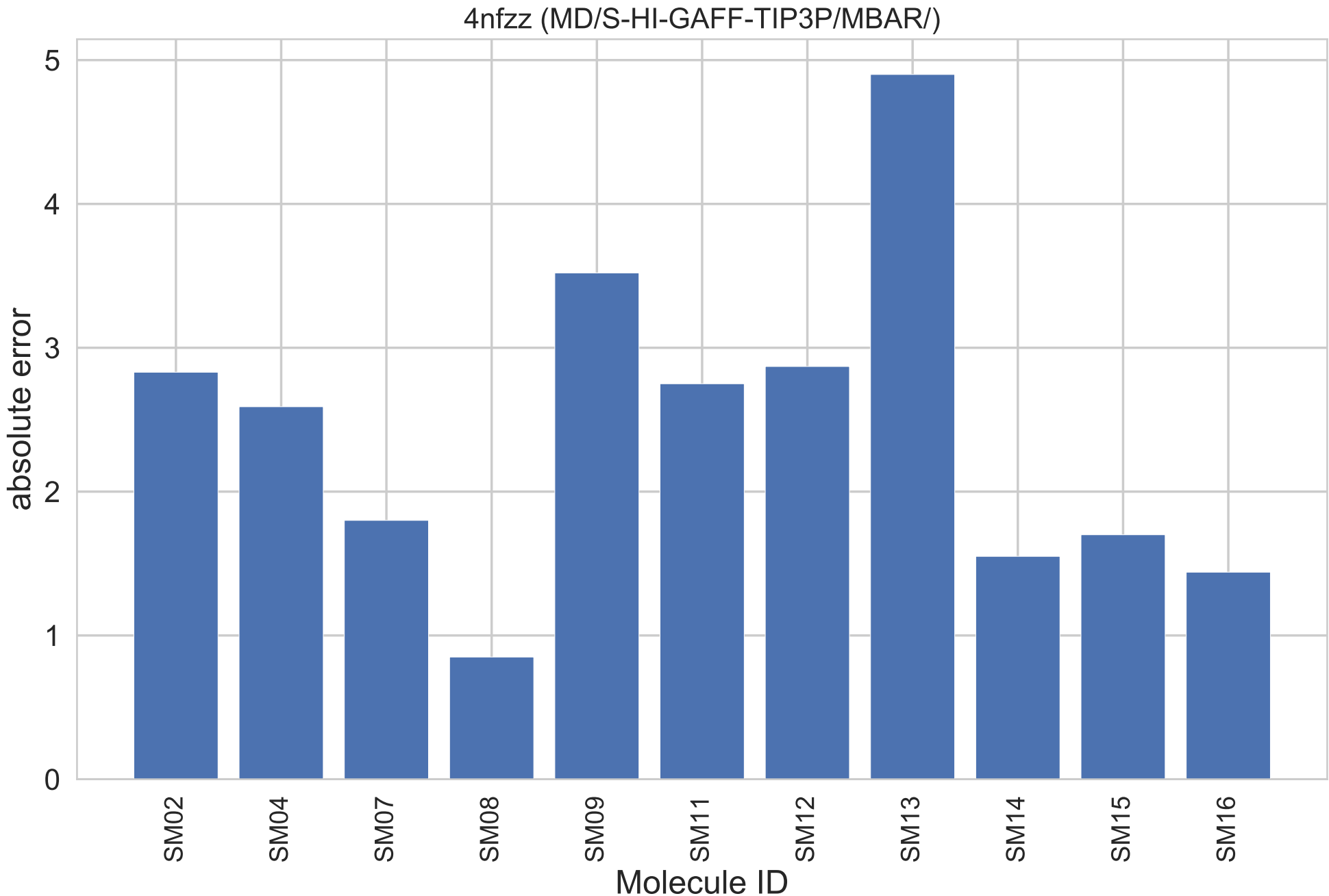
4nfzz (MD/S-HI-GAFF-TIP3P/MBAR/)
absolute error
0
1
2
3
4
5
SM02
SM04
SM07
SM08
SM09
SM11
SM12
SM13
SM14
SM15
SM16
Molecule ID