

PDBj, wwPDB, and their activities

In July 2000, the Protein Data Bank Japan (PDBj, <https://pdbj.org/>) at the Institute for Protein Research (IPR), Osaka University, started. Since then, PDBj has accepted new structures of biological macromolecules from researchers mainly in Asia and Middle East regions, and processed them for the common PDB database that has high qualities. Since then, the PDBj has become the leading data center of this region, as one of the four members of the wwPDB (worldwide PDB, <https://wwpdb.org/>): the RCSB-PDB and the BMRB (BioMagResBank) in USA, and the PDBe-EBI in the EU. The head of the PDBj changed in April 2017 from Prof. Haruki Nakamura of IPR, Osaka University, to Prof. Genji Kurisu of the same institute.

The PDBj has also developed several characteristic web services and provided them freely to structural biologists and bioinformatics researchers around the world.

In addition, PDBj-BMRB group was founded in PDBj at the early days so as to process and edit chemical shifts information in collaboration with the BMRB. The structural data taken from the recent cryo-EM (Electron Microscopy) technique have also been accepted and processed. These activities of the PDBj are now supported by JST-NBDC (Japan Science and Technology Agency - National Bioscience Database Center, <http://biosciencedbc.jp/>), and Osaka University.

The wwPDB registers more than 10,000 structures of biological macromolecules such as proteins and nucleic acids every year, and has determined a total of over 136,000 structures in the world as of December 2017. So far, PDBj has processed about 22 % of total entries in collaboration with other wwPDB members. The members gather frequently to discuss current issues and future progress of the wwPDB.

Message from the new head

Genji Kurisu, Professor, Institute for Protein Research, Osaka University



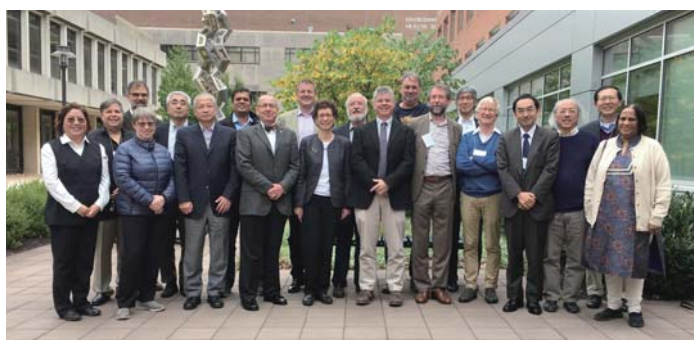
I'm serving as a successor of Prof. Haruki Nakamura, the former head of PDBj. Let me introduce myself. I got a Ph.D from Osaka University in 1997, where my major was protein crystallography. From April 1st, 1997, I started my academic carrier at the Institute for Protein Research (IPR), Osaka University, as a research associate. After studying at Purdue University for about two years, I moved to the Department of Life Sciences, University of Tokyo, as an independent associate professor in 2004. After five years working at Tokyo, I have returned to my home university, Osaka University, as a full professor of protein crystallography at IPR. As a depositor, I have 77 deposited coordinates in the PDB, and have served as an advisor to PDBj from 2010. In 2017, I began my new role as the head of PDBj and have a concurrent professorship in the Laboratory of Protein Databases, IPR.

The PDB has a long history and has matured greatly over the years. However, there are some newly arising issues that should be addressed immediately, such as how to incorporate hybrid structural biology methods and how to validate high resolution cryo-TEM structures. I'll do my best to fulfill my new role and would like to thank all structural biologists and PDBj users for their kind cooperation and continuous encouragement.

wwPDB Advisory Committee Meeting in 2017

The advisory committee meeting of the Worldwide Protein Data Bank (wwPDB-AC) was held at the Center for Integrative Proteomics Research, Rutgers University, USA, on October 13th, 2017. The wwPDB-AC consists of two advisors nominated from each wwPDB partner, representatives from the International Union of Crystallography and macromolecular EM community, and the wwPDB regional associate members (from India and China). The representatives from PDBj-AC were Profs. Tsuyoshi Inoue (Osaka Univ.) and Kei Yura (Ochanomizu Univ.). The agenda included: Introduction and Overview of the wwPDB, Partner meeting and Outreach activities, Macromolecular Crystallography, 3D Electron Microscopy and NMR Spectroscopy, and Looking ahead and Questions for the AC and general discussion. In the executive session, following specific proposals were recommended: 1) Proposal to take an enhanced approach for DOI resolution of PDB entries; 2) Proposal to adjust the terms of reference for the Advisory Committee; 3) Proposal to enter negotiations with EMDB with the intention to invite the EMDB to become a full partner in the wwPDB

organization; 4) Recommendation from the wwPDB Partners on the process for adding new regional wwPDB Partners; and 5) Recommendation to provide Mogul geometry standards for ligands restraints within the context of a PDB entry. Next wwPDB-AC meeting is scheduled to be held at Cambridge, UK on November 2nd, 2018.



24th Congress and General Assembly of the International Union of Crystallography

The 24th Congress and General Assembly of the International Union of Crystallography (IUCr 2017) was held in Hyderabad, India, from 21st to 28th August, 2017.

In the congress, we discussed the educational use of database in the symposium titled "Structural databases as teaching tools - Part A macromolecules". Researchers involved in databases management such as Jaime Prilusky of Proteopedia, Shuchismita Dutta of RCSB PDB, and Sameer Velankar of PDBe gave presentations about their services and activities. From PDBj, Hirofumi Suzuki gave the presentation titled "Play with 3D structure data of biomolecules", which was about PDBj' s educational contents on the Web and outreach activities such as our booth exhibition in Science Agora, an

annual scientific event held in Tokyo, Japan.

We, wwPDB, also exhibited a booth to discuss and explain wwPDB deposition system and foundation organization directly with attendees.

In the conference, a number of keynote lectures and microsymbosia about cryo-EM structural biology and methodology symbolized drastic growing of structural biology using cryo-EM.



wwPDB fan for giveaway



From left: Matthew Conroy (PDBe), Hirofumi Suzuki (PDBj), Chun-Jung Chen (NSRRC), and Atsushi Nakagawa (PDBj)

Topics

New extensions in the PDBj Mine

The PDBj Mine relational database (RDB) is the main backend database at PDBj. It can be also locally installed on the user's computers

(<https://pdbj.org/help/mine2-rdb-local-install> for instructions) or be accessed via the RESTful web service (see <https://pdbj.org/help/rest-interface>). The entire RDB dump file as well as weekly update files are downloadable at our FTP site (<ftp://ftp.pdbj.org/mine2>). The RDB schema (<https://pdbj.org/mine-rdb-docs>) is nearly compatible with the PDBx/mmCIF dictionary and a wide range of example SQL queries are available as a tutorial (<https://pdbj.org/help/mine2-sql>).

In addition to PDB entries, the wwPDB maintains and provides the Chemical Component Dictionary, the Chemical Component Model data (CCM) as well as the Biologically

Interesting Molecule Reference Dictionary (BIRD). For more information, please refer to <https://www.wwpdb.org/data/ccd> and <https://www.wwpdb.org/data/bird>. Last year, we integrated these data into the PDBj Mine. The tables related to CCD, CCM and BIRD can be found under the schema (namespace) "cc", "ccmodel" and "prd", respectively. By combining these data with PDB entries, many interesting queries can be executed. For example, it is now possible to search all the PDB entries having a given InchKey or CSD (Cambridge Structure Database) ID. Please refer to <https://pdbj.org/help/mine2-sql> for some examples.

Changes in OneDep system and PDB Archive

1. Enriched model files (V5.0) conforming to OneDep data standards now available in the PDB FTP archive [July 2017]

The model files in the PDB FTP archive have been updated to V5.0 of the PDBx/mmCIF dictionary. All V5.0 PDB model files have better organized content and conform to the revised data model used within the wwPDB OneDep System. Both PDBx/mmCIF and XML formats have been updated. Legacy PDB format files may not contain all of the remediated information.

2. OneDep provides a new option to deposit small angle scattering data in SASBDB released [July 2017]

Depositors are asked to input SASBDB accession ID or deposit data to SASBDB through OneDep system for their SAXS/SANS data. Some limited data such as status of the session, OneDep ID and publication information are shared with SASBDB.

3. Implementation of PDB entry versioning and better revision history to improve PDB archive management [October 2017]

At present, revised atomic coordinates for an existing released PDB entry are assigned a new accession code, and the prior entry is obsoleted. wwPDB has introduced a versioning system to enable depositor-initiated or wwPDB-initiated updates to previously released PDB entries while retaining the same PDB accession code.

In October 2017, wwPDB released the new versioned FTP archive at <ftp://ftp-versioned.pdbj.org/> for structural model files in PDBx/mmCIF and PDBML formats as the first stage. File names in the versioned FTP archive will conform to a new naming scheme. For example, the first initial release of PDB entry 1abc would have the following form under the new file-naming scheme: `pdb_00001abc_xyz_v1-0.cif.gz` where `pdb_00001abc` is new PDB accession code for entry 1abc; `xyz` stands for coordinate content; `cif` indicates the file format.

Please refer to the past wwPDB news for more information.

In the 2018 phase of the project, wwPDB will enable depositor-initiated updates of coordinates.

4. Five Easy Steps to PDB deposition with OneDep brochure

A new brochure that outlines the 5 Easy Steps to PDB Deposition with OneDep is available for download at wwPDB site.

PDBj provides its translations in Japanese, Chinese and Korean for download at <https://pdbj.org/info/data-deposition>.

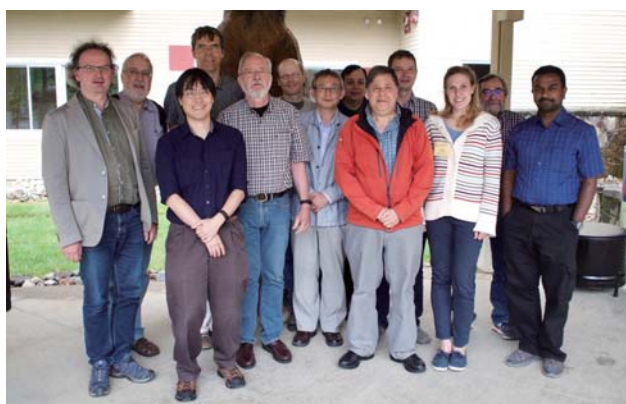


Development of tools for conversion of Validation Report in XML and RDF

PDBj-BMRB group has been developing tools for conversion of Validation Report into XML and RDF format, which may help to objectively assess the quality of structure coordinates deposited to OneDep. The conversion technology is based on established methods by Kinjo et al., (Nuc. Acid. Res. 2012, 40) and Yokochi et al. (J. Biomed. Sem. 2016, 7(16)) in the international collaboration with wwPDB. This approach will increase more interoperability of automation for quality validation of the deposited structure coordinates with complicated data structure.

NEF meeting on Sunday River, USA at June 12th - 15th

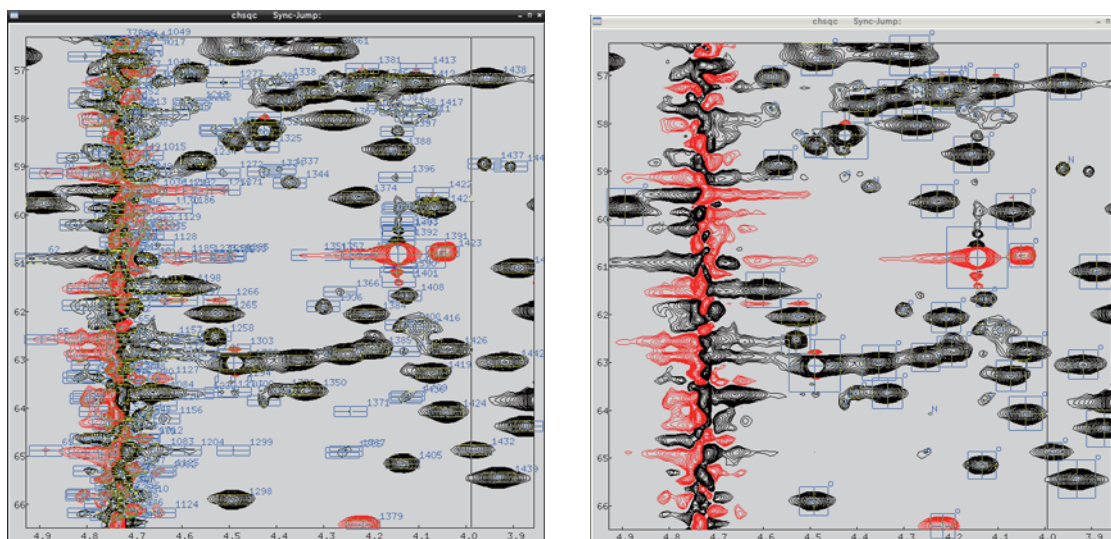
Validation Task Force meeting for NMR data Exchange Format (NEF) organized by wwPDB was held at Sunday River in USA from June 12th to 15th, 2017 in conjunction with the Gordon Research Conference 2017. The annual plans were discussed about development and deployment of tools for conversion of PDBx/mmCIF format into NEF and its related dictionary. More practical way for quantitative assessments of data quality was also issued to make a vision of additional mandatory items for NMR structure deposition such as NOE peak lists.



NMR-VTF NEF meeting, in Sunday River, USA

Deep Learning technology applied to highly automated data analysis in MagRO

New version of an integrated NMR analysis tool, MagRO has been released. The image recognition by Deep Learning technology was implemented in the tool, which can eliminate a large number of noise peaks at a high accuracy like a human vision. The new function is promising not only to expedite automation of NMR analysis but also to provide a possibility to objectively assess the quality of data (Kobayashi et al., under review).

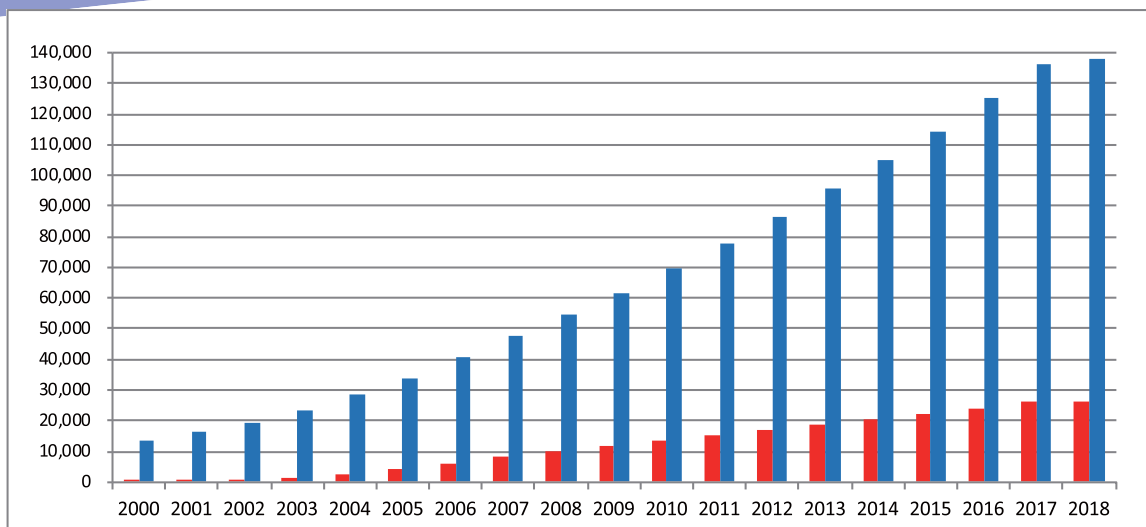


A part of the regions of 2D ¹³C-CT HSQC spectra, before (left) and after (right) Deep Learning filter.

Data Growth

Statics for PDB Structures that are deposited and processed by wwPDB/PDBj
The statics is also available on the wwPDB web page: <https://www.wwpdb.org/stats/deposition>

■ Total available structures ■ Total structures processed by PDBj



The number of PDB entries released as of February 14, 2018 (excludes obsolete entries)

Event Report

Various activities for the introduction of PDBj and its web services

- Osaka University ICHO festival
-Exhibition of protein structures using a 3D viewer developed by PDBj
(April 30, 2017, at Osaka University Suita Campus)
- The All-in-one Joint Workshop 2017
(May 27, 2017, Shizuoka)
- PDBj Luncheon Seminar
at the 17th Annual Meeting of the Protein Science Society of Japan
(June 22, 2017, Sendai)
- PDBj Luncheon Seminar
at the 55th Annual Meeting of the Biophysical Society of Japan
(September 21, 2017, Kumamoto)
- PDBj Luncheon Seminar at the 6th Joint Conference
on Informatics in Biology, Medicine and Pharmacology
(September 27, 2017, Sapporo)
- Science Agora 2017
(November 24-26, 2017, Tokyo)
※A scientific event supported by Japan Science and Technology Agency
- PDBj Luncheon Seminar
at the Annual Meeting of Crystallographic Society of Japan
(November 24, 2017, Hiroshima)
- Exhibition booth for the Life Science Databases
at the Consortium of Biological Sciences (ConBio) 2017
(December 6-9, 2017, Kobe)
- PDBj & BINDS Workshop
(February 20, 2018, at Osaka University Suita Campus)
- PDBj Luncheon Seminar
at the 138th Annual Meeting of the Pharmaceutical Society of Japan
(March 27, 2018, Kanazawa)



ICHO Festival



Luncheon Seminar at BSJ 2017



Luncheon Seminar at CrSJ 2017



Science Agora 2017



PDB j & BINDS Workshop

*Materials of the seminars and workshops are available at our web page:
<https://pdbj.org/info/previous-workshop>

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