



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 01:34 PM EDT

PDB ID : 6NLT
Title : Apo structure of the T130K mutant of ANT-4
Authors : Selvaraj, B.; Cuneo, M.J.
Deposited on : 2019-01-09
Resolution : 1.90 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 : **FAILED**
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) : 2.35.1

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 1.90 Å.

There are no overall percentile quality scores available for this entry.

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4682 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 Kanamycin nucleotidyltransferase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| | | | Total | C | N | O | S | | | |
| 1 | A | 253 | 2058 | 1308 | 335 | 400 | 15 | 0 | 4 | 0 |
| 1 | B | 252 | 2064 | 1309 | 336 | 406 | 13 | 0 | 7 | 0 |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|---------------------|------------|
| A | -2 | GLY | - | expression tag | UNP P05057 |
| A | -1 | SER | - | expression tag | UNP P05057 |
| A | 0 | HIS | - | expression tag | UNP P05057 |
| A | 130 | LYS | THR | engineered mutation | UNP P05057 |
| B | -2 | GLY | - | expression tag | UNP P05057 |
| B | -1 | SER | - | expression tag | UNP P05057 |
| B | 0 | HIS | - | expression tag | UNP P05057 |
| B | 130 | LYS | THR | engineered mutation | UNP P05057 |

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|------------|---------|---------|---------|
| 2 | A | 2 | Total 2 | Ca 2 | 0 | 0 |
| 2 | B | 1 | Total 1 | Ca 1 | 0 | 0 |

- Molecule 3 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|-----|-------|----------|--------------|----------|---------|---------|
| 3 | A | 289 | Total 289 | O 289 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|------------|--------------|-----------------|--------------|----------|----------------|----------------|
| 3 | B | 268 | Total 268 | O 268 | 0 | 0 |

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

3 Data and refinement statistics i

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

| Property | Value | Source |
|--|---|-----------|
| Space group | P 21 21 21 | Depositor |
| Cell constants a, b, c, α , β , γ | 57.25Å 97.65Å 101.08Å 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.39 – 1.90 | Depositor |
| % Data completeness (in resolution range) | 99.0 (49.39-1.90) | Depositor |
| R_{merge} | 0.04 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $\langle I/\sigma(I) \rangle$ ¹ | 2.81 (at 1.90Å) | Xtrriage |
| Refinement program | PHENIX (1.13_2998: ???) | Depositor |
| R, R_{free} | 0.175 , 0.215 | Depositor |
| Wilson B-factor (Å ²) | 18.5 | Xtrriage |
| Anisotropy | 0.360 | Xtrriage |
| L-test for twinning ² | $\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$ | Xtrriage |
| Estimated twinning fraction | 0.010 for -h,l,k | Xtrriage |
| Total number of atoms | 4682 | wwPDB-VP |
| Average B, all atoms (Å ²) | 22.0 | wwPDB-VP |

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.66% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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.

4 Model quality [i](#)

4.1 Standard geometry [i](#)

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4.2 Too-close contacts [i](#)

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4.3 Torsion angles [i](#)

4.3.1 Protein backbone [i](#)

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4.3.2 Protein sidechains [i](#)

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

4.3.3 RNA [i](#)

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

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

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

4.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

4.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 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.

4.7 Other polymers [i](#)

There are no such residues in this entry.

4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

5 Fit of model and data [i](#)

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

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

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

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5.3 Carbohydrates [i](#)

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5.4 Ligands [i](#)

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5.5 Other polymers [i](#)

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