

Published quarterly by the
Research Collaboratory for Structural Bioinformatics Protein Data Bank

NEWSLETTER



www.pdb.org • info@rcsb.org

Weekly RCSB PDB news is available online at www.pdb.org

Contents

MESSAGE FROM THE RCSB PDB 1

DATA DEPOSITION AND ANNOTATION

Deposition Statistics 2

wwPDB News 2

Validate Entries Before Deposition 2

DATA QUERY, REPORTING, AND ACCESS

Enhanced Sequence Display 3

Browse the PDB by GO Terms, EC Number,
 Source Organism, and More 3

Build Complex Queries with *Advanced Search* .. 4

Website Statistics 4

OUTREACH AND EDUCATION

Explore a Structural View of Biology

Using PDB-101 4

Meetings and Events 5

New Publications 5

Narrated RCSB PDB Tutorial Updated 6

Congratulations to Science Olympiad
 Protein Modeling National Champions 6

EDUCATION CORNER by Brandon Bryn, AAAS
*New Report Proposes Historic Renovation of
 Undergraduate Biology Education
 in the United States* 6

REFERENCES 7

**RCSB PDB PARTNERS, MANAGEMENT,
 AND STATEMENT OF SUPPORT** 8

SNAPSHOT: JULY 1, 2011

74,140 released atomic coordinate entries

ENTRIES BY MOLECULE TYPE		ENTRIES BY EXPERIMENTAL TECHNIQUE	
68,651	proteins, peptides, and viruses	64,633	X-ray
3,185	protein/nucleic acid complexes	8,945	NMR
2,265	nucleic acids	371	electron microscopy
39	other	36	hybrid
		155	other

RELATED EXPERIMENTAL DATA FILES

54,054	structure factors
6,245	NMR restraints
93	NMR chemical shifts

PDB 40

**Special Anniversary at the
 Cold Spring Harbor Laboratory
 October 28-30, 2011**

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

Program

This special event will begin with an evening reception, dinner, and oral session on Friday, October 28th and conclude with lunch on Sunday, October 30, 2011.

Presentations by our distinguished speakers will include:

- Cheryl Arrowsmith *Structural and chemical biology of the readers and writers of the histone code*
- David Baker *Prediction and design of macromolecular structures, functions, and interactions*
- Ad Bax *An NMR view of the interaction between viral fusion proteins and phospholipids*
- Axel Brunger *Challenges for structure determination at low resolution*
- Stephen K. Burley *Growth, globalization, and future of the PDB*
- Wah Chiu *CryoEM of molecular machines*
- Angela Gronenborn *Synergy between NMR and CryoEM: Novel findings for HIV capsid function*
- Richard Henderson *What is needed to make single particle electron cryomicroscopy reach its true potential*
- Wayne Hendrickson *SLAC1 and the splendor of atomic resolution*
- Mei Hong *Membrane protein solid-state NMR: Elucidating the influenza M2 structure and mechanism*
- So Iwata *Overcoming challenges of membrane protein crystallography*
- Louise Johnson *Structural biology: From early days to the present and possibilities for the future*
- T. Alwyn Jones *Model building man; an endangered species*
- Brian Matthews *Protein crystallography: Getting in on the ground floor*
- Jane Richardson *Studying and polishing the PDB's macromolecules*
- Michael Rossmann *The PDB: A historical perspective*
- Andrej Sali *Determining architectures of macromolecular assemblies by aligning interaction networks to electron microscopy density maps*
- David Searls *Macromolecular linguistics*
- Susan Taylor *Evolution of protein kinases: Insights from the structural kinome*
- Janet Thornton *Abstracting knowledge from protein structures for biology in the 21st century*
- Soichi Wakatsuki *Coevolution of synchrotron radiation technologies with protein X-ray crystallography*
- Kurt Wüthrich *Structural biology by NMR and the PDB*

Pricing

Regular packages (Registration with housing, \$550) are all inclusive and cover registration, food, and housing. Registration without housing packages (\$350) include registration and food, but not housing.

The maximum number of participants is 350. Early registration is strongly encouraged as the meeting is expected to fill quickly.

Posters

The meeting will also host a session of poster presentations. To submit your abstract for consideration, please submit online following the link provided after registration.

Travel Awards

Limited funds are available to help students and early career scientists attend PDB40. Application information is available online.



Complete meeting details and registration information:
meetings.cshl.edu/meetings/pdb40.shtml



This newsletter is printed on recycled paper

Data Deposition and Annotation

Deposition Statistics

From April 1-June 30, 2011, 2336 experimentally-determined structures were deposited to the PDB archive. The entries were processed and annotated by wwPDB teams at the RCSB PDB, PDBe, and PDBj. 4542 have been deposited overall in 2011.

Of the structures deposited in the first half of 2011, 79.8% were deposited with a release status of "hold until publication"; 17.8% were released as soon as annotation of the entry was complete; and 2.4% were held until a particular date. 92.8% of these entries were determined by X-ray crystallographic methods; 92.8% were determined by NMR methods.

From April - June, 2068 structures were released in the PDB, with a total of 3973 structures released so far in 2011.



PDB Archive Version 4.0 to be Released July 13, 2011

As announced previously, the wwPDB has performed an ambitious review of the PDB archive resulting in a new set of corrected files that follow the PDB Exchange Dictionary v.4.0. These files will be released on July 13, 2011.

The review involved remediating complex problems, including the representation of biological assemblies, residual B factors, peptide inhibitors and antibiotics, and entries in nonstandard crystal frames. A description of the review and resulting changes and corrections is available as a PDF from the wwPDB website (wwpdb.org). Versioning and revision logs will be introduced with this release.

For PDB format files, only the entries that have been changed during this remediation will be updated (<17000). These changes will be identified as version 3.3 of the PDB file format. All files in PDBx/mmCIF and PDBML/XML formats will be updated to reflect the new schema updates. Any changes made to the data will be recorded in the PDBX_VERSION data category and a revision log made for this release that will be available from the wwPDB FTP site.

From July 13, 2011 onward, all new releases and modified entries released will follow the updated formats (PDBx/PDBML v 4.0 and PDB File Format 3.3). Revisions to released entries will be tracked and numbered in the PDBx/mmCIF formatted files.

Users who maintain local copies of the wwPDB FTP can download the new files via rsync (see www.wwpdb.org/downloads.html for more).

A time-stamped snapshot of the PDB archive before this release will be available from <ftp://snapshots.wwpdb.org/>.

Validate Entries Before Deposition

Depositors are encouraged to run data validation checks to monitor improvements made to structural models before deposition.

The RCSB PDB's online Validation Server (validate.rcsb.org) can be used to create validation reports outside of the deposition pipeline. Two options are available:

- In the plain text report option, the server first checks the format consistency of the coordinates in the PRECHECK step. The precheck will produce a brief report identifying any changes that need to be made in your data files in order to obtain a validation report. In the validation step, the server produces an Atlas entry, a summary report, and a collection of structural diagnostics including bond distance and angle comparisons, torsion angle comparisons, base morphology comparisons (for nucleic acids), and molecular graphic images. Reports from PROCHECK¹, NUCHECK², SFCheck³, and MolProbity⁴ are made available.
- A new PDF report option produces a report that contains high-level geometric and experimental checking results without listing the detailed geometry. This unofficial report is similar to the wwPDB's PDF report generated during the annotation process for depositors to include with their journal submissions.

The Validation Server is available from the RCSB PDB Deposition Services page at deposit.pdb.org.

The screenshot shows the 'Validation Server' interface. It includes a header with 'ADIT! Validation Server' and a sub-header 'Validation Tutorial | Possible Format Problems'. The main text says 'Generate Validation Reports to monitor improvements made to your structural model.' There are two options: 'Option 1: Validation Report with Detailed Geometry (Plain Text)' and 'NEW! Option 2: Validation Report with High-level Summary (PDF)'. Option 1 includes a 'Method:' dropdown set to 'X-ray' and a 'BEGIN' button. Option 2 includes fields for 'Upload coordinate file' and 'Upload structure factor file (X-ray only)', both with 'Browse...' buttons. It also has 'Select file type:' dropdowns for 'PDB', 'mmCIF', and 'mtz'. There are checkboxes for 'Select SF Validation Program(s) to include in report:' with options 'SFCHECK', 'REFMACS', and 'PHENIX'. A 'BEGIN' button is at the bottom right. A note at the bottom says 'When you are ready, use ADIT to deposit your entry. A Validation Report PDF that can be shared with journals will be sent to you after processing.'

The Validation Server (validate.rcsb.org)

Like the Worldwide PDB on facebook

The image shows a Facebook post from 'Worldwide PDB'. The post features a large graphic for the 'PDB40 Symposium' held from October 29-30, 2011, at Cold Spring Harbor Laboratory. The graphic includes the text 'PROTEIN DATA BANK' and 'BIOSE'. To the right of the graphic is a 'Like' button and the word 'Organization'. Below the graphic is a collage of various protein structures and scientific diagrams.

Data Query, Reporting, and Access

Enhanced Sequence Display

From each *Structure Summary* page, the **sequence** tab offers a diagram representation of the sequence. Each macromolecule chain can be annotated with domain assignments, secondary structure, and structural features such sites defined in the structure entry (*i.e.*, binding sites of ligands) and protein modifications (*i.e.*, posttranslational modifications). These annotations can be mapped on to the 3D view of the entry (jmol.sourceforge.net) for further exploration.

Chain A : PROTEIN (FERREDOXIN)

FASTA | Sequence & DSSP | Image

Polymer 1
Length: 106 residues
Chain Type: polypeptide(L)
Reference: UniProtKB P00214

Annotations

Add Annotations
Select

Domain Assignment: SCOP **d1b0va** Ferredoxin: 106 residues
[hide] [reference]

Secondary Structure: DSSP 33% helical (8 helices; 35 residues)
15% beta sheet (6 strands; 16 residues)
[hide] [reference]

Structural Feature: Protein Modification
0020 tris-L-cysteinylyl triiron tetrasulfide (3Fe-4S, iron-sulfur protein, metalloprotein)
RESID: AA0139 PSI-MOD: MOD:00148
0024 tetrakis-L-cysteinylyl tetrairon tetrasulfide (4Fe-4S, iron-sulfur protein, metalloprotein)
RESID: AA0140 PSI-MOD: MOD:00149

Protein Modification Legend

 tris-L-cysteinylyl triiron tetrasulfide (3Fe-4S, iron-sulfur protein, metalloprotein)
 tetrakis-L-cysteinylyl tetrairon tetrasulfide (4Fe-4S, iron-sulfur protein, metalloprotein)

Protein modifications mapped onto the sequence diagram and Jmol view of ferredoxin (PDB entry 1b0v)

The current list of annotations includes:

- SCOP: domain annotations
- CATH: domain annotations
- Domain Parser (DP): domain annotations processed with the DP algorithm
- Protein Domain Parser (PDP): domain annotations processed with the PDP algorithm
- Pfam: regions with Pfam annotations
- Interpro: regions with Interpro annotations
- DSSP: secondary structure assignment
- STRIDE: secondary structure assignment
- Author Sec. Struc: secondary structure assignment as provided by the entry's author
- **NEW** Protein Modification: protein modifications as detected with software
- **NEW** Site Record: author assigned and software-detected binding sites
- **NEW** Single Nucleotide Polymorphism (SNP): data from the LS-SNP database

Using the Display Parameters box, users can toggle between the display of unique chains and all chains. By default, only unique chains are displayed. This box can also toggle the display of the UniProtKB reference sequence.

Browse the PDB by GO Terms, EC Number, Source Organism, and More

Use the *Browse Database* option to explore the PDB archive using different hierarchical trees. Browsers are available to search for related terms and structures based upon the following classifications:

- Trees for **Biological Process**, **Cellular Component**, and **Molecular Function** are organized using the Gene Ontology Consortium's descriptions for gene products (GO, www.geneontology.org). PDB IDs and corresponding chain IDs have been mapped to GO terms by the SIFTS (pdbe.org/sifts) initiative.
- **Enzyme Commission** numbers. Search for enzymes by term or by partial or full EC number.
- **Membrane Transport proteins** organized using Transporter Classification (TC) Database system (www.tcdb.org)
- **Source Organism**, using organisms found in the NCBI Taxonomy database (www.ncbi.nlm.nih.gov/Taxonomy/taxonomyhome.html). These organisms are the source of the individual naturally-occurring polypeptides. The PDB source organism assignment is based on author/UniProtKB-specified mapping of polypeptides.
- **Genome Location** of various organisms. The genomes represented are a subset of the genomes in the NCBI genome database and whose curated sequences for genetic loci are archived at Entrez Gene (www.ncbi.nlm.nih.gov/gene). The top level in the hierarchy is the organism's genome. Each genome expands into chromosomes, which in turn expand into a list of loci on the chromosomes. Each locus is a link to retrieve structures associated with that locus.
- The **MeSH** terms used to classify publications indexed by the National Library of Medicine, and that appear in the entry's related PubMed abstract (Medical Subject Headings, www.ncbi.nlm.nih.gov/mesh).
- **SCOP** description of evolutionary and functional relationships from the Structural Classification of Proteins (scop.mrc-lmb.cam.ac.uk/scop).
- **CATH** clustering of proteins at 4 major levels from CATH: Protein Structure Classification (www.cathdb.info).

The *Browse Database* feature can be accessed under the Search widget in the left-hand menu. Each tab links to a different browser.

Transporter Classification Browser

Browse membrane transport proteins in the PDB archive using the Transporter Classification (TC) system from the Transporter Classification Database (www.tcdb.org).

Here you can **browse** the TCDB superfamilies, **view** the number of associated PDB structures, and **search** for the specific associated structures.

sodium

Find in Tree Next Previous

- 1: Channels/Pores
- 2: Electrochemical Potential-driven Transporters
 - 2.A: Porters (uniporters, symporters, antiporters)
 - 2.A.1: The Major Facilitator Superfamily (MFS)
 - 2.A.21: The Solute:Sodium Symporter (SSS) Family
 - 2.A.22: The Neurotransmitter:Sodium Symporter (NSS) Family
 - 2.A.23: The Dicarboxylate/Amino Acid:Cation (Na⁺ or H⁺) Symporter (DAACS) Family
 - 2.A.31: The Anion Exchanger (AE) Family
 - 2.A.33: The NhaA Na⁺:H⁺ Antiporter (NhaA) Family
 - 2.A.37: The Monovalent Cation:Proton Antiporter-2 (CPA2) Family
 - 2.A.38: The K⁺ Transporter (Trk) Family
 - 2.A.3: The Amino Acid-Polyamine-Organocation (APC) Family
 - 2.A.49: The Chloride Carrier/Channel (ClC) Family
 - 2.A.4: The Cation Diffusion Facilitator (CDF) Family
 - 2.A.56: The Tripartite ATP-independent Periplasmic Transporter (TRAP-T) Family
 - 2.A.57: The Equilibrative Nucleoside Transporter (ENT) Family
 - 2.A.6: The Resistance-Nodulation-Cell Division (RND) Superfamily
 - 2.A.7: The Drug/Metabolite Transporter (DMT) Superfamily
 - 2.A.9: The Cytochrome Oxidase Biogenesis (Oxa1) Family
 - 2.C: Ion-gradient-driven energizers
 - 3: Primary Active Transporters

Use the Transporter Classification Browser to find PDB's membrane transport proteins as organized by TC Database family (www.tcdb.org). The browser will autocomplete search terms with the matching classifications, and highlight locations on the tree.

Build Complex Queries with *Advanced Search*

Advanced Search provides the capability of combining multiple searches of specific types of data in a logical AND or OR. The result is a list of structures that comply with ALL or ANY of the search criteria, respectively.

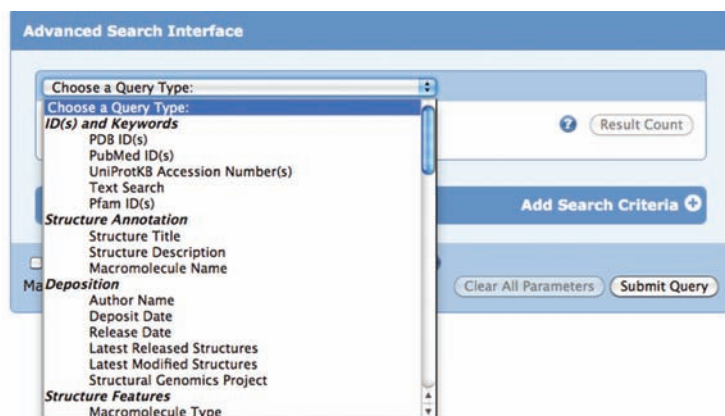
Individual data items are organized by category; contextual help and examples are available by selecting the question mark icon. Recently added items include protein modifications, Pfam ID, and EM structures with experimental data.

Currently, users can build searches based on:

- **ID(s) and Keywords:** PDB, PubMed, UniProtKB, Pfam IDs; text searching
- **Structure Annotation:** Structure title, description; and macromolecule name
- **Deposition:** Author name; Deposit Date; Release Date; Latest Released Structures; Latest Modified Structures; Structural Genomics Project
- **Structure Features:** Macromolecule Type; Number of Chains (asymmetric unit or biological assembly), entities; Models, and Disulfide Bonds; Molecular Weight; Secondary Structure Content; secondary structure length; SCOP, CATH, taxonomy
- **Sequence Features:** sequence; translated nucleotide sequence; sequence motif; chain length; protein modifications; genome location
- **Chemical Components:** name; ID; InChi descriptor; SMILES/SMARTS; molecular weight; chemical formula; binding affinity; has ligands; has modified residues
- **Biology:** Source; expression organism; Enzyme Classification; biological process; cell component; molecular function; Transporter Classification
- **Methods:** experimental method; X-ray resolution, R factor, diffraction source, reflections, cell dimensions, software, space group, crystal properties, detector; EM assembly
- **Publication:** citation; MeSH terms; PubMed abstract
- **Misc:** Has external links

The number of entries matching each individual query can be shown before running the full *Advanced Search*. Searches can be filtered by removing sequence similarity.

Queries built using *Advanced Search* can be stored in MyPDB to be run or modified at any time.



Combine different searches together to find structures and refine search results with *Advanced Search*. New queryable options include protein modifications, Pfam ID, and EM structures with experimental data.

Website Statistics

Access statistics for the second quarter of 2011 are shown.

Month	Unique Visitors	Number of Visits	Bandwidth
APRIL	230825	557911	763.04 GB
MAY	233123	561880	814.08 GB
JUNE	206456	507798	620.89 GB

Outreach and Education

Explore a Structural View of Biology Using PDB-101

PDB-101 is a new and unique view of the RCSB PDB that places educational materials front and center. It packages together the resources of interest to teachers, students, and the general public to promote exploration in the world of proteins and nucleic acids.

Clicking on the blackboard PDB-101 logo (or its related widget in the left-hand menu) reveals the education-centered website. This view offers easy navigation: select any *Molecule of the Month* article from the top bar menu or mouse over the PDB-101 pull-down to jump to other sections of PDB-101.



Click on the PDB-101 logo to access the education view; click on the blue logo in the top left at any time to access the main RCSB PDB website.

This initial release of PDB-101 offers:

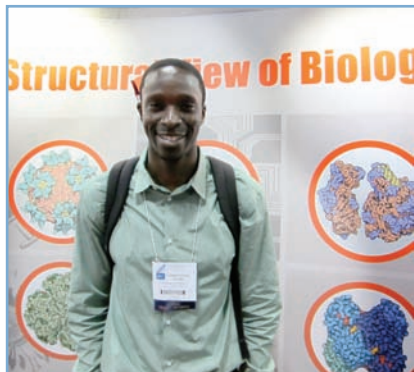
- **Structural View of Biology.** Built around the *Molecule of the Month* series, this feature promotes a top-down exploration of the PDB. Beginning with high-level functional categories, readers can browse through descriptive subcategories to access relevant articles that describe molecules in simple terms and access the related PDB entries. Mouseovers, pulldown menus, and carousels all offer easy navigational tools to promote learning.
- **Molecule of the Month series.** Since 2000, the RCSB PDB has published articles that describe the structure and function of a molecule along with interactive views, discussion topics, and links to structure examples. The collection of featured articles provides an annotated view of the PDB archive. With PDB-101, all *Molecule of the Month* issues appear on single pages, with links to printable PDF versions and downloadable high resolution images. They can be accessed through the pulldown menu in the top bar, the Structural View of Biology, and by archives organized by title, date, and category.
- Related **Educational Resources** and materials, including posters, animations, and classroom lessons and activities.

- **Understanding PDB Data**, a reference to help explore and interpret individual PDB entries. Broad topics include how to understand PDB data, how to visualize structures, how to read coordinate files, and potential challenges to exploring the archive.

PDB-101 will continue to be developed; we welcome your comments and suggestions.

To link directly to this view, use www.pdb.org/pdb-101.

Meetings and Events



At Experimental Biology, the RCSB PDB met with many users, including depositor Christopher Davies (Purdue University).

At the Experimental Biology meeting (April 9-13, Washington DC), the RCSB PDB met with researchers and educators at the exhibit booth. Attendees, particularly from the American Society for Biochemistry and Molecular Biology, were interested in the searching and reporting features of the RCSB PDB website.

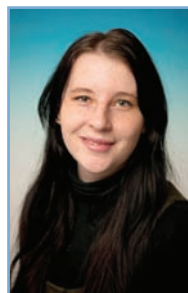
Rutgers Day, a full day of discovery and lively activities that showcase the varied resources, departments, and people at the university, was held April 30. The RCSB PDB was part of the Department of Chemistry & Chemical Biology's *Bonding With Chemistry* booth. Visitors of all ages built 3D DNA and virus structure models next to experiments and demonstrations of how chemistry impacts our lives.



Molecule building at Rutgers Day

The 2011 Meeting of the **American Crystallographic Association** (May 28-June 2, New Orleans, LA) was an active meeting. At the exhibition booth, visitors learned about new features such as the Validation Server, PDB-101, the wwPDB Common Tool for Deposition and Annotation, and much more. Director Helen Berman presented *Putting the data in data mining: Curating the PDB archive* as part of the *Use of Databases in Structural Biology* session. Lead annotator Jasmine Young described *The wwPDB Common*

Annotation and Deposition Tool Development in a poster presentation, and the RCSB PDB Poster Prize for best student poster presentation involving macromolecular crystallography was awarded.



At ACA, the RCSB PDB Poster Prize was awarded to **Briony Yorke** for *New Approaches to Time-Resolved Structural Studies of Macromolecules*. Briony Yorke¹, Arwen Pearson¹, Mike Webb¹, Robin Owen.² (¹The University of Leeds, Leeds, UK ²Diamond Light Source Ltd, Didcot, UK). Briony will receive a subscription to *Science* and a copy of *The International Tables of Crystallography Volume F*. Many thanks to the judges: Thomas Edwards (Emerald BioStructures), Katrina Forest (University of Wisconsin-Madison), and John Rose (The University of Georgia), and to Marcia Colquhoun and the ACA. The prize will also be awarded at the upcoming ISMB and IUCr meetings.

Future meetings include:

- **ISMB/ECCB**: At the 19th Annual International Conference on Intelligent Systems for Molecular Biology and 10th European Conference on Computational Biology (July 15-19; Vienna, Austria), Senior Scientist Andreas Prlic will describe *A Census of Internal Pseudo-Symmetries and Similarities in Protein Domains* at the Laptop/Poster session at 3DSig satellite meeting. Scientific Lead Peter Rose will help users Become an Expert User of the RCSB Protein Data Bank Website and Web Services at the Technology Track session on Monday, July 18 at 2:30 p.m.
- **Protein Society**: *The PDB at 40: Past, Present, and Future* will be discussed by Annotator Ezra Peisach during the poster presentations at this meeting (July 23-27; Boston, MA).
- **IUCr**: The XXII General Assembly and Congress of the International Union of Crystallography will be held August 22-30 in Madrid, Spain. Planned events include: a joint-wwPDB stand in the exhibition hall; a presentation on *The wwPDB and Future Perspectives in Sharing Macromolecular Structure Data* in the session on *Developments and directions for crystallographic databases* (Wednesday, August 24); an afternoon wwPDB Q&A session (Thursday, August 25); a discussion on *Validation of small molecule and macromolecular X-ray structures. What are the differences and how can we learn from each other?* by members of PDBe, CCDC, and RCSB PDB (Friday, August 26); and an introduction to *The wwPDB Working Format: A Simplified Application of CIF Technology* (Monday, August 29).
- **PDB 40**: Special symposium celebrating four decades of innovation in structural biology to be held October 28-30 at Cold Spring Harbor Laboratory. Early registration is strongly encouraged as the meeting is expected to fill quickly (meetings.cshl.edu/meetings/pdb40.shtml).

New Publications

The RCSB Protein Data Bank: site functionality and bioinformatics use cases (2011) *NCI-Nature Pathway Interaction Database Bioinformatics Primer* doi: [10.1038/pid.2011.1](https://doi.org/10.1038/pid.2011.1)

Miniseries: Illustrating the machinery of life: Eukaryotic cell panorama (2011) *Biochem Mol Biol Educ.* 39:91-101 doi:[10.1002/bmb.20494](https://doi.org/10.1002/bmb.20494)

The evolution of the RCSB Protein Data Bank website (2011) *WIREs Computational Molecular Science* doi:[10.1002/wcms.57](https://doi.org/10.1002/wcms.57)

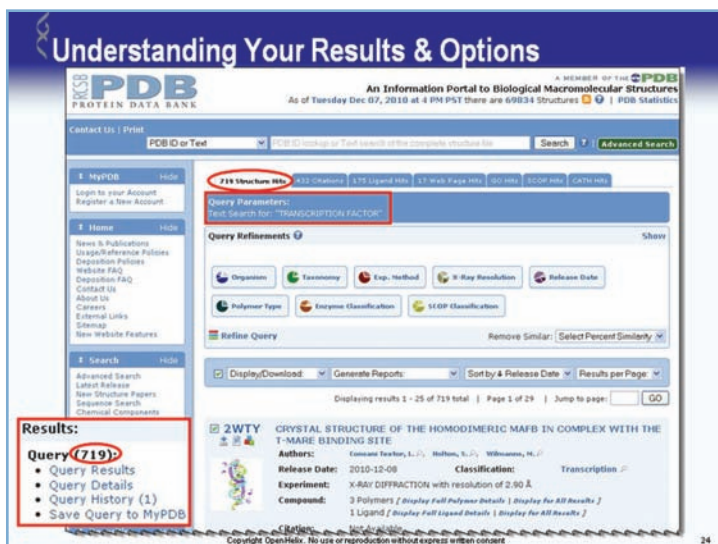
Narrated RCSB PDB Tutorial Updated

A comprehensive suite of RCSB PDB training materials is available at openhelix.com.

The updated training tools reflect many recent enhancements to the RCSB PDB site, including the data drill-down and data summary feature, updated ligand features such as a download page, images and binding affinity data, and new report types and visualization options.

The full tutorial runs for about an hour. Users can jump to any chapter: Introduction, Basic Searching & Browsing, Result Options, Structure Summary Page, Advanced Searching, Tools & Education, Summary, or Exercises.

The PowerPoint slides used as a basis for the tutorial, the suggested script for the slides, slide handouts, and exercises are all freely available for download and use as classroom content.



The narrated tutorial demonstrates and highlights how to use the tools found at www.pdb.org.

Congratulations to Science Olympiad Protein Modeling Champions

The National Science Olympiad Tournament was held May 20-21 at the University of Wisconsin at Madison.

Teams brought their A-game and some amazing prebuild models to the protein modeling competition.

The top scoring teams in this event were:

- 1) Liberal Arts and Science Academy (TX)
- 2) West Windsor-Plainsboro High School South (NJ)
- 3) Fairfax High School (VA)



The first place team from Liberal Arts and Science Academy received their award from Fred Berry, the VP of Academics at the Milwaukee School of Engineering.

Protein modeling will be offered as a 2012 event in the Science Olympiad; then it will be on hiatus from the tournament for two years as other events are incorporated. This event is managed by the MSOE Center for BioMolecular Modeling and hosted in NJ by the RCSB PDB. For protein modeling tips and news of interest to students and educators, follow us on [twitter@buildmodels](https://twitter.com/buildmodels).

Education Corner by Brandon Bryn, AAAS

New Report Proposes Historic Renovation of Undergraduate Biology Education in the United States

Traditional biology has experienced a renaissance in recent years, widening its reach to include newly pioneered disciplines such as genomics, proteomics, synthetic biology and systems biology. Yet, over the years, the fine art of undergraduate biology education has remained largely unchanged.

Now, after years of collaboration among biology students, professors, and researchers, the National Science Foundation (NSF), AAAS, and their partners have released *Vision and Change in Undergraduate Biology Education: A Call to Action* to chart a course for bringing more

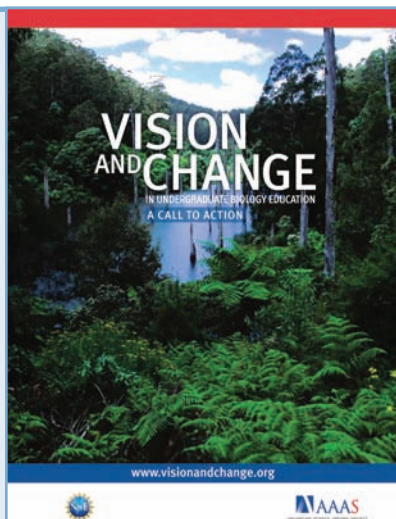
contemporary, multi-disciplinary instruction into undergraduate biology classrooms. For those concerned about—or directly involved with—the current state of biology education, this new report represents a significant step toward modernizing the ways that biological sciences are taught in universities across the United States.

“The publication of *Visions and Change* is a start,” said Bruce Alberts, the editor-in-chief of the journal *Science*. “It’s now time for action.”

“This report presents a blueprint for change,” added Judith Verbeke,

Reprinted with permission from the American Association for the Advancement of Science. This article is available from www.aaas.org/news/releases/2011/0223vision_change.shtml.

The full report *Vision and Change in Undergraduate Biology Education: A Call to Action*, can be accessed from visionandchange.org/finalreport



acting director of the Division of Biological Infrastructure at NSF. "We now need to work together to translate this vision into the changes necessary to effect a true transformation of undergraduate biology education."

The report, a comprehensive call to action, was released to the public on Saturday 19 February at the AAAS Annual Meeting in Washington, D.C. Yolanda George, deputy director of AAAS Education and Human Resources, organized the event and Alberts, a longtime advocate of science education, was there to discuss the report with faculty, reporters and policy-makers.

With funding from the NSF and support from the Howard Hughes Medical Institute and the National Institute of General Medical Sciences, AAAS led the effort to consult with top education experts, faculty members and students to develop the report. Across the board, there were serious concerns that biology education has become disconnected from the science as it's being practiced in the 21st century.

Undergraduate biology students have made it clear in focus groups that they are looking for relevance in their classrooms and labs. They want to be challenged, and they want to participate in real-world research that combines various disciplines.

With that in mind, the architects of *Vision and Change in Undergraduate Biology Education* set out to plot a strategy that would transform undergraduate biology education in America into a system that integrates the scientific process into all courses and provides student majors and non-majors with authentic research experiences and faculty members with a community of scholars to network with.

"Perhaps one of the most telling reflections of this report is the identi-

ty of science education as an active and growing discipline in its own right," said Cynthia Bauerle, senior program officer in Precollege and Undergraduate Education at Howard Hughes Medical Institute.

The infusion of science and technology into peoples' everyday lives, along with the emergence of novel interdisciplinary fields, has changed the way we view the world and made it clear that a transformation in biology education is necessary. Scientific leaps and bounds promise to open up a new world of opportunities and practical applications, including medical advances, alternative energy sources and fresh understandings of the behavioral and social sciences—in some cases, the moral and social tensions related to such advances as well. But to be ready for this changing landscape, undergraduate students need to be prepared to understand them and engage with them, even those who do not plan to become scientists.

The seeds of the Vision and Change report were sown in 2006, when the NSF education and biology directorates recognized the need within the biology community to discuss a shared vision for undergraduate biology education and the changes needed to achieve that vision. In 2007, AAAS coordinated a series of seven conversations across the country with prominent biology educators, administrators and stakeholders to seek direction on how to improve undergraduate biology instruction.

In 2009, a follow-up Vision and Change in Undergraduate Biology Education Conference in Washington, D.C., attracted more than 500 faculty, administrators, and students who continued that dialogue from the conversations and honed in on specific action items and practices that could make laboratory and classroom instruction more engaging. That same year, a group of 231 undergraduate students participated in focus groups that revealed their needs for biology education in the 21st Century.

According to Carol Brewer, former associate dean and emeritus professor of biology at the University of Montana and co-chair of the *Vision and Change* Advisory Board, the main goal of the convention was to be sure "that the science we are teaching is the same science we are doing."

The fruits of their labor are now available in the *Vision and Change* report—although publication of this report only represents the second-to-last step on the road to a modernized biology education in America. Implementing *Vision and Change* in educational practice and programs still remains a challenging task on the horizon.

To start, the report will be distributed to all who participated in the 2007 conversations or the 2009 conference, as well as to a host of grantees, provosts, deans, and biology department chairs across the country. Planning for a 2012 in Undergraduate Biology Education Conference is also already underway, focused on bringing the report into classrooms and labs across the nation.

References

1. R.A. Laskowski, M.W. McArthur, D.S. Moss, J.M. Thornton (1993) *J. Appl. Cryst.* 265:283-291.
2. Z. Feng, J. Westbrook, H.M. Berman (1998) NUCheck. NDB-407 Rutgers University, New Brunswick, NJ.
3. A.A. Vaguine, J. Richelle, S.J. Wodak (1999) *Acta Crystallogr.* D55:191-205.
4. S.C. Lovell, I.W. Davis, B.W. Arendall, P.I.W. de Bakker, J.M. Word, M.G. Prisant, J.S. Richardson, D.C. Richardson (2003) *Protein Struct. Funct. Genet.* 50:437-450.
5. K. Chen, G.J. Tilley, V. Sridhar, G.S.Prasad, C.D.Stout, F.A.Armstrong, B.K Burgess (1999) Alteration of the reduction potential of the [4Fe-4S](2+/+) cluster of *Azotobacter vinelandii* ferredoxin I. *J.Biol.Chem.* 274:36479-36487

RCSB PDB Partners

The RCSB PDB is managed by two partner sites of the Research Collaboratory for Structural Bioinformatics:



Rutgers, The State University of New Jersey
 Department of Chemistry and
 Chemical Biology
 610 Taylor Road
 Piscataway, NJ 08854-8087



San Diego Supercomputer Center and the Skaggs
 School of Pharmacy and Pharmaceutical Sciences
 University of California, San Diego
 9500 Gilman Drive
 La Jolla, CA 92093-0537



The RCSB PDB is a member of the
 Worldwide Protein Data Bank
 (www.wwpdb.org)

RCSB PDB Management

DR. HELEN M. BERMAN, Director
 Rutgers, The State University of New Jersey
berman@rcsb.rutgers.edu

DR. MARTHA QUESADA, Deputy Director
 Rutgers, The State University of New Jersey
mquesada@rcsb.rutgers.edu

DR. PHILIP E. BOURNE, Associate Director
 San Diego Supercomputer Center and the Skaggs School of
 Pharmacy and Pharmaceutical Sciences,
 University of California, San Diego
bourne@sdsc.edu

A list of current RCSB PDB Team Members is available from
www.pdb.org.

STATEMENT OF SUPPORT: *The RCSB PDB is supported by funds from the National Science Foundation, the National Institute of General Medical Sciences, the Office of Science, Department of Energy, the National Library of Medicine, the National Cancer Institute, the National Institute of Neurological Disorders and Stroke, and the National Institute of Diabetes & Digestive & Kidney Diseases.*