



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:16 AM UTC

PDB ID : 8K9S / pdb_00008k9s
Title : Crystal structure of plasmodium LysRS complexing with ASP3026 derived LysRS inhibitor 1 (ADKI1)
Authors : Zhou, J.; Xia, M.; Yang, G.; Li, P.; Fang, P.
Deposited on : 2023-08-01
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

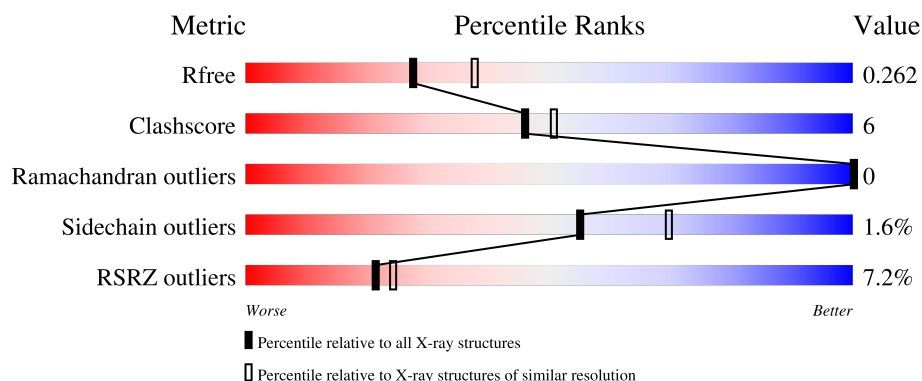
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	516	5% 83% 12% 5%
1	B	516	9% 76% 16% 7%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8115 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 Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	0	0
			3883	2504	647	715	17			
1	B	479	Total	C	N	O	S	0	0	0
			3831	2471	633	710	17			

There are 18 discrepancies between the modelled and reference sequences:

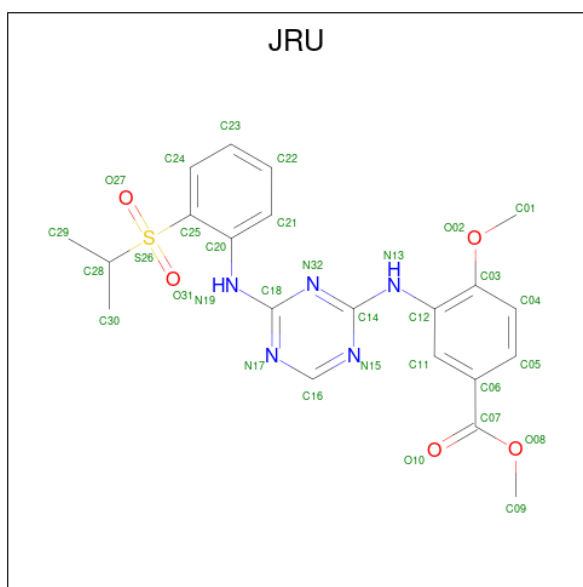
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP A0A024X378
A	584	GLY	-	expression tag	UNP A0A024X378
A	585	GLY	-	expression tag	UNP A0A024X378
A	586	HIS	-	expression tag	UNP A0A024X378
A	587	HIS	-	expression tag	UNP A0A024X378
A	588	HIS	-	expression tag	UNP A0A024X378
A	589	HIS	-	expression tag	UNP A0A024X378
A	590	HIS	-	expression tag	UNP A0A024X378
A	591	HIS	-	expression tag	UNP A0A024X378
B	76	MET	-	initiating methionine	UNP A0A024X378
B	584	GLY	-	expression tag	UNP A0A024X378
B	585	GLY	-	expression tag	UNP A0A024X378
B	586	HIS	-	expression tag	UNP A0A024X378
B	587	HIS	-	expression tag	UNP A0A024X378
B	588	HIS	-	expression tag	UNP A0A024X378
B	589	HIS	-	expression tag	UNP A0A024X378
B	590	HIS	-	expression tag	UNP A0A024X378
B	591	HIS	-	expression tag	UNP A0A024X378

- Molecule 2 is LYSINE (CCD ID: LYS) (formula: C₆H₁₅N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	6	2	2		
2	B	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 3 is methyl 4-methoxy-3-[[4-[(2-propan-2-ylsulfonyl)phenyl]amino]-1,3,5-triazin-2-yl]amino]benzoate (CCD ID: JRU) (formula: $C_{21}H_{23}N_5O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			32	21	5	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			32	21	5	5	1		

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

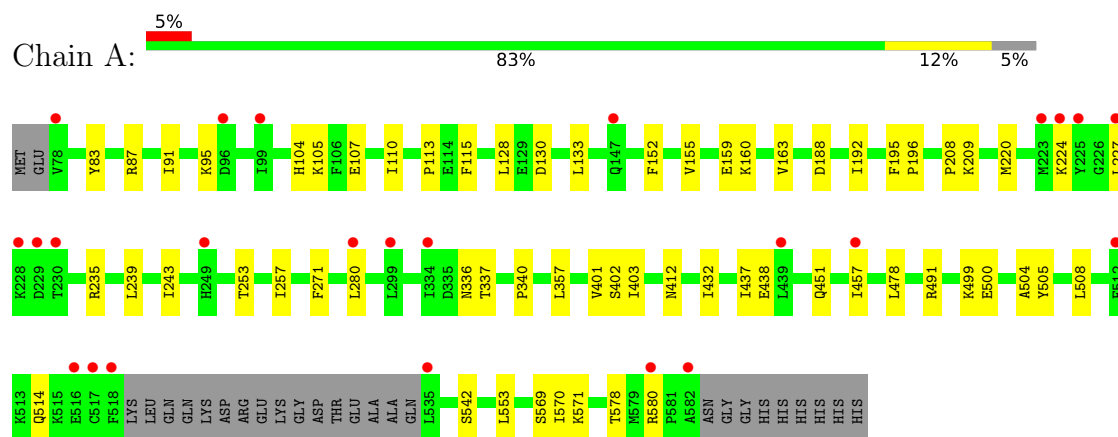
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	174	Total	O	0	0
			174	174		
5	B	131	Total	O	0	0
			131	131		

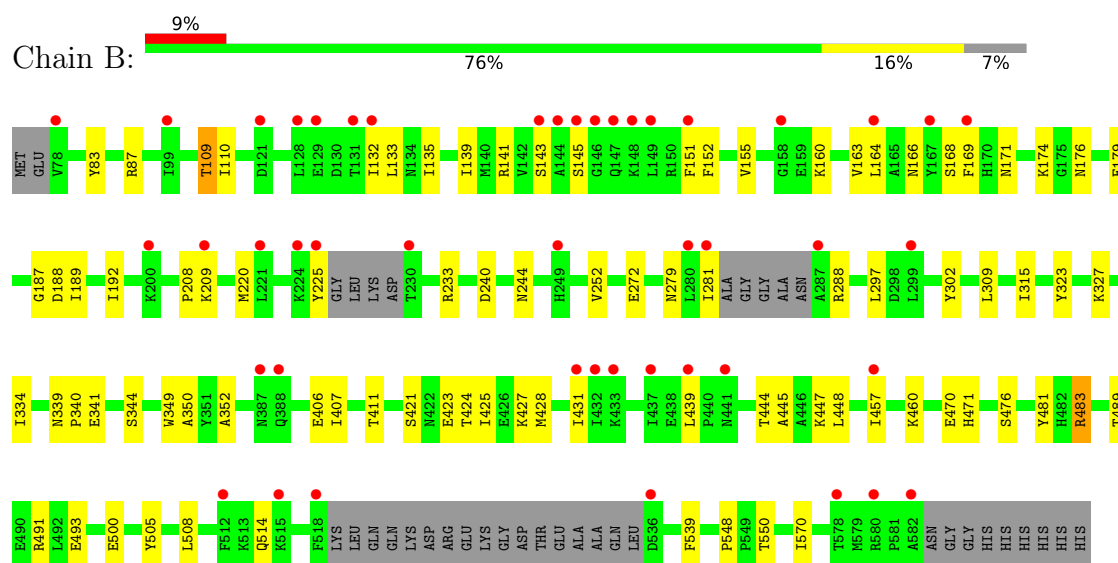
3 Residue-property plots [i](#)

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: Lysine-tRNA ligase



• Molecule 1: Lysine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.46Å 95.89Å 167.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.25 – 2.35 48.25 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.3 (48.25-2.35) 99.2 (48.25-2.35)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.76 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.219 , 0.263 0.218 , 0.262	Depositor DCC
R_{free} test set	2417 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	46.2	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8115	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JRU, MES

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	0/3980	0.32	0/5395
1	B	0.12	0/3926	0.34	0/5319
All	All	0.12	0/7906	0.33	0/10714

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

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	3883	0	3754	38	0
1	B	3831	0	3698	55	0
2	A	10	0	12	0	0
2	B	10	0	12	0	0
3	A	32	0	0	1	0
3	B	32	0	0	1	0
4	B	12	0	12	1	0
5	A	174	0	0	3	0
5	B	131	0	0	1	0
All	All	8115	0	7488	89	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 6.

All (89) 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:483:ARG:HH11	1:B:483:ARG:HG3	1.46	0.80
1:B:350:ALA:HA	1:B:550:THR:HG22	1.66	0.76
1:A:478:LEU:HD23	1:A:514:GLN:HE22	1.54	0.72
1:B:87:ARG:NH2	1:B:188:ASP:OD1	2.23	0.71
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.73	0.70
1:B:315:ILE:HG21	1:B:550:THR:HG21	1.75	0.67
1:B:110:ILE:HG21	1:B:133:LEU:HD13	1.75	0.67
1:B:279:ASN:HB2	1:B:281:ILE:HG12	1.78	0.65
1:A:87:ARG:NH2	1:A:188:ASP:OD1	2.29	0.65
1:A:580:ARG:HD3	1:B:297:LEU:HD22	1.80	0.64
1:B:166:ASN:HB3	1:B:169:PHE:CD1	2.34	0.62
1:A:155:VAL:HG12	1:A:160:LYS:HG3	1.81	0.62
1:A:107:GLU:HA	4:B:603:MES:H62	1.82	0.61
1:B:166:ASN:HB3	1:B:169:PHE:HD1	1.65	0.61
1:B:421:SER:O	1:B:425:ILE:HG13	2.02	0.60
1:B:423:GLU:OE1	1:B:423:GLU:N	2.30	0.59
1:B:508:LEU:HD22	1:B:514:GLN:HG2	1.84	0.59
1:B:240:ASP:OD1	1:B:244:ASN:ND2	2.36	0.58
1:B:281:ILE:HG13	1:B:302:TYR:HB2	1.85	0.58
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.86	0.58
1:B:427:LYS:O	1:B:431:ILE:HD12	2.03	0.58
1:B:483:ARG:HH11	1:B:483:ARG:CG	2.17	0.57
1:B:309:LEU:HD13	1:B:539:PHE:HB2	1.87	0.57
1:B:500:GLU:HG2	3:B:602:JRU:O31	2.04	0.57
1:B:135:ILE:HG22	1:B:192:ILE:HB	1.87	0.56
1:A:491:ARG:HA	1:A:505:TYR:HB3	1.87	0.56
1:A:500:GLU:HG2	3:A:602:JRU:O31	2.06	0.55
1:B:132:ILE:O	1:B:132:ILE:HD12	2.07	0.55
1:A:253:THR:O	1:A:257:ILE:HG12	2.07	0.55
1:A:104:HIS:HE1	1:B:481:TYR:O	1.90	0.55
1:A:337:THR:HG21	1:A:499:LYS:HE2	1.90	0.54
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.89	0.54
1:A:508:LEU:HD22	1:A:514:GLN:HG2	1.90	0.54
1:A:227:LEU:HD11	1:A:239:LEU:HB3	1.89	0.53
1:A:412:ASN:ND2	5:A:704:HOH:O	2.37	0.53
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.45	0.52
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.93	0.51
1:A:357:LEU:HD13	1:A:504:ALA:HB1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:VAL:HB	1:A:457:ILE:HD11	1.93	0.51
1:A:110:ILE:HG21	1:A:133:LEU:HD13	1.93	0.50
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.93	0.50
1:A:271:PHE:HZ	1:B:252:VAL:HA	1.76	0.50
1:A:438:GLU:O	1:A:451:GLN:NE2	2.34	0.50
1:B:176:ASN:HB3	1:B:179:GLU:HB3	1.94	0.50
1:A:235:ARG:NH2	1:A:580:ARG:O	2.32	0.49
1:B:132:ILE:O	1:B:133:LEU:HD23	2.13	0.49
1:B:471:HIS:NE2	1:B:493:GLU:OE1	2.46	0.49
1:B:407:ILE:O	1:B:411:THR:HG22	2.11	0.49
1:B:339:ASN:HB2	1:B:570:ILE:HD13	1.94	0.48
1:B:406:GLU:OE2	1:B:460:LYS:NZ	2.32	0.48
1:A:113:PRO:HG3	1:A:159:GLU:HG3	1.96	0.48
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.49	0.47
1:A:280:LEU:HD12	1:A:280:LEU:H	1.80	0.47
1:A:570:ILE:HG22	1:A:571:LYS:HE2	1.96	0.47
1:A:105:LYS:HE2	1:A:107:GLU:HG2	1.98	0.46
1:B:424:THR:O	1:B:428:MET:HG3	2.16	0.46
1:B:548:PRO:O	1:B:550:THR:HG23	2.15	0.46
1:B:155:VAL:HG12	1:B:160:LYS:HG3	1.96	0.46
1:B:470:GLU:HA	1:B:489:THR:O	2.16	0.46
1:A:209:LYS:HD2	5:A:778:HOH:O	2.16	0.45
1:A:115:PHE:CE2	1:A:196:PRO:HB3	2.51	0.45
1:A:130:ASP:N	1:A:130:ASP:OD1	2.50	0.45
1:B:139:ILE:O	1:B:187:GLY:N	2.46	0.45
1:A:91:ILE:O	1:A:95:LYS:HG2	2.16	0.45
1:B:233:ARG:HG2	1:B:240:ASP:CG	2.43	0.45
1:B:171:ASN:HB2	1:B:209:LYS:HD2	1.99	0.44
1:A:336:ASN:ND2	5:A:714:HOH:O	2.51	0.44
1:B:143:SER:OG	1:B:151:PHE:HB2	2.17	0.44
1:B:141:ARG:HE	1:B:141:ARG:HB3	1.60	0.43
1:B:349:TRP:CD2	1:B:352:ALA:HB2	2.53	0.43
1:A:504:ALA:HB2	1:A:553:LEU:HG	2.00	0.43
1:B:483:ARG:HG3	1:B:483:ARG:NH1	2.21	0.43
1:B:334:ILE:HG12	1:B:340:PRO:HD3	2.00	0.43
1:A:83:TYR:HB2	1:A:220:MET:HE2	2.00	0.43
1:B:444:THR:HG23	1:B:447:LYS:H	1.83	0.43
1:A:432:ILE:HG23	1:A:437:ILE:O	2.19	0.42
1:B:83:TYR:CD2	1:B:220:MET:HG3	2.54	0.42
1:B:109:THR:HG22	1:B:110:ILE:HG22	2.01	0.42
1:B:309:LEU:CD1	1:B:539:PHE:HB2	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327:LYS:HD2	1:B:341:GLU:HG2	2.01	0.42
1:B:145:SER:HB3	1:B:151:PHE:HE2	1.85	0.41
1:B:424:THR:HG22	1:B:428:MET:HE2	2.01	0.41
1:A:340:PRO:HG2	1:A:578:THR:HG21	2.02	0.41
1:B:225:TYR:CB	5:B:812:HOH:O	2.68	0.41
1:B:491:ARG:HA	1:B:505:TYR:HB3	2.03	0.41
1:A:128:LEU:O	1:A:195:PHE:HB2	2.20	0.41
1:A:224:LYS:HA	1:A:243:ILE:HG23	2.02	0.41
1:B:445:ALA:HA	1:B:448:LEU:HD12	2.02	0.40
1:A:569:SER:OG	1:A:571:LYS:HG2	2.21	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	485/516 (94%)	473 (98%)	12 (2%)	0	100	100
1	B	471/516 (91%)	463 (98%)	8 (2%)	0	100	100
All	All	956/1032 (93%)	936 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	413/464 (89%)	410 (99%)	3 (1%)	76	86
1	B	412/464 (89%)	402 (98%)	10 (2%)	43	57
All	All	825/928 (89%)	812 (98%)	13 (2%)	55	70

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	SER
1	A	403	ILE
1	A	542	SER
1	B	109	THR
1	B	164	LEU
1	B	168	SER
1	B	174	LYS
1	B	189	ILE
1	B	288	ARG
1	B	344	SER
1	B	439	LEU
1	B	476	SER
1	B	483	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	104	HIS
1	A	162	GLN
1	A	355	ASN
1	A	459	ASN
1	A	462	ASN
1	A	514	GLN
1	B	162	GLN
1	B	279	ASN
1	B	459	ASN
1	B	462	ASN

5.3.3 RNA ⓘ

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](#)

5 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	$\# Z > 2$
2	LYS	A	601	-	8,9,9	0.84	1 (12%)	7,10,10	0.97	1 (14%)
2	LYS	B	601	-	8,9,9	0.82	1 (12%)	7,10,10	1.03	1 (14%)
3	JRU	B	602	-	34,34,34	6.02	12 (35%)	42,48,48	3.66	13 (30%)
3	JRU	A	602	-	34,34,34	6.03	13 (38%)	42,48,48	4.23	14 (33%)
4	MES	B	603	-	12,12,12	2.18	1 (8%)	15,16,16	2.08	5 (33%)

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
2	LYS	A	601	-	-	1/9/9/9	-
2	LYS	B	601	-	-	3/9/9/9	-
3	JRU	B	602	-	-	10/28/28/28	0/3/3/3
3	JRU	A	602	-	-	11/28/28/28	0/3/3/3
4	MES	B	603	-	-	5/6/14/14	0/1/1/1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	JRU	O27-S26	23.05	1.64	1.44
3	B	602	JRU	O31-S26	23.02	1.64	1.44
3	B	602	JRU	O27-S26	22.99	1.64	1.44
3	A	602	JRU	O31-S26	22.94	1.64	1.44
4	B	603	MES	C8-S	-7.29	1.67	1.77
3	B	602	JRU	O08-C07	-6.72	1.18	1.33
3	A	602	JRU	O08-C07	-6.39	1.19	1.33
3	B	602	JRU	O10-C07	6.12	1.39	1.22
3	A	602	JRU	O10-C07	5.95	1.39	1.22
3	A	602	JRU	C18-N19	5.54	1.48	1.36
3	B	602	JRU	C18-N19	5.22	1.47	1.36
3	A	602	JRU	C14-N13	4.85	1.46	1.36
3	B	602	JRU	C14-N13	4.50	1.45	1.36
3	A	602	JRU	C18-N17	-2.54	1.31	1.34
3	B	602	JRU	C18-N17	-2.41	1.31	1.34
3	A	602	JRU	O08-C09	-2.35	1.40	1.45
3	A	602	JRU	C12-N13	2.26	1.46	1.39
3	A	602	JRU	C20-N19	2.26	1.46	1.39
3	A	602	JRU	C06-C07	2.21	1.54	1.50
2	A	601	LYS	OXT-C	-2.21	1.23	1.30
3	B	602	JRU	C12-N13	2.20	1.45	1.39
3	B	602	JRU	C25-S26	2.20	1.83	1.78
3	B	602	JRU	C20-N19	2.20	1.45	1.39
2	B	601	LYS	OXT-C	-2.19	1.23	1.30
3	A	602	JRU	C14-N15	-2.13	1.31	1.34
3	B	602	JRU	C14-N15	-2.13	1.31	1.34
3	B	602	JRU	O08-C09	-2.12	1.40	1.45
3	A	602	JRU	C25-S26	2.09	1.83	1.78

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	JRU	C16-N17-C18	11.93	120.89	113.27
3	B	602	JRU	C16-N17-C18	11.77	120.79	113.27
3	A	602	JRU	O08-C07-C06	11.29	129.23	112.31
3	A	602	JRU	O31-S26-O27	-10.76	108.99	118.72
3	B	602	JRU	C16-N15-C14	10.35	119.89	113.27
3	A	602	JRU	C16-N15-C14	10.21	119.79	113.27
3	B	602	JRU	O31-S26-O27	-9.27	110.34	118.72
3	A	602	JRU	N17-C18-N32	-7.49	119.18	126.42
3	B	602	JRU	N17-C18-N32	-6.81	119.83	126.42
3	A	602	JRU	N15-C14-N32	-6.64	120.00	126.42
3	A	602	JRU	C09-O08-C07	6.39	128.08	115.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	JRU	N15-C14-N32	-5.98	120.64	126.42
3	B	602	JRU	N17-C16-N15	-5.91	119.63	128.58
3	A	602	JRU	N17-C16-N15	-5.61	120.10	128.58
3	B	602	JRU	O08-C07-C06	5.59	120.69	112.31
4	B	603	MES	C5-N4-C3	5.44	120.57	108.84
3	A	602	JRU	O08-C07-O10	-4.54	114.62	123.46
3	B	602	JRU	O02-C03-C12	3.79	119.53	114.81
3	A	602	JRU	C18-N32-C14	3.45	120.03	113.85
3	B	602	JRU	C25-C20-N19	-3.25	118.50	121.50
3	B	602	JRU	C18-N32-C14	2.99	119.21	113.85
4	B	603	MES	C7-N4-C3	2.97	119.14	111.24
3	A	602	JRU	O02-C03-C12	2.77	118.26	114.81
3	A	602	JRU	C05-C06-C07	2.73	126.41	120.40
3	B	602	JRU	C25-S26-C28	2.66	111.58	105.70
2	B	601	LYS	OXT-C-O	-2.59	118.20	124.08
3	B	602	JRU	C01-O02-C03	-2.54	113.79	117.51
3	B	602	JRU	O02-C03-C04	-2.53	120.04	124.30
3	A	602	JRU	C11-C06-C07	-2.49	115.24	120.09
2	A	601	LYS	OXT-C-O	-2.46	118.51	124.08
4	B	603	MES	C7-N4-C5	2.30	117.36	111.24
3	A	602	JRU	C25-C20-N19	-2.28	119.40	121.50
4	B	603	MES	O2S-S-C8	2.14	109.96	106.73
4	B	603	MES	O1S-S-C8	2.12	109.94	106.73

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	JRU	N17-C18-N19-C20
3	A	602	JRU	N32-C18-N19-C20
3	A	602	JRU	C29-C28-S26-C25
3	A	602	JRU	C29-C28-S26-O27
3	A	602	JRU	C29-C28-S26-O31
3	A	602	JRU	C30-C28-S26-C25
3	A	602	JRU	C30-C28-S26-O27
3	A	602	JRU	C30-C28-S26-O31
3	B	602	JRU	C29-C28-S26-C25
3	B	602	JRU	C29-C28-S26-O27
3	B	602	JRU	C29-C28-S26-O31
3	B	602	JRU	C30-C28-S26-C25
3	B	602	JRU	C30-C28-S26-O27
3	B	602	JRU	C30-C28-S26-O31

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Mol	Chain	Res	Type	Atoms
4	B	603	MES	C8-C7-N4-C3
4	B	603	MES	C7-C8-S-O2S
4	B	603	MES	C7-C8-S-O3S
3	A	602	JRU	O10-C07-O08-C09
3	A	602	JRU	C06-C07-O08-C09
3	B	602	JRU	N32-C18-N19-C20
3	B	602	JRU	N15-C14-N13-C12
3	B	602	JRU	N32-C14-N13-C12
3	B	602	JRU	N17-C18-N19-C20
4	B	603	MES	C8-C7-N4-C5
4	B	603	MES	C7-C8-S-O1S
3	A	602	JRU	C24-C25-S26-O31
2	B	601	LYS	CG-CD-CE-NZ
2	B	601	LYS	CA-CB-CG-CD
2	B	601	LYS	CE-CD-CG-CB
2	A	601	LYS	CG-CD-CE-NZ

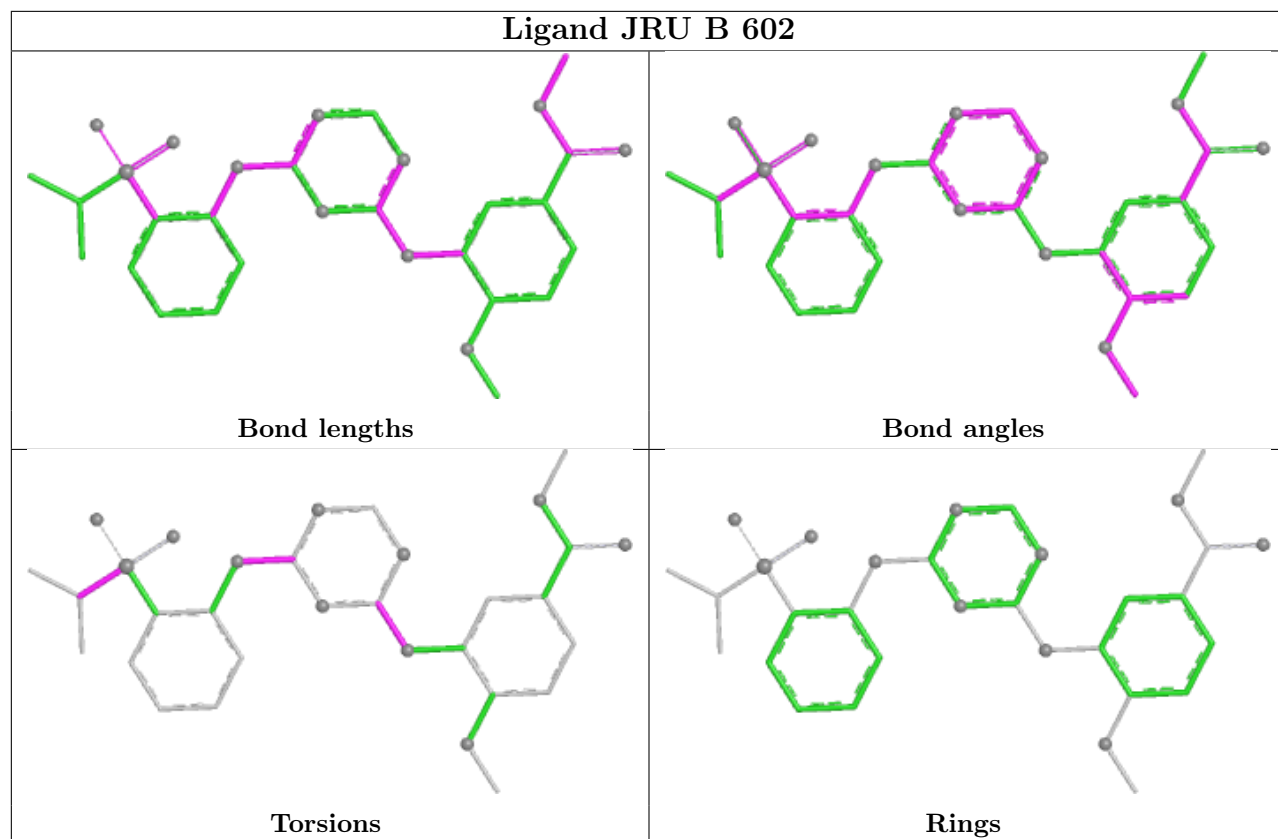
There are no ring outliers.

3 monomers are involved in 3 short contacts:

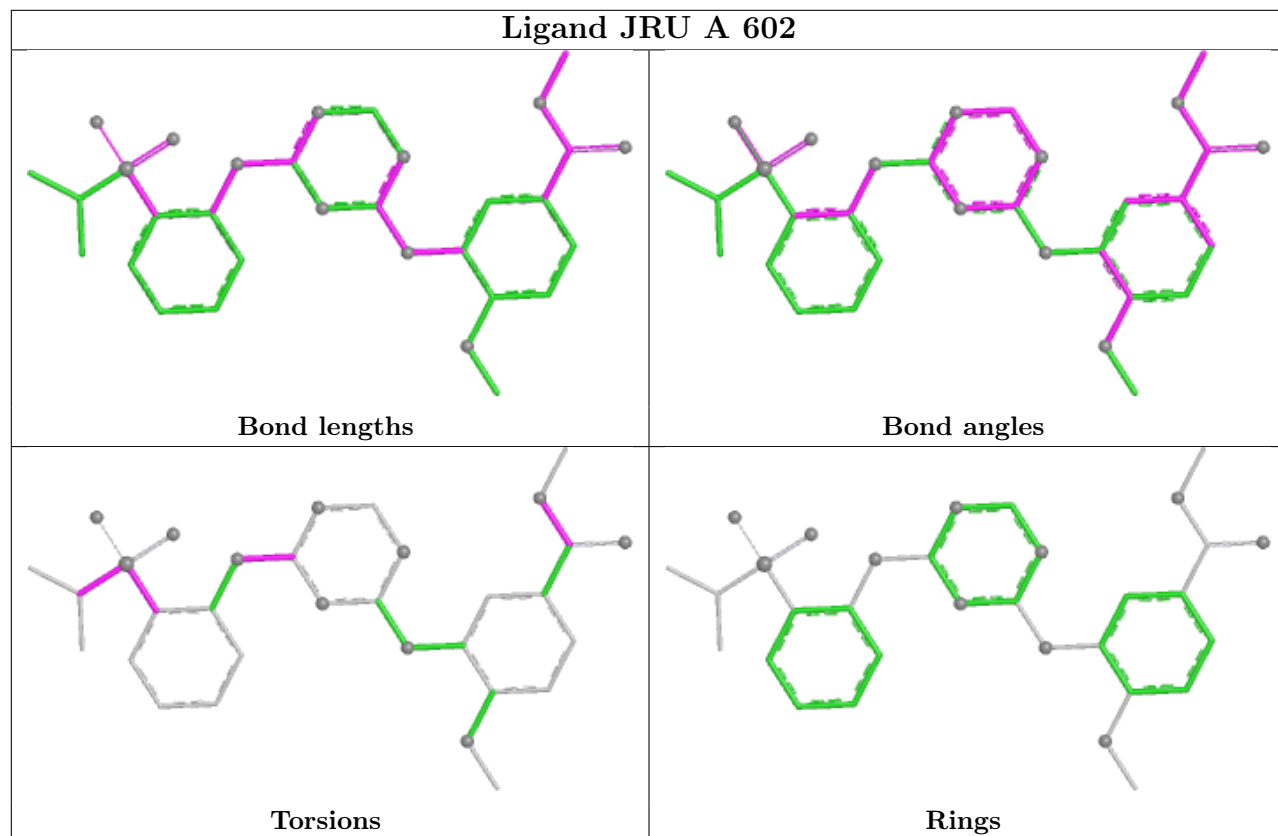
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	602	JRU	1	0
3	A	602	JRU	1	0
4	B	603	MES	1	0

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 JRU B 602



Ligand JRU A 602



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	489/516 (94%)	0.49	24 (4%)	35 41	32, 50, 73, 93	0
1	B	479/516 (92%)	0.77	46 (9%)	13 16	31, 61, 96, 125	0
All	All	968/1032 (93%)	0.63	70 (7%)	21 24	31, 54, 88, 125	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	518	PHE	5.3
1	A	512	PHE	5.1
1	B	280	LEU	5.0
1	A	229	ASP	5.0
1	A	225	TYR	4.5
1	B	78	VAL	4.4
1	B	582	ALA	4.4
1	A	78	VAL	4.3
1	A	518	PHE	4.3
1	B	147	GLN	4.2
1	B	146	GLY	4.0
1	B	225	TYR	4.0
1	B	145	SER	4.0
1	B	144	ALA	3.7
1	B	281	ILE	3.5
1	B	121	ASP	3.5
1	A	582	ALA	3.5
1	A	535	LEU	3.5
1	B	437	ILE	3.4
1	A	228	LYS	3.4
1	B	99	ILE	3.2
1	B	387	ASN	3.2
1	A	516	GLU	2.8
1	A	147	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	224	LYS	2.7
1	B	149	LEU	2.7
1	B	536	ASP	2.7
1	A	223	MET	2.6
1	A	99	ILE	2.6
1	A	299	LEU	2.5
1	A	457	ILE	2.5
1	B	439	LEU	2.5
1	B	515	LYS	2.5
1	B	169	PHE	2.4
1	B	167	TYR	2.4
1	B	158	GLY	2.4
1	B	432	ILE	2.4
1	B	128	LEU	2.4
1	B	164	LEU	2.4
1	B	132	ILE	2.3
1	A	517	CYS	2.3
1	B	287	ALA	2.3
1	A	580	ARG	2.3
1	B	143	SER	2.3
1	B	457	ILE	2.3
1	B	441	ASN	2.3
1	A	230	THR	2.3
1	B	230	THR	2.3
1	B	578	THR	2.3
1	A	227	LEU	2.2
1	B	224	LYS	2.2
1	A	334	ILE	2.2
1	B	151	PHE	2.2
1	B	129	GLU	2.1
1	A	249	HIS	2.1
1	B	249	HIS	2.1
1	B	512	PHE	2.1
1	B	148	LYS	2.1
1	B	433	LYS	2.1
1	A	439	LEU	2.1
1	B	431	ILE	2.1
1	B	131	THR	2.1
1	B	209	LYS	2.1
1	B	299	LEU	2.1
1	B	580	ARG	2.1
1	A	96	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	200	LYS	2.0
1	B	388	GLN	2.0
1	A	280	LEU	2.0
1	B	221	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](#)

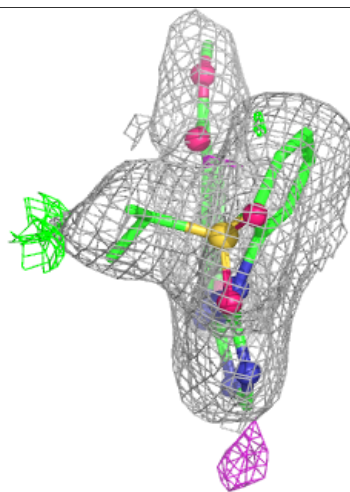
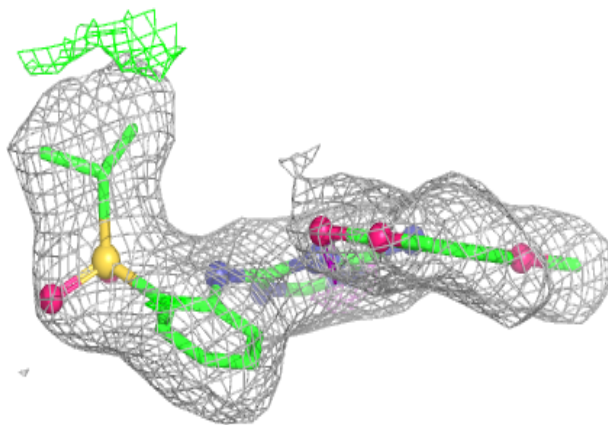
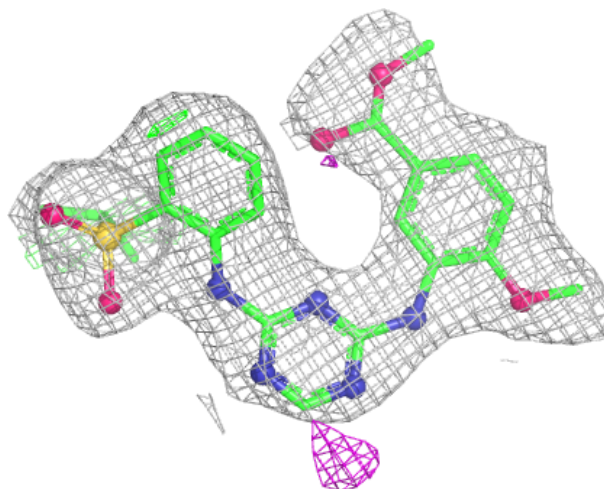
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
2	LYS	B	601	10/10	0.85	0.14	44,47,64,66	0
3	JRU	A	602	32/32	0.88	0.12	42,50,60,63	0
3	JRU	B	602	32/32	0.91	0.12	43,58,70,77	0
4	MES	B	603	12/12	0.92	0.10	43,49,56,57	0
2	LYS	A	601	10/10	0.95	0.08	33,38,43,46	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.

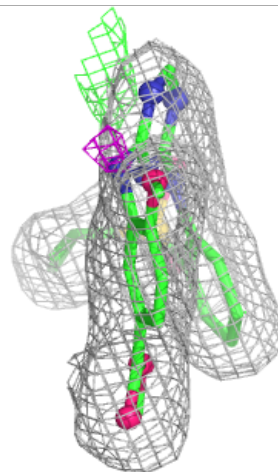
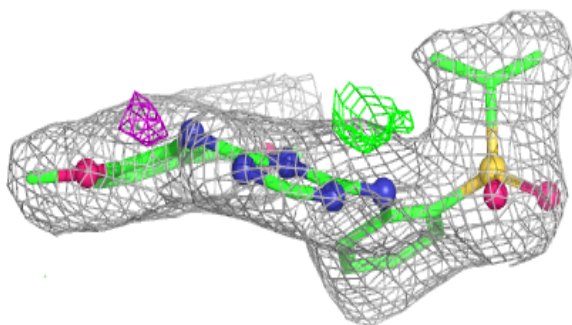
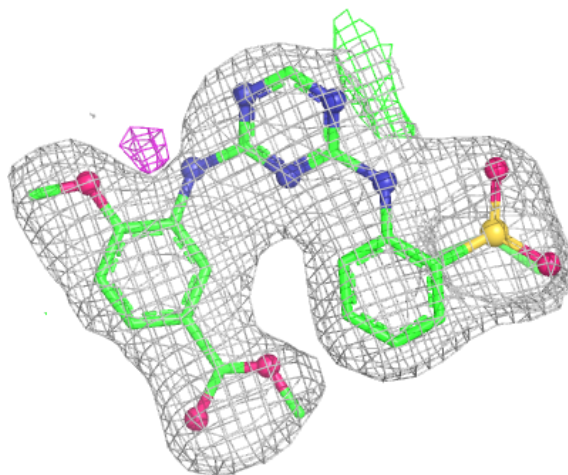
Electron density around JRU A 602:

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



Electron density around JRU B 602:

$2mF_o-DF_c$ (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.