

In Vacuo harmonically
restrained minimisation
4PTI: 1,072 atoms

CHARMM
PD



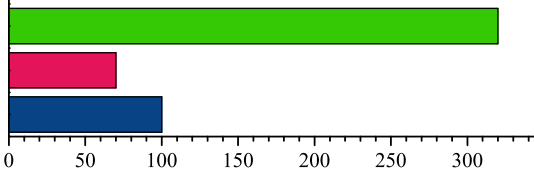
Molecular Dynamics
GB/SA
Ubiquitin: 1,230 atoms

Tinker
Amber8
PD



Molecular Dynamics
Explicit Solvent
45Å Periodic
Boundary Conditions
Ubiquitin: 7,050 Atoms

Tinker
NAMD2
PD



Relative Execution Time (%)