

-- STATS maxD --

min ESS = 159.761593253283

max BMK = 0.126182216120012

max MCSE = 6.42254269046651

all stationary: FALSE

burn: 0

max rel.err.: 2.23493058951696

-- STATS 1D --

min ESS = 3138.31833579998

max BMK = 0.0500317296791733

max MCSE = 1.99188371848435

all stationary: TRUE

burn: 0

max rel.err.: 2.26719408362239

-- STATS 2D --

min ESS = 3628.4100814237

max BMK = 0.0452272057516114

max MCSE = 1.8162633340519

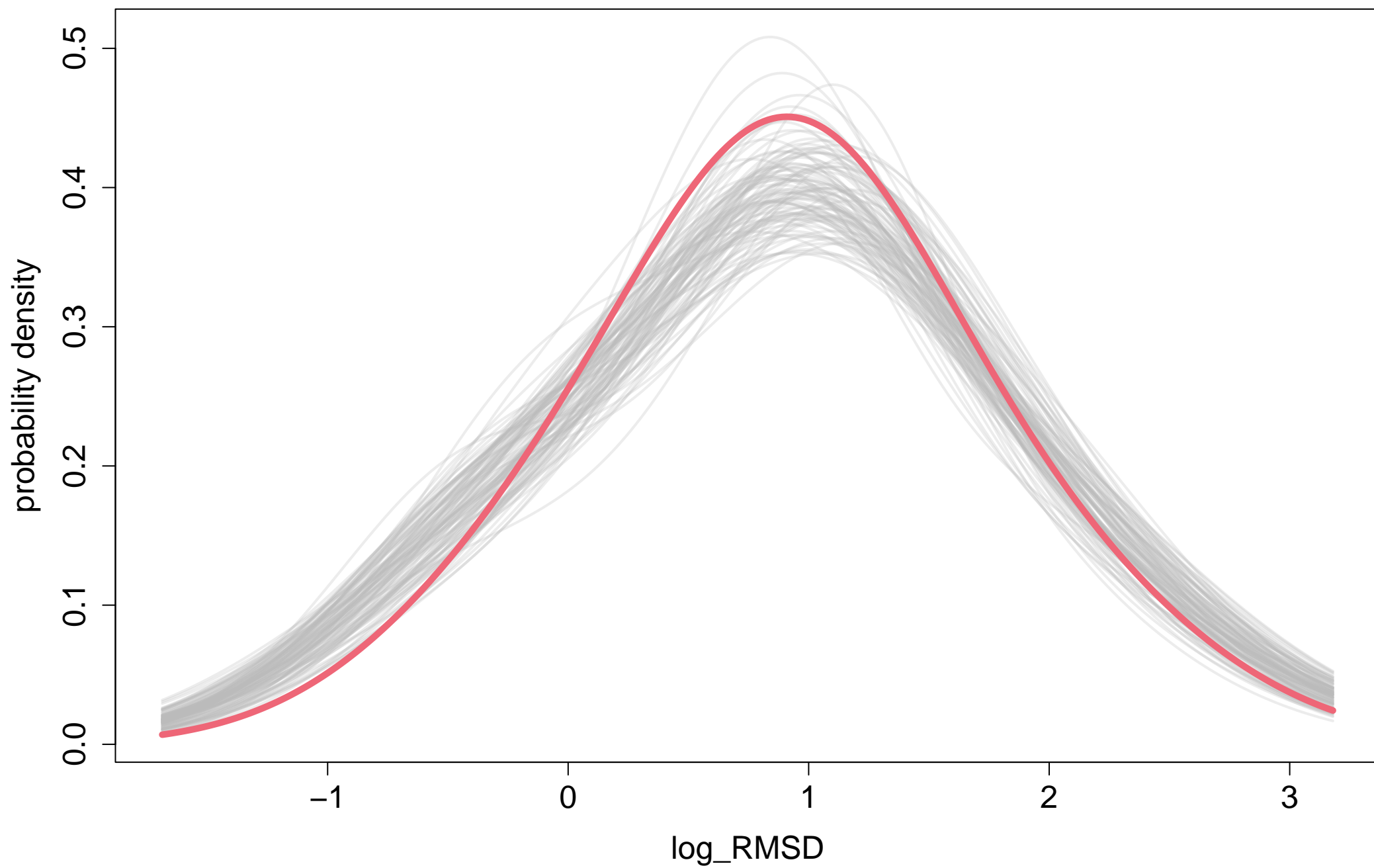
all stationary: TRUE

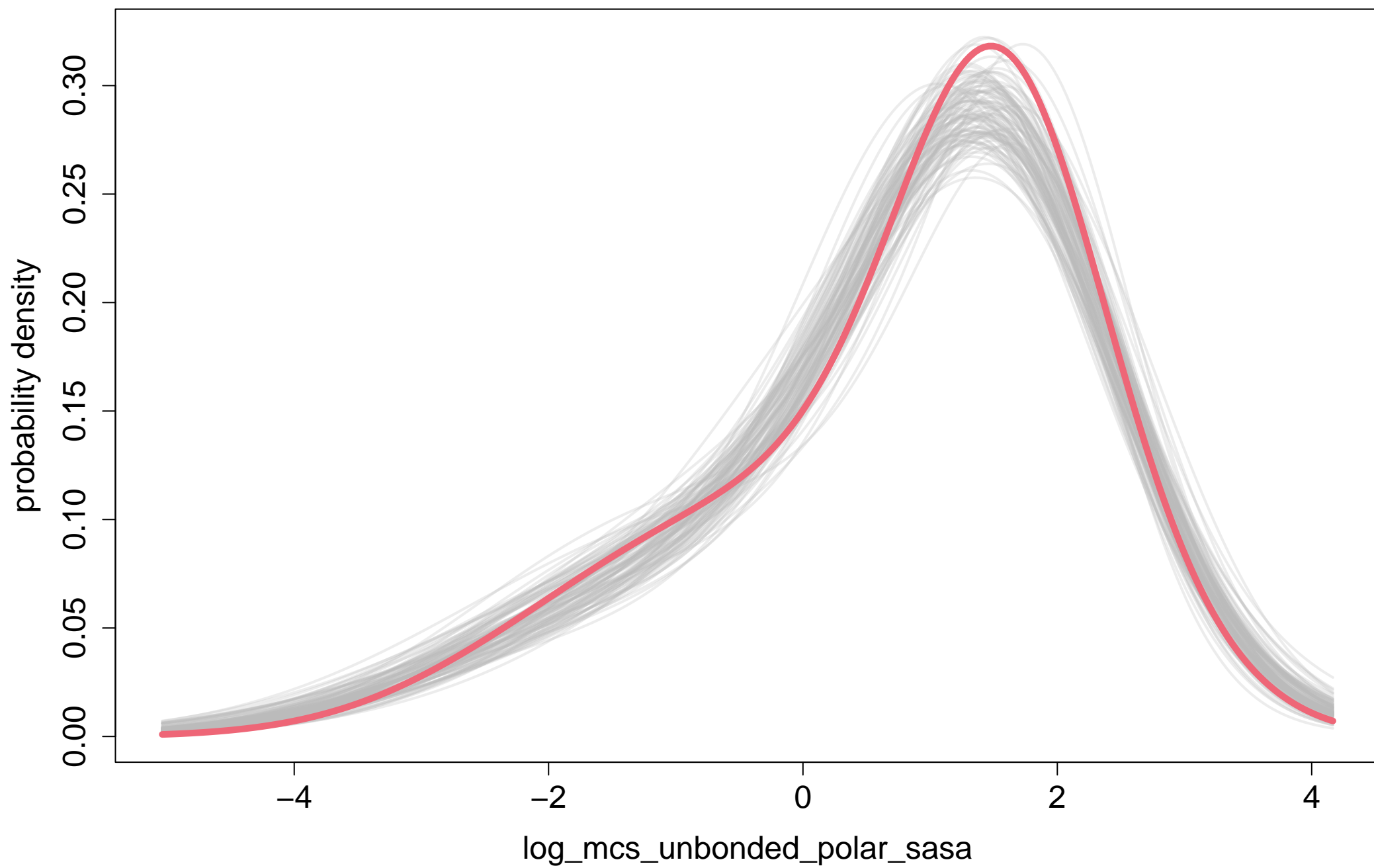
burn: 0

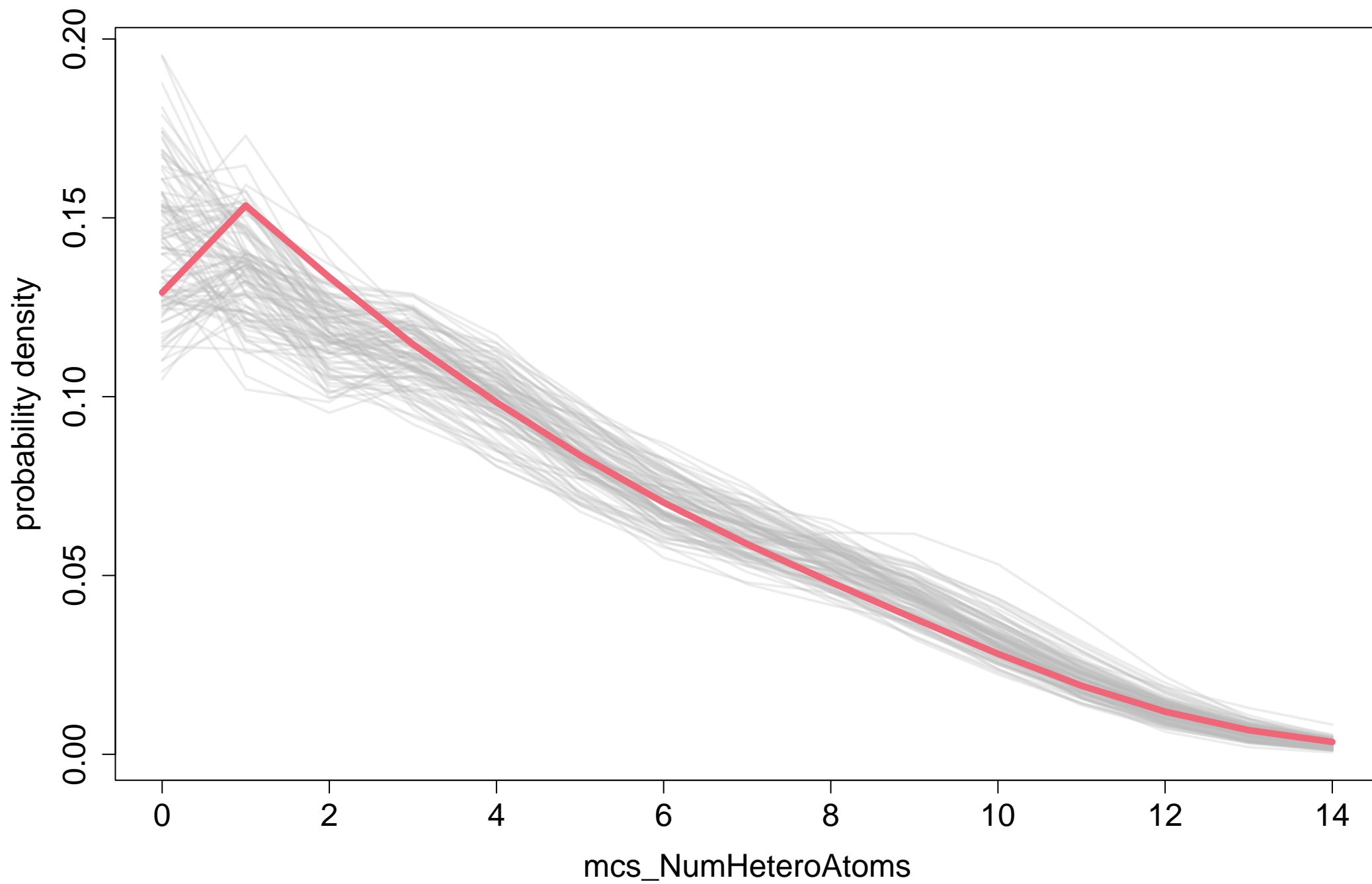
max rel.err.: 1.74575645540611

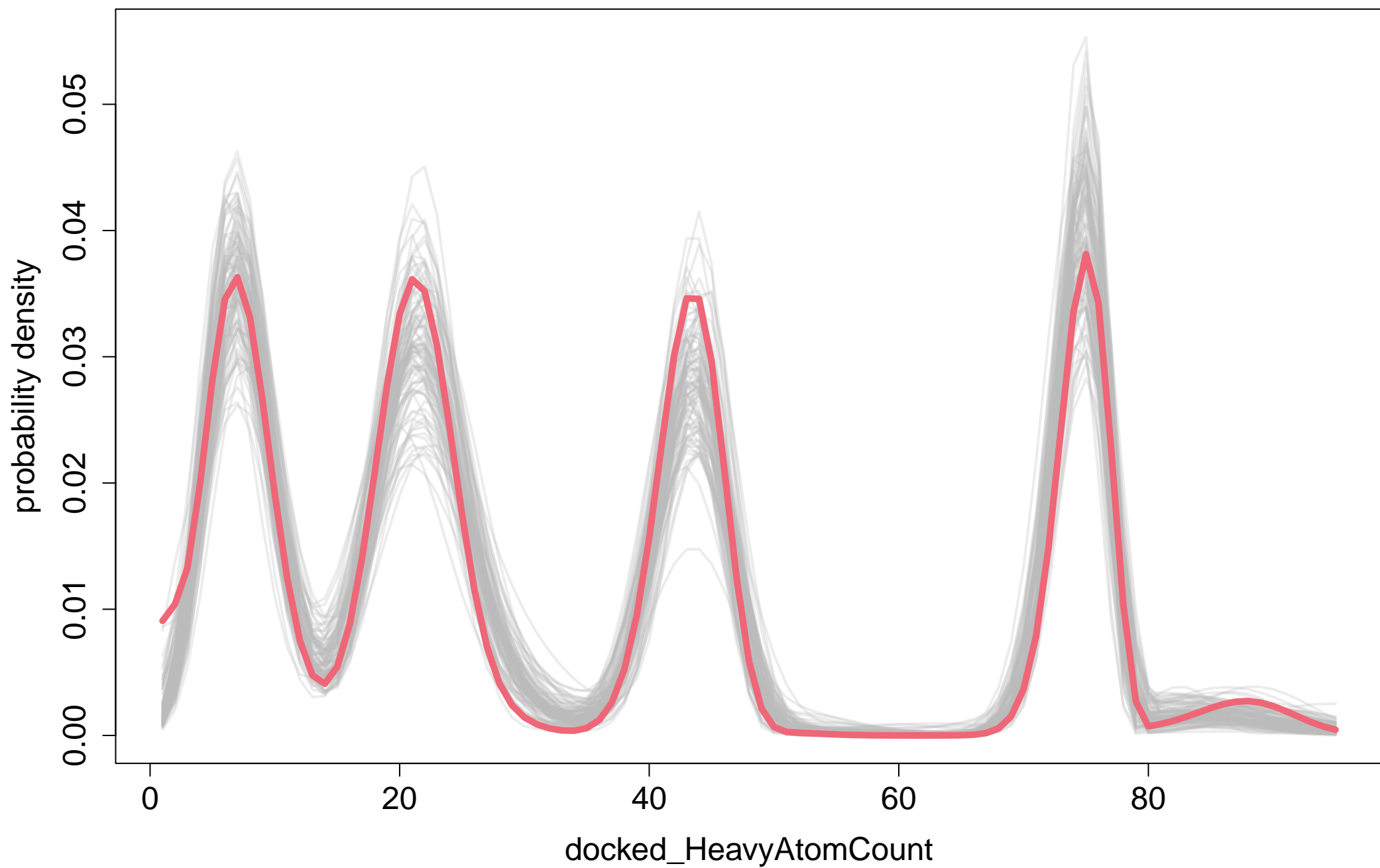
Occupied clusters: 9 of 16

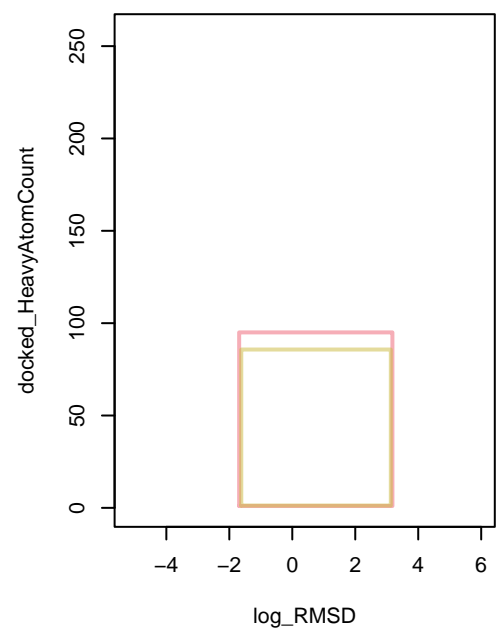
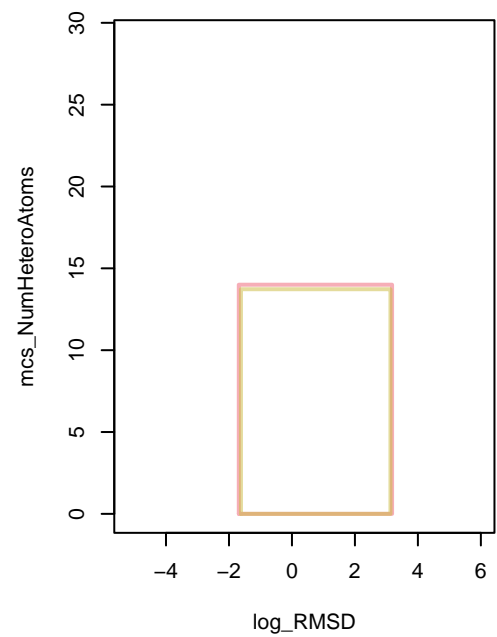
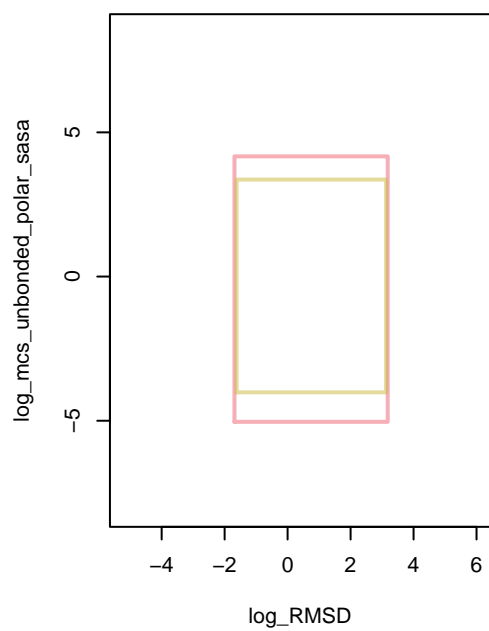
LL: -2160 +- 6.9



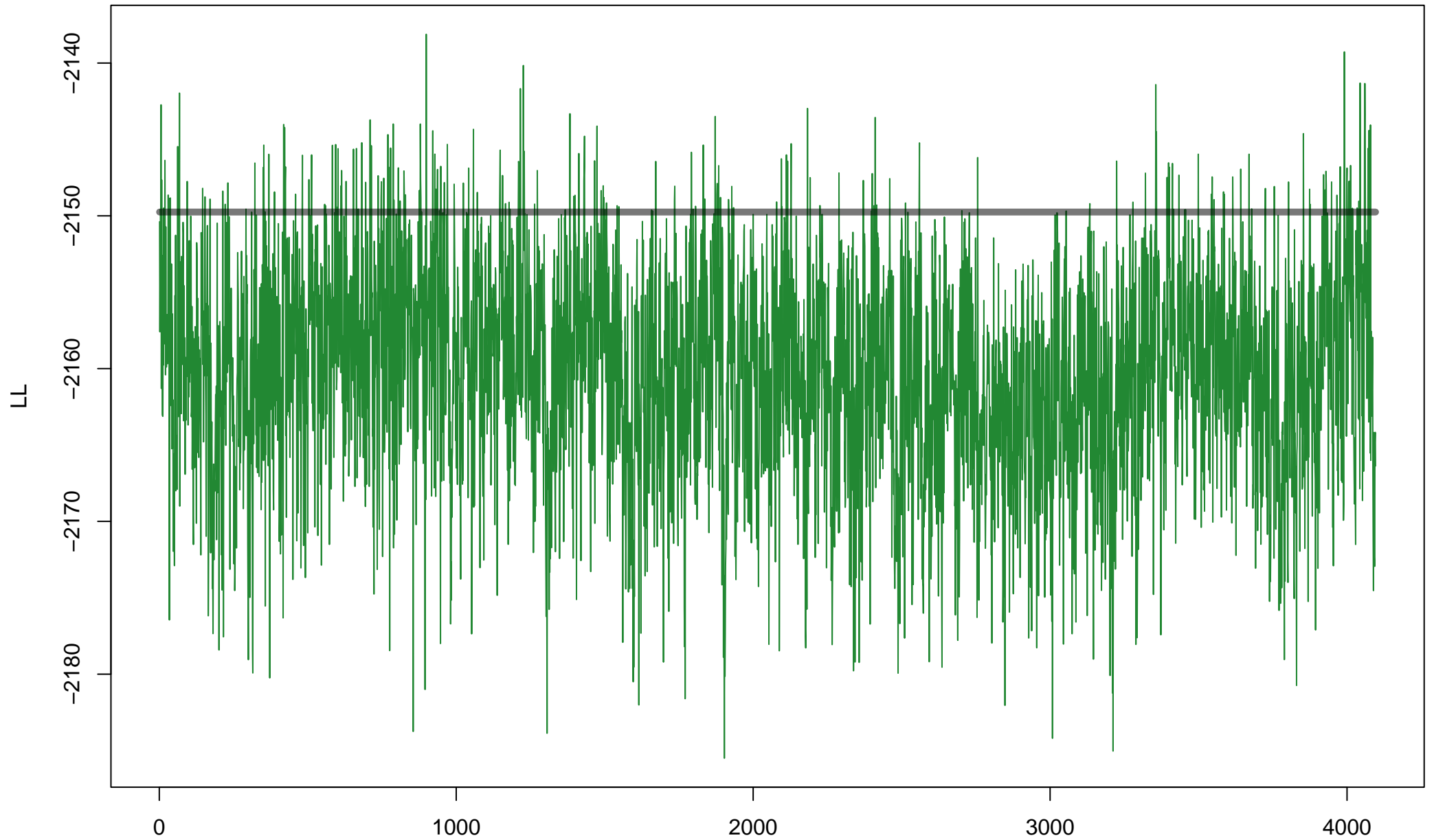




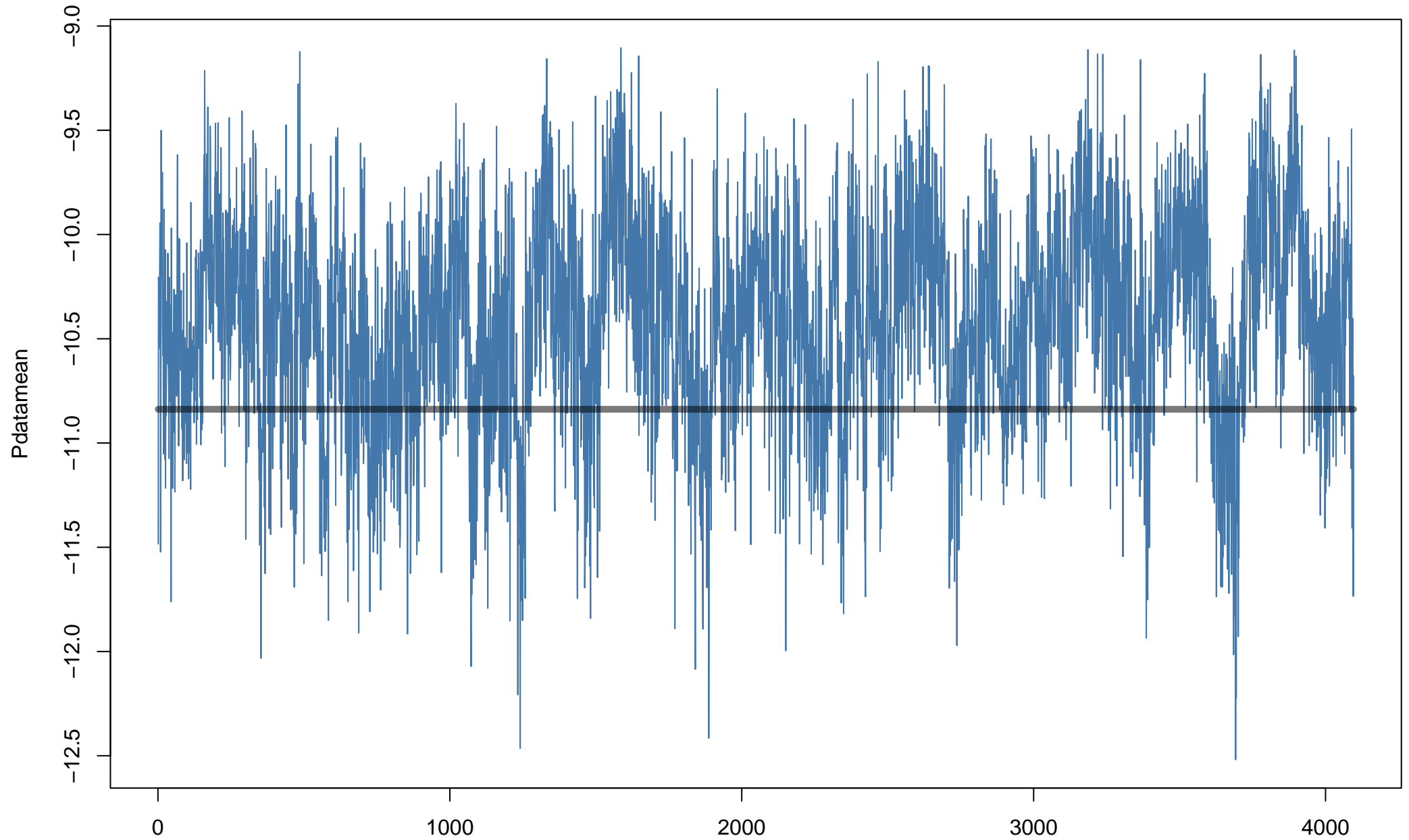




LL

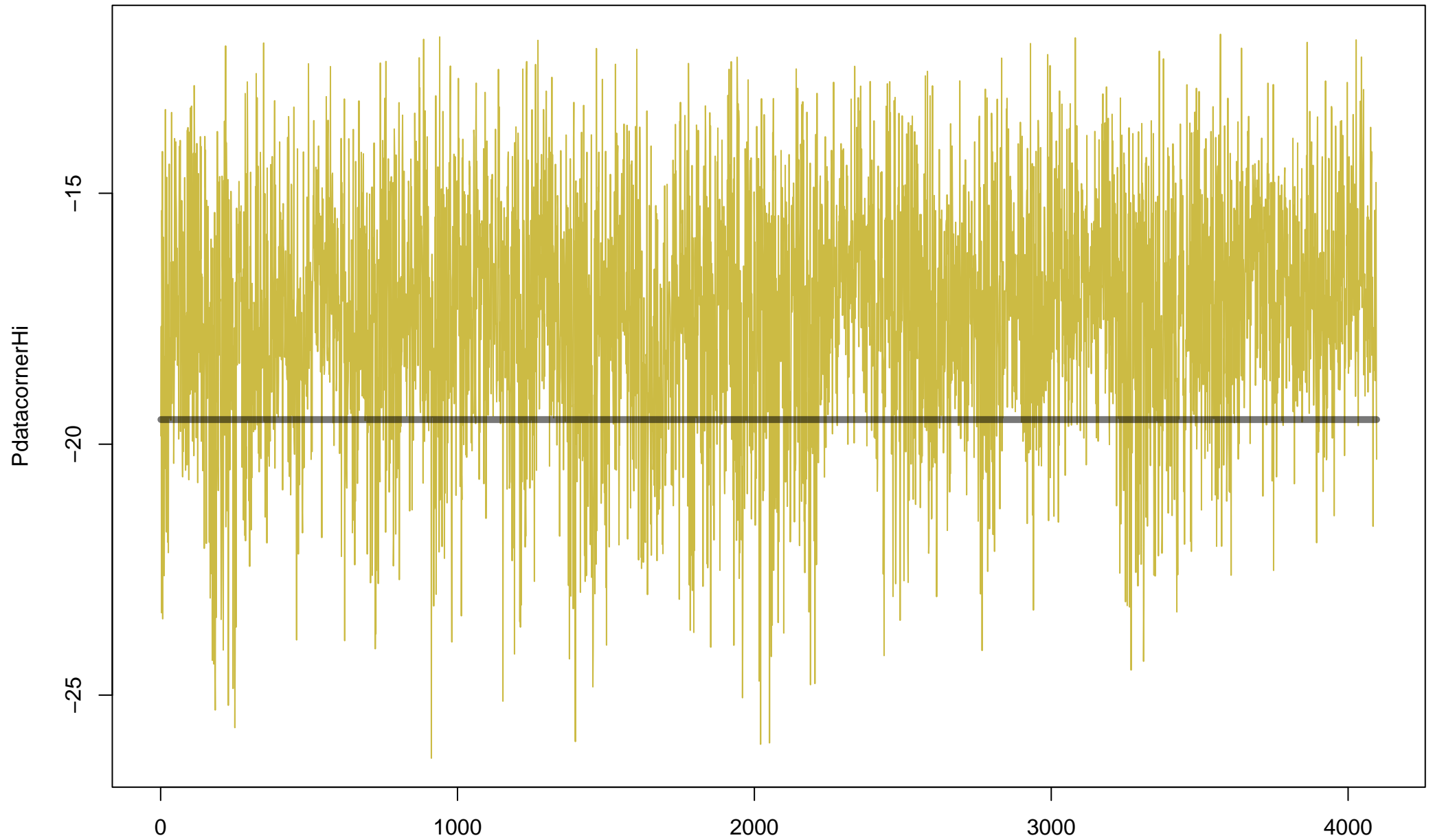


**Pdatamean**  
**ESS = 160 | BMK = 0.0799 | MCSE(6.27) = 6.42 | stat: TRUE | burn: 0 | rel.err: 0.836**



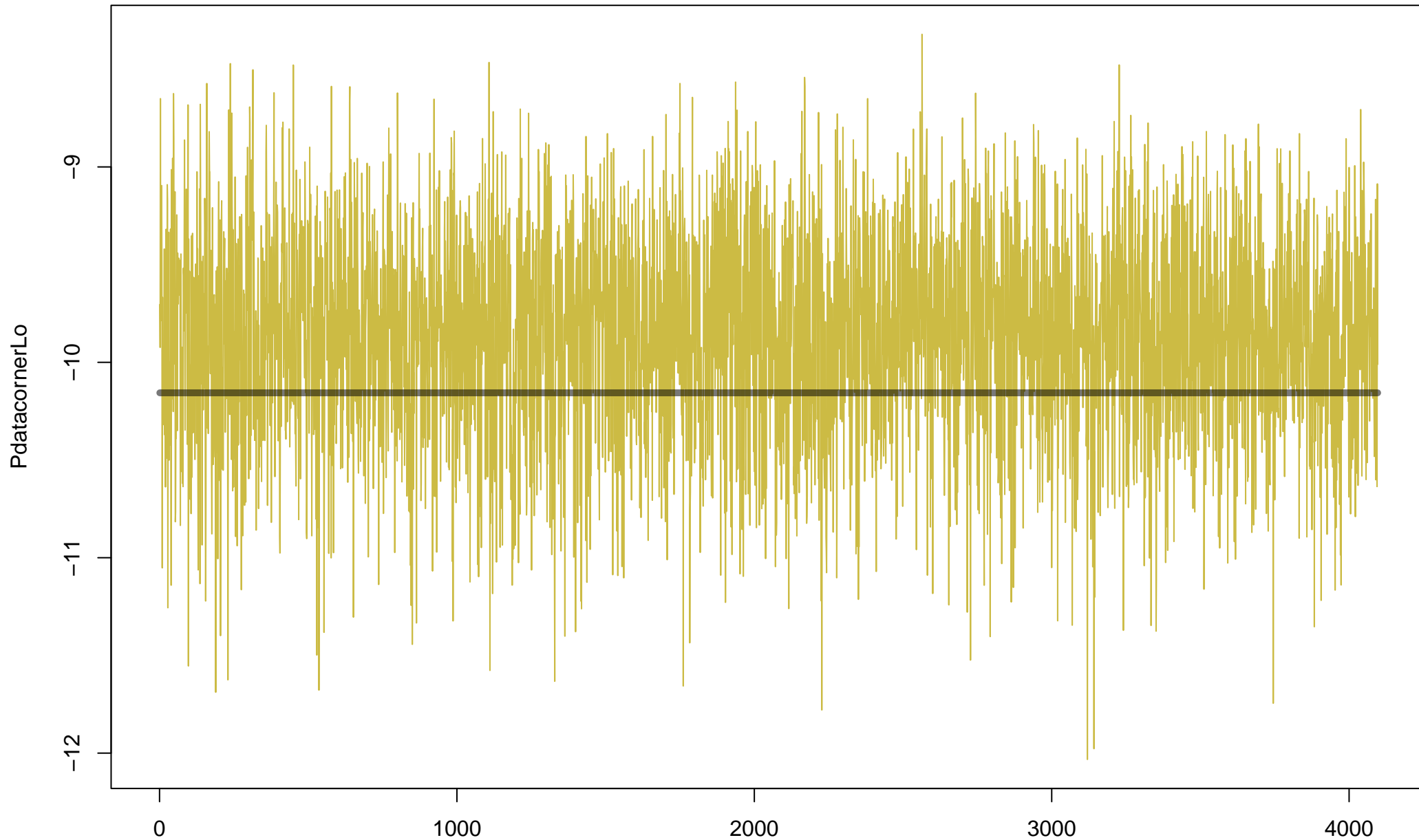


**PdatacornerHi**  
**ESS = 4100 | BMK = 0.126 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: 0.351**

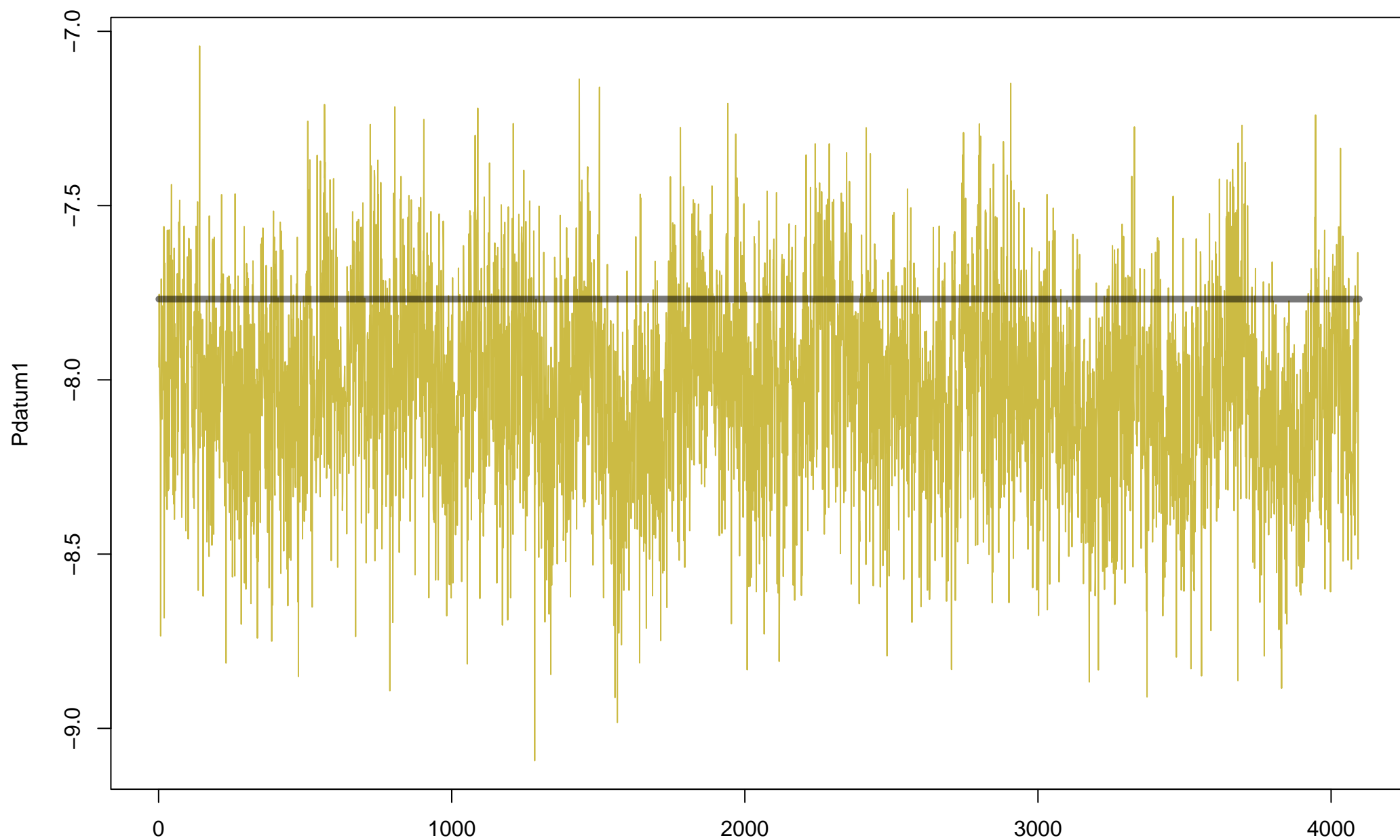


# PdatacornerLo

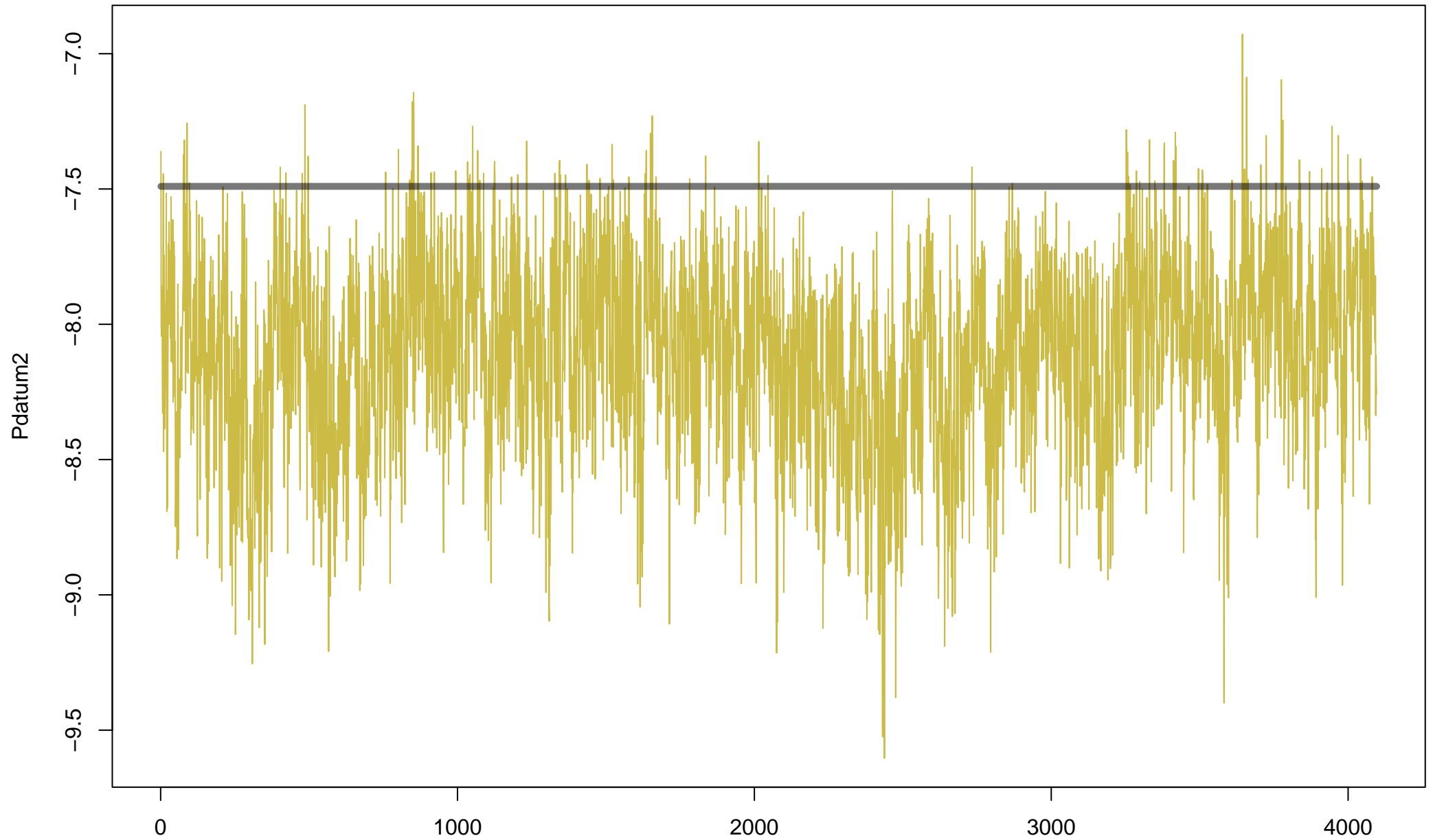
ESS = 3670 | BMK = 0.0438 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: 0.661



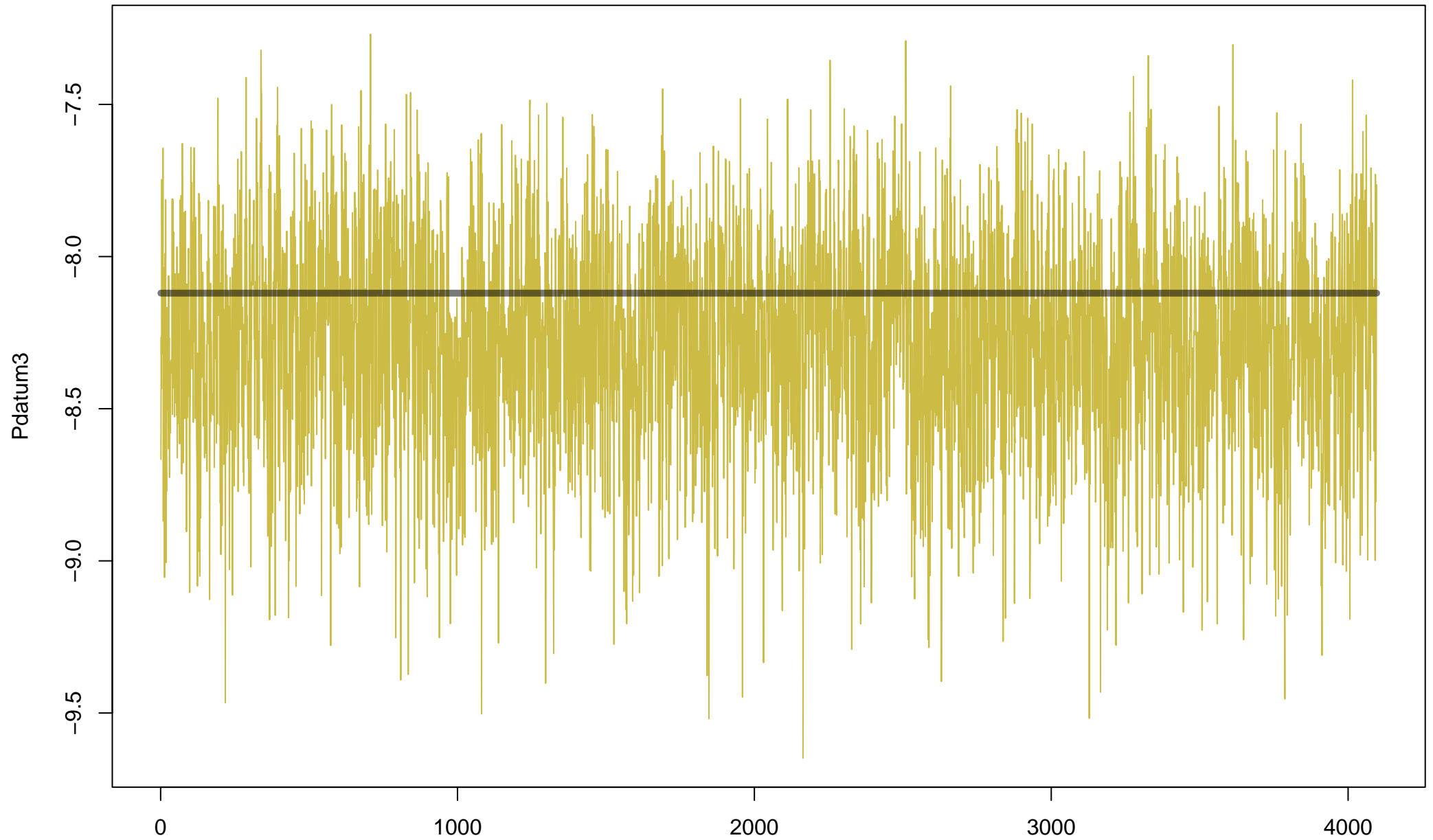
**Pdatum1**  
**ESS = 380 | BMK = 0.0517 | MCSE(6.27) = 4.06 | stat: TRUE | burn: 0 | rel.err: -0.862**



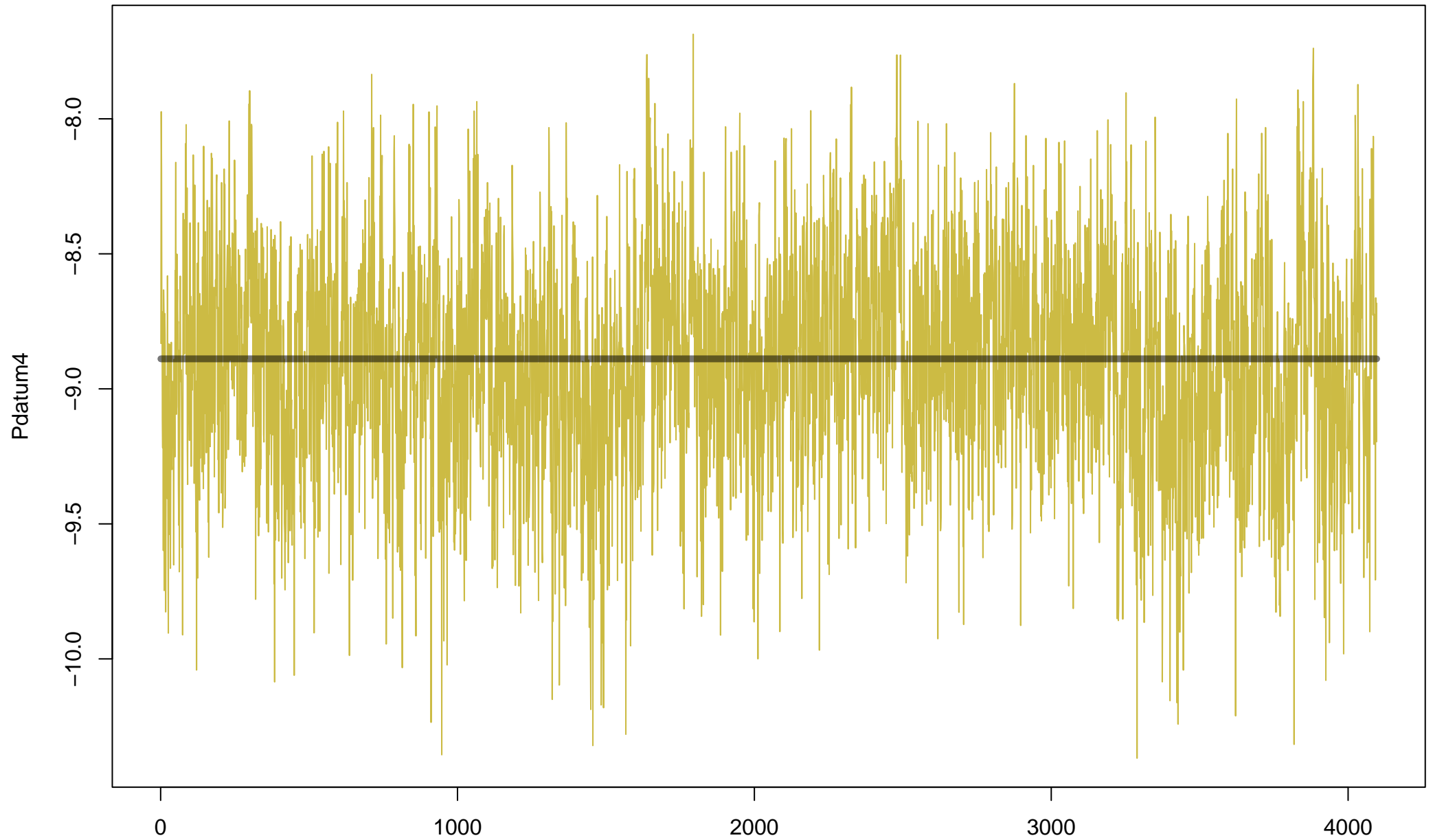
**Pdatum2**  
**ESS = 346 | BMK = 0.0442 | MCSE(6.27) = 5.3 | stat: TRUE | burn: 0 | rel.err: -2.23**



**Pdatum3**  
**ESS = 1840 | BMK = 0.0433 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: -0.321**

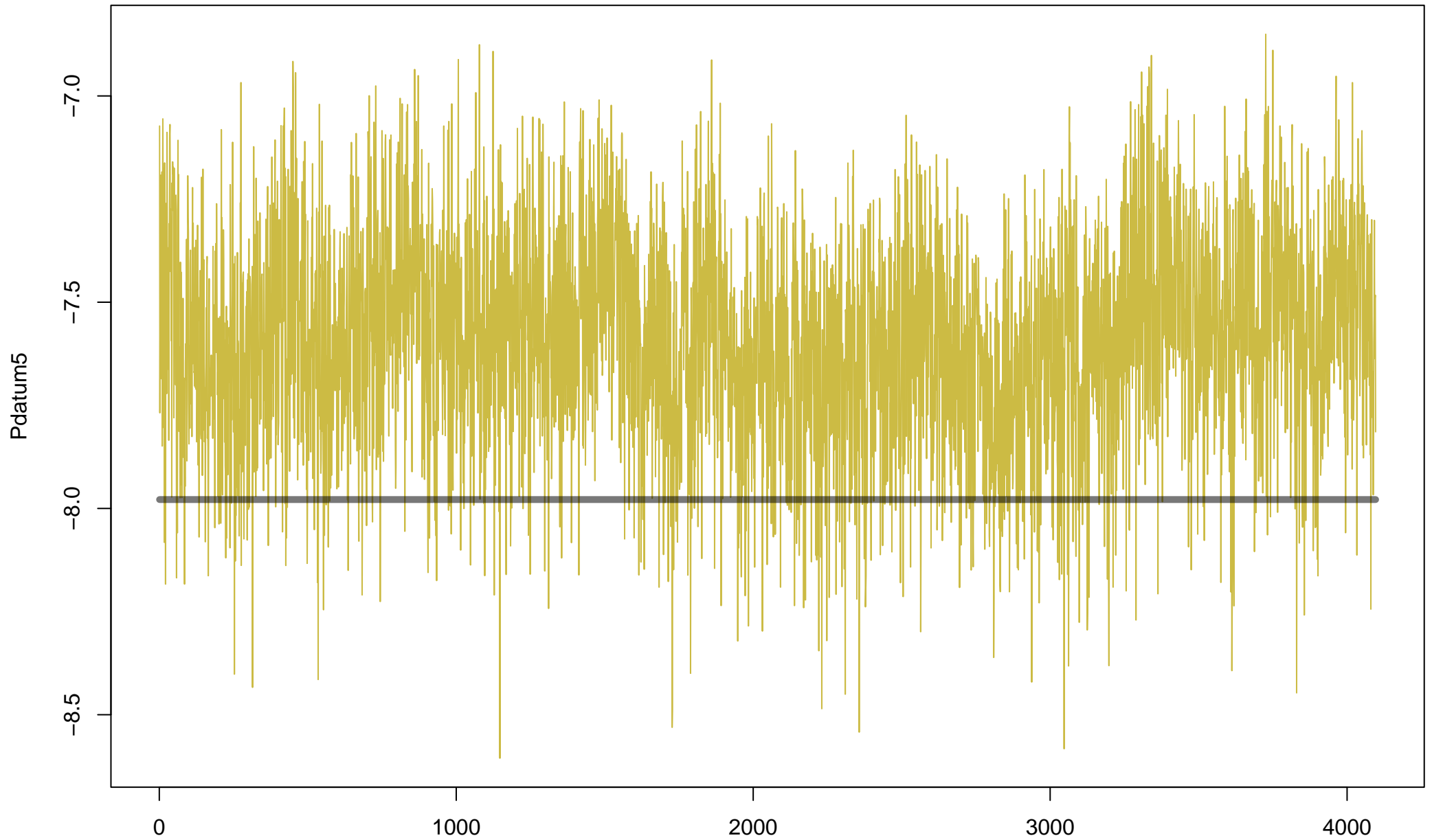


**Pdatum4**  
**ESS = 900 | BMK = 0.0438 | MCSE(6.27) = 3.75 | stat: TRUE | burn: 0 | rel.err: 0.149**



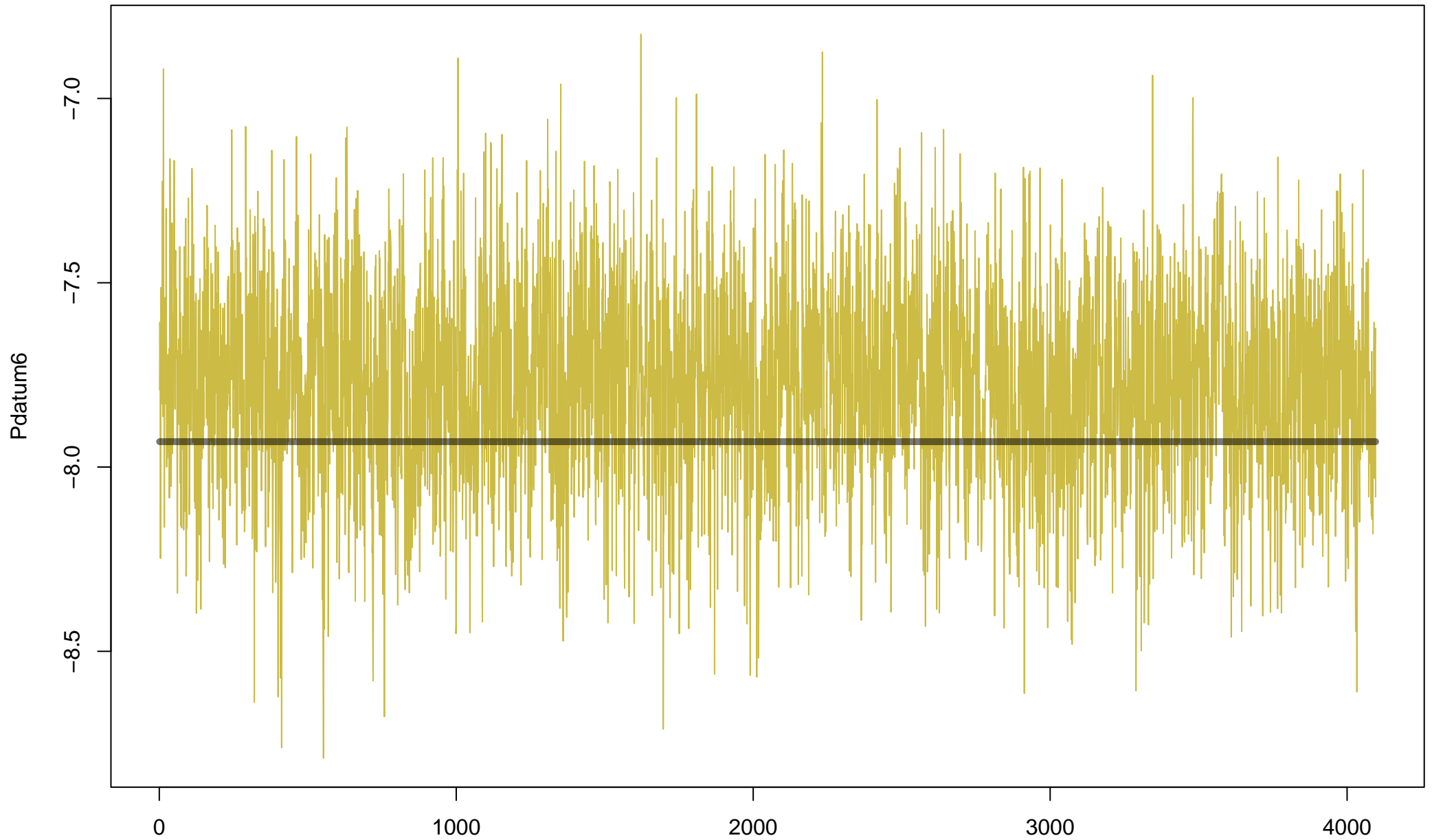
**Pdatum5**

**ESS = 318 | BMK = 0.0543 | MCSE(6.27) = 4.23 | stat: TRUE | burn: 0 | rel.err: 1.35**



**Pdatum6**

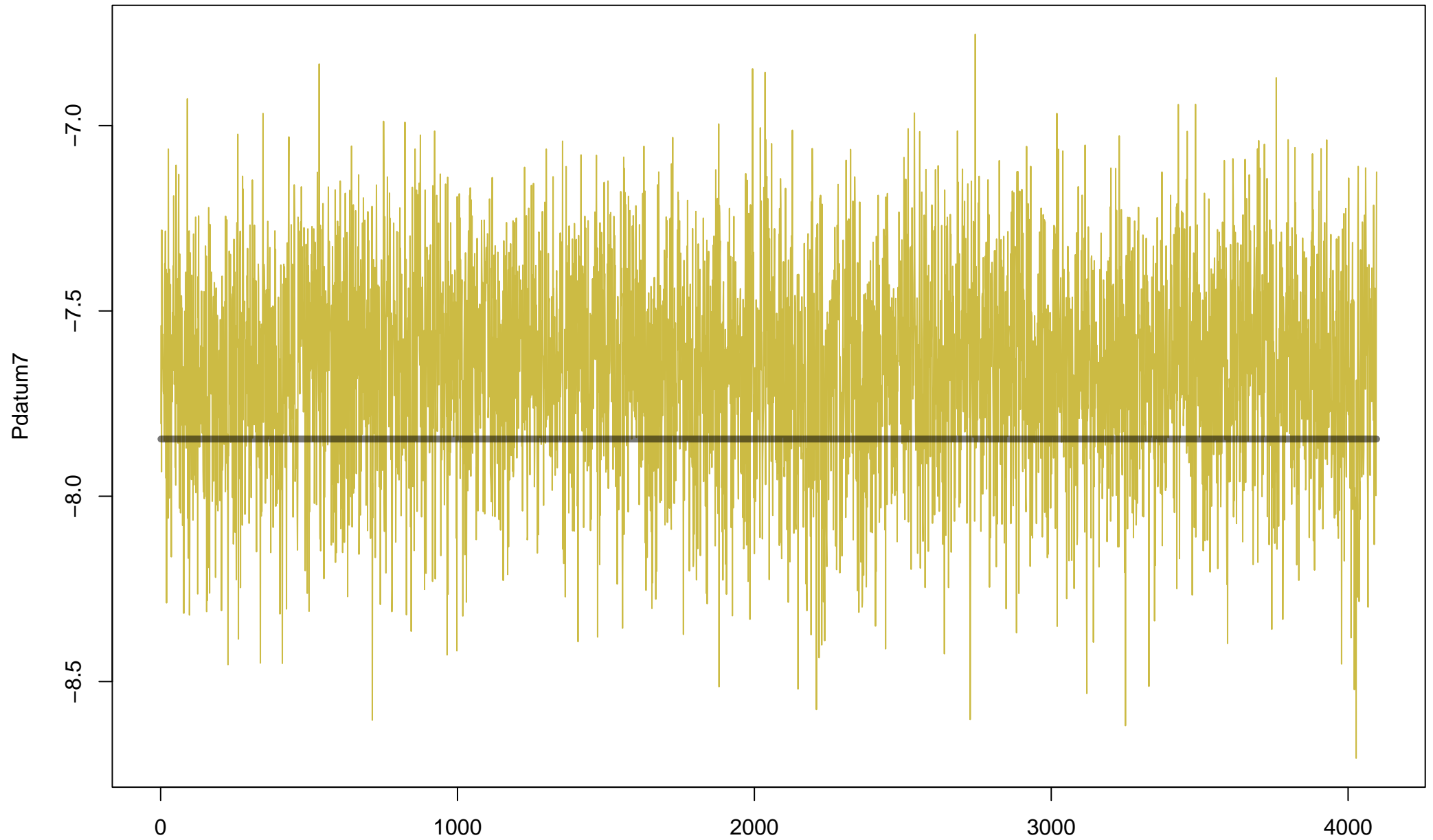
**ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: 0.651**





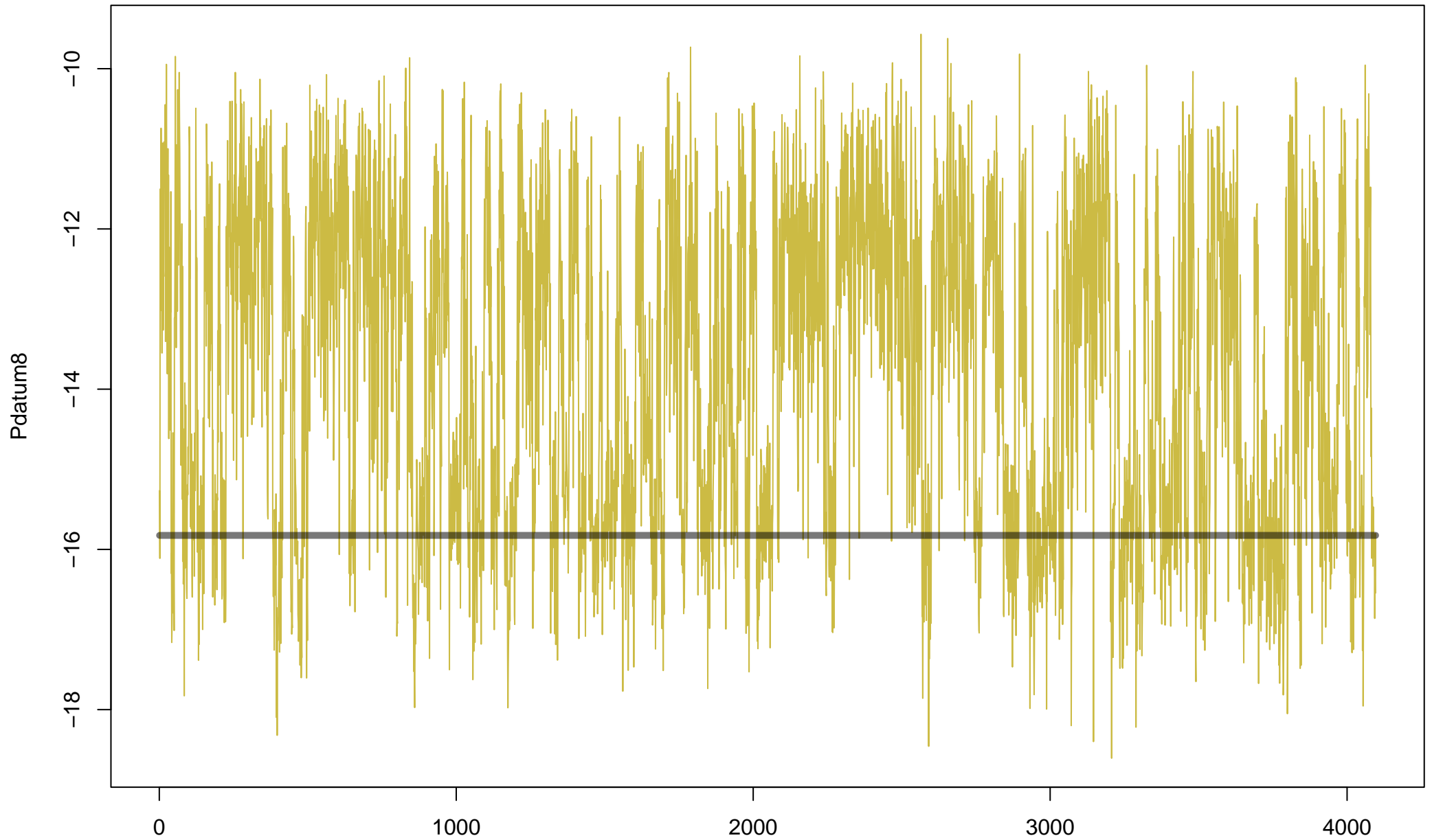
**Pdatum7**

**ESS = 4100 | BMK = 0.0336 | MCSE(6.27) = 1.88 | stat: FALSE | burn: 0 | rel.err: 0.757**

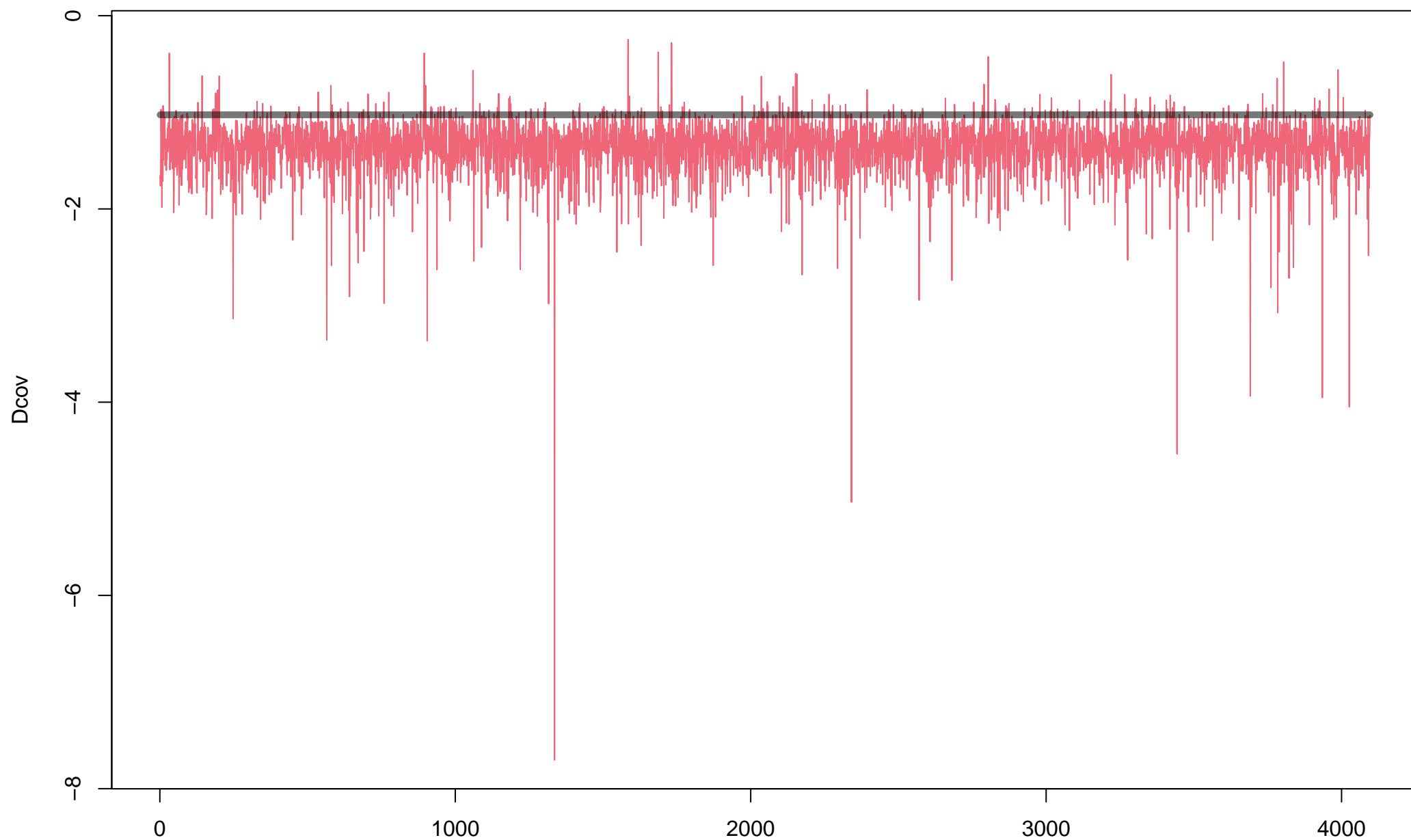


**Pdatum8**

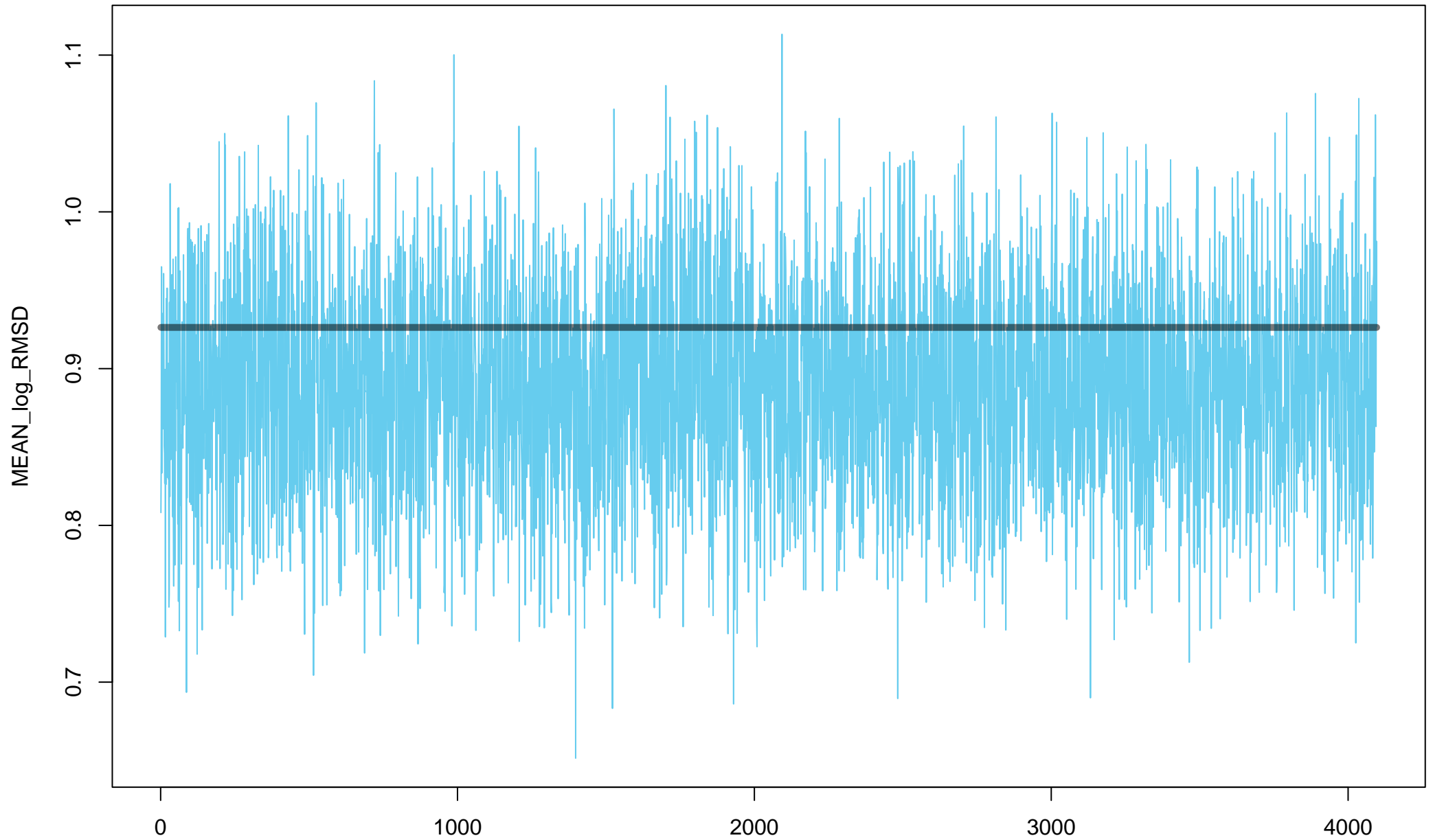
**ESS = 481 | BMK = 0.0464 | MCSE(6.27) = 4.3 | stat: TRUE | burn: 0 | rel.err: 0.591**



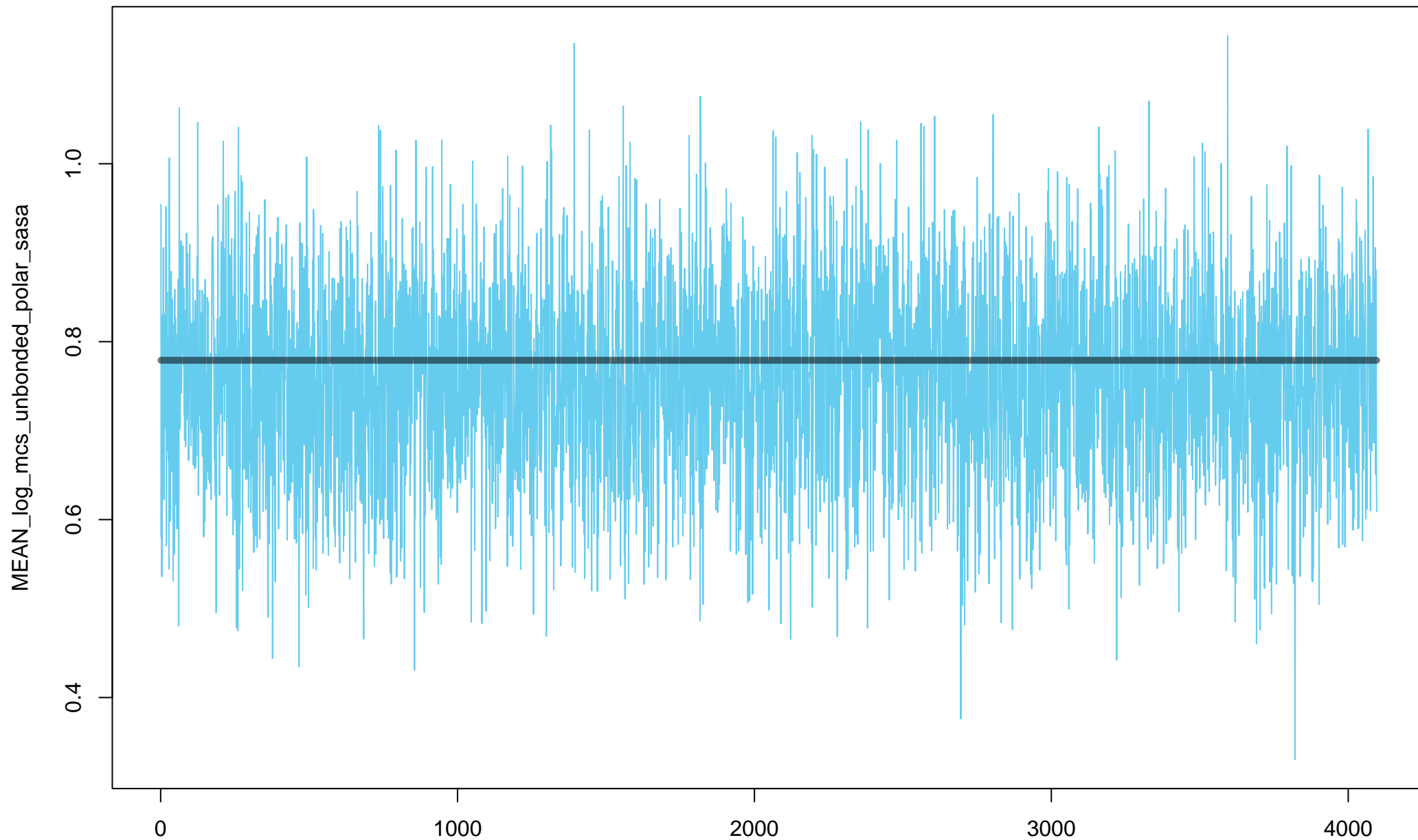
**Dcov**  
**ESS = 4100 | BMK = 0.0622 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 1.35**



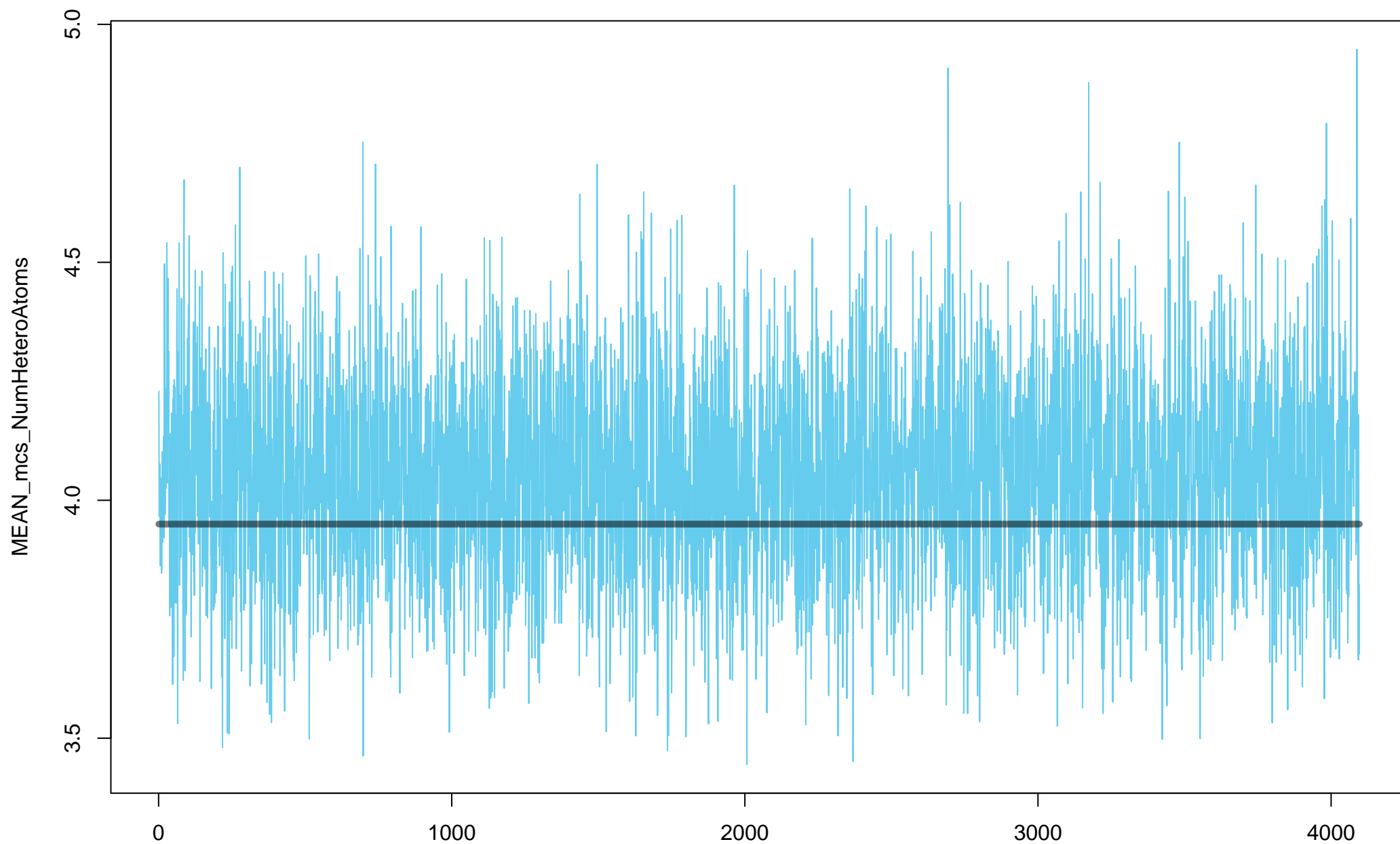
**MEAN\_log\_RMSD**  
**ESS = 4100 | BMK = 0.0437 | MCSE(6.27) = 1.48 | stat: TRUE | burn: 0 | rel.err: -0.589**



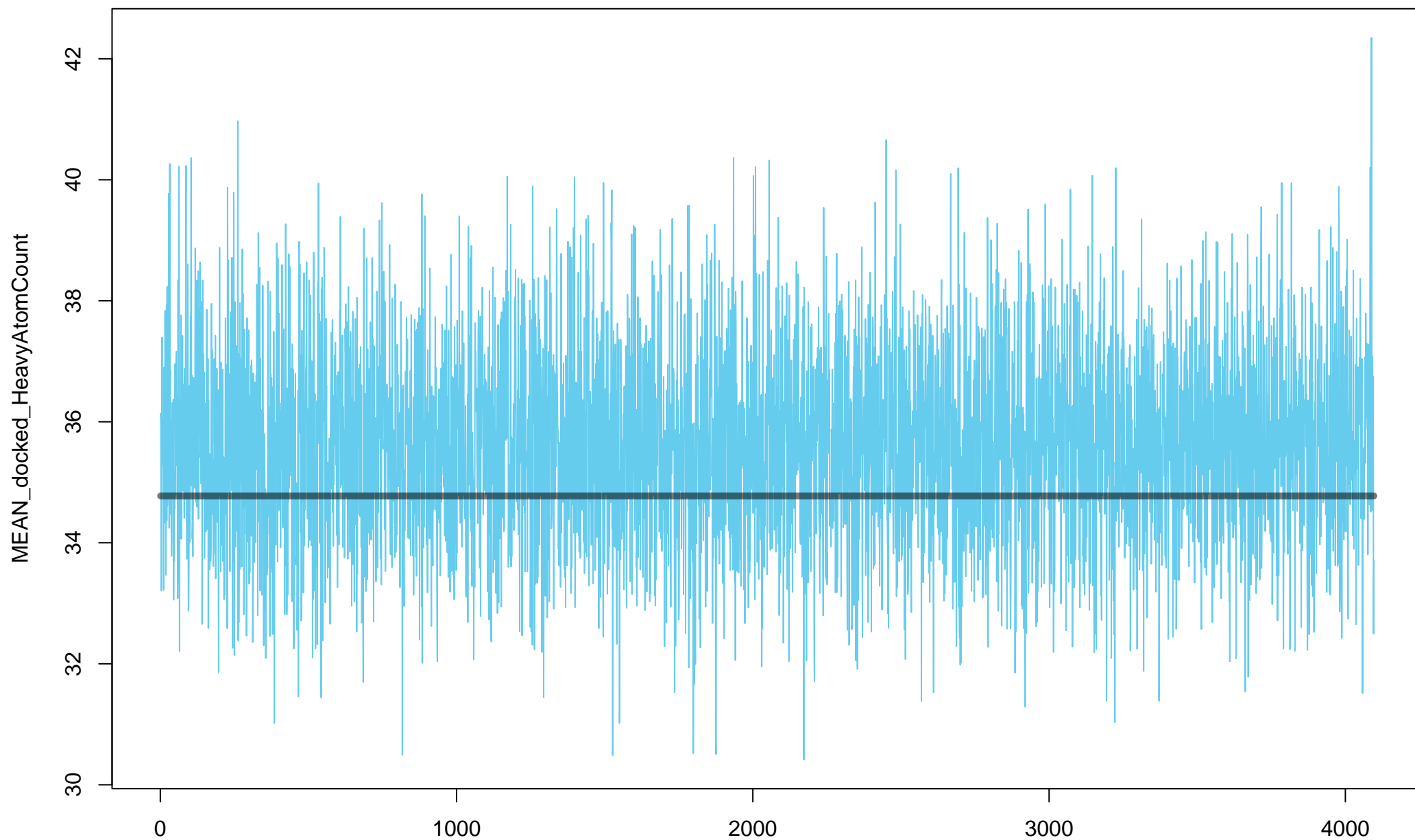
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 4100 | BMK = 0.0266 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0 | rel.err: -0.205**



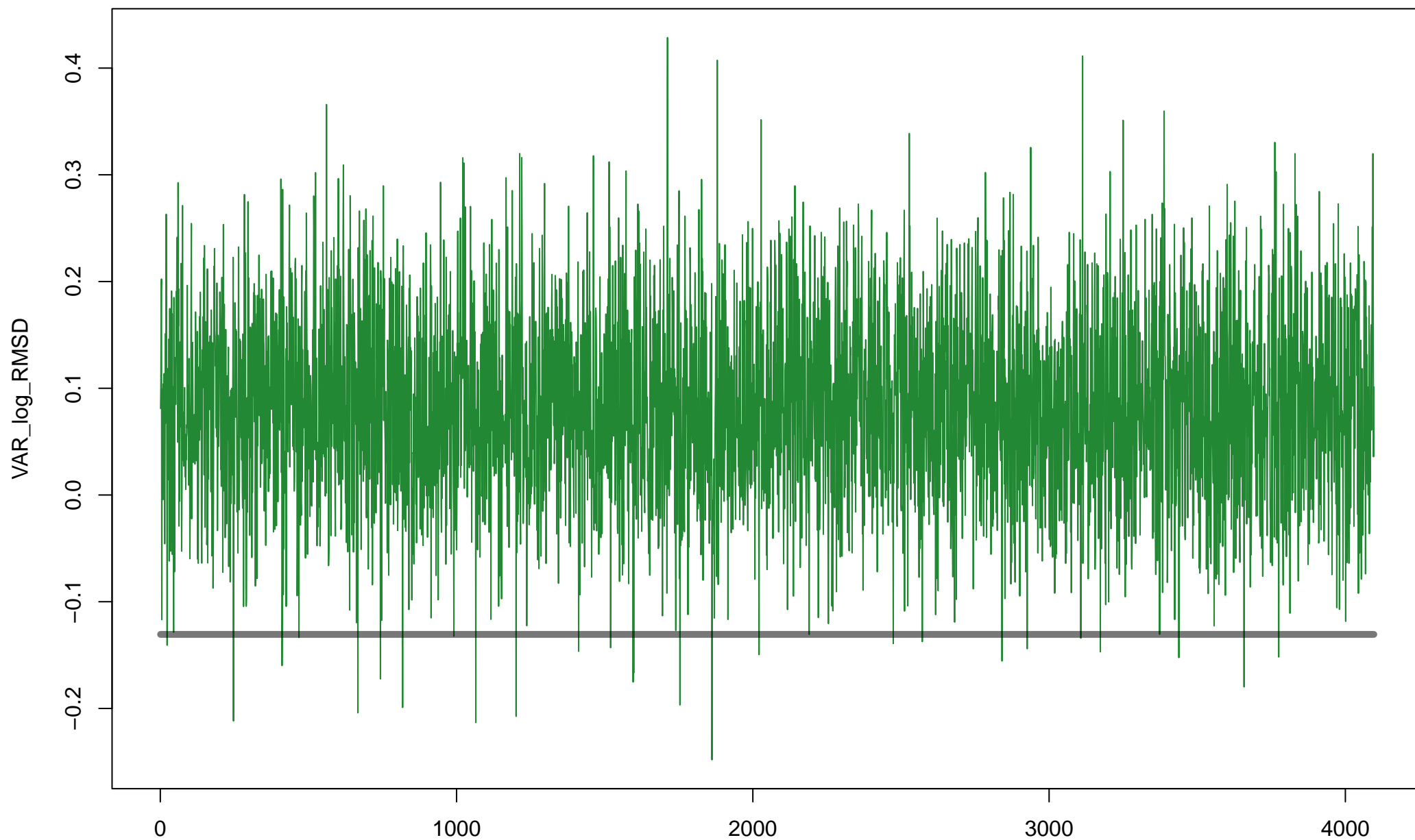
**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 4100 | BMK = 0.0415 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.491**



**MEAN\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.04 | MCSE(6.27) = 1.37 | stat: TRUE | burn: 0 | rel.err: 0.519**

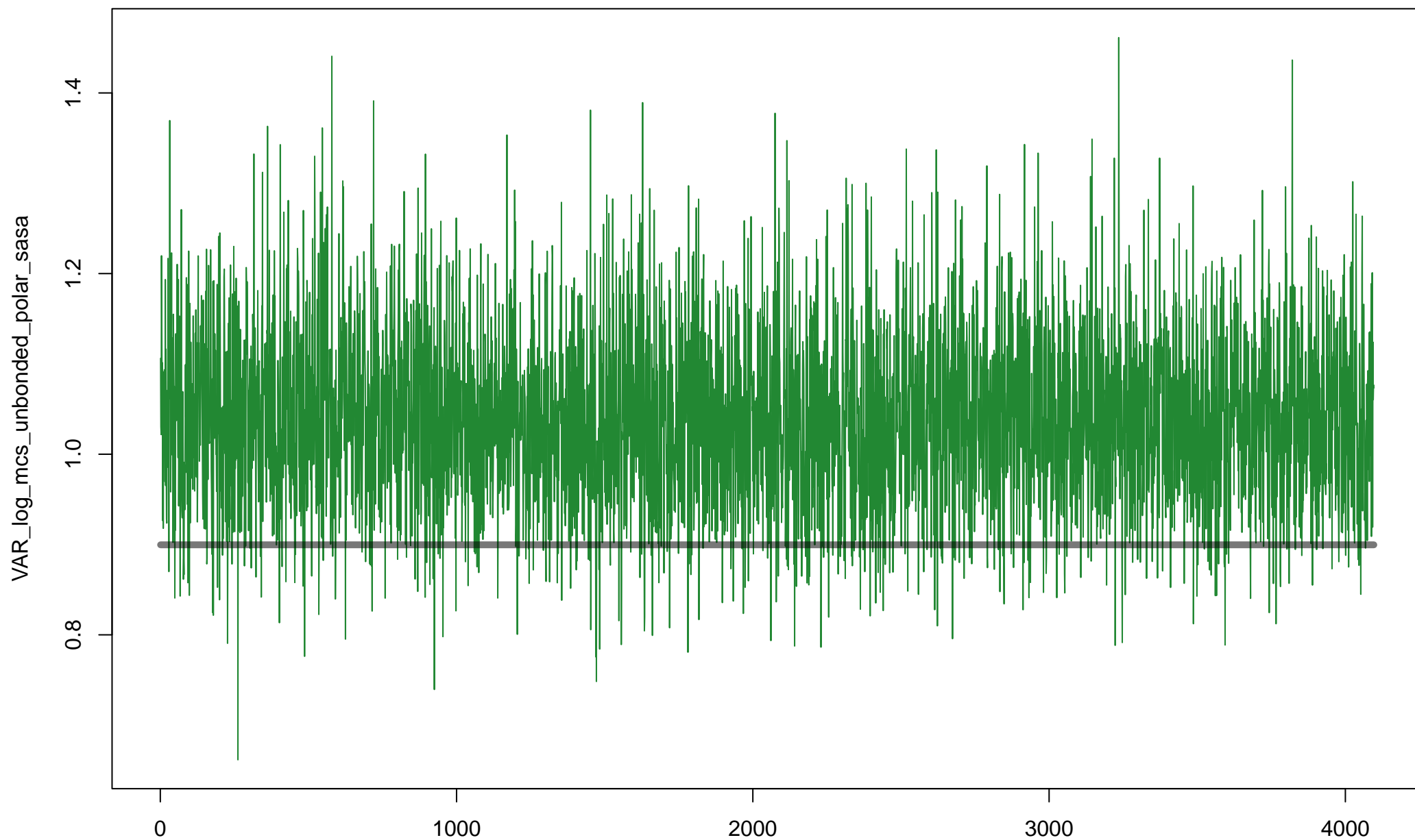


**VAR\_log\_RMSD**  
**ESS = 4100 | BMK = 0.0444 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 2.27**

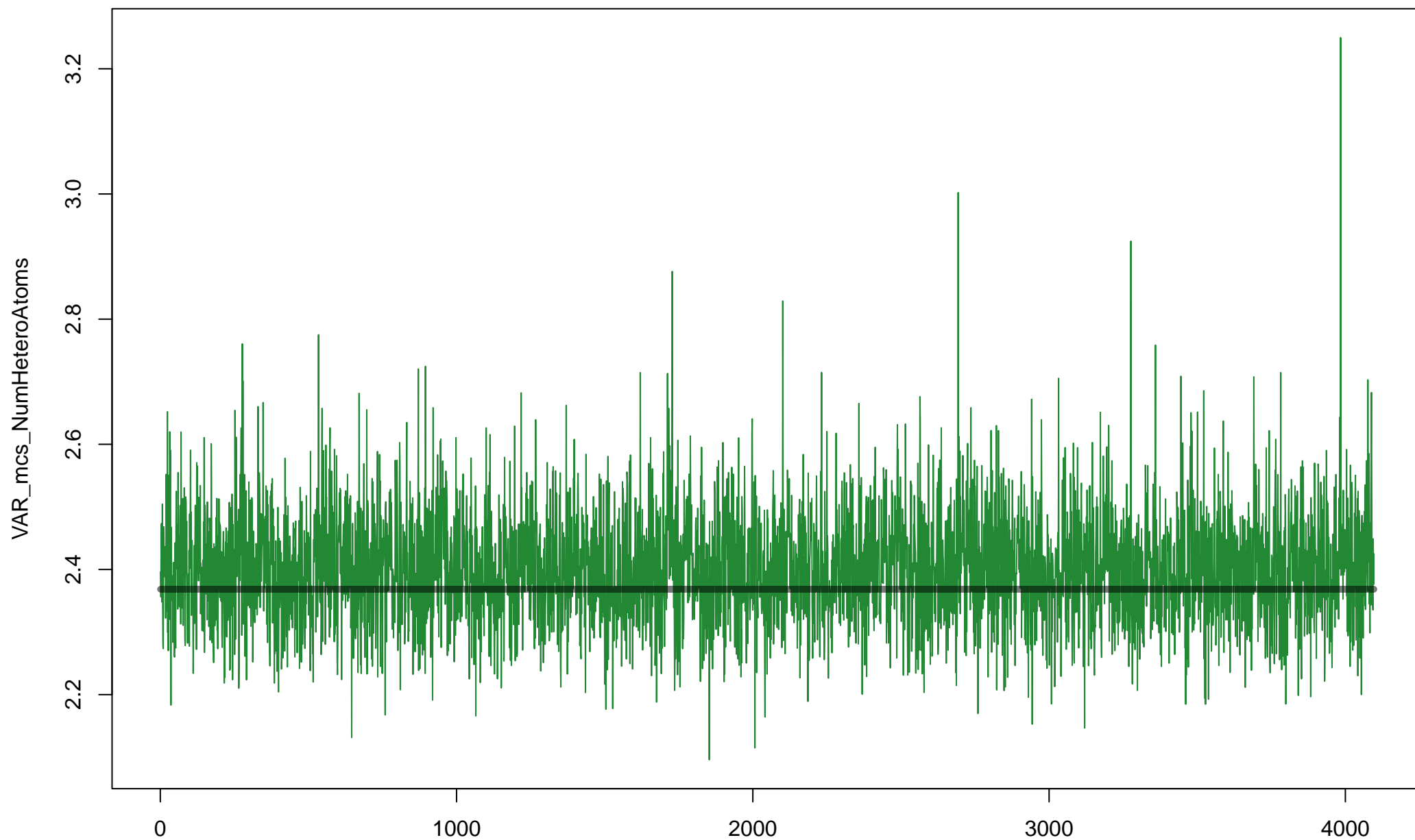




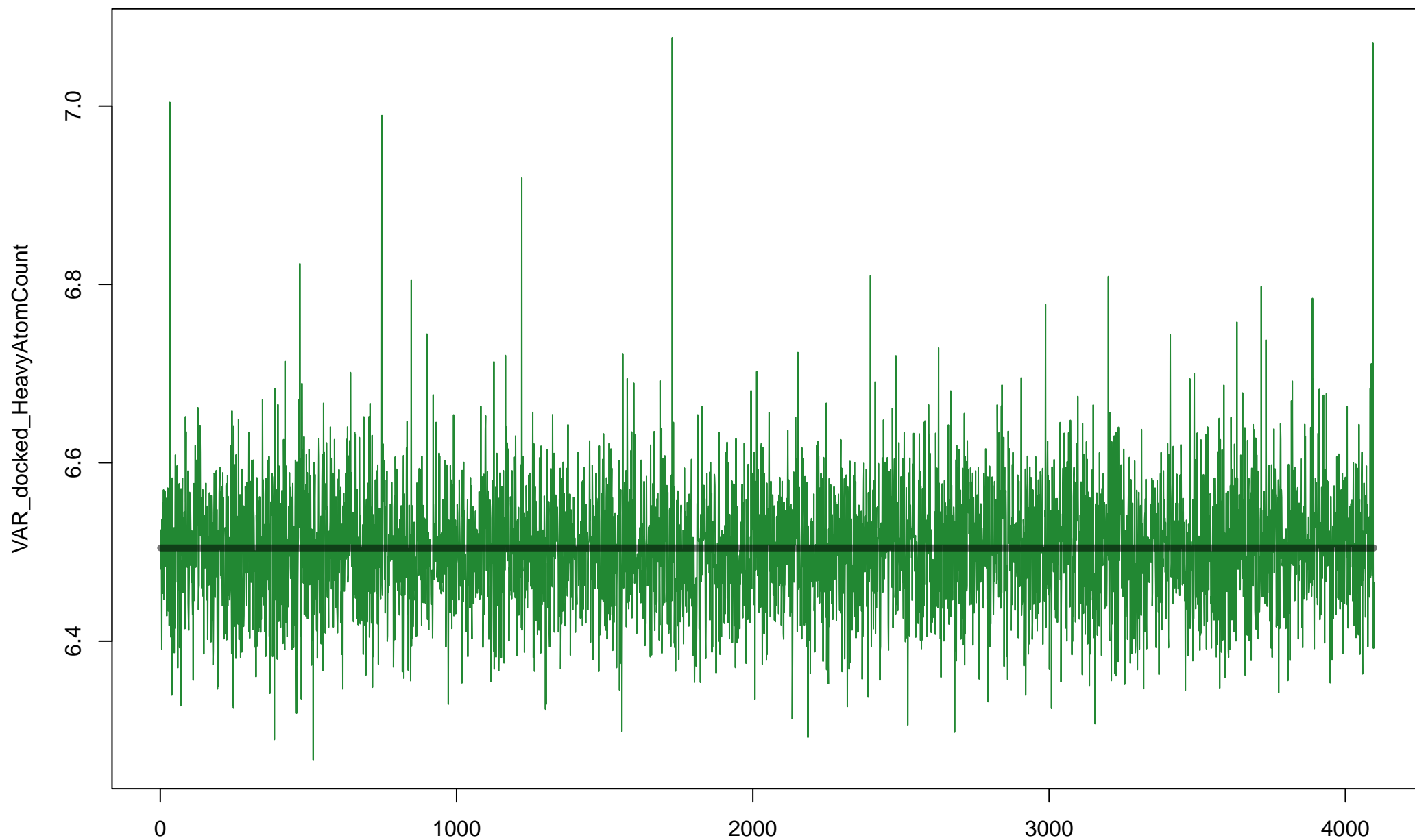
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 4100 | BMK = 0.0431 | MCSE(6.27) = 1.2 | stat: TRUE | burn: 0 | rel.err: 1.35**



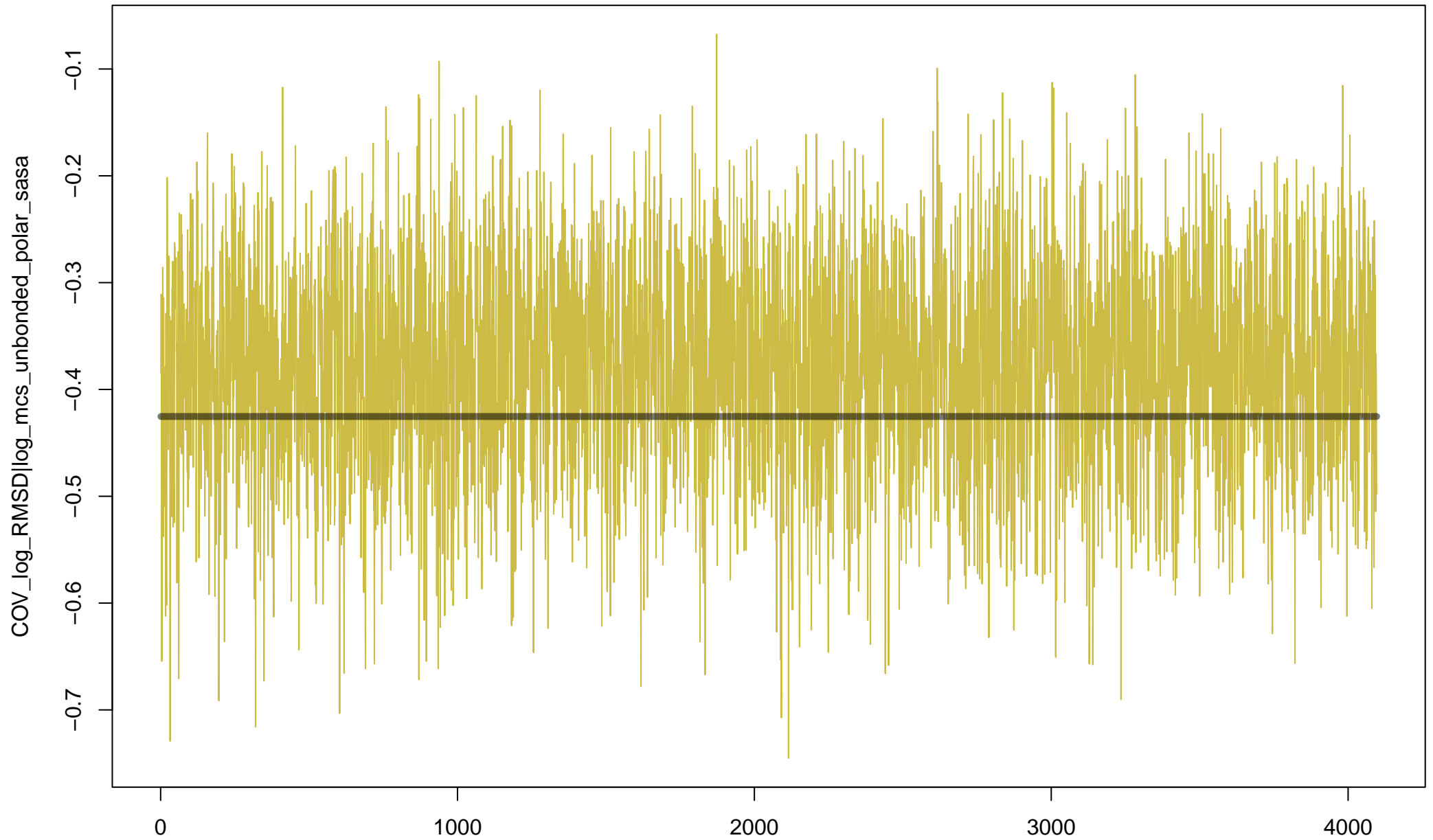
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 3140 | BMK = 0.05 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 0.402**



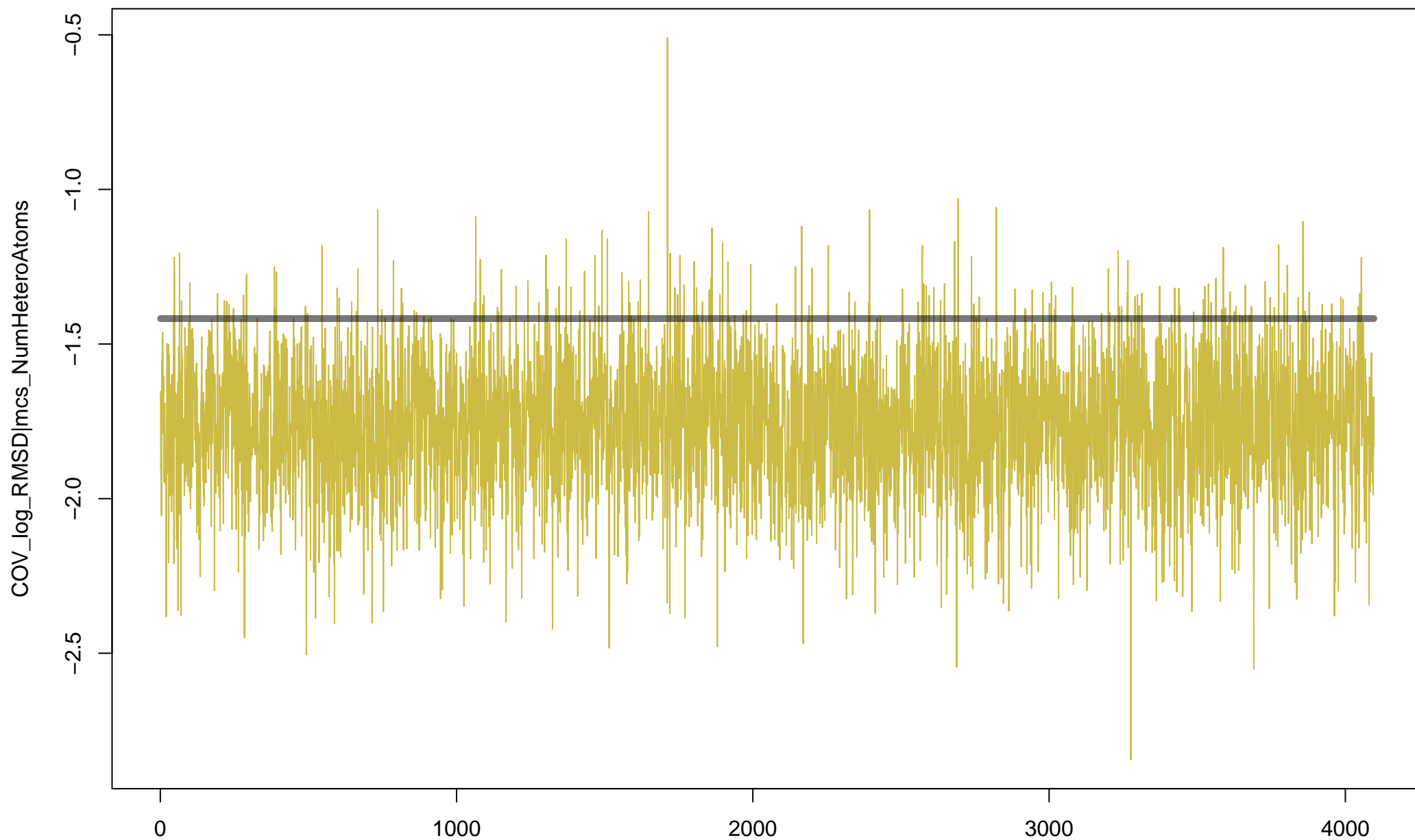
**VAR\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0454 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: 0.0485**



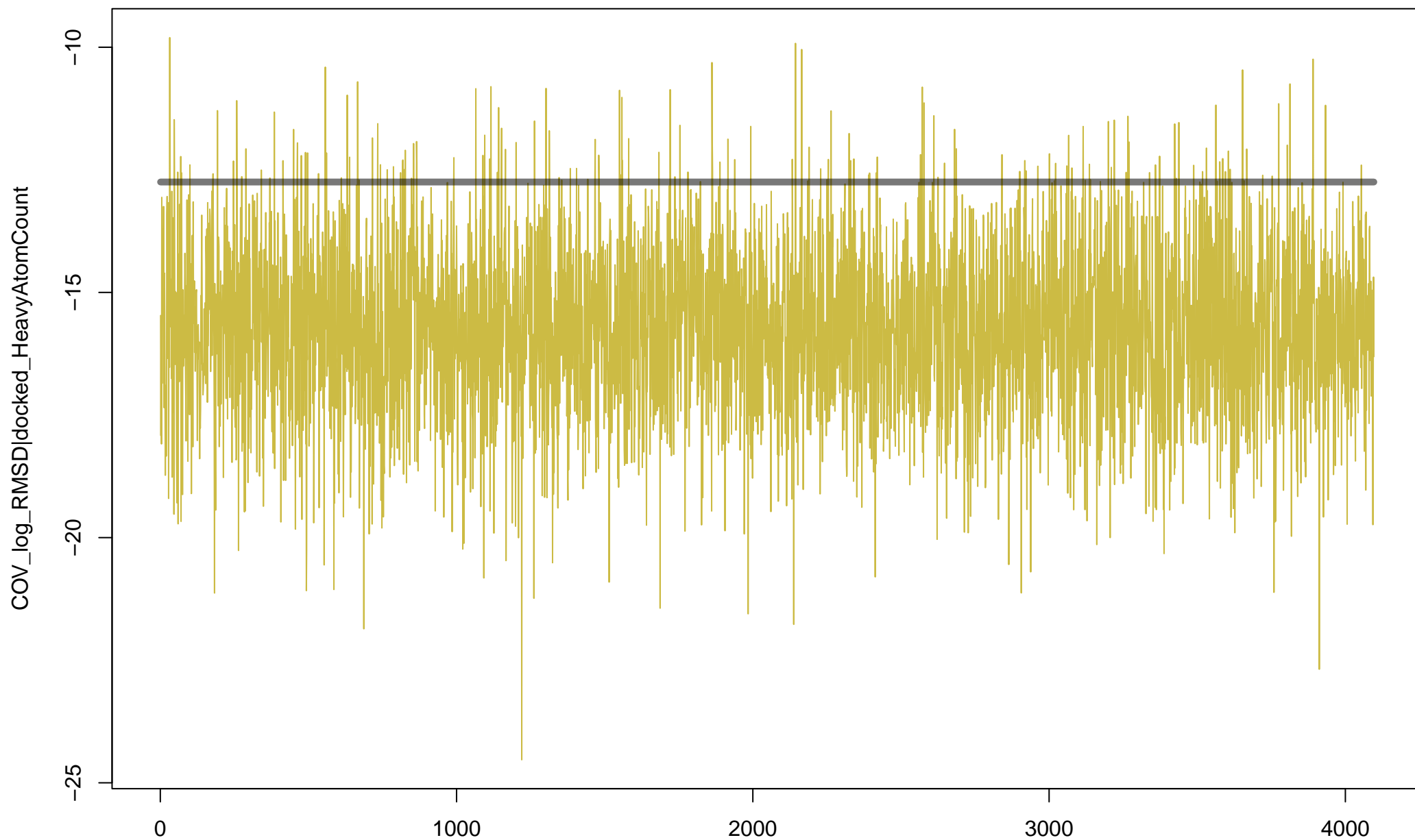
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 3630 | BMK = 0.026 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: 0.474**



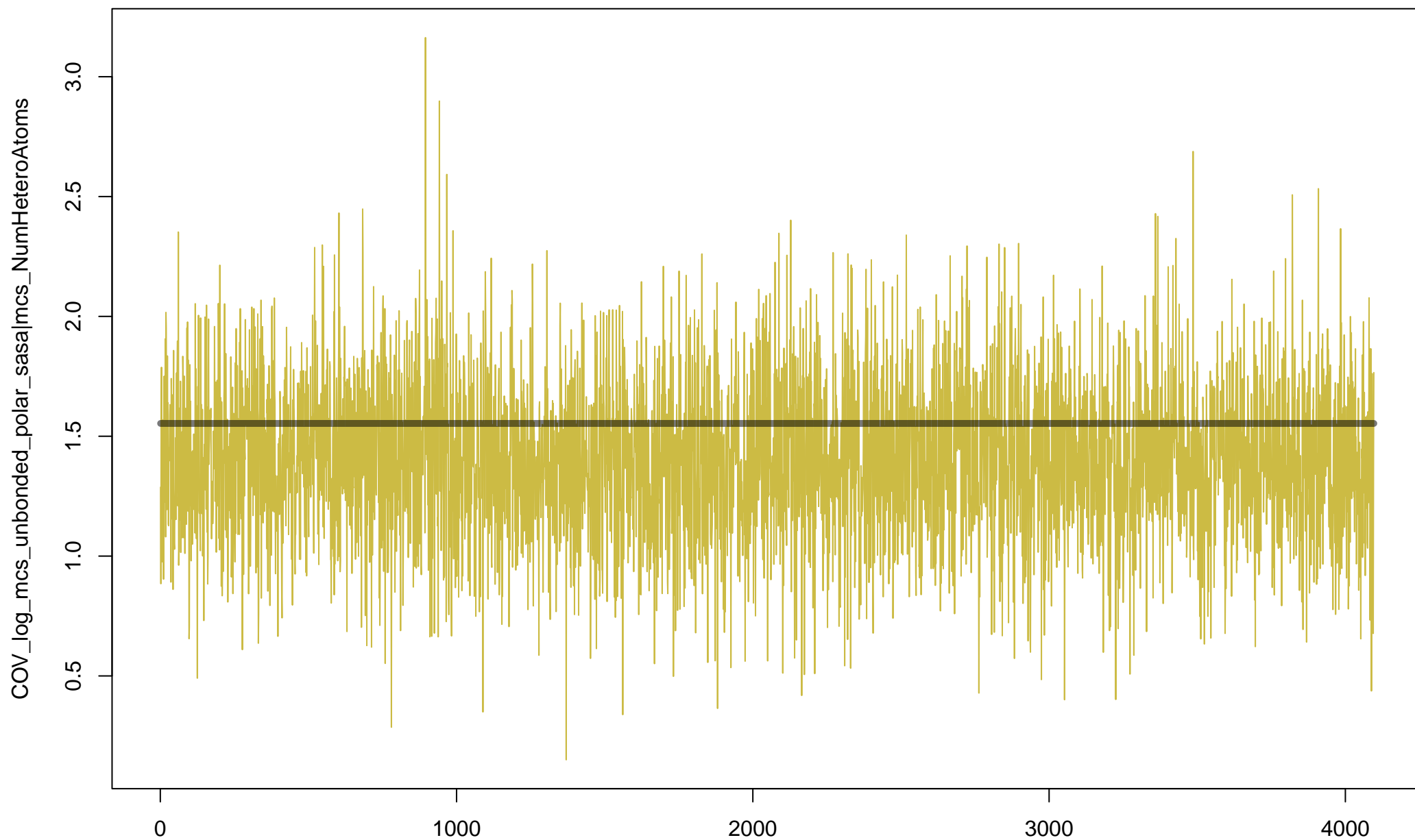
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 4100 | BMK = 0.0452 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: -1.6**



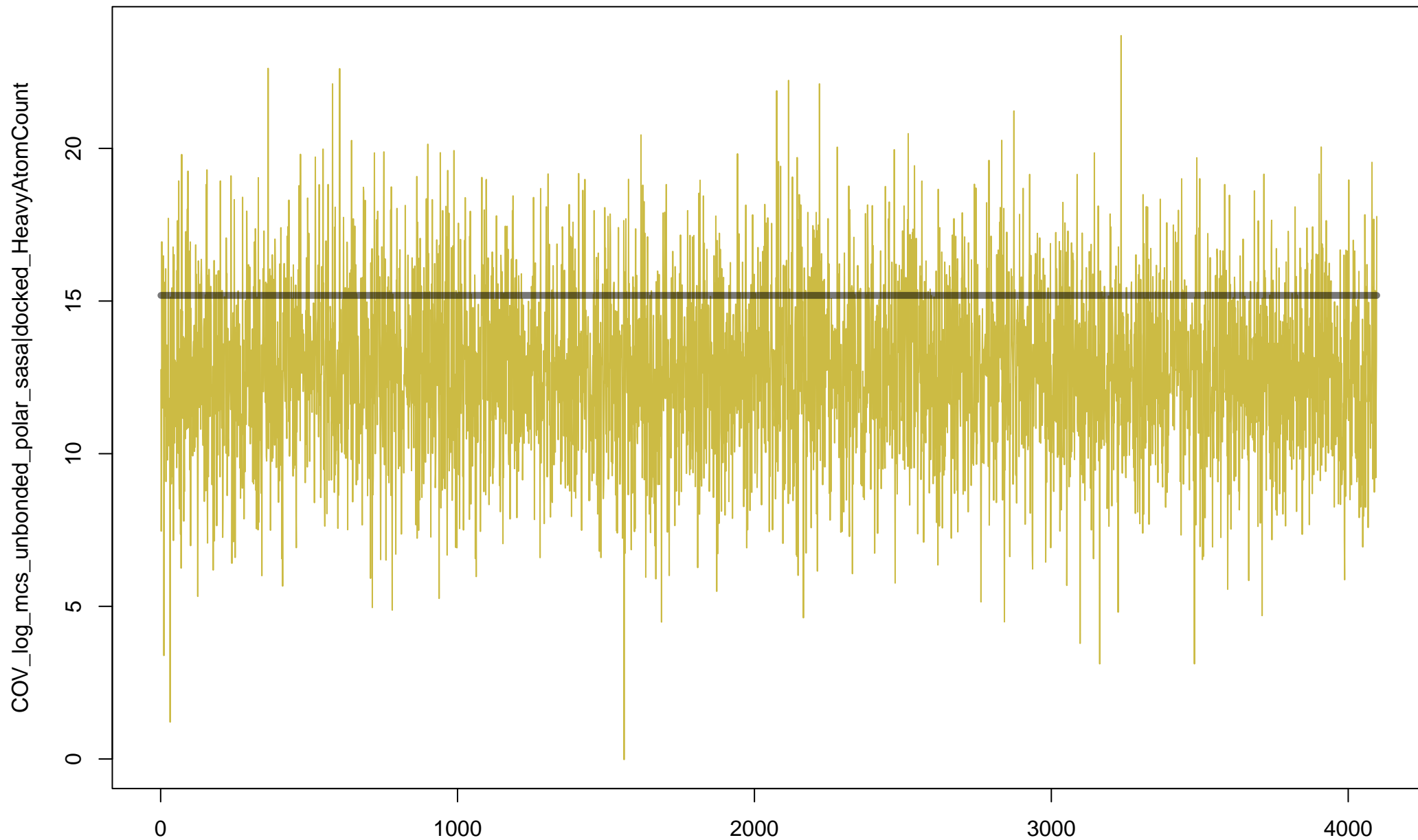
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0384 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: -1.75**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 4100 | BMK = 0.0445 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: -0.465**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.035 | MCSE(6.27) = 1.34 | stat: TRUE | burn: 0 | rel.err: -0.919**





**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0442 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.467**

