ESRF	**Experiment title:** Structure-function relationship in metalloproteins	**Experiment number**: mx88
Beamline: ID14-4	**Date of experiment**: from: 1st of August 2003 to: 2nd of August 2003	**Date of report**: 21/8-2003
Shifts: 3	**Local contact(s)**: Didier Nurizzo	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Gert Winther Pedersen*
Pernille Harris*
Hans E. M. Christensen
Michael S. E. Nielsen

Report:

Ferredoxin from the *Pyrococcus furiosus* is a small iron-sulphur containing protein, which has been characterised extensively by different techniques. We have been able to get small plate-like crystals which are difficult to work with because of the very high mosaic spread (the spots are lying on lines when the incoming beam is perpendicular to the stacking directions of the plates. One data set was collected to 2.2 Å on ID29 on an orthorhombic crystal form. We collected data on ID14-4 on two new crystal forms. One data set was collected to 1.5 Å and the other data set to 1.75 Å. All data sets are about 90% complete, because we removed the worst looking part of the data. Despite the horrible looks of the diffraction pattern, we have been able to solve the structure by molecular replacement with the ferredoxin from *Thermotoga maritima.* The refinement is currently under progress and the electron density maps look good.

The di-haem protein cytochrome *c*4 from *Pseudomonas stutzerii* is used as a model system for cooperative behaviour between metal centres. We have done previous work where we have characterized the oxidized and reduced form of the protein. We have crystallized a mutant protein, where we assume that the hydrogen network between the haem groups has been. We succeeded in collecting two data sets to 3.0 Å on very small crystals of this mutant protein. We chose the small crystals, since we have previously seen that these crystals tend to as like twin crystals.

Blue copper nitrite reductase is a key enzyme in the global nitrification cycle. We have crystallized a new form of this enzyme and collected data to 2.0 Å.