

Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 08:31 AM EDT

PDB ID : 6MLJ

Title : Crystal structure of the periplasmic Lysine-, Arginine-, Ornithine-binding pro-

tein (LAO) S70A mutant from Salmonella typhimurium complexed with argi-

nine

Authors: Romero-Romero, S.; Vergara, R.; Espinoza-Perez, G.; Rodriguez-Romero, A.

Deposited on : 2018-09-27

Resolution : 1.60 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 (i)) were used in the production of this report:

MolProbity : FAILED

Mogul : 1.8.5 (274361), CSD as541be (2020)

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 1.60 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 4052 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.

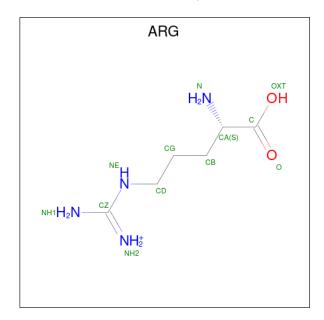
• Molecule 1 is a protein called Lysine/arginine/ornithine transport protein.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace | |
|-----|-------|----------|-------|------|-----|-----|---------|---------|-------|---|
| 1 | Λ | 237 | Total | С | N | О | S | 0 | 7 | 0 |
| 1 | А | 231 | 1842 | 1166 | 305 | 366 | 5 | 0 | (| |
| 1 | D | 237 | Total | С | N | О | S | 0 | 6 | 0 |
| 1 | Ъ | 231 | 1836 | 1163 | 305 | 363 | 5 | 0 | U | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue Modelled Ac | | Actual | Comment | Reference |
|-------|-------------------------|-----|--------|---------------------|----------------|
| A | 70 | ALA | SER | engineered mutation | UNP A0A0F6B499 |
| В | 70 | ALA | SER | engineered mutation | UNP A0A0F6B499 |

• Molecule 2 is ARGININE (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf |
|-----|-------|----------|-------------|--------|--------|--------|---------|---------|
| 2 | A | 1 | Total 12 | C 6 | N 4 | O 2 | 0 | 0 |

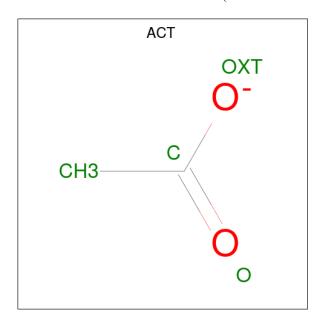
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| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|----------------------|---------|---------|
| 2 | В | 1 | Total C N O 12 6 4 2 | 0 | 0 |

• Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



| Mol | Chain | Residues | Ato | ms | | ZeroOcc | AltConf |
|-----|-------|----------|---------|--------|--------|---------|---------|
| 3 | A | 1 | Total 4 | C 2 | O 2 | 0 | 0 |

• Molecule 4 is water.

| Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|--------------------|---------|---------|
| 4 | A | 171 | Total O 171 171 | 0 | 0 |
| 4 | В | 175 | Total O 175 175 | 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 | 58.09Å 37.24Å 102.04Å | Depositor |
| a, b, c, α , β , γ | 90.00° 90.01° 90.00° | Веровног |
| Resolution (Å) | 38.34 - 1.60 | Depositor |
| % Data completeness | 99.1 (38.34-1.60) | Depositor |
| (in resolution range) | , | - |
| R_{merge} | 0.10 | Depositor |
| R_{sym} | (Not available) | Depositor |
| $< I/\sigma(I) > 1$ | 2.89 (at 1.59Å) | Xtriage |
| Refinement program | REFMAC 5.8.0238 | Depositor |
| R, R_{free} | 0.192 , 0.224 | Depositor |
| Wilson B-factor (A^2) | 13.9 | Xtriage |
| Anisotropy | 0.108 | Xtriage |
| L-test for twinning ² | $< L > = 0.44, < L^2> = 0.26$ | Xtriage |
| Estimated twinning fraction | 0.377 for h,-k,-l | Xtriage |
| Reported twinning fraction | 0.545 for H, K, L | Depositor |
| reported twinning fraction | 0.455 for -h,-k,l | Depositor |
| Outliers | 0 of 58580 reflections | Xtriage |
| Total number of atoms | 4052 | wwPDB-VP |
| Average B, all atoms (Å ²) | 18.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 6.64% 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)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Mol Type Chain Res Link | | | | Bo | nd leng | $	ag{ths}$ | Bond angles | | |
|------|-------------------------|-------|-----|-------|----------|---------|------------|-------------|------|----------|
| MIOI | Type | Chain | Res | LIIIK | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 2 | ARG | В | 301 | - | 10,11,11 | 0.91 | 0 | 11,13,13 | 1.81 | 3 (27%) |
| 2 | ARG | A | 301 | - | 10,11,11 | 1.63 | 2 (20%) | 11,13,13 | 1.51 | 1 (9%) |
| 3 | ACT | A | 302 | - | 3,3,3 | 0.71 | 0 | 3,3,3 | 1.16 | 0 |

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|------------|-------|
| 2 | ARG | В | 301 | - | - | 0/11/11/11 | - |
| 2 | ARG | A | 301 | - | - | 1/11/11/11 | - |

All (2) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(A) | $Ideal(\AA)$ |
|-----|-------|-----|------|-------|-------|-------------|--------------|
| 2 | A | 301 | ARG | OXT-C | -3.19 | 1.20 | 1.30 |
| 2 | A | 301 | ARG | O-C | 3.10 | 1.31 | 1.22 |

All (4) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Atoms Z | | $\operatorname{Ideal}({}^{o})$ |
|-----|-------|-----|------|----------|---------|--------|--------------------------------|
| 2 | A | 301 | ARG | CB-CG-CD | 3.90 | 123.76 | 112.05 |
| 2 | В | 301 | ARG | CB-CG-CD | 3.85 | 123.61 | 112.05 |
| 2 | В | 301 | ARG | OXT-C-CA | 2.82 | 122.98 | 113.38 |
| 2 | В | 301 | ARG | OXT-C-O | -2.80 | 117.72 | 124.09 |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| \mathbf{Mol} | Chain | Res | Type | Atoms |
|----------------|-------|-----|------|------------|
| 2 | A | 301 | ARG | N-CA-CB-CG |

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)

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.

