



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2024 – 02:07 PM JST

PDB ID : 8K9U  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : 1.13  
EDS : 2.37.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

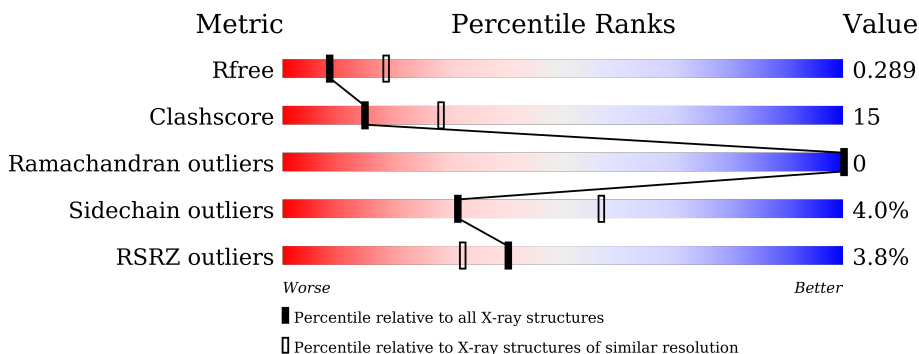
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

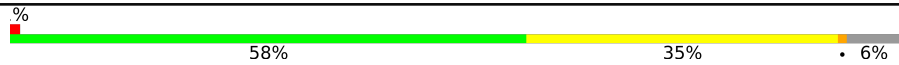

The reported resolution of this entry is 2.83 Å.

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))
$R_{free}$	130704	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (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  $\geq 3$ , 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	 % 58% 35% • 6%
1	B	516	 6% 61% 30% • 8%

## 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
			Total	C	N	O	S			
1	A	486	3826	2465	634	711	16	0	0	0
1	B	477	3725	2390	621	697	17	0	0	0

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

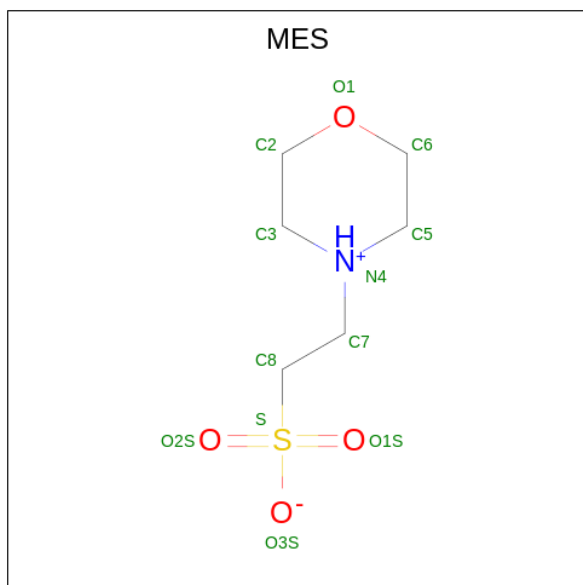
- Molecule 2 is LYSINE (three-letter code: LYS) (formula: C<sub>6</sub>H<sub>15</sub>N<sub>2</sub>O<sub>2</sub>).



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

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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

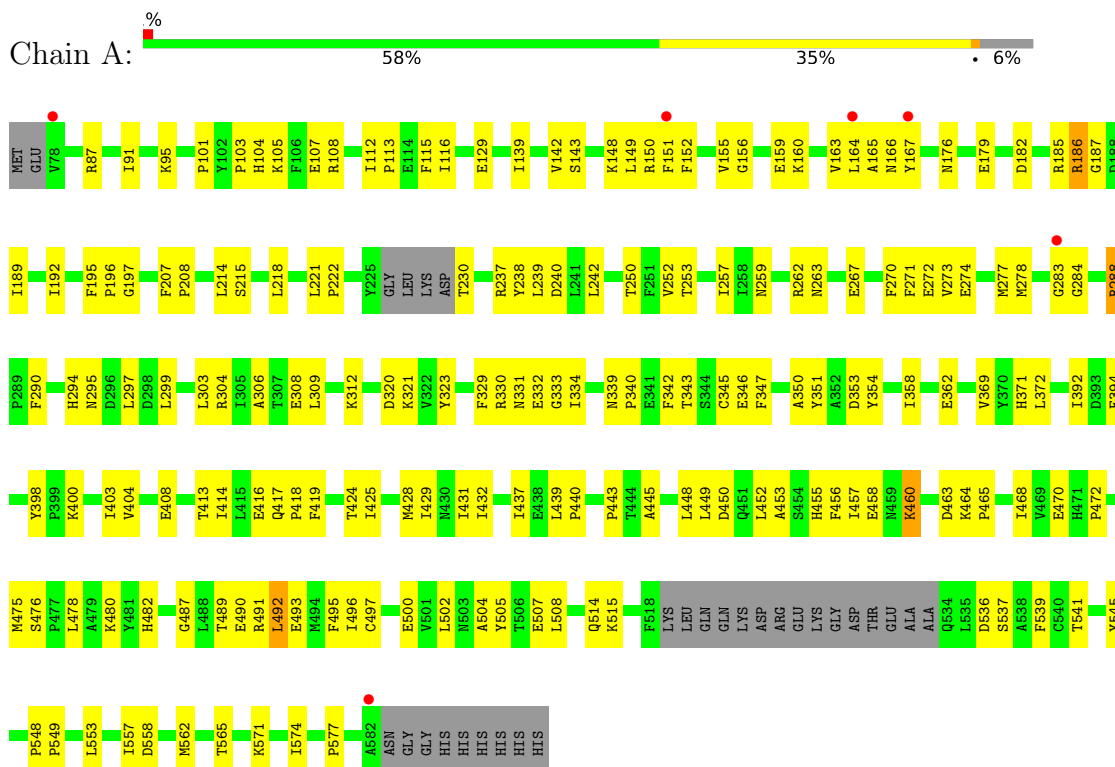
- Molecule 5 is water.

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

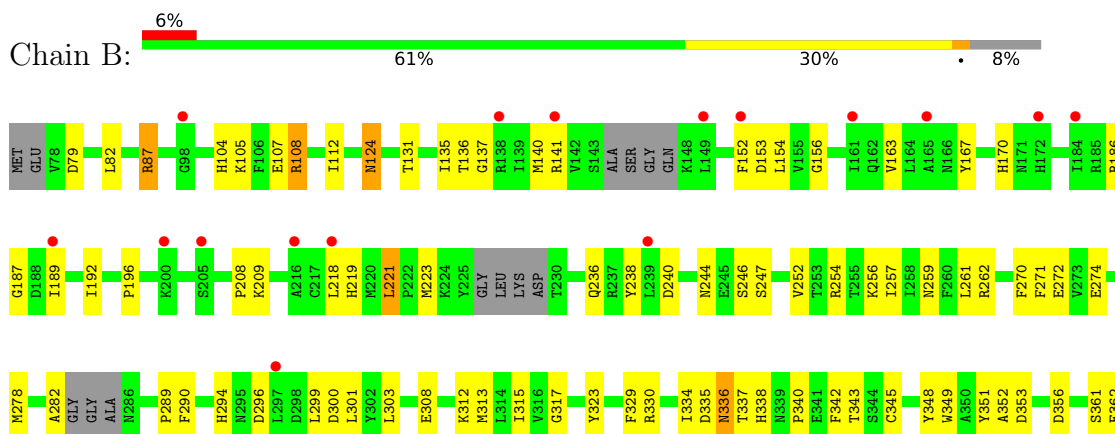
### 3 Residue-property plots i

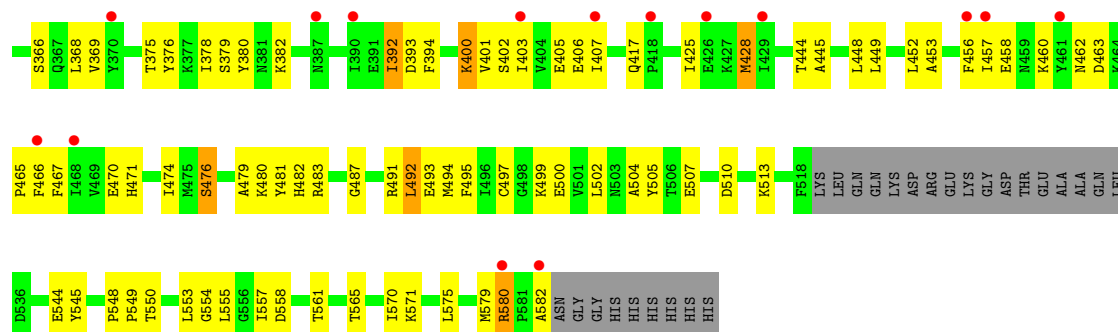
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.81Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.225 , 0.283 0.230 , 0.289	Depositor DCC
$R_{free}$ test set	1252 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtrriage
Anisotropy	0.010	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 37.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	7739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, JSL

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	0.31	0/3921	0.52	0/5321
1	B	0.28	0/3812	0.52	0/5178
All	All	0.30	0/7733	0.52	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 [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	3826	0	3654	130	0
1	B	3725	0	3525	118	0
2	A	10	0	12	0	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	227	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 15.

All (227) 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: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
1:B:492:LEU:HG	1:B:504:ALA:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:380:TYR:HD2	1:B:497:CYS:HG	1.56	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:332:GLU:HB2	3:A:602:JSL:C04	2.42	0.50
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:579:MET:HA	1:B:579:MET:HE3	1.94	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: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: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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:417:GLN:HA	1:A:418:PRO:C	2.36	0.44
1:A:91:ILE:O	1:A:95:LYS:HG3	2.18	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: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
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:312:LYS:HD3	1:B:507:GLU:CD	2.39	0.43
1:B:476:SER:HB2	1:B:479:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:THR:O	1:B:565:THR:OG1	2.23	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: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
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: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:495:PHE:CE2	1:B:500:GLU:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:278:MET:HE3	1:B:301:LEU:HD12	2.02	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:B:244:ASN:C	1:B:246:SER:H	2.25	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 [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	480/516 (93%)	473 (98%)	7 (2%)	0	<a href="#">100</a> <a href="#">100</a>

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [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	403/464 (87%)	390 (97%)	13 (3%)	39	63
1	B	390/464 (84%)	371 (95%)	19 (5%)	25	47
All	All	793/928 (86%)	761 (96%)	32 (4%)	31	57

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	113	PRO
1	A	166	ASN
1	A	186	ARG
1	A	230	THR
1	A	288	ARG
1	A	295	ASN
1	A	416	GLU
1	A	450	ASP
1	A	460	LYS
1	A	476	SER
1	A	478	LEU
1	A	492	LEU
1	A	571	LYS
1	B	87	ARG
1	B	107	GLU
1	B	108	ARG
1	B	124	ASN
1	B	221	LEU

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Mol	Chain	Res	Type
1	B	223	MET
1	B	247	SER
1	B	336	ASN
1	B	379	SER
1	B	392	ILE
1	B	400	LYS
1	B	428	MET
1	B	476	SER
1	B	483	ARG
1	B	492	LEU
1	B	493	GLU
1	B	558	ASP
1	B	571	LYS
1	B	580	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	295	ASN
1	A	339	ASN
1	A	371	HIS
1	B	263	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides 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
3	JSL	B	603	-	31,32,32	6.15	7 (22%)	40,45,45	3.52	11 (27%)
2	LYS	B	602	-	8,9,9	0.80	1 (12%)	9,10,10	1.17	2 (22%)
2	LYS	A	601	-	8,9,9	0.81	1 (12%)	9,10,10	1.21	2 (22%)
3	JSL	A	602	-	31,32,32	6.22	6 (19%)	40,45,45	2.97	12 (30%)
4	MES	B	601	-	12,12,12	2.25	1 (8%)	14,16,16	2.38	5 (35%)

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	JSL	B	603	-	-	11/24/24/24	0/3/3/3
2	LYS	B	602	-	-	2/9/9/9	-
2	LYS	A	601	-	-	0/9/9/9	-
3	JSL	A	602	-	-	8/24/24/24	0/3/3/3
4	MES	B	601	-	-	2/6/14/14	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	JSL	O25-S24	23.94	1.65	1.44
3	B	603	JSL	O29-S24	23.69	1.65	1.44
3	A	602	JSL	O29-S24	23.48	1.65	1.44
3	B	603	JSL	O25-S24	23.22	1.65	1.44
4	B	601	MES	C8-S	-7.55	1.66	1.77
3	A	602	JSL	C12-N11	4.81	1.46	1.36
3	B	603	JSL	C12-N11	4.79	1.46	1.36
3	A	602	JSL	C16-N17	4.70	1.46	1.36
3	B	603	JSL	C16-N17	4.67	1.46	1.36
3	A	602	JSL	C18-N17	2.34	1.46	1.39
3	A	602	JSL	C10-N11	2.32	1.46	1.39
3	B	603	JSL	C10-N11	2.32	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	603	JSL	C18-N17	2.21	1.46	1.39
2	A	601	LYS	OXT-C	-2.14	1.23	1.30
2	B	602	LYS	OXT-C	-2.12	1.23	1.30
3	B	603	JSL	O02-C03	2.01	1.40	1.37

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	603	JSL	O29-S24-O25	-12.09	107.61	118.71
3	A	602	JSL	O29-S24-O25	-9.77	109.75	118.71
3	A	602	JSL	N15-C16-N30	-8.04	118.93	126.55
3	B	603	JSL	O25-S24-C26	-7.82	102.71	107.97
3	A	602	JSL	N13-C12-N30	-7.67	119.28	126.55
3	B	603	JSL	N13-C12-N30	-7.56	119.38	126.55
3	B	603	JSL	N15-C16-N30	-7.29	119.65	126.55
3	B	603	JSL	O29-S24-C26	6.84	112.58	107.97
3	B	603	JSL	N15-C14-N13	-5.36	120.21	128.60
4	B	601	MES	C5-N4-C3	5.00	120.08	108.83
3	A	602	JSL	N15-C14-N13	-4.94	120.88	128.60
3	A	602	JSL	C16-N30-C12	4.47	121.47	113.89
3	B	603	JSL	O25-S24-C23	4.39	116.34	107.76
3	B	603	JSL	C23-C18-N17	-4.14	117.54	121.45
3	A	602	JSL	O02-C03-C10	4.11	119.84	114.80
3	B	603	JSL	C22-C23-S24	3.91	122.85	116.83
3	B	603	JSL	C16-N30-C12	3.87	120.45	113.89
4	B	601	MES	O3S-S-C8	3.62	111.62	105.77
3	A	602	JSL	O25-S24-C26	3.50	110.32	107.97
4	B	601	MES	C7-N4-C3	3.49	120.16	111.23
3	A	602	JSL	O29-S24-C26	3.46	110.30	107.97
4	B	601	MES	C7-N4-C5	3.33	119.74	111.23
3	A	602	JSL	C23-C18-N17	-3.29	118.34	121.45
3	B	603	JSL	O02-C03-C10	2.89	118.34	114.80
2	A	601	LYS	OXT-C-O	-2.65	118.08	124.09
2	B	602	LYS	OXT-C-O	-2.59	118.22	124.09
3	A	602	JSL	C01-O02-C03	-2.38	113.94	117.53
3	A	602	JSL	C22-C23-S24	2.29	120.36	116.83
3	A	602	JSL	O02-C03-C04	-2.25	120.25	124.12
2	A	601	LYS	OXT-C-CA	2.24	121.02	113.38
2	B	602	LYS	OXT-C-CA	2.19	120.83	113.38
4	B	601	MES	C2-C3-N4	-2.09	106.93	110.10

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	JSL	C18-C23-S24-O25
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	C18-C23-S24-O25
4	B	601	MES	N4-C7-C8-S
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
3	B	603	JSL	C18-C23-S24-O29
3	A	602	JSL	C22-C23-S24-O25
3	A	602	JSL	C22-C23-S24-O29
3	B	603	JSL	C22-C23-S24-O25
4	B	601	MES	C8-C7-N4-C3
3	B	603	JSL	C22-C23-S24-O29
3	A	602	JSL	C18-C23-S24-C26
3	B	603	JSL	C18-C23-S24-C26
3	A	602	JSL	C04-C05-O06-C07

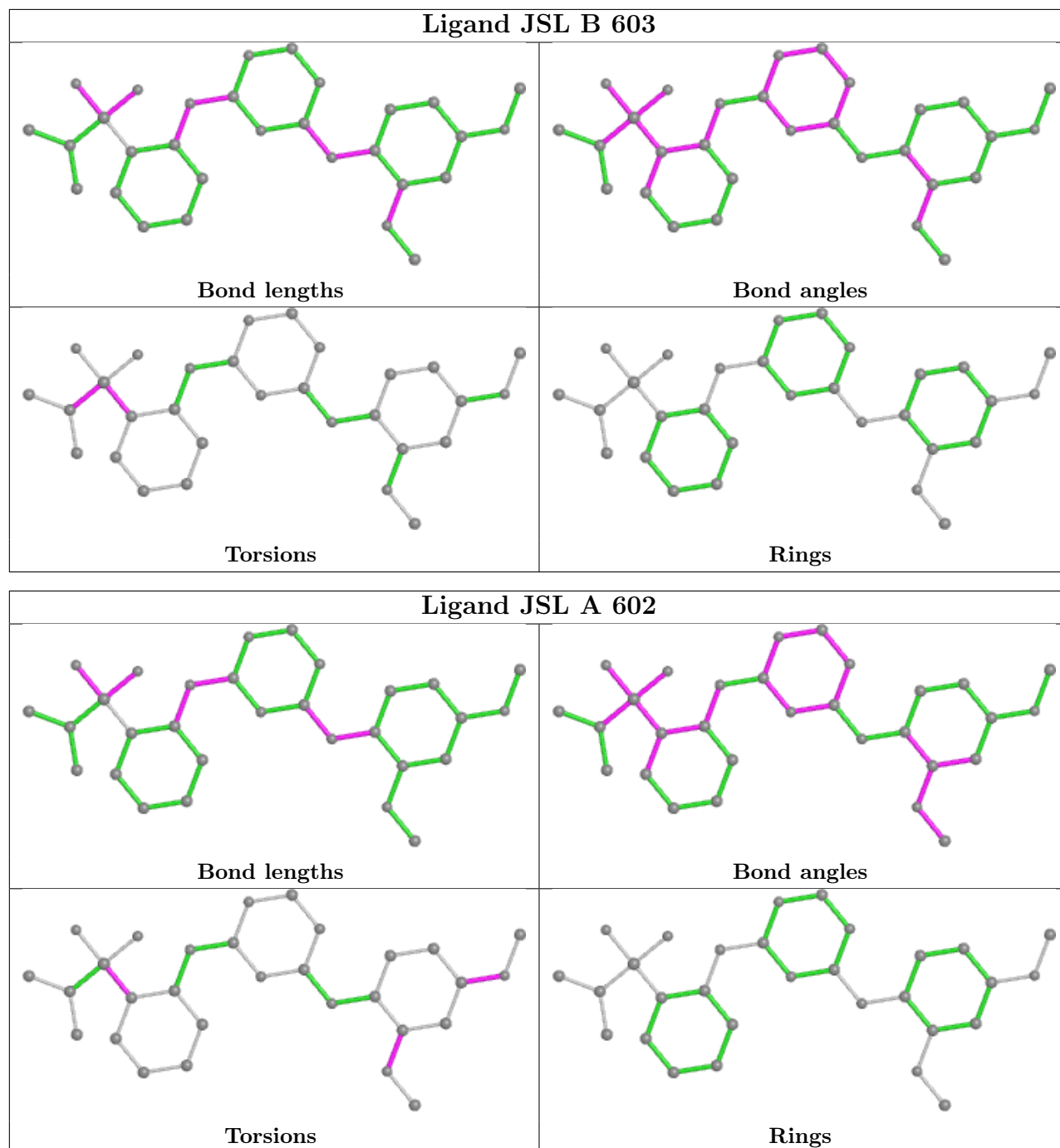
There are no ring outliers.

4 monomers are involved in 11 short contacts:

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

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	486/516 (94%)	0.15	6 (1%) 79 76	36, 62, 98, 127	0
1	B	477/516 (92%)	0.49	31 (6%) 18 13	37, 74, 130, 224	0
All	All	963/1032 (93%)	0.32	37 (3%) 40 32	36, 67, 117, 224	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	403	ILE	3.9
1	B	152	PHE	3.9
1	B	456	PHE	3.8
1	B	200	LYS	3.7
1	B	457	ILE	3.7
1	B	407	ILE	3.5
1	B	98	GLY	3.3
1	B	165	ALA	3.3
1	B	149	LEU	3.3
1	B	461	TYR	3.2
1	B	172	HIS	3.1
1	B	189	ILE	3.1
1	B	582	ALA	3.1
1	B	184	ILE	3.0
1	B	390	ILE	2.9
1	A	78	VAL	2.8
1	A	151	PHE	2.8
1	B	216	ALA	2.7
1	B	580	ARG	2.6
1	B	141	ARG	2.6
1	B	418	PRO	2.6
1	A	167	TYR	2.5
1	B	466	PHE	2.5
1	B	205	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	426	GLU	2.5
1	B	387	ASN	2.4
1	A	582	ALA	2.4
1	B	138	ARG	2.2
1	B	218	LEU	2.2
1	B	297	LEU	2.2
1	B	370	TYR	2.2
1	B	161	ILE	2.2
1	B	429	ILE	2.1
1	B	239	LEU	2.1
1	A	283	GLY	2.1
1	B	468	ILE	2.1
1	A	164	LEU	2.1

## 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 monosaccharides 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, 95<sup>th</sup> 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.

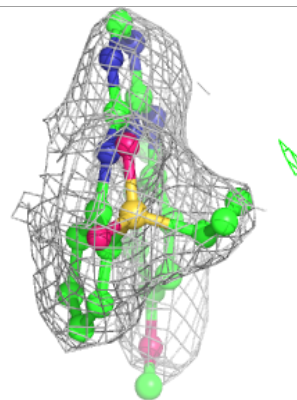
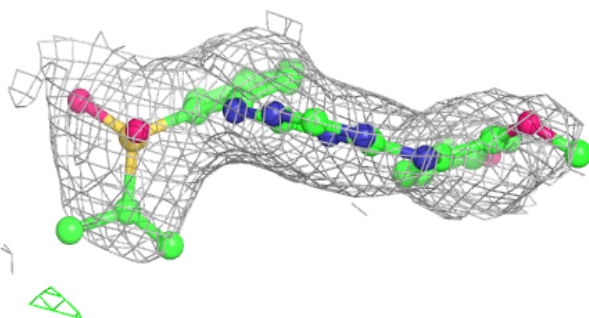
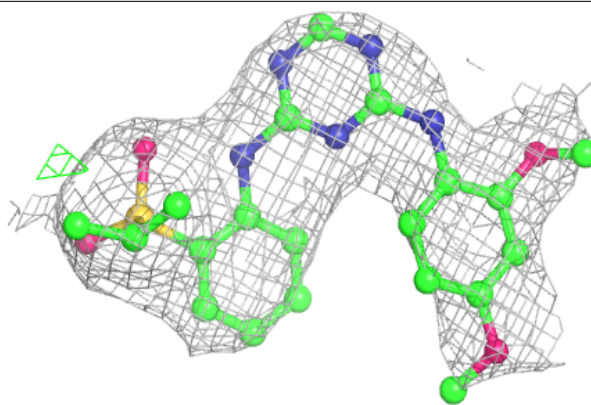
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	LYS	B	602	10/10	0.85	0.34	58,71,82,84	0
2	LYS	A	601	10/10	0.94	0.22	38,39,44,44	0
3	JSL	A	602	30/30	0.94	0.25	40,55,80,85	0
4	MES	B	601	12/12	0.94	0.21	47,56,64,65	0
3	JSL	B	603	30/30	0.95	0.19	52,60,68,80	0

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.

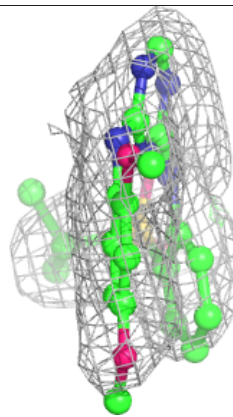
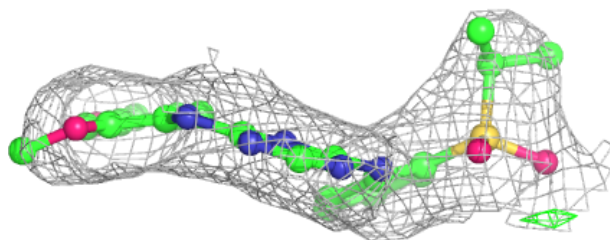
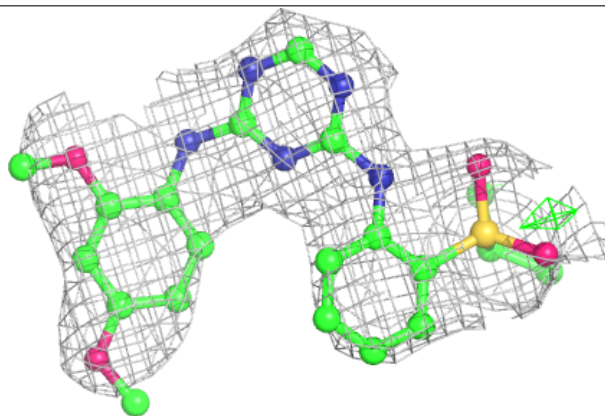


**Electron density around JSL A 602:**

$2mF_o-DF_c$  (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.