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Keywords: Phasing, ab initio, macromolecular crystallography, fragment search, ARCIMBOLDO, BORGES, SHREDDER, PHASER, SHELXE

MS4-O2 ARP/wARP 7.5 and beyond

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The ARP/wARP software for macromolecular model building is being continuously developed. Its recent release 7.5 (www.arp-warp.org), jointly with the CCP4 6.5, comes complete with additional innovations targeting protein model building at medium-to-low resolution range; including improved polypeptide recognition, NCS-restraints, atom update, estimation of solvent content and model accuracy, and an option to carry out SAD-refinement. The process of identifying and fitting of bound ligands now incorporates the 84 most common ligands and is able to use cif files defining bond, torsion and plane restraints.

Additionally, currently under development is the novel method of validating built protein fragments (presented in a dedicated poster at this meeting), as well as approaches to accurately estimating the quality of electron density maps and thus the phases. For the latter, a comprehensive scoring function has been designed that makes use of the distributions of third-order moment invariants computed throughout the density map. The distributions of the invariants have been shown to depend on the quality of phases, and the central moments of the distributions can conveniently capture the phase changes. The application of this method to decision-making, protocol guiding or validation in automated macromolecular structure solution and model building will be presented. This method is capable of ranking electron density maps within a resolution range from 2 to 6 Å and up to 80° phase error.

Keywords: ARP/wARP, software