Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 02:58 PM EDT

PDB ID	:	8UF5
Title	:	Catalytic domain of GtfB in complex with inhibitor G43
Authors	:	Schormann, N.; Deivanayagam, C.; Velu, S.
Deposited on	:	2023-10-03
Resolution	:	2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

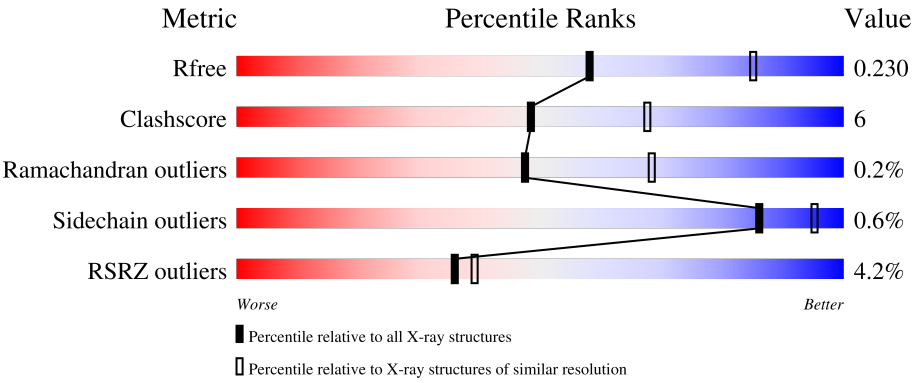
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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% 88% 9% .
1	B	869	5% 85% 10% .

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	1103	-	-	X	-
4	BTB	B	1103	-	-	X	-
6	EDO	B	1104	-	-	X	-
6	EDO	B	1105	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 13656 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	839	Total 6627	C 4176	N 1136	O 1299	S 16	0	1	0
1	B	831	Total 6522	C 4110	N 1116	O 1280	S 16	0	0	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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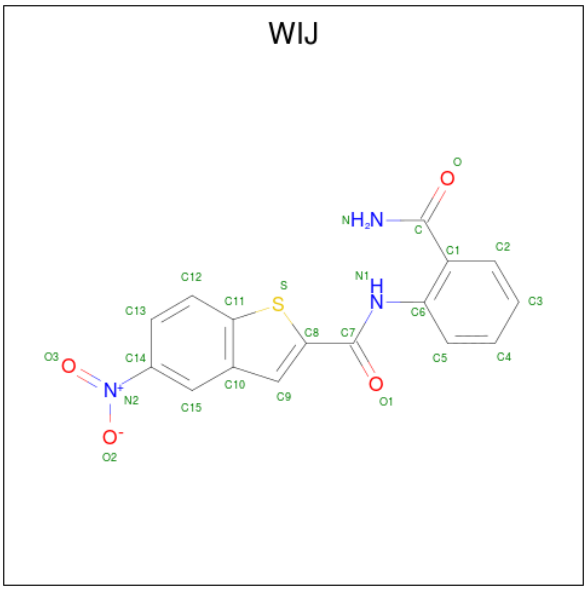
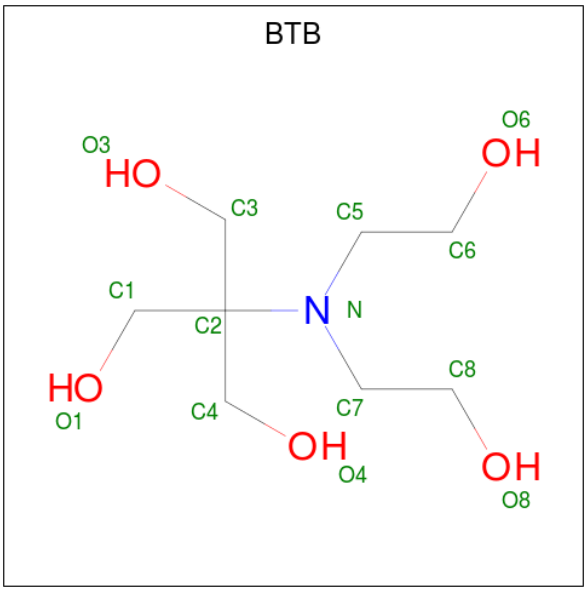
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ca 1 1	0	0

- Molecule 3 is N-(2-carbamoylphenyl)-5-nitro-1-benzothiophene-2-carboxamide (three-letter code: WIJ) (formula: $C_{16}H_{11}N_3O_4S$) (labeled as "Ligand of Interest" by depositor).



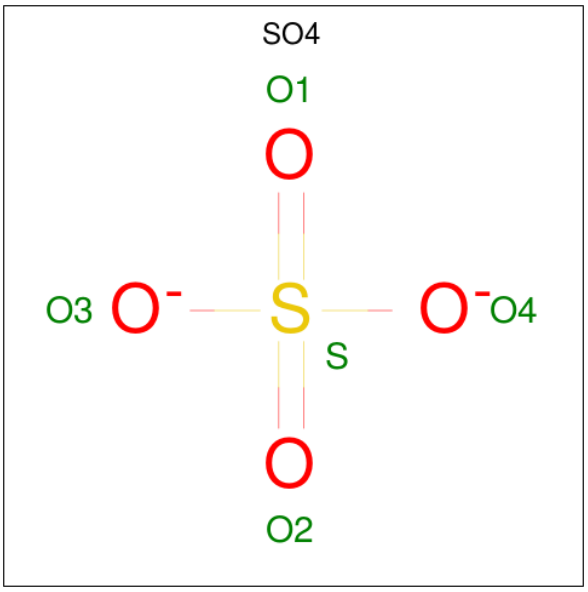
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O S 24 16 3 4 1	0	0
3	B	1	Total C N O S 24 16 3 4 1	0	0

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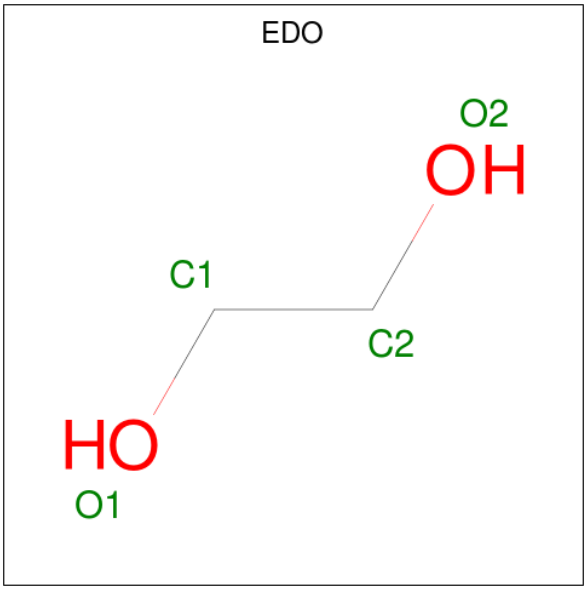
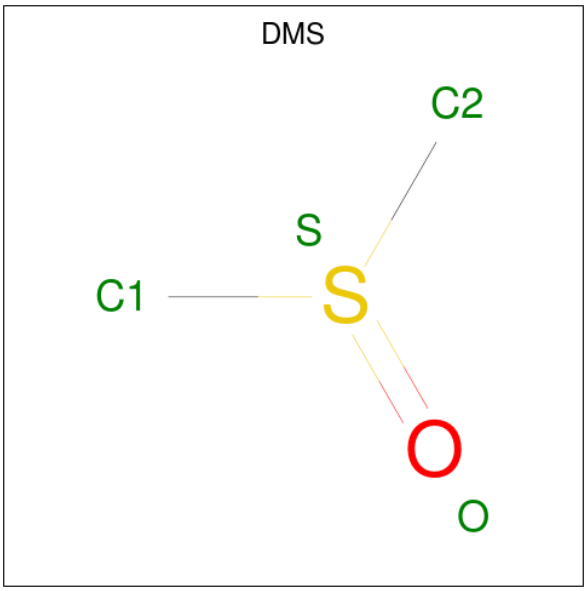
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0
5	B	1	Total O S 5 4 1	0	0

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0

- Molecule 7 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O S 4 2 1 1	0	0

- Molecule 8 is water.

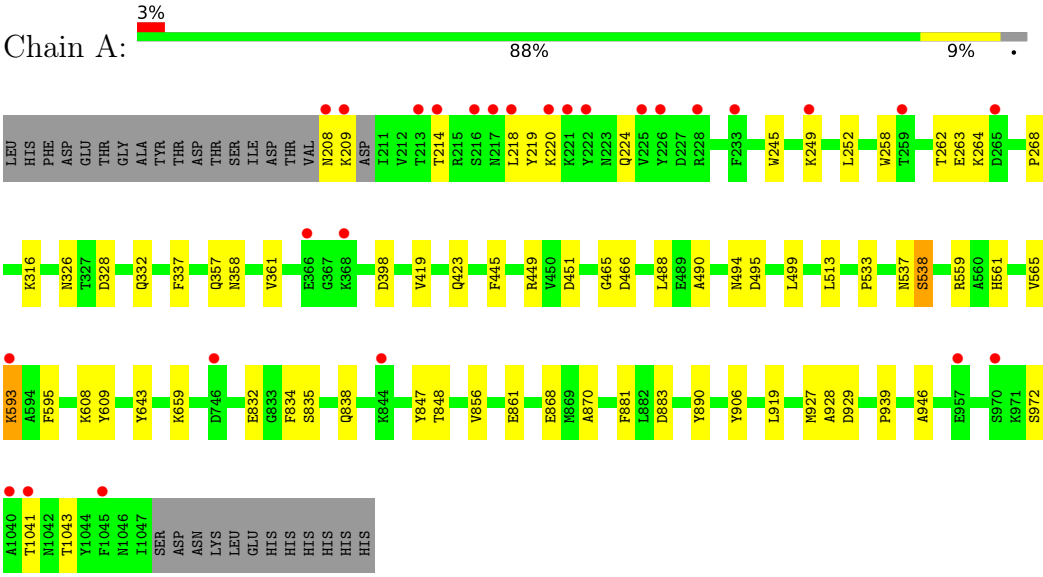
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	201	Total O 201 201	0	0
8	B	186	Total O 186 186	0	0

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.

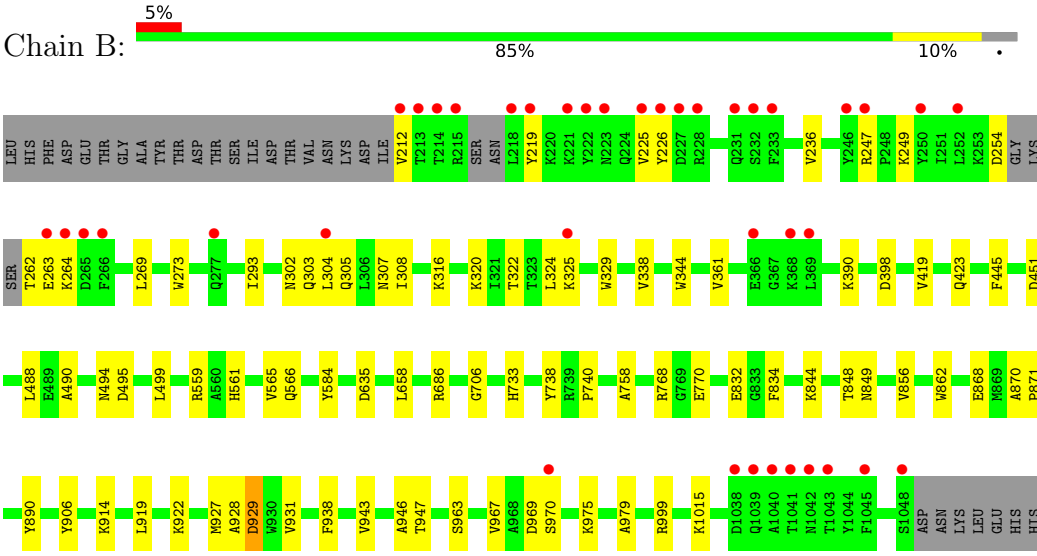
• Molecule 1: Glucosyltransferase-I

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	149.78Å 149.78Å 304.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.35 – 2.50 56.35 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (56.35-2.50) 100.0 (56.35-2.50)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.199 , 0.230 0.200 , 0.230	Depositor DCC
R_{free} test set	6050 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	38.8	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 44.9	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	0.93	EDS
Total number of atoms	13656	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, CA, BTB, WIJ, DMS, EDO

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	0.29	0/6765	0.49	0/9179
1	B	0.29	0/6656	0.49	0/9034
All	All	0.29	0/13421	0.49	0/18213

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	6627	0	6446	68	0
1	B	6522	0	6323	82	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	24	0	0	2	0
3	B	24	0	0	0	0
4	A	14	0	19	22	0
4	B	14	0	19	14	0
5	A	10	0	0	0	0
5	B	20	0	0	1	0
6	B	8	0	12	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	4	0	6	0	0
8	A	201	0	0	2	0
8	B	186	0	0	2	0
All	All	13656	0	12825	156	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 6.

All (156) 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:332:GLN:HG3	1:B:320:LYS:NZ	1.51	1.22
1:A:881:PHE:HE2	4:A:1103:BTB:C8	1.59	1.14
1:A:208:ASN:OD1	1:A:209:LYS:HG3	1.49	1.13
1:A:881:PHE:HE2	4:A:1103:BTB:H81	1.06	1.09
1:A:332:GLN:HG3	1:B:320:LYS:HZ2	0.94	1.07
1:A:881:PHE:CE2	4:A:1103:BTB:H81	1.90	1.06
1:A:218:LEU:HD11	8:A:1388:HOH:O	1.59	1.02
1:A:881:PHE:CE2	4:A:1103:BTB:C8	2.44	1.01
1:B:559:ARG:HH21	1:B:565:VAL:HG22	1.29	0.94
1:A:293:ILE:HG12	1:A:316:LYS:NZ	1.87	0.90
4:A:1103:BTB:H62	4:A:1103:BTB:H11	1.55	0.88
1:A:883:ASP:OD2	4:A:1103:BTB:H71	1.75	0.87
4:B:1103:BTB:H82	4:B:1103:BTB:O3	1.74	0.86
1:A:883:ASP:OD2	1:A:890:TYR:HB2	1.75	0.86
1:B:561:HIS:NE2	4:B:1103:BTB:H42	1.90	0.86
1:B:947:THR:HG22	1:B:963:SER:H	1.43	0.84
1:B:361:VAL:CG1	1:B:946:ALA:HB1	2.11	0.81
1:A:332:GLN:CG	1:B:320:LYS:NZ	2.41	0.79
1:A:513:LEU:HB2	1:A:538:SER:HB2	1.63	0.79
4:A:1103:BTB:H11	4:A:1103:BTB:C6	2.14	0.78
1:A:293:ILE:HD11	1:A:316:LYS:HD2	1.65	0.78
4:B:1103:BTB:H82	4:B:1103:BTB:C3	2.13	0.77
4:B:1103:BTB:H11	4:B:1103:BTB:C8	2.16	0.75
1:A:293:ILE:HG12	1:A:316:LYS:HZ2	1.50	0.74
1:B:226:TYR:HA	1:B:249:LYS:HG2	1.71	0.71
1:B:929:ASP:H	6:B:1105:EDO:H12	1.55	0.71
4:A:1103:BTB:H62	4:A:1103:BTB:C1	2.19	0.71
1:B:561:HIS:NE2	4:B:1103:BTB:C4	2.54	0.71
1:A:332:GLN:HG3	1:B:320:LYS:HZ1	1.56	0.70
1:B:733:HIS:NE2	6:B:1104:EDO:H21	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:881:PHE:HE2	4:A:1103:BTB:H82	1.53	0.69
1:A:293:ILE:HG12	1:A:316:LYS:HZ3	1.58	0.68
1:A:881:PHE:CE2	4:A:1103:BTB:H82	2.26	0.65
1:B:247:ARG:NE	1:B:262:THR:OG1	2.30	0.65
1:B:706:GLY:HA3	6:B:1104:EDO:H12	1.77	0.65
4:B:1103:BTB:H11	4:B:1103:BTB:O8	1.98	0.64
1:B:320:LYS:HD3	1:B:329:TRP:CH2	2.33	0.64
1:B:559:ARG:NH2	1:B:565:VAL:HG22	2.09	0.64
1:B:943:VAL:HG22	1:B:967:VAL:HG22	1.80	0.63
1:B:914:LYS:NZ	8:B:1202:HOH:O	2.30	0.63
1:B:325:LYS:HG2	1:B:325:LYS:O	1.99	0.63
1:A:883:ASP:OD2	4:A:1103:BTB:C7	2.47	0.62
1:A:593:LYS:NZ	1:B:304:LEU:HD11	2.15	0.61
1:B:566:GLN:OE1	4:B:1103:BTB:O6	2.19	0.60
1:A:593:LYS:HZ3	1:B:304:LEU:HD11	1.65	0.60
4:A:1103:BTB:O1	4:A:1103:BTB:O3	2.20	0.60
1:B:870:ALA:O	6:B:1105:EDO:H11	2.02	0.60
4:A:1103:BTB:C6	4:A:1103:BTB:H31	2.32	0.59
4:A:1103:BTB:H62	4:A:1103:BTB:H31	1.85	0.59
1:B:733:HIS:CE1	6:B:1104:EDO:H21	2.38	0.57
1:A:835:SER:HB3	1:A:838:GLN:HG3	1.85	0.57
1:B:361:VAL:HG12	1:B:946:ALA:HB1	1.86	0.56
1:A:533:PRO:HB3	1:A:537:ASN:HD22	1.70	0.56
1:B:834:PHE:CG	1:B:870:ALA:HB2	2.40	0.56
1:B:929:ASP:H	6:B:1105:EDO:C1	2.18	0.56
1:A:883:ASP:CG	4:A:1103:BTB:H71	2.26	0.56
1:B:293:ILE:HG12	1:B:316:LYS:NZ	2.21	0.56
1:B:303:GLN:NE2	1:B:307:ASN:OD1	2.38	0.56
1:B:212:VAL:HG22	1:B:212:VAL:O	2.04	0.55
1:A:848:THR:HB	1:A:906:TYR:HB3	1.88	0.55
1:B:738:TYR:OH	6:B:1104:EDO:H22	2.06	0.55
1:A:1041:THR:HB	1:A:1043:THR:HG23	1.89	0.54
1:B:320:LYS:HD3	1:B:329:TRP:CZ2	2.43	0.54
1:B:844:LYS:N	5:B:1109:SO4:O1	2.32	0.53
1:B:398:ASP:HB3	1:B:494:ASN:ND2	2.23	0.53
3:A:1102:WIJ:O	4:A:1103:BTB:O3	2.22	0.52
1:A:883:ASP:CG	4:A:1103:BTB:C8	2.77	0.52
1:B:264:LYS:HG2	1:B:264:LYS:O	2.09	0.52
1:B:269:LEU:HD23	1:B:273:TRP:HB3	1.92	0.52
1:B:848:THR:HB	1:B:906:TYR:HB3	1.90	0.52
1:A:361:VAL:HG22	1:A:946:ALA:HB1	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:856:VAL:HG23	1:B:919:LEU:HD23	1.91	0.51
1:A:834:PHE:CG	1:A:870:ALA:HB2	2.45	0.51
1:B:868:GLU:HA	1:B:927:MET:HB3	1.93	0.51
1:B:947:THR:HG22	1:B:963:SER:N	2.20	0.51
1:B:938:PHE:CD2	1:B:970:SER:HA	2.46	0.51
1:B:488:LEU:HD11	1:B:499:LEU:HD13	1.93	0.50
1:A:588:MET:O	1:A:592:LYS:HG3	2.12	0.50
1:B:254:ASP:OD1	1:B:322:THR:HG21	2.11	0.50
1:A:214:THR:HA	1:A:220:LYS:HZ3	1.77	0.50
1:B:247:ARG:HH11	1:B:263:GLU:H	1.60	0.50
1:A:883:ASP:CG	4:A:1103:BTB:O8	2.50	0.49
1:A:445:PHE:CG	1:A:928:ALA:HB2	2.47	0.49
1:B:451:ASP:OD1	1:B:452:ALA:N	2.45	0.49
1:A:214:THR:HA	1:A:220:LYS:NZ	2.28	0.49
1:B:928:ALA:HA	6:B:1105:EDO:O1	2.12	0.49
3:A:1102:WIJ:O	4:A:1103:BTB:C3	2.61	0.49
1:B:490:ALA:HB1	1:B:495:ASP:OD2	2.13	0.48
1:A:466:ASP:HB3	1:A:996:LEU:HD22	1.94	0.48
1:A:419:VAL:O	1:A:423:GLN:HG2	2.14	0.48
1:A:643:TYR:CD1	1:A:848:THR:HG23	2.49	0.47
1:A:332:GLN:CG	1:B:320:LYS:HZ1	2.19	0.47
1:B:212:VAL:O	1:B:212:VAL:HG13	2.14	0.47
1:A:488:LEU:HD11	1:A:499:LEU:HD13	1.96	0.47
1:A:490:ALA:HB1	1:A:495:ASP:OD2	2.14	0.47
1:B:584:TYR:HB2	1:B:881:PHE:CE1	2.49	0.47
1:B:561:HIS:ND1	1:B:832:GLU:OE2	2.41	0.47
1:A:593:LYS:NZ	1:B:304:LEU:CD1	2.78	0.47
1:A:868:GLU:HA	1:A:927:MET:HB3	1.95	0.47
4:B:1103:BTB:C8	4:B:1103:BTB:C1	2.84	0.46
1:B:883:ASP:OD2	4:B:1103:BTB:H72	2.14	0.46
1:A:883:ASP:OD2	4:A:1103:BTB:O8	2.31	0.46
1:A:262:THR:C	1:A:264:LYS:H	2.19	0.46
1:A:293:ILE:CG1	1:A:316:LYS:HZ3	2.28	0.46
1:B:706:GLY:CA	6:B:1104:EDO:H12	2.43	0.46
4:B:1103:BTB:O1	4:B:1103:BTB:O4	2.07	0.45
1:A:326:ASN:HD21	1:A:328:ASP:CG	2.19	0.45
1:B:445:PHE:CG	1:B:928:ALA:HB2	2.52	0.45
1:B:302:ASN:OD1	1:B:305:GLN:HG3	2.16	0.45
1:B:733:HIS:CD2	6:B:1104:EDO:H21	2.51	0.45
1:B:849:ASN:ND2	8:B:1203:HOH:O	2.36	0.44
4:B:1103:BTB:H82	4:B:1103:BTB:H11	1.96	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:883:ASP:OD2	1:A:890:TYR:CB	2.56	0.44
1:A:659:LYS:NZ	1:A:861:GLU:OE2	2.28	0.44
1:A:466:ASP:HB3	1:A:996:LEU:CD2	2.48	0.44
1:A:245:TRP:CZ2	1:A:268:PRO:HG3	2.53	0.44
1:A:593:LYS:HZ3	1:B:304:LEU:CD1	2.31	0.44
1:A:252:LEU:HD13	1:A:258:TRP:CE2	2.53	0.44
1:B:856:VAL:HG13	1:B:922:LYS:HD2	2.00	0.44
1:B:247:ARG:NH1	1:B:263:GLU:H	2.15	0.43
1:B:890:TYR:CE1	4:B:1103:BTB:H12	2.53	0.43
1:B:883:ASP:OD1	4:B:1103:BTB:H61	2.18	0.43
1:B:979:ALA:O	1:B:1015:LYS:HD2	2.19	0.43
1:B:559:ARG:HD3	1:B:635:ASP:OD1	2.18	0.43
1:B:740:PRO:HD2	1:B:758:ALA:HB1	2.01	0.43
1:B:768:ARG:NH2	1:B:770:GLU:OE1	2.52	0.43
4:B:1103:BTB:H41	4:B:1103:BTB:H52	1.87	0.43
1:B:686:ARG:O	6:B:1104:EDO:H12	2.18	0.42
1:A:224:GLN:HG3	1:A:249:LYS:HE3	2.00	0.42
1:A:357:GLN:O	1:A:358:ASN:HB2	2.19	0.42
1:B:236:VAL:HG12	1:B:943:VAL:HG23	2.01	0.42
1:B:293:ILE:HG12	1:B:316:LYS:HZ2	1.83	0.42
1:A:561:HIS:ND1	1:A:832:GLU:OE2	2.39	0.42
1:B:658:LEU:HD13	1:B:862:TRP:HB3	2.01	0.42
1:A:608:LYS:HD2	1:A:609:TYR:CZ	2.54	0.42
1:A:328:ASP:HB3	1:B:324:LEU:HD13	2.01	0.42
1:A:883:ASP:OD1	4:A:1103:BTB:H81	2.20	0.42
1:B:419:VAL:O	1:B:423:GLN:HG2	2.20	0.41
1:B:320:LYS:HD3	1:B:329:TRP:CZ3	2.55	0.41
1:B:466:ASP:OD1	1:B:999:ARG:NH1	2.53	0.41
1:A:559:ARG:NH2	1:A:565:VAL:HG22	2.36	0.41
1:B:338:VAL:HG13	1:B:344:TRP:CE3	2.55	0.41
1:A:293:ILE:CG1	1:A:316:LYS:NZ	2.70	0.41
1:A:883:ASP:OD1	4:A:1103:BTB:C8	2.69	0.41
1:B:938:PHE:HB2	1:B:969:ASP:O	2.21	0.41
1:B:304:LEU:O	1:B:308:ILE:HG22	2.21	0.41
1:A:465:GLY:HA3	8:A:1207:HOH:O	2.21	0.40
1:B:453:VAL:HG21	1:B:488:LEU:HB3	2.02	0.40
1:A:286:TYR:CD1	1:A:337:PHE:HB2	2.56	0.40
1:A:856:VAL:HG23	1:A:919:LEU:HD23	2.02	0.40
1:B:225:VAL:O	1:B:249:LYS:HE3	2.21	0.40
1:B:871:PRO:HA	6:B:1105:EDO:C1	2.51	0.40
1:A:939:PRO:HD2	1:A:972:SER:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:451:ASP:OD2	1:B:931:VAL:HG13	2.20	0.40
1:A:398:ASP:HB3	1:A:494:ASN:ND2	2.37	0.40
1:A:449:ARG:NH1	1:A:451:ASP:OD1	2.53	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	836/869 (96%)	811 (97%)	23 (3%)	2 (0%)	47	68
1	B	823/869 (95%)	797 (97%)	25 (3%)	1 (0%)	51	73
All	All	1659/1738 (96%)	1608 (97%)	48 (3%)	3 (0%)	47	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	TYR
1	B	219	TYR
1	A	263	GLU

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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	708/738 (96%)	703 (99%)	5 (1%)	84 94
1	B	694/738 (94%)	691 (100%)	3 (0%)	91 97
All	All	1402/1476 (95%)	1394 (99%)	8 (1%)	86 95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	538	SER
1	A	593	LYS
1	A	595	PHE
1	A	847	TYR
1	A	929	ASP
1	B	390	LYS
1	B	929	ASP
1	B	975	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	280	GLN
1	A	303	GLN
1	A	307	ASN
1	A	537	ASN
1	B	277	GLN
1	B	1042	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
3	WIJ	A	1102	-	21,26,26	0.68	1 (4%)	24,37,37	0.93	1 (4%)
5	SO4	B	1110	-	4,4,4	0.14	0	6,6,6	0.07	0
6	EDO	B	1104	-	3,3,3	0.05	0	2,2,2	0.19	0
7	DMS	B	1106	-	3,3,3	0.26	0	3,3,3	0.07	0
3	WIJ	B	1102	-	21,26,26	0.72	1 (4%)	24,37,37	0.87	1 (4%)
4	BTB	A	1103	-	13,13,13	0.49	0	7,16,16	0.57	0
5	SO4	A	1104	-	4,4,4	0.91	0	6,6,6	0.21	0
5	SO4	B	1107	-	4,4,4	0.13	0	6,6,6	0.08	0
5	SO4	A	1105	-	4,4,4	0.16	0	6,6,6	0.20	0
6	EDO	B	1105	-	3,3,3	0.44	0	2,2,2	0.38	0
5	SO4	B	1108	-	4,4,4	0.12	0	6,6,6	0.13	0
5	SO4	B	1109	-	4,4,4	0.12	0	6,6,6	0.12	0
4	BTB	B	1103	-	13,13,13	0.59	0	7,16,16	1.60	2 (28%)

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	WIJ	A	1102	-	-	10/12/16/16	0/3/3/3
6	EDO	B	1104	-	-	1/1/1/1	-
3	WIJ	B	1102	-	-	8/12/16/16	0/3/3/3
4	BTB	A	1103	-	-	10/21/21/21	-
6	EDO	B	1105	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	B	1103	-	-	9/21/21/21	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1102	WIJ	C8-S	2.49	1.75	1.72
3	A	1102	WIJ	C8-S	2.31	1.75	1.72

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1103	BTB	O1-C1-C2	-3.45	101.99	111.44
3	A	1102	WIJ	C6-C1-C	3.00	123.66	121.72
3	B	1102	WIJ	C6-C1-C	2.48	123.32	121.72
4	B	1103	BTB	O4-C4-C2	-2.12	105.64	111.44

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	WIJ	C8-C7-N1-C6
3	A	1102	WIJ	N1-C7-C8-C9
3	A	1102	WIJ	O1-C7-C8-C9
3	B	1102	WIJ	C8-C7-N1-C6
3	B	1102	WIJ	N1-C7-C8-C9
3	B	1102	WIJ	O1-C7-C8-C9
4	A	1103	BTB	C1-C2-C4-O4
4	A	1103	BTB	C1-C2-N-C7
4	A	1103	BTB	C3-C2-N-C7
4	A	1103	BTB	C4-C2-N-C7
4	A	1103	BTB	C8-C7-N-C5
4	B	1103	BTB	C1-C2-C3-O3
4	B	1103	BTB	C4-C2-C3-O3
4	B	1103	BTB	N-C2-C3-O3
4	B	1103	BTB	C1-C2-N-C5
4	B	1103	BTB	C3-C2-N-C5
4	B	1103	BTB	C4-C2-N-C5
4	B	1103	BTB	C8-C7-N-C2
4	B	1103	BTB	N-C7-C8-O8
3	B	1102	WIJ	O1-C7-N1-C6
3	A	1102	WIJ	O1-C7-N1-C6

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Mol	Chain	Res	Type	Atoms
4	B	1103	BTB	N-C5-C6-O6
3	A	1102	WIJ	N-C-C1-C6
3	A	1102	WIJ	O-C-C1-C6
3	B	1102	WIJ	N-C-C1-C6
3	B	1102	WIJ	O-C-C1-C6
3	B	1102	WIJ	C5-C6-N1-C7
4	A	1103	BTB	C6-C5-N-C2
4	A	1103	BTB	O1-C1-C2-N
4	A	1103	BTB	N-C2-C4-O4
4	A	1103	BTB	C3-C2-N-C5
3	A	1102	WIJ	C5-C6-N1-C7
6	B	1104	EDO	O1-C1-C2-O2
3	A	1102	WIJ	C1-C6-N1-C7
3	A	1102	WIJ	N-C-C1-C2
3	B	1102	WIJ	C1-C6-N1-C7
4	A	1103	BTB	O1-C1-C2-C3
3	A	1102	WIJ	O-C-C1-C2

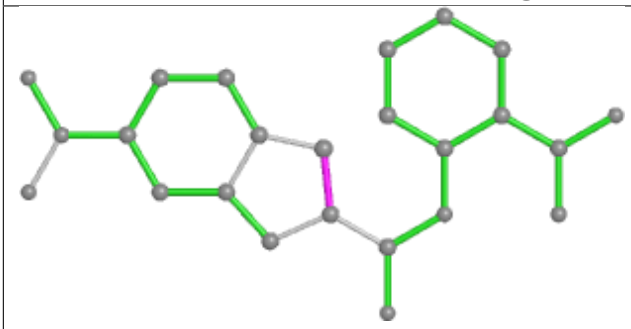
There are no ring outliers.

6 monomers are involved in 49 short contacts:

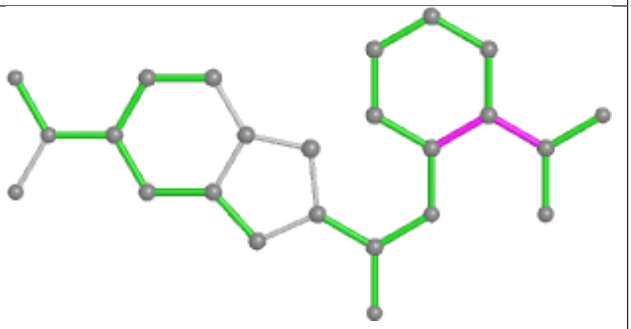
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	WIJ	2	0
6	B	1104	EDO	7	0
4	A	1103	BTB	22	0
6	B	1105	EDO	5	0
5	B	1109	SO4	1	0
4	B	1103	BTB	14	0

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.

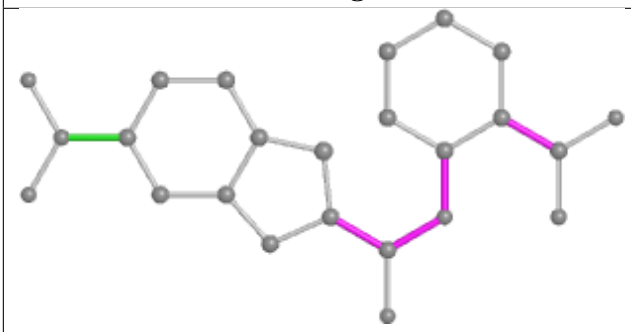
Ligand WIJ A 1102



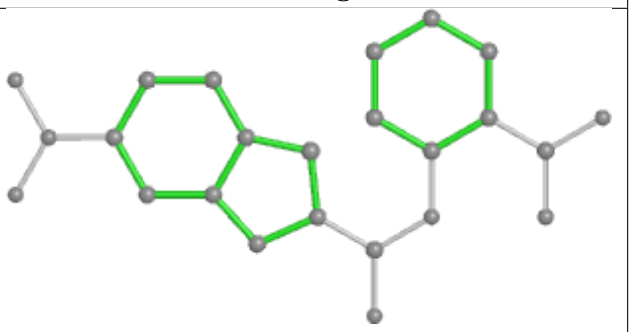
Bond lengths



Bond angles

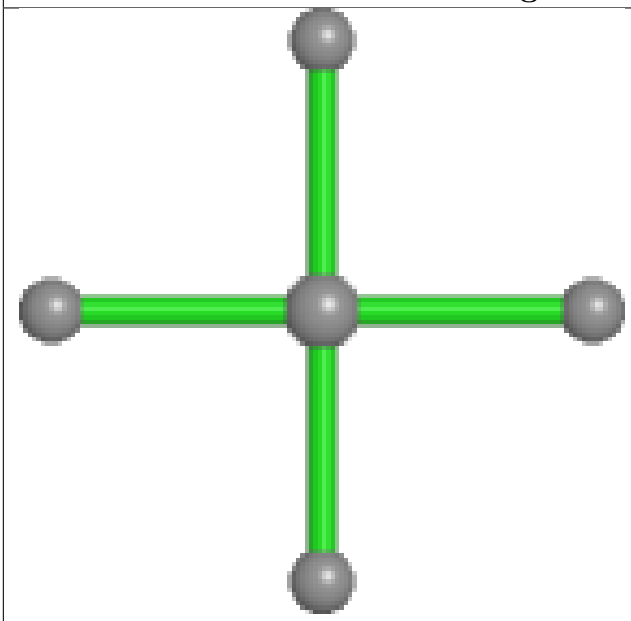


Torsions

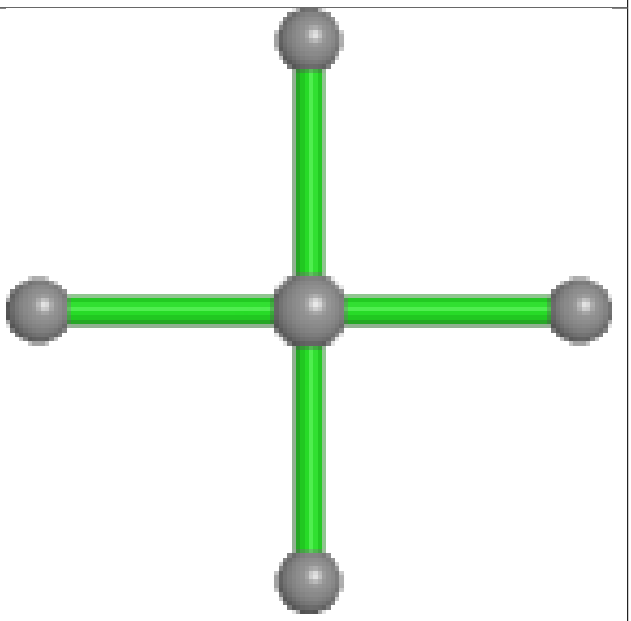


Rings

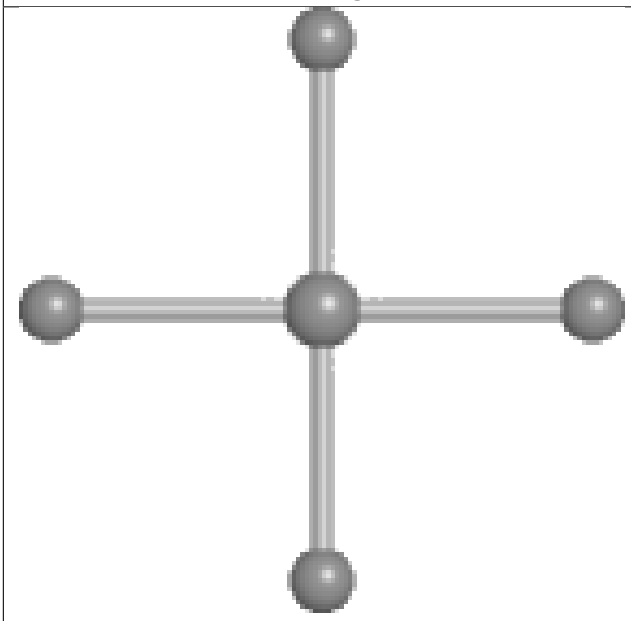
Ligand SO4 B 1110



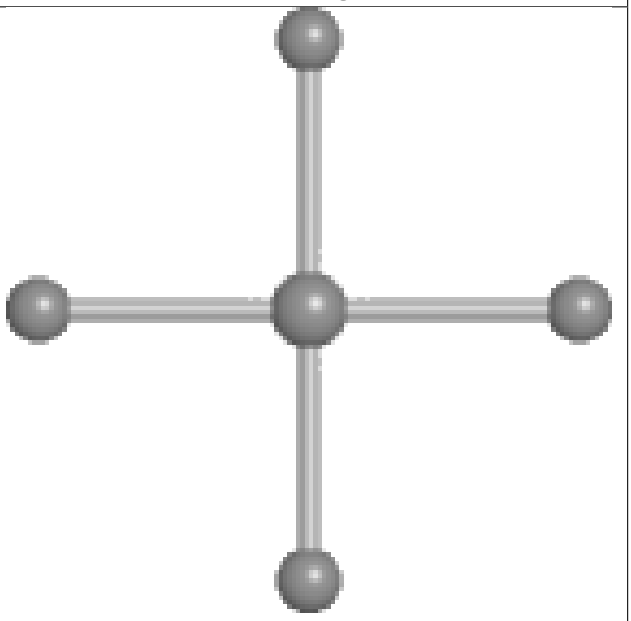
Bond lengths



Bond angles

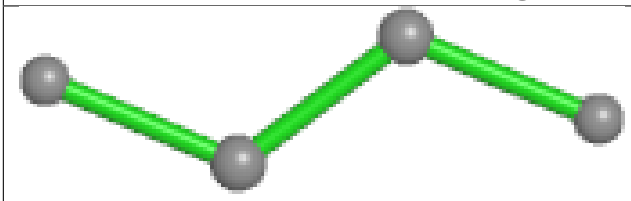


Torsions

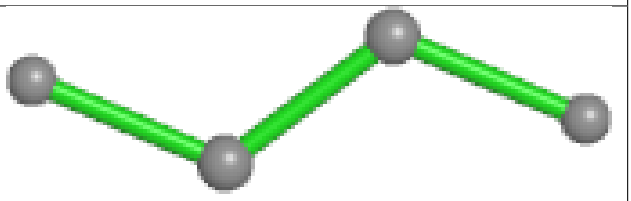


Rings

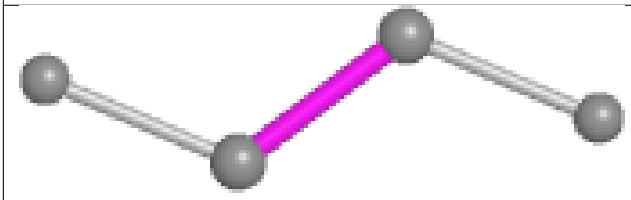
Ligand EDO B 1104



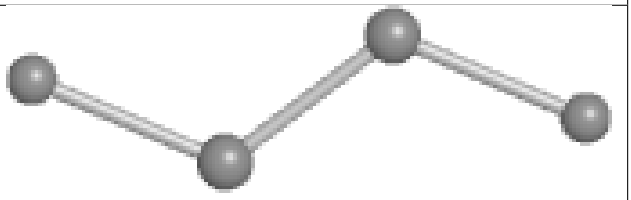
Bond lengths



Bond angles

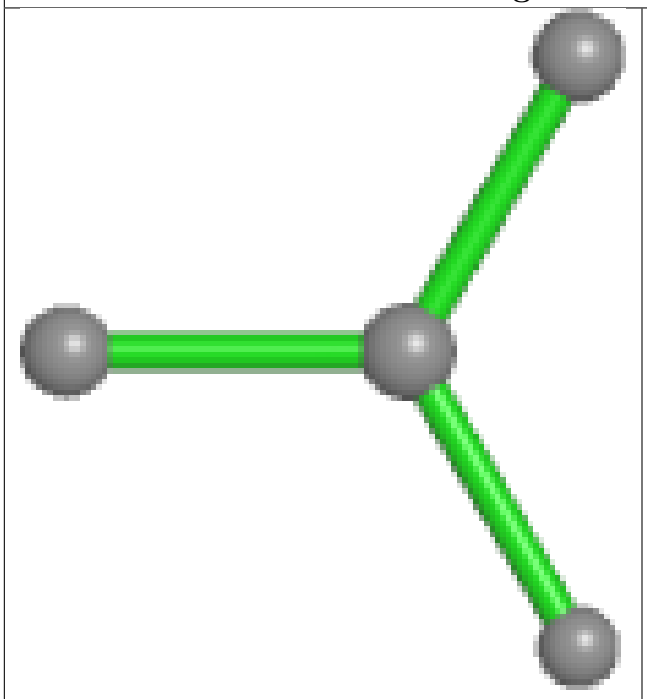


Torsions

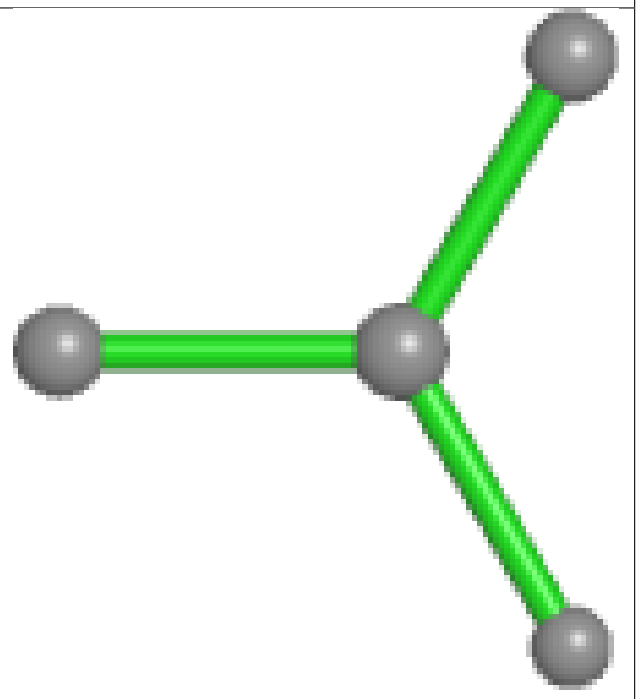


Rings

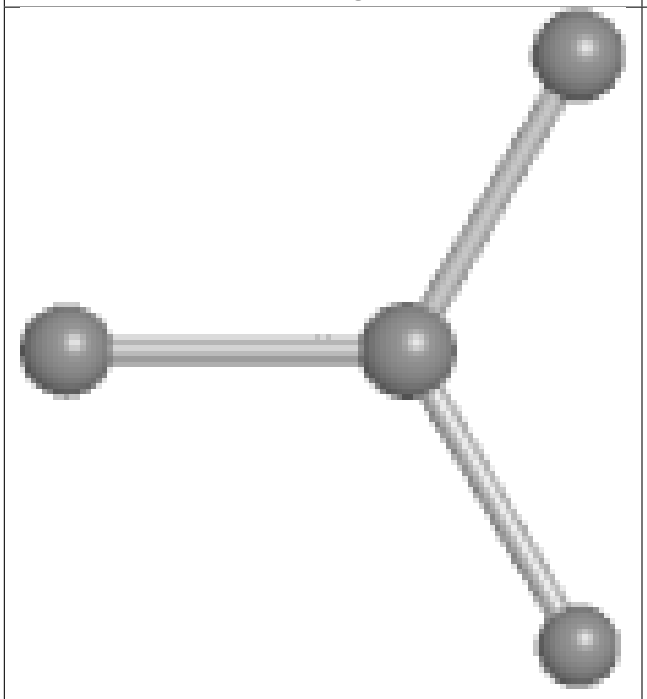
Ligand DMS B 1106



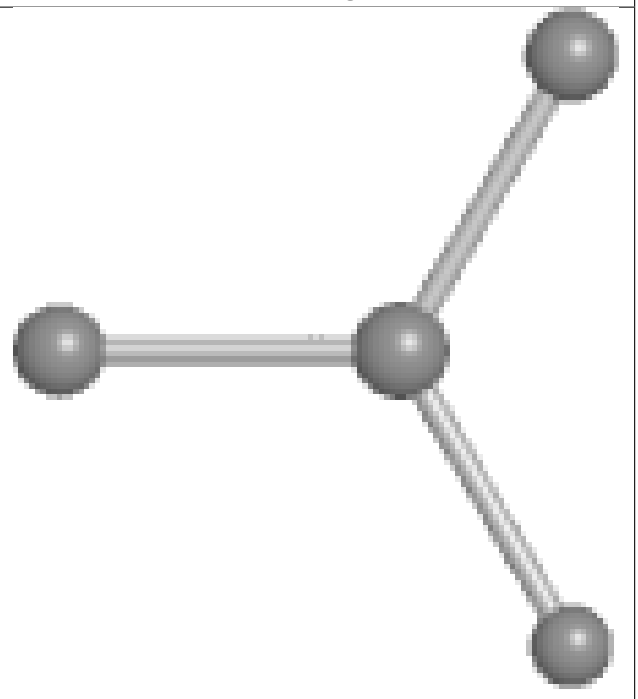
Bond lengths



Bond angles

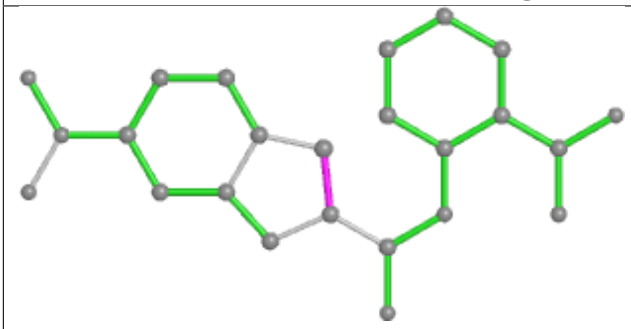


Torsions

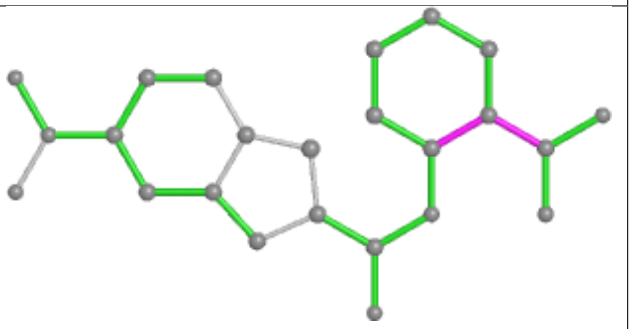


Rings

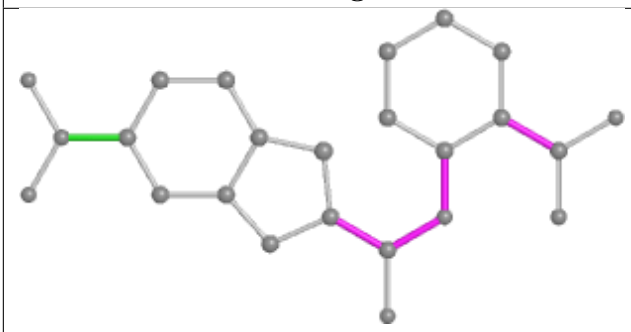
Ligand WIJ B 1102



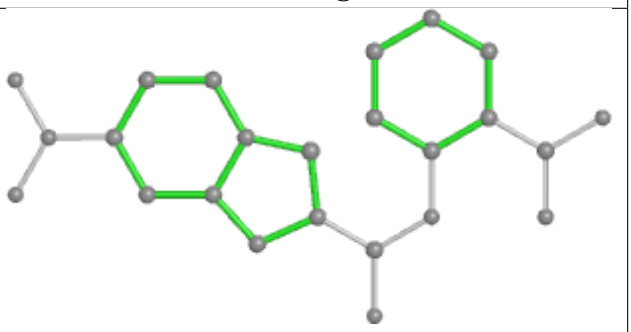
Bond lengths



Bond angles

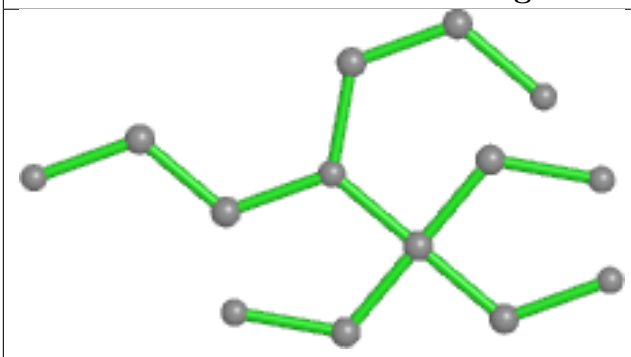


Torsions

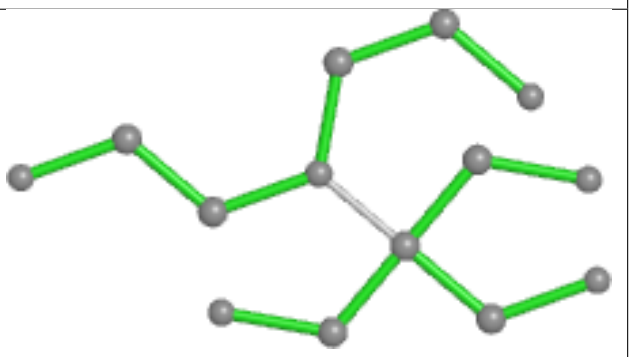


Rings

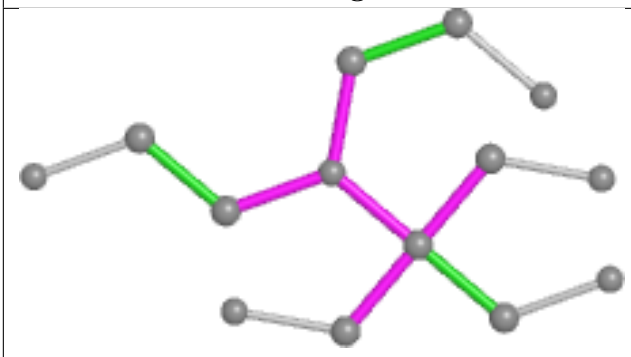
Ligand BTB A 1103



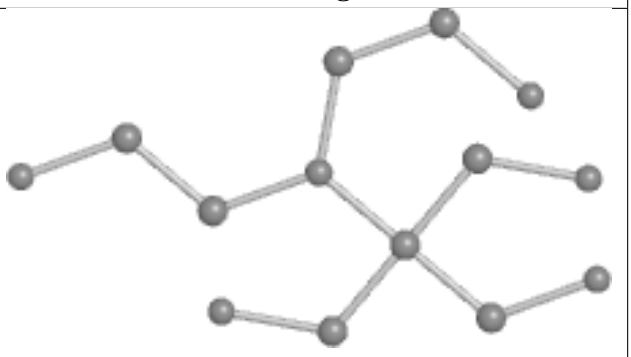
Bond lengths



Bond angles

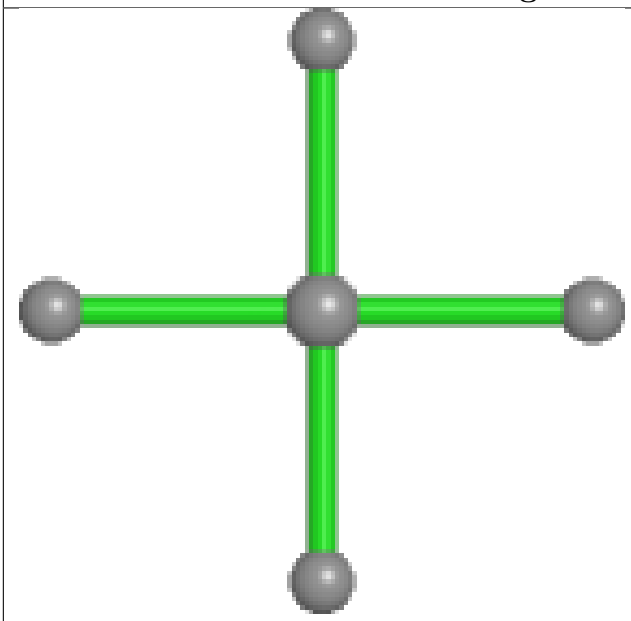


Torsions

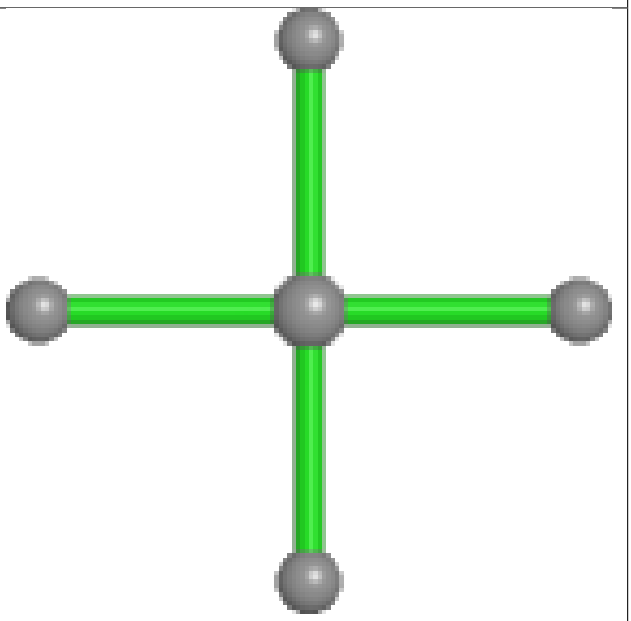


Rings

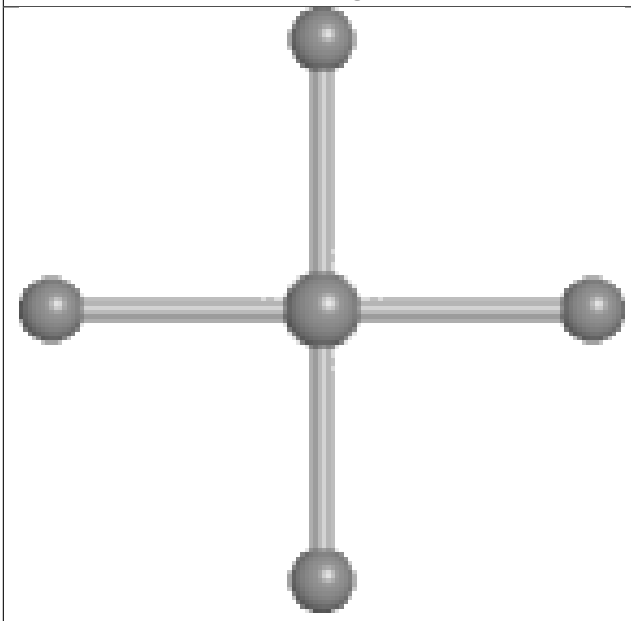
Ligand SO4 A 1104



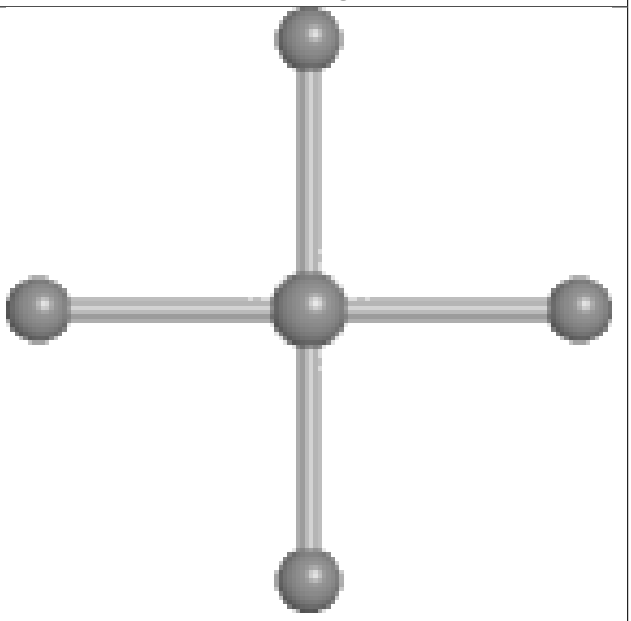
Bond lengths



Bond angles

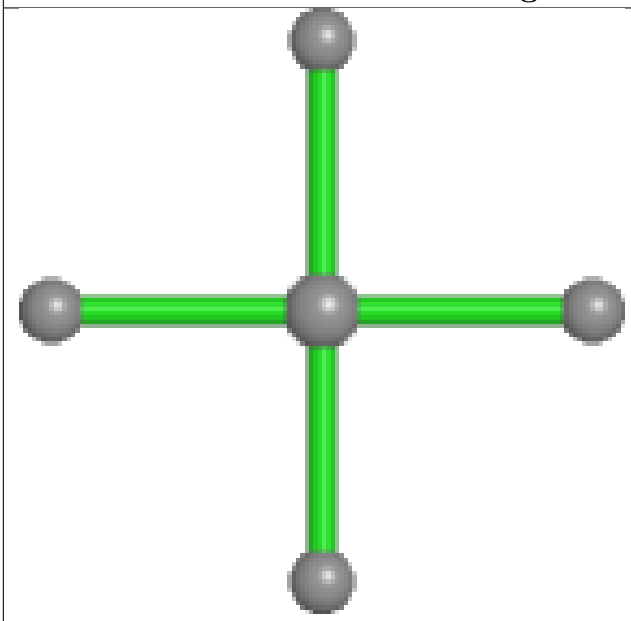


Torsions

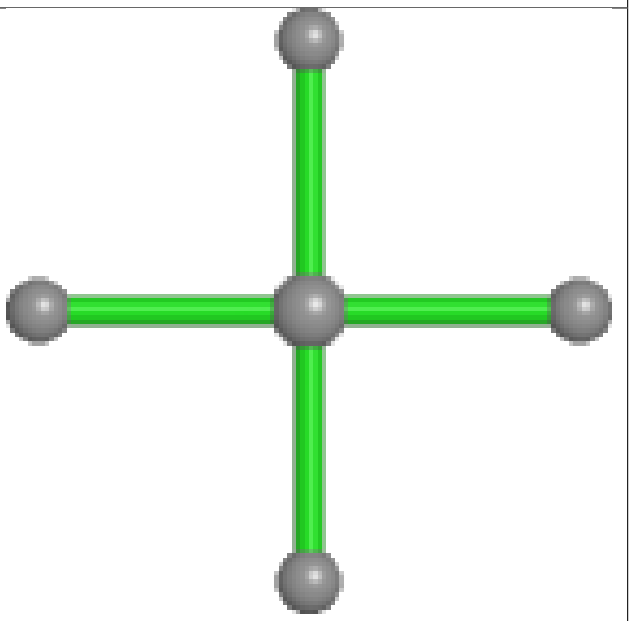


Rings

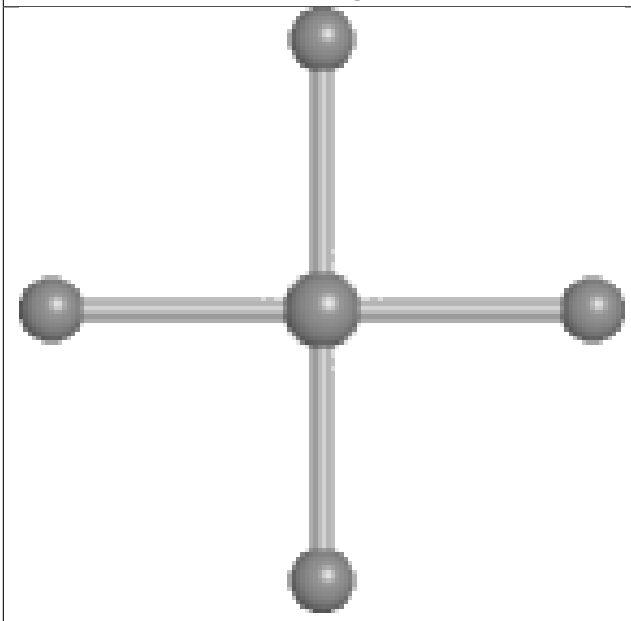
Ligand SO4 B 1107



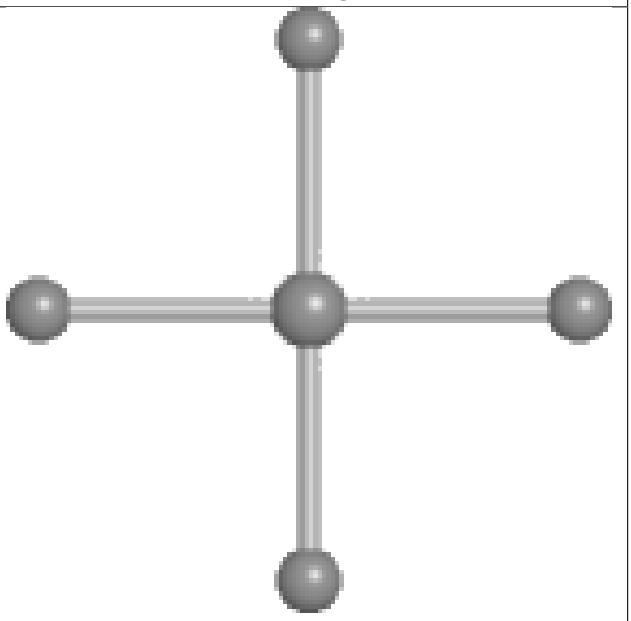
Bond lengths



Bond angles

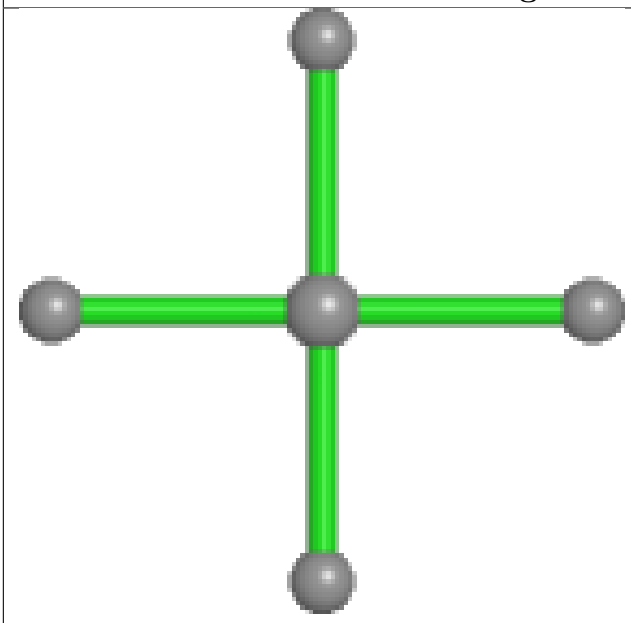


Torsions

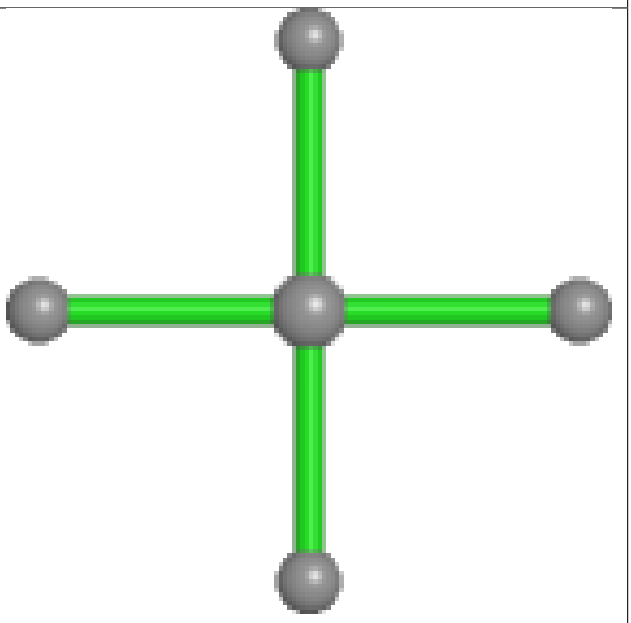


Rings

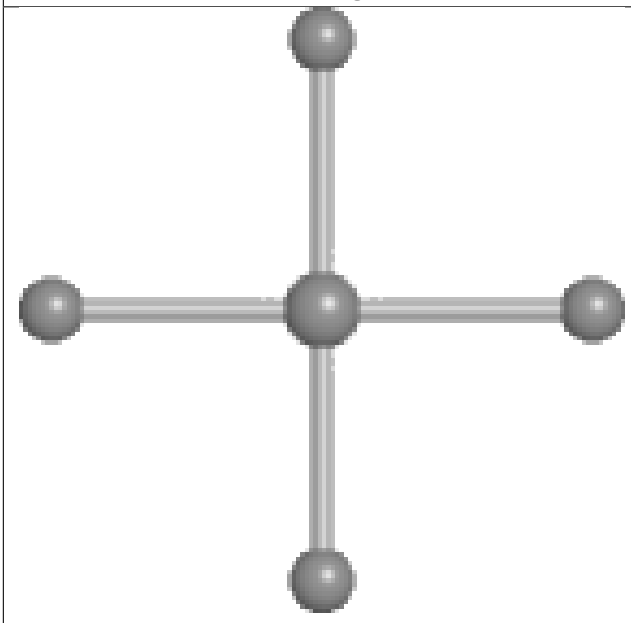
Ligand SO4 A 1105



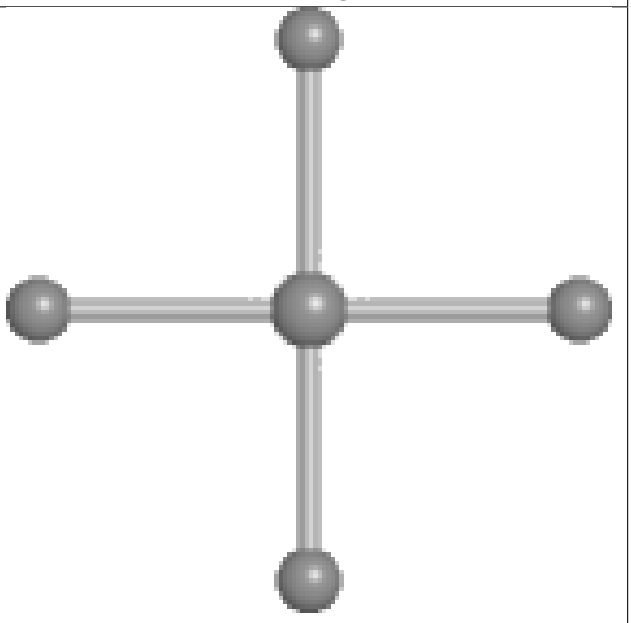
Bond lengths



Bond angles

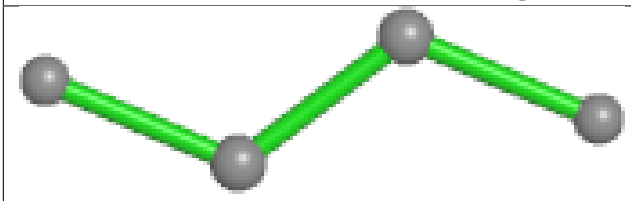


Torsions

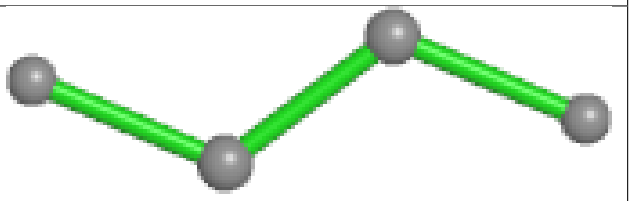


Rings

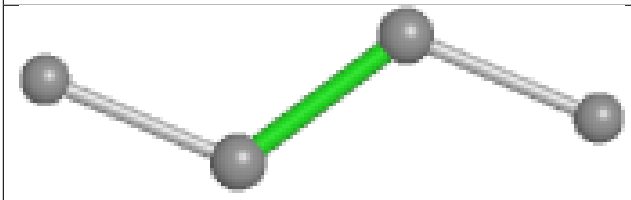
Ligand EDO B 1105



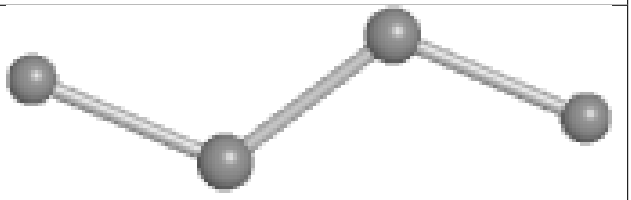
Bond lengths



Bond angles

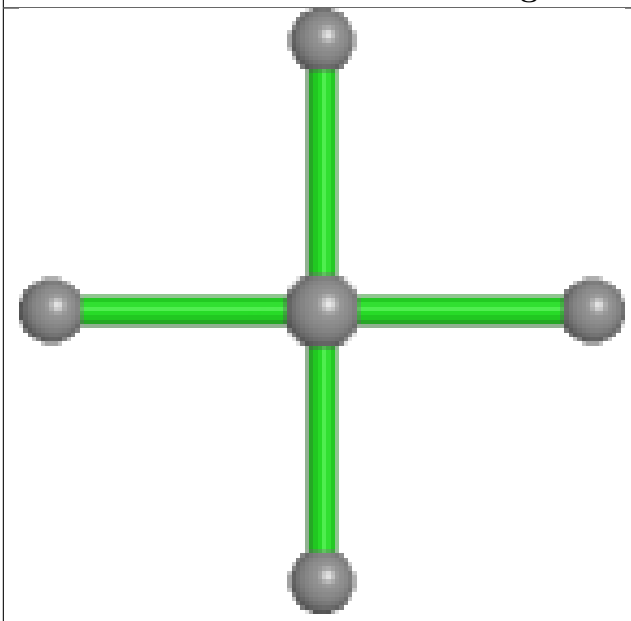


Torsions

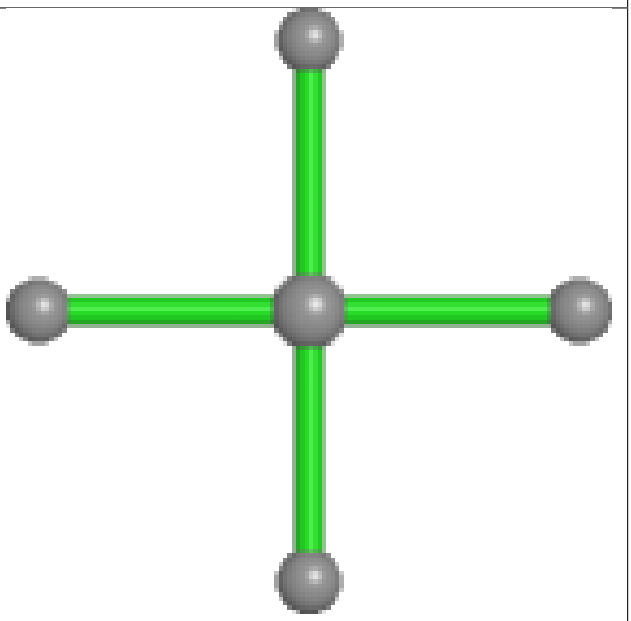


Rings

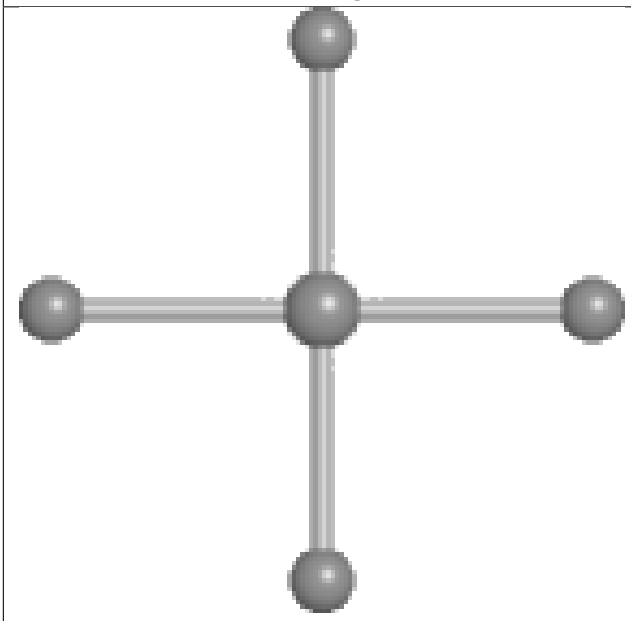
Ligand SO4 B 1108



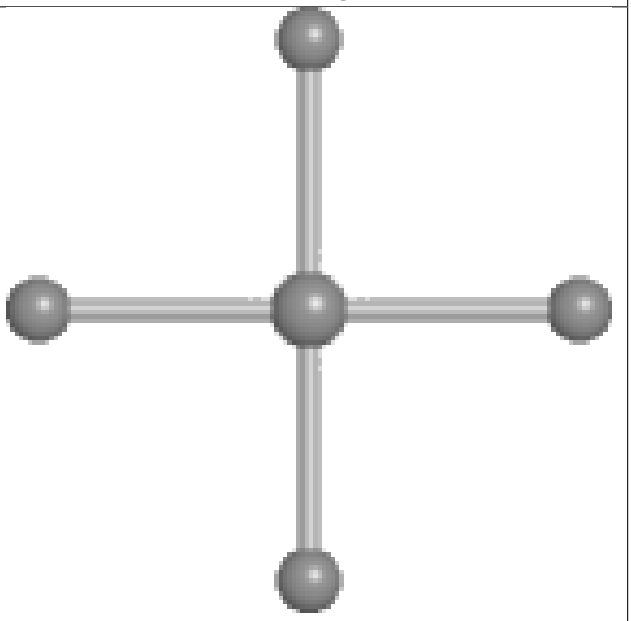
Bond lengths



Bond angles

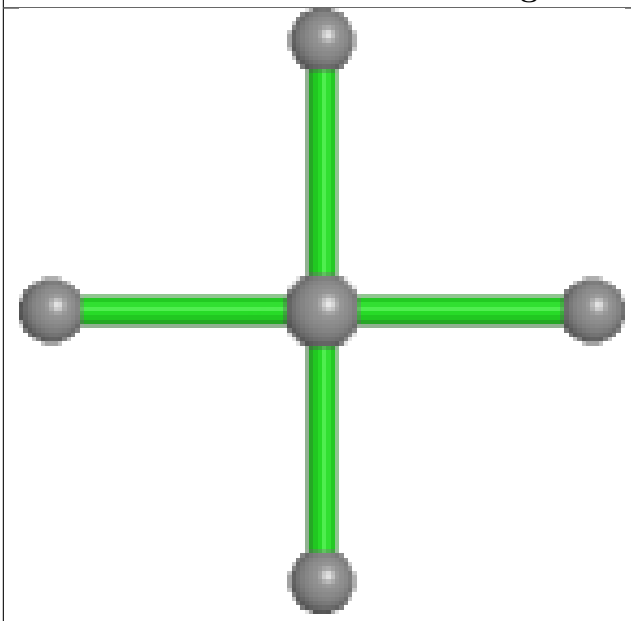


Torsions

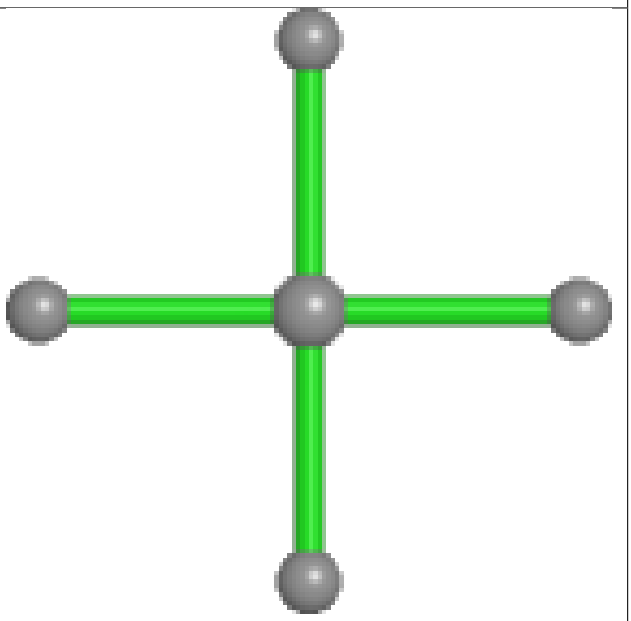


Rings

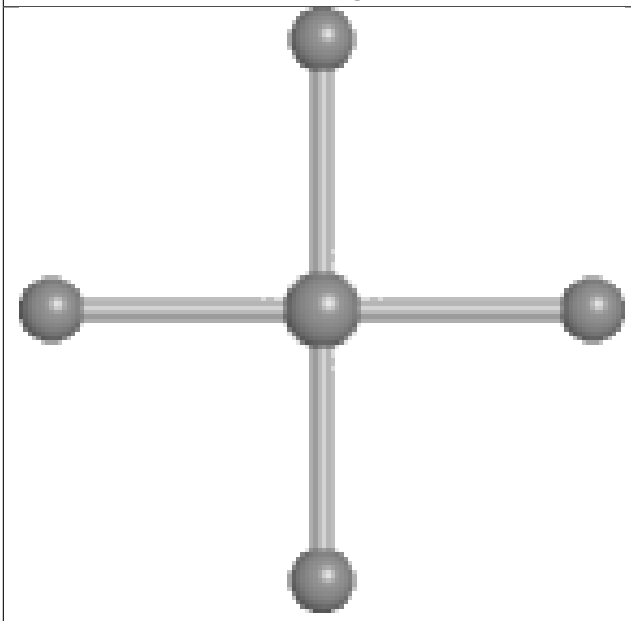
Ligand SO4 B 1109



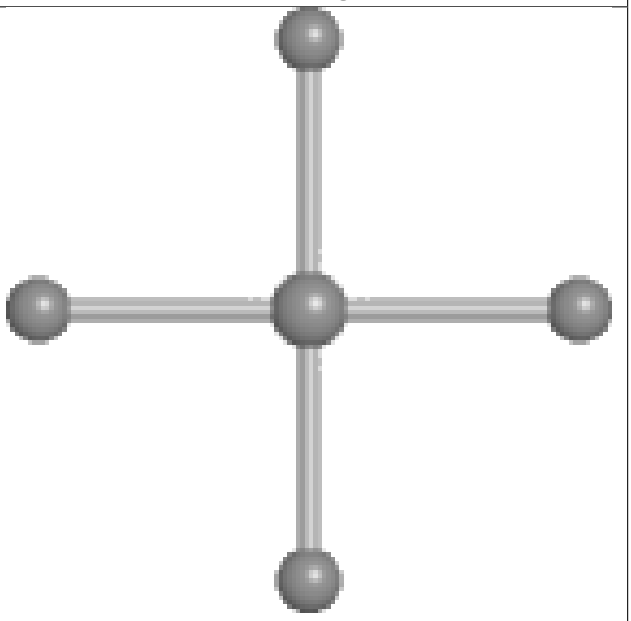
Bond lengths



Bond angles

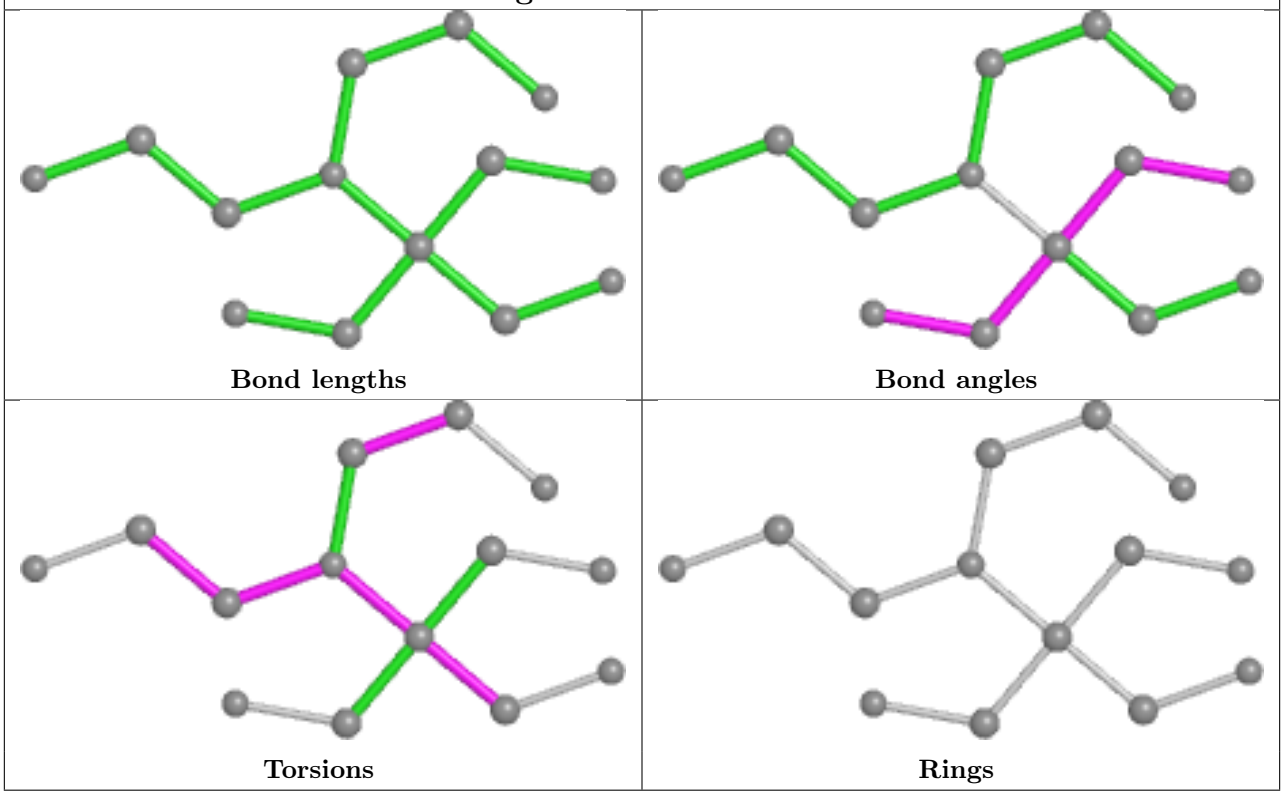


Torsions



Rings

Ligand BTB B 1103



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	839/869 (96%)	-0.00	28 (3%)	46	50	25, 39, 70, 108	0
1	B	831/869 (95%)	0.03	42 (5%)	28	29	23, 38, 83, 107	0
All	All	1670/1738 (96%)	0.02	70 (4%)	36	39	23, 39, 76, 108	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	214	THR	6.9
1	A	216	SER	5.6
1	B	218	LEU	5.3
1	B	1040	ALA	5.1
1	A	208	ASN	5.0
1	B	304	LEU	4.6
1	A	1041	THR	4.4
1	B	213	THR	4.4
1	B	259	THR	4.3
1	B	1045	PHE	4.2
1	B	1042	ASN	4.1
1	A	218	LEU	4.1
1	B	1041	THR	4.0
1	B	277	GLN	3.8
1	A	957	GLU	3.8
1	A	217	ASN	3.7
1	B	325	LYS	3.7
1	B	228	ARG	3.6
1	B	258	TRP	3.6
1	B	221	LYS	3.5
1	A	220	LYS	3.5
1	B	368	LYS	3.5
1	B	1043	THR	3.5
1	A	214	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	257	THR	3.3
1	B	219	TYR	3.3
1	A	228	ARG	3.3
1	B	250	TYR	3.2
1	B	252	LEU	3.1
1	A	222	TYR	3.1
1	B	233	PHE	3.1
1	A	225	VAL	3.1
1	B	366	GLU	3.1
1	B	263	GLU	3.1
1	A	213	THR	3.0
1	A	1040	ALA	3.0
1	B	1048	SER	3.0
1	B	1038	ASP	3.0
1	B	1039	GLN	2.9
1	A	265	ASP	2.9
1	B	215	ARG	2.9
1	A	233	PHE	2.9
1	B	226	TYR	2.9
1	B	264	LYS	2.9
1	A	226	TYR	2.8
1	A	970	SER	2.8
1	B	222	TYR	2.8
1	A	209	LYS	2.7
1	A	368	LYS	2.7
1	A	221	LYS	2.7
1	B	227	ASP	2.6
1	B	212	VAL	2.6
1	A	259	THR	2.5
1	B	265	ASP	2.5
1	B	246	TYR	2.5
1	B	232	SER	2.4
1	B	266	PHE	2.4
1	A	746	ASP	2.3
1	B	225	VAL	2.3
1	A	366	GLU	2.3
1	B	223	ASN	2.2
1	A	844	LYS	2.2
1	A	249	LYS	2.2
1	B	970	SER	2.2
1	A	593	LYS	2.1
1	A	1039	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	247	ARG	2.1
1	B	369	LEU	2.1
1	B	231	GLN	2.1
1	A	1045	PHE	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)

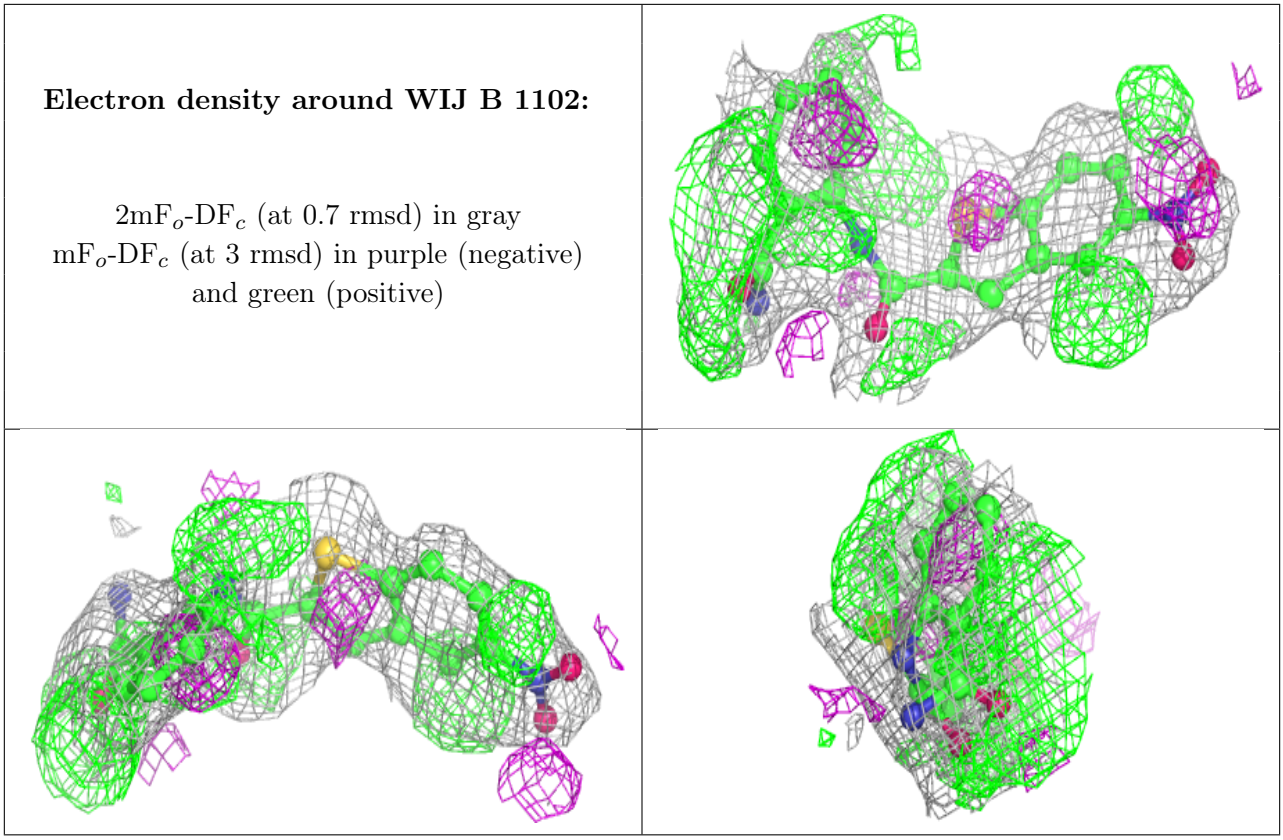
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
3	WIJ	B	1102	24/24	0.73	0.30	48,59,76,81	0
4	BTB	B	1103	14/14	0.73	0.36	44,58,75,79	0
7	DMS	B	1106	4/4	0.74	0.29	32,36,63,102	0
4	BTB	A	1103	14/14	0.76	0.33	42,53,73,81	0
3	WIJ	A	1102	24/24	0.85	0.24	38,56,68,79	0
5	SO4	B	1109	5/5	0.89	0.33	80,84,93,102	0
5	SO4	B	1110	5/5	0.90	0.44	79,83,94,117	0
5	SO4	A	1105	5/5	0.94	0.23	52,58,60,102	0
5	SO4	A	1104	5/5	0.94	0.24	56,73,75,87	0
5	SO4	B	1108	5/5	0.95	0.21	54,60,73,91	0
6	EDO	B	1104	4/4	0.95	0.42	32,38,41,42	0
5	SO4	B	1107	5/5	0.95	0.20	58,65,90,99	0
6	EDO	B	1105	4/4	0.96	0.33	38,43,49,51	0
2	CA	B	1101	1/1	0.98	0.14	36,36,36,36	0
2	CA	A	1101	1/1	0.99	0.11	34,34,34,34	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.

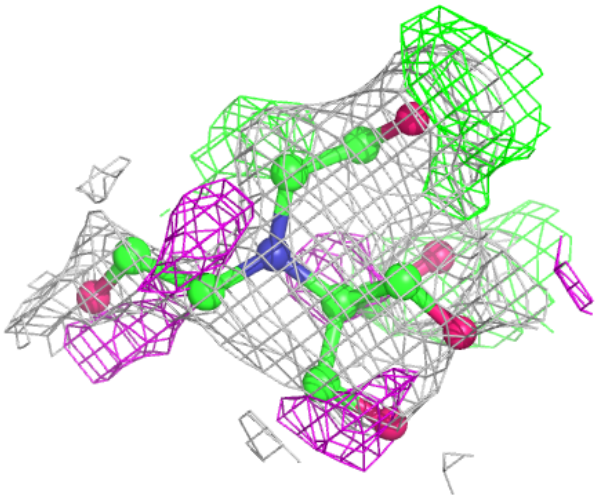
Electron density around WIJ B 1102:

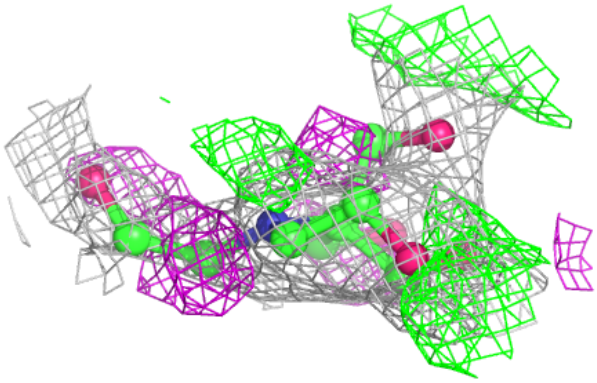
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

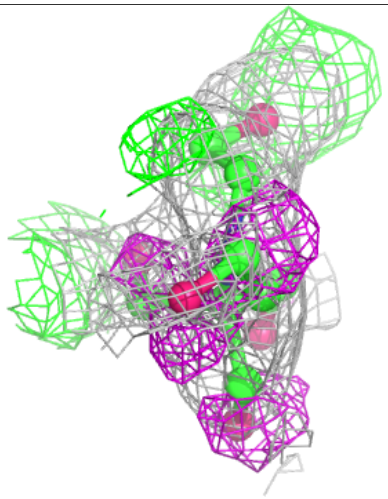


Electron density around BTB B 1103:

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

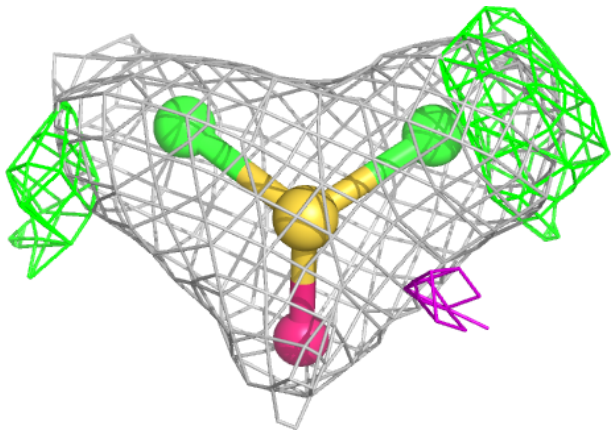


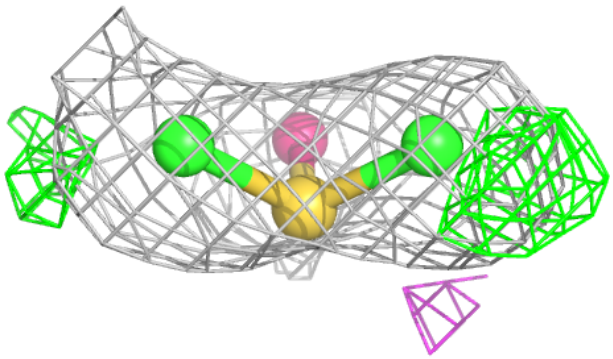


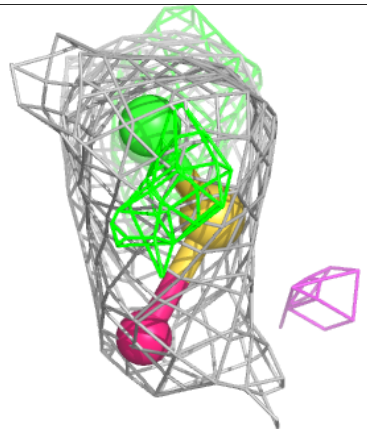


Electron density around DMS B 1106:

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

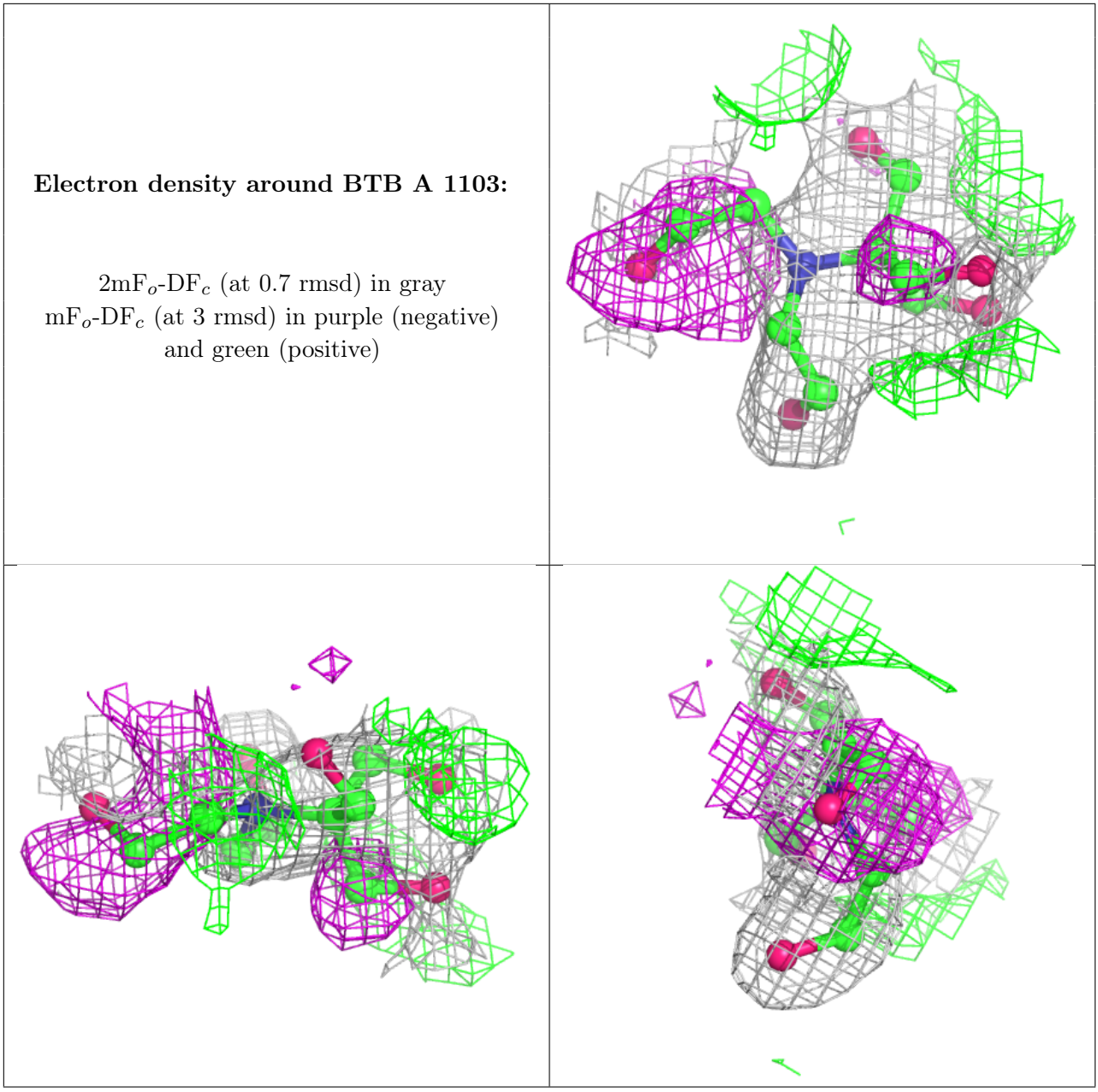






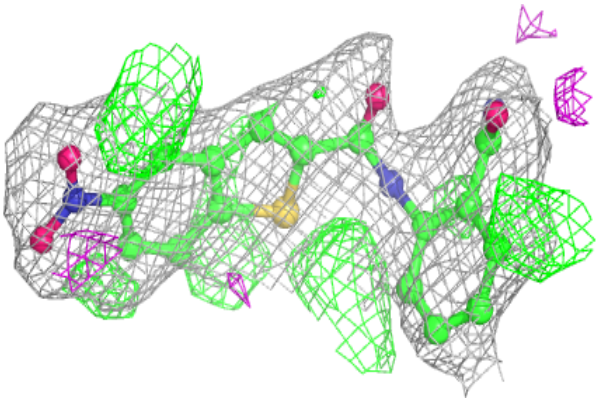
Electron density around BTB A 1103:

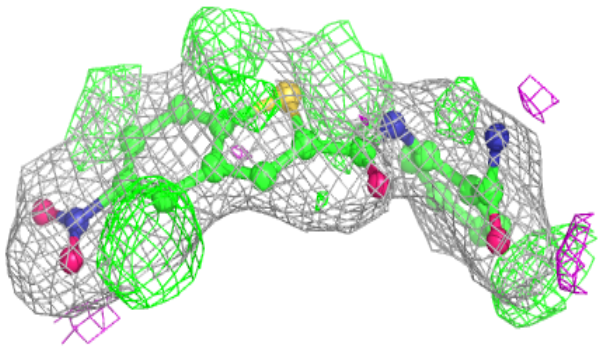
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

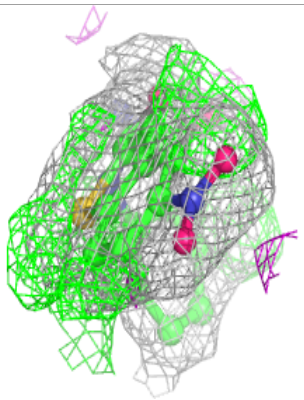


Electron density around WIJ A 1102:

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

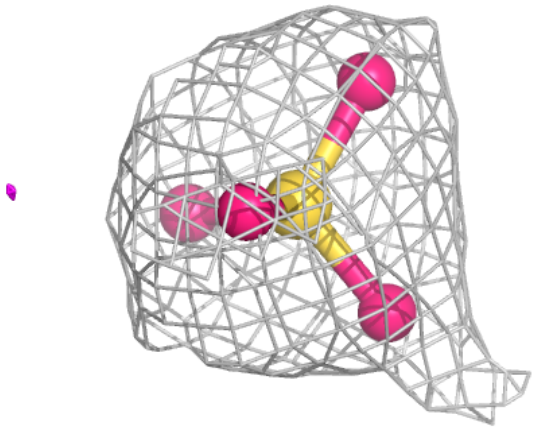


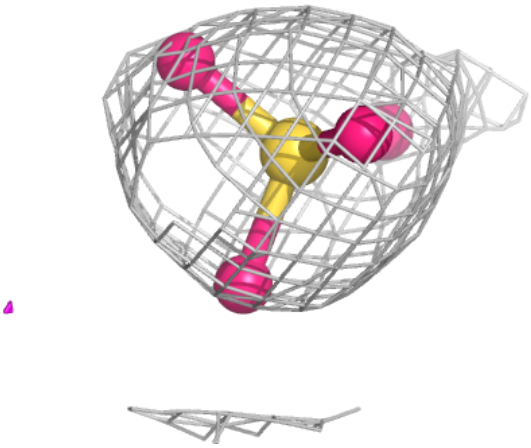


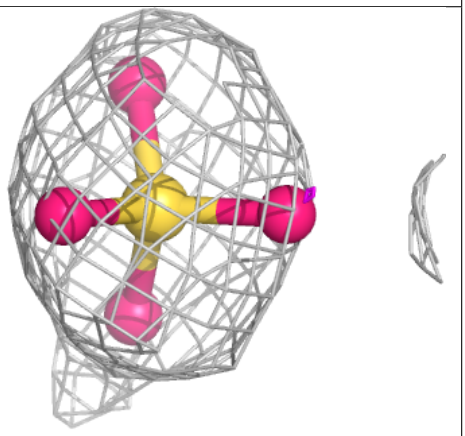


Electron density around SO4 B 1109:

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

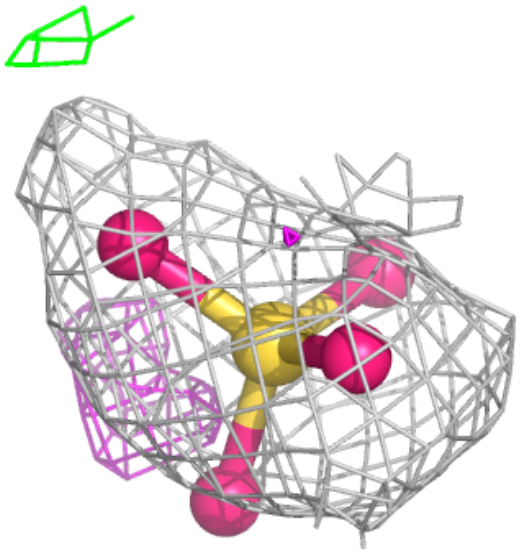


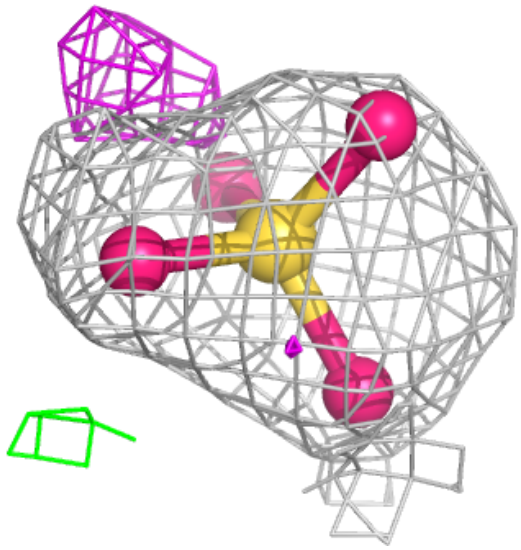


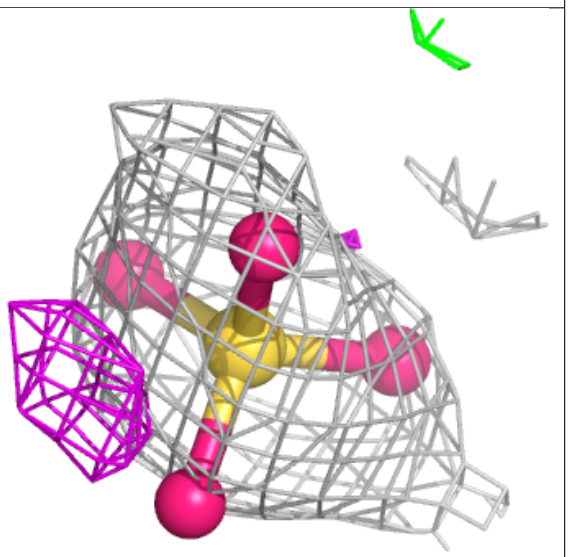


Electron density around SO4 B 1110:

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

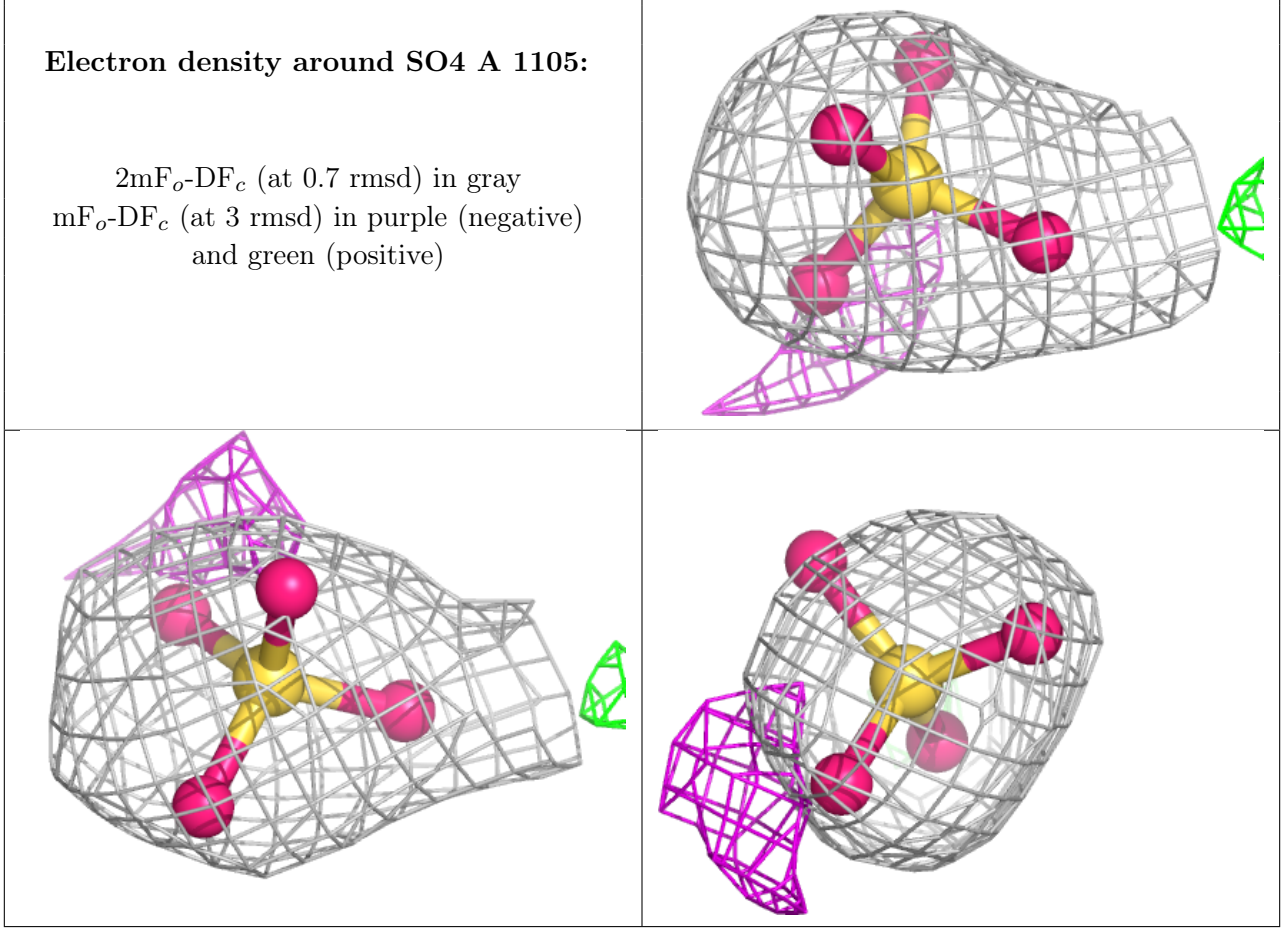






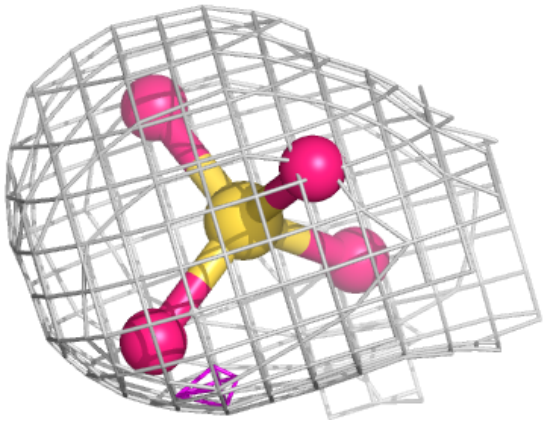
Electron density around SO4 A 1105:

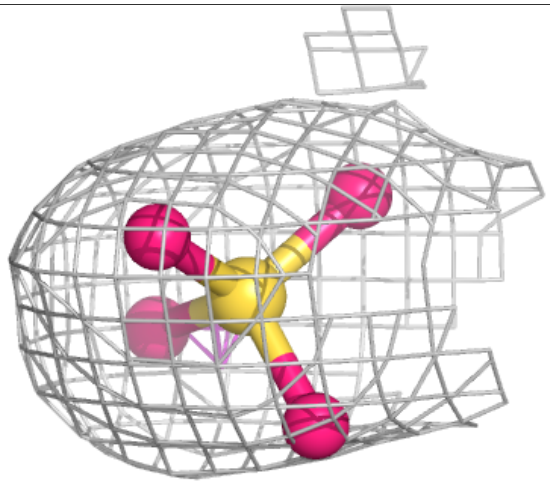
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

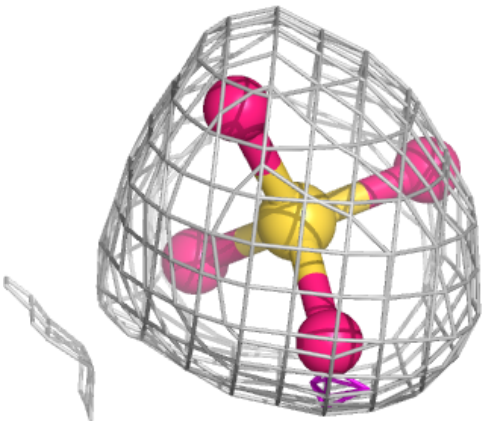


Electron density around SO4 A 1104:

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

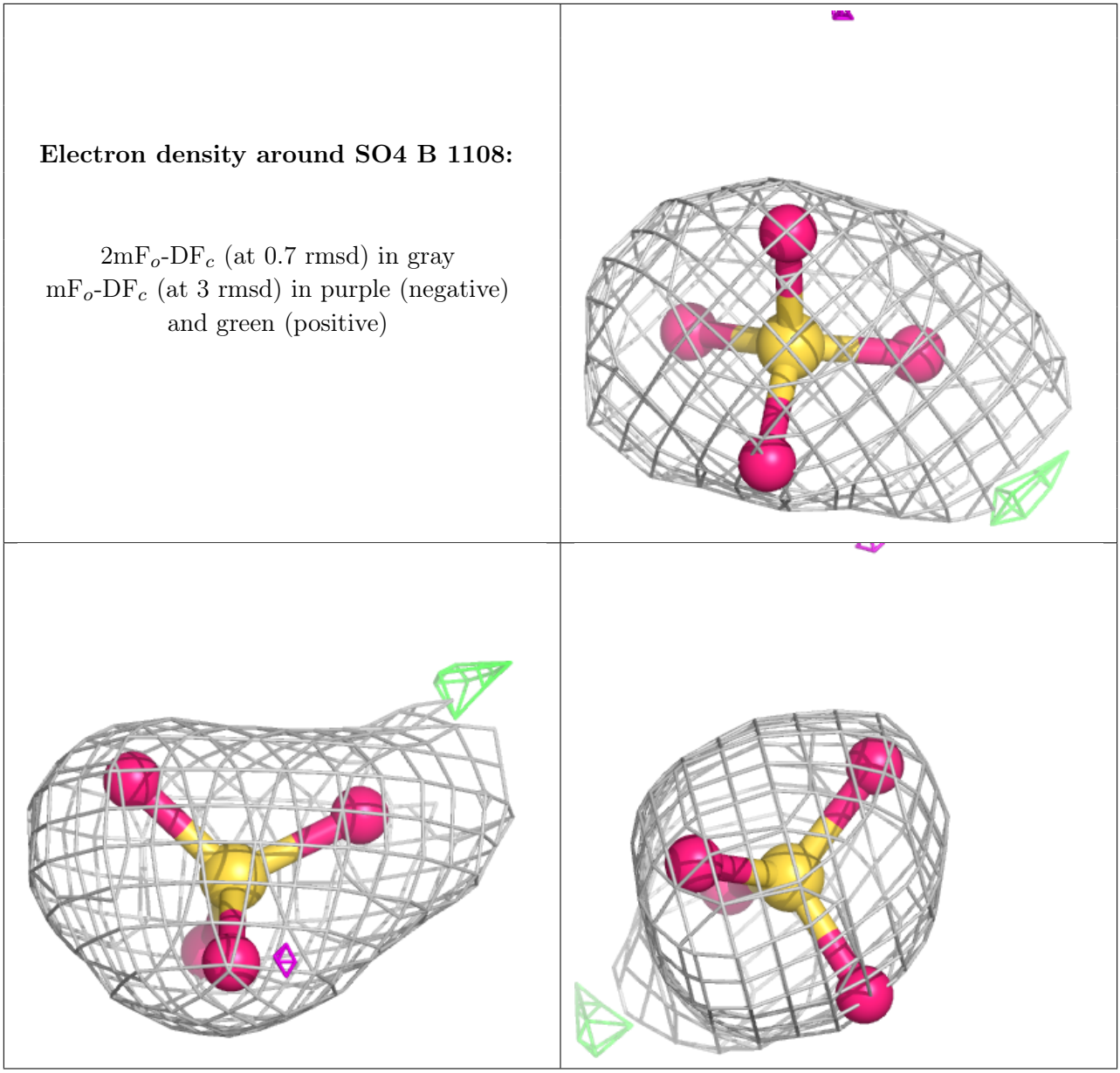






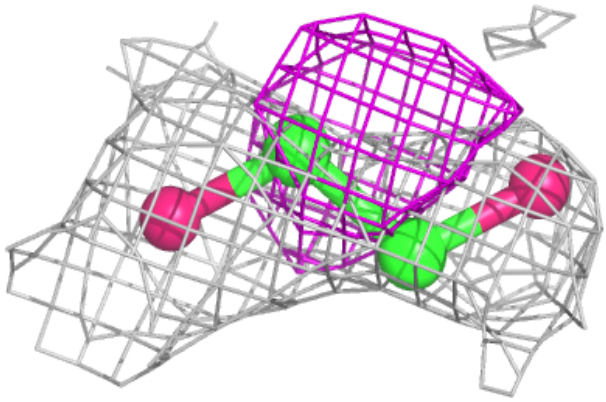
Electron density around SO4 B 1108:

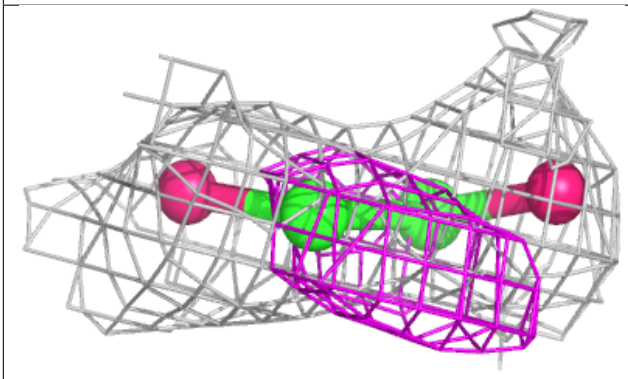
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

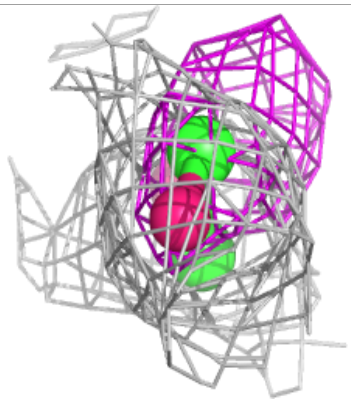


Electron density around EDO B 1104:

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

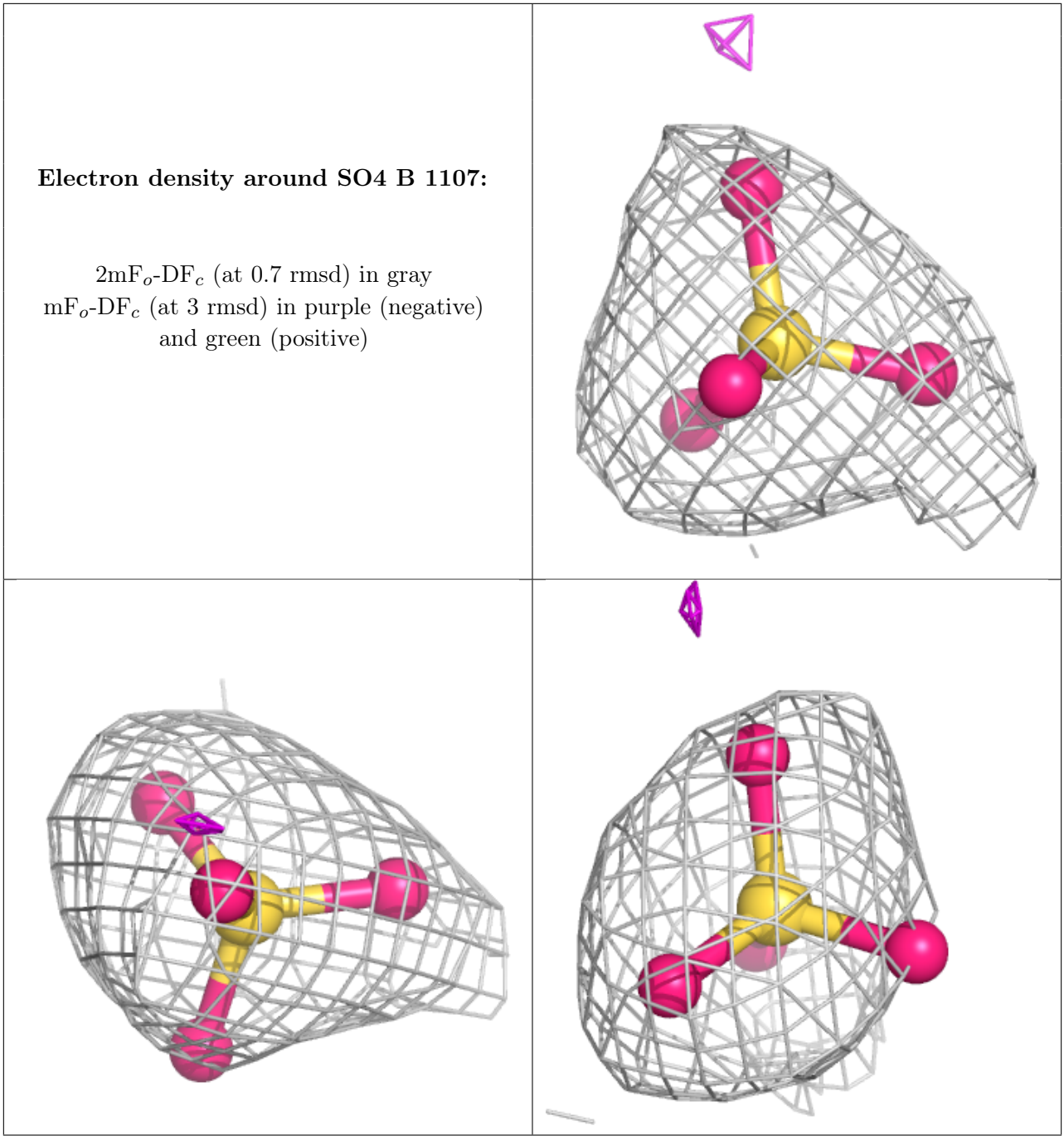






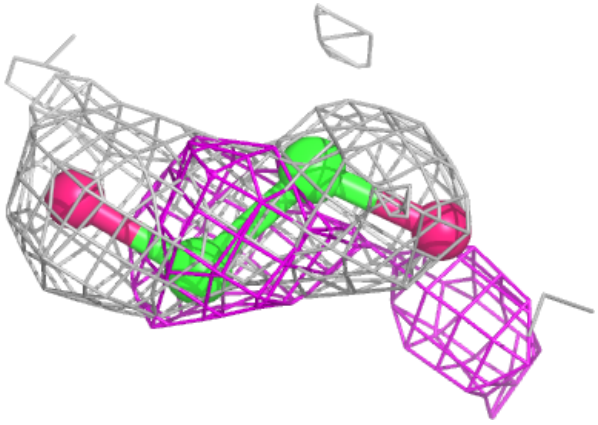
Electron density around SO4 B 1107:

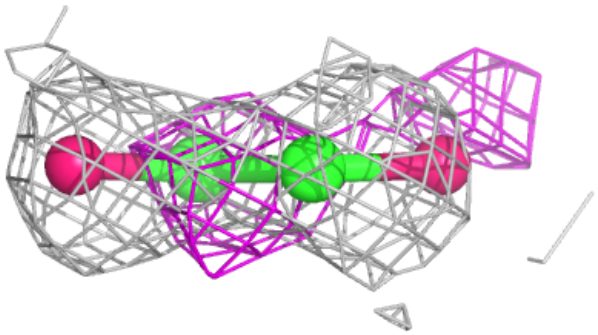
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

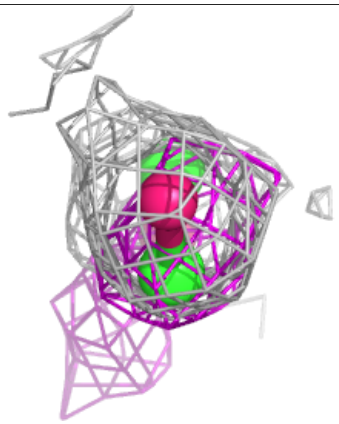


Electron density around EDO B 1105:

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

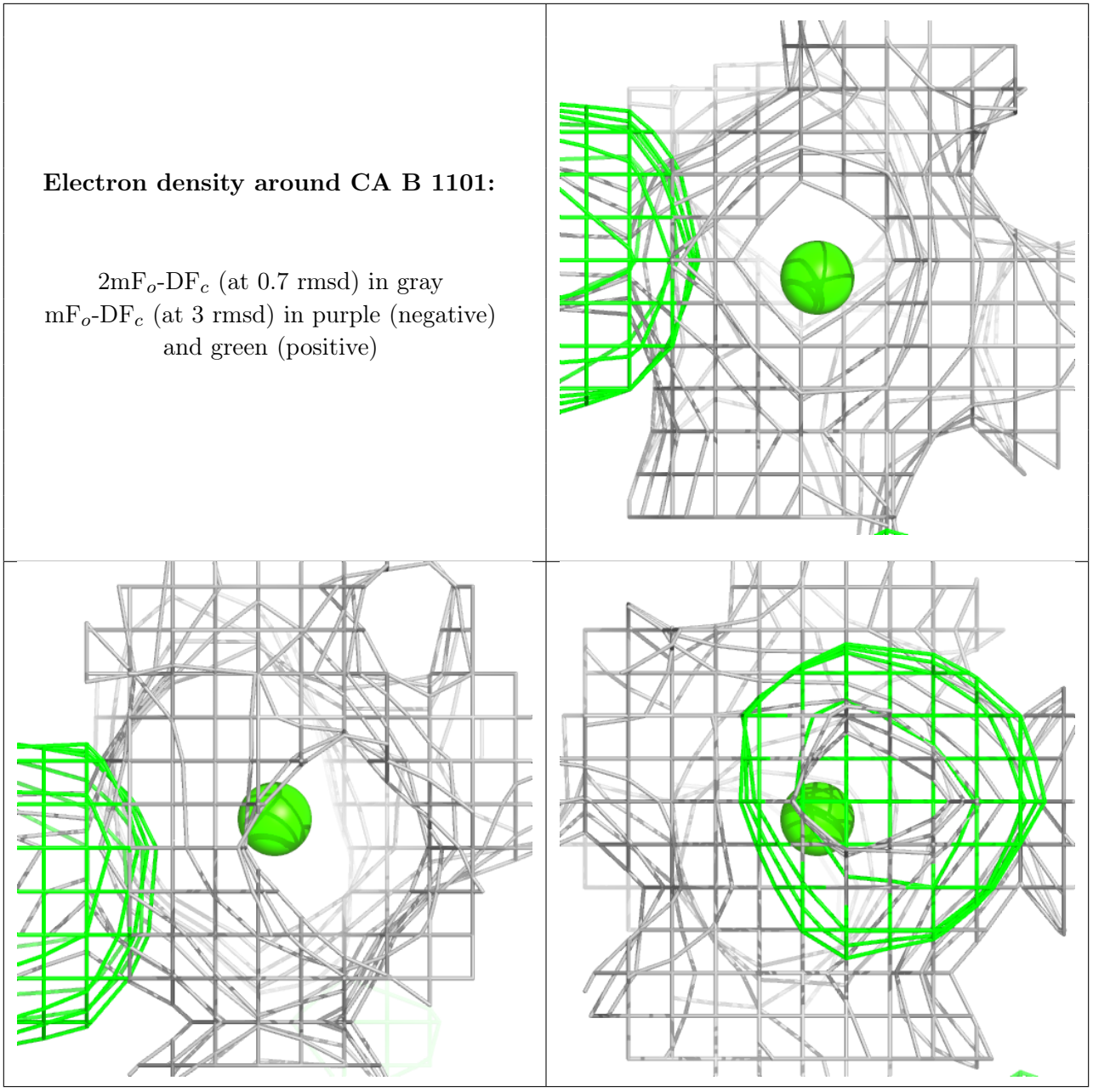






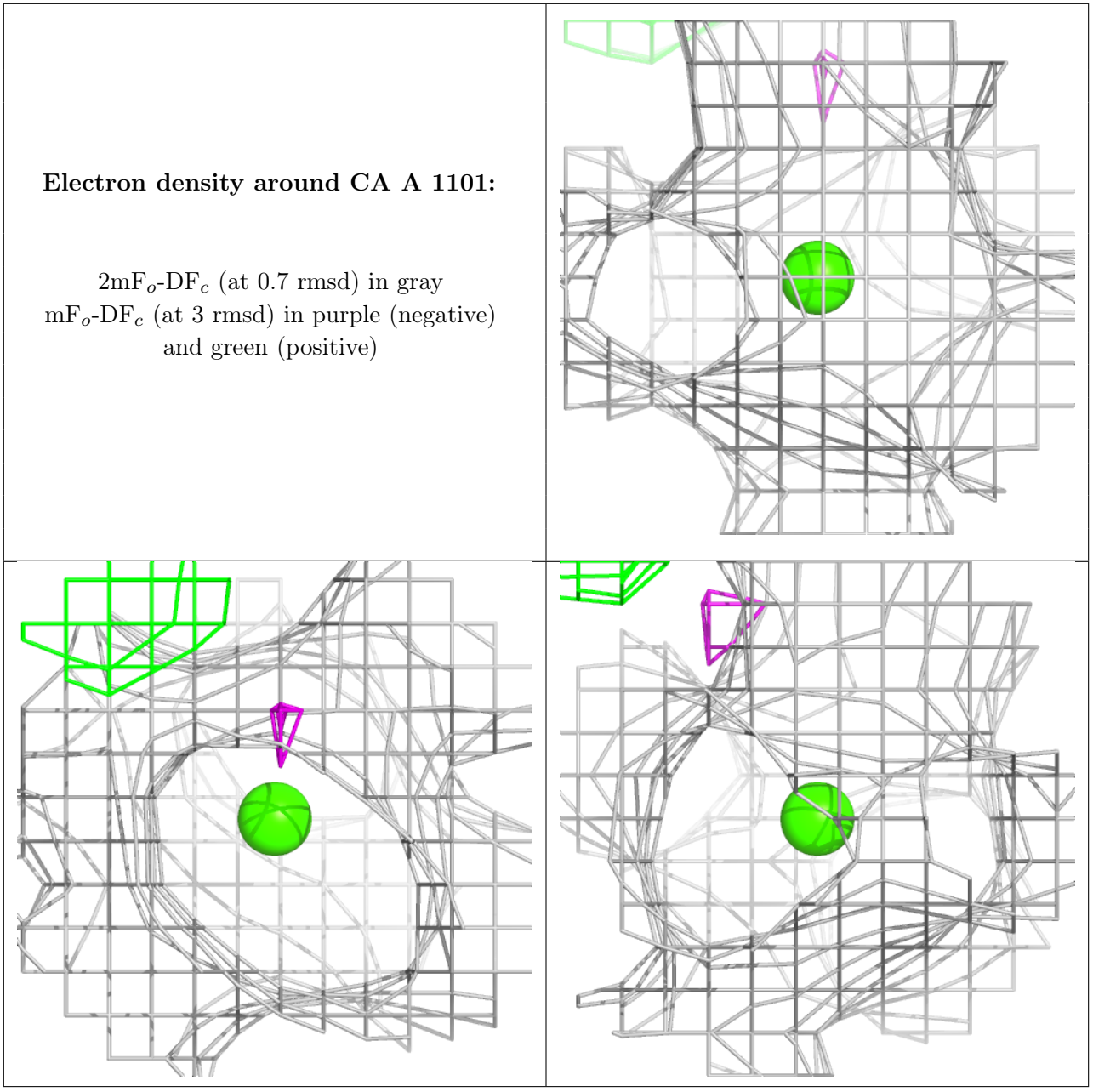
Electron density around CA B 1101:

$2mF_o$-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 1101:

$2mF_o$-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.