MAIN 2004: Model Building Beyond 100 Residues per Minute

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Model building of macromolecular structures at moderate resolution (around 2.8A and below) still requires user intervention to resolve the potential chain trace ambiguities, however, the classical approach by which amino acids are edited manually on one by one basis is becoming history. After an electron density map has been converted to a skeleton, the skeleton is used for recognition of secondary structure and main chain trace directly. Two consecutive screw turns are recognized as a helical structure, whereas beta structures are recognized from straight stretches of skeleton corresponding to at least five amino acids and their arrangements in pairs or sheets. After the secondary structure elements are established a combinatorial search of possible connectivities is used to further reduce the main chain ambiguities. The remaining ambiguities can be further resolved interactively by manual editing of the skeleton. The resolved skeleton then serves for building of the first main chain trace based on sp3 fragments positioned at the potential CA positions. If the resulting model looks satisfactory, it is converted to amino acid residues and enters refinement. Otherwise the resulting models can at any stage continue along the classical path of automated and manual model rebuilding, still using the same program with the same interactive 3D graphical user interface. (See http://www-bmb.ijs.si/)

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