Supplementary material

Will molecular dynamics simulations of proteins ever reach equilibrium?

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Figure S1. Protein conformational entropy from DDH analysis for the Gal3 simulations with the Lac and L02 ligands, as well as the difference in entropy of the two states, as a function of the length of the simulation. The entropy ($T\Delta S$ in kJ/mol at 300 K) is relative to the estimate at 500 ns. Only residues within 8 Å of L02 in the crystal structure were considered.

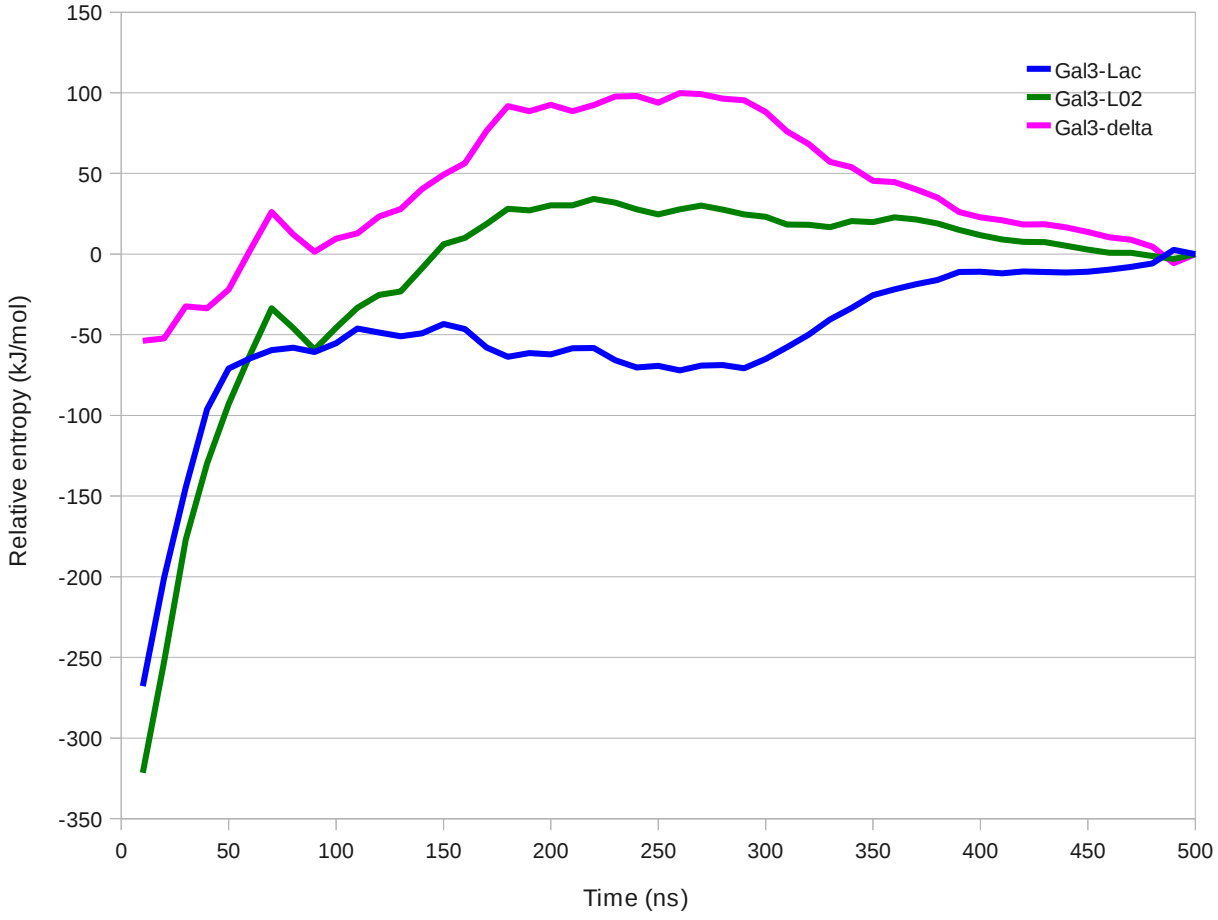

Figure S2. Entropy from VMA analysis for the Gal3 simulations with the Lac and L02 ligands,as well as the difference in entropy of the two states, as a function of the length of the simulation. The entropy ($T\Delta S$ in kJ/mol at 300 K) is relative to the estimate at 500 ns.

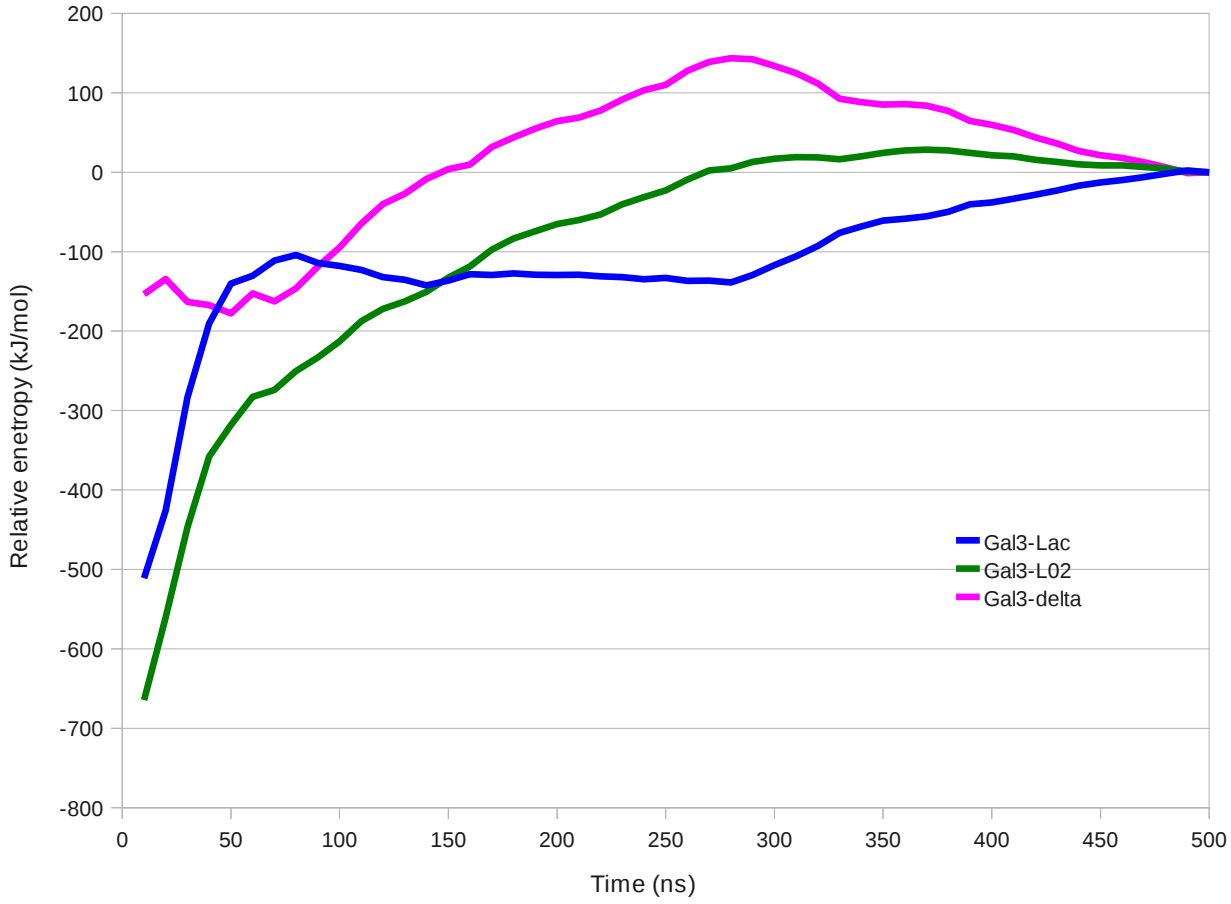

Figure S3. Entropy from QHA analysis for the Gal3 simulations with the Lac and L02 ligands, as well as the difference in entropy of the two states, as a function of the length of the simulation. The entropy ($T\Delta S$ in kJ/mol at 300 K) is relative to the estimate at 500 ns.

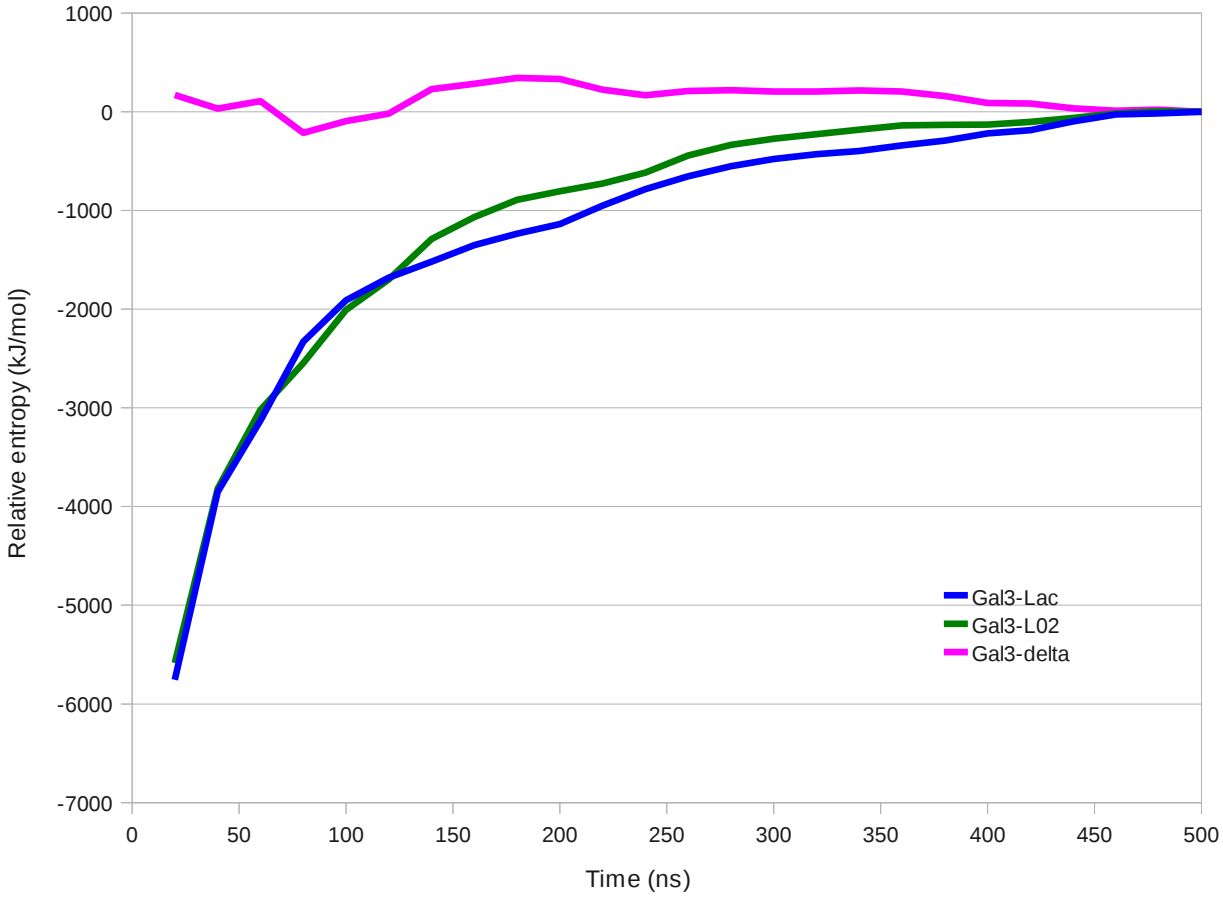

Figure S4. Root-mean square deviation (RMSD) during the MD simulation relative to the first snapshot of the production run.