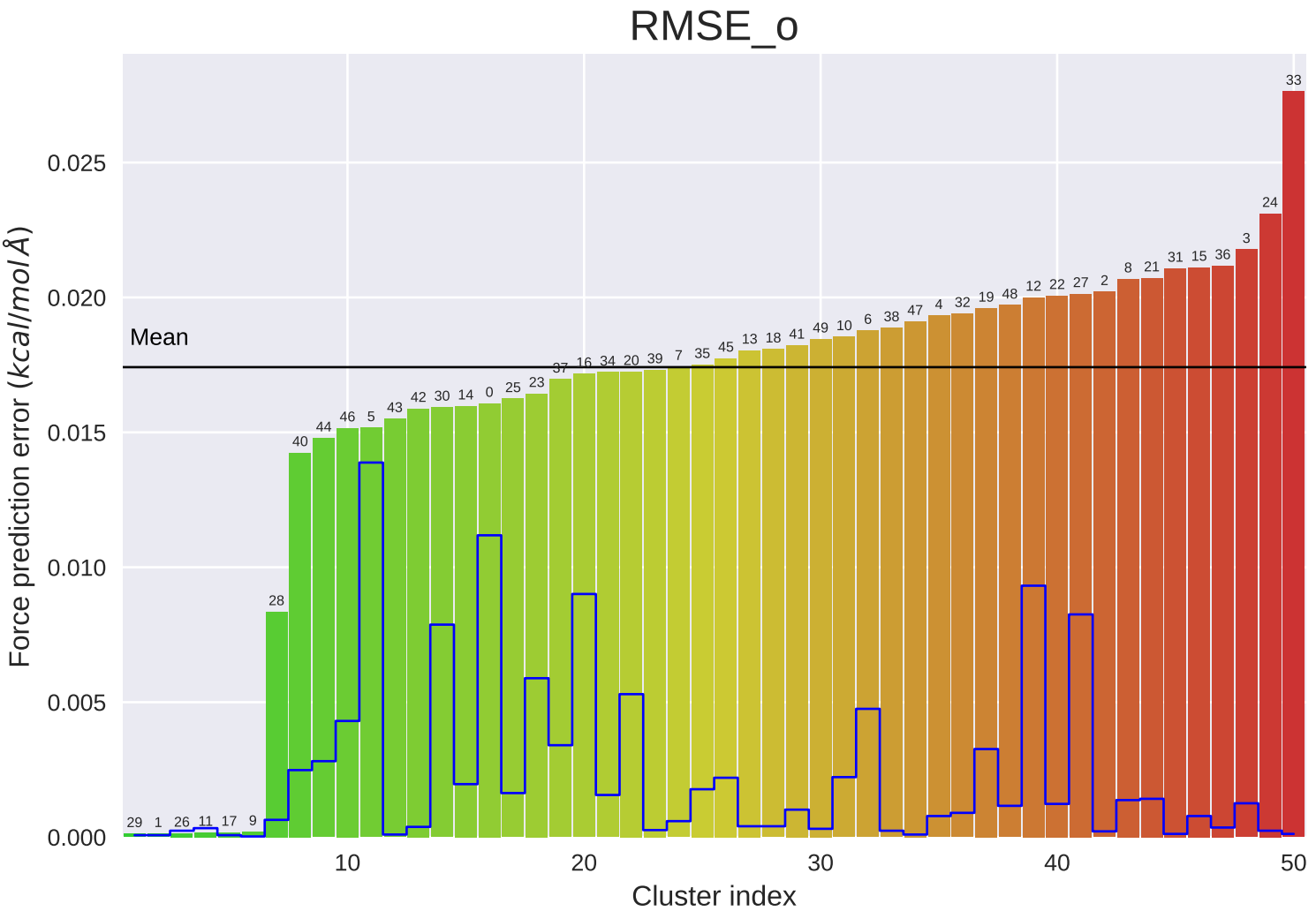
RMSE_o
Force prediction error (kcal/mol Å)
Cluster index
Mean
0.000
0.005
0.010
0.015
0.020
0.025
10
20
30
40
50
29 1 26 11 17 9 28 40 44 46 5 43 42 30 14 0 25 23 37 16 34 20 39 7 35 45 13 18 41 49 10 6 38 47 4 32 19 48 12 22 27 2 8 21 31 15 36 3 24 33