



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:34 PM UTC

PDB ID : 8K9X / pdb_00008k9x
Title : Crystal structure of plasmodium LysRS complexing with ASP3026 derived LysRS inhibitor 5 (ADKI5)
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.

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

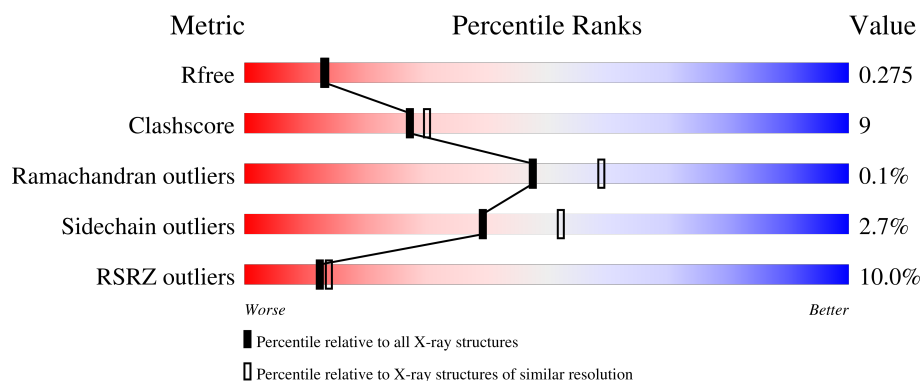
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	10% 72% 20% 7%
1	B	516	9% 77% 16% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7876 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.

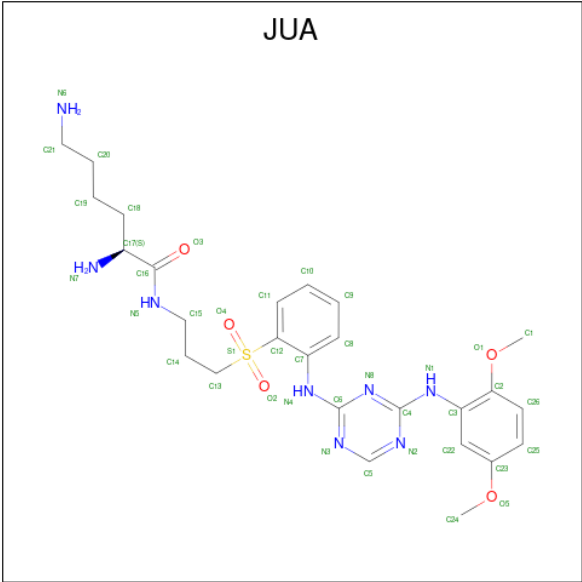
- Molecule 1 is a protein called Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3819	2470	632	701	16			
1	B	481	Total	C	N	O	S	0	0	0
			3825	2473	633	702	17			

There are 18 discrepancies between the modelled and reference sequences:

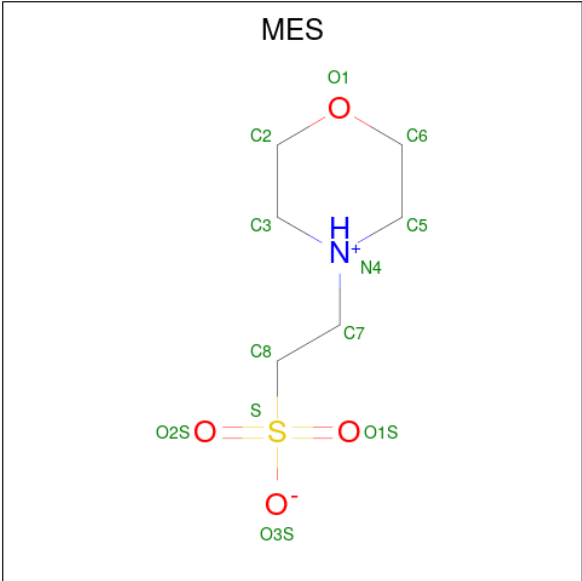
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP A0A024X378
A	584	GLY	-	expression tag	UNP A0A024X378
A	585	GLY	-	expression tag	UNP A0A024X378
A	586	HIS	-	expression tag	UNP A0A024X378
A	587	HIS	-	expression tag	UNP A0A024X378
A	588	HIS	-	expression tag	UNP A0A024X378
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 (2 {S})-2,6-bis(azanyl)- {N}-[3-[2-[4-[(2,5-dimethoxyphenyl)amino]-1,3,5-triazin-2-yl]amino]phenyl]sulfonylpropyl]hexanamide (CCD ID: JUA) (formula: C₂₆H₃₆N₈O₅S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			40	26	8	5	1		
2	B	1	Total	C	N	O	S	0	0
			40	26	8	5	1		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

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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	67	Total	O	0	0
			67	67		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	71.67Å 99.49Å 171.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.12 – 2.35 48.12 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.12-2.35) 99.1 (48.12-2.35)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.34Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.230 , 0.276 0.230 , 0.275	Depositor DCC
R_{free} test set	2000 reflections (3.86%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.670	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.9	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	0.94	EDS
Total number of atoms	7876	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 5.47% 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: MES, JUA

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	0.38	0/3914	0.59	2/5309 (0.0%)
1	B	0.39	0/3921	0.60	0/5319
All	All	0.39	0/7835	0.60	2/10628 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	418	PRO	N-CA-C	-5.50	102.30	111.26
1	A	419	PHE	N-CA-C	-5.04	106.96	113.01

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	3819	0	3666	77	0
1	B	3825	0	3666	64	1
2	A	40	0	0	2	0
2	B	40	0	0	1	0
3	A	24	0	24	5	0
4	A	61	0	0	3	0
4	B	67	0	0	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7876	0	7356	137	1

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 9.

All (137) 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:580:ARG:HD3	1:A:580:ARG:H	1.32	0.92
1:B:169:PHE:CB	4:B:704:HOH:O	2.28	0.81
1:B:169:PHE:HB2	4:B:704:HOH:O	1.80	0.80
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.63	0.78
1:B:308:GLU:HG3	1:B:348:TYR:OH	1.83	0.78
1:B:308:GLU:OE1	2:B:601:JUA:N7	2.18	0.77
1:B:439:LEU:HD21	1:B:443:PRO:HB3	1.66	0.76
1:B:337:THR:HG21	1:B:499:LYS:HD2	1.71	0.71
1:B:476:SER:OG	1:B:491:ARG:NH1	2.22	0.71
1:A:227:LEU:HD22	1:A:232:ILE:HD11	1.72	0.71
1:B:182:ASP:O	1:B:185:ARG:NH1	2.24	0.70
1:B:169:PHE:CD2	4:B:704:HOH:O	2.45	0.70
1:B:410:VAL:HG21	1:B:456:PHE:HB3	1.75	0.67
1:B:176:ASN:HD22	1:B:179:GLU:CD	2.03	0.66
1:B:464:LYS:HE3	4:B:718:HOH:O	1.96	0.66
1:A:231:GLU:OE2	1:A:235:ARG:NH2	2.31	0.64
1:A:407:ILE:HG13	1:A:457:ILE:HD11	1.77	0.64
1:B:308:GLU:HG3	1:B:348:TYR:HH	1.62	0.64
1:A:460:LYS:HG2	1:A:461:TYR:CD1	2.32	0.64
1:B:275:THR:HB	1:B:324:GLU:OE1	1.98	0.63
1:A:432:ILE:HG23	1:A:437:ILE:HB	1.80	0.63
1:A:495:PHE:CE2	1:A:500:GLU:HG3	2.35	0.62
1:A:295:ASN:H	1:B:331:ASN:HD21	1.49	0.61
1:A:495:PHE:CZ	1:A:500:GLU:HG3	2.35	0.61
1:A:295:ASN:ND2	1:B:331:ASN:OD1	2.34	0.60
1:B:169:PHE:N	4:B:704:HOH:O	2.26	0.60
1:B:150:ARG:HB2	1:B:165:ALA:HB3	1.84	0.60
1:B:169:PHE:CG	4:B:704:HOH:O	2.54	0.59
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.84	0.58
1:A:502:LEU:HD12	1:A:555:LEU:HD21	1.86	0.58
1:B:176:ASN:ND2	1:B:179:GLU:OE1	2.38	0.57
1:A:404:VAL:O	1:A:408:GLU:HG3	2.04	0.57
1:A:468:ILE:HD12	1:A:495:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:THR:HG22	1:B:304:ARG:HH11	1.69	0.56
1:A:408:GLU:HB3	1:A:413:THR:O	2.05	0.56
3:A:603:MES:O1S	1:B:108:ARG:NH1	2.39	0.55
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.88	0.55
1:B:164:LEU:HD23	1:B:207:PHE:CE2	2.42	0.55
1:A:460:LYS:HG2	1:A:461:TYR:HD1	1.70	0.55
1:A:294:HIS:HD2	1:A:296:ASP:H	1.55	0.55
1:B:382:LYS:HG3	1:B:497:CYS:SG	2.47	0.54
1:B:558:ASP:O	1:B:562:MET:HG3	2.06	0.54
1:A:107:GLU:HA	3:A:602:MES:H32	1.89	0.54
1:A:181:TYR:HA	1:A:184:ILE:HD12	1.89	0.53
1:A:201:LYS:N	1:A:201:LYS:HD2	2.23	0.53
1:A:386:GLU:OE1	1:A:386:GLU:N	2.27	0.53
1:A:419:PHE:HB2	1:A:474:ILE:HD11	1.91	0.53
1:A:463:ASP:HB2	4:A:743:HOH:O	2.08	0.53
1:B:129:GLU:H	1:B:129:GLU:CD	2.17	0.53
1:A:472:PRO:HD2	1:A:475:MET:SD	2.49	0.52
1:A:491:ARG:NH1	1:A:493:GLU:OE2	2.42	0.52
1:A:239:LEU:O	1:A:243:ILE:HG12	2.10	0.52
1:A:116:ILE:O	1:A:120:LYS:HB2	2.10	0.51
1:B:334:ILE:HG12	1:B:340:PRO:HD3	1.93	0.51
1:A:491:ARG:HG2	1:A:492:LEU:N	2.25	0.50
1:B:143:SER:OG	1:B:151:PHE:HB2	2.11	0.50
1:A:105:LYS:CG	3:A:602:MES:H22	2.41	0.50
1:A:226:GLY:C	1:A:227:LEU:HD23	2.37	0.50
1:A:467:PHE:HA	1:A:493:GLU:O	2.12	0.49
1:B:458:GLU:O	1:B:498:GLY:HA2	2.13	0.49
1:B:424:THR:O	1:B:428:MET:HG3	2.12	0.49
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.94	0.49
1:A:410:VAL:HG21	1:A:456:PHE:HB3	1.93	0.49
1:B:312:LYS:HZ1	1:B:478:LEU:HD12	1.78	0.48
1:B:312:LYS:NZ	1:B:478:LEU:HD12	2.29	0.48
1:A:330:ARG:HD2	2:A:601:JUA:C23	2.43	0.48
1:B:129:GLU:HA	1:B:195:PHE:CG	2.48	0.48
1:B:150:ARG:HH11	1:B:150:ARG:HG2	1.79	0.48
1:A:442:PRO:HG2	1:A:444:THR:HG23	1.97	0.47
1:A:112:ILE:HG12	1:A:135:ILE:HD11	1.97	0.47
1:A:470:GLU:OE2	1:A:482:HIS:NE2	2.45	0.47
1:A:150:ARG:HB2	1:A:165:ALA:HB3	1.97	0.47
1:A:390:ILE:HD11	1:A:497:CYS:SG	2.54	0.47
1:A:442:PRO:HG2	1:A:444:THR:CG2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:THR:HG21	1:A:431:ILE:HD13	1.97	0.46
1:B:470:GLU:HA	1:B:489:THR:O	2.15	0.46
1:A:278:MET:HE2	1:A:292:THR:HG21	1.98	0.46
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.99	0.45
1:A:470:GLU:HA	1:A:489:THR:O	2.16	0.45
1:B:319:ILE:HG22	1:B:322:VAL:HB	1.99	0.45
1:B:439:LEU:CD2	1:B:443:PRO:HB3	2.41	0.45
1:A:419:PHE:HB2	1:A:474:ILE:CD1	2.47	0.45
1:B:463:ASP:OD1	1:B:463:ASP:N	2.47	0.45
1:A:261:LEU:HD21	1:A:345:CYS:SG	2.57	0.45
1:A:166:ASN:HB3	1:A:169:PHE:CD2	2.52	0.45
1:A:278:MET:HE1	1:B:290:PHE:CD1	2.52	0.44
1:A:341:GLU:OE1	1:B:278:MET:HE2	2.18	0.44
1:A:349:TRP:NE1	3:A:603:MES:O3S	2.50	0.44
1:A:418:PRO:O	1:A:421:SER:HB3	2.17	0.44
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.88	0.43
1:B:234:TYR:CD2	1:B:579:MET:HE1	2.53	0.43
1:B:444:THR:HB	4:B:737:HOH:O	2.18	0.43
1:A:105:LYS:HG3	3:A:602:MES:H22	2.00	0.43
1:A:465:PRO:HB3	1:A:496:ILE:HG12	1.99	0.43
1:B:502:LEU:C	1:B:502:LEU:HD23	2.44	0.43
1:A:358:ILE:HG21	1:A:400:LYS:HE2	2.01	0.43
1:B:437:ILE:HD11	1:B:455:HIS:CE1	2.52	0.43
1:B:580:ARG:HB2	1:B:580:ARG:NH1	2.34	0.43
1:A:122:LEU:HD21	1:A:128:LEU:HD11	1.99	0.43
1:A:211:THR:C	1:A:212:ILE:HD13	2.44	0.42
1:B:278:MET:HE3	1:B:278:MET:HB2	1.66	0.42
1:A:176:ASN:OD1	1:A:179:GLU:N	2.47	0.42
1:B:580:ARG:HB2	1:B:580:ARG:HH11	1.85	0.42
1:A:299:LEU:HD23	1:A:299:LEU:HA	1.93	0.42
1:A:349:TRP:CG	1:A:352:ALA:HB2	2.54	0.42
1:B:142:VAL:HG22	1:B:152:PHE:CD1	2.54	0.42
1:A:245:GLU:H	1:A:245:GLU:CD	2.26	0.42
1:A:369:VAL:HG21	1:A:394:PHE:CG	2.54	0.42
1:B:111:SER:OG	1:B:114:GLU:HG3	2.19	0.42
1:A:502:LEU:HD11	1:A:553:LEU:HD11	2.01	0.41
1:A:176:ASN:HB3	1:A:179:GLU:HB3	2.02	0.41
1:A:313:MET:HE1	1:A:538:ALA:CB	2.51	0.41
1:A:417:GLN:O	1:A:418:PRO:C	2.63	0.41
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.89	0.41
1:A:469:VAL:HG23	1:A:470:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:579:MET:HE2	1:A:579:MET:HB3	1.84	0.41
1:B:105:LYS:HE3	1:B:105:LYS:HB2	1.88	0.41
1:B:494:MET:O	1:B:501:VAL:HG12	2.21	0.41
1:A:272:GLU:HB2	1:A:323:TYR:CZ	2.55	0.41
1:A:320:ASP:OD2	4:A:701:HOH:O	2.22	0.41
1:B:115:PHE:CE1	1:B:196:PRO:HB3	2.56	0.41
1:B:164:LEU:HD12	1:B:164:LEU:HA	1.88	0.41
1:B:335:ASP:OD1	1:B:336:ASN:N	2.54	0.41
1:B:223:MET:HE3	1:B:223:MET:HB3	1.71	0.41
1:B:347:PHE:C	1:B:347:PHE:CD1	2.98	0.41
1:B:478:LEU:HD22	1:B:514:GLN:HE22	1.86	0.41
1:A:280:LEU:HD21	1:A:299:LEU:HD13	2.02	0.41
1:A:474:ILE:H	1:A:474:ILE:HG12	1.64	0.41
1:A:308:GLU:HG2	1:A:348:TYR:OH	2.21	0.40
1:A:173:GLU:CD	1:A:173:GLU:C	2.89	0.40
1:A:234:TYR:HB3	1:A:577:PRO:HG2	2.02	0.40
1:A:482:HIS:O	4:A:702:HOH:O	2.22	0.40
1:A:556:GLY:HA3	2:A:601:JUA:O2	2.22	0.40
1:B:427:LYS:O	1:B:431:ILE:HG13	2.21	0.40
1:A:411:THR:O	1:A:411:THR:HG22	2.21	0.40
1:B:355:ASN:HB2	4:B:729:HOH:O	2.20	0.40
1:B:431:ILE:HG13	1:B:431:ILE:H	1.76	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:SER:OG	1:B:437:ILE:O[3_444]	2.05	0.15

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	473/516 (92%)	462 (98%)	10 (2%)	1 (0%)	43	52
1	B	473/516 (92%)	464 (98%)	9 (2%)	0	100	100
All	All	946/1032 (92%)	926 (98%)	19 (2%)	1 (0%)	48	59

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	417	GLN

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	403/464 (87%)	391 (97%)	12 (3%)	36	48
1	B	404/464 (87%)	394 (98%)	10 (2%)	42	55
All	All	807/928 (87%)	785 (97%)	22 (3%)	39	52

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	SER
1	A	180	CYS
1	A	186	ARG
1	A	192	ILE
1	A	227	LEU
1	A	232	ILE
1	A	344	SER
1	A	379	SER
1	A	421	SER
1	A	454	SER
1	A	478	LEU
1	A	492	LEU
1	B	85	GLU
1	B	99	ILE
1	B	122	LEU

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Mol	Chain	Res	Type
1	B	129	GLU
1	B	155	VAL
1	B	185	ARG
1	B	199	SER
1	B	275	THR
1	B	379	SER
1	B	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	294	HIS
1	A	295	ASN
1	A	459	ASN
1	B	236	GLN
1	B	244	ASN
1	B	294	HIS
1	B	331	ASN
1	B	430	ASN
1	B	435	HIS
1	B	455	HIS

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](#)

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	602	-	12,12,12	2.37	1 (8%)	15,16,16	2.54	8 (53%)
2	JUA	B	601	-	42,42,42	4.06	12 (28%)	54,56,56	3.16	16 (29%)
2	JUA	A	601	-	42,42,42	3.97	10 (23%)	54,56,56	3.38	16 (29%)
3	MES	A	603	-	12,12,12	2.33	1 (8%)	15,16,16	2.23	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
3	MES	A	602	-	-	1/6/14/14	0/1/1/1
2	JUA	B	601	-	-	4/35/35/35	0/3/3/3
2	JUA	A	601	-	-	5/35/35/35	0/3/3/3
3	MES	A	603	-	-	1/6/14/14	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JUA	O4-S1	16.12	1.66	1.44
2	B	601	JUA	O4-S1	16.06	1.65	1.44
2	B	601	JUA	O2-S1	15.58	1.65	1.44
2	A	601	JUA	O2-S1	14.79	1.64	1.44
3	A	602	MES	C8-S	-7.83	1.66	1.77
3	A	603	MES	C8-S	-7.83	1.66	1.77
2	A	601	JUA	C6-N4	6.61	1.50	1.36
2	B	601	JUA	C16-N5	6.28	1.48	1.33
2	A	601	JUA	C16-N5	6.27	1.48	1.33
2	B	601	JUA	C6-N4	6.23	1.49	1.36
2	B	601	JUA	C4-N1	5.95	1.49	1.36
2	A	601	JUA	C4-N1	5.65	1.48	1.36
2	A	601	JUA	C13-S1	3.85	1.85	1.77
2	B	601	JUA	C3-N1	3.57	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	JUA	C3-N1	3.17	1.48	1.39
2	B	601	JUA	C7-N4	3.04	1.48	1.39
2	B	601	JUA	O1-C2	2.94	1.41	1.37
2	A	601	JUA	C7-N4	2.92	1.47	1.39
2	B	601	JUA	O5-C23	2.91	1.43	1.37
2	B	601	JUA	C13-S1	2.83	1.83	1.77
2	A	601	JUA	O3-C16	-2.68	1.18	1.23
2	B	601	JUA	O3-C16	-2.61	1.18	1.23
2	B	601	JUA	C12-S1	2.30	1.83	1.78
2	A	601	JUA	C12-S1	2.17	1.83	1.78

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	JUA	C5-N2-C4	13.03	121.59	113.27
2	B	601	JUA	C5-N2-C4	11.73	120.77	113.27
2	A	601	JUA	C5-N3-C6	11.72	120.76	113.27
2	B	601	JUA	C5-N3-C6	9.75	119.50	113.27
2	A	601	JUA	O4-S1-O2	-7.96	109.92	118.45
2	B	601	JUA	N2-C4-N8	-7.41	119.25	126.42
2	A	601	JUA	N2-C4-N8	-7.07	119.59	126.42
2	A	601	JUA	N3-C6-N8	-6.86	119.78	126.42
2	A	601	JUA	N2-C5-N3	-6.43	118.85	128.58
2	B	601	JUA	N3-C6-N8	-6.38	120.25	126.42
3	A	602	MES	C5-N4-C3	5.58	120.86	108.84
3	A	603	MES	C5-N4-C3	5.53	120.76	108.84
2	B	601	JUA	N2-C5-N3	-5.51	120.24	128.58
2	B	601	JUA	O4-S1-O2	-5.05	113.04	118.45
2	B	601	JUA	C12-C7-N4	-4.98	116.91	121.50
3	A	602	MES	C2-C3-N4	-4.38	103.47	110.12
2	A	601	JUA	O4-S1-C13	4.36	115.32	108.18
2	B	601	JUA	O4-S1-C12	4.25	114.27	107.98
2	B	601	JUA	O2-S1-C12	3.87	113.71	107.98
2	B	601	JUA	C14-C13-S1	-3.51	103.51	113.33
2	B	601	JUA	O1-C2-C3	3.43	119.08	114.81
2	B	601	JUA	C6-N8-C4	3.42	119.98	113.85
2	A	601	JUA	O2-S1-C13	-3.38	102.65	108.18
2	A	601	JUA	C24-O5-C23	-3.37	110.28	117.50
2	B	601	JUA	C15-N5-C16	-3.30	116.62	122.55
3	A	603	MES	C7-N4-C5	3.13	119.57	111.24
2	A	601	JUA	C6-N8-C4	3.10	119.41	113.85
2	A	601	JUA	O2-S1-C12	2.98	112.38	107.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	MES	C7-N4-C5	2.89	118.95	111.24
3	A	602	MES	C7-N4-C3	2.83	118.78	111.24
2	B	601	JUA	C11-C12-S1	2.73	121.27	116.74
3	A	603	MES	O2S-S-C8	2.66	110.74	106.73
3	A	602	MES	O2S-S-C8	2.60	110.65	106.73
3	A	602	MES	O1S-S-C8	2.54	110.57	106.73
2	A	601	JUA	O1-C2-C3	2.37	117.77	114.81
3	A	603	MES	C2-C3-N4	-2.32	106.59	110.12
3	A	603	MES	C7-N4-C3	2.29	117.33	111.24
2	A	601	JUA	C1-O1-C2	-2.22	114.26	117.51
2	B	601	JUA	C11-C12-C7	2.16	122.05	120.29
3	A	602	MES	C8-C7-N4	-2.13	104.32	112.36
2	A	601	JUA	C12-C7-N4	-2.11	119.55	121.50
3	A	602	MES	C6-O1-C2	2.11	116.69	109.88
2	B	601	JUA	N1-C4-N8	2.08	124.05	116.90
2	A	601	JUA	N1-C4-N8	2.07	124.03	116.90
2	A	601	JUA	C11-C12-C7	2.05	121.96	120.29

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	JUA	S1-C13-C14-C15
3	A	603	MES	C8-C7-N4-C5
2	A	601	JUA	C25-C23-O5-C24
2	A	601	JUA	C22-C23-O5-C24
2	B	601	JUA	C14-C13-S1-O4
2	A	601	JUA	C16-C17-C18-C19
3	A	602	MES	C8-C7-N4-C3
2	A	601	JUA	C18-C19-C20-C21
2	B	601	JUA	C14-C13-S1-C12
2	A	601	JUA	N7-C17-C18-C19
2	B	601	JUA	C14-C13-S1-O2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

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

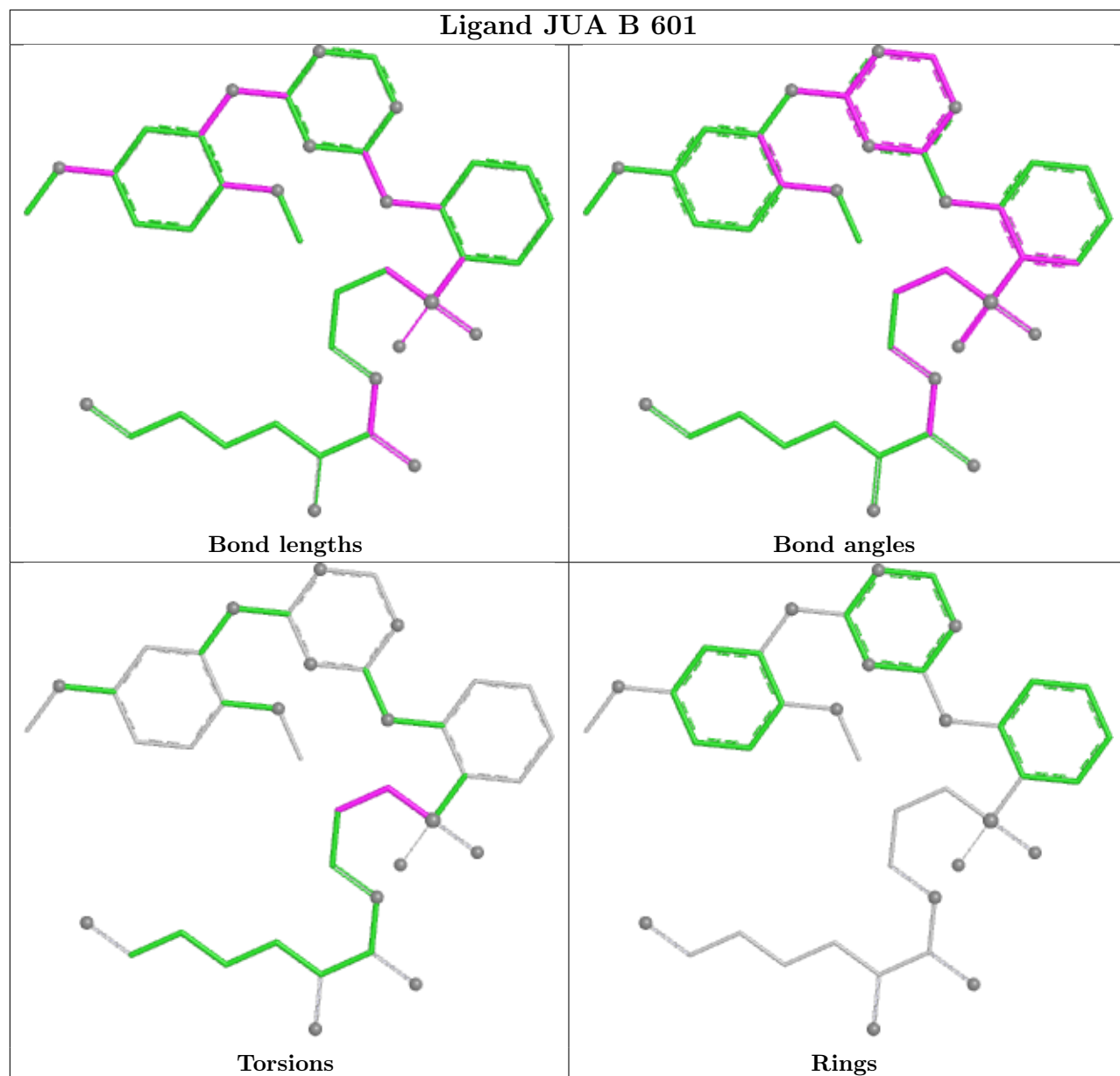
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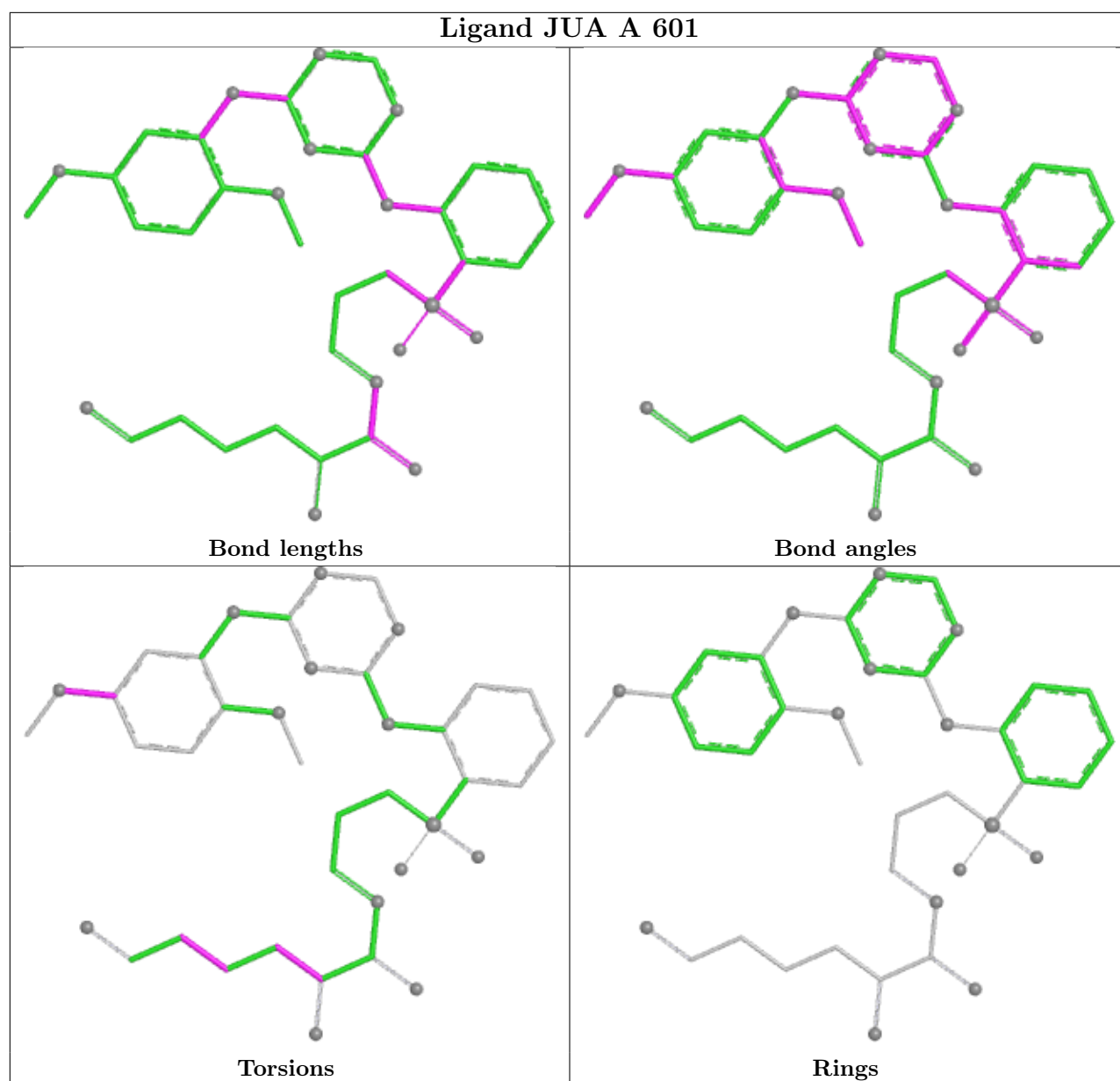
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	603	MES	2	0

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.

Ligand JUA B 601





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	481/516 (93%)	0.88	51 (10%)	11 13	35, 55, 84, 105	0
1	B	481/516 (93%)	0.84	45 (9%)	14 16	34, 56, 79, 101	0
All	All	962/1032 (93%)	0.86	96 (9%)	12 14	34, 55, 82, 105	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	282	ALA	5.4
1	A	518	PHE	5.1
1	A	230	THR	4.9
1	A	536	ASP	4.9
1	A	229	ASP	4.9
1	B	282	ALA	4.8
1	A	144	ALA	4.8
1	B	78	VAL	4.5
1	B	518	PHE	4.4
1	A	227	LEU	4.3
1	B	148	LYS	4.1
1	A	286	ASN	3.7
1	A	581	PRO	3.7
1	B	230	THR	3.5
1	B	387	ASN	3.5
1	B	147	GLN	3.5
1	B	99	ILE	3.4
1	A	142	VAL	3.4
1	A	225	TYR	3.3
1	A	143	SER	3.3
1	B	386	GLU	3.2
1	A	512	PHE	3.2
1	B	79	ASP	3.2
1	B	481	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	144	ALA	3.1
1	A	228	LYS	3.1
1	B	517	CYS	3.1
1	B	536	ASP	3.1
1	A	223	MET	3.1
1	A	420	ASP	3.0
1	B	229	ASP	3.0
1	A	538	ALA	2.8
1	B	287	ALA	2.8
1	B	131	THR	2.8
1	A	439	LEU	2.7
1	B	515	LYS	2.7
1	A	151	PHE	2.7
1	A	128	LEU	2.7
1	A	173	GLU	2.6
1	A	184	ILE	2.6
1	B	245	GLU	2.6
1	B	516	GLU	2.6
1	B	420	ASP	2.6
1	A	415	LEU	2.6
1	B	121	ASP	2.6
1	B	128	LEU	2.5
1	A	539	PHE	2.5
1	A	461	TYR	2.5
1	A	180	CYS	2.5
1	A	294	HIS	2.5
1	B	104	HIS	2.5
1	A	422	ASN	2.4
1	B	188	ASP	2.4
1	B	418	PRO	2.4
1	A	517	CYS	2.4
1	A	474	ILE	2.4
1	A	222	PRO	2.4
1	B	416	GLU	2.4
1	B	82	LEU	2.3
1	A	438	GLU	2.3
1	A	221	LEU	2.3
1	B	497	CYS	2.3
1	B	336	ASN	2.3
1	A	579	MET	2.3
1	A	580	ARG	2.3
1	A	147	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	174	LYS	2.3
1	A	199	SER	2.3
1	A	537	SER	2.3
1	A	149	LEU	2.2
1	A	478	LEU	2.2
1	B	334	ILE	2.2
1	A	245	GLU	2.2
1	A	437	ILE	2.2
1	B	512	PHE	2.2
1	A	200	LYS	2.2
1	B	578	THR	2.2
1	A	177	PHE	2.2
1	B	581	PRO	2.2
1	A	99	ILE	2.1
1	A	106	PHE	2.1
1	B	80	PRO	2.1
1	B	281	ILE	2.1
1	A	423	GLU	2.1
1	A	516	GLU	2.1
1	B	149	LEU	2.1
1	B	383	ASP	2.1
1	B	417	GLN	2.1
1	B	181	TYR	2.1
1	B	225	TYR	2.1
1	B	580	ARG	2.1
1	A	82	LEU	2.0
1	A	154	LEU	2.0
1	B	302	TYR	2.0
1	B	423	GLU	2.0
1	A	97	LYS	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

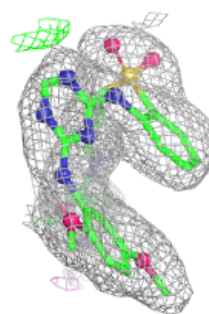
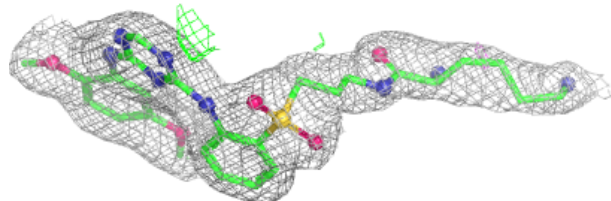
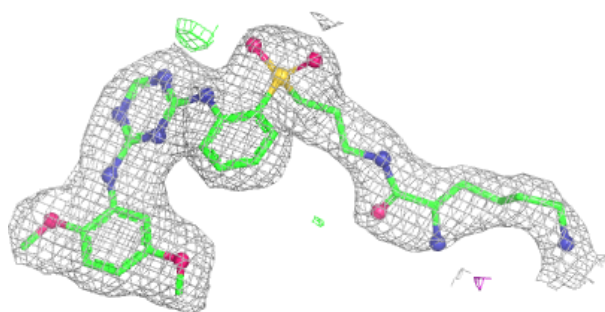
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

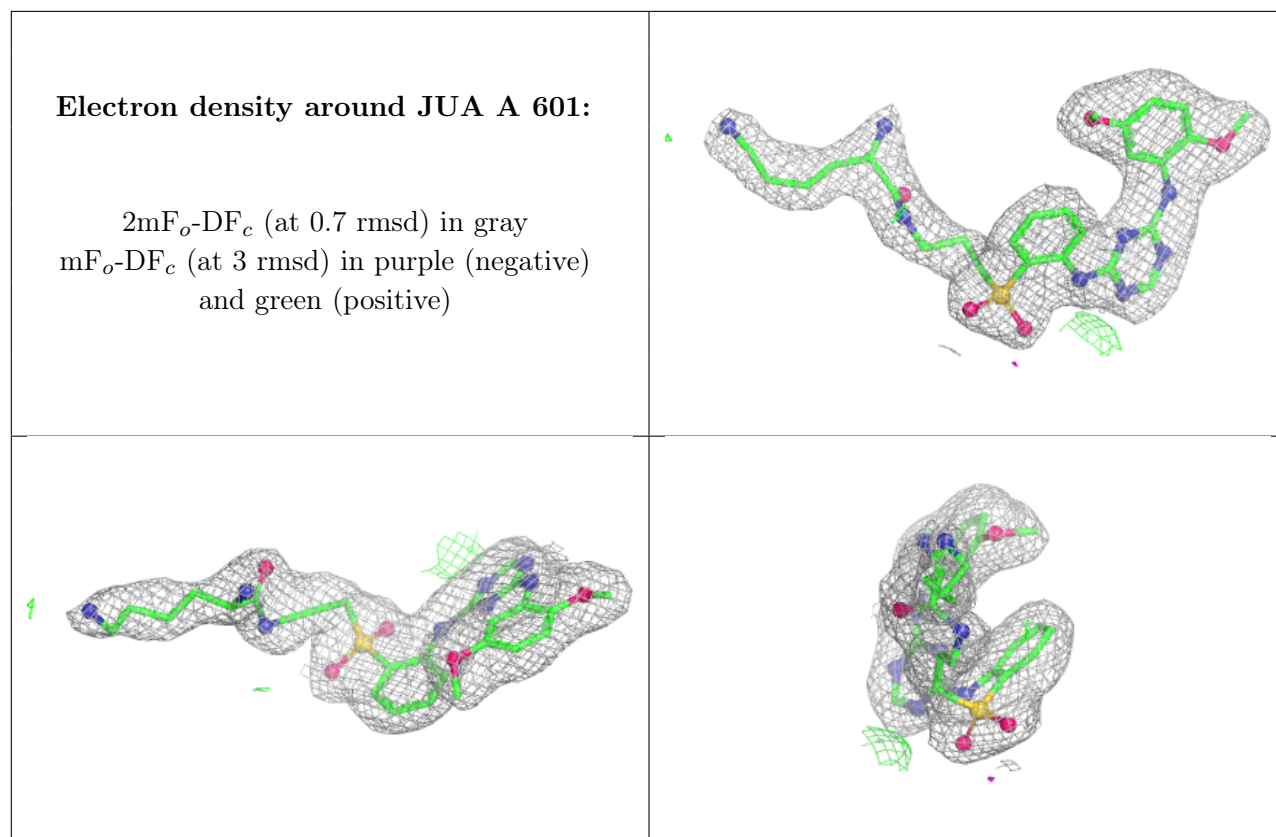
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MES	A	602	12/12	0.79	0.14	60,67,79,80	0
3	MES	A	603	12/12	0.89	0.11	52,58,66,67	0
2	JUA	B	601	40/40	0.93	0.10	44,52,60,61	0
2	JUA	A	601	40/40	0.95	0.09	36,43,53,55	0

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 JUA 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.