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# Escherichia coli's RfaH studied by all-atom Monte Carlo simulation (G)*

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RfaH is a compact two-domain multi-functional protein from the bacteria $Escherichia\ coli$ ($E.coli$). Its C-terminal domain (CTD) has been shown experimentally to be able to undergo a complete conformational change from an $\alpha$-helix bundle to a $\beta$-barrel structure. The $\alpha$-helix bundle to $\beta$-barrel fold switch accounts for the observed dual role of RfaH, whereby it regulates transcription as well as enhances translation. We employ all-atom Monte Carlo simulations to investigate the stabilities of the two structural forms of RfaH and the character of transition between them. Our simulations reveal that the stand-alone $\alpha$-helix CTD is relatively unstable despite the stabilizing interactions with the N-terminal domain (NTD). Moreover, we observe the stability of the stand-alone $\beta$-barrel conformation to be always higher than the $\alpha$-helix bundle structure. Thus, we conclude that the $\alpha$-helix bundle to $\beta$-barrel fold switch of the CTD in RfaH is thermodynamically favoured in our model.

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