

Supplementary Information

Monte Carlo Tightly Bound Ion model: Predicting ion binding properties of RNA with ion correlations and fluctuations

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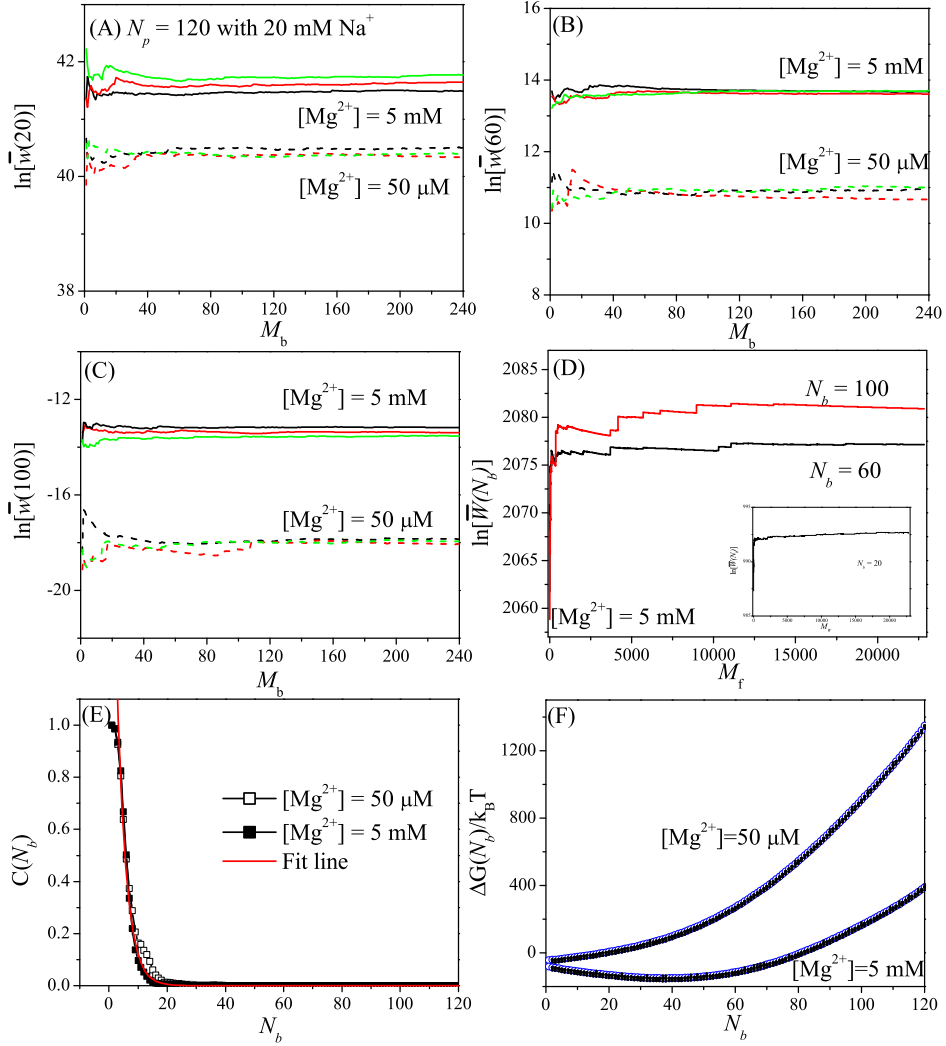


Figure S1: Tests of the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using a 120-nt RNA A-form helix as a test case. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 3.2 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

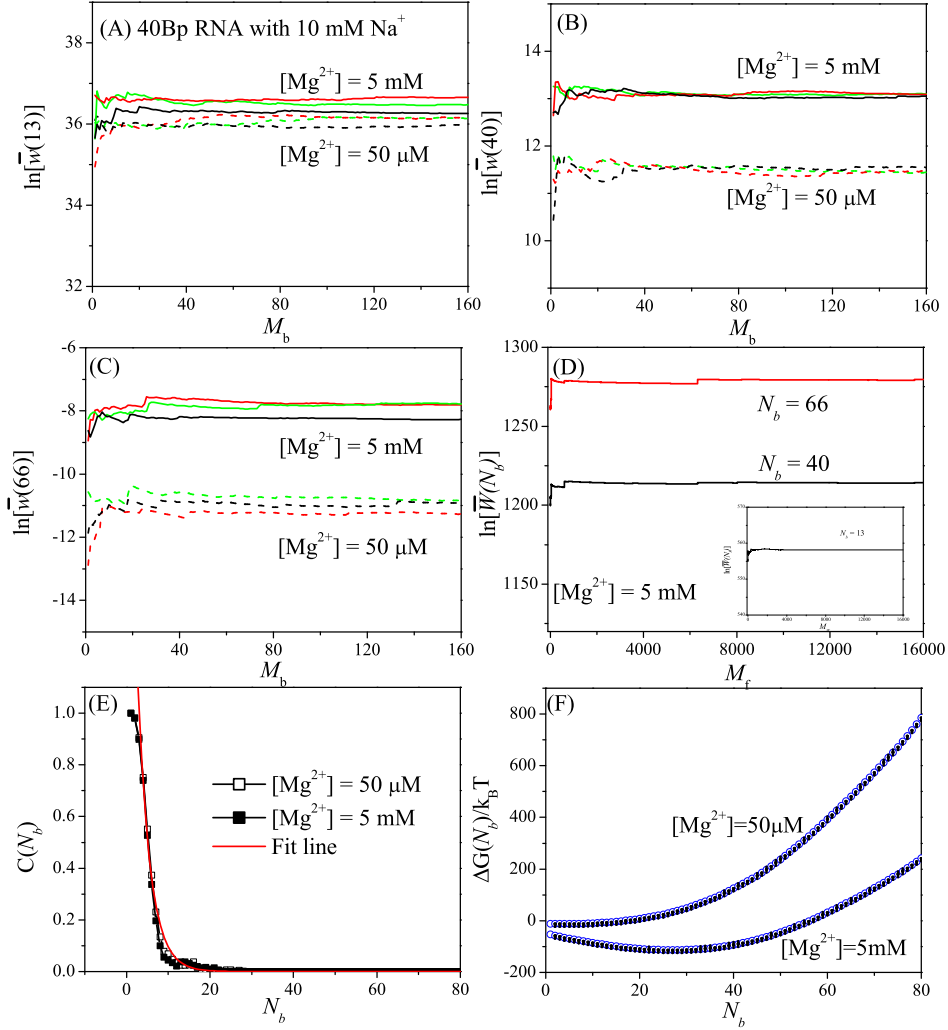


Figure S2: Tests for the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using 40-bp RNA helices. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 3.1 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

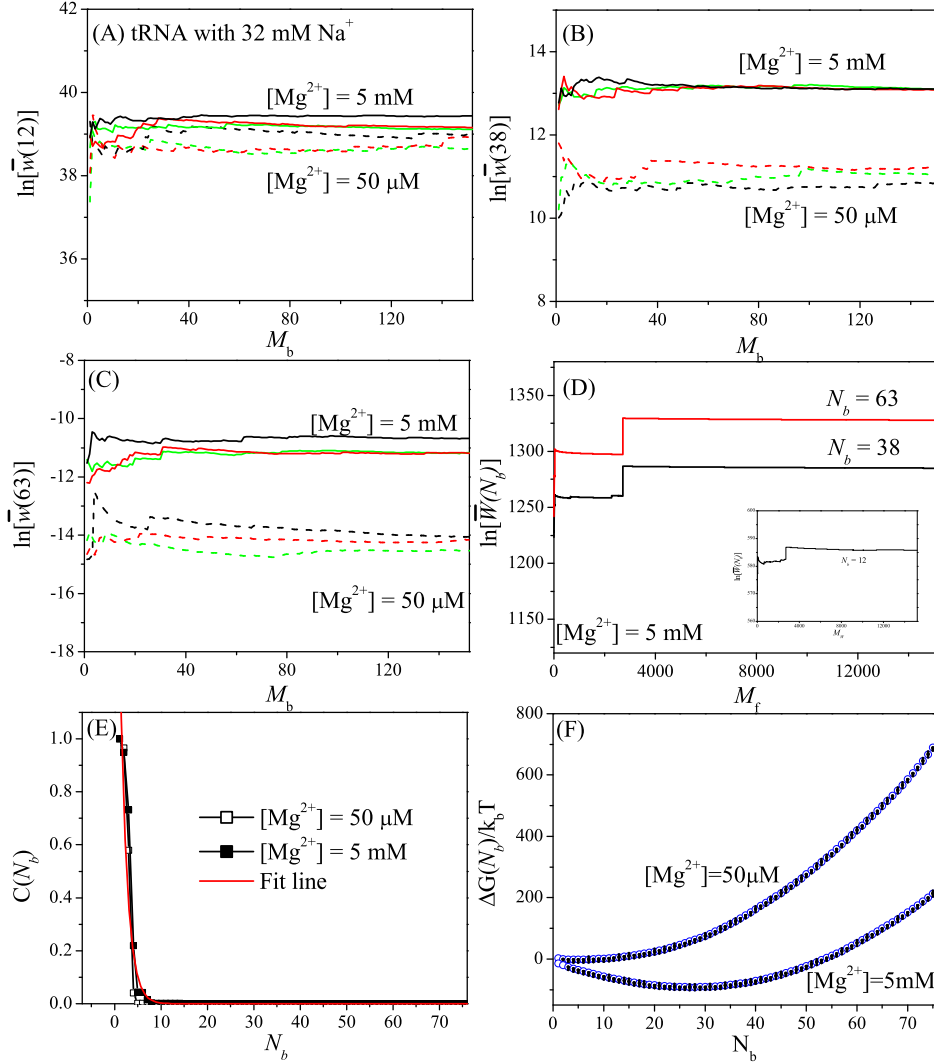


Figure S3: Tests for the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using tRNA. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 1.5 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

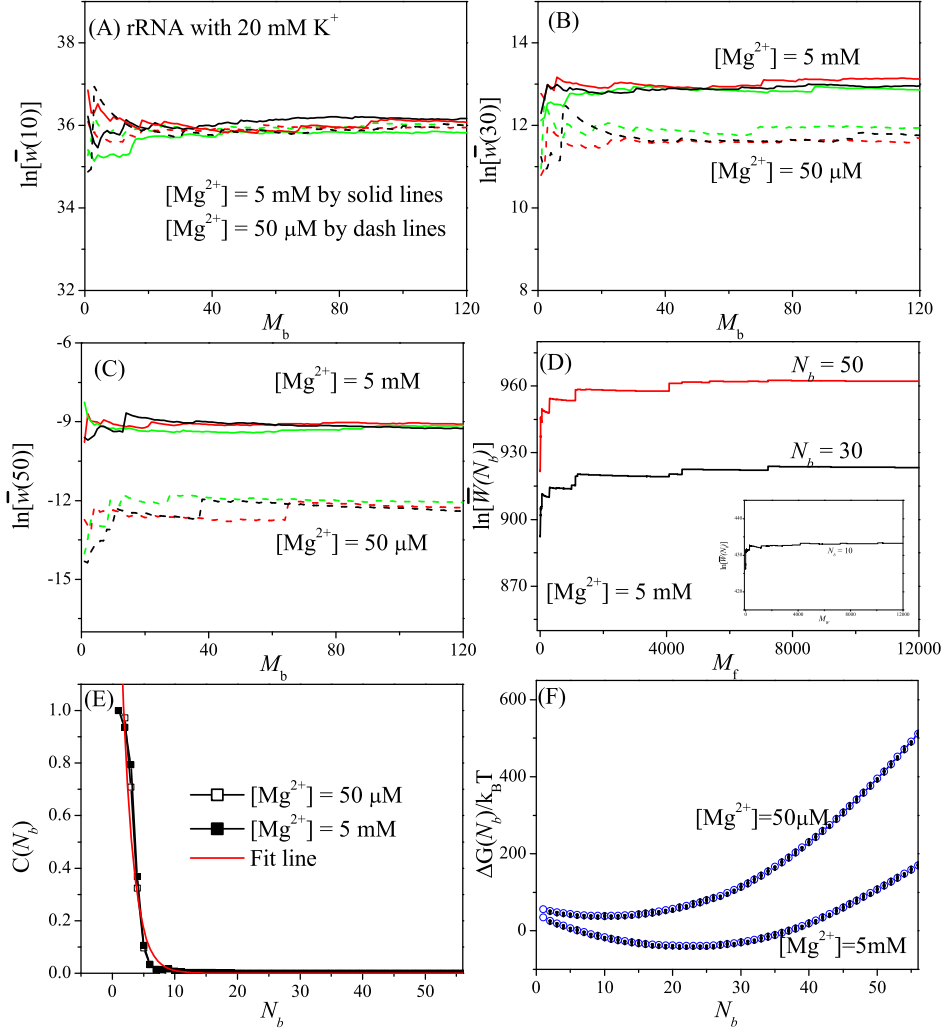


Figure S4: Tests for the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using rRNA. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 1.8 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

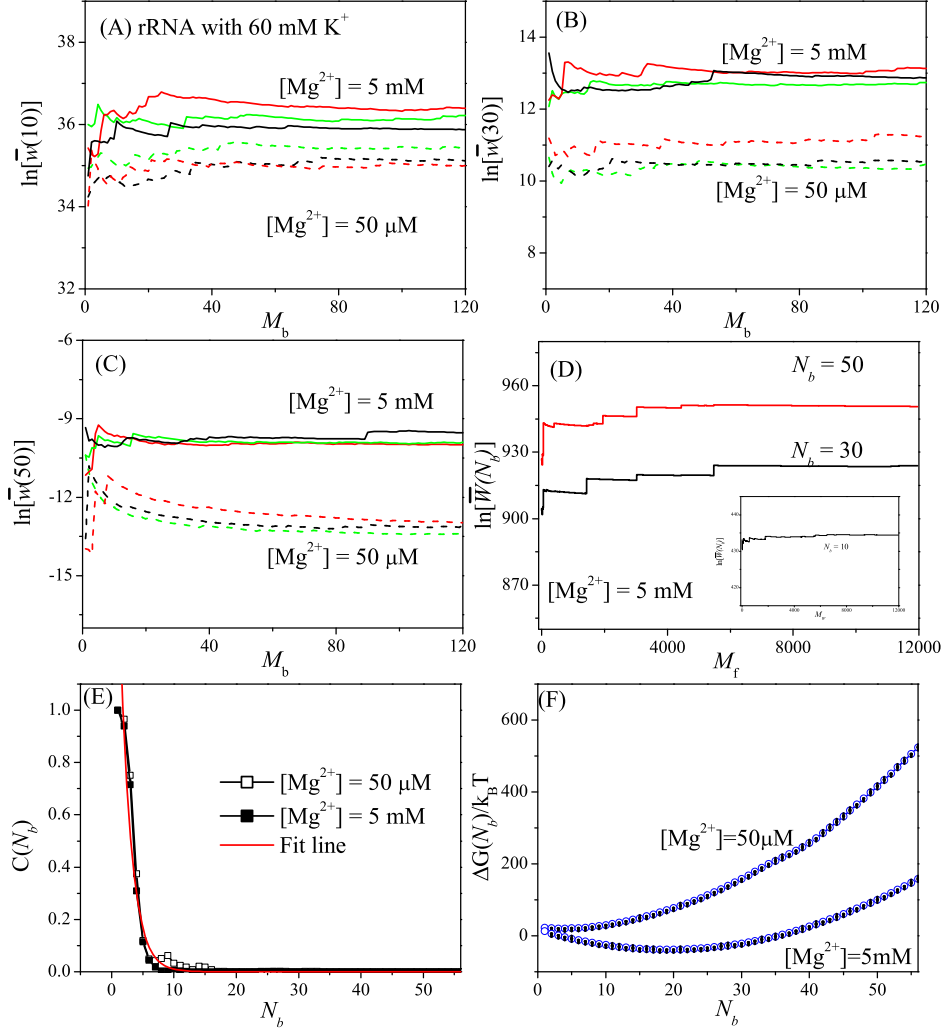


Figure S5: Tests for the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using rRNA. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 1.8 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

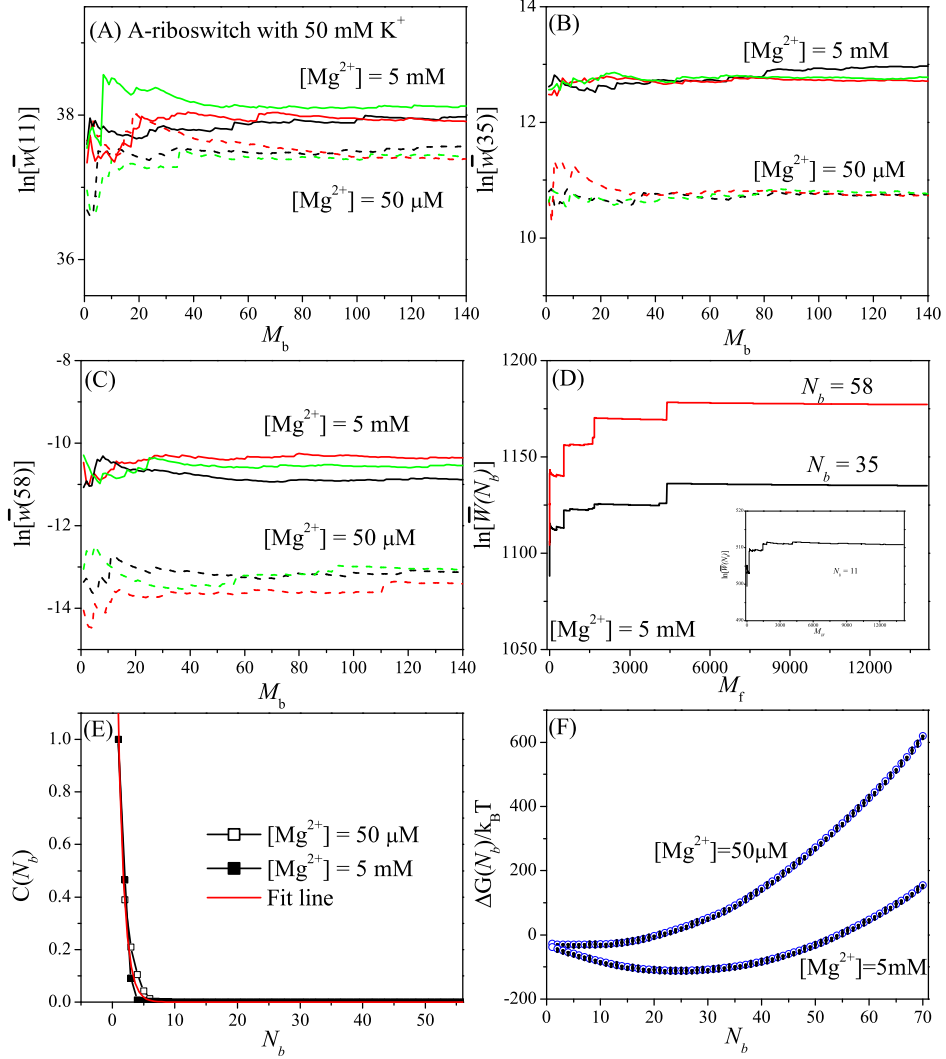


Figure S6: Tests for the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using A-riboswitch RNA. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 1.0 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

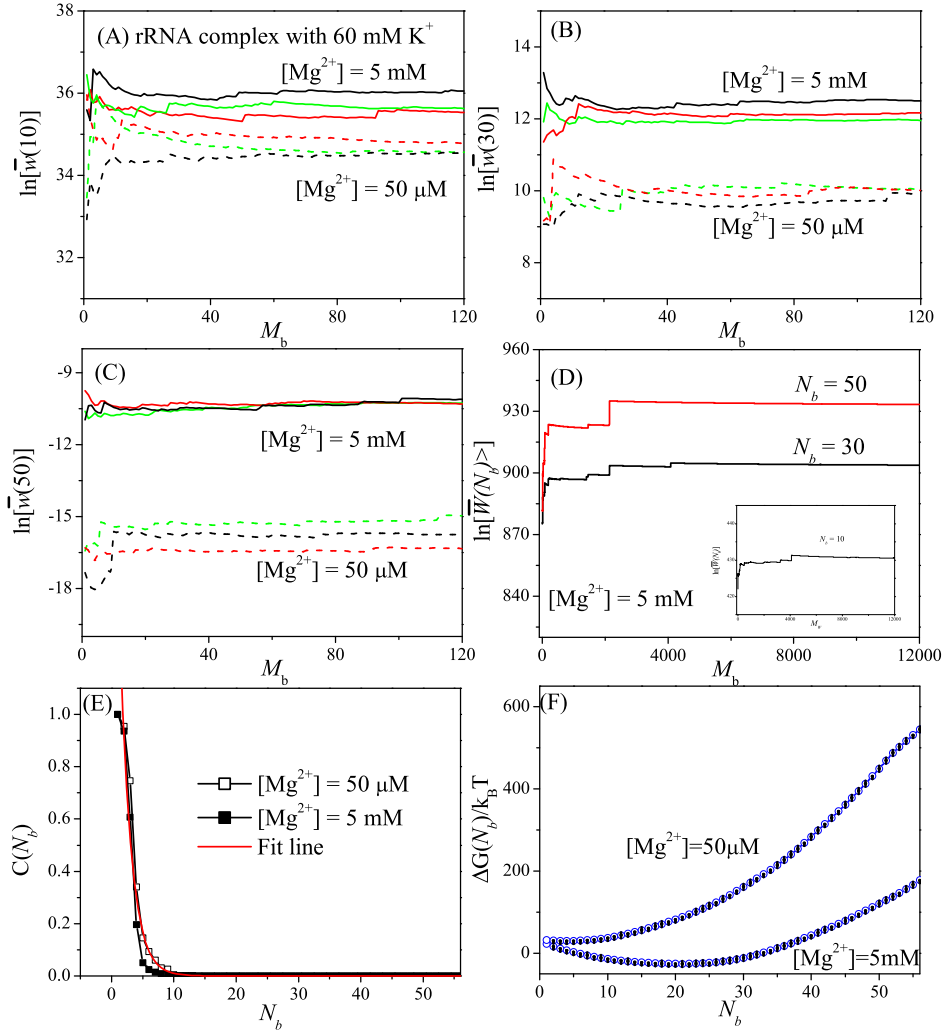


Figure S7: Tests for the robustness of the Monte Carlo sampling in the “insertion-deletion” algorithm using rRNA-protein complex. (A) $i = N_p/6$, (B) $i = N_p/2$, and (C) $i = 5N_p/6$ show the test results for the deletion process. (D) and the inset in (D) show the results for the Monte Carlo sampling of the insertion process. Here we adopt $N_b = N_p/6$ (inset), $N_b = N_p/2$ (black line), and $N_b = 5N_p/6$ (red line). (E) Correlation ($C(N_b)$) between the statistical weights before and after the deletion step. The characteristic correlation-specific TB ion number $N_b^{(\text{corr})}$ is found to be 1.8 for this system. (F) The free energy $\Delta G(N_b)$ as a function of N_b . The error bar shows the fluctuation for the different Monte Carlo samples of the TB ion distribution.

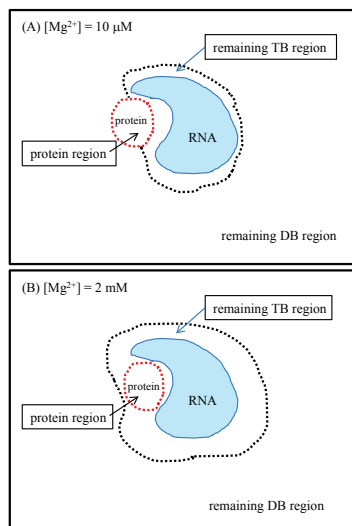


Figure S8: A schematic figure for the different regions for high and low Mg^{2+} concentrations, respectively. The region around the red dotted line is the location of the protein (the “protein region”). The region around the black dotted line is the TB region excluding the protein region and is called the “remaining TB region”. The rest region is called the “remaining DB region”. In (A), because the TB region is thin, part of protein region is in the DB region. The part of protein in the DB region belongs to the “remaining DB region”. In (B), the whole protein region is in the TB region.