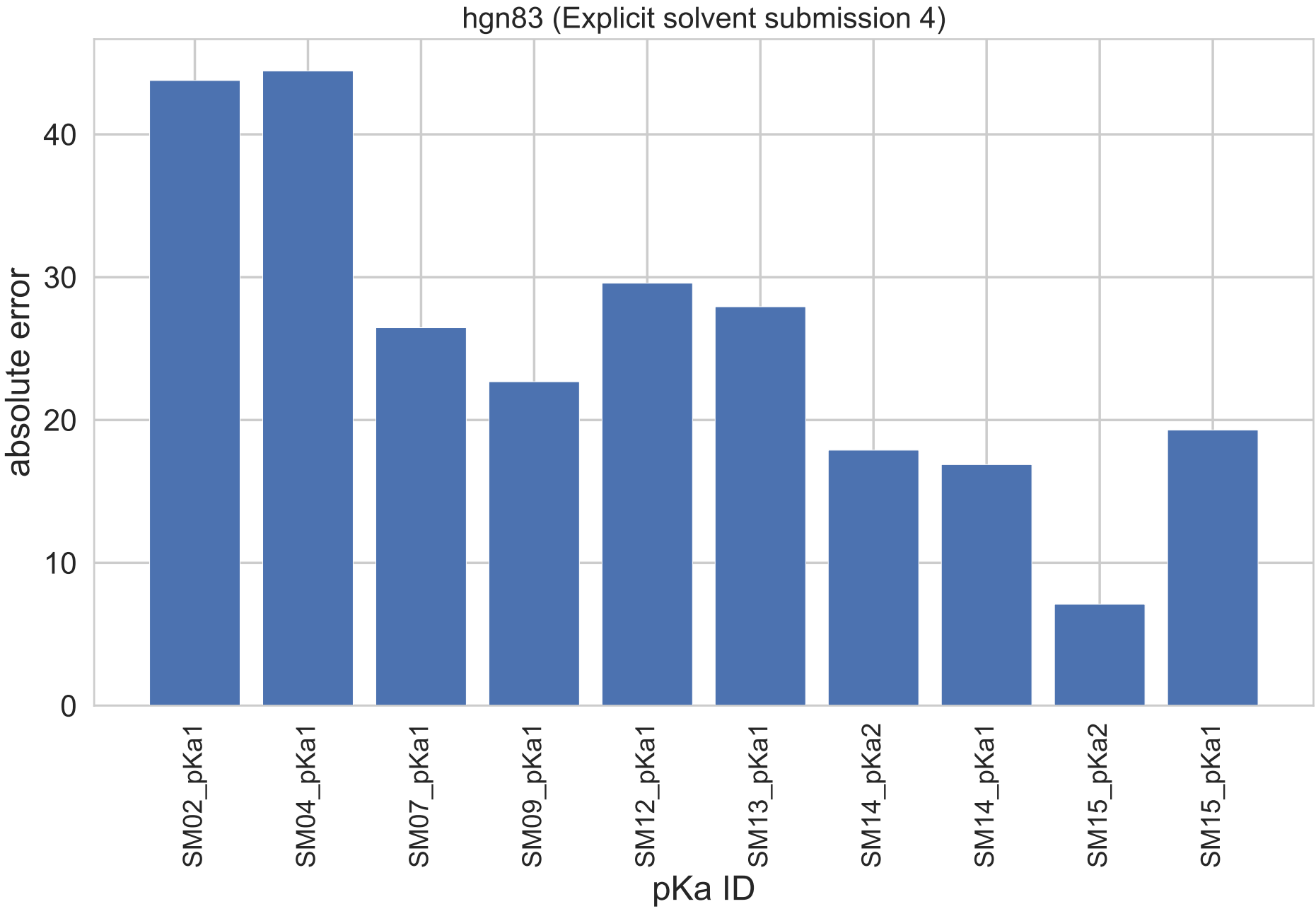
hgn83 (Explicit solvent submission 4)
absolute error
0
10
20
30
40
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa2
SM15_pKa1
pKa ID