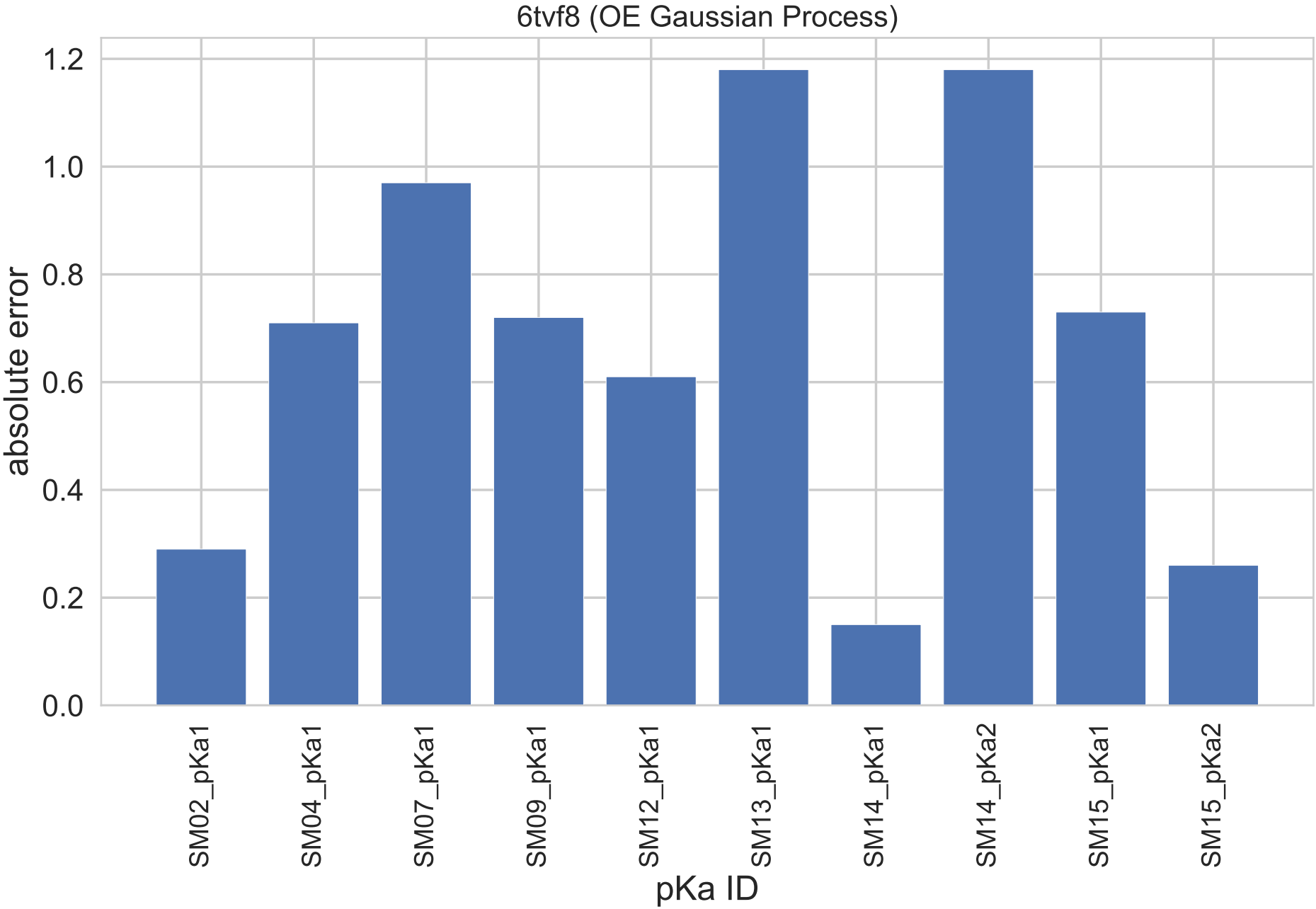
6tvf8 (OE Gaussian Process)
absolute error
1.2
1.0
0.8
0.6
0.4
0.2
0.0
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa1
SM14_pKa2
SM15_pKa1
SM15_pKa2
pKa ID