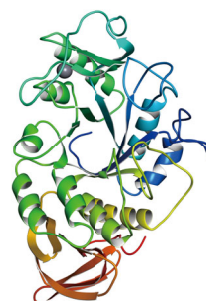
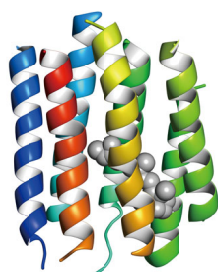
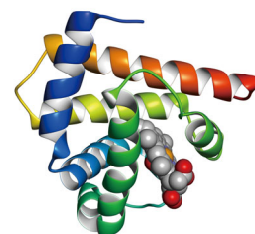
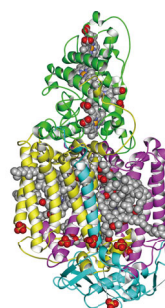
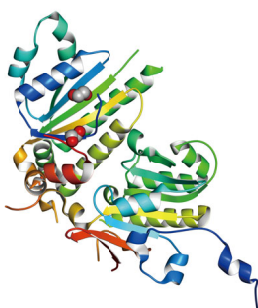
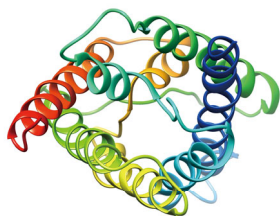
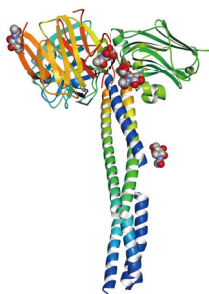
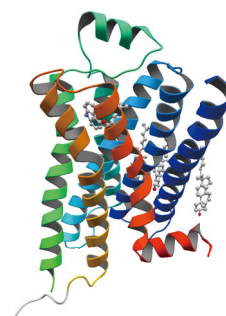
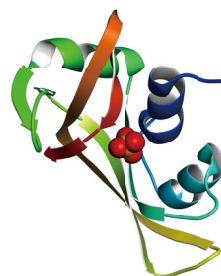
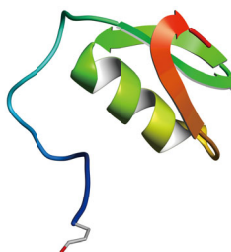
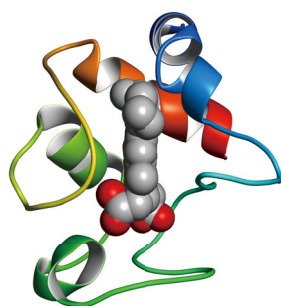
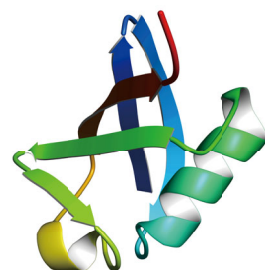
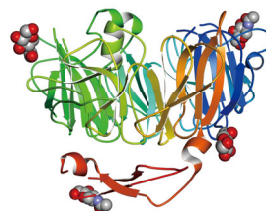
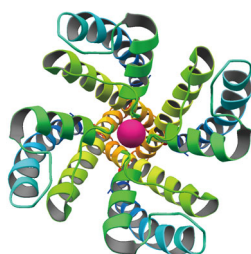
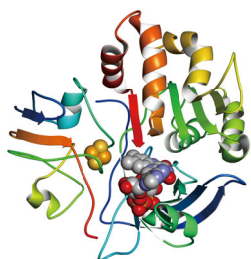
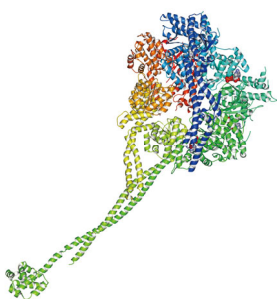
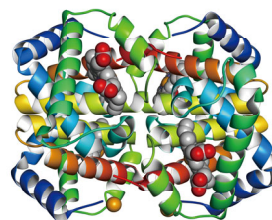
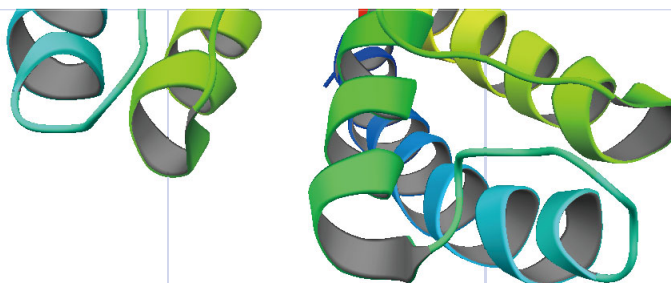


PDBj
Newsletter
March 2020
Vol. **21**





The 16th wwPDB Advisory Committee meeting

In 2019, we, PDBj, hosted the 16th annual wwPDB Advisory Committee (wwPDB AC) meeting on October 18, 2019, at the Institute for Protein Research (IPR), Osaka University.

The participants were Prof. Peter Rosenthal as the chair, Profs. Stephen K. Burley, Paul Adams, and Kirk L. Clark (RCSB-PDB), Profs. Sameer Velankar, David Brown, and Susan Lea (PDBe), Profs. John L. Markley, Jeffrey Hoch, Masatsune Kainosho, and Arthur Edison (BMRB), Profs. Sarah Butcher, Juha Huiskonen (EMDB), Profs. Genji Kurisu, Tsuyoshi Inoue, and Masaki Yamamoto (PDBj), Prof. Edward Baker (IUCr), Prof. Andrew R. Byrd (ISMAR) and Prof. Gerard Kleywegt (EBI). In addition, Profs. Wenqing Xu, Zhipu Luo (PDB-China) and Prof. Debasisa Mohanty (PDB-India) attended as associated members, while Profs. Daisuke Kohda, Kenji Mizuguchi and Yohei Miyanoiri attended the meeting as observers

In the morning, Prof. Genji Kurisu from PDBj explained the current and new wwPDB organization, the updated wwPDB vision and mission. Subsequently, the progress of the following items were reported: 1. Activities and plans of the wwPDB, 2. PDB / BMRB / EMDb Core Archive, 3. PDB Core Archive depositions / growth / download statistics, 4. BMRB / EMDb Core Archive growth statistics, 5. OneDep progress and goals, and 5. wwPDB biocurator productivity, DOI resolution and core member funding status.

Next, Profs. Wenqing Xu from PDB-China and Debasisa Mohanty from PDB-India, both of which will become the wwPDB's associate member, provided an explanation of their Data-in and Data-out activities and their plans for the future, as well as plans regarding the training of their staffs.

In the afternoon, Prof. Sameer Velankar reported the current situation regarding the future heading of the PDB core archive, improved ligand validation within OneDep, the new coordinate versioning system, registration of ORCID IDs, generation of ED map coefficient data for depositors, plans for coordinate versioning of legacy entries and the

planned remediation of carbohydrates. In addition, the current data distribution by the wwPDB partners was discussed and the future heading for distributing additional data, for which each partner site will establish a beta version of the PDB Core Archive that will contain additional annotations and data files, separate from the main FTP.

Next, Prof. John L. Markley reported the testing of new system and the continuing development of the NMR-STAR data dictionary. In addition, collaboration with NMRFAM and the release of the beta version of the small-molecule version of BMRBdep were also discussed. Finally, it was announced that Prof. John L. Markley will withdraw as the Co-Head of BMRB and will be replaced by Prof. Jeffrey Hoch as of April, 2020.

Next, Prof. Gerard Kleywegt reported the progress of the EM validation pipeline, the release plan of the new validation reports and the future plan for adding support for map segmentation data to the EMDb dictionary and the OneDep system.

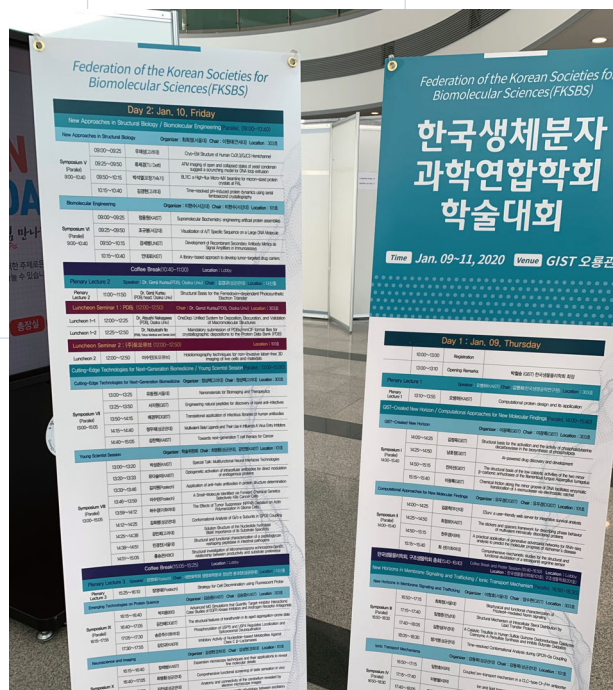
Finally, Prof. Stephen K. Burley asked some questions to the wwPDB AC and these were discussed, and finally the report from the wwPDB AC was replied to the wwPDB PIs



participants of the 16th wwPDB AC meeting at IPR, Osaka Univ.

The Federation of Korean Societies for Molecular & Biomedical Sciences (FKSBS)

The Federation of Korean Societies for Molecular & Biomedical Sciences (FKSBS) meeting was held in Gwangju, Korea, from January 9th to 11th, 2020. Prof. Young-Ho Lee from Korean Basic Science Institute kindly helped us to have our 1st PDBj seminar in Korea, where PDBj is in charge of Data-in activity of wwPDB. Genji Kurisu and Ju Yaen Kim attended FKSBS2020 meeting, and two oral presentations were given by Profs. Atsushi Nakagawa (Osaka University) and Nobutoshi Itoh (Tokyo Medical and Dental University). We introduced new functions of OneDep system, new Validation reports, newly introduced PDB-ID versioning and PDBx/mmCIF mandatory policy for MX users to Korean structural biologists. During the Q&A session after our presentations, some comments and questions came up from the audience, mainly concerning about the 3DEM validation and deposition. It must be important for PDBj to keep in touch with major Asian countries, through one of their scientific societies closely related to PDB activities. Finally, I'd like to express my sincere thanks to all members of 2020 FKSBS steering committee, including Prof. Young-Ho Lee (KBSI). (G.K.)



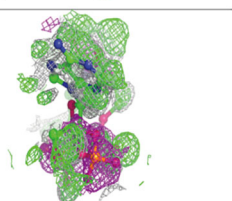
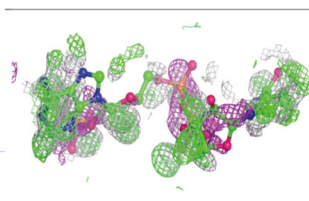
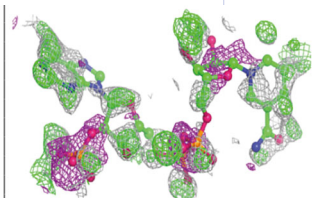
Improvements of the OneDep system

1 Improved ligand validation and electron density maps in the validation reportJun.,
2019

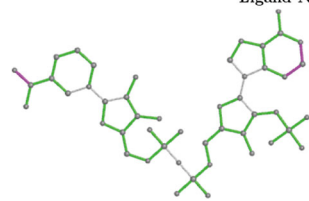
The improved wwPDB validation reports provide much clearer validation information for ligands. In addition to geometric validation for ligands, for PDB entries obtained via X-ray diffraction, the wwPDB validation report also presents images displaying the ligand and the surrounding electron density map. The electron density map coefficients ($2mF_o-DF_c$ and mF_o-DF_c) generated for wwPDB validation reports will be made available to end users in the PDB archive as new entries are released and when all validation reports are recalculated for existing entries.

Electron density around NAP A 1270:

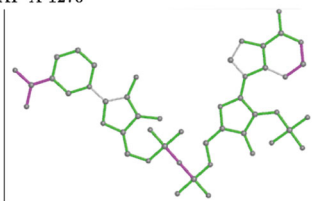
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



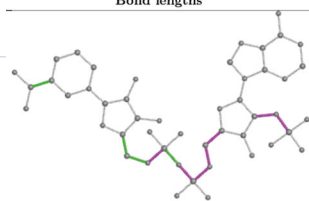
Ligand NAP A 1270



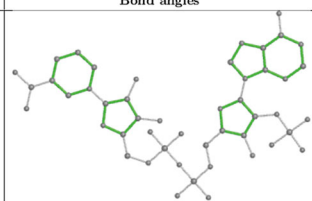
Bond lengths



Bond angles



Torsions



Rings

2 Mandatory PDBx/mmCIF format file submission for MX depositionsJul.,
2019

From July 1st 2019, PDBx/mmCIF is 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.

**3** Improve your released coordinates AND keep your original PDB IDAug.,
2019

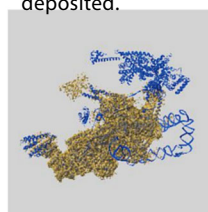
PDB versioning now allows all depositors to update their entries while retaining the same PDB accession code. Initially, i.e., since August 2019, this was limited to PDB entries that were submitted via the OneDep system, but we have since extended the versioning functionality to structures deposited via our legacy systems (ADIT and Autodep) from February 18, 2020. However, no changes to the deposited experimental data are allowed via this system.

4 Improved resolution of DOIs for PDB entriesOct.,
2019

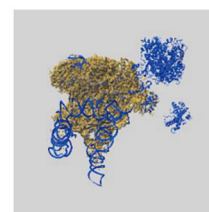
The wwPDB partners have improved the mechanism for the resolution of digital object identifiers (DOIs) associated with PDB entries and launched new wwPDB landing web-pages for each entry. These pages present basic information about the PDB structure, offer the model coordinates, experimental data and validation file downloads from the wwPDB FTP, and provide links to all the wwPDB partner websites for additional information (e.g. <https://doi.org/10.2210/pdb6l4p/pdb>).

5 Additional EM map validation now available through OneDepNov.,
2019

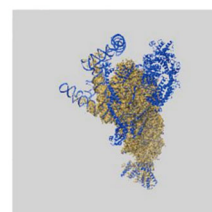
The wwPDB validation reports provided in the OneDep system now have additional validation for electron microscopy (EM) maps to help users identify potential discrepancies in their data. The process includes an analysis of the fitting of the PDB model to the EMDB map, represented at an amino acid level via residue-property plots and globally by a visual overlay of the map and the model. Fourier shell correlation (FSC) curves are also included to compare the reported and estimated resolution, in case either half maps or FSC data was deposited.



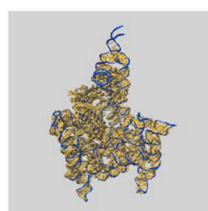
X



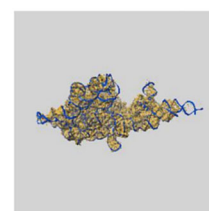
Y



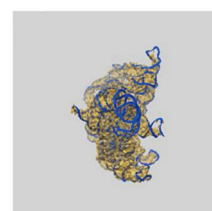
Z



X



Y

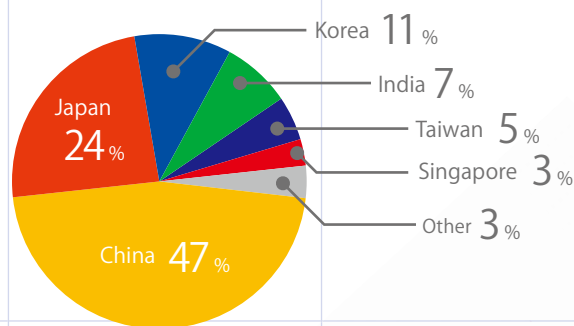


Z

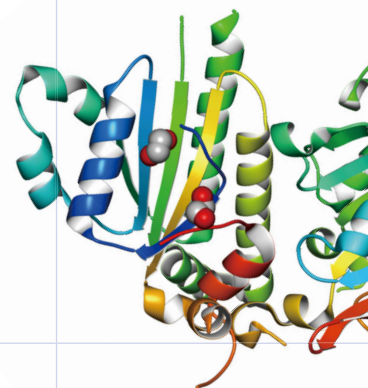
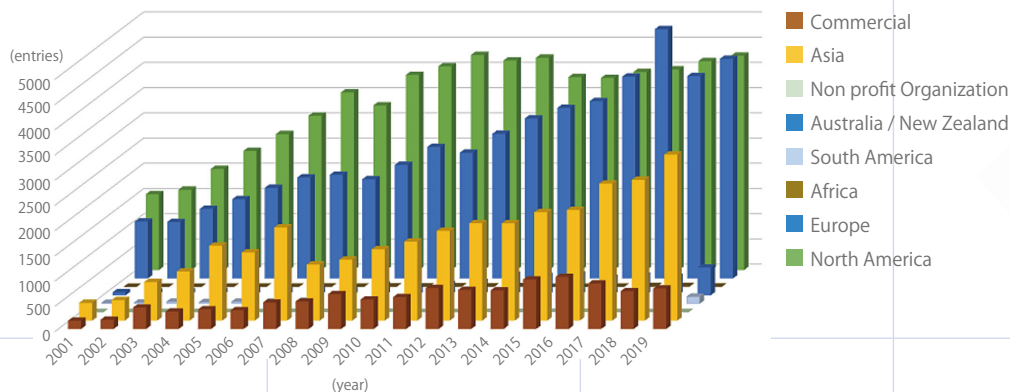
The lower part in the image shows the majority of the model fits well to the map.

6 EMD policy and procedures document now availableJan.,
2020

A comprehensive policy and procedures document for the EMDB archive has been drawn up by the EMDB team in order to ensure consistent and coherent rules for its data. The policy outlines the requirements for data deposition, accepted formats, entry modifications and release, which is now available to view on the EMDB website (<https://emdb-empiar.org/policies.html>).

Geographical distribution of
PDB depositions processed by
PDBj in 2019

Depositions By Depositor Location

Participation in BMRB AC meeting,
update of NMR data deposition system

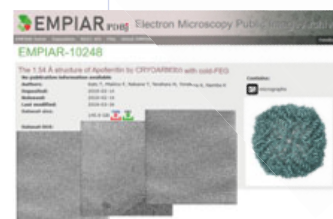
On March 30, 2019, Prof. Toshimichi Fujiwara participated in the BioMagResBank Advisory Committee (BMRB AC) at University of Wisconsin-Madison on behalf of PDBj-BMRB [Photo]. At the meeting, a new NMR data deposition system, BMRBDep, has been introduced. The University of Wisconsin already uses the BMRBDep as a default deposition system. PDBj-BMRB also begins accepting NMR data using the BMRBDep in May 2020. This will greatly improve user ex-perience at NMR data deposition.

Reference: doi: 10.1007/978-1-0716-0270-6_14.

OneDep data deposition with single file
in either NMR-STAR or NEF format

PDBj-BMRB is cooperating with development of OneDep, the data deposition system of wwPDB. As of March 2020, the OneDep system will begin accepting upload of NMR experimental data as a single file, either in NMR-STAR or NEF format. NEF is supported by the leading software in NMR structure determination, allowing data exchange among them. It is also expected not only to simplify the storage and distribution of NMR experimental data but also to improve quality of NMR data through validation packages implemented in the OneDep system. These changes will encourage reusing of the NMR data.

Reference: doi:10.1007/978-1-0716-0270-6_14



Recently, many atomic models determined by electron microscopy have been registered in PDB. Those models were constructed on 3D density maps, which were simultaneously registered in EMDB. Those 3D maps were calculated by huge amounts of 2D micrographic images, which were collected and distributed by EMPIAR database in UK. Images published in EMPIAR can be used for (1) validation of 3D maps, (2) lectures and workshops, and (3) developing new image analysis software. Because constructing of one 3D map requires 2D images with 100 GB to 10 TB, several sites have to be set to submit and distribute these data efficiently. We therefore establish the server "EMPIAR-PDBj" as the Asian mirroring site of EMPIAR. Images can be transferred not only by ftp and rsync, but also by the fast transferring software Aspera. The EMPIAR-PDBj team at Osaka University assists Japanese EM researchers with the transfer of big EM image data to EMPIAR. Instead of sending the data directly to the EBI (UK) via the internet, hard drives can also be sent to Osaka University by postal mail or via a courier service. As an alternative, internet transfer to our server in Osaka is also available. If you would like to take advantage of our submission services, please contact us first by e-mail (empiar-help@protein.osaka-u.ac.jp) before sending the data to us.

BSM-Arc: an archive for in silico models
and simulations

We establish the Biological Structure Model Archive (BSM-Arc, <https://bsma.pdbj.org>), which aims to collect raw data obtained via in silico methods related to structural biology, such as computationally modeled 3D structures and molecular dynamics trajectories. We welcome depositions of raw data and supplementary information corresponding to published, peer-reviewed papers.

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

PDBj exhibited booths at the following two events: "Science Festa 2019" on 18th August (Sun) at Herbis Hall, Osaka, and "Osaka University Co-Creation Bureau" on 30th November (Sat) at LaLaport EXPOCITY, Osaka. A wide



variety of people including children and adults participated; the total number was around 300 or 400 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

We 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.



The AR viewing of experimental facilities

We took the photos of experimental facilities used for structural analysis with 360 degrees camera. Utilizing the web service created by using it, they experienced just like they visited it on site, and we explained them.



Other Outreach Activities

The Joint Database Workshop AJACS Tokushima
6th June 2019, Tokushima

Luncheon Seminar at the 19th Annual Meeting of
the Protein Science
Society of Japan
28th June 2019, Hyogo

Luncheon Seminar at
the 8th Joint Conference on Informatics in Biology,
Medicine and Pharmacology
10th September 2019, Tokyo

Luncheon Seminar at the 57th Annual Meeting of
the Biophysical Society
of Japan
24th September 2019, Miyazaki

Poster presentation and workshop at
the symposium for the day of Togo (Integration)
5th October 2019, Tokyo

Symposium at the Annual Meeting of
Chem-Bio Informatics Society
23rd October 2019, Tokyo

Luncheon Seminar at
the Annual Meeting of Crystallographic Society of
Japan
19th November 2019, Ishikawa

BINDS joint seminar
27th November 2019, Ehime

Forum at the 42nd Annual Meeting of
the Molecular Biology Society of
Japan
3rd December 2019, Fukuoka

Luncheon Seminar at 2020 Federation of
the Korean Societies for
Biomolecular Sciences Conference
10th January 2020, Gwangju, Korea

IPR Seminar: PDBj and BINDS unit joint workshop
30th January 2020, Osaka



I would like to report the big event in PDBj this year. In October, PDBj hosted the worldwide Protein Data Bank Advisory Committee (wwPDB AC) meeting at Osaka University. The meeting was very fruitful and successful, which is owing to sincere contribution of all PDBj members and the kind financial support by the Protein Research Foundation. I greatly appreciate their kind help to host the wwPDB AC meeting. Let me express my unforgettable memory on the wwPDB AC meeting before. As you know already, Prof. Michael G. Rossmann from Purdue University who was a member of the wwPDB AC, passed away in May, 2019. Michael was my neighbor when I worked with Profs. William A. Cramer and Janet L. Smith at Purdue. He was a very brave and courageous man and my hero in Protein Crystallography. When the wwPDB AC meeting was held in Cambridge 2014, Michael and I went back together to the hotel after the dinner. He kindly asked me "Are you interested in the place where the 1st protein structure was solved?". I immediately replied YES and he kindly introduced me to the place where the different department currently exists. It is my good memory with Michael.

Prof. Haruki Nakamura, a former head of PDBj, also express his memorial message to him. "Late Professor Michael G. Rossmann was a member of the wwPDB Advisory Committee (wwPDB AC) from 2009 to 2014, and we invited him to Osaka University twice in 2009 and 2012. I had been a member of the wwPDB as the representative of the PDBj, and at those

wwPDB AC meetings I was always impressed by his thoughtful comments about the activities of the wwPDB. In particular, he had been very keen about the quality of PDB structural data and keeping the raw crystallographic experimental data, which was not easy in those days before the current Big Data era. Now, technologies to store big data have been very much developed and his idea becomes realistic. I notice that Michael was once a member of the US National Science Board, which discussed the scientific digital data collections. From their report, "Long-lived digital data collections: Enabling research and education in the 21st Century" issued in 2005, I learned a lot about the importance of archiving and validating scientific data. Michael must have understood the importance of archiving the raw experimental data and he had promoted the "data science" since many years ago. In that sense, we would appreciate not only his great contributions to structural biology and virology, but also those to the data science."

PDBj Head Prof., IPR, Osaka Univ. Genji KURISU

PDBj (Protein Data Bank Japan) is a project team, as a Joint Usage and Research activity of Institute for Protein Research, Osaka University, which maintains the single global PDB/BMRB/EMDB archives of macromolecular structures and provides integrated tools, in collaboration with the RCSB PDB, the BMRB in USA and the PDBe in EU. PDBj is supported by JST-NBDC and AMED-BINDS.

Protein Data Bank Japan

Staff

Head

Genji KURISU, Ph.D. (Prof., IPR, Osaka Univ.)

Group for PDB Database Curation

Atsushi NAKAGAWA, Ph.D.	(Prof., IPR, Osaka Univ.)
Yumiko KENGAKU	(IPR, Osaka Univ.)
Hasumi CHO, Ph.D.	(IPR, Osaka Univ.)
Yasuyo IKEGAWA	(IPR, Osaka Univ.)
Junko SATO	(IPR, Osaka Univ.)
Ju Yaen KIM, Ph.D.	(IPR, Osaka Univ.)

Group for BMRB

Toshimichi FUJIWARA, Ph.D.	(Prof., IPR, Osaka Univ.)
Chojiro KOJIMA, Ph.D.	(Prof., Yokohama National Univ.)
Yohei MIYANOIRI, Ph.D.	(Assoc. Prof., IPR, Osaka Univ.)
Takeshi IWATA	(IPR, Osaka Univ.)
Masashi YOKOCHI	(IPR, Osaka Univ.)

Group for EMPIAR

Kawabata TAKESEHI, Ph.D.	(Assoc. Prof., IPR, Osaka Univ.)
--------------------------	----------------------------------

Secretary

Ryoko SAKUMA (IPR, Osaka Univ.)

Contact

PDBj Office Tel: +81-6-6879-4311

PDBj Deposition Office Tel: +81-6-6879-8634

Research Center for State-of-the-Art Functional Protein Analysis,
Institute for Protein Research, Osaka University
3-2 Yamadaoka, Suita, Osaka 565-0871, JAPAN

Group for Development of new tools and services

Hiroyuki TOH, Ph.D.	(Prof., Kwansei Gakuin Univ.)
Reiko YAMASHITA	(IPR, Osaka Univ.)
Takahiro KUDOU	(IPR, Osaka Univ.)
Gert-Jan BEKKER, Ph.D.	(Assist. Prof., IPR, Osaka Univ.)

Collaboratory Researchers

Haruki NAKAMURA, Ph.D.	(Prof. Emer., Osaka Univ.)
Akira R. KINJO, Ph.D.	(Assoc. Prof., Universiti Brunei Darussalam)
Kei YURA, Ph.D.	(Prof., Waseda Univ.) for EM Navigator (Waseda Univ.) for EM Navigator (RIKEN SPring-8 Center)
Hirofumi SUZUKI, Ph.D.	(Prof., Waseda Univ.) for ProMode
Naofumi KOBAYASHI, Ph.D.	(Assoc. Prof., Kitasato Univ.) for ProMode
Hiroshi WAKO, Ph.D.	(Prof., Tokyo Medical and Dental Univ.)
Shigeru ENDO, Ph.D.	(Prof., Tohoku Univ.) for eF-site
Nobutoshi ITO, Ph.D.	(Prof., RIMD, Osaka Univ.)
Kengo KINOSHITA, Ph.D.	for SeqNavi, StructNavi, SeSAW, ASH, MAFFTash, Spanner and SFAS
Daron M. STANDLEY, Ph.D.	(Assoc. Prof., RIMD, Osaka Univ.) for MAFFTash
Kazutaka KATOH, Ph.D.	

Contact Form
<https://pdbj.org/contact>

