RCSB PDB PROTEIN DATA BANK

Summer 2006 • Number 30

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NEWSLETTER

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

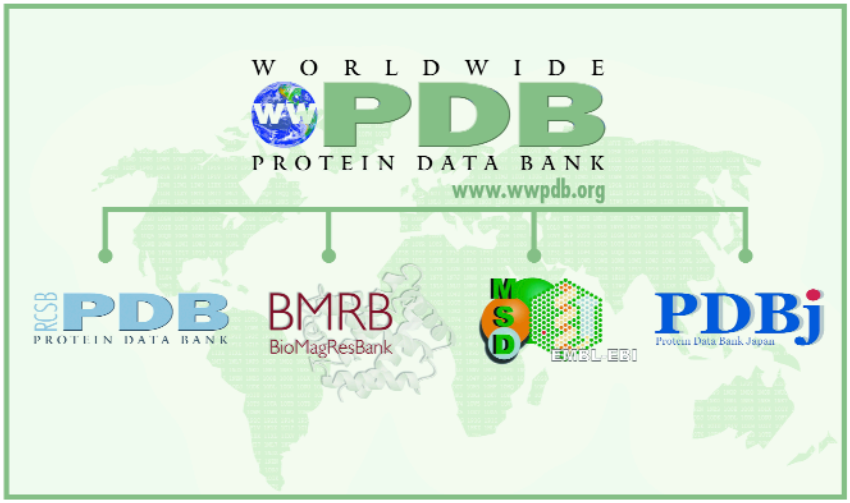
Contents

SNAPSHOT: JULY 1, 2006
37392 released atomic coordinate entries

MOLECULE TYPE		EXPERIMENTAL TECHNIQUE	
34221	proteins, peptides, and viruses	31655	X-ray
1627	nucleic acids	5531	NMR
1510	protein/nucleic acid complexes	126	electron microscopy
34	other	80	other
		21163	structure factor files
		3014	NMR restraint files

Participating RCSB Members:
Rutgers • SDSC/SKAGGS/UCSD
E-mail: info@rcsb.org
Web: www.pdb.org • FTP: ftp.rcsb.org
The RCSB PDB is a member of the wwPDB (www.wwpdb.org)

Message from the RCSB PDB



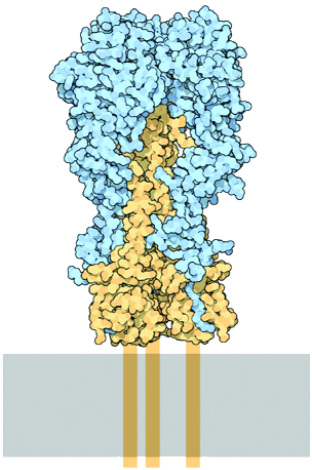
When it was established in 2003, the Worldwide Protein Data Bank (wwPDB) formalized a long-standing collaboration between founding members RCSB PDB, the Macromolecular Structure Database at the European Bioinformatics Institute (MSD-EBI), and Protein Data Bank Japan (PDBj).

The wwPDB recognizes the international character of the PDB and ensures that the archive will remain single and uniform.

During the past quarter, the BioMagResBank (BMRB) joined the wwPDB. The BMRB, located at the University of Wisconsin-Madison, is the archive for the experimental data gathered from NMR spectroscopic investigations of biological macromolecules. The BMRB group has created ADIT-NMR to enable authors to deposit experimental and coordinate data using a single tool. We look forward to developing future projects with the wwPDB.

APRIL 2006 MOLECULE OF THE MONTH: HEMAGGLUTININ (PDB ID: 1RUZ)

Gamblin, S.J., Haire, L.F., Russell, R.J., Stevens, D.J., Xiao, B., Ha, Y., Vasisht, N., Steinhauer, D.A., Daniels, R.S., Elliot, A., Wiley, D.C., Skehel, J.J. The structure and receptor binding properties of the 1918 influenza hemagglutinin. Science ***v303*** *pp.1838-1842, 2004*



Data Deposition and Processing

pdb_extract Now Supports NMR Depositions

The program pdb_extract[1], which has been simplifying the deposition of crystal structures, can now be used for NMR depositions. The latest version supports NMR-related information from the applications X-Plor/CNS/CNX, CYANA, and DYANA. Other enhancements made to the pdb_extract suite are detailed in the Version Release Notes available from the pdb_extract website.

pdb_extract minimizes errors and saves time during the deposition process since fewer data items have to be manually entered.

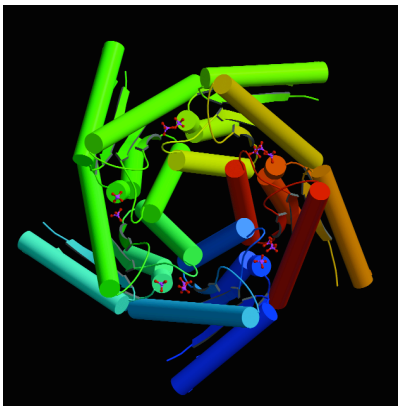
The program extracts key details from the output files produced by many X-ray crystallographic and NMR applications for use in the deposition process. The program merges these data into macromolecular Crystallographic Information File (mmCIF) data files that can be used with ADIT to perform validation and to add any additional information for PDB deposition.

pdb_extract can be used via web interface or downloadable workstation from pdb-extract.rcsb.org.

RCSB PDB Focus: Using Images from the RCSB PDB

The contents of the RCSB PDB are in the public domain. Online and printed resources are welcome to include PDB data and images from the RCSB PDB pages as long as the images are not being sold commercially. It is expected that the corresponding citations are included.

For example, the prepared images available for each structure (from the Structure Explorer pages) should cite the corresponding reference for the entry and the RCSB PDB:



PDB ID: 1DI0

B.C.Braden, C.A.Velikovsky, A.A.Cauerhff, I.Polikarpov, F.A.Goldbaum, Divergence in Macromolecular Assembly: X-Ray Crystallographic Structure Analysis of Lumazine Synthase from Brucella abortus, J.Mol.Biol. *297 pp. 1031 (2000). Image from the RCSB PDB (www.pdb.org: H.M.Berman, J.Westbrook, Z.Feng, G.Gilliland, T.N.Bhat, H.Weissig, I.N.Shindyalov, P.E.Bourne, The Protein Data Bank,* Nucleic Acids Research, *28 pp. 235-242 (2000)*

Pictures from Molecule of the Month features should also credit the illustrator David S. Goodsell of the Scripps Research Institute:

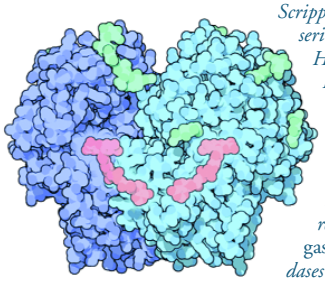


Image of glucose oxidase from David S. Goodsell's (The Scripps Research Institute) Molecule of the Month series at the RCSB PDB (www.pdb.org; Berman, H.M., Westbrook, J. Feng, Z., Gilliland, G., Bhat, T.N., Weissig, Shindyalov, I.N., Bourne, P.E. The Protein Data Bank, Nucleic Acids Research *v28 pp. 235-242, 2000); structure shown is 1gpe: Wohlfahrt, G., Witt, S., Hendle, J., Schomburg, D., Kalisz, H.M., Hecht, H.J. 1.8 and 1.9 Å resolution structures of the* Penicillium amagasakiense *and* Aspergillus niger *glucose oxidases as a basis for modelling substrate complexes. Acta Crystallogr., Sect.D v55 pp.969-977, 1999)*

A full list of related citations for the RCSB PDB is available online from the General Education section of the website.

PDB Archive Focus: Worldwide Data Annotation

Data from X-ray crystallographic, NMR, and cryo-electron microscopic experiments are deposited to the PDB archive by scientists from all over the world.

PDB data are processed by an international effort involving members of the wwPDB – the RCSB PDB, the Macromolecular Structure Database at the EMBL's European Bioinformatics Institute, and Protein Data Bank Japan. wwPDB annotators work with these data to make sure they are represented in the PDB archive in the best way possible. They run a series of checks, make corrections, and correspond with the depositors in an effort to make the data public as quickly and accurately as possible.

Statistics about the number of structures deposited, processed, and released by the wwPDB are available at www.wwpdb.org/stats.html.

Deposition Statistics

In the first half of 2006, 3547 structures were deposited to the PDB archive.

The entries were processed by the wwPDB teams at RCSB-Rutgers, MSD-EBI, and PDBj. Of the structures deposited, 70% were deposited with a release status of "hold until publication"; 17% were released as soon as annotation of the entry was complete; and 13% were held until a particular date.

81% of these entries were determined by X-ray crystallographic methods; 15% were determined by NMR methods; and 82% of all of these depositions were deposited with experimental data.

[1]Automated and accurate deposition of structures solved by X-ray diffraction to the Protein Data Bank. *Acta Crystallogr., Sect.D v60,* pp. 1833-1839, 2004.

Data Query, Reporting, and Access

RCSB PDB Offers Web Services

The RCSB PDB has introduced Web Services to help the software developer community build tools that interact more effectively with PDB data. Instead of storing coordinate files and related data locally, web services provide a way for software tools to interact with the RCSB PDB remotely.

The RCSB PDB's web services were implemented using Axis (ws.apache.org/axis) and include BLAST, FASTA, PubMed, and SNP queries. A complete list of web services and their WSDL description (Web Services Description Language in XML Format) is available.

Web services allow the developer community to build applications that are platform independent and require only a traditional HTTP connection. This is especially useful for developing in environments with relatively tight security constraints. Web services also provide a low-overhead approach to designing workflow applications that integrate remote services. Developers can write efficient and manageable tools without having to worry about low-level communication details. Using web services, programmers can write efficient workflow tools. For example, a developer could write a tool that interoperates between local data, PDB data, and NCBI data.

For general information on web services, please visit www.w3.org/2002/ws.

Automated Downloads of PDB Data

The RCSB PDB ftp site provides coordinate data (in PDB, mmCIF, and PDBML/XML formats) and experimental data. A web interface offers a way to download multiple data files from the archive. Scripts are also available to assist in the automated download of data from the ftp site:

ftp://snapshots.rcsb.org/rsyncSnapshots.sh
Makes a local copy of an annual snapshot or sections of the snapshot. This script is annotated to assist in downloading only sections of the archive. The time required to download the entire archive can be lengthy (18+ hours); however, the time required to download the coordinate data in a single format should be much less. While the amount of time depends upon network speed, our tests show that all of the coordinate files in PDB format from a snapshot can be downloaded in about 2 1/2 hours.

ftp://ftp.rcsb.org/pub/pdb/software/rsyncPDB.sh
Copies the current contents of the entire archive.

ftp://ftp.rcsb.org/pub/pdb/software/getPdbStructures.pl
Copies portions of the archive.

ftp://ftp.rcsb.org/pub/pdb/software/getPdbUpdate.pl
Copies the data from the weekly updates.

RSS Functionality at the RCSB PDB

An RSS (Really Simple Syndication) feed provides users with a list of newly updated structures as soon as they are available. RSS pushes information that can be read by client software (an RSS reader) that sits on your local computer. Rather than going to look for new PDB entries, they can come to you.

To start, download and install an RSS reader. Depending on your reader, either drag or click on the orange RSS icon from the top of the RCSB PDB home page (located just next to the latest release date) to add the URL for new structures to your RSS reader.

You will now be informed of new structures as they become available. Clicking on the update notice will take you to the list of new structures.

Some examples of RSS readers include:
- Google desktop (desktop.google.com)
- Firefox extensions called RSS Wiz or RSS Ticker (addons.mozilla.org/firefox/424)
- Safari (www.apple.com/macosx/features/safari)
- NetNewsWire (ranchero.com/netnewswire)
- IE7 Beta (www.microsoft.com/windows/ie/downloads/default.mspx)
- Firefox's "Live Bookmarks" (www.mozilla.com/firefox/livebookmarks.html)
- Vienna (www.opencommunity.co.uk/vienna2.html)

For more information on RSS, please see the following:
- RSS tutorial for webmasters (www.eopta.com/spec/rss-tutorial)
- Understanding and implementing RSS Content Feeds and Syndication (www.packtpub.com/files/RSS_and_Atom_Book_Chapter1_what_are_newsfeeds.pdf)
- Google RSS Readers (directory.google.com/Top/Reference/Libraries/Library_and_Information_Science/Technical_Services/Cataloguing/Metadata/RDF/Applications/RSS/News_Readers/)

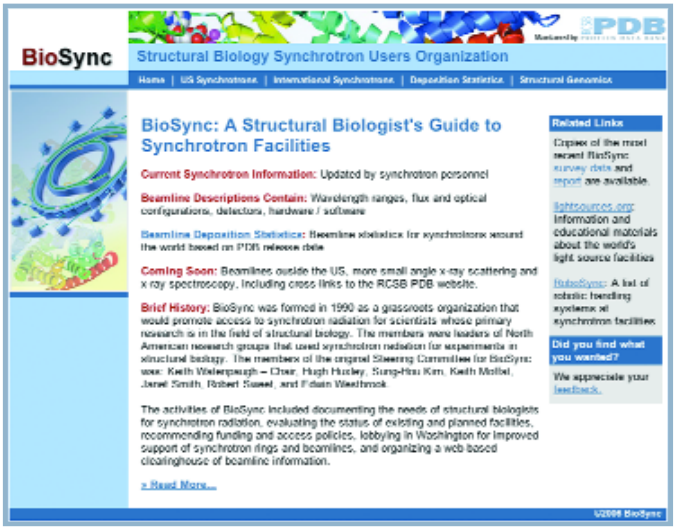
Website Statistics

Access statistics for www.pdb.org are given below for the second quarter of 2006.

MONTH	UNIQUE VISITORS	NUMBER OF VISITS	BANDWIDTH
APR	152,465	318,730	654.20 GB
MAY	157,055	336,815	539.67 GB
JUN	184,812	398,210	547.05 GB

Outreach and Education

BioSync is Alive and Growing



BioSync (Structural Biology Synchrotron Users Organization) was formed in 1990 as a grassroots organization intended to promote access to synchrotron radiation. It established a web-based clearing-house for beamline information at synchrotron facilities. The BioSync resource, originally designed and hosted by UCSD/SDSC, has been updated and is now being maintained by the RCSB PDB at BioSync.rcsb.org.

With its new look, the BioSync website currently contains updated descriptions of operational US synchrotron beamlines used for single crystal macromolecular crystallography. International sites and beam-lines are listed and will go 'live' as data is added for each one. PDB dep-osition statistics, grouped by site and beamline and cross-linked to the RCSB PDB, are also available.

Comments and suggestions are welcome at BioSync@deposit.rcsb.org.

Art of Science Exhibits at UCSD

Featuring images that explore the beauty found in structural biology, the RCSB PDB's Art of Science exhibit was on display with other artworks at Calit2 (University of California, San Diego) from June 9 – 30, 2006.

Molecule of the Month writer and illustrator David S. Goodsell (The Scripps Research Institute) provided additional watercolors, including a cross-section of blood serum, the interaction of HIV in the blood, and an illustration of a eukaryotic cytoplasm.

A wood carving of anthocyanidin synthatase, the natural pigment of berries, fruits and grapes, and a sculpture of human metalloelastase – both by Edgar Meyer (Texas A&M) – were also on display.

The show was exhibited at the CalIT2 building on the UCSD campus, next to the virtual reality visualization lab where "PDB-in-a-CAVE" demonstrations are run. The CAVE offers a room-sized space for users to interact with high-resolution video. Wearing stereo-glasses, the viewer can move through and around a projected biological macromolecule.

The Art of Science traveling exhibit includes pictures available from the RCSB PDB website and Molecule of the Month features. Since its beginnings at Rutgers University in New Jersey, the show has traveled to EMBL-Hamburg, Germany; University of Wisconsin-Madison; California State University, Fullerton; Purdue University; and Hyderabad, India. The RCSB PDB would like to see the Art of Science travel to other places. If you would be interested in sponsoring this exhibit at your institution, please let us know at info@rcsb.org.

David S. Goodsell: www.scripps.edu/mb/goodsell

Edgar Meyer: molecular-sculpture.com

RCSB PDB Poster Prize at ACA, ECM, ISMB, and AsCA

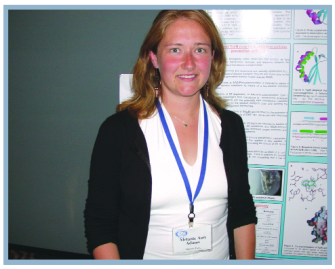
The RCSB PDB is pleased to announce the 2006 RCSB PDB Poster Prize, which recognizes student poster presentations at society meetings.

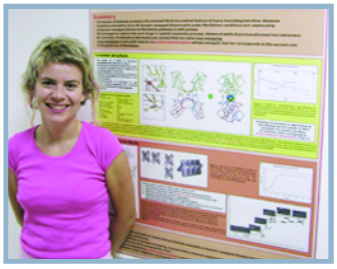
The prize will be awarded to the best posters related to macromolecular crystallography by undergraduate or graduate students at each of the meetings of the IUCr Regional Associates – the American Crystallographic Association (ACA), the European Crystallographic Association (ECM), and the Asian Crystallographic Association (AsCA).

At the Intelligent Systems for Molecular Biology (ISMB), the prize will be awarded to the best student poster in the "Structural Bioinformatics" category.

The awards consist of related educational books, and will be announced through the RCSB PDB website and newsletter. Information about previous winners and awards is available.

www.rcsb.org/pdb/static.do?p=general_information/about_pdb/poster_prize.html





The 2005 RCSB PDB Poster Prize winners: Melanie A. Adams at ACA and Sasa Jenko Kokalj at IUCr. (Not pictured: Andrew V. McDonnell and Alexandra Shulman-Peleg, co-winners at RECOMB)

Meetings and Exhibits

• NSTA – Jeff Milton met with teachers from around the country at the RCSB PDB's exhibit booth at the National Science Teacher's Association 54th National Conference on Science Education (April 6-9 in Anaheim, CA).

• MAMC – Annotator Massy Rajabzadeh presented the poster "Depositing Crystal Structures at the RCSB PDB in Five Simple Steps" and met with depositors at the 36th Mid-Atlantic Macromolecular Crystallography Meeting (June 1-3 at Wake Forest University in Winston-Salem, NC).

• Three-Dimensional Electron Microscopy – RCSB PDB Director Helen M. Berman described "How the History of the Protein Data Bank can inform the Future of Structural Biology" as one of the Keynote Lectures at the Gordon Conference on Three-Dimensional Electron Microscopy (June 25-30 at Il Ciocco, Barga, Italy).

PDB Education Corner:

Cheryl Campbell, New Providence High School

CHERYL CAMPBELL
graduated from Boise State University in Idaho in 1982 with a Bachelor of Science degree in Biology, and received her Masters in Teaching Natural Science from Rensselaer Polytechnic Institute in Troy, New York in 2002. After teaching for 13 years in Idaho in a small rural school, she moved to New Jersey and started teaching in New Providence. Through the years, she has taught Biology, Life Science, AP Biology, Honor's Biology, and Environmental Studies.

In October of 2005, I happened to notice a presentation on proteins while attending a convention for science teachers in New Jersey. I walked in and heard several people, including Christine Zardecki, talk about protein structure. The hands-on demonstrations with modeling kits[1] were fantastic, and I immediately knew I had to get the kits for my students. I ordered 10 kits and after using them, each class – Biology, Honor's Biology, and AP Biology – seemed to understand a little more about the three dimensional structures of proteins. The kits were such a success in the classroom that when I heard there was a competition on protein structure at the Science Olympiad… it didn't take much to convince the Biology Club to give the competition a try. The students worked early and late, trying to learn how to use the RasMol program and create a model of the TATA binding protein for the competition in January 2006. I am proud of the students who represented us at the Science Olympiad, and hope to participate again next year.

After the Olympiad, we were still thirsty to learn more from the structures in the PDB.

So on Wednesday, March 22, 2006, 10 juniors and seniors from New Providence High School (NJ) spent the day at Rutgers University listening and watching as scientists described and demonstrated their research projects.

We began our day with Dr. David A. Toke, our guide for a walking tour of the Rutgers University Cell and DNA Repository. He expertly described the steps in making cell lines that are being used to learn more about specific genes and their function. His own studies include taking a genetic approach to the study of addiction, longevity and many diseases. The students were particularly amazed at the size of the liquid nitrogen containers and the details required to insure both the privacy of data from human subjects and accuracy of data.

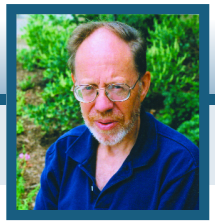
Next we had a chance to sit down and listen to Dr. Cathy Lawson (Department of Chemistry and Chemical Biology) describe how lysozyme crystals are grown. This was a very complicated talk, and the students were amazed at what the crystals look like and their role in the determination of protein structures.

Dr. Helen M. Berman, the director of the RCSB PDB, gave the students a great history of structural biology and the PDB. It is impressive to think of how much has become understood in the past 35 years.

After lunch, the students met two graduate students in Dr. Kathryn Uhrich's (Department of Chemistry and Chemical Biology) group – Min Jung Song and Jinzhong Wang. These students were the best. They showed us their experiments and talked about scientific discovery. The class saw how the process of learning by performing an experiment, and then rethinking their hypotheses using the results, worked in this laboratory.

The day was a great success. Each of my students gained some insight on how real research works. Experiences like this can help energize students to pursue science in their own college education and I would encourage more high school teachers to take advantage of what can be gained by interacting with the information in the PDB.

[1] Materials included the Mini-Toobers from3D Molecular Designs (http://www.3dmoleculardesigns.com), and the MSOE Model Lending Library (http://www.rpc.msoe.edu/lib/how.php)



PDB Community Focus:

Michael G. Rossmann

MICHAEL ROSSMANN *was born in Frankfurt (Main), Germany in 1930. He and his mother moved to England in 1939. He obtained a University of London B.Sc. degree in physics and mathematics. While teaching physics at the Royal Technical College in Glasgow (now the University of Strathclyde), he moonlighted at the University of Glasgow, obtaining a Ph.D. in chemical crystallography under the supervision of John Monteath Robertson. During that time, he married Audrey Pearson. His first two years of postdoctoral studies were in Bill Lipscomb's laboratory at the University of Minnesota where he spent some of his time writing some of the earliest crystallographic computer programs for structure determination and refinement. He returned to England in 1958 to join Max Perutz in Cambridge where he participated in the structure determination of horse oxy-hemoglobin at 5.5 Å resolution, thereby demonstrating the common evolutionary origin of oxygen carriers, such as hemoglobin and myoglobin. While in Cambridge and inspired by the hemoglobin results, he and David Blow established many of the techniques of modern macromolecular crystallography, including the molecular replacement method.*

In 1964, he moved to Purdue University. Initially, he studied dehydrogenases, discovering, in collaboration with Carl Brändén in Sweden and Len Banaszak at Washington University, that these proteins had a common NAD binding fold and, by extrapolation, that there existed a primordial nucleotide binding fold. He initiated his work on virus structure with a 1971 sabbatical half year with Bror Strandberg in Sweden. In 1985, he and his colleagues determined the structure of a common cold virus, the first animal virus to be determined to near atomic resolution, showing that there was a common origin of the capsid protein and assembly for simple RNA animal and plant viruses. This work had required the development of X-ray diffraction data processing techniques and the use of synchrotron methods, including the "American method" (still very much in favor among American politicians) of shooting first and thinking later (i.e. by-passing the old crystallographic technique of first "setting" crystals in order to be able to index the reflections).

He has continued to study numerous viruses, including the West Nile virus, the giant Mimivirus, and the bacteriophage T4. Currently, he is much involved in the use of cryo-electron microscopy (cryoEM) to extend the range of crystallography by combining low resolution cryoEM three-dimensional images with high resolution crystal structures of component proteins.

Q. *What was it like working in Cambridge in the 1950s? What made you decide to go to there at this time?*

A. Before I went to Cambridge, my interest in crystallography was fueled mainly by an interest in solving the phase problem for specific structures. I had heard a talk by Dorothy Hodgkin at the 1957 IUCr meeting in Montreal on the work in Cambridge by Perutz and Kendrew who were trying to solve the structure of proteins. With thousands of atoms per molecule, this seemed to be the ultimate challenge. Thus, when my postdoctoral time with Bill Lipscomb was nearing its end, I wrote a letter to Max Perutz asking whether he might have a job for me. He replied positively. Later, I discovered that many crystallographers thought that attempting to determine the structure of proteins was an unattainable objective and, hence, Max had had difficulty in finding helpers for his project. No doubt that was why he was now willing to take me into his small group.

Cambridge was a very new experience for me. Max's lab was a part of the famous Cavendish Laboratory where Rutherford, Thompson, and others had laid the foundations of nuclear physics. However, Max's group, initiated under the guidance of Sir Lawrence Bragg before he moved to the Royal Institution in London, had been expelled to a small hut outside the Austin wing of the Cavendish lab. My most important scientific education occurred during the morning coffee breaks when the approximately dozen occupants of the "MRC Hut" met in the crammed entrance area of the hut. This usually included Francis Crick, Sidney Brenner, John Kendrew, and Max. It is here that I began to realize that science is not only about solving puzzles, but, more importantly, recognizing what are the current significant problems susceptible to scientific investigation. We had relatively little contact with University activities, but Max had kindly arranged for me to be a "supervisor" for Peterhouse College. That required meeting with pairs of undergraduates and guiding them in their studies relevant to their current lecture courses. Like most people in England, I had always expected to find the best brains among Cambridge students, but I soon found that even in Cambridge there was quite a spread in ability.

The first year in Cambridge was especially exhilarating. This was the year that we determined the 5.5 Å structure of hemoglobin and recognized its evolutionary implications. This made an enormous impression on me and has guided my choice of research topics ever since. In the subsequent years, together with David Blow, I explored crystallographic techniques required in the potential determination of other protein structures based on my experience with the hemoglobin structure. It was David who suggested that we should study chymotrypsin together, a project that was subsequently brought to fruition by David and others after I had left Cambridge. These were exciting times, but I have been very fortunate in having experienced many more periods of frantic activity followed by great joy and satisfaction with new discoveries and understanding. Nevertheless, these first true adventures on the frontiers of science made a lasting and deep impression.

Q. *You were an early pioneer in methods development for protein crystallography. What drew you to this topic?*

A. To some extent, this question has been answered above. I gradually realized that the fun of solving crystallographic puzzles was merely a path to major discoveries in biology and medicine. The significance of the hemoglobin structure, recognized subsequently by a Nobel Prize to Max and John Kendrew, gave great satisfaction. Clearly, the daily fun of writing new computer programs and trying to solve the

little daily problems, such as how to scale data on different films, was a fairly certain path to discoveries of major importance.

Q. *You have always taken a strong interest in the PDB – why?*

A. During the important biological structure meeting at Cold Spring Harbor in 1971, Max called a meeting of all those who had coordinates of a protein structure. This included Fred Richards (ribonuclease), David Phillips (lysozyme), Jan Drenth (papain), and myself (lactate dehydrogenase). Max was concerned about the easy availability and preservation of coordinates. Walter Hamilton, of the Brookhaven National Lab, volunteered to be the curator, thus marking the beginning of the PDB. Sometime later, Fred Richards formed a steering committee that included me.

Although there were less than about a dozen structures in the early 70s, there was a tendency not to release coordinates except to friends. When Martha Ludwig and I were assistant editors to the *Journal of Biological Chemistry* (*JBC*), we instituted a policy that if a paper was dependent on a new set of coordinates, then these had to be deposited with the PDB. *JBC* was probably the first journal that had this policy. However, there were still quite a few published structures whose coordinates were unavailable in the PDB. Spurred on by need, I wrote a program that extracted coordinates from published stereo diagrams[1]. Fortunately, in those days, structural diagrams were usually merely a set of atomic positions joined by bonds. Ribbon diagrams had not yet become popular, although my wife had produced the first such figures based on models of carbonic anhydrase made by Anders Liljas and Bror Strandberg while we were on sabbatical leave in Uppsala[2]. At the 1976 Erice meeting, I made a plea for the compulsory deposition of coordinates for any published structure.

In more recent years, I have been concerned about maintaining funding and continuity of services by the PDB.

Q. *You have used crystallography to study structures ranging from small molecules to proteins to large viruses. Recently, you have been studying structures using cryo-electron microscopy. What do you see as the next challenge?*

A. For the PDB, there is a challenge for appropriate archiving of data derived from an increasing variety of physical techniques, including not only the final inferred coordinates, but also the raw data.

More generally, I see trends to look at structures of ever-increasing complexity to a point where the structures of equivalent objects are no longer sufficiently similar to permit crystallization or averaging of single particles observed by electron microscopy. Such problems may require using single particle diffraction techniques, high intensity synchrotron X-ray sources, and tomographic electron microscopic imaging. I expect that we will soon be looking at frozen vitrified single cells and, in the distant future, even observing living cells at near atomic resolution.

Clearly, such work will require ever larger PDB resources to make the results generally available and to avoid loss of information. I see the task of the PDB as being ever more challenging and more essential to all of science. I am seriously afraid of bureaucratic interference in the smooth development and growth of the PDB, which might have major negative impact on scientific progress.

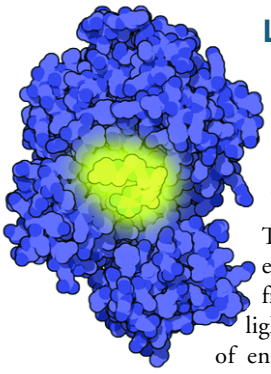
Q. *What would be your advice to someone just starting out in structural biology?*

A. Keep working in the lab. Enjoy your successes and share them with all who want to know. Find a mentor who can teach you a fundamental appreciation of science like I had the opportunity to learn in Cambridge. Never hide your ignorance, because then nobody can teach you. If you are not enjoying your studies, go and do something else.

Molecules of the Quarter:

Hemagglutinin, Glucose Oxidase, Luciferase

The **MOLECULE OF THE MONTH** *series explores the functions and significance of selected biological macromolecules for a general audience. The molecules featured this quarter were hemagglutinin, glucose oxidase, and luciferase. The complete Molecule of the Month features are accessible from the RCSB PDB home page.*



Luciferase (June 2006)

Do you remember the first time that you saw a firefly? If you live anywhere between the Rocky Mountains and the east coast of the US, you have probably chased fireflies since you were a child.

The cool yellowish light of fireflies is created by the enzyme luciferase, shown here from PDB entry 2d1s. The creation of light is not an easy process. It requires a lot of energy – a single photon of green light requires about the same energy as the breaking of eight ATP molecules. So, luciferase uses a very energetic process to create light. It has a cofactor, termed a luciferin, that forms a highly strained complex with oxygen, using an ATP molecule to help set everything up. When this oxygenated luciferin breaks, forming carbon dioxide in the process, it leaves behind a highly excited form that then emits the light.

PDB ID: 2D1S

Nakatsu, T., Ichiyama, S., Hiratake, J., Saldanha, A., Kobashi, N., Sakata, K., Kato, H. Structural basis for the spectral difference in luciferase bioluminescence Nature ***v440*** *pp.372-376, 2006*

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[2]Liljas, A. *et al.* Crystal structure of human carbonic anhydrase C. *Nat. New Biol.* **v.235** pp. 131-137, 1972.

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 (www.wwpdb.org)

RCSB PDB Management

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

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

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RCSB PROTEIN DATA BANK
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