SUPPLEMENTAL DATA

Catalytic Site Conformations in Human PNP by ^{19}F-NMR and Crystallography

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Running Title: ^{19}F-NMR of Human Purine Nucleoside Phosphorylase.

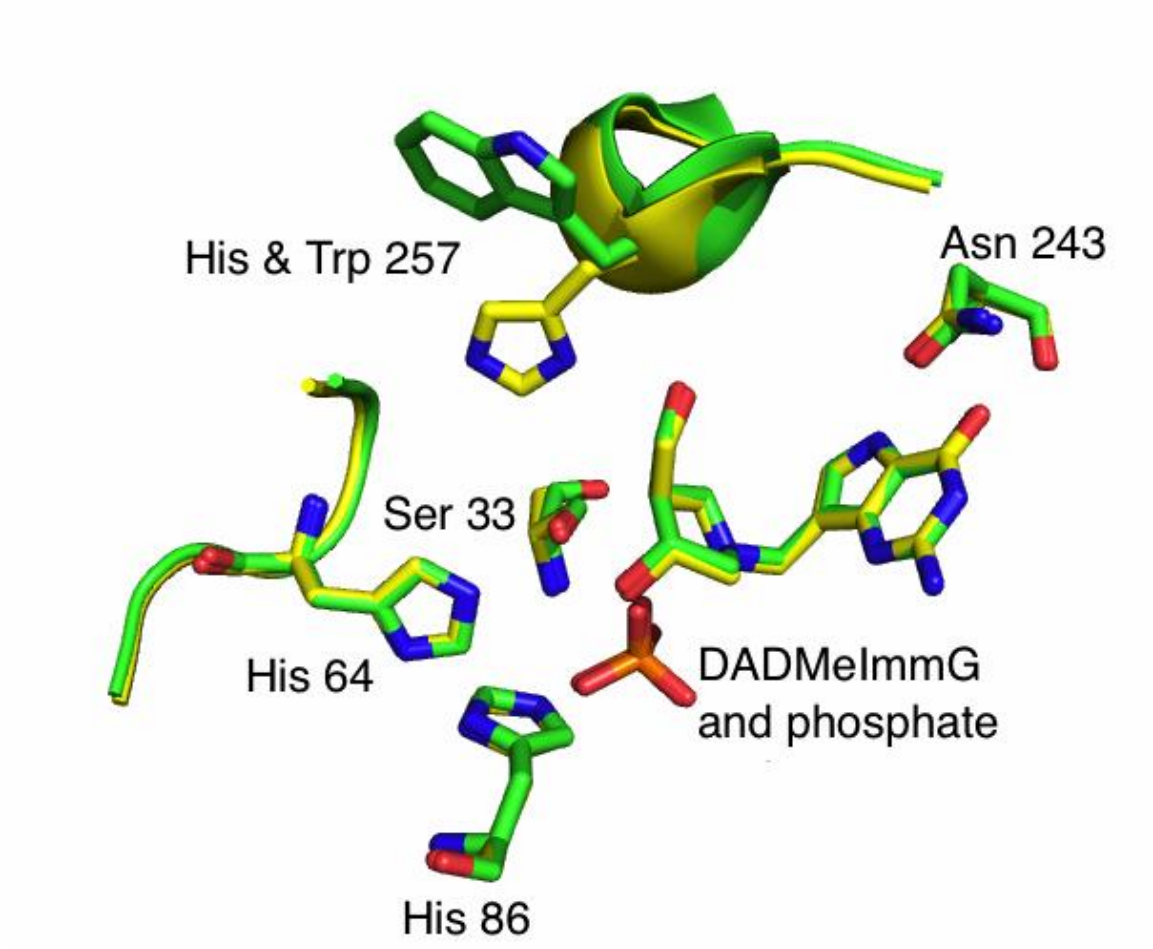

Figure S1:, related to Figure 4. Human PNP complexes; structural overlays of the catalytic site. (A). Overlap of the active site residues of WT PNP (yellow) and H257W-Leuko PNP (green) bound to DADMeImmG and phosphate.

Movie S1, related to Figures 4 and 7. The movie shows a secondary structural representation of phosphate bound human PNP (light brown) overlapped with a ribbon representation of the same structure (green). A conformational rearrangement in the active site of the green structure is shown upon binding of ligands (phosphate and the transition state analogue DADMeImmG). Movements are observed in the 257 region (show by the Trp257 residue) and the 64 loop (show by the His64 residue). Upon binding of ligands the PNP active site goes from a "open" to a "closed" conformation that can lead to catalysis.