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SNAPSHOT: APRIL 1, 2012

80402 released atomic coordinate entries

ENTRIES BY MOLECULE TYPE	ENTRIES BY EXPERIMENTAL TECHNIQUE
74460 proteins, peptides, and viruses	70436 X-ray
3569 protein/nucleic acid complexes	9335 NMR
2350 nucleic acids	421 electron microscopy
23 other	48 hybrid
	162 other

RELATED EXPERIMENTAL DATA FILES

59832	structure factors
6641	NMR restraints
406	NMR chemical shifts

Sound Science

Biomedical animator Drew Berry (Walter and Eliza Hall Institute of Medical Research) is known for his fantastic and detailed depictions of complex biomolecular systems. His award-winning work, which can be viewed online, in television and film, and in museums throughout the world, now appears in new and unusual venues thanks to a collaboration with the musician Björk.

Björk's latest project *Biophilia* manifests her love for music, technology, and nature in many ways: an album, iPad app, touring production (which includes a 24-woman Icelandic choir and a musical Tesla coil), and a music education initiative.

To accompany the song "Hollow," Björk's meditation on biological ancestry, Berry created a lush landscape for DNA to replicate (and sparkle) to the music. Molecular machines work at real-time speed, culminating in the appearance of Björk as a complex protein structure. Many of the molecular shapes, illustrated with great depth and rich color, were created with the help of crystal structure data from the PDB.

Recently released online, the animation is projected on screens throughout the venues hosting Björk's concerts, and is highlighted on stage during the performance of "Hollow." The related iPad app includes the "Hollow" movie and a "machine" that lets users queue up floating enzymes to interact with the replisome to create music.

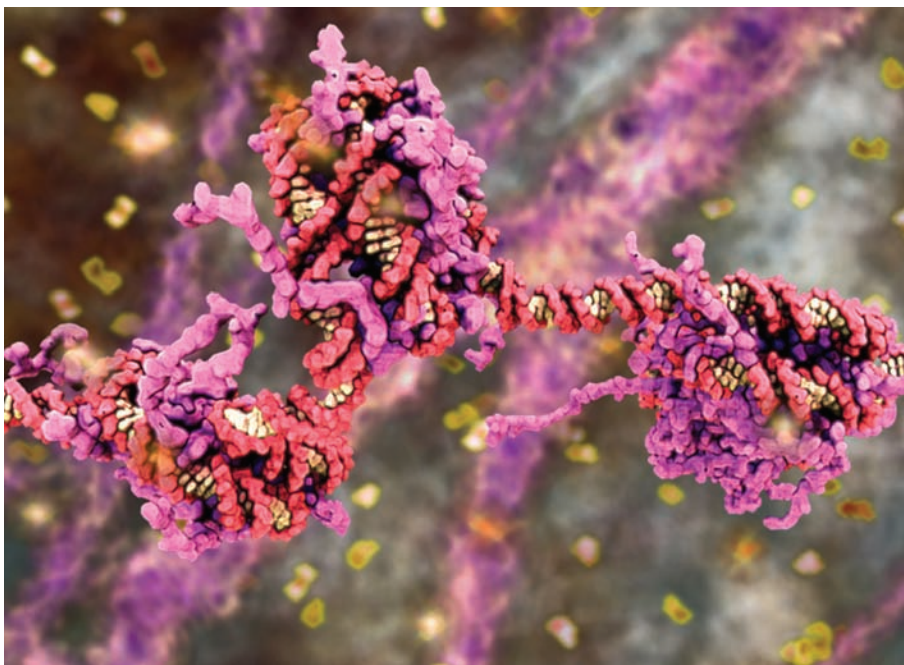


Image courtesy Drew Berry

The nucleosomes as seen in Hollow.

For more about Drew Berry's molecular animations, see bit.ly/wsGhIu
For more about Björk and *Biophilia*, see bjork.com
The video is online at youtu.be/Wa1A0pPc-ik



Data Deposition and Annotation

Volunteer Structures For Foldit



Foldit is an online game that attempts to predict the structure of a protein by taking advantage of humans' puzzle-solving intuitions and having people play competitively to fold the best proteins.

Gamers use the Foldit interface to build protein models based upon the amino acid sequence.

ADIT depositors can submit their sequences to serve as puzzle challenges for the Foldit community. When submitting an entry to the PDB, select the following options in the Release Status category:

- Release status for coordinates: Hold for 8 weeks
- Prerelease status for sequence information: Release Now
- CASP/CASP/other method development target: Foldit

The deposition will appear as a Foldit Target in the Unreleased Structures search. Foldit will use the prereleased sequence as a puzzle, and gamers will be able to compare their predicted models to the experimental data when it is released 8 weeks later.

Release Status			
Release status for coordinates	Help	Example	HOLD FOR PUBLICATION
Release status for structure factors	Help	Example	HOLD FOR PUBLICATION
Prerelease status for sequence information	Help	Example	RELEASE NOW
CASP/CASP/other method development target	Help	Example	?

CASD-NMR
 CASP
 Foldit
 GPCR Dock

Depositions can also be considered as targets for CASD-NMR, CASP, FoldIt, and GPCR Dock.

2012 Deposition Statistics

In the first quarter of 2012, 2470 experimentally-determined structures were deposited to the PDB archive.

82% were deposited with a release status of hold until publication; 14.6% were released as soon as annotation of the entry was complete; and 3.4% were held until a particular date. 93.0% of these entries were determined by X-ray crystallographic methods; 6.0% were determined by NMR methods.

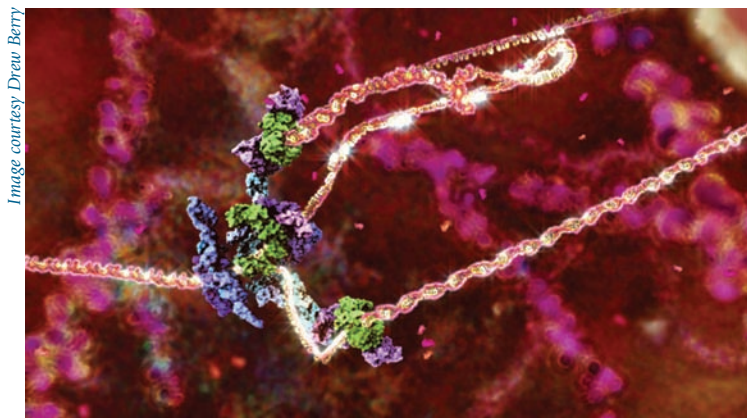


Image courtesy: Drew Berry

Drew Berry's replisome, from the video for Björk's Hollow.

wwPDB News



Electron Microscopy Validation Task Force Report

To improve validation methods in the PDB, the wwPDB has convened method-specific Task Forces to collect recommendations and develop consensus on additional validation that should be performed, and to identify software applications to perform validation tasks.

The 2011 X-ray Validation Task Force report¹ has been followed by the publication of **Outcome of the First Electron Microscopy Validation Task Force Meeting** in *Structure* (2012, 20:205-214).

At their 2010 inaugural meeting, this international group of 3DEM experts explored how to assess maps, models, and other data that are deposited into the EM Data Bank (EMDB) and PDB archives.

Many thanks to the authors and meeting participants: Richard Henderson (Co-chair, map validation), Andrej Sali (Co-chair, model validation), Matthew L. Baker, Bridget Carragher, Batsal Devkota, Kenneth H. Downing, Edward H. Egelman, Zukang Feng, Joachim Frank, Nikolaus Grigorieff, Wen Jiang, Steven J. Ludtke, Ohad Medalia, Pawel A. Penczek, Peter B. Rosenthal, Michael G. Rossmann, Michael F. Schmid, Gunnar F. Schröder, Alasdair C. Steven, David L. Stokes, John D. Westbrook, Willy Wriggers, Huanwang Yang, Jasmine Young, Helen M. Berman, Wah Chiu, Gerard J. Kleywegt, and Catherine L. Lawson.

1. A new generation of crystallographic validation tools for the Protein Data Bank. R.J. Read, P.D. Adams, W.B. Arendall III, A.T. Brunger, P. Emsley, R.P. Joosten, G.J. Kleywegt, E.B. Krissinel, T. Lutteke, Z. Otwinowski, A. Perrakis, J.S. Richardson, W.H. Sheffler, J.L. Smith, I.J. Tickle, G. Vriend, P.H. Zwart (2011) *Structure* 19: 1395-1412. doi:10.1016/j.str.2011.08.006

Data Query, Reporting, and Access

New Structures Widget

↑ New Structures
Hide

- Latest Release
- New Structure Papers
- Search Unreleased Entries

Available from the home page, the *New Structures* widget links to the latest structure released, the structure papers related to this release, and to the Unreleased Entry Search.

- **Latest Release:** The weekly update of new PDB entries can be explored and refined using the query results viewer
- **New Structure Papers:** A clickable list of citations associated with the entries in the latest PDB release
- **Unreleased Entries:** Find structures that are being processed or are on hold waiting for release. Data can be searched by PDB ID, author, title, status, sequence availability (some sequences are released in advance of the coordinates), and structural genomics project or center name.

The appearance of widgets on the RCSB PDB home page can be customized. For more, see the Winter 2012 Newsletter.

Ligand Summary Pages

Ligand Summary Pages provide information for all of the entries found in the wwPDB's Chemical Component Dictionary.

Similar to Structure Summary pages for PDB entries, Ligand Summary Pages are organized into widgets that highlight different types of information.

For example, view the Ligand Summary Page for caffeine (Ligand ID CFF) to access:

- **Chemical Component Summary:** an overview of the structure, including name, identifiers, synonyms, and SMILES and InCHI information
- **Related PDB Entries:** searches for other structures where the ligand appears as a free ligand
- **Related Ligands:** links to Summary Pages for similar ligands and stereoisomers, and automatically enters the ligand in the Chemical Structure Search tool to build related ligand searches
- **Ligand Image:** toggles between a static image and a 3D Jmol view
- **Links:** connects to information about the chemical component at external resources (BindingDB, HIC-Up, PDBChem, and more) and RCSB PDB's Ligand Expo

These summaries 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.

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



The Browse Database Icon

RCSB PDB's *Browse Database* feature explores 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 (GO) Consortium's descriptions for gene products. PDB IDs and corresponding chain IDs have been mapped to GO terms by the SIFTS initiative.
- **Enzyme Commission numbers.** Search for enzymes by name, or by partial or full EC number.
- **Membrane Transport proteins** organized using Transporter Classification (TC) Database system.

- **Source Organism**, using organisms found in the NCBI Taxonomy database. These organisms are the source of the individual naturally-occurring polypeptides. Source organism assignment in the PDB is based on author/UniProtKB-specified polypeptide mapping.
- **Genome Location of various organisms.** The genomes represented are a subset of those in NCBI's genome database with curate sequences for genetic loci archived at Entrez 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 associated structures.
- **MeSH (Medical Subject Headings)** that appear in the entry's related PubMed abstract.
- **SCOP** description of evolutionary and functional relationships from SCOP: Structural Classification of Proteins.
- **CATH** clustering of proteins at four major levels from CATH: Protein Structure Classification.

Click Browse from the top of any RCSB PDB page to access this feature.

Visualize Molecular Surfaces with Protein Workshop

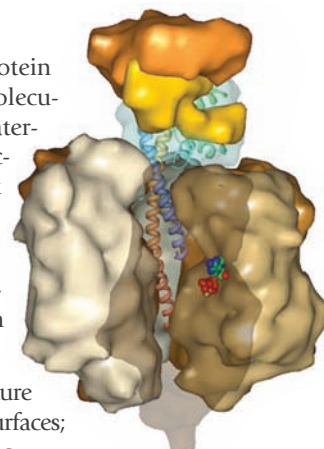
The molecular graphics program Protein Workshop² can be used to generate molecular surfaces to aid in the display of quaternary structure, protein-protein interactions, and binding sites. This robust feature is able to handle very large assemblies, such as virus capsids.

Surfaces are created for all macromolecule chains in a PDB entry using an algorithm from D. Xu and Y. Zhang.³

A detailed description for using this feature includes: how to create molecular surfaces; color by surface, chain, and entity; making a specific surface transparent; and tips.

Protein Workshop can be launched from every Structure Summary page using the link located underneath the image of the biomacromolecule.

The program can also be used to generate high resolution images for publication.



PDB ID 1e79
The structure of the central stalk in bovine F(1)-ATPase at 2.4 Å resolution.

C. Gibbons,
M.G. Montgomery,
A.G.W. Leslie, J.E. Walker
(2000) *Nat.Struct.Biol.*
7:1055-1061.

Website Statistics

Access statistics for the first quarter of 2012 are shown.

Month	Unique Visitors	Number of Visits	Bandwidth
JANUARY	242584	580,079	749.94 GB
FEBRUARY	258,865	628,875	877.04 GB
MARCH	255,442	613,853	825.07 GB

1. J.L. Moreland, A.Gramada, O.V. Buzko, Q. Zhang and P.E. Bourne (2005) The Molecular Biology Toolkit (MBT): A modular platform for developing molecular visualization applications. *BMC Bioinformatics* 6:21.
2. D. Xu and Y. Zhang. (2009) Generating Triangulated Macromolecular Surfaces by Euclidean Distance Transform. *PLoS ONE* 4:e8140.

wwPDB News



EM Maps Added to PDB Archive

The EM Data Bank (EMDB), the primary archive for experimentally-determined maps obtained using 3D electron microscopy methods, has joined the PDB archive (<ftp://ftp.wwpdb.org>). With the addition of EMD data, the physical size of the complete wwPDB archive is now approximately 180 GB. Sites that mirror the full wwPDB archive will need to increase storage capacity accordingly. Summary information regarding the merger and detailed specifications for data access are online at wwpdb.org/em.

Web Services for Accessing PDB Data

Web Services can help software developers build tools that efficiently interact with PDB data. Instead of storing coordinate files and related data locally, Web Services let software tools access the RCSB PDB remotely. Detailed documentation for accessing these Web Services is available.

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. Web Services can also be used to generate pre-defined summary and customizable reports for query results. A new service for accessing pre-released sequences in FASTA format has been recently added.

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

San Diego Festival of Science and Engineering

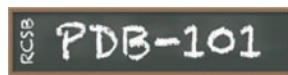


On Saturday, March 24, visitors to the RCSB PDB booth at the San Diego Festival of Science and Engineering's EXPO DAY learned about the basic building blocks of life by building 3D models of DNA and small proteins. They also watched animations of 3D proteins and nucleic acids, and took home posters and other materials about these fascinating structures.

EXPO DAY was the grand-slam-science-finale to a week of big events at San Diego State University, Balboa Park and California State University San Marcos. Activities included building what could be the world's longest DNA model, which was presented at the main stage at EXPO DAY.

Couldn't make it to San Diego? Build models of DNA and the dengue virus at home using PDFs from PDB-101 at bit.ly/xSfurM.

Visit PDB-101 for educational resources that explore a structural view of biology



PDB-101's *Structural View of Biology* promotes a top-down exploration of the PDB.

To start, select from high-level categories describing function: Protein Synthesis, Enzymes, Health and Disease, Biological Energy, Infrastructure and Communication, Biotechnology and Nanotechnology.

The Biological Energy category, for example, involves PDB structures that reveal how cells use chemical energy, light energy, electrical energy, and mechanical energy to power the processes of life. The structures are organized into the following subcategories:

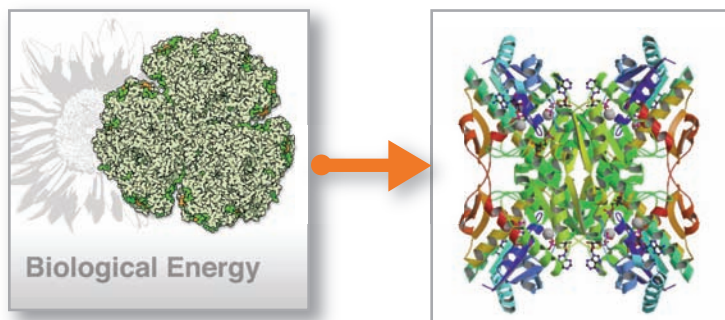
- Capturing the Energy in Food
- Photosynthesis
- Molecular Motors
- Creating and Capturing Light

These subcategories link to *Molecule of the Month* features related to the topic. Capturing the Energy in Food includes articles about structures such as pepsin (an enzyme that digests proteins), lactate dehydrogenase (which creates lactic acid as part of anaerobic respiration), and glycolytic enzymes (used to break down glucose).

Each article then links to special PDB-101 Structure Focus pages which highlight specific entries discussed in the article. These pages describe why the particular structure has been selected as an example, along with an interactive 3D view, sequence display, ligand information, and links to other structure examples discussed in the *Molecule of the Month* article. For example, the feature on glycolytic enzymes links to Structure Focus pages for all enzymes involved in glycolysis. These Focus pages are streamlined versions of the more complex Structure Summary pages available for all PDB entries.

The *Structural View of Biology* is a major part of PDB-101, the RCSB PDB resource that packages together materials and tools that promote exploration in the world of proteins and nucleic acids for teachers, students, and the general public. Click on the blackboard logo from the top of any RCSB PDB page to enter.

Other areas in PDB-101 include indexes of all *Molecule of the Month* articles; Educational Resources, with related tools, posters, tutorials, activities, lesson plans, and more; and the *Understanding PDB Data* reference for exploring and interpreting PDB data.



Phosphofructokinase
PDB ID: 4pfk

Explore biological function and related structures at PDB-101.

Modeling Proteins in New Jersey and California at the Science Olympiad

New Jersey

55 teams from New Jersey high schools demonstrated their understanding of protein structure at recent Science Olympiad competitions, and created 196 protein models along the way.

Science Olympiad tournaments consist of a series of events that test student knowledge in biology, earth science, chemistry, physics and technology. In New Jersey, protein modeling was one of the 25 events for high school teams at the regional and state competitions.

The focus of this year's event uses the example of the discovery and treatment of a rare, disease-causing genetic mutation to explore proteins involved in the regulation of apoptosis. The molecular story behind a mysterious bowel disease, Jmol, and related *Molecule of the Month* columns are key resources for preparation.

Teams submitted hand-built 3D models of the caspase protein found in PDB entry [1i3o](#) on the morning of the event. The models represented the protein backbone, with additional points awarded added details that highlighted important parts of the structure (such as the defective protein involved in the illness). During the event itself, the students quickly built models onsite (a portion of [1i3o](#) at regionals and PARP protein [3od8](#) at state) and answered questions on a written exam.

RCSB PDB members judged these competitions, and met with teams at the end of the day to discuss results. Many thanks to the RCSB PDB judges (Luigi Di Costanzo, Sutapa Ghosh, Brian Hudson, Huangwang Yang, Christine Zardecki, and Marina Zhuravleva), the NJ Science Olympiad organizers and volunteers, the host colleges, and to the MSOE Center for BioMolecular Modeling for the materials and design of this event.

California

Protein modeling was offered for the first time at the San Diego regional on February 18, 2012. The RCSB PDB held workshops to help introduce teams to the event, and members Peter Rose and Michael Gao judged the actual event. Congratulations to all of the teams that participated!

Protein modeling continues in 2012 at Science Olympiads across the country, culminating at the National Tournament in May. In 2013, the event will go on temporary hiatus as the Science Olympiad rotates in different events in the category of Physical Science & Chemistry.

The RCSB PDB will continue to update education-related news on twitter.com/buildmodels.

Top NJ Results

State:

1. JP Stevens
2. Princeton
3. East Brunswick

Southern Regional:

1. South Brunswick
2. West Windsor-Plainsboro North
3. Moorestown Friends

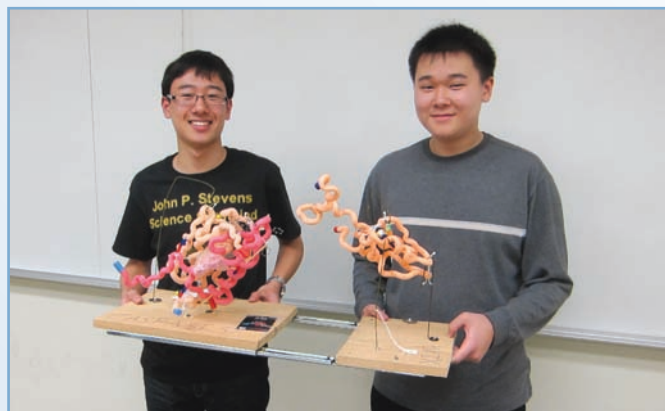
Central Regional:

1. JP Stevens
2. Hillsborough
3. Princeton II

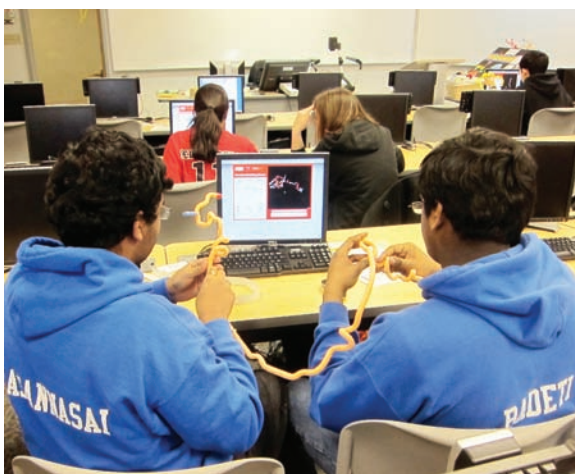
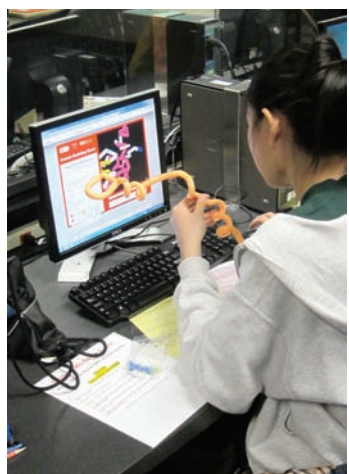
Northern Regional:

1. West Windsor-Plainsboro I
2. West Windsor-Plainsboro South II
3. Bergen County Academies

Full results are posted at education.pdb.org



Protein Modeling state champions from JP Stevens High School



Scenes from protein modeling events across NJ

Protein Society Honors RCSB PDB Director

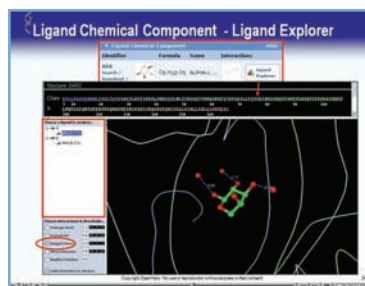


Helen Berman is the 2012 Awardee of the Carl Brändén Award of the Protein Society. The Award, sponsored by the Rigaku Corporation, is given to an outstanding protein scientist who has also made exceptional contributions in the areas of education and/or service to the science.

This award recognizes her accomplishments toward enabling a freely available and uniform worldwide archive of 3D structural information for biomedical research and education. Dr. Berman's passion for making structural data accessible and understandable by a broad community has driven the development of the Protein Data Bank into a vital and accessible international resource for biology. In the early 1970s, Berman was a champion of the open access of scientific information; while obvious today, at that time the concept of open access was truly visionary.

The award will be conferred at the 26th Annual Symposium of The Protein Society (August 5-8, 2012) in San Diego, CA. For the full list of awardees, please see proteinsociety.org.

Updated RCSB PDB Training Materials



OpenHelix has updated their free, online training materials to reflect many new RCSB PDB features, including the top bar searching feature with category options, auto-complete feature, improved macromolecule name queries, and PDB-101.

An online narrated tutorial, animated PowerPoint slides, handouts, and training exercises are available for download. Teachers and professors are encouraged to use these resources as classroom content. These files can be accessed from www.openhelix.com/pdb.

wwPDB News



Meeting Review Published

The Protein Data Bank at 40: Reflecting on the Past to Prepare for the Future

Structure 2012 20: 391-396 doi: 10.1016/j.str.2012.01.010

Education Corner by Hazel M. Holden, Ph.D. and Dan Toomey

Project CRYSTAL: Crystallographers Researching with Young Scientists, Teaching and Learning

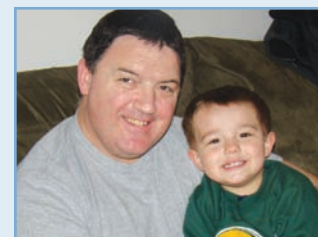
The concept of Project CRYSTAL (Crystallographers Researching with Young Scientists, Teaching and Learning) began by chance one spring day in March of 2007 in Madison, Wisconsin. My daughter, Kelsey Rayment, was complaining to her friends in school about having a mother as a scientist. She was overheard by her science teacher, Mr. Dan Toomey, who immediately asked her if I would come in and present my work to his class. When Dan called me and asked specifically what my research was about, I hesitated because I never expected a seventh grade teacher to even know about X-ray crystallography. To my surprise, Dan responded immediately because the previous year he had been involved with the SMART Teams, which is based at the Milwaukee School of Engineering (cbm.msos.edu). SMART stands for "Students Modeling A Research Topic," and the students involved with this program are matched to a mentor who then teaches them about the 3D structure of their favorite protein.

The first lecture to Dan's class was an eye-opening experience. I spoke to the students about X-ray crystallography and protein structure. To put things in the proper context, it is important to point out that these students did not even know what a covalent bond was, let alone a protein. I had to start my lecture off with a discussion of the periodic table and had to explain a bit about molecular bonding. What was fascinating, however, was to watch these students sit up in their seats when I explained how carbon monoxide binds to hemo-

HAZEL M. HOLDEN is a Professor of Biochemistry at the University of Wisconsin, Madison. Her present research interest focuses on the structure and function of enzymes involved in the biosynthesis of unusual deoxysugars. In her spare time she enjoys cycling and playing organ and piano. She is married to Professor Ivan Rayment, and they have two children, Kelsey and Harrison.



DAN TOOMEY has taught science for 7 years at Edgewood Campus School in Madison, Wisconsin. He is a Science Olympiad coach, a SMART team coach, Adjunct faculty member at Edgewood College's School of Education, and an NSF RET participant. In his spare time he enjoys spending time with his family, especially outdoors.



globin. Afterwards, they wrote me a thank-you note, and one of them remarked "Thank you, I learned how carbon monoxide kills you."

In the spring of 2008, Dan and I submitted a grant to the NSF to establish Project CRYSTAL. The proposal included both basic research on enzymes involved in unusual deoxysugar biosynthesis and biochemistry outreach to middle school students. Why did Dan and I choose to set up Project CRYSTAL specifically for these students rather than high school students? Because these young people are undergoing enormous changes both emotionally and physically, and by the time they reach high school it is almost too late to instill a joy for chemistry, biochemistry, and physics. Chemistry needs to be presented, with some rigor, at an earlier age than ninth grade.

The most important and fundamental question all of us can ask is how can we make chemistry exciting to these students and compete against their fascination with iPods, cell phones, and other high-tech gadgets. First and foremost, the chemistry has to be relevant to their everyday lives. When my husband, Ivan Rayment, and I were growing up we had chemistry sets, and we learned in our chemistry classes how to blow things up. But today, teaching students how to blow things up would not be well received. So how do we make chemistry exciting? We teach it in the context of biology, and in particular nutrition. This is an especially timely topic given the rising incidence of obesity among young people in the United States.

In 2009, Dan and I were awarded an NSF grant, and Project CRYSTAL "crystallized." The two founding graduate student mentors were Rachel Kubiak and Nate Bruender. Currently, Project CRYSTAL has two major missions: (1) to instill a love for chemistry in middle school students by studying the inner workings of nutrition, thereby leading to healthy life choices and (2) to provide a hands-on laboratory

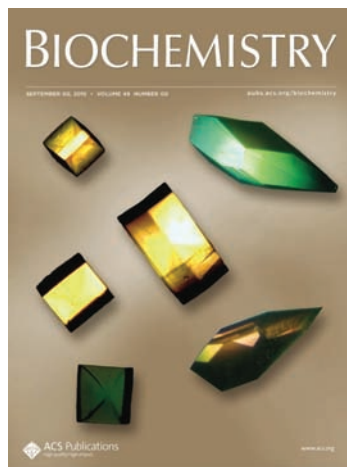
experience in an active, state-of-the-art research laboratory, thus fostering interest in a scientific career. To achieve the first mission, Dan, the graduate students, and I are developing teaching modules based upon the chemistry of sugars, fats, and proteins. These modules include the concepts of matter, electrons, neutrons, protons, atoms, molecules, and chemical bonding. We are hoping to eventually write a biochemistry textbook for middle school students.

To achieve the second goal, four middle school students have been coming to my laboratory once a week during the school year to participate in academic research. These students are learning fundamental techniques such as molecular cloning, protein purification, crystallization, X-ray data collection, and protein model building. Last year two of the students, Manpreet Kaur and Marie K. Avey, were co-authors on a paper published in *Biochemistry*,⁴ and their crystals were featured on its cover. These students also crystallized the enzyme AntD; a paper describing the structural analysis of this protein was recently published.⁵

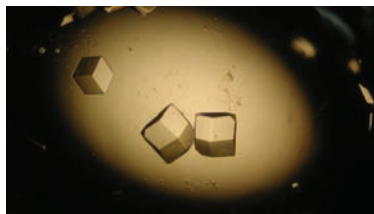
This year's group consists of Sarah, Melissa, Gwen, and Malaika, and they are being mentored by graduate students Rachel Kubiak and Becky Phillips. It has been a very exciting year so far, and these middle school students are getting close to having their first proteins over-expressed and purified. Crystallization trials will begin shortly if all goes well!

It has been an absolute privilege working with these middle school students, and all of us are grateful to the NSF for supporting this endeavor. More details concerning Project CRYSTAL can be found at www.projectcrystal.org.

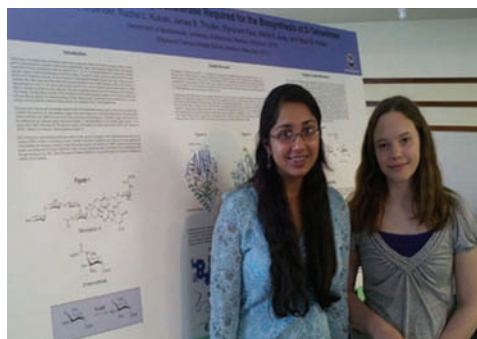
Manpreet and Marie at a poster session presenting their structure.



Crystals of AntD



Shown on the cover of *Biochemistry* are crystals of a novel C-3'-methyltransferase involved in the production of D-tetronitrose, an unusual sugar found attached to the antitumor agent tetrocarcin A or the antibiotic kijanimicin. The crystals were grown by Project CRYSTAL's Manpreet Kaur and Marie K. Avey.⁴



Rachel Kubiak watching the new students set up cloning experiments.



Becky Phillips with Melissa, Sarah, Malaika, and Gwen

4. N.A. Bruender, J.B. Thoden, M. Kaur, M.K. Avey, H.M. Holden (2010) Molecular architecture of a C-3'-methyltransferase involved in the biosynthesis of D-tetronitrose. *Biochemistry* 49:5891-5898. doi: 10.1021/bi100782b

5. R.L. Kubiak, H.M. Holden (2012) Structural studies of AntD: an N-Acyltransferase involved in the biosynthesis of D-anthrose. *Biochemistry* 51:867-878. doi: 10.1021/bi201650c

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
Center for Integrative Proteomics Research
174 Frelinghuysen 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)

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