b59 [#16X4,#16X3:1]~[#8X1:2] Sage 2.1.0 (regroup) 3500 Sage 2.2.1 Sage 2.2.1-sdata 3000 2500 2000 1500 1000 500 0 -0.06-0.04-0.020.02 0.04 0.00

Bond length error (A)