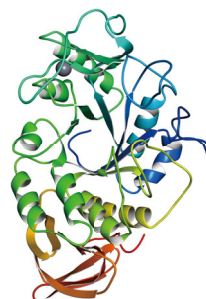
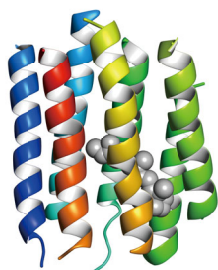
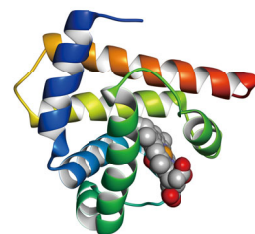
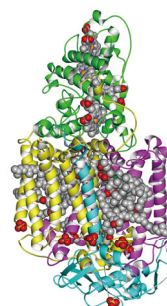
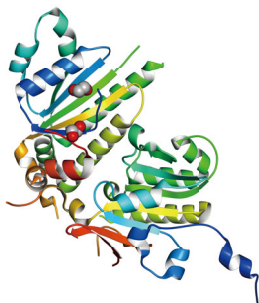
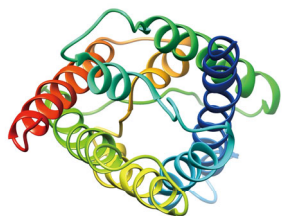
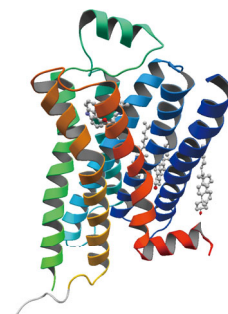
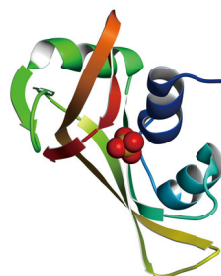
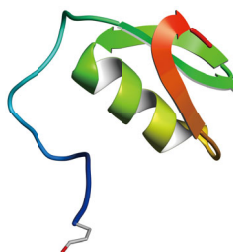
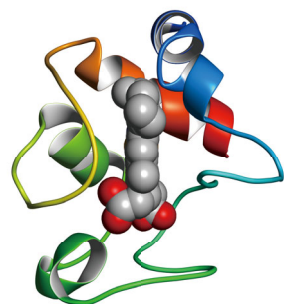
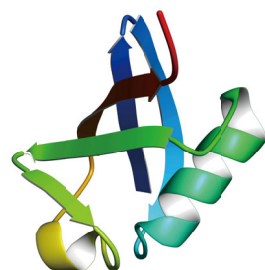
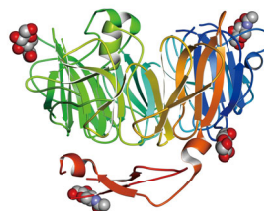
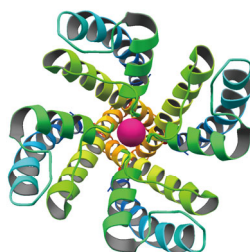
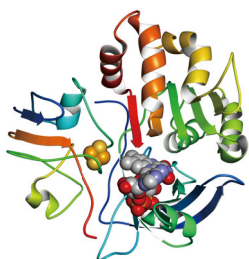
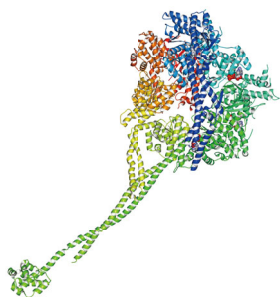
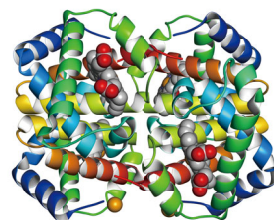
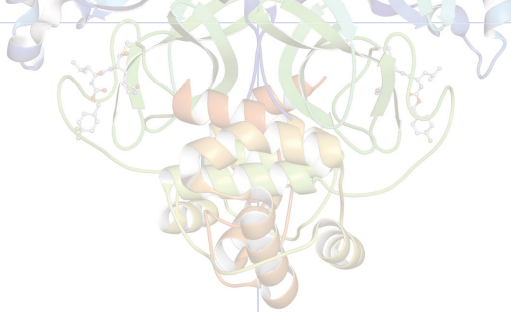


PDBj Newsletter

December 2021

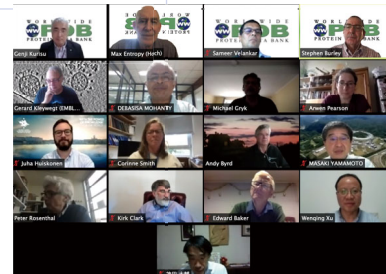
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The 17th wwPDB Advisory Committee Meeting

The wwPDB Advisory Committee meeting is annually held in autumn and rotationally hosted by one of the wwPDB core members. The 17th wwPDB AC meeting was originally scheduled to be hosted by BMRB at UConn Health. However, due to the COVID-19 pandemic, it was held virtually through the Zoom online system on September 30th and October 1, 2020. From PDBj, Genji Kurisu as the head of PDBj, and Drs. Masaki Yamamoto and Daisuke Kohda, as representatives of the PDBj Advisory Committee, attended this annual AC meeting. Status of Data-in activity under COVID-19 pandemic was reported, and the renewal of the charter scheduled for January 2021 and the successful relocation of BMRB from the University of Wisconsin-Madison to UConn Health were explained to the AC members. In the wwPDB AC meeting, the members discussed the future architecture of wwPDB and welcomed the scheduled participation of the Electron Microscopy Data Bank (EMDB) from 2021. They also exchanged ideas on how and when PDB China and PDB India will start their activities as wwPDB associate members under the COVID-19 pandemic situation. As one of the wwPDB core members, PDBj would like to greatly appreciate the contributions of the committee members', even at a midnight time for some members, for their specific and constructive suggestions.



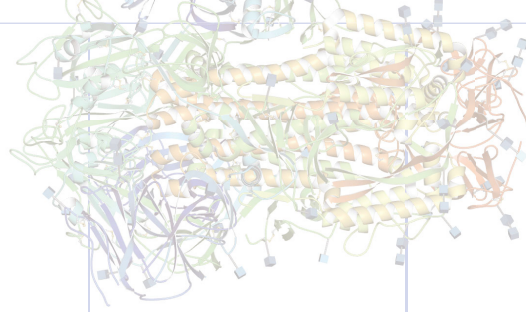
BMRB Advisory Committee Meeting 2021

The BMRB Advisory Committee meeting was usually held in spring at the University of Wisconsin-Madison, who managed BMRB activity in the USA. After relocation of the BMRB site to the UConn Health in 2021, the BMRB AC meeting was hosted by BMRB@UConn Health and held virtually through the Zoom online system on May 11 and 12, 2021 due to the COVID-19 pandemic. From PDBj, Genji Kurisu attended the AC meeting and presented the progress and plan of BMRBj activities as a representative of the BMRBj sub-group of PDBj. In the AC meeting, the members discussed the new BMRB-REDO type project. The regional contribution of BMRBj was approved, and further contributions will be much appreciated.

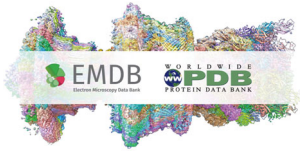
The updated new charter of wwPDB was signed and effective from January 2021

Our old charter signed in 2013 did not fit the current situation in certain aspects. We therefore updated the charter, and all wwPDB PIs, including EMDB and institutional representatives, signed a new charter that was effective from January 2021. The EMDB is now an official partner in the wwPDB. The EMDB was established in 2002 at EMBL European Bioinformatics Institute (EMBL-EBI). Since then, they have collaborated over a wide range of issues including the deposition/annotation/validation of EM based entries, together with the wwPDB core members. Since 2012, the EMDB archive has been officially released as a part of the wwPDB core archives (<ftp://ftp.pdbj.org/pub/>). Our updated new charter formalizes a long-standing relationship between the EMDB and wwPDB. The new charter also introduces the new category of wwPDB Associate members, which enables the establishment of new regional partners such as PDB China or PDB India. In the appendix to the new charter, we have defined the official file formats; PDBx/mmCIF as the primary format, and PDBML (XML) and RDF as the secondary format. PDBj is happy to see the RDF become an official format of wwPDB, as we have strongly encouraged the use of the RDF format together with JST-NBDC and DBCLS. The legacy PDB format will now be maintained only as a maximum effort and no more as an official format of PDB. Since its establishment, the PDB Core Archive has been managed as a public good according to the FAIR Principles. In support of the FAIR objectives, wwPDB has replaced its historical data access license with a standard open source license from Creative Commons, the CC0 1.0 Universal (CC0 1.0) Public Domain Dedication. The new CC0 license provides the same open access as the prior license. PDB data remain freely available to all PDB Users including commercial users.





EMDB becomes a partner in wwPDB



The Electron Microscopy Data Bank (EMDB), the public repository for electron cryo-microscopy maps and tomograms of

macromolecular complexes and subcellular structures, is now an official partner in the Worldwide Protein Data Bank (wwPDB) collaboration under a formal agreement.

(June 25, 2021)

Length of PDBID/CCD will be extended

wwPDB, in collaboration with the PDBx/mmCIF Working Group, has set plans to extend the length of ID codes for PDB and Chemical Component Dictionary (CCD) ID entries in the future. Entries containing these extended IDs will not be supported by the legacy PDB file format.

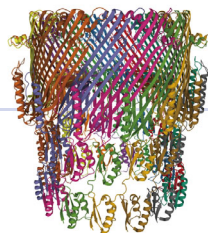
(April 20, 2021)

Modifications to support SHEET and ligand SITE records in June 2021

With the increase in size and complexity of PDB structures, legacy PDB format files will no longer be generated after June 8th 2021 for PDB entries for which the SHEET topology cannot be generated.

For these structures, wwPDB will continue to provide secondary structure information with helix and sheet information in the PDBx/mmCIF formatted file.

(March 16, 2021)



PDB:7cwu

Access improved carbohydrate data at the PDB

A new data representation method introduced for carbohydrates in PDB entries and reference data will improve the findability and interoperability of these molecules in macromolecular structures. The PDB archive now reflects:

- * Standardized Chemical Component Dictionary nomenclature following IUPAC-IUBMB recommendations
- * Uniform representation for oligosaccharides
- * Adoption of linear descriptors of carbohydrates commonly used by the glycoscience-community, using community tools
- * Annotated glycosylation sites in PDB structures

(July 28, 2020)

Consistent format for validation and coordinate data

We have started to provide wwPDB validation reports in PDBx/mmCIF format for all PDB depositions via OneDep. They have the same format as the PDB's structural data, making it easier to compare the structural data and the validation report with each other. They also make the data more logically organized and easier to work within the database. We provide validation reports in the PDBx/mmCIF format in PDB archives and EMDB archives.

(June 1, 2021)

Biocurator milestone: >10,000 depositions processed

Congratulations to wwPDB's Ms. Yumiko Kengaku on processing 10,000 depositions. Yumiko began her career as a biocurator in 2000 as a member of the newly-formed PDBj team



at her alma mater Osaka University. She is the first wwPDB biocurator to process more than 10,000 structures.

(April 6, 2021)

wwPDB EM validation reports now publicly available

The wwPDB archive has now been updated to include validation reports for every released set of EM model coordinates in the PDB and every released EMDB map entry. Validation reports provide quantitative and visual assessments of structure quality and enable archive-wide comparisons.

(January 12, 2021)

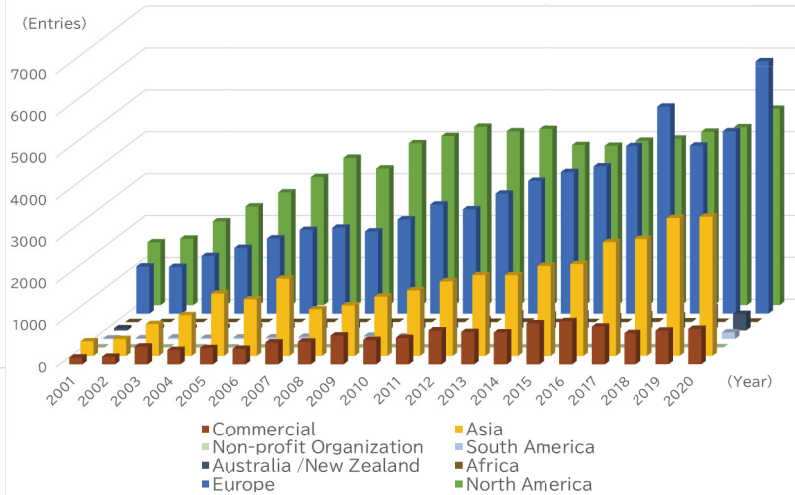
NMR restraints validation now available through OneDep

The wwPDB validation reports provided in OneDep now include restraints validation for NMR entries to help users identify potential discrepancies in their data.

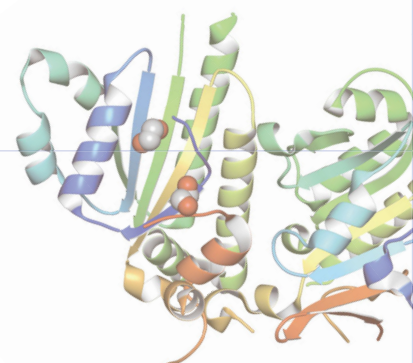
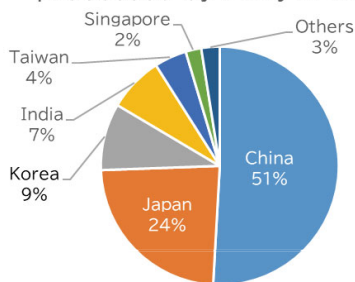
(December 6, 2020)

PDBj Data Growth

PDB Depositions By Depositor Location



Geographical distributions of PDB depositions processed by PDBj in 2020



PDBj BMRBj



BMRBj (Biological Magnetic Resonance Data Bank Japan), formerly known as PDBj-BMRB, is the group name for a regional NMR data repository site of PDBj. We will continue to provide services for the NMR community as before. We currently accept NMR experimental data through the OneDep, BMRBdep, and SMSDep systems.

The OneDep system accepts uploads of NMR experimental data as a single file, either in NEF (NMR Exchange Format) or NMR-STAR format. This makes it easier to archive, distribute, and reuse the NMR data. For most of the existing PDB-BMRB joint entries, BMRBj distributes an NEF archive. Each converted NEF data can be viewed as graphical content on our entry search page.

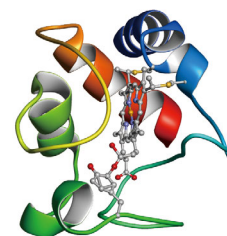
Depositors can now access a refreshed author view page to access uploaded or updated data files. The page contains detailed validation information and graphically represented summary content.



PDBj New Logo



We have also created a new PDBj logo. The design incorporates cytochrome c (PDBID: 1cyc), which was the first structure determined in Japan.





We are suffering under a global pandemic of coronavirus disease 2019 (COVID-19) since 2020. New positive cases of COVID-19 are being reported every day in Osaka. Some PDBj staff members are forced to work remotely from home following the rules and guidelines of Osaka University and the local government. Under this pandemic situation, many academic meetings and symposia were postponed or held as virtual conferences, which has been very dissatisfying and has dramatically changed our daily lives. The OneDep summit (April 2020), which was originally scheduled to be hosted by PDBj, was held virtually online, and the wwPDB AC meeting (October 2020) was hosted by BMRB and held online. In addition, our four prepared events to celebrate the 50th anniversary of PDB were all virtual: 1) a special symposium planned by the wwPDB Foundation and organized by the ASBMB, 2) PDB50 Sessions in the American Crystallographic Association organized by the RCSB PDB, 3) an EMBL conference held by PDBe, and 4) a satellite symposium of the annual meeting of the Biophysical Society of Japan organized by PDBj. I would like to thank all invited speakers, poster presenters, and PDBj friends and supporters who participated in the PDB50 Symposium in Asia entitled "50 years of the Protein Data Bank and the frontier of the Structural Biology in Asia" held on November 24, 2021. The PDB50 Symposium in Asia did not charge any registration fees and very successful. I greatly appreciate financial support from the Institute for Protein Research, Osaka University, the Biophysical Society of Japan, and the Protein Research Foundation.

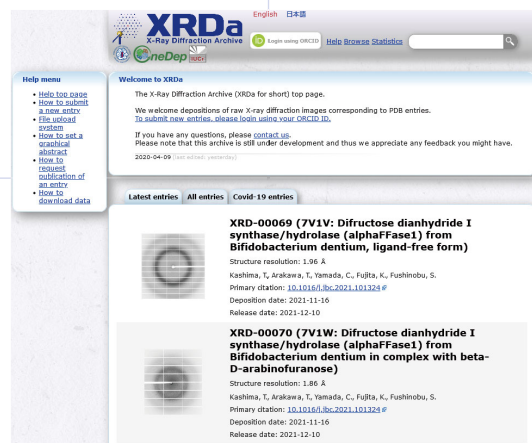
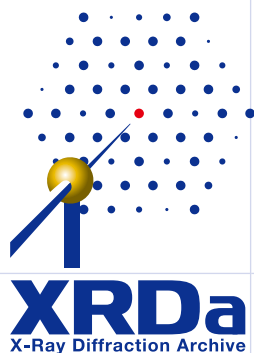
I would like to report on a topics directly related to COVID-19. Following the initial outbreak of the new coronavirus (SARS-CoV-2) in China, the first relevant X-ray structure of the SARS-CoV-2 main protease was deposited to the OneDep system at PDBj by Chinese researchers on January 26, 2020. In general, the new coordinates and related experimental data

(Structure Factors in case of MX) must be deposited to one of the wwPDB core members in advance of submitting a manuscript to an academic journal. Moreover, the deposited PDB data are normally kept confidential until the research paper that contains the relevant information is published, which is a consensus to ensure the originality of the authors' experiments in the structural biology community. However, protein structures constitute fundamental information that is actively used in structure-based drug discovery, and therefore, the immediate accumulation and timely release of structural data on SARS-CoV-2 proteins was highly desired. Therefore, under the agreement between RCSB PDB, PDBe, PDBj, and BMRB, we decided to contact each author (depositor) when the structure of a SARS-CoV-2 protein is deposited to PDB, and strongly recommend that the PDB coordinates and experimental data be released immediately without waiting for a journal publication (PDBj contacted the depositors in Asia and the Middle East). The Chinese team that solved the first SARS-CoV-2 protein structure kindly responded to our request. Indeed, most of the researchers have responded to our requests for immediate release of more than 1,600 entries in total following the first case. It was an unforgettable event that made me realize a the compassion and strength of the structural biology community of the structural biology community. I would like to thank all researchers who cooperated with us. Thank you very much and be safe.

PDBj has started X-ray Diffraction Archive (XRDa) for Asian depositors

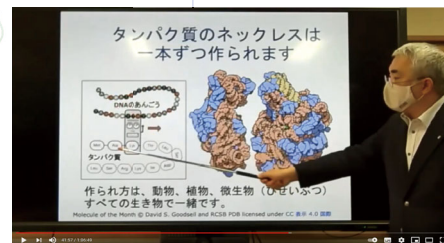
The worldwide Protein Data Bank (wwPDB) including PDBj has managed three core archives: Protein Data Bank (PDB) of atomic coordinates and crystallographic structure factors, Biological Magnetic Resonance Data Bank (BMRB) of experimental data for NMR experiments, and Electron Microscopy Data Bank (EMDB) of potential maps from single particle or sub-tomogram averaging in cryo-electron microscopy. In Asia, PDBj has already started the mirror site of BMRB as BMRBj, which curates and annotates the empirical NMR data locally in Osaka, Japan, and also started the brokering site of

EMPIAR (the Electron Microscopy Public Image Archive) from 2018 based on the bilateral agreement between EMBL-EBI and the Institute for Protein Research, Osaka University. EMPIAR at PDB (EMPIAR-PDBj) provided identical entries of EMPIAR at EMBL-EBI and helped local depositors transfer the images with large file sizes. However, there was no repository for raw diffraction images in Asia that are directly linked to more than 80% PDB entries. Although there are some X-ray diffraction archives in USA and Europe, none of them are managed by the wwPDB partner site. From 2020, PDBj has started our original diffraction archive named "X-ray Diffraction Archive" (XRDa, <https://xrda.pdbj.org>) that securely stores the experimental diffraction images from Asian depositors. You can easily deposit your diffraction images from your "My entries" page with ORCID iD login system of our web. Please deposit your diffraction images to PDBj.



Science Agora 2020

Genji Kurisu, as a representative of PDBj, gave a live lecture at Science Agora 2020 on November 22, 2020 (Sunday), which was watched by 100 people. The lecture was targeted at students in the upper elementary school, and he explained the fundamental knowledge of protein with demonstrations. You can also watch it on YouTube (<https://youtu.be/J60FFW85vyk>).



Science Fiesta 2021

We had an exhibit at "Science Fiesta 2021", the science event for young people. We prepared a web page (<https://numon.pdbj.org>) to explain the

structure of SARS-CoV-2 proteins, and also provided a tutorial movie (<https://youtu.be/31hkRkvGn9w>) of the page.



Example of Usage

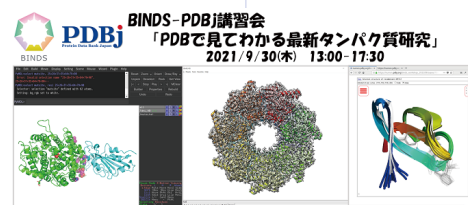
Molecular models created using 3D printing of structural data in the PDB are available on sale. These are models of a SARS-CoV-2 protein sold by Studio Midas.



BINDS-PDBj Workshop "Insight on Latest Protein Research via PDB"

We held a workshop on September 30, 2021 (Thursday) at 13:00-17:30 (JST=UTC+9).

In addition to lectures by X-ray, EM, and NMR researchers on their latest research results, a course was also conducted for the participants to observe the three-dimensional structure data by using a molecular viewer. Some of the lecture materials and movies are available from our website.



<https://pdbj.org/news/workshop20210930>

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