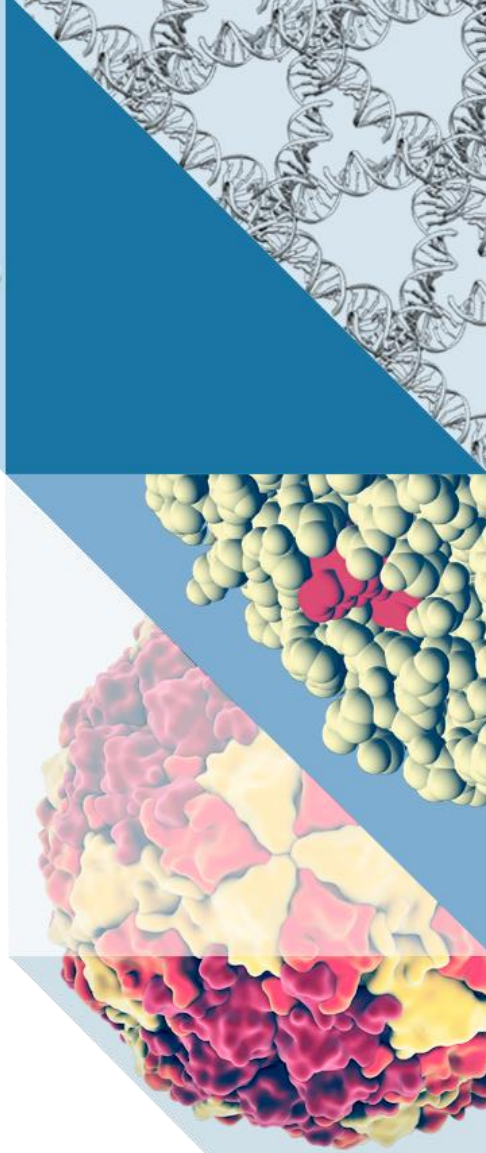
RCSB PDB
PROTEIN DATA BANK



Research Data Management for the PDB Archive: Unmerged Intensities, Structure Factors, Atomic Coordinates, and Metadata

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Director, RCSB Protein Data Bank

RUTGERS THE STATE UNIVERSITY OF NEW JERSEY
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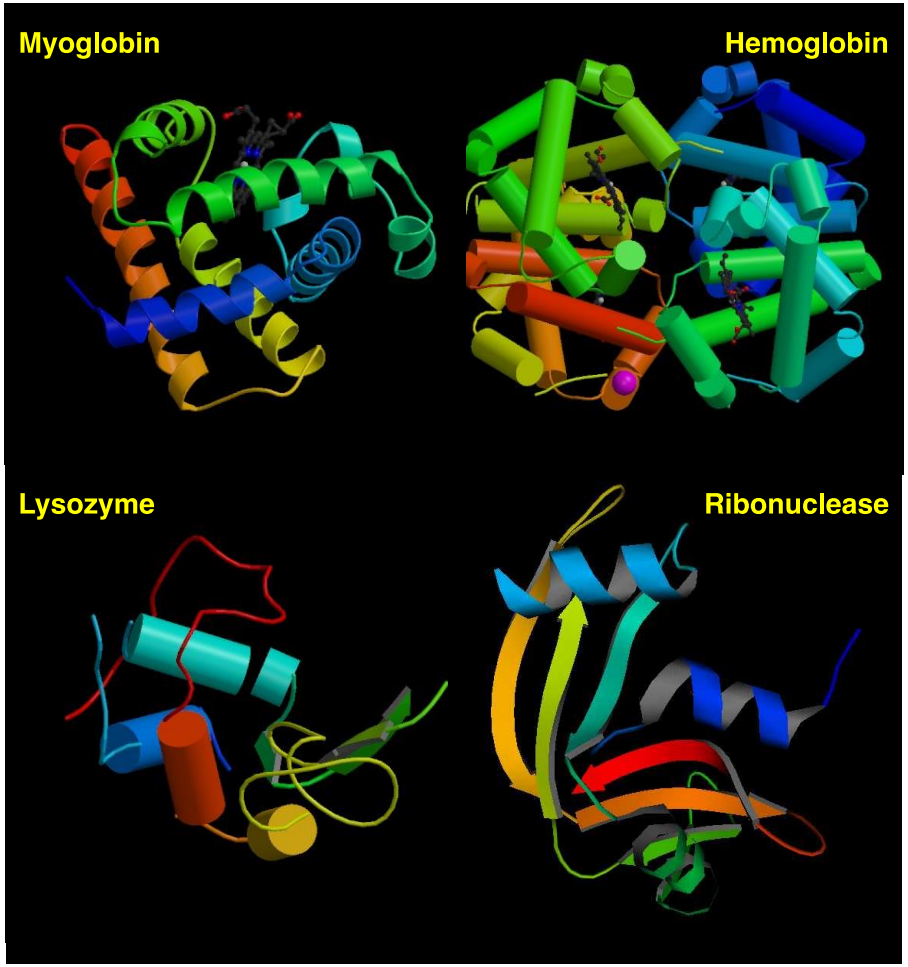
2017 ACA Meeting: Workshop

Outline

- History of the PDB Archive
- PDB Facts and Figures
- PDB Data Life Cycle/Unified OneDep System
- PDBx/mmCIF Working Group
- Evolution of the PDBx/mmCIF Data Dictionary
  - Structure Factors
  - Unmerged Intensities
  - Versioning
  - Updating of Atomic Coordinates
- Acknowledgements/wwPDB Foundation

Protein Data Bank Pioneered Open Access

- PDB 1st Open Access digital data resource in all of biology
- Founded 1971 with 7 X-ray structures
- Today, single global archive for experimental 3D macromolecular structure data
- Adhere to FAIR Principles

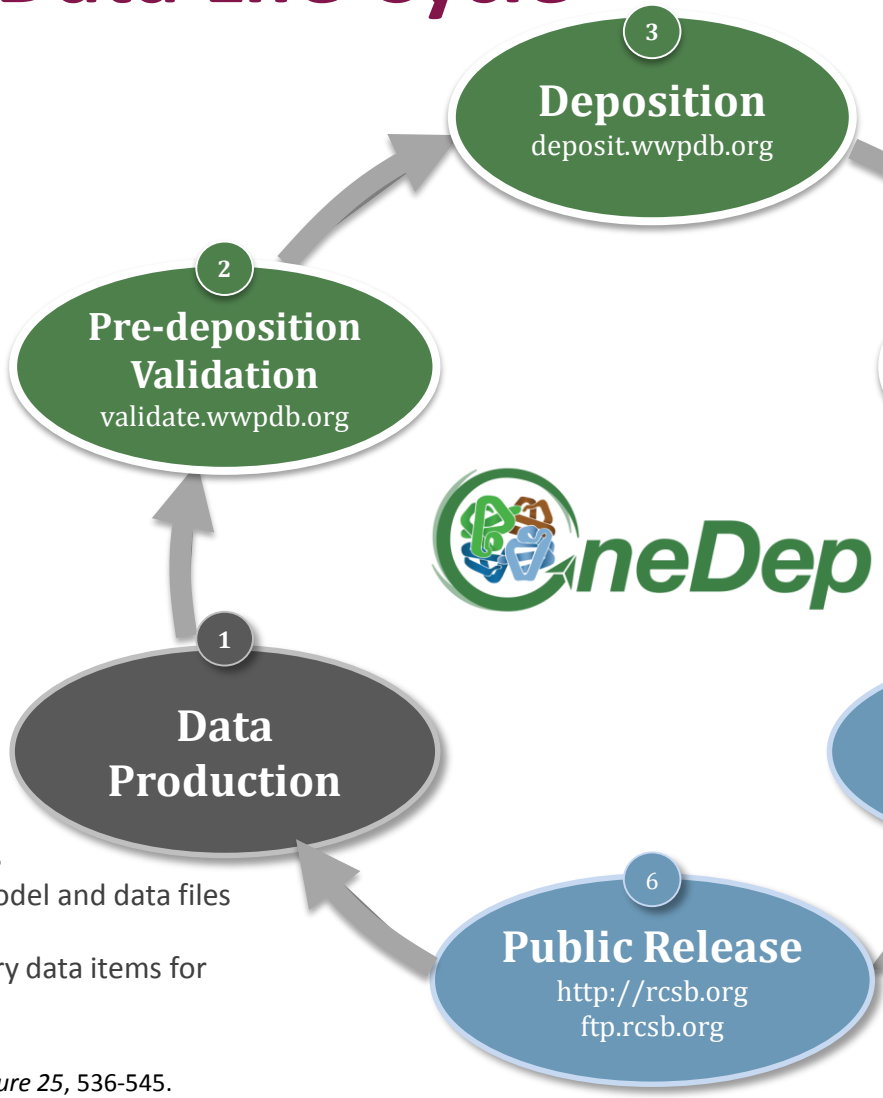


Some of the very first structures in the PDB

PDB: Massive Archive with Global Reach

- PDB safeguards >US$13 Billion worth of X-ray, NMR, and 3DEM data
- >130,000 structures freely available to Researchers, Educators/Students, and the Curious Public
- Archive growing at ~10%/year
- >1 Million Users worldwide served every year
- >1.5 Million structure data files downloaded/day
- Managed by worldwide collaboration (wwPDB)
- US PDB operations based at Rutgers/UCSD

PDB Data Life Cycle



wwPDB OneDep
Unified global deposition, biocuration, and validation system

Archive Keeper
RCSB PDB packages and re-distributes data to wwPDB partners

Structure Biologists
Generate atomic model and data files

Assemble mandatory data items for deposition

Data Users
Enables research in various fields

Data accessed *via* ftp download or web service

Young *et al.* (2017) *Structure 25*, 536-545.

PDBx/mmCIF Dictionary

- wwPDB manages PDB data using the macromolecular Crystallographic Information Framework (mmCIF)
- PDBx/mmCIF Dictionary contains >4400 data items for PX, NMR, and 3DEM (see mmcif.wwpdb.org)
- wwPDB PDBx/mmCIF Working Group coordinates evolution of the standard and implementation within software packages

- Working Group Roster

  Paul Adams (Chair)
  Jeff Bell
  Gerard Bricogne
  Paul Emsley
  Rasmus Fogh
  John Ionides
  Eugene Krissinel
  Nigel Moriarty
  Garib Murshudov
  Nicholas Sauter
  Mike Word

Going Beyond h, k, l, Fhkl, Sigma(Fhkl)

- h, k, l, Fhkl, Sigma(Fhkl) for refinement
- h, k, l, Fhklmap, ϕhklmap from Depositor interpretation
- h,k,l, Fhklnative, ϕhklnative from Depositor
- h,k,l, Fhkl+, Sigma(Fhkl)+, Fhkl-, Sigma(Fhkl)- for phasing from Depositor
- h,k,l, FhklDer#+, Sigma(FhklDer#+), FhklDer#-, Sigma(FhklDer#-) for phasing from Depositor

Unmerged Intensities

- Crystal ID
- Sweep ID
- Frame ID
- h, k, l, Ihkl, sigma(Ihkl), partiality
- Identifier for raw diffraction data image with location of peak centroid
- Misset Angles for crystal/sweep/frame
- Rotation Range

Versioning of the PDB Archive

- A new versioned data file naming convention:
  - Semantic version numbers (e.g., major-minor)
  - Uniform identification of data content types
  - Extended accession codes grandfathering of current 4-character codes

    pdb_00001abc_xyz_v2-0.cif.gz
- Versioned files contain additional audit records describing revision details at the granularity of PDBx/mmCIF data categories.
- A new FTP server will be deployed to host the versioned data files in parallel to the current FTP service

Updating of Atomic Coordinates

- Historical policy of obsoleting PDB entries upon coordinate data replacement has been revised
- Future coordinate replacements by the *Author of Record* will retain the original PDB entry code, incrementing the entry major version number
- Major versions of each entry (*i.e., the latest minor revision*) will be accessible from the primary wwPDB FTP archive

Acknowledgements

John Westbrook, Paul Adams,
wwPDB PDBx/mmCIF Working Group

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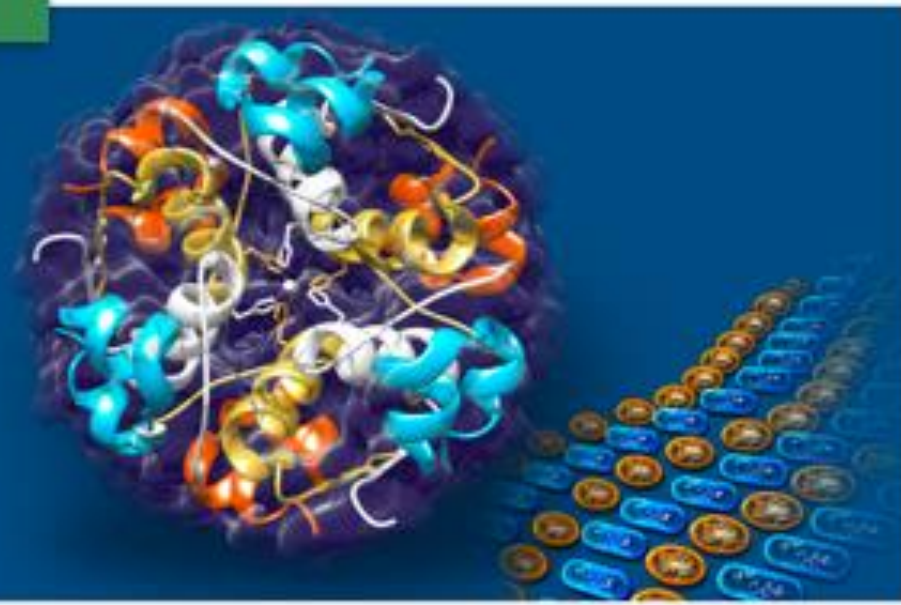
Support PDB's Spirit of Openness, Cooperation and Education

Worldwide Protein Data Bank Foundation

The wwPDB Foundation funds outreach activities of the wwPDB that are crucial to the future of the PDB archive, including workshops, symposia, and advisory meetings.

Visit **foundation.wwpdb.org** to make a donation.



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