MSE_o 3 9 13 41 26 49 16 15 2 0.4 Force prediction error (kcal/mol Å)² 4 10 47 19 0 40 44 14 31 45 18 48 6 17 12 28 39 1 32 33 36 37 27 25 30 8 Mean 0.3 29 35 22 24 0.2 0.1 0.0 10 20 30 40 50 Cluster index