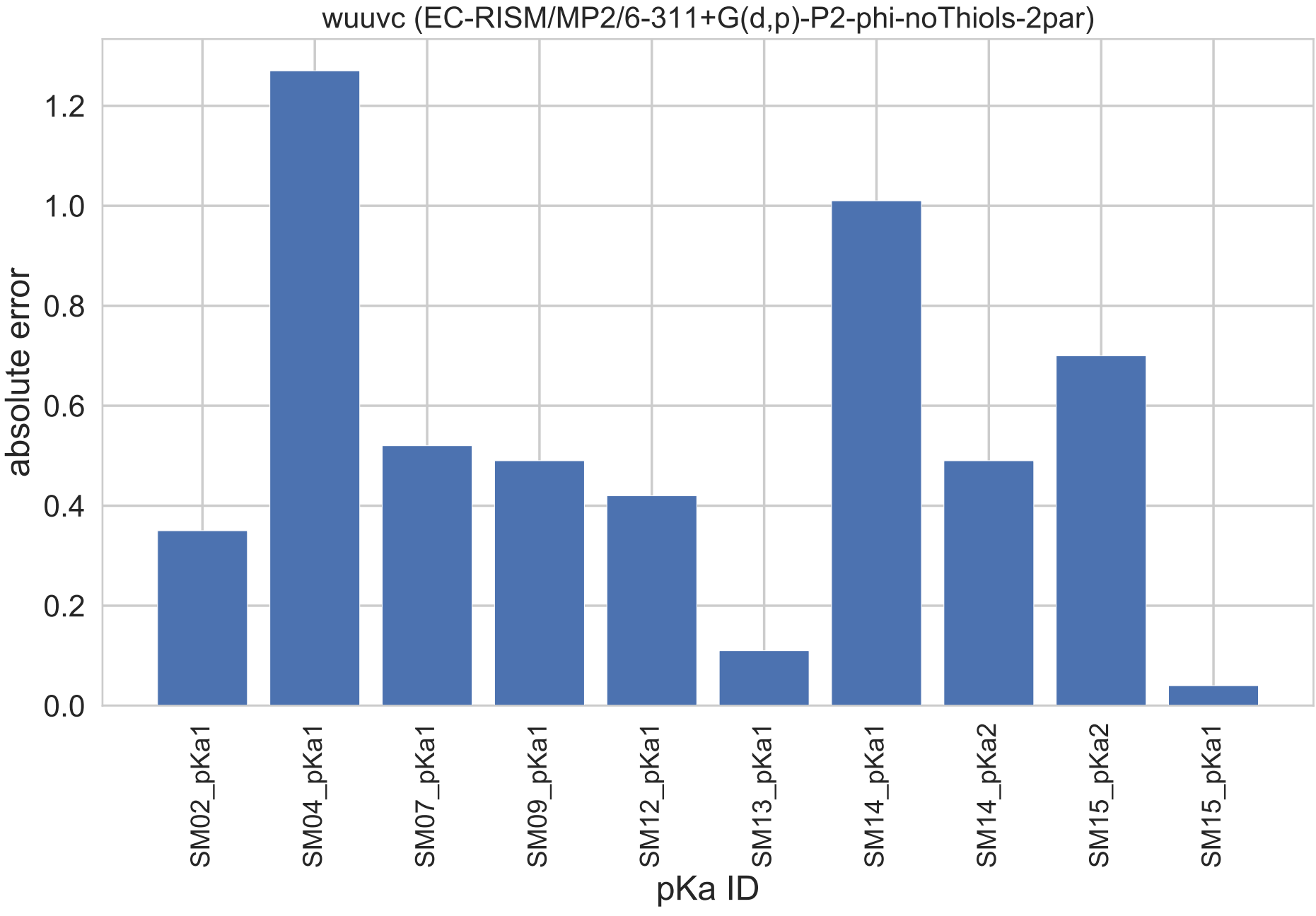
wuuvc (EC-RISM/MP2/6-311+G(d,p)-P2-phi-noThiols-2par)
absolute error
0.0
0.2
0.4
0.6
0.8
1.0
1.2
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa1
SM14_pKa2
SM15_pKa2
SM15_pKa1
pKa ID