

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

# NEWSLETTER



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Weekly RCSB PDB news is available online at [www.pdb.org](http://www.pdb.org)

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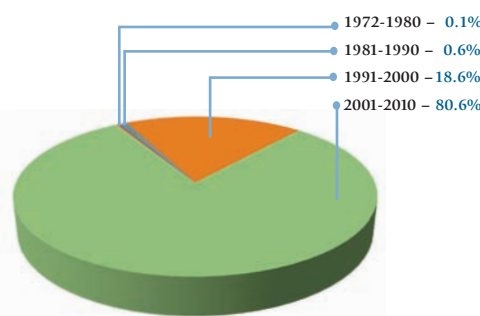
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## Message from the RCSB PDB

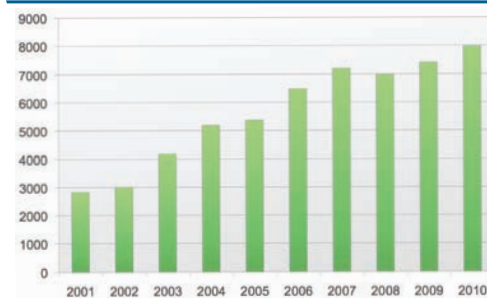
### From 7 to 70,000: The PDB Reaches a New Milestone

Entries released in the PDB by decade



56628 structures were released between 2001 and 2010.

Number of structures released per year (2001-2010)



Deposition and release statistics are available at [wwpdb.org](http://wwpdb.org).

As the year 2010 drew to a close, the number of biomacromolecular structures available in the Protein Data Bank (PDB) archive exceeded 70,000. The PDB archive has nearly tripled in size since the wwPDB was formed in 2003.

Today, the wwPDB receives approximately 25 new experimentally-determined structures from scientists each day for inclusion in the archive. In 2010, more than 260 million data files were downloaded or viewed online from wwPDB member sites. Users include structural biologists, computational biologists, biochemists, and molecular biologists in academia, government, and industry. Data are also used by educators and students furthering their understanding of biology.

Other wwPDB highlights from 2010 include the provision of Validation Report PDFs to depositors and the requirement of chemical shift data for NMR depositions. wwPDB members have also recently published papers that describe resources available from member sites.<sup>1-3</sup> wwPDB news and announcements are posted at [wwpdb.org](http://wwpdb.org) and available via RSS feed.

## SNAPSHOT: JANUARY 1, 2011

70,231 released atomic coordinate entries

ENTRIES BY MOLECULE TYPE		ENTRIES BY EXPERIMENTAL TECHNIQUE	
64,995	proteins, peptides, and viruses	61,011	X-ray
2,990	protein/nucleic acid complexes	8,702	NMR
2,208	nucleic acids	339	electron microscopy
38	other	29	hybrid
		150	other

## RELATED EXPERIMENTAL DATA FILES

50,414	structure factors
5,998	NMR restraints
1	NMR chemical shift

wwPDB organizations host PDB data deposition, processing, and distribution centers. wwPDB members are the RCSB PDB (USA), PDBe (UK), PDBj (Japan), and BMRB (USA).



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## Data Deposition and Annotation

### Deposition Statistics

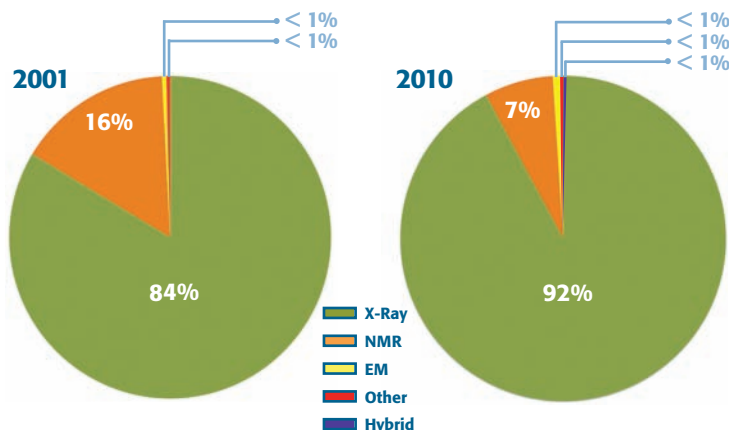
In the fourth quarter of 2010, 2123 experimentally-determined structures were deposited to the PDB archive for a total of 8865 entries deposited in the year.

Of the structures deposited in 2010, 77.0% were deposited with a release status of "hold until publication"; 19.2% were released as soon as annotation of the entry was complete; and 3.8% were held until a particular date.

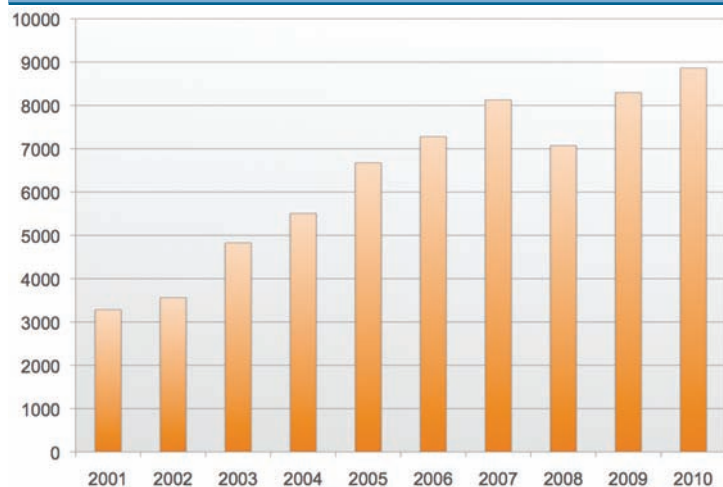
92.3% of these entries were determined by X-ray crystallographic methods; 6.8% were determined by NMR methods.

7,971 structures were released in the PDB archive in 2010. They account for 11% of the current total holdings of 70,231 entries.

Experimental type of entries deposited in the years 2001 and 2010

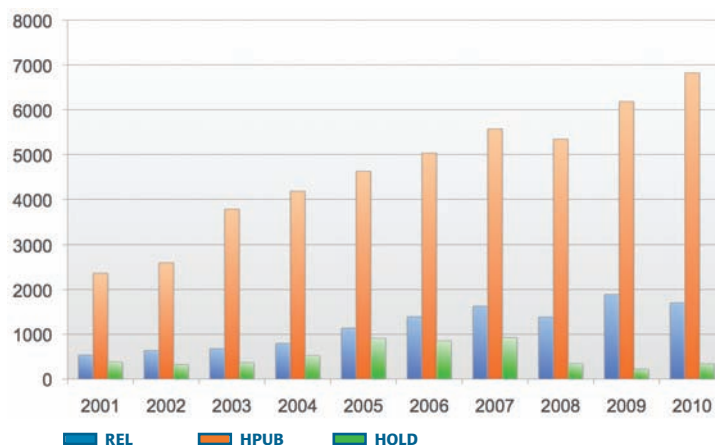


Number of entries deposited per year (2001 - 2010)



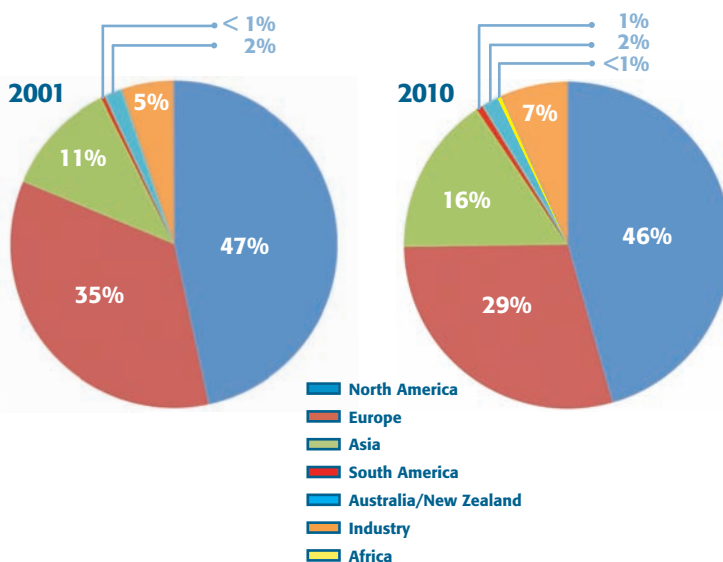
Deposited entries are processed and annotated by the wwPDB before release into the archive.

Release status for entries deposited in the years 2001 - 2010



Depending upon the hold status selected by the depositor, data release occurs when a depositor gives approval to the finalized entry (REL), the hold date has expired (HOLD), or the journal article describing the structure has been published (HPUB). A one-year limit on HOLD or HPUB was instituted in 2003.

Location of depositor for entries deposited in the years 2001 and 2010



### Deposition Session Restart IDs

Need more time to deposit an entry? ADIT 2.0 can email a restart ID to continue a deposition session at a later time.

Depositing a PDB entry can take place over a period of time using ADIT's "Session Restart ID" feature. Each deposition session has a single ID that can be emailed to the depositor and used to restart the session at a later date.

After initially uploading files, ADIT 2.0 runs checks for data format, validation, and sequence. On each of these pages, select "Click here to e-mail the session restart ID" to send an email containing the restart ID.

This identifier also appears in the title and the initial center panel of the ADIT editor window.

The unique case-sensitive restart ID, a combination of the date, time, computer IP, and session number, is generated automatically. It should be entered in the space provided on the ADIT home page to return to the deposition session. All entered data associated with a particular entry can be accessed using the restart ID until the "DEPOSIT NOW" button is selected, for up to six months after the session has been last updated.

## Data Query, Reporting, and Access

### 2010 Website Statistics

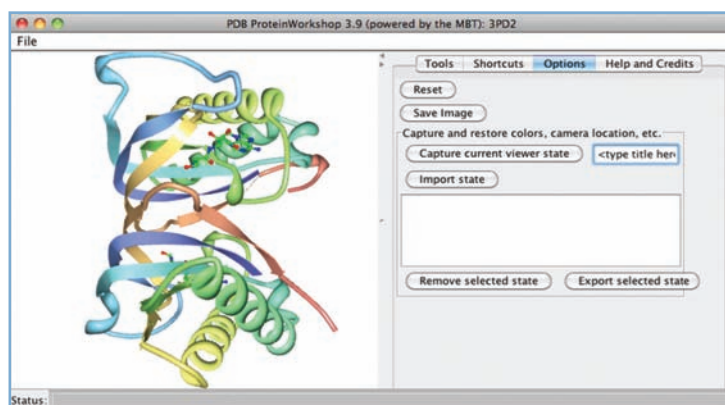
Month	Unique Visitors	Number of Visits	Bandwidth
JANUARY	176,655	422,065	755.87 GB
FEBRUARY	184,306	434,442	783.75 GB
MARCH	210,308	510,434	1,189.17 GB
APRIL	203,139	485,879	978.97 GB
MAY	199,620	473,973	1,058.45 GB
JUNE	174,582	429,274	869.39 GB
JULY	154,256	477,825	767.18 GB
AUGUST	159,350	396,199	783.32 GB
SEPTEMBER	201,919	477,825	1,344.88 GB
OCTOBER	235,083	556,548	1,434.02 GB
NOVEMBER	243,694	586,250	1,560.29 GB
DECEMBER	202,236	486,887	968.87 GB

## Latest Website Release

New and enhanced features were added to [www.pdb.org](http://www.pdb.org) at the beginning of December, including:

- **MyPDB storage of annotations.** Log in, view a *Structure Summary* page, and add a note about the entry in the *MyPDB Personal Annotations Widget*. That text will appear on that *Structure Summary* page, and on your MyPDB summary page of personal annotations, every time you log in.
- **Access to Transporter Classification information.** Browse membrane transport proteins in the PDB archive using the Transporter Classification (TC) system from the Transporter Classification Database ([www.tcdb.org](http://www.tcdb.org)).
- **Access to Structural Biology Knowledgebase data.** From an entry's *Structure Summary* page, users can see the related models, protein targets, biological annotations, clones, and more as provided by the SBKB ([sbkb.org](http://sbkb.org)).

For complete descriptions, see the *New Features Widget* on the RCSB PDB home page.



*Protein Workshop can be used to export high resolution images of structures. Shown: PDB ID 3pd2<sup>4</sup>*

## Binding Affinity Data Integration

Binding affinity data from BindingDB ([www.bindingdb.org](http://www.bindingdb.org)) and from BindingMOAD ([www.bindingmoad.org](http://www.bindingmoad.org)) have been integrated with the RCSB PDB website.

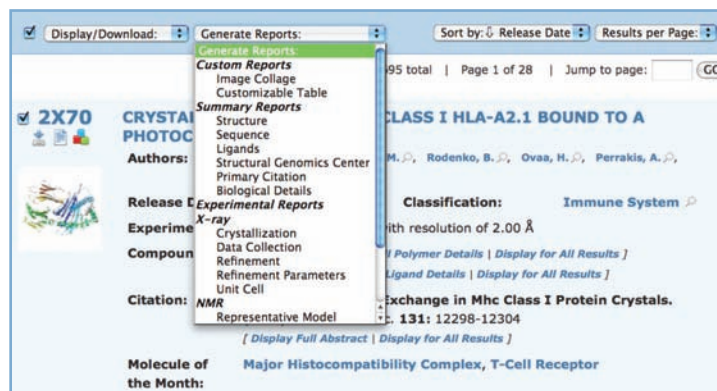
When available, binding constants and thermodynamic data will appear in the *External Ligand Annotations Widget* on *Structure Summary* pages and link to the corresponding external resource. If multiple experimental values are available for a measurement type, a range is listed.

External Ligand Annotations			Hide
Identifier	Binding Affinity data from BindingDB	Binding Affinity data from BindingMOAD	
117 Search Download	EC50: 2.5 nM IC50: 3.8 - 6.2 nM	IC50: 8 nM	

*The External Ligand Annotation Widget for PDB entry 1hwk<sup>5</sup>. Data in orange widgets on the RCSB PDB site are gathered from external resources.*

Users can search for PDB entries with particular binding affinity in these databases using a new *Advanced Search* option. Any available information from BindingDB and BindingMOAD can also be included in custom tabular reports.

## Creating Tabular Reports



*The Generate Reports pull-down menu. These reports offer convenient ways to view, export, and interact with query results.*

The *Generate Reports* pull-down menu on the *Structure Hits* tab offers different options for viewing a set of PDB entries. In addition to viewing a collage of structure images, users can create:

- A customized table of combinations of fields, including experimental, structural, and non-structural data; references to sequence databases (UniProtKB, Pfam), domain information (CATH, SCOP); literature (PubMed); and ontology terms (GO, MeSH)
- Pre-generated summary reports about structure, sequence, ligand, literature, and biological details
- Pre-generated experimental reports specific for X-ray or NMR structures

From the *Ligand Hits* tab, a report that includes the ligand ID, image, formula, molecular weight, name, SMILES, and the PDB IDs for the related entries can be created.

Once a report has been created, the interactive table interface can be used to sort the table; refine results using an online filter; show/hide/move columns; change the number of results shown per page; and resize the table itself. Tables can be exported into Excel and CSV formats.

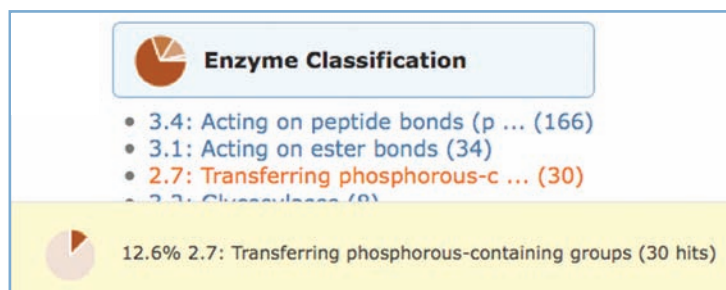


## New Data Distribution Summaries

RCSB PDB search results offer summary pie charts and summary links for standard characteristics of PDB entries that can be used to refine search results into subsets of interest. New charts for EC and SCOP classifications have been added to the list of available summary charts (resolution, release date, experimental method, polymer type, organism, taxonomy).

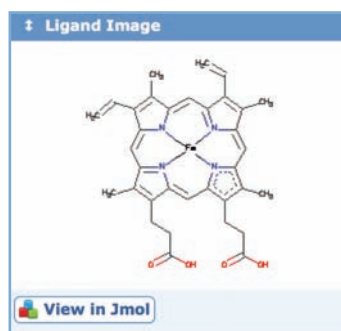
These drill-down options, or 'faceted search' options, provide a quick look at types of structures in the query results, and can be used to filter outliers or focus in on interesting results. Any combination of categories is possible: users can quickly select the high resolution entries from a structure type search; human-related entries from a sequence search; or the most recently released entries resulting from a chemical component search.

Charts can also be "hidden" for users who only want to view individual entries.



Distribution summaries can be used to quickly browse and refine search results.

## New Ligand Summaries



Users can toggle between a static image and a 3D Jmol view with the Ligand Image Widget.

or both. The *Related Ligands* widget links to summary pages for similar ligands and stereoisomers, and automatically enters the ligand in the RCSB PDB's *Chemical Structure Search* to build a search for a structurally similar ligand.

The *Links* widget lets users explore information related to the same chemical component at external resources (BindingDB, HIC-Up, PDBeChem and more) and the RCSB PDB's Ligand Expo.

These pages can be accessed by performing a ligand search, selecting a ligand from a PDB entry's *Structure Summary* page, and from the *Ligand Hits* tab for query results.

*Ligand Summary Pages* provide information about all of the entries found in the wwPDB's Chemical Component Dictionary. Similar to *Structure Summary* pages for PDB entries, widgets organize and highlight data on the page.

The *Chemical Component Summary* widget provides an overview of the structure, including name, identifiers, synonyms, and SMILES and InCHI information. A *Related Entries* widget links to all PDB entries where the ligand appears as a polymeric residue, a free ligand,

## Web Services

Web Services help software developers build tools that interact more effectively with PDB data. Instead of storing coordinate files and related data locally, Web Services let software tools interact with the RCSB PDB remotely. Documentation for accessing the RCSB PDB's Web Services is available from the Tools Widget in the left hand menu.

RESTful services exchange XML files in response to URL requests. RESTful search services return a list of IDs for Advanced Search and SMILES-based queries. RESTful fetch services return data when given IDs, including PDB entity descriptions, ligand information, third-party annotations for protein chains, and PDB to UniProtKB mappings. SOAP Web Services are also available.

Improvements are being made based on community feedback. Please let us know if there are website options that you think should be offered as a web service.

## Outreach and Education

### Molecules of 2010

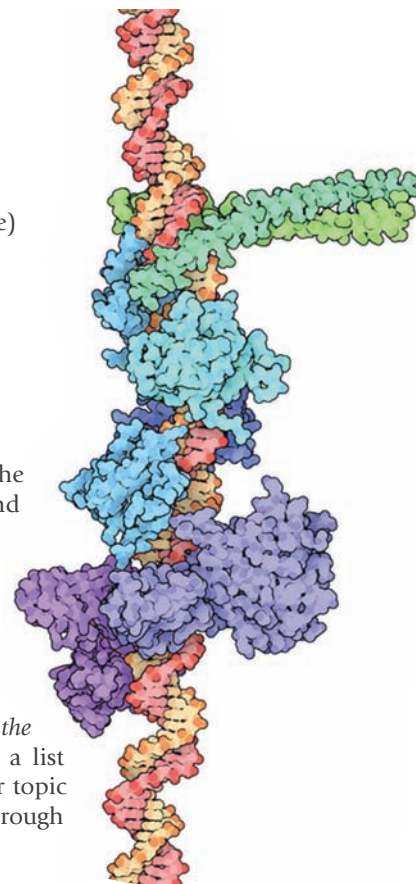
Since January 2000, the RCSB PDB's *Molecule of the Month* has been introducing readers to the structure and function of the many nucleic acids, proteins, and complex assemblies found in the PDB.

In 2010, the series looked at:

- 70S ribosomes (January)
- Enhanceosome (February)
- P-glycoprotein (March)
- Concanavalin A and circular permutation (April)
- Parvoviruses (May)
- Epidermal growth factor (June)
- Crystallins (July)
- Interferons (August)
- Isocitrate dehydrogenase (September)
- Riboswitches (October)
- Inteins (November)
- Adenovirus (December)

Out of these newer articles, the features on P-glycoprotein and 70S ribosomes were the most popular, with articles on hemoglobin and catalase the most read overall. *Molecule of the Month* articles were accessed close to 800,000 times in 2010.

The archive of all *Molecule of the Month* features is accessible by a list view, organized by date, title, or topic category, or by drilling down through categories and subcategories.



*Transcriptional enhanceosome* (PDB entries 1t2k<sup>6</sup>, 2pi0<sup>7</sup>, 2o6g<sup>8</sup> and 2o61<sup>8</sup>)

## Quick Survey on the Educational Uses of Molecular Visualization

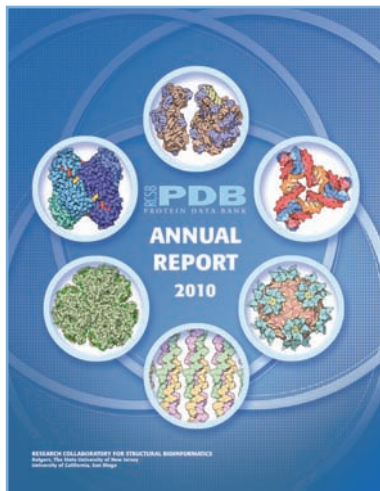
### Responses Needed:

<http://www.surveymonkey.com/s/62TL6ZJ>

To develop a systematic view of how molecular visualization is used in education, Paul Craig (Rochester University), Bob Bateman, and Lea Michel (University of Southern Mississippi) are surveying the biochemistry and molecular biology community. They plan to present the results at an upcoming meeting of the American Society for Biochemistry and Molecular Biology.

For related information, see the Spring 2010 RCSB PDB's Newsletter *Education Corner* on *A Proficiency Rubric for Biomacromolecular 3D Literacy* by Robert C. Bateman, Jr. and Paul A. Craig (<http://bit.ly/hsHhkz>).

## Annual Report Published



Download the 2010 Annual Report PDF from [www.pdb.org/ar10](http://www.pdb.org/ar10)

different activities in "data in" (data deposition, validation, and annotation), "data out" (data access, query, and reporting), and corresponding outreach and education activities.

The 2010 Annual Report for an overview of the RCSB PDB resource and its recent activities.

Since 2000, the Annual Report has provided yearly snapshots of the project. With this year's edition, printed reports will not be mailed directly to users. The report can be downloaded in PDF format from [www.pdb.org/ar10](http://www.pdb.org/ar10).

Aimed at the RCSB PDB's diverse community of PDB users in academia, industry, and education, the report highlights recent accomplishments in the report period of July 1, 2009 - June 30, 2010.

It explores the RCSB PDB's

## Poster Prize Awarded at AsCA



Takuya Yoshizawa

Takuya Yoshizawa received the poster prize at the 10<sup>th</sup> Conference of the Asian Crystallographic Association held in Busan, Korea (October 31 - November 3, 2010) for *Crystal structures of extra cellular dermal glycoprotein from carrot and xyloglucan specific endo-b-1,4-glucanase from Aspergillus aculeatus* by Takuya Yoshizawa<sup>1</sup>, Hiroshi Hashimoto<sup>1</sup>, Toshiyuki Shimizu<sup>2</sup>, Hisashi Hirano<sup>1</sup> and Mamoru Sato<sup>1</sup> (<sup>1</sup>Graduate School of Nanobioscience, Yokohama City University; <sup>2</sup>Graduate School of Pharmaceutical Sciences, The University of Tokyo).

Many thanks to the judges: Eunice Kim (Korea Institute of Science and Technology), Kunio Miki (Kyoto University), Zhi-Jie Liu (Institute of Biophysics, Chinese Academy of Sciences) and Soo Hyun Eom (Gwangju Institute of Science and Technology), and to Mitch Guss, Jenny Martin, and the Asian Crystallographic Association.

## Recent Meetings and Events

A variety of activities took place in Fall 2010.

The **Advisory Committees** of the RCSB PDB and the wwPDB met at the beginning of October 2010. The presentations and reports from these meetings are available online.

At the **New Jersey Science Convention** for area teachers, the RCSB PDB hosted an exhibit booth, and presented a hands-on workshop about the *Structure of tRNA and its interaction with the ribosome* (October 12-13, Somerset, NJ).

At Cold Spring Harbor Laboratory's course **X-ray Methods In Structural Biology** (October 11-26), John Westbrook presented *PDB Tools for Depositors*. He also gave a talk about the RCSB PDB at the **International Circular Dichroism and Bioinformatics Conference and EU/UK Annual CD Meeting** (December 3, Warwick University, UK).

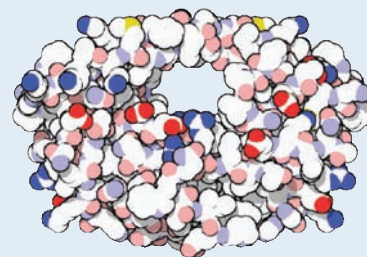
RCSB PDB Director Helen M. Berman received a *2010 Department of Chemistry Alumni Award* from the University of Pittsburgh. Associate Director Philip E. Bourne received the *Jim Gray eScience Award* from Microsoft Research.

## 25th Annual Meeting on HIV/AIDS-related Structural Biology

The NIH will sponsor the 25<sup>th</sup> annual meeting to discuss exciting progress made by structural biologists in the study of HIV.

This meeting will be held from March 28-30, 2011 on the NIH campus in Bethesda, MD. It is free and open to the public, but advance registration is required.

For more information, see [meetings.nigms.nih.gov/meetings/25thAIDSRelatedStructuralBiology](http://meetings.nigms.nih.gov/meetings/25thAIDSRelatedStructuralBiology)



Molecule of the Month's image of an HIV Protease<sup>2</sup>





## Education Corner by Jaime Prilusky, Ph.D., Weizmann Institute of Science

### Proteopedia: An online, collaborative 3D-encyclopedia of proteins & other molecules

As a wise man said, "A picture is worth a thousand words," and it happens to be true most of the time. Try to imagine this scene:

"The amino acid residues near the heme group in hemoglobin shift as the heme group converts between the non planar and the planar conformation by binding and releasing a molecule of O<sub>2</sub>." A description like this might elicit the proper mental image from an experienced crystallographer, and a somehow correct image from a biologist. You don't want to know what university or high-school students can make of it.

It's well known that the relationships between protein structures and functions are difficult to grasp, even for crystallographers. Masterpiece works like Goodsell's *Molecule of the Month* pages, with crisp and attractive drawings of molecules and easy-to-follow, accurate textual descriptions, greatly aided the understanding of the 'what,' 'why,' and 'when' around structures. Still, the connection between the words and the flat drawings are left as a mental exercise for the reader. And anything can happen when imagination flies.



Proteopedia came to the rescue with a simple concept: a web page (any platform, any browser) with a descriptive text, a '3D' structure that the user can rotate and change at will, and green 'hot' words between the text that interact with the 3D structure when clicked.

Before Proteopedia, the sequence of events while reading about structure and functions was something like this: first, read the description; then, imagine how this translates onto the static image.

With Proteopedia, the sequence of events is: click on the green words while reading the text description; then, observe the structure coming alive, rotating and changing its form to demonstrate what the text suggests. A whole new and rich experience of discovery for students and for teachers!

**JAIME PRILUSKY** ([Jaime.Prilusky@weizmann.ac.il](mailto:Jaime.Prilusky@weizmann.ac.il)) is the Head of the Bioinformatics Unit at the Weizmann Institute of Science in Rehovot, Israel. He received his Ph.D. in neuroendocrinology from the National University of Cordoba, Argentina in 1974, and was a professor at the National Technological University in Argentina before joining the Weizmann Institute in 1989.

An early online pioneer in bioinformatics, Jaime developed the first web interface to search and retrieve PDB data, called 3DB, and founded BioMOO (a virtual meeting place for biologists).

In addition to Proteopedia ([proteopedia.org](http://proteopedia.org)), his projects include OCA ([oca.weizmann.ac.il](http://oca.weizmann.ac.il)), a browser-database for protein structure/function and GeneCards ([www.genecards.org](http://www.genecards.org)), an electronic encyclopedia integrating information about the functions of human genes and their products, and of biomedical applications based on this knowledge. For more, see [miw.weizmann.ac.il](http://miw.weizmann.ac.il).

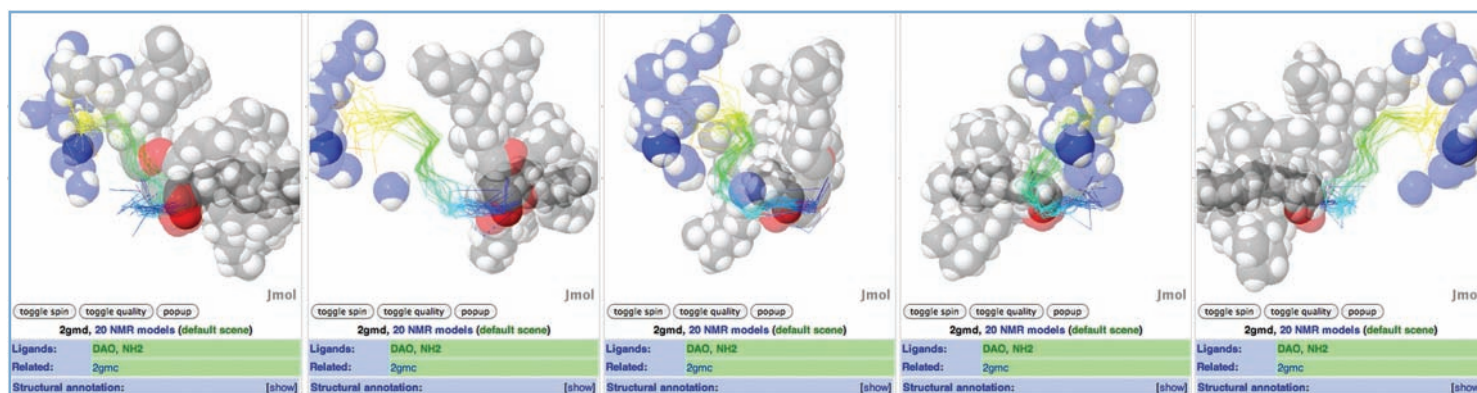
It's not surprising that education is one of the fields where Proteopedia's scenes have more impact. Teaching how data in a PDB file from a NMR experiment differs from that of an X-ray experiment might be possible, but it's easier if the student is able to compare, play, and manipulate representations of the 3D model of NMR and X-ray structures. This figure shows successive snapshots of a rotating representation of the PDB entry 2gmd, from an antimicrobial protein solved by NMR. The balanced use of solid and semi-transparent colors enhances the browsing of NMR structures.

Proteopedia was created in 2007 at the Weizmann Institute of Science, Israel, by Joel Sussman, Eran Hodis, and Jaime Prilusky, with brainstorming and suggestions from Israel Silman, John Moulton, and Eric Martz.<sup>10</sup> Since its creation, the number of users has grown steadily, as has the number of pages contributed by users and the range of fields where Proteopedia is being used.

Who's using [proteopedia.org](http://proteopedia.org)?

- High Schools as live support for classes, with richer interaction than a movie or a static image, and as support for student's self-paced learning.
- Universities, as live support for lectures and self-paced learning, as media for final projects and theses, and as a central topic for discussion at students' clubs.
- Researchers use Proteopedia as a source of information and as a secure shared collaboration site with remote partners.
- Journals as an Interactive 3D Complement (I3DC) for their papers.

Some Proteopedia pages become especially popular, indicating the role they play in the daily life of researchers and students. The most-accessed articles are *Teaching Scenes*, *Tutorials*, and *Educators' Pages*, *Avian Influenza Neuraminidase*, *Tamiflu and Relenza*, *Hemoglobin*,



View of 2gmd<sup>11</sup> in Proteopedia.

Acetylcholinesterase, HIV-1 Protease, Ribosome, Photosystem II, Lac Repressor, and Adenylyl Cyclase.

There are also Proteopedia pages on basic knowledge that help in understanding the data handled and maintained in the PDB, like *Atomic Coordinate File*, *Resolution*, *PDB Identification Code*, and *Protein Data Bank*.

Proteopedia couldn't exist without the structure files watched over by the wwPDB. The coordinates in the structure files provide the base for the 3D representation, and Proteopedia keeps a weekly updated selection of pages, including every one of the more than 70,000 PDB structures.

Creating Proteopedia pages with colorful live scenes is easy. The site contains text and video tutorials, and even 'crash course' instructions for the impatient. During our hands-on workshops, people start creating live 3D scenes in the first 30 minutes. When creating pages on Proteopedia, you may choose between different degrees of protection, depending on the namespace where the page is located, as described on the table. Workbench pages offer the ideal shared protected environment for collaboration. They are protected for read/write access, and the page creators may grant, to any Proteopedia user, read access to owned Workbench pages via provided tools.

Type of Page	Page Creator	Logged-in user	Anonymous user
Community domain	Read/Write	Read/Write	Read
Sandbox	Read/Write	Read/Write	Read
User domain	Read/Write	Read	Read
User Workbench	Read/Write	No access	No access

Levels of read/write access for Proteopedia creators and community editors

Finally, if you're searching for a topic to motivate your students or to discuss at your next talk, take a look at Proteopedia's Believe It or Not!, a page containing a list of useful, useless, or simply interesting facts about proteins, structures and what's around them. This page is automatically updated by OCA, the browser and database for structure and function.

Give [proteopedia.org](http://proteopedia.org) a chance to help you, your partners, and students to better explain and understand the relationship between structure and function.

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**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.*