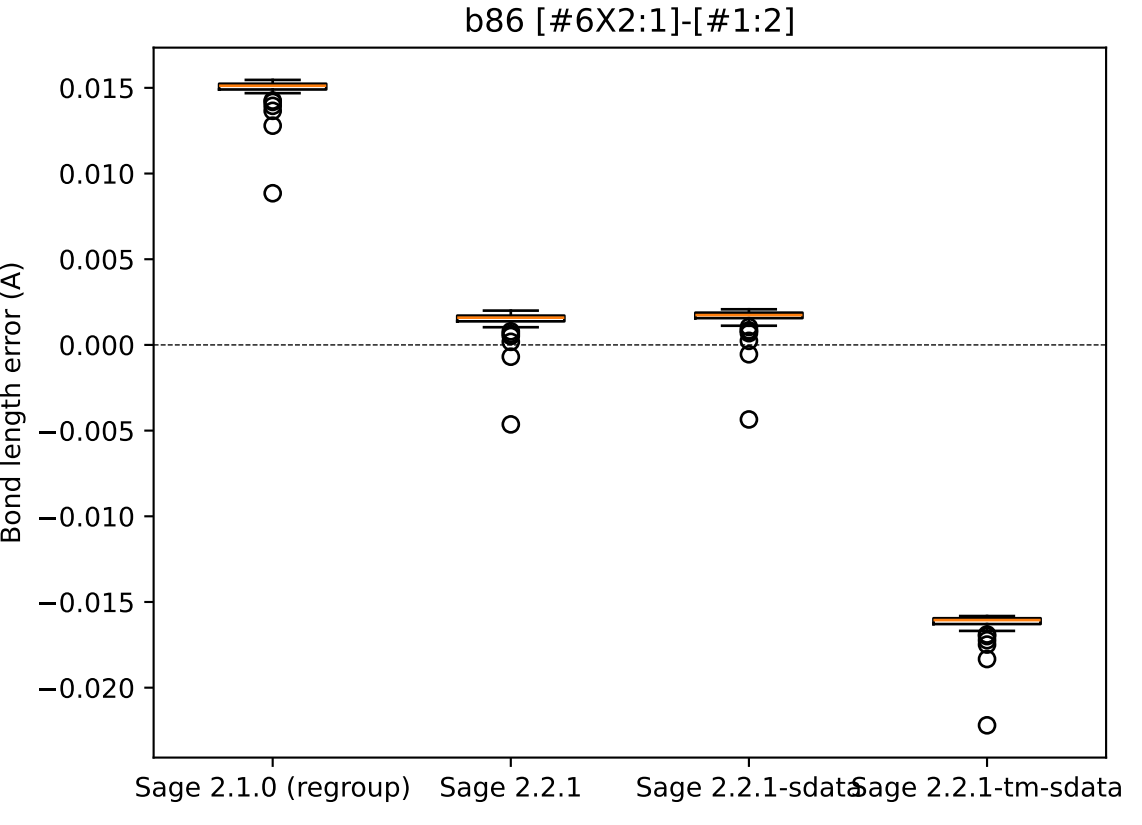
b86 [#6X2:1]-[#1:2]
Bond length error (A)
0.015
0.010
0.005
0.000
−0.005
−0.010
−0.015
−0.020
Sage 2.1.0 (regroup)
Sage 2.2.1
Sage 2.2.1-sdata
Sage 2.2.1-tm-sdata