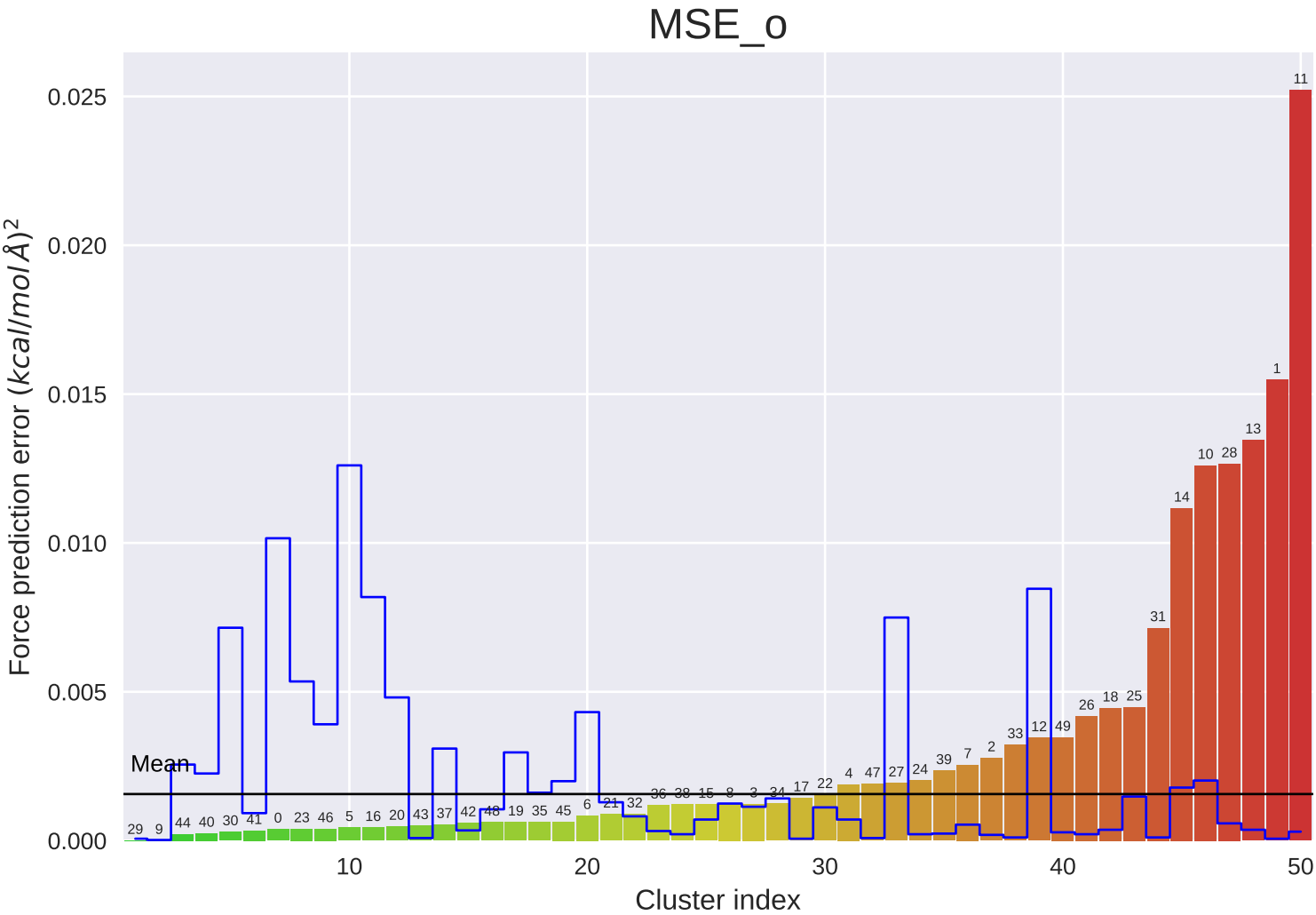
MSE_o
Force prediction error (kcal/mol Å)^2
0.025
0.020
0.015
0.010
0.005
0.000
Mean
29 9 44 40 30 41 0 23 46 5 16 20 43 37 42 48 19 35 45 6 21 32 36 38 15 8 3 34 17 22 4 47 27 24 39 7 2 33 12 49 26 18 25 31 14 10 28 13 1 11
10
20
30
40
50
Cluster index