

-- STATS maxD --

min ESS = 47.3197515443826

max BMK = 0.17693103594106

max MCSE = 9.34127867690484

all stationary: FALSE

burn: 1428

max rel.err.: 2.11241033875737

-- STATS 2D --

min ESS = 1840.27062576273

max BMK = 0.0610889572799121

max MCSE = 2.48856920325282

all stationary: TRUE

burn: 0

max rel.err.: 1.7839863701468

-- STATS 1D --

min ESS = 1740.84918026021

max BMK = 0.0532672886380778

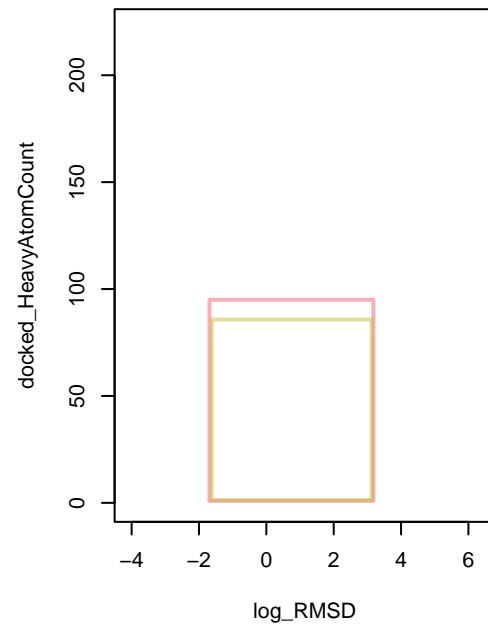
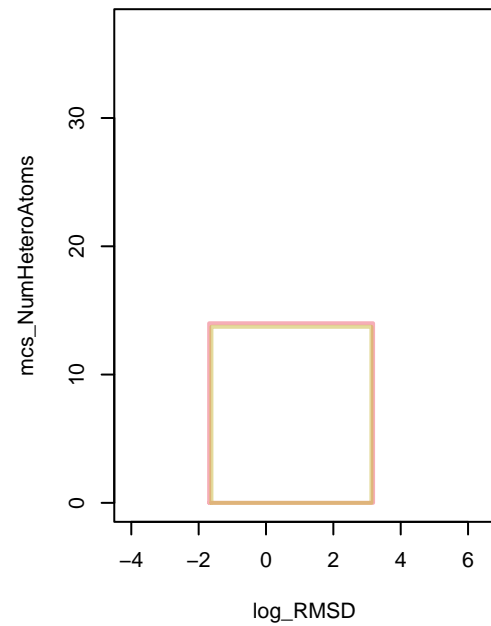
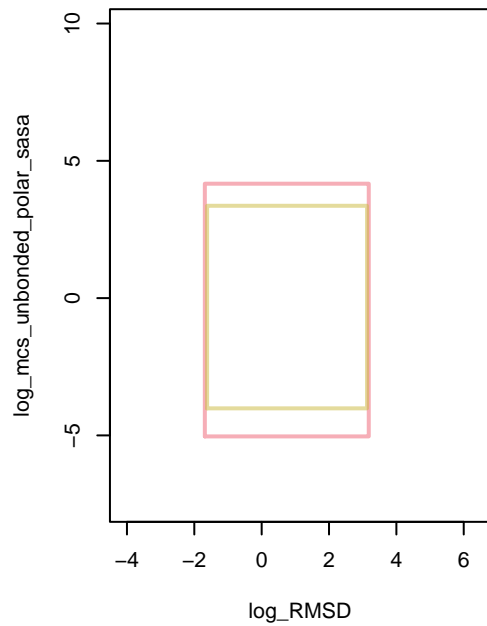
max MCSE = 2.51775076787936

all stationary: TRUE

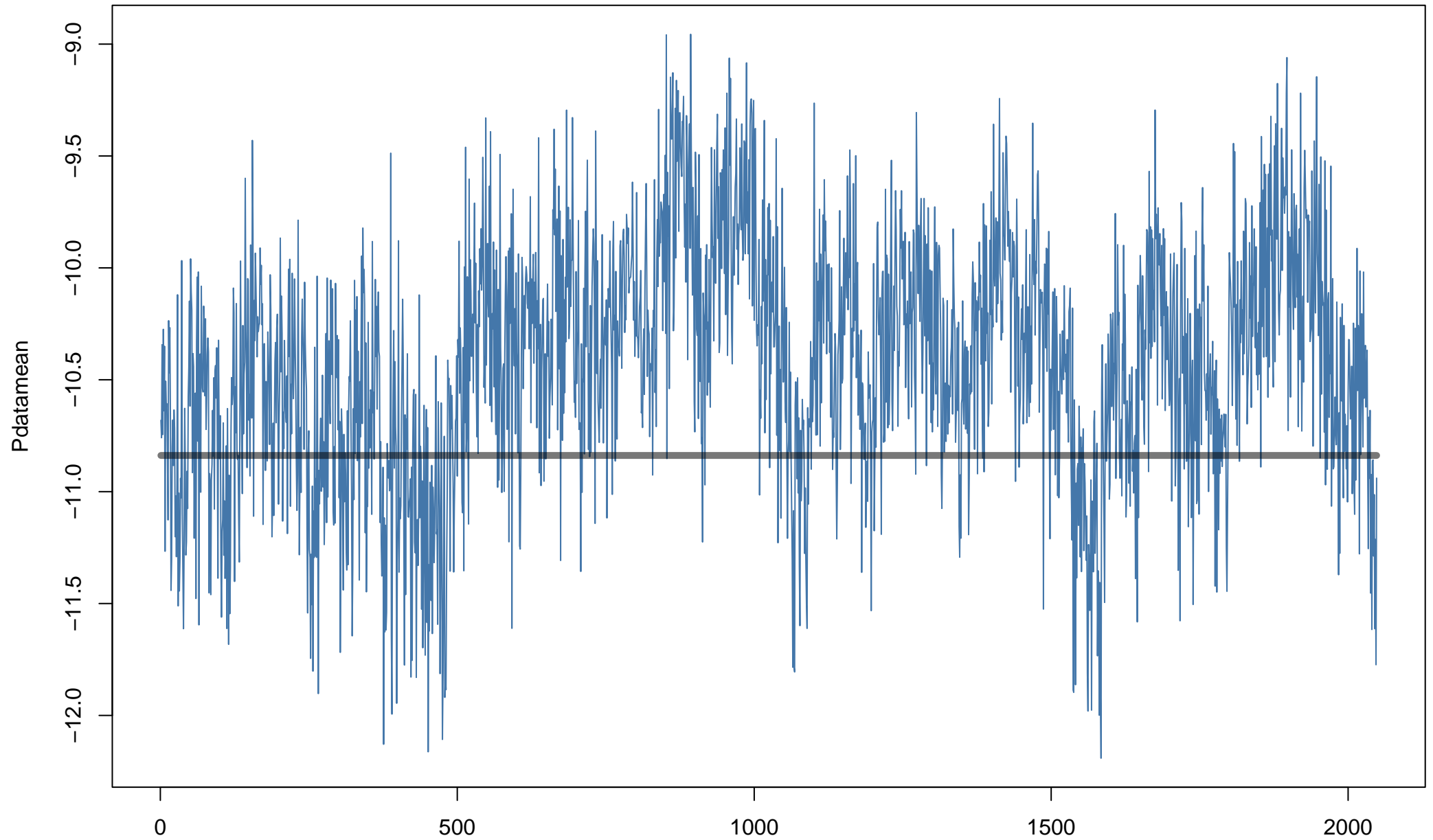
burn: 0

max rel.err.: 2.23903160795857

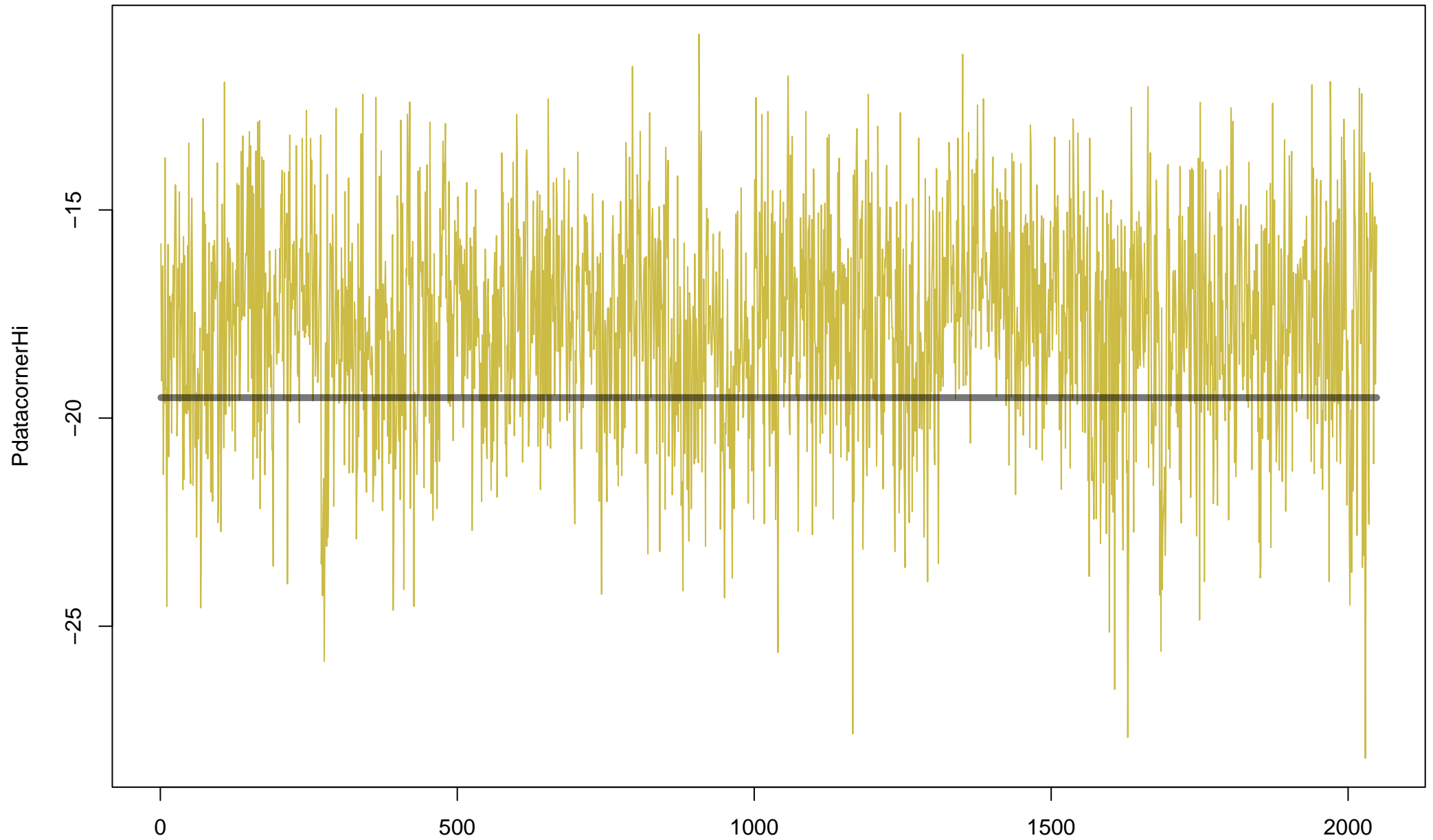
Occupied clusters: 10 of 16



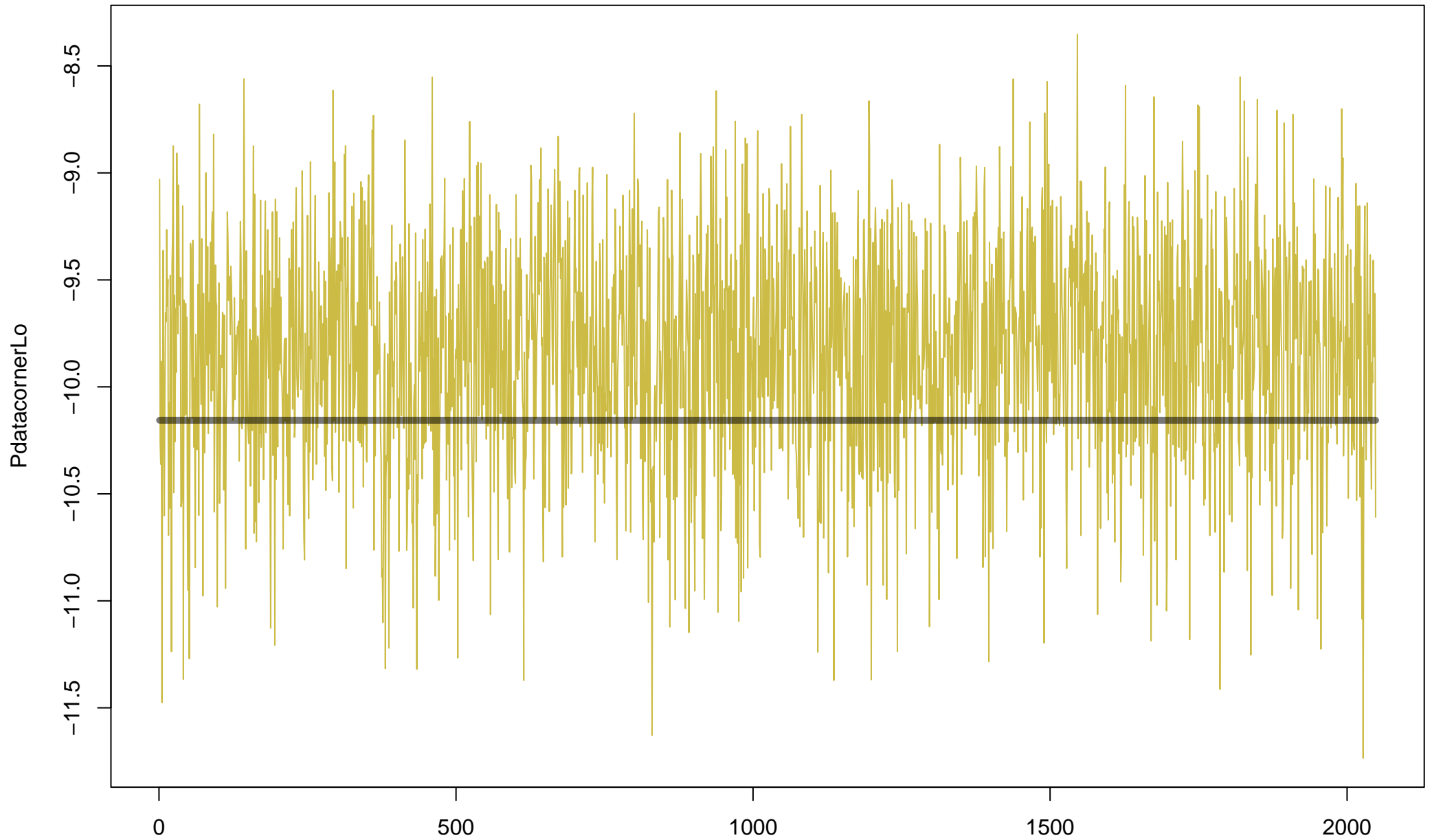
**Pdatamean**  
**ESS = 47.3 | BMK = 0.089 | MCSE(6.27) = 9.34 | stat: FALSE | burn: 0 | rel.err: 0.79**



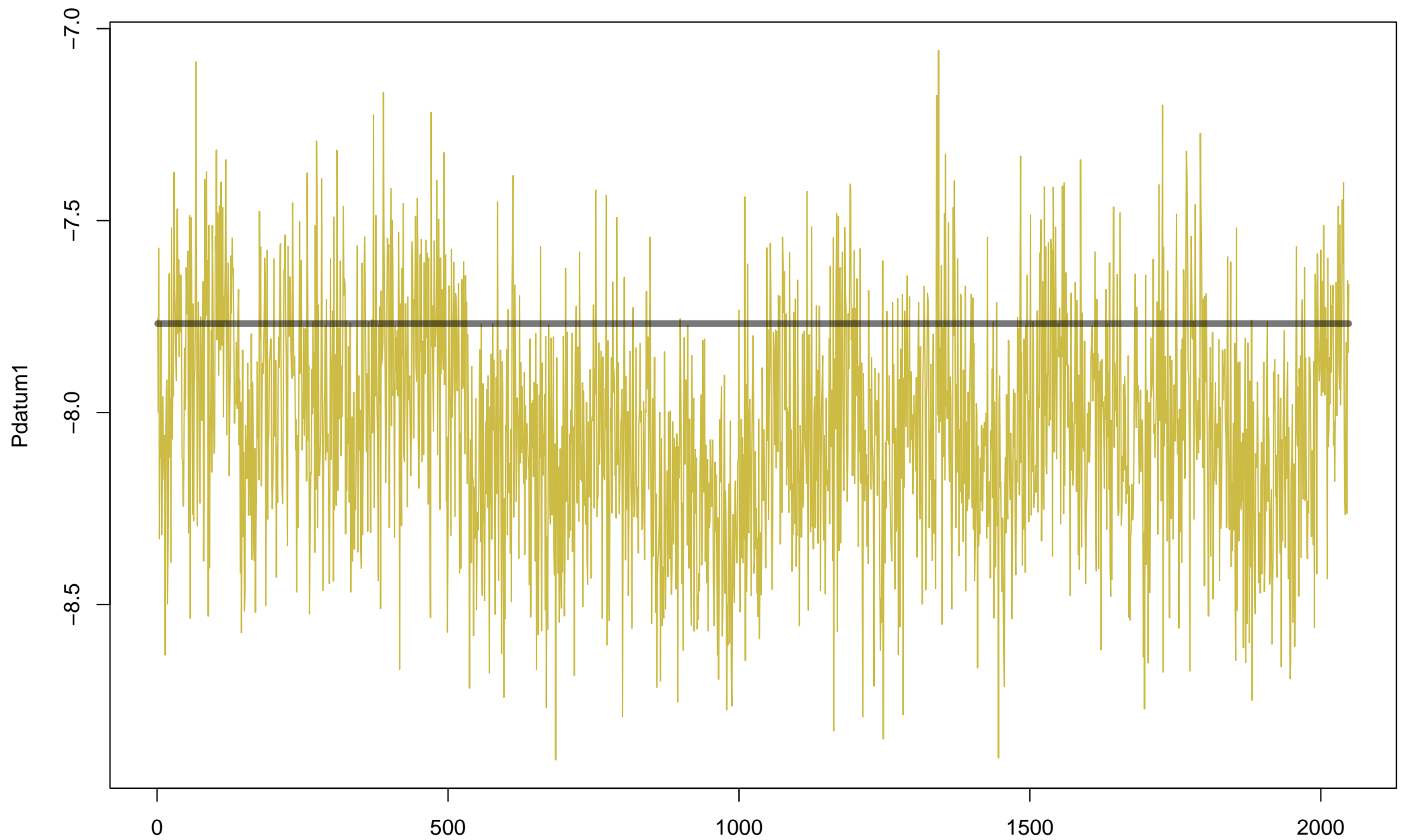
**PdatacornerHi**  
**ESS = 2050 | BMK = 0.177 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | rel.err: 0.258**



**PdatacornerLo**  
**ESS = 1550 | BMK = 0.0563 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: 0.712**

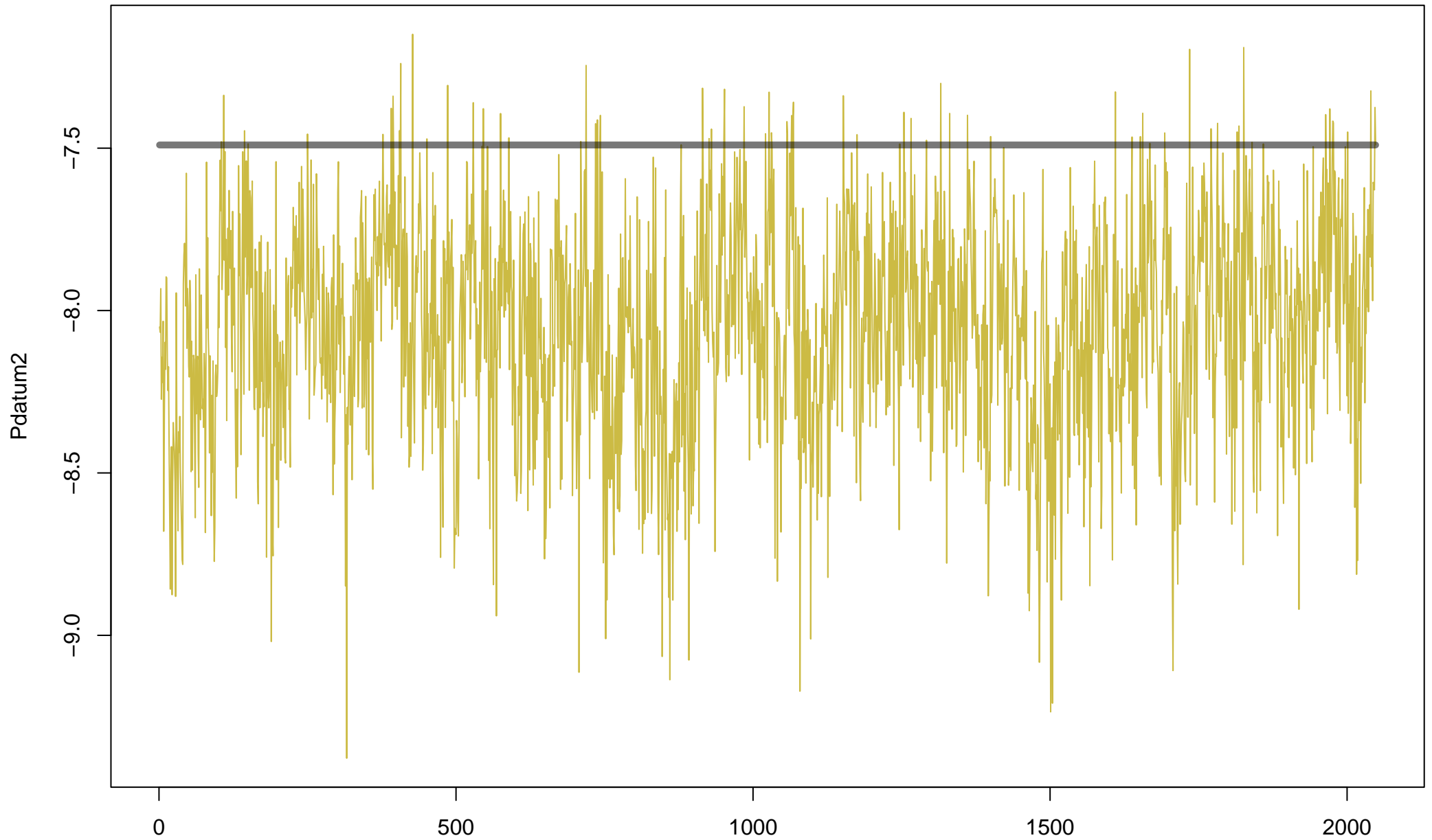


**Pdatum1**  
**ESS = 136 | BMK = 0.0424 | MCSE(6.27) = 6.3 | stat: FALSE | burn: 0 | rel.err: -0.85**



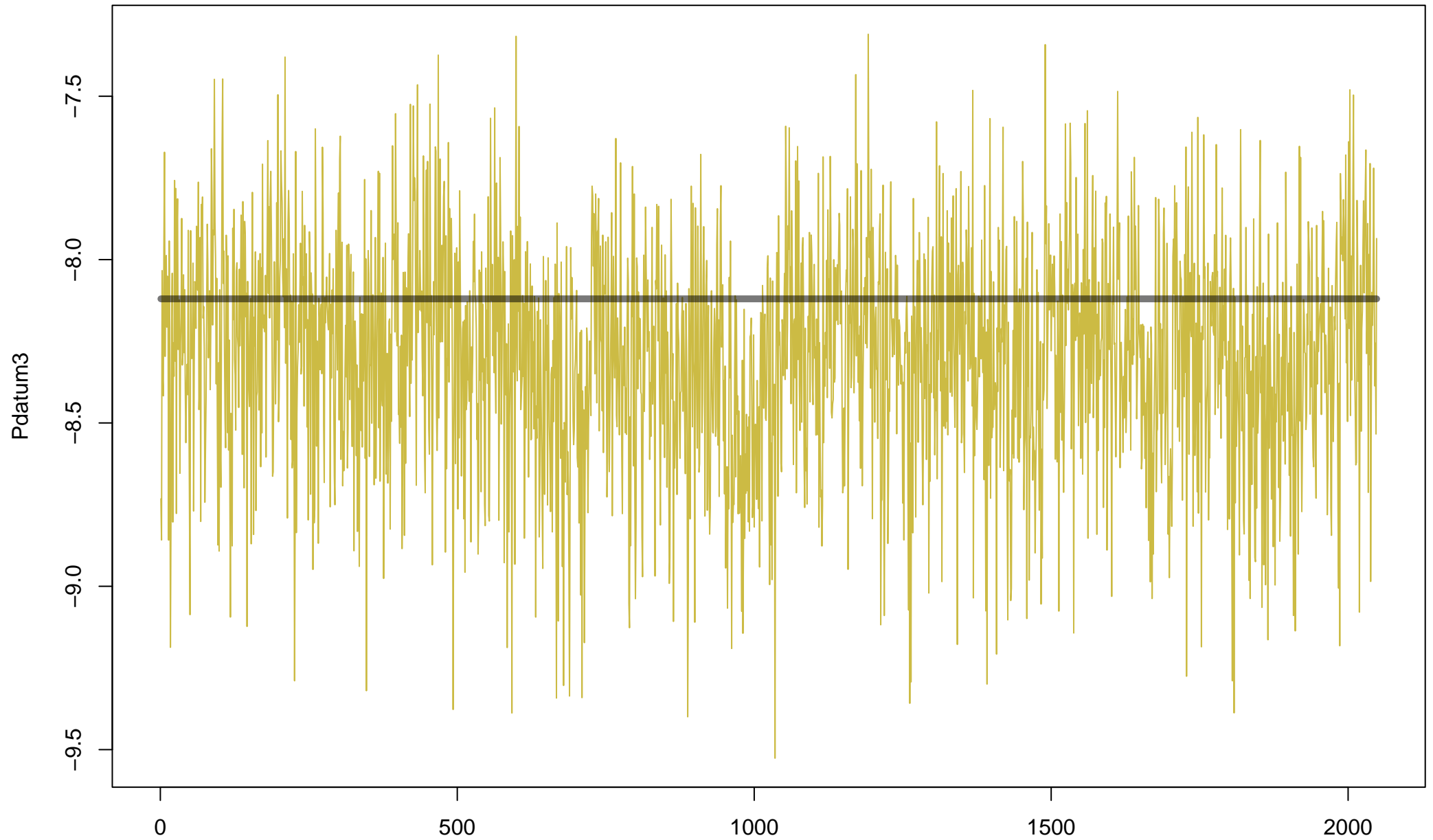
**Pdatum2**

**ESS = 333 | BMK = 0.0564 | MCSE(6.27) = 5.69 | stat: FALSE | burn: 0 | rel.err: -2.11**



**Pdatum3**

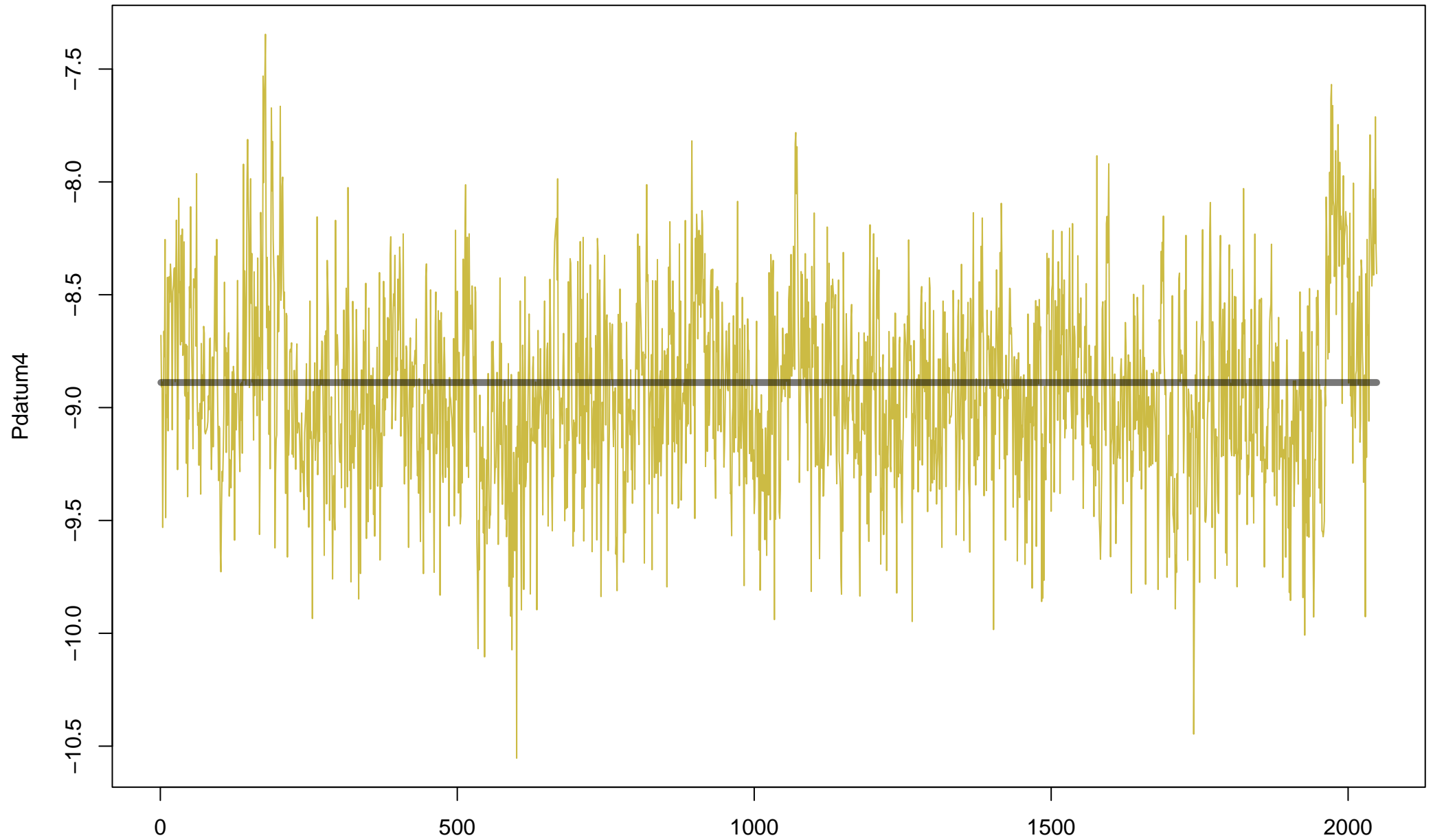
**ESS = 776 | BMK = 0.0369 | MCSE(6.27) = 4.42 | stat: FALSE | burn: 0 | rel.err: -0.386**





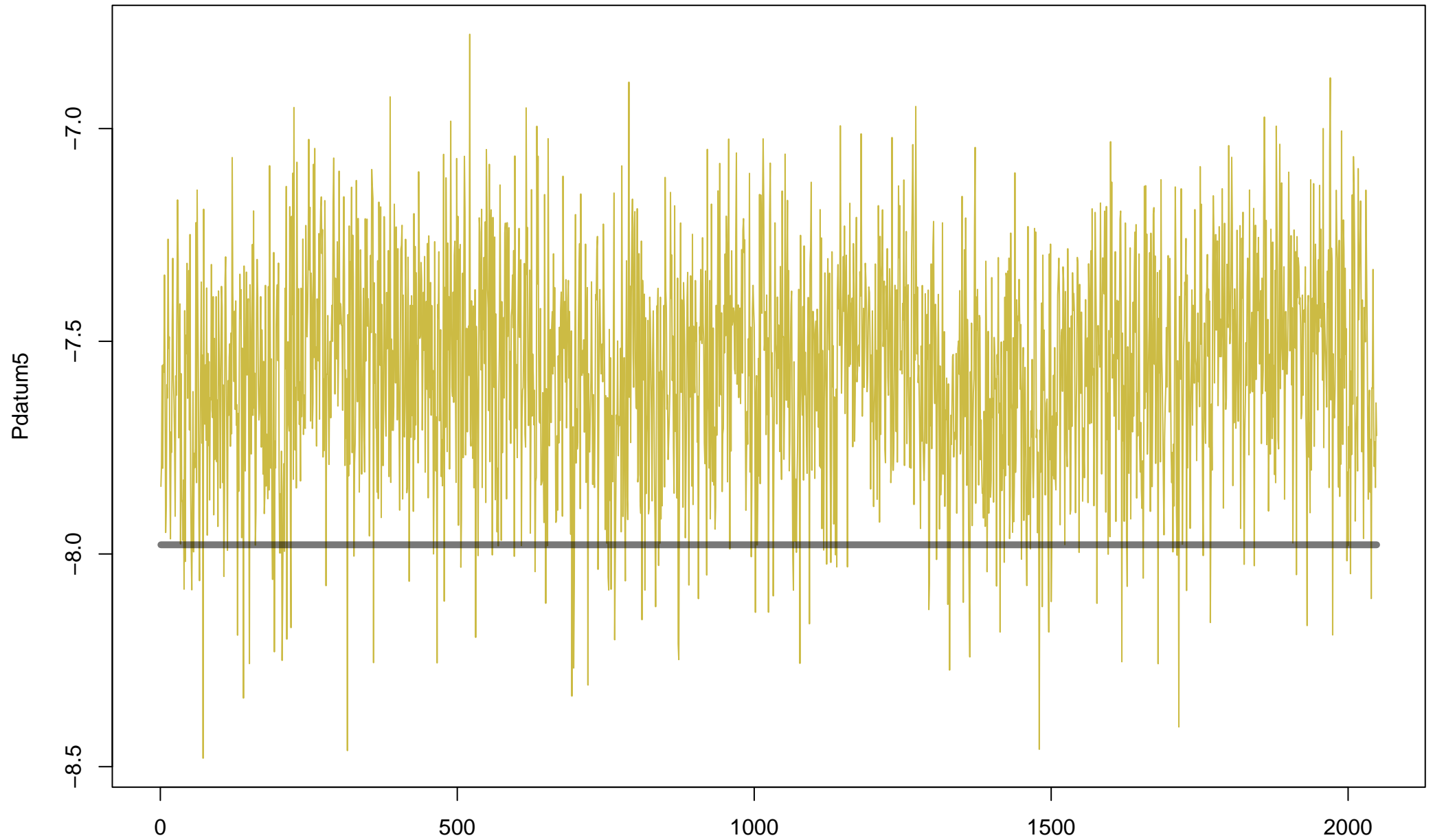
**Pdatum4**

**ESS = 209 | BMK = 0.0521 | MCSE(6.27) = 5.92 | stat: FALSE | burn: 0 | rel.err: 0.104**



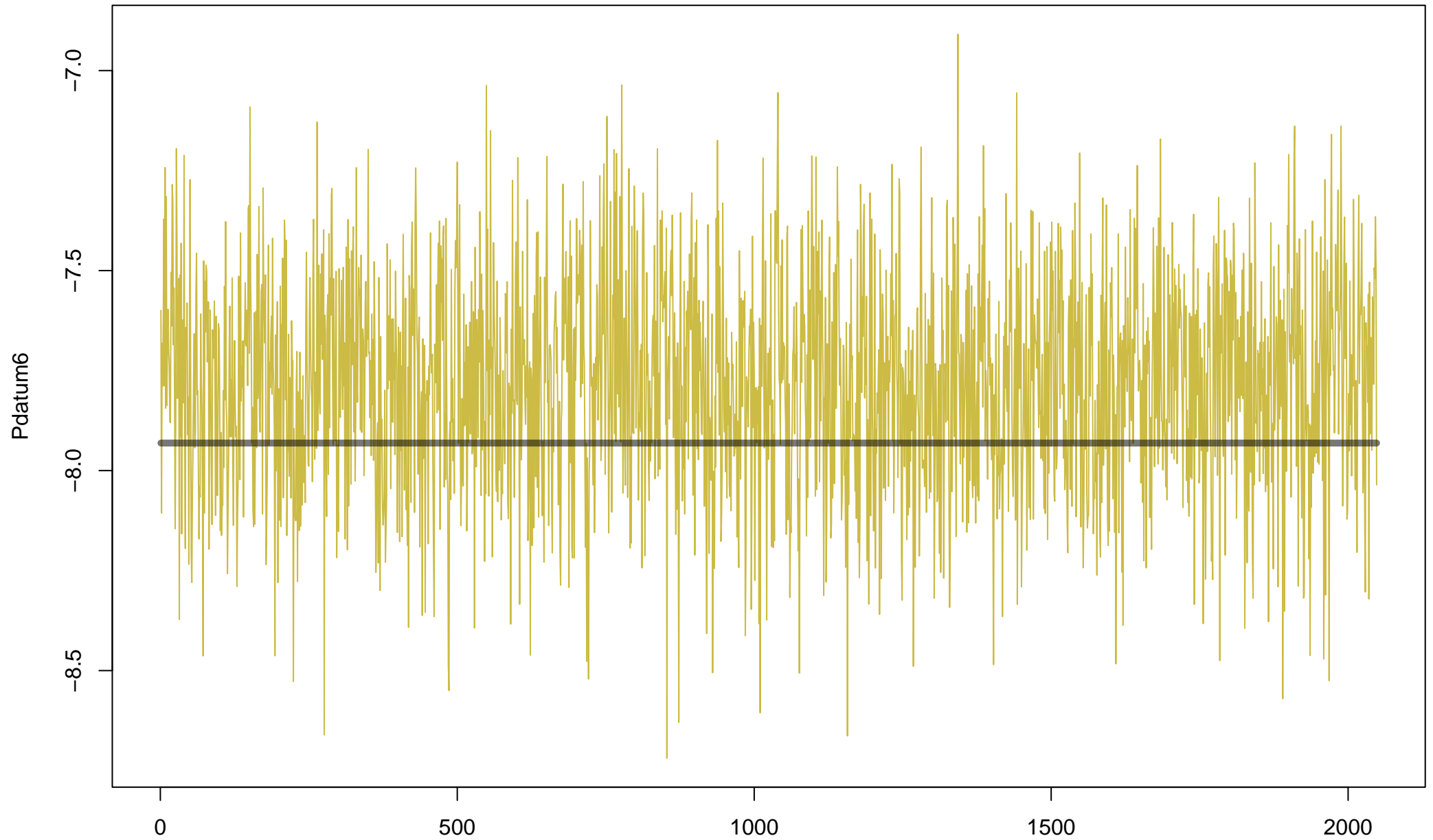
Pdatum5

ESS = 732 | BMK = 0.0338 | MCSE(6.27) = 3.7 | stat: FALSE | burn: 0 | rel.err: 1.43

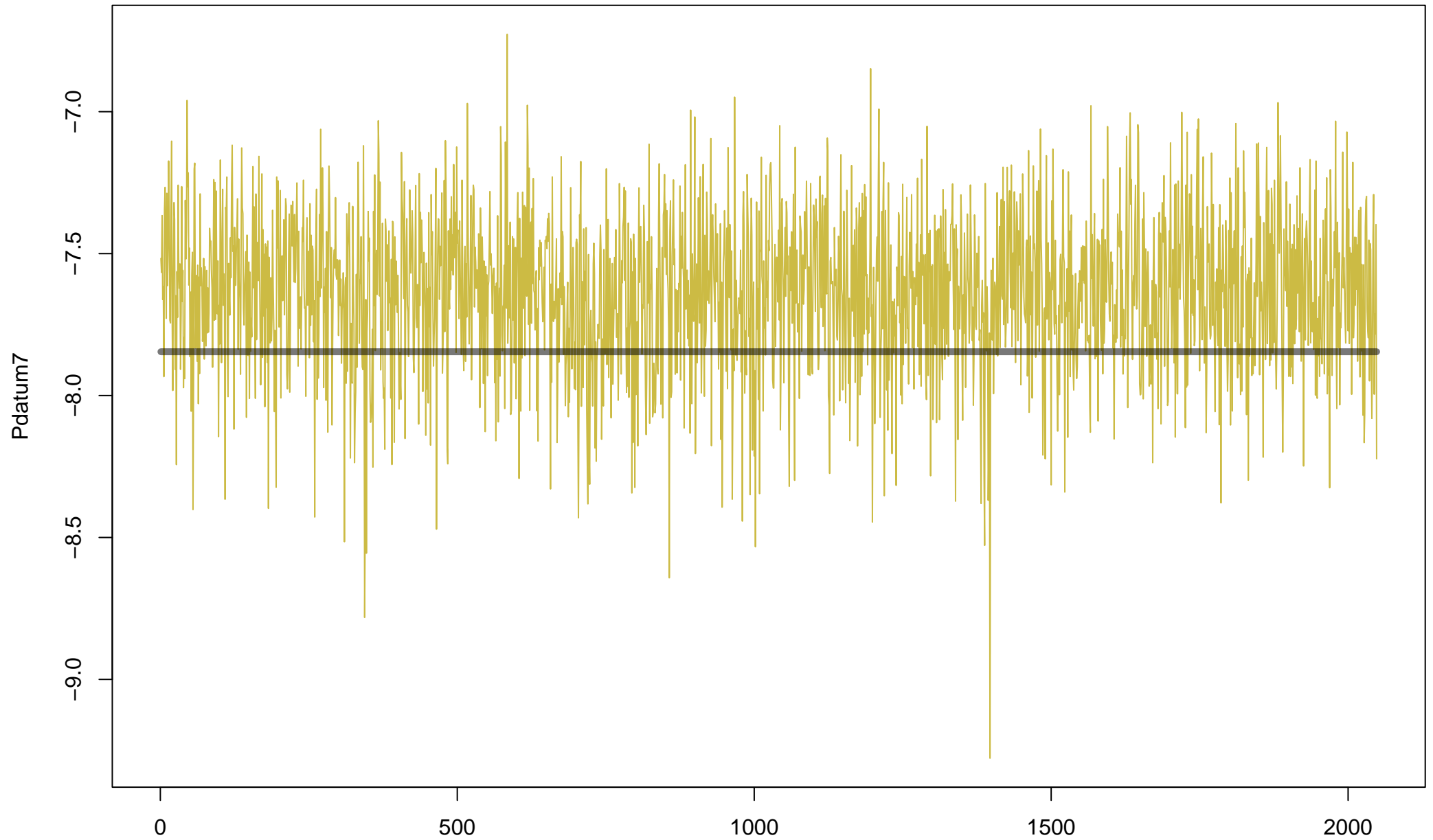


**Pdatum6**

**ESS = 1350 | BMK = 0.0267 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 0.633**

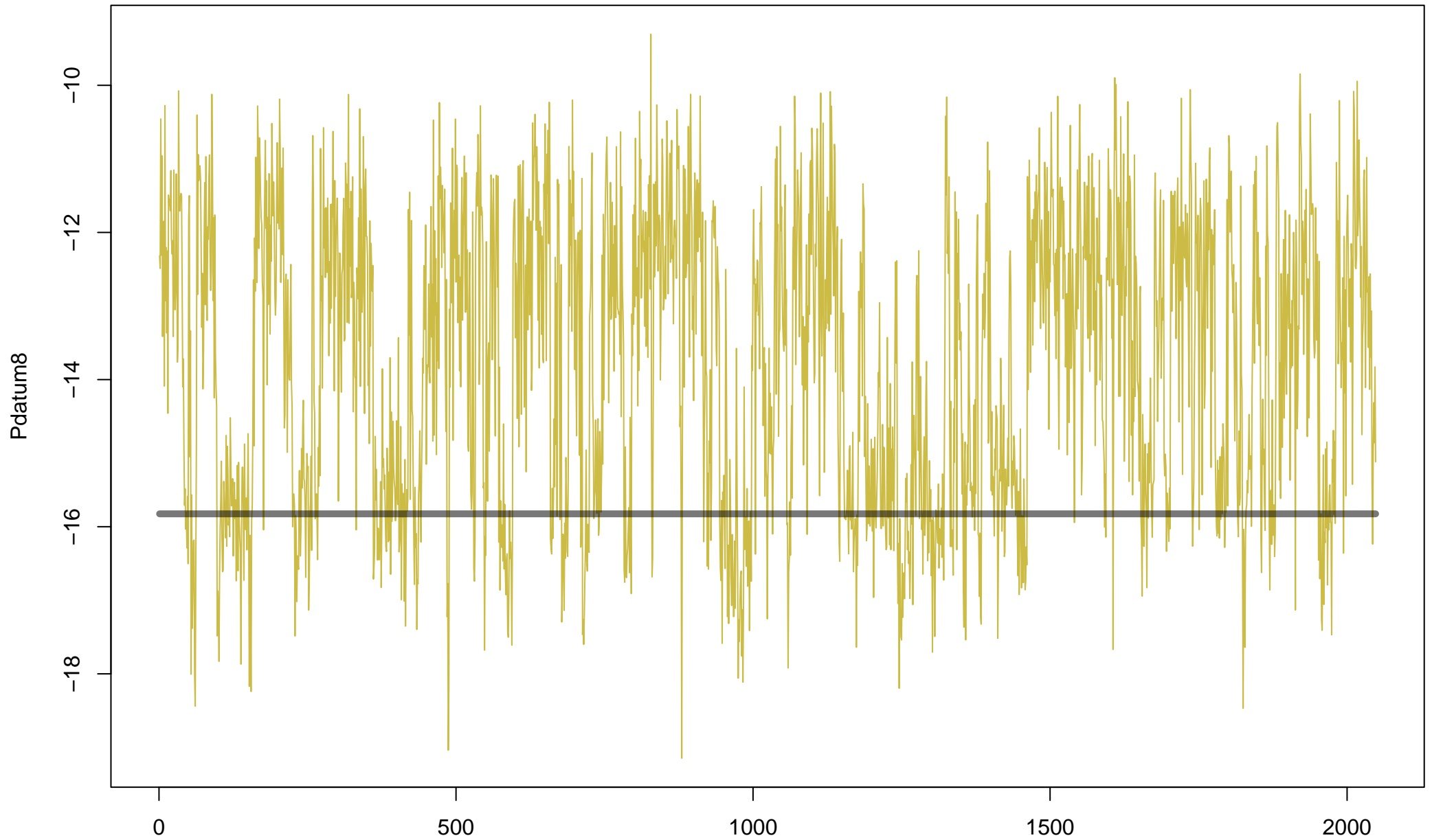


**Pdatum7**  
**ESS = 1830 | BMK = 0.0589 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | rel.err: 0.804**

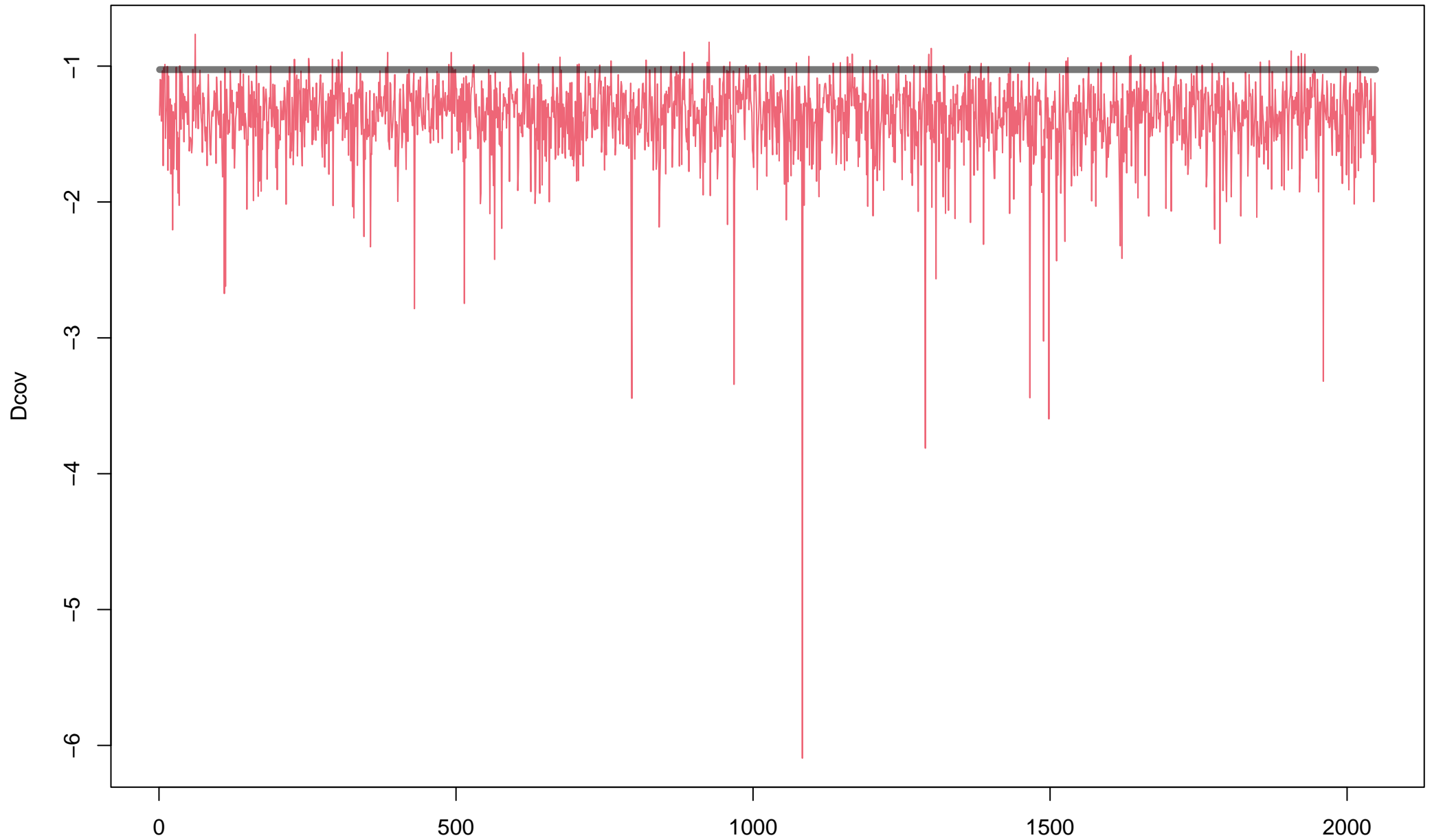


**Pdatum8**

**ESS = 249 | BMK = 0.102 | MCSE(6.27) = 5.14 | stat: TRUE | burn: 1428 | rel.err: 0.578**

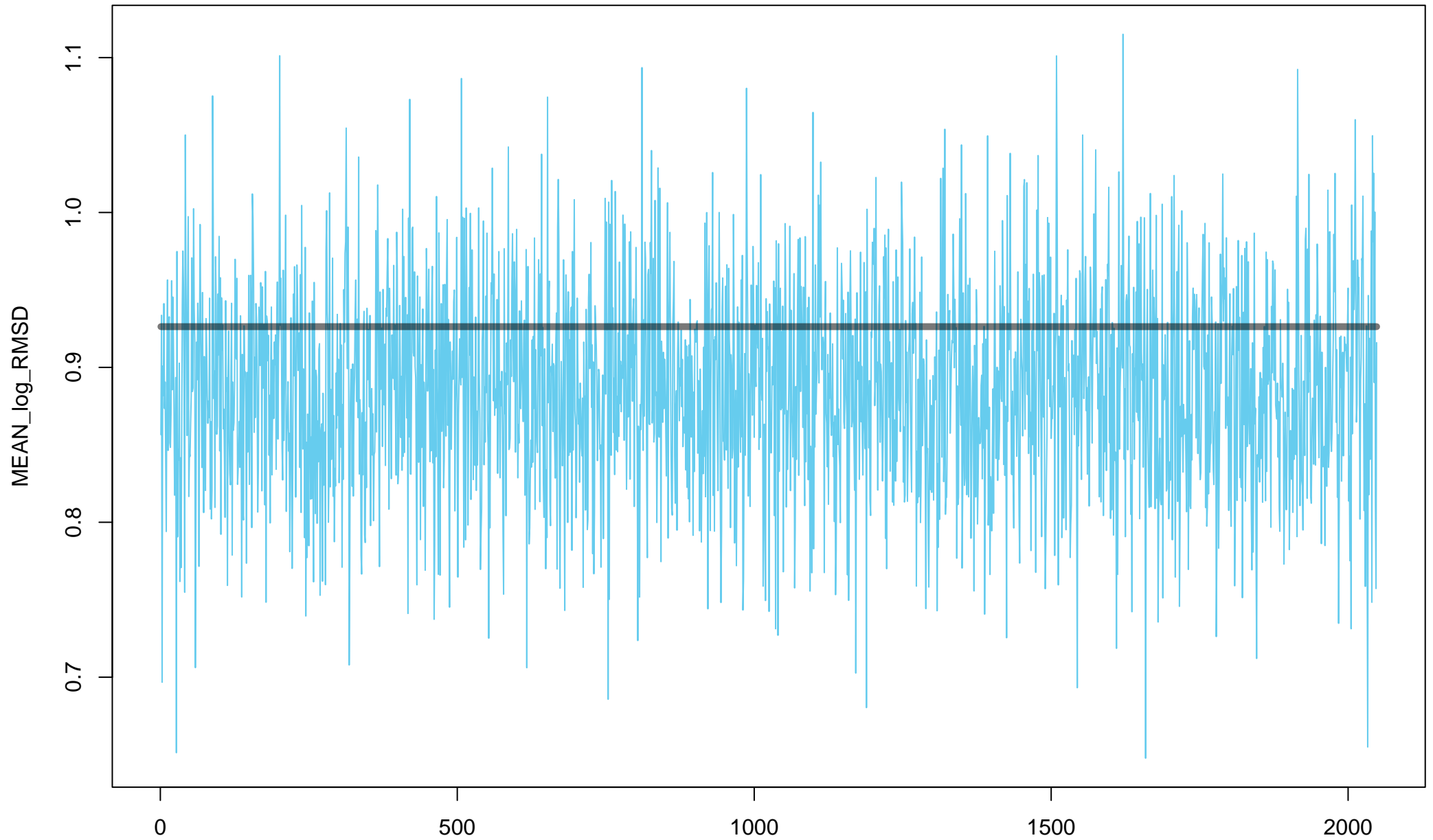


**Dcov**  
**ESS = 1480 | BMK = 0.0573 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | rel.err: 1.58**

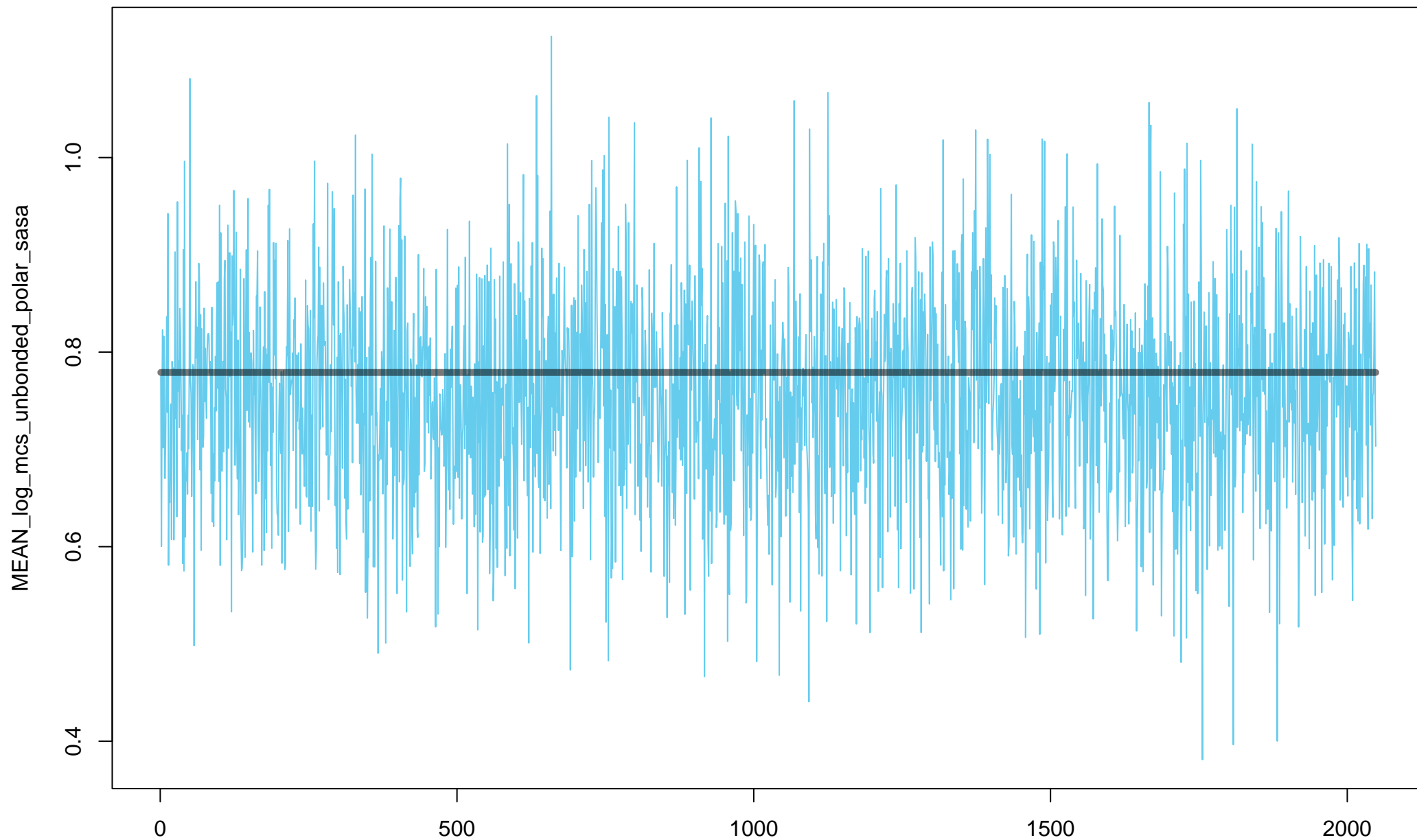


# MEAN\_log\_RMSD

ESS = 2050 | BMK = 0.0404 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 0 | rel.err: -0.611



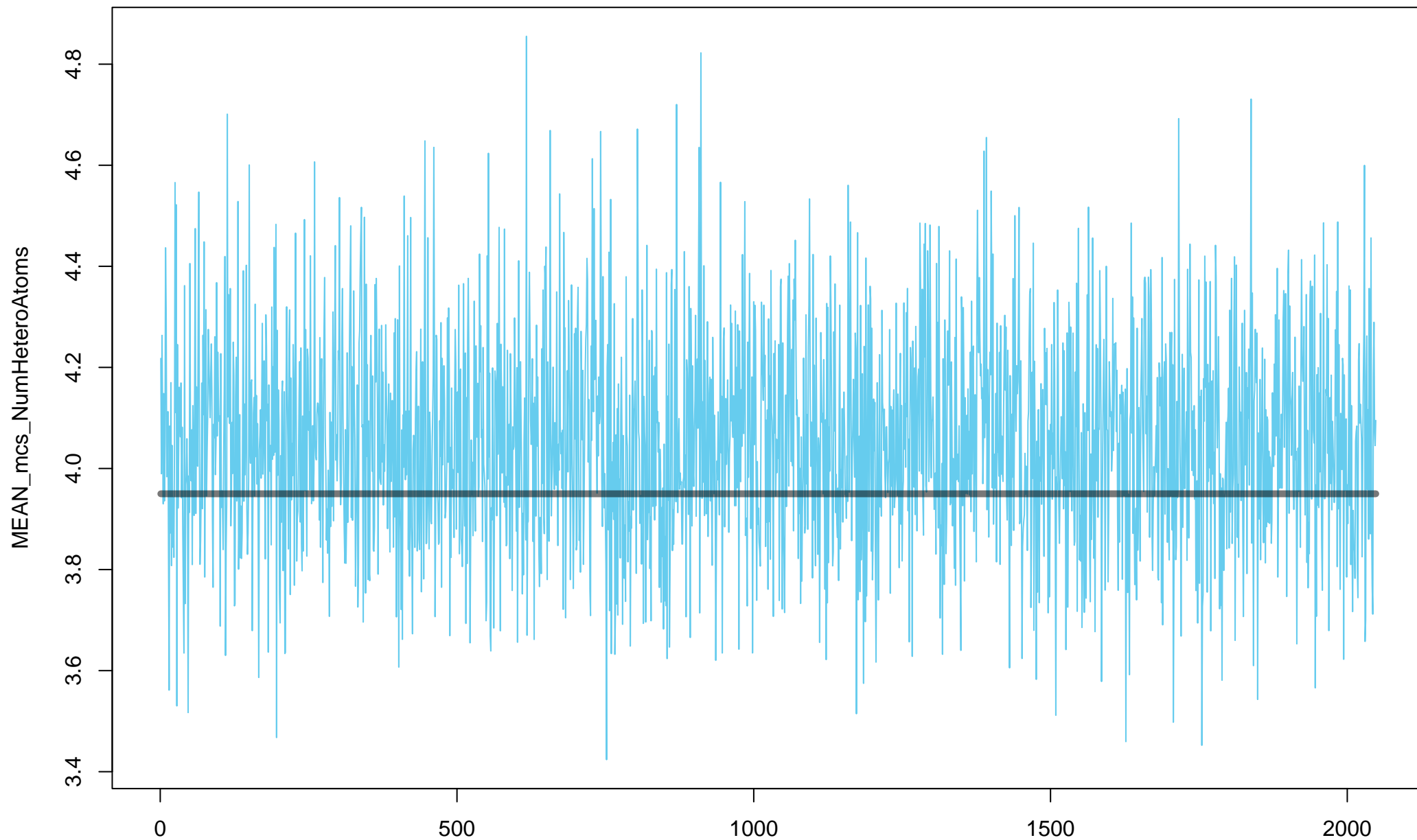
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: -0.231**





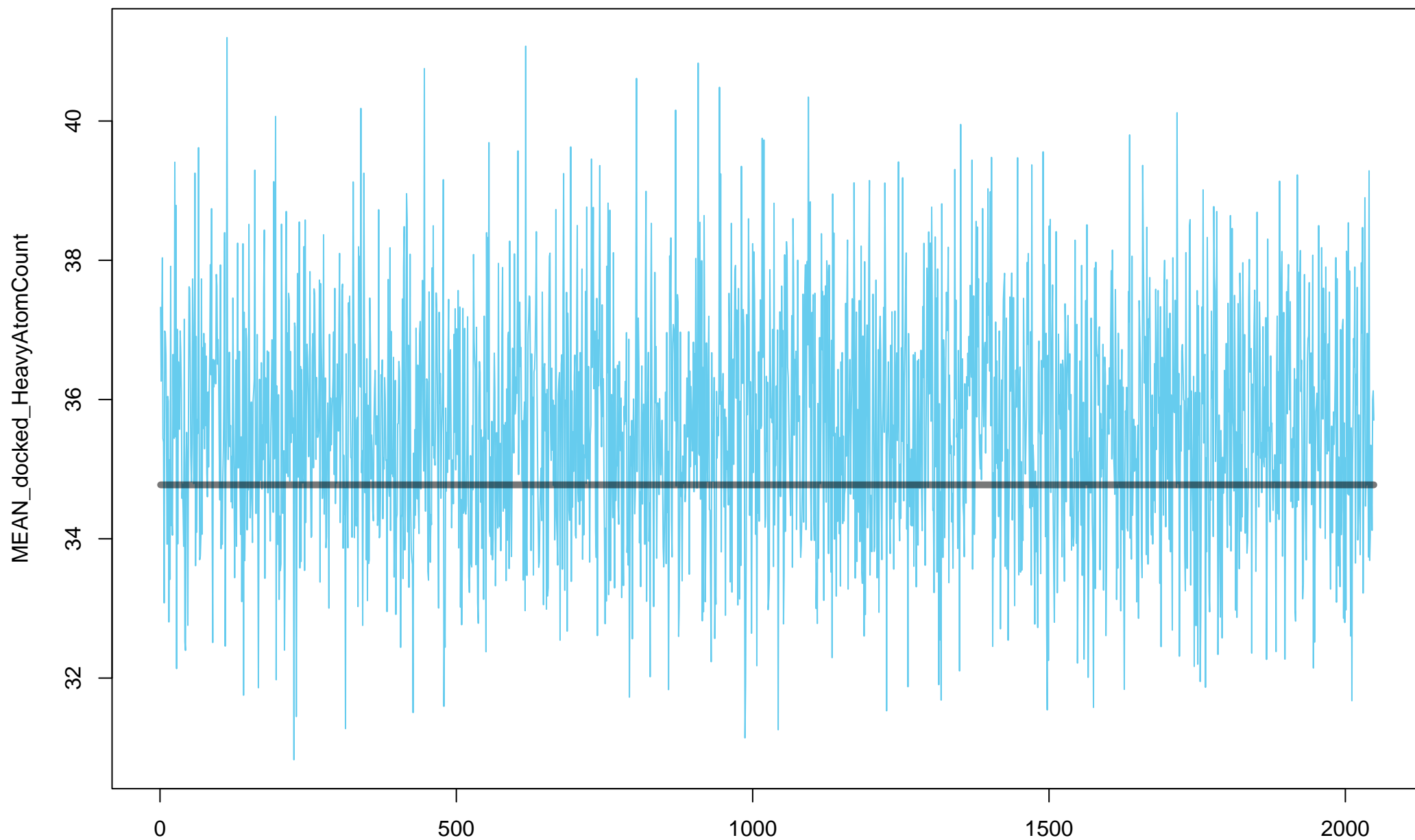
# MEAN\_mcs\_NumHeteroAtoms

ESS = 2050 | BMK = 0.0501 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: 0.504



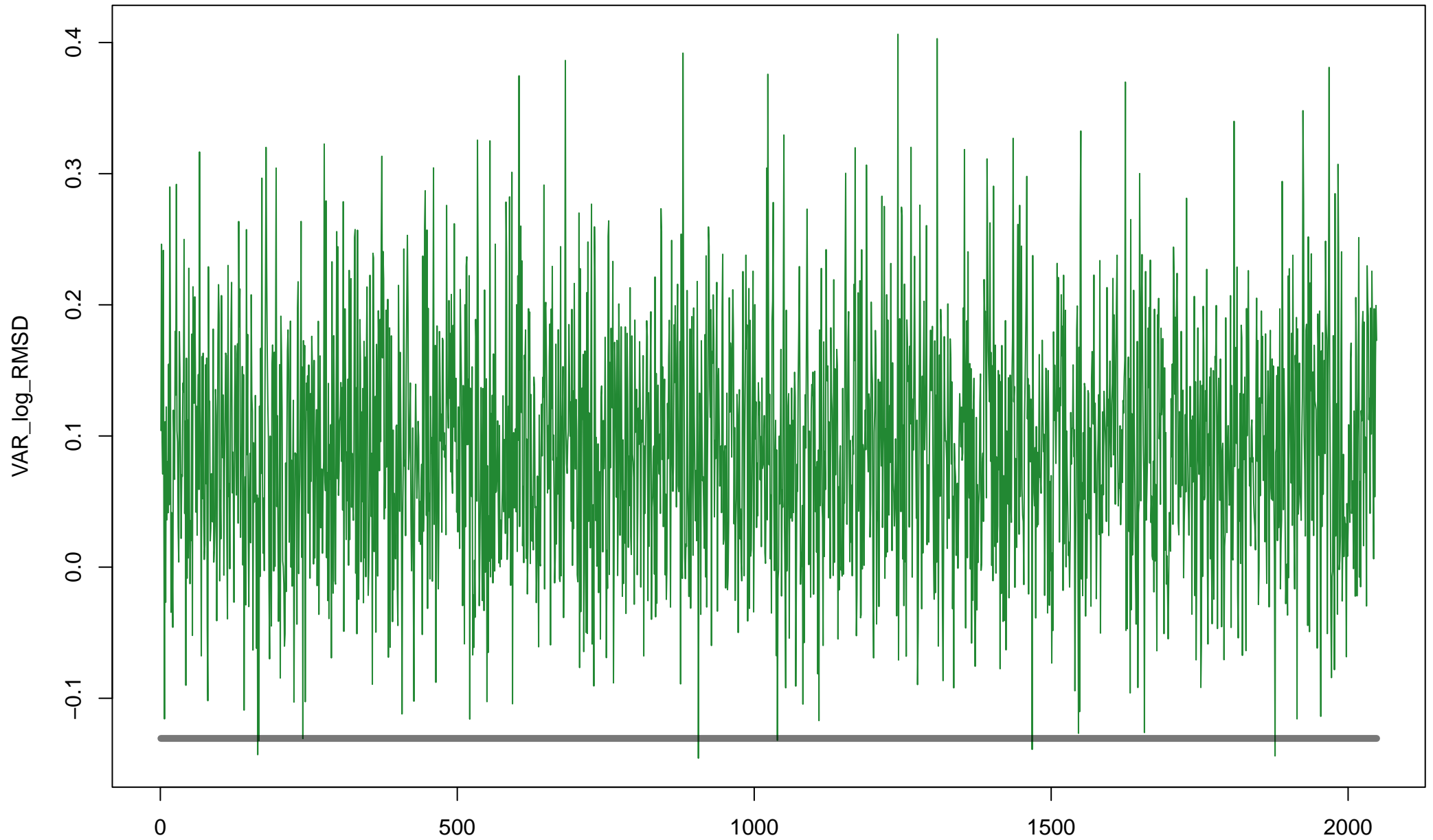
# MEAN\_docked\_HeavyAtomCount

ESS = 2050 | BMK = 0.0533 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0 | rel.err: 0.511

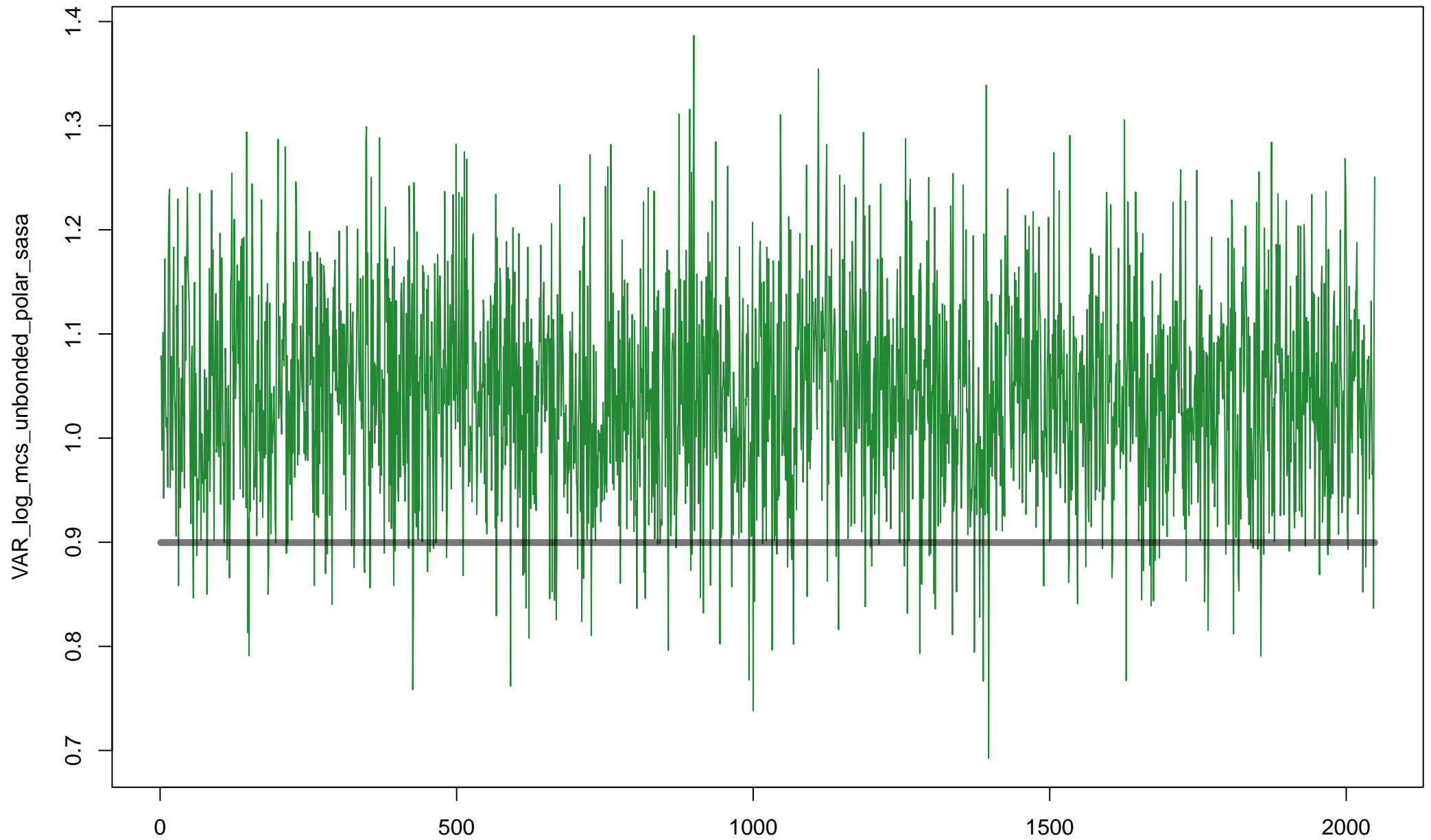


# VAR\_log\_RMSD

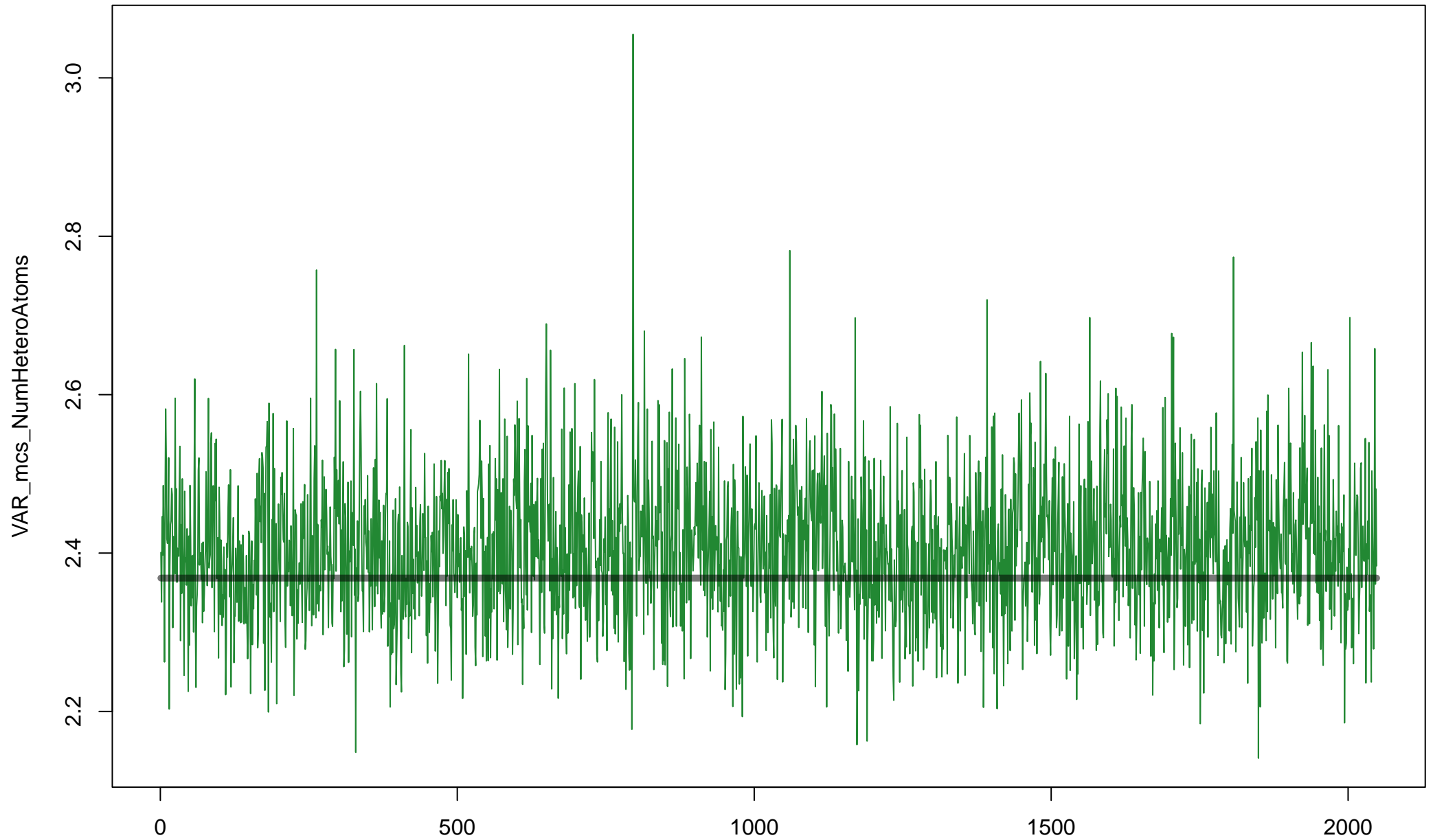
ESS = 2050 | BMK = 0.0348 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: 2.24



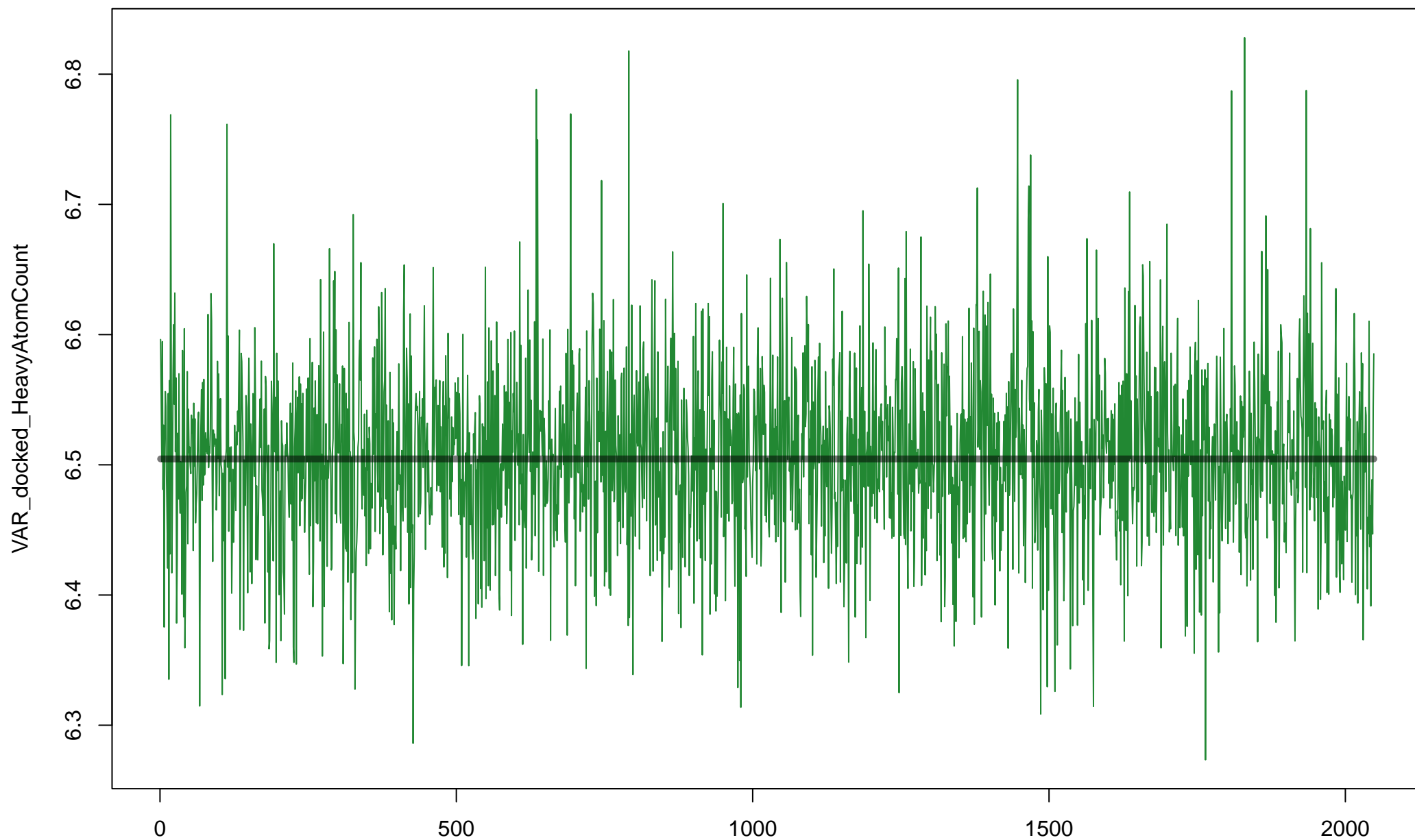
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0399 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 1.38**



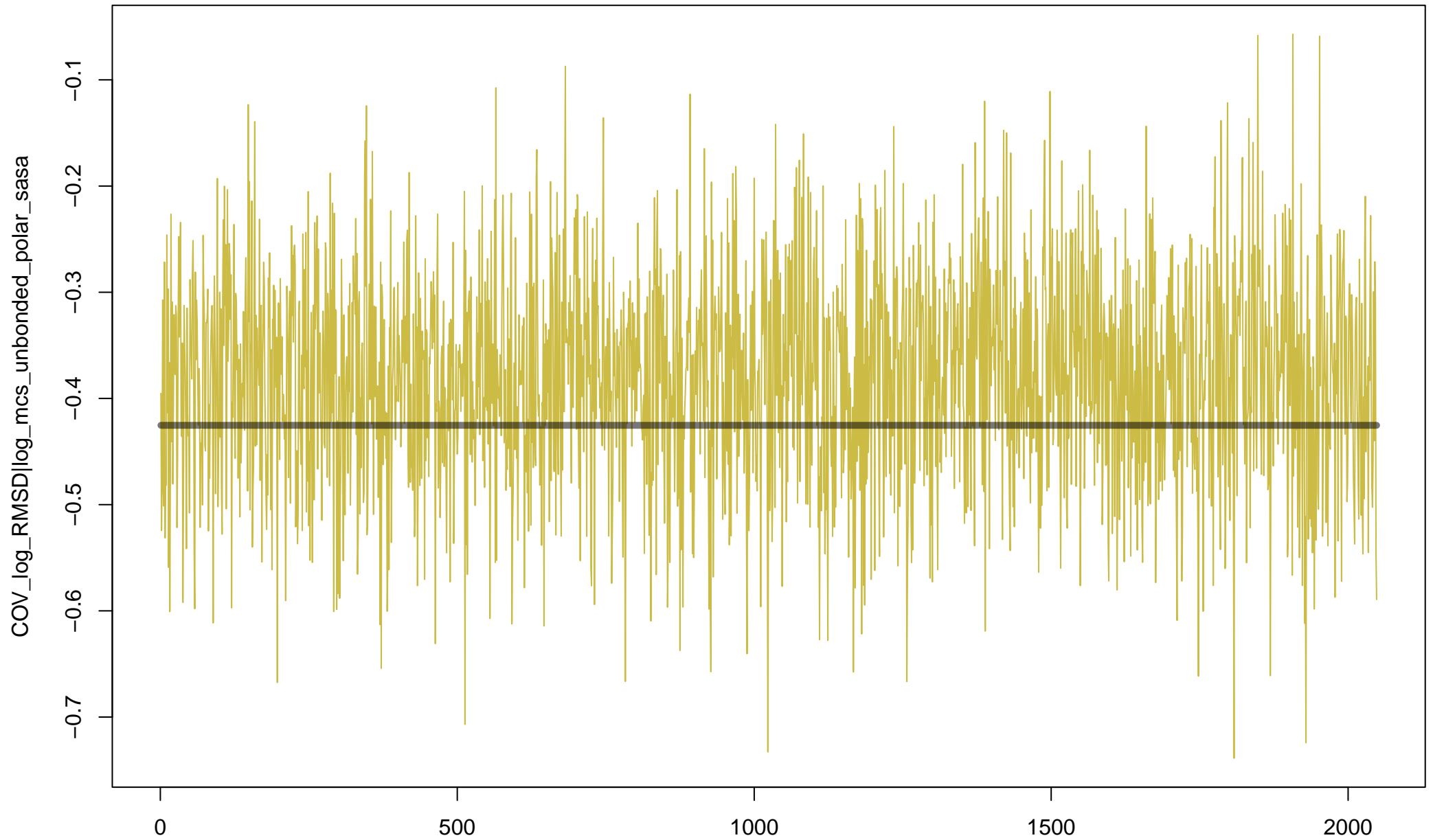
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1740 | BMK = 0.0434 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: 0.43**



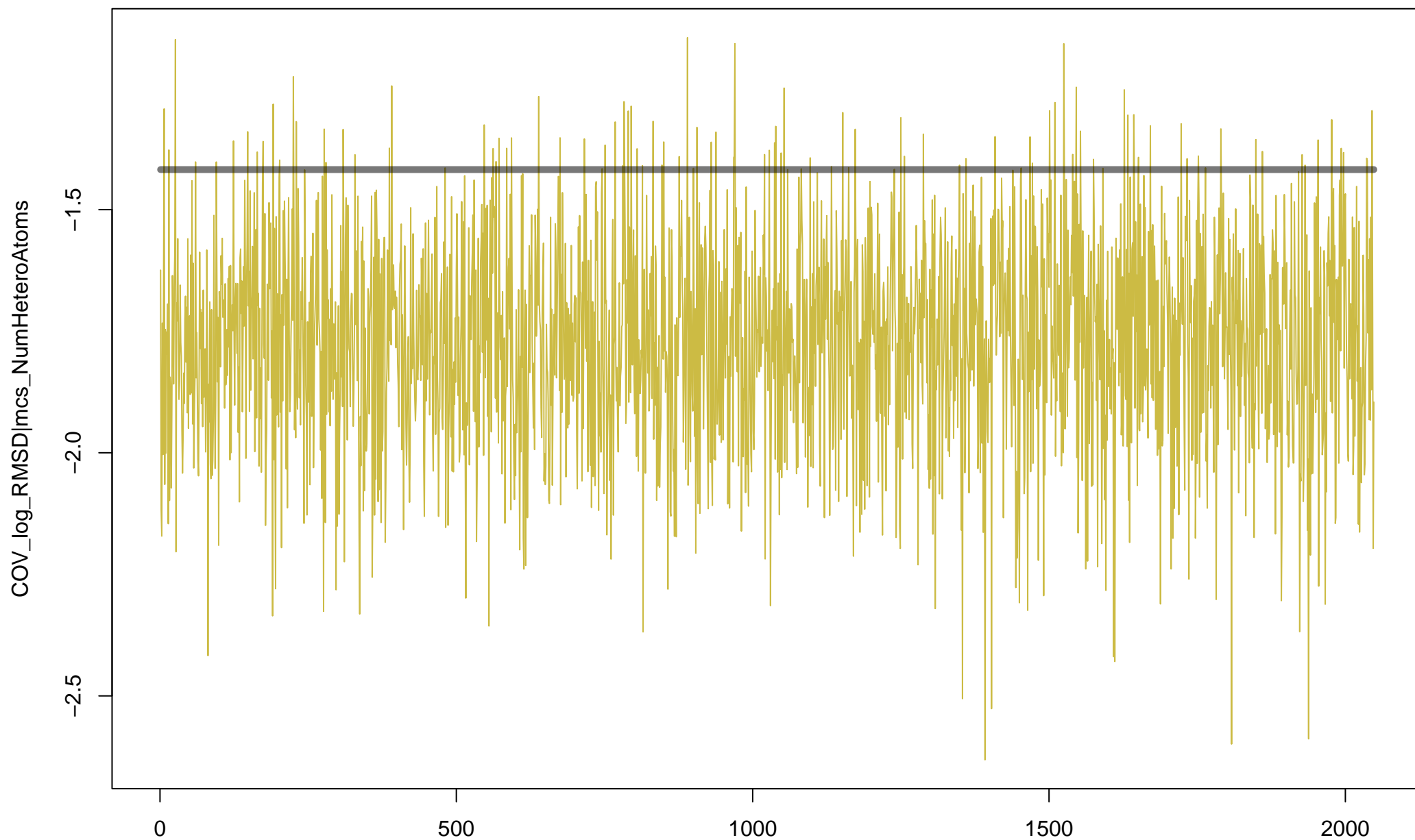
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.0635**



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.053 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | rel.err: 0.458**

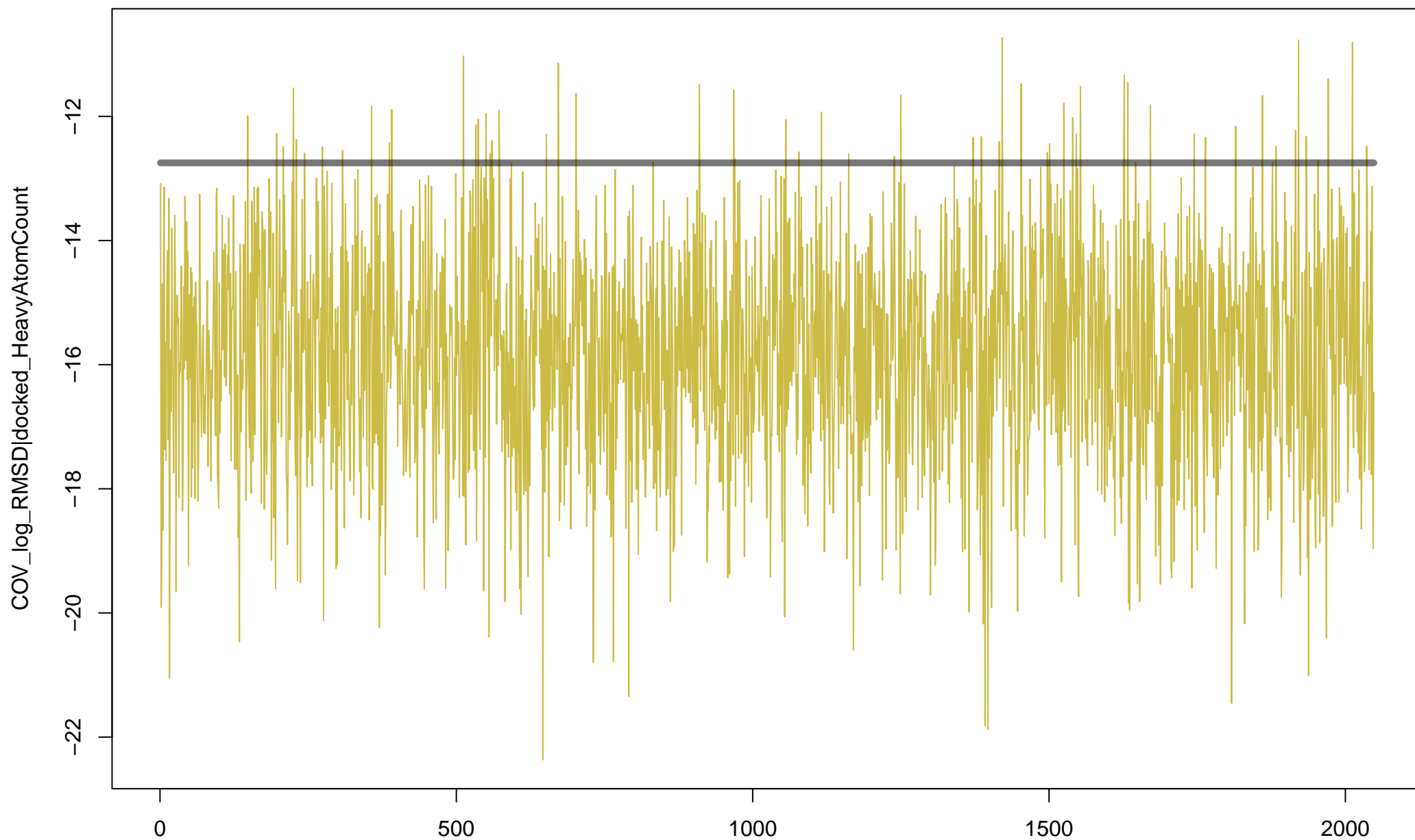


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0611 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | rel.err: -1.64**

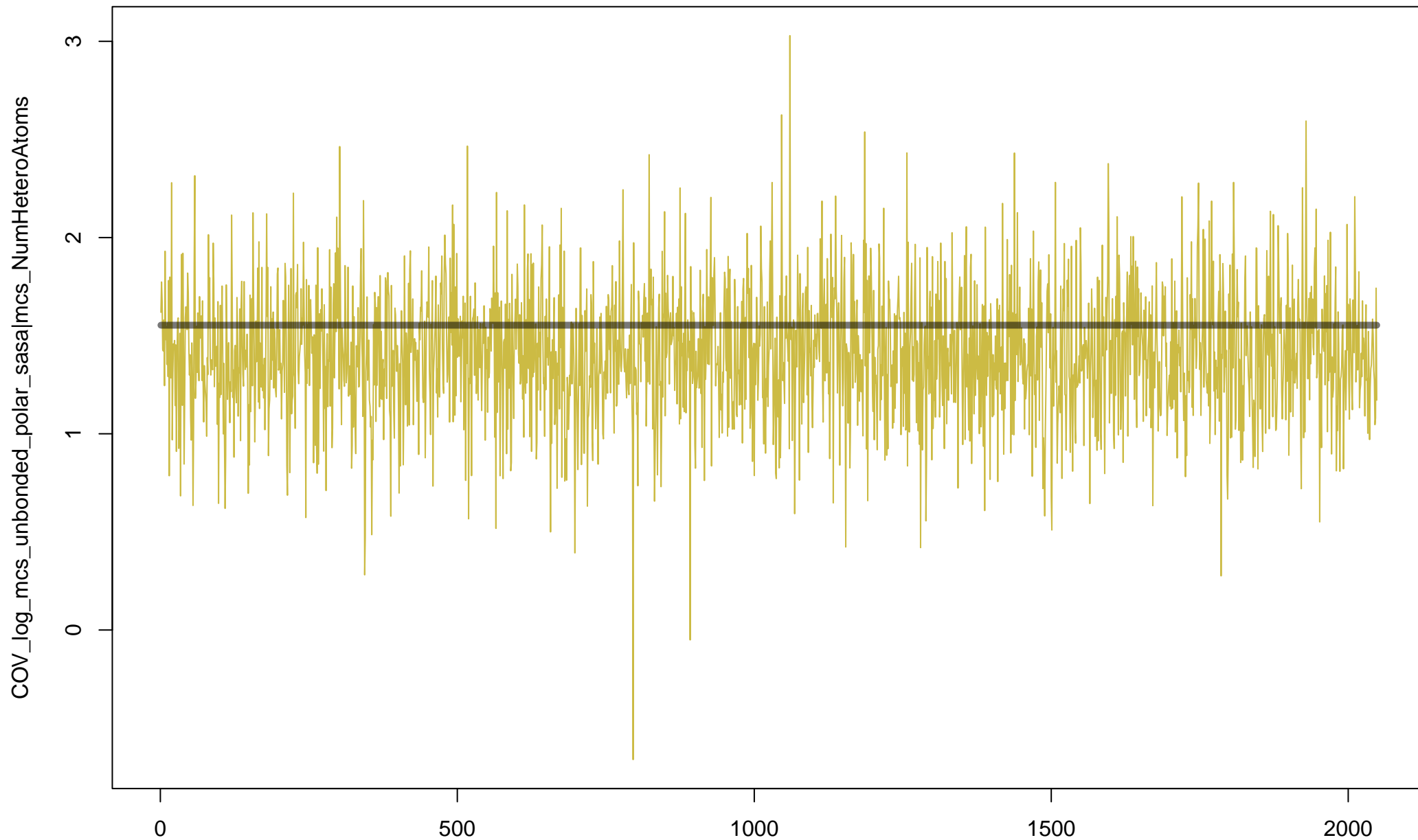




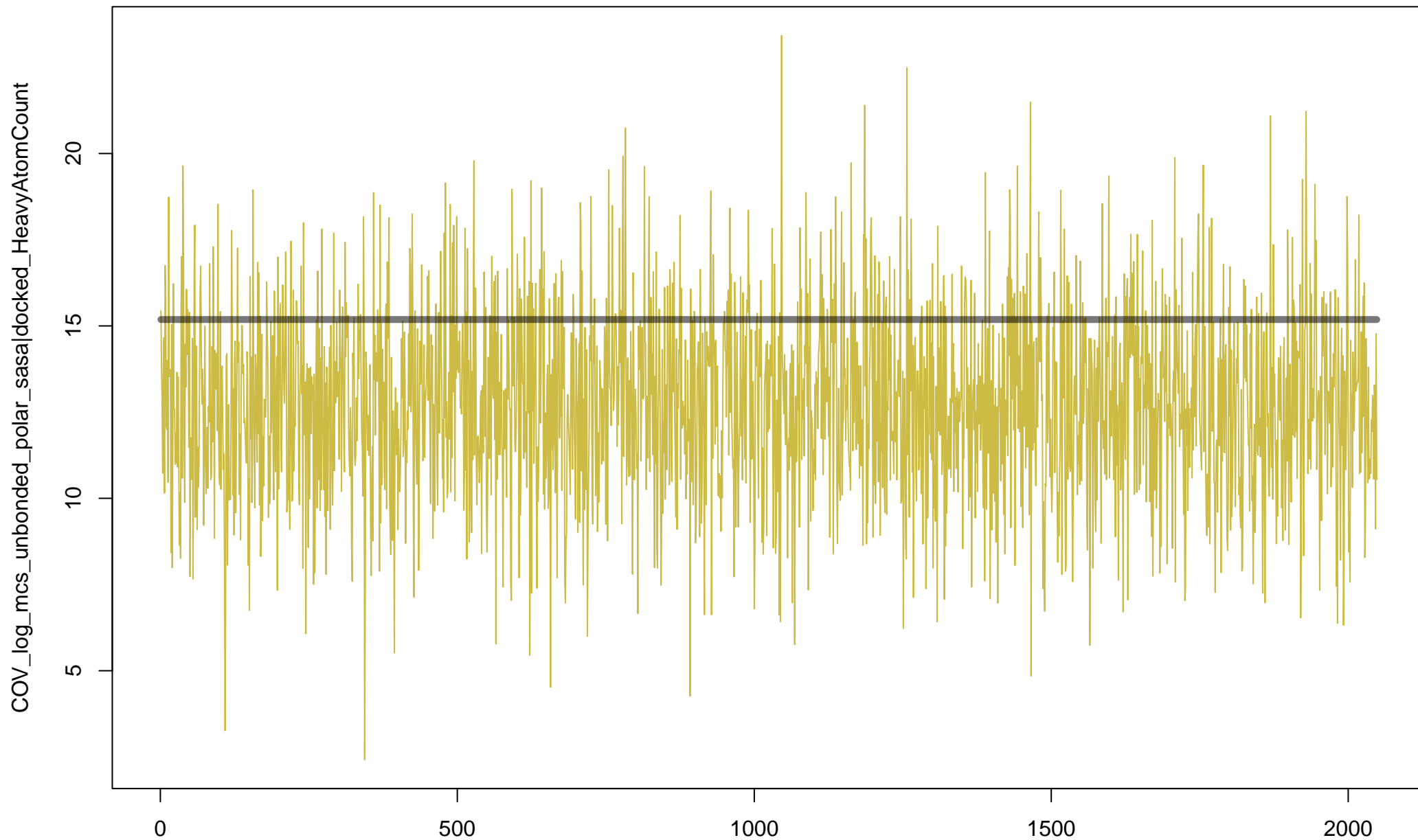
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 1840 | BMK = 0.0372 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: -1.78**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0573 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: -0.439**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0564 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: -0.904**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.038 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: 0.482**

