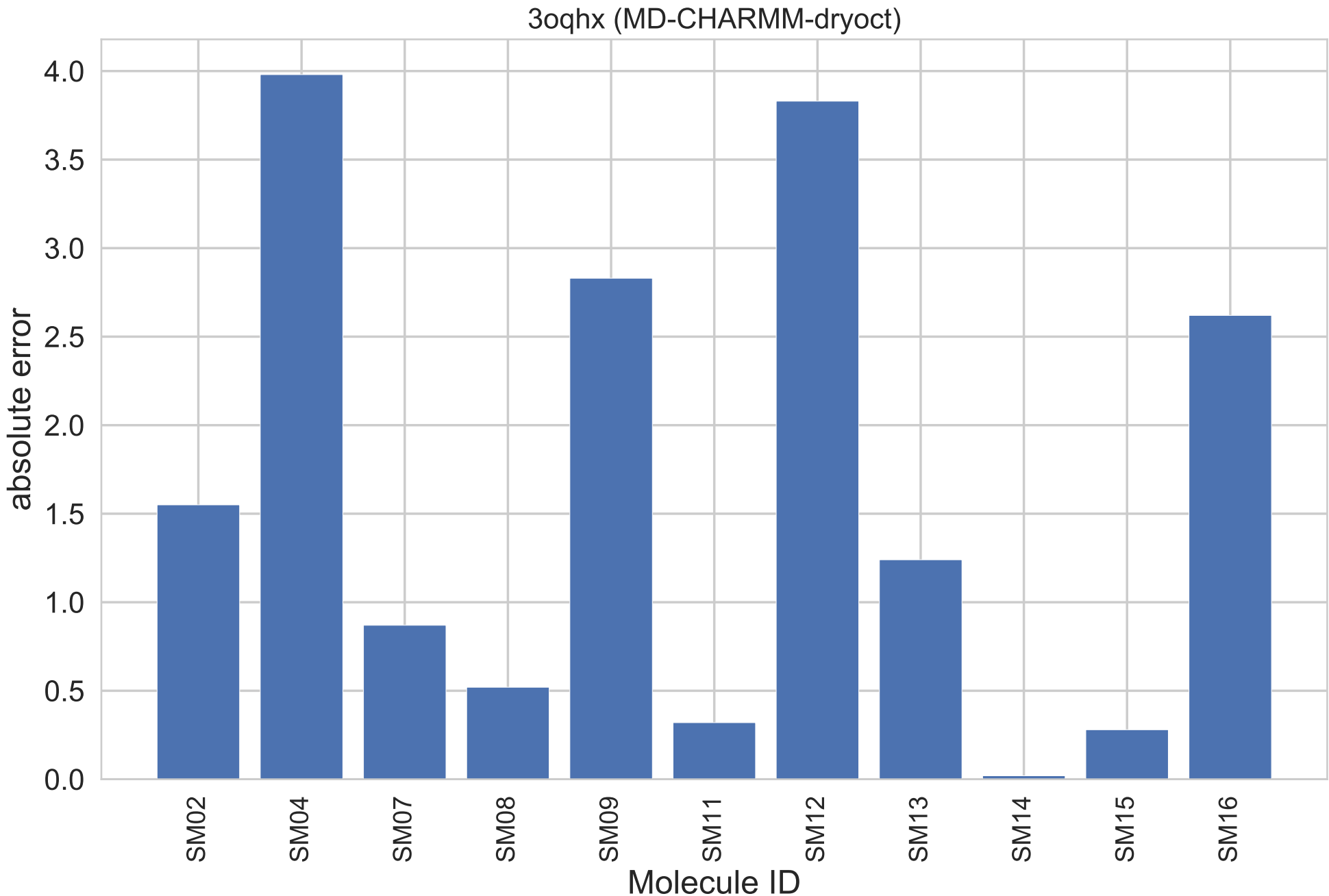
3oqhx (MD-CHARMM-dryoct)
absolute error
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
SM02
SM04
SM07
SM08
SM09
SM11
SM12
SM13
SM14
SM15
SM16
Molecule ID