

**Experiment title:**

The Structure Elucidation of the Membrane
Intrinsic Protein Complex Photosystem I by
X-Ray Crystallographic Methods

**Experiment
number:**

LS 419

Beamline:

ID2-BL4

Date of Experiment:

from: 27/04/96

to: 29/04/96

Date of Report:

27/08/96

Shifts:

6

Local contact(s):

Dr. A. Åberg, Dr. B. Rasmussen

Received at ESRF :

02 SEP 1996

Names and affiliations of applicants (*indicates experimentalists):

Wolf-Dieter Schubert, Olaf Klukas* , Norbert Krauß* and Wolfram Saenger
Institut für Kristallographie, Freie Universität Berlin, Takustraße 6, D-14195 Berlin,
Germany

*
Petra Fromme and Horst T. Witt
Max-Planck-Institut für Biophysikalische Chemie und Biochemie, Technische Universität
Berlin, Straße des 17. Juni 135, D-10623 Berlin, Germany

Report:

“X-ray crystallographic analysis of trimeric photosystem I (PS I) from *Synechococcus elongatus* has led to a first interpretation of an electron density at 6 Å resolution (Krauß et al., 1993). Important features of the PS I structure, as the positions of three [Fe₄S₄] clusters and numerous α-helices, were discernible from the map. The positions of those chlorophyll molecules involved in electron transfer or being part of the internal core antenna system of PS I (half of the expected number of ‘antenna’ chlorophyll molecules) were assigned tentatively.

Improvements in the protein purification procedures and the crystallization method led to crystals of reproducibly higher quality. Prior to our data collections at ESRF a native data set of 3.85 Å and several heavy atom derivative data sets suitable up to 4.5 Å map were available.

We collected data of platinum and mercury derivatives at the high-brilliance beamline ID2-BL4 at ESRF which were suitable up to 4.0 Å resolution and employed in the calculation of new MIR phases. From the interpretation of the corresponding electron density map a model resulted (Krauß et al., 1996), which is more complete and more accurate than the previous 6 Å model. 31 transmembrane α -helices were identified for which a reasonable assignment to individual PS I subunits could be proposed. In contrast to our 6 Å structure the arrangement of chlorophyll cofactors of electron transfer was found to be pseudo-symmetrical. Our model of the internal core antenna of PS I now consists of 65 chlorophyll molecules (20-25 chlorophyll molecules and the carotenoids still missing), forming a clustered net with each chlorophyll possessing at least one neighbour within a distance < 16 Å.

Diffraction data were collected at 4°C, because we could not establish conditions suitable for cryogenic data collection so far. During our last beam time at ESRF in 1996 and in our previous experiments at ID2-BL4 partial native data sets (up to 3.5 Å resolution) were collected compensating radiation damage by translating crystals parallel to the rotation axis after each individual image.

References:

Krauß, N., Hinrichs, W., Witt, I., Fromme, P., Pritzkow, W., Dauter, Z., Betzel, Ch., Wilson, K. S., Witt, H.T. & Saenger, W. (1993) Three-Dimensional Structure of System I of Photosynthesis at 6 Å Resolution. *Nature* 361, 326-331.

Krauß, N., Schubert, W.-D., Klukas, O., Fromme, I., Witt, H.T. & Saenger, W. (1996) Photosystem I at 4 Å Resolution: A Joint Photosynthetic Reaction Center and Core Antenna System. *Nature Struct. Biol.* (accepted).