



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:54 PM UTC

PDB ID : 8K9U / pdb_00008k9u
Title : Crystal structure of plasmodium LysRS complexing with ASP3026 derived LysRS inhibitor 2 (ADKI2)
Authors : Zhou, J.; Xia, M.; Yang, G.; Li, P.; Fang, P.
Deposited on : 2023-08-01
Resolution : 2.83 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

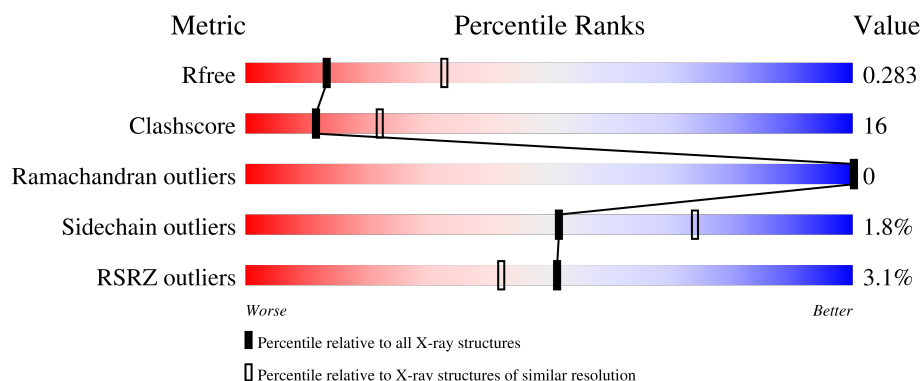
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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 5 unique types of molecules in this entry. The entry contains 7739 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.

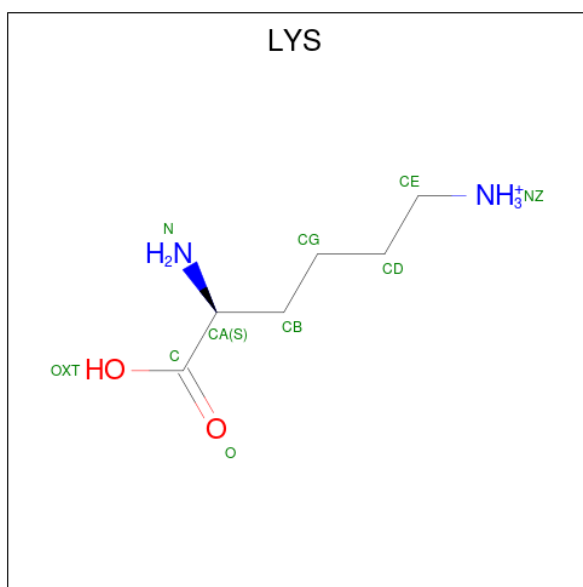
- Molecule 1 is a protein called Lysine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	486	Total	C	N	O	S	0	0	0
			3826	2465	634	711	16			
1	B	477	Total	C	N	O	S	0	0	0
			3725	2390	621	697	17			

There are 18 discrepancies between the modelled and reference sequences:

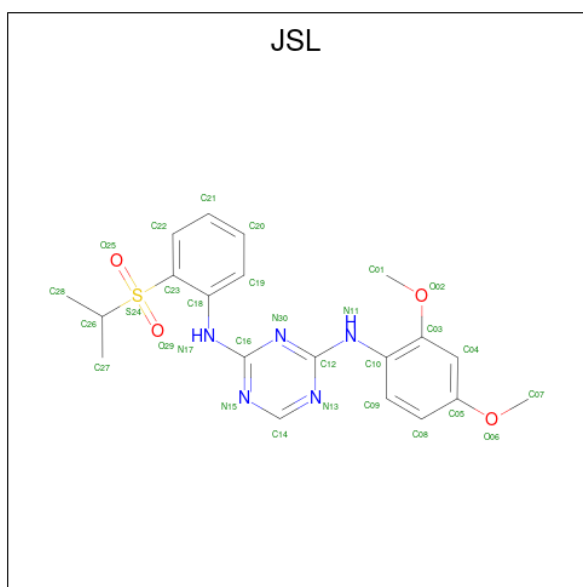
Chain	Residue	Modelled	Actual	Comment	Reference
A	76	MET	-	initiating methionine	UNP A0A024X378
A	584	GLY	-	expression tag	UNP A0A024X378
A	585	GLY	-	expression tag	UNP A0A024X378
A	586	HIS	-	expression tag	UNP A0A024X378
A	587	HIS	-	expression tag	UNP A0A024X378
A	588	HIS	-	expression tag	UNP A0A024X378
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 {N}4-(2,4-dimethoxyphenyl)- {N}2-(2-propan-2-ylsulfonylphenyl)-1,3,5-triazine-2,4-diamine (CCD ID: JSL) (formula: C₂₀H₂₃N₅O₄S) (labeled as "Ligand of Interest" by depositor).



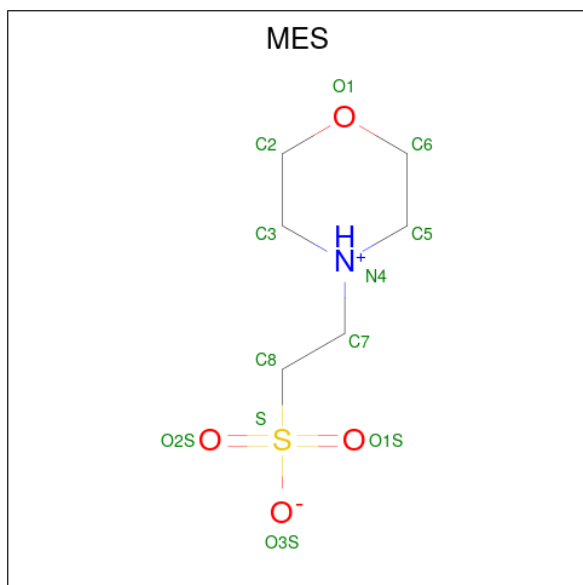
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			30	20	5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	0
			30	20	5	4	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		

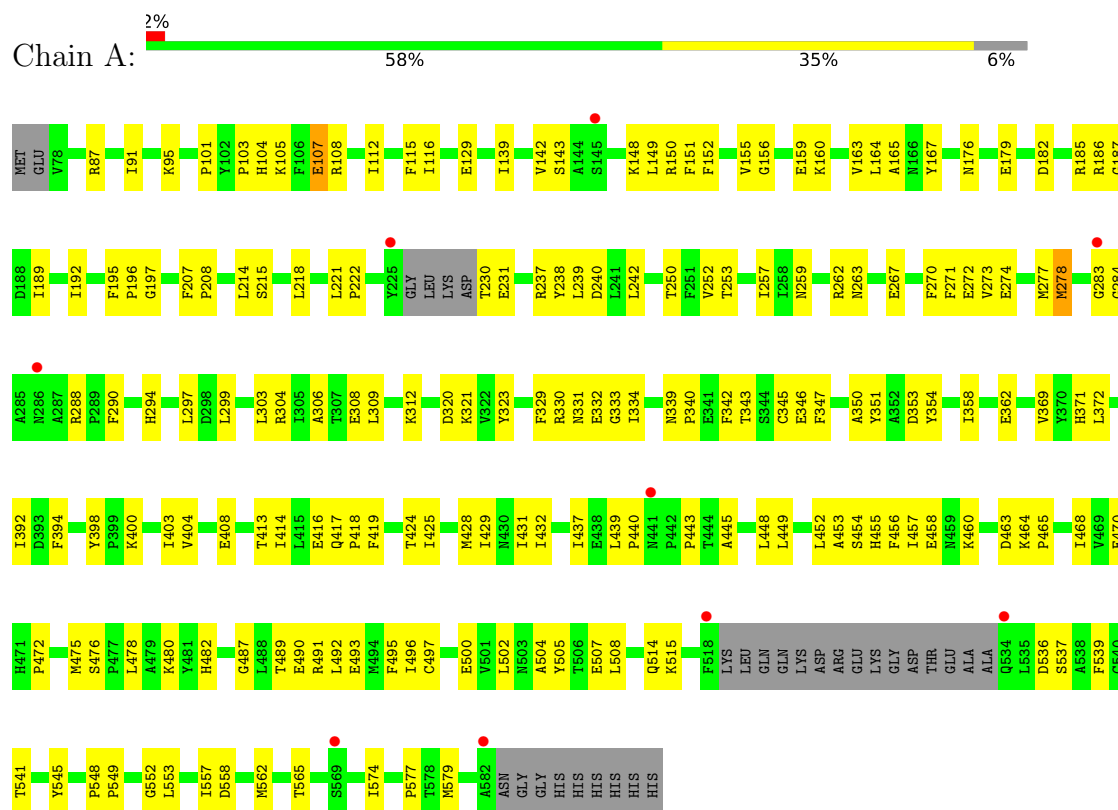
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		
5	B	38	Total	O	0	0
			38	38		

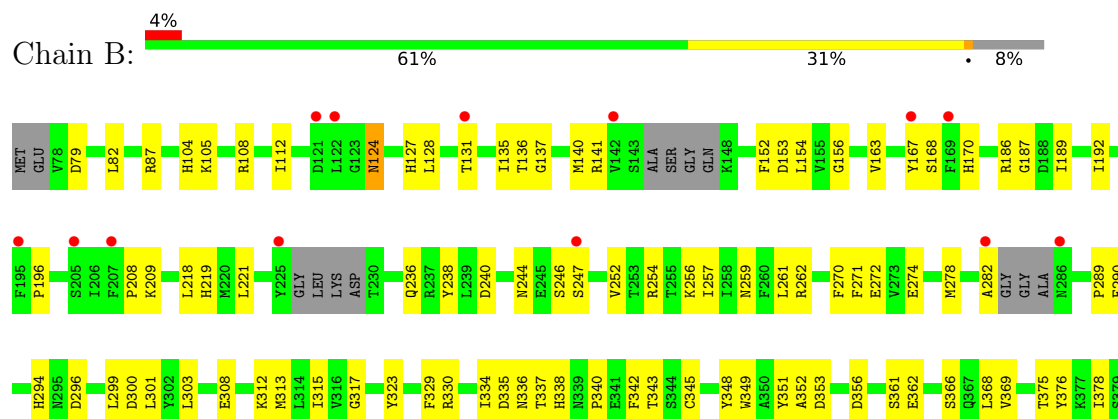
3 Residue-property plots

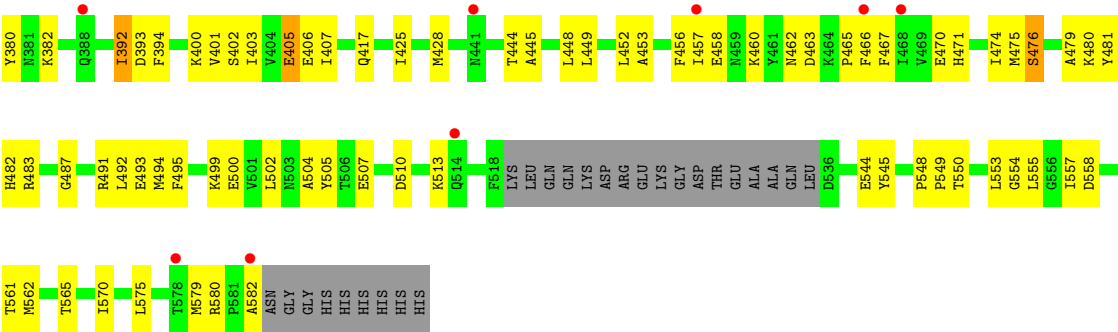
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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	69.72Å 92.26Å 162.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.74 – 2.83 46.74 – 2.83	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.74-2.83) 99.9 (46.74-2.83)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.05 (at 2.81Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.225 , 0.283 0.225 , 0.283	Depositor DCC
R_{free} test set	1252 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: JSL, 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	0.28	0/3921	0.42	0/5321
1	B	0.17	0/3812	0.40	0/5178
All	All	0.23	0/7733	0.41	0/10499

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	3826	0	3654	137	0
1	B	3725	0	3525	122	0
2	A	10	0	12	1	0
2	B	10	0	12	2	0
3	A	30	0	0	3	0
3	B	30	0	0	1	0
4	B	12	0	12	5	0
5	A	58	0	0	2	0
5	B	38	0	0	1	0
All	All	7739	0	7215	238	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 16.

All (238) 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:495:PHE:CE2	1:A:500:GLU:HG3	2.11	0.86
1:A:107:GLU:HA	4:B:601:MES:H62	1.61	0.83
1:B:192:ILE:HG23	1:B:208:PRO:HB3	1.63	0.81
1:A:152:PHE:HB2	1:A:163:VAL:HB	1.67	0.76
1:A:176:ASN:HB3	1:A:179:GLU:HB2	1.70	0.73
1:A:334:ILE:HG12	1:A:340:PRO:HD3	1.71	0.72
1:A:491:ARG:HA	1:A:505:TYR:HB3	1.71	0.72
1:A:104:HIS:HA	1:B:480:LYS:HE2	1.72	0.71
1:A:392:ILE:HD11	1:A:497:CYS:SG	2.31	0.70
1:B:257:ILE:HG12	1:B:368:LEU:HD11	1.72	0.70
1:A:182:ASP:O	1:A:185:ARG:NH2	2.24	0.70
1:A:548:PRO:HB3	1:B:189:ILE:HG21	1.73	0.69
1:B:406:GLU:HG2	1:B:457:ILE:HG23	1.73	0.69
1:A:439:LEU:HD11	1:A:443:PRO:HB3	1.74	0.68
1:A:257:ILE:HG12	1:A:372:LEU:HD11	1.74	0.68
1:B:337:THR:HG22	1:B:562:MET:HE1	1.75	0.68
1:B:502:LEU:HD11	1:B:553:LEU:HD11	1.77	0.67
1:A:189:ILE:HG22	1:A:214:LEU:HB2	1.77	0.66
1:B:112:ILE:HG12	1:B:135:ILE:HD11	1.78	0.66
1:B:167:TYR:HA	1:B:170:HIS:HB3	1.79	0.64
1:A:413:THR:HG21	1:A:431:ILE:HD11	1.79	0.63
1:A:492:LEU:HG	1:A:504:ALA:HB3	1.82	0.62
1:B:290:PHE:HB2	1:B:303:LEU:HB2	1.81	0.62
1:B:259:ASN:ND2	5:B:701:HOH:O	2.33	0.62
1:B:252:VAL:HG12	1:B:256:LYS:HE2	1.81	0.61
1:A:150:ARG:HB2	1:A:165:ALA:HB3	1.84	0.60
1:A:354:TYR:HB2	1:A:490:GLU:HB3	1.83	0.60
1:A:456:PHE:O	1:A:460:LYS:HE3	2.01	0.60
1:B:308:GLU:HG3	1:B:348:TYR:OH	2.02	0.60
1:B:79:ASP:HB3	1:B:82:LEU:HB3	1.84	0.59
1:B:353:ASP:OD1	1:B:356:ASP:N	2.31	0.59
1:A:449:LEU:HD13	1:A:472:PRO:HG2	1.84	0.59
1:B:407:ILE:HG13	1:B:457:ILE:HD11	1.84	0.59
1:A:253:THR:O	1:A:257:ILE:HG13	2.02	0.59
1:B:334:ILE:HG13	1:B:340:PRO:HD3	1.83	0.59
1:A:445:ALA:HA	1:A:448:LEU:HD12	1.84	0.58
1:A:502:LEU:HD11	1:A:553:LEU:HD11	1.84	0.58
1:B:378:ILE:HD11	1:B:392:ILE:HD12	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:LEU:HG	1:B:504:ALA:HB3	1.85	0.57
1:A:105:LYS:NZ	4:B:601:MES:O1	2.38	0.57
1:A:425:ILE:O	1:A:429:ILE:HG13	2.05	0.56
1:A:186:ARG:NH2	1:A:222:PRO:O	2.39	0.56
1:B:187:GLY:HA3	1:B:221:LEU:HD11	1.88	0.55
1:B:579:MET:HA	1:B:579:MET:HE3	1.88	0.55
1:B:428:MET:HG3	1:B:452:LEU:HD11	1.87	0.55
1:B:580:ARG:HH21	1:B:582:ALA:HA	1.72	0.55
3:B:603:JSL:O29	3:B:603:JSL:N17	2.40	0.55
1:A:274:GLU:OE2	1:B:254:ARG:NH2	2.38	0.54
1:A:139:ILE:O	1:A:187:GLY:N	2.34	0.54
1:A:312:LYS:NZ	1:A:507:GLU:OE1	2.37	0.54
1:B:491:ARG:HA	1:B:505:TYR:HB3	1.90	0.54
1:B:315:ILE:HG21	1:B:550:THR:HG21	1.90	0.53
1:A:237:ARG:NH1	1:A:240:ASP:OD2	2.40	0.53
1:A:320:ASP:HB3	1:A:350:ALA:HB3	1.91	0.53
1:A:351:TYR:N	1:A:549:PRO:O	2.32	0.53
1:A:192:ILE:HG23	1:A:208:PRO:HB3	1.91	0.53
1:B:453:ALA:O	1:B:458:GLU:HG3	2.09	0.53
1:A:262:ARG:NH1	1:A:272:GLU:OE2	2.41	0.53
1:A:417:GLN:OE1	1:A:487:GLY:HA3	2.10	0.52
1:A:493:GLU:HG3	1:A:502:LEU:O	2.09	0.52
1:B:362:GLU:OE2	1:B:400:LYS:NZ	2.26	0.52
1:A:470:GLU:OE2	1:A:482:HIS:NE2	2.43	0.52
1:A:536:ASP:HB3	1:A:539:PHE:H	1.74	0.52
1:B:402:SER:HB2	1:B:405:GLU:HG2	1.92	0.52
1:B:502:LEU:HD12	1:B:555:LEU:HD21	1.92	0.51
1:B:510:ASP:HB3	1:B:513:LYS:HB2	1.92	0.51
1:B:152:PHE:HB2	1:B:163:VAL:HB	1.92	0.51
1:B:337:THR:HG21	1:B:499:LYS:HG2	1.93	0.51
1:A:252:VAL:HA	1:B:271:PHE:CZ	2.45	0.51
3:A:602:JSL:N17	3:A:602:JSL:O29	2.44	0.51
1:B:221:LEU:HD12	1:B:221:LEU:H	1.75	0.51
1:B:240:ASP:OD1	1:B:244:ASN:ND2	2.31	0.51
1:A:290:PHE:HZ	1:B:294:HIS:HD2	1.58	0.50
1:A:458:GLU:HG2	1:A:495:PHE:CE2	2.46	0.50
1:A:330:ARG:HD2	3:A:602:JSL:C08	2.41	0.50
1:B:351:TYR:N	1:B:549:PRO:O	2.38	0.50
1:B:505:TYR:CZ	2:B:602:LYS:HE3	2.45	0.50
1:A:277:MET:HE3	1:A:329:PHE:HE2	1.76	0.50
1:A:332:GLU:HB2	3:A:602:JSL:C04	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:SER:O	1:A:541:THR:OG1	2.18	0.50
1:B:336:ASN:O	1:B:570:ILE:N	2.45	0.50
1:A:259:ASN:ND2	5:A:701:HOH:O	2.27	0.50
1:A:465:PRO:HB3	1:A:496:ILE:HG12	1.94	0.50
1:B:236:GLN:HB3	1:B:238:TYR:CZ	2.47	0.50
1:B:444:THR:O	1:B:448:LEU:HG	2.12	0.50
1:A:290:PHE:CZ	1:B:294:HIS:HD2	2.29	0.49
1:A:508:LEU:CD2	1:A:514:GLN:HB2	2.42	0.49
1:B:334:ILE:HD12	1:B:334:ILE:H	1.76	0.49
1:B:561:THR:O	1:B:565:THR:OG1	2.23	0.49
1:A:353:ASP:HB3	1:B:105:LYS:HD3	1.95	0.49
1:A:345:CYS:HB2	1:A:557:ILE:HD11	1.95	0.49
1:A:417:GLN:HA	1:A:418:PRO:C	2.36	0.49
1:A:294:HIS:NE2	1:B:340:PRO:HG2	2.27	0.49
1:A:297:LEU:HB3	1:A:299:LEU:HD12	1.93	0.49
1:A:369:VAL:HG21	1:A:394:PHE:CG	2.48	0.48
1:A:428:MET:HG2	1:A:452:LEU:HD11	1.94	0.48
1:B:290:PHE:CD2	1:B:329:PHE:HB3	2.48	0.48
1:A:333:GLY:HA2	1:B:296:ASP:OD2	2.12	0.48
1:B:369:VAL:HG12	1:B:375:THR:O	2.13	0.48
1:B:108:ARG:HB2	1:B:136:THR:HG23	1.96	0.48
1:B:382:LYS:NZ	1:B:462:ASN:OD1	2.47	0.48
1:A:108:ARG:NH2	4:B:601:MES:O1S	2.45	0.48
1:B:312:LYS:HD3	1:B:507:GLU:CD	2.39	0.47
1:A:455:HIS:O	1:A:460:LYS:NZ	2.43	0.47
1:B:294:HIS:CE1	1:B:296:ASP:HB2	2.49	0.47
1:A:343:THR:OG1	1:B:274:GLU:OE1	2.20	0.47
1:A:457:ILE:HG13	1:A:468:ILE:HD11	1.95	0.47
1:A:87:ARG:O	1:A:91:ILE:HG12	2.15	0.47
1:A:419:PHE:HA	1:A:424:THR:HG21	1.97	0.47
1:A:408:GLU:HG2	1:A:414:ILE:HA	1.96	0.47
1:B:343:THR:HB	1:B:557:ILE:HB	1.97	0.47
1:A:277:MET:HG3	1:B:329:PHE:HZ	1.80	0.47
1:B:494:MET:HB2	1:B:502:LEU:HD22	1.97	0.47
1:B:124:ASN:OD1	1:B:124:ASN:N	2.48	0.46
1:B:254:ARG:HB2	1:B:561:THR:HG21	1.96	0.46
1:B:299:LEU:HD12	1:B:300:ASP:H	1.79	0.46
1:B:137:GLY:HA3	1:B:154:LEU:HG	1.97	0.46
1:A:277:MET:HE3	1:A:329:PHE:CE2	2.50	0.46
1:A:330:ARG:HG3	1:A:342:PHE:HE1	1.81	0.46
1:A:103:PRO:HD2	1:A:214:LEU:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:VAL:HG12	1:A:160:LYS:HG3	1.98	0.46
1:A:218:LEU:HD12	1:B:544:GLU:HA	1.98	0.46
1:A:231:GLU:HB3	1:A:579:MET:HE1	1.98	0.46
1:B:278:MET:HE3	1:B:301:LEU:HD12	1.97	0.46
1:B:475:MET:HE2	1:B:475:MET:HB3	1.85	0.46
1:A:416:GLU:O	1:A:424:THR:OG1	2.33	0.45
1:A:288:ARG:O	1:A:331:ASN:N	2.44	0.45
1:A:470:GLU:HA	1:A:489:THR:O	2.16	0.45
1:B:452:LEU:HD23	1:B:456:PHE:HE2	1.81	0.45
1:A:263:ASN:O	1:A:267:GLU:HG3	2.15	0.45
1:A:271:PHE:CZ	1:B:252:VAL:HA	2.51	0.45
1:B:329:PHE:HA	1:B:340:PRO:O	2.15	0.45
1:B:470:GLU:OE2	1:B:482:HIS:NE2	2.46	0.45
1:A:439:LEU:HD12	1:A:440:PRO:HD2	1.97	0.45
1:B:499:LYS:HA	1:B:499:LYS:HD2	1.75	0.45
1:A:472:PRO:HD2	1:A:475:MET:SD	2.56	0.45
1:B:244:ASN:C	1:B:246:SER:H	2.25	0.45
1:A:574:ILE:O	1:A:577:PRO:HD3	2.17	0.45
1:B:366:SER:HB2	1:B:376:TYR:CE1	2.52	0.45
1:B:463:ASP:OD1	1:B:463:ASP:N	2.38	0.45
1:B:580:ARG:O	1:B:580:ARG:HG3	2.17	0.45
1:A:508:LEU:HD21	1:A:514:GLN:HB2	1.97	0.45
1:A:189:ILE:HG21	1:B:548:PRO:HB3	1.99	0.44
1:A:221:LEU:HD23	1:A:221:LEU:HA	1.83	0.44
1:A:290:PHE:HB2	1:A:303:LEU:HB2	1.99	0.44
1:A:91:ILE:O	1:A:95:LYS:HG3	2.18	0.44
1:B:127:HIS:C	1:B:128:LEU:HD12	2.42	0.44
1:A:347:PHE:CE2	1:A:553:LEU:HB3	2.52	0.44
1:A:284:GLY:HA3	1:A:306:ALA:HB3	1.99	0.44
1:B:425:ILE:HD11	1:B:445:ALA:HB2	2.00	0.44
1:A:362:GLU:HA	1:A:398:TYR:CE2	2.52	0.44
1:A:91:ILE:HG23	1:A:101:PRO:HG2	2.00	0.44
1:A:104:HIS:NE2	1:B:481:TYR:O	2.50	0.44
1:B:154:LEU:HD12	1:B:154:LEU:HA	1.89	0.44
1:A:250:THR:HG23	1:A:565:THR:HB	1.99	0.44
1:A:493:GLU:HA	1:A:502:LEU:O	2.17	0.44
1:A:270:PHE:HB3	1:A:323:TYR:HD1	1.83	0.43
1:A:552:GLY:C	2:A:601:LYS:HE2	2.43	0.43
1:A:112:ILE:O	1:A:116:ILE:HG13	2.18	0.43
1:A:143:SER:OG	1:A:151:PHE:HB2	2.19	0.43
1:A:242:LEU:HG	1:B:317:GLY:HA2	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:GLN:HG3	1:A:515:LYS:O	2.17	0.43
1:A:197:GLY:HA3	1:A:207:PHE:HE2	1.83	0.43
1:B:140:MET:O	1:B:186:ARG:NH1	2.46	0.43
1:B:270:PHE:HB3	1:B:323:TYR:CD1	2.53	0.43
1:B:401:VAL:HG21	1:B:460:LYS:HD3	2.01	0.43
1:A:150:ARG:NH1	5:A:708:HOH:O	2.51	0.43
1:A:270:PHE:HB3	1:A:323:TYR:CD1	2.54	0.43
1:B:170:HIS:HA	1:B:209:LYS:HA	1.99	0.43
1:A:403:ILE:HG23	1:A:404:VAL:HG23	2.00	0.43
1:B:476:SER:HB2	1:B:479:ALA:HB3	2.00	0.43
4:B:601:MES:H51	4:B:601:MES:H81	1.64	0.43
1:A:303:LEU:HB3	1:A:329:PHE:CD2	2.54	0.43
1:B:369:VAL:HG21	1:B:394:PHE:CG	2.54	0.43
1:B:548:PRO:O	1:B:550:THR:HG23	2.19	0.43
1:A:270:PHE:HA	1:A:321:LYS:HB3	1.99	0.43
1:A:463:ASP:OD1	1:A:464:LYS:HG2	2.18	0.43
1:A:358:ILE:HD12	1:A:400:LYS:HD2	2.00	0.42
1:A:419:PHE:CD2	1:A:472:PRO:HB3	2.54	0.42
1:B:467:PHE:CE1	1:B:494:MET:HG3	2.54	0.42
1:A:142:VAL:HG13	1:A:152:PHE:CE2	2.54	0.42
1:A:303:LEU:HD21	1:B:303:LEU:HD11	2.01	0.42
1:A:339:ASN:ND2	1:A:340:PRO:HD2	2.34	0.42
1:A:428:MET:HG2	1:A:452:LEU:CD1	2.48	0.42
1:B:335:ASP:OD1	1:B:338:HIS:N	2.46	0.42
1:B:349:TRP:NE1	4:B:601:MES:O2S	2.52	0.42
1:B:417:GLN:OE1	1:B:487:GLY:HA3	2.20	0.42
1:A:238:TYR:HB3	1:B:313:MET:O	2.20	0.42
1:A:283:GLY:HA3	1:A:309:LEU:HD11	2.01	0.42
1:A:545:TYR:CE1	1:B:219:HIS:HB2	2.55	0.42
1:B:345:CYS:O	1:B:554:GLY:HA2	2.20	0.42
1:B:403:ILE:HG21	1:B:471:HIS:HA	2.02	0.42
1:A:115:PHE:CE2	1:A:196:PRO:HB3	2.55	0.42
1:A:278:MET:HG2	1:A:303:LEU:HD23	2.00	0.42
1:B:141:ARG:HB3	1:B:153:ASP:HB2	2.02	0.42
1:B:254:ARG:NH2	1:B:343:THR:OG1	2.53	0.42
1:B:308:GLU:OE1	2:B:602:LYS:N	2.52	0.42
1:A:112:ILE:HD12	1:A:156:GLY:N	2.35	0.42
1:A:454:SER:HA	1:A:458:GLU:CD	2.44	0.42
1:B:330:ARG:HG3	1:B:342:PHE:HE1	1.84	0.42
1:B:466:PHE:CE1	1:B:495:PHE:HB2	2.54	0.42
1:A:371:HIS:HD2	1:A:372:LEU:HD23	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:MET:HE2	1:B:428:MET:HB2	1.91	0.42
1:A:432:ILE:HG23	1:A:437:ILE:O	2.20	0.42
1:A:164:LEU:HB3	1:A:207:PHE:CD1	2.55	0.41
1:B:262:ARG:NH1	1:B:272:GLU:OE2	2.53	0.41
1:B:393:ASP:O	1:B:465:PRO:HD2	2.20	0.41
1:B:449:LEU:HD12	1:B:474:ILE:HD11	2.01	0.41
1:A:271:PHE:CE1	1:B:252:VAL:HA	2.55	0.41
1:A:456:PHE:C	1:A:460:LYS:HE3	2.44	0.41
1:A:290:PHE:CD2	1:A:329:PHE:HB3	2.55	0.41
1:A:362:GLU:HG2	1:A:398:TYR:CD2	2.56	0.41
1:B:282:ALA:HB2	1:B:289:PRO:HB3	2.01	0.41
1:B:335:ASP:CG	1:B:338:HIS:HD1	2.29	0.41
1:B:495:PHE:CE2	1:B:500:GLU:HB2	2.56	0.41
1:A:480:LYS:HE3	1:B:104:HIS:HA	2.02	0.41
1:B:112:ILE:HD12	1:B:156:GLY:N	2.35	0.41
1:B:361:SER:HB2	1:B:467:PHE:HZ	1.86	0.41
1:A:558:ASP:O	1:A:562:MET:HG3	2.21	0.41
1:B:460:LYS:HB2	1:B:460:LYS:HE3	1.79	0.41
1:A:129:GLU:HA	1:A:195:PHE:CG	2.56	0.41
1:A:308:GLU:OE2	1:A:312:LYS:NZ	2.40	0.41
1:B:380:TYR:HB3	1:B:392:ILE:HD11	2.03	0.41
1:A:116:ILE:HD12	1:A:159:GLU:HB3	2.03	0.41
1:A:148:LYS:HG3	1:A:167:TYR:CD2	2.56	0.41
1:A:189:ILE:HB	1:A:215:SER:HB3	2.03	0.41
1:A:239:LEU:HD21	1:B:545:TYR:CD1	2.56	0.41
1:B:261:LEU:HD21	1:B:345:CYS:SG	2.61	0.41
1:A:453:ALA:O	1:A:457:ILE:HG12	2.21	0.40
1:B:87:ARG:HG2	1:B:218:LEU:HD23	2.03	0.40
1:A:277:MET:HA	1:A:304:ARG:HG2	2.03	0.40
1:B:131:THR:HG23	1:B:196:PRO:HD2	2.03	0.40
1:A:277:MET:HG3	1:B:329:PHE:CZ	2.56	0.40
1:A:346:GLU:HA	1:A:553:LEU:O	2.21	0.40
1:A:149:LEU:HD22	1:A:151:PHE:CE1	2.56	0.40
1:A:273:VAL:HB	1:B:575:LEU:CD1	2.51	0.40
1:B:349:TRP:CG	1:B:352:ALA:HB2	2.56	0.40
1:B:548:PRO:HG2	1:B:550:THR:HG22	2.03	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	480/516 (93%)	473 (98%)	7 (2%)	0	100	100
1	B	467/516 (90%)	453 (97%)	14 (3%)	0	100	100
All	All	947/1032 (92%)	926 (98%)	21 (2%)	0	100	100

There are no Ramachandran outliers to report.

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%)	398 (99%)	5 (1%)	63	80
1	B	390/464 (84%)	381 (98%)	9 (2%)	44	68
All	All	793/928 (86%)	779 (98%)	14 (2%)	51	74

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

Mol	Chain	Res	Type
1	A	107	GLU
1	A	230	THR
1	A	278	MET
1	A	476	SER
1	A	478	LEU
1	B	124	ASN
1	B	168	SER
1	B	247	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	392	ILE
1	B	405	GLU
1	B	476	SER
1	B	483	ARG
1	B	493	GLU
1	B	558	ASP

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	295	ASN
1	A	339	ASN
1	A	371	HIS
1	A	459	ASN
1	A	462	ASN
1	A	568	ASN
1	B	263	ASN
1	B	339	ASN
1	B	435	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](#)

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
4	MES	B	601	-	12,12,12	2.30	1 (8%)	15,16,16	2.27	5 (33%)
3	JSL	B	603	-	32,32,32	6.25	7 (21%)	39,45,45	3.93	10 (25%)
3	JSL	A	602	-	32,32,32	6.31	6 (18%)	39,45,45	3.66	11 (28%)
2	LYS	B	602	-	8,9,9	0.83	1 (12%)	7,10,10	1.03	1 (14%)
2	LYS	A	601	-	8,9,9	0.84	1 (12%)	7,10,10	1.07	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MES	B	601	-	-	2/6/14/14	0/1/1/1
3	JSL	B	603	-	-	10/24/24/24	0/3/3/3
3	JSL	A	602	-	-	7/24/24/24	0/3/3/3
2	LYS	B	602	-	-	2/9/9/9	-
2	LYS	A	601	-	-	0/9/9/9	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	JSL	O25-S24	24.72	1.65	1.44
3	B	603	JSL	O29-S24	24.46	1.65	1.44
3	A	602	JSL	O29-S24	24.24	1.65	1.44
3	B	603	JSL	O25-S24	23.98	1.65	1.44
4	B	601	MES	C8-S	-7.71	1.66	1.77
3	A	602	JSL	C12-N11	4.68	1.46	1.36
3	B	603	JSL	C12-N11	4.66	1.46	1.36
3	A	602	JSL	C16-N17	4.57	1.46	1.36
3	B	603	JSL	C16-N17	4.54	1.46	1.36
3	A	602	JSL	C18-N17	2.35	1.46	1.39
3	A	602	JSL	C10-N11	2.33	1.46	1.39
3	B	603	JSL	C10-N11	2.33	1.46	1.39
2	A	601	LYS	OXT-C	-2.23	1.23	1.30
3	B	603	JSL	C18-N17	2.22	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	602	LYS	OXT-C	-2.20	1.23	1.30
3	B	603	JSL	C23-S24	2.03	1.82	1.78

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	JSL	O29-S24-O25	-12.28	107.61	118.72
3	B	603	JSL	C14-N13-C12	10.85	120.21	113.27
3	B	603	JSL	C14-N15-C16	10.68	120.09	113.27
3	A	602	JSL	C14-N15-C16	10.53	120.00	113.27
3	A	602	JSL	O29-S24-O25	-9.92	109.75	118.72
3	A	602	JSL	C14-N13-C12	9.64	119.43	113.27
3	A	602	JSL	N15-C16-N30	-7.75	118.93	126.42
3	A	602	JSL	N13-C12-N30	-7.38	119.28	126.42
3	B	603	JSL	N13-C12-N30	-7.28	119.38	126.42
3	B	603	JSL	N15-C16-N30	-7.01	119.65	126.42
3	B	603	JSL	N15-C14-N13	-5.53	120.21	128.58
4	B	601	MES	C5-N4-C3	5.22	120.08	108.84
3	A	602	JSL	N15-C14-N13	-5.09	120.88	128.58
3	B	603	JSL	O25-S24-C23	4.69	116.34	107.81
3	B	603	JSL	C23-C18-N17	-4.29	117.54	121.50
3	A	602	JSL	C16-N30-C12	4.25	121.47	113.85
3	A	602	JSL	O02-C03-C10	4.04	119.84	114.81
3	B	603	JSL	C16-N30-C12	3.69	120.45	113.85
3	A	602	JSL	C23-C18-N17	-3.42	118.34	121.50
4	B	601	MES	C7-N4-C3	3.35	120.16	111.24
4	B	601	MES	C7-N4-C5	3.19	119.74	111.24
4	B	601	MES	O3S-S-C8	2.87	111.62	106.00
3	B	603	JSL	O02-C03-C10	2.83	118.34	114.81
2	A	601	LYS	OXT-C-O	-2.65	118.08	124.08
2	B	602	LYS	OXT-C-O	-2.59	118.22	124.08
3	A	602	JSL	C01-O02-C03	-2.43	113.94	117.51
3	A	602	JSL	O02-C03-C04	-2.22	120.25	124.08
4	B	601	MES	C2-C3-N4	-2.10	106.93	110.12

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	JSL	C22-C23-S24-O25
3	A	602	JSL	C22-C23-S24-O29
3	A	602	JSL	C18-C23-S24-O25

Continued on next page...

Continued from previous page...

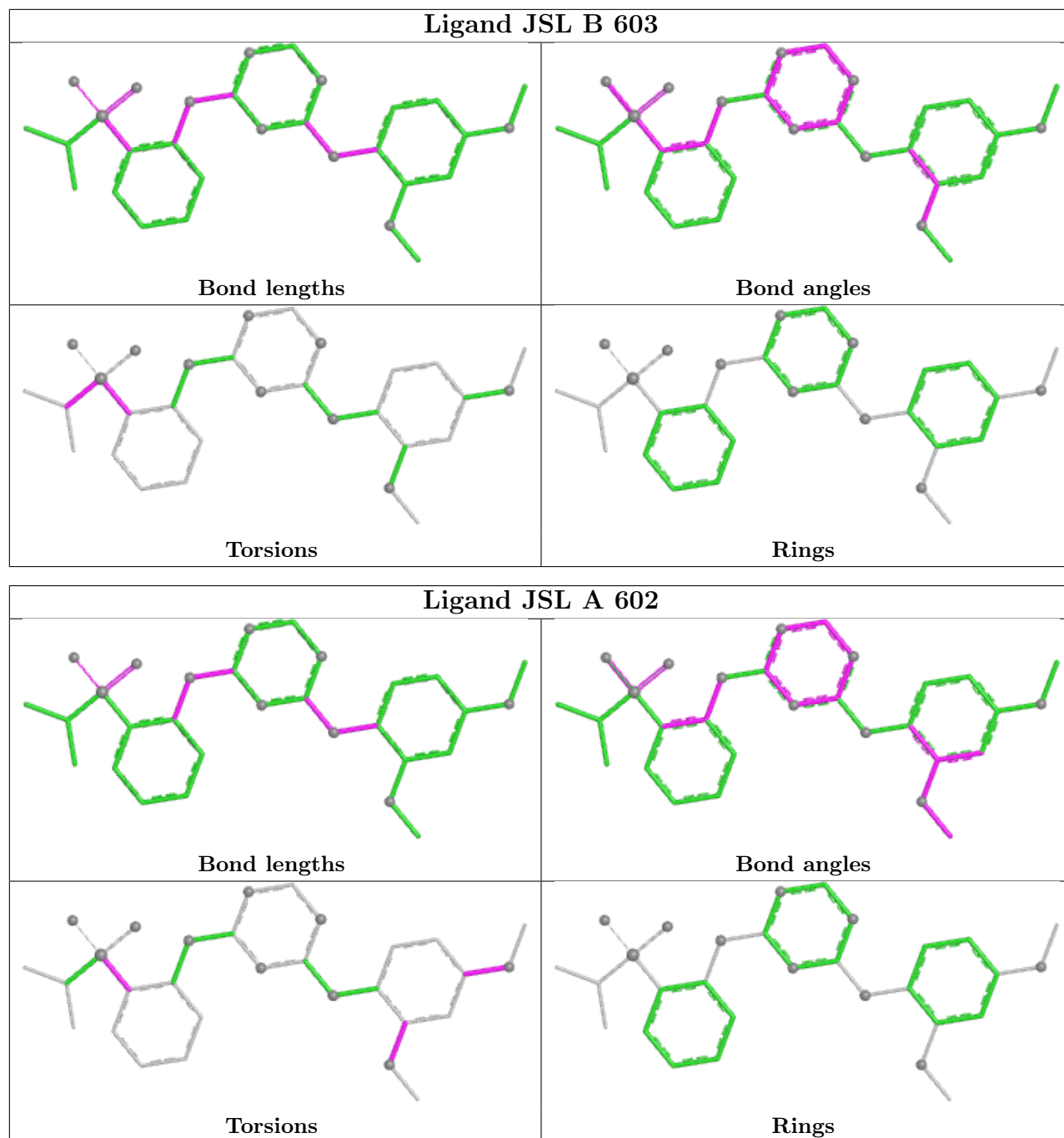
Mol	Chain	Res	Type	Atoms
3	A	602	JSL	C18-C23-S24-O29
3	B	603	JSL	C28-C26-S24-C23
3	B	603	JSL	C28-C26-S24-O25
3	B	603	JSL	C28-C26-S24-O29
3	B	603	JSL	C27-C26-S24-C23
3	B	603	JSL	C27-C26-S24-O25
3	B	603	JSL	C27-C26-S24-O29
3	B	603	JSL	C22-C23-S24-O25
3	B	603	JSL	C18-C23-S24-O25
3	A	602	JSL	C10-C03-O02-C01
3	A	602	JSL	C04-C03-O02-C01
2	B	602	LYS	CA-CB-CG-CD
2	B	602	LYS	CG-CD-CE-NZ
4	B	601	MES	C8-C7-N4-C3
4	B	601	MES	N4-C7-C8-S
3	B	603	JSL	C22-C23-S24-O29
3	B	603	JSL	C18-C23-S24-O29
3	A	602	JSL	C04-C05-O06-C07

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	MES	5	0
3	B	603	JSL	1	0
3	A	602	JSL	3	0
2	B	602	LYS	2	0
2	A	601	LYS	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	486/516 (94%)	0.14	9 (1%) 66 59	36, 62, 98, 127	0
1	B	477/516 (92%)	0.39	21 (4%) 39 30	37, 74, 130, 224	0
All	All	963/1032 (93%)	0.26	30 (3%) 51 42	36, 67, 117, 224	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	282	ALA	3.9
1	B	225	TYR	3.9
1	B	457	ILE	3.7
1	A	225	TYR	3.7
1	A	518	PHE	3.6
1	A	582	ALA	3.4
1	B	167	TYR	3.3
1	B	582	ALA	2.9
1	B	207	PHE	2.9
1	A	145	SER	2.7
1	B	286	ASN	2.7
1	B	169	PHE	2.6
1	B	466	PHE	2.6
1	B	142	VAL	2.6
1	B	578	THR	2.5
1	B	205	SER	2.5
1	A	286	ASN	2.5
1	B	121	ASP	2.4
1	B	247	SER	2.4
1	B	468	ILE	2.3
1	A	441	ASN	2.3
1	B	388	GLN	2.3
1	A	569	SER	2.3
1	B	122	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	441	ASN	2.2
1	B	195	PHE	2.2
1	A	283	GLY	2.1
1	A	534	GLN	2.1
1	B	131	THR	2.0
1	B	514	GLN	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](#)

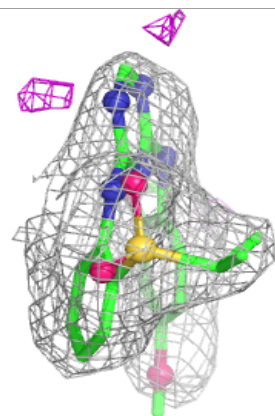
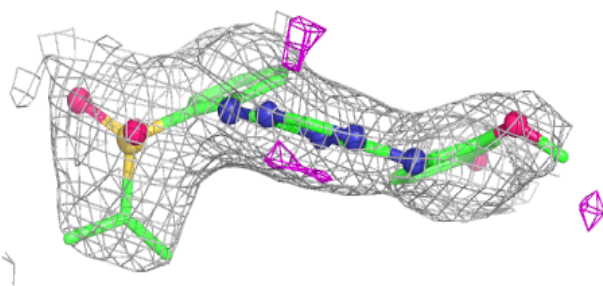
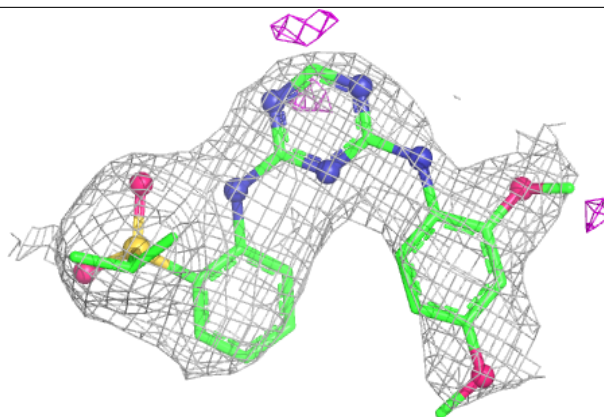
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	LYS	B	602	10/10	0.83	0.16	58,71,82,84	0
3	JSL	A	602	30/30	0.93	0.12	40,55,80,85	0
3	JSL	B	603	30/30	0.93	0.09	52,60,68,80	0
4	MES	B	601	12/12	0.93	0.11	47,56,64,65	0
2	LYS	A	601	10/10	0.94	0.09	38,39,44,44	0

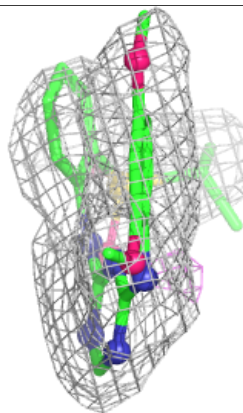
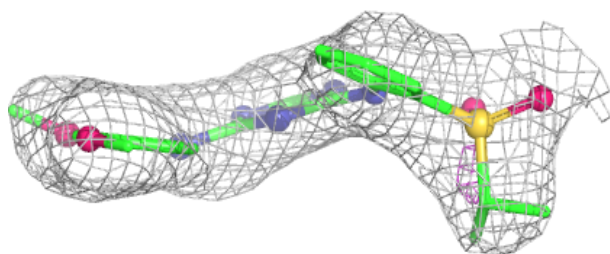
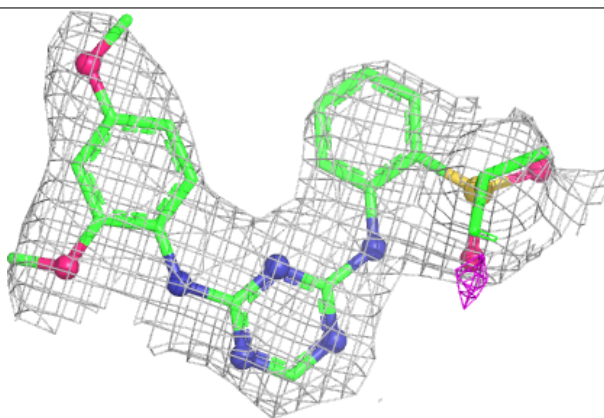
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JSL 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 JSL B 603:**

$2mF_o-DF_c$ (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.