MAE\_o 0.6 45 15 49 46 14 12 18 35 25 41 27 ttg 30 0.5 Force prediction error  $(kcal/mol\AA)$ Mean 33 40 7 6 37 43 0.4 31 22 4 0.3 0.2 0.1 0.0 10 20 30 40 50 Cluster index