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Supporting information for article:

Precipitant–ligand exchange technique reveals the ADP binding mode in *Mycobacterium tuberculosis* dethiobiotin synthetase

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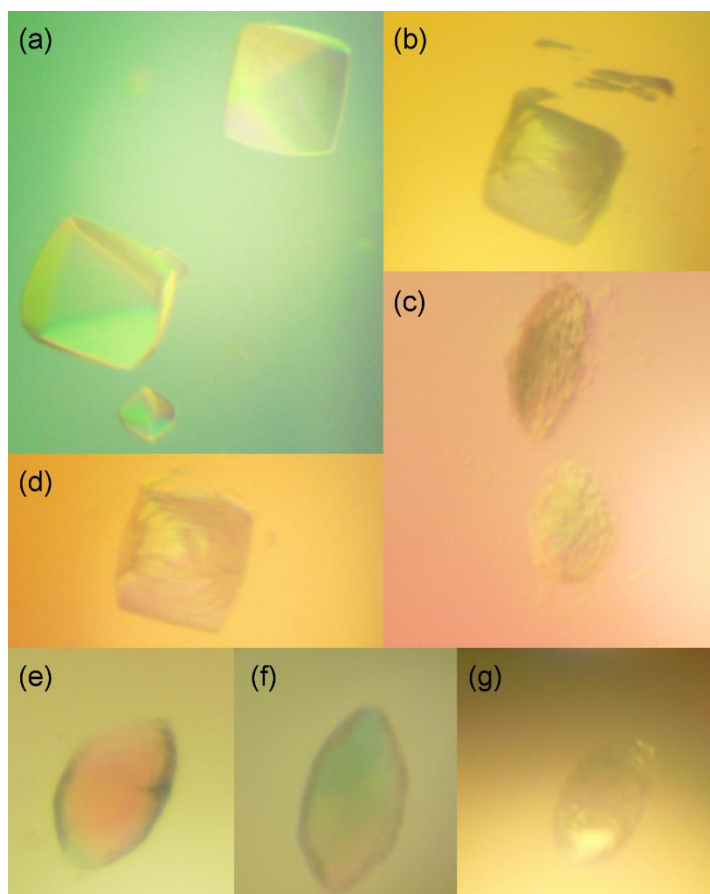


Figure S1 Pictures of *MtDTBS* crystals at various stages of precipitant-ligand exchange. (a) *MtDTBS* crystals grown from the sodium citrate growth condition (Materials and Methods) prior to exchange. (b, d) *MtDTBS* crystals immediately after being transferred into an exchange solution with 10 mM CTP. Cracking is visible, and sections of crystal have broken off (b). (c) crystals transferred into 10 mM CTP exchange solution that have undergone severe cracking and degradation. These crystals were deemed unlikely to produce acceptable X-ray diffraction, and the technique was optimised for shorter exchange times and higher ligand concentration. (e –g) *MtDTBS* crystals transferred into 100 mM CTP exchange solutions from citrate (e, f) and sulfate (g) growth conditions. These crystals were used to generate the crystallographic data for the CTP structures in this manuscript (PDB ID: 6E05, 6E05). The combination of a high concentration of CTP and a short exchange time resulted in minimal cracking and degradation. This allowed for acceptable X-ray diffraction quality and occupancy of the ligand.

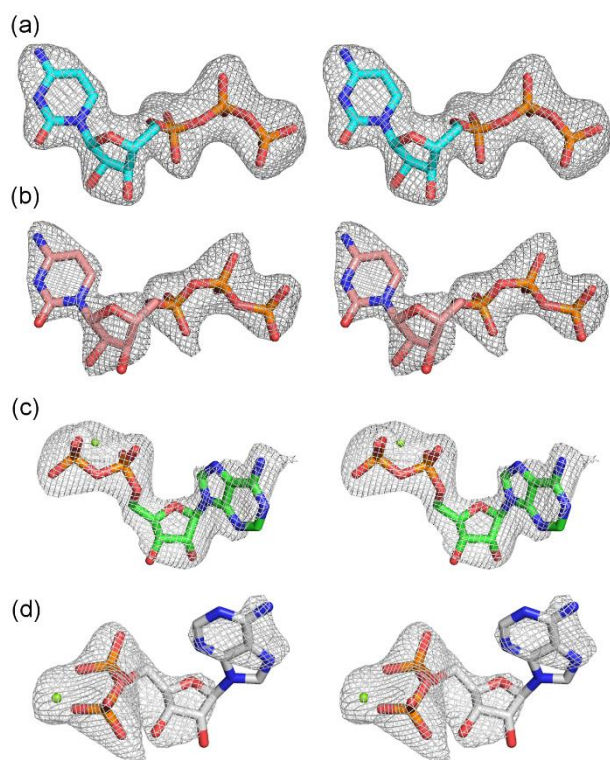


Figure S2 Walleye view of ligand Polder maps (3σ). CTP from precipitant-ligand exchange with crystals grown in (a) citrate and (b) sulfate. ADP from the two different conformations: (a) the ‘within’ DAPA pocket conformation (b) the ‘adjacent’ to DAPA pocket conformation.