



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:23 AM UTC

PDB ID : 8OQQ / pdb_00008oqq
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
in complex with Fragment-M-79
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2023-04-12
Resolution : 2.59 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

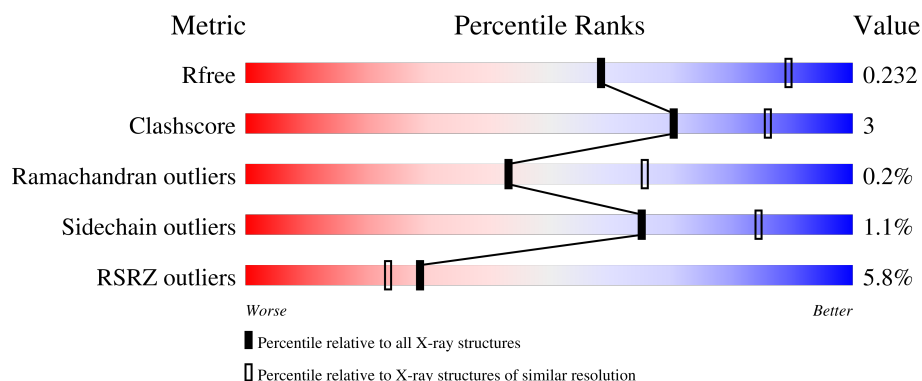
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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% 91% 7%
1	B	736	3% 91% 7%
2	C	403	5% 87% 11%
2	D	403	8% 86% 13%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17006 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	723	Total	C	N	O	S	0	0	0
			5379	3405	924	1030	20			
1	B	726	Total	C	N	O	S	0	0	0
			5397	3415	927	1034	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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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	397	Total	C	N	O	S	0	0	0
			2929	1828	520	566	15			
2	D	399	Total	C	N	O	S	0	0	0
			2942	1837	522	568	15			

- 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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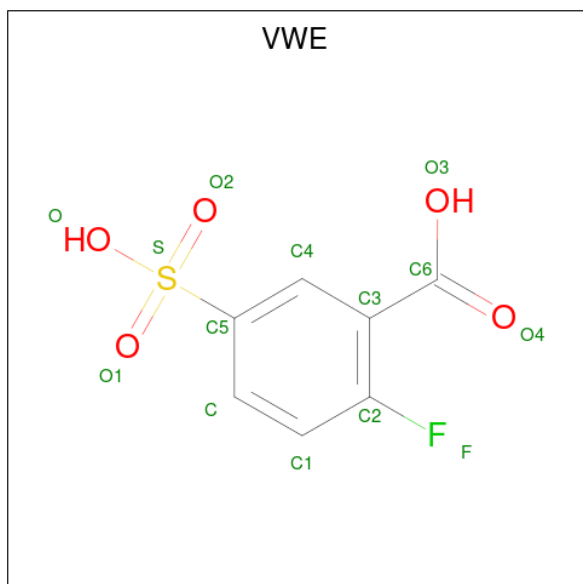
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	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	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is 2-fluoranyl-5-sulfo-benzoic acid (CCD ID: VWE) (formula: $C_7H_5FO_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	O	S	0	0
			14	7	1	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	F	O	S	0	0
			14	7	1	5	1		
5	B	1	Total	C	F	O	S	0	0
			14	7	1	5	1		
5	B	1	Total	C	F	O	S	0	0
			14	7	1	5	1		

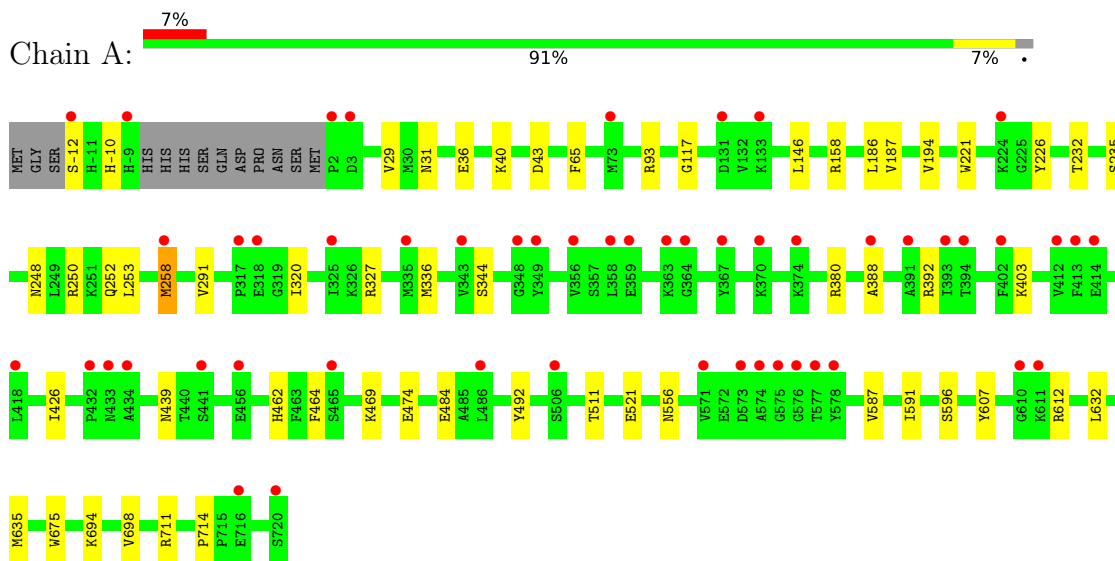
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	47	Total	O	0	0
			47	47		
6	B	68	Total	O	0	0
			68	68		
6	C	43	Total	O	0	0
			43	43		
6	D	28	Total	O	0	0
			28	28		

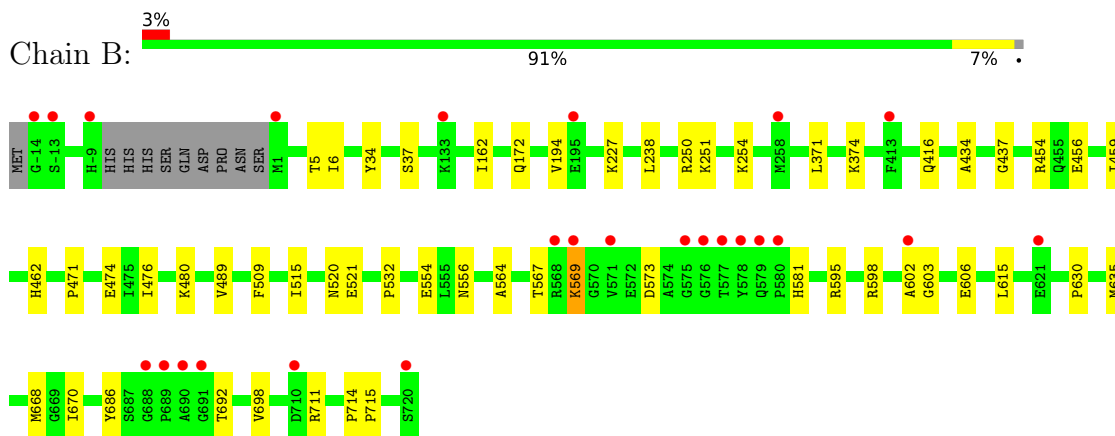
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

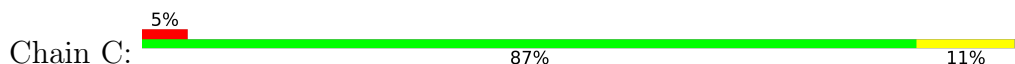
• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

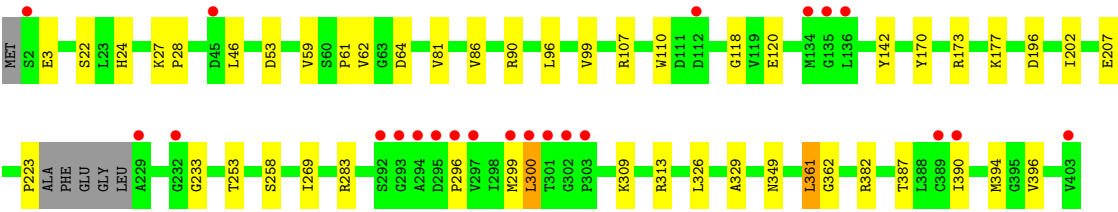


• Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

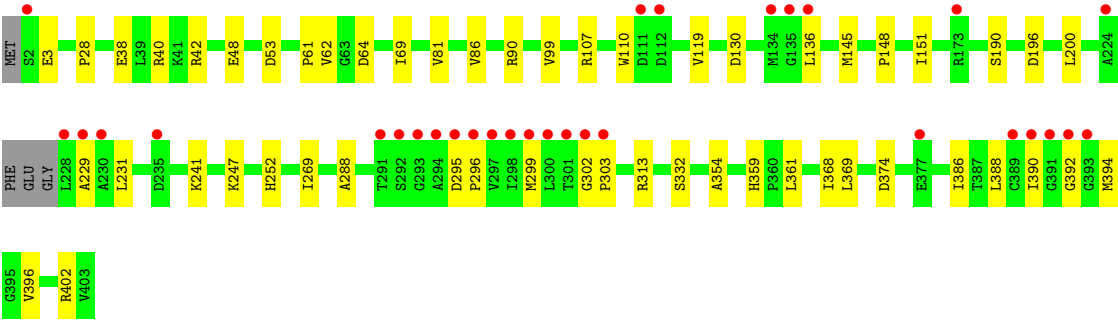
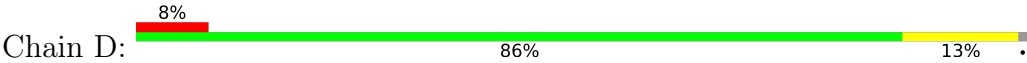


• Molecule 2: Putative acyltransferase Rv0859





● 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	250.34Å 134.02Å 119.75Å 90.00° 110.53° 90.00°	Depositor
Resolution (Å)	50.27 – 2.59 50.27 – 2.59	Depositor EDS
% Data completeness (in resolution range)	77.8 (50.27-2.59) 77.9 (50.27-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.196 , 0.231 0.196 , 0.232	Depositor DCC
R_{free} test set	4500 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17006	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% 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: VWE, GOL, 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	0.09	0/5479	0.25	0/7414
1	B	0.09	0/5497	0.26	0/7438
2	C	0.10	0/2972	0.29	0/4023
2	D	0.11	0/2985	0.30	0/4041
All	All	0.10	0/16933	0.27	0/22916

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	5379	0	5425	29	0
1	B	5397	0	5444	29	0
2	C	2929	0	2951	33	0
2	D	2942	0	2967	35	0
3	A	30	0	0	1	0
3	B	35	0	0	0	0
3	C	20	0	0	1	0
3	D	20	0	0	1	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	6	0	8	0	0
5	A	28	0	0	1	0
5	B	28	0	0	0	0
6	A	47	0	0	1	0
6	B	68	0	0	0	0
6	C	43	0	0	1	0
6	D	28	0	0	0	0
All	All	17006	0	16803	113	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 (113) 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:402:ARG:NH2	3:D:504:SO4:O3	2.22	0.72
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.73	0.69
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.74	0.68
1:B:595:ARG:NH1	1:B:603:GLY:O	2.27	0.66
2:C:27:LYS:NZ	2:D:136:LEU:O	2.29	0.65
2:C:296:PRO:HD3	2:D:81:VAL:HG21	1.81	0.63
1:A:158:ARG:NH1	6:A:901:HOH:O	2.31	0.62
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.83	0.60
1:B:250:ARG:NH1	2:C:142:TYR:O	2.34	0.60
1:A:698:VAL:HG13	1:A:714:PRO:HG3	1.83	0.60
2:C:96:LEU:HD23	2:C:396:VAL:HG13	1.84	0.59
2:D:252:HIS:HE1	2:D:332:SER:H	1.51	0.58
2:D:390:ILE:HD11	2:D:396:VAL:HG23	1.85	0.57
2:D:299:MET:HE2	2:D:392:GLY:H	1.69	0.57
2:D:190:SER:OG	2:D:374:ASP:OD2	2.18	0.57
3:A:808:SO4:O1	2:C:24:HIS:NE2	2.24	0.56
1:B:595:ARG:NH2	1:B:606:GLU:OE2	2.36	0.56
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.87	0.56
1:A:29:VAL:HG13	1:A:31:ASN:HD22	1.70	0.56
1:B:471:PRO:HG2	1:B:668:MET:HB3	1.88	0.56
2:C:62:VAL:HG12	2:D:62:VAL:HG22	1.88	0.55
2:C:258:SER:HB3	2:C:329:ALA:HA	1.89	0.55
2:D:148:PRO:HG2	2:D:151:ILE:HD12	1.89	0.54
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.44	0.53
2:C:22:SER:OG	2:C:207:GLU:OE2	2.24	0.52
1:B:5:THR:HG22	1:B:37:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:ASN:HB3	1:B:581:HIS:CE1	2.45	0.52
1:B:630:PRO:HG2	1:B:635:MET:HE2	1.91	0.52
1:B:564:ALA:HA	1:B:567:THR:HG22	1.92	0.51
2:D:241:LYS:NZ	2:D:295:ASP:OD1	2.43	0.51
1:A:250:ARG:HE	2:D:145:MET:HE3	1.75	0.51
2:C:283:ARG:NH1	6:C:601:HOH:O	2.44	0.51
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.45	0.51
2:C:28:PRO:HD2	2:C:64:ASP:HB3	1.93	0.51
2:D:390:ILE:HB	2:D:394:MET:HB2	1.92	0.51
1:A:632:LEU:HA	1:A:635:MET:HE3	1.93	0.51
2:D:302:GLY:N	2:D:303:PRO:HD2	2.27	0.50
1:A:-12:SER:O	1:A:93:ARG:NH1	2.45	0.50
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.92	0.50
2:C:223:PRO:HA	2:C:253:THR:HG22	1.94	0.49
2:D:38:GLU:HG3	2:D:42:ARG:HD2	1.94	0.49
1:A:258:MET:HE3	1:A:675:TRP:HB3	1.95	0.48
2:D:369:LEU:HD12	2:D:386:ILE:HD13	1.96	0.47
1:A:521:GLU:OE2	1:A:711:ARG:NE	2.37	0.47
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.96	0.47
2:C:173:ARG:HG2	2:C:177:LYS:HE2	1.97	0.47
2:C:299:MET:HG2	2:C:300:LEU:HD13	1.97	0.47
2:D:28:PRO:HD2	2:D:64:ASP:HB3	1.96	0.47
2:D:69:ILE:HD13	2:D:119:VAL:HG11	1.96	0.47
1:B:5:THR:HG21	1:B:34:TYR:HA	1.96	0.47
2:C:120:GLU:HG2	2:C:361:LEU:HB2	1.97	0.47
1:A:336:MET:HE2	1:A:439:ASN:HD21	1.80	0.47
2:D:229:ALA:C	2:D:231:LEU:H	2.23	0.47
1:A:29:VAL:HG13	1:A:31:ASN:ND2	2.30	0.46
1:A:320:ILE:HG21	1:A:484:GLU:HA	1.98	0.46
2:D:368:ILE:HD11	2:D:388:LEU:HD11	1.97	0.46
2:D:196:ASP:OD1	2:D:200:LEU:N	2.44	0.46
2:C:196:ASP:HB3	2:C:202:ILE:HD11	1.97	0.46
2:C:382:ARG:NE	3:C:501:SO4:O4	2.48	0.46
2:C:53:ASP:OD2	2:D:90:ARG:NH2	2.49	0.46
2:D:354:ALA:HB1	2:D:359:HIS:HB2	1.98	0.46
2:D:3:GLU:O	2:D:107:ARG:HG2	2.16	0.45
1:A:607:TYR:CE2	1:A:612:ARG:HG2	2.52	0.45
2:C:59:VAL:HG21	2:C:361:LEU:HB3	1.99	0.45
2:D:252:HIS:CE1	2:D:332:SER:H	2.34	0.45
1:A:327:ARG:NH1	1:A:403:LYS:O	2.50	0.45
1:B:521:GLU:OE2	1:B:711:ARG:NE	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:ASP:OD1	2:D:130:ASP:N	2.48	0.45
1:B:459:ILE:HG21	1:B:489:VAL:HG21	2.00	0.44
1:A:146:LEU:HD22	1:A:291:VAL:HG22	1.99	0.44
1:B:5:THR:HG22	1:B:37:SER:CB	2.47	0.44
1:B:515:ILE:HD12	1:B:670:ILE:HB	2.00	0.44
1:B:476:ILE:HG21	1:B:509:PHE:CE1	2.53	0.44
1:B:251:LYS:HD3	2:C:233:GLY:HA2	1.99	0.43
1:B:374:LYS:HB2	1:B:374:LYS:HE3	1.79	0.43
2:D:62:VAL:HG21	2:D:130:ASP:HA	2.00	0.43
1:A:36:GLU:HG3	1:A:40:LYS:HE3	1.99	0.43
1:A:596:SER:OG	5:A:806:VWE:O2	2.26	0.43
2:C:309:LYS:HE2	2:C:313:ARG:NH2	2.33	0.43
1:B:437:GLY:HA2	1:B:459:ILE:O	2.18	0.43
2:D:40:ARG:NE	2:D:48:GLU:OE2	2.52	0.43
2:C:170:TYR:HH	2:C:349:ASN:HD22	1.64	0.43
1:A:65:PHE:O	1:A:117:GLY:HA3	2.18	0.43
1:A:221:TRP:HA	1:A:226:TYR:CG	2.54	0.43
2:C:99:VAL:HG13	2:C:269:ILE:HD11	2.01	0.43
1:A:248:ASN:O	1:A:252:GLN:HG2	2.18	0.43
2:C:299:MET:HB3	2:C:300:LEU:HD22	2.02	0.42
2:C:390:ILE:HB	2:C:394:MET:HB2	2.01	0.42
2:C:110:TRP:CZ2	2:D:288:ALA:HA	2.55	0.42
1:B:5:THR:HG23	1:B:6:ILE:HG13	2.02	0.42
1:B:434:ALA:O	1:B:454:ARG:NH2	2.52	0.42
1:B:569:LYS:O	1:B:573:ASP:HB2	2.20	0.42
1:B:595:ARG:CZ	1:B:602:ALA:HB1	2.50	0.42
2:C:61:PRO:HG2	2:D:61:PRO:HG2	2.02	0.42
2:C:326:LEU:HD13	2:C:387:THR:HG23	2.01	0.42
1:B:456:GLU:HA	1:B:480:LYS:O	2.20	0.41
1:A:587:VAL:O	1:A:591:ILE:HG12	2.21	0.41
1:B:227:LYS:HD2	1:B:227:LYS:HA	1.82	0.41
1:B:686:TYR:O	1:B:692:THR:HA	2.20	0.41
1:A:388:ALA:O	1:A:392:ARG:HG3	2.21	0.41
2:C:90:ARG:NH2	2:D:53:ASP:OD2	2.51	0.41
2:D:390:ILE:HD12	2:D:394:MET:HB3	2.03	0.41
1:A:694:LYS:HE3	1:A:694:LYS:HB2	1.91	0.41
1:A:232:THR:O	1:A:235:SER:OG	2.38	0.41
1:A:186:LEU:HD12	1:A:186:LEU:HA	1.90	0.41
1:A:253:LEU:HD13	1:A:258:MET:HB2	2.03	0.41
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.92	0.41
2:C:118:GLY:HA3	2:C:362:GLY:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:464:PHE:HZ	1:A:511:THR:HG21	1.86	0.40
1:A:344:SER:OG	1:A:492:TYR:OH	2.34	0.40
1:A:-10:HIS:NE2	1:A:43:ASP:OD2	2.48	0.40
1:B:162:ILE:HD12	1:B:238:LEU:HD21	2.02	0.40
2:C:3:GLU:O	2:C:107:ARG:HG2	2.21	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	719/736 (98%)	682 (95%)	36 (5%)	1 (0%)	48	70
1	B	722/736 (98%)	699 (97%)	22 (3%)	1 (0%)	48	70
2	C	393/403 (98%)	381 (97%)	11 (3%)	1 (0%)	36	58
2	D	395/403 (98%)	375 (95%)	19 (5%)	1 (0%)	36	58
All	All	2229/2278 (98%)	2137 (96%)	88 (4%)	4 (0%)	43	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	361	LEU
2	D	361	LEU
1	B	556	ASN
1	A	556	ASN

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	554/566 (98%)	548 (99%)	6 (1%)	65	84
1	B	556/566 (98%)	548 (99%)	8 (1%)	59	81
2	C	306/310 (99%)	303 (99%)	3 (1%)	68	86
2	D	307/310 (99%)	305 (99%)	2 (1%)	76	89
All	All	1723/1752 (98%)	1704 (99%)	19 (1%)	65	84

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	187	VAL
1	A	194	VAL
1	A	258	MET
1	A	380	ARG
1	A	426	ILE
1	A	469	LYS
1	B	172	GLN
1	B	194	VAL
1	B	254	LYS
1	B	371	LEU
1	B	416	GLN
1	B	554	GLU
1	B	569	LYS
1	B	598	ARG
2	C	46	LEU
2	C	86	VAL
2	C	300	LEU
2	D	86	VAL
2	D	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	248	ASN
1	A	550	GLN
1	B	294	GLN
1	B	455	GLN
1	B	633	GLN

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Mol	Chain	Res	Type
2	C	327	ASN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

27 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	$\# Z > 2$
5	VWE	B	808	-	14,14,14	1.05	2 (14%)	21,21,21	0.87	2 (9%)
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	808	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	801	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	B	803	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	806	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.06	0
5	VWE	A	806	-	14,14,14	1.04	2 (14%)	21,21,21	0.88	2 (9%)
3	SO4	D	504	-	4,4,4	0.31	0	6,6,6	0.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	503	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.07	0
4	GOL	B	807	-	5,5,5	0.93	0	5,5,5	1.07	0
3	SO4	B	802	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.07	0
5	VWE	A	805	-	14,14,14	1.07	2 (14%)	21,21,21	0.86	2 (9%)
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	809	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	B	805	-	4,4,4	0.24	0	6,6,6	0.07	0
5	VWE	B	809	-	14,14,14	1.05	2 (14%)	21,21,21	0.88	2 (9%)
3	SO4	B	810	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.06	0
4	GOL	A	804	-	5,5,5	0.93	0	5,5,5	1.08	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
5	VWE	A	806	-	-	4/10/10/10	0/1/1/1
5	VWE	B	809	-	-	0/10/10/10	0/1/1/1
4	GOL	B	807	-	-	1/4/4/4	-
5	VWE	A	805	-	-	0/10/10/10	0/1/1/1
5	VWE	B	808	-	-	0/10/10/10	0/1/1/1
4	GOL	A	804	-	-	1/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	805	VWE	O4-C6	2.85	1.31	1.22
5	B	809	VWE	O4-C6	2.84	1.31	1.22
5	A	806	VWE	O4-C6	2.84	1.31	1.22
5	B	808	VWE	O4-C6	2.83	1.31	1.22
5	A	805	VWE	O3-C6	-2.59	1.22	1.30
5	B	808	VWE	O3-C6	-2.58	1.22	1.30
5	A	806	VWE	O3-C6	-2.55	1.22	1.30
5	B	809	VWE	O3-C6	-2.55	1.22	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	809	VWE	O4-C6-C3	-3.07	114.64	121.97
5	A	806	VWE	O4-C6-C3	-3.07	114.64	121.97
5	B	808	VWE	O4-C6-C3	-3.04	114.72	121.97
5	A	805	VWE	O4-C6-C3	-3.03	114.73	121.97
5	A	806	VWE	O3-C6-C3	2.37	122.01	115.28
5	B	809	VWE	O3-C6-C3	2.37	122.00	115.28
5	B	808	VWE	O3-C6-C3	2.36	121.98	115.28
5	A	805	VWE	O3-C6-C3	2.33	121.91	115.28

There are no chirality outliers.

All (6) torsion outliers are listed below:

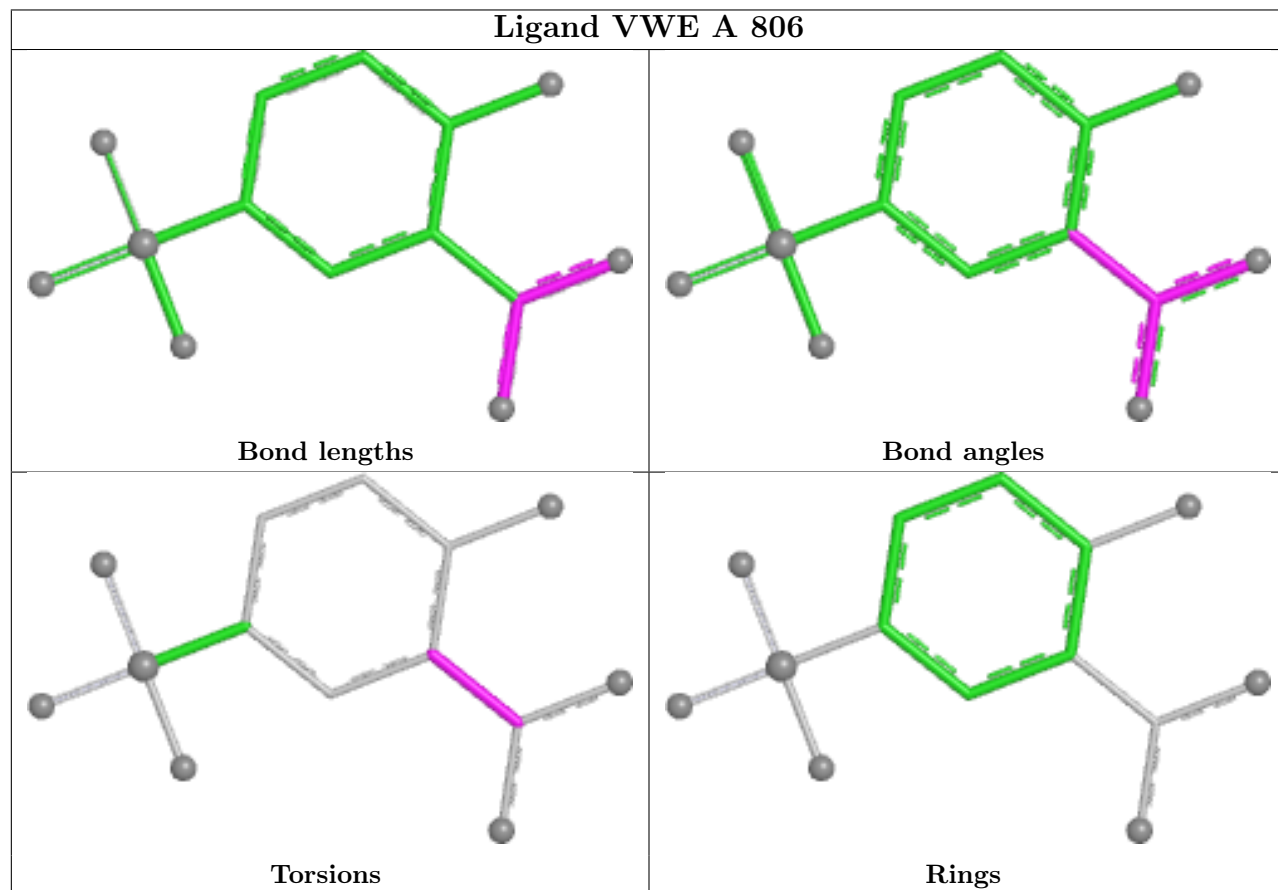
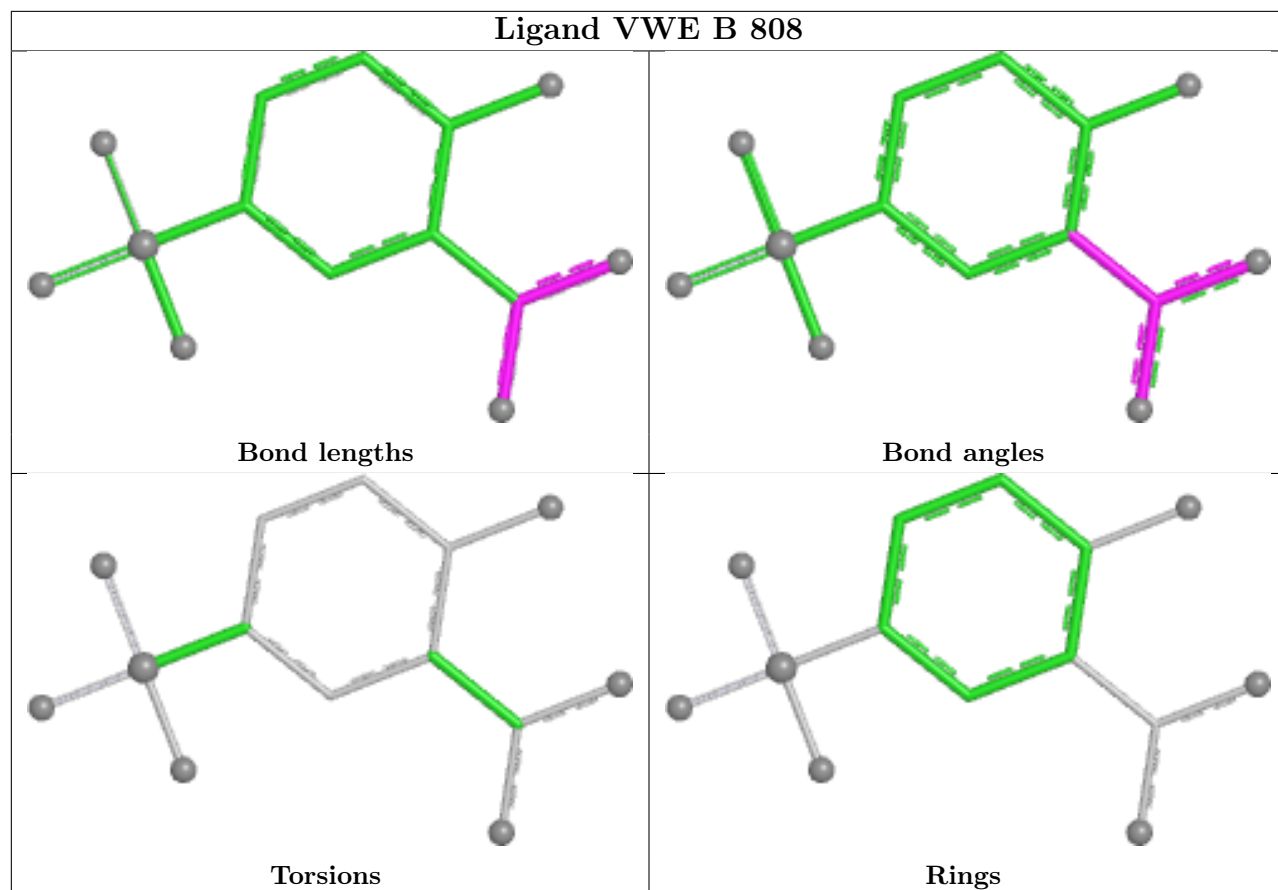
Mol	Chain	Res	Type	Atoms
5	A	806	VWE	C2-C3-C6-O4
4	A	804	GOL	O1-C1-C2-O2
4	B	807	GOL	O2-C2-C3-O3
5	A	806	VWE	C2-C3-C6-O3
5	A	806	VWE	C4-C3-C6-O3
5	A	806	VWE	C4-C3-C6-O4

There are no ring outliers.

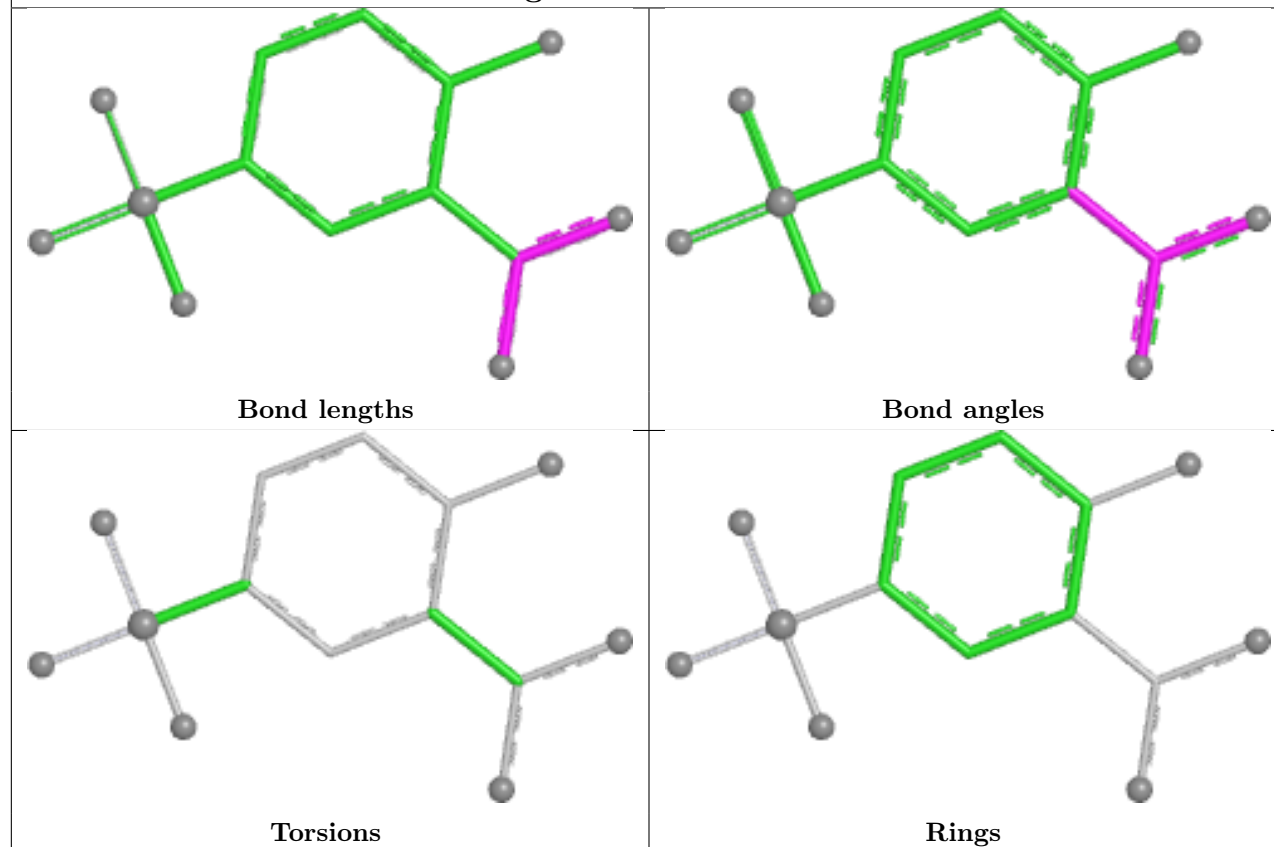
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	808	SO4	1	0
5	A	806	VWE	1	0
3	D	504	SO4	1	0
3	C	501	SO4	1	0

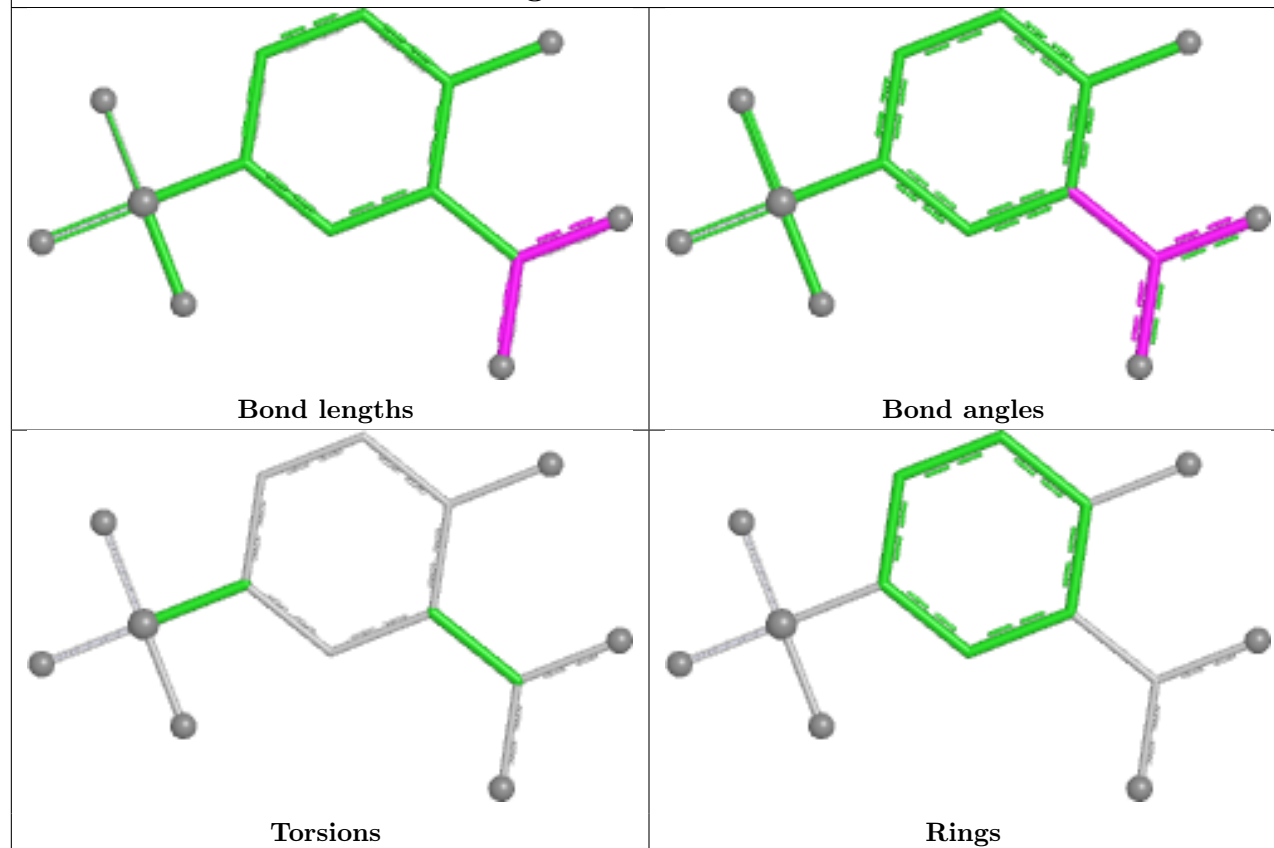
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



Ligand VWE A 805



Ligand VWE B 809



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	723/736 (98%)	0.53	52 (7%) 21 17	34, 66, 111, 164	0
1	B	726/736 (98%)	0.29	25 (3%) 48 42	36, 58, 97, 136	0
2	C	397/403 (98%)	0.20	22 (5%) 30 25	32, 51, 87, 126	0
2	D	399/403 (99%)	0.36	31 (7%) 19 15	33, 54, 93, 147	0
All	All	2245/2278 (98%)	0.36	130 (5%) 29 23	32, 58, 103, 164	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	294	ALA	5.9
2	D	390	ILE	5.6
2	C	293	GLY	5.6
2	D	301	THR	5.3
1	A	2	PRO	4.6
1	A	-9	HIS	4.6
2	D	296	PRO	4.5
2	D	391	GLY	4.5
2	C	301	THR	4.4
2	C	389	CYS	4.4
1	A	413	PHE	4.4
2	C	300	LEU	4.3
2	D	389	CYS	4.3
1	B	576	GLY	4.3
2	D	292	SER	4.3
1	B	578	TYR	4.2
2	D	228	LEU	4.1
2	C	294	ALA	4.0
2	D	302	GLY	3.9
1	B	577	THR	3.9
2	D	136	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
2	D	134	MET	3.8
1	A	335	MET	3.8
2	C	134	MET	3.7
2	D	303	PRO	3.6
1	B	1	MET	3.6
2	D	298	ILE	3.6
2	C	296	PRO	3.6
2	C	390	ILE	3.6
1	B	-14	GLY	3.6
2	D	230	ALA	3.6
1	B	690	ALA	3.5
1	B	-9	HIS	3.5
1	A	414	GLU	3.5
2	C	302	GLY	3.4
1	A	412	VAL	3.4
2	D	135	GLY	3.4
2	D	392	GLY	3.4
1	B	720	SER	3.3
2	C	232	GLY	3.2
1	A	574	ALA	3.2
2	D	293	GLY	3.1
2	D	297	VAL	3.1
1	A	575	GLY	3.1
1	B	688	GLY	3.0
1	A	364	GLY	3.0
1	B	579	GLN	3.0
1	B	-13	SER	2.9
2	C	299	MET	2.9
2	C	297	VAL	2.9
2	D	229	ALA	2.9
2	C	292	SER	2.9
2	D	299	MET	2.9
1	A	359	GLU	2.9
1	A	571	VAL	2.9
2	D	393	GLY	2.9
1	A	317	PRO	2.8
2	D	300	LEU	2.8
1	B	413	PHE	2.8
1	A	367	TYR	2.8
1	A	433	ASN	2.8
1	A	720	SER	2.8
2	D	295	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	348	GLY	2.8
2	C	229	ALA	2.8
1	A	356	VAL	2.8
1	A	394	THR	2.8
1	A	418	LEU	2.7
1	A	486	LEU	2.7
1	B	569	LYS	2.7
1	A	133	LYS	2.7
1	A	610	GLY	2.7
2	D	2	SER	2.7
1	A	388	ALA	2.7
1	A	318	GLU	2.6
1	B	133	LYS	2.5
1	A	-12	SER	2.5
1	A	578	TYR	2.5
2	C	45	ASP	2.5
1	A	374	LYS	2.5
1	A	465	SER	2.5
1	B	258	MET	2.5
1	A	577	THR	2.4
1	B	580	PRO	2.4
1	A	393	ILE	2.4
2	D	112	ASP	2.4
2	C	136	LEU	2.4
1	B	621	GLU	2.4
1	B	575	GLY	2.4
1	A	349	TYR	2.4
1	A	258	MET	2.3
2	C	303	PRO	2.3
2	D	173	ARG	2.3
1	A	3	ASP	2.3
1	A	343	VAL	2.3
1	A	73	MET	2.2
1	A	402	PHE	2.2
1	B	710	ASP	2.2
2	D	111	ASP	2.2
1	A	716	GLU	2.2
1	B	195	GLU	2.2
1	B	691	GLY	2.2
2	C	112	ASP	2.2
2	D	377	GLU	2.2
1	B	689	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	224	LYS	2.2
1	A	363	LYS	2.2
1	A	370	LYS	2.2
2	C	2	SER	2.2
2	C	403	VAL	2.1
1	A	456	GLU	2.1
1	A	441	SER	2.1
1	A	325	ILE	2.1
1	A	358	LEU	2.1
1	B	568	ARG	2.1
1	A	506	SER	2.1
1	A	391	ALA	2.1
2	D	291	THR	2.1
1	A	573	ASP	2.1
1	B	571	VAL	2.0
2	C	295	ASP	2.0
1	A	434	ALA	2.0
1	B	602	ALA	2.0
2	D	224	ALA	2.0
1	A	576	GLY	2.0
1	A	611	LYS	2.0
2	C	135	GLY	2.0
1	A	131	ASP	2.0
1	A	432	PRO	2.0
2	D	235	ASP	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 ⓘ

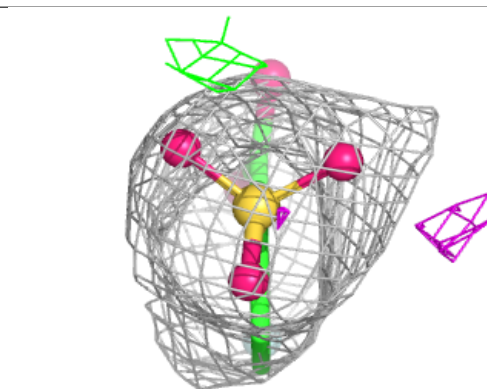
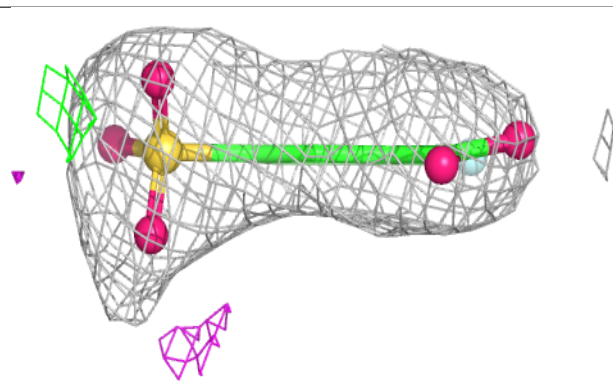
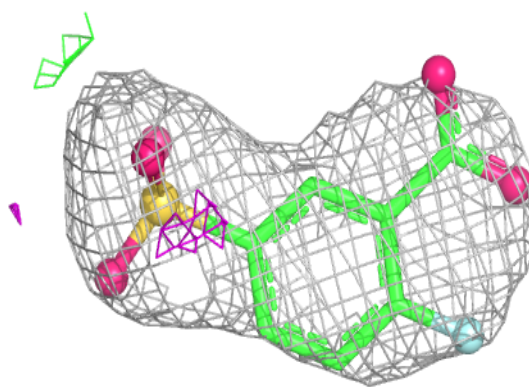
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SO4	B	804	5/5	0.68	0.15	78,89,103,108	5
3	SO4	D	504	5/5	0.73	0.22	99,107,141,147	2
3	SO4	A	807	5/5	0.75	0.11	103,106,117,131	0
3	SO4	D	502	5/5	0.78	0.10	99,108,122,140	0
3	SO4	A	808	5/5	0.78	0.14	122,123,146,151	0
3	SO4	B	810	5/5	0.79	0.12	93,102,126,134	0
3	SO4	B	805	5/5	0.80	0.08	94,96,127,130	0
3	SO4	C	504	5/5	0.81	0.08	89,91,114,124	0
3	SO4	C	503	5/5	0.85	0.09	99,99,117,134	0
3	SO4	C	501	5/5	0.85	0.09	80,82,119,122	0
3	SO4	B	803	5/5	0.86	0.16	57,63,74,83	5
3	SO4	A	801	5/5	0.87	0.12	72,86,108,112	0
3	SO4	A	802	5/5	0.88	0.09	90,94,104,111	0
4	GOL	B	807	6/6	0.88	0.18	52,61,69,86	0
3	SO4	B	806	5/5	0.89	0.11	54,56,66,67	5
4	GOL	A	804	6/6	0.89	0.14	54,55,67,69	0
3	SO4	B	801	5/5	0.89	0.12	80,97,115,124	0
3	SO4	B	802	5/5	0.90	0.12	79,86,90,96	0
3	SO4	A	809	5/5	0.90	0.08	93,97,112,145	0
3	SO4	A	803	5/5	0.90	0.12	38,55,60,63	5
3	SO4	D	501	5/5	0.90	0.10	83,88,92,99	0
5	VWE	A	805	14/14	0.90	0.12	79,83,97,106	0
5	VWE	B	808	14/14	0.90	0.15	62,92,102,105	0
5	VWE	B	809	14/14	0.90	0.12	82,96,109,135	0
3	SO4	D	503	5/5	0.92	0.16	72,72,89,99	0
5	VWE	A	806	14/14	0.92	0.10	74,90,104,108	0
3	SO4	C	502	5/5	0.94	0.11	59,73,90,94	0

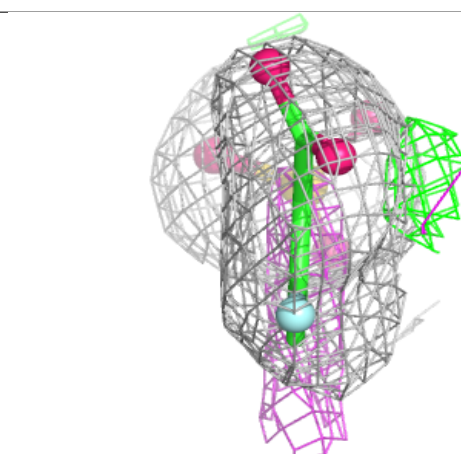
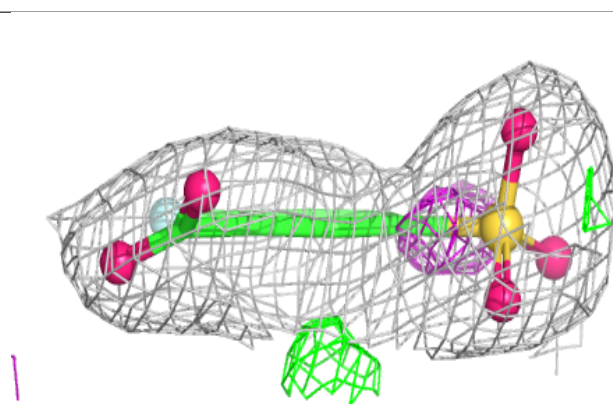
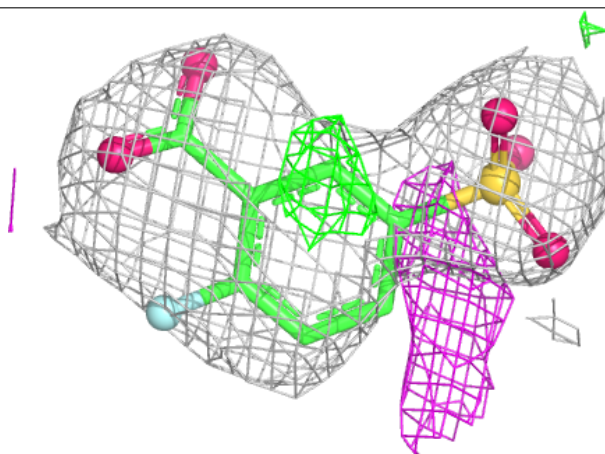
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around VWE A 805:

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

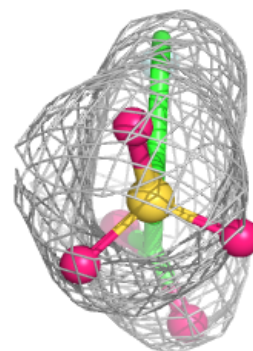
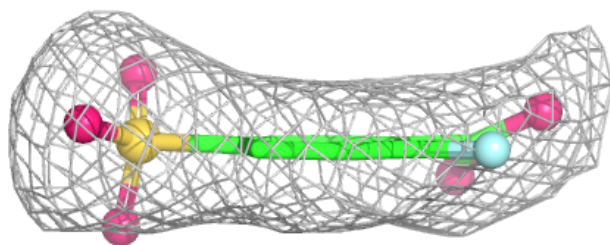
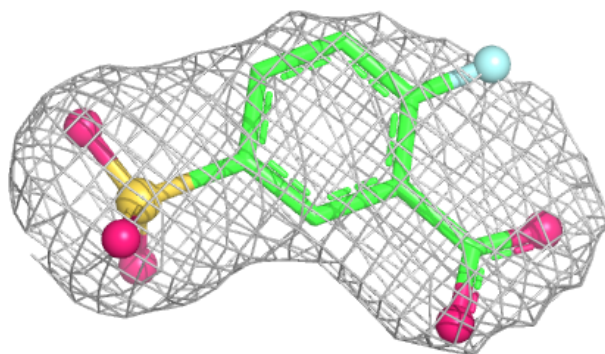
**Electron density around VWE B 808:**

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

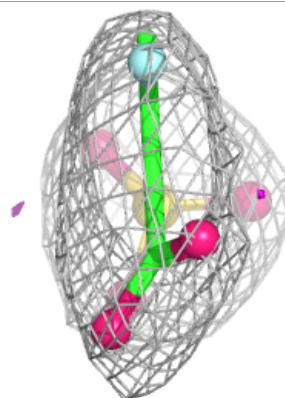
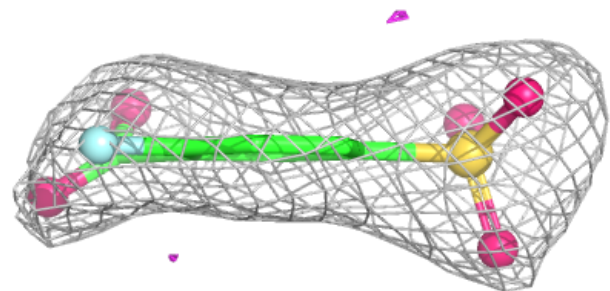
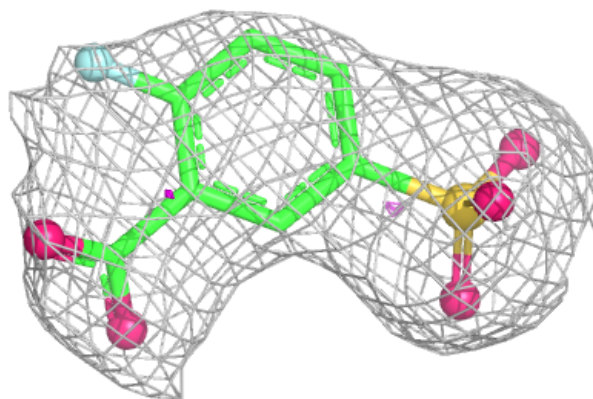


Electron density around VWE B 809:

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

**Electron density around VWE A 806:**

$2mF_o-DF_c$ (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.