

Volume 71 (2015)

Supporting information for article:

Structural plasticity in *Mycobacterium tuberculosis* uracil-DNA glycosylase (*MtUng*) and its functional implications

S. M. Arif, K. Geethanandan, P. Mishra, A. Surolia, U. Varshney and M. Vijayan

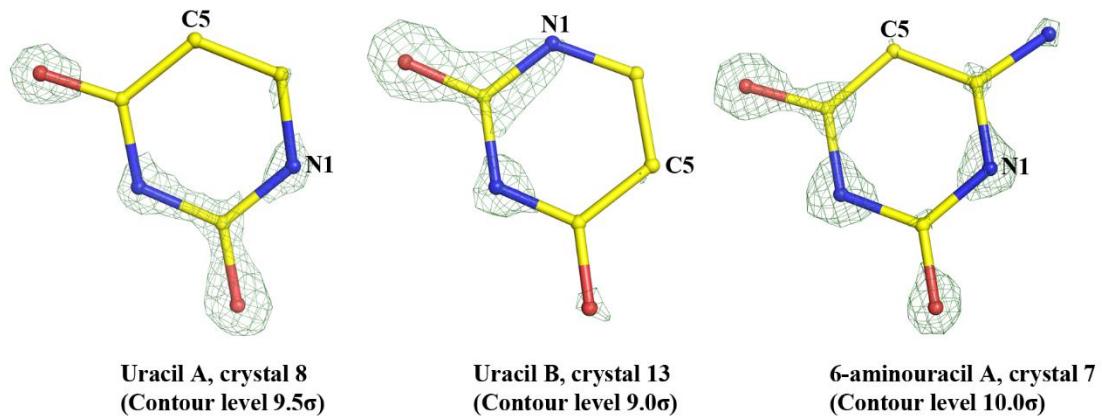
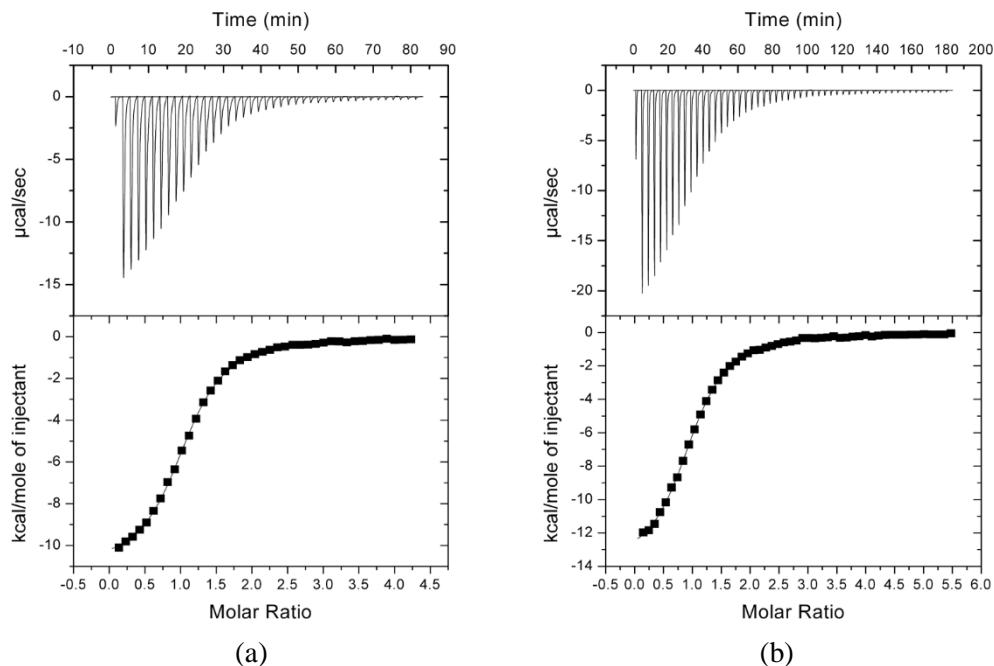


Figure S1 Typical electron densities for uracil and 6-aminouracil in simulated annealing $Fo-Fc$ omit maps with contour levels at which N1 and C5 can be discriminated.



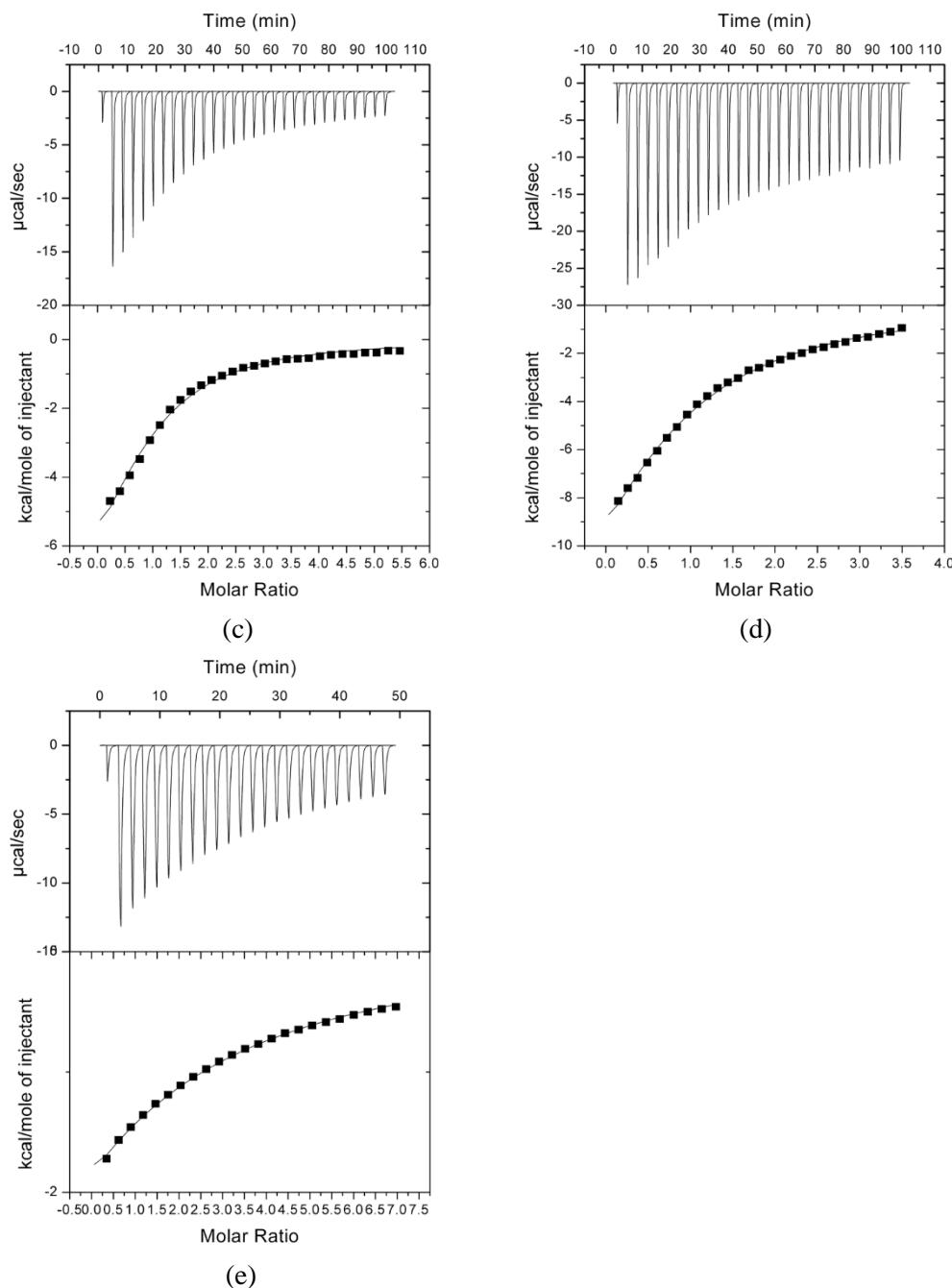


Figure S2 Isothermal titration calorimetry of (a) 6-aminouracil, (b) Uracil, (c) 2-thiouracil, (d) 5-nitouracil and (e) 5-fluorouracil, performed at 278K. The top panel in each graph shows the heat change elicited upon successive injections of ligand to the protein solution. The lower panel shows the binding isotherm as a function of molar ratio of ligand to enzyme. A theoretical curve was fitted to the integrated data using a one site model.

Table S1

(a) R.m.s deviations in C^α positions on pairwise superposition of the molecules in the 17 crystals.

(b) R.m.s deviations in C^a positions on pairwise superposition of domain 1 of the molecules in the 17 crystals.

(c) R.m.s deviations in C^a positions on pairwise superposition of the domain 2 sans residues 168-199 of the molecules in the 17 crystals.

(d) R.m.s deviations in C^a positions on pairwise superposition of the variable stretch (residues 168-199) of the molecules in the 17 crystals.