Evaluation of Performance of the Bio-Crystallography Beamline by Means of Refinement of High-Resolution Crystal Structure

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The purpose of this project is to evaluate the Bio-Crystallography Beamline (BL41XU) on the basis of the diffraction data of several proteins which have so far been investigated by using the beamlines of Photon Factory. The comparison of data sets of these protein crystals collected at the beamlines in both SPring-8 and Photon Factory enable us to evaluate the performance of the beamline. After the BL41XU beamline was open for users, the following proteins were employed in this study; 1) photolyase from *Anacystis nidulans*, 2) photosynthetic reaction center from *Chromatium tepidum*, 3) RepE from *E. coli*, 4) hydrogenase from *Desulfovibrio vulgaris*, 5) chitosanase from *Bacillus circulans*, 6) chaperonin 60 from *Paracoccus denitrificans*, 7) AhpC protein from *Amphibacillus xylanus*, 8) aldehyde reductase from *Sporobolomyces salmonicolor*. For most of protein samples, very clear and sharp diffraction patterns could be observed, which probably better qualitatively than those obtained at the Photon Factory In this report, preliminary results on *Anacystis* photolyase are presented.

Photolyases repair cyclobutane type dimers formed from adjacent pyrimidine bases, a major type of UV-induced lesion of DNA. Photolyase from the cyanobacterium, *Anacystis nidulans* is 53 kDa single chain protein containing two different chromophoric cofactors ($FADH^-$ and 8-hydroxy-5-deazaflavin, 8-HDF) in equimolar amounts. The crystal structure of *A. nidulans* photolyase was determined and refined to R = 0.197 at 1.8 Å resolution using X-ray diffraction data obtained with synchrotron radiation at the Photon Factory (T. Tamada, K. Kitadokoro, Y. Higuchi, K. Inaka, A. Yasui, P. E. de Ruiter, A. P. M. Eker, and K. Miki, *Nature Struct. Biol.*, **4**, 887-891, 1997).

The diffraction data collected by the oscillation method at the BL41XU beamline were processed at 1.7 Å resolution with the R_{merge} value of 0.077 and the completeness of 0.81. A diffraction pattern is shown in Figure. The crystal structure is refined using the diffraction data between 20-1.7 Å resolution. The present refined model has the R and R_{free} values of 0.25 and 0.28, respectively. The further refinement is now in progress.

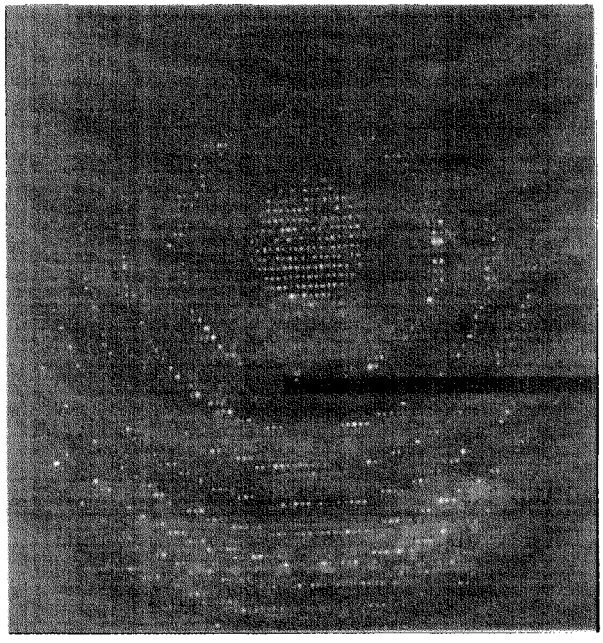

Figure. X-ray diffraction pattern of *A. nidulans* photolyase at the BL41XU baemline.