



	Experiment title: Crystallographic Investigations on Structure and Function of Photoactive Proteins	Experiment number: MX-134
Beamline: ID 29	Date of experiment: 15 July 2004 to 16 July 2004	Date of report: 28.02.2005
Shifts: 3	Local contact(s): Dr William SHEPARD	<i>Received at ESRF:</i>
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Report:

Photosystem II (PSII) is located in the thylakoid membrane of higher plants, algae and cyanobacteria that catalyzes the oxidation of water to atmospheric oxygen.

We are elucidating the three-dimensional structure of the PSII purified from the thermophilic cyanobacterium *Thermosynechococcus elongatus*. Up to now we obtained electron density maps at relatively low resolutions (Zouni *et al.* 2001), the most recent model determined at 3.2 Å (Biesiadka *et al.*, 2004), collected during the same proposal (MX134) period.

During the same proposal period we have collected datasets at 4 Å resolution at the Mn-edge and beyond. As there is quite some discussion about possible radiation damage specifically to the metal-sites, we planned to decrease the crystal temperature to 10 K.

The aim of this experiment was to collect dataset at Mn- and beyond at around 10 K to lower radiation damage around the redox-active Mn₄Ca cluster. These data should provide additional structural information on the geometry and coordination of the metal cluster.

A Helium cryostat was used to cool crystals to lower temperatures. The temperature of the specimen was about 15 to 20 K.

Several observations regarding data collection with the He-cryostat:

- high flow rates and perturbations of the cryo-stream caused vibration of the crystals. The vibration was especially strong when large crystals were mounted.

- prominent ice formation was observed on the crystal surface. Icing was dramatically increasing while fast rotating the crystal. Therefore inverse-beam data collection method was not applicable.

Several useful datasets were collected at the Mn-edge with a resolution of about 3.8 Å. The investigation of anomalous difference Fourier maps based on "Helium"-datasets revealed clear peaks at the location of the Mn-cluster. The appearance of these maps was different compared to 145K data, but higher resolution is needed for reliable interpretation of the structure of Mn₄Ca-cluster.

Reference

Biesiadka, J., Loll, B., Kern, J., Irrgang, K.-D. and Zouni, A. (2004) Crystal structure of cyanobacterial photosystem II at 3.2 Å resolution: a closer look at the Mn-cluster. *Phys Chem Chem Phys*, **6**, 4733-4736.