Computational Studies of P22 N Peptide-*box*B RNA Recognition

Michael R. Jones and Maria C. Nagan*

Truman State University, Department of Chemistry, Kirksville, MO

Lambdoid bacteriophage is a type of virus that invades *Escherichia coli* and manipulates the cell machinery to self-proliferate. One strategy of replication is to turn viral transcription on through the process known as antitermination. P22 N peptide recognition of *boxB* RNA signals this process to occur. Molecular dynamics studies of P22 N peptide-*box*B complexes have been undertaken to better understand the roles that arginine-rich motifs and water play in peptide-RNA recognition. Systems have been built under 200 mM KCl in the presence of explicit TIP4PEW water molecules and 55 ns of production run simulation time has been collected for six starting structures. Thermodynamic properties have been monitored for simulation convergence. The presence of hydrogen bonds between the RNA and the peptide have been compared across multiple models and sites of high water density have been examined to determine preferential water binding sites.