

Supplementary Figures

Mechanistic alternatives for peptide bond formation on the ribosome

Masoud Kazemi^{†‡}, Jaka Sočan[†], Fahmi Himo^{‡}, Johan Åqvist^{†*}*

[†]Department of Cell and Molecular Biology, Box 596, Uppsala University, BMC, SE-751 24
Uppsala, Sweden

[‡]Department of Organic Chemistry, Arrhenius Laboratory, Stockholm University, SE-106 91
Stockholm, Sweden

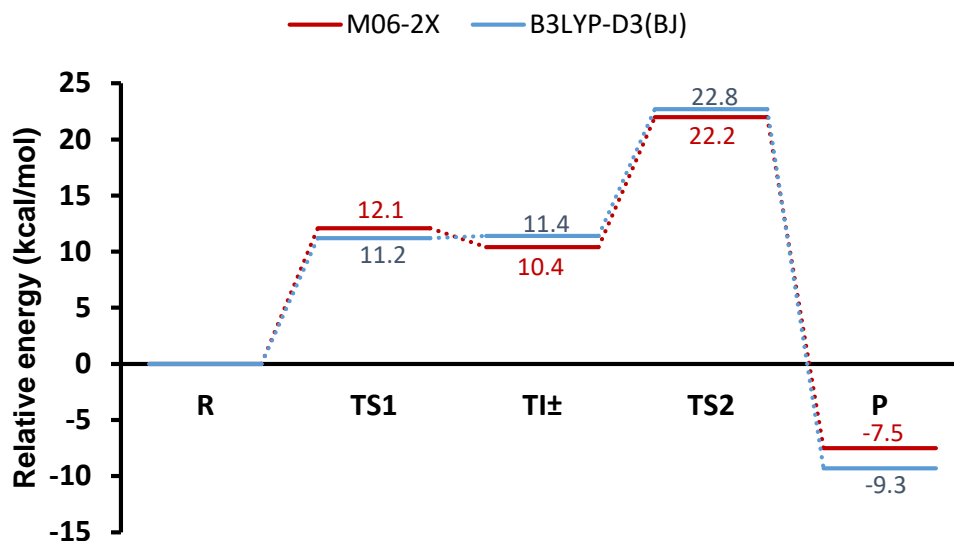


Figure S1. Calculated energetics of the proton shuttle mechanism involving a ten-membered transition state with M06-2X and B3LYP functionals.

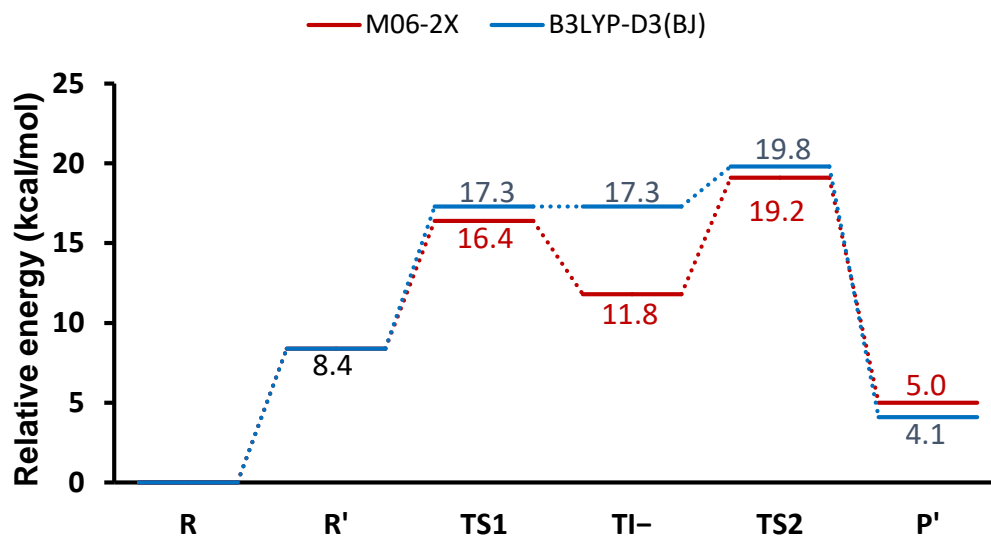


Figure S2. Calculated energetics of the general base catalyzed mechanism with M06-2X and B3LYP functionals.