



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 03:40 PM EDT

PDB ID : 8OQR / pdb_00008oqr
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
in complex with Fragment-M-80
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2023-04-12
Resolution : 2.40 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

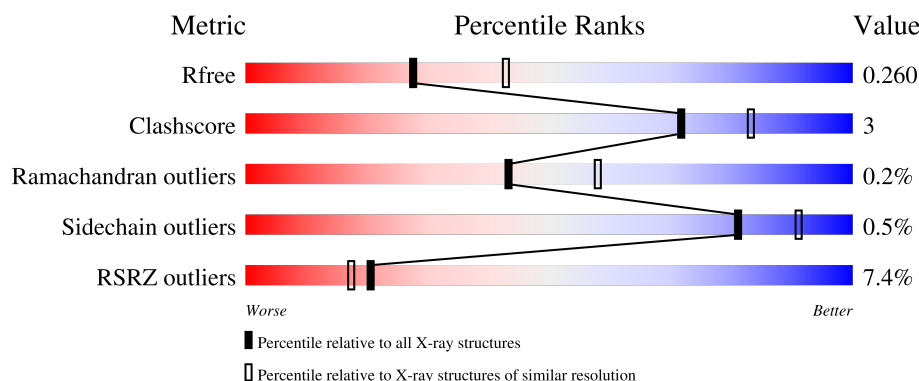
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	736	7% 92% 7%
1	B	736	7% 91% 8%
2	C	403	8% 87% 10%
2	D	403	7% 87% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17260 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 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5430	3434	936	1039	21			
1	B	728	Total	C	N	O	S	0	0	0
			5413	3424	931	1037	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	initiating methionine	UNP O53872
A	-14	GLY	-	expression tag	UNP O53872
A	-13	SER	-	expression tag	UNP O53872
A	-12	SER	-	expression tag	UNP O53872
A	-11	HIS	-	expression tag	UNP O53872
A	-10	HIS	-	expression tag	UNP O53872
A	-9	HIS	-	expression tag	UNP O53872
A	-8	HIS	-	expression tag	UNP O53872
A	-7	HIS	-	expression tag	UNP O53872
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression tag	UNP O53872
A	0	SER	-	expression tag	UNP O53872
B	-15	MET	-	initiating methionine	UNP O53872
B	-14	GLY	-	expression tag	UNP O53872
B	-13	SER	-	expression tag	UNP O53872
B	-12	SER	-	expression tag	UNP O53872
B	-11	HIS	-	expression tag	UNP O53872
B	-10	HIS	-	expression tag	UNP O53872
B	-9	HIS	-	expression tag	UNP O53872
B	-8	HIS	-	expression tag	UNP O53872
B	-7	HIS	-	expression tag	UNP O53872

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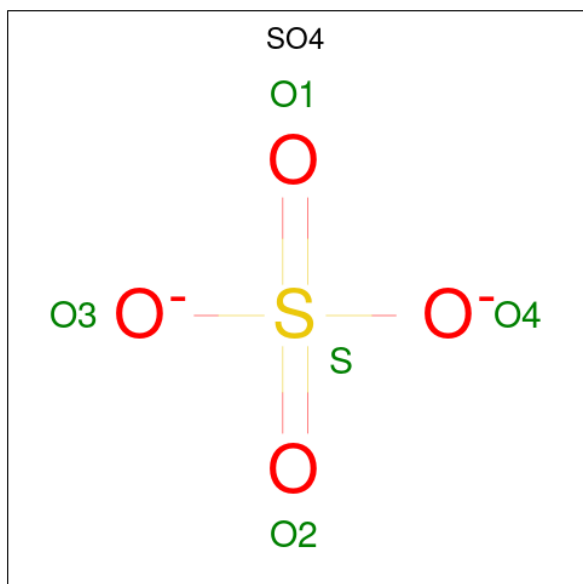
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression tag	UNP O53872
B	0	SER	-	expression tag	UNP O53872

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	391	Total	C	N	O	S	0	1	0
			2899	1810	515	560	14			
2	D	392	Total	C	N	O	S	0	0	0
			2897	1808	515	560	14			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



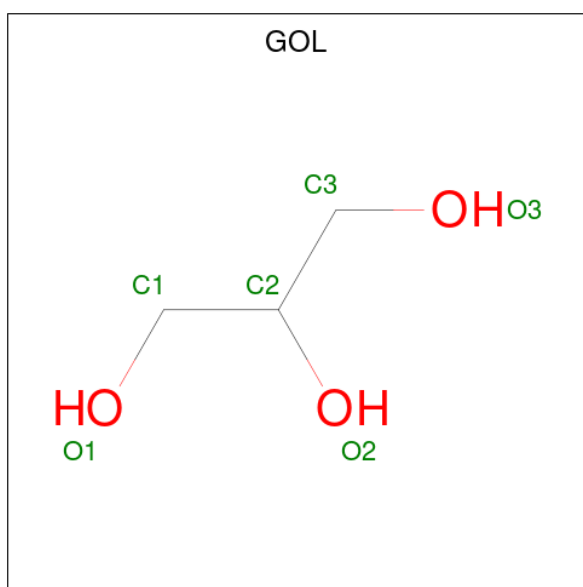
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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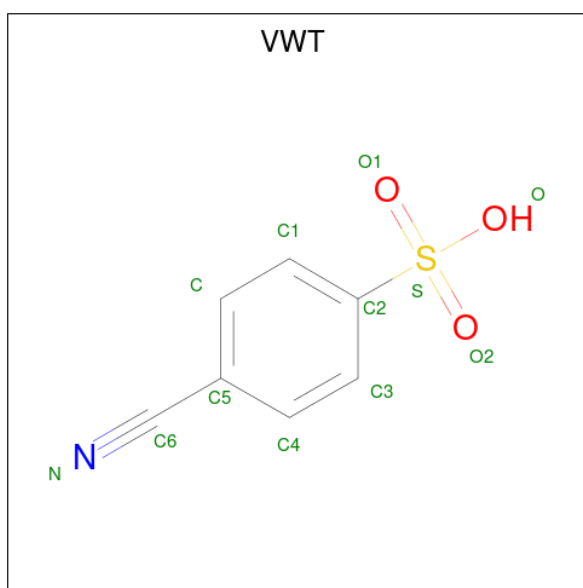
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is 4-cyanobenzenesulfonic acid (CCD ID: VWT) (formula: $C_7H_5NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O S 12 7 1 3 1	0	0
5	A	1	Total C N O S 12 7 1 3 1	0	0
5	A	1	Total C N O S 12 7 1 3 1	0	0
5	A	1	Total C N O S 12 7 1 3 1	0	0
5	B	1	Total C N O S 12 7 1 3 1	0	0
5	B	1	Total C N O S 12 7 1 3 1	0	0

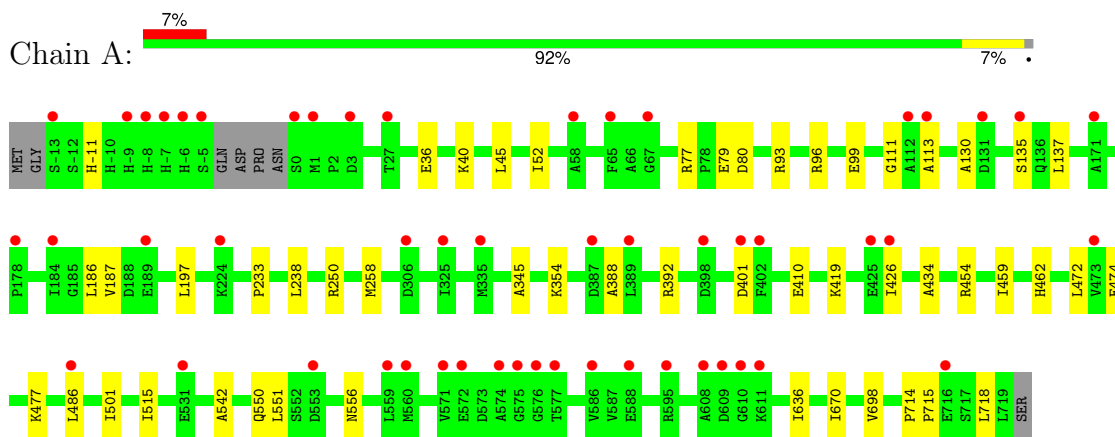
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	134	Total 134	O 134	0	0
6	B	154	Total 154	O 154	0	0
6	C	79	Total 79	O 79	0	0
6	D	77	Total 77	O 77	0	0

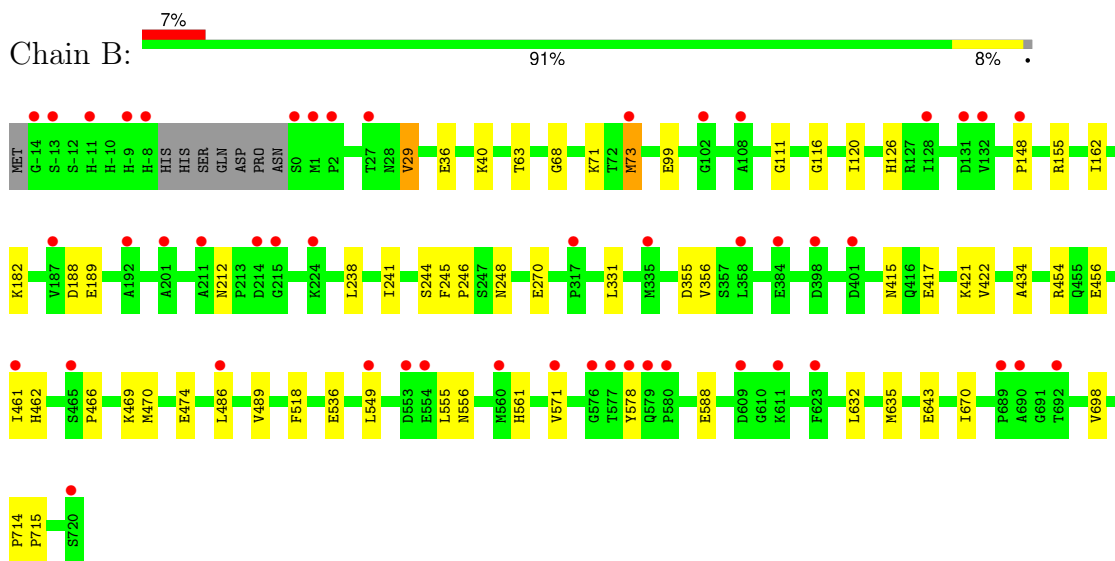
3 Residue-property plots [i](#)

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.

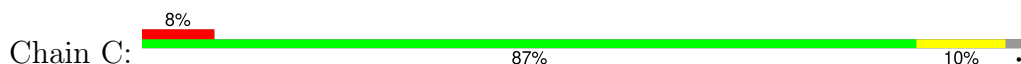
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

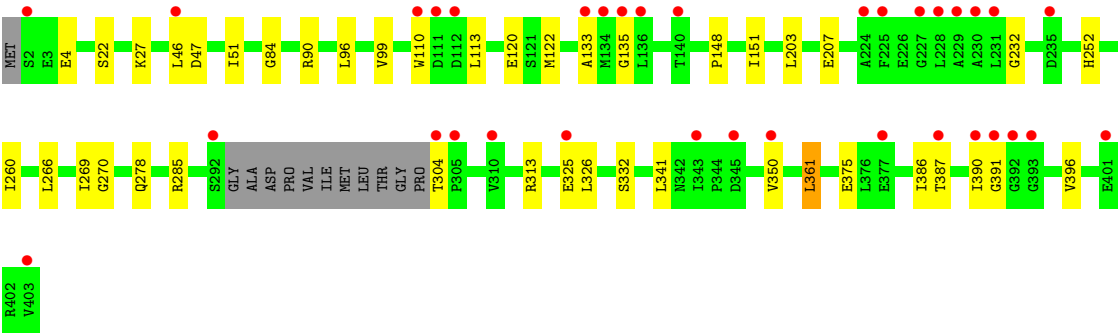


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

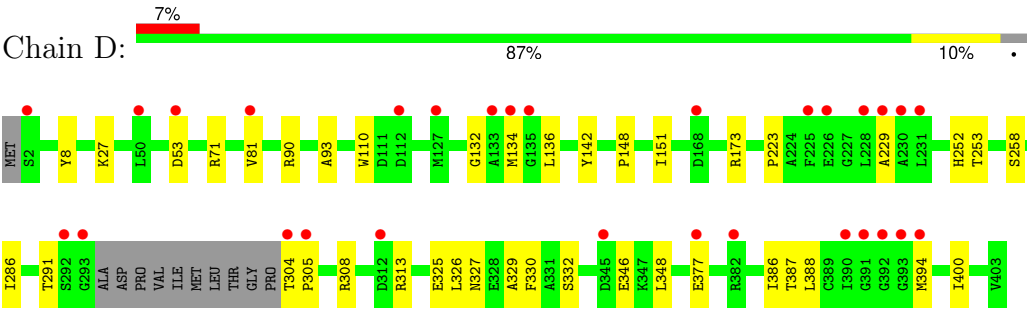


- Molecule 2: Putative acyltransferase Rv0859





● Molecule 2: Putative acyltransferase Rv0859



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	250.70Å 135.61Å 120.89Å 90.00° 110.27° 90.00°	Depositor
Resolution (Å)	47.92 – 2.40 47.92 – 2.40	Depositor EDS
% Data completeness (in resolution range)	79.9 (47.92-2.40) 79.9 (47.92-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.260 0.220 , 0.260	Depositor DCC
R_{free} test set	5817 reflections (3.93%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 34.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17260	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: SO4, VWT, GOL

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	0.11	0/5533	0.27	0/7487
1	B	0.11	0/5514	0.28	0/7461
2	C	0.12	0/2944	0.30	0/3982
2	D	0.12	0/2939	0.29	0/3975
All	All	0.11	0/16930	0.28	0/22905

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 [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	5430	0	5467	28	0
1	B	5413	0	5456	35	0
2	C	2899	0	2917	27	0
2	D	2897	0	2912	27	0
3	A	20	0	0	1	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	15	0	0	0	0
4	A	18	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	12	0	16	2	0
5	A	48	0	0	0	0
5	B	24	0	0	1	0
6	A	134	0	0	4	0
6	B	154	0	0	1	0
6	C	79	0	0	0	0
6	D	77	0	0	1	0
All	All	17260	0	16792	110	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 3.

All (110) 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)
2:D:173:ARG:NH2	2:D:348:LEU:O	2.14	0.79
2:D:148:PRO:HG2	2:D:151:ILE:HD13	1.77	0.67
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.79	0.64
1:A:477:LYS:HG3	1:A:486:LEU:HD21	1.80	0.63
1:B:63:THR:HA	1:B:111:GLY:HA3	1.80	0.63
1:B:73:MET:HE1	4:B:805:GOL:H11	1.81	0.63
1:A:250:ARG:NH1	2:D:142:TYR:O	2.32	0.62
1:B:270:GLU:HG2	2:D:27:LYS:HE2	1.82	0.62
2:C:84:GLY:HA2	2:D:394:MET:HE3	1.83	0.60
1:B:632:LEU:HA	1:B:635:MET:HE3	1.82	0.59
2:D:326:LEU:HD13	2:D:387:THR:HG23	1.84	0.59
1:A:550:GLN:NE2	6:A:902:HOH:O	2.31	0.59
2:D:93:ALA:HA	2:D:388:LEU:HD23	1.83	0.59
1:A:472:LEU:HD11	1:A:501:ILE:HG23	1.87	0.57
1:A:515:ILE:HD11	1:A:551:LEU:HD21	1.87	0.57
2:C:304:THR:HG23	2:C:341:LEU:HD11	1.87	0.57
3:A:804:SO4:O4	6:A:901:HOH:O	2.16	0.56
1:A:77:ARG:HG3	1:A:79:GLU:HG3	1.87	0.56
1:B:36:GLU:HG3	1:B:40:LYS:HE3	1.86	0.56
1:B:434:ALA:O	1:B:454:ARG:NH2	2.38	0.56
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.40	0.56
1:B:571:VAL:HG21	1:B:578:TYR:HB3	1.88	0.55
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.42	0.54
2:C:113:LEU:HD12	2:C:270:GLY:HA3	1.89	0.54
2:D:252:HIS:HE1	2:D:332:SER:H	1.55	0.53
1:A:345:ALA:O	1:A:392:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:354:LYS:NZ	6:A:909:HOH:O	2.42	0.52
1:A:459:ILE:HD11	1:A:486:LEU:HD13	1.91	0.52
1:B:212:ASN:ND2	6:B:910:HOH:O	2.41	0.52
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.91	0.52
1:A:258:MET:HG2	6:A:961:HOH:O	2.09	0.52
2:D:304:THR:HB	2:D:305:PRO:HD3	1.91	0.51
2:D:325:GLU:HB3	2:D:386:ILE:HG13	1.92	0.51
1:A:77:ARG:HG2	1:A:80:ASP:OD2	2.11	0.51
2:C:4:GLU:OE2	2:C:285:ARG:NH1	2.44	0.51
2:D:8:TYR:OH	2:D:271:SER:O	2.25	0.51
2:C:203:LEU:HD11	2:C:207:GLU:HG3	1.93	0.50
2:C:148:PRO:HD2	2:C:151:ILE:HD13	1.94	0.49
1:B:417:GLU:O	1:B:421:LYS:HG2	2.13	0.49
2:C:133:ALA:C	2:C:135:GLY:H	2.20	0.48
1:B:466:PRO:HD2	1:B:470:MET:HE2	1.95	0.48
1:B:126:HIS:NE2	1:B:189:GLU:OE2	2.33	0.48
1:A:434:ALA:O	1:A:454:ARG:NH1	2.46	0.48
1:B:73:MET:HE2	5:B:808:VWT:N	2.29	0.47
1:B:355:ASP:OD1	1:B:356:VAL:N	2.42	0.47
1:A:111:GLY:O	1:A:135:SER:OG	2.25	0.47
1:A:233:PRO:HA	1:A:238:LEU:HD23	1.97	0.47
1:B:241:ILE:O	1:B:244:SER:OG	2.29	0.47
1:A:130:ALA:HB2	1:A:197:LEU:HD11	1.97	0.47
1:A:96:ARG:NH1	1:A:99:GLU:OE2	2.44	0.47
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.97	0.46
2:C:252:HIS:HE1	2:C:332:SER:H	1.63	0.46
1:B:331:LEU:HD13	1:B:422:VAL:HG12	1.97	0.46
2:D:223:PRO:HA	2:D:253:THR:HG22	1.98	0.46
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.96	0.46
1:A:113:ALA:HB3	1:A:137:LEU:HD22	1.96	0.46
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.98	0.46
1:B:536:GLU:CD	1:B:549:LEU:HB2	2.41	0.45
2:C:326:LEU:HD13	2:C:387:THR:HG23	1.99	0.45
1:B:71:LYS:H	1:B:71:LYS:HD2	1.82	0.45
1:B:456:GLU:H	1:B:456:GLU:CD	2.25	0.45
2:C:51:ILE:HG12	2:C:113:LEU:HD23	1.99	0.45
1:A:715:PRO:HD2	1:A:718:LEU:HD12	1.98	0.44
1:B:461:ILE:HG12	1:B:489:VAL:HG11	1.99	0.44
2:D:308:ARG:NH2	6:D:601:HOH:O	2.27	0.44
2:C:390:ILE:HG12	2:C:391:GLY:H	1.83	0.44
2:D:286:ILE:HD13	2:D:400:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:325:GLU:HB3	2:C:386:ILE:HG13	1.99	0.43
2:D:252:HIS:CE1	2:D:330:PHE:HB3	2.53	0.43
1:B:162:ILE:HD12	1:B:238:LEU:HD21	2.00	0.43
2:C:266:LEU:HD23	2:C:266:LEU:HA	1.90	0.43
2:C:22:SER:OG	2:C:207:GLU:OE2	2.32	0.43
1:A:542:ALA:HB2	1:A:636:ILE:HG23	1.99	0.43
2:C:122:MET:HE2	2:C:260:ILE:HG23	2.00	0.43
1:B:116:GLY:O	1:B:120:ILE:HG12	2.18	0.43
1:A:698:VAL:HG13	1:A:714:PRO:HG3	2.01	0.43
1:B:248:ASN:OD1	2:C:232:GLY:HA2	2.18	0.43
1:A:388:ALA:O	1:A:392:ARG:HG3	2.19	0.43
1:B:245:PHE:HB2	1:B:246:PRO:HD3	2.00	0.42
2:C:47:ASP:HB3	2:C:278:GLN:HE22	1.84	0.42
1:B:466:PRO:HG2	1:B:469:LYS:HB2	2.01	0.42
1:A:-11:HIS:CD2	1:A:93:ARG:HG2	2.54	0.42
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.45	0.42
2:D:346:GLU:H	2:D:346:GLU:CD	2.28	0.42
2:D:71:ARG:HH22	2:D:81:VAL:HG13	1.83	0.42
2:C:27:LYS:NZ	2:D:136:LEU:O	2.53	0.42
2:C:46:LEU:HD12	2:C:278:GLN:HB3	2.02	0.42
1:B:29:VAL:HG13	1:B:68:GLY:HA2	2.02	0.41
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.88	0.41
2:D:252:HIS:CE1	2:D:332:SER:H	2.37	0.41
1:A:45:LEU:HD23	1:A:52:ILE:HD13	2.02	0.41
1:B:469:LYS:HB3	1:B:469:LYS:HE2	1.80	0.41
2:D:327:ASN:HB2	2:D:388:LEU:HD12	2.01	0.41
1:B:555:LEU:HD22	4:B:806:GOL:H2	2.03	0.41
1:A:426:ILE:HD13	1:A:426:ILE:HA	1.87	0.41
2:C:90:ARG:HH22	2:D:53:ASP:CG	2.28	0.41
2:D:90:ARG:NH1	2:D:291:THR:HG21	2.35	0.41
2:D:132:GLY:C	2:D:134:MET:H	2.29	0.41
2:D:258:SER:HB3	2:D:329:ALA:HA	2.02	0.41
1:B:182:LYS:NZ	1:B:188:ASP:O	2.53	0.41
2:D:93:ALA:HA	2:D:388:LEU:CD2	2.51	0.41
1:B:561:HIS:NE2	1:B:588:GLU:OE2	2.54	0.41
2:C:350:VAL:HG21	2:C:375:GLU:HG2	2.03	0.41
1:B:99:GLU:CD	1:B:155:ARG:HH21	2.28	0.40
1:B:415:ASN:OD1	1:B:417:GLU:HG2	2.20	0.40
2:C:133:ALA:C	2:C:135:GLY:N	2.79	0.40
1:A:410:GLU:OE2	1:A:419:LYS:NZ	2.50	0.40
2:C:120:GLU:HG2	2:C:361:LEU:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.98	0.40
2:C:96:LEU:HD23	2:C:396:VAL:HG13	2.02	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	725/736 (98%)	697 (96%)	27 (4%)	1 (0%)	48 64
1	B	724/736 (98%)	702 (97%)	20 (3%)	2 (0%)	36 50
2	C	388/403 (96%)	371 (96%)	16 (4%)	1 (0%)	36 50
2	D	388/403 (96%)	378 (97%)	9 (2%)	1 (0%)	36 50
All	All	2225/2278 (98%)	2148 (96%)	72 (3%)	5 (0%)	43 58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	229	ALA
1	A	556	ASN
1	B	556	ASN
1	B	148	PRO

5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/566 (99%)	557 (100%)	3 (0%)	81	91
1	B	558/566 (99%)	554 (99%)	4 (1%)	76	88
2	C	302/310 (97%)	302 (100%)	0	100	100
2	D	301/310 (97%)	300 (100%)	1 (0%)	86	93
All	All	1721/1752 (98%)	1713 (100%)	8 (0%)	81	91

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

Mol	Chain	Res	Type
1	A	187	VAL
1	A	401	ASP
1	A	670	ILE
1	B	29	VAL
1	B	73	MET
1	B	486	LEU
1	B	670	ILE
2	D	377	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	-9	HIS
1	A	-6	HIS
1	A	75	GLN
1	A	455	GLN
1	B	294	GLN
1	B	383	GLN
2	C	43	HIS
2	D	104	GLN
2	D	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

26 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	D	503	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	803	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	804	-	4,4,4	0.25	0	6,6,6	0.10	0
4	GOL	A	806	-	5,5,5	0.95	0	5,5,5	1.05	0
5	VWT	A	811	-	12,12,12	0.30	0	17,17,17	0.20	0
5	VWT	B	807	-	12,12,12	0.28	0	17,17,17	0.21	0
4	GOL	B	806	-	5,5,5	0.92	0	5,5,5	1.06	0
3	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	502	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	801	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	A	804	-	4,4,4	0.25	0	6,6,6	0.08	0
4	GOL	A	805	-	5,5,5	0.89	0	5,5,5	1.08	0
4	GOL	A	807	-	5,5,5	0.91	0	5,5,5	1.08	0
5	VWT	A	808	-	12,12,12	0.35	0	17,17,17	0.22	0
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.06	0
5	VWT	A	810	-	12,12,12	0.26	0	17,17,17	0.21	0
3	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.10	0
3	SO4	D	501	-	4,4,4	0.25	0	6,6,6	0.06	0
4	GOL	B	805	-	5,5,5	0.94	0	5,5,5	1.05	0
3	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
5	VWT	A	809	-	12,12,12	0.30	0	17,17,17	0.22	0
3	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.06	0
5	VWT	B	808	-	12,12,12	0.20	0	17,17,17	0.22	0
3	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	801	-	4,4,4	0.23	0	6,6,6	0.21	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	805	-	-	1/4/4/4	-
5	VWT	A	810	-	-	0/8/8/8	0/1/1/1
5	VWT	A	809	-	-	0/8/8/8	0/1/1/1
4	GOL	A	806	-	-	2/4/4/4	-
5	VWT	A	811	-	-	0/8/8/8	0/1/1/1
4	GOL	A	805	-	-	2/4/4/4	-
4	GOL	A	807	-	-	0/4/4/4	-
5	VWT	A	808	-	-	1/8/8/8	0/1/1/1
5	VWT	B	807	-	-	0/8/8/8	0/1/1/1
5	VWT	B	808	-	-	1/8/8/8	0/1/1/1
4	GOL	B	806	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	805	GOL	C1-C2-C3-O3
4	A	806	GOL	C1-C2-C3-O3
4	A	805	GOL	O2-C2-C3-O3
4	A	806	GOL	O2-C2-C3-O3
4	B	805	GOL	O1-C1-C2-O2
5	B	808	VWT	C3-C2-S-O
5	A	808	VWT	C3-C2-S-O

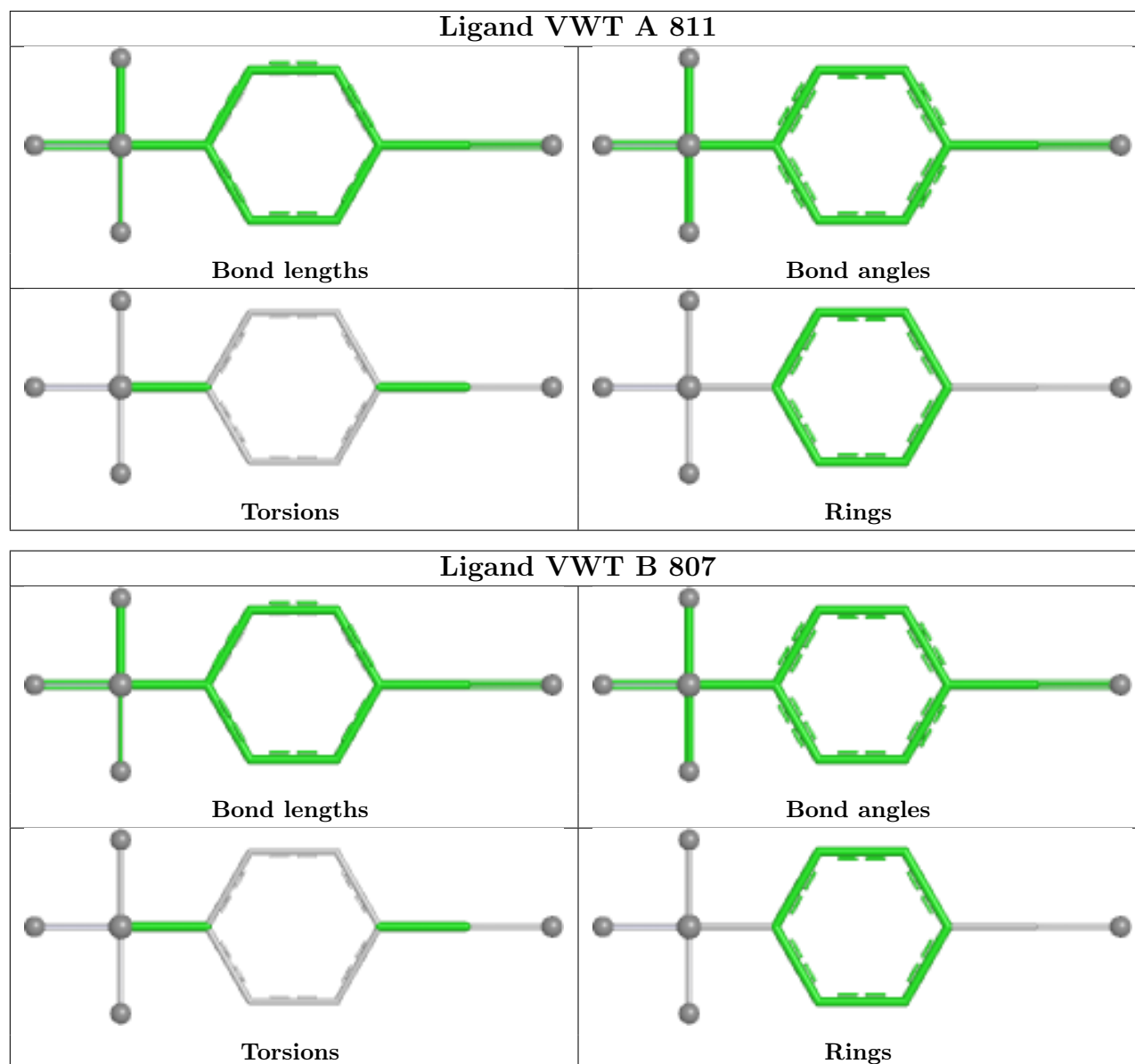
There are no ring outliers.

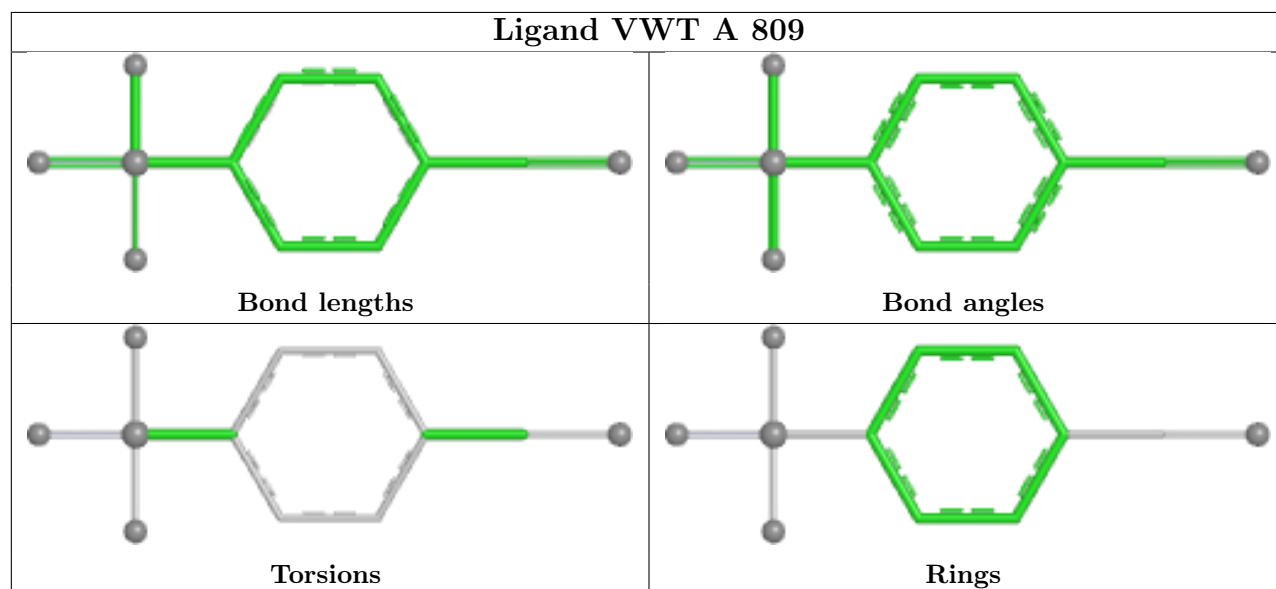
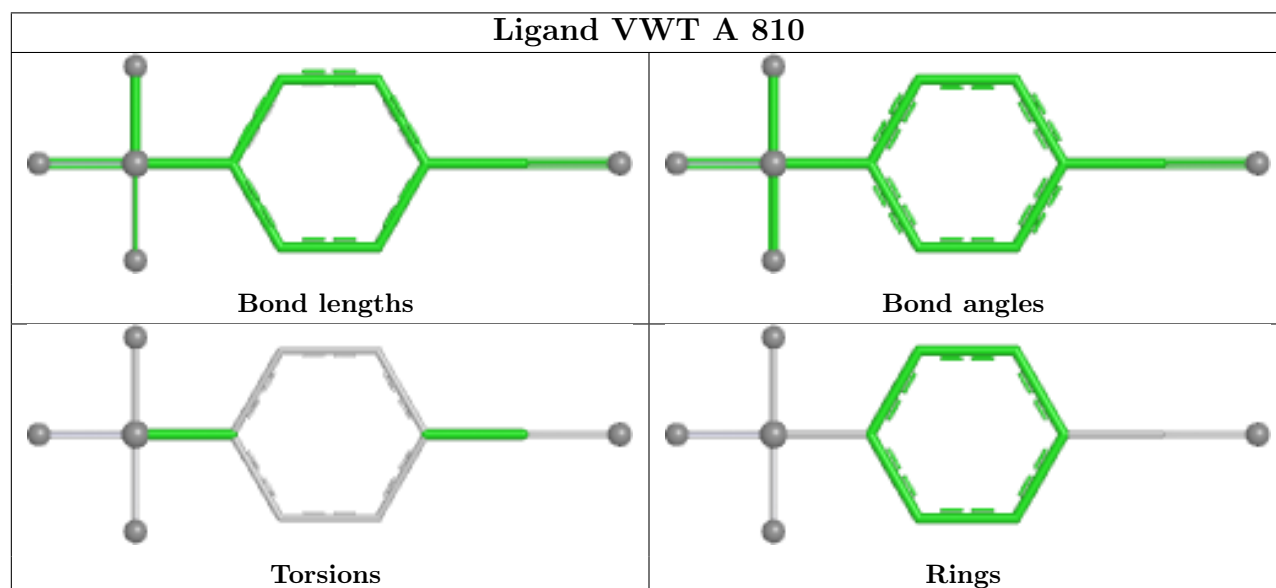
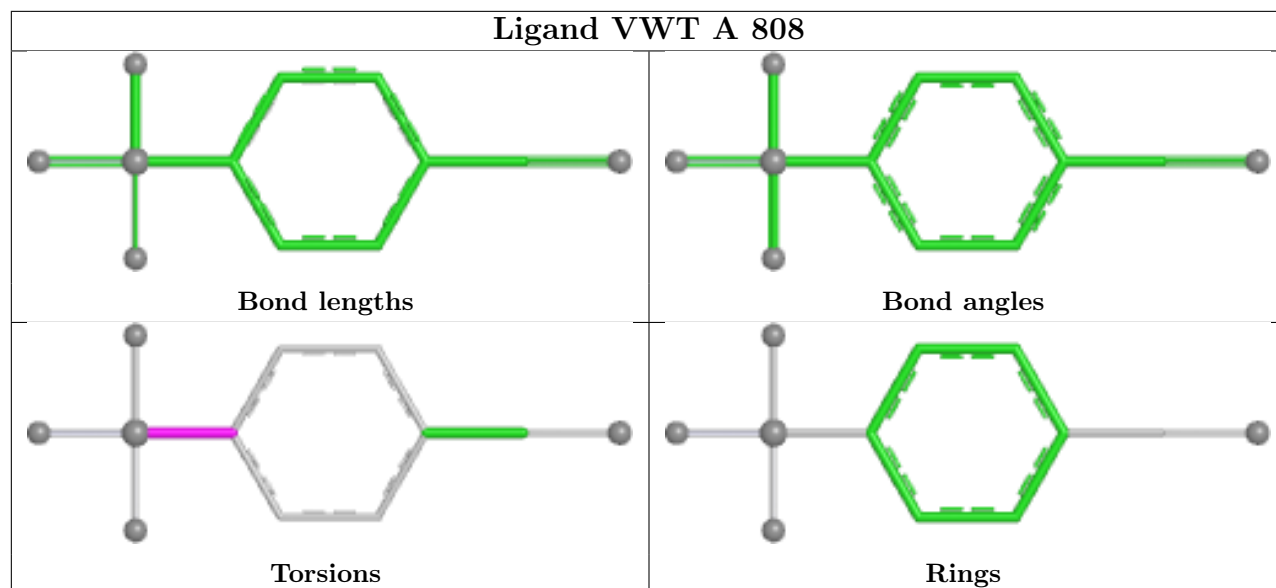
4 monomers are involved in 4 short contacts:

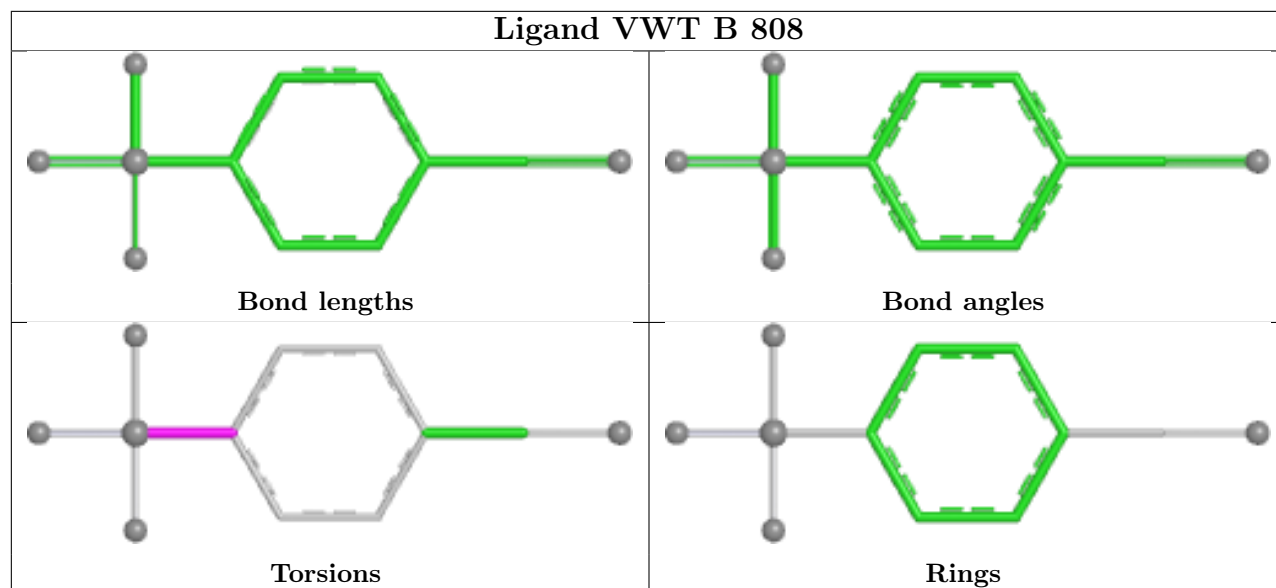
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	806	GOL	1	0
3	A	804	SO4	1	0
4	B	805	GOL	1	0
5	B	808	VWT	1	0

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	729/736 (99%)	0.67	52 (7%)	22	18	25, 47, 77, 117	0
1	B	728/736 (98%)	0.56	49 (6%)	24	20	25, 43, 72, 122	0
2	C	391/403 (97%)	0.75	34 (8%)	16	13	30, 44, 74, 136	1 (0%)
2	D	392/403 (97%)	0.69	30 (7%)	19	16	26, 44, 71, 133	0
All	All	2240/2278 (98%)	0.65	165 (7%)	20	17	25, 45, 75, 136	1 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	392	GLY	9.1
2	C	134	MET	8.8
1	B	578	TYR	8.0
1	B	577	THR	7.3
1	A	577	THR	6.1
1	B	720	SER	6.0
1	A	576	GLY	5.9
2	D	228	LEU	5.8
2	D	304	THR	5.7
1	A	575	GLY	5.5
1	B	-14	GLY	5.3
2	D	225	PHE	4.9
1	A	-5	SER	4.8
2	C	231	LEU	4.8
2	D	390	ILE	4.7
2	C	393	GLY	4.5
1	A	3	ASP	4.5
2	D	293	GLY	4.4
2	D	230	ALA	4.4
1	B	579	GLN	4.3
2	D	391	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	225	PHE	4.2
1	B	-8	HIS	4.2
2	C	304	THR	4.1
2	C	391	GLY	4.1
1	A	574	ALA	4.1
2	D	392	GLY	4.1
1	A	-13	SER	3.9
2	C	136	LEU	3.9
2	D	81	VAL	3.8
1	A	-9	HIS	3.7
1	A	113	ALA	3.7
1	A	486	LEU	3.7
2	C	390	ILE	3.7
1	B	131	ASP	3.7
1	B	486	LEU	3.6
1	B	576	GLY	3.6
2	D	231	LEU	3.6
2	D	393	GLY	3.5
2	D	112	ASP	3.5
1	B	1	MET	3.5
2	C	2	SER	3.5
1	B	571	VAL	3.4
1	A	426	ILE	3.4
2	D	226	GLU	3.4
1	A	559	LEU	3.3
1	A	389	LEU	3.3
2	C	325	GLU	3.3
2	C	292	SER	3.3
1	A	224	LYS	3.3
2	D	305	PRO	3.3
2	D	229	ALA	3.3
2	C	229	ALA	3.2
1	B	-13	SER	3.2
2	D	382	ARG	3.2
1	B	-11	HIS	3.2
2	C	228	LEU	3.2
2	D	2	SER	3.2
1	A	1	MET	3.1
1	A	571	VAL	3.1
2	C	227	GLY	3.1
1	A	306	ASP	3.1
2	C	111	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
2	C	112	ASP	3.1
1	B	0	SER	3.0
1	B	-9	HIS	3.0
2	D	135	GLY	3.0
1	B	609	ASP	2.9
2	C	305	PRO	2.9
1	A	611	LYS	2.9
2	D	394	MET	2.9
2	D	168	ASP	2.8
1	A	-7	HIS	2.8
2	C	230	ALA	2.8
1	B	317	PRO	2.8
2	C	387	THR	2.7
2	D	134	MET	2.7
1	B	102	GLY	2.7
1	A	184	ILE	2.7
2	D	345	ASP	2.7
1	B	128	ILE	2.6
1	B	580	PRO	2.6
1	B	465	SER	2.6
1	A	335	MET	2.6
1	B	187	VAL	2.6
2	C	133	ALA	2.6
1	A	178	PRO	2.5
2	C	403	VAL	2.5
1	A	0	SER	2.5
1	B	692	THR	2.5
1	A	65	PHE	2.5
1	A	171	ALA	2.5
1	A	608	ALA	2.5
1	B	27	THR	2.5
1	B	2	PRO	2.5
1	A	387	ASP	2.5
2	C	401	GLU	2.4
1	A	401	ASP	2.4
1	A	402	PHE	2.4
1	B	623	PHE	2.4
1	A	425	GLU	2.4
1	A	588	GLU	2.4
2	D	50	LEU	2.4
1	B	192	ALA	2.4
1	B	689	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	553	ASP	2.4
1	A	609	ASP	2.4
1	A	189	GLU	2.4
2	D	377	GLU	2.4
2	D	279	GLY	2.4
1	B	690	ALA	2.4
2	D	133	ALA	2.4
2	C	377	GLU	2.3
2	D	292	SER	2.3
1	A	67	GLY	2.3
1	B	553	ASP	2.3
1	A	572	GLU	2.3
1	B	384	GLU	2.3
1	B	549	LEU	2.3
1	A	112	ALA	2.3
1	B	215	GLY	2.3
2	C	135	GLY	2.3
1	B	398	ASP	2.3
1	B	132	VAL	2.3
1	A	560	MET	2.2
2	C	46	LEU	2.2
1	A	58	ALA	2.2
1	B	201	ALA	2.2
1	A	135	SER	2.2
1	B	401	ASP	2.2
2	D	53	ASP	2.2
1	A	595	ARG	2.2
1	A	586	VAL	2.2
1	B	461	ILE	2.2
2	C	310	VAL	2.2
1	A	-8	HIS	2.2
1	A	-6	HIS	2.2
1	A	398	ASP	2.2
1	B	611	LYS	2.2
2	C	350	VAL	2.1
1	B	73	MET	2.1
1	B	554	GLU	2.1
1	B	214	ASP	2.1
1	B	335	MET	2.1
1	B	211	ALA	2.1
1	A	131	ASP	2.1
2	D	312	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	127	MET	2.1
1	A	473	VAL	2.1
1	A	610	GLY	2.1
1	B	224	LYS	2.1
2	C	235	ASP	2.1
1	A	27	THR	2.1
1	A	716	GLU	2.1
2	C	343	ILE	2.1
1	B	148	PRO	2.1
2	C	224	ALA	2.0
2	C	140	THR	2.0
1	B	560	MET	2.0
1	B	108	ALA	2.0
1	A	531	GLU	2.0
1	B	358	LEU	2.0
1	A	325	ILE	2.0
2	C	110	TRP	2.0
2	C	345	ASP	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 oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.61	0.11	86,95,117,126	0
3	SO4	A	804	5/5	0.63	0.16	42,48,57,61	5
3	SO4	B	802	5/5	0.69	0.12	65,78,102,109	0
3	SO4	A	802	5/5	0.71	0.10	101,106,119,131	0
3	SO4	C	502	5/5	0.72	0.11	84,84,110,122	0

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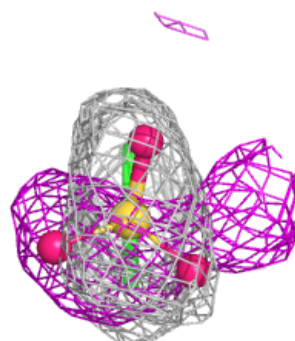
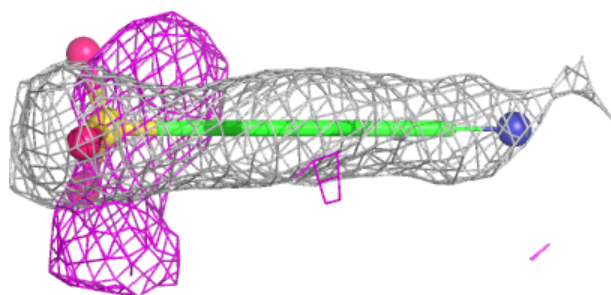
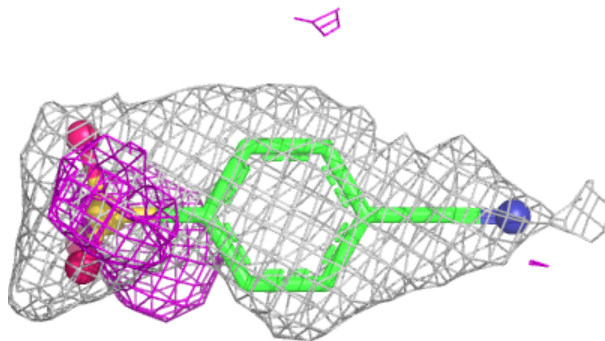
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	VWT	B	807	12/12	0.72	0.18	47,55,82,100	0
3	SO4	D	502	5/5	0.73	0.12	81,93,120,137	0
3	SO4	B	804	5/5	0.74	0.15	49,55,62,71	5
4	GOL	A	806	6/6	0.76	0.29	51,57,69,71	0
3	SO4	D	501	5/5	0.78	0.10	74,75,94,96	0
4	GOL	A	805	6/6	0.78	0.18	56,60,74,92	0
5	VWT	A	809	12/12	0.80	0.21	65,73,95,98	0
5	VWT	A	808	12/12	0.81	0.17	51,62,79,83	0
3	SO4	B	803	5/5	0.81	0.16	38,50,60,63	5
4	GOL	A	807	6/6	0.81	0.22	47,57,64,64	0
3	SO4	C	503	5/5	0.82	0.09	81,85,105,115	0
3	SO4	A	803	5/5	0.86	0.21	65,69,78,85	0
4	GOL	B	805	6/6	0.86	0.20	45,51,55,61	0
4	GOL	B	806	6/6	0.86	0.19	39,53,54,64	0
5	VWT	B	808	12/12	0.87	0.17	63,69,77,80	0
3	SO4	A	801	5/5	0.88	0.15	53,62,70,71	0
3	SO4	D	503	5/5	0.90	0.13	62,69,74,76	0
3	SO4	C	501	5/5	0.91	0.14	50,71,74,80	0
5	VWT	A	810	12/12	0.92	0.11	38,48,54,56	0
3	SO4	B	801	5/5	0.93	0.12	37,37,58,62	0
5	VWT	A	811	12/12	0.96	0.08	36,49,52,55	0

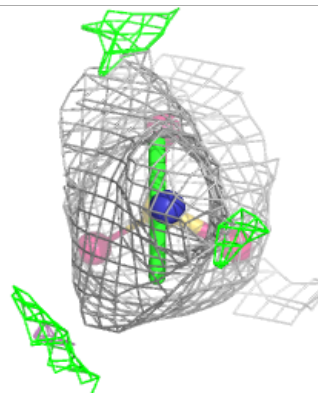
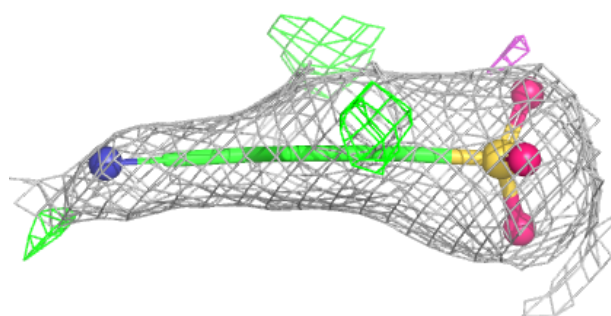
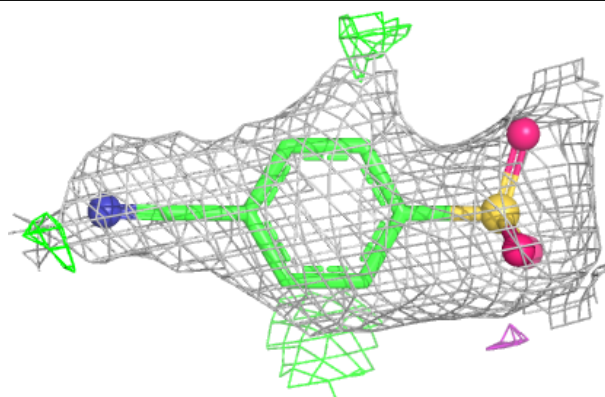
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VWT B 807:

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

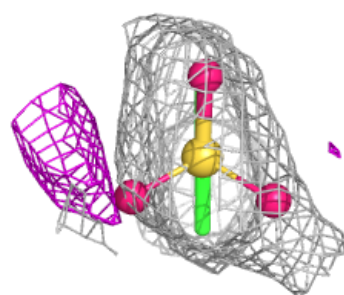
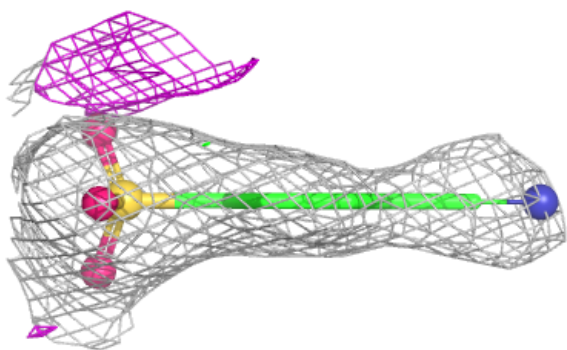
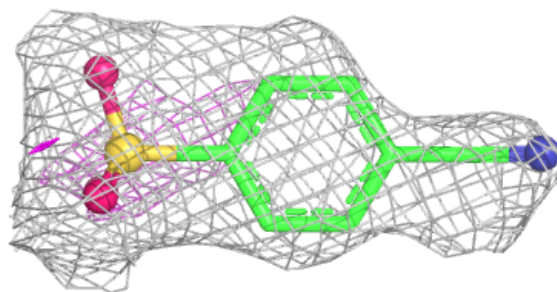
**Electron density around VWT A 809:**

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

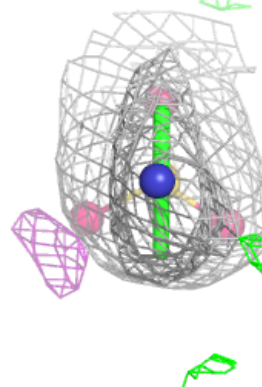
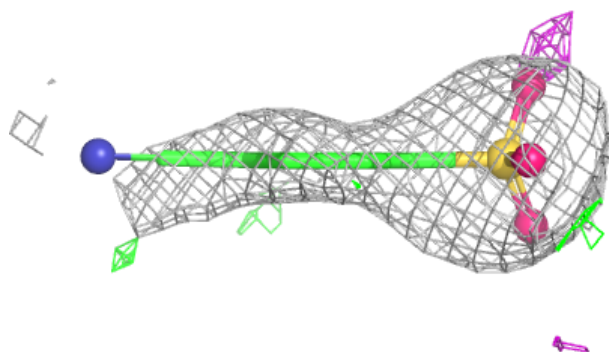
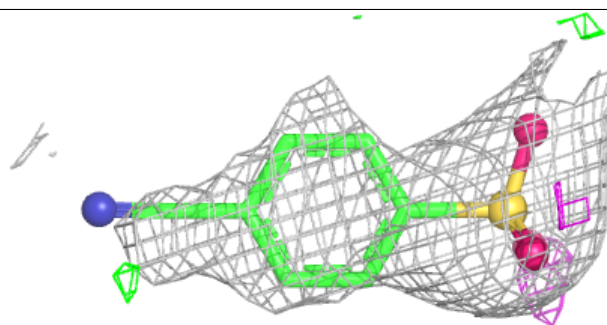


Electron density around VWT A 808:

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

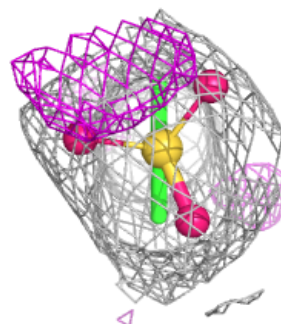
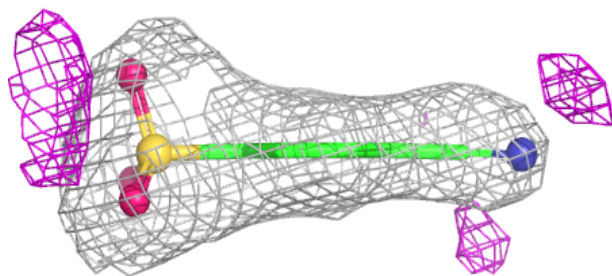
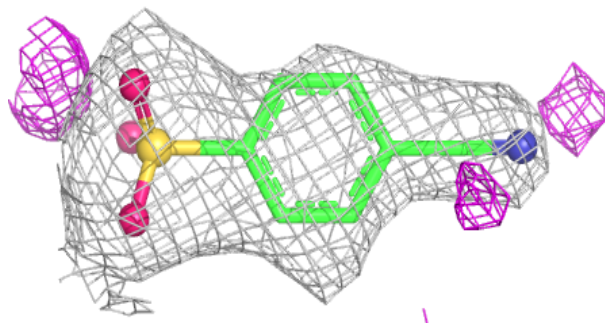
**Electron density around VWT B 808:**

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

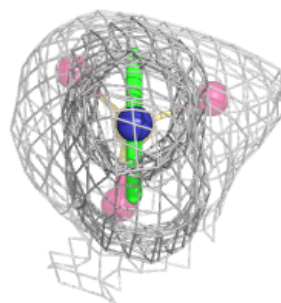
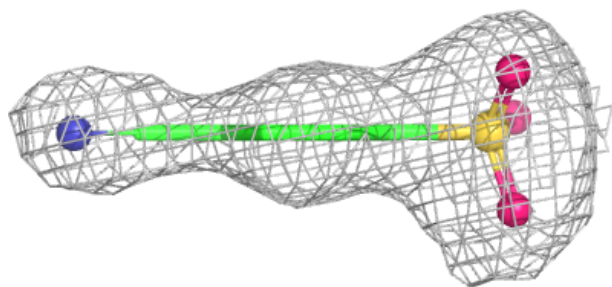
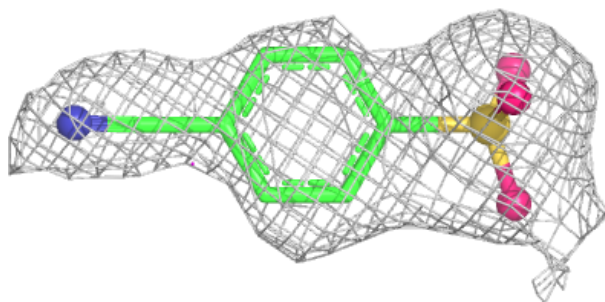


Electron density around VWT A 810:

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

**Electron density around VWT A 811:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.