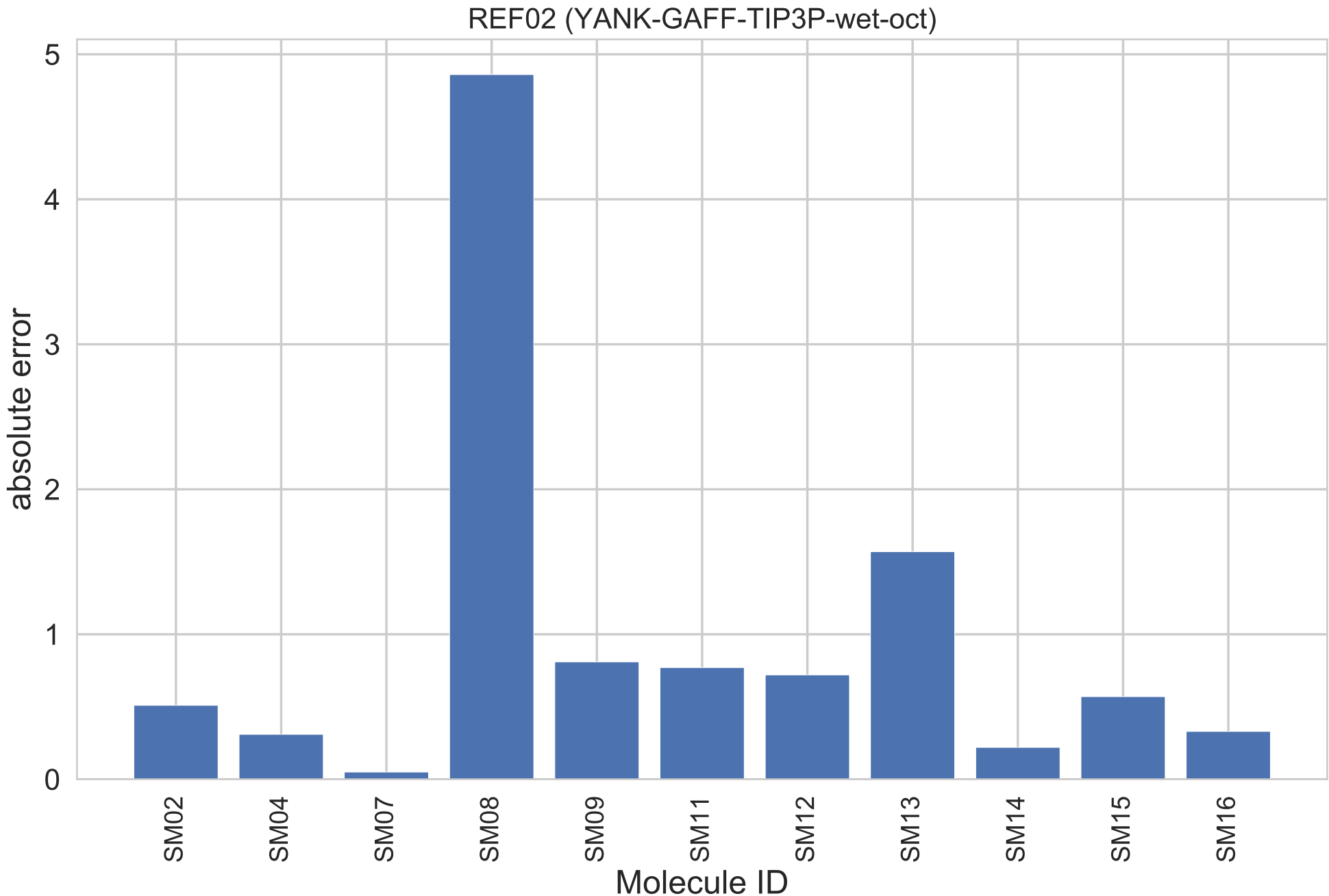
REF02 (YANK-GAFF-TIP3P-wet-oct)
absolute error
0
1
2
3
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SM02
SM04
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SM12
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SM16
Molecule ID