Full wwPDB X-ray Structure Validation Report

Oct 3, 2023 – 03:10 AM EDT

PDB ID : 6OLT
Title : Crosslinked Crystal Structure of Type II Fatty Acid Synthase Ketosynthase, FabF, and C12-crypto Aeryl Carrier Protein, AcpP
Deposited on : 2019-04-17
Resolution : 2.35 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 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) were used in the production of this report:

- MolProbity : FAILED
- Mogul : 1.8.5 (274361), CSD as541be (2020)
- Xtriage (Phenix) : 1.13
- EDS : FAILED
- buster-report : 1.1.7 (2018)
- 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

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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

There are 4 unique types of molecules in this entry. The entry contains 3867 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 3-oxoacyl-[acyl-carrier-protein] synthase 2.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>A</td>
<td>412</td>
<td>Total C N O S</td>
<td>0</td>
<td>16</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 2 is a protein called Acyl carrier protein.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
<th>Trace</th>
</tr>
</thead>
<tbody>
<tr>
<td>2</td>
<td>B</td>
<td>77</td>
<td>Total C N O S</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

- Molecule 3 is N-[2-(dodecanoylamino)ethyl]-N 3 -[(2R)-2-hydroxy-3,3-dimethyl-4-(phosphonoxy)butanoyl]-beta-alaminamide (three-letter code: MRJ) (formula: C_{23}H_{46}N_{3}O_{8}P) (labeled as "Ligand of Interest" by depositor).

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MRJ
```

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>A</td>
<td>1</td>
<td>Total C N O P</td>
<td>0</td>
<td>1</td>
</tr>
</tbody>
</table>
- Molecule 4 is water.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Residues</th>
<th>Atoms</th>
<th>ZeroOcc</th>
<th>AltConf</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>A</td>
<td>88</td>
<td>Total O &lt;br&gt;88 88</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>4</td>
<td>B</td>
<td>4</td>
<td>Total O &lt;br&gt;4 4</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

MolProbity and EDS failed to run properly - this section is therefore empty.
3 Data and refinement statistics

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

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Source</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space group</td>
<td>P 4 3 2 1 2</td>
<td>Depositor</td>
</tr>
<tr>
<td>Cell constants</td>
<td>86.45Å 86.45Å 115.16Å</td>
<td>Depositor</td>
</tr>
<tr>
<td>a, b, c, α, β, γ</td>
<td>90.00° 90.00° 90.00°</td>
<td>Depositor</td>
</tr>
<tr>
<td>Resolution (Å)</td>
<td>69.14 – 2.35</td>
<td>Depositor</td>
</tr>
<tr>
<td>% Data completeness</td>
<td>99.7 (69.14-2.35)</td>
<td>Depositor</td>
</tr>
<tr>
<td>Rmerge</td>
<td>0.33</td>
<td>Depositor</td>
</tr>
<tr>
<td>Rsyrm</td>
<td>(Not available)</td>
<td>Depositor</td>
</tr>
<tr>
<td>&lt;I/σ(I)&gt; &lt;1&gt;</td>
<td>1.36 (at 2.34Å)</td>
<td>Xtriage</td>
</tr>
<tr>
<td>Refinement program</td>
<td>PHENIX 1.13_2998</td>
<td>Depositor</td>
</tr>
<tr>
<td>R, Rfree</td>
<td>0.201 , 0.239</td>
<td>Depositor</td>
</tr>
<tr>
<td>Wilson B-factor (Å²)</td>
<td>39.5</td>
<td>Xtriage</td>
</tr>
<tr>
<td>Anisotropy</td>
<td>0.603</td>
<td>Xtriage</td>
</tr>
<tr>
<td>L-test for twinning²</td>
<td>&lt;</td>
<td>L</td>
</tr>
<tr>
<td>Estimated twinning fraction</td>
<td>No twinning to report.</td>
<td>Xtriage</td>
</tr>
<tr>
<td>Total number of atoms</td>
<td>3867</td>
<td>wwPDB-VP</td>
</tr>
<tr>
<td>Average B, all atoms (Å²)</td>
<td>59.0</td>
<td>wwPDB-VP</td>
</tr>
</tbody>
</table>

Xtriage’s analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 4.25% of the height of the origin peak. No significant pseudotranslation is detected.

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1Intensities estimated from amplitudes.
2Theoretical values of < |L| >, < L² > for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.
4 Model quality

4.1 Standard geometry

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

4.2 Too-close contacts

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

4.3 Torsion angles

4.3.1 Protein backbone

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

4.3.2 Protein sidechains

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

4.3.3 RNA

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

4.4 Non-standard residues in protein, DNA, RNA chains

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

4.5 Carbohydrates

There are no monosaccharides in this entry.

4.6 Ligand geometry

2 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).

<table>
<thead>
<tr>
<th>Mol</th>
<th>Type</th>
<th>Chain</th>
<th>Res</th>
<th>Link</th>
<th>Bond lengths</th>
<th>Bond angles</th>
</tr>
</thead>
</table>

| Counts | RMSZ | #|Z| > 2 | Counts | RMSZ | #|Z| > 2 |
|--------|------|-----|-----|------|--------|------|-----|
| 18,23,34 | 0.38 | 0 | 23,30,43 | 1.09 | 2 (8%) |
| 18,23,34 | 0.40 | 0 | 23,30,43 | 0.80 | 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.

<table>
<thead>
<tr>
<th>Mol</th>
<th>Type</th>
<th>Chain</th>
<th>Res</th>
<th>Link</th>
<th>Chirals</th>
<th>Torsions</th>
<th>Rings</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>MRJ</td>
<td>A</td>
<td>501[B]</td>
<td>1,2</td>
<td>-</td>
<td>7/27/29/41</td>
<td>-</td>
</tr>
<tr>
<td>3</td>
<td>MRJ</td>
<td>A</td>
<td>501[A]</td>
<td>1,2</td>
<td>-</td>
<td>6/27/29/41</td>
<td>-</td>
</tr>
</tbody>
</table>

There are no bond length outliers.

All (2) bond angle outliers are listed below:

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
<th>Atoms</th>
<th>Z</th>
<th>Observed(°)</th>
<th>Ideal(°)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>C37-C38-C39</td>
<td>-2.83</td>
<td>107.64</td>
<td>112.36</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>C37-N36-C34</td>
<td>-2.38</td>
<td>118.34</td>
<td>122.59</td>
</tr>
</tbody>
</table>

There are no chirality outliers.

All (13) torsion outliers are listed below:

<table>
<thead>
<tr>
<th>Mol</th>
<th>Chain</th>
<th>Res</th>
<th>Type</th>
<th>Atoms</th>
</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>A</td>
<td>501[A]</td>
<td>MRJ</td>
<td>C29-C32-C34-O35</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[A]</td>
<td>MRJ</td>
<td>C29-C32-C34-N36</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[A]</td>
<td>MRJ</td>
<td>O33-C32-C34-N36</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>O33-C32-C34-N36</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>N36-C37-C38-C39</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>N41-C42-C43-N1</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[A]</td>
<td>MRJ</td>
<td>O33-C32-C34-O35</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>C29-C32-C34-O35</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>C29-C32-C34-N36</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>C37-C38-C39-N41</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[B]</td>
<td>MRJ</td>
<td>C37-C38-C39-O40</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[A]</td>
<td>MRJ</td>
<td>O27-C28-C29-C30</td>
</tr>
<tr>
<td>3</td>
<td>A</td>
<td>501[A]</td>
<td>MRJ</td>
<td>O27-C28-C29-C31</td>
</tr>
</tbody>
</table>
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

4.7 Other polymers

There are no such residues in this entry.
4.8 Polymer linkage issues

There are no chain breaks in this entry.
5  Fit of model and data

5.1 Protein, DNA and RNA chains

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

5.2 Non-standard residues in protein, DNA, RNA chains

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

5.3 Carbohydrates

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

5.4 Ligands

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

5.5 Other polymers

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