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

Supplementary Information

Calculation of salt dependent free energy of binding of β-lactoglobulin homodimer formation and mechanism of dimer formation using molecular dynamics simulation and Three-dimensional Reference Interaction Site Model (3D-RISM): Diffuse salt ions and non-polar interaction between the monomers favour the dimer formation

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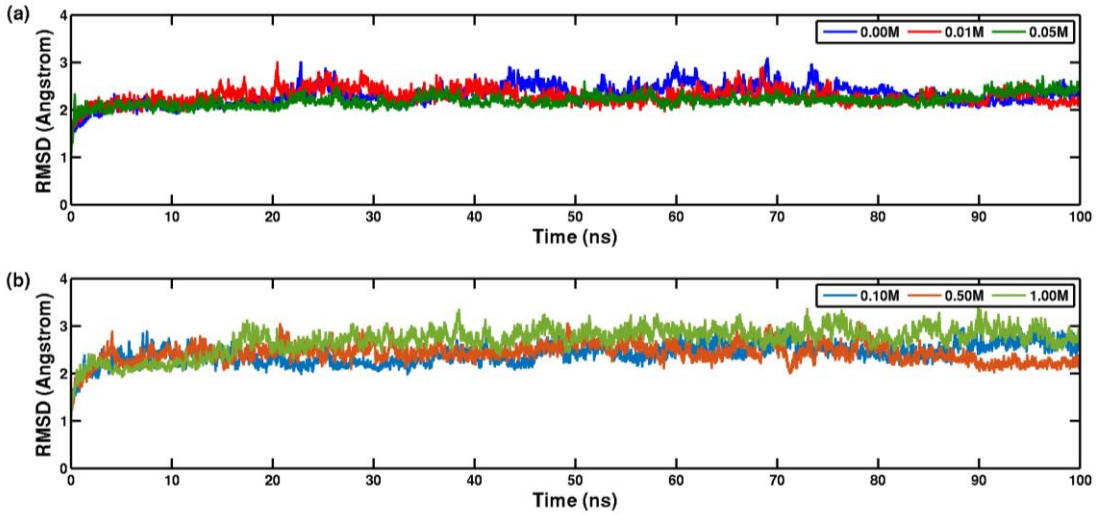

Figure S1. Root mean square deviation (RMSD) of β-lactoglobulin dimer (a) for 0.0, 0.01, 0.05 and (b) 0.10, 0.50 and 1.00M concentration of NaCl.

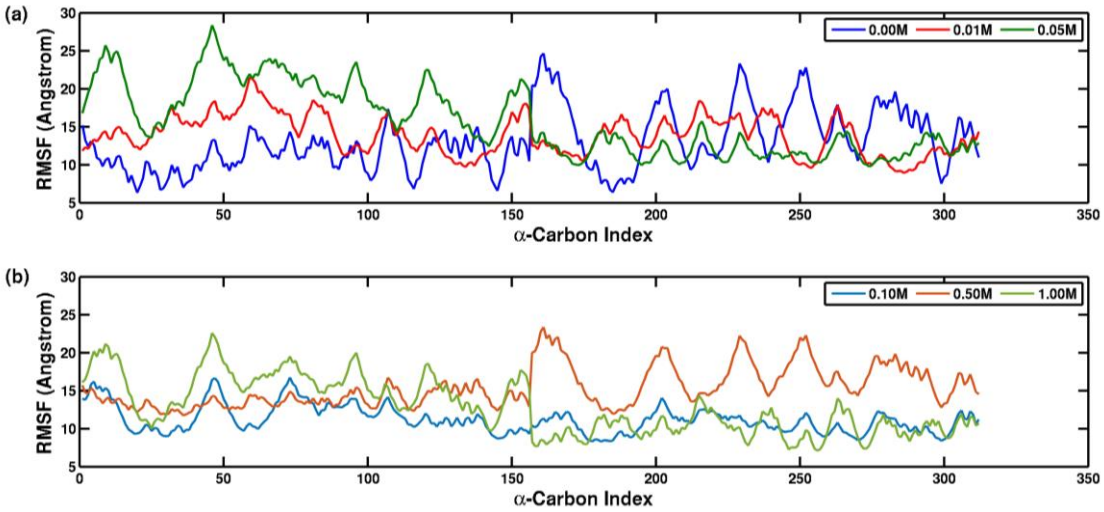

Figure S2. Root mean square fluctuation (RMSF) of β-lactoglobulin dimer (a) for 0.0, 0.01, 0.05 and (b) 0.10, 0.50 and 1.00M concentration of NaCl.

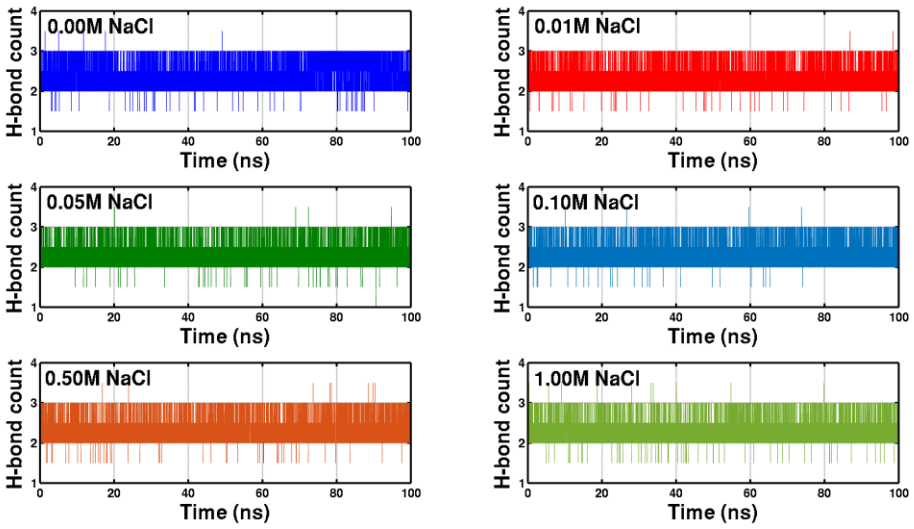

Figure S3: (a) Total H-bond count between D33 of one monomer and R40 of other monomer.

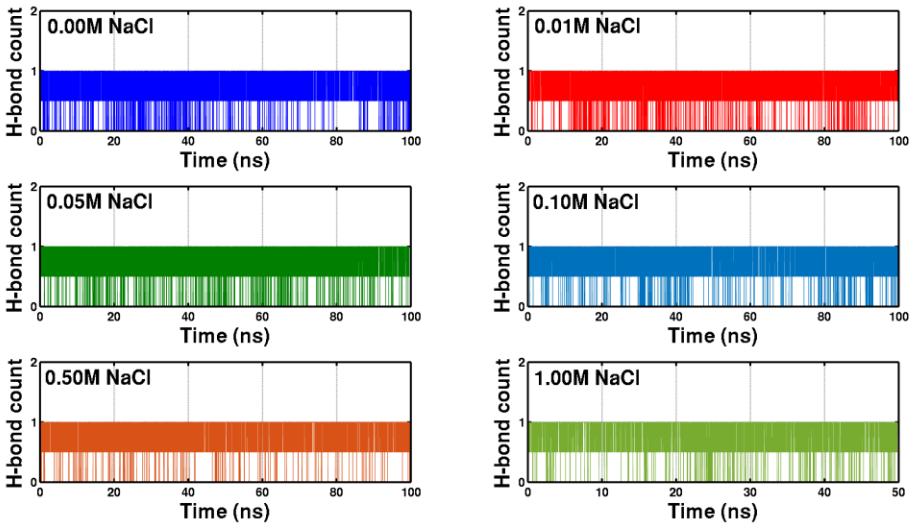

Figure S3: (b) Total H-bond count between D33 of one monomer and A34 of the other monomer.

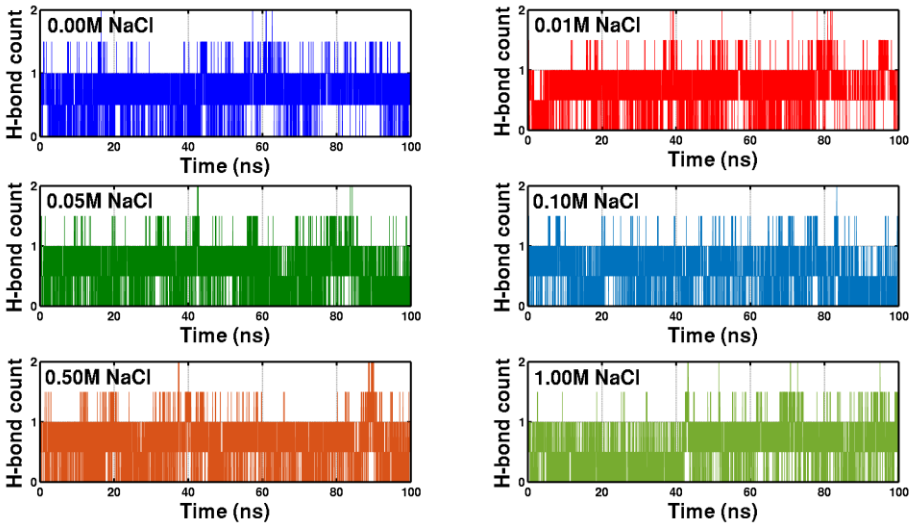

Figure S3: (c) Total H-bond count between H146 of one monomer and S150 of other monomer lying at the β-I-strands, at different salt concentrations.

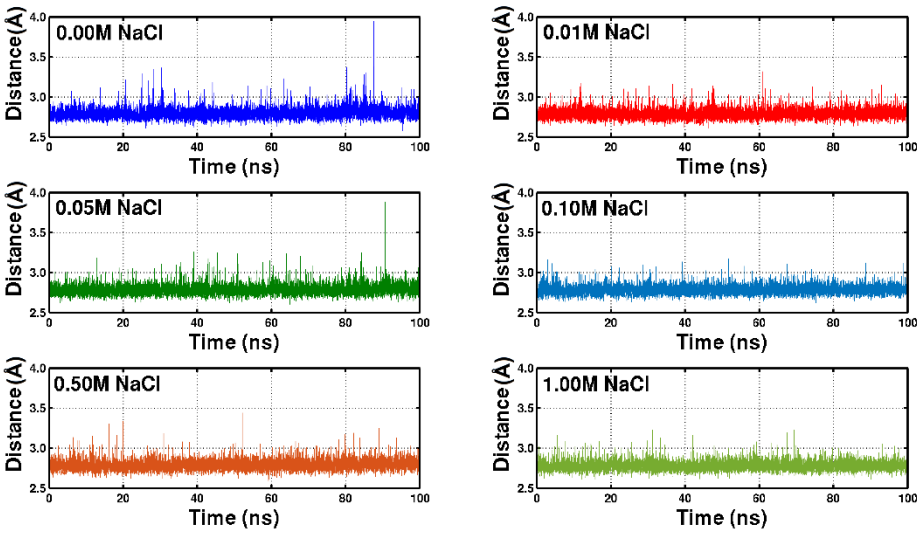

Figure S4: (a) Salt-bridge distance between D33 of one monomer and R40 of other monomer, both present in the AB loop region.

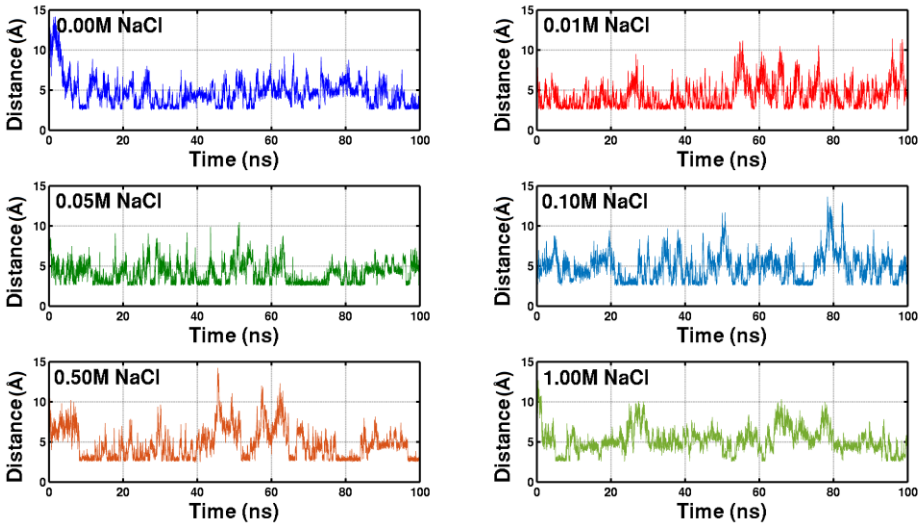

Figure S4: (b) Salt-bridge distance between E134 of one monomer and K141 of other monomer both present in the interface helix region, during 100ns simulation.

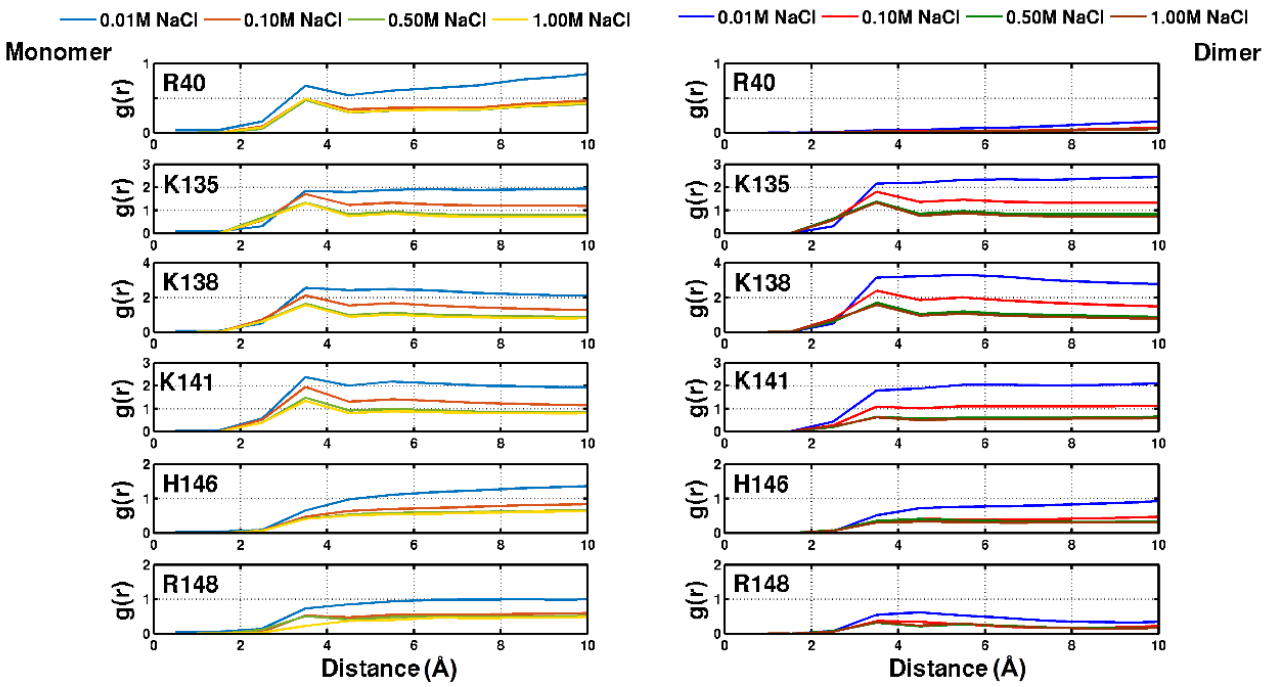

Figure S5: Pair correlation function between Cl^- ion and the center of the charged atom of the residues concerned.

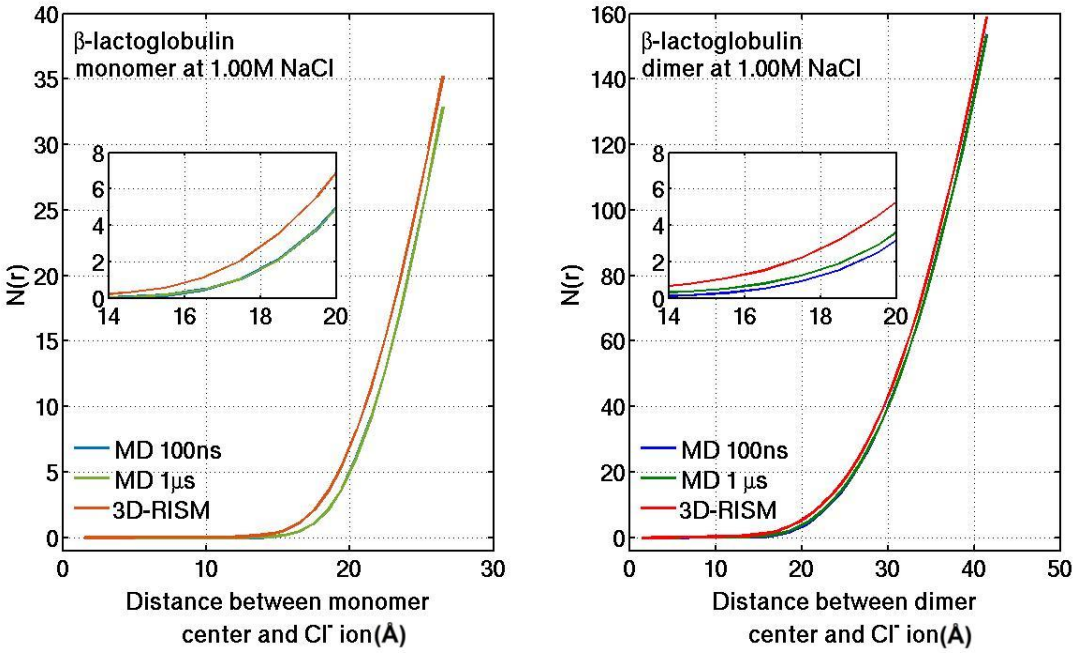

Fig S6: Variation of coordination number; N(r) of Cl^- ions from the center of the protein at 1.00M NaCl. For the monomer, there is essentially no difference between MD run of 100ns and 1 microsecond.

Table S1: The surface area of monomers and dimer obtained from MD simulation

NaCl Concentration	SASA monomer1 (Å2)	SASA monomer1 (Å2)	SASA dimer (Å2)
0.00M	7826.84 ± 192.32	7692.25 ± 191.78	14448.7 ± 248.79
0.01M	7998.94 ± 198.52	7653.86 ± 202.14	14468.5 ± 358.11
0.05M	7858.82 ± 204.57	7618.01 ± 206.34	14261.7 ± 246.99
0.10M	7699.56 ± 218.60	7727.83 ± 209.72	14447.4 ± 247.47
0.50M	7973.66 ± 216.73	7589.46 ± 199.44	14449.7 ± 288.36
1.00M	7682.56 ± 209.75	7578.93 ± 193.41	14706.5 ± 226.58

Table S2: A comparative study of standard deviations in relative binding free energy (ΔΔA) (in kcal/mol) with the number of frames for β-lactoglobulin dimer.

Concentration of NaCl (in M)	ΔΔA (for $T1_c$) for 25 frames	ΔΔA (for $T1_c$) for 50 frames
0.01	-8.11 ± 7.04	-8.76 ± 6.25
0.05	-11.53 ± 8.29	-12.70 ± 8.11
0.10	-17.06 ± 7.28	-16.45 ± 7.62
0.50	-12.78 ± 8.34	-12.18 ± 8.17
1.00	-8.47 ± 8.28	-9.75 ± 7.87