Iterative Model Building and Evaluation with Statistical Density Modification

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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 A. 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).

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