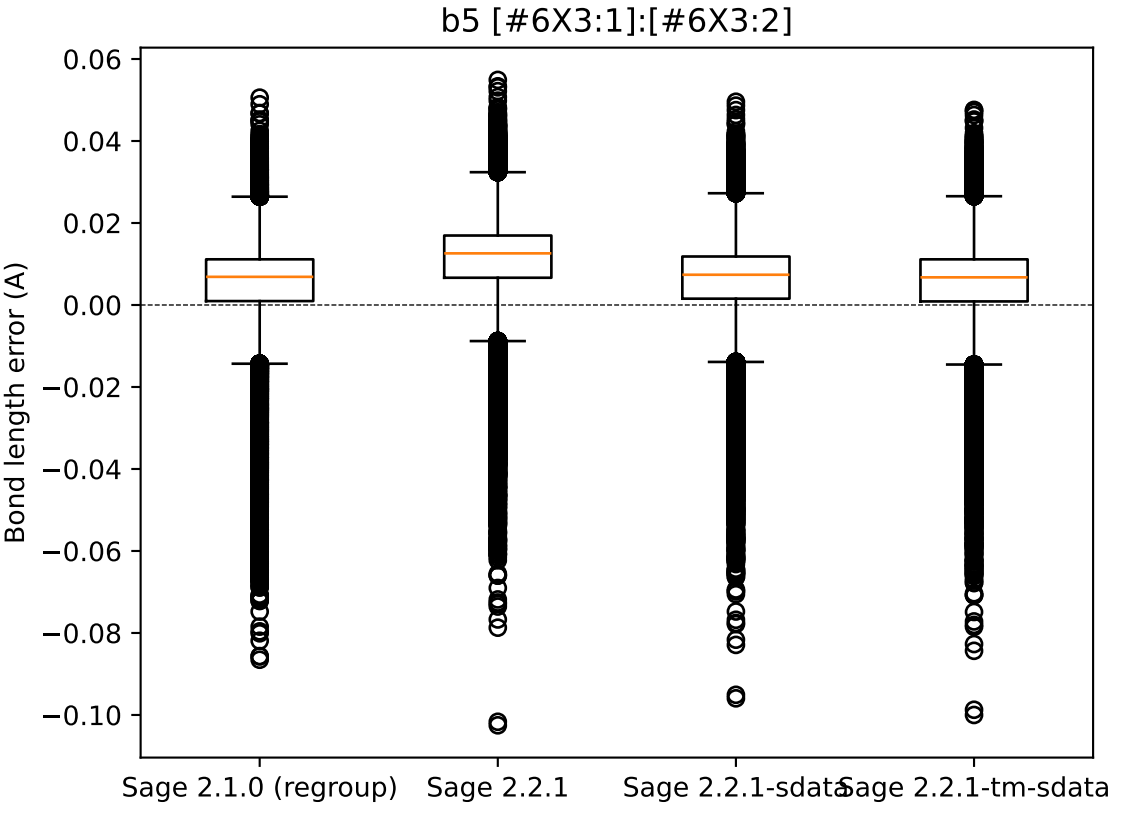
b5 [#6X3:1]:[#6X3:2]
Bond length error (A)
0.06
0.04
0.02
0.00
−0.02
−0.04
−0.06
−0.08
−0.10
Sage 2.1.0 (regroup)
Sage 2.2.1
Sage 2.2.1-sdata
Sage 2.2.1-tm-sdata