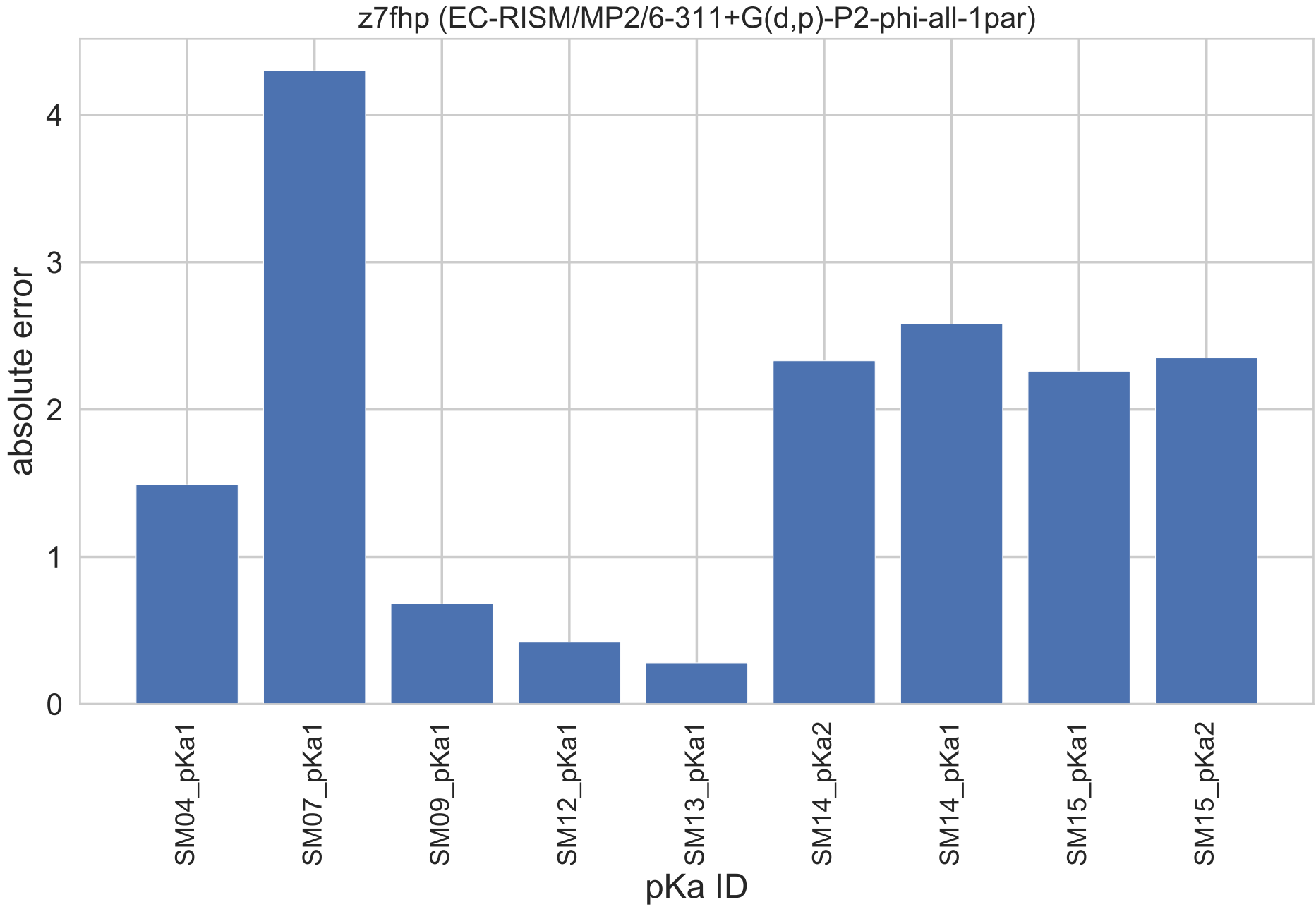
z7fhp (EC-RISM/MP2/6-311+G(d,p)-P2-phi-all-1par)
absolute error
0
1
2
3
4
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa1
SM15_pKa2
pKa ID