PDBj
Protein Data Bank Japan
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Message from the Head of PDBj

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I would like to express my sincere thanks to all structural biologists and PDBj users for their kind cooperation and continuous support. First, I'm reporting changes to the Protein Data Bank Japan (PDBj) staff members. Prof. Haruki Nakamura, the former head of PDBj, retired from Osaka University in March, 2018 and obtained the title of Professor Emeritus of Osaka University. He is the founder of PDBj and has grown it into a worldwide renowned data center in the structural biology community. I greatly appreciate his enormous contribution to PDBj. He is now working as a Program Supervisor of the Japan Agency for Medical Research and Development (AMED). Drs. Akira R. Kinjo and Hirofumi Suzuki were transitioned to new, exciting positions in Universiti Brunei Darussalam, Brunei, and Waseda University, Tokyo, respectively. They have developed core data-out services of PDBj since the early stages. Dr. Naohiro Kobayashi of the PDBj-BMRB group moved to the RIKEN SPring-8 Center in Yokohama. I'd like to thank my three colleagues for their sincere contributions to PDBj and hope they'll be successful in their respective new positions. As external collaborators, we will highly welcome their constructive suggestions.

Next, I will make an annual report of PDBj's activities. One of the most influential activities in 2018 was the start of EMPIAR (Electron Microscopy Public Image ARchive)-PDBj, under the agreement between IPR, Osaka University, and EMBL-EBI in UK. Our mirror site of EMPIAR became operational from December 2018. Secondly, the wwPDB has officially invited the Electron Microscopy Data Bank (EMDB) as the fifth core member and is making efforts on maintaining, growing and validating the EMDB data. The wwPDB shall also engage more in working with federated archives, such as SASBDB, EMPIAR or MX image archives. PDBj has a long history of co-maintaining the PDB and BMRB core archives, but Cryo-TEM and related methods are emerging so quickly that we need to catch up with this new trend.

Do you know how and when the conventional PDB format was introduced? In the third issue of the newsletter published by Brookhaven National Laboratory (BNL) in October, 1976, the following message was recorded;

"1976 (Oct. 15th), No. Sets Held (72), No. Sets Distributed (1101), No. Recipients (38).

These distribution statistics represent activity only at Brookhaven. Duplicate copies of the file are maintained at the Crystallographic Data Centre in Cambridge (England) and at the University of Tokyo (Japan). These sites distribute data independently. All of the new structures obtained since this past spring have been entered in the new 80-column format and work is proceeding on conversion of the old parameter sets to the new format."

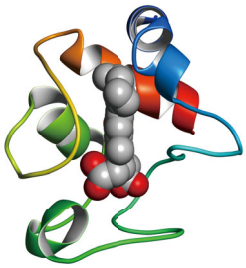


Fig.1 Crystal structure of cytochrome c

This was the announcement of the then new 80-column PDB format mandatory for the deposition of X-ray structures, which means that PDB format is more than 40 years old. I want to note that in the early 1970s, the master PDB data was sent from BNL to a team at the University of Tokyo, who then copied it to Nagoya Univ., Osaka Univ., and Kyushu Univ. Also, the data sets at that time included a deposition from Prof. Masao Kakudo, IPR, Osaka University, which was the sole deposition from Asia (PDB ID: 1CYC).

Lastly, in 2019, PDBj will continue to host several luncheon seminars at academic meetings throughout Japan to provide a good opportunity to discuss the leading archive of our community. The next wwPDB-AC meeting is scheduled to be held in Osaka, Japan, on October 18th, 2019 with the support of the Protein Research Foundation, Osaka, Japan. We will do our best as the host of this year's wwPDB-AC meeting in order to make it successful for both the wwPDB and PDBj itself.

About PDBj and wwPDB

PDBj has been in charge of the data processing in Asia and the Middle East region. In addition, we have developed several characteristic web services and provided them to structural biologists and bioinformatics researchers around the world. Furthermore, PDBj has established the PDBj-BMRB and EMPIAR-PDBj groups in collaboration with the BMRB and EMBL-EBI, respectively. Our activities are currently supported by JST-NBDC (Japan Science and Technology Agency - National Bioscience Database Center), Osaka University funded via MEXT (the Ministry of Science, Technology, Sports and Culture, Japan), and the AMED-BINDS (Basis for Supporting Innovative Drug Discovery and Life Science Research) project.

wwPDB AC meeting 2018 Report

The advisory committee meeting of the worldwide Protein Data Bank (wwPDB-AC) was held at Madingley Hall, Cambridge, UK on November 2nd, 2018. The wwPDB-AC consists of two advisors nominated by each wwPDB partner, representatives from the International Union of Crystallography and the macromolecular EM community, and wwPDB regional associate members (from India and China). The nominated representatives from PDBj-AC were Profs. Tsuyoshi Inoue (Osaka Univ.) and Masaki Yamamoto (RIKEN, SPring-8 Center). The agenda included: introduction and updated vision, mission and scope of the wwPDB; wwPDB community engagement; PDB core archive plans; BMRB core archive plans; questions and general discussion. In the executive session, one very important proposal was recommended: a plan to make PDBx/mmCIF Files mandatory for the deposition of X-ray Structures, which is scheduled to start from July 1st, 2019 (please also see page 3 for additional details.)

Fig.2 Attendees of the wwPDB-AC on 2018

AsCA2018 Report

Prof. Genji Kurisu and Dr. Takeshi Kawabata of PDBj attended the Asian Crystallographic Association (AsCA) 2018, which was held on December 2-5, 2018 at the University of Auckland, New Zealand. AsCA covers a wide range of crystallography, including not only crystallography of biopolymers, but also that of small compounds and inorganic materials, and new experimental techniques such as XFEL and neutron diffraction. Six keynotes and four plenary lectures were presented in a big hall, while 18 micro symposia were presented in three rooms in addition to the more than 250 posters that were on display. Among the 18 micro symposia, two symposia focused on Cryo-electron microscopy (Cryo-EM), indicating that many crystallographers are interested in using Cryo-EM. As the conference was held in the southern hemisphere, more than half of the participants came from Australia and New Zealand. According to the organizer, the number of Asian/Oceanic participants by country were Australia 106, New Zealand 86, Japan 86, China 47, Korea 3, and Taiwan 29. In addition, many speakers were invited from Europe and USA.

For the conference, Prof. Kurisu co-organized a micro symposium entitled “Database developments, validation and data mining” together with Dr. Amy Sarjeant from the Cambridge Crystallographic Data Centre. Here, Dr. James Hester explained data structures to describe crystallographic data, while Dr. Janet Newman talked about a database for crystallographic conditions. Dr. Stephen Burley from the RCSB-PDB, which currently processes deposited data from Oceania. Dr. Mathew Lightfoot from Cambridge Structural Database and Dr. Brian McMahon from IUCr also gave interesting talks. Dr. Burley explained PDB activities related to the validation of small compound ligand structures.

Dr. Kawabata provided a talk entitled “Databases and Web services from PDBj for Electron Microscopy,” which included an introduction of PDBj’s new mirroring database EMPIAR-PDBj for raw 2D images obtained by electron microcopy, as well as EM Navigator, Omokage Search, and the superimposing web service, gmfit. This year, PDBj introduced a new poster award to a student who presented excellent macromolecular structure work. PDBj appreciated the local organizers and referees led by Profs. Edward Baker and Kurt Krause, to help initiate our new award.

Fig.3 Speakers of the AsCA 2018 database session

Fig.4 The commendation ceremony of the PDBj poster prize.

OneDep Topics

Improvements of OneDep system and future plans

1. Data replacement prior to release; Privacy policy updated [May 2018]

In May 2018, OneDep improved the process of data replacement for PDB and EMDB entries, prior to their release. A new validation report is produced when a file is uploaded. Any major data errors or data inconsistencies between versions are displayed for review by the depositor so that these can be rectified prior to resubmission. We are also making sure that we are open and clear about how we handle personal data in OneDep. We have updated the wwPDB privacy policy to comply with the changes brought by the European Union data protection law (GDPR).

2. ORCIDs became mandatory for OneDep contact authors [July 2018]

ORCiD
Connecting Research and Researchers

In July 2018, ORCiD identifiers became mandatory for contact authors submitting PDB data using OneDep. This change supports wwPDB efforts to correctly attribute PDB structures to contact authors. At a later point, ORCiDs will be used to authenticate and reorganize access to deposition data within OneDep.

3. OneDep improves support for deposition of XFEL/SFX structures [October 2018]

In October 2018, the OneDep system for deposition, validation, and biocuration extended the range of metadata collected for structures solved by X-ray Free-Electron Laser (XFEL) and Serial Femtosecond Crystallography (SFX). Depositors can now provide details of the sample delivery, data measurement details such as focusing optics, pulse energy, frequency, and number of crystals used in new PDBx/mmCIF categories dedicated to XFEL and SFX experiments.

4. Mandatory mmCIF coordinate files for MX depositions [July 2019~]

PDBx/mmCIF will be the only format accepted for deposition of PDB structures resulting from macromolecular crystallography (MX), including X-ray, neutron, fiber, and electron diffraction methods via OneDep starting July 1st 2019. The deposition of PDBx/mmCIF format files will improve the efficiency of the deposition process and enhance validation through capture of the more extensive experimental metadata supported by PDBx/mmCIF, compared to the legacy PDB format. PDB entries with 100,000 or more atoms, and those with multiple character chain IDs are already not supported by the legacy PDB format. In addition, by 2021, we anticipate the PDB Chemical Component Identifier will need to be extended beyond three characters, which will necessarily result in the full retirement of files in the PDB Core Archive that utilize the legacy PDB format.

Refmac, Phenix.refine, and Buster programs can now output PDBx/mmCIF formatted files. For users of other structure determination/refinement software packages, the wwPDB provides stand-alone and web-based tools to convert legacy PDB format files into PDBx/mmCIF format: pdb_extract and MAXIT. More information on outputting and preparing PDBx/mmCIF format files for deposition can be found on the wwPDB website.

◆A request when referring to a PDB entry from your paper◆

Currently, PDB entries are collaboratively processed by wwPDB members; RCSB PDB, PDBe and PDBj. When you refer to your deposition, please describe it as shown in the examples below.

Example 1. “The coordinates and structure factors for the structures reported here have been deposited to the worldwide Protein Data Bank[1] and are available from Protein Data Bank Japan[2,3] with the accession codes ####.”

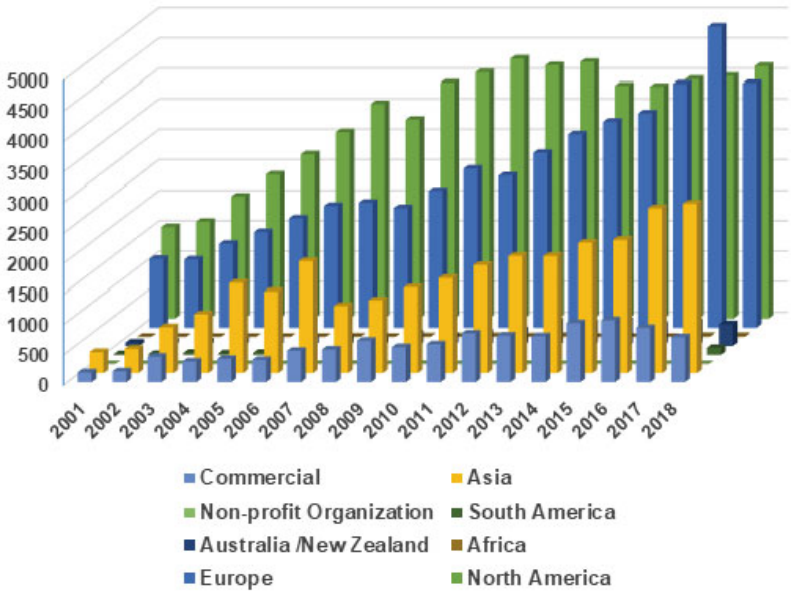
Example 2. “The cryo-EM density map has been deposited to the Electron Microscopy Data Bank[4] under accession number EMD-####. The atomic models of the cryo-EM structures have been deposited to the worldwide Protein Data Bank (wwPDB)[1] under the accession numbers #### and ####, respectively.”

Example 3. “The coordinates for [YOUR PROTEIN1] and [YOUR PROTEIN2] are available as PDB[5] entries #### and ####, respectively. The resonance assignment for [YOUR PROTEIN1] has been deposited to the Biological Magnetic Resonance Bank[6] as accession number ######.”

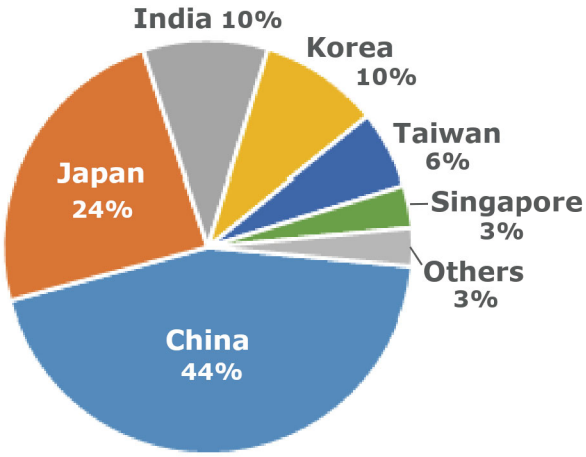
References
[1] Berman, H.M. et al. (2003). Nature Structural Biology 10 (12): 980.
[2] Kinjo, A.R. et al. (2018). Protein Science 27 (1): 95-102.
[3] Kinjo, A.R. et al. (2017). Nucleic Acids Research 45(D1), D282-D288.
[4] Lawson C.L. et al. (2016). Nucleic Acids Research 44(D1), D396-403.
[5] wwPDB consortium (2019). Nucleic Acids Research 47(D1), D520-D528.
[6] Ulrich E.L. et al. (2008). Nucleic Acids Research 36, D402-408.

Data Growth

Depositions By Depositor Location



Country distributions of Depositions processed by PDBj (2018)



BMRB Report

BMRB AC meeting 2018 at Wisconsin University of Madison, USA

The BioMagResBank Advisory Committee (BMRB AC) meeting was held at Wisconsin University of Madison on April 15th, 2018. Each representative research scientist presented their yearly contribution of NMR database entries to BMRB and their application, where the advisory committee subsequently assessed the activities and contributions to the life science database society. Also a new project leader, Prof. Jeffrey C. Hoch was introduced, and the time line for the replacement of the retiring Prof. John L. Markley was announced.

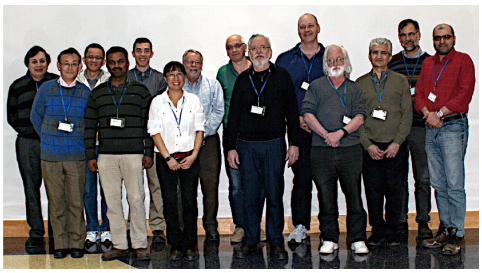


Fig.5 Attendees of the BMRB AC

Advanced and sophisticated Website for PDBj-BMRB

The PDBj-BMRB website and tools for converting the master BMRB format (NMR-STAR) to XML and RDF have been further updated. The top page provides a wide array of functions to search life science databases such as PDB, EMDB, Swiss-plot and Metabolomics as well as a gateway to each BMRB data entry, which includes rich information displaying not only the NMR parameters (assignment completeness and dynamics) but also PDB-IDs of homologues, PubMed-IDs of related papers, interaction partners and so on.

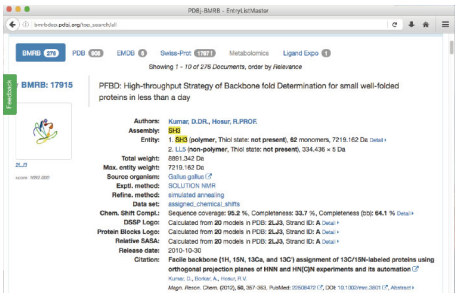


Fig.6 An example of search result on the webpage of PDBj-BMRB

Outreach 2018

PDBj has been active to hold luncheon seminars, workshops, and exhibitions to introduce our database, services and activities.

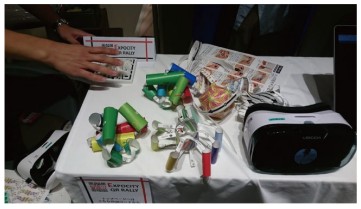
○Science Agora 2018 (held by Japan Science and Technology Agancy)

○Osaka University Co-Creation Bureau@EXPOCITY

PDBj held booths at the following two events for general public: Science Agora 2018 on Nov.11 & 12, 2018 at Telecom Center Building, Tokyo and Osaka University Co-Creation Bureau on Nov.17 at LaLaport EXPOCITY, Osaka. A wide variety of people including children and adults participated; the total number was about 500 people for each event. PDBj provided the following exhibitions at the booths:

Papermodels

Constructing molecular models such as proteins from a plain piece of paper by cutting, folding and gluing, which helps to better understand the structures of protein molecules. PDBj also utilized them to explain that linearly-connected amino acids spontaneously fold into a specific shape to serve their function. There are two types of paper model data: translations of originals that were provided by the RCSB-PDB; and PDBj's original creations. For both, the data in PDF format is downloadable at the PDBj Numon site (https://numon.pdbj.org/).



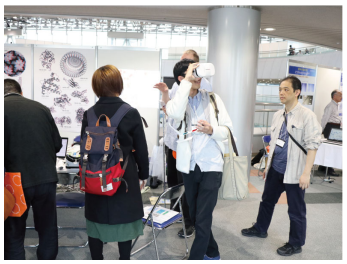
Molecular models produced by 3D printer

Molecular structural models made from plastic can be produced by a 3D printer. First, the molecular structural data is converted into 3D object data compatible with 3D printers (STL formatted files). To reduce the data size and increase the strength of the model, a surface model is usually selected. When the molecule is small, a spacefill representation in which each atom is shown as a sphere can also be used. Then the data is used by the 3D printer to produce a physical 3D model. We used the models to show that the shape of the cavity of the active site of proteins is central to the development of drugs.

Stereoscopic view of protein molecules

Visitors enjoyed viewing the shape of protein molecules via two unique services developed by PDBj. First is a VR molecular viewer to visualize molecules through a VR extension of our developed molecular viewer, Molmil, by using a modern smartphone with a relatively cheap VR goggle. The phone is to be mounted within the goggle after loading the VR scene, which can then be placed in front of the user's face. The demo showed several protein molecules floating in the air, surrounding the user, where the user can rotate around within the scene by rotating their head.

We also used Yorodumi Prime to view molecules by red-blue anaglyph glasses. Brief explanations aimed towards general people in combination with molecular anaglyph images that can be rotated and zoomed in/out by either mouse or finger actions gave visitors a glimpse of the wonderful world of molecular structures. This anaglyph view mode is also available from our website (https://numon.pdbj.org/) and we distributed paper glasses to visitors so they could enjoy viewing structures in stereo from their homes.



○Other Outreach Activities

＊ Materials of the seminars and workshops are available on our website: https://pdbj.org/info/previous-workshop

■PDBj Luncheon Seminar
at the 18th Annual Meeting of the Protein Science Society of Japan
June 28, 2018, Niigata

■PDBj Luncheon Seminar
at the 56th Annual Meeting of the Biophysical Society of Japan
September 16, 2018, Okayama

■PDBj Luncheon Seminar at the 7th Joint Conference on Informatics in Biology, Medicine and Pharmacology
September 20, 2018, Yamagata

■PDBj Luncheon Seminar
at the Annual Meeting of Crystallographic Society of Japan
November 11, 2018, Tokyo

■Exbition booth for the Life Science Databases at the 41st Annual Meeting of the Molecular Biology Society of Japan
November 28-30, 2018, Kanagawa

■The All-in-one Joint Workshop 2018/AJACS Bancho 2
January 28, 2019, Tokyo

■PDBj & BINDS Workshop
February 19, 2019, at Osaka University Suita Campus

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