Poster Presentations

[MS5-P23] First Results from Measurements at the New Neutron Diffractometer "BioDiff" T. E. Schrader[1], A. Ostermann[2], M. Monkenbusch[3], B. Laatsch[4], P. Jüttner[2], W. Petry[2] and D. Richter[3,5]

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The neutron diffractometer BioDiff is a joint project between the Forschungszentrum Jülich (FZJ/JCNS) and the Forschungs-Neutronenquelle Heinz Maier- Leibnitz (FRM II). The instrument BioDiff is especially designed to collect data from crystals with large unit cells. The main field of application is the structure analysis of proteins, especially the determination of hydrogen atom positions. Typical scientific questions addressed are the determination of protonation states of amino acid side chains and the characterization of the hydrogen bonding networks between the protein and an inhibitor or substrate. The orientation of water molecules in the active centre of the protein can also be determined (c. f. Fig. 1). The main advantage of the monochromatic instrument BioDiff is the possibility to adapt the wavelength between 2.4 Å and 5.6 Å to obtain a compromise between higher scattering yields at longer wavelengths and better resolution at smaller wavelengths. In this contribution the most recent results from the instrument BioDiff will be presented concentrating on the recently published measurements on the Toho-1 β- lactamase mutant R274N/R276N [1] and on myoglobin crystals [2]. The latter example will be given because it shows that data from BioDiff can be compared to similar instruments e. g. the BIX-3 in Japan. Here, the water network around the outer surface of the protein was investigated. Figure 1 nicely shows how the orientation of water molecules can be determined on the surface of the protein if the water molecules are fixed well enough due to a surrounding hydrogen bonding network.

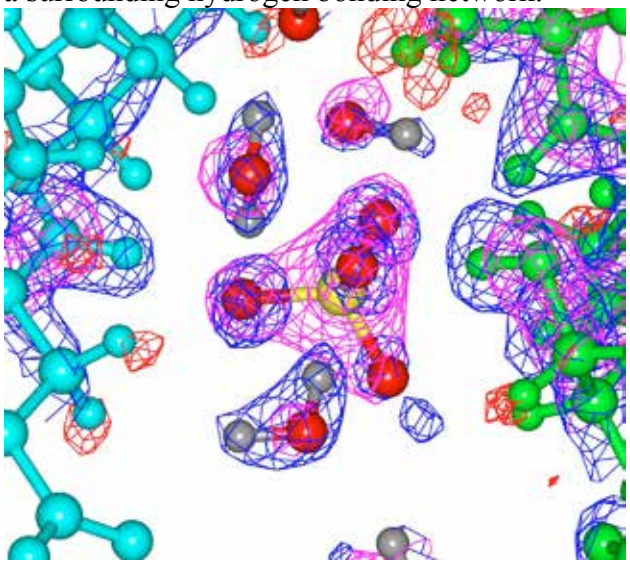

Figure 1 Water network in the contact region between two myoglobin molecules in the crystal. In the centre of picture a sulfate ion SO^{4-} is seen with the sulfur atom shown in yellow, the oxygen atoms shown in red. The deuterium atoms of the water molecules are coloured grey. The x-ray map is shown in magenta at a contour level of +2.7σ. The nuclear map is displayed at a contour level of -1.75σ in red and at +2.3σ in blue. Data partly taken from ref. [2]

[1] Tomanicek, Stephen J., Standaert, Robert F., Weiss, Kevin L., Ostermann, Andreas, Schrader, Tobias E., Ng, Joseph D. & Coates, Leighton (2013). *Journal of Biological Chemistry*, **288**, 4715-4722.
[2] Ostermann, A., Tanaka, I., Engler, N., Niimura, N.& Parak, F. G. (2002). *Biophys. Chem.*, **95**, 183

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