MAE_o 0.7 28 34 12 41 17 27 25 29 35 1 30 32 4 0 47 48 5 19 42 2 9 18 26 44 36 3 39 46 15 37 11 45 8 43 38 14 16 13 6 0.6 Force prediction error $(kcal/mol \text{\AA})$ 0.5 Mean 31 33 10 7 0.4 0.3 0.2 0.1 0.0 10 20 30 40 50

Cluster index