Macromolecular crystallography at the FRM II
The new neutron single crystal diffractometer BIODIFF

T.E. Schrader¹, A. Ostermann², M. Monkenbusch³, B. Laatsch³, Ph. Jüttner⁴, W. Petyş⁵, D. Richter⁶
¹Jülich Centre for Neutron Science JCNS, Forschungszentrum Jülich GmbH, Outstation at MLZ, Lichtenbergstr. 1, 85748 Garching, Germany
²Heinz Maier-Leibnitz Zentrum (MLZ), Technische Universität München, Lichtenbergstr. 1, 85748 Garching, Germany
³Jülich Centre for Neutron Science JCNS and Institute for Complex Systems ICS, Forschungszentrum Jülich GmbH, D-52425 Jülich,
⁴Zentralinstitut für Engineering und Technologie ZEA-1, Forschungszentrum Jülich GmbH, D-52425 Jülich

Neutron structure determination:
- Hydrogen atoms can be resolved even at a resolution of d_{min}=2.5Å
- Protonation states of amino acid side chains
- Deuterium exchange as a measure of flexibility and accessibility (discrimination between H (D)
- Solvent structure including hydrogen atoms can be analyzed
- Discrimination between neighbors in the periodic table is possible: e.g. N and O, Fe and Mn
- B-factors (σ²) of the hydrogen atoms can be compared with data of other techniques
- No radiation damage compared to measurements at synchrotrons

Hydration structure analysis:
- Example: myoglobin
- The hydrogen-bonding network strongly suggests
- Water network in the contact region between two myoglobin molecules in the crystal, in the centre of a sulfate ion SO₄⁻ 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 contour at a level of 2.7σ. The nuclear map is displayed at a contour level of 1.75σ in red and at 2.3σ in blue.

First instrument test with myoglobin:
- Neutron data from map calculation using the pdb-file 1L2K.pdb and the Biodiff data set:
- R=20.19 %
- Rwp=21.13 %

Water network in the contact region between two myoglobin molecules in the crystal, in the centre of a sulfate ion SO₄⁻ 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 contour at a level of 2.7σ. The nuclear map is displayed at a contour level of 1.75σ in red and at 2.3σ in blue.

First “user data-sets”:
- β-lactamase with bound BZB inhibitor
- First “user data-sets”:
- Summary of user experiments after 4 reactor cycles:

Next proposal deadline: May 2nd, 2014
userfrm2.tum.de
fq@frm2.tum.de
http://www.mlz-garching.de/biodiff