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Research Collaboratory for Structural Bioinformatics Protein Data Bank

RCSB PDB PROTEIN DATA BANK NEWSLETTER

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

Contents

SNAPSHOT: JULY 1, 2013

91761 released atomic coordinate entries

ENTRIES BY MOLECULE TYPE		ENTRIES BY EXPERIMENTAL TECHNIQUE	
84955	proteins and peptides	80936	X-ray
4234	protein/nucleic acid complexes	9987	NMR
2549	nucleic acids	615	electron microscopy
23	other	52	hybrid
		171	other

RELATED EXPERIMENTAL DATA FILES

70449	structure factors
7296	NMR restraints
1902	EMDB electron microscopy maps
1055	NMR chemical shifts

Message from the RCSB PDB

The RCSB PDB serves a wide variety of users interested in biology, including researchers, teachers, students, and the general public. To help keep our different user communities informed about RCSB PDB activities, we rely on a number of web- and email-based communication methods, including social media.

- RCSB PDB weekly news is the primary source for updates and related content. Detailed announcements of meetings and events, new tools, PDB-101 features, and descriptions of how to use RCSB PDB tools and services are posted with each regular update to the home page and to pdb-l@rcsb.org.
- wwPDB announcements and news are published at wwpdb.org. These notices then appear on the RCSB PDB home page in the wwPDB widget. An RSS feed is also available.
- Educational highlights are published on the PDB-101 home page, along with the latest *Molecule of the Month* column. *Molecule of the Month* articles are also pushed via an RSS feed.
- These news features are all posted on Facebook (www.facebook.com/RCSBPDB) and Twitter (@buildmodels), along with links to related news and other materials found at external resources.
- The quarterly newsletter combines RCSB PDB news with additional details, including deposition statistics and website usage information.

In addition, the newsletter's *Education Corner* shows how the PDB archive and RCSB PDB resources are used in classrooms all over the world. Past topics have ranged from a crystallography program for middle school students to the educational experiences that led recent RCSB PDB Poster Prize awardees to study structural biology in graduate school.

With RCSB PDB news and updates so readily available through electronic methods, we have decided to cease printing the paper edition of the quarterly newsletter. The current issue will be the last that is printed and mailed to our subscribers.

The newsletter will still be published online. We encourage all of our readers to sign up for quarterly newsletter email alerts at bit.ly/13XwVFP.

wwPDB is 10!

July 1, 2013 marks the 10th anniversary of the founding of the Worldwide Protein Data Bank.

The wwPDB consists of organizations that act as deposition, data processing and distribution centers for PDB data: RCSB PDB (USA), PDBe (Europe) and PDBj (Japan), and BMRB (USA). The wwPDB's mission is to maintain a single PDB archive of macromolecular structural data that is freely and publicly available to the global community.

Data Deposition and Annotation

wwPDB News

SAS Task Force Report Published

The wwPDB Small-Angle Scattering Task Force has published their *Report of the wwPDB Small-Angle Scattering Task Force: Data Requirements for Biomolecular Modeling and the PDB Structure* (2013) Jill Trewhella, Wayne A. Hendrickson, Gerard J. Kleywegt, Andrej Sali, Mamoru Sato, Torsten Schwede, Dmitri I. Svergun, John A. Tainer, John Westbrook and Helen M. Berman, *Structure* **21**: 875-881 **[doi: 10.1016/j.str.2013.04.020]**

The first meeting of the Small Angle Scattering (SAS) Task Force was sponsored by the wwPDB and held in July 2012 at the Center for Integrative Proteomics Research at Rutgers, The State University of New Jersey. The Task Force, chaired by Jill Trewhella, includes experts in SAS, crystallography, data archiving, and molecular modeling.

Recognizing the rapidly growing community of structural biology researchers that acquire and interpret SAS data in terms of increasingly sophisticated molecular models, the SAS Task Force made several recommendations. These include: development of a global repository for X-ray and neutron SAS data; creation of a standard dictionary of terms for data collection and for managing the SAS data repository; options for including SAS-derived shape and atomistic models along with specific information regarding the modeling protocol, uniqueness and uncertainty; development of criteria for assessment of data quality and accuracy. The Task Force also recommends that leaders from the various structural biology disciplines should jointly define what to archive in the PDB and what complementary archives might be needed, taking into account both scientific needs and funding.

This report by the wwPDB SAS Task Force follows recommendations recently published by wwPDB Validation Task Forces on X-ray and 3DEM. The report from the NMR Validation Task Force will be published shortly.

Landmark HIV Capsid Structures Follow New PDB Deposition and Release Procedures for Large Structures

Two complete HIV-capsid structures, both of unprecedented size, have been curated and made available in the archive following recently-announced procedures for the deposition and release of large structures. This represents a significant advance in the field of structural biology and a milestone for the PDB.

PDB entries 3J3Q and 3J3Y are models based on cryo-electron microscopy data and use of a molecular dynamics flexible-fitting method. They contain 1356 and 1176 protein chains, respectively, and over two million atoms each. The HIV-1 capsid is the protein envelope that encloses and protects the RNA genome of the virus. An important subject of study, the full capsid has been a difficult target for structural characterization due to its extremely large size and morphological variability.

Mature HIV-1 capsid structure by cryo-electron microscopy and all-atom molecular dynamics (2013) Gongpu Zhao, Juan R. Perilla, Ernest L. Yufenyuy, Xin Meng, Bo Chen, Jiying Ning, Jinwoo Ahn, Angela M. Gronenborn, Klaus Schulten, Christopher Aiken, Peijun Zhang, Nature **497***: 643-646* ***[doi: 10.1038/nature12162]***

EMDB entry EMD-5639 is the cryo-electron tomography reconstruction from which 3J3Q and 3J3Y were generated; related entry 3J34, derived from an 8.6 Ångström reconstruction of a capsid hexameric subunit in a helical assembly (EMD-5582), was used in the construction of both 3J3Q and 3J3Y.

In anticipation of greater numbers of PDB depositions, involving ever larger and more complex structures, often determined using multiple methods, the wwPDB has been developing a new system for deposition and annotation that will go into full production early in 2014. This system will support depositions of structures of any size, determined using diffraction, EM and/or NMR methods. Large structures that exceed the limitations of the PDB file format will be processed and released intact so that "split entries" become a thing of the past. Since the coordinate records in such large structures cannot be validly represented by the PDB file format, only an abbreviated PDB formatted file, containing authorship and citation details, will be provided in the FTP archive.

The wwPDB has also convened a Working Group for PDBx/mmCIF Data Deposition that includes representatives from the major X-ray structure-determination packages, and is chaired by Paul Adams (Lawrence Berkeley Laboratory; Phenix). To ease the transition from PDB to PDBx/mmCIF, the Working Group made recommendations about essential extensions required for large structures that have been incorporated. In addition, PDBx/mmCIF files suitable for deposition can now be created with recent versions of CCP4 (REFMAC 5.8) and Phenix (1.8.2) software packages. Both packages support the recommended extensions for large structures.

Prior to the release of the new deposition system in 2014, the wwPDB will accept, process, and then distribute the large files intact on the PDB FTP in the directory **/pub/pdb/data/large_structures**. In order to not break any current software, wwPDB curators will "split" such entries into a collection of PDB-format files that will be distributed on the PDB FTP following current release and formatting conventions. In 2014, all legacy split entries will be "reunited" and released intact (in PDBx/mmCIF format only) by the wwPDB.

The complete announcement on the deposition and release of large strucures is at **wwpdb.org**; users with questions about the new deposition system or the procedures for handling large structures should contact **info@wwpdb.org**.

10,000 NMR Entries

With the June 18, 2013 update, the number of entries released in the PDB archive determined using NMR spectroscopy passed the 10,000 mark.

Updated Version of MAXIT Available

MAXIT Version 8 includes a new option to assign ligands the same chain IDs as the adjacent polymers and incorporates several fixes to bugs.

This command-line program can also be used to:

- Read and write PDB and mmCIF format files, and translate between file formats
- Perform consistency checks on coordinates, sequence, and crystal data
- Automatically construct, transform, and merge information between formats
- Align residue numbering in the coordinates with the sequence
- Reorder and rename atoms in standard and nonstandard residues and ligands according to the wwPDB Chemical Component Dictionary

Visit **sw-tools.rcsb.org** to download MAXIT and other programs for processing and curating PDB data.

Deposition Statistics

In the second quarter of 2013, 2855 experimentally-determined structure coordinates and 138 3DEM maps were deposited to the archive. 5360 coordinate entries total have been deposited in the archive in 2013.

For the entries deposited this quarter, 84.1% were deposited with a release status of hold until publication; 13.2% were released as soon as annotation of the entry was complete; and 2.7% were held until a particular date. 91.9% of these entries were determined by X-ray crystallographic methods; 5.3% were determined by NMR methods.

During the same period, 2586 structures were released in the PDB.

Data Query, Reporting, and Access

Website Statistics

Access statistics for the second quarter of 2013 are shown.

Month	Unique Visitors	Number of Visits	Bandwidth
APRIL	369,516	811,545	1701.94 GB
MAY	337,920	765,033	1669.93 GB
JUNE	291,409	682,857	1387.67 GB

Beta Test RCSB PDB *Mobile* for Android

RCSB PDB users with Android phones or tablets using version 2.3 or higher of the Android OS can download beta version #2 of RCSB PDB *Mobile* from **www.rcsb.org/pdb/static.do?p=mobile/RCSBapp.html**.

RCSB PDB Mobile *for Android is in beta testing. The iOS version of RCSB PDB* Mobile *has been downloaded over 10,000 times.*

This free app provides fast, on-the-go access to the RCSB PDB. Options are available to search the entire PDB database, view the latest protein and nucleic acid structures released, access MyPDB, view the entire catalog of *Molecule of the Month* articles, and more. Structures can be interactively explored using the molecular viewer NDKMol (courtesy of Dr. Takanori Nakane, Kyoto University).

The Android edition of RCSB PDB *Mobile* is still under development. This beta release will "time out" in 2 months, by which time we anticipate the next generation app will be available from the Google Play Store. Please send any feedback to **quinn@sdsc.edu**.

Personalize the RCSB PDB with MyPDB

Access the MyPDB widget in the left-hand menu to create an account and then log in to access stored setting and functionalities:

Saved Query Manager. Use MyPDB to store any type of structure search, such as keyword, sequence, ligand, and any composite query built with Advanced Search. These queries can be run at any time with the click of a button.

Stored searches can also be set to run with each update. Email alerts (weekly or monthly) will be sent when new PDB entries matching the search are released.

A) Customizing the Query Manager

User Query (OK)	Motif Query For: CX{2,4}CX{12}HX{3,5}H	Yes	05/06/2013	05/07/2013	▸ ✕

B) MyPDB Query Manager

Name	Query Description	Email Notification	Last Run	Next Scheduled Run	Run Query (No Email)	Delete
GFP	gfp	Yes	04/30/2013	05/07/2013	▸	✕
2.7.11	EC Tree Search for 2.7....	Yes	04/30/2013	05/07/2013	▸	✕
User Query	Molecule : Catalase [A2A136, D9N167, P00432, P04040, P11934, P29422, P42321, P46206, P77872, Q3LSM1, Q834P5]	Yes	04/30/2013	05/07/2013	▸	✕
Zinc Fingers	Motif Query For: CX{2,4}CX{12}HX{3,5}H	Yes	05/06/2013	05/07/2013	▸	✕

Saved Query Manager Features. A) After saving a search to MyPDB, name it by clicking on the words `User Query` providing a more descriptive label. B) The manager can be used to change email notification settings, run queries, and delete saved searches.

Personal Annotations. Users can save personal annotations and notes on the Structure Summary tab of any PDB entry, and can add structures to a "favorites list". The Personal Annotations summary page provides easy access to all of these tagged structures and annotations.

User Account. Personal information (name, email address, account password, country, user type) can be updated at any time. All MyPDB account information is kept private and secure.

Browse the Anatomical Therapeutic Chemical Classification System to Find Structures

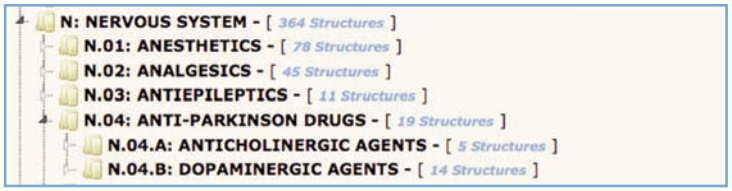
RCSB PDB's Browse Database feature explores the PDB archive using different hierarchical trees. The WHO Collaborating Centre (**www.whocc.no**) for Drug Statistics Methodology's Anatomical Therapeutic Chemical (ATC) classification system (**www.whocc.no/atc/structure_and_principles**) organizes drugs 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 be browsed using the ATC 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.

The browser opens up the top level in the hierarchy. Clicking on the arrow/folder icons expands the respective nodes. Clicking on the name of the node will retrieve all PDB IDs associated with that ATC code.

Structures having a particular ATC code (e.g., A12CC05) or name (e.g., Atorvastatin) can be found using the browser search box.

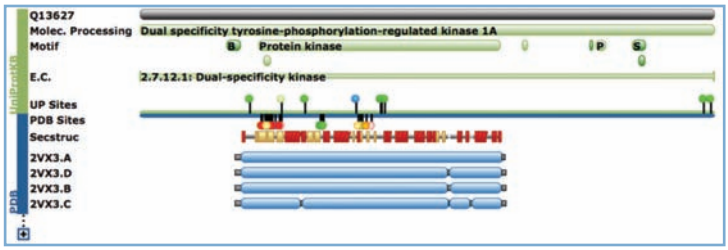
Other Browse options include GO Terms, Enzyme Classification, Transporter Classification, Source Organism, Genome Location, MeSH terms, SCOP, and CATH.



Use the Anatomical Therapeutic Chemical Classification Browser to find PDB structures

Map PDB Structures to Full-length Protein Sequences

The Protein Feature View visually summarizes how a full-length protein sequence from UniProtKB (**uniprot.org**)[1] corresponds to PDB entries. It also loads annotations from external databases (such as Pfam, **pfam.sanger.ac.uk**)[2] and homology models from the Protein Model Portal (**proteinmodelportal.org**).[3] Annotations visualizing predicted regions of protein disorder (computed with JRONN)[4] and hydrophobic regions (as computed using a sliding window approach) are also displayed.



Protein Feature View from the Structure Summary page for 2xv3.[5]

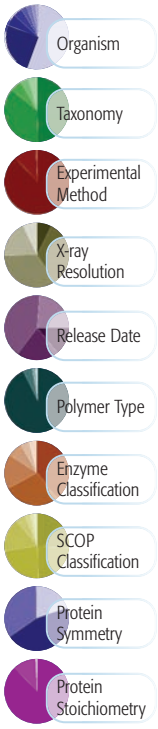
For individual entries, the Protein Feature View is available from the Molecular Description Widget on Structure Summary pages. The example shown for PDB ID 2vx3[5] illustrates how the ranges of a protein that have been observed in an experiment (in blue) correspond to the full length UniProtKB sequence (in grey). The secondary structure information from the PDB entry is also shown (helices in red, beta strands in yellow).

Various features that are known for the UniProtKB sequence are displayed in green as they correlate with regions in the PDB entry. Protein modifications and active site residues (from UniProtKB and the PDB entry) are also annotated. Moving the mouse cursor over the "lollipops" displays the residue label. Mousing over the images shown in the "Secstruc" row reveals secondary structure information from the entry.

This view can be expanded to map all PDB entries related to a single UniProtKB sequence by selecting the Protein Feature View link shown in this widget. By default, a few representative PDB entries are used to give an overview for which regions of the UniProtKB sequence PDB entries are available. Selecting the plus sign or the "Show All" button will expand the view to show all related PDB chains, which can then be sorted by resolution, length, and release date. These Protein View images can be exported as Scalable Vector Graphics (SVG) files.

The PDB to UniProtKB mapping is based on the data provided by the Structure integration with function, taxonomy and sequence (SIFTS; **pdbe.org/sifts**) initiative.[6]

Search the PDB Using Drill-down Pie Charts



Standard characteristics of PDB entries–organism, taxonomy, experimental method, X-ray resolution, release date, polymer type, EC, SCOP classification, protein symmetry, and protein stoichiometry–are used to create searchable data distribution summaries.

The Explore Archive widget on the home page provides a quick statistical overview of the PDB. Browse the charts individually, or view them all together by clicking on the "Show all" link. Clicking on a pie chart image will display a more detailed graphic that lists the percentages for the categories shown. Selecting one of the listed results will launch the corresponding structures in the Query Results Browser.

Data distribution drill-downs can also be used to refine search results and to explore the latest weekly update of PDB entries.

Any combination of categories is possible. Users can drill-down to quickly access high resolution entries from a structure type search; human-related entries from a sequence search; or the most recent PDB entries containing a particular ligand.

These charts can be hidden from the query results for users who want to only view the individual entries.

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 at **www.rcsb.org/pdb/software/rest.do**.

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.

Please let us know at **info@rcsb.org** if there are website options that you think should be offered as a web service.

1. UniProt Consortium. (2012) Reorganizing the protein space at the Universal Protein Resource (UniProt). *Nucleic Acids Res* **40**: D71-75.
2. M. Punta, P. C. Coggill, R. Y. Eberhardt, J. Mistry, J. Tate, C. Boursnell, N. Pang, K. Forslund, G. Ceric, J. Clements, A. Heger, L. Holm, E. L. Sonnhammer, S. R. Eddy, A. Bateman, R. D. Finn. (2012) The Pfam protein families database. *Nucleic Acids Res* **40**: D290-301.
3. K. Arnold, F. Kiefer, J. Kopp, J. N. Battey, M. Podvinec, J. D. Westbrook, H. M. Berman, L. Bordoli, T. Schwede. (2009) The Protein Model Portal. *Journal of structural and functional genomics* **10**: 1-8.
4. Z. R. Yang, R. Thomson, P. McNeil, R. M. Esnouf. (2005) RONN: the bio-basis function neural network technique applied to the detection of natively disordered regions in proteins. *Bioinformatics* **21**: 3369-3376.
5. A. K. Roos, M. Soundararajan, A. C. W. Pike, O. Fedorov, O. King, N. Burgess-Brown, C. Philips, P. Filippakopoulos, C. H. Arrowsmith, M. Wikstrom, A. Edwards, F. Vondelft, C. Bountra, S. Knapp. (2008) The Crystal Structure of the Human Dual Specificity Tyrosine-Phosphorylation-Regulated Kinase 1A. **doi:10.2210/pdb2vx3/pdb**
6. S. Velankar, J. M. Dana, J. Jacobsen, G. van Ginkel, P. J. Gane, J. Luo, T. J. Oldfield, C. O'Donovan, M. J. Martin, G. J. Kleywegt. (2013) SIFTS: Structure Integration with Function, Taxonomy and Sequences resource. *Nucleic Acids Res* **41**: D483-489.

Outreach and Education

Meetings and Events

The RCSB PDB built virus models at Rutgers Day, an event of discovery and lively activities that showcase the varied resources, departments, and people at the university.

RCSB PDB participated in a variety of community events, including the **San Diego Festival of Science and Engineering's Expo Day** (March 23) and **Rutgers Day** (April 27). Activities ranged from building DNA and viruses out of marshmallows to exploration of the RCSB PDB resource.

Curators and developers of biological databases convened at the Sixth International Biocuration Conference (April 7-10; Cambridge, UK). RCSB PDB's Lead Biocurator Jasmine Young presented a poster on *Curation at the PDB*.

At the **Experimental Biology** meeting (April 20-24; Boston, MA), RCSB PDB Director Helen M. Berman received the *2013 DeLano Award for Computational Biosciences* from 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 2013 award honors Prof. Berman's efforts to make data universally available.

The RCSB PDB also participated in the **National Science Teacher Association's Annual Meeting**, as described in this issue's *Education Corner*.

Upcoming meetings include:

ISMB/ECCB and 3Dsig: The International Society for Computational Biology and the European Conference on Computational Biology will meet July 19-23 in Berlin, Germany.

Presentations will include *What Bioinformaticians need to know about digital publishing beyond the PDF* (Associate Director Phil Bourne) and *New tools and visualization features at the RCSB PDB* (Peter Rose).

At the ISMB Special Interest Group meeting **Bioinformatics Open Source Conference** (BOSC), Andreas Prlić will present *Ten simple rules for the open development of scientific software*.

At the **3Dsig:Structural Bioinformatics & Computational Biophysics** satellite meeting, Associate Director Stephen Burley will give a keynote presentation on wwPDB: *Ensuring a freely accessible, singular archive of high quality macromolecular structure information*, and Peter Rose will present *A survey of protein stoichiometry and symmetry in the PDB* as a talk and a poster. The 3DSig poster *Aligning subunits of internally symmetric proteins with CE-Symm* by Spencer Bliven will also be presented. Associate Director Phil Bourne is one of the 3Dsig Program Chairs.

The RCSB PDB Poster Prize will be awarded for the best student poster presentation in the category of **Protein Structure and Function Prediction and Analysis**.

ACA: At the Annual Meeting of American Crystallographic Association (July 20-24; Honolulu, HI), the RCSB PDB will be exhibiting alongside the Structural Biology Knowledgebase. Director Helen Berman will present *The wwPDB: Ensuring a single, uniform archive of high quality data* during the session on Enabling Partnerships for Broader Crystallographic Data Accessibility. John Westbrook will present a poster and a tutorial in the Structure Validation session on *The New wwPDB Deposition and Annotation System*.

The RCSB PDB Poster Prize will be awarded for the best student poster presentation involving macromolecular crystallography.

ICSG2013-SLS: At Structural Life Science/Seventh International Conference on Structural Genomics (July 29-August 1; Sapporo, Japan), Stephen Burley will present *wwPDB: Ensuring a freely accessible, singular archive of high quality macromolecular structure information*.The RCSB PDB Poster Prize will be awarded for most creative use of the PDB.

ECM28: At the 28th Meeting of the European Crystallographic Association (August 25-28, Warwick, UK), John Westbrook will speak on *mmCIF and Structural Bioinformatics* as part of the August 25 satellite symposium on Crystallographic Information and Data Management organized by COMCIFS, the IUCr Committee for the Maintenance of the CIF Standard.

The RCSB PDB Poster Prize will be awarded for the best student poster presentation involving macromolecular crystallography.

wwPDB Symposium

A special public symposium sponsored by the wwPDB will be held on September 26, 2013 at Rutgers, The State University of New Jersey. *A Celebration of Open Access in Structural Biology: Recognizing the career and achievements of Professor Helen M. Berman* will include presentations from:

- Jean Baum (Rutgers, The State University of New Jersey)
- David L. Beveridge (Wesleyan University)
- Wayne Hendrickson (Columbia University)
- Stephen Neidle (University College London)
- Janet Thornton (European Bioinformatics Institute | EMBL Outstation - Hinxton)
- Soichi Wakatsuki (SLAC National Accelerator Laboratory | Stanford University)
- Cynthia Wolberger (Howard Hughes Medical Institute | Johns Hopkins University School of Medicine)

For more information, see **www.wwpdb.org/outreach2013.html**.

New Paper: Trendspotting in the PDB

A new paper from the RCSB PDB has been published that analyzes PDB data to identify developments and trends in structural biology:

Trendspotting in the Protein Data Bank

Helen M. Berman, Buvaneswari Coimbatore Narayanan, Luigi Di Costanzo, Shuchismita Dutta, Sutapa Ghosh, Brian P. Hudson, Catherine L. Lawson, Ezra Peisach, Andreas Prlić, Peter W. Rose, Chenghua Shao, Huanwang Yang, Jasmine Young, Christine Zardecki

FEBS Letters (2013) **587**: 1036-1045
doi: 10.1016/j.febslet.2012.12.029

A full list of RCSB PDB publications is available from **rcsb.org**.

Create High Resolution Images

Create or download publication-quality pictures of biomacromolecules with the RCSB PDB.

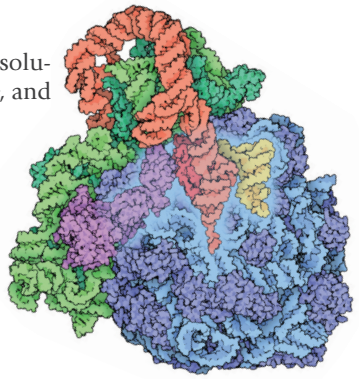
Several interactive, Java-based tools[7] can be used to visualize PDB data and create pictures. Protein Workshop offers easily customized views; Simple Viewer utilizes a quick ribbon display; and Ligand Explorer visualizes the interactions of bound ligands in protein and nucleic acids structures.

Each program can be used to create and save high-resolution images in JPEG, PNG, and TIFF formats. Using the Save Image dialog box from the File menu, users can specify the width and height of an image in pixels, inches, or millimeters.

From the educational PDB-101 site, high resolution TIFFs of *Molecule of the Month* illustrations can be downloaded and used in presentations and publications. The high resolution files are linked from each article, and available as an archive.

PDB-101 posters, including *The Structural Biology of HIV* and *Molecular Machinery: A Tour of the Protein Data Bank*, can be saved as high or low resolution PDFs.

Citation and usage information is available at **rcsb.org**.



Download high resolution images from Molecule of the Month articles. Shown: Transfer-Messenger RNA [doi: 10.2210/rcsb_pdb/mom_2013_1].

7. 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.

Education Corner

PDB-101 and the 2013 Meeting of the National Science Teachers Association

Science educators from around the world come together at annual meetings of the National Science Teachers Association (NSTA; **nsta.org**). Approximately 8,500 people attended this year's conference, held April 11-13 in San Antonio, Texas.

Through a workshop and exhibition booth, the RCSB PDB met with users (new and old) and demonstrated PDB-101 features and downloadable activities.

A new feature of the RCSB PDB stand was a "photo booth" that drew in many visitors. Attendees were asked to pose with their "favorite" molecule against a backdrop image of hundreds of *Molecule of the Month* images. Teachers were then asked to select their favorite molecule from among the most popular *Molecule of the Month* features. Their pictures and choices were posted to the RCSB PDB's Facebook page. When the results were tallied, Green Fluorescent Protein was shown to be the NSTA's favorite.

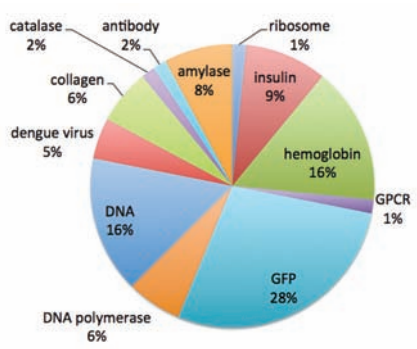
Molecule of the Month author David Goodsell presented a workshop on *Exploring Proteins and Nucleic Acids* at the PDB. He described all aspects of the structure determination pipeline, how to access PDB structures from the RCSB PDB website, and highlighted the PDB-101 resources described here.

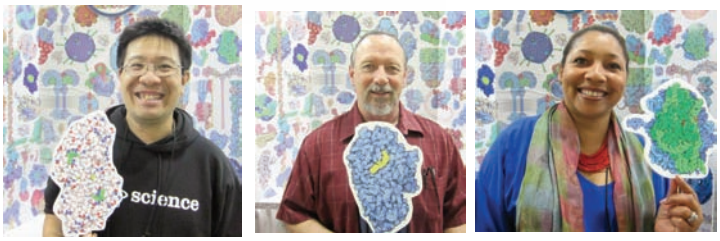
Protein and nucleic acid structure was a topic throughout the NSTA meeting, as seen in other presentations, workshops, and exhibit booths, including:

The WestEd workshop *Tangible Models and Augmented Reality: New Technology for High School Biology Classrooms* let teachers build physical 3D models of DNA and a virus structure. These physical models are linked with iPad programs that enhance the overall lesson (**www.wested.org**).

Science Take-Out presented a simple hands-on exercise that modeled how coded information in genes results in proteins with specific shapes that perform specific functions (**sciencetakeout.com**).

3D Molecular Designs/MSOE Center for BioMolecular Modeling offers kits to build physical models, such as the Insulin mRNA to Protein and DNA Starter Kits, and opportunities for professional development to educators (www.3dmoleculardesigns.com).





Teachers posed with their favorite molecule in the RCSB PDB's exhibit booth. All photos are posted at **www.facebook.com/RCSBPDB**.

PDB-101 Resources

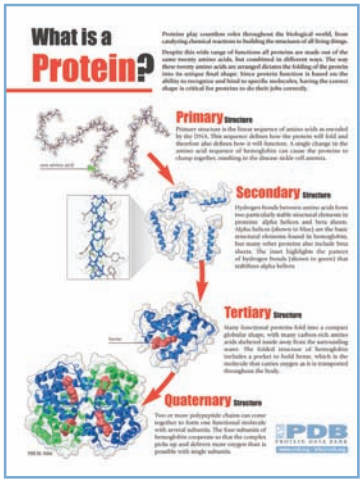
Throughout the NSTA meeting, attendees were presented with information and discussions about the PDB-101 website. Designed for teachers, students, and the general public, PDB-101 promotes exploration of the world of proteins and nucleic acids by packaging together educational resources and materials, including posters, animations, and classroom lessons and activities.

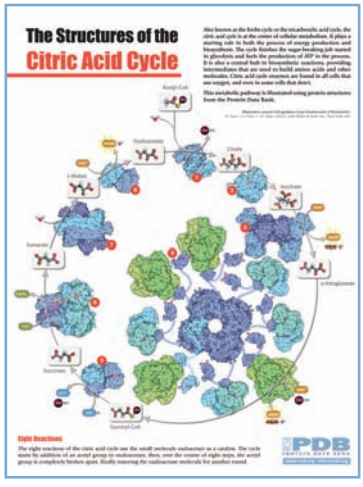
New features have been added to different sections of PDB-101:

Educational Resources: Posters/Exhibits

The flyer *What is a Protein?* introduces protein structure and function to beginners.

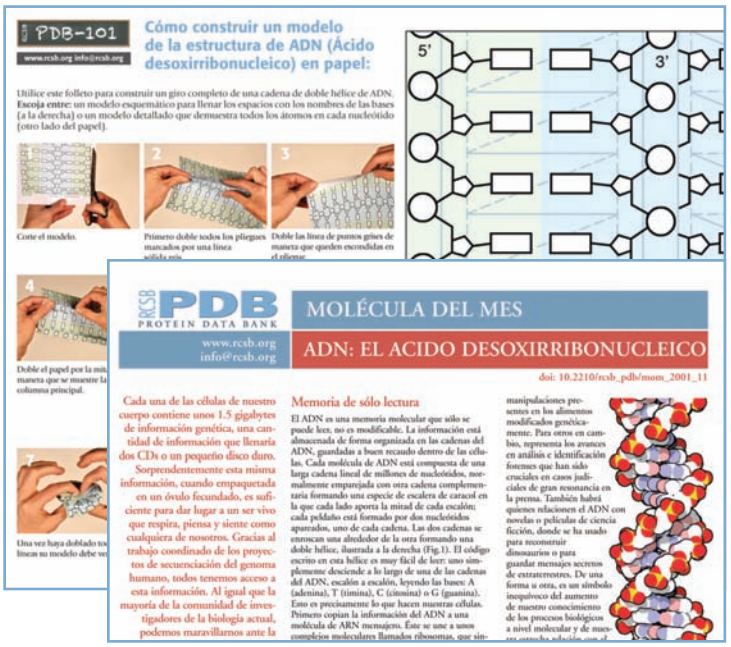
Structures of the Citric Acid Cycle illustrates the PDB structures involved in this important metabolic pathway.





Educational Resources: 3D Paper Models

DNA resources have been translated into Spanish, including the *Molecule of the Month* article and the paper model template.



Molecule of the Month

Articles describe the structure and function of a molecule, offer interactive views and discussion topics, and link to specialized pages to help explore specific example structures.

July's *Molecule of the Month* highlights the structure of the HIV capsid, and includes a downloadable PDF that can be folded into a 3D paper model (shown on the right).

Structural View of Biology

Built around the *Molecule of the Month* series, this browser promotes a top-down exploration of the PDB. Readers can travel through high-level functional categories (such as Protein Synthesis and Health and Disease) and descriptive subcategories (like Replication or Immune System) to access relevant articles that describe molecules in simple terms and provide specific examples.

Understanding PDB Data

Understanding PDB Data is a reference guide for exploring and interpreting individual PDB entries. Broad topics include how to understand PDB data, how to visualize structures, how to read coordinate files, and potential challenges to exploring the archive.

Author Profiles

Author Profiles offer historical and educational timelines of the structures associated with a particular researcher. Example profiles and searches for authors and structural genomics centers are available.

To visit PDB-101 from the main RCSB PDB site, click on the blackboard PDB-101 logo or its related widget in the left-hand menu. This view offers easy navigation: select any *Molecule of the Month* article from the top bar pull-down menu or choose one of the tabs to jump to other sections. Select the blue RCSB PDB logo from the top of the page at any time to return to the main website.

RCSB PDB PROTEIN DATA BANK NEWSLETTER

Web: www.rcsb.org
Email: info@rcsb.org
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RCSB PDB Partners

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

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

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

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