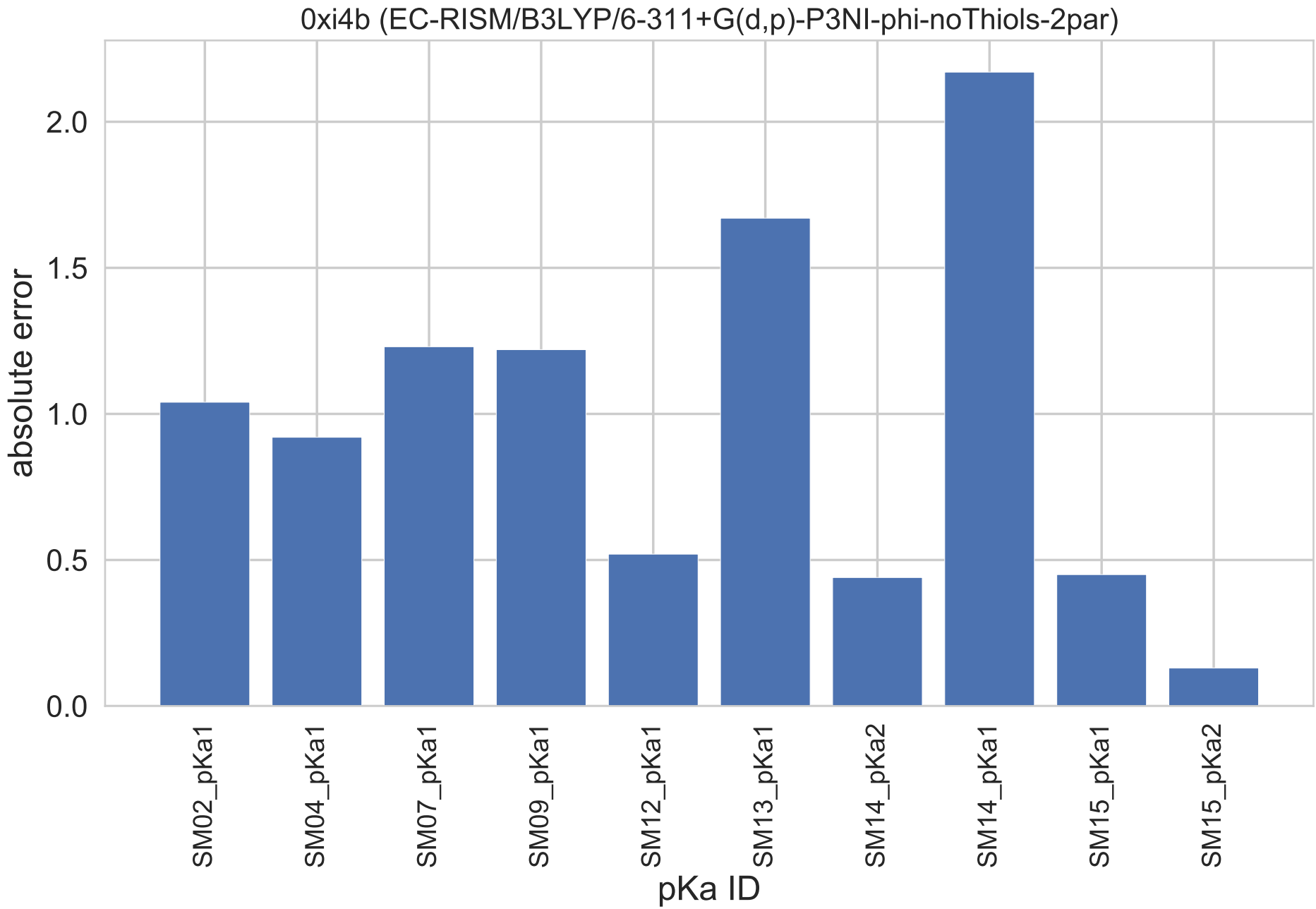
0xi4b (EC-RISM/B3LYP/6-311+G(d,p)-P3NI-phi-noThiols-2par)
absolute error
0.0
0.5
1.0
1.5
2.0
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa1
SM15_pKa2
pKa ID