

# Identifying and modelling low-occupancy states in macromolecular crystallography with Xtrapol8

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In time-resolved crystallography, a reaction intermediate can have such a low occupancy that it is hardly visible in the electron density. The same is true when ligand binding is studied but the apoprotein dominates the crystal. Several tools exist to unravel the structures of these low-occupancy states, one of them is Xtrapol8 [1]. Xtrapol8 allows to visualize the difference between two states by the calculation of a Bayesian weighted [2-3] Fourier difference map. Furthermore, it generates extrapolated structure factor amplitudes [4] that solely describe the low-occupancy state, enabling full modelling and refinement of the state. A brief overview of the methodology will be presented, along with examples and future developments.

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