



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 8UF5 / pdb_00008uf5
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 ⓘ 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

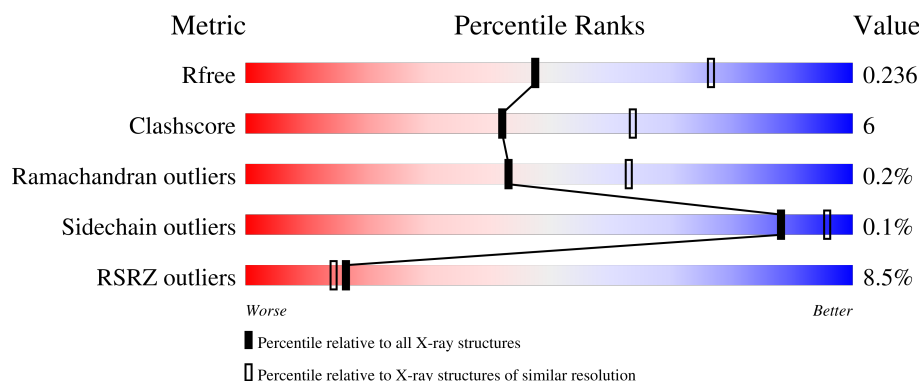
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	7% 88% 9% .
1	B	869	10% 84% 11% .

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

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	C	N	O	S	0	1	0
			6627	4176	1136	1299	16			
1	B	831	Total	C	N	O	S	0	0	0
			6522	4110	1116	1280	16			

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 (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

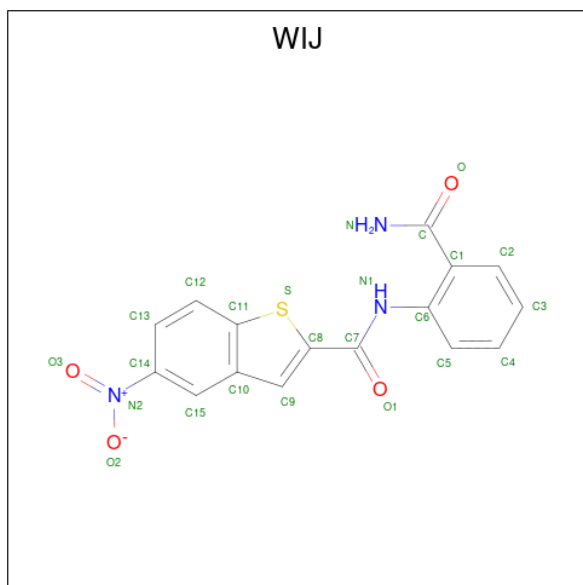
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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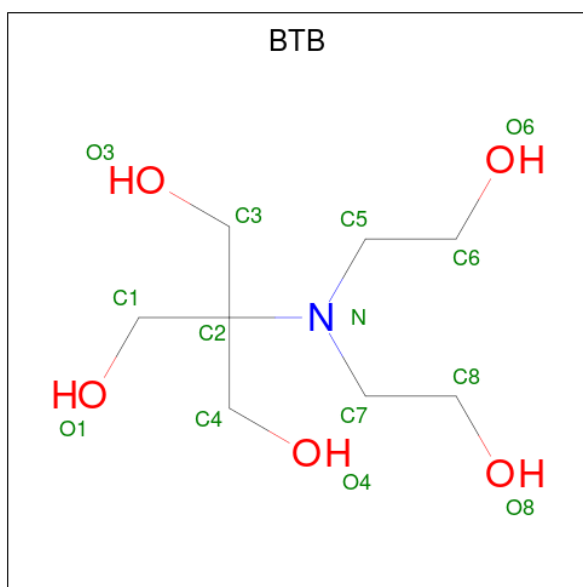
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		

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



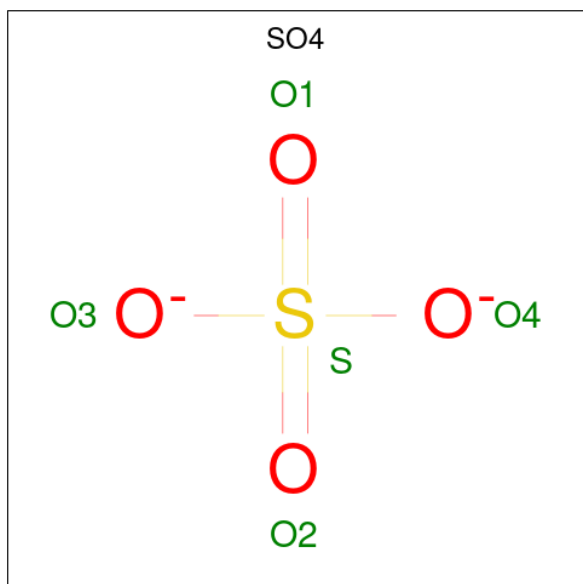
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			24	16	3	4	1		
3	B	1	Total	C	N	O	S	0	0
			24	16	3	4	1		

- Molecule 4 is 2-[BIS-(2-HYDROXY-ETHYL)-AMINO]-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: 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	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S) (labeled as "Ligand of Interest" by depositor).



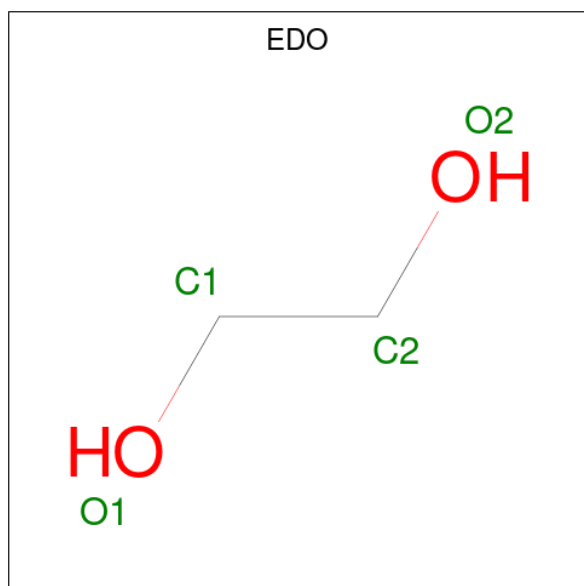
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		

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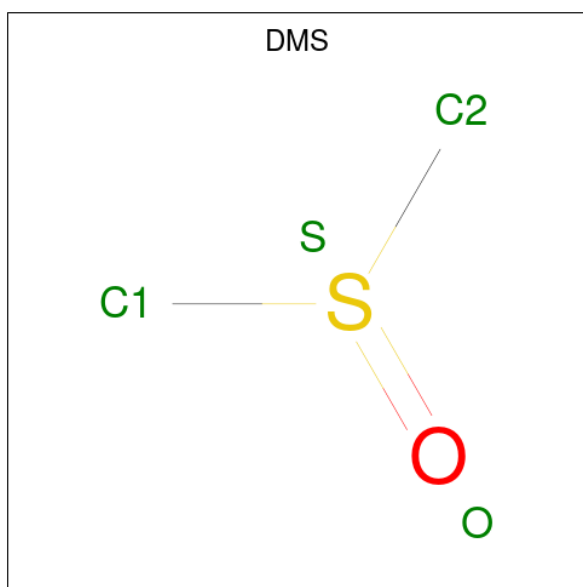
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS) (labeled as "Ligand of Interest" by depositor).



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

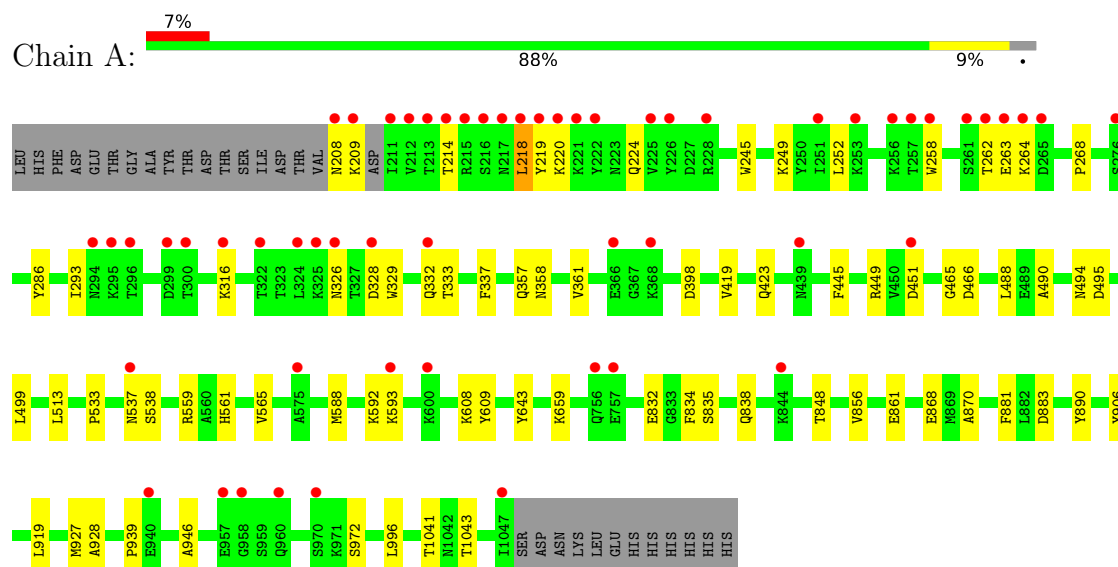
- Molecule 8 is water.

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

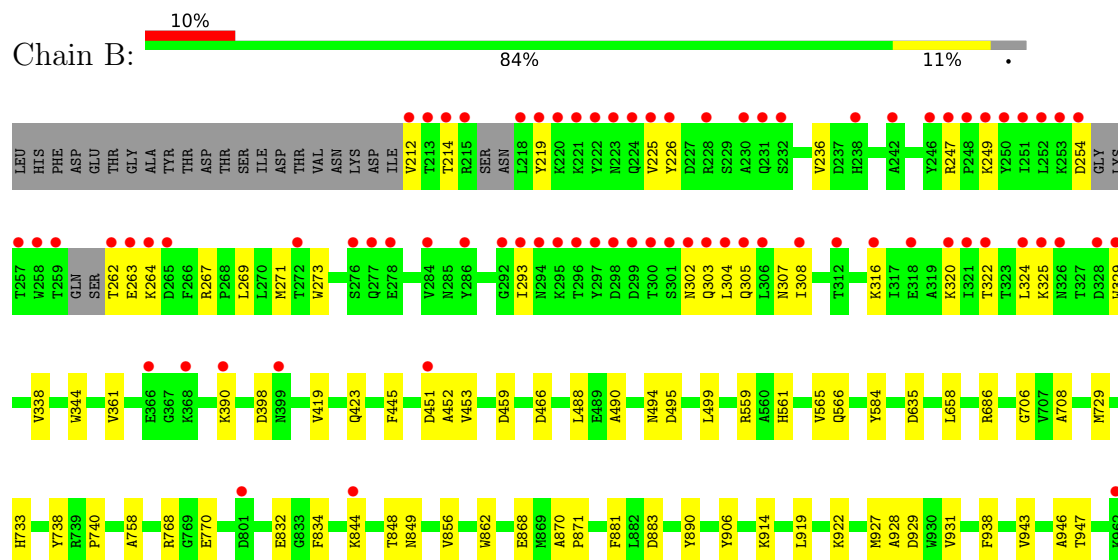
3 Residue-property plots [i](#)

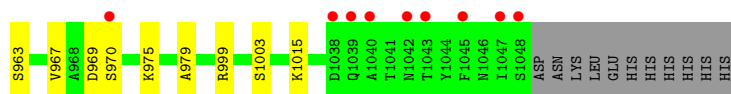
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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



• Molecule 1: Glucosyltransferase-I





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.199 , 0.230 0.207 , 0.236	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 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.23	0/6765	0.46	2/9179 (0.0%)
1	B	0.22	0/6656	0.46	1/9034 (0.0%)
All	All	0.23	0/13421	0.46	3/18213 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	THR	CB-CA-C	6.78	118.14	109.80
1	A	218	LEU	CA-C-N	5.95	132.91	121.54
1	A	218	LEU	C-N-CA	5.95	132.91	121.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6627	0	6446	70	0
1	B	6522	0	6323	87	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	14	0	19	23	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	13	0
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	163	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 (163) 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:881:PHE:CE2	4:A:1103:BTB:H81	1.90	1.06
1:A:332:GLN:HG3	1:B:320:LYS:HZ2	0.90	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:593:LYS:HZ3	1:B:304:LEU:HD11	1.55	0.71
1:B:561:HIS:NE2	4:B:1103:BTB:C4	2.54	0.71
1:B:733:HIS:NE2	6:B:1104:EDO:H21	2.06	0.70
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:B:729:MET:HE3	6:B:1104:EDO:H11	1.78	0.66
1:A:881:PHE:CE2	4:A:1103:BTB:H82	2.26	0.65
4:B:1103:BTB:O1	4:B:1103:BTB:O4	2.07	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: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:B:914:LYS:NZ	8:B:1202:HOH:O	2.30	0.62
1:A:883:ASP:CG	4:A:1103:BTB:H71	2.26	0.61
1:B:566:GLN:OE1	4:B:1103:BTB:O6	2.19	0.60
1:A:593:LYS:NZ	1:B:304:LEU:HD11	2.15	0.60
4:A:1103:BTB:O3	4:A:1103:BTB:O1	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:A:883:ASP:CG	4:A:1103:BTB:C8	2.77	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:214:THR:HA	1:A:220:LYS:HZ3	1.70	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:593:LYS:HZ3	1:B:304:LEU:CD1	2.20	0.54
1:A:883:ASP:CG	4:A:1103:BTB:O8	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:459:ASP:OD2	1:B:1003:SER:OG	2.22	0.53
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
1:B:708:ALA:HB2	1:B:729:MET:HE1	1.89	0.53
1:A:332:GLN:HG3	1:B:320:LYS:HZ1	1.62	0.53
3:A:1102:WIJ:O	4:A:1103:BTB:O3	2.22	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
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:A:262:THR:C	1:A:264:LYS:H	2.19	0.50
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:326:ASN:HD21	1:A:328:ASP:CG	2.19	0.50
1:B:247:ARG:HH11	1:B:263:GLU:H	1.60	0.50
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: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:293:ILE:HG12	1:B:316:LYS:HZ2	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:ARG:HD2	1:B:271:MET:HE1	1.97	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:293:ILE:CG1	1:A:316:LYS:HZ3	2.28	0.46
1:A:329:TRP:O	1:A:333:THR:OG1	2.33	0.46
1:B:706:GLY:CA	6:B:1104:EDO:H12	2.43	0.46
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
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: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:A:561:HIS:ND1	1:A:832:GLU:OE2	2.39	0.42
1:A:883:ASP:CG	4:A:1103:BTB:C7	2.92	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:A:332:GLN:CG	1:B:320:LYS:HZ1	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:ASP:CG	1:B:999:ARG:HH11	2.26	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
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

5.3.1 Protein backbone

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%)	43	63
1	B	823/869 (95%)	797 (97%)	25 (3%)	1 (0%)	48	68
All	All	1659/1738 (96%)	1608 (97%)	48 (3%)	3 (0%)	43	63

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 ⓘ

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	708/738 (96%)	708 (100%)	0	100	100
1	B	694/738 (94%)	692 (100%)	2 (0%)	86	94
All	All	1402/1476 (95%)	1400 (100%)	2 (0%)	88	96

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	390	LYS
1	B	975	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	260	GLN
1	A	280	GLN
1	A	290	GLN
1	A	303	GLN
1	A	305	GLN
1	A	307	ASN
1	A	341	GLN
1	A	386	ASN
1	A	532	ASN
1	A	537	ASN
1	A	673	ASN
1	A	855	ASN
1	A	1046	ASN
1	B	277	GLN
1	B	341	GLN
1	B	386	ASN
1	B	432	ASN
1	B	532	ASN
1	B	537	ASN
1	B	673	ASN

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Mol	Chain	Res	Type
1	B	735	ASN
1	B	855	ASN
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 oligosaccharides 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	$\# Z > 2$
4	BTB	B	1103	-	13,13,13	0.61	0	7,16,16	1.84	2 (28%)
5	SO4	B	1109	-	4,4,4	0.22	0	6,6,6	0.14	0
7	DMS	B	1106	-	3,3,3	0.26	0	3,3,3	0.07	0
6	EDO	B	1104	-	3,3,3	0.05	0	2,2,2	0.12	0
4	BTB	A	1103	-	13,13,13	0.50	0	7,16,16	0.61	0
5	SO4	B	1107	-	4,4,4	0.23	0	6,6,6	0.10	0
3	WIJ	B	1102	-	26,26,26	0.48	0	35,37,37	0.80	2 (5%)
5	SO4	B	1110	-	4,4,4	0.25	0	6,6,6	0.10	0
6	EDO	B	1105	-	3,3,3	0.41	0	2,2,2	0.39	0
5	SO4	A	1104	-	4,4,4	0.79	0	6,6,6	0.23	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SO4	A	1105	-	4,4,4	0.25	0	6,6,6	0.23	0
5	SO4	B	1108	-	4,4,4	0.22	0	6,6,6	0.13	0
3	WIJ	A	1102	-	26,26,26	0.44	0	35,37,37	0.84	1 (2%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BTB	B	1103	-	-	9/21/21/21	-
4	BTB	A	1103	-	-	10/21/21/21	-
3	WIJ	B	1102	-	-	8/14/16/16	0/3/3/3
6	EDO	B	1105	-	-	0/1/1/1	-
6	EDO	B	1104	-	-	1/1/1/1	-
3	WIJ	A	1102	-	-	9/14/16/16	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1103	BTB	O1-C1-C2	-4.00	101.99	111.40
3	A	1102	WIJ	C6-C1-C	3.05	123.66	121.67
3	B	1102	WIJ	C6-C1-C	2.53	123.32	121.67
4	B	1103	BTB	O4-C4-C2	-2.45	105.64	111.40
3	B	1102	WIJ	C13-C14-C15	2.04	122.73	120.11

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1102	WIJ	C8-C7-N1-C6
3	B	1102	WIJ	C8-C7-N1-C6
4	A	1103	BTB	O1-C1-C2-N
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

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Mol	Chain	Res	Type	Atoms
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	A	1102	WIJ	O1-C7-N1-C6
3	B	1102	WIJ	O1-C7-N1-C6
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
4	A	1103	BTB	C6-C5-N-C2
4	A	1103	BTB	O1-C1-C2-C4
3	B	1102	WIJ	N1-C7-C8-C9
3	B	1102	WIJ	C5-C6-N1-C7
4	A	1103	BTB	N-C2-C4-O4
4	A	1103	BTB	C3-C2-N-C5
3	A	1102	WIJ	N1-C7-C8-C9
3	A	1102	WIJ	N1-C7-C8-S
3	B	1102	WIJ	N1-C7-C8-S
3	A	1102	WIJ	C5-C6-N1-C7
6	B	1104	EDO	O1-C1-C2-O2
3	A	1102	WIJ	N-C-C1-C2
3	B	1102	WIJ	C1-C6-N1-C7
3	A	1102	WIJ	C1-C6-N1-C7

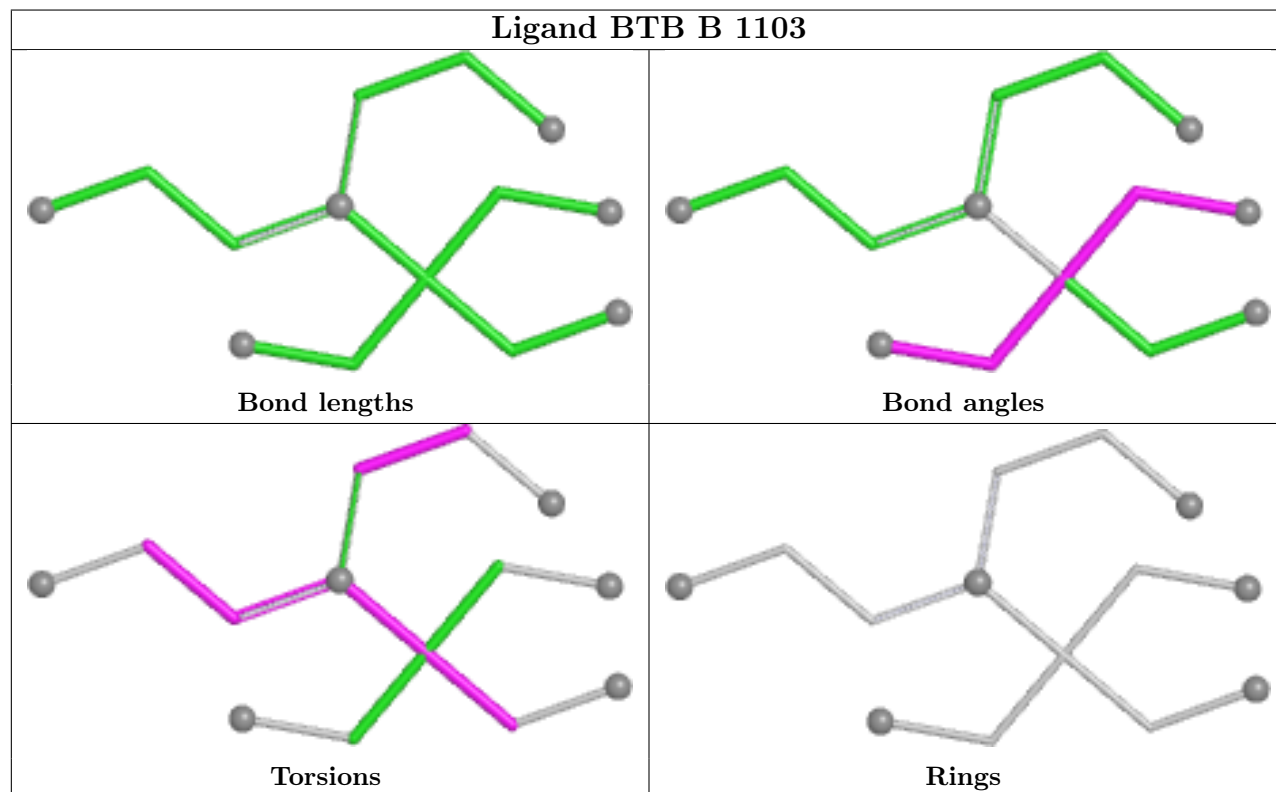
There are no ring outliers.

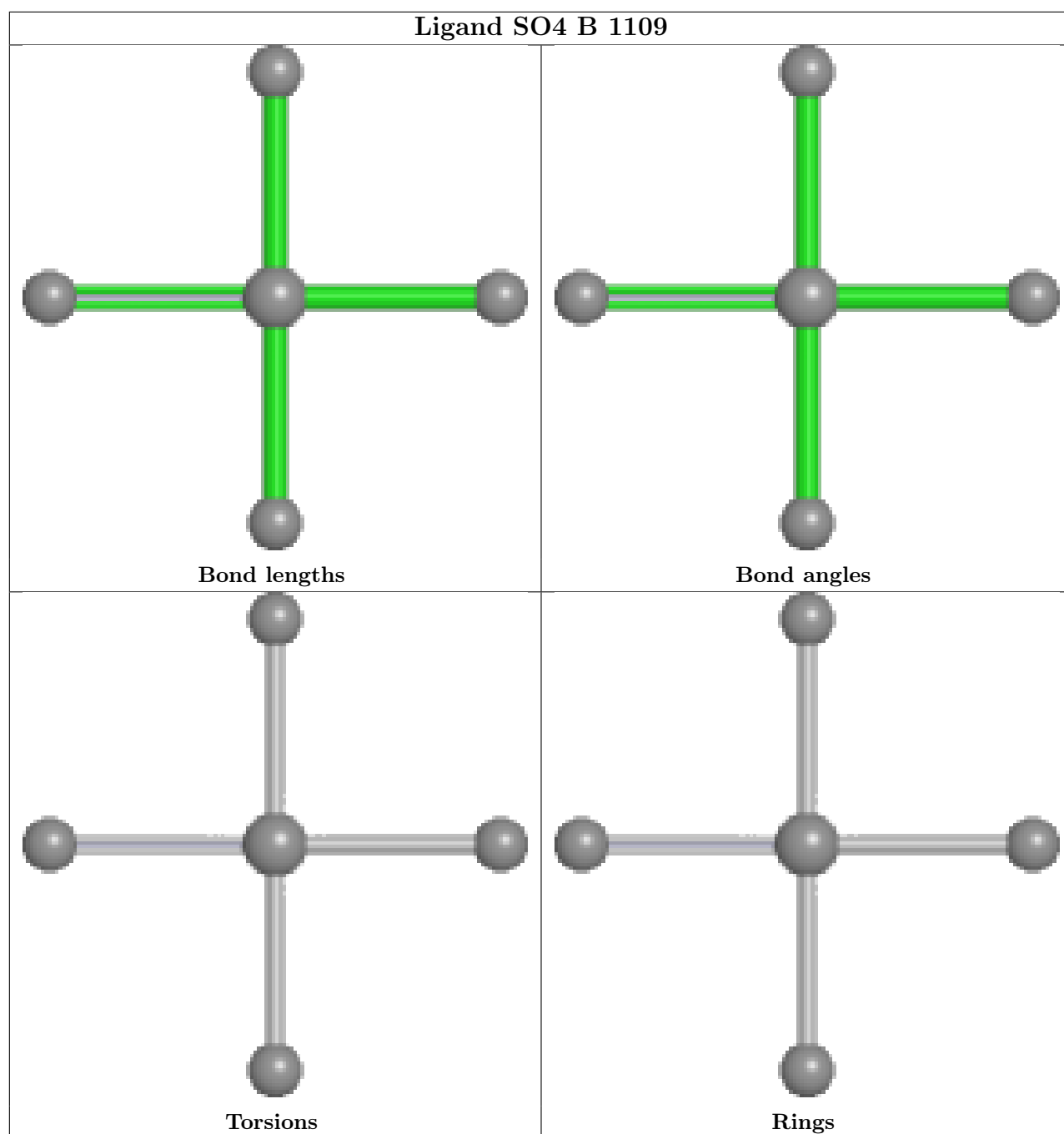
6 monomers are involved in 51 short contacts:

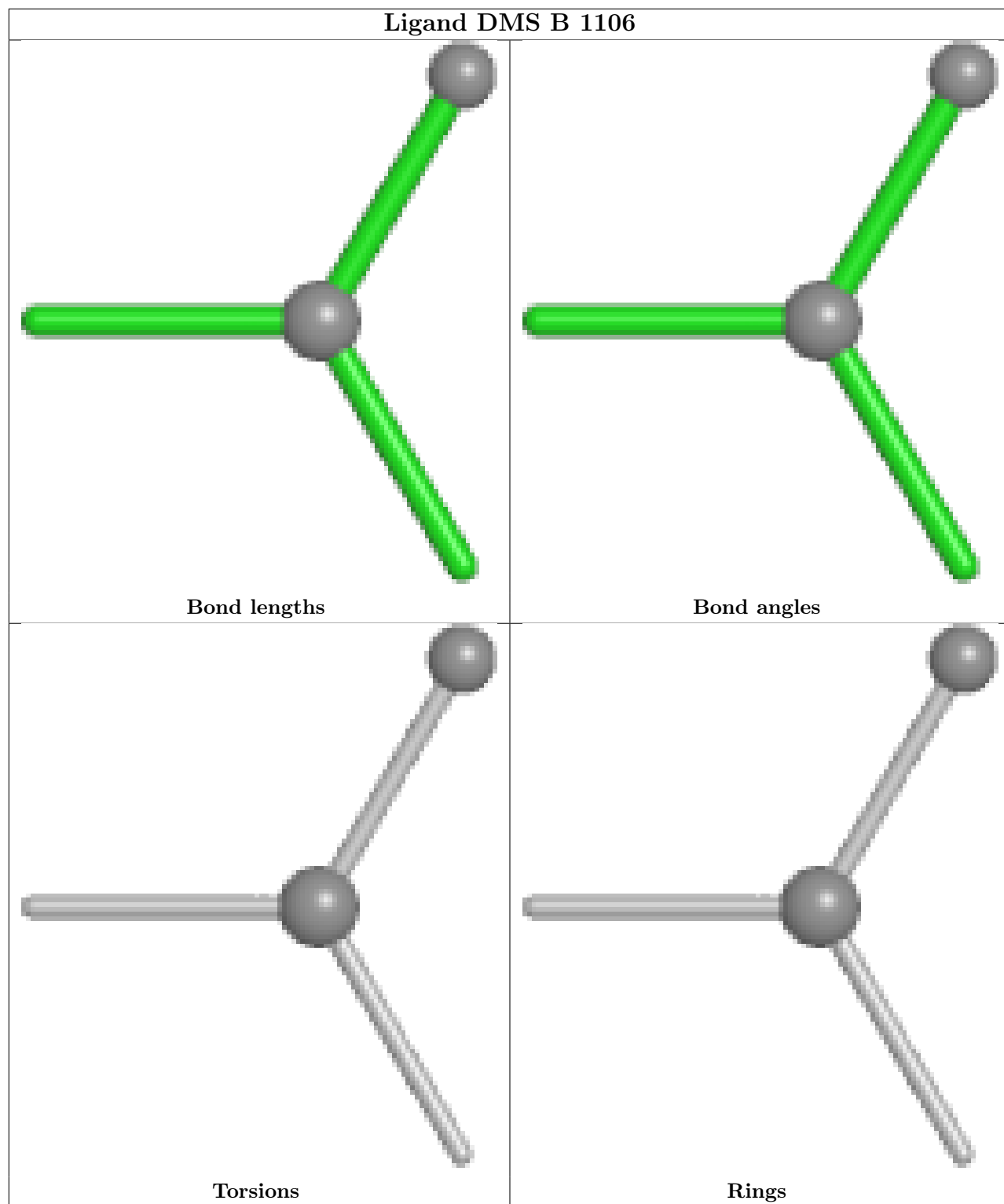
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1103	BTB	14	0
5	B	1109	SO4	1	0
6	B	1104	EDO	8	0
4	A	1103	BTB	23	0
6	B	1105	EDO	5	0
3	A	1102	WIJ	2	0

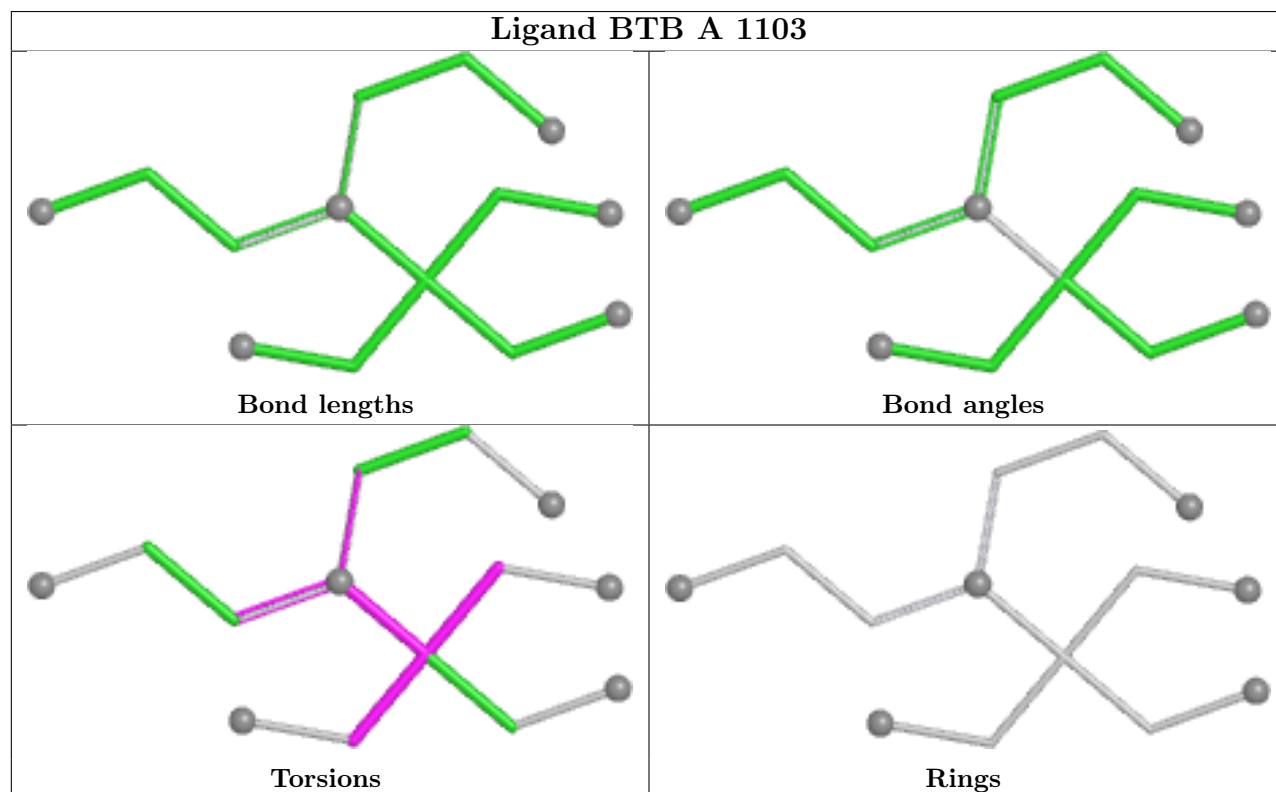
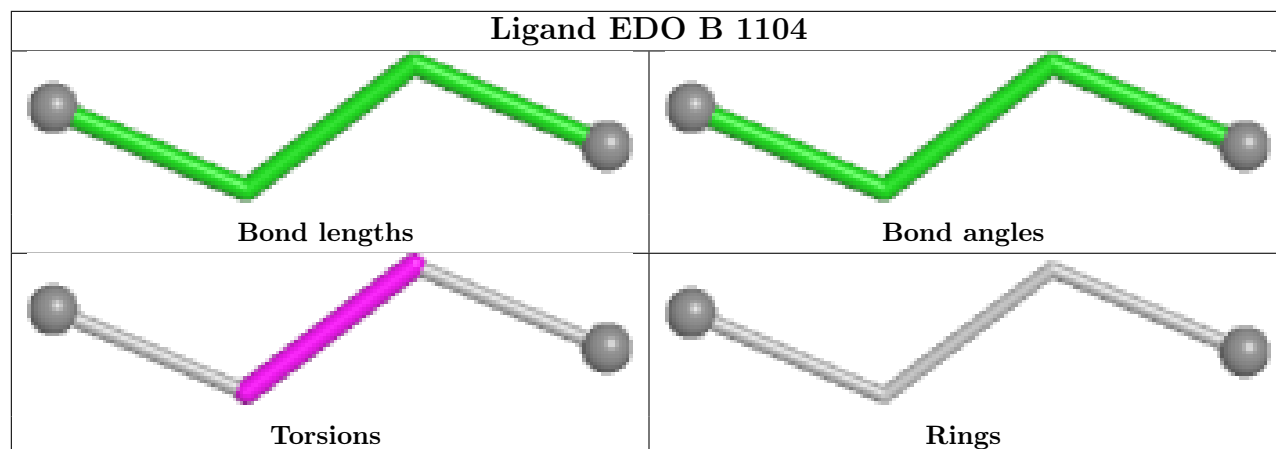
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

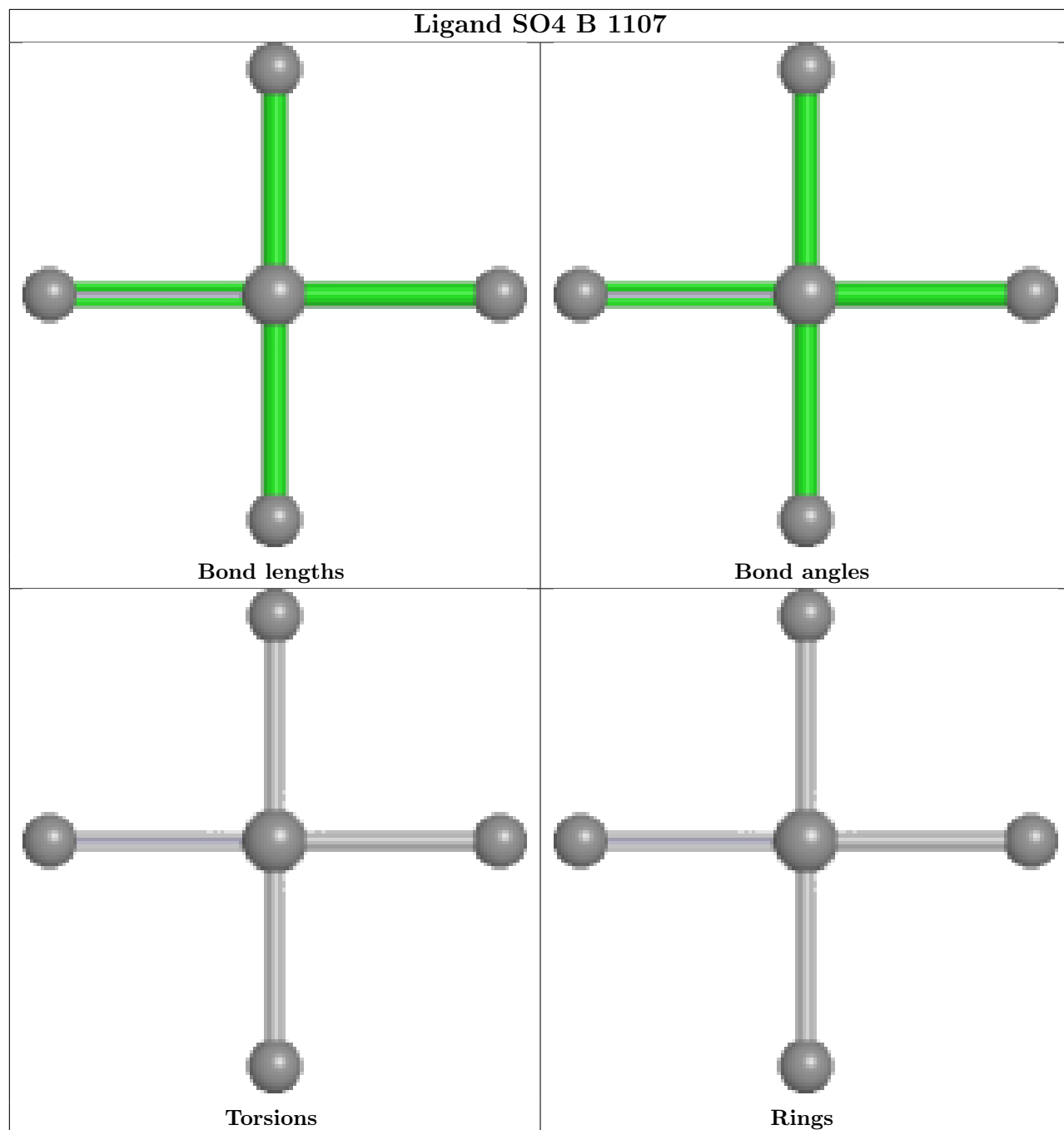
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

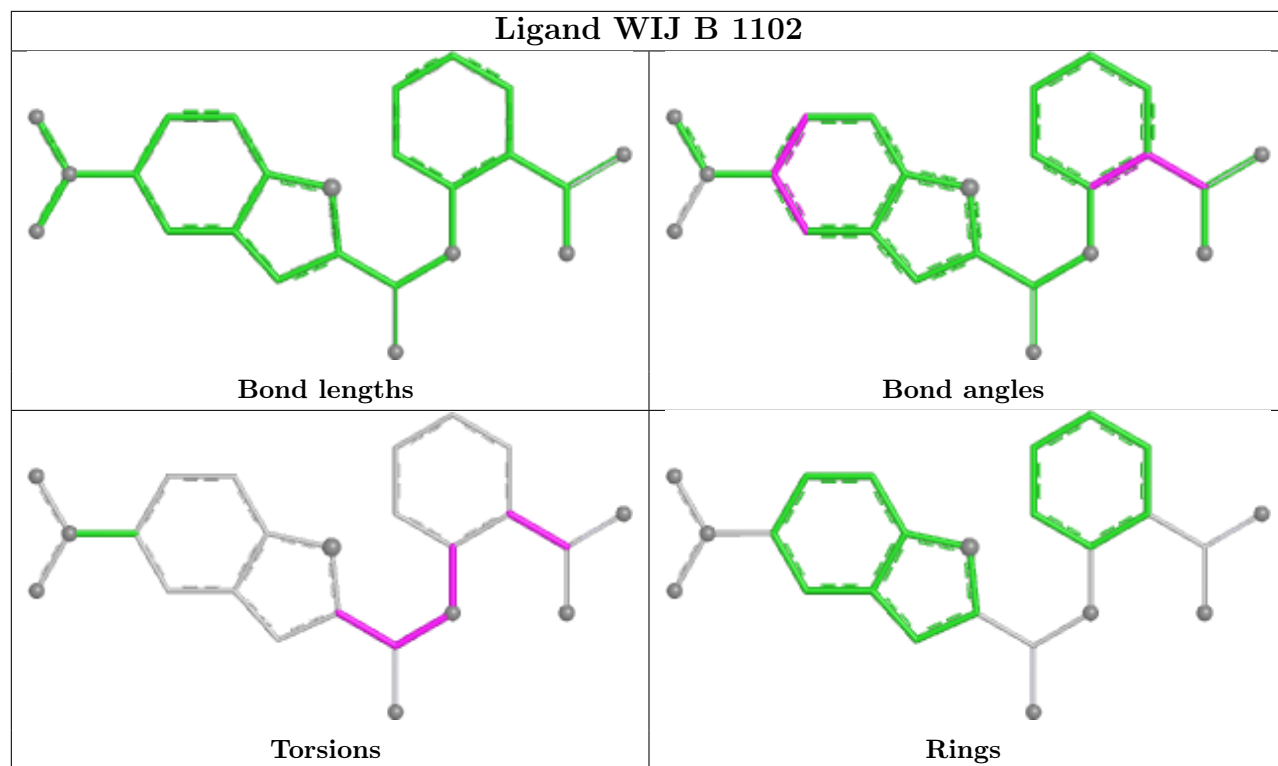


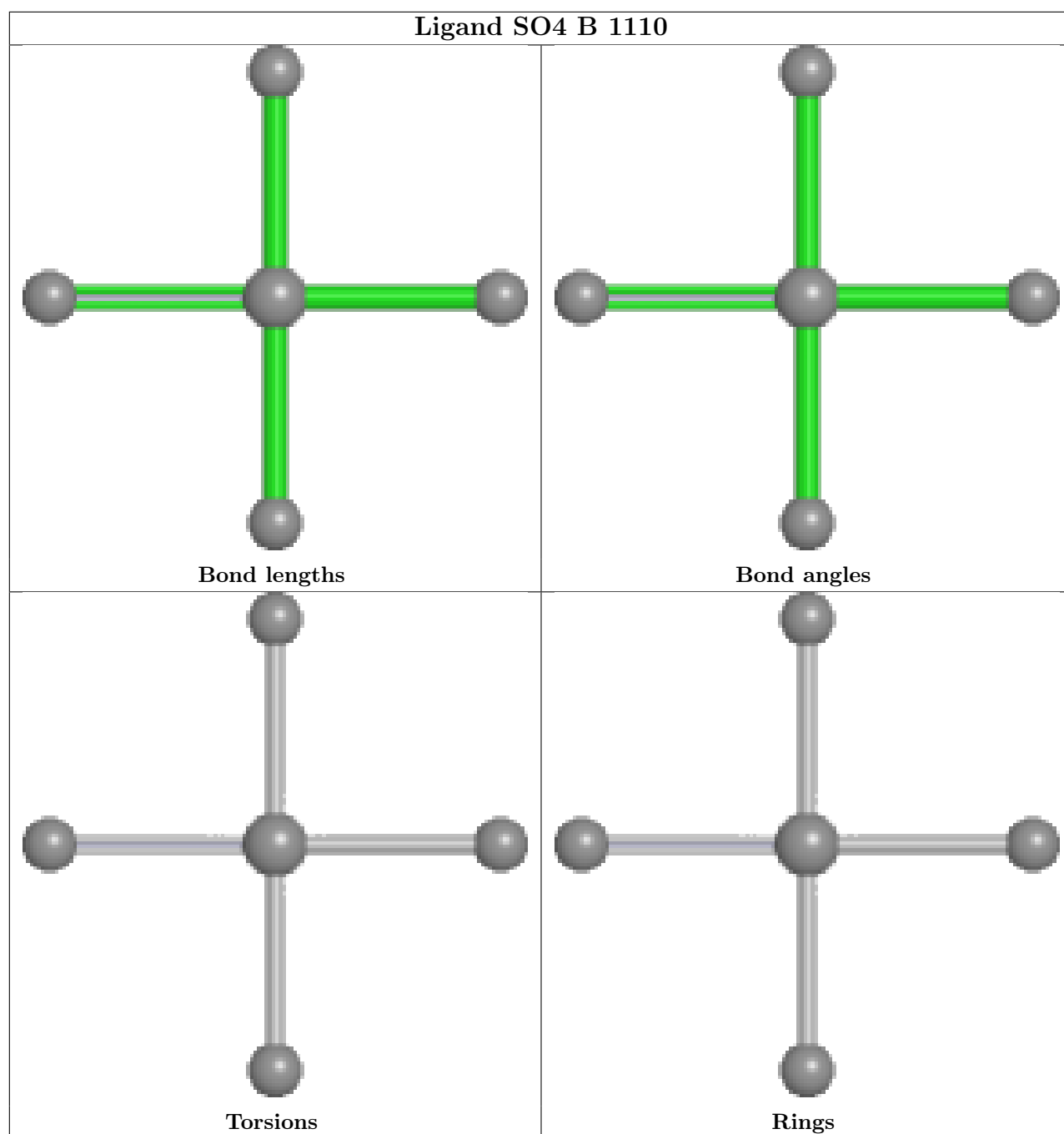


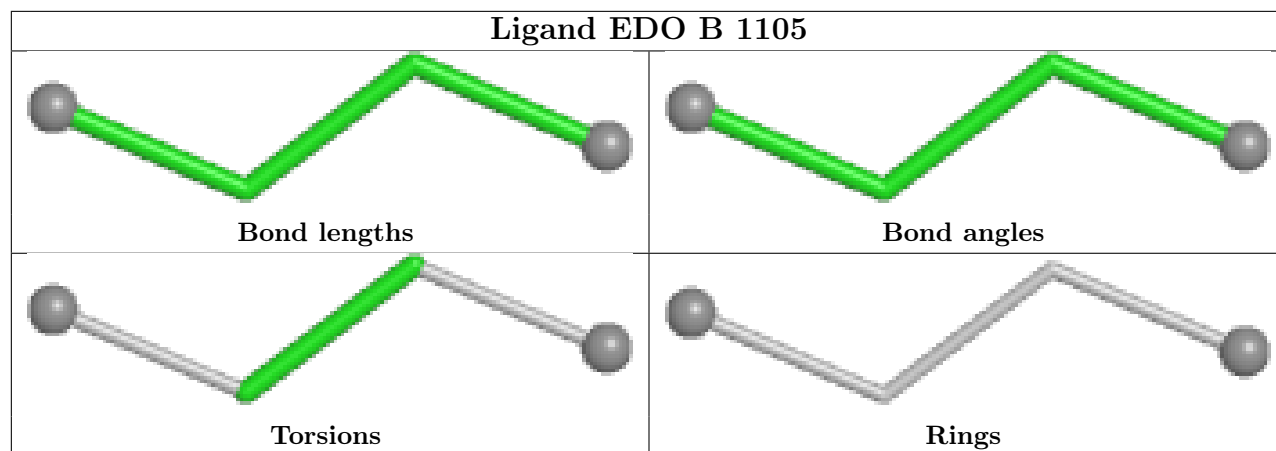


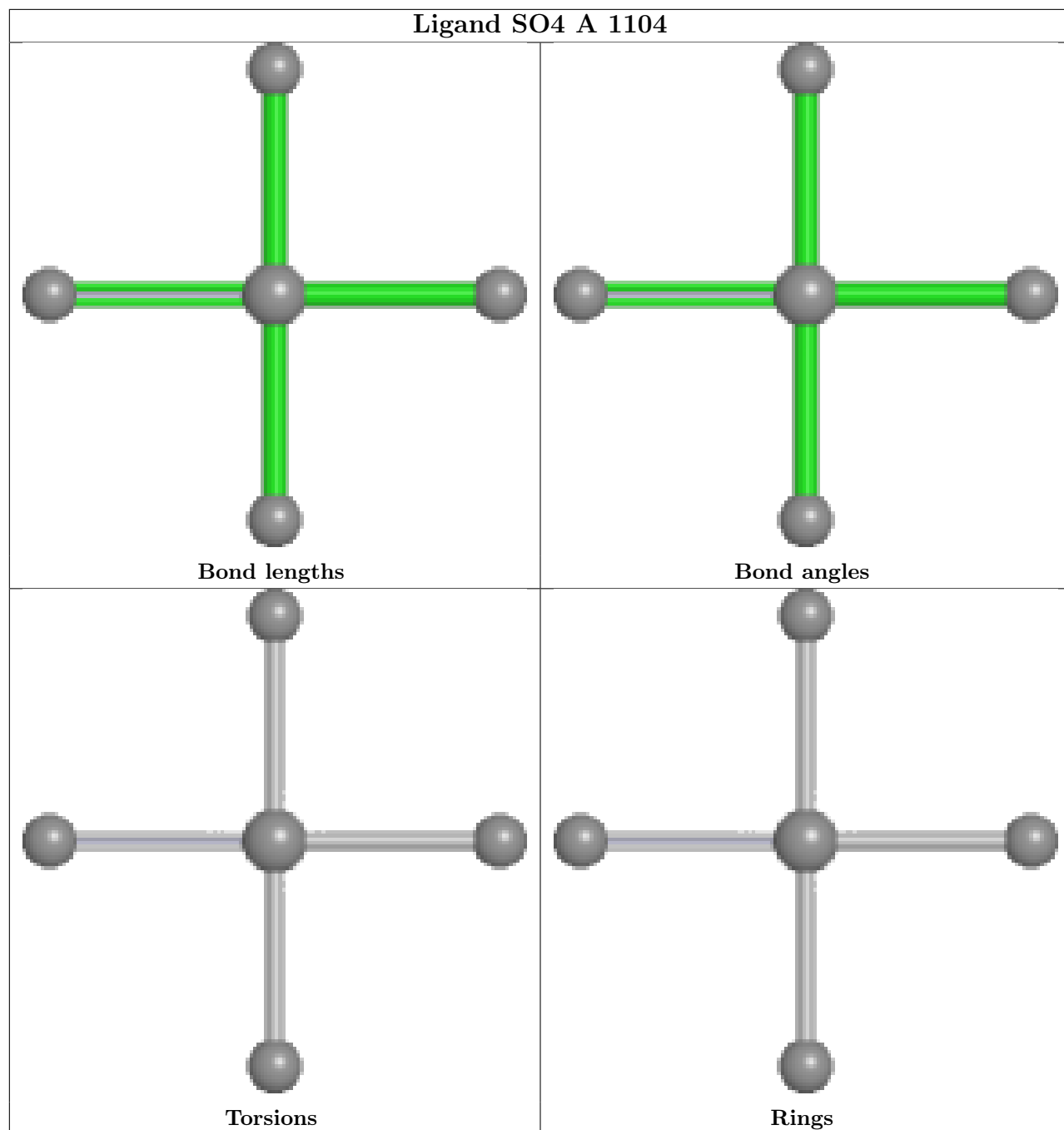


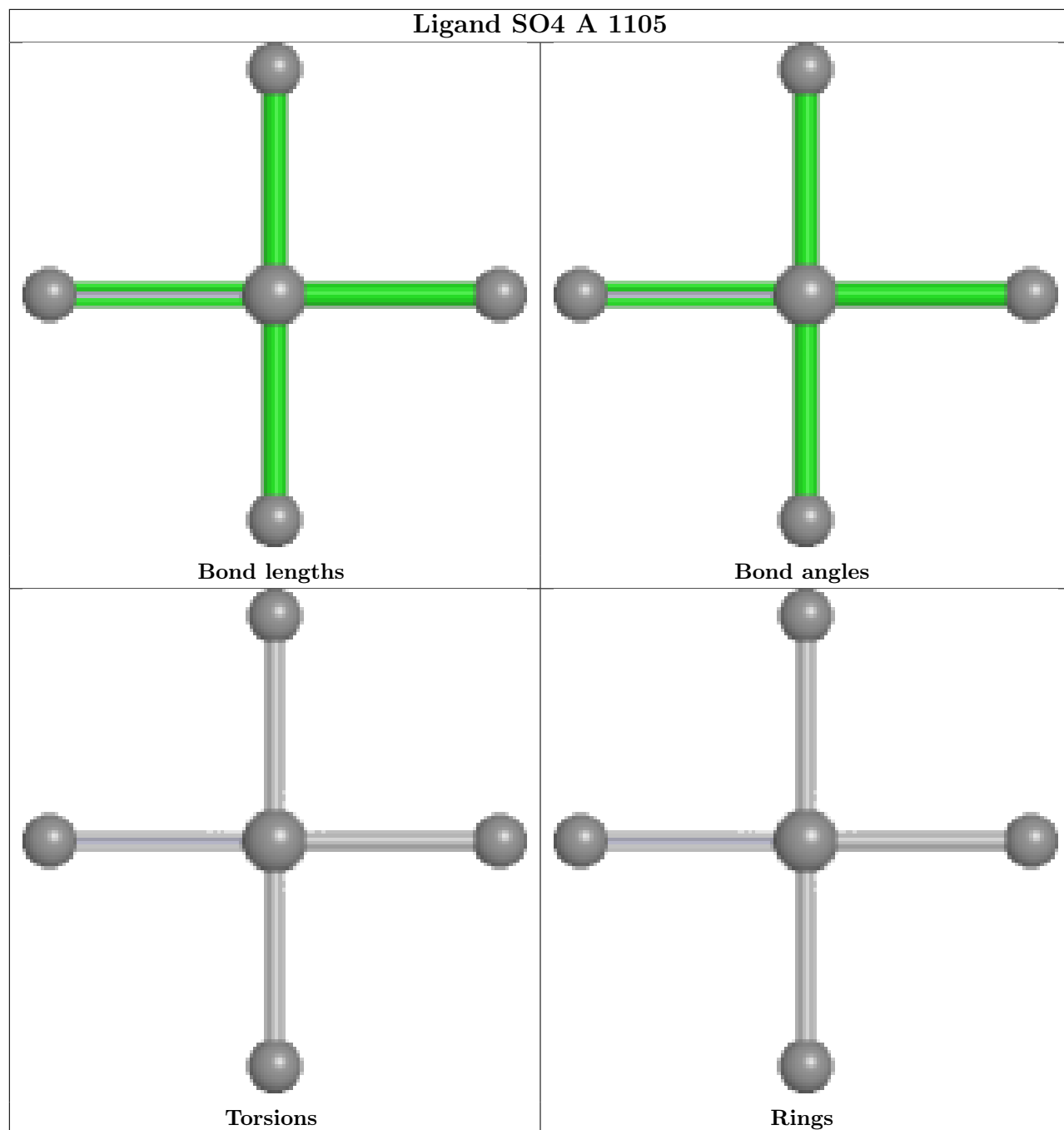


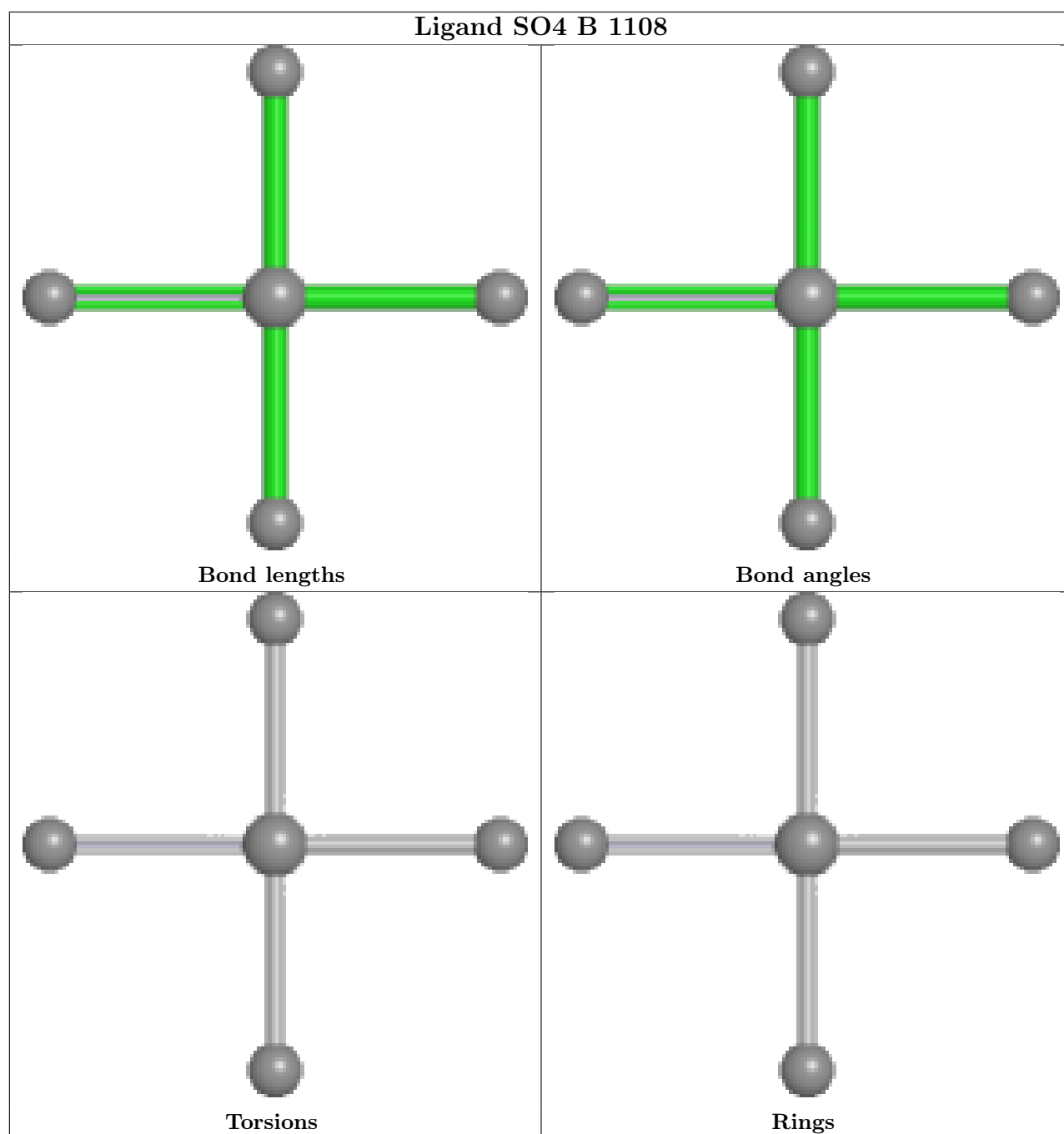


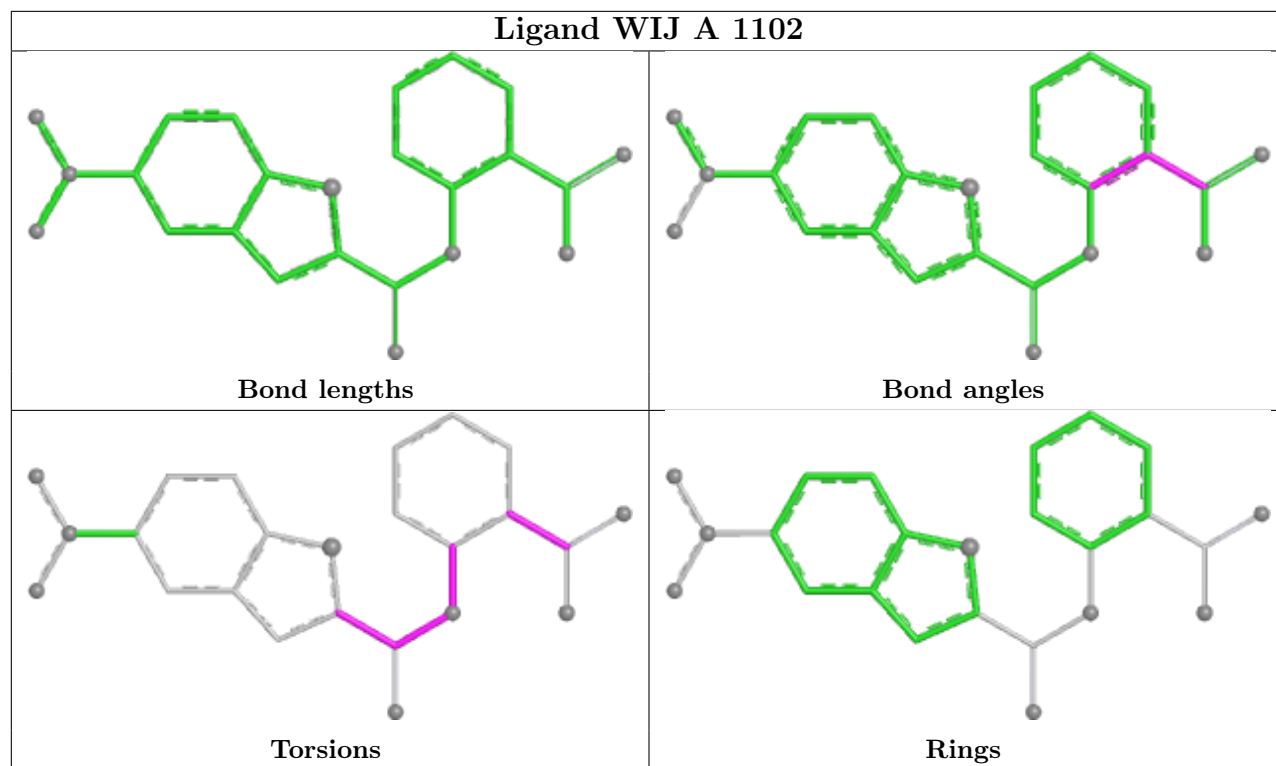












5.7 Other polymers [i](#)

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, 95th 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%)	0.27	57 (6%)	23	20	16, 39, 70, 108	1 (0%)
1	B	831/869 (95%)	0.34	85 (10%)	12	10	23, 38, 83, 107	0
All	All	1670/1738 (96%)	0.30	142 (8%)	16	14	16, 39, 76, 108	1 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	212	VAL	10.2
1	A	211	ILE	9.2
1	B	215	ARG	8.5
1	B	218	LEU	8.2
1	A	218	LEU	8.1
1	B	259	THR	7.0
1	B	262	THR	6.9
1	A	214	THR	6.7
1	A	209	LYS	6.6
1	B	1048	SER	6.2
1	A	213	THR	6.1
1	B	250	TYR	6.0
1	B	219	TYR	5.9
1	A	957	GLU	5.9
1	B	228	ARG	5.8
1	B	222	TYR	5.8
1	A	212	VAL	5.8
1	A	215	ARG	5.7
1	B	258	TRP	5.6
1	A	208	ASN	5.3
1	B	325	LYS	5.3
1	B	251	ILE	5.3
1	A	216	SER	5.2
1	B	252	LEU	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	249	LYS	5.0
1	A	970	SER	5.0
1	B	970	SER	4.9
1	A	221	LYS	4.8
1	A	257	THR	4.7
1	B	324	LEU	4.7
1	A	263	GLU	4.7
1	B	320	LYS	4.7
1	B	213	THR	4.7
1	B	304	LEU	4.7
1	B	254	ASP	4.6
1	B	214	THR	4.4
1	B	326	ASN	4.4
1	B	257	THR	4.3
1	B	224	GLN	4.2
1	B	263	GLU	4.2
1	B	220	LYS	4.2
1	A	217	ASN	4.1
1	B	277	GLN	4.1
1	B	221	LYS	4.1
1	A	264	LYS	4.0
1	B	264	LYS	4.0
1	B	316	LYS	3.9
1	A	368	LYS	3.8
1	B	1047	ILE	3.8
1	B	298	ASP	3.7
1	B	1043	THR	3.7
1	B	451	ASP	3.7
1	B	226	TYR	3.7
1	A	960	GLN	3.6
1	B	276	SER	3.5
1	B	265	ASP	3.4
1	B	295	LYS	3.4
1	B	303	GLN	3.4
1	A	1047	ILE	3.4
1	A	439	ASN	3.3
1	A	316	LYS	3.3
1	B	297	TYR	3.3
1	B	299	ASP	3.3
1	B	278	GLU	3.3
1	B	366	GLU	3.2
1	B	292	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	300	THR	3.2
1	A	757	GLU	3.2
1	A	265	ASP	3.1
1	B	294	ASN	3.1
1	B	1045	PHE	3.1
1	A	328	ASP	3.1
1	B	302	ASN	3.1
1	B	308	ILE	3.0
1	A	844	LYS	2.9
1	B	1039	GLN	2.9
1	A	219	TYR	2.9
1	A	326	ASN	2.9
1	A	296	THR	2.9
1	A	222	TYR	2.9
1	B	253	LYS	2.8
1	B	368	LYS	2.8
1	B	272	THR	2.8
1	A	322	THR	2.7
1	A	295	LYS	2.7
1	A	228	ARG	2.7
1	B	301	SER	2.7
1	B	322	THR	2.7
1	B	248	PRO	2.6
1	B	284	VAL	2.6
1	B	225	VAL	2.6
1	A	225	VAL	2.6
1	B	293	ILE	2.6
1	A	262	THR	2.5
1	A	258	TRP	2.5
1	B	801	ASP	2.5
1	A	600	LYS	2.5
1	B	399	ASN	2.5
1	B	962	LYS	2.5
1	B	844	LYS	2.4
1	B	230	ALA	2.4
1	B	232	SER	2.4
1	B	306	LEU	2.4
1	B	1042	ASN	2.4
1	A	276	SER	2.4
1	B	231	GLN	2.4
1	B	238	HIS	2.4
1	A	537	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	256	LYS	2.4
1	B	296	THR	2.4
1	A	261	SER	2.3
1	A	958	GLY	2.3
1	A	251	ILE	2.3
1	B	247	ARG	2.3
1	B	246	TYR	2.3
1	A	593	LYS	2.3
1	B	242	ALA	2.3
1	A	756	GLN	2.3
1	A	226	TYR	2.3
1	A	299	ASP	2.2
1	A	451	ASP	2.2
1	B	1040	ALA	2.2
1	A	325	LYS	2.2
1	B	223	ASN	2.2
1	B	318	GLU	2.2
1	B	305	GLN	2.1
1	A	324	LEU	2.1
1	B	328	ASP	2.1
1	B	329	TRP	2.1
1	A	220	LYS	2.1
1	A	253	LYS	2.1
1	B	390	LYS	2.1
1	B	1038	ASP	2.1
1	A	294	ASN	2.1
1	A	366	GLU	2.1
1	A	575	ALA	2.0
1	B	321	ILE	2.0
1	A	332	GLN	2.0
1	A	940	GLU	2.0
1	A	300	THR	2.0
1	B	312	THR	2.0
1	B	286	TYR	2.0

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

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

6.3 Carbohydrates

There are no oligosaccharides in this entry.

6.4 Ligands

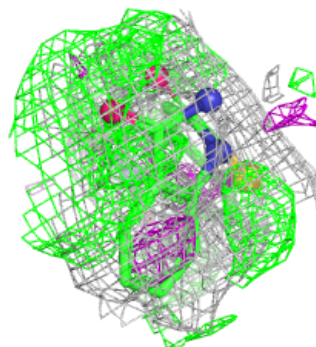
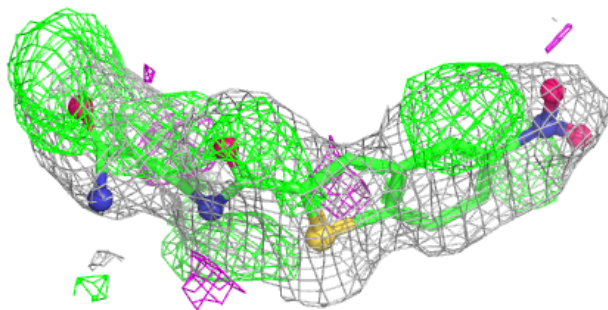
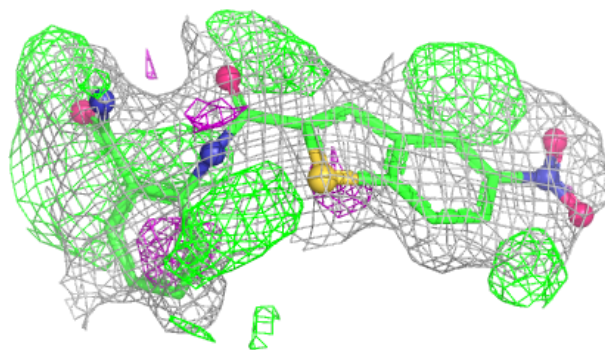
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	WIJ	B	1102	24/24	0.72	0.26	48,59,76,81	0
4	BTB	B	1103	14/14	0.72	0.27	44,58,75,79	0
3	WIJ	A	1102	24/24	0.77	0.21	38,56,68,79	0
4	BTB	A	1103	14/14	0.78	0.23	42,53,73,81	0
7	DMS	B	1106	4/4	0.81	0.23	32,36,63,102	0
5	SO4	B	1109	5/5	0.82	0.11	80,84,93,102	0
5	SO4	B	1110	5/5	0.84	0.11	79,83,94,117	0
6	EDO	B	1104	4/4	0.90	0.26	32,38,41,42	0
5	SO4	A	1104	5/5	0.91	0.15	56,73,75,87	0
5	SO4	B	1107	5/5	0.92	0.21	58,65,90,99	0
6	EDO	B	1105	4/4	0.93	0.29	38,43,49,51	0
5	SO4	B	1108	5/5	0.94	0.15	54,60,73,91	0
5	SO4	A	1105	5/5	0.94	0.19	52,58,60,102	0
2	CA	B	1101	1/1	0.99	0.03	36,36,36,36	0
2	CA	A	1101	1/1	0.99	0.02	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.

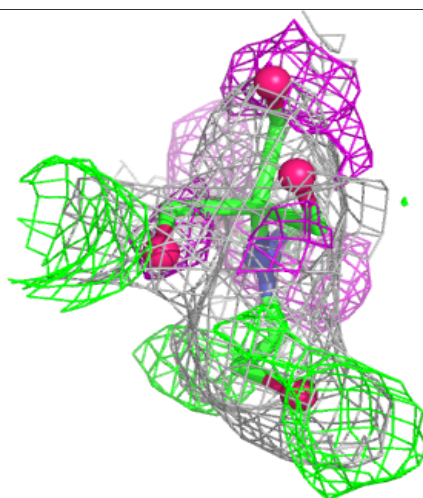
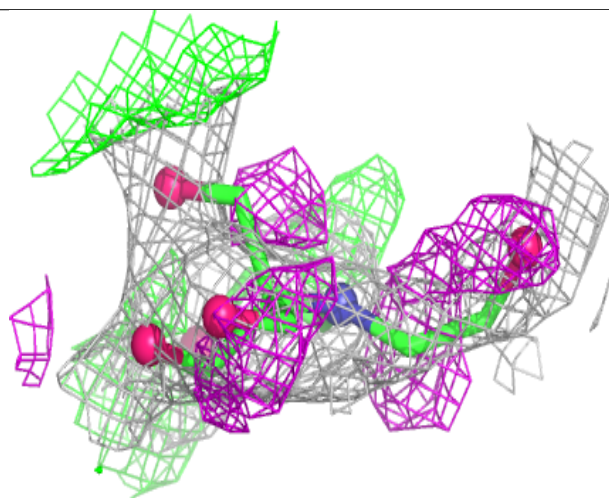
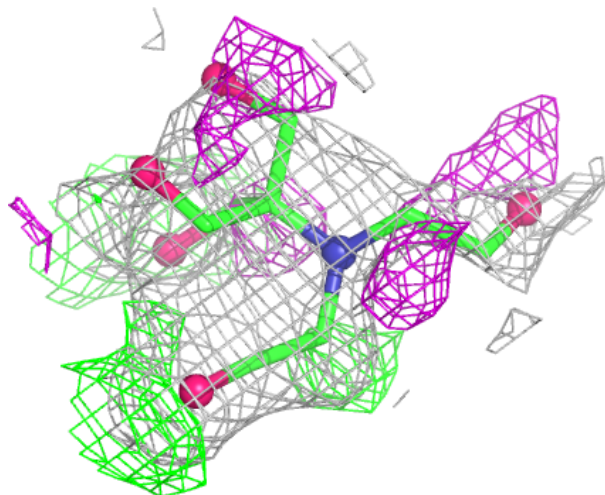
Electron density around WIJ B 1102:

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



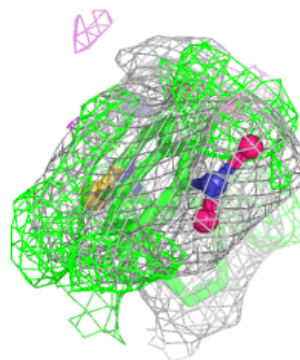
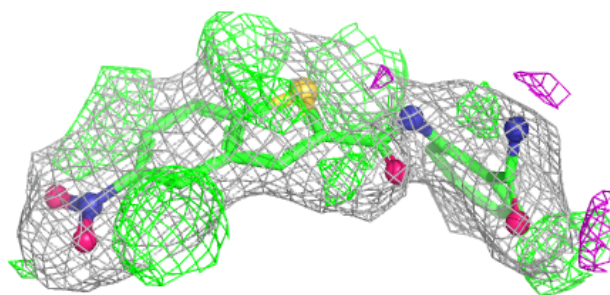
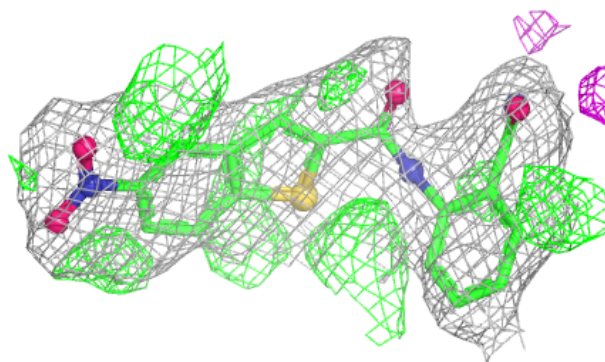
Electron density around BTB B 1103:

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



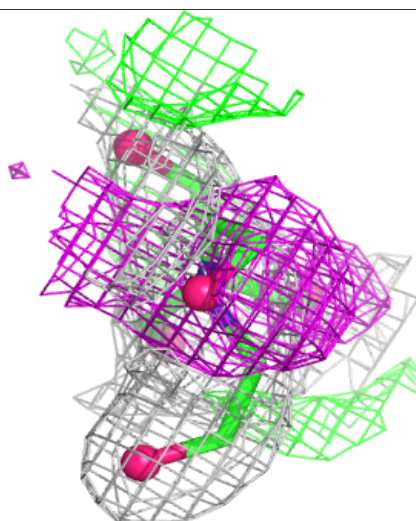
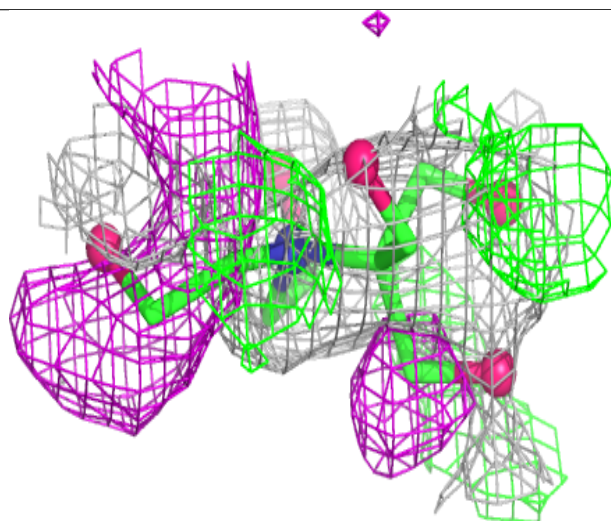
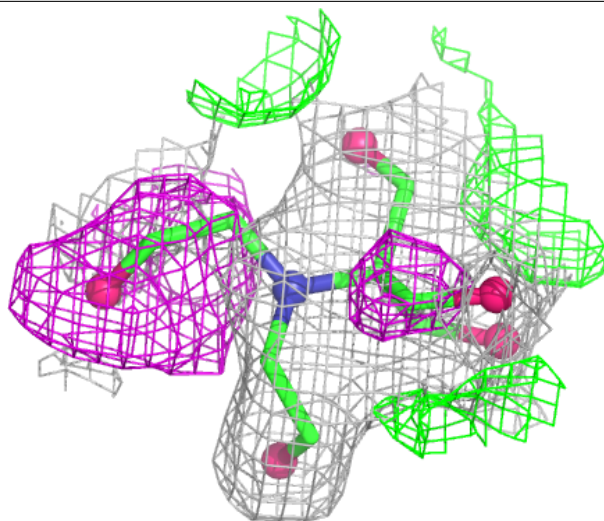
Electron density around WIJ A 1102:

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



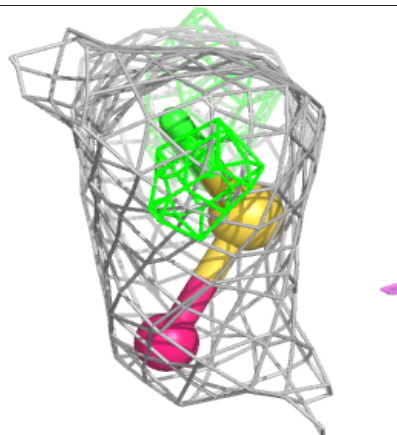
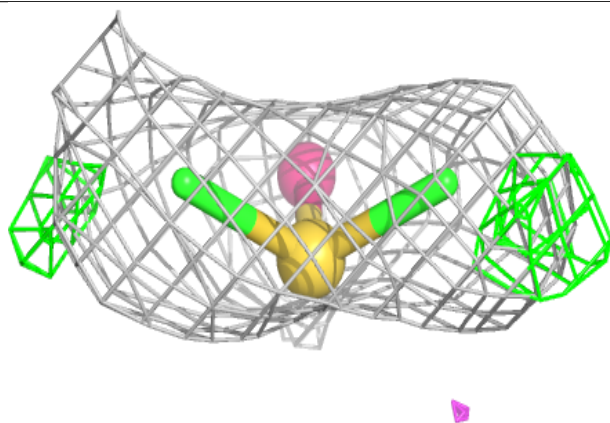
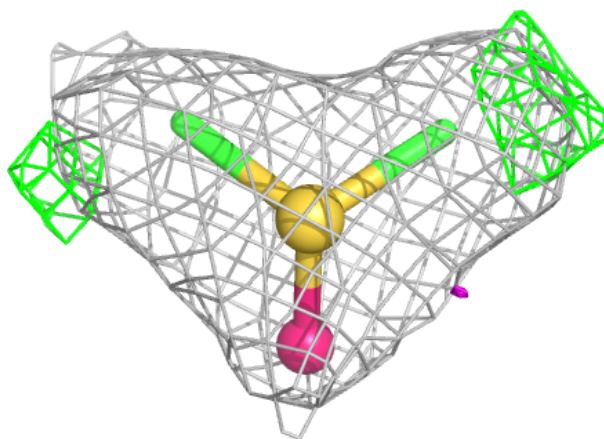
Electron density around BTB A 1103:

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



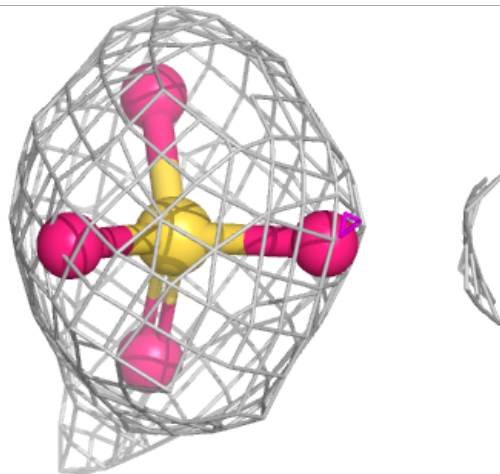
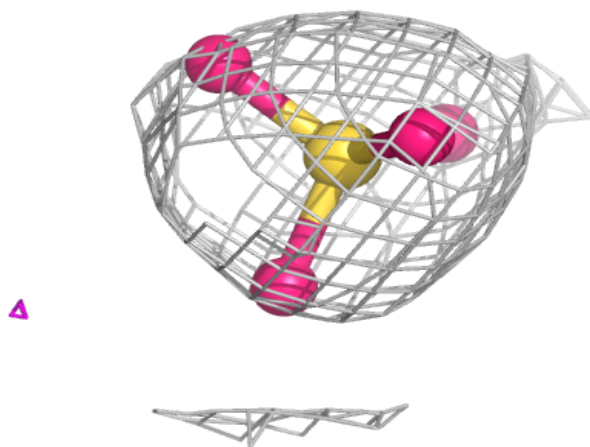
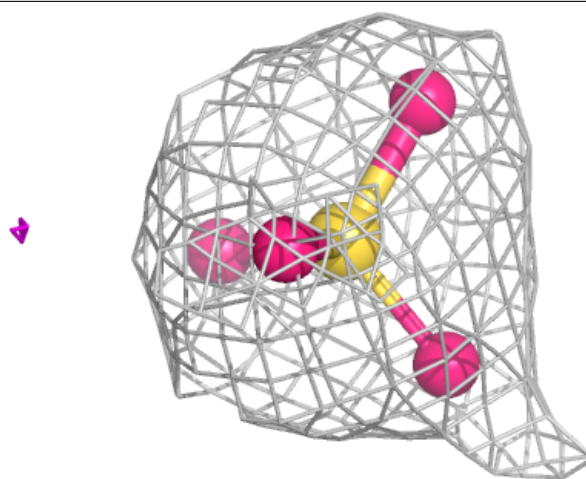
Electron density around DMS B 1106:

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



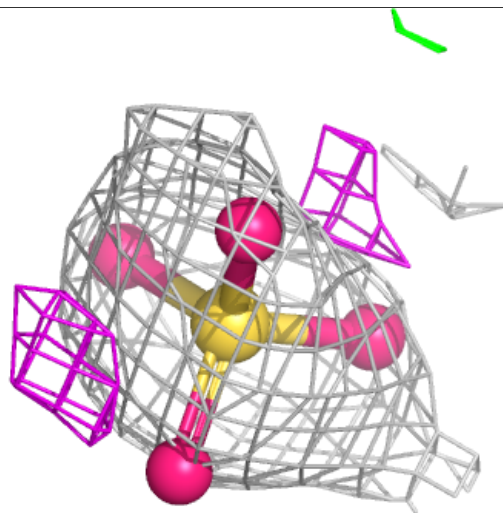
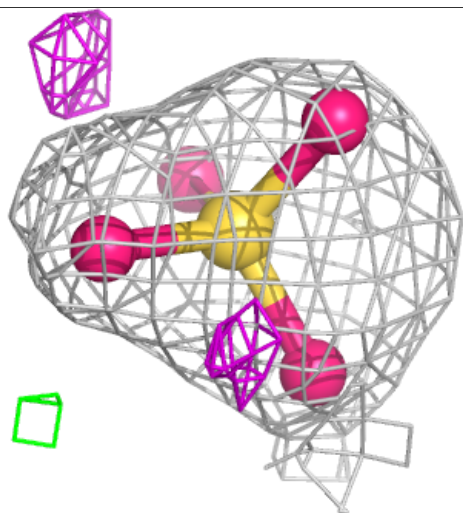
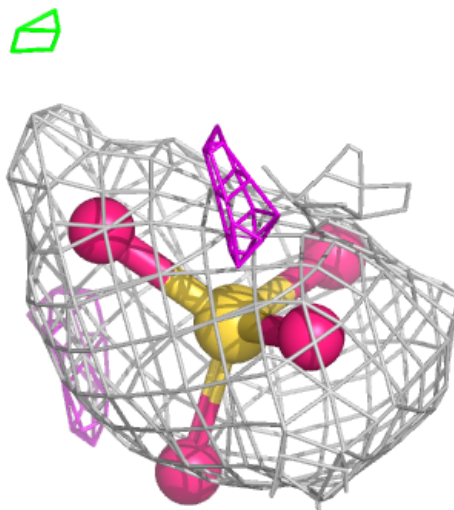
Electron density around SO4 B 1109:

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



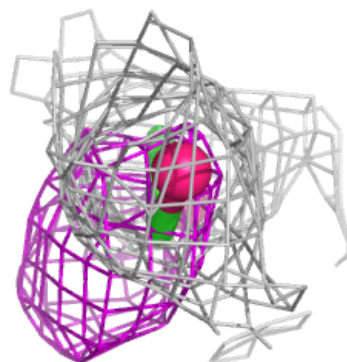
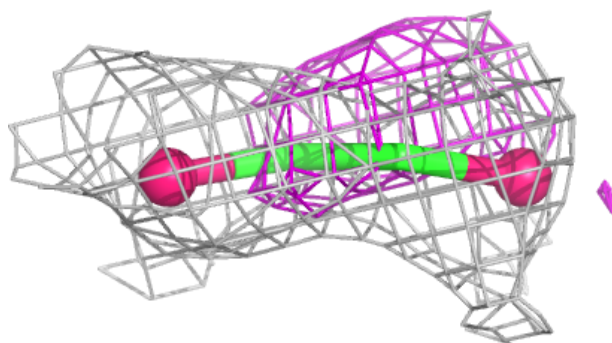
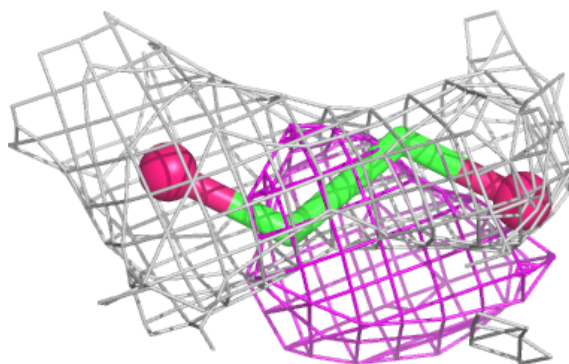
Electron density around SO4 B 1110:

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

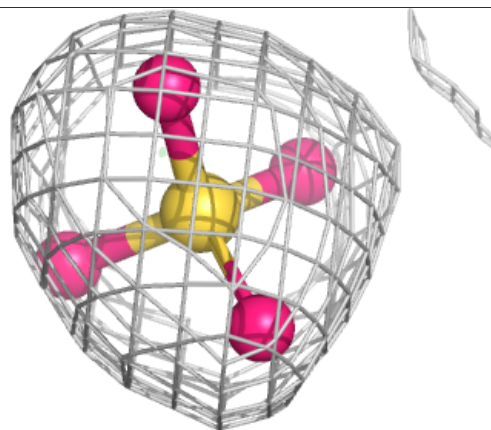
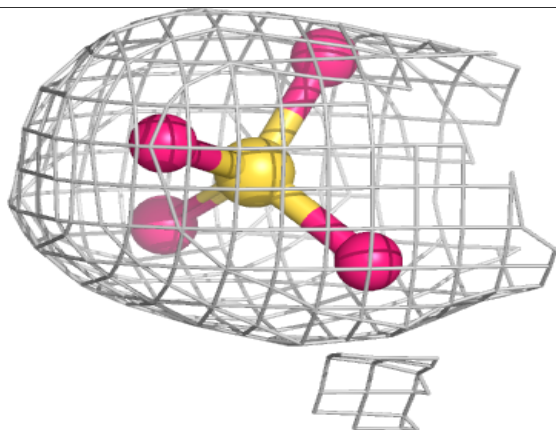
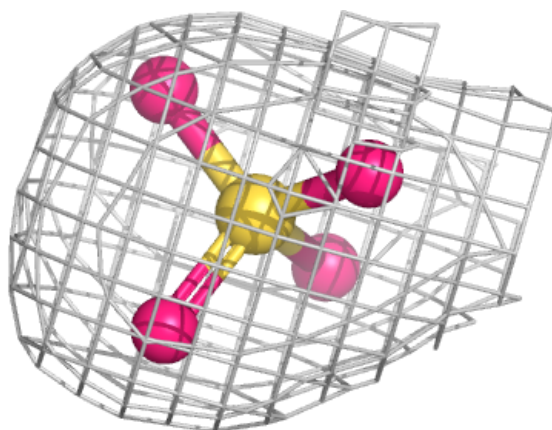


Electron density around EDO B 1104:

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

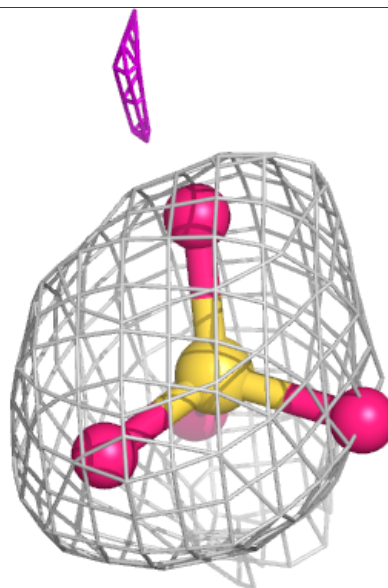
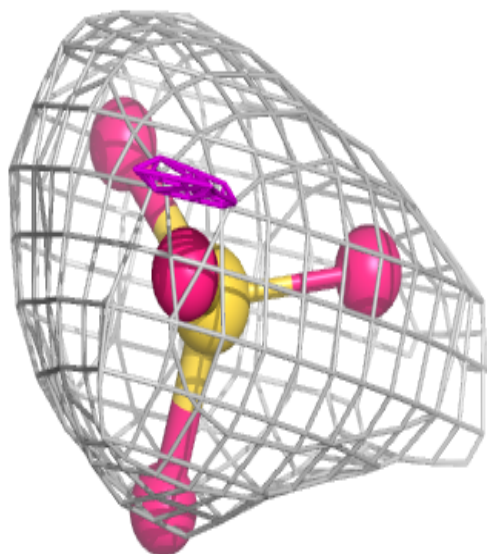
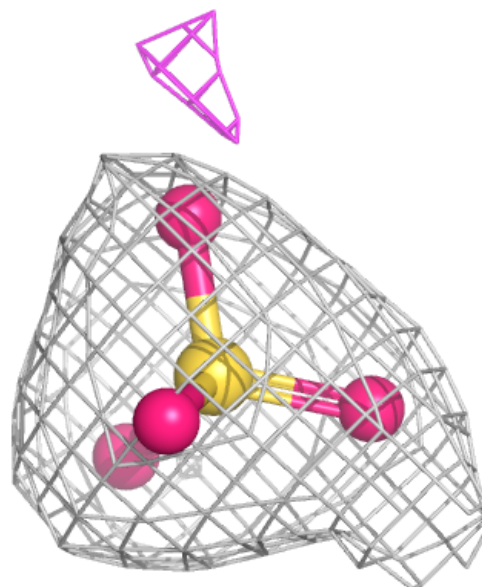
**Electron density around SO4 A 1104:**

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



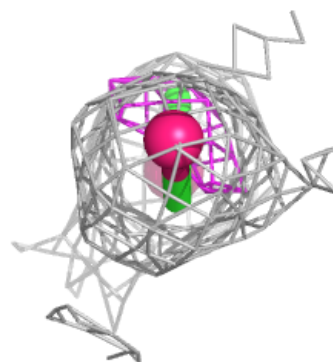
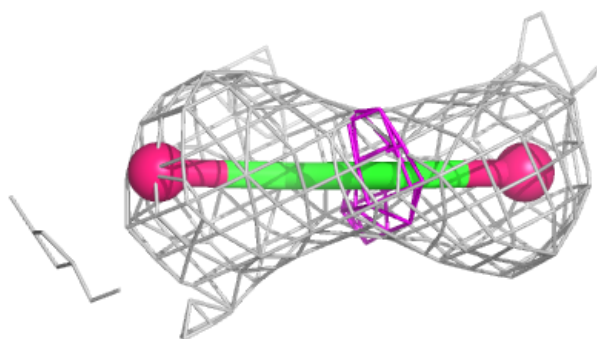
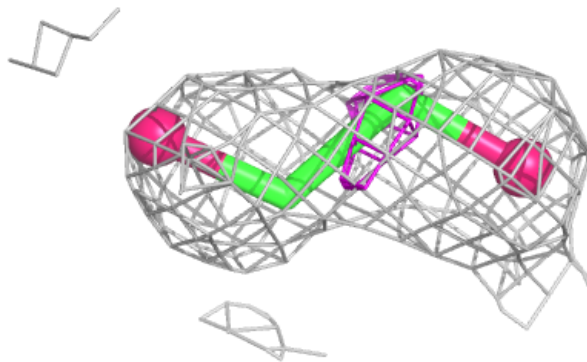
Electron density around SO4 B 1107:

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



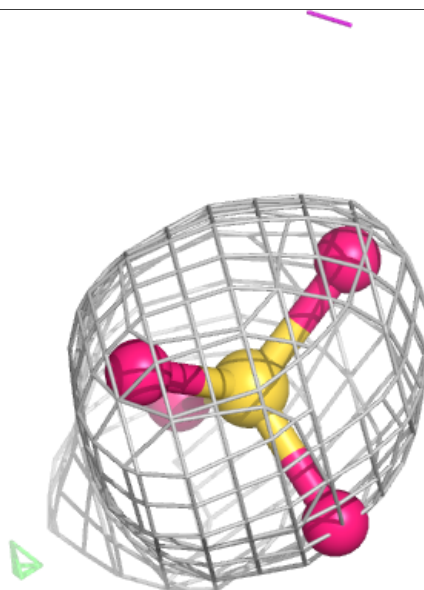
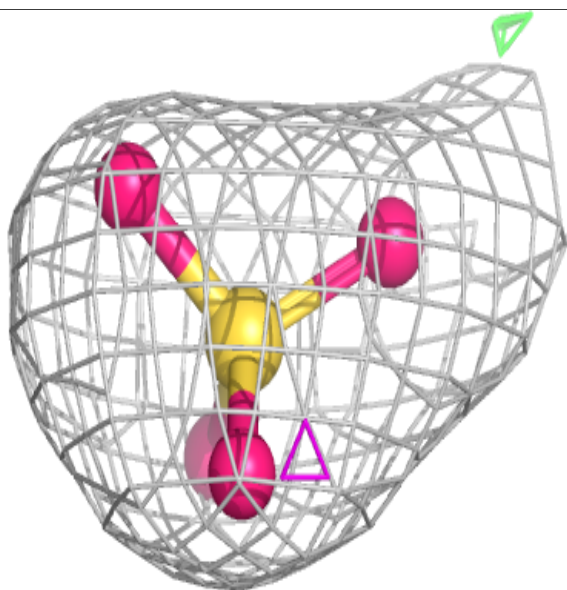
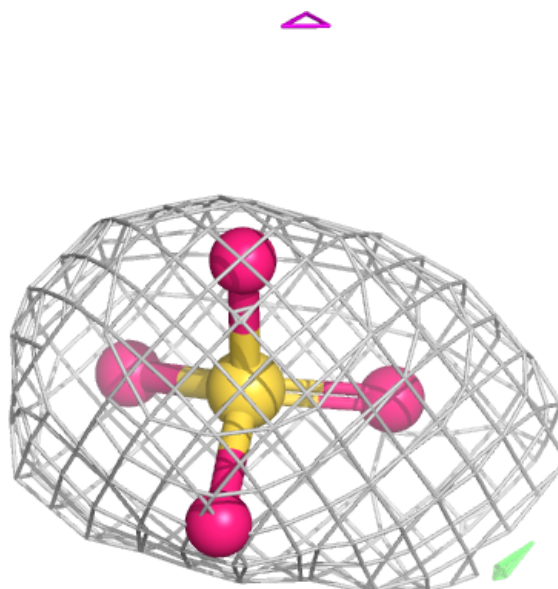
Electron density around EDO B 1105:

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



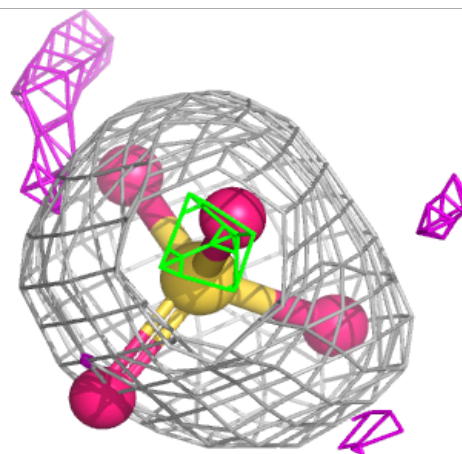
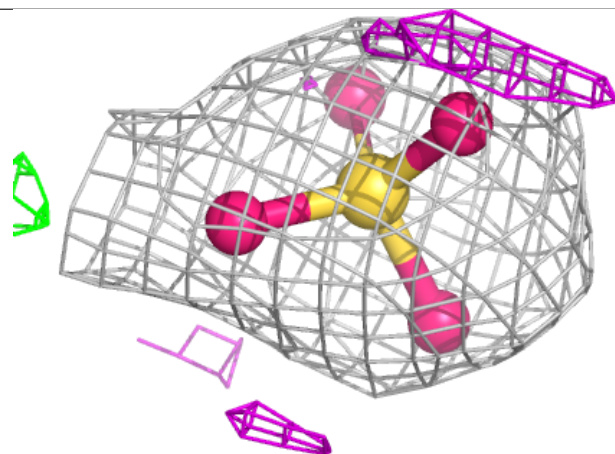
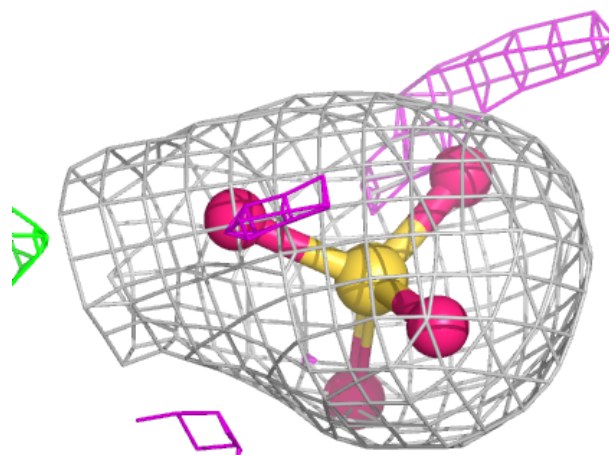
Electron density around SO4 B 1108:

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



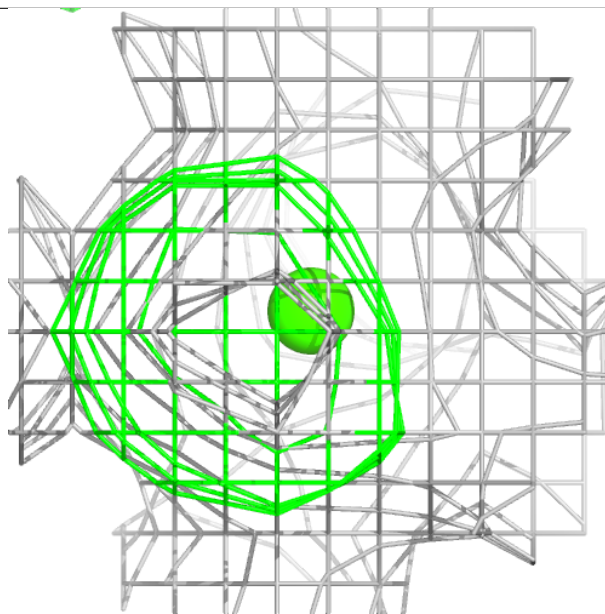
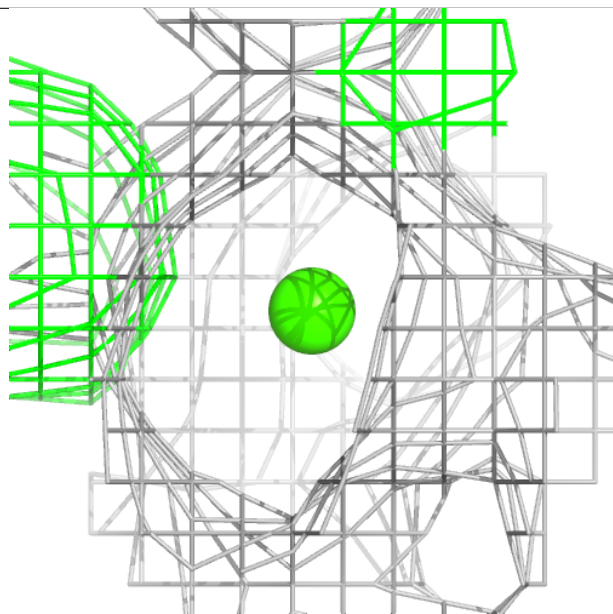
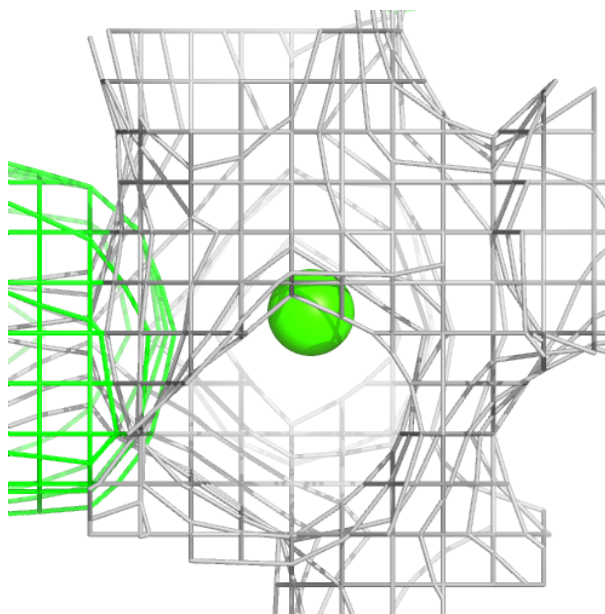
Electron density around SO4 A 1105:

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



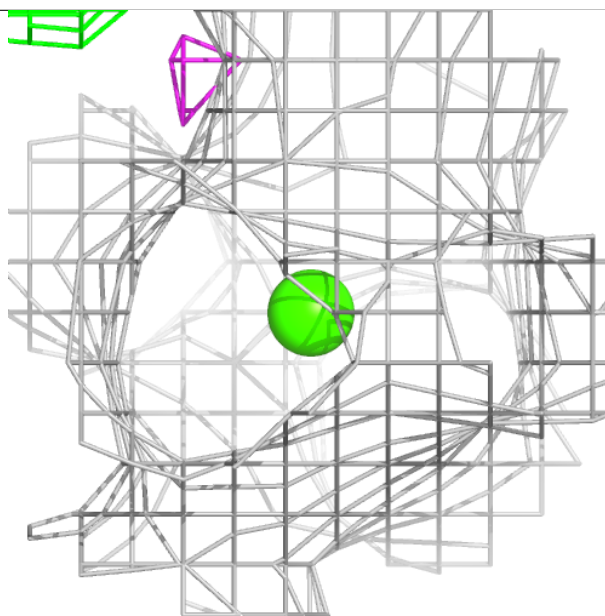
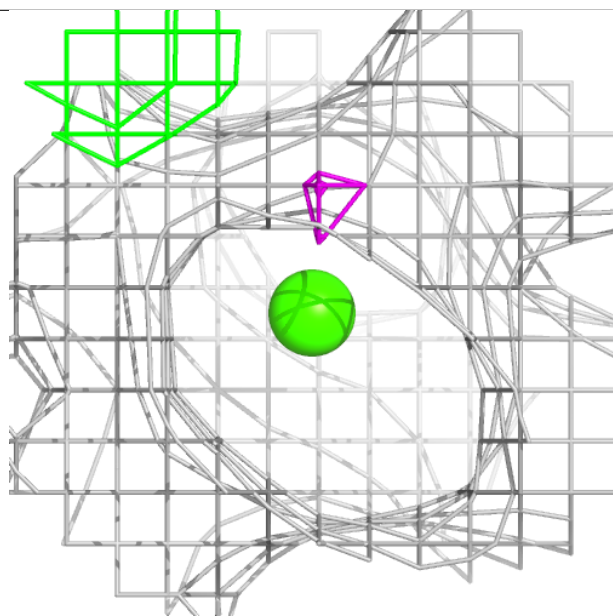
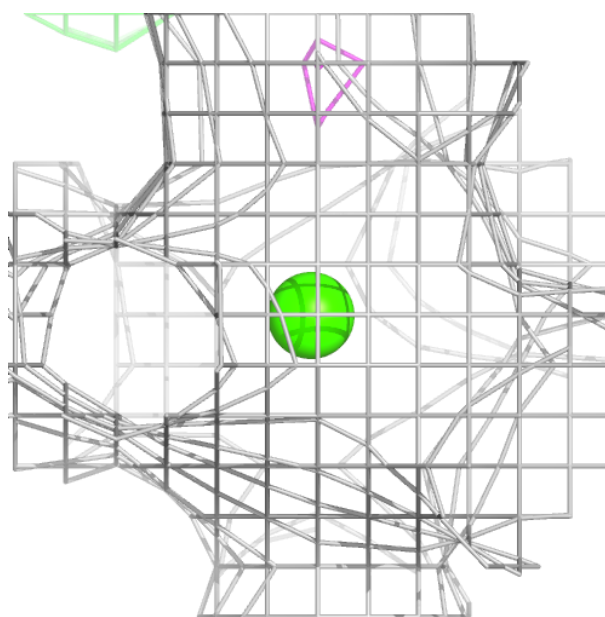
Electron density around CA B 1101:

$2mF_o-DF_c$ (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.