



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 16, 2024 – 12:32 am GMT

PDB ID : 8OQT  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

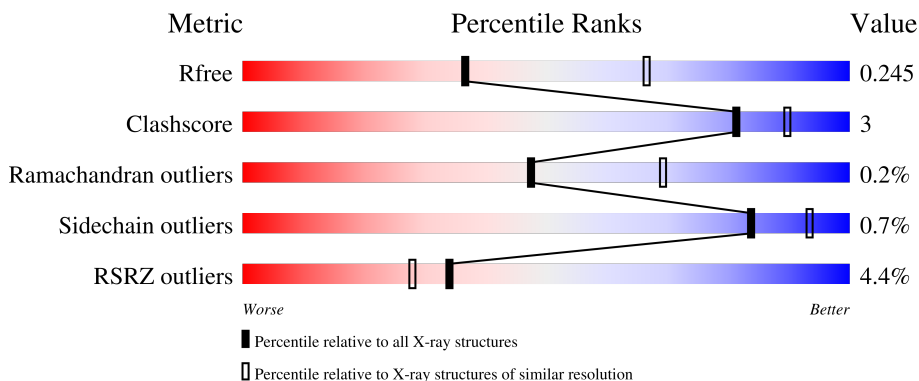
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

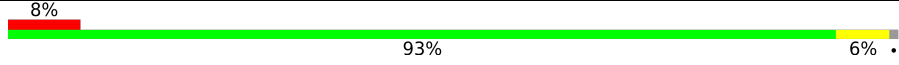
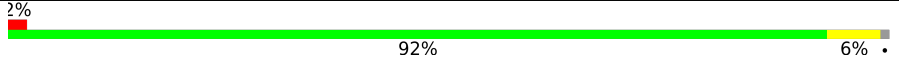
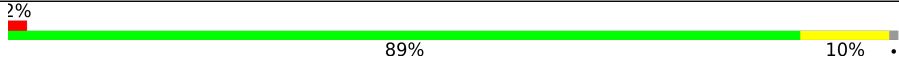
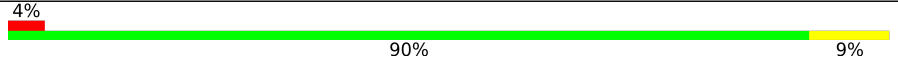
The reported resolution of this entry is 2.62 Å.

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))
$R_{free}$	130704	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (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  $\geq 3$ , 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	
1	B	736	
2	C	403	
2	D	403	

## 2 Entry composition [i](#)

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
			Total	C	N	O	S			
1	B	726	5391	3410	926	1034	21	0	0	0
1	A	729	5420	3428	934	1037	21	0	0	0

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

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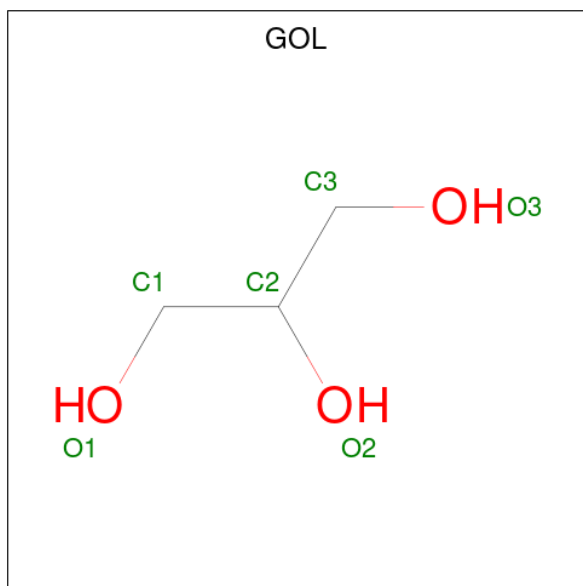
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	HIS	-	expression tag	UNP O53872
A	-5	SER	-	expression tag	UNP O53872
A	-4	GLN	-	expression tag	UNP O53872
A	-3	ASP	-	expression tag	UNP O53872
A	-2	PRO	-	expression tag	UNP O53872
A	-1	ASN	-	expression 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
			Total	C	N	O	S			
2	D	401	Total 2955	C 1845	N 524	O 570	S 16	0	0	0
2	C	400	Total 2944	C 1837	N 523	O 569	S 15	0	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



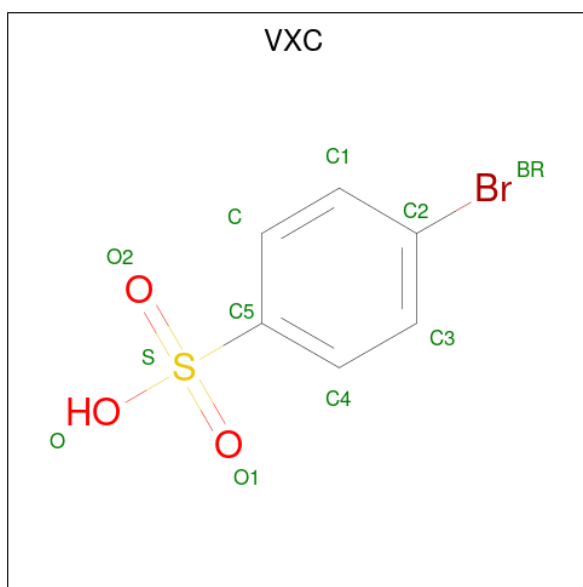
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	B	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	D	1	5	4	1	0	0
4	D	1	5	4	1	0	0

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

- Molecule 5 is 4-bromanylbenzenesulfonic acid (three-letter code: VXC) (formula: C<sub>6</sub>H<sub>5</sub>BrO<sub>3</sub>S) (labeled as "Ligand of Interest" by depositor).



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

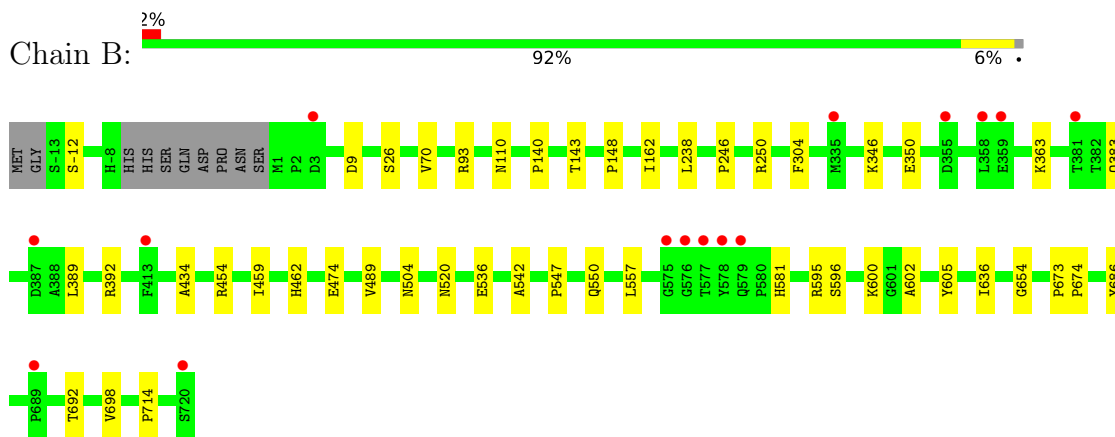
- Molecule 6 is water.

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		

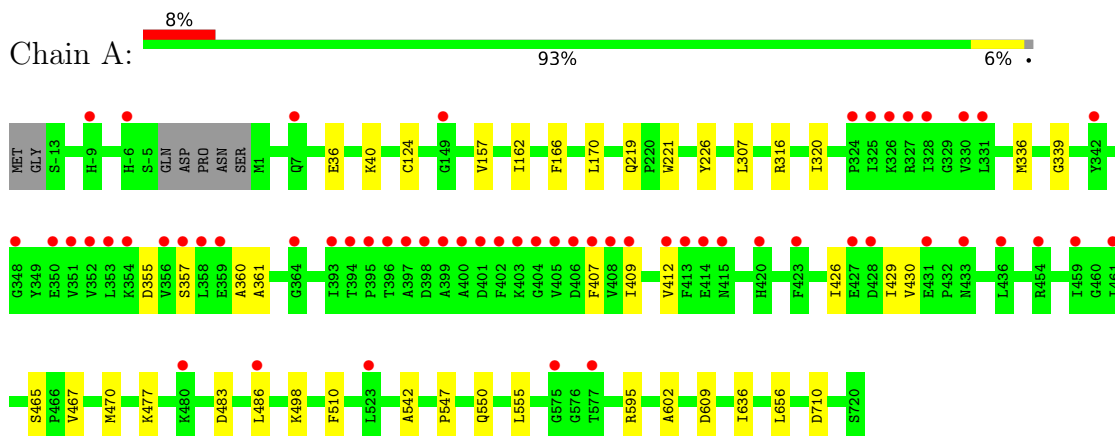
### 3 Residue-property plots [i](#)

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.

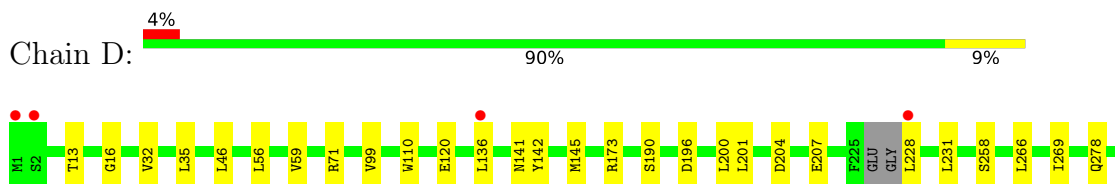
- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



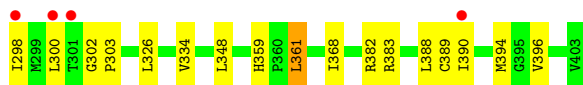
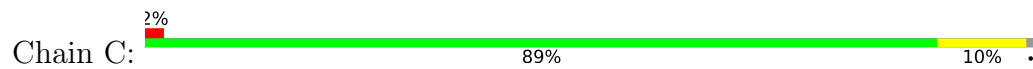
- Molecule 2: Putative acyltransferase Rv0859







• 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, $\alpha$ , $\beta$ , $\gamma$	247.48Å 133.23Å 115.93Å 90.00° 109.64° 90.00°	Depositor
Resolution (Å)	54.59 – 2.62 116.54 – 2.62	Depositor EDS
% Data completeness (in resolution range)	55.1 (54.59-2.62) 55.1 (116.54-2.62)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.50 (at 2.62Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.199 , 0.245 0.199 , 0.245	Depositor DCC
$R_{free}$ test set	2910 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.3	Xtrriage
Anisotropy	0.057	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 20.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	17002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, GOL, VXC

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	0.24	0/5523	0.45	0/7477
1	B	0.25	0/5492	0.46	0/7436
2	C	0.24	0/2987	0.49	0/4044
2	D	0.24	0/2998	0.49	0/4058
All	All	0.24	0/17000	0.47	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	21	1
1	B	5391	0	5415	25	1
2	C	2944	0	2960	25	0
2	D	2955	0	2981	25	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	30	0	0	0	0
5	A	33	0	0	0	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	88	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 (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:C:223:PRO:HA	2:C:253:THR:HG22	1.95	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: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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:229:ALA:C	2:C:231:LEU:H	2.22	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
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
1:B:536:GLU:OE2	1:B:605:TYR:OH	2.27	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 [\(i\)](#)

### 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%)	685 (94%)	39 (5%)	1 (0%)	51	74
1	B	722/736 (98%)	695 (96%)	26 (4%)	1 (0%)	51	74
2	C	396/403 (98%)	378 (96%)	17 (4%)	1 (0%)	41	62
2	D	397/403 (98%)	379 (96%)	17 (4%)	1 (0%)	41	62
All	All	2240/2278 (98%)	2137 (95%)	99 (4%)	4 (0%)	47	69

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 [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	557/566 (98%)	553 (99%)	4 (1%)	84	93
1	B	554/566 (98%)	548 (99%)	6 (1%)	73	88
2	C	306/310 (99%)	304 (99%)	2 (1%)	84	93
2	D	308/310 (99%)	308 (100%)	0	100	100
All	All	1725/1752 (98%)	1713 (99%)	12 (1%)	84	93

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	9	ASP
1	B	110	ASN
1	B	304	PHE
1	B	350	GLU
1	B	363	LYS
1	B	383	GLN
2	C	62	VAL

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Mol	Chain	Res	Type
2	C	300	LEU
1	A	307	LEU
1	A	483	ASP
1	A	555	LEU
1	A	609	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
4	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.04	0
3	GOL	A	802	-	5,5,5	0.91	0	5,5,5	0.95	0
4	SO4	A	806	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXC	A	810	-	11,11,11	0.22	0	16,16,16	0.12	0
4	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	B	807	-	4,4,4	0.14	0	6,6,6	0.05	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	VXC	B	811	-	11,11,11	0.27	0	16,16,16	0.17	0
4	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	A	805	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXC	B	809	-	11,11,11	0.22	0	16,16,16	0.19	0
4	SO4	A	803	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	506	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.07	0
4	SO4	D	501	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	B	804	-	4,4,4	0.14	0	6,6,6	0.05	0
5	VXC	B	810	-	11,11,11	0.22	0	16,16,16	0.12	0
4	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.06	0
4	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	GOL	A	801	-	5,5,5	0.88	0	5,5,5	1.03	0
4	SO4	A	807	-	4,4,4	0.15	0	6,6,6	0.05	0
5	VXC	A	808	-	11,11,11	0.26	0	16,16,16	0.19	0
3	GOL	B	803	-	5,5,5	0.92	0	5,5,5	1.01	0
4	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.04	0
4	SO4	D	505	-	4,4,4	0.13	0	6,6,6	0.06	0
4	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.06	0
3	GOL	B	802	-	5,5,5	0.89	0	5,5,5	1.01	0
5	VXC	A	809	-	11,11,11	0.21	0	16,16,16	0.12	0
4	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	808	-	4,4,4	0.14	0	6,6,6	0.06	0
3	GOL	B	801	-	5,5,5	0.90	0	5,5,5	0.98	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
3	GOL	A	802	-	-	4/4/4/4	-
3	GOL	B	801	-	-	2/4/4/4	-
5	VXC	B	809	-	-	0/6/6/6	0/1/1/1
5	VXC	A	810	-	-	0/6/6/6	0/1/1/1
3	GOL	A	801	-	-	0/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-
5	VXC	A	809	-	-	0/6/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	VXC	B	810	-	-	0/6/6/6	0/1/1/1
5	VXC	B	811	-	-	0/6/6/6	0/1/1/1
5	VXC	A	808	-	-	0/6/6/6	0/1/1/1
3	GOL	B	803	-	-	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:

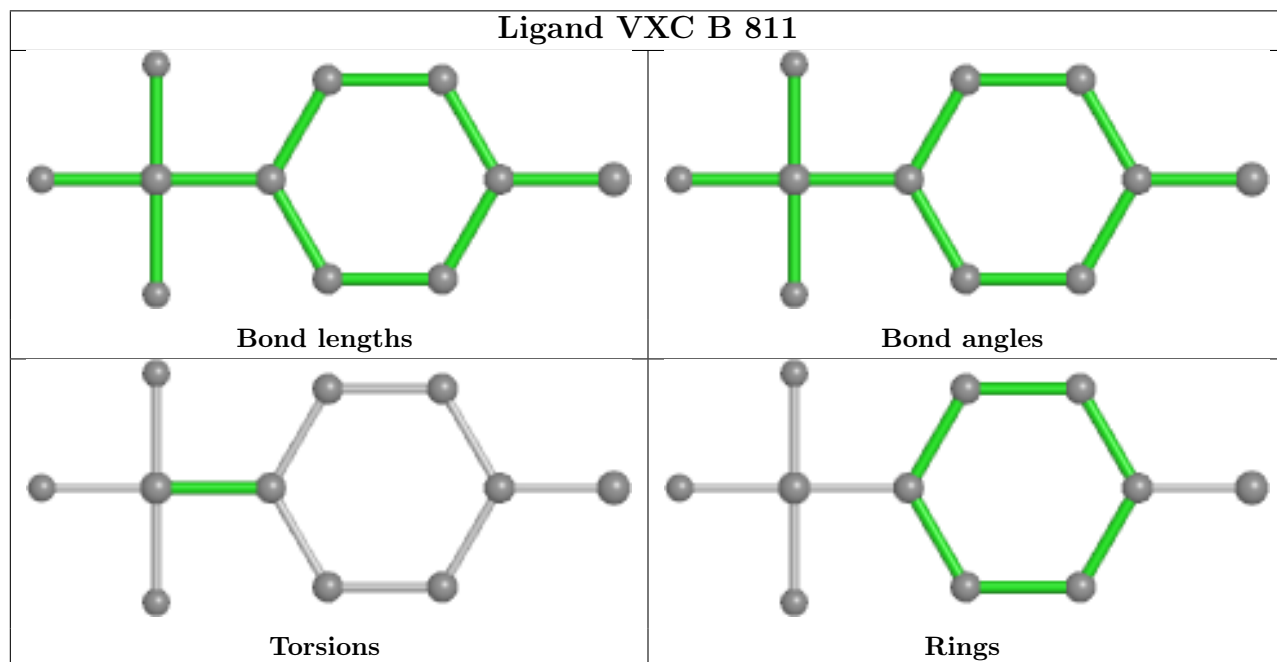
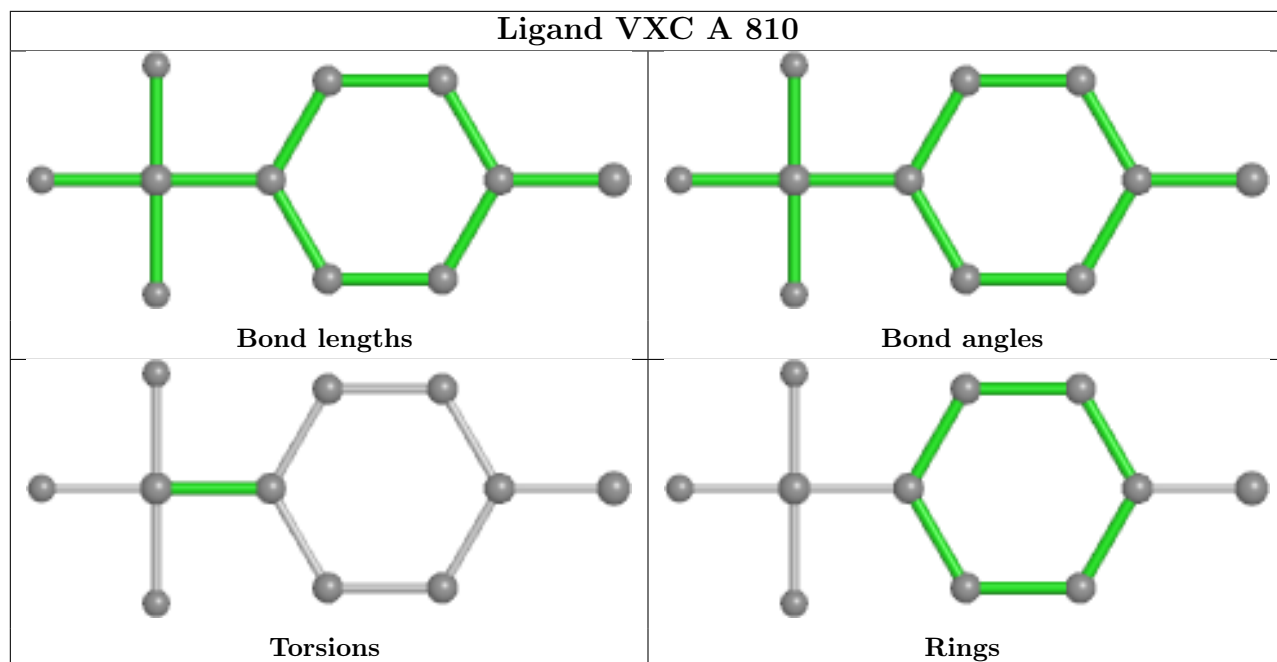
Mol	Chain	Res	Type	Atoms
3	B	801	GOL	C1-C2-C3-O3
3	B	802	GOL	O1-C1-C2-C3
3	B	803	GOL	O1-C1-C2-C3
3	A	802	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-C3
3	B	801	GOL	O2-C2-C3-O3
3	B	802	GOL	O1-C1-C2-O2
3	B	803	GOL	O1-C1-C2-O2
3	A	802	GOL	O2-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2

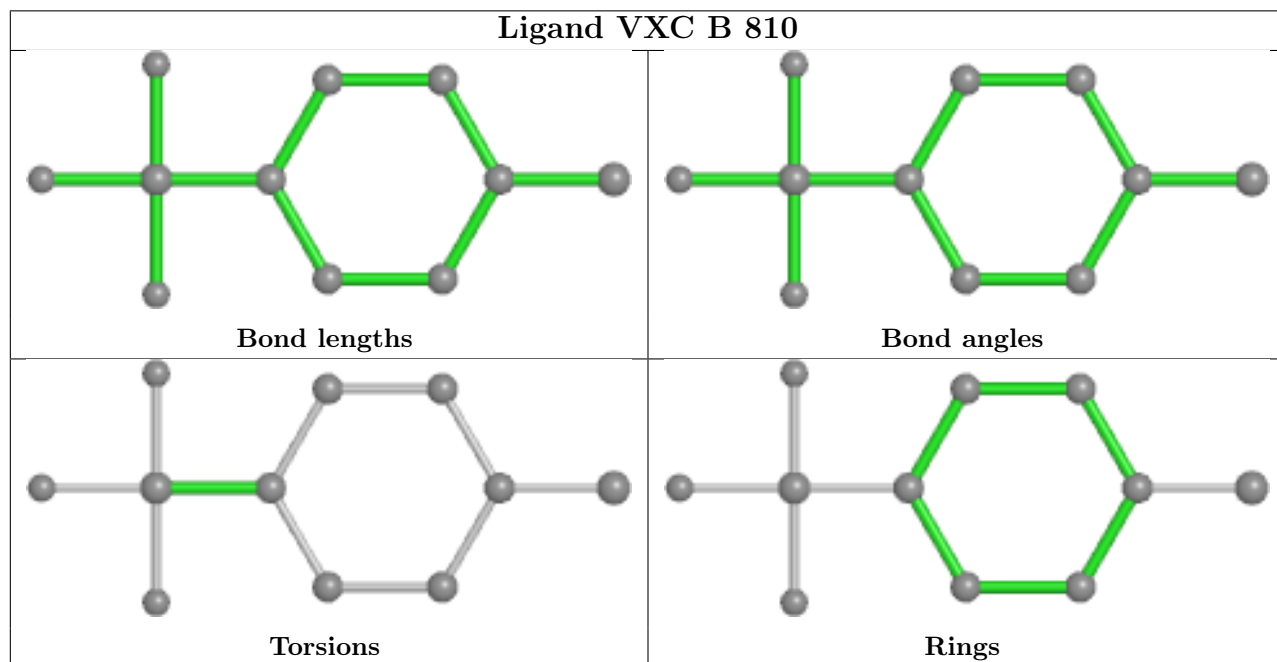
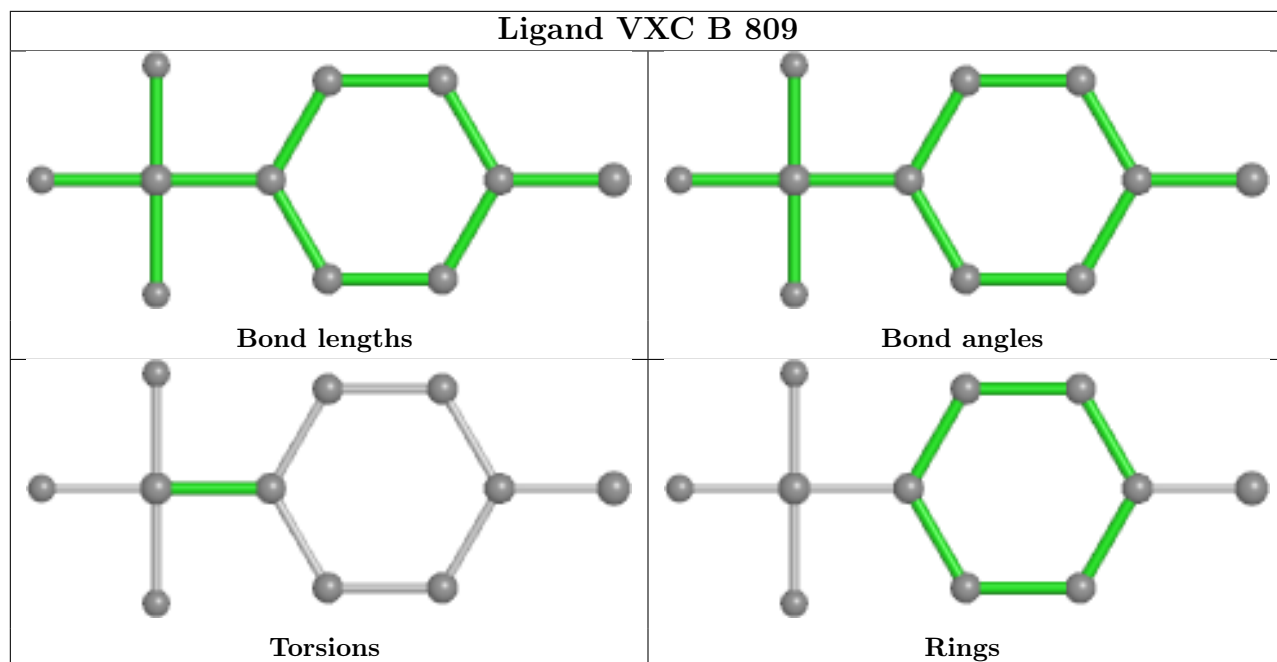
There are no ring outliers.

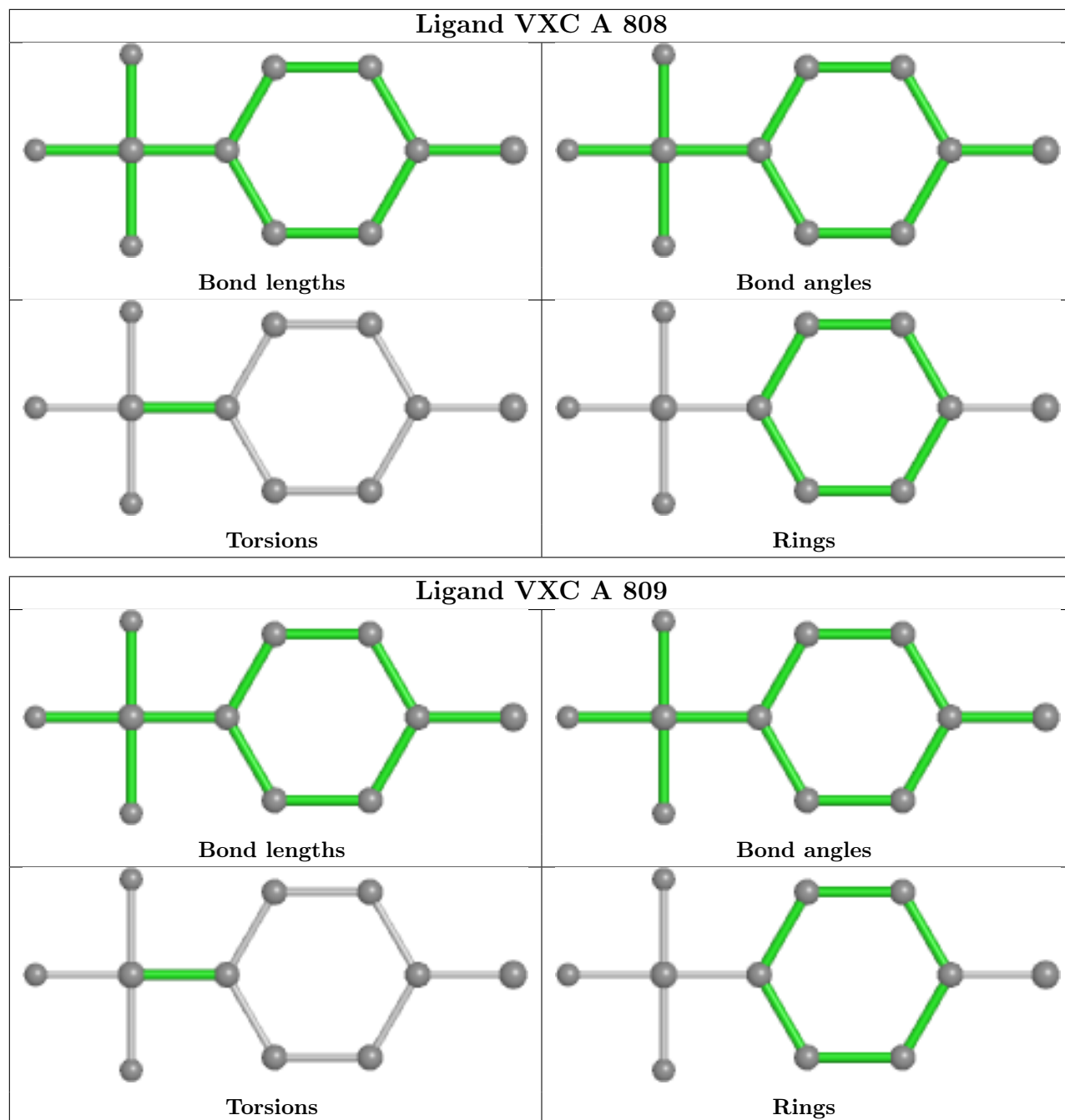
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	809	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	729/736 (99%)	0.41	59 (8%) 12 8	18, 45, 115, 162	0
1	B	726/736 (98%)	0.18	15 (2%) 63 58	18, 37, 88, 120	0
2	C	400/403 (99%)	0.23	10 (2%) 57 51	17, 34, 70, 138	0
2	D	401/403 (99%)	0.21	15 (3%) 41 35	15, 29, 73, 129	0
All	All	2256/2278 (99%)	0.27	99 (4%) 34 28	15, 37, 96, 162	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	228	LEU	9.5
1	A	401	ASP	9.1
2	C	294	ALA	7.8
2	D	2	SER	6.7
1	A	328	ILE	6.6
1	B	577	THR	6.2
1	A	433	ASN	6.1
1	A	352	VAL	6.0
2	C	301	THR	6.0
1	A	325	ILE	5.8
1	A	436	LEU	5.7
2	C	300	LEU	5.6
1	A	356	VAL	5.5
1	A	404	GLY	5.5
1	A	358	LEU	5.4
2	C	134	MET	5.3
1	A	354	LYS	5.3
1	A	-6	HIS	5.2
1	B	720	SER	5.2
1	A	400	ALA	5.1
1	A	407	PHE	5.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	331	LEU	5.0
1	A	398	ASP	4.6
2	C	295	ASP	4.6
1	A	359	GLU	4.6
1	B	359	GLU	4.5
2	D	1	MET	4.4
2	D	297	VAL	4.4
1	A	348	GLY	4.3
2	D	228	LEU	4.3
2	D	300	LEU	3.9
1	A	428	ASP	3.8
1	B	358	LEU	3.8
1	A	403	LYS	3.8
1	A	577	THR	3.6
2	C	296	PRO	3.6
2	C	297	VAL	3.4
1	A	413	PHE	3.4
1	A	423	PHE	3.3
1	A	351	VAL	3.3
1	B	689	PRO	3.3
1	A	326	LYS	3.2
1	A	454	ARG	3.2
1	A	396	THR	3.1
1	B	3	ASP	3.1
1	B	381	THR	3.1
1	A	350	GLU	3.1
2	D	294	ALA	3.0
2	C	390	ILE	3.0
1	A	427	GLU	2.9
1	A	364	GLY	2.9
1	B	335	MET	2.9
1	A	402	PHE	2.8
2	D	136	LEU	2.8
1	A	412	VAL	2.8
1	A	357	SER	2.8
1	A	459	ILE	2.7
1	A	405	VAL	2.7
2	D	298	ILE	2.7
2	C	298	ILE	2.7
1	A	415	ASN	2.7
1	B	413	PHE	2.7
1	B	575	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	486	LEU	2.6
1	A	342	TYR	2.6
1	A	327	ARG	2.6
1	A	461	ILE	2.6
2	D	304	THR	2.5
1	A	399	ALA	2.5
1	A	149	GLY	2.5
1	A	414	GLU	2.5
1	B	579	GLN	2.5
1	A	420	HIS	2.5
1	A	330	VAL	2.5
2	D	296	PRO	2.4
2	D	295	ASP	2.4
2	D	390	ILE	2.4
1	B	355	ASP	2.4
2	D	293	GLY	2.4
1	A	406	ASP	2.3
2	D	301	THR	2.3
1	A	523	LEU	2.3
1	A	409	ILE	2.3
1	A	575	GLY	2.2
2	D	389	CYS	2.2
1	B	387	ASP	2.2
1	A	397	ALA	2.2
1	A	480	LYS	2.2
1	A	408	VAL	2.2
1	B	578	TYR	2.2
1	A	393	ILE	2.2
1	A	353	LEU	2.2
1	B	576	GLY	2.1
1	A	394	THR	2.1
1	A	324	PRO	2.1
1	A	7	GLN	2.1
1	A	395	PRO	2.0
1	A	-9	HIS	2.0
1	A	431	GLU	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 [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

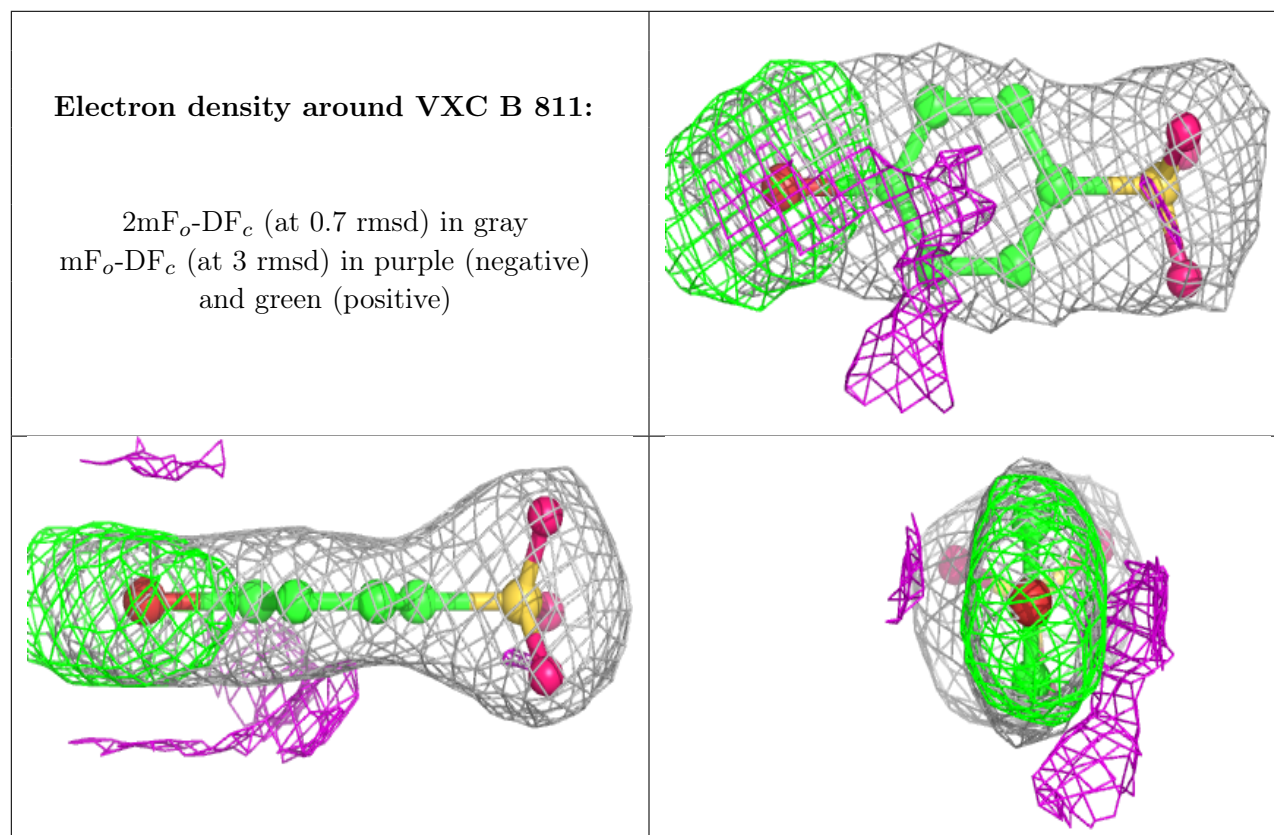
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	C	507	5/5	0.69	0.20	89,114,122,159	0
4	SO4	B	808	5/5	0.75	0.25	112,116,132,155	0
4	SO4	C	506	5/5	0.78	0.38	84,89,130,147	0
5	VXC	B	811	11/11	0.80	0.27	25,43,68,376	0
3	GOL	A	802	6/6	0.86	0.28	38,48,54,68	0
4	SO4	B	807	5/5	0.87	0.23	78,79,123,133	0
3	GOL	B	802	6/6	0.87	0.18	32,41,46,50	0
4	SO4	D	506	5/5	0.87	0.28	31,38,50,56	5
4	SO4	A	807	5/5	0.88	0.33	77,86,109,112	0
4	SO4	A	806	5/5	0.90	0.18	72,87,113,132	0
5	VXC	A	809	11/11	0.90	0.29	54,86,102,201	0
4	SO4	C	502	5/5	0.91	0.17	88,91,94,116	0
5	VXC	A	808	11/11	0.91	0.28	47,76,97,168	0
5	VXC	B	810	11/11	0.91	0.30	52,59,80,148	0
4	SO4	D	502	5/5	0.92	0.13	65,73,84,84	0
5	VXC	B	809	11/11	0.92	0.23	44,57,84,127	0
4	SO4	D	504	5/5	0.93	0.14	40,55,76,102	0
4	SO4	A	804	5/5	0.93	0.36	81,85,128,130	0
3	GOL	B	803	6/6	0.93	0.13	38,46,55,64	0
4	SO4	C	503	5/5	0.94	0.14	62,69,76,110	0
4	SO4	A	805	5/5	0.95	0.15	53,60,85,89	0
3	GOL	A	801	6/6	0.95	0.20	23,38,43,44	0
4	SO4	B	805	5/5	0.95	0.20	52,74,95,100	0
4	SO4	D	505	5/5	0.95	0.12	43,43,78,107	0
4	SO4	D	501	5/5	0.96	0.12	41,53,72,82	0
4	SO4	C	501	5/5	0.96	0.15	59,63,70,70	5
4	SO4	B	806	5/5	0.96	0.13	43,49,59,63	0
4	SO4	B	804	5/5	0.96	0.17	36,41,71,76	0
3	GOL	B	801	6/6	0.96	0.31	19,36,41,42	0
5	VXC	A	810	11/11	0.96	0.22	42,61,79,111	0
4	SO4	C	505	5/5	0.97	0.12	51,58,75,77	0
4	SO4	A	803	5/5	0.97	0.14	37,49,71,89	0

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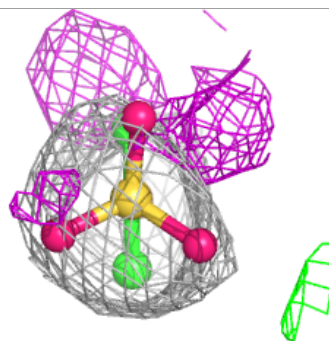
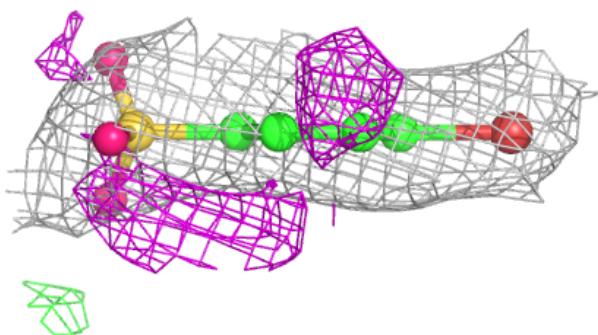
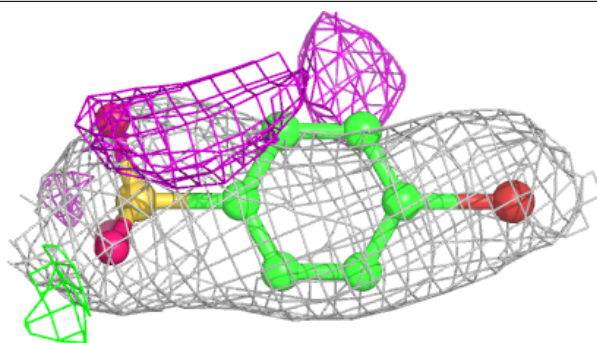
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	SO4	D	503	5/5	0.97	0.13	35,53,60,107	0
4	SO4	C	504	5/5	0.98	0.13	34,48,65,95	0

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.

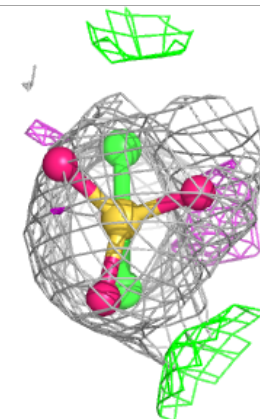
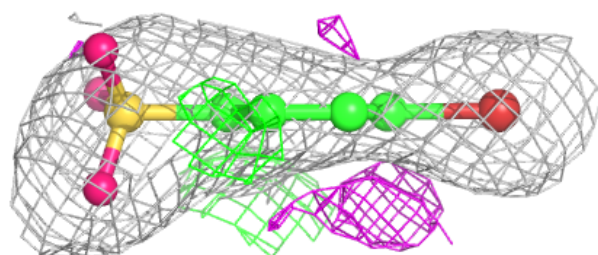
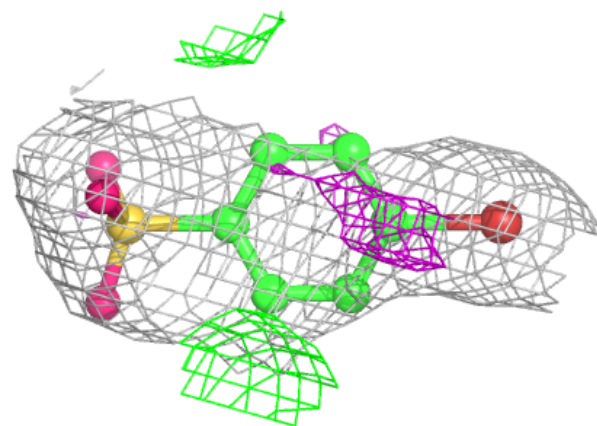


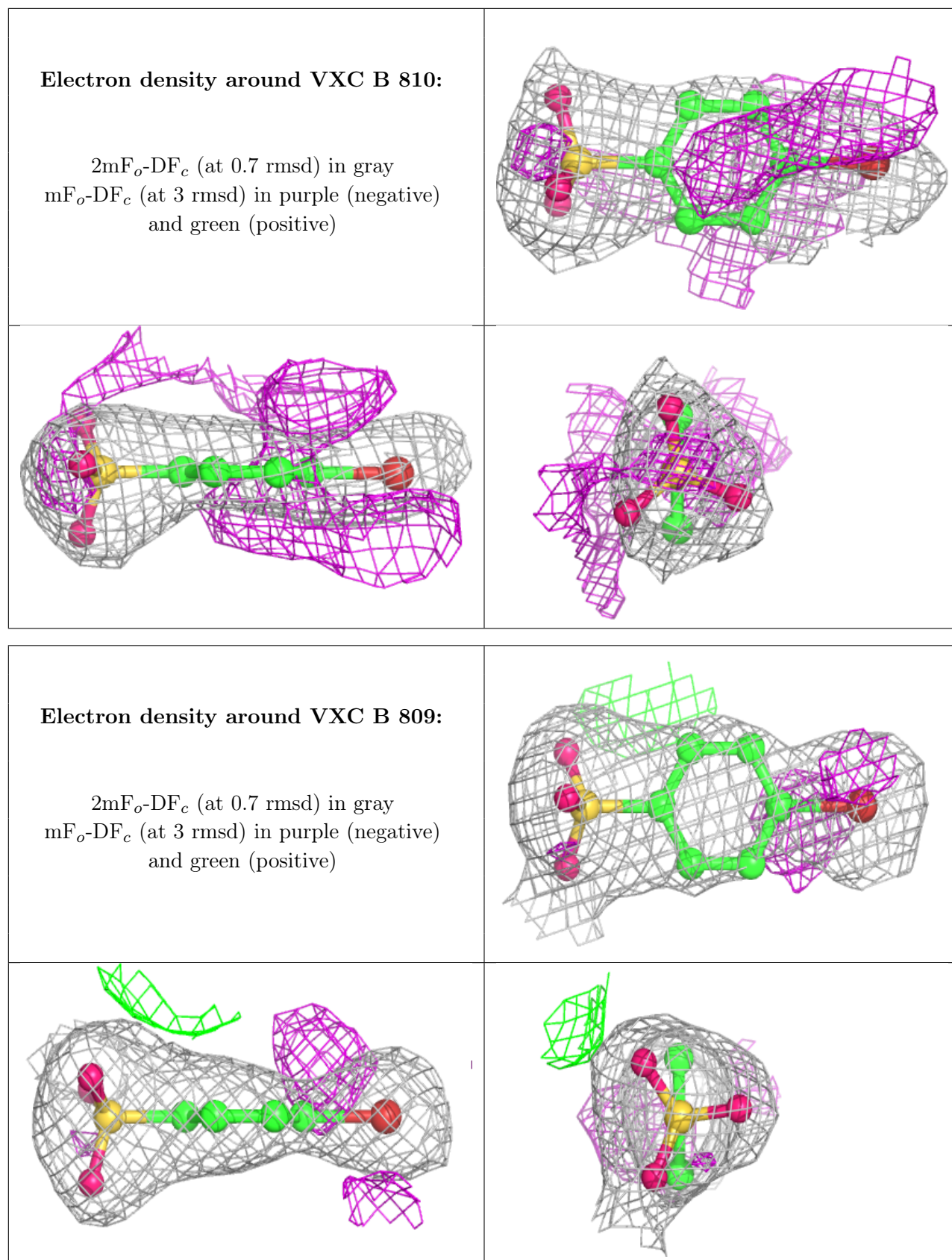
**Electron density around VXC A 809:**

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

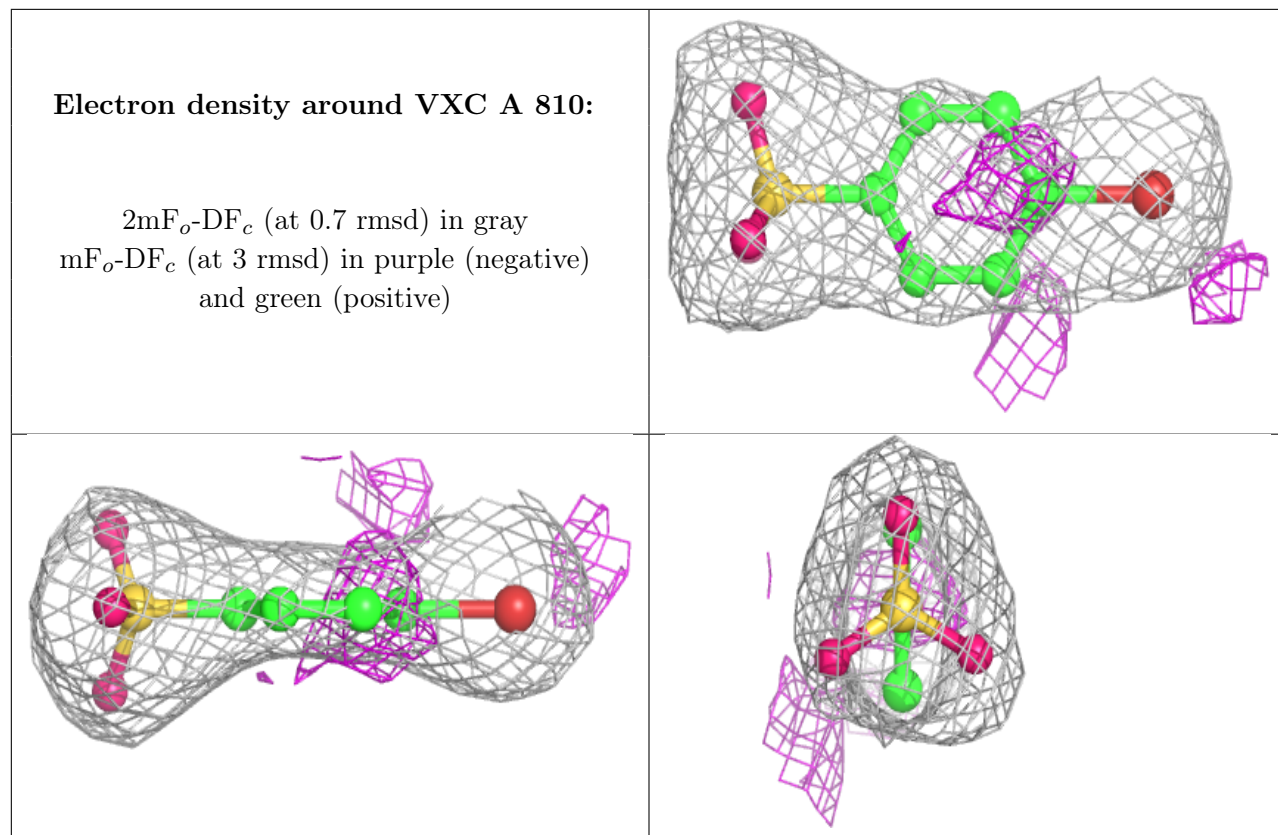
**Electron density around VXC A 808:**

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









## 6.5 Other polymers [i](#)

There are no such residues in this entry.