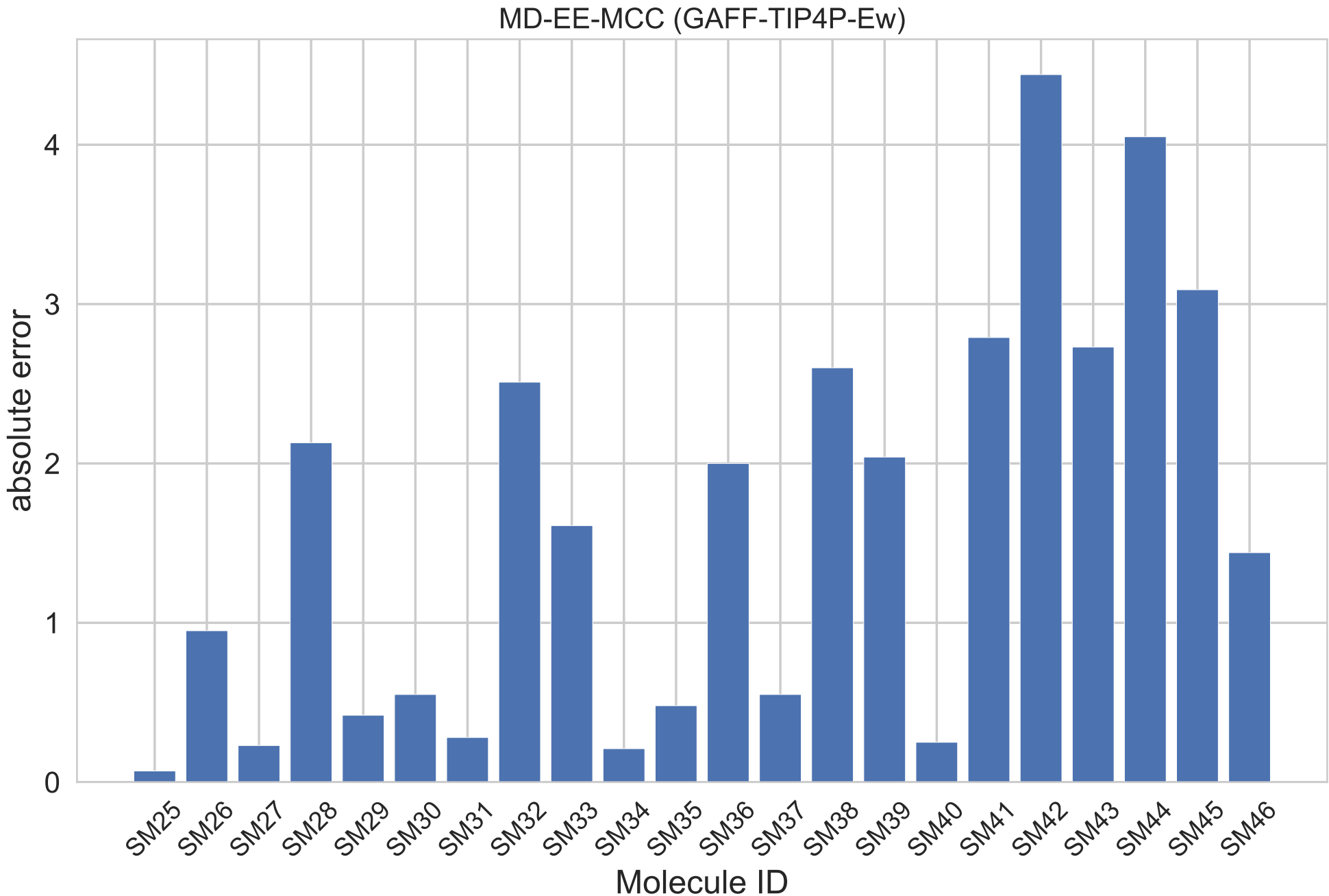
MD-EE-MCC (GAFF-TIP4P-Ew)
absolute error
0
1
2
3
4
SM25
SM26
SM27
SM28
SM29
SM30
SM31
SM32
SM33
SM34
SM35
SM36
SM37
SM38
SM39
SM40
SM41
SM42
SM43
SM44
SM45
SM46
Molecule ID