



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 01:47 AM UTC

PDB ID : 8PF8 / pdb_00008pf8
Title : Structure of Mycobacterium tuberculosis beta-oxidation trifunctional enzyme
in complex with Fragment-M-72
Authors : Dalwani, S.; Wierenga, R.K.; Venkatesan, R.
Deposited on : 2023-06-15
Resolution : 2.23 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

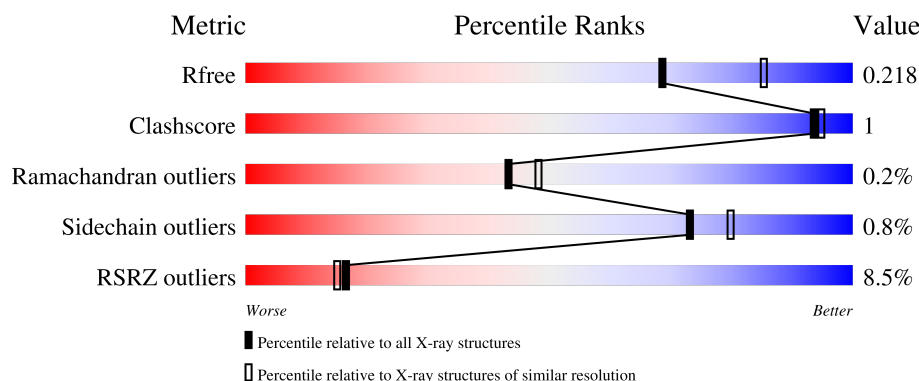
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.23 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	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	736	10% 96% ..
1	B	736	8% 95% ..
2	C	403	7% 95% 5%
2	D	403	8% 94% 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 17613 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 Probable fatty oxidation protein FadB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5429	3434	936	1038	21			
1	B	732	Total	C	N	O	S	0	0	0
			5450	3445	940	1044	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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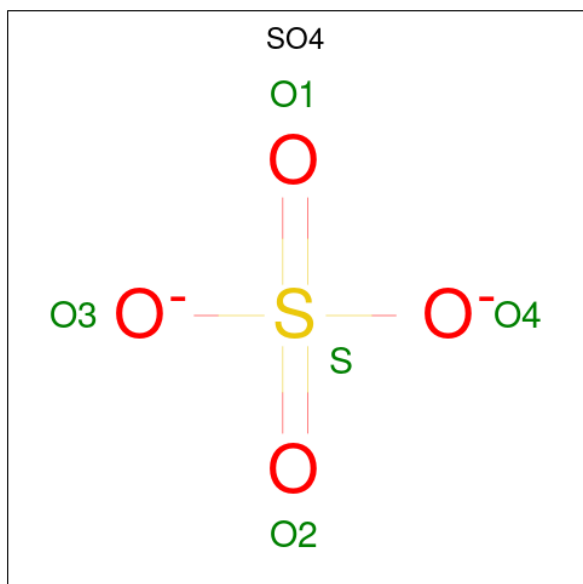
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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	HIS	-	expression tag	UNP O53872
B	-5	SER	-	expression tag	UNP O53872
B	-4	GLN	-	expression tag	UNP O53872
B	-3	ASP	-	expression tag	UNP O53872
B	-2	PRO	-	expression tag	UNP O53872
B	-1	ASN	-	expression 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	0	0
			2966	1853	525	573	15			
2	D	403	Total	C	N	O	S	0	0	0
			2971	1856	526	574	15			

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



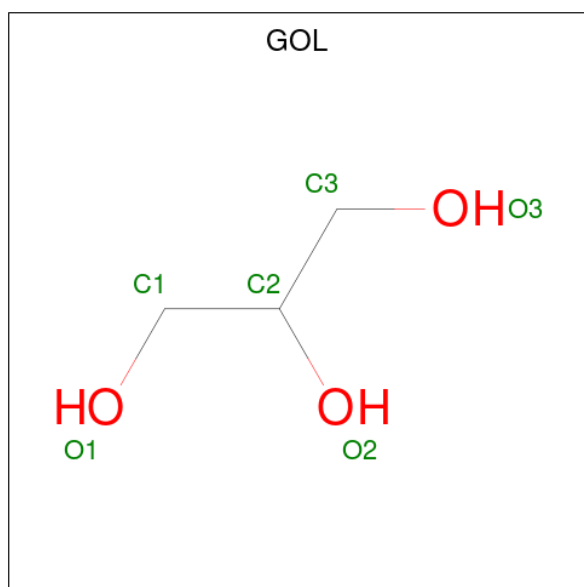
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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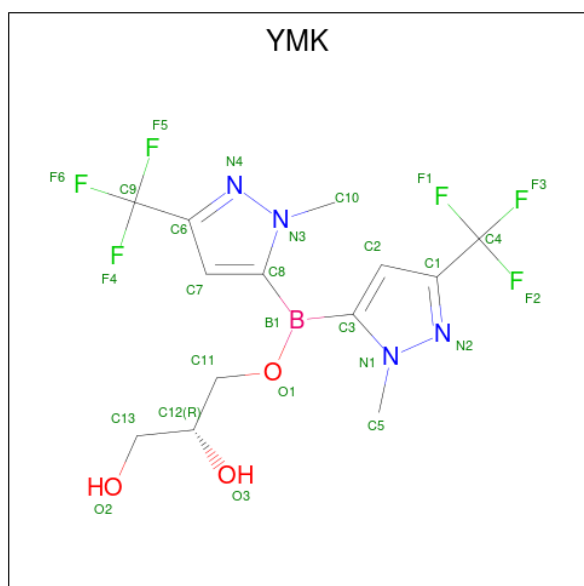
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

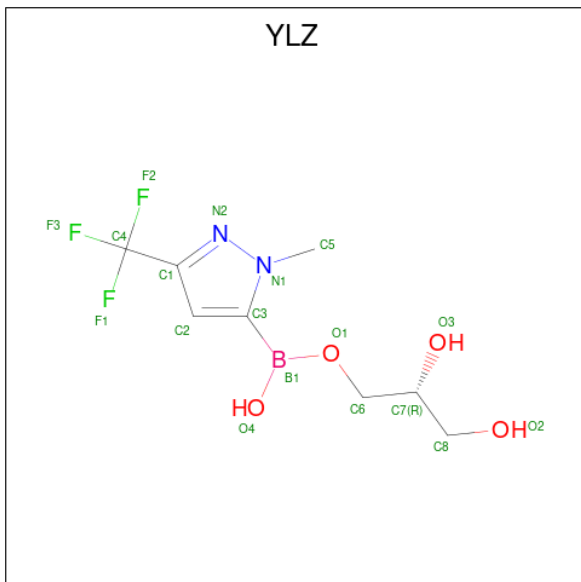
- Molecule 5 is (2 {R})-3-bis[2-methyl-5-(trifluoromethyl)pyrazol-3-yl]boranyloxypropan e-1,2-diol (CCD ID: YMK) (formula: $C_{13}H_{15}BF_6N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	B	C	F	N	O	0	0
			27	1	13	6	4	3		

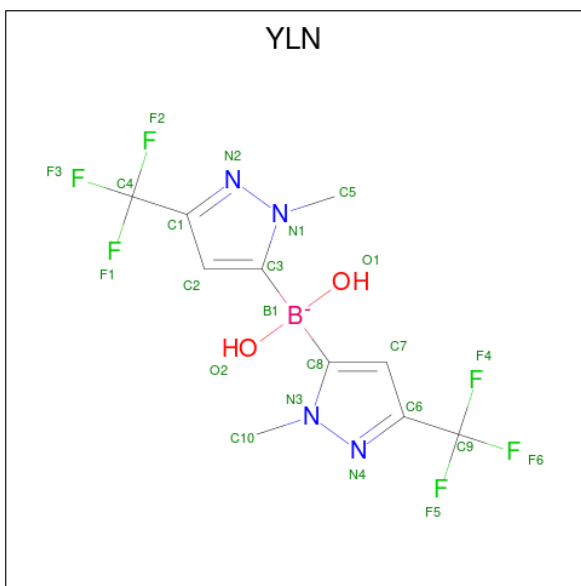
- Molecule 6 is [(2 {R})-2,3-bis(oxidanyl)propoxy]-[2-methyl-5-(trifluoromethyl)pyrazol-3-yl]

borinic acid (CCD ID: YLZ) (formula: $C_8H_{12}BF_3N_2O_4$) (labeled as "Ligand of Interest" by depositor).



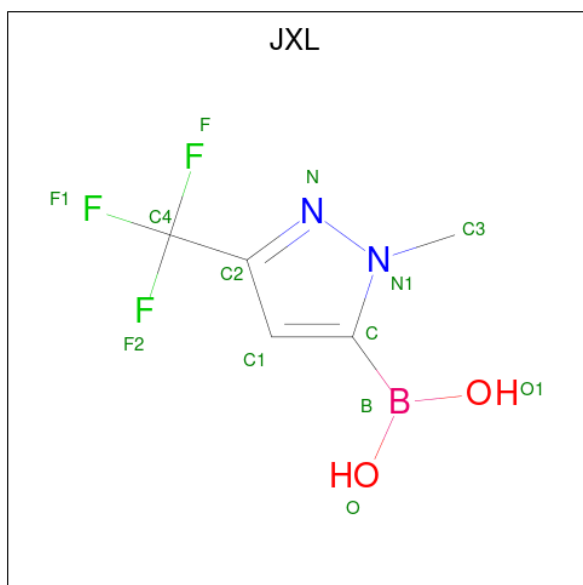
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	B	C	F	N	O		
6	A	1	18	1	8	3	2	4	0	0
6	B	1	18	1	8	3	2	4	0	0

- Molecule 7 is bis[2-methyl-5-(trifluoromethyl)pyrazol-3-yl]-bis(oxidanyl)boranuide (CCD ID: YLN) (formula: $C_{10}H_{10}BF_6N_4O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	B	C	F	N	O	0	0
			22	1	10	6	4	1		
7	B	1	Total	B	C	F	N	O	0	0
			22	1	10	6	4	1		

- Molecule 8 is [2-methyl-5-(trifluoromethyl)pyrazol-3-yl]boronic acid (CCD ID: JXL) (formula: $C_5H_6BF_3N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	B	C	F	N	O	0	0
			13	1	5	3	2	2		
8	A	1	Total	B	C	F	N	O	0	0
			13	1	5	3	2	2		
8	A	1	Total	B	C	F	N	O	0	0
			13	1	5	3	2	2		
8	B	1	Total	B	C	F	N	O	0	0
			13	1	5	3	2	2		
8	B	1	Total	B	C	F	N	O	0	0
			13	1	5	3	2	2		
8	B	1	Total	B	C	F	N	O	0	0
			13	1	5	3	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	116	Total	O	0	0
			116	116		

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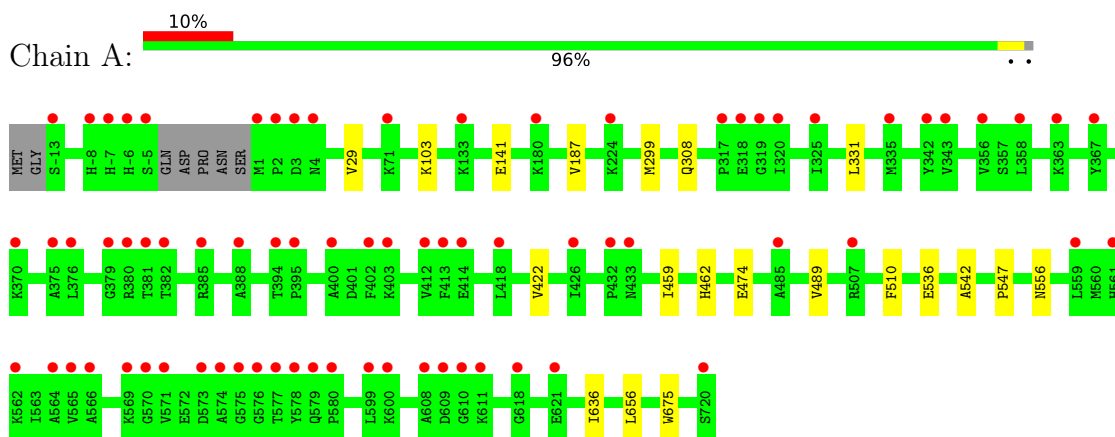
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	171	Total 171	O 171	0	0
9	C	111	Total 111	O 111	0	0
9	D	93	Total 93	O 93	0	0

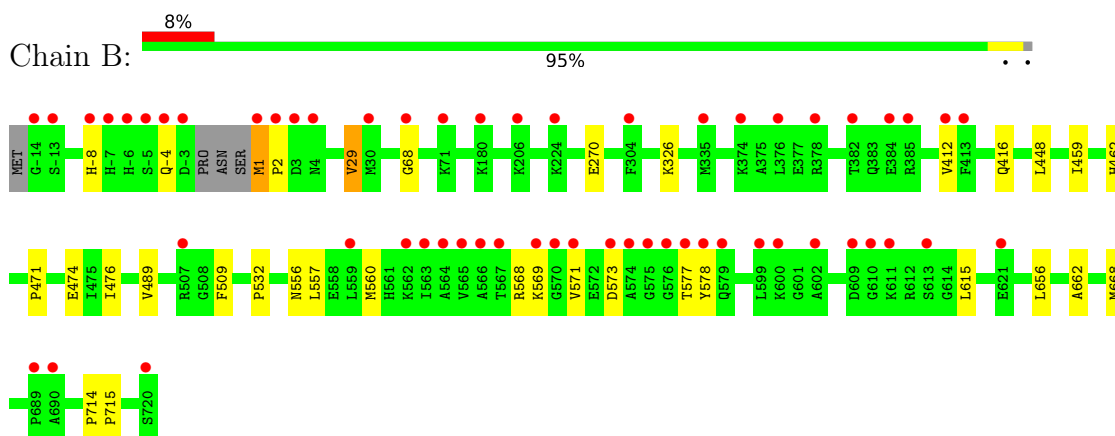
3 Residue-property plots

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

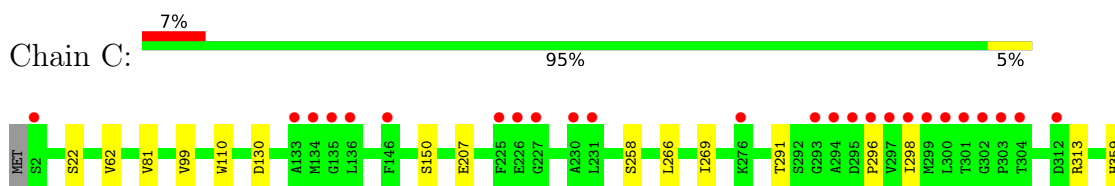
- Molecule 1: Probable fatty oxidation protein FadB

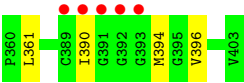


- Molecule 1: Probable fatty oxidation protein FadB

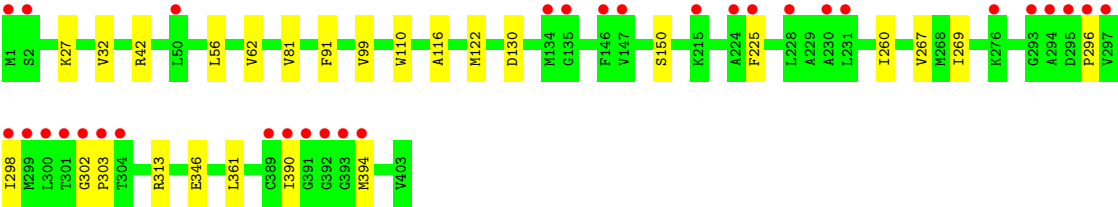


- Molecule 2: Putative acyltransferase Rv0859





● Molecule 2: Putative acyltransferase Rv0859



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	250.96Å 134.61Å 119.97Å 90.00° 110.44° 90.00°	Depositor
Resolution (Å)	112.42 – 2.23 112.42 – 2.23	Depositor EDS
% Data completeness (in resolution range)	72.7 (112.42-2.23) 72.7 (112.42-2.23)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.22Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.189 , 0.219 0.189 , 0.218	Depositor DCC
R_{free} test set	6595 reflections (3.65%)	wwPDB-VP
Wilson B-factor (Å ²)	46.8	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 34.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17613	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: YMK, GOL, SO4, YLZ, YLN, JXL

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	0.12	0/5532	0.28	0/7486
1	B	0.12	0/5553	0.28	0/7514
2	C	0.11	0/3011	0.30	0/4077
2	D	0.11	0/3016	0.31	0/4084
All	All	0.12	0/17112	0.29	0/23161

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	5429	0	5467	8	0
1	B	5450	0	5482	16	0
2	C	2966	0	2986	13	0
2	D	2971	0	2991	15	0
3	A	20	0	0	0	0
3	B	25	0	0	1	0
3	C	35	0	0	0	0
3	D	35	0	0	0	0
4	A	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	27	0	0	0	0
6	A	18	0	0	0	0
6	B	18	0	0	0	0
7	A	22	0	0	0	0
7	B	22	0	0	1	0
8	A	39	0	0	0	0
8	B	39	0	0	0	0
9	A	116	0	0	0	0
9	B	171	0	0	0	0
9	C	111	0	0	0	0
9	D	93	0	0	0	0
All	All	17613	0	16934	47	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 1.

All (47) 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:-8:HIS:HB2	1:B:-4:GLN:HE21	1.47	0.77
2:C:110:TRP:CD1	2:D:313:ARG:HD3	2.37	0.59
1:A:299:MET:HE2	1:A:675:TRP:HA	1.84	0.59
1:B:462:HIS:HB3	1:B:474:GLU:HB3	1.85	0.57
2:D:390:ILE:HB	2:D:394:MET:HG3	1.86	0.57
2:C:62:VAL:HG12	2:D:62:VAL:HG12	1.87	0.56
2:C:81:VAL:HG11	2:D:296:PRO:HD3	1.87	0.56
2:C:296:PRO:HD3	2:D:81:VAL:HG11	1.89	0.55
2:C:99:VAL:HG13	2:C:269:ILE:HD11	1.89	0.55
2:C:313:ARG:HD3	2:D:110:TRP:CD1	2.42	0.54
1:B:270:GLU:HG2	2:D:27:LYS:HE2	1.90	0.54
2:C:291:THR:HG22	2:C:396:VAL:HG22	1.92	0.51
1:A:462:HIS:HB3	1:A:474:GLU:HB3	1.93	0.50
1:B:29:VAL:HG13	1:B:68:GLY:HA2	1.94	0.49
2:C:22:SER:OG	2:C:207:GLU:OE2	2.23	0.49
2:D:302:GLY:N	2:D:303:PRO:HD2	2.27	0.49
1:B:557:LEU:HA	1:B:560:MET:HE3	1.94	0.48
2:C:390:ILE:HD11	2:C:396:VAL:HG23	1.95	0.48
2:D:99:VAL:HG13	2:D:269:ILE:HD11	1.96	0.48
2:C:62:VAL:HG11	2:C:130:ASP:HA	1.96	0.47
1:B:-8:HIS:HB3	3:B:807:SO4:O3	2.15	0.47
2:D:150:SER:HB2	2:D:225:PHE:CG	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ILE:HG21	1:A:489:VAL:HG21	1.97	0.45
2:D:62:VAL:HG11	2:D:130:ASP:HA	1.98	0.45
1:B:471:PRO:HG2	1:B:668:MET:HB3	1.98	0.45
1:A:510:PHE:CD1	1:A:656:LEU:HD11	2.52	0.45
1:B:714:PRO:HA	1:B:715:PRO:HD3	1.91	0.44
1:B:569:LYS:O	1:B:573:ASP:N	2.31	0.44
2:D:116:ALA:O	2:D:267:VAL:N	2.44	0.44
2:D:32:VAL:HG11	2:D:56:LEU:HD11	2.00	0.44
1:A:536:GLU:CD	1:A:547:PRO:HB2	2.43	0.43
1:B:1:MET:HA	1:B:2:PRO:HD3	1.83	0.43
2:C:258:SER:HB2	2:C:359:HIS:HB2	2.00	0.43
2:C:390:ILE:HB	2:C:394:MET:HB2	2.01	0.43
1:B:568:ARG:HD3	1:B:578:TYR:CD2	2.53	0.43
1:B:416:GLN:HG3	1:B:448:LEU:HD23	2.01	0.43
2:C:266:LEU:HD23	2:C:266:LEU:HA	1.82	0.43
2:D:91:PHE:HB2	2:D:390:ILE:CG2	2.49	0.43
1:B:459:ILE:HG21	1:B:489:VAL:HG21	2.01	0.42
2:D:122:MET:HE2	2:D:260:ILE:HG23	2.01	0.42
7:B:806:YLN:C7	7:B:806:YLN:C3	2.95	0.42
1:B:532:PRO:HB2	1:B:615:LEU:HD13	2.02	0.41
1:A:331:LEU:HD13	1:A:422:VAL:HG12	2.02	0.41
1:A:542:ALA:HB2	1:A:636:ILE:HG23	2.02	0.41
1:B:476:ILE:HG21	1:B:509:PHE:CE1	2.56	0.41
1:B:656:LEU:HD13	1:B:662:ALA:HB2	2.02	0.41
1:A:103:LYS:HE2	1:A:103:LYS:HB3	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	725/736 (98%)	701 (97%)	23 (3%)	1 (0%)	48 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	728/736 (99%)	707 (97%)	19 (3%)	2 (0%)	36	38
2	C	400/403 (99%)	387 (97%)	12 (3%)	1 (0%)	36	38
2	D	401/403 (100%)	390 (97%)	10 (2%)	1 (0%)	43	48
All	All	2254/2278 (99%)	2185 (97%)	64 (3%)	5 (0%)	43	48

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	361	LEU
2	C	361	LEU
1	A	556	ASN
1	B	556	ASN
1	B	412	VAL

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%)	556 (99%)	4 (1%)	76	81
1	B	562/566 (99%)	557 (99%)	5 (1%)	70	78
2	C	309/310 (100%)	307 (99%)	2 (1%)	78	83
2	D	309/310 (100%)	306 (99%)	3 (1%)	68	76
All	All	1740/1752 (99%)	1726 (99%)	14 (1%)	73	80

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

Mol	Chain	Res	Type
1	A	29	VAL
1	A	141	GLU
1	A	187	VAL
1	A	308	GLN
1	B	1	MET
1	B	29	VAL

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Mol	Chain	Res	Type
1	B	326	LYS
1	B	571	VAL
1	B	577	THR
2	C	150	SER
2	C	298	ILE
2	D	42	ARG
2	D	298	ILE
2	D	346	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	298	ASN
1	A	383	GLN
1	A	550	GLN
1	A	681	GLN
1	B	550	GLN
1	B	633	GLN
1	B	681	GLN
2	C	49	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

35 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	802	-	4,4,4	0.24	0	6,6,6	0.05	0
6	YLZ	B	805	-	15,18,18	0.31	0	19,26,26	0.23	0
3	SO4	B	804	-	4,4,4	0.24	0	6,6,6	0.08	0
7	YLN	B	806	1	17,23,24	3.44	1 (5%)	24,37,40	0.58	0
8	JXL	A	809	-	10,13,13	0.38	0	15,20,20	0.28	0
3	SO4	C	507	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	504	-	4,4,4	0.23	0	6,6,6	0.09	0
8	JXL	B	808	-	10,13,13	0.36	0	15,20,20	0.22	0
3	SO4	C	502	-	4,4,4	0.24	0	6,6,6	0.05	0
8	JXL	A	810	-	10,13,13	0.30	0	15,20,20	0.22	0
3	SO4	C	503	-	4,4,4	0.24	0	6,6,6	0.12	0
3	SO4	D	501	-	4,4,4	0.24	0	6,6,6	0.08	0
6	YLZ	A	807	-	15,18,18	0.34	0	19,26,26	0.23	0
3	SO4	C	501	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	A	804	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	D	507	-	4,4,4	0.24	0	6,6,6	0.04	0
8	JXL	B	809	-	10,13,13	0.32	0	15,20,20	0.20	0
3	SO4	C	505	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	A	801	-	4,4,4	0.24	0	6,6,6	0.06	0
8	JXL	B	810	-	10,13,13	0.37	0	15,20,20	0.26	0
3	SO4	D	506	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	B	803	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	C	506	-	4,4,4	0.24	0	6,6,6	0.05	0
3	SO4	D	502	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	D	503	-	4,4,4	0.24	0	6,6,6	0.08	0
3	SO4	B	801	-	4,4,4	0.23	0	6,6,6	0.12	0
3	SO4	D	505	-	4,4,4	0.23	0	6,6,6	0.08	0
5	YMK	A	806	-	22,28,28	0.34	0	29,43,43	0.23	0
3	SO4	B	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	0.08	0
3	SO4	B	807	-	4,4,4	0.24	0	6,6,6	0.11	0
3	SO4	C	504	-	4,4,4	0.23	0	6,6,6	0.06	0
7	YLN	A	808	1	17,23,24	3.43	1 (5%)	24,37,40	0.57	0
4	GOL	A	805	-	5,5,5	0.96	0	5,5,5	1.04	0
8	JXL	A	811	-	10,13,13	0.31	0	15,20,20	0.28	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
6	YLZ	B	805	-	-	4/10/17/17	0/1/1/1
7	YLN	B	806	1	-	0/12/20/24	0/2/2/2
8	JXL	A	809	-	-	0/8/10/10	0/1/1/1
6	YLZ	A	807	-	-	3/10/17/17	0/1/1/1
7	YLN	A	808	1	-	0/12/20/24	0/2/2/2
4	GOL	A	805	-	-	0/4/4/4	-
8	JXL	B	808	-	-	0/8/10/10	0/1/1/1
8	JXL	B	809	-	-	2/8/10/10	0/1/1/1
8	JXL	A	810	-	-	2/8/10/10	0/1/1/1
8	JXL	B	810	-	-	2/8/10/10	0/1/1/1
5	YMK	A	806	-	-	2/18/27/27	0/2/2/2
8	JXL	A	811	-	-	0/8/10/10	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	806	YLN	B1-O1	14.16	1.51	1.36
7	A	808	YLN	B1-O1	14.11	1.51	1.36

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	806	YMK	C3-B1-O1-C11
5	A	806	YMK	C8-B1-O1-C11
6	B	805	YLZ	C6-C7-C8-O2
8	A	810	JXL	O1-B-C-C1
8	A	810	JXL	O-B-C-C1
8	B	809	JXL	O1-B-C-C1
8	B	809	JXL	O-B-C-C1
8	B	810	JXL	O1-B-C-C1
8	B	810	JXL	O-B-C-C1
6	A	807	YLZ	C6-C7-C8-O2
6	B	805	YLZ	O3-C7-C8-O2
6	A	807	YLZ	O3-C7-C8-O2

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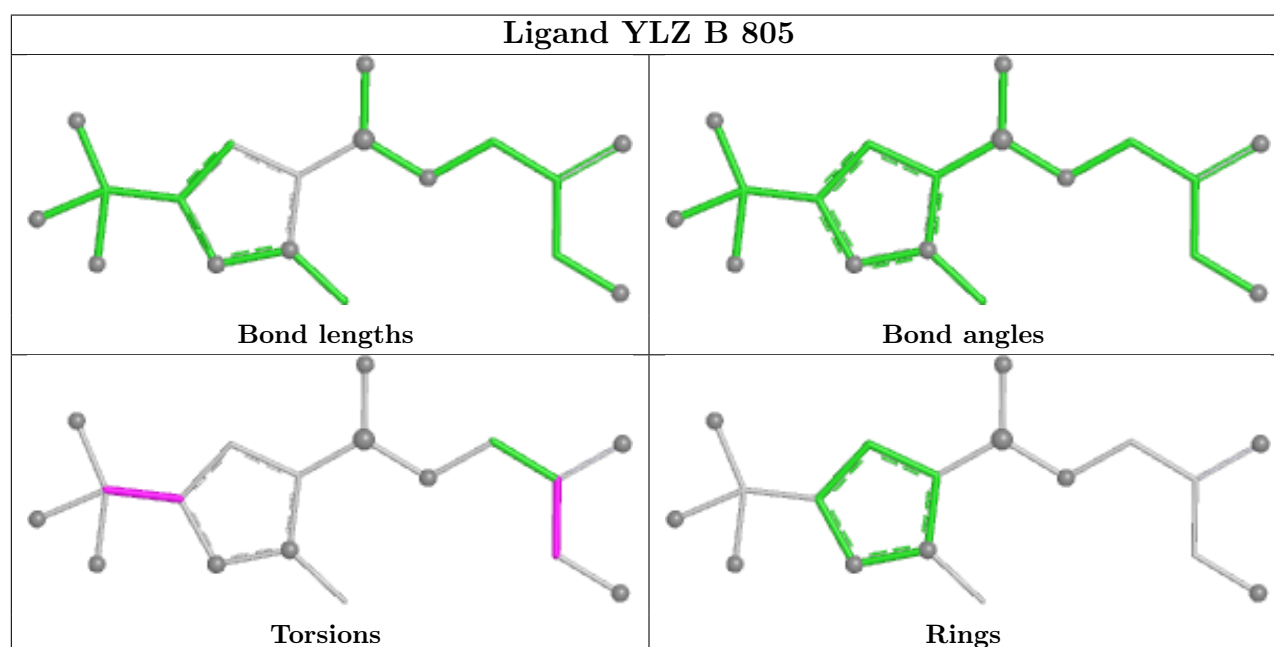
Mol	Chain	Res	Type	Atoms
6	B	805	YLZ	N2-C1-C4-F2
6	B	805	YLZ	C2-C1-C4-F2
6	A	807	YLZ	N2-C1-C4-F2

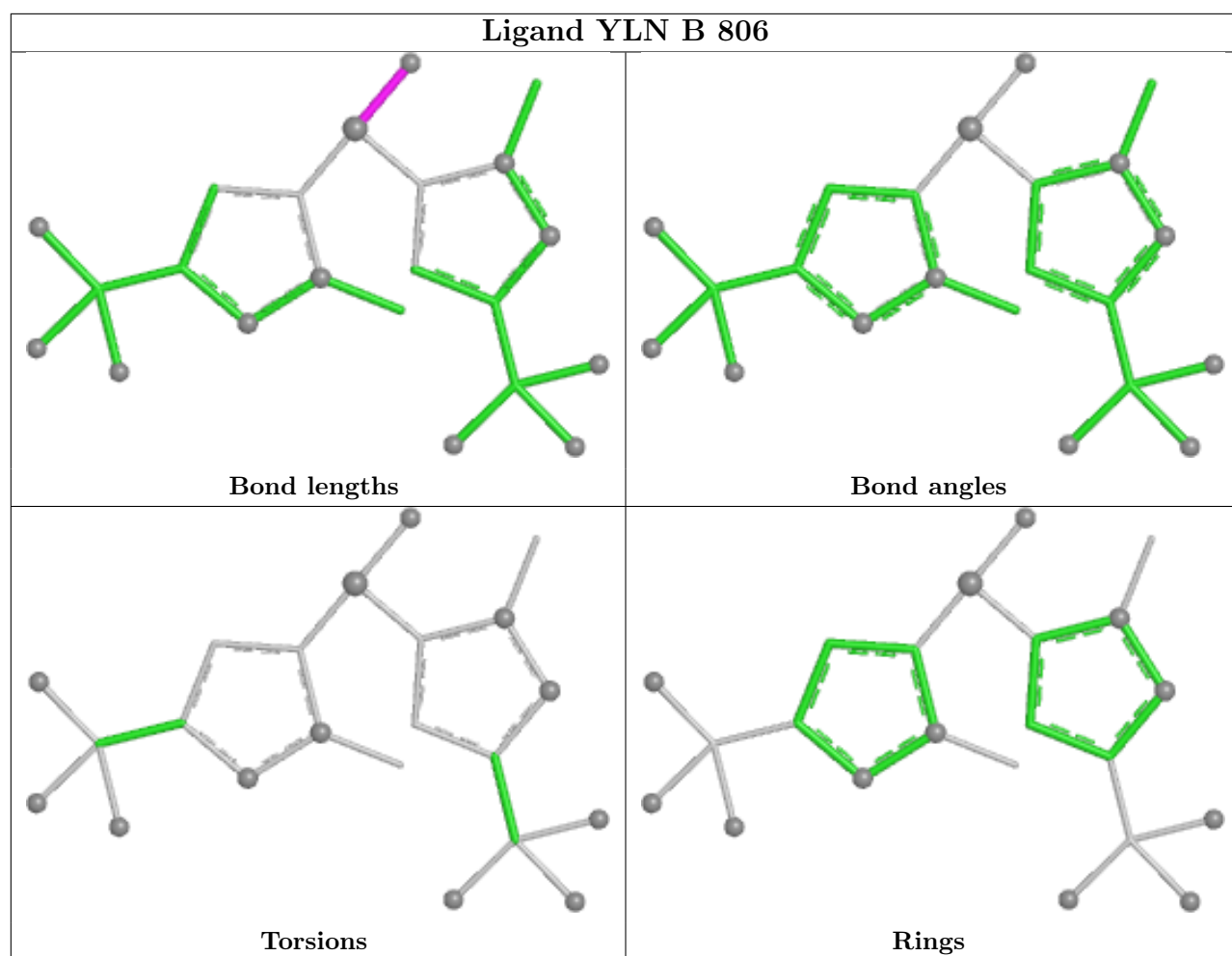
There are no ring outliers.

2 monomers are involved in 2 short contacts:

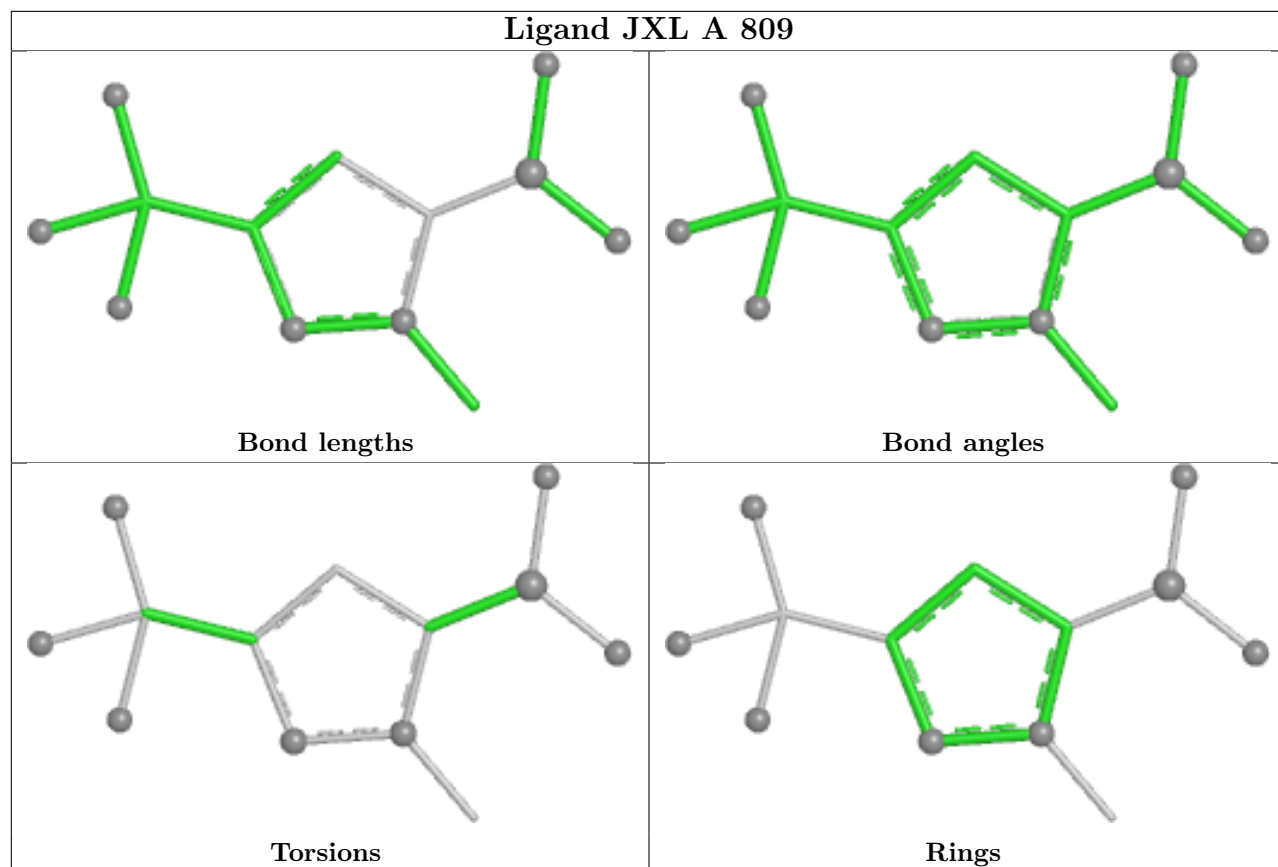
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	806	YLN	1	0
3	B	807	SO4	1	0

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.

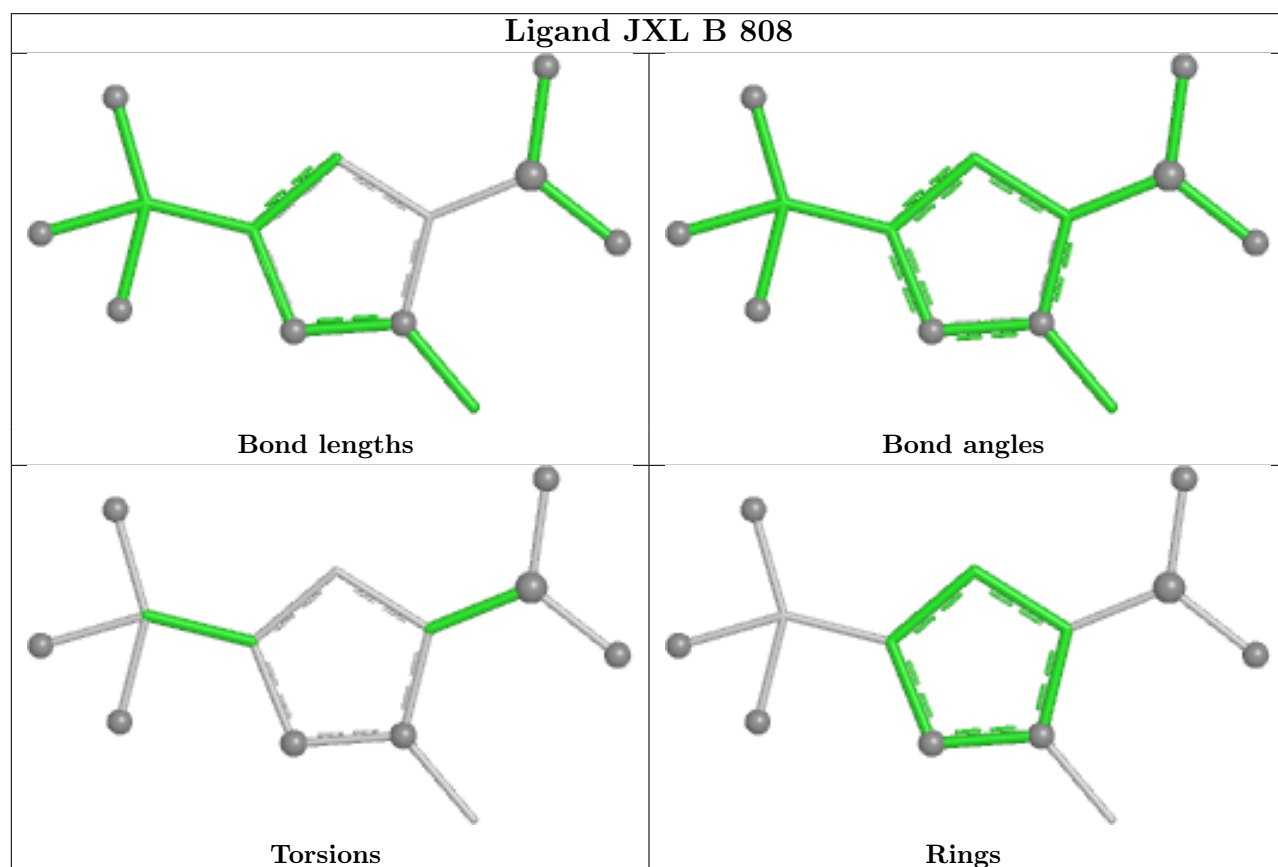




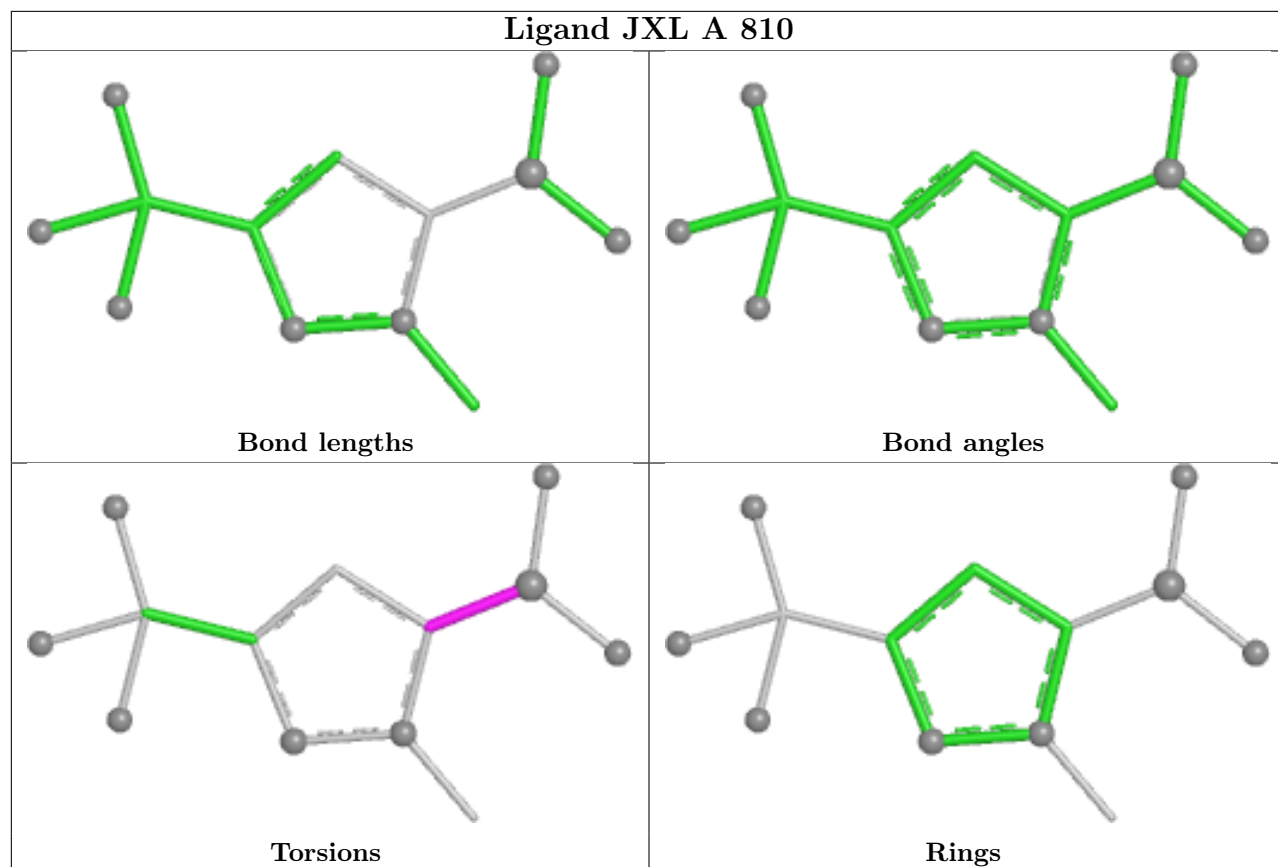
Ligand JXL A 809



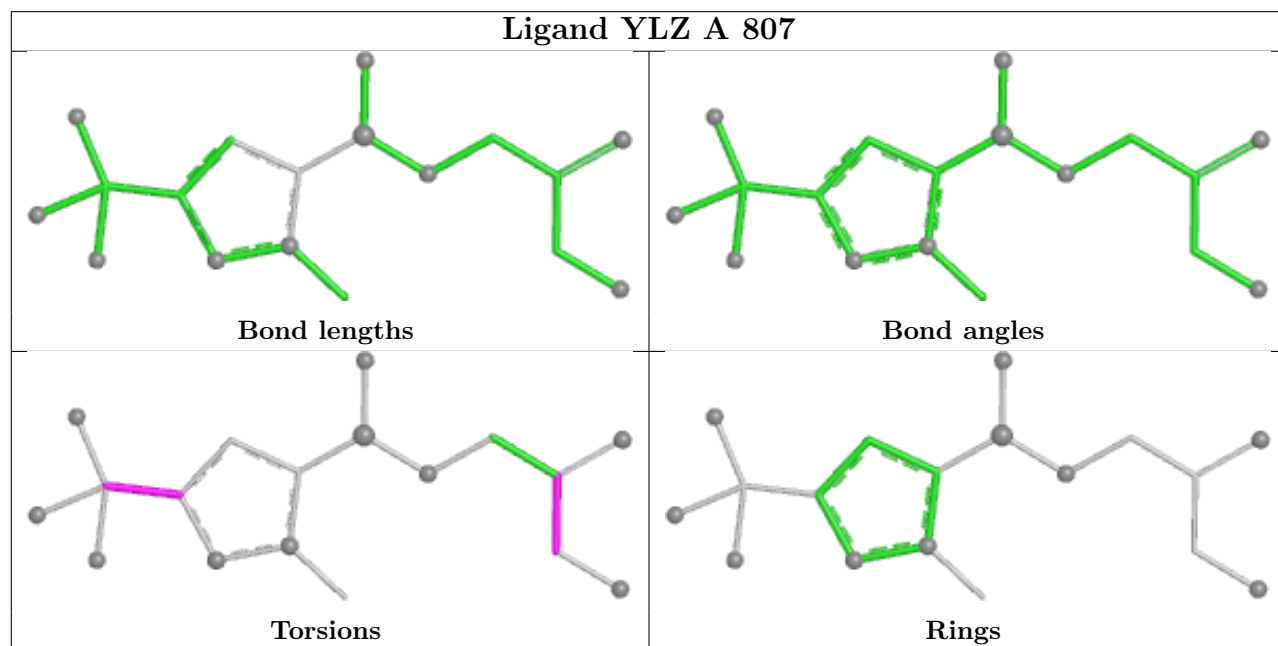
Ligand JXL B 808



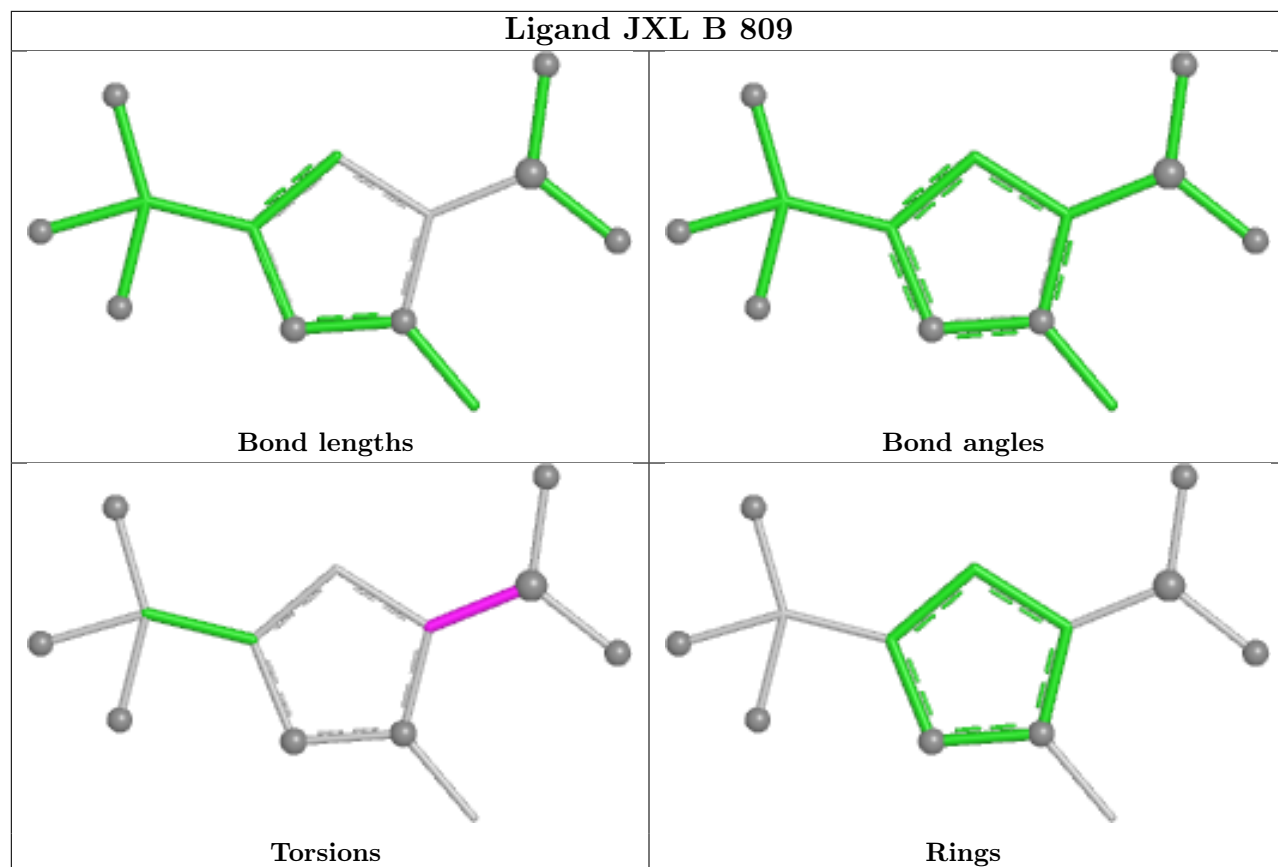
Ligand JXL A 810



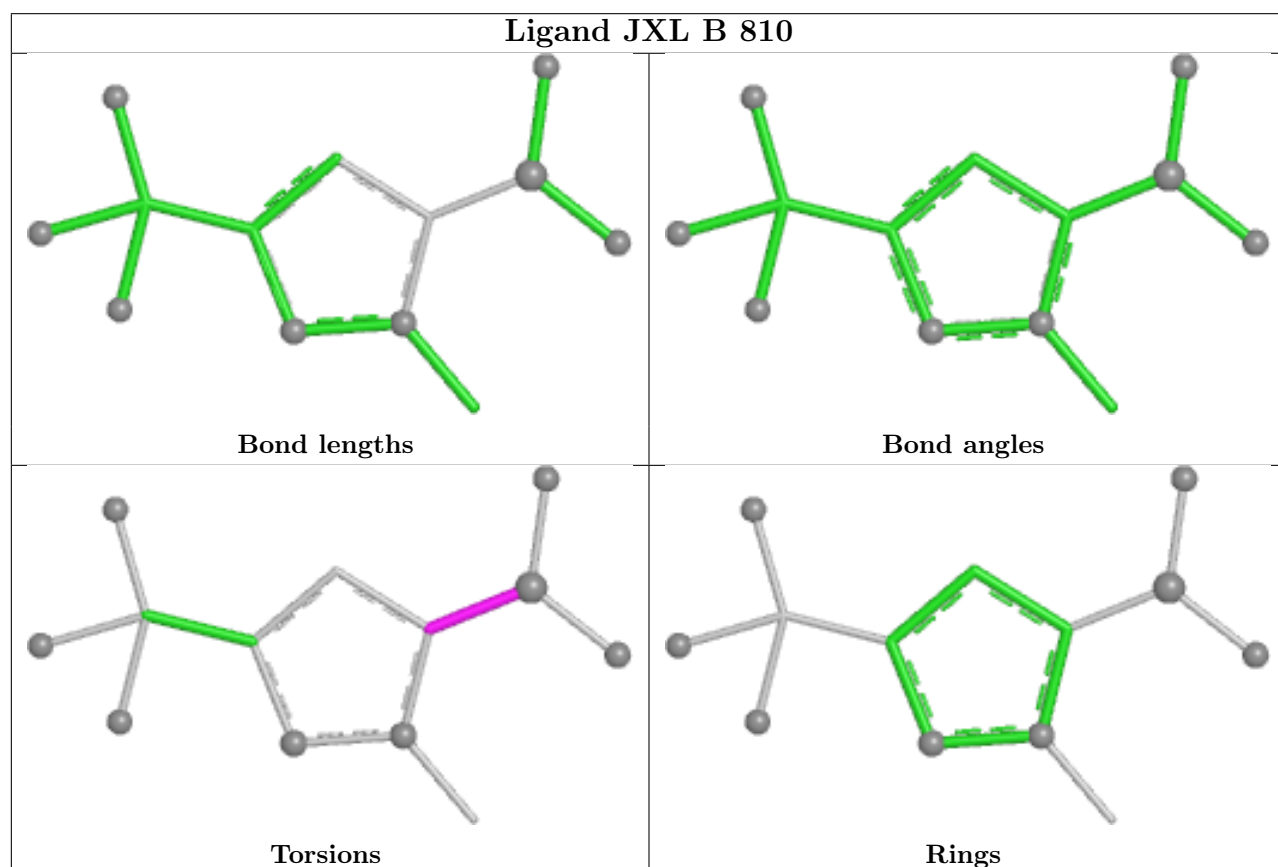
Ligand YLZ A 807

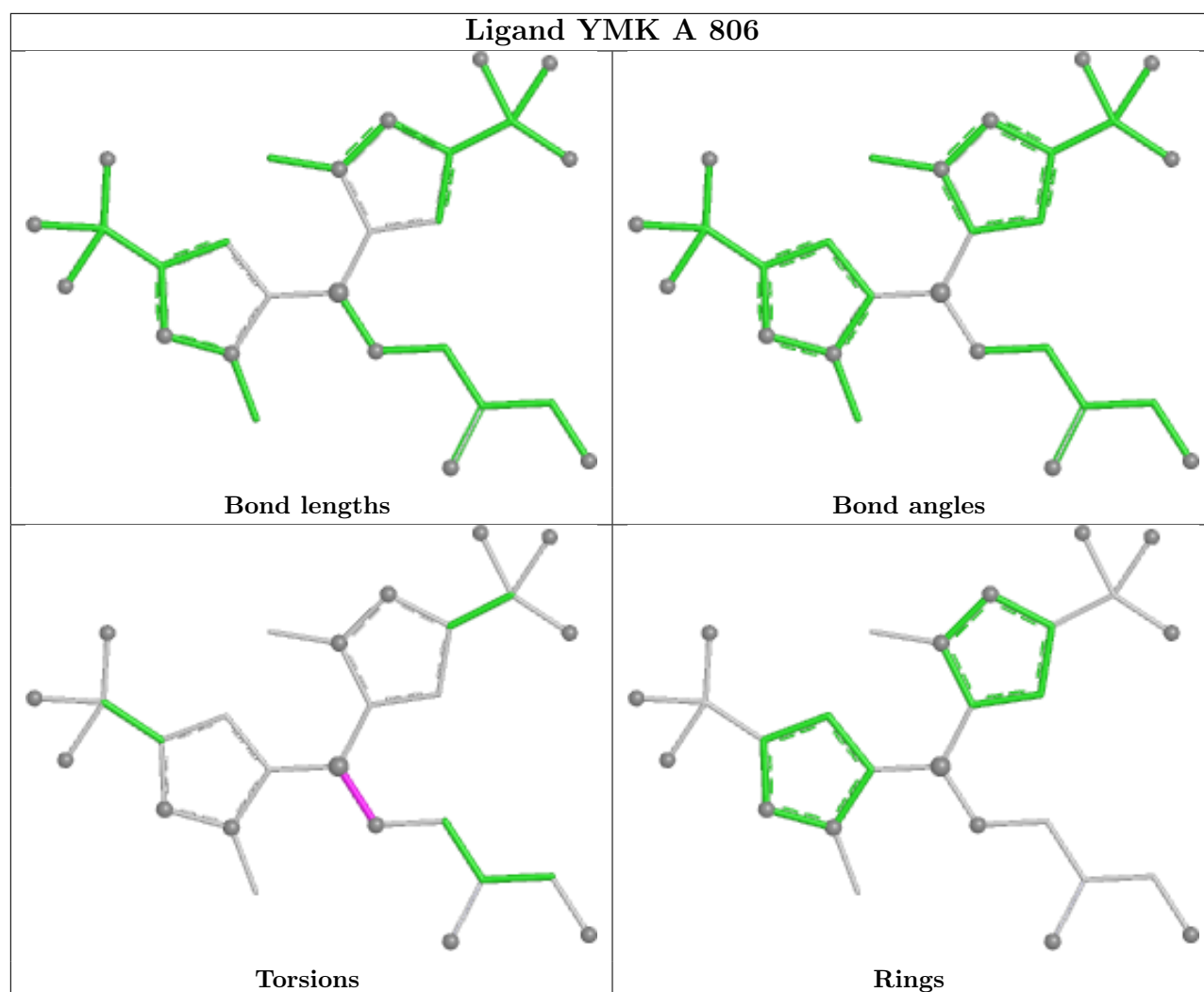


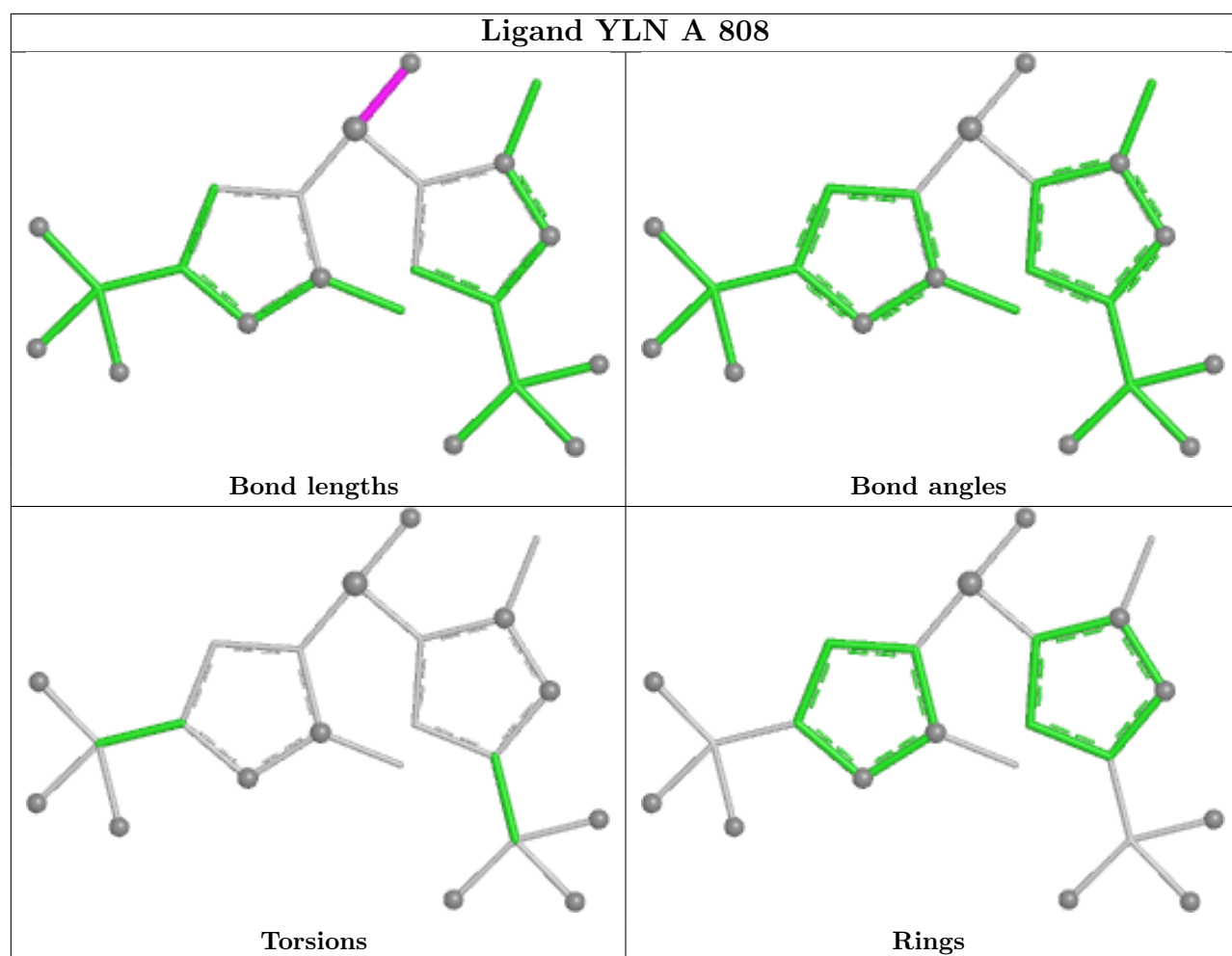
Ligand JXL B 809

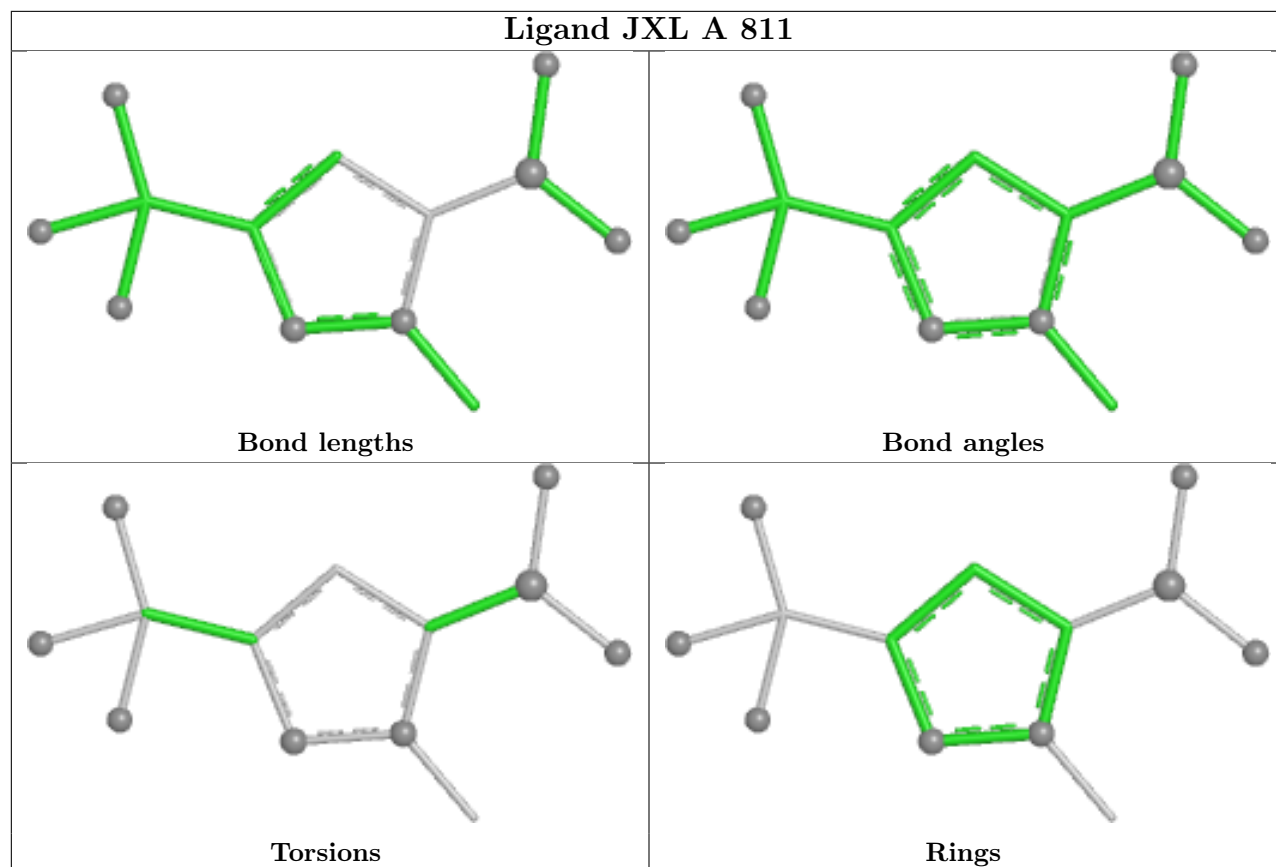


Ligand JXL B 810









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%)	0.52	74 (10%) 12 11	35, 58, 103, 153	0
1	B	732/736 (99%)	0.35	57 (7%) 19 17	34, 52, 92, 145	0
2	C	402/403 (99%)	0.17	30 (7%) 20 18	33, 48, 83, 114	0
2	D	403/403 (100%)	0.23	32 (7%) 18 16	32, 48, 87, 156	0
All	All	2266/2278 (99%)	0.35	193 (8%) 16 15	32, 52, 95, 156	0

All (193) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-14	GLY	9.5
1	A	720	SER	8.1
2	D	296	PRO	7.8
2	D	1	MET	7.7
2	D	390	ILE	6.7
1	A	574	ALA	6.5
2	D	391	GLY	6.3
2	C	301	THR	6.3
1	B	577	THR	6.2
2	D	302	GLY	6.1
2	C	231	LEU	5.9
1	B	720	SER	5.9
2	D	301	THR	5.9
2	C	390	ILE	5.5
1	A	559	LEU	5.4
2	C	389	CYS	5.2
1	B	413	PHE	4.9
2	D	303	PRO	4.9
2	C	300	LEU	4.9
2	C	302	GLY	4.9
2	D	297	VAL	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	575	GLY	4.8
1	A	1	MET	4.8
2	D	231	LEU	4.7
2	D	299	MET	4.7
1	A	-5	SER	4.5
2	D	389	CYS	4.3
1	A	376	LEU	4.3
2	C	303	PRO	4.3
1	A	-13	SER	4.3
1	B	611	LYS	4.3
1	B	-13	SER	4.2
2	D	2	SER	4.1
2	C	135	GLY	4.0
1	B	578	TYR	4.0
1	B	621	GLU	4.0
1	A	413	PHE	4.0
1	A	611	LYS	3.9
2	D	146	PHE	3.9
2	D	225	PHE	3.9
1	A	133	LYS	3.9
1	A	418	LEU	3.9
2	C	299	MET	3.8
2	C	391	GLY	3.8
2	C	2	SER	3.8
2	C	225	PHE	3.8
1	A	224	LYS	3.7
1	B	-5	SER	3.7
2	D	298	ILE	3.7
1	A	-7	HIS	3.7
1	B	-7	HIS	3.7
1	B	599	LEU	3.7
1	B	-4	GLN	3.6
2	C	134	MET	3.6
2	C	294	ALA	3.6
1	A	-8	HIS	3.6
1	B	1	MET	3.6
2	D	293	GLY	3.6
1	B	565	VAL	3.6
2	C	297	VAL	3.6
2	D	392	GLY	3.5
1	A	335	MET	3.5
1	B	600	LYS	3.5

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Mol	Chain	Res	Type	RSRZ
2	C	298	ILE	3.5
1	B	559	LEU	3.5
1	A	400	ALA	3.4
1	B	573	ASP	3.4
1	B	609	ASP	3.4
1	A	3	ASP	3.3
1	A	573	ASP	3.3
1	B	-3	ASP	3.3
2	D	300	LEU	3.3
1	A	2	PRO	3.3
1	A	319	GLY	3.2
1	A	610	GLY	3.2
1	B	3	ASP	3.2
1	A	180	LYS	3.2
1	A	577	THR	3.2
1	B	570	GLY	3.2
1	A	71	LYS	3.2
1	A	412	VAL	3.2
1	B	571	VAL	3.1
1	B	579	GLN	3.1
1	B	567	THR	3.1
2	D	294	ALA	3.1
1	B	385	ARG	3.1
2	C	295	ASP	3.0
1	A	569	LYS	3.0
2	D	393	GLY	3.0
1	B	-6	HIS	3.0
1	B	690	ALA	3.0
1	A	-6	HIS	3.0
2	C	293	GLY	3.0
1	A	579	GLN	2.9
1	B	575	GLY	2.9
1	B	576	GLY	2.9
1	A	388	ALA	2.9
1	A	385	ARG	2.9
2	D	295	ASP	2.9
1	A	580	PRO	2.9
1	B	689	PRO	2.9
1	B	562	LYS	2.9
1	B	564	ALA	2.9
1	A	618	GLY	2.8
1	A	317	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	296	PRO	2.8
1	A	578	TYR	2.8
1	B	574	ALA	2.8
2	C	133	ALA	2.8
2	D	228	LEU	2.8
2	D	224	ALA	2.8
1	B	412	VAL	2.8
1	A	380	ARG	2.8
1	B	563	ILE	2.8
2	D	135	GLY	2.8
1	A	621	GLU	2.8
1	A	433	ASN	2.7
2	C	392	GLY	2.7
2	D	215	LYS	2.7
1	A	382	THR	2.7
1	B	4	ASN	2.7
2	D	304	THR	2.7
1	B	610	GLY	2.7
2	D	394	MET	2.7
2	C	304	THR	2.6
1	A	414	GLU	2.6
1	A	370	LYS	2.6
1	A	600	LYS	2.6
1	B	224	LYS	2.6
1	B	378	ARG	2.6
1	B	374	LYS	2.6
2	C	393	GLY	2.6
1	B	569	LYS	2.6
2	C	230	ALA	2.5
2	D	134	MET	2.5
1	A	356	VAL	2.5
1	A	358	LEU	2.5
1	A	564	ALA	2.5
2	C	276	LYS	2.5
1	B	-8	HIS	2.5
1	A	565	VAL	2.5
2	D	50	LEU	2.5
1	A	375	ALA	2.5
1	A	403	LYS	2.5
1	A	608	ALA	2.5
1	A	570	GLY	2.5
2	C	227	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	318	GLU	2.5
1	A	342	TYR	2.5
1	B	376	LEU	2.5
1	A	609	ASP	2.5
1	A	395	PRO	2.5
2	C	226	GLU	2.4
1	B	304	PHE	2.4
1	B	71	LYS	2.4
1	B	30	MET	2.4
1	A	576	GLY	2.4
1	B	602	ALA	2.4
1	A	4	ASN	2.4
2	D	276	LYS	2.4
1	B	68	GLY	2.3
2	D	230	ALA	2.3
1	A	381	THR	2.3
1	A	571	VAL	2.3
2	C	312	ASP	2.3
1	A	432	PRO	2.3
1	A	562	LYS	2.3
1	A	599	LEU	2.2
1	A	507	ARG	2.2
2	D	147	VAL	2.2
1	A	561	HIS	2.2
1	A	363	LYS	2.2
1	A	485	ALA	2.2
1	A	566	ALA	2.2
1	A	367	TYR	2.2
2	C	146	PHE	2.2
1	B	2	PRO	2.2
1	B	206	LYS	2.2
1	A	320	ILE	2.2
1	B	335	MET	2.2
1	A	379	GLY	2.1
1	B	382	THR	2.1
1	B	566	ALA	2.1
1	A	325	ILE	2.1
1	A	426	ILE	2.1
1	A	343	VAL	2.1
1	B	613	SER	2.0
1	B	384	GLU	2.0
1	A	402	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	180	LYS	2.0
1	A	394	THR	2.0
2	C	136	LEU	2.0
1	B	507	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	802	5/5	0.48	0.23	76,76,82,85	5
8	JXL	A	809	13/13	0.74	0.23	79,91,110,113	0
3	SO4	C	505	5/5	0.77	0.09	98,102,112,122	0
3	SO4	C	501	5/5	0.78	0.15	102,112,126,155	0
3	SO4	D	505	5/5	0.79	0.24	68,72,91,98	5
3	SO4	C	504	5/5	0.80	0.12	88,94,106,134	0
8	JXL	B	809	13/13	0.80	0.18	69,84,98,98	0
3	SO4	B	803	5/5	0.81	0.10	108,130,147,166	0
8	JXL	A	810	13/13	0.82	0.17	68,78,93,94	0
8	JXL	B	808	13/13	0.82	0.23	81,98,107,109	0
3	SO4	A	801	5/5	0.82	0.12	70,80,101,112	0
3	SO4	D	507	5/5	0.83	0.12	69,75,98,103	0
3	SO4	B	807	5/5	0.85	0.11	89,91,95,99	0
3	SO4	D	506	5/5	0.85	0.13	103,107,125,129	1
3	SO4	A	802	5/5	0.85	0.11	93,95,108,128	0
5	YMK	A	806	27/27	0.85	0.18	66,84,105,107	0
3	SO4	B	801	5/5	0.86	0.13	67,69,93,98	0
3	SO4	A	804	5/5	0.87	0.14	57,61,66,66	5
4	GOL	A	805	6/6	0.88	0.20	66,75,82,90	0

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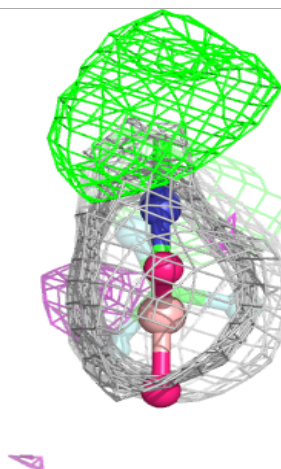
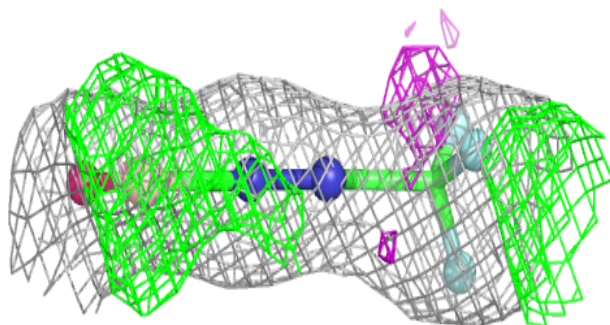
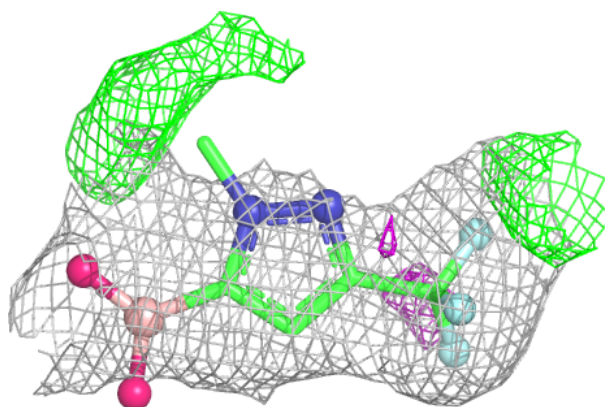
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	B	804	5/5	0.88	0.15	51,51,59,60	5
3	SO4	D	503	5/5	0.89	0.10	84,84,97,123	0
3	SO4	C	502	5/5	0.89	0.10	71,92,98,98	0
3	SO4	C	503	5/5	0.90	0.10	74,87,96,99	0
3	SO4	C	507	5/5	0.90	0.09	68,80,92,95	0
6	YLZ	A	807	18/18	0.90	0.14	63,70,80,88	0
6	YLZ	B	805	18/18	0.90	0.15	62,73,83,86	0
8	JXL	B	810	13/13	0.91	0.13	63,68,78,82	0
3	SO4	D	501	5/5	0.92	0.07	91,93,97,97	0
8	JXL	A	811	13/13	0.92	0.12	58,63,68,72	0
3	SO4	D	502	5/5	0.92	0.08	67,72,93,96	0
3	SO4	C	506	5/5	0.92	0.09	85,95,97,107	0
3	SO4	D	504	5/5	0.92	0.08	78,88,100,102	0
7	YLN	A	808	22/23	0.93	0.10	50,56,61,66	0
7	YLN	B	806	22/23	0.93	0.10	53,58,68,68	0
3	SO4	A	803	5/5	0.94	0.07	82,88,93,95	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.

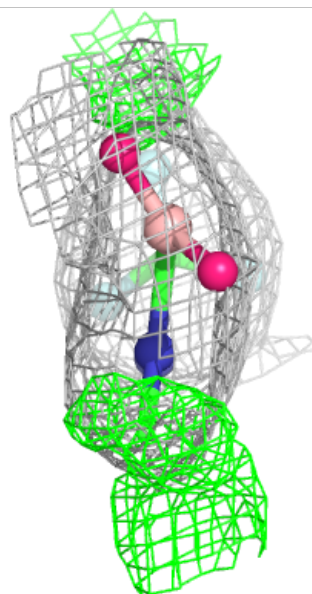
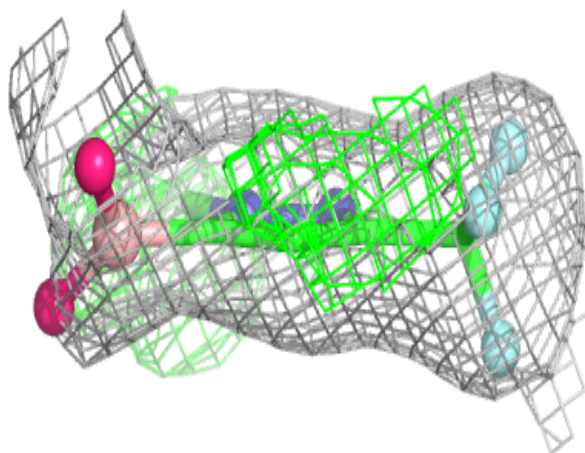
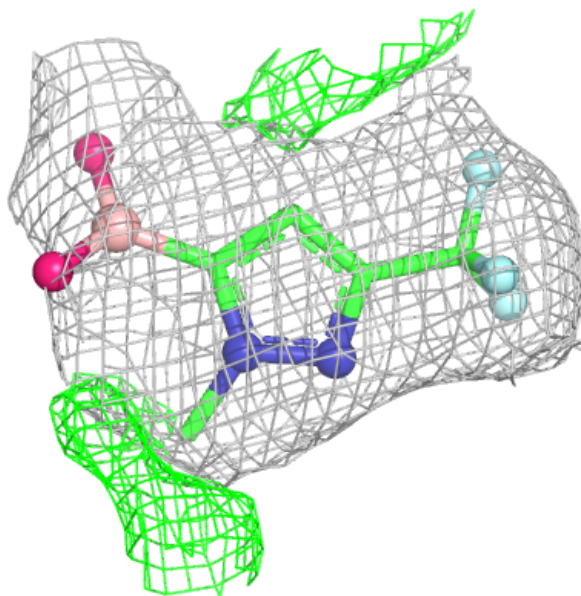
Electron density around JXL A 809:

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



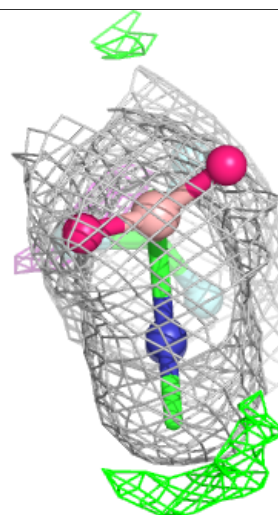
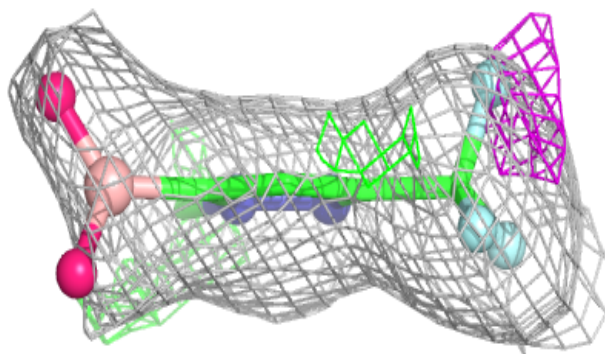
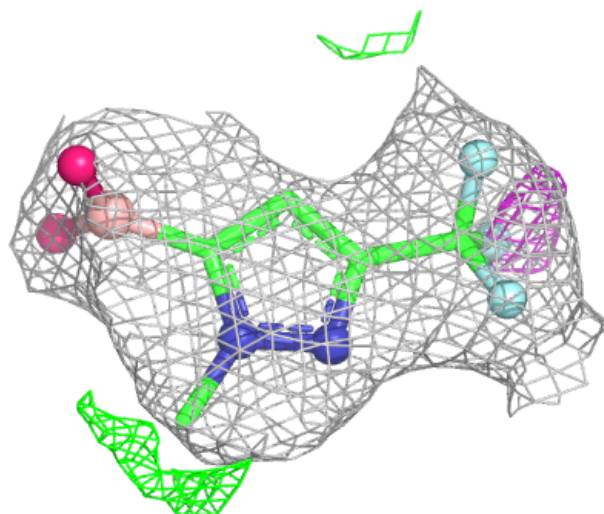
Electron density around JXL B 809:

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



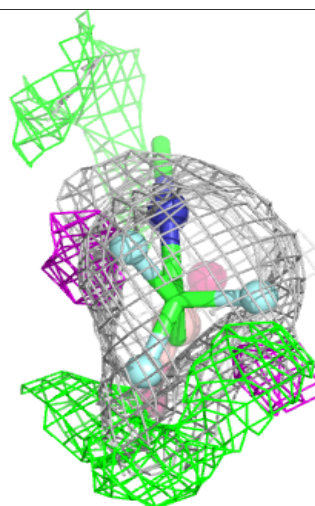
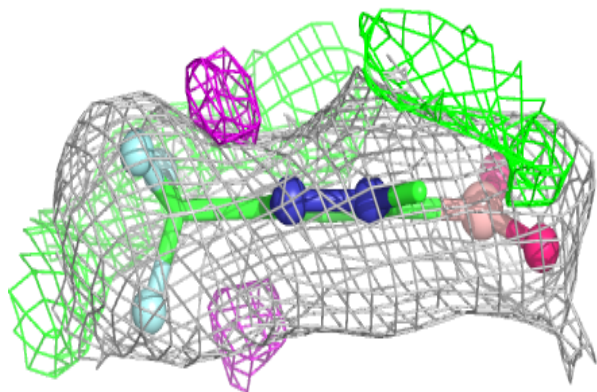
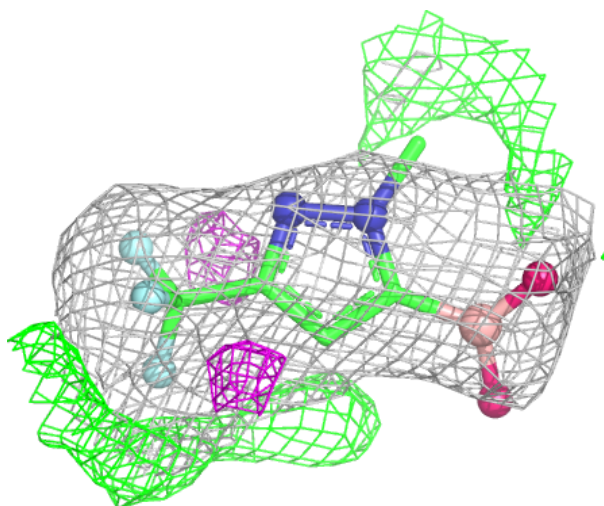
Electron density around JXL A 810:

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



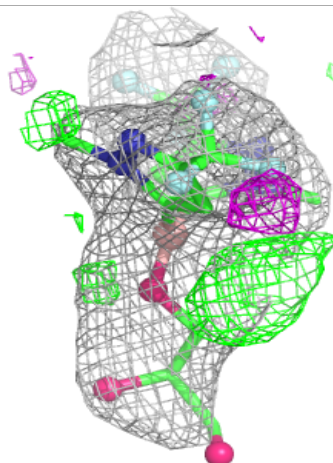
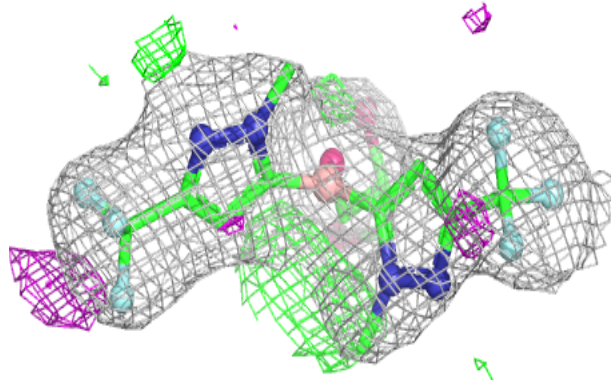
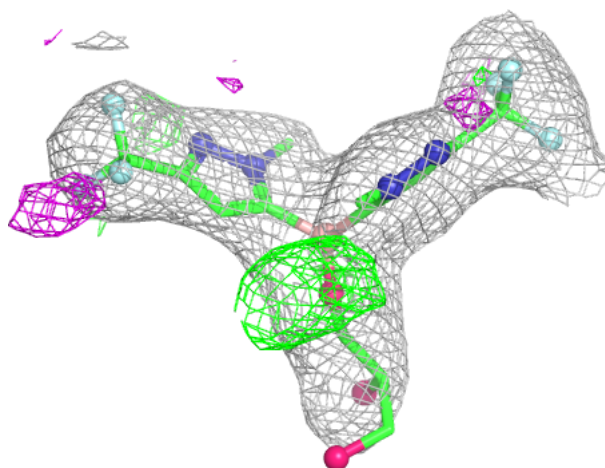
Electron density around JXL B 808:

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



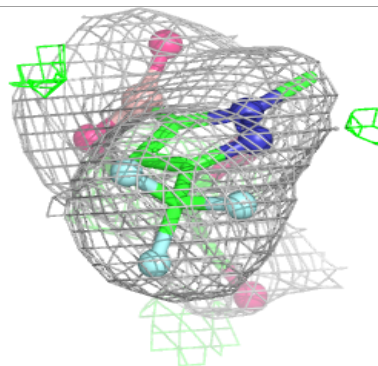
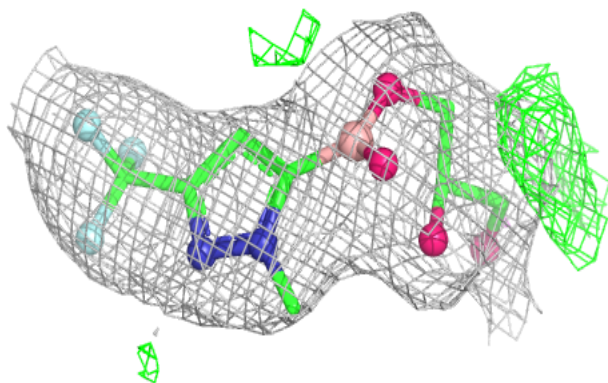
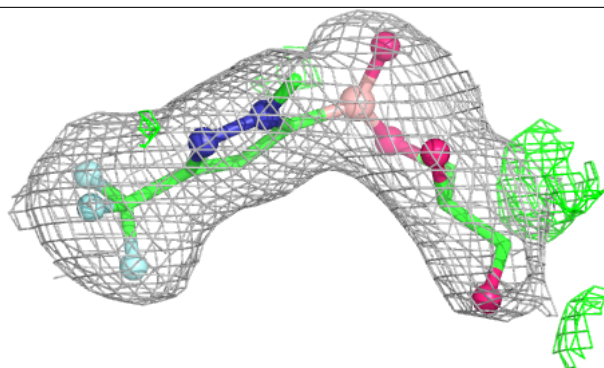
Electron density around YMK A 806:

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

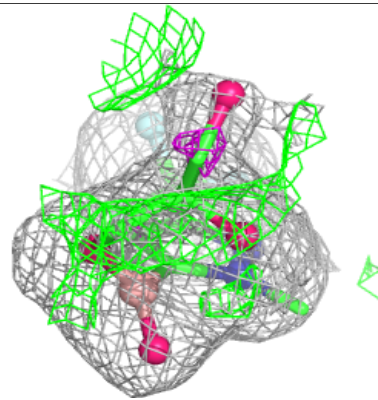
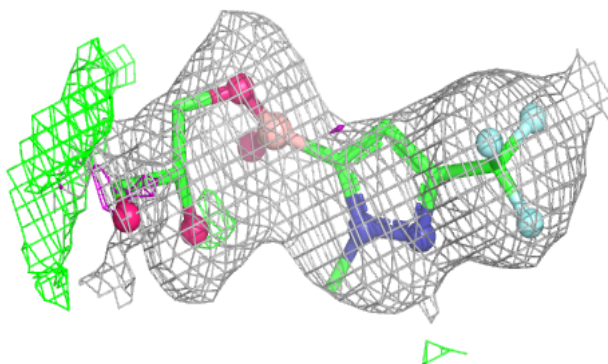
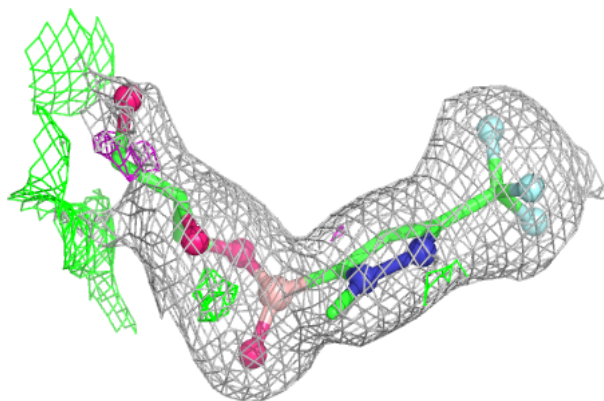


Electron density around YLZ A 807:

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

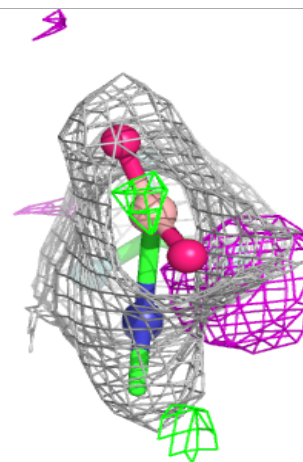
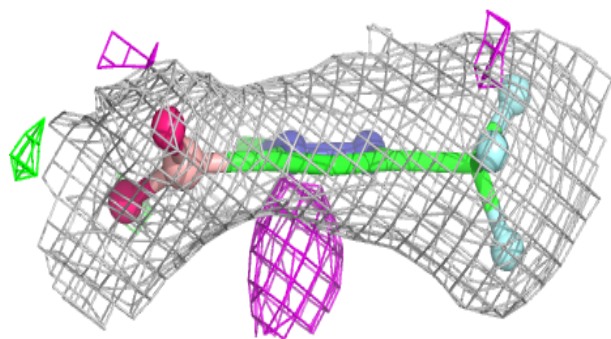
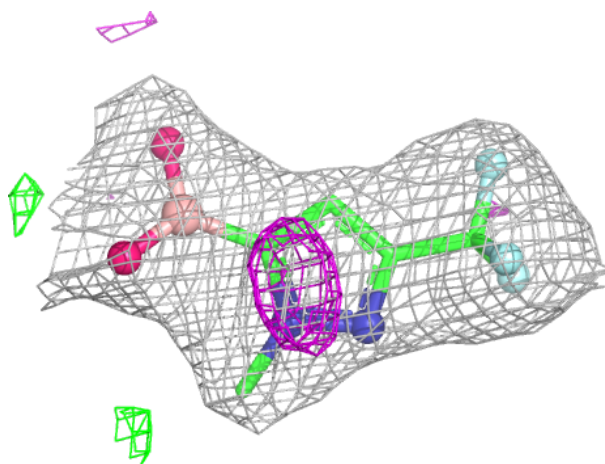
**Electron density around YLZ B 805:**

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



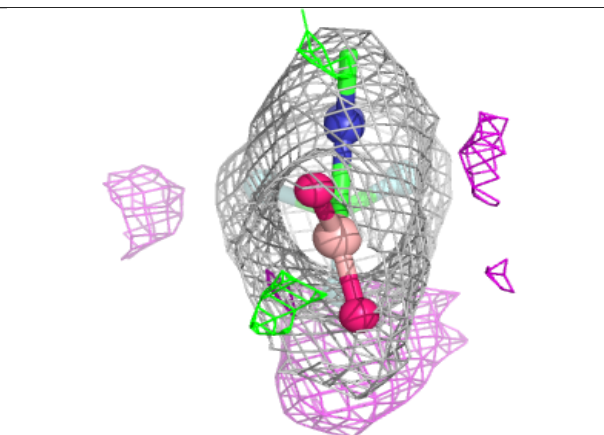
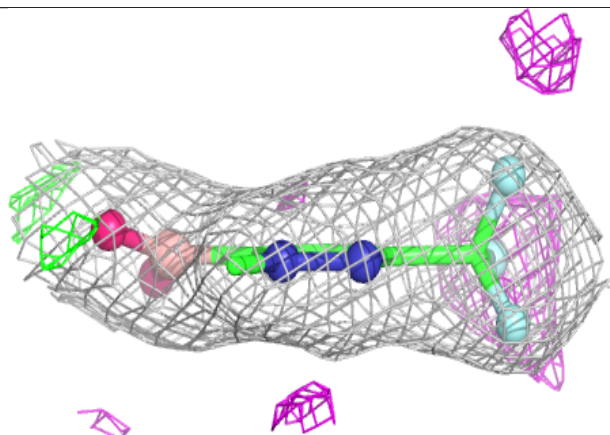
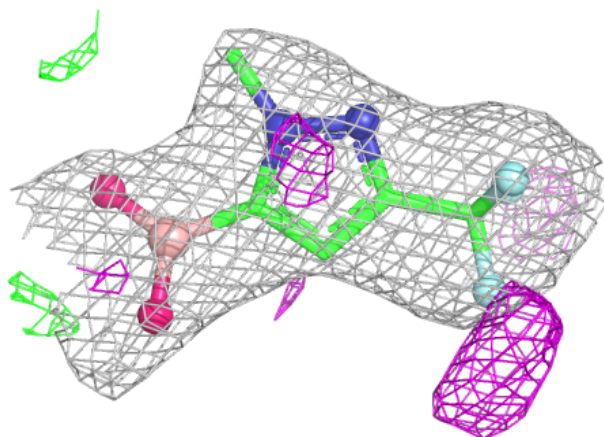
Electron density around JXL B 810:

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

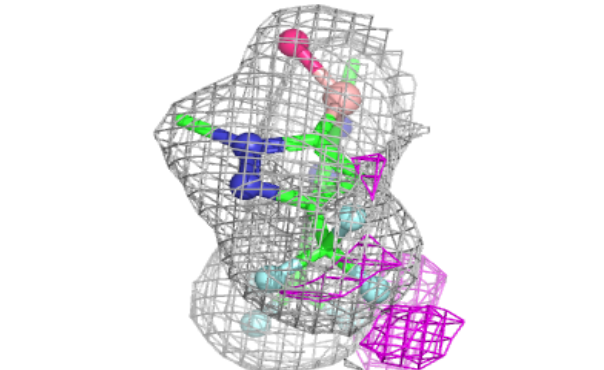
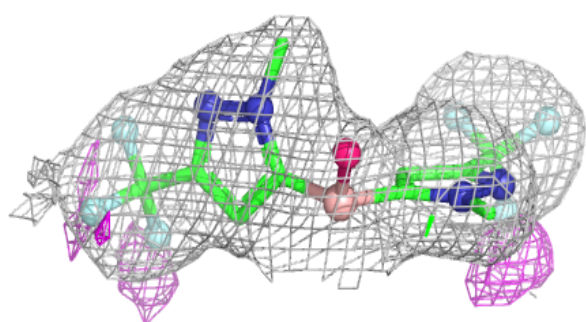
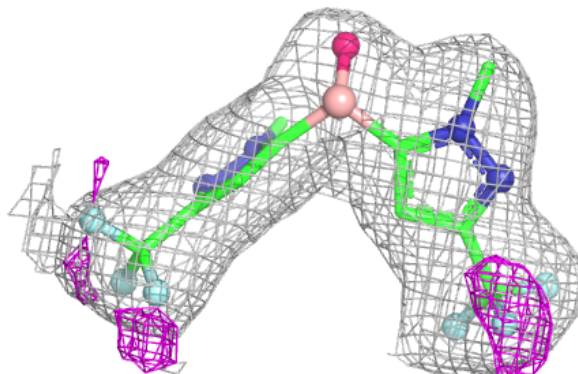


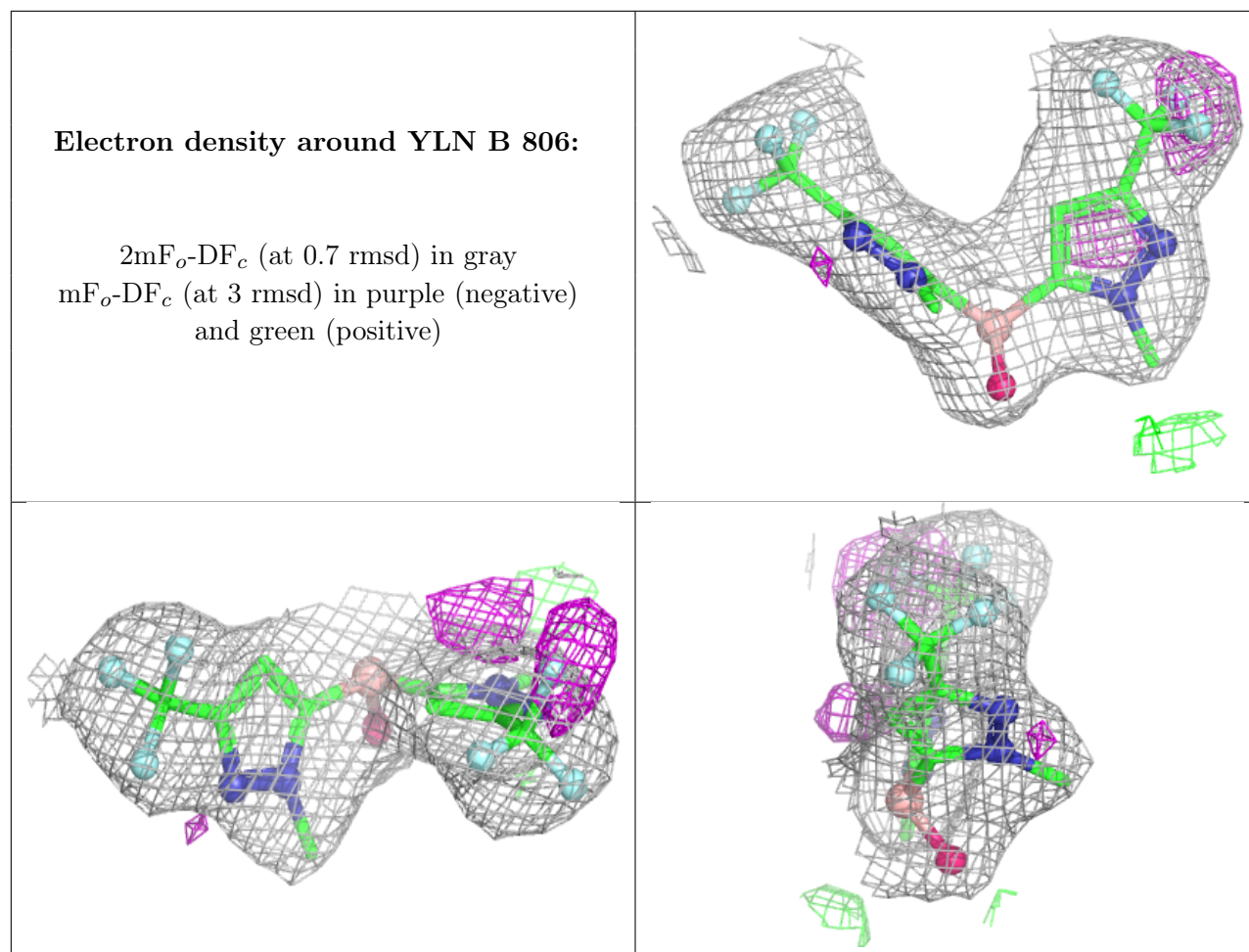
Electron density around JXL A 811:

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

**Electron density around YLN 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 ⓘ

There are no such residues in this entry.