

## W0180

**Data Collection From Macromolecular Crystals at Ultra High Resolution.** R. Sanishvili<sup>1</sup>, A. Mischler<sup>2</sup>, A. Joachimiak<sup>1</sup>, A. Podjarny<sup>2</sup>, <sup>1</sup> Biosciences Div., Argonne National Laboratory, Argonne, IL, USA, <sup>2</sup> IGBMC, CNRS, 1 rue Laurent Fries, Illkirch, France.

With the advent of modern beamlines at third generation synchrotrons, more and more crystallographic data at ultra high resolutions are being collected from macromolecular crystals. There are number of structures currently deposited in PDB with resolution of about 0.8 Å and few of them go beyond this barrier (e.g. crambin, 1EJG<sup>1</sup>; aldose reductase, 1US0<sup>2</sup>; and antifreeze protein 1UCS,<sup>3</sup>).

Structures at such resolutions lead to better understanding of function of proteins on atomic level. Dramatically increased ratio of observations to refined parameters allows interpretation of quantum calculations for macromolecules<sup>4</sup>, which previously was possible only for small molecules.

At present, numerous new synchrotron beamlines are being constructed around the World. This will give boost to ultra high resolution data collection. Firstly, due to more available beamtime for projects that cannot qualify as high throughput. Secondly, already acquired experience can be incorporated in design of new beamlines to address some of the limitations.

To this end, such limitations of current technology will be presented along with practical tips for data collection at ultra high resolutions.

<sup>1</sup>Jelsch, C., Teeter, M. M., et al.(2000) *Proc.Nat.Acad.Sci.USA* 97 pp. 3171

<sup>2</sup>Howard, E. I., Sanishvili, R., et al.(2004) *Proteins: Struct.,Funct., Genet.* 55 pp. 792

<sup>3</sup>Ko, T.-P., Robinson, H., et al. (2003) *Biophys. J.* 84 pp. 1228

<sup>4</sup>Muzet N, Guillot B, et al. (2003) *PNAS* 100 8742–7