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

Oct 2, 2023 – 04:52 AM EDT

| | | |
|---|---|---|
| PDB ID | : | 6NFJ |
| Title | : | Structure of Beta-Klotho in Complex with FGF19 C-terminal peptide |
| Authors | : | Kuzina, E.; Schlessinger, J.; Lee, S. |
| Deposited on | : | 2018-12-20 |
| Resolution | : | 3.19 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) 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 (i)

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

The reported resolution of this entry is 3.19 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 14271 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 Beta-klotho.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | A | 844 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6373 | 4149 | 1076 | 1126 | 22 | | | |
| 1 | D | 846 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 6129 | 3969 | 1051 | 1088 | 21 | | | |

There are 14 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 308 | GLN | ASN | engineered mutation | UNP Q86Z14 |
| A | 611 | GLN | ASN | engineered mutation | UNP Q86Z14 |
| A | 985 | ASN | - | expression tag | UNP Q86Z14 |
| A | 986 | LEU | - | expression tag | UNP Q86Z14 |
| A | 987 | TYR | - | expression tag | UNP Q86Z14 |
| A | 988 | PHE | - | expression tag | UNP Q86Z14 |
| A | 989 | GLN | - | expression tag | UNP Q86Z14 |
| D | 308 | GLN | ASN | engineered mutation | UNP Q86Z14 |
| D | 611 | GLN | ASN | engineered mutation | UNP Q86Z14 |
| D | 985 | ASN | - | expression tag | UNP Q86Z14 |
| D | 986 | LEU | - | expression tag | UNP Q86Z14 |
| D | 987 | TYR | - | expression tag | UNP Q86Z14 |
| D | 988 | PHE | - | expression tag | UNP Q86Z14 |
| D | 989 | GLN | - | expression tag | UNP Q86Z14 |

- Molecule 2 is a protein called Nanobody 30.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | B | 111 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 762 | 490 | 136 | 132 | 4 | | | |
| 2 | E | 113 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 763 | 488 | 135 | 136 | 4 | | | |

- Molecule 3 is a protein called Fibroblast growth factor 19.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | C | 19 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 122 | 77 | 19 | 25 | 1 | | | |
| 3 | F | 19 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 122 | 77 | 19 | 25 | 1 | | | |

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 | C 1 2 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 130.09Å 143.90Å 141.05Å<br>90.00° 90.90° 90.00° | Depositor |
| Resolution (Å) | 59.42 – 3.19 | Depositor |
| % Data completeness<br>(in resolution range) | 97.8 (59.42-3.19) | Depositor |
| $R_{merge}$ | (Not available) | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.11 (at 3.19Å) | Xtriage |
| Refinement program | PHENIX (1.13_2998: ???) | Depositor |
| R, $R_{free}$ | 0.280 , 0.320 | Depositor |
| Wilson B-factor (Å$^2$) | 77.8 | Xtriage |
| Anisotropy | 0.438 | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.38$, $< L^2 > = 0.21$ | Xtriage |
| Estimated twinning fraction | 0.064 for -h,-k,l | Xtriage |
| Total number of atoms | 14271 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 80.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 55.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2847e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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.

# 4 Model quality

## 4.1 Standard geometry

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

## 4.2 Too-close contacts

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

## 4.3 Torsion angles

### 4.3.1 Protein backbone

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

### 4.3.2 Protein sidechains

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

### 4.3.3 RNA

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

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

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

## 4.5 Carbohydrates

There are no monosaccharides in this entry.

## 4.6 Ligand geometry

There are no ligands in this entry.

## 4.7 Other polymers

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

## 5.1 Protein, DNA and RNA chains

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

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

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

## 5.3 Carbohydrates

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

## 5.4 Ligands

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

## 5.5 Other polymers

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