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Improved low-resolution crystallographic refinement with Phenix and Rosetta

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Refinement of macromolecular structures against low-resolution crystallographic data is limited by the ability of current methods to arrive at a high-quality structure with realistic geometry. We have developed a new method for crystallographic refinement which combines the Rosetta sampling methodology and all atom energy function with likelihood-based reciprocal space refinement in Phenix, and find, on a test set of difficult low-resolution refinement cases, that models refined with the new method have significantly improved model geometry, and in most cases, lower free R factors and RMS deviation to the final model. Integration of the software packages additionally makes advanced sampling methods used in structure prediction and design available for crystallographic refinement and model-building, and also provides a strategy for improving the Rosetta force field for better agreement with experimental data.

[1] *DiMaio et al. (2013) Nature Methods 10:1102-4.*

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