MAE_o 0.175 5 39 14 24 2 12 8 37 25 49 43 19 36 22 7 30 3 17 0 48 28 6 11 29 47 20 41 34 0.150 Force prediction error $(kcal/mol\mbox{\ensuremath{\ensuremath{A}}})$ Mean 46 21 10 1 26 15 35 44 32 0.125 33 27 18 40 0.100 38 31 4 13 9 45 0.075 0.050 0.025 0.000 10 20 30 40 50

Cluster index