M13.0B Time-Resolved Diffraction and Protein Dynamics

Chair: I. Schlicting
Co-Chair: J. Helliwell

Attendance: 215

The session on 'time-resolved crystallography and protein dynamics' was organized according to the title moving from X-ray crystallographic studies using 3D crystals, to electron microscopic studies using 2D crystals to simulations and molecular dynamics calculations. The session started with an overview on time-resolved crystallography by Greg Petsko (Brandeis University) describing the methods for and problems with triggering reactions in crystals. Both strategies for studying unstable species namely the Laue method on fast time scales and the slowing and trapping approches were summarized and illustrated with examples. Thus, the scene was set up perfectly for Hiroaki Kato (Kyoto University) who described a phosphorylation reaction of glutathion synthetase using photolysis of caged ATP to start the reaction. Time-resolved Laue and cryocrystallographic experiments were performed that showed the build-up of the phosphorylated transition state analog and the concomitant ordering of a loop. Richard Henderson (MRC) used electron microscopy, 2D crystals of wildtype bacterio-rhodopsin and of a mutant, photolysis and freeze trapping to look at the structure of the Mearly ? Mlate intermediate in bacteriorhodopsin. Janos Hajdu (Uppsala University)! reported results obtained by an EU collaboration on the use of free electron lasers for structure determination. Interestingly, simulations indicated that 10 fs pulse length might result in diffraction before the sample disappears in a plasma, whereas this seemed not to be true for 70 fs pulses. Protein dynamics were addressed by Gail Bradbrook (Grenoble) using molecular dynamics calculations. The importance of water molecules and protons was taken up again in the summary of the session by John Helliwell (Manchester University) who also addressed the complementarity of neutron diffraction experiments with atomic resolution X-ray studies.

Ilme Schlichting