



	<b>Experiment title:</b> Crystallographic Investigation of Structure and Function of Photosystems I and II	<b>Experiment number:</b> LS-2188
<b>Beamline:</b> ID14 2	<b>Date of experiment:</b> from: 28.06.-01.07.2002	<b>Date of report:</b> 28.04.03
<b>Shifts:</b> 9	<b>Local contact(s):</b> Dr. Steffi Arzt	<i>Received at ESRF:</i>
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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; hence we try to collect better native data set and derivative data sets to higher resolution. The new freezing protocol with decreased mosaicity made the data collection of heavy derivative obvious. We applied the quick soaking method for all heavy atom derivatives which were previously used to solve the phase problem for the 3.8 Å data set. We measured crystals after different soaking times in the heavy atom solutions. The following table gives an overview about the collected derivative data sets at the beamline ID 14 2:

compound	resolution [Å]	Completeness [%]	R <sub>sym</sub>	I/(σ)	mosaicity	soaking time [min]
Hg(Cl) <sub>2</sub>	4.6	82.0 (53.6)	0.101 (0.386)	10.7 (2.2)	0.8	10
Hg(SCN) <sub>2</sub>	4.1	86.7 (72.8)	0.092 (0.486)	11.6 (1.9)	0.6	15
Hg(SCN) <sub>2</sub>	4.2	86.6 (69.7)	0.082 (0.304)	10.1 (2.7)	0.6	40
Ta <sub>6</sub> Br <sub>12</sub>	4.3	83.2 (57.7)	0.097 (0.566)	11.4 (1.8)	0.6	30
Ta <sub>6</sub> Br <sub>12</sub>	4.1	88.9 (69.8)	0.079 (0.516)	12.6 (2.0)	0.6	20

Additionally we collected a native data-set to 97.6 % completeness data set of ~ 3.6 Å resolution. The resulting data set after processing with DENZO and SCALEPACK had a maximum resolution of 3.6 Å with R<sub>sym</sub>=0.088 and <I/σ(I)>=14.7 (R<sub>sym</sub>=0.460 and <I/σ(I)>=1.8).

We used the program SHARP to calculate new phases. With better phase information and better native data, we obtained improved maps. Finally we were able to get more detailed information about the missing loop regions and the position of the co-factors.

## 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.