



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 06:53 PM UTC

PDB ID : 6NTI / pdb_00006nti
Title : Neutron/X-ray crystal structure of AAC-VIa bound to kanamycin b
Authors : Cuneo, M.J.; Kumar, P.
Deposited on : 2019-01-29
Resolution : 2.30 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

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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	FAILED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

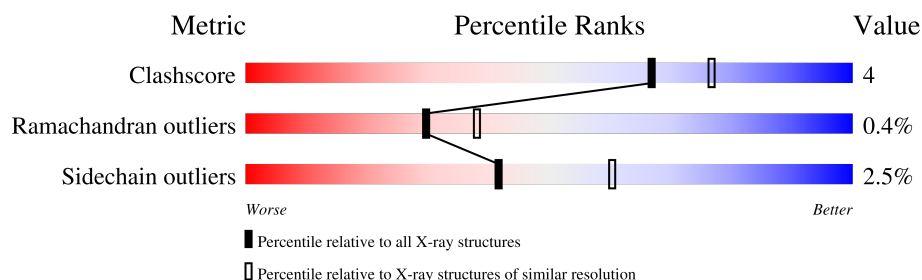
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION, NEUTRON DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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 ≥ 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 4726 atoms, of which 2014 are hydrogens and 581 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.

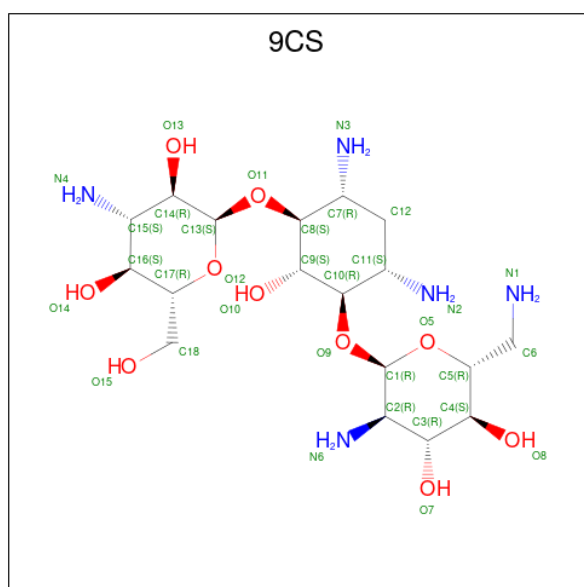
- Molecule 1 is a protein called Aminoglycoside N(3)-acetyltransferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
			Total	C	D	H	N	O	S			
1	A	268	4429	1281	425	1977	367	373	6	87	245	0

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 (1R,2S,3S,4R,6S)-4,6-DIAMINO-3-[(3-AMINO-3-DEOXY-ALPHA-D-GLUCOPYRANOSYL)OXY]-2-HYDROXYCYCLOHEXYL 2,6-DIAMINO-2,6-DIDEOXY-ALPHA-D-GLUCOPYRANOSIDE (CCD ID: 9CS) (formula: C₁₈H₃₇N₅O₁₀).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	D	H	N	O		
2	A	1	86	18	16	37	5	10	10	1

- Molecule 3 is MAGNESIUM ION (CCD ID: 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	70	Total	D	O	1	0
			210	140	70		

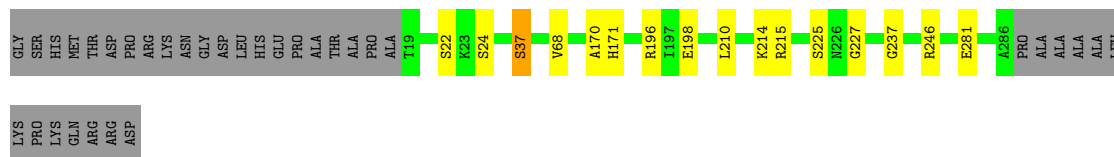
3 Residue-property plots [i](#)

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: Aminoglycoside N(3)-acetyltransferase

Chain A:  83% 5% 11%



4 Data and refinement statistics

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

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	51.36Å 86.06Å 77.60Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	14.00 – 2.30	Depositor
% Data completeness (in resolution range)	86.0 (14.00-2.30)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.237 , 0.257	Depositor
Wilson B-factor (Å ²)	41.1	Xtriage
Anisotropy	0.496	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4726	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 9CS, MG

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	0.63	18/3986 (0.5%)	0.48	0/5448

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	214[A]	LYS	C-N	14.65	1.53	1.33
1	A	214[B]	LYS	C-N	14.65	1.53	1.33
1	A	22[A]	SER	C-N	10.80	1.47	1.33
1	A	22[B]	SER	C-N	10.80	1.47	1.33
1	A	24[A]	SER	C-N	-7.29	1.24	1.33
1	A	24[B]	SER	C-N	-7.29	1.24	1.33
1	A	225[A]	SER	C-N	7.23	1.43	1.33
1	A	225[B]	SER	C-N	7.23	1.43	1.33
1	A	246[A]	ARG	C-N	-7.15	1.24	1.33
1	A	246[B]	ARG	C-N	-7.15	1.24	1.33
1	A	227[A]	GLY	C-N	6.42	1.41	1.33
1	A	227[B]	GLY	C-N	6.42	1.41	1.33
1	A	170[A]	ALA	C-N	-6.10	1.24	1.33
1	A	170[B]	ALA	C-N	-6.10	1.24	1.33
1	A	171[A]	HIS	C-N	5.33	1.41	1.33
1	A	171[B]	HIS	C-N	5.33	1.41	1.33
1	A	37[A]	SER	C-N	5.05	1.41	1.33
1	A	37[B]	SER	C-N	5.05	1.41	1.33

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

CLOSE-CONTACTS INFOmissingINFO

5.2 Torsion angles [i](#)

5.2.1 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	509/302 (168%)	492 (97%)	15 (3%)	2 (0%)	30	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	237[A]	GLY
1	A	237[B]	GLY

5.2.2 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%)	369 (97%)	10 (3%)	40	59

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37[A]	SER
1	A	37[B]	SER
1	A	68[A]	VAL
1	A	68[B]	VAL
1	A	198[A]	GLU
1	A	198[B]	GLU
1	A	210[A]	LEU
1	A	210[B]	LEU
1	A	215[A]	ARG

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Mol	Chain	Res	Type
1	A	215[B]	ARG

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

5.2.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.4 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.5 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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.

5.6 Other polymers [i](#)

There are no such residues in this entry.

5.7 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.