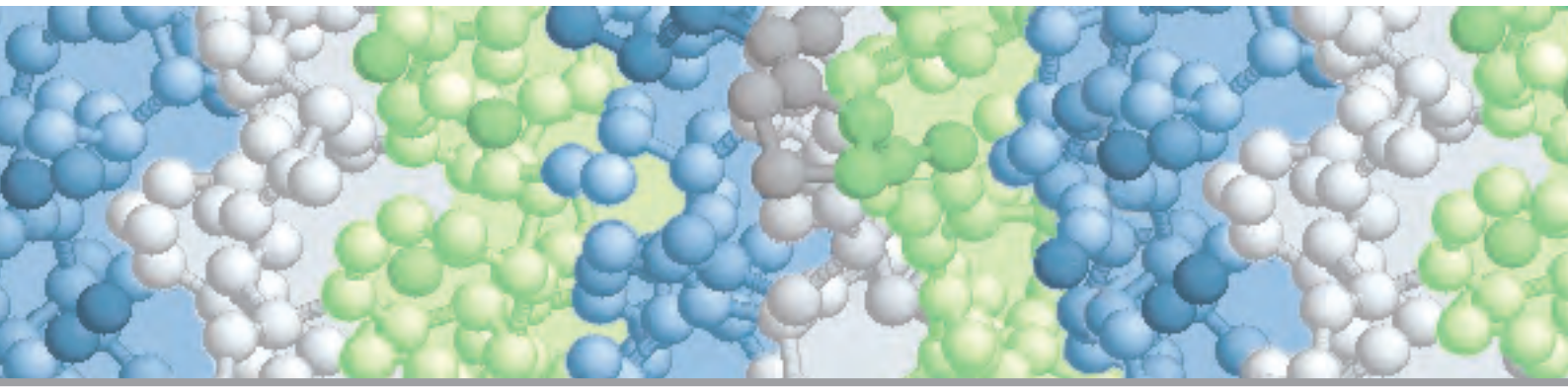
PDBj

Protein Data Bank Japan

http://www.pdbj.org/

News Letter Vol. 8, No. 1

June 2006



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

News

Announcement

In April, 2006, PDBj (Protein Data Bank Japan) started the renewed project for the development of structural databases of biological macromolecules supported by BIRD (Institute of Bioinformatics Research and Development)-JST (Japan Science and Technology Agency).

Every year, the wwPDB (worldwide Protein Data Bank) registers more than 6,000 structures of biological macromolecules such as proteins and nucleic acids determined all over the world, and it gave us a total of more than 37,000 structures as of June, 2006. As one of the wwPDB members, PDBj collaborates to maintain the PDB database with the other international members, RCSB-PDB in the United States, MSD-EBI in the EU, and BMRB (BioMagResBank), who is a new member and manages the database for biological NMR experimental data. PDBj will also develop its own services.

In the renewed project, in addition to continuously curating, editing and validating much more deposited structure data, and maintaining their quality, we will start to develop new databases covering solid-state NMR data and electron density data observed by high-resolution electron microscopy experiments. Thus, by applying the most advanced information technology such as Grid, PDBj will construct more useful and informative databases

In particular, collaborating with MSD-EBI and RCSB-PDB, PDBj is going construct a database for the electron density maps by high-resolution microscopy, single particle analysis, and tomography of biological supramolecules and membrane proteins, a field in which many Japanese researchers contribute. In 2006, PDBj hired a new researcher who has experience in EM experiments and analysis, and will start to develop the database.

The information of atom coordinates is essentially analogue data, and so a quick query search is highly desired for the analogue information such as the molecular shape and the surface shape. PDBj is going to develop a new Grid system, where such tough queries are rapidly processed using many CPUs, distributed in many places in Japan. In addition, PDBj will integrate several services, which we have so far developed, so as to construct a new portal site, which offers information about function and evolution of proteins. This could give us effective tools for function annotation of newly analyzed proteins.

In October, 2006, the wwPDBAC (wwPDB Advisory Committee) meeting will be held in Tokyo, where all the wwPDB members and the advisory boards will gather to discuss issues of the current situation and the future progress of the wwPDB.

PDBj will continuously develop its own graphic viewer, jV, and the educational database of protein structures (eProtS). We will also make timely tutorial courses for users and beginners of the PDB database.

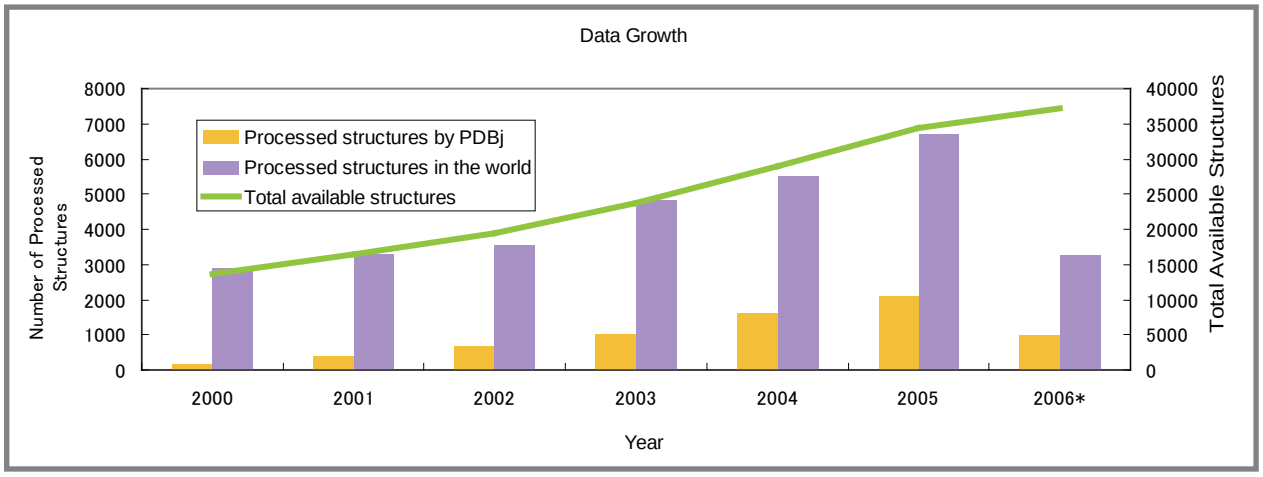
We hope for your support and collaboration.

The 6th Annual Meeting of the Protein Science Society of Japan

The 6th Annual Meeting of the Protein Science Society of Japan was held on April 24th- 26th 2006 at Kyoto International Conference Hall. We introduced our activities and Structure Query Service at the lunchon-seminar on 26th. It drew an audience of 120 or more. We have received valuable comments on our services through the questionnaire.

Statistics

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



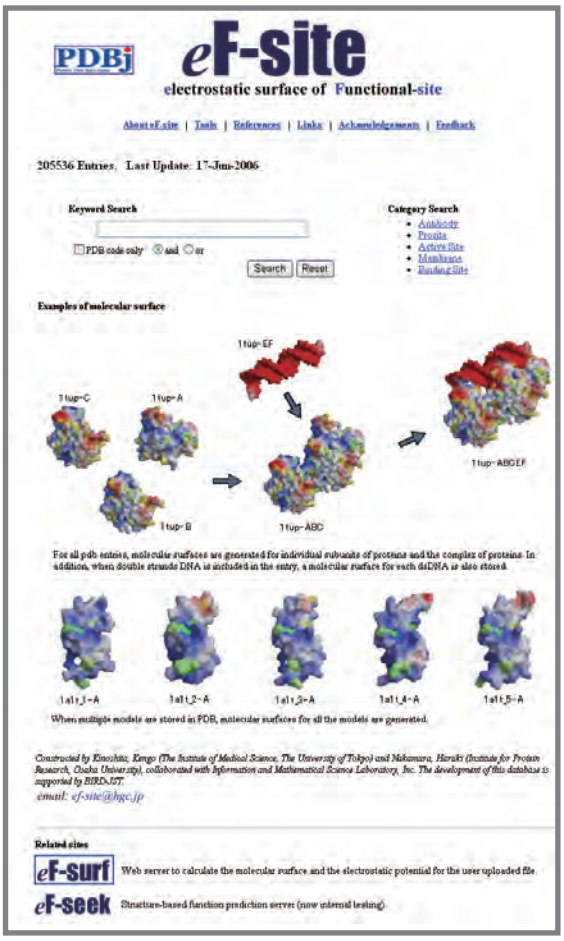
* Last updated : June, 2006

Services

*e*F-site

The database eF-site (electrostatic surface of functional site) for the molecular surfaces with the electrostatic potential and hydrophobic properties has so far been developed at PDBj. It now contains 205,536 molecular surface entries as of June 17, 2006, which cover almost all the PDB entries. Those data are updated every week with the addition of new entries in the PDB.

In addition, we, PDBj, proceed to construct mirror sites of our databases. For the eF-site database, the server of the eF-site@HGC (Human Genome Center, The University of Tokyo: http://ef-site.hgc.jp/eF-site/) is completely synchronized with that of the eF-site@IPR (Institute for Protein Research, Osaka University: http://ef-site.protein.osaka-u.ac.jp/eF-site/), and so the users can choose either at their convenience.



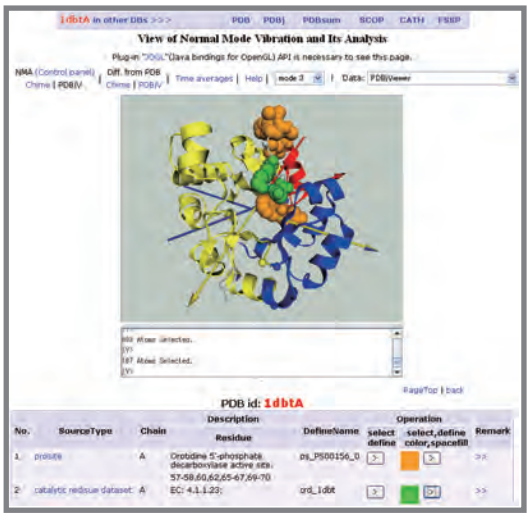
The eF-site frontpage.

jV3.2

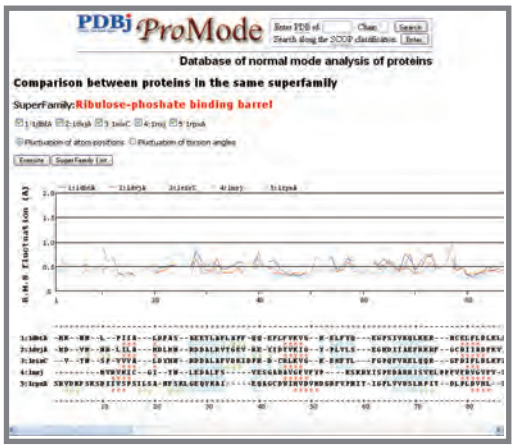
The new version of the PDBjViewer, jV, is now released (ver 3.2). The new command “show site” was added in this version, which enables jV to download the data from the databases in the similar way to that of “show xps3” . In addition, some known bugs were fixed and the stability of jV was much improved. Furthermore, the new user manual is now available at http: //ef-site.hgc.jp/eF-site/jV/ jV3_User'sGuide.pdf. The new manual is written in a tutorial style and covers the latest functionalities of jV3.2.

*Pro*Mode (database of normal mode analysis of protein structures)

Several new functions have been installed on *Pro*Mode. (1) Animation of vibrational motion of protein structure can be displayed by the jV viewer in addition to Chime. The animation with a cartoon model, which is only available on jV, is more impressive when observing protein motions. (2) Knowledge information such as PROSITE motifs and catalytic residues are listed below the animation window in *Pro*Mode, if any. The relevant residues can be highlighted on the animation easily. It is interesting to relate such residues to a dynamic structure of the protein (e.g., dynamic domains defined by DynDom which are distinguishable by colors in *Pro*Mode). (3) The new pages to compare fluctuations of homologous proteins (proteins classified into the same superfamily in the SCOP database) have been created. The homologous proteins are structurally aligned by ASH, and then the fluctuations of atomic positions and dihedral angles are plotted in the same chart. In some regions the fluctuations of the residues are comparable to each other and in other regions they have more variety. Such kinds of information are useful to understand the dynamic structure of proteins.

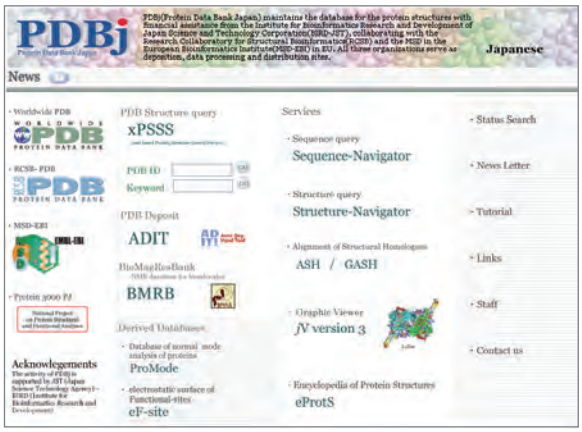


The animation window by jV and the knowledge information list in ProMode.



The page of comparison among homologous proteins in ProMode.

Renewed Top Page!!

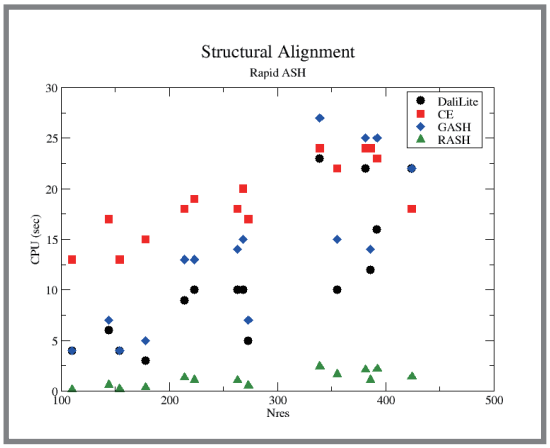


Structure Navigator RT (β version)

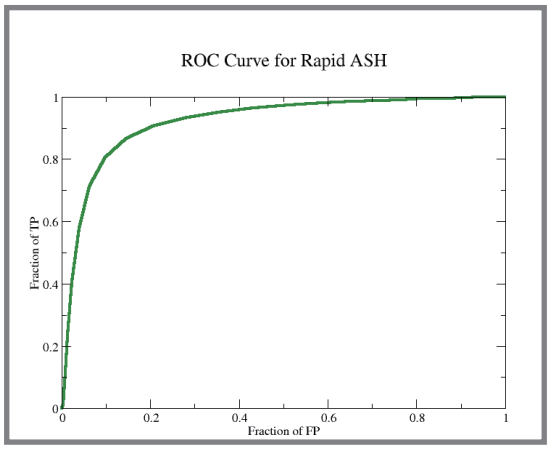
It has long been our goal to offer structure-based queries at PDBj. Now, with Structure Navigator RT (β version), a real-time structure query service, it is possible. Structure Navigator RT works by rapidly aligning a query structure to representative structures, then mapping the remaining PDB structures onto the representatives using stored alignments. The entire query process can be done in seconds to minutes.

The first goal in constructing Structure Navigator RT was to develop a rapid structure alignment algorithm we call Rapid ASH (RASH). On the right we show the improvement in terms of speed for RASH compared to DaliLite, CE, and GASH. Also shown is the accuracy in terms of an ROC curve. This accuracy is evaluated based on 8,581,970 structure pairs as described by Kolodny et al. (J. Mol. Biol. (2005) 346, 1173-1188.

Although RASH is much faster than DaliLite or CE, it is still not fast enough for real-time structure based queries. We also needed a means of sorting alignments based on their expected structural similarity. We defined a structural descriptor vector for the query and for each template in our database consisting of the length of the structure, percent helical content, percent strand content, radius of gyration, and contact order. Using these descriptors, templates could be aligned rapidly.

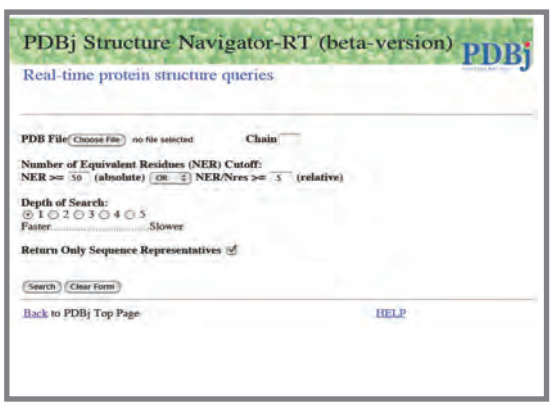


Improved speed of RASH.

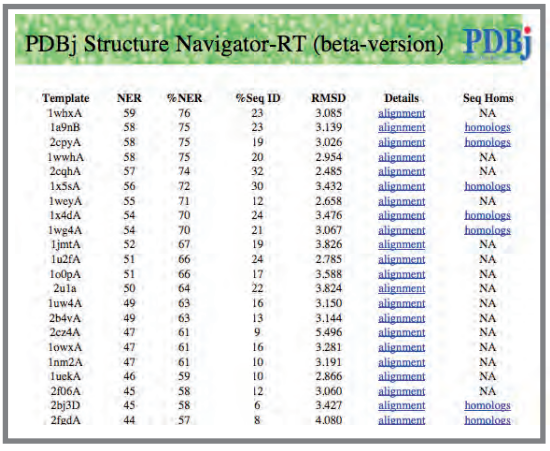


Accuracy in domain assignment by RASH.

The top page of Structure Navigator RT is similar to that of Structure Navigator except that there is a window for uploading a PDB formatted file. The results are then returned in seconds to minutes, and are clustered by sequence family. The actual alignments and superpositions are similar in format to Structure Navigator, and can be viewed online or downloaded.



RASH top page.



Template	NER	%NER	%Seq ID	RMSD	Details	Seq Homs
1whxA	59	76	23	3.085	alignment	NA
1a9nB	58	75	23	3.139	alignment	homologs
2cpyA	58	75	19	3.026	alignment	homologs
1wwhA	58	75	20	2.954	alignment	NA
2cqhA	57	74	32	2.485	alignment	NA
1x5sA	56	72	30	3.432	alignment	homologs
1weyA	55	71	12	2.658	alignment	NA
1x4dA	54	70	24	3.476	alignment	homologs
1wg4A	54	70	21	3.067	alignment	homologs
1jmtA	52	67	19	3.826	alignment	NA
1u2fA	51	66	24	2.785	alignment	NA
1o0pA	51	66	17	3.588	alignment	NA
2u1a	50	64	22	3.824	alignment	NA
1uw4A	49	63	16	3.150	alignment	NA
2b4vA	49	63	13	3.144	alignment	NA
2cz4A	47	61	9	5.496	alignment	NA
1owxA	47	61	16	3.281	alignment	NA
1nm2A	47	61	10	3.191	alignment	NA
1uekA	46	59	10	2.866	alignment	NA
2f06A	45	58	12	3.060	alignment	NA
2bj3D	45	58	6	3.427	alignment	homologs
2fedA	44	57	8	4.080	alignment	homologs

RASH results page.

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