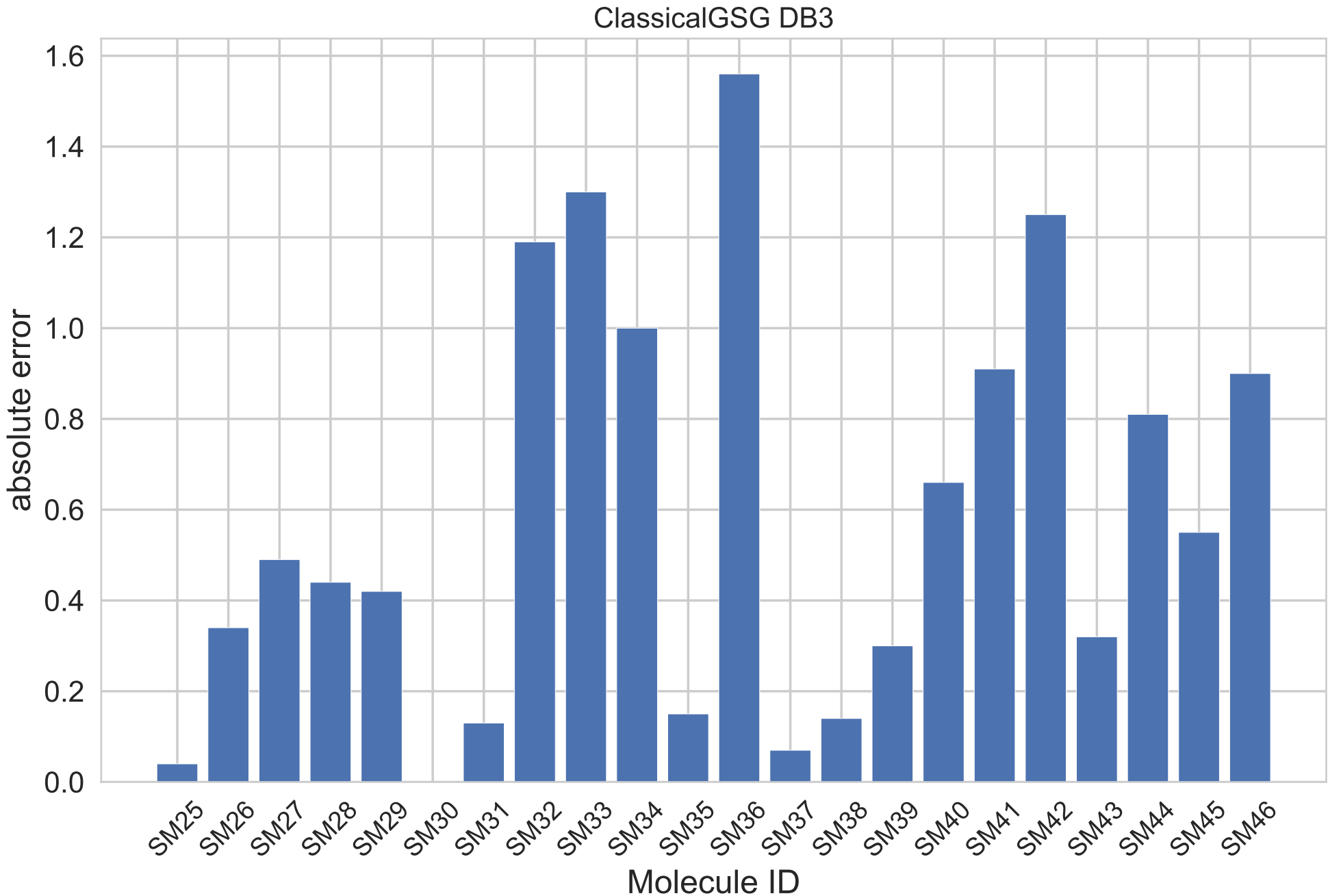
ClassicalGSG DB3
absolute error
1.6
1.4
1.2
1.0
0.8
0.6
0.4
0.2
0.0
SM25
SM26
SM27
SM28
SM29
SM30
SM31
SM32
SM33
SM34
SM35
SM36
SM37
SM38
SM39
SM40
SM41
SM42
SM43
SM44
SM45
SM46
Molecule ID