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**Supporting information for article:**

# Chasing the structural diversity of the transcription regulator *Mycobacterium tuberculosis* HigA2

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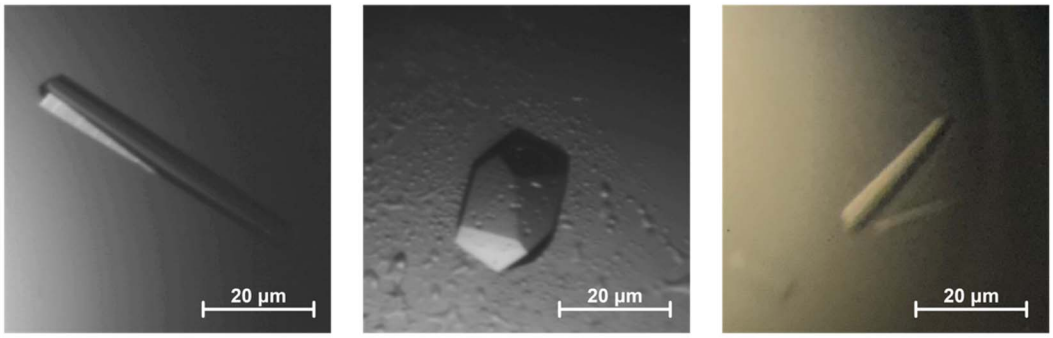


**Figure S1** Morphology of $_{Mt}$HigA2 crystals. Three protein crystals differ from each other in crystal shapes and sizes.

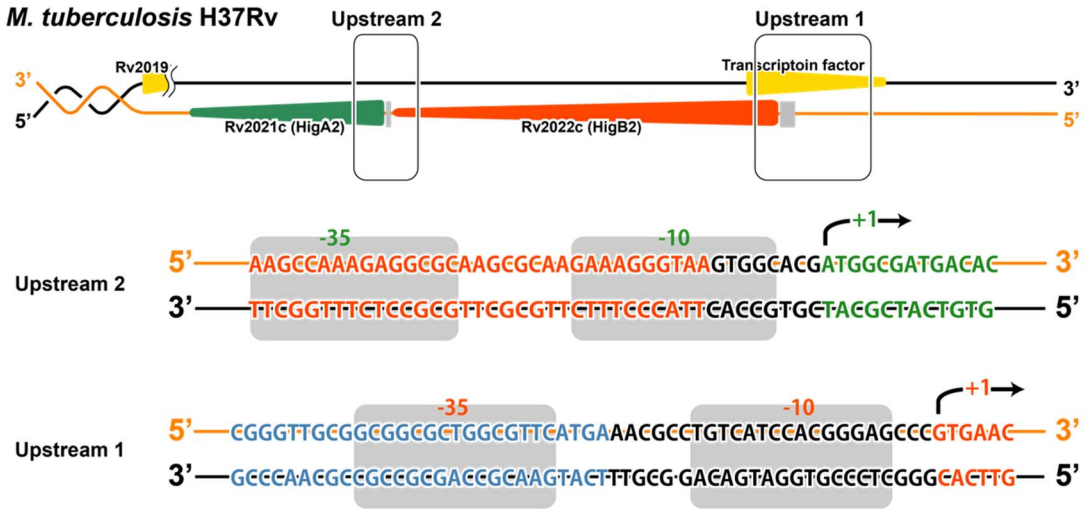


**Figure S2** Organization of $_{Mt}$HigBA2 operon and expected promoter sequence. The putative -10 box and -35 box are denoted. The DNA sequence tried for interaction assay were highlighted as grey colour.

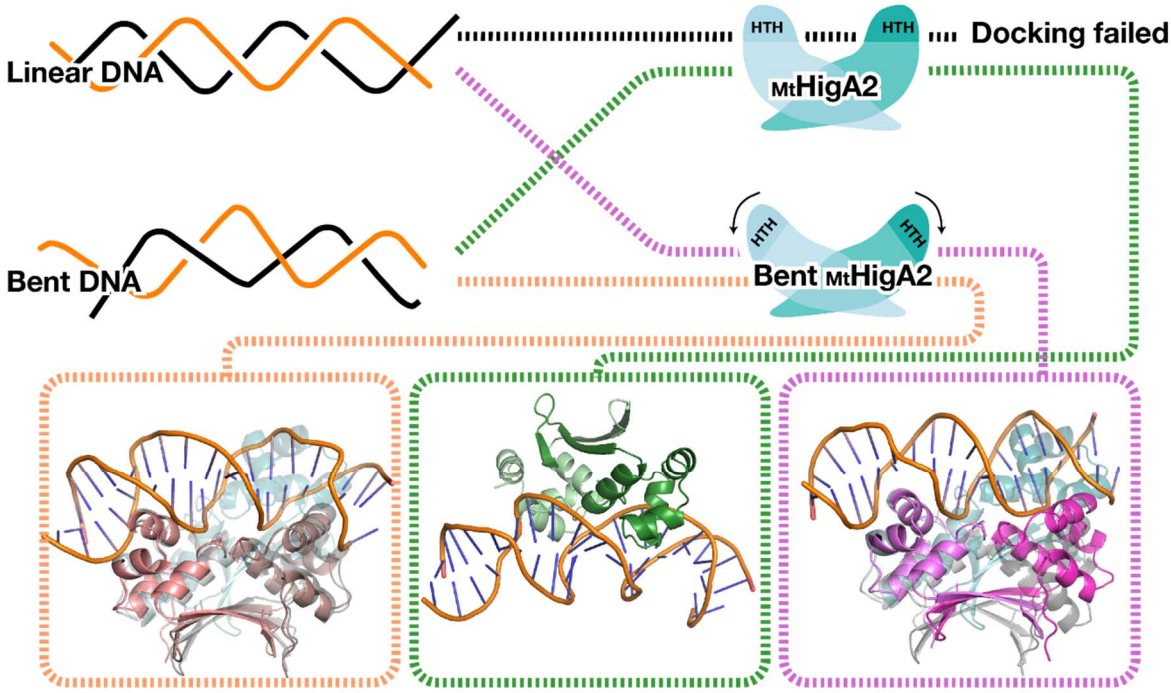


**Figure S3** Proposed interaction between the $_{Mt}$HigA2 and DNA. Total 4 sets of docking simulation were tried but linear $_{Mt}$HigA2 failed to recognize linear DNA. The lowest scored DNA-bound model was identified when bent $_{Mt}$HigA2 was docked to bent DNA (coloured in salmon, weighted ClusPro score of -2103). When the linear $_{Mt}$HigA2 is docked to bent DNA, the wrong binding model was resulted, showing solvent-exposed HTH motifs (coloured in green, weighted ClusPro score of -1595). Linear $_{Mt}$HigA2 was successfully docked to bent DNA, but distorted β-lid is observed in docked model (coloured in magenta, weighted ClusPro score of -2003). Linear $_{Mt}$HigA2 (light cyan) and modelled bent $_{Mt}$HigA2 (light grey) are aligned based on HTH motif and superimposed.