b52 [#16X2,#16X1-1,#16X3+1:1]-[#6X3:2] 0 0 0 0 0 0 0

0.05

0.00

-0.05

-0.10

-0.15

-0.20

-0.25

Bond length error (A)

Sage 2.1.0 (regroup) Sage 2.2.1 Sage 2.2.1-sdat&age 2.2.1-tm-sdata