# Full wwPDB X-ray Structure Validation Report ⓘ

May 4, 2024 – 06:10 pm BST

| | | |
|---|---|---|
| PDB ID | : | 6RC3 |
| Title | : | Crystal structure of NAD kinase 1 from Listeria monocytogenes in complexe with an adenine derivative |
| Authors | : | Gelin, M.; Labesse, G. |
| Deposited on | : | 2019-04-11 |
| Resolution | : | 2.31 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 | : | 4.02b-467 |
| Mogul | : | 1.8.4, CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36.2 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36.2 |

PERCENTILES INFOmissingINFO

# 1 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2133 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.

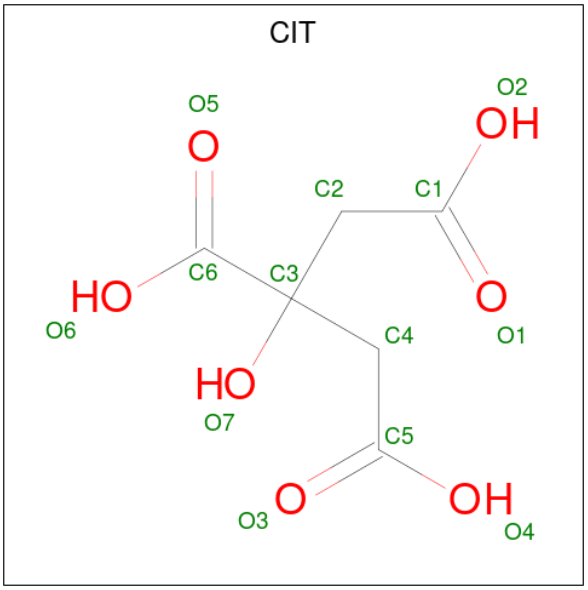
- Molecule 1 is a protein called NAD kinase 1.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 258 | Total | C | N | O | S | 0 | 2 | 0 |
| | | | 2050 | 1315 | 343 | 383 | 9 | | | |

There are 8 discrepancies between the modelled and reference sequences:

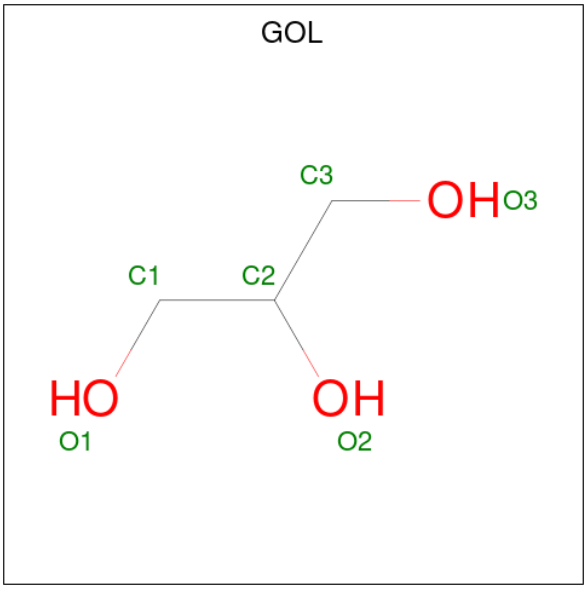
| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 265 | LEU | - | expression tag | UNP Q8Y8D7 |
| A | 266 | GLU | - | expression tag | UNP Q8Y8D7 |
| A | 267 | HIS | - | expression tag | UNP Q8Y8D7 |
| A | 268 | HIS | - | expression tag | UNP Q8Y8D7 |
| A | 269 | HIS | - | expression tag | UNP Q8Y8D7 |
| A | 270 | HIS | - | expression tag | UNP Q8Y8D7 |
| A | 271 | HIS | - | expression tag | UNP Q8Y8D7 |
| A | 272 | HIS | - | expression tag | UNP Q8Y8D7 |

- Molecule 2 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



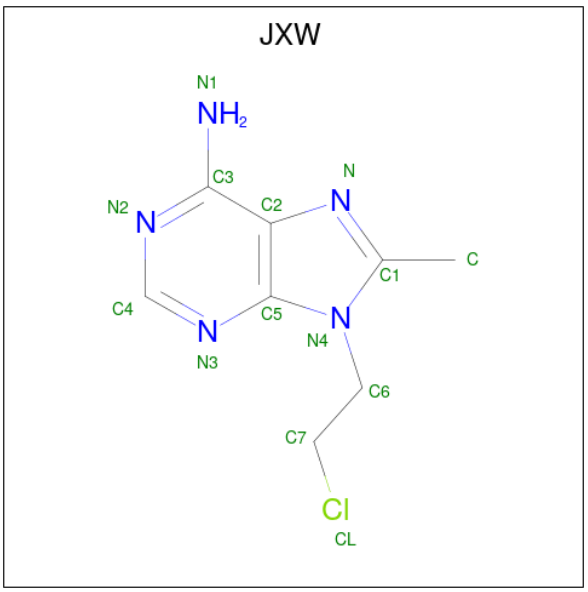
| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 2 | A | 1 | Total C O<br>13 6 7 | 0 | 0 |

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).




| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|---|---|---|---|---|---|
| 3 | A | 1 | Total C O<br>6 3 3 | 0 | 0 |

- Molecule 4 is 9-(2-chloroethyl)-8-methyl-purin-6-amine (three-letter code: JXW) (formula: $C_8H_{10}ClN_5$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|---|---|
| 4 | A | 1 | Total | C | Cl | N | 0 | 0 |
| | | | 14 | 8 | 1 | 5 | | |

- Molecule 5 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| 5 | A | 50 | Total | O | 0 | 0 |
| | | | 50 | 50 | | |

SEQUENCE-PLOTS INFOmissingINFO

## 2 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | I 2 2 2 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 62.83Å 73.91Å 118.46Å<br>90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 36.95 – 2.31<br>59.23 – 2.32 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 74.2 (36.95-2.31)<br>74.2 (59.23-2.32) | Depositor<br>EDS |
| $R_{merge}$ | 0.06 | Depositor |
| $R_{sym}$ | 0.06 | Depositor |
| $< I/\sigma(I) >$ [1] | 8.00 (at 2.32Å) | Xtriage |
| Refinement program | PHENIX 1.14_3260 | Depositor |
| R, $R_{free}$ | 0.208 , 0.238<br>0.208 , 0.238 | Depositor<br>DCC |
| $R_{free}$ test set | 917 reflections (9.99%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 47.0 | Xtriage |
| Anisotropy | 0.077 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.34 , 68.4 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.48$, $< L^2 > = 0.32$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.93 | EDS |
| Total number of atoms | 2133 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 59.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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.

# 3 Model quality

## 3.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: JXW, GOL, CIT

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 | 0.25 | 0/2112 | 0.43 | 0/2854 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

## 3.2 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 | 2050 | 0 | 1986 | 12 | 0 |
| 2 | A | 13 | 0 | 5 | 1 | 0 |
| 3 | A | 6 | 0 | 8 | 0 | 0 |
| 4 | A | 14 | 0 | 0 | 0 | 0 |
| 5 | A | 50 | 0 | 0 | 0 | 0 |
| All | All | 2133 | 0 | 1999 | 12 | 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 3.

All (12) 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:108:LYS:HG2 | 1:A:115:GLU:HG2 | 1.81 | 0.60 |
| 1:A:38:ILE:HG21 | 1:A:90:LEU:HD11 | 1.88 | 0.54 |
| 1:A:65:ILE:HG21 | 1:A:86:LEU:HD21 | 1.90 | 0.53 |
| 1:A:160:THR:HA | 1:A:164:ASN:HB3 | 1.95 | 0.49 |
| 1:A:90:LEU:HD23 | 1:A:248:PHE:HZ | 1.77 | 0.49 |
| 1:A:24:PHE:HD1 | 1:A:29:MET:HG3 | 1.82 | 0.45 |
| 1:A:66:GLY:HA3 | 1:A:76:ALA:HA | 2.00 | 0.44 |
| 1:A:182:THR:HG22 | 1:A:198:PRO:HB3 | 2.01 | 0.42 |
| 1:A:172:MET:HE1 | 1:A:178:ALA:HB3 | 2.01 | 0.41 |
| 1:A:101:PRO:HG2 | 1:A:157:PRO:HG2 | 2.02 | 0.41 |
| 1:A:100:TYR:OH | 2:A:301:CIT:O6 | 2.38 | 0.41 |
| 1:A:24:PHE:CD1 | 1:A:29:MET:HG3 | 2.56 | 0.41 |

There are no symmetry-related clashes.

## 3.3 Torsion angles (i)

### 3.3.1 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 | 254/272 (93%) | 242 (95%) | 12 (5%) | 0 | 100 100 |

There are no Ramachandran outliers to report.

### 3.3.2 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 | 222/237 (94%) | 217 (98%) | 5 (2%) | 50 66 |

All (5) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|---|---|---|---|
| 1 | A | 60 | ASP |
| 1 | A | 123 | GLU |
| 1 | A | 172 | MET |
| 1 | A | 247 | ARG |
| 1 | A | 251 | PHE |

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

#### 3.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

### 3.5 Carbohydrates (i)

There are no monosaccharides in this entry.

### 3.6 Ligand geometry (i)

3 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).

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\| > 2$ | Counts | RMSZ | $\#\|Z\| > 2$ |
| 3 | GOL | A | 302 | - | 5,5,5 | 0.88 | 0 | 5,5,5 | 1.01 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 4 | JXW | A | 303 | - | 11,15,15 | 0.76 | 0 | 9,21,21 | 1.26 | 2 (22%) |
| 2 | CIT | A | 301 | - | 12,12,12 | 1.03 | 0 | 17,17,17 | 1.52 | 1 (5%) |

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 |
|---|---|---|---|---|---|---|---|
| 3 | GOL | A | 302 | - | - | 0/4/4/4 | - |
| 4 | JXW | A | 303 | - | - | 2/3/3/3 | 0/2/2/2 |
| 2 | CIT | A | 301 | - | - | 7/16/16/16 | - |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 2 | A | 301 | CIT | O6-C6-C3 | 3.99 | 119.98 | 113.05 |
| 4 | A | 303 | JXW | C2-C3-N1 | 2.36 | 123.94 | 120.35 |
| 4 | A | 303 | JXW | C7-C6-N4 | -2.27 | 109.97 | 112.60 |

There are no chirality outliers.

All (9) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 2 | A | 301 | CIT | C2-C3-C6-O5 |
| 2 | A | 301 | CIT | C2-C3-C6-O6 |
| 2 | A | 301 | CIT | O7-C3-C6-O5 |
| 2 | A | 301 | CIT | O7-C3-C6-O6 |
| 4 | A | 303 | JXW | N4-C6-C7-CL |
| 2 | A | 301 | CIT | C2-C3-C4-C5 |
| 2 | A | 301 | CIT | C6-C3-C4-C5 |
| 4 | A | 303 | JXW | C7-C6-N4-C5 |
| 2 | A | 301 | CIT | O7-C3-C4-C5 |

There are no ring outliers.

1 monomer is involved in 1 short contact:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|---|---|---|---|---|---|
| 2 | A | 301 | CIT | 1 | 0 |

## 3.7 Other polymers (i)

There are no such residues in this entry.

## 3.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

# 4 Fit of model and data

## 4.1 Protein, DNA and RNA chains

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, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|
| 1 | A | 258/272 (94%) | 0.15 | 2 (0%) 86 89 | 25, 57, 90, 107 | 44 (17%) |

All (2) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 110 | GLY | 4.3 |
| 1 | A | 31 | TYR | 2.2 |

## 4.2 Non-standard residues in protein, DNA, RNA chains

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

## 4.3 Carbohydrates

There are no monosaccharides in this entry.

## 4.4 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, $95^{th}$ 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$^2$) | Q<0.9 |
|---|---|---|---|---|---|---|---|---|
| 3 | GOL | A | 302 | 6/6 | 0.82 | 0.13 | 76,77,78,78 | 0 |
| 4 | JXW | A | 303 | 14/14 | 0.82 | 0.22 | 78,84,93,97 | 0 |
| 2 | CIT | A | 301 | 13/13 | 0.85 | 0.20 | 81,85,88,88 | 0 |

## 4.5 Other polymers (i)

There are no such residues in this entry.