Re-factoring the B-factor: enabling intuitive structural-disorder analysis and multi-dataset crystallographic parameterisation.

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Displacement parameters (or temperature factors, or B-factors) describe the positional disorder of an atom in an atomic model. Though they typically constitute at least 20% of atomic model parameters and contain detailed information about atomic motions, they are difficult to interpret and are thus little-used in quantitative structural analysis. Furthermore, the permitted complexity of an atomic disorder model is strongly restricted by the resolution of the crystallographic data. We present a new approach for decomposing molecular disorder into a hierarchical series of contributions, which provides an intuitive basis for quantitative structural analysis. Additionally, this formalism allows for the simultaneous parameterisation of closely-related macromolecular structures, decreasing the data-parameter ratio and reducing overfitting, particularly for low resolution models. We demonstrate the visualisation of disorder in several biologically-relevant systems, and show that multi-crystal experiments offer an opportunity to improve our understanding of dynamics within macromolecular crystals.