



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:20 PM UTC

PDB ID : 8K9W / pdb_00008k9w
Title : Crystal structure of plasmodium LysRS complexing with ASP3026 derived LysRS inhibitor 4 (ADKI4)
Authors : Zhou, J.; Xia, M.; Yang, G.; Li, P.; Fang, P.
Deposited on : 2023-08-01
Resolution : 2.30 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

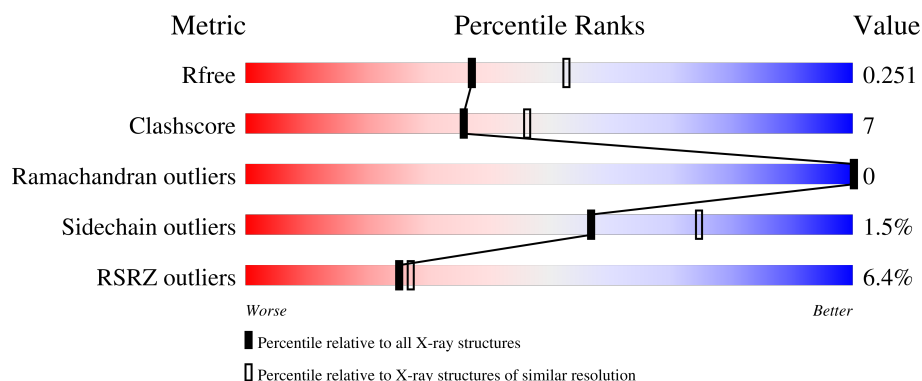
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	
1	B	516	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7727 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.

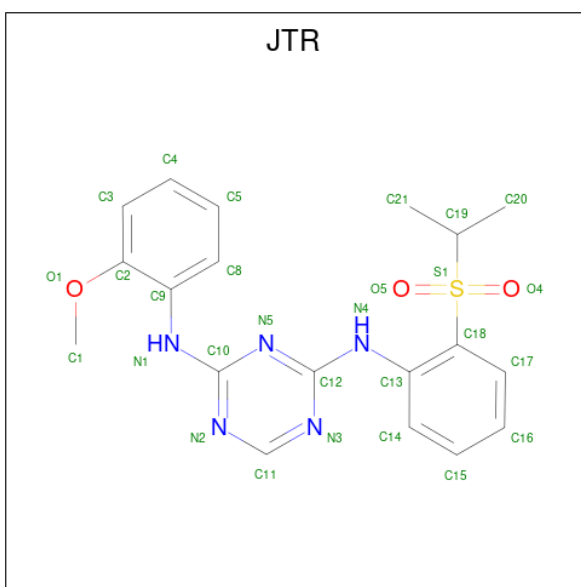
- Molecule 1 is a protein called Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	476	Total	C	N	O	S	0	0	0
			3741	2419	620	687	15			
1	B	482	Total	C	N	O	S	0	0	0
			3770	2436	626	691	17			

There are 18 discrepancies between the modelled and reference sequences:

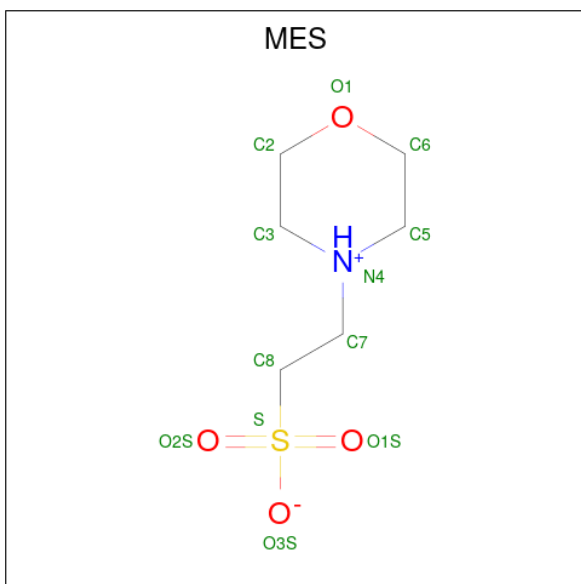
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP A0A024X378
A	584	GLY	-	expression tag	UNP A0A024X378
A	585	GLY	-	expression tag	UNP A0A024X378
A	586	HIS	-	expression tag	UNP A0A024X378
A	587	HIS	-	expression tag	UNP A0A024X378
A	588	HIS	-	expression tag	UNP A0A024X378
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 {N}2-(2-methoxyphenyl)- {N}4-(2-propan-2-ylsulfonylphenyl)-1,3,5-triazine-2,4-diamine (CCD ID: JTR) (formula: C₁₉H₂₁N₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			28	19	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			28	19	5	3	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

Continued on next page...

Continued from previous page...

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

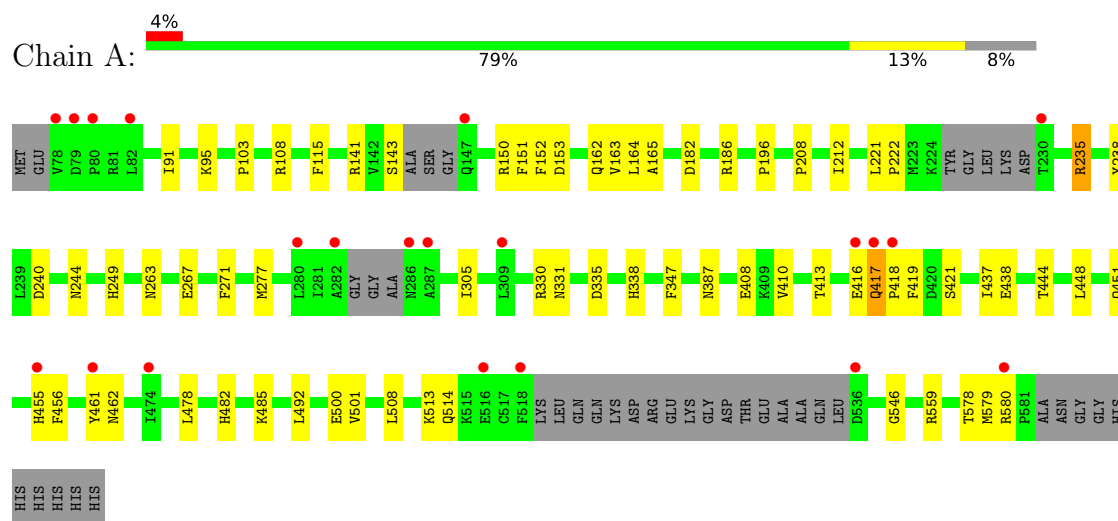
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total	O	0	0
			61	61		
4	B	75	Total	O	0	0
			75	75		

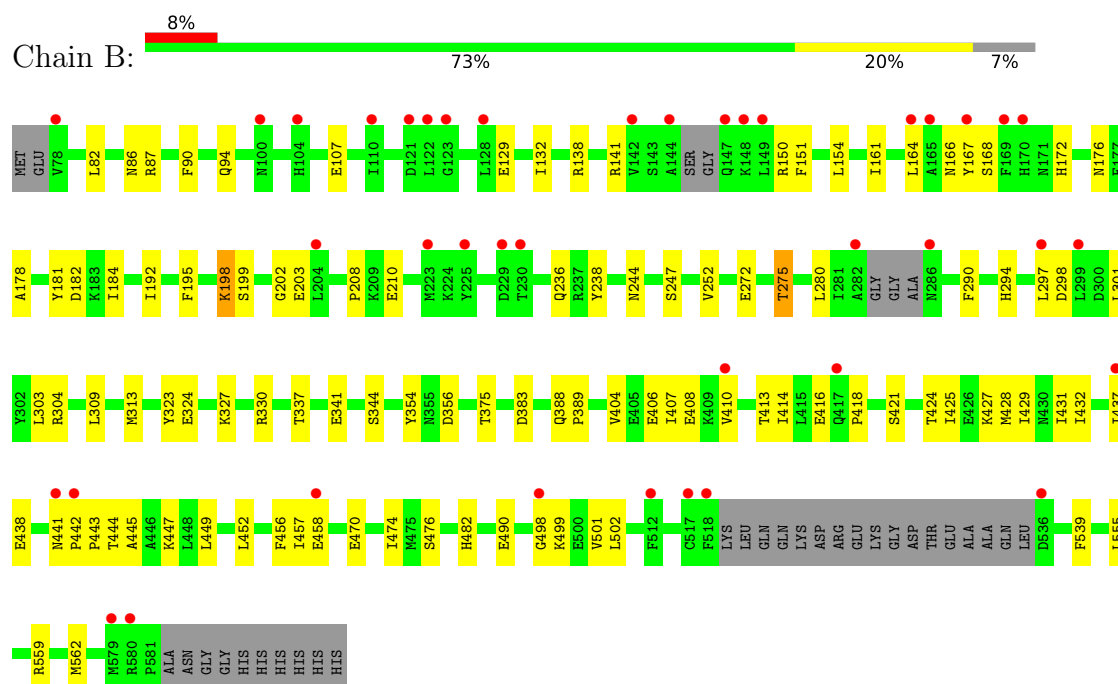
3 Residue-property plots [i](#)

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	71.92Å 95.55Å 168.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.45 – 2.30 32.45 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (32.45-2.30) 99.9 (32.45-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.29Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.214 , 0.251 0.214 , 0.251	Depositor DCC
R_{free} test set	2000 reflections (3.82%)	wwPDB-VP
Wilson B-factor (Å ²)	56.9	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7727	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.98% 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: JTR, 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	0.27	0/3835	0.45	2/5211 (0.0%)
1	B	0.33	0/3865	0.51	0/5250
All	All	0.30	0/7700	0.48	2/10461 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	417	GLN	CA-C-N	-5.40	113.09	119.84
1	A	417	GLN	C-N-CA	-5.40	113.09	119.84

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	ARG	Sidechain

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	3741	0	3550	44	0
1	B	3770	0	3556	68	0
2	A	28	0	0	0	0
2	B	28	0	0	2	0
3	A	24	0	24	3	0
4	A	61	0	0	2	0
4	B	75	0	0	2	0
All	All	7727	0	7130	108	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 7.

All (108) 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:A:249:HIS:CD2	4:A:706:HOH:O	2.35	0.79
1:B:441:ASN:HA	1:B:443:PRO:N	1.99	0.77
1:B:181:TYR:HA	1:B:184:ILE:HD12	1.69	0.73
1:B:441:ASN:HA	1:B:442:PRO:C	2.16	0.70
1:B:354:TYR:HB2	1:B:490:GLU:HG2	1.75	0.69
1:B:444:THR:HG23	1:B:447:LYS:H	1.56	0.69
1:B:199:SER:OG	1:B:203:GLU:N	2.26	0.69
1:A:235:ARG:NH2	1:A:580:ARG:O	2.26	0.68
1:B:421:SER:O	1:B:425:ILE:HG13	1.94	0.68
1:B:425:ILE:O	1:B:429:ILE:HG13	1.95	0.67
1:B:275:THR:HB	1:B:324:GLU:OE1	1.96	0.66
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.78	0.65
1:A:482:HIS:CE1	1:A:485:LYS:HG3	2.30	0.65
1:B:337:THR:HG21	1:B:499:LYS:HD2	1.79	0.65
1:B:172:HIS:HD2	4:B:747:HOH:O	1.78	0.64
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.81	0.63
1:B:176:ASN:HA	4:B:747:HOH:O	2.00	0.61
1:B:164:LEU:O	1:B:208:PRO:HD2	2.03	0.58
1:A:263:ASN:O	1:A:267:GLU:HG3	2.05	0.56
1:B:424:THR:O	1:B:428:MET:HG3	2.05	0.56
1:B:166:ASN:OD1	1:B:168:SER:OG	2.23	0.54
1:B:427:LYS:O	1:B:431:ILE:HG13	2.08	0.54
1:A:335:ASP:HB3	1:A:338:HIS:HB2	1.90	0.53
1:B:141:ARG:HH22	1:B:151:PHE:HB2	1.72	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ARG:NH1	1:A:221:LEU:O	2.43	0.52
1:B:129:GLU:HG2	1:B:195:PHE:CE2	2.44	0.52
1:B:458:GLU:O	1:B:498:GLY:HA2	2.10	0.51
1:B:82:LEU:O	1:B:86:ASN:ND2	2.42	0.51
1:B:272:GLU:HB2	1:B:323:TYR:CZ	2.45	0.51
1:B:164:LEU:CD2	1:B:166:ASN:HB2	2.41	0.50
1:B:244:ASN:O	1:B:247:SER:OG	2.29	0.50
1:B:441:ASN:HA	1:B:443:PRO:CD	2.42	0.50
1:A:410:VAL:HG21	1:A:456:PHE:HB3	1.94	0.50
1:A:508:LEU:HD12	1:A:514:GLN:HG2	1.94	0.49
1:B:236:GLN:HG2	1:B:238:TYR:CZ	2.47	0.49
1:B:559:ARG:HA	1:B:562:MET:HE3	1.93	0.49
1:A:417:GLN:O	1:A:419:PHE:N	2.46	0.49
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.48	0.48
1:A:500:GLU:HG2	1:A:559:ARG:NH1	2.28	0.48
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.94	0.48
1:B:418:PRO:HB2	1:B:421:SER:HB3	1.94	0.48
1:B:452:LEU:HD22	1:B:456:PHE:HE2	1.78	0.48
1:B:502:LEU:HD12	1:B:555:LEU:HD21	1.96	0.48
1:B:150:ARG:HH12	1:B:182:ASP:CG	2.23	0.47
1:A:437:ILE:HD13	1:A:455:HIS:HD2	1.80	0.47
1:A:578:THR:C	1:A:579:MET:HG3	2.39	0.47
1:A:461:TYR:C	1:A:462:ASN:HD22	2.21	0.47
1:B:167:TYR:HE1	1:B:172:HIS:HE2	1.63	0.47
1:A:408:GLU:HG2	1:A:413:THR:O	2.15	0.46
1:B:388:GLN:HG2	1:B:389:PRO:HD2	1.97	0.46
1:B:275:THR:HG22	1:B:304:ARG:HH11	1.81	0.46
1:B:432:ILE:HG22	1:B:437:ILE:O	2.16	0.46
1:B:327:LYS:NZ	1:B:341:GLU:OE2	2.47	0.45
1:B:404:VAL:O	1:B:408:GLU:HG3	2.16	0.45
3:A:603:MES:H51	1:B:356:ASP:OD1	2.16	0.45
1:B:280:LEU:HD23	1:B:301:LEU:CD2	2.46	0.45
1:B:176:ASN:OD1	1:B:178:ALA:N	2.49	0.45
1:B:330:ARG:HD3	2:B:601:JTR:C5	2.46	0.45
1:A:416:GLU:O	1:A:417:GLN:C	2.60	0.45
1:B:164:LEU:HD21	1:B:166:ASN:HB2	1.99	0.44
1:B:449:LEU:CD1	1:B:474:ILE:HD11	2.46	0.44
1:A:347:PHE:CD1	1:A:347:PHE:C	2.95	0.44
1:A:478:LEU:HA	1:A:514:GLN:HE22	1.83	0.44
1:B:297:LEU:O	1:B:298:ASP:C	2.59	0.44
1:A:186:ARG:HH12	1:A:222:PRO:C	2.25	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:LEU:HD23	1:B:161:ILE:HD11	1.98	0.44
1:A:141:ARG:HB3	1:A:153:ASP:HB2	1.99	0.44
1:A:150:ARG:NH1	1:A:182:ASP:OD1	2.48	0.44
1:A:305:ILE:O	1:A:330:ARG:NH1	2.50	0.44
1:A:578:THR:O	1:A:579:MET:HG3	2.18	0.44
1:B:428:MET:HE3	1:B:452:LEU:HD12	2.00	0.44
2:B:601:JTR:N5	2:B:601:JTR:C14	2.80	0.44
1:A:387:ASN:OD1	1:A:387:ASN:N	2.51	0.44
1:B:437:ILE:O	1:B:438:GLU:C	2.59	0.44
1:A:115:PHE:CE2	1:A:196:PRO:HB3	2.52	0.43
1:A:438:GLU:O	1:A:451:GLN:NE2	2.51	0.43
1:B:309:LEU:HD23	1:B:539:PHE:HB2	2.00	0.43
1:B:428:MET:HE1	1:B:449:LEU:HG	2.00	0.43
1:A:103:PRO:HG3	1:A:212:ILE:HD11	2.01	0.43
1:B:198:LYS:HD2	1:B:202:GLY:HA2	2.00	0.43
1:A:508:LEU:HD11	1:A:513:LYS:HB2	2.01	0.42
1:B:290:PHE:HB2	1:B:303:LEU:HB2	2.01	0.42
1:B:90:PHE:O	1:B:94:GLN:HG2	2.19	0.42
1:A:277:MET:HE3	1:A:277:MET:HB3	1.68	0.42
1:A:150:ARG:HB2	1:A:165:ALA:HB3	2.02	0.42
1:B:132:ILE:O	1:B:132:ILE:HD12	2.19	0.42
1:B:470:GLU:HG2	1:B:482:HIS:CD2	2.55	0.42
1:B:87:ARG:HD2	1:B:87:ARG:HA	1.80	0.42
1:A:164:LEU:O	1:A:208:PRO:HD2	2.20	0.41
1:A:418:PRO:HG2	1:A:421:SER:HB3	2.02	0.41
1:A:91:ILE:O	1:A:95:LYS:HG3	2.20	0.41
1:B:406:GLU:O	1:B:410:VAL:HG22	2.20	0.41
1:A:143:SER:OG	1:A:151:PHE:HB2	2.20	0.41
1:A:238:TYR:HE1	1:B:313:MET:HE3	1.86	0.41
3:A:602:MES:H32	1:B:107:GLU:HA	2.02	0.41
1:B:444:THR:O	1:B:445:ALA:C	2.64	0.41
1:A:108:ARG:HD2	3:A:603:MES:O3S	2.21	0.41
1:A:240:ASP:OD1	1:A:244:ASN:ND2	2.38	0.41
1:B:432:ILE:H	1:B:432:ILE:HG13	1.65	0.41
1:A:249:HIS:HD2	4:A:706:HOH:O	1.93	0.40
1:A:444:THR:O	1:A:448:LEU:HG	2.21	0.40
1:A:271:PHE:HZ	1:B:252:VAL:HA	1.87	0.40
1:A:331:ASN:OD1	1:B:294:HIS:HD2	2.04	0.40
1:A:546:GLY:O	1:B:138:ARG:NH2	2.51	0.40
1:B:416:GLU:H	1:B:424:THR:HG23	1.86	0.40
1:A:330:ARG:HG2	1:A:330:ARG:HH11	1.87	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:HH22	1:B:151:PHE:CB	2.32	0.40
1:B:408:GLU:HB3	1:B:413:THR:O	2.22	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	466/516 (90%)	457 (98%)	9 (2%)	0	100	100
1	B	474/516 (92%)	457 (96%)	17 (4%)	0	100	100
All	All	940/1032 (91%)	914 (97%)	26 (3%)	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	392/464 (84%)	389 (99%)	3 (1%)	73	86
1	B	388/464 (84%)	379 (98%)	9 (2%)	44	63
All	All	780/928 (84%)	768 (98%)	12 (2%)	57	75

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

Mol	Chain	Res	Type
1	A	162	GLN
1	A	492	LEU
1	A	501	VAL
1	B	198	LYS
1	B	210	GLU
1	B	275	THR
1	B	344	SER
1	B	375	THR
1	B	383	ASP
1	B	414	ILE
1	B	476	SER
1	B	501	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	GLN
1	A	176	ASN
1	A	338	HIS
1	A	412	ASN
1	A	455	HIS
1	A	462	ASN
1	A	514	GLN
1	B	86	ASN
1	B	92	GLN
1	B	279	ASN
1	B	294	HIS
1	B	295	ASN
1	B	388	GLN
1	B	514	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	MES	A	603	-	12,12,12	2.19	1 (8%)	15,16,16	2.30	5 (33%)
2	JTR	A	601	-	30,30,30	6.31	6 (20%)	36,42,42	3.82	12 (33%)
3	MES	A	602	-	12,12,12	2.18	1 (8%)	15,16,16	2.23	5 (33%)
2	JTR	B	601	-	30,30,30	6.23	5 (16%)	36,42,42	3.94	10 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	603	-	-	1/6/14/14	0/1/1/1
2	JTR	A	601	-	-	8/22/22/22	0/3/3/3
3	MES	A	602	-	-	1/6/14/14	0/1/1/1
2	JTR	B	601	-	-	7/22/22/22	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JTR	O4-S1	23.75	1.65	1.44
2	A	601	JTR	O5-S1	23.66	1.65	1.44
2	B	601	JTR	O4-S1	23.43	1.64	1.44
2	B	601	JTR	O5-S1	23.38	1.64	1.44
3	A	603	MES	C8-S	-7.34	1.67	1.77
3	A	602	MES	C8-S	-7.22	1.67	1.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	JTR	C12-N4	4.51	1.46	1.36
2	A	601	JTR	C12-N4	4.47	1.45	1.36
2	A	601	JTR	C10-N1	4.29	1.45	1.36
2	B	601	JTR	C10-N1	4.12	1.45	1.36
2	B	601	JTR	C10-N2	-2.19	1.31	1.34
2	A	601	JTR	C12-N3	-2.02	1.31	1.34
2	A	601	JTR	C13-N4	2.00	1.45	1.39

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	JTR	C11-N3-C12	11.65	120.72	113.27
2	A	601	JTR	C11-N3-C12	11.61	120.69	113.27
2	B	601	JTR	C11-N2-C10	11.21	120.43	113.27
2	A	601	JTR	C11-N2-C10	11.11	120.37	113.27
2	B	601	JTR	O5-S1-O4	-10.84	108.92	118.72
2	A	601	JTR	O5-S1-O4	-9.27	110.33	118.72
2	A	601	JTR	N3-C12-N5	-6.68	119.96	126.42
2	B	601	JTR	N3-C12-N5	-6.60	120.04	126.42
2	A	601	JTR	N2-C10-N5	-6.38	120.26	126.42
2	B	601	JTR	N2-C11-N3	-6.07	119.39	128.58
2	B	601	JTR	N2-C10-N5	-6.03	120.59	126.42
2	A	601	JTR	N2-C11-N3	-6.00	119.50	128.58
3	A	603	MES	C5-N4-C3	5.74	121.21	108.84
3	A	602	MES	C5-N4-C3	5.28	120.21	108.84
2	B	601	JTR	O1-C2-C9	3.78	119.53	114.81
3	A	603	MES	C7-N4-C3	3.67	121.03	111.24
2	A	601	JTR	O1-C2-C9	3.60	119.30	114.81
3	A	602	MES	C7-N4-C3	3.13	119.58	111.24
2	A	601	JTR	C12-N5-C10	3.00	119.23	113.85
3	A	603	MES	O1S-S-C8	2.80	110.95	106.73
2	B	601	JTR	C12-N5-C10	2.78	118.83	113.85
3	A	602	MES	C7-N4-C5	2.70	118.44	111.24
3	A	602	MES	C2-C3-N4	-2.60	106.17	110.12
2	B	601	JTR	C1-O1-C2	-2.49	113.86	117.51
2	B	601	JTR	O1-C2-C3	-2.46	120.16	124.30
2	A	601	JTR	C13-N4-C12	-2.25	122.36	129.22
3	A	602	MES	O3S-S-C8	2.23	110.37	106.00
2	A	601	JTR	O1-C2-C3	-2.22	120.55	124.30
3	A	603	MES	O3S-S-C8	2.21	110.32	106.00
3	A	603	MES	C7-N4-C5	2.13	116.92	111.24
2	A	601	JTR	C1-O1-C2	-2.13	114.39	117.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	JTR	C18-S1-C19	2.02	110.17	105.70

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	JTR	N3-C12-N4-C13
2	A	601	JTR	N5-C12-N4-C13
2	A	601	JTR	C20-C19-S1-C18
2	A	601	JTR	C20-C19-S1-O4
2	A	601	JTR	C20-C19-S1-O5
2	A	601	JTR	C21-C19-S1-C18
2	A	601	JTR	C21-C19-S1-O4
2	A	601	JTR	C21-C19-S1-O5
2	B	601	JTR	C20-C19-S1-C18
2	B	601	JTR	C20-C19-S1-O4
2	B	601	JTR	C20-C19-S1-O5
2	B	601	JTR	C21-C19-S1-C18
2	B	601	JTR	C21-C19-S1-O4
2	B	601	JTR	C21-C19-S1-O5
3	A	602	MES	C8-C7-N4-C5
3	A	603	MES	C8-C7-N4-C5
2	B	601	JTR	C17-C18-S1-O4

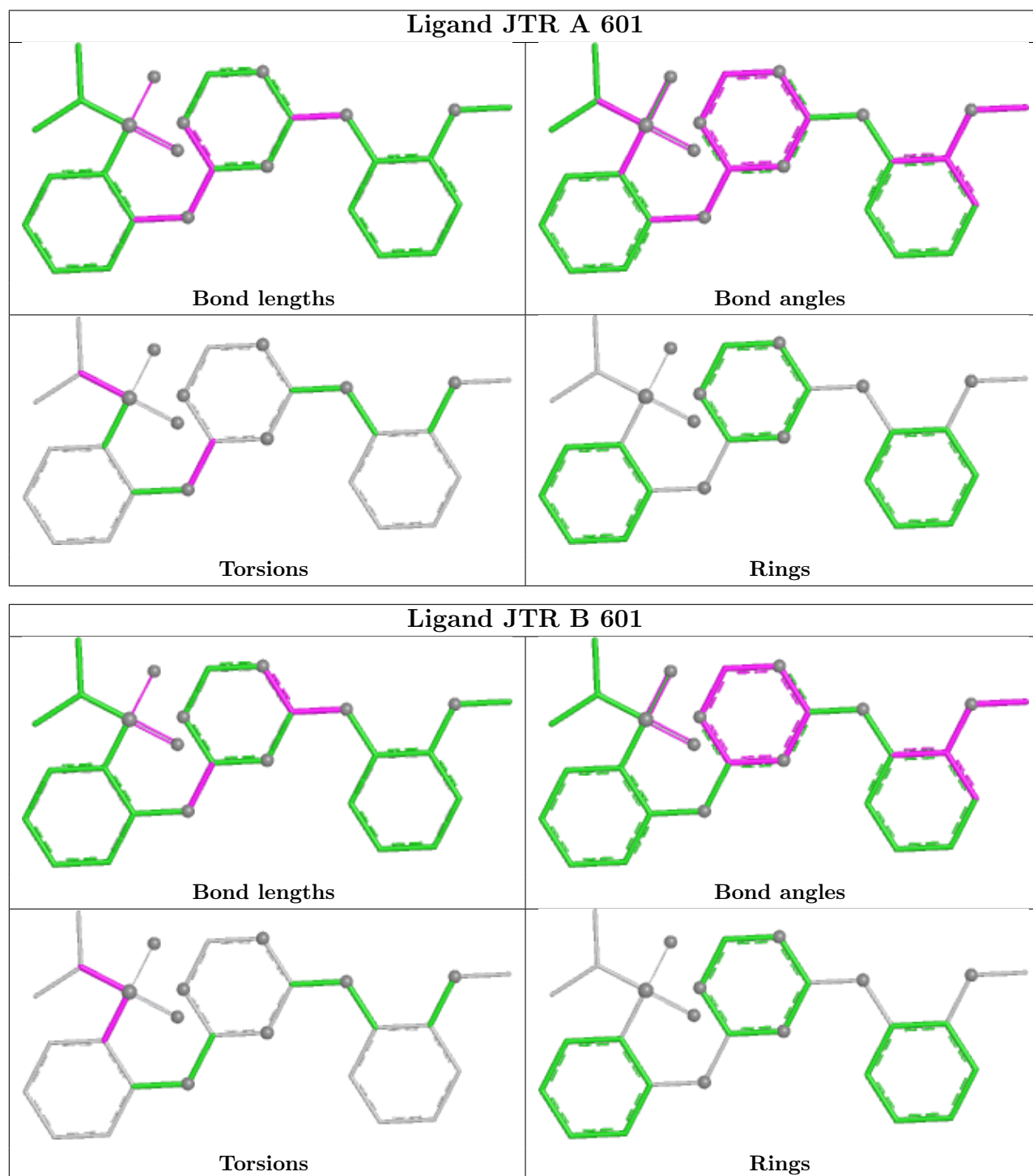
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	MES	2	0
3	A	602	MES	1	0
2	B	601	JTR	2	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	476/516 (92%)	0.41	21 (4%)	39 41	45, 65, 101, 155	0
1	B	482/516 (93%)	0.63	40 (8%)	17 19	42, 76, 131, 186	0
All	All	958/1032 (92%)	0.52	61 (6%)	25 27	42, 70, 120, 186	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	ALA	5.2
1	B	78	VAL	4.7
1	B	282	ALA	4.2
1	B	286	ASN	4.0
1	B	165	ALA	4.0
1	A	230	THR	4.0
1	A	78	VAL	3.9
1	B	144	ALA	3.9
1	A	286	ASN	3.9
1	B	148	LYS	3.9
1	A	518	PHE	3.3
1	B	164	LEU	3.3
1	B	121	ASP	3.2
1	A	147	GLN	3.2
1	B	225	TYR	3.1
1	B	110	ILE	3.1
1	A	461	TYR	3.1
1	A	287	ALA	3.0
1	B	147	GLN	2.9
1	B	123	GLY	2.9
1	B	297	LEU	2.9
1	A	417	GLN	2.8
1	B	122	LEU	2.8
1	A	580	ARG	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	536	ASP	2.7
1	B	458	GLU	2.6
1	B	518	PHE	2.6
1	B	417	GLN	2.6
1	B	229	ASP	2.5
1	B	512	PHE	2.5
1	B	128	LEU	2.5
1	B	149	LEU	2.4
1	B	442	PRO	2.4
1	B	437	ILE	2.4
1	A	280	LEU	2.4
1	B	167	TYR	2.3
1	B	299	LEU	2.3
1	B	169	PHE	2.3
1	B	536	ASP	2.3
1	A	80	PRO	2.3
1	B	223	MET	2.3
1	B	498	GLY	2.2
1	A	516	GLU	2.2
1	A	474	ILE	2.2
1	B	142	VAL	2.2
1	A	416	GLU	2.2
1	A	82	LEU	2.2
1	A	309	LEU	2.2
1	A	455	HIS	2.2
1	B	104	HIS	2.2
1	B	517	CYS	2.2
1	A	79	ASP	2.1
1	B	580	ARG	2.1
1	B	441	ASN	2.1
1	B	204	LEU	2.1
1	B	100	ASN	2.1
1	A	418	PRO	2.1
1	B	410	VAL	2.1
1	B	230	THR	2.0
1	B	170	HIS	2.0
1	B	579	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

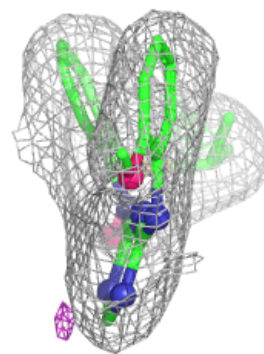
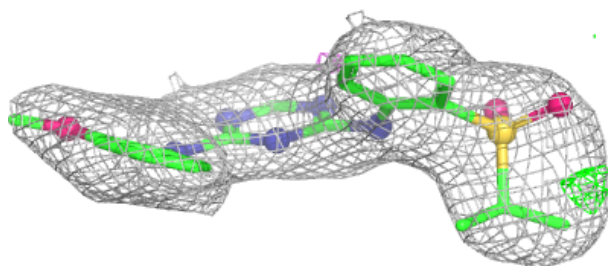
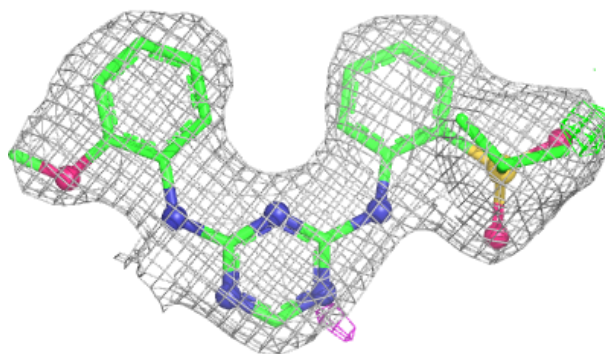
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	JTR	A	601	28/28	0.88	0.12	60,67,74,76	0
3	MES	A	602	12/12	0.93	0.09	66,71,78,80	0
3	MES	A	603	12/12	0.93	0.10	54,57,60,62	0
2	JTR	B	601	28/28	0.94	0.10	61,70,75,76	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.

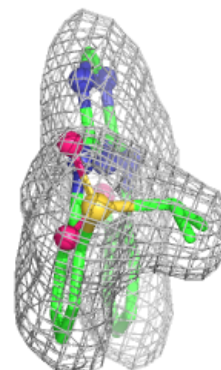
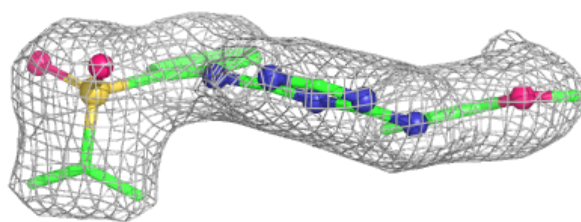
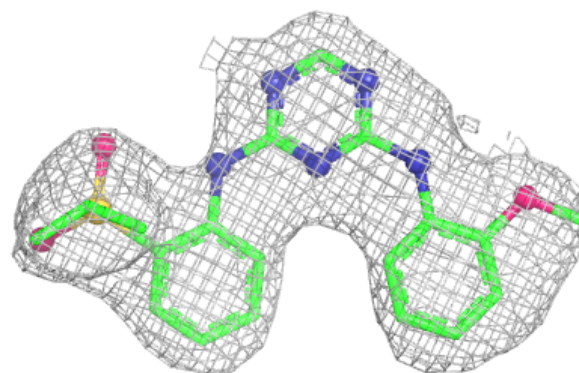
Electron density around JTR A 601:

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 JTR B 601:

$2mF_o-DF_c$ (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.