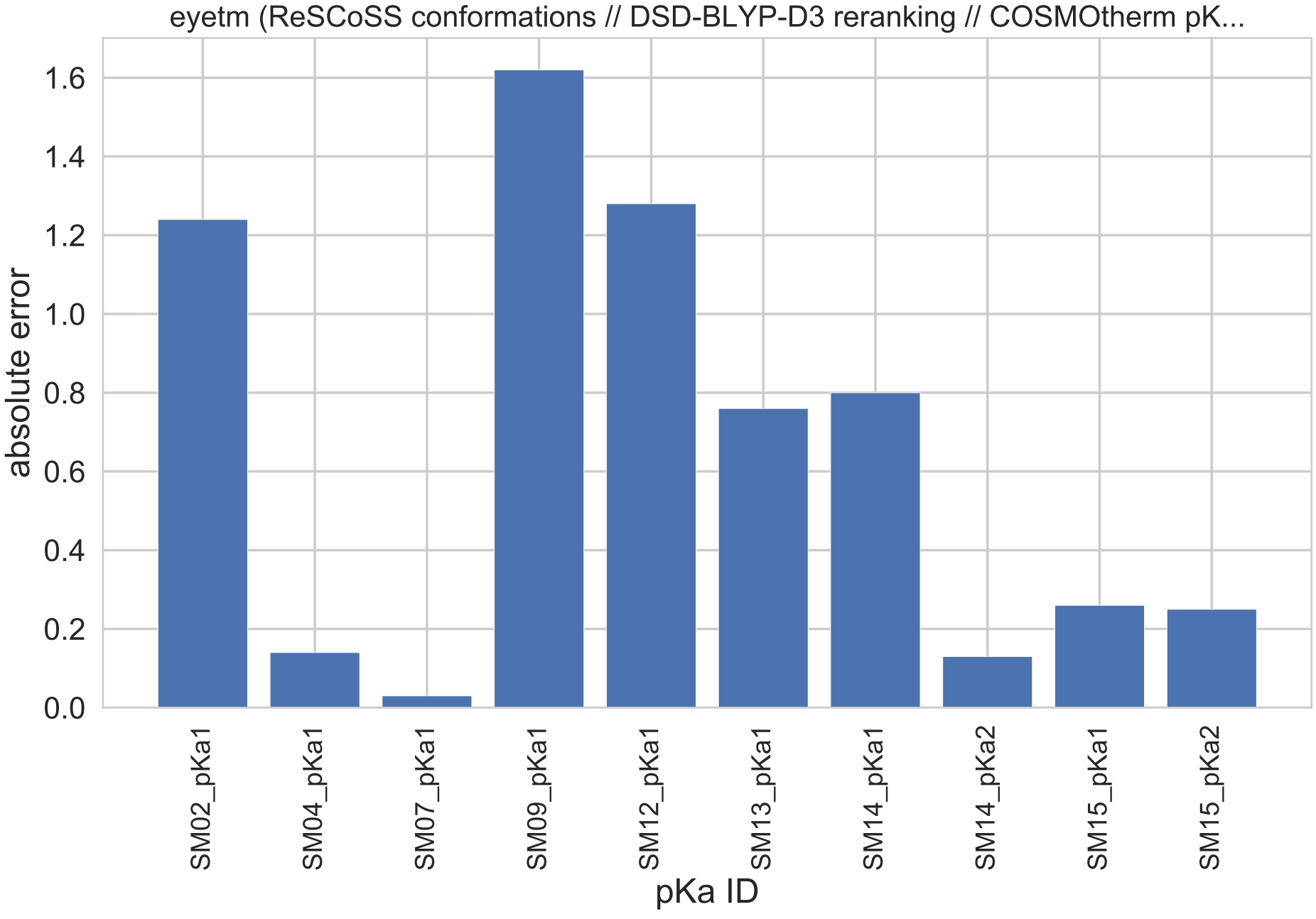
eyetm (ReSCoSS conformations // DSD-BLYP-D3 reranking // COSMOtherm pK...
absolute error
0.0
0.2
0.4
0.6
0.8
1.0
1.2
1.4
1.6
SM02_pKa1
SM04_pKa1
SM07_pKa1
SM09_pKa1
SM12_pKa1
SM13_pKa1
SM14_pKa1
SM14_pKa2
SM15_pKa1
SM15_pKa2
pKa ID