



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 17, 2024 – 01:38 pm BST

PDB ID : 8OQN
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 : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
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) : 2.37.1

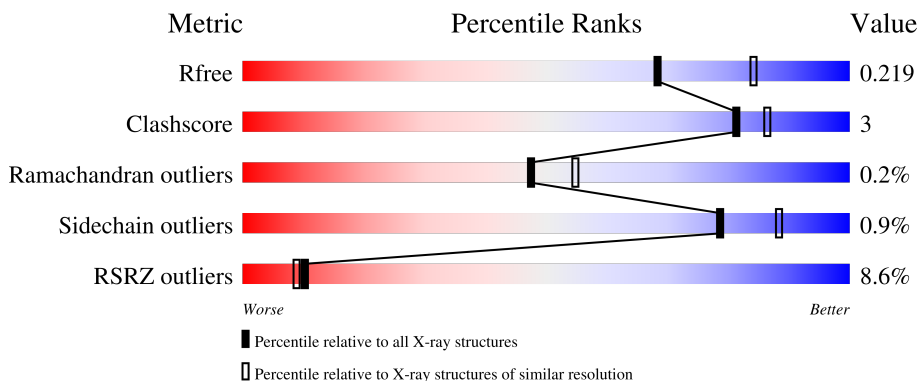
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

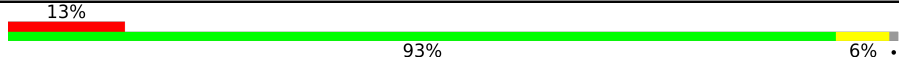
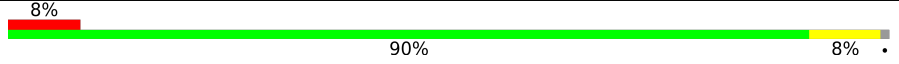
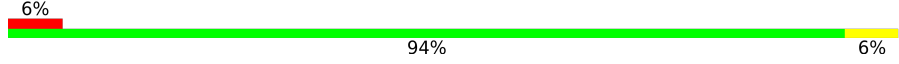
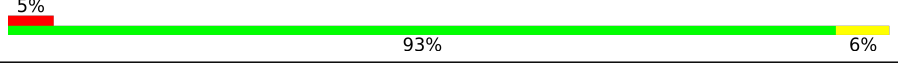
The reported resolution of this entry is 2.20 Å.

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}	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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	 13% 93% 6%
1	B	736	 8% 90% 8%
2	C	403	 6% 94% 6%
2	D	403	 5% 93% 6%

2 Entry composition i

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
			Total	C	N	O	S			
1	A	729	5430	3434	936	1039	21	0	0	0
1	B	728	5414	3424	931	1038	21	0	0	0

There are 32 discrepancies between the modelled and reference sequences:

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

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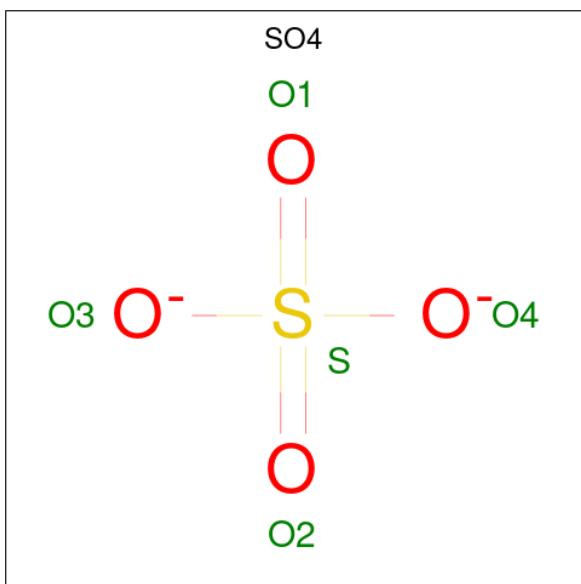
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression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

- Molecule 2 is a protein called Putative acyltransferase Rv0859.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	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 (three-letter code: SO4) (formula: O₄S).



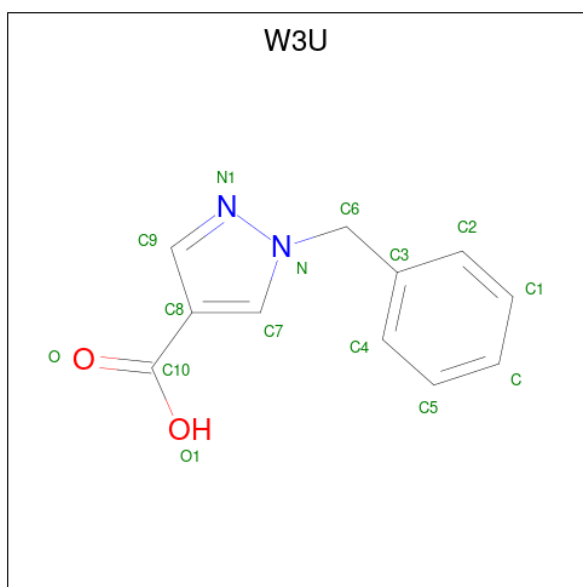
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is 1-benzyl-1H-pyrazole-4-carboxylic acid (three-letter code: W3U) (formula: $C_{11}H_{10}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 5 is water.

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

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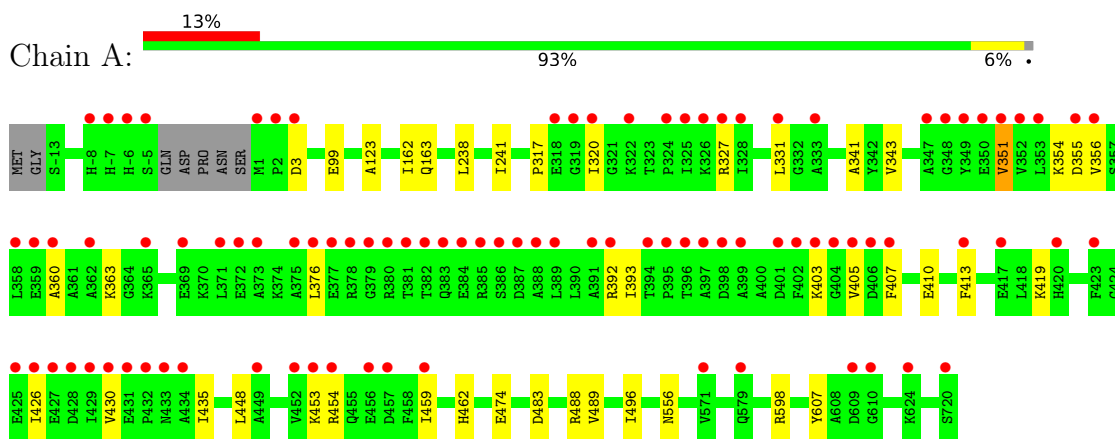
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	46	Total O 46 46	0	0
5	C	57	Total O 57 57	0	0
5	D	48	Total O 48 48	0	0

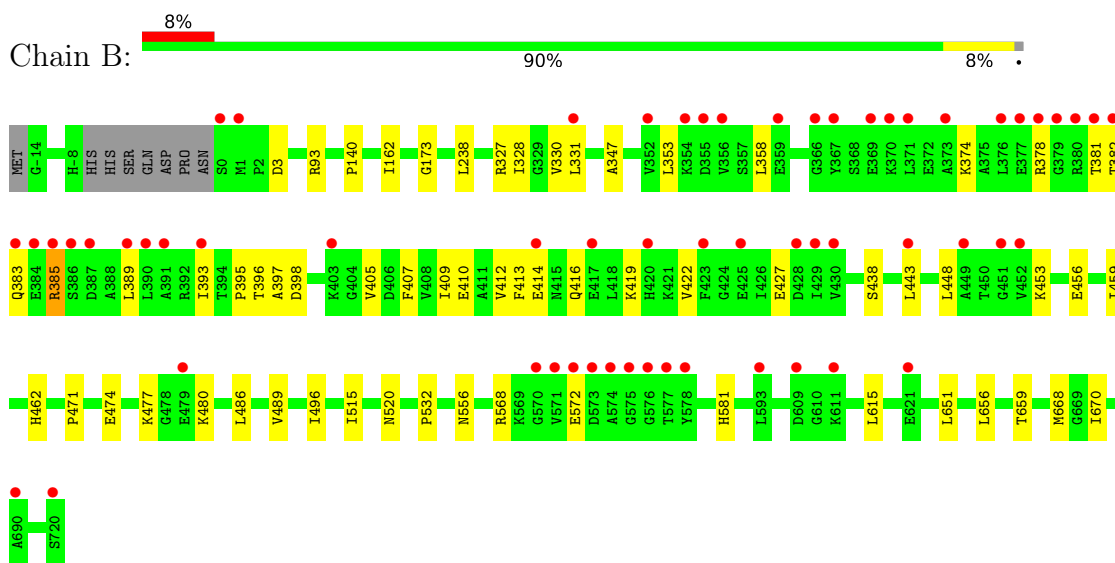
3 Residue-property plots [i](#)

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

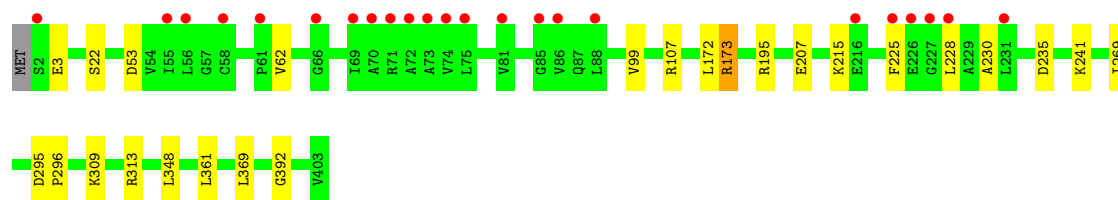


- Molecule 1: 3-hydroxyacyl-CoA dehydrogenase



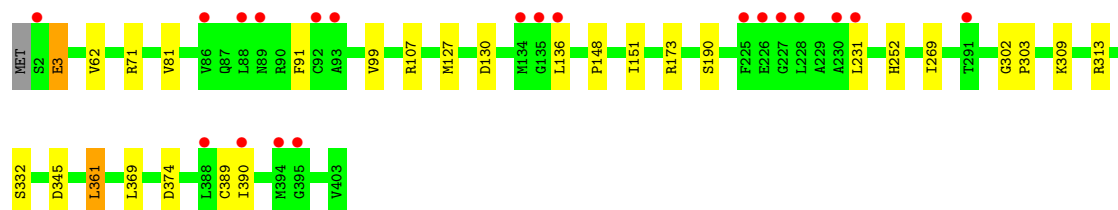
- Molecule 2: Putative acyltransferase Rv0859





● Molecule 2: Putative acyltransferase Rv0859

Chain D: 5% 93% 6%



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)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.193 , 0.221 0.191 , 0.219	Depositor DCC
R_{free} test set	9084 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	52.4	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
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

Xtrriage'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	0.25	0/5533	0.48	0/7487
1	B	0.25	0/5515	0.48	0/7462
2	C	0.25	0/3020	0.51	0/4089
2	D	0.25	0/3020	0.51	0/4089
All	All	0.25	0/17088	0.49	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	26	0
1	B	5414	0	5456	34	0
2	C	2972	0	2994	14	0
2	D	2972	0	2994	18	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	88	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 (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: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
1:B:471:PRO:HG2	1:B:668:MET:HE3	1.77	0.66
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: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: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:459:ILE:HG21	1:B:489:VAL:HG21	1.93	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:413:PHE:O	1:A:419:LYS:NZ	2.44	0.48
2:D:62:VAL:HG21	2:D:130:ASP:HA	1.94	0.48
1:B:419:LYS:HA	1:B:422:VAL:HG22	1.94	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
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: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
2:D:389:CYS:C	2:D:390:ILE:HG13	2.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:190:SER:OG	2:D:374:ASP:OD2	2.33	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: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%)	51 60
1	B	724/736 (98%)	696 (96%)	27 (4%)	1 (0%)	51 60
2	C	401/403 (100%)	390 (97%)	10 (2%)	1 (0%)	47 55
2	D	401/403 (100%)	391 (98%)	9 (2%)	1 (0%)	47 55
All	All	2251/2278 (99%)	2174 (97%)	73 (3%)	4 (0%)	47 55

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 [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	560/566 (99%)	556 (99%)	4 (1%)	84	91
1	B	558/566 (99%)	555 (100%)	3 (0%)	88	94
2	C	310/310 (100%)	306 (99%)	4 (1%)	69	81
2	D	310/310 (100%)	306 (99%)	4 (1%)	69	81
All	All	1738/1752 (99%)	1723 (99%)	15 (1%)	78	88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP
1	A	351	VAL
1	A	376	LEU
1	A	407	PHE
1	B	3	ASP
1	B	385	ARG
1	B	389	LEU
2	C	53	ASP
2	C	173	ARG
2	C	228	LEU
2	C	235	ASP
2	D	3	GLU
2	D	136	LEU
2	D	173	ARG
2	D	345	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	163	GLN

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](#)

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	$\# Z > 2$
4	W3U	B	811	-	15,16,16	0.22	0	18,21,21	0.42	0
3	SO4	D	504	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	804	-	4,4,4	0.14	0	6,6,6	0.06	0
4	W3U	B	810	-	15,16,16	0.19	0	18,21,21	0.38	0
3	SO4	B	802	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	807	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	804	-	4,4,4	0.14	0	6,6,6	0.04	0
4	W3U	A	807[A]	-	15,16,16	0.22	0	18,21,21	0.38	0
3	SO4	C	504	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	801	-	4,4,4	0.14	0	6,6,6	0.05	0
4	W3U	B	813	-	15,16,16	0.20	0	18,21,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	W3U	B	809[B]	-	15,16,16	0.22	0	18,21,21	0.40	0
4	W3U	B	808	-	15,16,16	0.24	0	18,21,21	0.37	0
3	SO4	C	506	-	4,4,4	0.14	0	6,6,6	0.06	0
4	W3U	A	806	-	15,16,16	0.23	0	18,21,21	0.40	0
3	SO4	A	801	-	4,4,4	0.14	0	6,6,6	0.05	0
4	W3U	B	809[A]	-	15,16,16	0.20	0	18,21,21	0.40	0
3	SO4	D	501	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	501	-	4,4,4	0.14	0	6,6,6	0.06	0
4	W3U	A	808	-	15,16,16	0.26	0	18,21,21	0.36	0
4	W3U	A	805	-	15,16,16	0.23	0	18,21,21	0.35	0
4	W3U	B	812	-	15,16,16	0.20	0	18,21,21	0.46	0
3	SO4	D	506	-	4,4,4	0.15	0	6,6,6	0.04	0
3	SO4	B	803	-	4,4,4	0.14	0	6,6,6	0.06	0
3	SO4	C	507	-	4,4,4	0.14	0	6,6,6	0.04	0
3	SO4	D	503	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	505	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	A	802	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	805	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	C	503	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	B	806	-	4,4,4	0.14	0	6,6,6	0.07	0
3	SO4	A	803	-	4,4,4	0.14	0	6,6,6	0.05	0
3	SO4	D	502	-	4,4,4	0.14	0	6,6,6	0.06	0
4	W3U	A	809	-	15,16,16	0.21	0	18,21,21	0.39	0
3	SO4	D	505	-	4,4,4	0.14	0	6,6,6	0.05	0
4	W3U	A	807[B]	-	15,16,16	0.24	0	18,21,21	0.37	0
3	SO4	C	502	-	4,4,4	0.14	0	6,6,6	0.07	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	B	811	-	-	1/6/8/8	0/2/2/2
4	W3U	B	813	-	-	1/6/8/8	0/2/2/2
4	W3U	B	809[B]	-	-	0/6/8/8	0/2/2/2
4	W3U	B	809[A]	-	-	0/6/8/8	0/2/2/2
4	W3U	B	810	-	-	1/6/8/8	0/2/2/2
4	W3U	B	808	-	-	2/6/8/8	0/2/2/2
4	W3U	A	806	-	-	1/6/8/8	0/2/2/2
4	W3U	A	808	-	-	1/6/8/8	0/2/2/2
4	W3U	B	812	-	-	0/6/8/8	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	W3U	A	805	-	-	0/6/8/8	0/2/2/2
4	W3U	A	809	-	-	2/6/8/8	0/2/2/2
4	W3U	A	807[A]	-	-	0/6/8/8	0/2/2/2
4	W3U	A	807[B]	-	-	0/6/8/8	0/2/2/2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

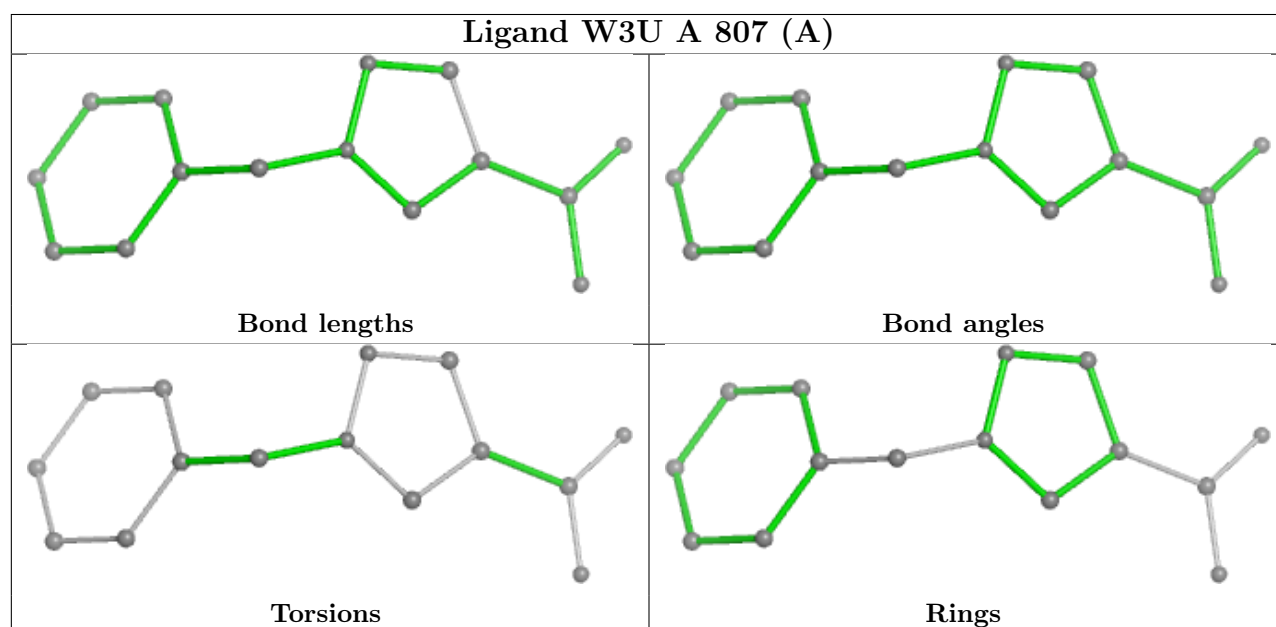
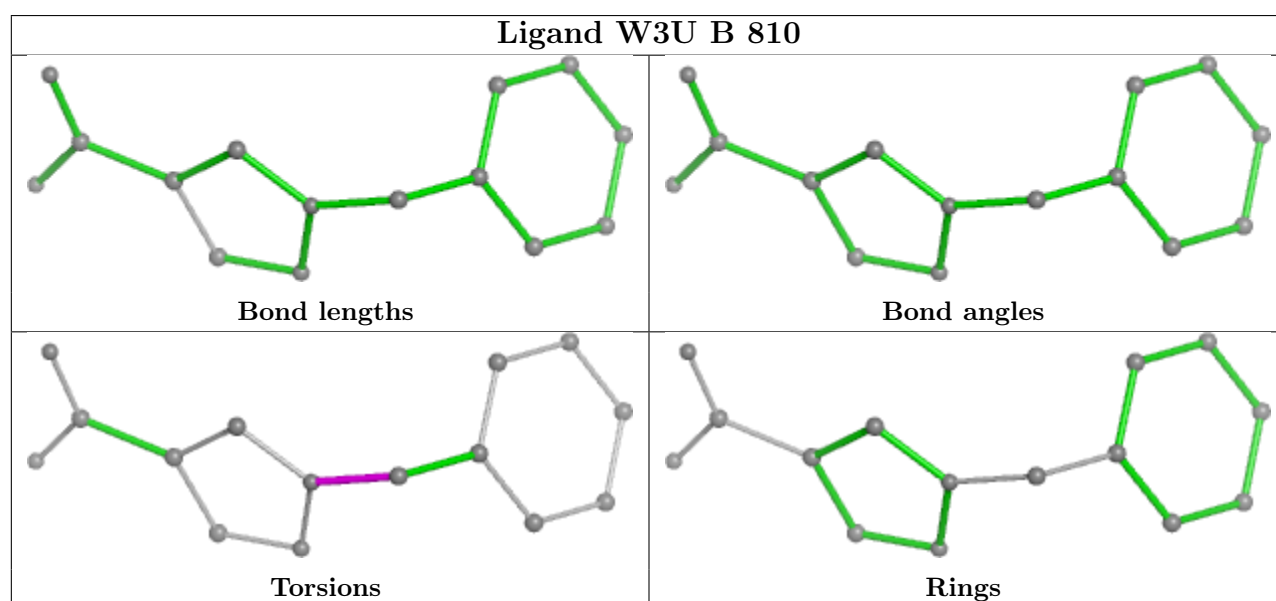
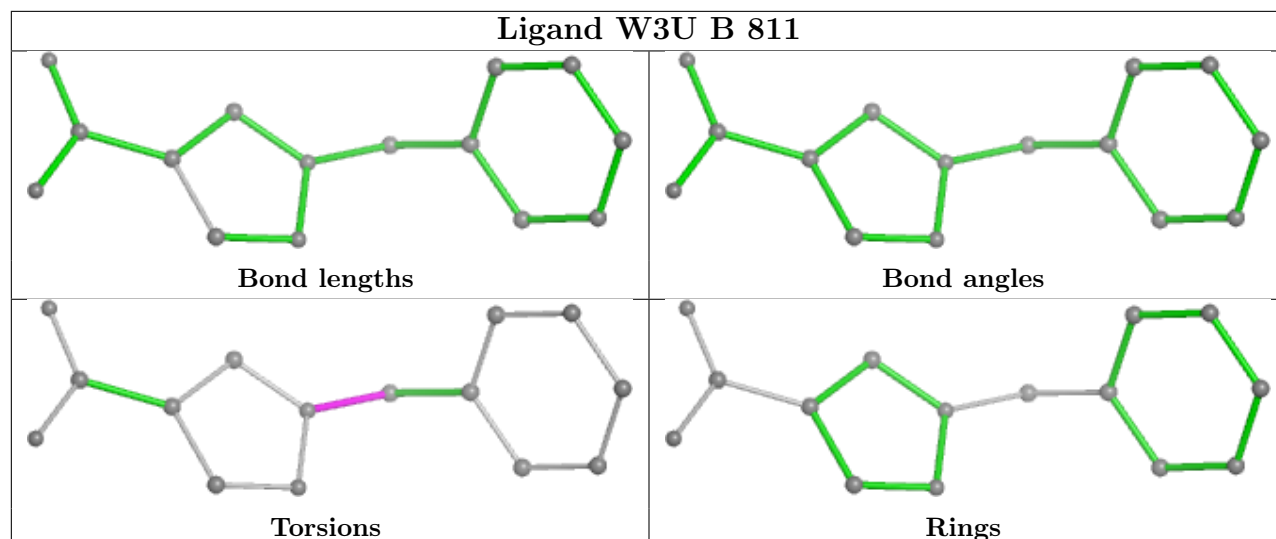
Mol	Chain	Res	Type	Atoms
4	A	808	W3U	C3-C6-N-C7
4	A	809	W3U	C3-C6-N-C7
4	B	808	W3U	C3-C6-N-C7
4	B	813	W3U	C3-C6-N-C7
4	B	808	W3U	C3-C6-N-N1
4	A	806	W3U	C3-C6-N-C7
4	B	810	W3U	C3-C6-N-C7
4	B	811	W3U	C3-C6-N-C7
4	A	809	W3U	C3-C6-N-N1

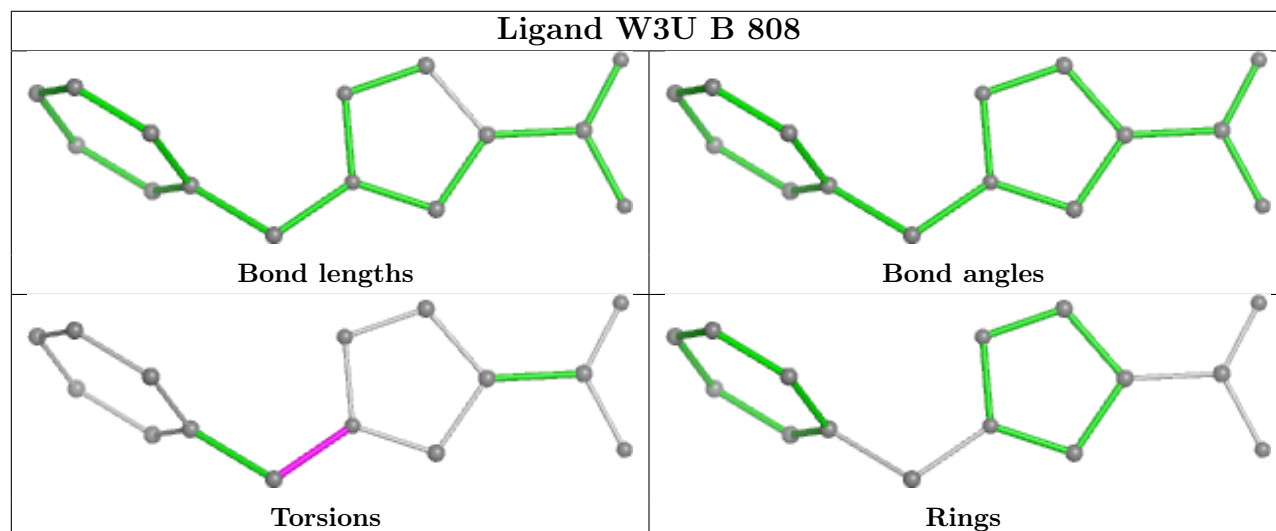
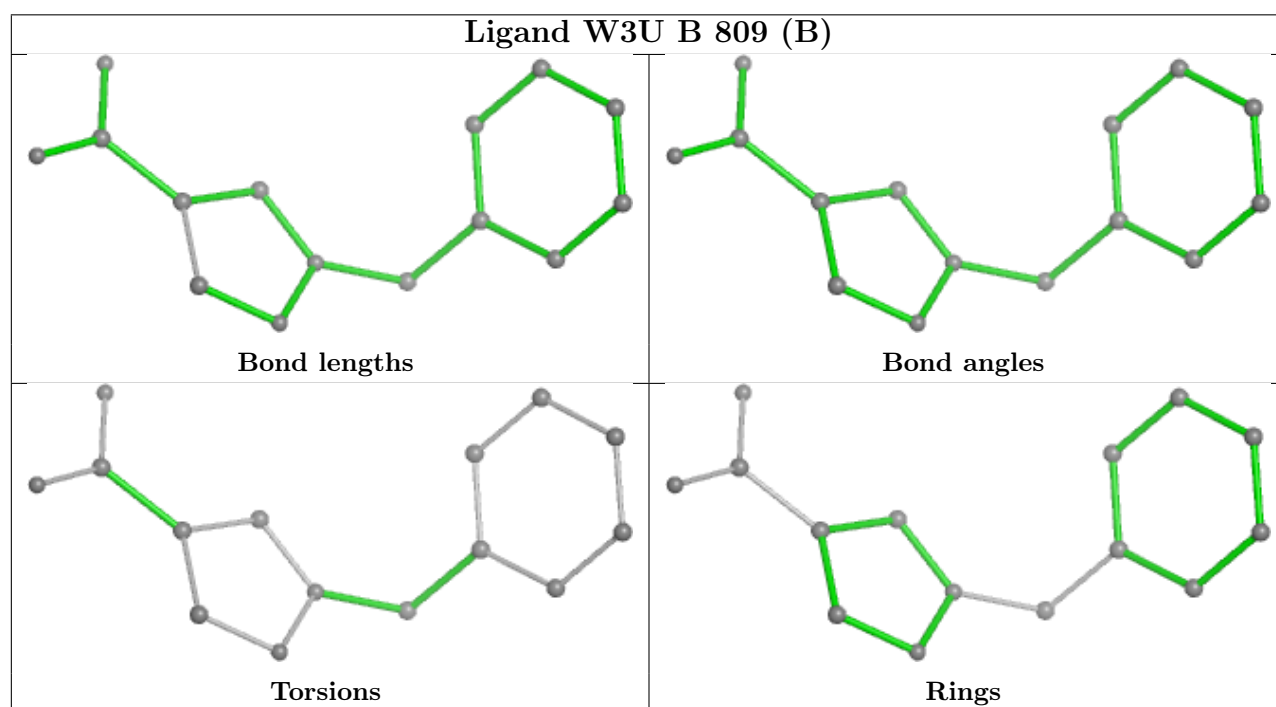
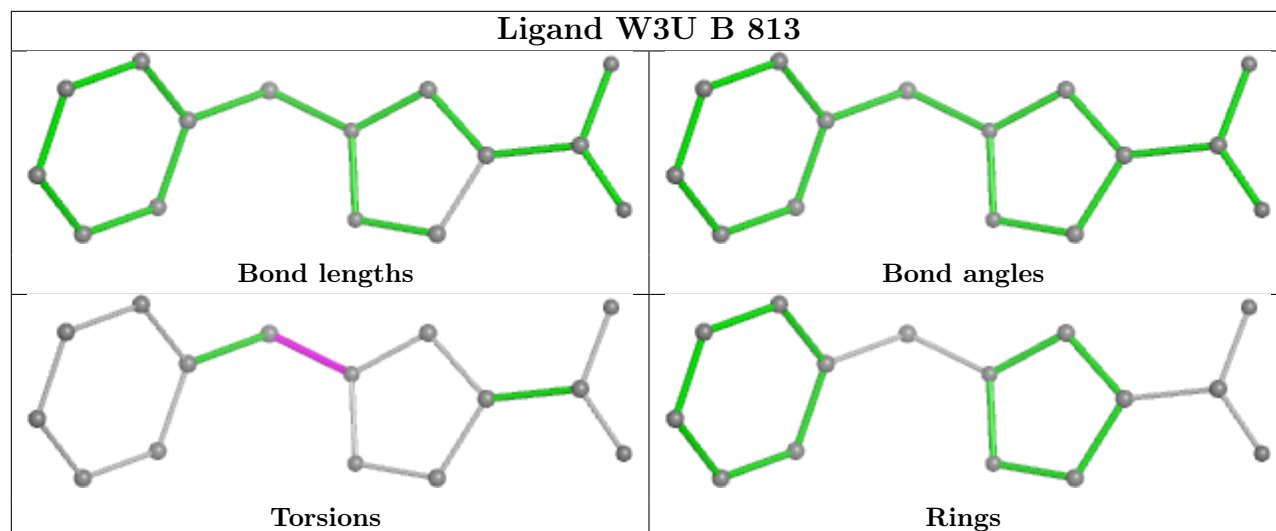
There are no ring outliers.

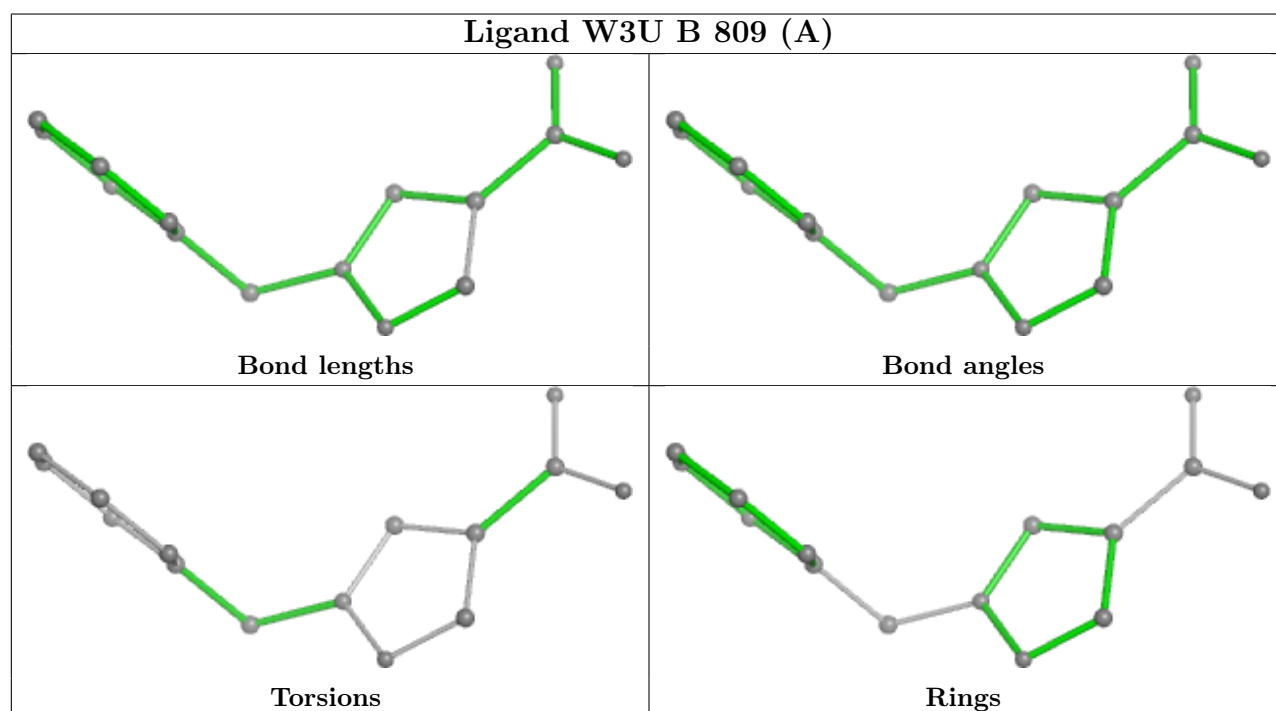
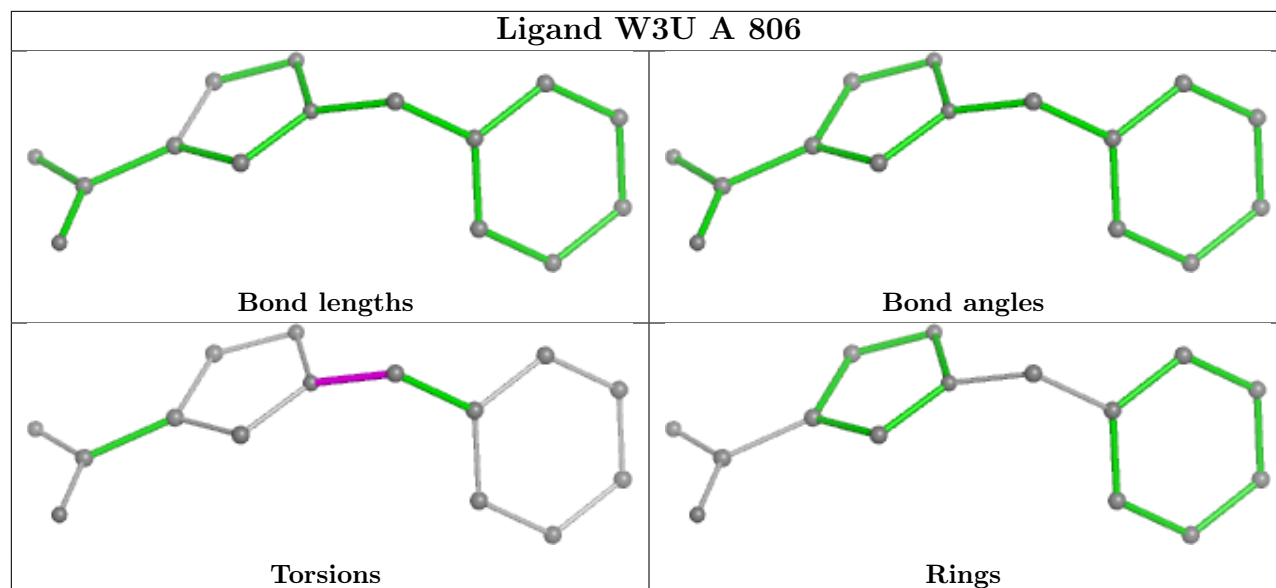
3 monomers are involved in 3 short contacts:

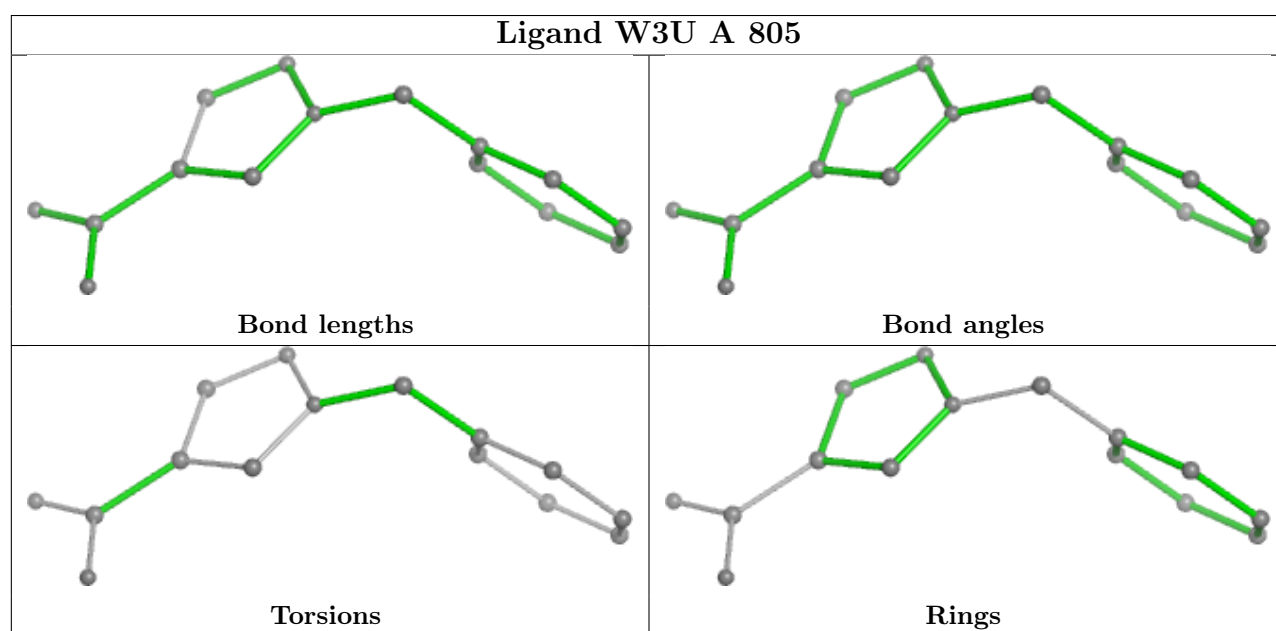
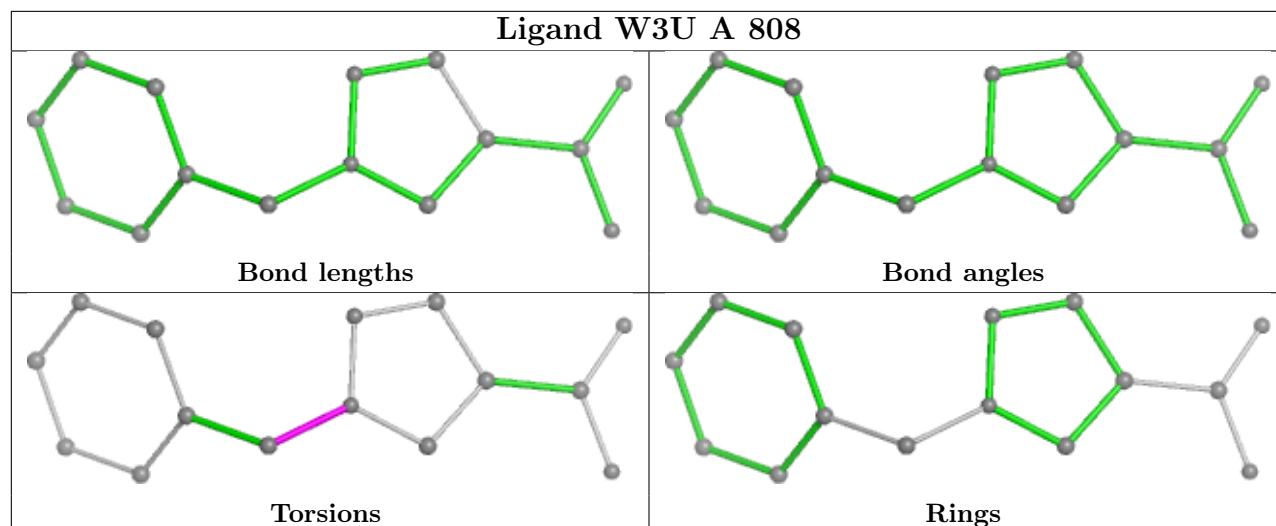
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	807[A]	W3U	1	0
3	B	805	SO4	1	0
3	C	503	SO4	1	0

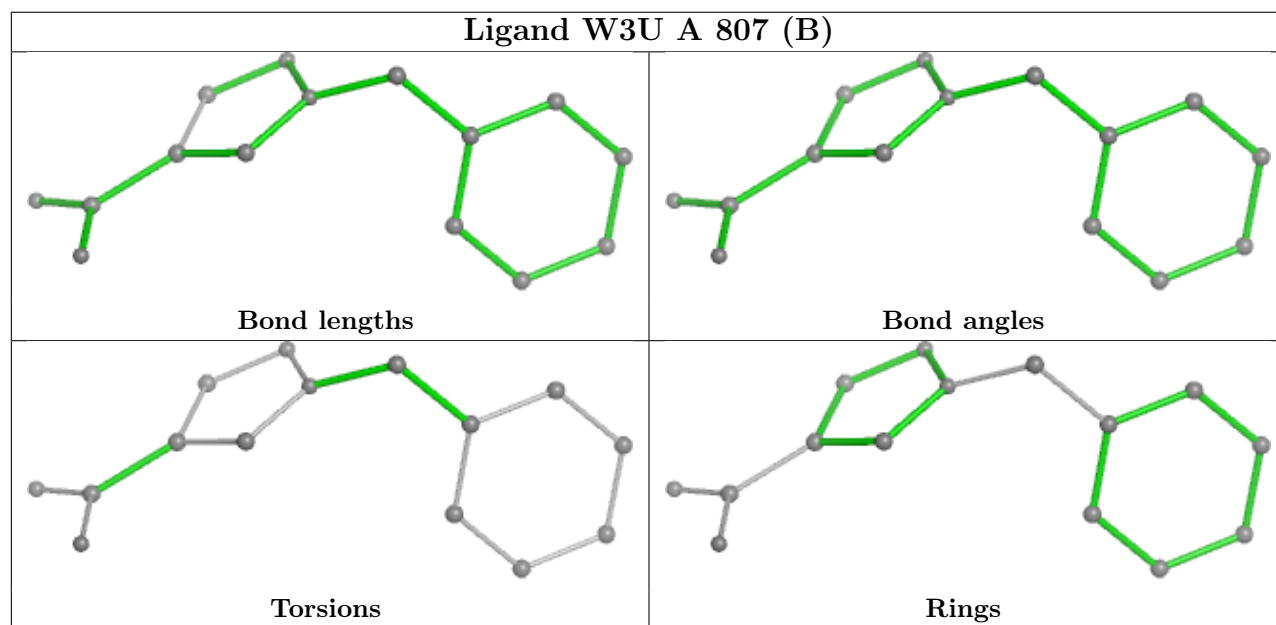
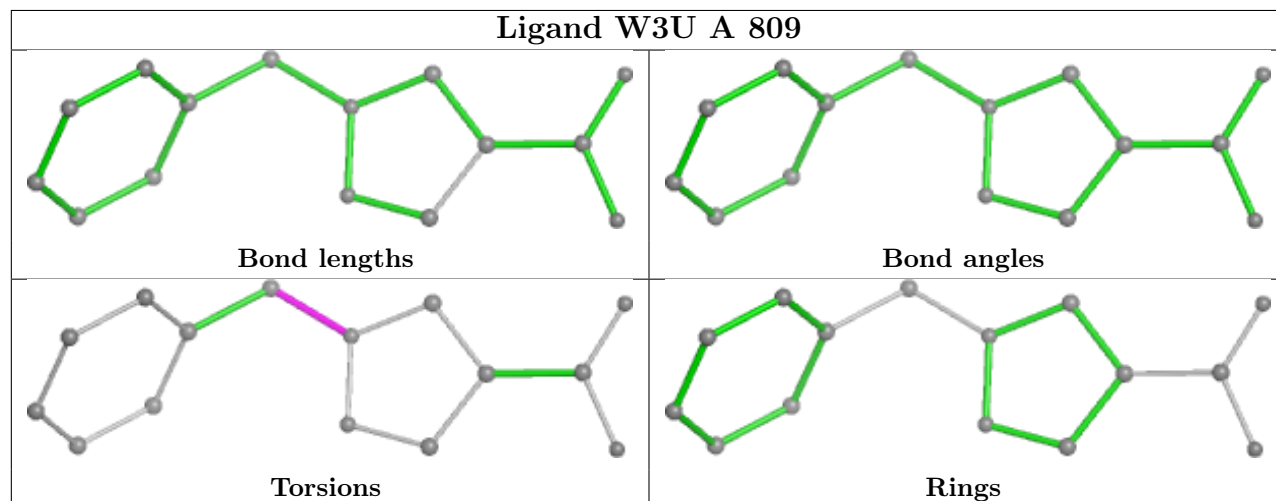
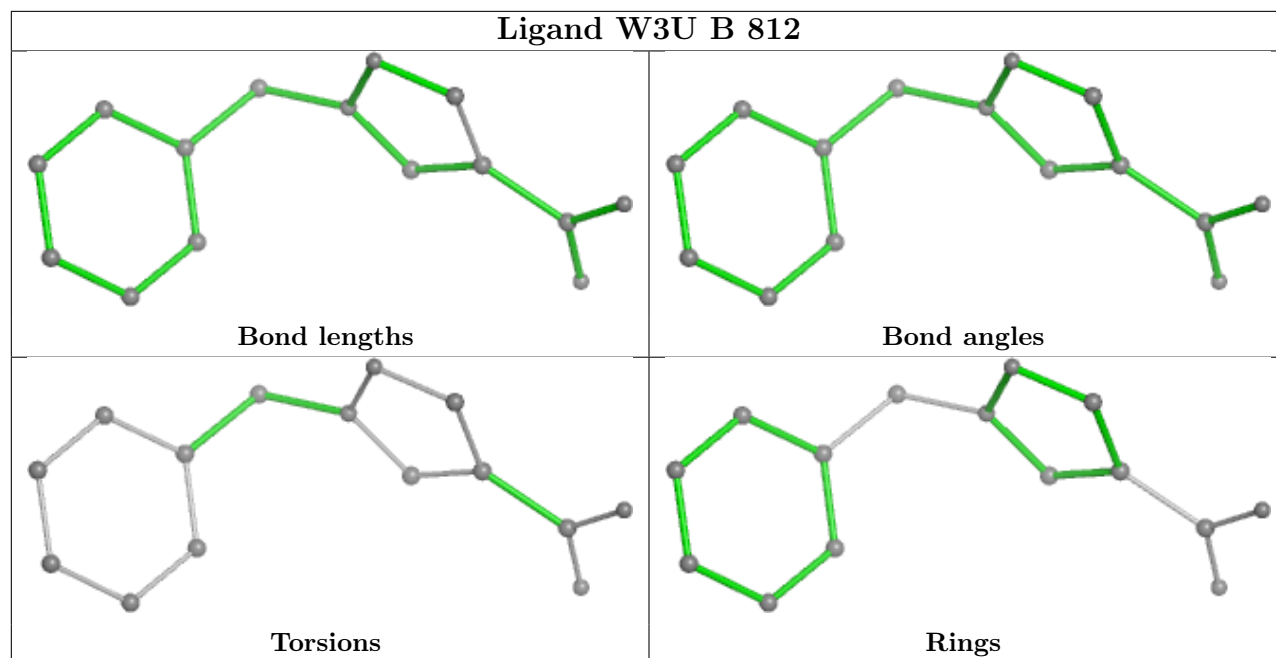
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











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%)	0.44	93 (12%) 3 3	41, 69, 145, 179	0
1	B	728/736 (98%)	0.30	59 (8%) 12 10	39, 63, 131, 182	0
2	C	402/403 (99%)	0.28	23 (5%) 23 22	36, 50, 76, 158	0
2	D	402/403 (99%)	0.31	20 (4%) 28 27	39, 56, 86, 140	0
All	All	2261/2278 (99%)	0.34	195 (8%) 10 9	36, 60, 135, 182	0

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	382	THR	9.3
1	B	389	LEU	7.9
1	A	433	ASN	6.9
1	A	385	ARG	6.8
1	B	385	ARG	6.7
1	A	403	LYS	6.4
2	C	225	PHE	5.9
2	C	226	GLU	5.8
1	A	389	LEU	5.7
1	A	371	LEU	5.5
1	B	387	ASP	5.5
1	A	384	GLU	5.4
1	A	407	PHE	5.3
1	A	432	PRO	5.3
1	A	387	ASP	5.3
1	A	375	ALA	5.3
1	A	402	PHE	5.2
2	D	225	PHE	5.0
2	D	134	MET	5.0
1	A	405	VAL	4.9
1	A	328	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	383	GLN	4.8
1	A	404	GLY	4.8
1	A	352	VAL	4.8
1	A	-6	HIS	4.7
1	B	390	LEU	4.6
1	A	453	LYS	4.6
1	B	577	THR	4.6
1	B	573	ASP	4.5
1	A	376	LEU	4.5
1	A	423	PHE	4.5
1	A	429	ILE	4.5
1	A	383	GLN	4.4
1	A	382	THR	4.4
1	A	454	ARG	4.4
1	B	720	SER	4.4
1	A	406	ASP	4.3
1	B	377	GLU	4.3
2	D	136	LEU	4.2
1	B	381	THR	4.2
2	D	228	LEU	4.2
1	A	324	PRO	4.1
1	B	609	ASP	4.0
1	B	373	ALA	4.0
1	A	358	LEU	4.0
1	B	378	ARG	3.9
1	A	427	GLU	3.9
1	A	381	THR	3.9
1	A	377	GLU	3.9
1	A	388	ALA	3.9
1	B	376	LEU	3.8
1	A	-5	SER	3.8
1	A	327	ARG	3.8
1	A	456	GLU	3.8
1	B	386	SER	3.8
1	A	373	ALA	3.8
1	B	371	LEU	3.8
1	A	325	ILE	3.8
1	A	428	ASP	3.7
1	B	393	ILE	3.7
2	D	226	GLU	3.6
2	C	86	VAL	3.6
1	A	348	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	609	ASP	3.6
1	A	449	ALA	3.5
1	A	397	ALA	3.5
1	B	384	GLU	3.5
1	B	356	VAL	3.5
1	A	359	GLU	3.5
1	A	399	ALA	3.4
1	A	401	ASP	3.4
1	B	1	MET	3.4
1	A	318	GLU	3.4
1	A	425	GLU	3.4
1	A	378	ARG	3.4
1	B	452	VAL	3.3
1	A	380	ARG	3.3
2	C	2	SER	3.3
2	D	2	SER	3.2
1	A	320	ILE	3.2
1	A	360	ALA	3.2
1	B	429	ILE	3.2
1	A	3	ASP	3.2
2	D	231	LEU	3.2
1	A	398	ASP	3.2
2	D	92	CYS	3.1
1	A	379	GLY	3.1
1	A	322	LYS	3.1
1	A	579	GLN	3.0
1	B	0	SER	3.0
1	A	2	PRO	3.0
1	A	319	GLY	3.0
1	A	430	VAL	3.0
1	A	610	GLY	3.0
1	B	355	ASP	3.0
1	A	434	ALA	3.0
1	B	417	GLU	2.9
1	A	349	TYR	2.9
1	B	367	TYR	2.9
2	D	88	LEU	2.9
2	D	291	THR	2.9
1	B	451	GLY	2.9
2	D	227	GLY	2.8
1	A	452	VAL	2.8
1	B	574	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	571	VAL	2.8
1	A	431	GLU	2.8
1	B	575	GLY	2.8
1	A	720	SER	2.8
1	B	576	GLY	2.8
1	B	420	HIS	2.8
1	B	430	VAL	2.8
1	A	395	PRO	2.8
2	C	227	GLY	2.7
2	C	228	LEU	2.7
1	A	362	ALA	2.7
2	D	135	GLY	2.7
2	C	58	CYS	2.7
1	B	380	ARG	2.7
1	A	350	GLU	2.7
1	B	391	ALA	2.7
1	B	449	ALA	2.7
1	B	690	ALA	2.7
1	B	578	TYR	2.7
1	B	428	ASP	2.7
1	B	331	LEU	2.7
1	A	417	GLU	2.7
1	A	426	ILE	2.6
1	B	370	LYS	2.6
2	D	93	ALA	2.6
1	A	326	LYS	2.6
1	A	392	ARG	2.6
1	A	396	THR	2.6
2	D	388	LEU	2.6
1	A	413	PHE	2.6
2	D	390	ILE	2.6
1	A	356	VAL	2.5
1	B	611	LYS	2.5
1	B	571	VAL	2.5
1	A	386	SER	2.5
1	A	-7	HIS	2.5
1	B	366	GLY	2.5
1	B	354	LYS	2.5
1	B	379	GLY	2.5
1	B	369	GLU	2.5
1	B	425	GLU	2.5
1	B	572	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	333	ALA	2.5
1	B	443	LEU	2.4
1	A	347	ALA	2.4
1	A	-8	HIS	2.4
1	A	457	ASP	2.4
2	C	70	ALA	2.4
1	A	394	THR	2.4
1	B	359	GLU	2.4
2	C	216	GLU	2.4
2	C	75	LEU	2.3
2	D	86	VAL	2.3
2	C	74	VAL	2.3
1	B	570	GLY	2.3
1	A	420	HIS	2.3
2	C	88	LEU	2.2
1	A	365	LYS	2.2
1	B	621	GLU	2.2
1	A	353	LEU	2.2
1	A	372	GLU	2.2
2	C	81	VAL	2.2
1	A	459	ILE	2.2
2	C	72	ALA	2.2
2	D	394	MET	2.2
1	A	351	VAL	2.2
2	D	395	GLY	2.2
1	B	479	GLU	2.2
1	B	593	LEU	2.2
1	B	423	PHE	2.2
2	C	85	GLY	2.2
2	D	230	ALA	2.2
1	B	414	GLU	2.1
2	C	55	ILE	2.1
2	C	69	ILE	2.1
2	C	56	LEU	2.1
1	A	391	ALA	2.1
2	C	73	ALA	2.1
2	C	61	PRO	2.1
2	C	66	GLY	2.1
2	C	231	LEU	2.1
1	B	403	LYS	2.1
1	A	369	GLU	2.1
2	D	89	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	355	ASP	2.1
1	A	331	LEU	2.0
2	C	71	ARG	2.0
1	A	1	MET	2.0
1	A	624	LYS	2.0
1	B	352	VAL	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 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	803	5/5	0.71	0.19	85,89,103,107	5
4	W3U	A	809	15/15	0.72	0.32	102,111,125,127	0
4	W3U	A	808	15/15	0.75	0.34	89,108,126,128	0
3	SO4	A	801	5/5	0.82	0.22	124,126,143,154	0
3	SO4	D	505	5/5	0.82	0.40	80,80,94,103	5
4	W3U	B	809[A]	15/15	0.83	0.34	70,77,84,86	15
4	W3U	B	809[B]	15/15	0.83	0.34	71,82,91,93	15
4	W3U	A	807[A]	15/15	0.84	0.37	74,85,90,93	15
4	W3U	A	807[B]	15/15	0.84	0.37	74,83,90,93	15
3	SO4	B	805	5/5	0.85	0.23	115,117,141,156	0
4	W3U	B	810	15/15	0.85	0.24	61,94,108,112	0
3	SO4	C	505	5/5	0.86	0.39	114,122,138,164	0
4	W3U	B	813	15/15	0.86	0.25	92,101,118,118	0
4	W3U	B	808	15/15	0.87	0.18	98,119,139,144	0
3	SO4	B	806	5/5	0.88	0.41	69,71,78,80	5
4	W3U	B	812	15/15	0.89	0.31	56,88,118,118	0
3	SO4	C	507	5/5	0.89	0.20	65,66,78,79	5

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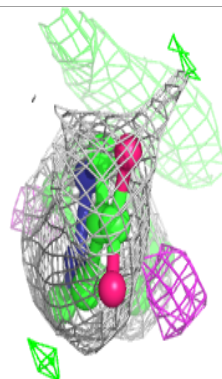
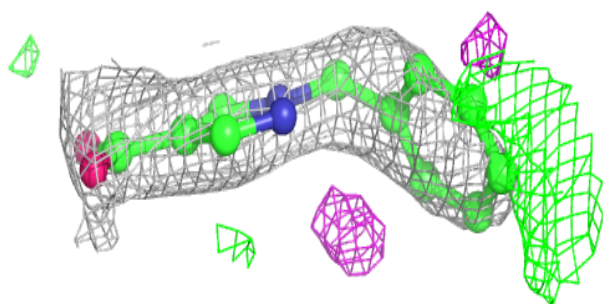
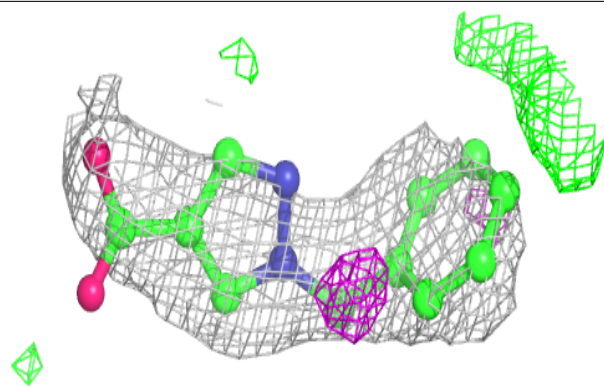
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	C	504	5/5	0.90	0.21	102,104,140,164	0
3	SO4	B	801	5/5	0.90	0.21	59,70,80,85	5
3	SO4	A	804	5/5	0.91	0.49	118,129,164,167	0
3	SO4	C	506	5/5	0.91	0.09	77,77,101,113	0
3	SO4	C	503	5/5	0.91	0.21	89,100,115,140	0
3	SO4	A	803	5/5	0.91	0.14	72,73,76,80	5
4	W3U	A	805	15/15	0.91	0.15	58,79,93,97	0
3	SO4	D	506	5/5	0.93	0.08	122,124,128,130	5
3	SO4	A	802	5/5	0.94	0.14	99,110,126,127	0
3	SO4	D	502	5/5	0.94	0.20	85,89,107,114	0
4	W3U	B	811	15/15	0.94	0.14	60,72,85,89	0
3	SO4	D	503	5/5	0.94	0.33	100,116,126,143	0
3	SO4	B	804	5/5	0.94	0.18	73,73,85,89	5
4	W3U	A	806	15/15	0.95	0.15	69,73,82,83	0
3	SO4	B	802	5/5	0.95	0.17	77,99,108,117	0
3	SO4	D	501	5/5	0.96	0.08	96,101,105,105	0
3	SO4	B	807	5/5	0.96	0.15	134,135,140,142	0
3	SO4	C	501	5/5	0.97	0.09	74,78,86,93	0
3	SO4	D	504	5/5	0.98	0.16	71,85,87,89	0
3	SO4	C	502	5/5	0.98	0.19	71,75,77,101	0

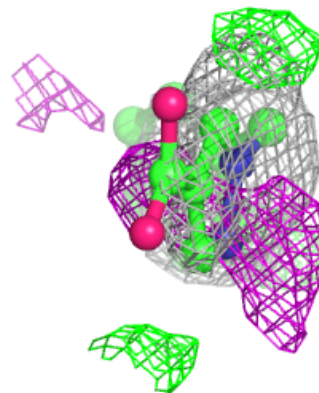
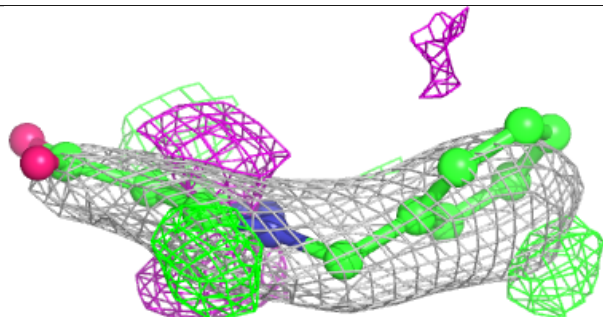
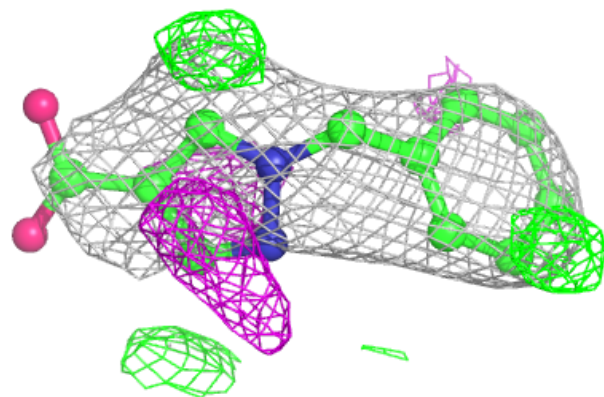
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around W3U A 809:

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

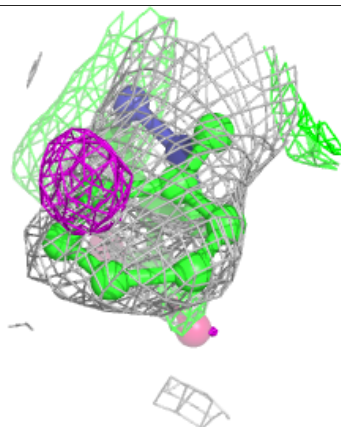
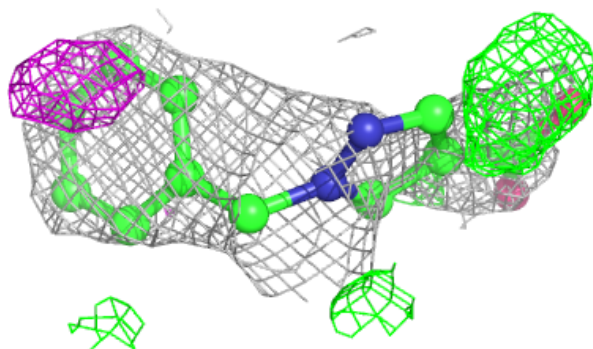
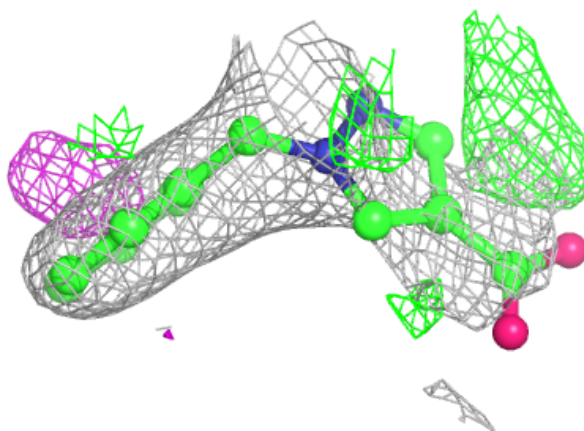
**Electron density around W3U A 808:**

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

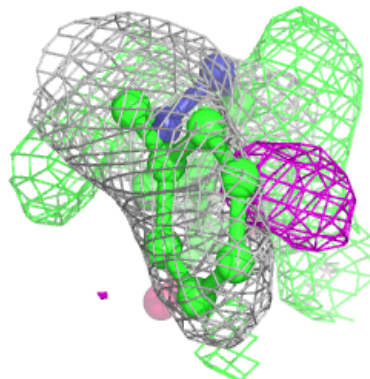
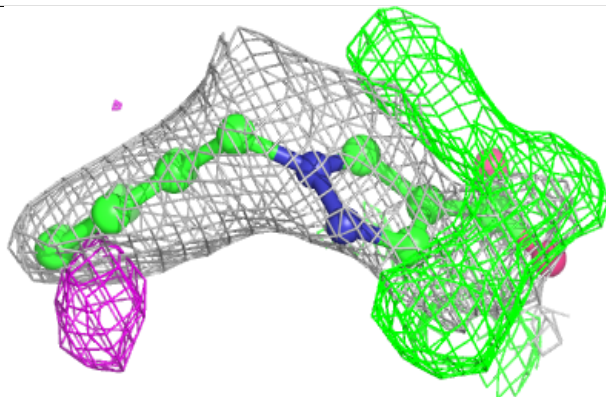
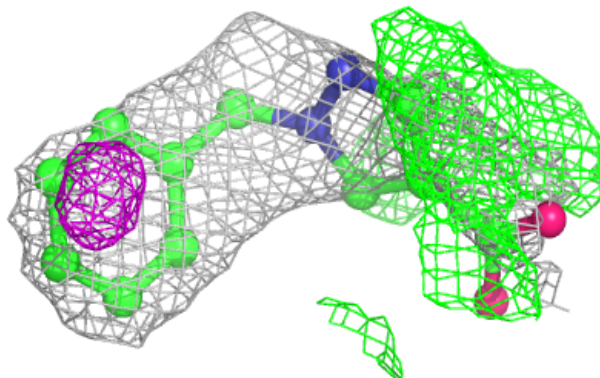


Electron density around W3U B 809 (A):

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

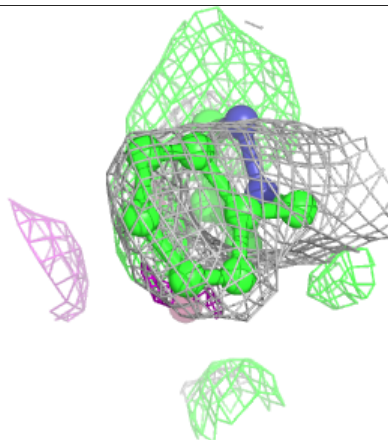
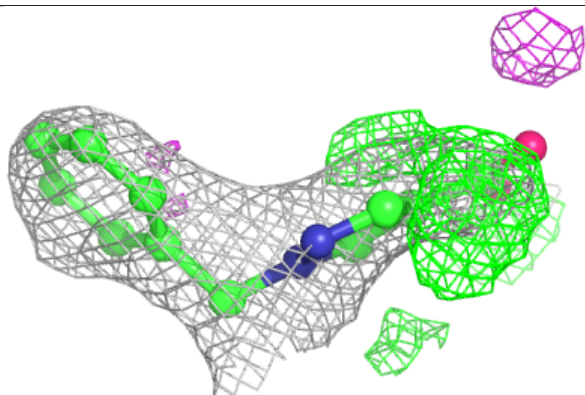
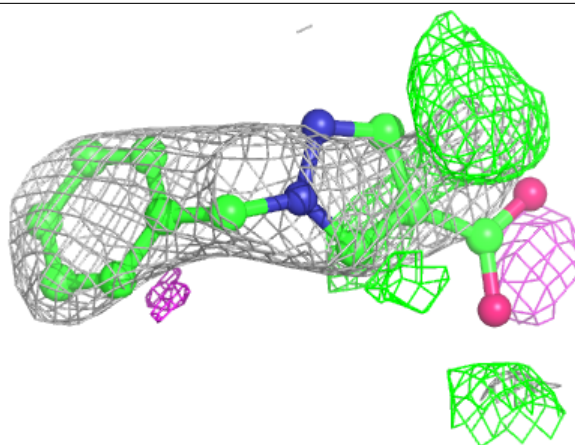
**Electron density around W3U B 809 (B):**

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



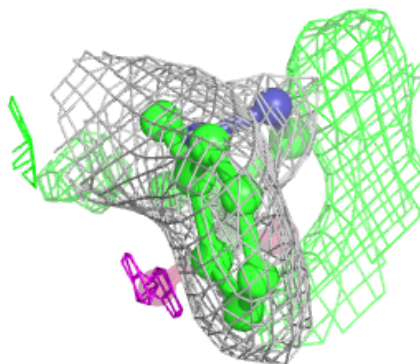
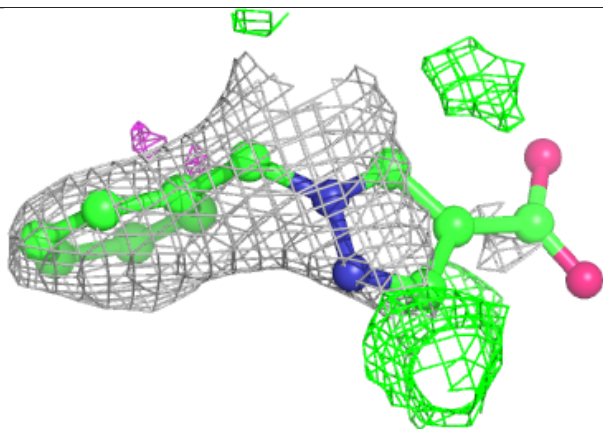
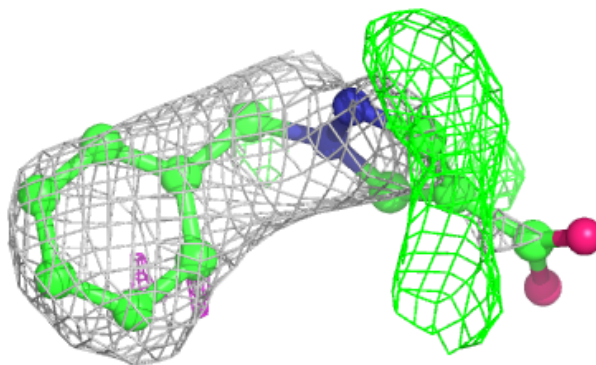
Electron density around W3U A 807 (A):

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

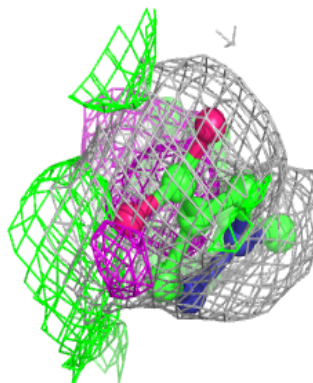
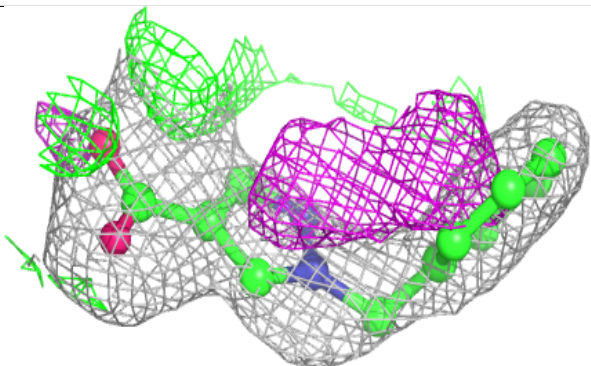
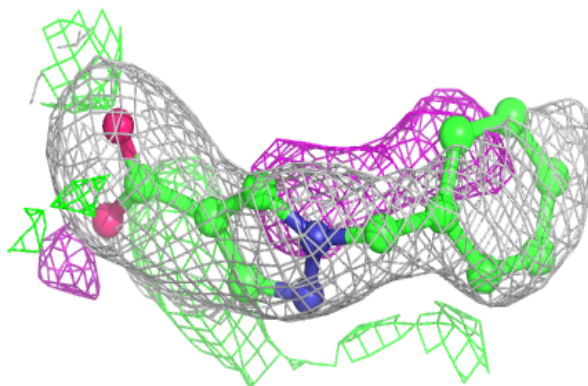


Electron density around W3U A 807 (B):

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

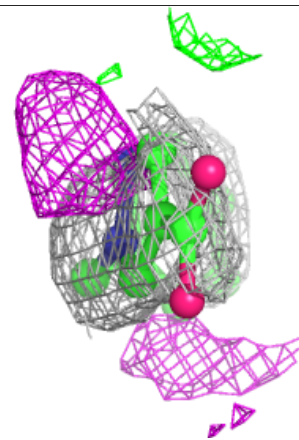
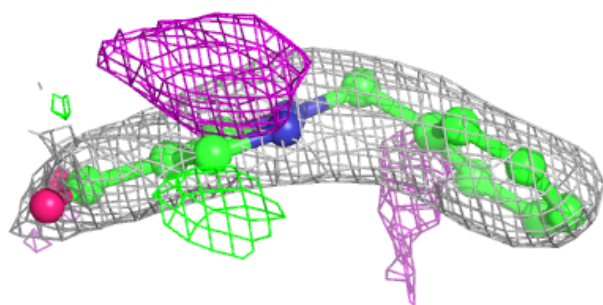
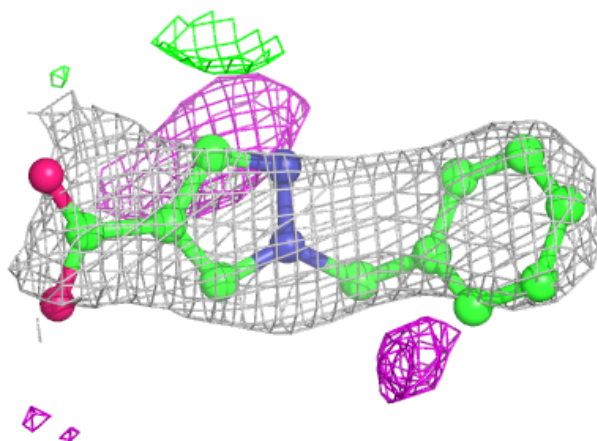
**Electron density around W3U B 810:**

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

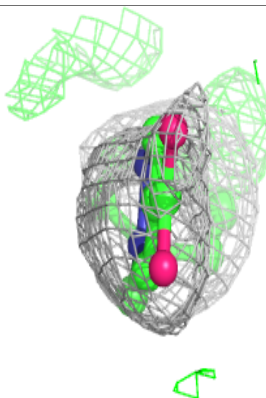
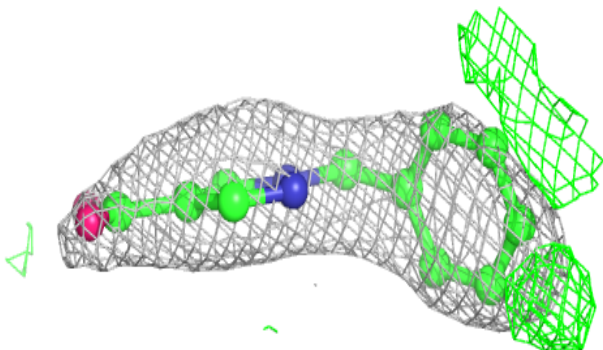
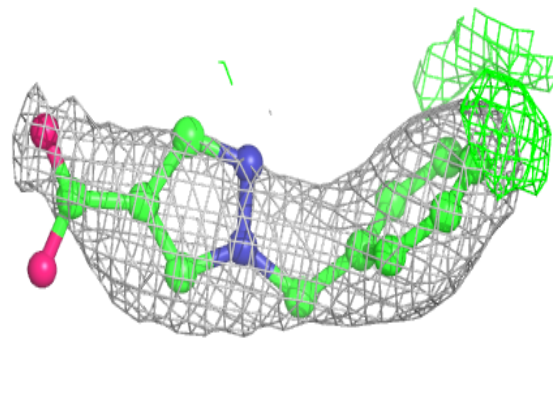


Electron density around W3U B 813:

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

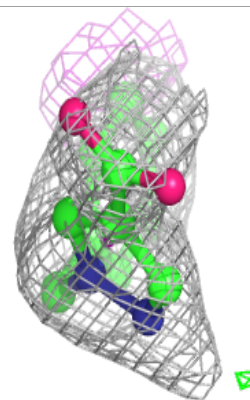
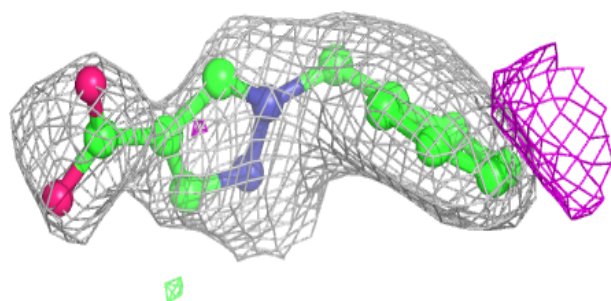
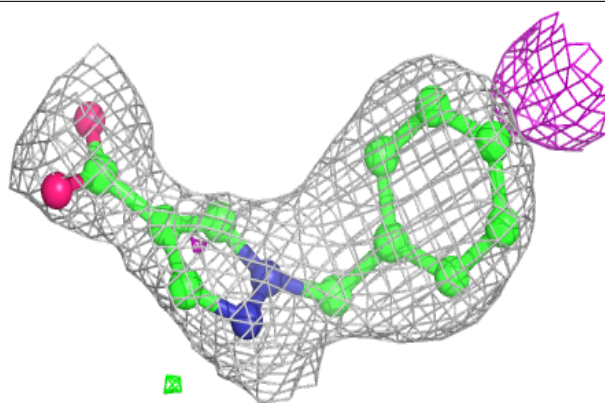
**Electron density around W3U B 808:**

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

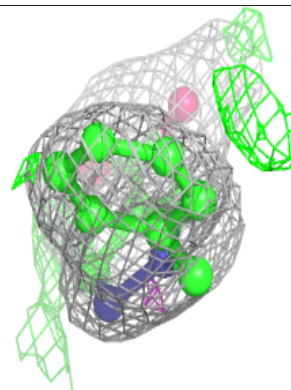
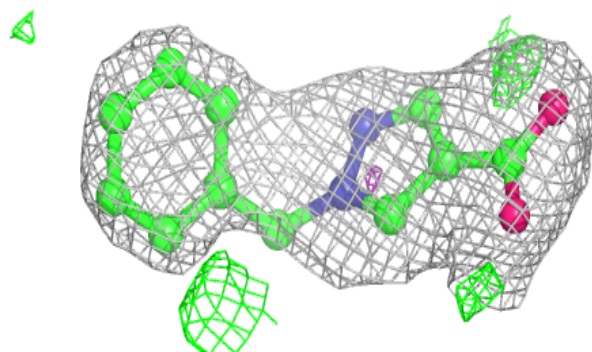
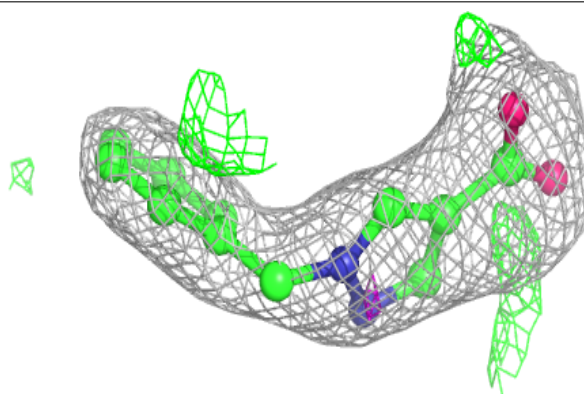


Electron density around W3U B 812:

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

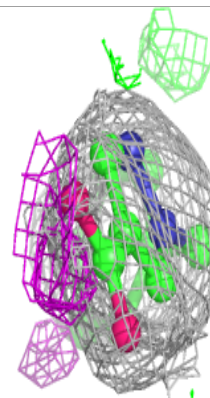
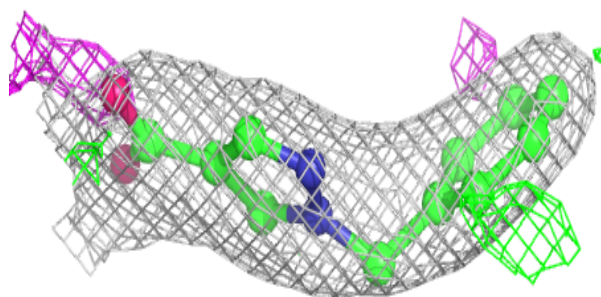
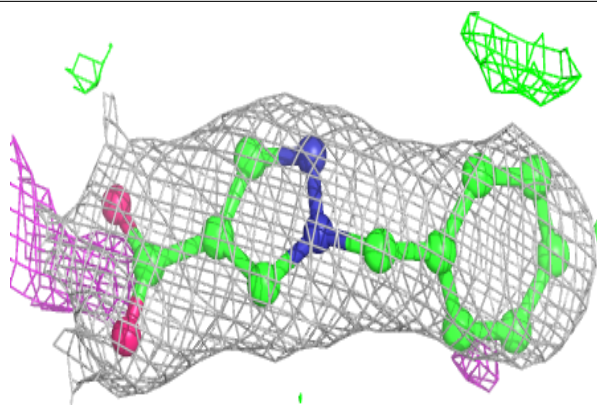
**Electron density around W3U A 805:**

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

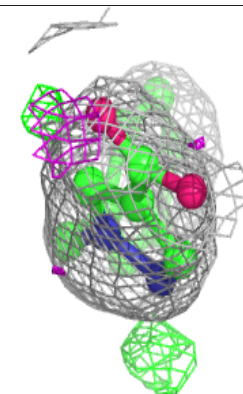
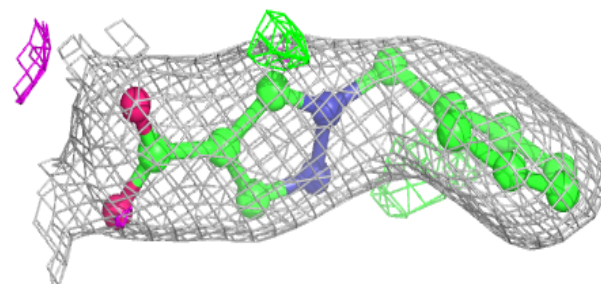
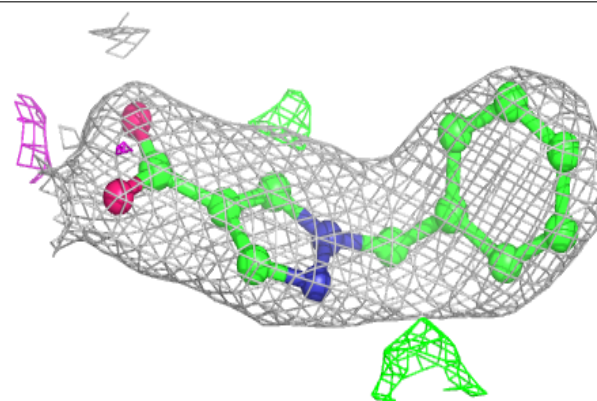


Electron density around W3U B 811:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.