



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 07:05 pm BST

PDB ID : 9R8Z / pdb\_00009r8z  
Title : METTL3/14 complex with switchable fragment  
Authors : Bayliss, R.; Maddison, L.; Richards, M.W.  
Deposited on : 2025-05-18  
Resolution : 2.21 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 : 4-5-2 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

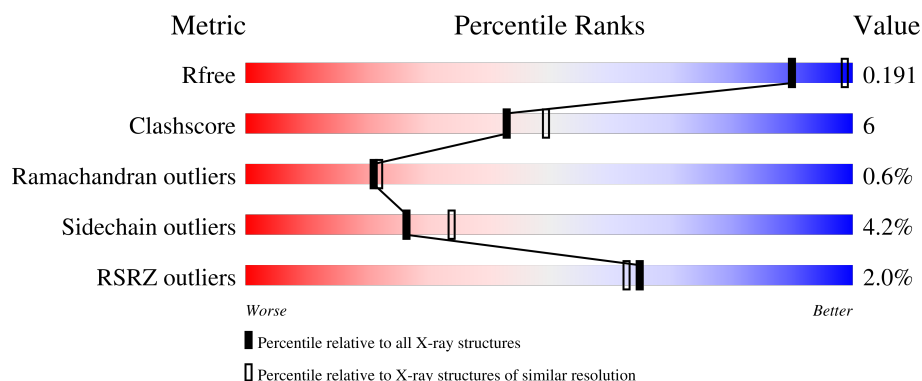
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

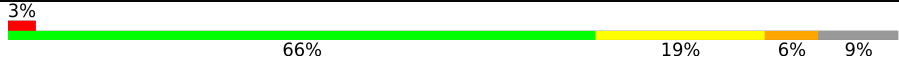

The reported resolution of this entry is 2.21 Å.

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	7682 (2.24-2.20)
Clashscore	190562	8402 (2.24-2.20)
Ramachandran outliers	187476	8303 (2.24-2.20)
Sidechain outliers	187428	8304 (2.24-2.20)
RSRZ outliers	180081	7683 (2.24-2.20)

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	224	
2	B	348	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4231 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 N(6)-adenosine-methyltransferase catalytic subunit METTL3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	203	Total	C	N	O	S	0	0	0
			1643	1050	293	290	10			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	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	285	Total	C	N	O	S	0	1	0
			2325	1478	402	433	12			

There are 2 discrepancies between the modelled and reference sequences:

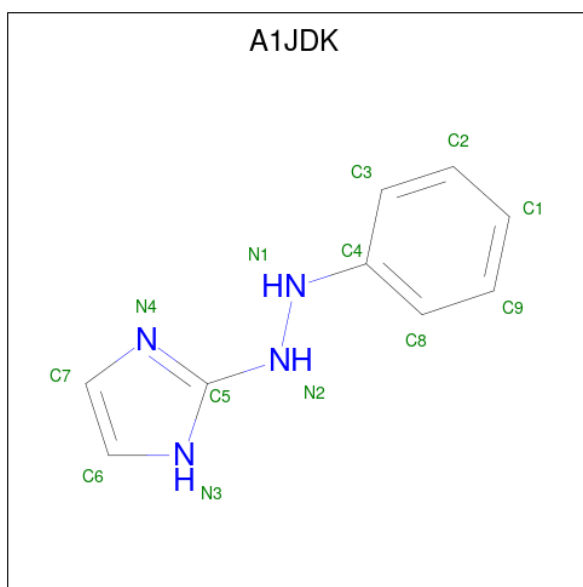
Chain	Residue	Modelled	Actual	Comment	Reference
B	109	GLY	-	expression tag	UNP Q9HCE5
B	110	SER	-	expression tag	UNP Q9HCE5

- Molecule 3 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C<sub>2</sub>H<sub>6</sub>OS).



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

- Molecule 4 is 1-(1 {H}-imidazol-2-yl)-2-phenyl-diazane (CCD ID: A1JDK) (formula: C<sub>9</sub>H<sub>10</sub>N<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			13	9	4		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		

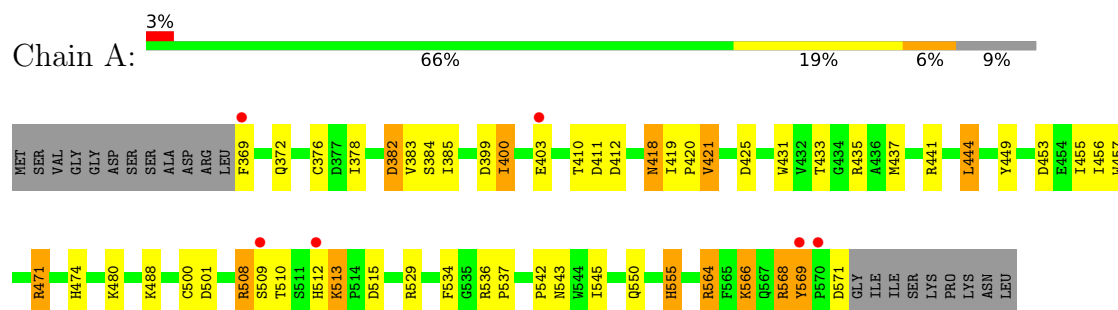
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	62	Total	O	0	0
			62	62		
6	B	166	Total	O	0	0
			166	166		

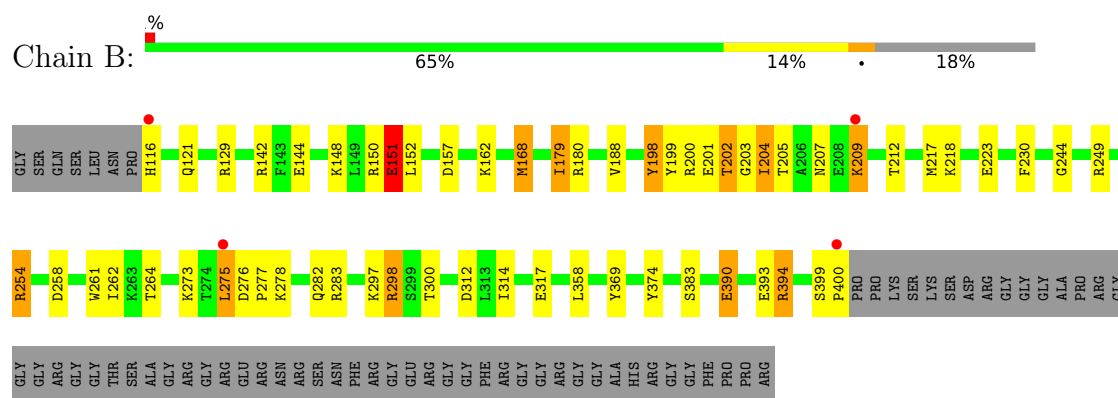
### 3 Residue-property plots [i](#)

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: N(6)-adenosine-methyltransferase catalytic subunit METTL3



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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.83Å 100.83Å 117.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.57 – 2.21 76.57 – 2.21	Depositor EDS
% Data completeness (in resolution range)	100.0 (76.57-2.21) 100.0 (76.57-2.21)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.88)	Depositor
R, $R_{free}$	0.174 , 0.227 0.183 , 0.191	Depositor DCC
$R_{free}$ test set	1486 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.3	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 49.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	4231	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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: A1JDK, CL, DMS

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	0.97	1/1688 (0.1%)	1.65	32/2296 (1.4%)
2	B	1.03	3/2383 (0.1%)	1.64	30/3231 (0.9%)
All	All	1.00	4/4071 (0.1%)	1.64	62/5527 (1.1%)

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	2
2	B	0	4
All	All	0	6

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	121	GLN	C-O	7.30	1.32	1.24
2	B	179	ILE	CB-CG1	-5.44	1.42	1.53
2	B	314	ILE	C-O	-5.29	1.18	1.24
1	A	508	ARG	NE-CZ	5.17	1.38	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	200	ARG	N-CA-CB	9.65	124.00	110.01
2	B	151	GLU	CB-CG-CD	8.59	127.21	112.60
2	B	205	THR	CA-CB-OG1	-8.57	96.75	109.60
1	A	410	THR	CA-CB-OG1	-7.95	97.68	109.60
1	A	569	TYR	CB-CA-C	7.63	120.70	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	258	ASP	CA-CB-CG	7.63	120.23	112.60
1	A	444	LEU	N-CA-CB	-7.54	99.07	110.01
2	B	168	MET	CG-SD-CE	-7.43	84.56	100.90
1	A	437	MET	CB-CG-SD	-7.43	90.42	112.70
2	B	393	GLU	N-CA-CB	7.20	120.71	110.12
1	A	513	LYS	CB-CA-C	-7.13	99.32	110.02
2	B	198	TYR	N-CA-CB	6.90	122.06	110.32
1	A	508	ARG	CD-NE-CZ	6.86	134.00	124.40
1	A	369	PHE	CA-CB-CG	6.69	120.49	113.80
2	B	148	LYS	CB-CA-C	6.58	122.73	110.70
1	A	382	ASP	CA-CB-CG	6.57	119.17	112.60
2	B	198	TYR	CB-CA-C	-6.48	96.64	110.32
1	A	471	ARG	CB-CG-CD	6.45	126.14	111.30
2	B	282	GLN	N-CA-CB	-6.45	100.32	110.06
1	A	412	ASP	CA-CB-CG	6.43	119.03	112.60
2	B	298	ARG	CB-CA-C	-6.41	98.77	110.63
2	B	200	ARG	CB-CA-C	-6.32	100.95	110.88
1	A	555	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	534	PHE	CA-C-N	6.11	126.15	120.34
1	A	534	PHE	C-N-CA	6.11	126.15	120.34
1	A	437	MET	CB-CA-C	6.03	121.79	110.63
2	B	393	GLU	CB-CA-C	-6.01	100.81	110.79
1	A	500	CYS	CB-CA-C	-5.95	98.09	110.40
1	A	569	TYR	CA-CB-CG	5.90	124.52	113.90
1	A	441	ARG	CD-NE-CZ	5.87	132.62	124.40
2	B	218	LYS	N-CA-CB	5.84	120.08	110.39
1	A	501	ASP	CA-CB-CG	5.79	118.39	112.60
2	B	283	ARG	CA-CB-CG	-5.78	102.53	114.10
2	B	390	GLU	CB-CA-C	5.73	120.42	110.68
2	B	209	LYS	CB-CG-CD	5.72	124.45	111.30
1	A	437	MET	CG-SD-CE	-5.72	88.32	100.90
1	A	471	ARG	NE-CZ-NH2	-5.72	114.06	119.20
2	B	312	ASP	CB-CA-C	-5.70	104.15	111.22
1	A	418	ASN	CA-CB-CG	-5.70	106.90	112.60
1	A	444	LEU	CB-CA-C	5.67	119.79	110.88
2	B	273	LYS	N-CA-CB	5.65	118.44	110.36
1	A	571	ASP	CA-CB-CG	5.63	118.23	112.60
1	A	435	ARG	CG-CD-NE	-5.61	99.66	112.00
2	B	298	ARG	N-CA-CB	5.56	118.78	110.22
2	B	142	ARG	NE-CZ-NH2	5.54	124.19	119.20
2	B	116	HIS	CB-CA-C	5.40	120.35	110.10
1	A	403	GLU	CB-CA-C	5.35	118.29	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	433	THR	N-CA-CB	-5.32	102.78	111.66
2	B	157	ASP	CA-CB-CG	5.28	117.88	112.60
2	B	162	LYS	CB-CG-CD	5.25	123.37	111.30
1	A	515	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	435	ARG	CB-CG-CD	5.23	123.33	111.30
2	B	261	TRP	O-C-N	5.22	129.26	123.05
2	B	212	THR	CA-CB-OG1	-5.20	101.79	109.60
1	A	455	ILE	CA-C-N	-5.19	115.73	122.94
1	A	455	ILE	C-N-CA	-5.19	115.73	122.94
2	B	144	GLU	N-CA-CB	-5.11	101.46	109.78
2	B	217	MET	CG-SD-CE	5.10	112.13	100.90
1	A	453	ASP	CA-CB-CG	5.10	117.70	112.60
2	B	244	GLY	O-C-N	5.09	127.13	122.19
2	B	150	ARG	NE-CZ-NH1	-5.07	116.43	121.50
1	A	411	ASP	CA-CB-CG	5.02	117.62	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	510	THR	Peptide
1	A	564	ARG	Sidechain
2	B	129	ARG	Sidechain
2	B	249	ARG	Sidechain
2	B	254[A]	ARG	Sidechain
2	B	394	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	1643	0	1612	28	0
2	B	2325	0	2269	28	0
3	A	8	0	12	0	0
3	B	12	0	18	1	0
4	A	13	0	0	0	0
5	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	62	0	0	2	1
6	B	166	0	0	1	1
All	All	4231	0	3911	49	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (49) 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:474:HIS:HB3	2:B:298:ARG:NH1	1.89	0.86
1:A:471:ARG:NH2	2:B:399:SER:HA	2.05	0.71
2:B:254[B]:ARG:NH2	6:B:601:HOH:O	2.23	0.71
2:B:180:ARG:NH1	2:B:223:GLU:HG3	2.06	0.70
1:A:474:HIS:HB3	2:B:298:ARG:CZ	2.27	0.64
1:A:372:GLN:HB3	1:A:555:HIS:O	2.02	0.59
2:B:168:MET:HE3	2:B:369:TYR:HA	1.84	0.59
2:B:168:MET:CE	2:B:369:TYR:HD1	2.15	0.59
1:A:383:VAL:HG23	1:A:421:VAL:HG11	1.86	0.57
1:A:419:ILE:N	1:A:420:PRO:CD	2.69	0.56
2:B:168:MET:HE1	2:B:374:TYR:HB2	1.88	0.56
1:A:449:TYR:CD1	1:A:488:LYS:HB2	2.40	0.56
2:B:383:SER:H	3:B:501:DMS:H13	1.70	0.55
1:A:513:LYS:O	6:A:901:HOH:O	2.19	0.53
1:A:542:PRO:O	1:A:543:ASN:HB2	2.09	0.52
1:A:568:ARG:O	1:A:568:ARG:NE	2.42	0.52
1:A:474:HIS:CB	2:B:298:ARG:NH1	2.70	0.50
1:A:456:ILE:HD11	2:B:262:ILE:HD11	1.94	0.50
2:B:198:TYR:O	2:B:202:THR:HB	2.12	0.50
2:B:390:GLU:OE2	2:B:394:ARG:HD3	2.12	0.50
2:B:199:TYR:O	2:B:203:GLY:N	2.38	0.49
2:B:202:THR:HG22	2:B:204:ILE:HB	1.94	0.49
1:A:449:TYR:CE1	1:A:488:LYS:HB2	2.49	0.48
2:B:275:LEU:O	2:B:276:ASP:C	2.57	0.48
1:A:456:ILE:HD11	2:B:262:ILE:CD1	2.43	0.48
2:B:168:MET:O	2:B:358:LEU:HA	2.13	0.47
1:A:512:HIS:O	1:A:513:LYS:HD3	2.14	0.46
1:A:566:LYS:O	1:A:569:TYR:O	2.33	0.46
2:B:202:THR:CG2	2:B:204:ILE:HG12	2.45	0.46
1:A:474:HIS:ND1	2:B:298:ARG:NH2	2.64	0.45
2:B:179:ILE:HG21	2:B:179:ILE:HD13	1.67	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LEU:HD23	1:A:449:TYR:HB2	2.00	0.43
2:B:188:VAL:HA	2:B:230:PHE:O	2.19	0.43
2:B:168:MET:HE3	2:B:369:TYR:HD1	1.81	0.43
1:A:418:ASN:C	1:A:420:PRO:HD2	2.44	0.43
6:A:918:HOH:O	2:B:400:PRO:HD3	2.19	0.42
1:A:382:ASP:CG	1:A:384:SER:HG	2.28	0.42
1:A:457:TRP:O	1:A:480:LYS:HA	2.20	0.42
2:B:264:THR:OG1	2:B:317:GLU:HA	2.20	0.42
2:B:275:LEU:O	2:B:277:PRO:N	2.53	0.42
2:B:151:GLU:O	2:B:152:LEU:C	2.62	0.42
1:A:431:TRP:CD2	1:A:513:LYS:HD2	2.54	0.42
1:A:372:GLN:O	1:A:545:ILE:HA	2.20	0.42
1:A:385:ILE:O	1:A:564:ARG:NH2	2.52	0.42
1:A:400:ILE:O	1:A:400:ILE:HG23	2.20	0.41
2:B:168:MET:CE	2:B:369:TYR:CD1	3.00	0.41
1:A:536:ARG:HB3	1:A:537:PRO:HD2	2.03	0.41
1:A:512:HIS:O	1:A:512:HIS:CD2	2.74	0.41
1:A:399:ASP:OD1	1:A:399:ASP:C	2.64	0.41

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:956:HOH:O	6:B:752:HOH:O[3_455]	2.11	0.09

## 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	201/224 (90%)	188 (94%)	11 (6%)	2 (1%)	12	11
2	B	284/348 (82%)	271 (95%)	12 (4%)	1 (0%)	30	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	485/572 (85%)	459 (95%)	23 (5%)	3 (1%)	21	22

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	CYS
1	A	509	SER
2	B	204	ILE

### 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	178/197 (90%)	169 (95%)	9 (5%)	21	26
2	B	253/295 (86%)	244 (96%)	9 (4%)	31	40
All	All	431/492 (88%)	413 (96%)	18 (4%)	26	34

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	378	ILE
1	A	400	ILE
1	A	421	VAL
1	A	425	ASP
1	A	508	ARG
1	A	529	ARG
1	A	550	GLN
1	A	566	LYS
1	A	568	ARG
2	B	151	GLU
2	B	201	GLU
2	B	202	THR
2	B	207	ASN
2	B	209	LYS
2	B	275	LEU

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Mol	Chain	Res	Type
2	B	278	LYS
2	B	297	LYS
2	B	300	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	495	ASN
1	A	496	GLN
1	A	512	HIS
1	A	550	GLN
2	B	122	HIS
2	B	308	ASN
2	B	332	HIS
2	B	382	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 for Mogul analysis.

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	DMS	A	801	-	3,3,3	0.53	0	3,3,3	0.50	0
3	DMS	B	502	-	3,3,3	1.17	0	3,3,3	0.46	0
3	DMS	B	501	-	3,3,3	0.97	0	3,3,3	0.67	0
4	A1JDK	A	803	-	13,14,14	2.10	2 (15%)	13,17,17	2.39	4 (30%)
3	DMS	A	802	-	3,3,3	0.68	0	3,3,3	0.48	0
3	DMS	B	503	-	3,3,3	0.52	0	3,3,3	0.42	0

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	A1JDK	A	803	-	-	1/4/5/5	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	803	A1JDK	N1-N2	-6.72	1.25	1.39
4	A	803	A1JDK	C5-N3	-2.05	1.32	1.35

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	A1JDK	C7-N4-C5	6.72	108.31	103.42
4	A	803	A1JDK	C7-C6-N3	2.75	110.56	106.41
4	A	803	A1JDK	C6-N3-C5	-2.64	105.48	108.08
4	A	803	A1JDK	C6-C7-N4	-2.13	106.41	109.82

There are no chirality outliers.

All (1) torsion outliers are listed below:

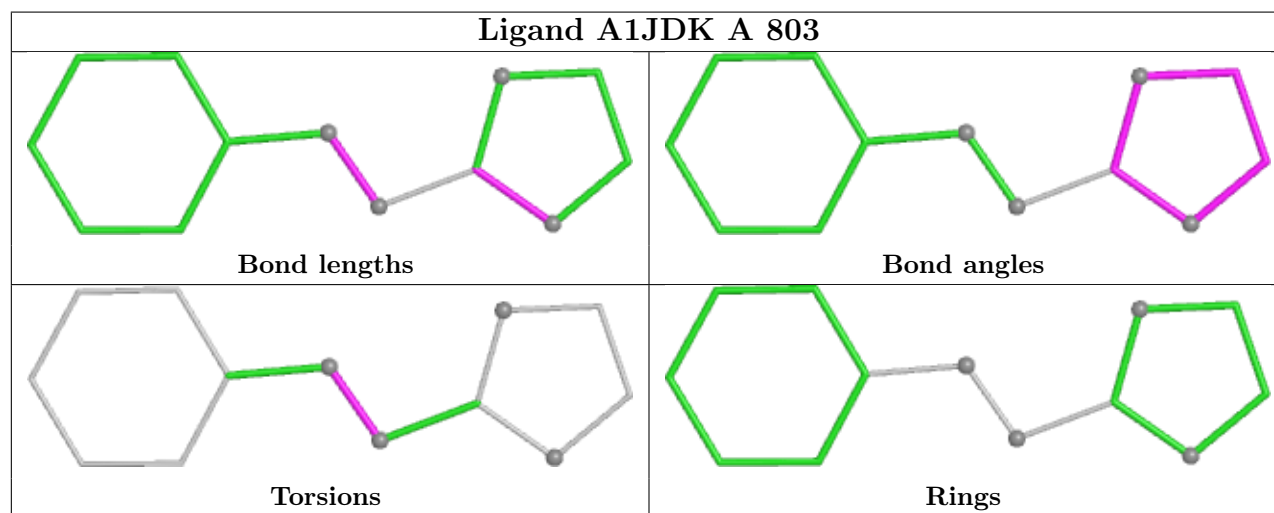
Mol	Chain	Res	Type	Atoms
4	A	803	A1JDK	C4-N1-N2-C5

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	DMS	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	203/224 (90%)	0.24	6 (2%) 52 50	36, 70, 114, 143	0
2	B	285/348 (81%)	-0.28	4 (1%) 73 72	21, 48, 98, 124	1 (0%)
All	All	488/572 (85%)	-0.07	10 (2%) 65 63	21, 55, 109, 143	1 (0%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	275	LEU	4.2
1	A	369	PHE	3.7
1	A	570	PRO	3.6
1	A	509	SER	3.3
1	A	569	TYR	2.9
1	A	512	HIS	2.7
2	B	209	LYS	2.4
2	B	116	HIS	2.3
1	A	403	GLU	2.3
2	B	400	PRO	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](#)

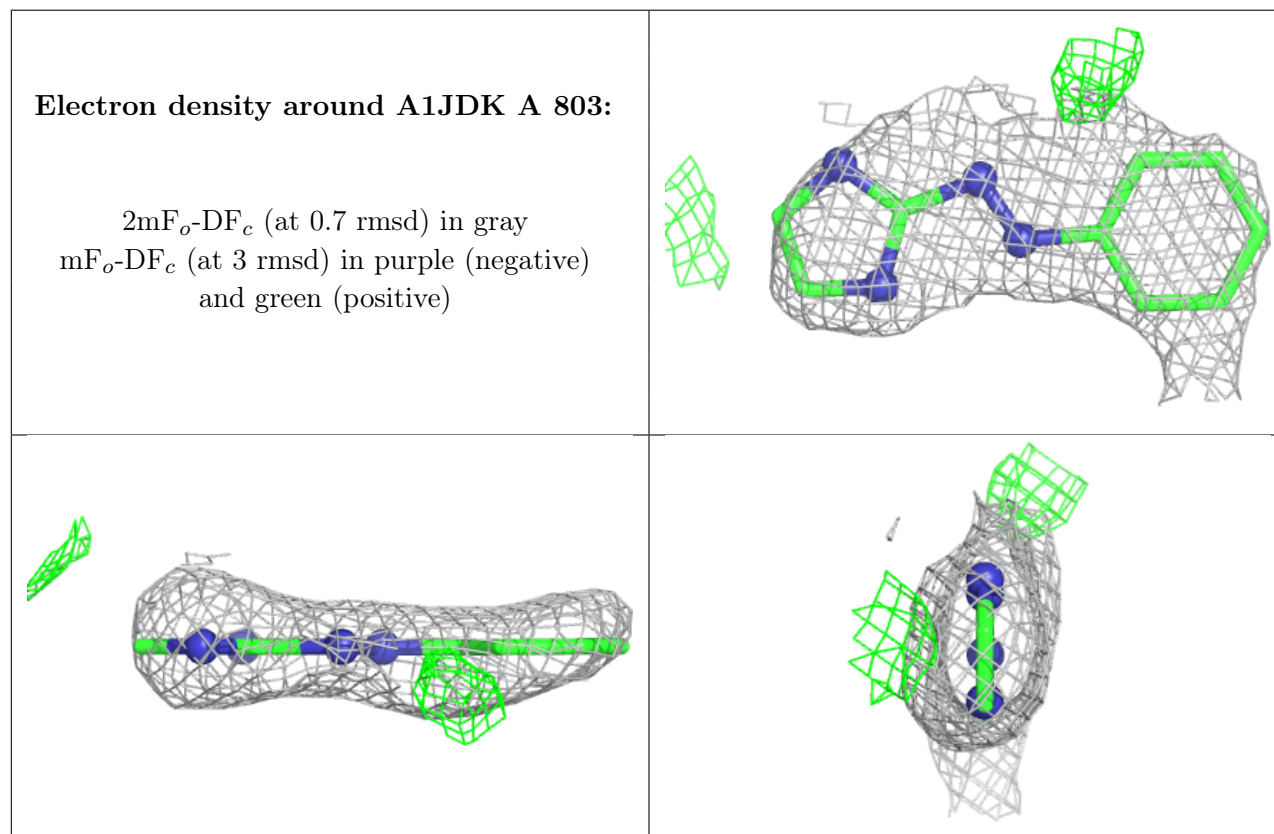
There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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
3	DMS	A	802	4/4	0.54	0.25	99,108,128,145	0
3	DMS	B	501	4/4	0.71	0.25	61,74,78,99	0
3	DMS	B	503	4/4	0.78	0.24	90,104,120,127	0
3	DMS	B	502	4/4	0.81	0.26	66,83,105,115	0
4	A1JDK	A	803	13/13	0.84	0.17	100,108,117,120	0
5	CL	A	804	1/1	0.92	0.13	86,86,86,86	0
5	CL	A	805	1/1	0.94	0.15	85,85,85,85	0
3	DMS	A	801	4/4	0.98	0.07	49,54,55,55	0

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.