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# A tutorial for learning and teaching crystallography

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## Introduction

Based on the data collected during the DGK workshop on *'X-Ray Difffraction Data Collection using Synchrotron Radiation'* held at BESSY (Berlin) in August 2007, we have created a tutorial for teaching and learning macromolecular crystallography. The tutorial consists of five experiments. It covers all the information needed to repeat the whole experiments or parts of them starting from the crystallisation and ending with the structure solution. The diffraction images are also provided.
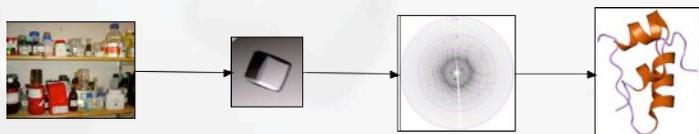


## Contents

- biological information about the protein
- crystallisation conditions
- crystal soaking and cryo-conditions
- data collection parameters
- data processing and scaling
- structure determination steps
- results
- references

## Download

http://www.embl-hamburg.de/Xray_Tutorial/
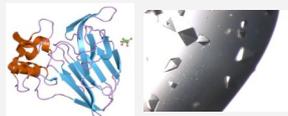
http://www.mx.bessy.de/bessy-ws/bessy.html
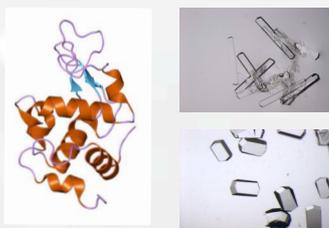
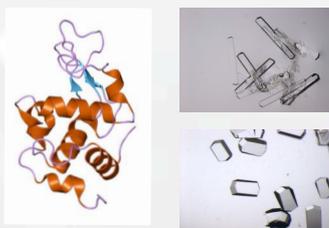## The Five Experiments

1) S-SAD
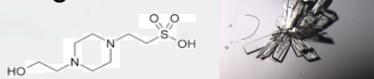on cubic Zn-free insulin

2) MAD
on bromide soaked thaumatin

3) Molecular Replacement
on monoclinic lysozyme

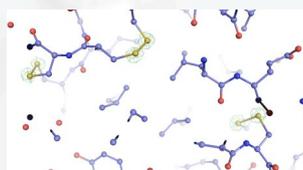4) Identification of bound solvent ions in tetragonal lysozyme

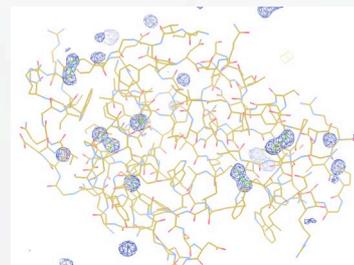5) Identification of a bound ligand in tetragonal lysozyme



## Reference
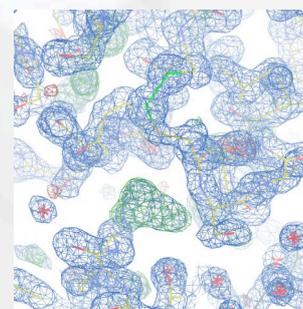
Faust et al., *J. Appl. Cryst.* (in press)

## Results



The final model of insulin superimposed onto the anomalous difference electron density map. The map is contoured at 8.0 $\sigma$.



Refined structure of lysozyme with the anomalous difference electron density map contoured at 4.0 $\sigma$. The disulfide bridges can be easily located as well as the bound chloride ions.



Electron density map of monoclinic lysozyme. The $(2F_o\text{-}F_c, \alpha_c)$-map is contoured at 1.2 $\sigma$ (blue), the $(F_o\text{-}F_c, \alpha_c)$-map at ± 3.0 $\sigma$ (green/red). The bound nitrate ions can be clearly discerned in the map.
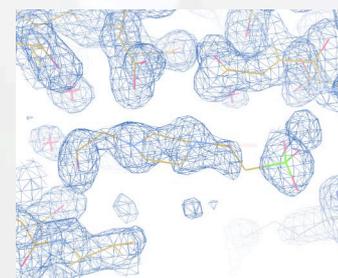


Electron density map of tetragonal lysozyme around the bound HEPES molecule after refinement. The $(2F_o\text{-}F_c, \alpha_c)$-map is contoured at 1.0 $\sigma$.