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Supplementary Material

The Role of Metal Ions in Substrate Recognition and Stability of Concanavalin A: A Molecular Dynamics Study

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Figure S1. The plot showing RMSD between the crystal structure (1CVN) of ConA tetramer and the structures extracted from the trajectories of all the four simulations (E1 to E4) of the monomer (top), dimer (middle) and tetramer (bottom).

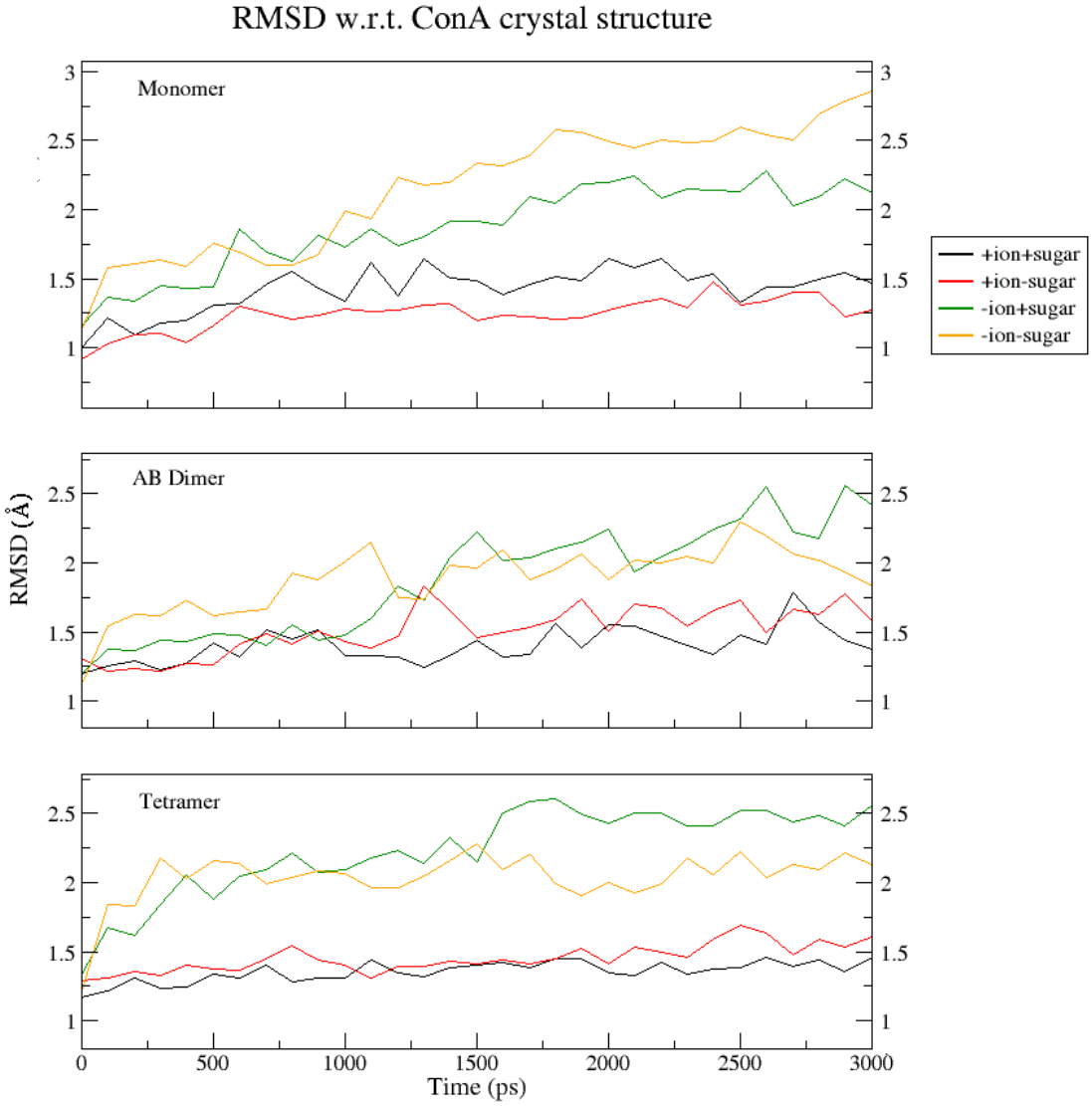

Figure S1

Figure S2. Plot depicting the variation of the radius of gyration for the monomer (top), AB dimer (middle), and tetramer (bottom) of ConA in various MD trajectories. Black, red, green and orange colored lines depict the results for E1, E2, E3 & E4 simulations, respectively.

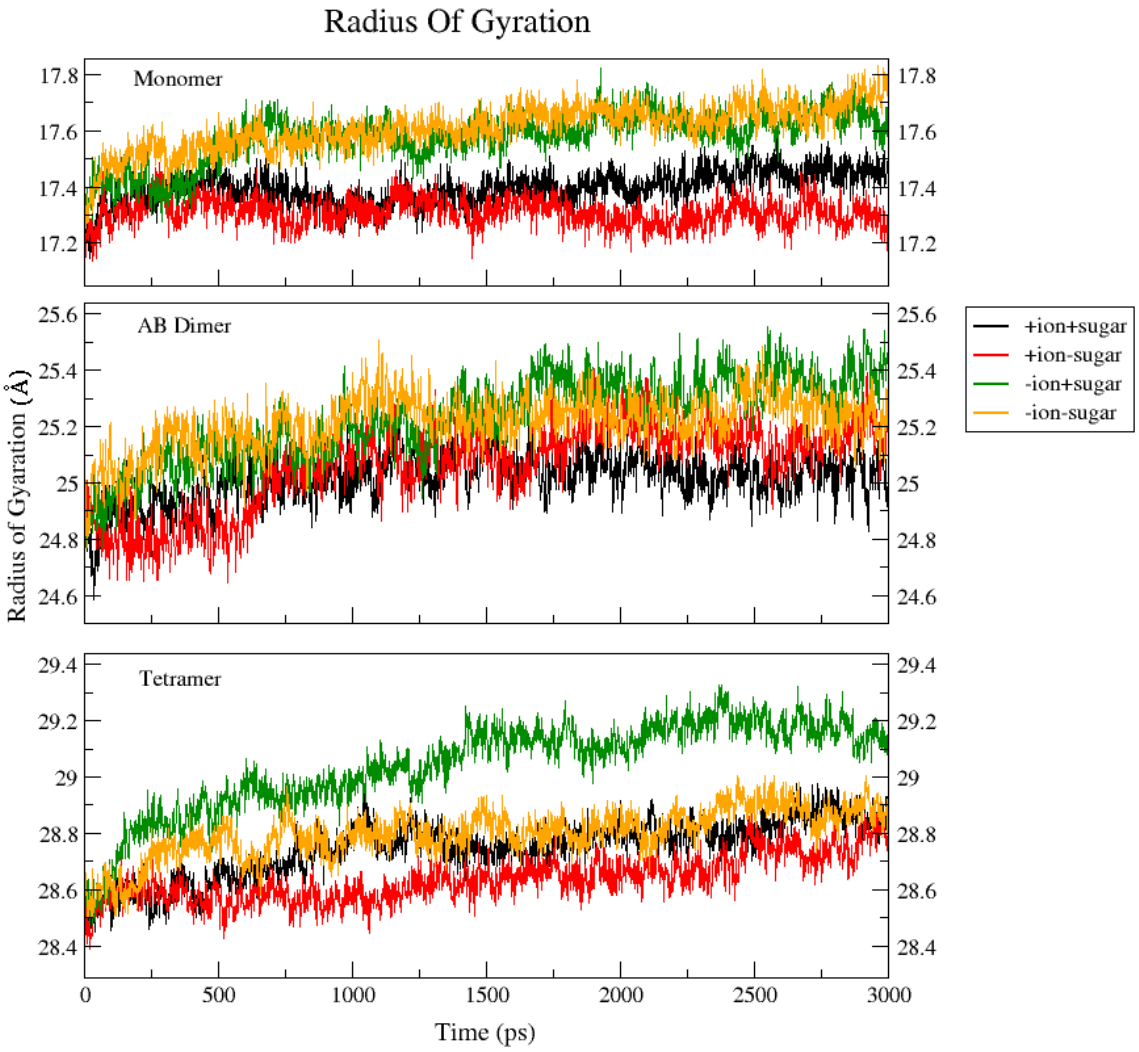

Figure S2

Figure S3. The plot showing the theoretical residue-wise BFs computed from the MD trajectories for (a) the four chains of ConA tetramer and (b) monomer and AB dimer during the four different simulation conditions, E1, E2, E3 and E4. The results from the four different simulations (E1, E2, E3, and E4) have been shown using black, red, green, and orange lines, respectively.

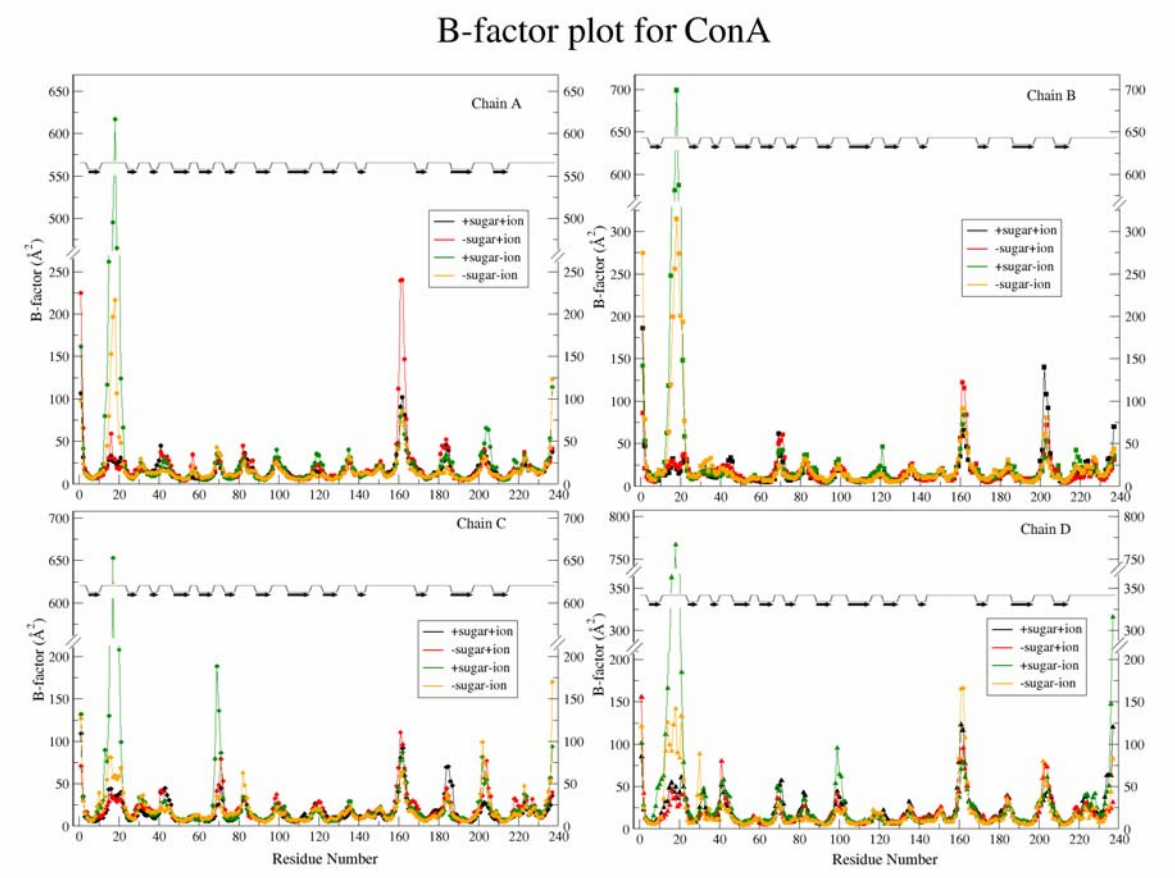

Figure S3 (a)

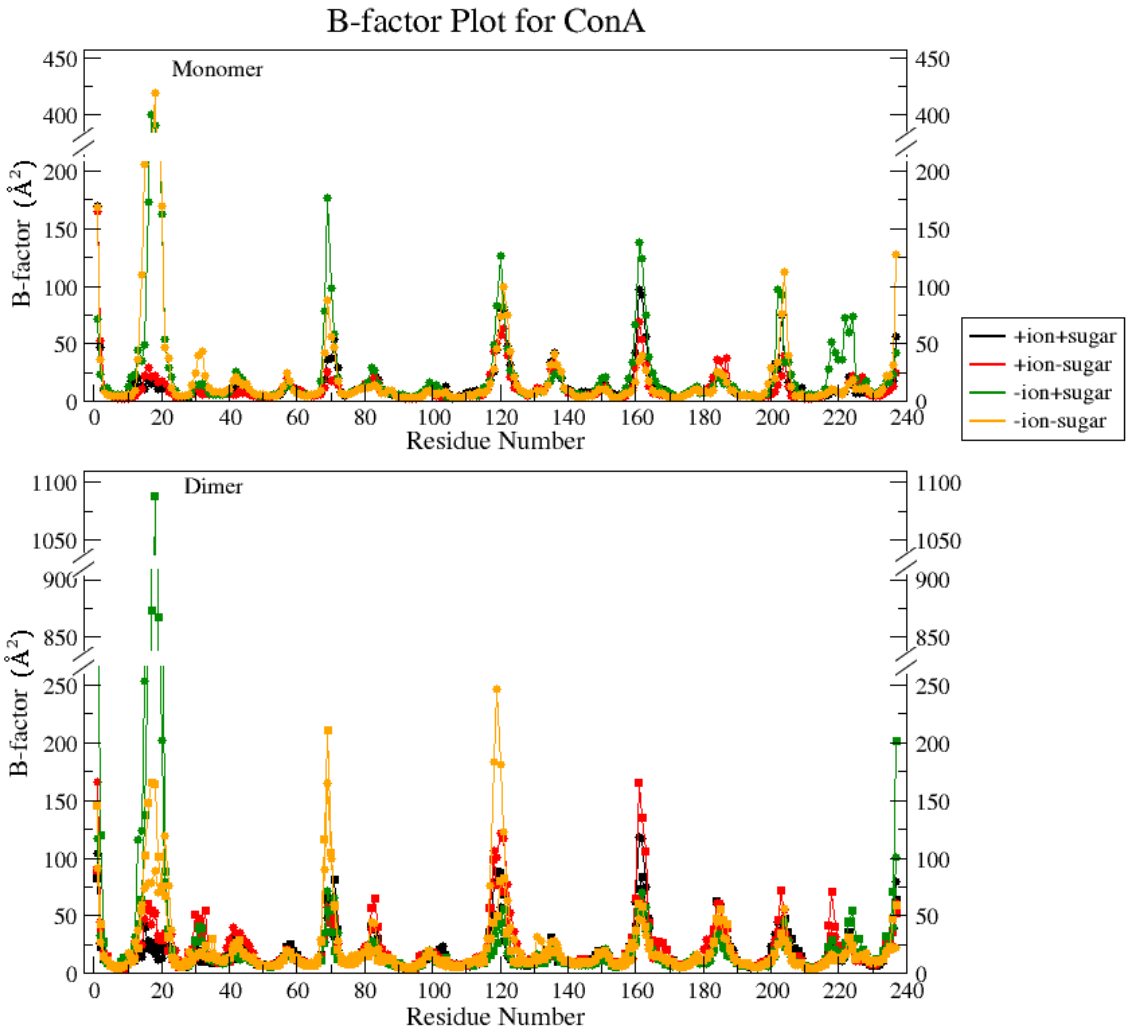
B-factor Plot for ConA
Monomer
Dimer
B-factor (Å²)
Residue Number
+ion+sugar
+ion-sugar
-ion+sugar
-ion-sugar

Figure S3 (b)

Figure S4. The variation of the non-polar solvent accessible surface area for ConA during the 3ns simulations have been shown for monomer (top), AB dimer (middle), and tetramer (bottom), respectively.

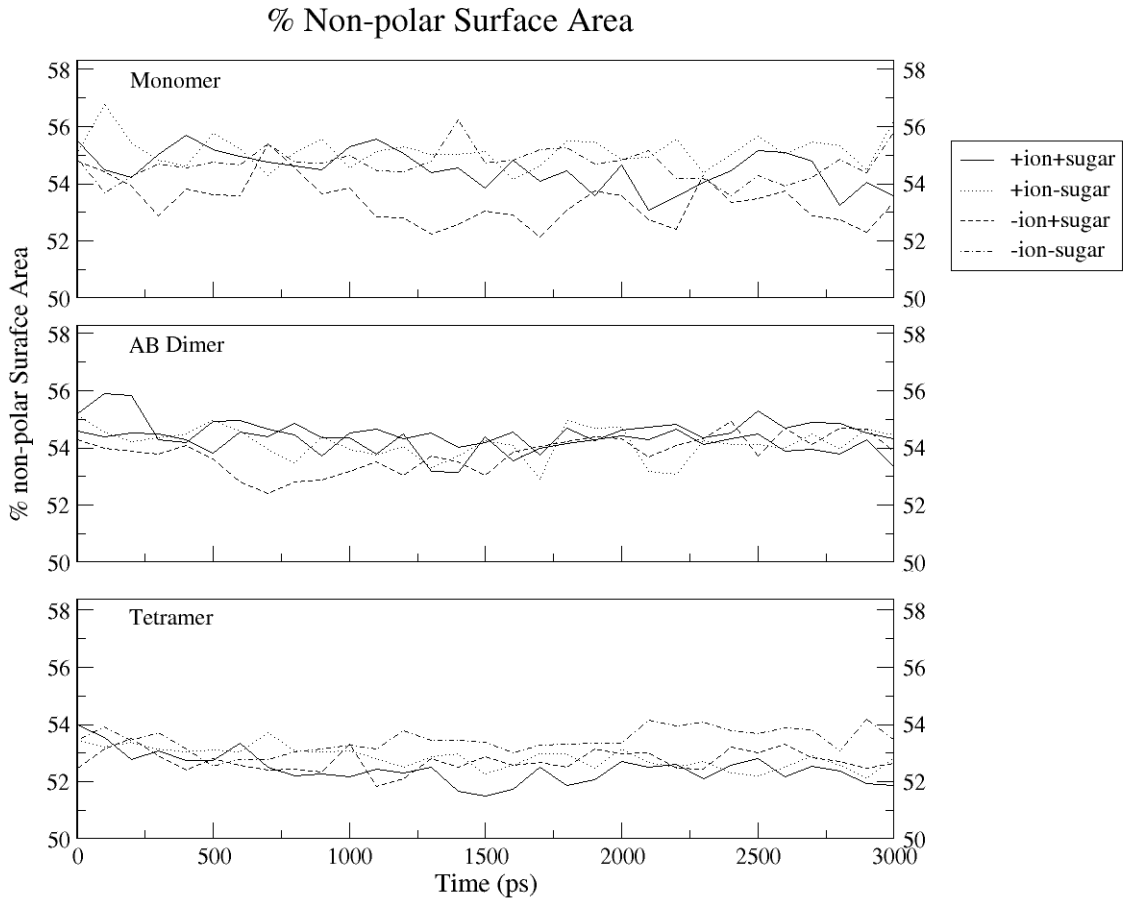

Figure S4

Figure S5. The total number of hydrogen bonds involving main chain and side chains in structures saved at an interval of 100 ps during the 3 ns simulations of monomer, AB dimer and tetramer of ConA. **(a)** main-chain to main-chain (M-M) hydrogen bonds **(b)** hydrogen bonds involving side chains (S-M/S). Both panels have used the same depiction scheme for different simulations as in previous figures.

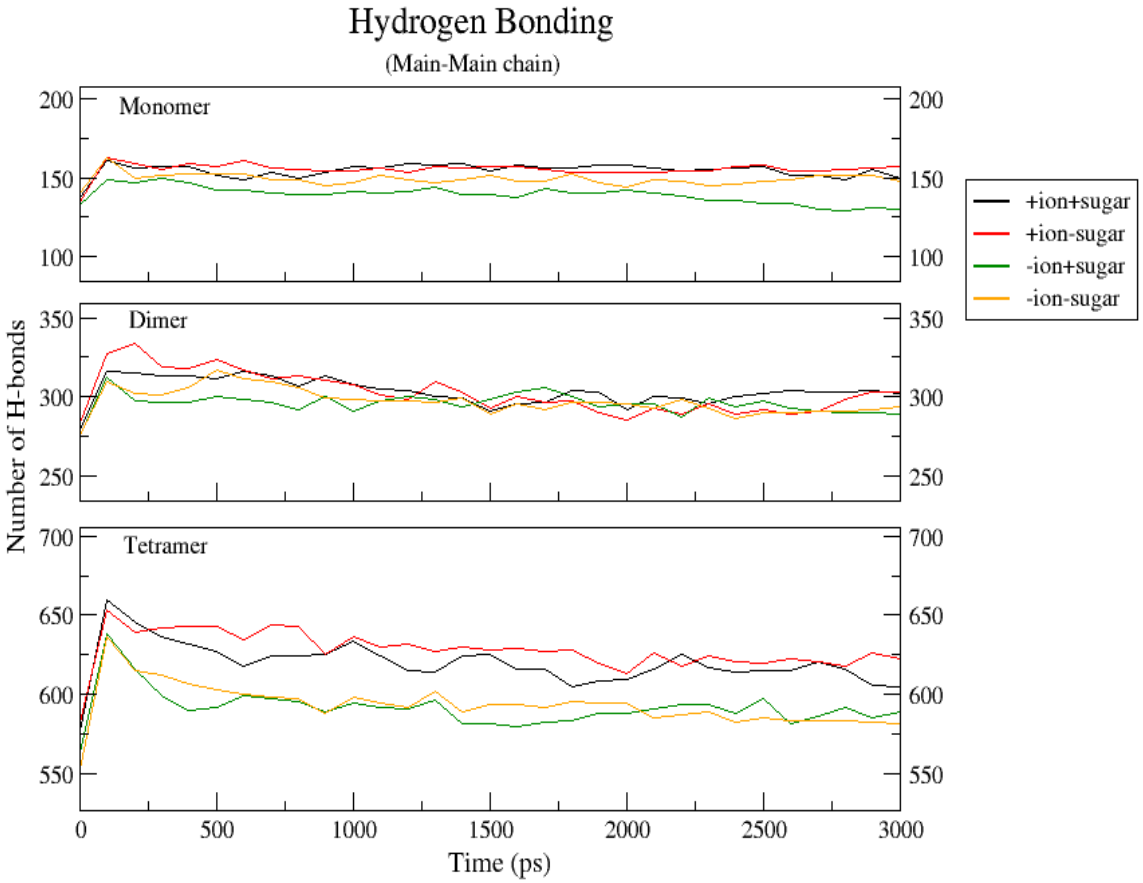

Figure S5 (a)

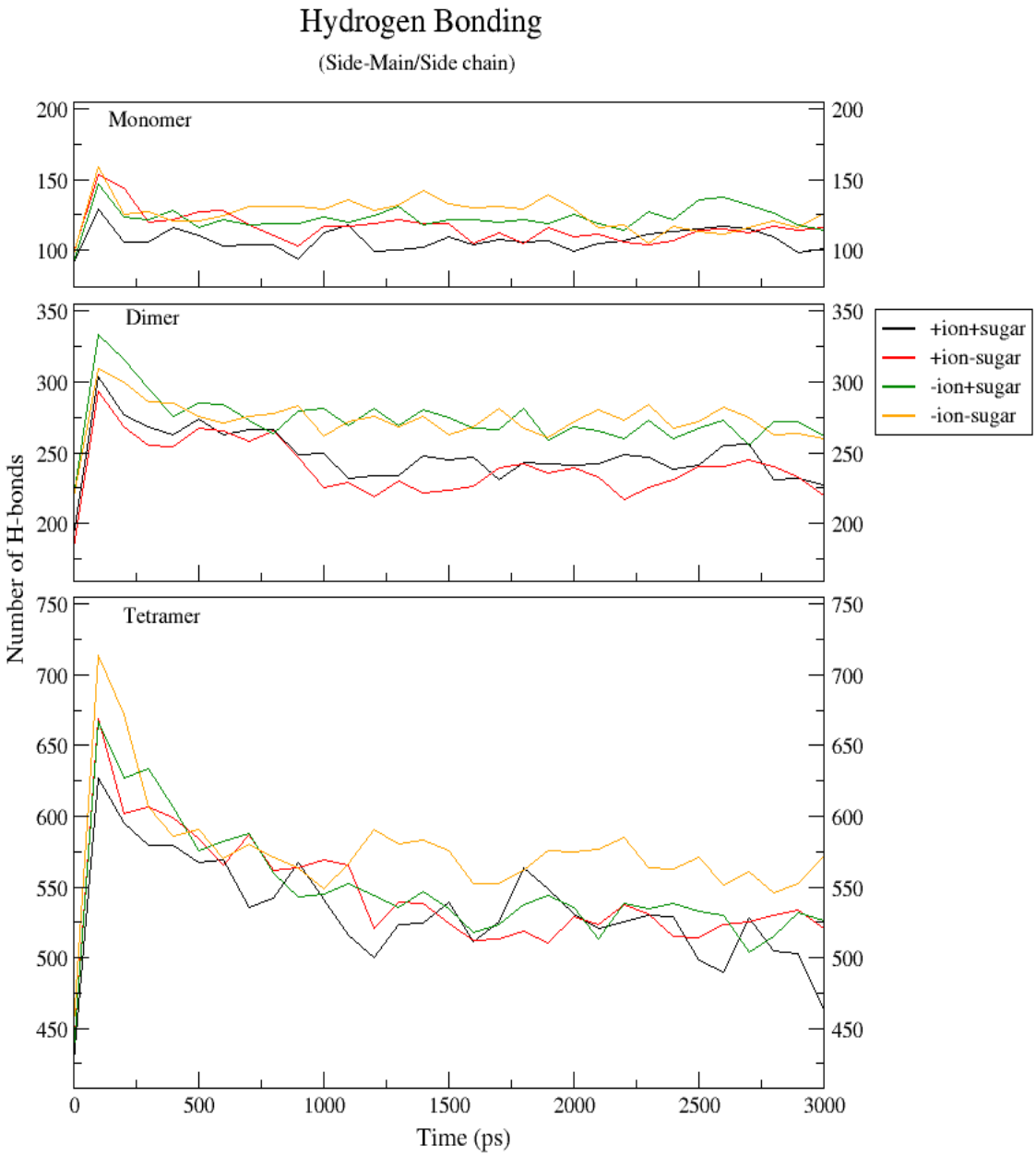
Hydrogen Bonding
(Side-Main/Side chain)
Monomer
Dimer
Tetramer
Number of H-bonds
Time (ps)
+ion+sugar
+ion-sugar
-ion+sugar
-ion-sugar

Figure S5 (b)

Figure S6. The percentage occupancy of various hydrogen bonds involving main chain and side chains in structures sampled at an interval of 100 ps during the 3 ns simulations of substrate bound ConA tetramer (top panel) in presence and (bottom panel) absence of the ions.

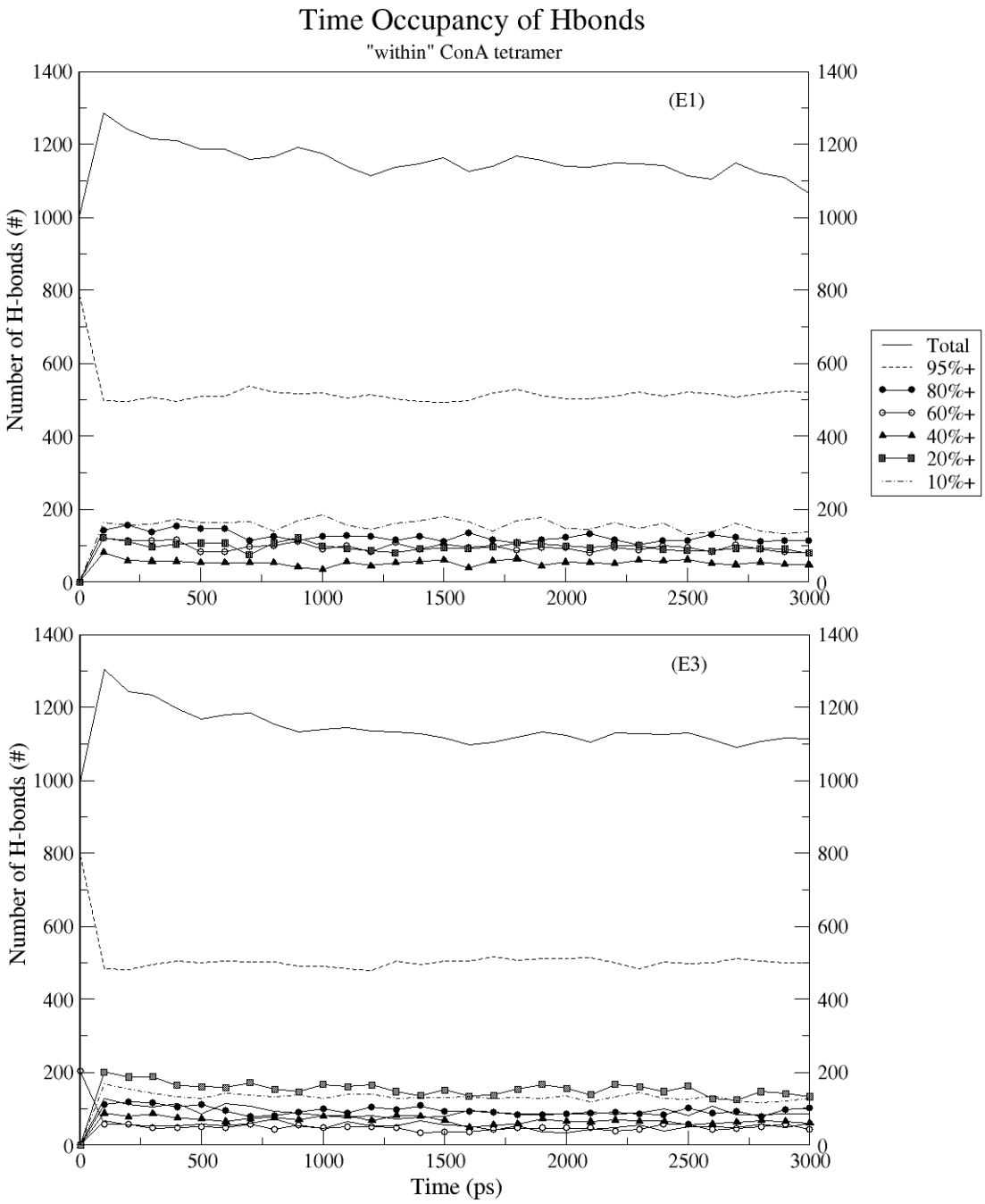

Figure S6

Figure S7. RMSD plot of the monomeric ConA for the 7ns simulations in absence of metal ions. The RMSD values for the loops, β-sheet core and whole protein have been plotted separately.

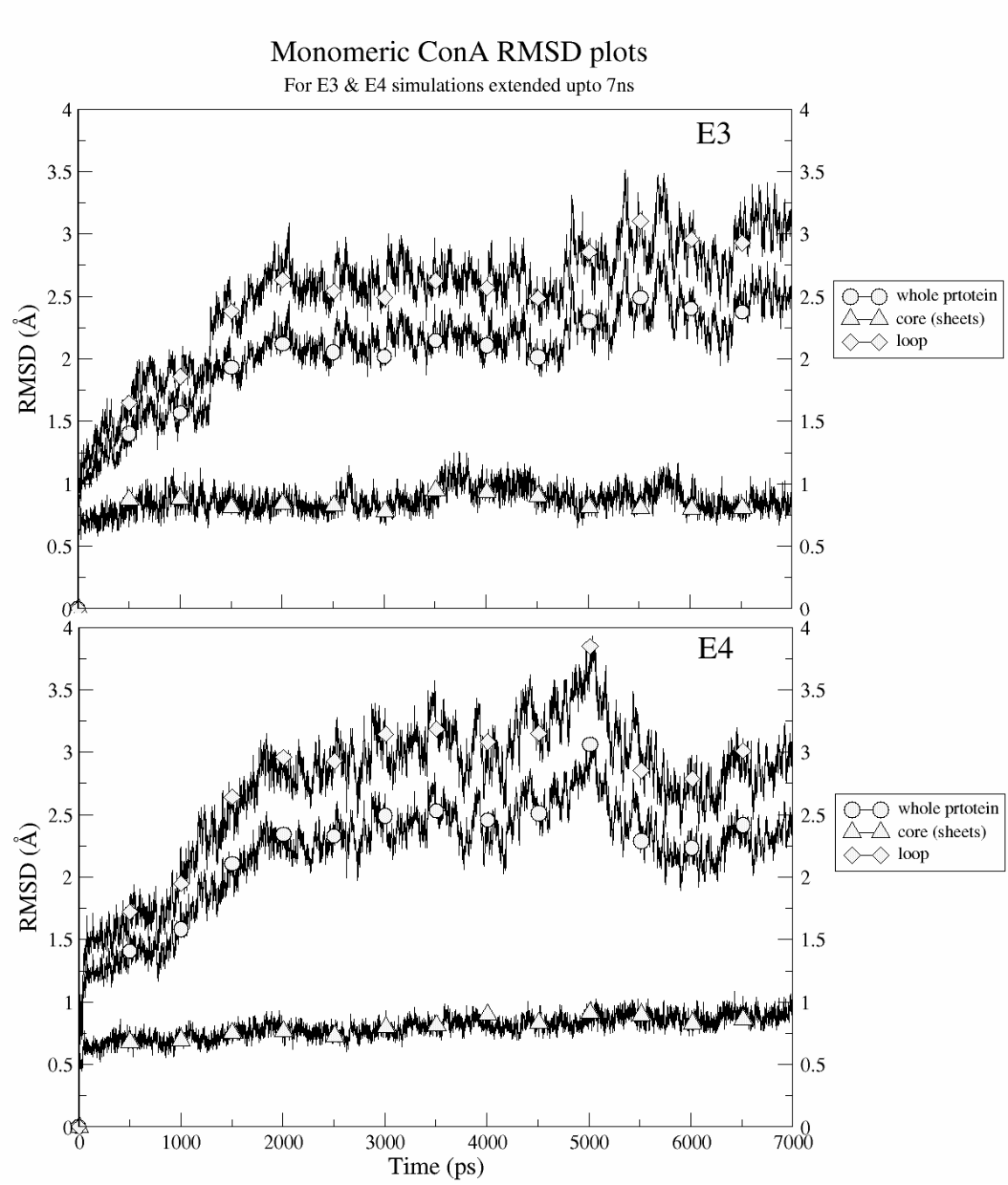

Figure S7

Figure S8. The residue-wise RMSD plot for ConA dimer (final structure from E2 simulation) with respect to 1GKB. The rRMSDs for the two chains of ConA dimer have been plotted separately. The secondary structural states for various residues are annotated (the arrows indicate β sheets and lines indicate loop regions).

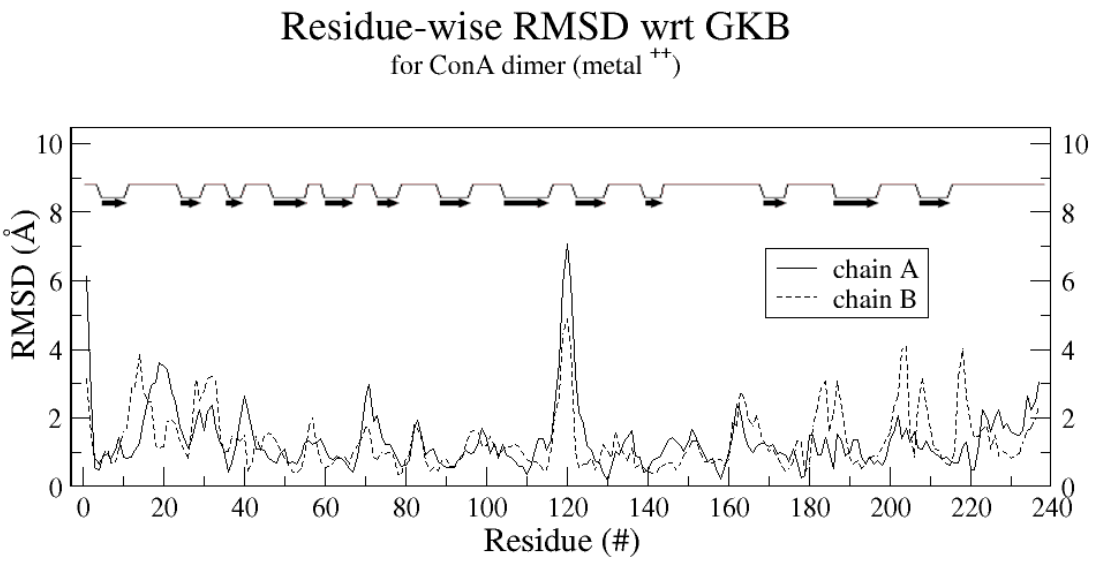

Figure S8