

Poster Presentation

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Recent developments in ARP/wARP

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The ARP/wARP software project [1,2] includes an automated model building and refinement for macromolecular crystal structure determination. It is based on the results of two decades of extensive research and development in the areas of X-ray crystallography, informatics, data mining, and statistical pattern recognition. With the use of computationally efficient methods ARP/wARP provides easy-to-use pipelines for building models of proteins and their complexes with bound nucleotides and small-molecule ligands.

Here we present recent innovations of ARP/wARP that improve performance at resolutions 3.0-3.5 Å and enable interpretation of cryo-electron microscopy (cryo-EM) density maps. The main-chain tracing tools for both proteins and nucleic acids have been advanced to yield more reliable models with improved local stereochemistry. A new protein side-chain docking module has been developed and now provides better performance, particularly at low resolution. This enabled a provision of a new, fully automated tool for building atomic models of proteins and nucleic acids into cryo-EM maps at resolutions better than 3.5 Å. Finally, the ARP/wARP web-server has been completely redesigned and provides a more intuitive interface to all the ARP/wARP functionalities. Most recent version of ARP/wARP and the web-service are available at <http://www.embl-hamburg.de/ARP/>.

[1] Langer, G.G. et. al. (2008), Nat. Protoc. 3(7), 1171-1179.

[2] Langer G.G. et. al. (2013), Acta Cryst. D69, 635-641.

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