Supplementary material

Figure S1. Radial distribution function of water solvent calculated by averaging over the 10ps molecular dynamics simulation of the cytosine solution: $g_{HwHw}(r)$ (dotted black line), $g_{OwOw}(r)$ (solid red line), $g_{OwHw}(r)$ (dashed blue line). Ow denotes oxygen atoms of water molecules and Hw hydrogen atoms. See Table 1 for numerical specification of position and height of first peaks and computational details for detailed description.



Figure S2. Distribution of angles of hydrogen bonds formed between amide group of the base and oxygen atom of water: N9-H9...Ow (solid black line) in adenine, N1-H1...Ow (solid red line) and N9-H9...Ow (solid blue line) in guanine, N1-H1...Ow (solid green line) in cytosine, N1-H1...Ow (solid pink line) and N3-H3...Ow (solid purple line) in thymine.



Figure S3. Radial pair distribution functions for water hydrogen atoms Hw and N2 atom of the guanine: RDF calculated for all water molecules (solid black line), and only for those that are not bounded to hydrogen atoms of amino group (solid red line). See computational details for detailed description.



Figure S4. Distribution of angles of hydrogen bonds formed between water hydrogen atoms Hw and carbonyl group of the base: C6=O6...Hw (solid black line) in guanine, C2=O2...Hw (solid red line) in cytosine, C2=O2...Hw (solid green line) and C4=O4...Hw (solid blue line) in thymine.



Figure S5. Radial pair distribution functions for water molecules around the each Hydrogen atom of CH₃ site in thymine. See computational details for detailed description.





Let us assume that N=C1 double bond is always vector a, and N-C2 single bond is always vector b. Then vector c is cross-product of vectors a and b. After assigning N-Hw H-bond as vector d, we are using dot product of vectors c and d to calculate angle β . Finally, value for angle α is calculated according to following equations:

 $\alpha = \begin{cases} 90^{\circ} + \beta, & \text{if } \beta \le 90^{\circ}; \\ \beta - 270, & \text{if } \beta > 90^{\circ}. \end{cases}$