MS22.03.13 3DBASE - A MACROMOLECULAR STRUCTURE DATABASE. E.E.Abola, J.Prilusky, N.O.Manning, J.L.Sussman, Chemistry Department, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY, 11973-5000 USA and Bioinformatics Unit, Weizmann Institute of Science, 76100 Rehovot, Israel

The Protein Data Bank (PDB) is an archive of experimentally- determined three-dimensional structures of biological macromolecules. We will describe the new relational database, 3DBase, that represents the structural, biological, chemical, and bibliographic information found in the PDB archives.

3DBase is constructed with the SYBASE DBMS and the Object Protocol Model (OPM) and OPM data management tools developed by Victor Markowitz's group at Lawrence Berkeley National Laboratory. SYBASE provides a powerful and robust environment for data management, the OPM tools allow rapid development of SYBASE databases, while OPM's object-oriented view provides a scientifically intuitive representation of data.

Objects have been incorporated into the database schema that allow for description and access of 3-dimensional information from a number of viewpoints. Crystallographers can access a full description of the diffraction study via the oExperiment Object, while structural data on the biologically active molecule are accessed through oMacromolecule. 3DBase also includes facilities for extended annotation by outside users of any accessible object.

Access to 3DBase is provided primarily through a Web browser constructed using the Genera software package developed by Stan Letovsky of Johns Hopkins Medical Institutes. In addition to accessing data stored in 3DBase, the browser provides links to entries in other databases. Graphical views of molecules are provided in the browser by use of Roger Sayle's Rasmol program along with graphical annotation commands stored in the database. In the future, multiple interfaces to 3DBase will be provided with support for queries of increased complexity.

The PDB is supported by a combination of Federal Government Agency funds and user fees. Support is provided by the U.S. National Science Foundation, the U.S. Public Health Service, National Institutes of Health, National Center for Research Resources, National Institutes of General Medical Sciences, National Library of Medicine, and the U.S. Department of Energy under contract DE-AC02-76CH00016.

PS22.03.14 PROTEIN DATA BANK - WHERE WE ARE TODAY. N.O.Manning, E.E.Abola, F.C.Bernstein, J.A.Callaway, F.M.Cummings, B.R.Deroski, P.A.Esposito, A.Forman, P.A.Langdon, M.D.Libeson, J.E.McCarthy, J.Prilusky, J.P.Rose, R.K.Shea, J.L.Sikora, D.R.Stampf, S.Swaminathan, D.Xue, and J.L.Sussman, Chemistry Department, Brookhaven National Laboratory, P.O. Box 5000, Upton, NY, 11973-5000 USA

The Protein Data Bank (PDB) is an archive of experimentally- determined three-dimensional structures of biological macromolecules, serving a global community of researchers, educators, and students. Accessible on the World Wide Web at URL http://www.pdb.bnl.gov, the PDB is easily queried via a Web Browser form, and specific structures can be viewed, downloaded, or studied via links to other biological databases.

The PDB has successfully responded to the rapidly-increasing number of depositions by implementing more efficient, semi-automatic procedures for both data deposition and entry processing. The quality of released PDB coordinate entries is ensured by validation procedures that include WhatCheck by Gert Vriend and Rob Hooft of EMBL, as well as by batch quality assurance measures developed by the PDB. New collaborations have also helped the PDB provide better service to our users.

The new PDB Contents Guide which details the exact format of atomic coordinate entries was recently released. This Contents Guide is helpful to several communities, assisting depositors in preparing their entries for deposition, guiding software and information resource developers, and helping users of the PDB to understand the contents of coordinate entries. Additionally, this format description is crucial in the effort to produce CIF-compliant data files from PDB entries. A review of the past year's achievements will be presented.

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