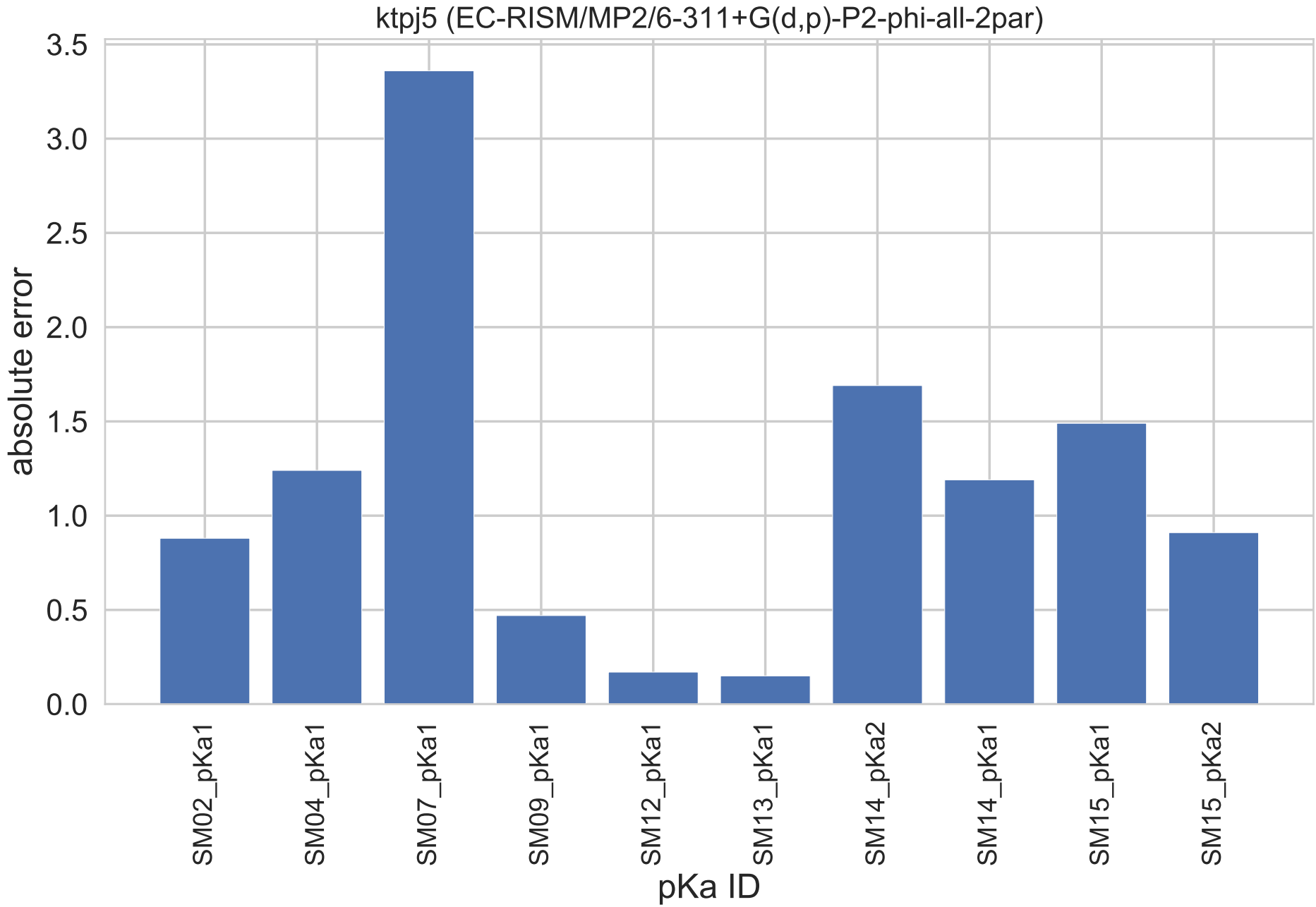
ktpj5 (EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-2par)
absolute error
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa1
SM15_pKa2
pKa ID