

Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2024 – 07:09 pm BST

PDB ID : 8RLJ

Title: Structure of the apo form of PIB-1 in an Orthorombic space group

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Deposited on : 2024-01-03

Resolution : 2.45 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 (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 (1)) 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) : 2.37.1

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 2.45 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 2 unique types of molecules in this entry. The entry contains 18086 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 Class C beta-lactamese-related serine hydrolase.

| Mol | Chain | Residues | | Ato | oms | | | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 1 | A | 346 | Total | С | N | О | S | 0 | 0 | 0 |
| 1 | Λ | 340 | 2739 | 1730 | 488 | 514 | 7 | | 0 | |
| 1 | В | 385 | Total | С | N | О | S | 0 | 0 | 0 |
| 1 | Ъ | 369 | 3041 | 1927 | 536 | 571 | 7 | 0 | U | |
| 1 | С | 386 | Total | С | N | О | S | 0 | 0 | 0 |
| 1 | | 360 | 3048 | 1932 | 537 | 572 | 7 | 0 | U | |
| 1 | D | 382 | Total | С | N | O | S | 0 | 0 | 0 |
| 1 | D | 302 | 3020 | 1916 | 533 | 564 | 7 | 0 | U | |
| 1 | E | 383 | Total | С | N | Ο | S | 0 | 0 | 0 |
| 1 | Ľ | 303 | 3033 | 1923 | 534 | 569 | 7 | 0 | U | U |
| 1 | F | 372 | Total | С | N | О | S | 0 | 0 | 0 |
| 1 | I. | 312 | 2953 | 1874 | 520 | 552 | 7 | 0 | U | |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|------------------|----------------|
| A | 25 | PRO | ALA | cloning artifact | UNP A0A1J0J3U4 |
| В | 25 | PRO | ALA | _ | UNP A0A1J0J3U4 |
| С | 25 | PRO | ALA | cloning artifact | UNP A0A1J0J3U4 |
| D | 25 | PRO | ALA | cloning artifact | UNP A0A1J0J3U4 |
| Е | 25 | PRO | ALA | cloning artifact | UNP A0A1J0J3U4 |
| F | 25 | PRO | ALA | cloning artifact | UNP A0A1J0J3U4 |

• Molecule 2 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2 | A | 37 | Total O 37 37 | 0 | 0 |
| 2 | В | 43 | Total O 43 43 | 0 | 0 |
| 2 | С | 63 | Total O 63 63 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 2 | D | 51 | Total O 51 51 | 0 | 0 |
| 2 | E | 35 | Total O 35 35 | 0 | 0 |
| 2 | F | 23 | Total O 23 23 | 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 | 77.76Å 100.82Å 269.67Å | Depositor |
| a, b, c, α , β , γ | 90.00° 90.00° 90.00° | Depositor |
| Resolution (Å) | 49.55 - 2.45 | Depositor |
| % Data completeness | 99.8 (49.55-2.45) | Depositor |
| (in resolution range) | | |
| R_{merge} | (Not available) | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | 0.64 (at 2.45Å) | Xtriage |
| Refinement program | PHENIX dev_4746, PHENIX dev_4746 | Depositor |
| R, R_{free} | 0.222 , 0.271 | Depositor |
| Wilson B-factor (A^2) | 37.2 | Xtriage |
| Anisotropy | 0.464 | Xtriage |
| L-test for twinning ² | $< L > = 0.47, < L^2> = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 18086 | wwPDB-VP |
| Average B, all atoms (\mathring{A}^2) | 51.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.

²Theoretical 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.



¹Intensities estimated from amplitudes.

4 Model quality (i)

4.1 Standard geometry (i)

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

4.2 Too-close contacts (i)

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

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

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

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)

There are no ligands in this entry.

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)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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

