



	Experiment title: Crystallographic Investigations on Structure and Function of Photoactive Proteins	Experiment number: MX-134
Beamline: ID 29	Date of experiment: 28 April 2004 to 29 April 2004	Date of report: 28.02.2005
Shifts: 3	Local contact(s): Dr. Gordon LEONARD	<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.

The aim of the experiment was to collect dataset at Mn edge to obtain structural information on the redox active site, the two Mn-clusters which are present in PSII dimer. The previous resolution of these data was limited to 4.8 Å.

Three prominent maxima at 4.0381, 6.5390 and 7.1120 keV corresponding to Ca, Mn and Fe could be identified. Whereas the Ca and Mn are part of the Mn-Ca-complex, Fe²⁺ are bound to the haem groups of cyt *b*-449 and cyt *c*-550 and there is a non-haem Fe²⁺.

We collected altogether six dataset (3 at the Mn-edge and 3 at the Ca-edge). In Table 1 the two dataset with the best data statistics are given.

Table1: Summary of dataset for anomalous diffraction data. Values in parentheses apply to highest resolution shell.

Dataset	Mn-edge	Ca-edge
Wavelength (Å)	1.89	1.910
Resolution ^a (Å)	40 - 4.0 (4.07 - 4.00)	40 - 4.0 (4.07 - 4.00)
Unique reflections	76,072	77,931
R_{sym} ^a	0.060 (0.398)	0.064 (0.419)
Completeness ^a (%)	96.0 (91.9)	98.1 (90.2)
I/sig(I) ^a	16.0 (2.7)	17.4 (3.5)
Redundancy	3.3	4.6

$$^a R_{\text{sym}} = \sum_h \sum_i |I_{h,i} - \langle I_h \rangle| / \sum_h \sum_i I_{h,i}$$

The anomalous electron density maps of the dataset beyond the Mn-edge showed only one single strong peak in the same location as the much larger peak originating from the Mn-Ca-cluster. In agreement with the EXAFS scan, it was attributed to Ca²⁺.

Reference

Zouni, A., Witt, H.-T., Kern, J., Fromme, P., Krauß, N., Saenger, W., Orth, P. (2001) Crystal structure of photosystem II from *Synechococcus elongatus* at 3.8 Å resolution. *Nature* **409**, 739-743.

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.