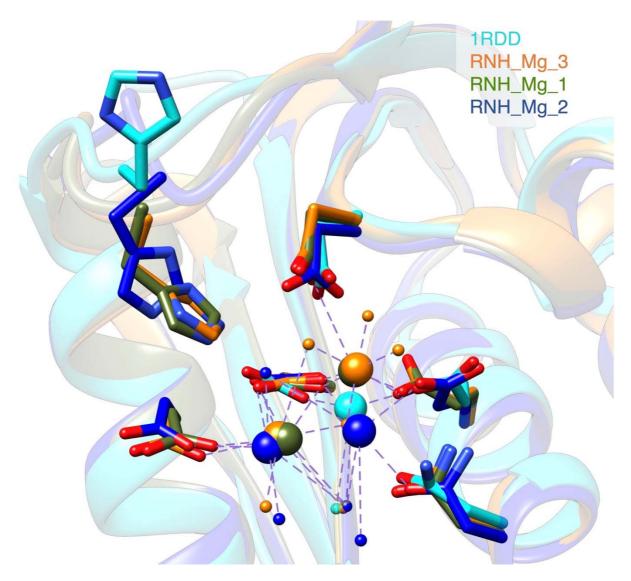


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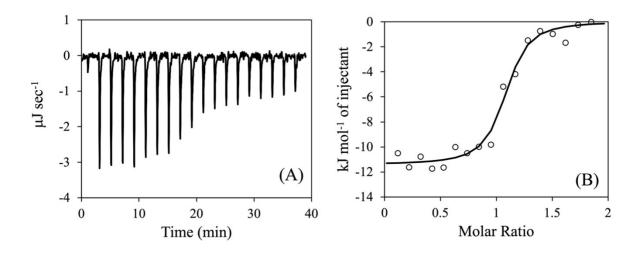
Supporting information for article:

Pivotal role of a conserved histidine in *Escherichia coli* ribonuclease HI as proposed by X-ray crystallography

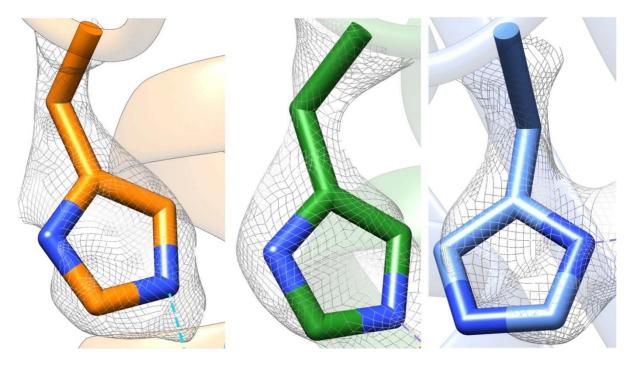
Zengwei Liao, Takuji Oyama, Yumi Kitagawa, Katsuo Katayanagi, Kosuke Morikawa and Masayuki Oda



**Figure S1** Comparison of Mg<sup>2+</sup> coordination patterns in the *E. coli* RNase HI crystal structures. Dark olive green: RNH\_Mg\_1, blue: RNH\_Mg\_2 Orange: RNH\_Mg\_3, cyan: one Mg<sup>2+</sup> bound *E. coli* RNase HI (PDB entry 1RDD). Note that one Mg<sup>2+</sup> position (upper right) of two Mg<sup>2+</sup> sites looks like a single metal, because of nearly perfect overlapping.



**Figure S2** ITC measurements of the interaction between RNase HI and  $Zn^{2+}$ . (A) The ZnCl<sub>2</sub> solution was injected into the RNase HI solution. (B) Integrated data was fitted using one-site model. The three independent experiments gave  $n = 0.99 \pm 0.15$ ,  $K_d = 1.09 (\pm 0.60) \mu$ M, and  $\Delta H = 11.7 (\pm 0.6)$  kJ mol<sup>-1</sup>.



**Figure S3**  $2F_{o}$ - $F_{c}$  electron density maps (level: 1.3  $\sigma$ ) of His124 in RNH\_Mg\_3, RNH\_Zn\_1 and RNH\_Zn\_2 respectively. The His124 in each structure is zoomed in and the angle is adjusted to show the complete map of the whole imidazole sidechain.