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RCSB PDB PROTEIN DATA BANK NEWSLETTER

Contents

SNAPSHOT: APRIL 1, 2010

64,357 released atomic coordinate entries

MOLECULE TYPE		EXPERIMENTAL TECHNIQUE	
59,564	proteins, peptides, and viruses	55,596	X-ray
2,124	nucleic acids	8,316	NMR
2,631	protein/nucleic acid complexes	283	electron microscopy
		21	hybrid
38	other	141	other

44,986 structure factor files
5,607 NMR restraint files

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E-mail: info@rcsb.org
Web: www.pdb.org • FTP: ftp.wwpdb.org

The RCSB PDB is a member of the wwPDB (www.wwpdb.org)

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

Message from the RCSB PDB

New Features Widget

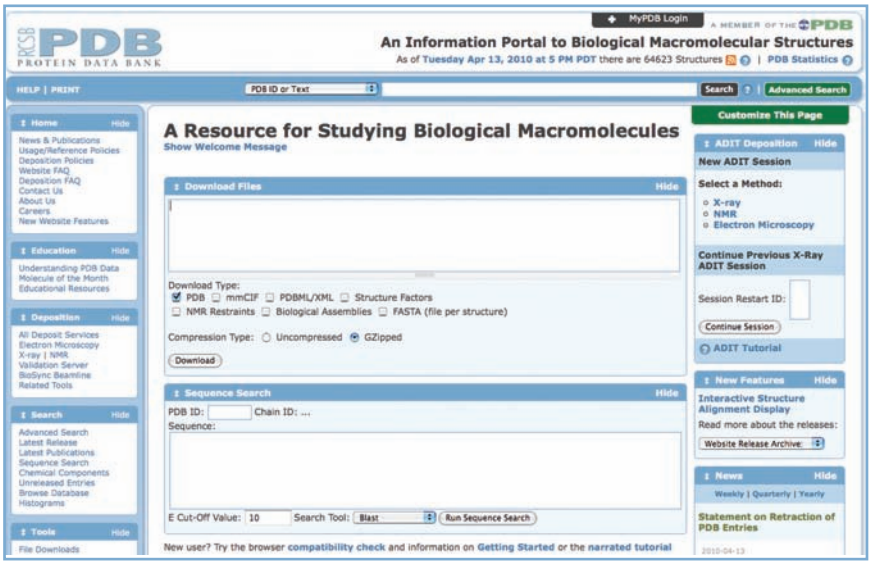
In March, many new features were added to the website, including improved ligand search options, pre-calculated pairwise structure alignments, enhancements to viewing query results and tabular reports, and much more.

An overview can be found in the **New Features** Widget box on the home page. This widget scrolls through a list of the new features, and links to descriptions of all recent major website additions.

All widgets with a dark blue bar on top can be moved around on the page by dragging the arrow buttons, hidden by selecting "Hide," or included in a customized view.

The Customize This Page button in the top right corner lets users select which widgets are displayed by default. To only see query-related options, the *Molecule of the Month* can be replaced with forms to download files and search by sequence.

Other widgets that can be displayed on the home page include the **RCSB PDB Comparison Tool** for running pairwise structural and sequence alignments, the **ADIT Deposition** Widget, and the **Featured Molecule** Widget which displays the RCSB PDB's *Molecule of the Month* and the Protein Structure Initiative's *Featured Molecule*.



This example shows the RCSB PDB home page customized to show the Download Files *and* Sequence Search *widgets in the middle. The* ADIT Deposition *widget, which lets users start or continue a new deposition session, appears on the right. Other widgets can be set to appear at the bottom of the page or simply hidden.*

Data Deposition and Processing

Deposition Statistics

In the first quarter of 2010, 2065 experimentally-determined structures were deposited to the PDB archive. The entries were processed and annotated by wwPDB teams at the RCSB PDB, PDBe, and PDBj.

Of the structures deposited, 74.7% were deposited with a release status of "hold until publication"; 22.6% were released as soon as annotation of the entry was complete; and 2.7% were held until a particular date. 92.5% of these entries were determined by X-ray crystallographic methods; 6.9% were determined by NMR methods.

During the same time period, 2027 structures were released in the PDB.

wwPDB News

Changes to the wwPDB Policy for Depositing Polypeptide Structures

The wwPDB now accepts polypeptide structure depositions of all gene products; all naturally-occurring, non-ribosomally synthesized peptides, such as antibiotics; and all peptidic repeat units of larger polymers, such as fibrous and amyloid polymers. In addition, non-naturally occurring synthetic peptides with at least 24 residues will be accepted for deposition.

Consistent with earlier policy, depositions of polynucleotide and polysaccharide structures of 4 or more residues are also accepted. For more information, see the wwPDB Policy Guide at www.wwpdb.org.

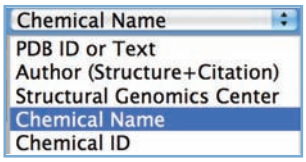
Initial Release REVDAT Dates

The PDB archive can be accessed at FTP sites at the RCSB PDB, PDBe, and PDBj. The update schedules for these sites have been coordinated to be simultaneous. All updates now occur at the target time of Wednesday 00:00 UTC (Coordinated Universal Time). As of March 31, 2010, the initial release date reflected in the REVDAT record mirrors the Wednesday release. The file's timestamp of the Friday before release will not be changed.

Data Query, Reporting, and Access

Improved Ligand Searching

Searching for ligands using the RCSB PDB's Advanced Search, Chemical Structure Search, or top-bar pulldown search has been improved.

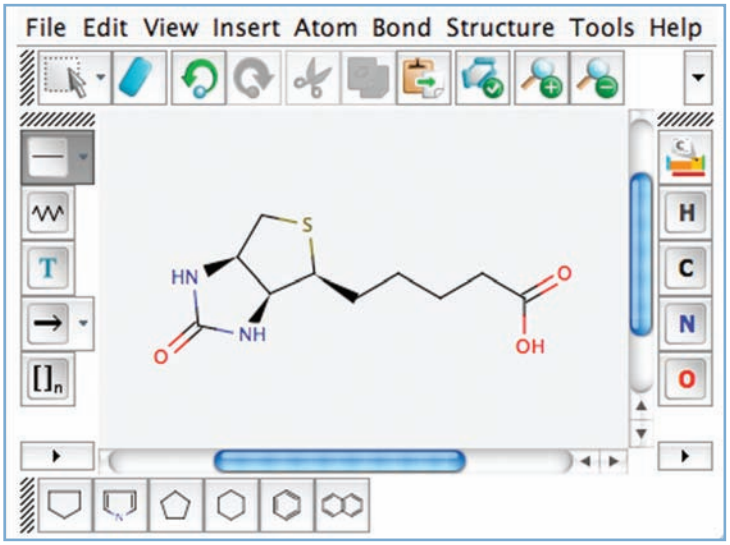


The **Chemical Name** search from the top-bar pulldown menu on every page returns matches to names of small molecules in the wwPDB Chemical Component Dictionary and any synonyms. Searches by **Chemical Name** or **Chemical ID** will return structures with matching components that are free ligands or are part of a protein or nucleic acid chain.

In the **Advanced Search**, searches can be customized to look for free and/or polymeric chemical components. A "sounds like" option searches for misspelled or incomplete chemical component names. **Advanced Searches** using SMILES strings use a similarity (instead of dissimilarity) threshold while specifying polymeric type.

The **Chemical Structure Search** (available from the left hand **Search** menu under **Chemical Components**) utilizes the latest version of the MarvinSketch[1] applet (5.3.0.1).

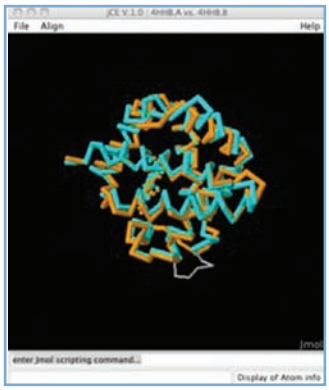
Screencasts are available to help explore these features at www.rcsb.org/pdb/static.do?p=general_information/screencasts.jsp



Users can perform exact, similar, or substructure search by drawing components or loading and editing SMILES strings or chemical IDs into the tool.

Comparison Tool for Exploring Sequence and Structure Alignments

The **Comparison Tool** calculates pairwise sequence and structure alignments using different methods. This feature is available on the Compare Structures web page (under **Tools** in the left menu) and as a downloadable web widget.



The current sequence alignments possible are blast2seq,[2] Needleman-Wunsch,[3] and Smith-Waterman.[4] Structure alignments can be performed using FATCAT[5] and CE[6] through a Java applet launched from the RCSB PDB site. Mammoth,[7] TM-Align,[8] and TopMatch[9] structure alignments will be launched at their related external sites.

This functionality is also integrated with the Sequence Clusters offered from each entry's Sequence Similarity tab. Users can select a pair of chains from a given sequence cluster, and then run either sequence or structure alignments. For example, the Sequence Similarity tab for entry 4hhb offers sequence clusters at different similarity cutoffs. Users can select a pair of chains from a given sequence cluster (95% for this example), and then run the sequence or structure alignments available from the Comparison Tool.

Advanced Search: Sequence Motif

Advanced Search lets users build queries of specific types of data. To look for structures with a particular Sequence Motif, try using one of these techniques with the Sequence Features>Sequence Motif option. Users can query for an exact sequence or for a sequence pattern using regular expression syntax, as shown below. Regular expressions are powerful notations for defining complex sequence patterns.

• Short Sequence Fragments
The sequence motif search, unlike BLAST or FASTA, can search for short sequence fragments of any size, such as NPPTP

• Wildcard Searches
Use an 'X' in the sequence for wildcard searching. For example, XPPXP can be entered to look for SH3 domains using the consequence sequence -X-P-P-X-P (where X is a variable residue and P is proline)

• Multiples of Variable Residues
The {n} notation can be used, where n is the number of variable residues. To query a motif with 7 variables between residues W and G, and 20 variable residues between G and L, try WX{7}GX{20}L

• Ranges of Variable Residues
The {n,m} notation can be used to indicate ranges of variable residues, where n is the minimum and m the maximum number of repetitions. For example, the zinc finger motif that binds Zn in a DNA-binding domain can be expressed as: CX{2,4}CX{12}HX{3,5}H

• Motifs at the Beginning of a Sequence
The '^' operator searches for sequence motifs at the beginning of a protein sequence. Two ways of looking for sequences with N-terminal histidine tags are: ^HHHHHH and ^H{6}

• Alternative Residues
Square brackets specify alternative residues at a particular position. To search for a Walker (P loop) motif that binds ATP or GTP, try: [AG]XXXXGK[ST]

The search will look for sequences with A or G, followed by 4 variable residues, then G K, and finally S or T.

Time-stamped Copies of PDB Archive Available via FTP

A snapshot of the PDB archive (ftp.wwpdb.org) as of January 4, 2010 has been added to ftp://snapshots.wwpdb.org/. Snapshots of the PDB have been archived annually since 2004. It is hoped that these snapshots will provide readily identifiable data sets for research on the PDB archive.

The directory 20100104 includes the 62,388 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 indicate 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.

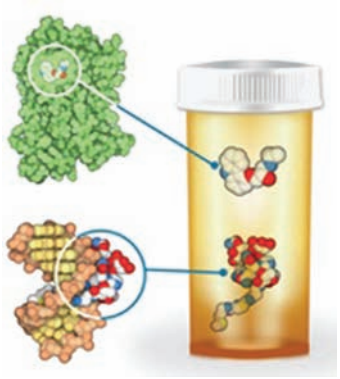
Website Statistics

Website access statistics for the first quarter of 2010 are given below.

Month	Unique Visitors	Number of Visits	Bandwidth
JANUARY 2010	176655	422065	755.87 GB
FEBRUARY 2010	184306	434442	783.75 GB
MARCH 2010	210308	510434	1189.17 GB

Outreach and Education

Poster Download: *How Do Drugs Work?*



A new poster that explores different kinds of protein-drug structures found in the PDB archive is available for download as a poster (26 x 38") and flyer (8 1/2 x 11").

How Do Drugs Work? was inspired by the success and enduring popularity of 2002's poster on *Molecular Machinery: A Tour of the Protein Data Bank.* That poster, which depicts many PDB structures drawn to scale, is also available.

Written and illustrated in a style similar to the *Molecule of the Month* series, the poster uses PDB structures to discuss antibiotics and antivirals, chemotherapy, drug metabolism, drugs of signaling proteins, and lifestyle drugs.

All posters and flyers are available from the **RCSB PDB's Educational Resources** page. Printed copies will be distributed at scientific and educational meetings.

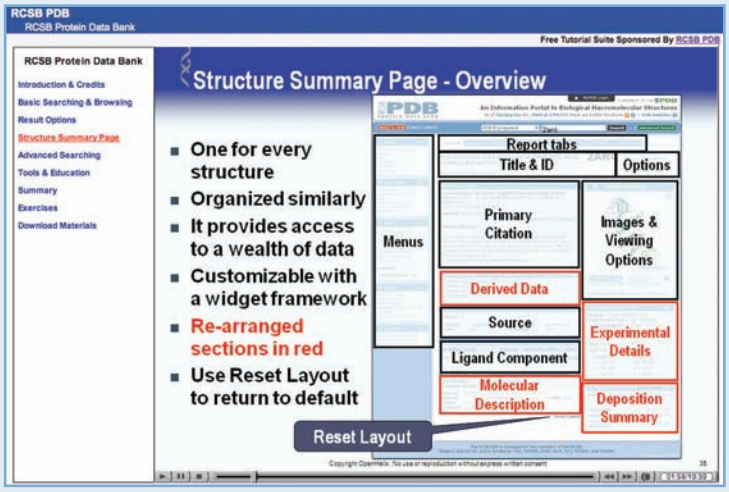
Online Narrated Tutorial Demonstrates How to Use the RCSB PDB

Comprehensive training materials to introduce users to the features and functionality of the RCSB PDB are now freely available at **openhelix.com**.

The new training tools include an online narrated tutorial that demonstrates basic and advanced searches, how to generate reports, the different options for exploring individual structures, and many of the resources and tools available at the RCSB PDB for research and education. The full tutorial runs for about an hour, and can be navigated by specific chapters.

The animated PowerPoint slides used as a basis for the tutorial can be downloaded, along with slide handouts and exercises. These materials are freely available for teachers and professors to create classroom content.

OpenHelix has also created **Quick Reference Cards** for the RCSB PDB that highlight search strategies, features and functionality. The cards can be ordered at **openhelix.com** at no cost; shipping is free within the United States.



In addition to viewing the narrated tutorial, users can download slides and exercises that illustrate how to use the RCSB PDB searching and reporting functions at **www.openhelix.com/pdb**.

NJ Science Olympiad Protein Modeling Results

High school teams across New Jersey demonstrated their understanding of hemagglutinin, neuraminidase, and protein structure at Science Olympiad competitions held across the state.

At the RCSB PDB-sponsored protein modeling trial event, teams submitted their hand-built 3D models of a hemagglutinin protein with an abstract to be judged by staff from the RCSB PDB. These models were enhanced with different features to help tell the story of hemagglutinin's function. At the competition, teams quickly built a model of a selected protein region using Jmol and completed a written exam with questions about protein structure and influenza. Teams used the *Molecule of the Month* and other RCSB PDB resources to help prepare for this event. 35 teams competed in this event at three regional tournaments in January.

The top scoring teams were:

Southern Regional
January 9, 2010
Camden County College

1. Cherry Hill High School East
2. MATES Academy
3. The Lawrenceville School

Cherry Hill East and their prebuild model of hemagglutinin. A rubric was used to award points for the accuracy of the model and for the addition of materials that illustrated the function of the protein.

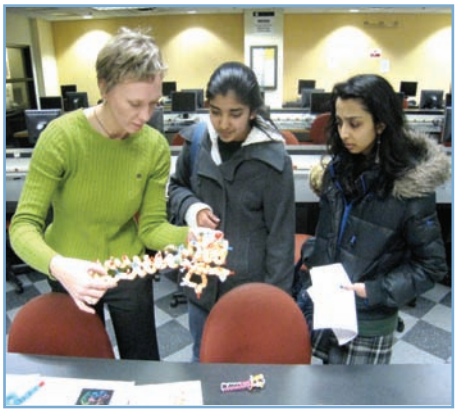
Central Regional
January 12, 2010
Union County College

1. South Brunswick
2. Westfield
3. Hillsborough

The team from South Brunswick marked the beta sheets in their model after viewing them in Jmol.

Northern Regional
January 14, 2010
New Jersey Institute of Technology

1. West Windsor Plainsboro South
2. Livingston
3. Princeton



Annotator Marina Zhuravleva reviews the scoring for West Windsor Plainsboro South's prebuild model with the team.

At the state finals (March 16, Middlesex County College), where the top scoring teams at all NJSO events compete, 24 teams participated. The top scores went to first place West Windsor Plainsboro North, second place West Windsor Plainsboro South, and third place New Providence.

Special thanks to our all of our judges from the RCSB PDB, the NJ Science Olympiad organizers, and to the MSOE Center for BioMolecular Modeling[10] for developing this event nationwide.

Information and resources about this event are posted at **education.pdb.org** and on **twitter.com/buildmodels**.

The state champions from West Windsor Plainsboro High School North.

For more information on the NJ Science Olympiad, please see **njscienceolympiad.org**.

Recent and Upcoming Meetings and Events

The RCSB PDB presented along with the PSI SGKB at the 54th **Annual Meeting of the Biophysical Society** (February 20-24) in San Francisco, CA. Attendees stopped by the exhibit booth to meet with staff, see demonstrations of new features, and to take home the latest RCSB PDB materials. A poster on Education and Outreach at the RCSB Protein Data Bank was also presented by Christine Zardecki.

At the **National Science Teachers Association's National Conference** (March 18-21) in Philadelphia, PA, the RCSB PDB met with teachers at levels ranging from middle school to college. Teachers new to the resource were enthusiastic about incorporating features such as the *Molecule of the Month* in their classes, while current users were pleased to pick up materials such as the *How Do Drugs Work?* poster.

RCSB PDB staff introduced students of all ages to protein structure and function by building 3D models of virus structures at **Princeton's Science and Engineering Expo** (March 18) and the **San Diego Science Festival Expo Day** (SDSF; March 27).

Future meetings this summer include the 18th Annual International Conference on **Intelligent Systems for Molecular Biology** (July 11-13, Boston, MA); the **American Crystallographic Association's** meeting (July 24-29, Chicago, IL); the **Protein Society** (August 1-5, San Diego, CA), and a half day symposium on *The PDB and Chemistry* at the **American Chemical Society's** National Meeting & Exposition (August 22-26, Boston, MA).

John Westbrook at the Biophysical Society.

Virus building at SDSF.

Education Corner by Robert C. Bateman, Jr. and Paul A. Craig

A Proficiency Rubric for Biomacromolecular 3D Literacy

ROBERT BATEMAN *(robert.bateman@usm.edu) is a Professor of Biochemistry at the University of Southern Mississippi, where he has been a faculty member since 1988. He holds a bachelor's degree in biochemistry from Louisiana State University and a doctorate in biochemistry from the University of North Carolina at Chapel Hill. He performed postdoctoral work at the UT-Southwestern Medical Center at Dallas and did a sabbatical with Jane and David Richardson in 1999. His website is* ***ocean.otr.usm.edu/~w304739/****.*

PAUL CRAIG *(paul.craig@rit.edu), a member of the RCSB PDB Advisory Committee, is a Professor of Biochemistry and Bioinformatics at the Rochester Institute of Technology, where he has been a faculty member since 1993. He holds a bachelor's degree in chemistry from Oral Roberts University and a doctorate in biological chemistry from the University of Michigan. His postdoctoral work at the Henry Ford Hospital (Detroit, MI) was followed by a sabbatical at the San Diego Supercomputer Center with the RCSB PDB's Philip Bourne in 2002. His website is* ***people.rit.edu/pac8612/****.*

Biochemistry educators use a burgeoning variety of tools to teach concepts in higher order molecular structure, but continue to struggle with how to assess the effectiveness of these tools and approaches in promoting student learning. Resolution of this issue is important if we are to compare studies of teaching effectiveness. As a step towards this, we are expanding on the idea of molecular 3D literacy[11; 12] to propose a set of standards for achieving a level of proficiency in structural biology concepts appropriate to various educational levels. Such standards should not only provide a framework for assessment of teaching efficacy by novice and experienced instructors alike, but also enlighten developers of molecular visualization tools as they consider the education-oriented end-user.

Based on our own experiences over decades of teaching structural concepts in biochemistry,[11-14] we considered several factors in developing such a set of standards for molecular 3D literacy. First, we framed the standards in terms of a one-page proficiency rubric. While there are undoubtedly those who would argue that it is too limiting, we believe that anything more comprehensive will simply not be useful to most instructors who use these standards as a basis for assessing the effectiveness of teaching structural concepts. Second, we divided the rubric into three columns to correlate proficiency levels with the appropriate educational objectives of the course. This makes it not only useful in a wide variety of educational settings ranging from high school to graduate school, but enables its direct use in assessing advanced courses. Third, the rubric should be as independent of the teaching modality and technology as possible, *i.e.*, it needs to separate the concepts from the tools. It would therefore be valuable in assessing learning with any kind of molecular visualization tool including hard models, graphic rendering programs like Jmol[15] and PyMOL[16], simulations, animations, interactive games, haptics, *etc.* Fourth, the rubric is intentionally broad enough to cover a variety of biomacromolecules and is thus not limited to the usual protein structure concepts.

As we use different molecular visualization tools with students and demonstrate them to colleagues who teach at levels from secondary school through college, we find that their fascination with the beauty of the images and animations interferes with higher level thinking about the structures themselves. One of the goals of establishing the rubric is to introduce users to critical thinking concerning the 3D data they encounter. Some items in the rubric directly address this issue: atomic geometry and structural model skepticism. Other items gauge the user's ability to employ the molecular visualization software as something other than a black box: structure-function relationships, topology, and connectivity.

The proficiency rubric shown here has been reproduced from the original at **ocean.otr.usm.edu/~w304739/MolVisProf.pdf**. It is composed of a one-page grid followed by a one-page legend of the categories included. These categories address information in alternate renderings, molecular motion, structure-function relationships, limitations of molecular models, geometric constraints, recognition of higher order symmetry, chain topology, intermolecular interactions, monomer and het group recognition, and construction/annotation. This last category is not so much a concept as the ability to apply the other molecular concepts to a new situation.

Since this is intended to be a tool that will benefit everyone who teaches biomacromolecular structure concepts, we ask the community to assist in refining this tool by providing feedback directly to one of us and by using the rubric in your courses. If you develop a grading/assessment rubric of your own that is tailored to your purposes, please send us a copy along with information about your course and your contact information so we can properly acknowledge your contribution.

PROPOSED ASSESSMENT RUBRIC FOR BIOMACROMOLECULAR 3D LITERACY

DEFINITION OF TERMS:

Alternate Renderings: Rendering of a macromolecular structure such as a protein or nucleic acid structure in various ways from the simplest possible way (connections between alpha carbons) to illustration of secondary structure (ribbons) to surface rendering and space filling.

Kinematics: Animated motion simulating conformational changes involved in ligand binding or catalysis, or other molecular motion/dynamics.

Structure-Function Relationship: Active/binding sites, microenvironments, nucleophiles, redox centers, *etc.*

Structural Model Skepticism: Recognition of the limitations of models to describe the structure of macromolecules.

Atomic Geometry: three atom and four atom (dihedral) angles, metal size and metal-ligand geometries, steric clashes.

Symmetry Recognition: recognition of symmetry elements within both single chain and oligomeric macromolecules.

Topology and Connectivity: Following the chain direction through the molecule, translating between 2D topology mapping and 3D rendering.

Intermolecular Interactions: covalent and noncovalent bonding governing ligand binding and subunit-subunit interactions.

Construction and Annotation: ability to build macromolecular models, either physical or computerized, and, where possible, add commentary, either written or verbal, to tell a molecular story.

Monomer Recognition: recognition of both native and modified amino acids, nucleotides, sugars, and other biomonomer units. Understanding of their physical and chemical properties, particularly regarding functional groups.

Het Group Recognition: metals and metal clusters, posttranslational additions such as glycosylation, phosphorylation, lipid attachment, *etc.*

The authors thank Drs. Ricky Cox and Brian Zoltowski for their helpful comments.

Reprinted from **ocean.otr.usm.edu/~w304739/MolVisProf.pdf** *with permission.*

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	Introductory Biology (Novice level)	Biochemistry/Cell Biology (Amateur level)	Structural biology graduate student (Expert level)
Alternate Renderings	Views alternate renderings as different molecules or giving different properties to molecule.	Sees alternate renderings as different views of the same molecule. Understands basic information conveyed by each.	Understands the limitations and information to be gained by each type of molecular rendering.
Kinematics	Sees animation as cartoon rather than as structural motion.	Recognition of molecular hinges and movement of both backbone and sidechains during conformational change.	Understands the limitations and information to be gained by various types of animations. Creates and evaluates animations.
Structure-Function Relationship	Vague notion of active/binding sites or functional groups. Can visualize nucleic acid grooves.	Recognition of the role the structure of the binding site plays in function. Can reasonably predict the effect of a mutation on function. Sees relationships between structurally homologous binding sites which may not have sequence homology.	Sees beyond the binding site to the role of the overall structure in function. Can extract information and relationships from figures in publications or presentations.
Structural Model Skepticism	Acceptance of physical or graphic structure as portrayed.	Understands fundamental limitations of models derived from either experimental or theoretical means.	Is able to query model with visual inspection and validation tools to identify flaws.
Atomic Geometry	Unable to recognize problematic bond angles or gain information from them.	Recognizes obvious problems with bond angles and geometries. Is able to measure dihedral angles and identify secondary structures.	Is able to propose alternative structural interpretations that may resolve problems. Recognizes relationship of metal ligand geometry to redox state and potential function.
Symmetry/ Asymmetry Recognition	Able to see simple rotational axes of symmetry.	Able to orient molecule to illustrate axes of symmetry. Recognizes helical handedness and dipoles.	Recognizes symmetry in oligomers as well as monomers (e.g., fused gene duplications). Recognizes significant charge asymmetries.
Topology and Connectivity	Able to see overall shape of molecule and general chain winding.	Able to determine chain direction from visual inspection. Able to draw a linear topology map illustrating secondary structure sequencing.	Able to draw a 2D topology map of supersecondary structure from a 3D structural model. Recognizes common protein folds and possible evolutionary relationships.
Molecular Interactions	Able to discern key intramolecular interactions such as hydrogen bonding or charge interactions.	Able to recognize specific intermolecular interactions (H bonding, salt bridges, *etc.*).	Able to recognize nonspecific forces at interfaces, i.e. packing and hydrophobic interactions.
Construction and Annotation	Able to build only the simplest molecular model.	Able to construct a macromolecular model from a coordinate set and provide brief annotation.	Able to read a PDB file and construct a detailed, labeled model making appropriate use of color, animations, and alternate renderings from it.
Monomer Recognition	Able to distinguish between dissimilar monomers.	Recognizes all native monomer groups and their physical properties.	Recognizes unusual or modified monomer groups and surmises their physical and functional properties.
Het Group Recognition	Does not recognize significant additions to the biopolymer chain.	Recognizes common het groups such as common metals and glycans.	Recognizes unusual/unexpected het groups and surmises their physical and functional properties.

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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 Worldwide Protein Data Bank (www.wwpdb.org)

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A list of current RCSB PDB Team Members is available from www.pdb.org.

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