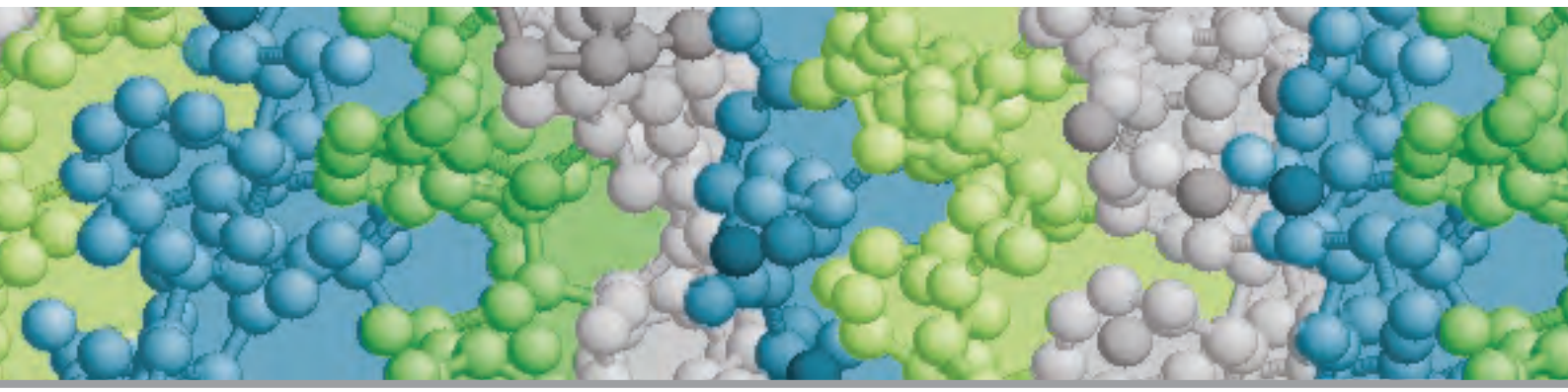
PDBj
Protein Data Bank Japan

http://www.pdbj.org/

News Letter Vol. 9, No. 1

August 2007



PDBj is maintained at the Protein Research Institute, Osaka University, and supported by Japan Science and Technology Agency.

News

About the wwPDB Remediation Project

The evolution of experimental methods, functional knowledge of proteins, and methods used to process PDB data has introduced inconsistencies into the archive. The wwPDB has remediated these data to create a more uniform archive. The new archive is now available starting August 1, 2007 from ftp://ftp.wwpdb.org/ and from our mirror site: ftp://pdb.protein.osaka-u.ac.jp/v3/. In addition, all the data that are viewed on our browsing system (xPSSS) are based on these Remediated PDB data (Version 3.1).

There are several essential changes including even the atom nomenclature, and so application programs may not work without modifications. So far, several tools, which can parse the Remediated data, have been developed, and they are available from: http://remediation.wwpdb.org/software.html. Our graphics viewer, jV3.4 (http://www.pdbj.org/jV/), can also parse and display the Remediated data (Version 3.1), in addition to the previous PDB data (Version 2.3). Moreover, a nomenclature converter system from the Remediated data (Version 3.1) to the previous PDB data (version 2.3) is available at: http://util.wwpdb.org/.

The results of these remediation efforts can be found in the remediated coordinate files. Highlights include the following:

Sequence: Updated references to databases and taxonomies and resolved differences between chemical and macromolecular sequences

Citation: Verified and updated primary citation assignments

Assembly and virus Information: Improved representation of deposited and experimental coordinate frames, symmetry, and frame transformations

Nucleic acid labeling: Deoxy and ribose nucleotides assigned separate chemical definitions. The DNA forms are relabeled as DA, DC, DG, DT, and DI. RNA forms remain labeled as A, G, C, U, I.

Beamline data: Beamline and synchrotron facility names have been made consistent with BioSync.

Atom nomenclature: Standardized to reflect changes in the Chemical Component Dictionary (http://remediation.wwpdb.org/tutorial.html), which contains the following:

* Use of IUPAC nomenclature for standard amino acid and nucleotides, with the exception of the well-established conventions for C-terminal atoms OXT and HXT
* More conventional atom labeling
* Addition of model and idealized coordinates
* Use of chemical descriptors (e.g. SMILES, InChI) and systematic names
* Stereochemical assignments
* Removal of redundant ligands
* Creation of a companion dictionary of amino acid variants to provide additional nomenclature information for the protonation states of standard amino acids in N-terminal, C-terminal, and free forms. This dictionary also includes common side chain protonation states.

The previous PDB data (version 2.3) dated on July 31, 2007 are now frozen, but they can be downloaded from the ftp site: ftp://pdb.protein.osaka-u.ac.jp/pub/pdb/ and from our PDBj Web page, http://www.pdbj.org/remediation/, by identifying each PDBID.

The 7th Annual Meeting of the Protein Science Society of Japan

The 7th Annual Meeting of the Protein Science society of Japan was held from 24th to 26th May, 2007 at the Sendai International Center in Sendai. We introduced our activities, including the announcement of remadiated PDB files and BMRB services.

Snapshots of the 7th PSSJ.

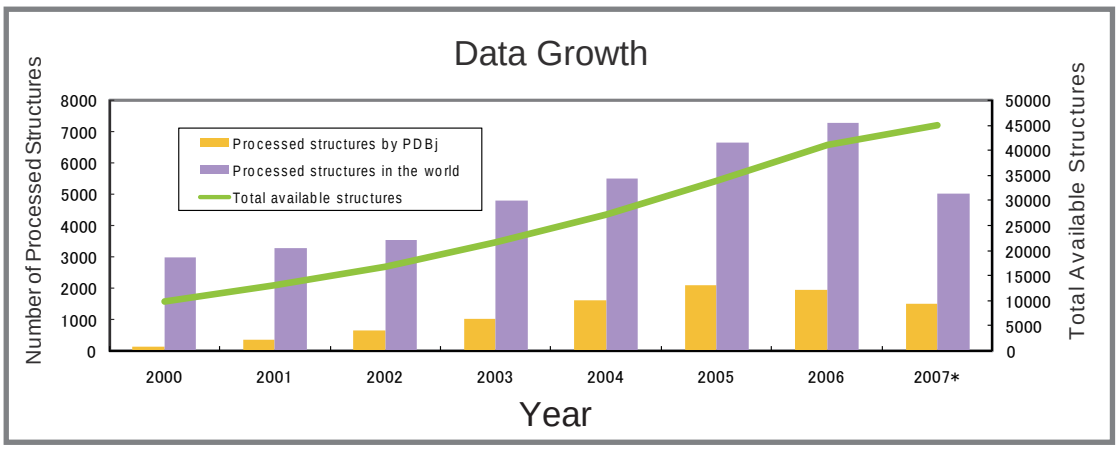
Ichou Festival

The annual university festival, known as Ichousai, was held at Osaka University on April 30th and May 1st. The laboratories and institutes were opened to the public, including high school students. We introduced the eProtS database, which is described further in this issue.

Snapshot of Ichou Festival.

Statistics

The statistics data is available at the wwPDB page (http://www.wwpdb.org/stats.html).



* Last updated : July 31, 2007

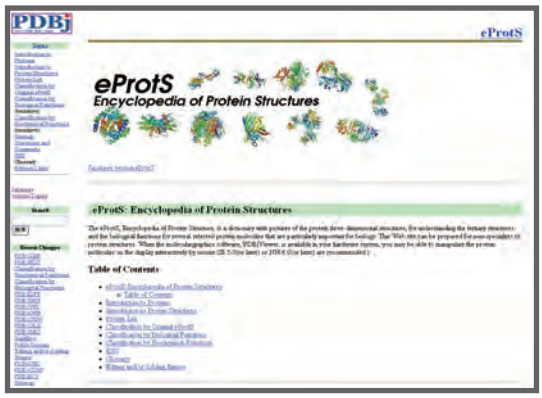
Services

eProtS: Explaining protein structures to non-specialists

eProtS stands for the ``encyclopedia of Protein Structures.'' It contains descriptions of many protein structures of general interest, in terms of their biological and/or social contexts, and structural features.

eProtS is especially targeted at non-specialists such as advanced high school or college students, or even professional scientists in other fields. The contents are available both in Japanese and in English.

In order to catch up with the ever increasing PDB entries, we have developed a Wiki version of eProtS. If you are a structural biologist and want to explain your favorite protein to the general public, please contribute!



The eProtS frontpage.

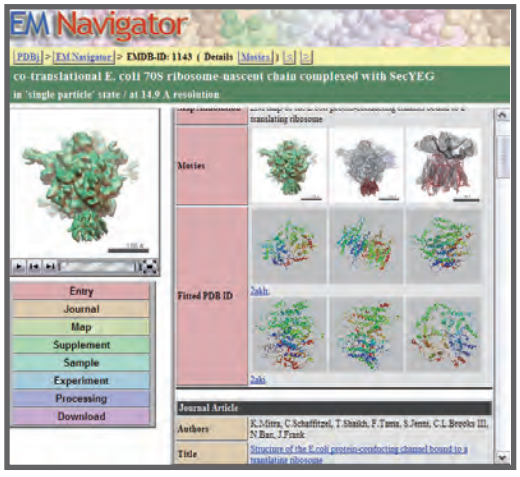
EM Navigator - Electron microscopy data browser

Many readers of this newsletter might not know much about electron microscopic (EM) structure analysis. EM Navigator, our new service for browsing EM structure data, has been constructed so that even non experts can easily browse and enjoy 3D EM data.

Traditionally, EM structure data have not been user-friendly. It is often very hard to recognize the 3D structures by just seeing the figures in the papers or web pages. In the case of atomic coordinates of proteins, we can easily get the 3D views using jV on the PDBj web site or by opening the downloaded data using some popular software such as RasMol. The 3D maps from EM structural analyses have been deposited to the EM Databank managed by MSD-EBI, which is also a member of wwPDB. However, it requires some skill and effort to visualize the map data as shown in the papers. The barriers are much higher for viewing the structures combined with other data, such as the fitted atomic coordinates.

We are now constructing movies for each data entry in the EMDB, and are embedding them in the EM Navigator web pages. You will easily get the 3D views with detailed information using a web browser without installing special software. Further, movies will be added, such as views with the fitted atomic models and zoomed up images around important regions. Moreover, we are making the site more useful by including snapshots of PDB data along with the EM data, the images of the supplementary information deposited by authors, and so on.

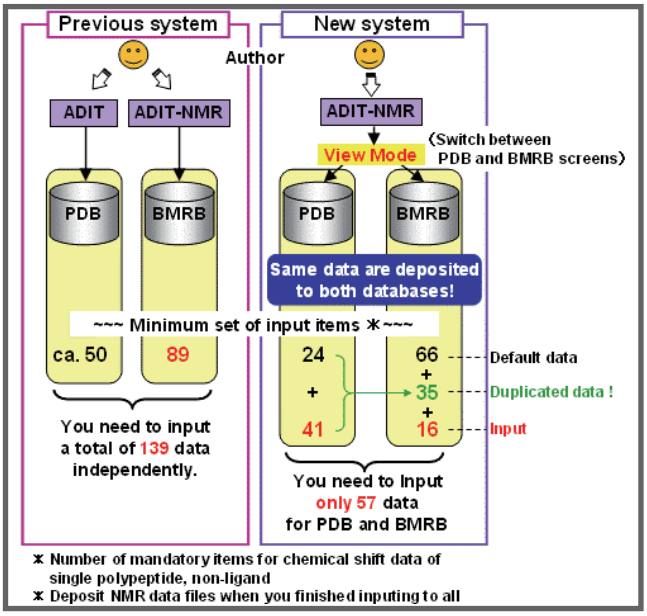
Our goal is not only to have an easy-to-use enjoyable site, but to build some analytical services as well, making use of other database entries in the future.



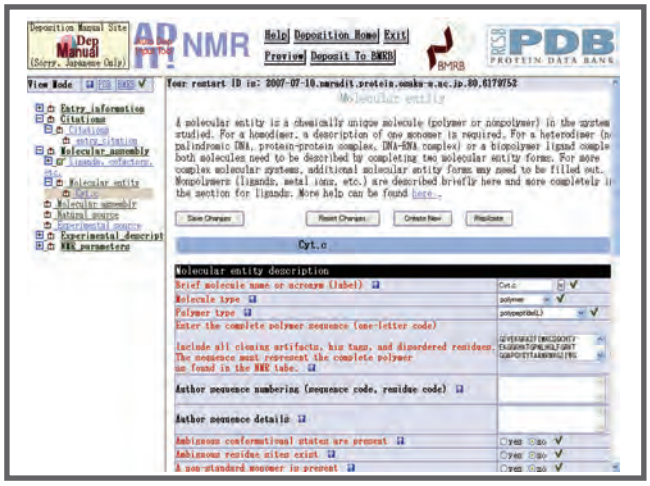
The EM Navigator frontpage.

New Data Deposition Website ADIT-NMR

A new version of ADIT-NMR, the data deposition website of BMRB (BioMagResBank, University of Wisconsin-Madison), has been released at BioMagResBank in September, 2006 and at PDBj in May, 2007. Previously, researchers had to input data and upload files of assigned NMR data to BMRB, and atomic coordinates to PDB deposition websites, individually. However, these deposition websites are now integrated into a single website. In the new ADIT-NMR (http://nmradit.protein.osaka-u.ac.jp/bmrb-adit), some items in data categories such as citation and general entry information, description of molecules and source are input only once. Such data can be shared with BMRB and PDB depositions. Also, many default values are indicated, and researchers can select values from pulldown menus. The summary of these improvements is shown in the right figure. We expect that these changes will contribute to reducing the deposition workload for researchers.



The difference between the new and previous system of BMRB and PDB data deposition.



The session screen on the new ADIT-NMR. (http://nmradit.protein.osaka-u.ac.jp/bmrb-adit)

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