



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 07:05 PM UTC

PDB ID : 8OQT / pdb_00008oqt
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
in complex with Fragment-M-91
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2023-04-12
Resolution : 2.62 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

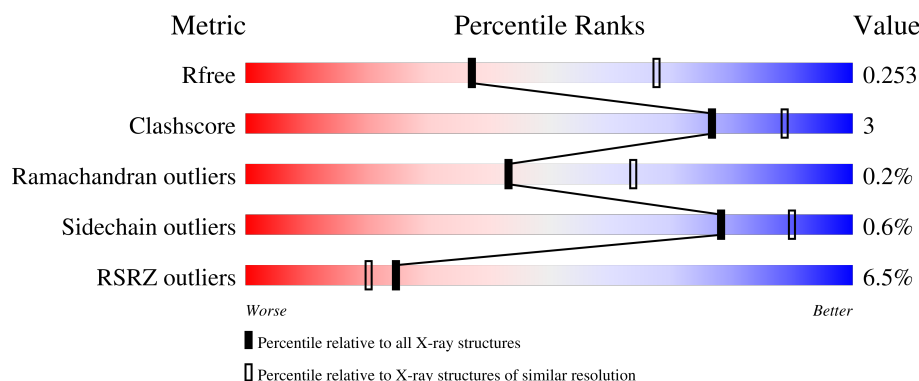
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.62 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	10% 93% 6%
1	B	736	4% 92% 7%
2	C	403	5% 88% 11%
2	D	403	5% 89% 10%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17002 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	B	726	Total	C	N	O	S	0	0	0
			5391	3410	926	1034	21			
1	A	729	Total	C	N	O	S	0	0	0
			5420	3428	934	1037	21			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

Continued on next page...

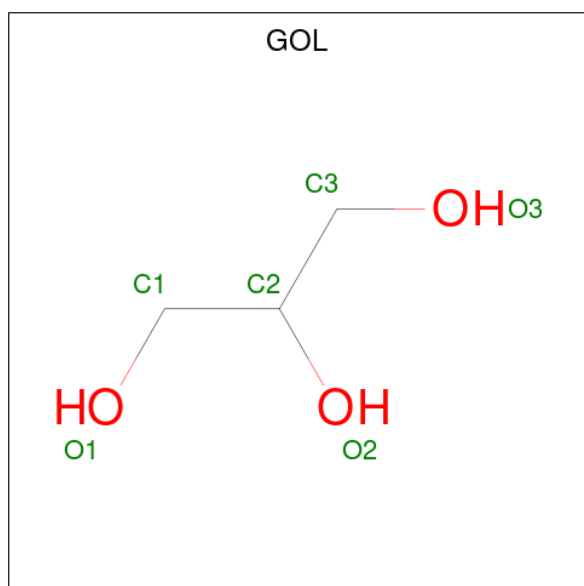
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	401	Total	C	N	O	S	0	0	0
			2955	1845	524	570	16			
2	C	400	Total	C	N	O	S	0	0	0
			2944	1837	523	569	15			

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



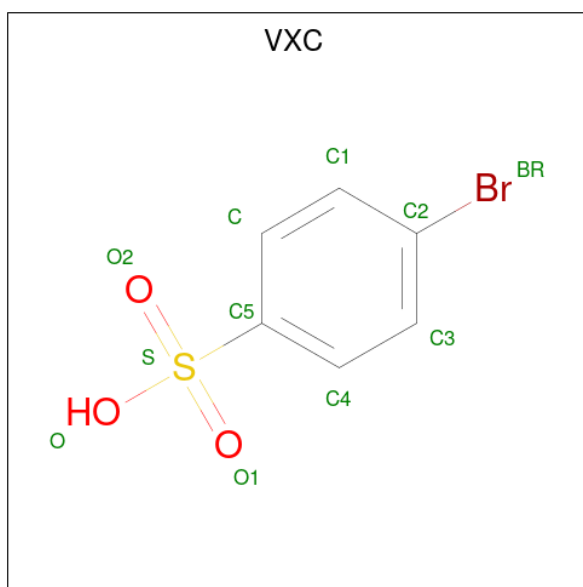
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 5 is 4-bromanylbenzenesulfonic acid (CCD ID: VXC) (formula: $\text{C}_6\text{H}_5\text{BrO}_3\text{S}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	Br	C	O	S	0	0
			11	1	6	3	1		
5	B	1	Total	Br	C	O	S	0	0
			11	1	6	3	1		
5	B	1	Total	Br	C	O	S	0	0
			11	1	6	3	1		
5	A	1	Total	Br	C	O	S	0	0
			11	1	6	3	1		
5	A	1	Total	Br	C	O	S	0	0
			11	1	6	3	1		
5	A	1	Total	Br	C	O	S	0	0
			11	1	6	3	1		

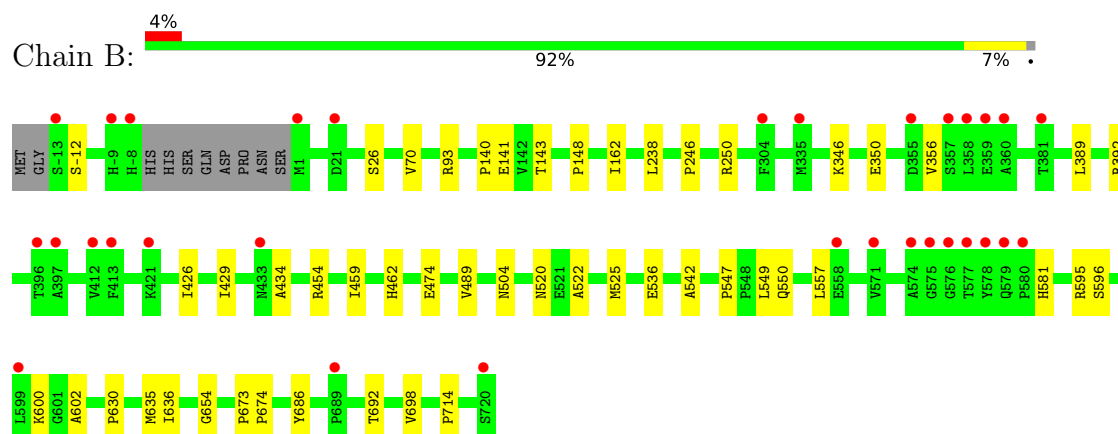
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	25	Total	O	0	0
			25	25		
6	D	19	Total	O	0	0
			19	19		
6	C	15	Total	O	0	0
			15	15		
6	A	22	Total	O	0	0
			22	22		

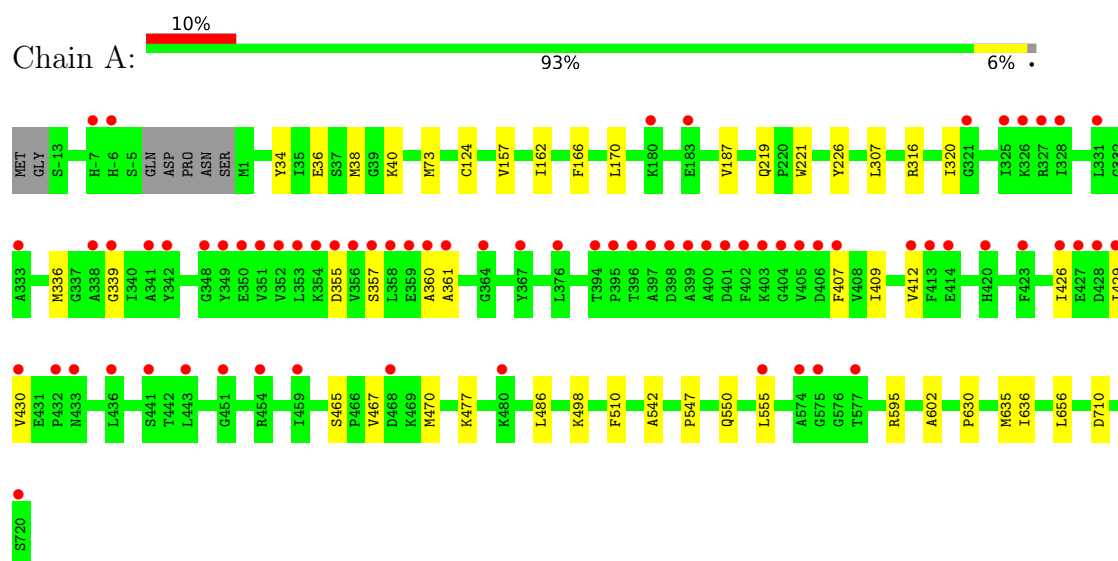
3 Residue-property plots [i](#)

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.

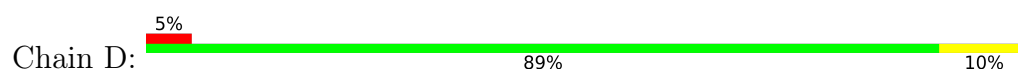
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

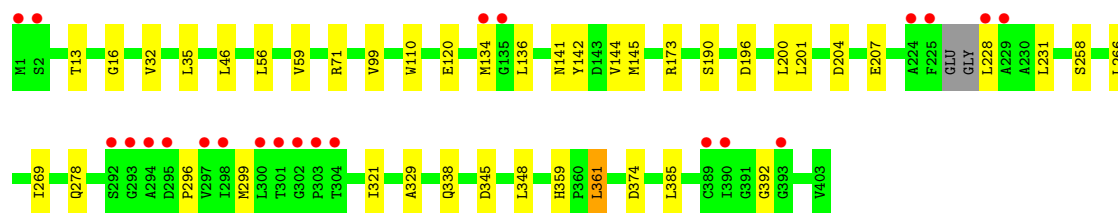


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

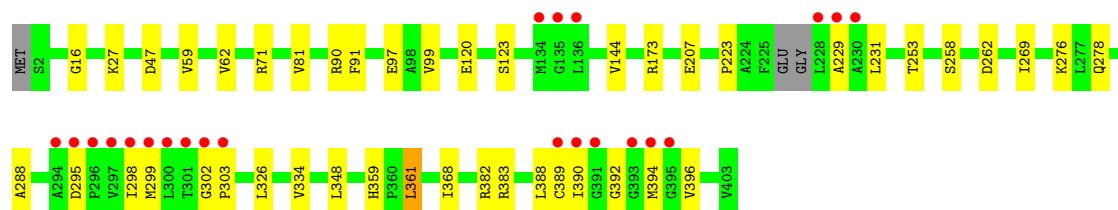
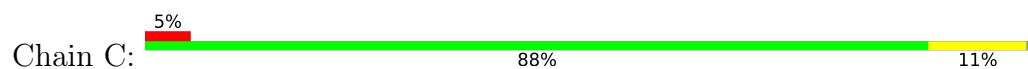


- Molecule 2: Putative acyltransferase Rv0859





● 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	247.48Å 133.23Å 115.93Å 90.00° 109.64° 90.00°	Depositor
Resolution (Å)	54.59 – 2.62 54.59 – 2.62	Depositor EDS
% Data completeness (in resolution range)	55.1 (54.59-2.62) 55.1 (54.59-2.62)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.62Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.199 , 0.245 0.209 , 0.253	Depositor DCC
R_{free} test set	2910 reflections (2.73%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.6	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	0.91	EDS
Total number of atoms	17002	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.05% 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, VXC, 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	0.08	0/5523	0.23	0/7477
1	B	0.10	0/5492	0.26	0/7436
2	C	0.09	0/2987	0.27	0/4044
2	D	0.09	0/2998	0.25	0/4058
All	All	0.09	0/17000	0.25	0/23015

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	5420	0	5442	25	1
1	B	5391	0	5415	27	1
2	C	2944	0	2960	26	0
2	D	2955	0	2981	27	0
3	A	12	0	16	0	0
3	B	18	0	24	0	0
4	A	25	0	0	0	0
4	B	25	0	0	0	0
4	C	35	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	30	0	0	0	0
5	A	33	0	0	1	0
5	B	33	0	0	1	0
6	A	22	0	0	0	0
6	B	25	0	0	0	0
6	C	15	0	0	0	0
6	D	19	0	0	0	0
All	All	17002	0	16838	97	1

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 (97) 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:C:299:MET:HE2	2:C:392:GLY:H	1.54	0.72
1:B:250:ARG:HH12	2:D:145:MET:HG2	1.55	0.72
2:D:338:GLN:NE2	2:D:345:ASP:OD1	2.18	0.70
1:B:389:LEU:HD23	1:B:392:ARG:HH21	1.58	0.68
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.75	0.68
2:D:173:ARG:NH2	2:D:348:LEU:O	2.27	0.68
2:D:120:GLU:HG2	2:D:361:LEU:HB2	1.79	0.65
1:B:434:ALA:O	1:B:454:ARG:NH2	2.30	0.64
2:C:295:ASP:HB3	2:C:298:ILE:HG22	1.80	0.63
2:D:136:LEU:O	2:C:27:LYS:NZ	2.32	0.62
2:D:190:SER:OG	2:D:374:ASP:OD2	2.18	0.60
1:A:426:ILE:HD12	1:A:429:ILE:HD12	1.83	0.59
2:C:173:ARG:NH2	2:C:348:LEU:O	2.30	0.59
1:A:316:ARG:NH1	1:A:320:ILE:O	2.35	0.59
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.85	0.58
1:B:557:LEU:HD12	1:B:596:SER:HA	1.84	0.58
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.86	0.58
1:A:477:LYS:HD3	1:A:486:LEU:HD22	1.86	0.58
1:A:630:PRO:HG2	1:A:635:MET:HE2	1.86	0.57
1:B:346:LYS:HA	1:B:389:LEU:HD22	1.86	0.56
2:C:47:ASP:HB3	2:C:278:GLN:HE22	1.71	0.55
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.87	0.55
1:A:357:SER:HB3	1:A:360:ALA:HB3	1.87	0.54
1:B:162:ILE:HD12	1:B:238:LEU:HD21	1.89	0.54
2:D:258:SER:HB2	2:D:359:HIS:HB2	1.89	0.54
1:B:522:ALA:HA	1:B:525:MET:HE3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:MET:SD	1:A:465:SER:OG	2.66	0.53
1:A:157:VAL:HG13	1:A:162:ILE:HA	1.92	0.51
1:A:470:MET:O	1:A:498:LYS:NZ	2.33	0.50
2:D:321:ILE:HG21	2:D:385:LEU:HB2	1.94	0.50
2:C:390:ILE:HD12	2:C:394:MET:HB2	1.93	0.50
2:D:299:MET:HE2	2:D:392:GLY:H	1.77	0.49
2:C:91:PHE:HB2	2:C:390:ILE:HG23	1.93	0.49
2:C:120:GLU:HG2	2:C:361:LEU:HB2	1.95	0.49
2:D:228:LEU:HD13	2:D:231:LEU:HD12	1.94	0.48
1:B:698:VAL:HG13	1:B:714:PRO:HG3	1.95	0.48
1:A:407:PHE:CE2	1:A:409:ILE:HD11	2.48	0.48
2:C:302:GLY:N	2:C:303:PRO:HD2	2.28	0.48
2:D:71:ARG:CZ	2:C:394:MET:HG2	2.44	0.47
2:C:123:SER:OG	2:C:262:ASP:OD2	2.28	0.47
1:A:73:MET:HE2	5:A:810:VXC:BR	2.69	0.47
2:C:223:PRO:HA	2:C:253:THR:HG22	1.95	0.47
2:C:229:ALA:C	2:C:231:LEU:H	2.22	0.47
1:A:355:ASP:HB3	1:A:361:ALA:HB2	1.97	0.47
1:A:339:GLY:HA3	1:A:467:VAL:HB	1.97	0.46
1:A:166:PHE:HA	1:A:170:LEU:HB2	1.97	0.46
2:D:196:ASP:OD1	2:D:200:LEU:N	2.49	0.45
2:D:32:VAL:HG11	2:D:56:LEU:HD11	1.98	0.45
1:A:547:PRO:HG2	1:A:550:GLN:HB3	1.97	0.45
1:B:250:ARG:NH1	2:D:145:MET:HG2	2.28	0.45
2:D:134:MET:HE2	2:D:144:VAL:HG21	1.98	0.45
2:C:90:ARG:HE	2:C:97:GLU:HG2	1.82	0.45
1:A:426:ILE:O	1:A:430:VAL:HG22	2.18	0.44
1:A:357:SER:O	1:A:361:ALA:N	2.46	0.44
1:A:221:TRP:HA	1:A:226:TYR:CG	2.52	0.44
2:C:258:SER:HB2	2:C:359:HIS:HB2	1.98	0.44
2:C:368:ILE:HD11	2:C:388:LEU:HD11	2.00	0.44
1:B:140:PRO:O	1:B:143:THR:OG1	2.34	0.44
1:B:520:ASN:HB3	1:B:581:HIS:CD2	2.52	0.44
1:B:673:PRO:HA	1:B:674:PRO:HD3	1.90	0.44
2:D:258:SER:HB3	2:D:329:ALA:HA	1.99	0.44
1:B:-12:SER:O	1:B:93:ARG:HD2	2.18	0.44
1:A:36:GLU:HG3	1:A:40:LYS:HE3	2.00	0.44
1:A:542:ALA:HB2	1:A:636:ILE:HG23	2.00	0.44
1:B:542:ALA:HB2	1:B:636:ILE:HG23	1.99	0.43
2:C:71:ARG:HH22	2:C:81:VAL:HG22	1.83	0.43
2:D:13:THR:HG23	2:D:35:LEU:HD11	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:MET:HE3	1:A:73:MET:HB2	1.97	0.43
2:D:201:LEU:HD11	2:D:204:ASP:HB3	2.00	0.43
2:D:59:VAL:HG21	2:D:361:LEU:HB3	2.01	0.43
1:B:536:GLU:CD	1:B:549:LEU:HB2	2.43	0.43
2:D:46:LEU:HD12	2:D:278:GLN:HB3	2.01	0.43
2:D:296:PRO:HD3	2:C:81:VAL:HG21	2.00	0.43
1:B:246:PRO:HG2	2:D:141:ASN:HB3	2.01	0.42
1:B:250:ARG:HG2	2:D:142:TYR:CE2	2.54	0.42
1:B:596:SER:OG	1:B:600:LYS:HG3	2.18	0.42
1:B:504:ASN:ND2	1:B:654:GLY:O	2.50	0.42
1:B:70:VAL:HG22	5:B:809:VXC:BR	2.75	0.42
1:B:547:PRO:HG2	1:B:550:GLN:HB3	2.02	0.42
1:A:34:TYR:HE1	1:A:38:MET:HE2	1.84	0.42
1:B:686:TYR:O	1:B:692:THR:HA	2.19	0.42
2:C:382:ARG:HG3	2:C:383:ARG:HG3	2.01	0.42
1:B:595:ARG:CZ	1:B:602:ALA:HB1	2.50	0.41
2:C:16:GLY:HA2	2:C:207:GLU:HG2	2.02	0.41
2:C:390:ILE:HD11	2:C:396:VAL:HG23	2.02	0.41
1:A:426:ILE:HG13	1:A:430:VAL:HG13	2.01	0.41
2:D:110:TRP:CZ2	2:C:288:ALA:HA	2.56	0.41
1:A:124:CYS:O	1:A:219:GLN:NE2	2.50	0.41
2:C:59:VAL:HG21	2:C:361:LEU:HB3	2.02	0.41
1:A:595:ARG:CZ	1:A:602:ALA:HB1	2.51	0.41
2:D:16:GLY:HA2	2:D:207:GLU:HG2	2.02	0.40
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.56	0.40
2:C:326:LEU:HD23	2:C:334:VAL:HA	2.03	0.40
1:B:630:PRO:HG2	1:B:635:MET:HE2	2.03	0.40
2:C:303:PRO:HD3	2:C:389:CYS:HA	2.04	0.40
1:B:536:GLU:OE1	1:B:547:PRO:HB2	2.21	0.40
2:D:266:LEU:HD23	2:D:266:LEU:HA	1.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:SER:OG	1:A:710:ASP:OD2[1_556]	2.12	0.08

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	725/736 (98%)	685 (94%)	39 (5%)	1 (0%)	48	69
1	B	722/736 (98%)	695 (96%)	26 (4%)	1 (0%)	48	69
2	C	396/403 (98%)	378 (96%)	17 (4%)	1 (0%)	36	56
2	D	397/403 (98%)	379 (96%)	17 (4%)	1 (0%)	36	56
All	All	2240/2278 (98%)	2137 (95%)	99 (4%)	4 (0%)	43	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	361	LEU
2	C	361	LEU
1	A	412	VAL
1	B	148	PRO

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	557/566 (98%)	554 (100%)	3 (0%)	81	91
1	B	554/566 (98%)	549 (99%)	5 (1%)	70	86
2	C	306/310 (99%)	303 (99%)	3 (1%)	68	85
2	D	308/310 (99%)	308 (100%)	0	100	100
All	All	1725/1752 (98%)	1714 (99%)	11 (1%)	78	90

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	141	GLU
1	B	350	GLU
1	B	356	VAL
1	B	426	ILE
1	B	429	ILE
2	C	62	VAL
2	C	144	VAL
2	C	276	LYS
1	A	187	VAL
1	A	307	LEU
1	A	555	LEU

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

Mol	Chain	Res	Type
1	B	163	GLN
1	B	248	ASN
1	B	294	GLN
2	D	198	ASN
2	D	349	ASN
1	A	-8	HIS
1	A	252	GLN
1	A	550	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

34 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	VXC	B	809	-	11,11,11	0.22	0	16,16,16	0.19	0
3	GOL	A	801	-	5,5,5	0.90	0	5,5,5	1.11	0
4	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	501	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.06	0
3	GOL	B	803	-	5,5,5	0.95	0	5,5,5	1.09	0
4	SO4	C	507	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.08	0
3	GOL	B	802	-	5,5,5	0.92	0	5,5,5	1.09	0
4	SO4	D	502	-	4,4,4	0.23	0	6,6,6	0.09	0
5	VXC	A	809	-	11,11,11	0.19	0	16,16,16	0.12	0
4	SO4	B	805	-	4,4,4	0.24	0	6,6,6	0.09	0
4	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	A	807	-	4,4,4	0.24	0	6,6,6	0.08	0
4	SO4	A	804	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	A	806	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	A	805	-	4,4,4	0.24	0	6,6,6	0.09	0
5	VXC	A	810	-	11,11,11	0.20	0	16,16,16	0.12	0
3	GOL	B	801	-	5,5,5	0.93	0	5,5,5	1.06	0
4	SO4	B	807	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	D	504	-	4,4,4	0.24	0	6,6,6	0.07	0
4	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.08	0
4	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.08	0
5	VXC	B	811	-	11,11,11	0.27	0	16,16,16	0.17	0
3	GOL	A	802	-	5,5,5	0.93	0	5,5,5	1.03	0
4	SO4	B	806	-	4,4,4	0.24	0	6,6,6	0.10	0
5	VXC	A	808	-	11,11,11	0.27	0	16,16,16	0.19	0
4	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.06	0
4	SO4	B	808	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	VXC	B	810	-	11,11,11	0.20	0	16,16,16	0.12	0
4	SO4	A	803	-	4,4,4	0.23	0	6,6,6	0.08	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	VXC	B	809	-	-	0/6/6/6	0/1/1/1
3	GOL	A	801	-	-	0/4/4/4	-
3	GOL	A	802	-	-	4/4/4/4	-
5	VXC	B	811	-	-	0/6/6/6	0/1/1/1
5	VXC	A	808	-	-	0/6/6/6	0/1/1/1
5	VXC	A	809	-	-	0/6/6/6	0/1/1/1
5	VXC	A	810	-	-	0/6/6/6	0/1/1/1
5	VXC	B	810	-	-	0/6/6/6	0/1/1/1
3	GOL	B	801	-	-	2/4/4/4	-
3	GOL	B	803	-	-	2/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

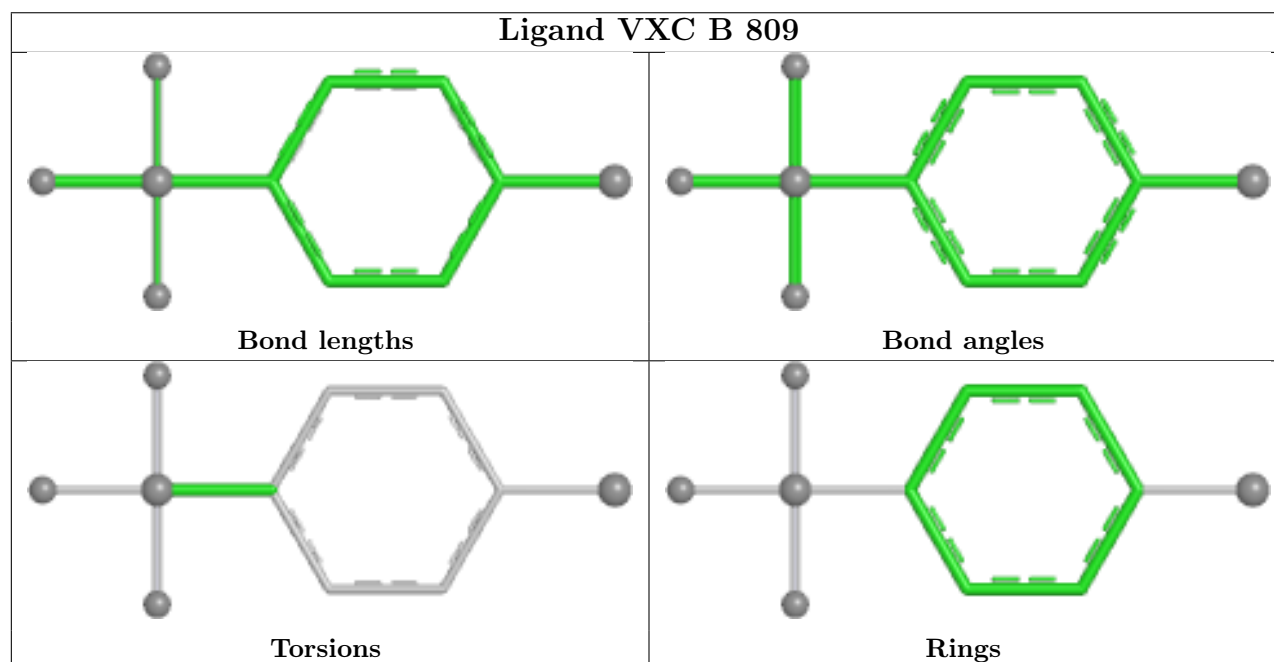
Mol	Chain	Res	Type	Atoms
3	B	801	GOL	C1-C2-C3-O3
3	B	802	GOL	O1-C1-C2-C3
3	B	803	GOL	O1-C1-C2-C3
3	A	802	GOL	O1-C1-C2-C3
3	A	802	GOL	C1-C2-C3-O3
3	B	801	GOL	O2-C2-C3-O3
3	B	802	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-O2
3	A	802	GOL	O2-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2

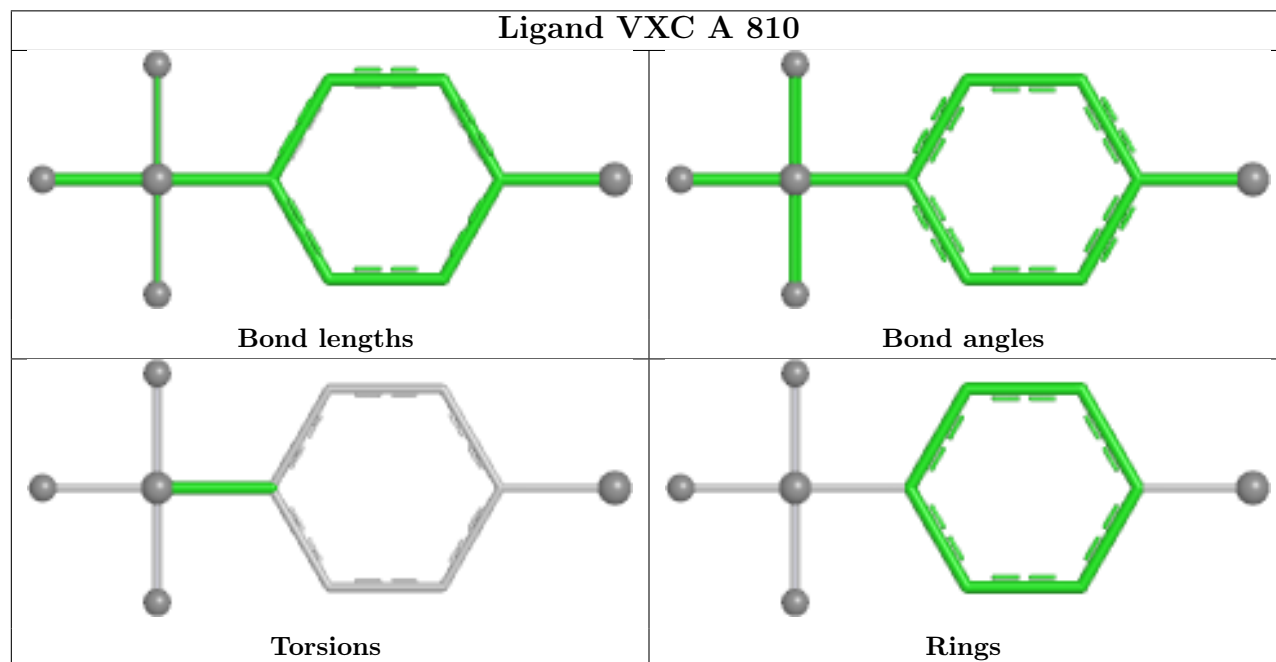
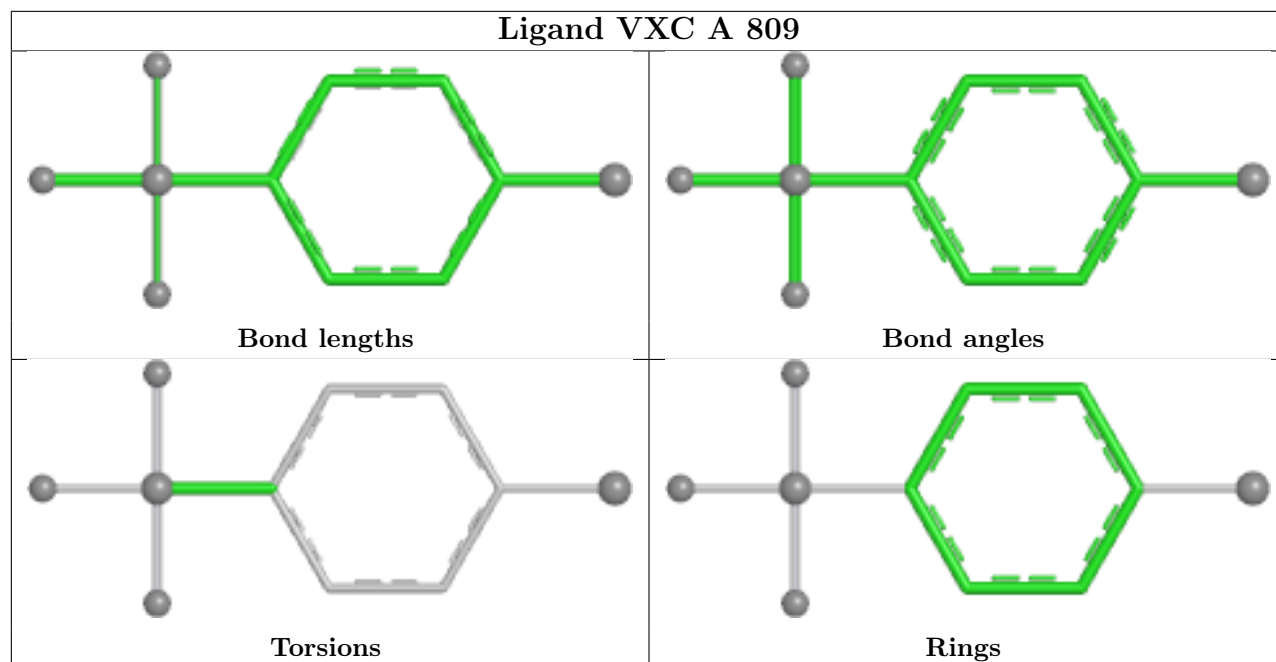
There are no ring outliers.

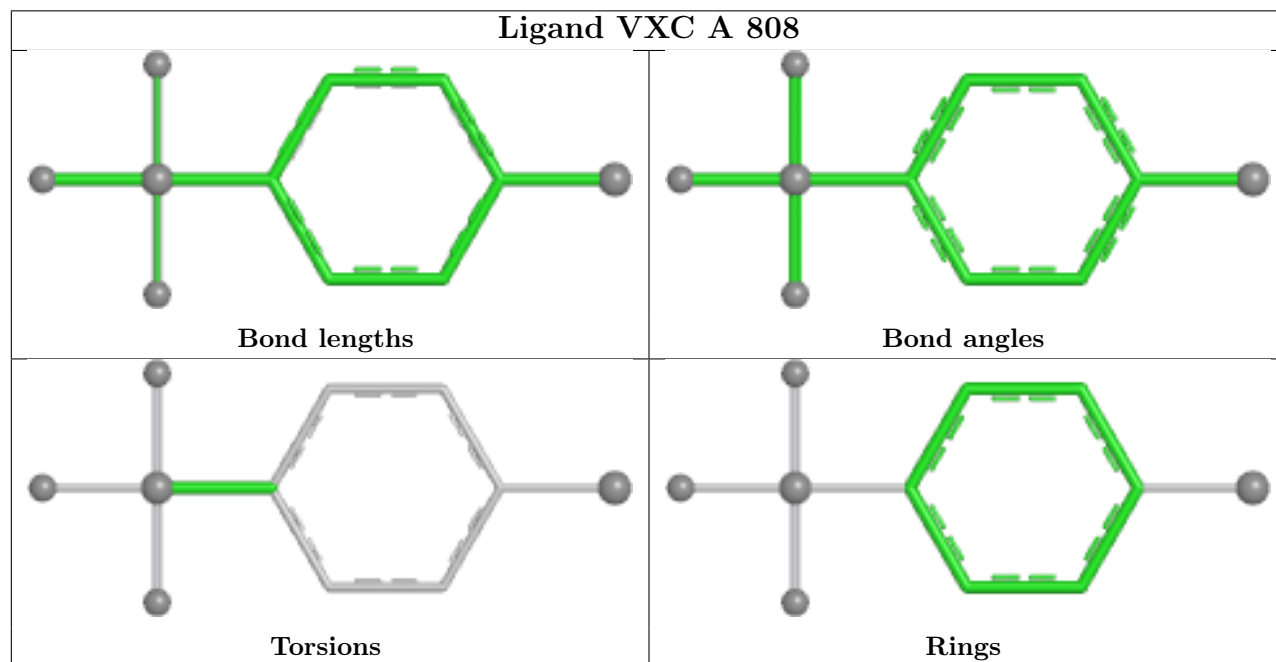
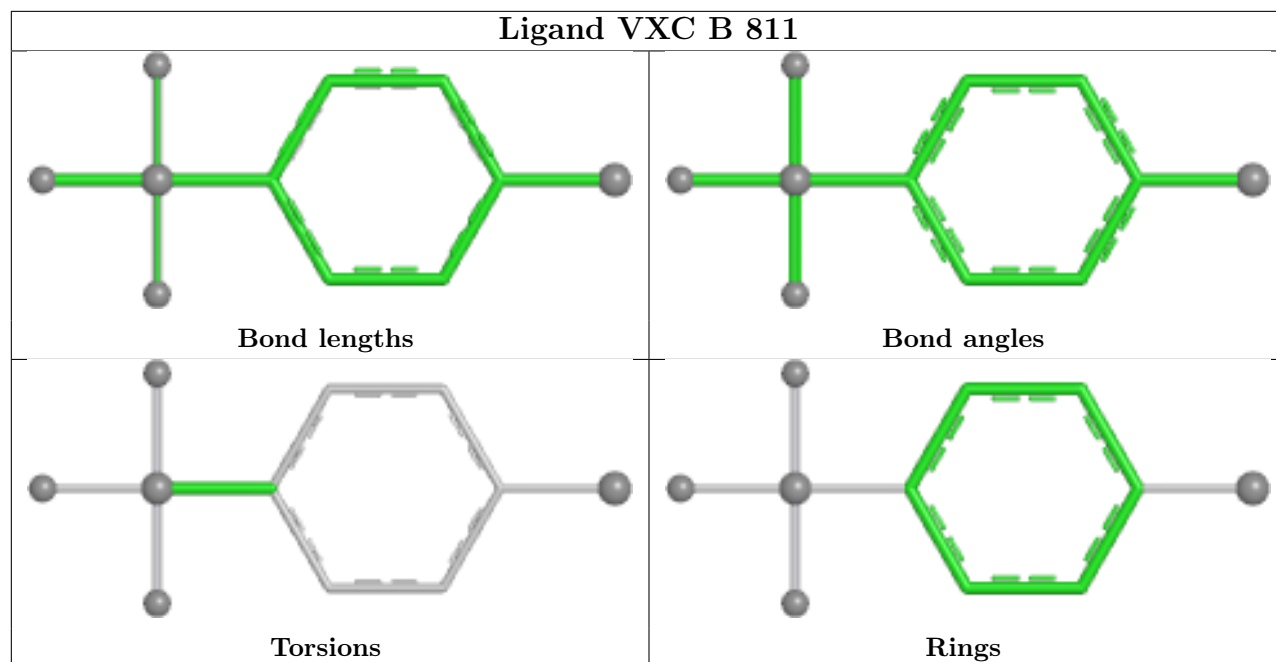
2 monomers are involved in 2 short contacts:

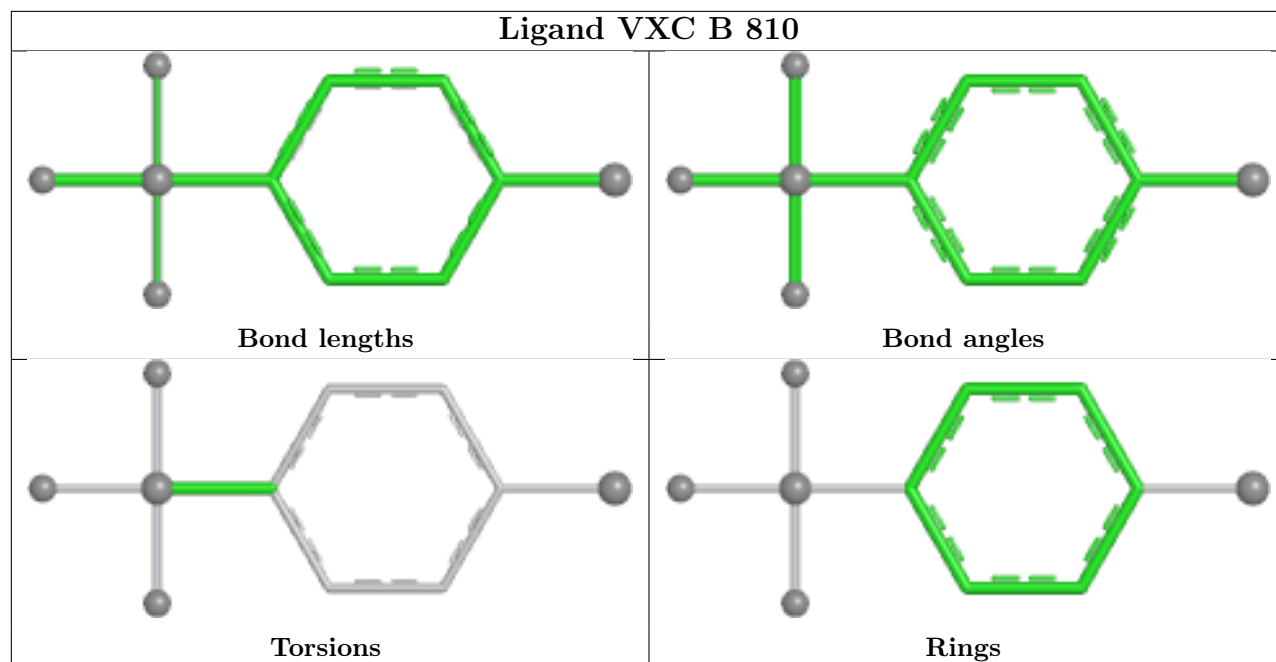
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	809	VXC	1	0
5	A	810	VXC	1	0

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%)	0.34	71 (9%) 13 10	18, 45, 115, 162	0
1	B	726/736 (98%)	0.01	31 (4%) 40 34	18, 37, 88, 120	0
2	C	400/403 (99%)	-0.09	22 (5%) 30 25	17, 34, 70, 138	0
2	D	401/403 (99%)	-0.13	22 (5%) 30 25	15, 29, 73, 129	0
All	All	2256/2278 (99%)	0.08	146 (6%) 25 20	15, 37, 96, 162	0

All (146) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	228	LEU	8.4
1	A	359	GLU	7.2
1	A	352	VAL	6.6
1	A	356	VAL	6.3
1	A	325	ILE	5.9
2	D	293	GLY	5.8
1	A	354	LYS	5.8
1	A	405	VAL	5.8
1	B	359	GLU	5.5
1	A	328	ILE	5.2
1	B	413	PHE	5.1
1	A	402	PHE	5.0
1	A	413	PHE	5.0
1	A	400	ALA	4.9
2	D	1	MET	4.8
1	A	331	LEU	4.7
1	A	349	TYR	4.7
1	B	358	LEU	4.5
1	A	404	GLY	4.4
1	A	358	LEU	4.4
1	A	575	GLY	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	2	SER	4.2
1	A	407	PHE	4.2
1	A	395	PRO	4.2
2	D	228	LEU	4.1
2	C	136	LEU	4.1
1	A	399	ALA	3.9
1	A	396	THR	3.9
2	D	389	CYS	3.9
1	A	423	PHE	3.9
1	A	357	SER	3.9
2	C	230	ALA	3.8
1	A	-6	HIS	3.8
1	A	454	ARG	3.8
1	B	360	ALA	3.8
1	A	401	ASP	3.7
1	B	355	ASP	3.7
1	A	429	ILE	3.7
1	A	432	PRO	3.7
2	D	301	THR	3.6
2	C	294	ALA	3.6
2	C	134	MET	3.6
1	A	397	ALA	3.5
1	A	406	ASP	3.5
2	D	297	VAL	3.5
2	D	225	PHE	3.4
2	D	390	ILE	3.3
1	A	427	GLU	3.3
2	C	295	ASP	3.3
1	A	412	VAL	3.2
1	B	574	ALA	3.2
1	B	421	LYS	3.2
2	D	300	LEU	3.2
1	A	451	GLY	3.2
1	B	720	SER	3.2
2	D	224	ALA	3.2
1	A	403	LYS	3.1
1	A	342	TYR	3.1
1	A	577	THR	3.1
2	C	301	THR	3.1
2	C	300	LEU	3.0
1	A	426	ILE	3.0
1	A	351	VAL	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	298	ILE	2.9
2	C	390	ILE	2.9
1	A	364	GLY	2.9
2	C	389	CYS	2.9
1	B	577	THR	2.9
1	A	433	ASN	2.8
1	A	341	ALA	2.8
1	A	350	GLU	2.8
1	A	398	ASP	2.8
2	D	294	ALA	2.8
1	A	355	ASP	2.8
1	B	412	VAL	2.8
1	B	689	PRO	2.7
2	D	134	MET	2.7
1	B	578	TYR	2.7
1	A	436	LEU	2.7
1	A	326	LYS	2.6
1	A	348	GLY	2.6
2	C	296	PRO	2.6
1	B	571	VAL	2.6
2	D	302	GLY	2.6
2	C	302	GLY	2.6
1	B	304	PHE	2.6
1	A	720	SER	2.5
2	D	292	SER	2.5
2	C	391	GLY	2.5
2	D	295	ASP	2.5
1	B	558	GLU	2.5
1	A	574	ALA	2.5
1	B	381	THR	2.5
1	A	361	ALA	2.5
1	A	441	SER	2.5
1	A	183	GLU	2.5
1	A	459	ILE	2.4
1	B	580	PRO	2.4
1	A	430	VAL	2.4
1	A	180	LYS	2.4
2	D	298	ILE	2.4
1	B	-13	SER	2.4
1	B	575	GLY	2.4
1	B	576	GLY	2.4
1	A	414	GLU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	339	GLY	2.3
2	C	297	VAL	2.3
1	A	333	ALA	2.3
2	D	135	GLY	2.3
1	B	433	ASN	2.3
1	A	321	GLY	2.3
1	B	599	LEU	2.3
1	A	338	ALA	2.3
2	C	394	MET	2.2
2	D	303	PRO	2.2
2	D	393	GLY	2.2
1	B	1	MET	2.2
1	A	480	LYS	2.2
1	A	360	ALA	2.2
1	A	367	TYR	2.2
2	C	303	PRO	2.2
2	C	393	GLY	2.2
1	A	428	ASP	2.2
1	B	357	SER	2.2
1	B	-8	HIS	2.2
1	A	443	LEU	2.1
1	A	-7	HIS	2.1
1	A	420	HIS	2.1
1	B	397	ALA	2.1
2	C	229	ALA	2.1
1	A	353	LEU	2.1
1	B	-9	HIS	2.1
2	C	395	GLY	2.1
1	B	579	GLN	2.1
1	A	376	LEU	2.1
1	A	555	LEU	2.1
1	B	21	ASP	2.0
2	C	135	GLY	2.0
1	A	468	ASP	2.0
2	D	229	ALA	2.0
1	B	335	MET	2.0
1	B	396	THR	2.0
1	A	394	THR	2.0
2	D	304	THR	2.0
2	C	299	MET	2.0
1	A	327	ARG	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.

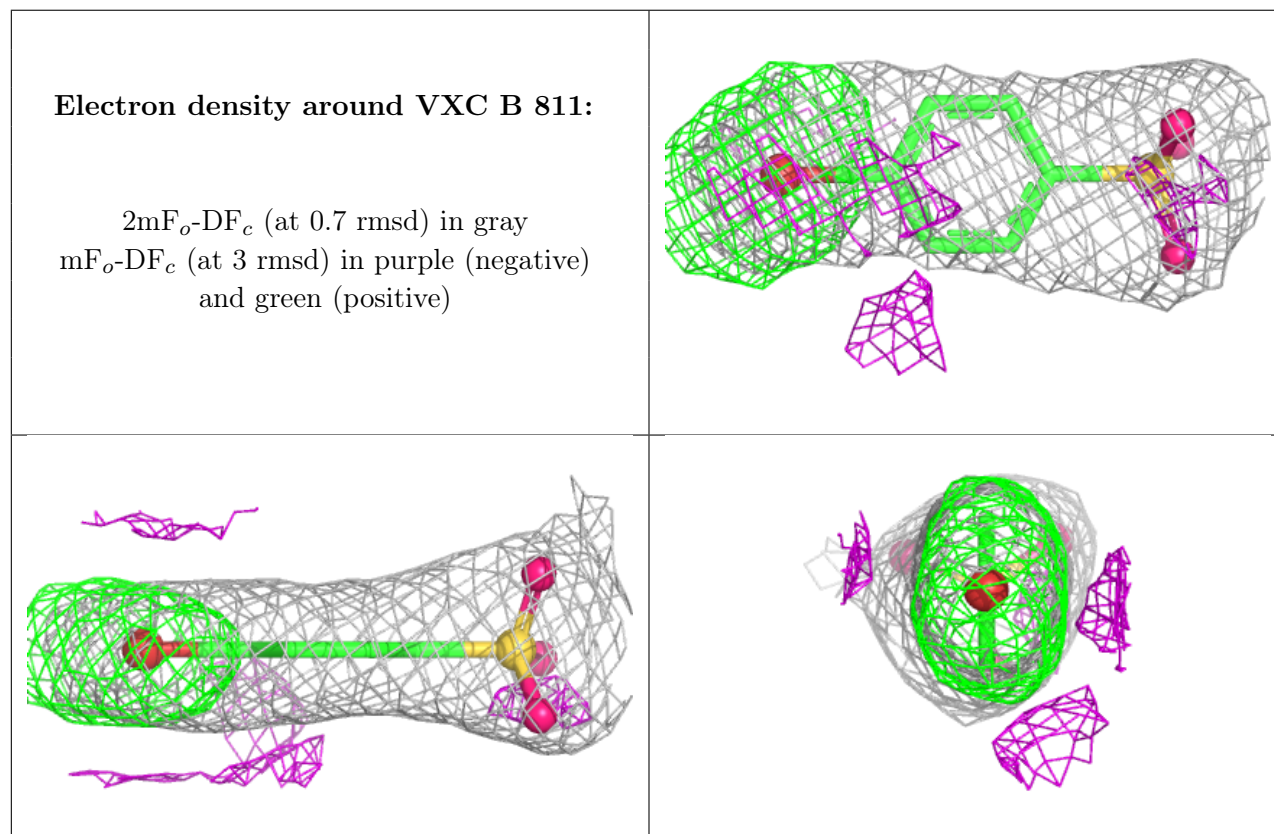
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	B	808	5/5	0.52	0.14	112,116,132,155	0
4	SO4	C	506	5/5	0.72	0.12	84,89,130,147	0
3	GOL	A	802	6/6	0.77	0.19	38,48,54,68	0
4	SO4	B	807	5/5	0.78	0.09	78,79,123,133	0
4	SO4	C	507	5/5	0.78	0.12	89,114,122,159	0
4	SO4	C	502	5/5	0.79	0.12	88,91,94,116	0
4	SO4	A	807	5/5	0.79	0.11	77,86,109,112	0
3	GOL	B	802	6/6	0.80	0.15	32,41,46,50	0
5	VXC	B	811	11/11	0.80	0.23	25,43,68,376	0
3	GOL	B	803	6/6	0.81	0.14	38,46,55,64	0
5	VXC	A	809	11/11	0.82	0.18	54,86,102,201	0
4	SO4	D	502	5/5	0.83	0.13	65,73,84,84	0
4	SO4	A	806	5/5	0.84	0.09	72,87,113,132	0
4	SO4	D	501	5/5	0.85	0.17	41,53,72,82	0
4	SO4	D	506	5/5	0.86	0.13	31,38,50,56	5
5	VXC	A	808	11/11	0.87	0.14	47,76,97,168	0
4	SO4	A	804	5/5	0.88	0.11	81,85,128,130	0
5	VXC	B	810	11/11	0.89	0.12	52,59,80,148	0
4	SO4	C	503	5/5	0.89	0.12	62,69,76,110	0
4	SO4	B	805	5/5	0.89	0.21	52,74,95,100	0
4	SO4	D	504	5/5	0.89	0.14	40,55,76,102	0
4	SO4	C	501	5/5	0.90	0.10	59,63,70,70	5
3	GOL	A	801	6/6	0.90	0.13	23,38,43,44	0
4	SO4	D	505	5/5	0.91	0.11	43,43,78,107	0
4	SO4	B	806	5/5	0.91	0.10	43,49,59,63	0
3	GOL	B	801	6/6	0.92	0.12	19,36,41,42	0
4	SO4	A	805	5/5	0.92	0.10	53,60,85,89	0

Continued on next page...

Continued from previous page...

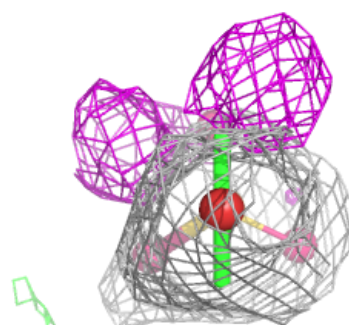
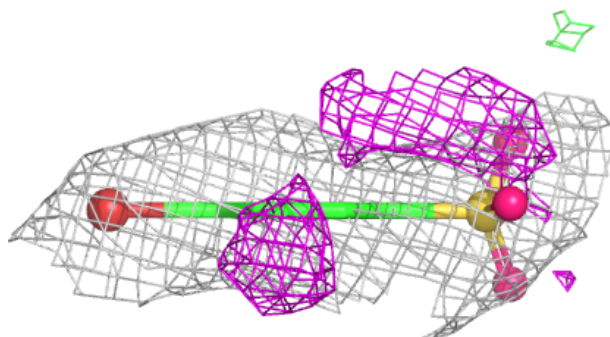
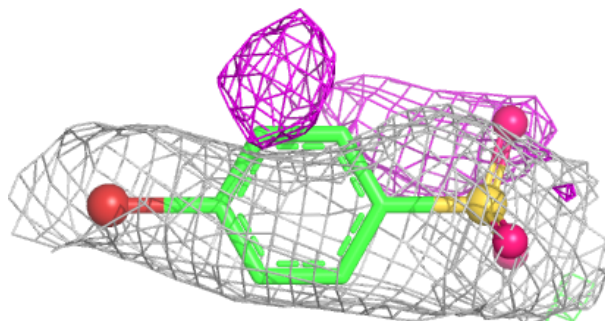
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	SO4	A	803	5/5	0.93	0.09	37,49,71,89	0
5	VXC	B	809	11/11	0.93	0.12	44,57,84,127	0
4	SO4	C	505	5/5	0.94	0.11	51,58,75,77	0
4	SO4	D	503	5/5	0.95	0.13	35,53,60,107	0
4	SO4	C	504	5/5	0.95	0.14	34,48,65,95	0
4	SO4	B	804	5/5	0.95	0.11	36,41,71,76	0
5	VXC	A	810	11/11	0.95	0.10	42,61,79,111	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.

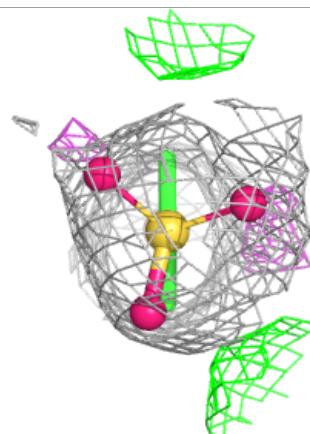
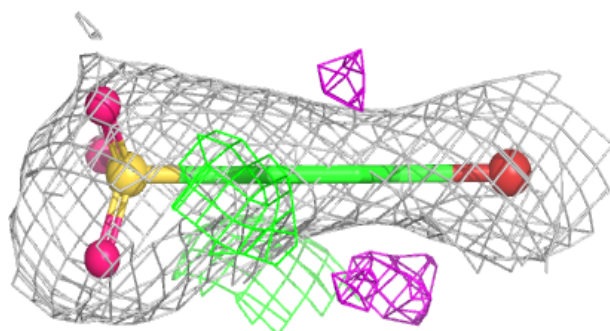
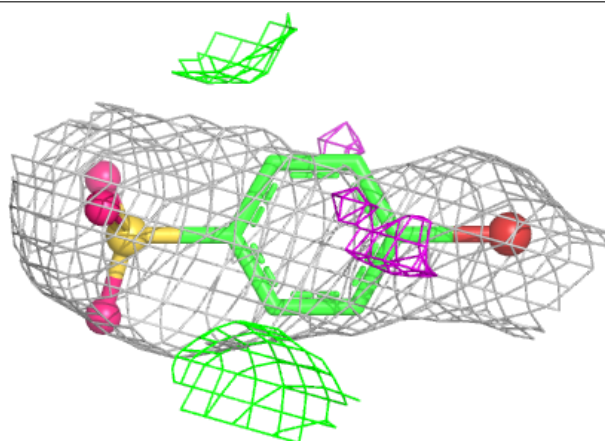


Electron density around VXC A 809:

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

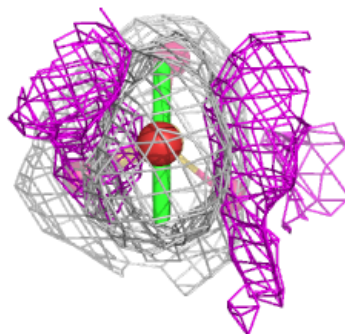
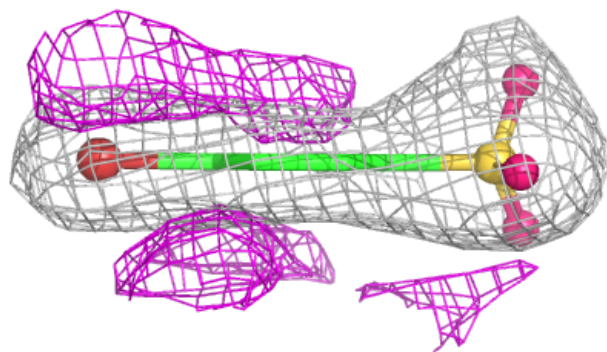
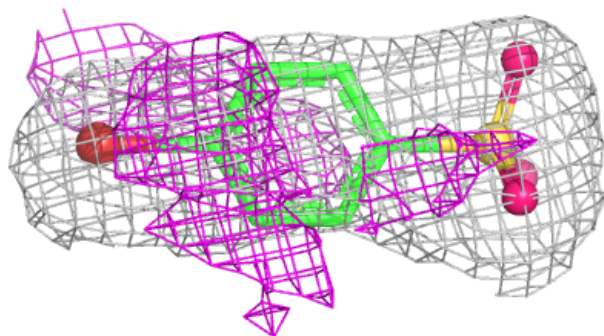
**Electron density around VXC A 808:**

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

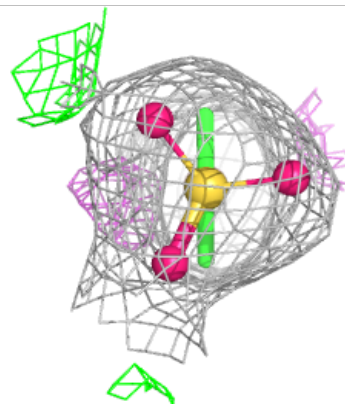
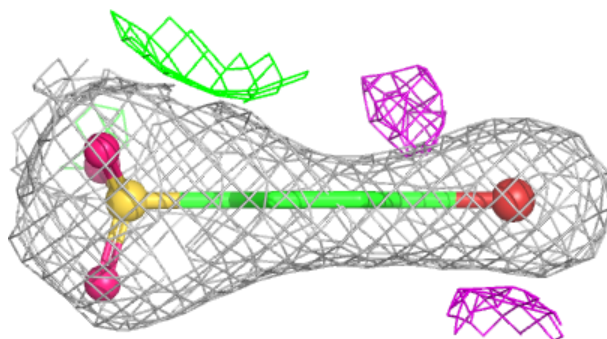
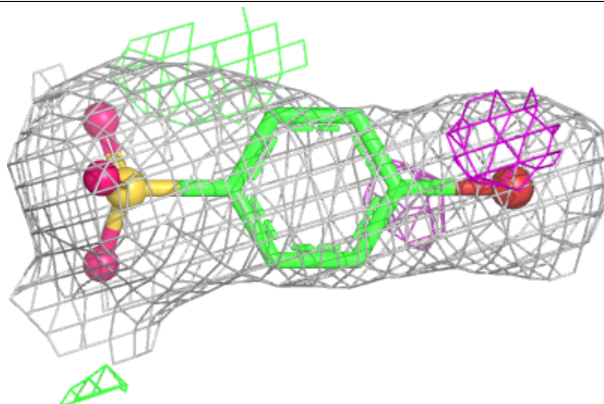


Electron density around VXC B 810:

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

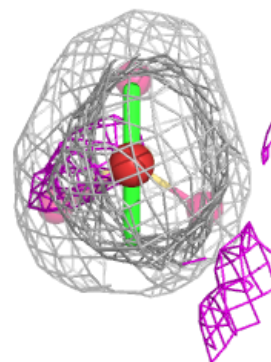
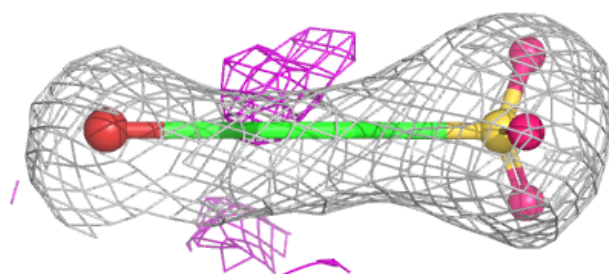
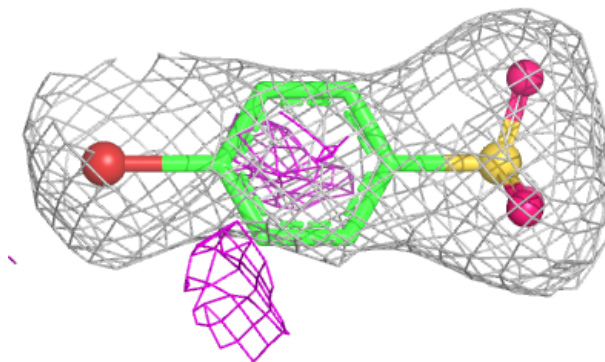
**Electron density around VXC B 809:**

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



Electron density around VXC 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.