



# wwPDB X-ray Structure Validation Summary Report i

Apr 9, 2014 – 07:24 PM EDT

PDB ID : 4MLN  
Title : Crystal of PhnZ bound to (R)-2-amino-1-hydroxyethylphosphonicacid  
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Deposited on : 2013-09-06  
Resolution : 2.10 Å(reported)

This is a wwPDB validation summary report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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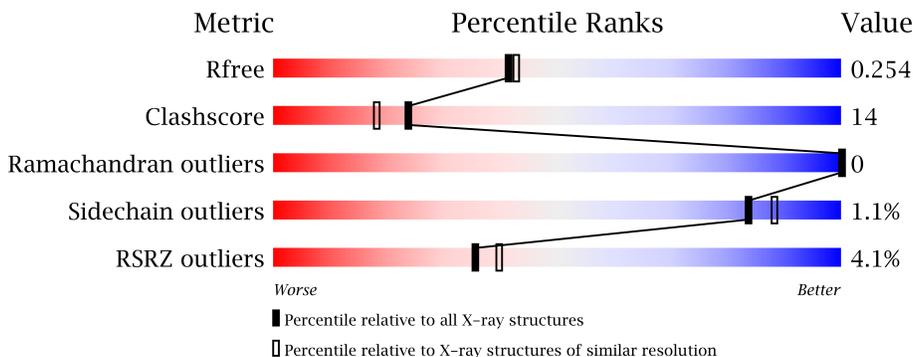
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : **FAILED**  
Xtriage (Phenix) : dev-1439  
EDS : stable22978  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22978

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 66092                       | 3012 (2.10-2.10)                                      |
| Clashscore            | 79885                       | 3649 (2.10-2.10)                                      |
| Ramachandran outliers | 78287                       | 3610 (2.10-2.10)                                      |
| Sidechain outliers    | 78261                       | 3611 (2.10-2.10)                                      |
| RSRZ outliers         | 66119                       | 3013 (2.10-2.10)                                      |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 196    |                  |
| 1   | B     | 196    |                  |

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 2976 atoms, of which 14 are hydrogens and 0 are deuterium.

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 Predicted HD phosphohydrolase PhnZ.

| Mol | Chain | Residues | Atoms |     |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 1   | A     | 182      | 1394  | 875 | 240 | 270 | 9 | 0       | 1       | 0     |
| 1   | B     | 182      | 1410  | 883 | 246 | 272 | 9 | 1       | 0       | 0     |

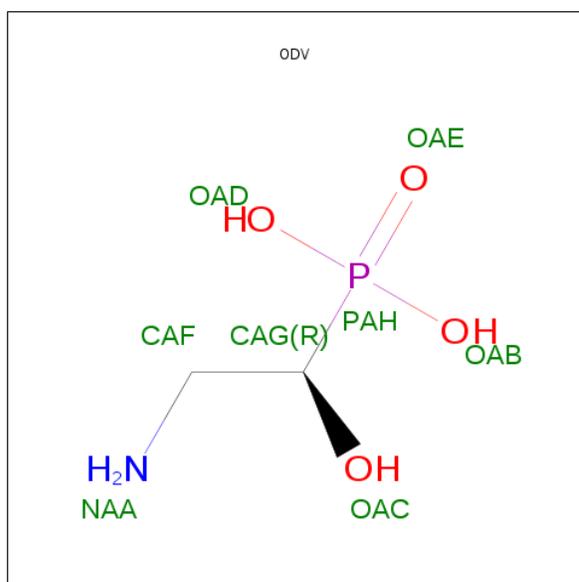
There are 12 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 191     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| A     | 192     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| A     | 193     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| A     | 194     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| A     | 195     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| A     | 196     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| B     | 191     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| B     | 192     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| B     | 193     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| B     | 194     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| B     | 195     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |
| B     | 196     | HIS      | -      | EXPRESSION TAG | UNP D0E8I5 |

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

- Molecule 3 is [(1R)-2-AMINO-1-HYDROXYETHYL]PHOSPHONICACID (three-letter code: ODV) (formula: C<sub>2</sub>H<sub>8</sub>NO<sub>4</sub>P).



| Mol | Chain | Residues | Atoms |   |   |   |   | ZeroOcc | AltConf |   |
|-----|-------|----------|-------|---|---|---|---|---------|---------|---|
|     |       |          | Total | C | H | N | O |         |         | P |
| 3   | A     | 1        | 15    | 2 | 7 | 1 | 4 | 1       | 0       | 0 |
| 3   | B     | 1        | 15    | 2 | 7 | 1 | 4 | 1       | 0       | 0 |

- Molecule 4 is water.

| Mol | Chain | Residues | Atoms            | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4   | A     | 65       | Total O<br>65 65 | 0       | 0       |
| 4   | B     | 73       | Total O<br>73 73 | 0       | 0       |



## 4 Data and refinement statistics (i)

| Property  | Value   | Source           |
|---|---|------------------|
| Space group   | P 21 21 21  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 66.63Å 74.91Å 75.81Å<br>90.00° 90.00° 90.00°                | Depositor        |
| Resolution (Å)  | 19.90 – 2.10<br>19.90 – 2.10                                | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 99.8 (19.90-2.10)<br>99.8 (19.90-2.10)                      | Depositor<br>EDS |
| $R_{merge}$   | (Not available)   | Depositor        |
| $R_{sym}$   | 0.11  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.28 (at 2.09Å)   | Xtriage          |
| Refinement program  | PHENIX (phenix.refine: 1.8.1_1168)                          | Depositor        |
| R, $R_{free}$   | 0.196 , 0.254<br>0.196 , 0.254                              | Depositor<br>DCC |
| $R_{free}$ test set   | 1133 reflections (5.00%)                                    | DCC              |
| Wilson B-factor (Å <sup>2</sup> )                                       | 33.1  | Xtriage          |
| Anisotropy  | 0.211   | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.38 , 48.5   | EDS              |
| Estimated twinning fraction   | 0.039 for -h,l,k  | Xtriage          |
| L-test for twinning   | $\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$ | Xtriage          |
| Outliers  | 0 of 22671 reflections                                      | Xtriage          |
| $F_o, F_c$ correlation  | 0.95  | EDS              |
| Total number of atoms   | 2976  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 31.0  | wwPDB-VP         |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: FE, ODV

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     | 0.39         | 0/1422  | 0.51        | 0/1917  |
| 1   | B     | 0.40         | 0/1435  | 0.50        | 0/1931  |
| All | All   | 0.40         | 0/2857  | 0.51        | 0/3848  |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts i

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 1394  | 0        | 1290     | 47      | 0            |
| 1   | B     | 1410  | 0        | 1320     | 31      | 1            |
| 2   | A     | 2     | 0        | 0        | 0       | 0            |
| 2   | B     | 2     | 0        | 0        | 0       | 0            |
| 3   | A     | 8     | 7        | 1        | 0       | 0            |
| 3   | B     | 8     | 7        | 1        | 0       | 0            |
| 4   | A     | 65    | 0        | 0        | 10      | 1            |
| 4   | B     | 73    | 0        | 0        | 6       | 0            |
| All | All   | 2962  | 14       | 2612     | 78      | 1            |

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

The worst 5 of 78 close contacts within the same asymmetric unit are listed below.

| Atom-1          | Atom-2         | Distance(Å) | Clash(Å) |
|-----------------|----------------|-------------|----------|
| 1:B:20:ARG:NH1  | 4:B:369:HOH:O  | 1.88        | 1.05     |
| 1:B:72:MET:CE   | 1:B:129:THR:HB | 1.91        | 1.01     |
| 1:A:123:SER:O   | 4:A:358:HOH:O  | 1.80        | 0.98     |
| 1:B:72:MET:HE1  | 1:B:129:THR:HB | 1.47        | 0.94     |
| 1:B:25:ILE:HD13 | 1:B:29:ILE:N   | 1.84        | 0.93     |

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

| Atom-1         | Atom-2               | Distance(Å) | Clash(Å) |
|----------------|----------------------|-------------|----------|
| 1:B:44:ARG:NH2 | 4:A:354:HOH:O[4_455] | 1.93        | 0.27     |

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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     | 177/196 (90%) | 169 (96%) | 8 (4%)  | 0        | 100         | 100 |
| 1   | B     | 176/196 (90%) | 171 (97%) | 5 (3%)  | 0        | 100         | 100 |
| All | All   | 353/392 (90%) | 340 (96%) | 13 (4%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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     | 139/168 (83%) | 138 (99%) | 1 (1%)   | 91          | 94 |
| 1   | B     | 143/168 (85%) | 141 (99%) | 2 (1%)   | 78          | 83 |
| All | All   | 282/336 (84%) | 279 (99%) | 3 (1%)   | 84          | 88 |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 166 | GLN  |
| 1   | B     | 44  | ARG  |
| 1   | B     | 162 | GLU  |

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

### 5.3.3 RNA [i](#)

There are no RNA chains in this entry.

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

Mogul failed to run properly - this section will therefore be empty.

## 5.5 Carbohydrates [i](#)

Mogul failed to run properly - this section will therefore be empty.

## 5.6 Ligand geometry [i](#)

Mogul failed to run properly - this section will therefore be empty.

## 5.7 Other polymers [i](#)

Mogul failed to run properly - this section will therefore be empty.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

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

### 6.1 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<sup>th</sup> 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 <sup>2</sup> ) | Q<0.9  |
|-----|-------|---------------|--------|---------------|-----------------------|--------|
| 1   | A     | 182/196 (92%) | 0.21   | 7 (3%) 38 43  | 20, 33, 53, 60        | 1 (0%) |
| 1   | B     | 182/196 (92%) | 0.03   | 8 (4%) 33 37  | 14, 27, 44, 53        | 1 (0%) |
| All | All   | 364/392 (92%) | 0.12   | 15 (4%) 35 40 | 14, 30, 49, 60        | 2 (0%) |

The worst 5 of 15 RSRZ outliers are listed below:

| Mol | Chain | Res | Type | RSRZ |
|-----|-------|-----|------|------|
| 1   | B     | 25  | ILE  | 5.2  |
| 1   | B     | 69  | PHE  | 3.7  |
| 1   | B     | 116 | ALA  | 3.5  |
| 1   | A     | 112 | VAL  | 3.5  |
| 1   | A     | 168 | ASP  | 3.3  |

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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 | RSR  | LLDF  | B-factors( $\text{\AA}^2$ ) | Q<0.9 |
|-----|------|-------|-----|-------|------|-------|-----------------------------|-------|
| 3   | ODV  | A     | 203 | 8/8   | 0.15 | 0.38  | 22,31,44,44                 | 0     |
| 2   | FE   | A     | 202 | 1/1   | 0.13 | -0.05 | 21,21,21,21                 | 0     |
| 3   | ODV  | B     | 203 | 8/8   | 0.12 | -0.49 | 20,27,48,48                 | 0     |
| 2   | FE   | B     | 202 | 1/1   | 0.12 | -0.77 | 18,18,18,18                 | 0     |
| 2   | FE   | B     | 201 | 1/1   | 0.10 | -1.30 | 19,19,19,19                 | 0     |
| 2   | FE   | A     | 201 | 1/1   | 0.09 | -2.50 | 22,22,22,22                 | 0     |

## 6.5 Other polymers

There are no such residues in this entry.