Investigating the ion dependence of the first unfolding step of GTPase-Associating Center ribosomal RNA

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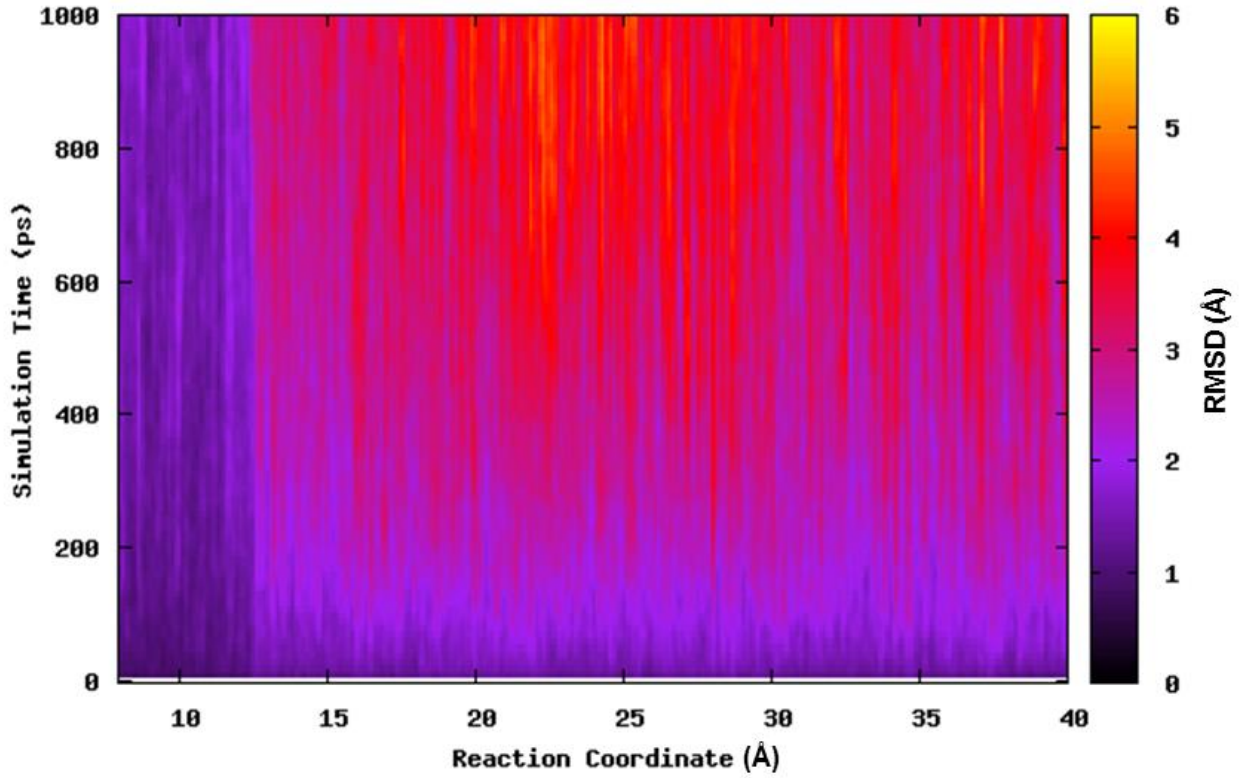
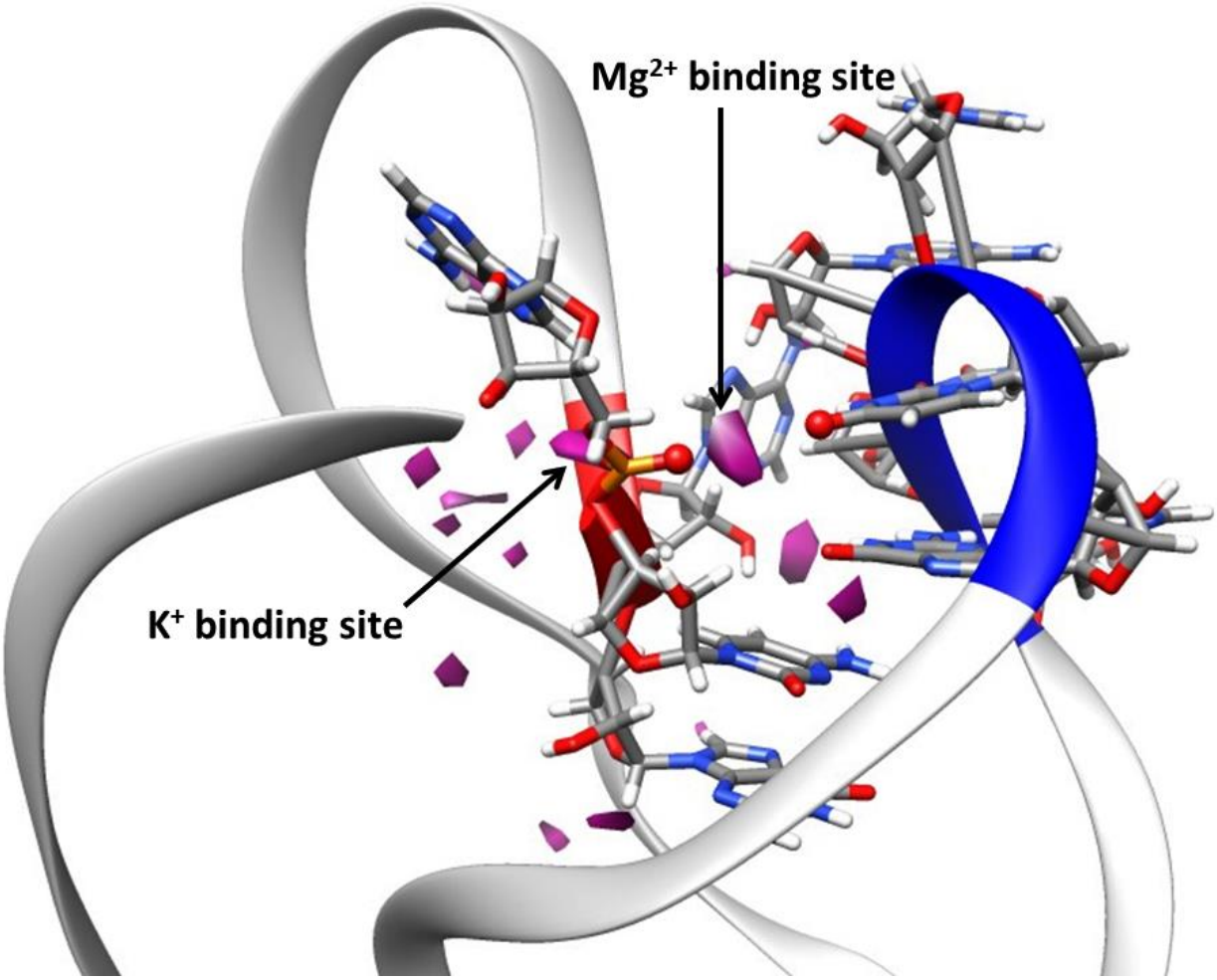
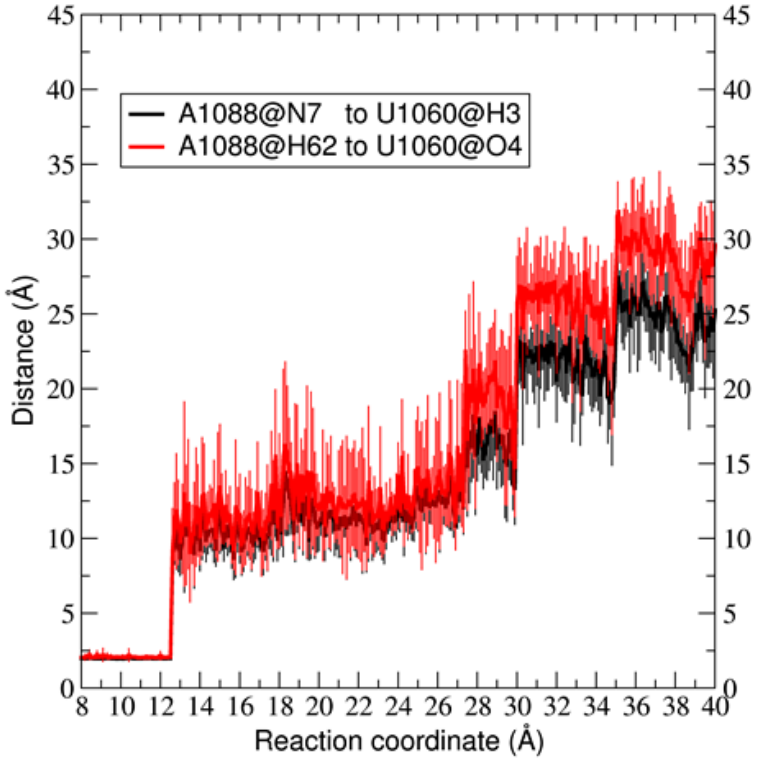
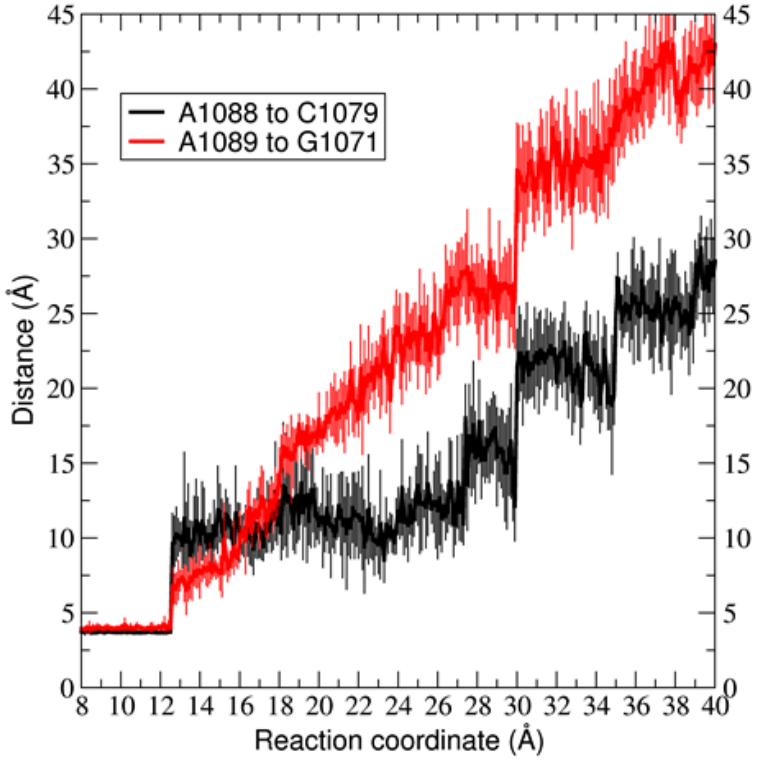


Supporting Figure 1. Root mean square deviation along each umbrella trajectory with reference to the umbrella initial structure in one copy of US-boundMg simulations with no excess $MgCl_2$. The figure is not shown for other umbrella sampling simulations because of the similarity to this figure.

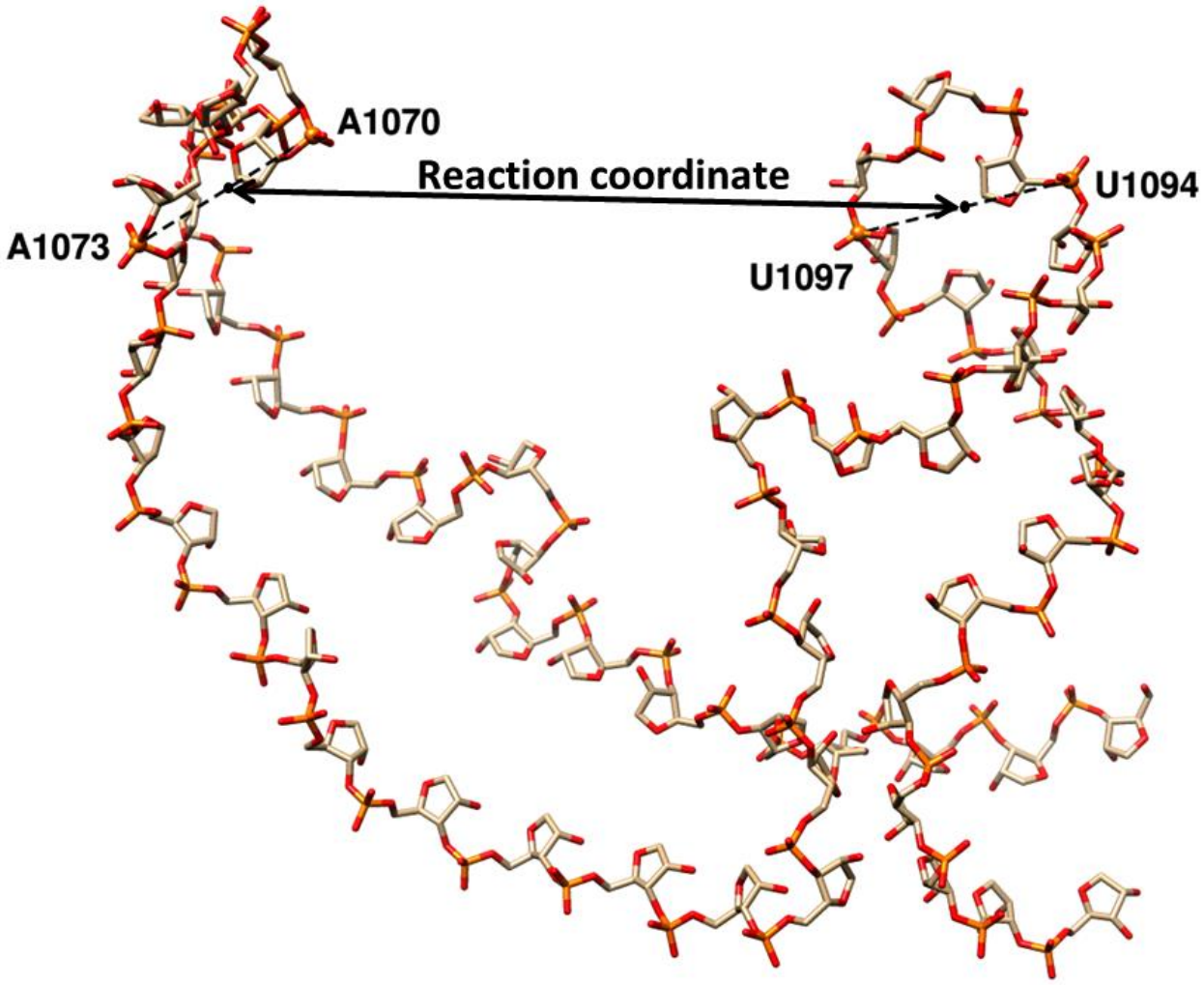


Supporting Figure 2. Part of the *GAC* RNA average structure over cumulative 2 ns production data of umbrellas 9.0-9.9 Å (close to the crystal structure with reaction coordinate value of 9.6 Å) in two independent sets of simulations with neutralizing potassium. The purple diamonds represent positions occupied by potassium 2000 times the evenly-distributed potassium would occupy. Potassium ions accumulate in the potassium and magnesium binding sites when the ions are free in simulations (black plot in **Error! Reference source not found.**2).

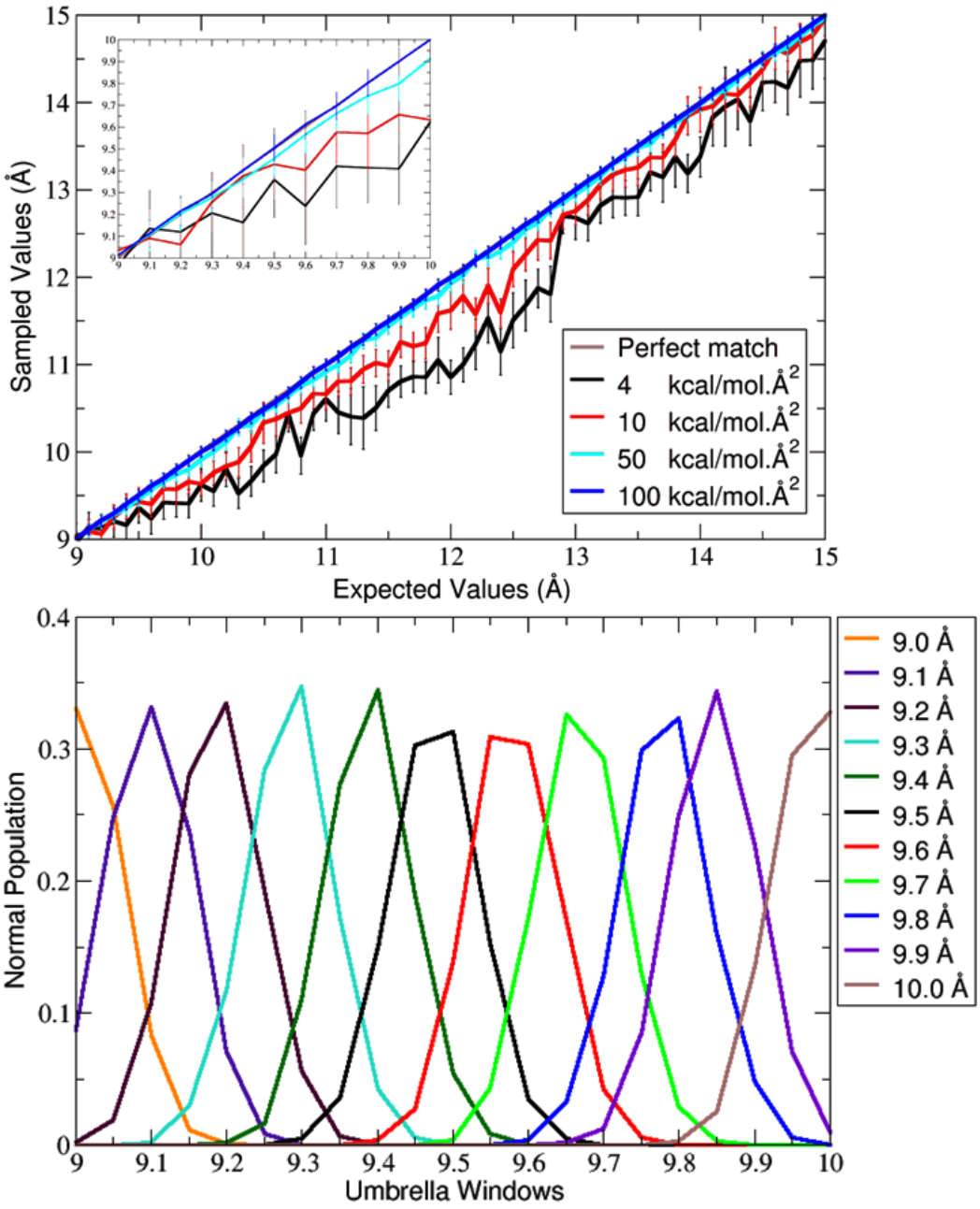

A1088@N7 to U1060@H3
A1088@H62 to U1060@O4
Distance (Å)
Reaction coordinate (Å)


A1088 to C1079
A1089 to G1071
Distance (Å)
Reaction coordinate (Å)

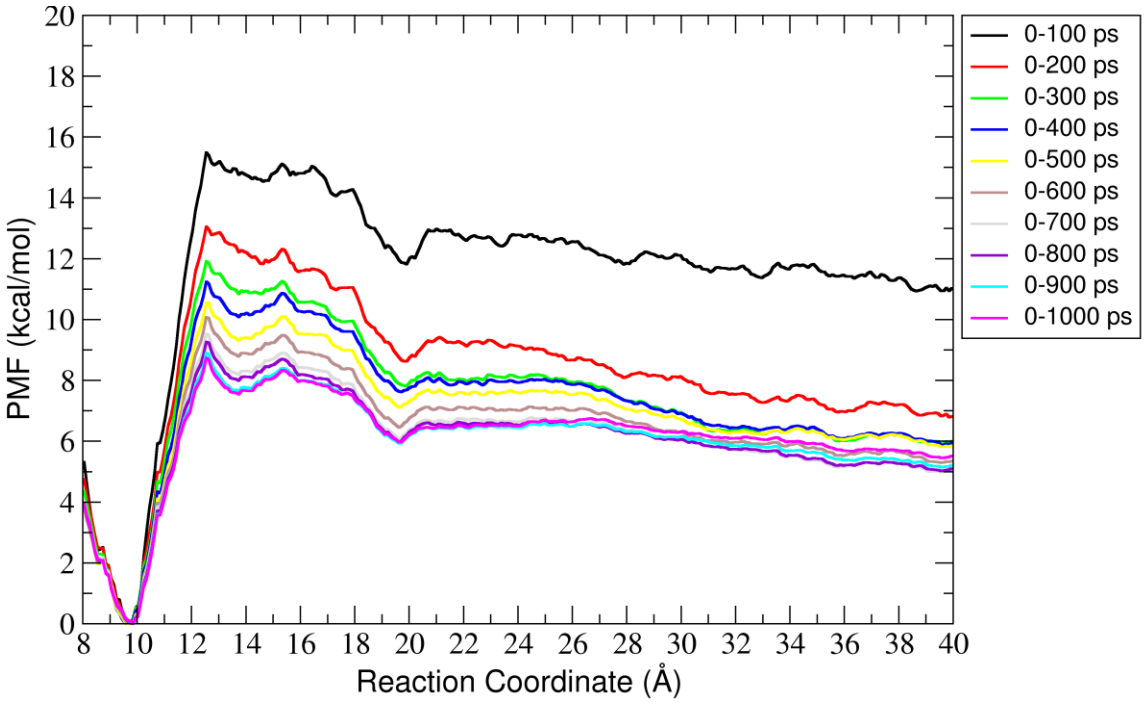
Supporting Figure 3. Top: Hydrogen bond distances between A1088 and U1060 along the reaction coordinate. **Bottom:** Distances between the center of masses of base atoms of A1088 and C1079; and between the center of masses of base atoms of A1089 and G1071 along the reaction coordinate which are representative of the stacking interactions between these two pairs of bases. The data is gathered are from combined umbrella samplings with bound and unbound bridging Mg^{2+} with error bars representing the standard deviations between different runs.



Supporting Figure 4. The reaction coordinate distance (double-headed arrow) used in umbrella sampling simulations which is the distance from the center of mass of phosphorus atoms of A1070 and A1073 to the center of mass of phosphorus atoms of U1094 and U1097, shown on the initial structure of the 40.0 Å umbrella window. The hydrogen and base atoms are not shown for clarity and the phosphorus atoms of the indicated four residues are shown with orange spheres.



Supporting Figure 5. Top: Sampled vs. expected values for umbrellas close to the minimum PMF of the system with no excess $MgCl_2$ in presence of the bound Mg^{2+}, sampled with different force constants. **Bottom:** Histograms of the sampled values close to the minimum PMF for the system sampled with 100 kcal/mol-Å^2 force constant.



Supporting Figure 6. Evolution of the PMF plots in one copy of US-boundMg simulations with no excess $MgCl_2$ in presence of the bound Mg^{2+}, with adding 100 ps chunks of data.

Supporting Text: Cpptraj scripts

- **Displacing the bound magnesium for the first umbrella window:**

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trajout step7.rst restart

- **Grid analysis for Supporting Figure 2:**

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