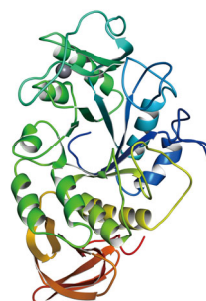
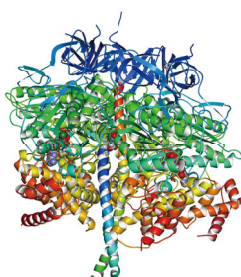
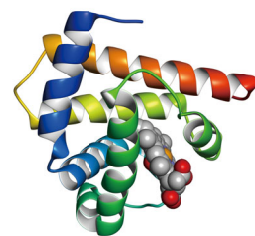
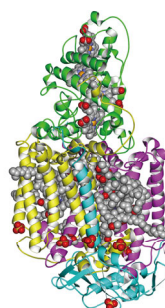
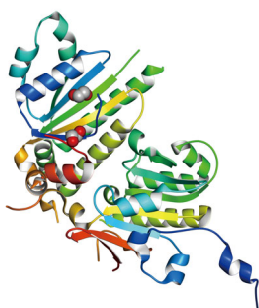
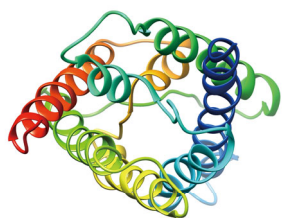
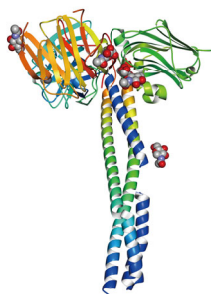
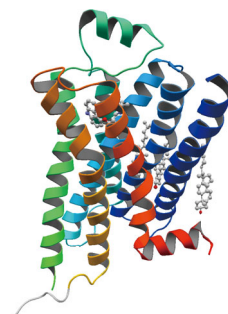
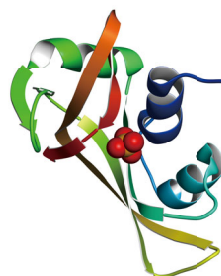
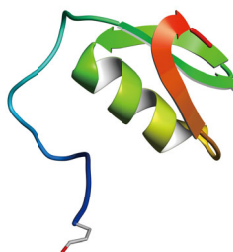
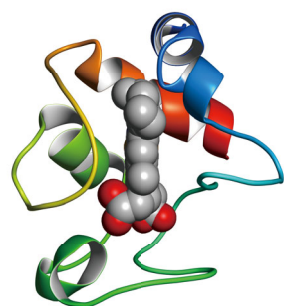
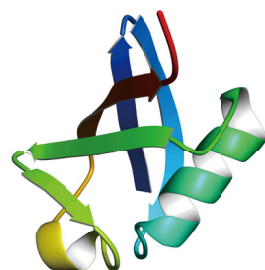
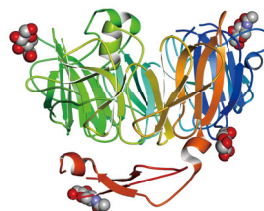
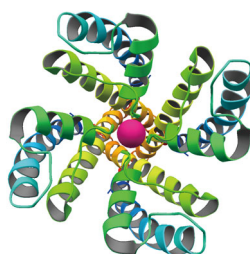
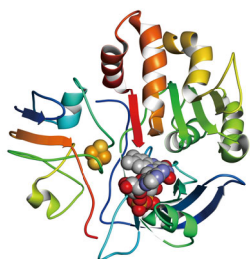
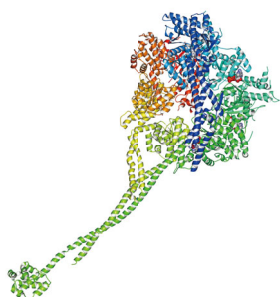
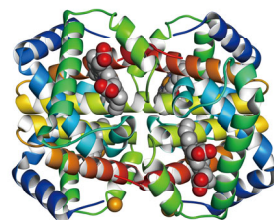
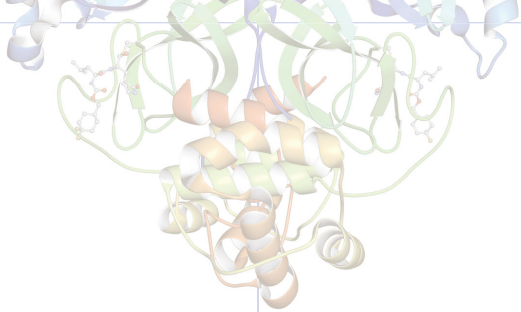


PDBj Newsletter

March 2024

Vol. 24





wwPDB Advisory Committee

The wwPDB Advisory Committee (wwPDB AC) meeting is held in autumn and rotated and hosted by one of the wwPDB core members. On October 27th, 2023, EMDDB hosted the 20th wwPDB AC meeting in a hybrid format. Most of the wwPDB PIs attended the meeting locally from the Hinxton campus of EMBL-EBI in the UK, whereas all wwPDB AC members joined remotely via the Zoom online system. As representatives of the PDBj Advisory Committee, Genji Kurisu, as head of PDBj, and Drs. Toshiya Senda (KEK Photon Factory) and David Hsiao (Academia Sinica, Taiwan), attended this annual AC meeting. The status of all wwPDB core archives and OneDep development was reported. In the wwPDB AC meeting, the advisors discussed the threats posed by the current war in Ukraine to the wwPDB Open Access Model, the BMRB funding update, and the structure of wwPDB AC. As one of the wwPDB core members, PDBj would greatly appreciate the contribution of committee members to concrete and constructive suggestions, even at this late date. PDBj will host the next Advisory Committee meeting in October 2024.



OneDep Summit 2023



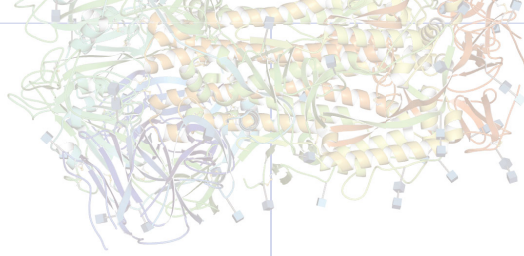
The OneDep Summit was held at the Genome Campus in Hinxton, UK, from October 29th to 30th 2023. At this annual conference, developers and biocurators of OneDep, the common data deposition system of wwPDB, gathered to discuss the long-term development goals of the OneDep system, annotation guidelines, and future challenges. We are currently facing the following challenges: a growing number of depositions, increasing amounts of experimental data, particularly EM maps,

and the complexity of depositions and annotations for a series of multiple entries. The OneDep development team discussed the renewal plan for data exchange among PDB sites and improvements in system reliability, performance, and usability. The PDB biocurator team explored ideas for enhancing the efficiency of annotation processes and the treatment of series depositions. Decisions made at the OneDep Summit will contribute to guiding the future development of the OneDep system. Since this event, internal meetings have continued to establish detailed requirements and implementation strategies.

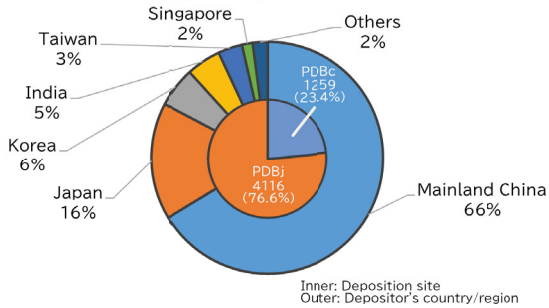
The PDBj Advisory Committee Meeting

The PDBj Advisory Committee meeting was held online at 10 am on March 6th, 2023, via the Zoom online system. Staff from our primary funder, JST-NBDC, including Professor Takashi Itoh of Kyushu University (a program supervisor), joined the meeting as observers. Professor Kurisu presented the activity report for 2022 and the activity plan for 2023. In 2022, PDB China was inaugurated, and PDBj provided on-site training for two Chinese biocurators from Shanghai. Following the on-site training at PDBj, these biocurators returned to China and processed a few of the Chinese entries in 2022. Additionally, the status of the original activities of PDBj, EMPIAR-PDBj, XRDa (X-tal Raw Diffraction Archive), and BSM-Arc (Biological Structural Molde Archive) were reported. Finally, Professor Kurisu reported the succession of Dr. Junichi Saito from Kyowa Hakko Kirin Co. by Dr. Satoshi Sogabe from Axcelead Drug Discovery Partners and expressed his sincere appreciation of Dr. Saito's contribution to PDBj.

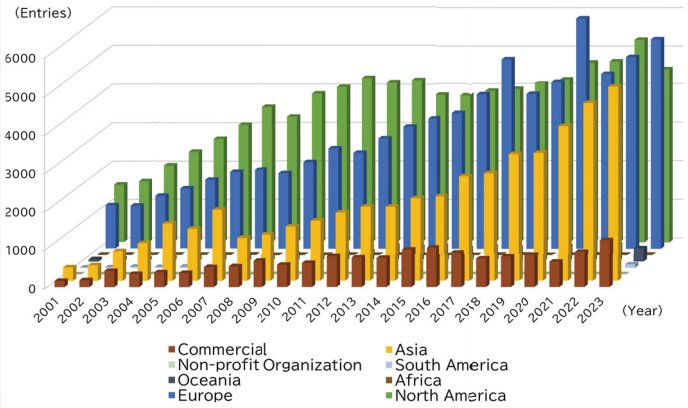




Geographical distributions of PDB depositions processed by PDBj and PDBc in 2023



PDB Depositions By Depositor Location



In 2023, more than 16,000 new PDB entries were released, of which approximately 30% were deposited by institutes in the Asian region. For certain entries from Mainland China, we re-assigned them to PDB China for processing.

Achieved 10000 entries in the PDB deposition processes



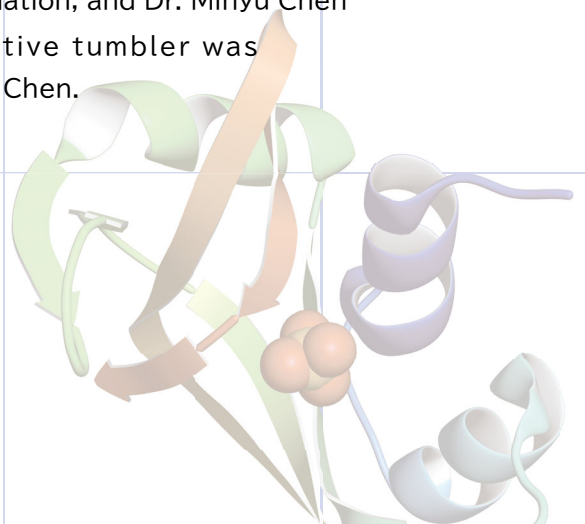
Dr. Minyu Chen, a PDBj biocurator since 2007, has processed over 10,000 PDB depositions.

She is the second PDBj biocurator to reach this milestone, following Yumiko Kengaku, and the fifth in the wwPDB.

(Feb 13th 2024)



(Above) Toshiharu Hase, head of the Protein Research Foundation, and Dr. Minyu Chen
(Left) The commemorative tumbler was presented to Dr. Chen.



Model CIF: Data Format for Structural Models Derived Using Computational Methods

The Model CIF Working Group has developed a data format “Model CIF,” for structural models derived using computational methods. This is an extension of “PDBx/mmCIF,” which is a descriptive format for experimentally determined molecular structure data and is the standard format for PDB.

(Jan 31st, 2023)

Regarding the Termination of Data Provision in PDB Format Due to CCD 5-digit Conversion

Until now, the Chemical Component Dictionary (CCD) ID, used to identify compounds when describing PDB data, has been defined to be three characters or less. Still, as ID resources have been exhausted, this will no longer be possible. Issue a 5-character alphanumeric code (we do not use the 4-character code to avoid confusion with the PDB ID). Data for PDB entries containing 5-character CCD IDs is not provided in PDB format because 5-character CCD IDs cannot be written in PDB format.

(Mar 8th, Sep 14th, and Dec 14th, 2023)

ORCiD Authentication in OneDep

When registering PDB data using OneDep, you can now register and view the data using ORCiD authentication. Previously, authentication was required for each registered session. However, when using ORCiD authentication, re-authenticating for each session is no longer necessary, and all registered sessions can be viewed in a list.

(Mar 28th and Dec 20th, 2023)

wwPDB 20th Anniversary

In July 2003, the wwPDB was founded by the RCSB PDB, PDBe, and PDBj, and this year marks its 20th anniversary. Later, BMRB and EMDB joined as members.



(Jul 9th, 2023)

Distribution of EMDB Metadata in PDBx/mmCIF Format

To date, EMDB metadata has been distributed in the XML format; however, we have now started distributing this data in the PDBx/mmCIF format. This is anticipated to facilitate interoperability between PDB and EMDB data.

(Oct 4th, 2023)

Improvement of Information on Peptide Residues in the CCD

In the Chemical Component Dictionary (CCD), a data item indicating the atoms comprising the main chain of a peptide has been added, and the nomenclature of atoms has been standardized.

(Jul 27th and Nov 15th, 2023)

Standardization of NMR Experimental Data Deposited in the PDB

wwPDB has released an archive in which experimental data (chemical shifts and restriction information) for NMR structures previously deposited in PDB have been converted from software-specific formats to both NMR-STAR and NEF formats supported by the NMR community. In the future, it is planned that wwPDB will only accept single files in either NMR-STAR or NEF format for NMR experimental data deposition and that the use of supporting software-specific formats will be discontinued.

(Jun 14th, 2023)

Release of the Next-generation Archive Repository

We have released the PDB next-generation archive repository (NextGen).

This repository is an extended PDB archive that includes external database resources such as UniProt, SCOP2, and Pfam, as well as structural model data that is maintained in the conventional PDB archive. Moreover, it includes information regarding intra-molecular connectivity.

NextGen is available from the following site:

<https://ftp-nextgen.pdbj.org>

(Feb 7th and Jul 5th, 2023)

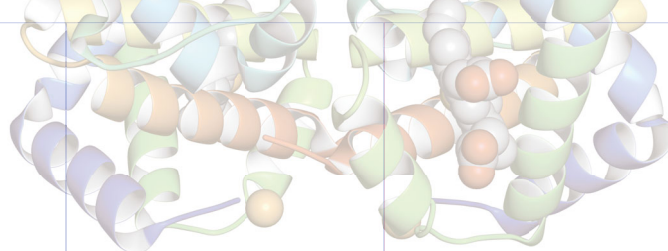
Improvement of Starting Model Information

To improve information relating to starting models for X-ray, electron microscopy, and NMR methods, we have introduced the following new PDBx/mmCIF category:

`_pdbx_initial_refinement_model`

This clarifies the source of the initial model information (e.g., PDB, AlphaFoldDB, and RoseTTAFold) and makes it easier to distinguish between experimentally and computationally obtained models.

(Feb 1st, 2023)



Conferences, etc.

We introduced the latest trends in PDB, future activity policies, the OneDep deposition system, etc. at academic conferences.

May 18 th , 2023	The 27 th ann. mtg of the Taiwan biophys. society (Taiwan Tzu Chi Univ.)	seminar
Jun 25 th -Jul 1 st , 2023	BioHackathon 2023 (Kagawa Intl. Conf. Hall)	devel. mtg
Jul 5 th , 2023	The 23 rd PSSJ (Nagoya Intl. Conf. Hall)	luncheon seminar
Aug 22 nd -29 th , 2023	The 26 th IUCr (Melbourne Conv. & Exh. Centre)	booth exh.
Sep 8 th , 2023	IIBMP2023 (Kashiwa-no-ha Conf. Center)	luncheon seminar
Oct 5 th , 2023	Togo-no-hi symposium 2023 (Miraikan)	Oral Pres.
Oct 29 th , 2023	Ann. mtg of CRSJ (Yamaguchi Univ. Tokiwa Campus)	luncheon semr./ booth
Nov 2 nd , 2023	The 96 th ann. mtg of the Jp. Biochem. Soc. (Fukuoka Intl. Conf. Hall)	seminar
Nov 15 th , 2023	The 61 st ann. mtg of the Biophys. Soc. of Jp (Nagoya Intl. Conf. Hall)	luncheon seminar

Events for General People

During 2023, we held the following events for the general public, in which we explained protein molecules and their functions using stereoscopic views and red-blue anaglyph glasses.

Jul 6 th , 2023	Sakura science program 2023 (IPR, Osaka Univ.)
Jul 8 th , 2023	Osaka Univ. co-creation day@EXPOCITY (lalaport EXPOCITY)
Jul 29 th and Aug 1 st , 2023	IPR seminar for senior high school students (IPR, Osaka Univ.)

Biophysical Society of Japan wwPDB Student Presentation Award



At the 61st Annual Meeting of the Biophysical Society of Japan held in November 2023 at the Nagoya International Conference Center, PDB Outstanding Student Awards were awarded to three oral presentations given by outstanding students. This commemorates the 20th anniversary of establishing the International Protein Structure Data Bank (wwPDB) in 2023. The award winners and their presentation titles are as follows.

Keisuke Kasahara (Dept. Bioeng., Grad. Sch. Eng., Univ. Tokyo) “Thermodynamic analysis of Fv-supercharged antibody-antigen interactions and control of interaction parameters”

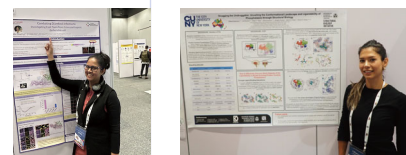
Katsuhiko Minami (National Institute of Genetics, Graduate Institute for Advanced Studies, SOKENDAI) “Replication-dependent histone (Repli-Histo) labeling revealed that chromatin motion can determine DNA replication timing”

Kyle Ian Peter Le Huray (University of Leeds, Leeds, UK)

“Harnessing the power of machine learning and high-throughput molecular dynamics simulations to predict protein-lipid interactions”

IUCr wwPDB Biomolecule Poster Award

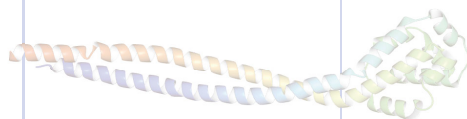
At the 26th Conference of the International Crystallographic Association (IUCr2023) held in Melbourne, Australia, from August 22nd (Tue) to August 29th (Tue), 2023, we set up an exhibition booth and presented awards to outstanding students. Poster awards were presented. The award winners are as follows:



Akila Pilapitiya, Lilian Hor, Jason Paxman, and Begoña Heras, “The crystal structure of the toxin EspC from enteropathogenic *Escherichia coli* reveals approaches to combat diarrheal infections” , La Trobe University

Liliana Guerrero (1), Ali Ebrahim (1), Blake T. Riley (1), Minyoung Kim (1,2), Qingqiu Huang (3), Aaron D. Finke (3), and Daniel A. Keedy (1,4)

, “Drugging the Undruggable: Unveiling the Conformational Landscape and Ligandability of Phosphatases through Structural Biology” , (1) Structural Biology Initiative, CUNY Advanced Science Research Center (2) Department of Molecular Biology, Princeton University (3) Cornell High Energy Synchrotron Source (CHESS), Cornell University and (4) Department of Chemistry and Biochemistry, City College of New York



I was a biocurator before?



At the International Union of Crystallography Congress (IUCr) held in Melbourne, Australia, in August 2023, I met my old friend, Dr. Jiansheng Jiang of the National Institute of Allergy & Infectious Diseases, USA (photo), with whom I shared good memories from more than 20 years ago. In 1998, Prof. Yoshimasa Kyogoku, a director of the Institute for Protein Research (IPR) at the time, decided to send me to the Brookhaven National Laboratory (BNL), Long Island, NY, USA, to learn data-annotation for the PDB entries. I spent 3 months there in early 1999, and it was Dr. Jiang who taught me how to process the PDB entries in BNL. I processed a few entries under his kind guidance. Soon thereafter, the PDB activity moved from BNL to Rutgers University, and the relationship between BNL and IPR was severed; however, this was the starting point of my relationship with PDB. In November 2023, I had the opportunity to present a talk on PDBj at the symposium of the Japanese Biochemical Society held in Fukuoka. The organizer of this symposium was Prof. Takashi Ito, a research supervisor of the Database Integration Coordination Program (DICP) of JST-NBDC, who asked me to present my thoughts on data-driven research and describe the target of my current DICP project, as well as what I had in mind as an experimental scientist when I started the DB activity. At this symposium, I expressed my opinion that it is necessary to ensure the “high quality” of PDB as one of the fundamental databases that support data-driven research with full use of AI. I also explained why I became involved in PDB, mentioning that “PDB has always been close to me since I was very young, and I cannot imagine my institute without PDB.” This idea came back to me, partly through my reunion with Dr. Jiang last summer. The events of last year indeed presented excellent opportunities for me to reflect on my encounters with PDB.

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Protein Data Bank Japan

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