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MAIN in 2004: Model Building at 100 Residues per Minute. Dusan Turk, Biochemistry and Molecular Biology, Jozef Stefan Institute, Jamova 39, Ljubljana, 1000 SLOVENIA.

Automation of interactive macromolecular crystal structure determination process needs to fulfill two requirements: The tools applied should be automated to the extent that a user does not have to provide additional manual input but their triggering and the results should appear on the screen under interactive time restraints (a user's mind did not get enough time to wonder away). In order to achieve these two goals the MAIN routines for automated model building were rewritten more or less from scratch. The new map skeletonization algorithm follows the ridges of electron density maps. The resulting skeleton serves as the searching path for recognition of secondary structure and main chain: Two sequential screw turns are recognized as the smallest element of a helical structure, whereas recognition of beta structure is based on straight stretches corresponding to at least five amino acids and their arrangements in pairs and sheets. During the next step connections between the secondary structure elements are establisehd on a combinatorial search basis. The resulting labeled skeleton is used for building of the first main chain trace based on sp3 fragments positioned at the potential CA positions. If the model looks satisfactory, it is converted to amino acid residues, from where it enters sequence assignment step and refinement. If the model is not satisfactory, then it is used as a starting point for a density modification procedure, which includes refinement and phase combination. Alternatively, a user can manually edit the skeleton (breaking false connections and building new ones) and restart the main chain tracing procedure. The resulting models can be further process 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/".