

Hydrogen and Hydration DataBase for Bio-Macromolecules (HHDB)

Ryota Kuroki¹, Toshiyuki Chatake¹, Kazuo Kurihara¹, Takashi Ohhara¹, Hisao Umino¹, Raul E. Cachau³, Michael Blaber⁴, Nobuo Niimura^{1,2}, ¹*Neutron Science Research Center, Japan Atomic Energy Research Institute (JAERI)*. ²*Institute of Applied Beam Science, Graduate School of Science and Engineering, Ibaraki University*. ³*Advanced Biomedical Computing Center, National Cancer Institute at Frederick*. ⁴*Department of Chemistry and Biochemistry, Florida State University*. E-mail: r-kuroki@neutrons.tokai.jaeri.go.jp

Solvation, desolvation and hydrogen bonding are key energetic contributors to biopolymer folding, dynamics and molecular recognition; however, no systematic, high-resolution stereochemical database dedicated to the characterization and analysis of hydrogen bonding exists. We have created a hydrogen and hydration database for bio-macromolecules (HHDB; <http://hhdb.tokai.jaeri.go.jp>) that categorizes all hydrogen atoms and hydration water molecules including hydrogen atoms in proteins. The HHDB includes H-bond data only from direct determination of hydrogen atoms by neutron diffraction, and certain extremely high resolution x-ray diffraction data. The HHDB provides a graphical user interface for the visualization of all hydrogen atom positions in proteins and solvent, and all hydrogen bonding (H-bond) interactions. For example, one type of plot featured in the database places the hydrogen atom positions at the origin and plots the direction of the H-bond donor along the horizontal axis, allowing the user to visualize the distribution of the acceptor atoms, distance and angle. The HHDB provides researchers with a much-needed resource for understanding and analyzing hydrogen-bonding.

Keywords: neutron diffraction, protein, hydrogen bond