

## E0046

**Iterative Model Building and Evaluation With Statistical Density Modification.** T. Terwilliger, Bioscience Div., Los Alamos National Laboratory, MS M888, Los Alamos, NM 87545 USA.

Automated model-building beginning with an FFT-based search for helices and sheets and followed by chain extension using tripeptide fragments from high-resolution structures and pattern-based probabilistic identification of side chains has been successful in automated model building for maps with resolution as low as 3 Å. Model-building can be combined with refinement and statistical density modification to improve the quality and completeness of atomic models of macromolecules and to evaluate the quality of atomic models. A useful tool in removing model bias is prime-and-switch phasing. In this technique a substantially correct model containing some atoms in incorrect positions is used to estimate ("prime") initial phases, and a second source of phase information such as a flat solvent region is used without reference to the original phase probabilities in density modification. After prime-and-switch phasing the density at incorrect atomic positions is often considerably decreased compared to that at correct positions. This technique has been incorporated as an integral part of iterative model-building and refinement in the PHENIX software (<http://www.phenix-online.org>).