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Supplemental Information

Hexahydrated Mg^{2+} Binding and Outer-Shell Dehydration on RNA Surface

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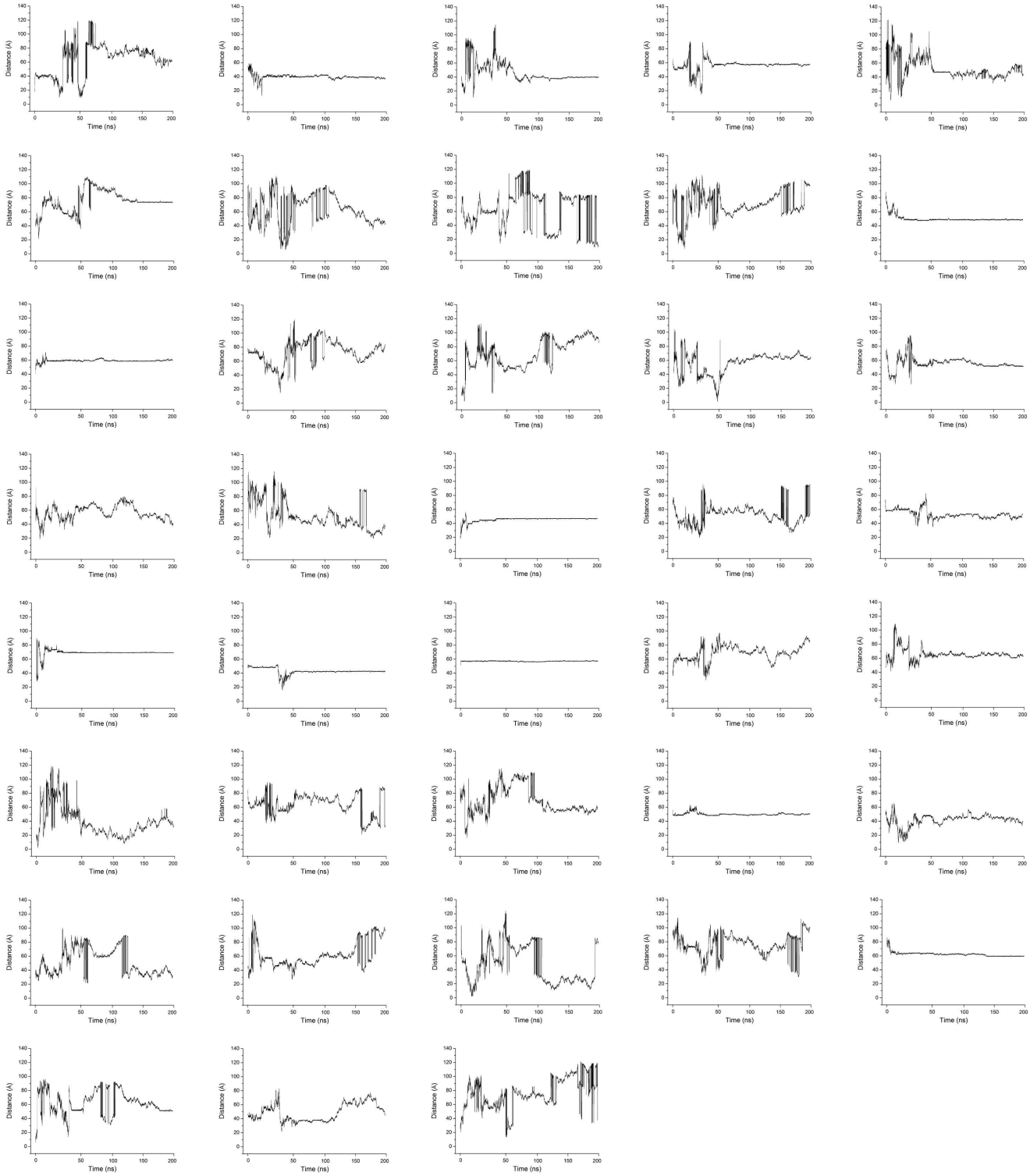

Figure S1: Coordinate variations (relative to the initial coordinates) of all the 38 Mg^{2+} ions in tRNA-water-ion solution system during a 200 ns MD simulation. Small coordinate variation indicates Mg^{2+} ion binding to the tRNA surface.

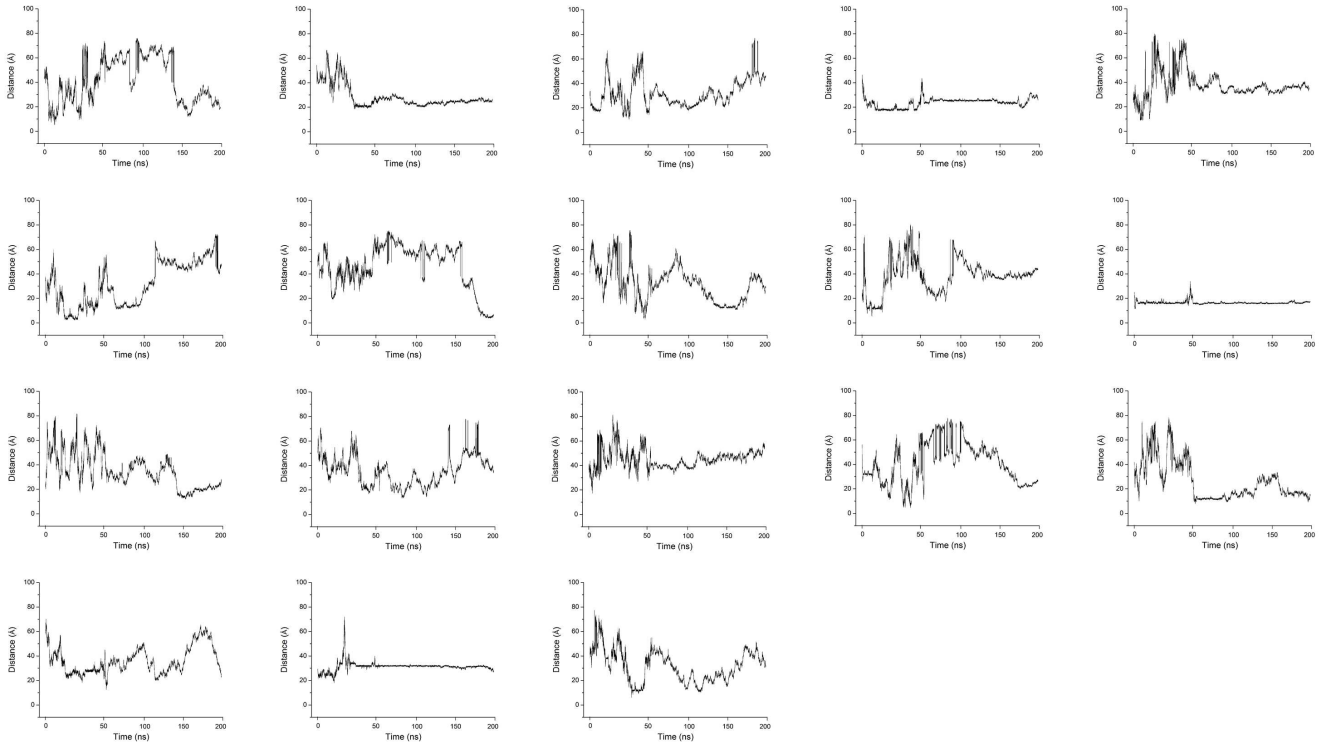

Figure S2: Coordinate variations (relative to the initial coordinates) of all 18 Mg^{2+} ions in mRNA-water-ion solution system during 200 ns MD simulation. Small coordinate variation indicates Mg^{2+} ion binding to the mRNA surface.

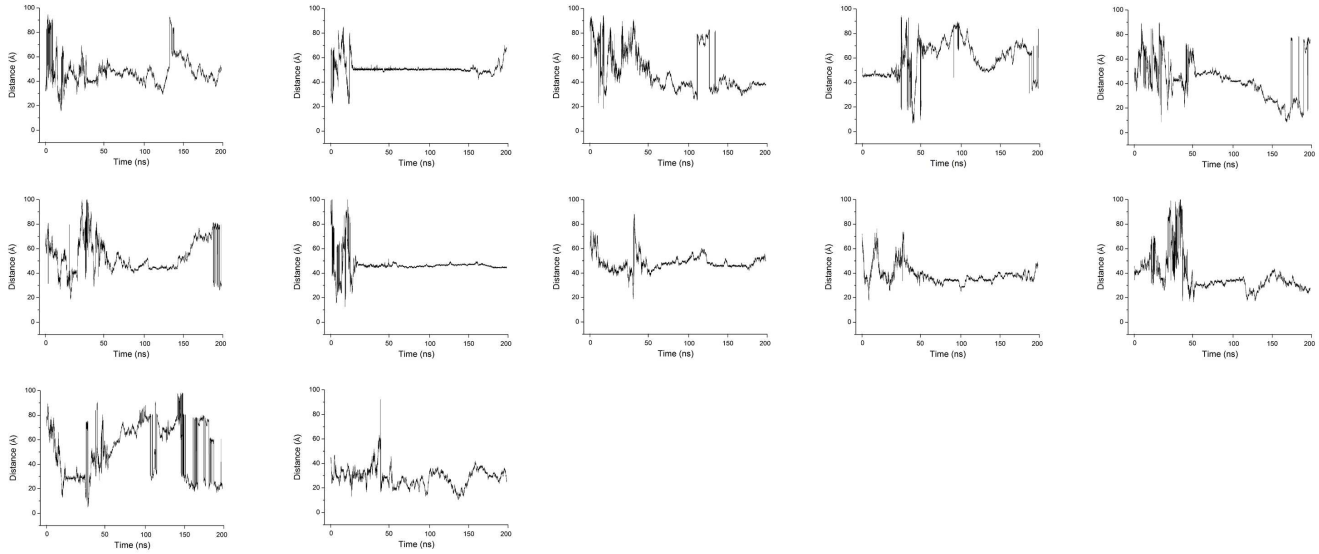

Figure S3: Coordinate variations of all the 12 Mg^{2+} ions in the BWYV RNA-water-ion solution system during the 200 ns MD simulation. Small coordinate variation indicates Mg^{2+} ion binding to the BWYV RNA surface.

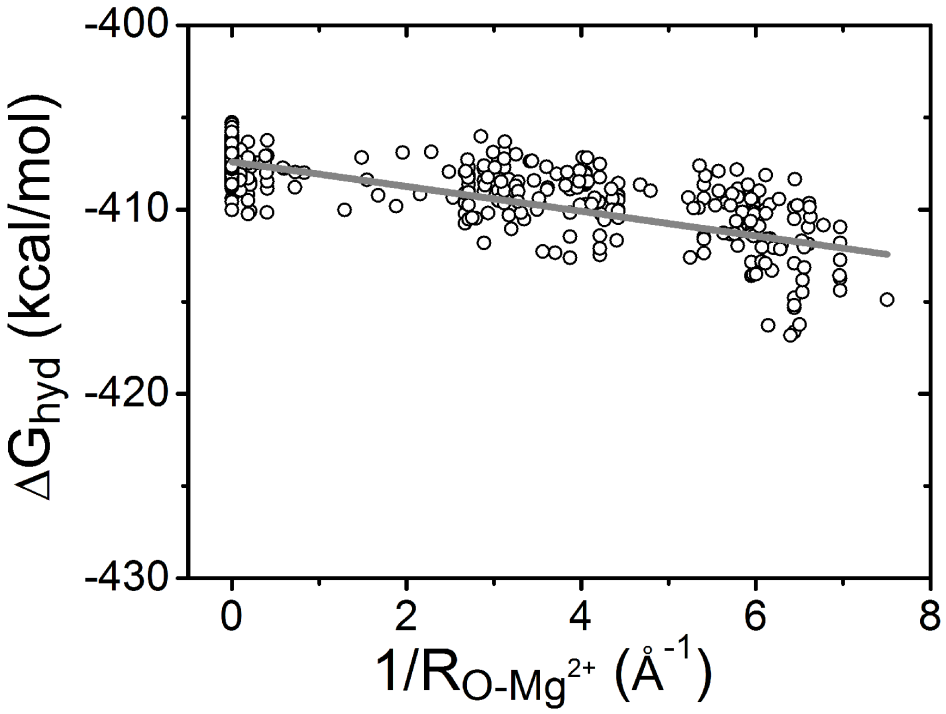

Figure S4: Relationship between the hydration free energy ΔG_{hyd} and $1/R_{O-Mg^{2+}}$ values of mRNA structure. The gray line is fitted by equation: ΔG_{hyd} = -0.67/$R_{O-Mg^{2+}}$-407.41.

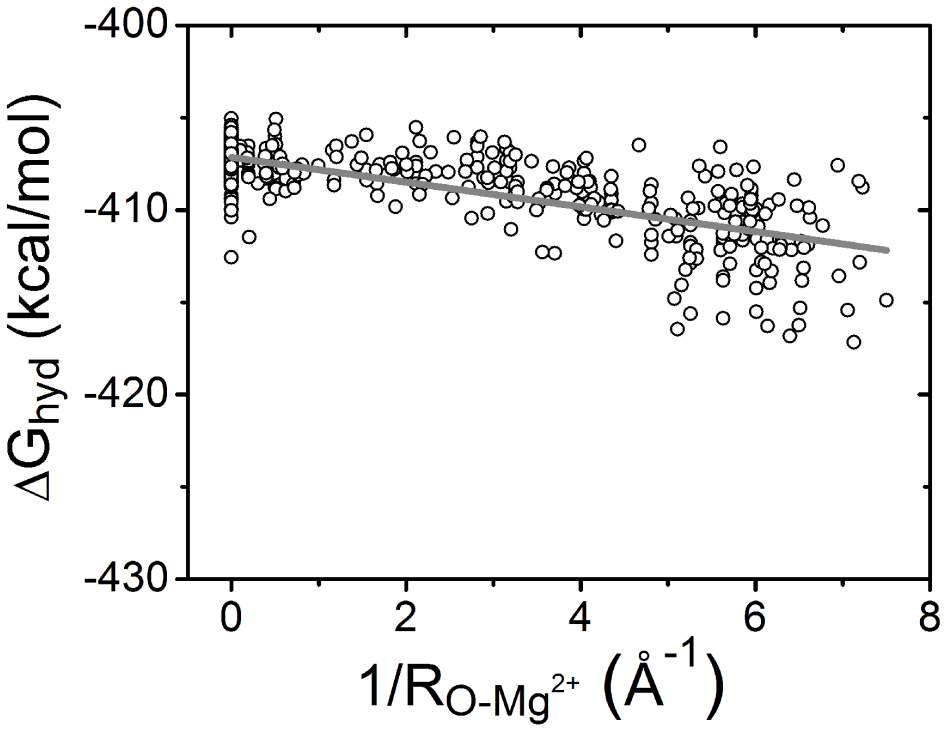

Figure S5: Relationship between the hydration free energy ΔG_{hyd} and $1/R_{O-Mg^{2+}}$ values of BWYV RNA structure. The gray line is fitted by equation: ΔG_{hyd} = -0.67/$R_{O-Mg^{2+}}$-407.26.

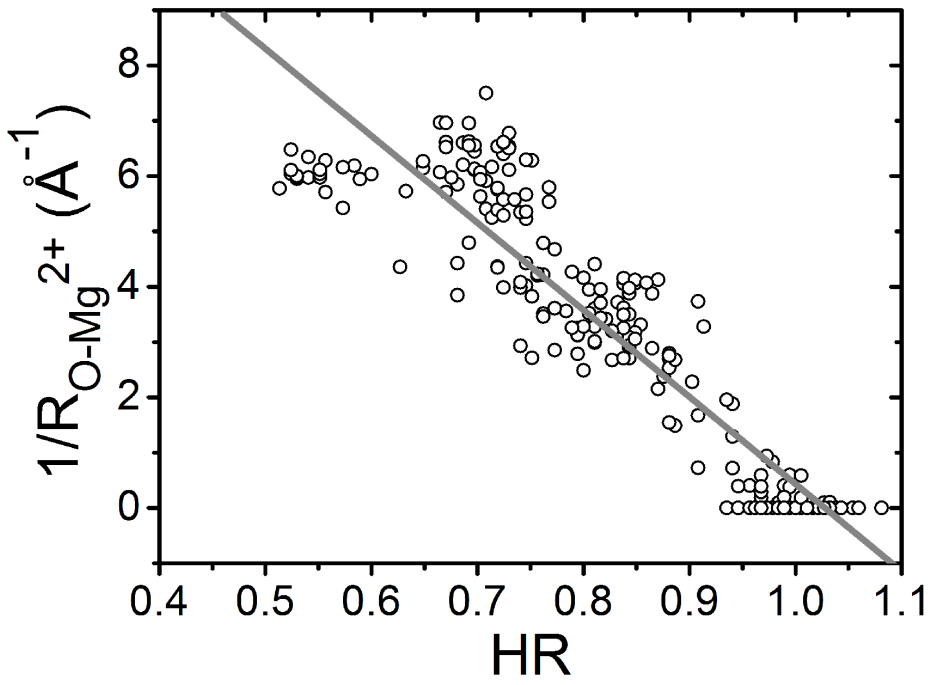

Figure S6: Relationship between $1/R_{O-Mg^{2+}}$ values and hydration ratio (HR) of mRNA structure. The gray line is fitted by equation: $1/R_{O-Mg^{2+}}$ = -15.74D_{hyd}+16.17.

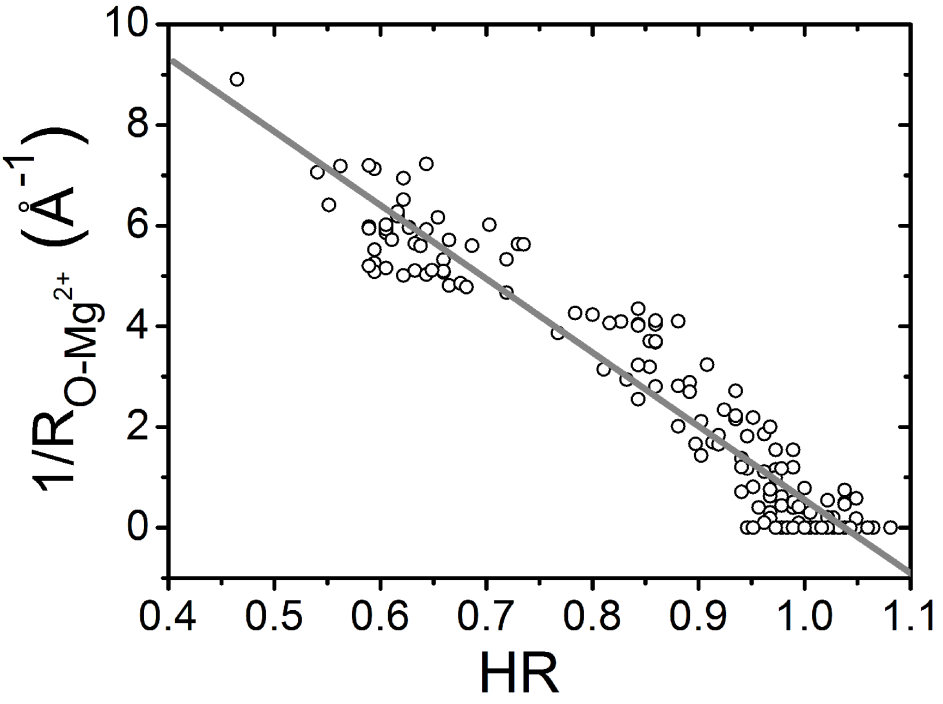

Figure S7: Relationship between $1/R_{O-Mg^{2+}}$ values and hydration ratio (HR) of BWYV RNA structure. The gray line is fitted by equation: $1/R_{O-Mg^{2+}}$ = -14.62D_{hyd}+15.18.