

# wwPDB X-ray Structure Validation Summary Report (i)

#### Sep 14, 2020 – 09:43 AM BST

PDB ID : 6TTX

Title : Crystal structure of the human METTL3-METTL14 complex bound to Com-

pound 5 (ASI M3M 051)

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Deposited on : 2019-12-30

Resolution : 2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity: 4.02b-467

Mogul : 1.8.5 (274361), CSD as541be (2020)

Xtriage (Phenix) : 1.13

EDS : FAILED

buster-report : 1.1.7 (2018)

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

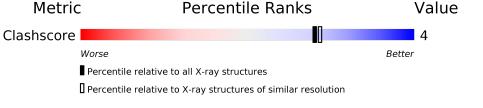
Validation Pipeline (wwPDB-VP) : 2.14.4.dev1

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	Similar resolution
10100110	$(\#  ext{Entries})$	$(\#  ext{Entries},  ext{resolution range}( ext{Å}))$
Clashscore	141614	9178 (2.00-2.00)

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 on 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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain				
1	A	580	31% • 66%				
2	В	456	48%		• 49%		



# 2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 3768 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.

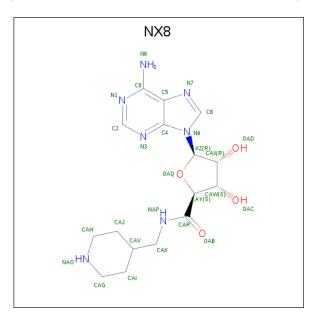
• Molecule 1 is a protein called N6-adenosine-methyltransferase catalytic subunit.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
1	Λ	197	Total	С	N	О	S	0	2	0
1	A	197	1568	1010	270	278	10	0	3	

• Molecule 2 is a protein called N6-adenosine-methyltransferase non-catalytic subunit.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace		
2	В	233	Total 1849	C 1193	N 309	O 334	S 13	0	1	0

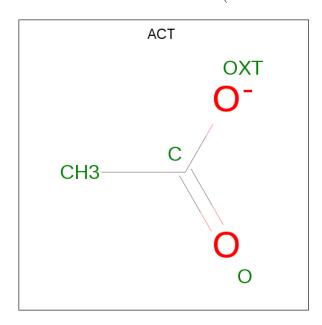
• Molecule 3 is  $(2 \{S\},3 \{S\},4 \{R\},5 \{R\})$ -5-(6-aminopurin-9-yl)-3,4-bis(oxidanyl)-  $\{N\}$ -(pip eridin-4-ylmethyl)oxolane-2-carboxamide (three-letter code: NX8) (formula:  $C_{16}H_{23}N_7O_4$ ) (labeled as "Ligand of Interest" by author).



N	/Iol	Chain	Residues	Atoms		ZeroOcc	AltConf		
	3	A	1	Total 27	C 16	N 7	O 4	0	0



 $\bullet$  Molecule 4 is ACETATE ION (three-letter code: ACT) (formula:  $\mathrm{C_2H_3O_2}).$ 



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

 $\bullet$  Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	133	Total O 133 133	0	0
5	В	187	Total O 187 187	0	0

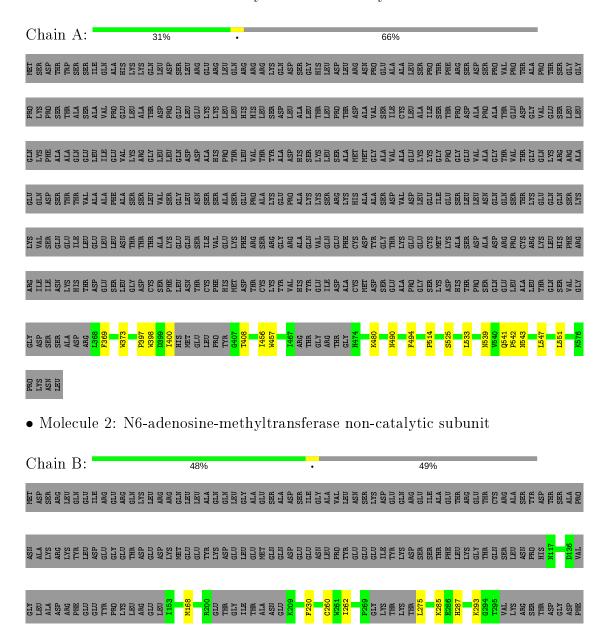


# 3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

• Molecule 1: N6-adenosine-methyltransferase catalytic subunit







GLU
ARG
GLY
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GLY
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GLY
ARG



# 4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants	64.21	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $120.00^{\circ}$	Depositor
Resolution (Å)	44.77 - 2.00	Depositor
% Data completeness	99.6 (44.77-2.00)	Depositor
(in resolution range)	,	_
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.40 \; ({\rm at} \; 2.00 {\rm \AA})$	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
$R, R_{free}$	0.191 , $0.217$	Depositor
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.136	Xtriage
L-test for twinning <sup>2</sup>	$< L > = 0.49, < L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.033  for -h,-k,l	Xtriage
Total number of atoms	3768	wwPDB-VP
Average B, all atoms $(\mathring{A}^2)$	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 3.99% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;sup>2</sup>Theoretical values of <|L|>,  $< L^2>$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: NX8, 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		
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z  > 5	
1	A	0.43	0/1616	0.59	0/2199	
2	В	0.46	0/1896	0.59	0/2574	
All	All	0.45	0/3512	0.59	0/4773	

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	1568	0	1520	13	0
2	В	1849	0	1756	13	0
3	A	27	0	0	0	0
4	В	4	0	3	0	0
5	A	133	0	0	1	1
5	В	187	0	0	1	1
All	All	3768	0	3279	24	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 4.

The worst 5 of 24 close contacts within the same asymmetric unit are listed below, sorted by their



clash magnitude.

Atom-1	Atom-2	$egin{array}{l}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	Clash overlap (Å)
2:B:321:ILE:O	2:B:321:ILE:HD12	1.74	0.87
2:B:168:MET:HE1	2:B:374:TYR:HB2	1.67	0.76
1:A:456[A]:ILE:HG12	2:B:285:LYS:HE2	1.79	0.64
1:A:457:TRP:CE2	1:A:514:PRO:HG3	2.42	0.55
2:B:230:PHE:CE1	2:B:339:LEU:HD22	2.44	0.53

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	$egin{array}{l}  ext{Interatomic} \  ext{distance} \ ( ext{Å}) \end{array}$	$egin{array}{c}  ext{Clash} \  ext{overlap } ( ext{Å}) \end{array}$
5:A:813:HOH:O	5:B:700:HOH:O[6_664]	2.14	0.06

#### 5.3 Torsion angles (i)

#### 5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

### 5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 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)

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).

Mal	Mol Type Ch	Chain	Res	Link	Bond lengths			Bond angles		
MIGI		Chain			Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ACT	В	501	-	1,3,3	9.85	1 (100%)	0,3,3	0.00	-
3	NX8	A	601	-	27,30,30	5.85	10 (37%)	30,43,43	2.20	7 (23%)

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	${f Res}$	Link	Chirals	${f Torsions}$	Rings
3	NX8	A	601	_	-	4/9/37/37	1/4/4/4

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	${f Z}$	$\operatorname{Observed}(\operatorname{\AA})$	$\operatorname{Ideal}( ext{\AA})$
3	A	601	NX8	CAX-CAZ	-17.53	1.27	1.53
3	A	601	NX8	OAQ-CAZ	15.79	1.63	1.41
3	A	601	NX8	CAW-CAY	-15.18	1.34	1.53
4	В	501	ACT	СН3-С	9.85	1.61	1.48
3	A	601	NX8	OAQ-CAY	5.59	1.51	1.43

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^o)$	$\operatorname{Ideal}({}^o)$
3	A	601	NX8	OAQ-CAY-CAR	-5.82	101.39	111.11
3	A	601	NX8	CAK-NAP-CAR	-4.51	114.06	122.67
3	A	601	NX8	N3-C2-N1	-4.28	121.99	128.68
3	A	601	NX8	CAY-CAR-NAP	3.77	120.14	115.47
3	A	601	NX8	CAX-CAW-CAY	3.60	105.83	101.64

There are no chirality outliers.



All (4) torsion outliers are listed below:

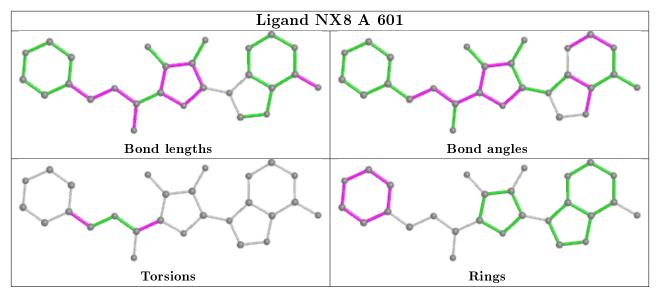
Mol	Chain	Res	Type	Atoms
3	A	601	NX8	NAP-CAK-CAV-CAJ
3	A	601	NX8	NAP-CAK-CAV-CAI
3	A	601	NX8	OAB-CAR-CAY-OAQ
3	A	601	NX8	NAP-CAR-CAY-OAQ

All (1) ring outliers are listed below:

Mol	Chain	${f Res}$	Type	${f Atoms}$
3	A	601	NX8	CAG-CAH-CAI-CAJ-CAV-NAO

No monomer is involved in short contacts.

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 then 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)

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates (i)

EDS failed to run properly - this section is therefore empty.

#### 6.4 Ligands (i)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers (i)

EDS failed to run properly - this section is therefore empty.

