ESRF	**Experiment title:** Crystallographic Investigation of Structure and Function of Photosystems I and II	**Experiment number**: LS-2188
Beamline: ID14 2	**Date of experiment**: from: 22.02.2003 to: 24.02.2003	**Date of report**: 10.01.2004
Shifts: 6	**Local contact(s)**: Dr Elena Micossi	*Received at ESRF:*

Names and affiliations of applicants (* indicates experimentalists):

Jacek Biesiadka*, Bernhard Loll*and Wolfram Saenger
Institut für Chemie/Kristallographie, Freie Universität Berlin, Takustr. 6, D - 14195 Berlin

Athina Zouni*, Jan Kern*
Max-Volmer-Institut für Biophsykalische Chemie und Biochemie, Technische Universität Berlin, Strasse des 17. Juni 135, D - 10623 Berlin

Norbert Krauss
Institut für Biochemie, Universitäts-Klinikum Charité der Humboldt-Universität Berlin, Monbijoustr. 2, D - 10117 Berlin

Report:

During beamtime allocation LS-2188, we collected a full data set at ID14-2. Data statistics are summarized in following table:

Data set	**native**
X-ray source	ESRF (Grenoble), ID14-2
Wavelength (Å)	0.933
Resolution* (Å)	50 - 3.3
Unique reflections	122,001
R_{sym}*	0.106 (0.681)
Completeness* (%)	91.3 (56.1)
I/sig(I) *	12.8 (2.0)
Redundancy	3.6

*Values in parentheses apply to highest resolution shell.

These was the data set with the highest resolution, collected by our BAG in Grenoble. The model of PSII contains 38,000 atoms corresponding to nearly 70% of the expected total number of atoms. Refinement of coordinates with CNS converged at R/R_{free} of 0.36/0.42. Despite relatively good quality of electron density maps, reliable sequence assignment was only possible in regions with specific sequence landmarks. Therefore, amino acid side chains

of fragments of the structure where sequence assignment was ambiguous were truncated and modeled as poly-Ala or Cα-trace, resulting in a final structure containing 24,180 atoms. The refinement of these data set, reached an intermediate state, where we could assigne the amino acid sequence of most of the subunits. Furthermore we identified cofactors in the electron density, which have not seen before.