

Ultra-high Resolution Measurement at BL41XU of SPring-8

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A proton and an electron play an important role to chemical reaction through biomacromolecules. In order to elucidate the reaction by X-ray crystallography, it is essential to make clear the structure in atomic resolution below 0.7 Å. The measurement in such resolution is achieved by not only improving the sample crystal but also optimizing the equipment of the beamline. BL41XU at SPring-8 with the high brilliance is the most suitable for such data collection.

In this time, we improved the optics, the control system and the setup procedure of BL41XU. Especially, in order to realize the diffraction measurement in ultra-high resolution, the beamline was adjusted to obtain the beam stability in a short wavelength (< 0.6 Å).

Example data collection was performed at 100 K, using the crystal of Endopolygalacturonase I. The X-ray was set at 0.6 Å, and R-Axis V (Rigaku) was used as the detector. To acquire the complete data set, two data, in which the camera length was different, were collected. Consequently, diffraction spots were visible to a resolution of 0.62 Å. Intensity data were integrated and scaled, and R_{sym} of overall and outer shell (0.70-0.68 Å) were 3.2 and 30.0 %, respectively. As a result of structural refinement using SHELXL, R and R_{free} value of the obtained structure, in which 3,416 non-hydrogen atoms and 2,181 hydrogen atoms are included, is 9.72 and 10.78 %, respectively. Some other data are under analysis.

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