b10 [#6X3:1](=[#8X1+0])-[#7X3:2] Sage 2.1.0 (regroup) 4000 Sage 2.2.1 Sage 2.2.1-sdata 3500 3000 2500 Count 2000 1500 1000 500 0 -0.10-0.050.00 0.05

Bond length error (A)