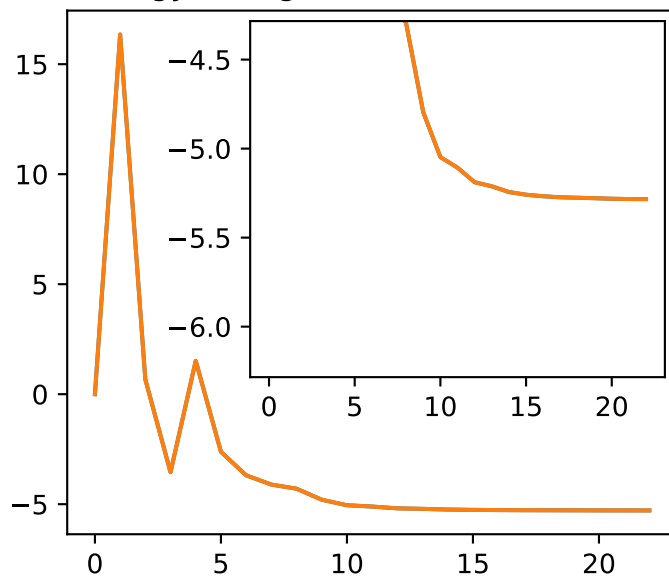
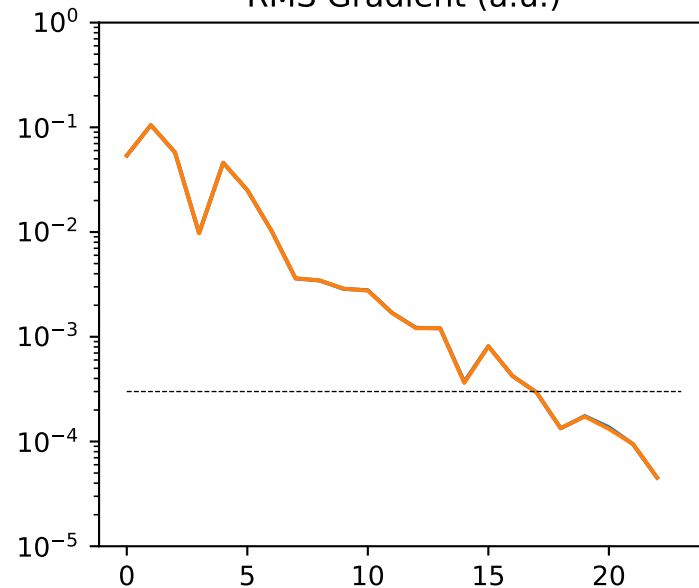


Optimization performance for psb3-qmmm-meci

Energy change, from start (kcal/mol)



RMS Gradient (a.u.)



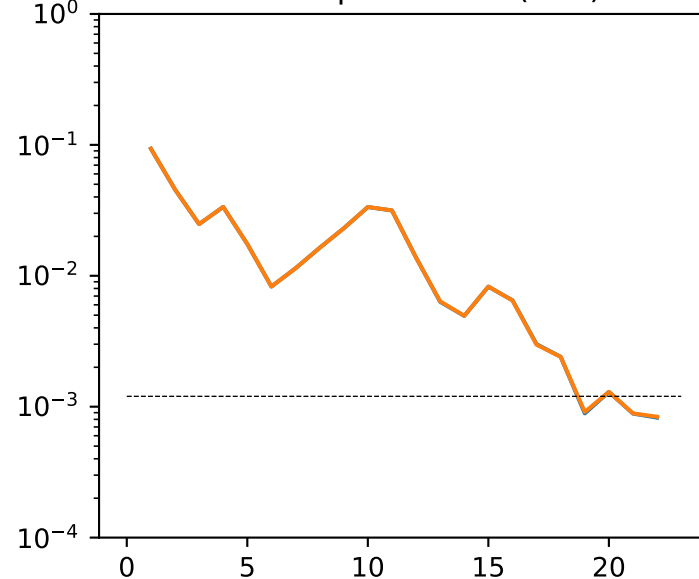
Max Gradient (a.u.)



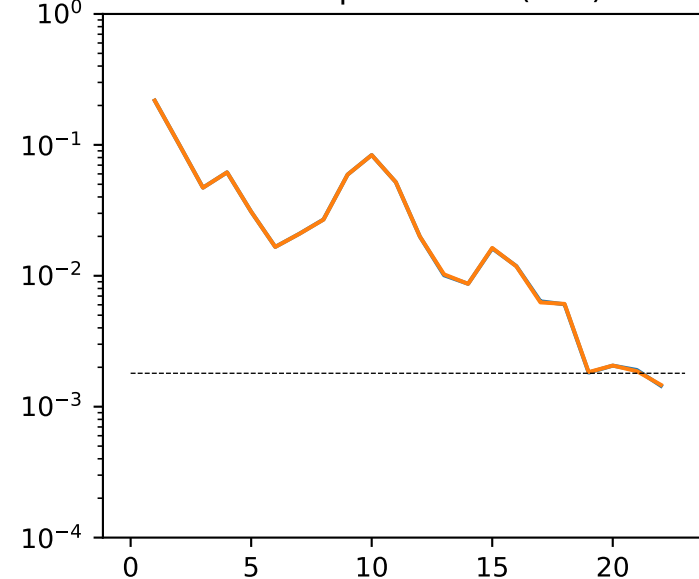
Energy change per step (a.u.)



RMS Displacement (a.u.)



Max Displacement (a.u.)



Optimization Cycle

2022-09-08 Converged N=22 v1.0 Converged N=22