

-- STATS maxD --

min ESS = 25.831684608135

max BMK = 0.143860111113758

max MCSE = 10.2464703121841

all stationary: FALSE

burn: 2040

max rel.err.: 2.14996201291285

-- STATS 1D --

min ESS = 1578.90761411563

max BMK = 0.065360920036416

max MCSE = 2.79028252634216

all stationary: TRUE

burn: 0

max rel.err.: 2.28292707034922

-- STATS 2D --

min ESS = 1597.89593655313

max BMK = 0.0629987372488306

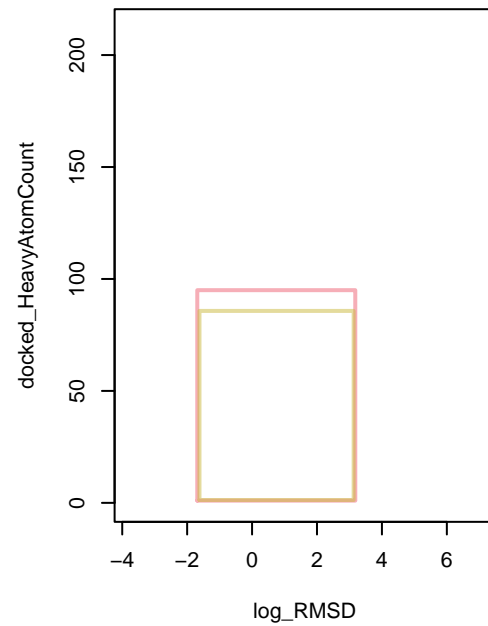
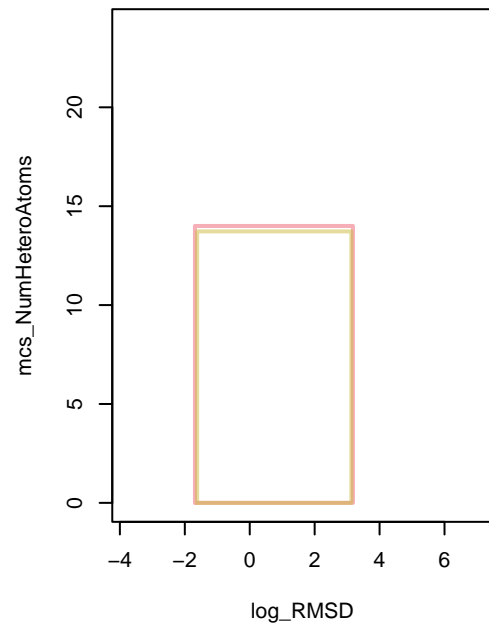
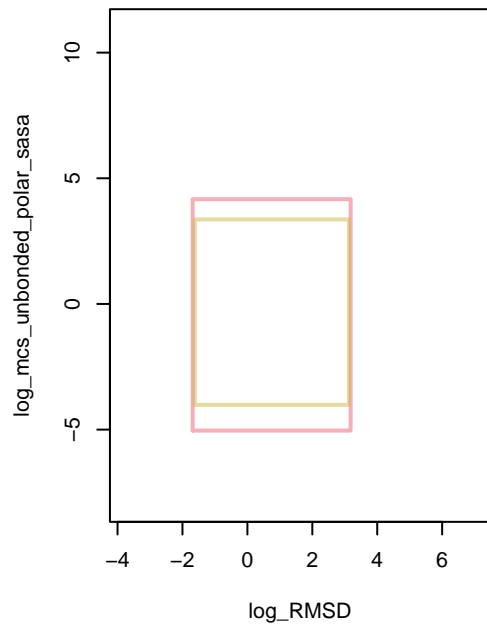
max MCSE = 2.91346002203466

all stationary: TRUE

burn: 0

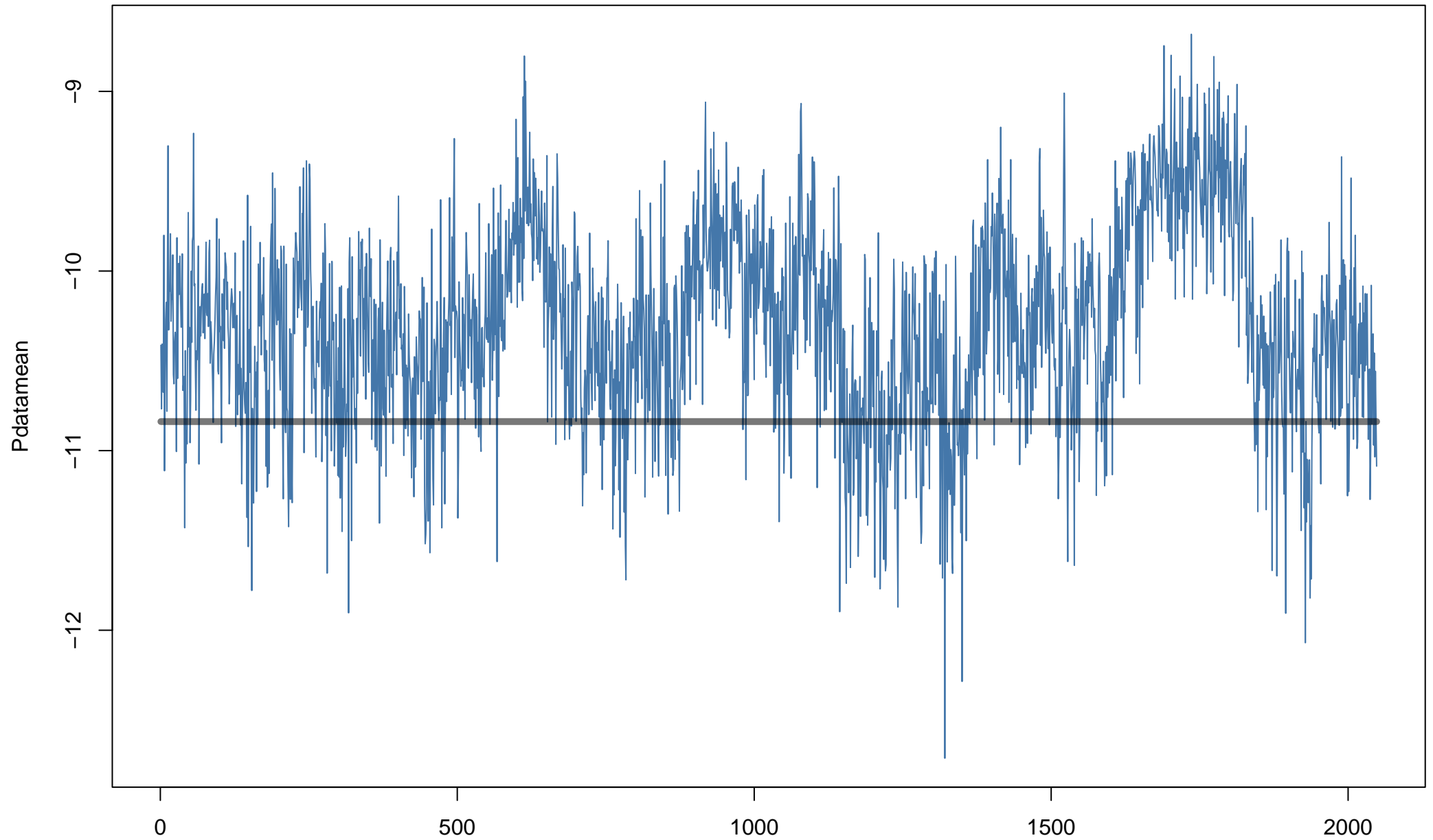
max rel.err.: 1.7385923829972

Occupied clusters: 9 of 16

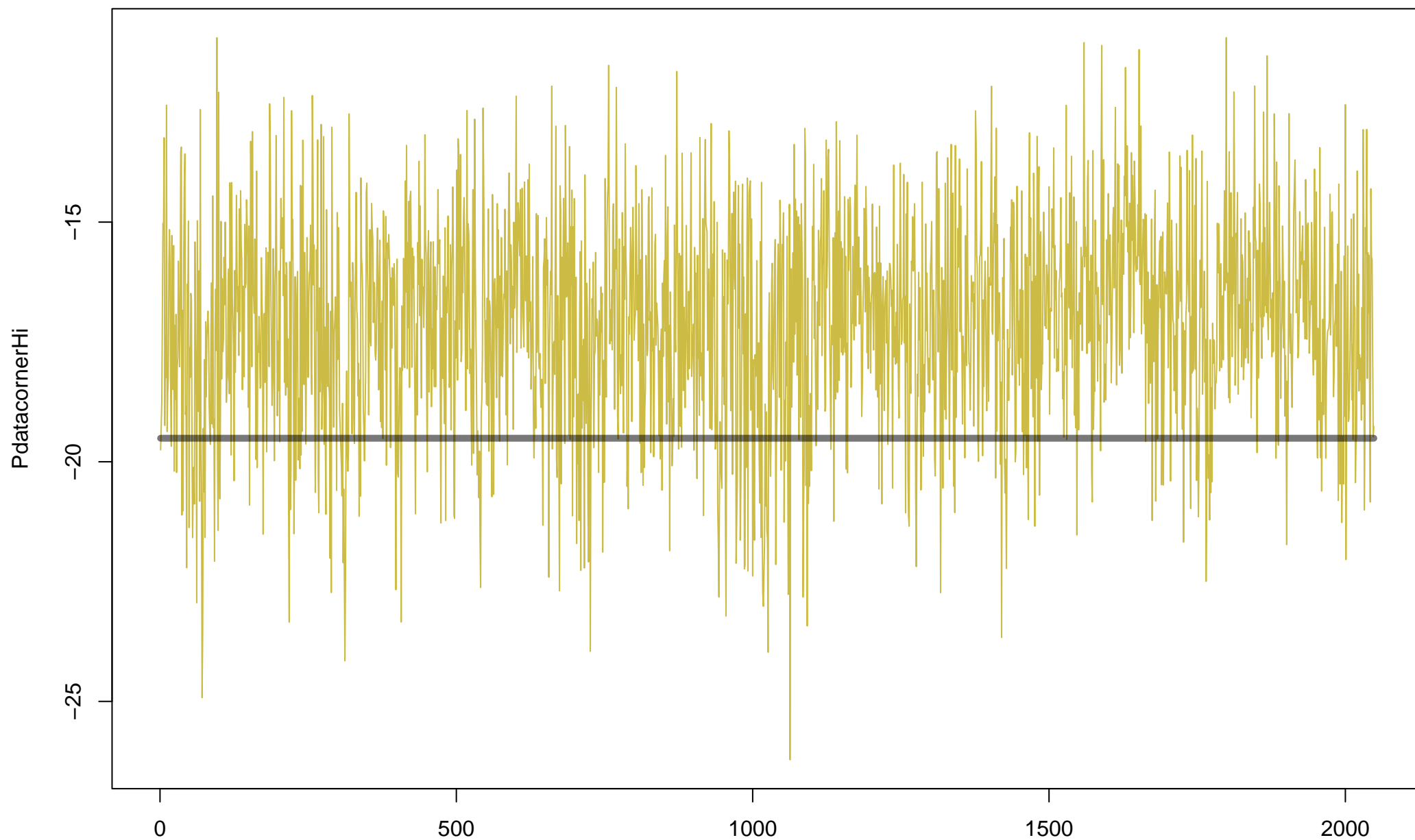


**Pdatamean**

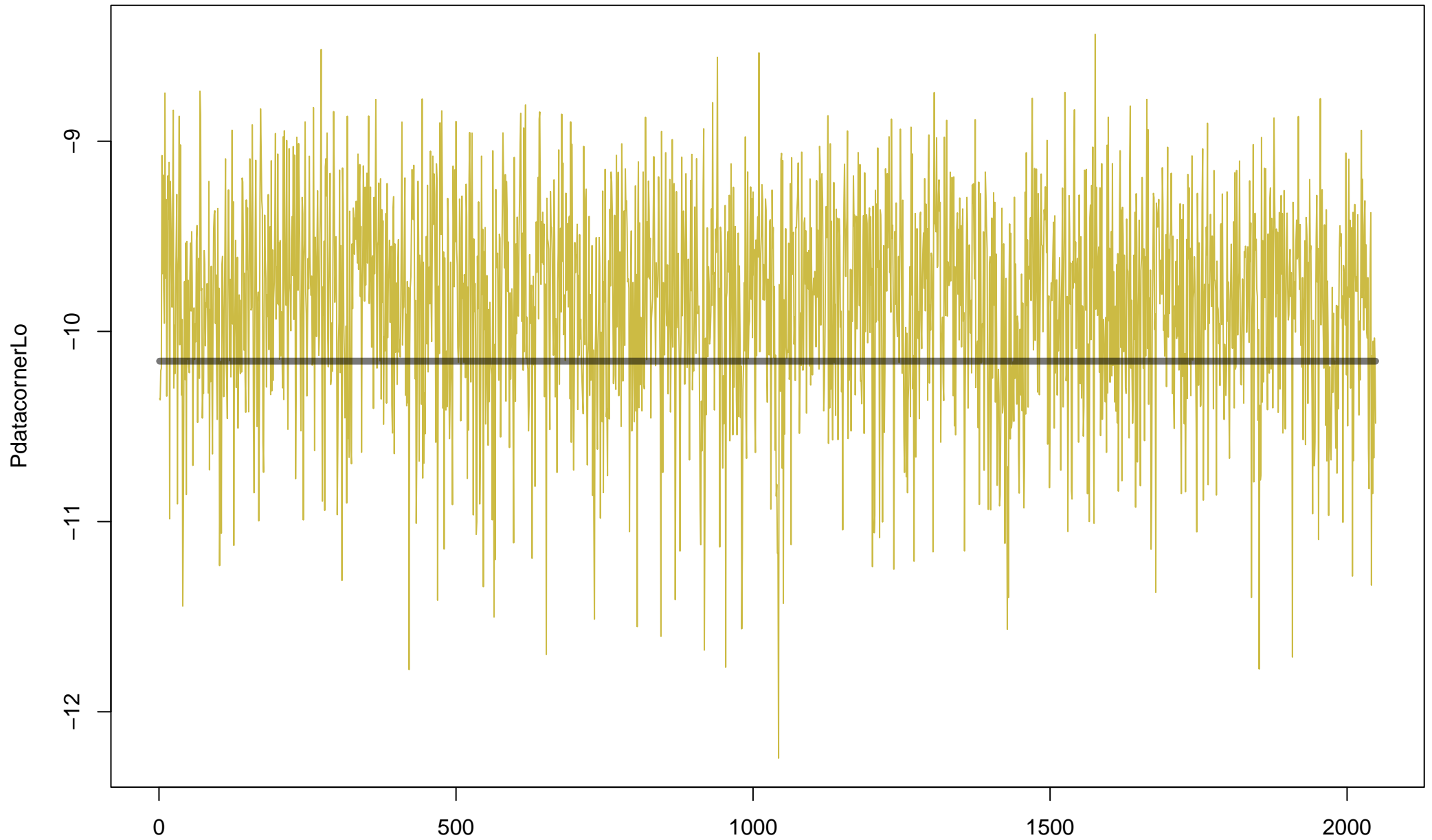
**ESS = 25.8 | BMK = 0.144 | MCSE(6.27) = 10.2 | stat: FALSE | burn: 2040 | rel.err: 0.877**



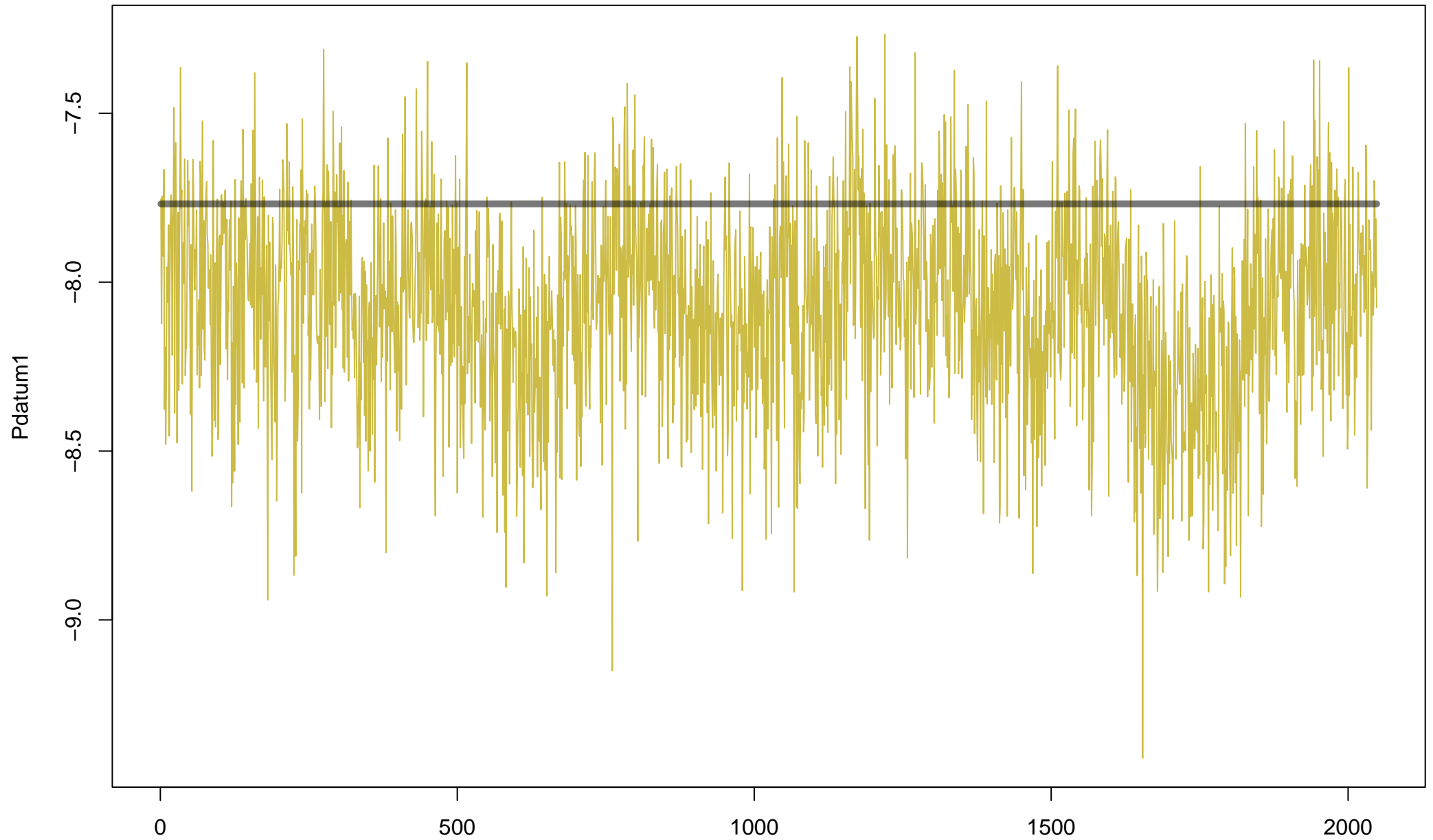
**PdatacornerHi**  
**ESS = 1350 | BMK = 0.136 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 0.28**



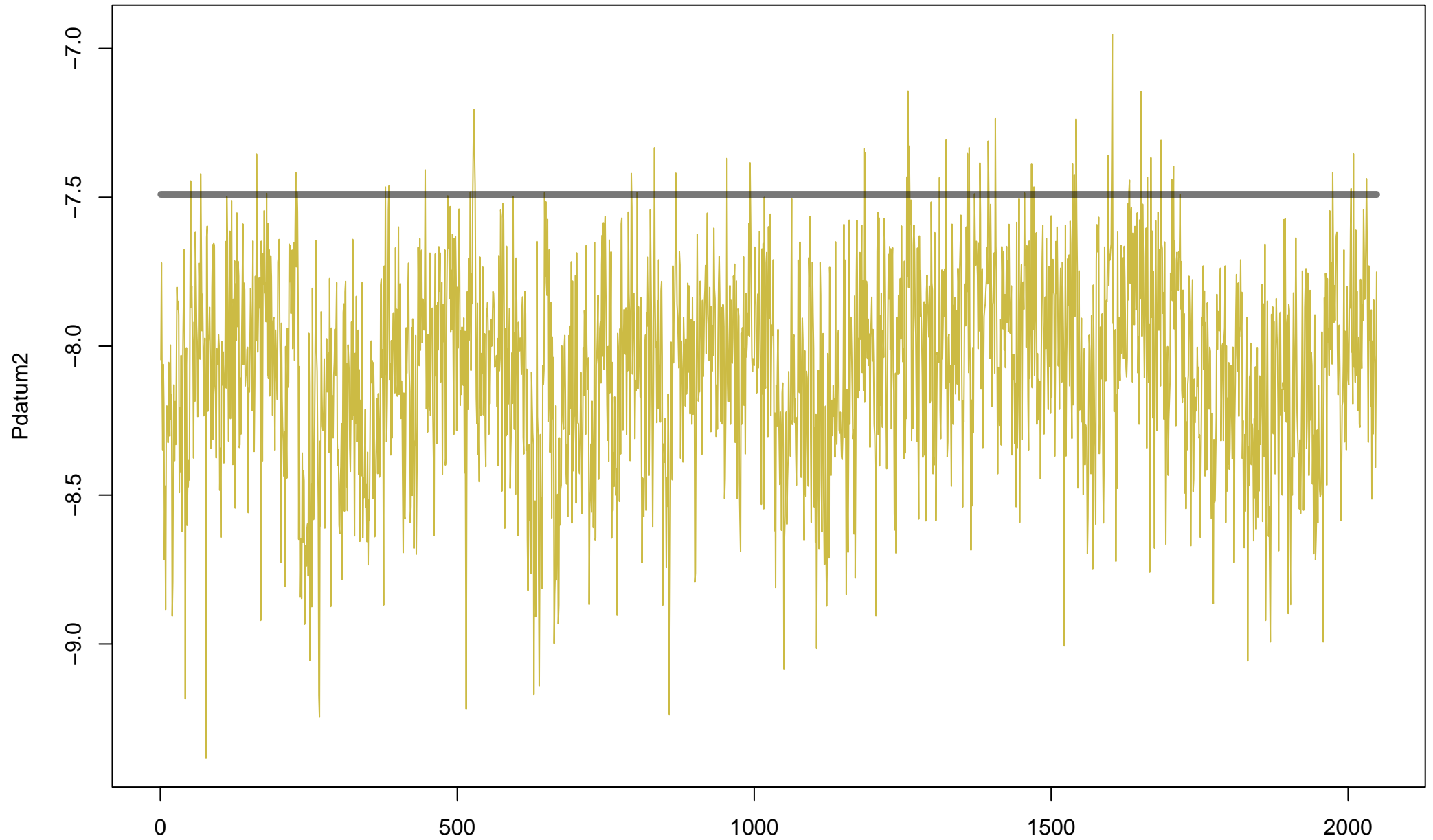
**PdatacornerLo**  
**ESS = 1660 | BMK = 0.0538 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: 0.708**



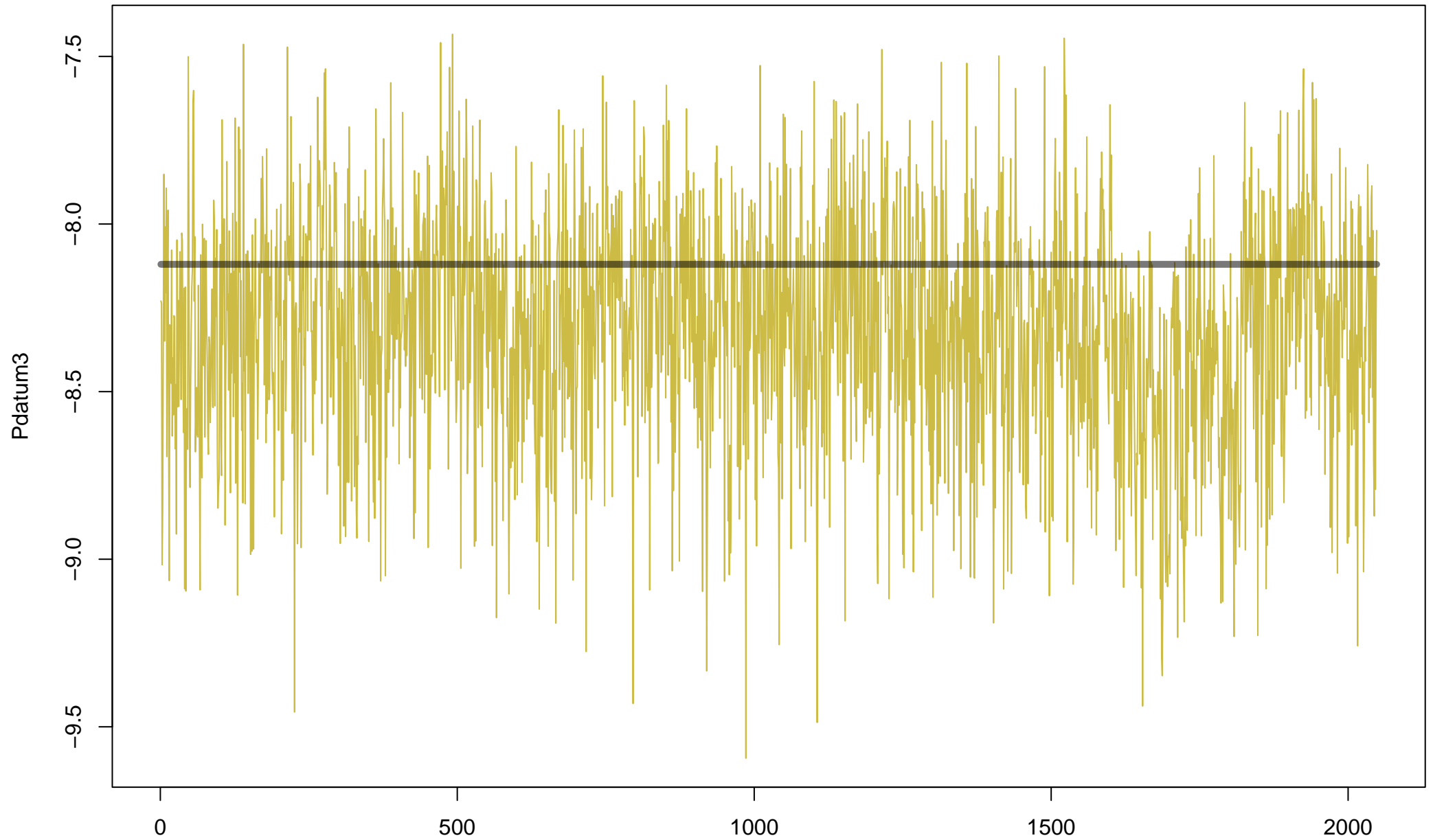
**Pdatum1**  
**ESS = 171 | BMK = 0.0573 | MCSE(6.27) = 5.9 | stat: FALSE | burn: 0 | rel.err: -1.08**



**Pdatum2**  
**ESS = 308 | BMK = 0.0694 | MCSE(6.27) = 5.66 | stat: TRUE | burn: 0 | rel.err: -2.15**

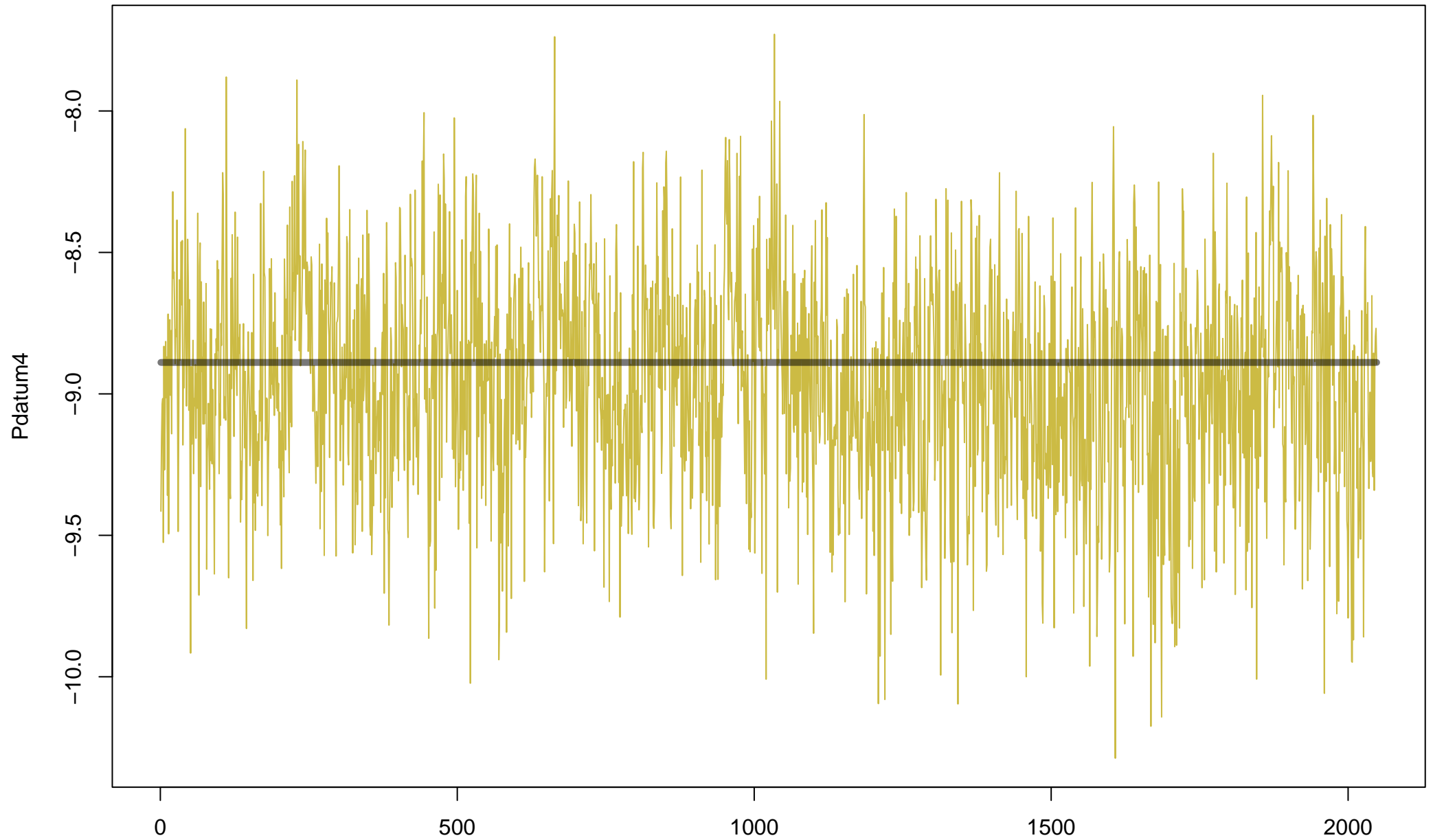


**Pdatum3**  
**ESS = 726 | BMK = 0.0664 | MCSE(6.27) = 4.08 | stat: TRUE | burn: 0 | rel.err: -0.47**



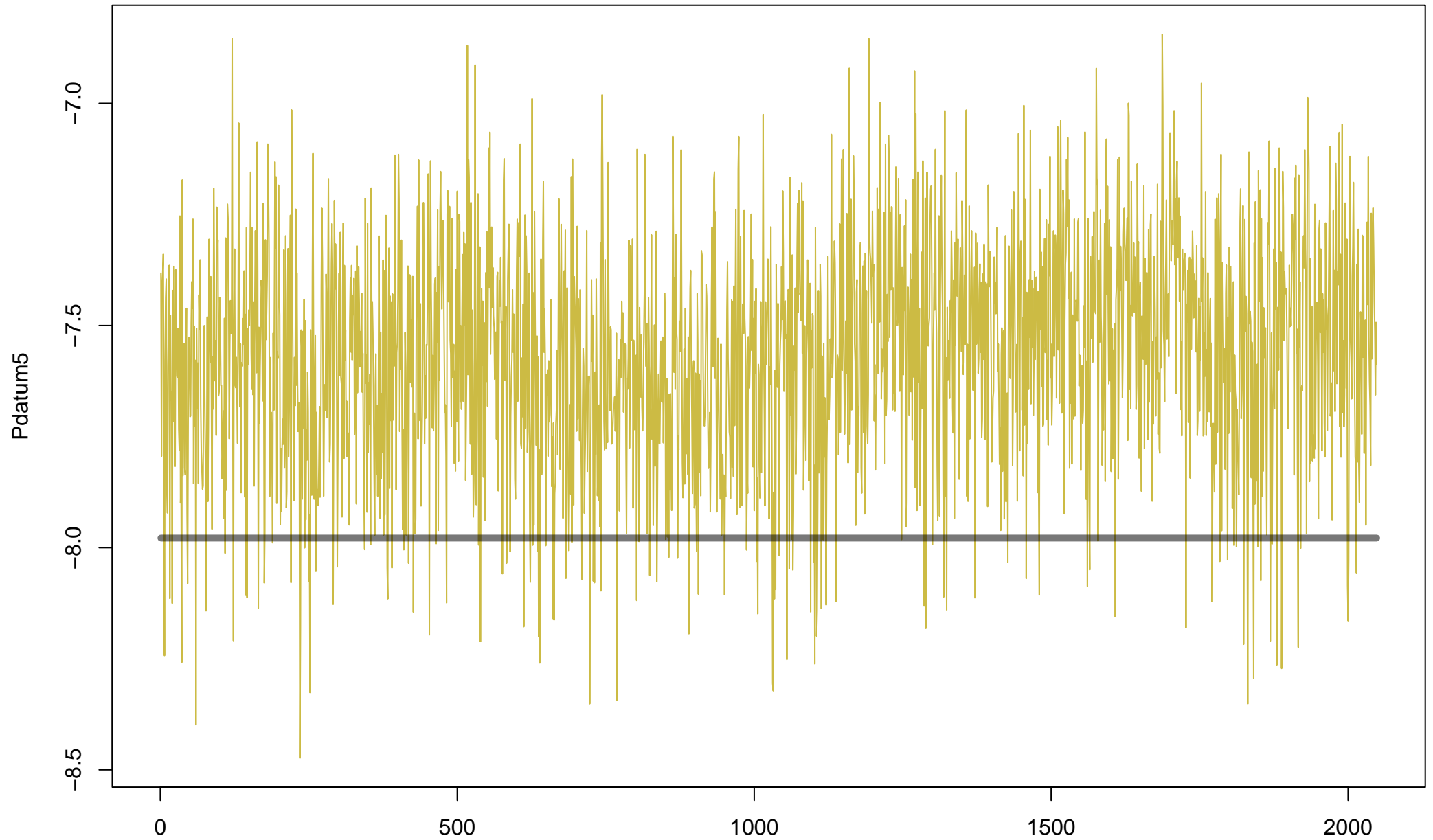


**Pdatum4**  
**ESS = 701 | BMK = 0.106 | MCSE(6.27) = 4.87 | stat: TRUE | burn: 0 | rel.err: 0.0136**



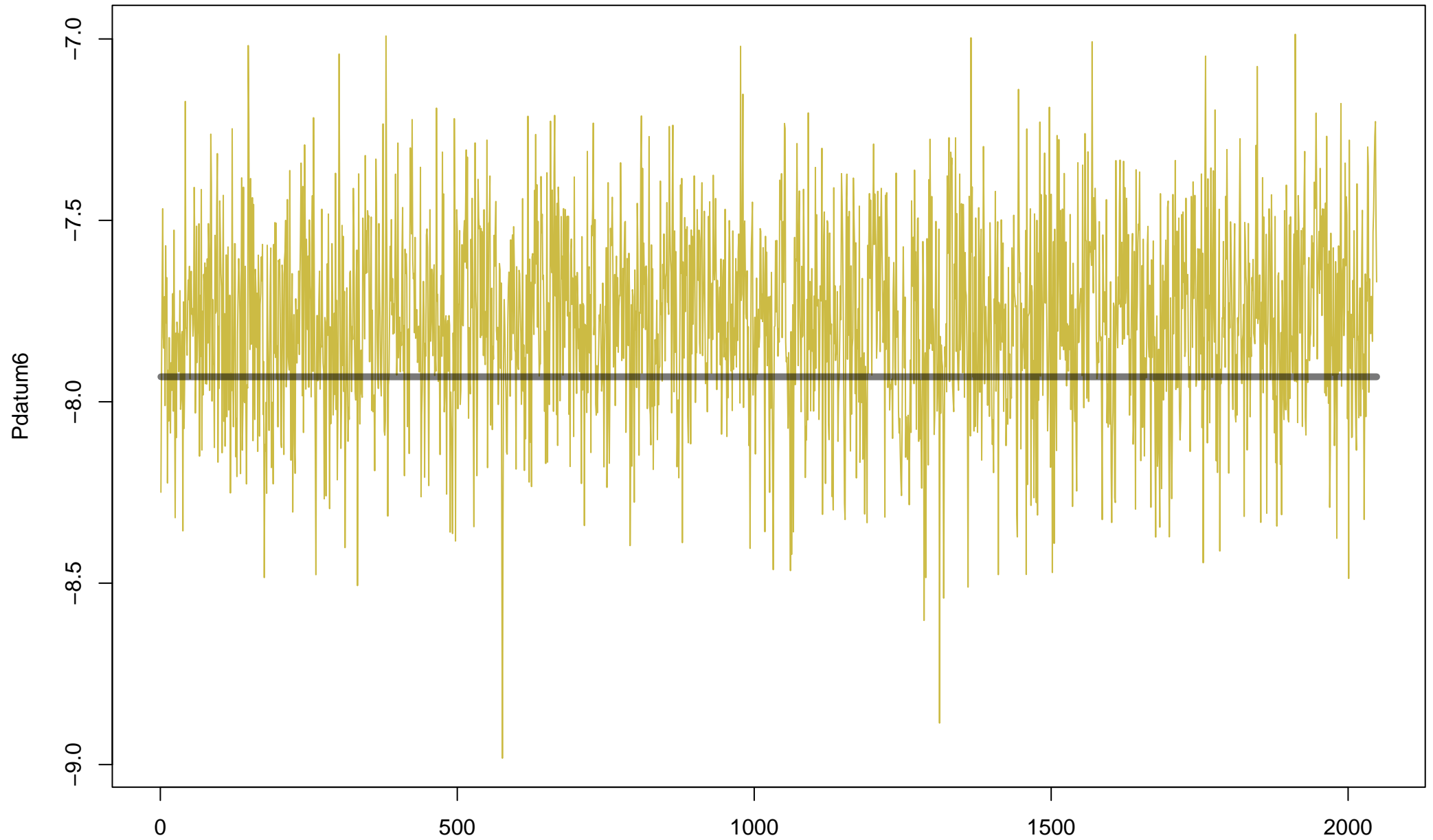
**Pdatum5**

**ESS = 399 | BMK = 0.127 | MCSE(6.27) = 4.39 | stat: FALSE | burn: 0 | rel.err: 1.43**



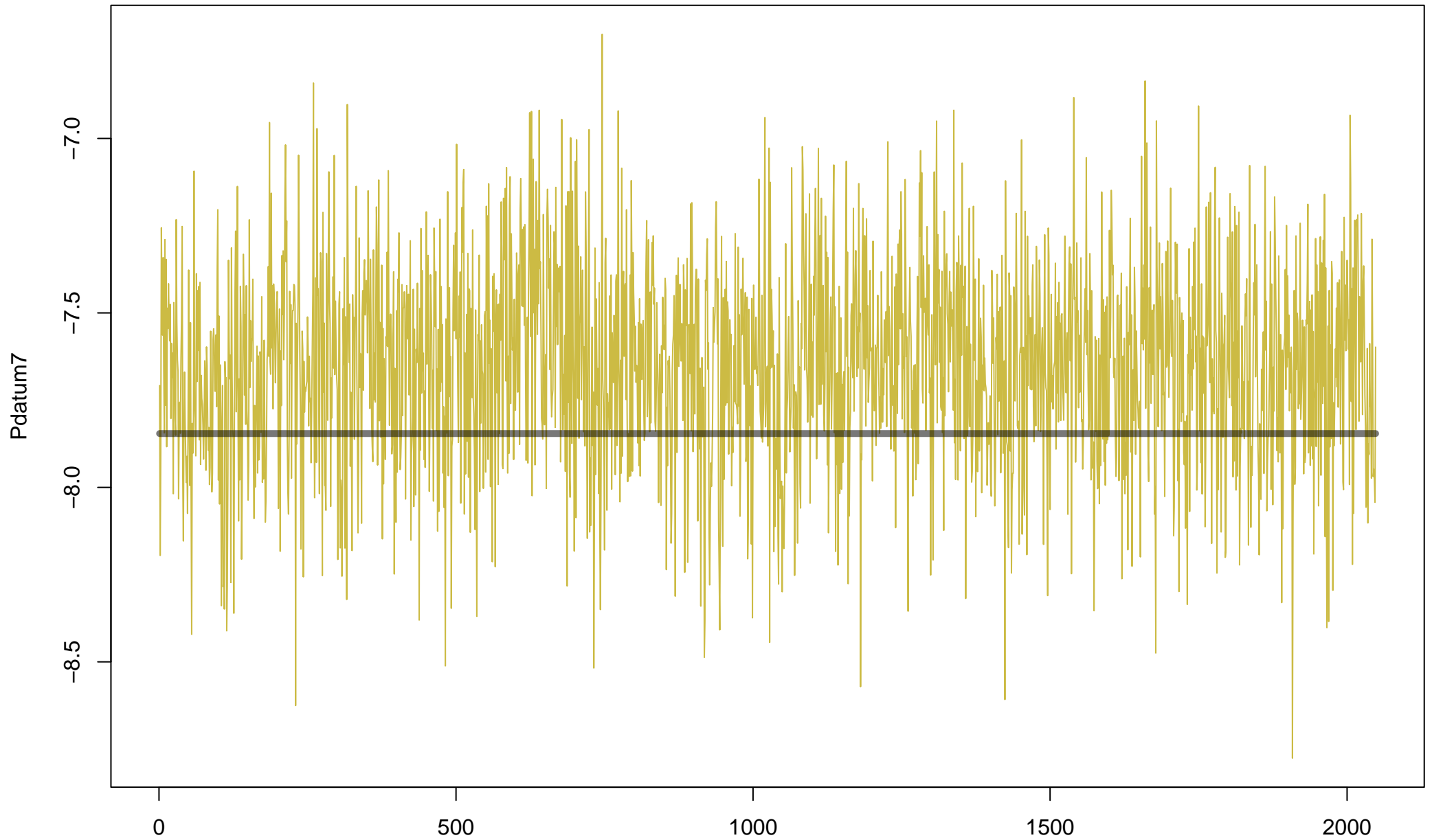
**Pdatum6**

**ESS = 1460 | BMK = 0.0609 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 0.66**



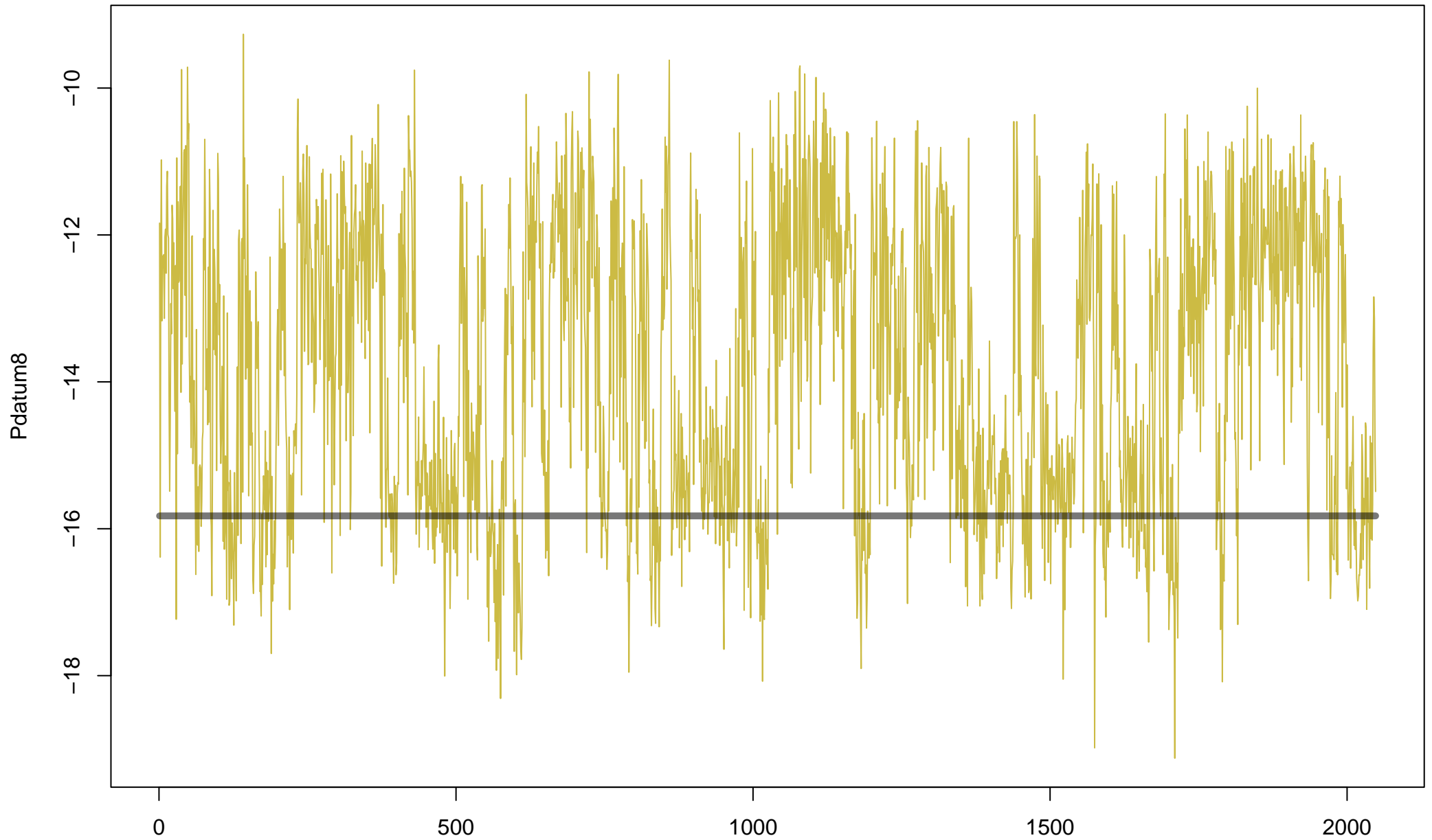
**Pdatum7**

**ESS = 1360 | BMK = 0.0341 | MCSE(6.27) = 3.65 | stat: FALSE | burn: 0 | rel.err: 0.735**



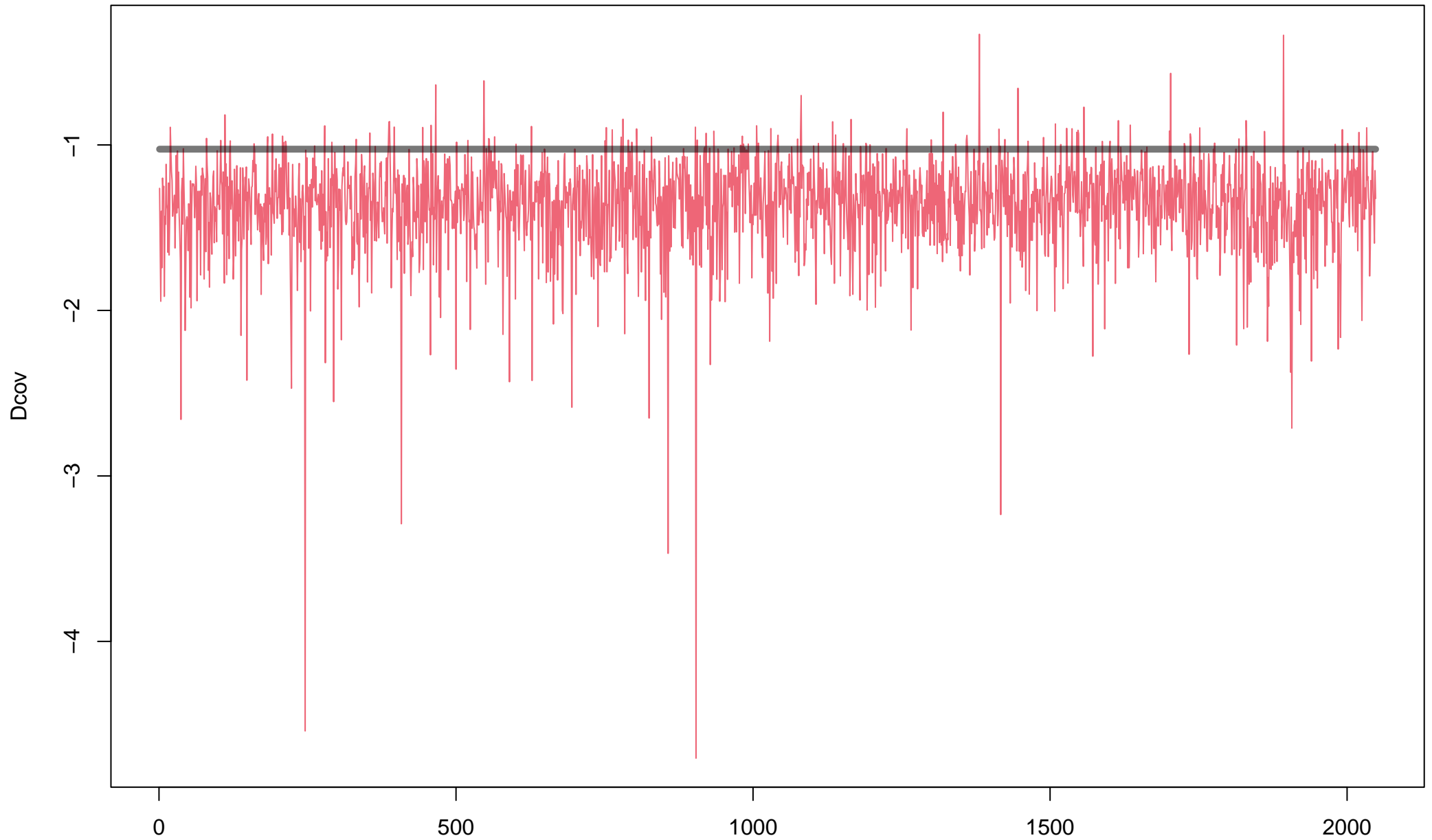
**Pdatum8**

**ESS = 277 | BMK = 0.083 | MCSE(6.27) = 5.36 | stat: TRUE | burn: 0 | rel.err: 0.541**

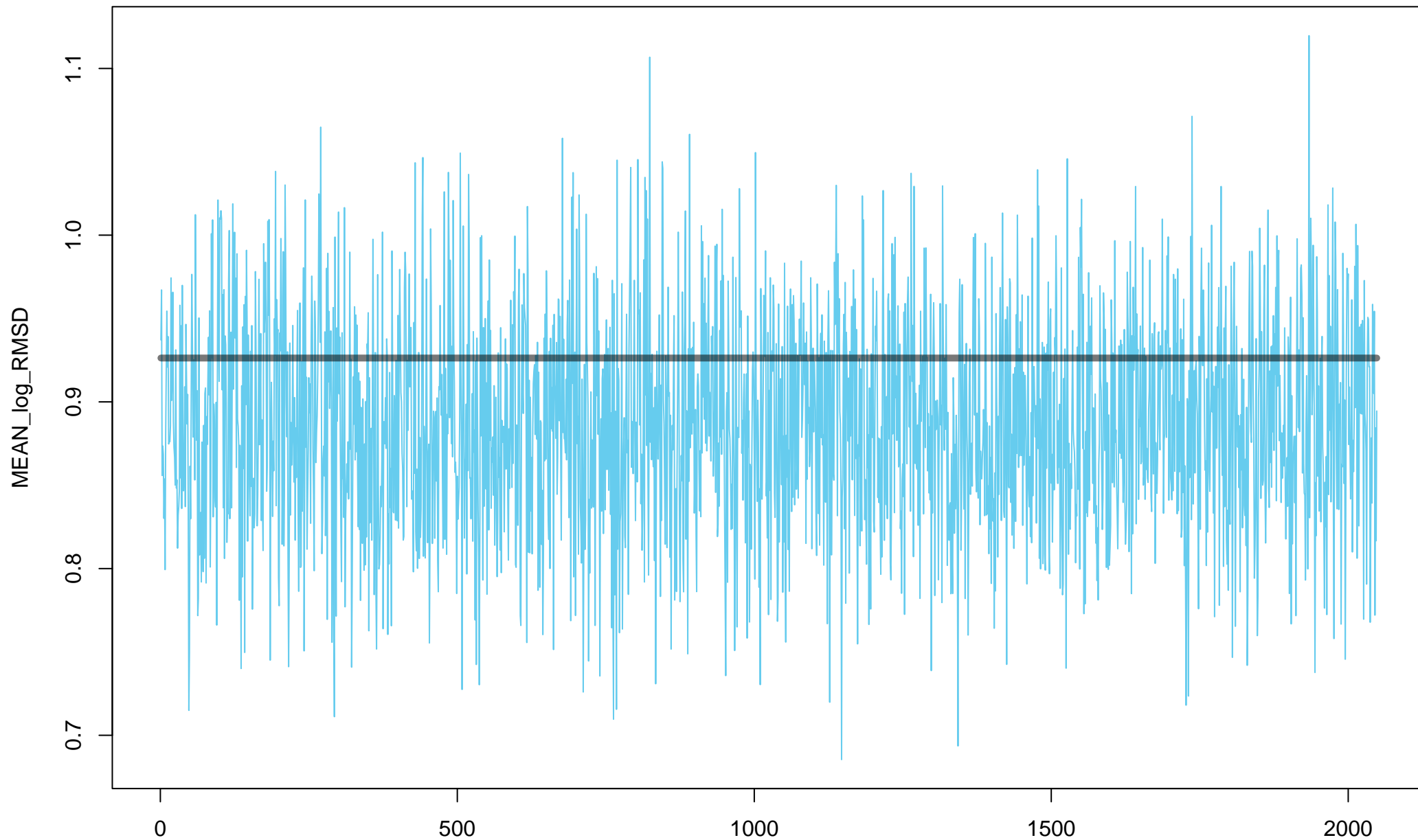


Dcov

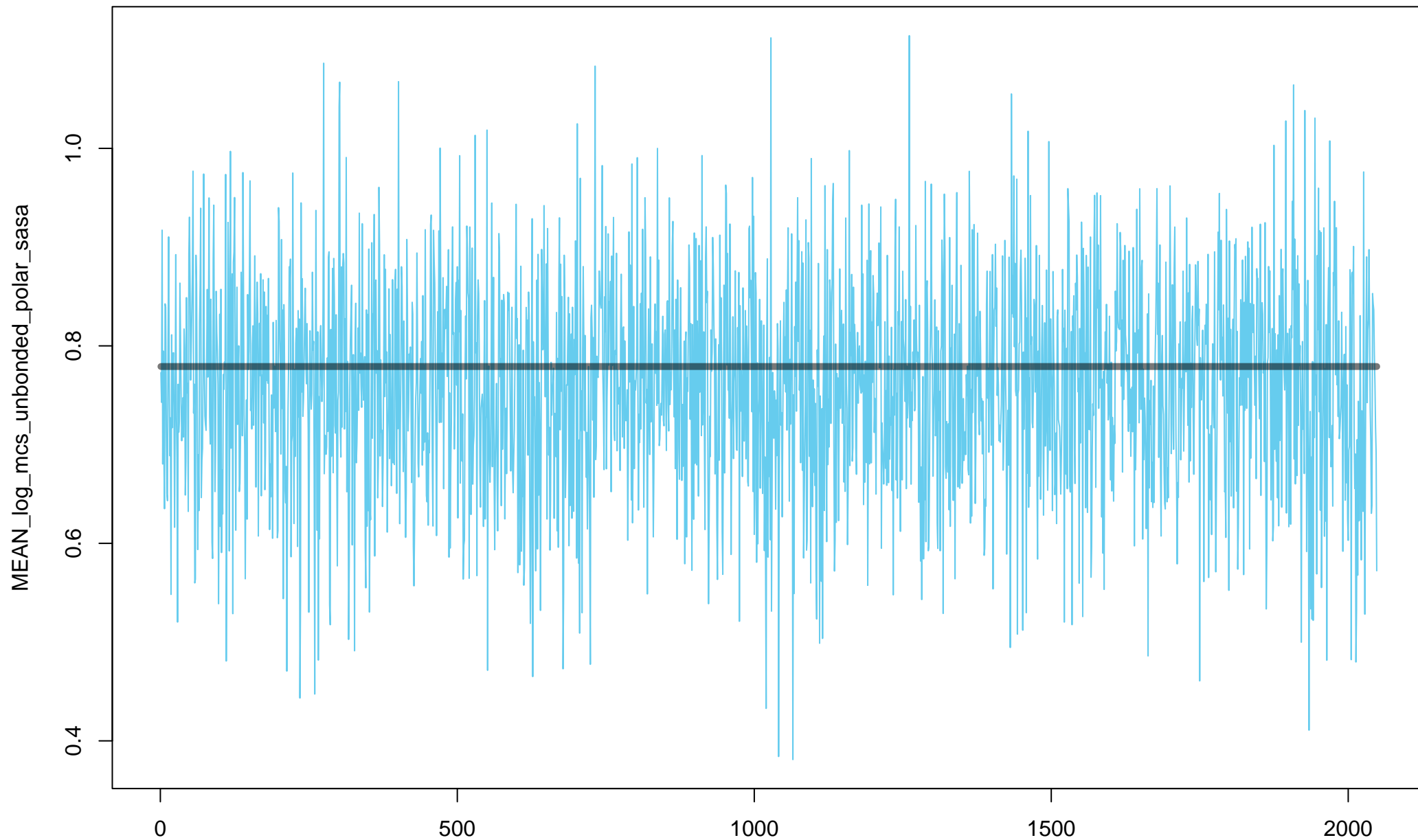
ESS = 2050 | BMK = 0.0739 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 1.42



**MEAN\_log\_RMSD**  
**ESS = 1580 | BMK = 0.0654 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: -0.613**



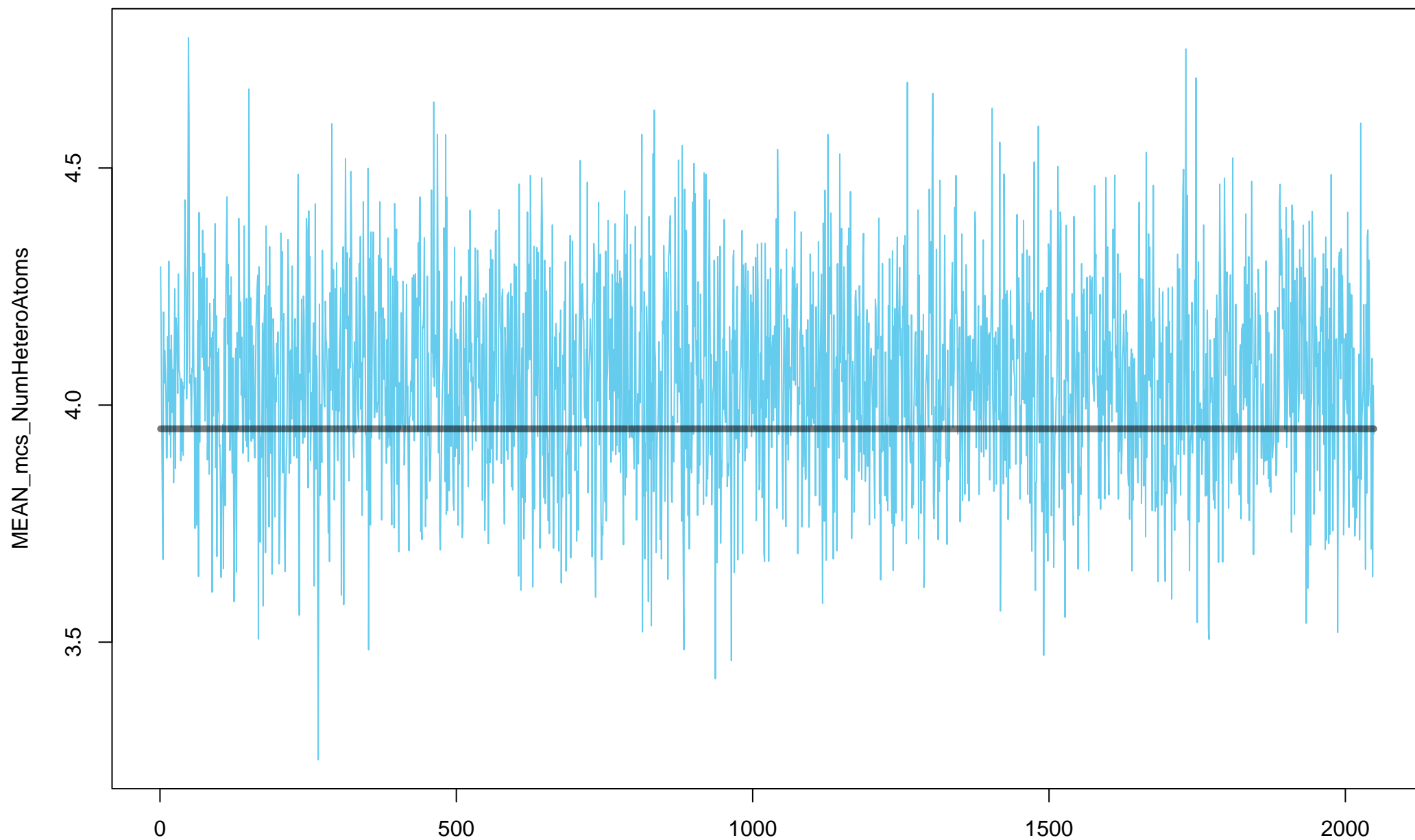
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0345 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: -0.194**





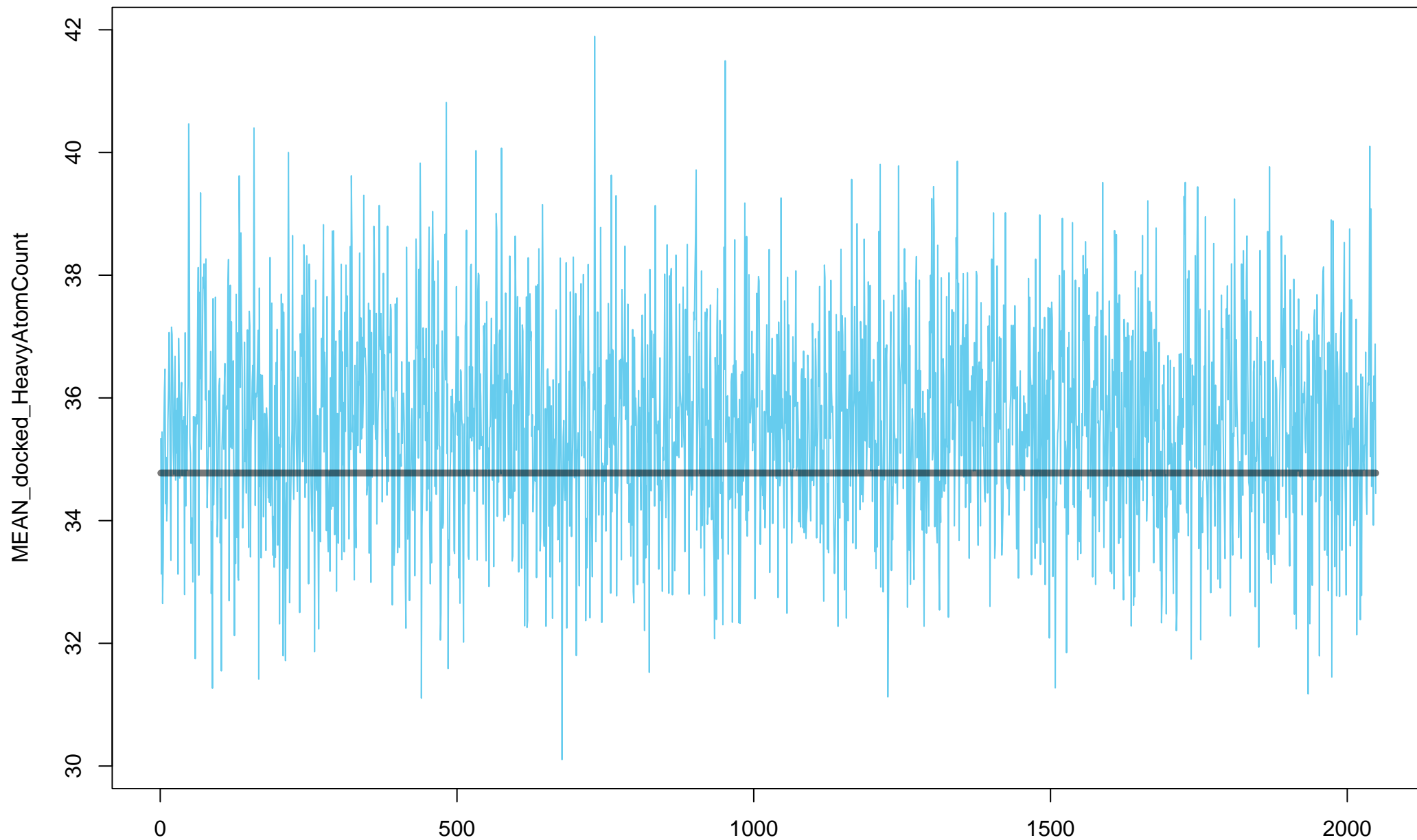
# MEAN\_mcs\_NumHeteroAtoms

ESS = 2050 | BMK = 0.0457 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: 0.487

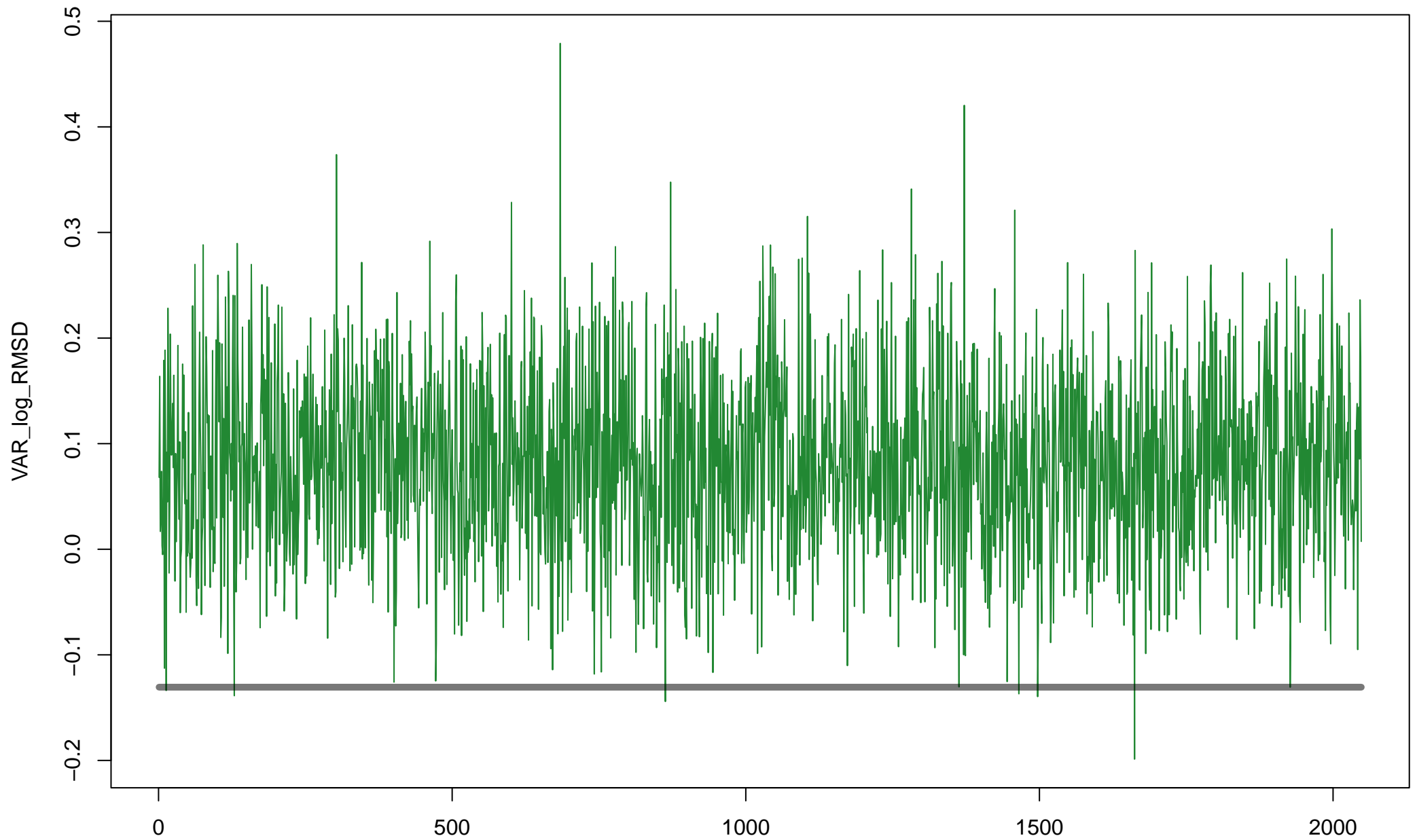


# MEAN\_docked\_HeavyAtomCount

ESS = 1840 | BMK = 0.0494 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: 0.501

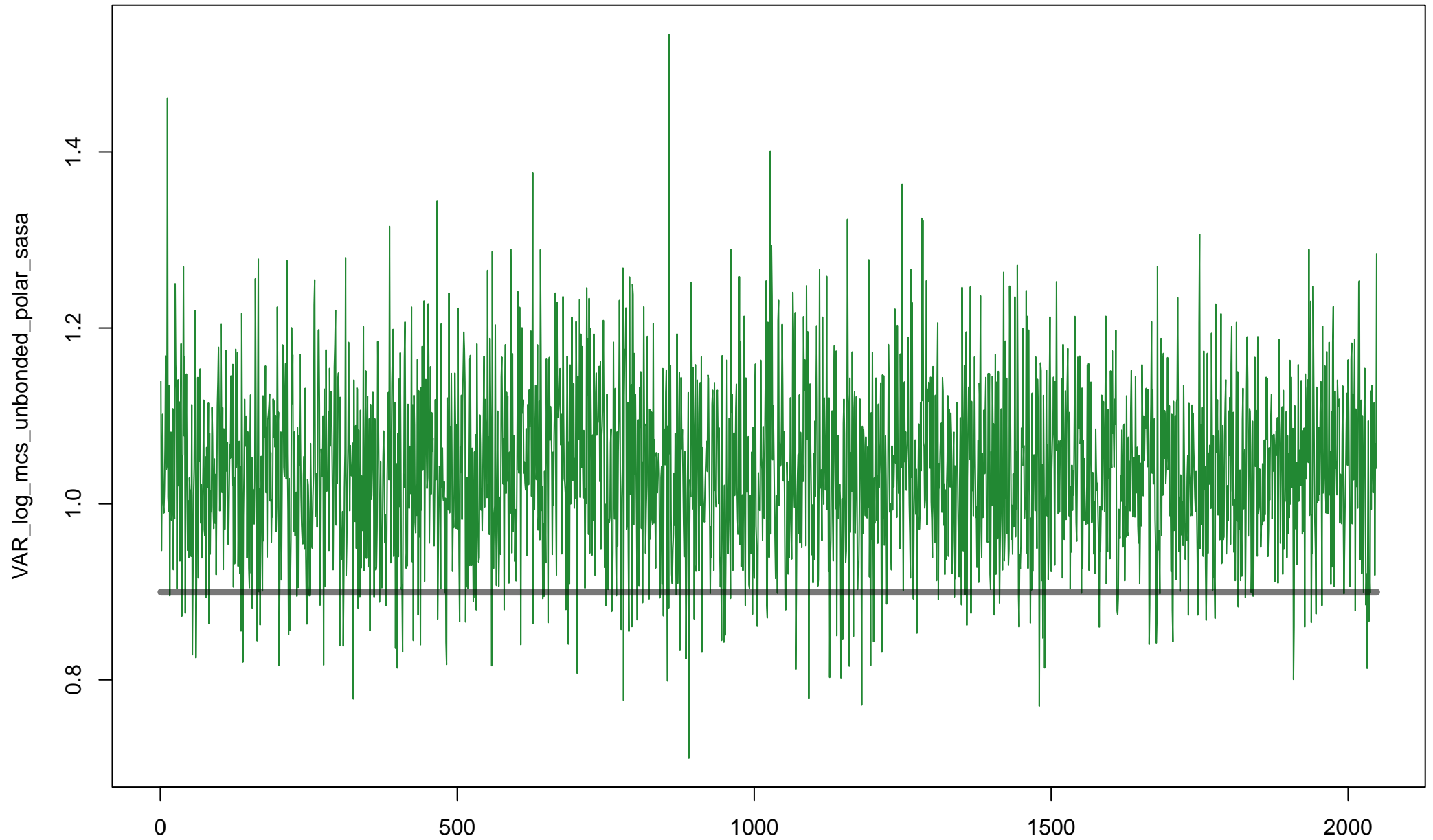


**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 2.28**

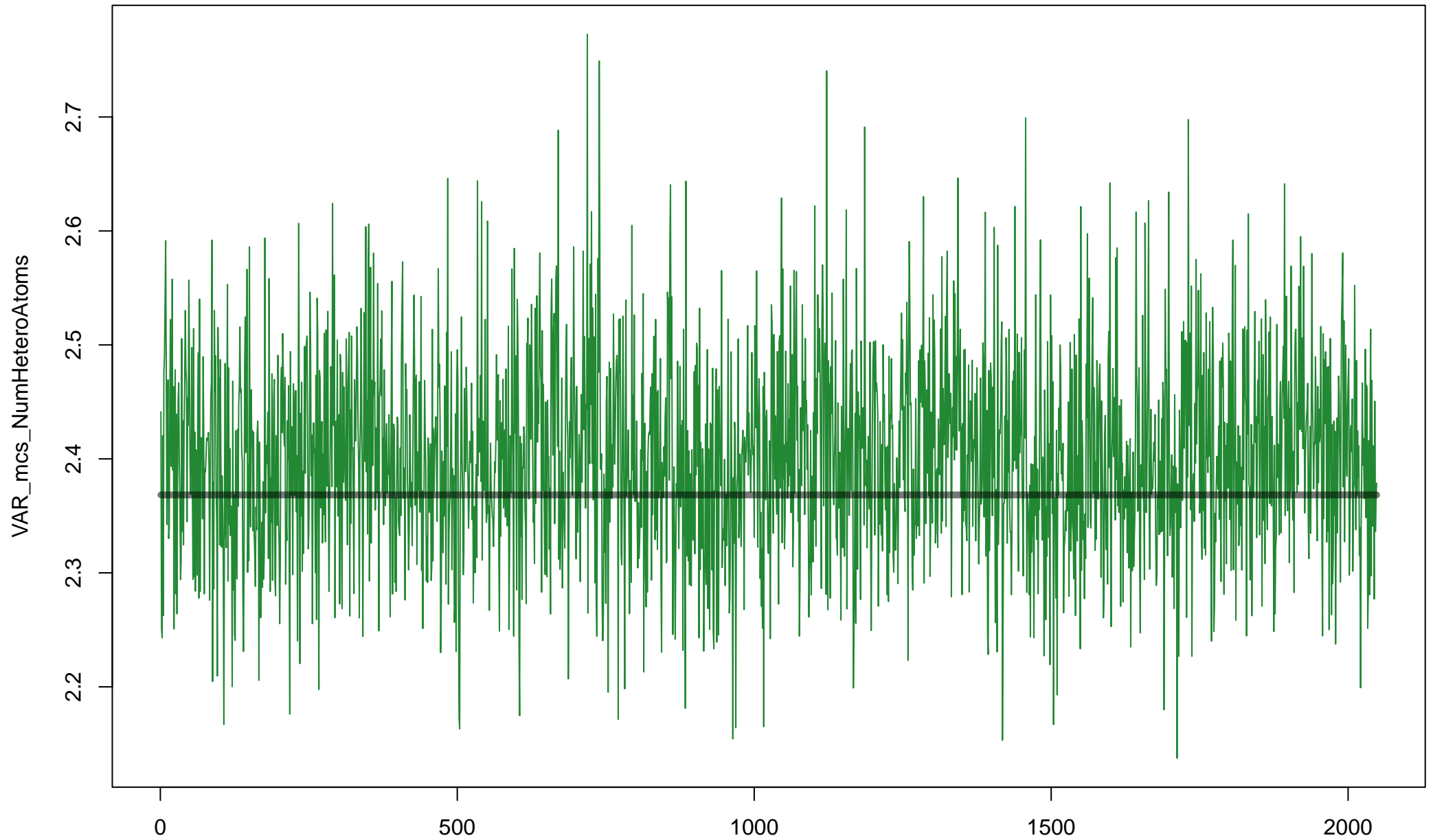


VAR\_log\_mcs\_unbonded\_polar\_sasa

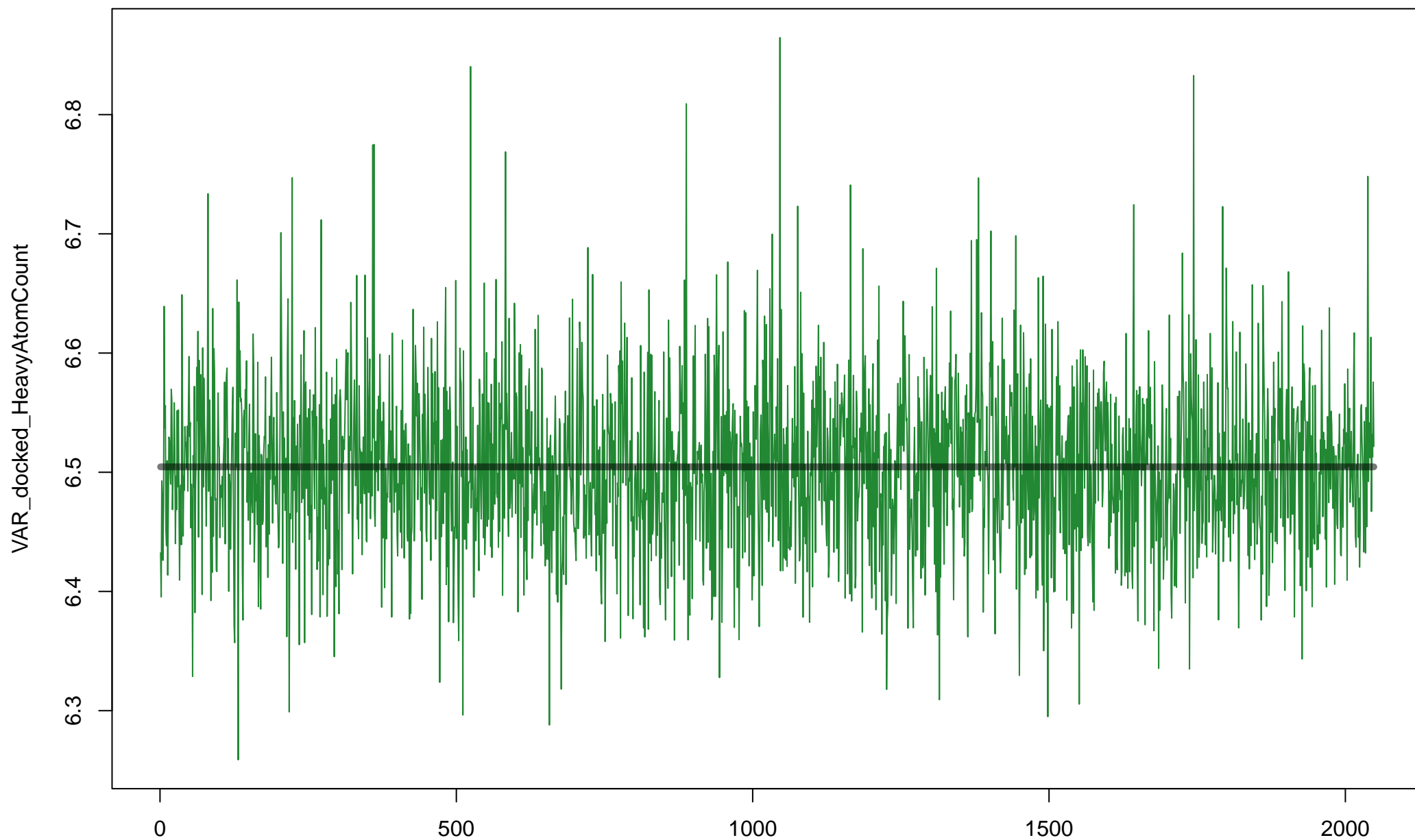
ESS = 2050 | BMK = 0.0506 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: 1.32



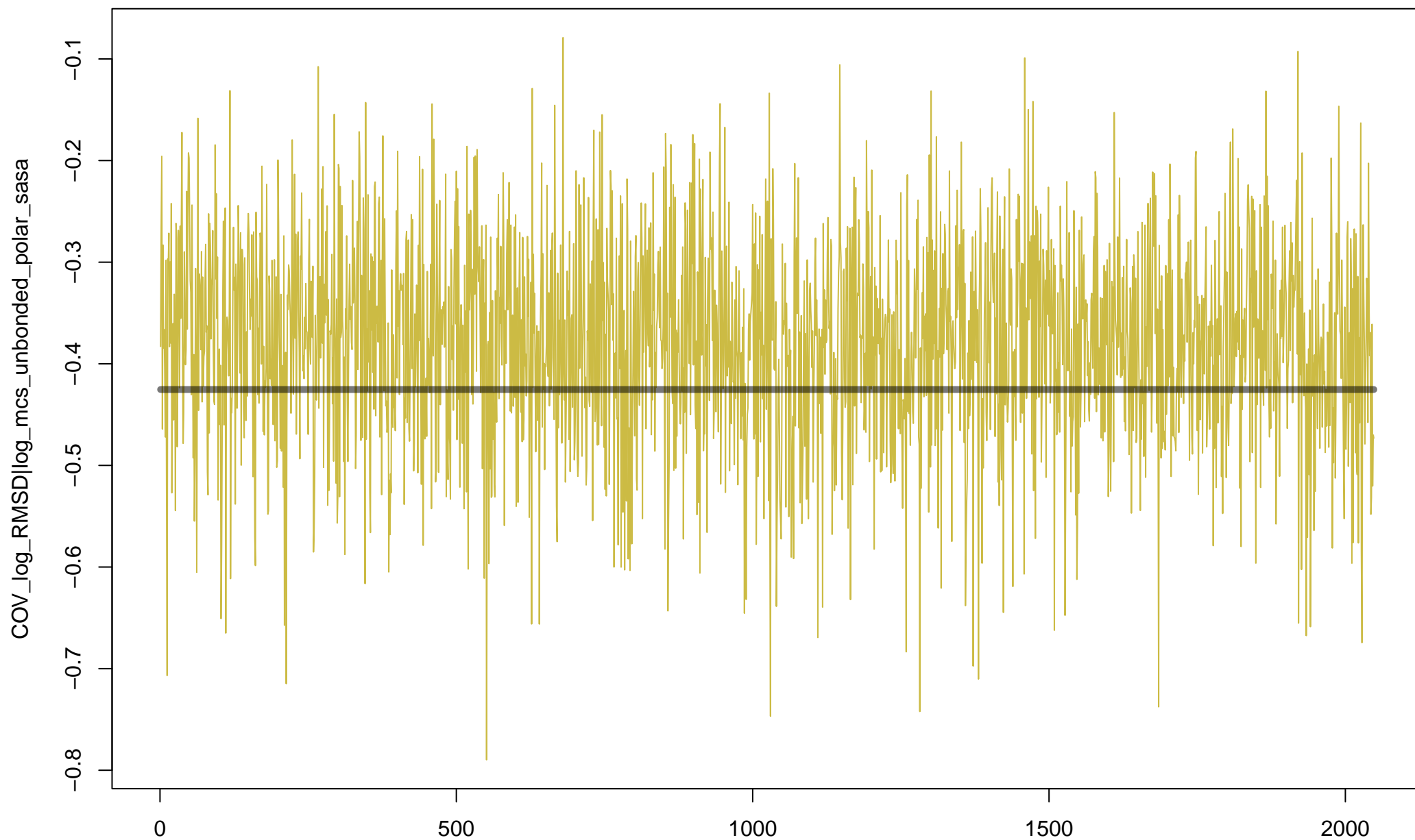
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1720 | BMK = 0.0569 | MCSE(6.27) = 2.79 | stat: TRUE | burn: 0 | rel.err: 0.42**



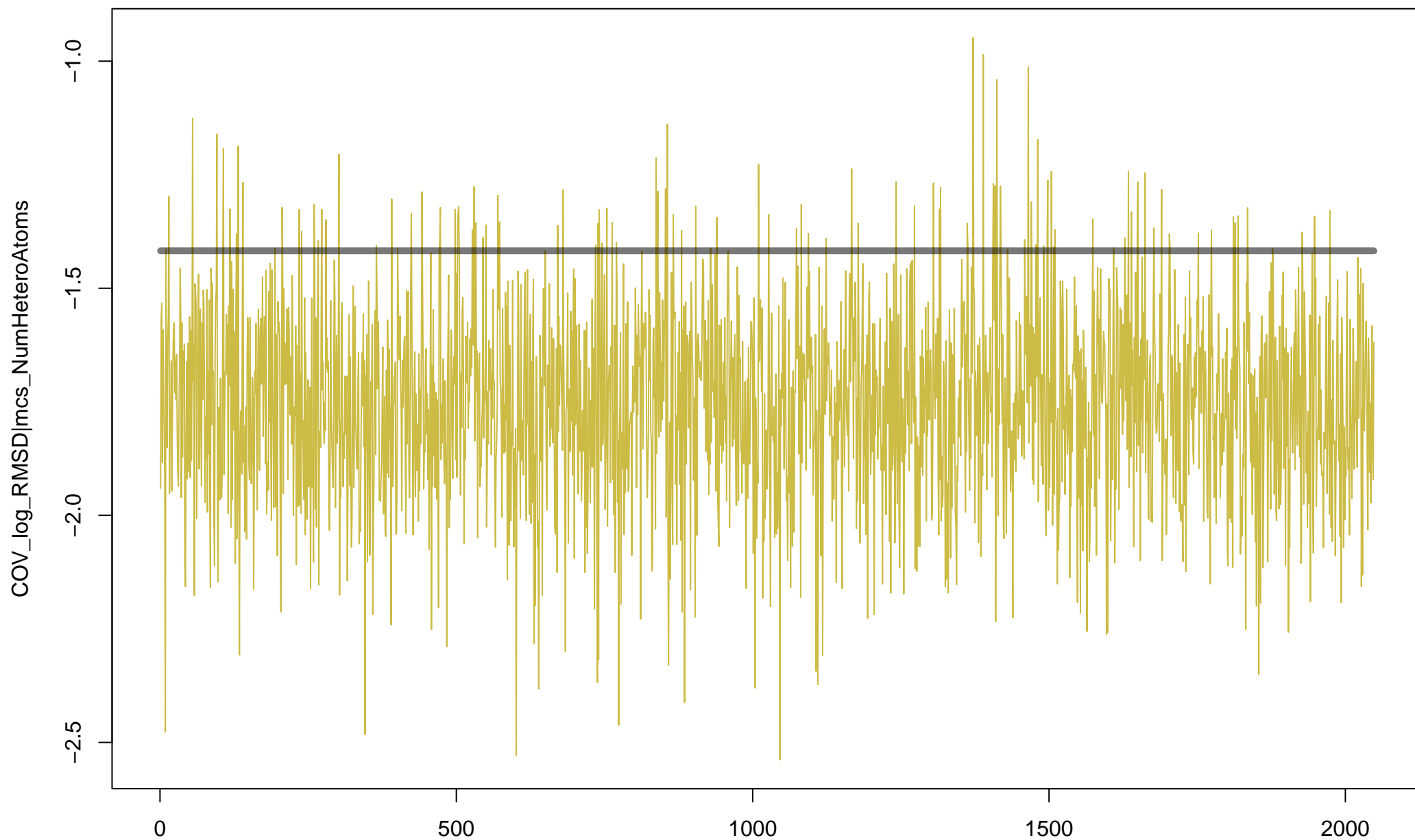
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0604 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0 | rel.err: 0.0325**



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0511 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0 | rel.err: 0.457**

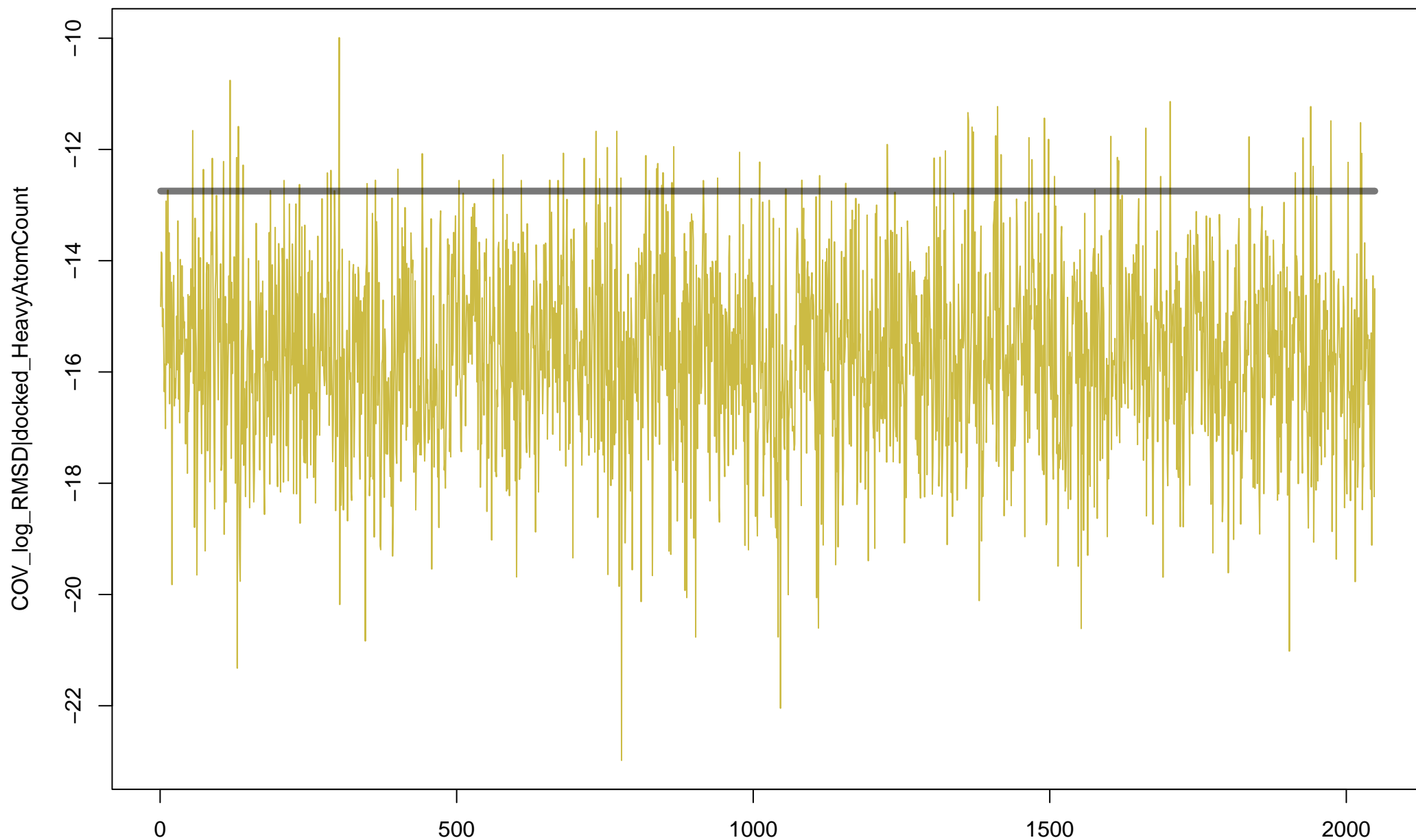


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1690 | BMK = 0.063 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: -1.59**

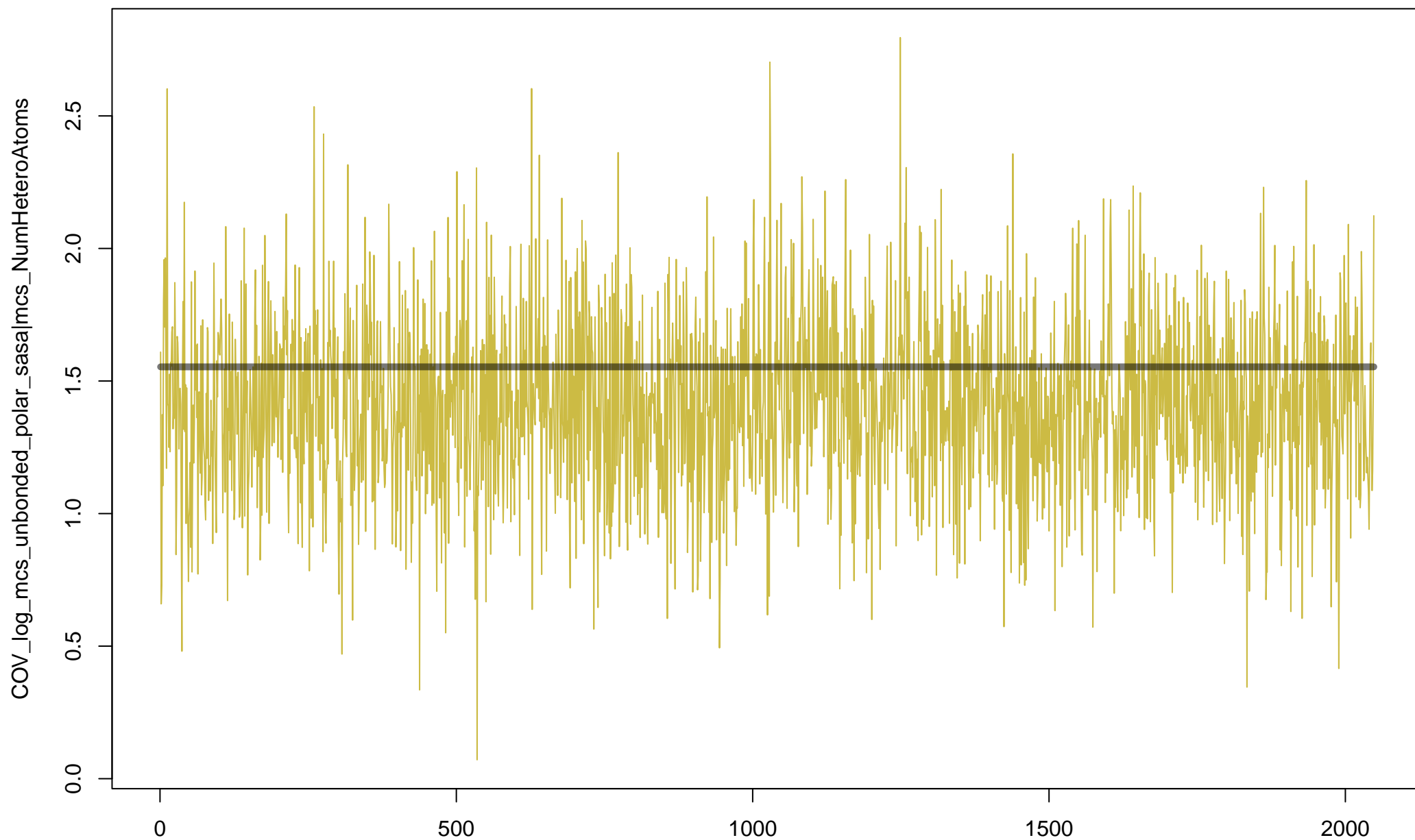




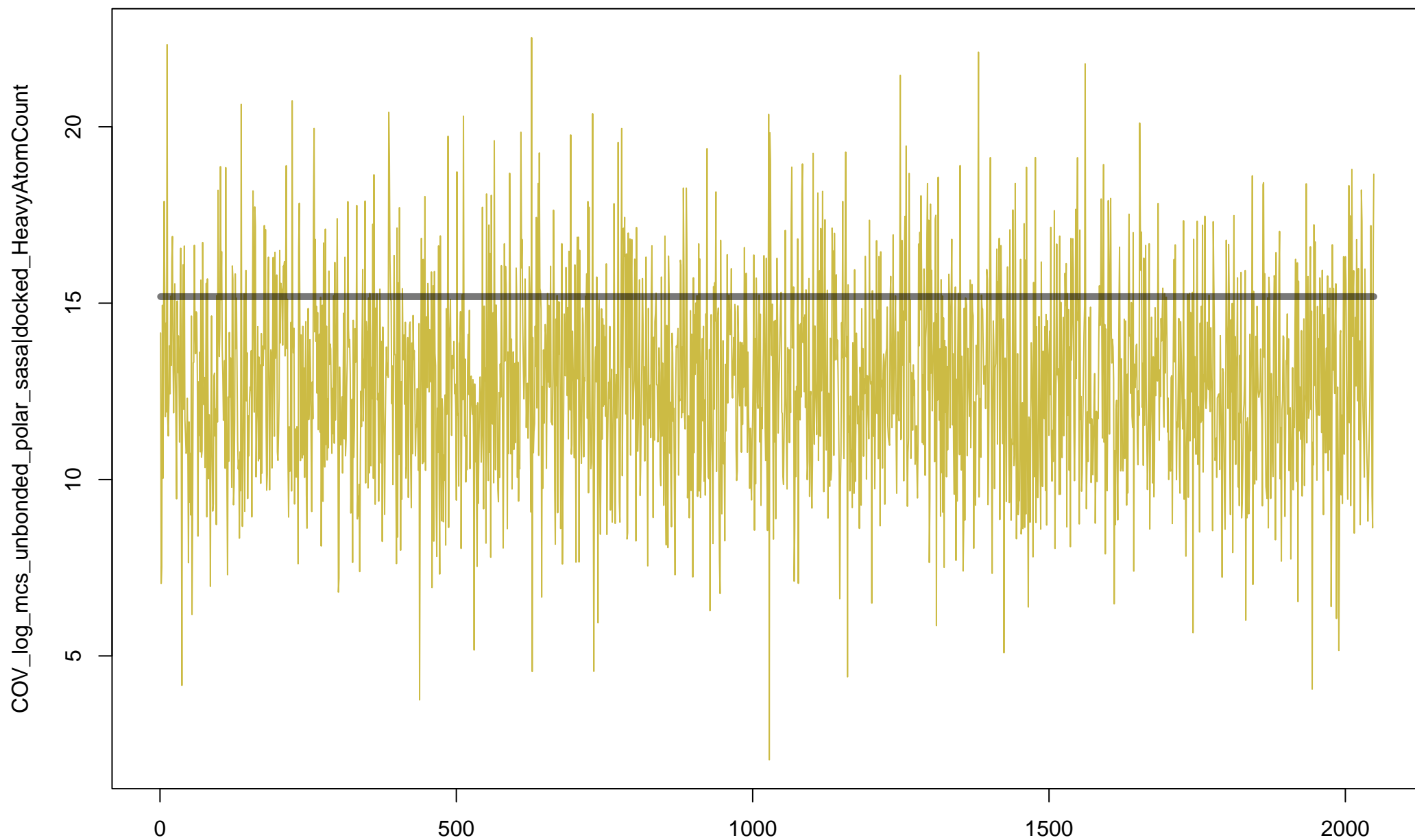
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1600 | BMK = 0.0481 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: -1.74**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0566 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: -0.433**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0443 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: -0.888**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: 0.435**

