RMSE_o 43 42 3 1 31 47 0 21 2 30 45 9 44 8 15 46 4 48 5 32 Mean 17 49 35 38 41 22 34 16 20 18 19 0.020 Force prediction error $(kcal/mol\mbox{\ensuremath{\ensuremath{A}}})$ 39 25 10 28 7 0.015 26 12 0.010 0.005 14 29 24 0.000 10 20 30 40 50 Cluster index