



	Experiment title: Crystallographic Investigations on Structure and Function of Photoactive Proteins	Experiment number: MX-134
Beamline: ID14 2	Date of experiment: from: 04 April 2003 to: 07 April 2003	Date of report: 28.02.2005
Shifts: 9	Local contact(s): Dr. David Richard HALL	<i>Received at ESRF:</i>
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Report:

Photosystem II (PSII) is located in the thylakoid membrane of higher plants, algae and cyanobacteria that catalyzes the oxidation of water to atmospheric oxygen. X-ray diffraction data of PSII from the cyanobacterium *Thermosynechococcus elongatus* were collected at ESRF beamline ID14-2 ($\lambda=0.933$ Å) at 100 K (Table 1). Fine-tuning of crystallization conditions and an improved cooling protocol yielded low mosaic crystals diffracting to 2.9 Å maximum resolution. However, due to strong anisotropic diffraction the final dataset had to be truncated beyond 3.2 Å resolution. In the crystal structure at 3.2 Å resolution, several loop regions of the principal protein subunits are now defined that were not interpretable previously at 3.8 Å resolution and the amino acid sequence could be assigned to the central subunits.

Table 1: Data collection statistics

Data set	native
X-ray source	ESRF (Grenoble), ID14-2
Wavelength (Å)	0.933
Resolution* (Å)	50 - 3.2 (3.26 - 3.20)
Unique reflections	133,566
R_{sym}^*	0.106 (0.681)
Completeness* (%)	91.3 (56.1)
$I/\text{sig}(I)^*$	12.8 (2.0)
Redundancy	4.7

Ankylosing Spondylitis (AS) is an autoimmune disease genetically linked to HLA-B27. The subtype HLA-B*2705 of this MHC class I molecule is strongly associated with AS while HLA-B*2709 is not. The only difference between the two alleles is the HLA heavy chain (HC) at position 116 (Asp in B*2705 and His in B*2709). We have collected diffraction data to atomic resolution (Table 2) and determined the structures of both subtypes in complex with a nonapeptide by molecular replacement.

Table 2: Crystallographic Data and Refinement Statistics.

Data collection	HLA-B*2705 : pGR	HLA-B*2709 : pGR
Space group	P2 ₁	P2 ₁
Unit cell (<i>a,b,c</i> [Å])	51.0, 82.1, 65.3; 108.7	51.0, 81.9, 65.4; 108.9
Resolution [Å] ^a	50.0 – 1.4 (1.42 – 1.40)	30.0 – 1.12 (1.12 – 1.10)
Unique reflections	97993 (4386)	196702 (9285)
Completeness [%] ^a	97.9 (87.7)	95.8 (90.4)
I/σ ^a	28.0 (7.9)	20.8 (2.7)
R_{sym} ^{a, b}	0.039 (0.112)	0.043 (0.288)

Reference

Biesiadka, J., Loll, B., Kern, J., Irrgang, K.-D. and Zouni, A. (2004) Crystal structure of cyanobacterial photosystem II at 3.2 Å resolution: a closer look at the Mn-cluster. *Phys Chem Chem Phys*, **6**, 4733-4736.