

-- STATS maxD --

min ESS = 74.4387755126867

max BMK = 0.1531676162531

max MCSE = 7.81467578232566

all stationary: FALSE

burn: 816

max rel.err.: 2.15182031904781

-- STATS 1D --

min ESS = 1344.62579005673

max BMK = 0.071875100127486

max MCSE = 2.97538382163338

all stationary: FALSE

burn: 0

max rel.err.: 2.25737564192647

-- STATS 2D --

min ESS = 1909.68711454513

max BMK = 0.0579770197243112

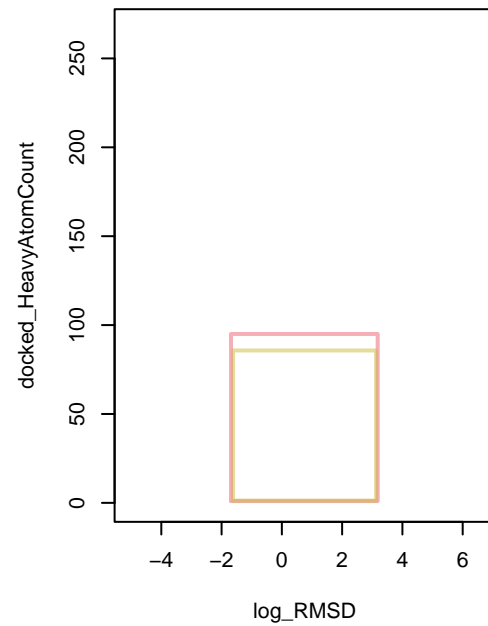
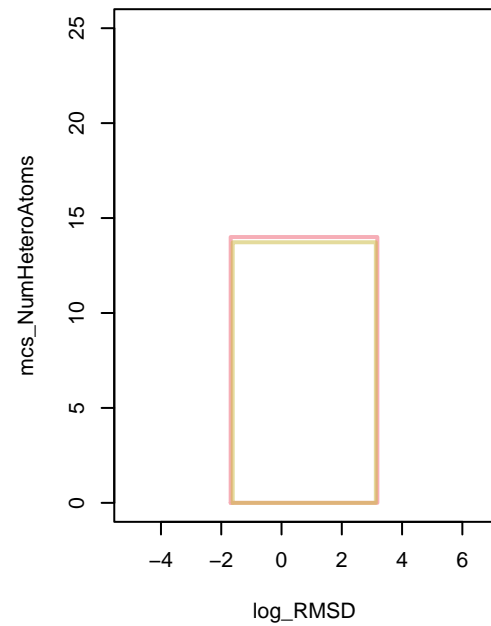
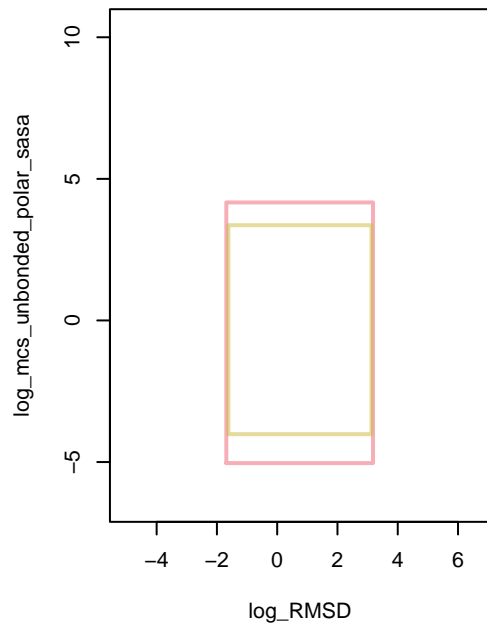
max MCSE = 2.76503004800683

all stationary: TRUE

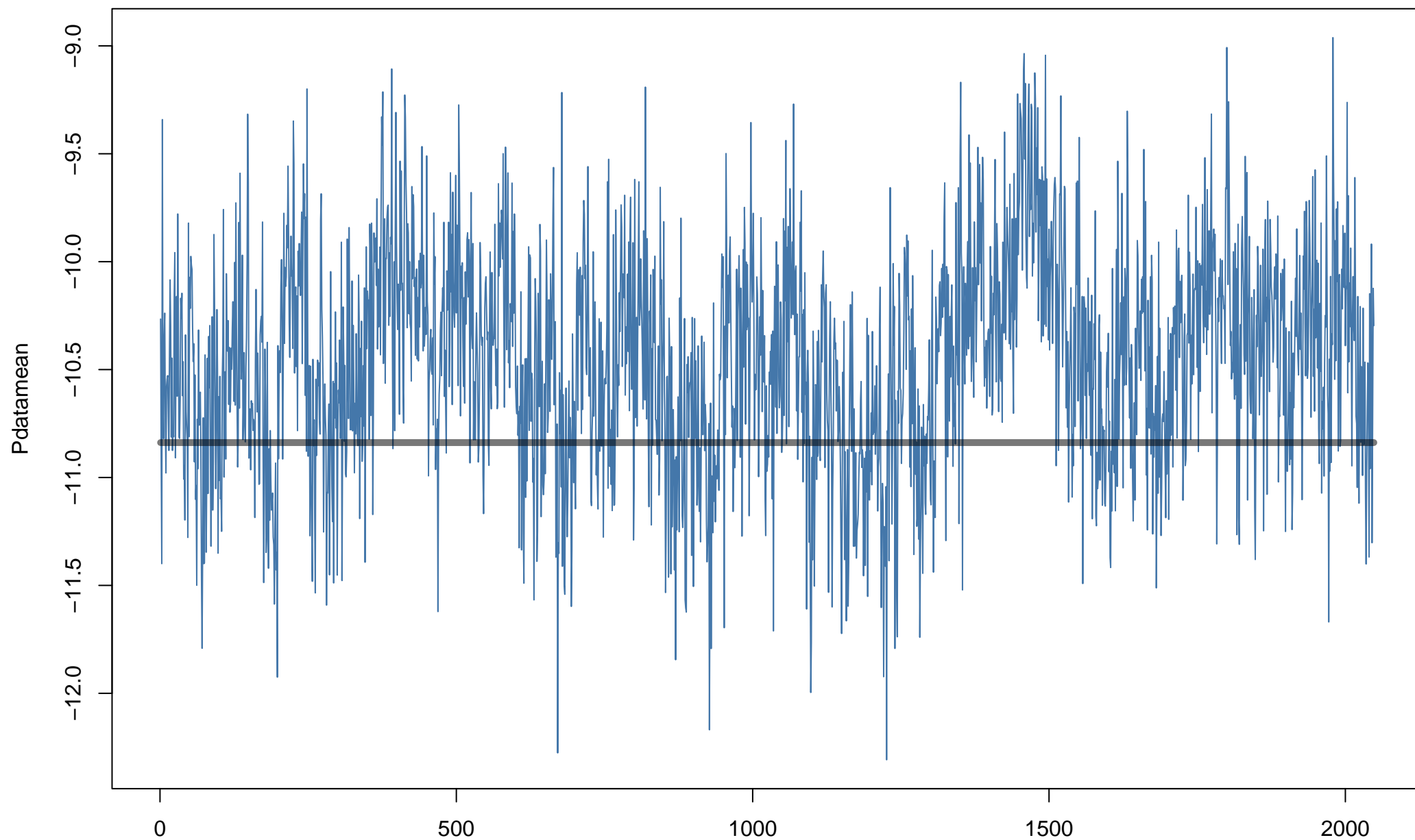
burn: 0

max rel.err.: 1.73586507878291

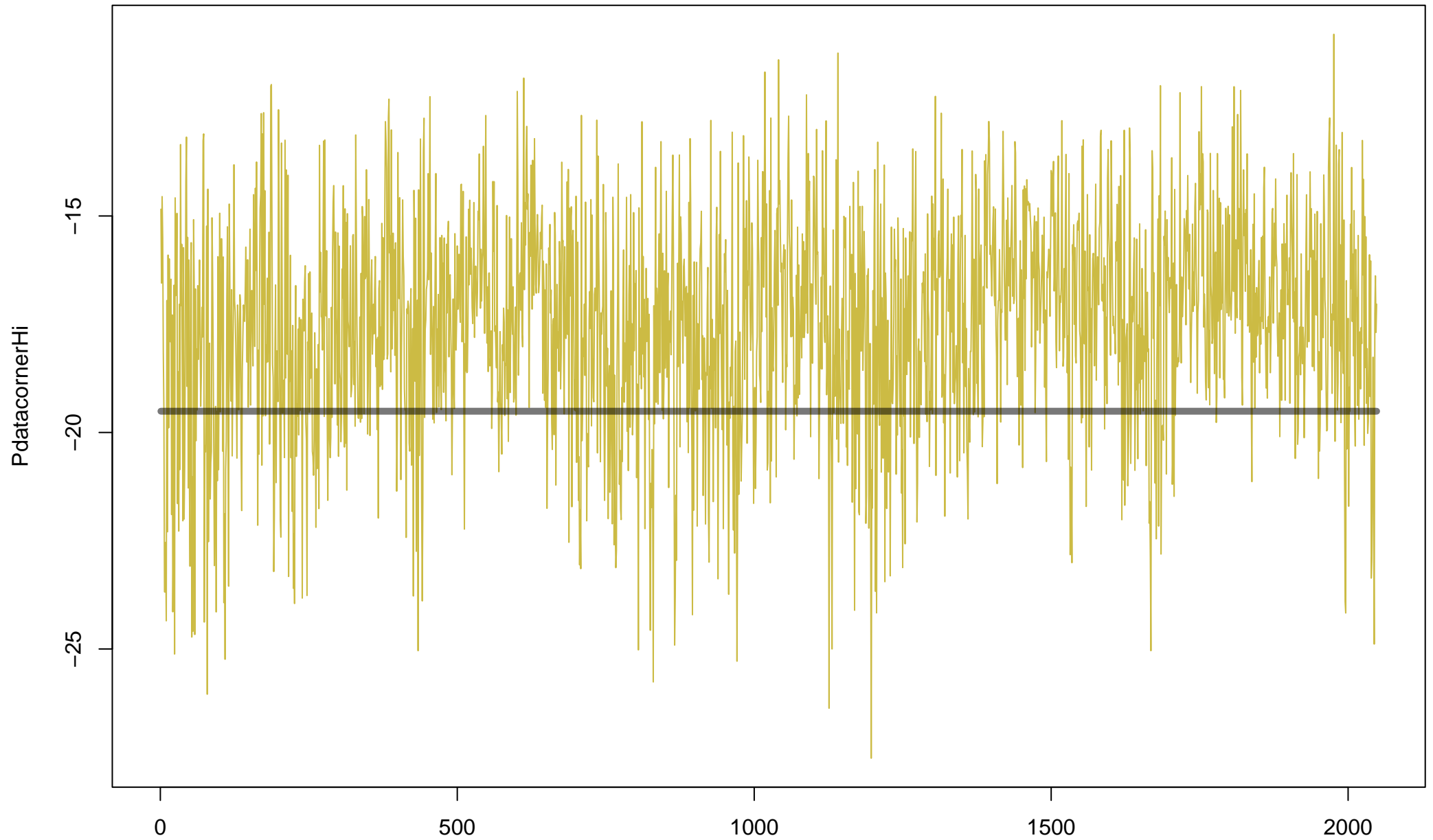
Occupied clusters: 9 of 16



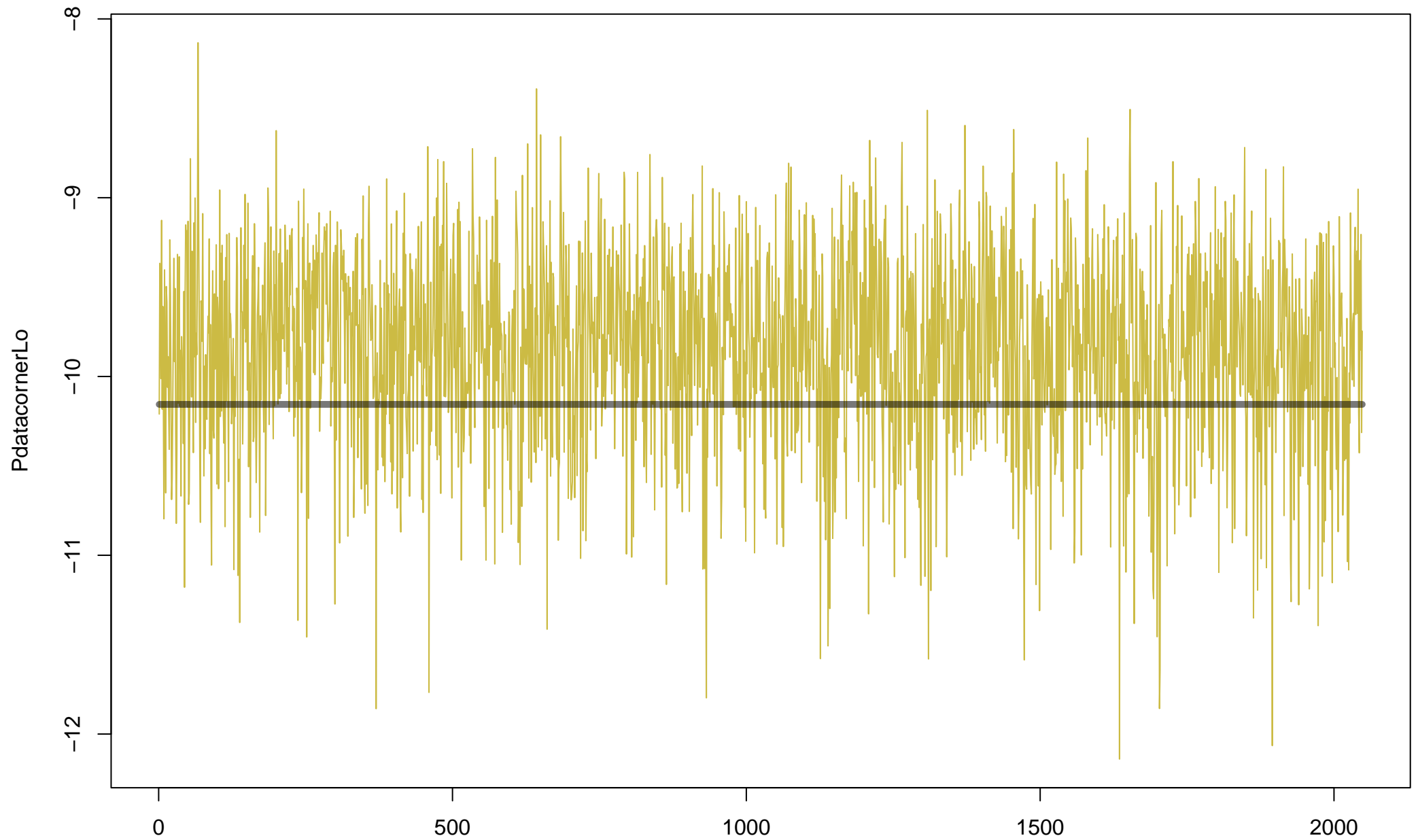
**Pdatamean**  
**ESS = 74.4 | BMK = 0.0734 | MCSE(6.27) = 7.81 | stat: FALSE | burn: 0 | rel.err: 0.765**



**PdatacornerHi**  
**ESS = 1880 | BMK = 0.153 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 0.273**

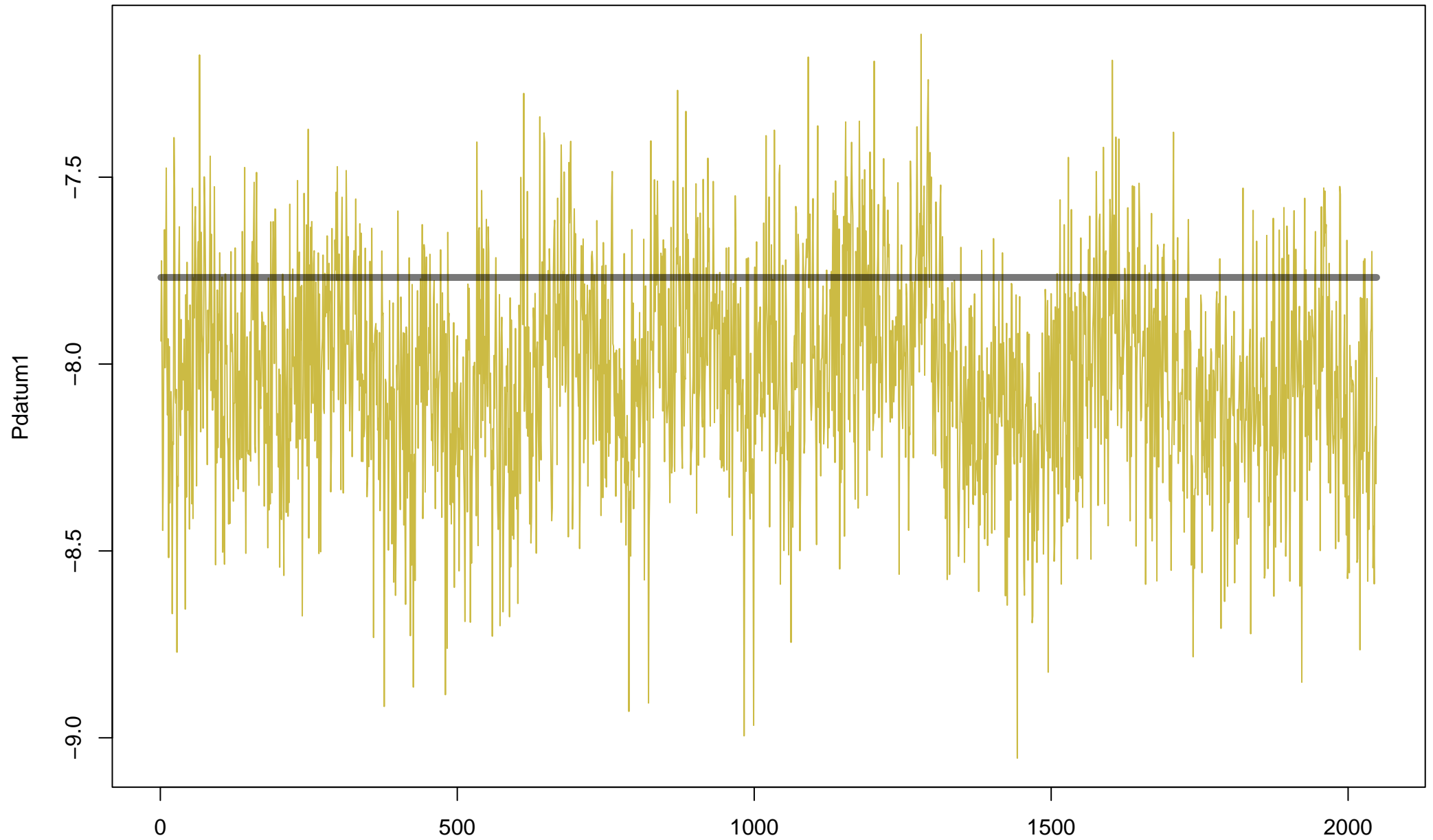


**PdatacornerLo**  
**ESS = 1770 | BMK = 0.0579 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: 0.681**



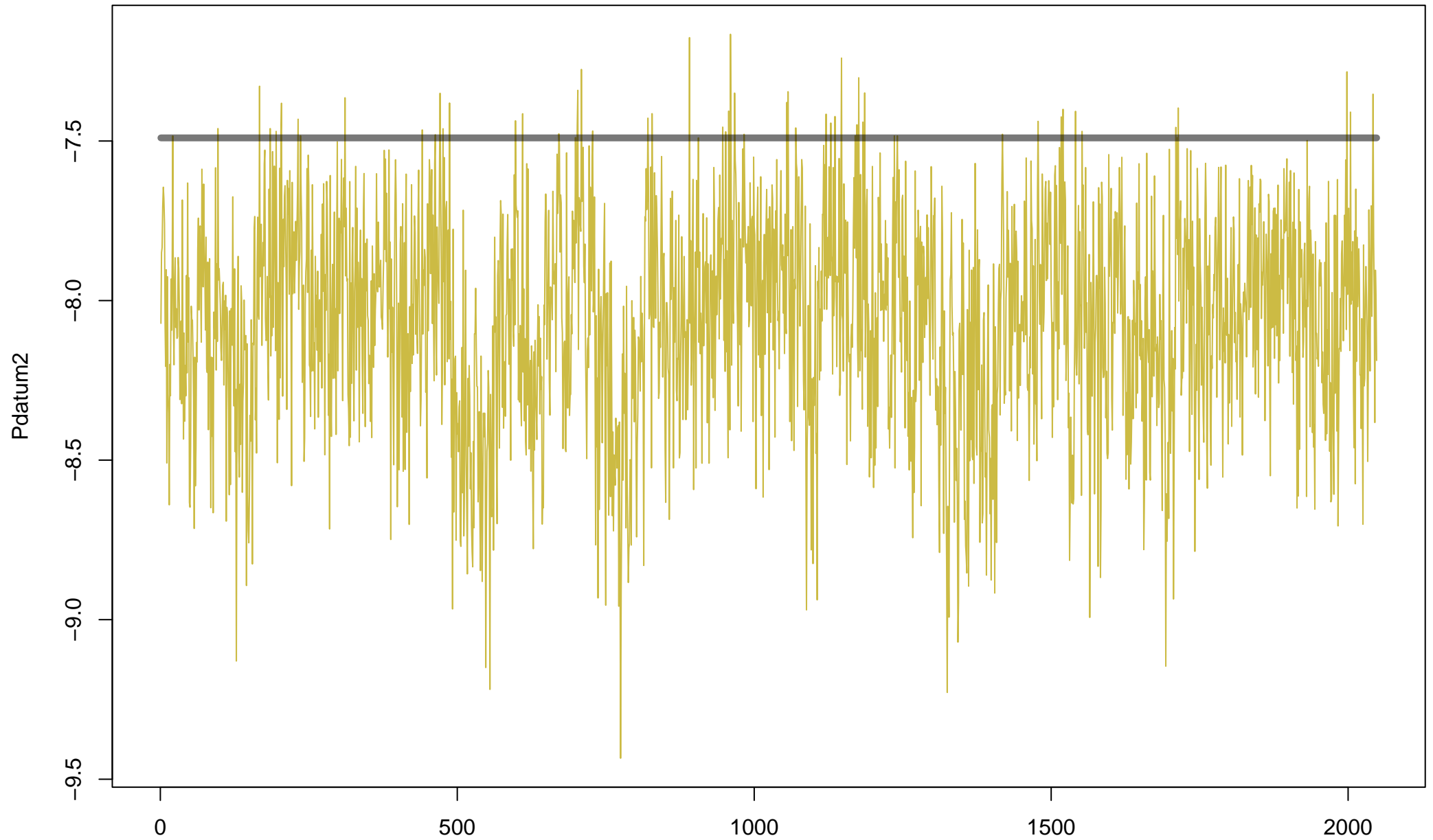
**Pdatum1**

**ESS = 171 | BMK = 0.0523 | MCSE(6.27) = 5.56 | stat: TRUE | burn: 0 | rel.err: -0.866**

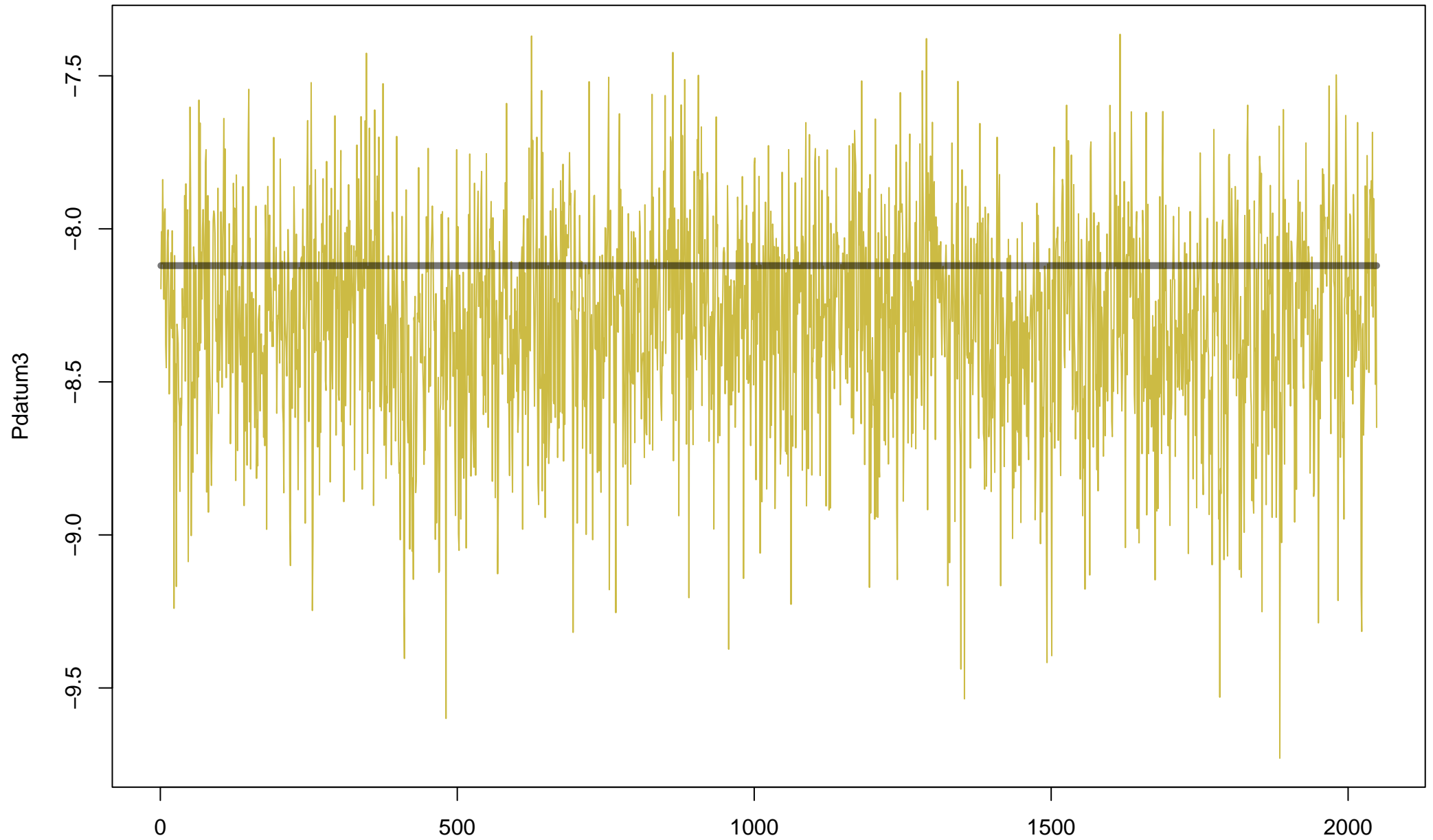


**Pdatum2**

**ESS = 266 | BMK = 0.0281 | MCSE(6.27) = 5.91 | stat: TRUE | burn: 0 | rel.err: -2.15**



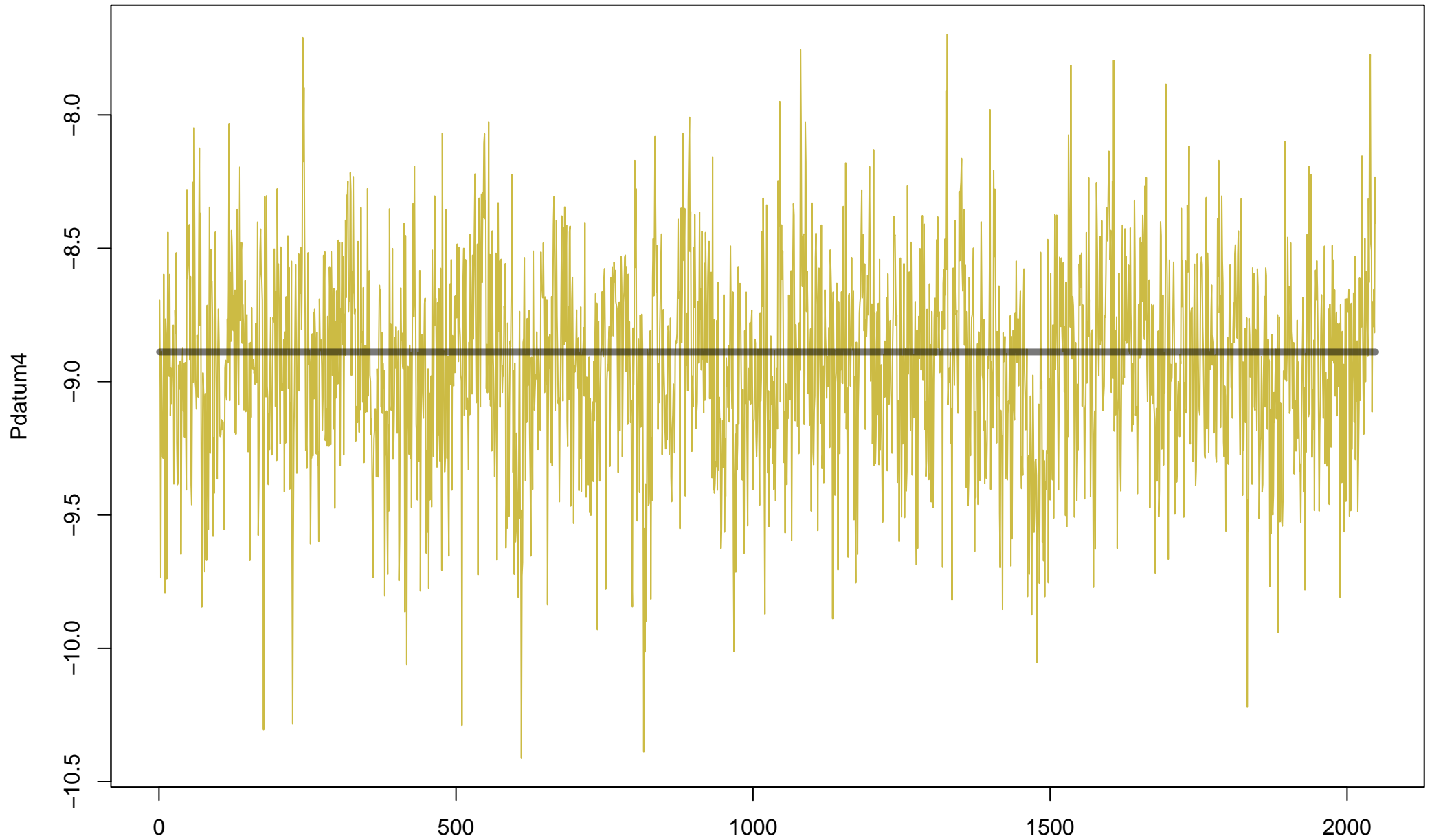
**Pdatum3**  
**ESS = 751 | BMK = 0.03 | MCSE(6.27) = 2.94 | stat: TRUE | burn: 0 | rel.err: -0.417**



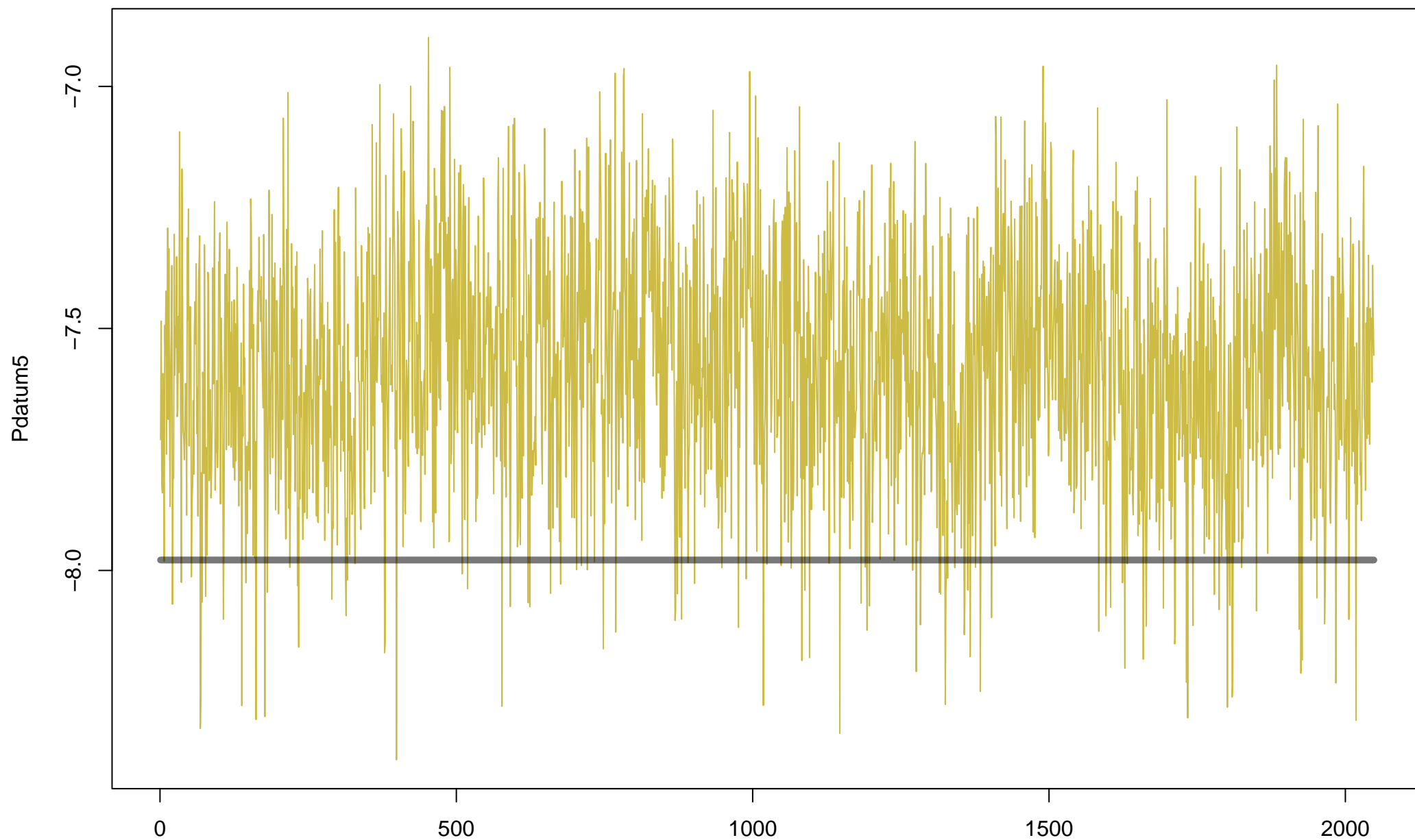


**Pdatum4**

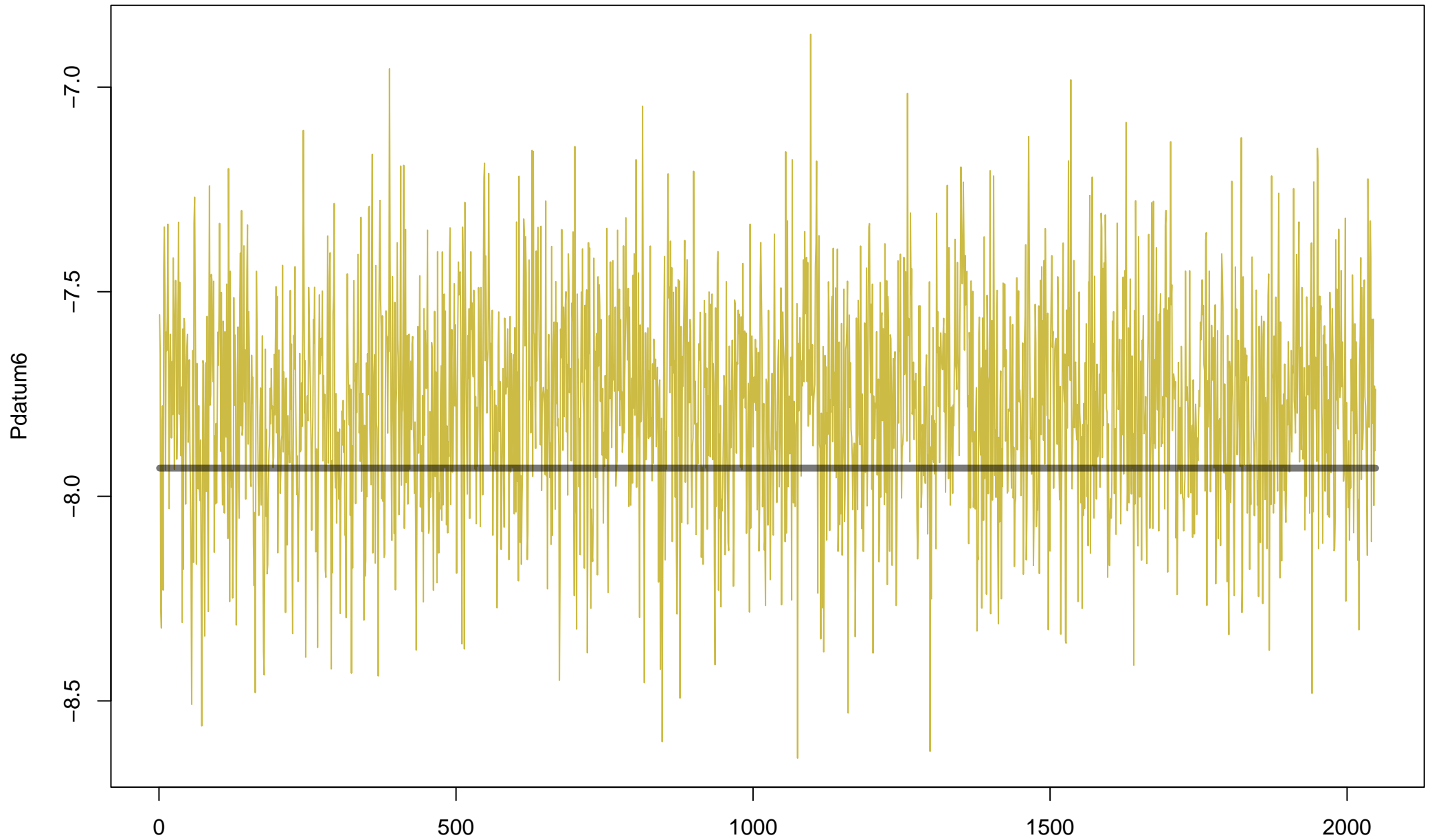
**ESS = 722 | BMK = 0.0568 | MCSE(6.27) = 3.99 | stat: TRUE | burn: 0 | rel.err: 0.0464**



**Pdatum5**  
**ESS = 293 | BMK = 0.0528 | MCSE(6.27) = 4.16 | stat: TRUE | burn: 0 | rel.err: 1.43**

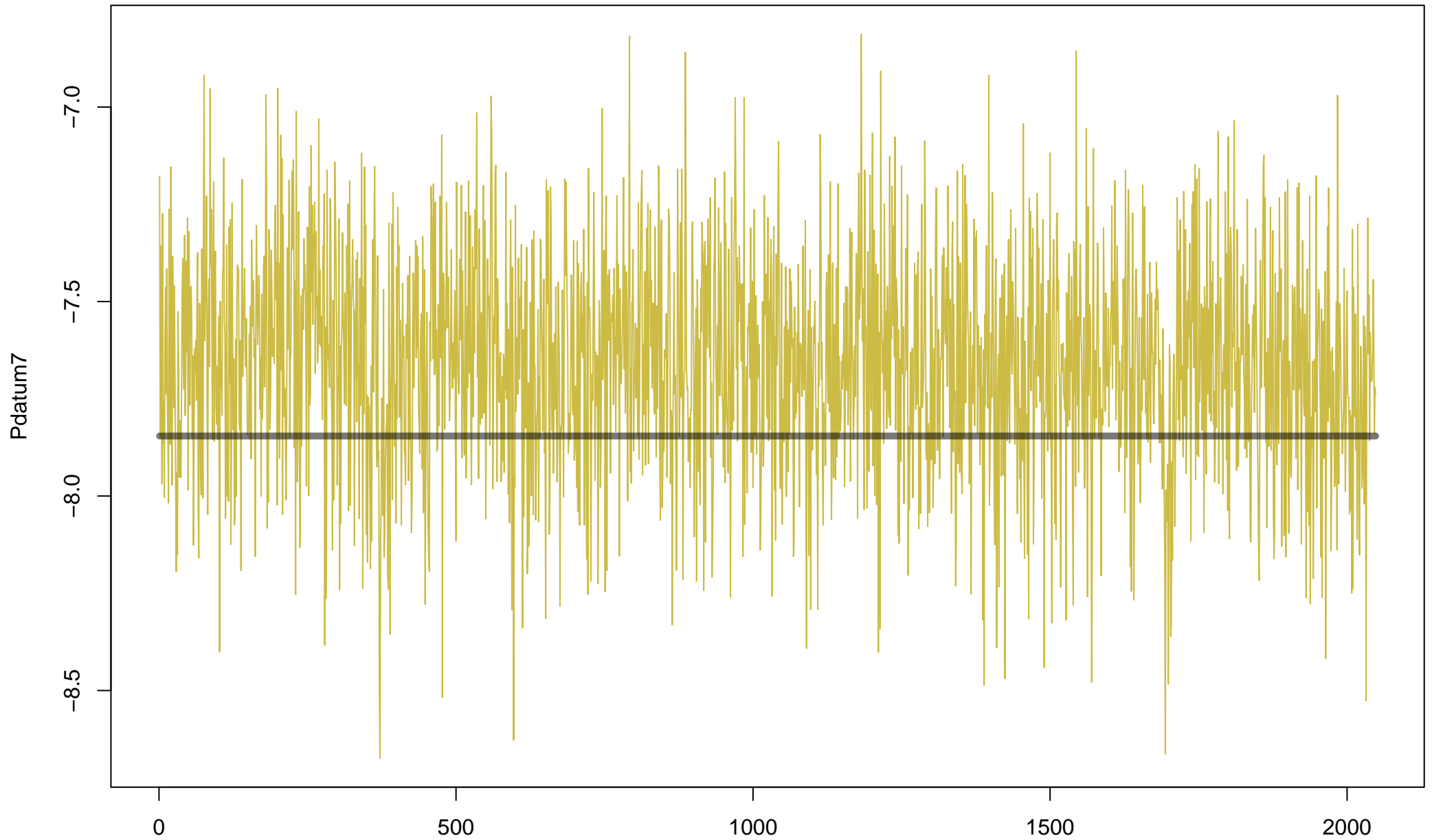


**Pdatum6**  
**ESS = 1610 | BMK = 0.038 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0 | rel.err: 0.675**



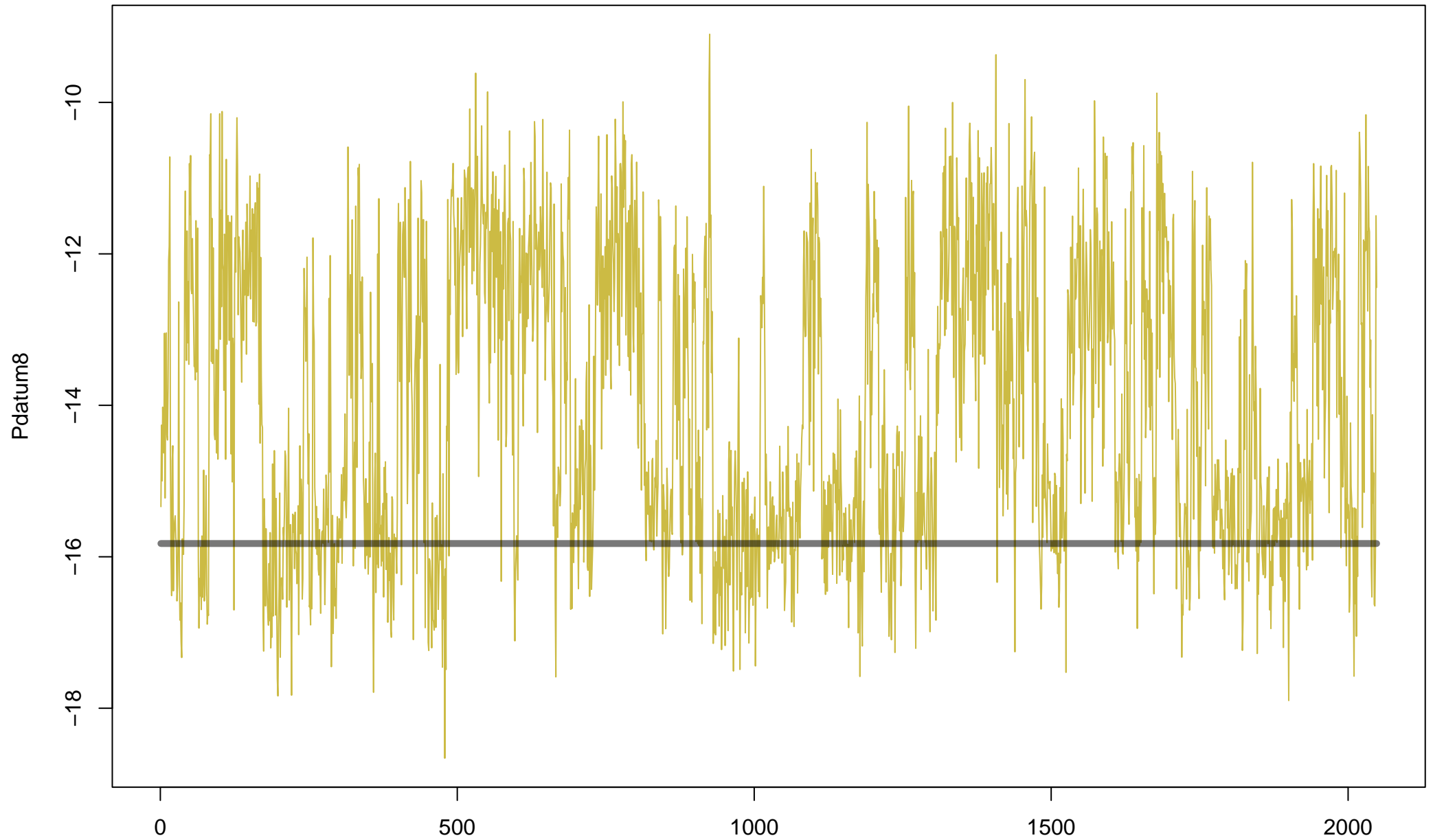
**Pdatum7**

**ESS = 1700 | BMK = 0.0723 | MCSE(6.27) = 3.08 | stat: FALSE | burn: 0 | rel.err: 0.73**

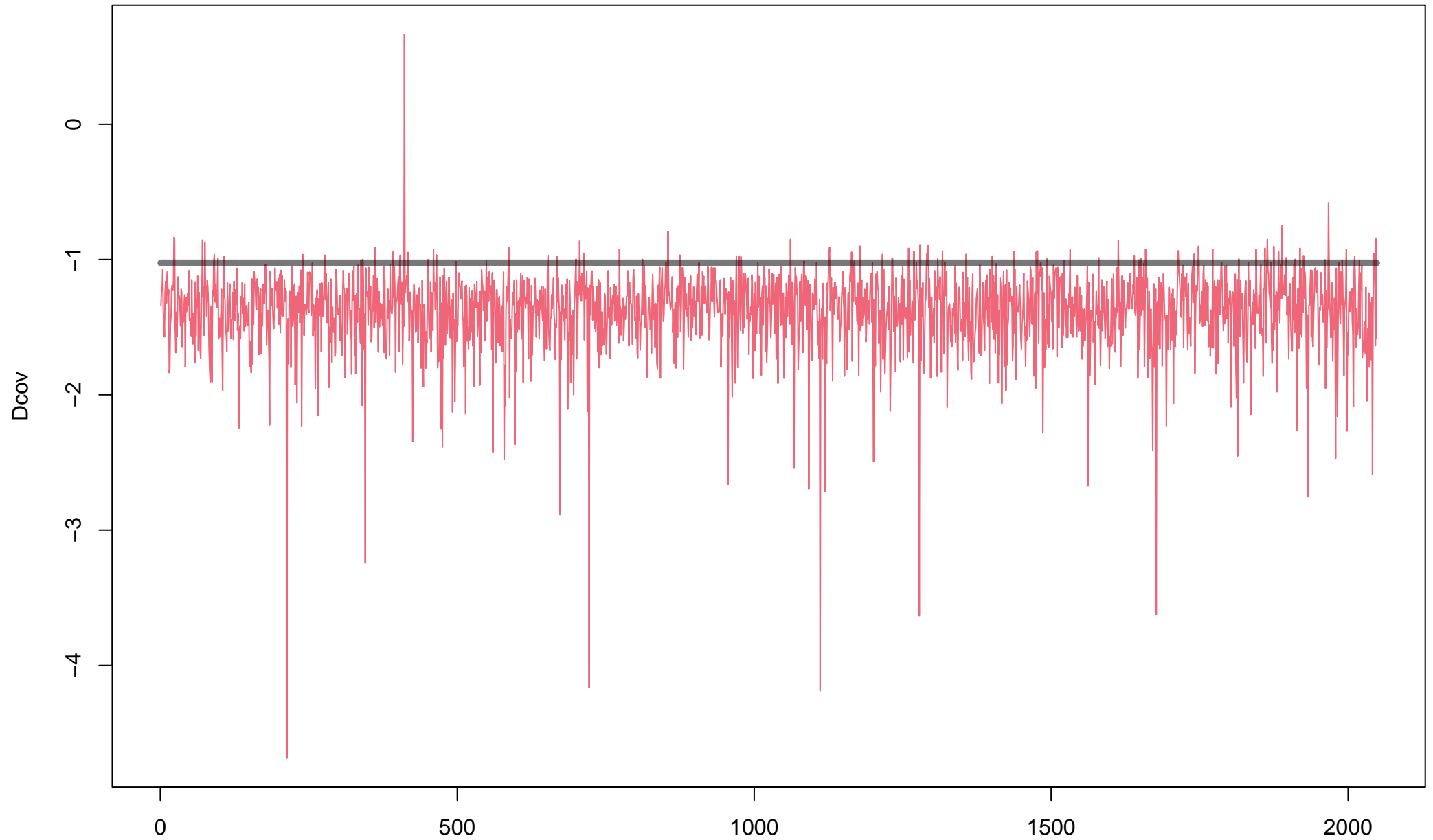


**Pdatum8**

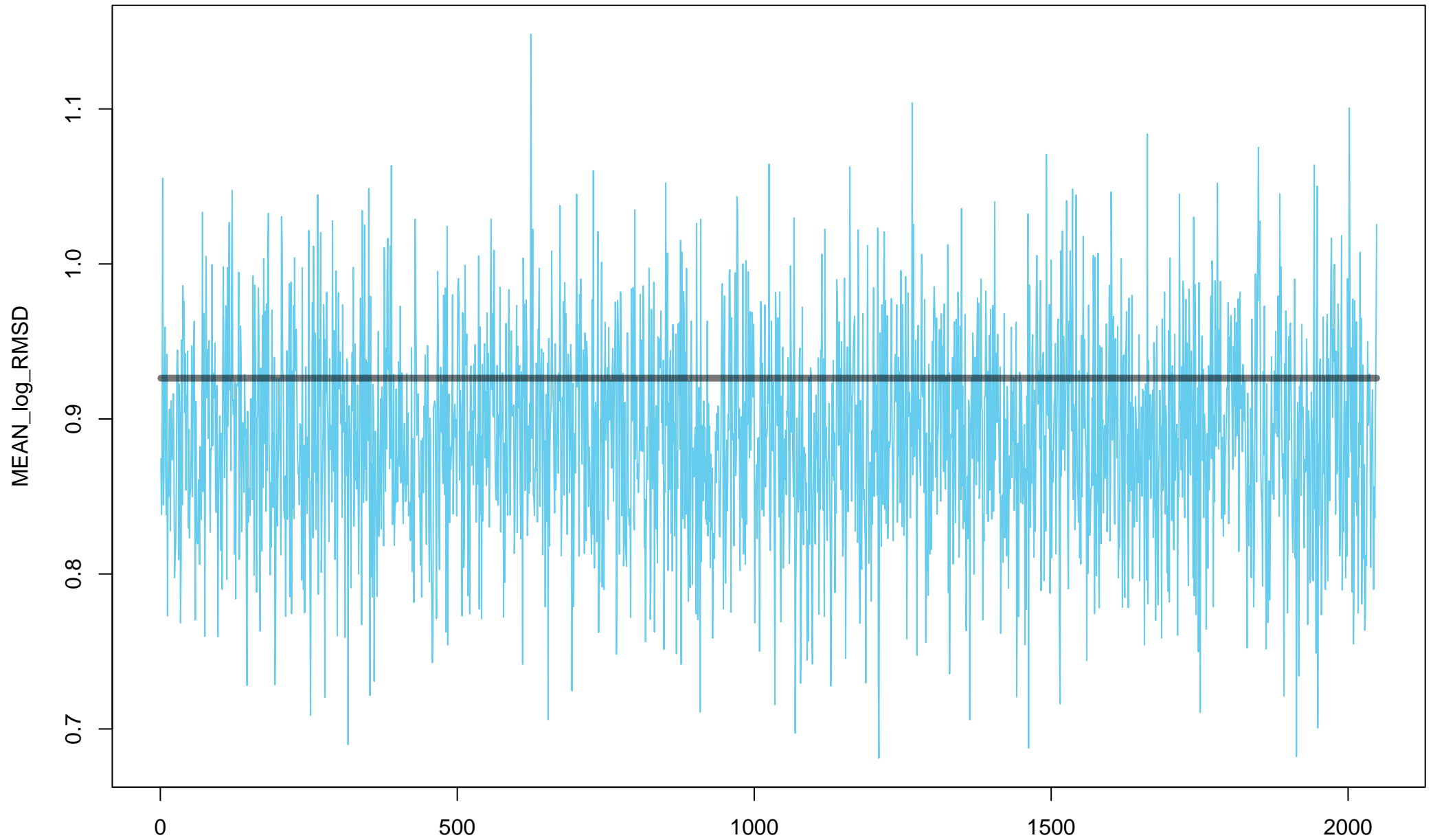
**ESS = 213 | BMK = 0.103 | MCSE(6.27) = 5.89 | stat: TRUE | burn: 816 | rel.err: 0.497**



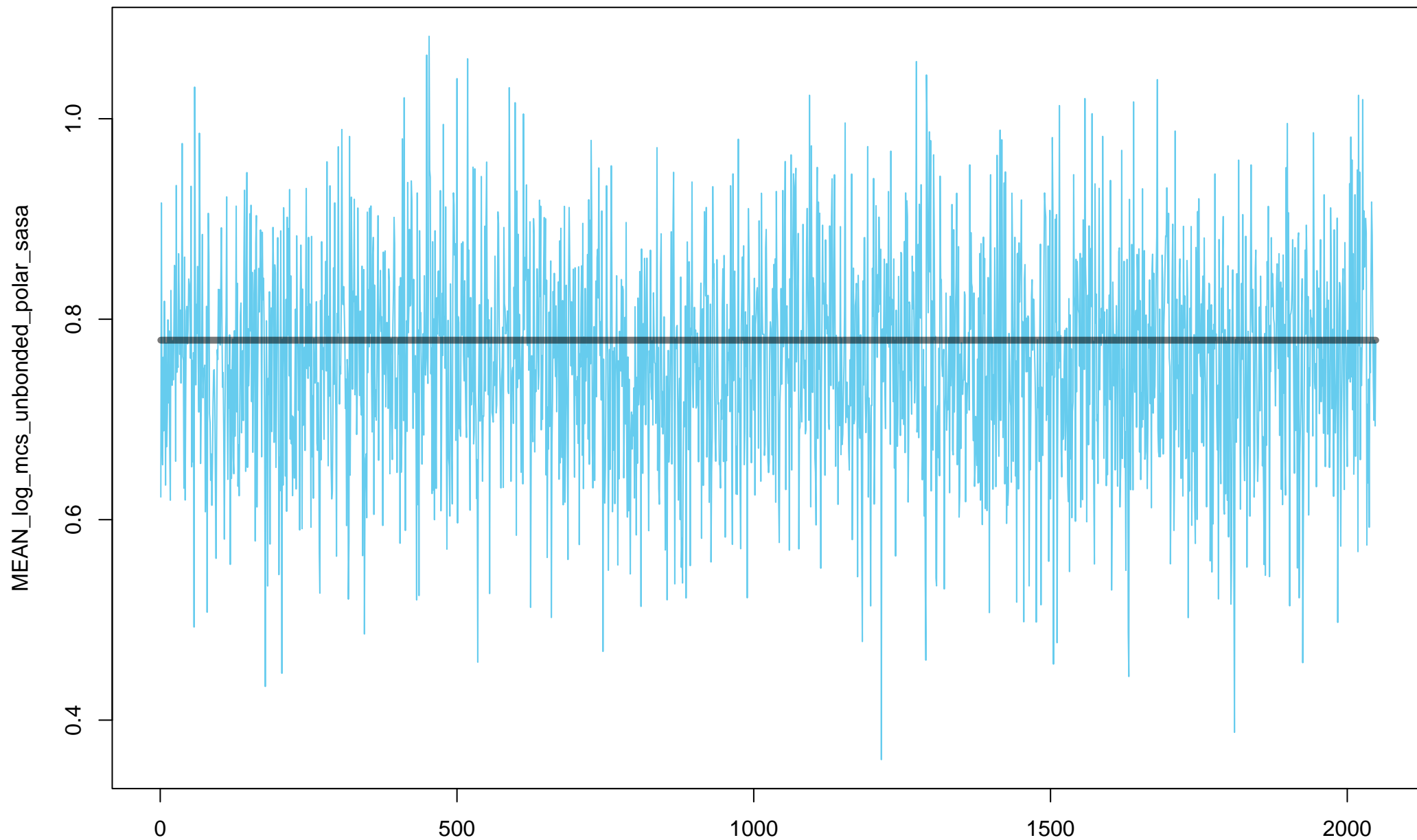
**Dcov**  
**ESS = 2050 | BMK = 0.0733 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: 1.26**



**MEAN\_log\_RMSD**  
**ESS = 1800 | BMK = 0.045 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: -0.549**



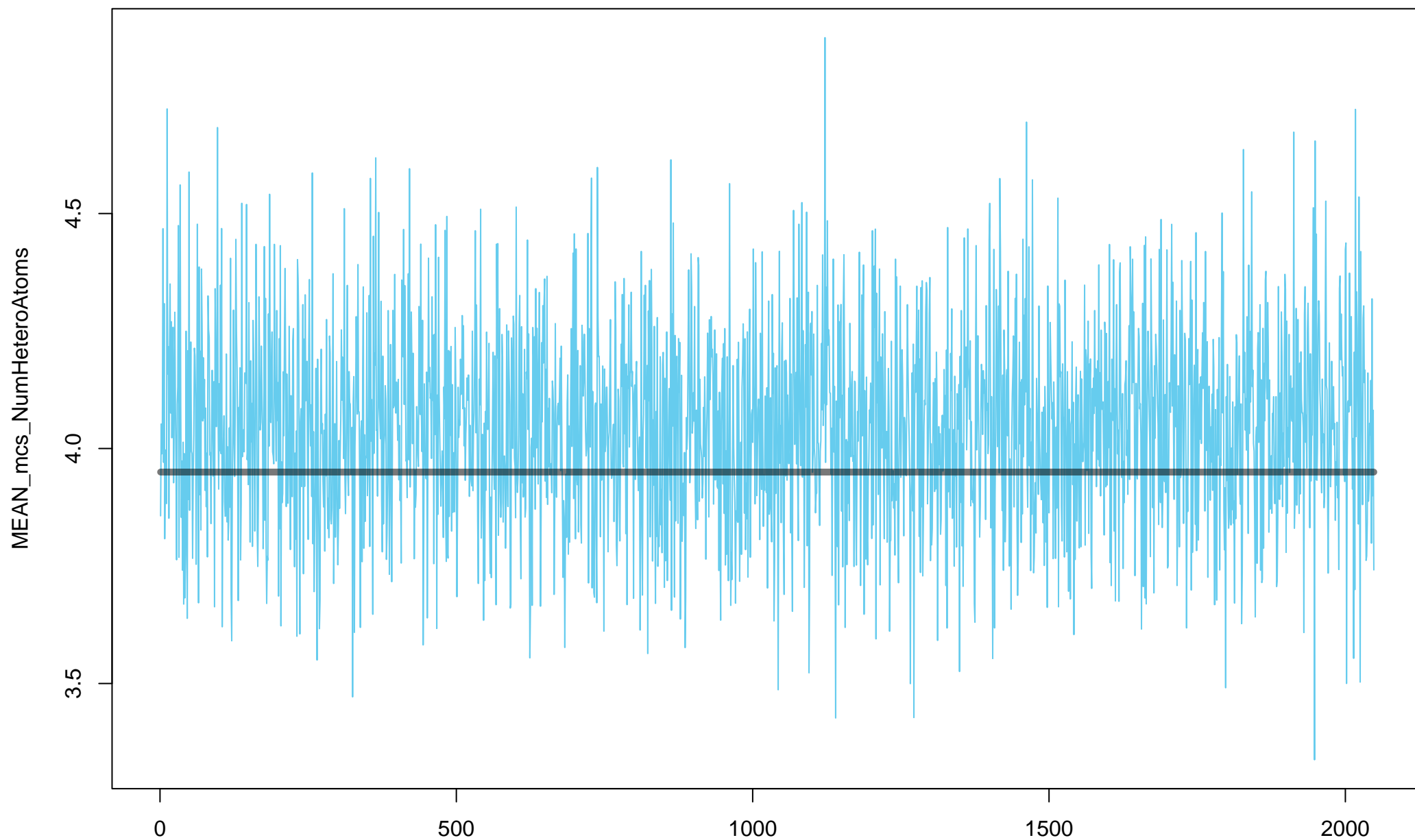
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1920 | BMK = 0.0489 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: -0.186**



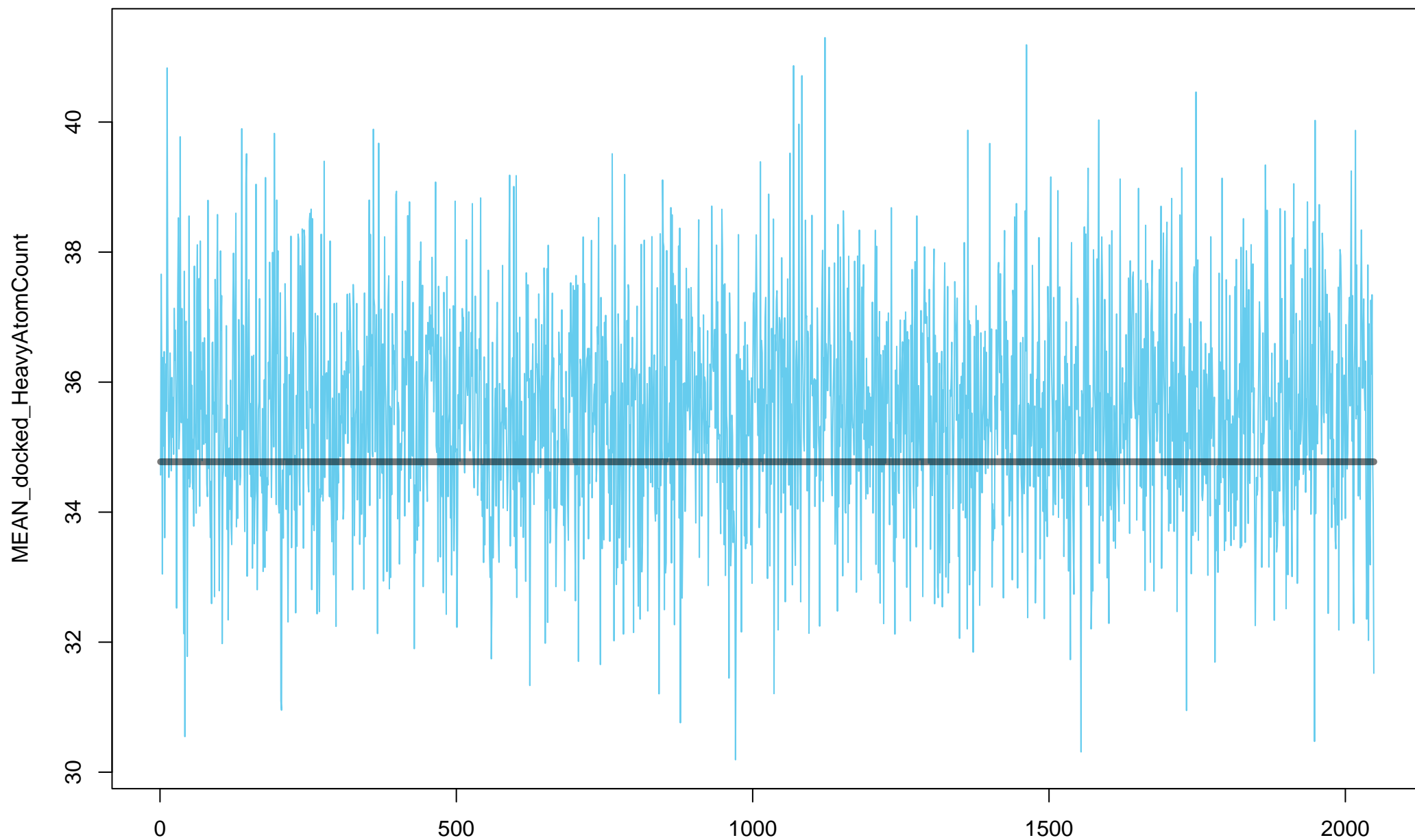


# MEAN\_mcs\_NumHeteroAtoms

ESS = 2050 | BMK = 0.0515 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: 0.454

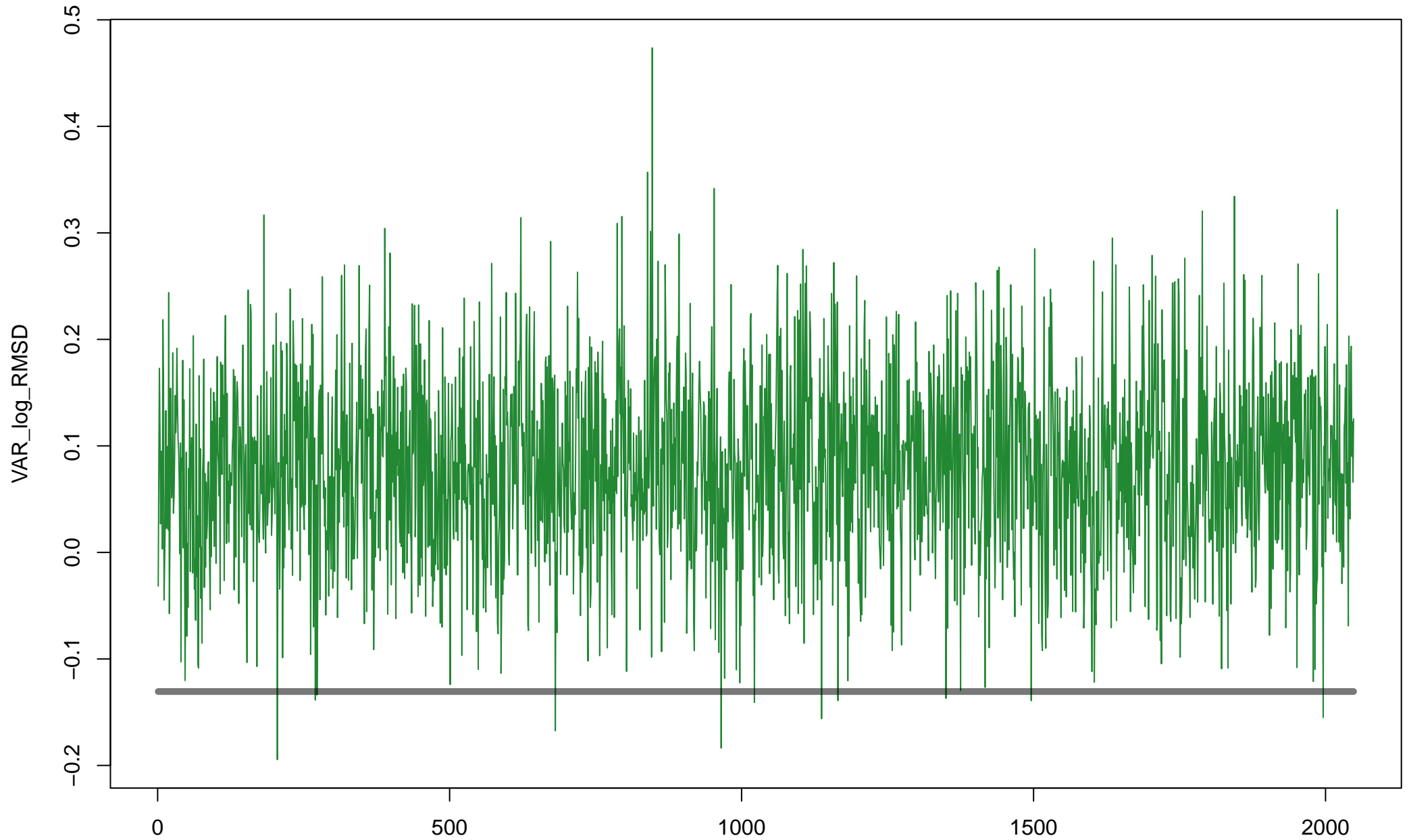


**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0392 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.478**

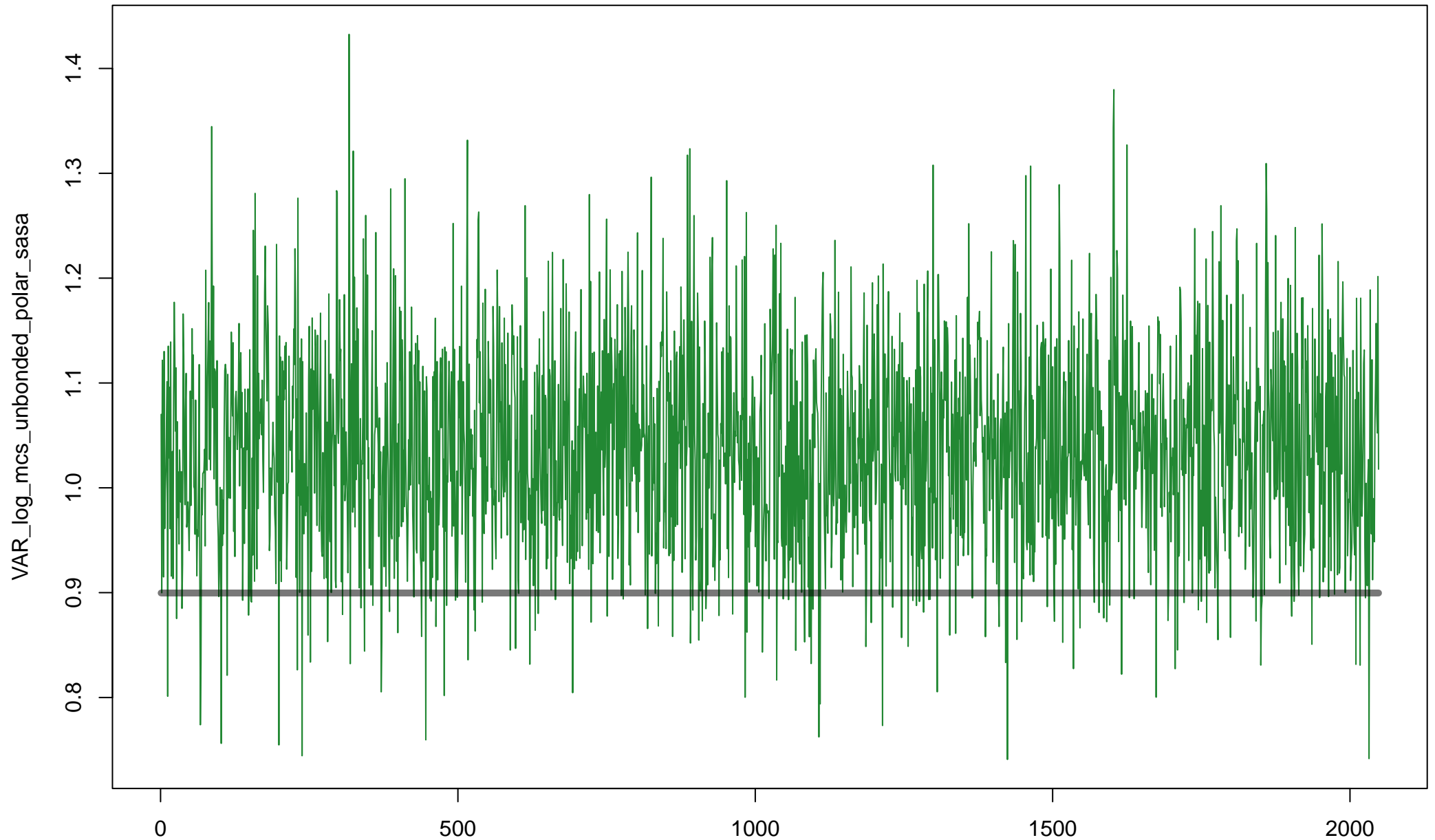


# VAR\_log\_RMSD

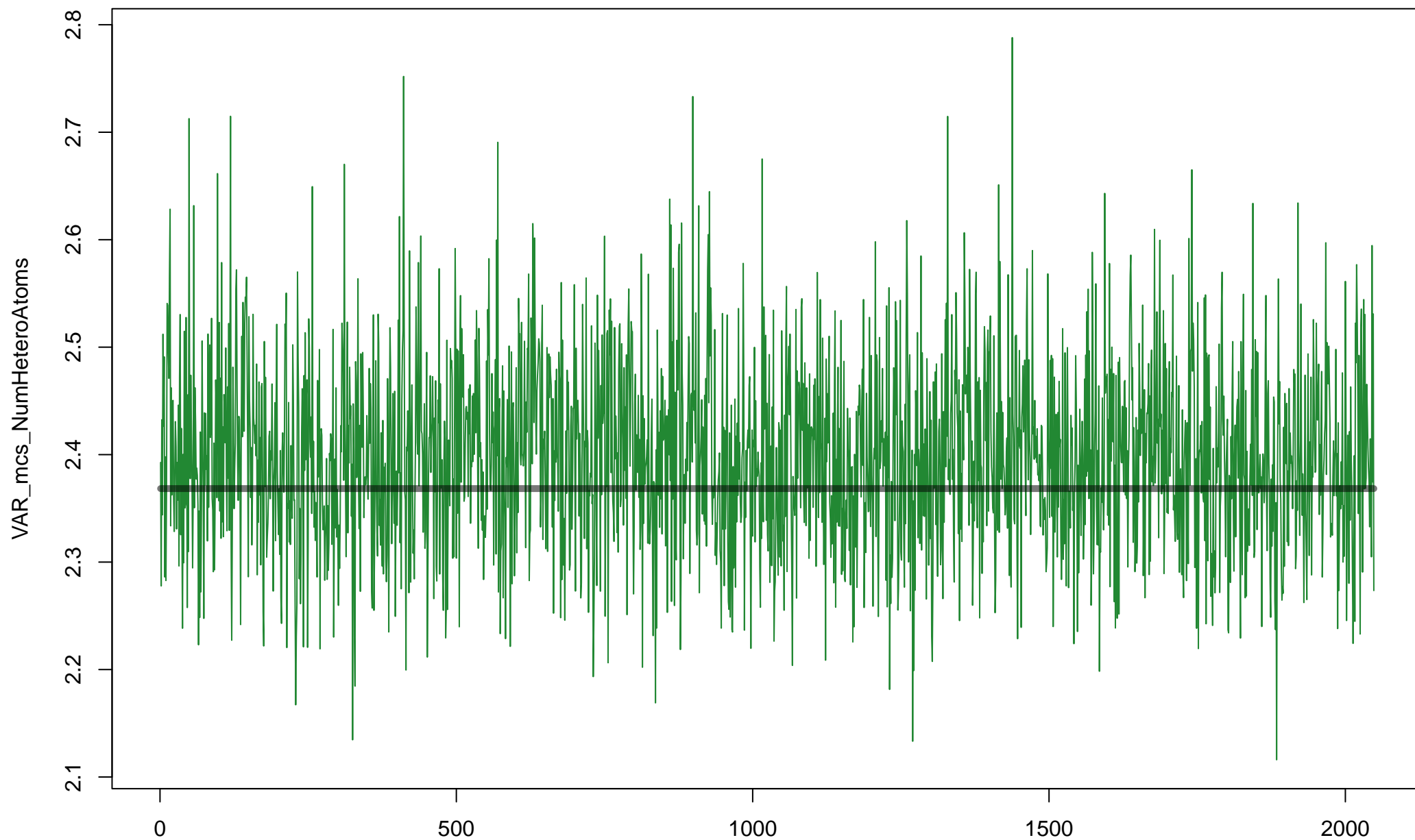
ESS = 2050 | BMK = 0.0569 | MCSE(6.27) = 2.61 | stat: FALSE | burn: 0 | rel.err: 2.26



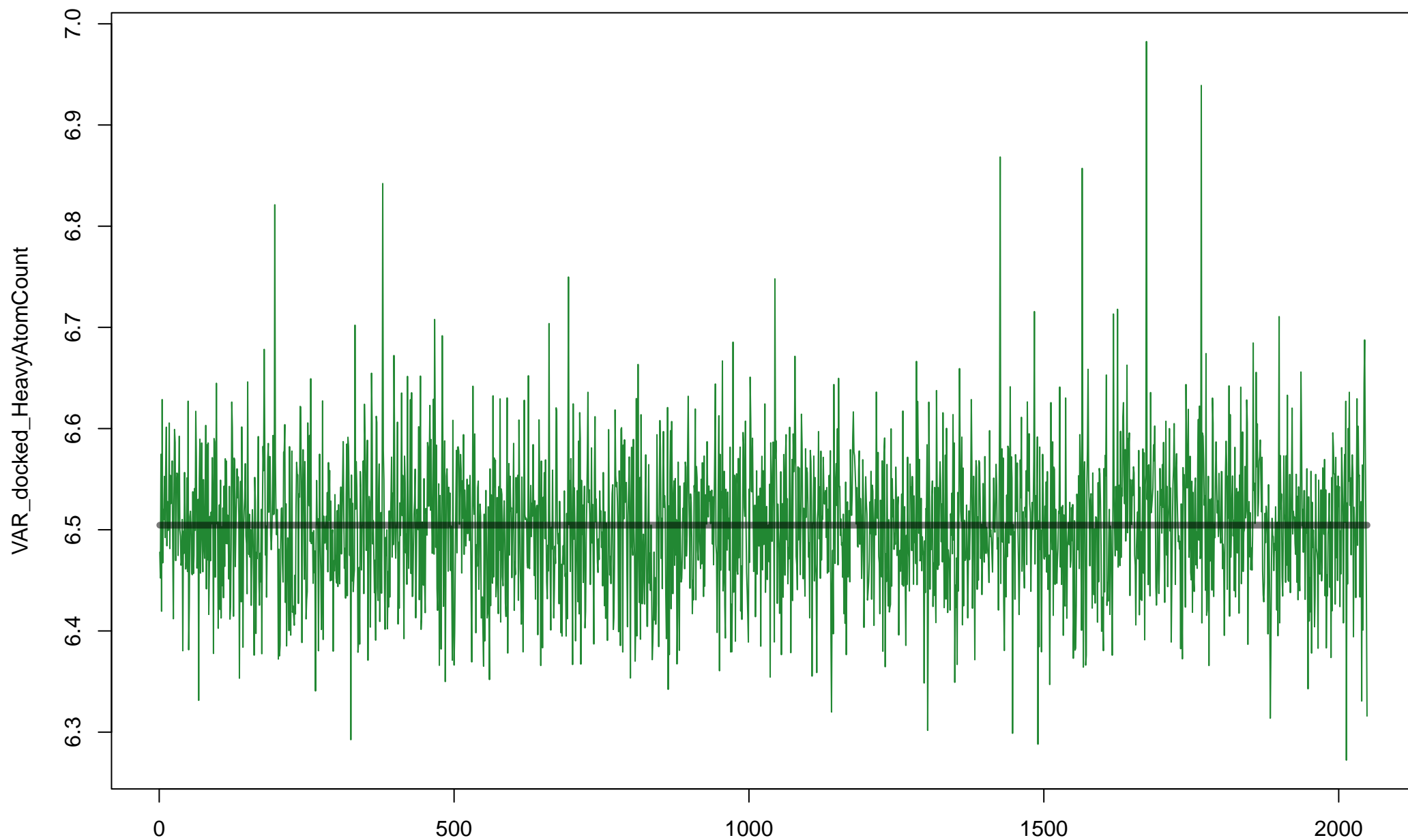
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0368 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 1.36**



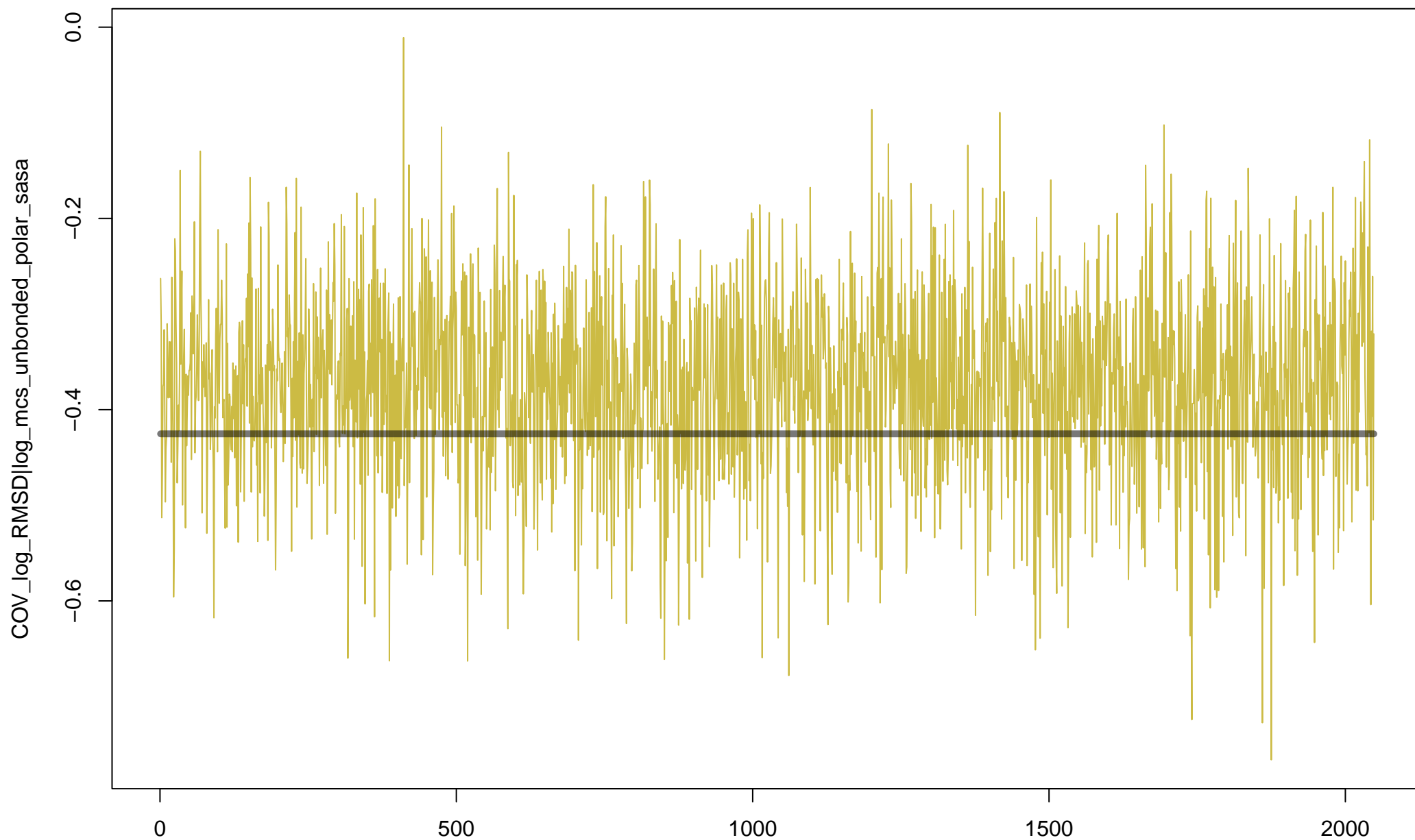
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1340 | BMK = 0.0485 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: 0.383**



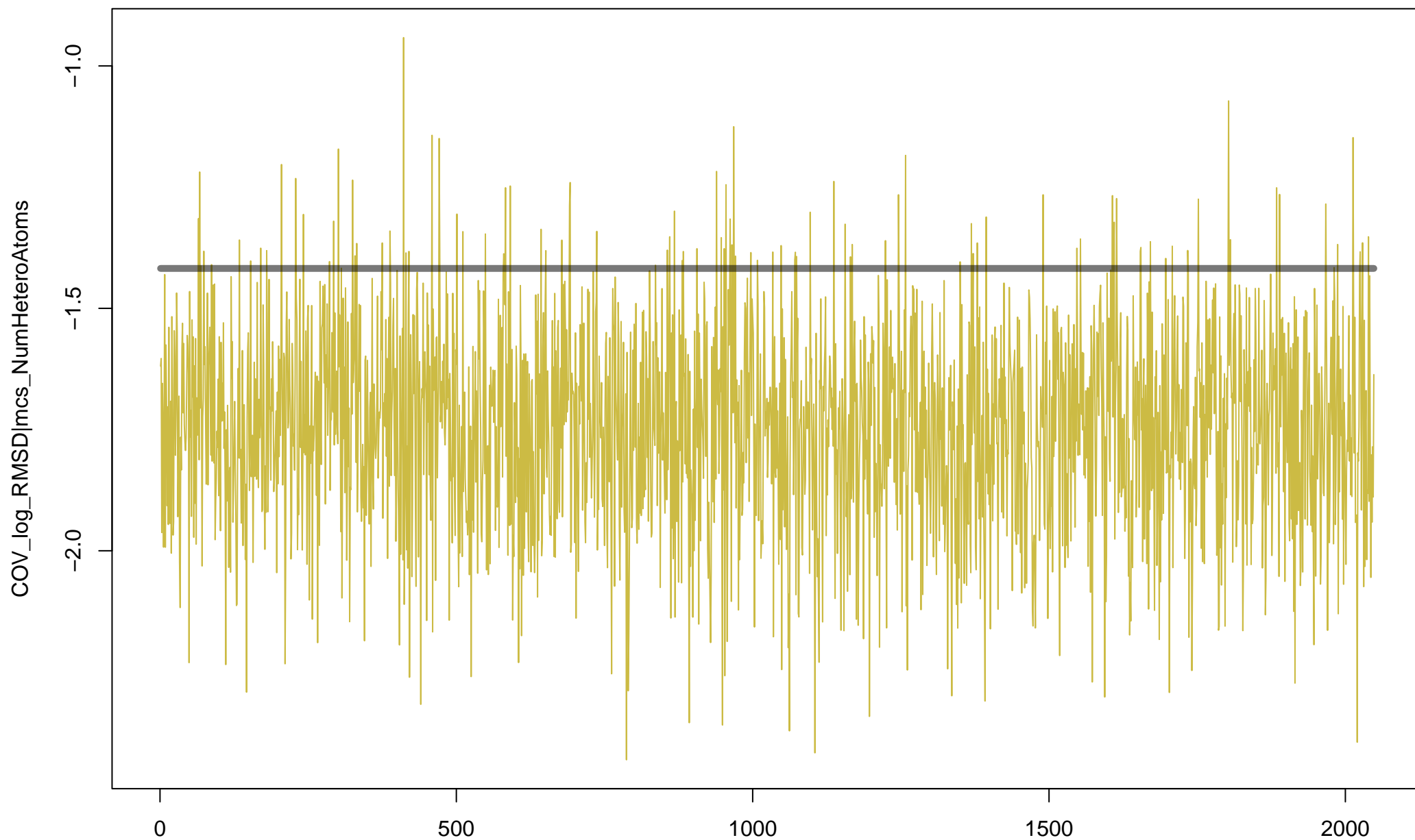
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0719 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: 0.0355**



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1910 | BMK = 0.0552 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: 0.531**

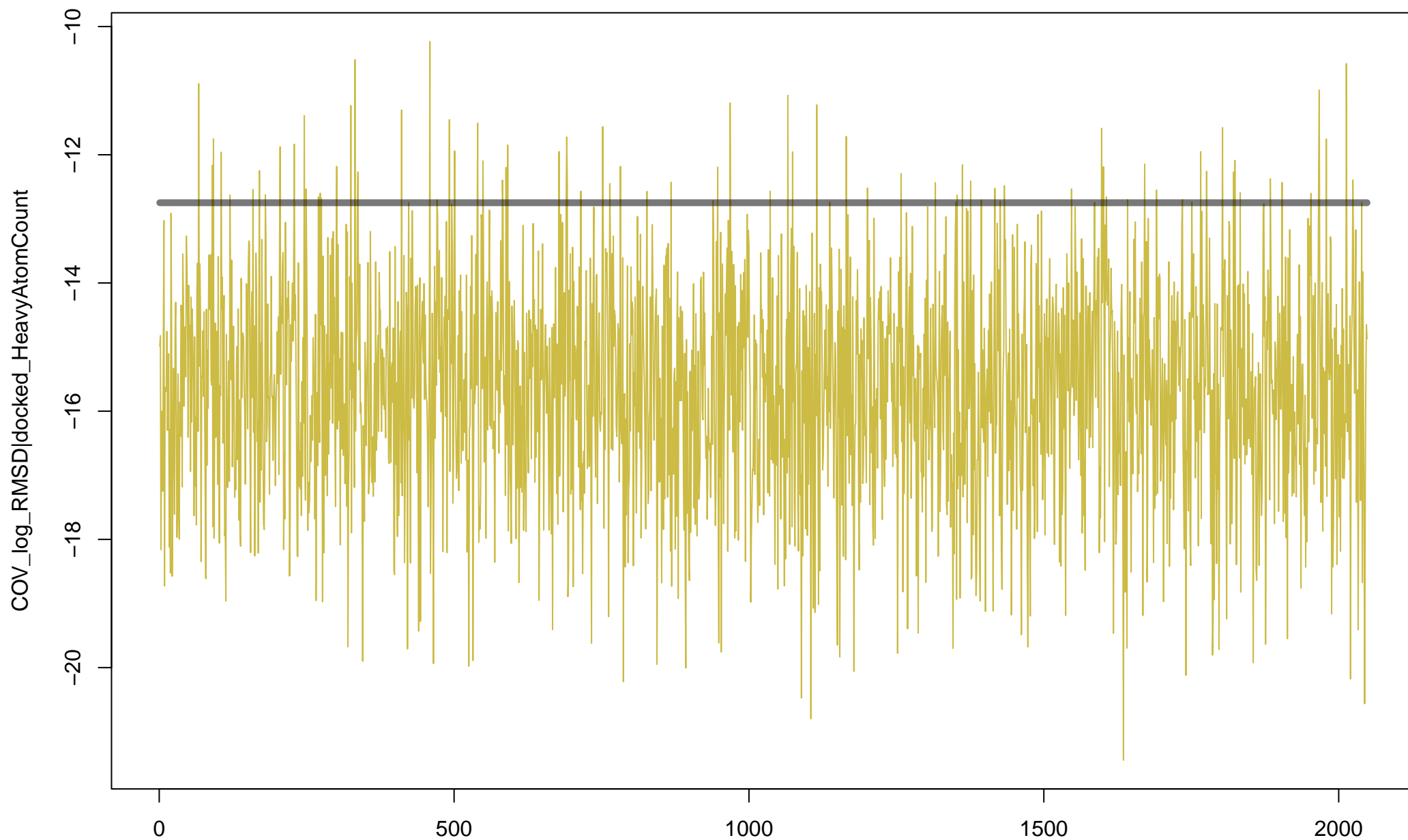


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | rel.err: -1.59**

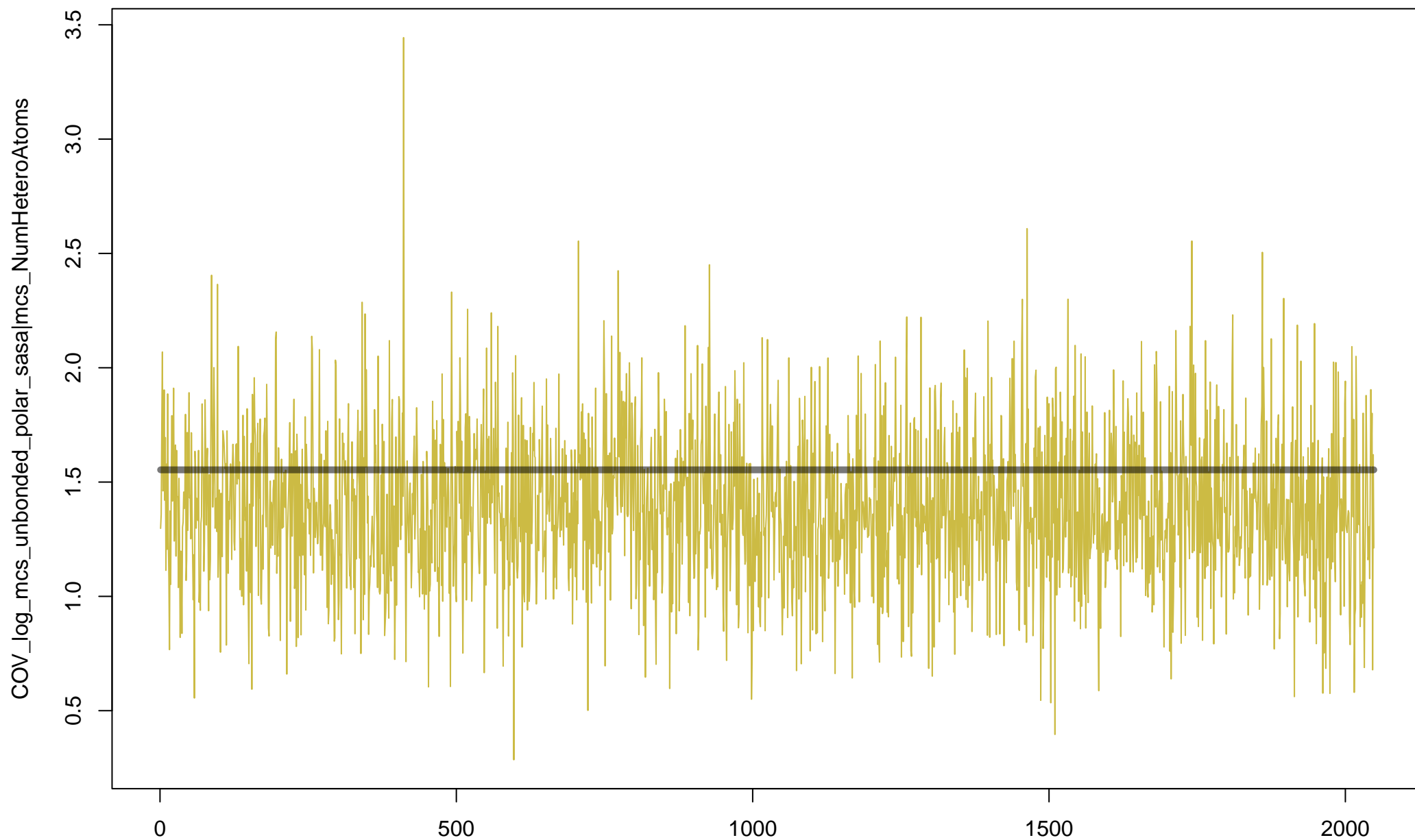




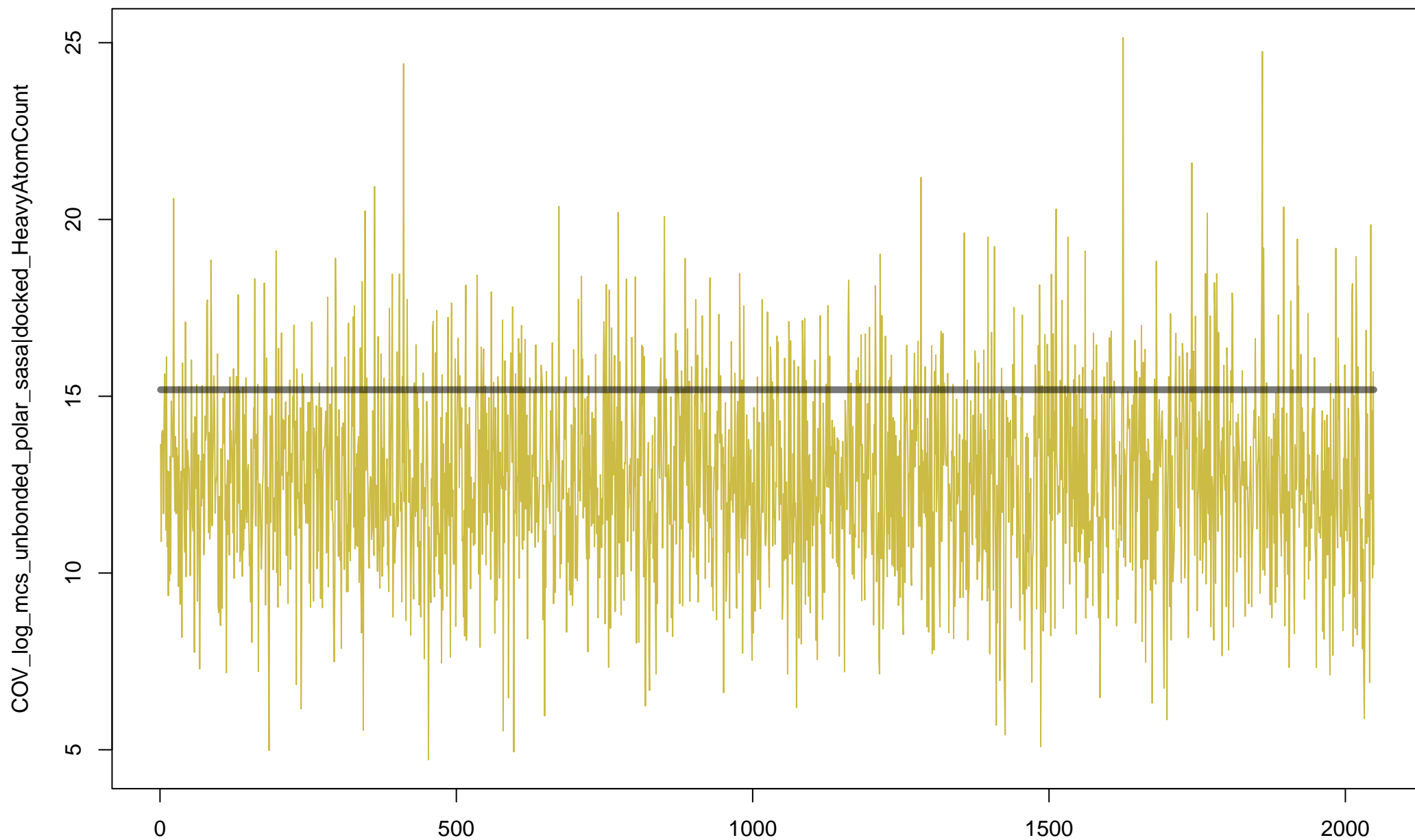
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0498 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: -1.74**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0526 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | rel.err: -0.501**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0393 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: -0.964**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.058 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: 0.428**

