



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 4, 2020 – 01:29 pm BST

PDB ID : 6NTJ  
Title : Neutron/X-ray crystal structure of AAC-VIa bound to gentamicin C1A  
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Deposited on : 2019-01-29  
Resolution : 1.90 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](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.

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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)  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
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) : 2.11

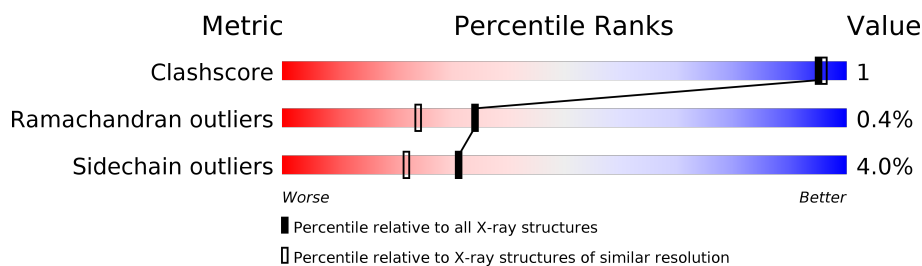
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION, NEUTRON DIFFRACTION*

The reported resolution of this entry is 1.90 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))
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	302	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 4952 atoms, of which 2007 are hydrogens and 737 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 Aminoglycoside N(3)-acetyltransferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	267	Total	C	D	H	N	O	S	152	244	0
			4417	1278	427	1968	366	372	6			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP C4NV15
A	-1	SER	-	expression tag	UNP C4NV15
A	0	HIS	-	expression tag	UNP C4NV15

- Molecule 2 is a ligand with the chemical component id LLL but its atom names do not match the existing wwPDB Chemical Component Dictionary definition for LLL. ERROR THIS SHOULD NOT HAPPEN FOLLOWING ANNOTATION.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	D	H	N	O		6	1
			82	19	12	39	5	7			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	154	Total	D	O	0	0
			452	298	154		

**i**

Note EDS failed to run properly.

- Molecule 1: Aminoglycoside N(3)-acetyltransferase

ALA	GLY	
ALA	SER	
LEU	HIS	
LYS	MET	
PRO	THR	
LYS	ASP	
GLN	PRO	
ARG	ARG	
ARG	LYS	
ASP	ASN	
	GLY	
	ASP	
	LEU	
	HIS	
	GLU	
	PRO	
	ALA	
	THR	
	ALA	
	PRO	
	ALA	T19
		R28
		R36
		Y40
		L75
		N80
		E96
		L99
		D92
		I119
		R124
		I165
		P208
		L209
		L210
		R215
		Q263
		R283
		A284
		A285
		ALA
		PRO
		ALA
		ALA

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.32Å 86.23Å 51.00Å 90.00° 120.40° 90.00°	Depositor
Resolution (Å)	43.11 – 1.90	Depositor
% Data completeness (in resolution range)	98.3 (43.11-1.90)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.24 (at 1.89Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, $R_{free}$	0.157 , 0.200	Depositor
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.357	Xtriage
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
Total number of atoms	4952	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.36% 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: MG, LLL

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	1.07	4/3976 (0.1%)	1.06	16/5434 (0.3%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	86[A]	GLU	CD-OE2	5.90	1.32	1.25
1	A	86[B]	GLU	CD-OE2	5.90	1.32	1.25
1	A	80[A]	TRP	CB-CG	5.04	1.59	1.50
1	A	80[B]	TRP	CB-CG	5.04	1.59	1.50

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283[A]	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	283[B]	ARG	NE-CZ-NH1	-7.70	116.45	120.30
1	A	215[A]	ARG	CB-CG-CD	-7.02	93.35	111.60
1	A	215[B]	ARG	CB-CG-CD	-7.02	93.35	111.60
1	A	36[A]	ARG	NE-CZ-NH2	-6.64	116.98	120.30

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	2449	1968	161	0	0
2	A	43	39	0	0	0
3	A	1	0	0	0	0
4	A	452	0	0	1	0
All	All	2945	2007	161	1	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 1.

All (1) 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)
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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	507/302 (168%)	489 (96%)	17 (3%)	1 (0%)	47 38

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	PRO

### 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	379/226 (168%)	363 (96%)	16 (4%)	30	20

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89[B]	LEU
1	A	92[A]	ASP
1	A	165[A]	ILE
1	A	89[A]	LEU
1	A	165[B]	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 3 ligands modelled in this entry, 1 could not be matched to an existing wwPDB Chemical Component Dictionary definition at this stage and 1 is monoatomic - leaving 1 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



## 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 ⓘ

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

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

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

### 6.3 Carbohydrates ⓘ

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

### 6.4 Ligands ⓘ

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

### 6.5 Other polymers ⓘ

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