RMSE\_o 5 3 46 32 49 22 31 17 40 37 42 43 44 35 38 20 47 41 16 19 18 1 30 23 7 48 21 15 4 9 2 0 33 0.020 Mean Force prediction error  $(kcal/mol\mbox{\ensuremath{\ensuremath{A}}})$ 28 25 10 39 13 6 0.015 27 36 12 0.010 26 11 0.005 14 24 29 0.000 10 20 30 40 50 Cluster index