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Quantum refinement for neutron macromolecular crystallography

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Neutron crystallography is a powerful method to determine the positions of hydrogen atoms in macromolecular structures. However, it is sometimes hard to judge what would constitute a chemically reasonable model, and the geometry of H atoms depends more on the surroundings (for example the formation of hydrogen bonds) than heavy atoms, so that the empirical geometry information for the hydrogen atoms used to supplement the experimental data is often less accurate. These problems may be reduced by using quantum-mechanical calculations, allowing to extract the maximal amount of information from the neutron data. We have recently implemented quantum refinement interfacing the widely used structure-refinement software Phenix and the freely available quantum mechanical software ORCA. This opens for quantum-mechanically supported structure determination with all structure methods available in Phenix, including neutron crystallography and overcomes some of the limitations in our previous implementation.

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