MAE_o 26 24 47 35 1 13 41 15 33 8 37 3 42 0.07 11 30 19 49 29 21 39 18 6 44 45 10 0.06 Force prediction error $(kcal/mol\mbox{\ensuremath{\ensuremath{A}}})$ 23 34 0 Mean 27 16 4 40 14 7 38 48 31 20 0.05 22 36 17 2 43 12 5 25 0.04 9 32 28 0.03 0.02 0.01 0.00 10 20 30 40 50

Cluster index