ESRF

Experiment title:
X-Ray Crystallographic Investigations on the Structures and Functions of the Photosystem I and II

Experiment number:
LS-1932

Beamline:
ID14 2

Date of experiment:
from: 31 March 2001 to: 01 April 2001

Date of report:
28.08.2001

Received at ESRF:

Shifts:
6

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Report:

The present model of photosystem II (PSII) from the thermophilic cyanobacterium *Synechococcus elongatus* at 3.8 Å (Zouni et al., 2001) lacks many important details, as the amino acid side chains, the orientation of many cofactors - especially the Mn-cluster - and the position of some subunits. The aim of this experiment was to obtain a more detailed model for the PSII.

The proceeding experiment LS-1932 at the beamline ID 14 2 led to complete data set from a native crystal. The data were collected on a ADSC Q4 CCD detector and the wavelength λ=0.934 to 90.6 % complete data set of ~ 3.5 Å resolution. The resulting data set after processing with DENZO and SCALEPACK had a maximum resolution of 3.6 Å with R_{sym}=0.14 and $<I/\sigma(I)>$=5.8 (R_{sym}=0.47 and $<I/\sigma(I)>$=2.0).

Improved electron density maps were obtained using 3.6 Å native data set and experimental phases (Zouni et al., 2001) combined with calculated phases derived from an incomplete model of PSII. Phase combination was performed using the program SIGMAA (CCP4, 1994). After density modification and phase extension using the CNS program in solvent flipping mode, we were able to partially trace the missing loops connecting transmembrane helices and some of the not yet traced protein mass on the lumenal side. The model was subjected to refine a polyalanine trace using rigid-body minimisation and simulated annealing procedures, both with MLHL (maximum likelihood with phase probability distribution), crystallographic target and bulk solvent correction (performed in CNS). In addition to the previous model (Zouni et al., (2001), *Nature* **409**, 739-743) we could trace some of the connecting loops within the core complex proteins D1, D2, CP43 and CP47. We could also locate fragments of protein on the lumenal side, possibly belonging to the extrinsic 12 kDa protein (psbU). The new model also shows the structures of the chlorophylls more clearly, which could help to model the excitation energy transfer in the antenna system.

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.