Supporting information for "Distal Proton Shuttle Mechanism of Ribosome Catalysed Peptide Bond Formation – A DFT study"

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Table S1. NBO charge of the important atoms in the reaction species.

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Figure S1. Schematic representation of the energy profiles of the distal proton shuttle mechanism. The PCM continuum solvation model with the dielectric constant of 4, 24 and 78 was introduced to mimic the water environment. ZPE correction is also included. The overall energy barriers are very close under different dielectric constants, which validates the QM model used in this paper.
Figure S2. Schematic representation of the energy profile for the peptide bond formation with W3 involved in proton transfer in the rate-limiting step.
Figure S3 Geometries of reaction species including RC, INT, TS2 and Pr in the distal proton shuttle pathway. Hydrogen bonds are represented by dashed lines. Important geometric parameters are labeled. The hydrogen bond length is measured as the distance between two heavy atoms (in red).
Table S3. Cartesian coordinates of the RC, TS1, INT, TS2 and P in the distal proton shuttle mechanism.

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