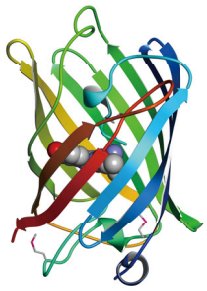
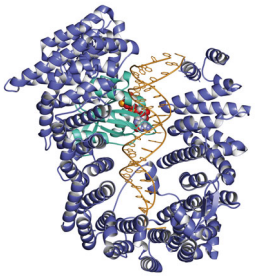
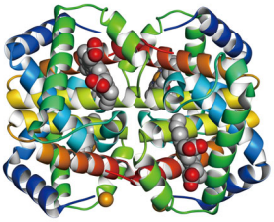
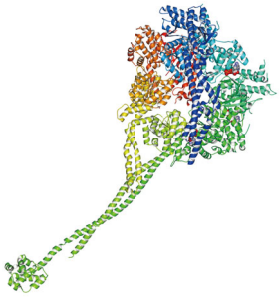
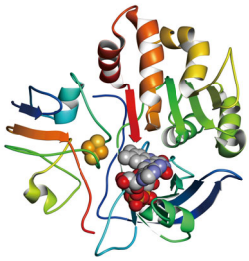
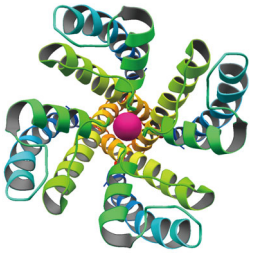
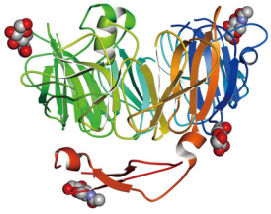
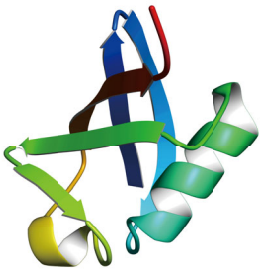
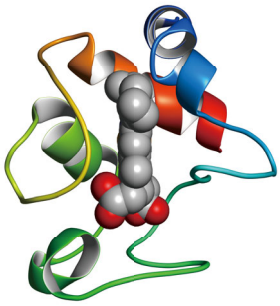
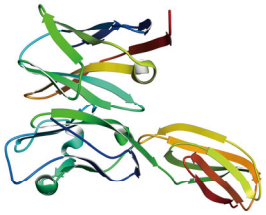
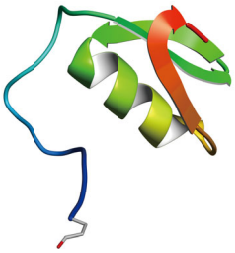
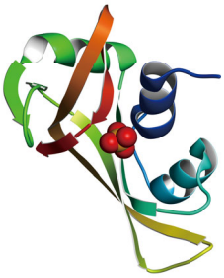
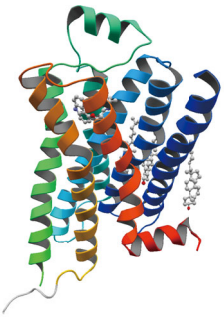
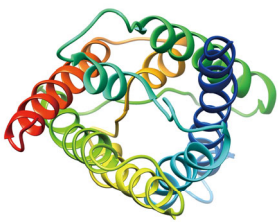
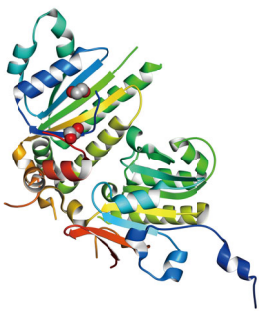
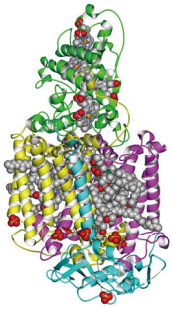
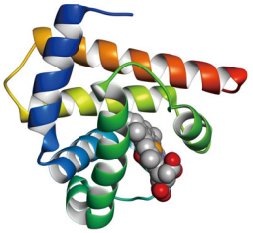
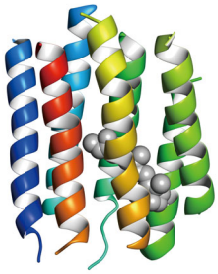
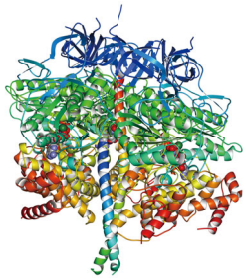



PDBj Newsletter

March 2025

Vol. 25


wwPDB Advisory Committee Meeting

The wwPDB Advisory Committee (wwPDB AC) meeting is held annually in autumn and is hosted on a rotationally by one of the wwPDB core members. The 21st wwPDB AC meeting was hosted by PDBj and held in a remote format on October 18th, 2024. The wwPDB Summit, which includes OneDep Developer and Biocurator meetings, was held on October 16th, 17th, and 18th, 2024, and hosted onsite by PDBj. Thus most of the wwPDB PIs participated in the wwPDB AC meeting remotely from the Senri Hankyu Hotel near Osaka University. All wwPDB AC members joined via Zoom. Genji Kurisu, the head of PDBj, along with Drs. Toshiya Senda (KEK Photon Factory) and Kyeong Kyu Kim (Sungkyunkwan University School of Medicine, Republic of Korea), attended this annual AC meeting as representatives of the PDBj AC. During the meeting, reports were presented on the status of all wwPDB core archives, the transition plan of PDB China to core membership, and funding updates for wwPDB core members. Advisors also discussed OneDep developments and wwPDB policies regarding the obsolescence of entries. As one of the wwPDB core members, PDBj appreciates the valuable contributions of the committee members, especially those who joined very late hours in their respective time zones, for their highly specific and constructive suggestions. The wwPDB Summit and AC meeting were financially supported by JST-NBDC and the Protein Research Foundation. The next wwPDB Summit and AC meeting will be hosted by BMRB in May and October 2025, respectively.

wwPDB Summit 2024

wwPDB Summit 2024 was held at the Senri Hankyu Life Science Center from October 16th to 18th, 2024. OneDep developers and PDB biocurators discussed the challenges of the OneDep system, streamlining data deposition, and reviewing software development management. In particular, reducing the complexity of inputting common metadata in multiple-entry studies has been marked as an urgent issue, and further discussions will continue. In addition, the current software development style was revised to allow the OneDep system to be deployed in cloud environments, and the efficiency of annotation and ensuring uniform quality at each site were discussed.

PDBj AC meeting (for fiscal years 2023 and 2024)

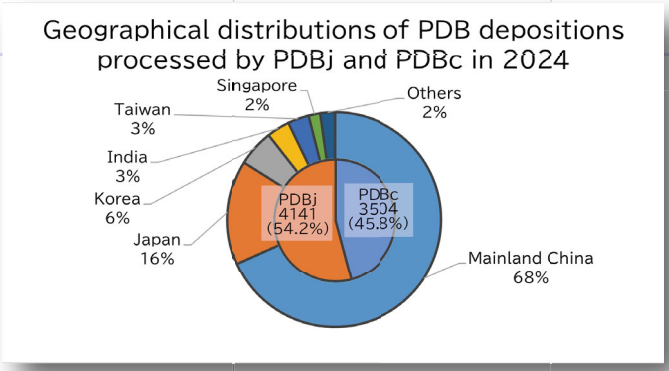
FY2023 (April 2023 – March 2024)

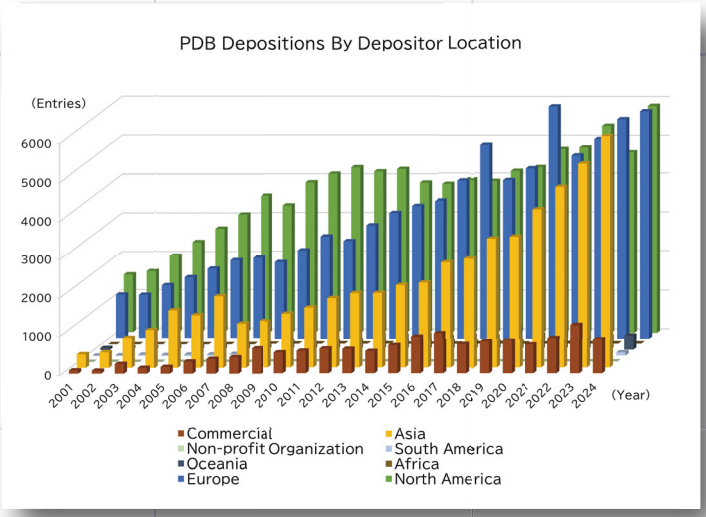
The FY2023 PDBj AC meeting was held via Zoom at 1:00 PM on March 13th, 2024. Members of our primary funding agency, JST-NBDC, including the program supervisor Prof. Takashi Itoh of Kyushu University, participated in the meeting as observers. Prof. Kurisu presented an activity report for FY2023 and an activity plan for FY2024. PDB China was successfully launched in 2023, and PDBj provided extensive support for its establishment. Additionally, the 20th anniversary event of wwPDB, including the three Best Presentation Awards at the Biophysical Society of Japan Annual Meeting was reported. Updates on PDBj's original activities, including EMPIAR-PDBj and BMRBj, were also provided. Finally, Prof. Kurisu reported on the transition of the PDBj AC membership with Prof. Chwan-Deng Hsiao from Academia Sinica, Taiwan, who was succeeded by Prof. Nei-Li Chan from the Medical School of National Taiwan University. Prof. Kurisu expresses appreciation for Dr. Hsiao's valuable contributions to PDBj. For further details, please refer to the AC report at pdbj.org.

FY2024 (April 2024 – March 2025)

The FY2024 PDBj AC meeting was held via Zoom at 1:00 PM on February 13th, 2025. Three members from our primary funding agency, JST NBDC, including the program supervisor, Prof. Takashi Itoh of Kyushu University, participated as observers. Prof. Kurisu has presented an activity report for FY2024 and an activity plan for FY2025. In 2024, PDBj launched a new UniProt portal page, highlighting its most recommended query entry and new Sequence Navigator Pro service. In December 2024, PDBj hosted an exhibition booth for wwPDB and PDBj at the Conference of the Asian Crystallographic Association and presented the wwPDB Foundation Best Poster Awards to three distinguished presenters. Finally, Prof. Kurisu commented that after PDB China became a full member, PDBj would be able to allocate more resources to data-out activities and OneDep development. Therefore, PDBj has been actively working to establish PDB China in Shanghai.

PDBj Data Growth





PDB entries from the Asian region were first accepted by PDBj, and those from mainland China were then assigned to PDBc for processing. In 2024, approximately 46% of PDB entries submitted to PDBj (approximately 66% of entries from mainland China) were processed by PDBc annotators.

PDBj Topics

Started providing compound data files with ideal coordinates in SDF/MOL format

We began by providing data files with ideal atomic conformations in SDF/MOL format. Each file can be downloaded from the PDB archive. The URL is as follows:

wwPDB https://files.wwpdb.org/pub/pdb/refdata/chem_comp/

PDBj https://files.pdbj.org/pub/pdb/refdata/chem_comp/

We also provide the combined files that include each chemical compound file. The URL is as follows:

wwPDB https://files.wwpdb.org/pub/pdb/data/monomers/components-pub.sdf.gz

PDBj https://files.pdbj.org/pub/pdb/data/monomers/components-pub.sdf.gz

(Feb 13th 2024)

Released user guide for PDBx/mmCIF format data

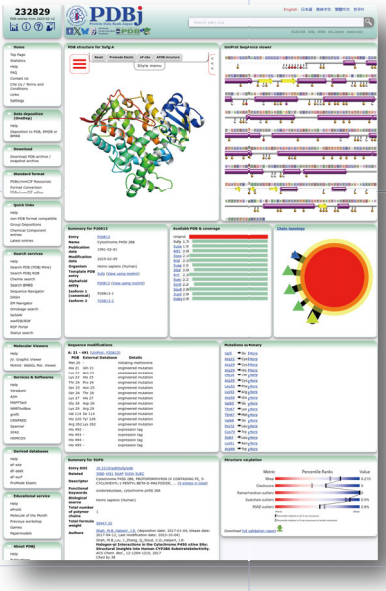
A new user guide for the PDBx/mmCIF format was published. The URL is as follows:

https://mmcif.wwpdb.org/docs/user-guide/guide.html

Please refer to this document when working with this format.

(Jun 20th 2024)

Launched new portal site linking gene mutation information with protein sequence and three-dimensional structure information



The Institute for Protein Research, Osaka University, and PDBj, together with the Tohoku Medical Megabank Organization (ToMMo) at Tohoku University, have built a portal site linking gene mutation information for Japanese people with protein sequence and three-dimensional structure information, and have released it as a new PDBj service.

https://pdbj.org/uniprot/

This site links the gene mutation information stored in the Japanese Multi-Omics Reference Panel (jMorp) constructed by ToMMo. It also implements a tool for easily displaying mutations in the three-dimensional structure of proteins. The correspondence between gene mutations and three-dimensional protein structures is complicated; however, our portal site makes it easy to check for correspondence.

(Left) A new portal site connecting Japanese gene mutation information published in PDBj with protein sequences and structures (example: UniProt ID: P20813).

(Nov 1st ,2024)

Termination of FTP download service on wwPDB site

The wwPDB site (ftp.wwpdb.org) will abolish the FTP download service because current major web browsers no longer support downloading via the FTP protocol. The PDBj ftp site (ftp.pdbj.org) will continue providing FTP services for the time being.

(Oct 31st ,2024)

Nobel Prize in Chemistry 2024

The 2024 Nobel Prize in Chemistry was awarded for achievements in computational protein design and structural prediction. The PDB data served as a training set for developing methods for these tasks, which were recognized by the award.

(Oct 18th ,2024)

Once the preprint is published, PDB entry will also be made public

The wwPDB has a policy of releasing deposited PDB entries to the public that, "when a paper is published, the corresponding PDB entry will also be made public," and we have decided to include bioRxiv preprints in this published paper.

(Oct 17th ,2024)

Standardization of protein modification description in PDB data

The method for describing protein chemical modifications (PCM) and post-translational modifications (PTM) in PDB data, which has been inconsistent until now, has been standardized. This is expected to improve the searchability. This change is gradually reflected in existing public entries.

(Oct 9th ,2024)

PDB Archive has started publishing data on structures determined by IHM

Structural data solved using the "Integrative and Hybrid structure determination Method (IHM)," which combines multiple experimental and computational methods, have been published in PDB-IHM (formerly PDB-Dev) until now. We began publishing them in the PDB archive (https://files.wwpdb.org/pub/pdb_ihm/).

We also added links to the relevant PDB-IHM pages on the landing pages of each PDB entry.

(Oct 3rd ,2024)

PDBj

Outreach

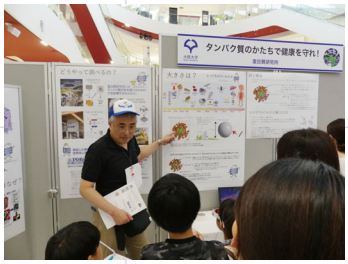
Conferences, etc.

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

Jun 13th, 2024	The 24th PSSJ (Sapporo Conf. Center)	luncheon seminar
Jun 24th–28th, 2024	IUPAB 2024 (Kyoto Itnl. Conf. Center)	booth exh.
Aug 22nd, 2024	ICMRBS 2024 (Coex, Seoul, Korea)	luncheon seminar
Oct 5th, 2024	Togo-no-hi symposium 2024 (Shinagawa the Grand Hall)	poster pres.
Oct 22nd–23rd, 2024	The 22nd IPR Retreat (Icho Kaikan, Osaka Univ.)	poster pres.
Oct 24th, 2024	APBJC2024 (Naha Cultural Arts Theater NAHArt)	luncheon seminar
Nov 10th, 2024	Annual meeting of CrSJ 2024 (Nagoya Univ.)	luncheon seminar
Dec 1st–6th, 2024	The 18th AsCA (Sunway Univ, Malaysia)	booth exh. and poster award

Events for general public

On June 29th, 2024, we exhibited a booth at the "Osaka University Co-Creation DAY @ EXPOCITY" held at LaLaport EXPOCITY, where we used red and cyan glasses for stereoscopic vision and paper models to explain protein molecules and their functions.



AsCA poster award

As part of the wwPDB Foundation's activities, PDBj awarded the Poster Award to the following three people at the Asian Union of Crystallographers Congress (AsCA2024) held in Kuala Lumpur, Malaysia in December 2024. Award certificates were sent by AsCA, and prizes were sent by the wwPDB Foundation. We would like to thank the AsCA Executive Committee for serving as judges.

Salma Dienta Salsabila

(Gwangju Institute of Sci. and Tech.)
for Structural Mechanistic Insights into the Function of Phosphatidylethanolamine N-Methyltransferase PmtA Mediating Bacterial Phosphatidylcholine Synthesis

Se-Young Son

(Ewha Womans University)
for Structural Investigation of the Docking Domain Assembly from Trans-At Polyketide Synthases

Yeon-Ju Jung

(Ewha Womans University)
for Unveiling Thermostable sPLA2 from Scisciorella Marina: Enhanced Stability and Biotransformation for Industrial Applications

Booth exhibition (IUPAB2024, AsCA2024)

PDBj exhibited at the International Union of Biological Chemistry (IUPAB2024) held in Kyoto in June 2024 and at the Asian Union of Crystallographers Meeting in Kuala Lumpur, Malaysia in December 2024. At the exhibition booth, we introduced our activities using PDBj brochures, as well as wwPDB activities.

Left: Professor Juha Huiskonen (University of Helsinki, Finland), a member of the wwPDB Management AC, and Professor Kurisu, director of PDBj, at the IUPAB2024 booth.

Right: Professor Sun-Shin Cha (Ewha Women's University, South Korea), a PDB submitter, and Professor Kurisu, the director of PDBj, at the AsCA2024 booth.

PDBj

Episode

Nobel Prize in Chemistry 2024

The 2024 Nobel Prize in Chemistry was awarded to Professor David Baker (University of Washington), Dr. Demis Hassabis (DeepMind), and Dr. John Jumper (DeepMind) for their contributions to the computational protein design and protein structure prediction. As a member of wwPDB, the PDB core archive serves as a training dataset for innovative molecular design and structure prediction methods, I would like to extend my congratulations to the laureates. This award highlighted the importance of maintaining and openly sharing the updated PDB core archive as a freely accessible resource. Although I am not an expert in protein design or structure prediction, I strongly feel the profound impact of their work as a researcher in a related field. A Nature News article published last year quoted Dr. Jumper's remark at a DeepMind press briefing: 'It's humbling every time we train [AlphaFold] on years of effort. Each data point is the years of effort from someone.'"[*1]. Professor Helen M. Berman, former director of the RCSB PDB, also emphasized the significance of experimental data in AI-driven scientific breakthroughs in the same issue of Nature. When asked, 'Does it speak to the importance of experimental data for powering AI breakthroughs in science?" She responded: "Yes, 100%. People will say, 'Oh, well the PDB data are really special.' However, we know why this is unique. It took a long, long time to figure out how to handle the data, how to represent the data, and how to collect the data.[*2] The contributions of this year's laureates will accelerate a new era in protein science, enabling more dynamic, detailed, and extensive descriptions of protein molecules in combination with existing experimental structural biology methods. In line with advancements in computational science recognized by the Nobel Prize, wwPDB continues to emphasize structures determined by the integrated/hybrid method (PDB-IHM), which incorporates complementary techniques beyond crystallography, NMR, and cryo-electron microscopy. We hope that this Nobel Prize in Chemistry will serve as a catalyst for further advancements in data-driven research, including PDB-IHM.

*1 Callaway, E. Nature, 634, 525, 2024 *2 Callaway, E. Nature 634, 1028, 2024

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Protein Data Bank Japan

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