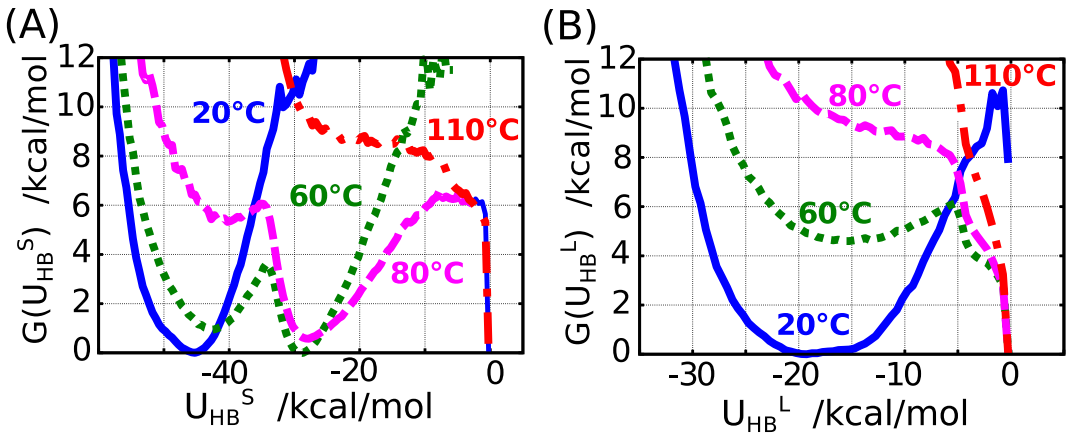

Figure S1: Free energy profiles of the hydrogen bond energy of two stems (A; $U_{\mathrm{HB}}^{\mathrm{S}}$) and two loops (stem-loop interactions) (B; $U_{\mathrm{HB}}^{\mathrm{L}}$) at $C = 500$ mM and $f = 0$.

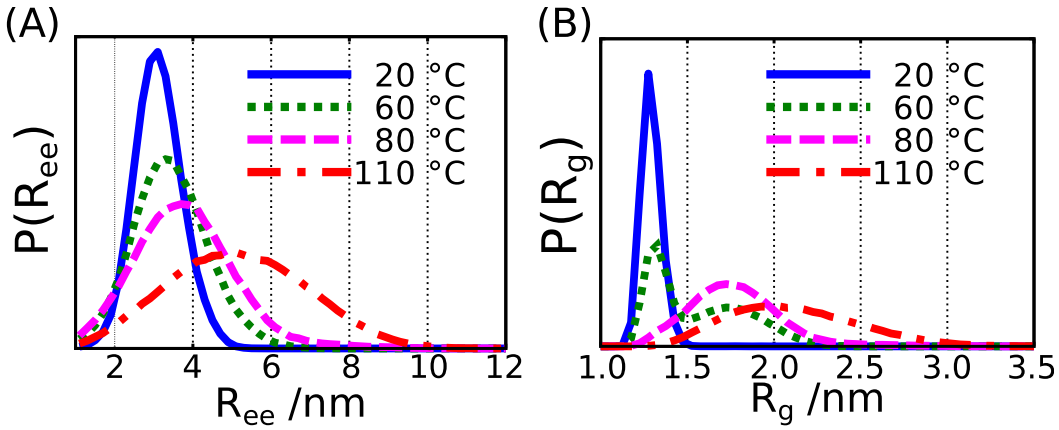

Figure S2: Probability distributions of the molecular extension (A; R_{ee}) and radius of gyration (B; R_{g}) at $C = 500$ mM and $f = 0$.

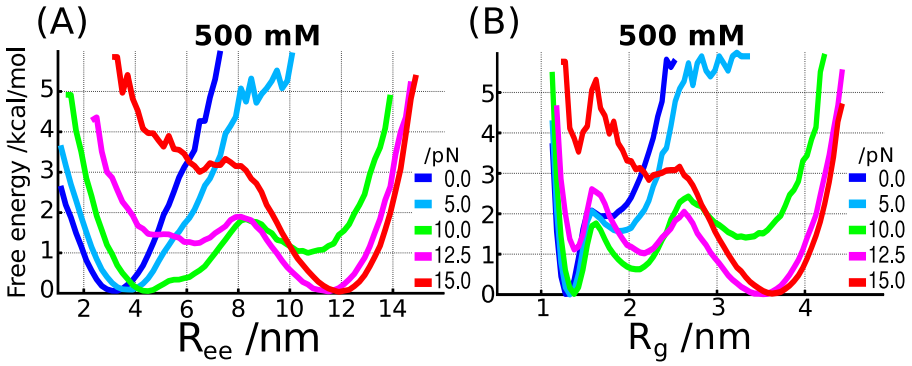

Figure S3: Free energy profiles as a function of R_{ee} (A) and R_{g} (B) at 500 mM of monovalent salt.

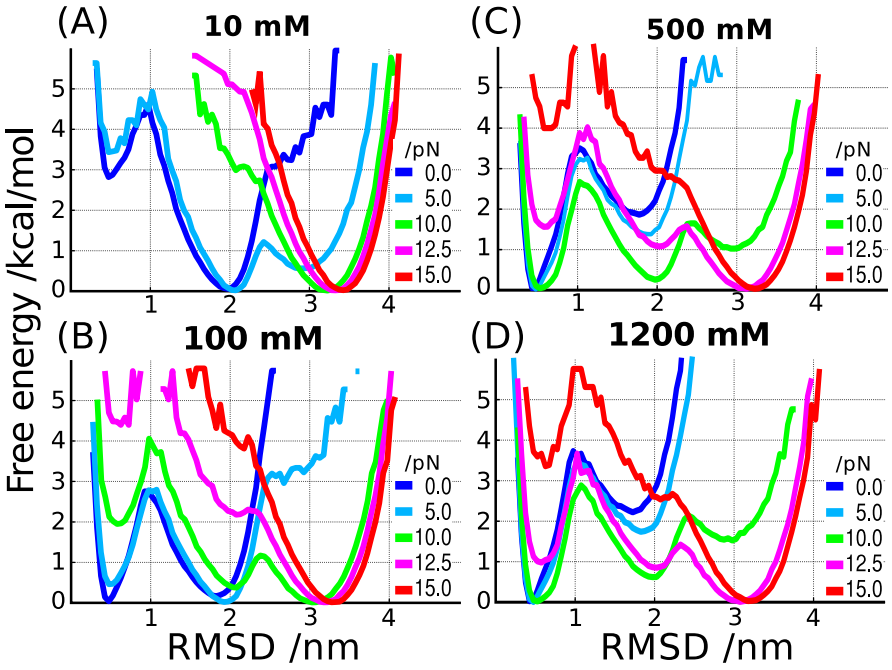

Figure S4: Free energy profiles as a function of RMSD at four different salt concentrations, 10 mM (A), 100 mM (B), 500 mM (C), and 1200 mM (D).

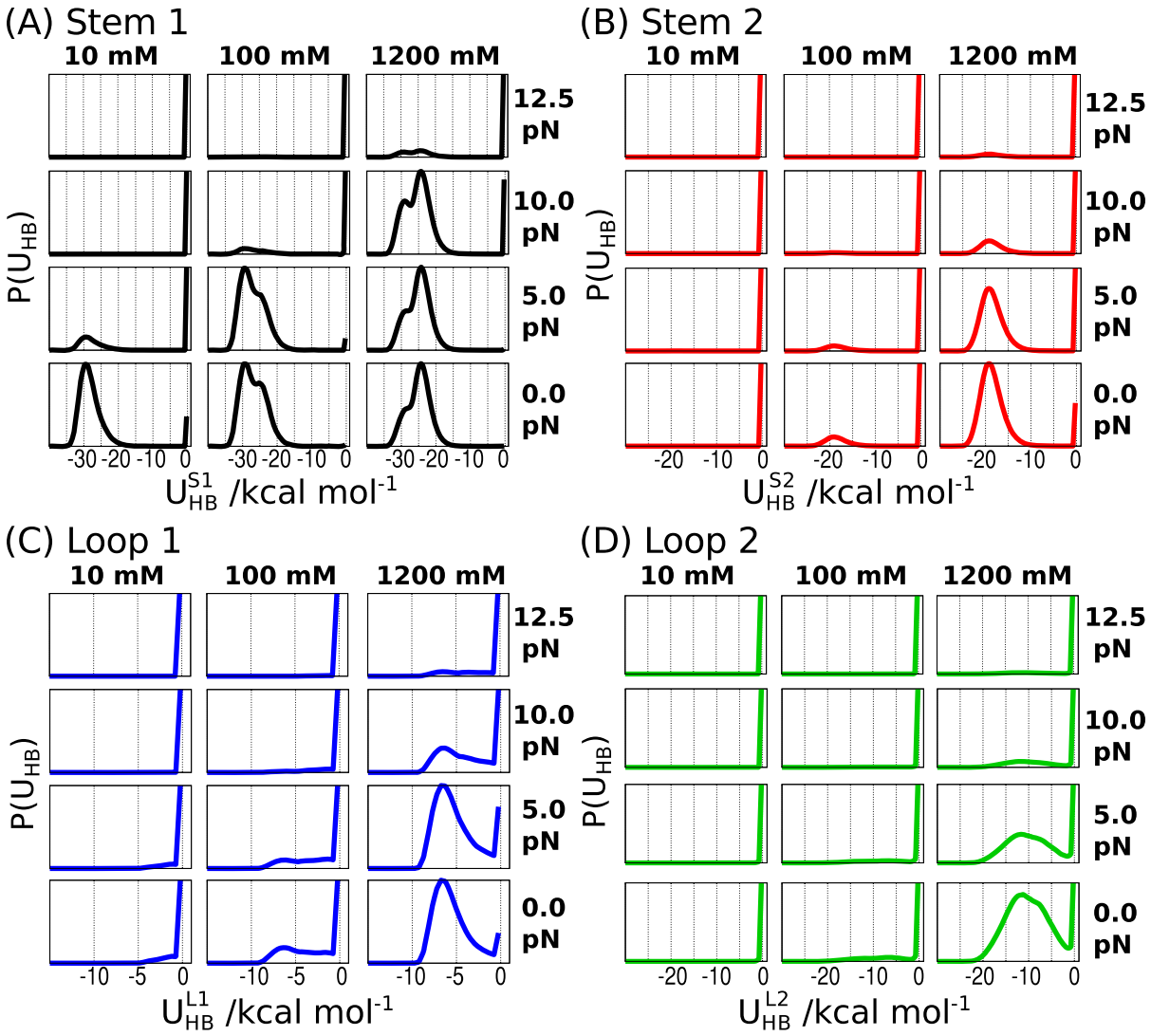

Figure S5: Probability distributions of hydrogen-bond energy. (A) Distribution of the total hydrogen bond energy. (B-E) Distributions of hydrogen bond energies for individual structural elements (B) Stem1; (C) Stem 2; (D) Loop 1 (E) Loop2. The salt concentrations and force values are explicitly indicated.

	Nucleotide pair	Interaction type (atoms)
1	C3b - G18b	canonical b.p.
2	G4b -C17b	canonical b.p.
3	C5b - G16b	canonical b.p.
4	G6b - C15b	canonical b.p.
5	G7b - C14b	canonical b.p.
6	C10b - G28b	canonical b.p.
7	C11b - G27b	canonical b.p.
8	G12b - C26b	canonical b.p.
9	G4b - A20b	N2 - N3
10	G4s - A20b	O2′ - N1
11	C5b - A20s	O2 - O2′
12	G6s - A21p	O2′ - OP1
13	G7b - A24b	N2 - N1; N3 - N6
14	C8b - G12b	N4 - N7; N3 - O6
15	C8b - A25b	O2 - N6
16	C8b - C26b	O2 - N4
17	C14s - A25b	O2′ - N1
18	C14b - A25b	O2 - N6
19	C15s - A23b	O2′ - N1
20	C15b - A23b	O2 - N6
21	G16b - A21p	N2 - OP2
22	G16s - A21b	O2′ - N7
23	C17N - A20s	O2 - O2′

Table S1: List of hydrogen bonding interactions in BWYV PK. First 8 pairs correspond canonical base pairs forming stems S1 and S2. Other 15 pairs are all tertially interactions forming either L1 or L2. Since we use the three-interaction-site model, a letter "s", "b" or "p" is put following each nucleotide number to indicate one of sugar, base, or phosphate, respectively.