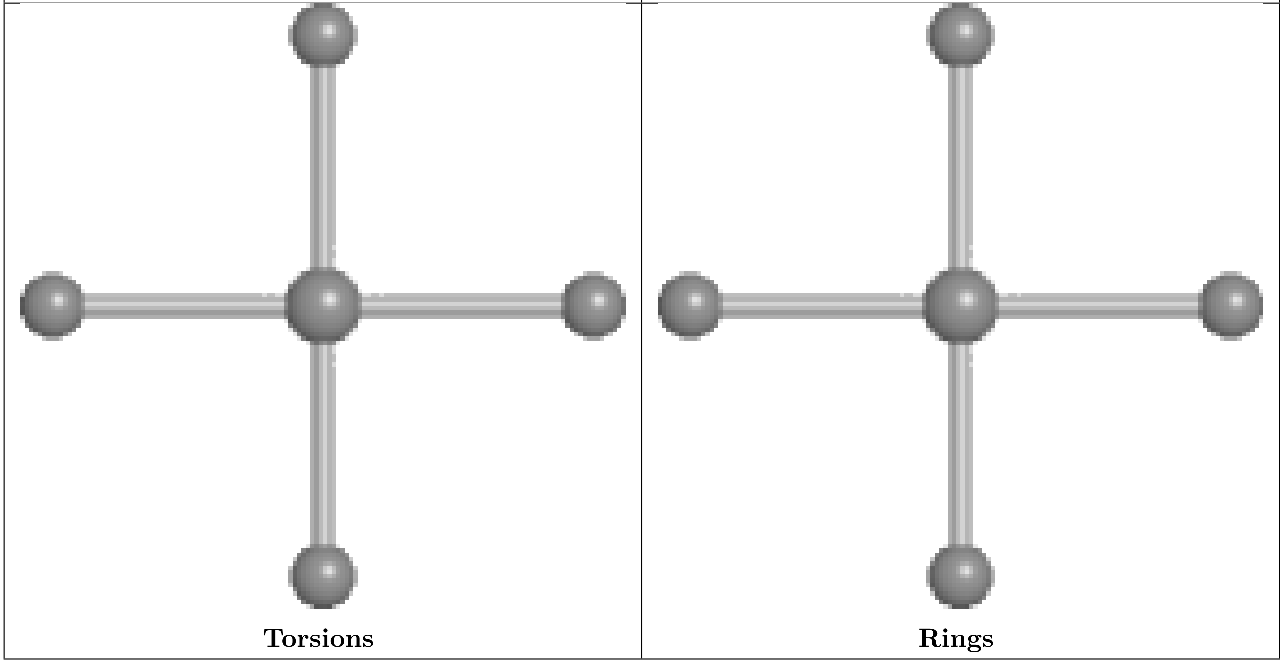


Torsions **Rings**

Ligand SO4 A 424

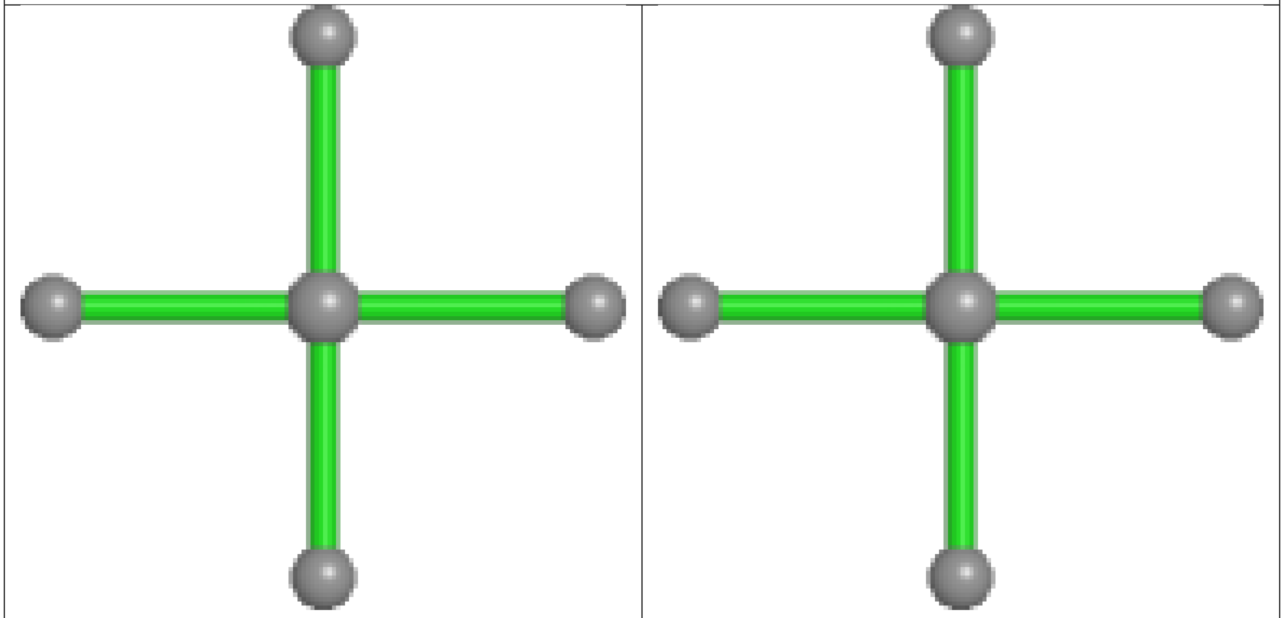


Bond lengths **Bond angles**



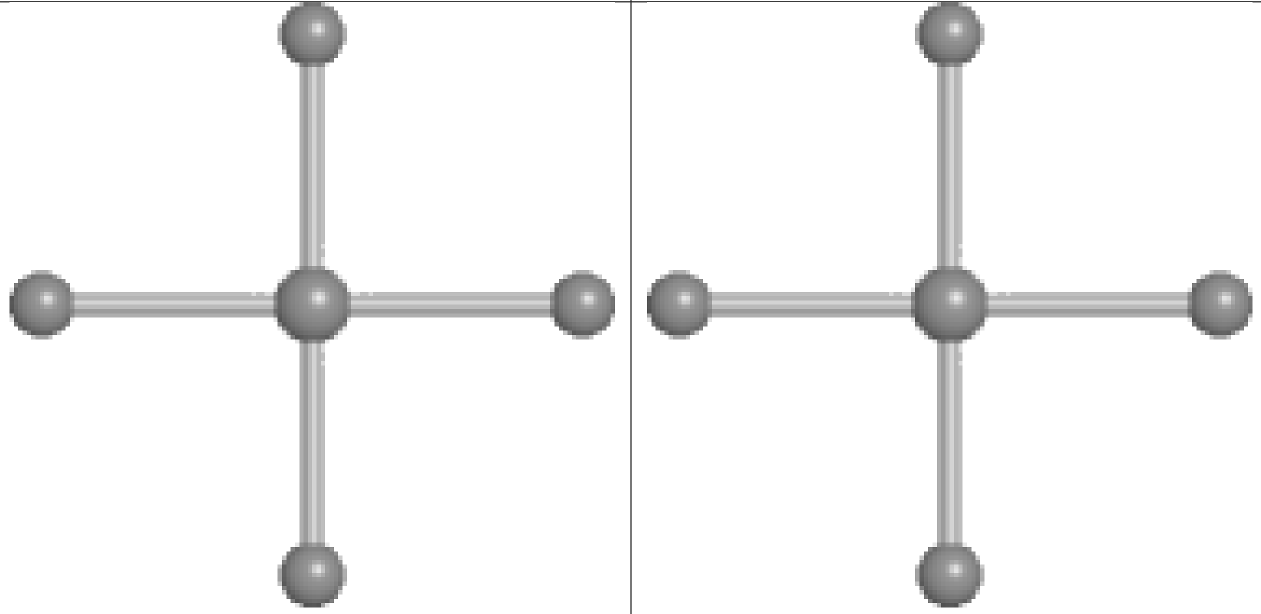
Torsions **Rings**

Ligand SO4 B 404



Bond lengths

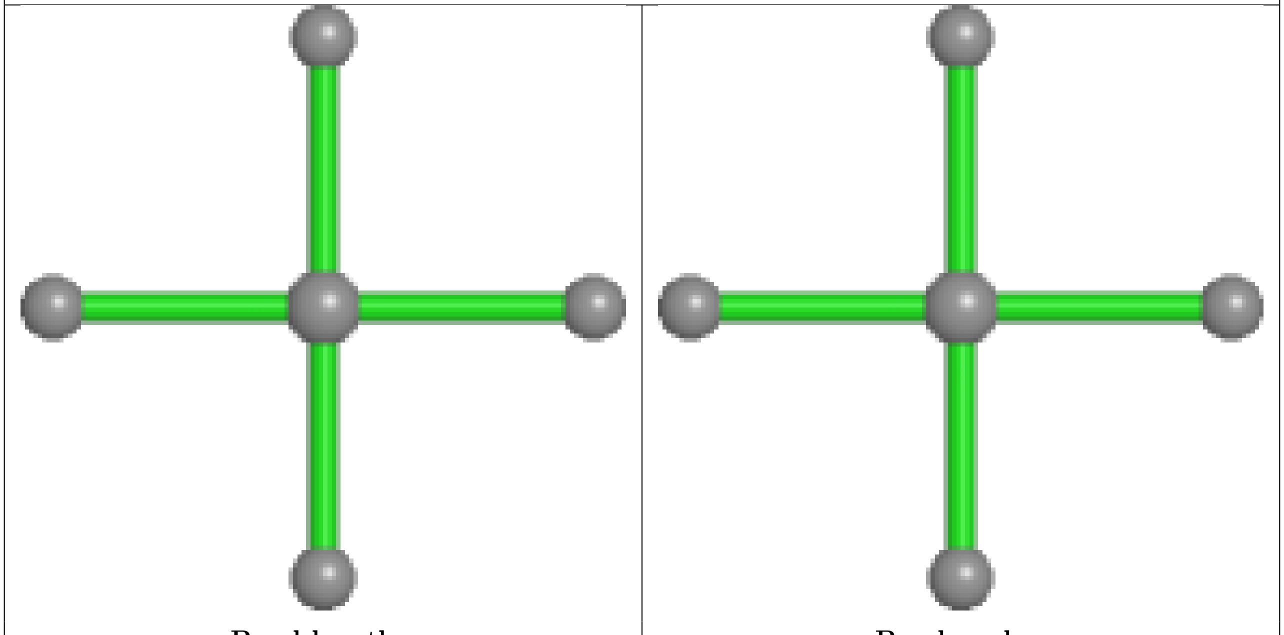
Bond angles



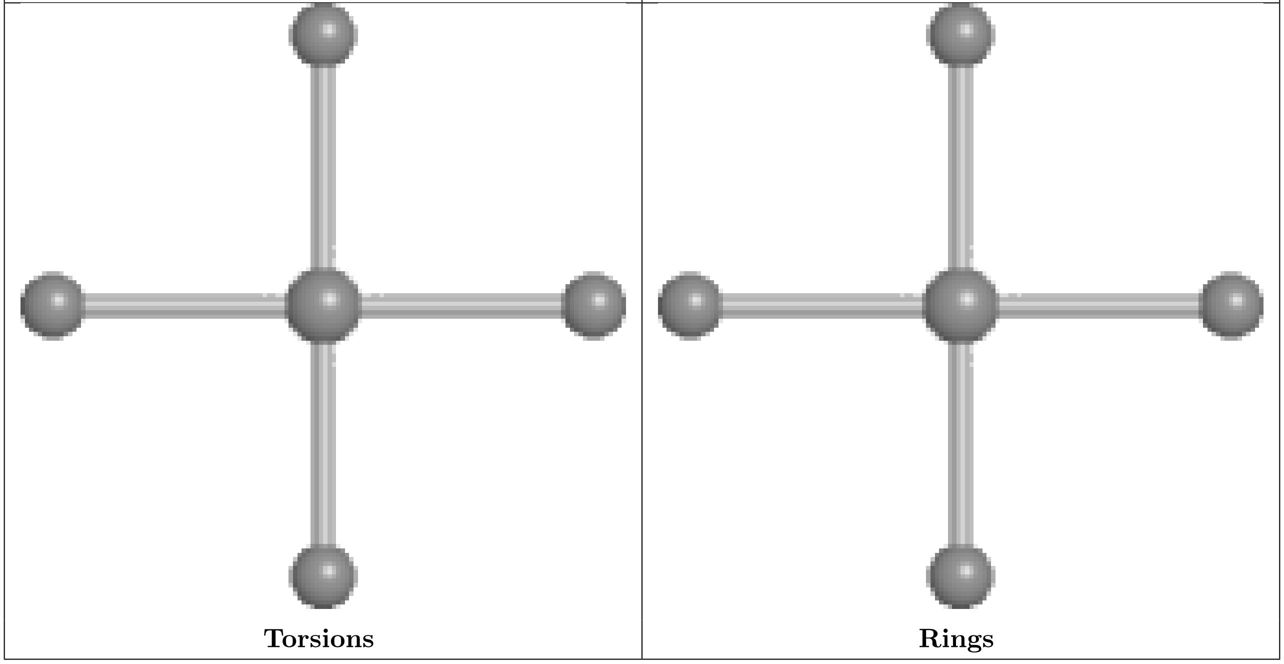
Torsions

Rings

Ligand SO4 A 411

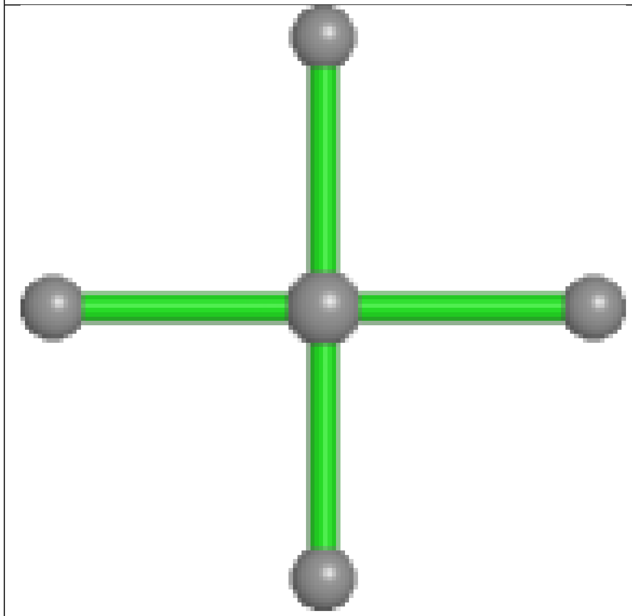


Bond lengths **Bond angles**

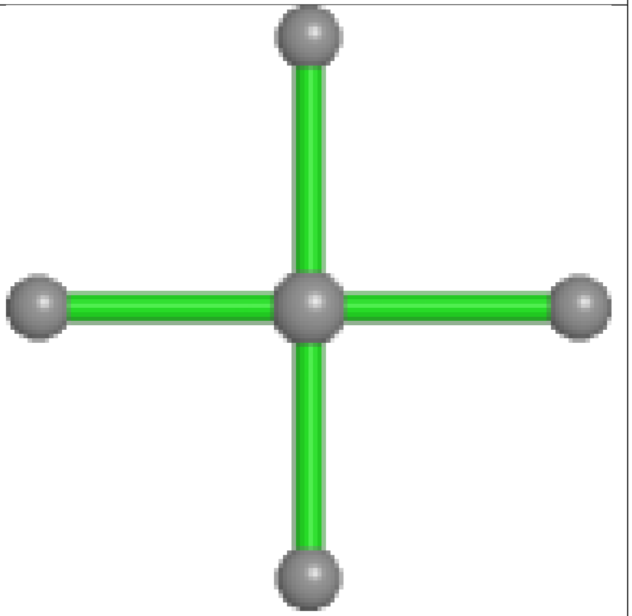


Torsions **Rings**

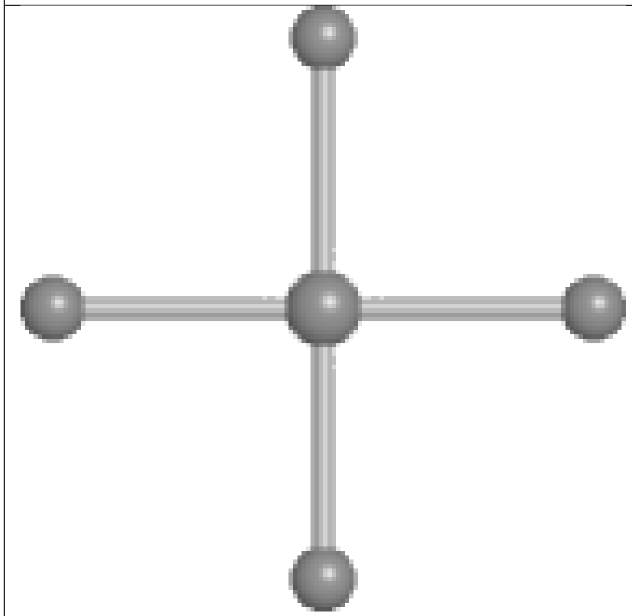
Ligand SO4 A 415



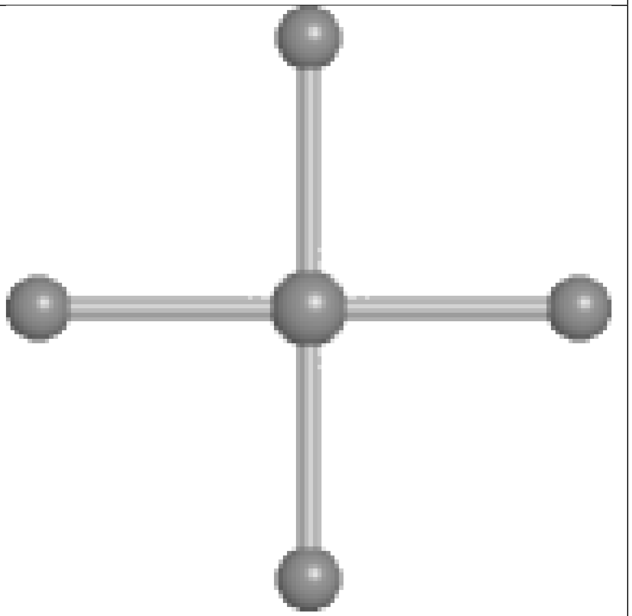
Bond lengths



Bond angles

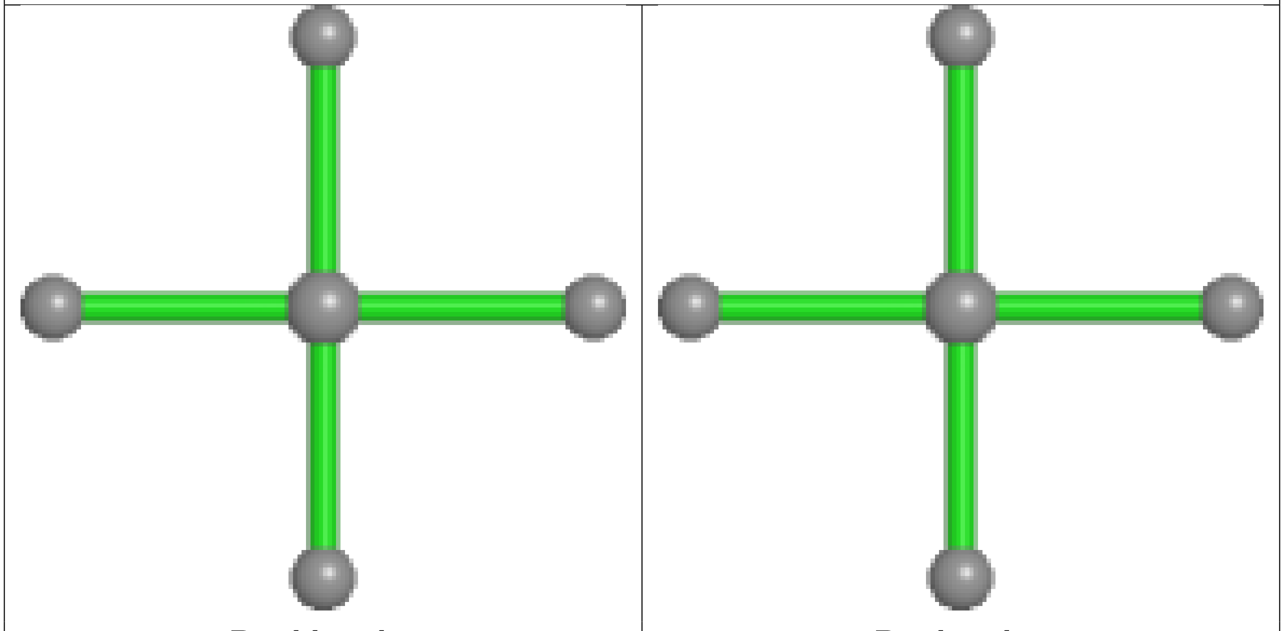


Torsions

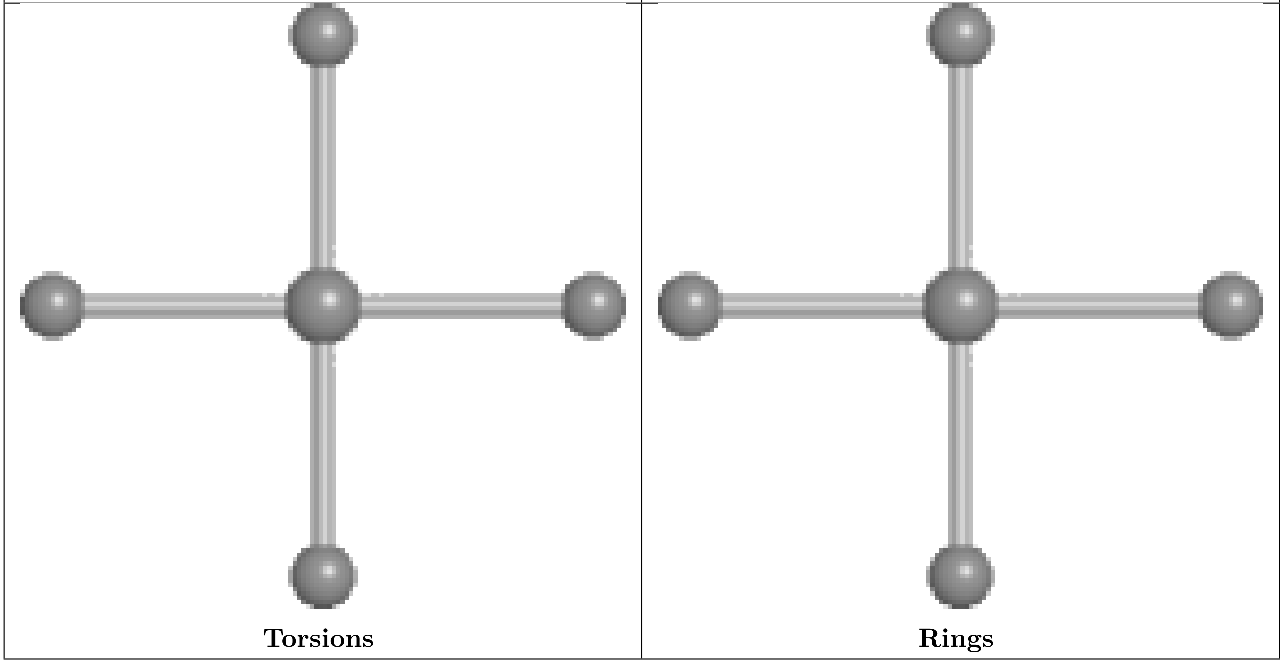


Rings

Ligand SO4 A 414

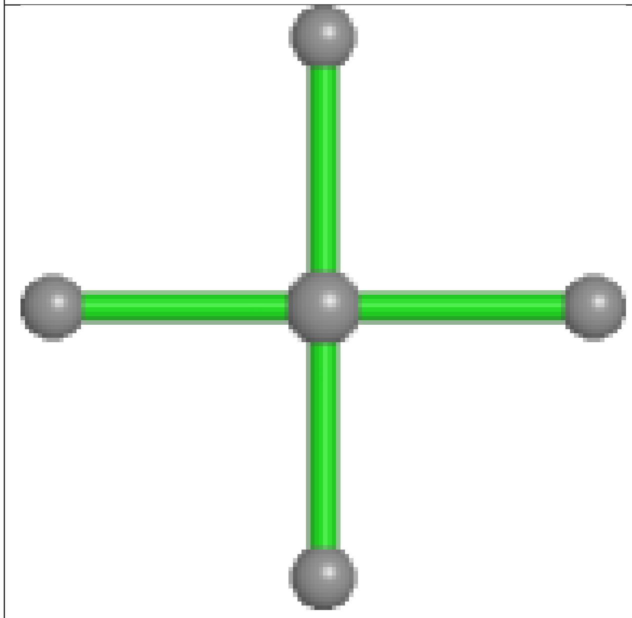


Bond lengths **Bond angles**

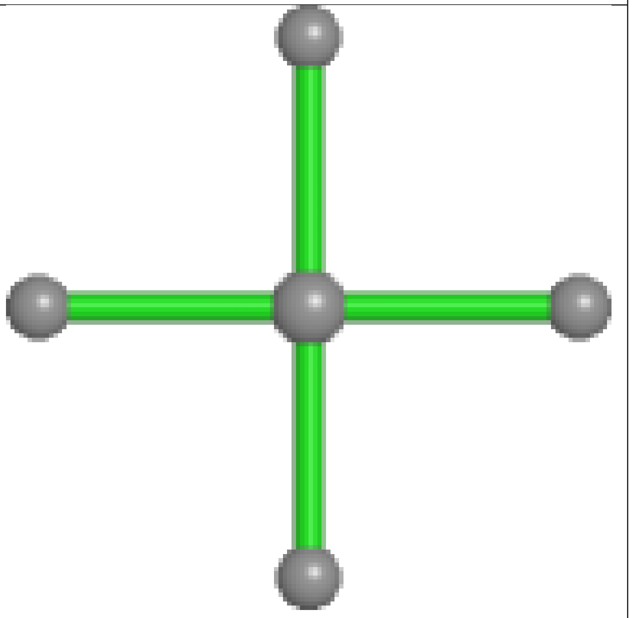


Torsions **Rings**

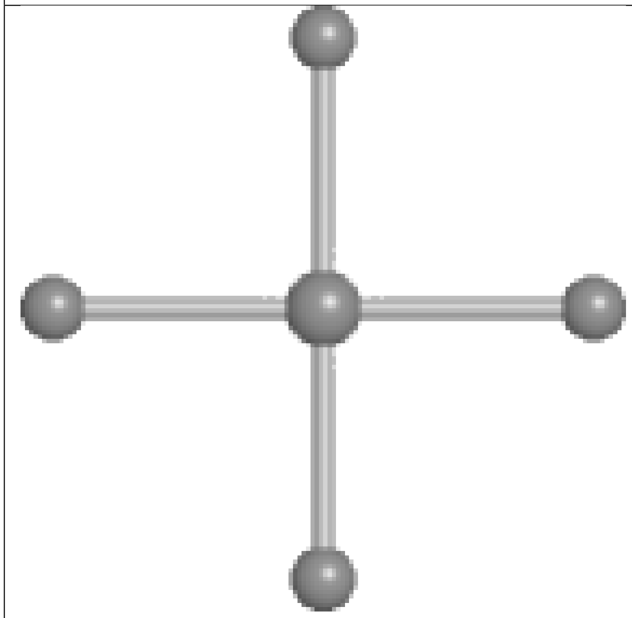
Ligand SO4 A 420



Bond lengths



Bond angles



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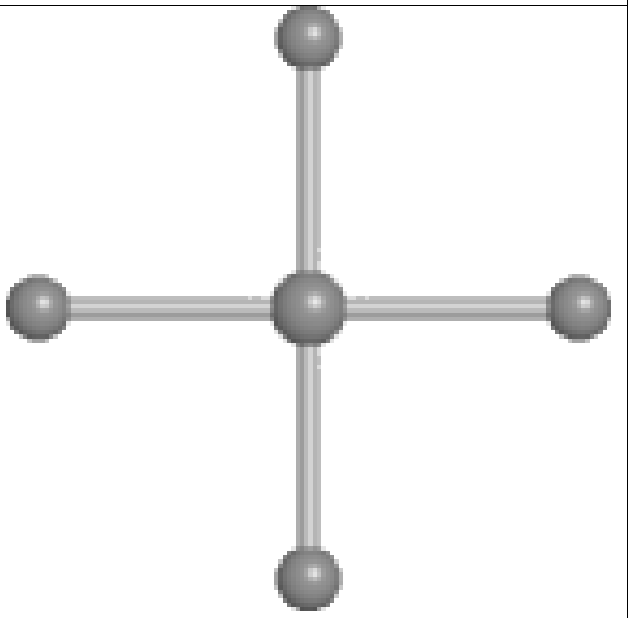
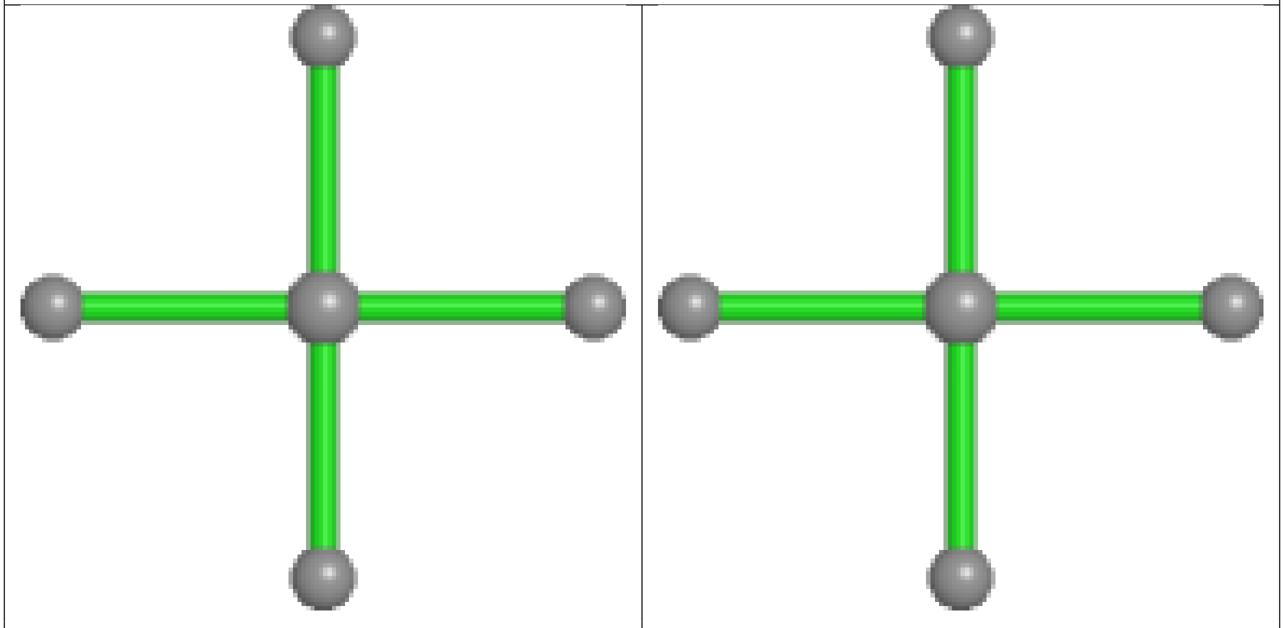


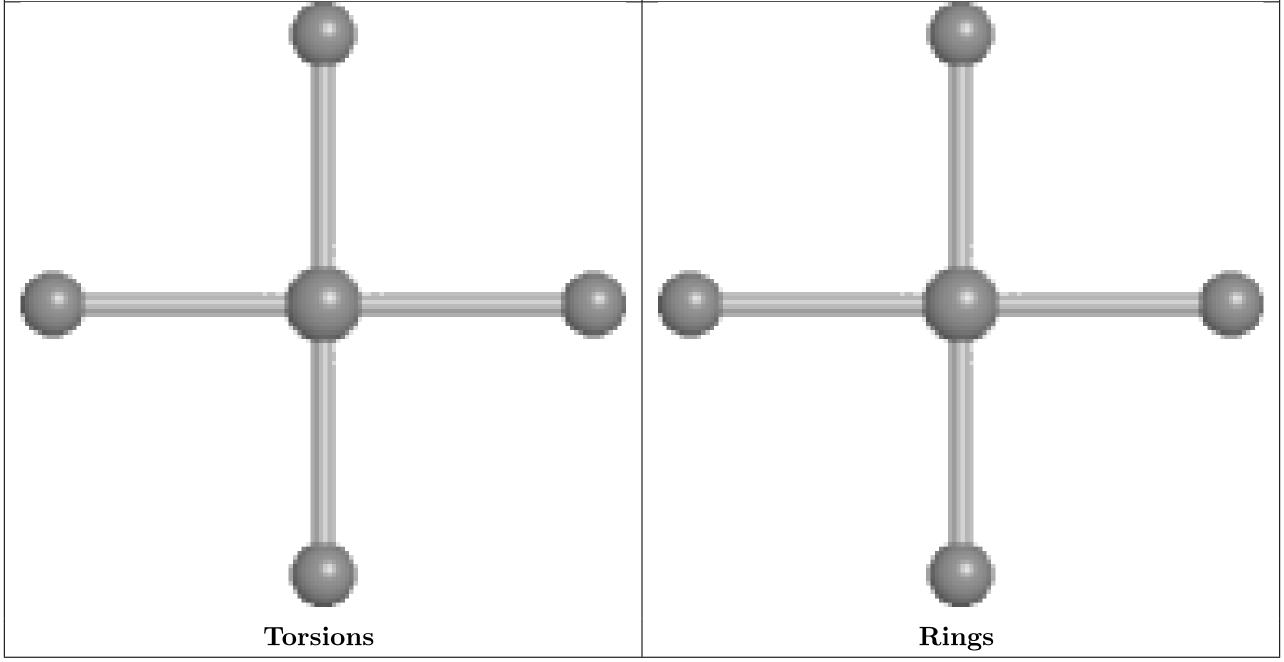
Rings

Ligand SO4 A 418



Bond lengths

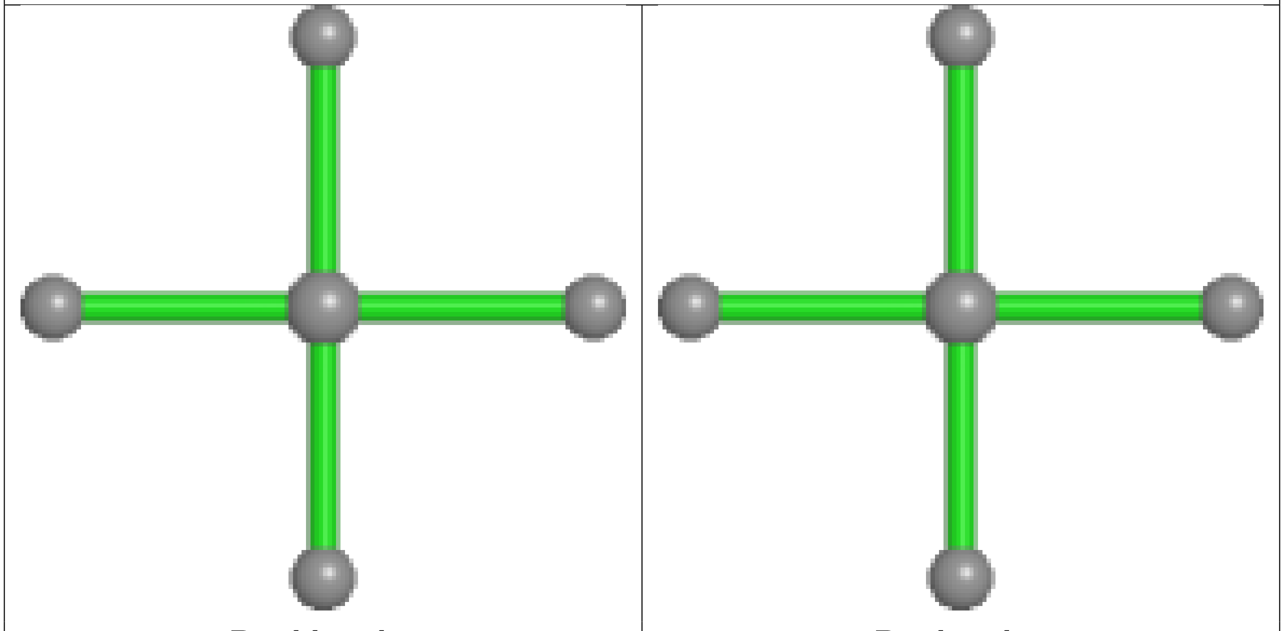
Bond angles



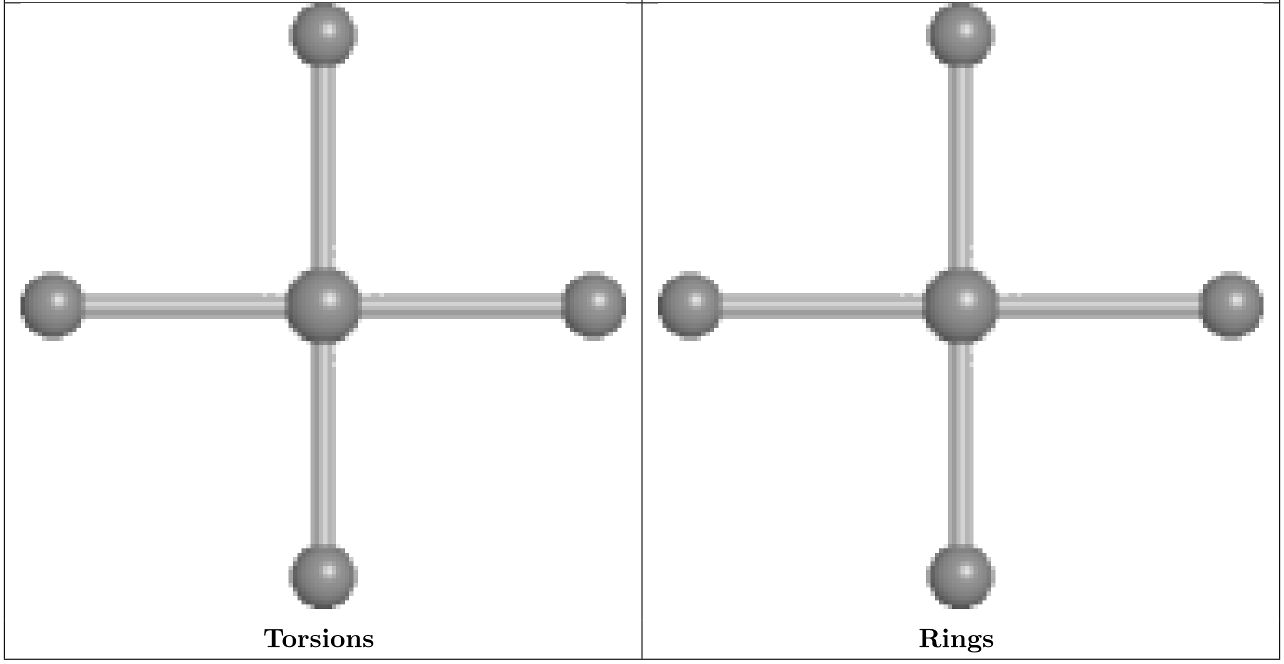
Torsions

Rings

Ligand SO4 A 419

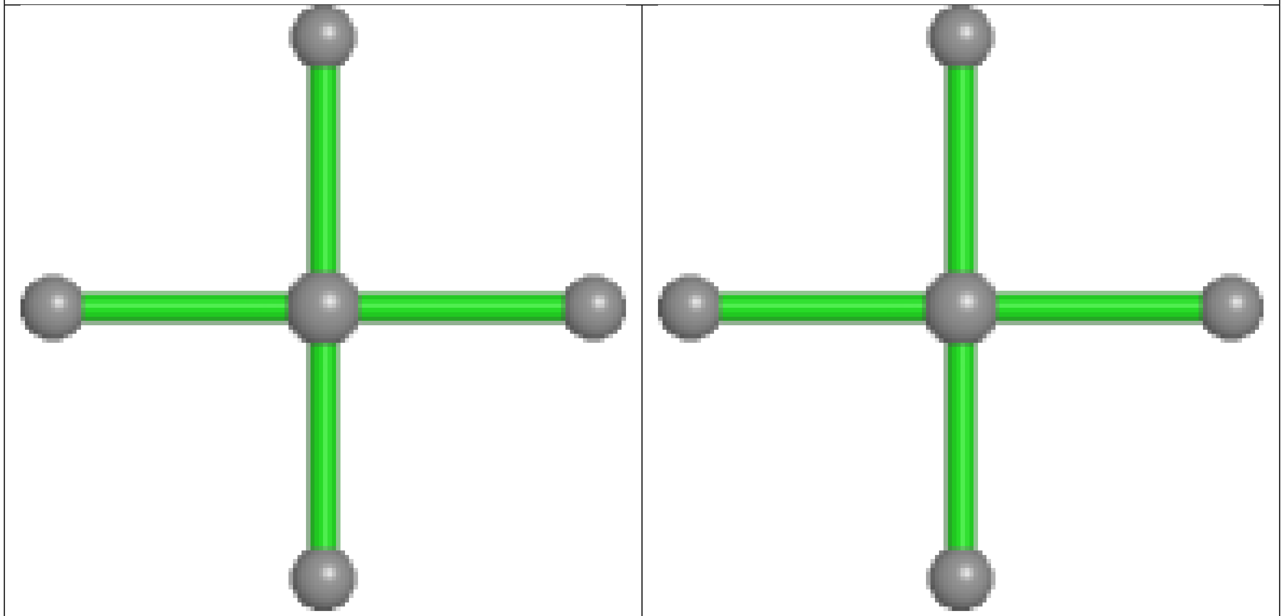


Bond lengths **Bond angles**



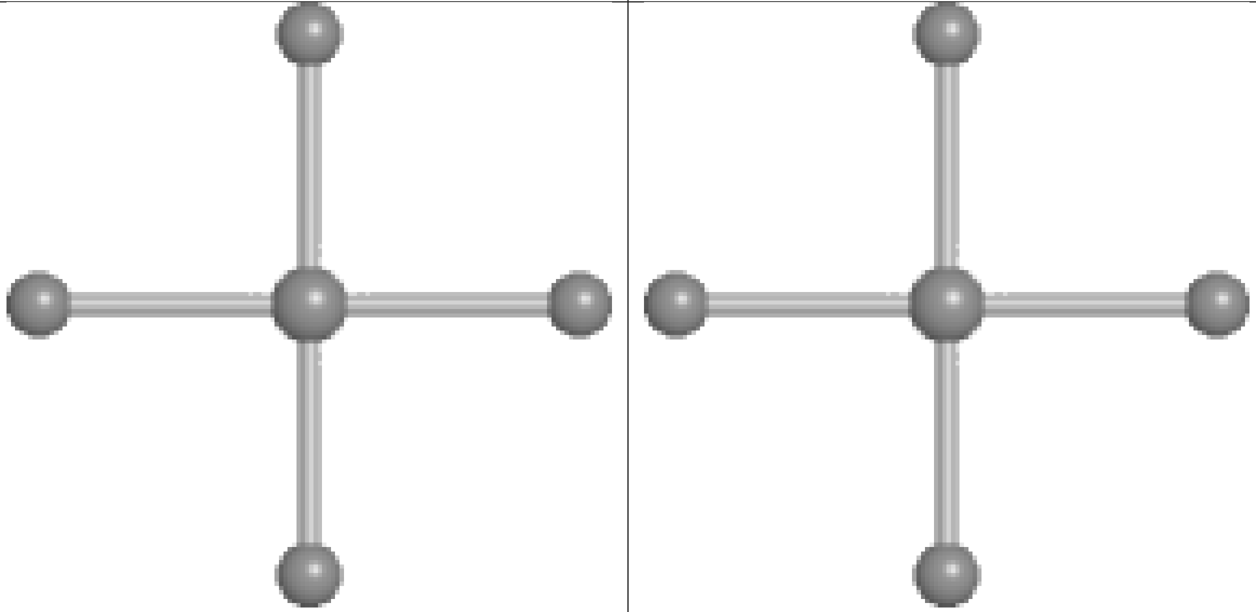
Torsions **Rings**

Ligand SO4 A 422



Bond lengths

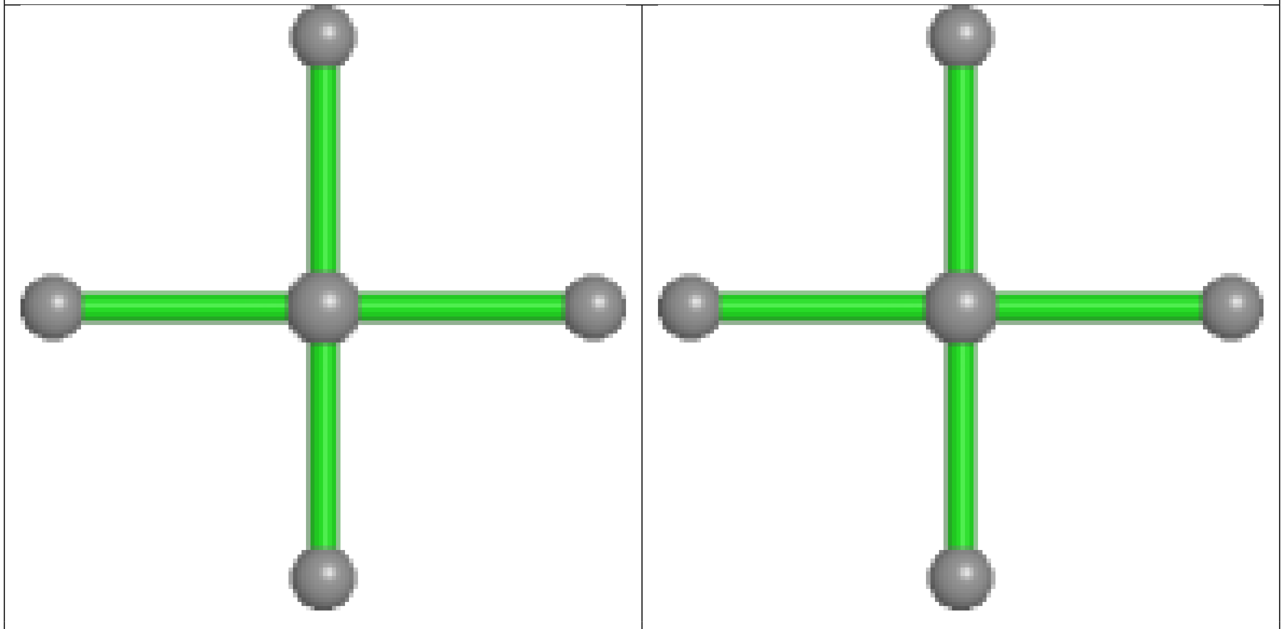
Bond angles



Torsions

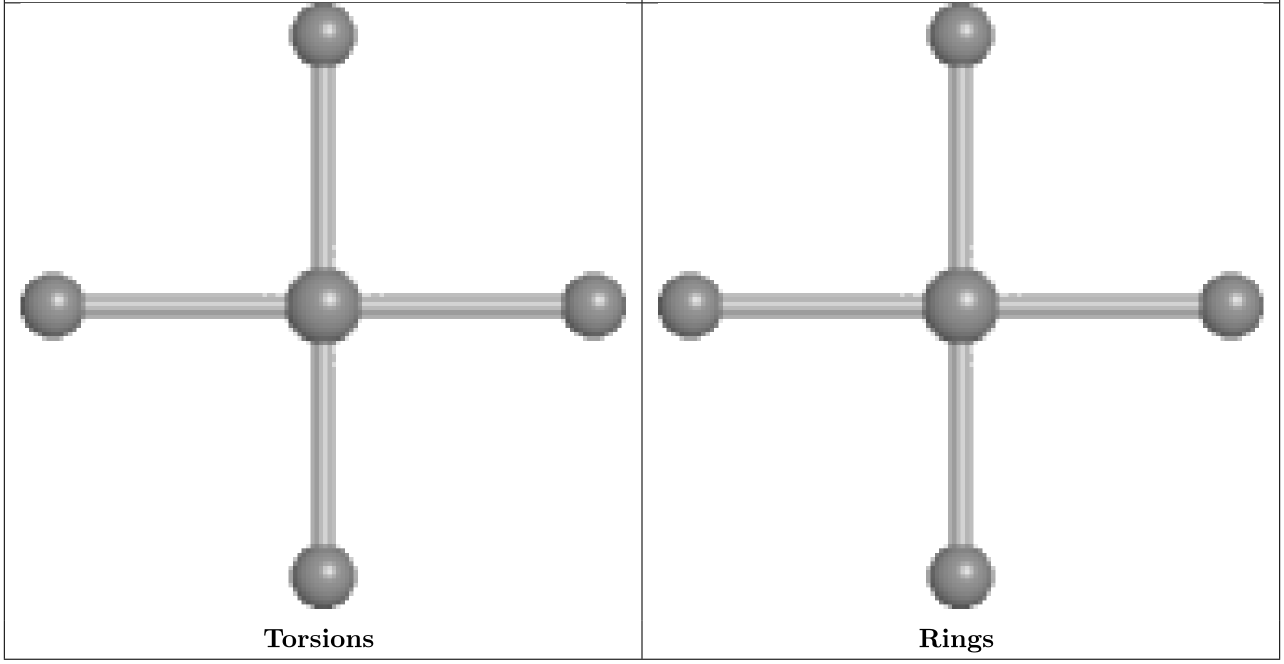
Rings

Ligand SO4 B 410



Bond lengths

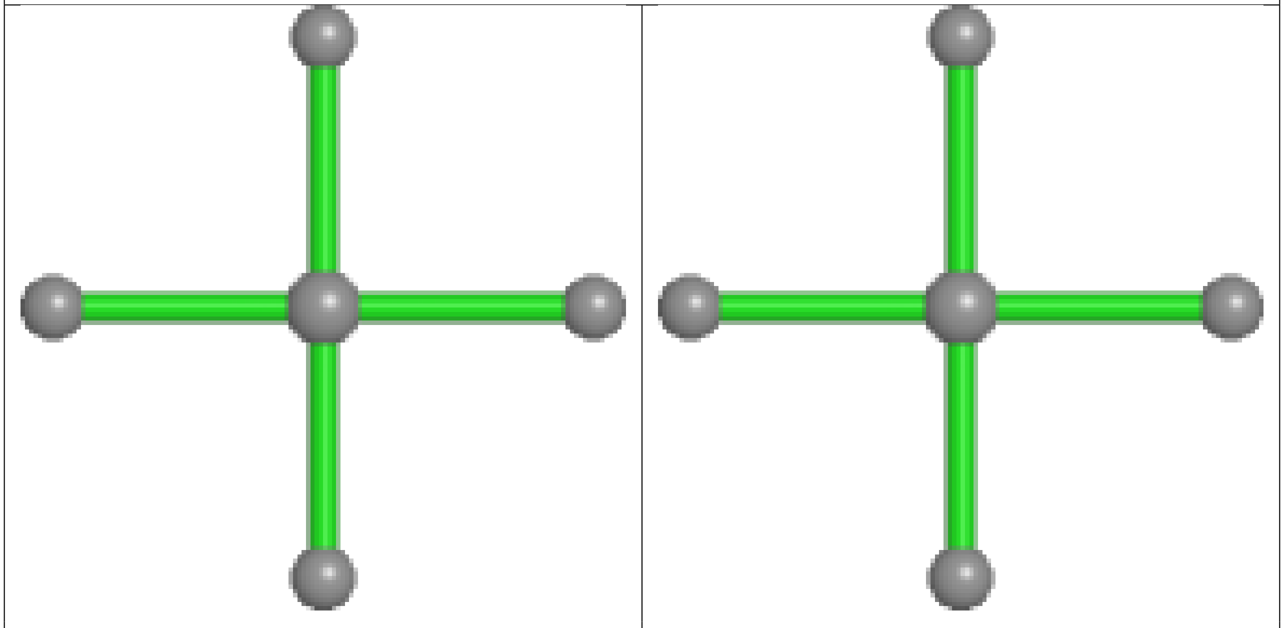
Bond angles



Torsions

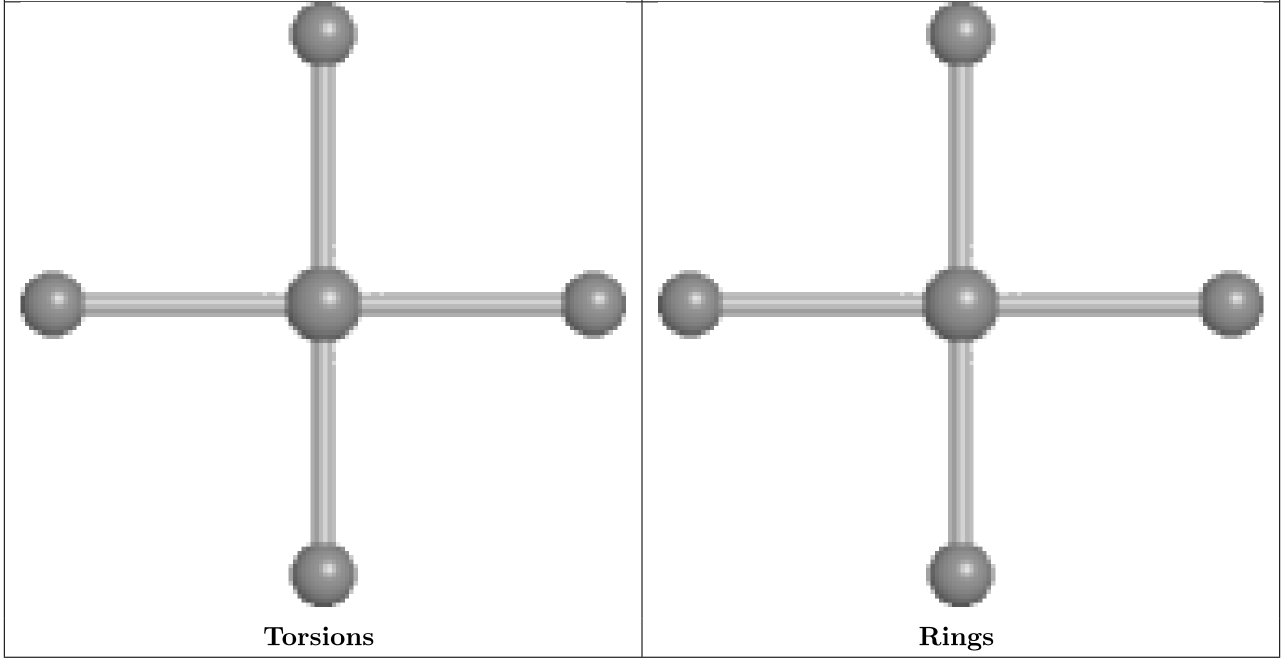
Rings

Ligand SO4 A 421



Bond lengths

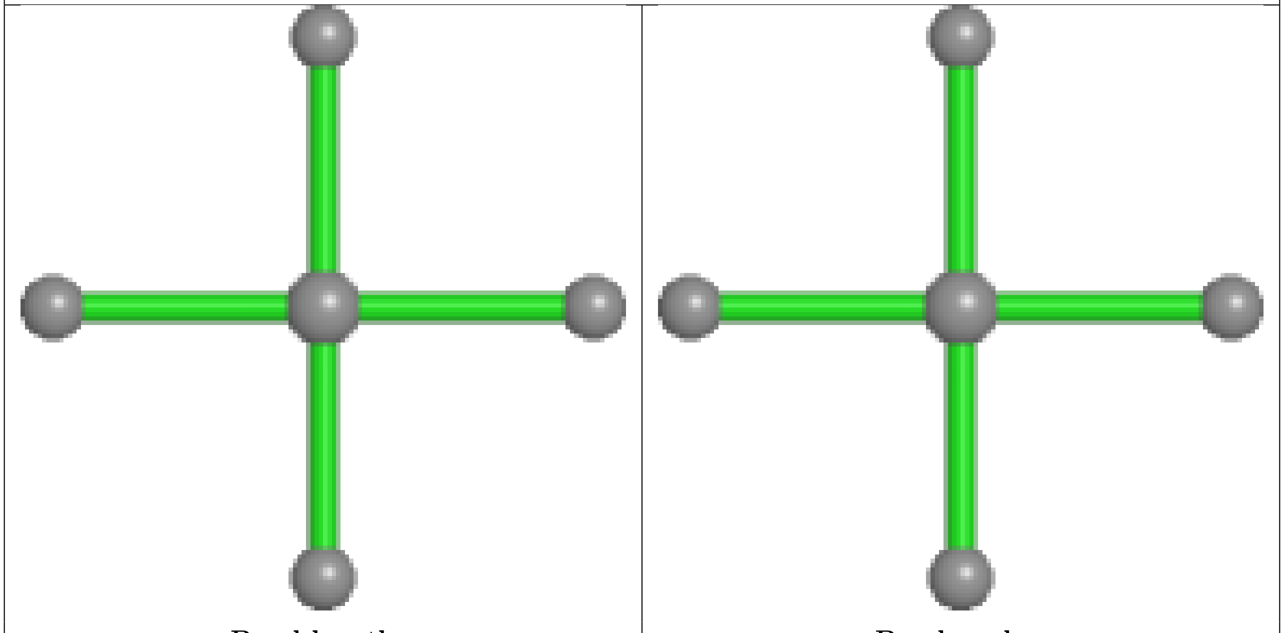
Bond angles



Torsions

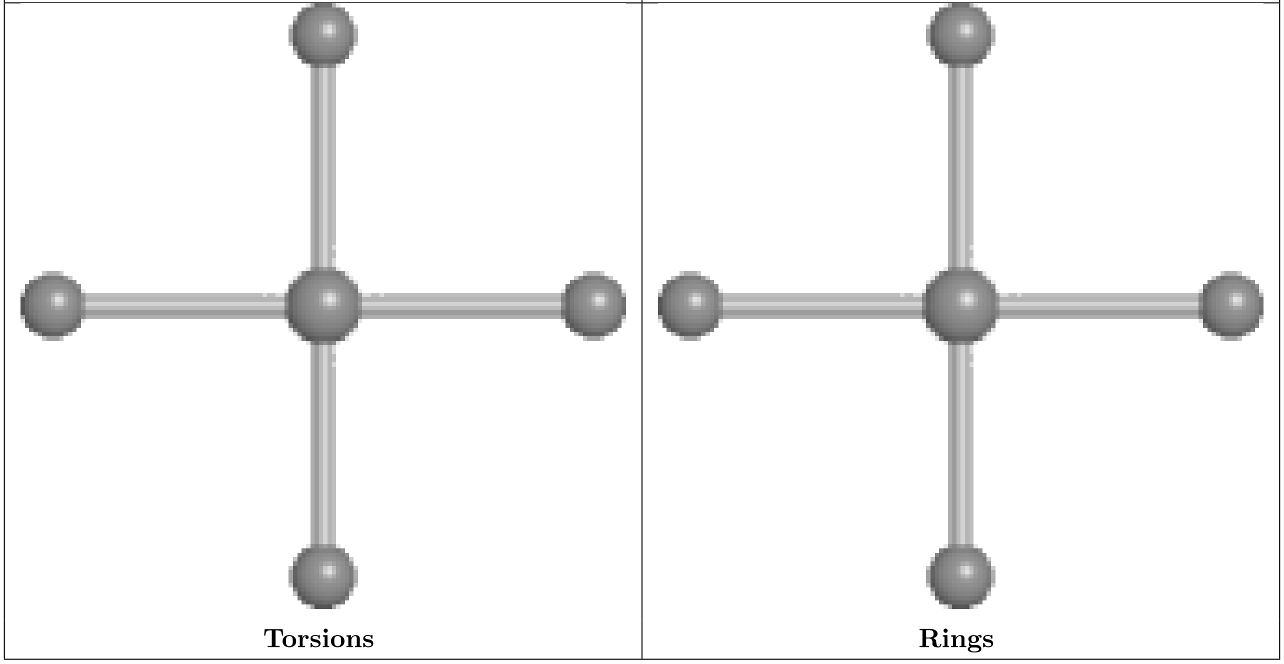
Rings

Ligand SO4 A 405



Bond lengths

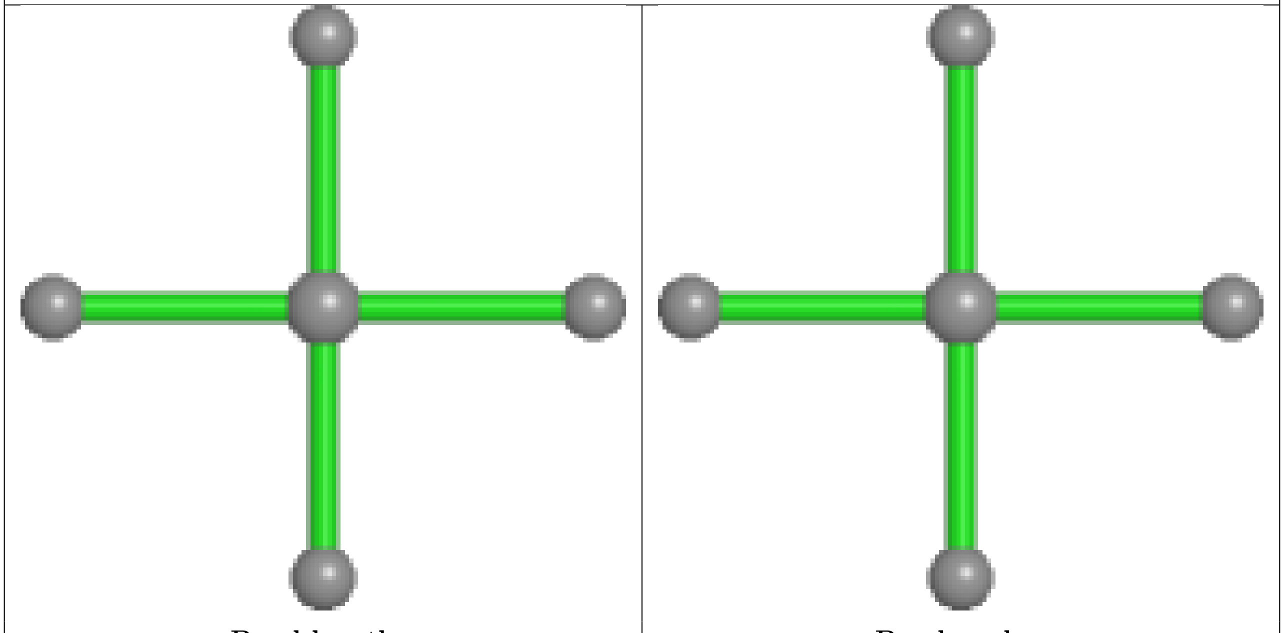
Bond angles



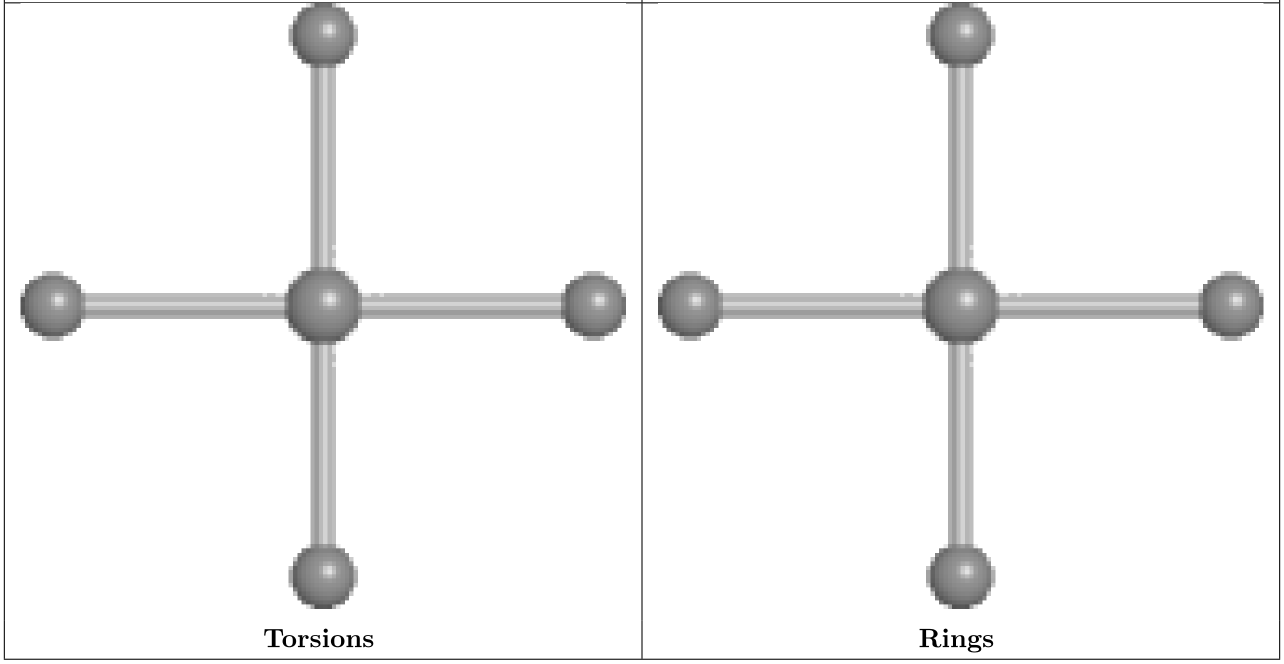
Torsions

Rings

Ligand SO4 B 409

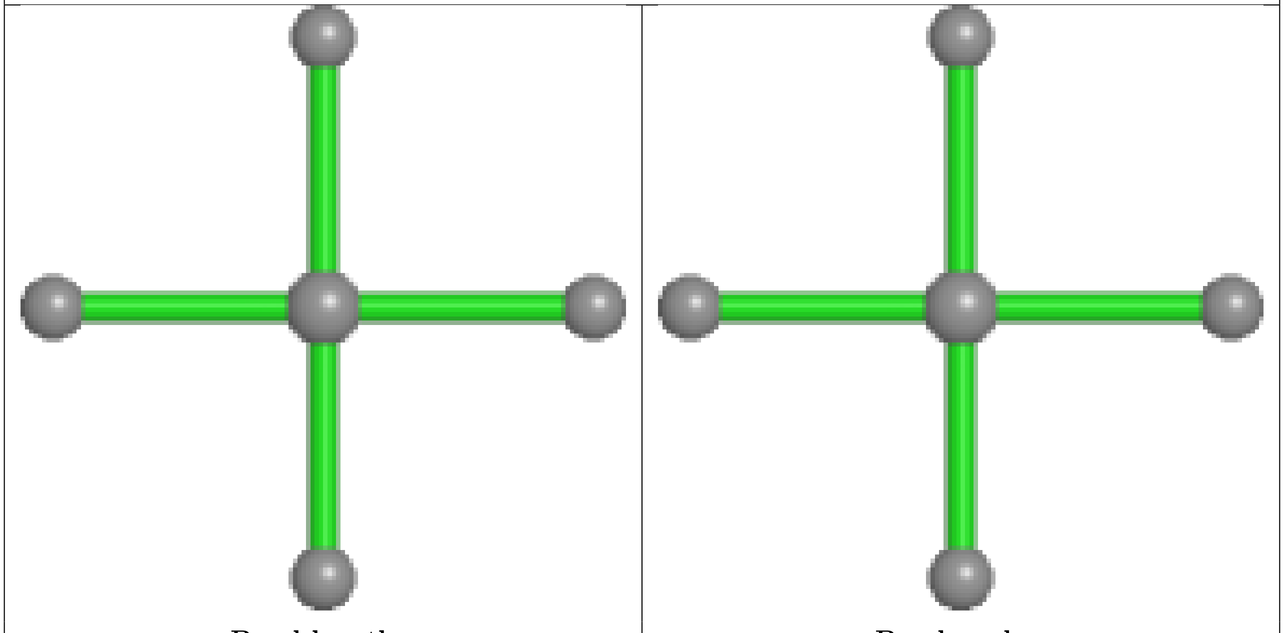


Bond lengths **Bond angles**

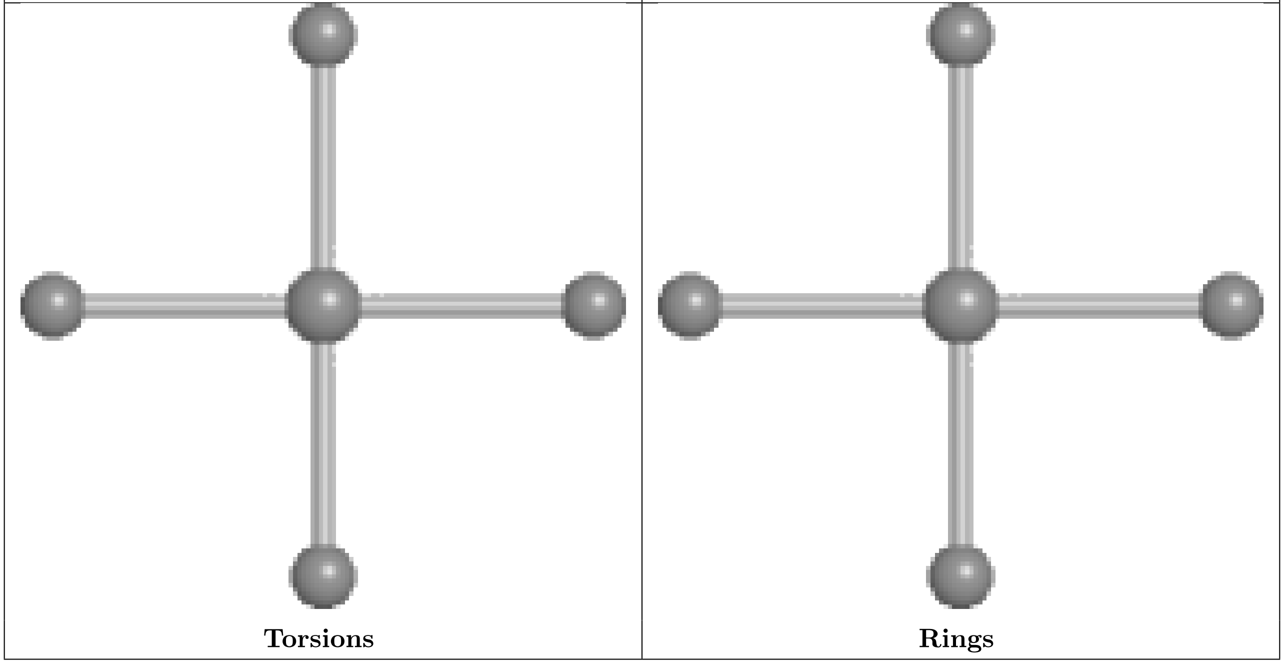


Torsions **Rings**

Ligand SO4 B 417

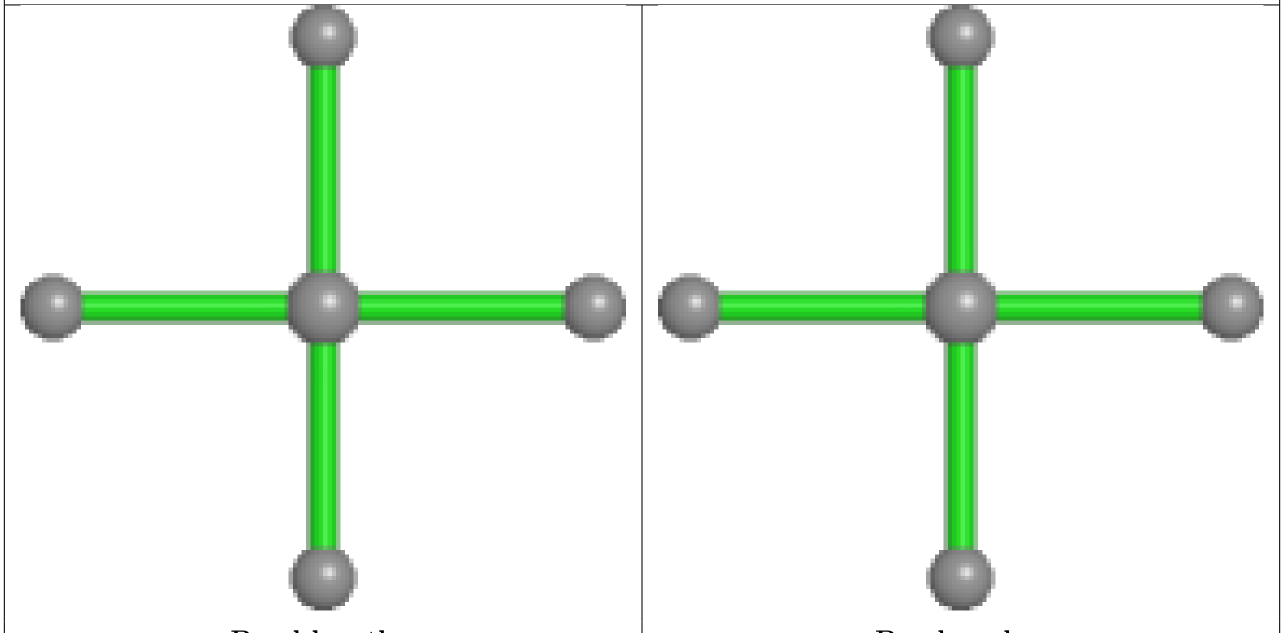


Bond lengths **Bond angles**



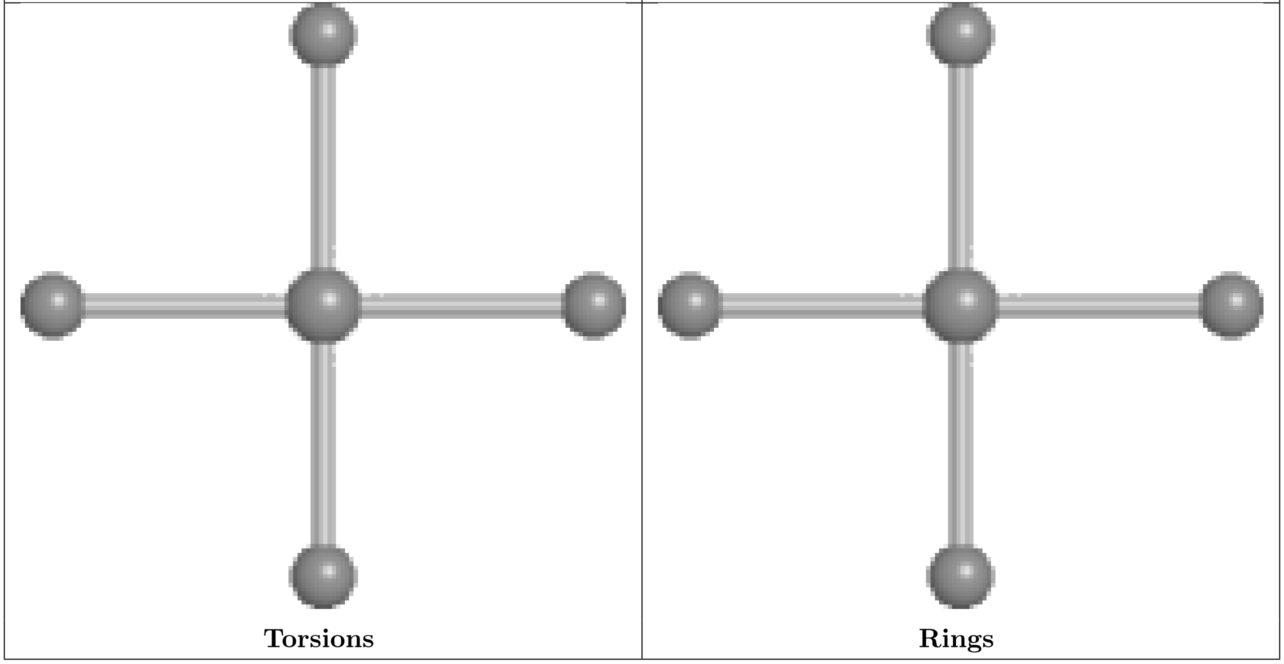
Torsions **Rings**

Ligand SO4 B 425



Bond lengths

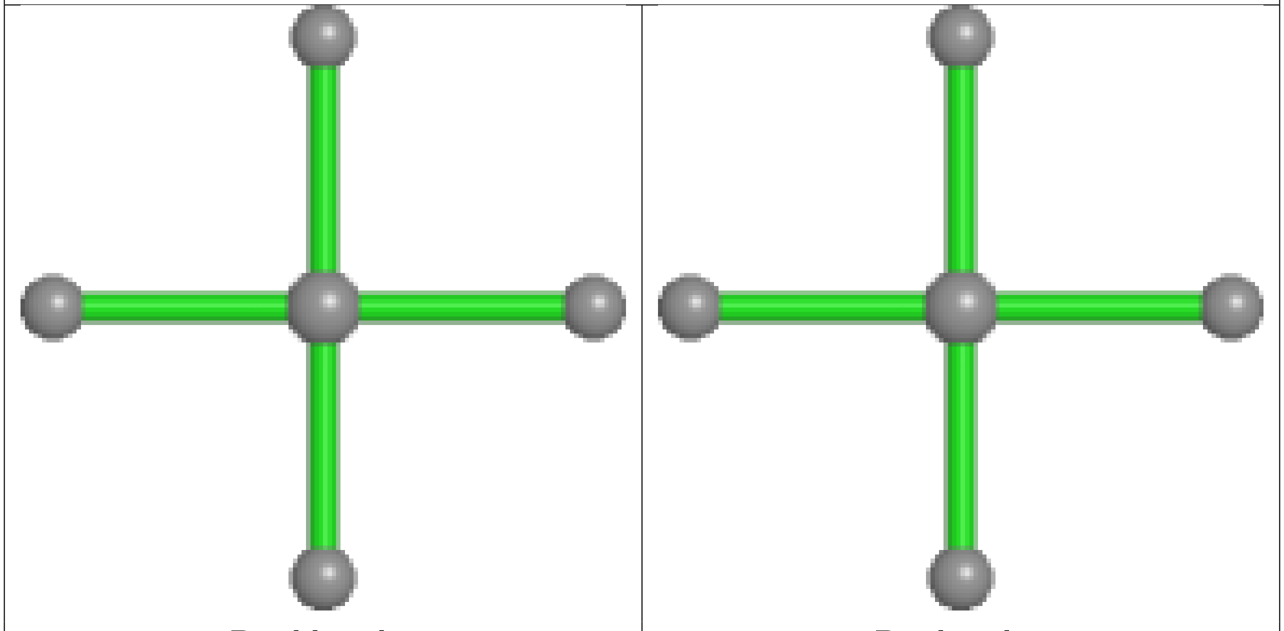
Bond angles



Torsions

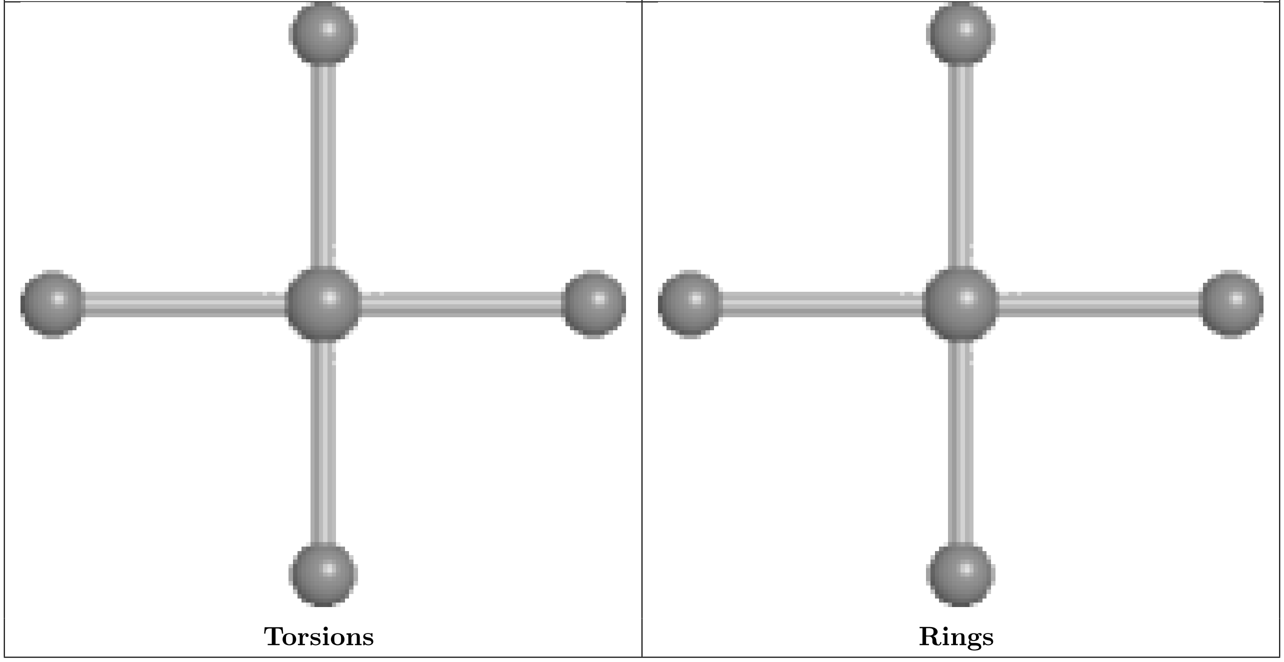
Rings

Ligand SO4 B 416



Bond lengths

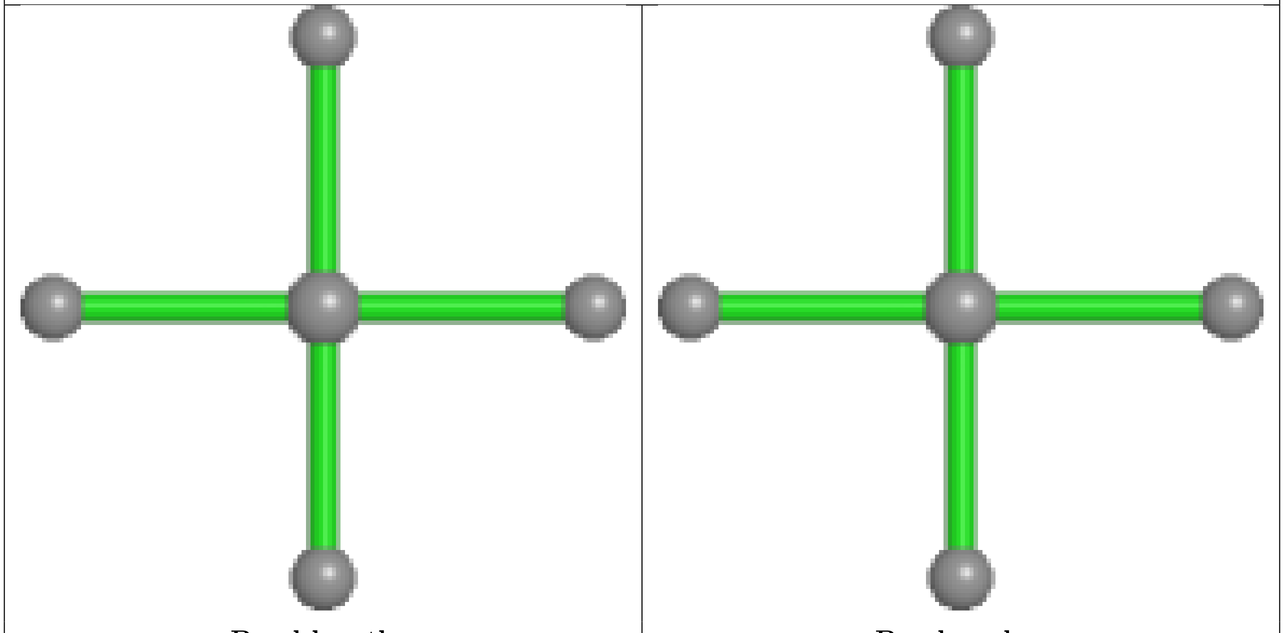
Bond angles



Torsions

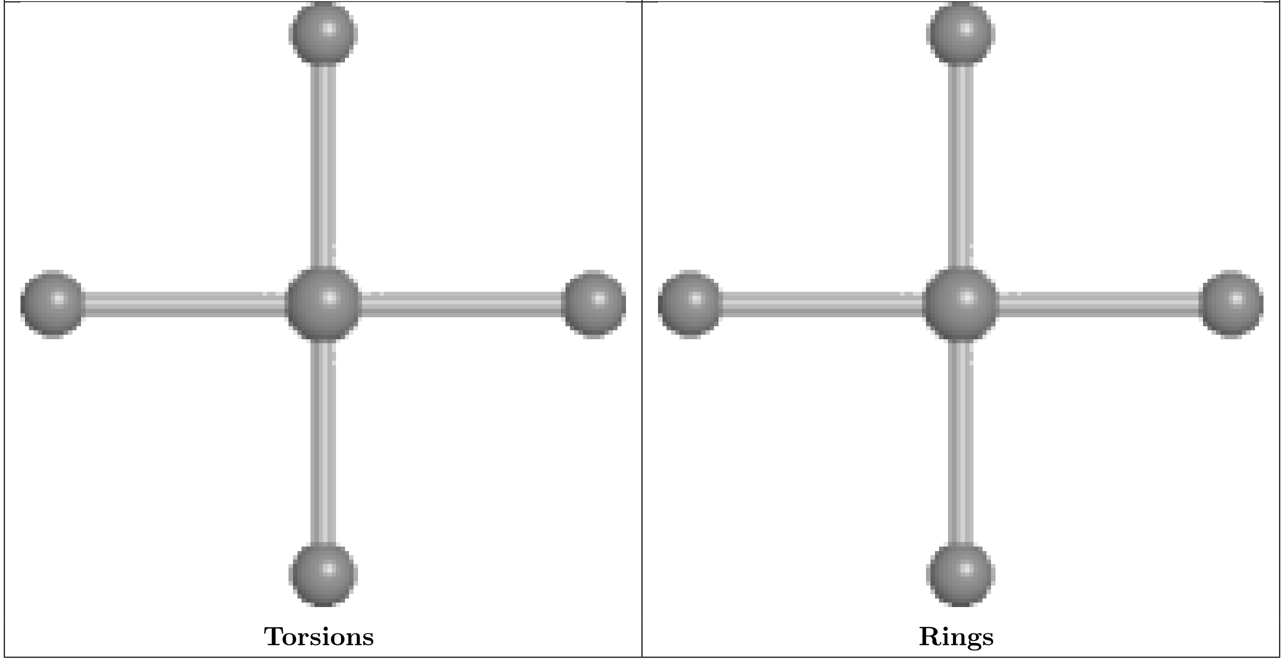
Rings

Ligand SO4 A 412



Bond lengths

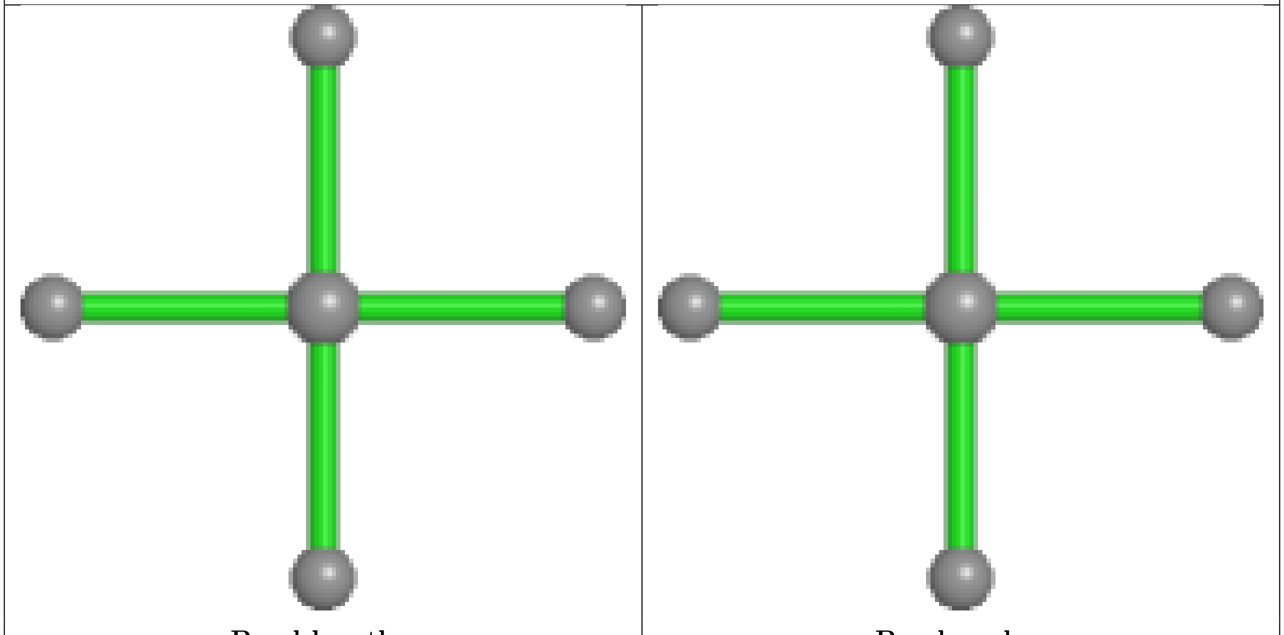
Bond angles



Torsions

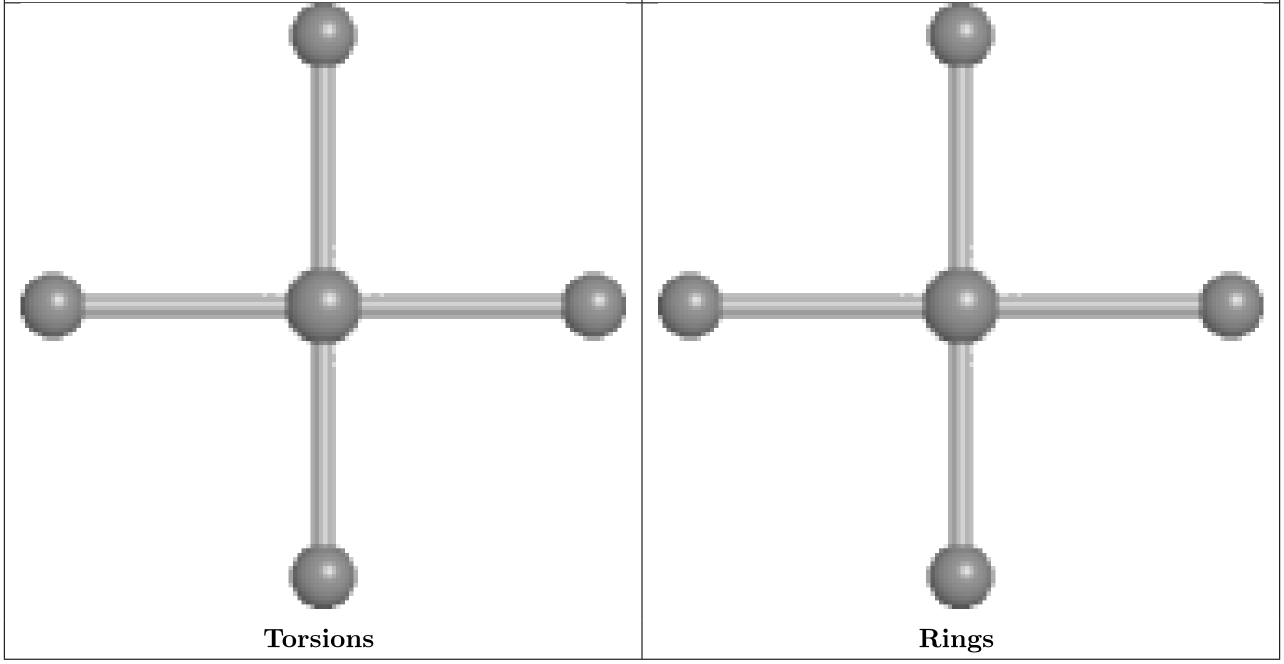
Rings

Ligand SO4 B 424



Bond lengths

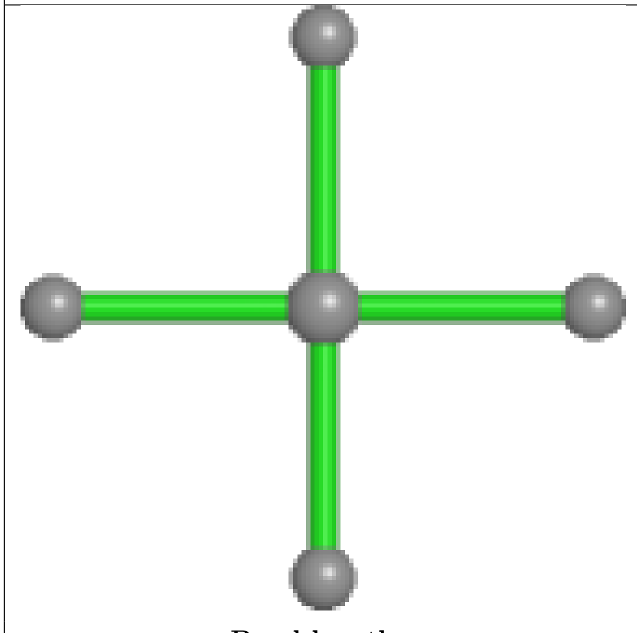
Bond angles



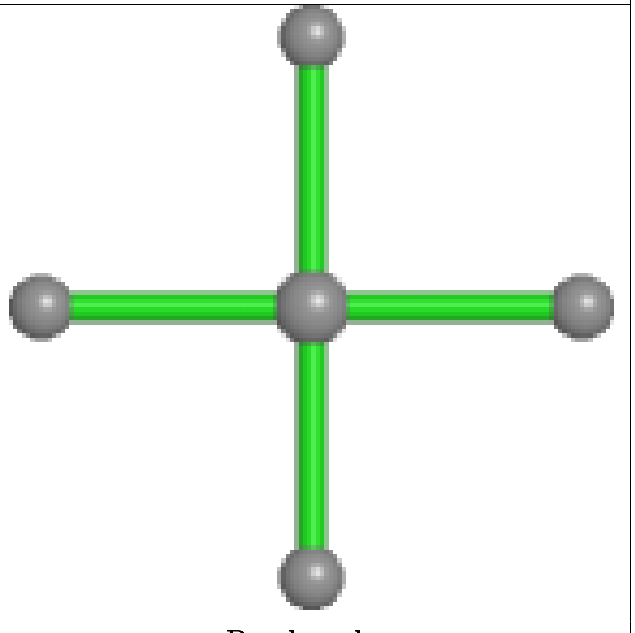
Torsions

Rings

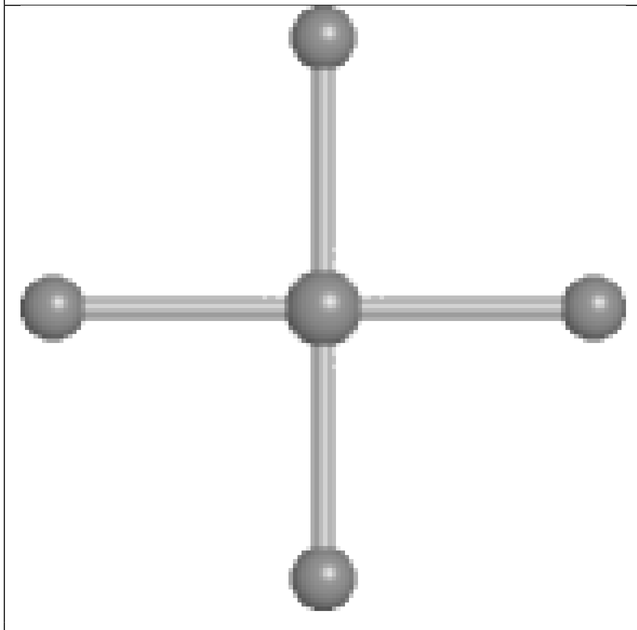
Ligand SO4 A 413



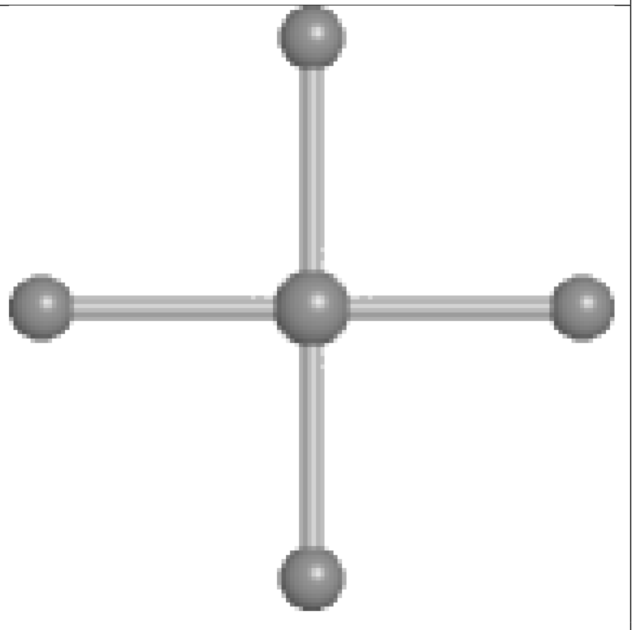
Bond lengths



Bond angles

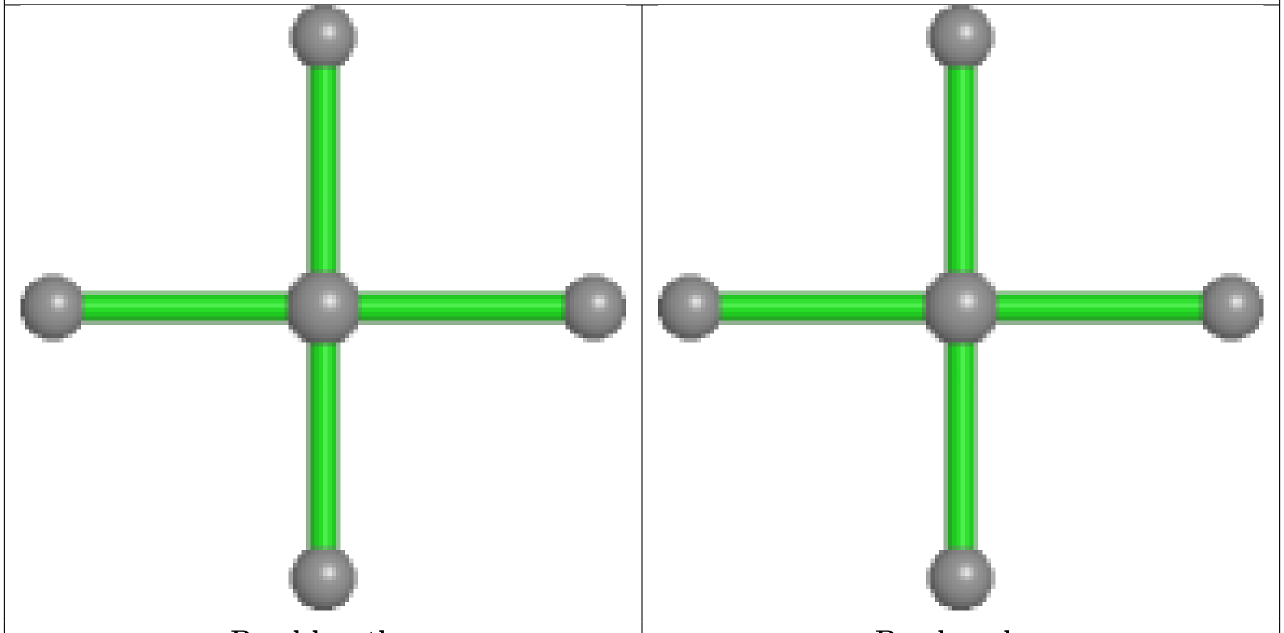


Torsions



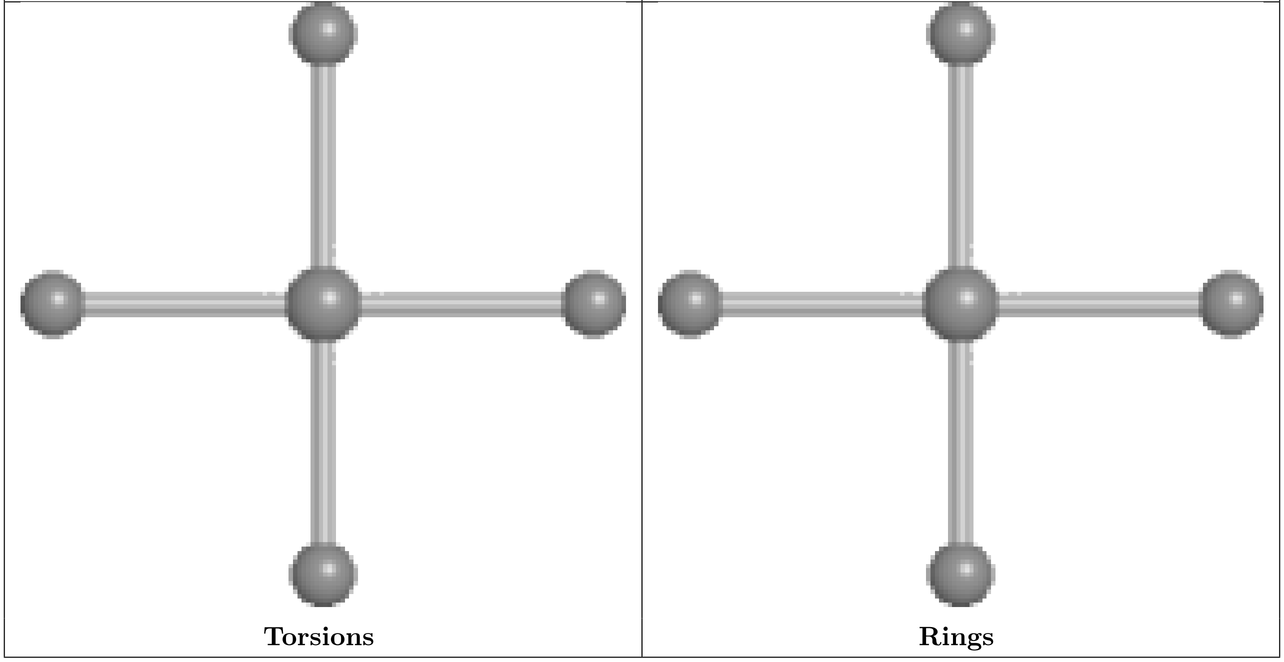
Rings

Ligand SO4 B 423



Bond lengths

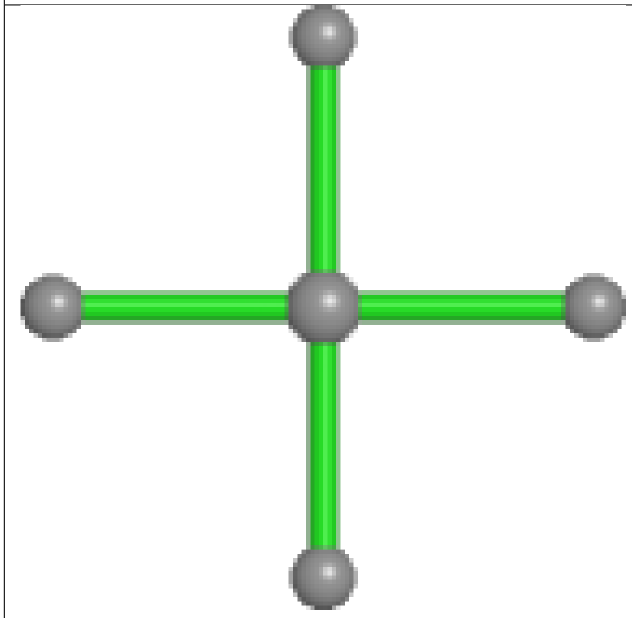
Bond angles



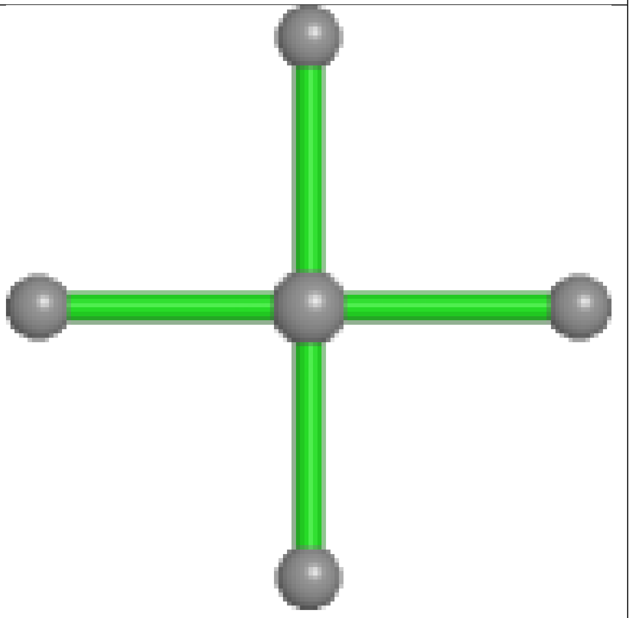
Torsions

Rings

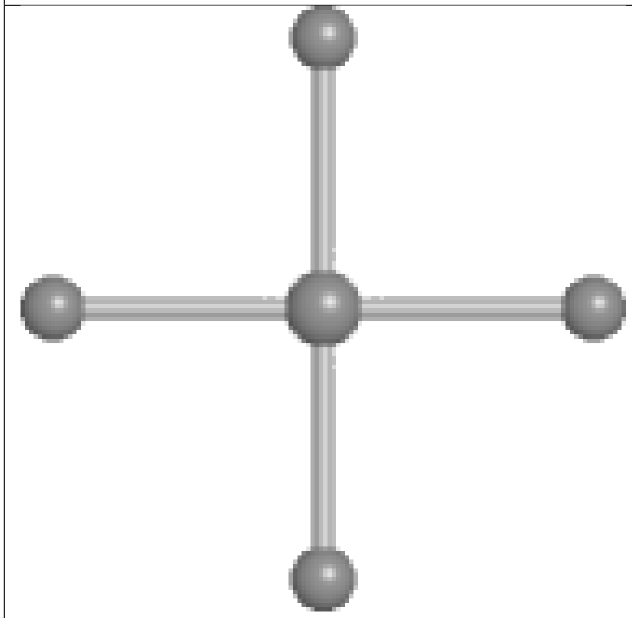
Ligand SO4 A 407



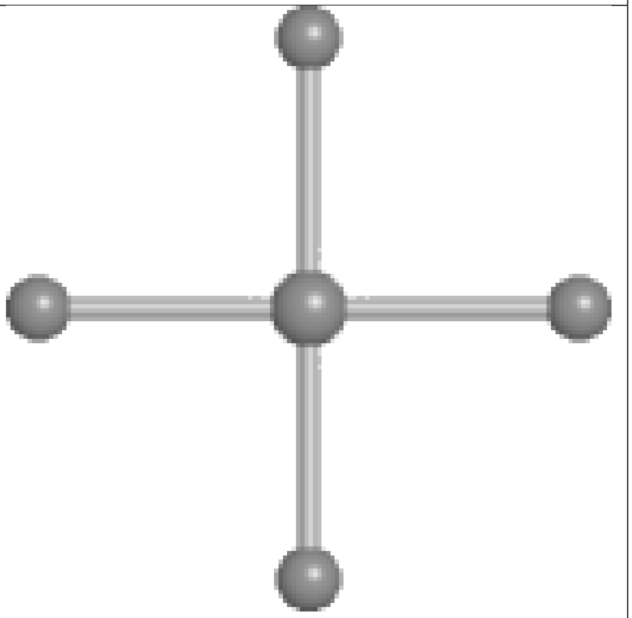
Bond lengths



Bond angles

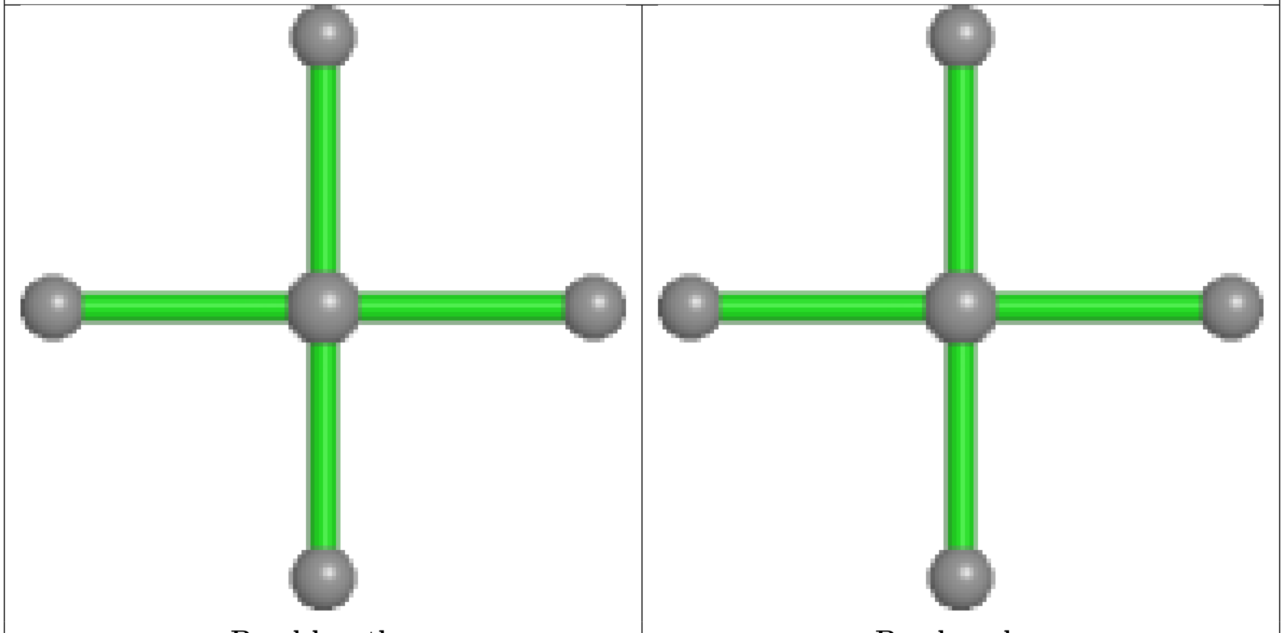


Torsions



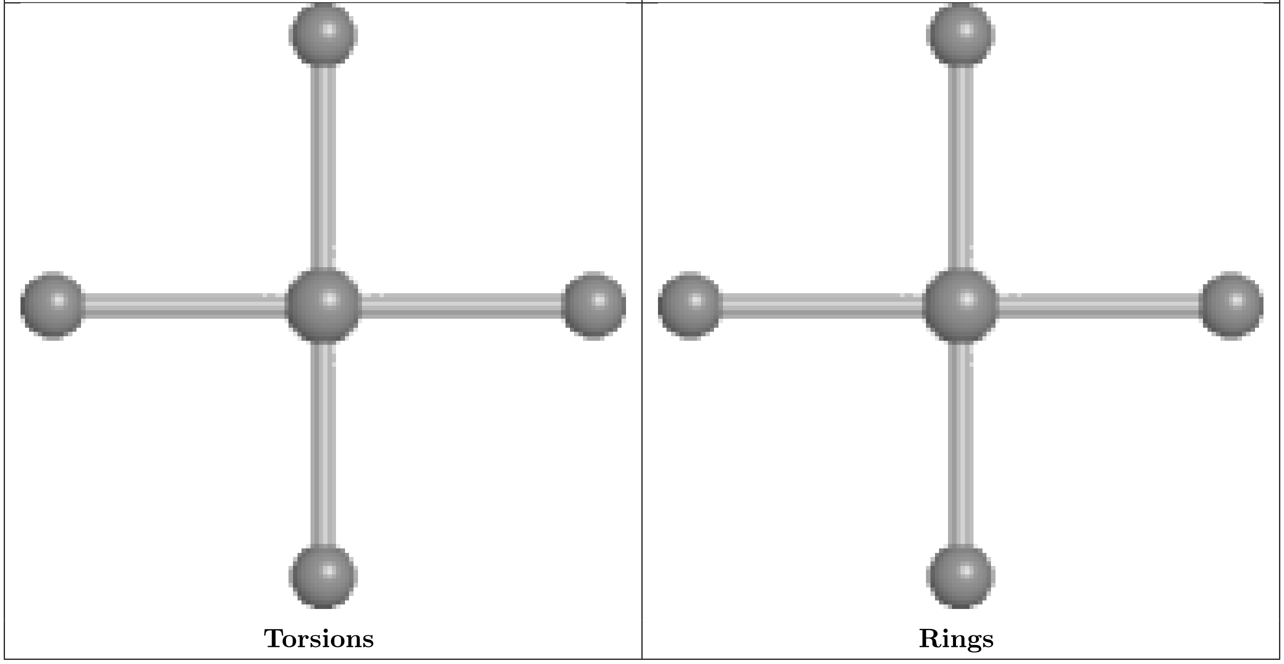
Rings

Ligand SO4 B 411



Bond lengths

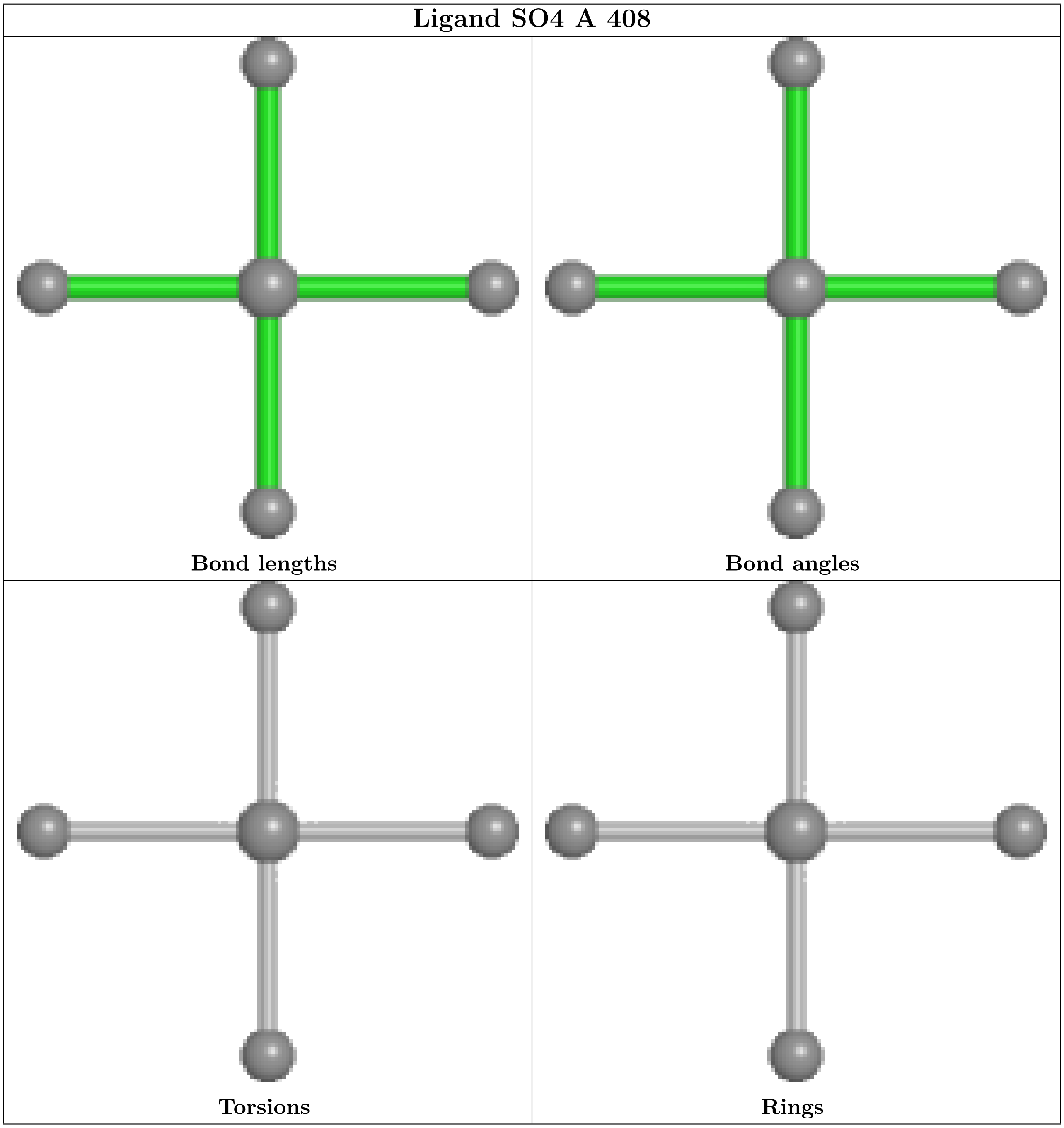
Bond angles



Torsions

Rings

Ligand SO4 A 408



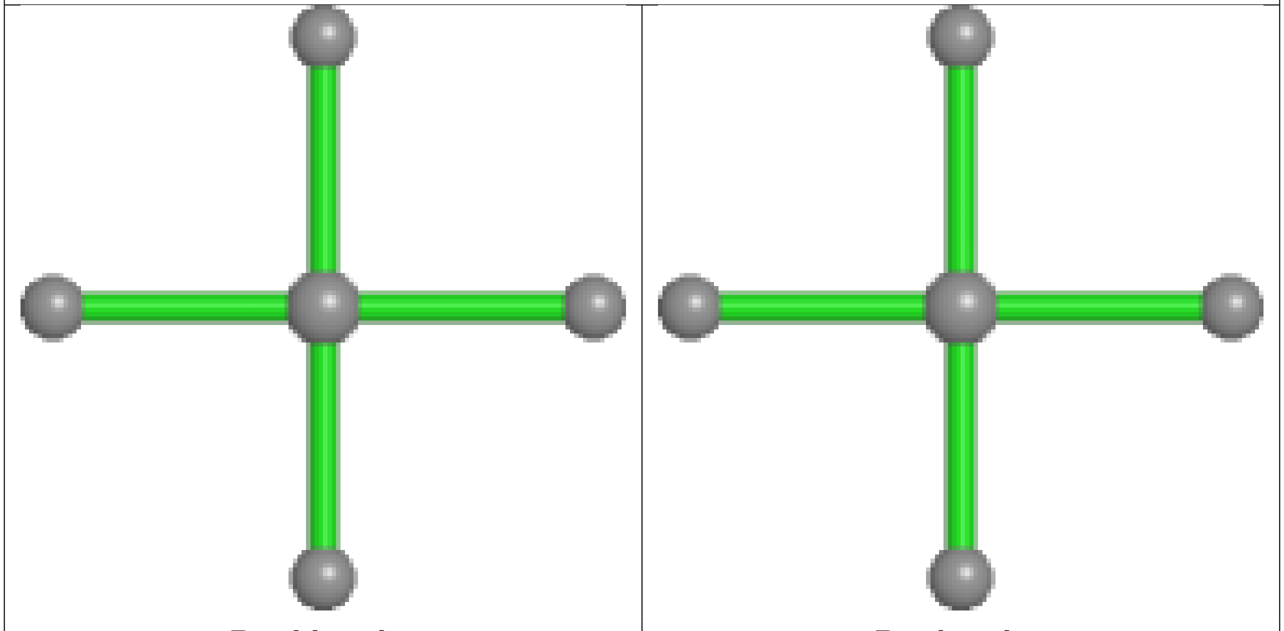
Bond lengths

Bond angles

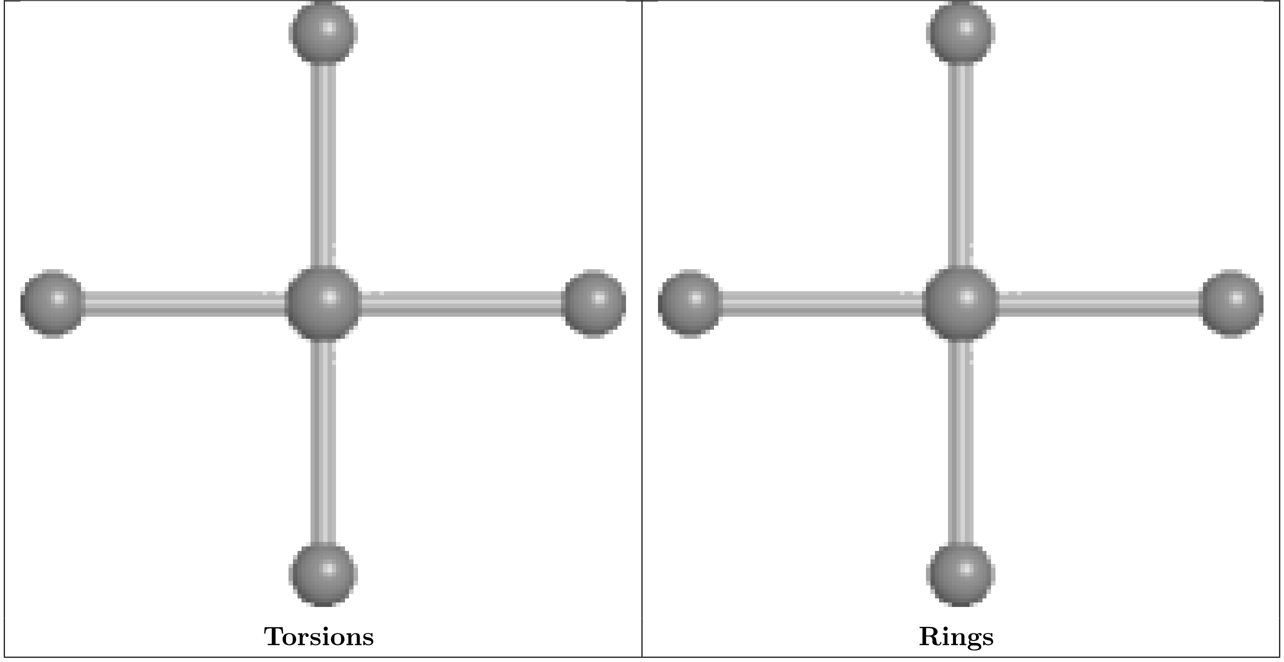
Torsions

Rings

Ligand SO4 B 420

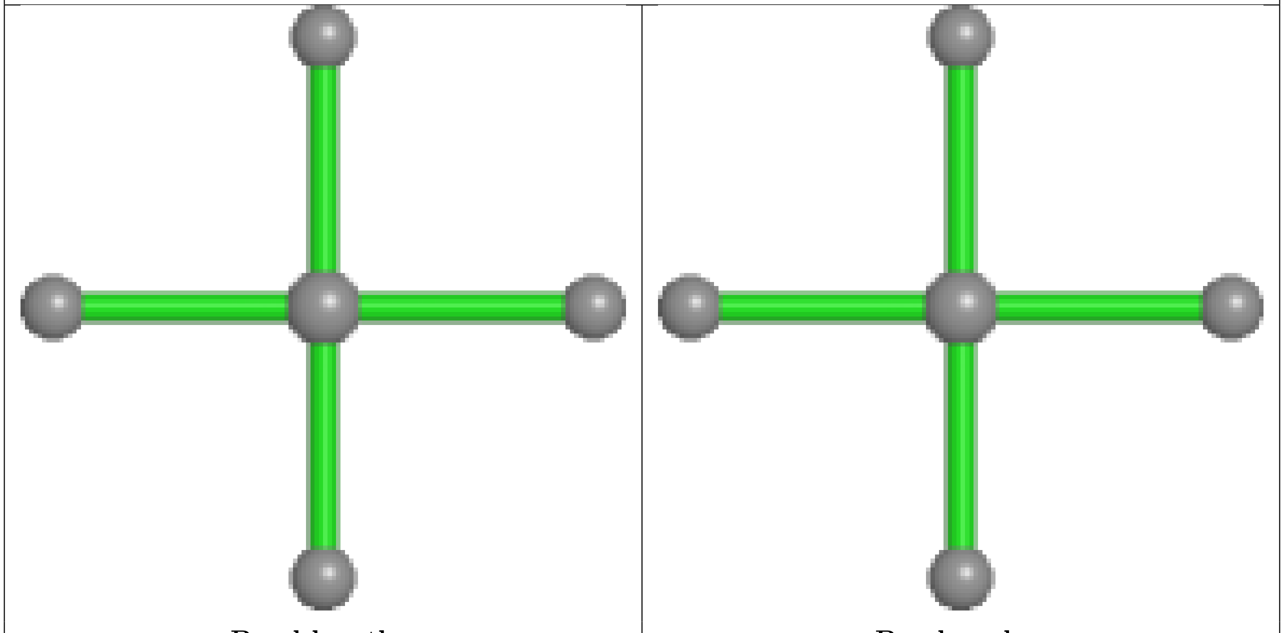


Bond lengths **Bond angles**

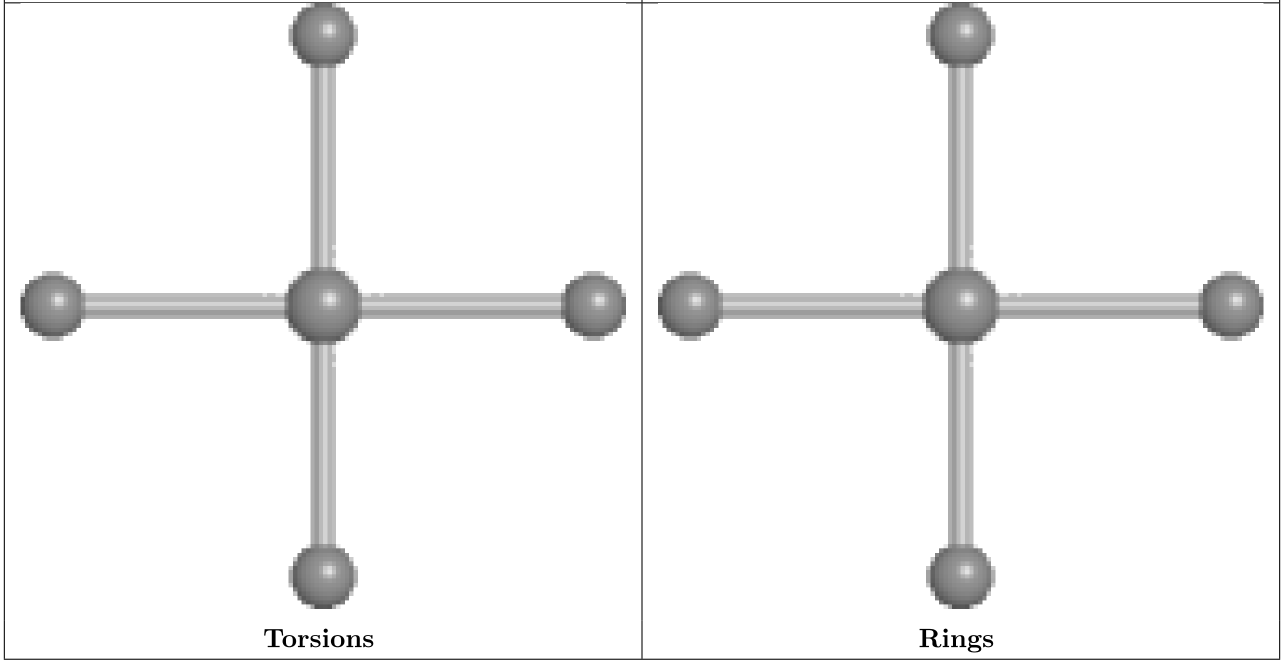


Torsions **Rings**

Ligand SO4 B 426

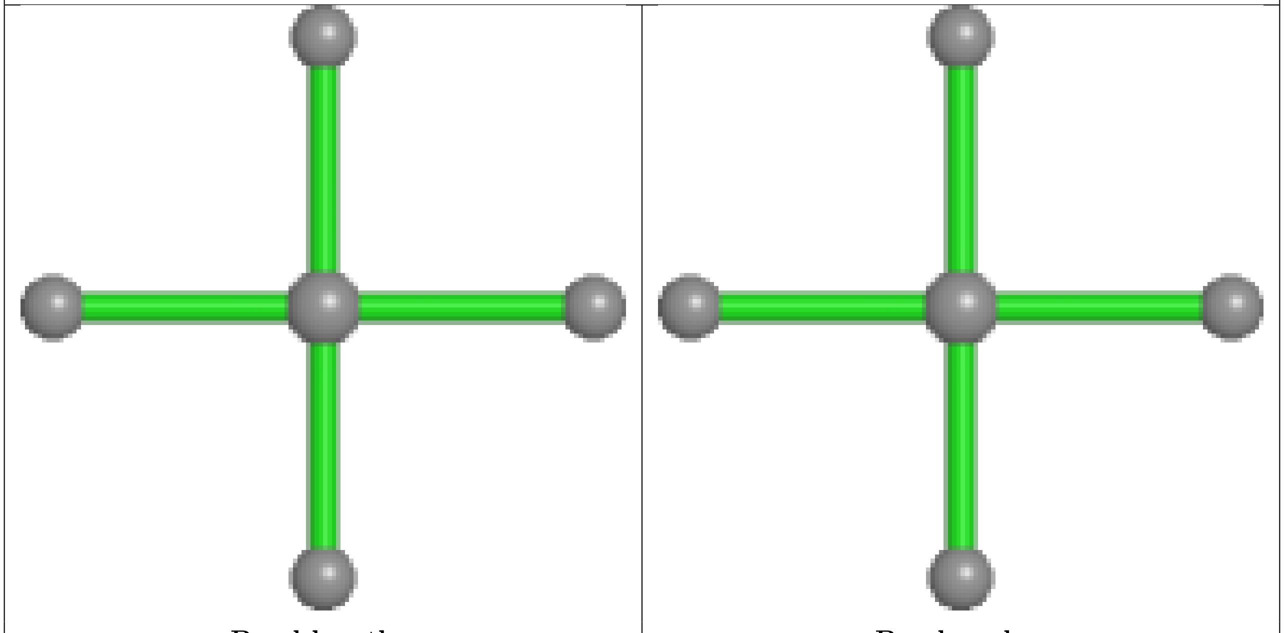


Bond lengths **Bond angles**



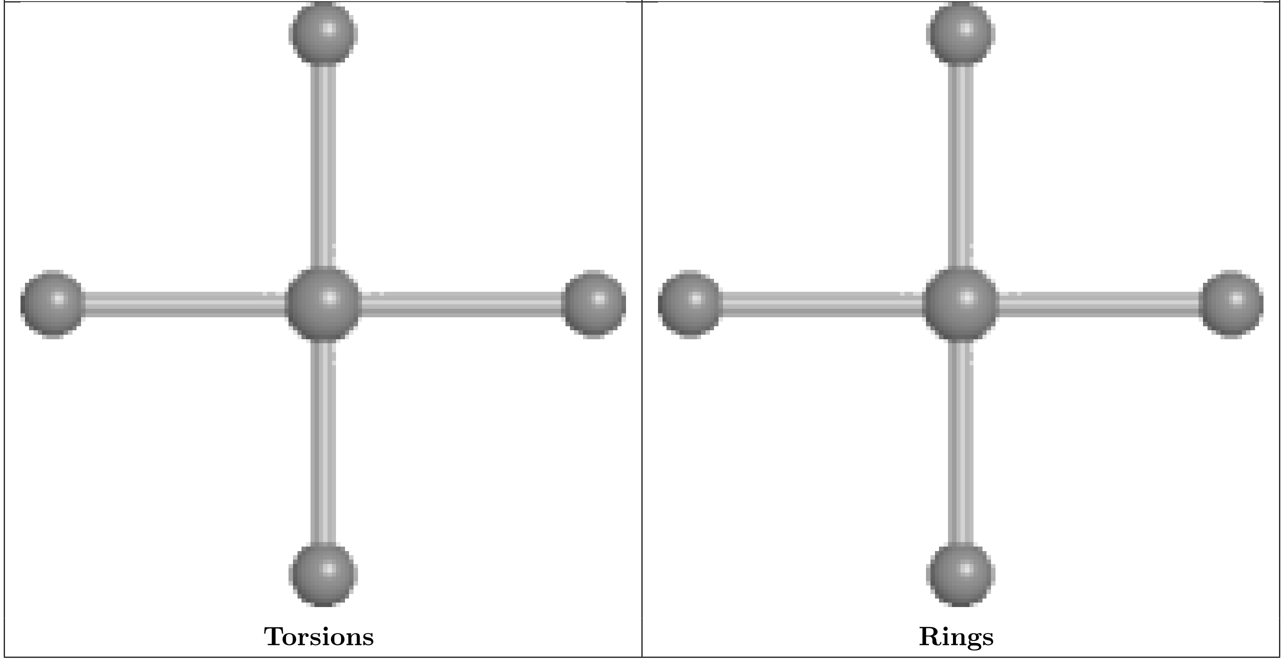
Torsions **Rings**

Ligand SO4 A 410



Bond lengths

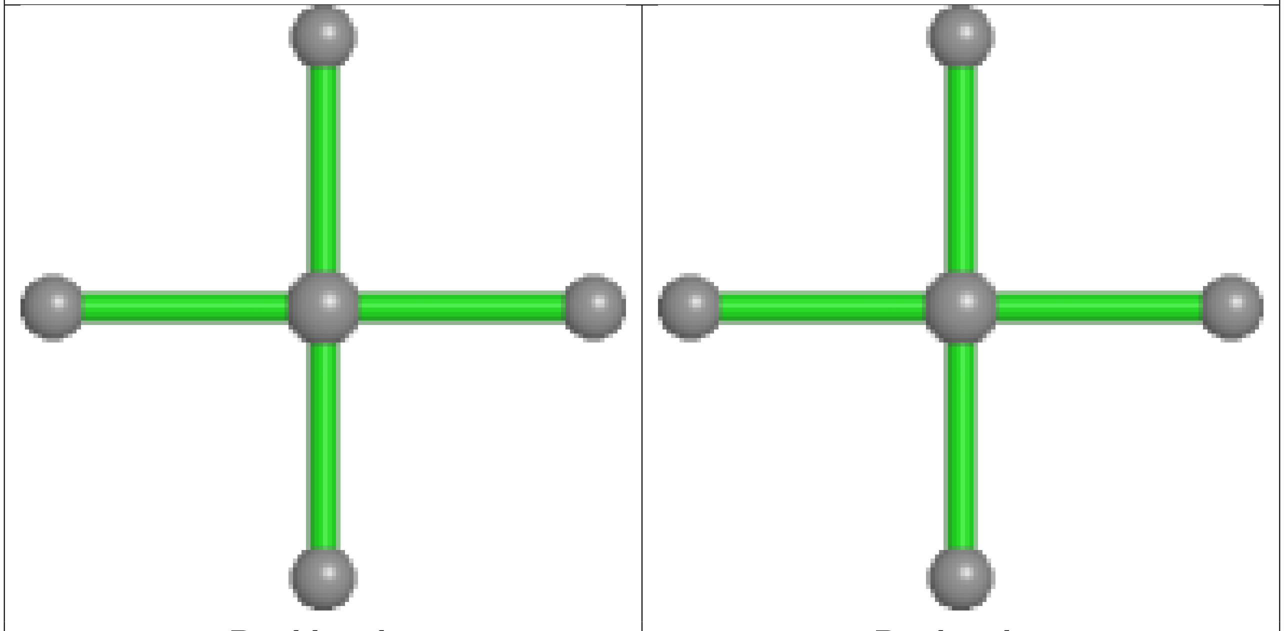
Bond angles



Torsions

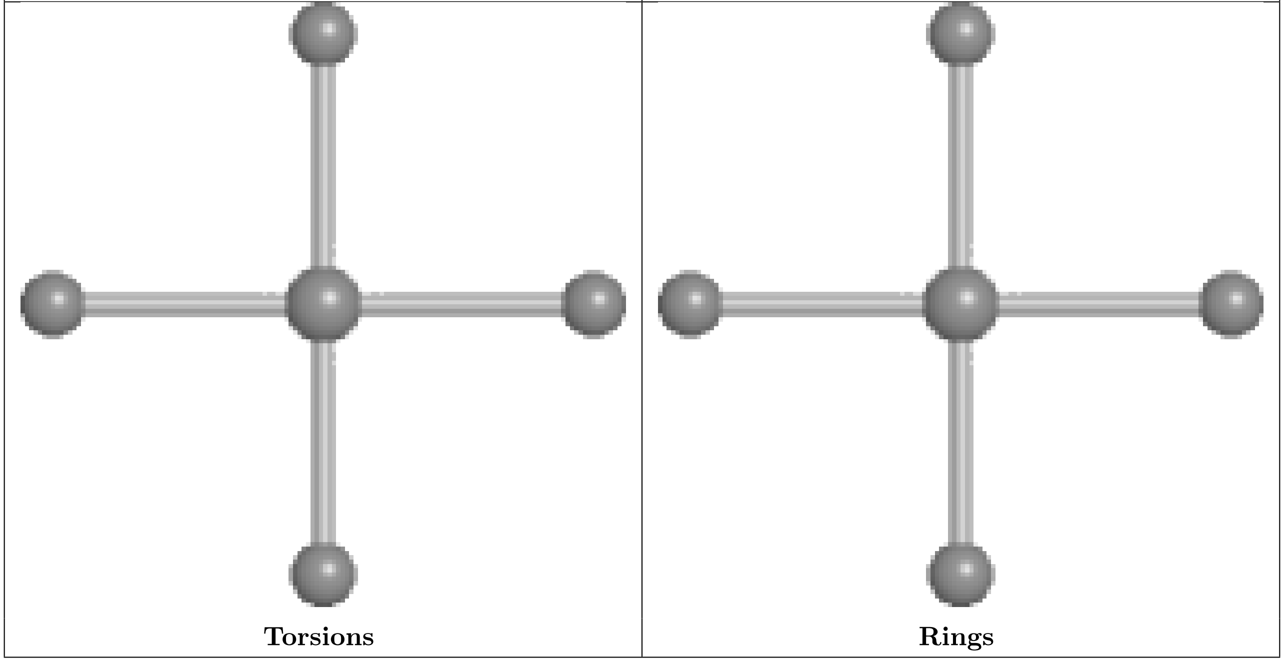
Rings

Ligand SO4 B 406



Bond lengths

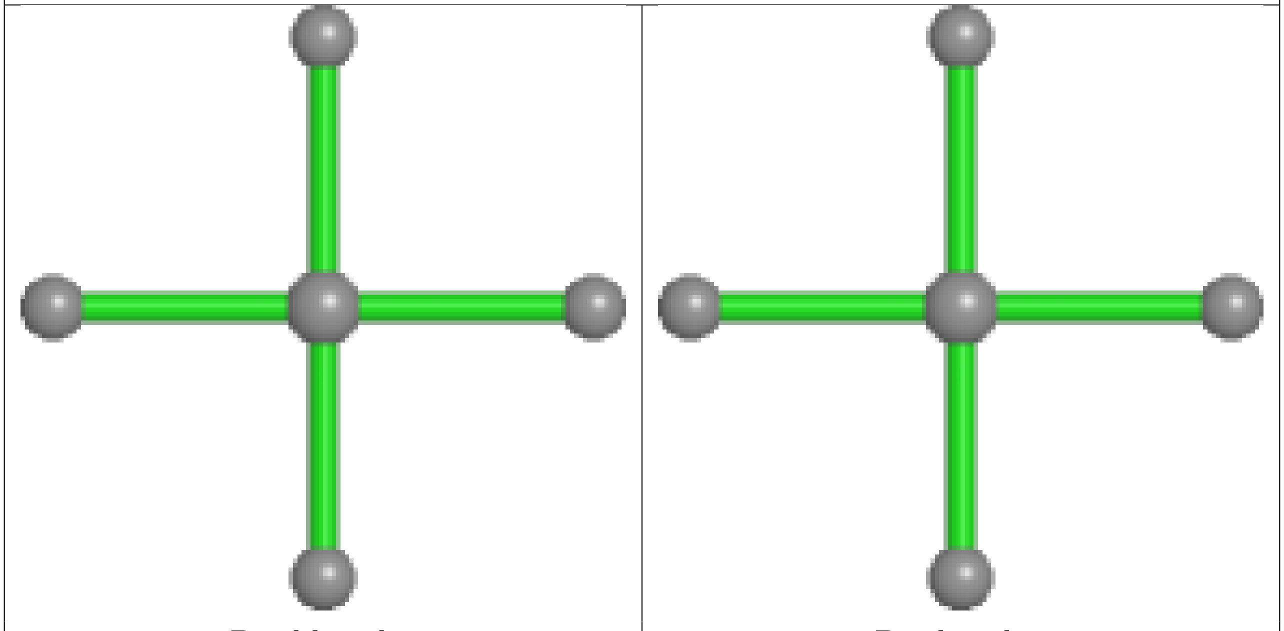
Bond angles



Torsions

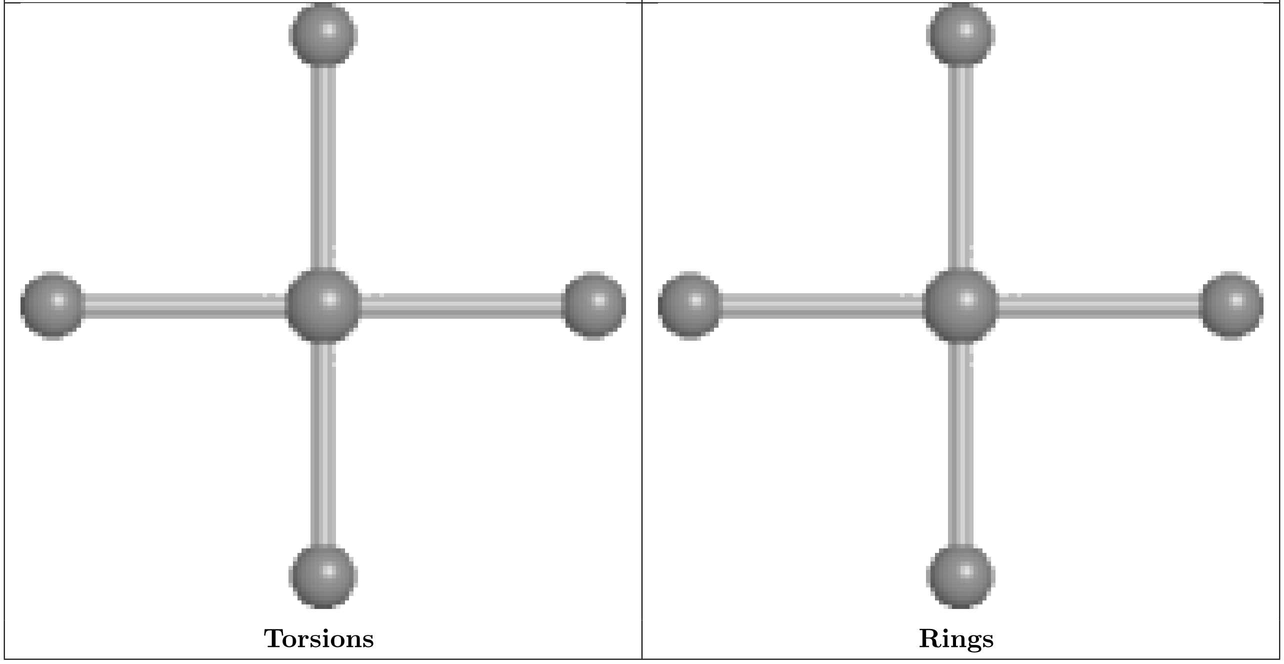
Rings

Ligand SO4 B 407



Bond lengths

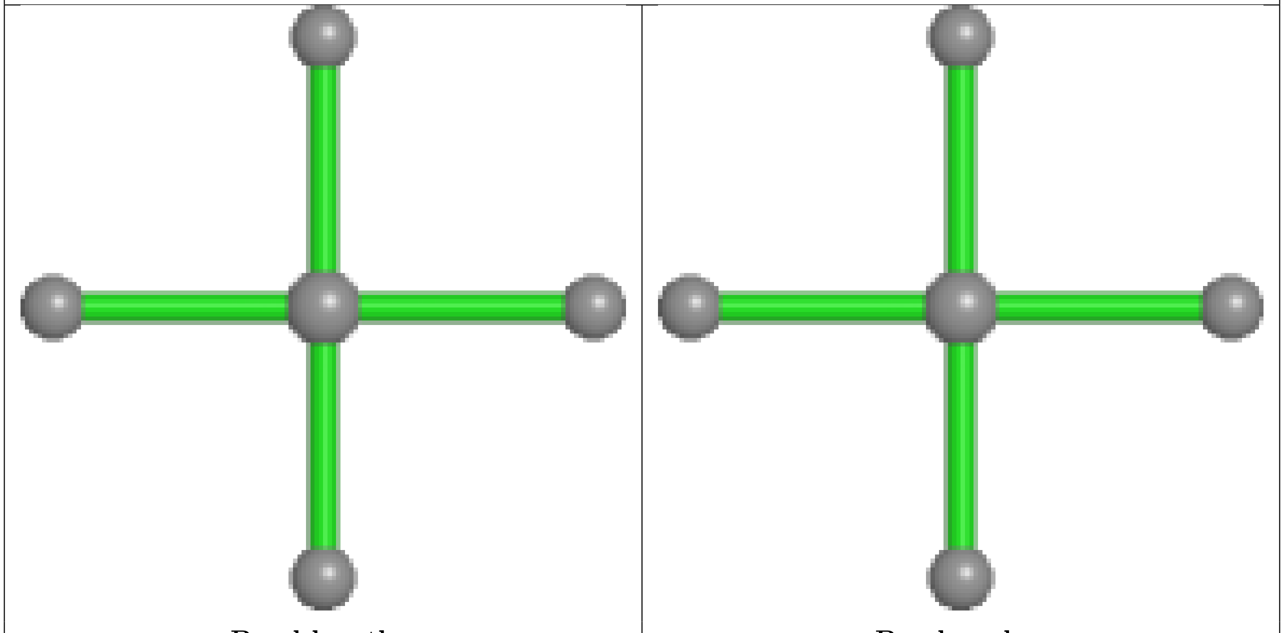
Bond angles



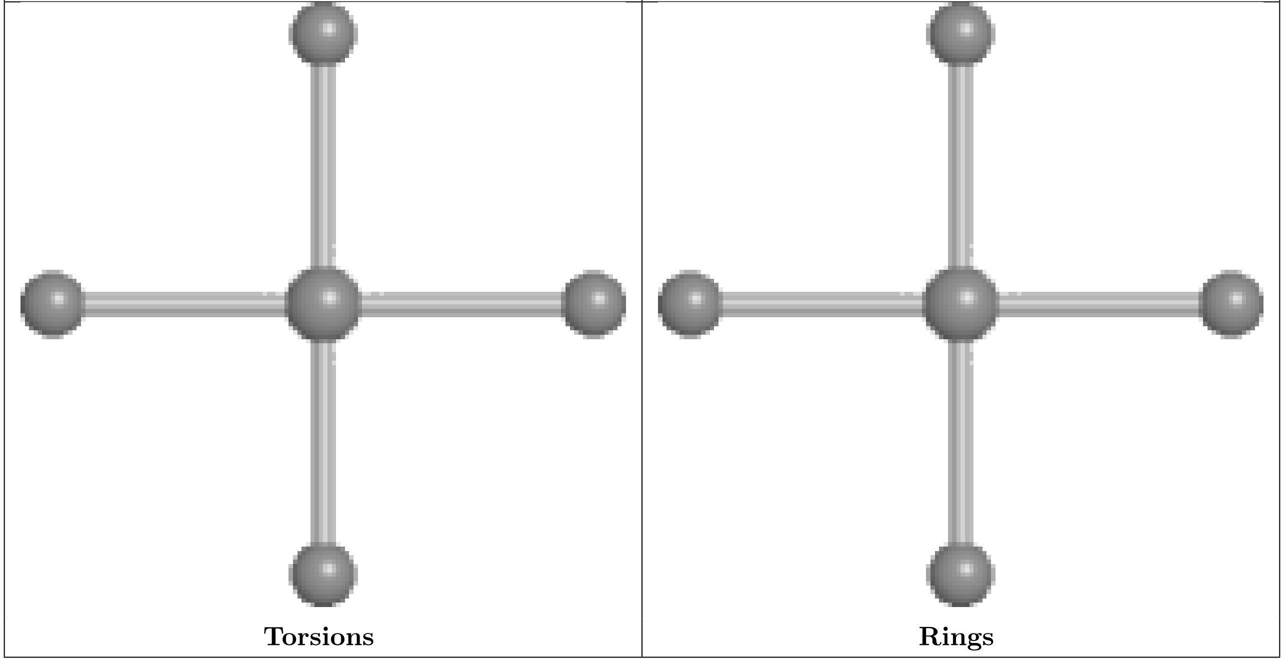
Torsions

Rings

Ligand SO4 B 413

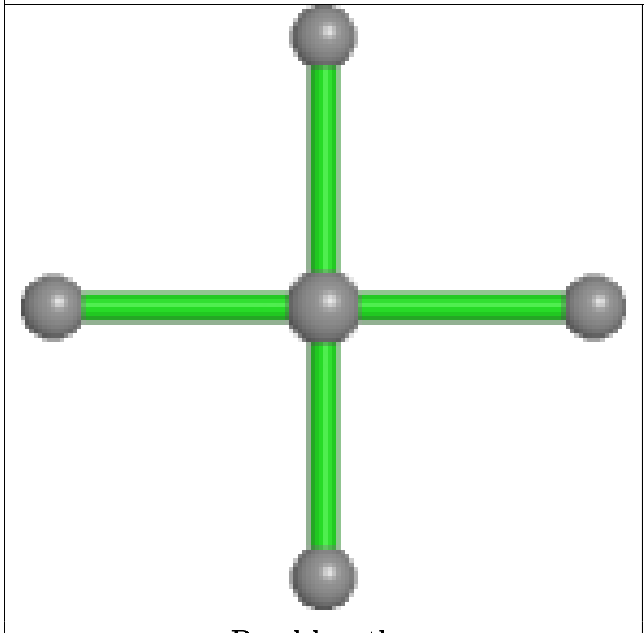


Bond lengths Bond angles

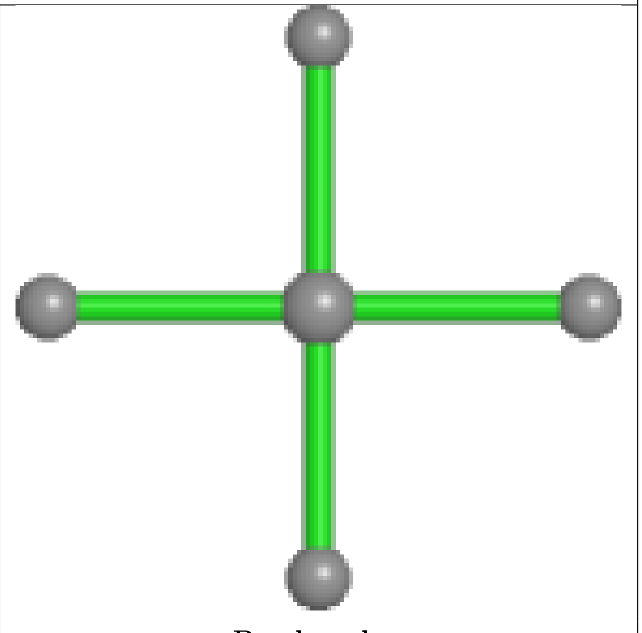


Torsions Rings

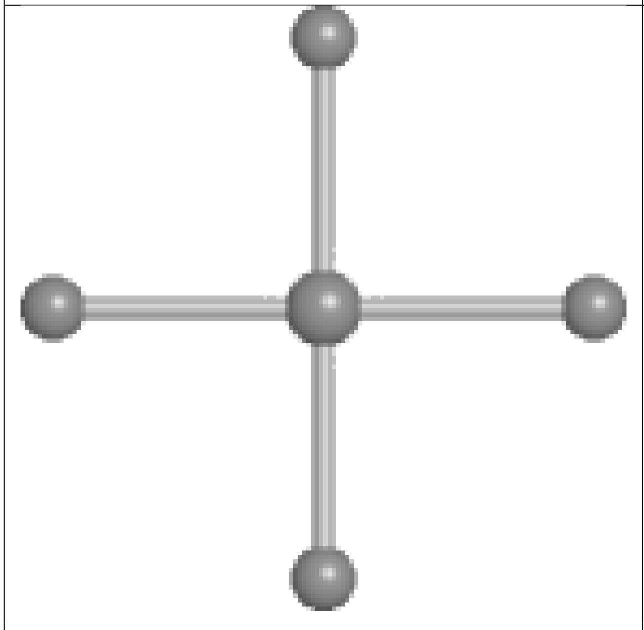
Ligand SO4 B 412



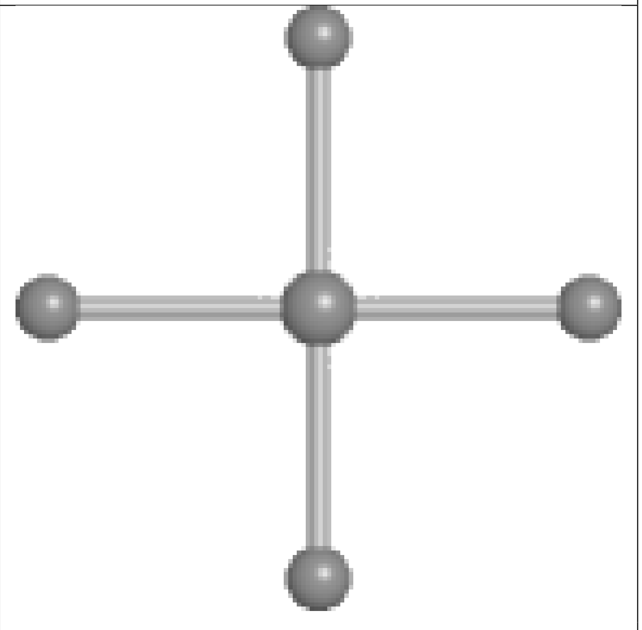
Bond lengths



Bond angles

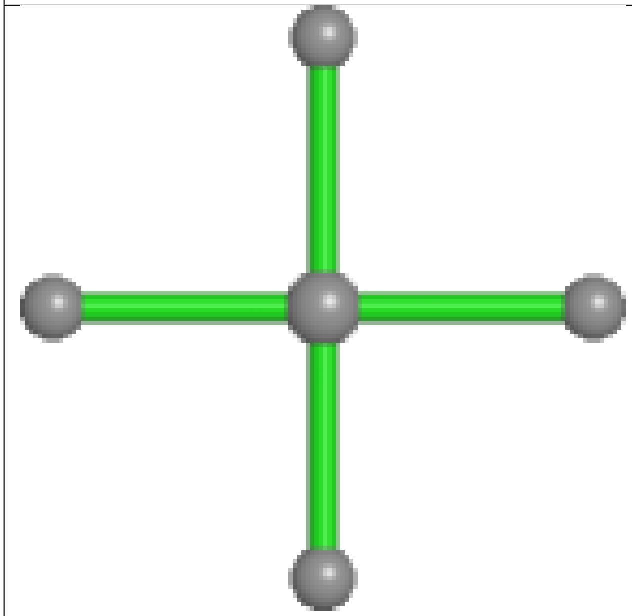


Torsions

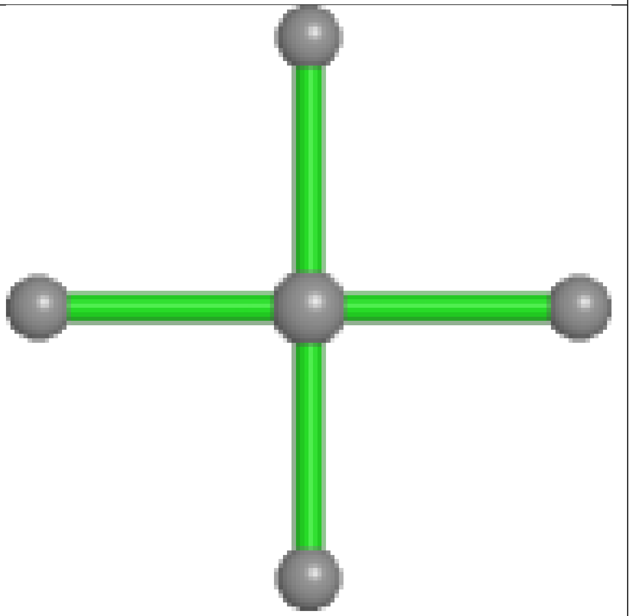


Rings

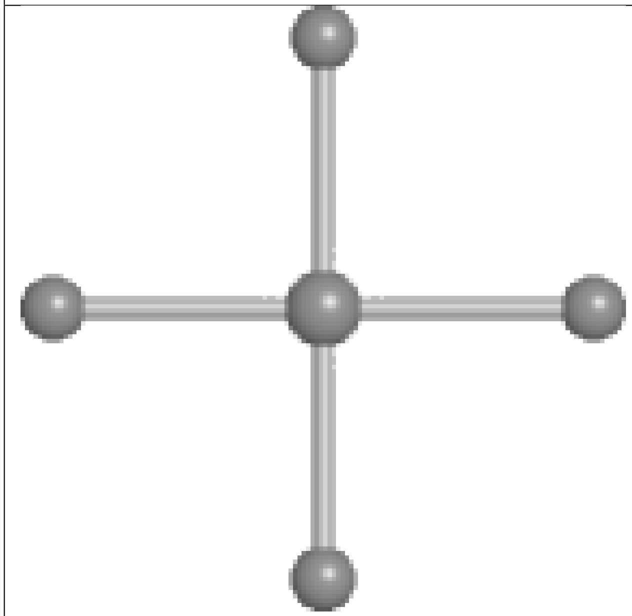
Ligand SO4 A 404



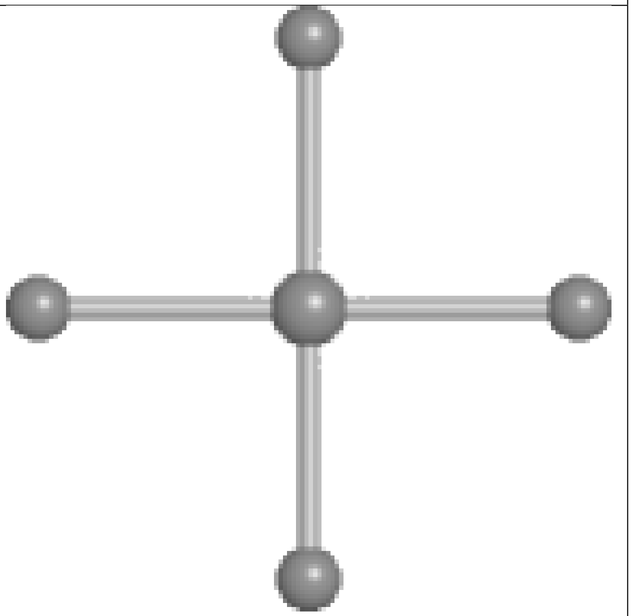
Bond lengths



Bond angles

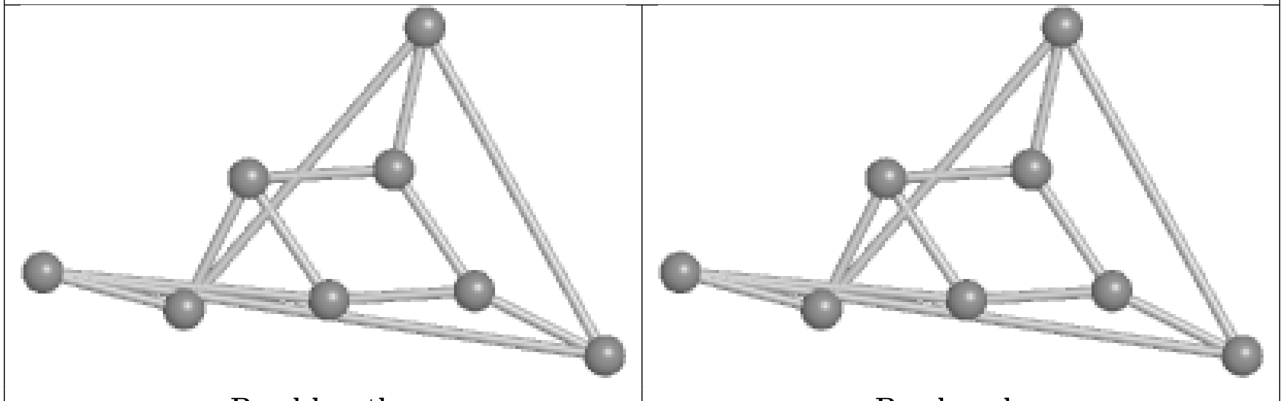


Torsions



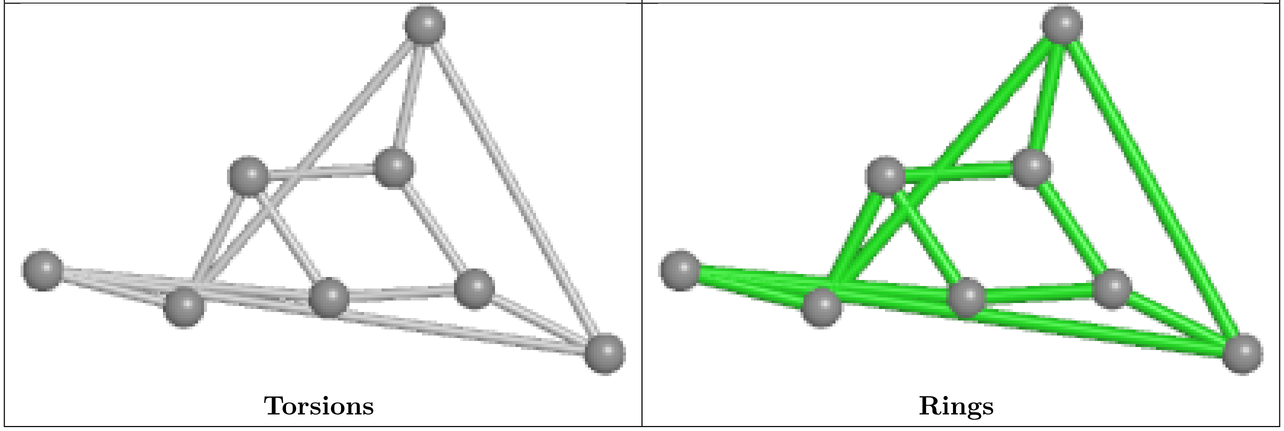
Rings

Ligand SF4 B 403



Bond lengths

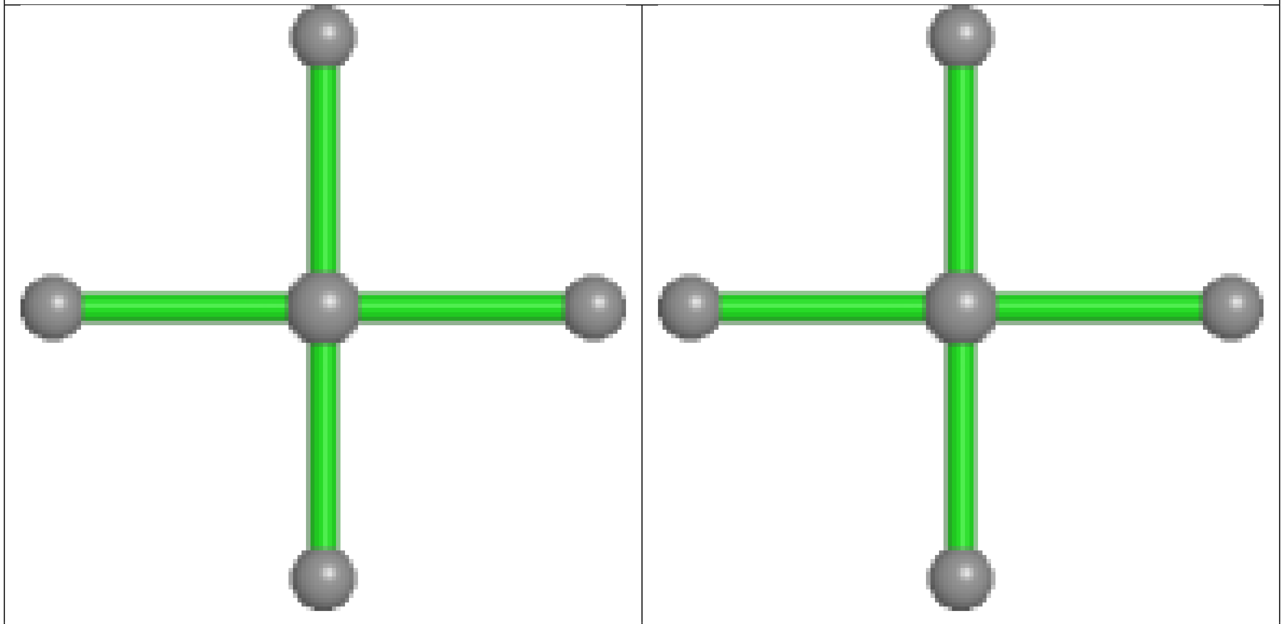
Bond angles



Torsions

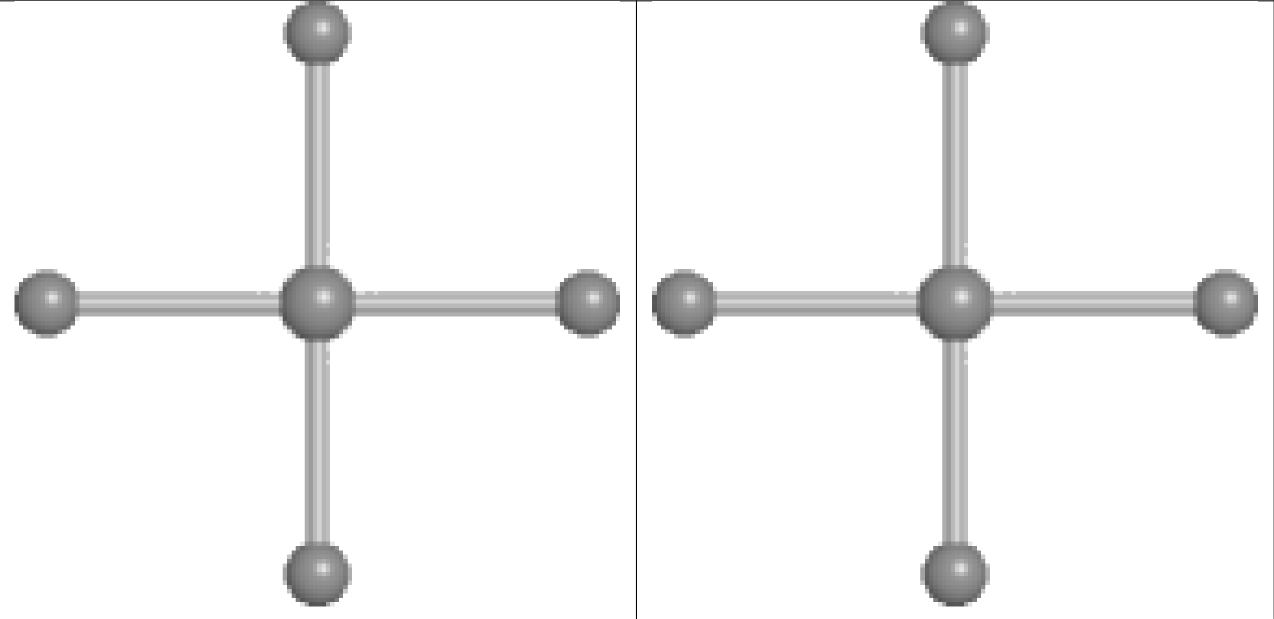
Rings

Ligand SO4 A 417



Bond lengths

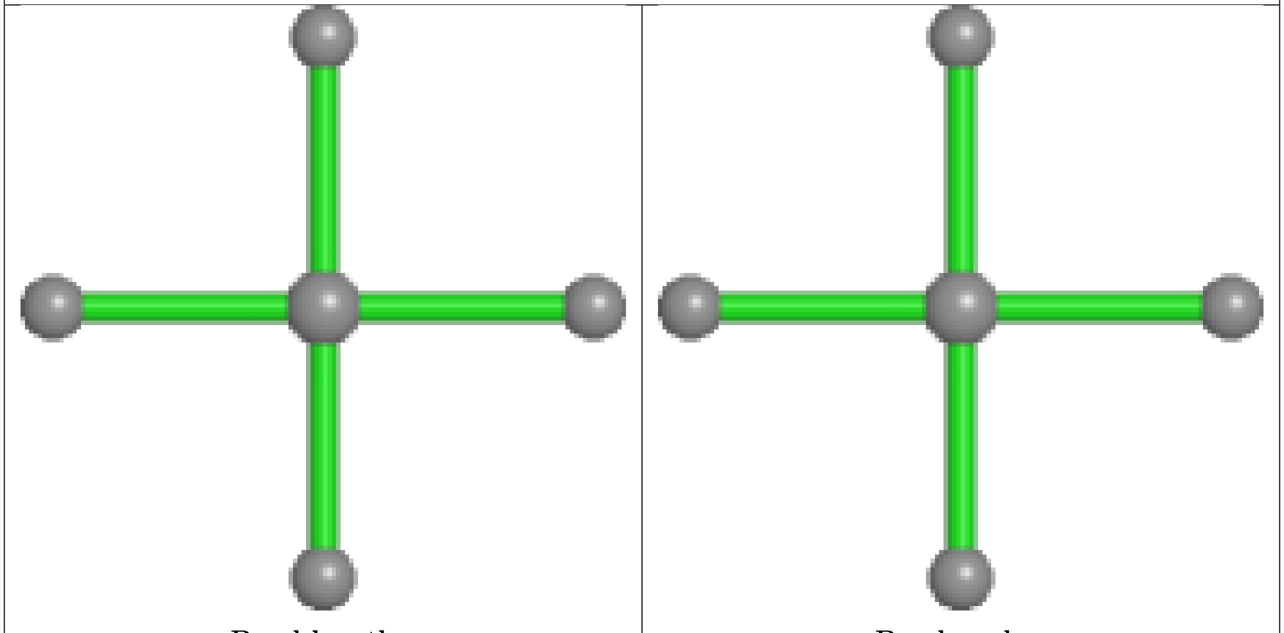
Bond angles



Torsions

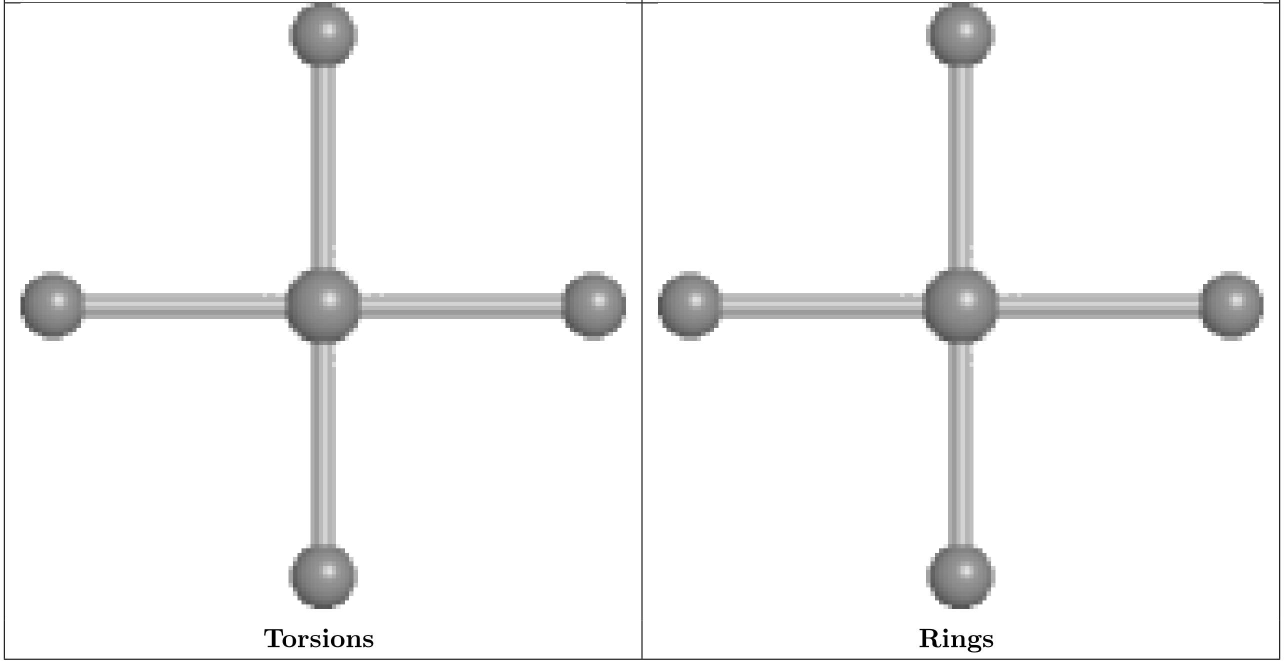
Rings

Ligand SO4 B 414



Bond lengths

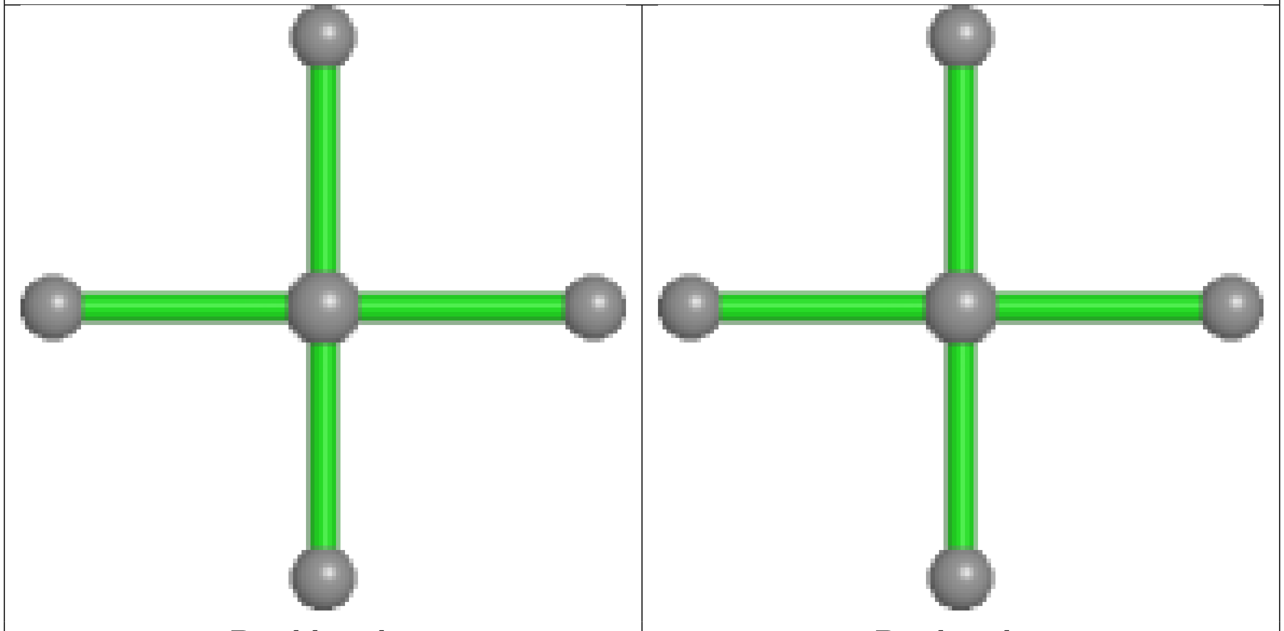
Bond angles



Torsions

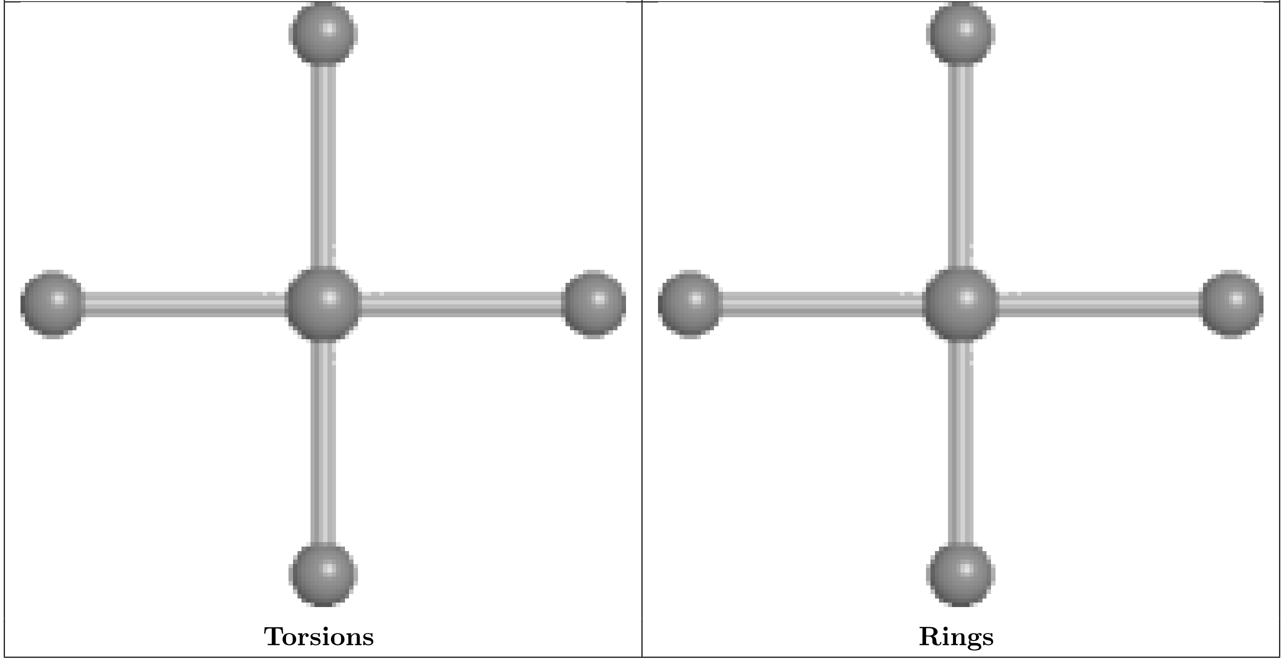
Rings

Ligand SO4 A 425



Bond lengths

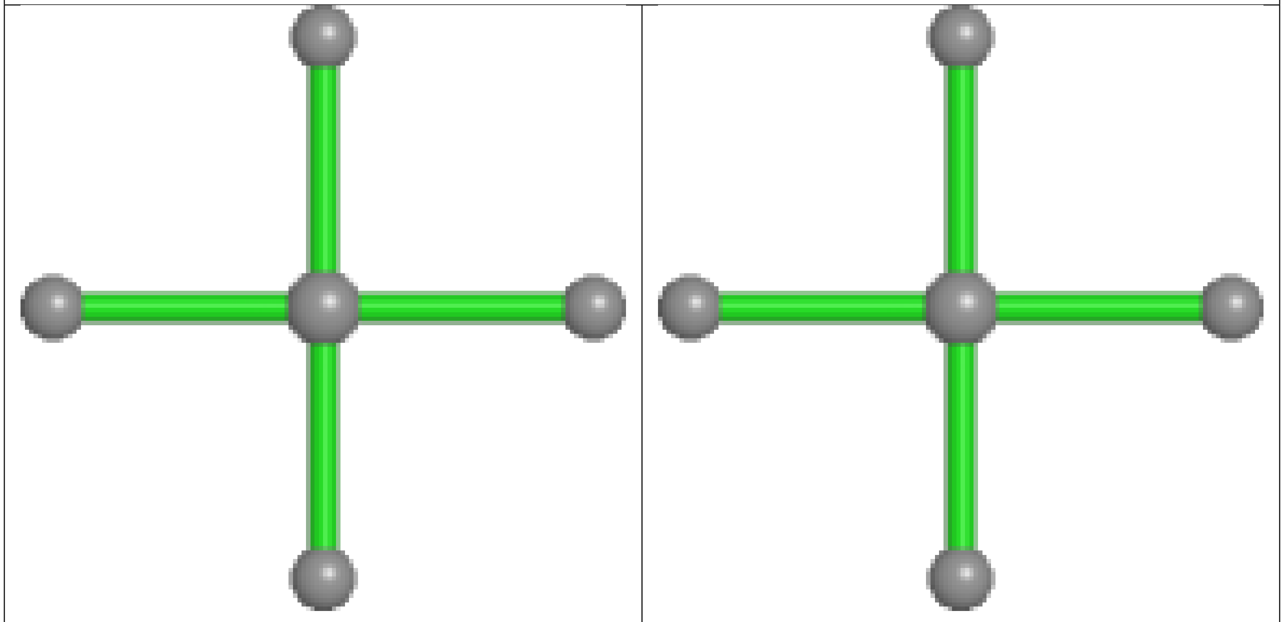
Bond angles



Torsions

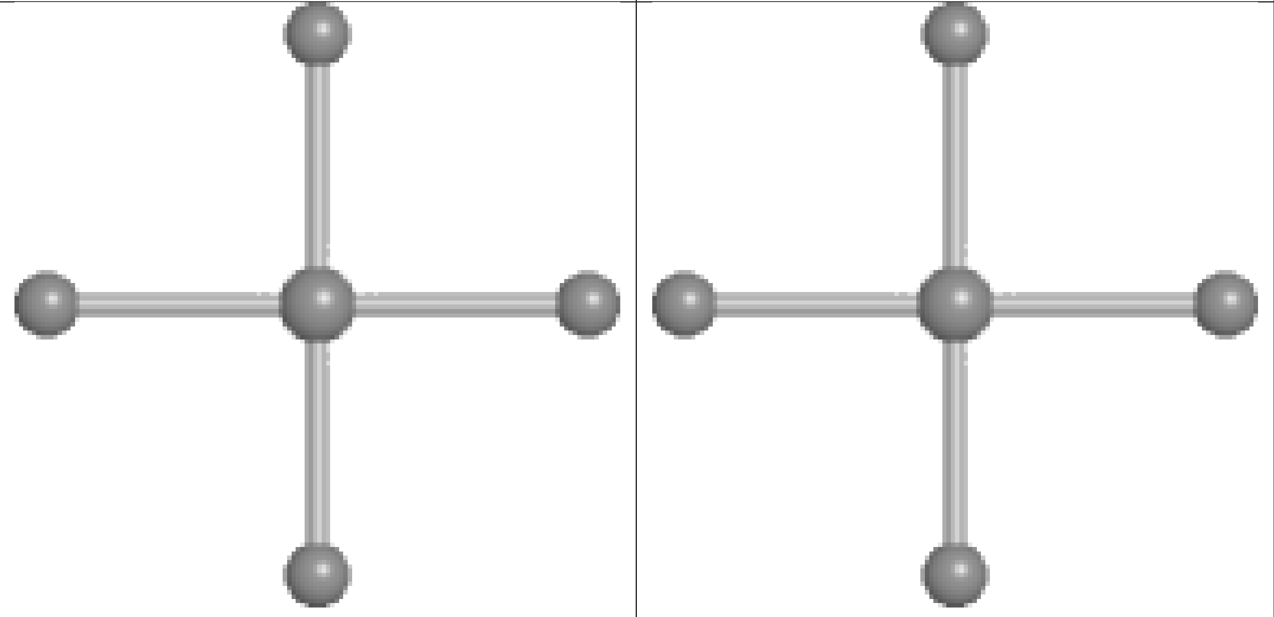
Rings

Ligand SO4 B 422



Bond lengths

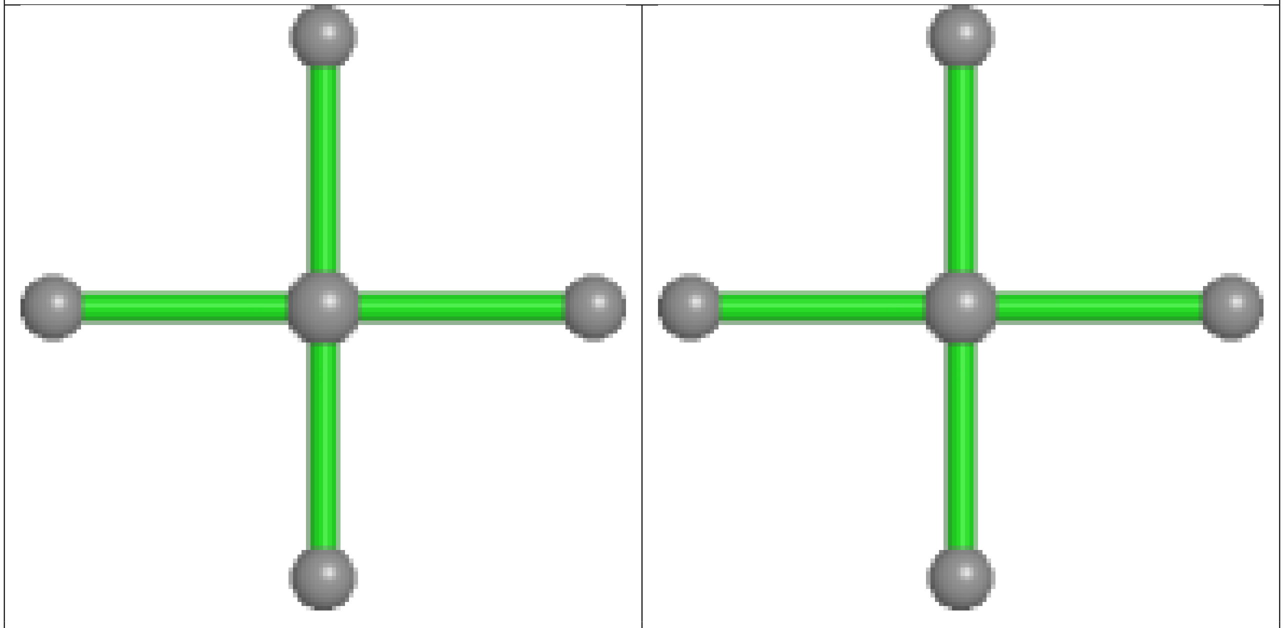
Bond angles



Torsions

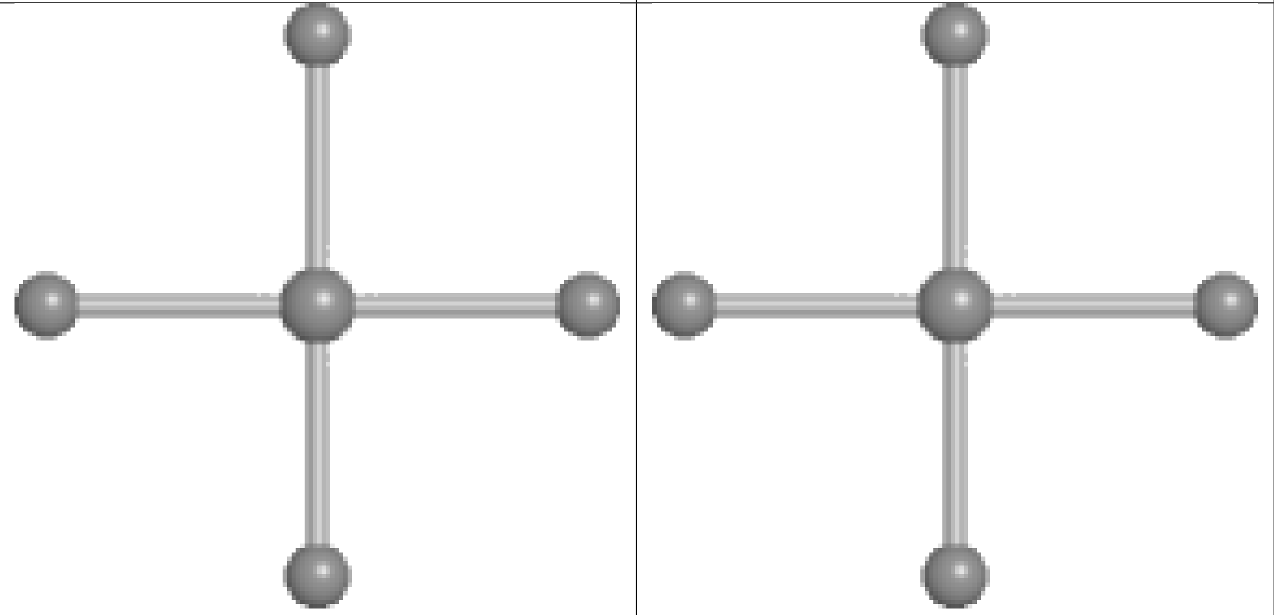
Rings

Ligand SO4 A 423



Bond lengths

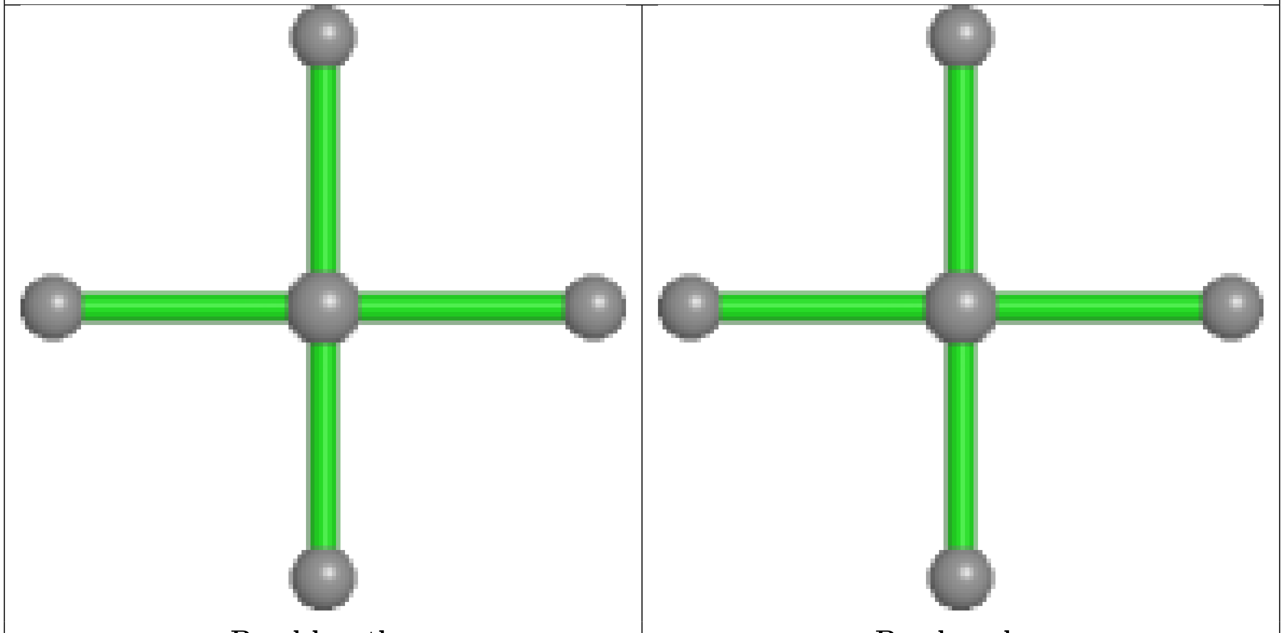
Bond angles



Torsions

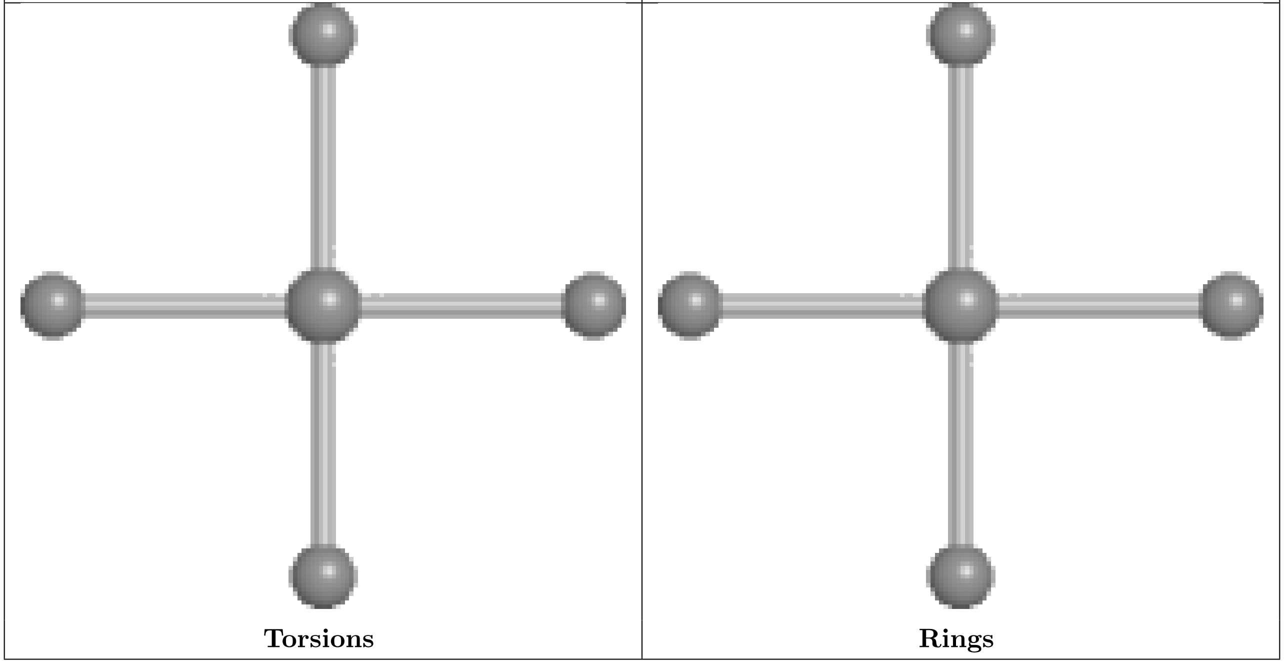
Rings

Ligand SO4 B 405



Bond lengths

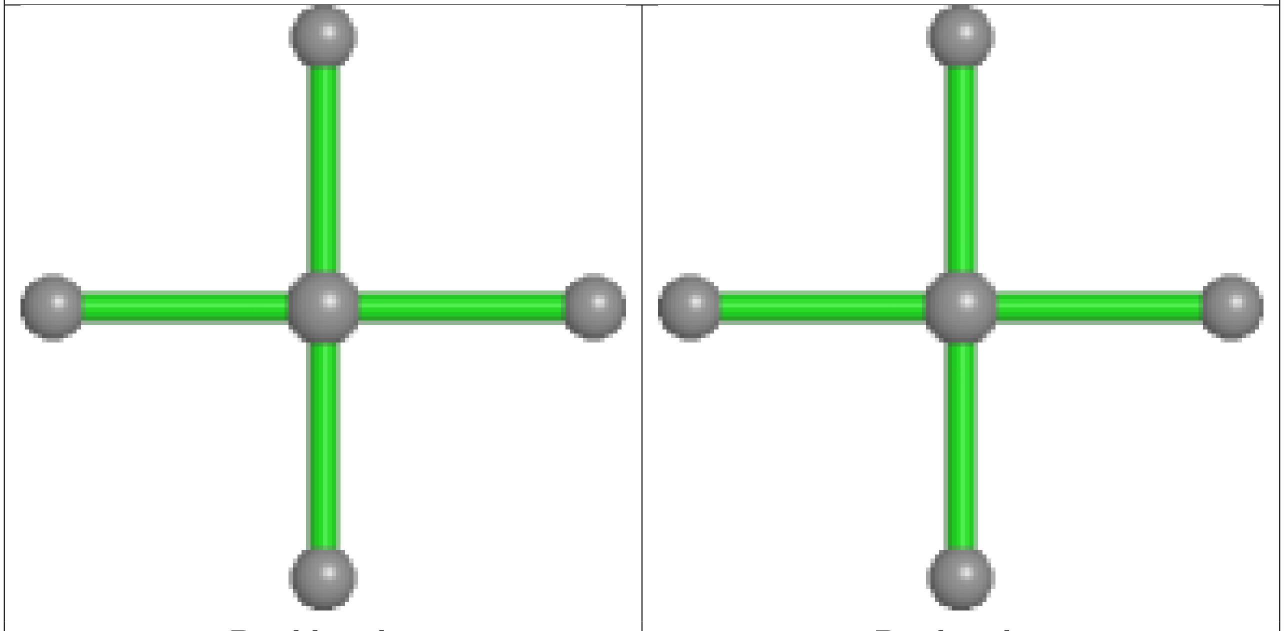
Bond angles



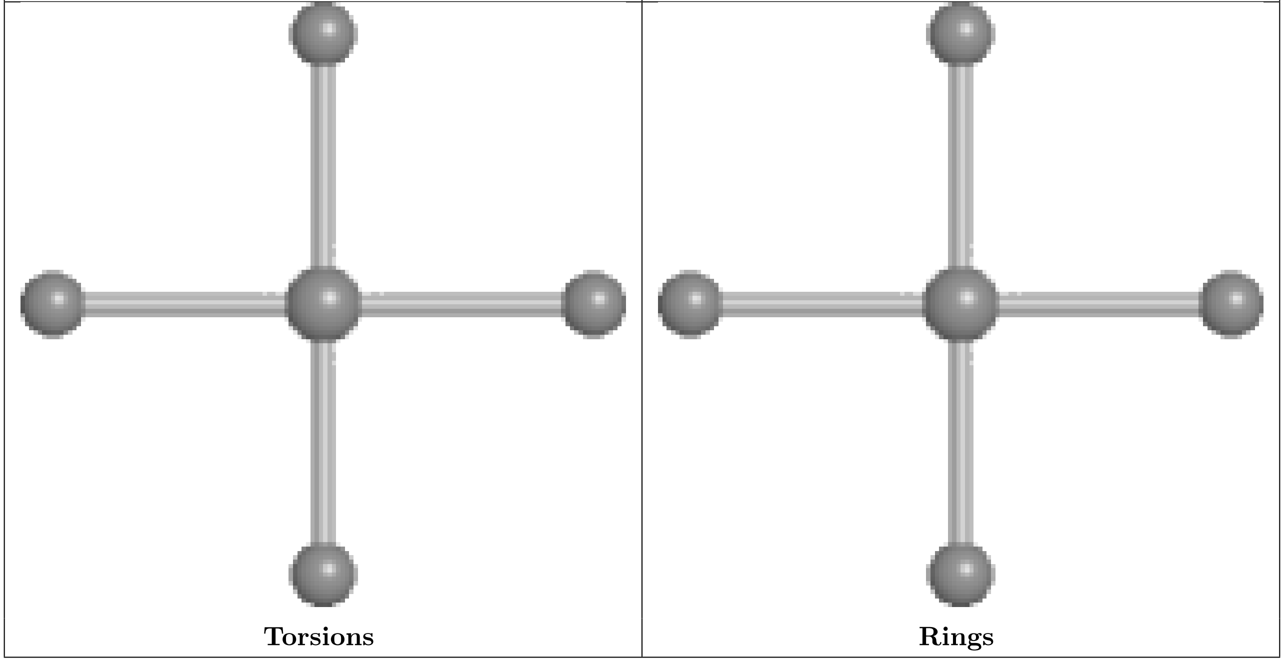
Torsions

Rings

Ligand SO4 B 419

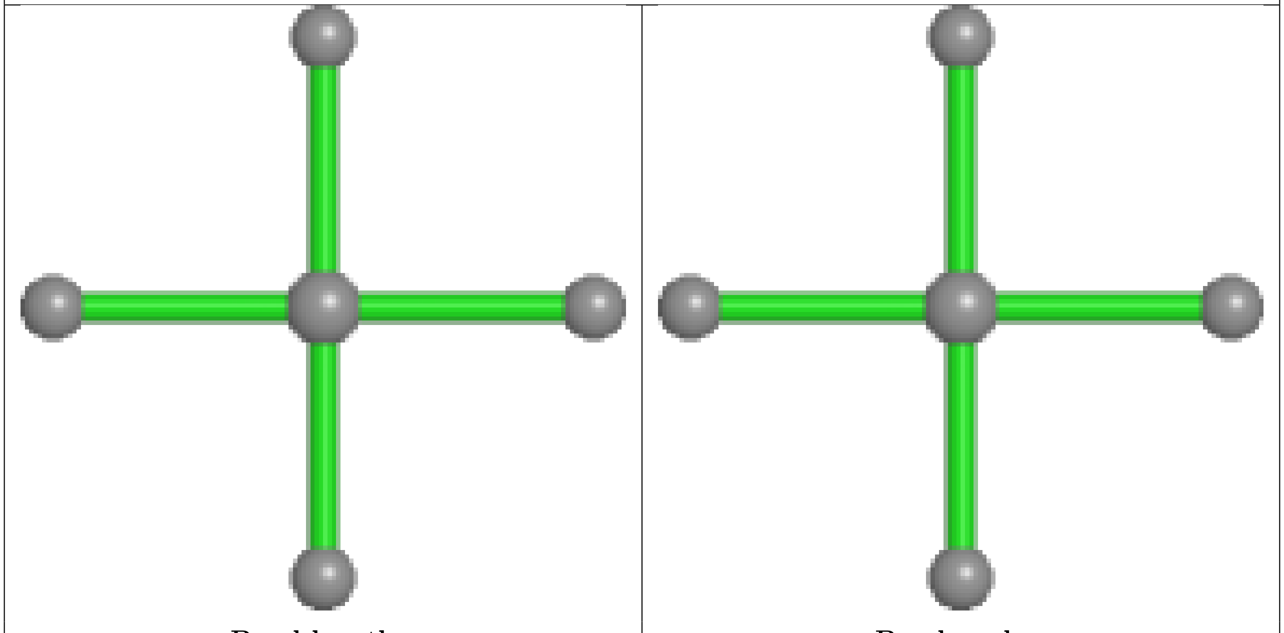


Bond lengths **Bond angles**

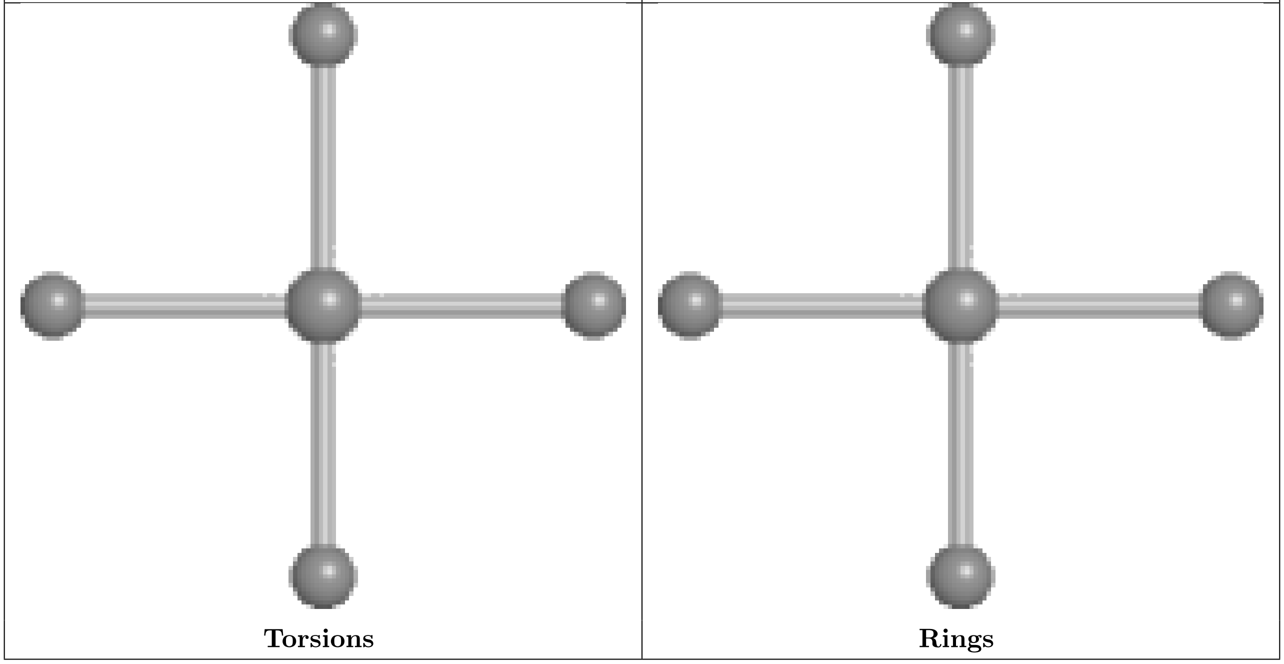


Torsions **Rings**

Ligand SO4 A 409

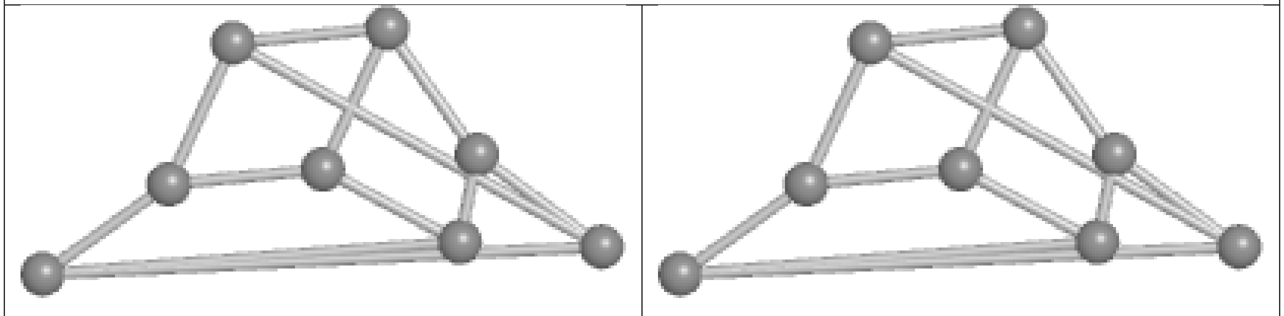


Bond lengths Bond angles



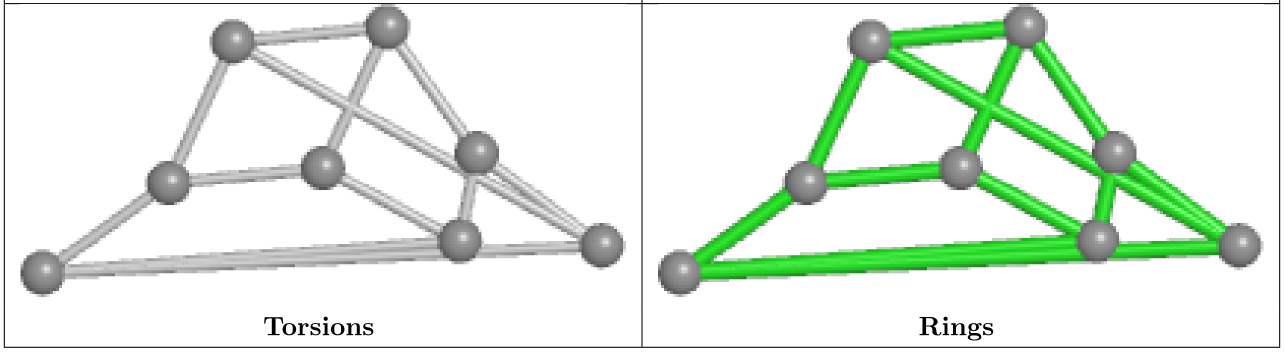
Torsions Rings

Ligand SF4 A 403



Bond lengths

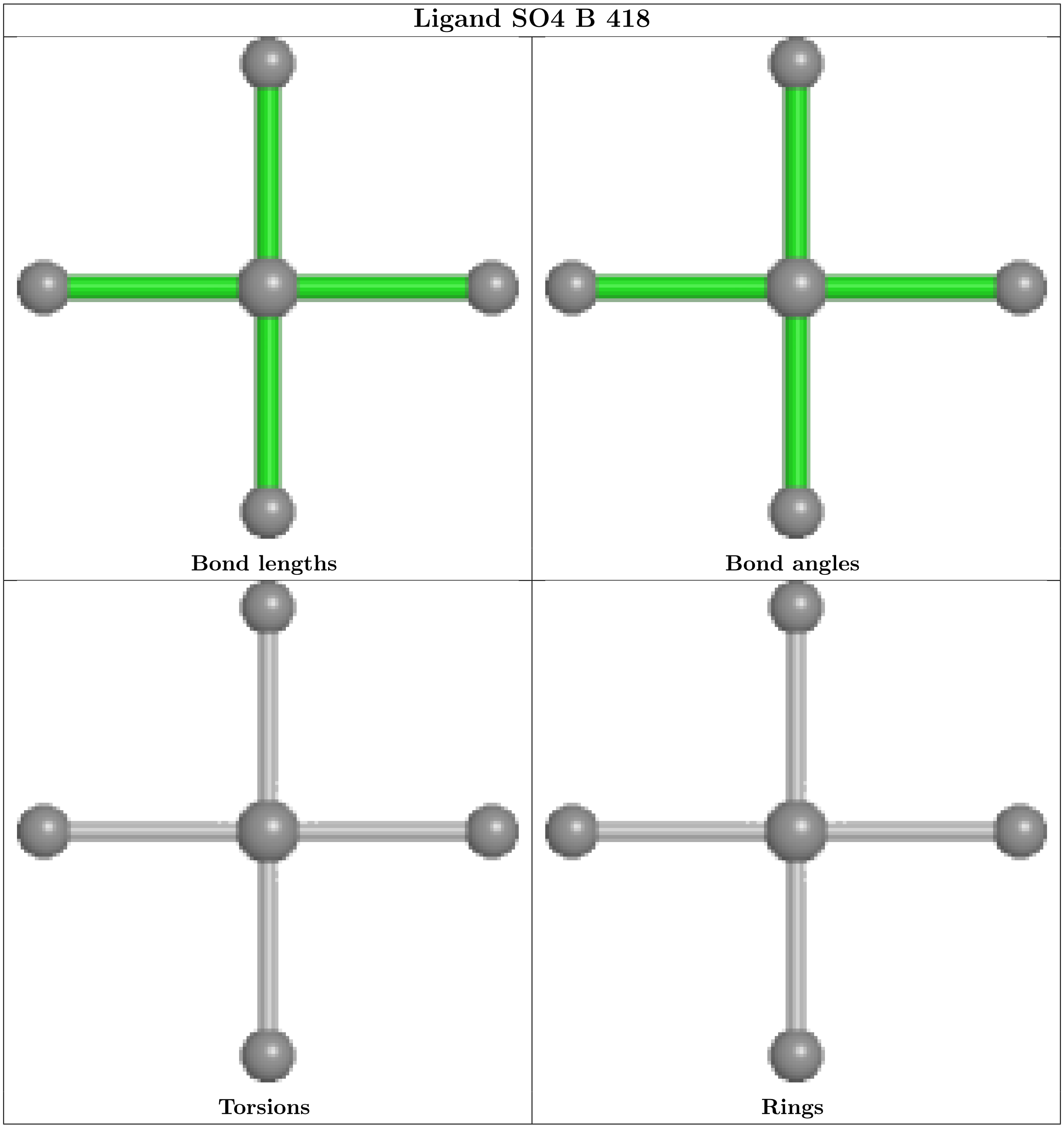
Bond angles



Torsions

Rings

Ligand SO4 B 418



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	297/308 (96%)	0.57	44 (14%)	2	1	41, 83, 193, 217	0
2	B	298/311 (95%)	0.46	36 (12%)	4	2	39, 87, 165, 220	0
All	All	595/619 (96%)	0.51	80 (13%)	3	2	39, 85, 190, 220	0

All (80) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	235	TYR	9.8
2	B	284	ILE	8.4
1	A	296	VAL	6.9
1	A	284	ILE	6.6
1	A	292	GLU	6.2
1	A	295	LYS	6.0
2	B	234	PRO	5.8
1	A	307	GLU	5.7
2	B	311	PHE	5.6
1	A	283	LYS	5.5
2	B	89	GLY	5.4
2	B	283	LYS	5.3
1	A	126	ASP	4.9
2	B	93	TYR	4.9
2	B	308	LYS	4.9
1	A	308	LYS	4.7
1	A	199	HIS	4.5
1	A	191	ALA	4.5
1	A	289	SER	4.4
2	B	233	CYS	4.3
1	A	290	ALA	4.2
1	A	299	TYR	4.1
2	B	144	PHE	3.9
2	B	307	GLU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	92	GLY	3.8
1	A	128	ILE	3.8
2	B	309	SER	3.8
1	A	291	THR	3.8
1	A	125	LEU	3.7
1	A	235	TYR	3.6
1	A	298	SER	3.6
2	B	236	SER	3.5
1	A	93	TYR	3.5
2	B	91	GLU	3.4
2	B	237	CYS	3.4
1	A	192	PHE	3.3
1	A	194	GLY	3.2
1	A	1	MET	3.2
1	A	124	ASN	3.2
1	A	196	SER	3.1
2	B	306	LEU	3.0
2	B	138	THR	2.8
2	B	199	HIS	2.8
2	B	95	THR	2.7
2	B	90	ILE	2.7
2	B	239	SER	2.7
1	A	274	GLU	2.7
1	A	302	ASN	2.6
1	A	92	GLY	2.6
1	A	237	CYS	2.6
1	A	268	ARG	2.5
2	B	124	ASN	2.5
1	A	138	THR	2.5
1	A	90	ILE	2.5
1	A	222	GLU	2.5
1	A	275	LEU	2.4
2	B	305	ILE	2.4
2	B	188	LYS	2.4
1	A	254	ASN	2.4
2	B	288	LEU	2.4
2	B	285	CYS	2.4
2	B	123	THR	2.4
2	B	99	ASP	2.3
2	B	94	ARG	2.3
1	A	270	LEU	2.3
2	B	191	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	197	LEU	2.3
1	A	144	PHE	2.2
1	A	91	GLU	2.2
1	A	100	ALA	2.2
2	B	229	HIS	2.2
1	A	94	ARG	2.2
2	B	293	VAL	2.2
1	A	186	ASP	2.2
1	A	127	GLU	2.2
1	A	89	GLY	2.1
1	A	99	ASP	2.1
1	A	88	GLU	2.1
2	B	299	TYR	2.1
2	B	280	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	B	420	5/5	0.41	0.65	248,248,248,248	0
5	SO4	B	412	5/5	0.47	0.36	227,227,227,227	0
5	SO4	A	421	5/5	0.52	0.41	194,194,194,195	0
5	SO4	A	422	5/5	0.55	0.54	193,193,193,194	0
5	SO4	B	411	5/5	0.55	0.46	241,241,241,241	0
5	SO4	B	424	5/5	0.58	0.59	248,248,248,249	0
5	SO4	A	424	5/5	0.60	0.48	190,190,191,191	0
5	SO4	A	419	5/5	0.63	0.23	195,195,195,195	0
5	SO4	A	423	5/5	0.65	0.51	221,221,221,221	0

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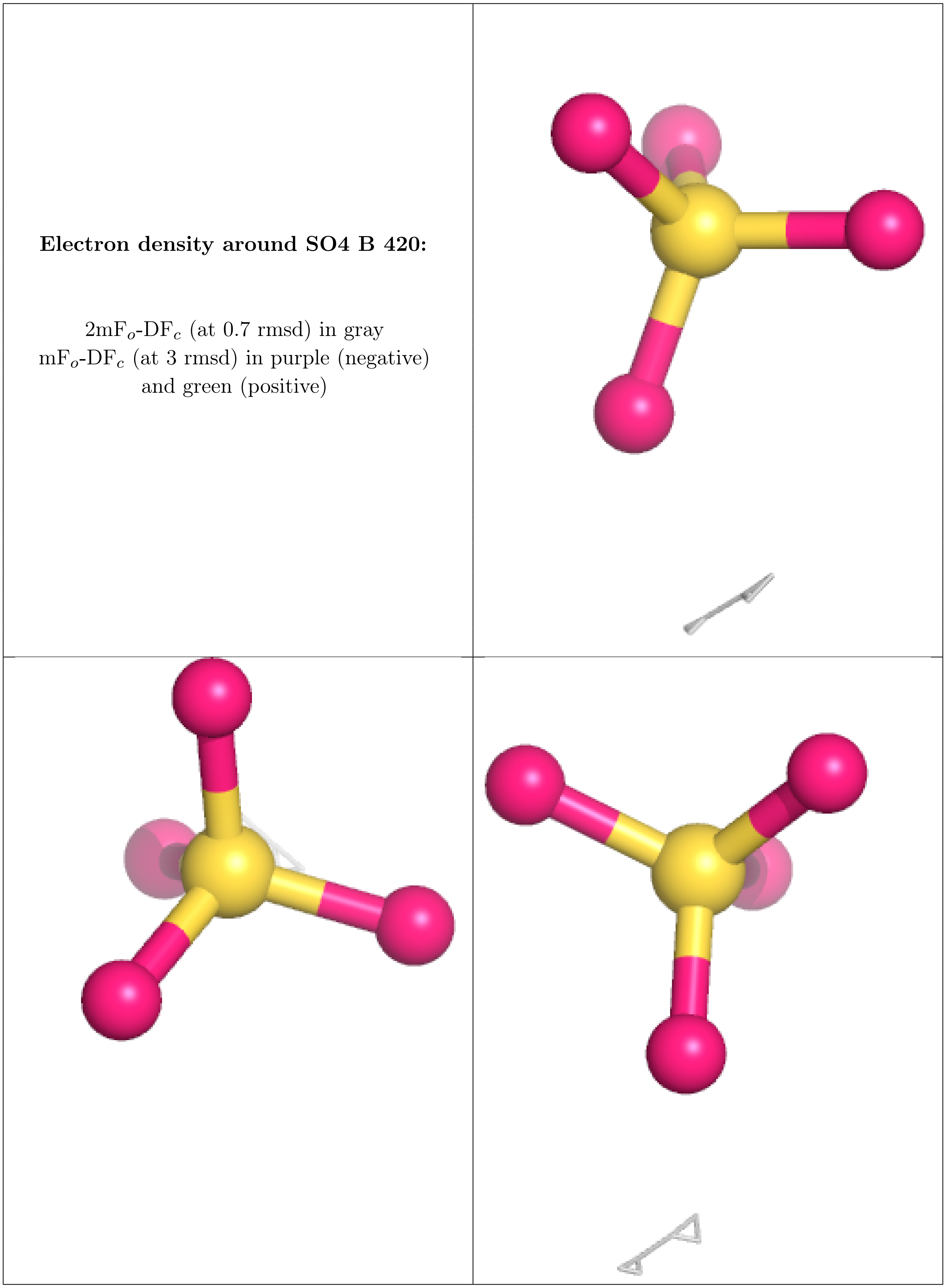
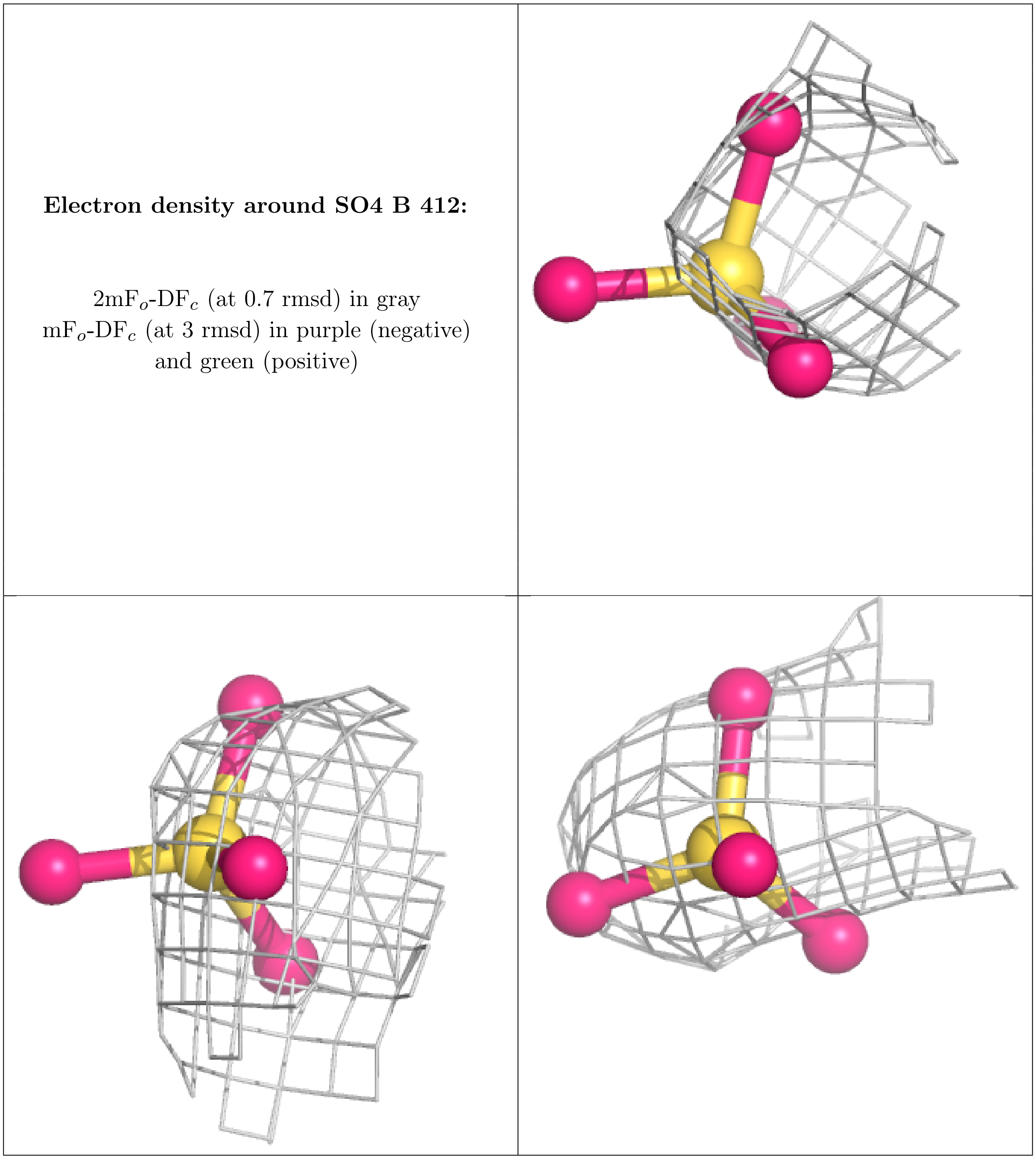
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\AA^2$)	Q<0.9
5	SO4	B	419	5/5	0.65	0.24	169,170,170,170	0
5	SO4	A	407	5/5	0.66	0.36	186,186,186,186	0
5	SO4	A	415	5/5	0.70	0.76	204,204,204,204	0
5	SO4	A	414	5/5	0.71	0.27	179,180,180,180	0
5	SO4	B	409	5/5	0.72	0.25	160,160,160,161	0
5	SO4	B	416	5/5	0.74	0.20	180,181,181,181	0
5	SO4	B	417	5/5	0.75	0.41	194,194,194,194	0
5	SO4	B	415	5/5	0.76	0.33	179,179,180,180	0
5	SO4	A	420	5/5	0.76	0.15	198,198,198,198	0
5	SO4	A	409	5/5	0.78	0.21	208,209,209,209	0
5	SO4	A	406	5/5	0.78	0.32	153,154,154,154	0
5	SO4	B	425	5/5	0.78	0.36	189,189,189,189	0
5	SO4	A	418	5/5	0.79	0.32	179,179,179,180	0
5	SO4	B	413	5/5	0.82	0.53	151,151,151,151	0
5	SO4	A	417	5/5	0.82	0.25	180,180,180,181	0
5	SO4	B	418	5/5	0.84	0.25	168,168,168,168	0
5	SO4	B	421	5/5	0.85	0.44	222,222,222,222	0
5	SO4	B	422	5/5	0.86	0.27	187,187,187,187	0
5	SO4	B	423	5/5	0.86	0.67	195,195,196,196	0
5	SO4	A	405	5/5	0.87	0.29	151,151,151,151	5
5	SO4	A	410	5/5	0.88	0.22	148,148,149,149	0
5	SO4	A	408	5/5	0.88	0.26	163,163,163,164	0
5	SO4	B	410	5/5	0.89	0.23	189,189,189,189	0
5	SO4	A	411	5/5	0.90	0.26	173,173,173,173	0
5	SO4	B	404	5/5	0.90	0.31	148,148,148,148	0
5	SO4	B	414	5/5	0.91	0.13	164,164,164,165	0
5	SO4	A	416	5/5	0.91	0.10	143,143,143,143	0
3	ZN	B	402	1/1	0.91	0.06	165,165,165,165	0
5	SO4	A	412	5/5	0.91	0.17	138,138,139,139	0
5	SO4	B	426	5/5	0.92	0.23	171,172,172,172	0
5	SO4	A	425	5/5	0.93	0.36	138,138,138,139	0
5	SO4	A	404	5/5	0.93	0.26	117,117,117,118	0
5	SO4	A	413	5/5	0.94	0.32	156,156,156,156	0
5	SO4	B	406	5/5	0.94	0.15	141,141,141,141	0
5	SO4	B	407	5/5	0.94	0.14	149,149,149,149	5
5	SO4	B	408	5/5	0.95	0.16	127,127,128,128	0
5	SO4	B	405	5/5	0.96	0.22	97,99,99,99	0
3	ZN	A	402	1/1	0.96	0.09	125,125,125,125	0
4	SF4	B	403	8/8	0.97	0.09	110,110,111,112	8
4	SF4	A	403	8/8	0.98	0.08	103,103,103,104	8
3	ZN	A	401	1/1	1.00	0.12	63,63,63,63	0
3	ZN	B	401	1/1	1.00	0.11	63,63,63,63	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 B 420:

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

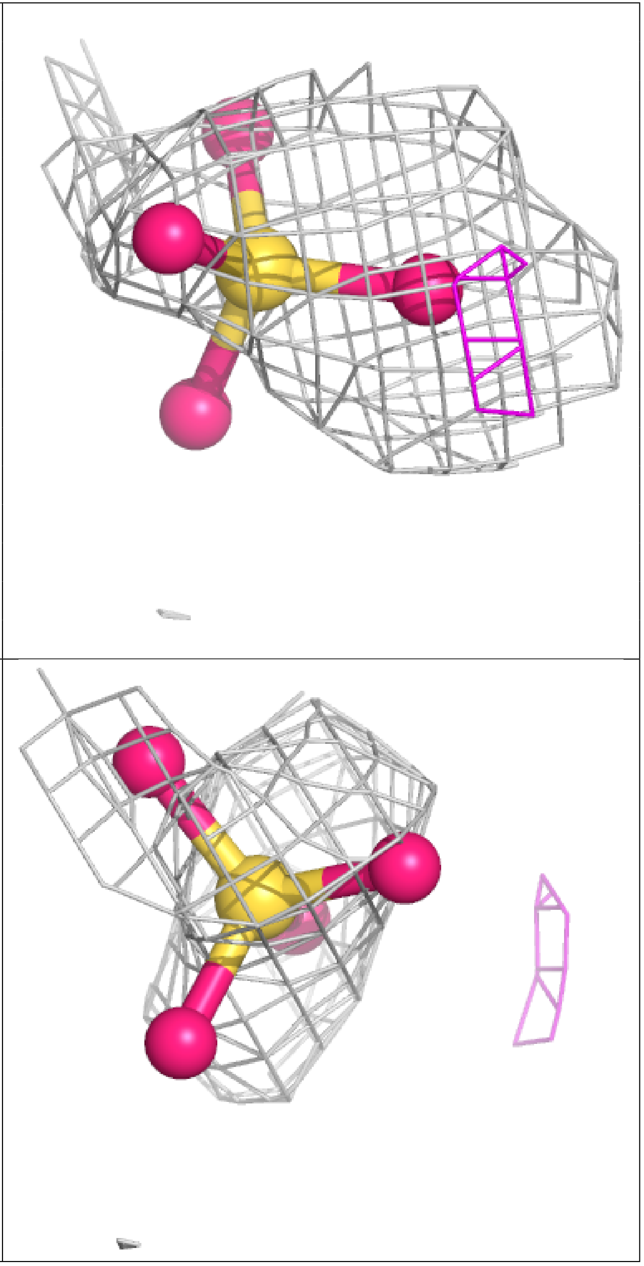


Electron density around SO4 B 412:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

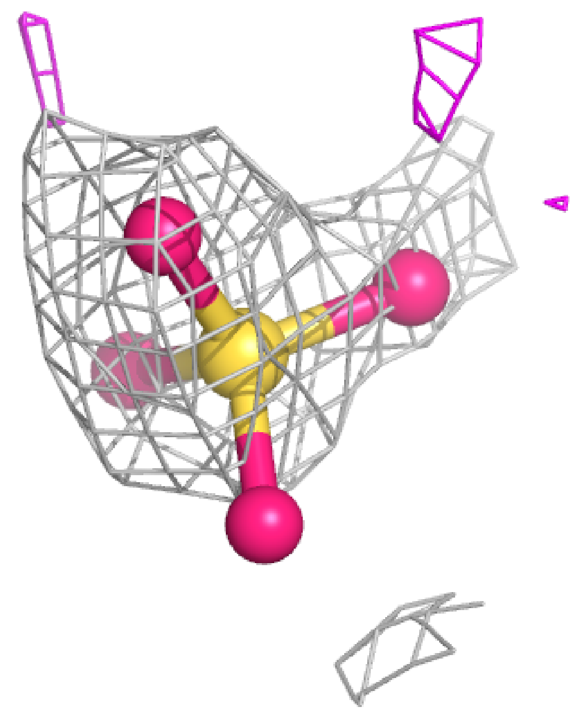
Electron density around SO4 A 421:

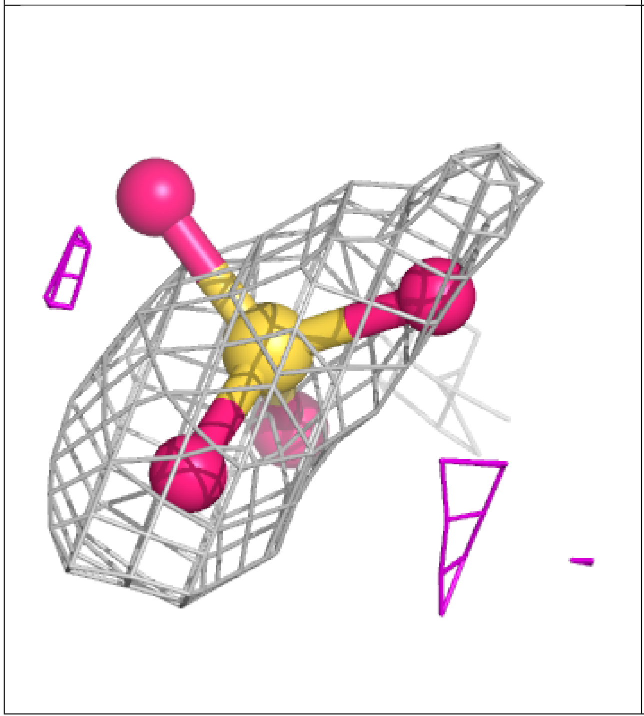
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

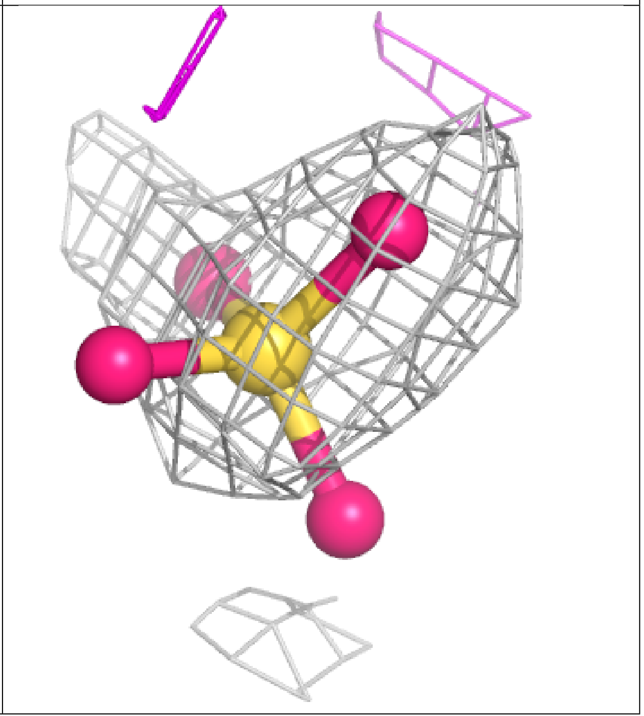


Electron density around SO4 A 422:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





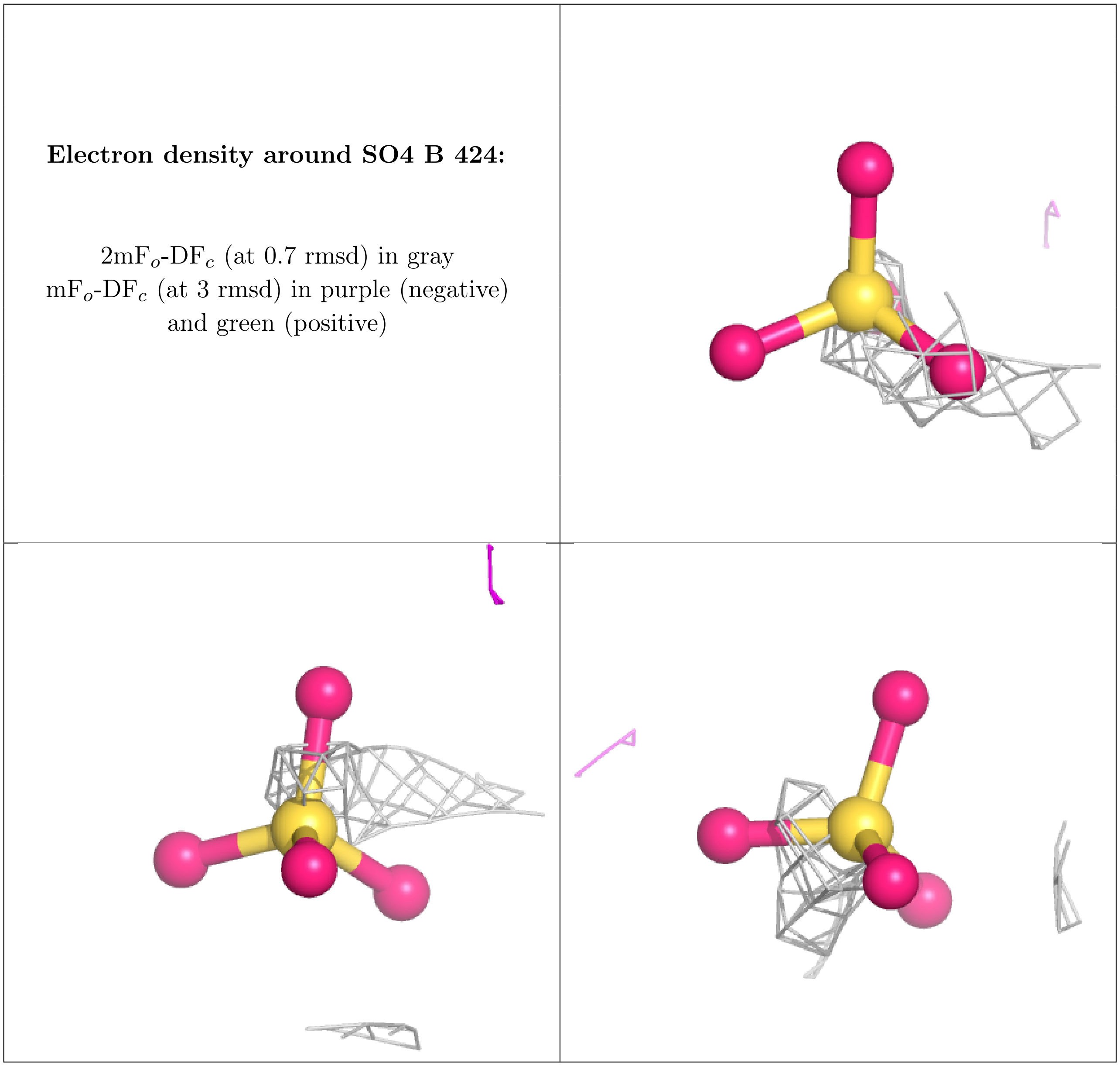


Electron density around SO4 B 411:

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 B 424:

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 424:

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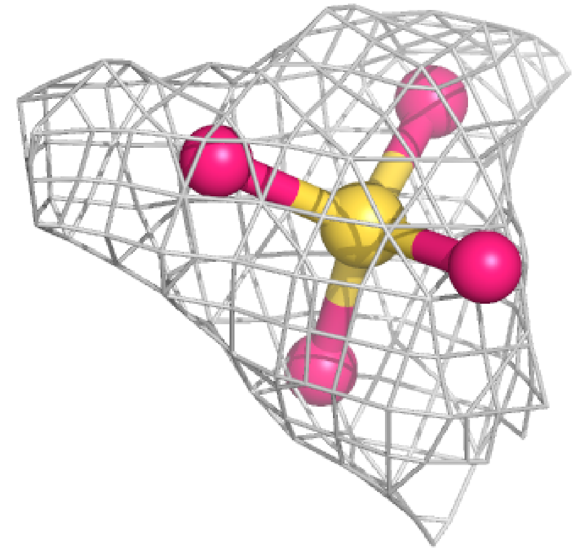
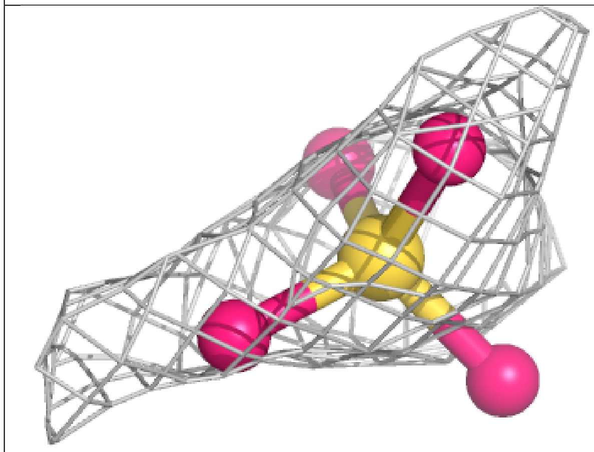
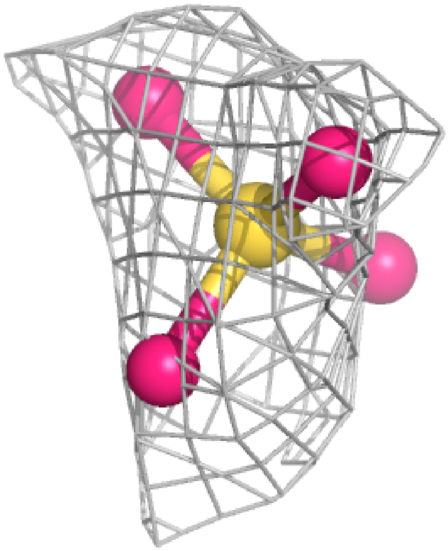
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

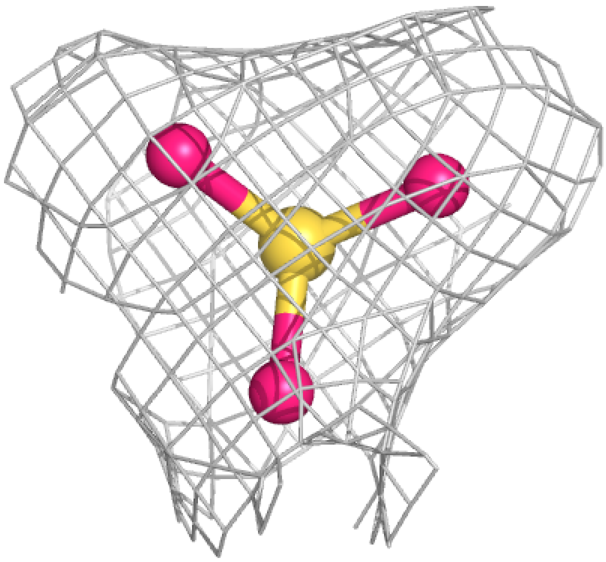


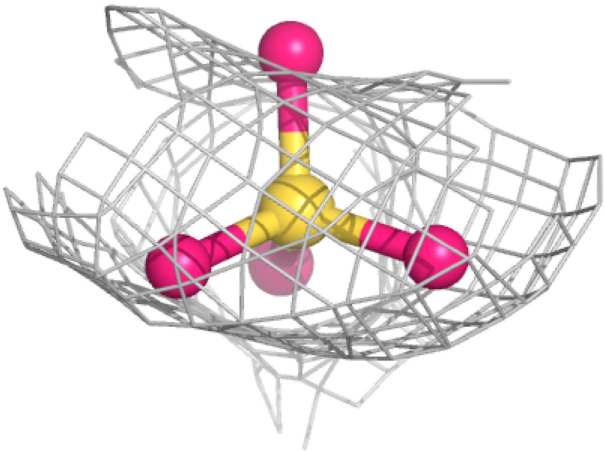


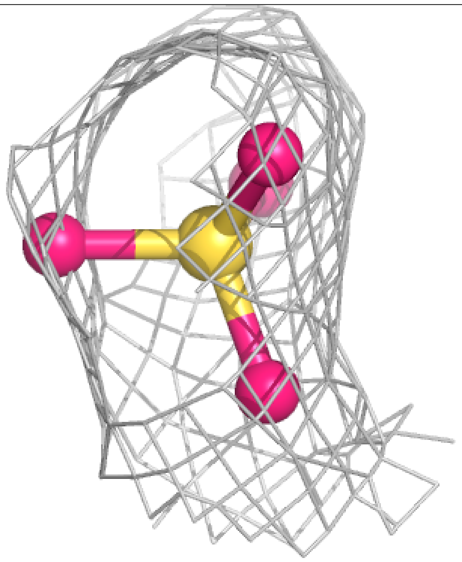


Electron density around SO4 A 419:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

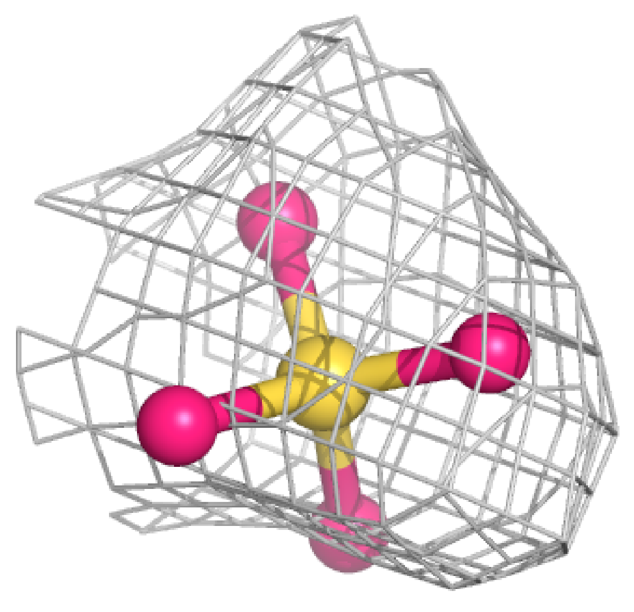


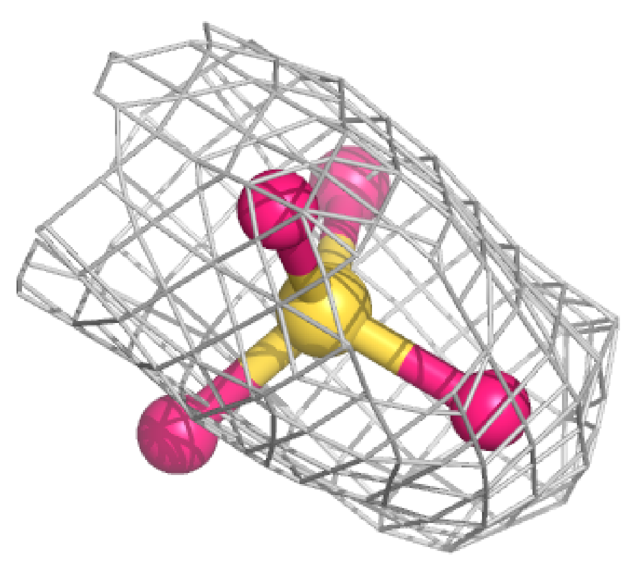


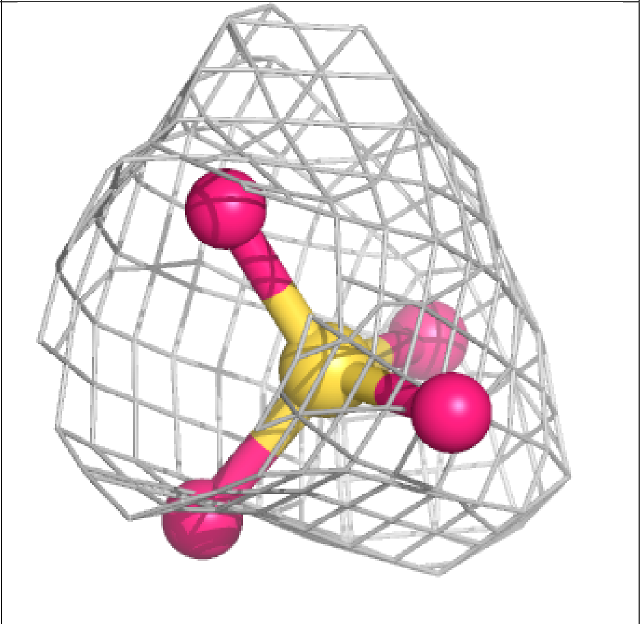


Electron density around SO4 A 423:

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

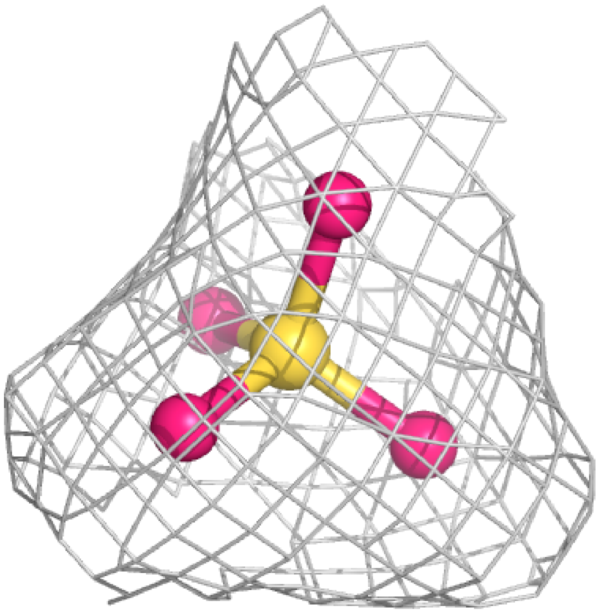


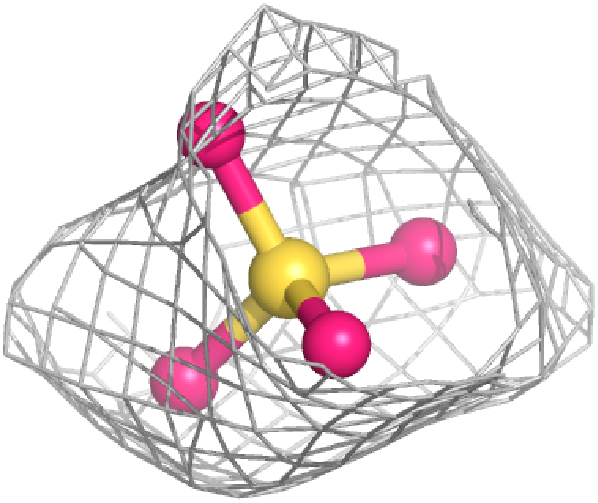


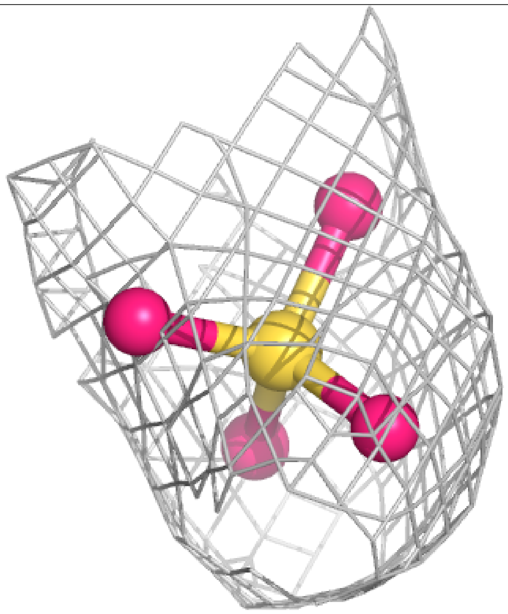


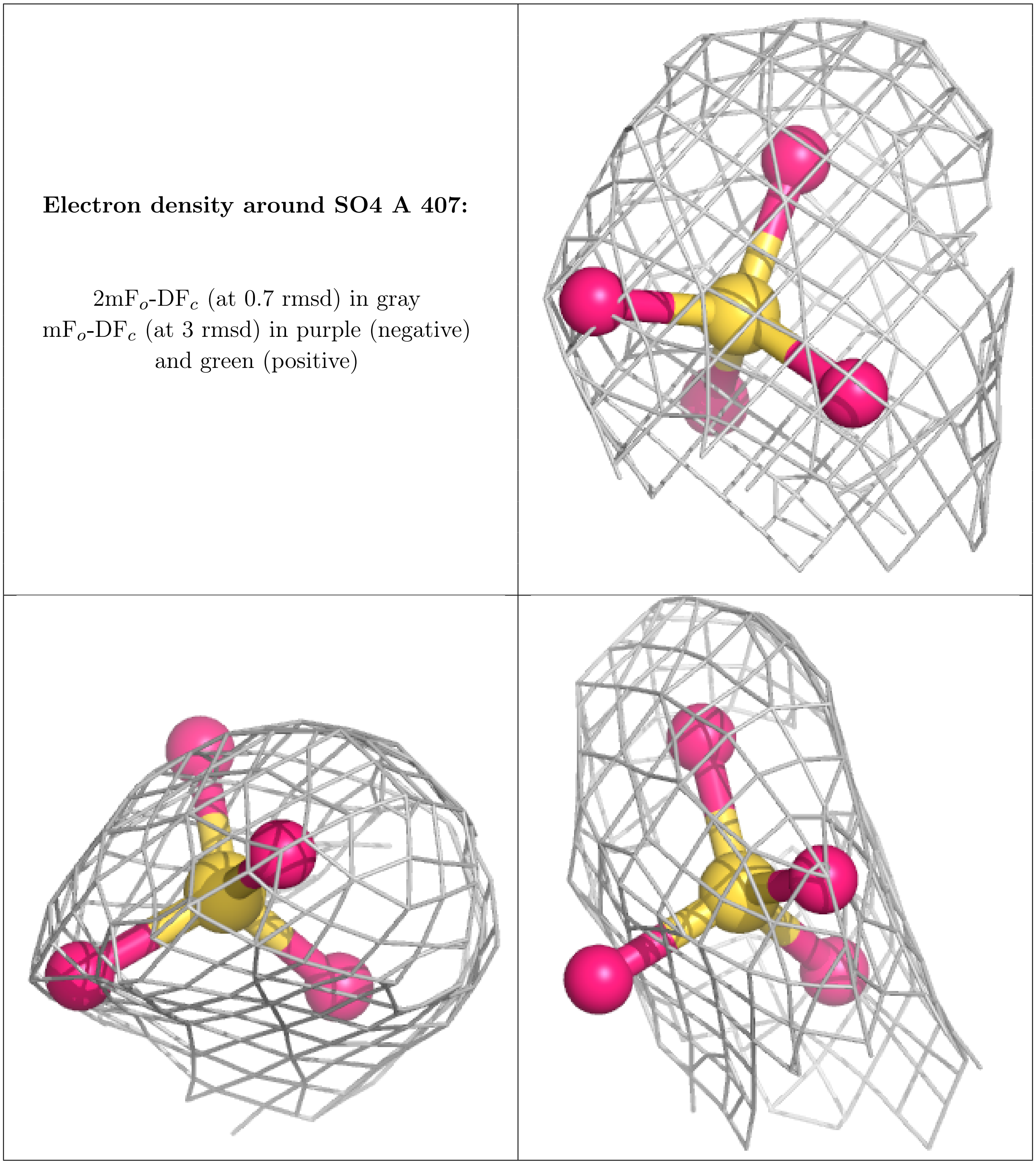
Electron density around SO4 B 419:

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



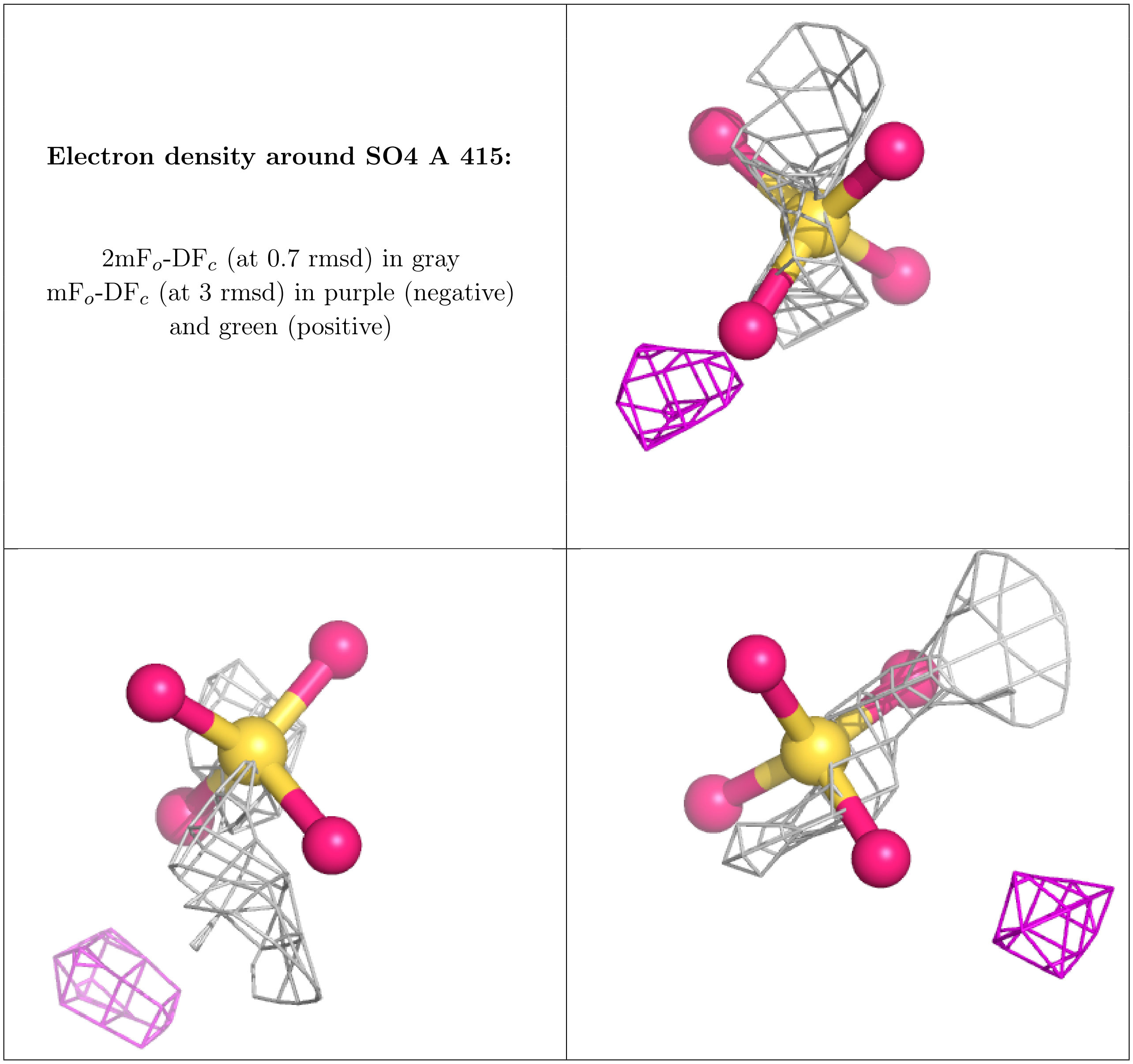






Electron density around SO4 A 407:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

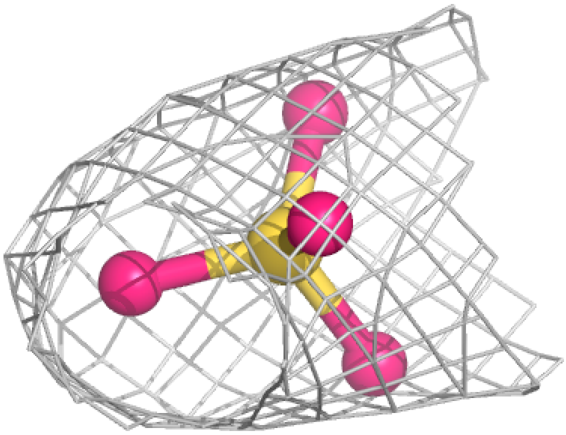


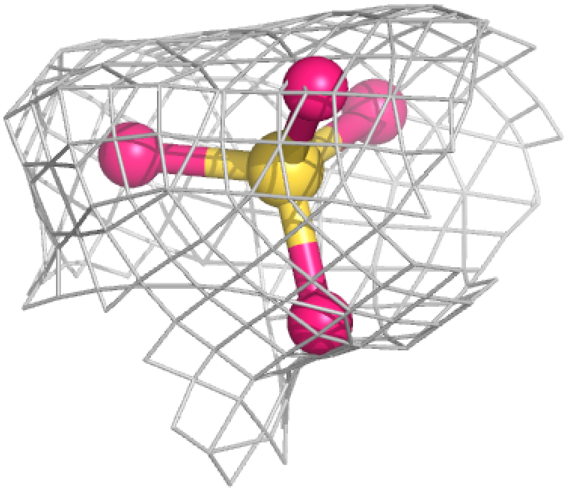
Electron density around SO4 A 415:

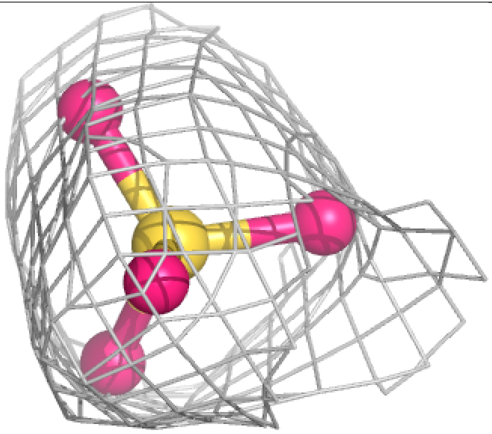
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 A 414:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

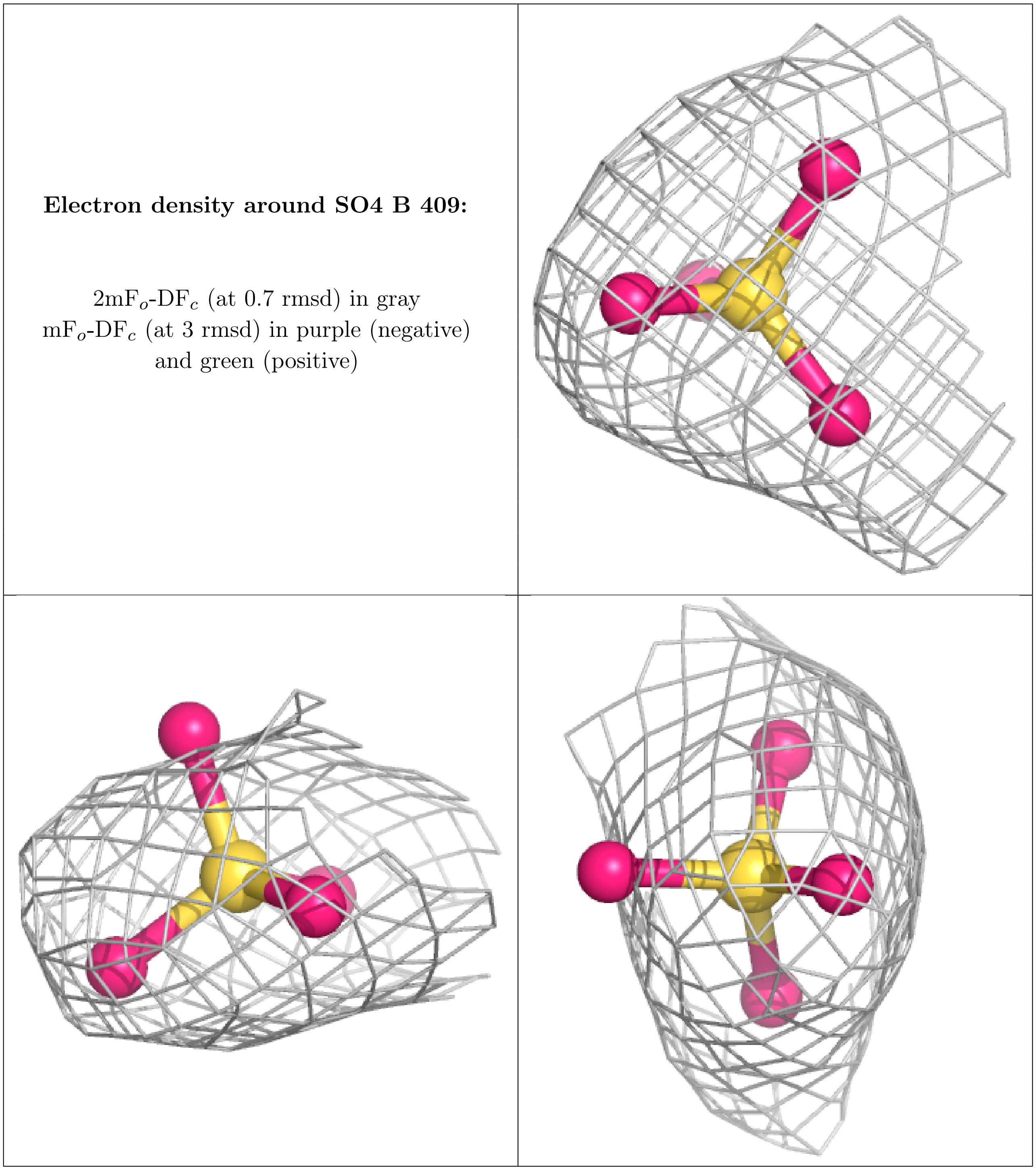






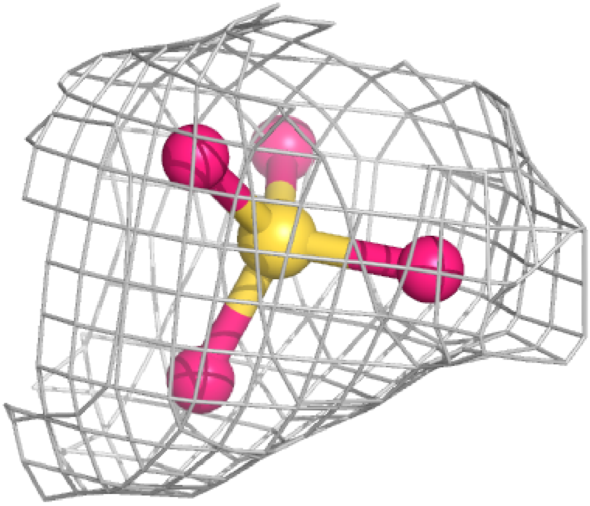
Electron density around SO4 B 409:

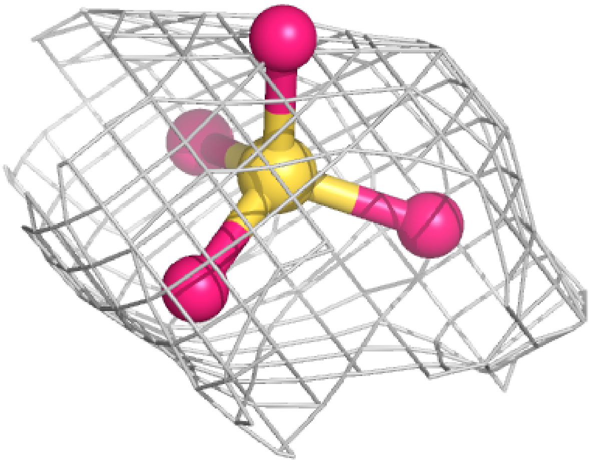
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

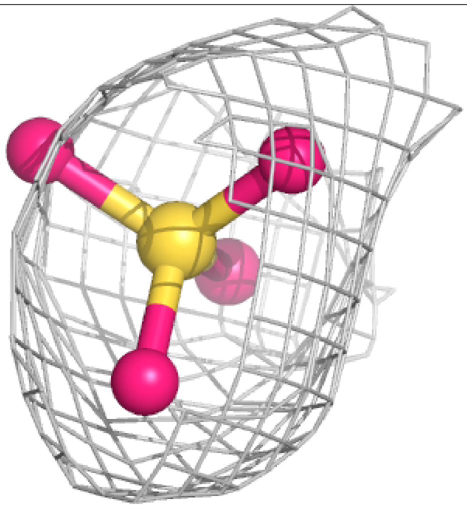


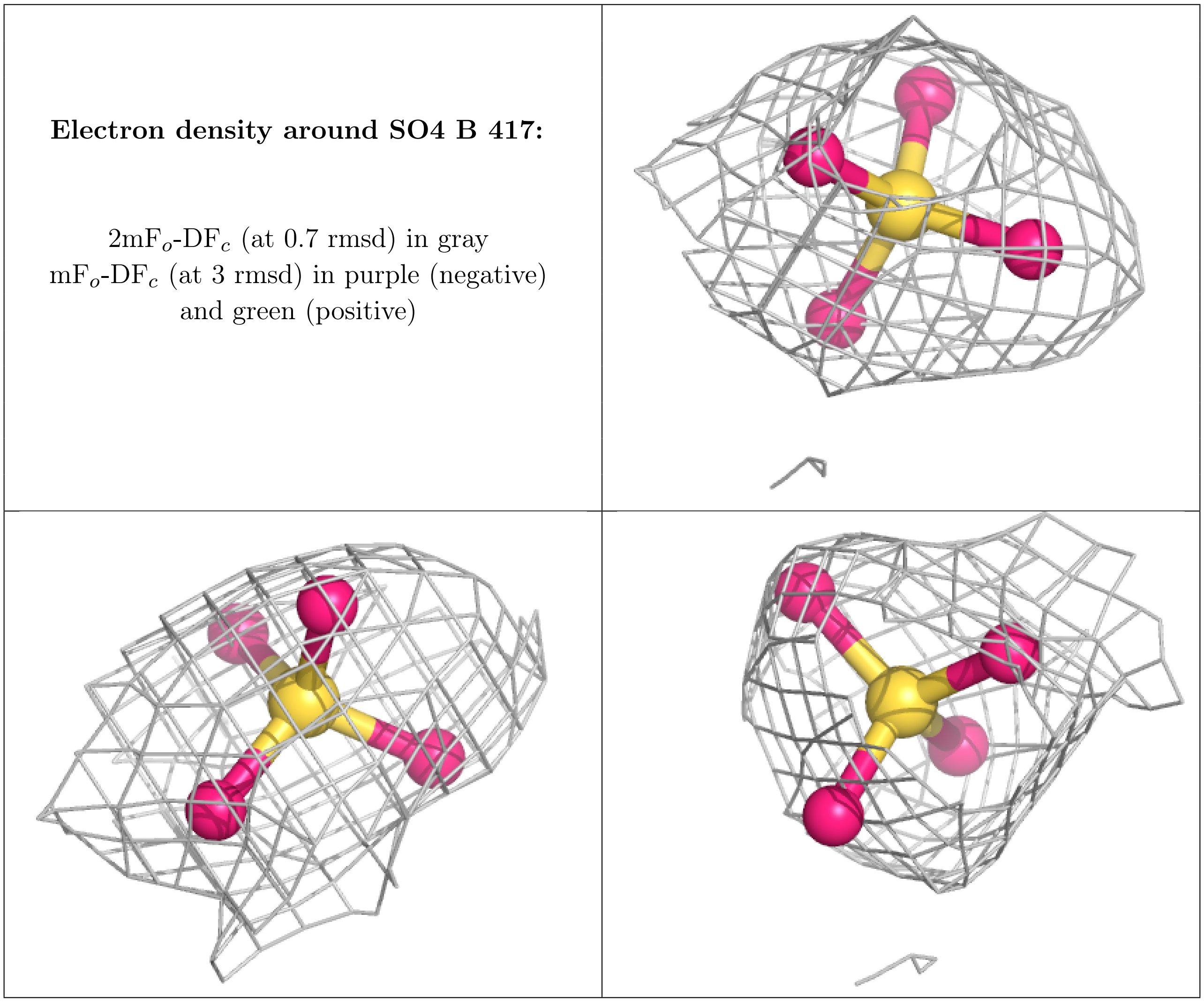
Electron density around SO4 B 416:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







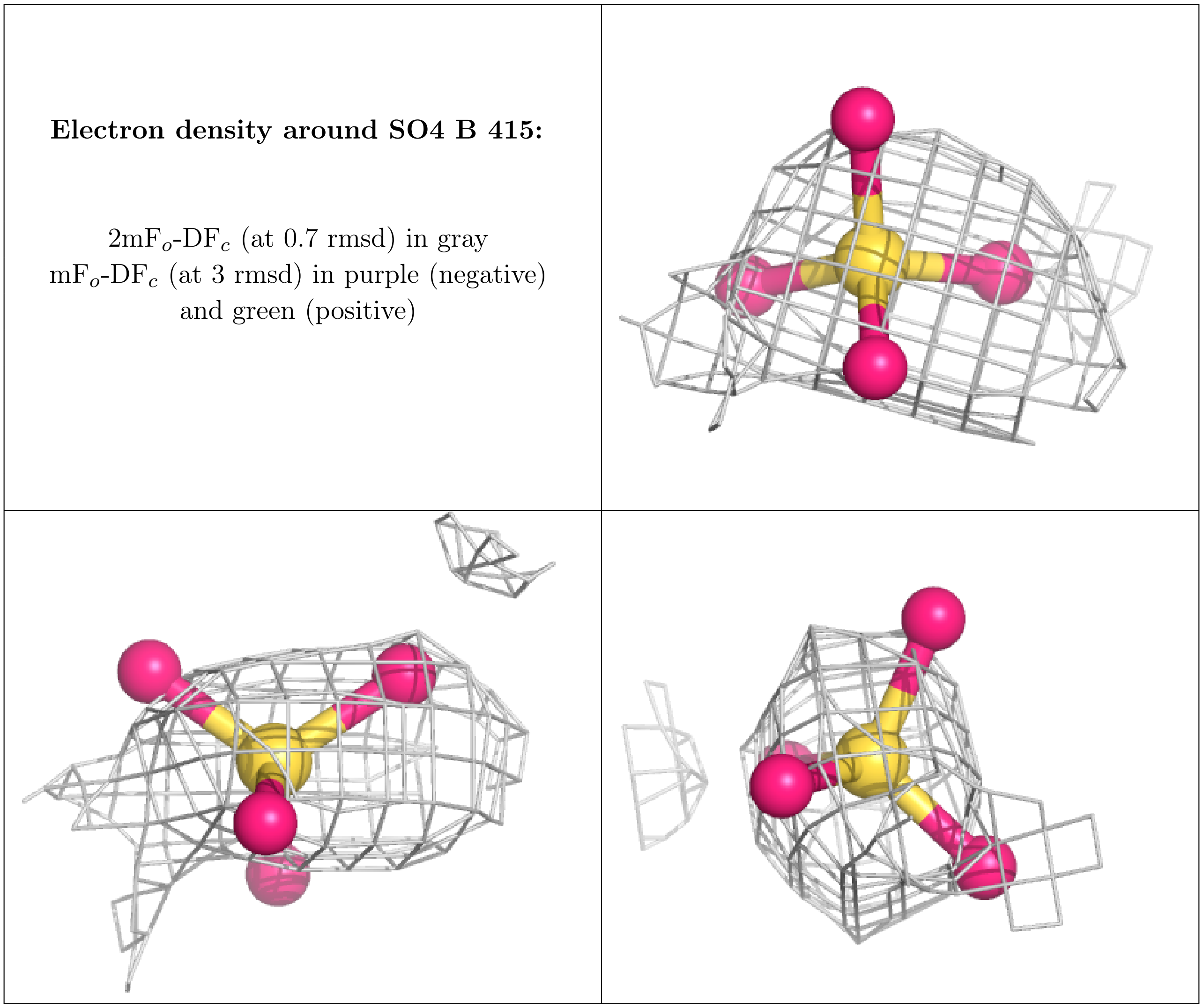


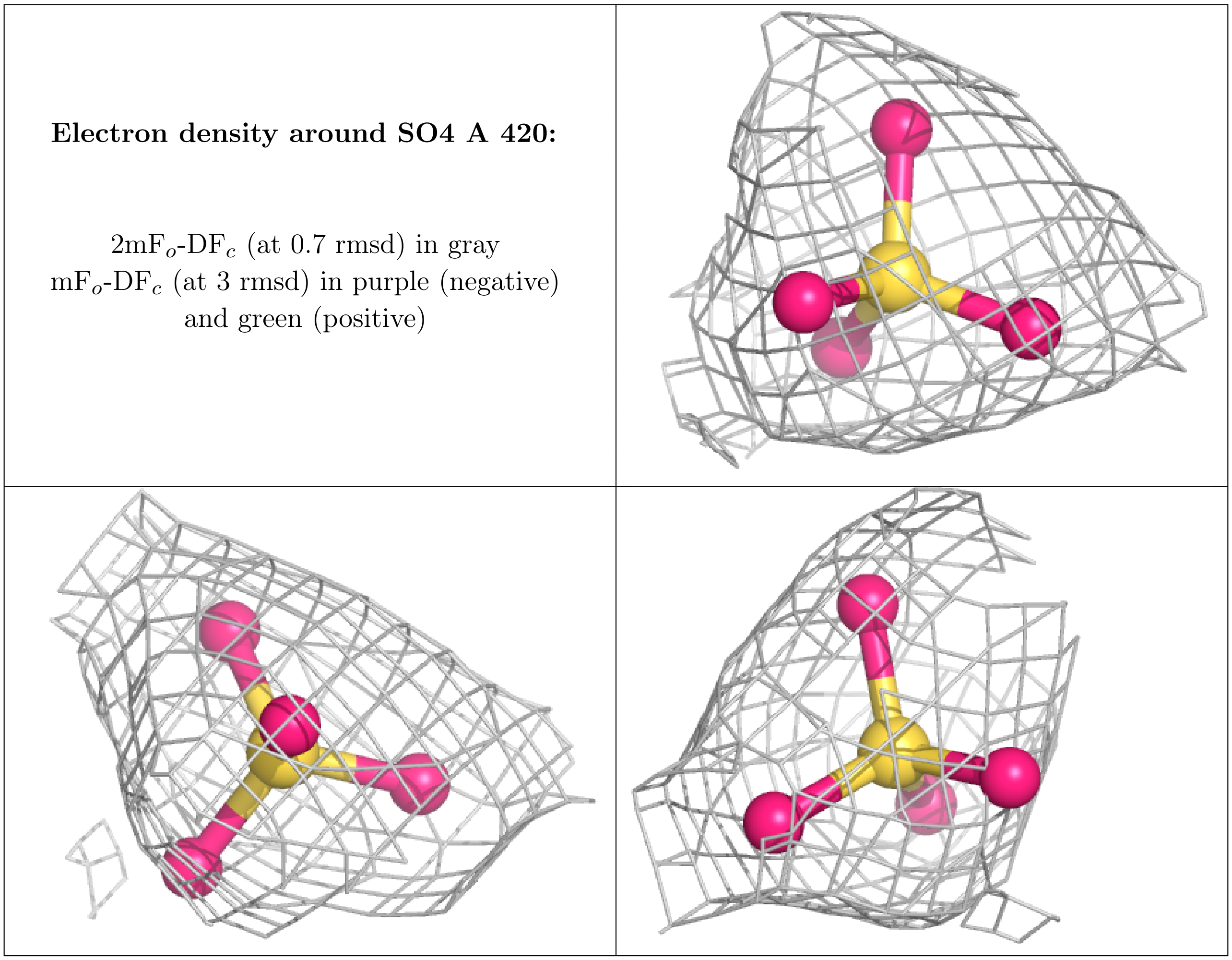
Electron density around SO4 B 417:

$2mF_o$-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 415:

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



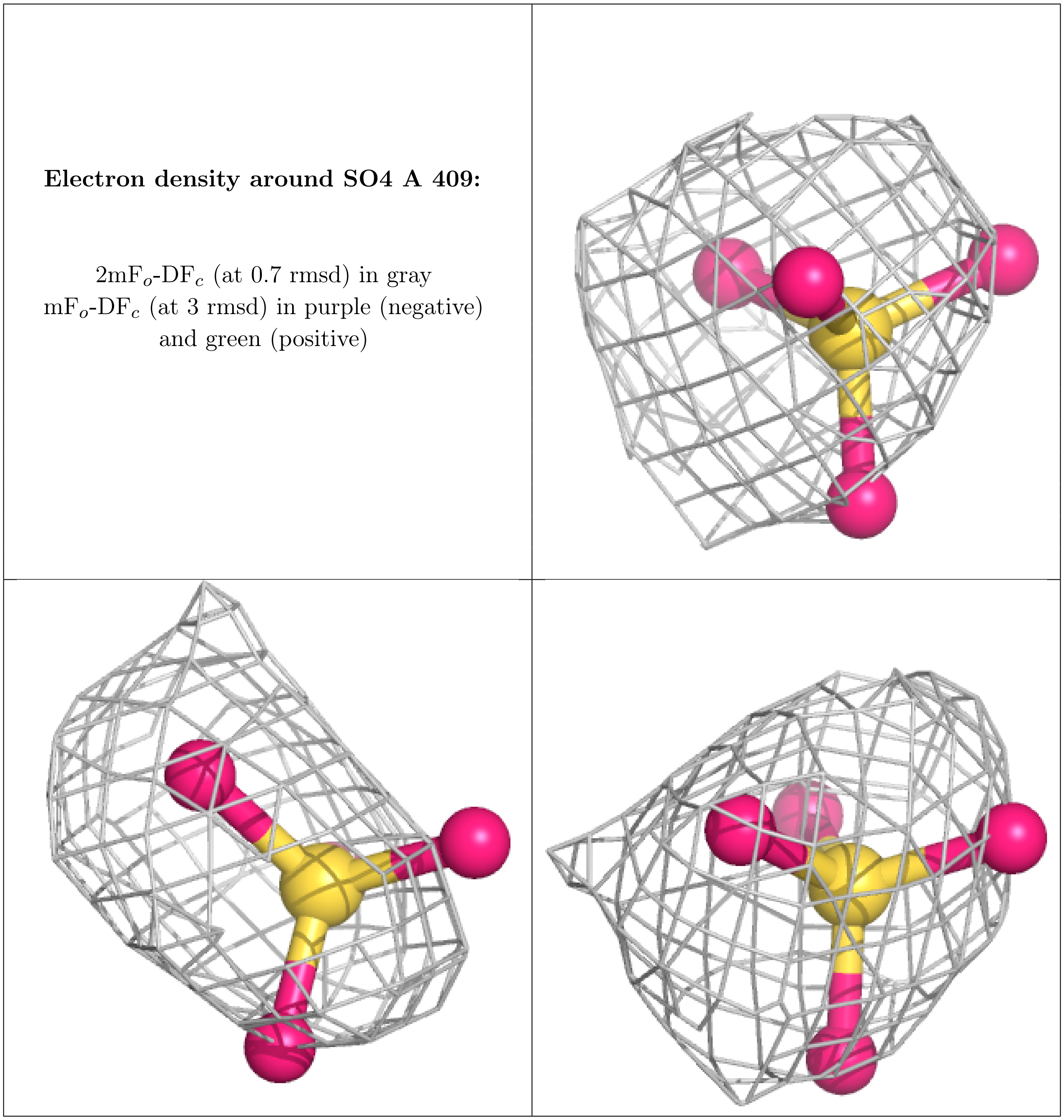


Electron density around SO4 A 420:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

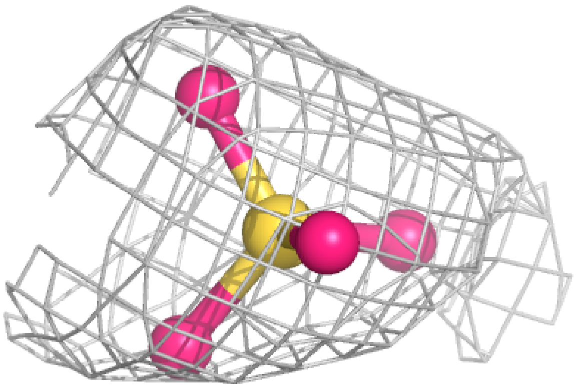
Electron density around SO4 A 409:

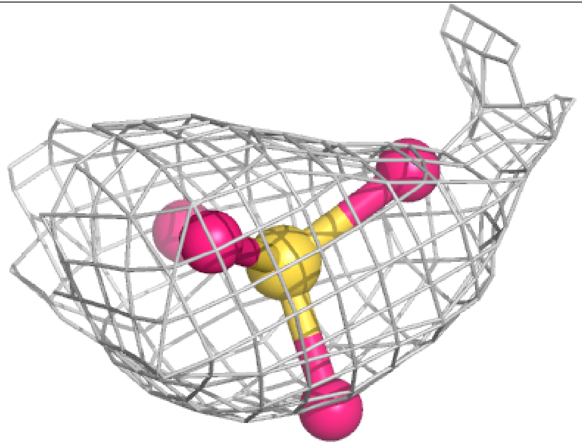
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

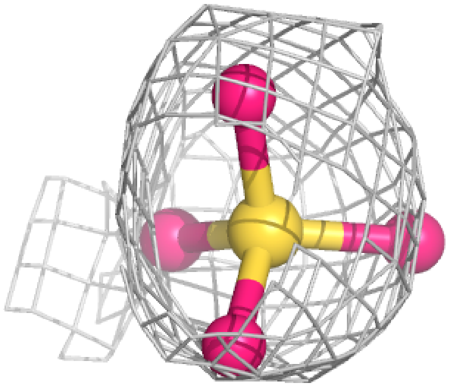


Electron density around SO4 A 406:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

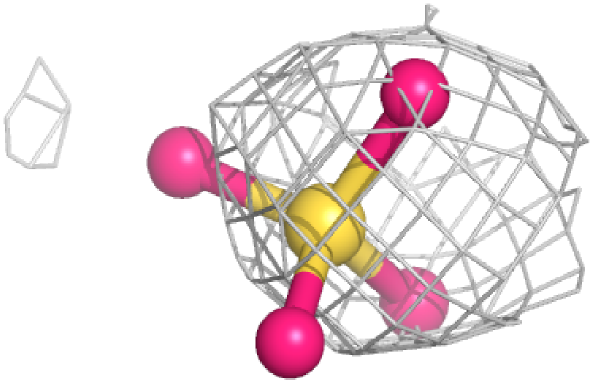


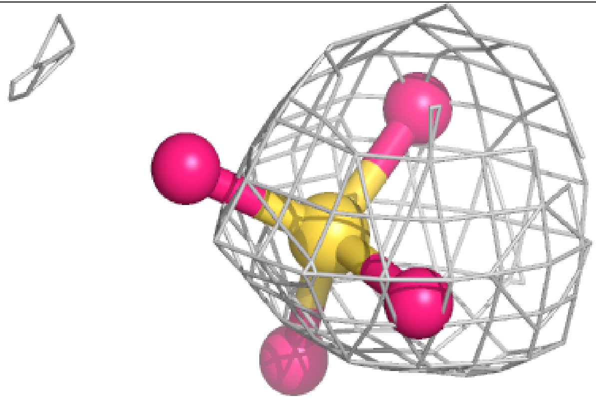


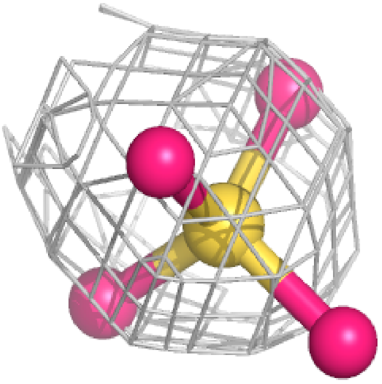


Electron density around SO4 B 425:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

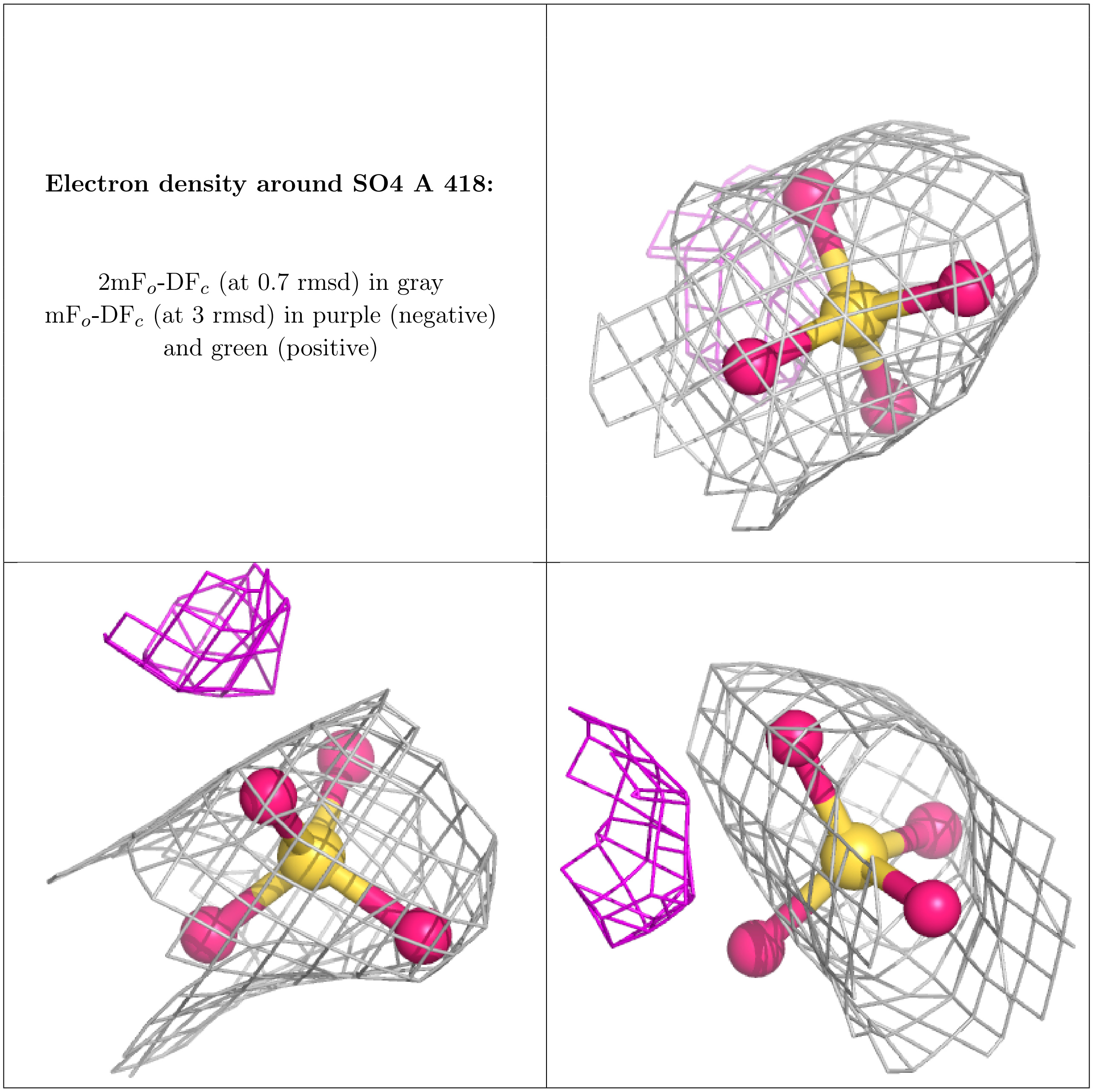


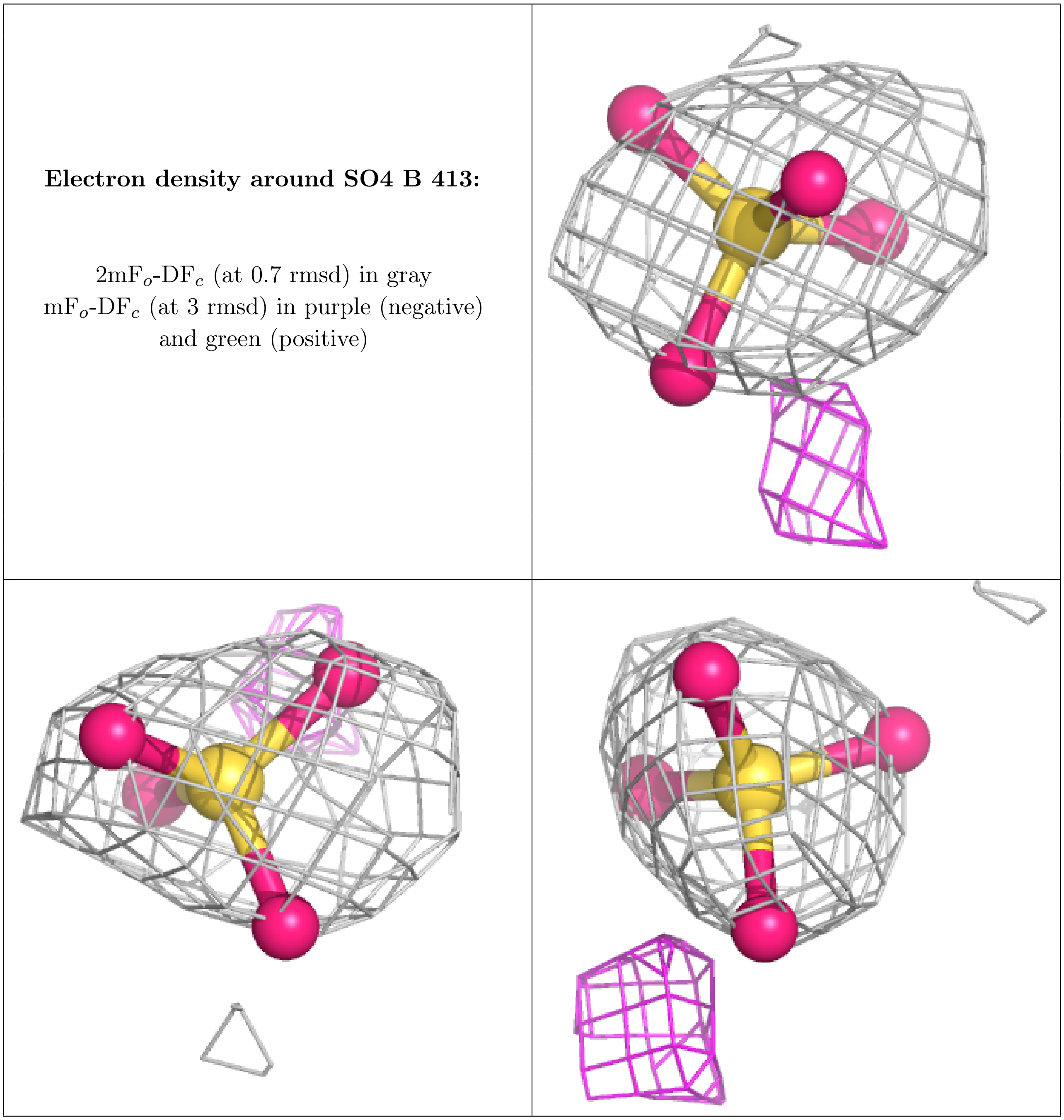




Electron density around SO4 A 418:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



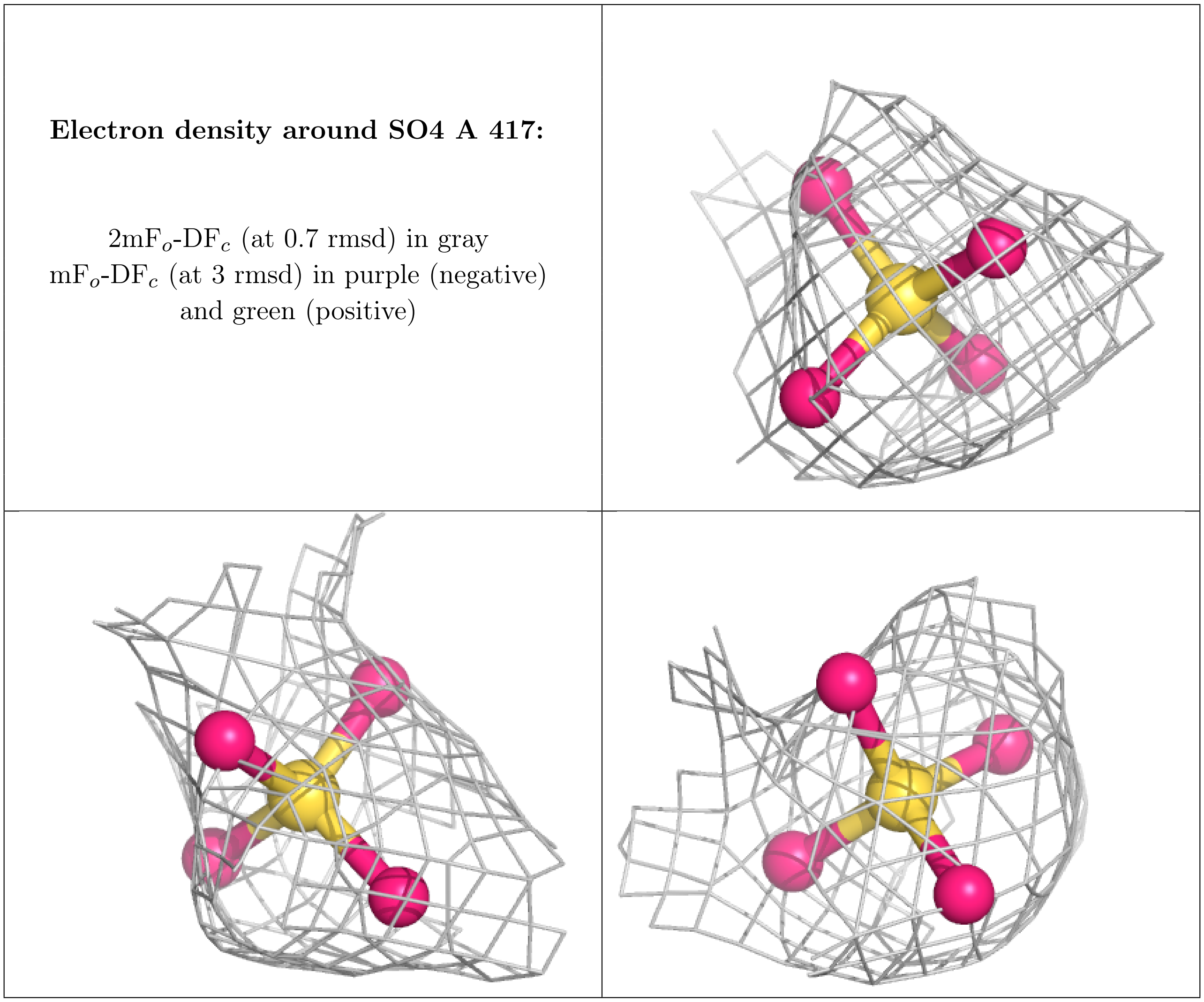


Electron density around SO4 B 413:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

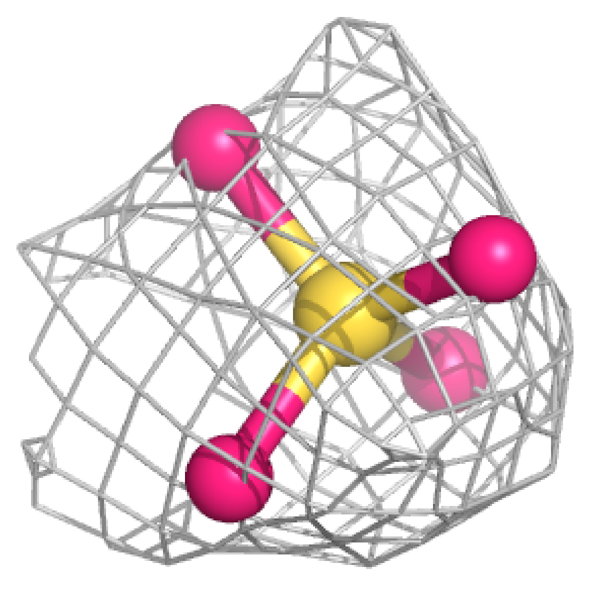
Electron density around SO4 A 417:

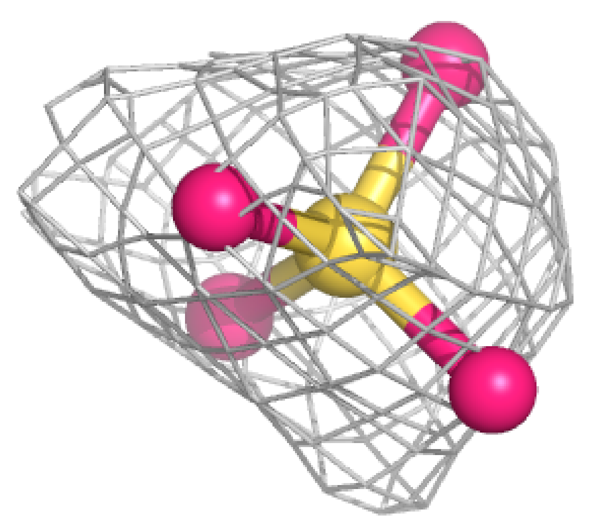
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

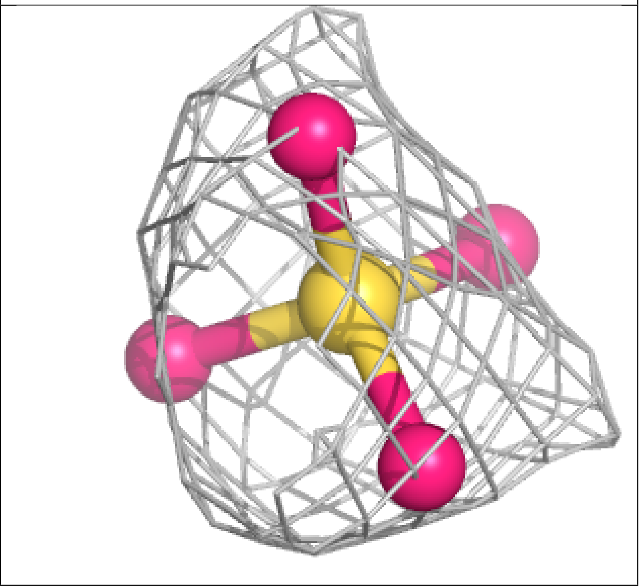


Electron density around SO4 B 418:

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

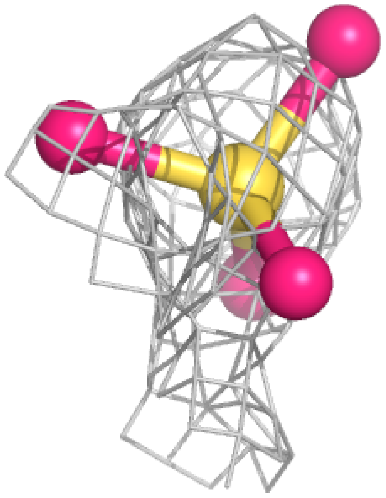


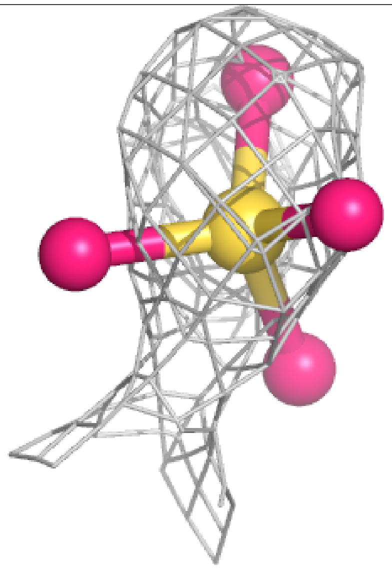


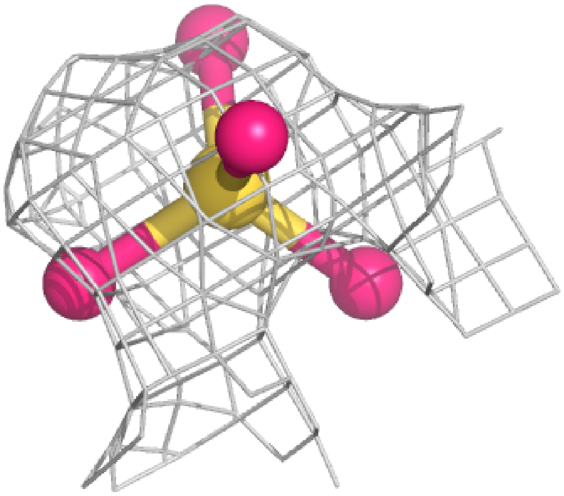


Electron density around SO4 B 421:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

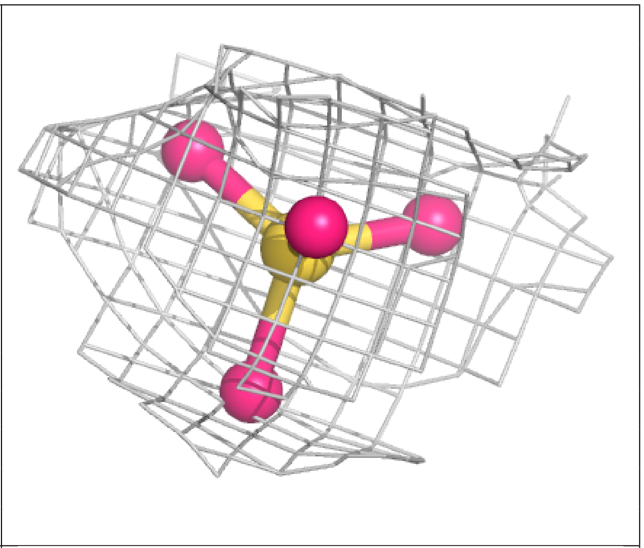


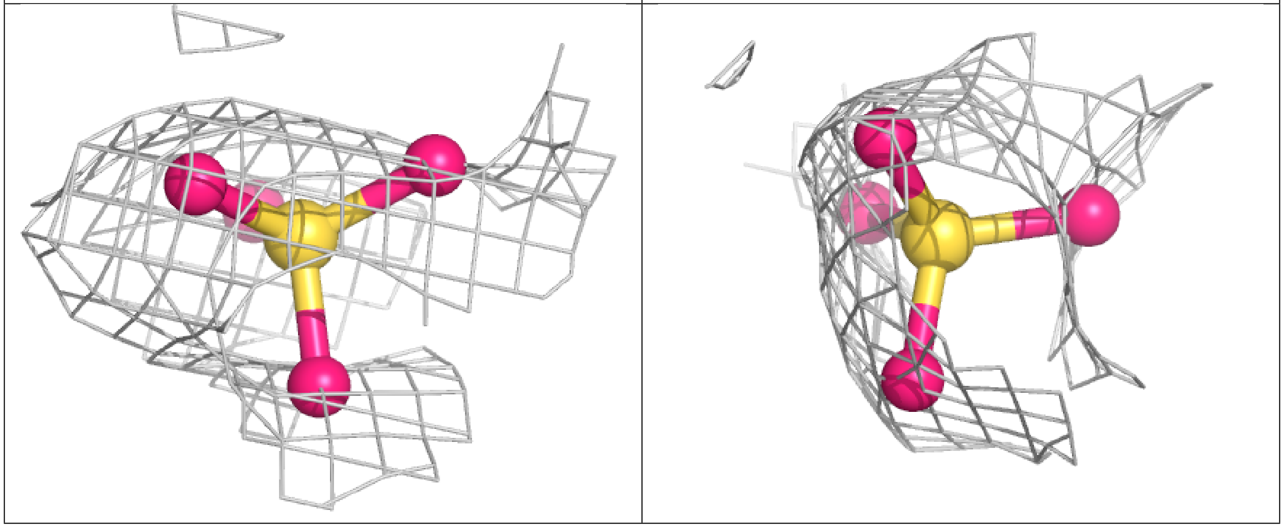


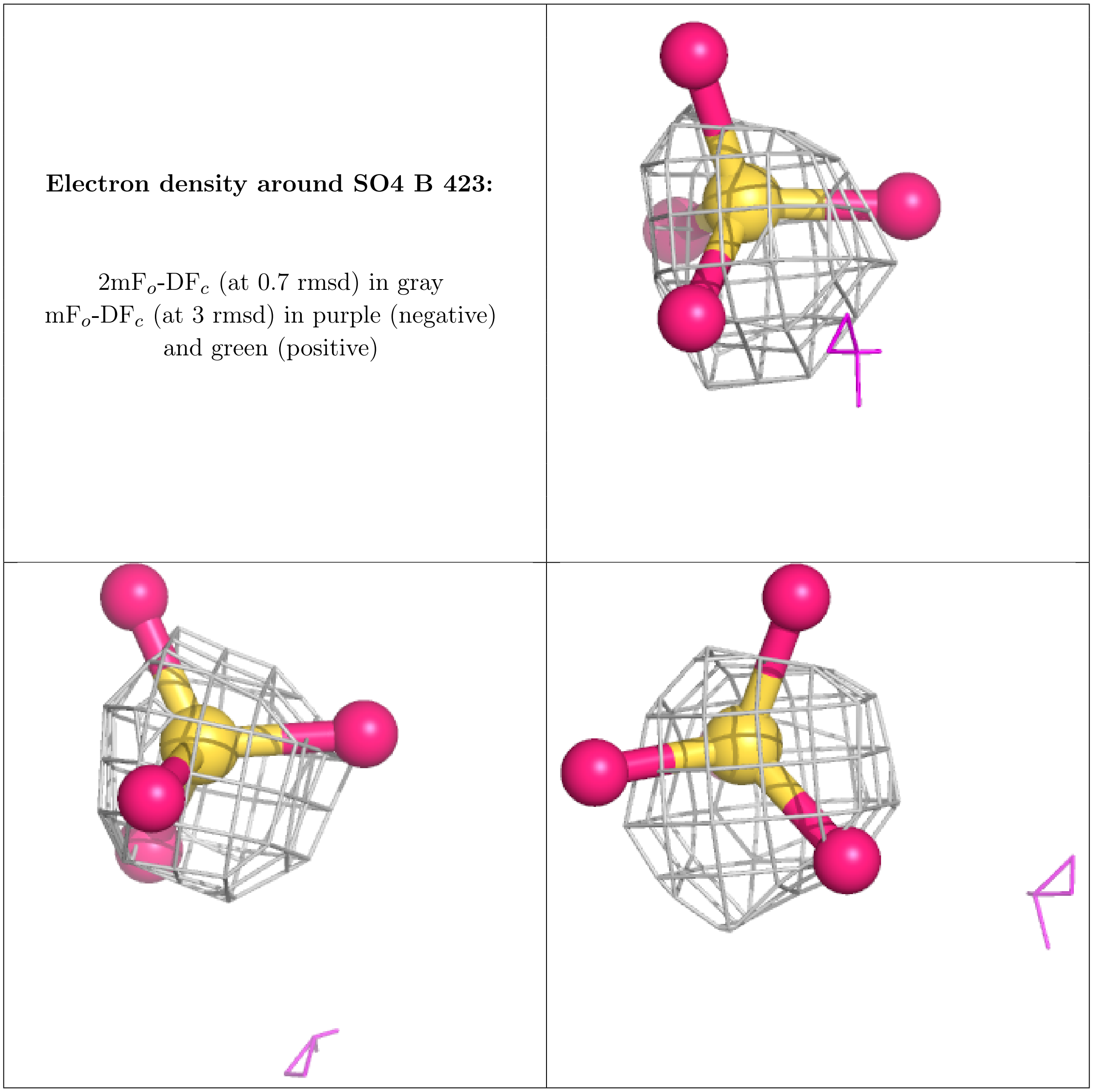


Electron density around SO4 B 422:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





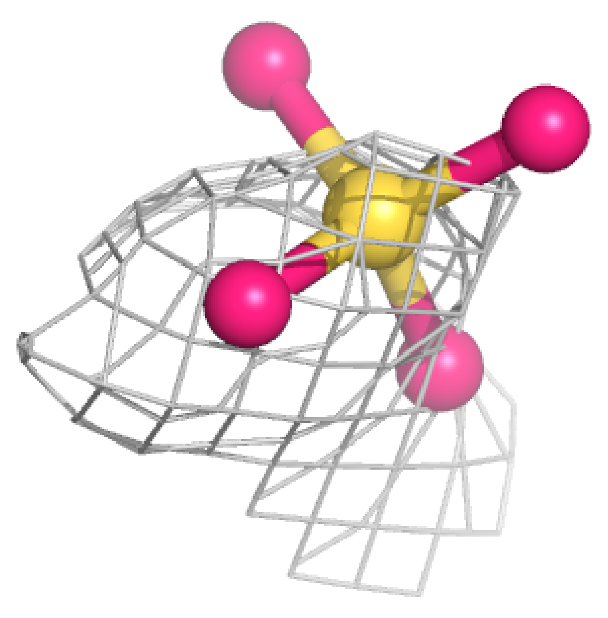


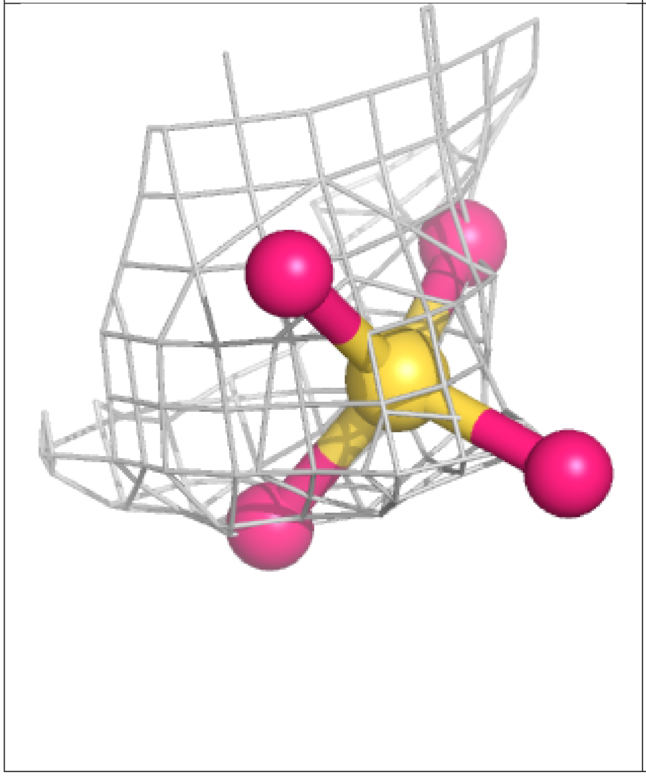
Electron density around SO4 B 423:

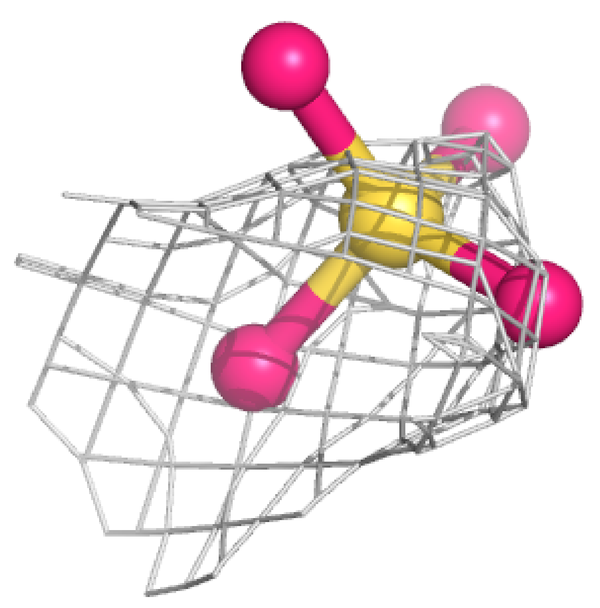
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

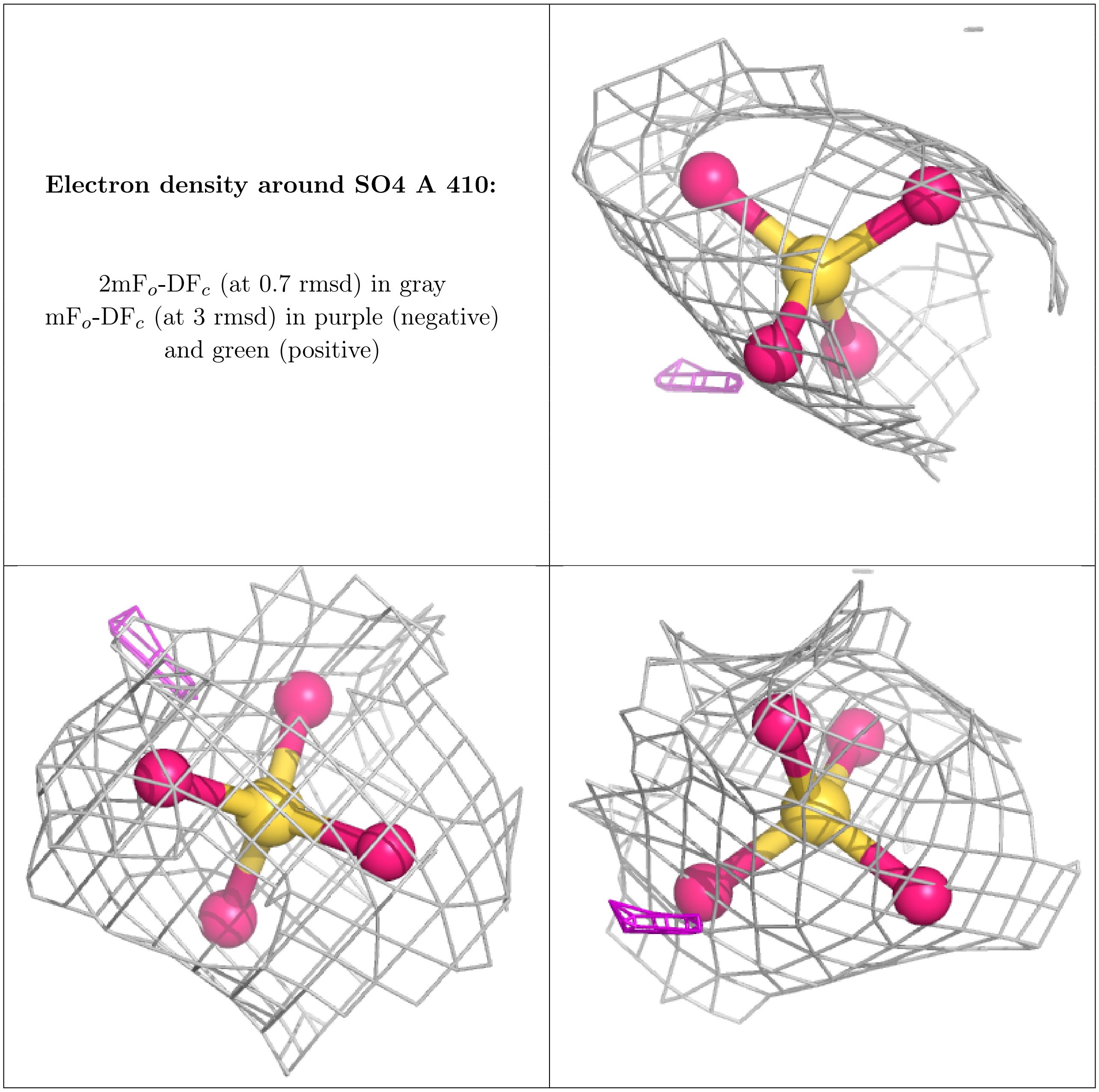
Electron density around SO4 A 405:

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







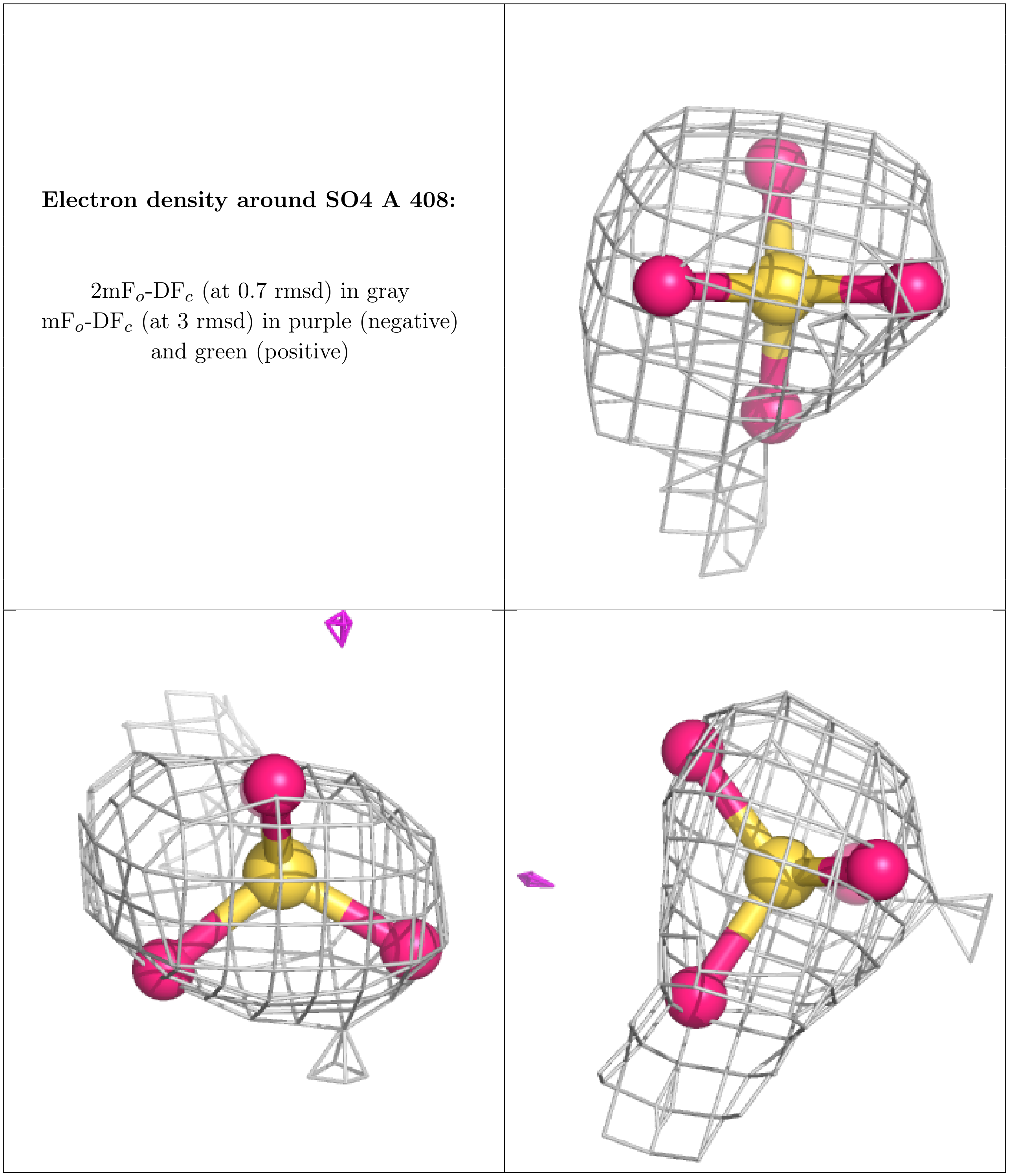


Electron density around SO4 A 410:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

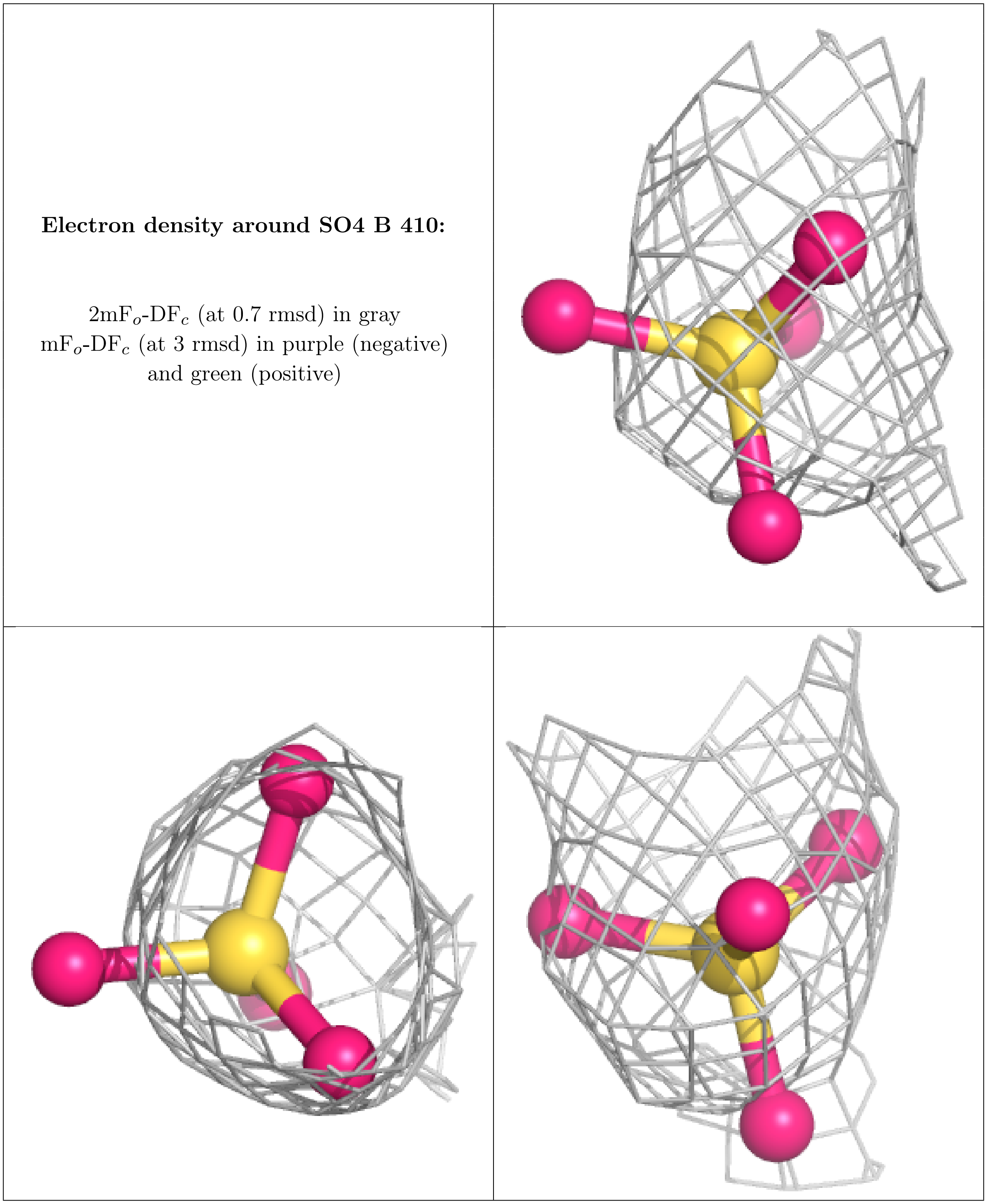
Electron density around SO4 A 408:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



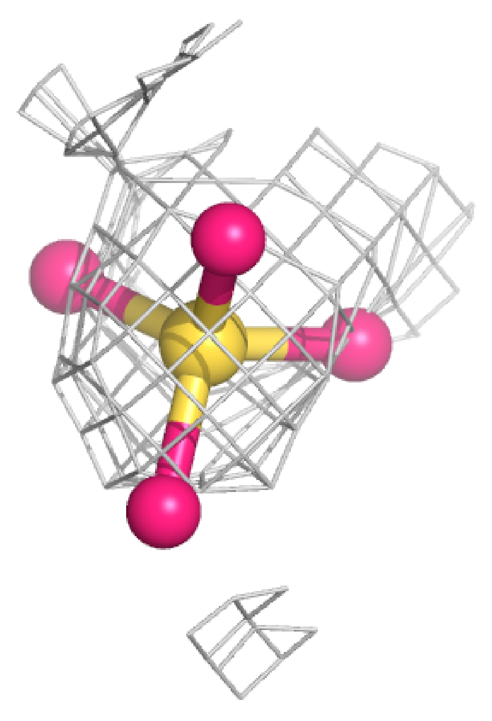
Electron density around SO4 B 410:

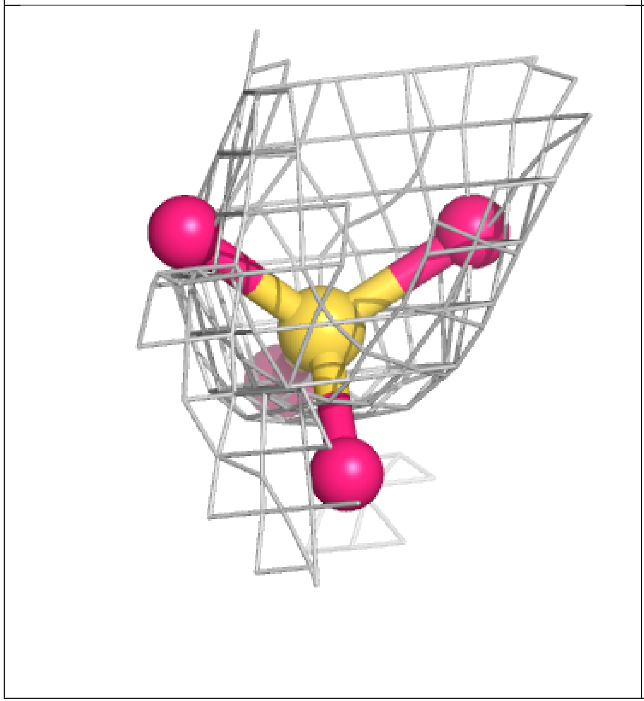
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

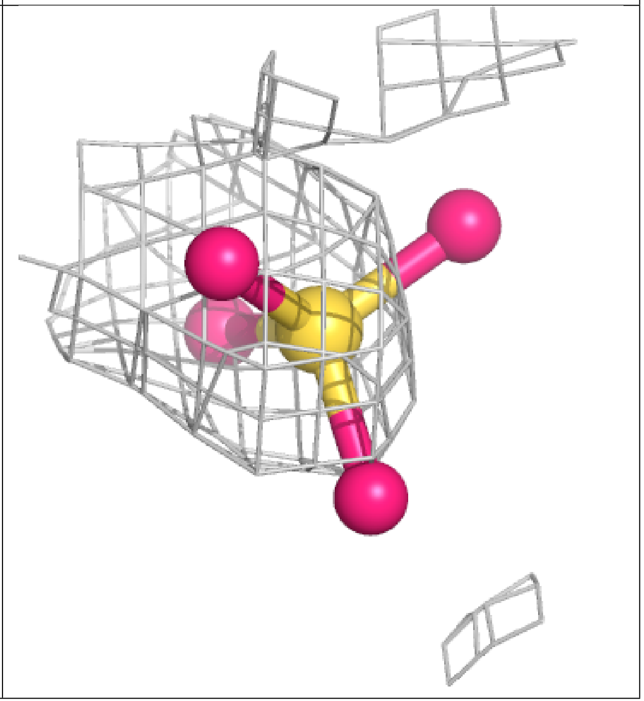


Electron density around SO4 A 411:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

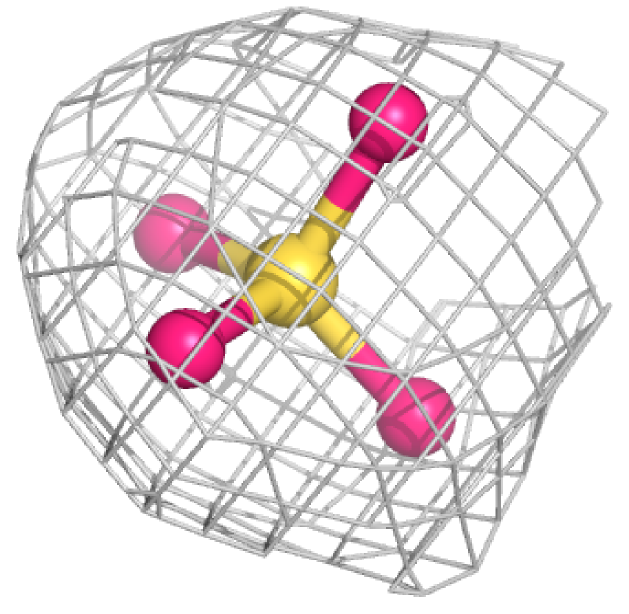


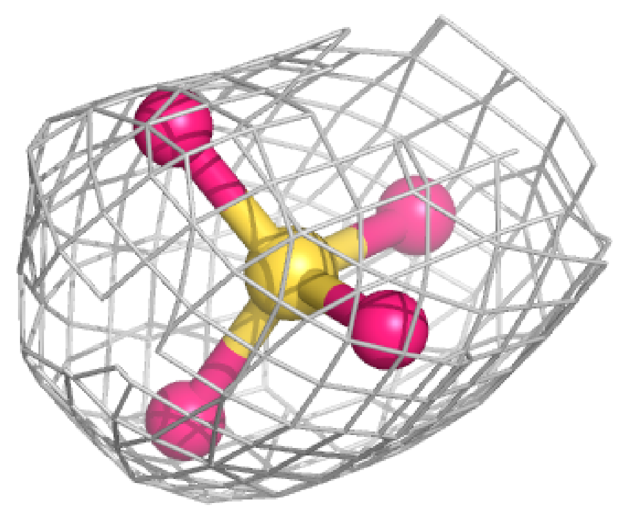


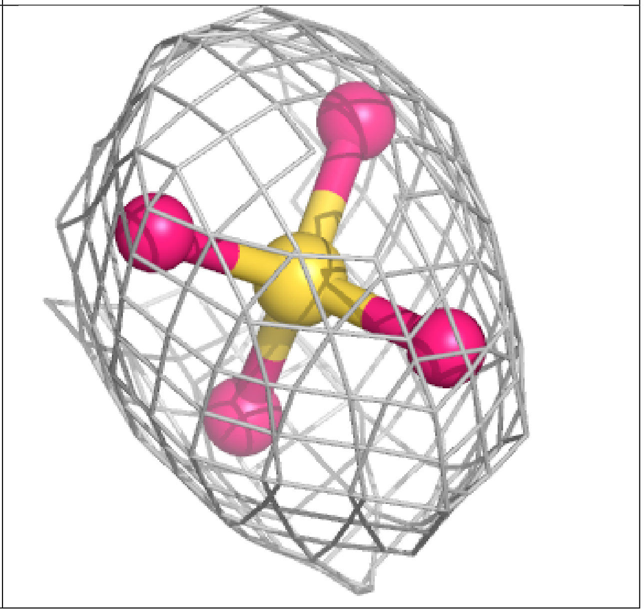


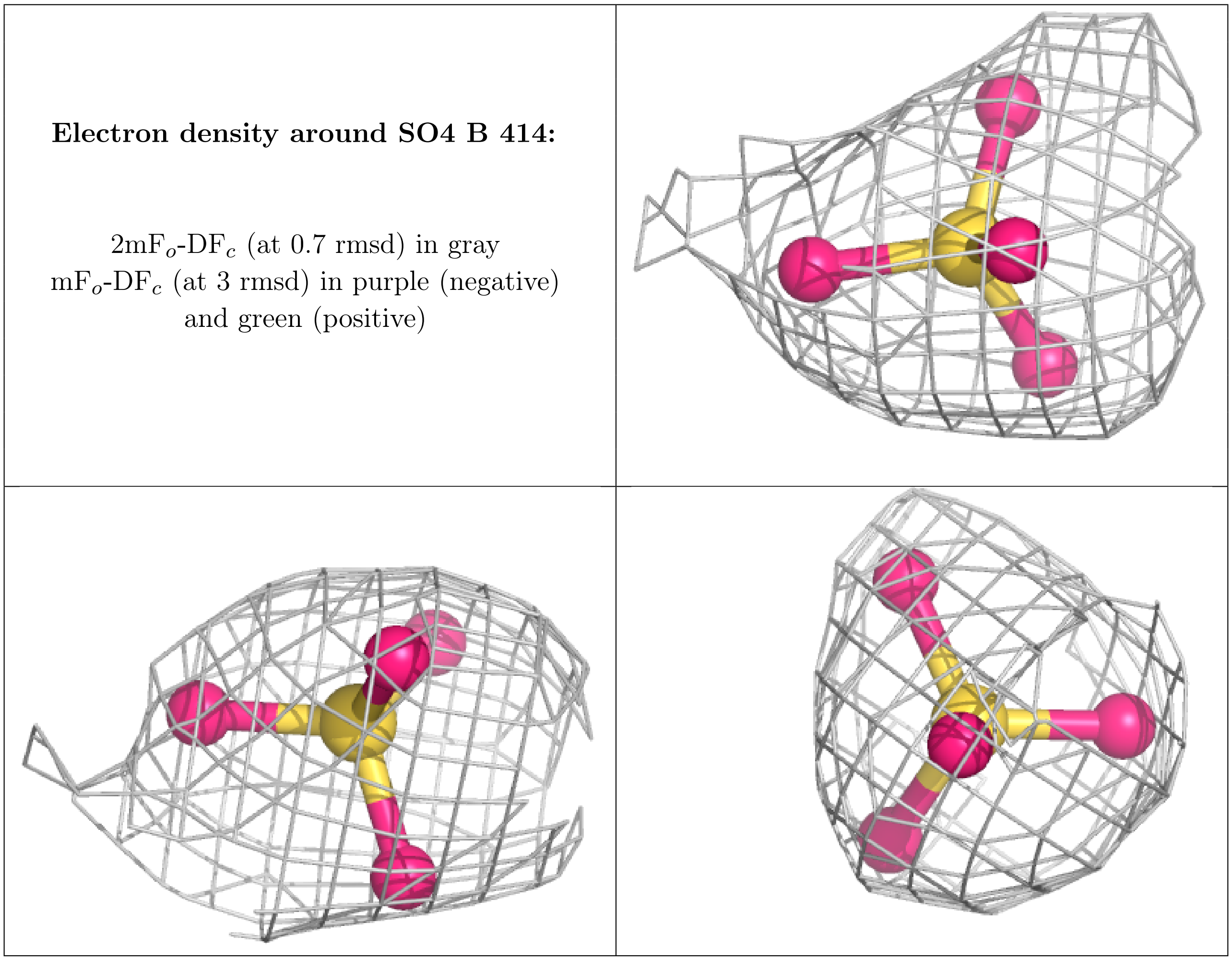
Electron density around SO4 B 404:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







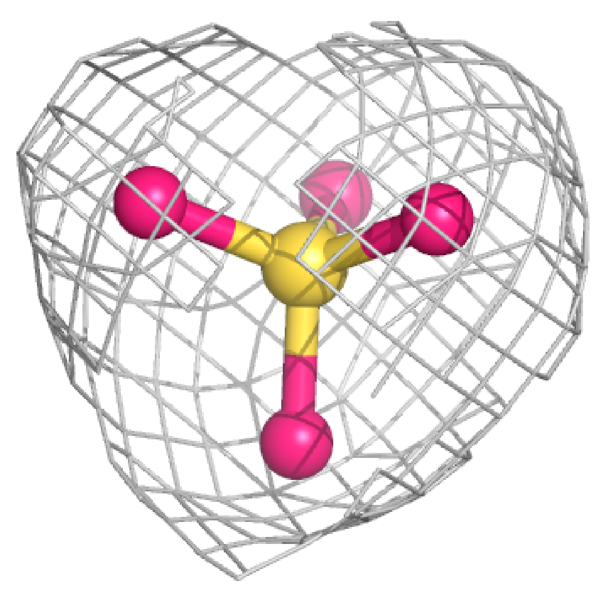


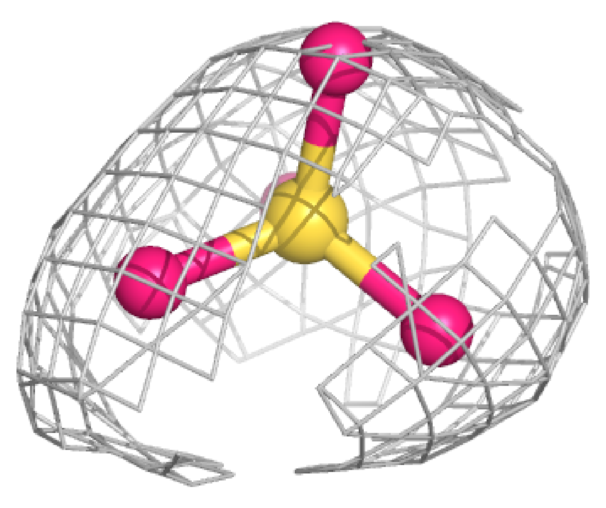
Electron density around SO4 B 414:

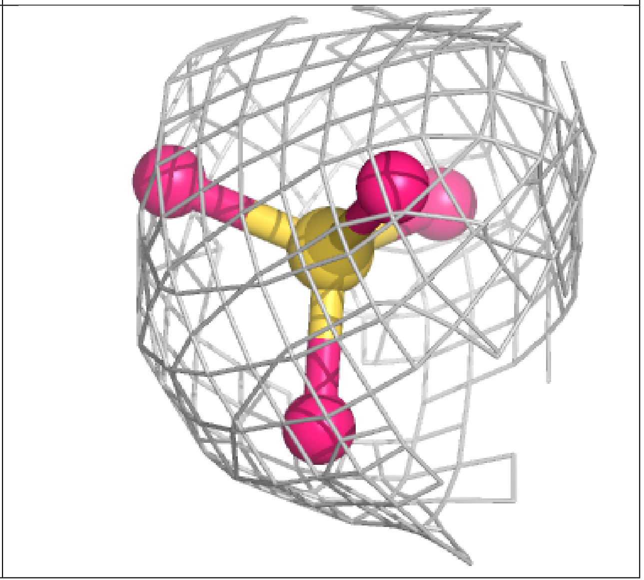
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

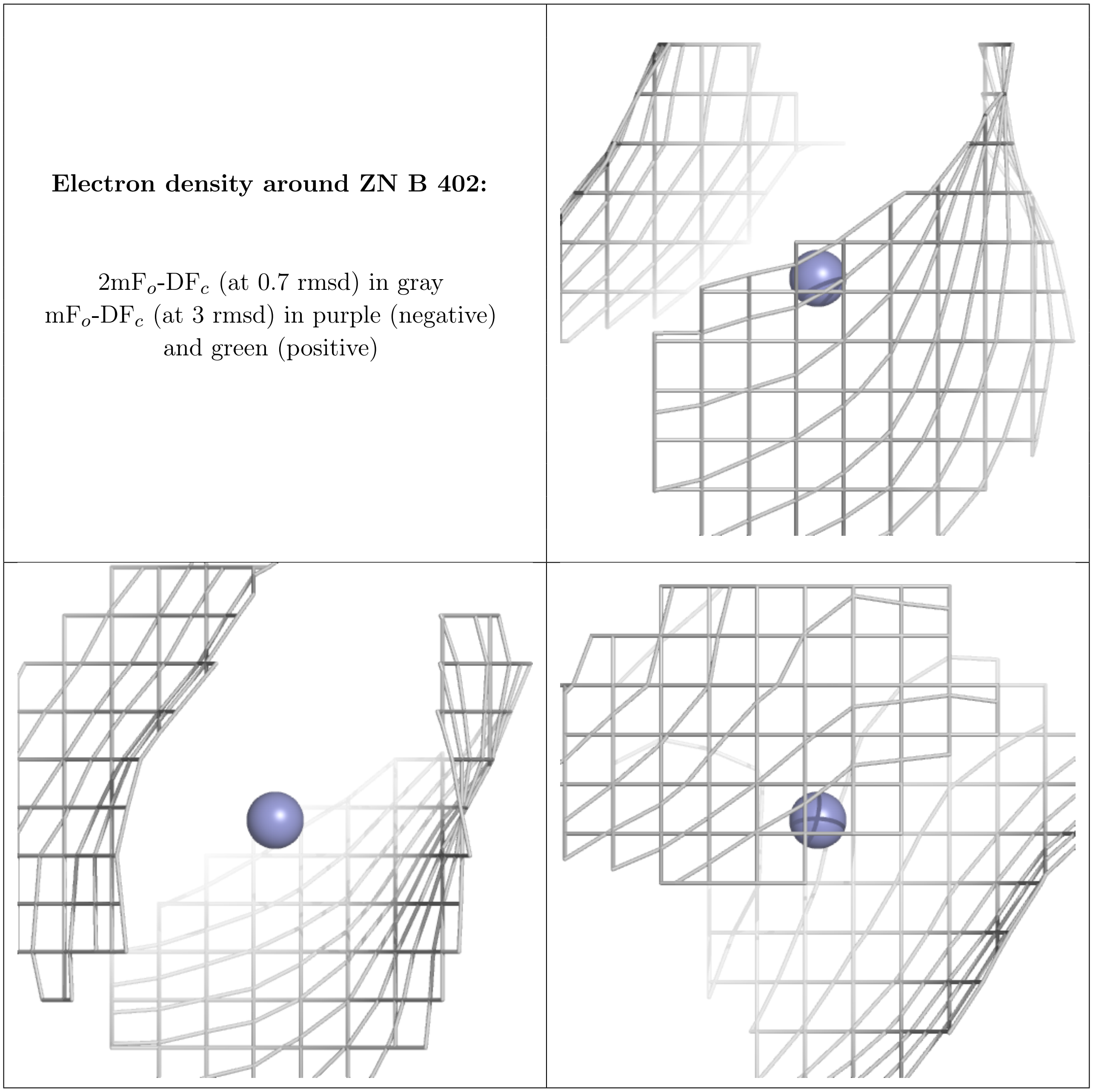
Electron density around SO4 A 416:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)







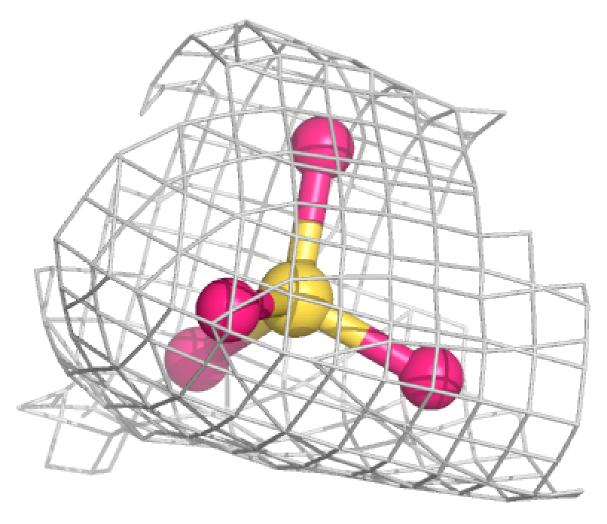


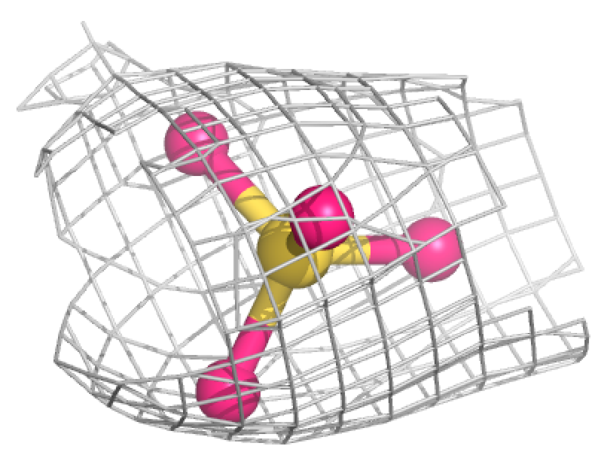
Electron density around ZN B 402:

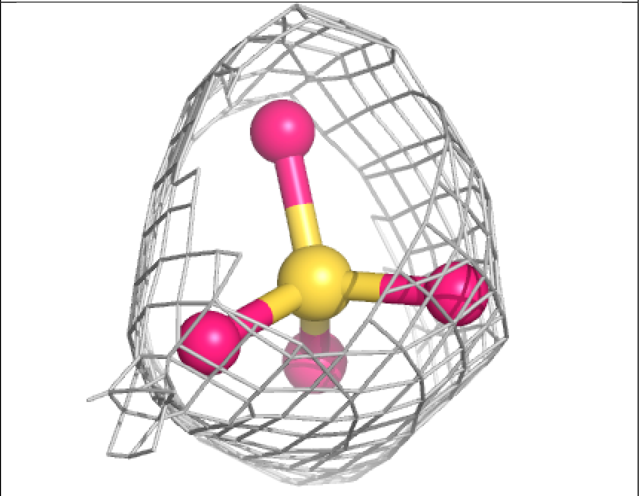
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around SO4 A 412:

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

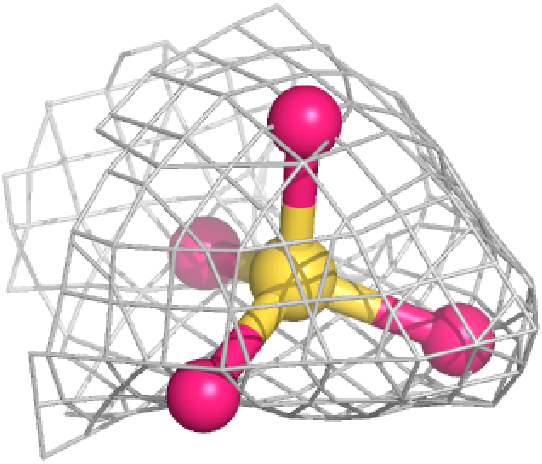


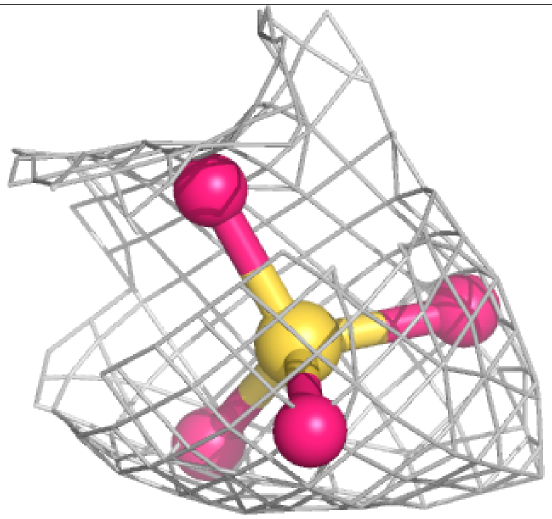


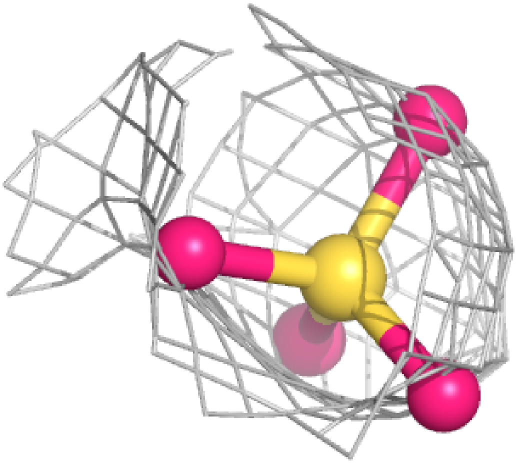


Electron density around SO4 B 426:

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

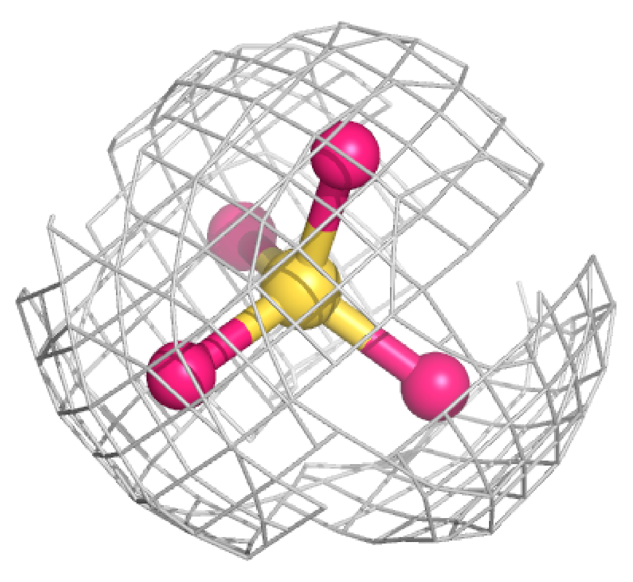


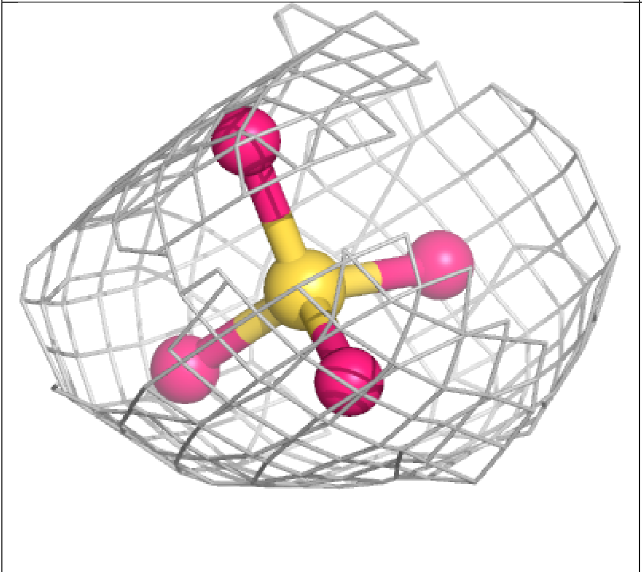


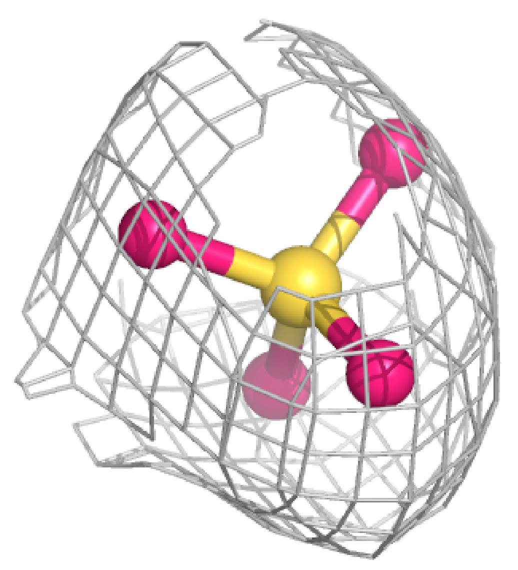


Electron density around SO4 A 425:

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

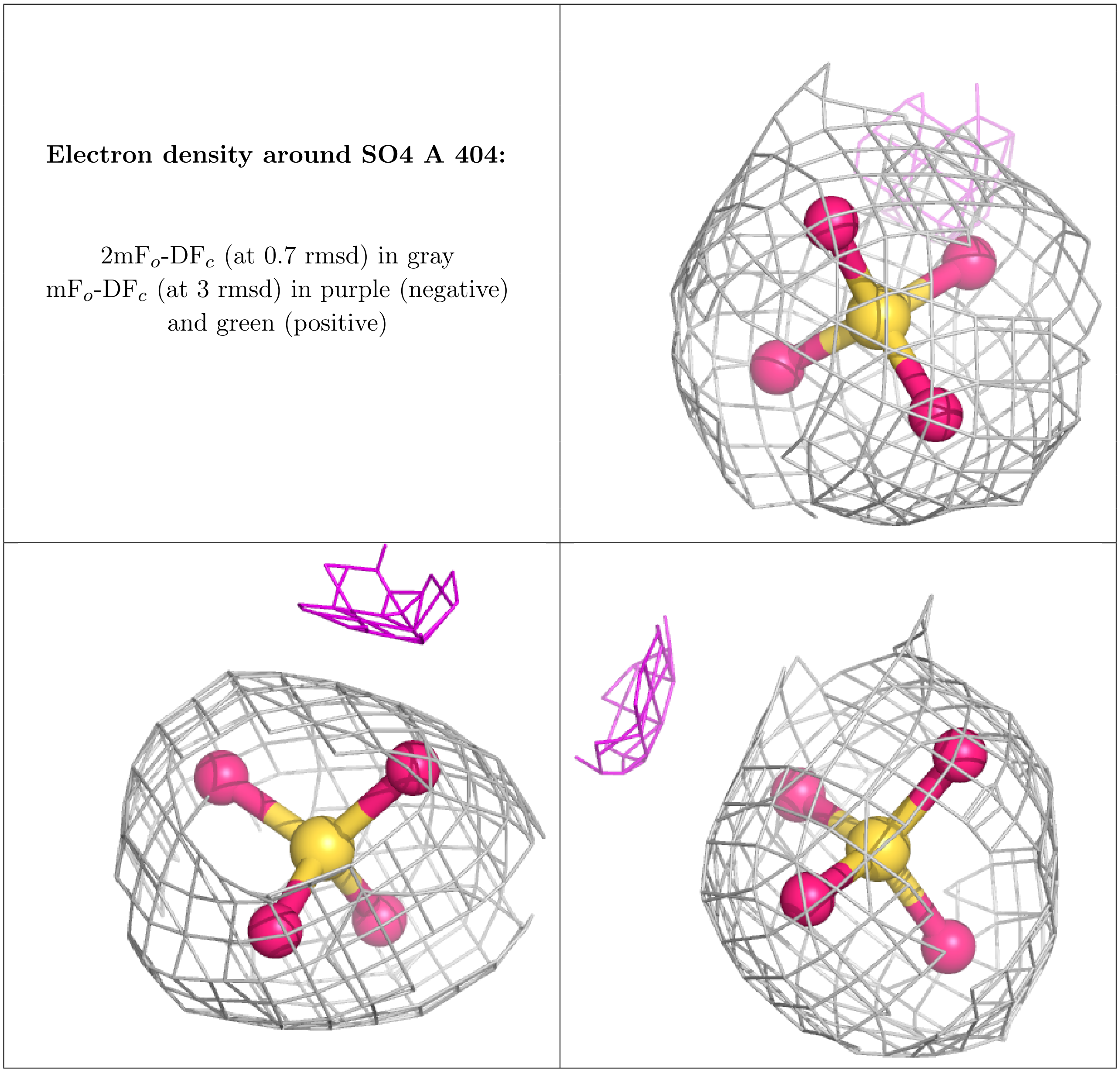






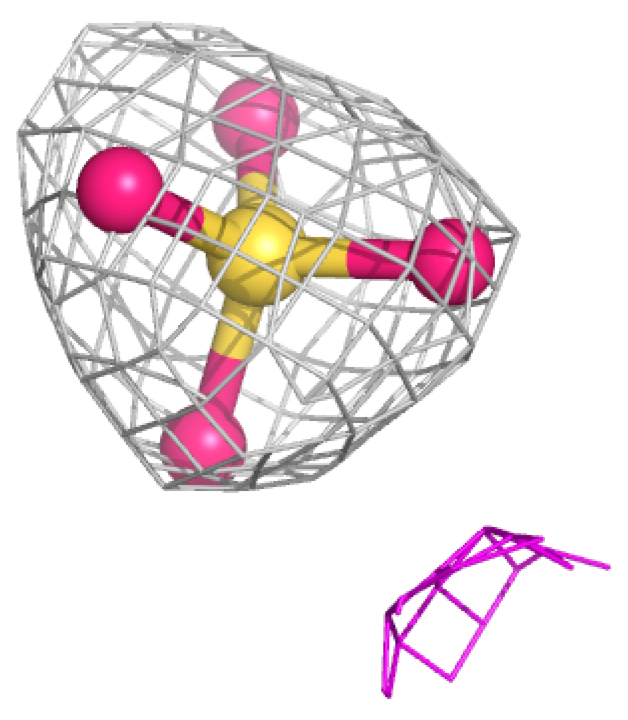
Electron density around SO4 A 404:

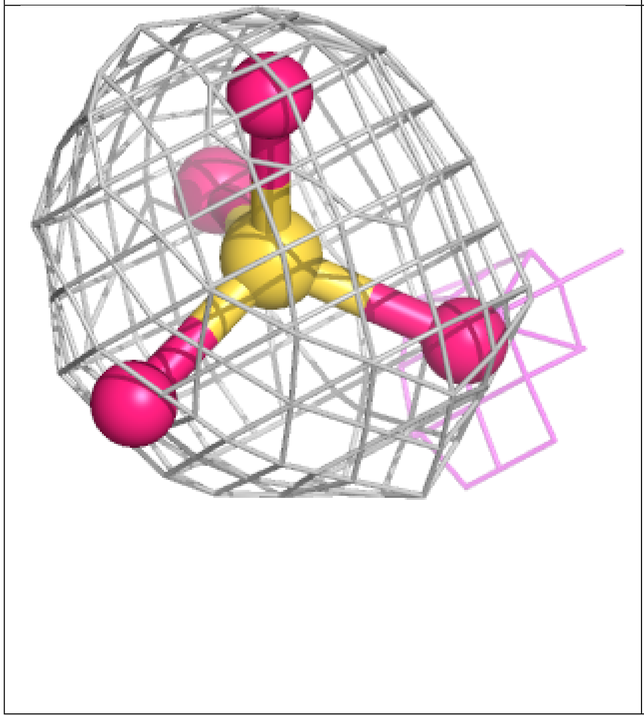
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

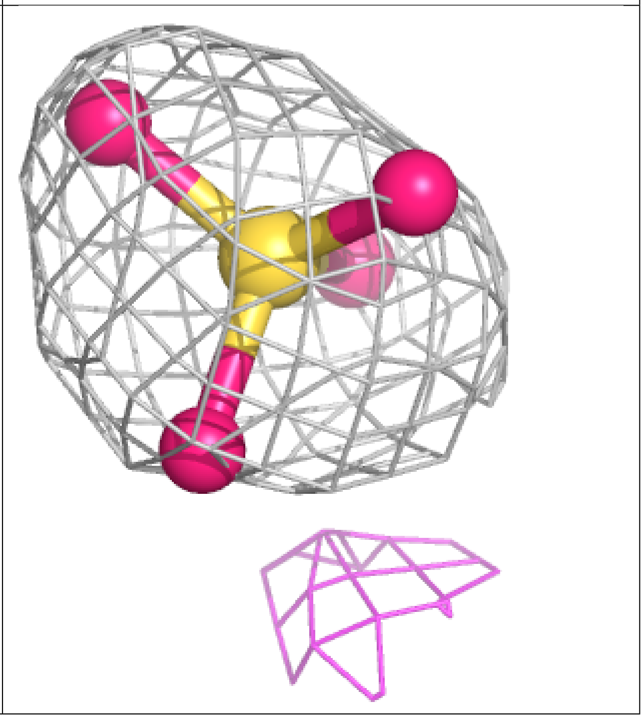


Electron density around SO4 A 413:

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

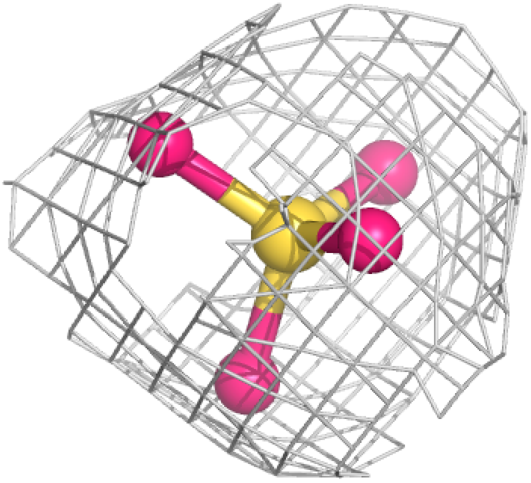


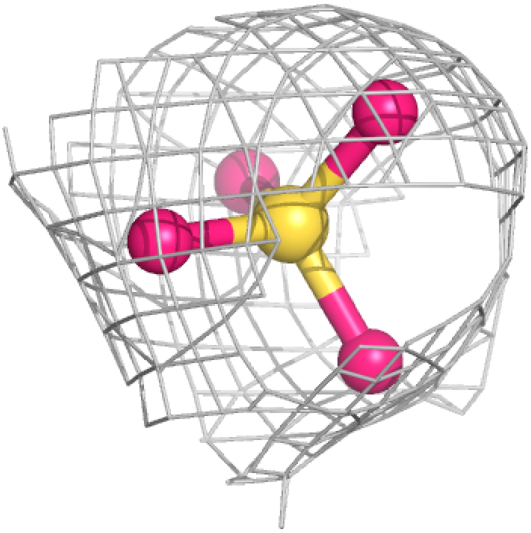


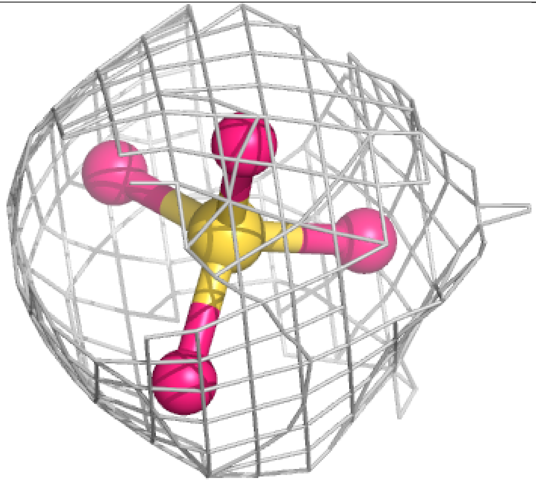


Electron density around SO4 B 406:

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

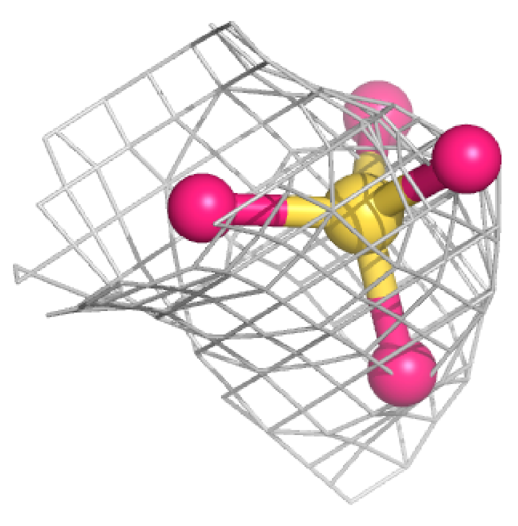


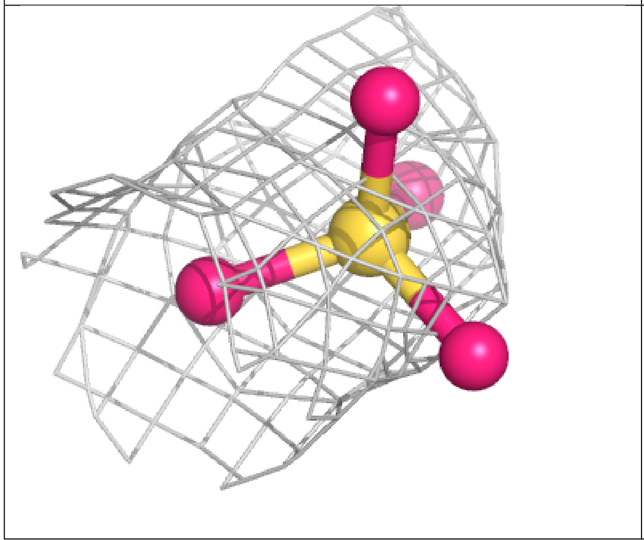


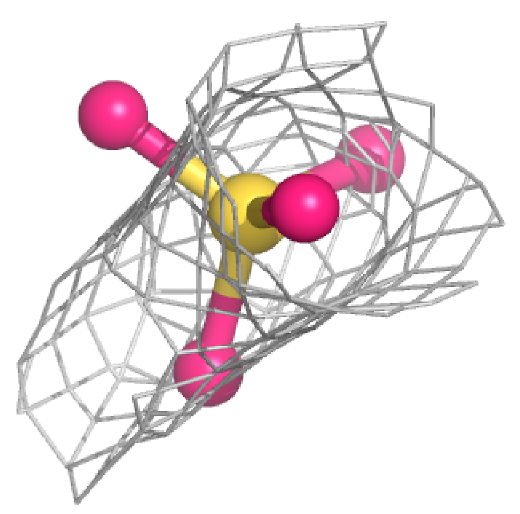


Electron density around SO4 B 407:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

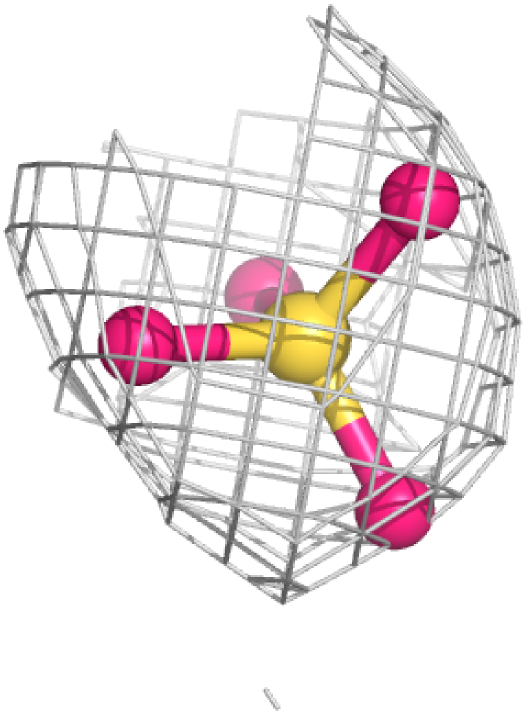


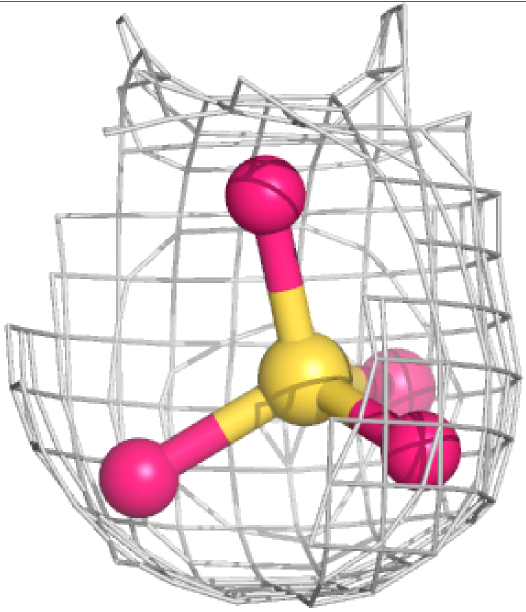


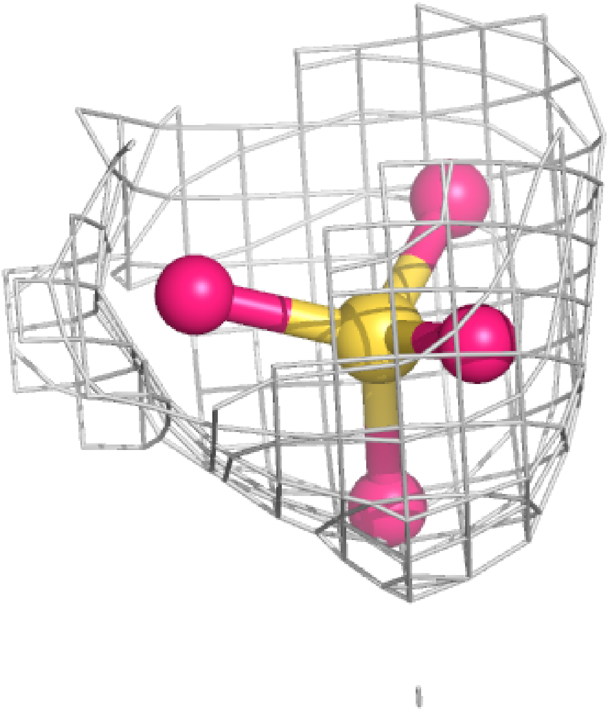


Electron density around SO4 B 408:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

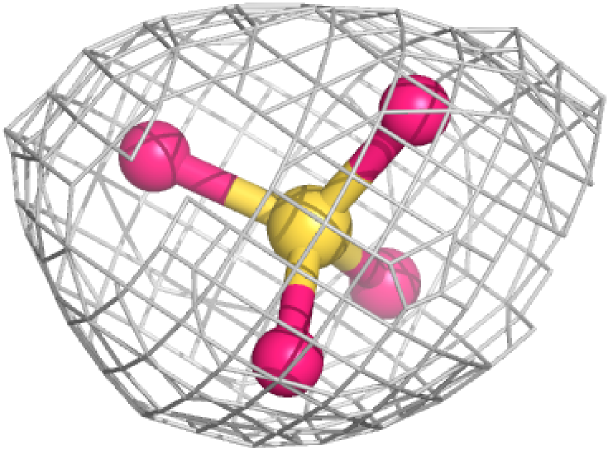


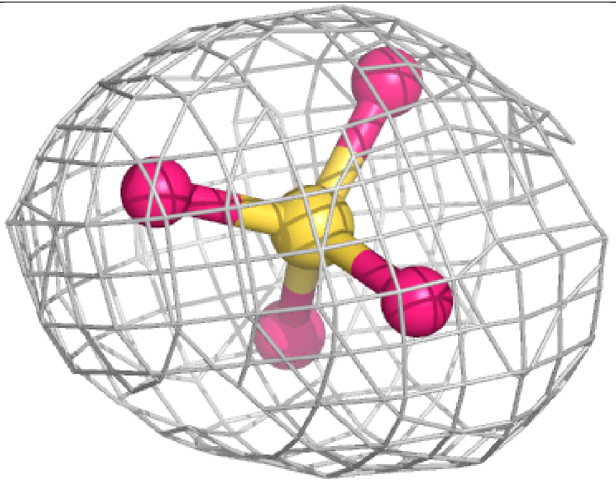


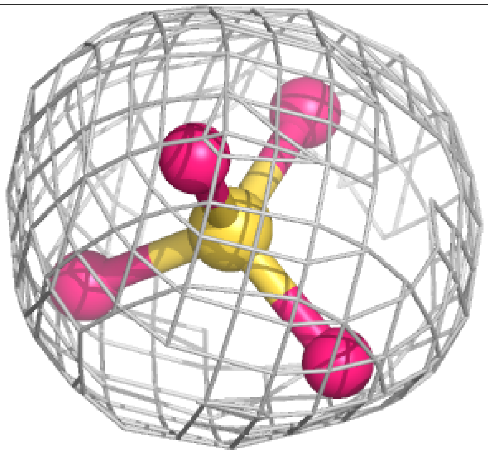


Electron density around SO4 B 405:

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

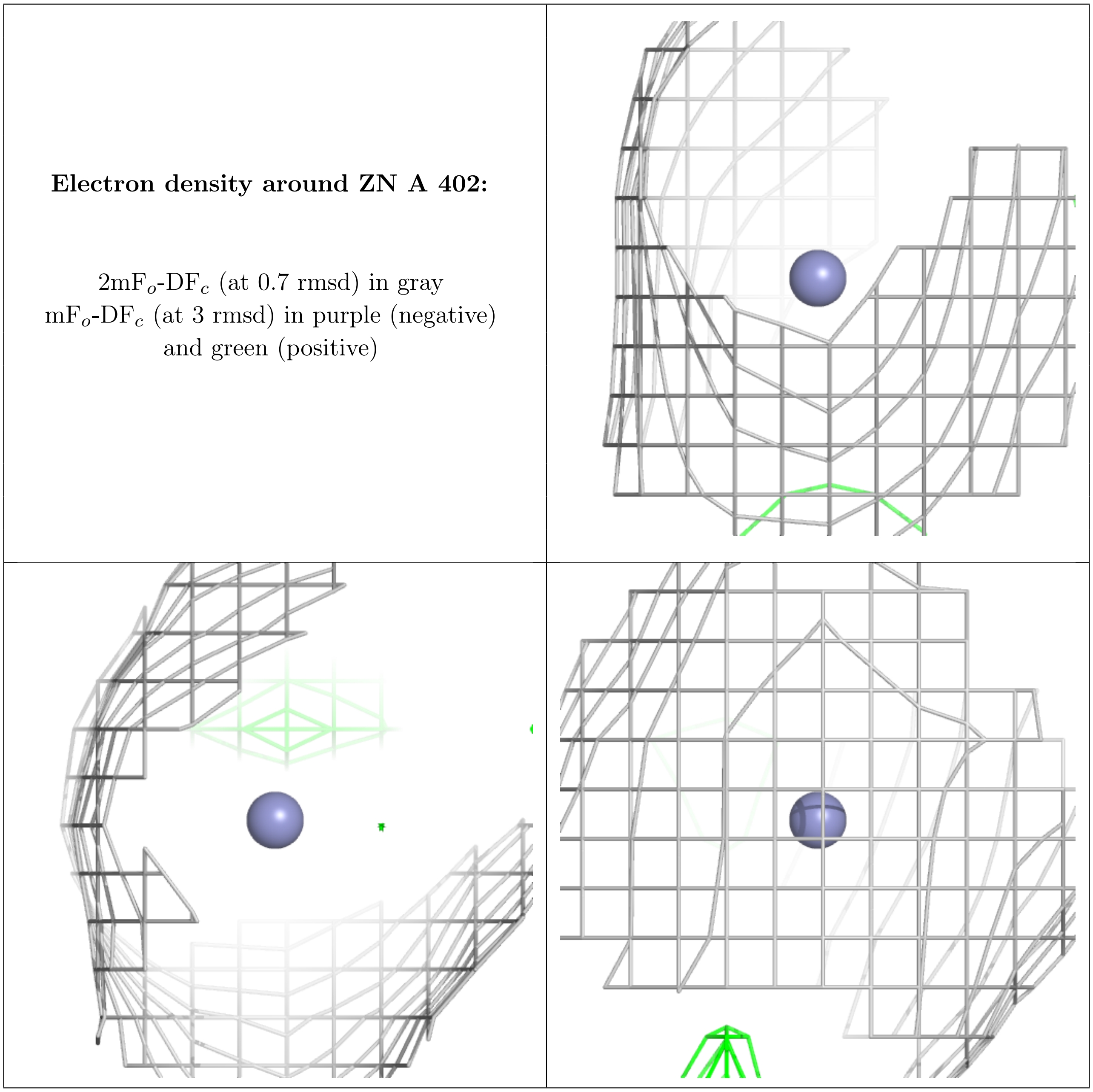


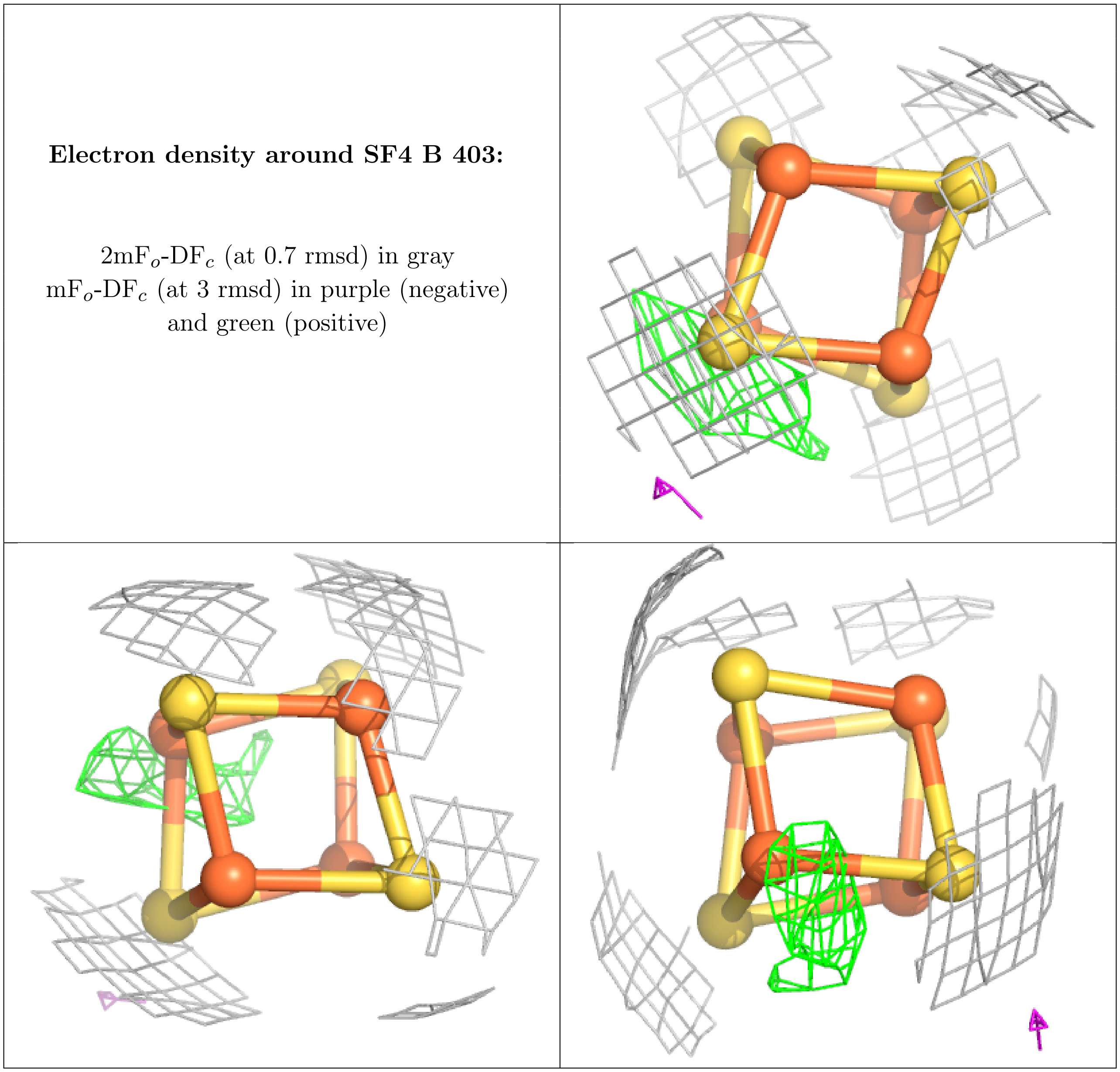




Electron density around ZN A 402:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



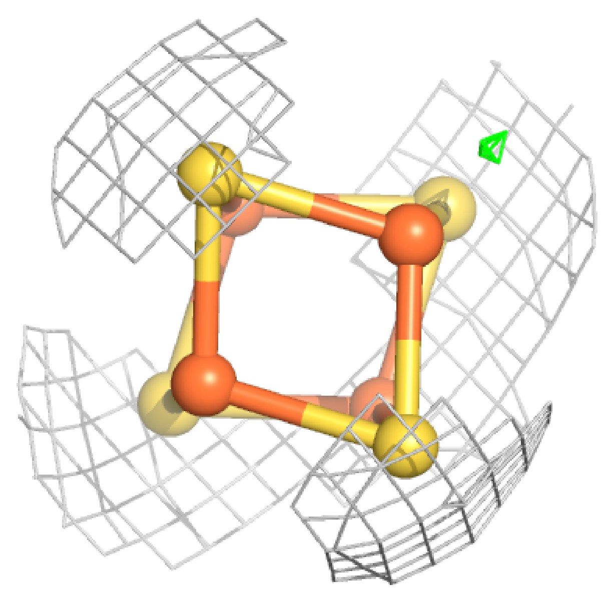


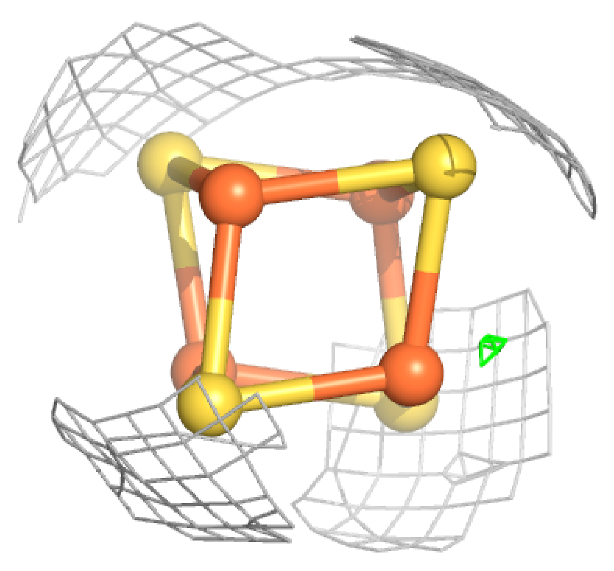
Electron density around SF4 B 403:

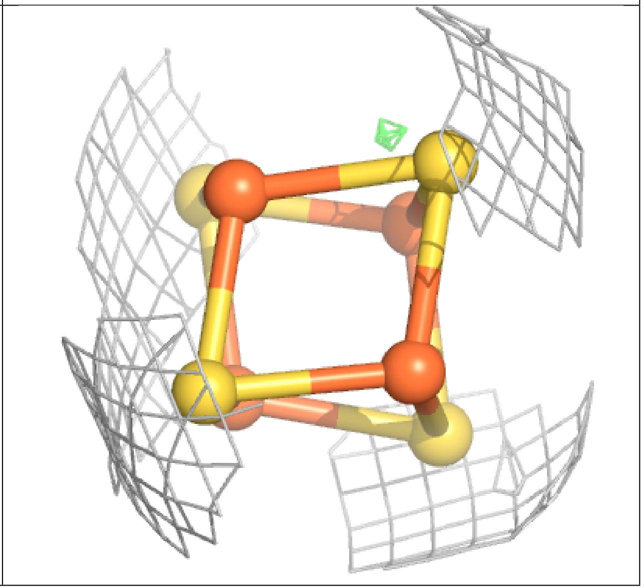
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

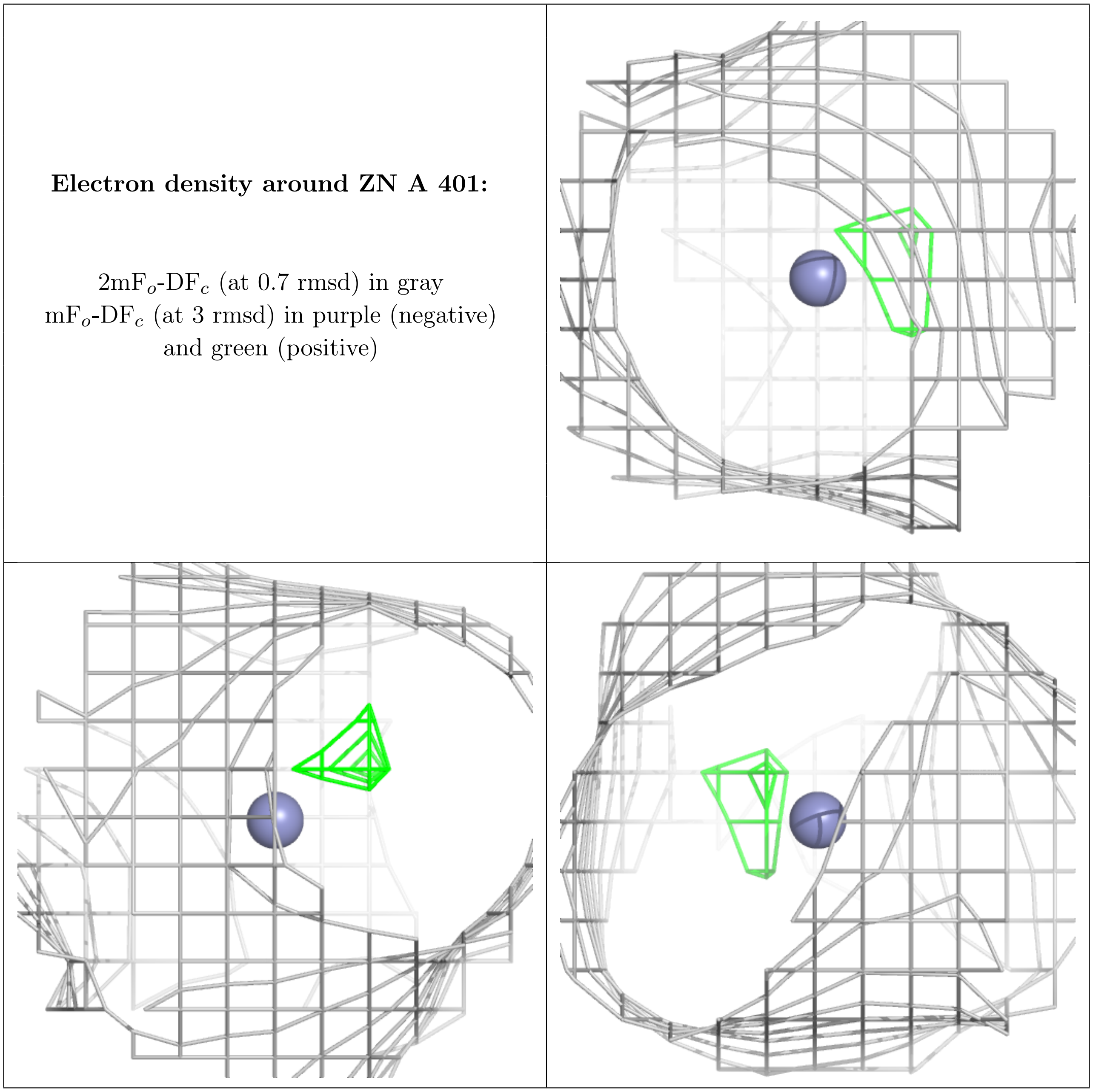
Electron density around SF4 A 403:

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



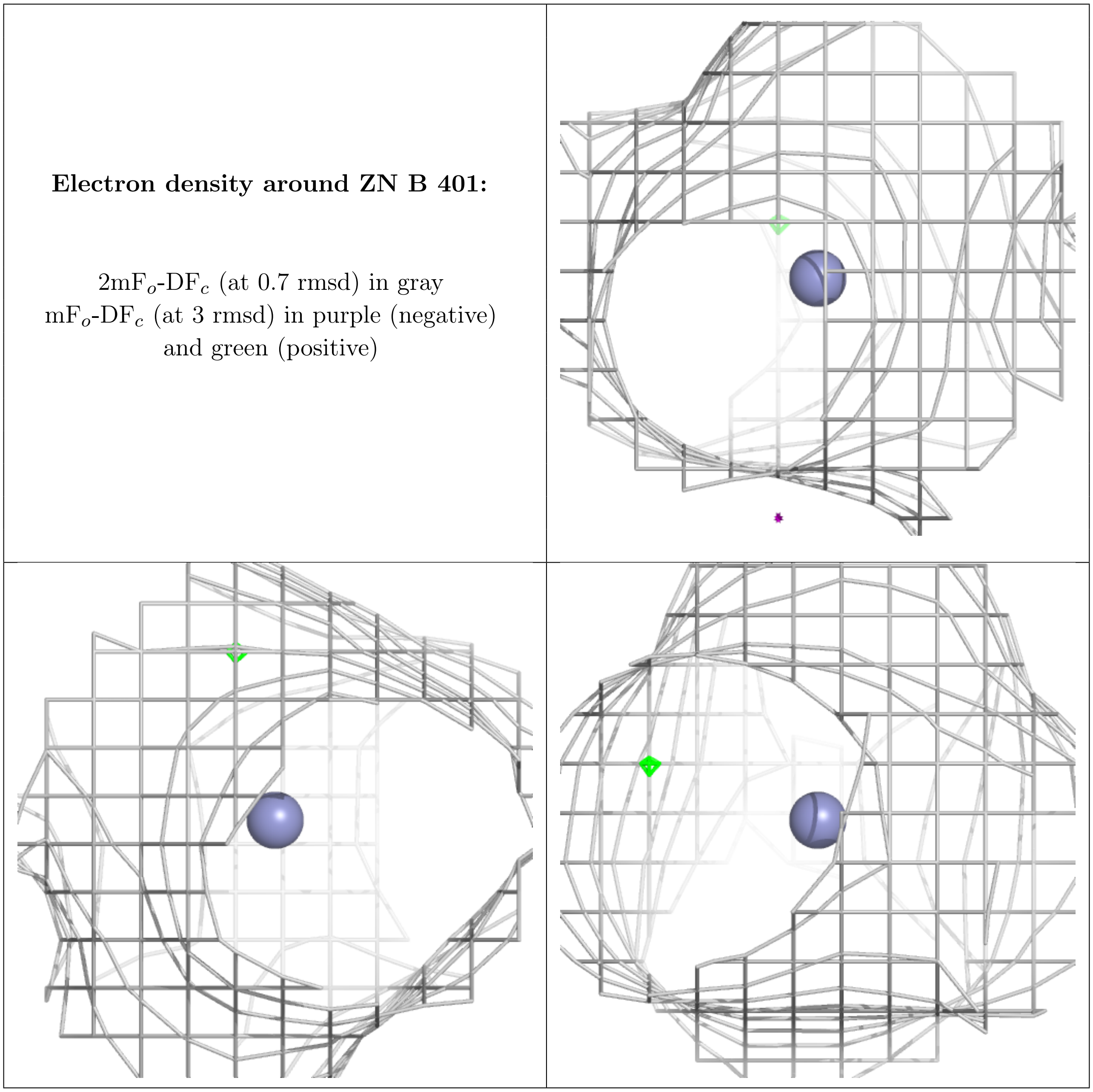






Electron density around ZN A 401:

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 ZN 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.