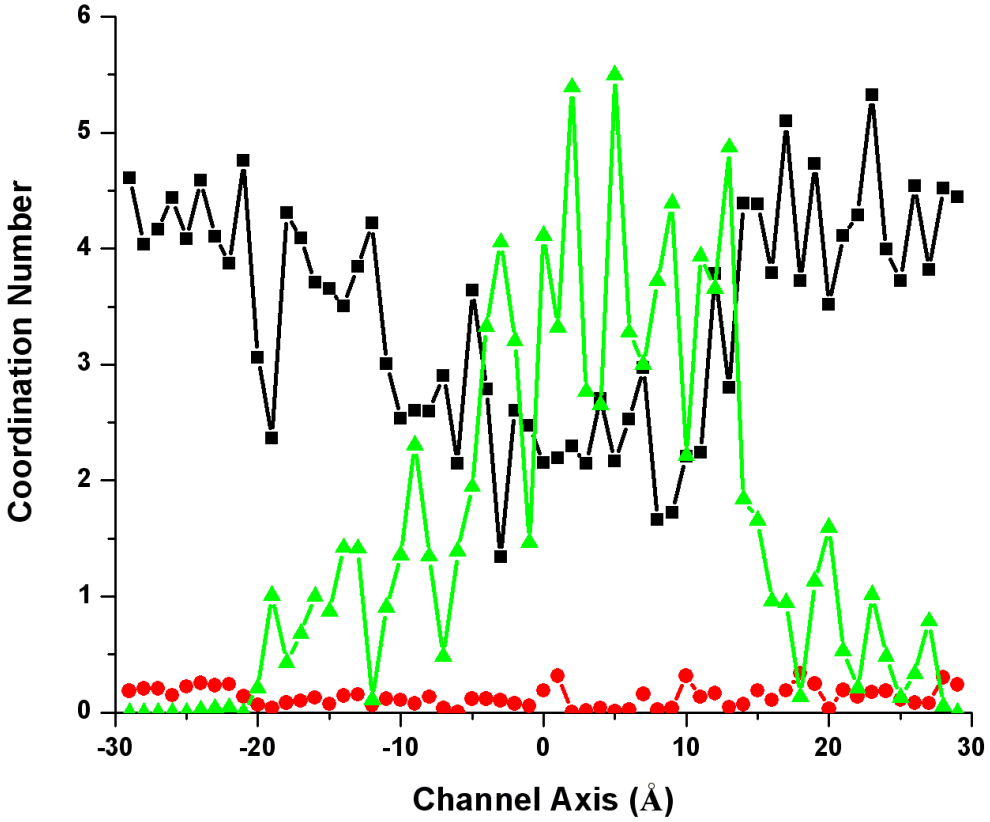
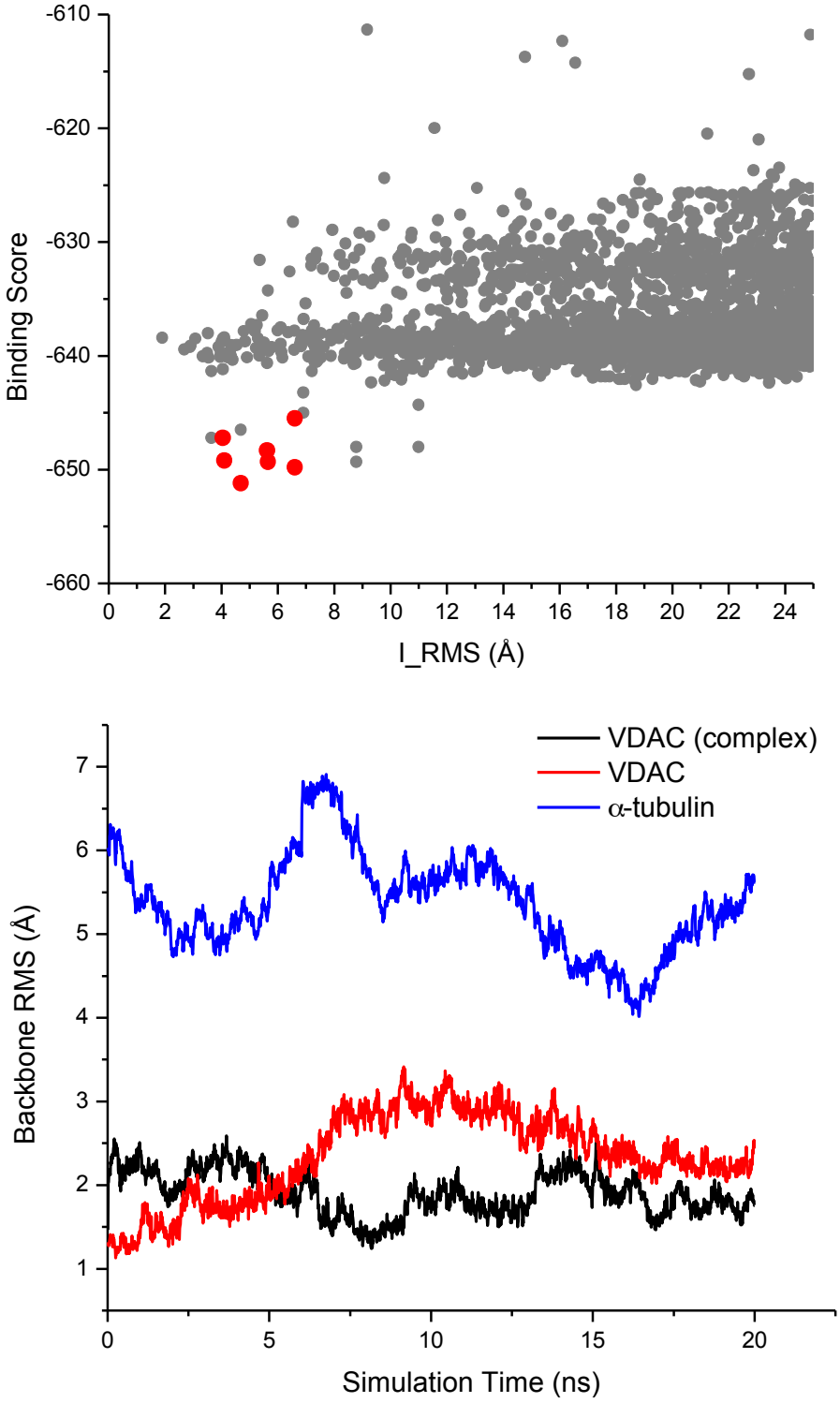
Supplementary Figures



Supplemental Figure 1: The position-dependent coordination number of ATP molecule. N(K+) is shown as black squares, N(Cl-) red circles and N(Protein) as green triangles. Contact analysis was performed by averaging of heavy atoms contacts within a sphere with R=3.5 Å.

Supplemental Figure 2: Interface energies of VDAC/α-Tubulin Complex vs. I_RMS from ROSETTA PROTEIN-PROTEIN Docking. The low-energy decoys chosen for further refinement with MD are shown in red. and RMSF for heavy atoms.



Supplemental Figure 3: Summary of cumulative charge transfer from five independent simulations for open VDAC1 channel. The contributions from anion and cation currents are shown.