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Research Collaboratory for Structural Bioinformatics Protein Data Bank

## NEWSLETTER

RCSB  
PDB  
PROTEIN DATA BANK

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

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## SNAPSHOT: OCTOBER 1, 2011

76,132 released atomic coordinate entries

ENTRIES BY MOLECULE TYPE	ENTRIES BY EXPERIMENTAL TECHNIQUE
70,513 proteins, peptides, and viruses	66,482 X-ray
3,290 protein/nucleic acid complexes	9,073 NMR
2,305 nucleic acids	376 electron microscopy
24 other	46 hybrid
	155 other

## RELATED EXPERIMENTAL DATA FILES

55,882	structure factors
6,374	NMR restraints
178	NMR chemical shifts

## Message from the RCSB PDB



At the end of October, the Worldwide PDB will host a symposium to celebrate the anniversary of the Protein Data Bank (PDB). In its 40<sup>th</sup> year, the PDB contains more than 76,000 entries that are deposited and used by researchers and students from around the globe.

Only a few structures were available in the beginning. October's *Molecule of the Month*, abstracted here, highlights these early *PDB Pioneers*.

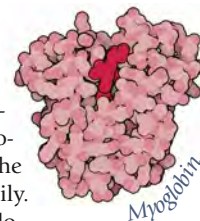
PDB40 information and registration is at [meetings.cshl.edu/meetings/pdb40.shtml](http://meetings.cshl.edu/meetings/pdb40.shtml)

## PDB Pioneers

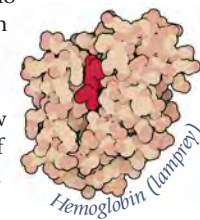
Structural biology was born in 1958 with John Kendrew's atomic structure of myoglobin, and in the following decade, the field grew rapidly. By the early 1970s, there were a dozen atomic structures of proteins, and researchers were discovering that they had a gold mine of information. However, the coordinate files for these structures are quite large, and in the days before the internet, it was difficult for individual researchers to share these large files with the growing number of interested structural biologists around the world. The PDB archive was created to solve this problem. Depositors would send their coordinates to the PDB, who would then mail them to interested users. To celebrate the 40<sup>th</sup> anniversary of the PDB, you can explore the historic protein structures that inspired the creation of the archive.

## Carrying Oxygen

John Kendrew's structure of myoglobin (1mbn) revealed the folding of protein chains for the first time, and showed how protein chains interact with prosthetic groups and with ligands. Max Perutz's structure of hemoglobin (2dhb) extended this story, showing how four similar chains can associate and regulate the binding of ligands through small changes in shape. The early PDB also included one additional protein from this family. A hemoglobin from lamprey (2lhb), which is intermediate between myoglobin and hemoglobin, regulates its action by transitioning between monomers and dimers.



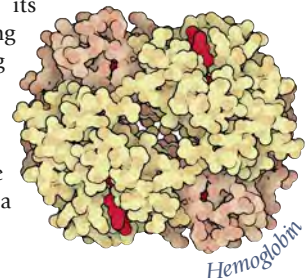
Myoglobin



Hemoglobin (lamprey)

## Enzyme Active Sites

The early PDB also included several structures of enzymes, revealing how protein chains fold to form chemical catalysts. DC Phillips' structure of lysozyme (1lyz), solved in 1965 and added to the PDB in 1975, revealed that enzymes have a form-fitting active site, and with some careful modeling, his group proposed that lysozyme distorts its substrate, making it easier to cleave. Several protein-cutting enzymes were included on the PDB magnetic tapes, including carboxypeptidase (3cpa), subtilisin (1sbt), chymotrypsin (2cha), and papain (9pap), as well as a small inhibitory protein, pancreatic trypsin inhibitor (4pti). The largest structure in the early PDB was the oligomeric enzyme lactate dehydrogenase (6ldh), composed of four chains with a groundbreaking 334 amino acids each.



Hemoglobin

The complete *Molecule of the Month* can be found at [dx.doi.org/10.2210/rcsb\\_pdb/mom\\_2011\\_10](http://dx.doi.org/10.2210/rcsb_pdb/mom_2011_10)



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## Data Deposition and Annotation

### Deposition Statistics

From July 1 - September 30, 2011, 2393 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. 6939 have been deposited overall in 2011.

During the same time quarter, 2025 structures were released in the PDB.

Of the structures deposited in 2011 so far, 79.9% were deposited with a release status of "hold until publication"; 17.9% were released as soon as annotation of the entry was complete; and 2.2% were held until a particular date. 92.8% of these entries were determined by X-ray crystallographic methods; 6.3% were determined by NMR methods.

### Validate Structure Factor Diffraction Data with SF-Tool

SF-Tool is a streamlined, web-based tool for validating structure factor diffraction data files. The latest release includes support for neutron and hybrid experiments; incorporates checks from REFMAC<sup>1</sup>, PHENIX<sup>2</sup>, and SFCHECK<sup>3</sup>; and converts multiple data sets into a single mmCIF file.

Visit [sf-tool.rcsb.org](http://sf-tool.rcsb.org) to:

- Validate model coordinates against structure factor data for X-ray and neutron data
- Easily convert structure factor files between different formats (mmCIF, MTZ, CNS/CNX, XPLOR, SHELX, TNT, HKL2000, SCALEPACK, D\*Trek, SAINT, and more)
- Check for and validate twinned or detwinned data

Documentation for this program is available. Questions, comments, and suggestions should be sent to [deposit@deposit.rcsb.org](mailto:deposit@deposit.rcsb.org).

### New pdb\_extract Release



Version 3.11 of `pdb_extract` has been released as an online web tool and a downloadable workstation program.

`pdb_extract` minimizes errors and saves time during the deposition process by extracting key details from the output files produced by many X-ray crystallographic and NMR applications. The program merges these data into macromolecular Crystallographic Information File (mmCIF) data files that can be used with ADIT for validation and deposition.

New features include:

- Supports data from hybrid method experiments
- Parses NCS and TLS ranges in BUSTER and REFMAC
- Improved mtz to mmCIF conversion
- Assesses quality of X-ray data

Complete details are available in the release notes and manual. Tutorials are available.

Depositors can upload files into the `pdb_extract` webserver or download the latest workstation version at [pdb-extract.rcsb.org](http://pdb-extract.rcsb.org).



## wwPDB News

### wwPDB News: Archive Version 4.0 Released

PDB Archive Version 4.0 was released in July. These files follow the PDB Exchange Dictionary v.4.0 and contain the results of remediating complex problems, including the representation of biological assemblies, residual B factors, peptide inhibitors and antibiotics, and entries in nonstandard crystal frames.

For PDB format files, only the entries changed during this remediation have been updated (<17000). These changes are identified as version 3.3 of the PDB file format. All files in PDBx/mmCIF and PDBML/XML formats reflect the new schema updates. Any changes made to the data are recorded in the PDBX\_VERSION data category.

From July 13, 2011 onward, all new releases and modified entries will follow the updated formats. Revisions to released entries will be tracked and numbered in the PDBx/mmCIF formatted files.

A description of the review and resulting changes and corrections is available from the wwPDB website ([wwpdb.org](http://wwpdb.org)). These data reflect the wwPDB's continuing commitment to providing accurate and detailed data to users worldwide.

## Data Query, Reporting, and Access

### New Website Release

[www.pdb.org](http://www.pdb.org) offers many new features for searching and browsing, including:

- **Explore Archive widget:** Tour the PDB archive by "drilling down" on significant properties of structures like *Organism* and *Polymer* type with just a few clicks using the home page's new Explore Archive widget. This widget provides a statistical overview of the PDB. Users can browse the charts individually, or view them all together by clicking on the "Show all" link.

This widget applies the same drill-down options available from each set of search results to the contents of the entire archive.

The screenshot shows the 'Explore Archive' widget with several category buttons: Organism, Taxonomy, Exp. Method, X-Ray Resolution, Release Date, Polymer Type, Enzyme Classification, and SCOP Classification. A 'Show all' button is at the bottom. The 'Organism' category is selected, showing a list of organisms with their respective PDB entry counts:

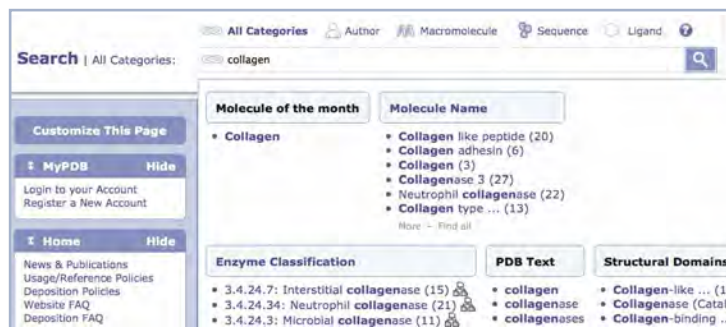
- Homo sapiens (18192)
- Escherichia coli (4469)
- Mus musculus (3267)
- Saccharomyces cerevisiae
- Bos taurus (1915)
- Rattus norvegicus (1627)
- Escherichia coli K-12 (1181)
- Other (40015)

Quickly see how many PDB entries are in a given category with the Explore Archive widget.



- **Top search bar:** The redesigned top search bar helps users easily and intuitively create both broad and precise searches. Start typing to access a suggestion box of related terms and links to searches. This box can be used to search a variety of categories, or limited to citation author, macromolecule name, sequence, or ligand.

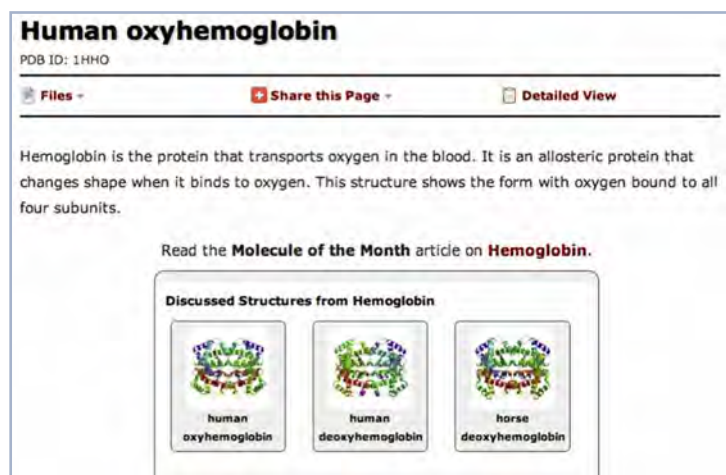
The order of results of a PDB text search or a sequence search is now based on the relevance of the term (for a text search) or the alignment score (for a sequence search).



Entering text in the All Categories top bar search returns search suggestions, organized by topic. Select any link to find all structures matching the query in that category.

- **PDB-101 Structure Focus:** Learn about the individual entries discussed in *Molecule of the Month* articles. Each Structure Focus page provides a description that explains why it was selected as an example structure, and offers an interactive 3D representation of the structure, sequence display, ligand information, and links to any other articles discussed in the *Molecule of the Month* feature.

PDB-101 is a unique view of the RCSB PDB that packages together the resources of interest to teachers, students, and the general public.



Top of Structure Focus page for hemoglobin entry 1hho.

- **Search for structures by protein modification.** The Protein Modification Browser was constructed based on protein modification ontology (PSI-MOD) from the Proteomics Standards Initiative ([www.psidev.info](http://www.psidev.info)). From here, users can browse protein residue modifications, view the number of associated PDB entries, and search for associated structures.

The related Advanced Search options have been expanded to include the protein modification source type (Name, Keyword, RESID,

PSI-MOD, and Chemical Component Dictionary) and the associated name/ID of the modification.

Check out the *What's New* page for complete descriptions of the newest RCSB PDB website features.



PSI-MOD Protein Modification Browser is one of the ways users can browse through the PDB. To view all of the options, select the Browse link from the top menu bar.

## Different Ways To Explore New Entries

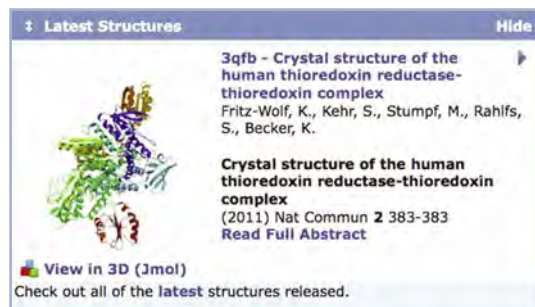
On average, 170 new entries are released into the PDB archive each week. The RCSB PDB offers different ways of exploring these new entries:

- The **Latest Structures** widget on the home page provides a slideshow of individual entries. It displays the entry title, image, citation, and a link to the PubMed abstract, if available. Users can pause the show at any point to read the entire abstract, click on the entry title to view the entry's *Structure Summary* page, or go straight to the Jmol view of the entry.

- The **New Structures** widget provides easy access to the Latest Structures added with the most recent weekly update. The structures will appear in the Query Result Browser, where users can drill through the structures by category (organism, taxonomy, experimental method, and more), generate reports, and download structure and sequences files.

The widget also links to a listing of the publications newly associated with PDB structures during the latest weekly update. This list includes links to the related PDB entry, the PubMed abstract, and related articles, and the unreleased entry search.

- The **MyPDB** service can be set to run saved searches with each update. Email alerts (weekly or monthly) will be sent when new entries matching the search are released in the PDB archive.



The Latest Structures widget, located on the home page, cycles through newly released entries.

## Website Statistics

Access statistics for the third quarter of 2011 are shown.

Month	Unique Visitors	Number of Visits	Bandwidth
JULY	187344	470491	589.52 GB
AUGUST	189681	467477	642.00 GB
SEPTEMBER	242775	567725	683.56 GB

## Outreach and Education

### Tools for Education

PDB-101 packages together resources that promote exploration in the world of proteins and nucleic acids for teachers, students, and the general public. Major topics include:


- **Structural View of Biology.** Built around the *Molecule of the Month* series, this feature promotes a top-down exploration of the PDB. Starting 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.** 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 these articles provides an annotated view of the PDB archive. *Molecule of the Month* columns appear on single pages, with links to printable PDF versions and downloadable high-resolution images. They can be accessed using the pulldown menu in the top bar, through the Structural View of Biology interface, and by archives organized by title, date, and category.
- **Related Educational Resources and materials,** including posters, animations, and classroom lessons and activities. Recently, a poster and animation of the structure of the HIV virus was added.
- **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.



Click on the blackboard logo from any page to enter PDB-101.

to enter PDB-101, click on the blackboard PDB-101 logo or its related widget in the left-hand menu to reveal an education-centered website. This view offers easy navigation: select any *Molecule of the Month* article from the top bar menu or mouse over the upper-left PDB-101 pulldown menu to jump to other sections. Select the blue RCSB PDB logo from the top of the page at any time to access RCSB PDB deposition and query services from the main website.

to enter PDB-101, click on the blackboard PDB-101 logo or its related widget in the left-hand menu to reveal an education-centered website. This view offers easy navigation:

Related materials for learning about the RCSB PDB website include a suite of tools (narrated tutorial, slides, and exercises) from [open-helix.com](http://open-helix.com); short online screencasts that demonstrate how to use different RCSB PDB tools; and contextual help and examples available where a  appears.

To link directly to this view, use [www.pdb.org/pdb-101](http://www.pdb.org/pdb-101).

### Meetings and Events

At the 19<sup>th</sup> Annual International Conference on Intelligent Systems for Molecular Biology (ISMB) and 10<sup>th</sup> European Conference on Computational Biology (July 15-19; Vienna, Austria), Senior Scientist Andreas Prlić described *A Census of internal pseudo-symmetries and similarities in protein domains* at the Laptop/Poster session of the 3Dsig satellite meeting. Scientific Lead Peter Rose helped users *Become an expert user of the RCSB Protein Data Bank website and Web Services* at the Technology Track session.

At the 25<sup>th</sup> anniversary symposium of the Protein Society (July 23-27, 2011; Boston, MA), annotator Ezra Peisach discussed *The PDB at 40: Past, Present, and Future* during the poster presentations.

At the XXII General Assembly and Congress of the International Union of Crystallography (IUCr, August 22-30, Madrid, Spain), the RCSB PDB participated in many events with the wwPDB. In addition to a wwPDB exhibit booth and an open wwPDB Q&A Session, there were several presentations.



wwPDB members in the exhibition hall.



Speakers of the Validation, error detection and fraud prevention session.





Martha Quesada and the poster on the Common Tool for Deposition and Annotation. Depositors also participated in a survey about the deposition process.

RCSB PDB Director Helen M. Berman discussed *The wwPDB and future perspectives in sharing macromolecular structure data* as part of the session *Developments and directions for crystallographic databases*, chaired by RCSB PDB's Senior Software Architect John Westbrook and Saulius Gražulis (Vilnius University).

John Westbrook also gave a presentation on *The wwPDB Working Format: A simplified application of CIF technology during the session Archiving, exchange, and retrieval of scientific data in the 21<sup>st</sup> century*.

RCSB PDB annotator Marina Zhuravleva, together with Swanand Gore (PDBe) and Matthew Lightfoot (CCDC), talked about the *Validation of small molecule and macromolecular X-ray structures. What are the differences and how can we learn from each other?* during the session on *Validation, error detection and fraud prevention*.

A poster on *The wwPDB Common Tool for Deposition and Annotation* was presented by RCSB PDB Deputy Director Martha Quesada. Depositors at the meeting gave feedback on the development of the tool, and completed surveys about their thoughts on the deposition process.

## Poster Prizes

The RCSB PDB Poster Prize is awarded for the best student poster presentations at selected meetings.



Serah Kimani

At IUCr, the award went to Serah Kimani for *Unexpected reactions resulting from mutating catalytic residues in an amidase reveal the role of the catalytic unit* (Serah Kimani,<sup>a</sup> Trevor Sewell,<sup>b</sup> <sup>a</sup>Department of Molecular and Cell Biology, University of Cape Town, Cape Town (South Africa). <sup>b</sup>Electron Microscope Unit, University of Cape Town, Cape Town (South Africa)).

The judging committee also recognized Adriana Kantcheva with an honorable mention for *Structure of the chloride dependent E290S-LeuT mutant from Aquifex aeolicus* (Adriana K. Kantcheva,<sup>a</sup> Anne-Marie Lund Winther,<sup>a</sup> Matthias Quick,<sup>b</sup> Jonathan A. Javitch,<sup>b</sup> and Poul Nissen,<sup>a</sup>



Adriana Kantcheva

<sup>a</sup>Center for Structural Biology, Dept. Molecular Biology, University of Aarhus (Denmark). <sup>b</sup>Center for Molecular Recognition, Dept. Pharmacology, Columbia University, New York).

Many thanks to the judges, who worked through all six days of poster presentations: Bernhard Rupp (k.k.Hofkristallamt), Kam Zhang (RIKEN), Manfred Weiss (Helmholtz-Zentrum Berlin), Jochen Mueller Dieckmann (EMBL-Hamburg), George Phillips (University Wisconsin-Madison), Clyde Smith (Stanford Synchrotron Radiation Laboratory), Miroslav Cygler (National Research Council Canada). Special thanks to the Poster Judging Committee Chair Katherine Kantardjieff (California State University San Marcos) and to the IUCr.



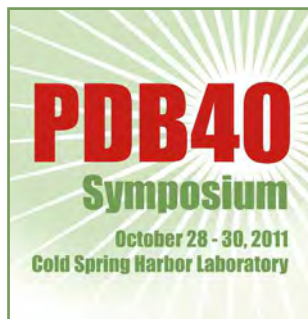
Tammy Cheng

At ISMB, Tammy Cheng received the award for *Structural biology meets systems biology: Gauging the systemic impact of non-synonymous single nucleotide polymorphisms* (Tammy M. K. Cheng<sup>1</sup>, Linda Jeffery<sup>2</sup>, Lucas Goehring<sup>3</sup>, Yu-En Lu<sup>4</sup>, Jacqueline Hayles<sup>2</sup>, Bela Novak<sup>5</sup>, Paul A. Bates,<sup>1</sup> <sup>1</sup>Biomolecular Modelling Laboratory, Cancer Research UK London Research Institute; <sup>2</sup>Cell Cycle Laboratory, Cancer Research UK London Research Institute; <sup>3</sup>Max Planck Institute for Dynamics and

Self-Organization, Göttingen, Germany; <sup>4</sup>Computer Laboratory, University of Cambridge, UK; <sup>5</sup>Department of Biochemistry, University of Oxford, UK).

Many thanks to the judges: Emidio Capriotti (Stanford), Jeroen de Ridder (Delft University of Technology), Javier Diaz (University of Toronto), Nils Gehlenborg (Harvard Medical School), Milana Frenkel-Morgenstern (Weizmann Institute), Arik Harel (Rutgers), Edda Kloppmann (Technische Universität München), Nathan Nehrt (University of Maryland, Baltimore County), Venkata P. Satagopam (EMBL Heidelberg), Christian Schäfer, Andrea Schafferhans, Markus Schmidberger (Technische Universität München). Thanks also to Poster Committee Chair Yana Bromberg (Rutgers University) and to the International Society for Computational Biology.

## PDB40 Symposium



The symposium will begin at 5:30 p.m. with a special reception and dinner on Friday, October 28, and end after lunch on Sunday, October 30.

The speaker program and poster abstracts have been posted on the meeting site at [meetings.cshl.edu/meetings/pdb40.shtml](http://meetings.cshl.edu/meetings/pdb40.shtml).

Registration will be open until all available spaces have been filled.

## Education Corner by Christopher M. Smith, Ph.D

### The Anatomy of Vision: Insights into Molecular Modeling for the Middle Schooler

Most young scientists (middle/high schoolers) today are pretty savvy when it comes to the use of computers, cell phones, and social media networks. And they are very adept at using these tools for entertainment, so our challenge as educators is how to redirect this expertise and familiarity to further their education. As scientists, we can easily say that visualizing a protein in 3D using a molecular graphics program is pretty cool, but the reality is it pales in comparison to the 3D animations students use in computer gaming.<sup>4</sup> So how do we engage these technologically savvy students? The answer (or at least one of them) lies in making the “science” topic relevant to them and in presenting it within the context of the world around them. A “topic” cannot be made relevant to them if it is taught in isolation from the rest of the world (or all other topics), so it must be integrated! This “integration” is the subject of this exercise to teach middle school (and sometimes sixth-grade) students “molecular modeling”; what it is, why it is important, and how it is used to advance our knowledge.

The end point of this exercise is to have the students use CN3D (or any other visualization application) to explore the various structural elements of the rhodopsin protein (1gu8). Keep in mind that my science objective is for the students to learn something about molecular modeling; everything else that I talk about is just a set of tools to engage their interest and active participation. I generally begin my “molecular modeling” presentation with a few comments about computer gaming (an interest of theirs), and drawing analogies to molecular modeling (an interest of mine). But the real story ... the real fun begins when we start to talk about the anatomy and physiology of the eye. This is a topic that appears to always be interesting to the students, especially the visually impaired. You can use any general anatomical rendition of the eye that is available via practically any web resource. My preference is the very simple *Human Eye* image (Figure 1) because it depicts a cross-section of the eye with insets focusing on smaller and smaller details of that anatomy, *i.e.*, general eye anatomy, the structure of the retinal tissue layer, a close-up of a light-sensing Rod, and a depiction of the rhodopsin protein in the Rod membrane. A description and walk-through of general eye anatomy includes exhaustive comments about protein composition and packing in the cornea to maintain clarity while providing strength and elasticity. I place an extreme emphasis on the health of the eye, especially the cornea, and perhaps “scare” the students a little with a couple of analogies and interesting discussions on the nature of proteins. For example, the cornea is much like the white of a chicken egg and it can and will turn irreversibly “white” if exposed to extremes of heat or chemicals (*e.g.*, acetone found in nail polish remover—you can actually demonstrate the latter in class, which really catches their attention). I usually follow with a short, general



**CHRISTOPHER SMITH** is the Director of Education, Outreach & Training at the Center for Theoretical Biological Physics housed at the University of California San Diego ([ctbp.ucsd.edu](http://ctbp.ucsd.edu)).

The NSF-funded CTBP, a collaboration between UCSD and The Salk Institute for Biological Studies, encompasses a broad array of research

and training activities at the forefront of the biology-physics interface. CTBP's mission is to conduct and foster research aimed at providing a quantitative framework for unraveling the workings of complex biological processes. Research within CTBP focuses on the following broadly defined areas: Cellular Tectonics Gene Regulatory Networks, and Computational Approaches to Intracellular and Intercellular Communication.

Christopher's research interests encompass DNA and protein sequence and structural analysis and the computational tools facilitating these analyses. Current research focuses on the development of user-friendly interfaces for computational tools and databases for the end-user (researcher and educator). He has developed web-based resources for educators (*e.g.*, the CMSMBR, Discovery Tools), IT training workshops for educators, health-care professionals and researchers and is actively engaged in K-16 education projects. Christopher's education interests encompass the integration of information technology and science into K-16 and informal education.

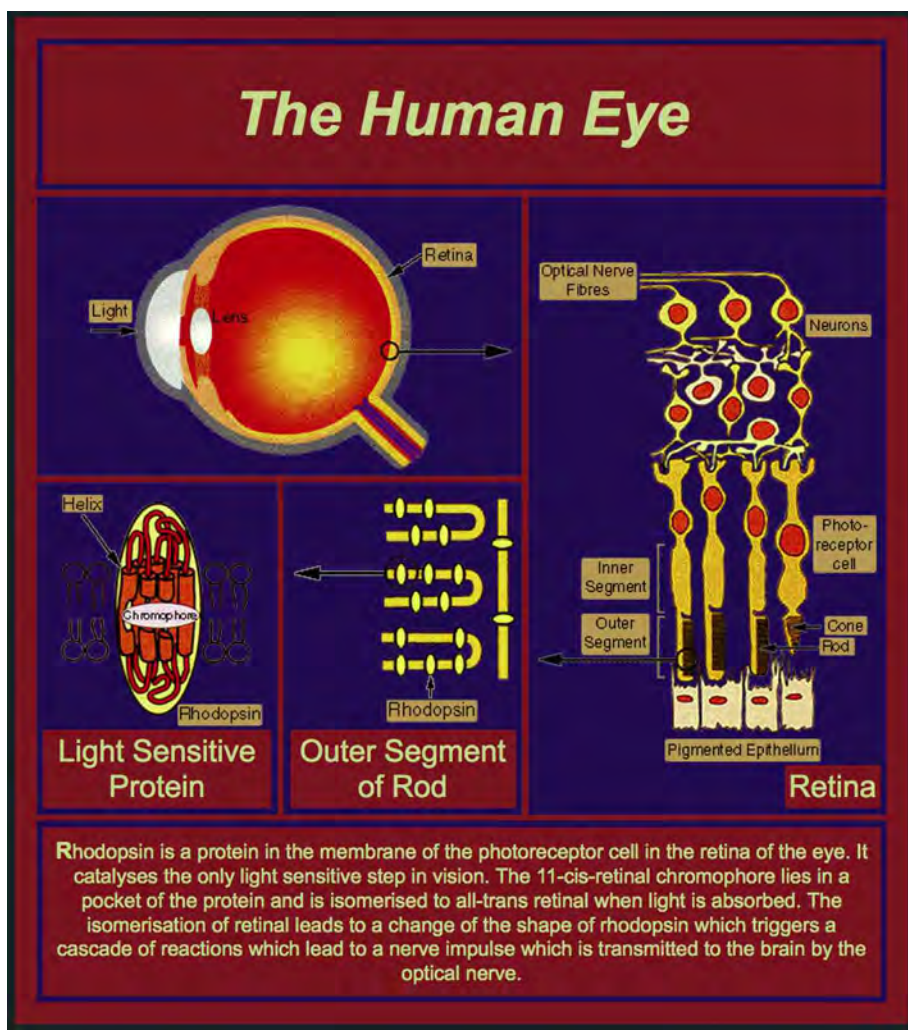
description of protein folding and unfolding, and the concept of conformational changes. This is followed by an explanation and demonstration of how a conformational change in rhodopsin is elicited by a photon of light. *This is vision in the making.* The demonstration is a beautiful animation of the photoisomerization process as a photon of light hits a membrane embedded rhodopsin protein (see [www.blackwellpublishing.com/matthews/rhodopsin.html](http://www.blackwellpublishing.com/matthews/rhodopsin.html)). As students view the animation (again and again!), I also introduce the concept of light (photons), elements of protein secondary structure, and a description of retinal; where it is from and why it is important. For example, I usually ask the students if they have ever heard the expression, “eat your carrots, they are good for you (your vision),” then follow by introducing the nomenclature of organisms, *e.g.*, the carrot (*Daucus carota*), and how its scientific name is related to the compound “carotene,” a metabolic precursor to “retinal”—the key ingredient of rhodopsin, essential for sight. Now that the students have grasped the “relationships,” *i.e.*, these many topics are taught in “context,” we begin our exploration of the rhodopsin. You can start with Jmol, but many students like the stand-alone aspect and additional functionality of independent programs, so I invariably use Cn3D (NIH; [www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml](http://www.ncbi.nlm.nih.gov/Structure/CN3D/cn3d.shtml)). Once each student has Cn3D up and running with rhodopsin on the screen, you can walk through the various secondary structural elements, including the location of retinal, and talk about the significance of the parallel grouping of alpha helices, hydrophobicity, *etc.*



The important thing is that the students are allowed to explore the model and ask questions. I also strongly emphasize that students try different visualization parameters (sticks, balls; color-schemes, etc.) and when they ask me "What is it?", I ask them what they see and how it is different from their previous representation. I interject into their answers additional detail on the structure that the particular parameter highlights. And soon enough, the students are exploring all the advanced, nook and cranny features of the program ... not because I said so, but because of their curiosity. Sometimes the students will want to explore other proteins, so you may want to be prepared with a list of suggestions. My recommendations are protein toxins in the venom of "cool" animals; Charybotoxin (Death Stalker Scorpion; **1tsk**), Conotoxin (Cone Shell; **1hje**), Tetrodotoxin (Fahaka Puffer Fish; **1rmk**), and Convulxin (Rattlesnake; **1uos**). The other interesting tidbit that can be added to the toxin structure discussion is the relative sizes of these proteins, and the significance this has physiologically and chemically as these toxins are distributed throughout the body (quickly) and with such drastic, immediate effects.

A final note—if you do this exercise with your students, be prepared to field questions for days and weeks later as the students do their own exploration of the Protein Data Bank.

Figure 1. Human Eye image available from [www2.mrc-lmb.cam.ac.uk/groups/GS/eye.html](http://www2.mrc-lmb.cam.ac.uk/groups/GS/eye.html) (reprinted courtesy of Gebhard Schertler, Paul Scherrer Institute, Switzerland)



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