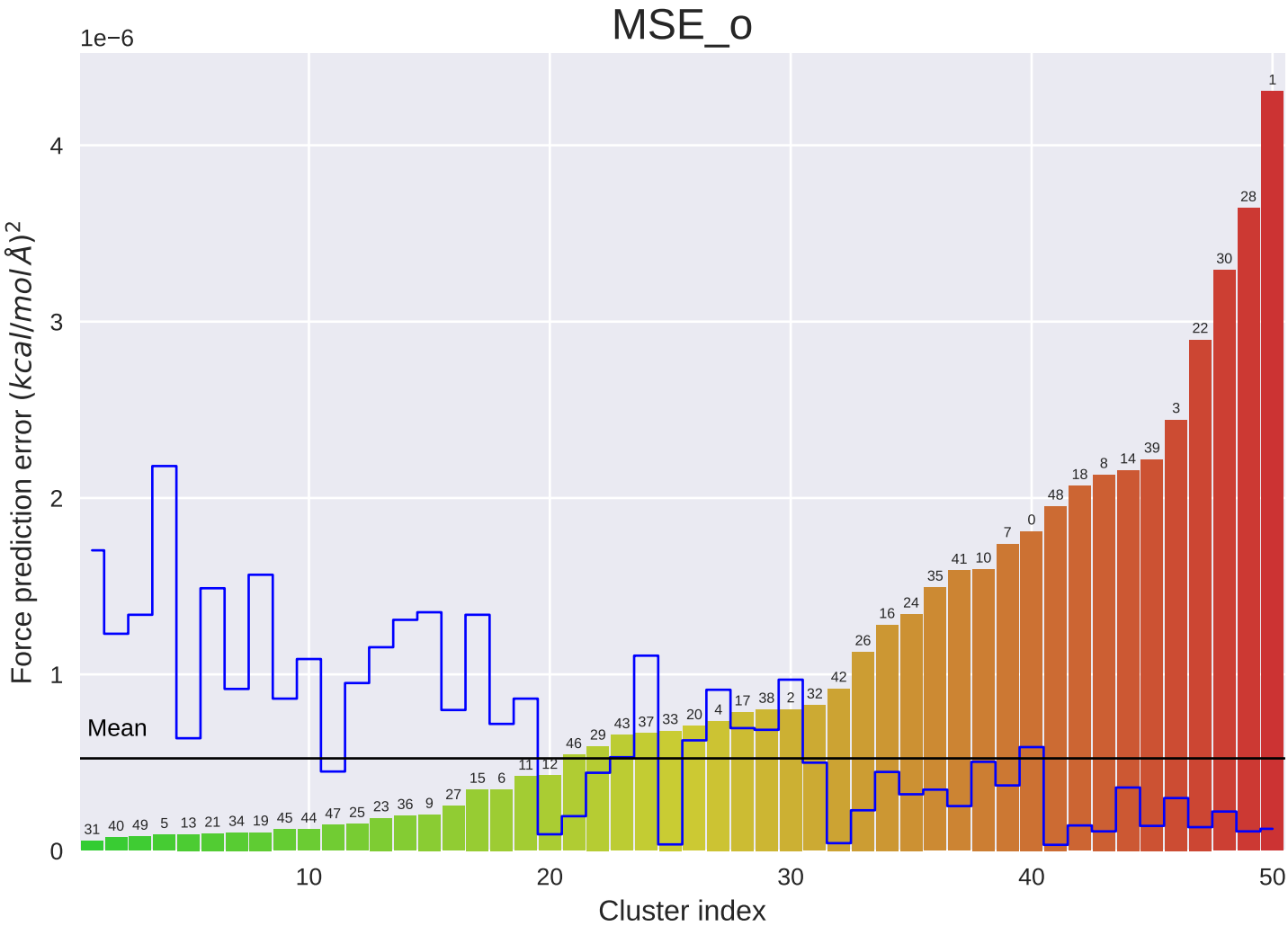
MSE_o
1e−6
Force prediction error (kcal/mol Å)²
Cluster index
Mean
0
1
2
3
4
10
20
30
40
50
31 40 49 5 13 21 34 19 45 44 47 25 23 36 9 27 15 6 11 12 46 29 43 37 33 20 4 17 38 2 32 42 26 16 24 35 41 10 7 0 48 18 8 14 39 3 22 30 28 1