b24 [#6X2:1]-[#6:2] 700 Sage 2.1.0 (regroup) Sage 2.2.1 600 Sage 2.2.1-sdata 500 400 Count 300 200 100 0 -0.03-0.02-0.010.03 0.04 0.00 0.01 0.02

Bond length error (A)