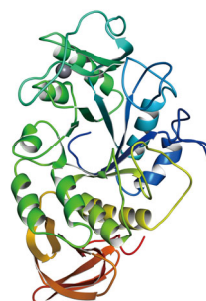
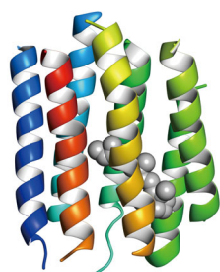
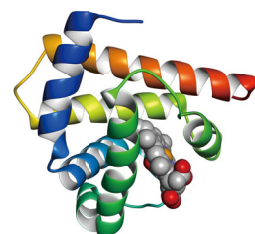
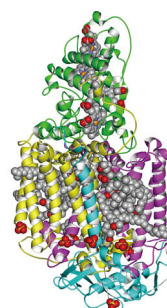
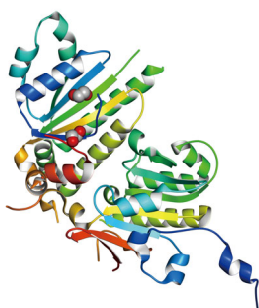
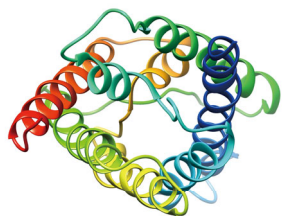
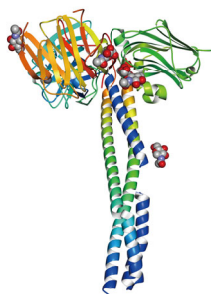
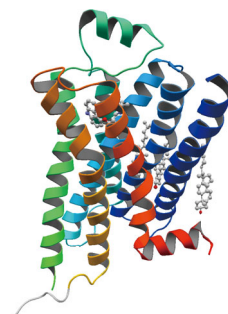
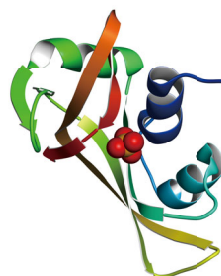
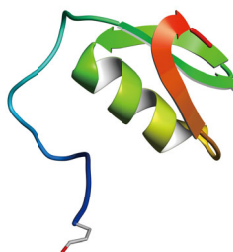
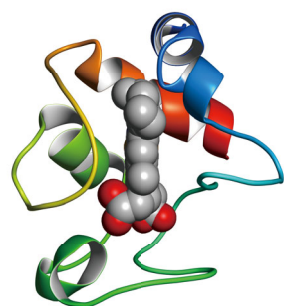
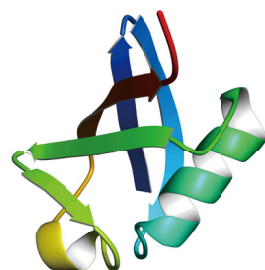
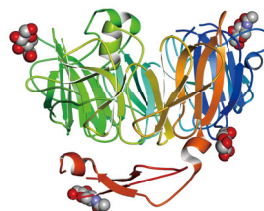
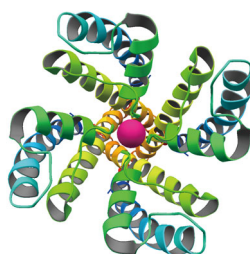
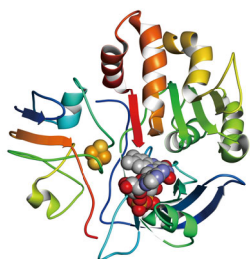
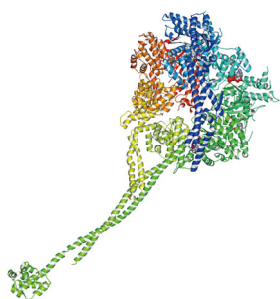
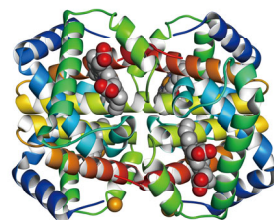
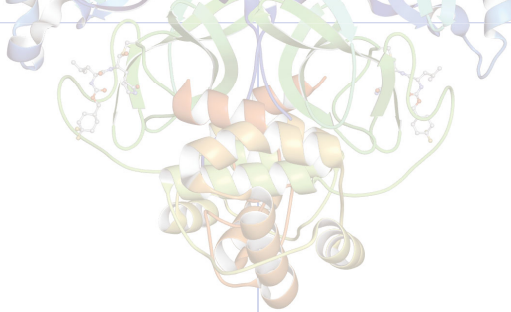


# PDBj Newsletter

March 2023

## Vol. 23



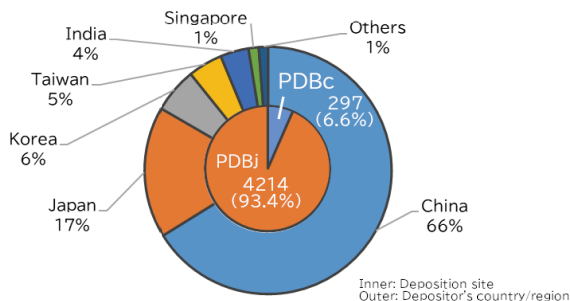


## wwPDB Advisory Committee

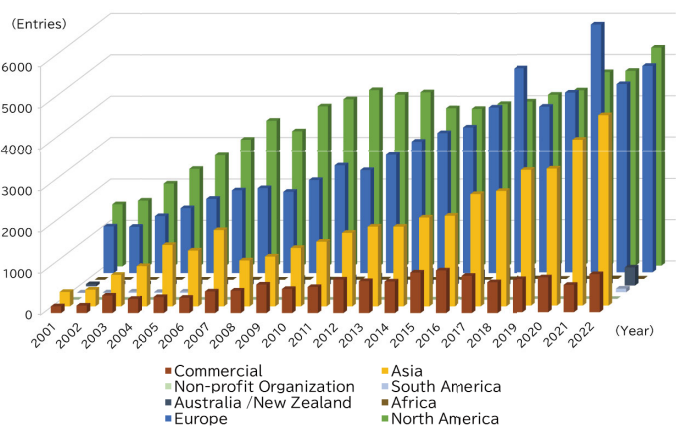
The wwPDB Advisory Committee (AC) was held online from 21:30 to 24:25 on November 14th, 2022, via Zoom. The PDBj representatives this year were Prof. Toshiya Senda from Photon Factory, KEK, and Prof. David Hsiao from Academia Sinica, Taiwan. Before the remote meeting, the wwPDB members prepared and circulated the current status of the three core archives and activity reports to the AC members. During the remote meeting, the wwPDB AC discussed the following topics: Training plan of PDB China Biocurators, closer collaboration with CASP, CAPRI, etc.; further automated group depositions related to the fragment screening, etc., BMRB Funding renewal challenges, and withdrawal of the FTP protocol for downloading PDB archives. The AC report will be uploaded as soon as this is received. We thank the two PDBj representatives who attended the AC meeting even at midnight in the Asian time zone.



Geographical distributions of PDB depositions processed by PDBj and PDBc in 2022

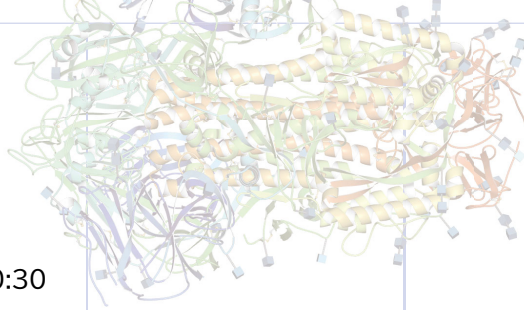


PDB Depositions By Depositor Location



After on-site training at PDBj, two biocurators from Shanghai started processing data remotely using the designated OneDep system provided by PDBj. Entries assigned by PDBj will be remotely processed until the OneDep system is fully installed at PDBc in Shanghai. In 2022, 297 entries were processed from mainland China, which is 6.6% of the entire Asian and 10% of Chinese depositions.





## PDBj Advisory Committee Meeting

The PDBj Advisory Committee meeting was held online from 10:30 on March 10th, 2022, via the Zoom. Staff from our main funder, JST NBDC, including a program supervisor, Prof. Takashi Itoh of Kyushu University, joined the meeting as observers. Prof. Kurisu presented the activity report of 2021 and the activity plan of 2022. Since 2021 was a special year celebrating the 50th anniversary of the PDB, PDBj hosted two international symposiums and served as a guest editor of the special issue of *J. Biochem.* published by the Japanese Biochemical Society. During the meeting, advisors actively discussed the topics on how to validate the expanding number of Cryo-EM structures and emerging AlphaFold2 predicted structures. 2022 was a grant renewal year for PDBj, and Prof. Kurisu explained a new plan to open a branch office of PDBj at the Protein Research Foundation, Minoh-city, Osaka. Advisors enthusiastically expressed their wishes to renew the grant from JST NBDC. Finally, Prof. Kurisu reported the retirement of Prof. Bong-Jin Lee from Seoul National University, Korea, and greatly appreciated his contribution to PDBj.

## OneDep Summit 2022

From May 10th (Tue) to May 12th (Thu), 2022, An annual developer meeting for the OneDep system, a common data deposition system of wwPDB, was held to decide the long-term development goals for this system. Among the topics discussed at the meeting, the introduction of five-character CCD IDs and additional user authentication mechanisms (such as ORCID) may impact PDB deposition soon.

## RDF Summit 4



From January 26th (Thu) to January 30th (Mon), 2023, representatives of biological databases gathered in Kyoto to participate in RDF Summit 4, which aims to strengthen the collaboration among databases and facilitate users to reuse archived data. We discussed a variety of issues: (1) updating huge data sets, archived in DDBJ, UniProt, PDBj, and PubChem; (2) creating each data model using common standards; and (3) technical and financial infrastructure to maintain these data archives. There was a presentation visualizing data models to help users to understand the ontologies of each database.

## AsCA PDBj Poster Award

PDBj has been awarding the PDBj Poster Award since 2018 for outstanding presentations by young scientists at conferences in Asia and the Middle East for which PDBj is responsible for PDB registration. At the 17th Asian Crystallographic Association (AsCA2022) held at



Ramada Plaza Jeju Hotel, Korea, October 30 - November 2, 2022, the 3rd PDBj Poster Award winner was honored.

The winner was Dr. Hyunmin Kim (Seoul National University, Korea), whose poster presentation was entitled "Molecular basis for effector protein recognition by Legionella Type IVB coupling protein complex." Prof. Chun-Jung Chen of NSRRC, Taiwan, presented the award certificate, a commemorative book as the supplementary gift and PDBj novelty goods.

The selection was made by the selection committee members appointed by the Executive Committee of AsCA2022. We appreciate the local executive committee and the selection committee members.

## Deprecation of FTP File Download Protocol in the PDB Archive

Currently, we provide the PDB Archive download service via HTTPS, FTP, and rsync protocols, but we will stop the FTP protocol for the wwpdb.org domain on November 1, 2024. We will keep the service by these three protocols at the pdbj.org domain for the time being.

(November 2, 2022)

## Update of the wwPDB Charter

The wwPDB charter was updated in 2021 and recognizes three founding members (RCSB PDB in the US, PDBe in the UK, PDBj in Japan) and two specialized data resource members (BMRB in US/Japan, EMDB in the UK) as regular members, which operate three core data archives (PDB, BMRB, EMDB). The new associate member category has also been described.

(October 13, 2022)

## Rename the PDB Archive Domain

Currently, we provide the PDB Archive download service on the ftp.wwpdb.org domain for all protocols, but the hostname will be changed from September 2023, and access will only be available under the following host names.

FTP : ftp.wwpdb.org

HTTPS : files.wwpdb.org

RSYNC : rsync.wwpdb.org

(August 24, 2022)

## Extension of CCDID and PDBID

To preparing for the shortage of ID resources, the digits of CCDID (Chemical Component Dictionary ID), currently limited to three, and the PDBID, now four, will be expanded to five and eight, respectively.

PDB entries with extended CCD or PDB IDs codes will be distributed in PDBx/mmCIF format only.

(October 13, 2022)

## Improvement of the Validation Report for EM Structures by using the Q Score

Since September 23, 2022, the wwPDB to provide improved validation reports for EM structures by incorporating the Q score.

(July 26, 2022)

## Paper of the PDBx/mmCIF Format Published

A paper by wwPDB and the PDBx/mmCIF working group members on the PDBx/mmCIF format, a fundamental information description tool in structural biology, was published in a special issue of the *Journal of Molecular Biology, Computational Resources for Molecular Biology 2022*.

PDBx/mmCIF Ecosystem: Foundational Semantic Tools for Structural Biology

John D. Westbrook, Jasmine Y. Young, Chenghua Shao, Zukang Feng, Vladimir Guranovic, Catherine L. Lawson, Brinda Vallat, Paul D. Adams, John M. Berrisford, Gerard Bricogne, Kay Diederichs, Robbie P. Joosten, Peter Keller, Nigel W. Moriarty, Oleg V. Sobolev, Sameer Velankar, Clemens Vonrhein, David G. Waterman, Genji Kurisu, Helen M. Berman, Stephen K. Burley, and Ezra Peisach

(2022) *Journal of Molecular Biology* **434**: 167599 doi: 10.1016/j.jmb.2022.167599

This paper is dedicated to the late John D. Westbrook, who established the PDBx/mmCIF data dictionary and format and contributed to the foundation for the current Protein Data Bank (PDB) archive (wwPDB.org).

(June 29, 2022)

## IPR Seminar for Senior High School Students

We held the IPR Seminar for senior high school students at the Institute for Protein Research, Osaka University, on July 30 (Sat) and August 8 (Mon), 2022. Students were provided with a hands-on workshop using PDBj's educational website for general users "PDBj Numon" to experience the stereoscopic view of molecules and other features of PDBj.

## Luncheon Seminar at the 22nd annual meeting of the PSSJ

We held a luncheon seminar at the 22nd Annual Meeting of the Protein Science Society of Japan at the Tsukuba International Congress Center on Thursday, June 9, 2022, to introduce the recent activities of the PDBj and the activity plans of wwPDB. We also introduced tools and services provided by PDBj for analyzing, editing, and depositing structural data.

## Luncheon Seminar at IIBMP2022

We held a luncheon seminar at the Japan Bioinformatics Society Annual Meeting and the 11th United Institute of Biomedical Informatics Conference (IIBMP2022) at Senri Life Science Center (Toyonaka, Osaka) on Tuesday, September 13, 2022, to introduce PDBj's recent activities and plans to promote the advanced use and application of PDB data. We also conducted a questionnaire survey to promote the utilization of PDB data.

## The 17th AsCA2022 Luncheon Seminar

We held a luncheon seminar at the 17th Conference of the Asian Crystallographic Association (AsCA2022) in Jeju, Korea, on Monday, October 31, 2022, to introduce recent activities related to PDB and OneDep, the common PDB deposition system in each wwPDB site.



## The Day of "Togo-no-hi" Symposium 2022

We gave an oral presentation on the PDB at Togo's Day Symposium 2022, held online on Tuesday, October 5. We also gave poster presentations on the PDB, BMRB, EMDB, and EMPIAR.

## The 31st Science Festival for Youth in Osaka

We exhibited a structural explanation of the SARS-CoV-2 proteins at the 31st Science Festival for Youth (Science Fiesta) Osaka held at Otani Junior and Senior High School (Osaka city) on August 20-21, 2022.



<https://youtu.be/8c2lD-0l3gw>

## Annual Meeting of the CrSJ

PDBj presented a talk entitled "Recent activities of PDBj and the future activity plan of wwPDB" at the Annual Meeting of the Crystallographic Society of Japan held in Nishinomiya, Hyogo, Japan, on November 26th, 2022, to eighty-eight Japanese depositors in the audience. We asked several questions through Google form and there were several active discussions, such as "how to re-upload withdrawn entries to OneDep" or "Possibilities of large experimental data of XFEL of about 40 TB to our Xtal Raw Data Archive (XRDa)."

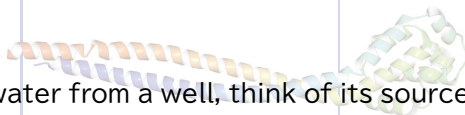
## Booth Exhibition at the 60th Biophysics Society of Japan

We exhibited a booth at the 60th Annual Meeting of the Biophysical Society of Japan held at Hakodate Arena and Hakodate Civic Hall in Hakodate, Hokkaido, from September 28 (Wed) to 30 (Fri), 2022. We conducted a detailed questionnaire survey on the use of integrated data concerning the integrated portal to be developed as a new project of JST NBDC, and we could collect many questionnaires.

## Annual Meeting of the Molecular Biology Society of Japan

We introduced the PDB database and our activities at the forum "Database Applications in Life Sciences" at the 44th Annual Meeting of the Molecular Biology Society of Japan held at Makuhari Messe on Wednesday, November 30, 2022. About 60 people attended the forum, including both on-site and online participants.

## Be grateful



“When you drink water from a well, think of its source” is a Chinese proverb that means “be grateful.” I learned this in school and remembered when we wrote a commentary entitled “History of Protein Data Bank Japan: Standing at the beginning of the age of structural genomics” in a special issue of Biophysical Reviews to celebrate Prof. Haruki

Nakamura’s 70th birthday. This article includes the recollections of our early history: a mirror site of Brookhaven PDB before Prof. Nakamura’s move to Osaka University, and his contribution to start the Data-in activity by PDBj in 2000 with strong help from RCSB PDB, the establishment of the wwPDB in 2003 and the unique and original secondary databases or tools developed by PDBj (<https://doi.org/10.1007/s12551-022-01021-w>). Our Data-in contribution was just 5% of all depositions worldwide when we started the local data processing in 2000. However, last year, we processed 28% of global depositions to the wwPDB. I emphasized two points in the commentary: the first is that with his great foresight, Prof. Nakamura planned, budgeted, and implemented not just a mirror site but also regional deposition (Data-in) and unique data distribution (Data-out) services in Asia. The second is that the start of our regional Data-in service was technically supported by the RCSB PDB at that time. In 2022, the number of depositions from Asia (4,749) to PDBj is almost equal to that from Europe and Africa to PDBe (4,757). The number in 2018 was 2,801 to PDBj and 4,025 to PDBe, respectively. The growth of Asian depositions is so remarkable that the wwPDB invited PDB China last year to be an associate member as the wwPDB advisory committee recommended. To support the launch of PDB China in Shanghai, PDBj hosted two visiting annotators from Shanghai in August 2022 and provided two-months intensive on-site training similar to that given to us by RCSB PDB 22 years ago. Being grateful to the people who dug a well, I strongly consider that we need to address the future requirements securely and timely whenever needed to promote greater progress.

Genji Kurisu, Ph.D. Osaka University

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