
Growth, Globalization, and Future of the Protein Data Bank

Stephen K. Burley, Eli Lilly & Co.


October 28th 2011



wwpdb.org

Acknowledgements

- Helen Berman - RCSB PDB
 - Gerard Kleywegt - PDBe
 - John Markley - BMRB
 - Haruki Nakamura - PDBj
-
- Phil Bourne - RCSB PDB
 - Martha Quesada - RCSB PDB
 - Christine Zardecki - RCSB PDB



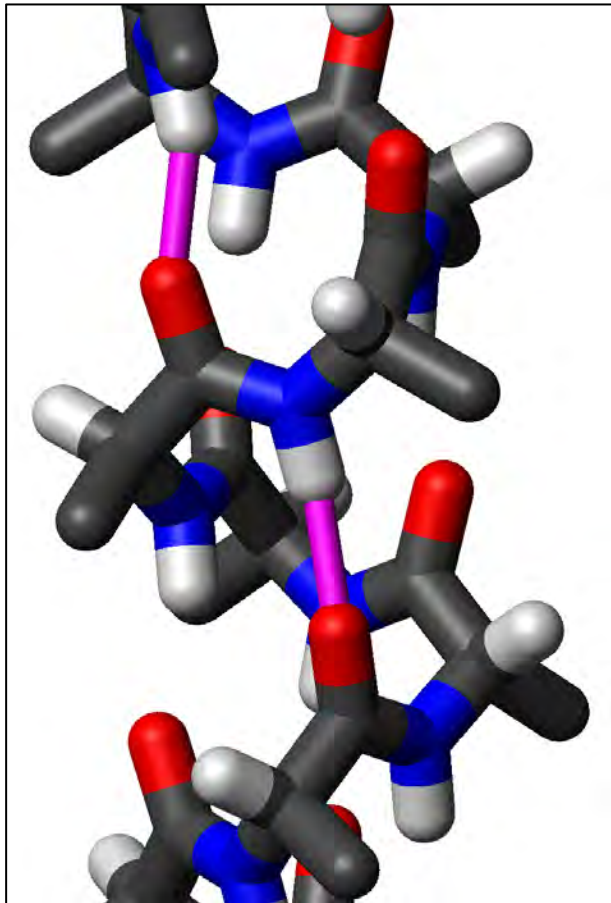
“We may anticipate that the chemist of the future who is interested in biomolecules will come to rely upon a new structural chemistry, and that great progress will be made, through this technique, in biology and medicine.”

Linus Pauling, Nobel Lecture 1954



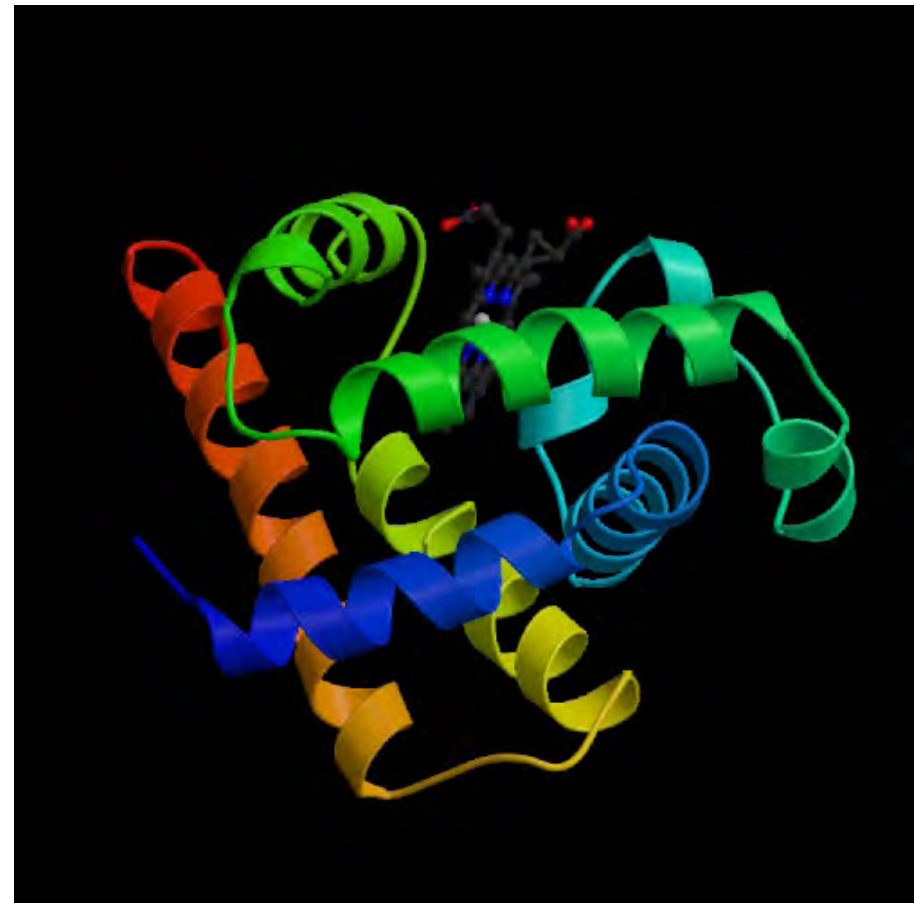
Chemistry → Biological Structure

α -Helix



Pauling and Corey (1951)

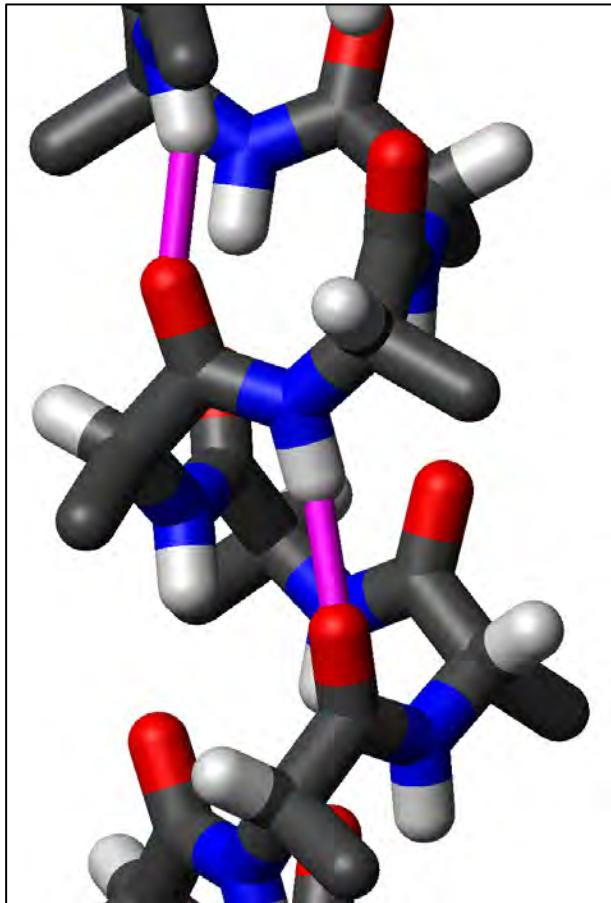
Myoglobin



Kendrew *et al.* (1958)

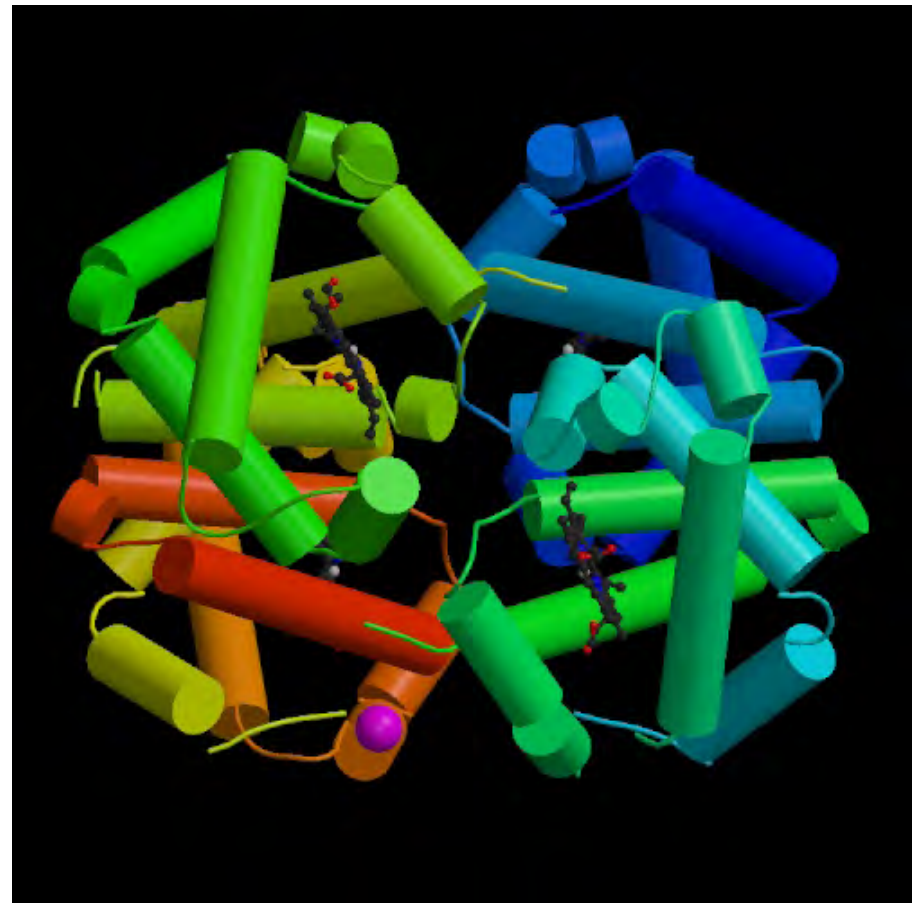
Chemistry → Biological Structure

α -Helix



Pauling and Corey (1951)

Hemoglobin

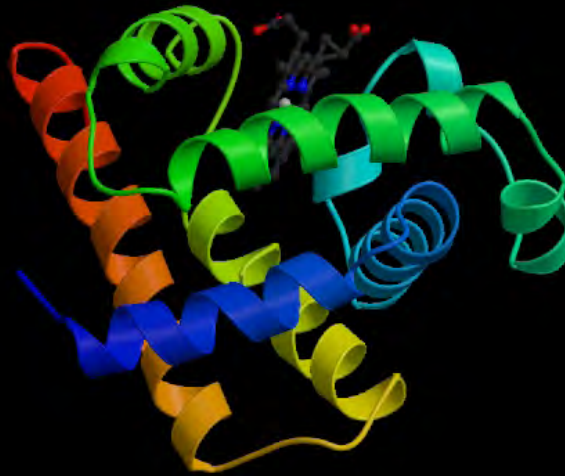


Perutz *et al.* (1959)

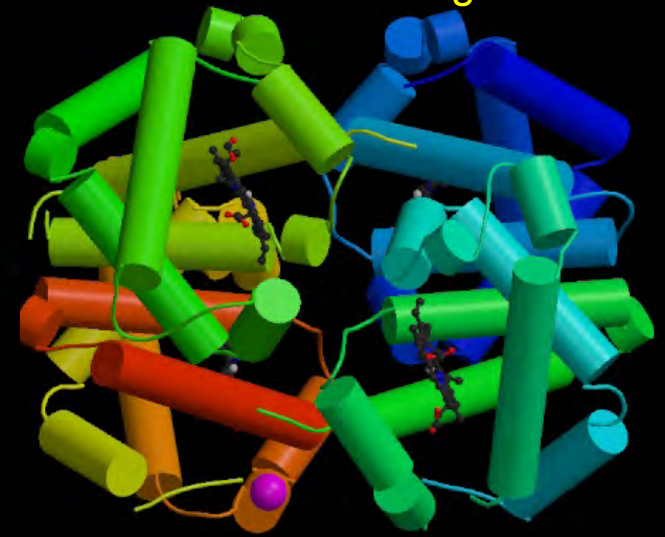
By the
mid-1960s
things
were
getting
out of
hand!

Something
had to be
done ...

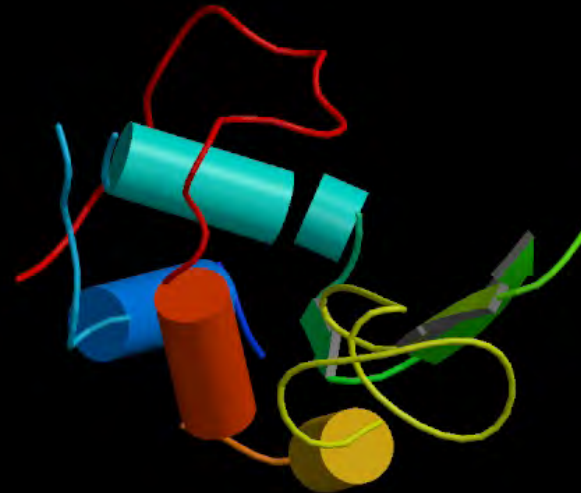
Myoglobin-1958



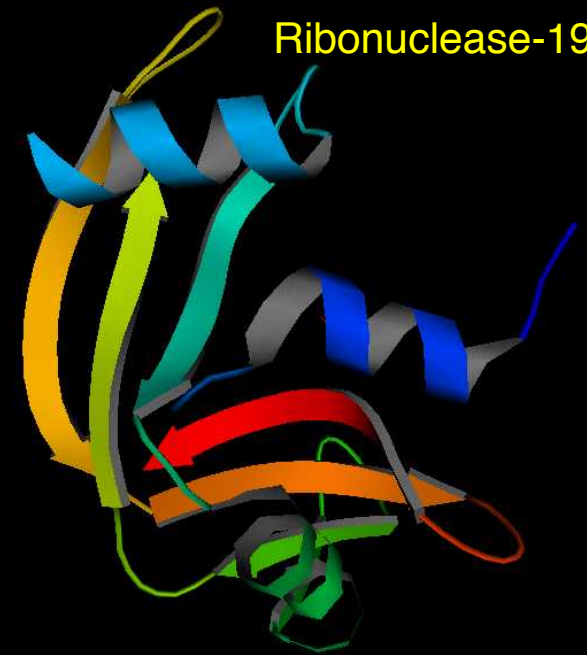
Hemoglobin-1959



Lysozyme-1965



Ribonuclease-1965





**First Electronic, Open Access
Resource for the Biological Sciences**



CSHL Symposia June 4-11 1971

- “Structure and Function of Proteins at the Three-Dimensional Level”
- Organizer: James D. Watson
- Advisors: Aaron Klug, William N. Lipscomb, Max Perutz, David C. Phillips, and Frederic M. Richards

PDB is Born in 1971

- Protein Data Bank found its first home at Brookhaven National Laboratory with only 7 structures
- Founding Director: Walter C. Hamilton
- Announced in *Nature New Biology* with the following caveat:

“The success of the proposed system will depend on the response of protein crystallographers supplying data.”

CRYSTALLOGRAPHY

Protein Data Bank

A repository system for protein crystallographic data will be operated jointly by the Crystallographic Data Centre, Cambridge, and the Brookhaven National Laboratory. The system will be responsible for storing atomic coordinates, structure factors and electron density maps and will make these data available on request. Distribution will be on magnetic tape in machine-readable form whenever possible. There will be no charge for the service other than handling costs. Files will be updated as new material is received. The total holding will be announced annually in the organic bibliographic volumes of the reference series "Molecular Structures and Dimensions" published by the Crystallographic Data Centre and the International Union of Crystallography by Oosthoek's, Utrecht.

The success of the proposed system will depend on the response of the protein crystallographers supplying data. These will be accepted either "raw" or refined, in machine-readable form or as manuscripts. Laboratories intending to join the scheme should communicate with Mrs Olga Kennard or Dr D. G. Watson at the University Chemical Laboratories, Lensfield Road, Cambridge, who are responsible for the organization of the system. Data can be submitted to Cambridge or to Dr W. C. Hamilton at the Brookhaven National Laboratory, Upton, New York 11973, where the data will be computer processed.

The two centres will maintain identical files and both will provide data services. The new data bank is intended to supplement existing publication media so that depositing material in this form is not a substitute for the publication of the results of structural investigations in a scientific journal.



**Growth of the PDB:
The Singular Archive for
Macromolecular Structure Data**



1987: Users Compel Deposition

Yale University

Department of Molecular Biophysics
and Biochemistry
260 Whitney Avenue
P.O. Box 6666
New Haven, Connecticut 06511
Telephone:
203 432-5620

28 October 1987

Dear Colleague,

We are writing to you because of our increasing concern with the preservation of and access to macromolecular structure data and the derived molecular models. It is our intent to send the enclosed letter to the editors of a number of major journals in which such studies are usually published. The content of the letter is self explanatory. The details of the proposal, which will certainly evolve, are less important than the general thrust. We hope very much that you would be willing to cosign this letter.

Since we are trying to get as much support as possible, it is unrealistic to attempt to get all of the original signatures on one letter. If you will join us, we ask that you sign and date the second copy of the final page and return it to F.M.Richards in the enclosed envelope.

Sincerely yours,

Frederic M. Richards
Frederic M. Richards

Richard E. Dickerson
Richard E. Dickerson

Jane S. Richardson
Jane S. Richardson

Michael G. Rossmann
Michael G. Rossmann

David C. Richardson
David C. Richardson

David R. Davies
David R. Davies

Joseph Kraut
Joseph Kraut

Don C. Wiley
Don C. Wiley

Stephen C. Harrison
Stephen C. Harrison

Distribution List for Draft Deposition Guidelines

IUCr Commission on Biological Macromolecules

Current members:

G. Dodson
S. Borisov
P. M. Colman
M. N. G. James
B. W. Matthews
D. Moras
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J. S. Richardson
M. G. Rossmann

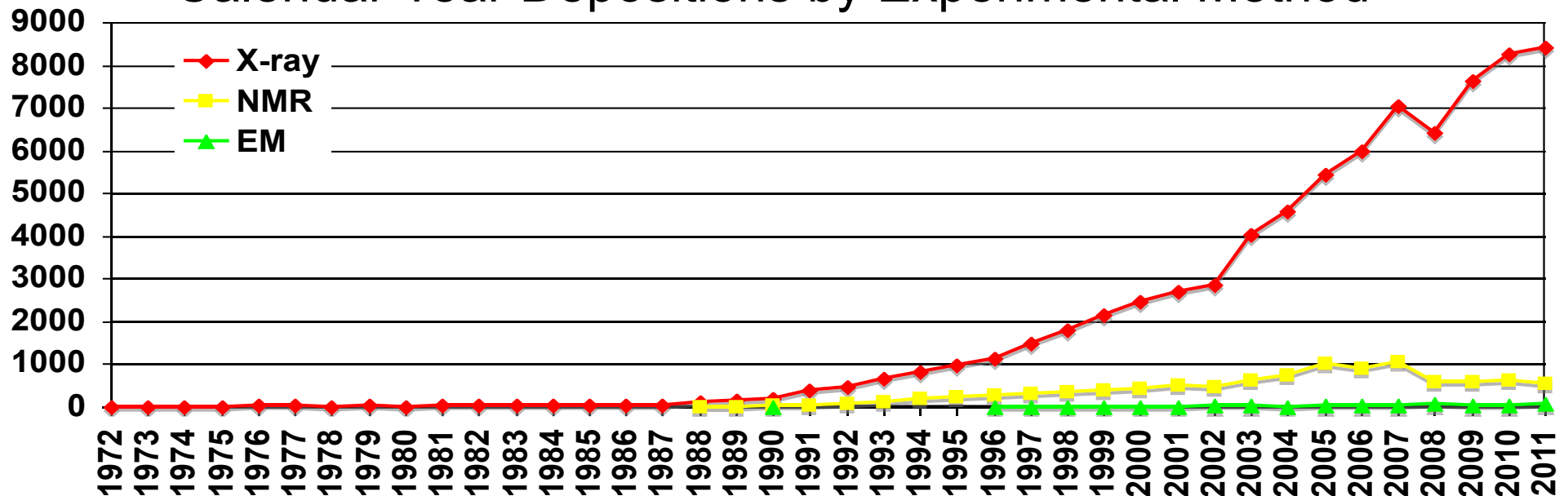
U. S. Funding Agencies

J. C. Norvell
M. Cassman
A. Kowalsky

10,000-Fold Growth in Four Decades

- 7 → >76,000 entries
- 2011 will see ~9,000 depositions
- Electron Microscopy is beginning to hit its stride

Calendar Year Depositions by Experimental Method

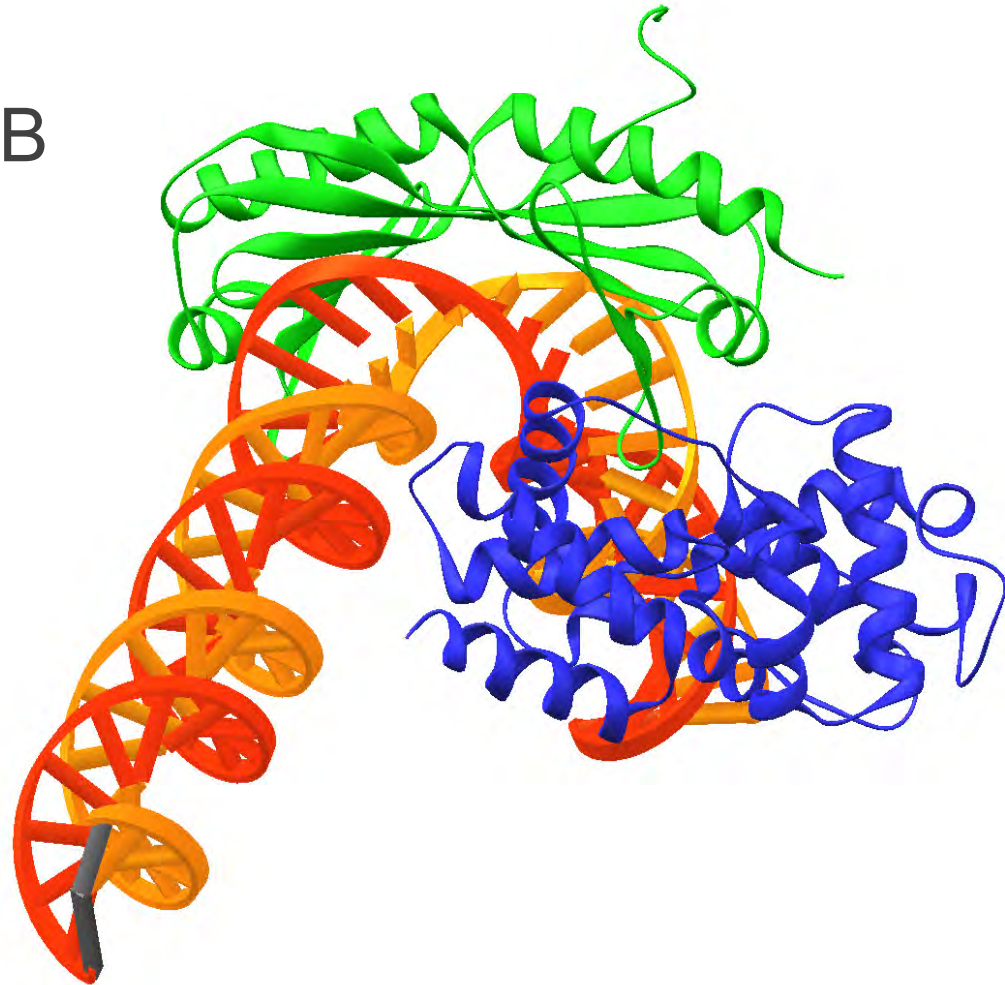


20 Person Years → 20 Person Days

- Faster and Faster Computing
- Graphical Display (Geis → Frodo → O → COOT → ...)
- Simulated Annealing Refinement
- Gene Cloning/Protein Expression Systems
- Protein Purification/Engineering
- Crystallization Strategies (Factorial, LCP, ...)
- Data Collection: Cryogenics/Area Detectors
- Synchrotron Beamlines → MAD/SAD Phasing
- Automated Map Interpretation/Model Building
- Micro Focus X-ray Beamlines

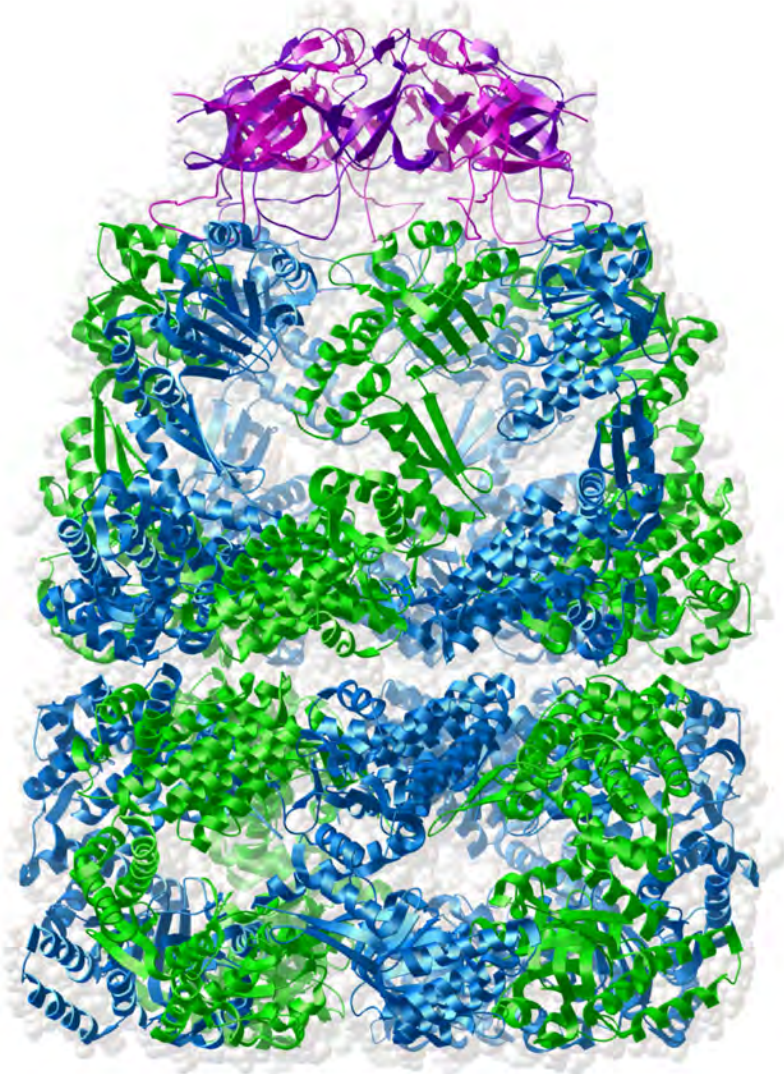
Function Follows Form

- TBP+DNA+TFIIB



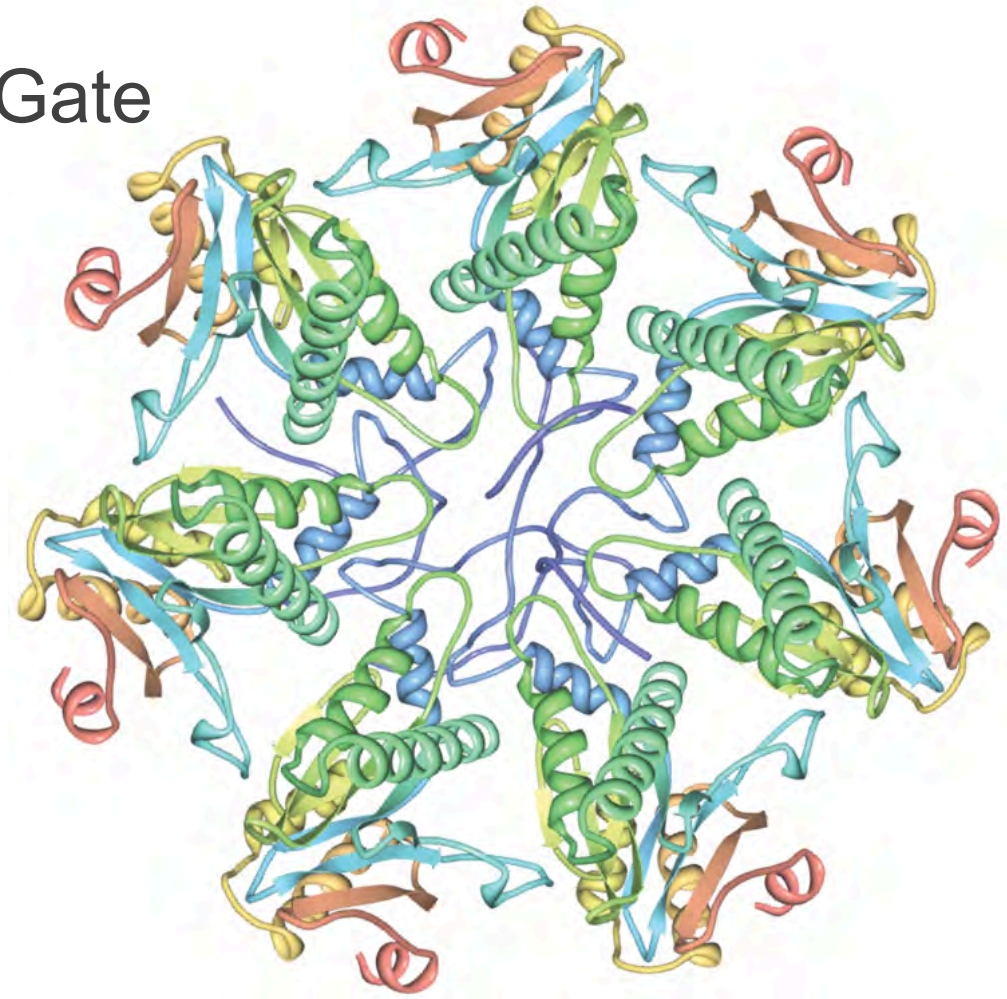
Function Follows Form

- GroEL-GroES



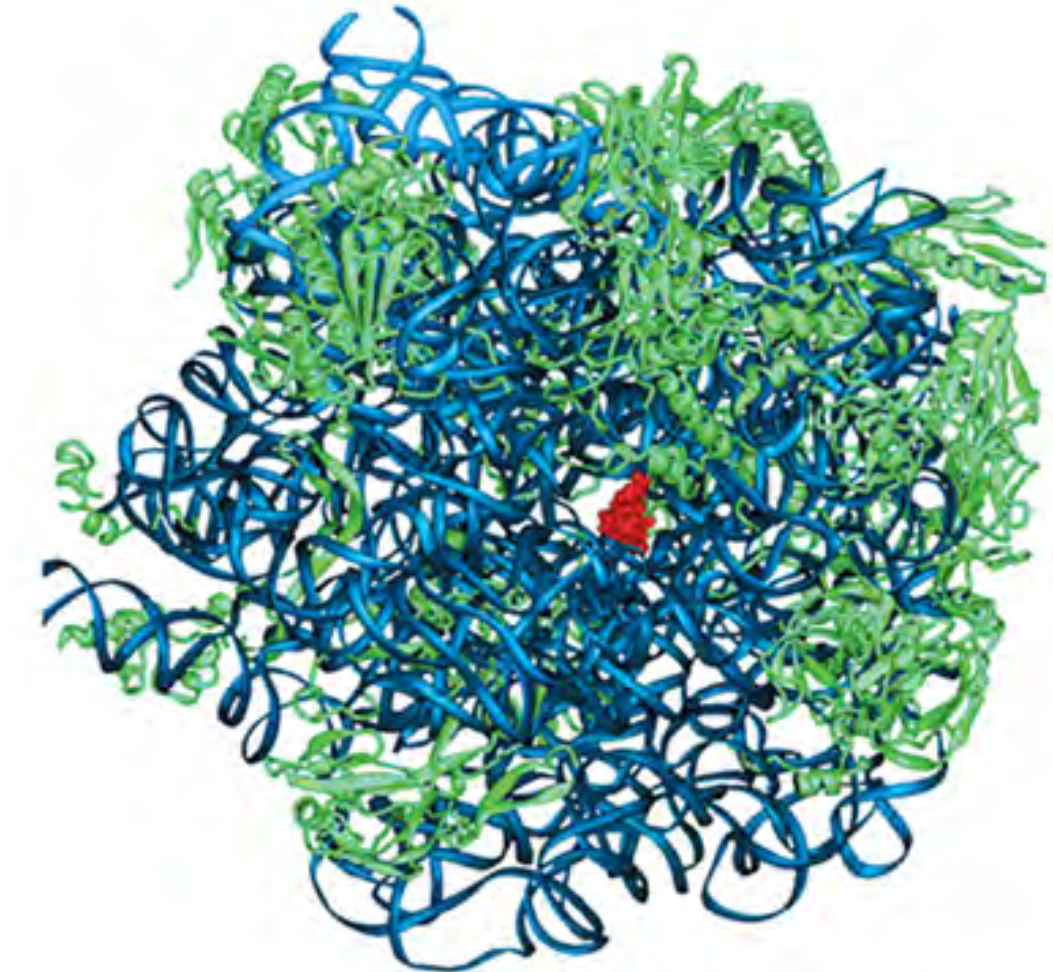
Function Follows Form

- Archaeal Proteasome Gate



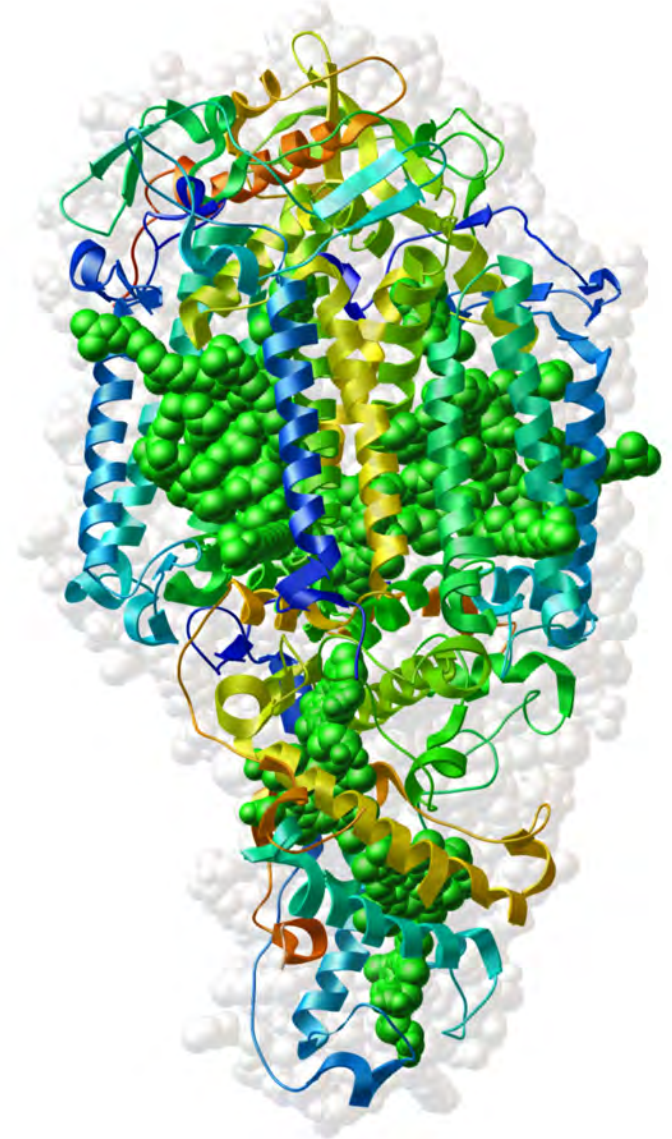
Function Follows Form

- Ribosome



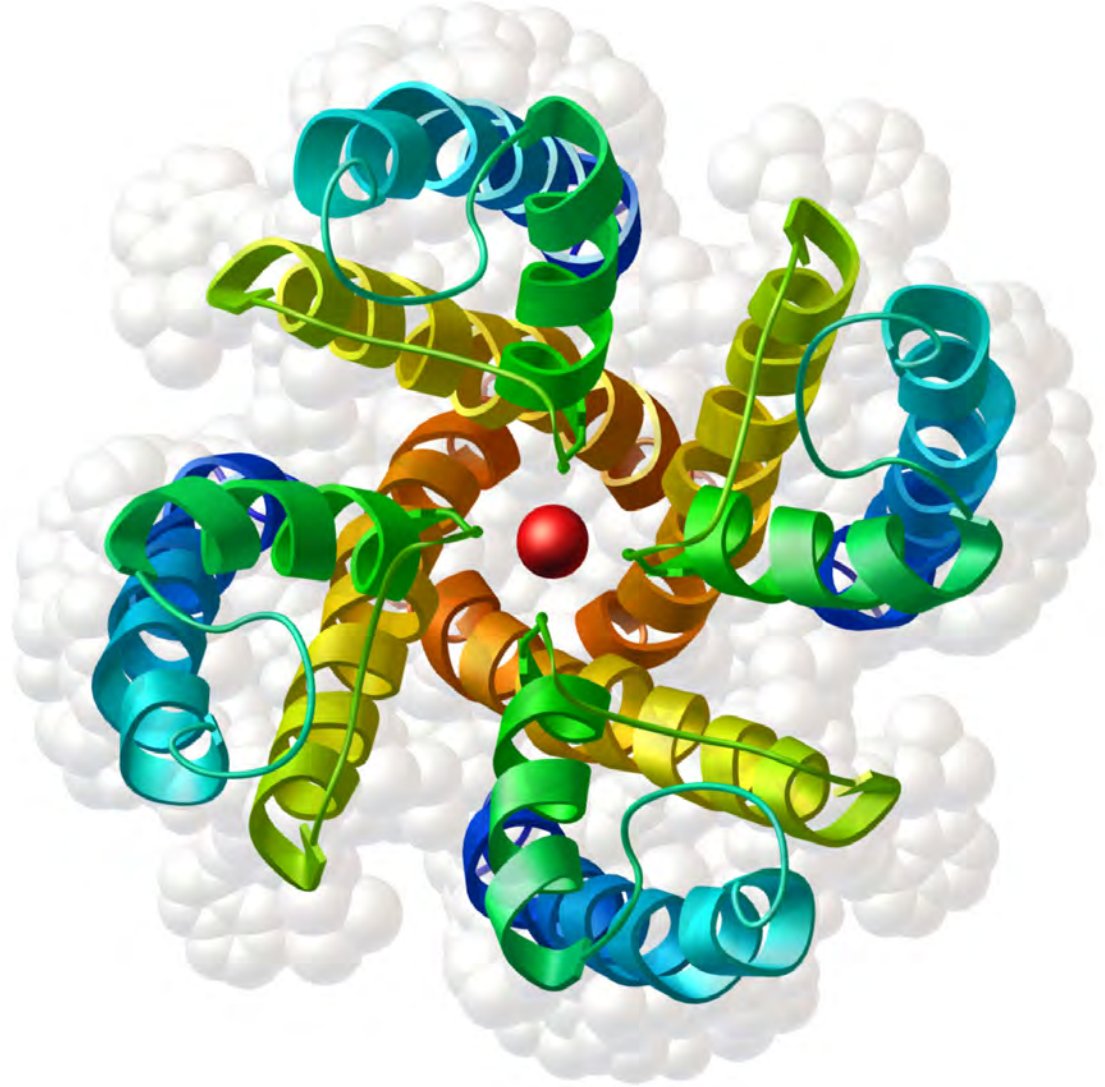
Function Follows Form

- Photosynthetic Reaction Center



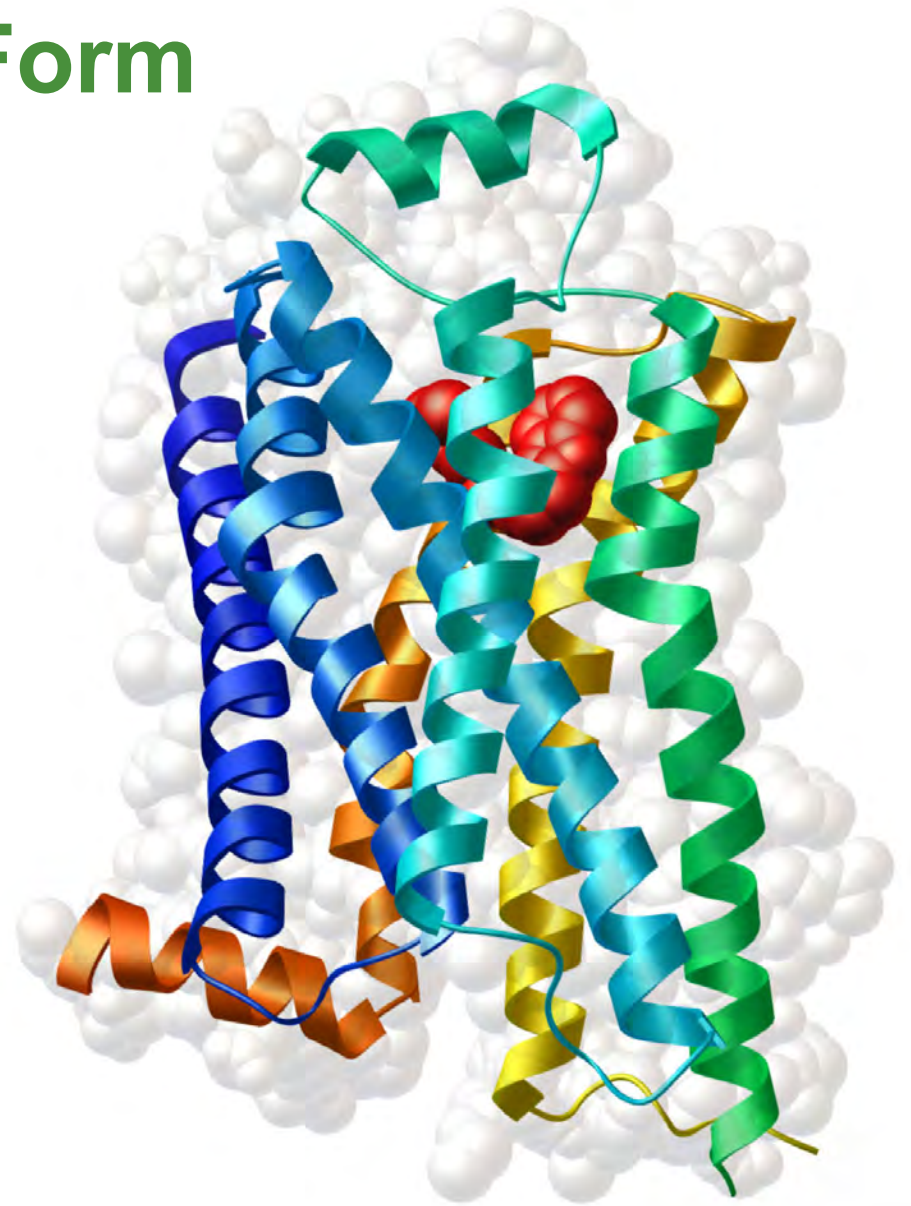
Function Follows Form

- K⁺ Channel



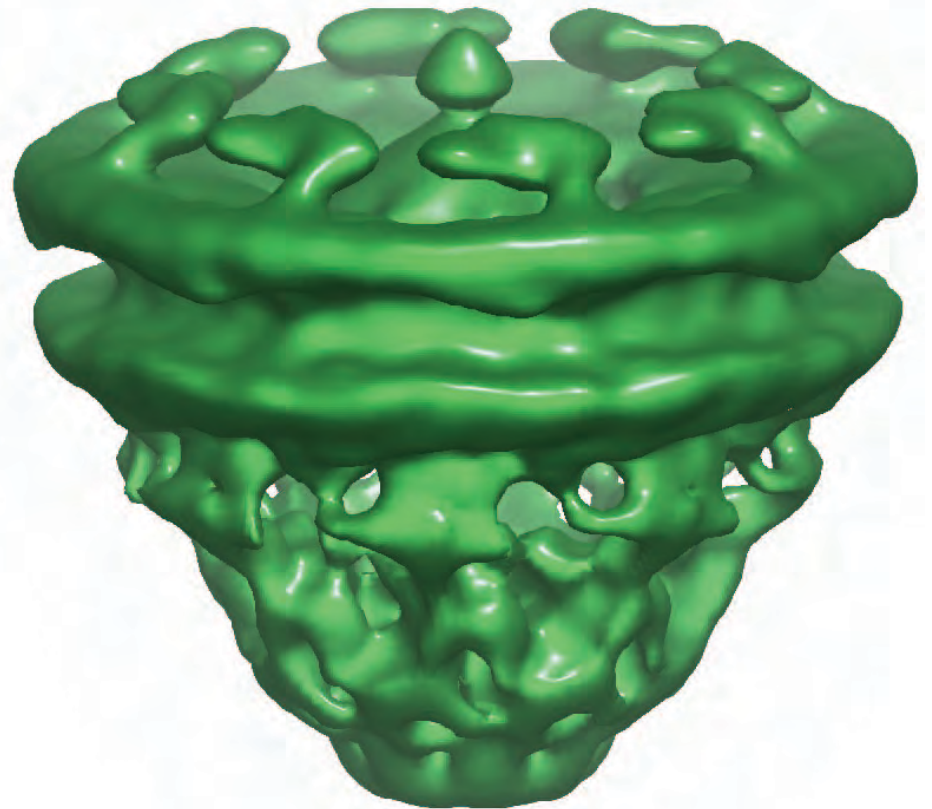
Function Follows Form

- β Adrenergic GPCR



Function Follows Form

- Nuclear Pore Complex



PDB Downloads~210 Million in 2010!



■ RCSB PDB

■ PDBe

■ PDBj

“Science knows no country, because knowledge belongs to humanity and is the torch that illuminates the world.”

Louis Pasteur

Globalization of the PDB



wwpdb.org

wwPDB Established in 2003

- Membership
 - RCSB PDB (Research Collaboratory for Structural Bioinformatics - Rutgers University/UC San Diego)
 - PDBj (Osaka University)
 - PDBe (EMBL EBI)
 - BMRB (University of Wisconsin)*
- MOU signed July 1st 2003; Amended in 2007*
- Announced in *Nature Structural Biology*

Announcing the worldwide Protein Data Bank

In recognition of the growing international and interdisciplinary nature of structural biology, three organizations have formed a collaboration to oversee the newly formed worldwide Protein Data Bank (wwPDB; <http://www.wwpdb.org/>). The Research Collaboratory for Structural Bioinformatics (RCSB), the Macromolecular Structure

mentation will be kept publicly available and the distribution sites will mirror the PDB archive using identical contents and subdirectory structure. However, each member of the wwPDB will be able to develop its own web site, with a unique view of the primary data, providing a variety of tools and resources for the global community.

description conventions of the PDB exchange dictionary. In addition, the legacy PDB format would not be modified unless there is a compelling reason for a change. Should such a situation occur, all three wwPDB members would have to agree on the changes and give the structural biology community 90 days advance notice.

wwPDB Today

Advisory Committee Meeting 2011



Leadership



PDBj
Protein Data Bank Japan



RCSB PDB
PROTEIN DATA BANK

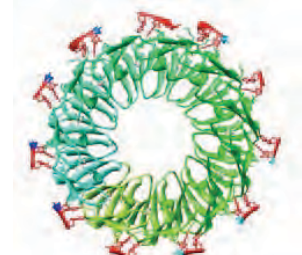
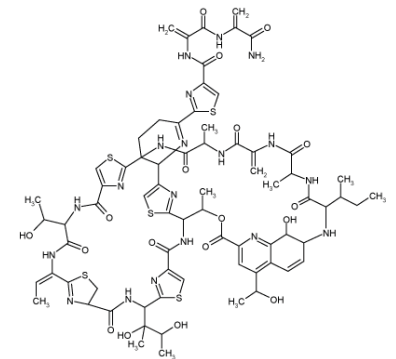
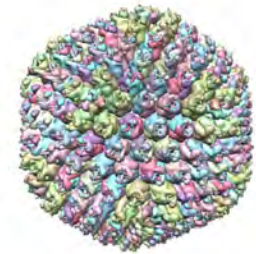
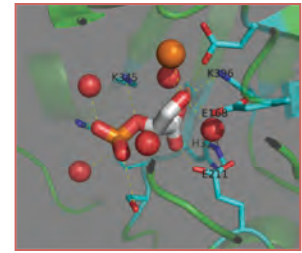
EMBL-EBI PDBe
PROTEIN DATA BANK EUROPE

wwPDB Member Responsibilities

- Members collaborate on “Data In”
 - Issue PDB IDs
- RCSB PDB serves as the Archive Keeper
 - Manage PDB IDs
 - Sole write access
- Members compete on “Data Out”
 - Distribute Identical Data
 - “Market Place of Ideas” concept

wwPDB Archive Remediation

- 2007: Sequences/Chemistry, Viruses ...
- 2009: New Record Types, Enhanced Annotations, Database References, Various Corrections ...
- 2011: Peptide Antibiotics, Biological Assemblies, Tagging Entries ...
- 2012: Next!



Please visit <http://www.wwpdb.org>



Access the PDB FTP:
RCSB PDB PDBe PDBj
Archive Download
Chemical Component Dictionary
Deposit Data to the PDB:
RCSB PDB PDBe
PDBj BMRB
Search for Structures:
RCSB PDB PDBe
PDBj BMRB
PDB Archive Snapshots:
RCSB PDB PDBj
Instructions to Journals
Documentation
Format
Annotation and Policies
Workshops and Task Forces
X-ray Validation
NMR Validation
wwPDBAC

The Worldwide Protein Data Bank (wwPDB) consists of organizations that act as deposition, data processing and distribution centers for PDB data. The founding members are **RCSB PDB** (USA), **PDBe** (Europe) and **PDBj** (Japan)¹. The **BMRB** (USA) group joined the wwPDB in 2006. The mission of the wwPDB is to maintain a single Protein Data Bank Archive of macromolecular structural data that is freely and publicly available to the global community.

This site provides information about services provided by the individual member organizations and about projects undertaken by the wwPDB.

wwPDB Statement on Retraction of PDB Entries

21-October-2011

PDB40 Symposium Update

Celebrate four decades of innovation in structural biology with the wwPDB October 28-30, 2011 at CSHL. View the preliminary program ([PDF](#)) and poster abstracts ([PDF](#)). Limited space is available--**register today!**




14-October-2011

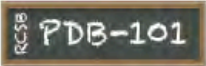
First contours of a vision for the future of validation at the PDB

The Worldwide Protein Data Bank (wwPDB; www.wwpdb.org) is pleased to direct PDB depositors and users to the recommendations of the wwPDB X-ray Validation Task Force (VTF) that were published in the journal *Structure* this week (2011, vol. 19: 1395-1412).


RCSB PDB






PROTEIN DATA BANK









PDB-101

A MEMBER OF THE  **PDB**

An Information Portal to Biological Macromolecular Structures

As of **Tuesday Oct 11, 2011 at 5 PM PDT** there are **76495** Structures | [PDB Statistics](#) |   

[All Categories](#) |  Author |  Macromolecule |  Sequence |  Ligand | 

Search | All Categories: 

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- Validation Server
- BioSync Beamlines/Facilities
- Related Tools


Biological Macromolecular Resource

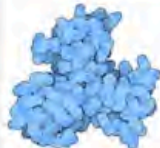
Full Description

[Featured Molecules](#) **Hide**

Structural View of Biology List View of Archive By: [Title](#) | [Date](#) | [Category](#)

 **Enzymes** 

**Molecule of the Month**
PDB Pioneers
Structural biology was born in 1958 with John Kendrew's atomic structure of myoglobin, and in the following decade, the field grew rapidly. By the early 1970's, there were a dozen atomic structures of proteins, and researchers were discovering that they had a goldmine of information.
[Full Article](#)

**Protein Structure Initiative Featured System**
Bacterial Armor
Researchers at MCSG have revealed the inner workings of a surface layer protein, showing how bacteria attach their form-fitting protein coats.
[Full Article](#) | [Archive](#) | [PSI Structural Biology Knowledgebase](#)


[New Structures](#) **Hide**

- Latest Release
- New Structure Papers
- Search Unreleased Entries

[New Features](#) **Hide**

PDB-101: Mobile Access to Molecule of the Month

Latest features released:

Website Release Archive: 

[wwPDB News](#) **Hide**

PDB40 Symposium
October 28 - 30, 2011
Cold Spring Harbor Laboratory

PDBj

PDBj
Protein Data Bank Japan

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- ADIT-NMR

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- PDB/RDF, chem_comp/RDF
- Latest Release Search
- Sequence-Navigator
- Structure-Navigator
- SeSAW
- Ligand Binding Sites (GIRAF)
- EM Navigator
- Search NMR Data (BMRB)
- Status Search



Service and Software >>

- jV: Graphic Viewer
- Yorodumi
- Protein Globe
- ASH
- MAFFTash
- SEALA



PDBj (Protein Data Bank Japan) maintains a centralized PDB archive of macromolecular structures and provides integrated tools, in collaboration with the [RCSB](#), the [BMRB](#) in USA and the [PDBe](#) in EU. PDBj is supported by [JST-NBDC](#) and [Osaka University](#).

Deposition

[Data Deposition Information >>](#)

[PDB Deposition](#)  [NMR Data Deposition](#) 

Search

[Search PDB](#)  [Search NMR Data](#) 

PDB ID or Keyword

Accession number
 Deposition code

[Advanced Search >>](#)

What's new

18-Aug-2011

76495
[entries available on 12 Oct., 2011](#)
00:00(UTC) / 09:00(JST)

WORLDWIDE **PDB**
PROTEIN DATA BANK

eProtS
Encyclopedia of Protein Structures

Protein Globe

DBCLS
Database Center for Life Science

PDBe

Enter search term, accession number or PDBe service name



SEARCH

FEEDBACK

PDBe Tools

Latest release

PDB entries
PDB compounds
EMDB entries
PDB entry status

Deposit

PDB (AutoDep)
EMDB (EmDep)

Search

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About us

EMBL-EBI's Protein Data Bank in Europe (PDBe) is the European resource for the collection, organisation and dissemination of data on biological macromolecular structures. [More...](#) [Contact us](#)

PDBe Notification:

Due to essential maintenance at the EBI, PDBe services as well as PDB and EMDB deposition tools will be unavailable between Friday 21 Oct 11am BST and Monday 24 Oct 11am BST. Other wwPDB and EMDB deposition sites will not be affected. We apologise for any inconvenience this may cause.



As of 12 October 2011 the PDB contains **76495** entries ([latest entries](#), [latest compounds](#)) and EMDB contains **1160** entries ([latest](#))

Quick access

Sequence search

PDBe feature

RSS feeds

One-click access to PDB data

Enter a PDB ID code and click a button below for more information about the PDB entry:

Entry summary

Download PDB file

Download other files

Quaternary structure

Similar structures

Motifs and sites

Retrieve PDB entries using an external database identifier:



PubMed



Search

Find a random PDB entry ...

Quips



Phaser - a "stunning" method for solving crystal structures

Latest News

18 October 2011

PDBe service interruption 21-24 October [More...](#)

17 October 2011

New Quips episode about PHASER and the first structure it helped solve [More...](#)

14 October 2011

First contours of a vision for

BMRB



Biological Magnetic Resonance Data Bank

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BMRB

BioMagResBank

BMRB Data Listed By:

[Macromolecular types](#)[NMR spectral parameters](#)[Kinetics](#)[Thermodynamics](#)[Restrains](#)[Structure](#)[Time-domain sets](#)[Solid-state NMR](#)[Unfolded proteins](#)[Binding Data](#)[Diseases](#)

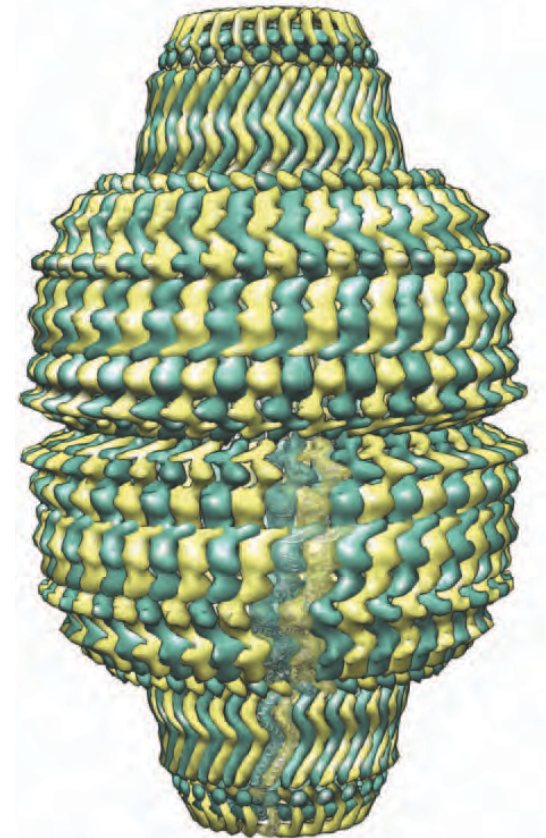
PDB of the Future



wwpdb.org

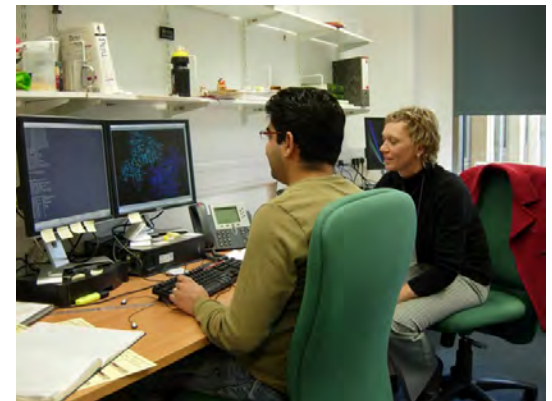
What: Responding to User Needs

- Higher deposition rates
- Increasingly complex structures
- Enhanced validation
- Expanded annotation
- Hybrid methods

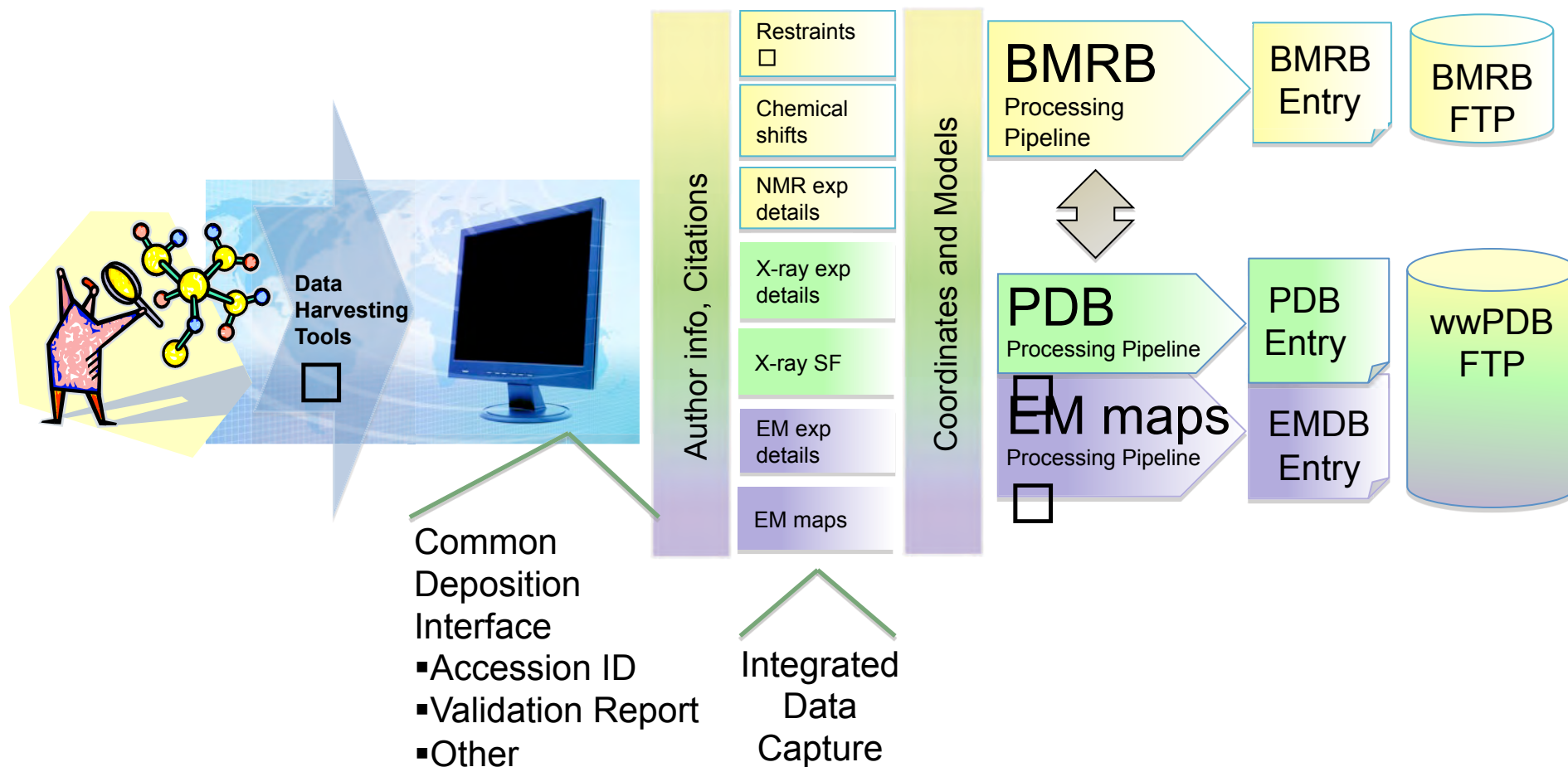


Why: What's In It For ...

- Depositors
 - Interactive Deposition Interface
 - Validation/Annotation
 - Increased Efficiency
 - Support New/Hybrid Methods
- Annotators
 - Increased Throughput
 - Advanced Annotation
- Researchers/Educators
 - Highest Quality Archive

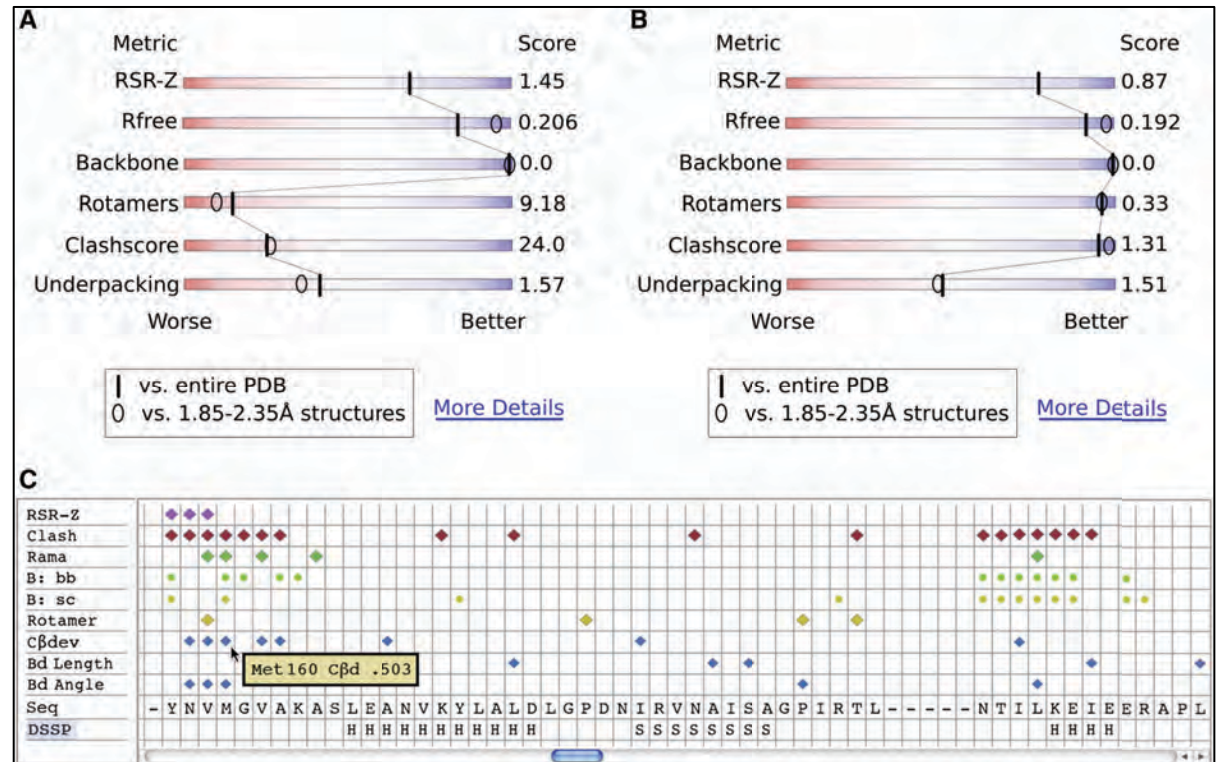


How: Common Deposition Tool



How: Enhanced Validation Systems

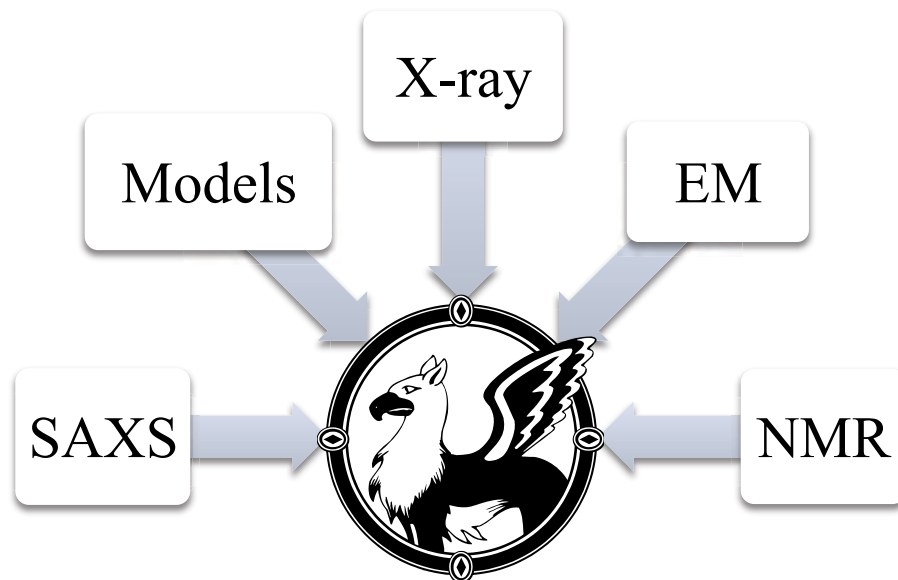
- User Driven
- Transparent
- Interpretable



From *A new generation of crystallographic validation tools for the Protein Data Bank*
Read et al. (2011) *Structure* 19, 1395-1412.

How: Hybrid Methods → New Biology

- Today: Combined Neutron/X-ray Structures
- Tomorrow: Scientist's Choice



- Extensible Dictionary
- Modular System

**Plus ça change
(Plus c'est la même chose)**

The more things change
(The more they remain the same)



wwpdb.org

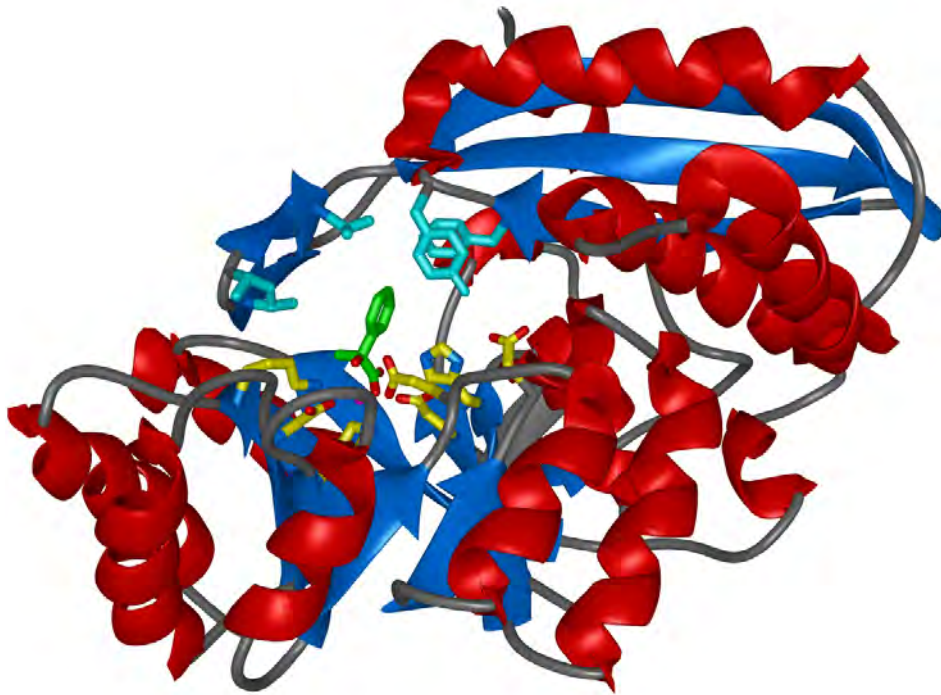
1971: What does it Look Like?



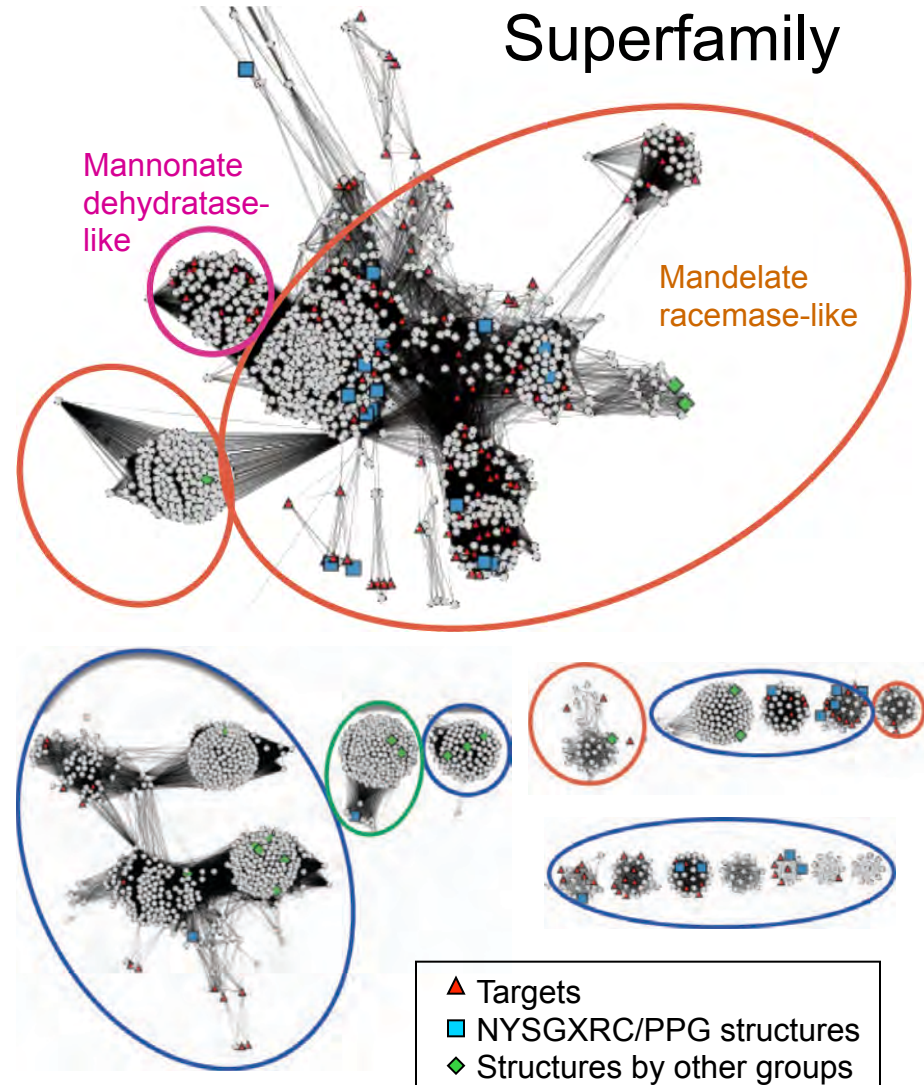
Sperm Whale Myoglobin—Kendrew *et al.* (Irving Geis)

2011: What does it Look Like?

Triosphosphate Isomerase
($\alpha\beta$)₈ Barrel Superfold from
Phillips *et al.* occurs in
~5% of all proteins



Enolase Superfamily



PDB40 **Symposium**

October 28 - 30, 2011
Cold Spring Harbor Laboratory

**Come celebrate four
decades of innovation in
structural biology**

Speakers

- Cheryl Arrowsmith, University of Toronto, Canada
- David Baker, University of Washington
- Ad Bax, NIH/DHHS/NIDDK/LCP
- Axel Brunger, Stanford University/HHMI
- Stephen K. Burley, Eli Lilly & Co.
- Wah Chiu, Baylor College of Medicine
- Johann Deisenhofer, UT Southwestern Medical Center
- Angela Gronenborn, University of Pittsburgh
- Richard Henderson, MRC Lab. of Molecular Biology
- Wayne Hendrickson, Columbia University
- Mei Hong, Iowa State University
- Brian Matthews, University of Oregon
- Jane Richardson, Duke University Medical Center
- Michael Rossmann, Purdue University
- Andrej Sali, University of California, San Francisco
- David Searls, Independent Consultant
- Susan Taylor, University of California, San Diego
- Janet Thornton, EMBL EBI, Hinxton
- Soichi Wakatsuki, IMMS-KEK
- Kurt Wüthrich, The Scripps Research Institute, ETH Zürich

meetings.cshl.edu/meetings/pdb40.shtml