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Report:

Crystals of photsystem I (PS I) isolated from the thermophilic cyanobacterium ***Synechococcus elongatus*** have been used to investigate the three-dimensional structure of this multi-subunit membrane embedded protein pigment complex. Structural information was obtained from an electron density map at 4 Å resolution (Krauß et al., 1996; Schubert et al., 1997) resulting in a model consisting of the α-helices including some interhelical links, the iron sulfur clusters, most of the chlorophyll ***a*** cofactors and one phylloquinone position.

A major step towards an improvement of the structure analysis was achieved establishing suitable conditions for collection of X-ray diffraction data under cryogenic conditions. At 100 K PS I crystals can be irradiated for several hours at one position with the intense X-ray beam at beam line ID2 until significant loss in diffraction quality is observed. Because of the large size of the crystals (typical dimensions are 0.5 x 0.5 x 1 $.0\,mm^3$) and small diameter of the X-ray beam at ID2 (between 100 x 100 and 150 x 150 μm^2) data collection can be continued irradiating the same crystal at different positions. Freezing of the crystals is accompanied by a change of the space group from hexagonal $P6_3$ (a = 286 Å, c = 167 Å) at 277 K to monoclinic $P2_1$ (a = 277 Å, b = 165 Å, c = 283 A, $\beta = 119°$) at 100 K with one

PS 1 trimer in the asymmetric unit. This opens an additional route to phase improvement by density modification using the molecular averaging method.

During the experiment at ID2, maximum priority was given to collection of a complete native data set of ≈ 3 Å resolution. Native data were collected using a Marresearch imaging plate detector with a scanning radius of 172.5 mm and the maximum wavelength available at this beam line, which is 1.39 Å, in order to get the maximum anomalous scattering signal of the iron atoms (36 per asymmetric unit) which can be achieved under the experimental conditions. The resulting data set after processing the raw data with programs DENZO and SCALEPACK (Otwinowski and Minor) has a maximum resolution of 2.9 Å with R_{sym} = 0.17 between 3.0 and 2.9 Å and they are 98 % complete up to 4.5 A. Unfortunately, the completeness in the higher resolution shells drops continuously to a minimum of 52 % between 3.0 and 2.9 Å because of the increasing number of overlapping reflection profiles due to the large unit cell constants and the high mosaicity of the crystal (0.8°). The high quality of the data is reflected by the anomalous Patterson function, which clearly shows the peaks corresponding to the difference vectors between the iron atoms in the Harker section (u ½ w).

Data sets of two mercury derivative crystals prepared under different conditions were collected using a scanning radius of 150 mm. The crystals diffracted to at least 3.2 Å resolution. Evaluation of the data is in progress.

References

Krauß, N., Schubert, W.-D., Klukas, O., Fromme, P., Witt, H.T. & Saenger, W. (1996) Photosystem I at 4 Å Resolution Represents the First Structural Model of Joint Photosynthetic Reaction Centre and Core Antenna System. *Nature Struct. Biol.* 3,965-973.

Schubert, W.-D., Klukas, O., Krauß, N., Saenger, W., Fromme, P. & Witt, H.T. (1997) Photosystem *I* of *Synechococcus elongatus* at 4 Å Resolution: Comprehensive Structure Analysis. J. ***Mol. Biol. 272,741-769.***