

W0636

On-going Developments Aimed at Improving the Success Rate of Challenging Structure Determinations. G. Bricogne, Global Phasing Ltd., Sheraton House, Castle Park, Cambridge CB3 0AX, United Kingdom

The pursuit of high throughput in structure determination has stimulated an unprecedented level of coordinated effort between developers of instruments and of software towards increasing degrees of automation in the determination of macromolecular crystal structures. Some of its concrete achievements, such as the automated screening of large numbers of crystals, are already contributing valuable help to investigators wanting to tackle challenging projects.

This talk will describe a number of further on-going developments, all based on (or guided by) improved statistical analyses of the reality of experiments and of data, which are specifically aimed at providing greater help still to such projects. They include the design and on-line monitoring of experiments (smart data collection), and the systematic use of unmerged data, together with new likelihood functions based on them, to accommodate the effects of radiation damage in scaling, in phasing from weak signals, and in structure refinement.