Molecular dynamics (MD) is a powerful technique for studying protein dynamics and here we apply it to three inter-related problems. Firstly, in our MD simulations, we implement distance restraints derived from G-protein coupled receptor (GPCR) activation experiments, such as site-directed spin labelling, to simulate the active form of GPCRs\(^1\). GPCRs are dynamic proteins and the resultant instability, which may be captured by simulation, is one of the reasons why the proteins are difficult to crystallize. Secondly, We have used a range of techniques based on MD simulations of the inactive and active receptors to understand the stabilizing effect of the nine mutations that were used to stabilize the beta(1)-adrenergic receptor\(^2\) to enhance crystallization\(^3\). Our explanation of the thermostabilization is partly based on Berezovsky’s closed loop hypothesis\(^4\) in which the basic folding unit is a closed loop of about 25-35 residues held together at the loop ends (locks) and so thirdly we also present evidence to support this protein folding hypothesis.