



Supplementary Fig. 1: *Top* Electron density maps for the product molecule in chain C of data set 2 (inhibitor cocrystallisation; $2F_o - F_c$ in blue contoured at 1σ , negative $F_o - F_c$ in red contoured at -3σ , positive $F_o - F_c$ in green contoured at 3σ within 1.6 \AA), second representation is rotated 90° . *Bottom* Chemical structure of the catalytic product 6,7-dimethyl-8-(D-ribose)lumazine and the commercially available, weak binding inhibitor ($K_i = 210 \text{ \mu M}$ vs *S. pombe* and 95 \mu M vs *M. tuberculosis* LS (Talukdar *et al.*, 2009)) used for initial co-crystallisation studies.

Talukdar, A., Breen, M., Bacher, A., Illarionov, B., Fischer, M., Georg, G., Ye, Q. Z. & Cushman, M. (2009). *J Org Chem* 74, 5123-5134.