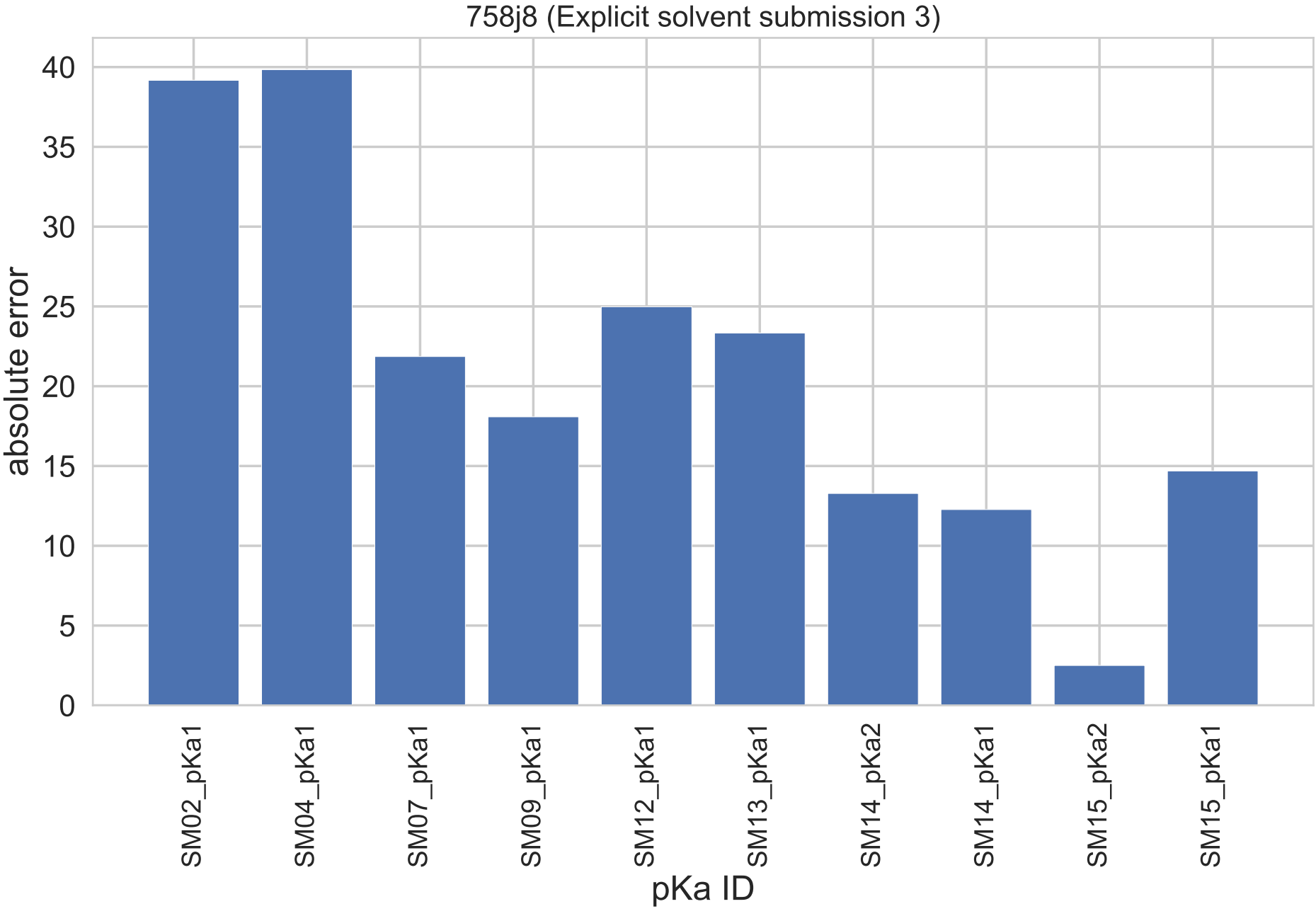
758j8 (Explicit solvent submission 3)
absolute error
0
5
10
15
20
25
30
35
40
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa2
SM14_pKa1
SM15_pKa2
SM15_pKa1
pKa ID