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Macromolecular Neutron Diffraction at the Heinz Maier-Leibnitz Zentrum MLZ

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Neutron single crystal diffraction provides an experimental method for the direct location of hydrogen and deuterium atoms in biological macromolecules, thus providing important complementary information to that gained by X-ray crystallography. At the MLZ the neutron single crystal diffractometer BIODIFF, a joint project of the Forschungszentrum Jülich and the FRM II, is dedicated to structure determination of proteins. Typical scientific questions address the determination of protonation states of amino acid side chains, the orientation of individual water molecules and the characterization of the hydrogen bonding network between the protein active centre and an inhibitor or substrate. This knowledge is often crucial towards understanding the specific function and behaviour of an enzyme. BIODIFF is designed as a monochromatic diffractometer and is able to operate in the wavelength range of 2.4 Å to about 5.6 Å. This allows to adapt the wavelength to the size of the unit cell of the sample crystal. Data collection at cryogenic temperatures is possible, allowing studies of cryo-trapped enzymatic intermediates. Some recent examples will be presented to illustrate the potential of neutron macromolecular crystallography.

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