b86 [#6X2:1]-[#1:2] 60 Sage 2.1.0 (regroup) Sage 2.2.1 Sage 2.2.1-sdata 50 40 Count 30 20 10

-0.0050-0.00250.0000 0.0025 0.0050 0.0075 0.0100 0.0125 0.0150 Bond length error (A)