b16 [#6X4:1]-[#8X2H0:2] 1400 Sage 2.1.0 (regroup) Sage 2.2.1 Sage 2.2.1-sdata 1200 Sage 2.2.1-tm-sdata 1000 800 Count 600 400 200 0 -0.20-0.15-0.10-0.050.05 0.10 0.00

Bond length error (A)