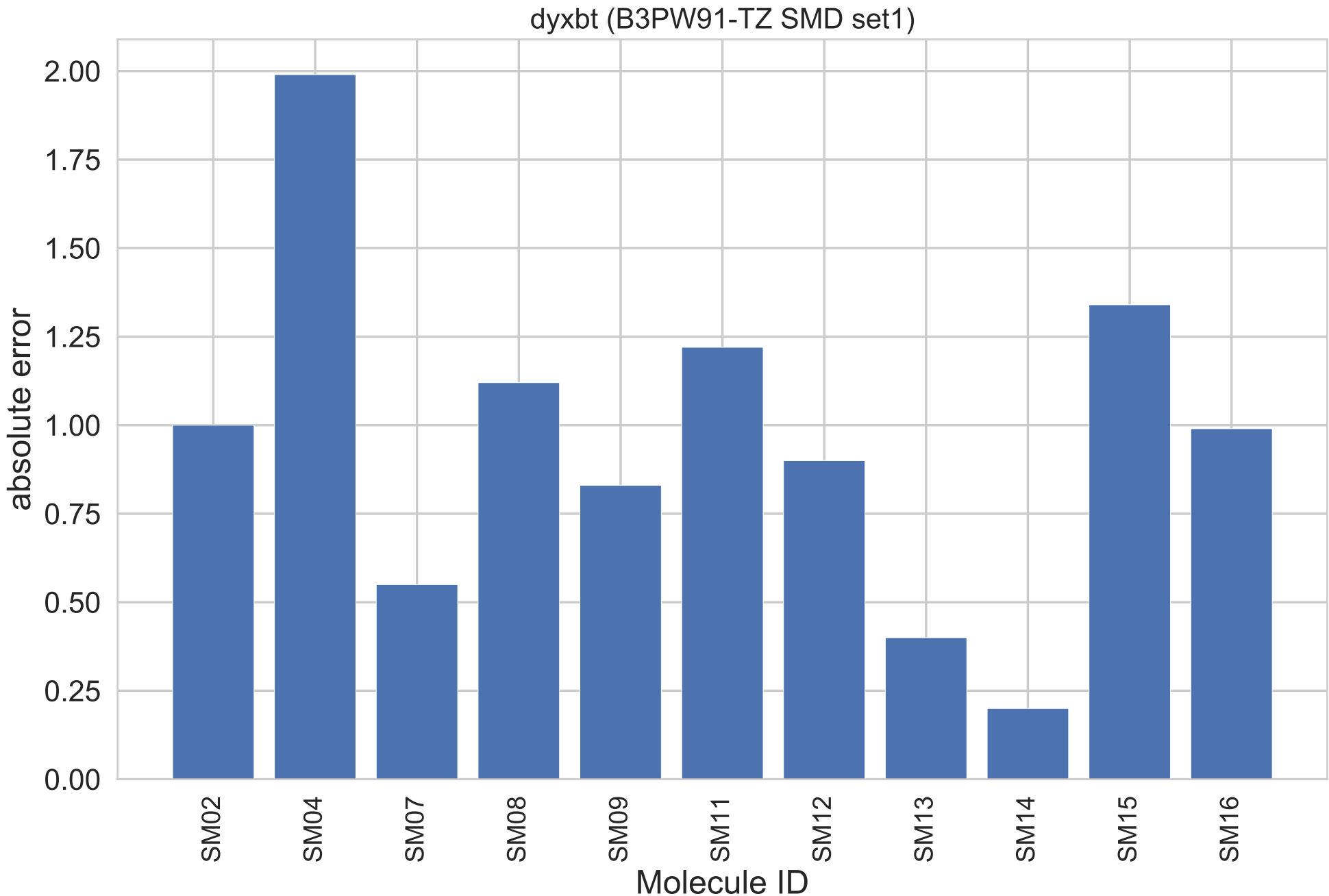
dyxbt (B3PW91-TZ SMD set1)
absolute error
2.00
1.75
1.50
1.25
1.00
0.75
0.50
0.25
0.00
SM02
SM04
SM07
SM08
SM09
SM11
SM12
SM13
SM14
SM15
SM16
Molecule ID