Reducing dynamical electron scattering reveals hydrogen atoms

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Compared with X-rays, electron diffraction faces a crucial challenge: dynamical electron scattering compromises structure solution and its effects can only be modelled in specific cases. Dynamical scattering can be reduced experimentally by decreasing crystal size but not without a penalty, as it also reduces the overall diffracted intensity. In this article it is shown that nanometre-sized crystals from organic pharmaceuticals allow positional refinement of the hydrogen atoms, even whilst ignoring the effects of dynamical scattering during refinement. To boost the very weak diffraction data, a highly sensitive hybrid pixel detector was employed. A general likelihood-based computational approach was also introduced for further reducing the adverse effects of dynamic scattering, which significantly improved model accuracy, even for protein crystal data at substantially lower resolution.
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