

# Protein Data Bank (PDB) Archive and the wwPDB Partnership

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[wwpdb.org](http://wwpdb.org)

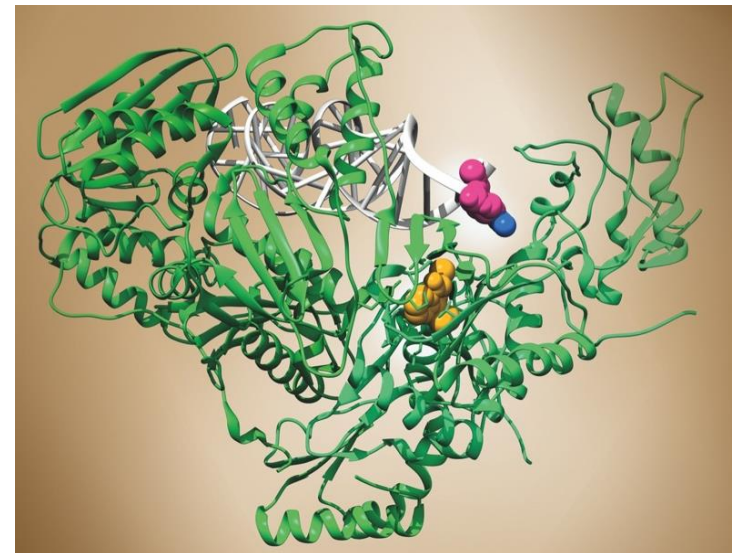
# Protein Data Bank

- Global archive of experimental macromolecular structure data central to basic and applied research and education in biology and biomedicine
- First open access digital data resource in biology (est. 1971 with 7 entries)
- Single global archive of experimental 3D structures of proteins, DNA, and RNA (>124,000 entries today)
  - Primary data for structural biology, computational biology, drug discovery, ...
  - Complements GenBank and UniProt sequence databases
- All data freely available without restrictions on usage (we adhere to the FAIR Principles)



**ABL tyrosine-kinase inhibited by Imatinib for treatment of chronic myeloid leukemia (CML).**

PDB ID 2hyy Cowan-Jacob *et al.* (2007) *Acta Crystallographica D*63: 80-93.



**HIV-1 reverse transcriptase complex with DNA and nevirapine**

PDB ID 3v81 Das *et al.* (2012) *Nature Structural and Molecular Biol* ogy19: 253-259.

# wwPDB Partners/Responsibilities



- Partners share “Data In” responsibilities
  - Biocurate new depositions
  - Define deposition and annotation policies
  - Implement community validation standards
- Partners distribute identical data *via* FTP
- Partners provide complementary “Data Out” resources
- Advised by an international committee of experts

# PDB Facts and Figures

- Archival Contents
  - >124,000 Structures Released since 1971
  - ~11,000 New Structures Deposited/Year
- Global User Base
  - ~30,000 Depositors Worldwide
  - >1 Million Unique Users/Year  
from 192/195 UN-recognized sovereign nations
- Impacts all of Biology and Medicine
  - >500 Million Data Files Downloaded/Year
  - ~1.5 Million Data Files Downloaded/Day
  - >200 derived data resources repackage PDB data

# 1. wwPDB Operations/Funding

**Founding wwPDB Partners operate collaboratively from regional data centers in US, EU, and Asia**

- US-based RCSB PDB is funded from US sources
- EU-based PDBe is funded from UK and EU sources
- Japan-based PDBj is funded from Japanese source

**BioMagResBank (BMRB) joined wwPDB in 2006**

- BMRB US operations funded from US sources
- BMRB Japan operations funded from Japanese source

# 1. wwPDB Funding Sources

- **RCSB PDB (USA):** Core Operations – NSF-administered Cooperative Agreement (~90%; 5yrs; NSF/NIH/DoE); Value-added Activities – NIH/NSF (~10%; 3-5yrs)
- **PDBe (Europe):** Core Operations – EBML (~50%; 3-5yrs), BBSRC (~6%; 1-2yrs), and Wellcome Trust (~20%; 5yrs); Value-added Activities – EMBL/EU/BBSRC/Wellcome Trust (~24%; 1-3yrs)
- **PDBj (Asia):** Core Operations – JST NBDC (~80%; 3yrs) Value-added Activities – MEXT (~20%; 1-3yrs)
- **BMRB<sub>Madison</sub>:** Core Operations – NIH NIGMS (~80%; 5yrs) Value-added Activities – NIH NIGMS (~20%; 5 yrs)
- **BMRB<sub>Osaka</sub>:** Core Operations – JST NBDC (~80%; 3yrs) Value-added Activities – MEXT (~20%; 1-3yrs)

## 2. User Communities

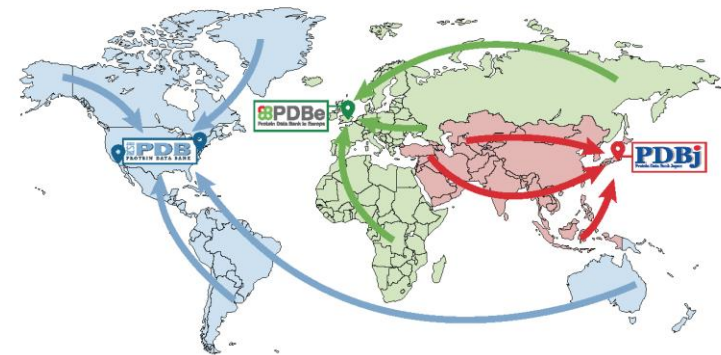
- **Data Producers:** Structural biologists worldwide (crystallography, nuclear magnetic resonance, and electron microscopy)
- **Primary Data Consumers:** Researchers, Educators, and Students worldwide in basic and applied biology, medicine, allied health professions, bioinformatics, chemistry, physics, engineering, computer science, statistics/biostatistics, materials science, mathematics, plant sciences, animal husbandry, ecology, ...
- **Other Data Consumers:** Patients, Patient's Families, Patient Advocates, Artists, Journalists, Media Outlets, and Curious Public worldwide

## 2. User Communities

- **Data Producers:**  
~30,000 registered depositors adding  
~11,000 new structures/yr  
(Archive growth~9%/yr)
- **Data Consumers:**  
>1 million unique users/yr
- **Data Rates:** ~1.5 million data files downloaded/day;  
>500 million data files downloaded/year
- **Pharmaceutical Cos**  
use PDB archive inside company firewalls daily



Depositor Locations



Biocuration Workload Distribution



Data Download Locations



# 3. Data Utilization/Monitoring

- **Basic and Applied Researchers** in every area of biology, medicine, and biotechnology, and selected areas of chemistry, physics, materials science, engineering, computer science, statistics/biostatistics, and mathematics worldwide
- **Educators and Students**
  - Graduate/Professional Schools
  - Technical/Undergraduate Colleges
  - Schools (Kindergarten→High School)
- **Other Users:** Science Funders, > 200 Derived Data Resources, Patients, Patient's Families, Patient Advocates, Artists, Journalists, Media Outlets, and the Curious Public worldwide

# 3. Data Utilization/Monitoring

- **Citation of wwPDB Peer Reviewed Publications**
  - >20,000 total citations and ~2000 annual citations of publications from wwPDB Partners
  - Track Citations *versus* Research Areas
- **PDB Structure Identifiers** now being “cited” nearly as frequently as our peer reviewed publications
- **Protein Data Bank** appears in >3,000 issued US patents
- **PDB Data File Downloads**
  - wwPDB FTP Sites: ~370 million in 2015
  - wwPDB Partner Websites:~165 million in 2015

## 4. Impact of Losing PDB Archive

- Current PDB holdings exceed 124,000 experimentally determined 3D structures of biological macromolecules
- Estimated cost of replicating each PDB entry ranges from US\$50,000 to >US\$250,000
- Conservative cost of replicating the PDB archive (assuming an average unit cost of US\$100,000) gives

**PDB Replacement Cost > US\$12.5 billion**

# 4. Impact of Losing PDB Archive

- Research progress would be slowed in every area of biology and medicine and related fields worldwide
- >200 Derived Data Resources (e.g., UniProt, model organism data bases) would no longer be able to repackage PDB data
- Drug discovery innovation in the the pharmaceutical and biotechnology industry would be slowed (impacting work on novel targets and mechanisms of action, and NCEs)
- Biology and medical education in schools, colleges, research universities, and graduate and profession schools would be compromised
- Patients, Patient's Families, and Patient Advocates forced to make less informed choices re treatment/management

# 5. Contingency Planning

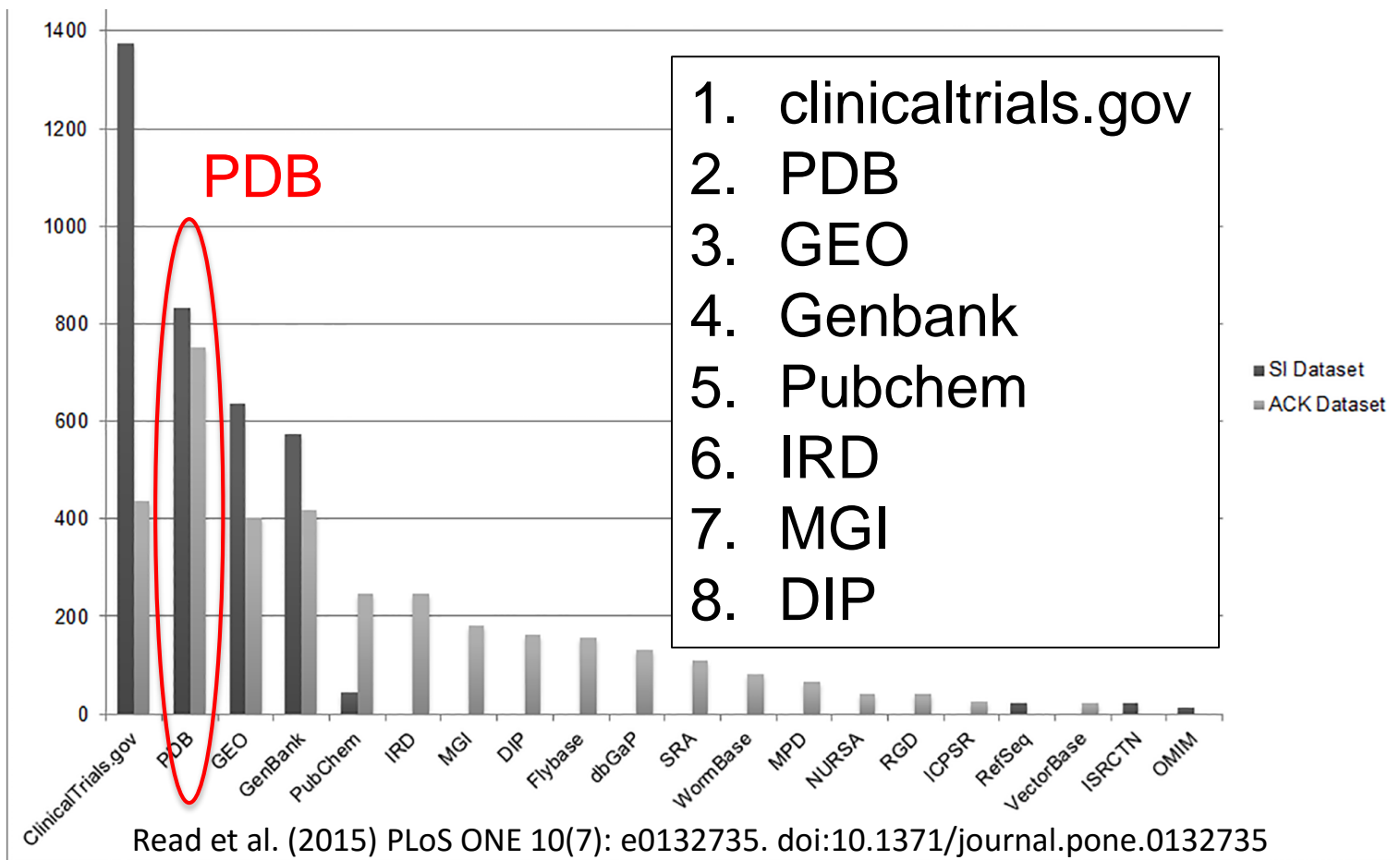
- **Scenario 1: Single wwPDB Partner loses funding**
  - Surviving wwPDB Partners could continue providing global data access
  - Surviving wwPDB Partners would need additional funding to shoulder increased data deposition/biocuration/validation burdens coming from geographic area no longer served
- **Scenario 2: All wwPDB Partners lose funding**
  - Current PDB archive FTP tree contents could be transferred to a data commons
  - All data deposition/biocuration/validation operations would cease → no growth in the PDB archive

# 6. Challenges Facing the wwPDB

- 1. Year-on-Year growth in number of PDB depositions and their complexity** (needing more human biocuration effort)
- 2. Technology/infrastructure required to keep pace with rapid methodological advances** (e.g., Hybrid methods, XFEL)
- 3. Short duration of current funding cycles**
- 4. Current funding mechanisms are not fit for purpose**
  - Tailored for 3-5 year duration research grants
  - Emphasis on discovery *versus* meeting infrastructure needs
- 5. Declining funding levels in all wwPDB Partner geographies over the past decade plus**
- 6. Lack of distinction in the Big Data Resource Funding Debate between Primary Data Archival Resources and Secondary Data Resources that aggregate other peoples data** (i.e., Huffington Post's of Biology)

# 6. Challenges Facing the wwPDB

Common locations where data from NIH-funded work published in 2011 was shared, based on PubMed SI field and PMC ACKnowledgements



# Protein Data Bank (PDB) Archive and the wwPDB Partnership

## Worldwide Protein Data Bank Co-Leaders

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John L. Markley, Ph.D. — BMRB

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