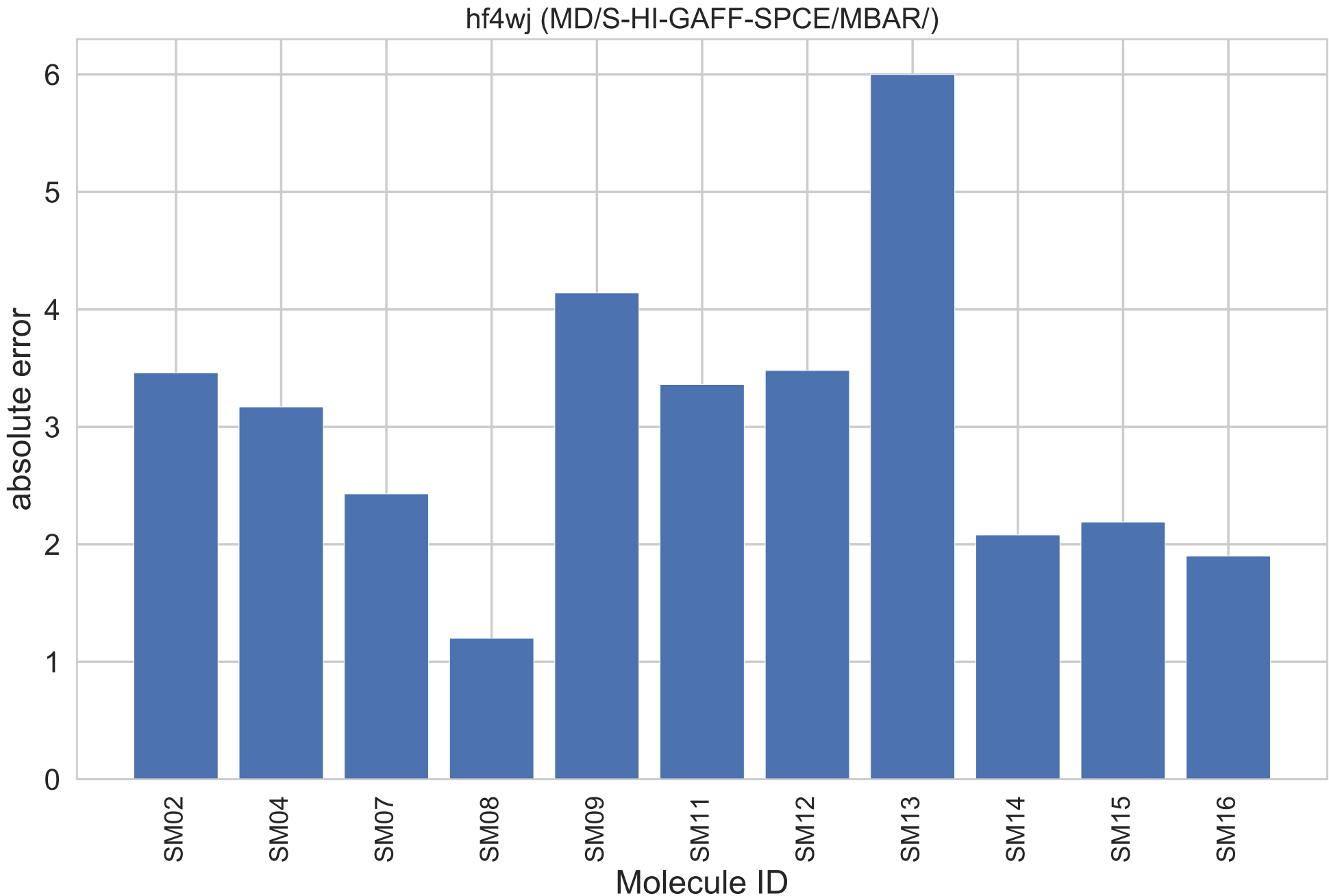
hf4wj (MD/S-HI-GAFF-SPCE/MBAR/)
absolute error
0
1
2
3
4
5
6
SM02
SM04
SM07
SM08
SM09
SM11
SM12
SM13
SM14
SM15
SM16
Molecule ID