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Research Collaboratory for Structural Bioinformatics Protein Data Bank

RCSB PDB PROTEIN DATA BANK NEWSLETTER

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Contents

SNAPSHOT: APRIL 1, 2013

89212 released atomic coordinate entries

ENTRIES BY MOLECULE TYPE

82570	proteins and peptides
4099	protein/nucleic acid complexes
2520	nucleic acids
23	other

ENTRIES BY EXPERIMENTAL TECHNIQUE

78608	X-ray
9869	NMR
514	electron microscopy
52	hybrid
169	other

RELATED EXPERIMENTAL DATA FILES

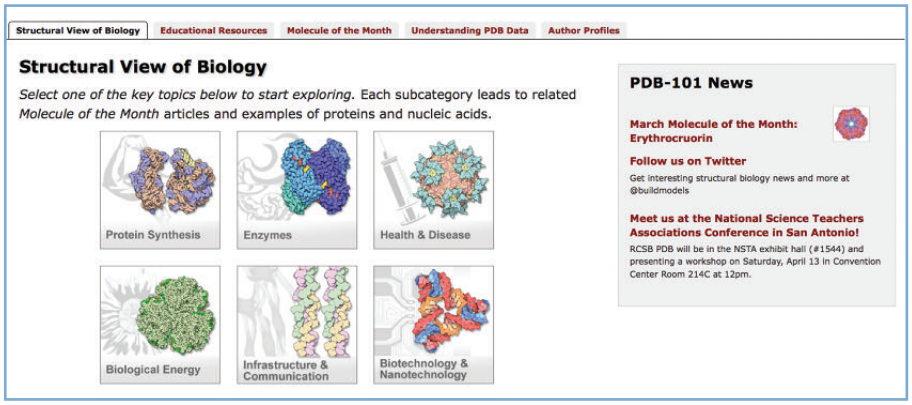
68096	structure factors
7178	NMR restraints
1797	EMDB electron microscopy maps
936	NMR chemical shifts

Message from the RCSB PDB

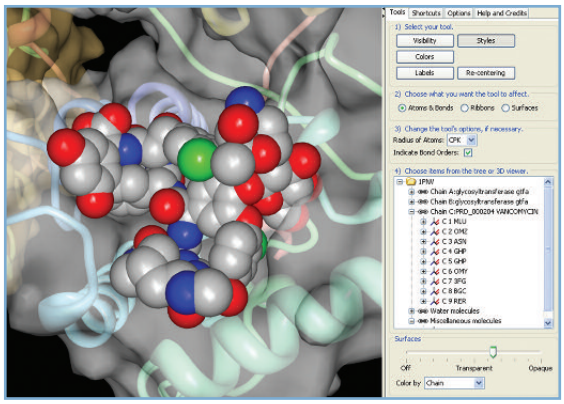
New and enhanced features have been added to the RCSB PDB, including:

- The Simple Search available from the top menu bar has a cleaner and simpler look and feel. The search form offers the same search suggestion capabilities.
- A new Browse Database option can be used to find structures using the Anatomical Therapeutic Chemical (ATC) Classification System for drugs from the WHO Collaborating Centre for Drug Statistics Methodology.
- Jmol pages now include an updated Display Options menu, new scripting options, tabs for domains and ligands, and the JavaScript beta version of Jmol.
- Information about protein stoichiometry and symmetry have been integrated into drill down charts and Advanced Search. Symmetry features can be highlighted in Jmol.
- Options to search, view annotations, and visualize about the peptide-like antibiotic and inhibitor molecules described in the wwPDB's Biologically Interesting molecule Reference Dictionary.

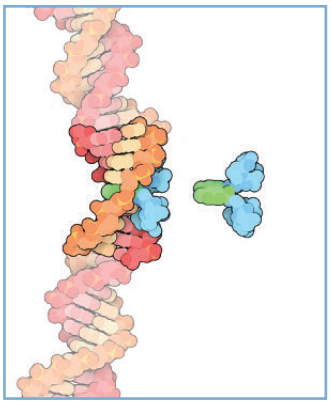
See the **What's New** page for more new features and examples.



PDB-101 has new tabs for easier access to Educational Materials, Molecule of the Month, *Understanding PDB Data, and Author Profiles.* ***PDB-101 News*** *has been added.*



Protein Workshop view of vancomycin PRD_000204 as seen in PDB ID 1pnv.



April's Molecule of the Month *looks at the BIRD molecule actinomycin*

Data Deposition and Annotation

Deposition Statistics

In the first quarter of 2013, 2501 experimentally-determined structure coordinates and 127 3DEM maps were deposited to the archive.

84% were deposited with a release status of hold until publication; 13.5% were released as soon as annotation of the entry was complete; and 2.6% were held until a particular date. 92.6% of these entries were determined by X-ray crystallographic methods; 5.7% were determined by NMR methods.

During the same period, 2166 structures were released in the PDB.

wwPDB News

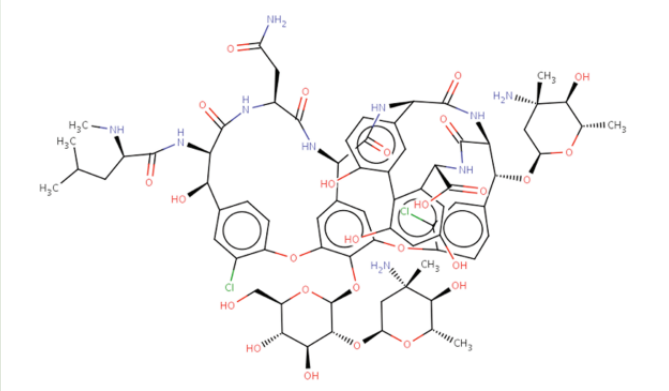
The Biologically Interesting Molecule Reference Dictionary (BIRD) for Peptide-like Antibiotic and Inhibitor Molecules

The wwPDB's Biologically Interesting molecule Reference Dictionary (BIRD) describes antibiotics, peptide inhibitors, and other complex biological ligands. To help define and represent these biologically interesting molecules, BIRD contains chemical descriptions, sequence and linkage information, and functional and classification information as taken from the core structures and from external resources.

All PDB entries containing these molecules have been annotated using this dictionary, with corresponding BIRD ID code contained only in the PDBx-formatted file. The use of BIRD will greatly improve the consistency of peptide-like antibiotic and inhibitor molecules in the PDB.

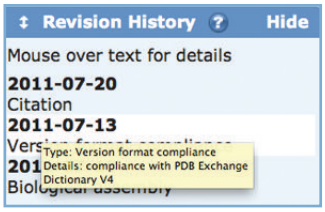
BIRD is available on the wwPDB FTP server adjacent to the Chemical Component Dictionary at ftp.wwpdb.org/pub/pdb/data/bird/prd/.

These data reflect the wwPDB's continuing commitment to providing accurate and detailed data to users worldwide.



Chloroorienticin A has a disaccharide and a monosaccharide decorating the peptide core (PRD_000203)

Revision History Widget



The Revision History box shows the modification date and a summary description; mousing over the text provides additional details.

Structure Summary pages offer a variety of information about an entry, organized into different widget boxes that can be moved around on the page.

The Revision History widget box displays the details of changes made to an entry's mmCIF/PDBx file after the initial release. The details of these changes have been recorded in the category PDBX_VERSION since July 2011 (see the wwpdb.org for more information).

These descriptions are more detailed than the information stored in REVDAT records, which indicate what records have been changed in the PDB format file for the entry.

Data Query, Reporting, and Access

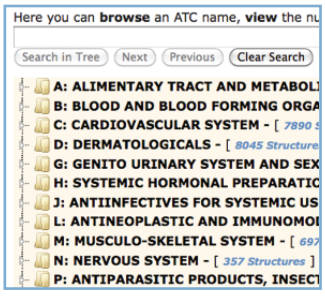
Access Drugs and Drug Targets in the PDB

New features for exploring drugs found in PDB entries were recently added to the website.

Auto-complete suggestions of stereoisomers when searching for ibuprofen.

Stereoisomers The integration of drug and drug target data from DrugBank (www.drugbank.ca) has been extended to include stereoisomer matches. Searches for a given drug name will now return the different stereoisomers of the drug. For example, a Simple Search for ibuprofen in the top bar will suggest the different stereoisomers associated with the drug.

DrugBank Widget A new Drug Info widget available from Ligand Summary pages lists the corresponding data from DrugBank (when available). The widget contains DrugBank ID, drug name, groups, brand name, and more, with links to the corresponding data at DrugBank. A sequence search based on the drug target sequence can be launched from this widget. For an example, see the Ligand Summary page for BP (Ibuprofen).

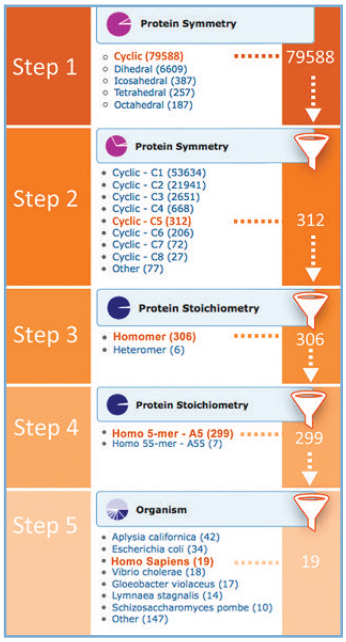


Enter search terms or browse through categories to find PDB structures in a given Anatomical Therapeutic Chemical class.

Browse Database using ATC The WHO Collaborating Centre for Drug Statistics Methodology's Anatomical Therapeutic Chemical (ATC) classification system organizes drugs into five levels according to the organ or system on which they act and/or their therapeutic and chemical characteristics. The RCSB PDB database can now be browsed using this system. Select the ATC tab from the Browse Database interface to navigate through the drug classification hierarchy, view the number of associated PDB structures, and access the related entries.

Distribution of PDB Data by Protein Stoichiometry and Symmetry

Distribution drill-downs for protein stoichiometry and symmetry (at 95% sequence identity threshold) have been added to the Explore Archive widget on the home page. The stoichiometry and symmetry information comes from the first biological assembly associated with the entry.



The drill-downs can be applied successively. For example to find C5 symmetric homo-pentameric human proteins one would use the following sequence of drill-downs:

Step 1: Protein Symmetry Cyclic

Step 2: Protein Symmetry C5

Step 3: Protein Stoichiometry Homomer

Step 4: Protein Stoichiometry A5

Step 5: Organism *Homo sapiens*

Drill-downs, including options for stoichiometry or symmetry, can also be used to further refine search results from the query result browser page.

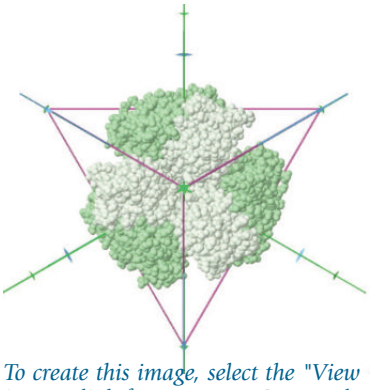
Advanced Search can also be used to search for structures based on protein stoichiometry and symmetry.

3D Visualization of Protein Symmetry

To facilitate the exploration of symmetry, several options are available from the 3D Jmol views of structure:

Default Orientations Users can toggle between canonical views of structure that highlight symmetry: sides and back, and along unique n-fold symmetry axes.

Symmetry axes and polyhedra Symmetry axes and symbols representing folds (dyad for 2-fold, triad for 3-fold axis, or in general a polygon for n-fold axis) can be displayed with a structure. Users can select to view the protein enclosed in a polyhedron that matches its symmetry.



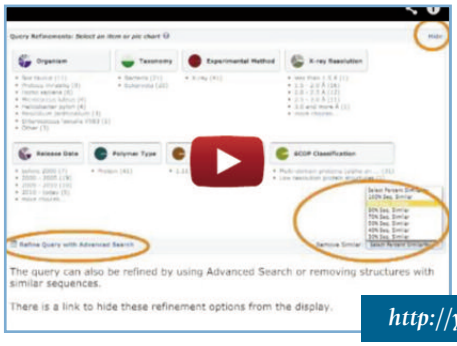
To create this image, select the "View in 3D" link for PDB ID 1G63, and then select Jmol options polyhedron: on; axes: on; style: CPK; color: symmetry; and deselect background: black.

Colored by symmetry or subunit Structures can be colored by symmetry, sequence (subunits with >= 95% sequence identity shown in the same color), or by subunit.

Pseudosymmetry The default view shows symmetry based on a 95% sequence identity threshold. Since some structures will display pseudosymmetry when using a 30% sequence identity threshold, an option lets users toggle between the two options.

To access Jmol on the RCSB PDB site, select the "View in 3D" link on any entry's Structure Summary page. Protein symmetry is calculated for all entries containing at least one protein chain, including asymmetric units and all biological assemblies (except for entries split among several PDB files due to their size).

Quick Tour of Search Results



A new video demonstrates the different options available for exploring search results at the RCSB PDB website.

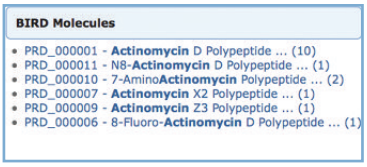
http://youtu.be/G3mA1UFUKps

Search, View Annotations, and Visualize Peptide-like Antibiotic and Inhibitor Molecules

BIRD stands for the wwPDB's Biologically Interesting molecule Reference Dictionary, and contains information about the representation of peptide-like antibiotic and inhibitor molecules in the PDB archive. New RCSB PDB website features utilize BIRD data to provide improved searching and visualization options for these molecules:

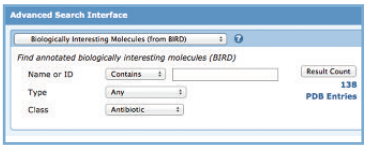
Search BIRD Molecules

Simple Search: Biologically interesting Molecules from BIRD can be searched by typing a name (vancomycin), a BIRD ID (PRD_000204), type (glycopeptide), or class (antibiotic) in the top search bar. Suggestions will appear under the BIRD Molecules category.



Autosuggestions from a Simple Search for actinomycin

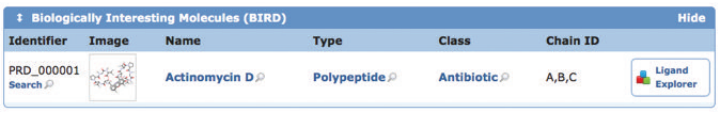
Advanced Search: Biologically interesting Molecules from BIRD can also be searched from the advanced search menu. Search by text/name, BIRD type (structural classification of the entity), or BIRD class (broad definition of the entity function).



Advanced Search options for querying BIRD

View Annotations from BIRD: The BIRD widget on an entry's Structure Summary page will display the ID, image, name, type, class, and chain location for any such molecules in the entry. Ligand Explorer can be launched to view the molecule and binding site in 3D.

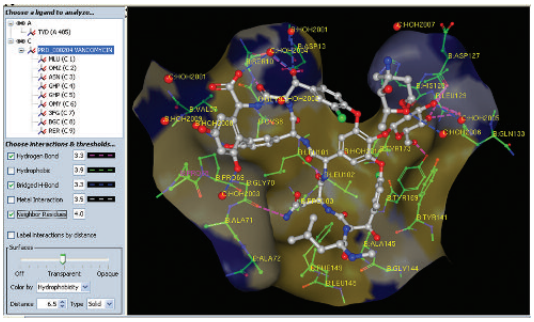
As with other Structure Summary page features, the examples displayed (ID, name, type, and class) can be used to find other PDB entries with the same characteristics.



BIRD widget from PDB ID 1a7y

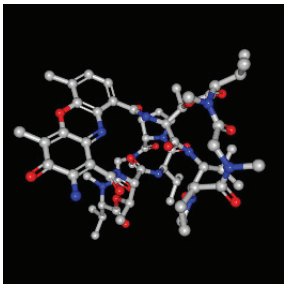
Visualize BIRD Molecules

Ligand Explorer: Ligand Explorer can be launched from the BIRD Widget to visualize these molecules and their binding sites. The program can center on other molecules by clicking on a name or identifier from the left hand menu. Intermolecular interactions such as hydrogen bond or hydrophobic interactions and a binding site surface can be turned on for the active ligand.

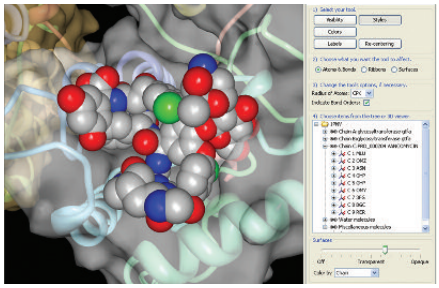


Ligand Explorer view of Vancomycin PRD_000204.

Protein Workshop: In Protein Workshop, BIRD molecules are listed in the right hand menu and can be manipulated as with any other macromolecule chain or ligand. Protein Workshop can be launched from any entry's Structure Summary page.



Protein Workshop view of actinomycin D as seen in PDB ID 1a7y.



Protein Workshop view of vancomycin PRD_000204 as seen in PDB ID 1pnv.

wwPDB News

Time-stamped Copies of the PDB Archive

A snapshot of the PDB archive (**ftp.wwpdb.org**) as of January 1, 2013 has been added to **ftp://snapshots.wwpdb.org/**. Snapshots have been archived annually since January 2005 to provide readily identifiable data sets for research on the PDB archive.

The directory 20130101 includes the 87,090 experimentally-determined coordinate files and related experimental data that were available at that time. Coordinate data are available in PDB, mmCIF, and XML formats. The date and time stamp of each file indicates the last time the file was modified.

The script at **ftp://snapshots.wwpdb.org/rsyncSnapshots.sh** may be used to make a local copy of a snapshot or sections of the snapshot.

Website Statistics

Access statistics for the first quarter of 2013 are shown.

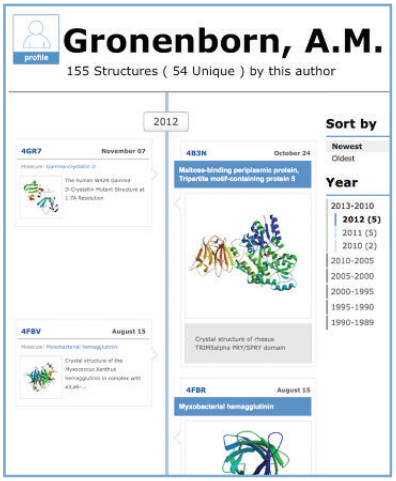
Month	Unique Visitors	Number of Visits	Bandwidth
JANUARY	308,327	703,069	1785.92 GB
FEBRUARY	317,729	683,177	1866.81 GB
MARCH	346,548	765,109	1529.32 GB

Outreach and Education

Author Profiles: Timeline Display of a Researcher's Structures

Author Profiles are a unique historical and educational tool offering a timeline display of all structures associated with a particular researcher. Structures are sorted by deposition date, with the first instance of a protein or protein complex highlighted. Images are linked to the Structure Summary page for the entry.

A search box is provided to search by author or structural genomics center name. Author Profile URLs are permanent links that can be copied and shared.



A.M. Gronenborn's Author Profile

Portable Molecules (of the Month)

Read Molecule of the Month *articles using RCSB PDB* Mobile.

The RCSB PDB *Mobile* app for Apple iOS provides fast access to PDB searching and molecular visualization.

The entire catalog of *Molecule of the Month* articles is available. Each feature describes important biological molecules and how they function with descriptive text and illustrations. The molecules used as examples in the articles can be further explored and viewed in 3D.

A version of the app for the Android will be announced shortly.

Poster Prize Awarded at AsCA

Yohta Fukuda

The RCSB PDB Poster Prize went to Yohta Fukuda at the Joint Meeting of the Asian Crystallographic Association (AsCA), Society of Crystallographers in Australia and New Zealand (SCANZ) and the BRAGG Symposium (December 2 - 6, 2012, Adelaide, Australia) for *Atomic resolution structure of copper-containing nitrite reductase provides insights into common properties of type 2 copper-containing enzymes* (Yohta Fukuda,[1] Taro Tamada,[2] Hideto Takami,[3] Tsuyoshi Inoue,[1] Masaki Nojiri;[1] [1]Osaka University, [2]Japan Atomic Energy Agency, [3]Japan Agency of Marine-Earth Science and Technology).

Yohta will receive *Computational Structural Biology* (Torsten Schwede, Manuel C. Peitsch, editors) and *International Tables of Crystallography* Volume F.

Many thanks to Charlie Bond (University of Western Australia) and AsCA.

ASBMB Honors RCSB PDB Director

Helen Berman is the 2013 Awardee of the DeLano Award for Computational Biosciences of the American Society for Biochemistry and Molecular Biology. The Award, established by family, friends and colleagues to honor the legacy of Warren L. DeLano, recognizes scientists for the most accessible and innovative development or application of computer technology to enhance research in the life sciences at the molecular level.

This award recognizes her accomplishments toward enabling a freely available and uniform worldwide archive of 3D structural information for biomedical research and education. Prof. 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 ASBMB's Annual Meeting (April 20-24, 2013) in Boston, MA. Prof. Berman will present her award lecture, *PDB as a public resource for enabling protein science*, on Monday, April 22. For the full list of awardees, please see **asbmb.org**.

Art of Science exhibits in Giza, Egypt

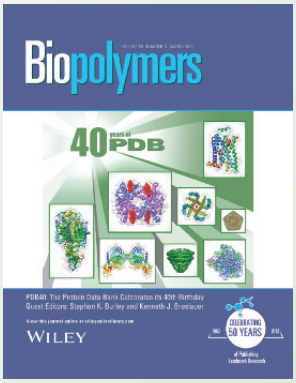
SIRA CORP recently displayed the Art of Science *show.*

SIRA CORP hosted a Protein Science Museum using images from the RCSB PDB's *Art of Science* exhibit. The event was part of the Biotechnology Symposium 2013 held March 16, 2013 at Cairo University. The first of its kind in Egypt, this display and event targeted junior researchers as well as Biotechnology undergraduate students.

SIRA CORP is a consulting and training company focusing on bridging the gap between Egypt and the advanced world in critical science and technology disciplines. For more information, see **www.sira-corp.com** and **www.facebook.com/SiraCorpBiotechnology.**

wwPDB News

Special issue of Biopolymers Continues PDB40 Celebration



The March 2013 issue of *Biopolymers* contains six invited contributions based on presentations made at the October 2011 symposium held at Cold Spring Harbor Laboratory that commemorated 40 years of the Protein Data Bank archive.

This special issue was edited by Stephen K. Burley and Kenneth J. Breslauer, and begins with an editorial describing the history of the PDB from its beginnings through the 2011 celebration.

Articles include:

- *PDB40: The Protein Data Bank celebrates its 40th birthday*, Stephen K. Burley
- *Studying and polishing the PDB's macromolecules*, Jane S. Richardson and David C. Richardson
- *Abstracting knowledge from the Protein Data Bank*, Nicholas Furnham, Roman A. Laskowski and Janet M. Thornton
- *The impact of influenza hemagglutinin fusion peptide length and viral subtype on its structure and dynamics*, Justin L. Lorieau, John M. Louis and Ad Bax
- *Sweet entanglements–protein: Glycan interactions in two HIV-inactivating lectin families*, Leonardus M. I. Koharudin and Angela M. Gronenborn
- *A primer in macromolecular linguistics*, David B. Searls

The issue concludes with an article by the wwPDB directors describing *The Future of the Protein Data Bank.*

The program and selected presentations from the October 2011 meeting are available online from the wwPDB website.

Biopolymers
Special Issue: PDB40: The Protein Data Bank Celebrates its 40th Birthday
Volume 99, Issue 3, pages 165–222, March 2013
http://onlinelibrary.wiley.com/doi/10.1002/bip.v99.3/issuetoc

Education Corner by Rachel Kramer Green, Ph.D.

The Ins and Outs of the RCSB PDB Help Desk: What do we learn from our users? What do they learn from us?

Did you ever wonder what happens when you fill out the form on the "Contact Us" page (Figure 1) at the RCSB PDB website? Who is going to answer you? What types of questions do your colleagues ask?

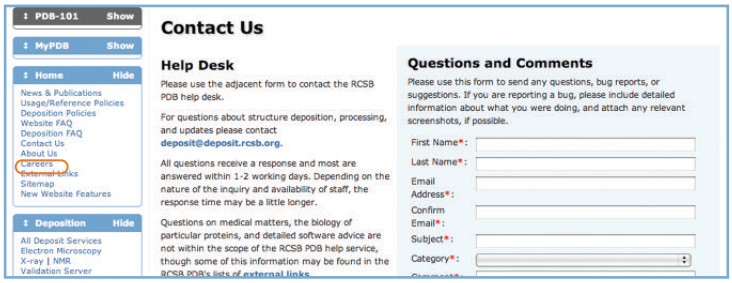


Figure 1: The Contact Us page.

The RCSB PDB Help Desk supports people from all over the world who write daily for assistance with the website, archive and general structural biology. About 1000 electronic conversations are initiated by nearly as many unique users in any given year. Many queries also lead to additional questions and clarifications. Questions come from students new to structural biology, users interested in the general study of science, and domain experts from various disciplines that utilize PDB data.

Once you press the "Send your feedback" button, a copy of your question or comment is delivered to me to answer or triage to other members of the RCSB PDB team. Simultaneously, a ticket is loaded into our tracking system so that we are sure to follow-up on each and every message. From that point, a team of scientists, computer specialists, and educators are available to assist with your needs.

Managing the Help Desk

From my college days, I was fascinated by the idea of a crystal as an orderly array of molecules. Once in graduate school I learned that not only was this a cool thing, but that from it you could figure out what the stuff in the crystal looked like and then how it worked. I have also always been an avid reader, fascinated by words and the use of the English language. As the long self-proclaimed "grammar police" with a grandmother who would send me back my letters with spelling and grammatical mistakes corrected, editing and writing were always close competitors with science as my main intellectual interest. After editing both my high school and college newspapers while exploring and majoring in chemistry, the idea of explaining and teaching science to lay people was always intriguing to me.

My work with the RCSB PDB's Help Desk has allowed me to do just that. Users write in from all over the world, and I have been fascinated by the different written cadences and expression with which users from different nationalities write. But, don't worry too much about your English when you write, I always enjoy figuring out what you are asking. On occasion, an email arriving in Italian or German has even provided me the opportunity to try out Google Translate.

RACHEL KRAMER GREEN, *received her Ph.D. in 1998 in Chemistry from Rutgers University. Her research thesis, conducted in the laboratory of Professor Helen M. Berman was entitled* The X-ray Crystallographic Studies of Collagen-like Peptides. *As she was concluding her degree, the management of the PDB was moving from Brookhaven National Laboratories to the RCSB PDB. Rachel coordinated the transition of data processing for the PDB from Brookhaven to the RCSB. Following the move of her family to Denver, Colorado in 1999, Rachel continued to work remotely for the RCSB PDB performing a variety of jobs including assisting in website development, writing electronic and print outreach materials as well as managing the help desk. Rachel is now in her 13th year of working for the RCSB PDB project.*

In fact, that is one of the things that I love most about my job. Each question is a bit of a mystery. Some are more easily solved with a single link or comment, and others require some research and consultation with my colleagues. What is the user asking? Do we provide anything that will help? Do we need to develop something that will? If there is a problem, can we correct it easily, or will it take some extended effort?

People also write with all levels of experience. Some ask for help with homework with interesting questions. Others are power users of the archive and website whom I am privileged to have been able to help over the course of years.

Some Common Types of Questions

Over the years, the types of questions have changed as ever-continuing website development and data remediation efforts have made the resource much more usable and accurate. Questions and comments to the email help desk have become much more about research queries and suggestions for new features than about things that need to be

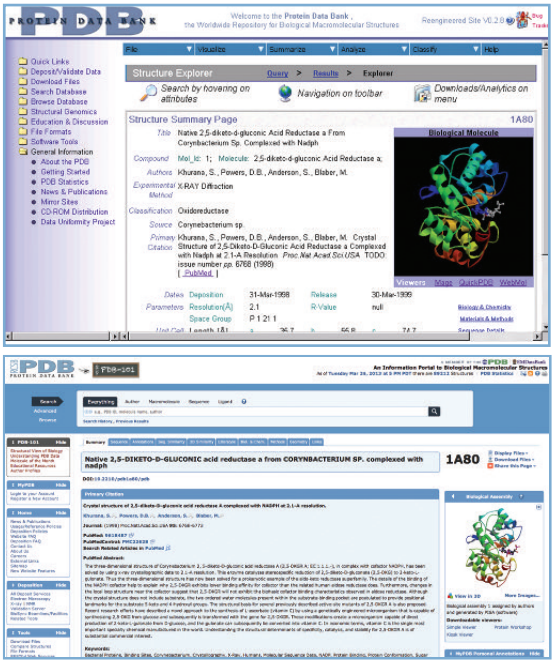


Figure 2: The structure summary page for entry 1A80 circa 2003 and now.

changed, more easily found, or fixed. Look and feel updates to the website over the years (Figure 2) have made access to the website and the underlying data a much more user-friendly experience.

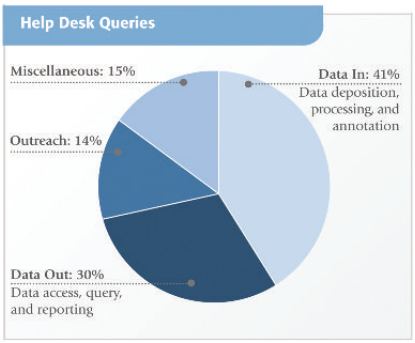


Figure 3: From the 2012 RCSB PDB Annual Report - types of questions to the help desk.

While you write about many, varied types of things, questions to the Help Desk tend to be evenly split between deposit and query-related issues with the remainder concerning outreach, file format, problems with service (these often stem from external firewall issues), the use of molecular viewers, and data download questions (Figure 3).

One deposit-related category that appears frequently is a user writing to let us know that a citation has been published and that the corresponding structure entry can thus be released. While we do use an internal scanning tool to identify new PubMed entries and receive citation notifications from journal representatives, email messages from authors and users alike are very helpful in our efforts to release entries in a timely manner.

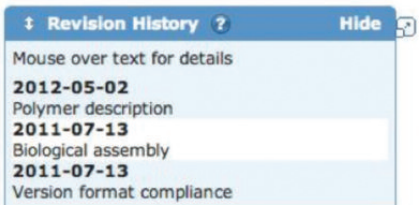


Figure 4: The Revision History widget was created in response to user requests.

Frequently, user questions regarding various aspects of the site lead to improvements and the implementation of new features. Such comments help us to identify in which areas users are most interested and where we should place our development efforts. For example, frequent requests for a version of RCSB PDB *Mobile* for the Android platform led to work in this area. As a result, an app is now in alpha testing. Also the desire of users to be able to easily review changes that have been made to PDB files led to the implementation of a "Revision History" feature on the Structure Summary pages (Figure 4).

One area of regular interest is how to conduct a particular search or how to generate a report of a particular type of information available in the database. These types of questions let us know the kinds of searches in which users are interested, and show us areas where we may need to add functionality. Many improvements that have been made to searching and reporting features (such as the recent addition of an option to search by method used for structure solution – MAD, SAD, Molecular Replacement, *etc.*) have in a large part stemmed from user comments and suggestions.

File format is another area that generates many queries to the Help Desk. Whether for deposition or programming purposes, detailed explanations and direction to the appropriate places in the documentation are given. One common question regards the difference between the sequence found in the SEQRES records and that found in the coordinate records. In general, the SEQRES records and FASTA sequence gives the entire sequence studied (even if some of it was not experimentally observed) and the coordinate section gives only what was experimentally observed. In a PDB format file, REMARK 465 lists discrepancies between the SEQRES and the coordinate section. Along with visual and functional improvements to the sequence tab of the Structure Summary page, sequence-related questions to the Help Desk led to the development of the section "Primary Sequences and the PDB Format" on PDB-101's "Looking at Structures" resource and more detailed documentation on the website.

Interaction with the user community also alerts us to problems on the site or inaccuracies in the archive of which we might otherwise be unaware. Often we can provide a quick fix for these problems (even within the day or week), and other times the solution may require a data remediation effort, for example when new information becomes available over time, or a complicated fix to the site.

The Help Desk and Outreach

The Help Desk is one of the many tools the RCSB PDB utilizes in its outreach efforts. In 2012, ~13% questions related to outreach and education. Interactions with journals, publishers, teachers and students regarding our images and educational materials both promote our activities and provide us with valuable feedback about the features that are most used and new ones that may be helpful to the community.

Many outreach-related emails include requests for permission to reprint a particular image in materials both in English and a variety of other languages. These questions come from a vast sampling of the community, including journal and textbook authors and editors; doctoral students completing their theses; creators of webpages, posters, animations, sculptures, and online educational materials; documentary producers; teachers and professors for use in their lectures and classroom materials, and many others. Many are referred to the RCSB PDB Policies & References page. One recent request led to the inclusion of a *Molecule of the Month* image on the NPR science blog post by Robert Krulwich on the different ways proteins can be visualized.

Many users are interested to learn how the popular *Molecule of the Month* images are created. I am able to direct these queries to an interview with the author and illustrator of the series, David Goodsell, that was published in our newsletter in 2003.

Other questions relate to our print and electronic publications – the newsletter, annual report, posters, and online tutorials. We also occasionally receive queries regarding the history of the PDB and RCSB PDB.

Tracking System

Many of the improvements that we have made regarding user-satisfaction have resulted from the institution of an issue-tracking system for the Help Desk that is integrated with our website development tracking system. This system ensures that users receive timely responses and gives us the ability to notify users when their issues and suggestions have been resolved or implemented. Using the tracker also enables us to have an overview of new features that would be of interest to the most users.

We have also found the tracking system to be useful to monitor when busy and slow periods occur. For example, as you might imagine, the end of summer and the period between Christmas and New Year's are particularly light times.

Over the years, I have learned so much from all of you about your interests. And every once in a while someone writes from here in Colorado and I grin to myself that I am undercover "right next door" (although now the secret is out). And sometimes, someone writes about a collagen-related structure and I get to discuss a little bit about this molecule that I came to love. Recently, I realized that I miss my users when you are quiet… so please, keep up the emails. I love to hear from you.

RCSB PDB PROTEIN DATA BANK NEWSLETTER

Web: www.rcsb.org
Email: info@rcsb.org
FTP: ftp.wwpdb.org

RCSB PDB Partners

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

RUTGERS

Rutgers, The State University of New Jersey
Center for Integrative Proteomics Research
174 Frelinghuysen Road
Piscataway, NJ 08854-8087

UCSD SDSC • SKAGGS SCHOOL of PHARMACY and PHARMACEUTICAL SCIENCES

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

WORLDWIDE PDB PROTEIN DATA BANK

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

RCSB PDB Management

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

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

DR. STEPHEN K. BURLEY, Associate Director
Rutgers, The State University of New Jersey
sburley@proteomics.rutgers.edu

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

A list of current RCSB PDB Team Members is available from ww.rcsb.org.

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RCSB PROTEIN DATA BANK
www.rcsb.org • info@rcsb.org

Rutgers, The State University of New Jersey
Center for Integrative Proteomics Research
174 Frelinghuysen Road
Piscataway, NJ 08854-8087
USA