Recent activities of PDBj and wwPDB

Genji Kurisu
Institute for Protein Research, Osaka University

Since 2001, PDBj has been managed at Institute for Protein Research, Osaka University as a member of the wwPDB, to curate and process the deposited data for an open and single archive.

wwPDB Architecture

PDBj is in charge of processing and annotating the depositions from Asian and Middle-east regions

deposit.wwpdb.org

PDB Core Archive Depositions

- 12,179 depositions in 2018.
- Rapid growth in 3DEM
  - Exceeded NMR depositions

<table>
<thead>
<tr>
<th>Method</th>
<th>2017 Depositions</th>
<th>2018 Depositions</th>
</tr>
</thead>
<tbody>
<tr>
<td>MX</td>
<td>17,889 (91.1%)</td>
<td>15,897 (87.0%)</td>
</tr>
<tr>
<td>NMR</td>
<td>460 (3.5%)</td>
<td>418 (3.4%)</td>
</tr>
<tr>
<td>EMDB</td>
<td>874 (5.2%)</td>
<td>1140 (6.4%)</td>
</tr>
<tr>
<td>Other</td>
<td>26 (0.2%)</td>
<td>27 (0.2%)</td>
</tr>
</tbody>
</table>

2018 Processing Sites

- RCSB PDB: 34%
- PSDB: 33%
- PDBe: 23%
- PDBj: 1%

2018 Depositor Locations

- North America: 38%
- Europe: 36%
- Asia: 15%
- South America: 6%
- Oceania: 4%
- Africa: 2%
- Other: 3%

PDB Core Archive Growth

* As of 3 Sep 2019
PDB Core Archive Downloads

More than 1.8 million/day!

• As of 3 Sep 2019

Geographic Origins of FTP downloads; 2012-2015

PDB Core Archive Update I

Ligand Validation
• Adapted software from Global Phasing Ltd. under a formal agreement
• Provides geometrical quality in 2D depiction
• Provides electron density fit for X-ray
• Now mandatory at deposition: identification of Ligand/s Of Interest (LOI, author’s research focus)

PDB Core Archive Update II

Coordinate Versioning
• To improve data quality in the PDB archive
• Depositors can now make corrections to existing structures in the PDB Core Archive by updating the atomic coordinates while preserving the original PDB identifier.
• Deployed on July 27th 2019 for all structures that were originally deposited via OneDep (Phase one)
• First coordinate replacement (PDB entry 5T26) versioned at FTP on August 7th 2019 following reviewers’ comments based on the wwPDB validation reports
  • With PDB prefix and extension of 4 characters (e.g., from “1ABC” to “PDB_00001ABC”)
  • Example: PDB_00001ABC_XYZ_V2.cif.gz

PDB Core Archive Update III

Use of ORCID
• To enable better management of incoming data
• To credit PDB entries by author unambiguously
• 25% of the unique depositors provided ORCID ids
• 3342 unique PIs with ORCID ids
PDB Core Archive Plans

- **ED map coefficients**
  - ED map coefficients have been provided to depositors during biocuration for new entries
  - As part of annual recalculation of validation reports, the ED map coefficients will be provided for existing entries at the wwPDB FTP site for better interpretation of the ligand validation by user community.

- **Coordinate Versioning (Legacy entries)**
  - Create OneDep deposition sessions
  - Enable authors access and login
  - Entries will be versioned at versioned FTP

wwPDB 2018-2019 Publications

Mandatory mmCIF deposition announced on 3rd April 2019
https://doi.org/10.1107/S2059783319004522
I/HM manuscript was submitted.

Atomic coordinates in PDBx/mmCIF

<table>
<thead>
<tr>
<th>Serial</th>
<th>Type</th>
<th>Chain</th>
<th>Unit</th>
<th>X</th>
<th>Y</th>
<th>Z</th>
<th>Temperature</th>
<th>Occupancy</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>38.840</td>
<td>0.236</td>
<td>1.012</td>
<td>1.00</td>
<td>34.65</td>
</tr>
<tr>
<td>2</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>38.356</td>
<td>-0.999</td>
<td>0.357</td>
<td>1.00</td>
<td>42.26</td>
</tr>
<tr>
<td>3</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>37.098</td>
<td>-1.547</td>
<td>1.056</td>
<td>1.00</td>
<td>41.25</td>
</tr>
<tr>
<td>4</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>36.619</td>
<td>-0.946</td>
<td>2.028</td>
<td>1.00</td>
<td>29.44</td>
</tr>
<tr>
<td>5</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>39.398</td>
<td>-2.114</td>
<td>0.379</td>
<td>1.00</td>
<td>40.70</td>
</tr>
<tr>
<td>6</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>36.610</td>
<td>-2.666</td>
<td>0.495</td>
<td>1.00</td>
<td>32.67</td>
</tr>
<tr>
<td>7</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>35.411</td>
<td>-3.244</td>
<td>1.202</td>
<td>1.00</td>
<td>34.90</td>
</tr>
<tr>
<td>8</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>35.683</td>
<td>-4.740</td>
<td>1.081</td>
<td>1.00</td>
<td>38.30</td>
</tr>
<tr>
<td>9</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>36.827</td>
<td>-5.147</td>
<td>0.747</td>
<td>1.00</td>
<td>28.59</td>
</tr>
<tr>
<td>10</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>34.063</td>
<td>-2.660</td>
<td>0.823</td>
<td>1.00</td>
<td>24.49</td>
</tr>
<tr>
<td>11</td>
<td>ATOM</td>
<td>A</td>
<td>1</td>
<td>33.031</td>
<td>-3.308</td>
<td>1.686</td>
<td>1.00</td>
<td>20.37</td>
</tr>
</tbody>
</table>

Acknowledgements