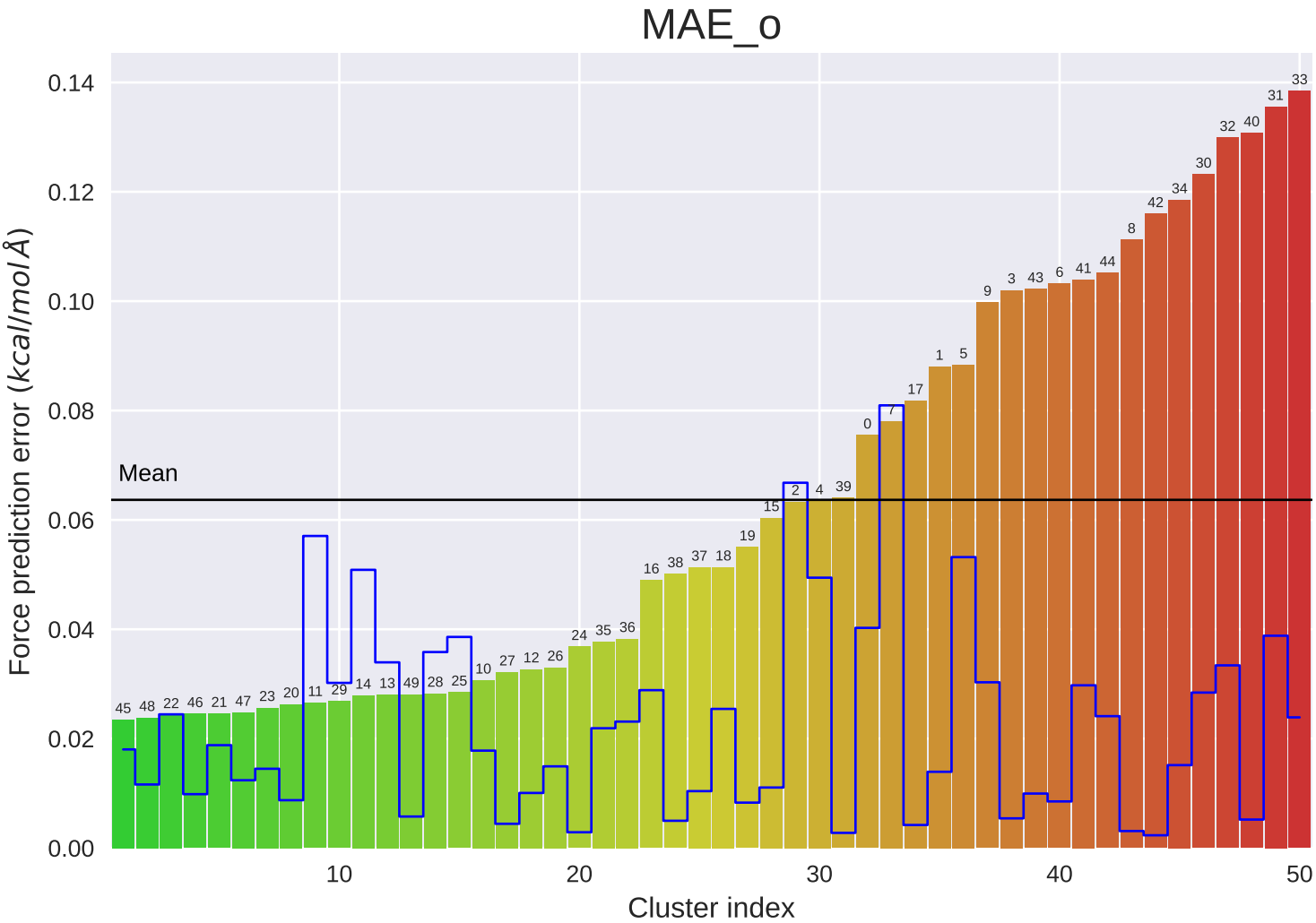
MAE_o
Force prediction error (kcal/mol Å)
0.14
0.12
0.10
0.08
0.06
0.04
0.02
0.00
Mean
45 48 22 46 21 47 23 20 11 29 14 13 49 28 25 10 27 12 26 24 35 36 16 38 37 18 19 15 2 4 39 0 7 17 1 5 9 3 43 6 41 44 8 42 34 30 32 40 31 33
10
20
30
40
50
Cluster index