

-- STATS maxD --

min ESS = 124.545184068825

max BMK = 0.145444094212262

max MCSE = 7.2625187490411

all stationary: FALSE

burn: 0

max rel.err.: 2.14226721846499

-- STATS 1D --

min ESS = 2743.6687133882

max BMK = 0.0551534242319819

max MCSE = 1.79135581289609

all stationary: TRUE

burn: 0

max rel.err.: 2.26513201569589

-- STATS 2D --

min ESS = 3860.97436205184

max BMK = 0.0434234763655092

max MCSE = 1.75249267071461

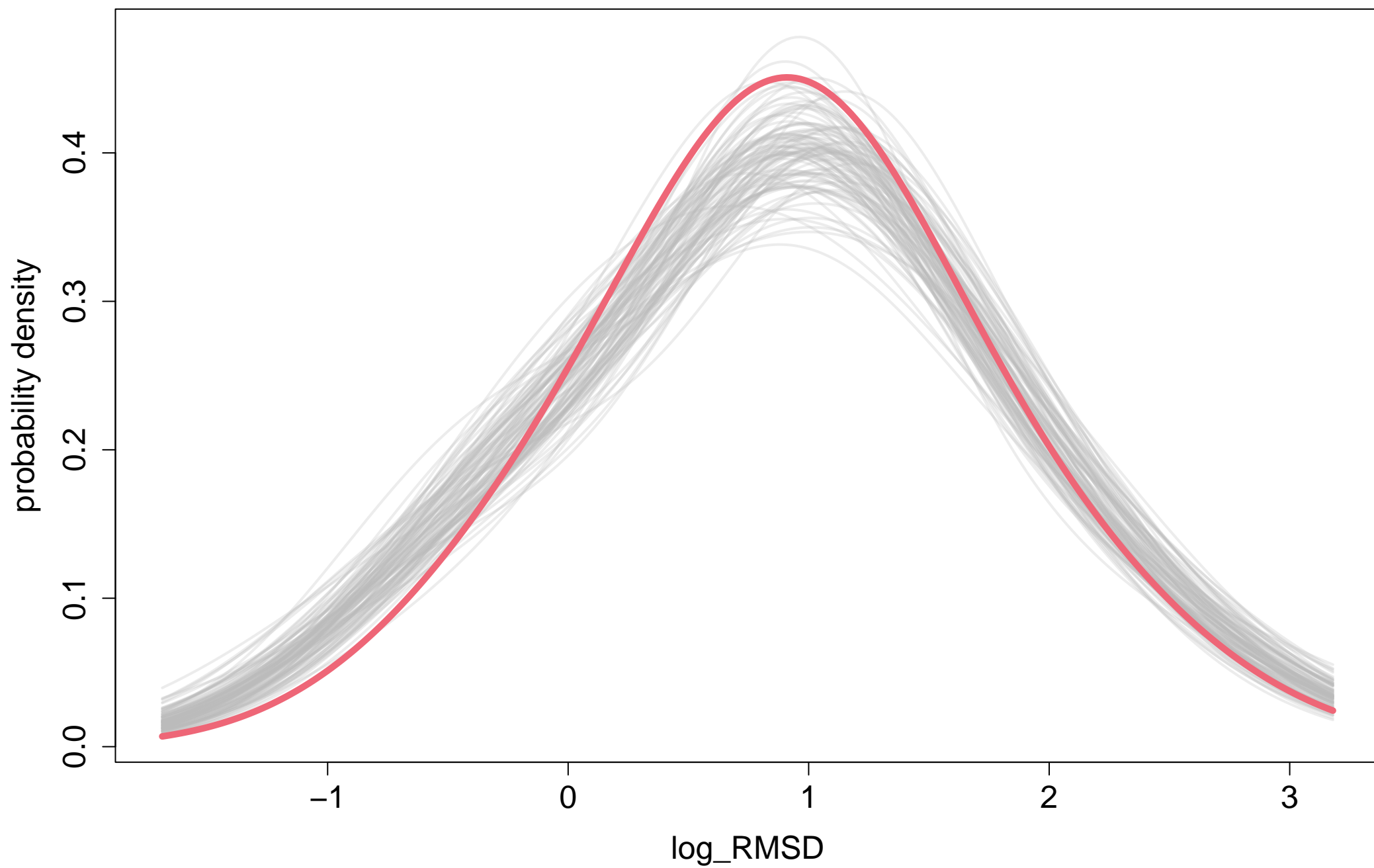
all stationary: TRUE

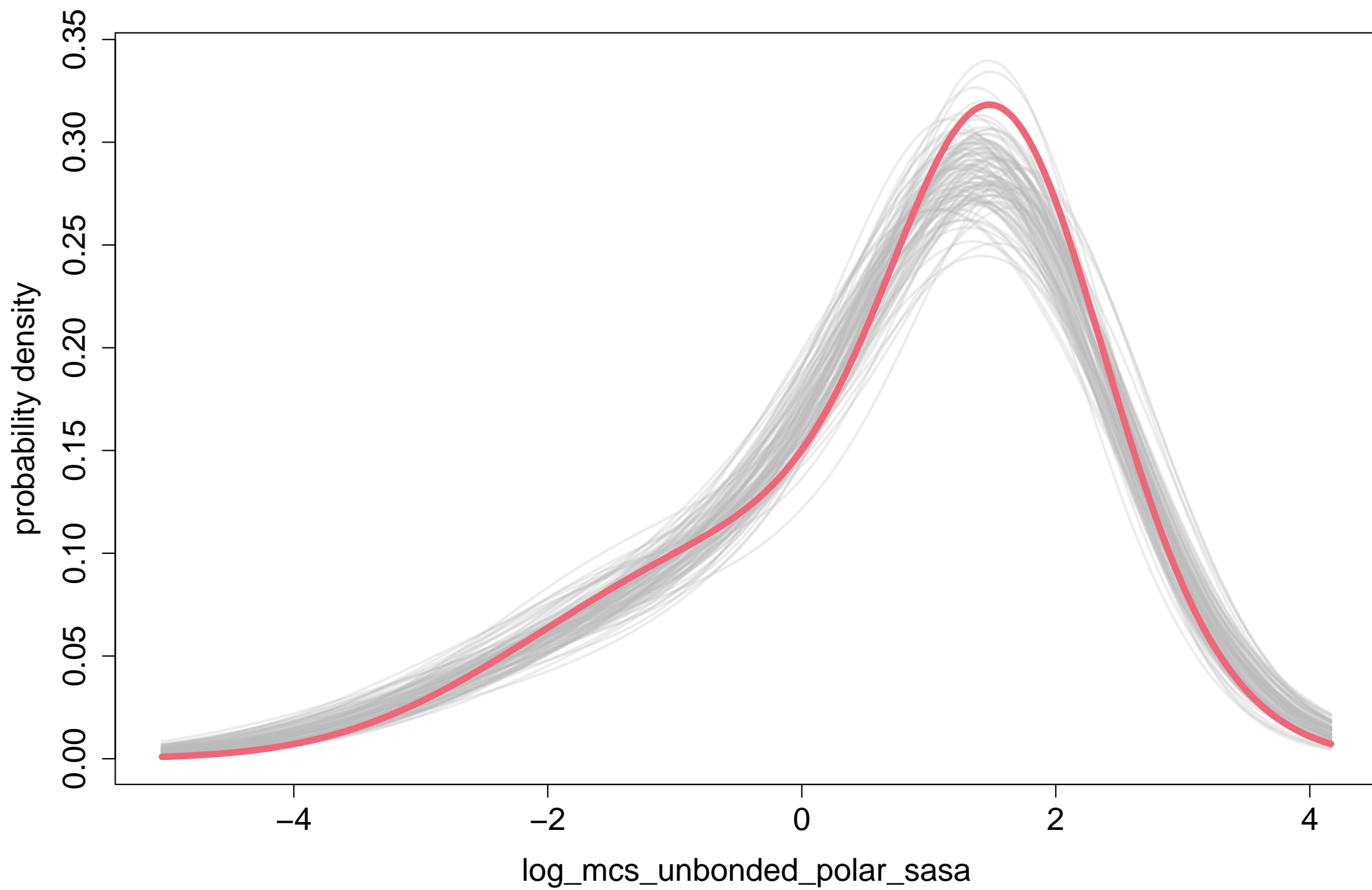
burn: 0

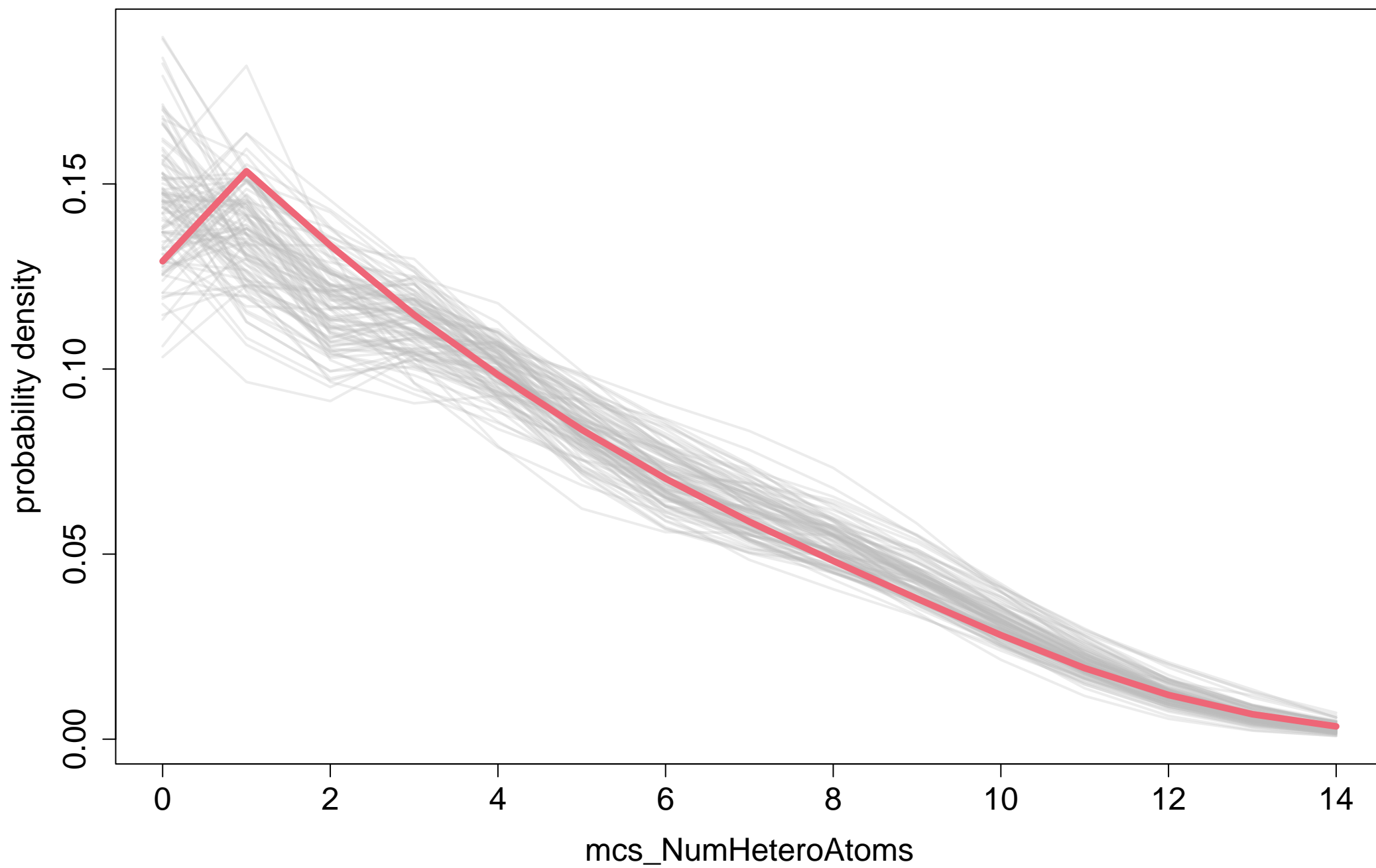
max rel.err.: 1.75152693069975

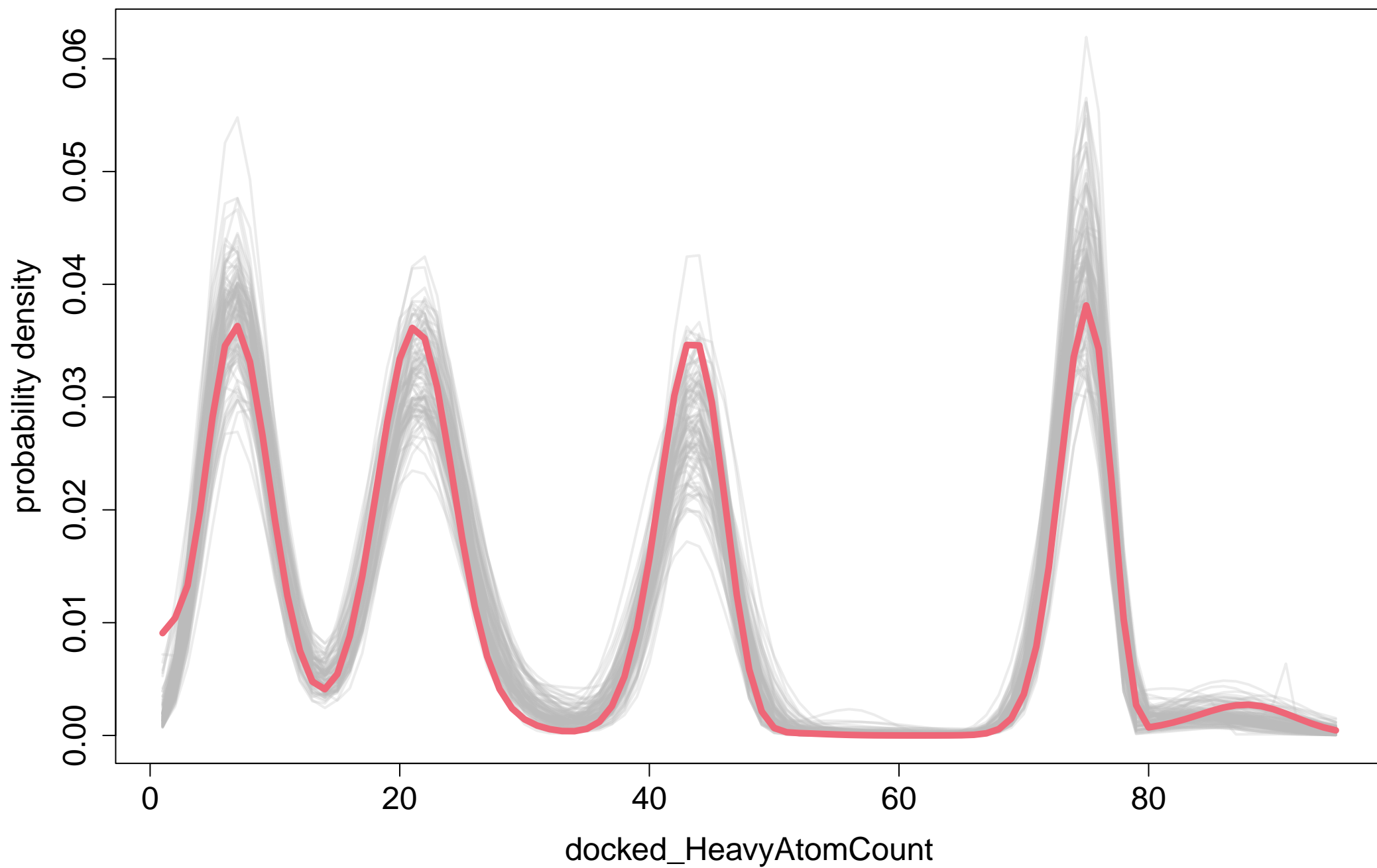
Occupied clusters: 9 of 16

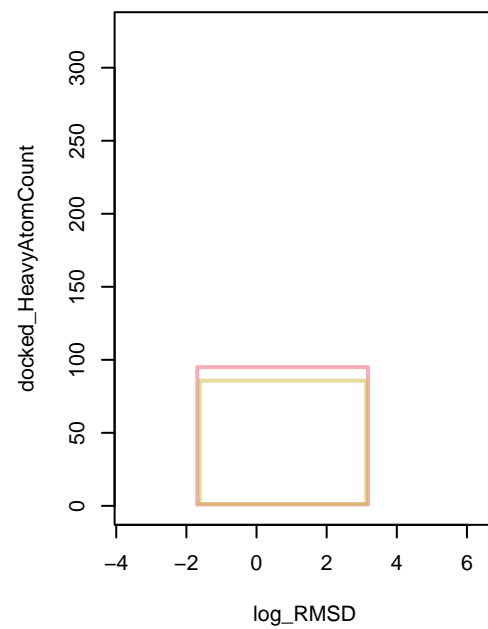
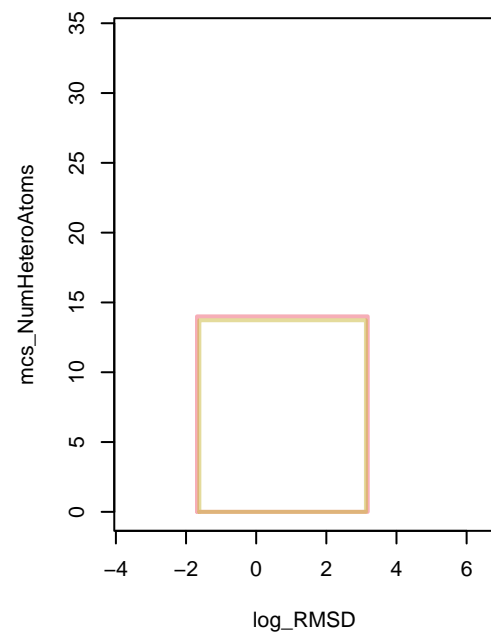
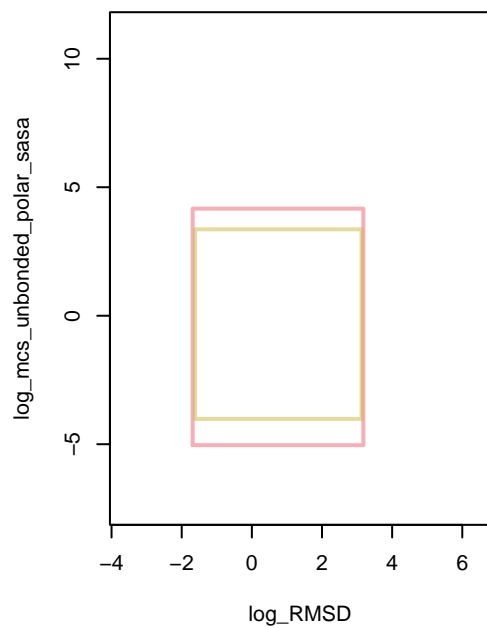
LL: -2160 +- 6.71



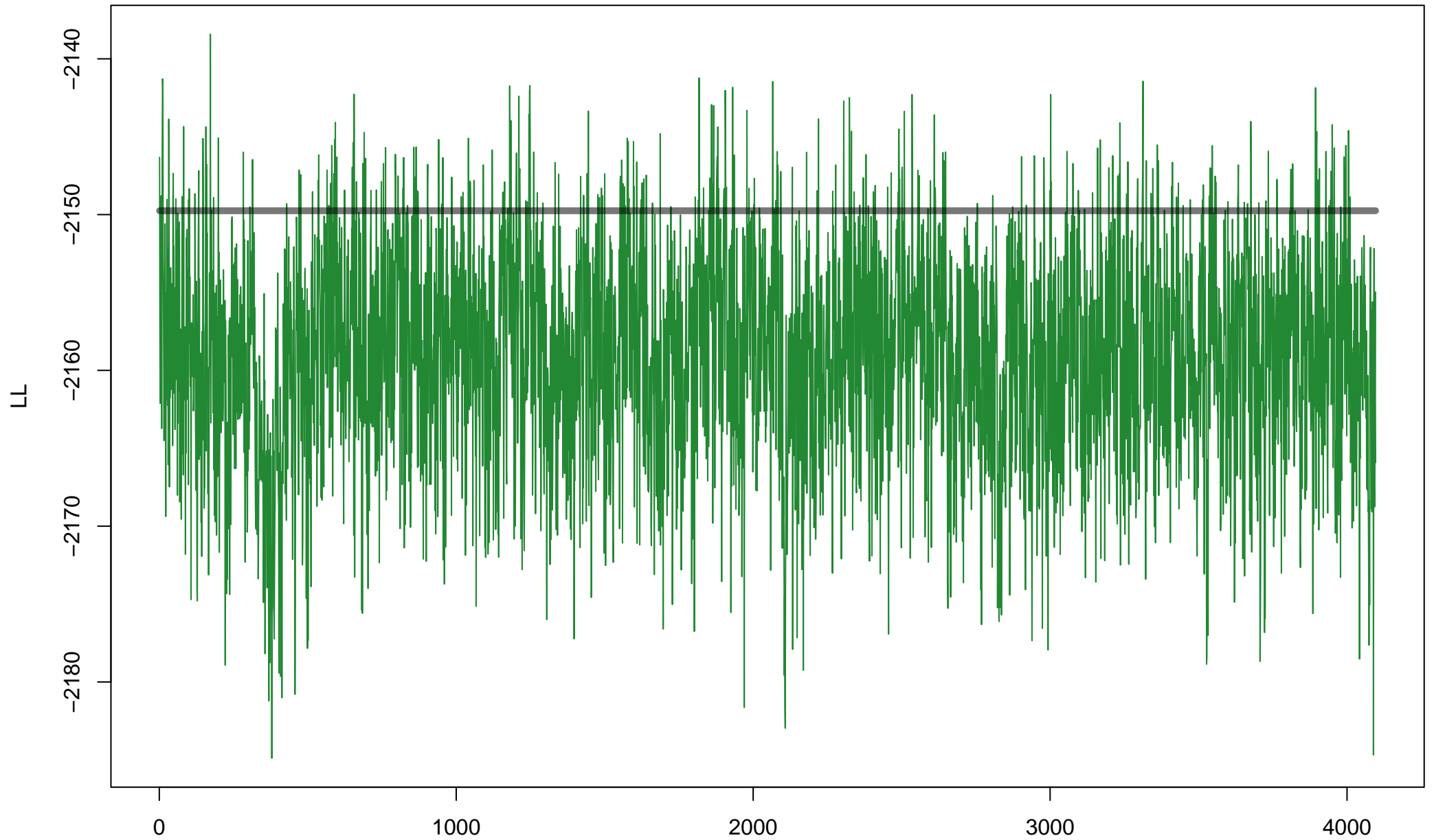




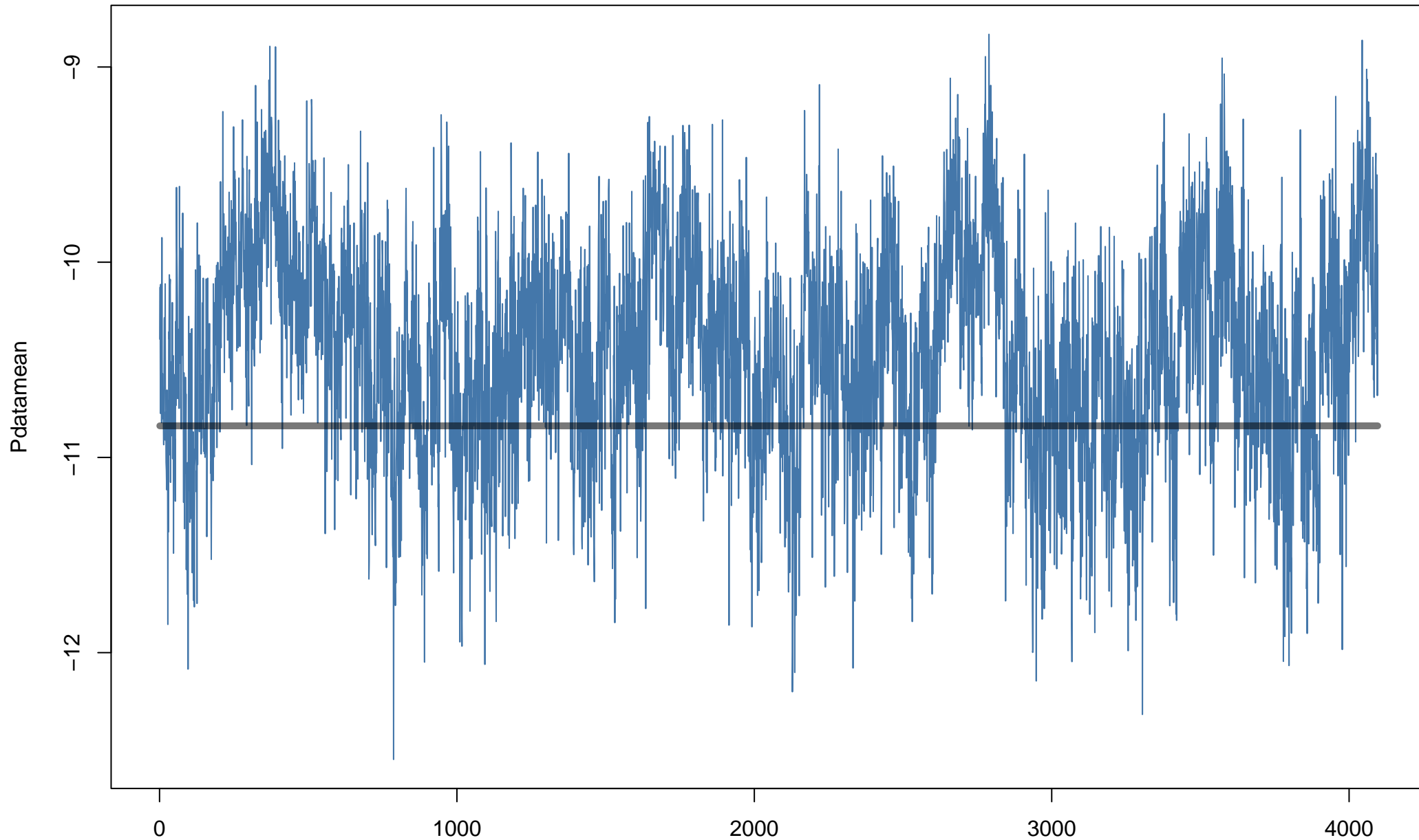




LL

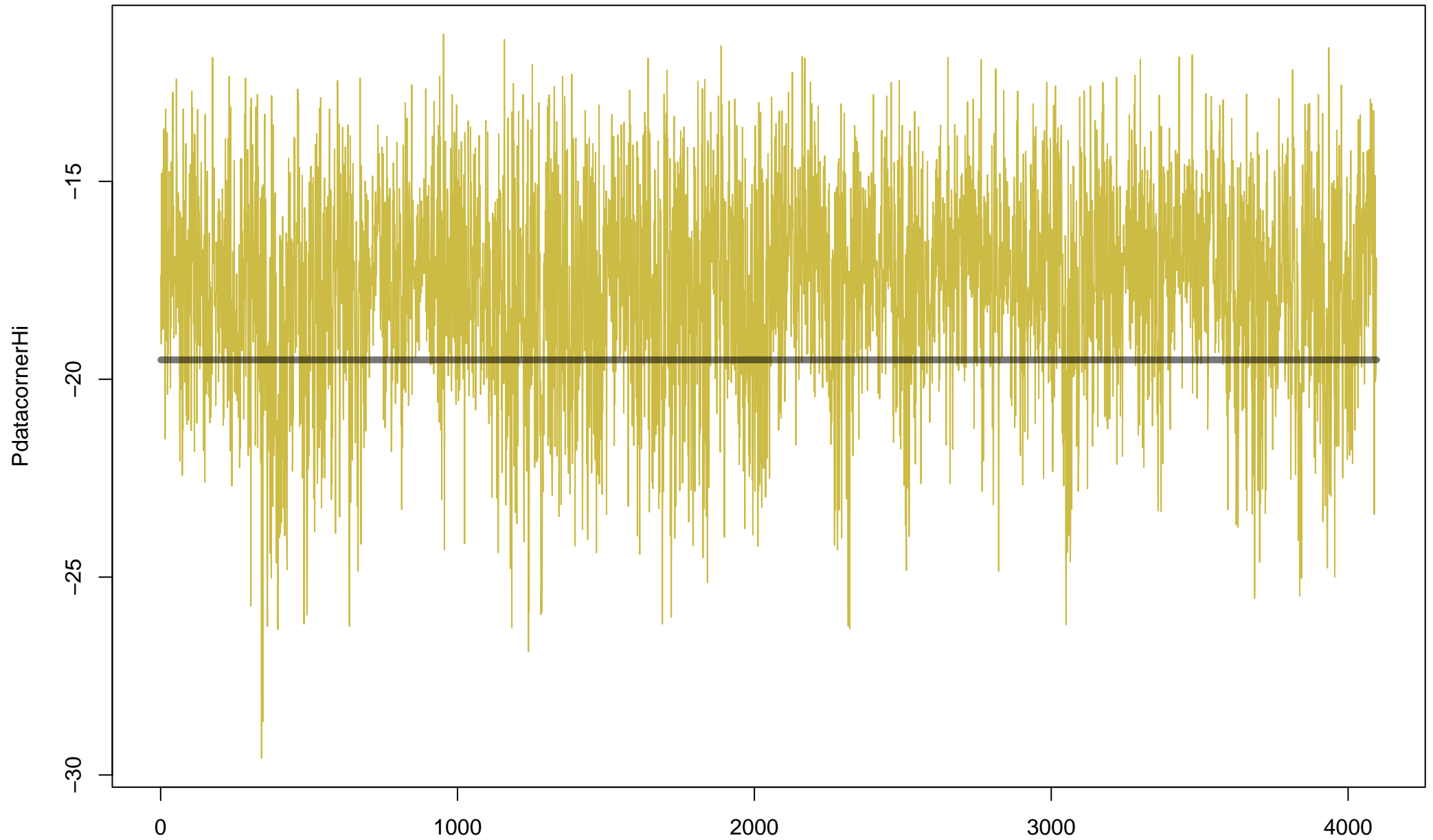


**Pdatamean**  
**ESS = 125 | BMK = 0.0718 | MCSE(6.27) = 7.26 | stat: FALSE | burn: 0 | rel.err: 0.744**



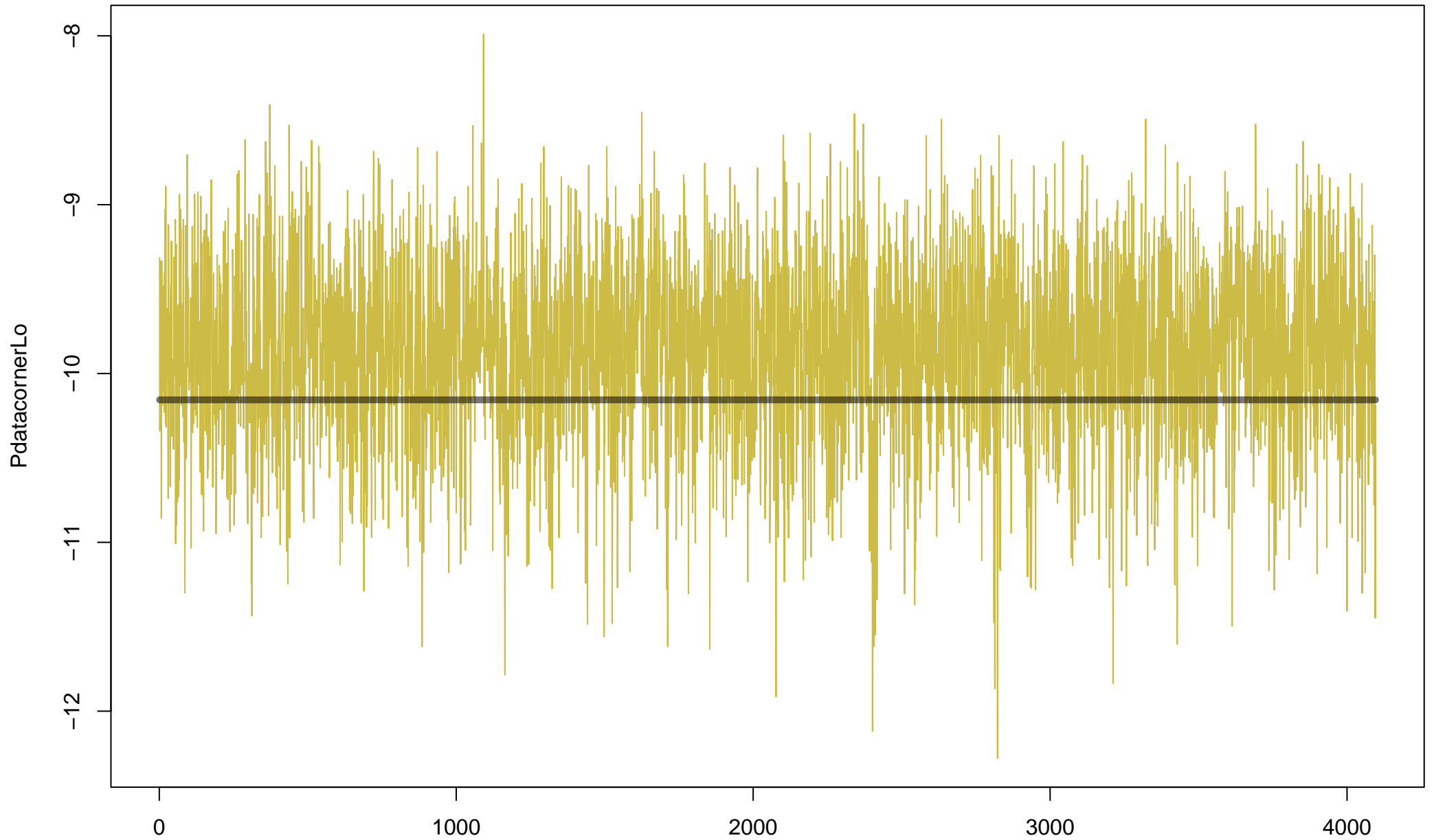


**PdatacornerHi**  
**ESS = 4100 | BMK = 0.145 | MCSE(6.27) = 1.53 | stat: TRUE | burn: 0 | rel.err: 0.309**

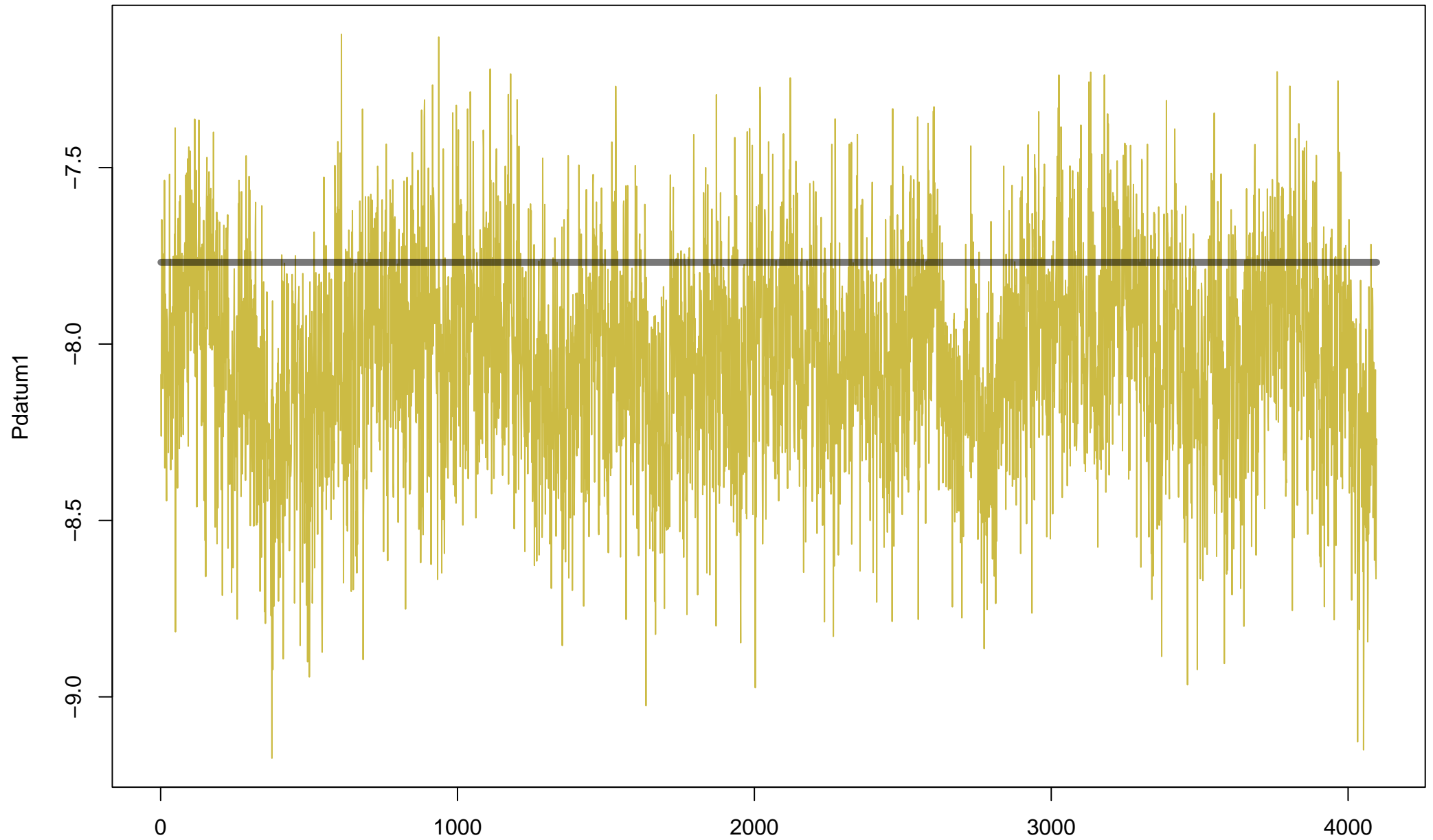


# PdatacornerLo

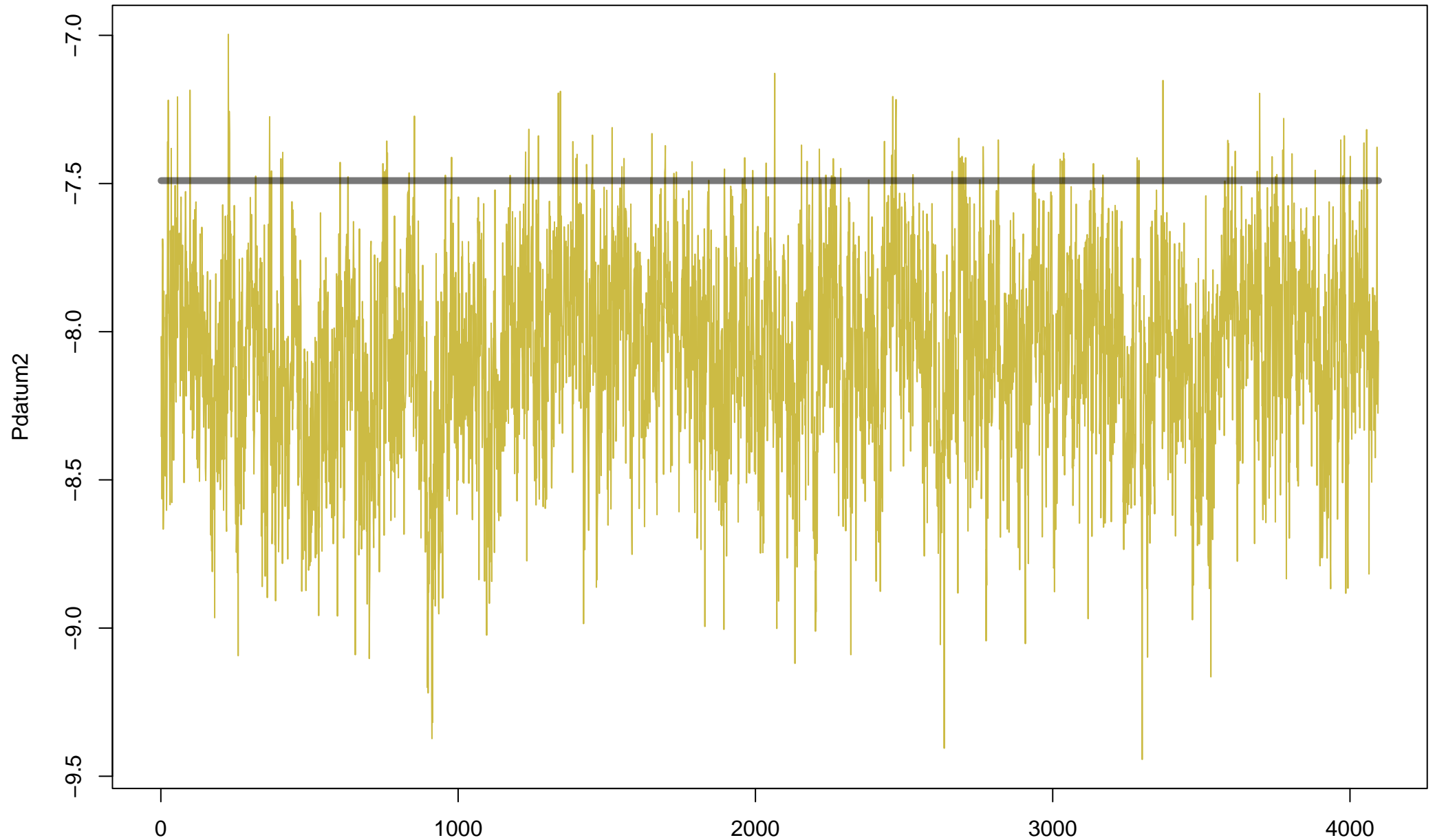
ESS = 3030 | BMK = 0.0357 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: 0.669



**Pdatum1**  
**ESS = 516 | BMK = 0.041 | MCSE(6.27) = 4.65 | stat: TRUE | burn: 0 | rel.err: -0.844**

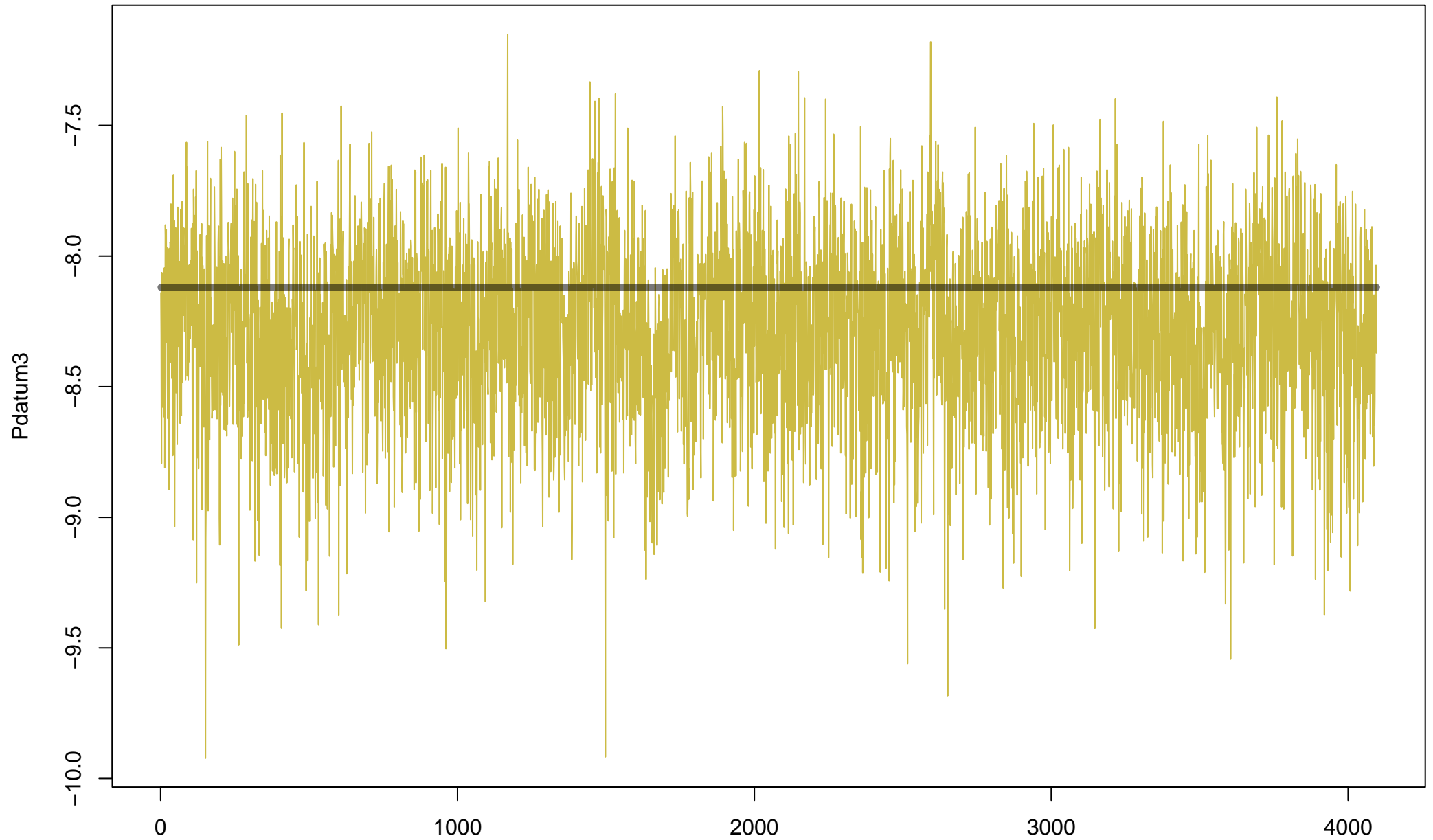


**Pdatum2**  
**ESS = 528 | BMK = 0.0595 | MCSE(6.27) = 4.17 | stat: TRUE | burn: 0 | rel.err: -2.14**



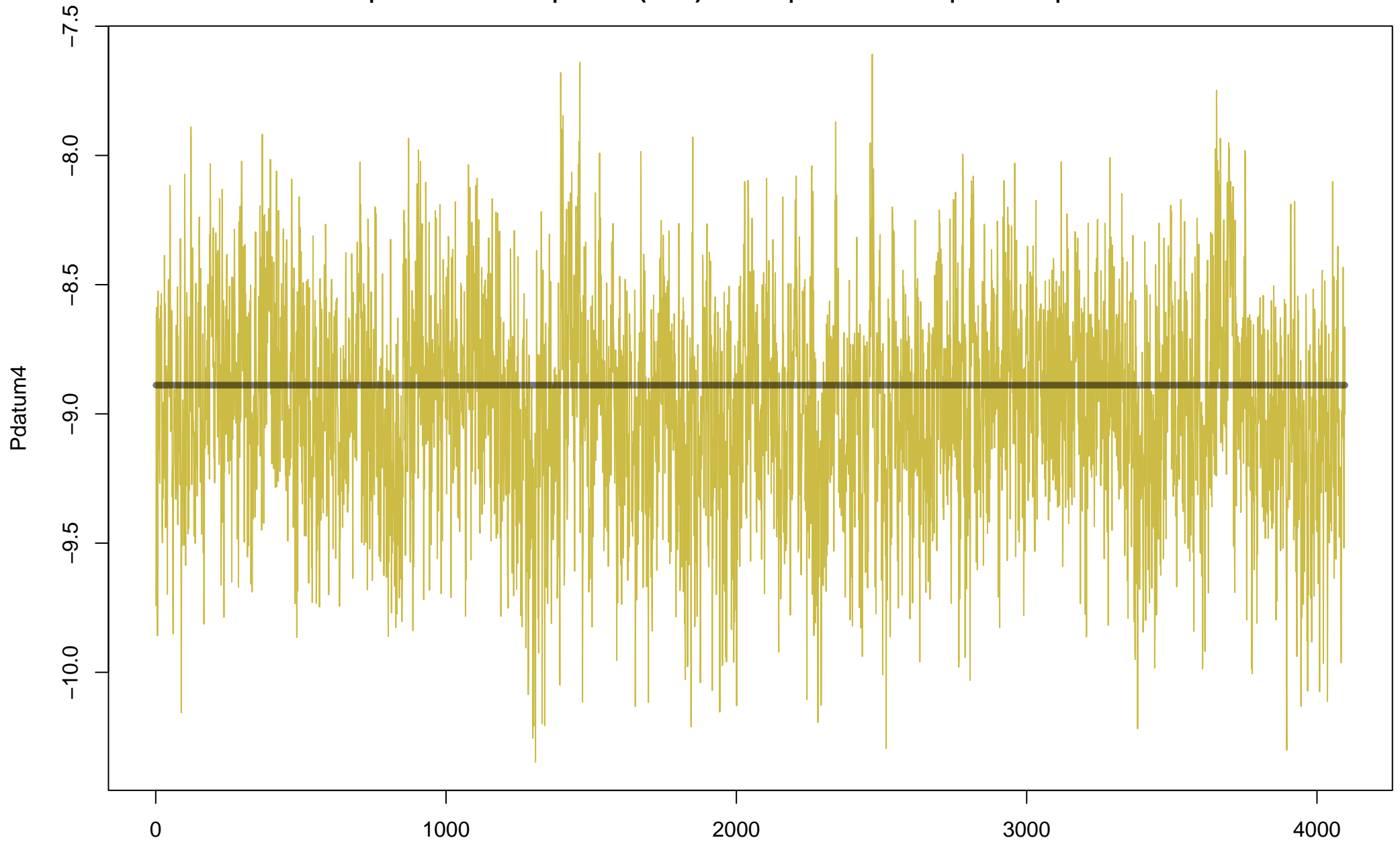
**Pdatum3**

**ESS = 1550 | BMK = 0.0288 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | rel.err: -0.311**



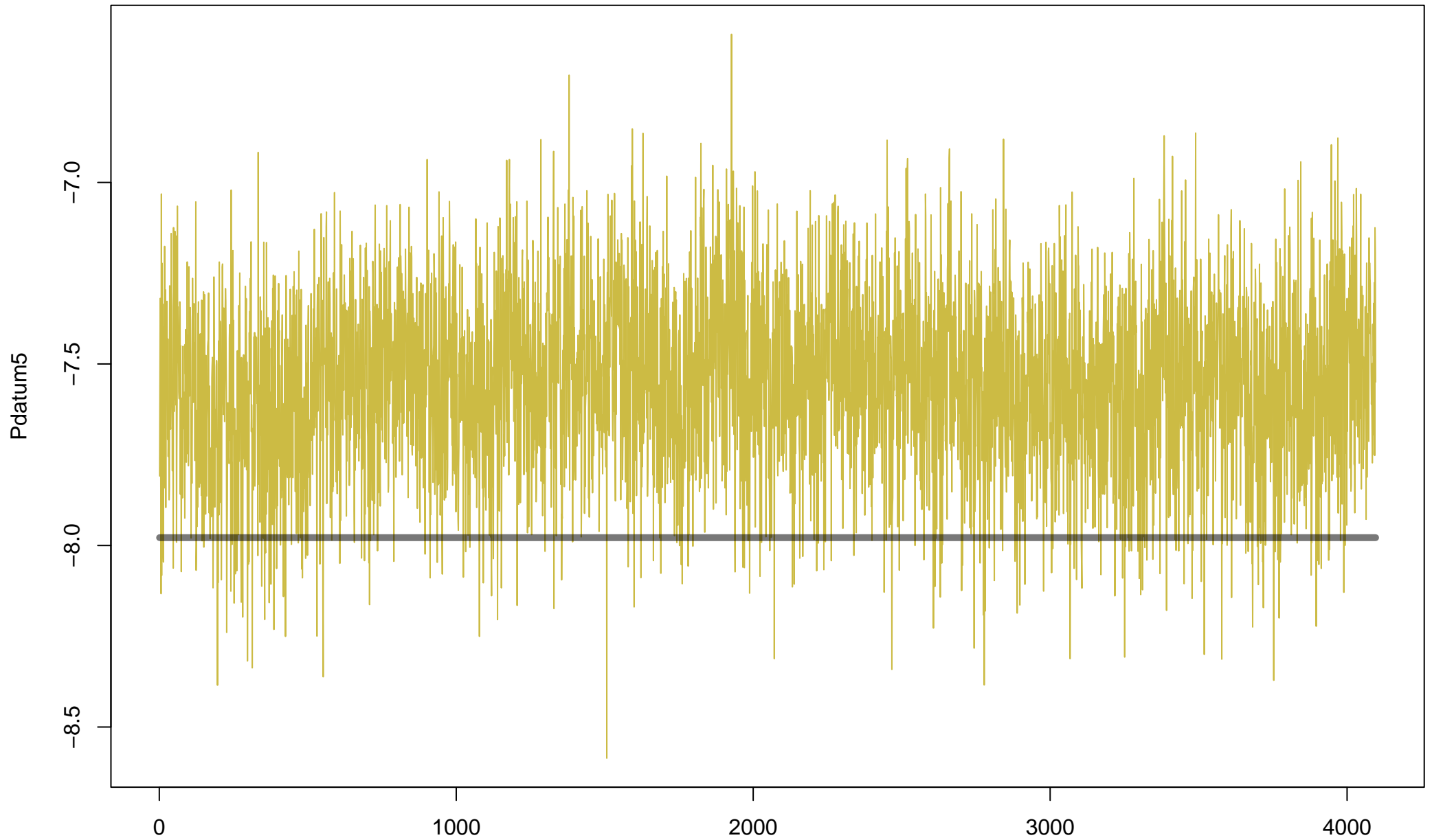
**Pdatum4**

**ESS = 717 | BMK = 0.0454 | MCSE(6.27) = 4.14 | stat: FALSE | burn: 0 | rel.err: -0.00611**



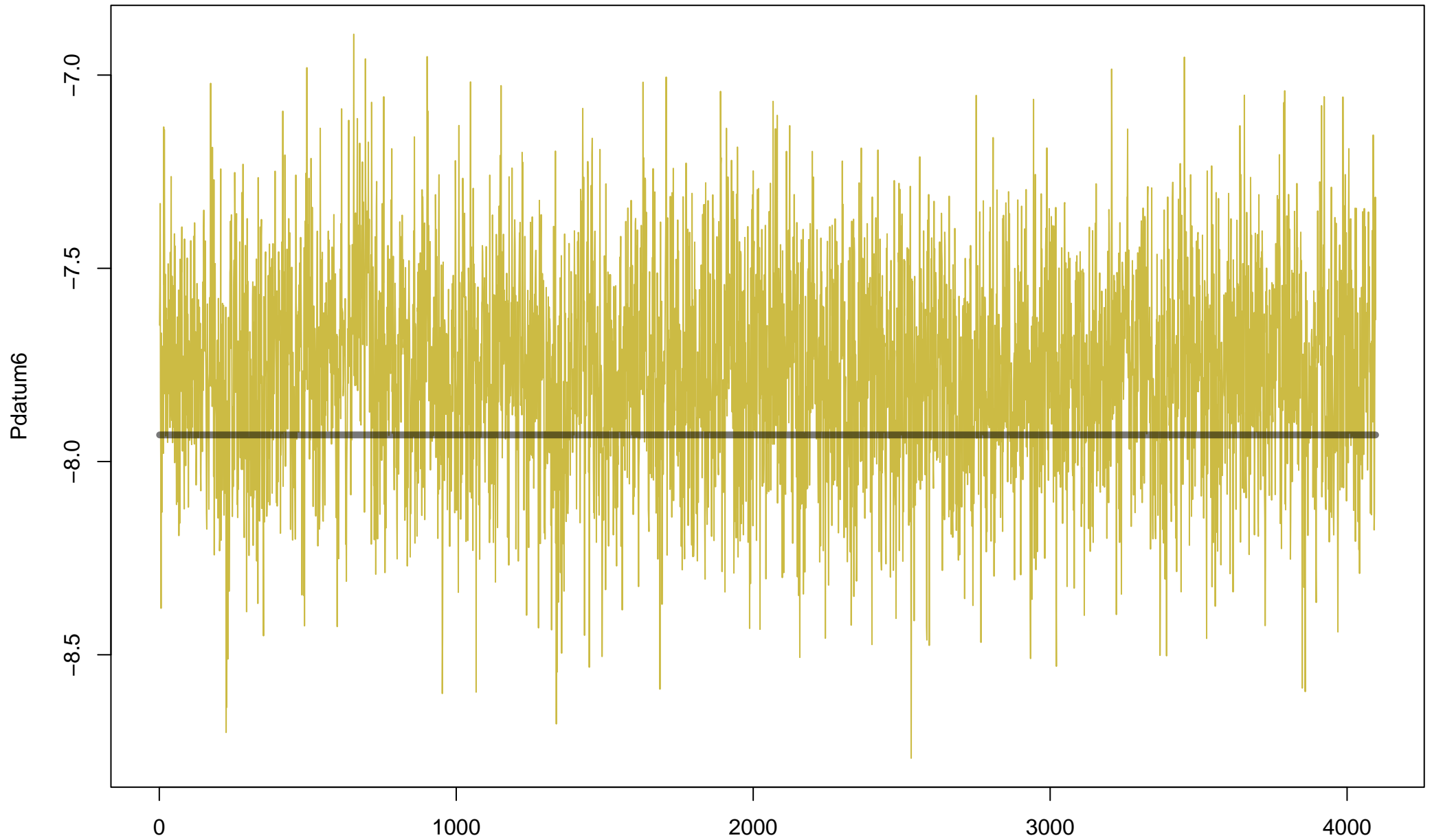
**Pdatum5**

**ESS = 852 | BMK = 0.0332 | MCSE(6.27) = 3.03 | stat: FALSE | burn: 0 | rel.err: 1.47**



**Pdatum6**

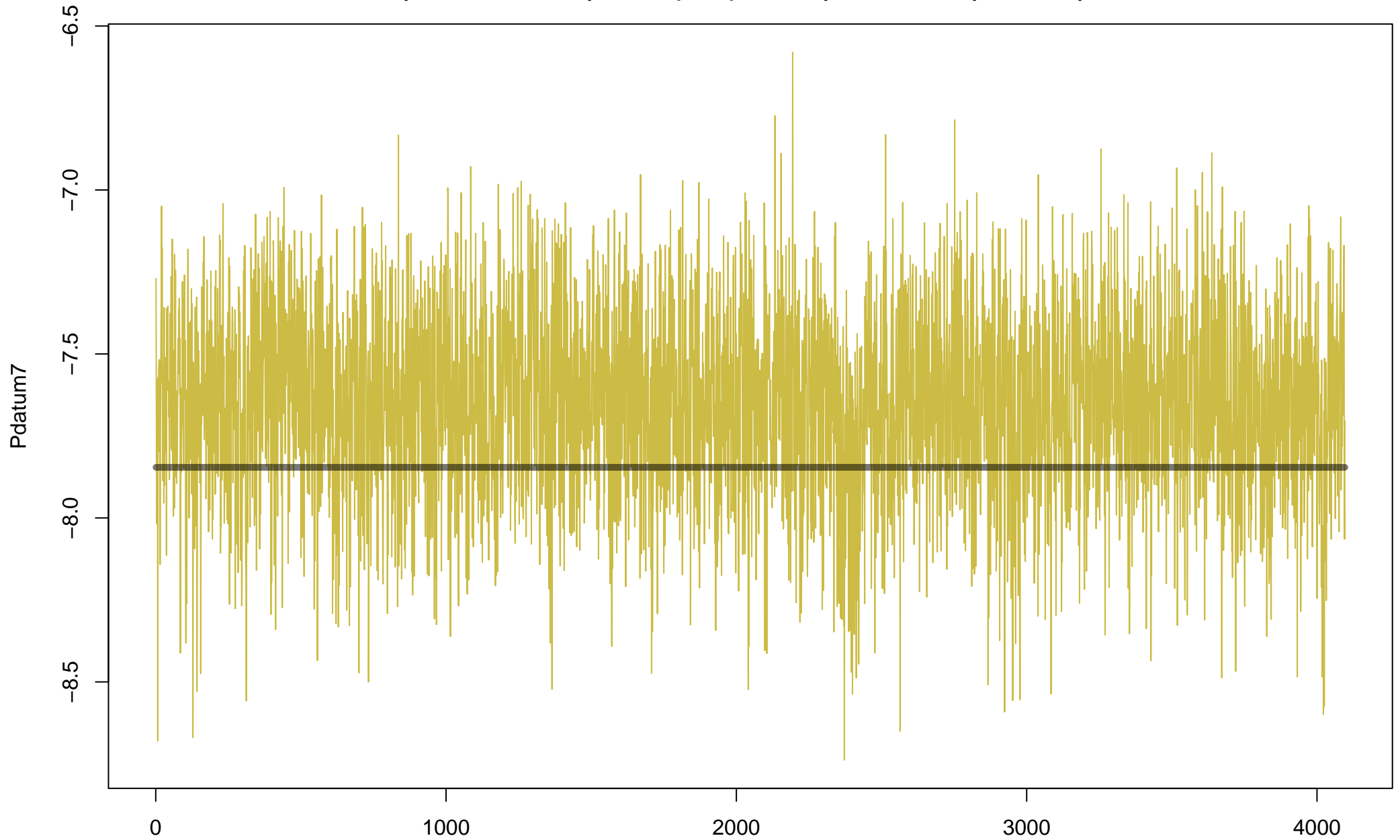
**ESS = 2210 | BMK = 0.0349 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 0.686**





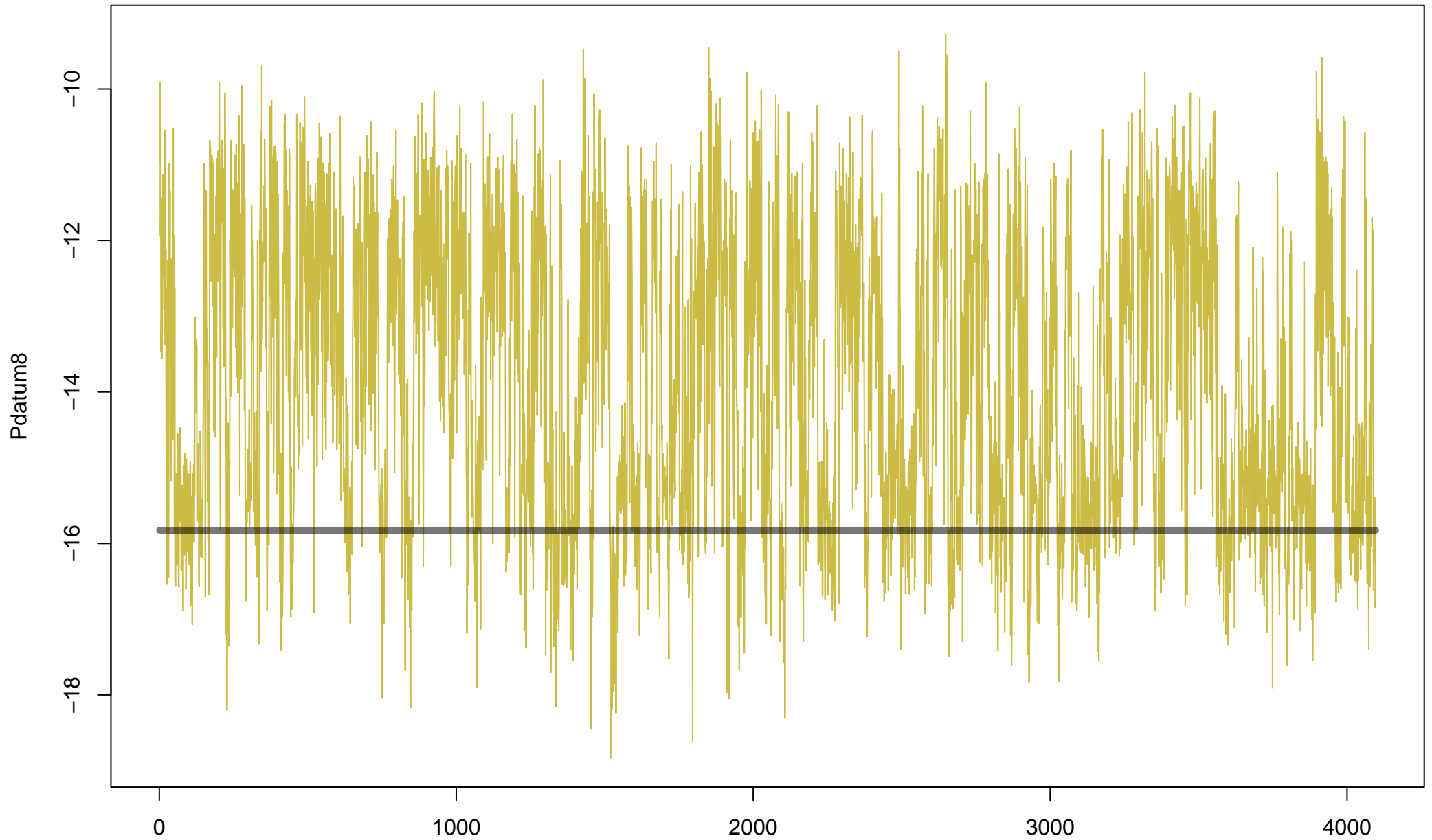
**Pdatum7**

**ESS = 1930 | BMK = 0.0474 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.743**



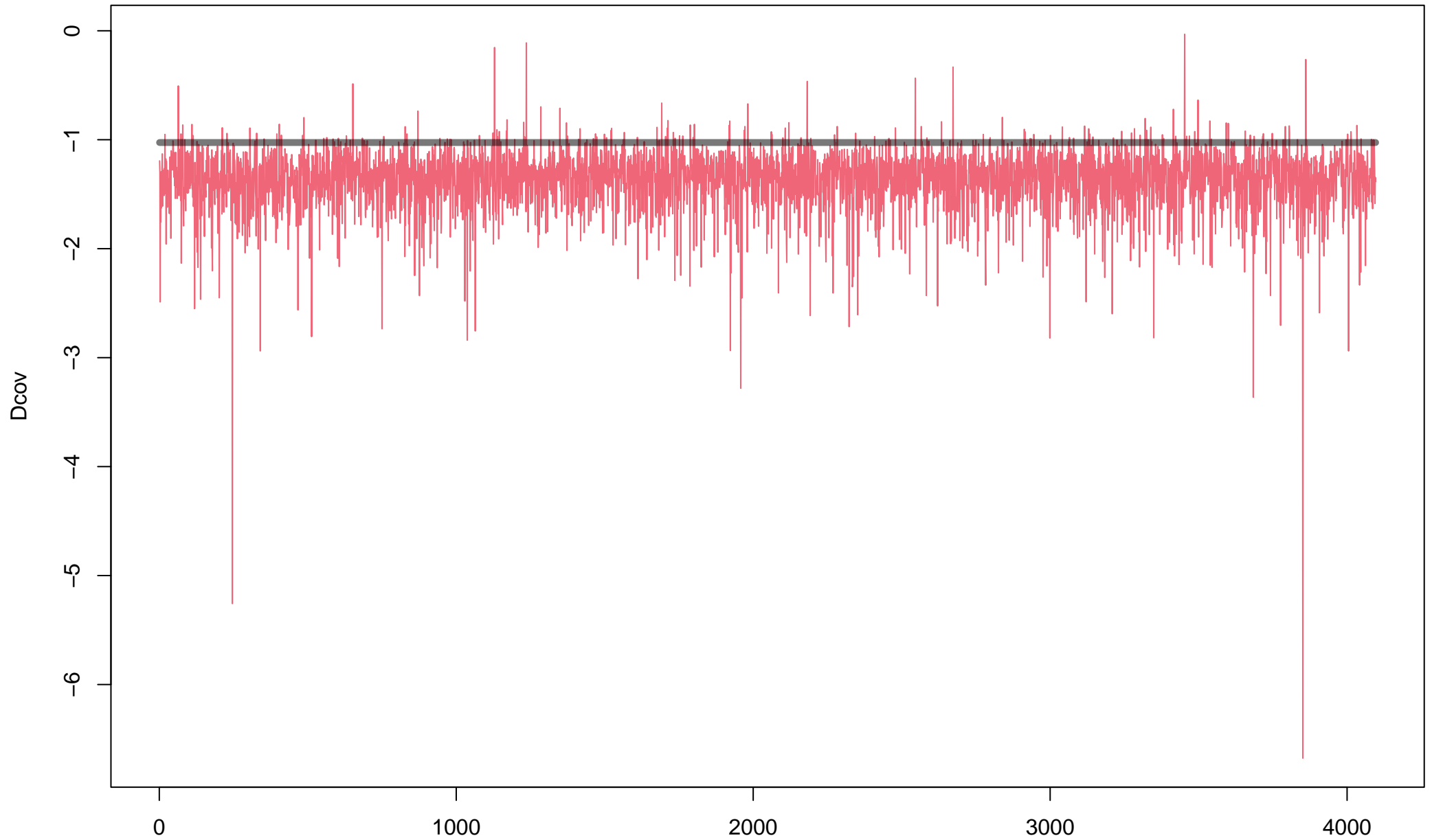
**Pdatum8**

**ESS = 547 | BMK = 0.141 | MCSE(6.27) = 3.86 | stat: TRUE | burn: 0 | rel.err: 0.534**

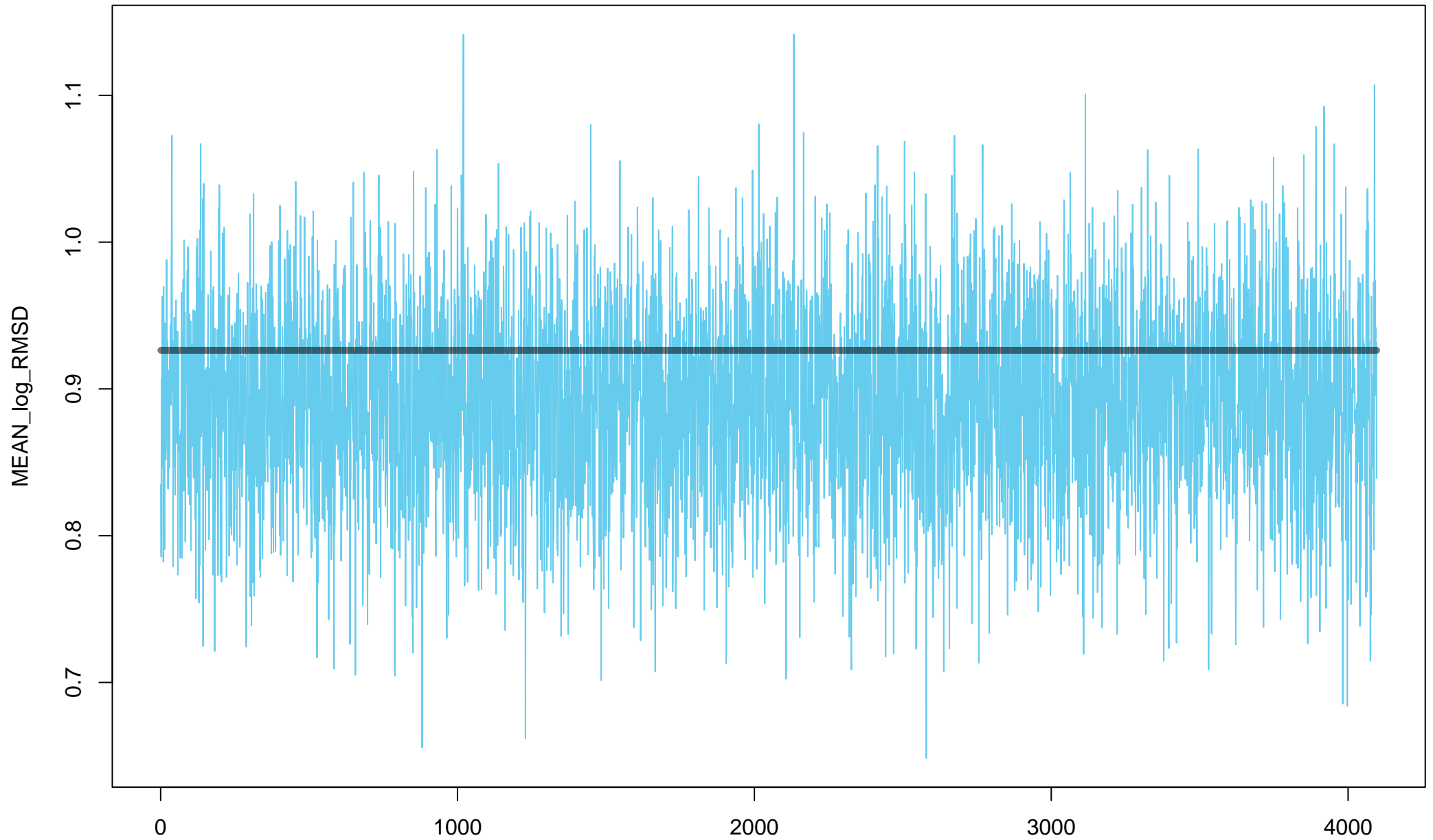


**Dcov**

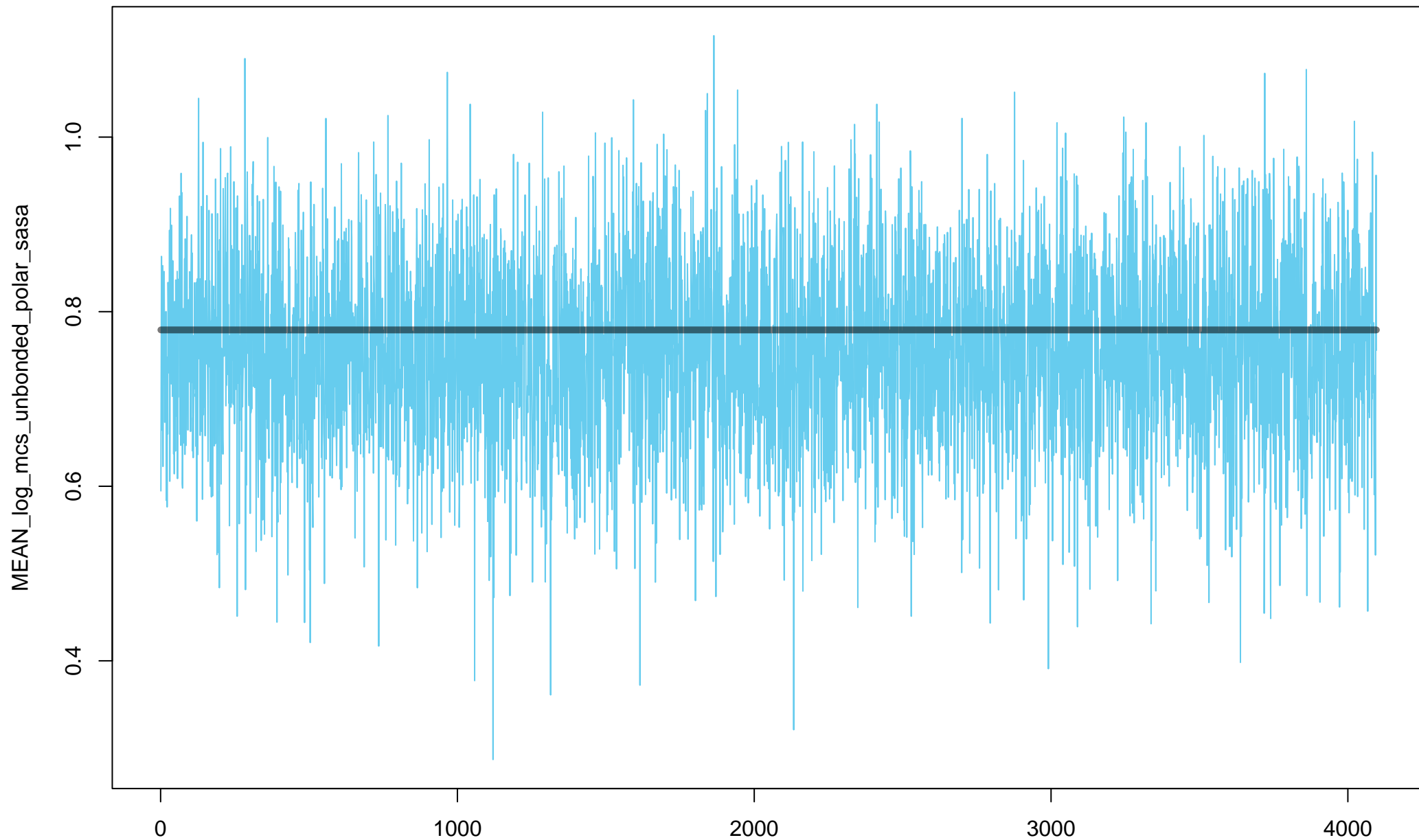
**ESS = 4100 | BMK = 0.0617 | MCSE(6.27) = 1.39 | stat: TRUE | burn: 0 | rel.err: 1.38**



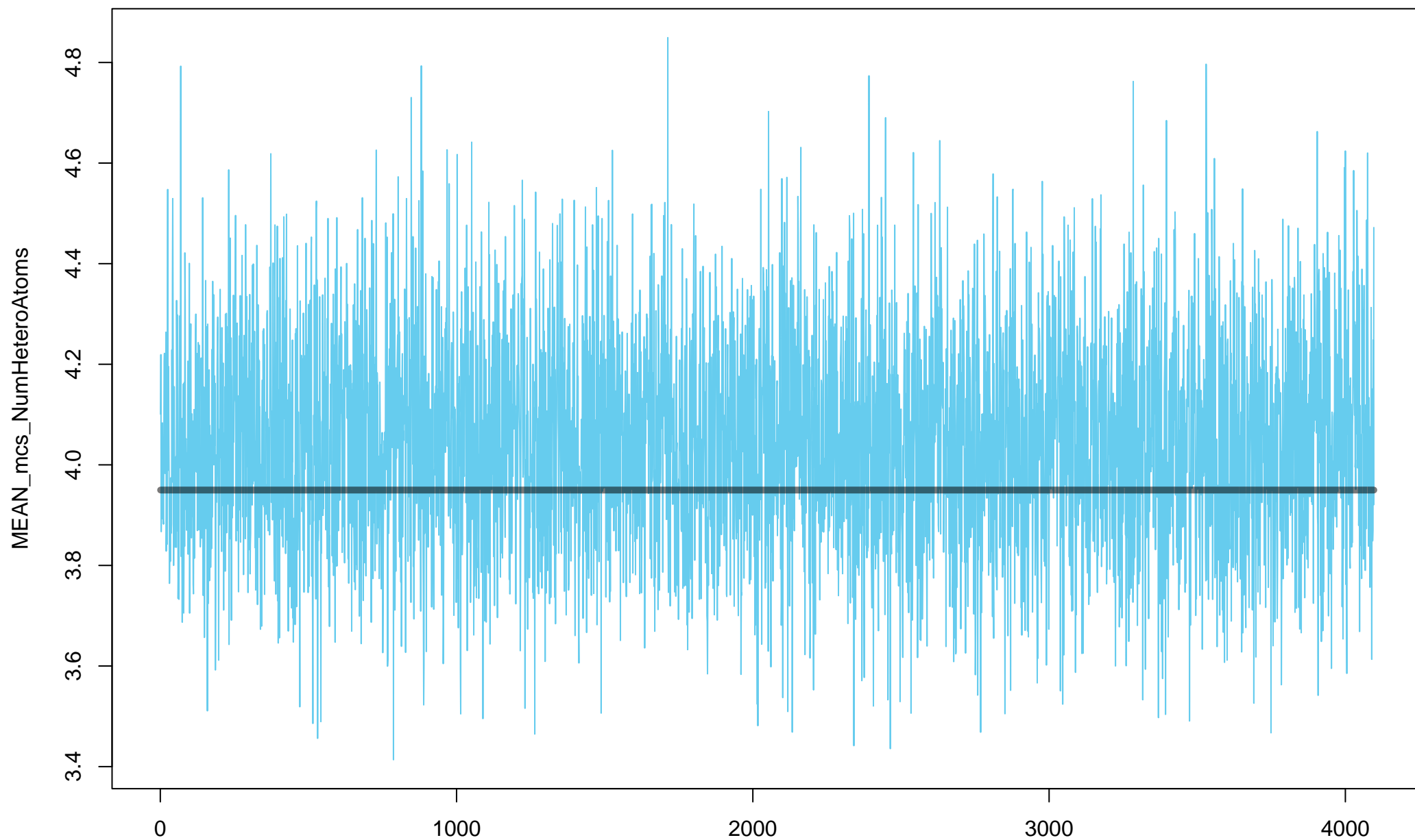
**MEAN\_log\_RMSD**  
**ESS = 4100 | BMK = 0.0382 | MCSE(6.27) = 1.39 | stat: TRUE | burn: 0 | rel.err: -0.56**



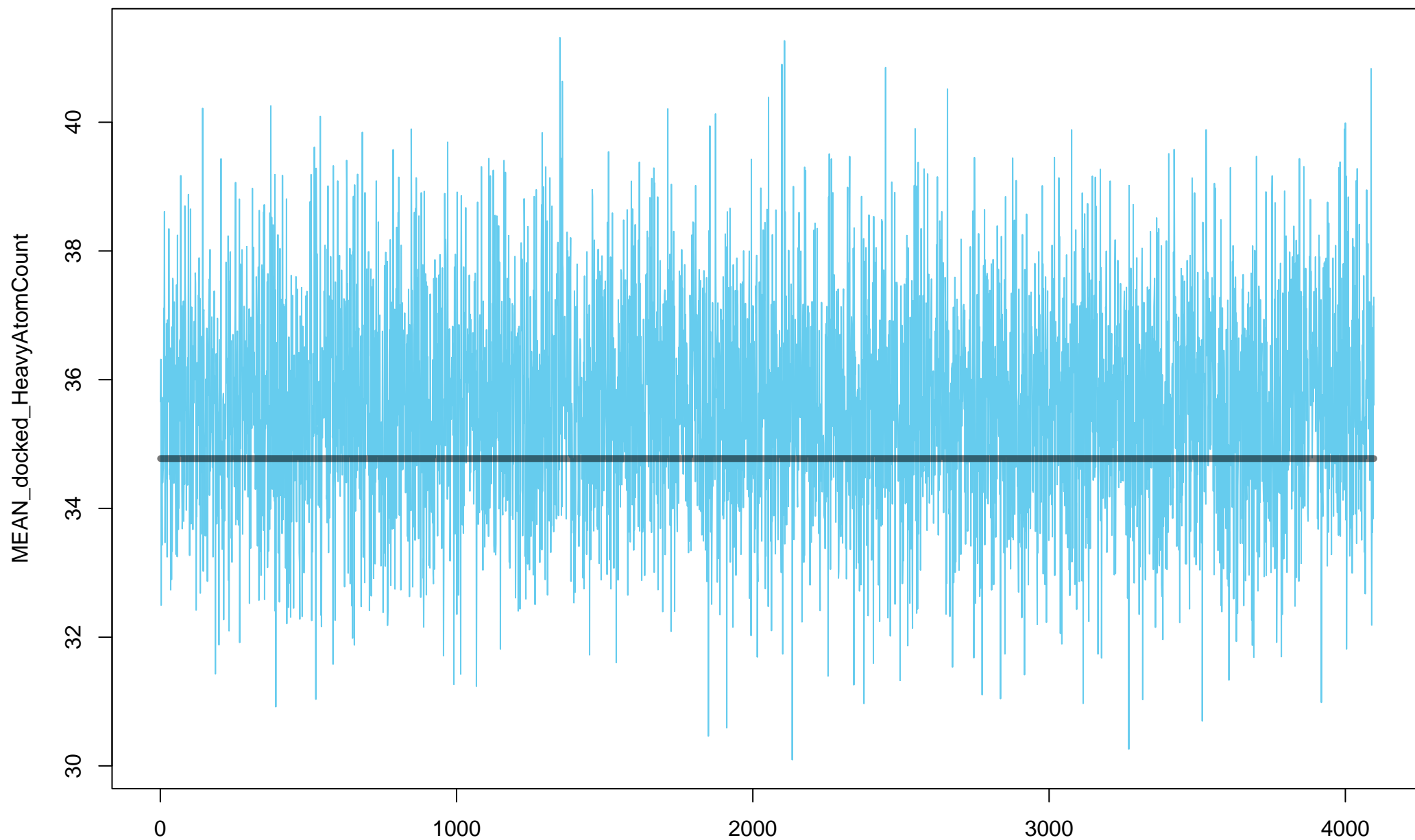
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 4100 | BMK = 0.0254 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: -0.237**



**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 4100 | BMK = 0.0369 | MCSE(6.27) = 1.4 | stat: TRUE | burn: 0 | rel.err: 0.458**

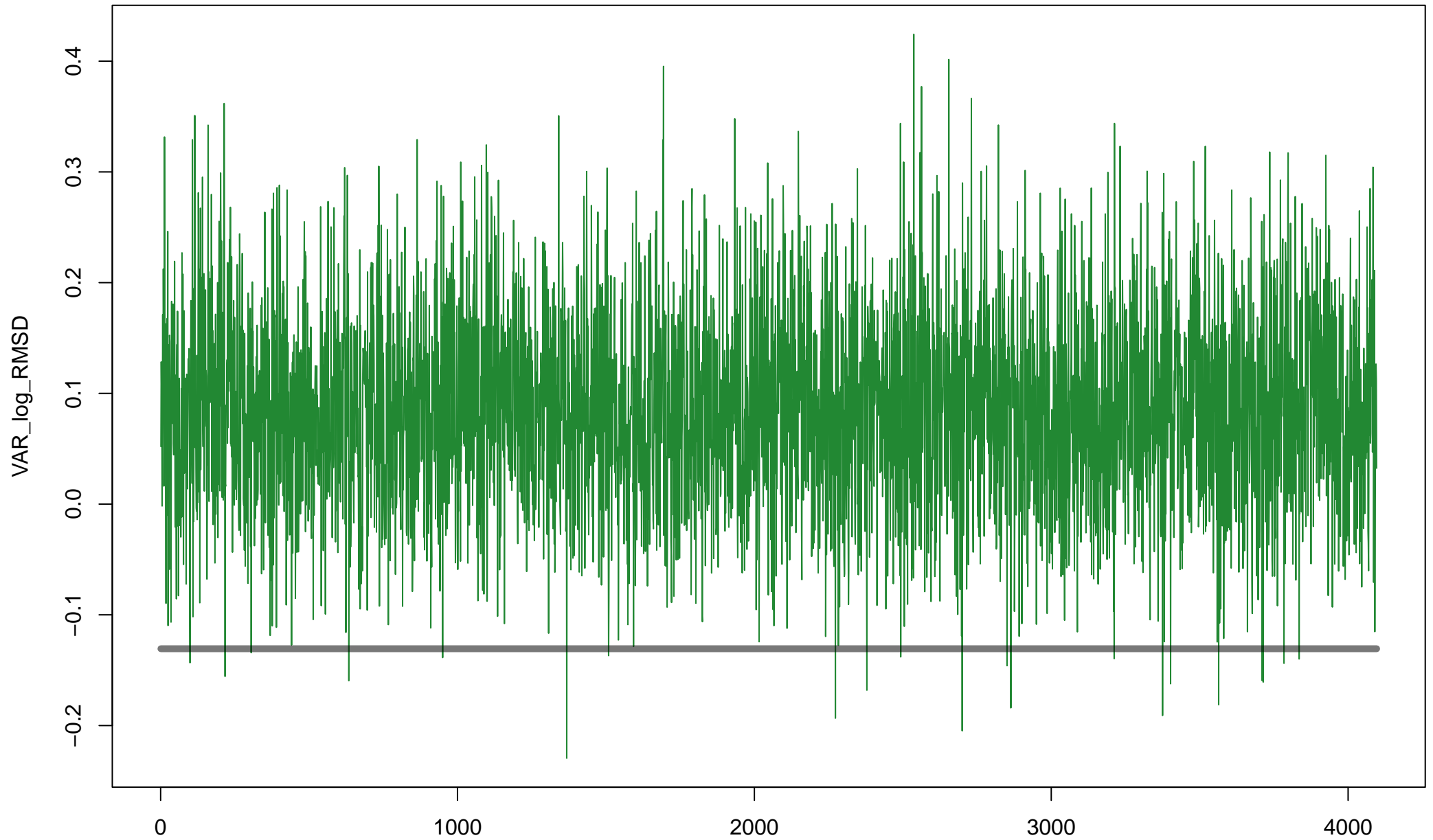


**MEAN\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0254 | MCSE(6.27) = 1.46 | stat: TRUE | burn: 0 | rel.err: 0.511**



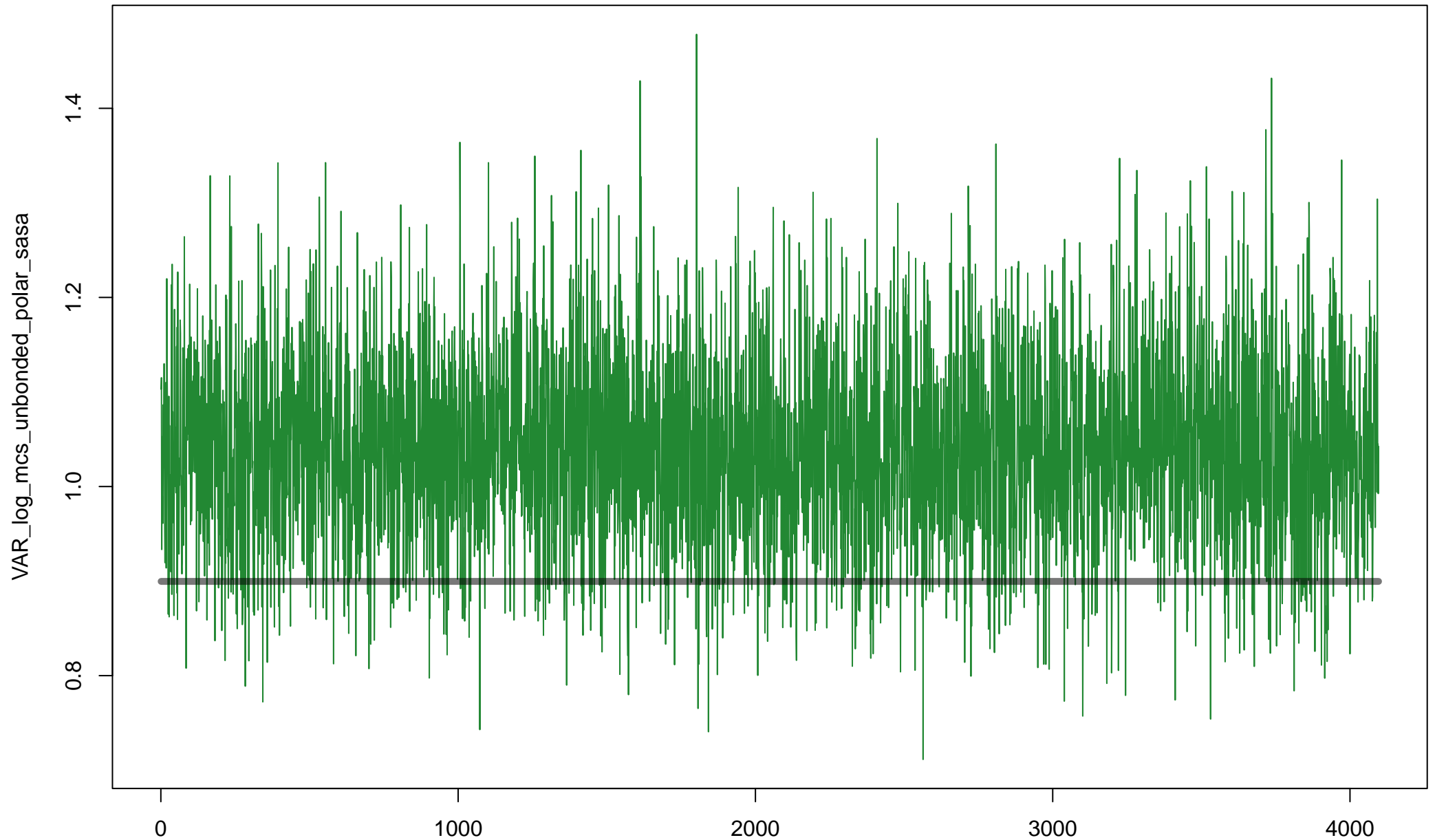
# VAR\_log\_RMSD

ESS = 4100 | BMK = 0.0365 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: 2.27

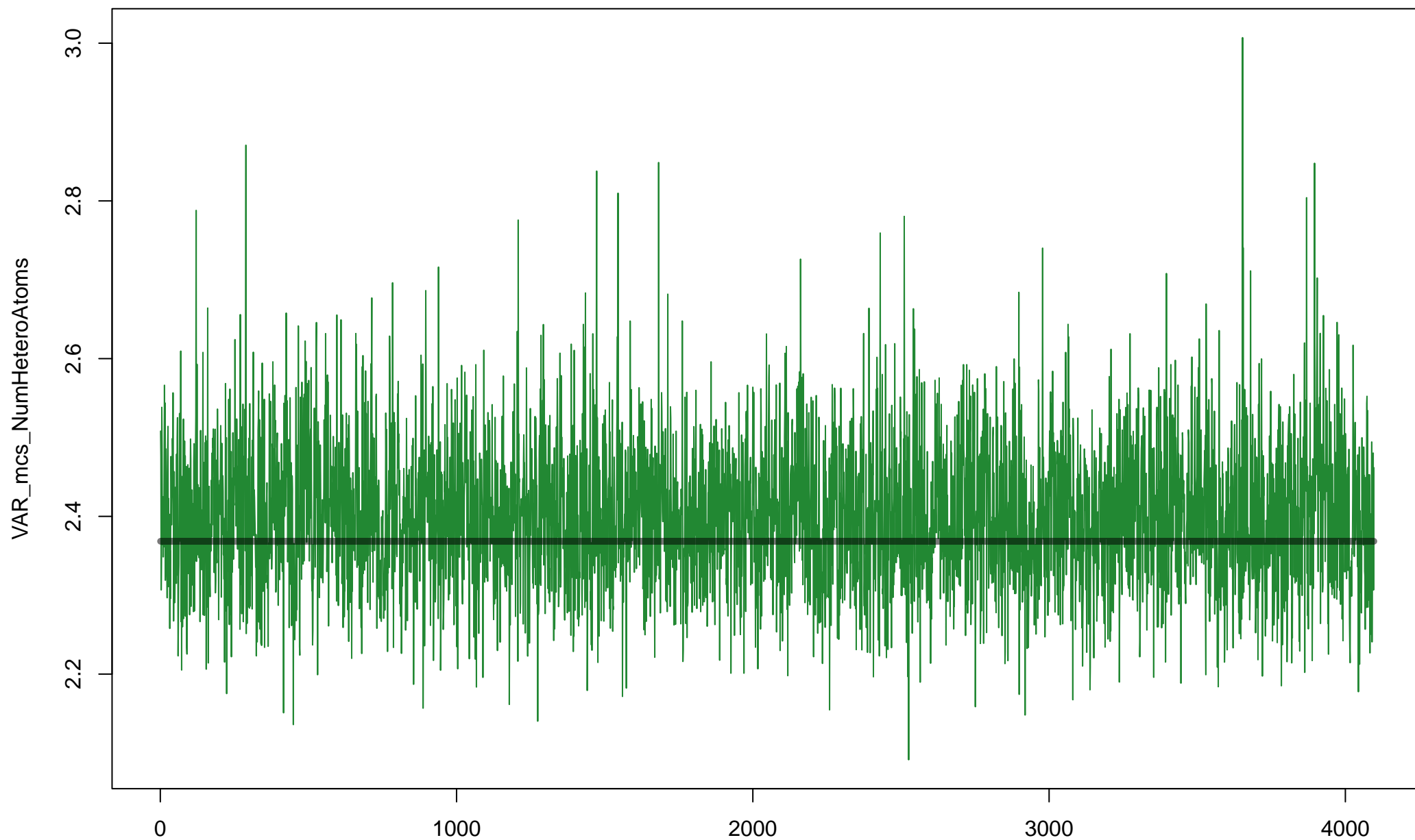




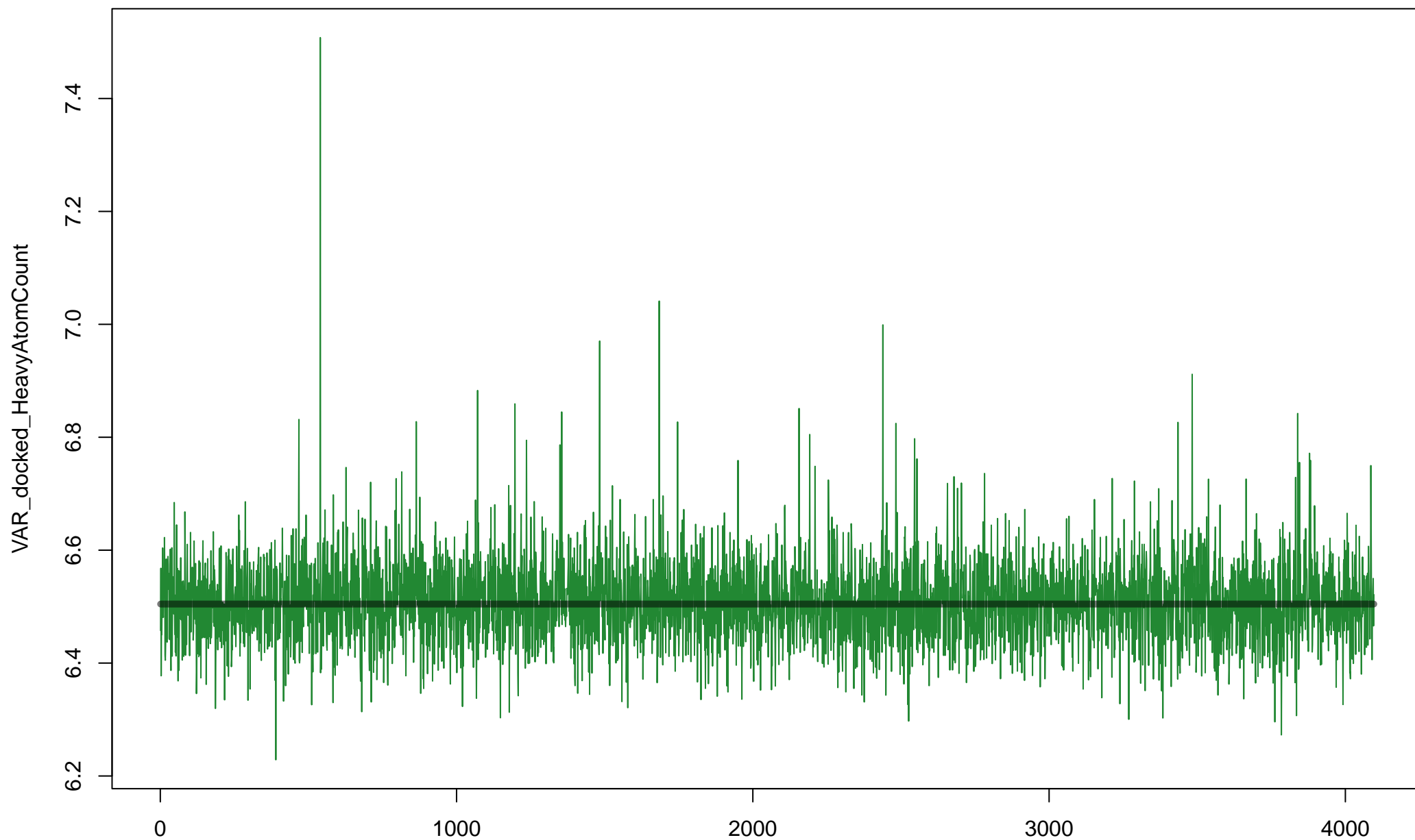
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 4000 | BMK = 0.0351 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: 1.34**



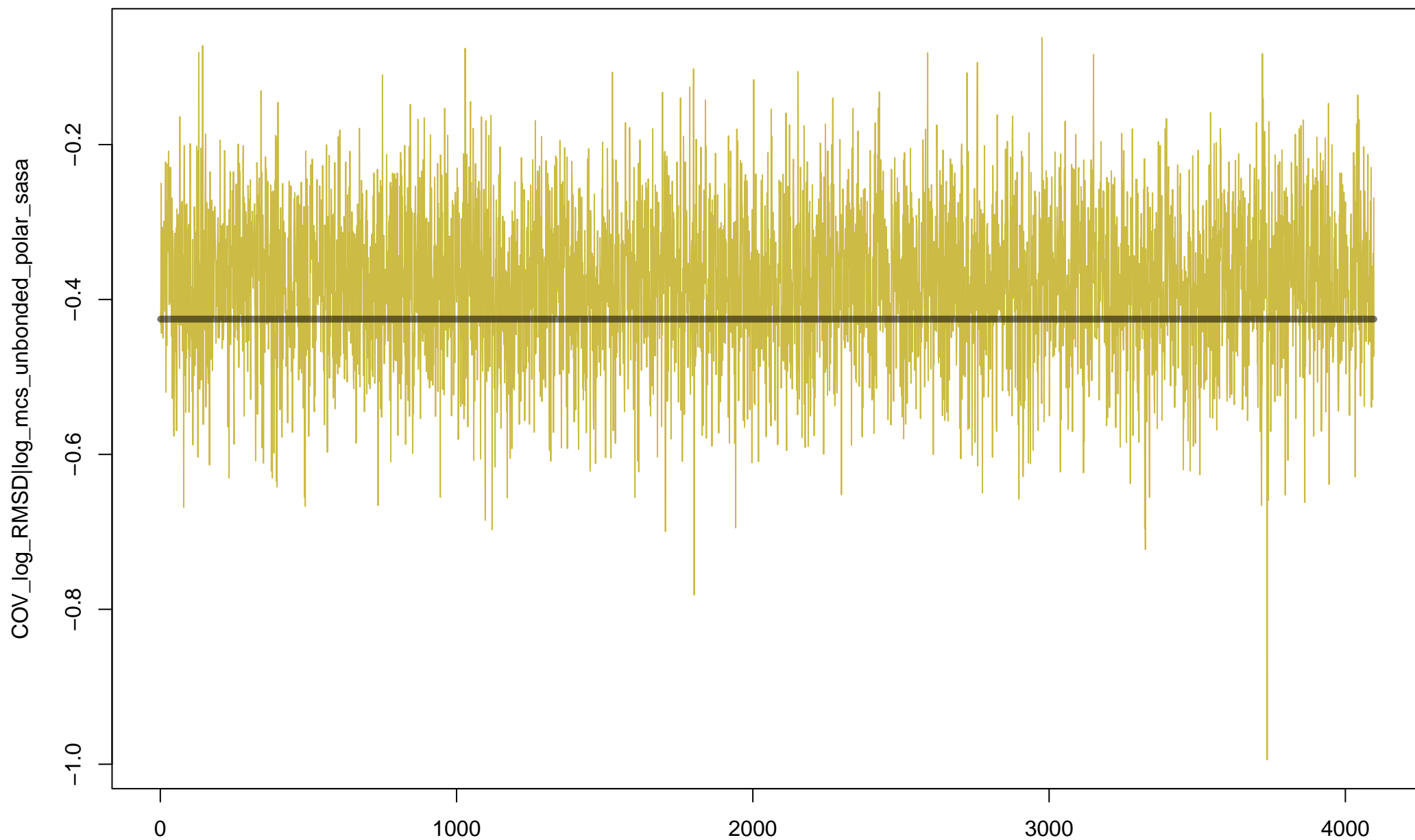
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2740 | BMK = 0.0512 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.392**



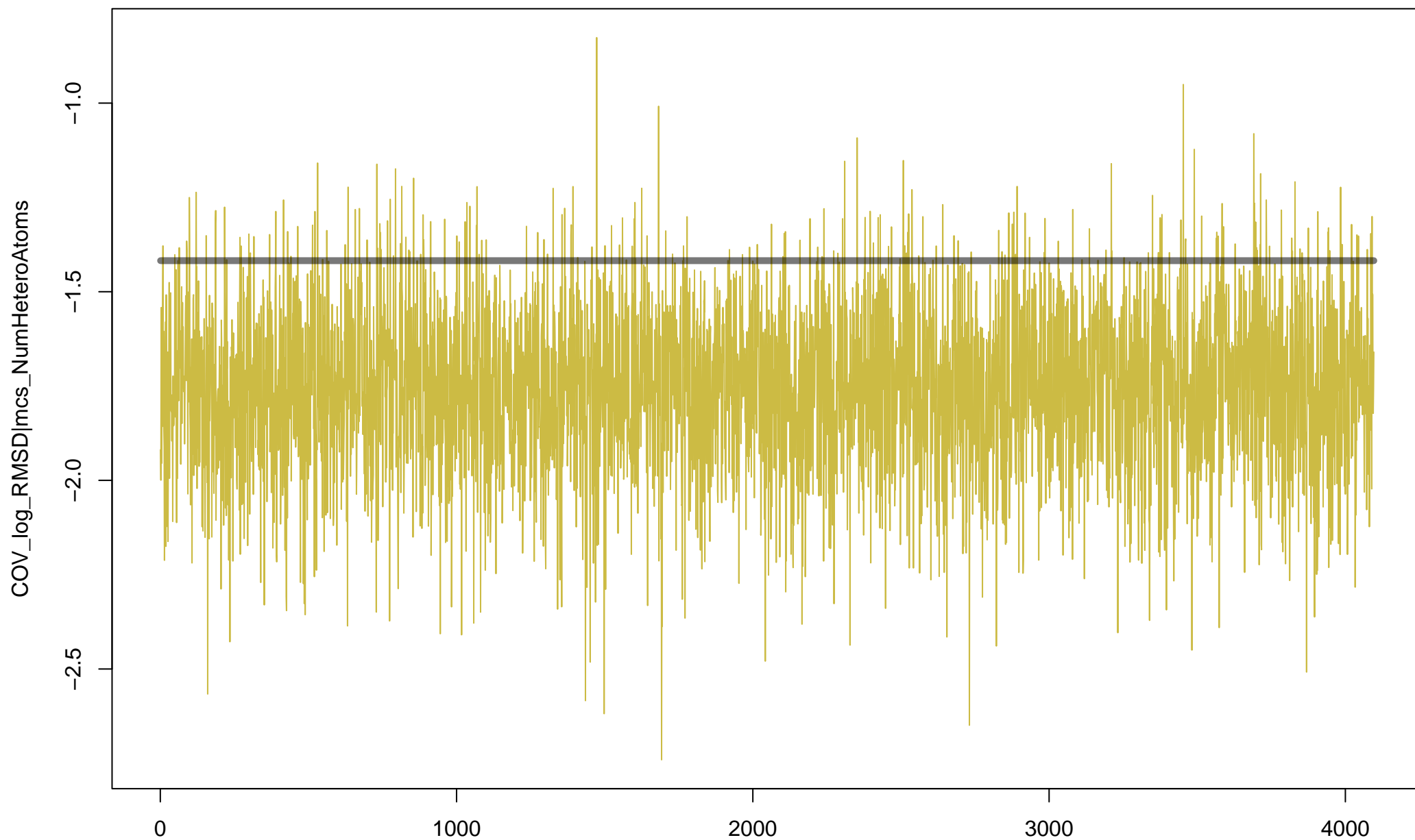
**VAR\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0552 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: 0.0723**



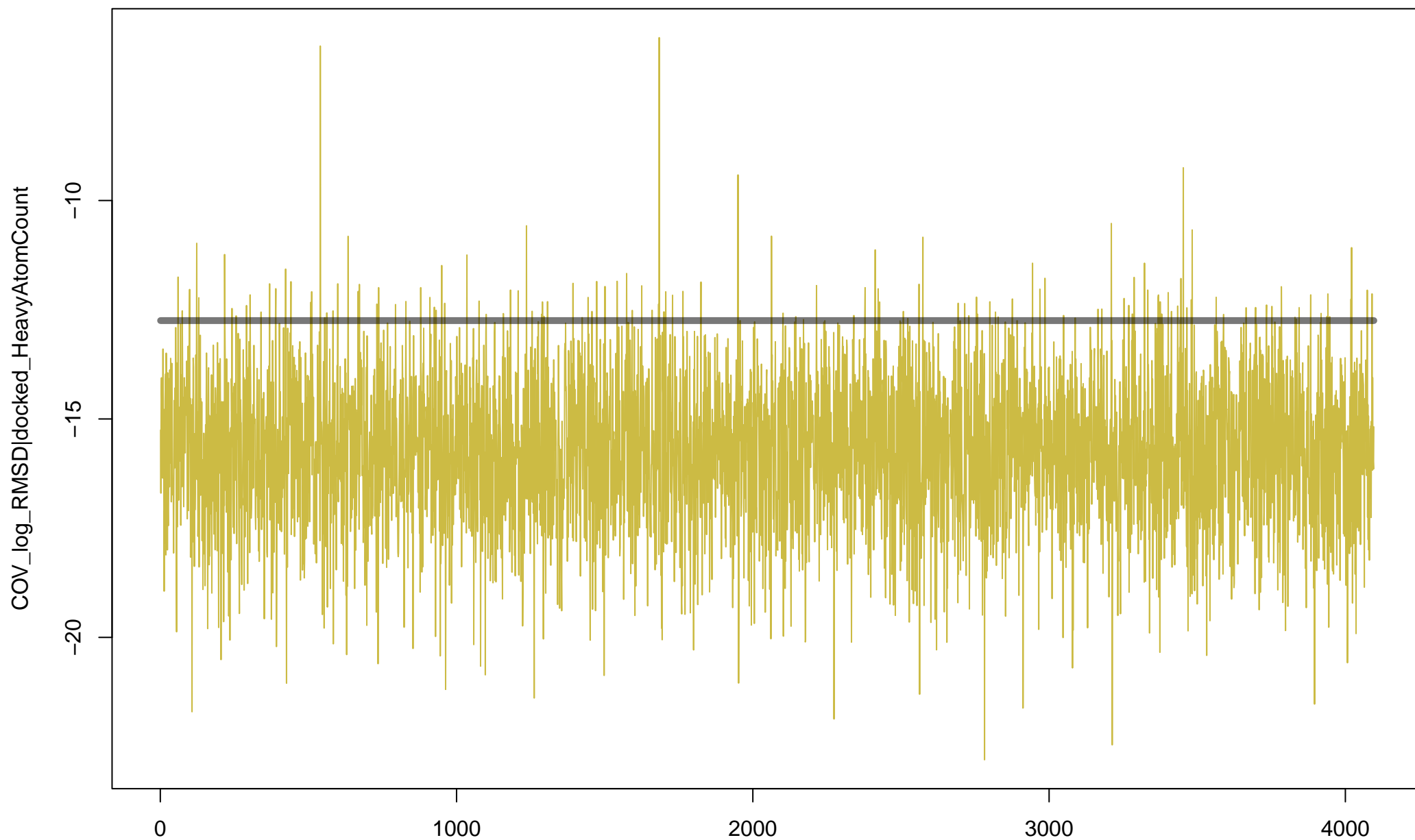
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 4100 | BMK = 0.0356 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0 | rel.err: 0.468**



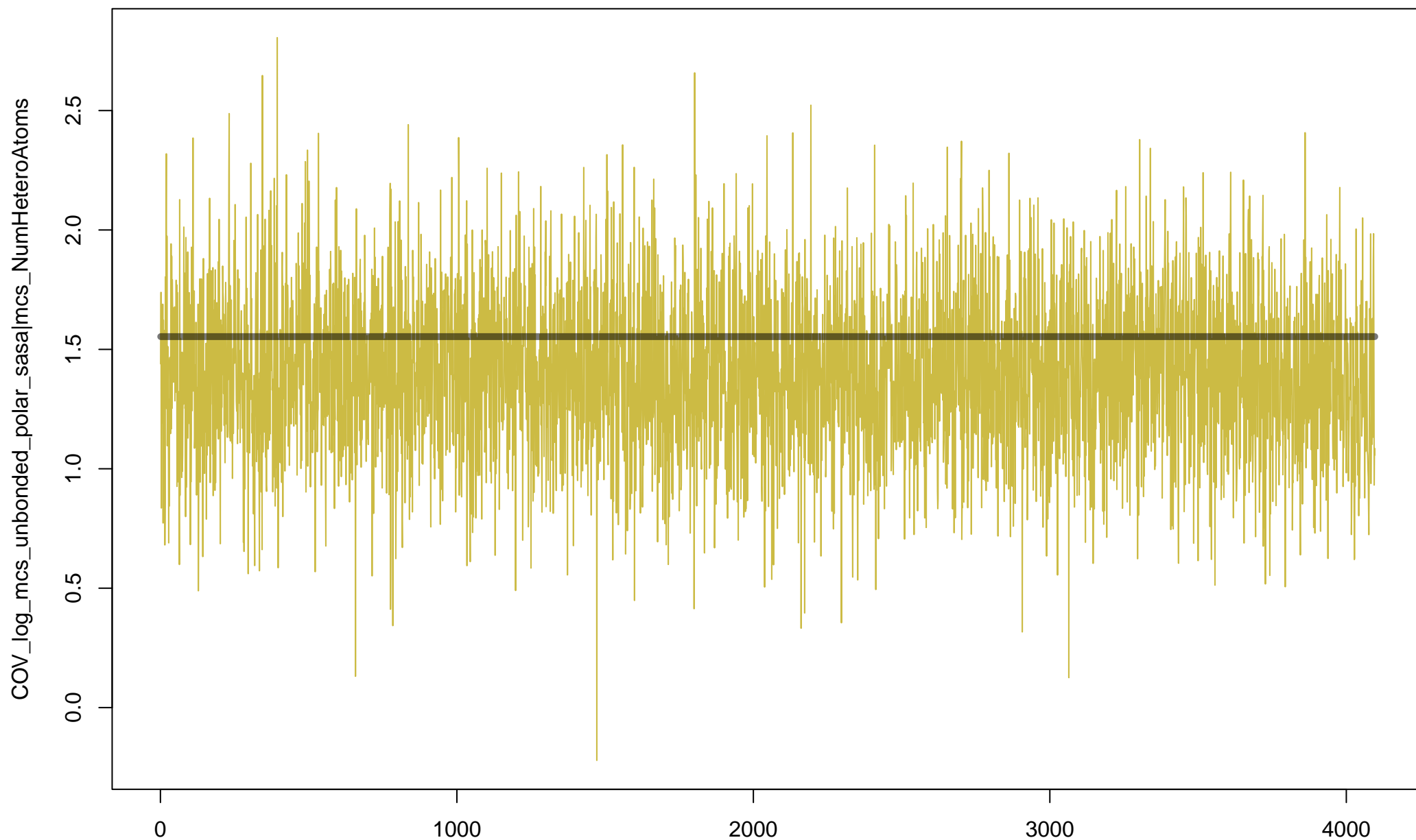
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 3860 | BMK = 0.039 | MCSE(6.27) = 1.75 | stat: TRUE | burn: 0 | rel.err: -1.56**



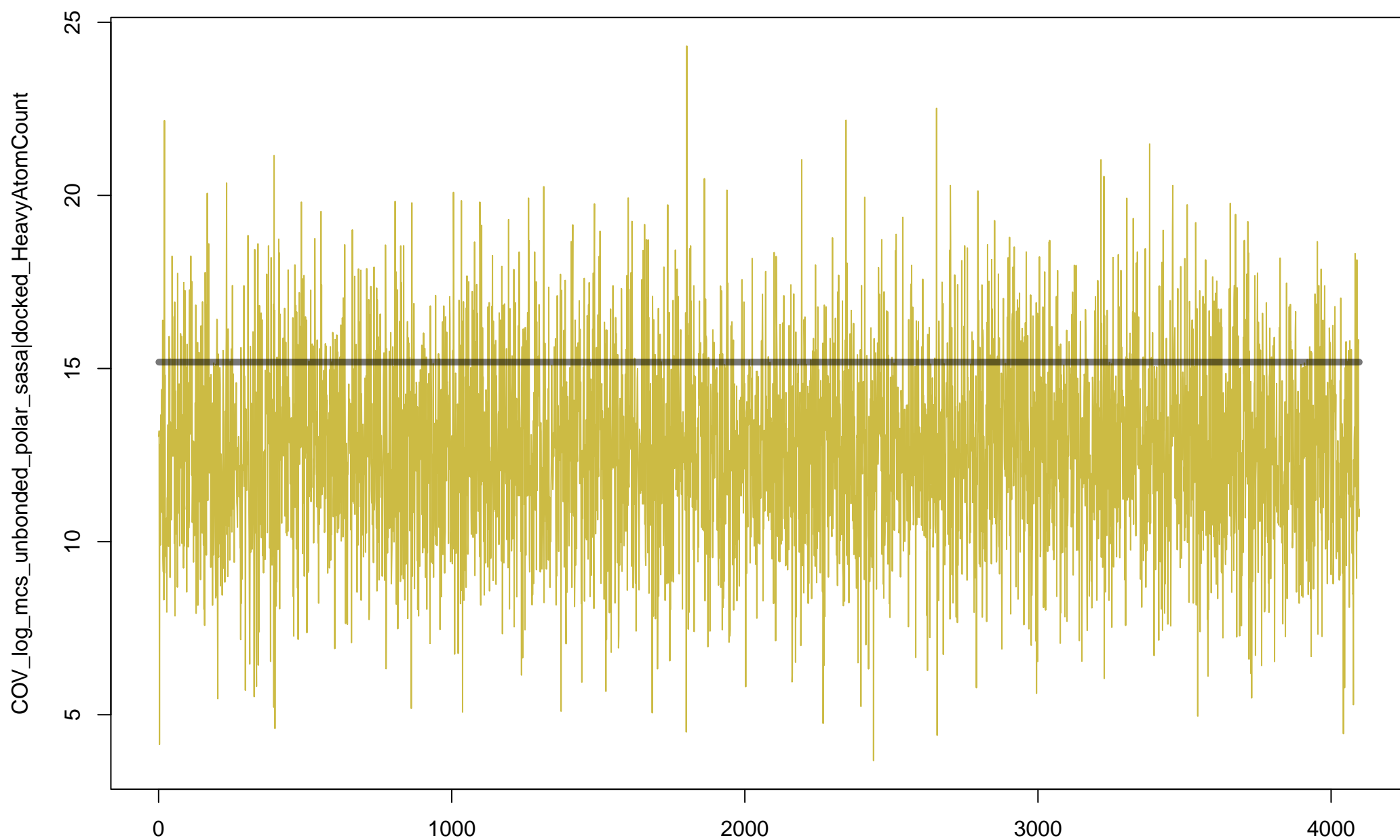
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0365 | MCSE(6.27) = 1.38 | stat: TRUE | burn: 0 | rel.err: -1.75**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 4100 | BMK = 0.0405 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: -0.478**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0261 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0 | rel.err: -0.925**





**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0434 | MCSE(6.27) = 1.36 | stat: TRUE | burn: 0 | rel.err: 0.462**

