Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2023 – 10:54 PM EDT

PDB ID	:	8FG8
Title	:	Catalytic domain of GtfB in complex with inhibitor 2-[(2,4,5-Trihydroxyphenyl)methylidene]-1-benzofuran-3-one
Authors	:	Schormann, N.; Deivanayagam, C.; Velu, S.
Deposited on	:	2022-12-12
Resolution	:	2.35 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 ⓘ 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 ⓘ) were used in the production of this report:

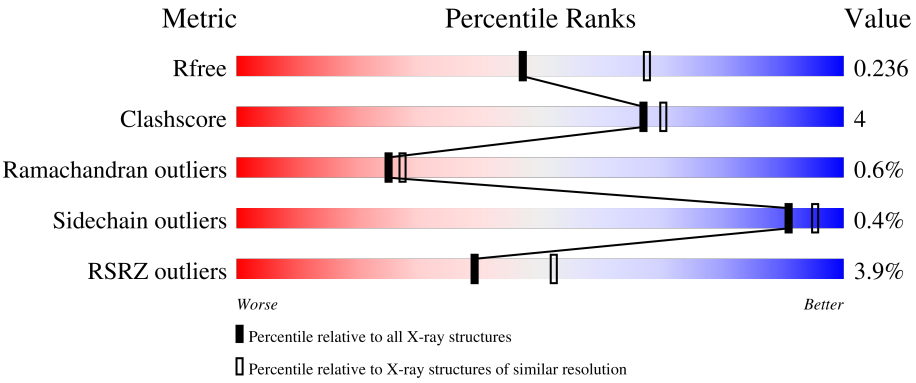
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	869	3% 90% 6% ·
1	B	869	4% 87% 7% · 5%

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
4	BTB	A	1203	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13759 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 Glucosyltransferase-I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	835	Total 6595	C 4154	N 1132	O 1293	S 16	0	0	0
1	B	824	Total 6470	C 4074	N 1110	O 1270	S 16	0	1	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1052	LEU	-	expression tag	UNP P08987
A	1053	GLU	-	expression tag	UNP P08987
A	1054	HIS	-	expression tag	UNP P08987
A	1055	HIS	-	expression tag	UNP P08987
A	1056	HIS	-	expression tag	UNP P08987
A	1057	HIS	-	expression tag	UNP P08987
A	1058	HIS	-	expression tag	UNP P08987
A	1059	HIS	-	expression tag	UNP P08987
B	1052	LEU	-	expression tag	UNP P08987
B	1053	GLU	-	expression tag	UNP P08987
B	1054	HIS	-	expression tag	UNP P08987
B	1055	HIS	-	expression tag	UNP P08987
B	1056	HIS	-	expression tag	UNP P08987
B	1057	HIS	-	expression tag	UNP P08987
B	1058	HIS	-	expression tag	UNP P08987
B	1059	HIS	-	expression tag	UNP P08987

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0

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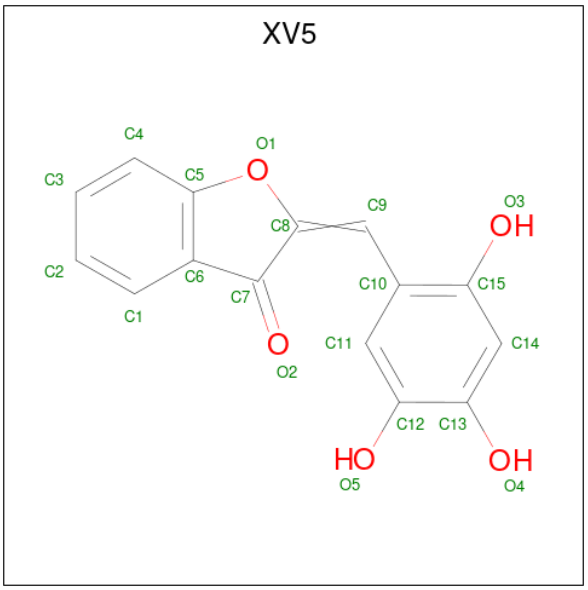
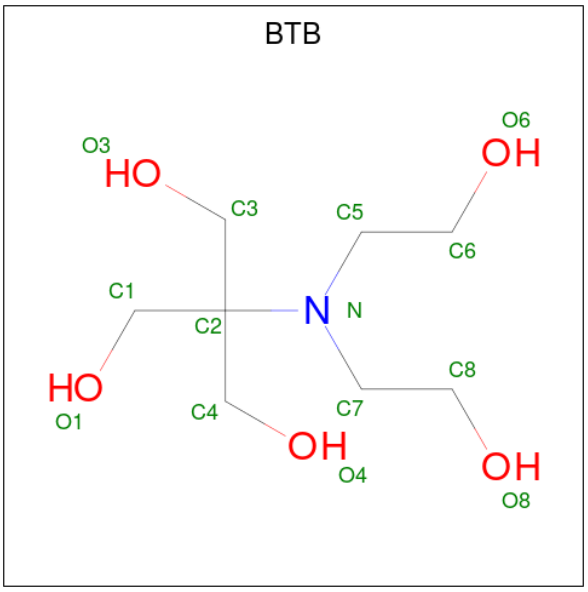
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Ca 2 2	0	0

- Molecule 3 is (2Z)-2-[(2,4,5-trihydroxyphenyl)methylidene]-1-benzofuran-3(2H)-one (three-letter code: XV5) (formula: $C_{15}H_{10}O_5$) (labeled as "Ligand of Interest" by depositor).



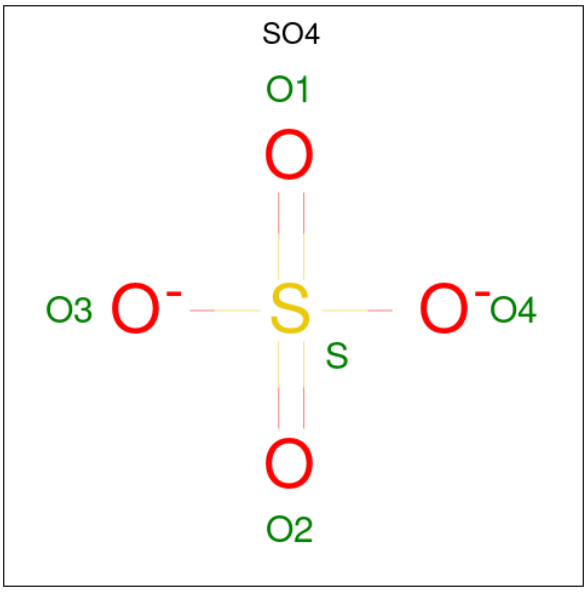
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 20 15 5	0	0
3	B	1	Total C O 20 15 5	0	0

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: BTB) (formula: $C_8H_{19}NO_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	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	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.

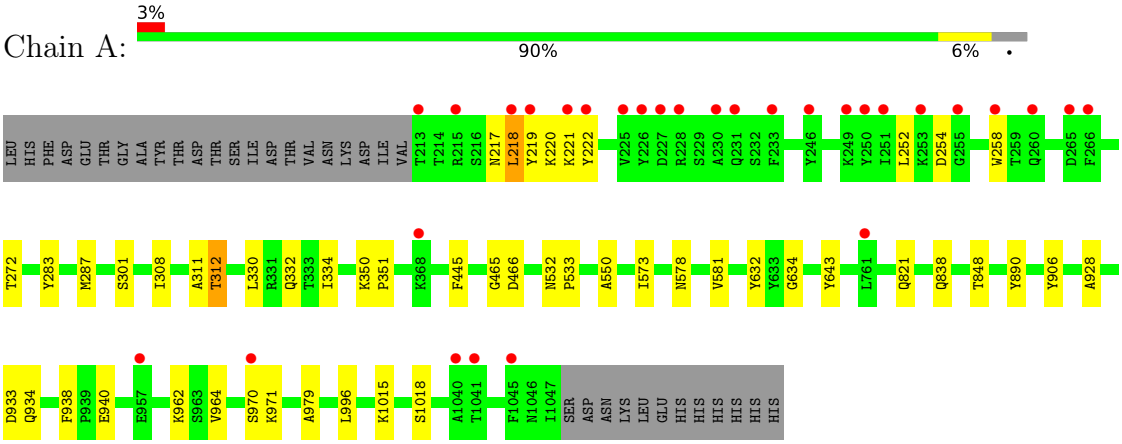
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	245	Total O 245 245	0	0
6	B	258	Total O 258 258	0	0

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.

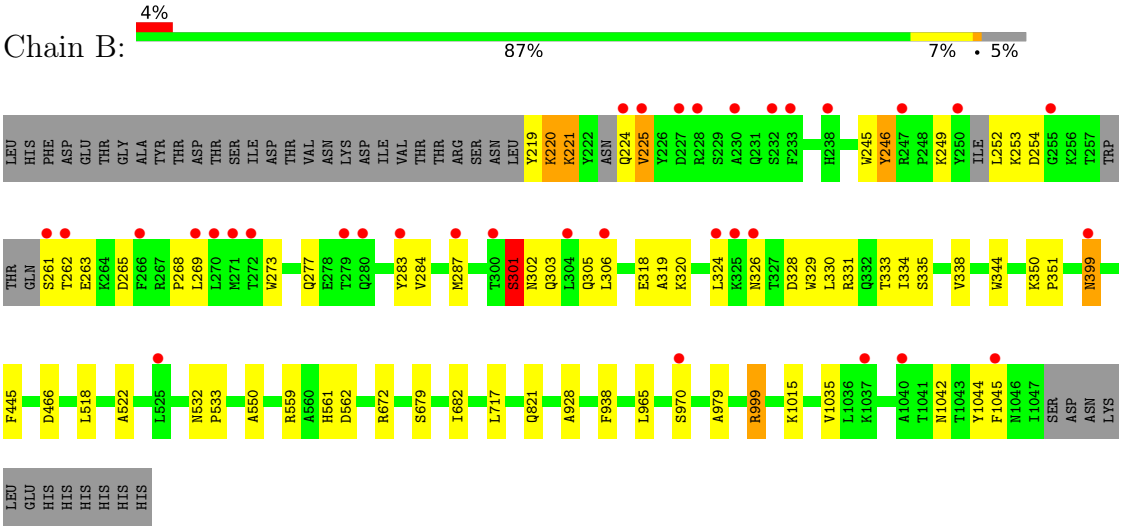
• Molecule 1: Glucosyltransferase-I

Chain A:



• Molecule 1: Glucosyltransferase-I

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.46Å 150.46Å 304.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.04 – 2.35 73.04 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.1 (73.04-2.35) 96.1 (73.04-2.35)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0257, PHENIX 1.16_3549	Depositor
R, R_{free}	0.205 , 0.233 0.208 , 0.236	Depositor DCC
R_{free} test set	6850 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	48.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 34.7	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	0.95	EDS
Total number of atoms	13759	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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: BTB, SO4, XV5, CA

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	0.65	0/6734	0.76	0/9138
1	B	0.65	0/6603	0.77	1/8958 (0.0%)
All	All	0.65	0/13337	0.76	1/18096 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	559	ARG	NE-CZ-NH1	5.61	123.11	120.30

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	6595	0	6422	38	0
1	B	6470	0	6261	54	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
3	A	20	0	0	2	0
3	B	20	0	0	1	0
4	A	14	0	19	7	0
4	B	14	0	19	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	50	0	0	0	0
5	B	70	0	0	0	0
6	A	245	0	0	3	0
6	B	258	0	0	2	0
All	All	13759	0	12721	100	0

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

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:SER:O	1:B:338:VAL:HG12	1.84	0.76
1:B:284:VAL:HG21	1:B:306:LEU:HD22	1.69	0.74
1:A:838:GLN:HE22	1:A:848:THR:HG21	1.52	0.74
1:B:338:VAL:HG23	1:B:344:TRP:CE3	2.25	0.71
1:A:573:ILE:CG2	1:A:581:VAL:HG21	2.24	0.67
4:B:1203:BTB:O3	4:B:1203:BTB:O8	2.13	0.65
1:B:277:GLN:HG2	1:B:303:GLN:HG2	1.79	0.64
1:A:573:ILE:HG21	1:A:581:VAL:HG21	1.79	0.64
1:B:1042:ASN:HB3	6:B:1308:HOH:O	1.97	0.64
1:A:252:LEU:O	1:A:254:ASP:O	2.16	0.63
1:A:838:GLN:NE2	1:A:848:THR:HG21	2.13	0.63
1:B:219:TYR:O	1:B:221:LYS:N	2.27	0.60
1:B:320:LYS:HE3	1:B:324:LEU:HD11	1.82	0.60
1:B:329:TRP:O	1:B:333:THR:HG23	2.03	0.59
1:A:217:ASN:O	1:A:218:LEU:HB2	2.02	0.58
1:A:962:LYS:H	1:A:964:VAL:CG2	2.15	0.58
1:B:330:LEU:O	1:B:330:LEU:HD13	2.03	0.58
1:A:962:LYS:O	1:A:964:VAL:HG23	2.06	0.55
1:A:962:LYS:H	1:A:964:VAL:HG23	1.71	0.55
1:B:254:ASP:OD1	1:B:319:ALA:N	2.40	0.54
1:B:561:HIS:NE2	4:B:1203:BTB:H81	2.23	0.54
1:A:643:TYR:HB2	1:A:848:THR:HG22	1.90	0.54
1:A:332:GLN:NE2	1:B:329:TRP:HB2	2.22	0.54
4:B:1203:BTB:O1	4:B:1203:BTB:H62	2.08	0.54
1:B:965:LEU:HB2	1:B:1035:VAL:HG11	1.91	0.53
3:A:1202:XV5:C2	6:A:1536:HOH:O	2.57	0.53
1:A:218:LEU:CD2	1:A:272:THR:HB	2.38	0.53
3:A:1202:XV5:C2	6:A:1463:HOH:O	2.57	0.53
1:A:283:TYR:CE1	1:A:287:MET:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:LEU:O	1:B:334:ILE:HG22	2.10	0.52
1:B:326:ASN:ND2	1:B:328:ASP:HB2	2.25	0.52
1:A:578:ASN:O	1:A:581:VAL:HG23	2.11	0.51
1:B:1035:VAL:HG13	1:B:1044:TYR:CE2	2.45	0.51
1:A:962:LYS:C	1:A:964:VAL:HG23	2.31	0.51
1:B:329:TRP:CZ3	1:B:330:LEU:HD23	2.46	0.51
1:A:308:ILE:O	1:A:311:ALA:O	2.29	0.50
1:B:326:ASN:HD22	1:B:328:ASP:HB2	1.77	0.50
1:B:254:ASP:CG	1:B:319:ALA:HA	2.32	0.50
1:B:979:ALA:O	1:B:1015:LYS:HD2	2.11	0.50
1:A:330:LEU:O	1:A:334:ILE:HG12	2.12	0.50
1:A:218:LEU:HG	1:A:219:TYR:N	2.26	0.50
1:B:399:ASN:ND2	6:B:1306:HOH:O	2.44	0.50
1:B:254:ASP:OD1	1:B:319:ALA:HA	2.12	0.49
1:B:252:LEU:HD23	1:B:252:LEU:O	2.12	0.49
1:B:221:LYS:O	1:B:249:LYS:HE3	2.12	0.49
1:A:332:GLN:HE22	1:B:329:TRP:HB2	1.78	0.49
4:A:1203:BTB:O3	4:A:1203:BTB:C7	2.61	0.49
1:A:848:THR:OG1	1:A:906:TYR:HB3	2.13	0.49
1:B:224:GLN:O	1:B:225:VAL:HG22	2.12	0.49
1:A:222:TYR:HB3	1:A:258:TRP:CZ3	2.48	0.48
1:B:283:TYR:CE1	1:B:287:MET:HG3	2.48	0.48
1:A:979:ALA:O	1:A:1015:LYS:HD2	2.14	0.48
1:A:933:ASP:HB3	1:A:934:GLN:OE1	2.14	0.48
1:B:320:LYS:NZ	1:B:324:LEU:HD21	2.29	0.47
1:A:938:PHE:CD2	1:A:970:SER:HA	2.50	0.47
1:B:254:ASP:OD1	1:B:318:GLU:C	2.53	0.47
1:B:225:VAL:HA	1:B:246:TYR:HE2	1.79	0.47
1:B:329:TRP:CH2	1:B:330:LEU:HD23	2.50	0.47
1:B:532:ASN:N	1:B:533:PRO:CD	2.79	0.46
1:B:254:ASP:OD1	1:B:319:ALA:CA	2.64	0.45
1:B:938:PHE:CD2	1:B:970:SER:HA	2.51	0.45
4:A:1203:BTB:O3	4:A:1203:BTB:H71	2.16	0.45
4:A:1203:BTB:H51	4:A:1203:BTB:O4	2.17	0.45
1:A:550:ALA:HB3	1:A:821:GLN:HB3	1.99	0.45
1:A:890:TYR:CD2	4:A:1203:BTB:H72	2.52	0.45
1:B:350:LYS:HB3	1:B:351:PRO:HA	1.99	0.45
1:B:225:VAL:HA	1:B:246:TYR:CE2	2.53	0.44
1:B:550:ALA:HB3	1:B:821:GLN:HB3	2.00	0.44
1:A:218:LEU:HG	1:A:219:TYR:H	1.81	0.43
1:B:268:PRO:HG3	1:B:330:LEU:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ASP:OD2	4:B:1203:BTB:O8	2.36	0.43
1:B:252:LEU:O	1:B:254:ASP:N	2.41	0.43
1:A:970:SER:O	1:A:1018:SER:HA	2.18	0.43
1:B:269:LEU:HD21	1:B:273:TRP:CE3	2.54	0.43
1:B:245:TRP:CZ2	1:B:331:ARG:HG2	2.53	0.43
1:B:261:SER:C	1:B:263:GLU:H	2.22	0.43
1:B:320:LYS:CE	1:B:324:LEU:HD11	2.46	0.43
1:A:532:ASN:N	1:A:533:PRO:CD	2.82	0.42
4:A:1203:BTB:O4	4:A:1203:BTB:C5	2.68	0.42
1:B:261:SER:N	1:B:265:ASP:CB	2.83	0.42
1:B:466:ASP:OD2	1:B:999:ARG:HD2	2.20	0.42
1:A:445:PHE:CG	1:A:928:ALA:HB2	2.54	0.42
1:A:311:ALA:O	1:A:312:THR:CB	2.68	0.42
1:B:301:SER:HB3	1:B:302:ASN:H	1.75	0.41
1:A:465:GLY:HA3	6:A:1348:HOH:O	2.20	0.41
1:B:672:ARG:O	1:B:682:ILE:HA	2.21	0.41
4:A:1203:BTB:H81	4:A:1203:BTB:H52	1.92	0.41
3:B:1202:XV5:O1	3:B:1202:XV5:O3	2.38	0.41
1:A:220:LYS:HG2	1:A:221:LYS:H	1.86	0.41
1:A:466:ASP:HB3	1:A:996:LEU:CD2	2.51	0.41
1:A:632:TYR:CE2	1:A:634:GLY:HA3	2.56	0.41
1:B:302:ASN:O	1:B:303:GLN:C	2.59	0.41
1:A:350:LYS:HB3	1:A:351:PRO:HA	2.03	0.41
1:A:890:TYR:CD1	4:A:1203:BTB:H12	2.56	0.40
1:A:940:GLU:HB2	1:A:971:LYS:HB2	2.03	0.40
1:B:561:HIS:NE2	4:B:1203:BTB:C8	2.84	0.40
1:B:445:PHE:CG	1:B:928:ALA:HB2	2.56	0.40
1:B:518:LEU:HD12	1:B:522:ALA:HB3	2.04	0.40
1:B:338:VAL:CG2	1:B:344:TRP:CE3	3.00	0.40
1:B:679:SER:HB3	1:B:717:LEU:HD13	2.03	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	833/869 (96%)	799 (96%)	31 (4%)	3 (0%)	34 38
1	B	817/869 (94%)	784 (96%)	26 (3%)	7 (1%)	17 17
All	All	1650/1738 (95%)	1583 (96%)	57 (4%)	10 (1%)	25 27

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	LEU
1	B	301	SER
1	B	305	GLN
1	A	301	SER
1	B	220	LYS
1	B	262	THR
1	B	1045	PHE
1	B	225	VAL
1	B	253	LYS
1	A	312	THR

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	706/738 (96%)	706 (100%)	0	100 100
1	B	686/738 (93%)	680 (99%)	6 (1%)	78 87
All	All	1392/1476 (94%)	1386 (100%)	6 (0%)	91 95

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	220	LYS
1	B	221	LYS
1	B	246	TYR

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Mol	Chain	Res	Type
1	B	301	SER
1	B	399	ASN
1	B	999	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	756	GLN
1	A	855	ASN
1	B	305	GLN
1	B	855	ASN
1	B	934	GLN

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 31 ligands modelled in this entry, 3 are monoatomic - leaving 28 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	1207	-	4,4,4	0.35	0	6,6,6	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	SO4	B	1206	-	4,4,4	0.36	0	6,6,6	0.08	0
5	SO4	B	1212	-	4,4,4	0.32	0	6,6,6	0.12	0
3	XV5	A	1202	-	22,22,22	0.40	0	31,32,32	0.56	0
5	SO4	A	1206	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	A	1213	-	4,4,4	0.30	0	6,6,6	0.08	0
5	SO4	B	1214	-	4,4,4	0.36	0	6,6,6	0.13	0
5	SO4	B	1208	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	B	1207	-	4,4,4	0.37	0	6,6,6	0.08	0
5	SO4	A	1204	-	4,4,4	0.34	0	6,6,6	0.06	0
5	SO4	A	1205	-	4,4,4	0.34	0	6,6,6	0.05	0
5	SO4	B	1215	-	4,4,4	0.36	0	6,6,6	0.07	0
5	SO4	B	1213	-	4,4,4	0.33	0	6,6,6	0.16	0
4	BTB	A	1203	-	13,13,13	1.71	1 (7%)	7,16,16	1.09	0
5	SO4	B	1210	-	4,4,4	0.33	0	6,6,6	0.08	0
5	SO4	B	1217	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	B	1216	-	4,4,4	0.35	0	6,6,6	0.07	0
5	SO4	A	1208	-	4,4,4	0.34	0	6,6,6	0.11	0
5	SO4	A	1209	-	4,4,4	0.32	0	6,6,6	0.18	0
5	SO4	B	1209	-	4,4,4	0.28	0	6,6,6	0.12	0
5	SO4	A	1210	-	4,4,4	0.33	0	6,6,6	0.10	0
3	XV5	B	1202	2	22,22,22	0.40	0	31,32,32	0.60	0
5	SO4	A	1212	-	4,4,4	0.29	0	6,6,6	0.13	0
5	SO4	B	1205	-	4,4,4	0.34	0	6,6,6	0.08	0
5	SO4	A	1211	-	4,4,4	0.34	0	6,6,6	0.08	0
4	BTB	B	1203	2	13,13,13	1.39	1 (7%)	7,16,16	0.93	0
5	SO4	B	1204	-	4,4,4	0.28	0	6,6,6	0.26	0
5	SO4	B	1211	-	4,4,4	0.32	0	6,6,6	0.10	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
3	XV5	B	1202	2	-	4/4/16/16	0/3/3/3
3	XV5	A	1202	-	-	4/4/16/16	0/3/3/3
4	BTB	B	1203	2	-	6/21/21/21	-
4	BTB	A	1203	-	-	10/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1203	BTB	C2-N	6.06	1.60	1.48
4	B	1203	BTB	C2-N	4.88	1.58	1.48

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1202	XV5	C7-C8-C9-C10
3	A	1202	XV5	O1-C8-C9-C10
3	A	1202	XV5	C11-C10-C9-C8
3	A	1202	XV5	C15-C10-C9-C8
3	B	1202	XV5	C7-C8-C9-C10
3	B	1202	XV5	O1-C8-C9-C10
3	B	1202	XV5	C11-C10-C9-C8
4	A	1203	BTB	O1-C1-C2-C4
4	A	1203	BTB	C1-C2-C3-O3
4	A	1203	BTB	C1-C2-C4-O4
4	A	1203	BTB	C3-C2-C4-O4
4	A	1203	BTB	N-C2-C4-O4
4	A	1203	BTB	C4-C2-N-C5
4	A	1203	BTB	C8-C7-N-C5
4	B	1203	BTB	O1-C1-C2-C4
4	B	1203	BTB	C1-C2-C3-O3
4	B	1203	BTB	C3-C2-C4-O4
3	B	1202	XV5	C15-C10-C9-C8
4	A	1203	BTB	N-C7-C8-O8
4	A	1203	BTB	C1-C2-N-C5
4	A	1203	BTB	C3-C2-N-C5
4	B	1203	BTB	N-C2-C3-O3
4	B	1203	BTB	N-C2-C4-O4
4	B	1203	BTB	C1-C2-C4-O4

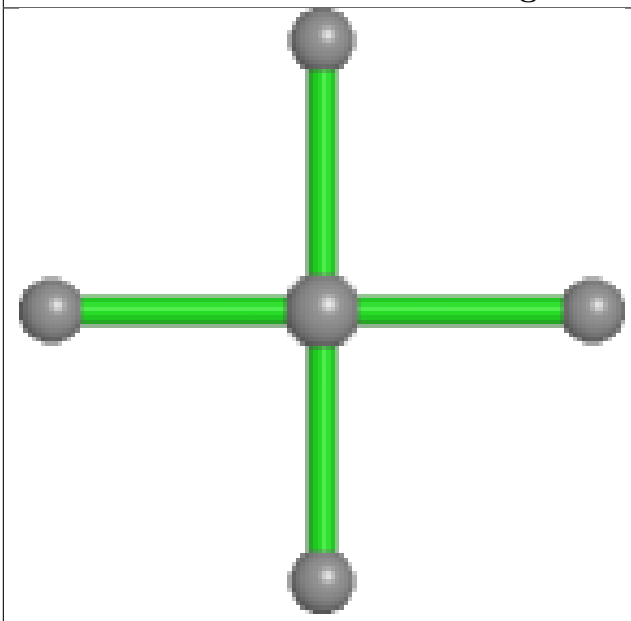
There are no ring outliers.

4 monomers are involved in 15 short contacts:

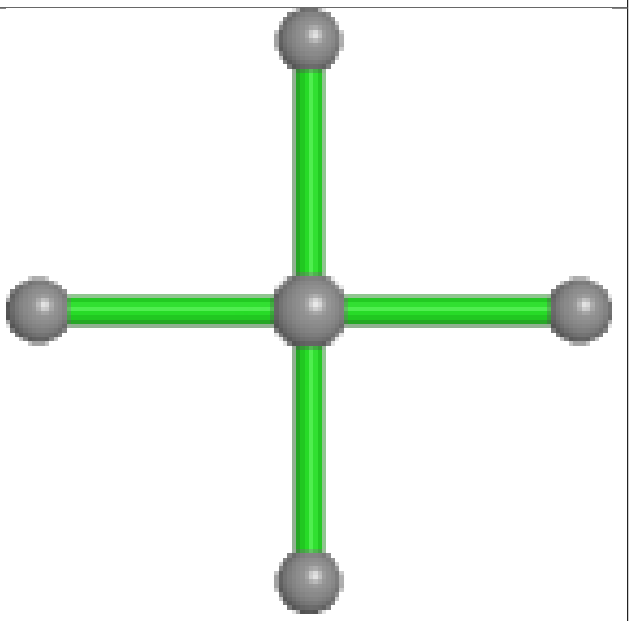
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1202	XV5	2	0
4	A	1203	BTB	7	0
3	B	1202	XV5	1	0
4	B	1203	BTB	5	0

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

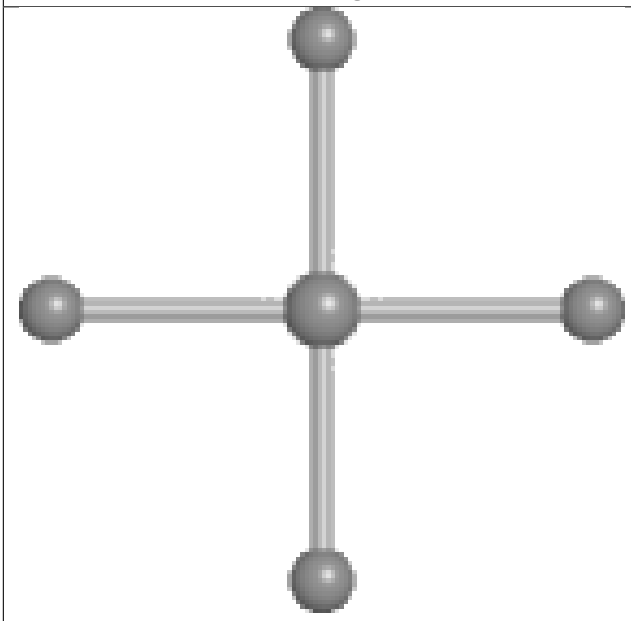
Ligand SO4 A 1207



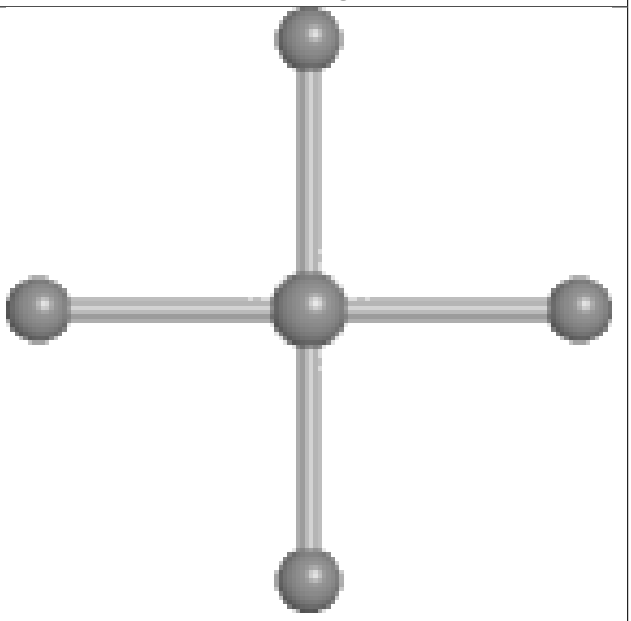
Bond lengths



Bond angles

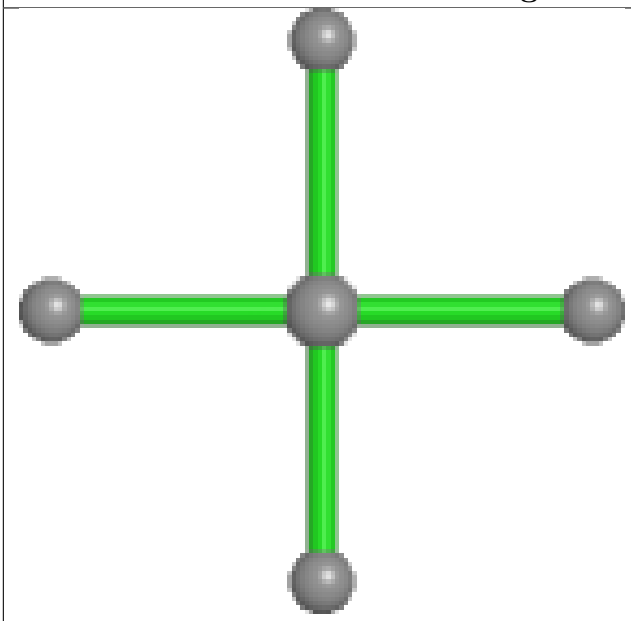


Torsions



Rings

Ligand SO4 B 1206



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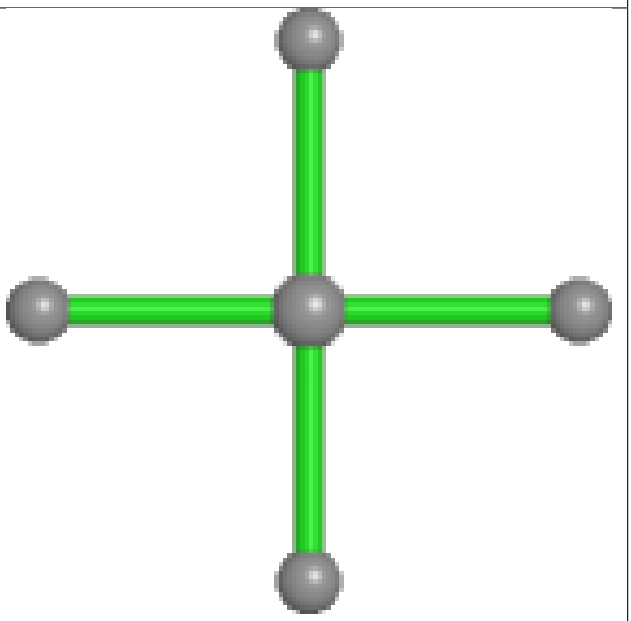

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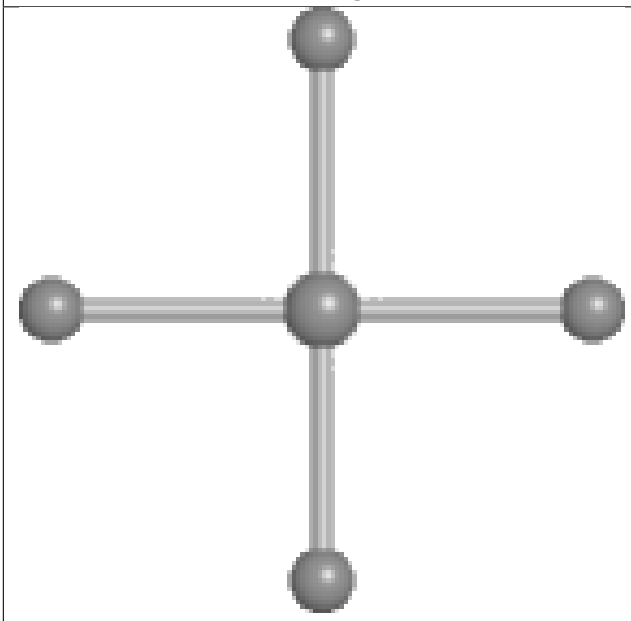

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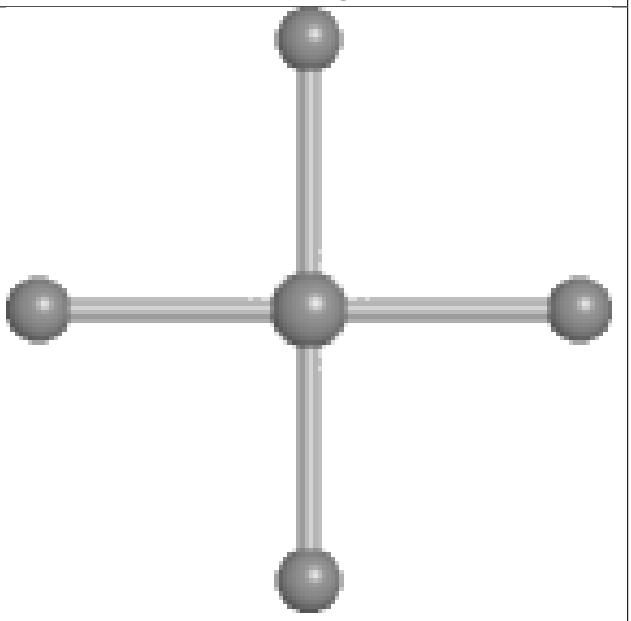
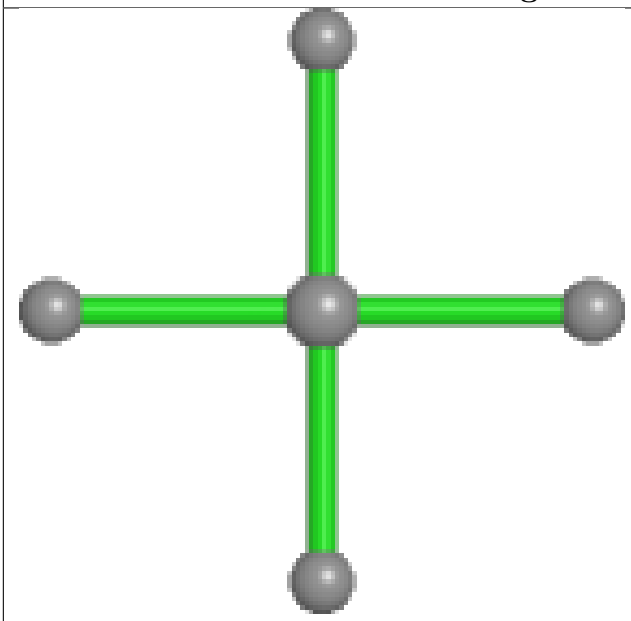


Rings

Ligand SO4 B 1212



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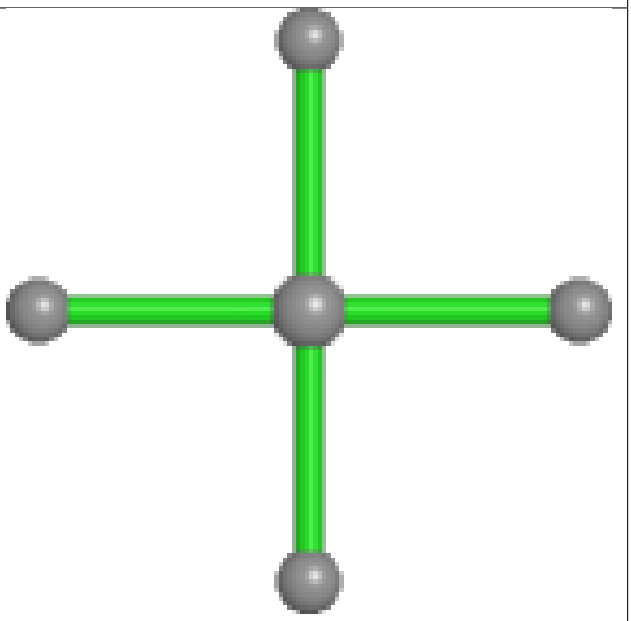
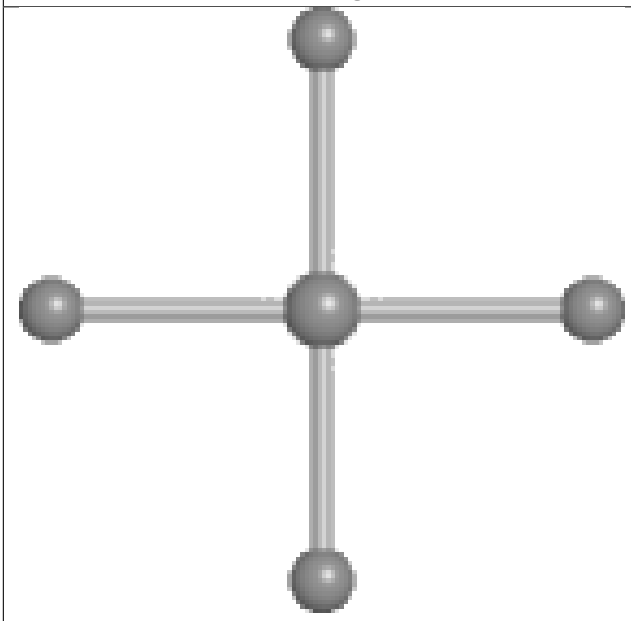


Bond angles



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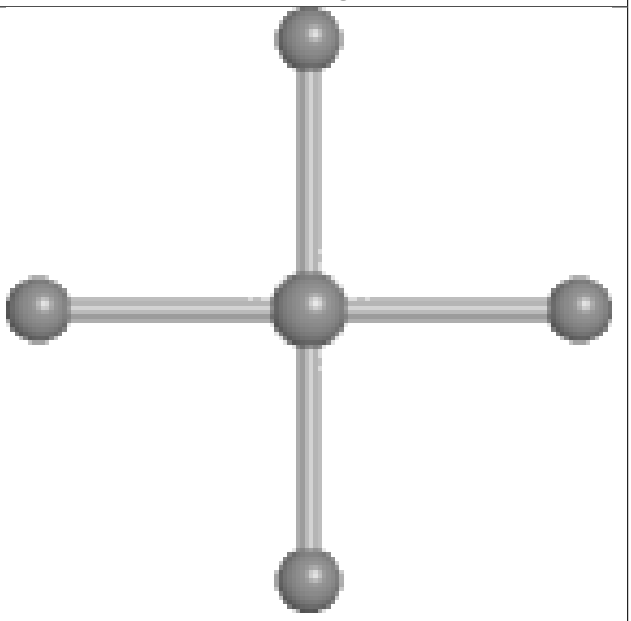
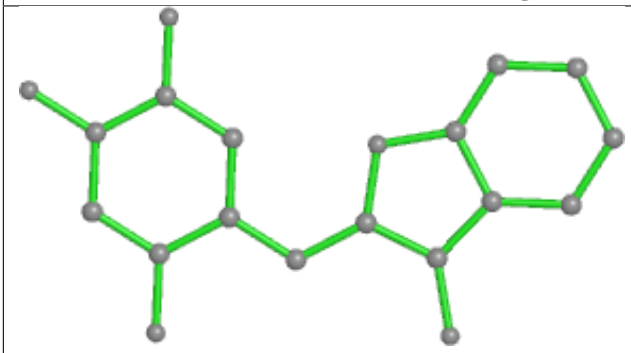


Rings

Ligand XV5 A 1202



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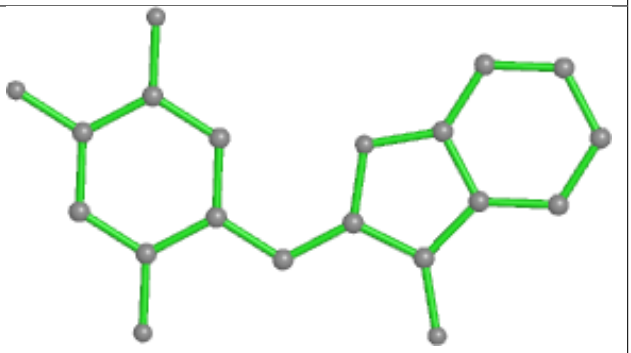

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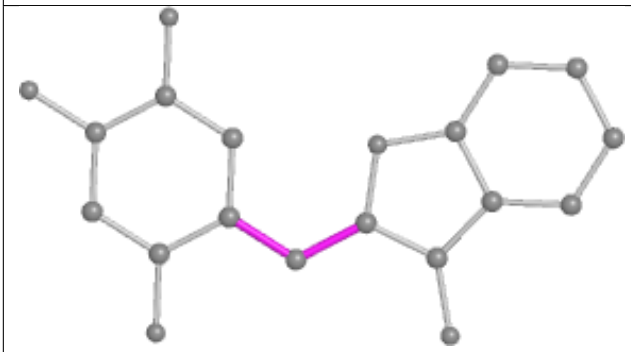

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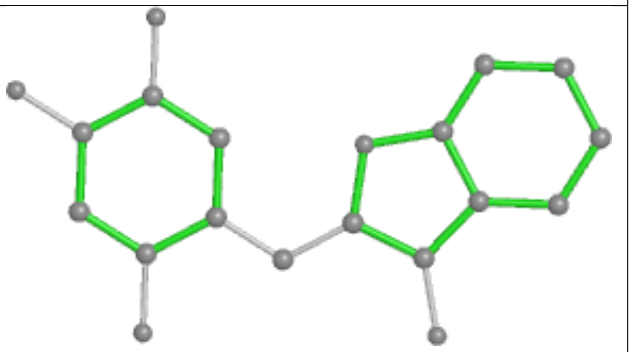
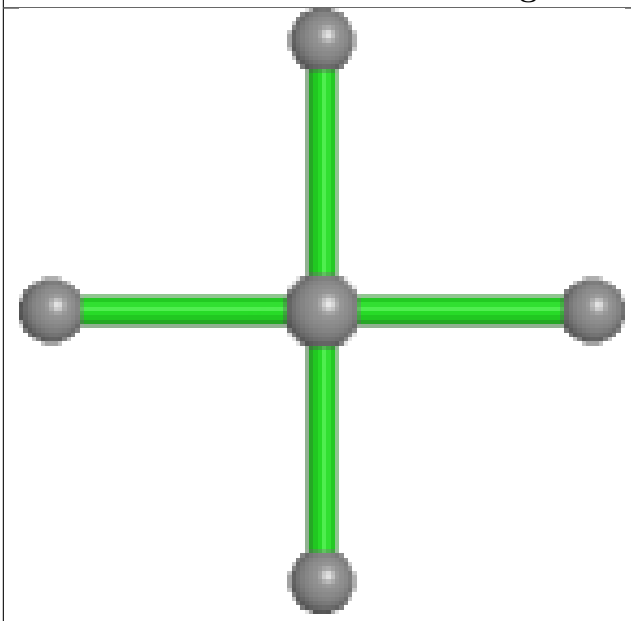


Rings

Ligand SO4 A 1206



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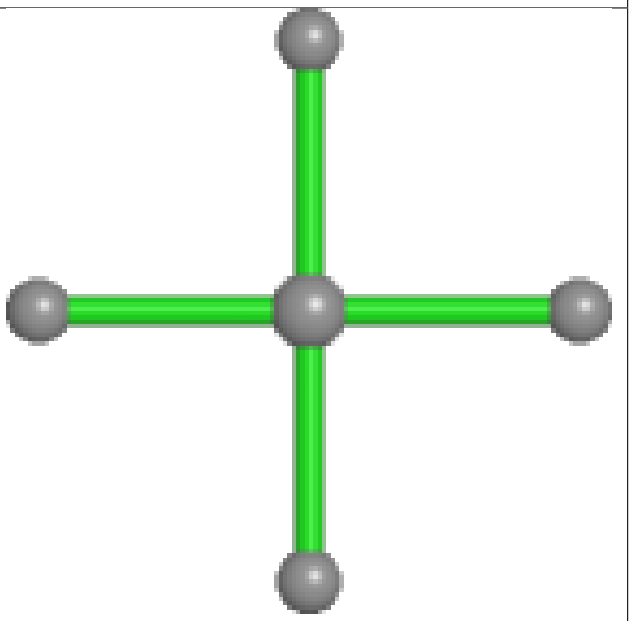

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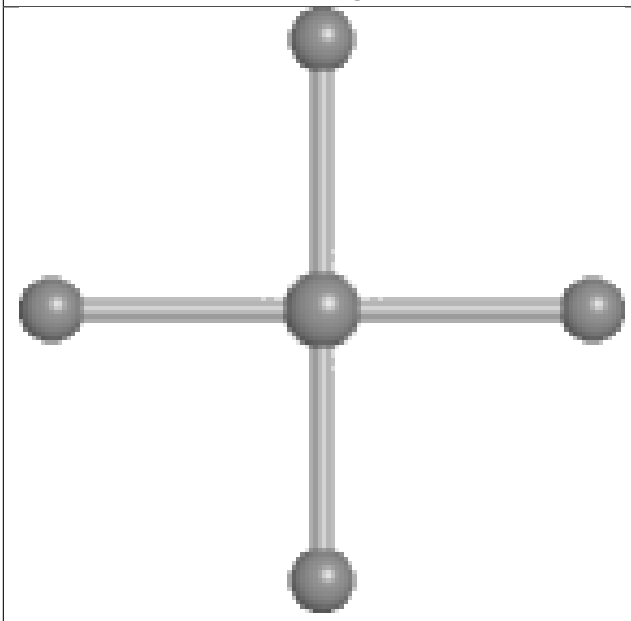

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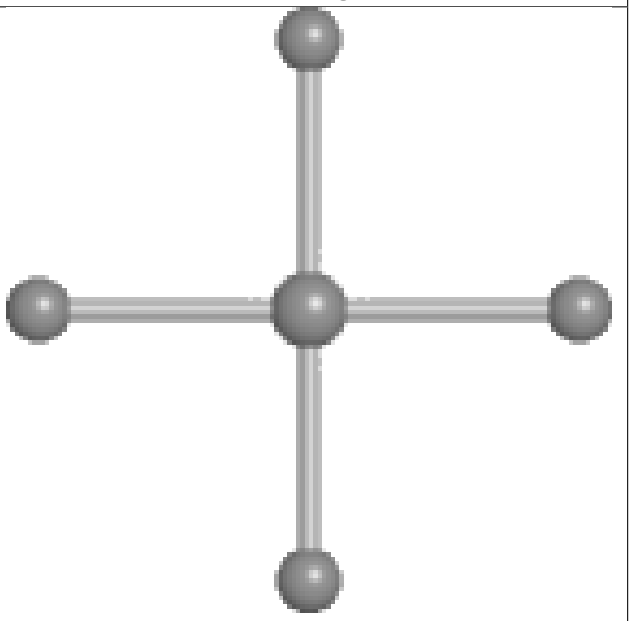
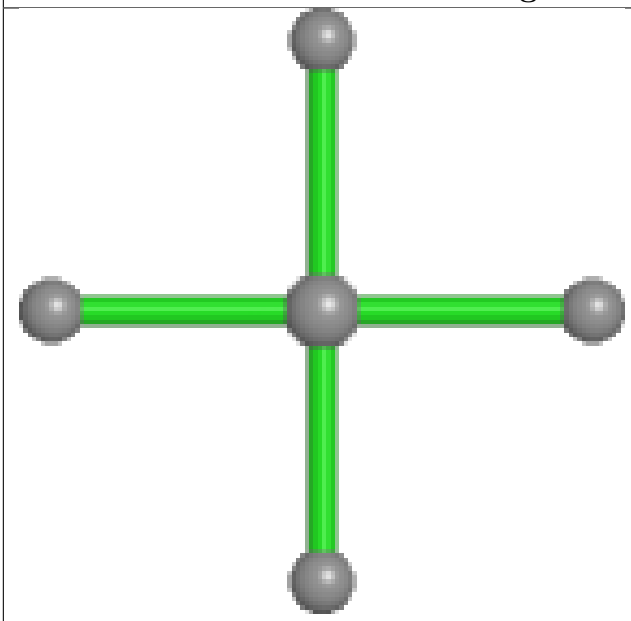


Rings

Ligand SO4 A 1213



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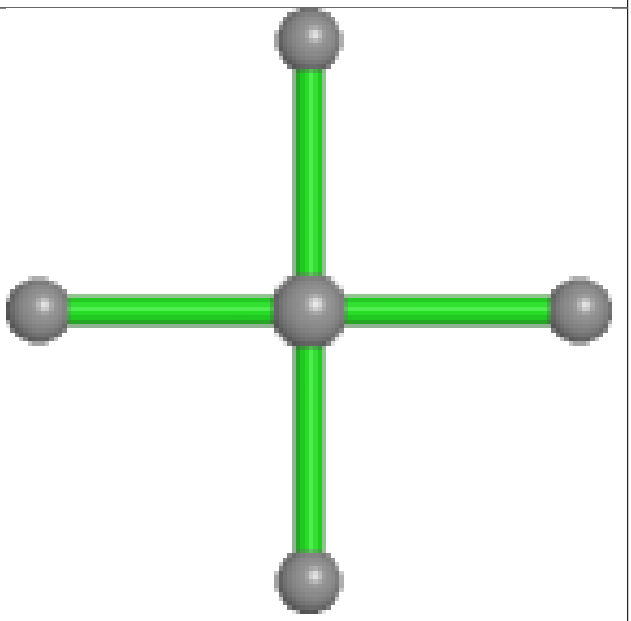

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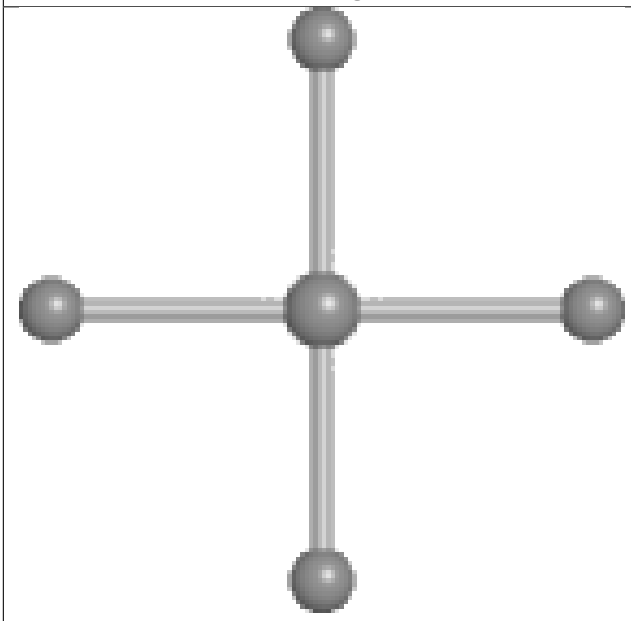

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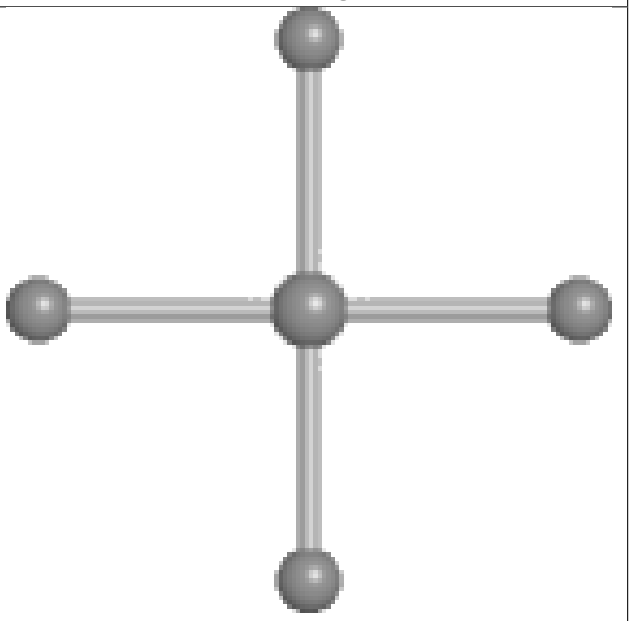
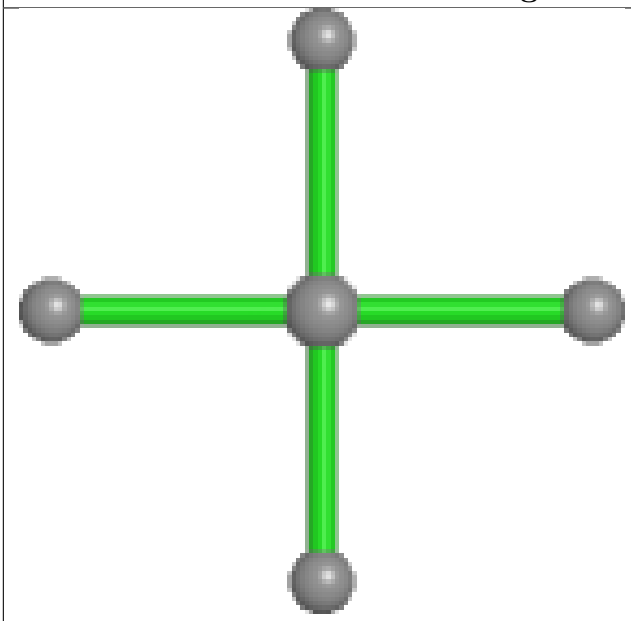
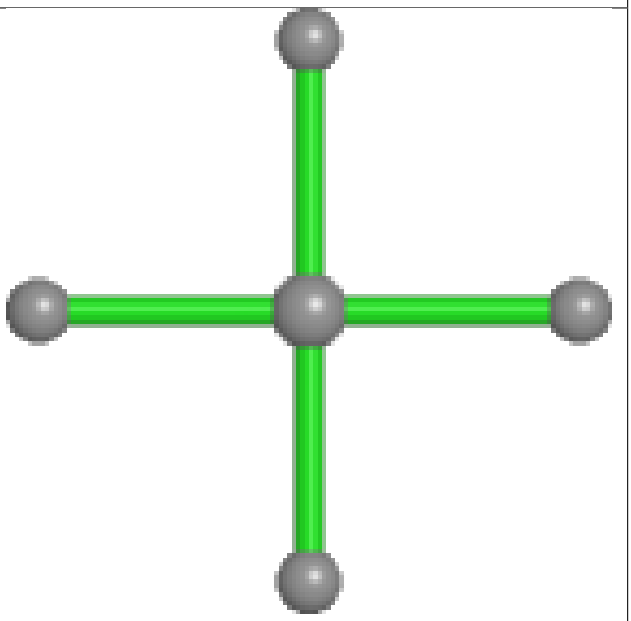


Rings

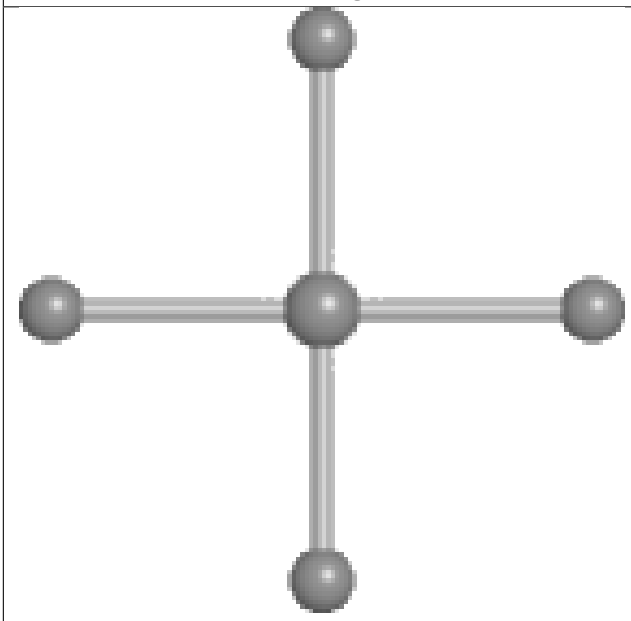
Ligand SO4 B 1214



Bond lengths



Bond angles



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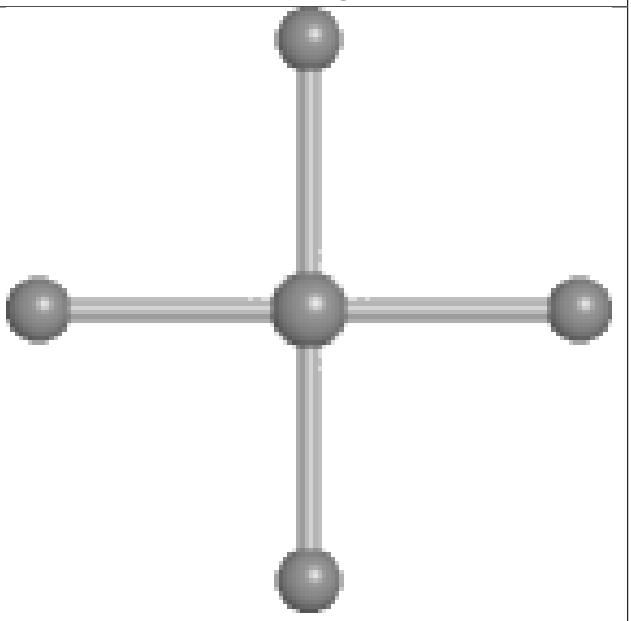
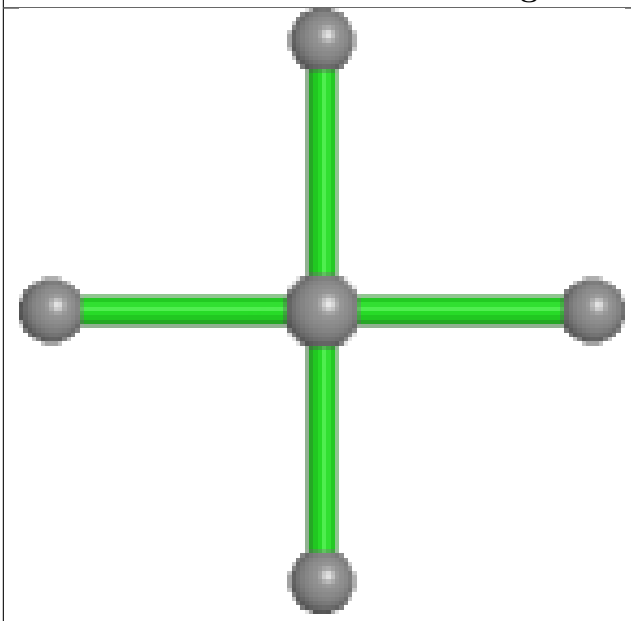
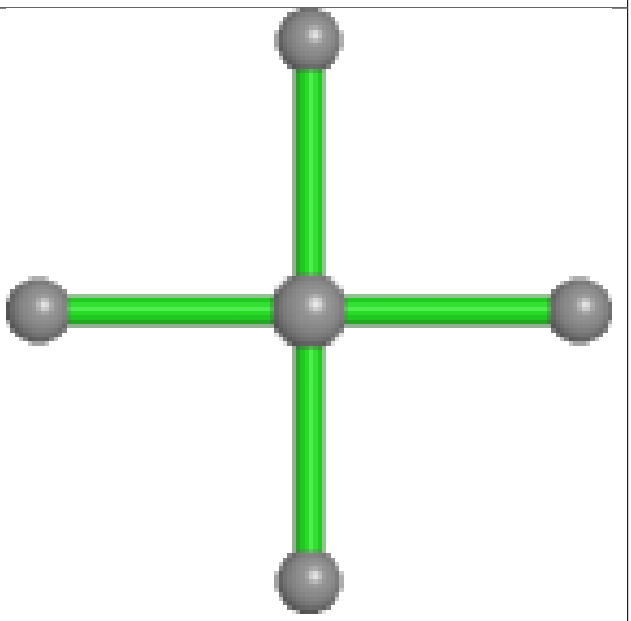


Rings

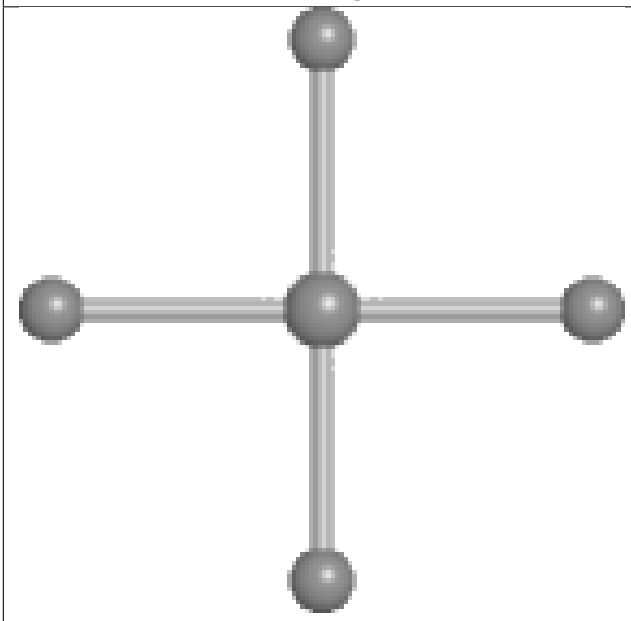
Ligand SO4 B 1208



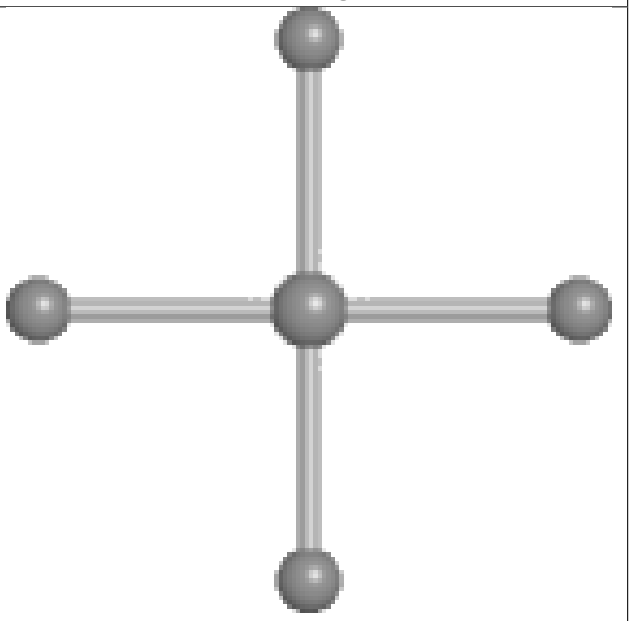
Bond lengths



Bond angles

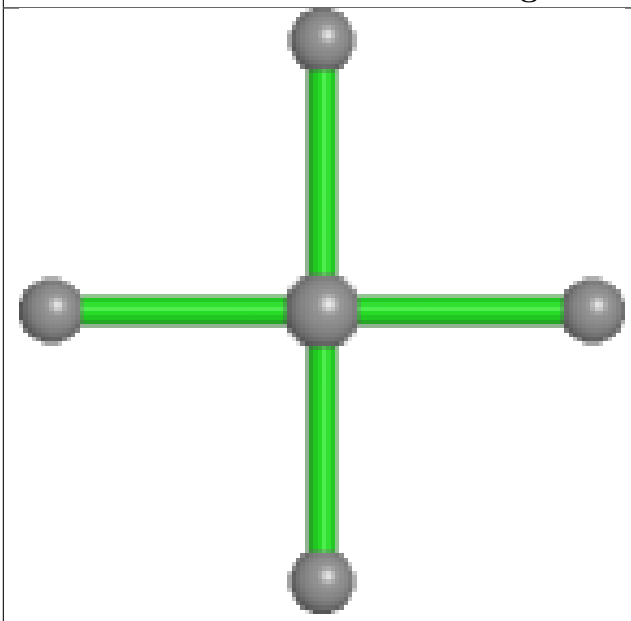


Torsions

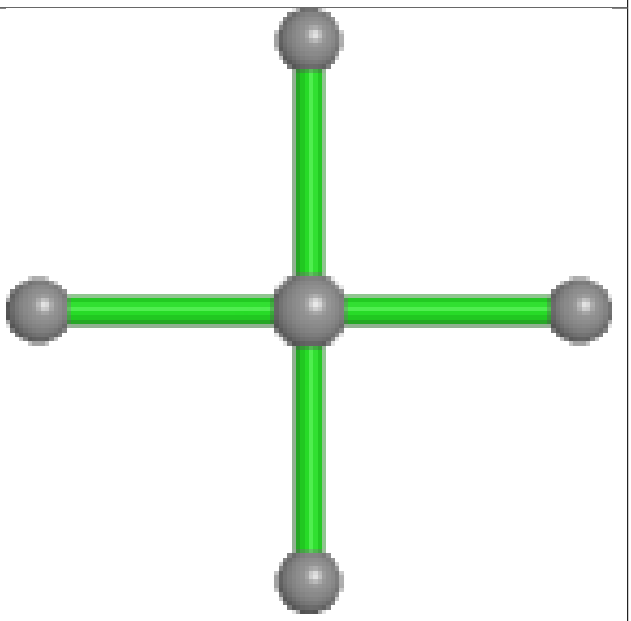


Rings

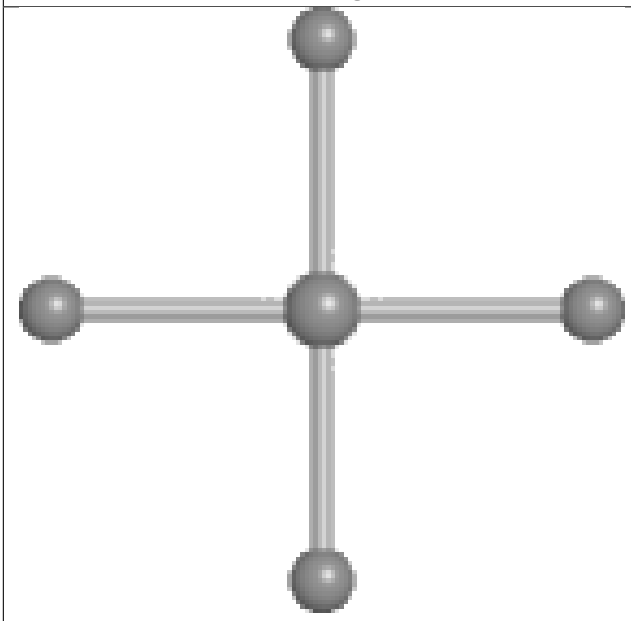
Ligand SO4 B 1207



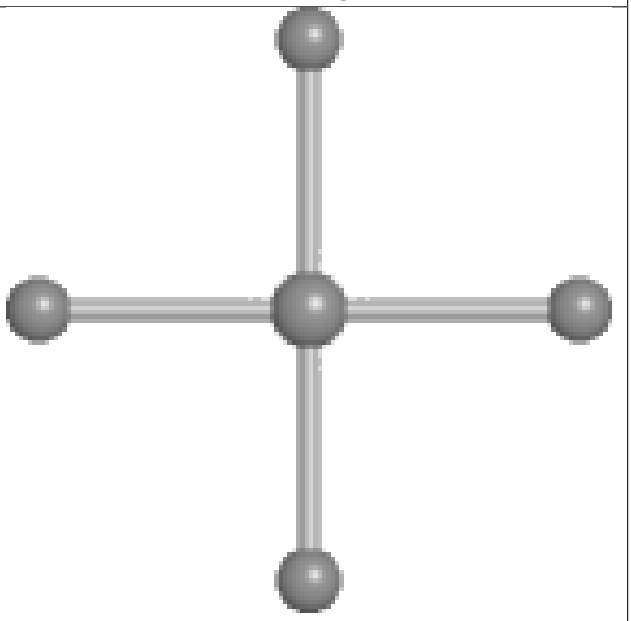
Bond lengths



Bond angles

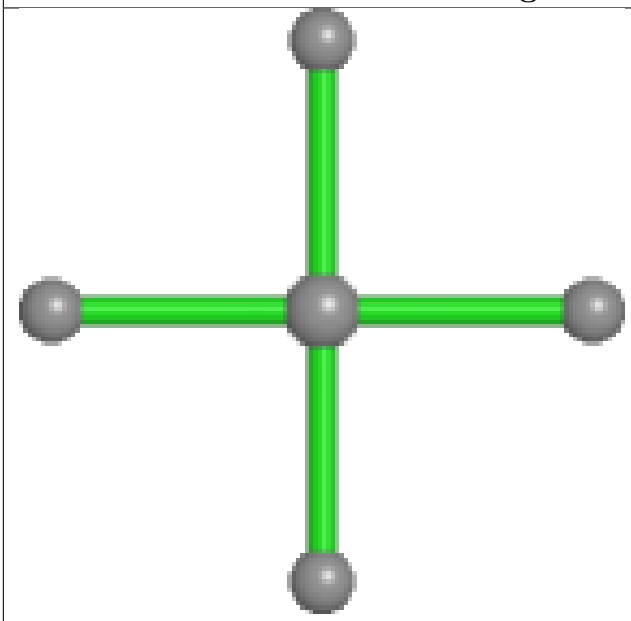


Torsions



Rings

Ligand SO4 A 1204



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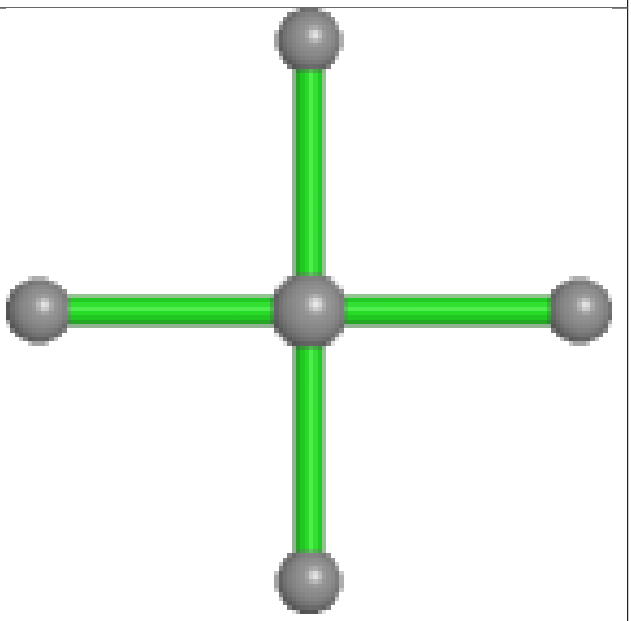
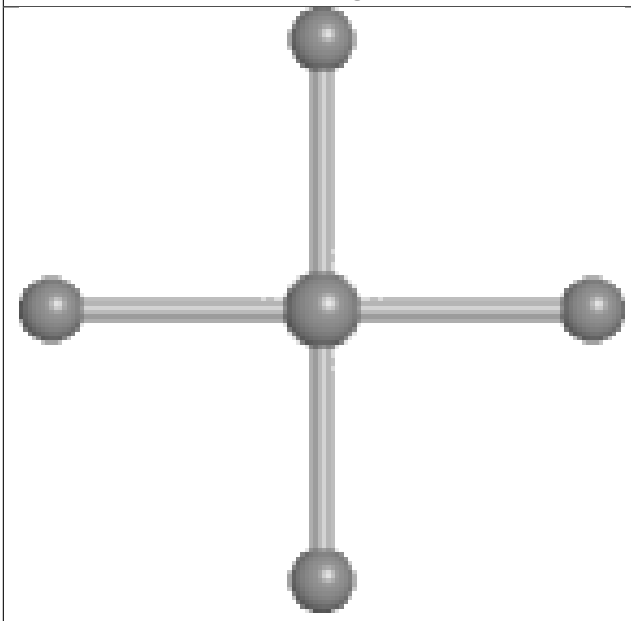
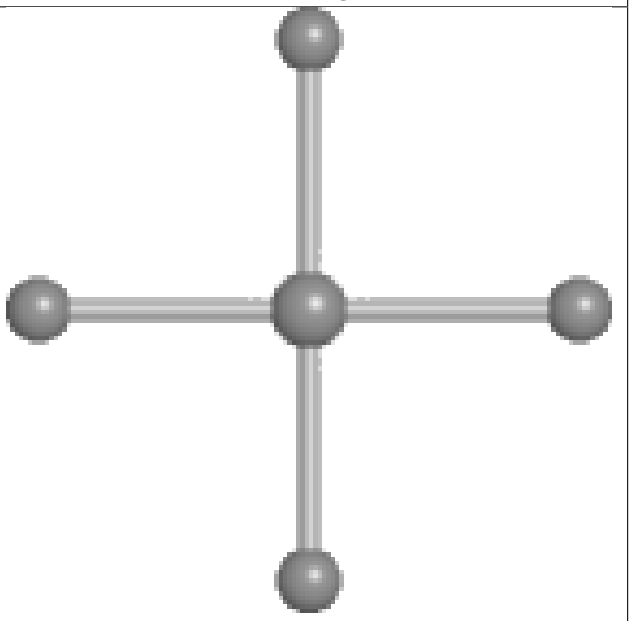


Bond angles

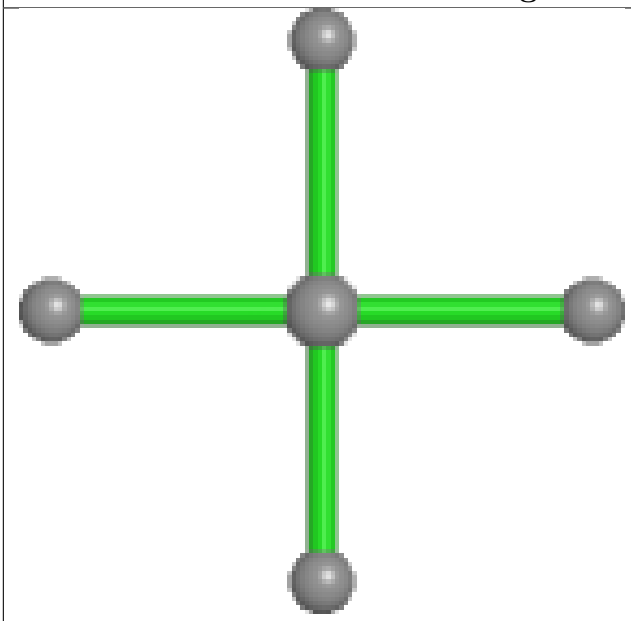


Torsions



Rings

Ligand SO4 A 1205



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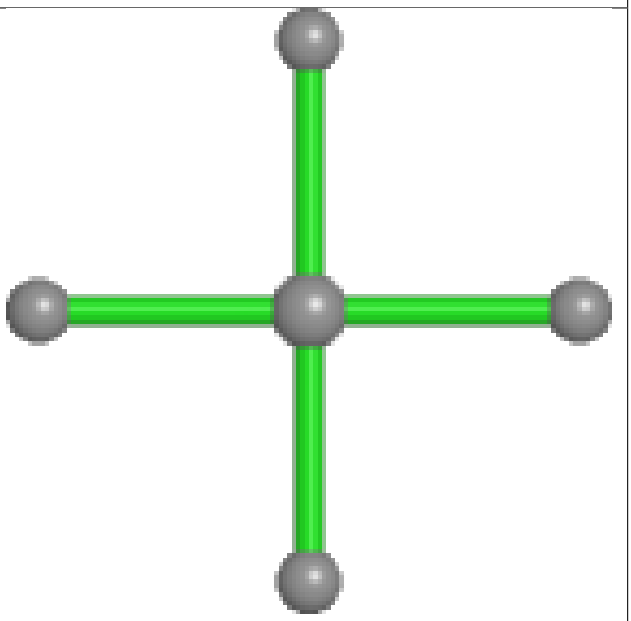
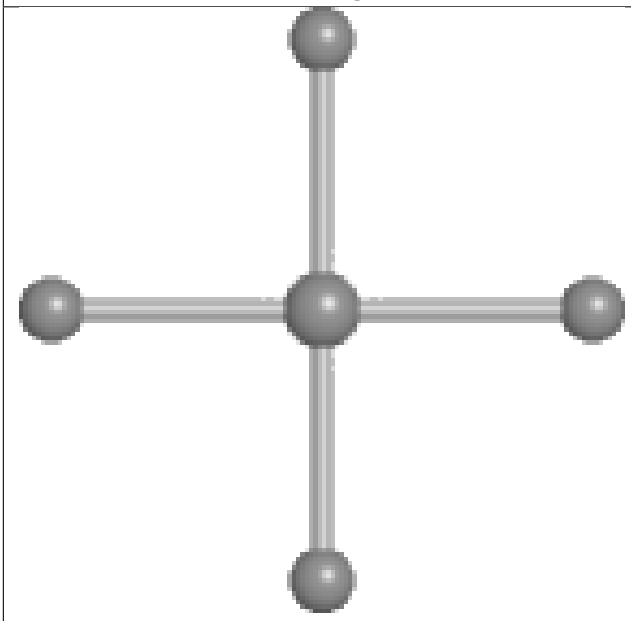
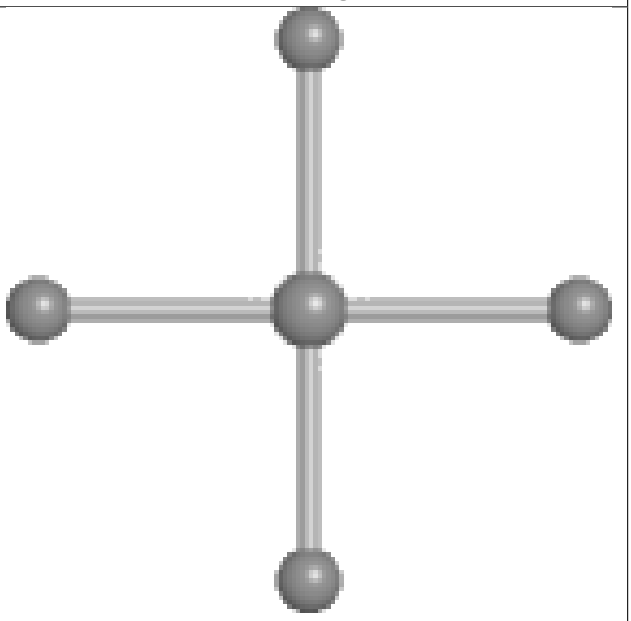


Bond angles

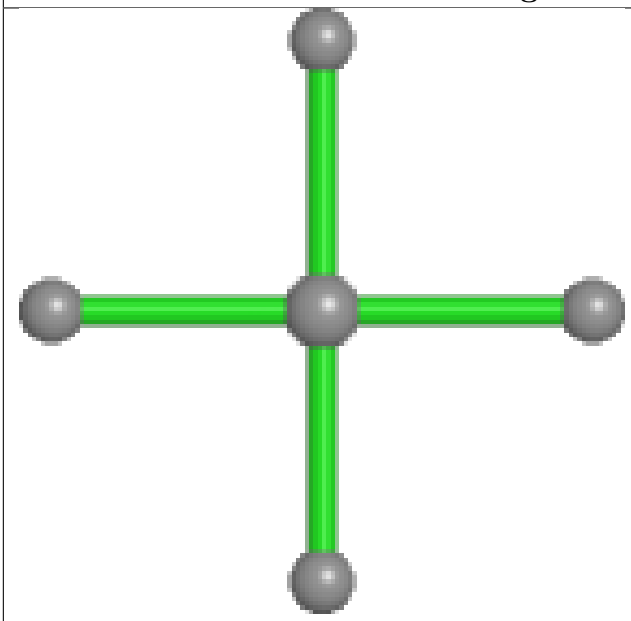


Torsions



Rings

Ligand SO4 B 1215



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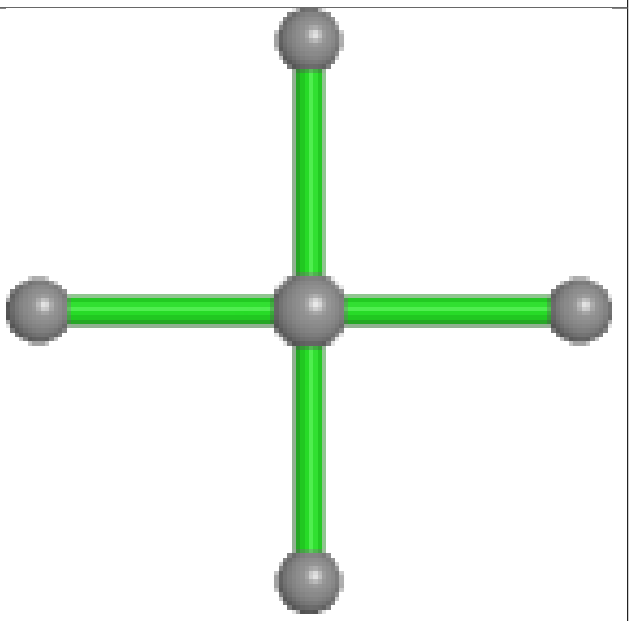
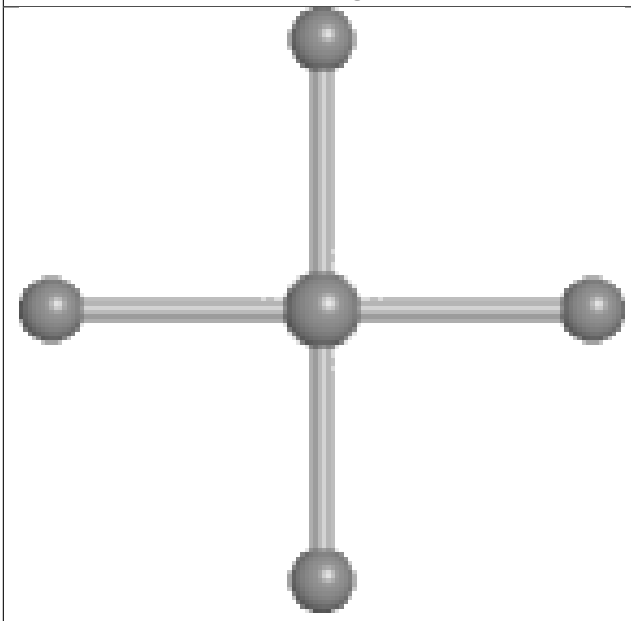
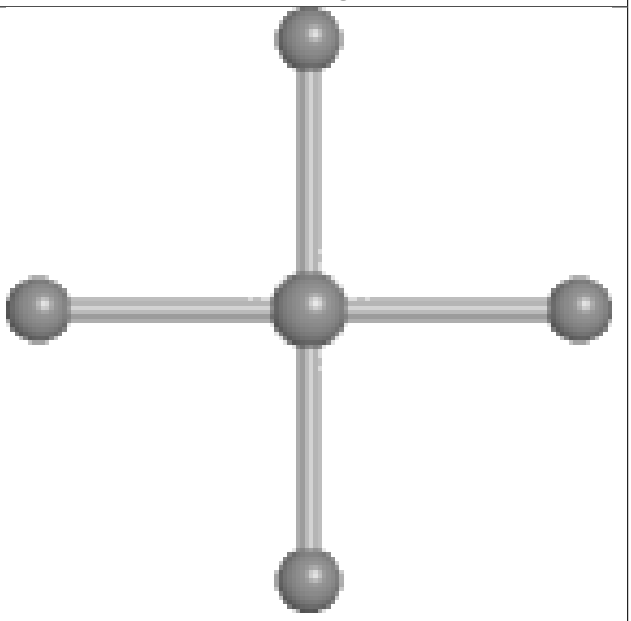


Bond angles

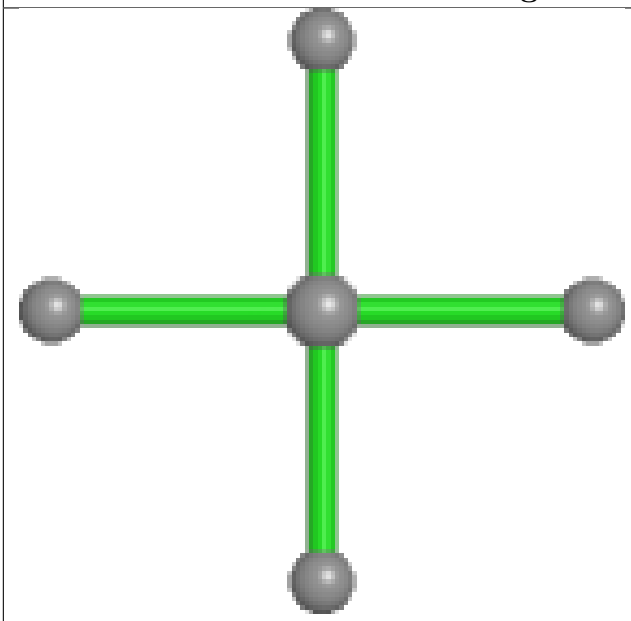


Torsions

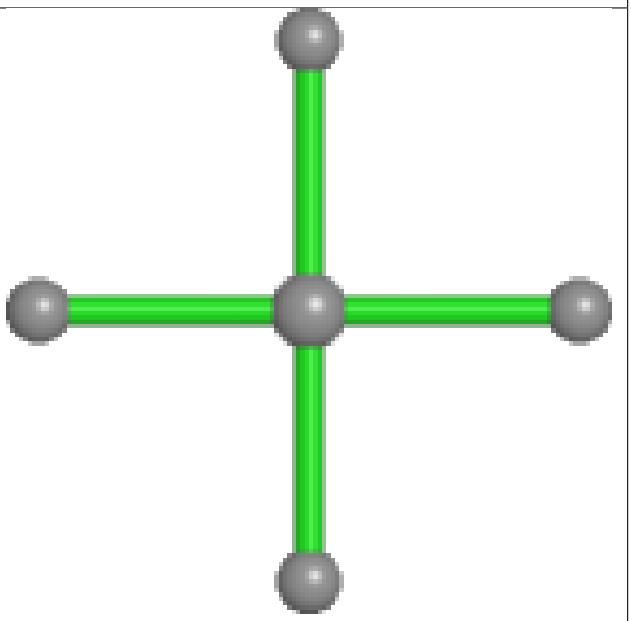


Rings

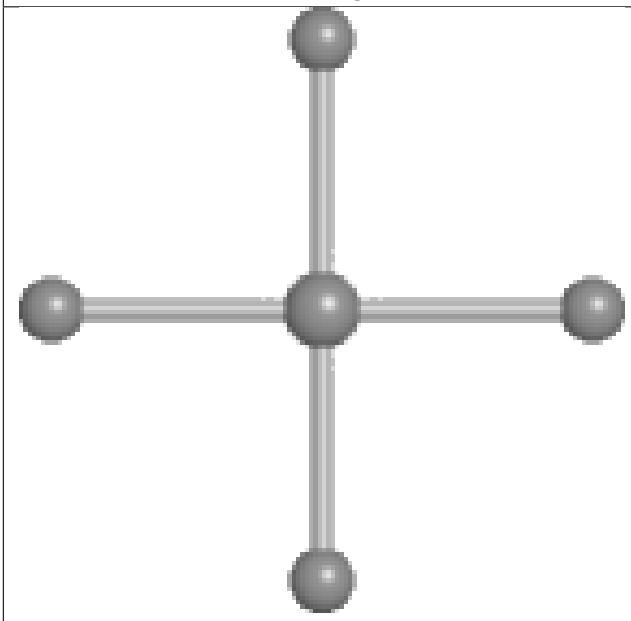
Ligand SO4 B 1213



Bond lengths



Bond angles



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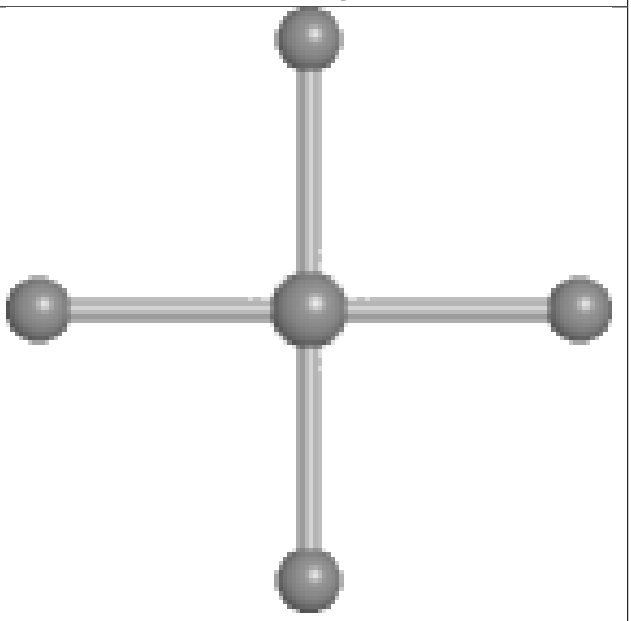
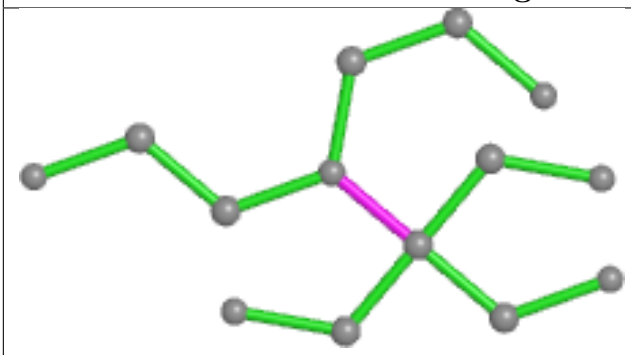


Rings

Ligand BTB A 1203



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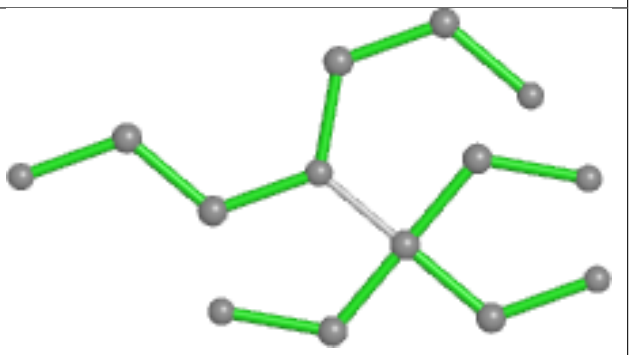
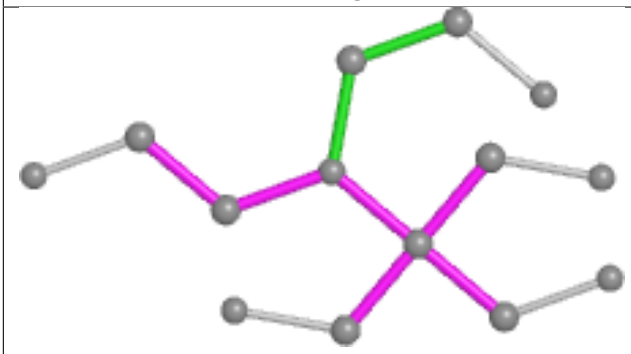


Bond angles



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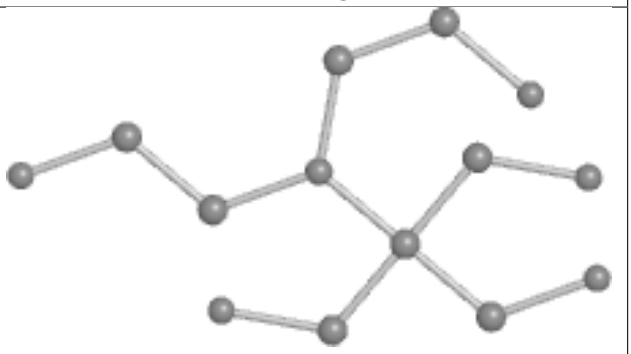
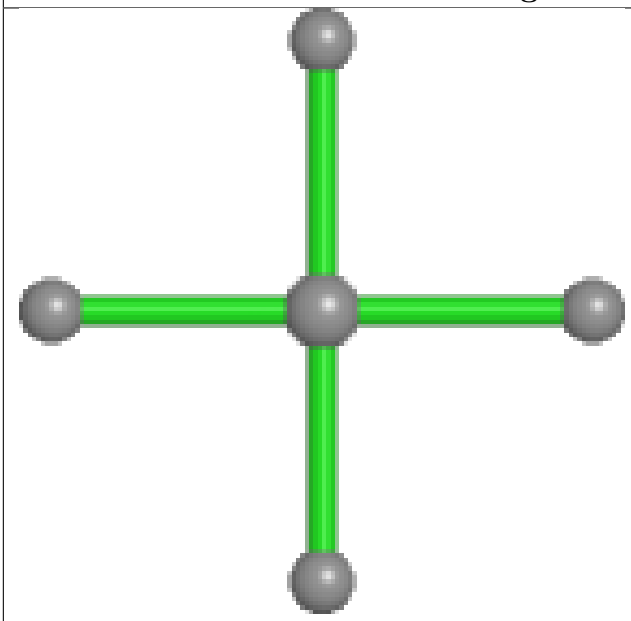


Rings

Ligand SO4 B 1210



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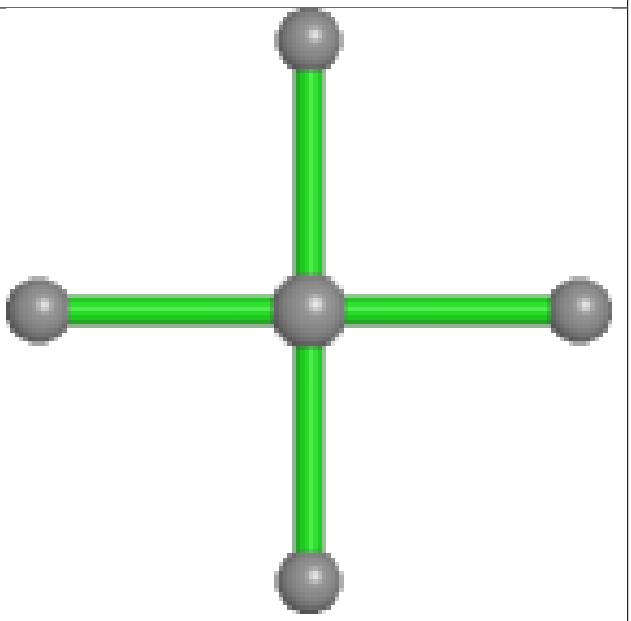
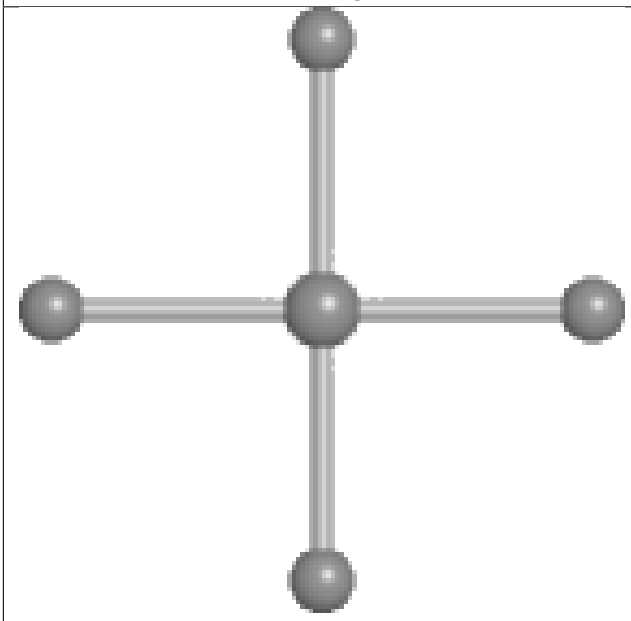


Bond angles



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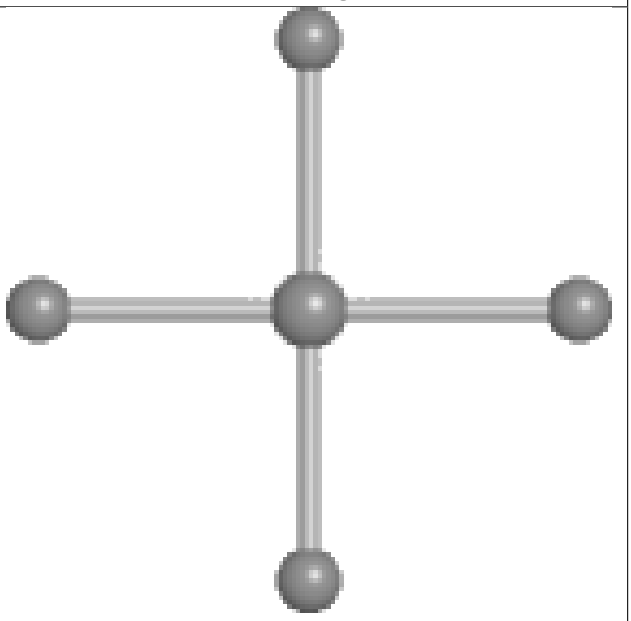
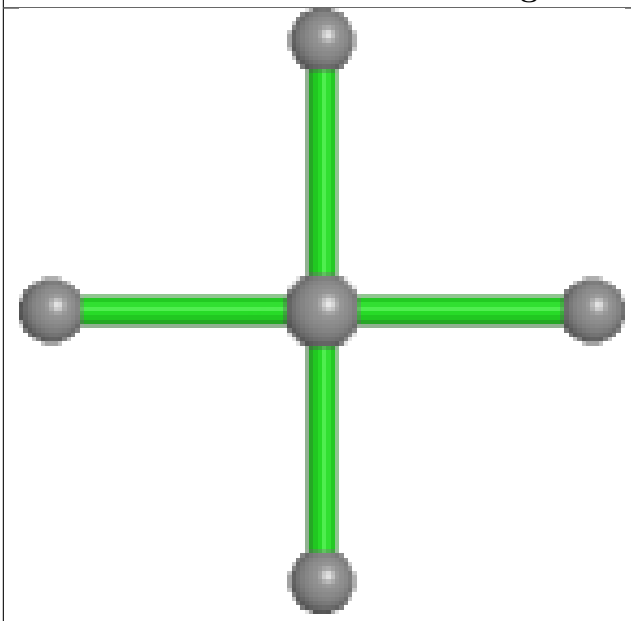


Rings

Ligand SO4 B 1217



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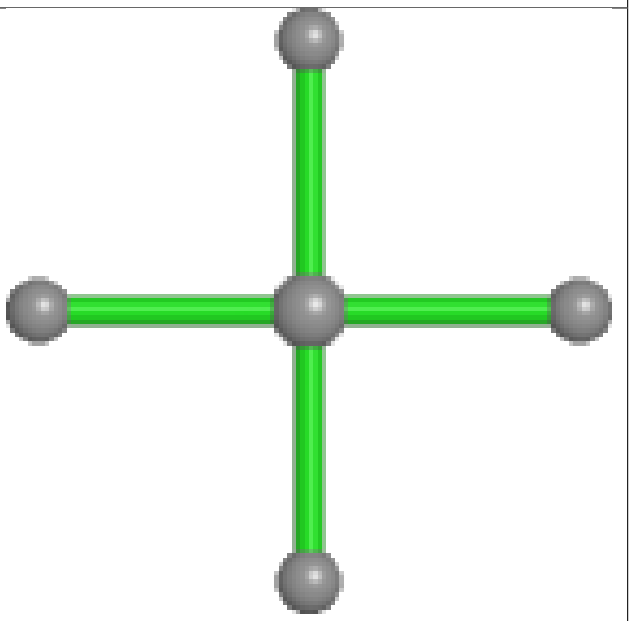
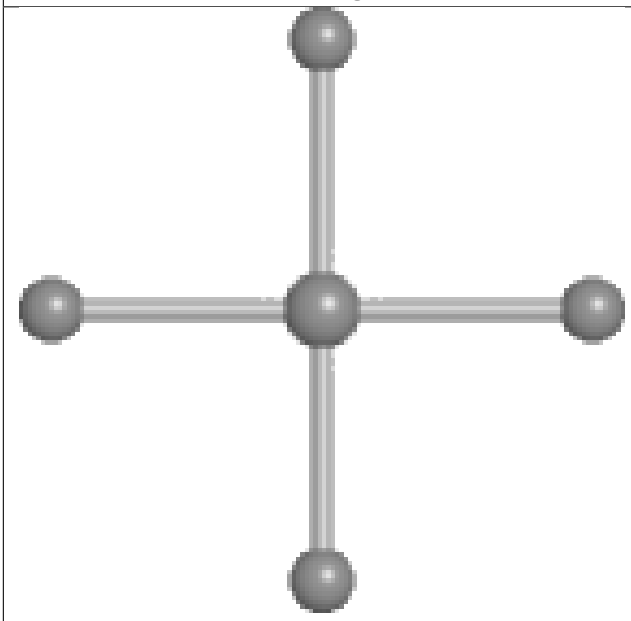


Bond angles



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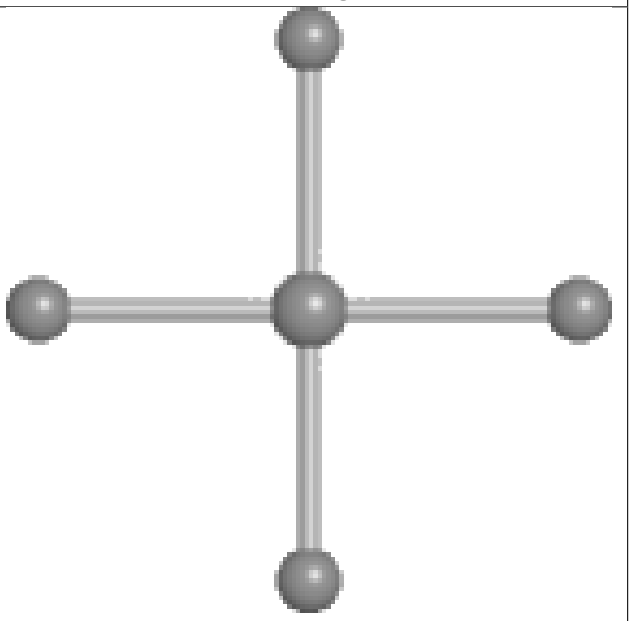
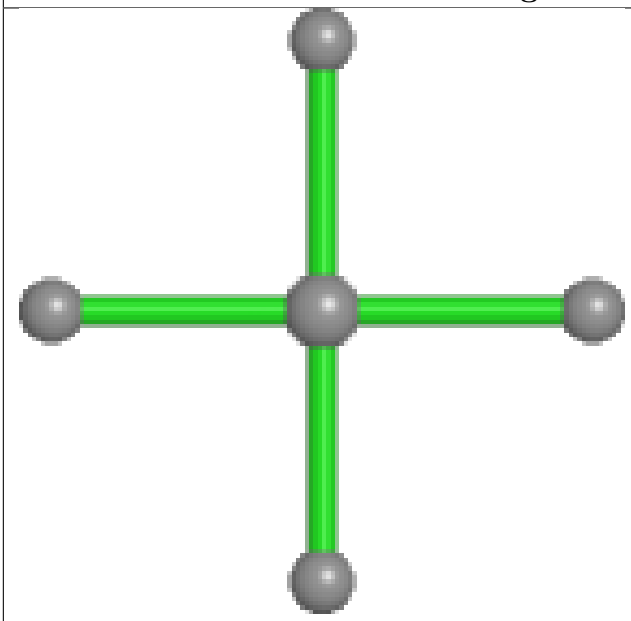


Rings

Ligand SO4 B 1216



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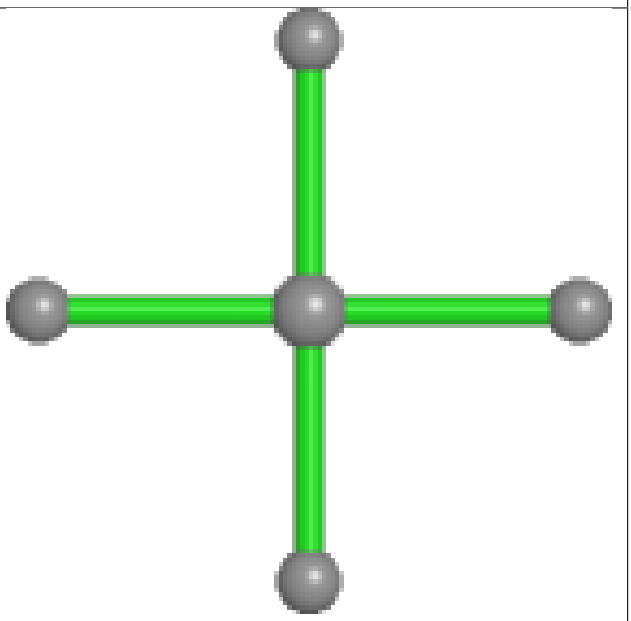
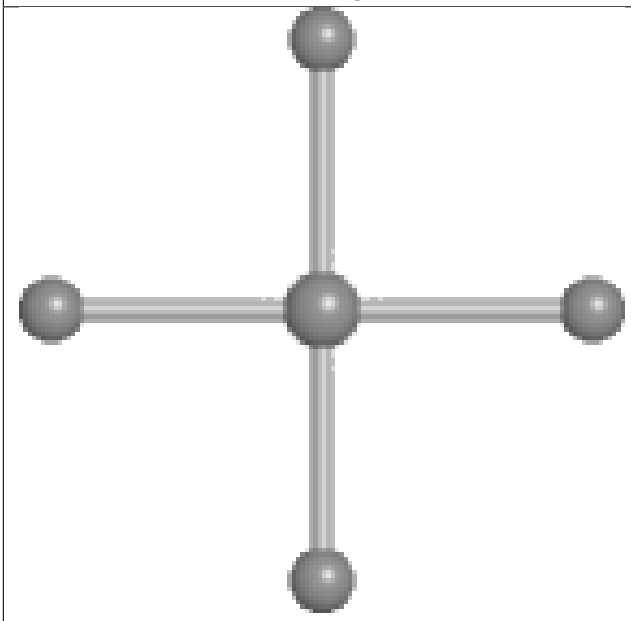


Bond angles



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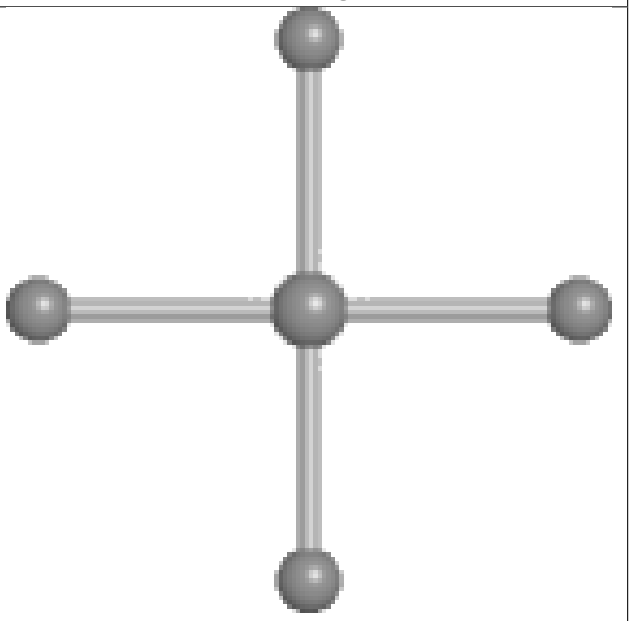
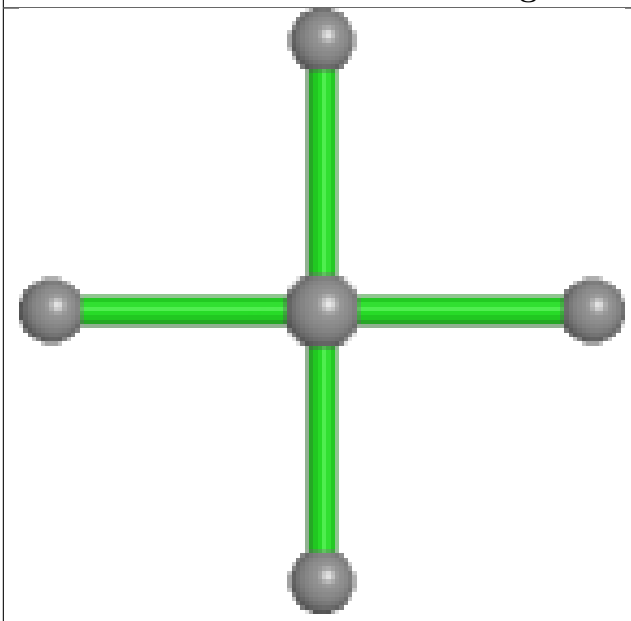


Rings

Ligand SO4 A 1208



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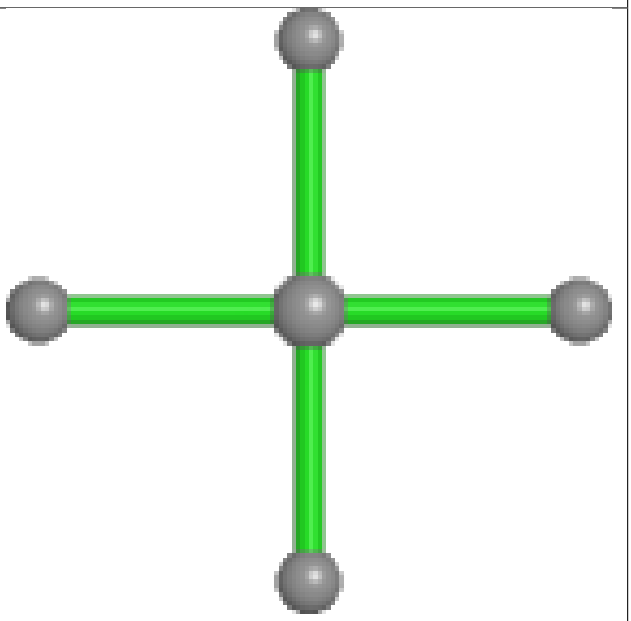
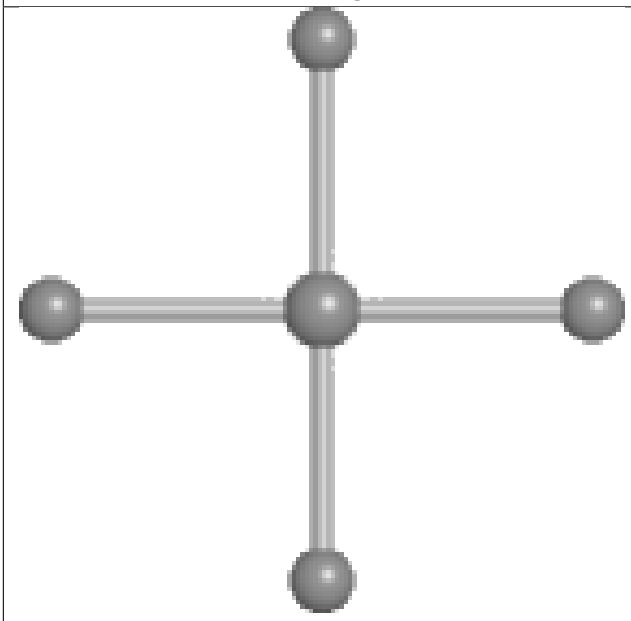
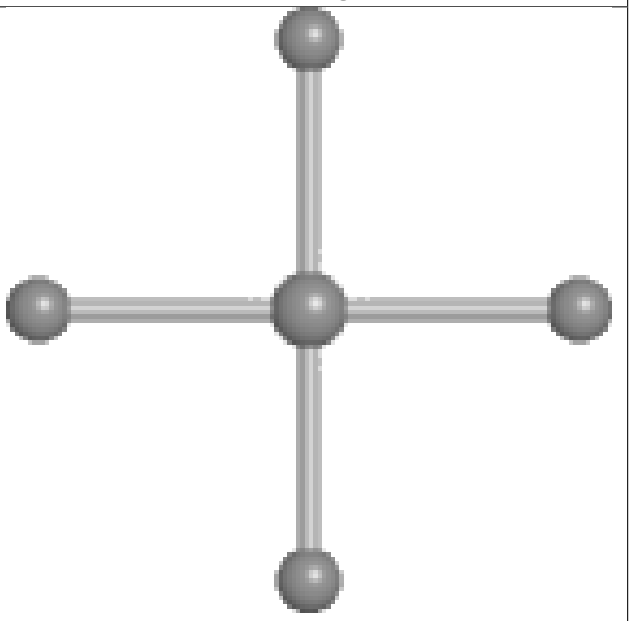


Bond angles

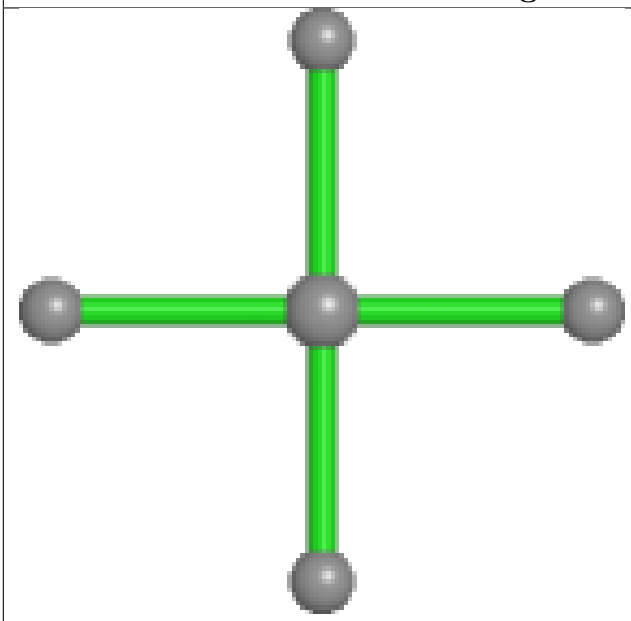


Torsions

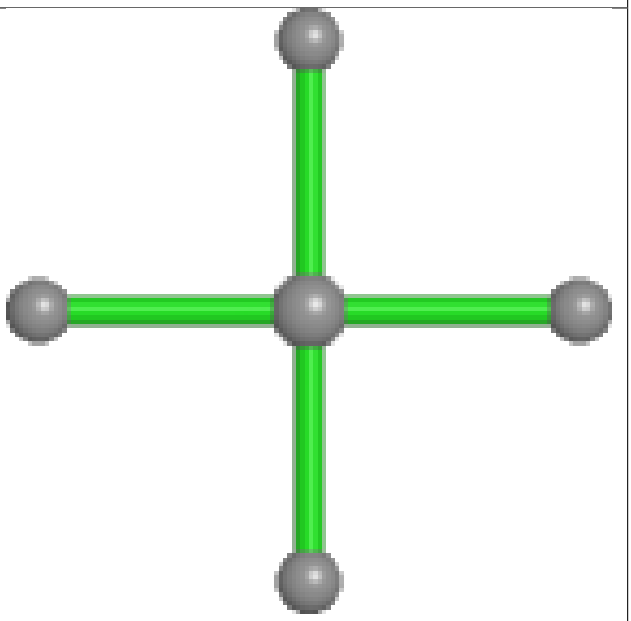


Rings

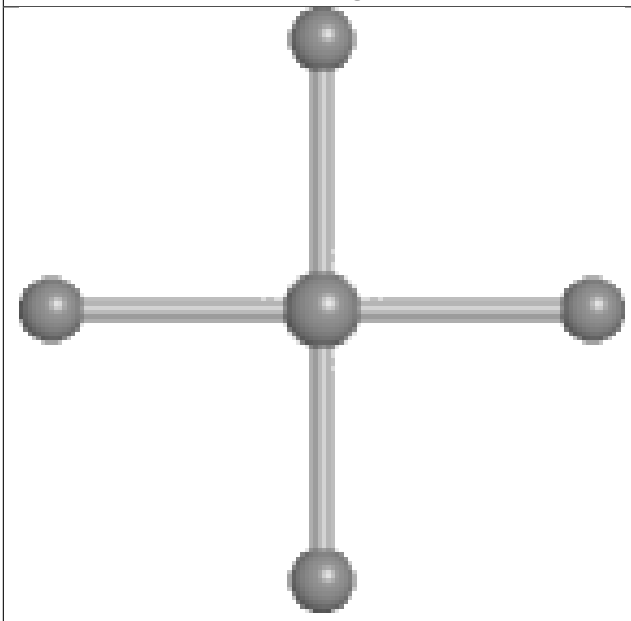
Ligand SO4 A 1209



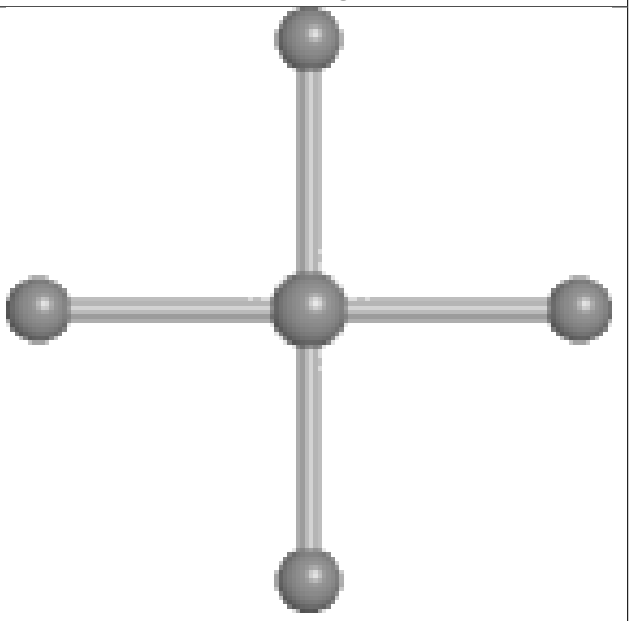
Bond lengths



Bond angles

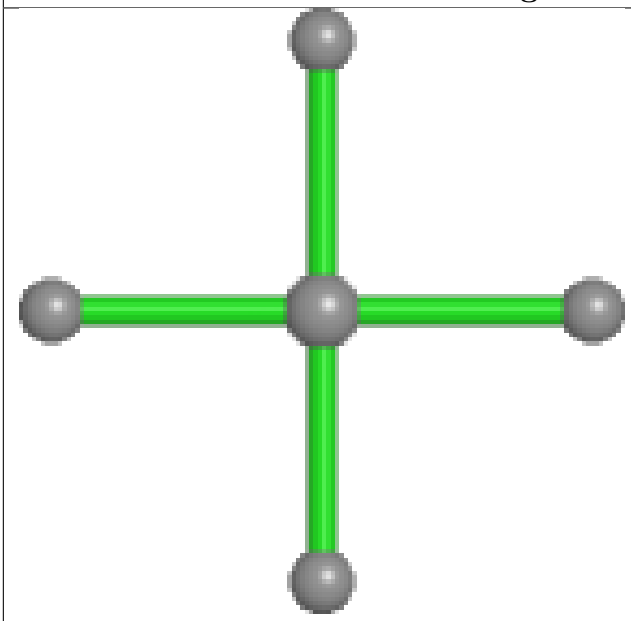


Torsions



Rings

Ligand SO4 B 1209



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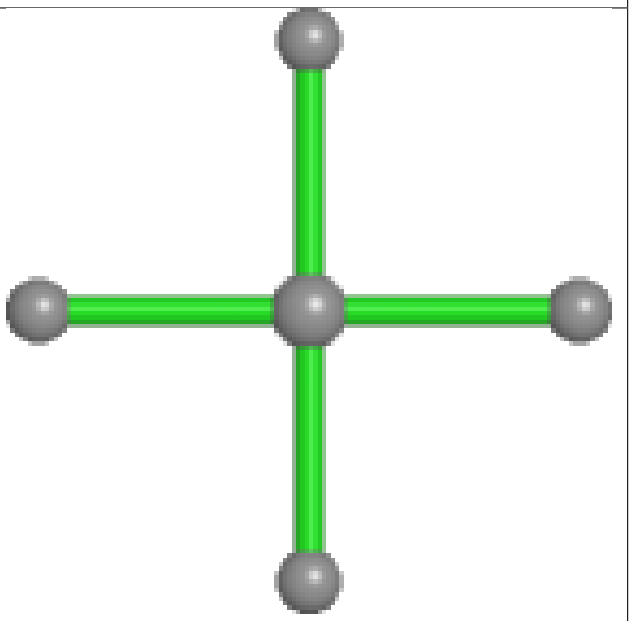
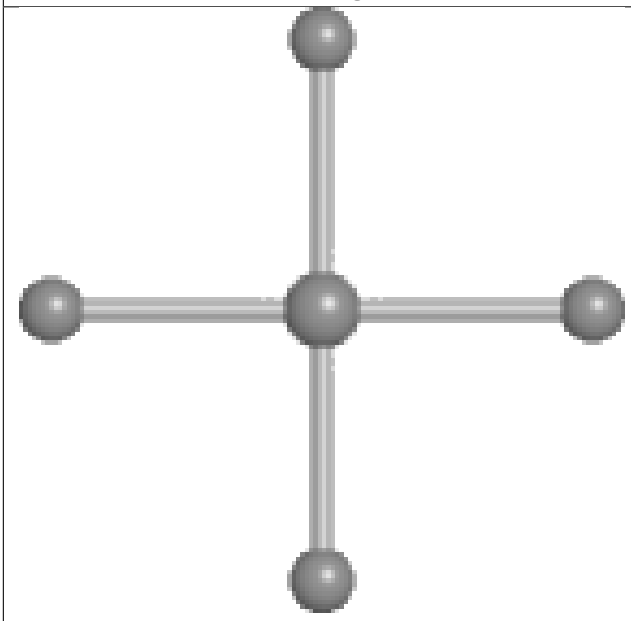
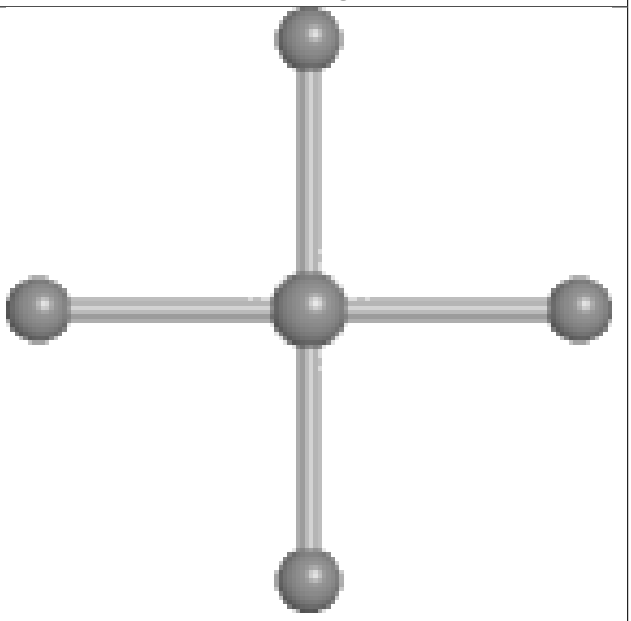


Bond angles

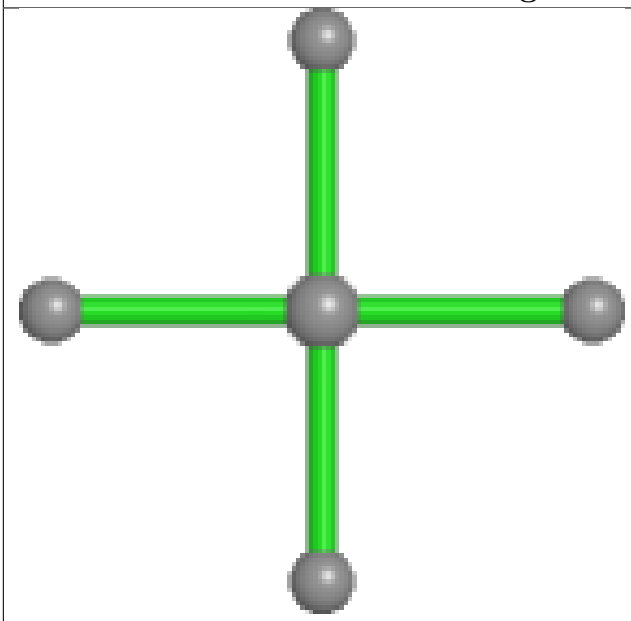


Torsions



Rings

Ligand SO4 A 1210



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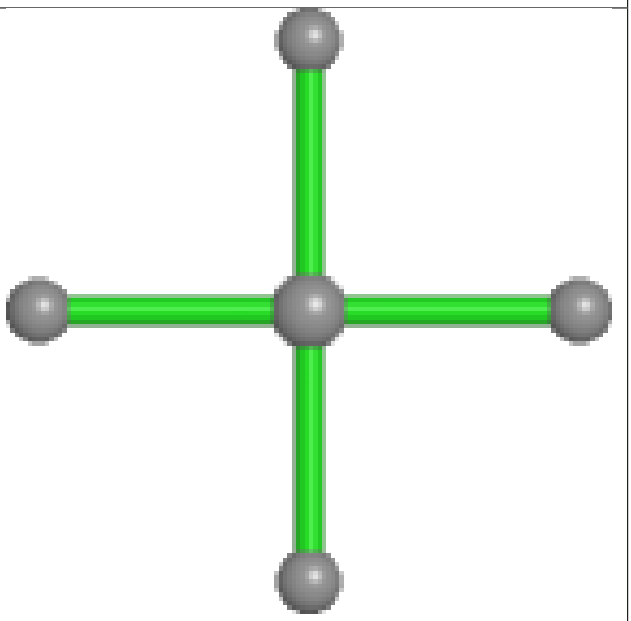
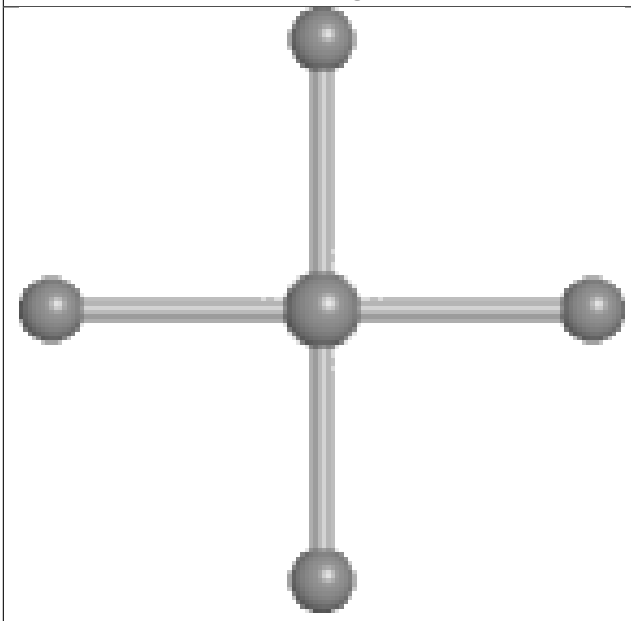
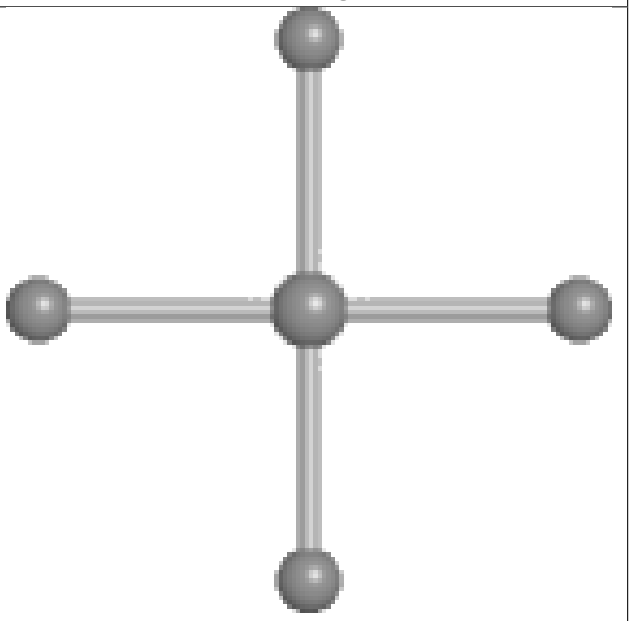


Bond angles

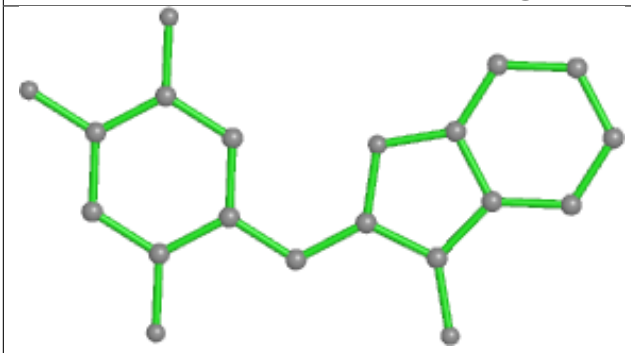


Torsions

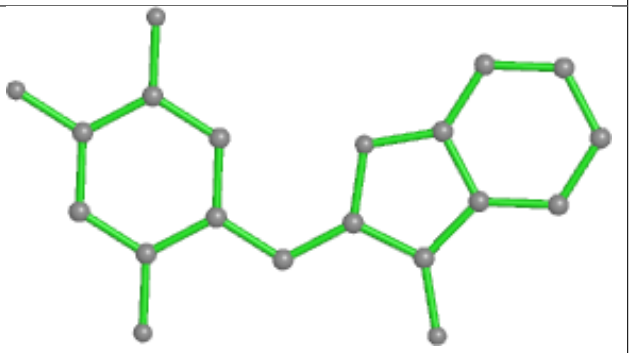


Rings

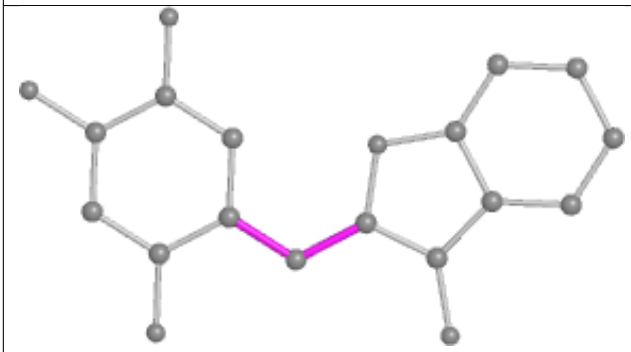
Ligand XV5 B 1202



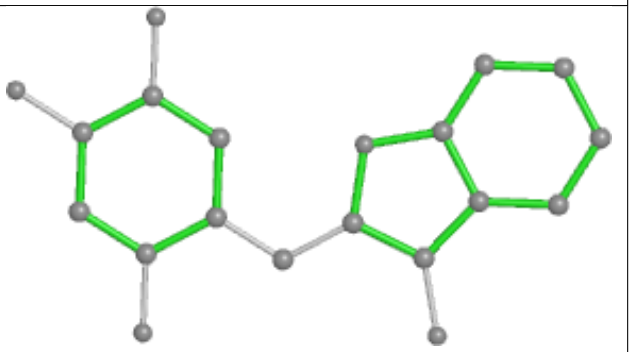
Bond lengths



Bond angles

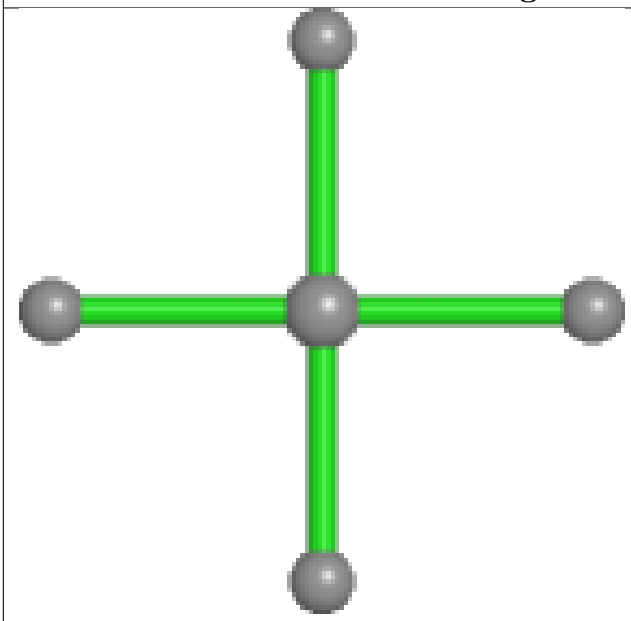


Torsions

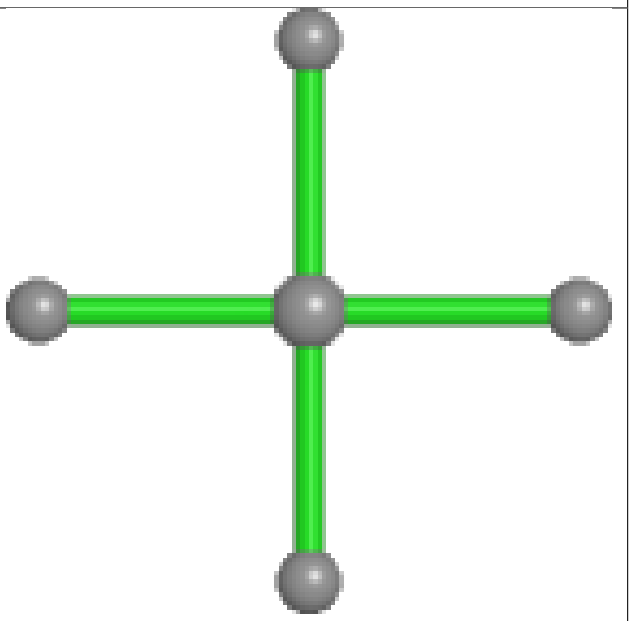


Rings

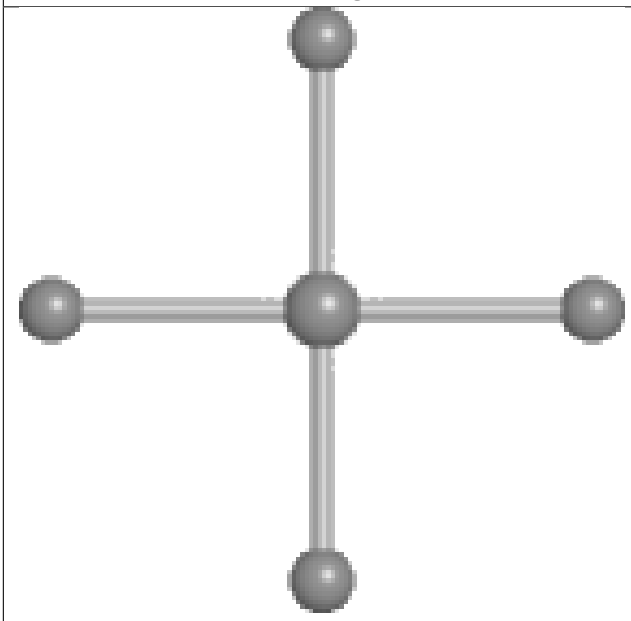
Ligand SO4 A 1212



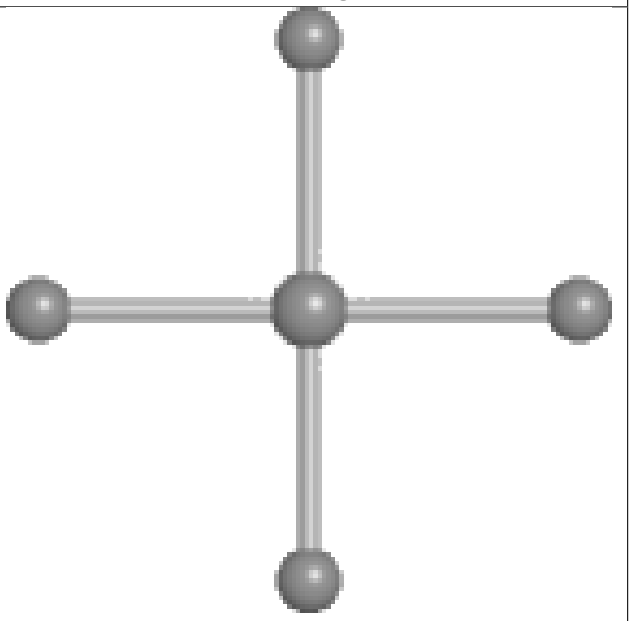
Bond lengths



Bond angles

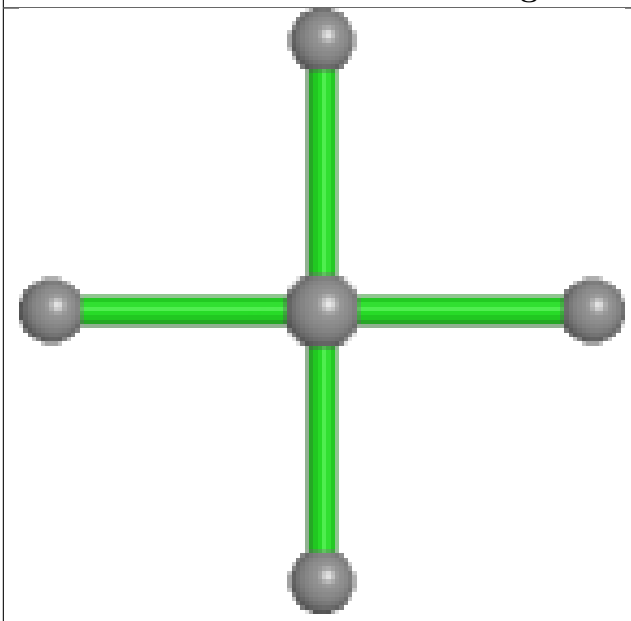


Torsions

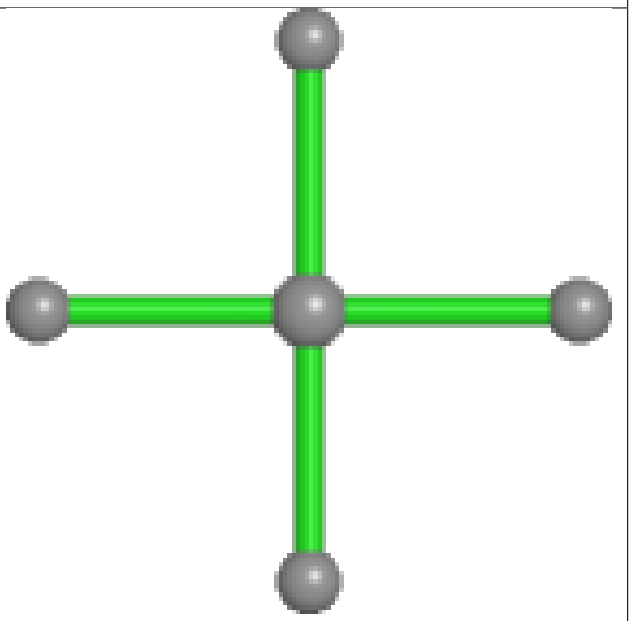


Rings

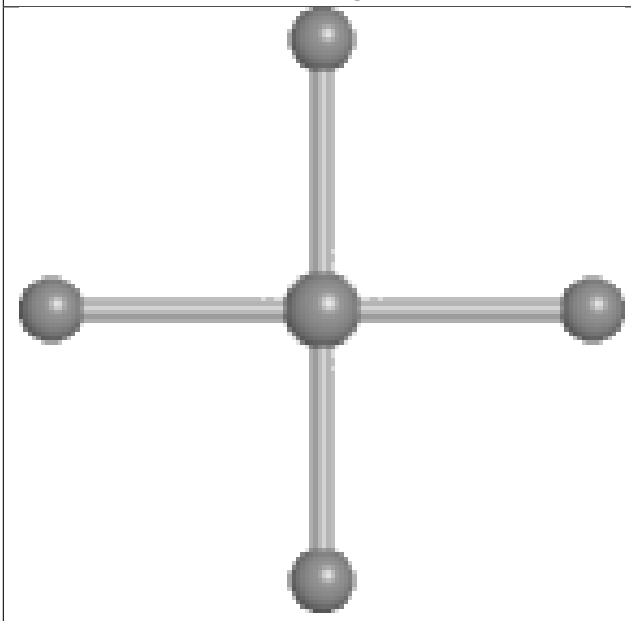
Ligand SO4 B 1205



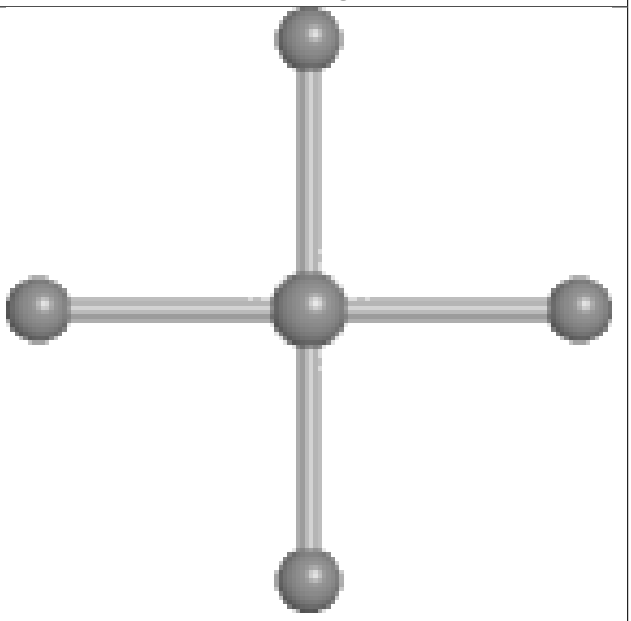
Bond lengths



Bond angles

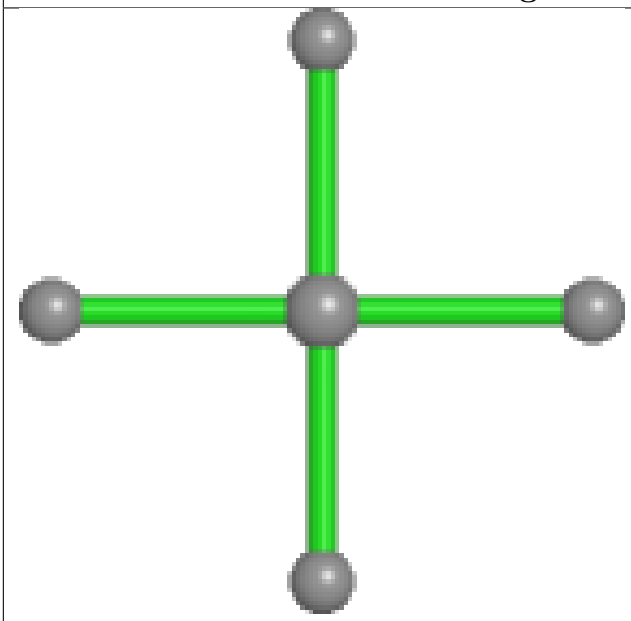


Torsions

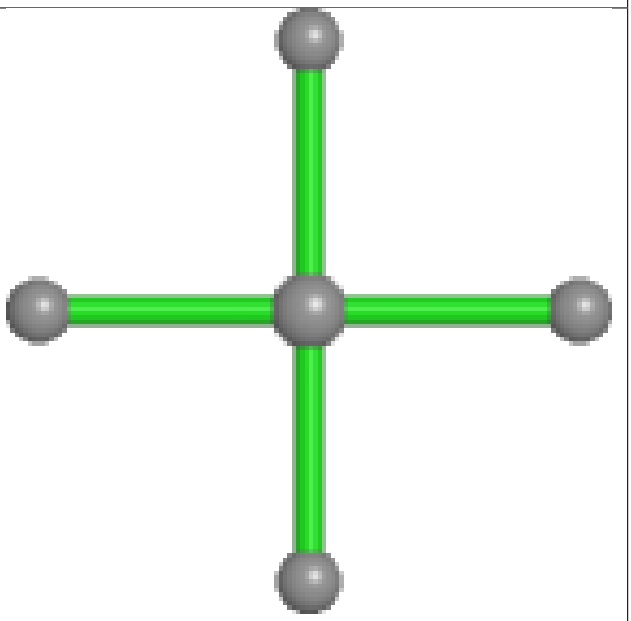


Rings

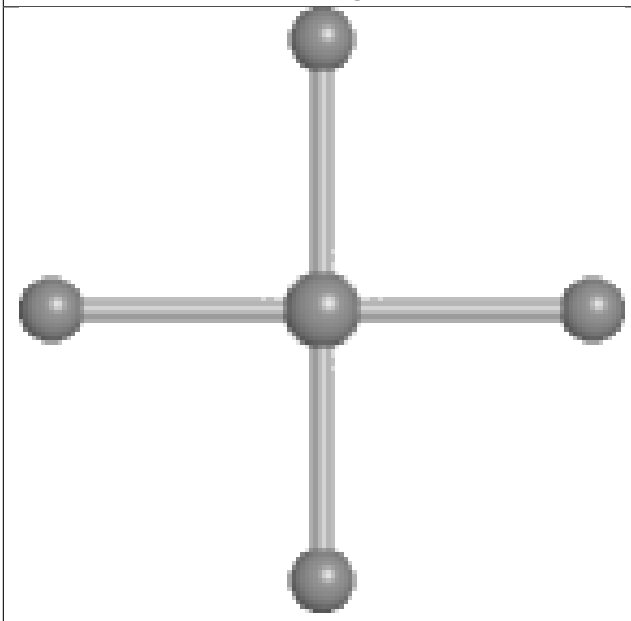
Ligand SO4 A 1211



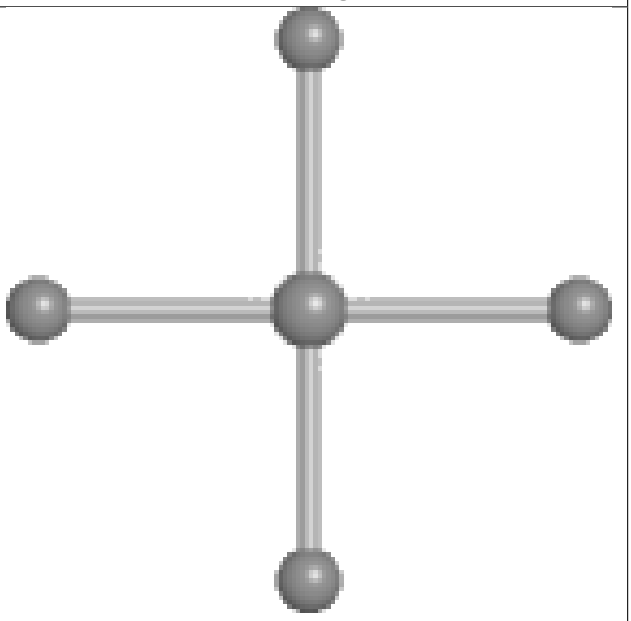
Bond lengths



Bond angles

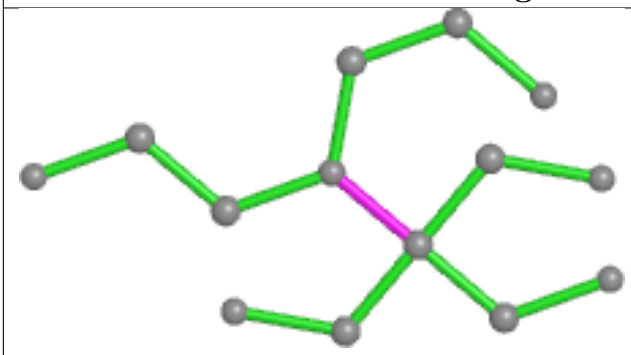


Torsions

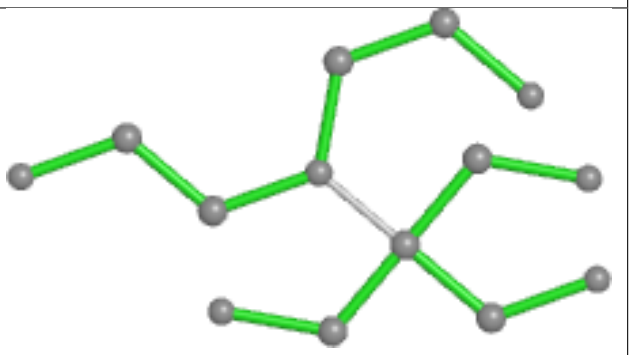


Rings

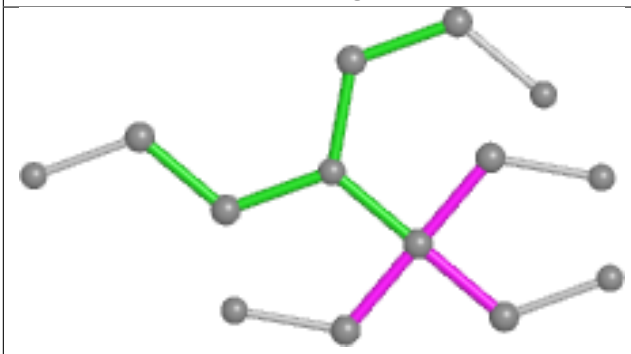
Ligand BTB B 1203



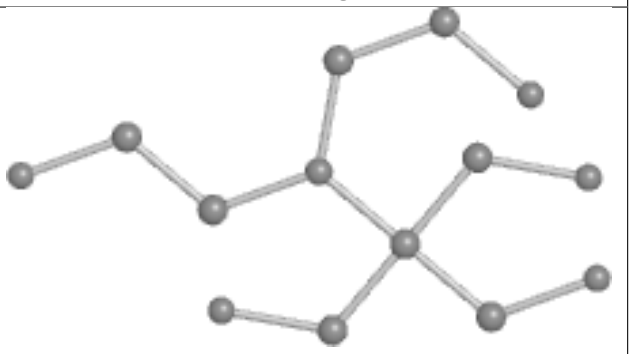
Bond lengths



Bond angles

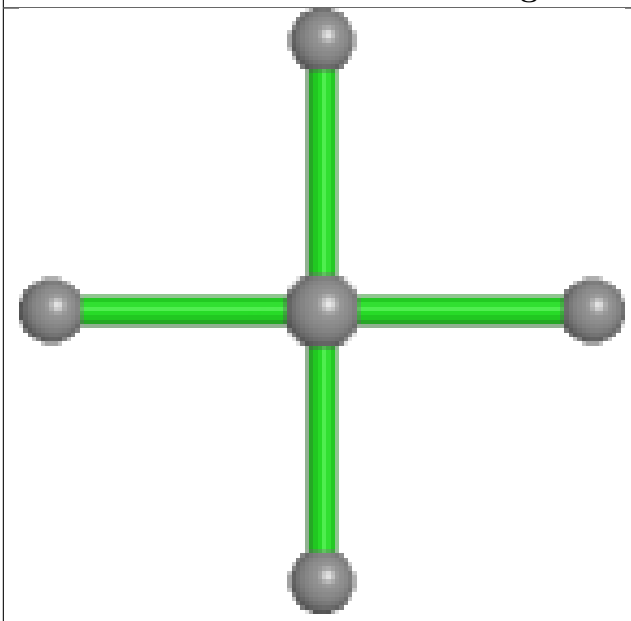


Torsions

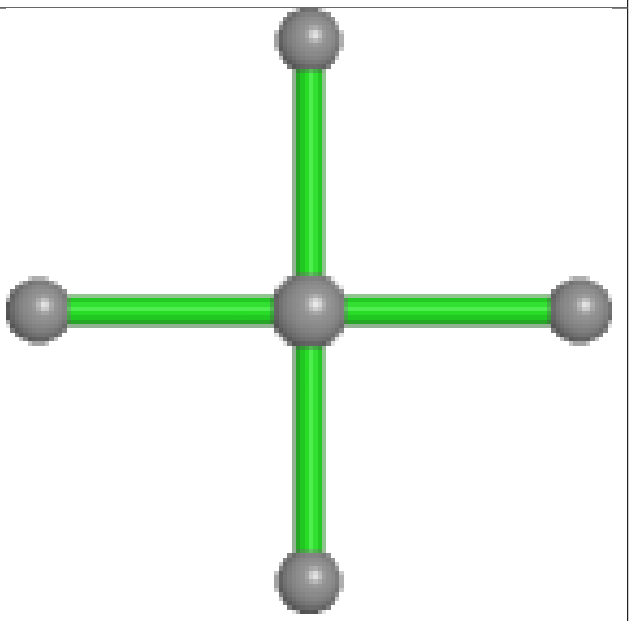


Rings

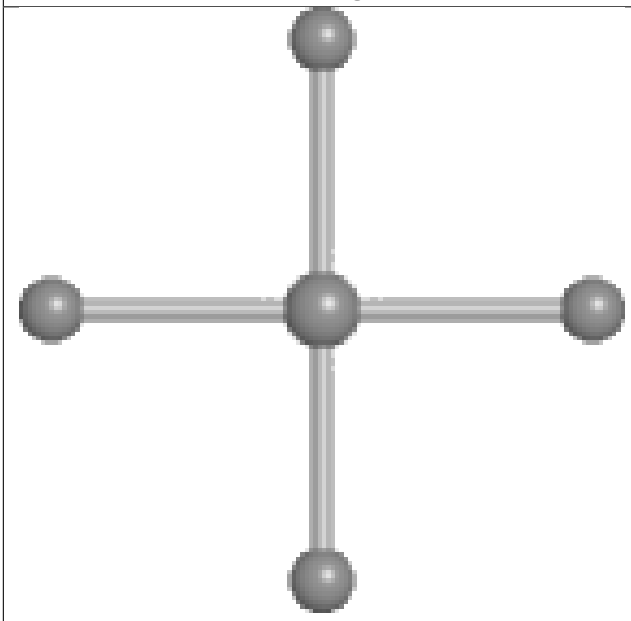
Ligand SO4 B 1204



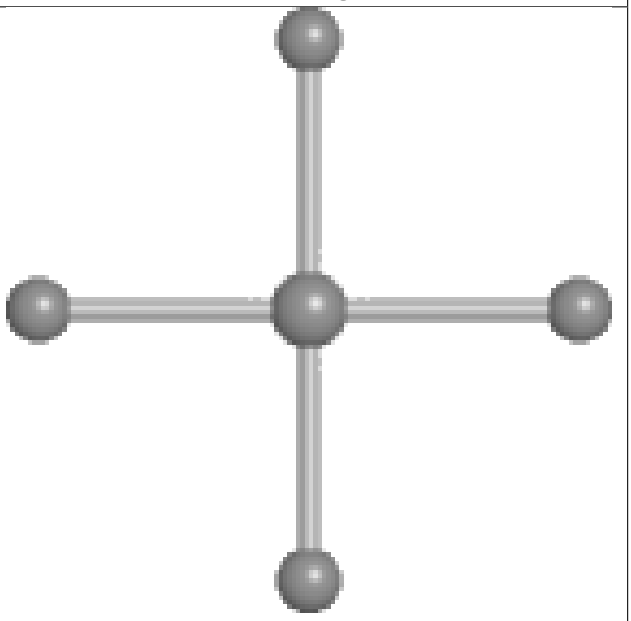
Bond lengths



Bond angles

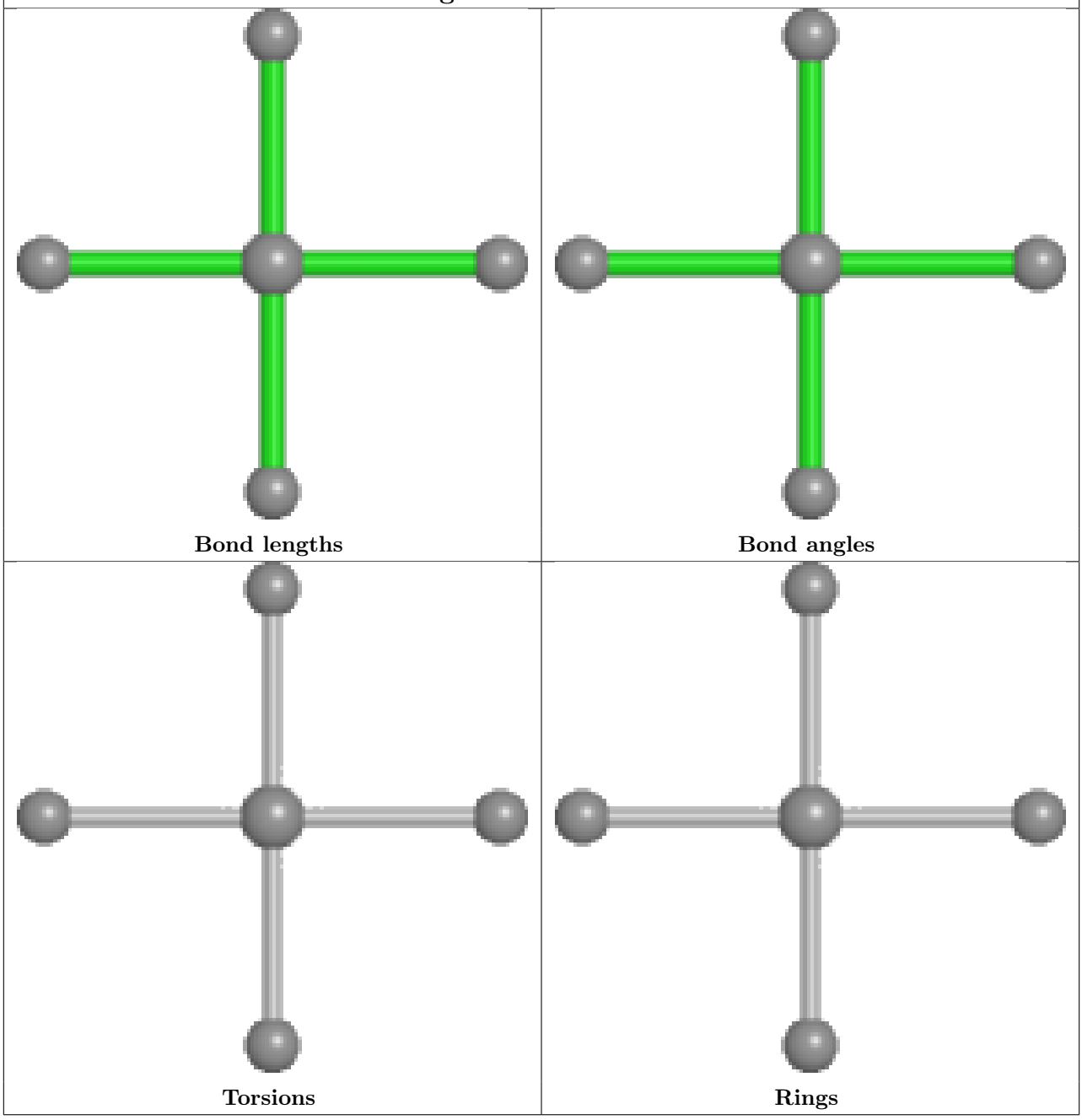


Torsions



Rings

Ligand SO4 B 1211



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	835/869 (96%)	0.03	30 (3%)	42	55	34, 52, 92, 131	0
1	B	824/869 (94%)	0.09	34 (4%)	37	49	31, 49, 113, 145	0
All	All	1659/1738 (95%)	0.06	64 (3%)	39	52	31, 50, 107, 145	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	304	LEU	7.4
1	B	271	MET	5.0
1	B	228	ARG	4.9
1	B	233	PHE	4.4
1	B	1040	ALA	4.4
1	A	228	ARG	4.2
1	B	325	LYS	4.2
1	B	266	PHE	3.9
1	A	218	LEU	3.8
1	B	1045	PHE	3.7
1	A	1041	THR	3.5
1	B	232	SER	3.5
1	B	272	THR	3.4
1	A	226	TYR	3.4
1	A	260	GLN	3.3
1	B	230	ALA	3.3
1	B	324	LEU	3.2
1	B	287	MET	3.2
1	A	233	PHE	3.1
1	A	255	GLY	3.1
1	A	231	GLN	3.1
1	B	326	ASN	3.1
1	B	262	THR	3.0
1	A	215	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	225	VAL	2.9
1	B	225	VAL	2.9
1	A	251	ILE	2.8
1	A	970	SER	2.7
1	B	306	LEU	2.7
1	A	249	LYS	2.7
1	B	255	GLY	2.7
1	B	227	ASP	2.7
1	B	283	TYR	2.6
1	A	253	LYS	2.6
1	B	250	TYR	2.6
1	A	213	THR	2.6
1	A	957	GLU	2.6
1	A	219	TYR	2.6
1	A	222	TYR	2.6
1	B	970	SER	2.5
1	B	270	LEU	2.5
1	A	1045	PHE	2.5
1	A	1040	ALA	2.5
1	B	269	LEU	2.4
1	A	221	LYS	2.4
1	A	266	PHE	2.4
1	B	1037	LYS	2.3
1	B	238	HIS	2.3
1	B	279	THR	2.3
1	B	247	ARG	2.3
1	B	399	ASN	2.3
1	A	761	LEU	2.2
1	A	227	ASP	2.2
1	A	258	TRP	2.2
1	A	265	ASP	2.2
1	B	261	SER	2.2
1	A	246	TYR	2.1
1	A	250	TYR	2.1
1	B	224	GLN	2.1
1	B	280	GLN	2.1
1	A	368	LYS	2.1
1	B	300	THR	2.0
1	B	525	LEU	2.0
1	A	230	ALA	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
5	SO4	B	1204	5/5	0.74	0.20	68,78,103,111	0
3	XV5	B	1202	20/20	0.75	0.24	62,81,90,91	0
3	XV5	A	1202	20/20	0.75	0.22	72,84,95,100	0
5	SO4	A	1207	5/5	0.80	0.21	105,107,116,125	0
5	SO4	B	1209	5/5	0.80	0.21	90,103,118,126	0
5	SO4	A	1211	5/5	0.84	0.28	101,107,115,115	0
5	SO4	A	1210	5/5	0.86	0.26	84,99,104,109	0
5	SO4	B	1206	5/5	0.86	0.13	106,114,122,124	0
5	SO4	A	1206	5/5	0.86	0.19	107,118,124,125	0
5	SO4	B	1216	5/5	0.87	0.17	94,112,115,122	0
5	SO4	B	1217	5/5	0.87	0.13	111,112,122,126	0
5	SO4	A	1212	5/5	0.89	0.21	79,85,101,104	0
4	BTB	B	1203	14/14	0.90	0.33	52,70,78,82	0
5	SO4	A	1205	5/5	0.90	0.16	113,122,125,127	0
4	BTB	A	1203	14/14	0.91	0.23	52,77,86,97	0
5	SO4	A	1209	5/5	0.91	0.14	68,74,94,104	0
5	SO4	B	1215	5/5	0.91	0.17	103,105,112,122	0
5	SO4	A	1213	5/5	0.91	0.24	85,97,100,105	0
2	CA	B	1218	1/1	0.91	0.11	85,85,85,85	0
5	SO4	B	1214	5/5	0.92	0.19	90,103,108,112	0
5	SO4	B	1207	5/5	0.92	0.23	108,111,117,122	0
5	SO4	A	1208	5/5	0.93	0.17	87,97,100,109	0
5	SO4	B	1212	5/5	0.93	0.15	80,83,92,97	0
5	SO4	B	1211	5/5	0.95	0.23	81,82,88,95	0
5	SO4	B	1210	5/5	0.95	0.14	94,98,107,107	0
5	SO4	B	1208	5/5	0.96	0.14	85,87,98,101	0
5	SO4	B	1213	5/5	0.96	0.11	86,91,98,100	0

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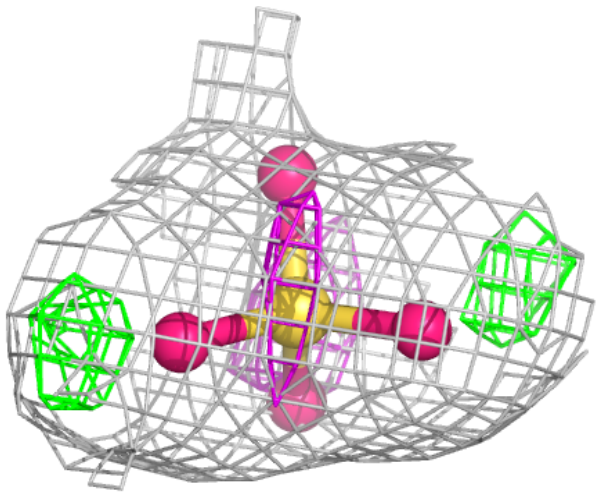
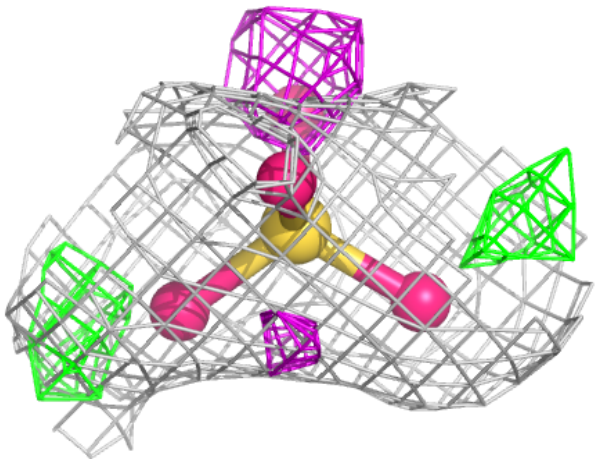
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	A	1204	5/5	0.98	0.12	70,71,80,80	0
5	SO4	B	1205	5/5	0.98	0.09	67,69,73,76	0
2	CA	A	1201	1/1	0.99	0.09	40,40,40,40	0
2	CA	B	1201	1/1	1.00	0.12	42,42,42,42	0

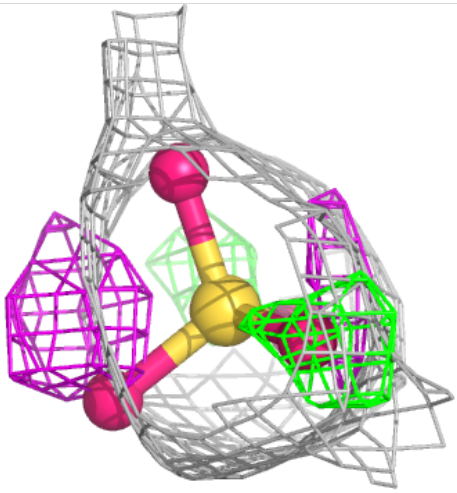
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SO4 B 1204:

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

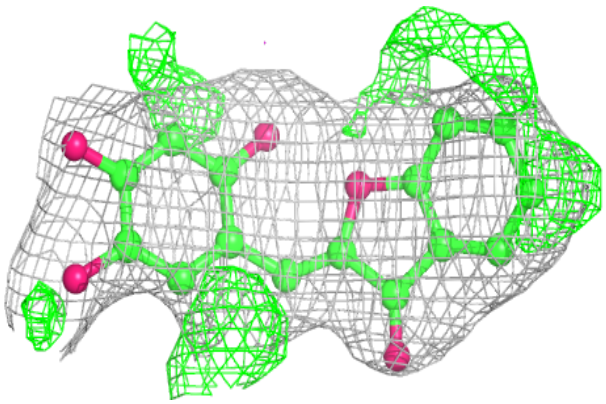


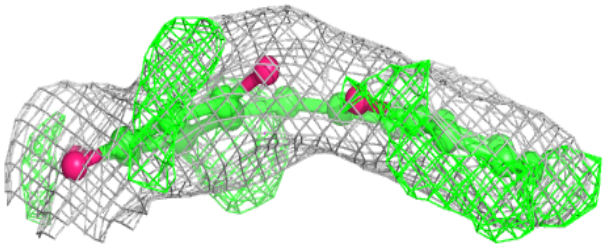


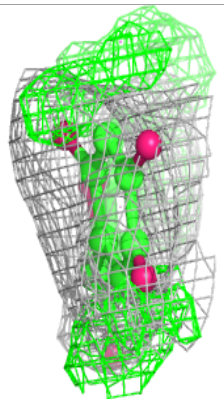


Electron density around XV5 B 1202:

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

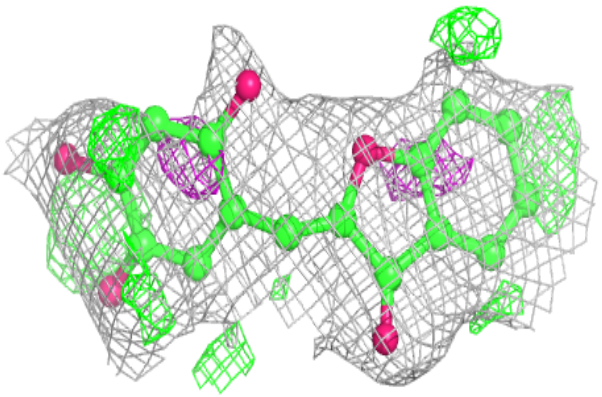


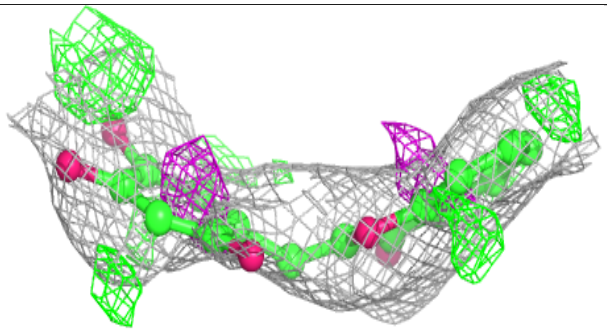


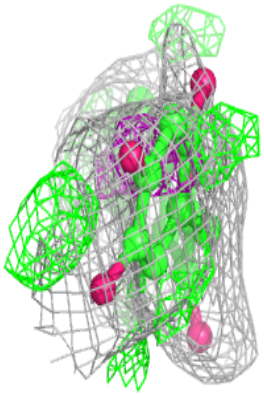


Electron density around XV5 A 1202:

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

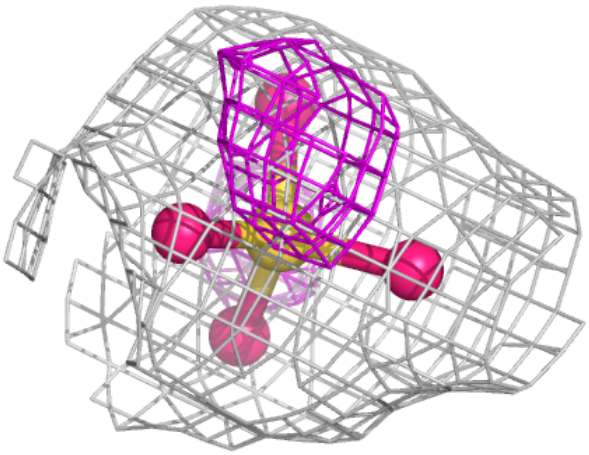


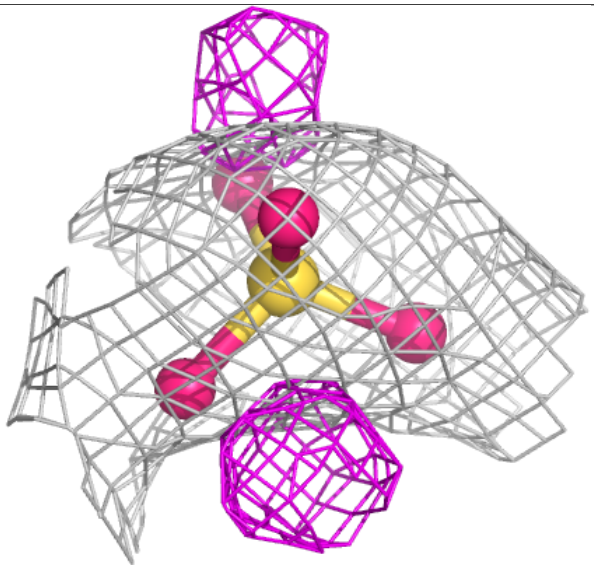


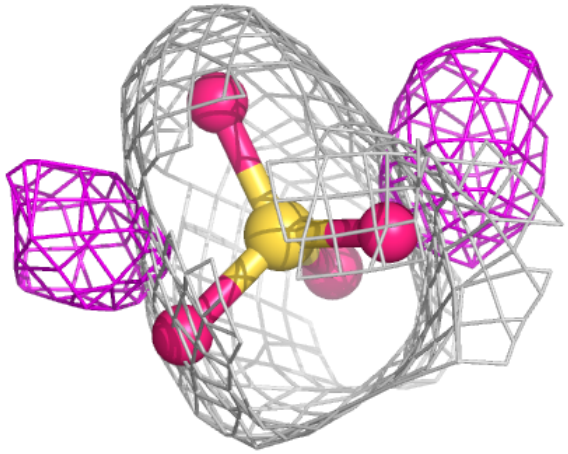


Electron density around SO4 A 1207:

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

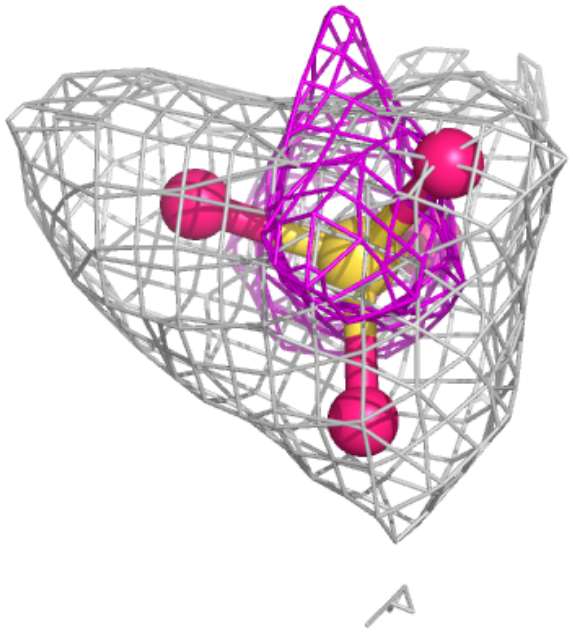


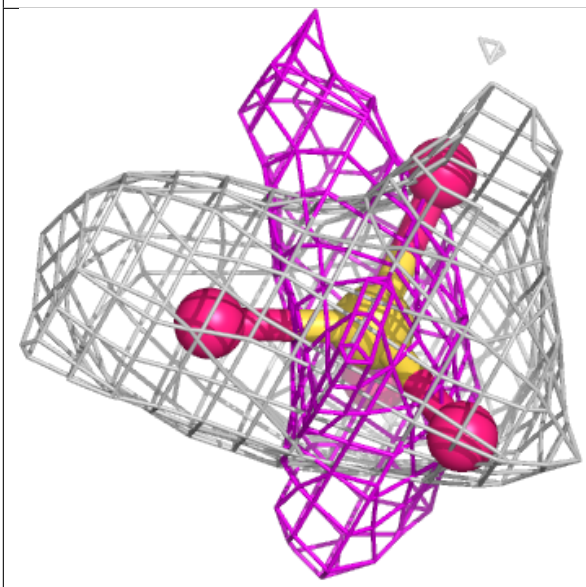


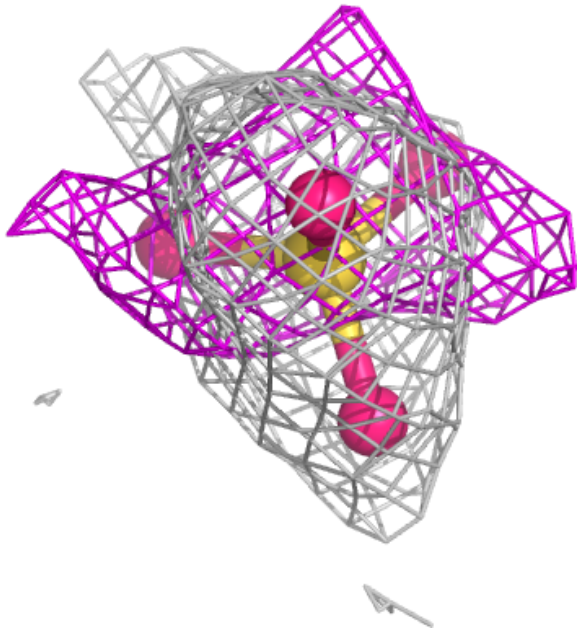


Electron density around SO4 B 1209:

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

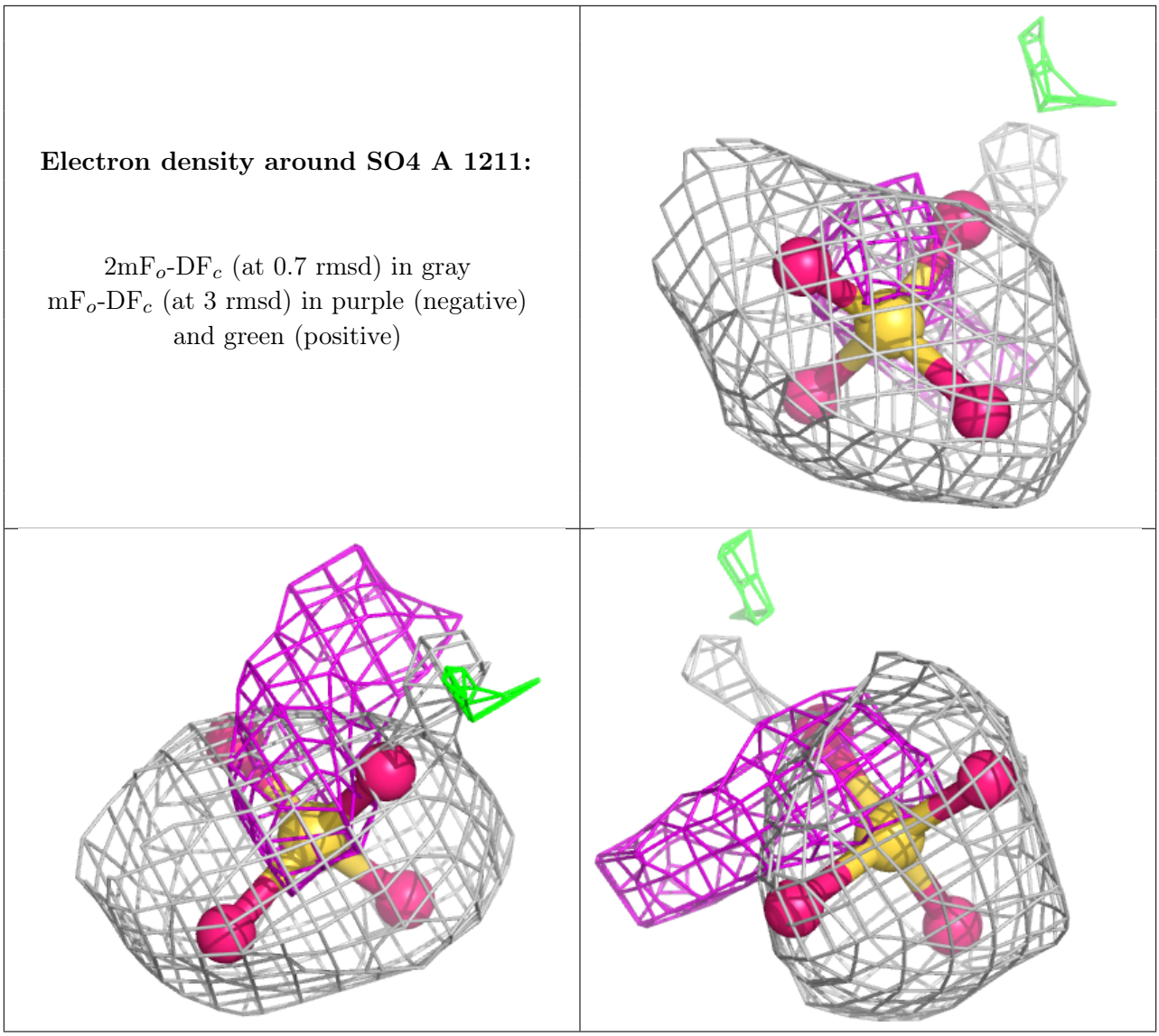






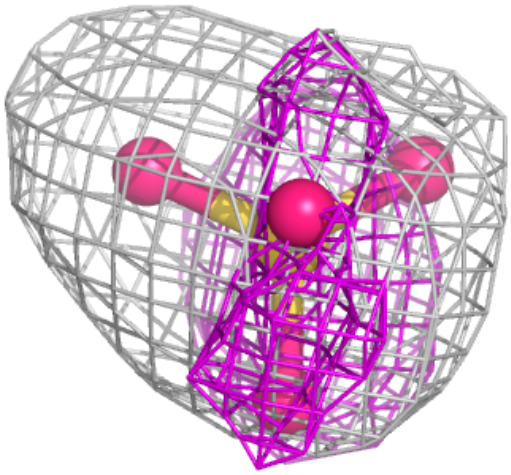
Electron density around SO4 A 1211:

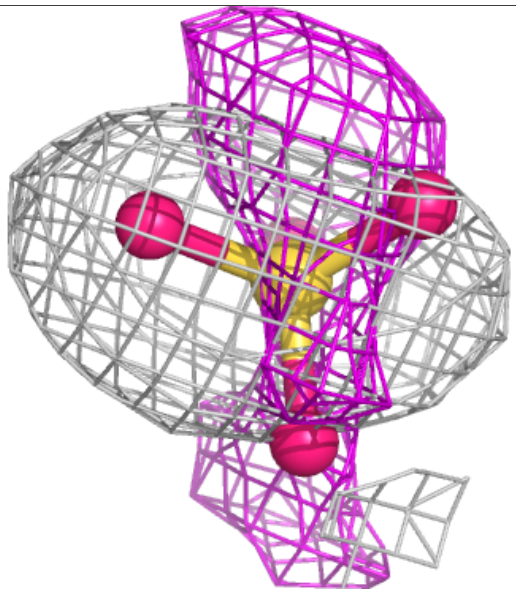
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

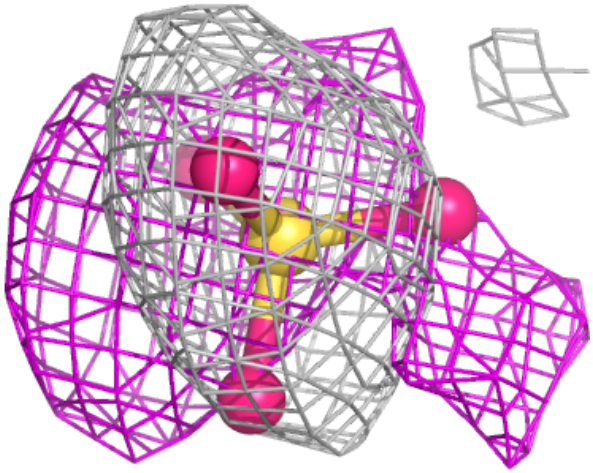


Electron density around SO4 A 1210:

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

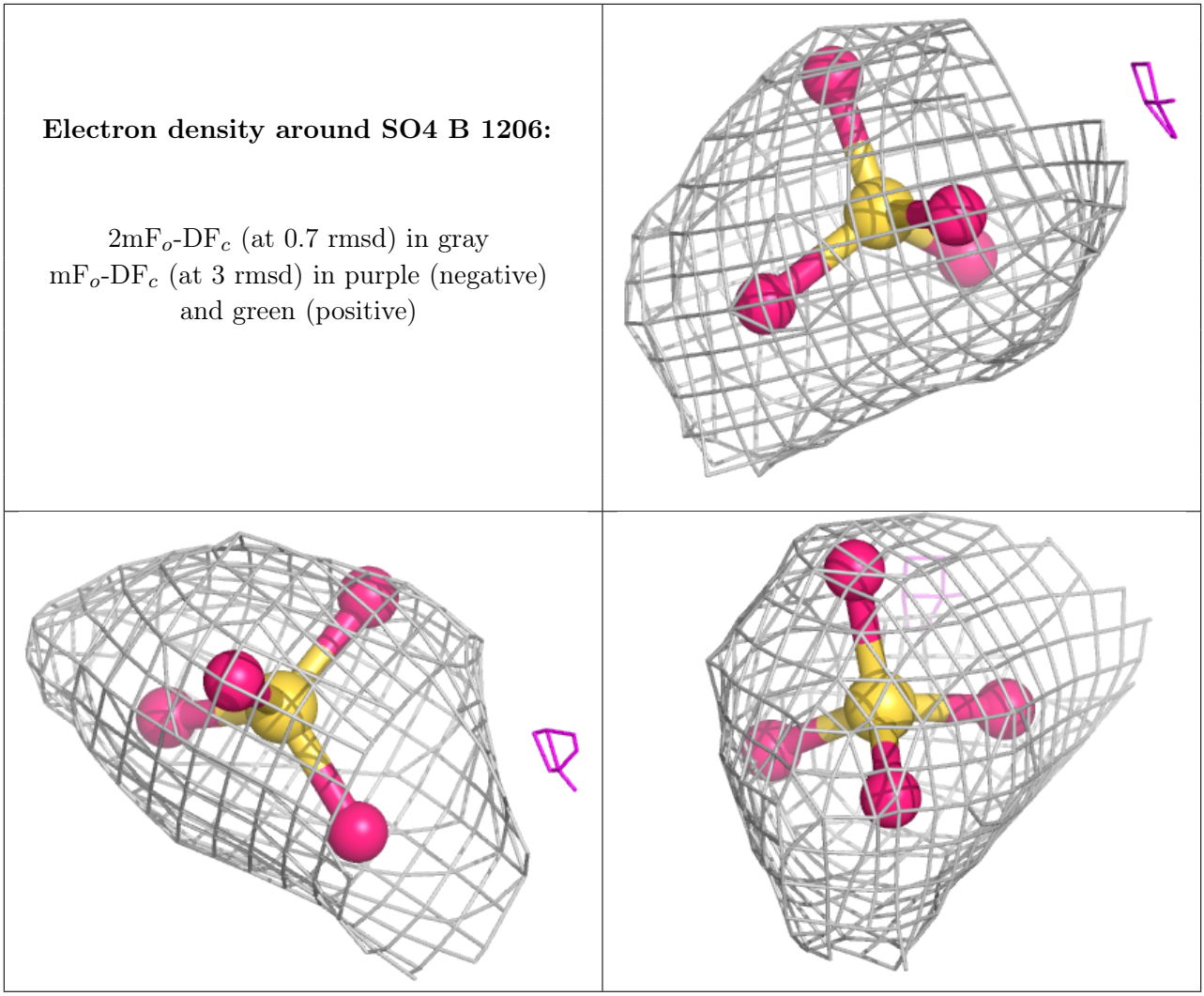






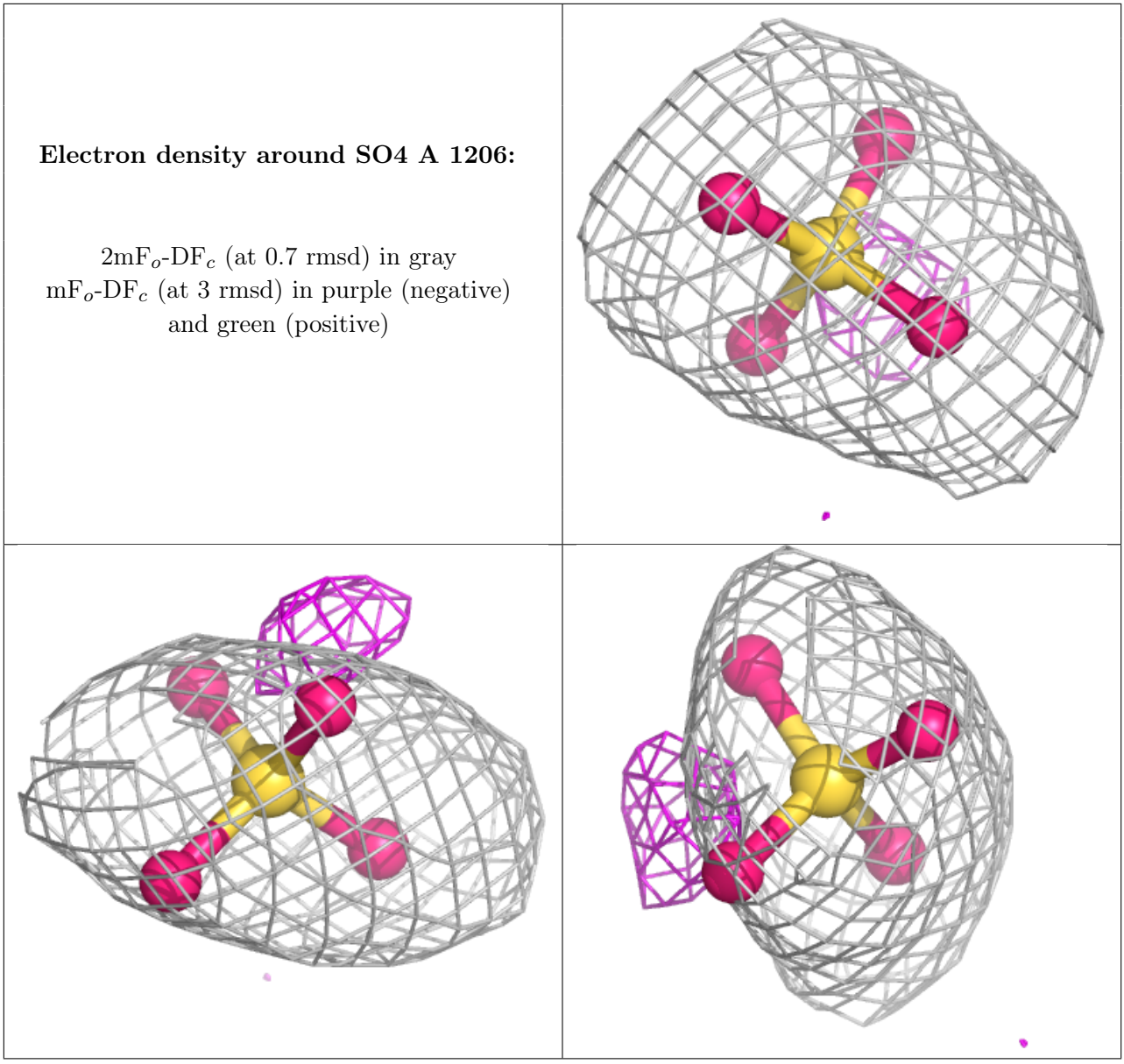
Electron density around SO4 B 1206:

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



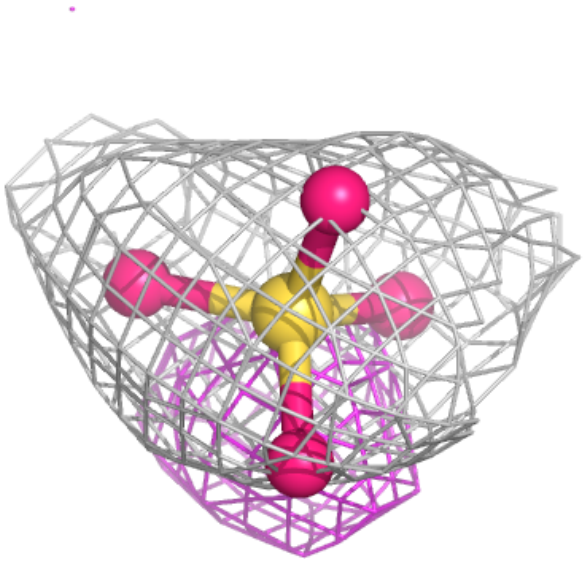
Electron density around SO4 A 1206:

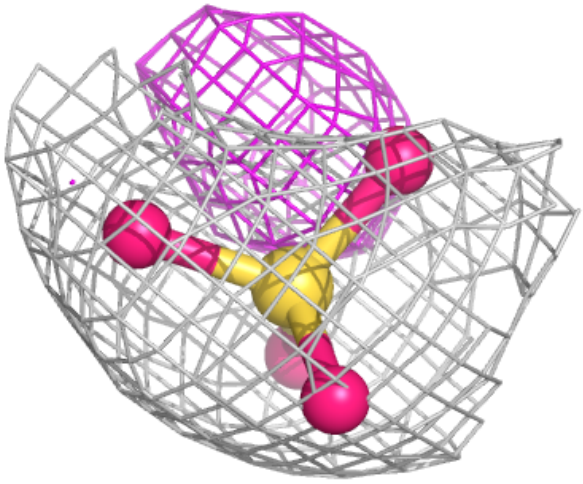
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

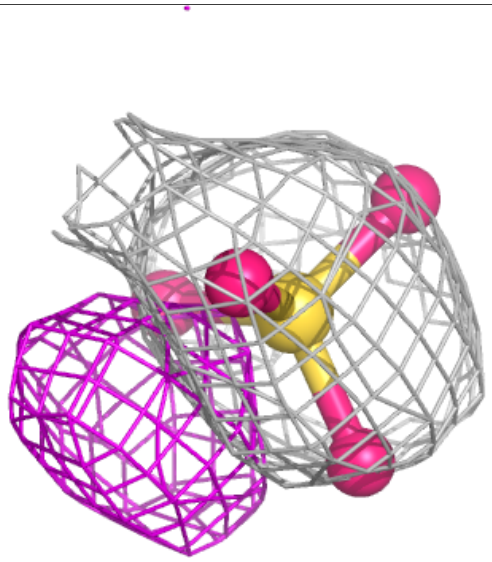


Electron density around SO4 B 1216:

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

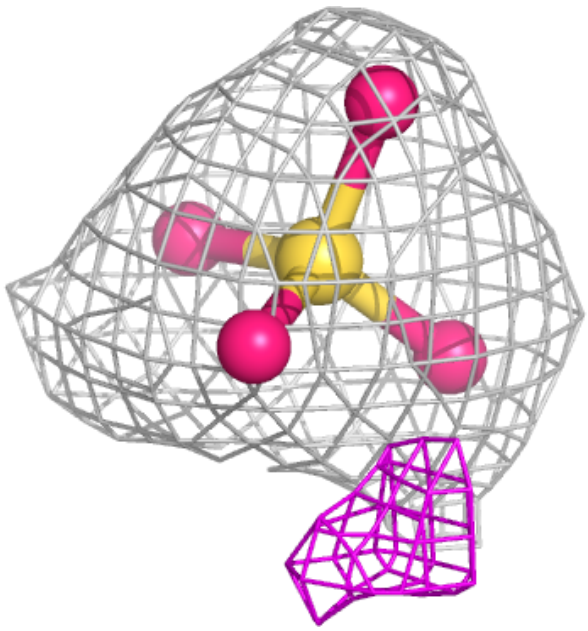


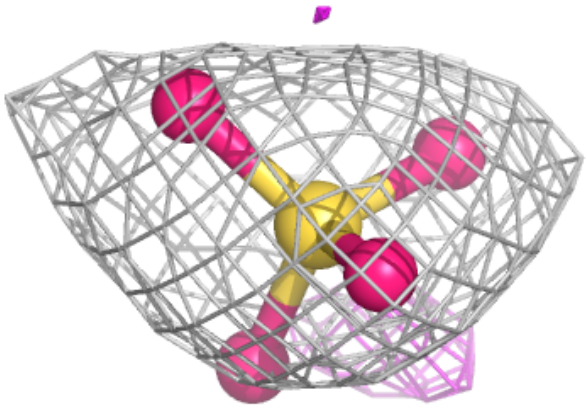


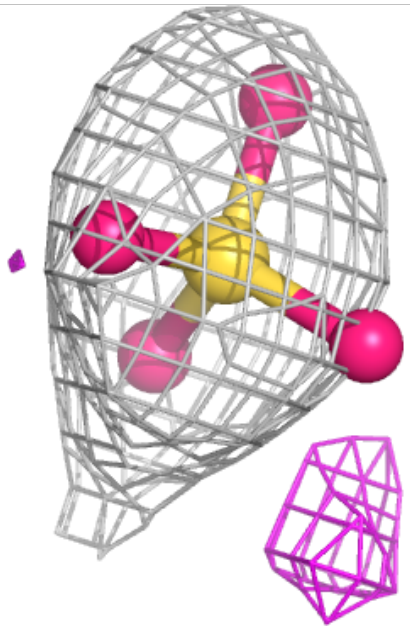


Electron density around SO4 B 1217:

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

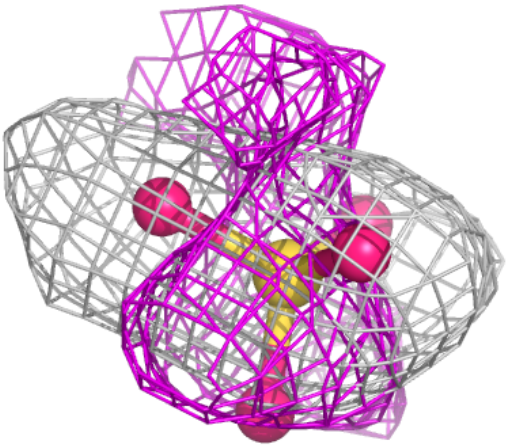


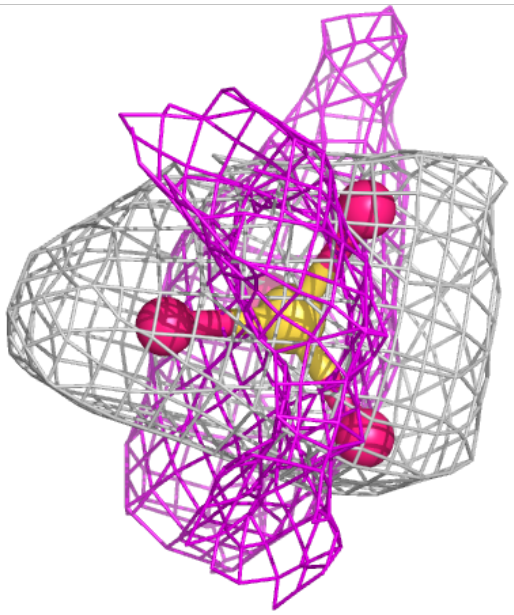


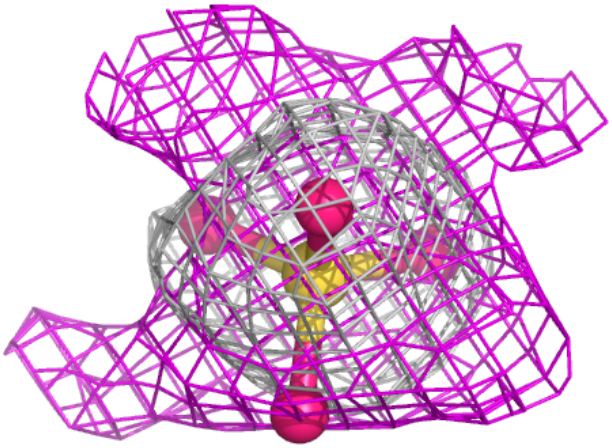


Electron density around SO4 A 1212:

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

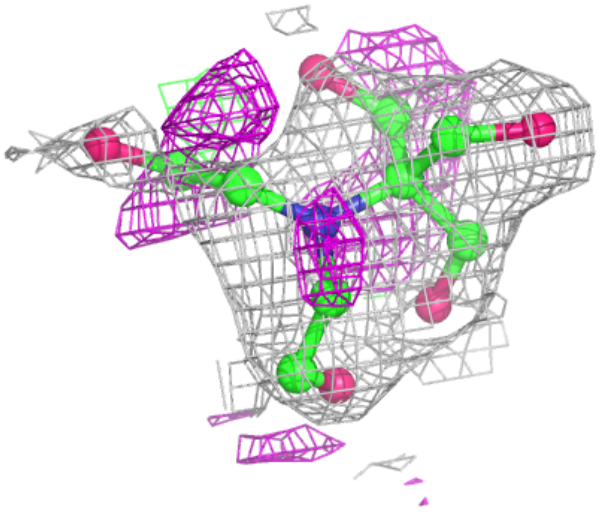


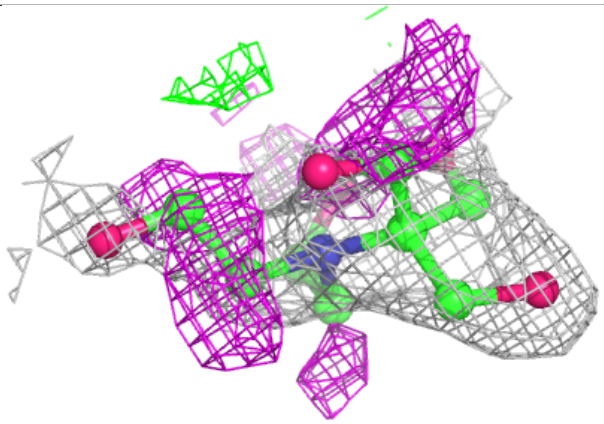


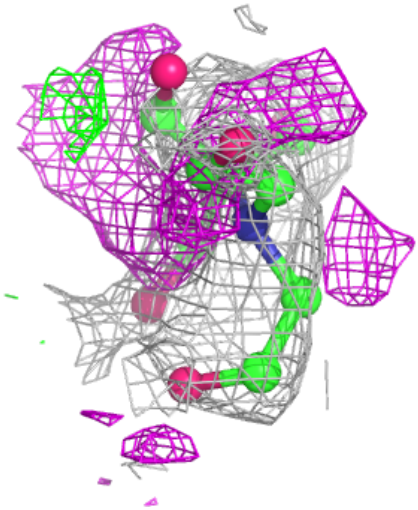


Electron density around BTB B 1203:

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

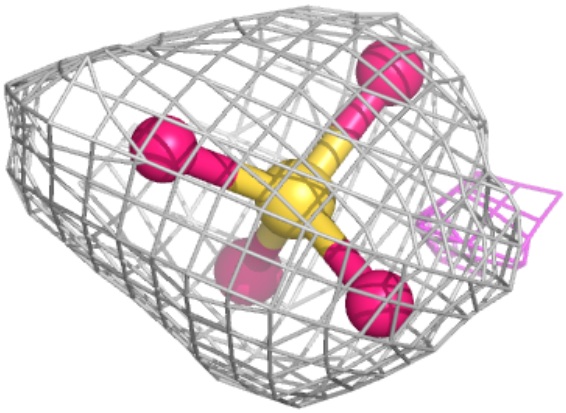


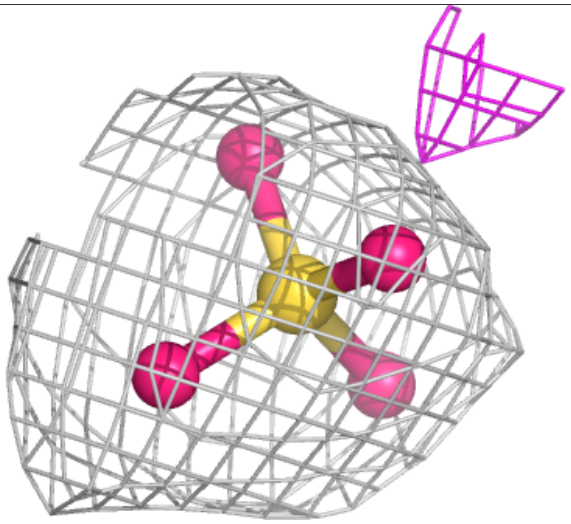


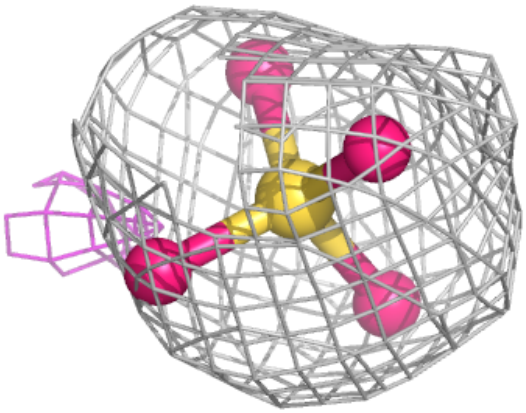


Electron density around SO4 A 1205:

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

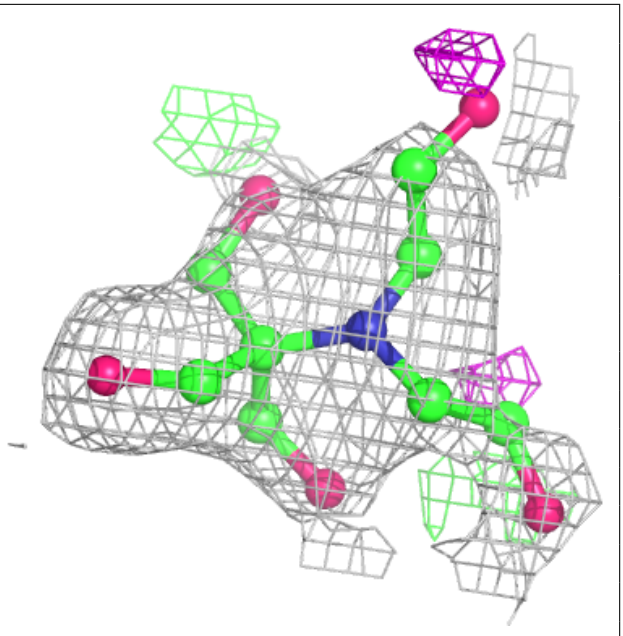


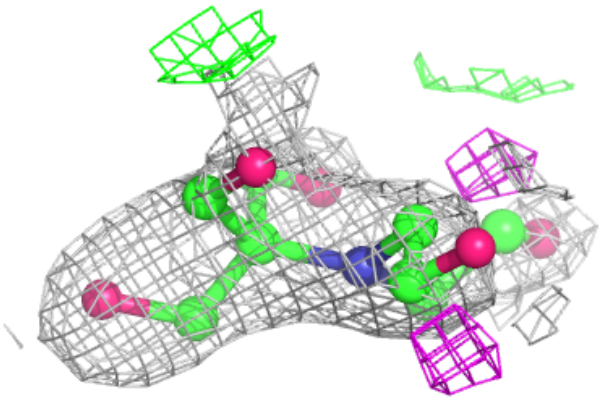


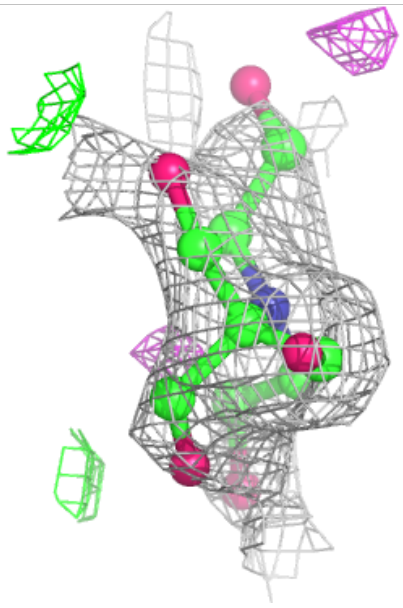


Electron density around BTB A 1203:

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

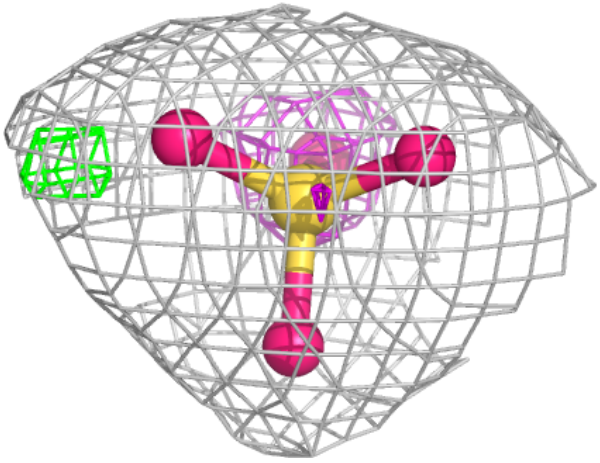


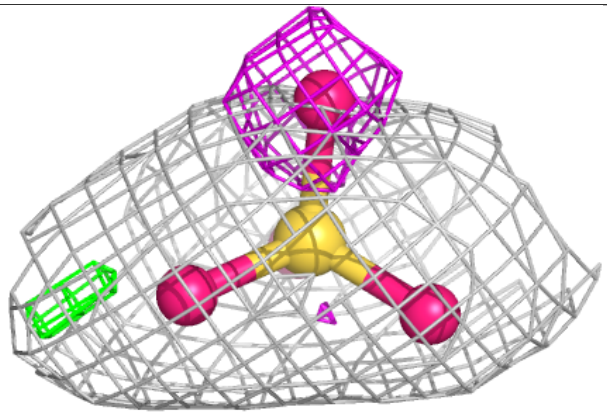


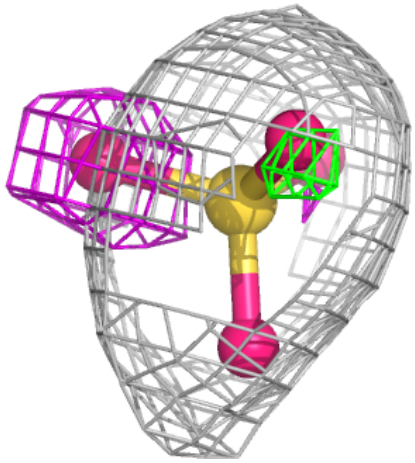


Electron density around SO4 A 1209:

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

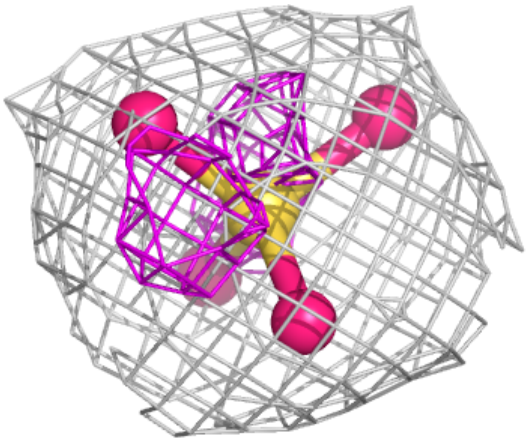


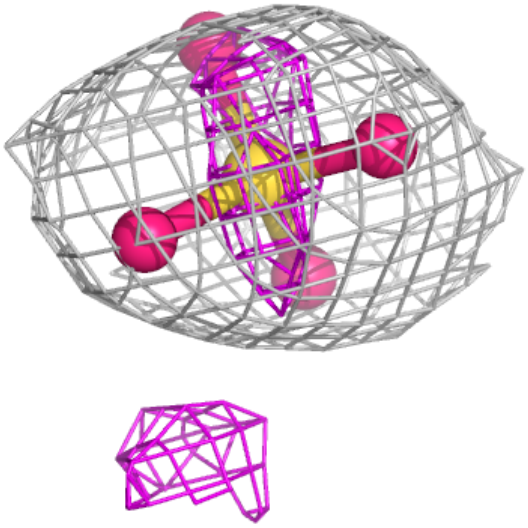


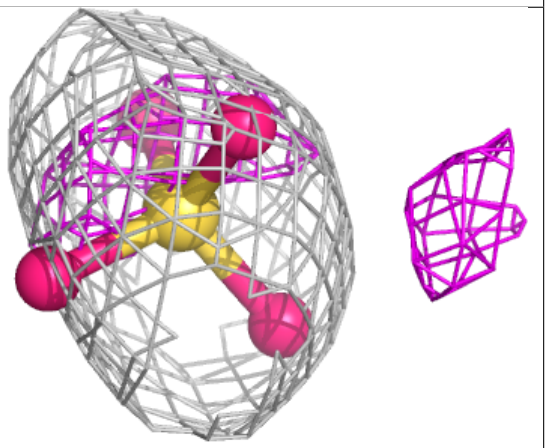


Electron density around SO4 B 1215:

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

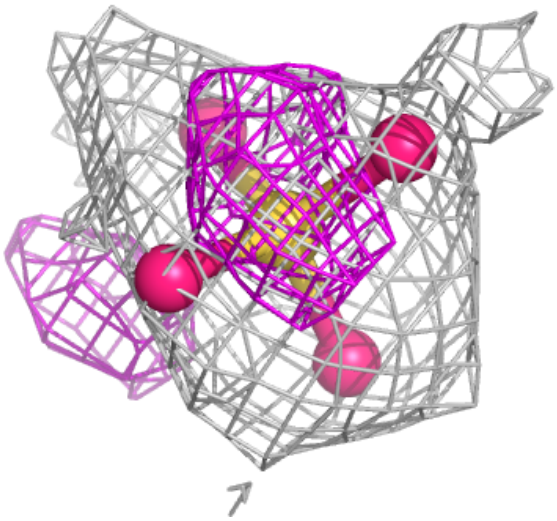


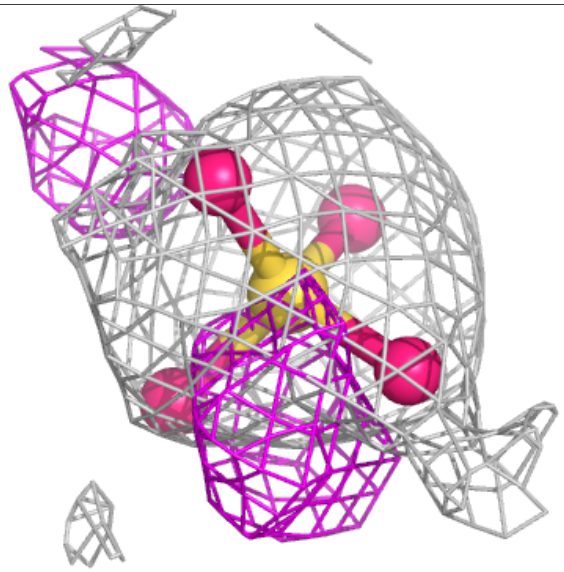


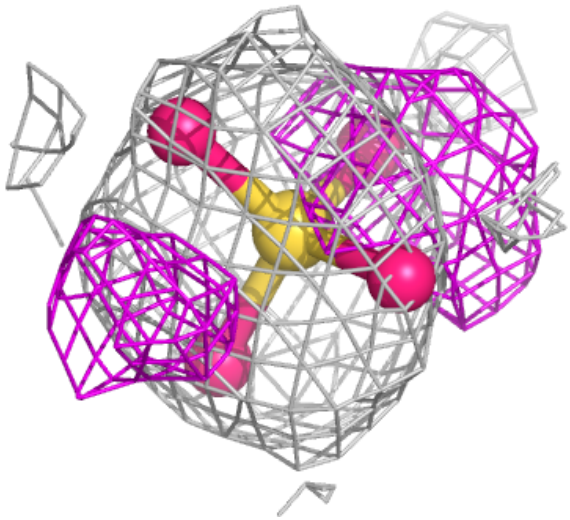


Electron density around SO4 A 1213:

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

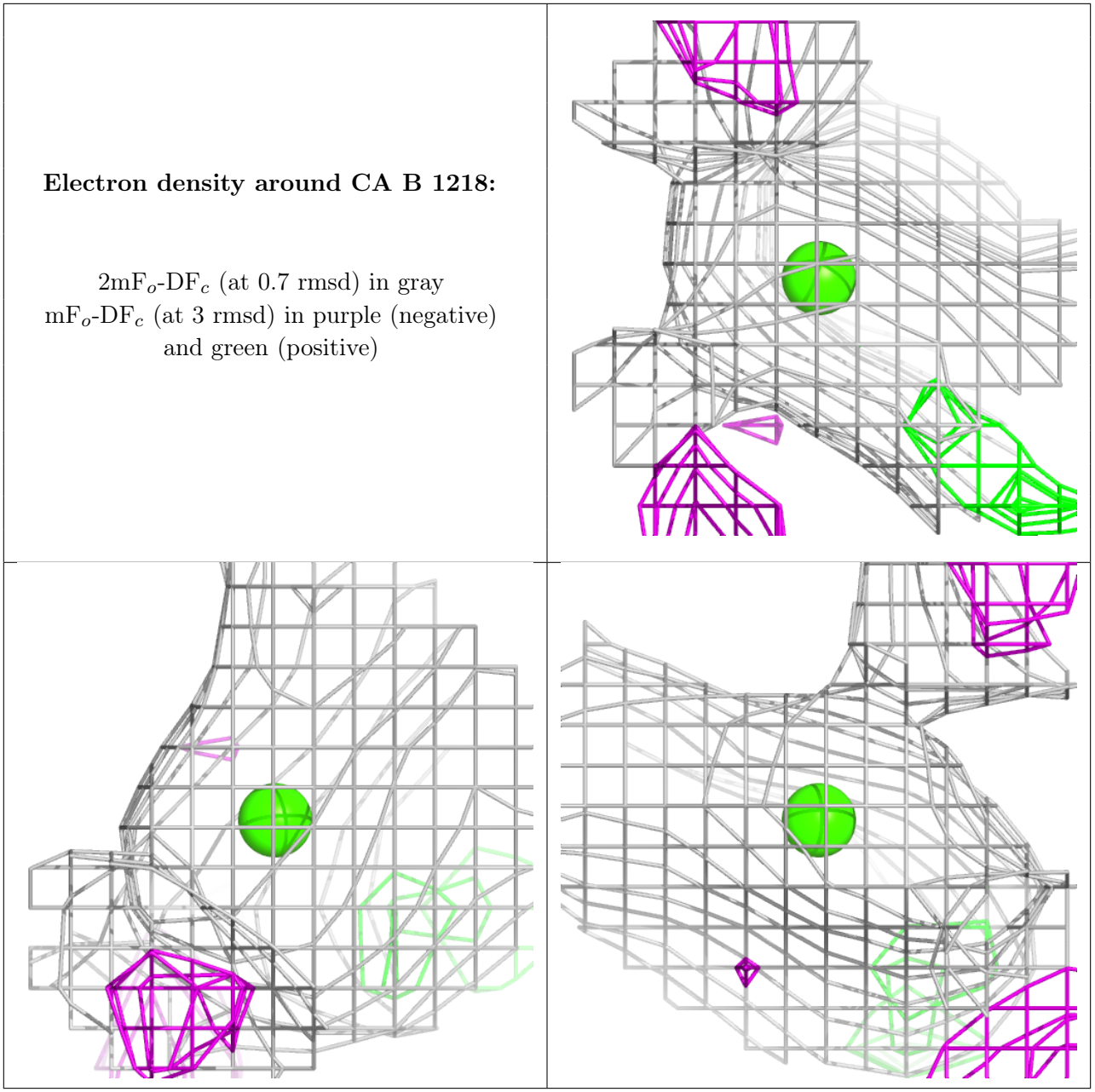






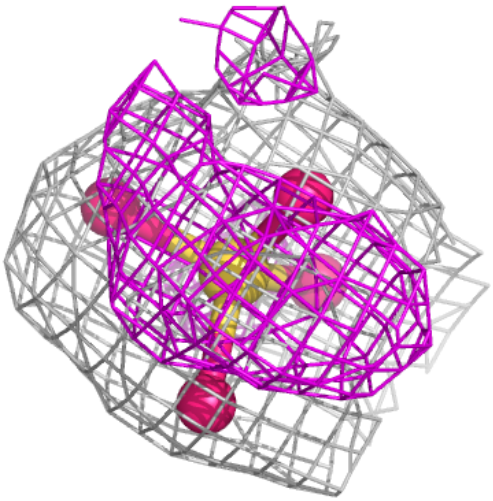
Electron density around CA B 1218:

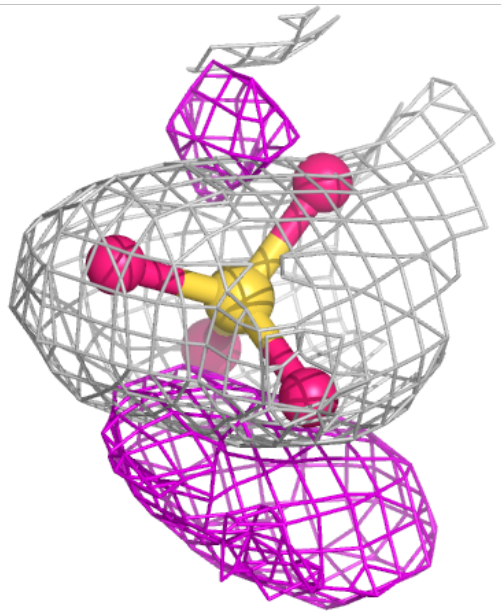
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

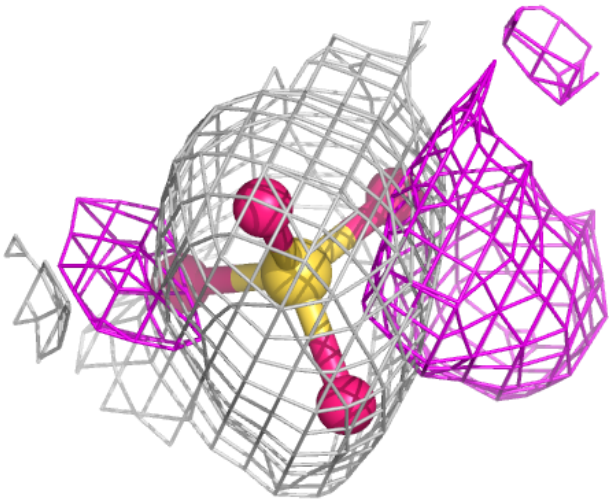


Electron density around SO4 B 1214:

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

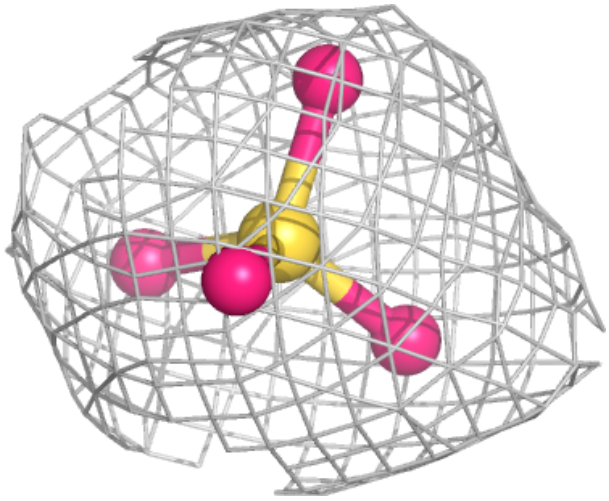


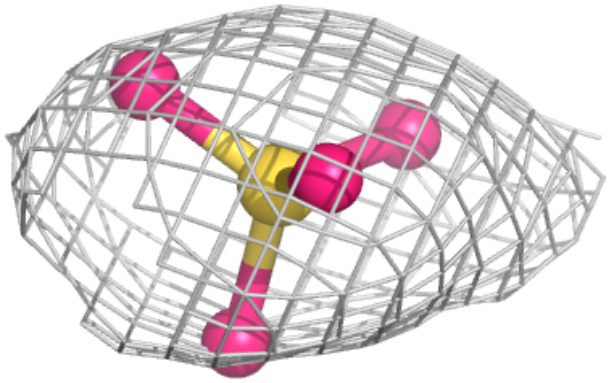


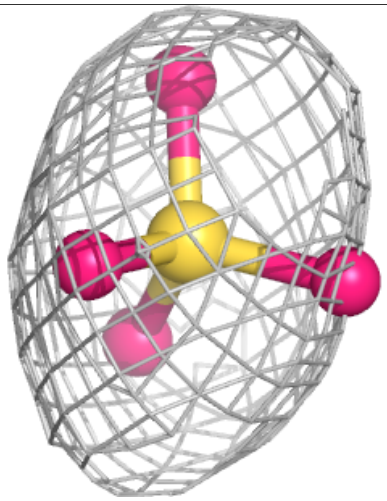


Electron density around SO4 B 1207:

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

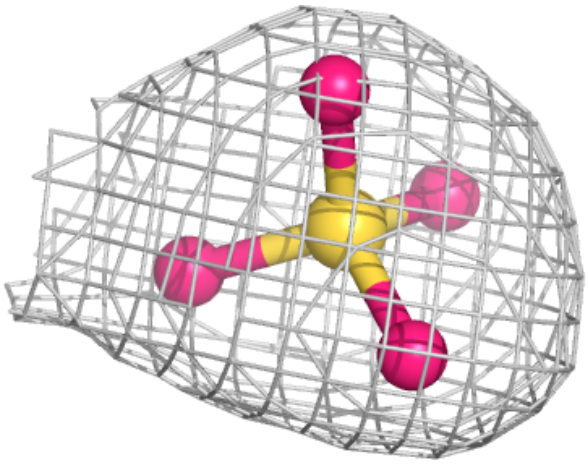


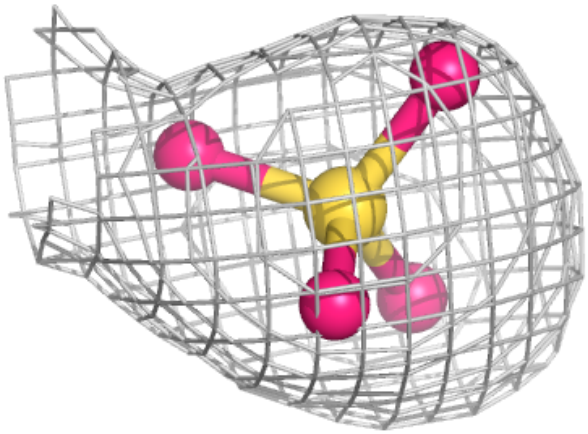


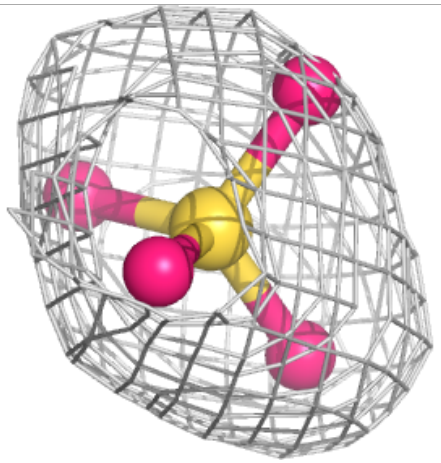


Electron density around SO4 A 1208:

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

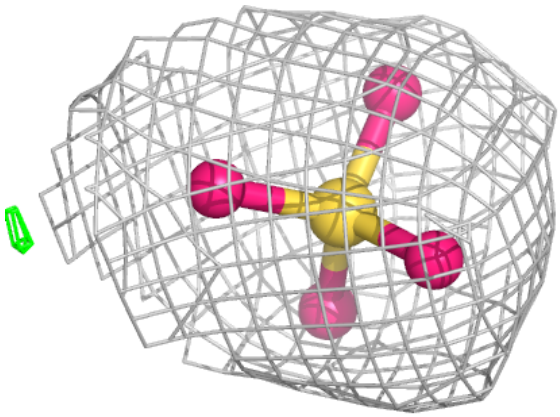


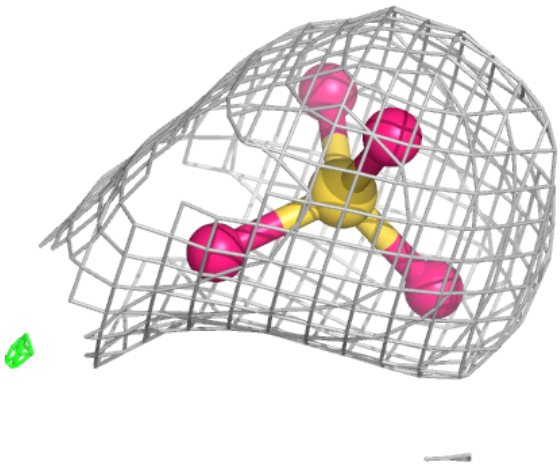


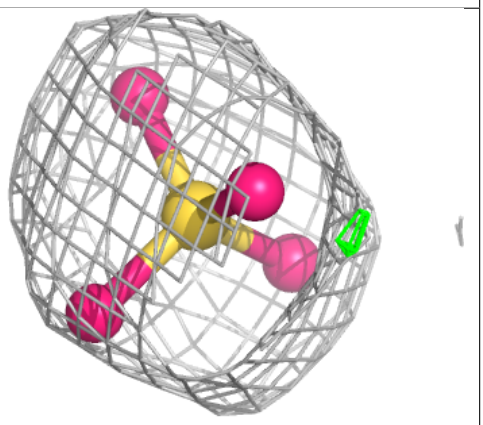


Electron density around SO4 B 1212:

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

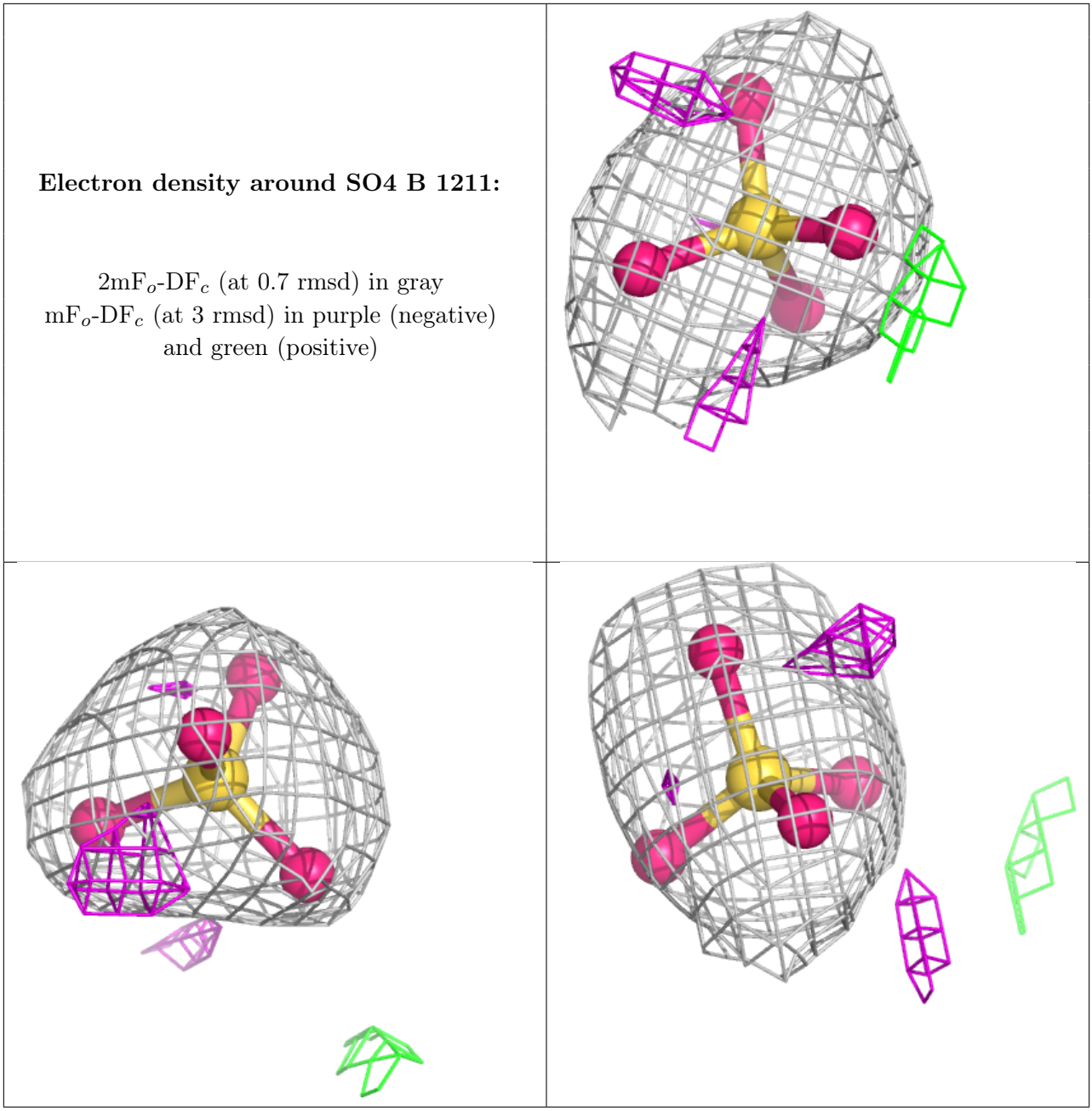






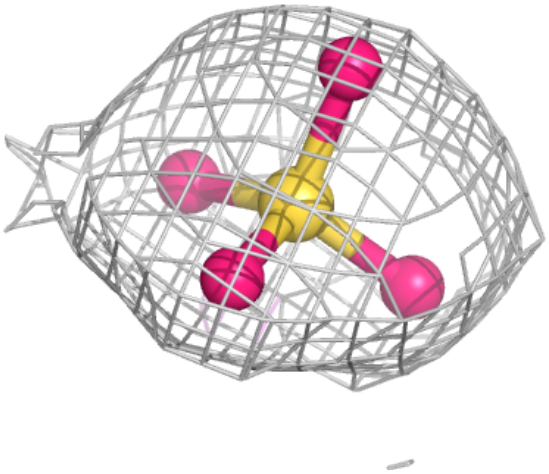
Electron density around SO4 B 1211:

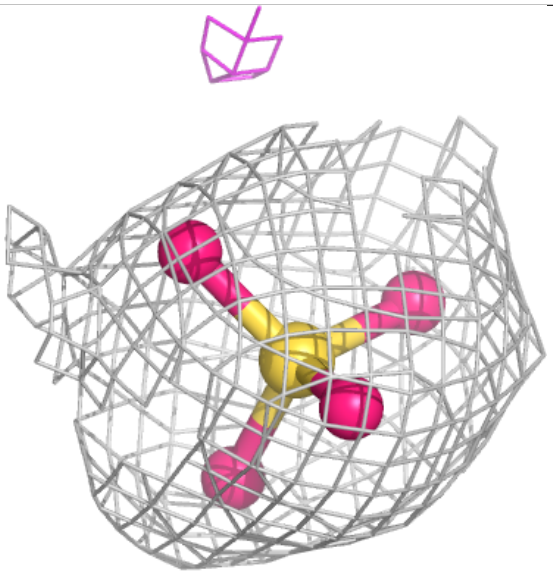
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

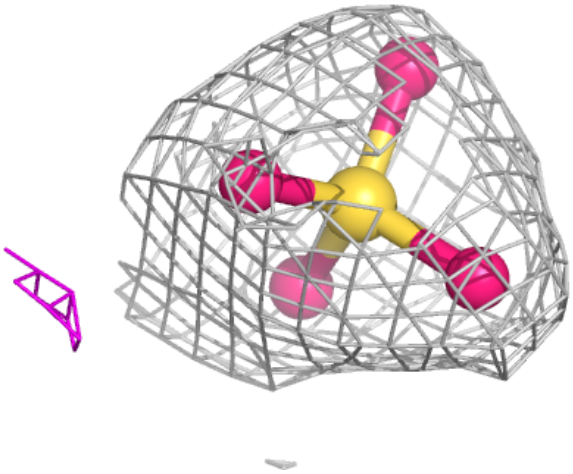


Electron density around SO4 B 1210:

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

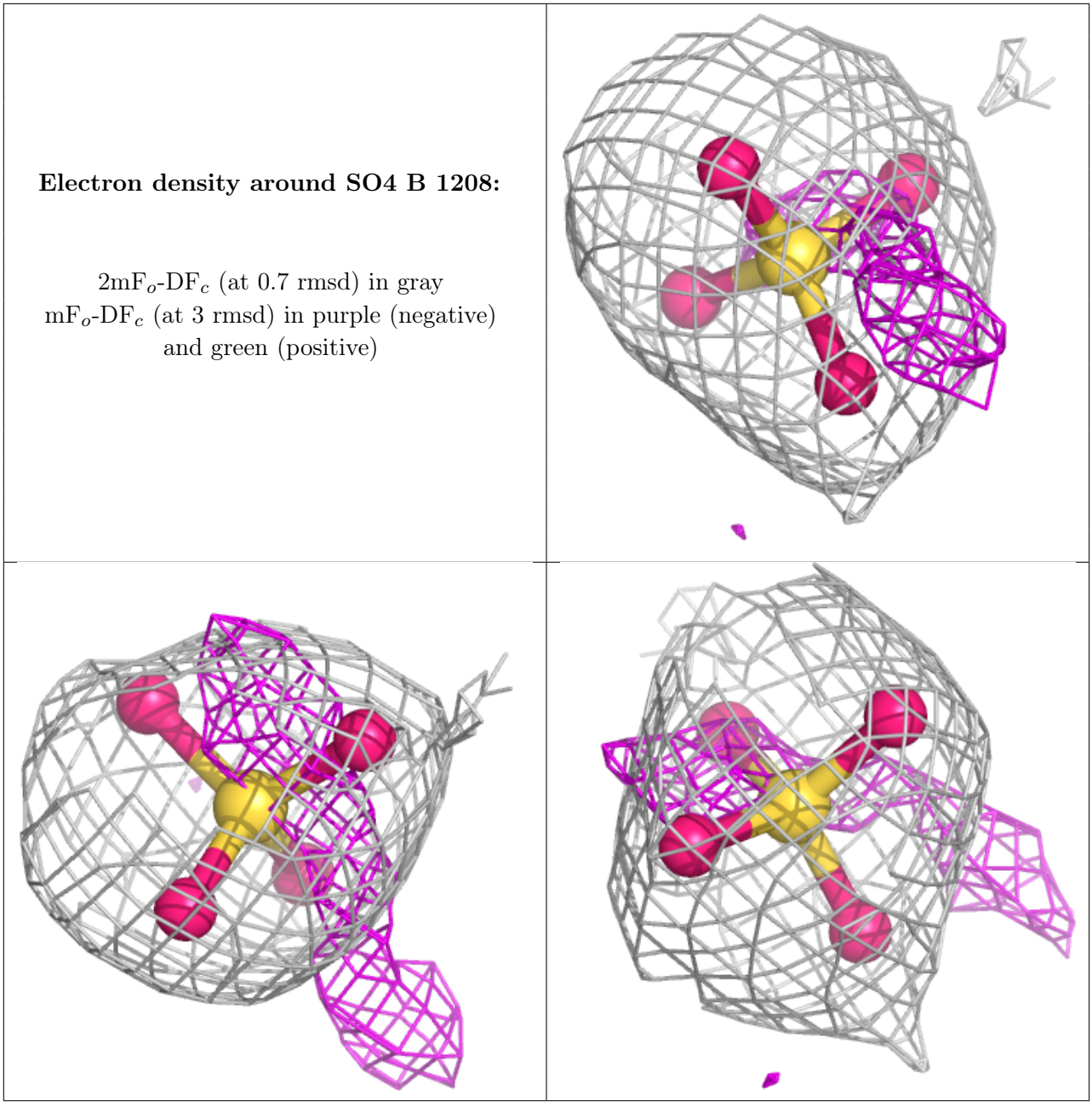






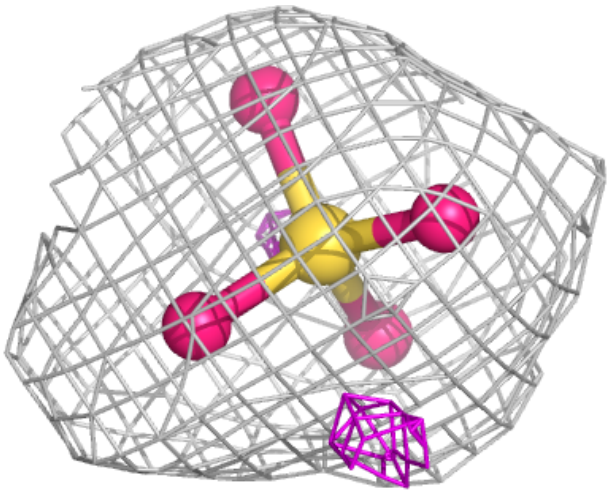
Electron density around SO4 B 1208:

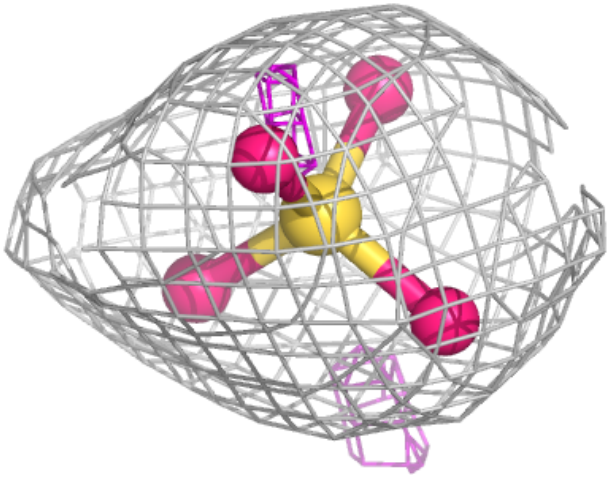
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

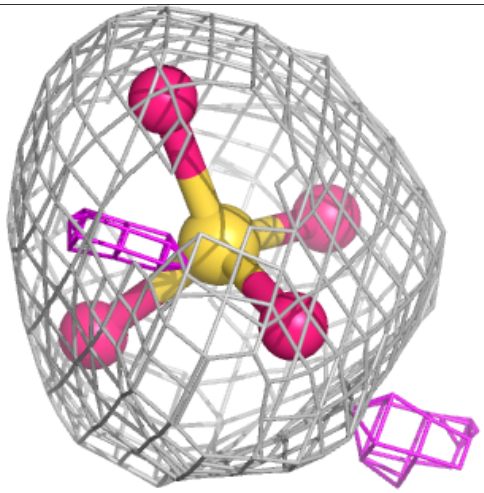


Electron density around SO4 B 1213:

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

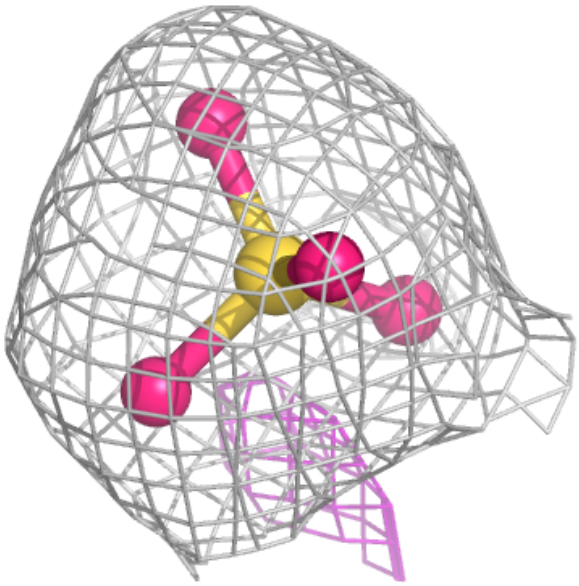


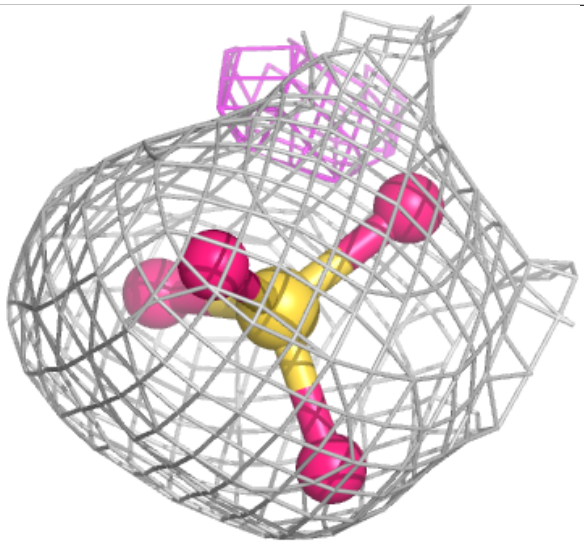


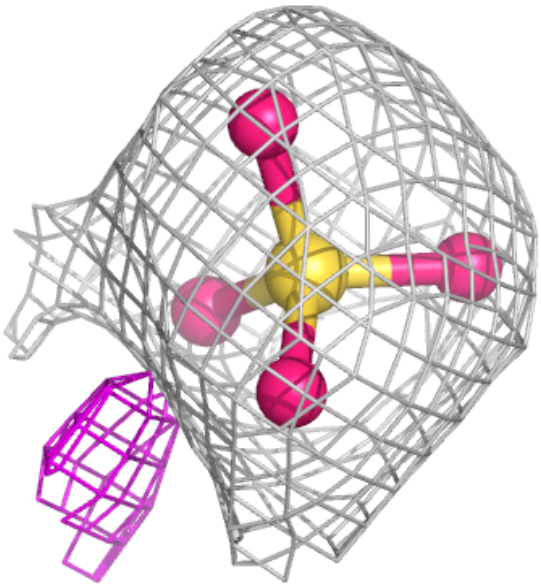


Electron density around SO4 A 1204:

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

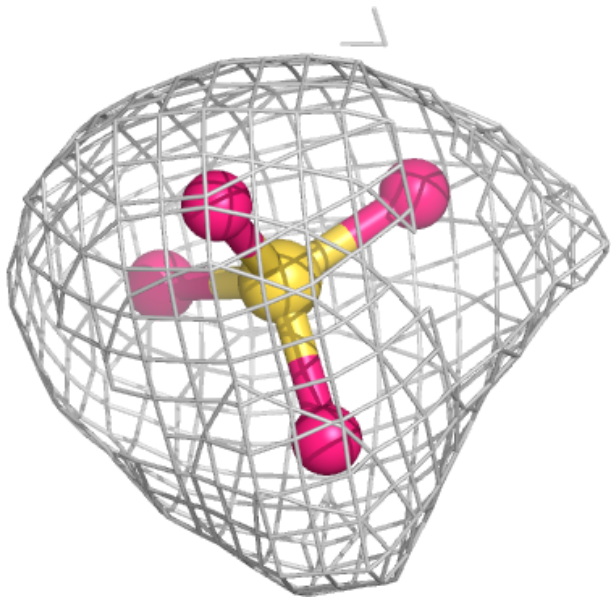


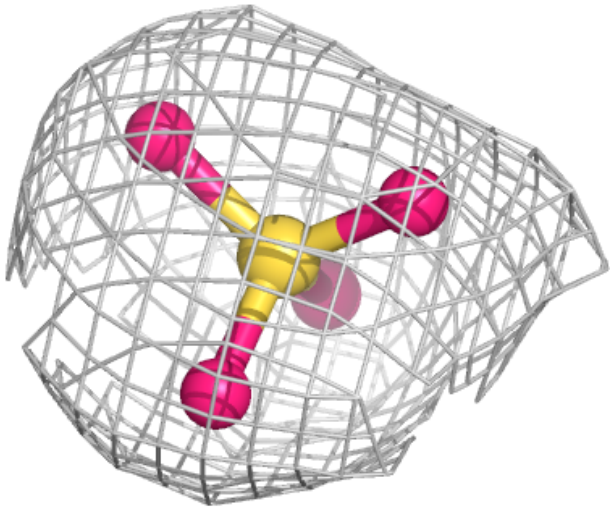


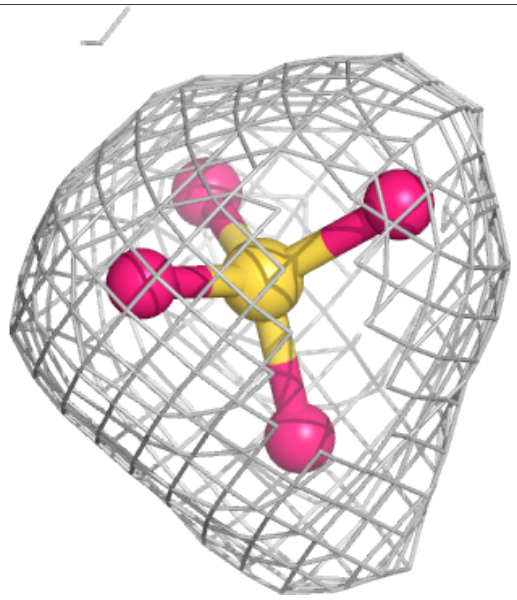


Electron density around SO4 B 1205:

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

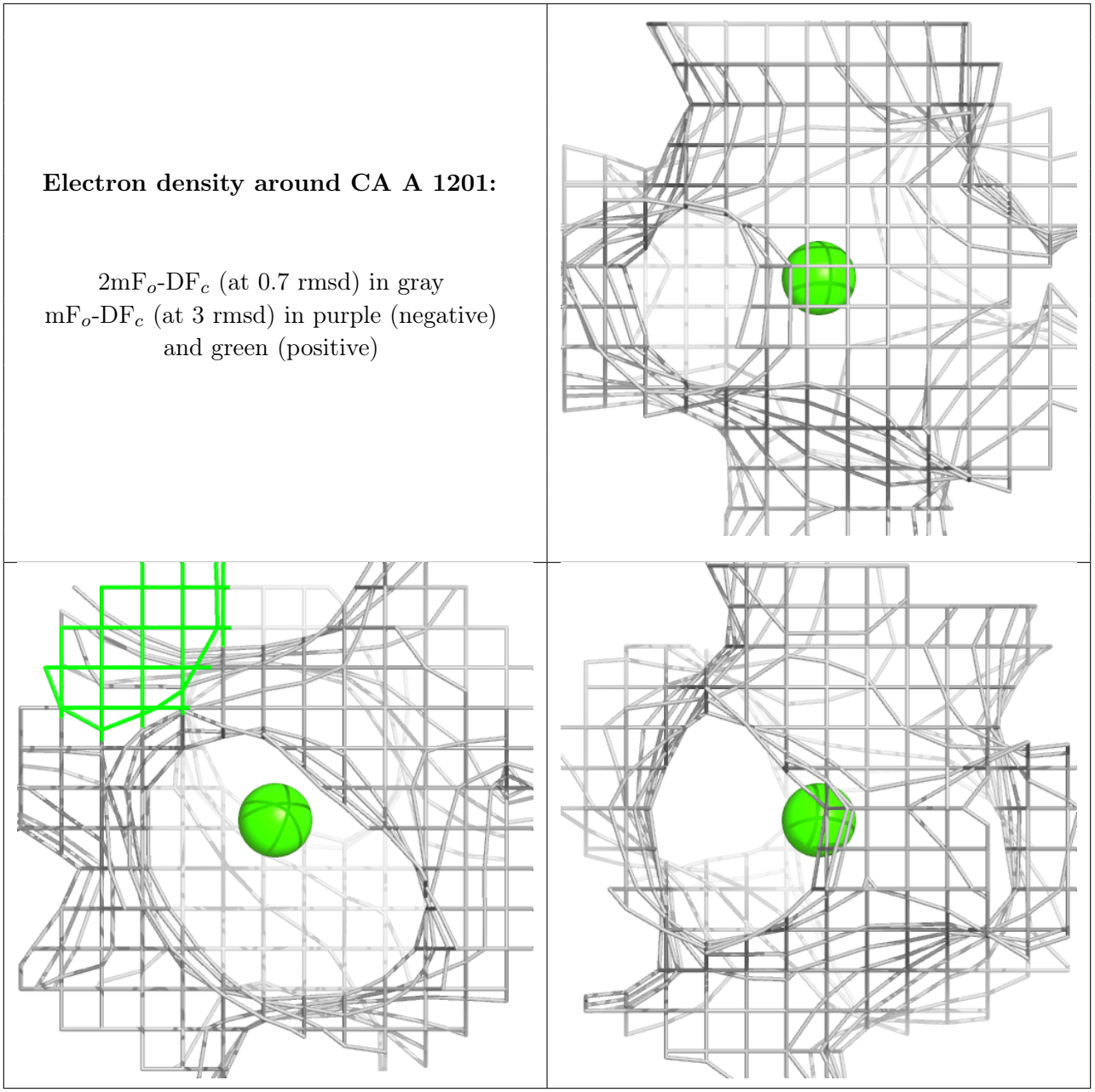






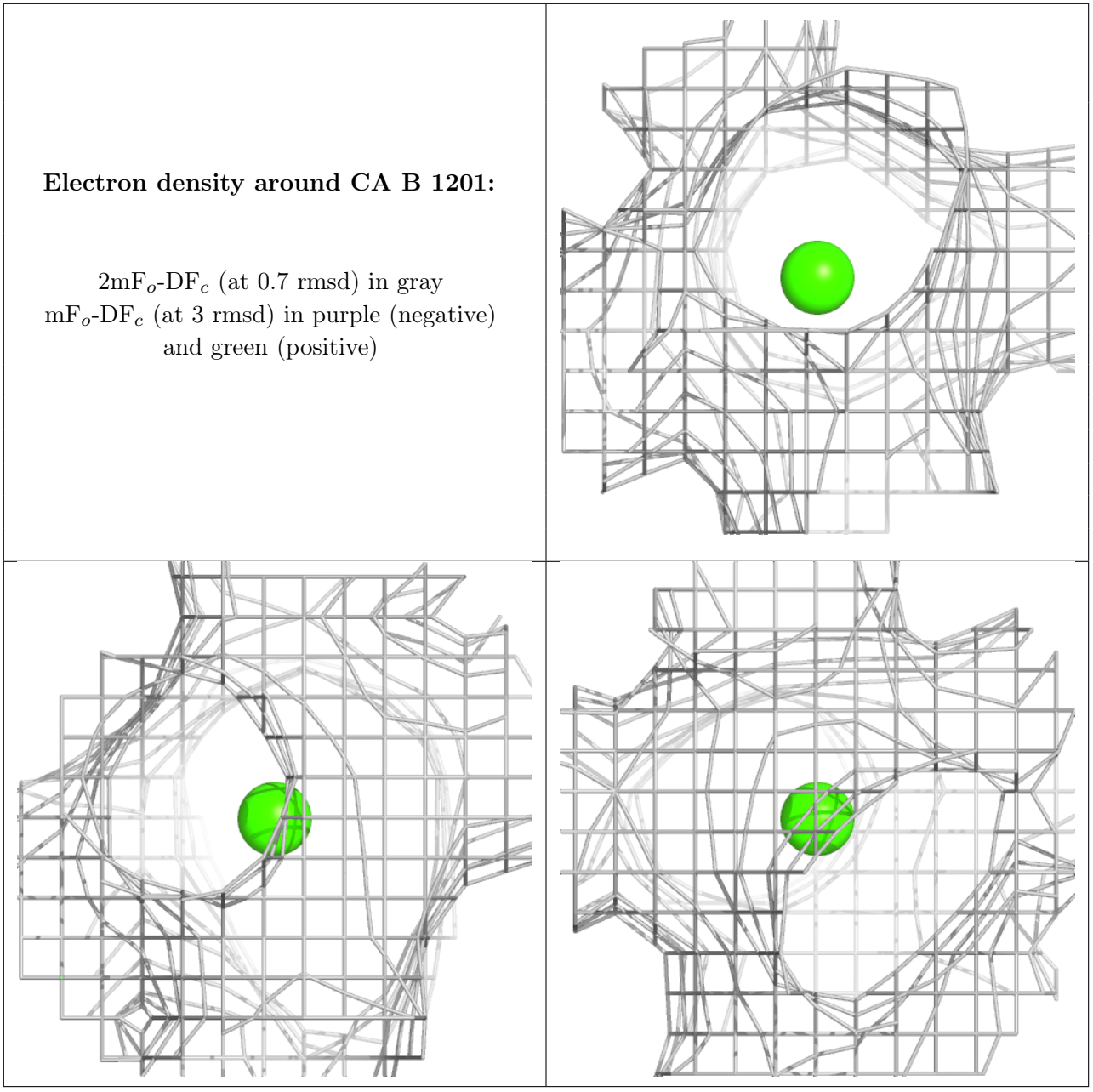
Electron density around CA A 1201:

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



Electron density around CA B 1201:

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



6.5 Other polymers (i)

There are no such residues in this entry.