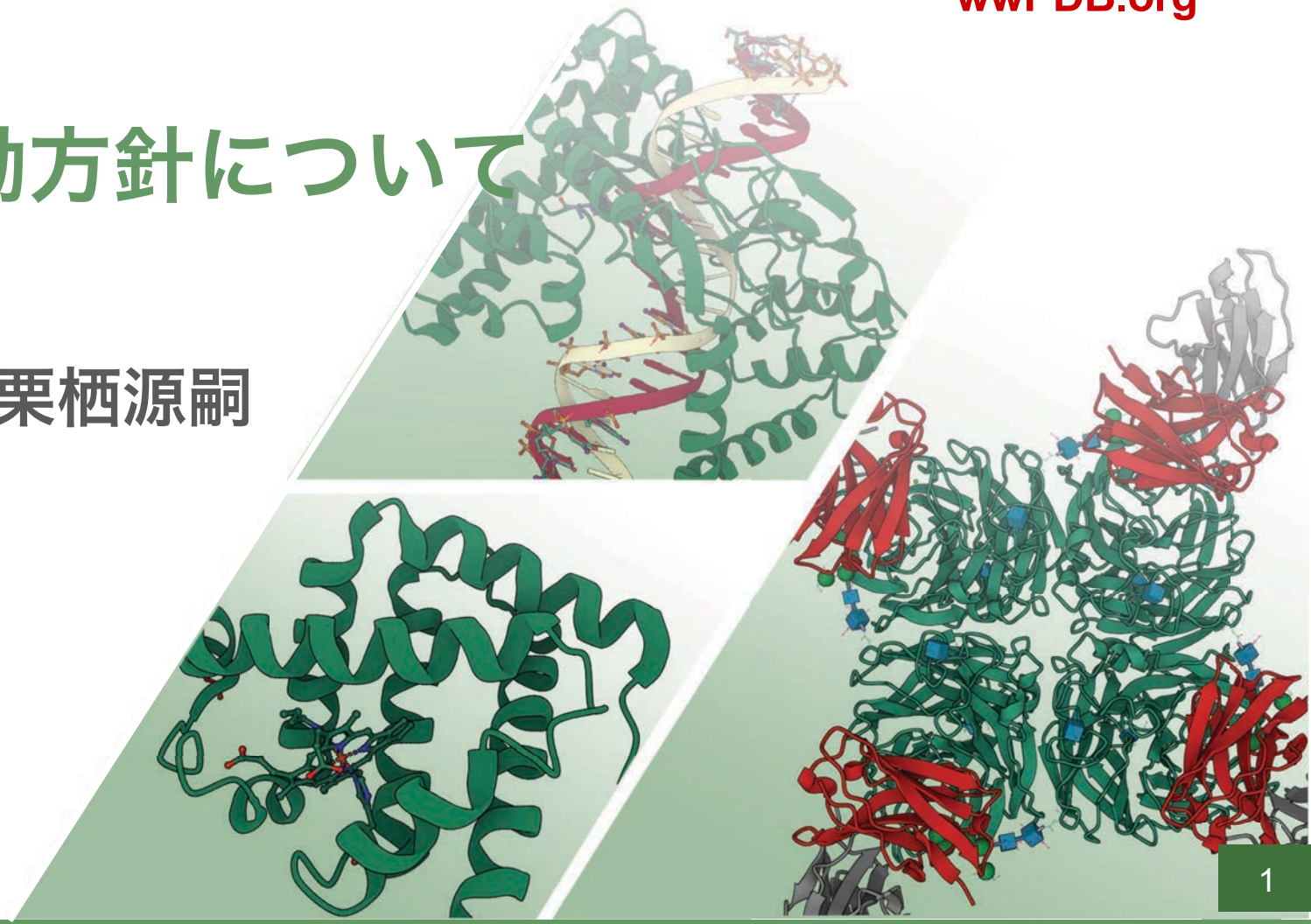
PDBj
Protein Data Bank Japan

WORLDWIDE PDB
PROTEIN DATA BANK

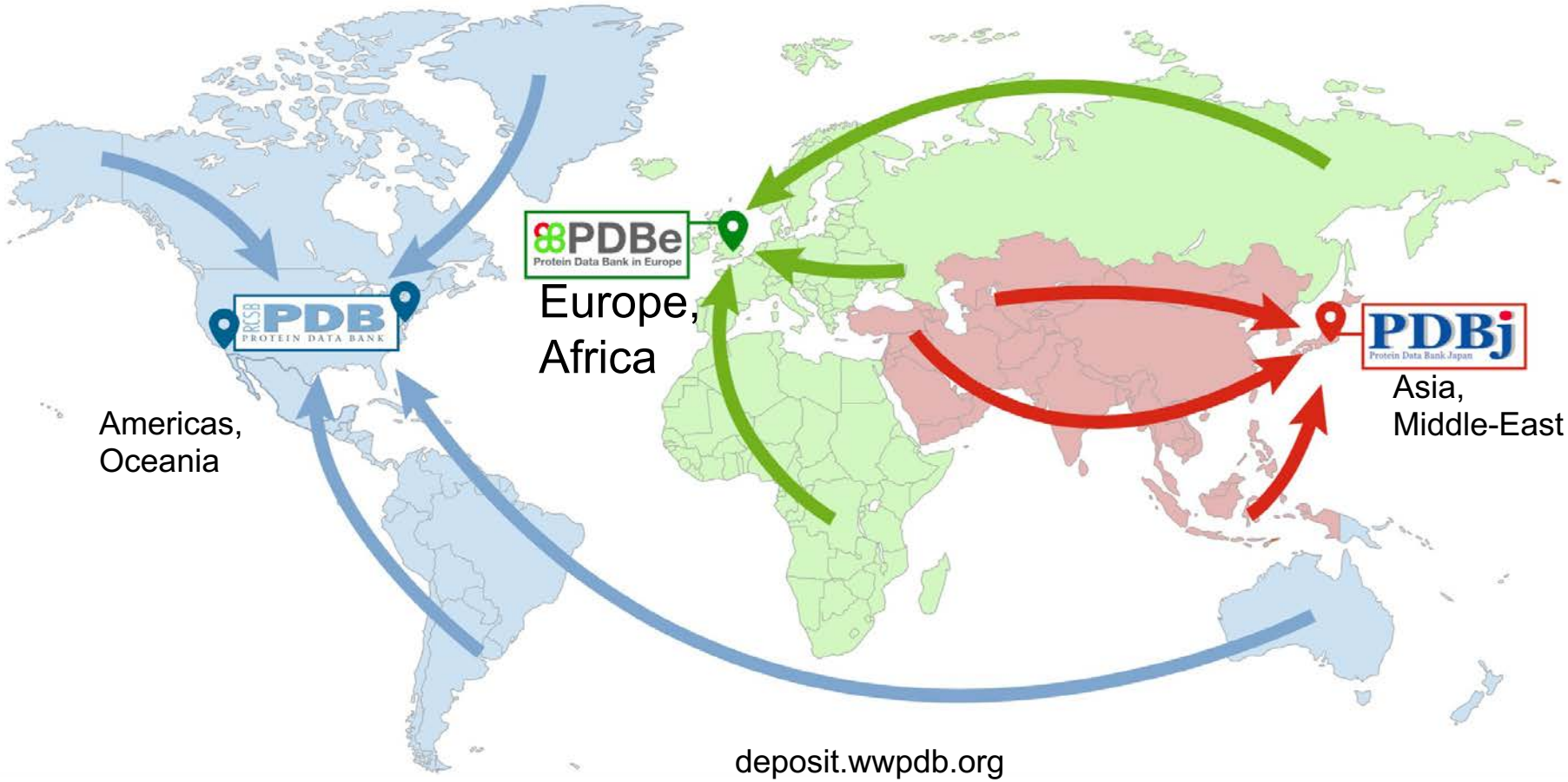
wwPDB.org

PDBjの最近の活動と wwPDBの今後の活動方針について

大阪大学蛋白質研究所　栗栖源嗣

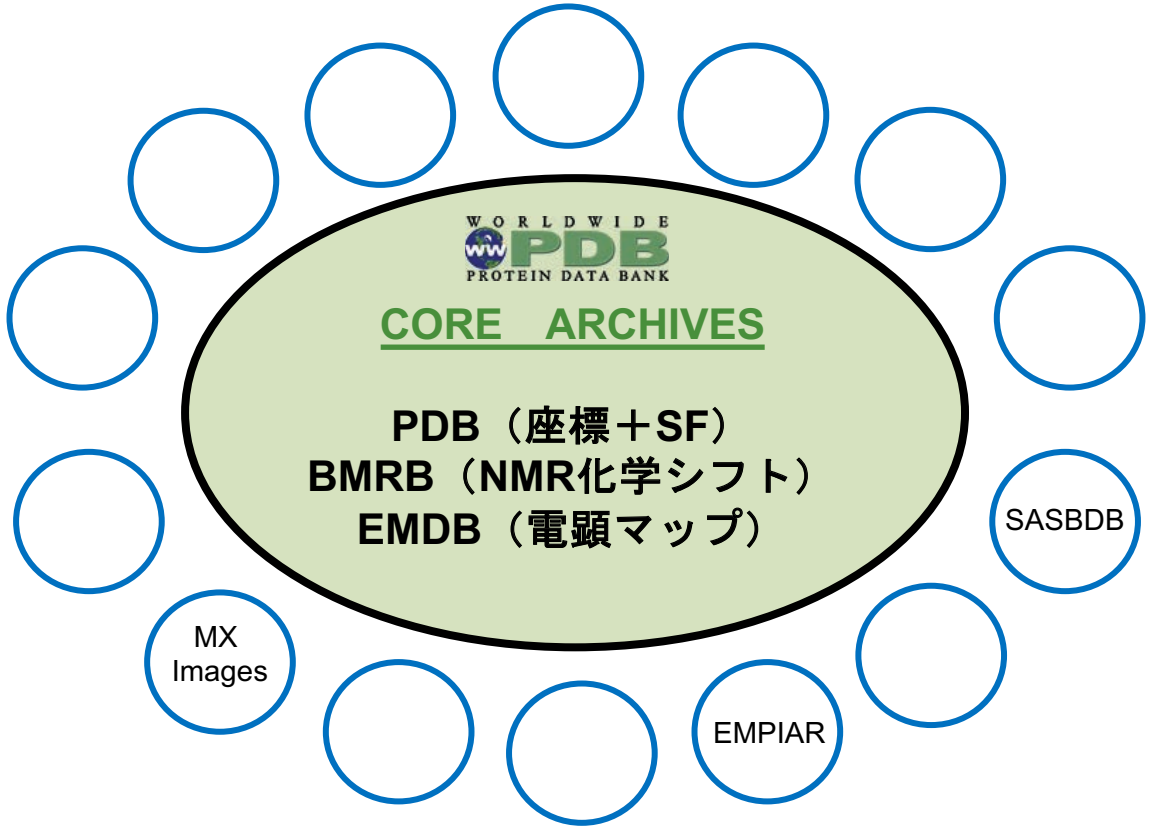


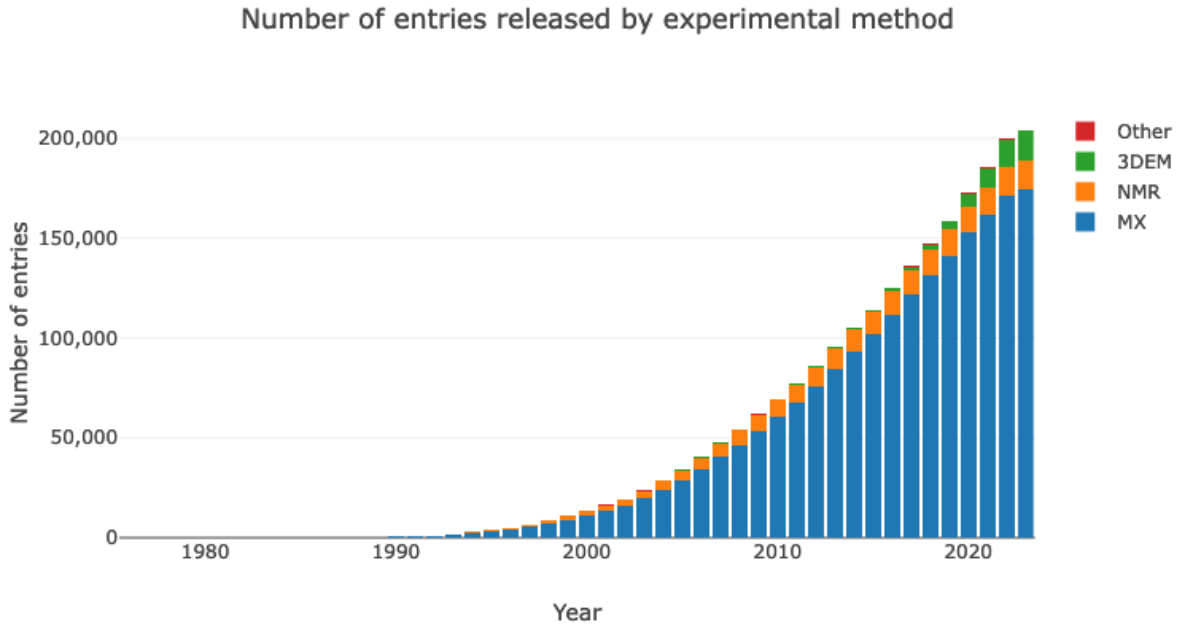
PDBは国際共同プロジェクト



日米欧でデータを相互交換して毎水曜（日本時間9時）に同じデータを公開

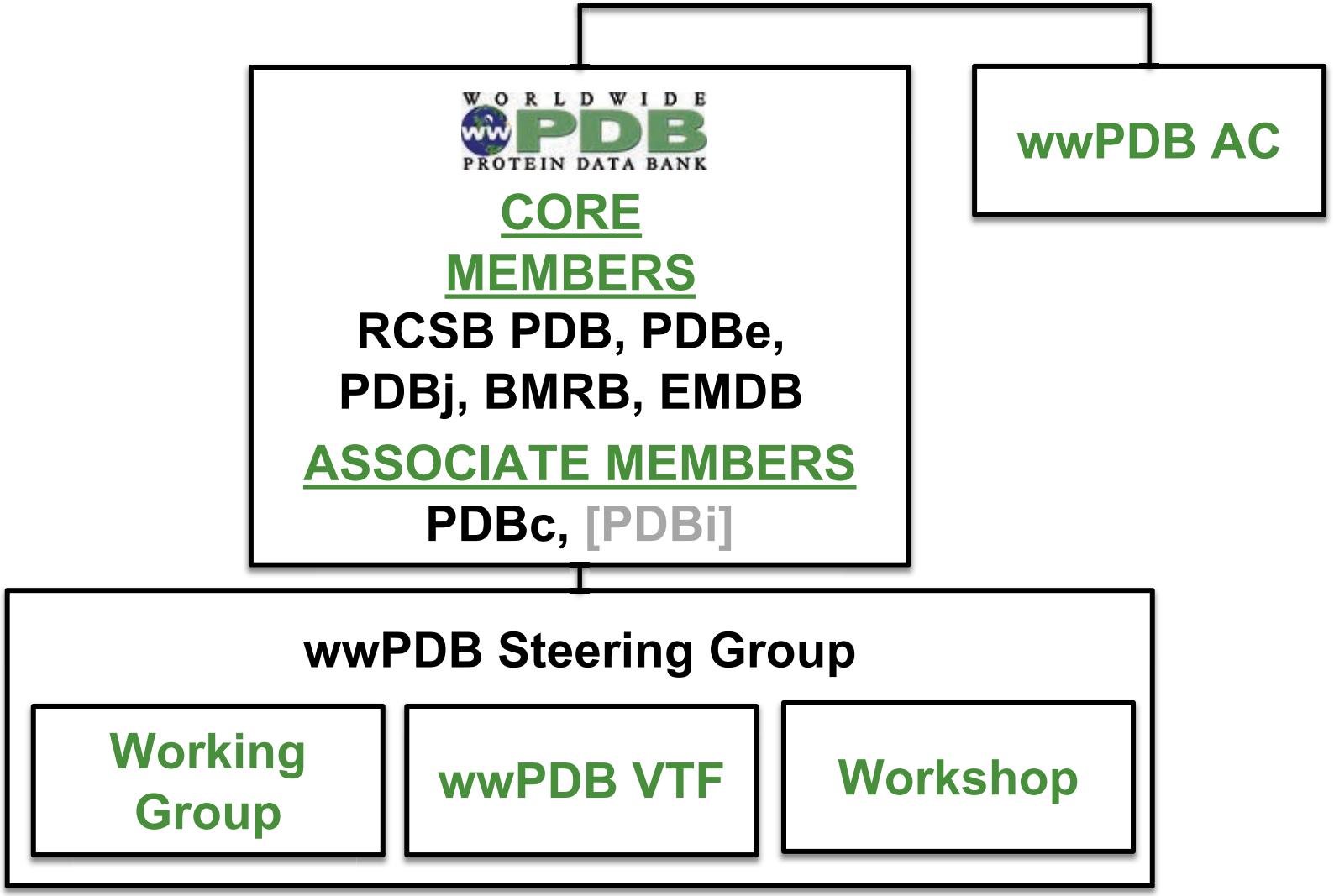
wwPDBは3つのArchiveを運営している



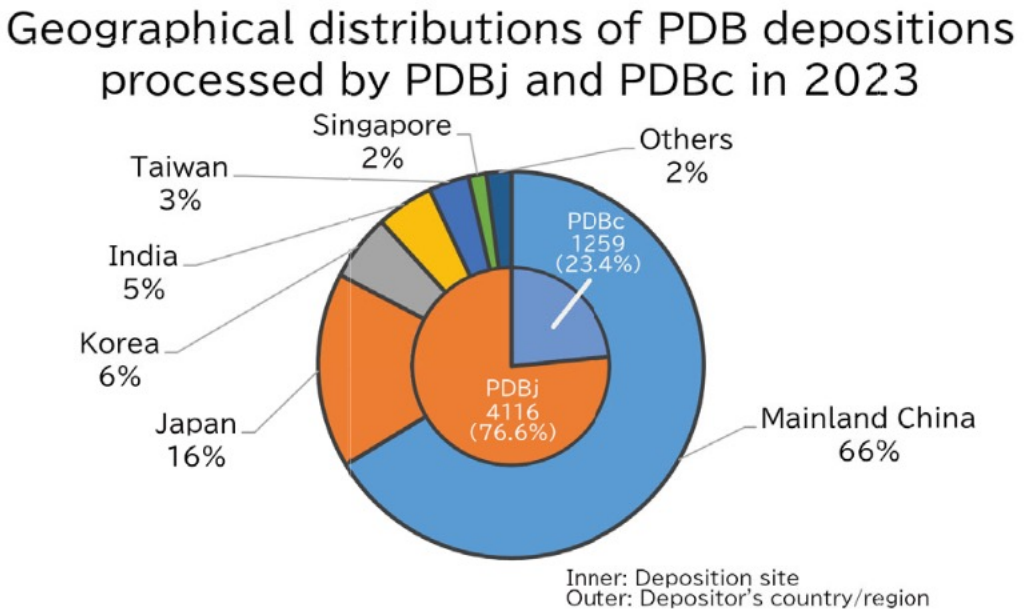


3

国際組織wwPDBが運営（2022に中国参入）



PDBcの4名のアノテータが中国大陸からのエントリーを処理



letters to the editor

STRUCTURAL BIOLOGY

ISSN 2059-7983

Announcing the launch of Protein Data Bank China as an Associate Member of the Worldwide Protein Data Bank Partnership

Wenqing Xu,[a]* Sameer Velankar,[b]* Ardan Patwardhan,[c] Jeffrey C. Hoch,[d] Stephen K. Burley[e,f]* and Genji Kurisu[g,h]*

Received 1 July 2023
Accepted 21 July 2023

Edited by R. J. Read, University of Cambridge, United Kingdom

This paper is dedicated to the International Union of Crystallography on the occasion of its 75th anniversary.

Keywords: macromolecular crystallography; nuclear magnetic resonance; three-dimensional cryo-electron microscopy; Protein Data Bank; Biological Magnetic Resonance Bank; Electron Microscopy Data Bank; Worldwide Protein Data Bank.

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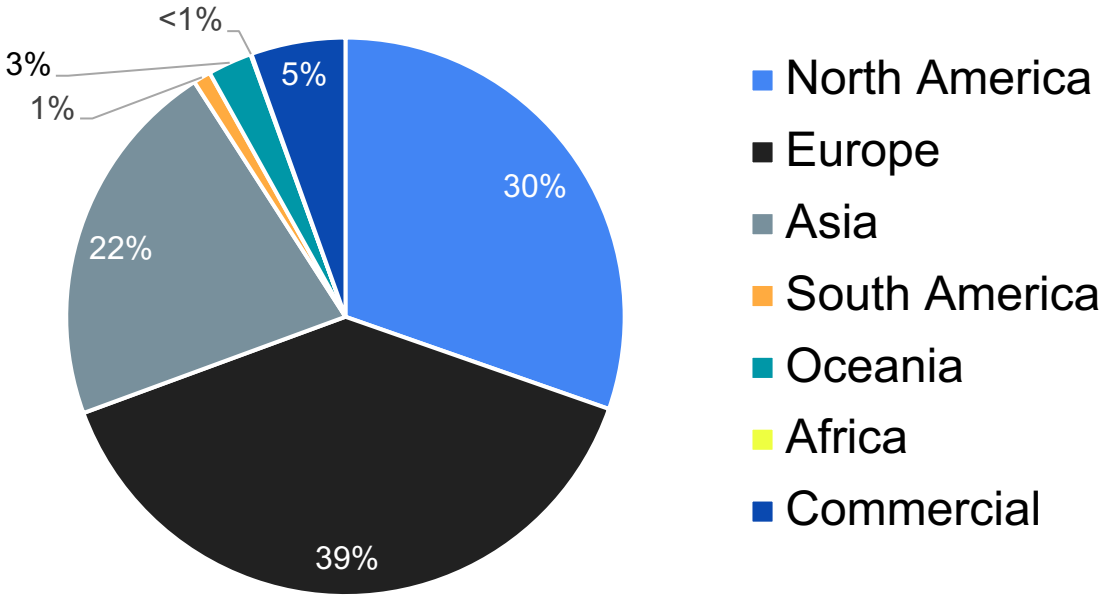
The Protein Data Bank (PDB) is the single global archive of atomic-level, three-dimensional structures of biological macromolecules experimentally determined by macromolecular crystallography, nuclear magnetic resonance spectroscopy or three-dimensional cryo-electron microscopy. The PDB is growing continuously, with a recent rapid increase in new structure depositions

- PDB China が完全に立ち上がるまで登録は全てPDBjに行っていただきます
- PDB China が完全に立ち上がった後も香港と台湾の登録者はPDBcとPDBjを選べるようにします
- PDB Chinaが完全に立ち上がった後は，PDBjがオセアニアもカバーする予定です

アジア発のデータ数増加は欧米を凌駕

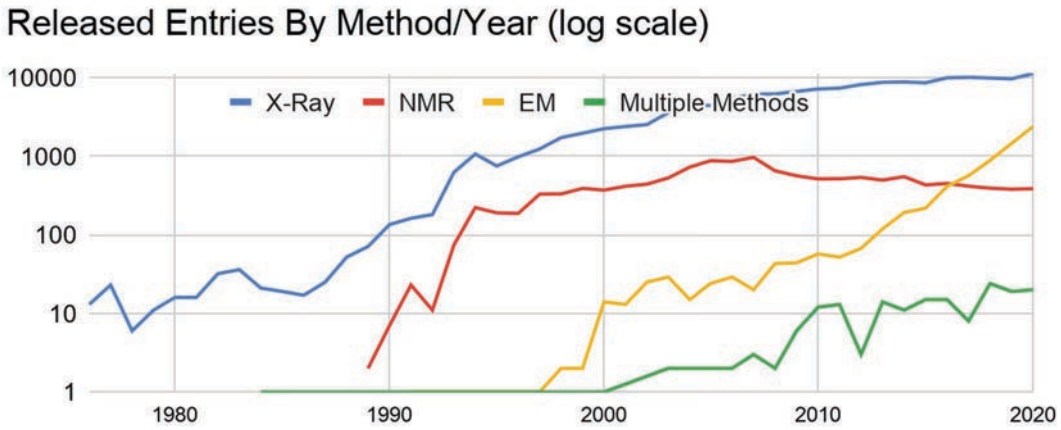
全22万件エントリーの地域内訳

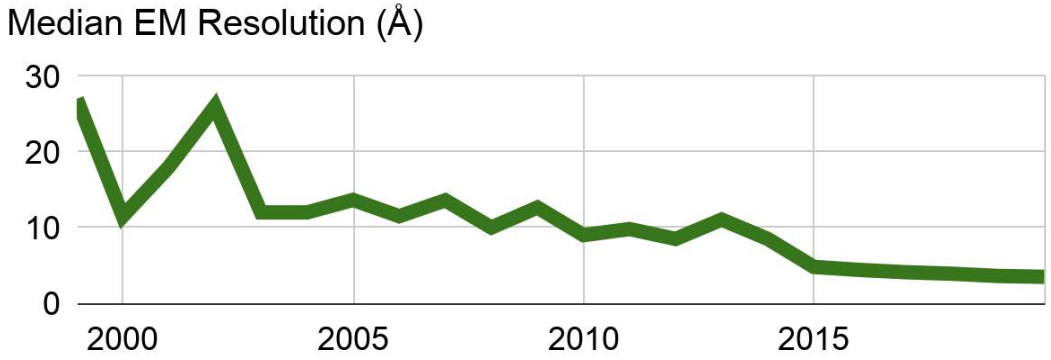


PDBjで処理したエントリー数の推移

PDB Archiveの推移（1）

- 220,000件を超える専門家が編集処理したデータをCC0 1.0 として自由に利用可能
  - ❖ 年率 ~8%でデータ量が増加
- 全世界で >400 を超える外部データベースで活用されている
- 2020年集計でクライオ電顕のエントリーが
  - ❖ 前年比60%増
  - ❖ 原子分解能 (~1Å)に到達するエントリーもで始めた





CoreTrustSeal certification renewed through April 2024 (CoreTrustSeal.org)

PDB Archiveの推移（2）

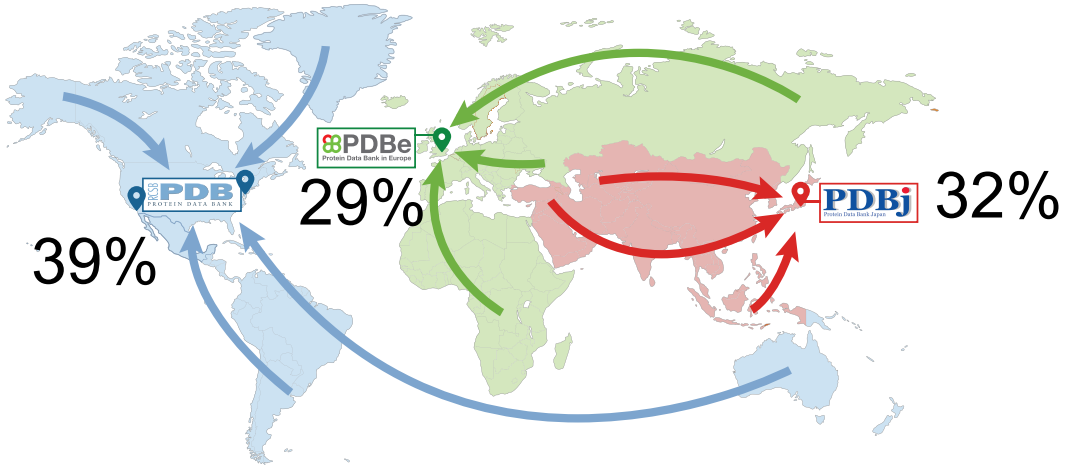
- 2023年1年間に限ると，アジア地区のデータ量増加率が他地域よりも多いので，PDBjの登録・編集の割合は**約32%に増加**
(5,376/17,064 = 0.315)

  ➡ **中国発のエントリー数の急増**

- 機械学習による予測構造を併用した構造解析の増加。結晶解析の位相問題解決にも貢献。

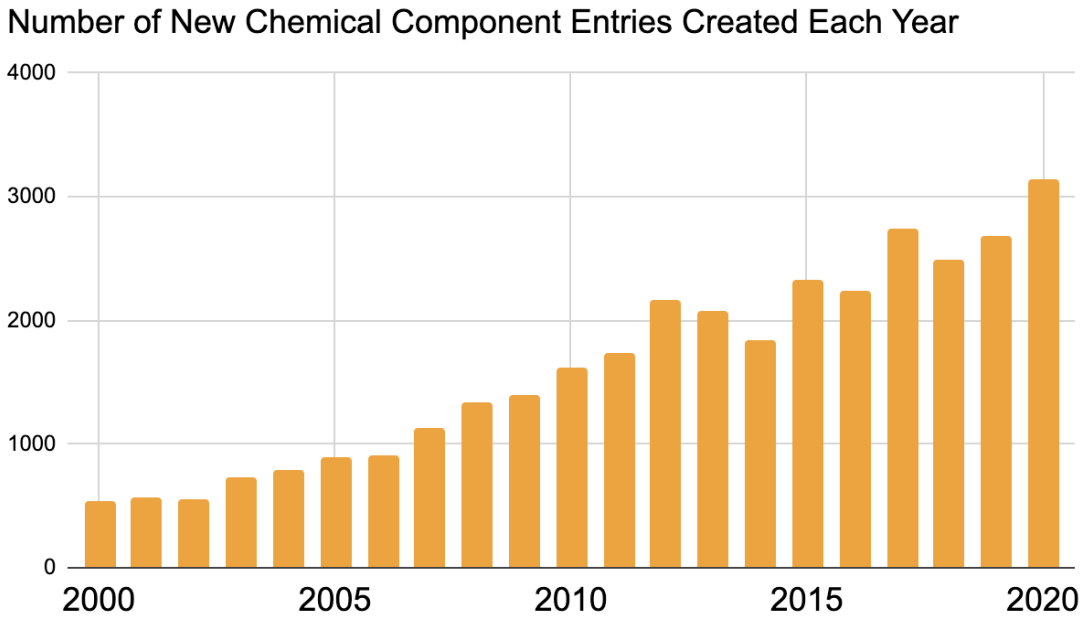
  ➡ 構造予測手法（AlphaFold2等）を併用した**Integrated/Hybrid構造解析に対応した検証レポートの構築**

2023年1年間の内訳



アナウンス１：化合物IDが５桁になる

- PDBフォーマットでつかう**３文字の化合物IDが足りなくなりました。**
- 以降の新規データは**PDBx/mmCIFでのみ提供されています。**
- 新しいエントリーを**PDBフォーマットでは提供できません。**



アナウンス２：PDB IDは8桁になる

- 4文字のPDB IDも近い将来枯渇します
- 既に8文字のPDB IDでデータが提供されています
  wwpdb.org/pdb?id=**pdb_00006lu7**
- **既に提供を開始しています！**

実験データのアーカイブを加速しよう

PDBj Protein Data Bank Japan
as a member of WORLDWIDE PDB PROTEIN DATA BANK

IUCrJ
ISSN 2052-2525
BIOLOGY | MEDICINE

Findable Accessible Interoperable Re-usable (FAIR) diffraction data are coming to protein crystallography

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‡ Chairman of the IUCr Committee on Data.
§ Chairman of the IUCr Commission on Biological Macromolecules.
¶ Member of the IUCr Commission on Biological Macromolecules.
‡‡ Section Editor *Acta Cryst. D*.
§§ Section Editor *Acta Cryst. F*.
¶¶ Main Editor *Journal of Applied Crystallography*.
‡‡‡ Main Editor *IUCrJ*.

Keywords: FAIR; diffraction data; IUCr policy.

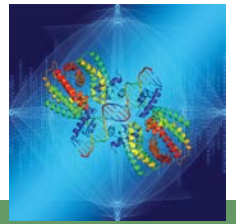
The unprecedented progress of modern science is driven, to a large extent, by the fast propagation of information. Descriptions of experiments and results, and their interpretation, are no longer disseminated solely in peer-reviewed scientific publications, but are frequently distributed through non-reviewed publication platforms as preprints, entries to data repositories, databases *etc.* As a result of ever faster computers and internet connections, many experimental results are now available instantaneously at the click of a mouse, irrespective of the location of the source or consumer.

In many instances, experiments performed and interpreted by one scientific group stimulate the interest of other scientists enough to spur research in further laboratories. Not infrequently, the results of these follow-up experiments are in disagreement with the previously obtained results and/or interpretations (Baker, 2016), notably in psychology and the clinical sciences. In some cases, the original results cannot even be reproduced well enough to allow follow-up experiments to commence (Prinz *et al.*, 2011).

Repeating an entire experiment performed by others is usually not feasible because of the significant time, effort and funds it would require (Baker, 2015). So the question is, what should be done in this new era? How can new technical developments be best exploited for furthering science and the scientific output?

The structural biology community has always been at the forefront of sharing processed, *i.e.* analysed, results. Since its creation in 1971, the Protein Data Bank (PDB; Berman *et al.*, 2000) has become an indispensable daily resource for hundreds of thousands of scientists. Initially, the PDB curated only the molecular structure coordinate files, but since 2008 the deposition of the processed diffraction data, *i.e.* intensities or structure-factor amplitudes, has been mandatory for each derived coordinate set. At present, all serious scientific journals require the deposition of the coordinates of the structures and the associated diffraction data as well as the submission of a PDB validation report with the manuscript for review. Notable also is a recent initiative by *Science* of the introduction of a Statistical Board of Reviewing Editors (McNutt, 2014*a*,*b*). This is an initiative similar to the practice of some referees insisting on access to the underpinning crystallographic data (Helliwell, 2018). Certainly, the PDB is an indispensable resource not only for structural biology but for all modern biological, biomedical and biochemical science (Burley *et al.*, 2019).

However, even with diffraction data being a part of every macromolecular crystallographic deposition in the PDB, and even assuming 'perfect' data reduction and processing of the original diffraction images, some experimental information, *e.g.* diffuse



STRUCTURAL BIOLOGY
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A public database of macromolecular diffraction experiments

Marek Grabowski,[a]‡ Karol M. Langner,[a]‡§ Marcin Cymborowski,[a] Przemyslaw J. Porebski,[a,b] Piotr Sroka,[a] Heping Zheng,[a] David R. Cooper,[a] Matthew D. Zimmerman,[a] Marc-André Elsliger,[c] Stephen K. Burley[d,e] and Wladek Minor[a]*

[a]Department of Molecular Physiology and Biological Physics, University of Virginia, Charlottesville, VA 22904, USA, [b]Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, Niezapominajek 8, 30-239 Cracow, Poland, [c]Department of Integrative Structural and Computational Biology, The Scripps Research Institute, La Jolla, CA 90237, USA, [d]RCSB Protein Data Bank; Center for Integrative Proteomics Research; Institute for Quantitative Biomedicine; Rutgers Cancer Institute of New Jersey; Department of Chemistry and Chemical Biology, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA, and [e]San Diego Supercomputer Center and Skaggs School of Pharmacological Sciences, University of California, San Diego, La Jolla, CA 92093, USA. *Correspondence e-mail: wladek@iwonka.med.virginia.edu

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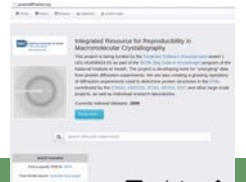
Edited by T. O. Yeates, University of California, USA

‡ The first two authors contributed equally.
§ Present address: Google Inc., Mountain View, CA 94043, USA.

Keywords: diffraction experiment; protein crystallography; repository; data; metadata; IRRMC.

The low reproducibility of published experimental results in many scientific disciplines has recently garnered negative attention in scientific journals and the general media. Public transparency, including the availability of 'raw' experimental data, will help to address growing concerns regarding scientific integrity. Macromolecular X-ray crystallography has led the way in requiring the public dissemination of atomic coordinates and a wealth of experimental data, making the field one of the most reproducible in the biological sciences. However, there remains no mandate for public disclosure of the original diffraction data. The Integrated Resource for Reproducibility in Macromolecular Crystallography (IRRMC) has been developed to archive raw data from diffraction experiments and, equally importantly, to provide related metadata. Currently, the database of our resource contains data from 2920 macromolecular diffraction experiments (5767 data sets), accounting for around 3% of all depositions in the Protein Data Bank (PDB), with their corresponding partially curated metadata. IRRMC utilizes distributed storage implemented using a federated architecture of many independent storage servers, which provides both scalability and sustainability. The resource, which is accessible *via* the web portal at http://www.proteindiffraction.org, can be searched using various criteria. All data are available for unrestricted access and download. The resource serves as a proof of concept and demonstrates the feasibility of archiving raw diffraction data and associated metadata from X-ray crystallographic studies of biological macromolecules. The goal is to expand this resource and include data sets that failed to yield X-ray structures in order to facilitate collaborative efforts that will improve protein structure-determination methods and to ensure the availability of 'orphan' data left behind for various reasons by individual investigators and/or extinct structural genomics projects.



1. Introduction

Issues with the reproducibility of published experimental results have recently attracted attention in many different scientific fields (Collins & Tabak, 2014). The lack of availability of original, primary scientific data represents a major factor contributing to reproducibility problems (Iqbal *et al.*,

Archive for Xtal Diffraction Images

PDBj Protein Data Bank Japan
as a member of wwPDB WORLDWIDE PROTEIN DATA BANK

XRDa X-Ray Diffraction Archive
English 日本語
Login using ORCID
ヘルプ エントリー探検 統計情報

Help menu

- Help top page
- How to submit a new entry
- File upload system
- How to set a graphical abstract
- How to request publication of an entry
- How to download data

XRDaへようこそ

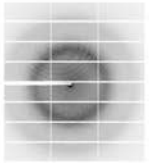
The X-Ray Diffraction Archive (XRDa for short) top page.

We welcome depositions of raw X-ray diffraction images corresponding to PDB entries.
To submit new entries, please login using your ORCID ID.

If you have any questions, please contact us.
Please note that this archive is still under development and thus we appreciate any feedback you might have.

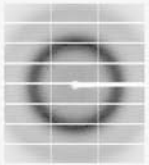
2020-04-09 (last edited: 3 months ago)

Latest entries | All entries | Covid-19 entries



7V1X: Difructose dianhydride I synthase/hydrolase (alphaFFase1) from Bifidobacterium dentium in complex with beta-D-fructofuranose

Structure resolution: 1.76 Å
Kashima, T., Arakawa, T., Yamada, C., Fujita, K., Fushinobu, S.
DOI: 10.1016/j.jbc.2021.101324
Deposition date: 2021-11-16
Release date: 2021-11-16



7DNN: Crystal structure of the AgCarB2-C2 complex with homoorientin

Structure resolution: 2.25 Å
Senda, M., Kumano, T., Watanabe, S., Kobayashi, M., Senda, T.
Deposition date: 2021-08-19
Release date: 2021-10-20

5AUI: Crystal structure of Ferredoxin

XRDa X-Ray Diffraction Archive
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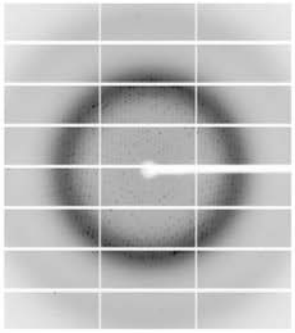
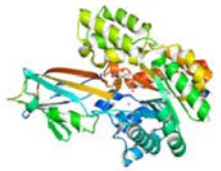
7dnn: Crystal structure of the AgCarB2-C2 complex with homoorientin

Authors:	Senda, M., Kumano, T., Watanabe, S., Kobayashi, M., Senda, T.
R-work:	0.19630
R-free:	0.24710
Unit cell edges (Å):	73.905 x 102.511 x 136.09
Unit cell angles (°):	90, 90, 90
Resolution:	47.97 Å - 2.25 Å
Space group:	P 21 21 2
Primary citation	
PDBj website for 7dnn	
Entry:	Download (1.03 GB)





Dataset CarB homologue3-homoorientin complex

Number of frames	440
Distance (mm)	257.1
Oscillation width (°)	0.5
Wavelength (Å)	1
Equipment	DECTRIS PILATUS 2M-F
Beamline	PHOTON FACTORY BEAMLINE AR-NE3A

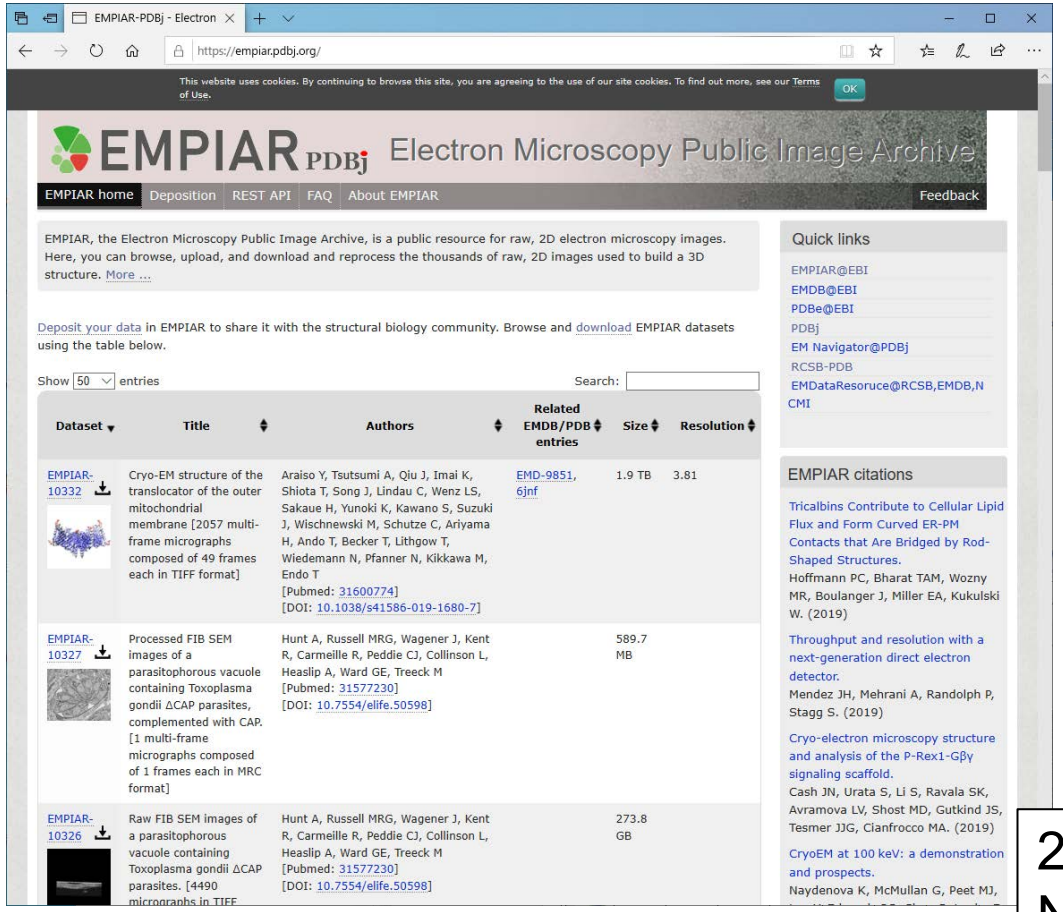
ファイルマネージャー

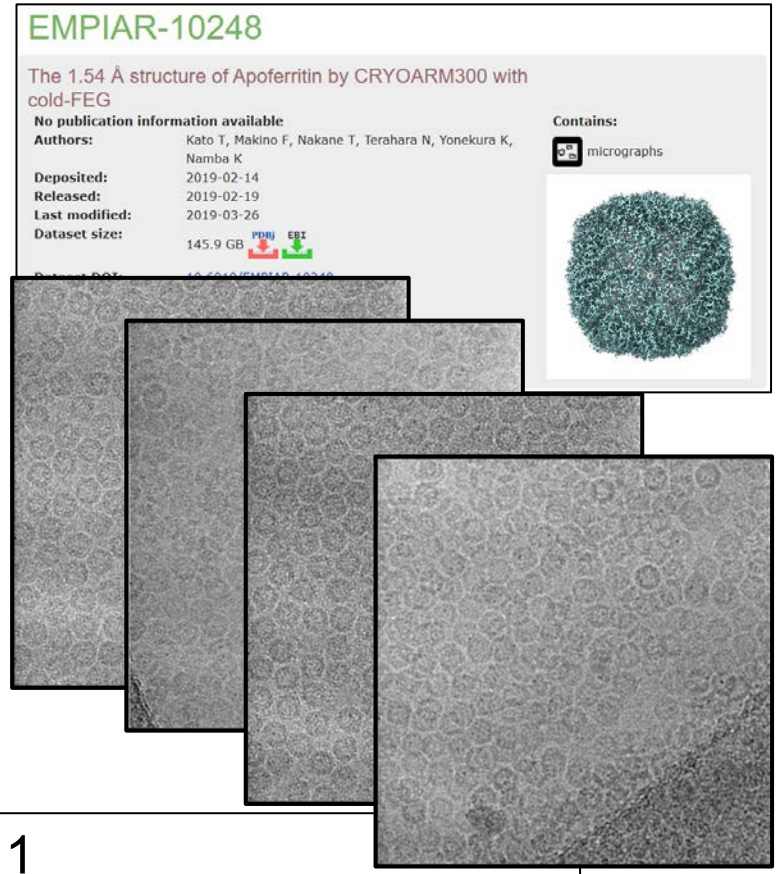
Path: /

名	説明	サイズ	変更日
data			

https://xrda.pdbj.org

EMPIAR-PDBj started from Dec. 2018





2024/6/11
Number of whole entries: 1714
Entries from Japan : 123

https://empiar.pdbj.org

NEW

PDB-Dev will be rebranded as “PDB-IHM”

PDBj Protein Data Bank Japan
as a member of wwPDB WORLDWIDE PROTEIN DATA BANK

Structure
Letter to the Editor
CellPress

PDB-Dev: a Prototype System for Depositing Integrative/Hybrid Structural Models

Stephen K. Burley,[1,2,3,*] Genji Kurisu,[4] John L. Markley,[5] Haruki Nakamura,[4] Sameer Velankar,[6] Helen M. Berman,[1] Andrej Sali,[7] Torsten Schwede,[8] and Jill Trewhella[9,10]
[1]RCSB Protein Data Bank, Institute for Quantitative Biomedicine, Rutgers, The State University of New Jersey, Piscataway, NJ 08854, USA
[2]Skaggs School of Pharmacy and Pharmaceutical Sciences and San Diego Supercomputer Center, University of California, San Diego, La Jolla, CA 92093, USA
[3]Rutgers Cancer Institute of New Jersey, Rutgers, The State University of New Jersey, New Brunswick, NJ 08903, USA
[4]Protein Data Bank Japan (PDBj), Institute for Protein Research, Osaka University, Osaka 565-0871, Japan
[5]BMRB, BioMagResBank, Biochemistry Department, University of Wisconsin-Madison, Madison, WI 53706, USA
[6]Protein Data Bank in Europe (PDBe), European Molecular Biology Laboratory, European Bioinformatics Institute (EMBL-EBI), Wellcome Genome Campus, Hinxton, Cambridgeshire CB10 1SD, UK
[7]Department of Bioengineering and Therapeutic Sciences, Department of Pharmaceutical Chemistry, California Institute for Quantitative Biosciences, University of California, San Francisco, UCSF MC 2552, Byers Hall at Mission Bay, 1700 4th Street, Suite 503B, San Francisco, CA 94158, USA
[8]SIB Swiss Institute of Bioinformatics and Biozentrum, University of Basel, Klingelbergstrasse 50-70, 4056 Basel, Switzerland
[9]School of Life and Environmental Sciences, The University of Sydney, Sydney, NSW 2006, Australia
[10]Department of Chemistry, University of Utah, Salt Lake City, UT 84112, USA
*Correspondence: stephen.burley@rcsb.org
http://dx.doi.org/10.1016/j.str.2017.08.001

With this Letter to the Editor, the Worldwide PDB (wwPDB) Partnership (wwpdb.org) and the wwPDB Integrative/Hybrid (I/H) Methods Task Force would like to announce public release of a prototype system for depositing I/H structural models, PDB-Development (or “PDB-Dev”) (Vallat et al., 2016c). The URL for PDB-Dev is https://pdb-dev.wwpdb.org.

Essential mechanisms in biology frequently involve large macromolecular assemblies (or machines). In favorable cases, their structures can be determined by X-ray crystallography or nuclear magnetic resonance (NMR) spectroscopy or hydrogen/deuterium exchange, cryo-electron tomography with sub-tomogram averaging, correlative fluorescent light microscopy, and various proteomics and bioinformatics analyses (Ward et al., 2013). I/H approaches have yielded informative structural models of very large macromolecular assemblies, such as the nuclear pore complex and its sub-complexes, the type III secretion system needle, the proteosomal lid sub-complex, the ESCRT-I complex, and an RNA ribosome-binding element from the turnip crinkle virus genome. Despite great need, there are, at present, no standard hybrid). These experimental and computational scientists, together with wwPDB representatives, contributed to the workshop. Three breakout groups discussed challenges involved in managing I/H structural models and their supporting experimental data. Five consensus recommendations emerging from the meeting were summarized in a White Paper published in *Structure* (Sali et al., 2015), the most important of these being the urgent need for creation of data standards and establishment of a federated system of data resources to standardize representation, validation, archiving, and dissemination

ARTICLE IN PRESS
Database

IHMCIF: An Extension of the PDBx/mmCIF Data Standard for Integrative Structure Determination Methods

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