

-- STATS maxD --

min ESS = 140.667595900426

max BMK = 0.14702016661042

max MCSE = 7.21300393553351

all stationary: FALSE

burn: 0

max rel.err.: 1.92020151897835

-- STATS 2D --

min ESS = 1895.52777906317

max BMK = 0.0643941796923661

max MCSE = 2.60392035320313

all stationary: TRUE

burn: 0

max rel.err.: 1.81066157426604

-- STATS 1D --

min ESS = 2048

max BMK = 0.067761729728456

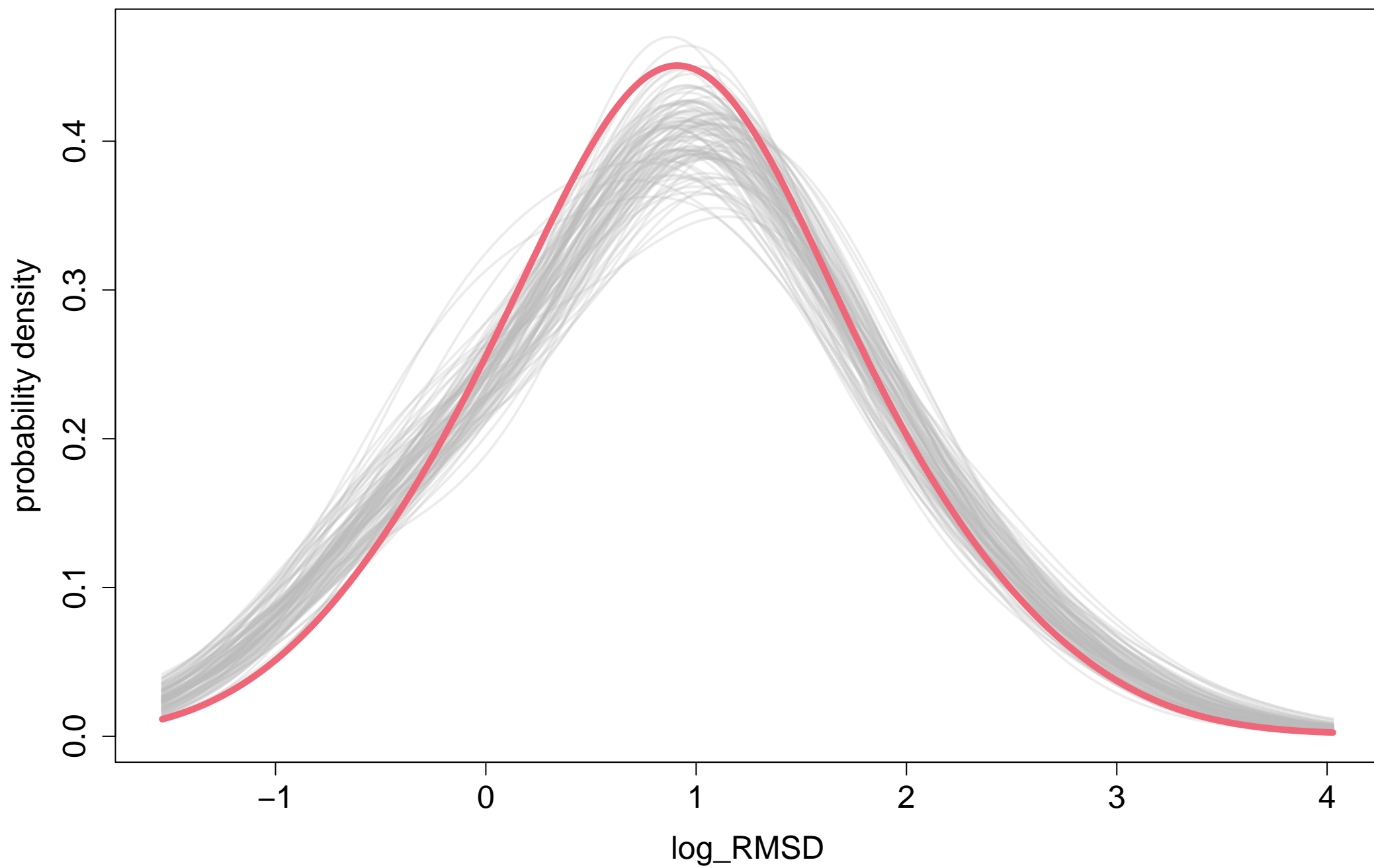
max MCSE = 2.42055275469433

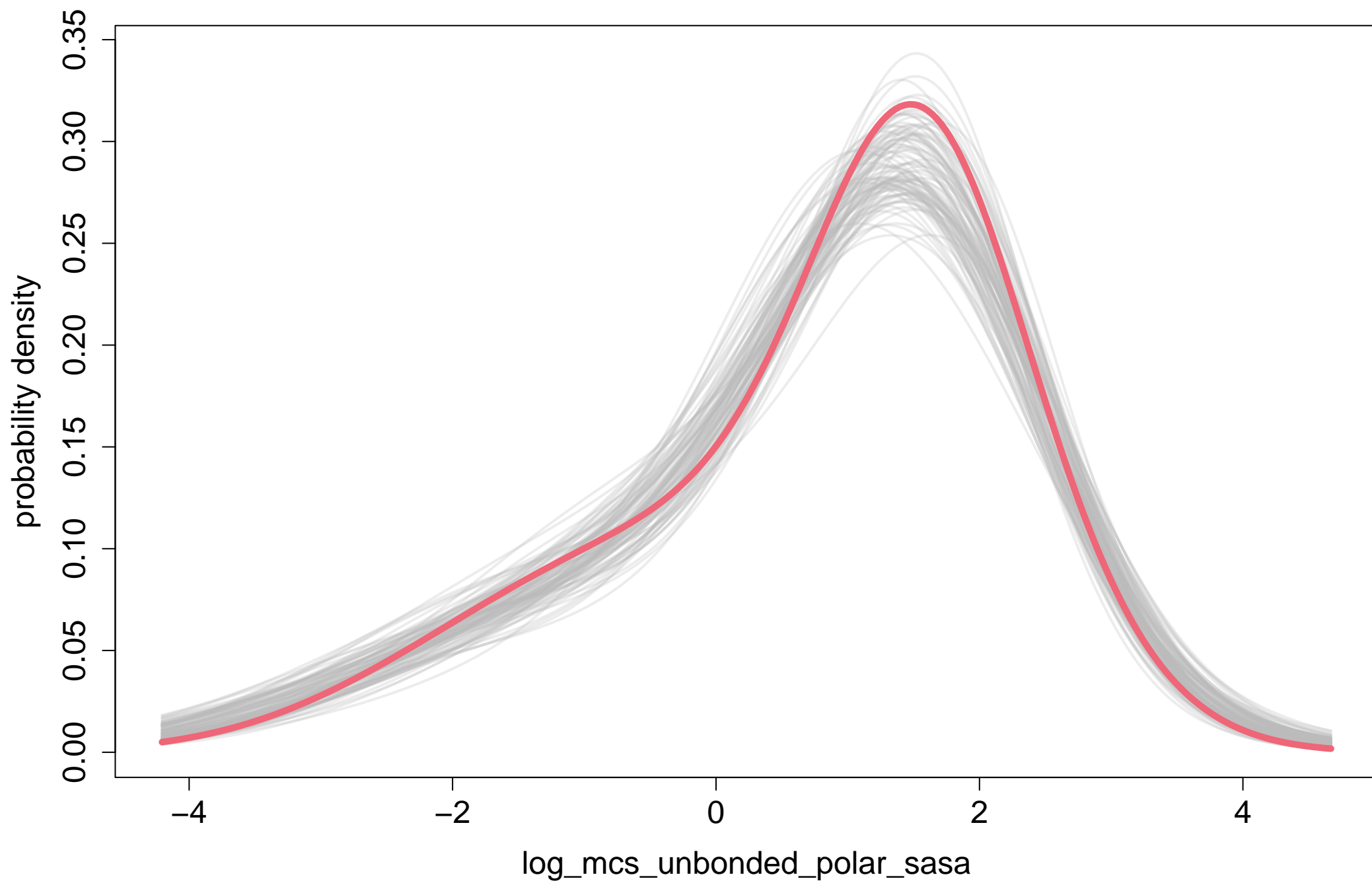
all stationary: TRUE

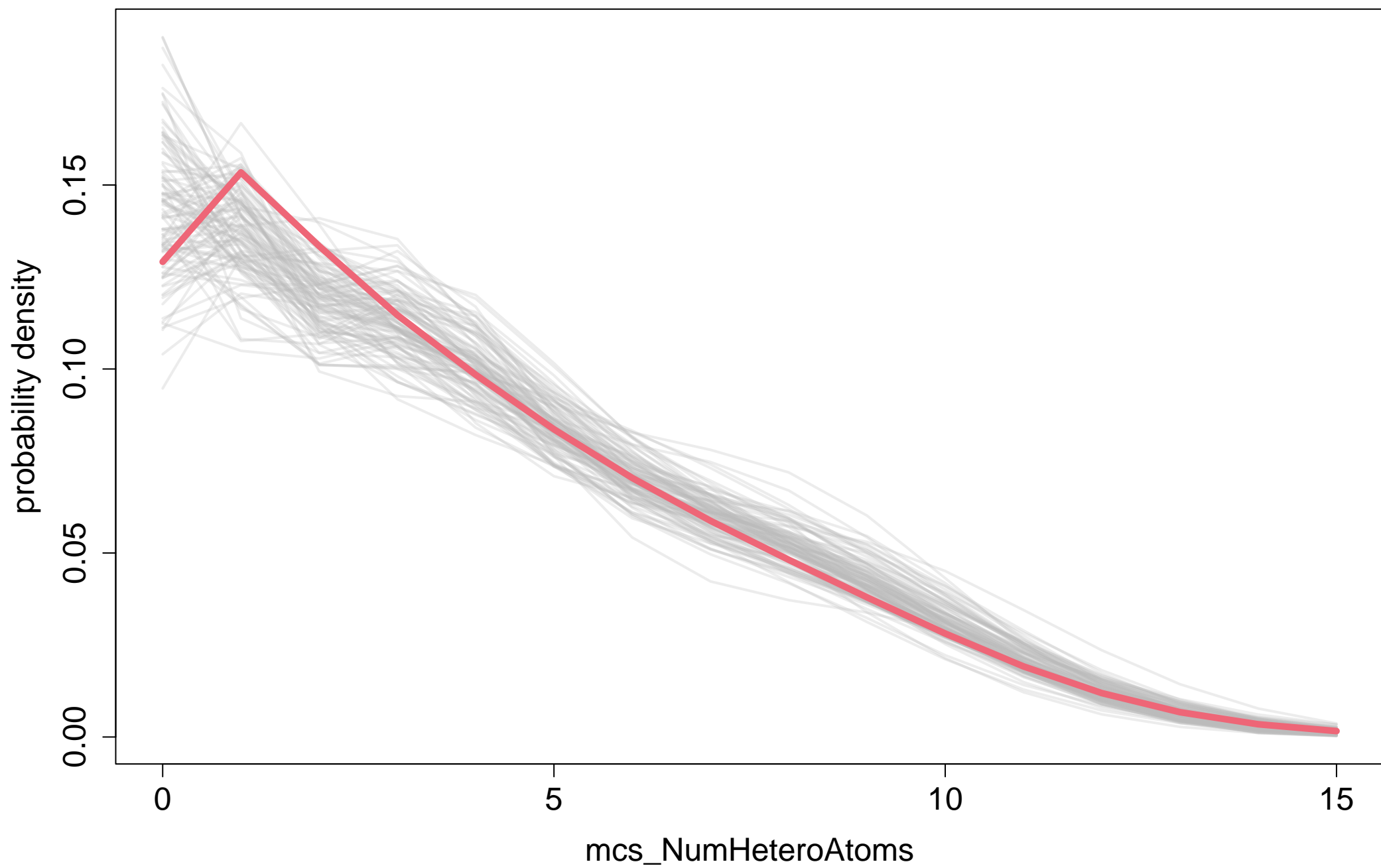
burn: 0

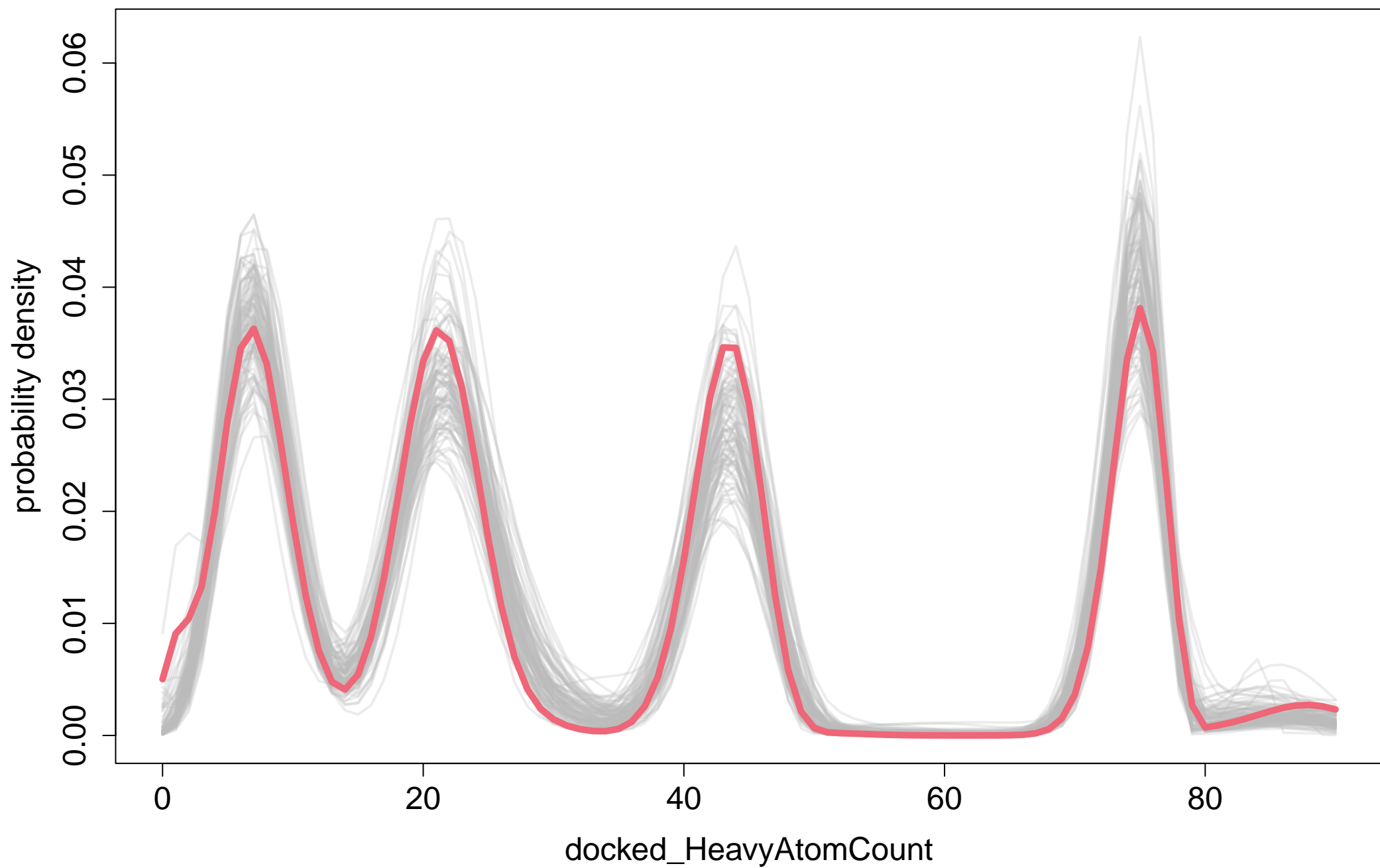
max rel.err.: 2.27123814715788

LL: -2200 +- 13.1

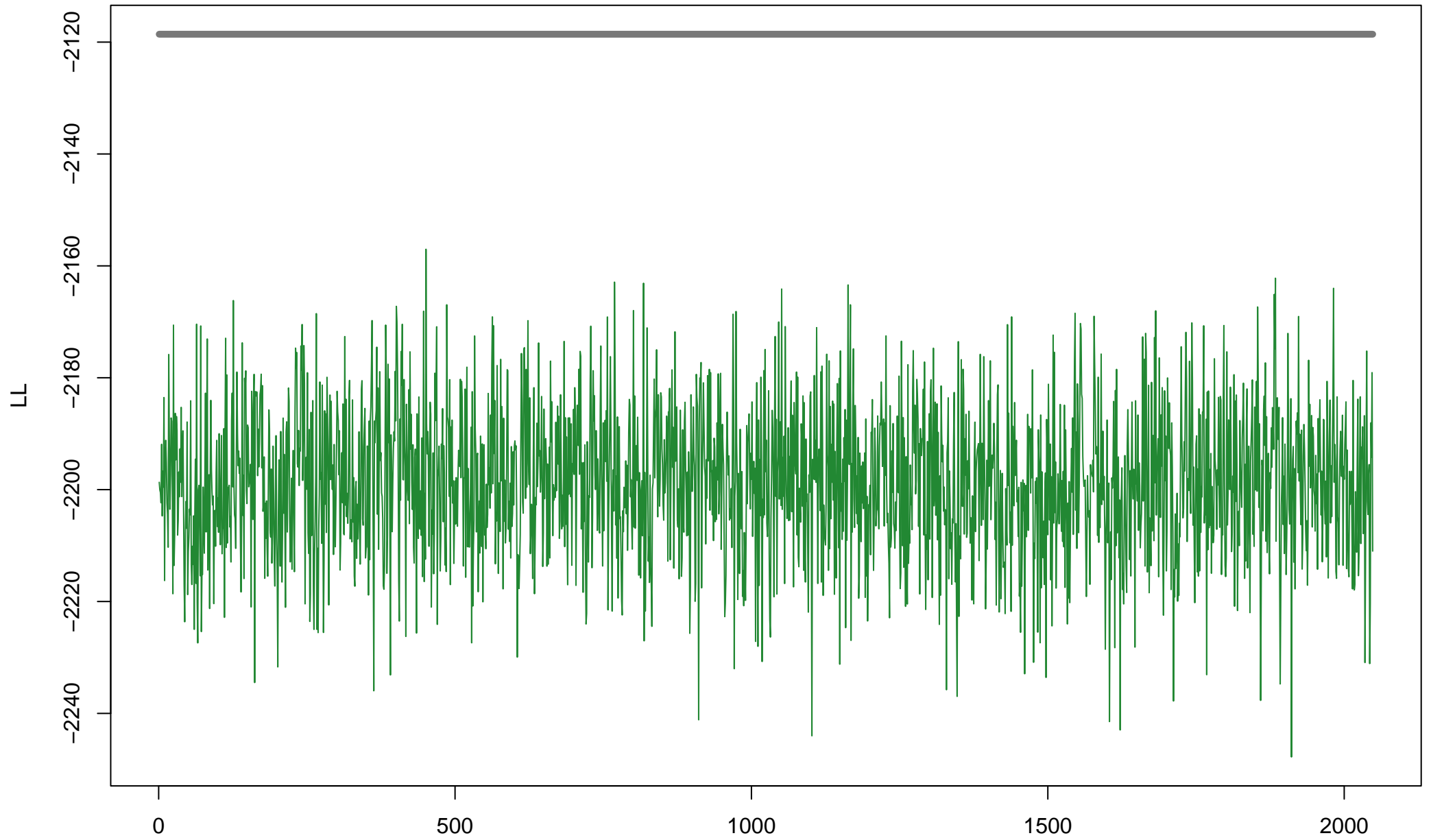




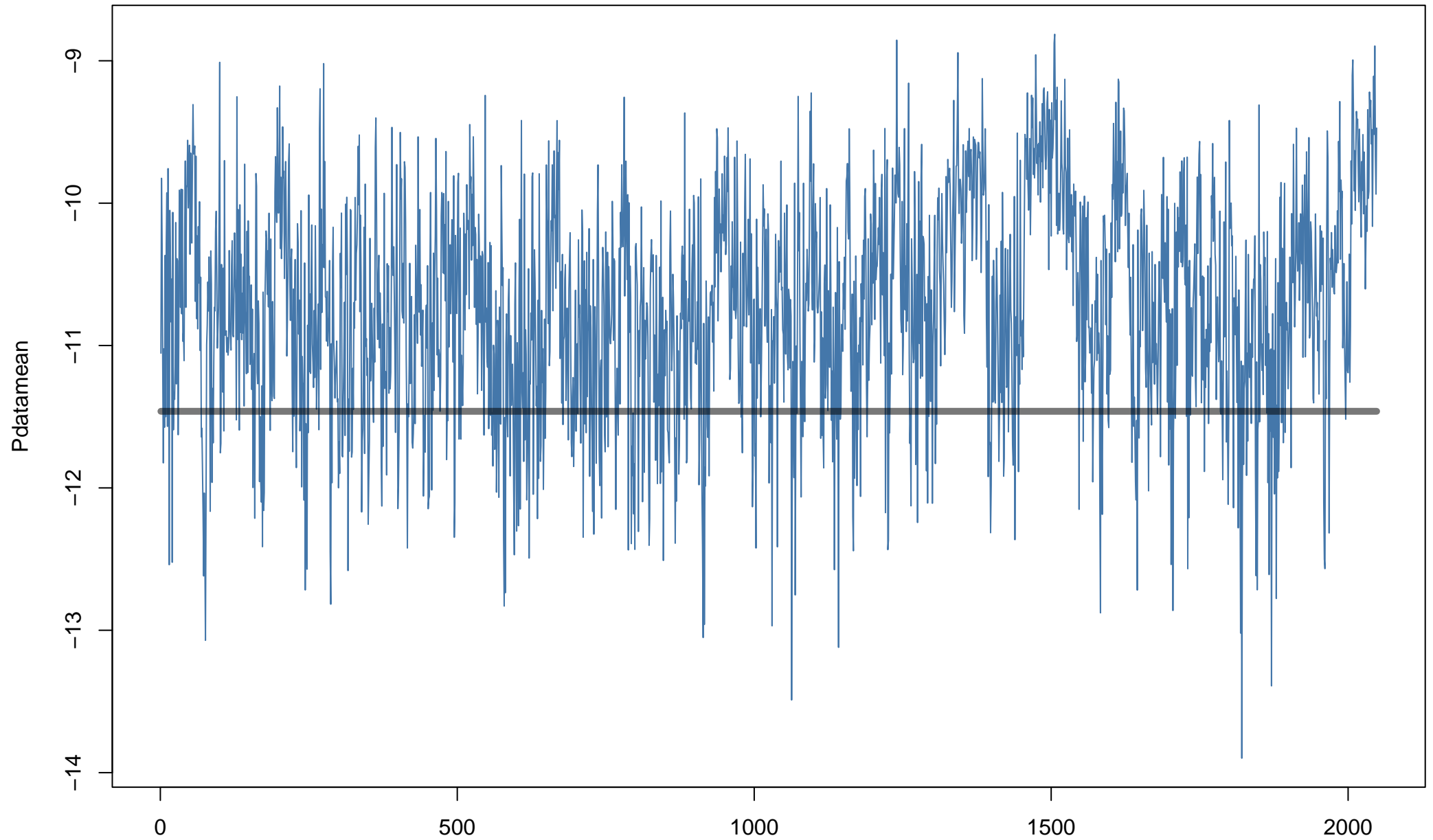




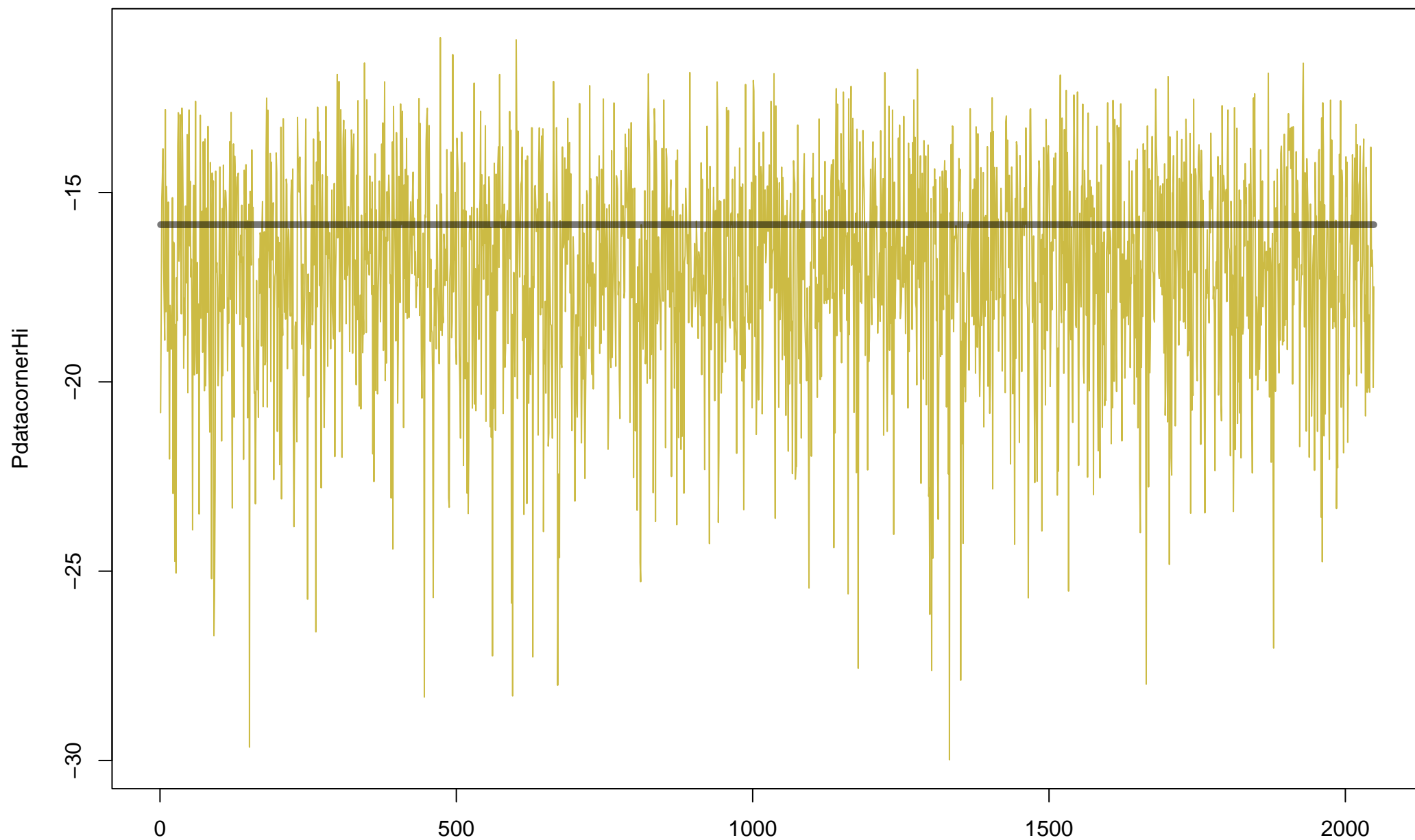
LL



**Pdatamean**  
**ESS = 141 | BMK = 0.147 | MCSE(6.27) = 7.21 | stat: TRUE | burn: 0 | rel.err: 0.855**

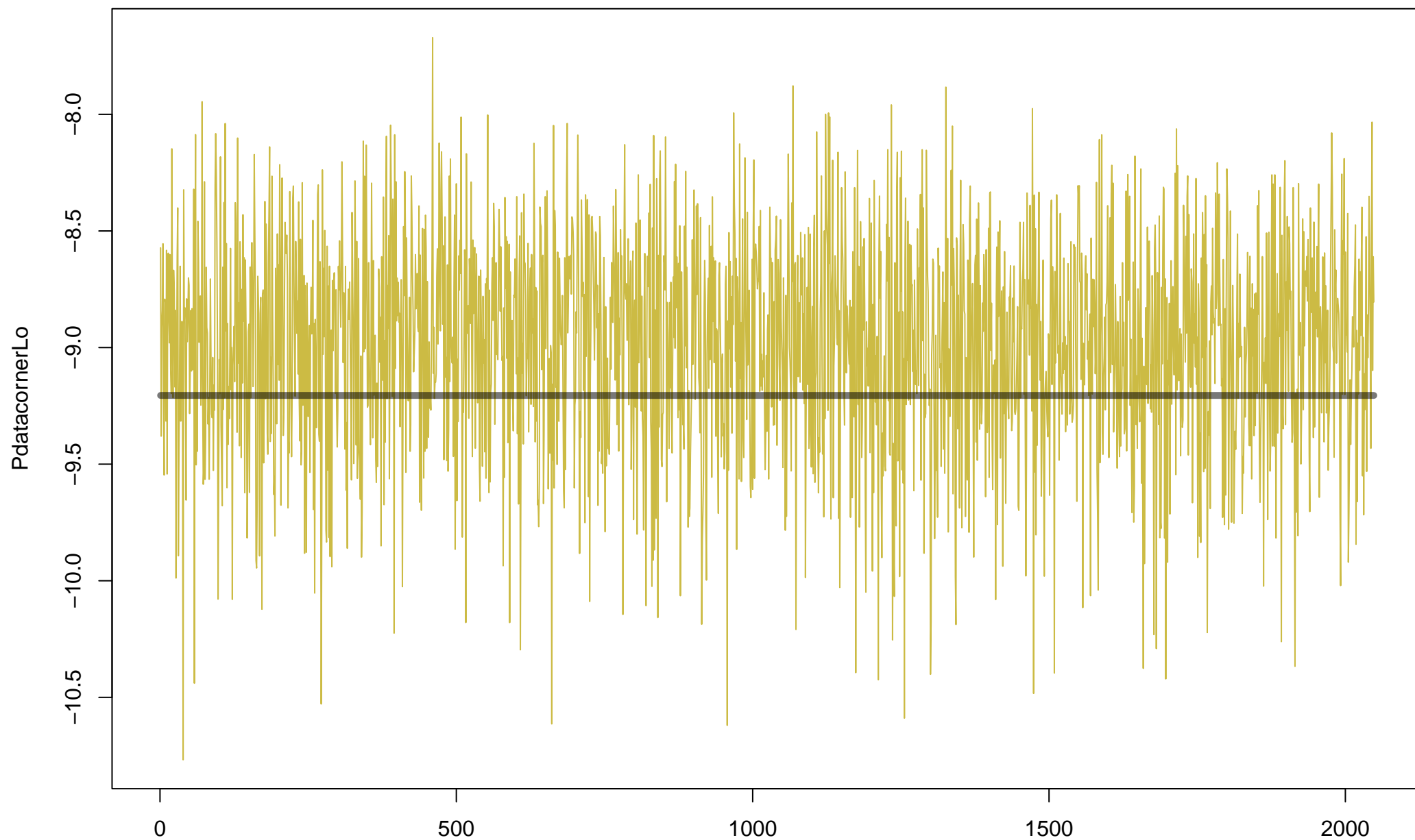


**PdatacornerHi**  
**ESS = 2050 | BMK = 0.13 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: 0.247**

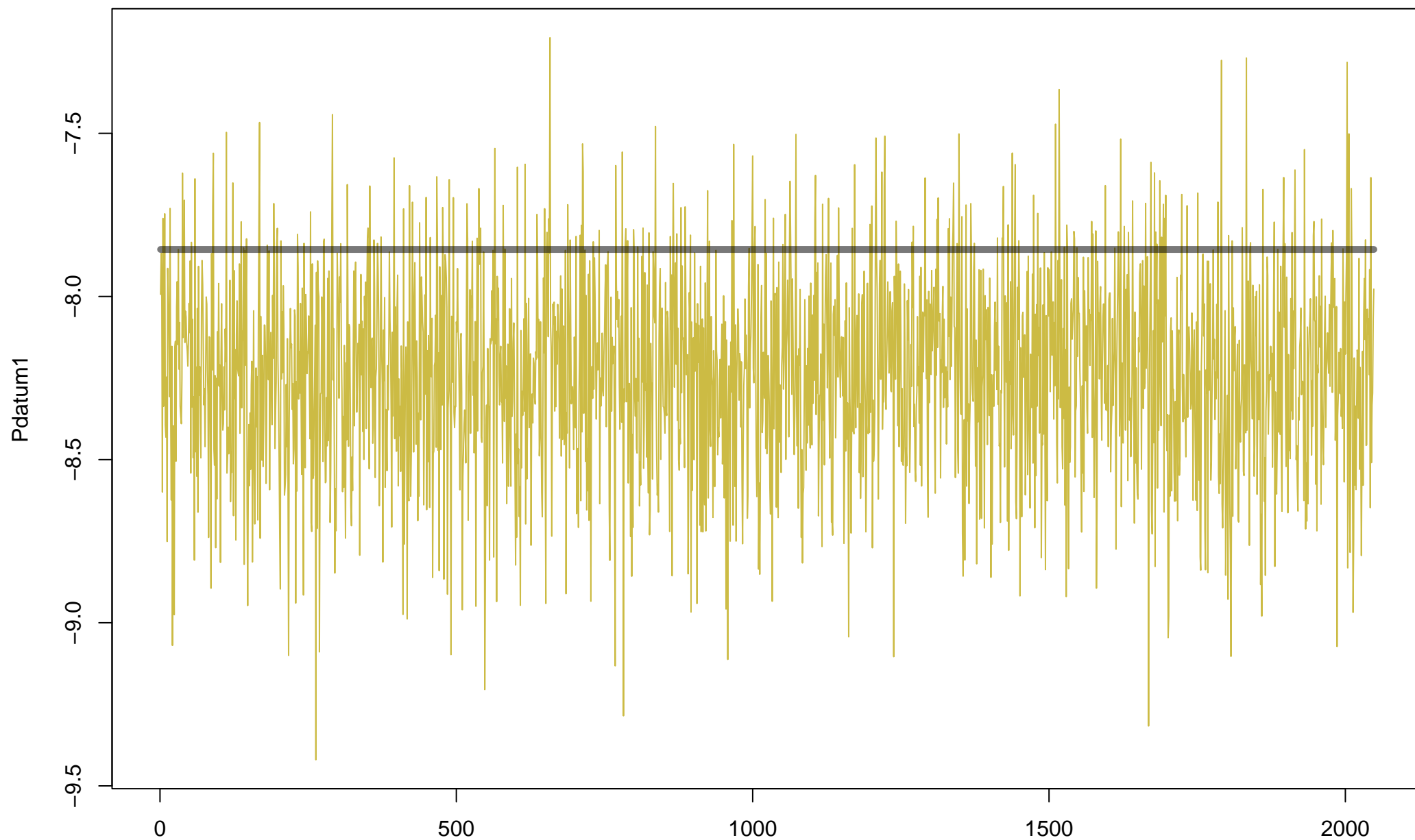




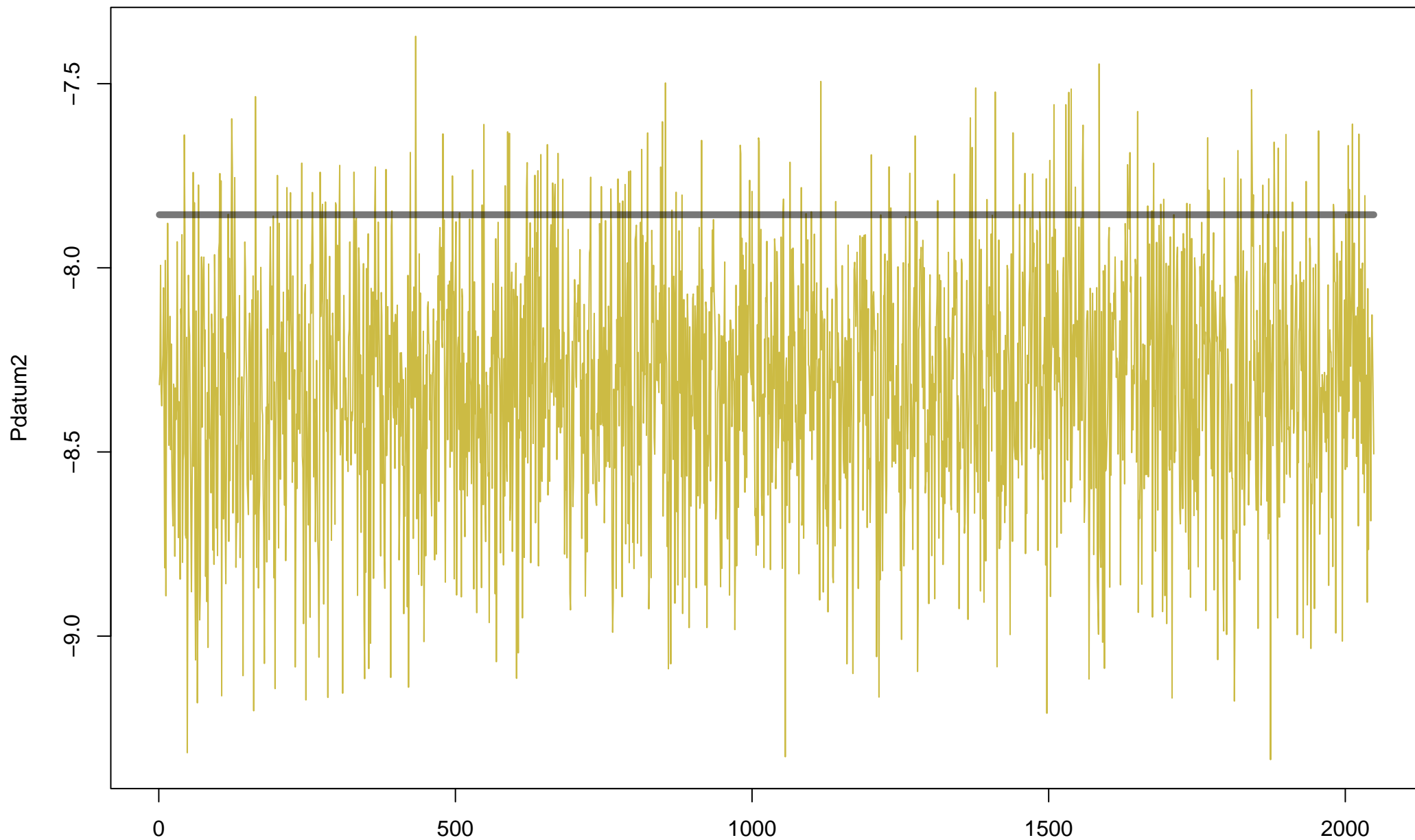
**PdatacornerLo**  
**ESS = 2050 | BMK = 0.0477 | MCSE(6.27) = 1.76 | stat: TRUE | burn: 0 | rel.err: 0.615**



**Pdatum1**  
**ESS = 1920 | BMK = 0.0521 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: -1.32**

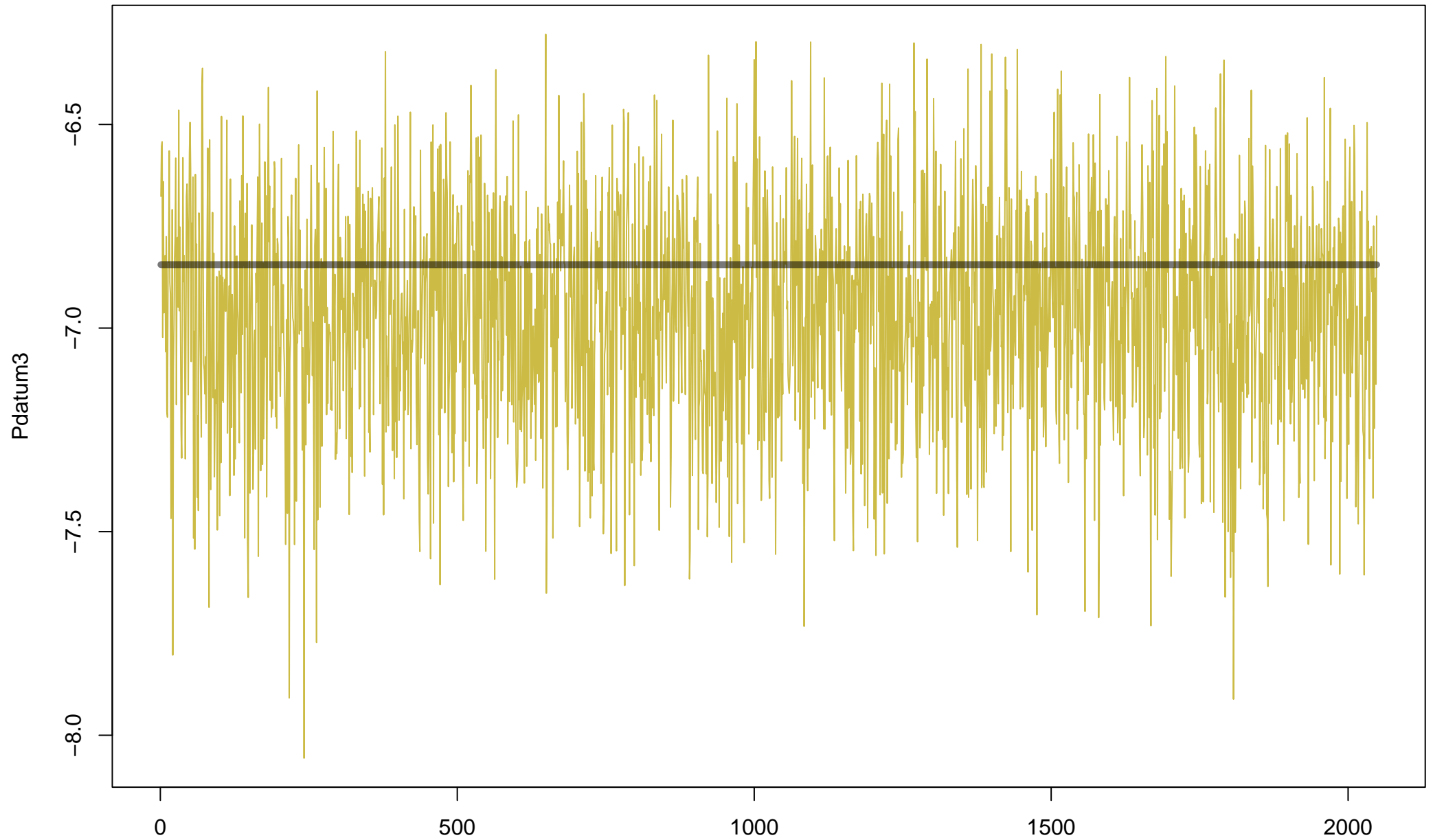


**Pdatum2**  
**ESS = 2020 | BMK = 0.0572 | MCSE(6.27) = 2.5 | stat: FALSE | burn: 0 | rel.err: -1.58**

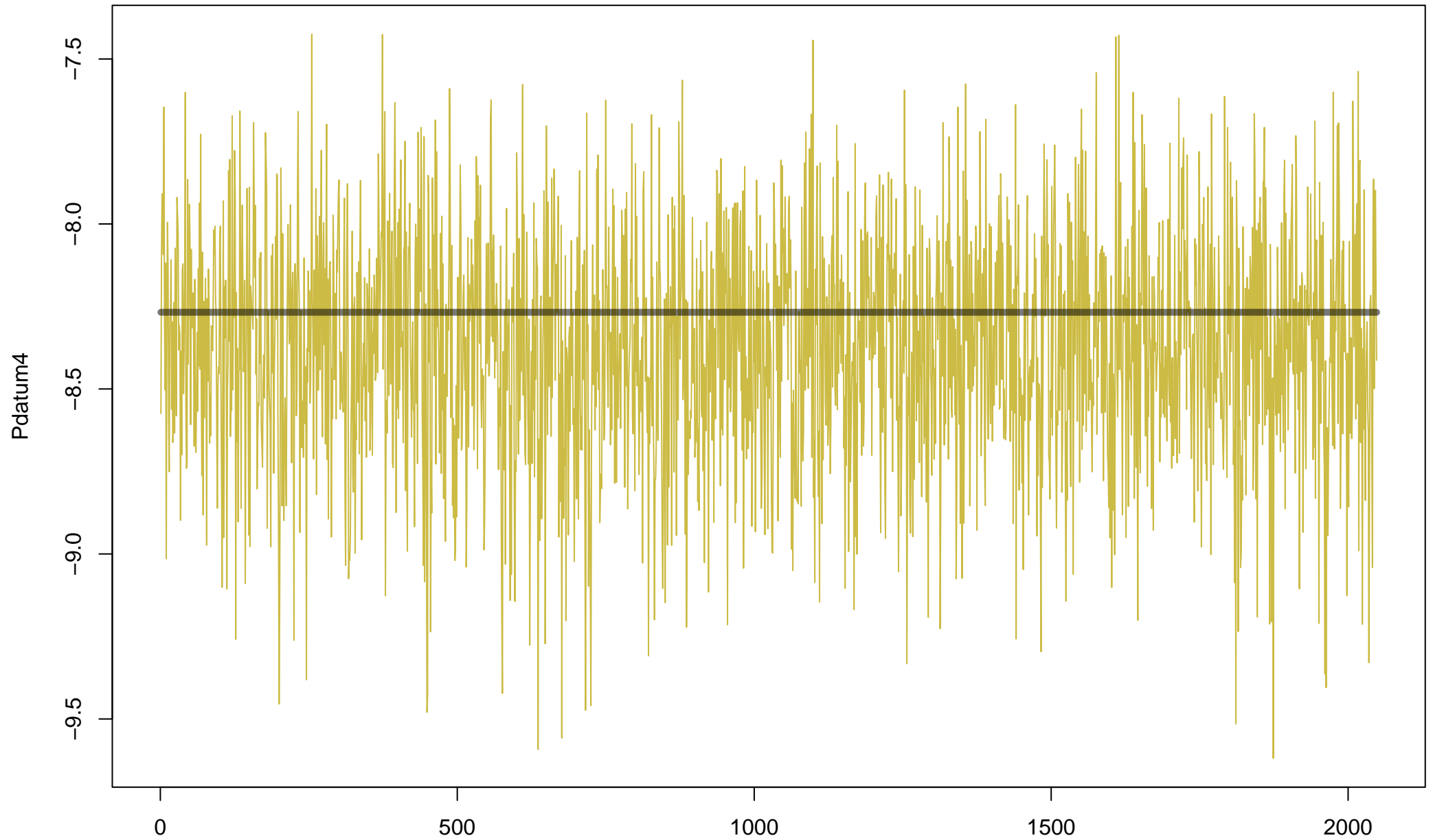


**Pdatum3**

**ESS = 2050 | BMK = 0.0342 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0 | rel.err: -0.356**

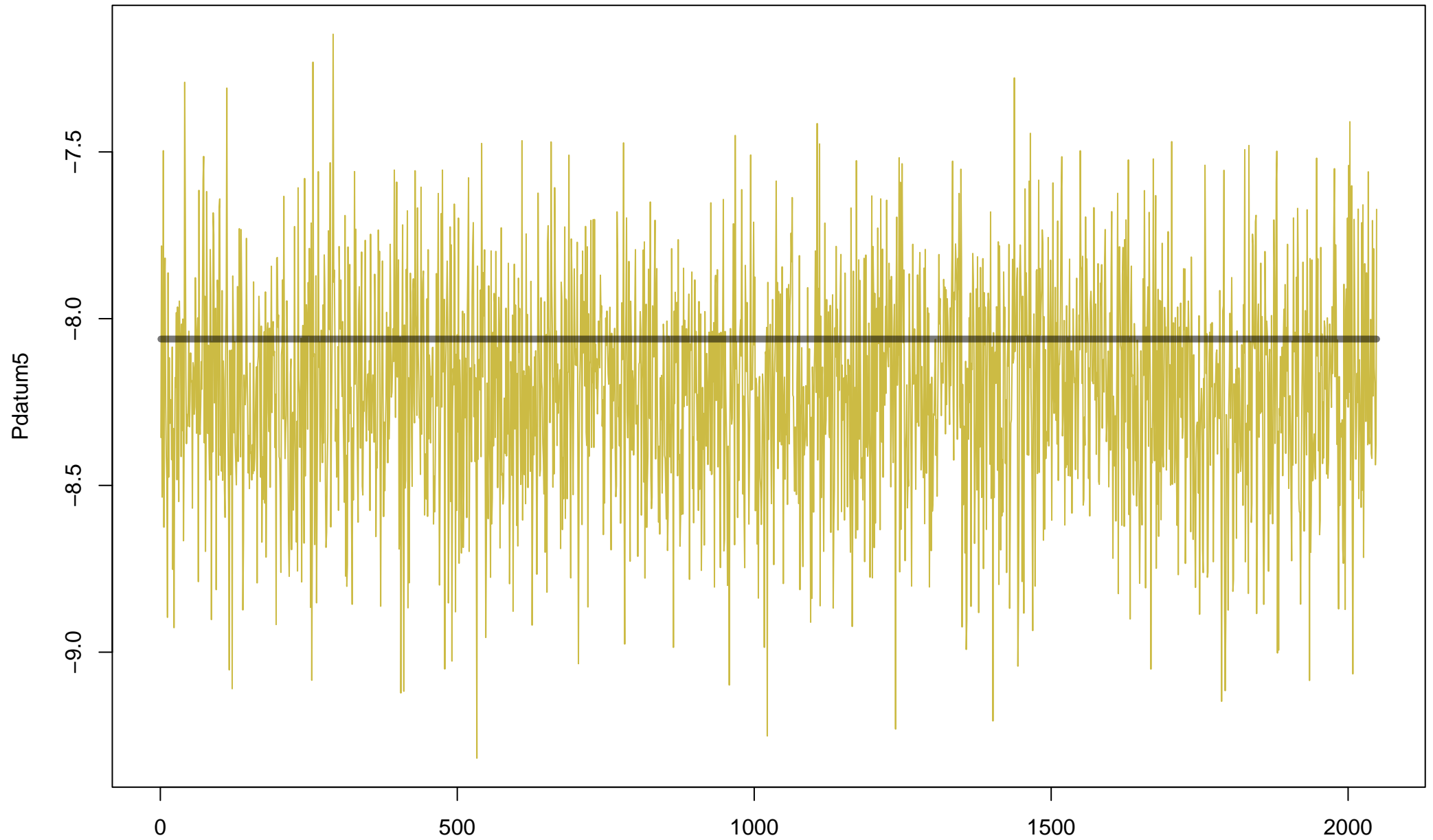


**Pdatum4**  
**ESS = 1770 | BMK = 0.0304 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: -0.151**



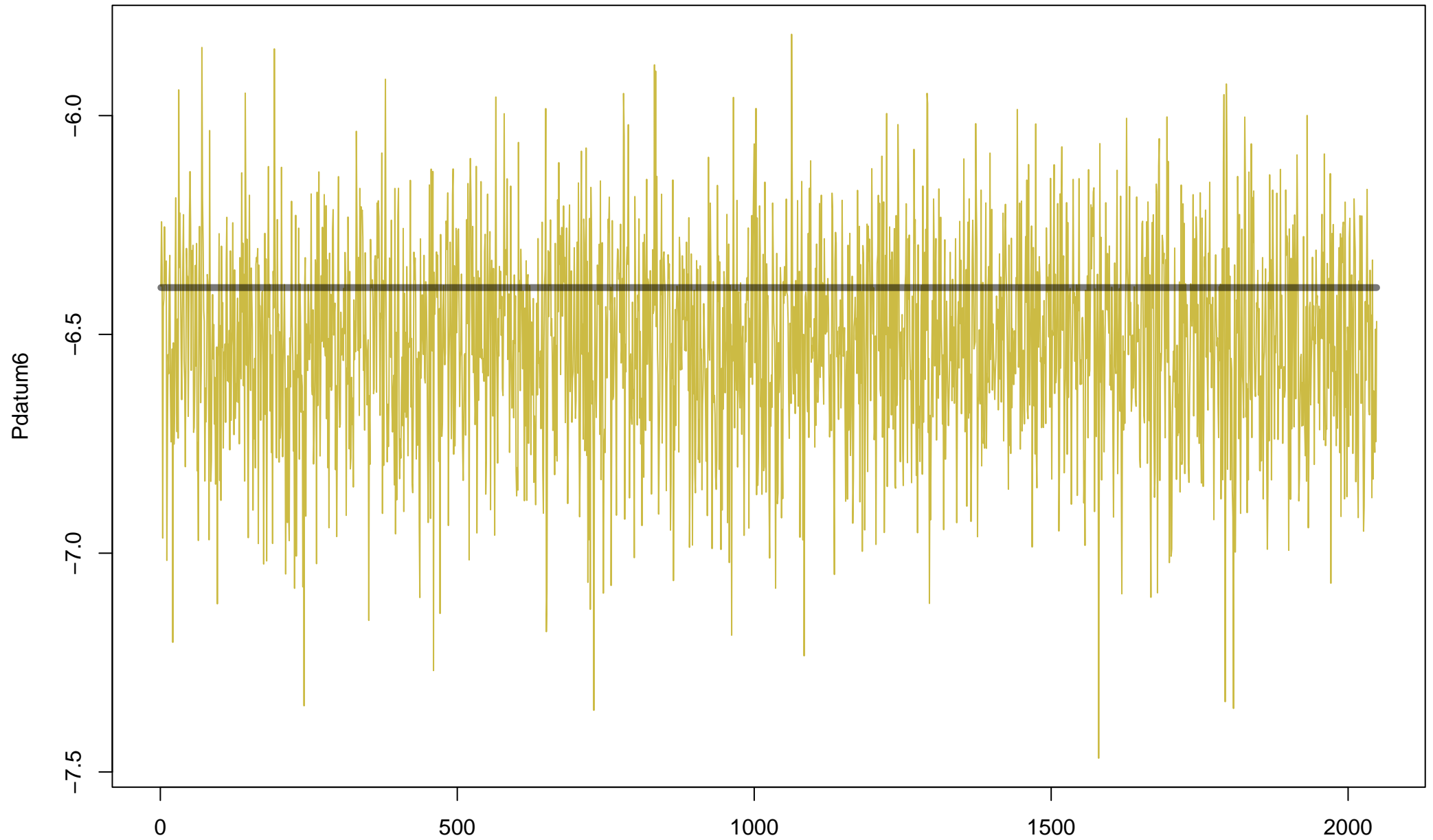
**Pdatum5**

**ESS = 2050 | BMK = 0.0444 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0 | rel.err: -0.338**



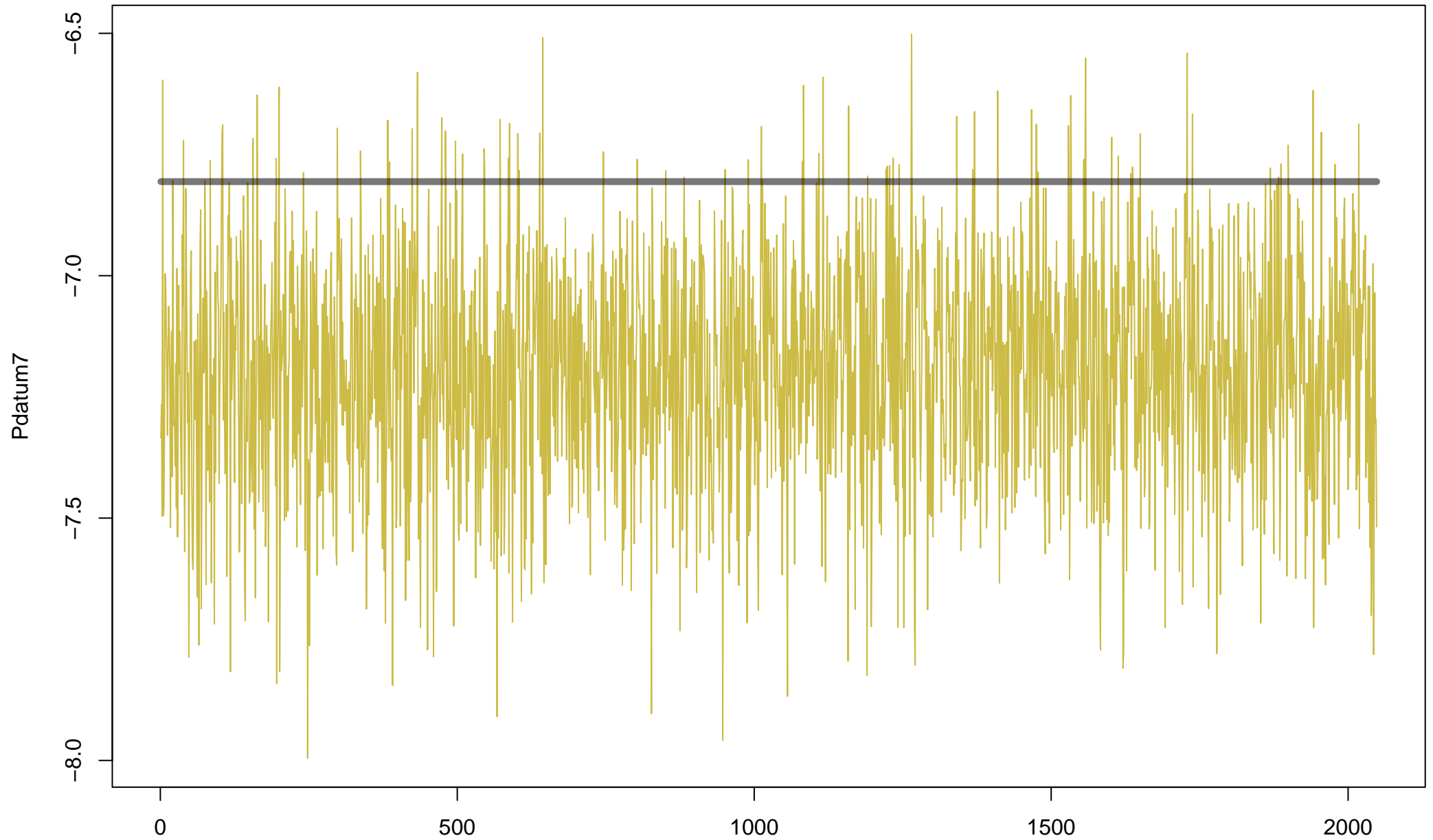
**Pdatum6**

**ESS = 2050 | BMK = 0.0514 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: -0.475**



Pdatum7

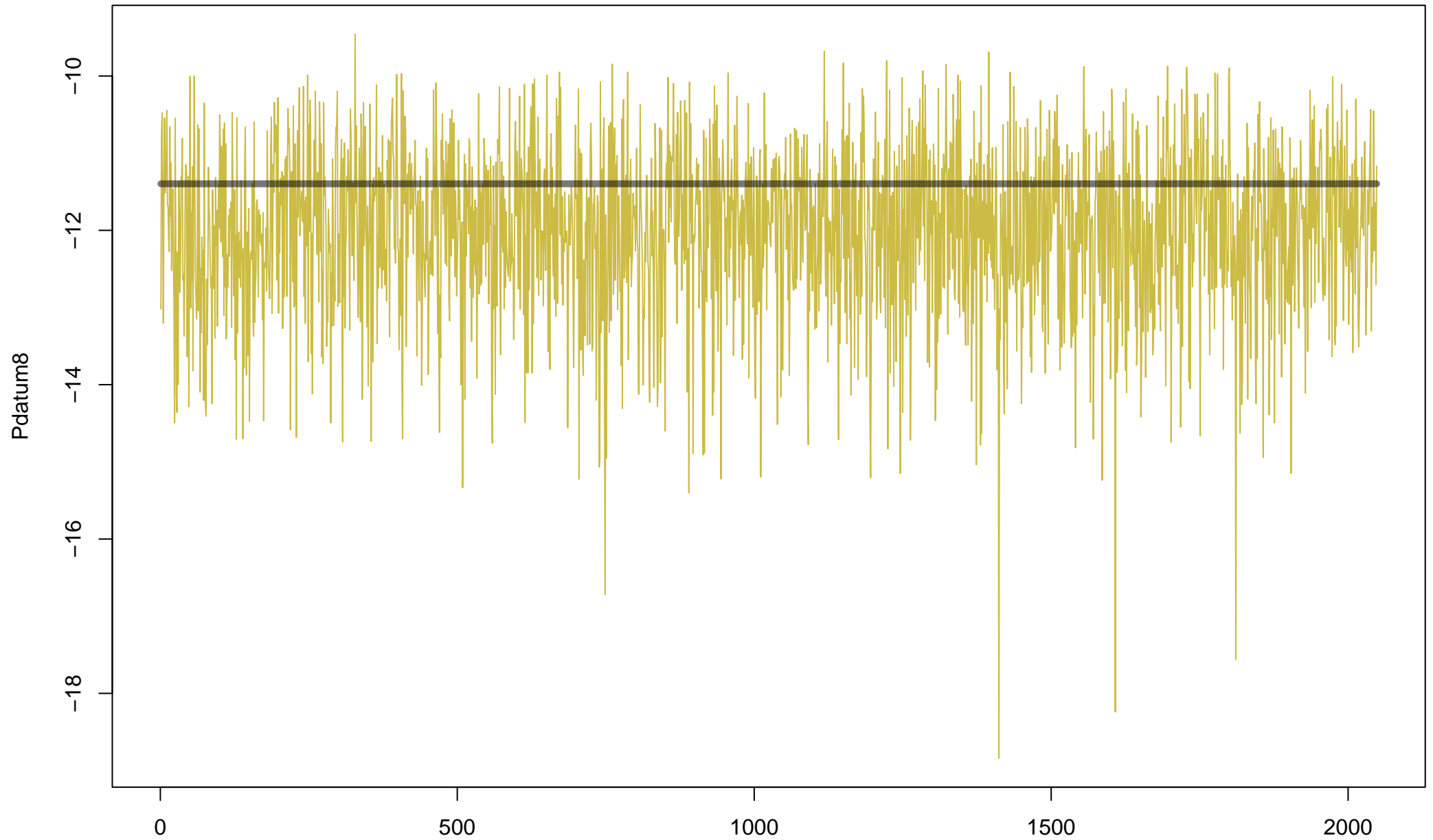
ESS = 2050 | BMK = 0.0521 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: -1.92





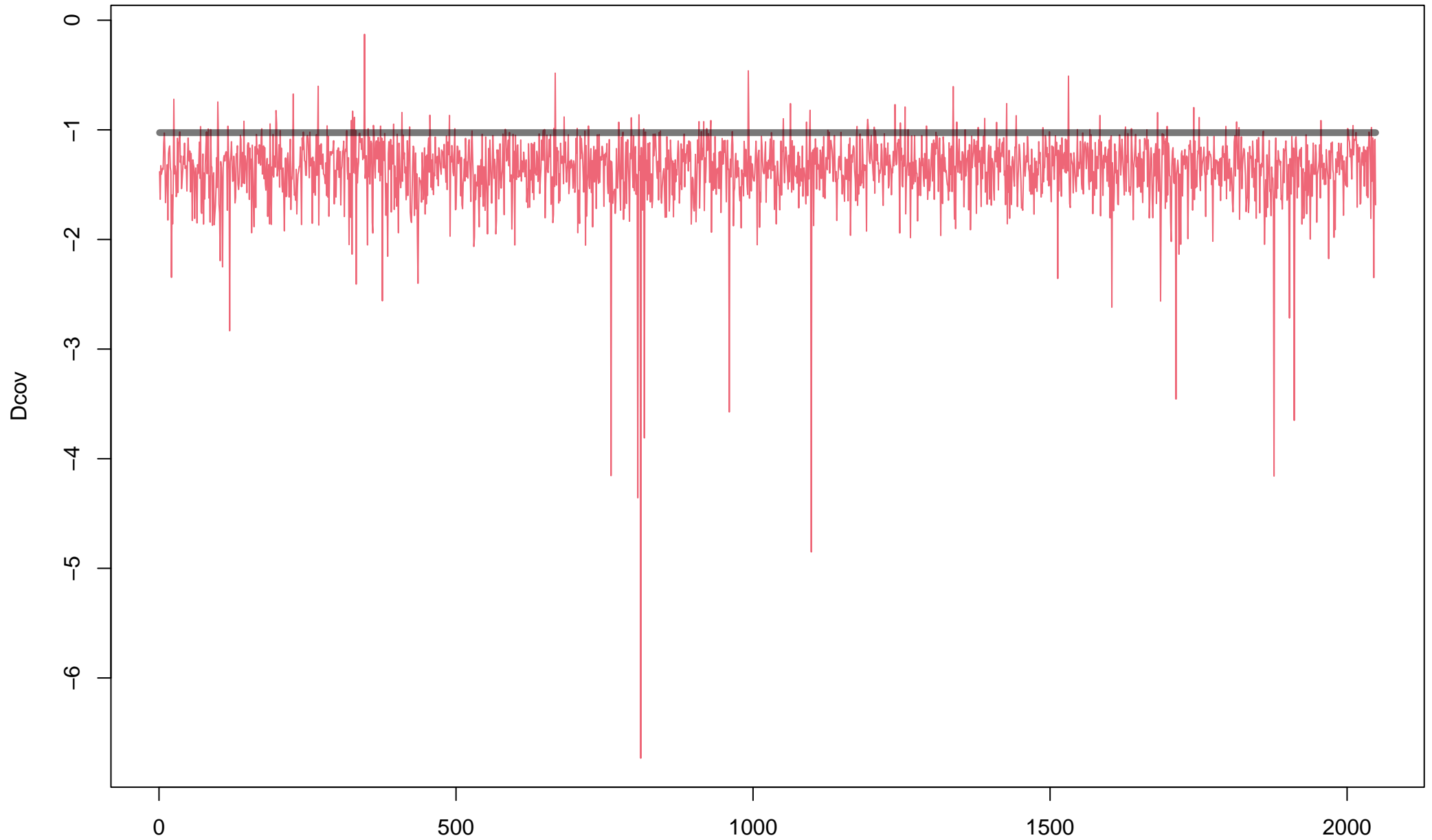
**Pdatum8**

**ESS = 1620 | BMK = 0.0568 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: -0.15**

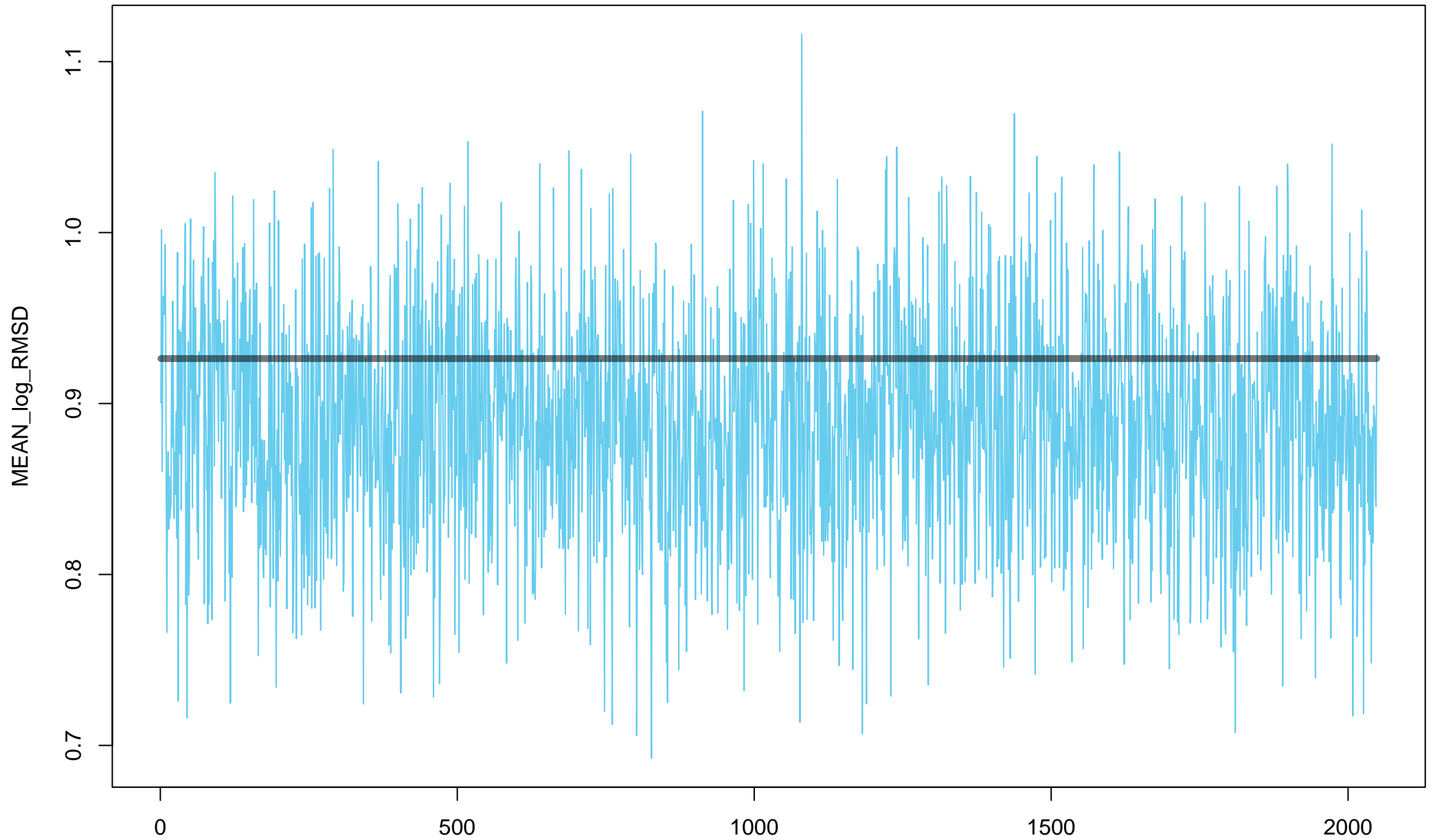


Dcov

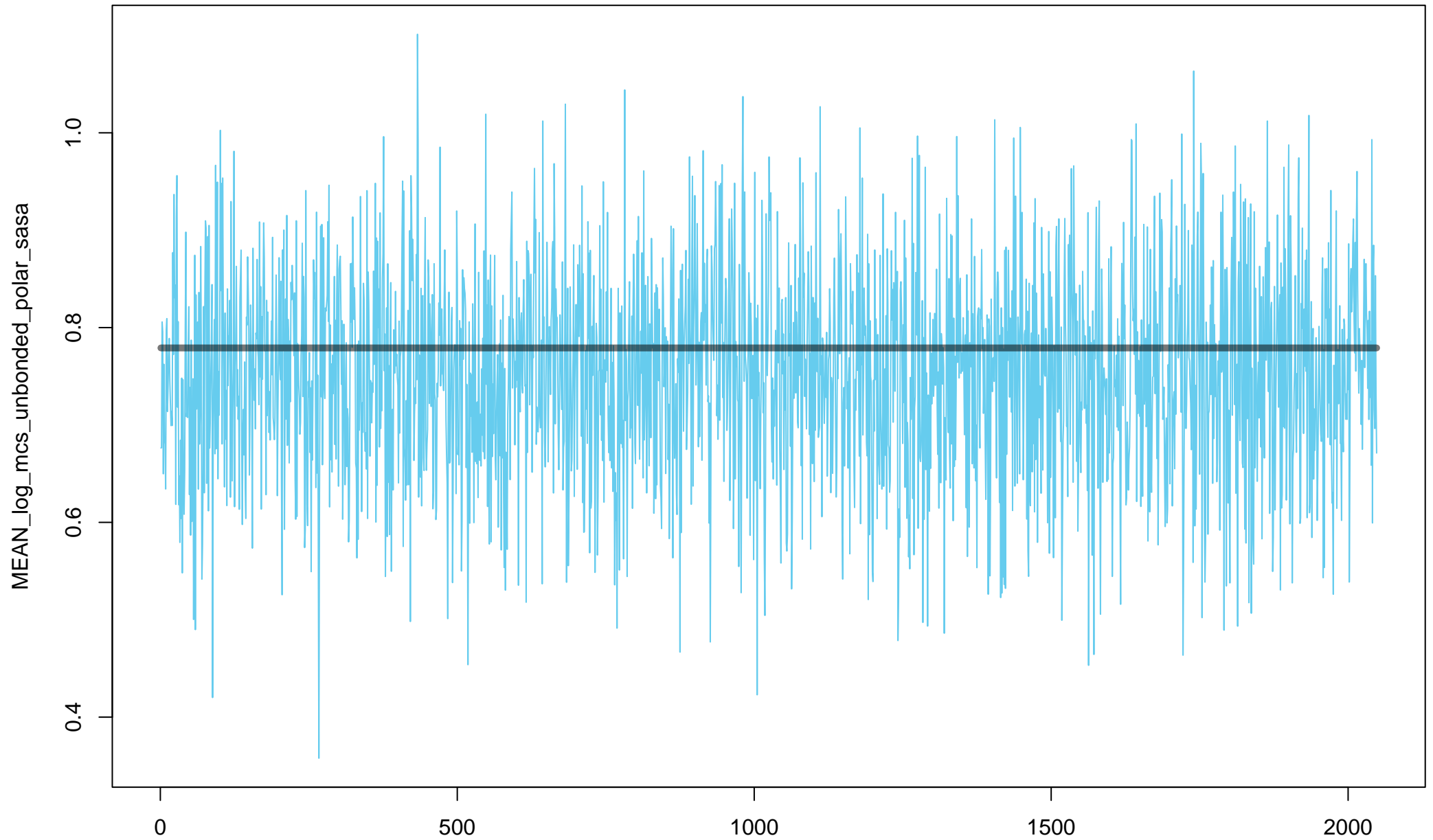
ESS = 2050 | BMK = 0.0733 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0 | rel.err: 1.35



**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.032 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: -0.589**

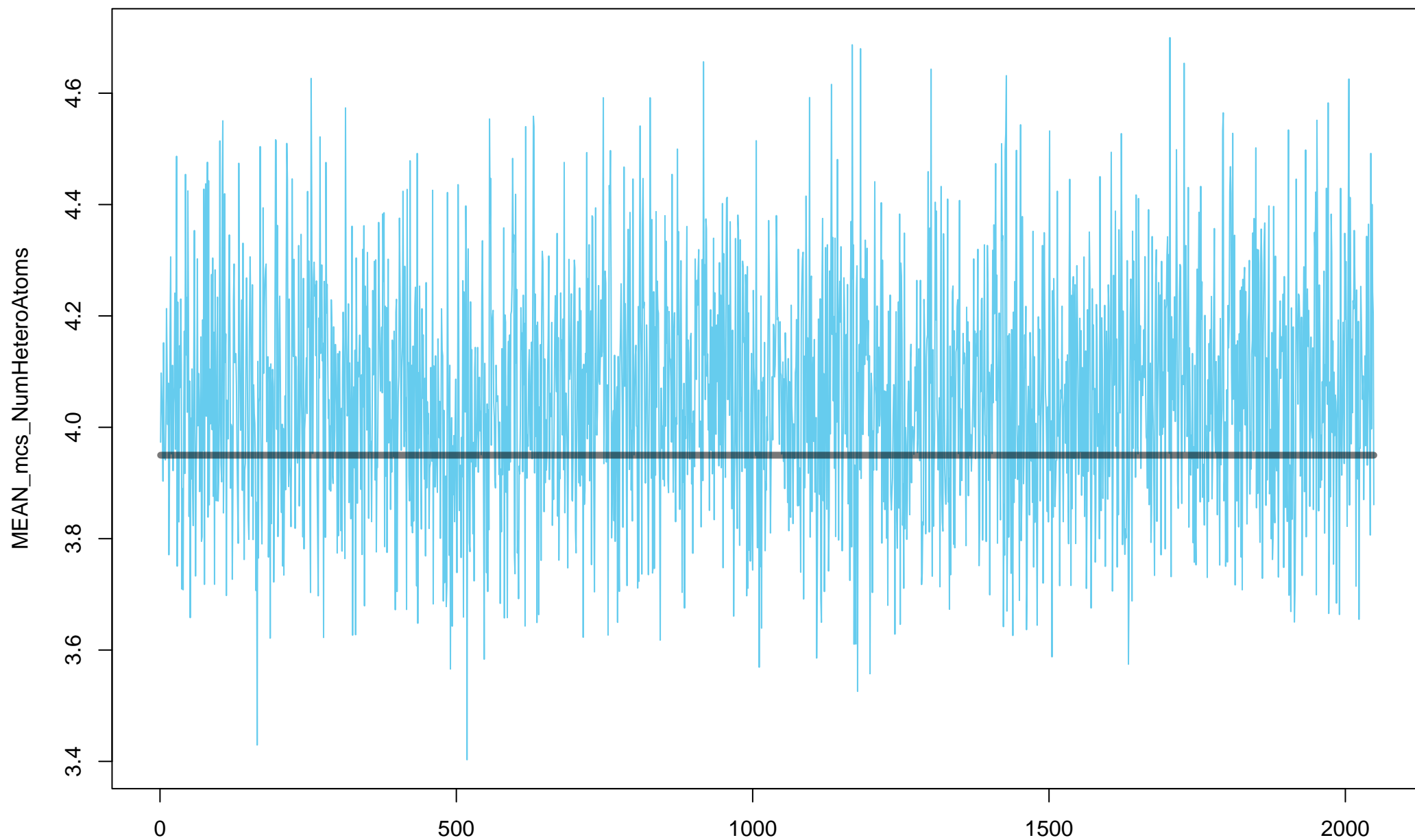


**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: -0.255**

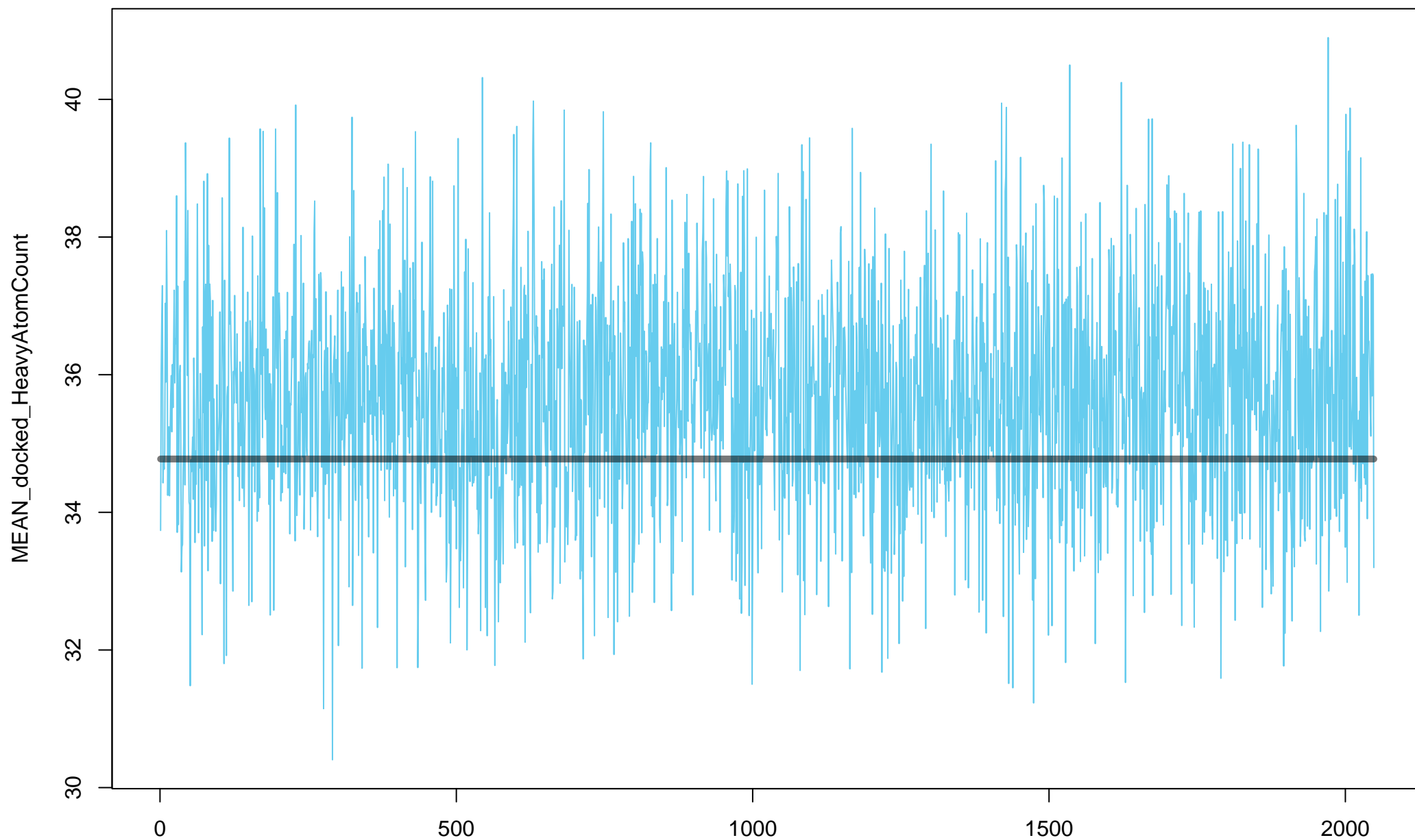


# MEAN\_mcs\_NumHeteroAtoms

ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.538

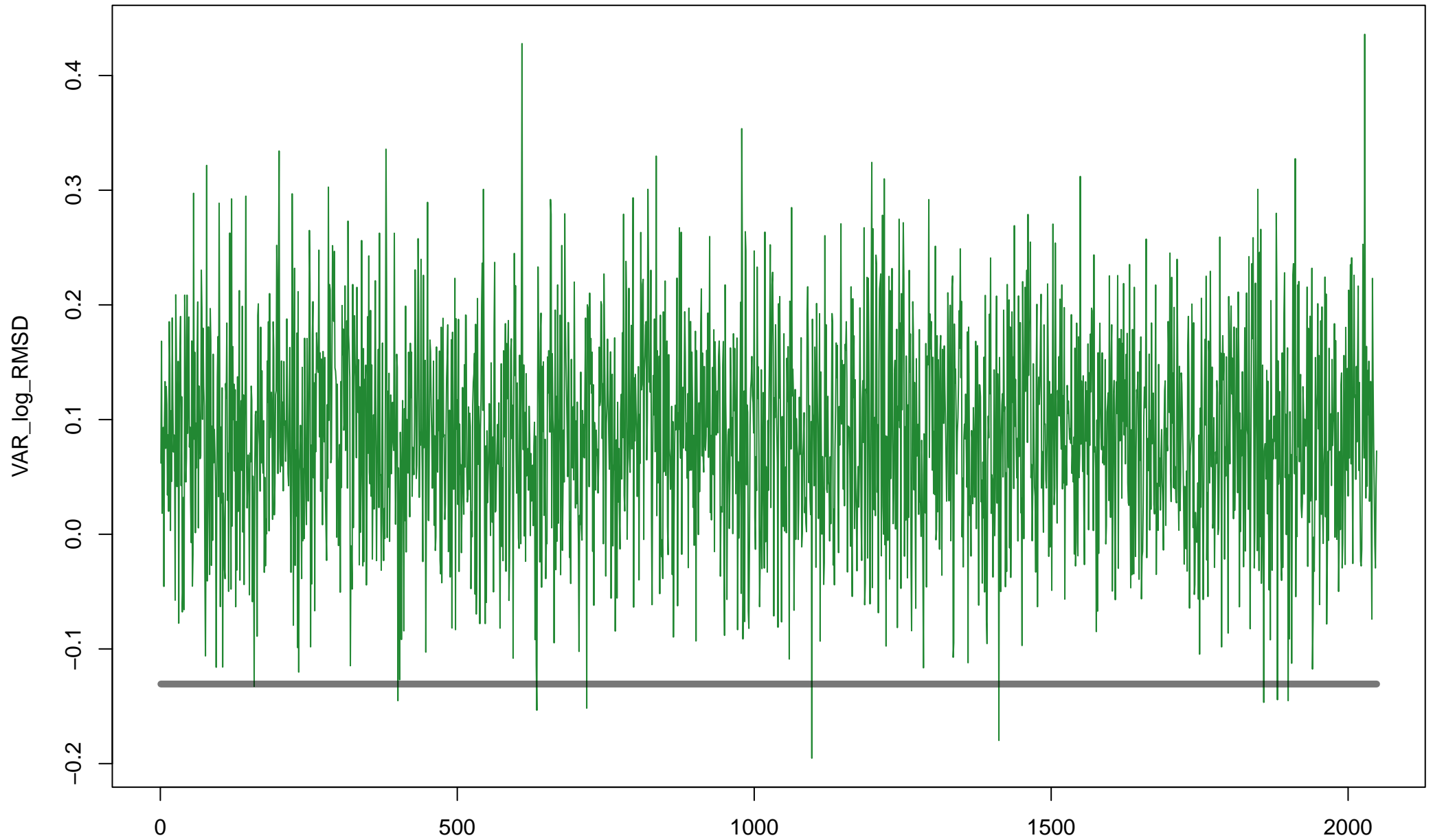


**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0334 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 0.557**

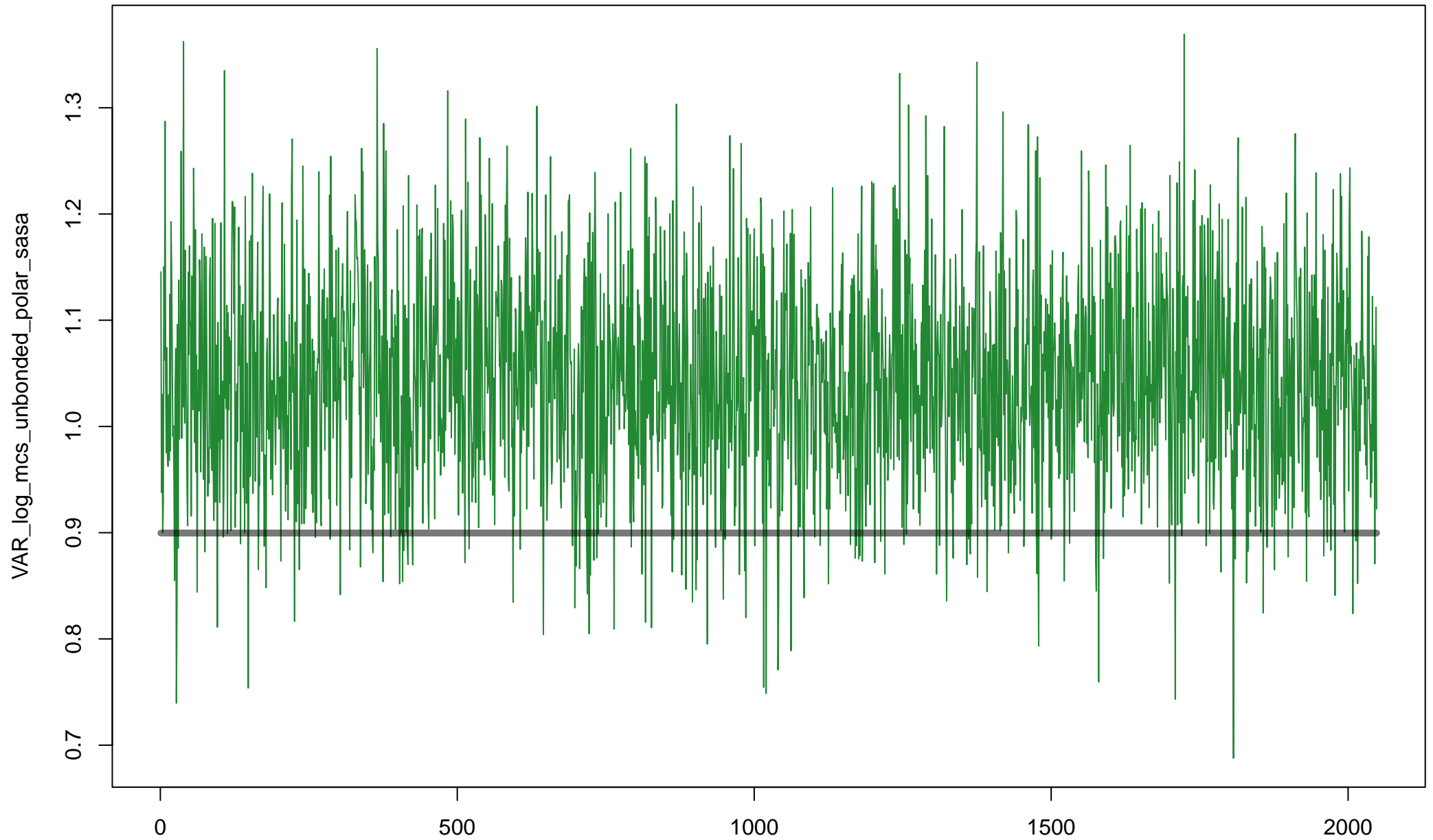


# VAR\_log\_RMSD

ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: 2.27

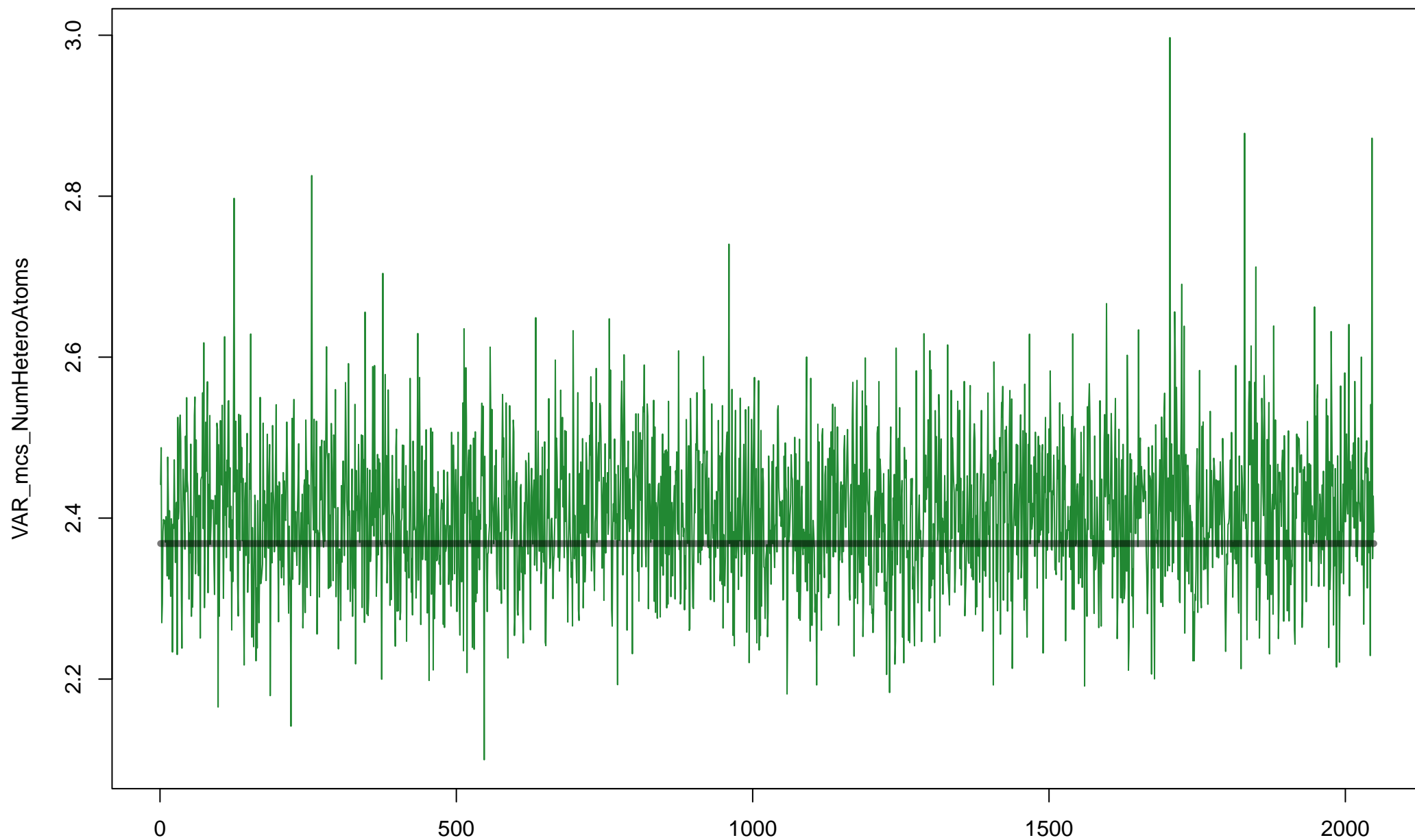


**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0375 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: 1.39**

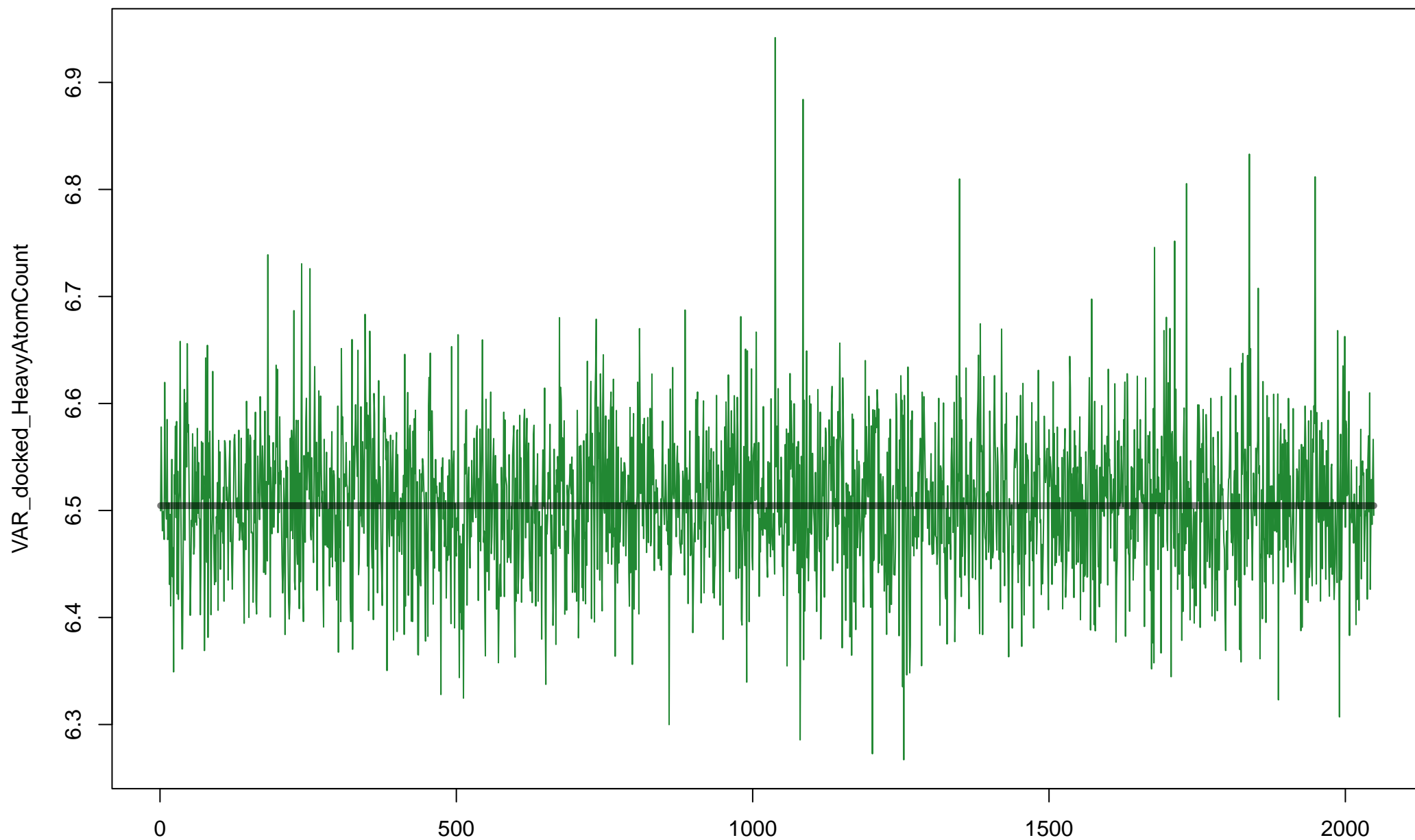




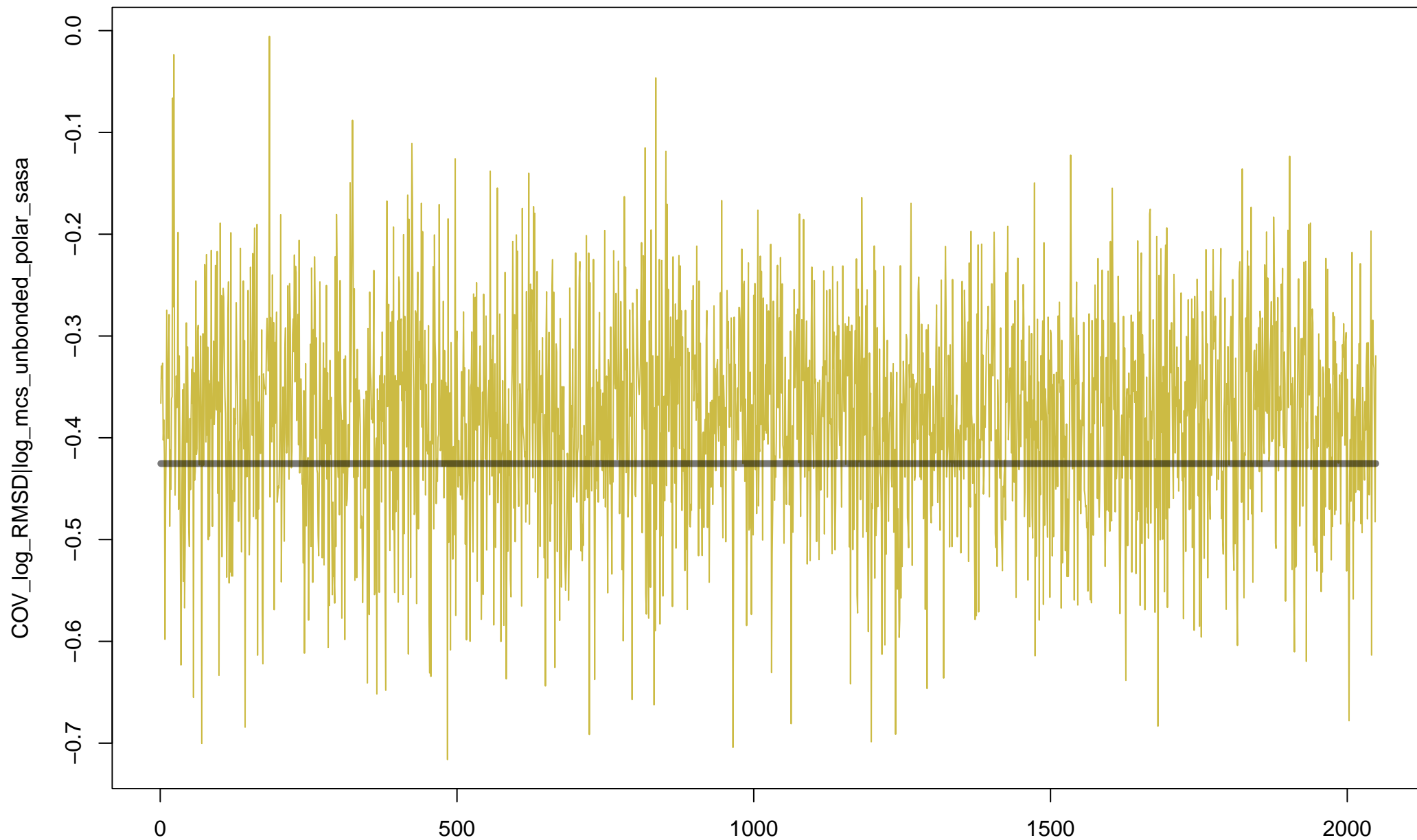
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0567 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: 0.452**



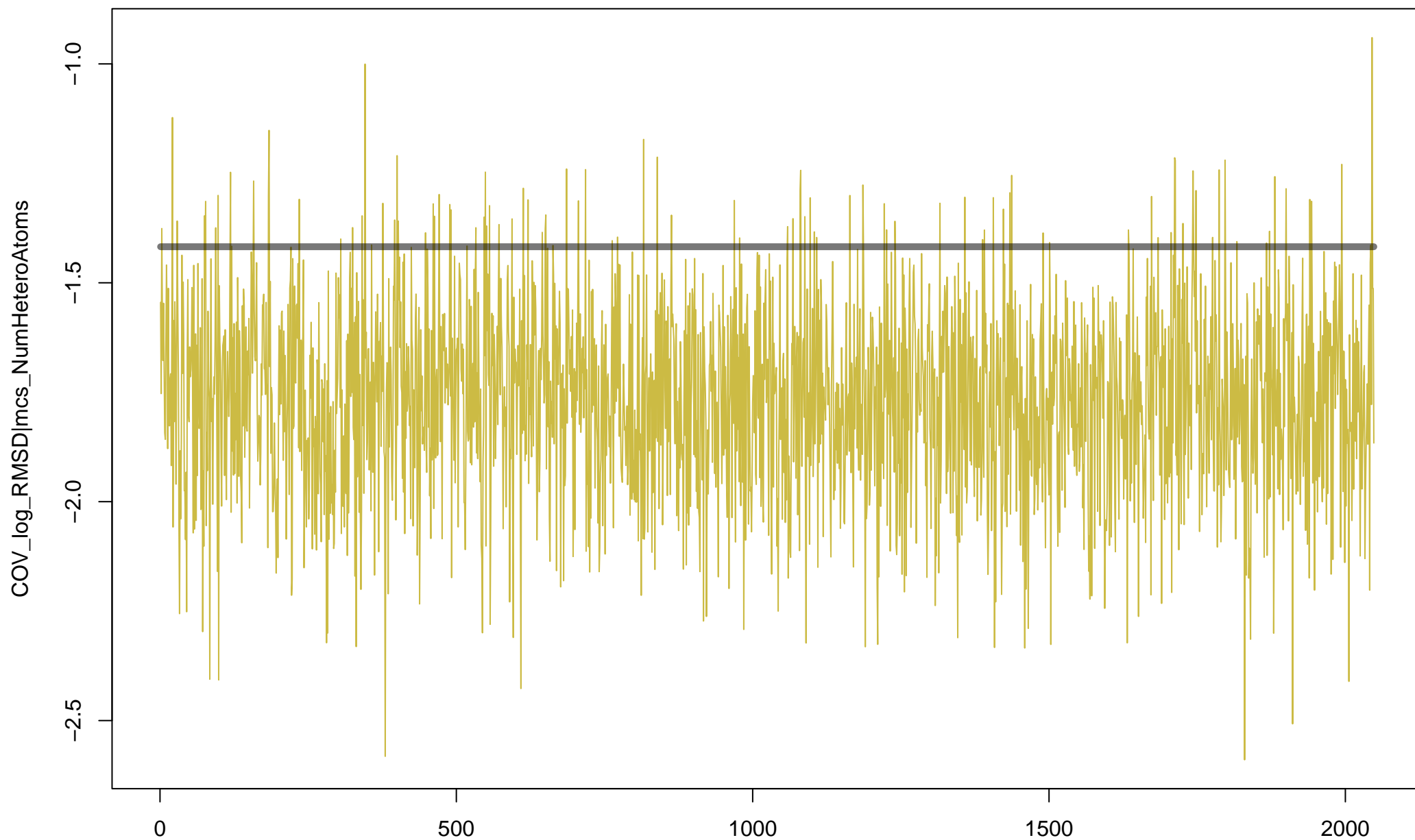
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0678 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: 0.0876**



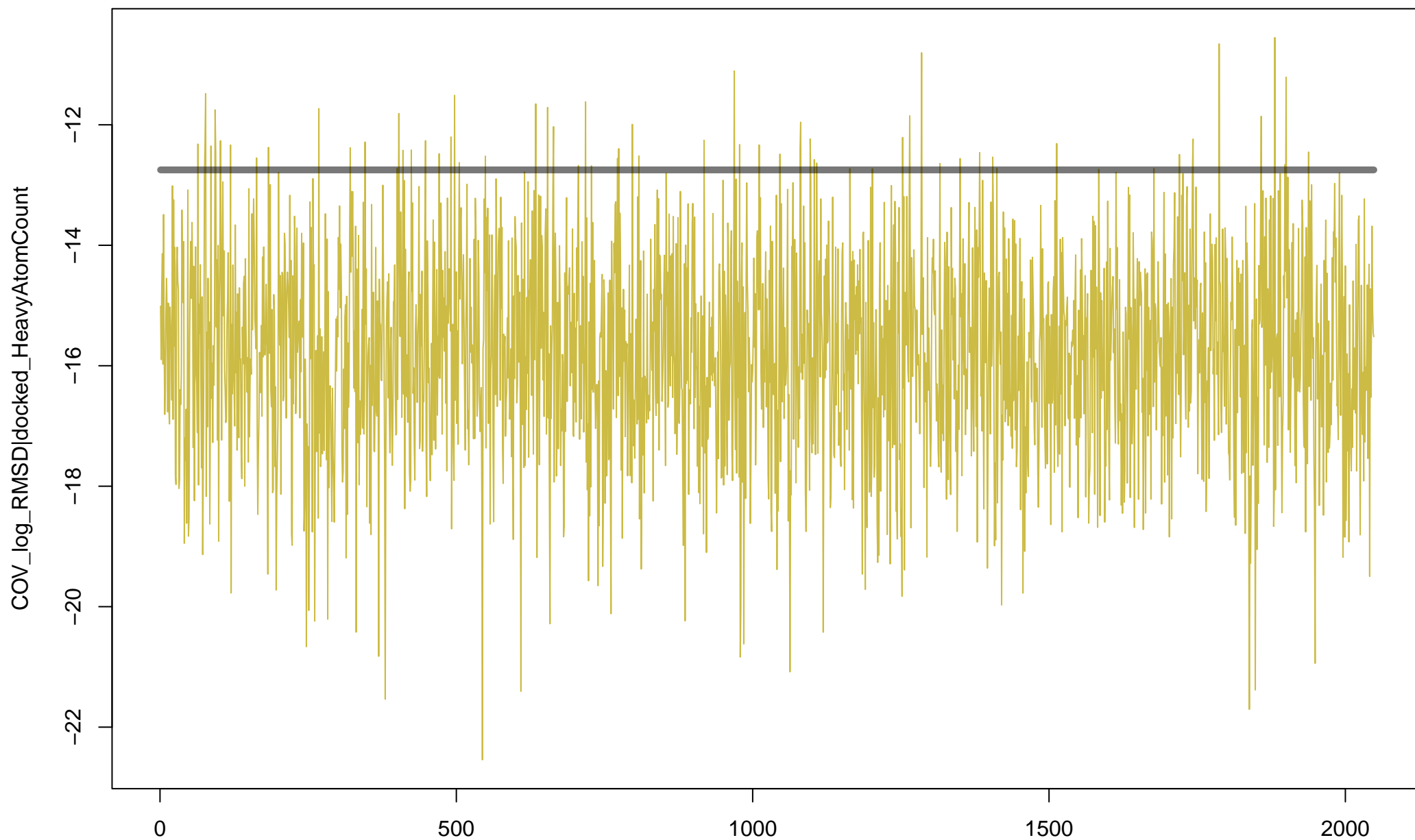
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0644 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: 0.423**



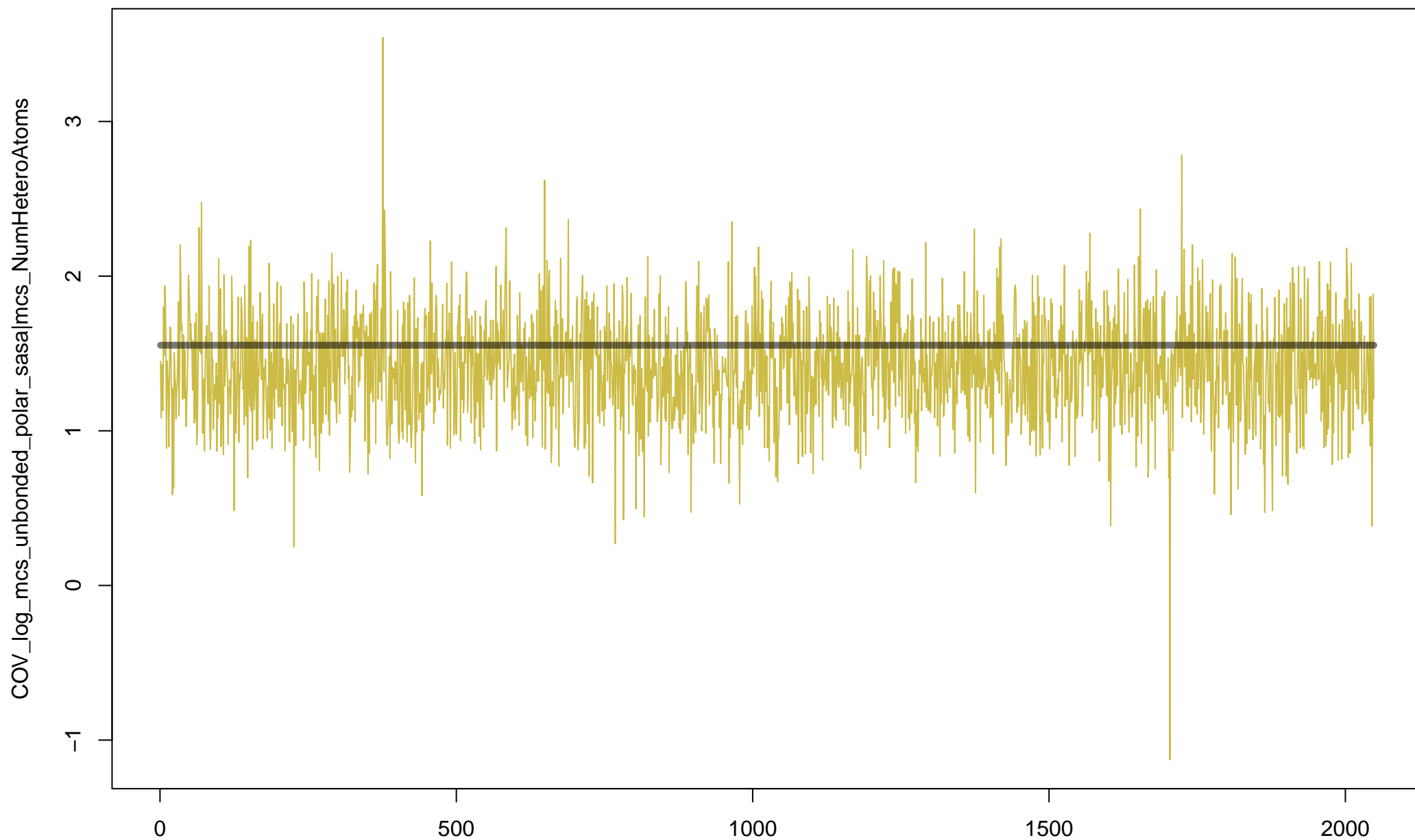
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0403 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: -1.61**



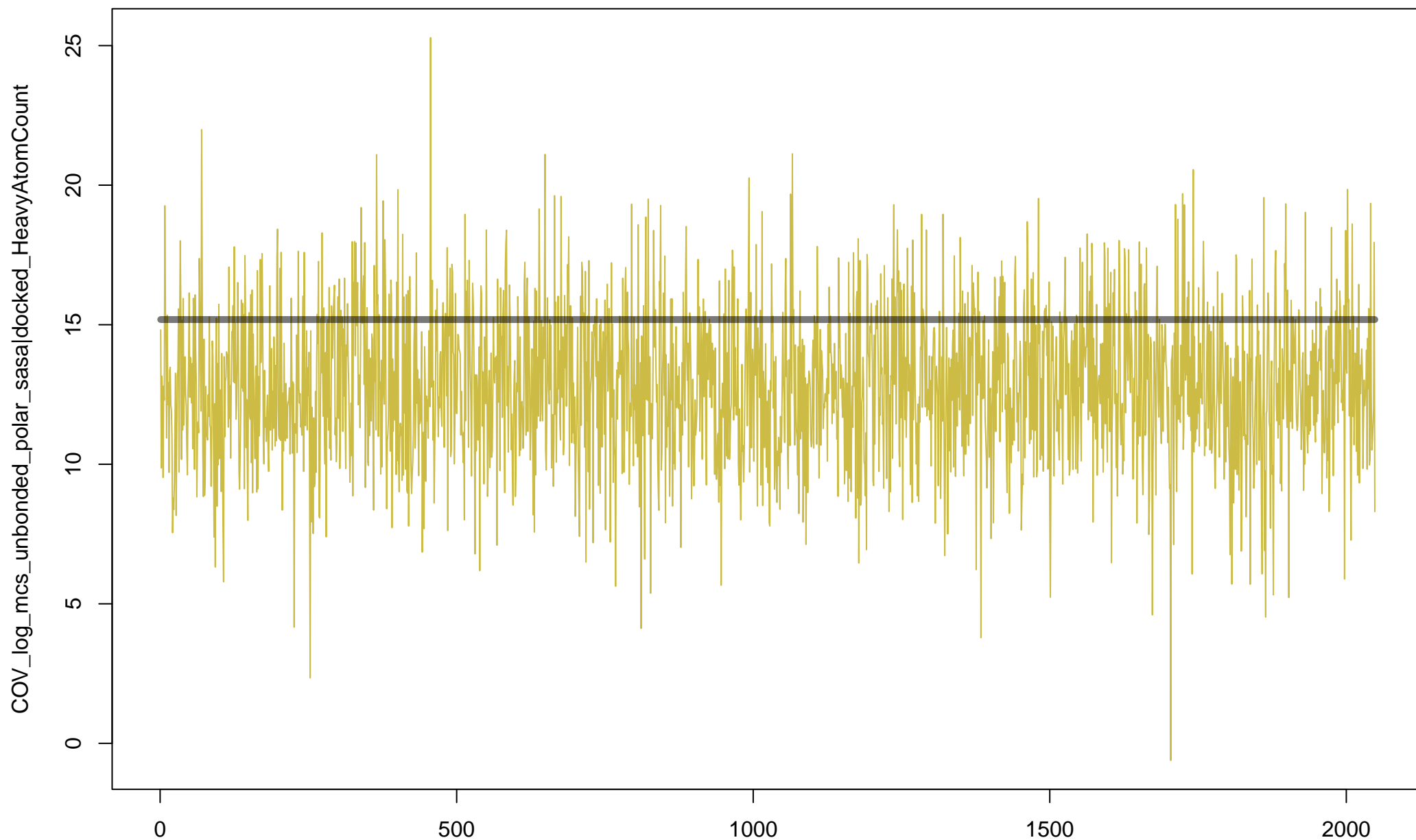
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0533 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: -1.81**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 1900 | BMK = 0.0531 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: -0.416**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 1910 | BMK = 0.0469 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0 | rel.err: -0.876**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0453 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: 0.54**

