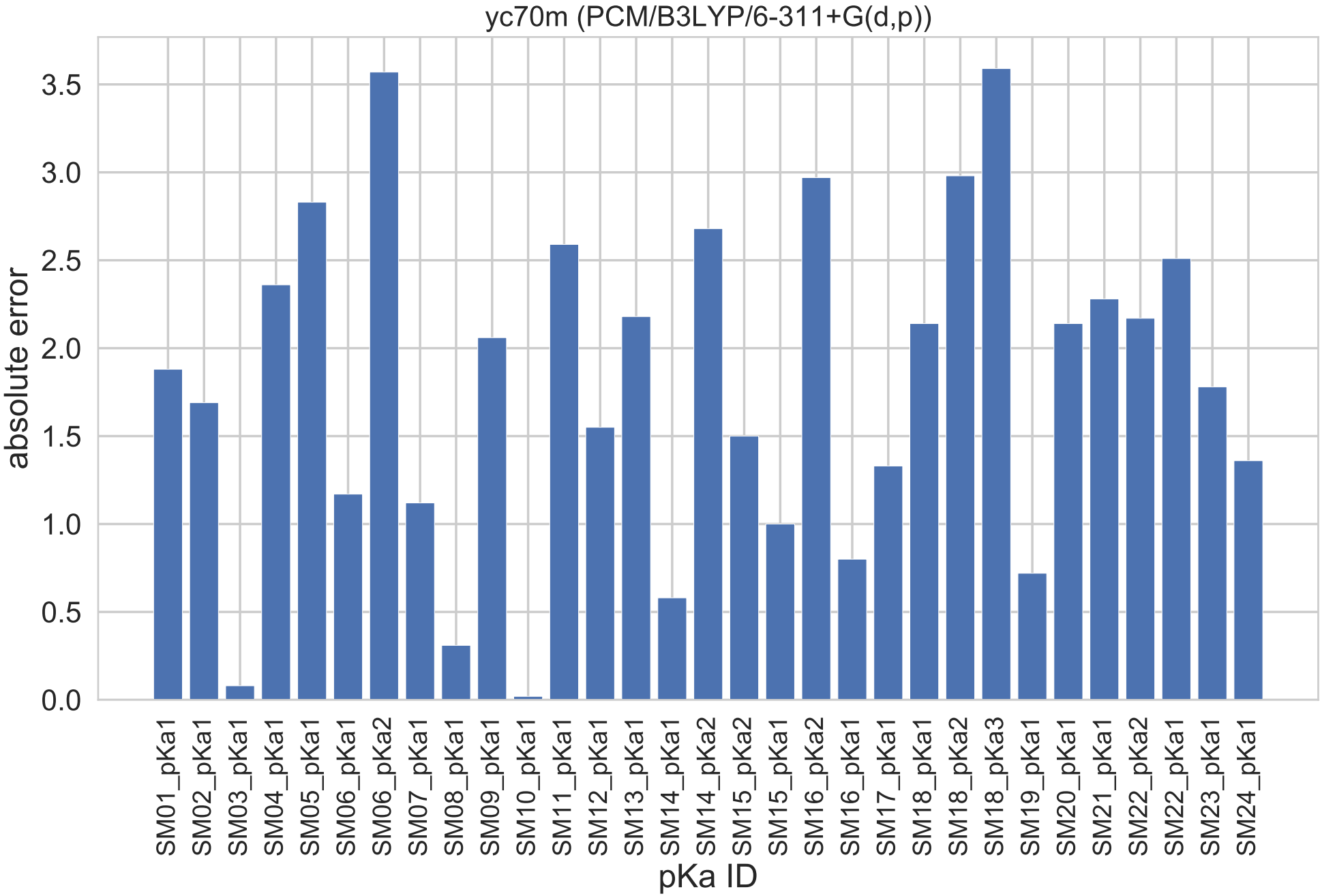
yc70m (PCM/B3LYP/6-311+G(d,p))
absolute error
0.0
0.5
1.0
1.5
2.0
2.5
3.0
3.5
SM01_pKa1
SM02_pKa1
SM03_pKa1
SM04_pKa1
SM05_pKa1
SM06_pKa1
SM06_pKa2
SM07_pKa1
SM08_pKa1
SM09_pKa1
SM10_pKa1
SM11_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa1
SM14_pKa2
SM15_pKa2
SM15_pKa1
SM16_pKa2
SM16_pKa1
SM17_pKa1
SM18_pKa1
SM18_pKa2
SM18_pKa3
SM19_pKa1
SM20_pKa1
SM21_pKa1
SM22_pKa2
SM22_pKa1
SM23_pKa1
SM24_pKa1
pKa ID