

-- STATS maxD --

min ESS = 155.685412973418

max BMK = 0.12295507793789

max MCSE = 6.7717608617198

all stationary: FALSE

burn: 1632

max rel.err.: 2.06212947358124

-- STATS 2D --

min ESS = 2048

max BMK = 0.047633949943371

max MCSE = 2.4935379876555

all stationary: TRUE

burn: 0

max rel.err.: 1.80664001834303

-- STATS 1D --

min ESS = 1531.15427488669

max BMK = 0.0655621800407998

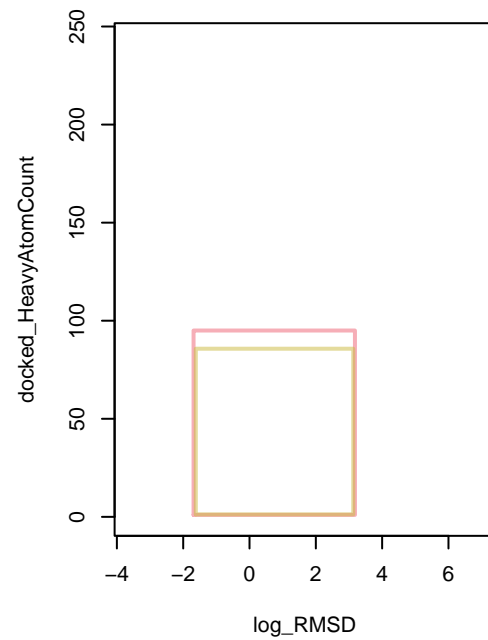
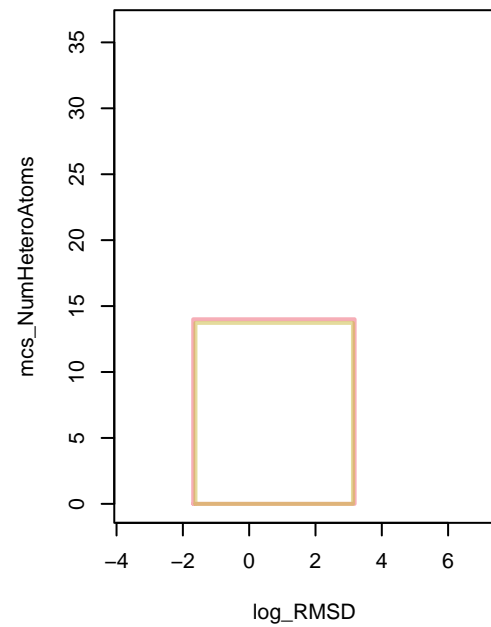
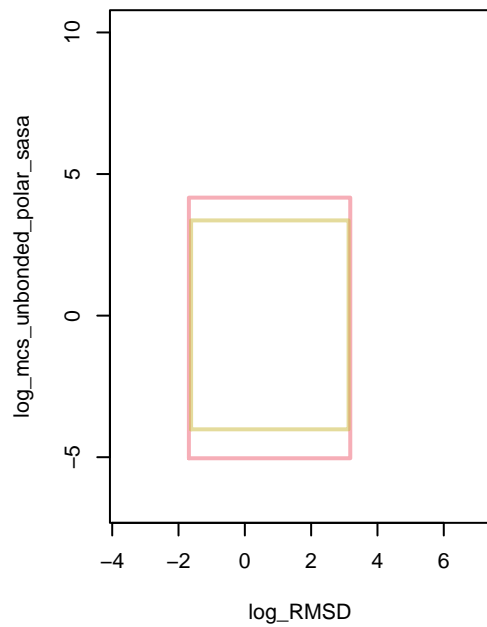
max MCSE = 3.43567124002789

all stationary: TRUE

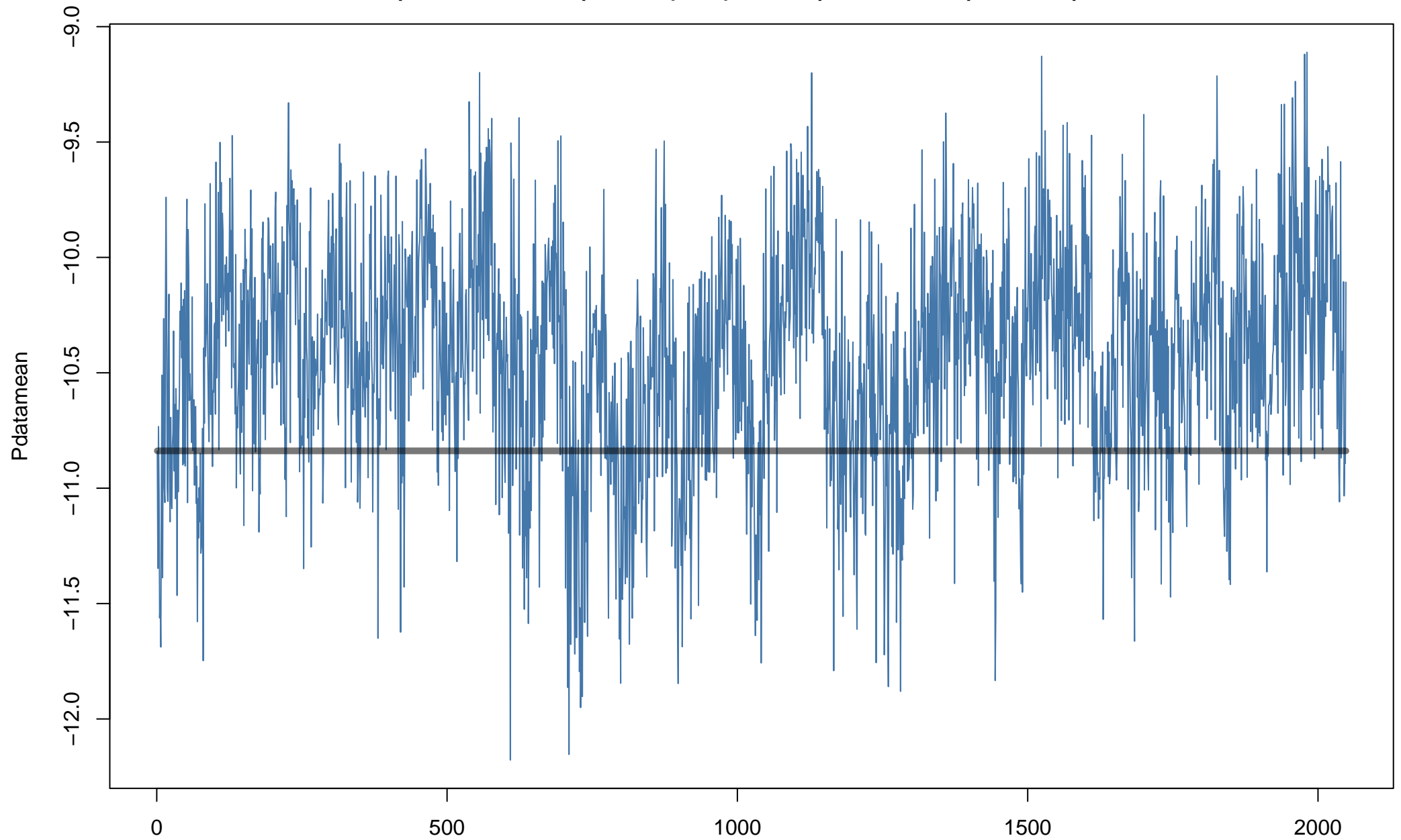
burn: 0

max rel.err.: 2.32983497273179

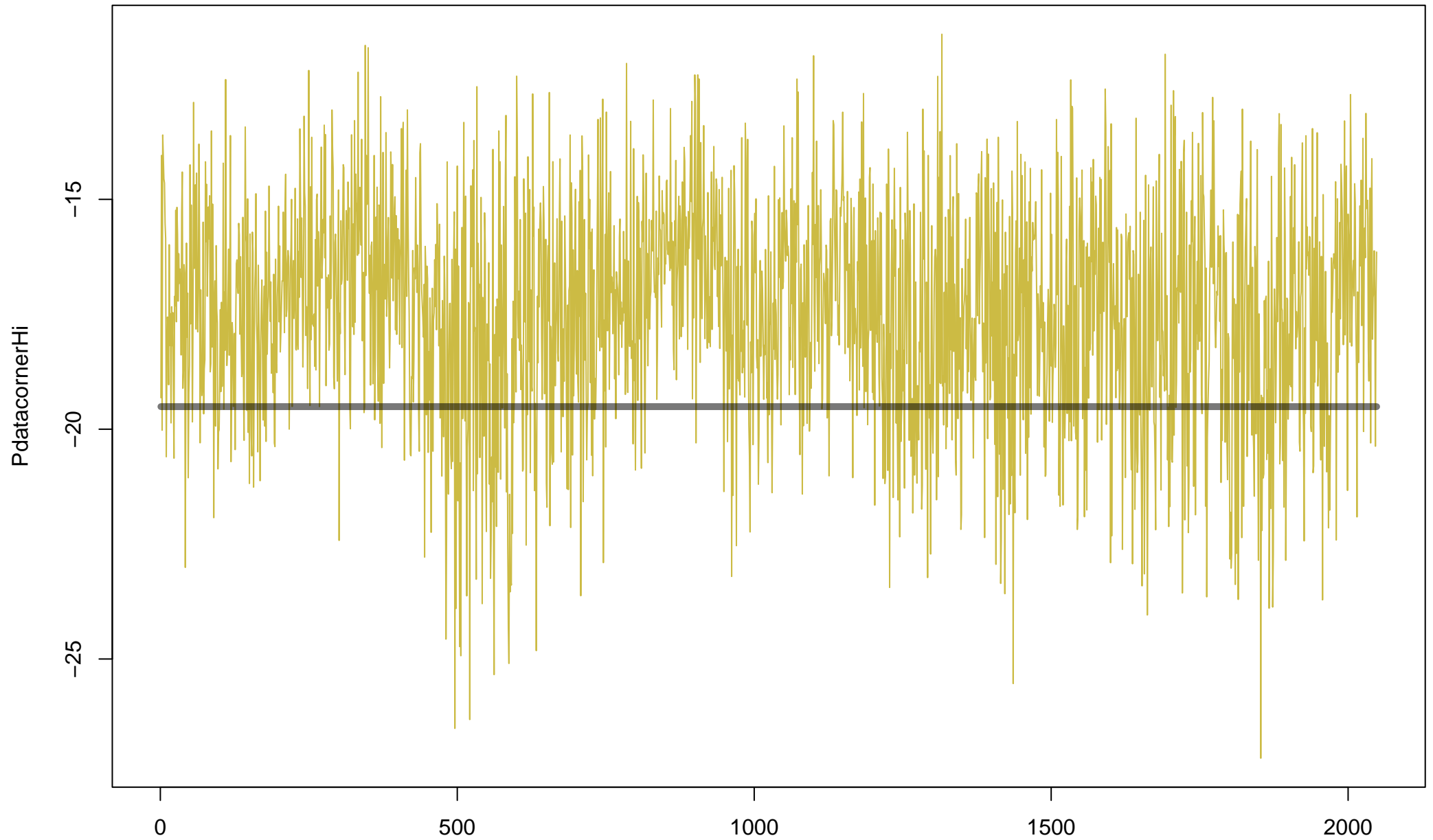
Occupied clusters: 10 of 16



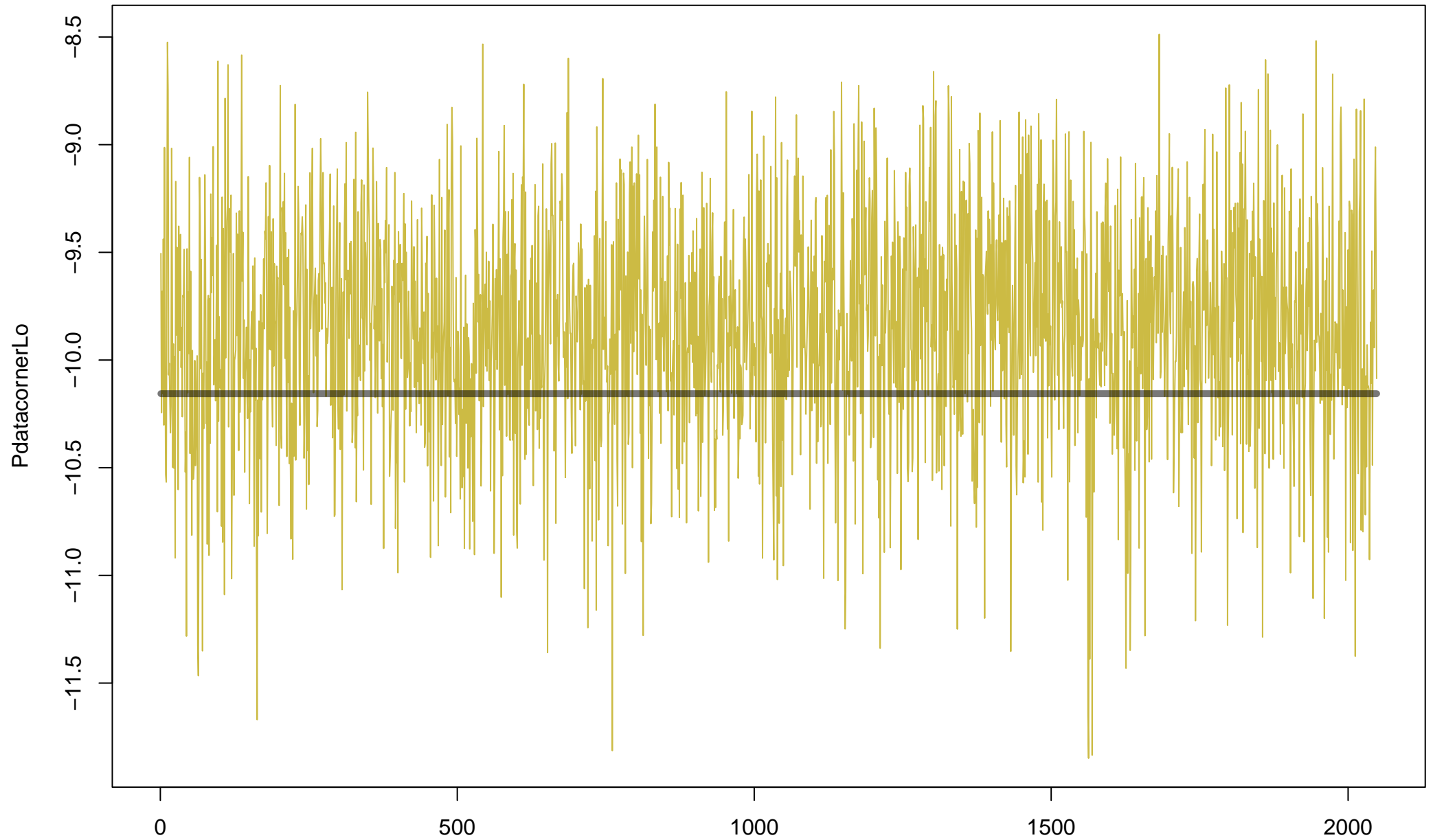
**Pdatamean**  
**ESS = 156 | BMK = 0.0619 | MCSE(6.27) = 6.77 | stat: TRUE | burn: 0 | rel.err: 0.862**



**PdatacornerHi**  
**ESS = 1250 | BMK = 0.123 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 0.323**

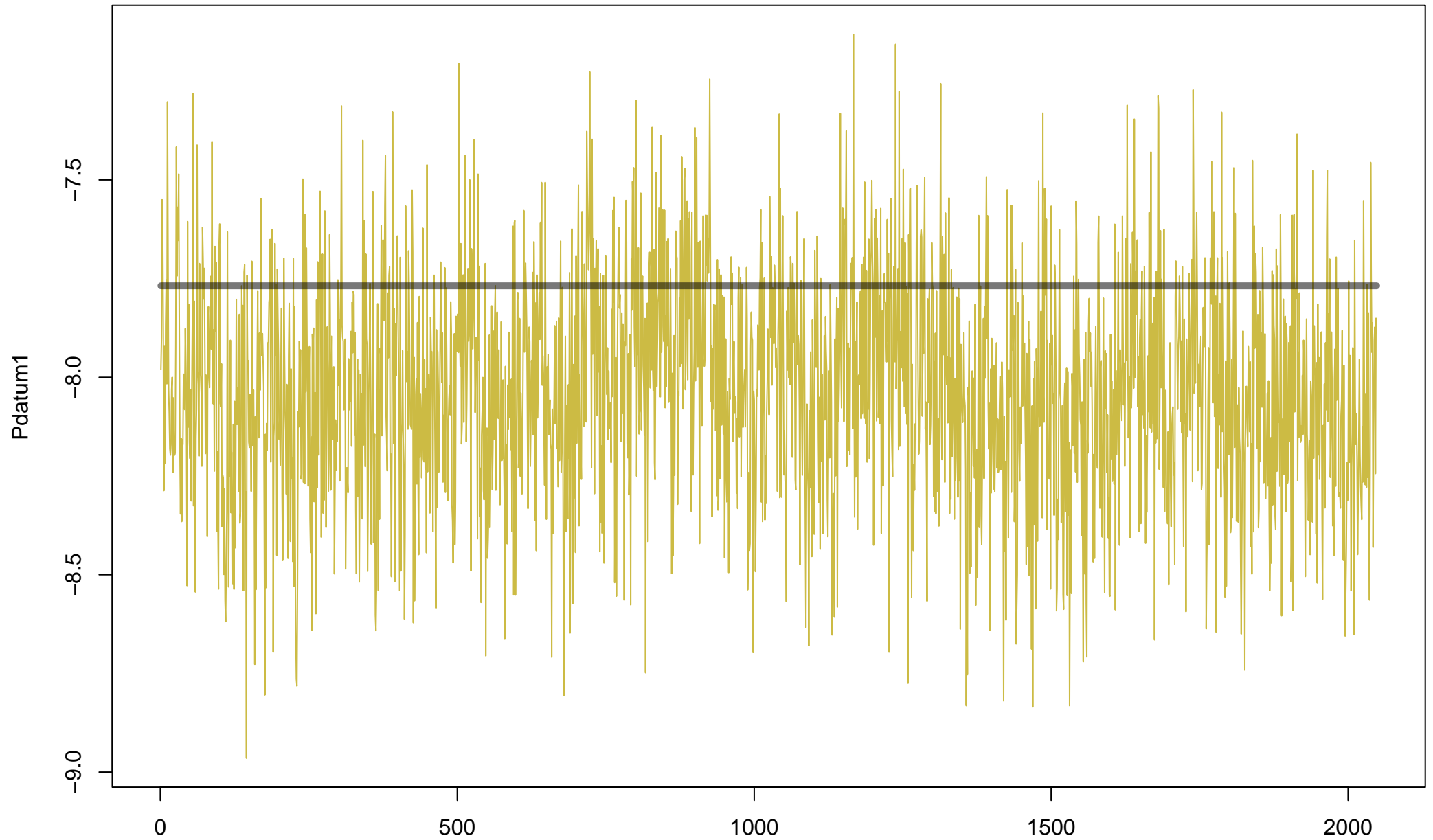


**PdatacornerLo**  
**ESS = 1870 | BMK = 0.066 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 0.686**

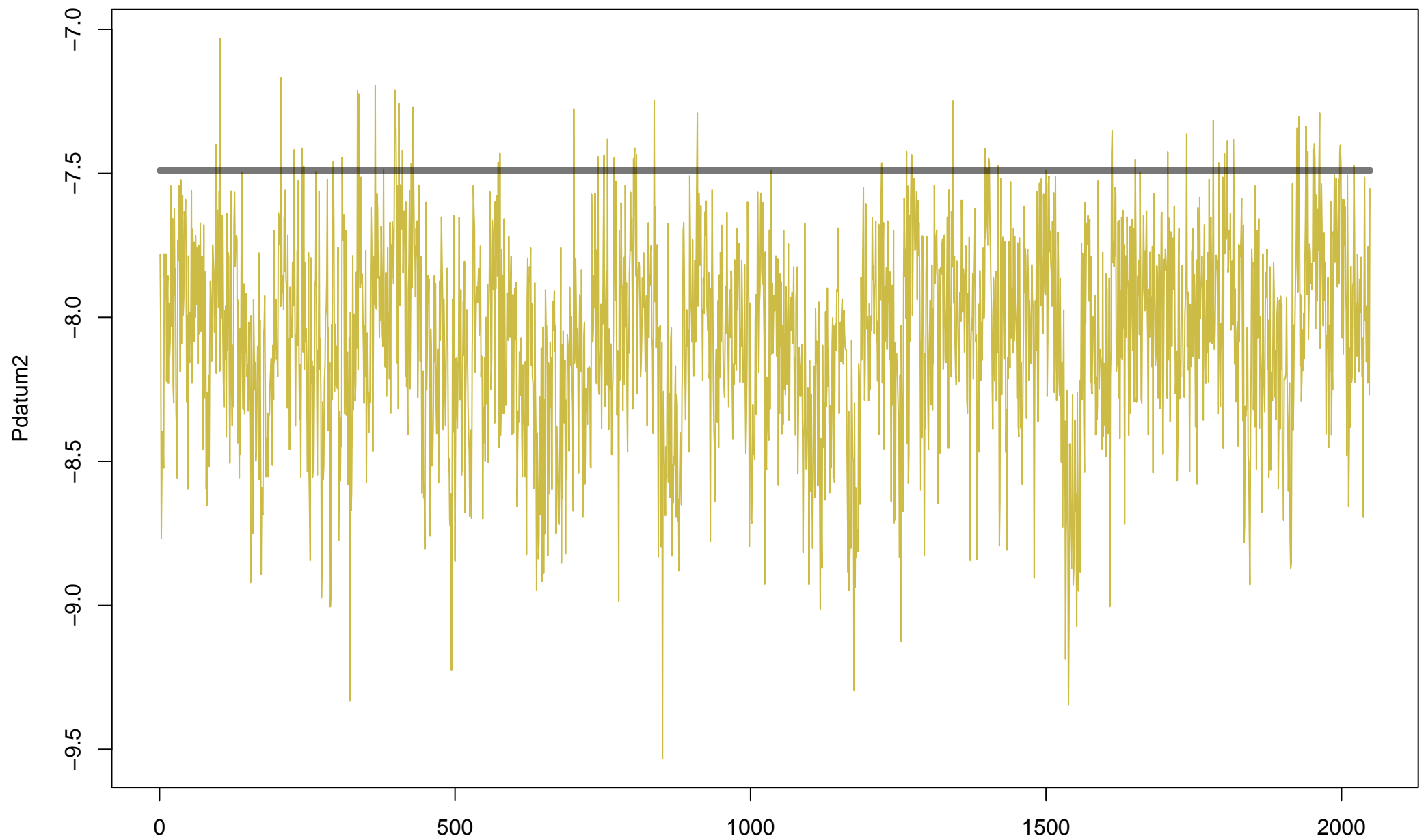


**Pdatum1**

**ESS = 424 | BMK = 0.0448 | MCSE(6.27) = 4.29 | stat: TRUE | burn: 0 | rel.err: -0.874**

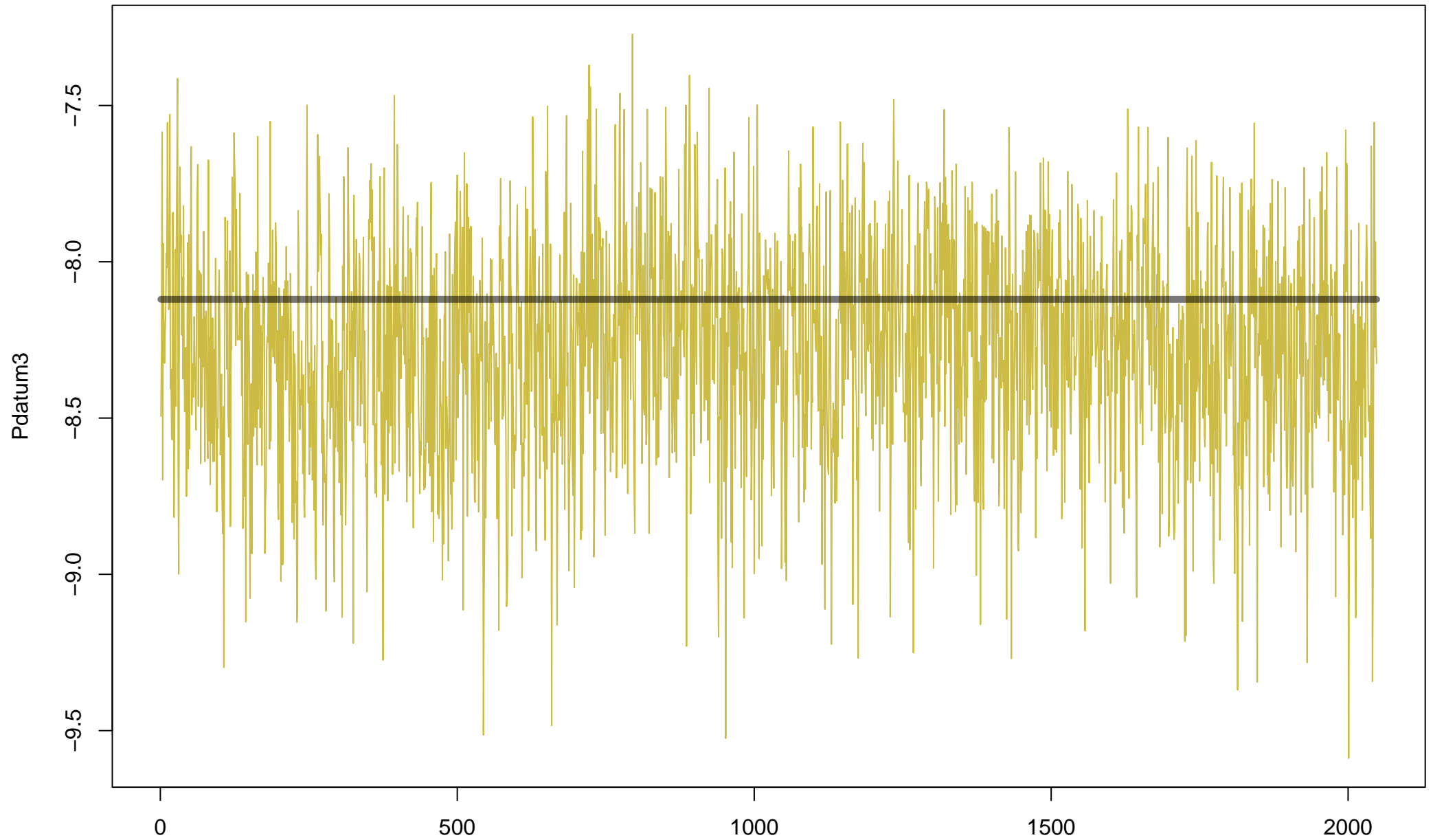


**Pdatum2**  
**ESS = 235 | BMK = 0.0727 | MCSE(6.27) = 5.73 | stat: TRUE | burn: 0 | rel.err: -2.06**



**Pdatum3**

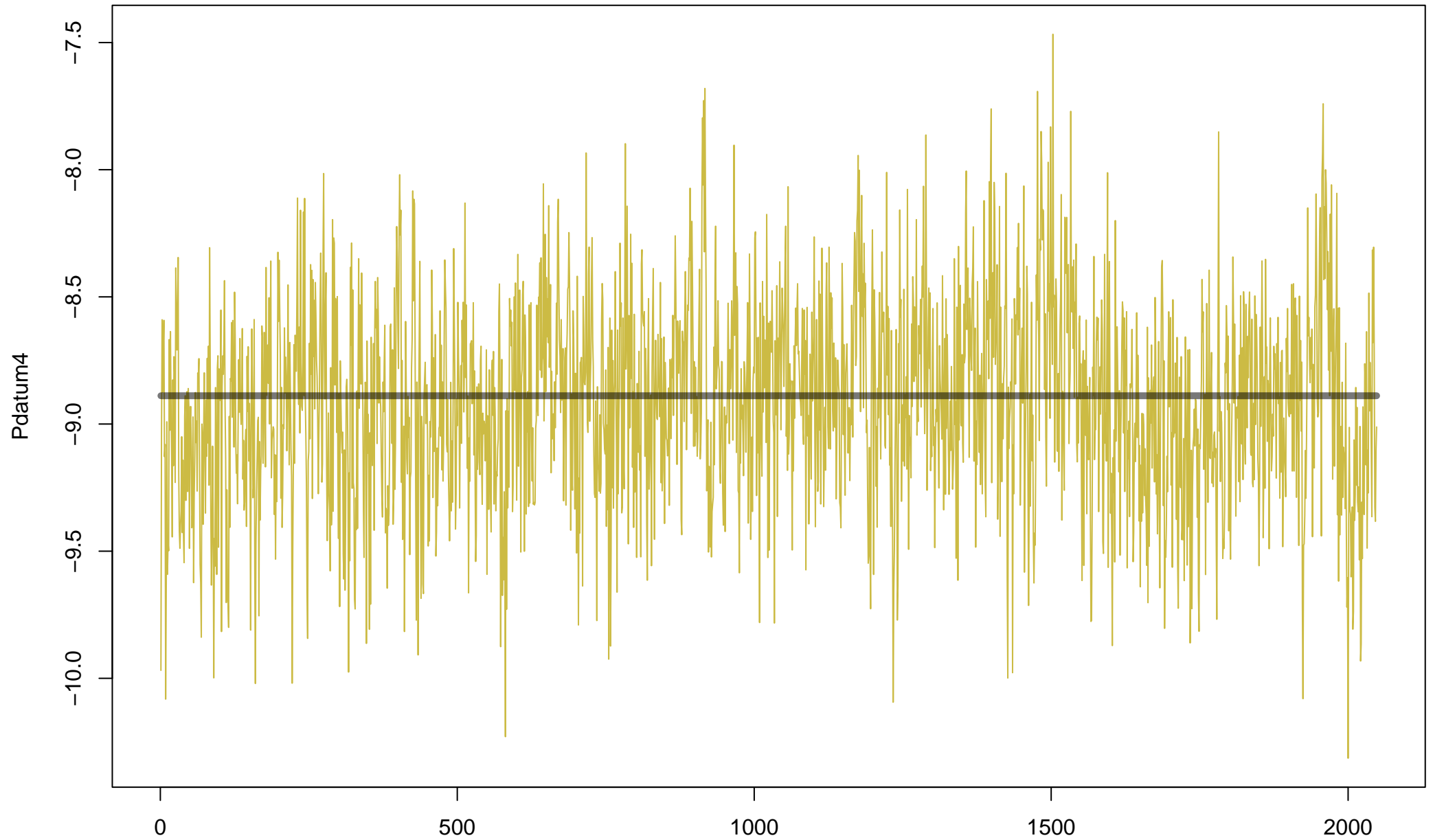
**ESS = 1460 | BMK = 0.0738 | MCSE(6.27) = 3.17 | stat: TRUE | burn: 0 | rel.err: -0.317**





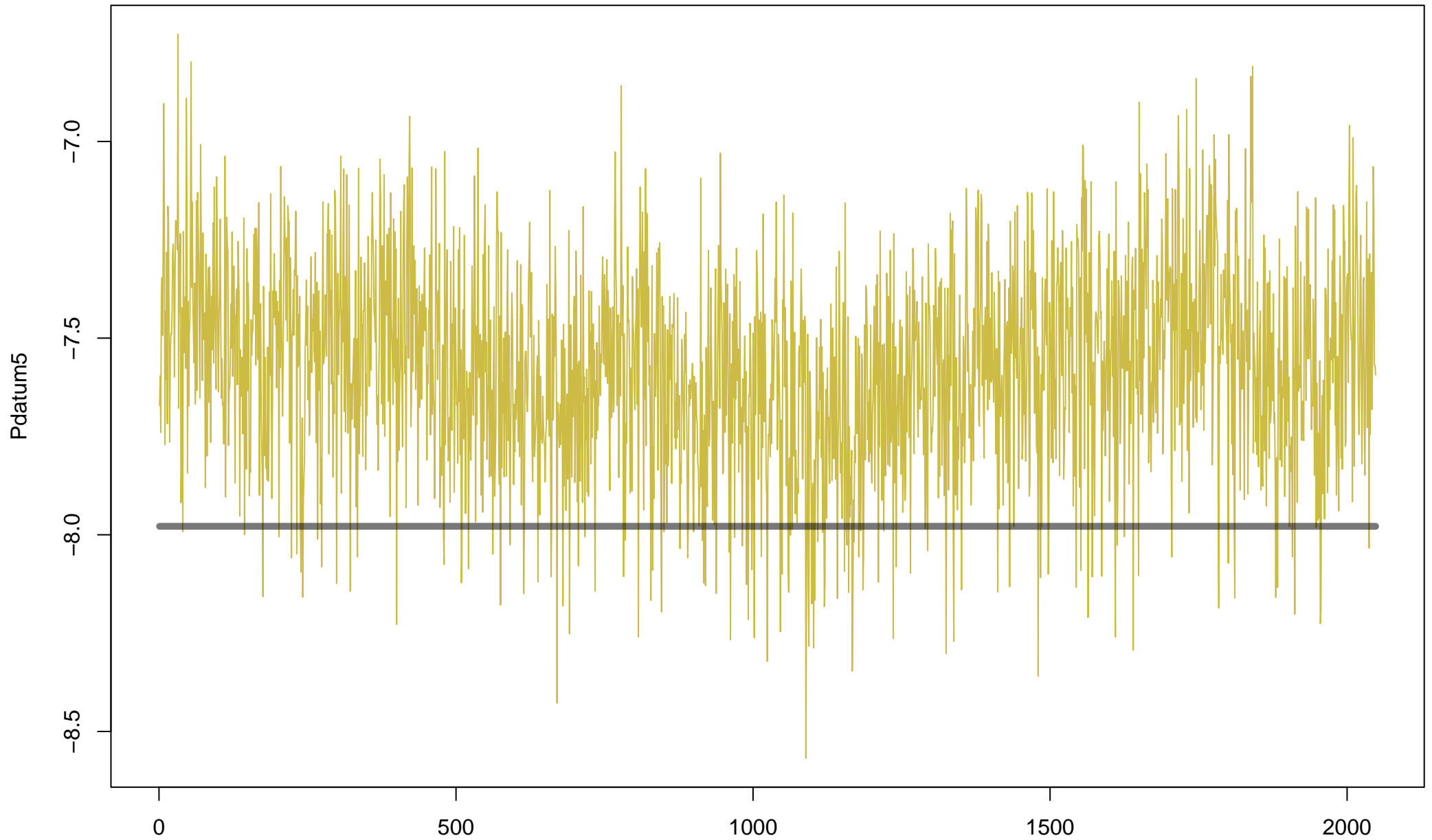
**Pdatum4**

**ESS = 513 | BMK = 0.0647 | MCSE(6.27) = 5.37 | stat: FALSE | burn: 0 | rel.err: 0.118**



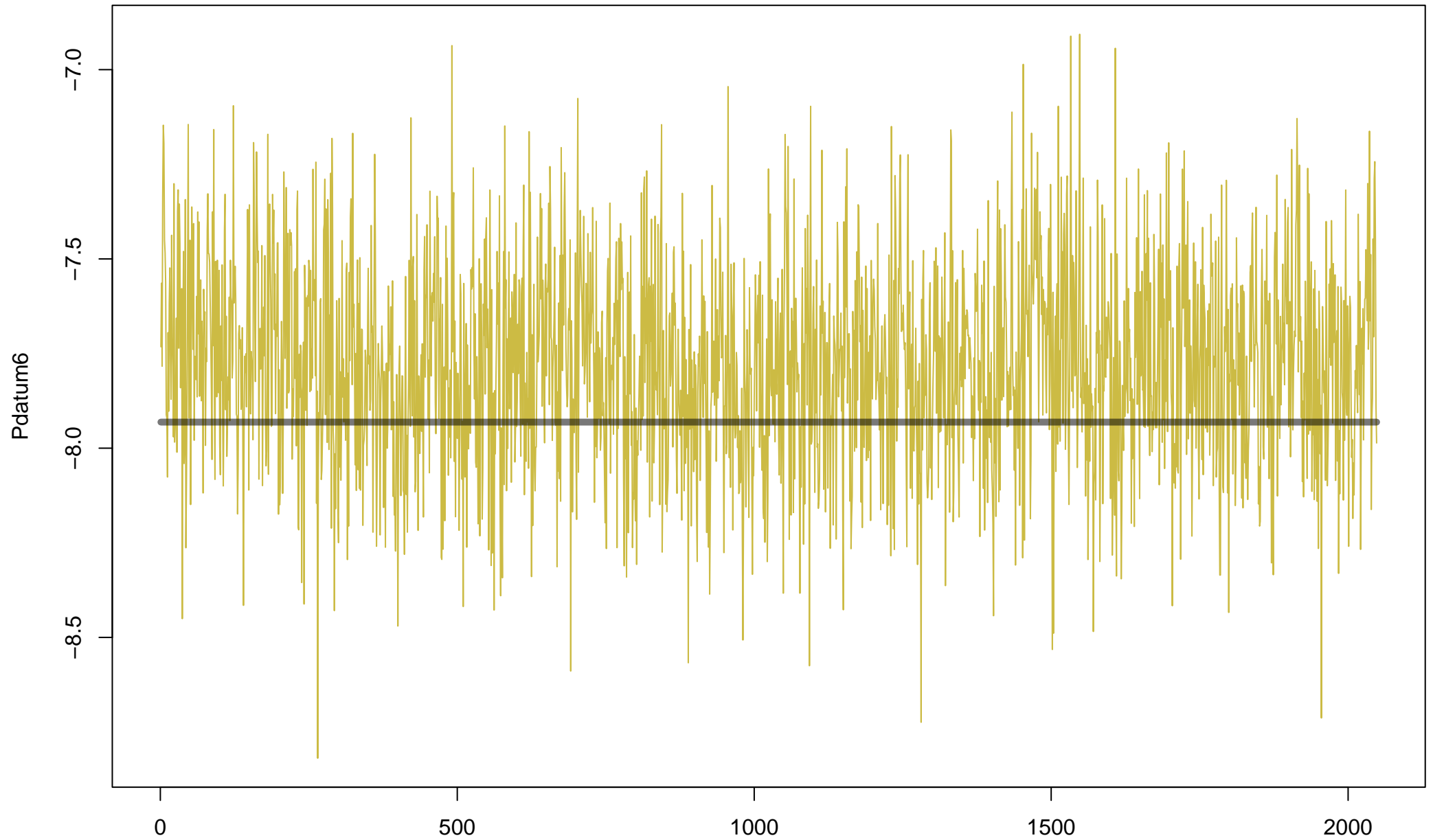
**Pdatum5**

**ESS = 161 | BMK = 0.044 | MCSE(6.27) = 5.34 | stat: FALSE | burn: 0 | rel.err: 1.39**

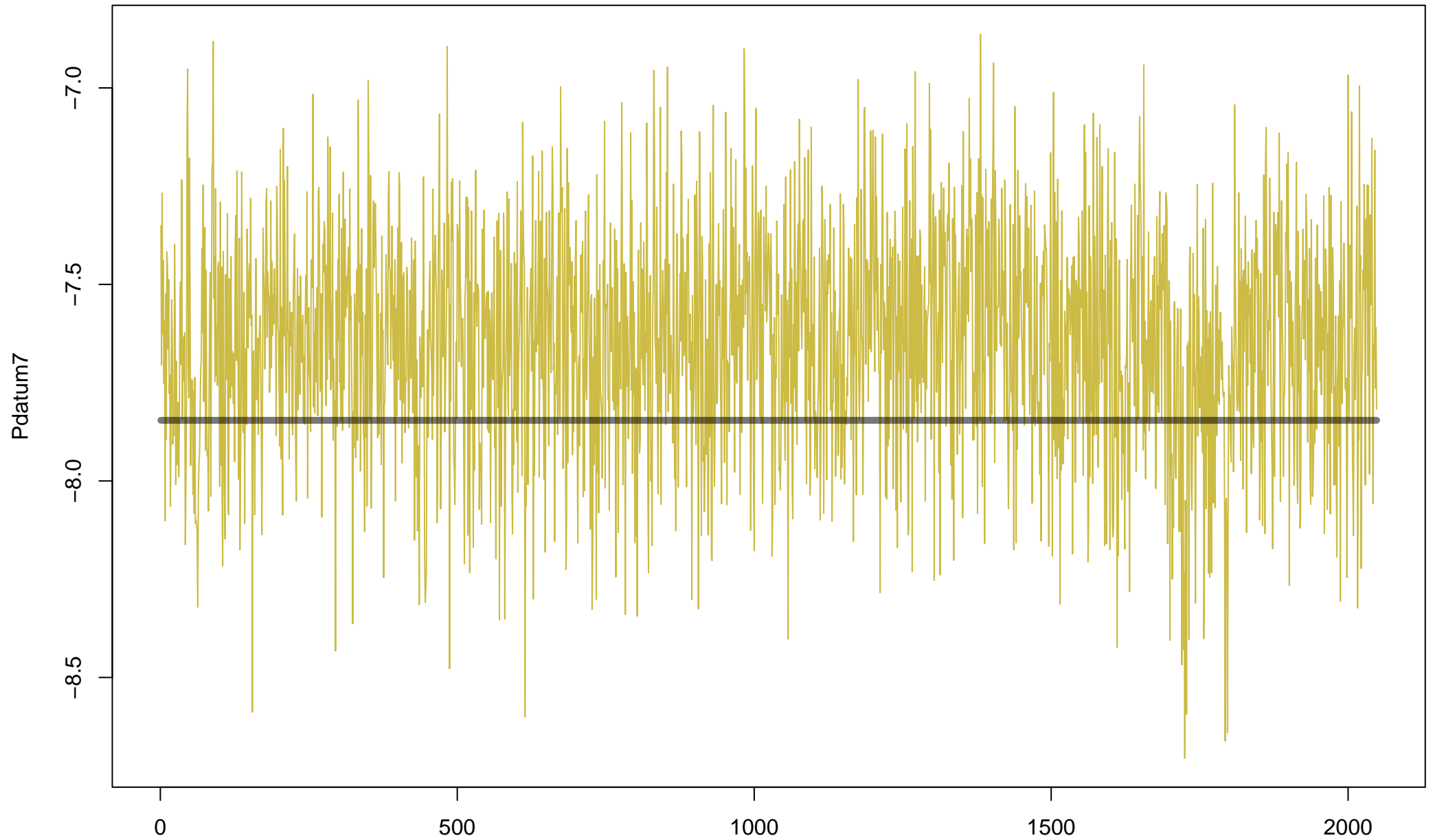


**Pdatum6**

**ESS = 1120 | BMK = 0.047 | MCSE(6.27) = 3.28 | stat: FALSE | burn: 0 | rel.err: 0.627**

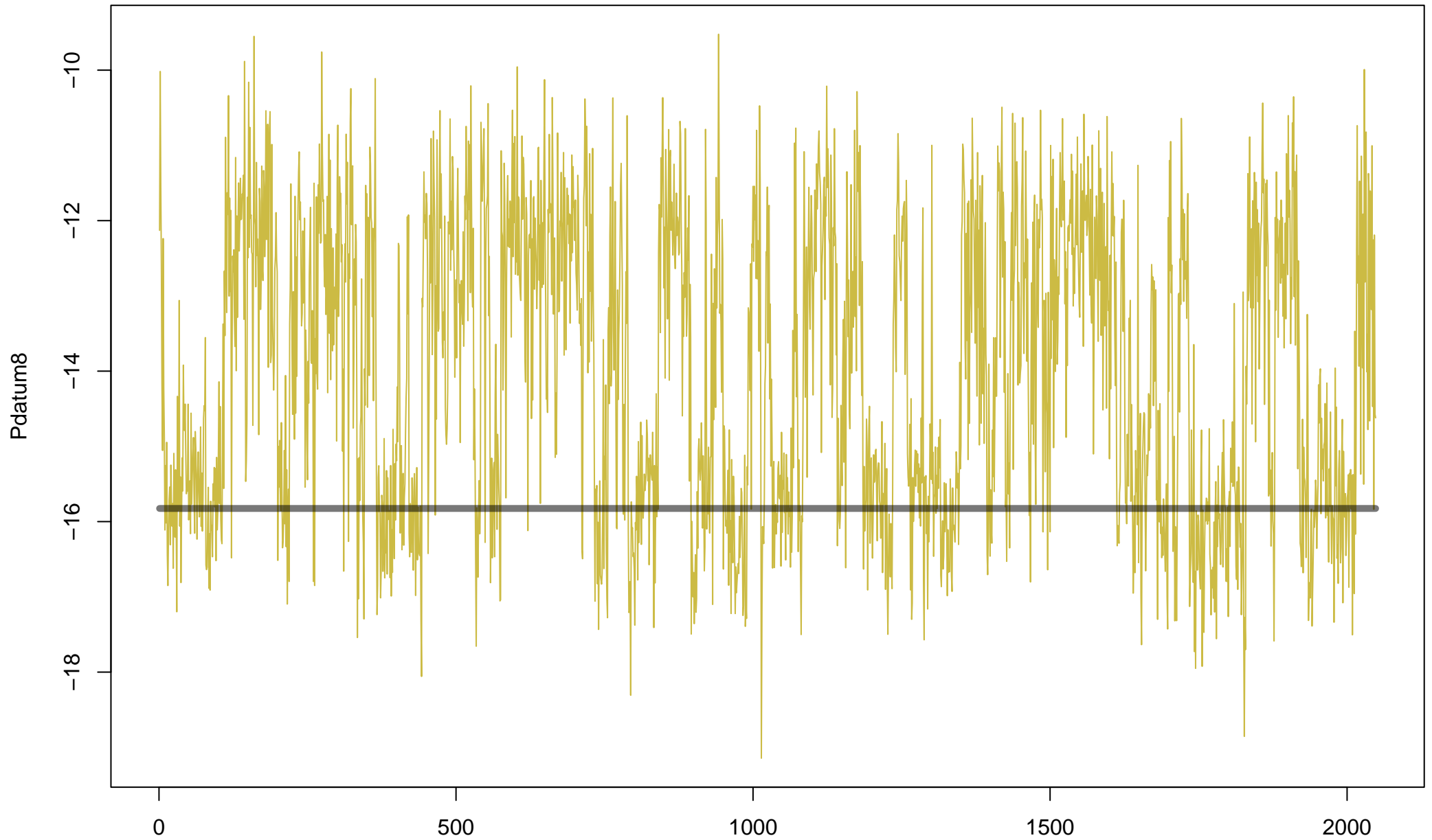


**Pdatum7**  
**ESS = 1280 | BMK = 0.038 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: 0.754**

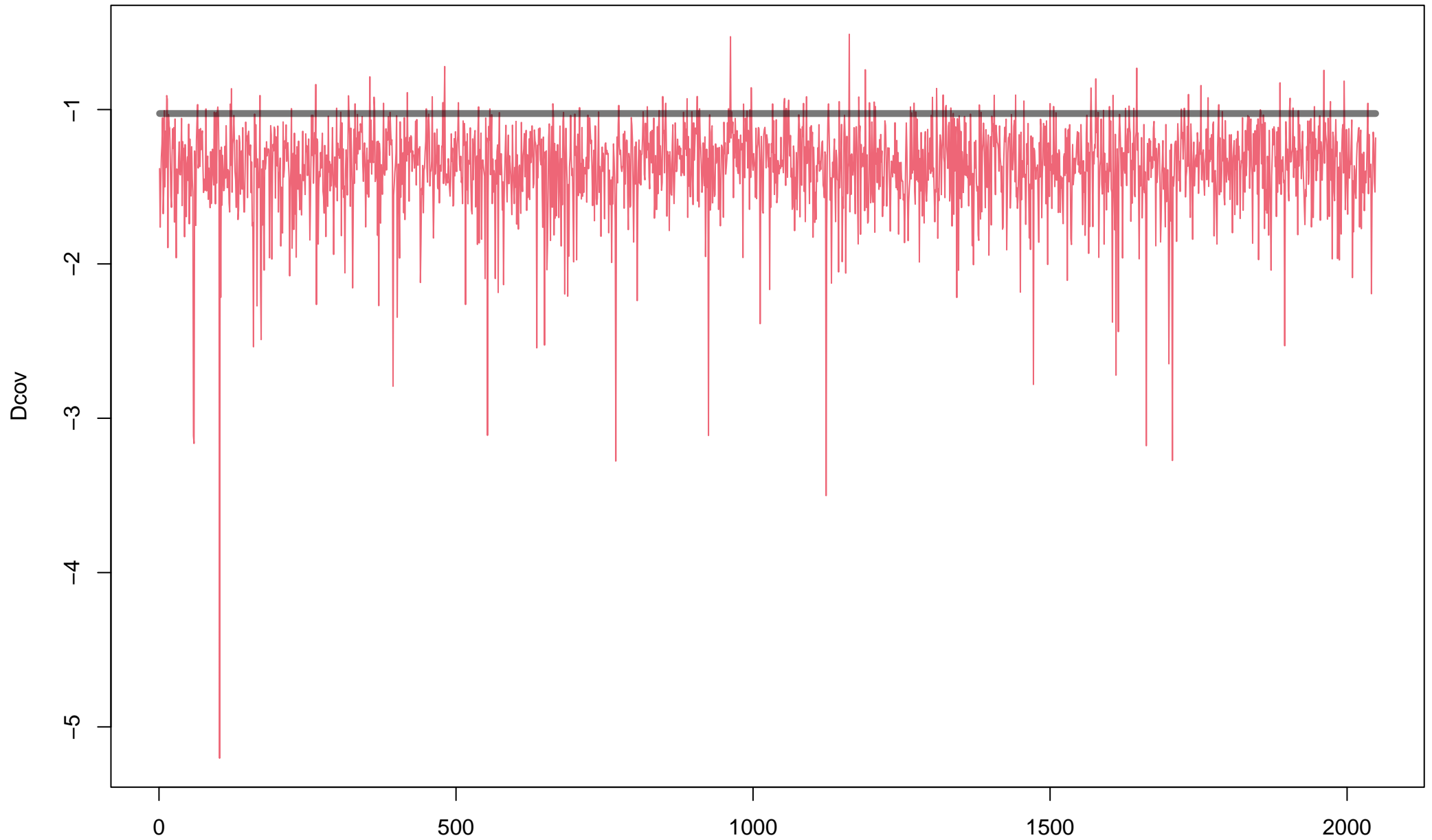


**Pdatum8**

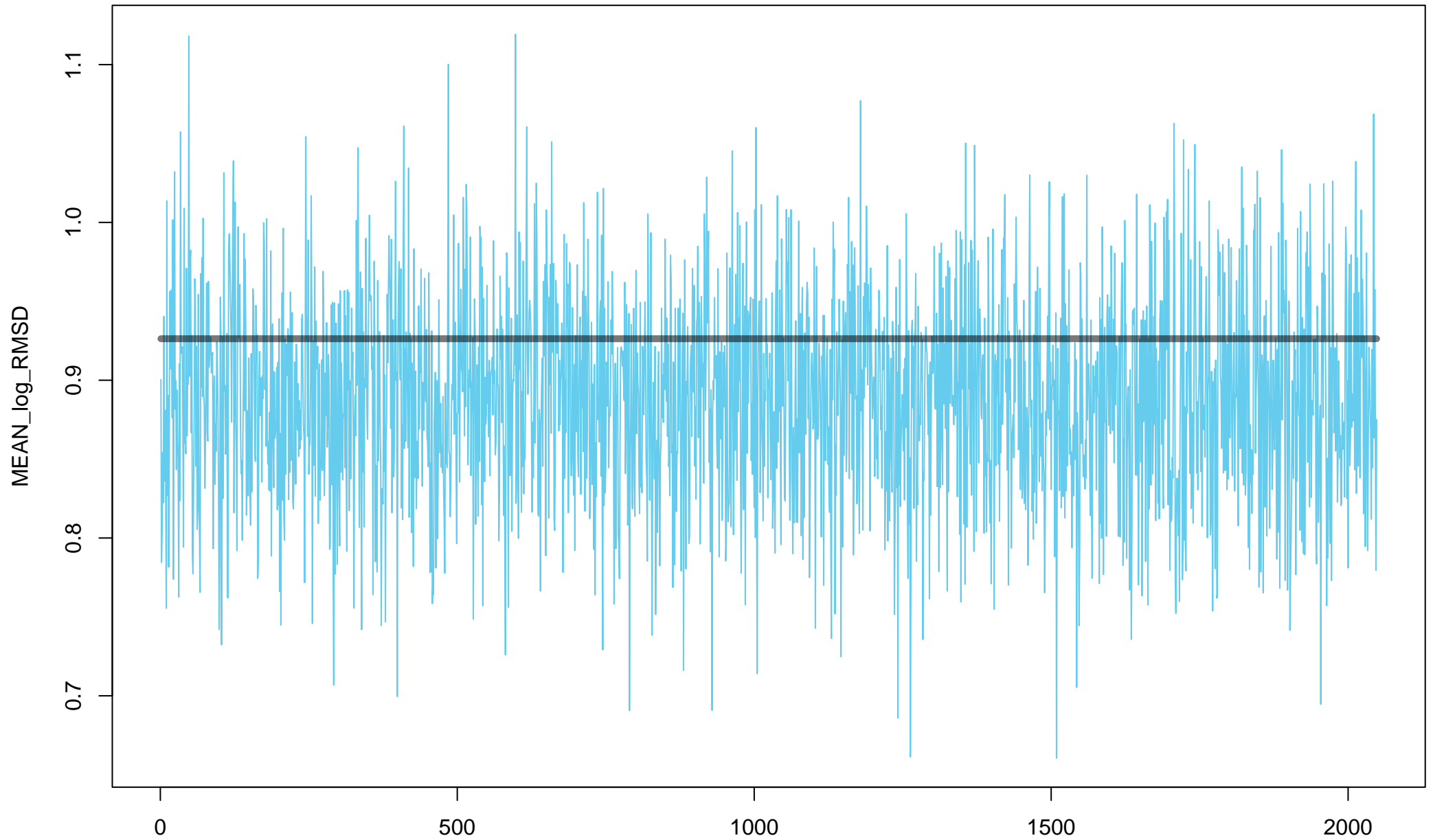
**ESS = 327 | BMK = 0.115 | MCSE(6.27) = 5.33 | stat: TRUE | burn: 1632 | rel.err: 0.549**



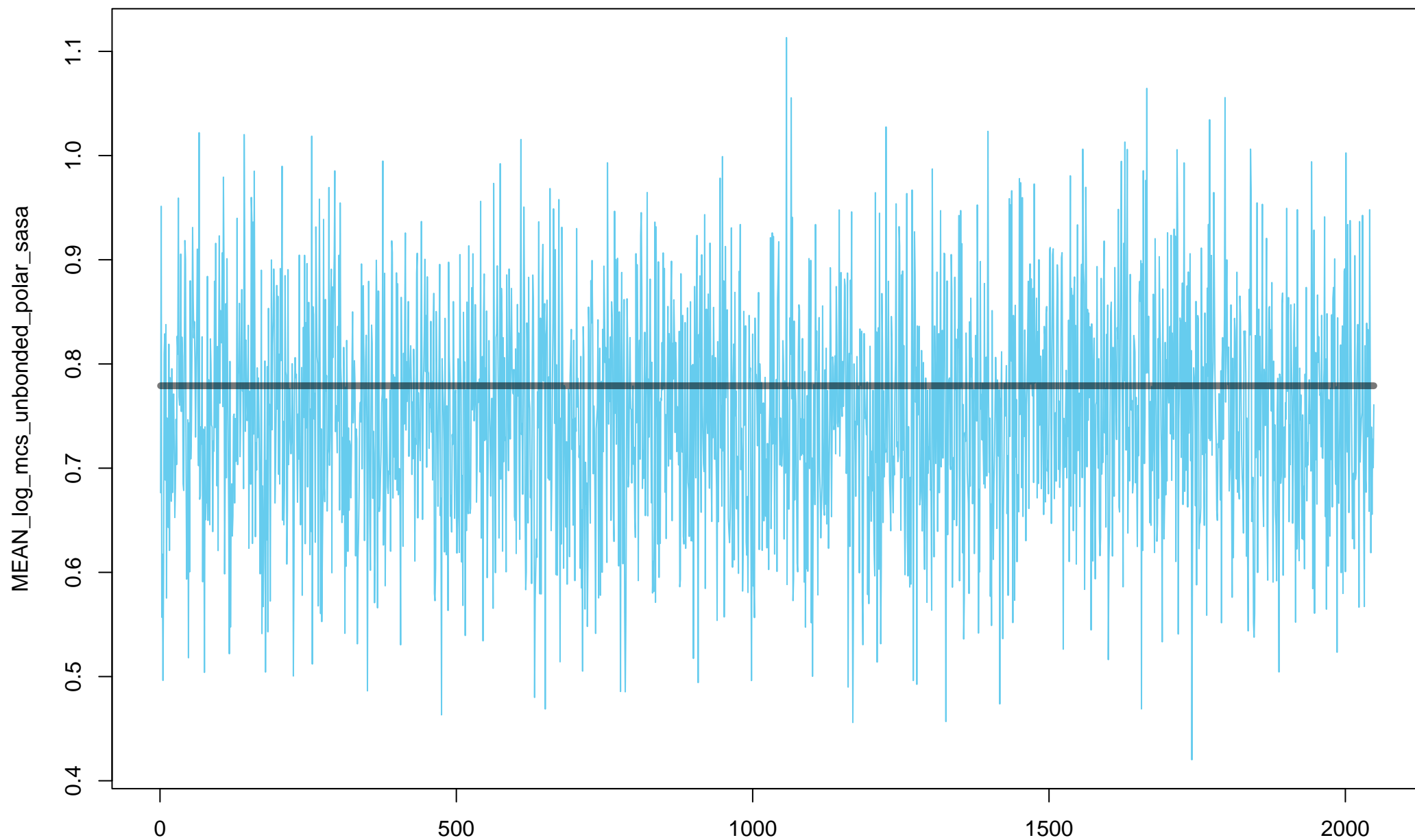
**Dcov**  
**ESS = 2050 | BMK = 0.0554 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 1.47**



**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0387 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: -0.584**



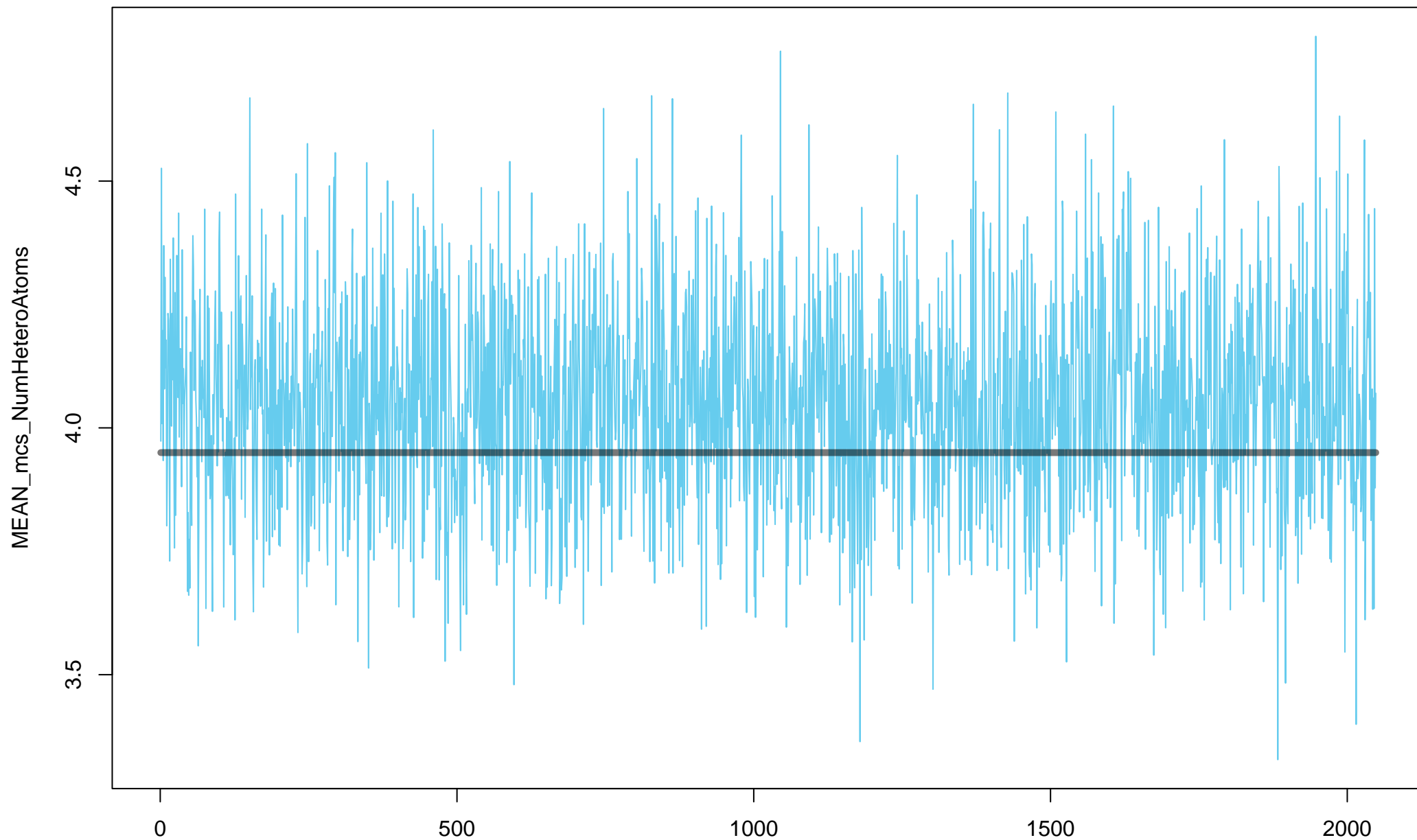
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1590 | BMK = 0.0471 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: -0.262**





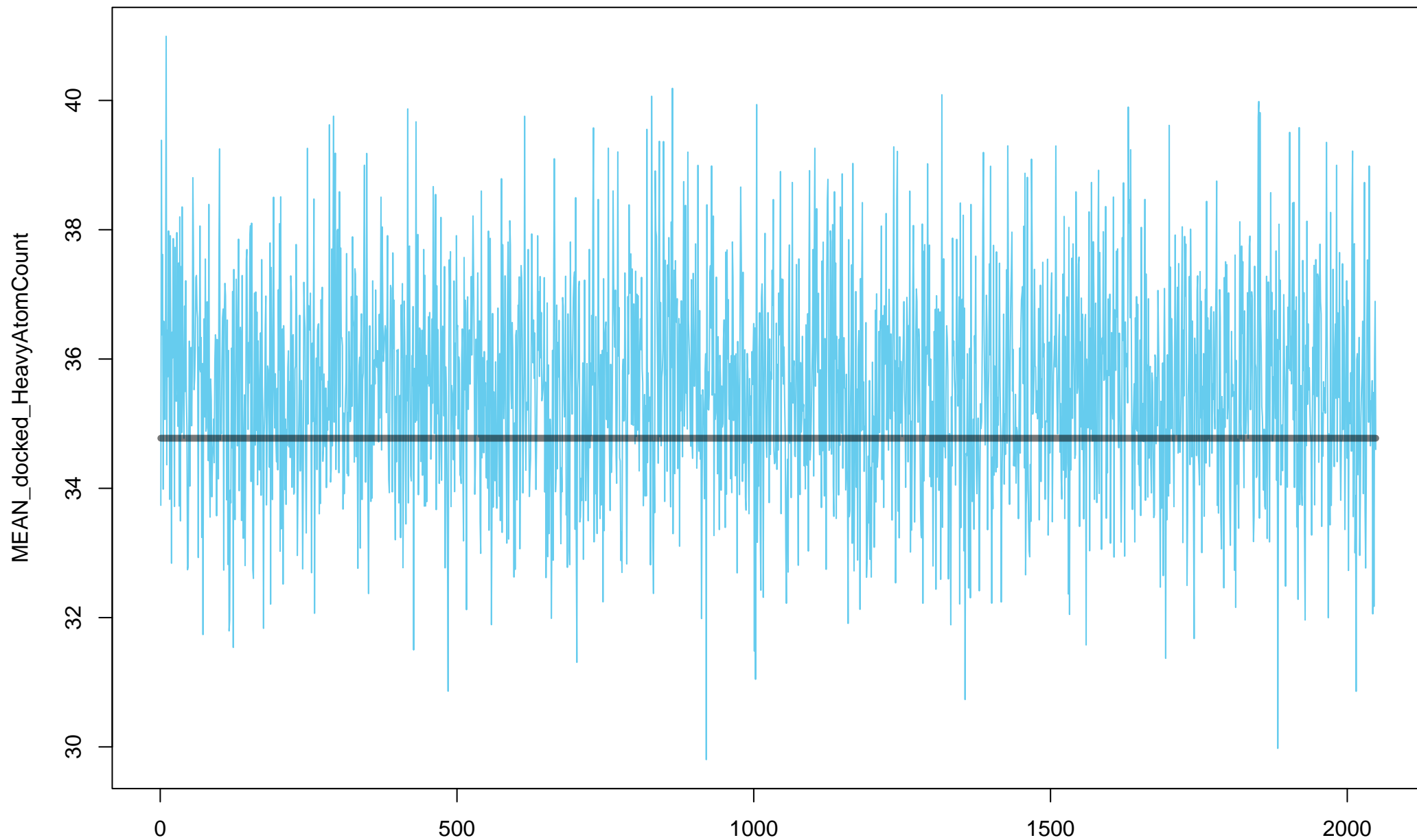
# MEAN\_mcs\_NumHeteroAtoms

ESS = 2050 | BMK = 0.0374 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: 0.478



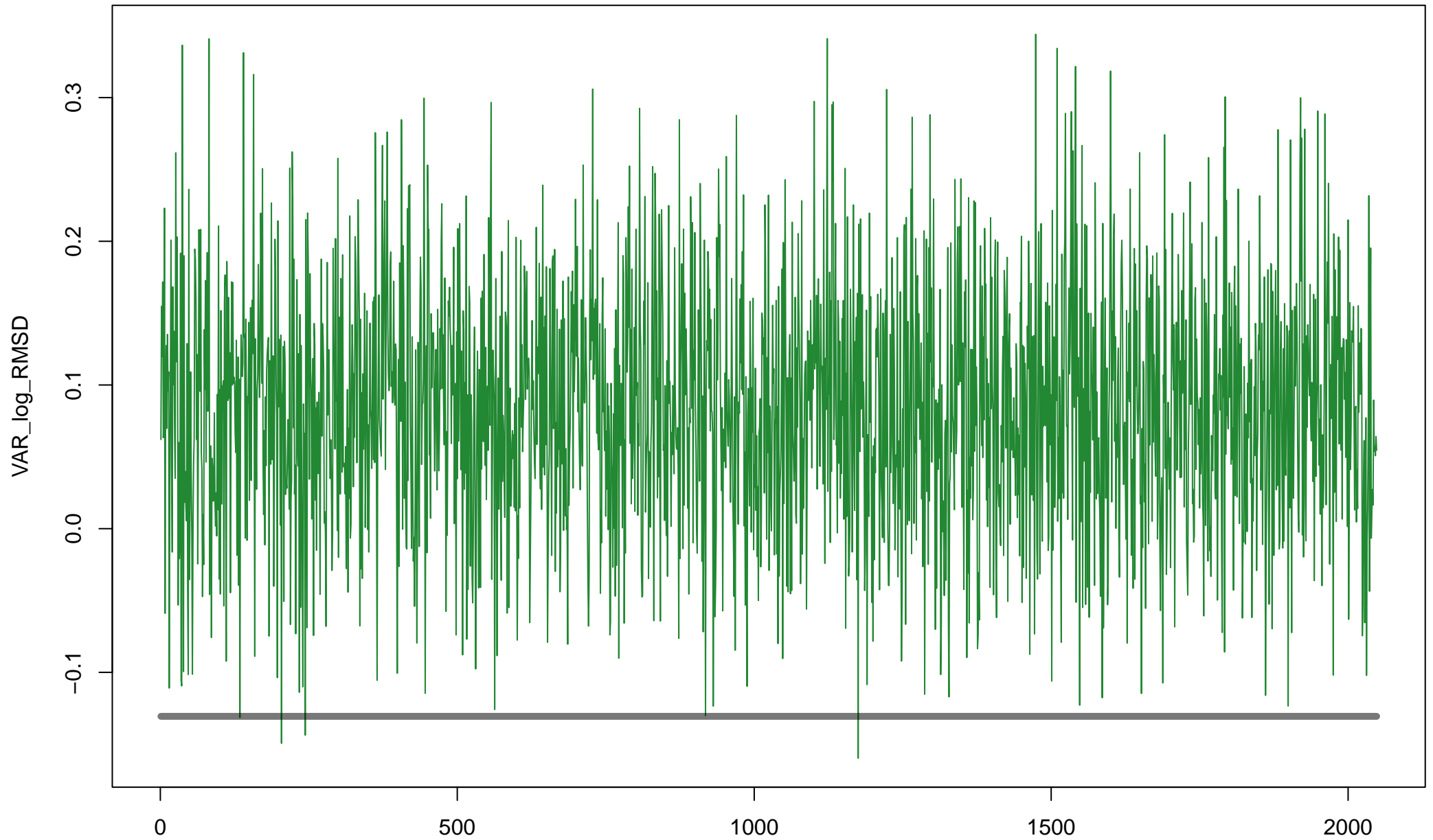
# MEAN\_docked\_HeavyAtomCount

ESS = 2050 | BMK = 0.0409 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.497

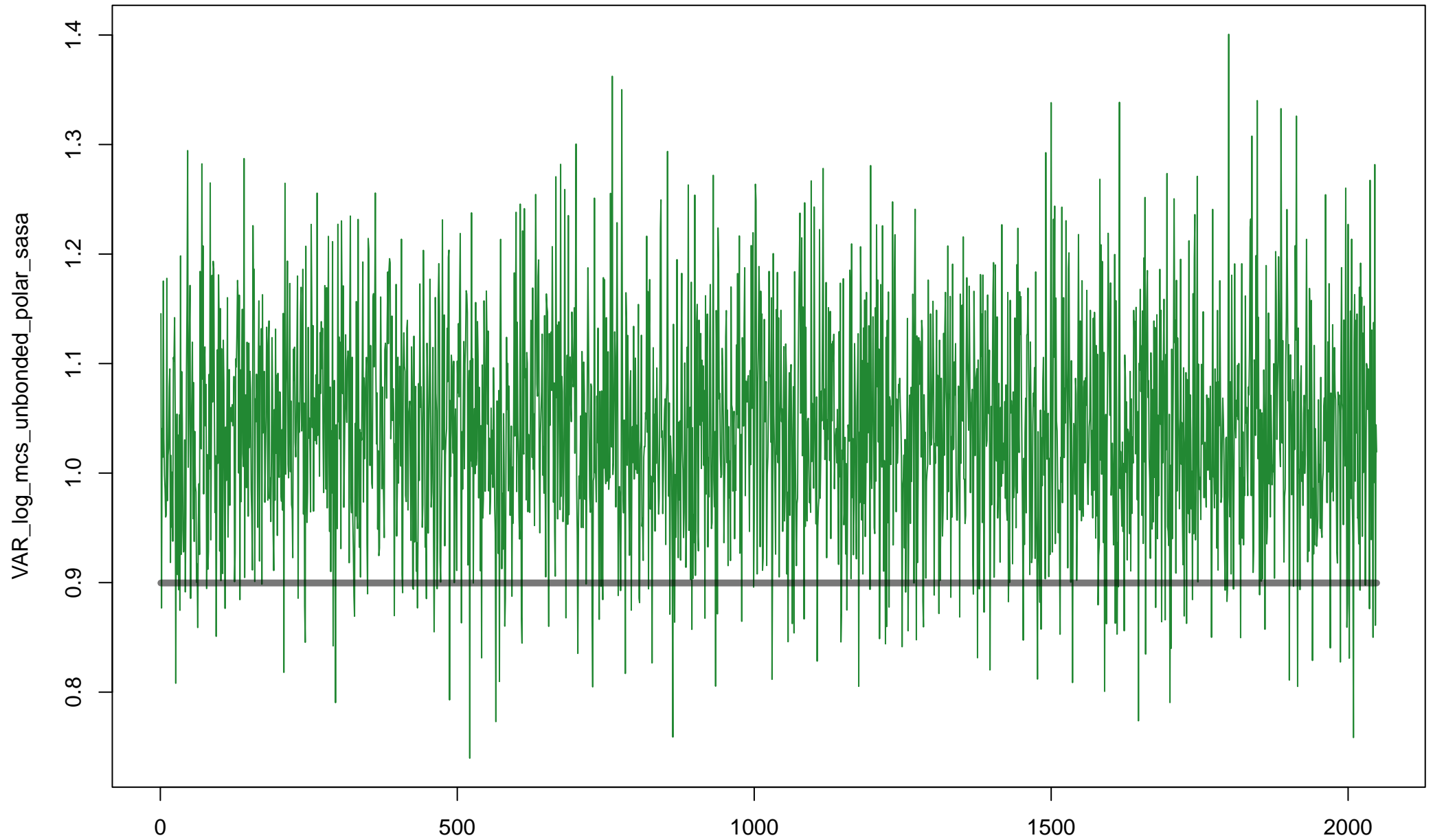


# VAR\_log\_RMSD

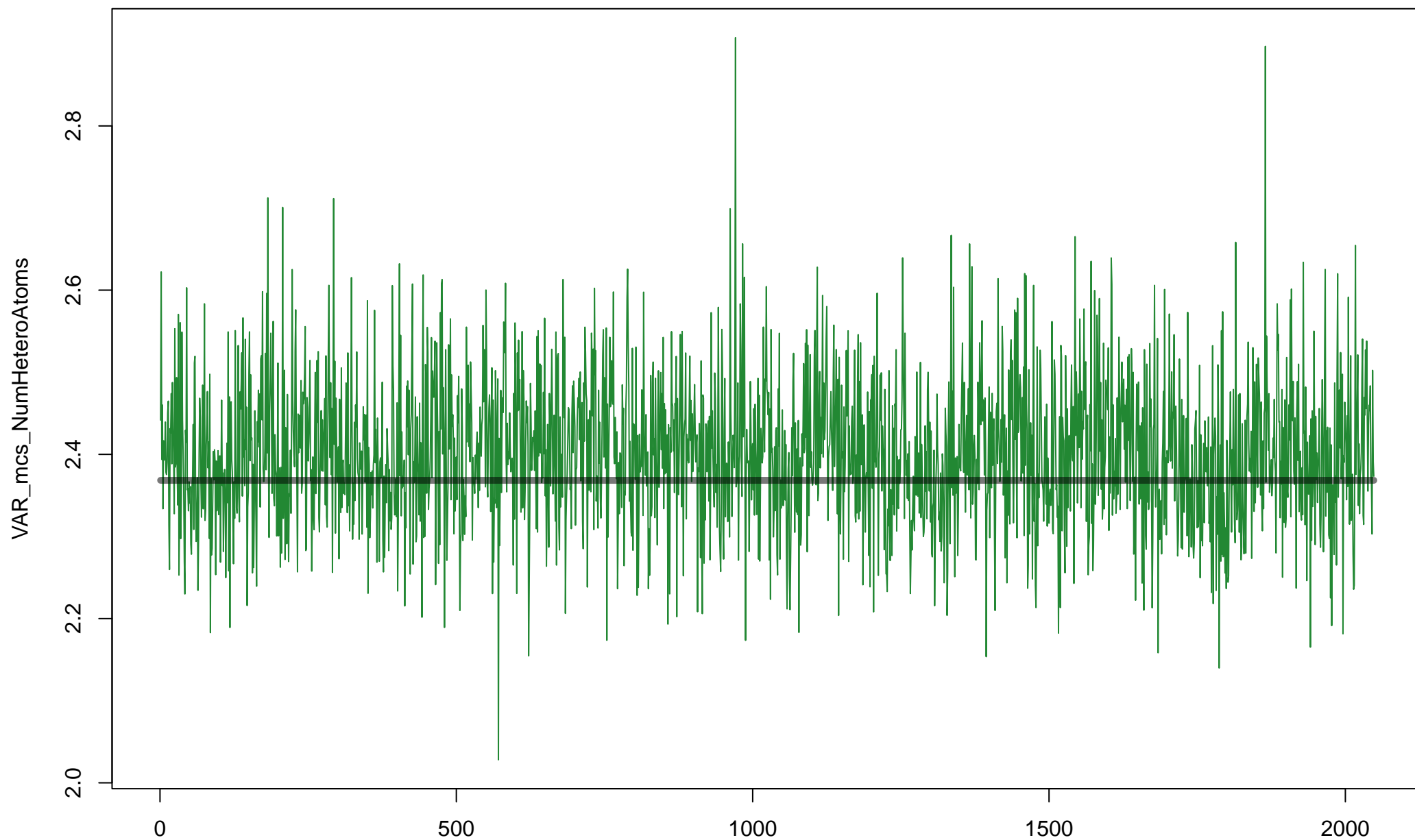
ESS = 2050 | BMK = 0.0363 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: 2.33



**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: 1.38**

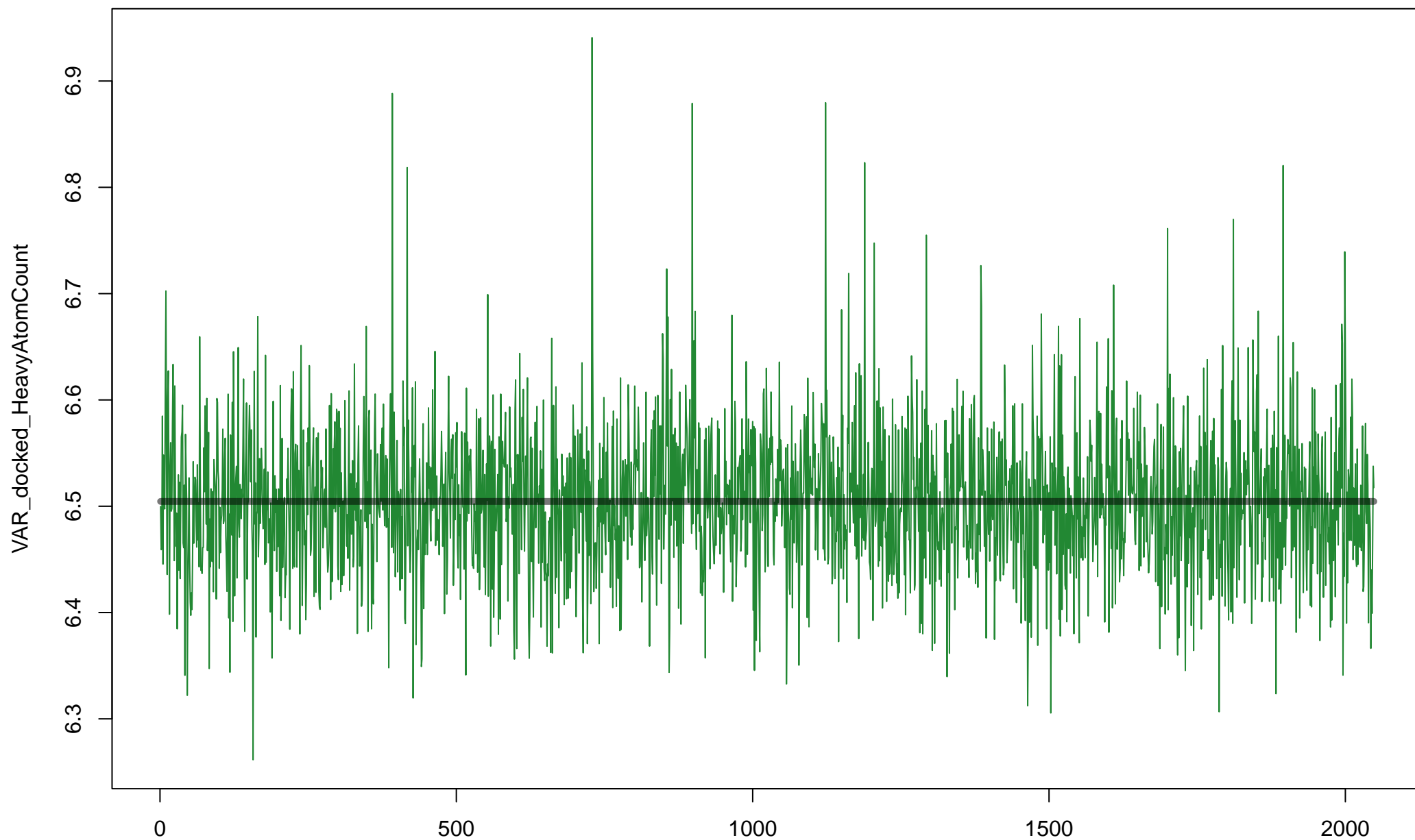


**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1530 | BMK = 0.0656 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: 0.407**

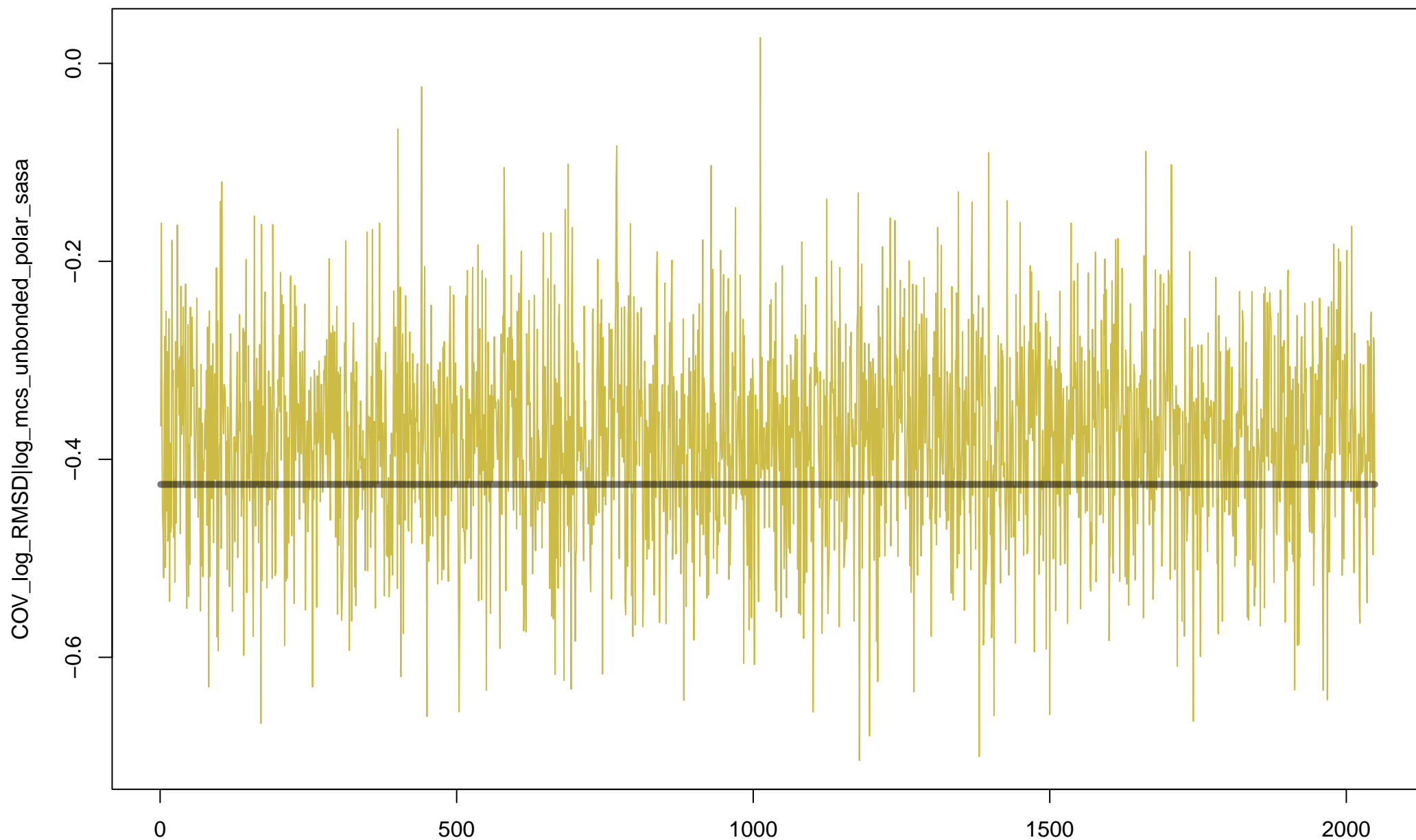


# VAR\_docked\_HeavyAtomCount

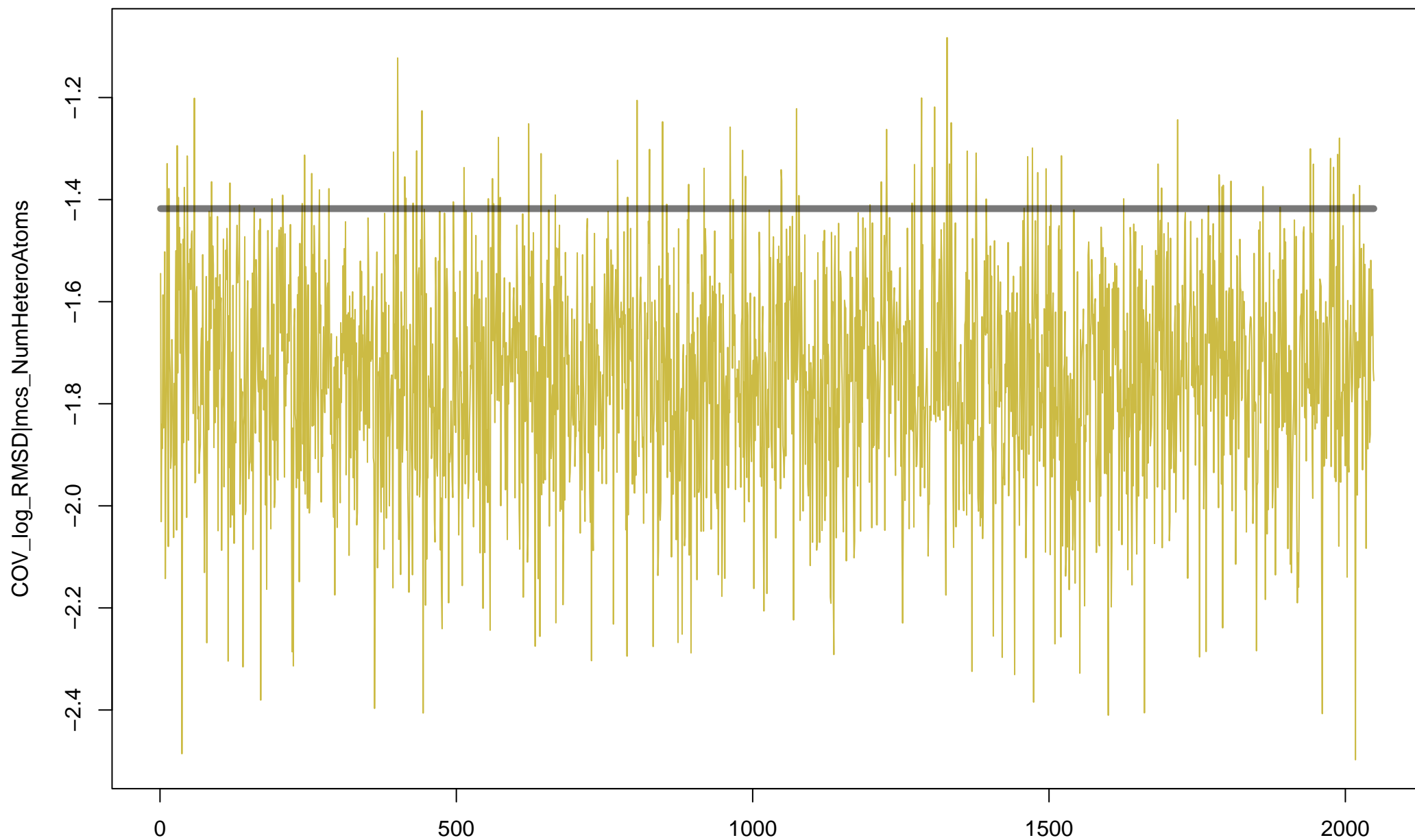
ESS = 2050 | BMK = 0.0581 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: 0.042



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0476 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: 0.47**

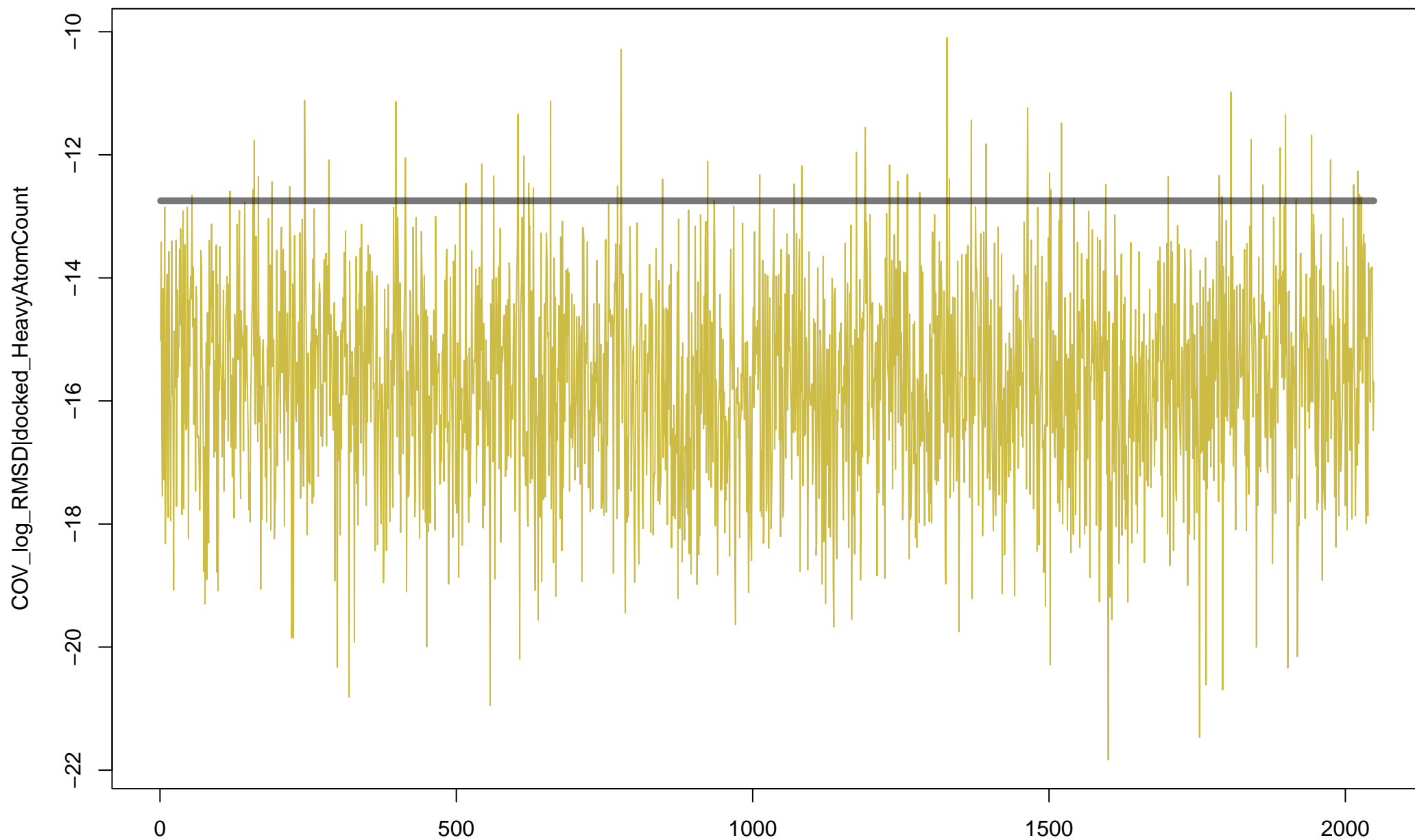


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0375 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: -1.57**

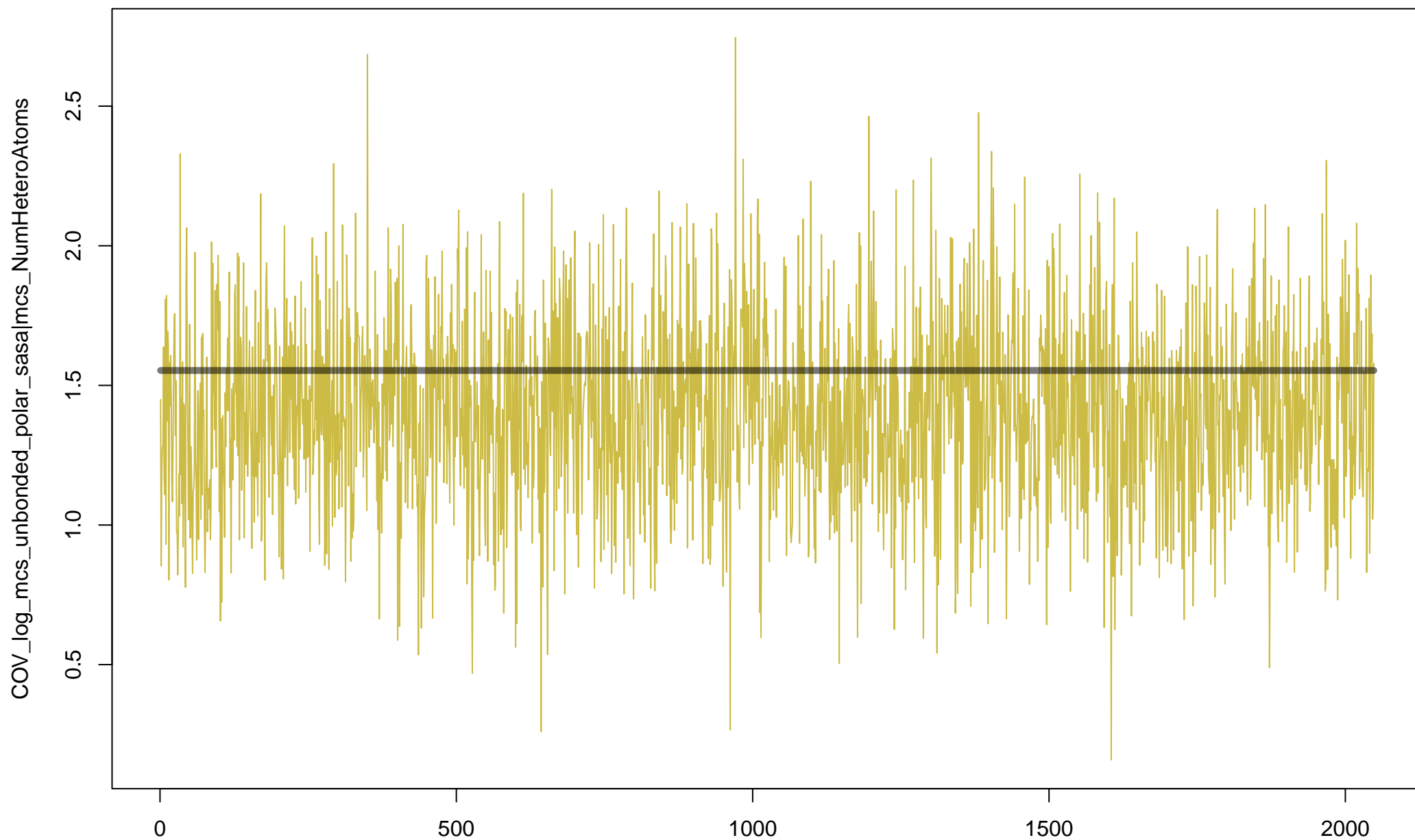




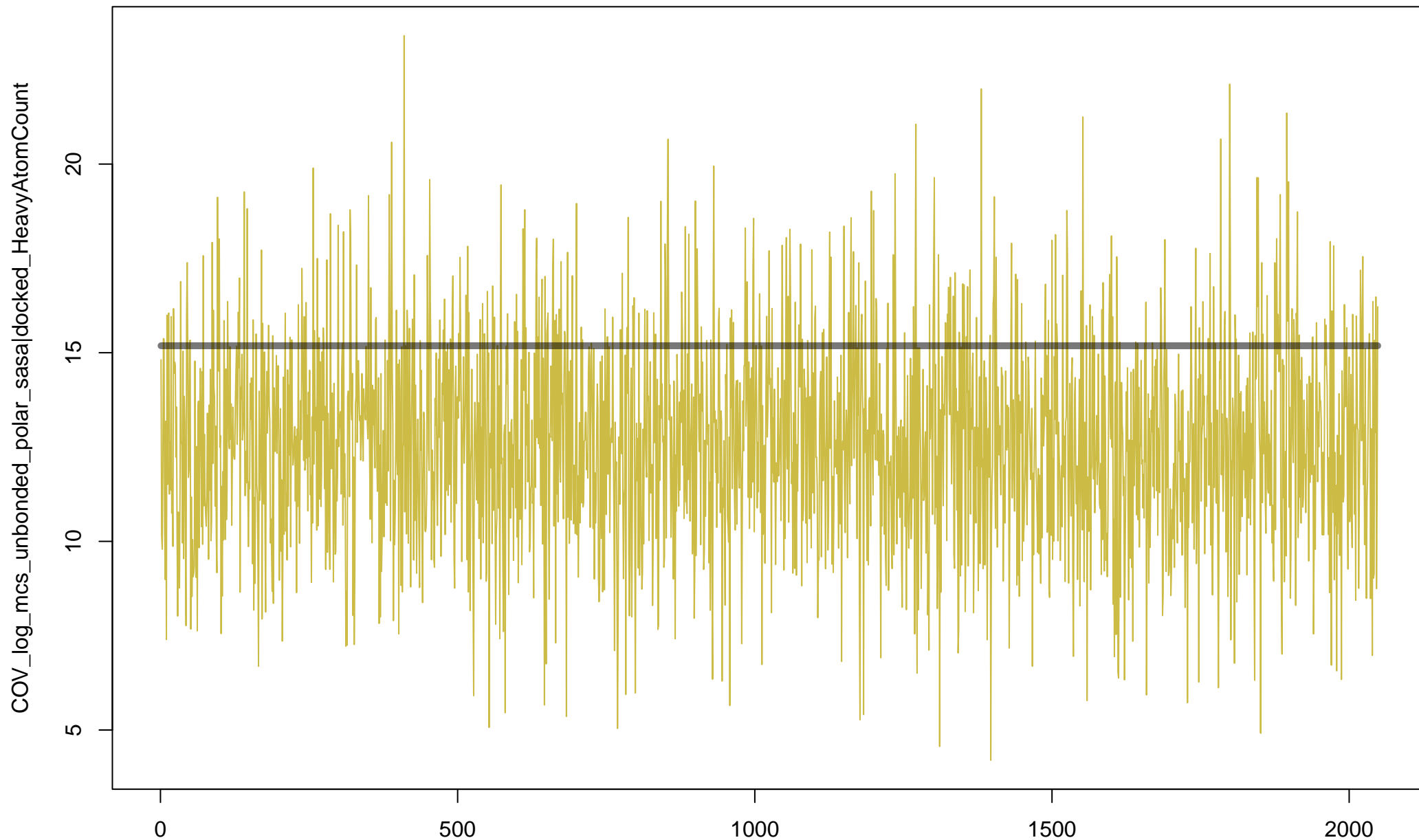
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0275 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | rel.err: -1.81**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0456 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: -0.463**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.041 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: -0.955**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0379 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 0.473**

