



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:42 PM UTC

PDB ID : 8OQN / pdb_00008oqn
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
in complex with Fragment-M-53
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2023-04-12
Resolution : 2.20 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

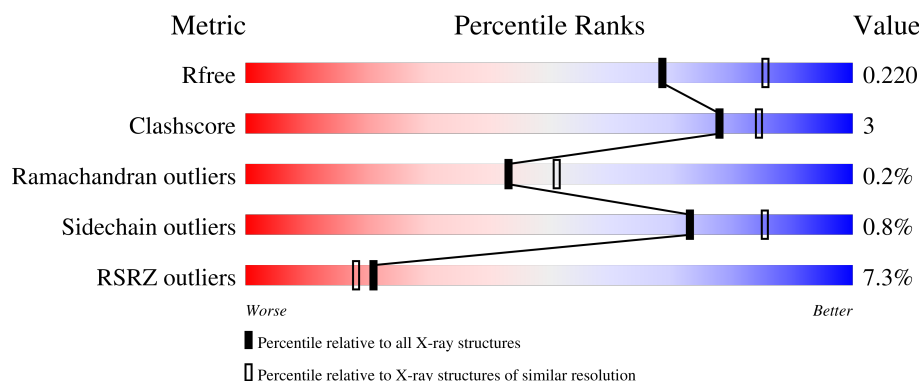
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	8% 93% 6%
1	B	736	9% 89% 10%
2	C	403	5% 94% 6%
2	D	403	5% 93% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17291 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 3-hydroxyacyl-CoA dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5430	3434	936	1039	21			
1	B	728	Total	C	N	O	S	0	0	0
			5414	3424	931	1038	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	402	Total	C	N	O	S	0	1	0
			2972	1857	526	574	15			
2	D	402	Total	C	N	O	S	0	1	0
			2972	1857	526	574	15			

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



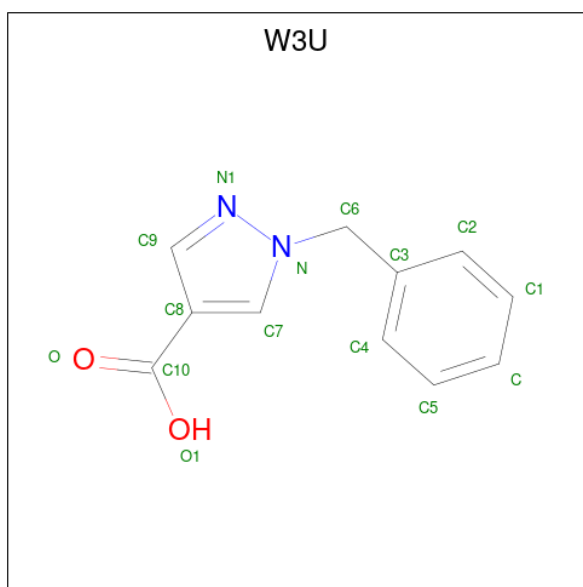
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	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	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		
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 1-benzyl-1H-pyrazole-4-carboxylic acid (CCD ID: W3U) (formula: C₁₁H₁₀N₂O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	A	1	Total	C	N	O	0	1
			30	22	4	4		
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	A	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	1
			30	22	4	4		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		
4	B	1	Total	C	N	O	0	0
			15	11	2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	37	Total	O	0	0
			37	37		

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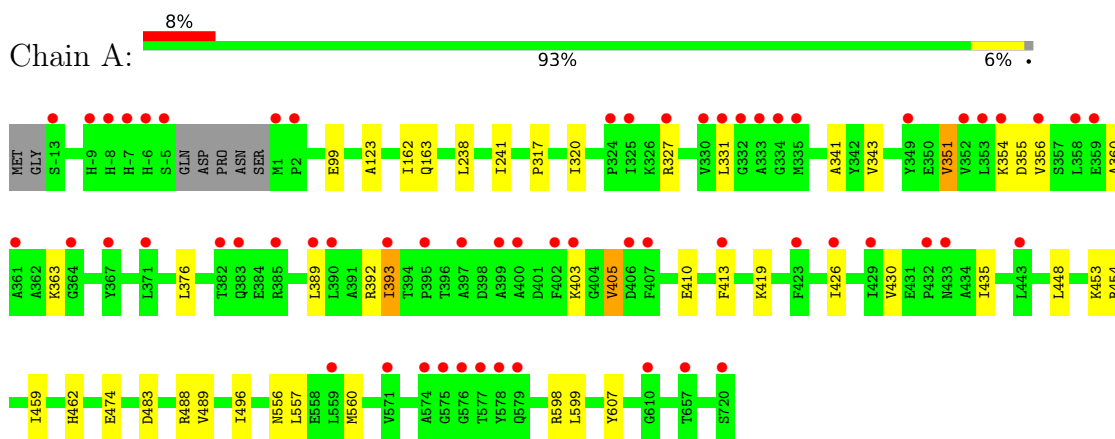
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	46	Total 46	O 46	0	0
5	C	57	Total 57	O 57	0	0
5	D	48	Total 48	O 48	0	0

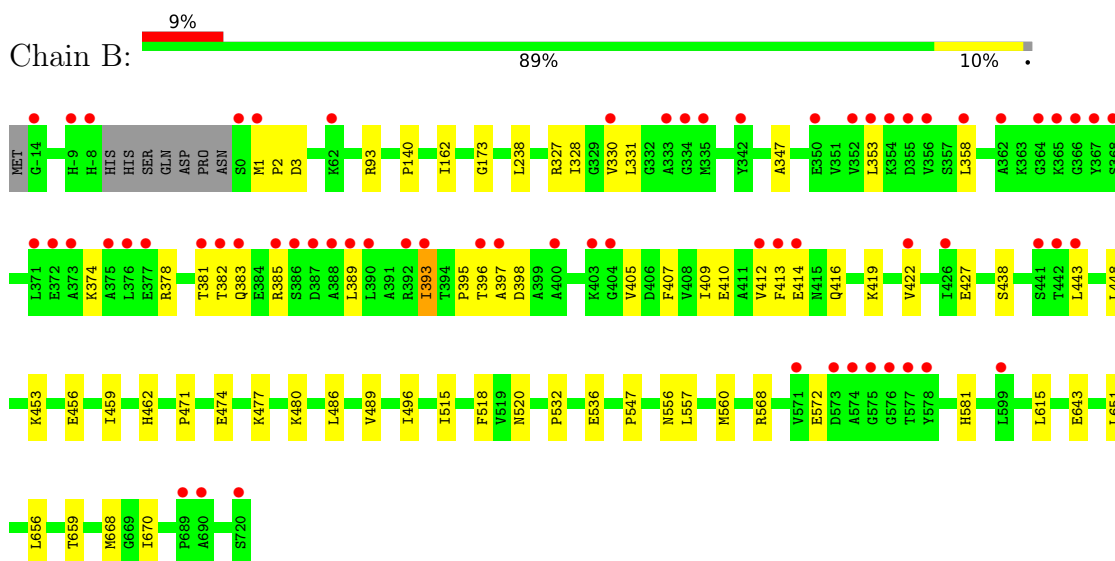
3 Residue-property plots [i](#)

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

- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

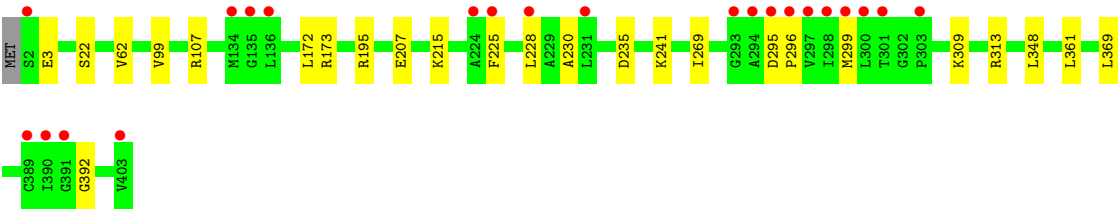


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase

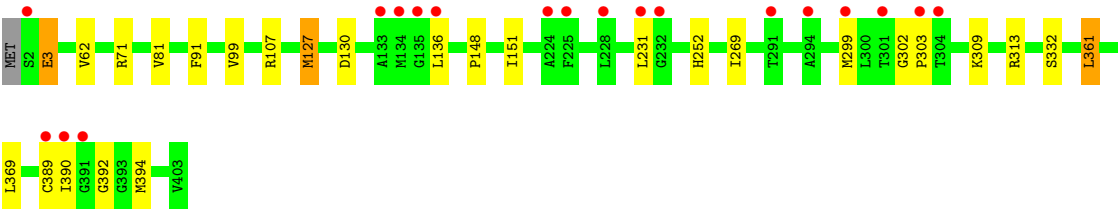
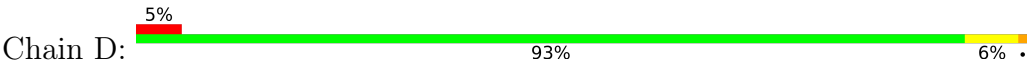


- Molecule 2: Putative acyltransferase Rv0859





● Molecule 2: Putative acyltransferase Rv0859



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	247.31Å 134.03Å 116.41Å 90.00° 109.70° 90.00°	Depositor
Resolution (Å)	48.98 – 2.20 48.98 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.98-2.20) 99.6 (48.98-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.221 0.192 , 0.220	Depositor DCC
R_{free} test set	9091 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17291	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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, W3U

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	0/5533	0.27	0/7487
1	B	0.11	0/5515	0.29	0/7462
2	C	0.11	0/3020	0.31	0/4089
2	D	0.10	0/3020	0.30	0/4089
All	All	0.10	0/17088	0.29	0/23127

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5430	0	5467	27	0
1	B	5414	0	5456	38	0
2	C	2972	0	2994	15	0
2	D	2972	0	2994	19	0
3	A	20	0	0	0	0
3	B	35	0	0	1	0
3	C	35	0	0	1	0
3	D	30	0	0	0	0
4	A	90	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	105	0	0	0	0
5	A	37	0	0	0	0
5	B	46	0	0	1	0
5	C	57	0	0	0	0
5	D	48	0	0	0	0
All	All	17291	0	16911	95	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 (95) 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:396:THR:HG22	1:B:398:ASP:H	1.36	0.89
1:A:360:ALA:HA	1:A:363:LYS:HE2	1.73	0.71
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.78	0.64
2:D:252:HIS:HE1	2:D:332:SER:H	1.44	0.64
1:B:410:GLU:HG3	1:B:438:SER:HA	1.82	0.62
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.83	0.61
1:B:557:LEU:HA	1:B:560:MET:HE3	1.83	0.61
1:B:471:PRO:HG2	1:B:668:MET:HE3	1.84	0.59
1:B:381:THR:HG22	1:B:383:GLN:H	1.65	0.59
1:A:405:VAL:HB	1:A:430:VAL:HG12	1.84	0.59
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.85	0.58
2:C:309:LYS:HE2	2:C:313:ARG:HH22	1.69	0.58
1:A:419:LYS:HD3	1:A:448:LEU:HD21	1.86	0.58
1:B:331:LEU:HB2	1:B:410:GLU:HA	1.87	0.56
2:C:299:MET:HE2	2:C:392:GLY:H	1.71	0.56
2:C:22:SER:OG	2:C:207:GLU:OE2	2.20	0.55
1:B:374:LYS:O	1:B:378:ARG:HG2	2.07	0.55
1:B:477:LYS:HD2	1:B:486:LEU:HD22	1.89	0.54
1:A:343:VAL:HG12	1:A:496:ILE:HB	1.89	0.54
2:C:173:ARG:NH2	2:C:348:LEU:O	2.32	0.54
1:B:358:LEU:N	1:B:397:ALA:HB2	2.23	0.54
1:B:427:GLU:OE1	1:B:453:LYS:N	2.35	0.54
1:A:355:ASP:OD1	1:A:356:VAL:N	2.40	0.53
2:D:91:PHE:HB2	2:D:390:ILE:HG23	1.90	0.53
2:D:252:HIS:CE1	2:D:332:SER:H	2.26	0.53
1:A:426:ILE:HG22	1:A:430:VAL:HG13	1.90	0.53
1:B:1:MET:HE3	1:B:2:PRO:HD2	1.91	0.52
1:B:459:ILE:HG21	1:B:489:VAL:HG21	1.93	0.51

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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	0.50
1:A:320:ILE:HD11	1:A:483:ASP:HB3	1.92	0.50
1:B:93:ARG:NH2	5:B:902:HOH:O	2.45	0.50
2:C:99:VAL:HG11	2:C:369:LEU:CD2	2.42	0.49
2:D:302:GLY:N	2:D:303:PRO:HD2	2.27	0.49
2:D:62:VAL:HG21	2:D:130:ASP:HA	1.94	0.48
2:D:389:CYS:C	2:D:390:ILE:HG13	2.39	0.48
1:B:419:LYS:HA	1:B:422:VAL:HG22	1.94	0.48
1:A:413:PHE:O	1:A:419:LYS:NZ	2.44	0.48
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.96	0.47
1:B:353:LEU:O	1:B:395:PRO:HA	2.14	0.47
1:B:568:ARG:O	1:B:572:GLU:HG3	2.14	0.47
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.97	0.47
1:A:241:ILE:HG22	2:D:231:LEU:HD21	1.97	0.47
2:D:99:VAL:HG11	2:D:369:LEU:HD22	1.97	0.47
2:C:62:VAL:HG12	2:D:62:VAL:HG22	1.96	0.46
2:D:390:ILE:HG21	2:D:394:MET:HE3	1.98	0.46
1:B:456:GLU:HA	1:B:480:LYS:O	2.16	0.46
2:D:3:GLU:O	2:D:107:ARG:HG2	2.15	0.46
1:B:412:VAL:HG22	1:B:413:PHE:H	1.81	0.46
1:B:532:PRO:HB2	1:B:615:LEU:HD13	1.98	0.46
2:C:392:GLY:O	2:D:71:ARG:NH2	2.38	0.46
1:A:99:GLU:HB3	1:A:123:ALA:O	2.15	0.46
1:B:416:GLN:HG3	1:B:443:LEU:HD22	1.97	0.46
2:D:303:PRO:HD3	2:D:389:CYS:HA	1.97	0.46
1:A:162:ILE:HD12	1:A:238:LEU:HD21	1.97	0.45
1:A:453:LYS:HG3	1:A:454:ARG:H	1.82	0.45
1:A:557:LEU:HA	1:A:560:MET:HE3	1.97	0.45
1:A:327:ARG:HB3	1:A:405:VAL:HG22	1.98	0.45
1:B:443:LEU:HD13	1:B:448:LEU:HD21	1.98	0.45
2:C:241:LYS:HE2	2:C:295:ASP:OD1	2.17	0.45
2:D:148:PRO:HD2	2:D:151:ILE:HD13	1.99	0.45
1:B:382:THR:HB	1:B:385:ARG:HB3	1.98	0.45
1:A:341:ALA:HB1	1:A:351:VAL:HG21	1.98	0.44
1:A:426:ILE:O	1:A:430:VAL:HG22	2.17	0.44
2:D:309:LYS:HE2	2:D:313:ARG:HH22	1.82	0.44
1:B:414:GLU:HA	1:B:419:LYS:NZ	2.31	0.44
2:C:195:ARG:NH1	3:C:503:SO4:O4	2.36	0.44
1:A:317:PRO:HB2	1:A:320:ILE:HD13	1.98	0.44
1:B:358:LEU:HD12	1:B:396:THR:O	2.17	0.44
2:C:3:GLU:O	2:C:107:ARG:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:299:MET:HE2	2:D:392:GLY:H	1.83	0.43
1:A:331:LEU:HB2	1:A:410:GLU:HA	1.99	0.43
1:B:347:ALA:HB2	1:B:496:ILE:HA	2.01	0.43
2:D:127:MET:HG3	2:D:361:LEU:HD11	1.99	0.43
1:A:435:ILE:HD11	1:A:488:ARG:HD3	1.99	0.43
1:A:351:VAL:HG22	1:A:393:ILE:HA	2.00	0.43
2:C:99:VAL:HG11	2:C:369:LEU:HD21	2.00	0.43
1:B:162:ILE:HD12	1:B:238:LEU:HD21	2.01	0.42
1:B:536:GLU:CD	1:B:547:PRO:HB2	2.44	0.42
1:A:403:LYS:O	1:A:430:VAL:HA	2.18	0.42
1:B:659:THR:N	3:B:805:SO4:O1	2.46	0.42
1:A:354:LYS:NZ	1:A:426:ILE:HD11	2.35	0.42
1:B:515:ILE:HD12	1:B:670:ILE:HB	2.02	0.42
1:B:330:VAL:HA	1:B:409:ILE:O	2.20	0.41
1:B:393:ILE:H	1:B:393:ILE:HG13	1.67	0.41
2:C:172:LEU:HD22	2:C:215:LYS:HG3	2.03	0.41
1:A:163:GLN:NE2	4:A:807[A]:W3U:N1	2.69	0.41
1:B:327:ARG:HB2	1:B:405:VAL:HA	2.03	0.41
1:B:518:PHE:HB2	1:B:643:GLU:CD	2.45	0.41
1:A:598:ARG:HG3	1:A:607:TYR:CE2	2.56	0.40
2:C:296:PRO:HD3	2:D:81:VAL:HG11	2.02	0.40
1:A:392:ARG:H	1:A:392:ARG:HG2	1.56	0.40
2:C:225:PHE:O	2:C:230:ALA:HB2	2.22	0.40
1:B:140:PRO:HA	1:B:173:GLY:HA3	2.03	0.40
1:B:328:ILE:HG12	1:B:407:PHE:HB3	2.03	0.40
1:B:651:LEU:HD23	1:B:656:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	725/736 (98%)	697 (96%)	27 (4%)	1 (0%)	48	57
1	B	724/736 (98%)	696 (96%)	27 (4%)	1 (0%)	48	57
2	C	401/403 (100%)	390 (97%)	10 (2%)	1 (0%)	43	51
2	D	401/403 (100%)	391 (98%)	9 (2%)	1 (0%)	43	51
All	All	2251/2278 (99%)	2174 (97%)	73 (3%)	4 (0%)	43	51

All (4) Ramachandran outliers are listed below:

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

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	560/566 (99%)	554 (99%)	6 (1%)	65	79
1	B	558/566 (99%)	555 (100%)	3 (0%)	81	90
2	C	310/310 (100%)	308 (99%)	2 (1%)	78	89
2	D	310/310 (100%)	307 (99%)	3 (1%)	68	81
All	All	1738/1752 (99%)	1724 (99%)	14 (1%)	73	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	351	VAL
1	A	376	LEU
1	A	389	LEU
1	A	393	ILE
1	A	405	VAL
1	A	599	LEU
1	B	3	ASP

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Mol	Chain	Res	Type
1	B	389	LEU
1	B	393	ILE
2	C	228	LEU
2	C	235	ASP
2	D	3	GLU
2	D	127	MET
2	D	136	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	294	GLN
1	A	433	ASN
1	A	455	GLN
1	A	550	GLN
1	A	648	GLN
1	A	681	GLN
1	B	75	GLN
1	B	163	GLN
1	B	504	ASN
1	B	550	GLN
1	B	633	GLN
2	D	338	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

37 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.07	0
4	W3U	B	811	-	16,16,16	0.12	0	21,21,21	0.40	0
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.08	0
4	W3U	A	806	-	16,16,16	0.12	0	21,21,21	0.38	0
4	W3U	A	809	-	16,16,16	0.17	0	21,21,21	0.39	0
3	SO4	B	807	-	4,4,4	0.24	0	6,6,6	0.10	0
4	W3U	A	807[A]	-	16,16,16	0.15	0	21,21,21	0.38	0
3	SO4	B	803	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	806	-	4,4,4	0.23	0	6,6,6	0.09	0
3	SO4	B	802	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	501	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
4	W3U	A	805	-	16,16,16	0.16	0	21,21,21	0.40	0
4	W3U	A	807[B]	-	16,16,16	0.15	0	21,21,21	0.39	0
4	W3U	B	809[A]	-	16,16,16	0.16	0	21,21,21	0.38	0
4	W3U	B	813	-	16,16,16	0.20	0	21,21,21	0.45	0
4	W3U	B	810	-	16,16,16	0.15	0	21,21,21	0.41	0
4	W3U	B	808	-	16,16,16	0.15	0	21,21,21	0.37	0
4	W3U	B	809[B]	-	16,16,16	0.15	0	21,21,21	0.36	0
3	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	801	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	805	-	4,4,4	0.23	0	6,6,6	0.07	0
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.08	0
4	W3U	A	808	-	16,16,16	0.18	0	21,21,21	0.47	0
3	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	504	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.10	0
4	W3U	B	812	-	16,16,16	0.17	0	21,21,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	A	802	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	803	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	503	-	4,4,4	0.24	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
4	W3U	A	808	-	-	0/8/8/8	0/2/2/2
4	W3U	B	809[B]	-	-	0/8/8/8	0/2/2/2
4	W3U	B	812	-	-	0/8/8/8	0/2/2/2
4	W3U	A	805	-	-	0/8/8/8	0/2/2/2
4	W3U	B	811	-	-	0/8/8/8	0/2/2/2
4	W3U	A	807[B]	-	-	0/8/8/8	0/2/2/2
4	W3U	B	809[A]	-	-	0/8/8/8	0/2/2/2
4	W3U	B	813	-	-	0/8/8/8	0/2/2/2
4	W3U	A	806	-	-	0/8/8/8	0/2/2/2
4	W3U	A	809	-	-	2/8/8/8	0/2/2/2
4	W3U	B	810	-	-	0/8/8/8	0/2/2/2
4	W3U	B	808	-	-	2/8/8/8	0/2/2/2
4	W3U	A	807[A]	-	-	0/8/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

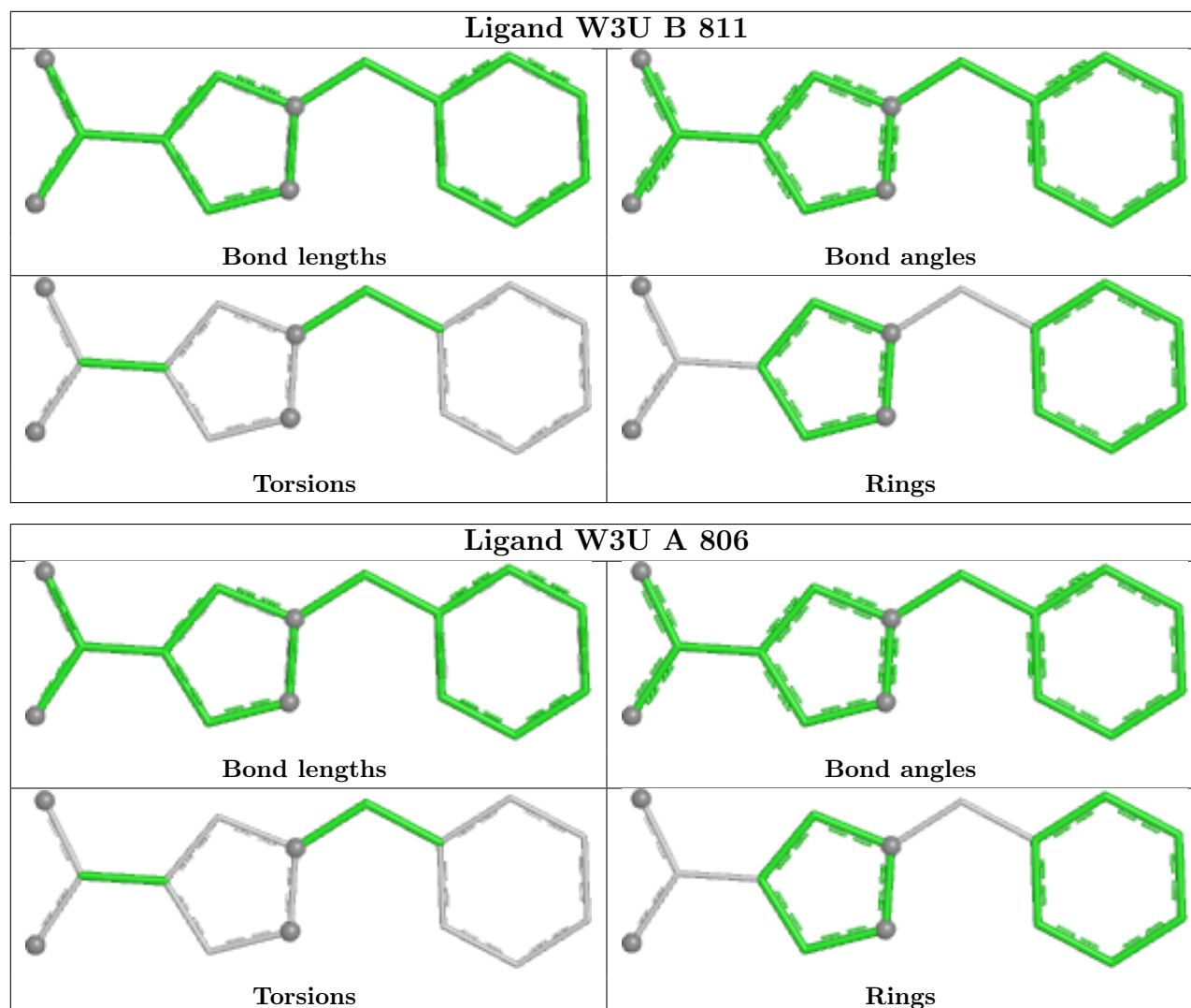
Mol	Chain	Res	Type	Atoms
4	B	808	W3U	C3-C6-N-C7
4	B	808	W3U	C3-C6-N-N1
4	A	809	W3U	C3-C6-N-C7
4	A	809	W3U	C3-C6-N-N1

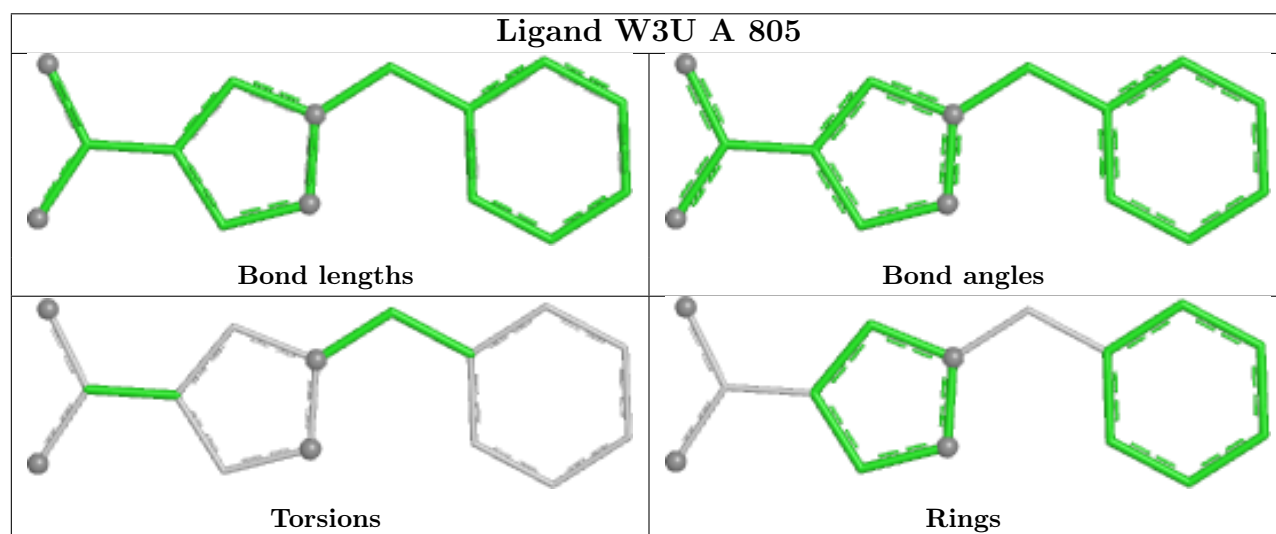
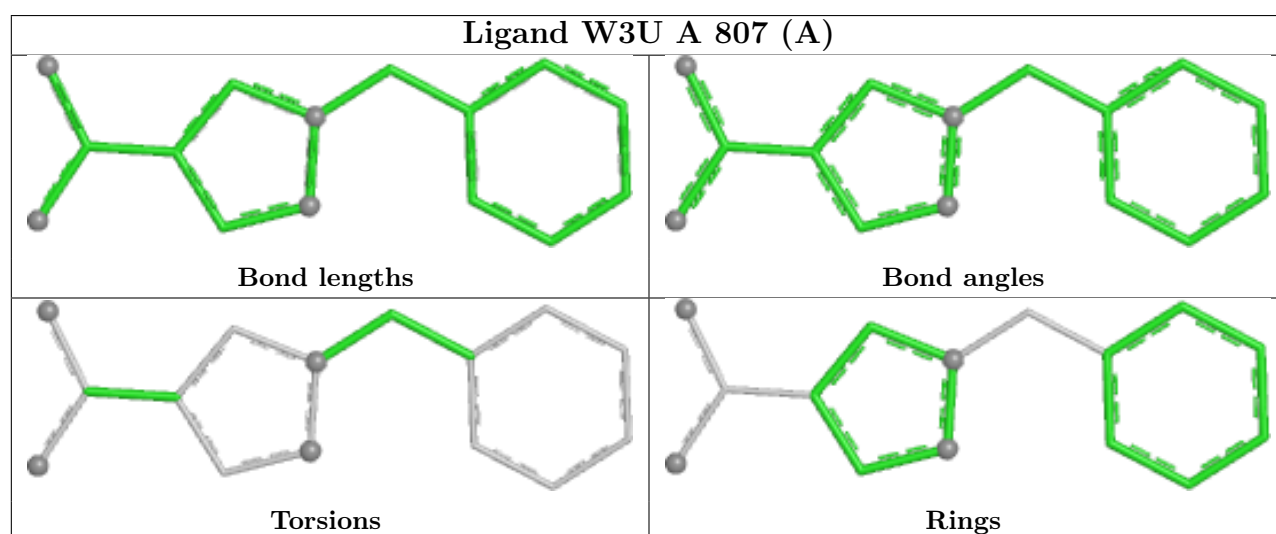
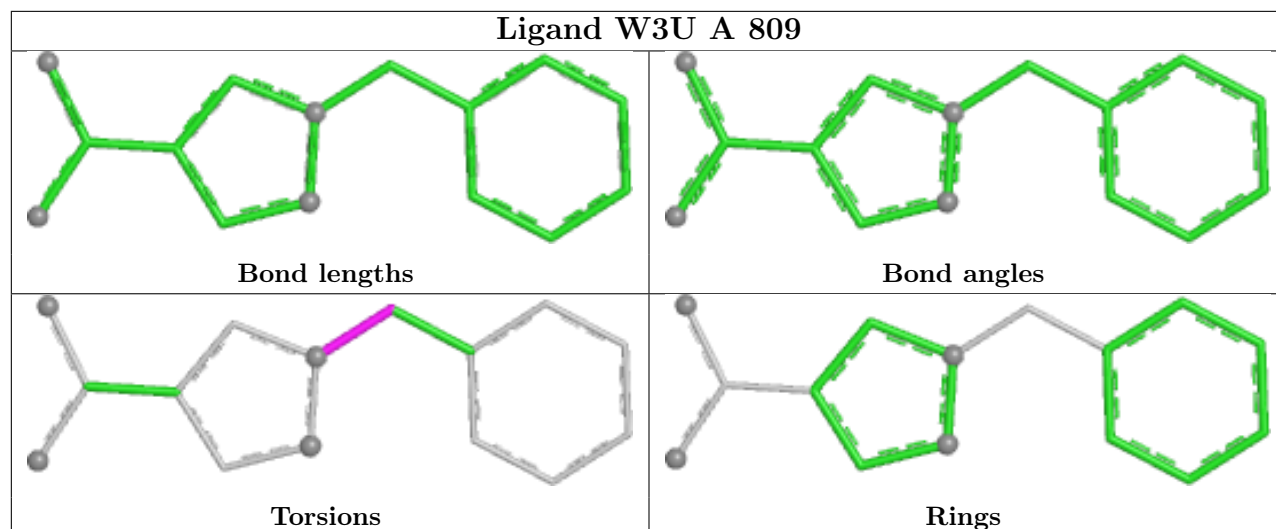
There are no ring outliers.

3 monomers are involved in 3 short contacts:

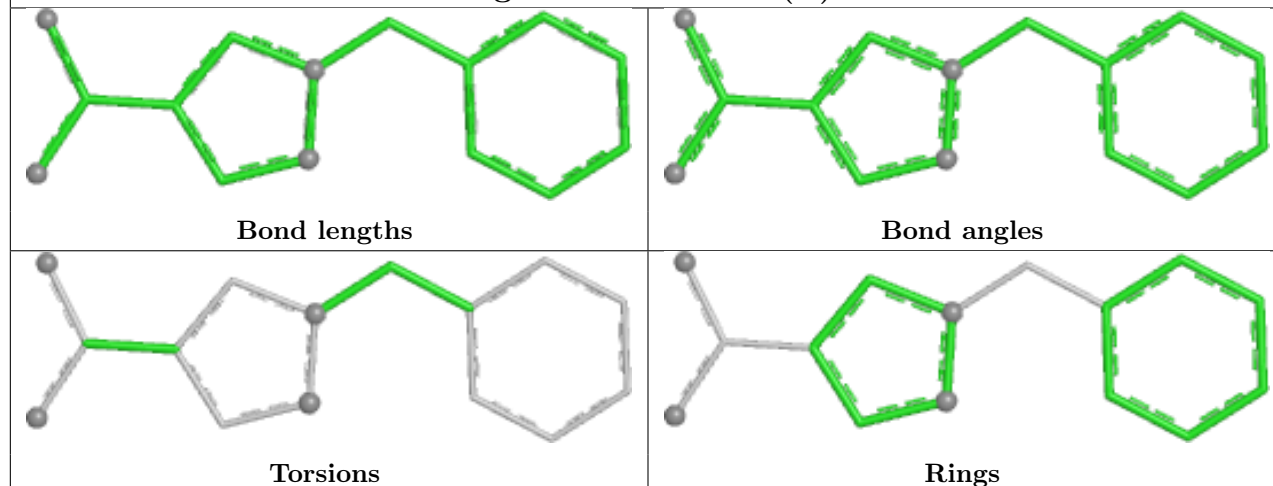
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807[A]	W3U	1	0
3	B	805	SO4	1	0
3	C	503	SO4	1	0

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.

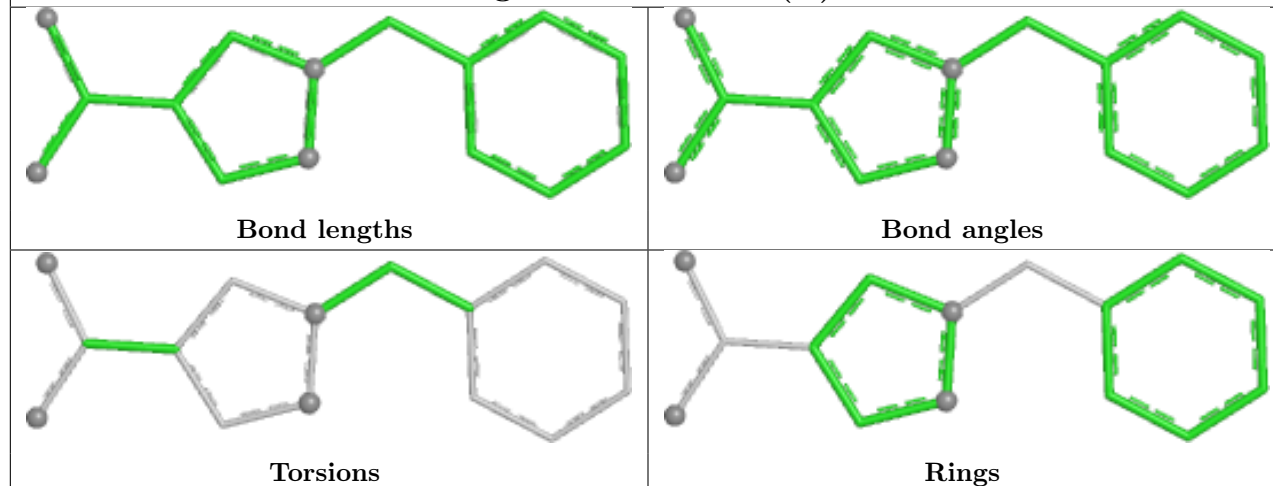




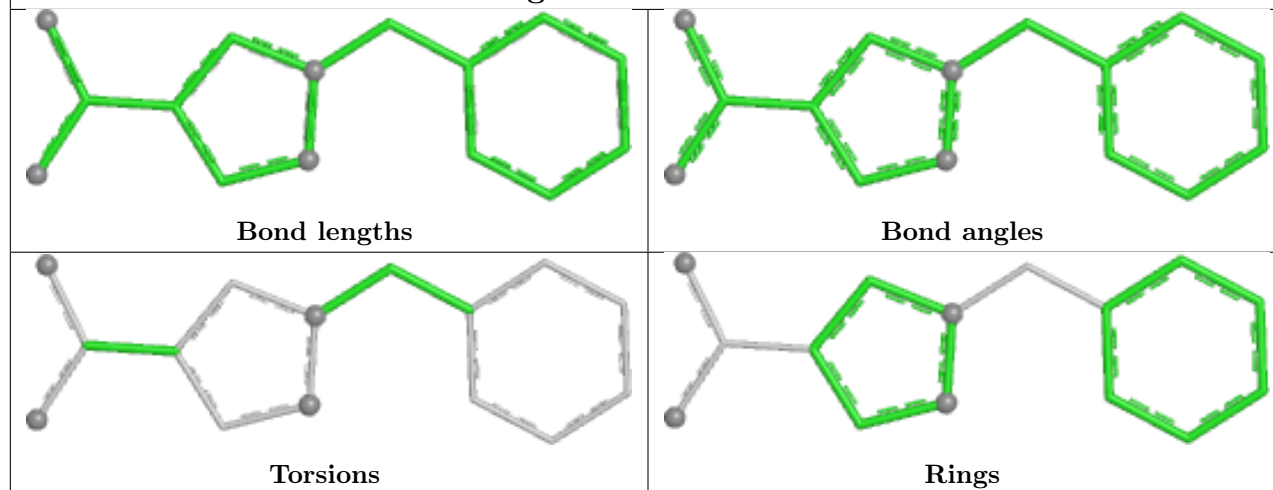
Ligand W3U A 807 (B)

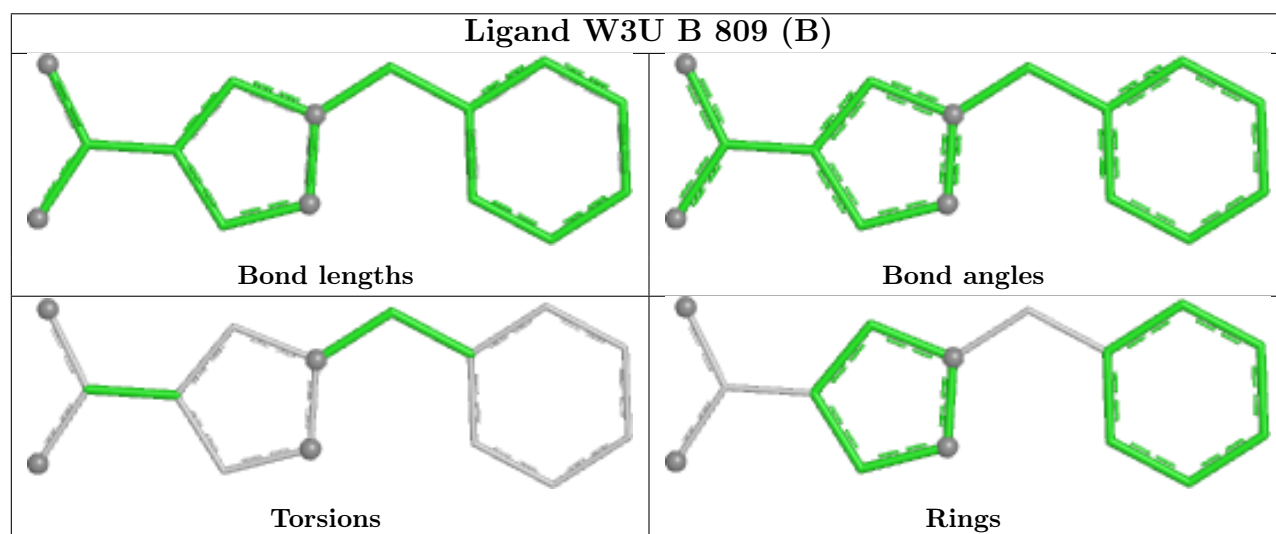
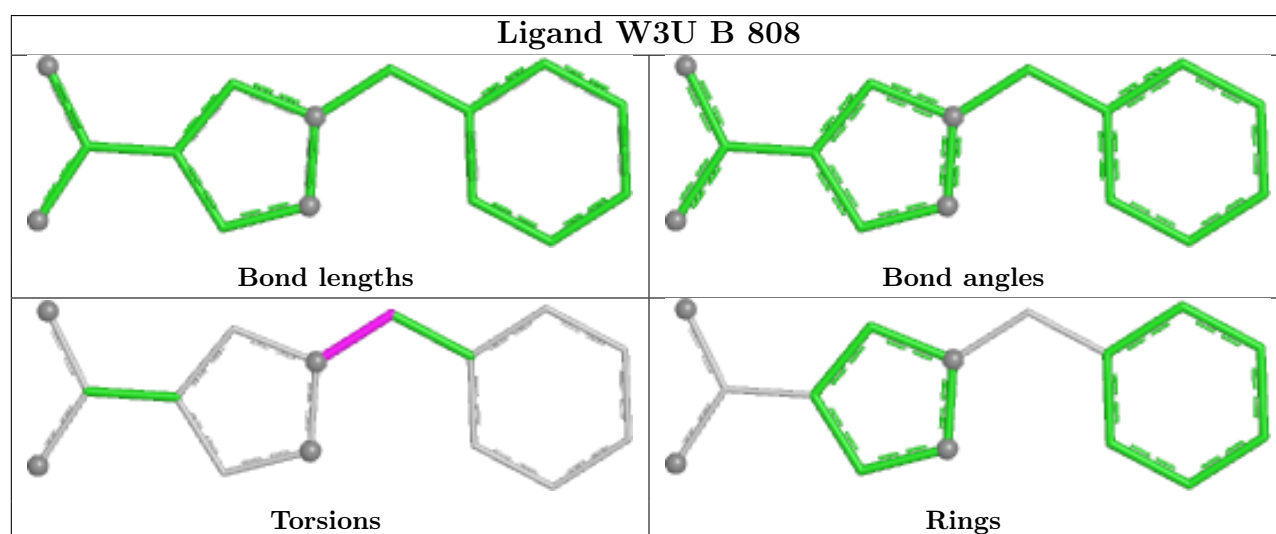
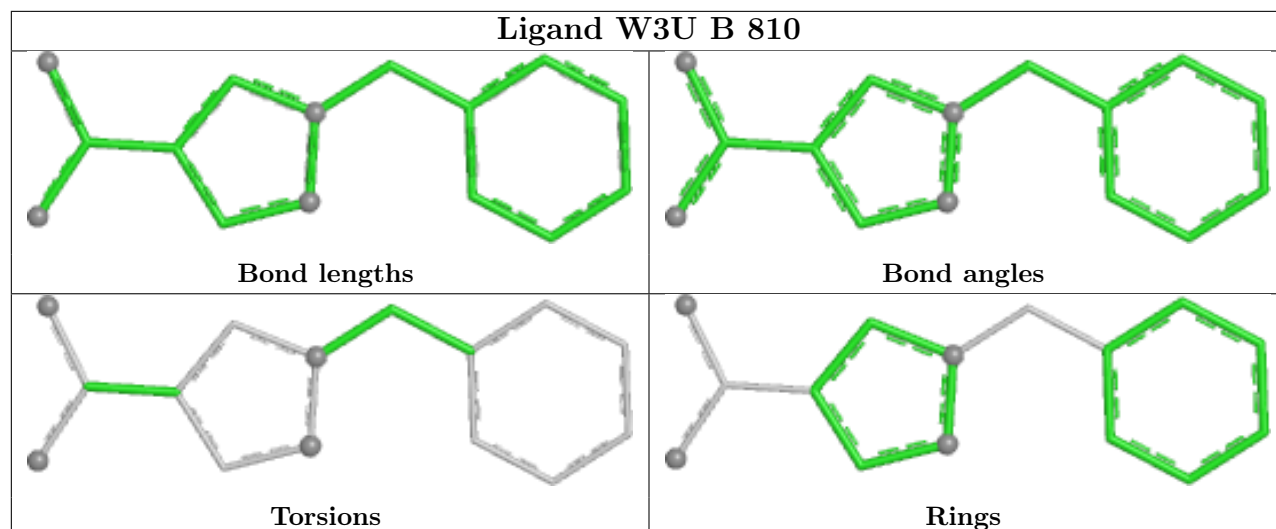


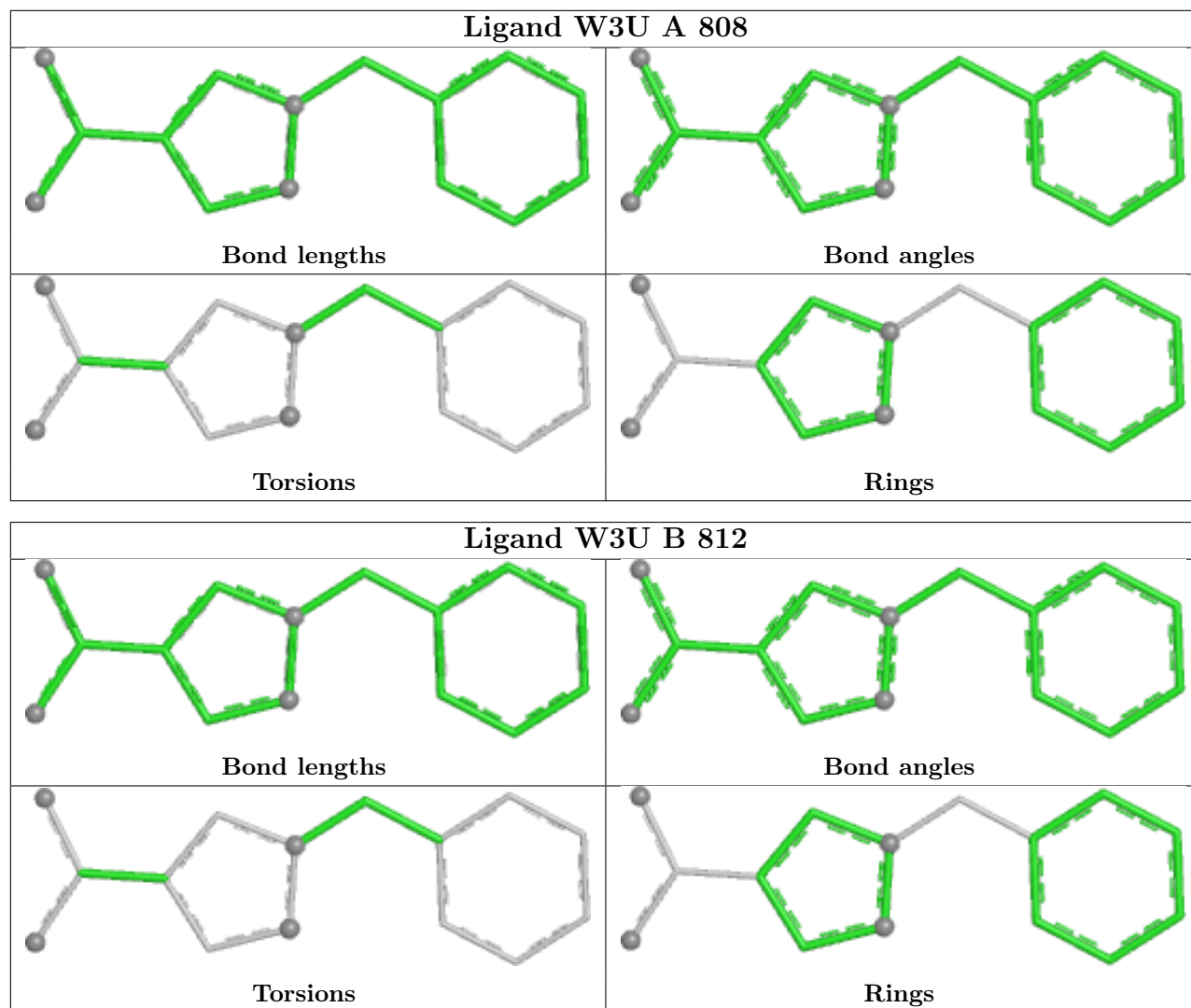
Ligand W3U B 809 (A)



Ligand W3U B 813







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%)	0.45	60 (8%) 17 15	41, 69, 145, 179	0
1	B	728/736 (98%)	0.39	65 (8%) 15 13	39, 63, 131, 182	0
2	C	402/403 (99%)	-0.03	22 (5%) 30 27	32, 50, 76, 158	1 (0%)
2	D	402/403 (99%)	0.14	19 (4%) 36 33	35, 56, 86, 140	1 (0%)
All	All	2261/2278 (99%)	0.29	166 (7%) 21 18	32, 60, 135, 182	2 (0%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	136	LEU	8.3
1	B	390	LEU	8.0
2	D	134	MET	6.3
2	D	225	PHE	5.6
1	B	389	LEU	5.3
2	D	228	LEU	5.1
2	C	225	PHE	5.0
1	B	382	THR	5.0
1	B	368	SER	4.8
1	B	388	ALA	4.6
1	B	385	ARG	4.6
1	B	413	PHE	4.4
1	A	399	ALA	4.3
1	B	367	TYR	4.2
1	A	426	ILE	4.2
1	A	358	LEU	4.1
1	B	371	LEU	4.1
2	C	134	MET	4.0
2	D	135	GLY	4.0
1	B	393	ILE	4.0
1	A	574	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
2	C	294	ALA	3.9
2	D	133	ALA	3.8
2	C	301	THR	3.8
2	C	228	LEU	3.8
1	A	413	PHE	3.8
1	B	578	TYR	3.7
2	C	136	LEU	3.7
2	D	231	LEU	3.7
1	B	-8	HIS	3.7
1	A	402	PHE	3.6
1	A	400	ALA	3.6
1	B	441	SER	3.6
1	B	577	THR	3.6
2	D	224	ALA	3.5
2	C	2	SER	3.5
1	B	356	VAL	3.5
1	A	-6	HIS	3.4
2	D	2	SER	3.4
1	B	442	THR	3.4
2	C	299	MET	3.3
1	A	371	LEU	3.3
1	A	2	PRO	3.3
1	B	397	ALA	3.2
1	B	335	MET	3.2
1	A	-7	HIS	3.2
1	A	429	ILE	3.2
1	A	579	GLN	3.2
1	B	342	TYR	3.1
1	A	-5	SER	3.1
2	D	294	ALA	3.1
1	A	1	MET	3.1
2	D	301	THR	3.0
1	B	690	ALA	3.0
1	B	353	LEU	3.0
1	B	386	SER	3.0
1	A	367	TYR	3.0
1	A	720	SER	3.0
1	A	432	PRO	3.0
1	B	354	LYS	2.9
1	B	383	GLN	2.9
2	D	232	GLY	2.9
1	A	397	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	389	CYS	2.9
1	B	576	GLY	2.9
2	D	303	PRO	2.9
1	A	353	LEU	2.9
2	C	224	ALA	2.9
1	A	325	ILE	2.9
1	B	1	MET	2.9
1	A	333	ALA	2.8
1	A	393	ILE	2.8
1	A	577	THR	2.8
1	A	576	GLY	2.8
2	C	390	ILE	2.8
1	A	423	PHE	2.8
1	B	355	ASP	2.8
1	B	365	LYS	2.8
2	C	297	VAL	2.8
2	D	299	MET	2.7
1	B	412	VAL	2.7
1	A	389	LEU	2.7
1	A	407	PHE	2.7
1	A	-13	SER	2.7
1	A	390	LEU	2.7
1	B	375	ALA	2.7
1	A	-9	HIS	2.6
1	A	352	VAL	2.6
1	B	334	GLY	2.6
1	A	324	PRO	2.6
1	B	720	SER	2.6
1	B	373	ALA	2.6
1	B	392	ARG	2.6
1	B	366	GLY	2.6
1	B	396	THR	2.6
2	C	135	GLY	2.6
1	B	403	LYS	2.6
1	B	358	LEU	2.5
1	A	406	ASP	2.5
1	A	610	GLY	2.5
1	B	330	VAL	2.5
1	B	400	ALA	2.5
1	A	356	VAL	2.5
1	B	574	ALA	2.5
1	B	-9	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	C	300	LEU	2.5
1	B	0	SER	2.4
2	D	390	ILE	2.4
1	B	-14	GLY	2.4
2	C	296	PRO	2.4
1	A	349	TYR	2.4
2	C	293	GLY	2.4
1	A	657	THR	2.4
2	C	389	CYS	2.4
1	B	352	VAL	2.4
1	A	335	MET	2.4
1	B	350	GLU	2.4
1	B	689	PRO	2.4
1	B	414	GLU	2.4
1	A	559	LEU	2.3
2	C	231	LEU	2.3
1	A	354	LYS	2.3
1	A	403	LYS	2.3
1	A	578	TYR	2.3
2	C	391	GLY	2.3
1	B	571	VAL	2.3
1	B	599	LEU	2.3
1	A	575	GLY	2.3
1	A	385	ARG	2.3
1	A	359	GLU	2.3
1	A	361	ALA	2.3
1	B	376	LEU	2.2
1	B	387	ASP	2.2
1	A	395	PRO	2.2
1	A	332	GLY	2.2
1	A	334	GLY	2.2
1	B	364	GLY	2.2
1	A	382	THR	2.2
1	B	404	GLY	2.2
1	A	327	ARG	2.2
1	A	364	GLY	2.2
1	B	377	GLU	2.2
2	D	304	THR	2.2
2	C	298	ILE	2.2
1	A	443	LEU	2.1
1	A	330	VAL	2.1
2	C	295	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	362	ALA	2.1
1	B	573	ASP	2.1
2	C	303	PRO	2.1
2	D	291	THR	2.1
1	B	62	LYS	2.1
1	A	-8	HIS	2.1
1	B	443	LEU	2.1
1	A	571	VAL	2.1
1	B	381	THR	2.0
1	A	383	GLN	2.0
1	A	433	ASN	2.0
1	B	426	ILE	2.0
1	B	422	VAL	2.0
2	C	403	VAL	2.0
1	B	575	GLY	2.0
2	D	391	GLY	2.0
1	B	372	GLU	2.0
1	B	333	ALA	2.0
1	A	331	LEU	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
3	SO4	B	803	5/5	0.47	0.14	85,89,103,107	5
3	SO4	D	506	5/5	0.56	0.14	122,124,128,130	5
3	SO4	B	807	5/5	0.65	0.09	134,135,140,142	0
3	SO4	A	804	5/5	0.67	0.11	118,129,164,167	0

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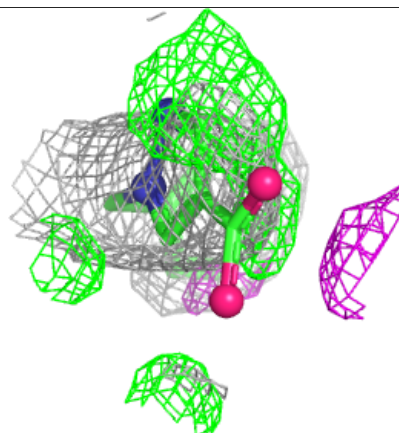
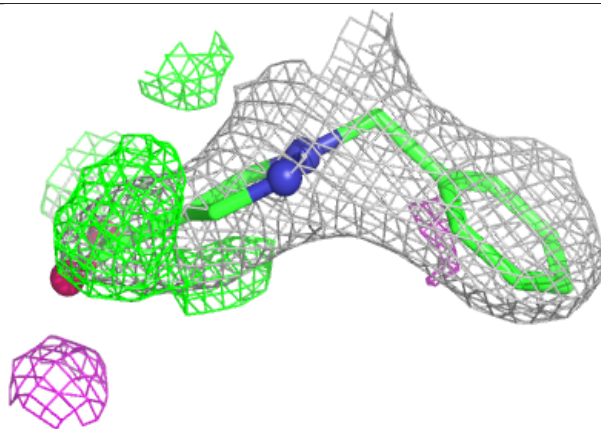
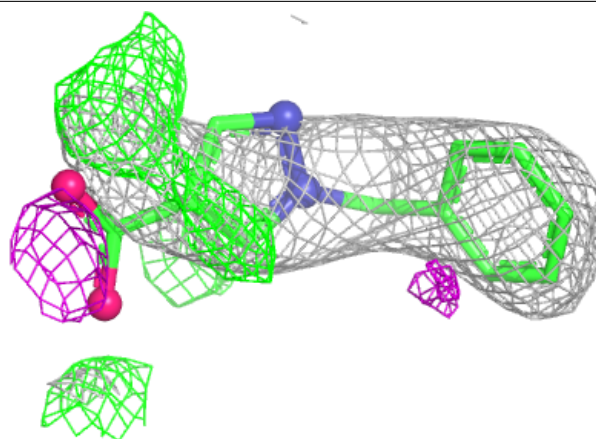
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	C	505	5/5	0.69	0.13	114,122,138,164	0
3	SO4	B	805	5/5	0.71	0.09	115,117,141,156	0
3	SO4	A	803	5/5	0.74	0.12	72,73,76,80	5
3	SO4	D	505	5/5	0.74	0.16	80,80,94,103	5
3	SO4	C	504	5/5	0.74	0.11	102,104,140,164	0
3	SO4	A	801	5/5	0.76	0.08	124,126,143,154	0
4	W3U	A	807[A]	15/15	0.76	0.30	74,85,90,93	15
4	W3U	A	807[B]	15/15	0.76	0.30	74,83,90,93	15
3	SO4	C	503	5/5	0.77	0.09	89,100,115,140	0
3	SO4	B	802	5/5	0.77	0.10	77,99,108,117	0
3	SO4	B	801	5/5	0.77	0.14	59,70,80,85	5
3	SO4	C	507	5/5	0.77	0.17	65,66,78,79	5
3	SO4	D	503	5/5	0.78	0.09	100,116,126,143	0
4	W3U	A	808	15/15	0.78	0.28	89,108,126,128	0
4	W3U	B	810	15/15	0.78	0.26	61,94,108,112	0
4	W3U	A	809	15/15	0.80	0.23	102,111,125,127	0
3	SO4	A	802	5/5	0.80	0.09	99,110,126,127	0
4	W3U	B	809[B]	15/15	0.81	0.27	71,82,91,93	15
4	W3U	B	809[A]	15/15	0.81	0.27	70,77,84,86	15
3	SO4	B	804	5/5	0.83	0.09	73,73,85,89	5
4	W3U	B	813	15/15	0.83	0.20	92,101,118,118	0
3	SO4	B	806	5/5	0.86	0.14	69,71,78,80	5
4	W3U	B	812	15/15	0.86	0.13	56,88,118,118	0
4	W3U	B	808	15/15	0.86	0.21	98,119,139,144	0
3	SO4	C	506	5/5	0.87	0.08	77,77,101,113	0
4	W3U	A	805	15/15	0.87	0.17	58,79,93,97	0
3	SO4	D	502	5/5	0.90	0.07	85,89,107,114	0
3	SO4	C	501	5/5	0.90	0.08	74,78,86,93	0
3	SO4	D	501	5/5	0.90	0.07	96,101,105,105	0
4	W3U	A	806	15/15	0.91	0.15	69,73,82,83	0
4	W3U	B	811	15/15	0.91	0.15	60,72,85,89	0
3	SO4	D	504	5/5	0.94	0.06	71,85,87,89	0
3	SO4	C	502	5/5	0.94	0.07	71,75,77,101	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.

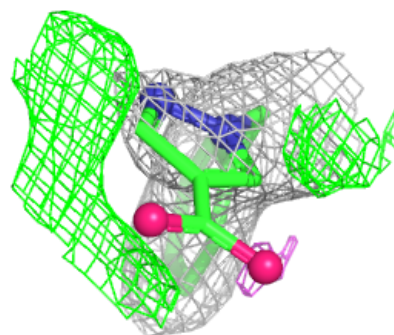
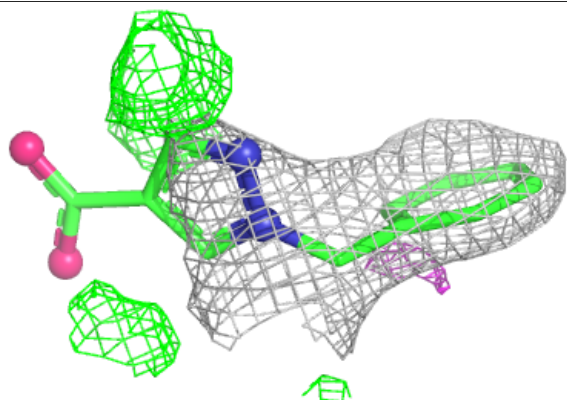
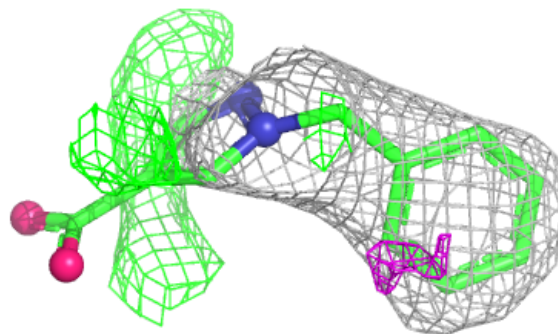
Electron density around W3U A 807 (A):

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

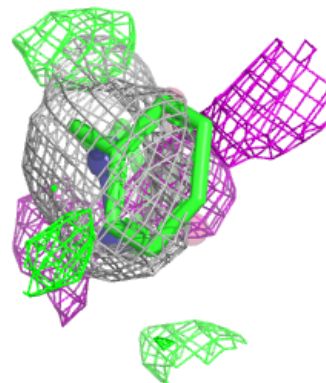
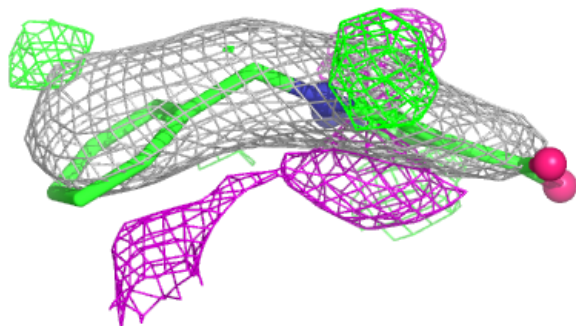
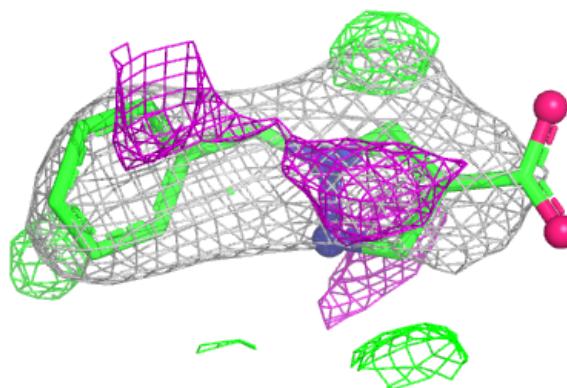


Electron density around W3U A 807 (B):

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

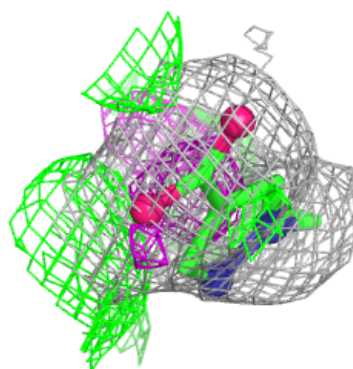
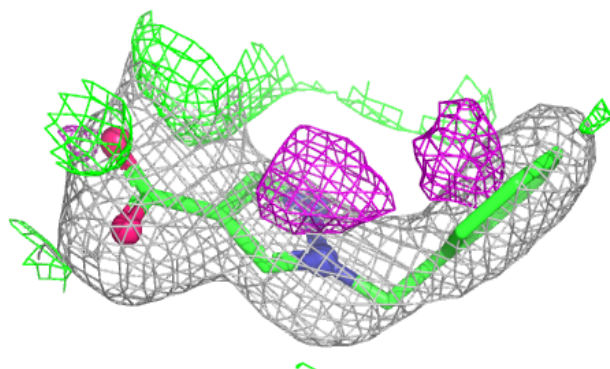
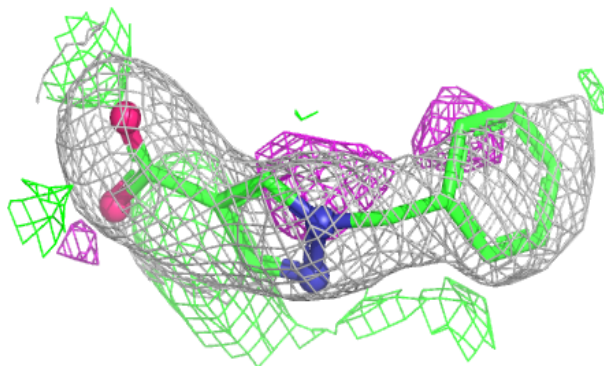
**Electron density around W3U A 808:**

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

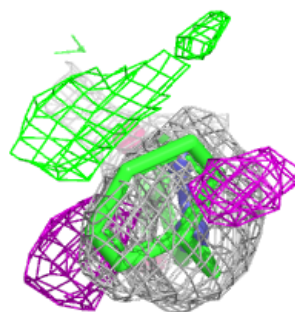
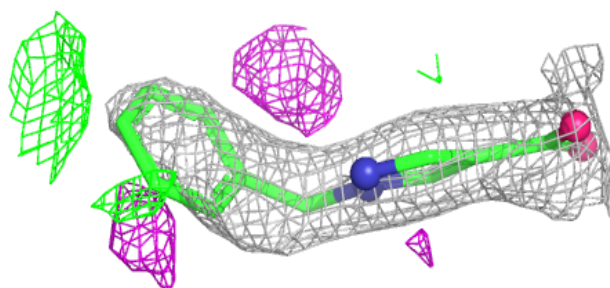
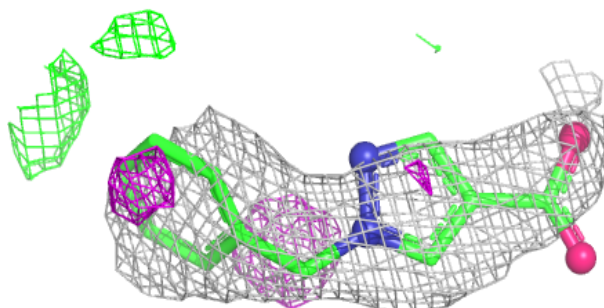


Electron density around W3U B 810:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

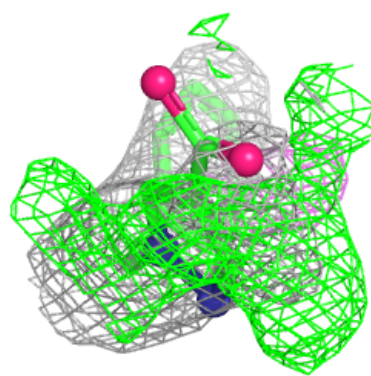
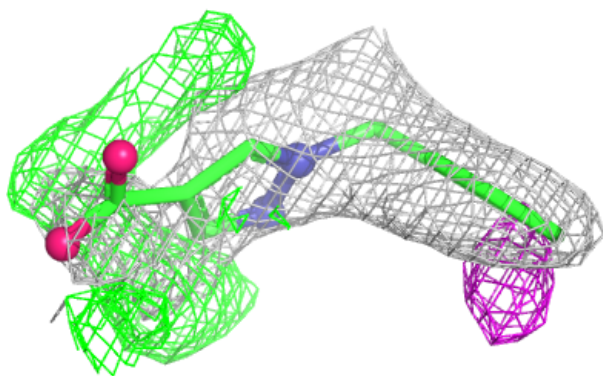
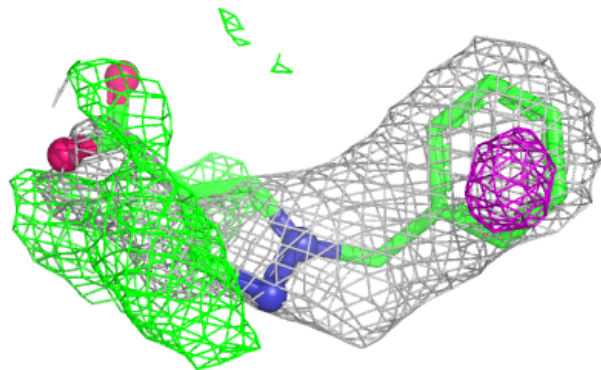
**Electron density around W3U A 809:**

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

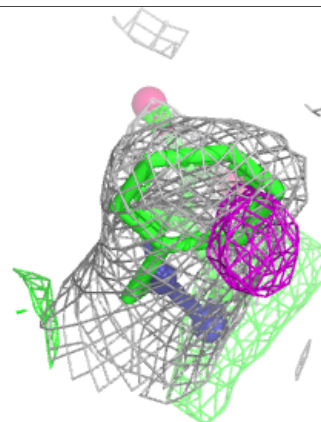
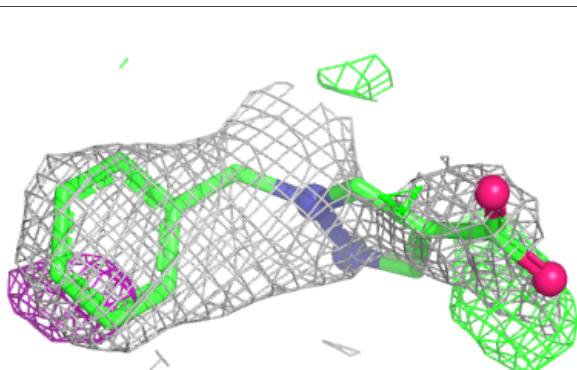
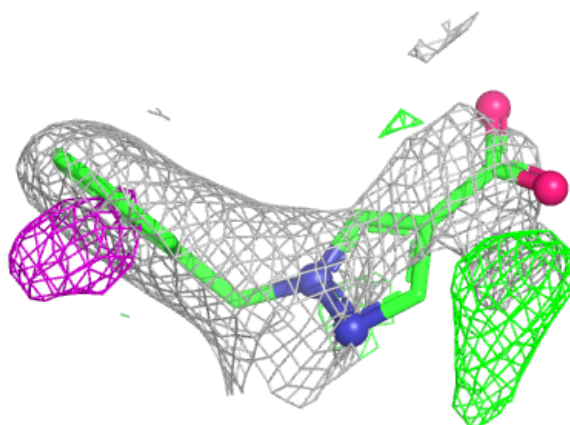


Electron density around W3U B 809 (B):

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

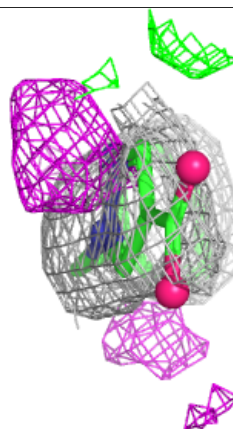
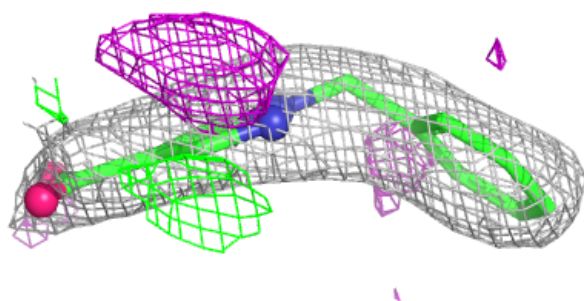
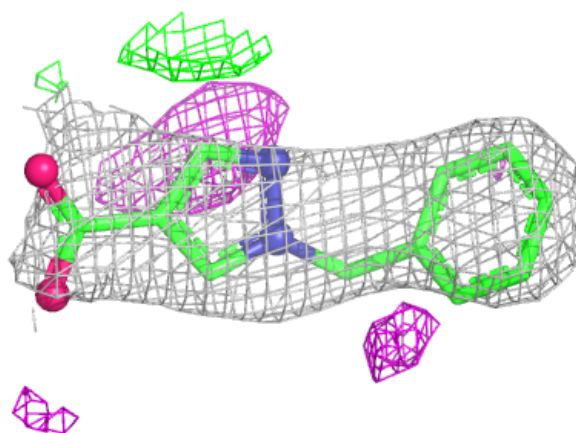
**Electron density around W3U B 809 (A):**

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

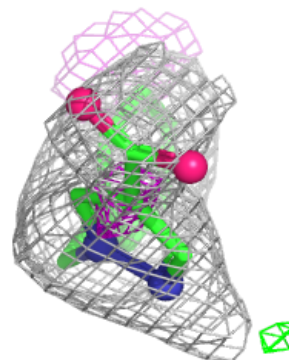
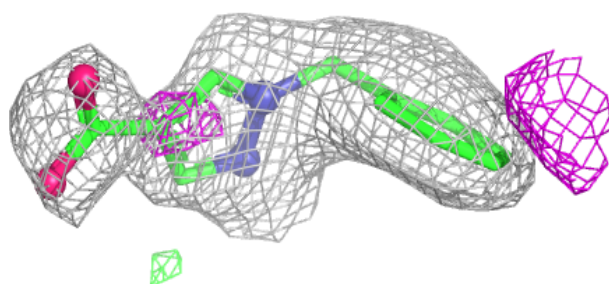
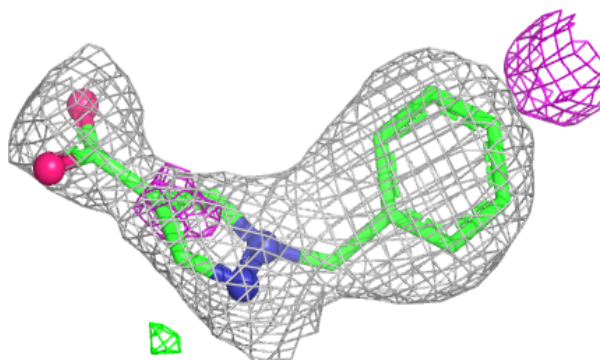


Electron density around W3U B 813:

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

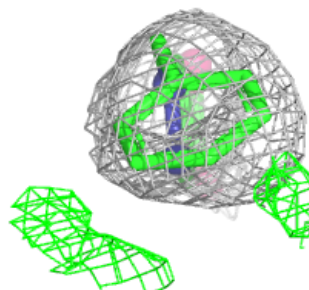
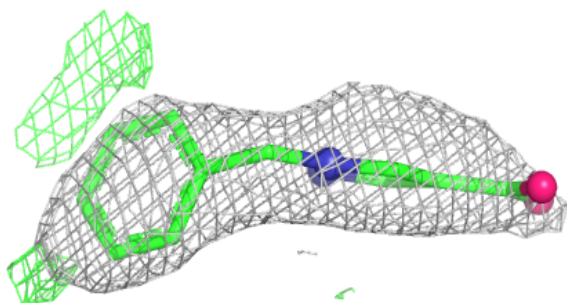
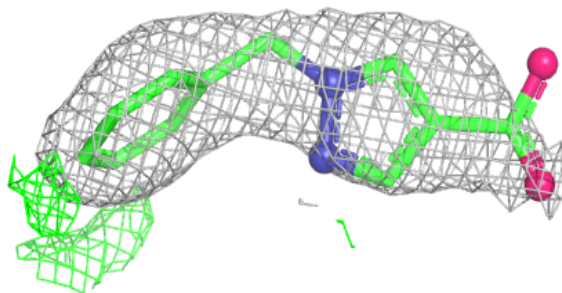
**Electron density around W3U B 812:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

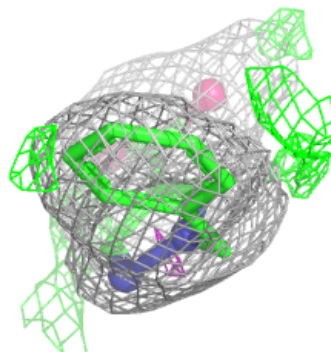
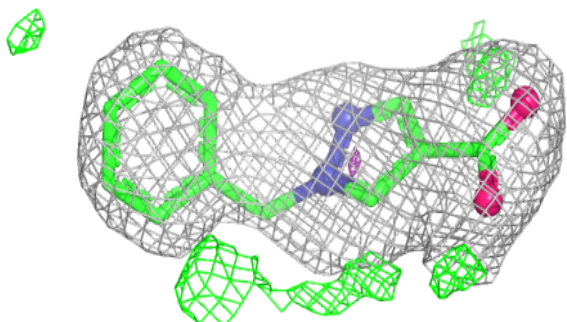
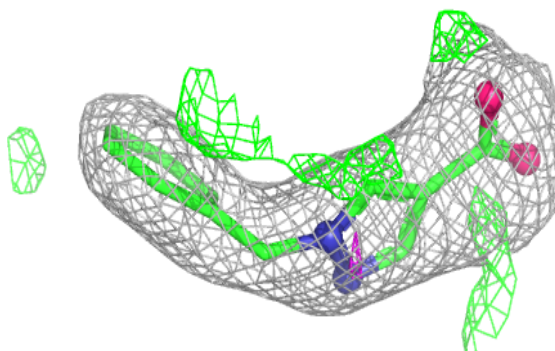


Electron density around W3U B 808:

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

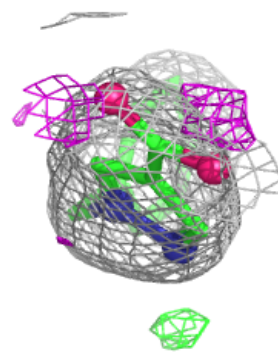
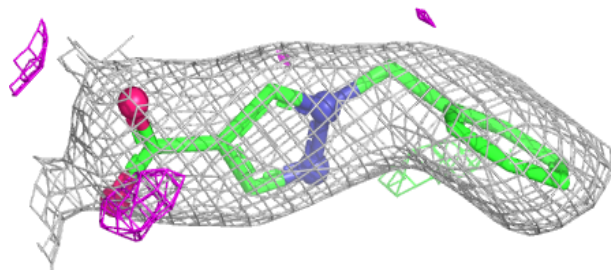
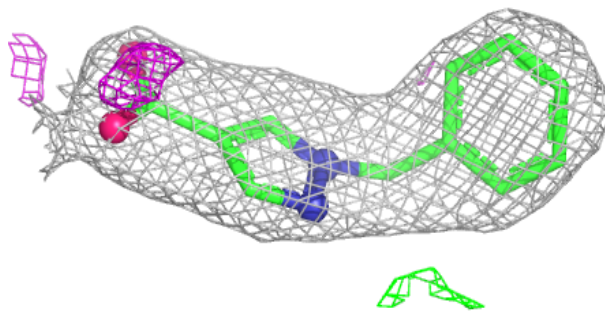
**Electron density around W3U A 805:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

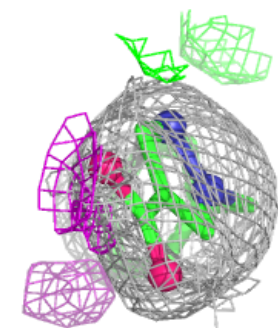
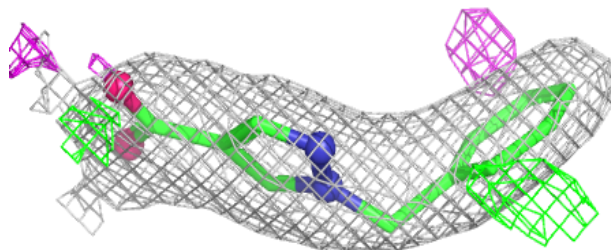
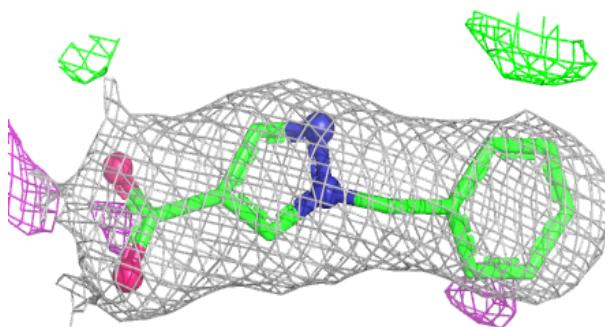


Electron density around W3U A 806:

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

**Electron density around W3U B 811:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.