*Article*

# Self-Association of Antimicrobial Peptides: A Molecular Dynamics Simulation Study on Bombinin

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1

# Supplementary Material
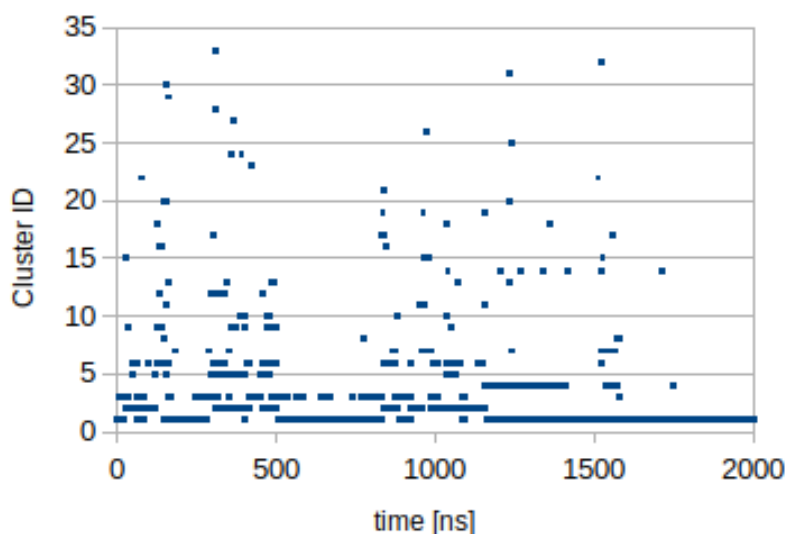


**Figure S 1.** Cluster population along the 2 $\mu$s trajectory of the single bombinin H2 monomer in water.
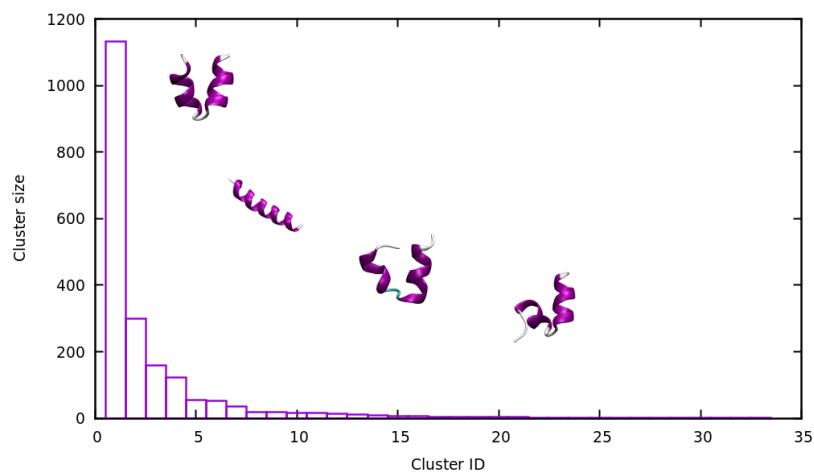
**Figure S 2.** Clusters' size and centroids of the four biggest clusters.
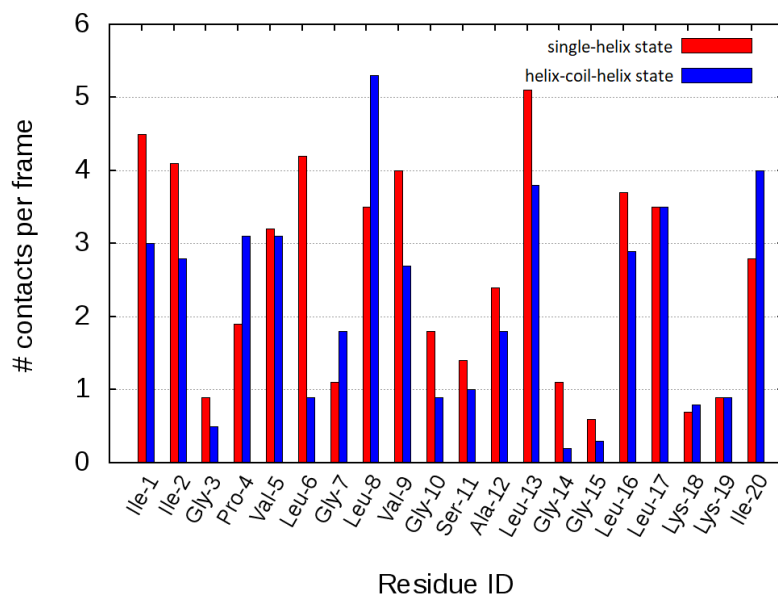


**Figure S 3.** Intermolecular contacts per frame for each of the residues in the bombinin H2 molecule in the single-helix and the helix-coil-helix states for the solution of 27 bombinin H2 monomers.
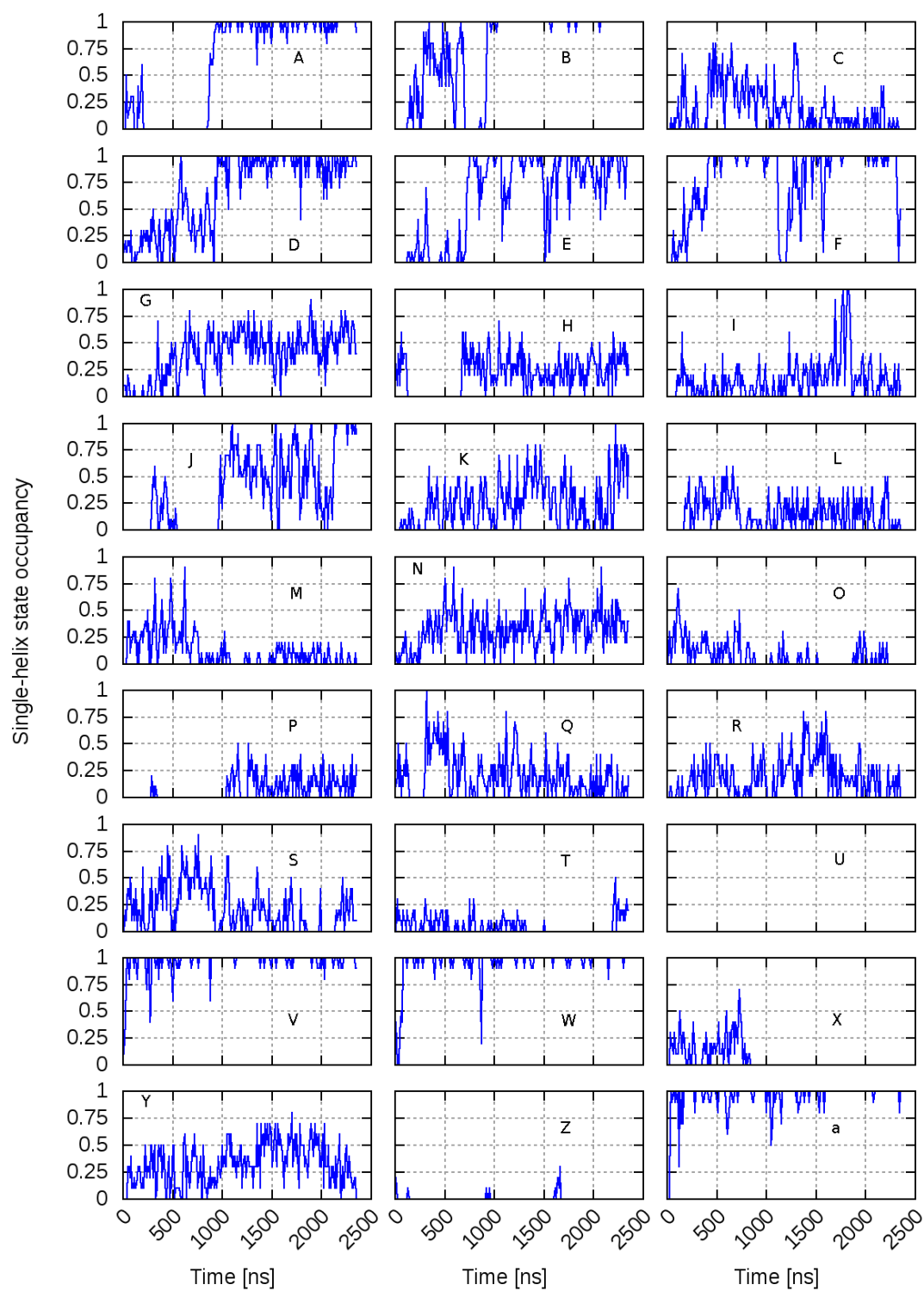
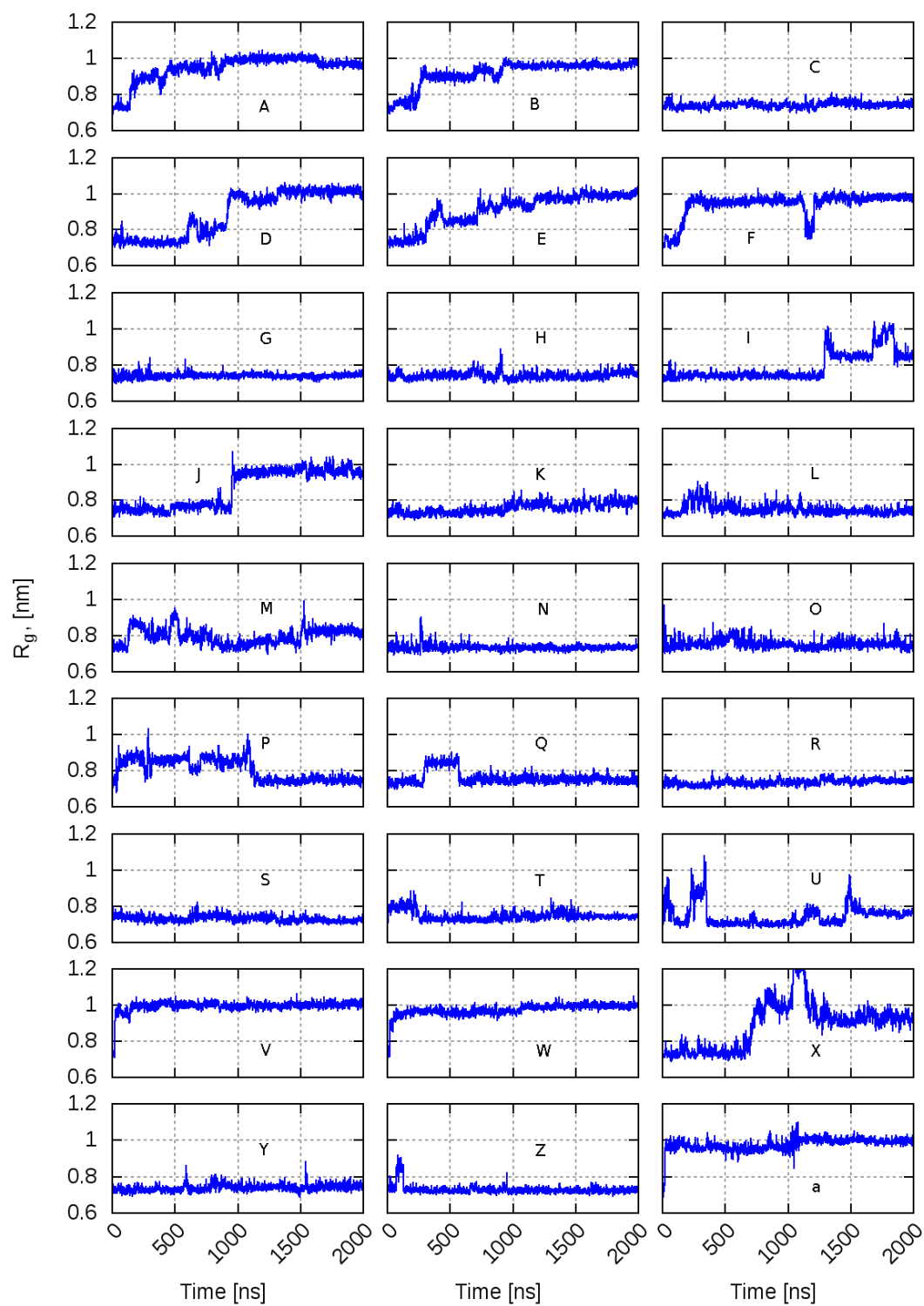**Figure S 4.** Single-helix state occupancy for each of the 27 peptide chains.

**Figure S 5.** Gyration radius for each of the 27 peptide chains.