Figure S2. Comparison of I-TASSER and AlphaFold models of PfATP4. Left: global structural alignment of PfATP4 models produced by AlphaFold (blue) and I-TASSER (tan) with inset window displaying the drug-binding pocket. Arrow indicates the primary structural perturbation in the drug binding pocket, a displacement of helices a_5 and a_6 downwards by approximately 6Å in the AlphaFold model compared to the I-TASSER models. Right: AlphaFold Confidence Map coloured by pLDDT score (source: exported from AlphaFold structural repository with UniProt identifier A0A143ZZK9).