b72 [#6:1]-[#35:2] 40 Sage 2.1.0 (regroup) Sage 2.2.1 35 Sage 2.2.1-sdata Sage 2.2.1-tm-sdata 30 25 Count 20 15 10 5 0.04 -0.03-0.02-0.010.00 0.01 0.02 0.03 0.05

Bond length error (A)