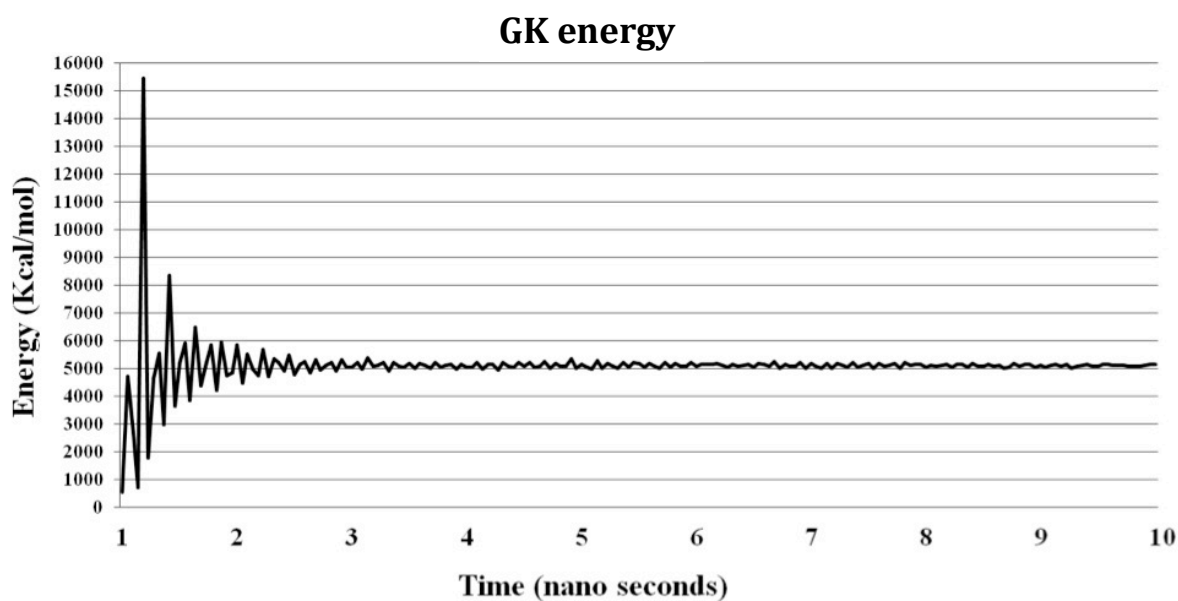
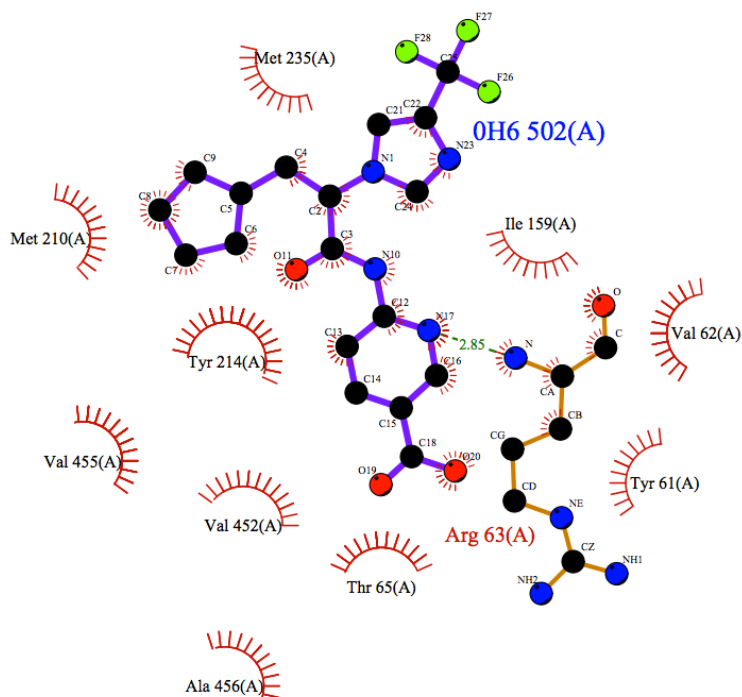


Supplementary Figure 1: X-Ray crystallographic structure of human glucokinase obtained from PDB (ID: 1V4S)

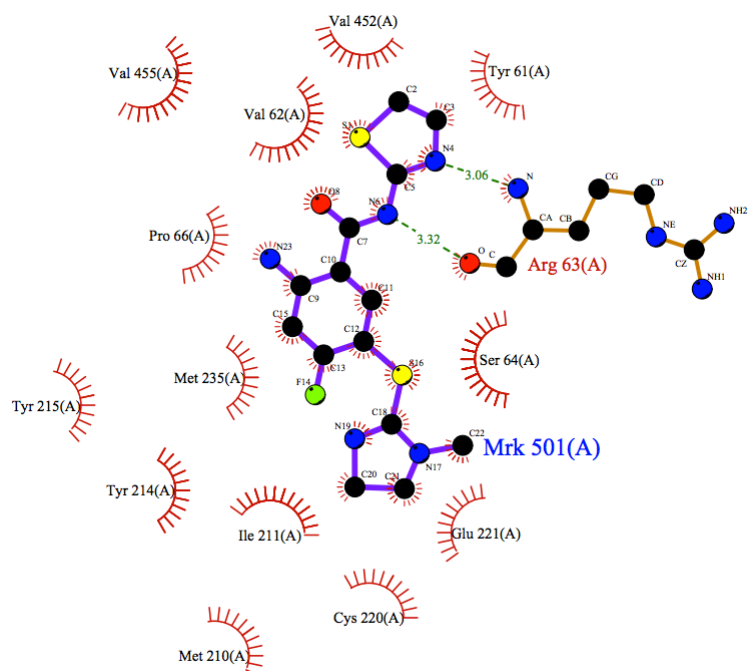


Supplementary Figure 2: Energy plot of GK generated during molecular dynamics simulation for the run time of 10 ns. The plot showing the stabilization of trajectories near 5000 Kcal/mol after 2 ns of run time

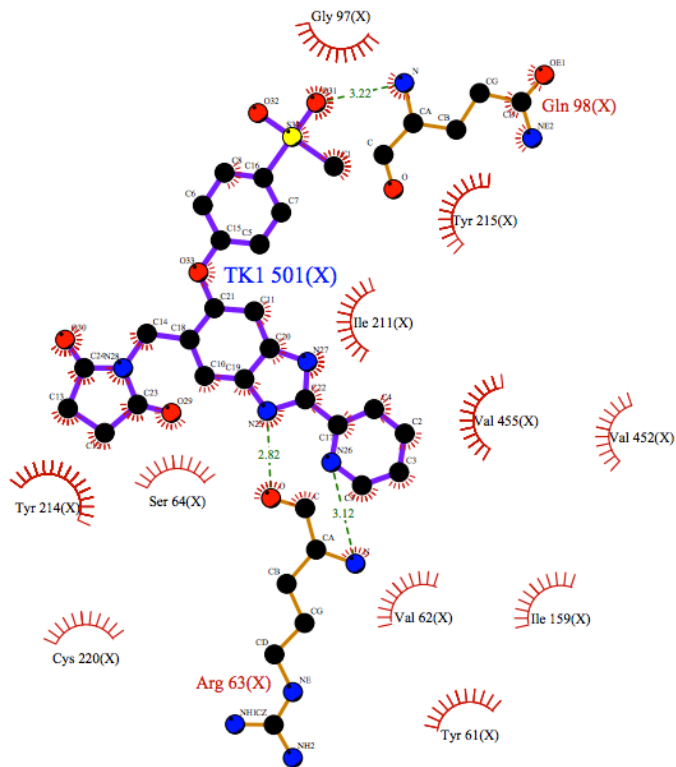
GK = glucokinase



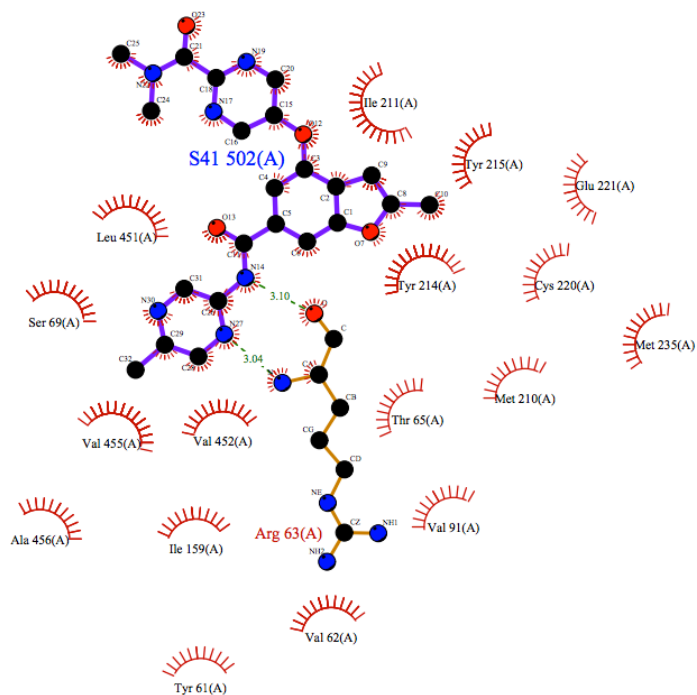
Supplementary Figure 3: Ligand plot of 3VF6



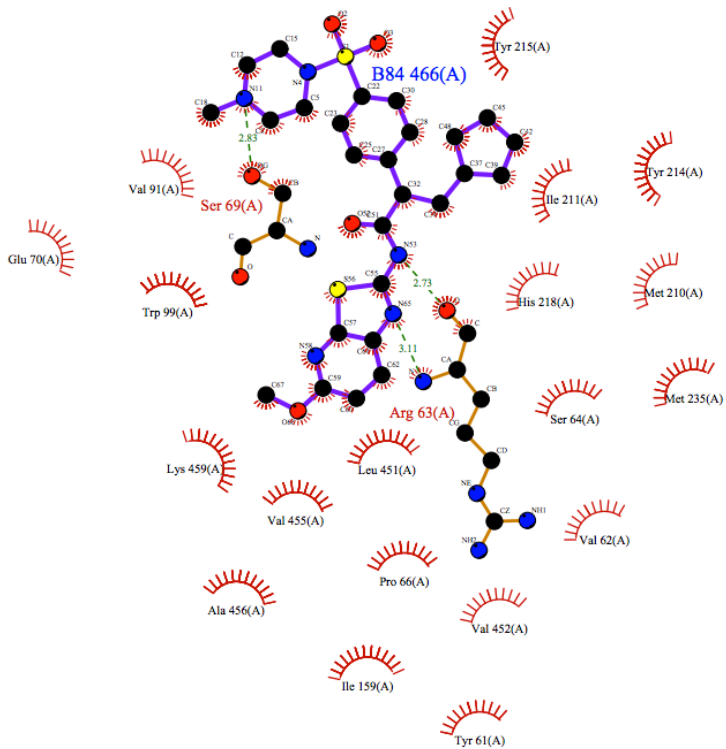
Supplementary Figure 4: Ligand plot of 3ID8



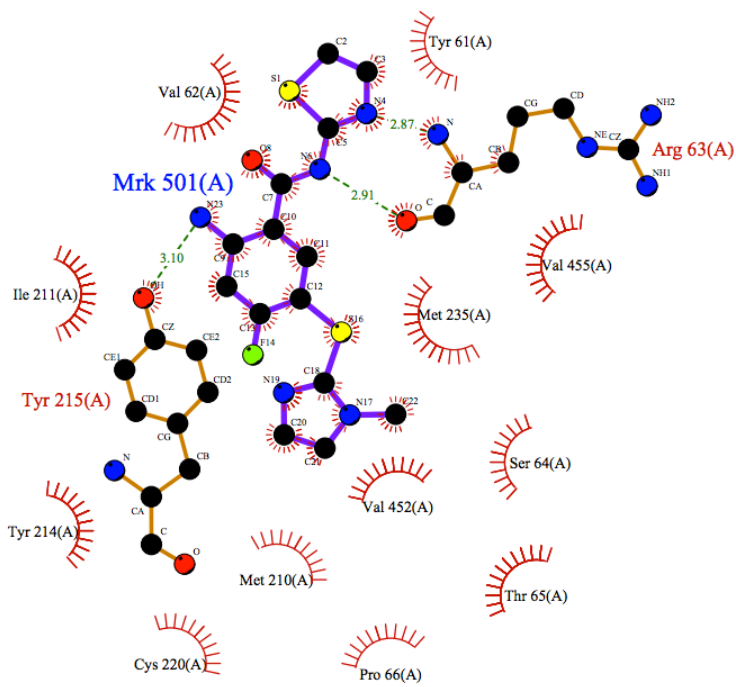
Supplementary Figure 5: Ligand plot of 3H1V



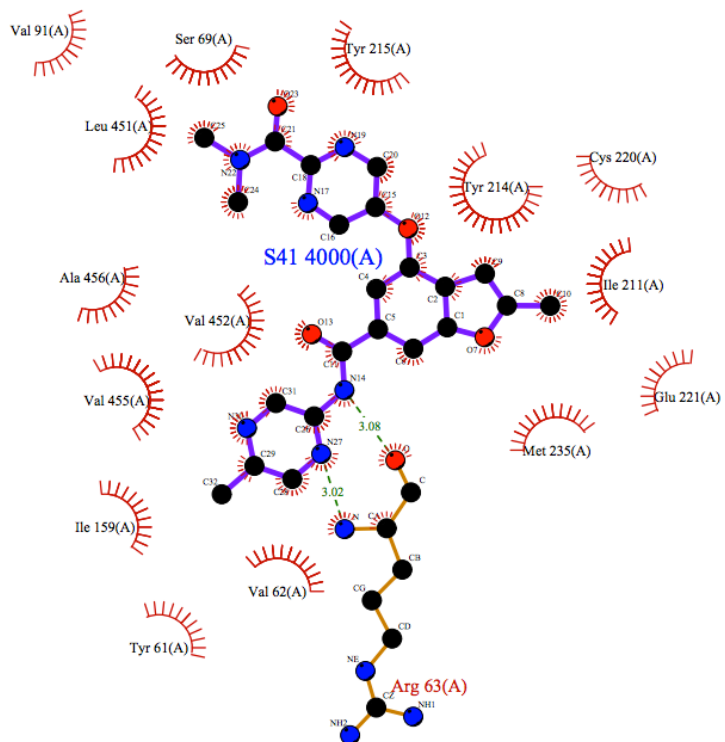
Supplementary Figure 6: Ligand plot of 4DHY



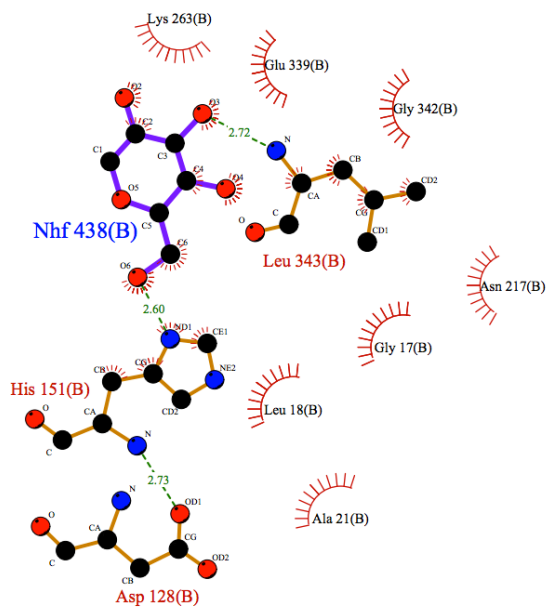
Supplementary Figure 7: Ligand plot of 3IMX



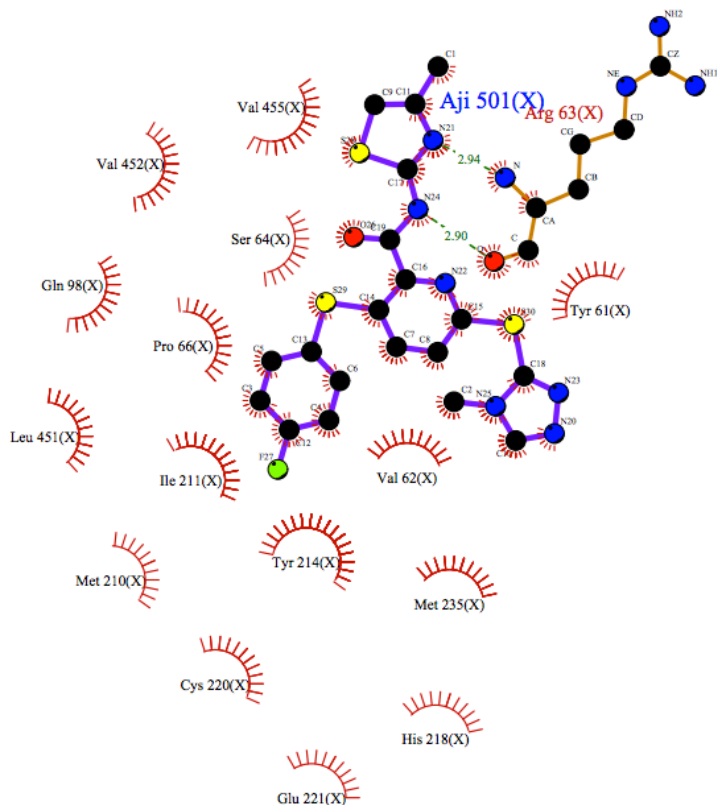
Supplementary Figure 8: Ligand plot of 3F9M



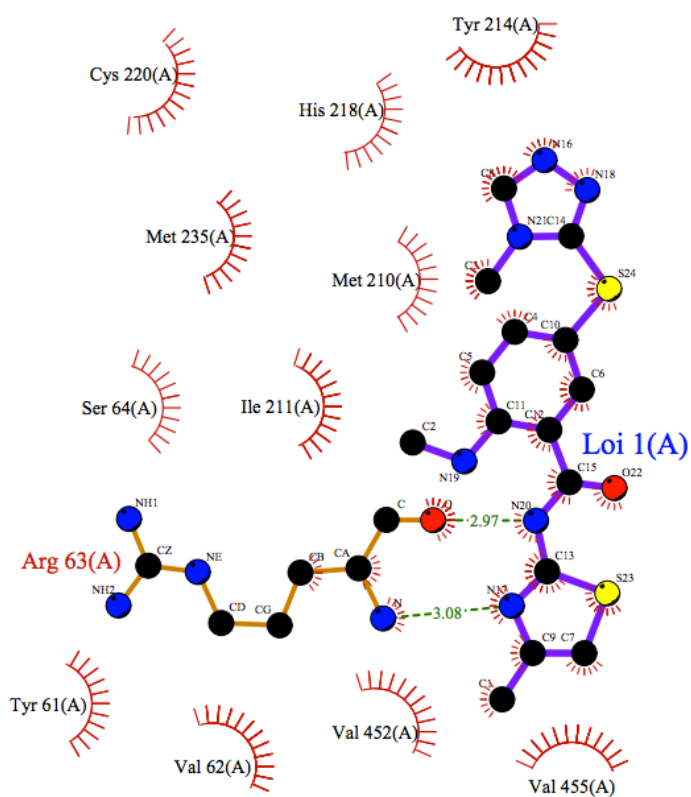
Supplementary Figure 9: Ligand plot of 3S41



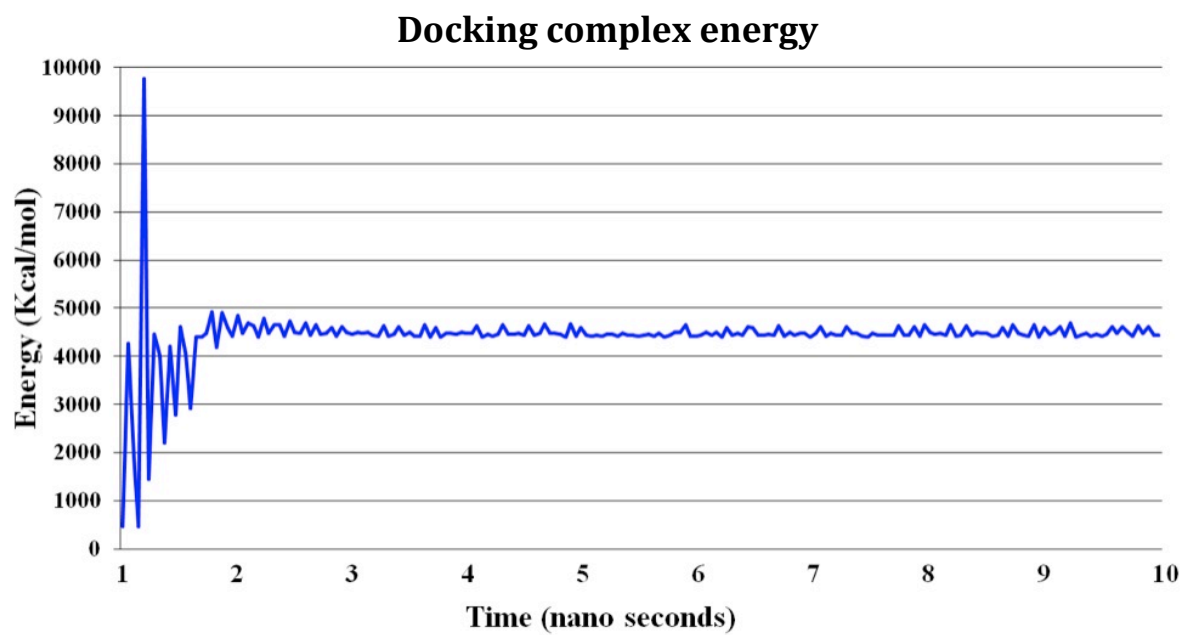
Supplementary Figure 10: Ligand plot of 3FRO



Supplementary Figure 11: Ligand plot of 3A0I



Supplementary Figure 12: Ligand plot of 3GOI



Supplementary Figure 13: Energy plot of GK-PD24 complex generated during molecular dynamics simulations of 10 ns run time

GK-PD24 = glucokinase pyridone derivative 24