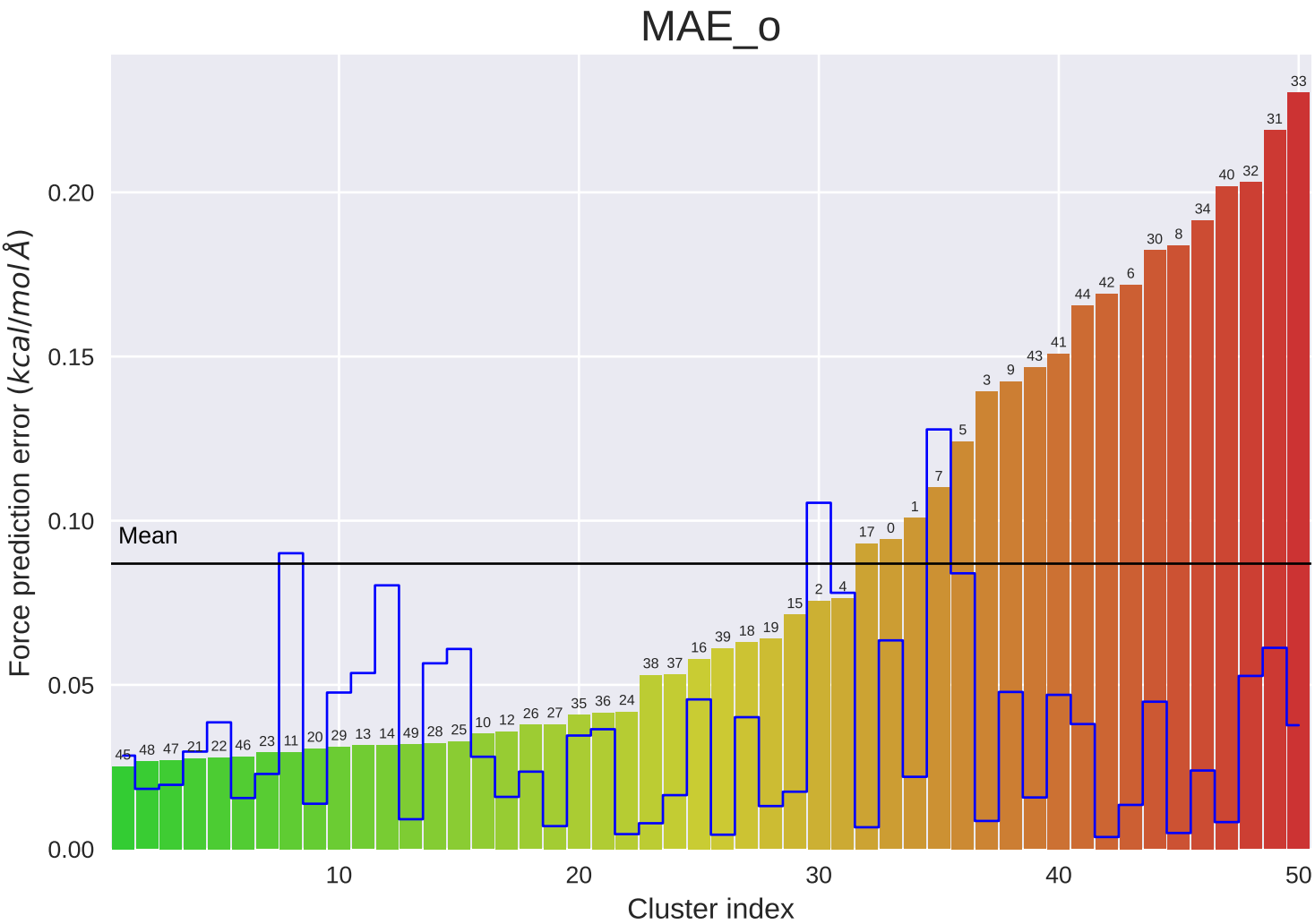
MAE_o
Force prediction error (kcal/mol Å)
Cluster index
Mean
0.00
0.05
0.10
0.15
0.20
10
20
30
40
50
45 48 47 21 22 46 23 11 20 29 13 14 49 28 25 10 12 26 27 35 36 24 38 37 16 39 18 19 15 2 4 17 0 1 7 5 3 9 43 41 44 42 6 30 8 34 40 32 31 33