



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2026 – 02:39 pm BST

PDB ID : 29VD / pdb\_000029vd  
Title : Crystal structure of the human METTL3-METTL14 in complex with STC-15  
Authors : Bedi, R.K.; Caflisch, A.  
Deposited on : 2026-04-09  
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](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>.

---

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 : 1.8.4, CSD as541be (2020)  
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

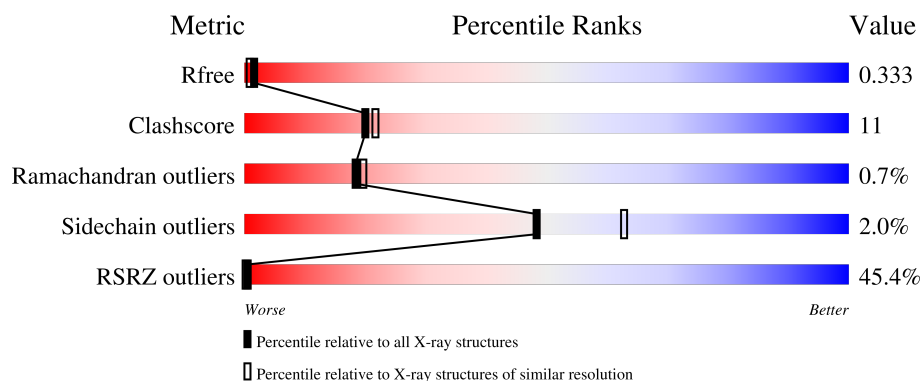
# 1 Overall quality at a glance

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  $\geq 3$ , 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	228	<div> <div>38%</div> <div>64%</div> <div>25%</div> <div>10%</div> </div>
2	B	307	<div> <div>37%</div> <div>65%</div> <div>12%</div> <div>22%</div> </div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3543 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 N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1591	1022	279	281	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	353	MET	-	initiating methionine	UNP Q86U44

- Molecule 2 is a protein called N(6)-adenosine-methyltransferase non-catalytic subunit METTL14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	238	Total	C	N	O	S	0	1	0
			1836	1181	309	333	13			

There are 18 discrepancies between the modelled and reference sequences:

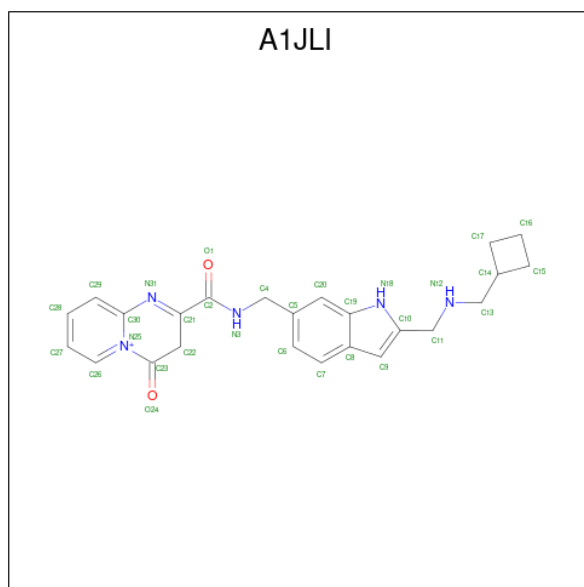
Chain	Residue	Modelled	Actual	Comment	Reference
B	89	MET	-	initiating methionine	UNP Q9HCE5
B	90	HIS	-	expression tag	UNP Q9HCE5
B	91	HIS	-	expression tag	UNP Q9HCE5
B	92	HIS	-	expression tag	UNP Q9HCE5
B	93	HIS	-	expression tag	UNP Q9HCE5
B	94	HIS	-	expression tag	UNP Q9HCE5
B	95	HIS	-	expression tag	UNP Q9HCE5
B	96	SER	-	expression tag	UNP Q9HCE5
B	97	SER	-	expression tag	UNP Q9HCE5
B	98	GLY	-	expression tag	UNP Q9HCE5
B	99	ARG	-	expression tag	UNP Q9HCE5
B	100	GLU	-	expression tag	UNP Q9HCE5
B	101	ASN	-	expression tag	UNP Q9HCE5
B	102	LEU	-	expression tag	UNP Q9HCE5

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	103	TYR	-	expression tag	UNP Q9HCE5
B	104	PHE	-	expression tag	UNP Q9HCE5
B	105	GLN	-	expression tag	UNP Q9HCE5
B	106	GLY	-	expression tag	UNP Q9HCE5

- Molecule 3 is {N}-[[2-[(cyclobutylmethylamino)methyl]-1 {H}-indol-6-yl]methyl]-4-oxid anylidene-3 {H}-pyrido[1,2-a]pyrimidin-5-ium-2-carboxamide (CCD ID: A1JLI) (formula: C<sub>24</sub>H<sub>26</sub>N<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		

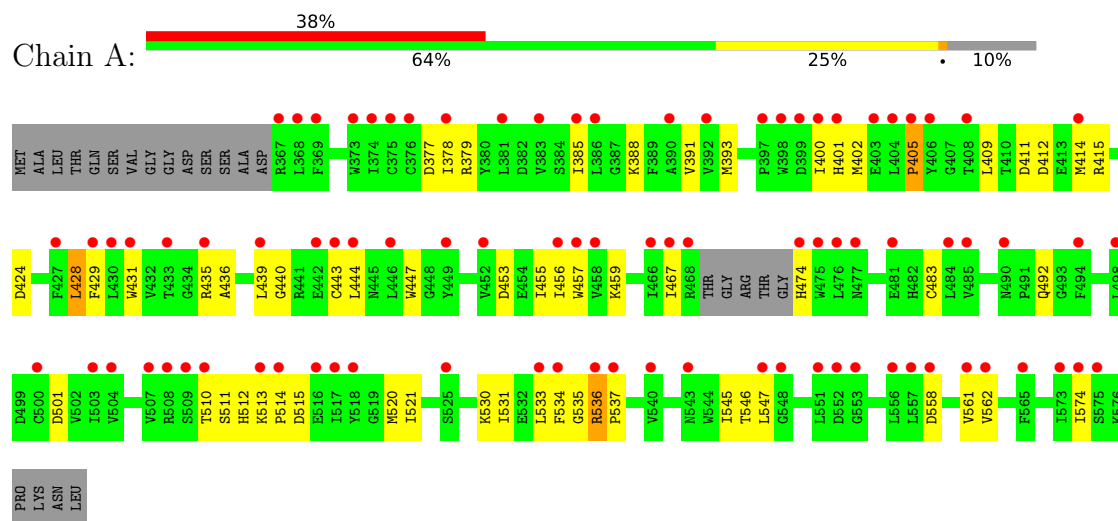
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	35	Total	O	0	0
			35	35		
5	B	46	Total	O	0	0
			46	46		

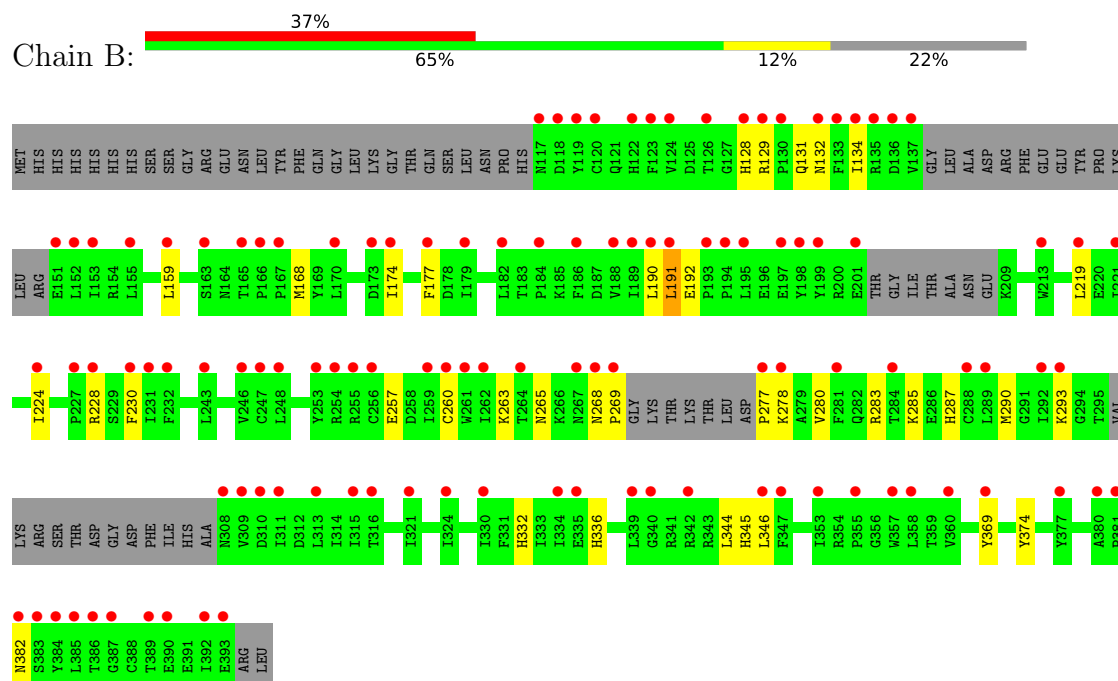
### 3 Residue-property plots [i](#)

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: N6-adenosine-methyltransferase catalytic subunit



- Molecule 2: N(6)-adenosine-methyltransferase non-catalytic subunit METTL14



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.25Å 64.25Å 226.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	54.04 – 2.35 54.04 – 2.35	Depositor EDS
% Data completeness (in resolution range)	98.9 (54.04-2.35) 98.9 (54.04-2.35)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.18 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.274 , 0.337 0.275 , 0.333	Depositor DCC
$R_{free}$ test set	1209 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.0	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 46.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.077 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	3543	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A1JLI, ACT

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	0.42	0/1634	0.67	3/2230 (0.1%)
2	B	0.41	0/1886	0.64	1/2567 (0.0%)
All	All	0.42	0/3520	0.66	4/4797 (0.1%)

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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	405	PRO	CA-CB-CG	-8.89	87.61	104.50
1	A	405	PRO	N-CD-CG	-8.04	91.13	103.20
2	B	280	VAL	N-CA-C	-6.73	106.23	112.96
1	A	405	PRO	CA-N-CD	-5.00	104.99	112.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	536	ARG	Sidechain

## 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	1591	0	1497	41	1
2	B	1836	0	1697	37	0
3	A	31	0	0	4	0
4	B	4	0	3	0	0
5	A	35	0	0	9	1
5	B	46	0	0	9	1
All	All	3543	0	3197	76	2

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 11.

All (76) 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:385:ILE:O	5:A:701:HOH:O	1.92	0.88
1:A:409:LEU:HB2	1:A:414:MET:HE2	1.63	0.78
2:B:382:ASN:OD1	5:B:501:HOH:O	2.05	0.73
1:A:537:PRO:O	5:A:702:HOH:O	2.07	0.71
1:A:561:VAL:HA	5:A:701:HOH:O	1.94	0.67
1:A:393:MET:HG3	1:A:429:PHE:HB2	1.77	0.67
2:B:219:LEU:O	5:B:502:HOH:O	2.12	0.66
1:A:531:ILE:HD12	1:A:545:ILE:O	1.95	0.66
1:A:424:ASP:OD2	5:A:704:HOH:O	2.14	0.65
1:A:388:LYS:NZ	5:A:708:HOH:O	2.31	0.63
1:A:515:ASP:OD1	5:A:705:HOH:O	2.16	0.62
2:B:128:HIS:CE1	2:B:269:PRO:HG2	2.34	0.62
2:B:263:LYS:NZ	5:B:509:HOH:O	2.30	0.61
2:B:278:LYS:H	2:B:278:LYS:CD	2.15	0.59
2:B:277:PRO:HD2	2:B:278:LYS:HD3	1.84	0.59
2:B:129:ARG:NH1	2:B:263:LYS:O	2.35	0.58
1:A:391:VAL:HB	1:A:530:LYS:HG2	1.85	0.58
2:B:132:ASN:ND2	2:B:265:ASN:OD1	2.36	0.58
1:A:521:ILE:HG22	5:A:723:HOH:O	2.02	0.57
1:A:436:ALA:HA	1:A:439:LEU:HB3	1.86	0.57
2:B:278:LYS:H	2:B:278:LYS:HD3	1.71	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:ASP:OD2	2:B:283:ARG:HA	2.08	0.54
2:B:382:ASN:O	5:B:504:HOH:O	2.18	0.54
2:B:168:MET:HE3	2:B:369:TYR:HD1	1.73	0.54
1:A:455:ILE:HD13	1:A:520:MET:HE1	1.88	0.54
1:A:378:ILE:HD11	1:A:534:PHE:H	1.73	0.53
2:B:190:LEU:HD12	2:B:191:LEU:H	1.73	0.53
1:A:377:ASP:OD1	1:A:379:ARG:HB2	2.08	0.52
1:A:558:ASP:O	1:A:562:VAL:HG23	2.10	0.52
2:B:168:MET:CE	2:B:369:TYR:HD1	2.24	0.51
1:A:456:ILE:HD13	2:B:260[B]:CYS:SG	2.51	0.51
1:A:431:TRP:CE3	1:A:483:CYS:HB2	2.46	0.50
2:B:344:LEU:HG	5:B:506:HOH:O	2.11	0.49
1:A:474:HIS:N	5:A:703:HOH:O	2.45	0.49
1:A:457:TRP:CE3	1:A:514:PRO:HD3	2.47	0.49
2:B:190:LEU:HG	2:B:345:HIS:CD2	2.48	0.49
2:B:192:GLU:O	5:B:505:HOH:O	2.19	0.48
1:A:536:ARG:HE	3:A:601:A1JLI:C6	2.26	0.48
2:B:131:GLN:O	2:B:134:ILE:HD12	2.15	0.47
2:B:332:HIS:CE1	5:B:516:HOH:O	2.67	0.47
1:A:393:MET:CG	1:A:429:PHE:HB2	2.44	0.46
1:A:400:ILE:O	1:A:402:MET:N	2.48	0.46
1:A:459:LYS:HB2	1:A:459:LYS:HE3	1.46	0.46
1:A:443:CYS:HB3	1:A:447:TRP:CZ2	2.50	0.46
1:A:510:THR:O	1:A:512:HIS:HD2	1.98	0.46
1:A:513:LYS:HB3	3:A:601:A1JLI:C15	2.46	0.46
2:B:168:MET:HE3	2:B:369:TYR:HA	1.98	0.46
2:B:168:MET:HE1	2:B:374:TYR:HB2	1.97	0.46
2:B:260[A]:CYS:SG	2:B:287:HIS:CE1	3.09	0.45
2:B:168:MET:CE	2:B:369:TYR:CD1	3.00	0.45
1:A:428:LEU:HD22	1:A:429:PHE:N	2.32	0.44
1:A:440:GLY:O	1:A:444:LEU:HB2	2.18	0.44
1:A:412:ASP:OD1	1:A:415:ARG:NH1	2.47	0.44
2:B:191:LEU:HD13	2:B:346:LEU:HB2	2.00	0.44
1:A:536:ARG:HE	3:A:601:A1JLI:C5	2.31	0.43
1:A:535:GLY:HA3	1:A:546:THR:CG2	2.48	0.43
1:A:536:ARG:O	1:A:537:PRO:C	2.60	0.43
2:B:228:ARG:HA	2:B:293:LYS:O	2.18	0.43
2:B:336:HIS:CE1	5:B:516:HOH:O	2.71	0.42
1:A:431:TRP:CD2	1:A:483:CYS:HB2	2.54	0.42
1:A:535:GLY:HA3	1:A:546:THR:HG23	2.02	0.42
2:B:277:PRO:HG2	2:B:278:LYS:HZ2	1.84	0.42

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:536:ARG:NH2	3:A:601:A1JLI:C7	2.83	0.41
2:B:174:ILE:HA	2:B:177:PHE:HB3	2.02	0.41
2:B:190:LEU:O	5:B:506:HOH:O	2.21	0.41
1:A:531:ILE:HD11	1:A:547:LEU:HG	2.02	0.41
2:B:230:PHE:HD2	2:B:290:MET:HE3	1.85	0.41
2:B:278:LYS:HD3	2:B:278:LYS:N	2.34	0.41
2:B:268:ASN:N	2:B:269:PRO:HD3	2.36	0.41
1:A:411:ASP:CG	1:A:435:ARG:HH22	2.29	0.41
1:A:455:ILE:CD1	1:A:520:MET:HE1	2.51	0.41
2:B:159:LEU:HD23	2:B:159:LEU:HA	1.94	0.41
2:B:168:MET:HE3	2:B:369:TYR:CD1	2.54	0.41
5:A:703:HOH:O	2:B:257:GLU:OE2	2.21	0.41
1:A:378:ILE:CD1	1:A:534:PHE:H	2.33	0.40
2:B:260[B]:CYS:SG	2:B:285:LYS:HD2	2.61	0.40

All (2) 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:A:492:GLN:NE2	5:A:702:HOH:O[5_665]	2.07	0.13
5:B:515:HOH:O	5:B:530:HOH:O[4_455]	2.15	0.05

## 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	201/228 (88%)	186 (92%)	12 (6%)	3 (2%)	8	7
2	B	229/307 (75%)	216 (94%)	13 (6%)	0	100	100
All	All	430/535 (80%)	402 (94%)	25 (6%)	3 (1%)	18	20

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	467	ILE
1	A	574	ILE
1	A	401	HIS

### 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	161/200 (80%)	156 (97%)	5 (3%)	35	47
2	B	185/274 (68%)	183 (99%)	2 (1%)	65	79
All	All	346/474 (73%)	339 (98%)	7 (2%)	48	63

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	405	PRO
1	A	428	LEU
1	A	453	ASP
1	A	511	SER
1	A	533	LEU
2	B	191	LEU
2	B	224	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	539	ASN
2	B	121	GLN
2	B	128	HIS
2	B	282	GLN
2	B	366	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

2 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	ACT	B	401	-	3,3,3	1.54	1 (33%)	3,3,3	1.26	0
3	A1JLI	A	601	-	30,35,35	3.03	15 (50%)	33,49,49	2.09	9 (27%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	A1JLI	A	601	-	-	0/14/33/33	0/4/5/5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A1JLI	C29-C30	7.41	1.53	1.40
3	A	601	A1JLI	C20-C19	6.26	1.49	1.39
3	A	601	A1JLI	C10-N18	5.93	1.45	1.37
3	A	601	A1JLI	C21-N31	4.42	1.40	1.30
3	A	601	A1JLI	C26-N25	3.98	1.43	1.36
3	A	601	A1JLI	C19-N18	3.90	1.45	1.38
3	A	601	A1JLI	C11-C10	3.47	1.54	1.49

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	A1JLI	C2-N3	3.32	1.39	1.33
3	A	601	A1JLI	C9-C10	3.23	1.43	1.37
3	A	601	A1JLI	C28-C27	3.19	1.46	1.38
3	A	601	A1JLI	C13-C14	3.12	1.57	1.51
3	A	601	A1JLI	C13-N12	2.87	1.51	1.47
3	A	601	A1JLI	C4-C5	2.74	1.57	1.51
3	A	601	A1JLI	C30-N31	-2.64	1.34	1.38
4	B	401	ACT	CH3-C	2.47	1.59	1.49
3	A	601	A1JLI	C11-N12	2.39	1.53	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	A1JLI	O24-C23-N25	-4.70	115.82	122.48
3	A	601	A1JLI	C11-C10-C9	-4.12	126.75	131.38
3	A	601	A1JLI	C20-C19-C8	-3.95	120.31	122.86
3	A	601	A1JLI	C29-C30-N31	3.92	123.93	115.36
3	A	601	A1JLI	C4-N3-C2	3.28	126.48	122.08
3	A	601	A1JLI	C19-C8-C9	3.02	109.23	106.79
3	A	601	A1JLI	C11-N12-C13	2.71	123.57	113.86
3	A	601	A1JLI	O1-C2-N3	-2.58	118.57	123.30
3	A	601	A1JLI	C21-C2-N3	2.15	120.55	116.18

There are no chirality outliers.

There are no torsion outliers.

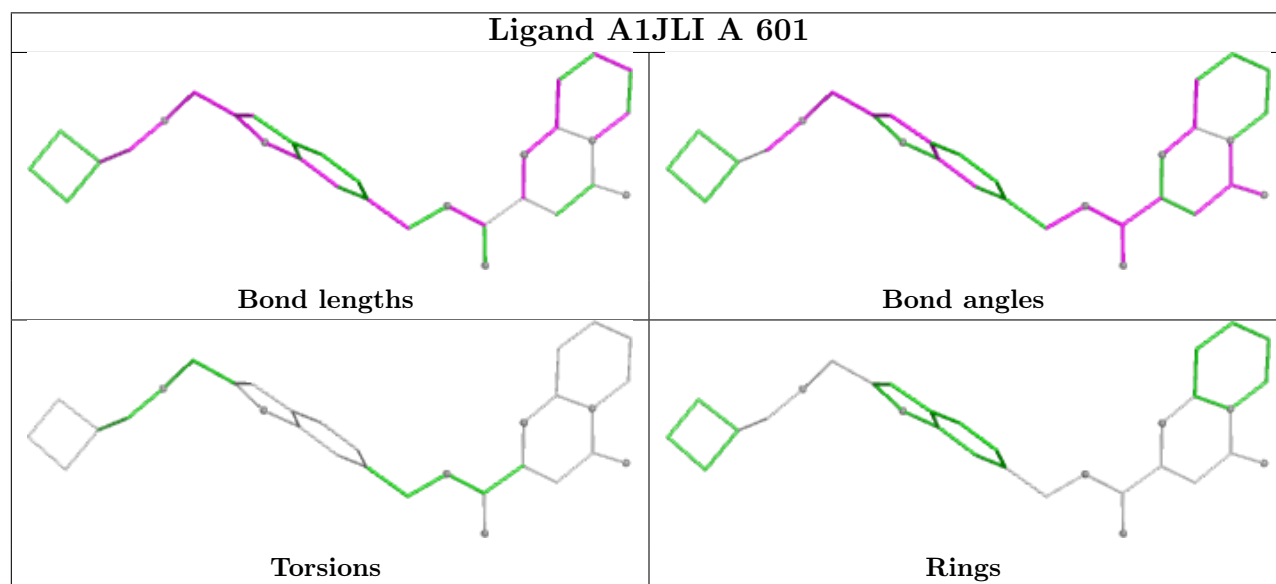
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	A1JLI	4	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, 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	205/228 (89%)	1.98	87 (42%) <b>0</b> <b>0</b>	30, 44, 65, 72	0
2	B	238/307 (77%)	2.12	114 (47%) <b>0</b> <b>0</b>	23, 43, 70, 77	1 (0%)
All	All	443/535 (82%)	2.06	201 (45%) <b>0</b> <b>0</b>	23, 43, 67, 77	1 (0%)

All (201) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	119	TYR	7.3
2	B	311	ILE	7.2
2	B	310	ASP	6.3
1	A	386	LEU	5.7
1	A	557	LEU	5.6
2	B	309	VAL	5.6
1	A	565	PHE	5.4
2	B	384	TYR	5.3
2	B	289	LEU	5.3
1	A	378	ILE	5.1
2	B	377	TYR	4.8
1	A	405	PRO	4.6
1	A	558	ASP	4.6
1	A	429	PHE	4.5
2	B	392	ILE	4.5
2	B	118	ASP	4.5
2	B	152	LEU	4.4
2	B	387	GLY	4.3
2	B	256	CYS	4.1
2	B	281	PHE	4.1
1	A	507	VAL	4.0
2	B	292	ILE	4.0
1	A	504	VAL	3.9
2	B	153	ILE	3.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	177	PHE	3.8
2	B	334	ILE	3.8
1	A	368	LEU	3.8
1	A	509	SER	3.8
1	A	401	HIS	3.8
2	B	221	ILE	3.7
1	A	446	LEU	3.7
2	B	308	ASN	3.7
2	B	248	LEU	3.6
1	A	514	PRO	3.6
2	B	179	ILE	3.6
2	B	385	LEU	3.5
2	B	277	PRO	3.5
2	B	381	PRO	3.5
2	B	117	ASN	3.5
2	B	390	GLU	3.5
2	B	193	PRO	3.4
2	B	231	ILE	3.4
1	A	477	ASN	3.4
1	A	547	LEU	3.3
2	B	191	LEU	3.3
2	B	261	TRP	3.3
1	A	573	ILE	3.3
1	A	551	LEU	3.3
2	B	170	LEU	3.3
1	A	385	ILE	3.3
2	B	163	SER	3.3
2	B	227	PRO	3.2
1	A	449	TYR	3.2
1	A	392	VAL	3.2
1	A	533	LEU	3.2
1	A	400	ILE	3.2
1	A	516	GLU	3.2
1	A	397	PRO	3.2
2	B	224	ILE	3.2
1	A	444	LEU	3.2
1	A	398	TRP	3.1
2	B	330	ILE	3.1
1	A	485	VAL	3.1
2	B	155	LEU	3.1
1	A	561	VAL	3.1
1	A	474	HIS	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	369	PHE	3.0
1	A	404	LEU	3.0
1	A	452	VAL	3.0
2	B	262	ILE	3.0
1	A	457	TRP	3.0
1	A	390	ALA	3.0
2	B	340	GLY	3.0
2	B	186	PHE	3.0
1	A	383	VAL	3.0
2	B	128	HIS	3.0
2	B	246	VAL	2.9
2	B	288	CYS	2.9
1	A	466	ILE	2.9
2	B	151	GLU	2.9
2	B	259	ILE	2.9
1	A	552	ASP	2.9
2	B	380	ALA	2.9
2	B	120	CYS	2.9
2	B	134	ILE	2.9
1	A	548	GLY	2.8
2	B	293	LYS	2.8
1	A	536	ARG	2.8
2	B	130	PRO	2.8
1	A	458	VAL	2.8
1	A	376	CYS	2.8
1	A	510	THR	2.8
2	B	228	ARG	2.8
2	B	159	LEU	2.8
1	A	439	LEU	2.8
2	B	122	HIS	2.8
2	B	189	ILE	2.8
1	A	513	LYS	2.8
1	A	574	ILE	2.7
2	B	389	THR	2.7
1	A	373	TRP	2.7
2	B	182	LEU	2.7
2	B	123	PHE	2.7
2	B	315	ILE	2.7
1	A	467	ILE	2.7
2	B	230	PHE	2.7
1	A	562	VAL	2.7
1	A	553	GLY	2.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	324	ILE	2.7
1	A	534	PHE	2.6
1	A	367	ARG	2.6
2	B	137	VAL	2.6
2	B	194	PRO	2.6
2	B	243	LEU	2.6
2	B	357	TRP	2.6
2	B	268	ASN	2.6
2	B	360	VAL	2.6
1	A	556	LEU	2.5
1	A	508	ARG	2.5
1	A	540	VAL	2.5
2	B	195	LEU	2.5
1	A	431	TRP	2.5
2	B	124	VAL	2.5
2	B	269	PRO	2.5
1	A	517	ILE	2.5
2	B	126	THR	2.4
1	A	494	PHE	2.4
2	B	232	PHE	2.4
2	B	198	TYR	2.4
1	A	403	GLU	2.4
2	B	355	PRO	2.4
2	B	264	THR	2.4
2	B	316	THR	2.4
1	A	575	SER	2.4
1	A	374	ILE	2.4
2	B	346	LEU	2.4
2	B	197	GLU	2.4
2	B	201	GLU	2.4
1	A	484	LEU	2.4
1	A	475	TRP	2.4
2	B	132	ASN	2.3
2	B	184	PRO	2.3
2	B	174	ILE	2.3
2	B	188	VAL	2.3
1	A	399	ASP	2.3
2	B	386	THR	2.3
1	A	456	ILE	2.3
2	B	247	CYS	2.3
1	A	490	ASN	2.3
2	B	173	ASP	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	B	253	TYR	2.3
1	A	468	ARG	2.3
2	B	255	ARG	2.3
2	B	347	PHE	2.3
1	A	430	LEU	2.3
1	A	476	LEU	2.3
1	A	375	CYS	2.3
1	A	433	THR	2.3
2	B	260[A]	CYS	2.2
2	B	342	ARG	2.2
2	B	199	TYR	2.2
2	B	369	TYR	2.2
2	B	213	TRP	2.2
2	B	321	ILE	2.2
2	B	339	LEU	2.2
1	A	500	CYS	2.2
1	A	525	SER	2.2
2	B	129	ARG	2.2
1	A	414	MET	2.2
2	B	136	ASP	2.2
1	A	481	GLU	2.2
2	B	335	GLU	2.2
2	B	393	GLU	2.2
1	A	406	TYR	2.1
2	B	135	ARG	2.1
1	A	427	PHE	2.1
1	A	537	PRO	2.1
2	B	133	PHE	2.1
1	A	443	CYS	2.1
2	B	254	ARG	2.1
1	A	503	ILE	2.1
2	B	167	PRO	2.1
1	A	381	LEU	2.1
2	B	313	LEU	2.1
1	A	518	TYR	2.1
2	B	284	THR	2.1
2	B	383	SER	2.1
2	B	190	LEU	2.1
1	A	543	ASN	2.1
2	B	267	ASN	2.1
2	B	166	PRO	2.1
2	B	278	LYS	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	498	LEU	2.0
1	A	435	ARG	2.0
1	A	408	THR	2.0
1	A	442	GLU	2.0
2	B	165	THR	2.0
2	B	219	LEU	2.0
2	B	358	LEU	2.0
2	B	382	ASN	2.0
2	B	353	ILE	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](#)

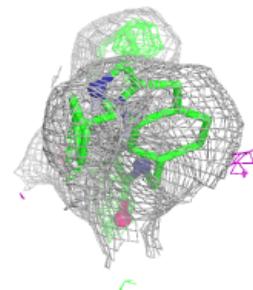
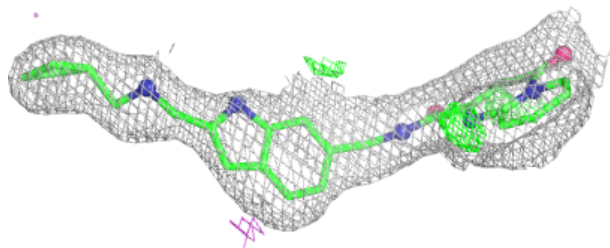
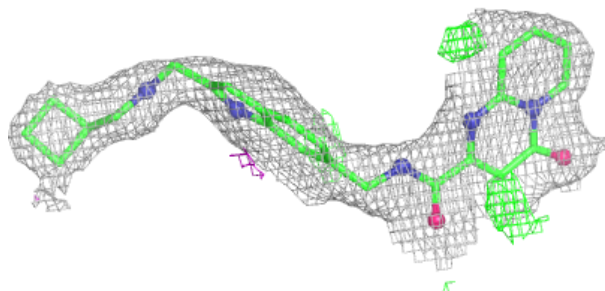
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	A1JLI	A	601	31/31	0.83	0.16	37,45,50,51	0
4	ACT	B	401	4/4	0.84	0.15	37,38,44,44	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 A1JLI A 601:**

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



## 6.5 Other polymers [i](#)

There are no such residues in this entry.