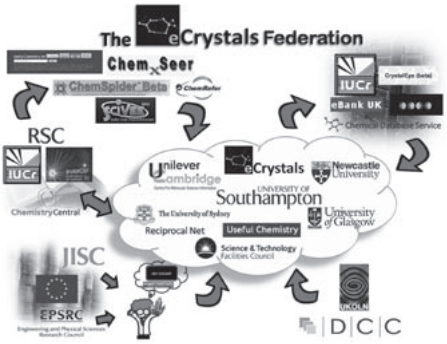
chem.soton.ac.uk) is establishing a network of such crystallographic data repositories across an international group of laboratories. Data is being harvested by CCDC and the CDS and the project is working with IUCr, RSC, Chemistry Central and Nature to establish protocols for scaleable harvesting mechanisms across the network. By engaging data centres, librarians, researchers, publishers and information providers we are developing approaches to the preservation and curation of scientific data in open repositories (the UK Digital Curation Centre is a partner). A demonstration and strategies for installation and population of eCrystals repositories at new sites will be outlined, based on experiences of early adopter sites.



Keywords: publishing, database preparation, software for crystallography

P24.04.05

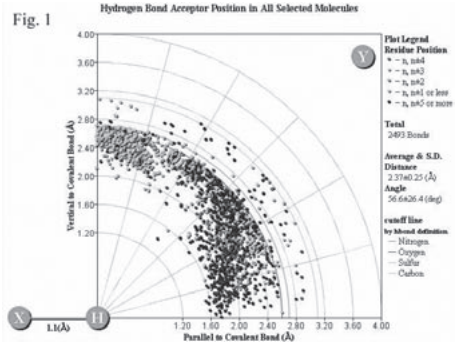
Acta Cryst. (2008). A**64**, C627

Development of hydrogen and hydration database for biomolecules (HHDB)

Nobuo Okazaki[1], Takashi Ohhara[1], Hisao Umino[1], Toshiyuki Chatake[2], Kazuo Kurihara[1], Raul E Cachau[3], Michael Blaber[4], Nobuo Niimura[5], Ryota Kuroki[1]
[1]Japan Atomic Energy Agency, Quantum Beam Science Directorate, Research Group for Molecular Structural Biology, 2-4, Shirakata-Shirane, Tokai, Ibaraki, 319-1195, Japan, [2]Kyoto University Research Reactor Institute, [3]Advanced Biomedical Computing Center, National Cancer Institute at Frederick, [4]Department of Chemistry and Biochemistry, Florida State University, [5]Graduate School of Science and Engineering, Ibaraki University, E-mail：okazaki.nobuo@jaea.go.jp

In protein molecules, key energetic contributors are solvation, desolvation and hydrogen bonding. They contribute protein folding, dynamics and molecular recognition. As a result, more elaborate studies of hydrogen atoms will be great help to recognize protein structures and obtain new findings of them. However, we do not have system which dedicated to characterization and analysis of hydrogen bonding. Therefore, we have developed a database for hydrogen and hydration water molecules. That database named Hydrogen and Hydration Database for Biomolecules (HHDB; http://hhdb.tokai-sc.jaea.go.jp/). Hydrogen bond data stored to HHDB use hydrogen atom coordinates determined directly by neutron diffraction and certain extremely high resolution x-ray diffraction. HHDB provides graphical user interface, users can use it through web browser. HHDB can visualize hydrogen atom positions in protein and solvent, and hydrogen bonding interactions. Figure 1 shows HHDB plot example. In this plot, hydrogen atom is placed at the origin, and each point represents hydrogen bond distance and angle. We are improving the web user interfaces and the performance for usability.

Fig. 1



Keywords: neutron diffraction, protein, hydrogen bond

P24.04.06

Acta Cryst. (2008). A**64**, C627

Protein-protein interactions: Structural features and empirical estimation of free energy of binding

Pinak Chakrabarti, Mainak Guharoy
Bose Institute, Department of Biochemistry, P1/12 CIT Scheme VIIM, Kolkata, W. Bengal, 700054, India, E-mail：pinak@boseinst.ernet.in

An analysis of protein-protein complexes has shown that the average interface area (the accessible surface area, ASA, on the two components that gets buried on complex formation) is ~2000 Å^2 [1] and that the interface can be dissected into core and rim regions with the former being composed of residues that are more conserved than those in the latter [2]. There is an approximate linear relation between the change in the surface area buried (δASA) and the change in free energy of binding (δδG) obtained from alanine scanning mutagenesis. This relationship has now been used to predict the free energy of binding (δG). The experimental δG varies linearly with the interface area (or the number of atoms buried in the complex), but plateaus off beyond ~1600 Å^2, indicating that the energy gained from burying additional surface area is used for conformational changes associated with larger interfaces. Further, the interface can be dissected into secondary structural segments [3]. The β and NR-classes of interfaces have a relatively lower δG than α- and $\alpha\beta$-classes.

References
[1] Chakrabarti, P. and Janin, J. Dissecting protein-protein recognition sites. Proteins, 47, 334-343 (2002).
[2] Guharoy, M. and Chakrabarti, P. Conservation and relative importance of residues across protein-protein interfaces. Proc. Natl. Acad. Sci. USA, 102, 15447-15452 (2005).
[3] Guharoy, M. and Chakrabarti, P. Secondary structure based analysis and classification of biological interfaces: identification of binding motifs in protein-protein interactions. Bioinformatics, 23, 1909-1918 (2007).

Keywords: protein-protein interactions, free energy of binding, molecular recognition

P24.07.07

Acta Cryst. (2008). A**64**, C627–628

Defining a protein: Mining the protein structure database

Boguslaw Stec, B.V.L.S. Prasad, Ying Zhang, Adam Godzik
Burnham Institute for Medical Research, IIDC, 10901 N. Torrey Pines Rd., La Jolla, CA, 92037, USA, E-mail：bstec@burnham.org

Rapid increase of structural information expressed in the explosive growth of the PDB allows for rigorous studies of two links in a central biology paradigm: a sequence-structure and a structure-function relationship. We constructed a database of redundant protein structures by application of sequence- based methods (CD-HIT). Subsequently, we clustered the structures belonging to a single protein sequence by structural methods (BOSv3) and derived a global