Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Probing the conformational dynamics of an Ago-RNA complex in water/meoh solution.

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Supplementary Information

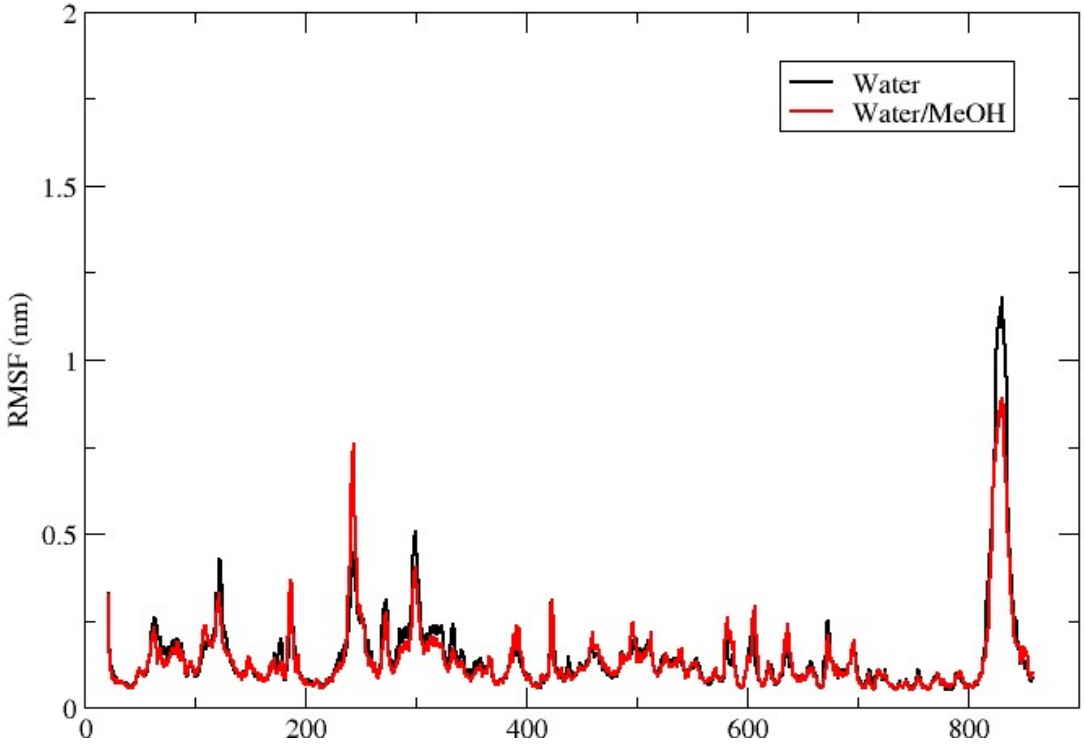

Figure S1 Per-residue C**α**-RMSF calculated for the simulation performed in water (black line) and water/meoh (red line)

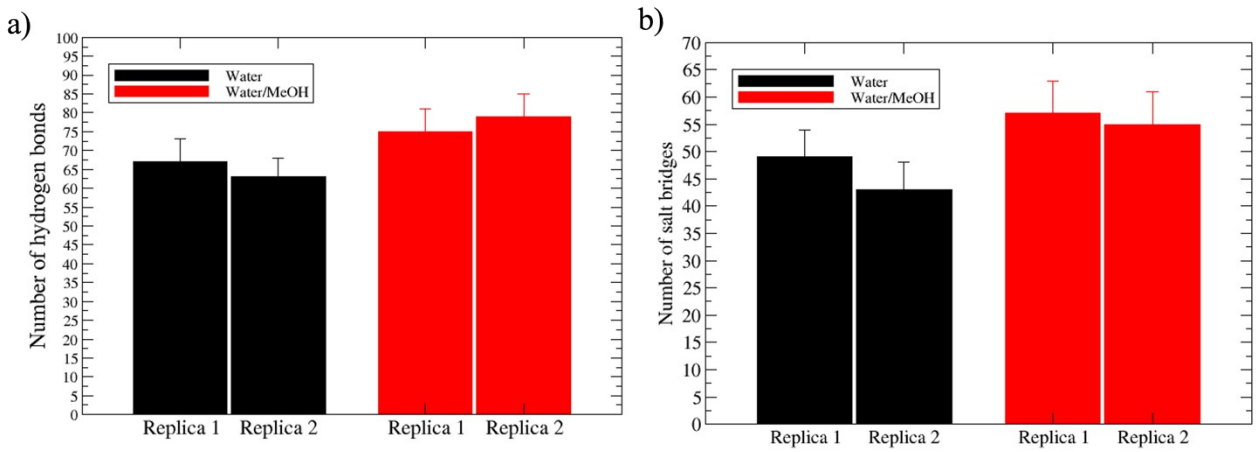

Figure S2 (a) Number of hydrogen bonds between protein and RNA. (b) Number of salt bridges involving Arginine and Lysine with phosphates of the RNA backbone.

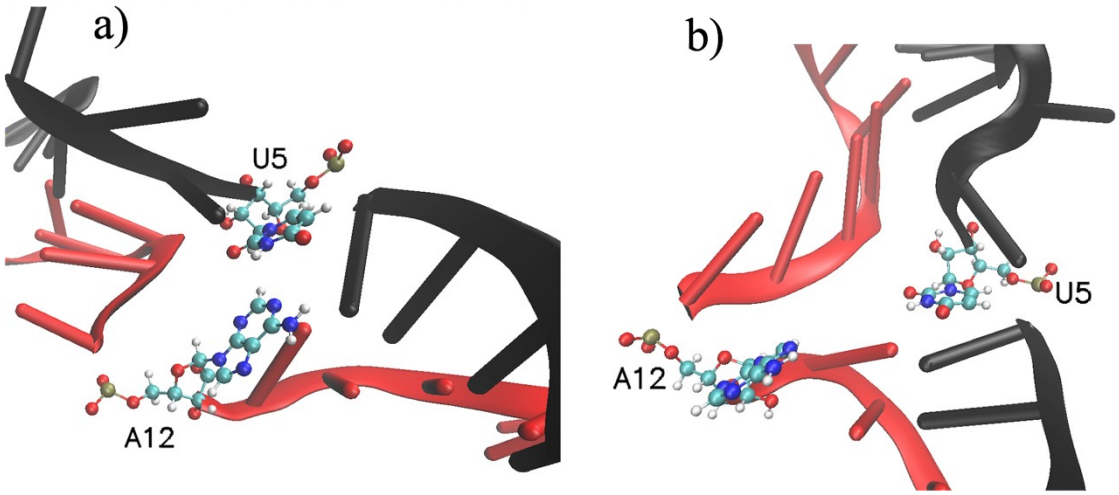

Figure S3 (a)guide A12 and target U5 by starting crystallographic structure (b) middle structure from the most populated cluster in water/meoh simulation.

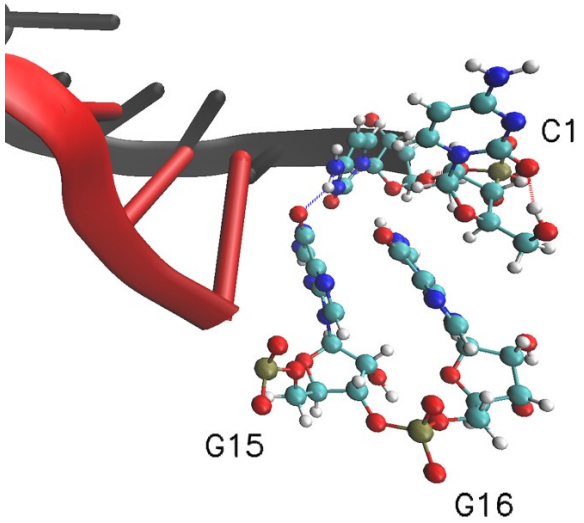

Figure S4 middle cluster structure retrieved from water simulation showing interaction with unpaired gC1 and tG16

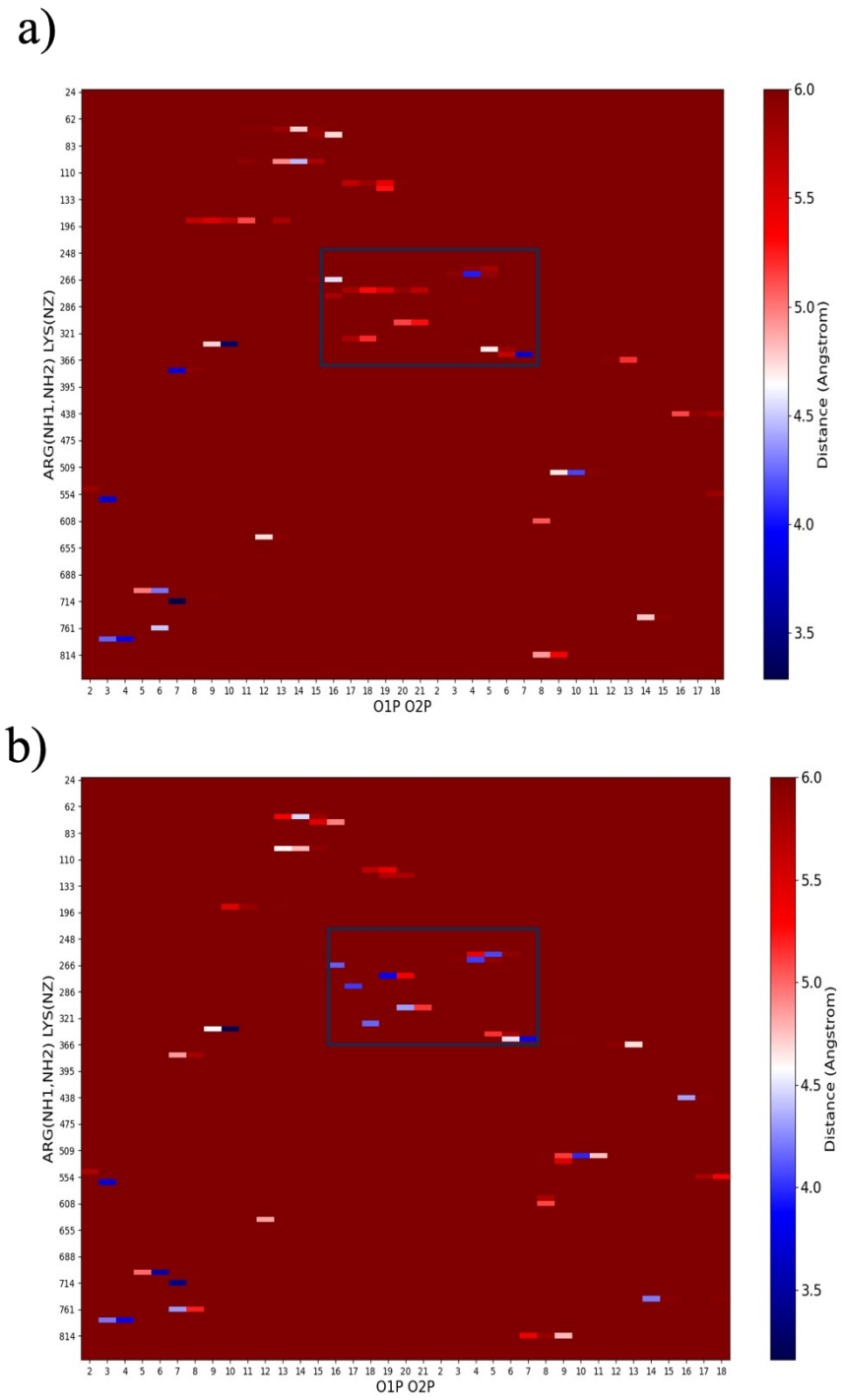

Figure S5 Salt-bridge per-residue contact map in water (a) and water/meoh (b) within a cut-off of 6.0 Å between Ago(y-axis) and RNA(x-axis). The per-residue salt bridge mean-distances have been computed between O1P-O2P center of mass and NH1-NH2 center of mass in case of ARG residues. For LYS, the mean distances have been calculated between O1P-O2P center of mass and NZ atom

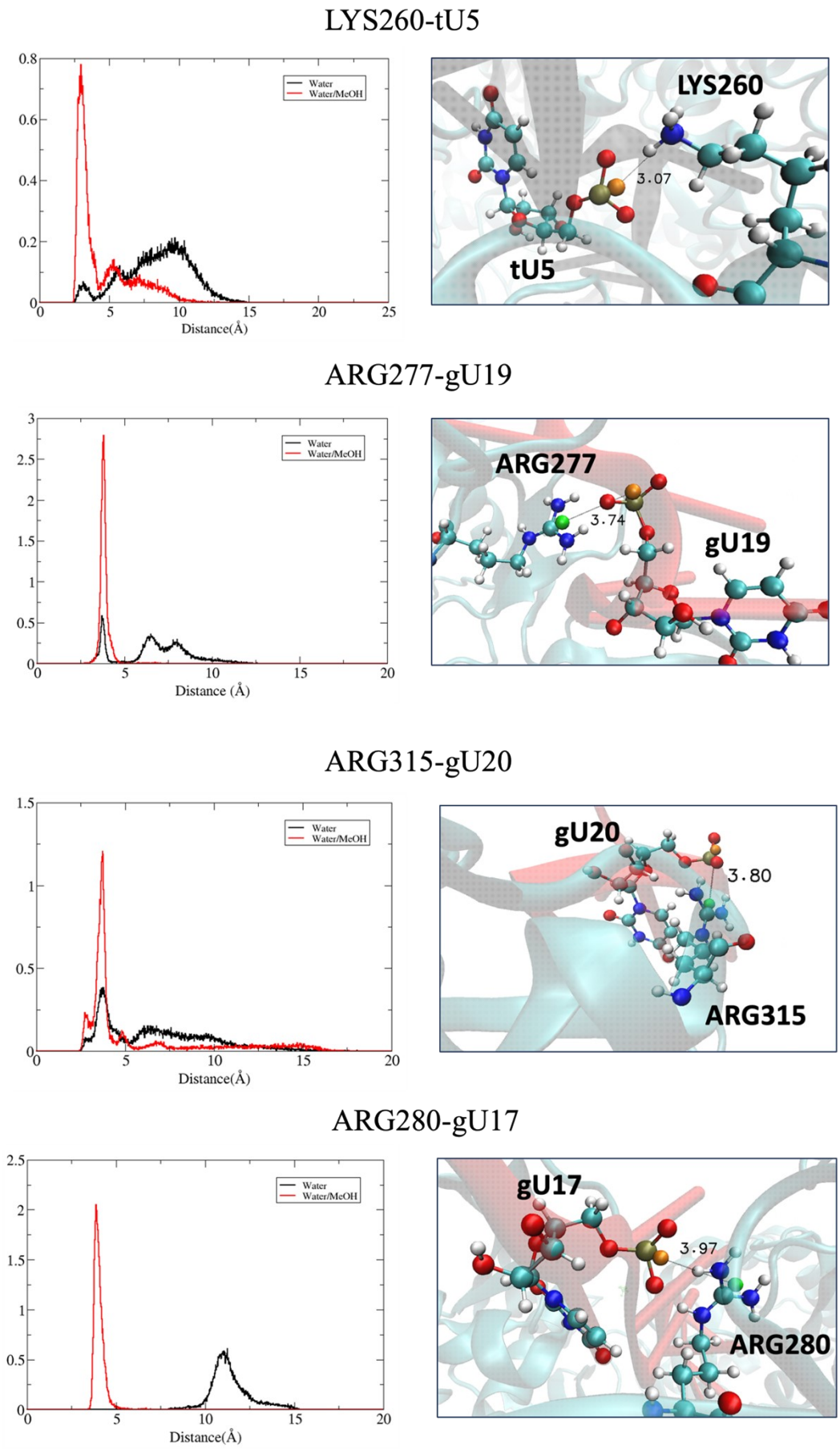

Figure S6. Analysis of distances between O1P-O2P center of mass and NH1-NH2 center-of-mass for arginine-phosphate couple and O1P-O2P center-of-mass and NZ atom for lysine-phosphate couple. Left panel, normalized distance distribution. Right panel, representative snapshot illustrating the salt bridge interaction. NH1-NH2 and O1P-O2P centers of mass are displayed as dummy atoms colored respectively in green and orange.

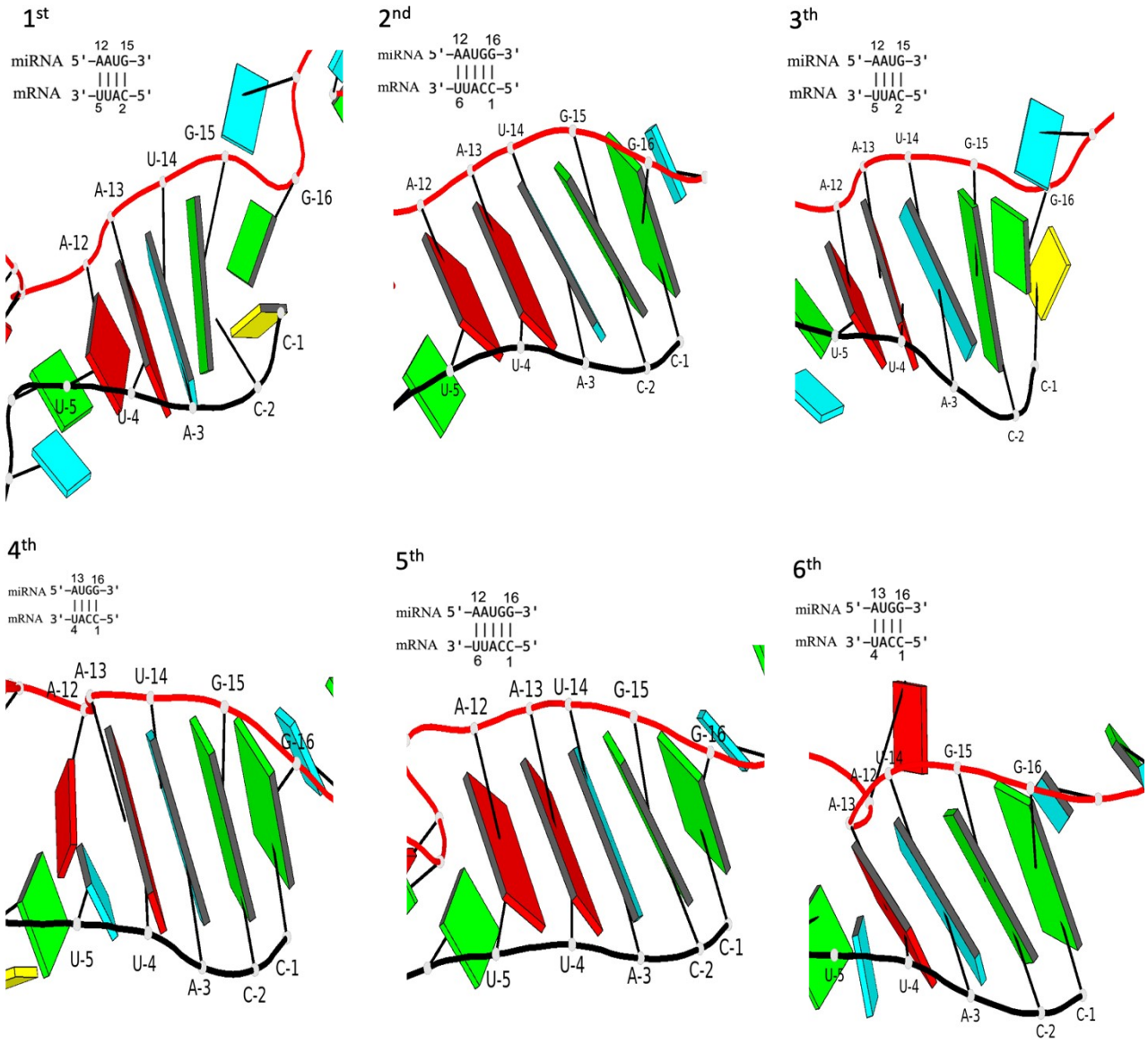

Figure S7 Representative structures of the base pair in the supplementary duplex extracted from the 1st, 2nd, 3th,4th, 5th and 6th most populated clusters, showing the variation of the status of the base pairs along the trajectories collected in water.

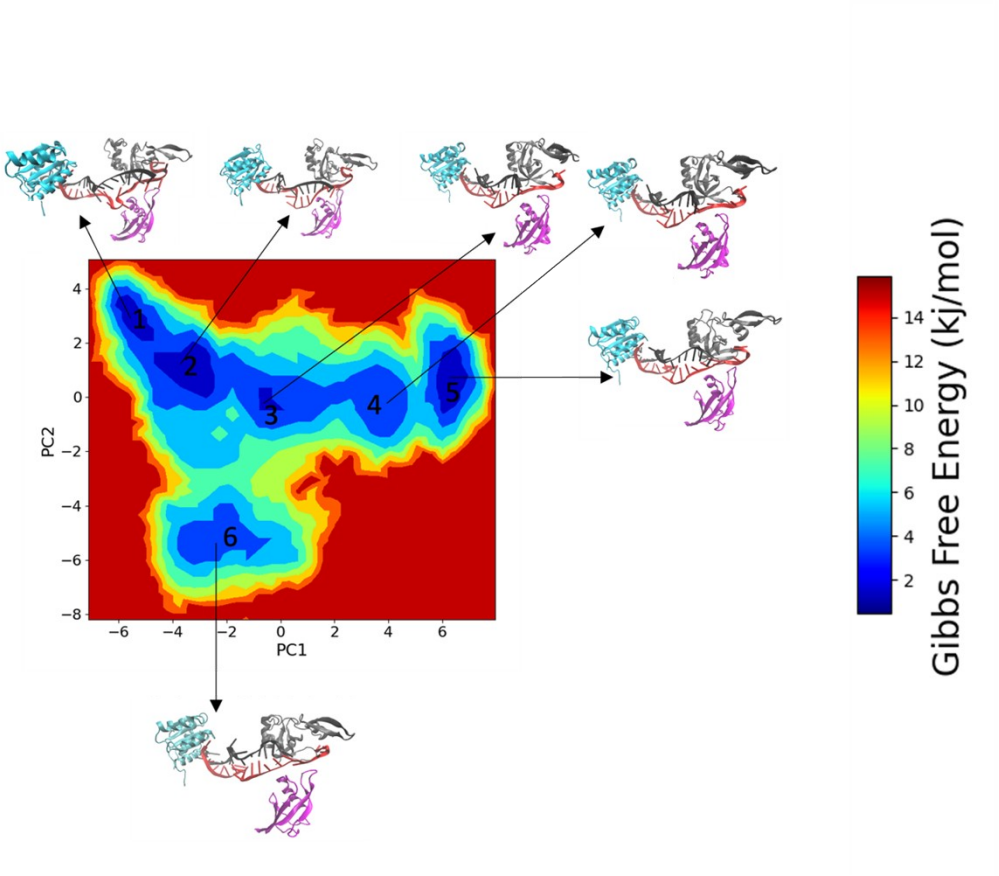

Figure S8. Details of complex conformation along PC1 and PC2 describing structural variations in the recognized local minima from the FEL computed in water system. For protein only PAZ, MID and N domains are present for clarity.

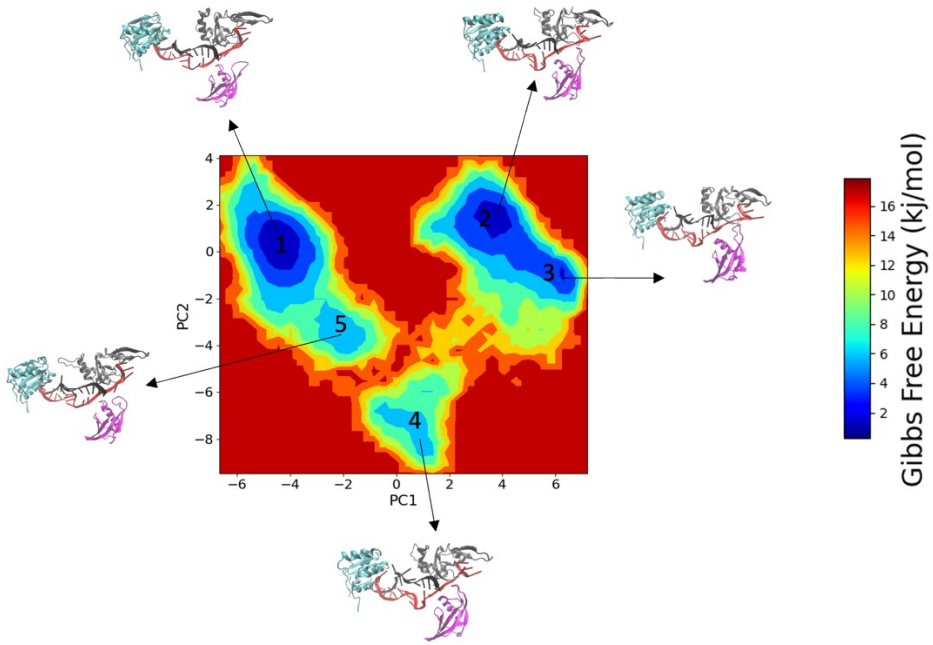

Figure S9. Details of complex conformation along PC1 and PC2 describing structural variations in the recognized local minima from the FEL computed in water/meoh system. For protein only PAZ, MID and N domains are present for clarity.