# What neutrons can do for you:
# The single crystal neutron diffractometer BIODIFF at the Heinz Maier-Leibnitz Zentrum (MLZ) and a short excursion to Small-angle neutron diffraction

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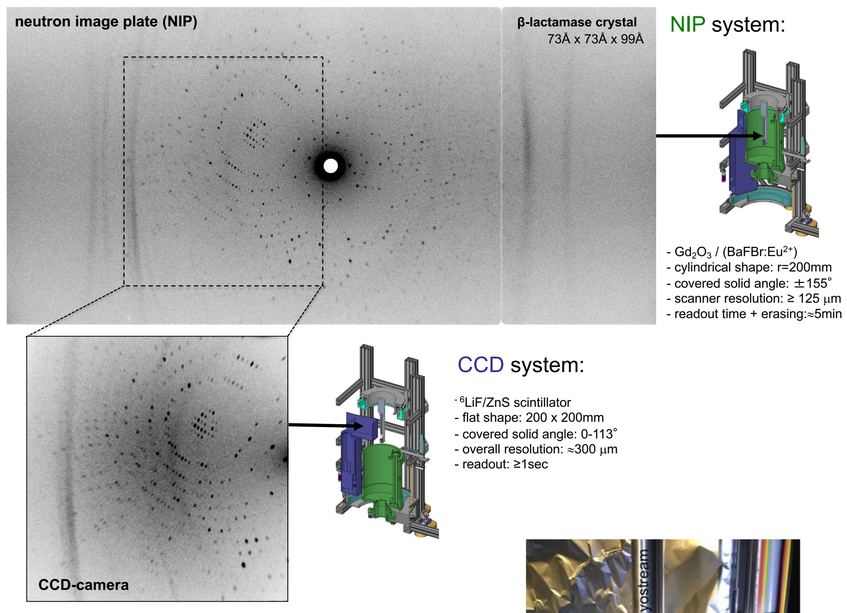
## Instrument Description

**BIODIFF** is operated in collaboration between the FRM II and the Forschungszentrum Jülich. It is optimised for studies of crystals with large unit cells and its main application lies in the structural analysis of protein crystals.

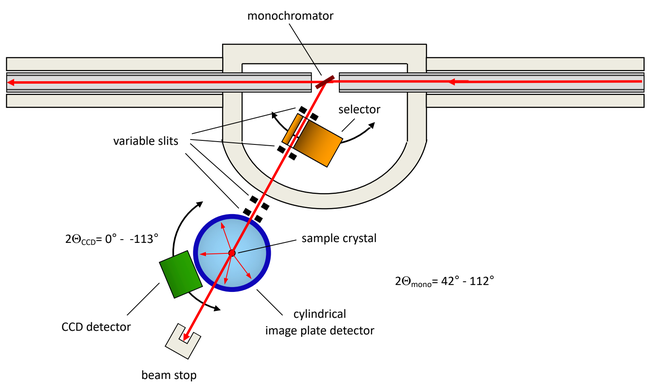
**Important instrument parameters:**

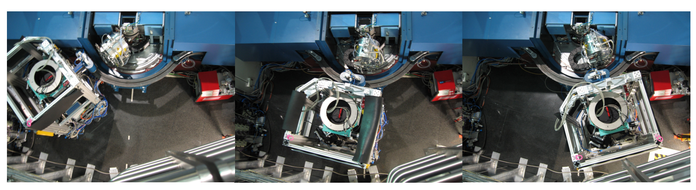
| | |
|---|---|
| **Neutron guide** | NL-1, supermirror m=2 |
| **Monochromator** | PG002, mosaicity: 0.4 – 0.5°<br>wavelength range with selector: 2.4 - 5.6 Å<br>wavelength range without selector: 2.4 - 6.1 Å |
| **Higher order filter** | velocity selector, transmission: 87% for 2.4 Å |
| **Collimation** | adjustable slits, down to ∅ = 1 mm |
| **Wavelength resolution** for 2.4 Å | $\Delta\lambda/\lambda$ = 2.9% |
| **Divergence** (no slits) for 2.4 Å | horizontal: 0.8° FWHM<br>vertical: 0.7° FWHM |
| **Main detector** | neutron image plate (cylindrical), radius= 20 cm; angular range: ±152° horizontal; ±48° vertical, pixel size: 125, 250, 500 μm² |
| **Auxiliary detector** | CCD camera with scintillator: 200 x 200 mm<br>distance to sample: 100 mm<br>CCD: 2048 x 2048 pixel; pixel size: 13.5 μm²<br>spatial resolution: 300 μm² |
| **Sample environment** | Oxford Cryosystems Cryostream 700 plus: 90 – 500 K, several FRM II/JCNS standard sample environments |

**Neutron IP and CCD detector system:**

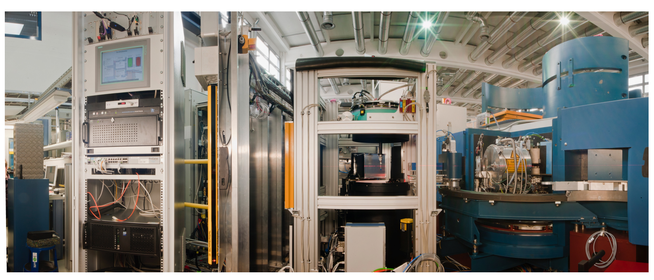



## Schematic view of the instrument:



Wavelength change possible within < 30 min



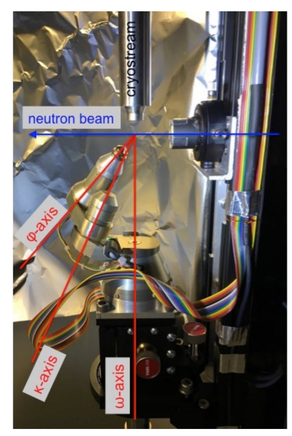
Instrument side view with shielding removed

## Sample environment:

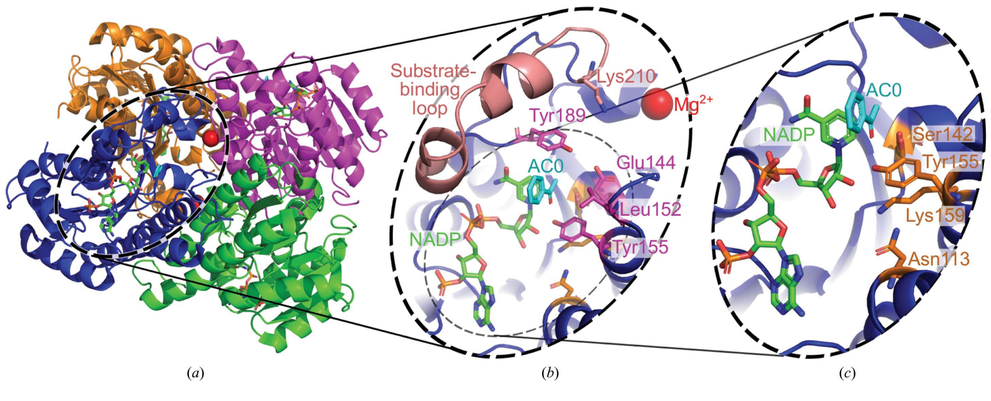
Mini-kappa-goniometer
➞ optimizing data collection strategy

Standard Oxford cryostream 700+
➞ temperature range 90 – 500 K

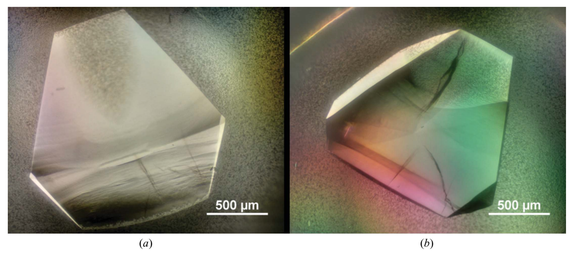
Closed cycle cryostat
➞ temperature range 4 – 300 K



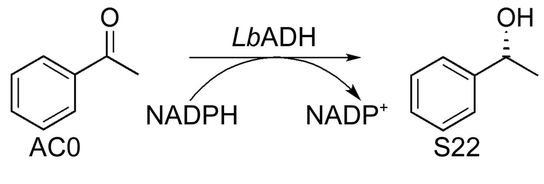

## Alcoholdehydrogenase, in collaboration with Prof. Dr. Weuster-Botz (TUM)



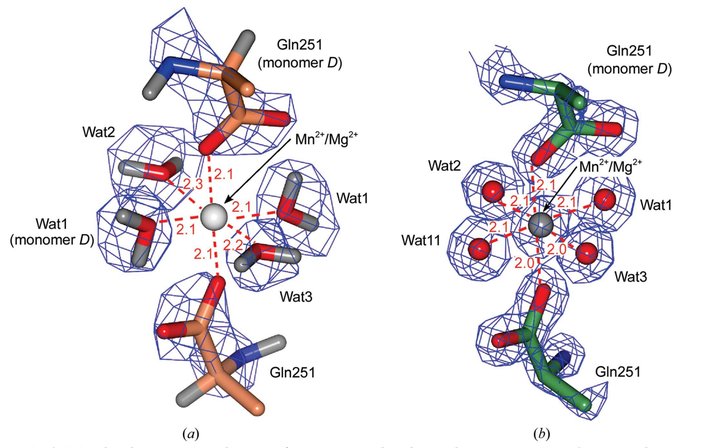

*Structural arrangement of LbADH in complex with NADP, acetophenone (AC0) and Mg2+ (PDB entry 1zk4). (a) Overall tetrameric arrangement of LbADH. The monomers are shown as differently coloured ribbon representations and the Mg2+ ion as a sphere; the NADP cofactor and AC0 substrate are highlighted as stick models (green and cyan, respectively). (b) Enlargement of the substrate and co-substrate binding region and (c) enlargement of the catalytic centre. Figure* from *Acta Cryst. (2018). F74*




*Microscopic images of (a) the largest ( 1.0 mm³) and (b) the best neutron-diffracting His6-tagged LbADH crystal ( 0.7 mm³).*

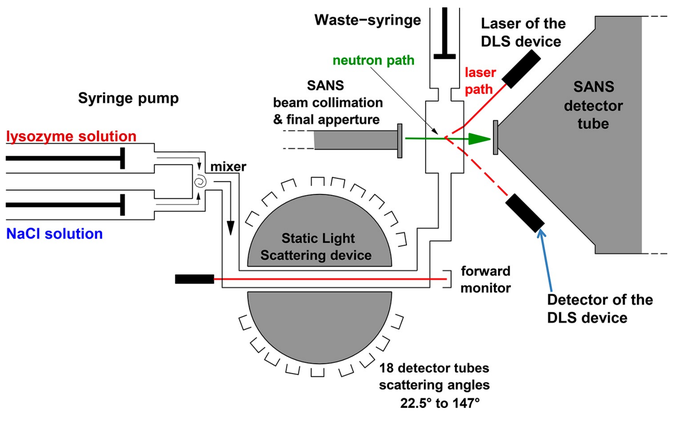



Figures taken from Hermann et al. *Acta Cryst. (2018). F74*

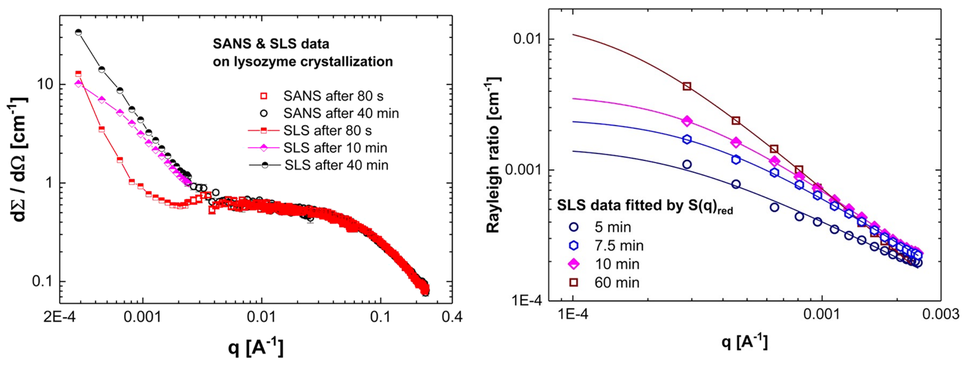



*Mg2+/Mn2+-binding site coordinating four water molecules and connecting two C-terminal Gln251 residues of the biological unit. A difference OMIT map (Fo - DFc) for both Gln251 residues, all water molecules and Mn2+/Mg2+ is contoured at 2.5 . Red dashed lines indicate the coordination sphere for Mn2+/Mg2+. Distances are given in Å . (a) The nuclear scattering map for the neutron structure (orange; PDB entry 6h1m) shows no detectable density at the ion-binding site. Mn2+/Mg2+ was modelled in the neutron structure. (b) The electron scattering map for the X-ray structure (green; PDB entry 6h07) reveals clear density at the ion-binding site.*

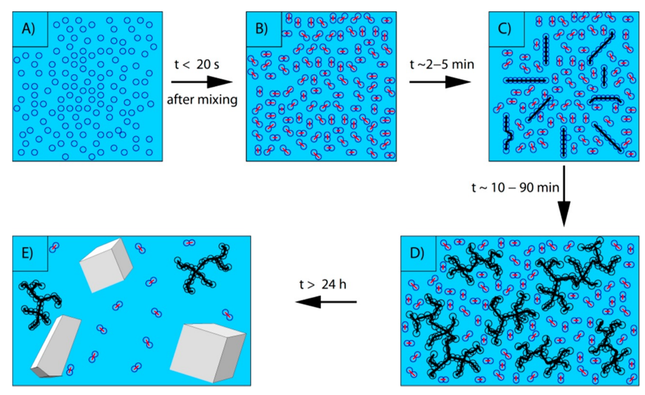
## Crystallization kinetics of lysozyme as seen with different scattering techniques




Experimental set-up at the beamline




Figures taken from Heigl et al. *Cryst. Growth Des. 2018, 18, 1483−1494*




Final model of crystallization process

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