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

Dec 3, 2023 – 02:03 pm GMT

| | | |
|---|---|---|
| PDB ID | : | 1UVI |
| Title | : | The structural basis for RNA specificity and Ca2 inhibition of an RNA-dependent RNA polymerase phi6p2 with 6nt RNA |
| Authors | : | Salgado, P.S.; Makeyev, E.V.; Butcher, S.; Bamford, D.; Stuart, D.I.; Grimes, J.M. |
| Deposited on | : | 2004-01-21 |
| Resolution | : | 2.15 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:

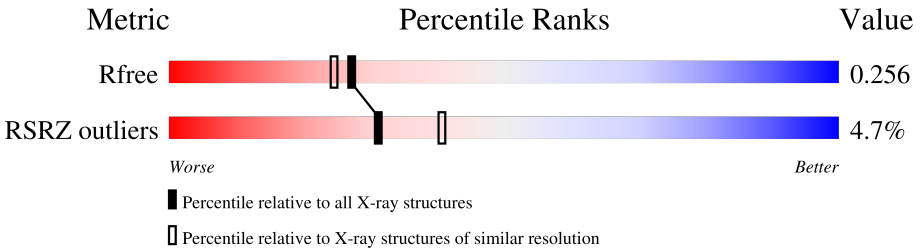
| | | |
|---|---|---|
| MolProbity | : | FAILED |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | 2.36 |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Refmac | : | 5.8.0158 |
| CCP4 | : | 7.0.044 (Gargrove) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.36 |

# 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 2.15 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)) |
|---|---|---|
| $R_{free}$ | 130704 | 1479 (2.16-2.16) |
| RSRZ outliers | 127900 | 1456 (2.16-2.16) |

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

# 2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16447 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 RNA-directed RNA polymerase.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | S | | | |
| 1 | A | 664 | 5265 | 3342 | 914 | 977 | 32 | 0 | 0 | 0 |
| 1 | B | 664 | 5265 | 3342 | 914 | 977 | 32 | 0 | 0 | 0 |
| 1 | C | 664 | 5265 | 3342 | 914 | 977 | 32 | 0 | 0 | 0 |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| A | 456 | MET | ILE | conflict | UNP P11124 |
| B | 456 | MET | ILE | conflict | UNP P11124 |
| C | 456 | MET | ILE | conflict | UNP P11124 |

- Molecule 2 is a RNA chain called 5'-R(*UP*UP*UP*UP*CP*CP)-3'.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | Total | C | N | O | P | | | |
| 2 | D | 4 | 77 | 36 | 10 | 28 | 3 | 0 | 0 | 0 |
| 2 | E | 4 | 77 | 36 | 10 | 28 | 3 | 0 | 0 | 0 |
| 2 | F | 4 | 77 | 36 | 10 | 28 | 3 | 0 | 0 | 0 |

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mn | | |
| 3 | A | 1 | 1 | 1 | 0 | 0 |
| 3 | B | 1 | 1 | 1 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | Mn | | |
| 3 | C | 1 | 1 | 1 | 0 | 0 |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms | | ZeroOcc | AltConf |
|---|---|---|---|---|---|---|
| | | | Total | O | | |
| 4 | A | 116 | 116 | 116 | 0 | 0 |
| | | | Total | O | | |
| 4 | B | 192 | 192 | 192 | 0 | 0 |
| | | | Total | O | | |
| 4 | C | 109 | 109 | 109 | 0 | 0 |
| | | | Total | O | | |
| 4 | D | 1 | 1 | 1 | 0 | 0 |

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# 3 Data and refinement statistics (i)

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 105.13Å 93.71Å 140.74Å<br>90.00° 101.22° 90.00° | Depositor |
| Resolution (Å) | 19.93 – 2.15<br>19.93 – 2.15 | Depositor<br>EDS |
| % Data completeness<br>(in resolution range) | 97.8 (19.93-2.15)<br>97.9 (19.93-2.15) | Depositor<br>EDS |
| $R_{merge}$ | 0.13 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 1.92 (at 2.15Å) | Xtriage |
| Refinement program | CNS 1.1 | Depositor |
| R, $R_{free}$ | 0.230 , 0.256<br>0.230 , 0.256 | Depositor<br>DCC |
| $R_{free}$ test set | 7208 reflections (5.06%) | wwPDB-VP |
| Wilson B-factor (Å$^2$) | 27.7 | Xtriage |
| Anisotropy | 0.631 | Xtriage |
| Bulk solvent $k_{sol}$(e/Å$^3$), $B_{sol}$(Å$^2$) | 0.39 , 43.2 | EDS |
| L-test for twinning[2] | $< \|L\| > = 0.50$, $< L^2 > = 0.33$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| $F_o$,$F_c$ correlation | 0.94 | EDS |
| Total number of atoms | 16447 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 33.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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.

# 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)

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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)

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### 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)

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 | 664/664 (100%) | 0.15 | 28 (4%) | 36 | 45 | 17, 30, 52, 102 | 0 |
| 1 | B | 664/664 (100%) | 0.16 | 19 (2%) | 51 | 61 | 17, 28, 51, 102 | 0 |
| 1 | C | 664/664 (100%) | 0.40 | 41 (6%) | 20 | 27 | 18, 31, 53, 103 | 0 |
| 2 | D | 4/6 (66%) | 1.91 | 1 (25%) | 0 | 0 | 115, 116, 122, 128 | 0 |
| 2 | E | 4/6 (66%) | 2.84 | 3 (75%) | 0 | 0 | 115, 116, 123, 129 | 0 |
| 2 | F | 4/6 (66%) | 2.39 | 2 (50%) | 0 | 0 | 115, 116, 123, 129 | 0 |
| All | All | 2004/2010 (99%) | 0.25 | 94 (4%) | 31 | 41 | 17, 30, 53, 129 | 0 |

All (94) RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | C | 607 | ARG | 11.1 |
| 1 | C | 603 | ALA | 10.8 |
| 1 | B | 606 | ALA | 9.5 |
| 1 | C | 606 | ALA | 9.1 |
| 1 | B | 609 | ALA | 8.6 |
| 1 | C | 604 | SER | 8.4 |
| 1 | C | 608 | GLN | 8.4 |
| 1 | A | 606 | ALA | 8.0 |
| 1 | C | 609 | ALA | 8.0 |
| 1 | C | 664 | ARG | 7.7 |
| 1 | C | 610 | GLY | 6.7 |
| 1 | C | 612 | ALA | 6.6 |
| 1 | B | 608 | GLN | 6.6 |
| 1 | A | 664 | ARG | 6.0 |
| 1 | A | 605 | MET | 6.0 |
| 1 | C | 216 | LYS | 5.9 |
| 1 | A | 1 | PRO | 5.9 |
| 1 | B | 610 | GLY | 5.6 |
| 1 | B | 664 | ARG | 5.4 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | B | 607 | ARG | 5.4 |
| 1 | A | 607 | ARG | 5.1 |
| 1 | B | 603 | ALA | 5.0 |
| 1 | C | 215 | PRO | 4.8 |
| 1 | B | 604 | SER | 4.7 |
| 1 | C | 537 | ARG | 4.6 |
| 1 | B | 1 | PRO | 4.5 |
| 1 | C | 1 | PRO | 4.3 |
| 1 | C | 2 | ARG | 4.2 |
| 1 | C | 611 | LEU | 4.2 |
| 1 | B | 576 | TRP | 4.1 |
| 1 | A | 609 | ALA | 4.1 |
| 1 | B | 537 | ARG | 4.0 |
| 1 | C | 254 | GLU | 4.0 |
| 1 | A | 217 | THR | 3.9 |
| 1 | B | 216 | LYS | 3.9 |
| 1 | C | 605 | MET | 3.8 |
| 2 | F | 8 | C | 3.7 |
| 1 | A | 216 | LYS | 3.7 |
| 1 | B | 612 | ALA | 3.6 |
| 1 | C | 506 | ARG | 3.6 |
| 1 | C | 470 | ARG | 3.5 |
| 1 | A | 610 | GLY | 3.5 |
| 1 | A | 254 | GLU | 3.5 |
| 1 | A | 659 | ARG | 3.4 |
| 1 | C | 505 | SER | 3.4 |
| 1 | C | 217 | THR | 3.4 |
| 1 | C | 63 | ASP | 3.3 |
| 2 | E | 7 | C | 3.3 |
| 1 | A | 576 | TRP | 3.3 |
| 1 | C | 596 | LEU | 3.2 |
| 2 | E | 5 | U | 3.2 |
| 1 | C | 556 | ASP | 3.2 |
| 1 | C | 535 | GLY | 3.1 |
| 2 | D | 5 | U | 3.1 |
| 2 | E | 8 | C | 3.1 |
| 1 | C | 592 | LYS | 3.1 |
| 1 | C | 259 | ASP | 3.1 |
| 1 | B | 613 | GLU | 3.0 |
| 1 | A | 506 | ARG | 3.0 |
| 1 | A | 652 | GLU | 3.0 |
| 1 | B | 2 | ARG | 2.9 |

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| Mol | Chain | Res | Type | RSRZ |
|---|---|---|---|---|
| 1 | A | 270 | ARG | 2.9 |
| 1 | A | 215 | PRO | 2.9 |
| 1 | A | 505 | SER | 2.7 |
| 1 | A | 373 | GLU | 2.7 |
| 1 | A | 603 | ALA | 2.6 |
| 1 | A | 611 | LEU | 2.6 |
| 1 | C | 461 | LYS | 2.5 |
| 1 | C | 373 | GLU | 2.5 |
| 1 | A | 219 | LYS | 2.5 |
| 2 | F | 5 | U | 2.5 |
| 1 | C | 214 | ASP | 2.4 |
| 1 | C | 219 | LYS | 2.4 |
| 1 | C | 308 | LEU | 2.4 |
| 1 | C | 602 | VAL | 2.4 |
| 1 | A | 2 | ARG | 2.3 |
| 1 | A | 239 | GLN | 2.3 |
| 1 | C | 593 | ARG | 2.3 |
| 1 | C | 279 | LEU | 2.2 |
| 1 | B | 535 | GLY | 2.2 |
| 1 | A | 259 | ASP | 2.2 |
| 1 | C | 408 | ILE | 2.2 |
| 1 | A | 214 | ASP | 2.2 |
| 1 | C | 534 | SER | 2.1 |
| 1 | C | 536 | VAL | 2.1 |
| 1 | B | 479 | LYS | 2.1 |
| 1 | A | 656 | ARG | 2.1 |
| 1 | A | 645 | LEU | 2.1 |
| 1 | A | 613 | GLU | 2.1 |
| 1 | B | 321 | VAL | 2.1 |
| 1 | C | 309 | ASN | 2.1 |
| 1 | C | 262 | ASP | 2.1 |
| 1 | C | 218 | GLY | 2.0 |
| 1 | B | 457 | LEU | 2.0 |

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

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

## 5.3 Carbohydrates (i)

There are no monosaccharides in this entry.

## 5.4 Ligands (i)

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 | MN | B | 1665 | 1/1 | 0.98 | 0.06 | 26,26,26,26 | 0 |
| 3 | MN | A | 1665 | 1/1 | 0.99 | 0.08 | 29,29,29,29 | 0 |
| 3 | MN | C | 1665 | 1/1 | 0.99 | 0.05 | 30,30,30,30 | 0 |

## 5.5 Other polymers (i)

There are no such residues in this entry.