RMSE\_o 0.14 5 35 15 36 14 41 30 43 19 8 37 16 6 34 11 17 47 2 12 0 3 29 26 25 7 49 42 20 28 22 Mean 0.12 Force prediction error  $(kcal/mol\mbox{\it Å})$ 24 44 27 39 40 18 31 23 9 4 13 45 38 0.10 0.08 0.06 0.04 0.02 0.00 10 20 30 40 50 Cluster index