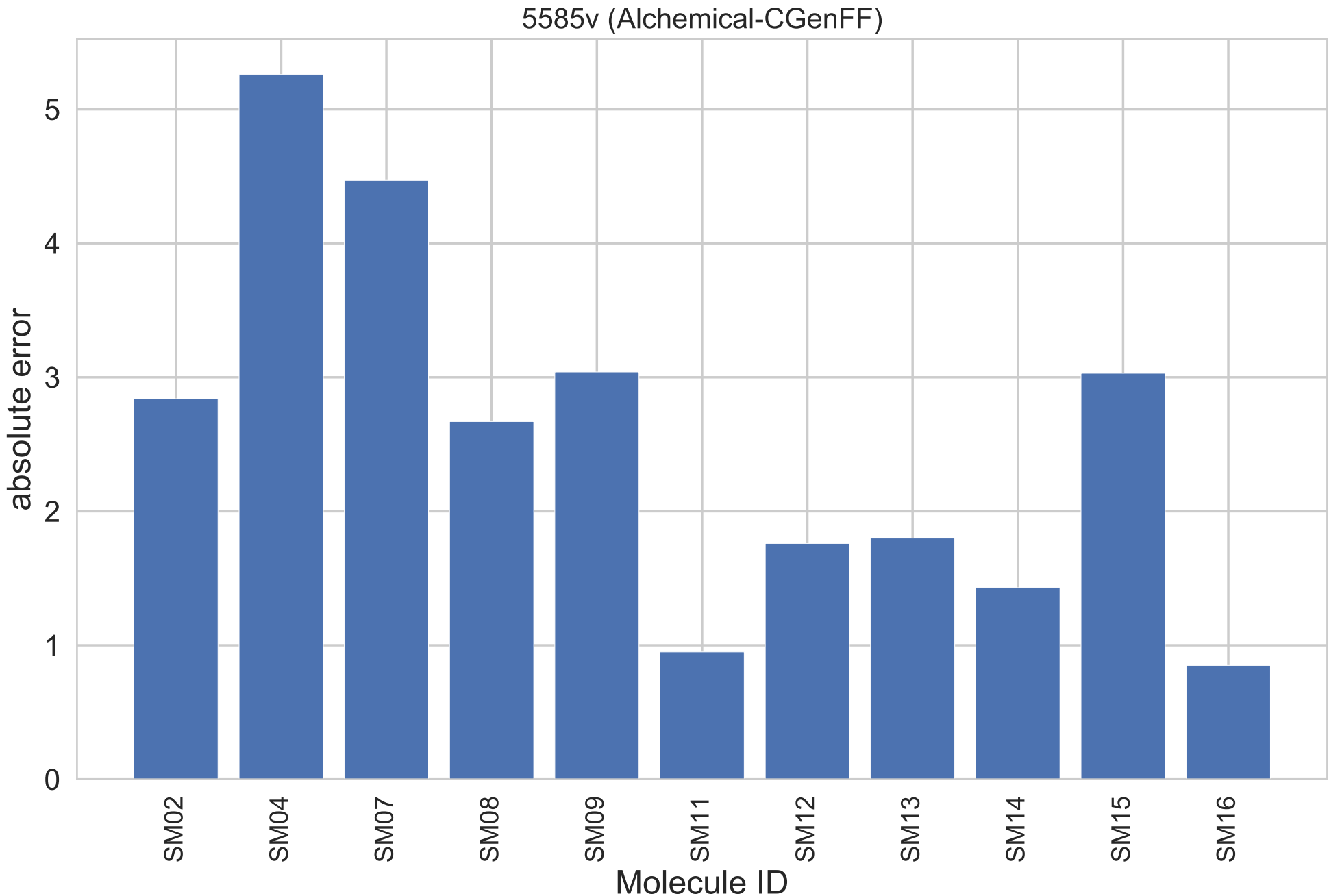
5585v (Alchemical-CGenFF)
absolute error
0
1
2
3
4
5
SM02
SM04
SM07
SM08
SM09
SM11
SM12
SM13
SM14
SM15
SM16
Molecule ID