RMSE_o 2 0 13 16 26 20 44 48 35 34 41 39 36 9 15 19 27 3 12 1 32 0.7 10 28 49 5 Mean 46 40 31 45 7 6 37 43 18 38 25 30 8 33 Force prediction error $(kcal/mol \text{\AA})$ 0.6 42 14 22 24 4 29 0.5 21 0.4 0.3 0.2 0.1 0.0 10 20 30 40 50 Cluster index