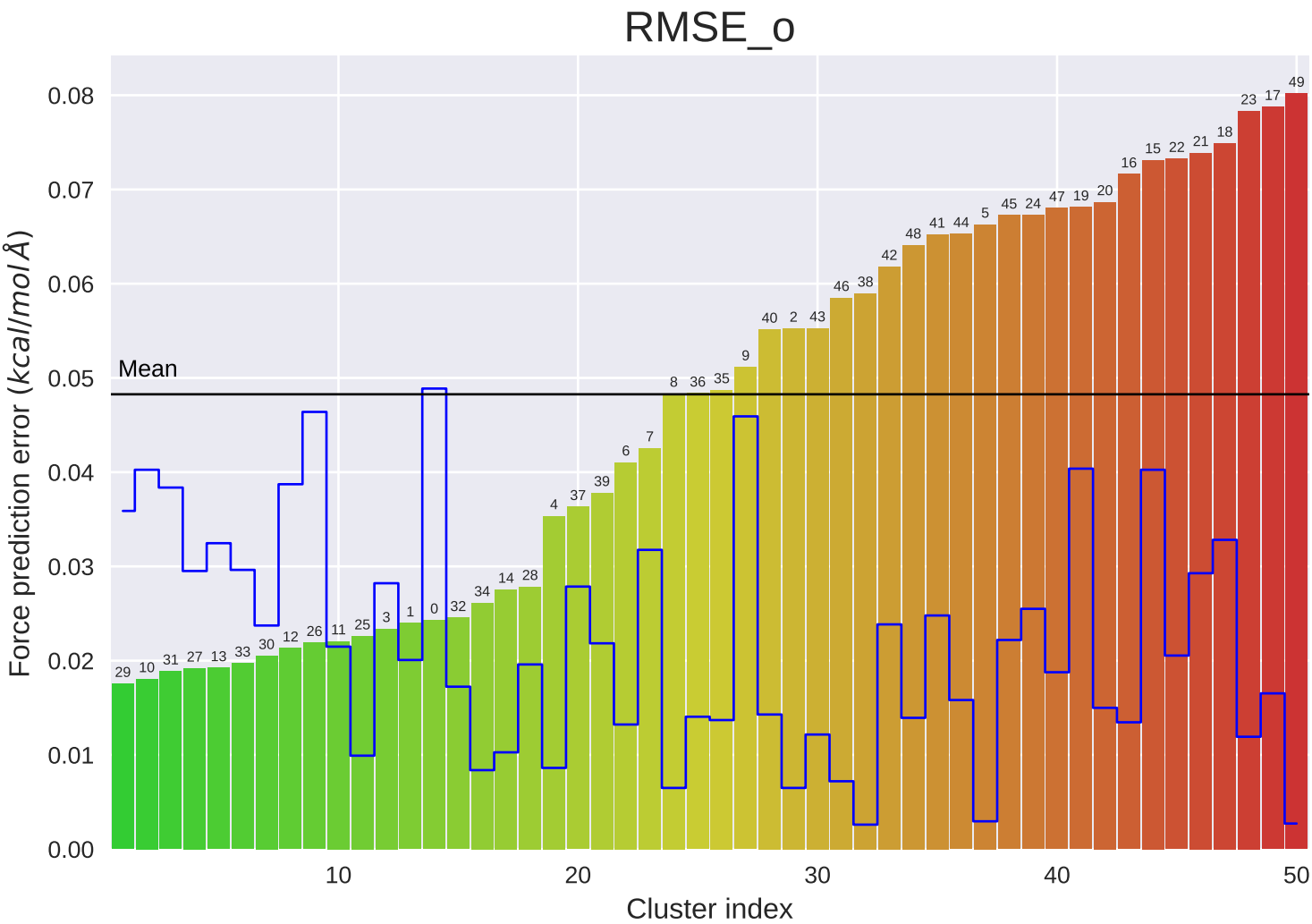
RMSE_o
Mean
Force prediction error (kcal/mol Å)
Cluster index
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0.07
0.08
10
20
30
40
50
29 10 31 27 13 33 30 12 26 11 25 3 1 0 32 34 14 28 4 37 39 6 7 8 36 35 9 40 2 43 46 38 42 48 41 44 5 45 24 47 19 20 16 15 22 21 18 23 17 49