Poster Presentation

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New tools for automated model completion and refinement

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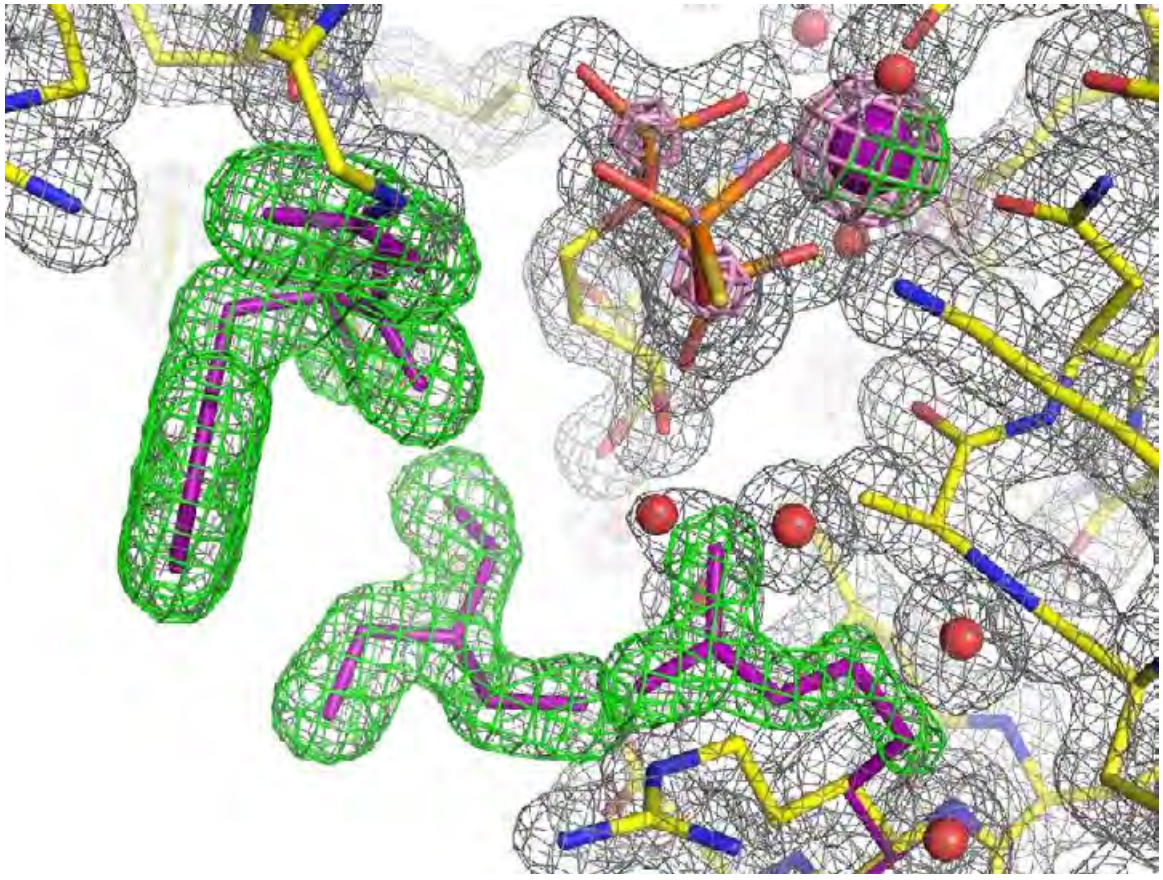
Although macromolecular crystallography has been greatly accelerated by the development of automated software for data processing, phasing, and model building, most structures require significant manual intervention to yield a truly final model. In addition to missing individual protein or nucleic residues, this may include the addition of alternate conformations, ligands (both free and covalently bound), elemental ions, or modified amino acids. We have developed a number of tools to streamline several of these steps within the Phenix software suite (Adams et al. 2010): 1) an automated pipeline for the determination of ligand-bound structures by molecular replacement (Echols et al. 2014a); 2) placement of elemental ions during refinement (Echols et al. 2014b), as an extension of solvent placement; 3) fitting of additional conformations of protein residues into difference density. These tools reliably reproduce published structures in a majority of test cases, and in several instances identify details omitted by the original authors. Their low false positive rate makes them suitable for use in high-throughput workflows.

[1] *P.D. Adams et al., Acta Crystallographica D, 2010, 66, 213-221,* ***[2]*** *N. Echols et al., Acta Crystallographica D, 2014a, 70, 144-154,* ***[3]*** *N. Echols et al., Acta Crystallographica D, 2014b, in press*



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