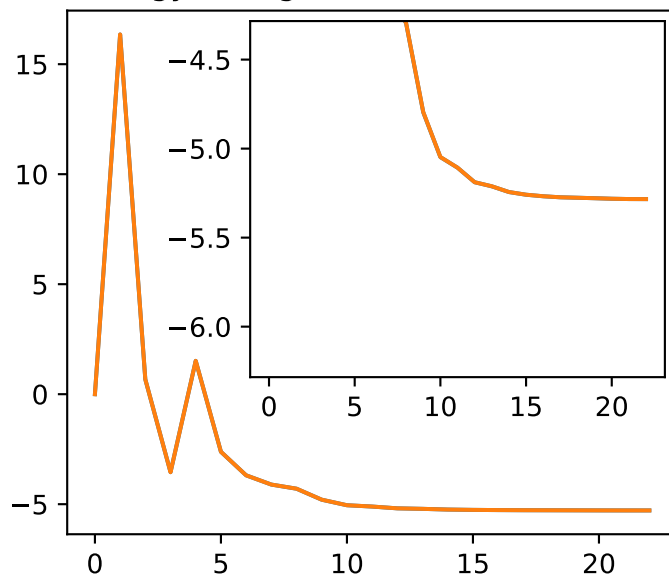
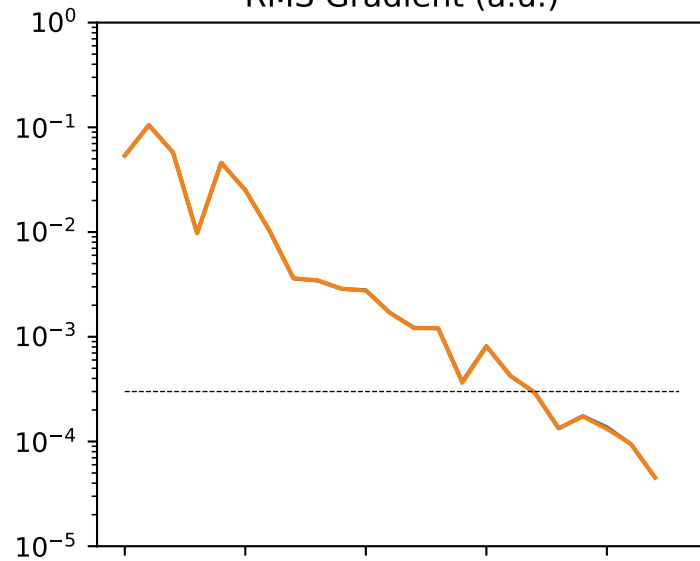


# Optimization performance for psb3-qmmm-meci

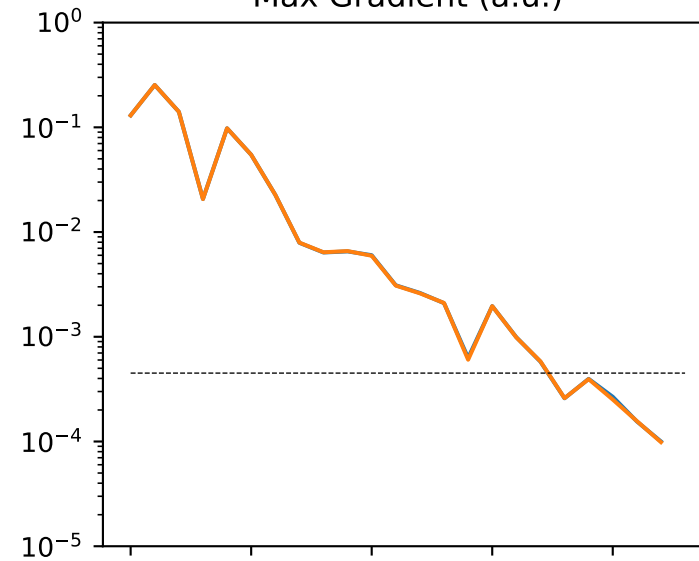
Energy change, from start (kcal/mol)



RMS Gradient (a.u.)



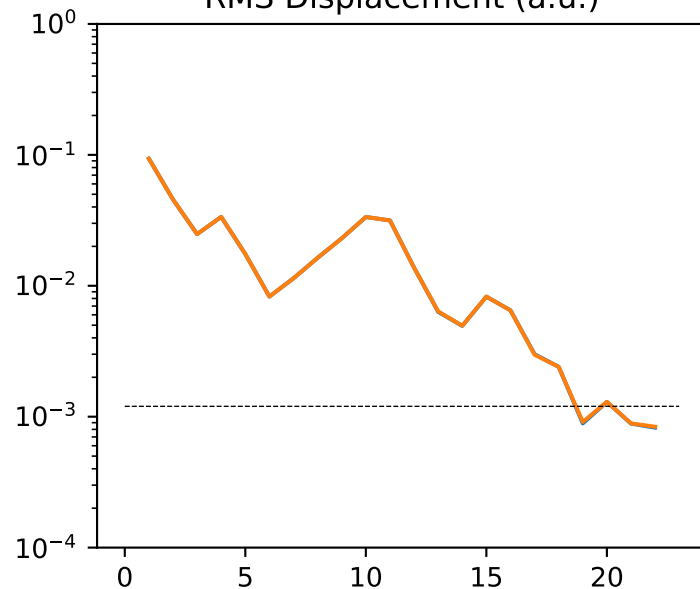
Max Gradient (a.u.)



Energy change per step (a.u.)



RMS Displacement (a.u.)



Max Displacement (a.u.)



2022-09-08 Converged N=22

v1.0 Converged N=22