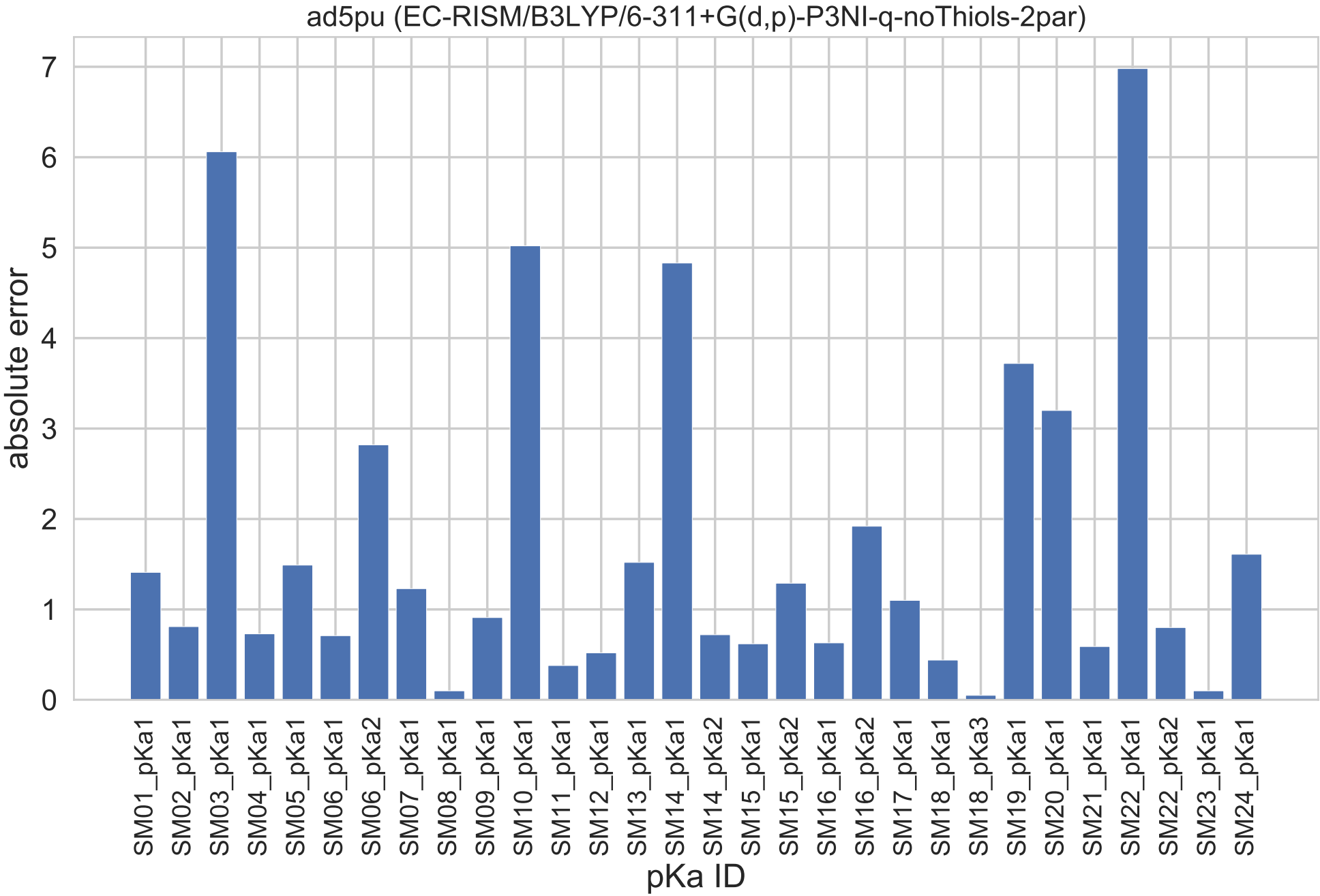
ad5pu (EC-RISM/B3LYP/6-311+G(d,p)-P3NI-q-noThiols-2par)
absolute error
0
1
2
3
4
5
6
7
SM01_pKa1
SM02_pKa1
SM03_pKa1
SM04_pKa1
SM05_pKa1
SM06_pKa1
SM06_pKa2
SM07_pKa1
SM08_pKa1
SM09_pKa1
SM10_pKa1
SM11_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa1
SM14_pKa2
SM15_pKa1
SM15_pKa2
SM16_pKa1
SM16_pKa2
SM17_pKa1
SM18_pKa1
SM18_pKa3
SM19_pKa1
SM20_pKa1
SM21_pKa1
SM22_pKa1
SM22_pKa2
SM23_pKa1
SM24_pKa1
pKa ID