

wwPDB X-ray Structure Validation Summary Report (i)

Oct 5, 2023 – 06:14 AM EDT

PDB ID : 6VR1

Title : Complex of HLA-A2, a class I MHC, with a p53 peptide Authors : Wu, D.; Pierce, B.G.; Gallagher, D.T.; Mariuzza, R.A.

Deposited on : 2020-02-06

Resolution : 2.37 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 (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) : 2.35.1

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 2.37 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 4 unique types of molecules in this entry. The entry contains 6514 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 MHC class I antigen.

| \mathbf{Mol} | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | | | |
|----------------|-------|----------|-------|------|-----|---------|---------|-------|---|---|--|
| 1 | Λ | 275 | Total | С | N | О | S | 0 | 0 | 0 | |
| 1 | Λ | 210 | 2219 | 1389 | 402 | 419 | 9 | 0 | | | |
| 1 | D | 275 | Total | С | N | О | S | 0 | 0 | 0 | |
| | 210 | 2184 | 1371 | 388 | 416 | 9 | | | | | |

There are 36 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| A | 0 | MET | _ | initiating methionine | UNP Q861F7 |
| A | 276 | GLY | - | expression tag | UNP Q861F7 |
| A | 277 | GLY | - | expression tag | UNP Q861F7 |
| A | 278 | GLY | - | expression tag | UNP Q861F7 |
| A | 279 | LEU | - | expression tag | UNP Q861F7 |
| A | 280 | ASN | - | expression tag | UNP Q861F7 |
| A | 281 | ASP | - | expression tag | UNP Q861F7 |
| A | 282 | ILE | - | expression tag | UNP Q861F7 |
| A | 283 | PHE | - | expression tag | UNP Q861F7 |
| A | 284 | GLU | - | expression tag | UNP Q861F7 |
| A | 285 | ALA | - | expression tag | UNP Q861F7 |
| A | 286 | GLN | - | expression tag | UNP Q861F7 |
| A | 287 | LYS | - | expression tag | UNP Q861F7 |
| A | 288 | ILE | - | expression tag | UNP Q861F7 |
| A | 289 | GLU | - | expression tag | UNP Q861F7 |
| A | 290 | TRP | - | expression tag | UNP Q861F7 |
| A | 291 | HIS | - | expression tag | UNP Q861F7 |
| A | 292 | GLU | - | expression tag | UNP Q861F7 |
| D | 0 | MET | - | initiating methionine | UNP Q861F7 |
| D | 276 | GLY | | expression tag | UNP Q861F7 |
| D | 277 | GLY | - | expression tag | UNP Q861F7 |
| D | 278 | GLY | - | expression tag | UNP Q861F7 |
| D | 279 | LEU | - | expression tag | UNP Q861F7 |
| D | 280 | ASN | | expression tag | UNP Q861F7 |
| D | 281 | ASP | _ | expression tag | UNP Q861F7 |

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|----------------|------|------------|-------|
| COHABABACA | | DIEUIUU | DUIUE |
| 0 0 1000100000 | | | |

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| D | 282 | ILE | - | expression tag | UNP Q861F7 |
| D | 283 | PHE | - | expression tag | UNP Q861F7 |
| D | 284 | GLU | - | expression tag | UNP Q861F7 |
| D | 285 | ALA | - | expression tag | UNP Q861F7 |
| D | 286 | GLN | - | expression tag | UNP Q861F7 |
| D | 287 | LYS | - | expression tag | UNP Q861F7 |
| D | 288 | ILE | - | expression tag | UNP Q861F7 |
| D | 289 | GLU | - | expression tag | UNP Q861F7 |
| D | 290 | TRP | - | expression tag | UNP Q861F7 |
| D | 291 | HIS | - | expression tag | UNP Q861F7 |
| D | 292 | GLU | - | expression tag | UNP Q861F7 |

 \bullet Molecule 2 is a protein called Beta-2-microglobulin.

| Mol | Chain | Residues | Atoms | | | ZeroOcc | AltConf | Trace | | |
|-----|-------|----------|--------------|----------|----------|----------|---------|-------|---|---|
| 2 | В | 100 | Total 801 | C 511 | - 1 | O 150 | S 3 | 0 | 0 | 0 |
| 2 | Е | 100 | Total 806 | C 516 | N 137 | O 149 | S 4 | 0 | 0 | 0 |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|-----------------------|------------|
| В | 1 | MET | - | initiating methionine | UNP P61769 |
| Е | 1 | MET | - | initiating methionine | UNP P61769 |

• Molecule 3 is a protein called Cellular tumor antigen p53 peptide.

| Mol | Chain | Residues | ${f Atoms}$ | | | ZeroOcc | AltConf | Trace | | |
|-----|-------|----------|-----------------|----|----|---------|---------|-------|---|---|
| 2 | D | 0 | O Total C N O S | 0 | 0 | | | | | |
|) | 1 | 9 | 77 | 45 | 17 | 13 | 2 | 0 | 0 | |
| 9 | 0 | 0 | Total | С | N | О | S | 0 | 0 | 0 |
| J | Q | 9 | 77 | 45 | 17 | 13 | 2 | U | U | 0 |

• Molecule 4 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4 | A | 161 | Total O 161 161 | 0 | 0 |
| 4 | В | 28 | Total O 28 28 | 0 | 0 |

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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|------------------|---------|---------|
| 4 | D | 95 | Total O 95 95 | 0 | 0 |
| 4 | Е | 52 | Total O 52 52 | 0 | 0 |
| 4 | Р | 10 | Total O 10 10 | 0 | 0 |
| 4 | Q | 4 | Total O 4 4 | 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 1 21 1 | Depositor |
| Cell constants | 71.33Å 79.73Å 85.85Å | Depositor |
| a, b, c, α , β , γ | 90.00° 101.68° 90.00° | Depositor |
| Resolution (Å) | 20.00 - 2.37 | Depositor |
| % Data completeness | 99.6 (20.00-2.37) | Depositor |
| (in resolution range) | , | • |
| R_{merge} | 0.11 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | 2.21 (at 2.37Å) | Xtriage |
| Refinement program | REFMAC 5.8.0238 | Depositor |
| R, R_{free} | 0.217 , 0.274 | Depositor |
| Wilson B-factor (\mathring{A}^2) | 37.4 | Xtriage |
| Anisotropy | 0.620 | Xtriage |
| L-test for twinning ² | $ < L >=0.48, < L^2>=0.31$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 6514 | wwPDB-VP |
| Average B, all atoms (Å ²) | 41.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.51% 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.

