

-- STATS maxD --

min ESS = 142.264080778136

max BMK = 0.117980622864252

max MCSE = 6.89093211359896

all stationary: FALSE

burn: 0

max rel.err.: 2.17133114975167

-- STATS 1D --

min ESS = 2984.33624440196

max BMK = 0.0471441449735093

max MCSE = 1.84788844374762

all stationary: TRUE

burn: 0

max rel.err.: 2.27126072319875

-- STATS 2D --

min ESS = 3789.95339395361

max BMK = 0.0405371552624997

max MCSE = 1.77766566030369

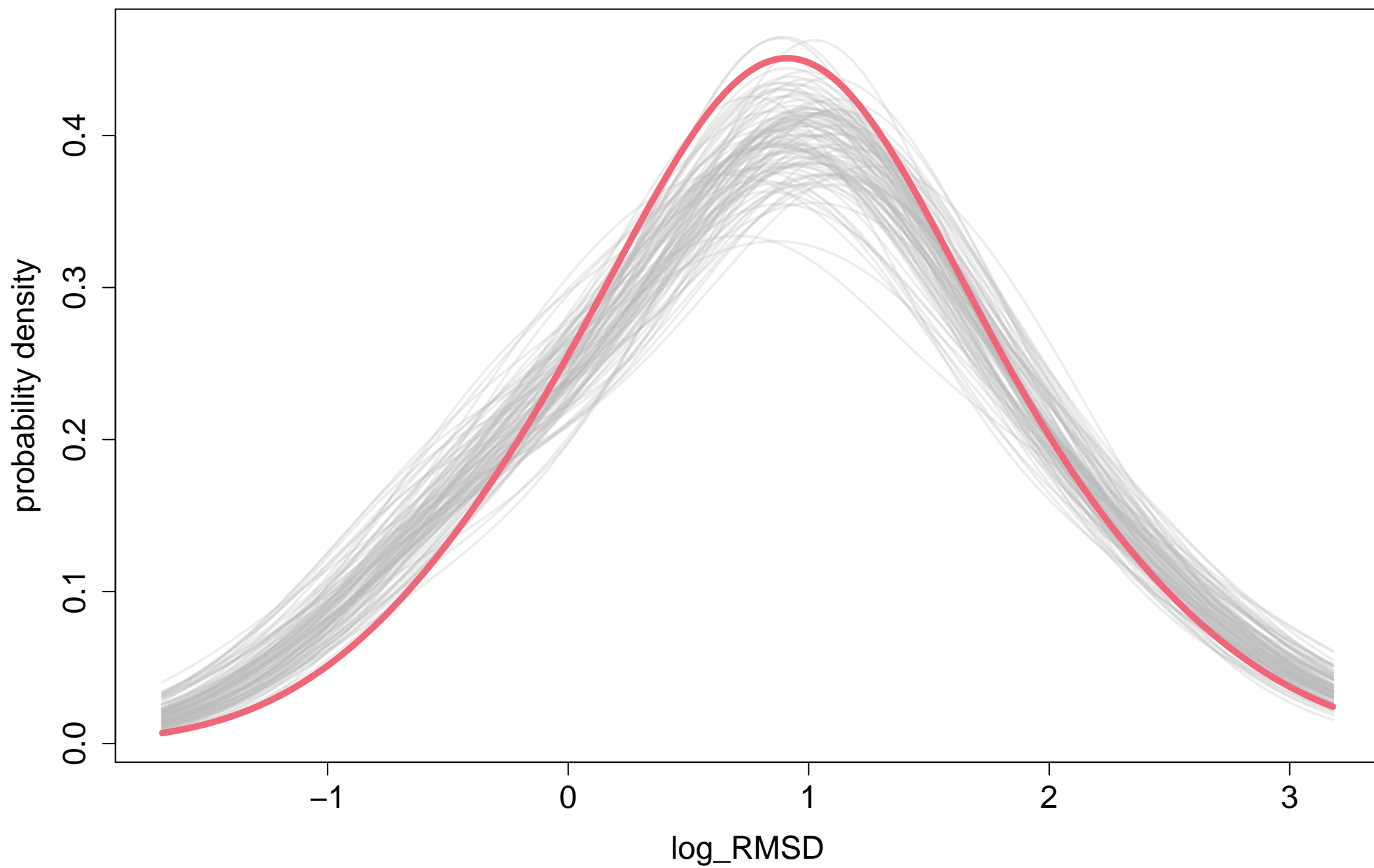
all stationary: TRUE

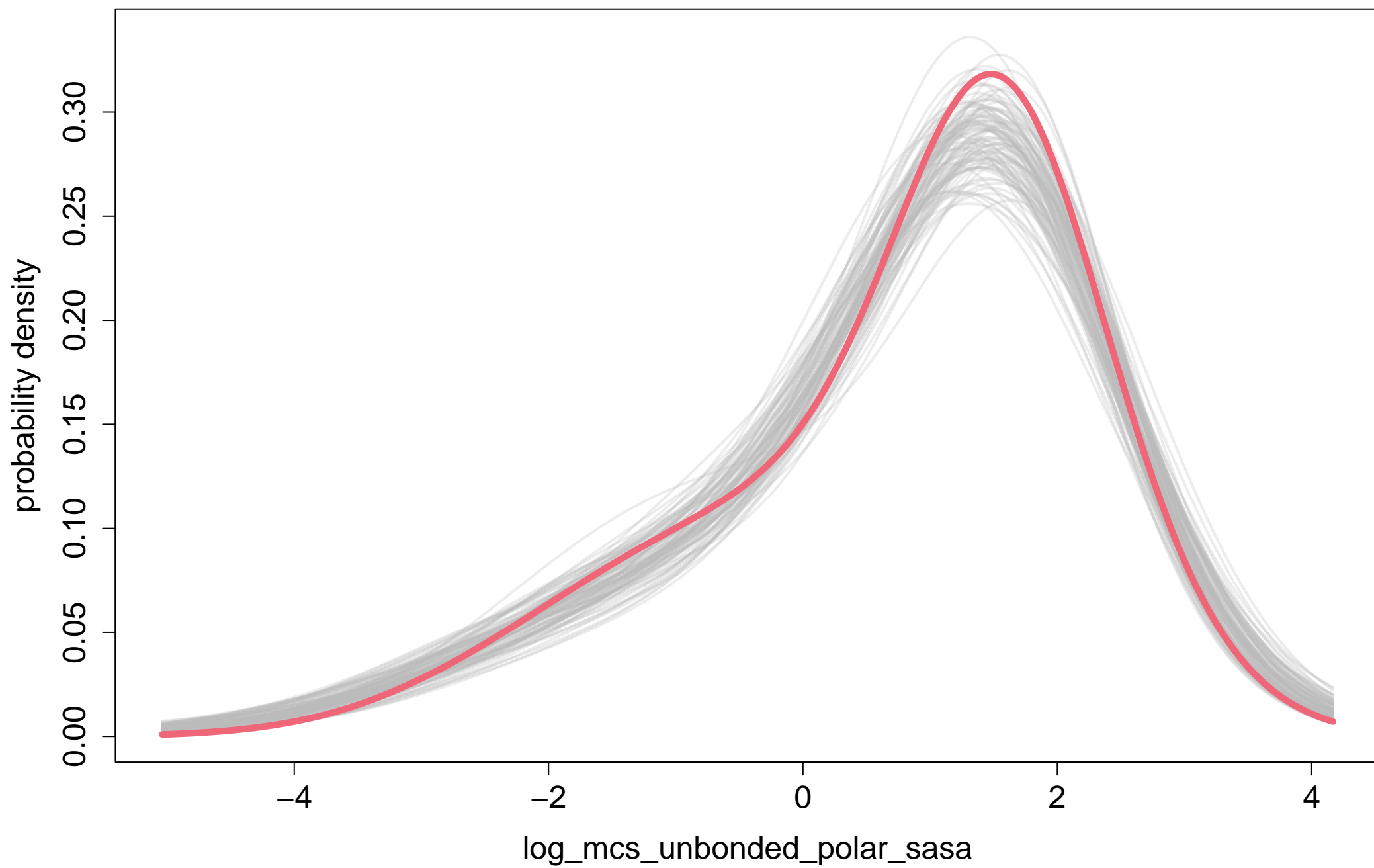
burn: 0

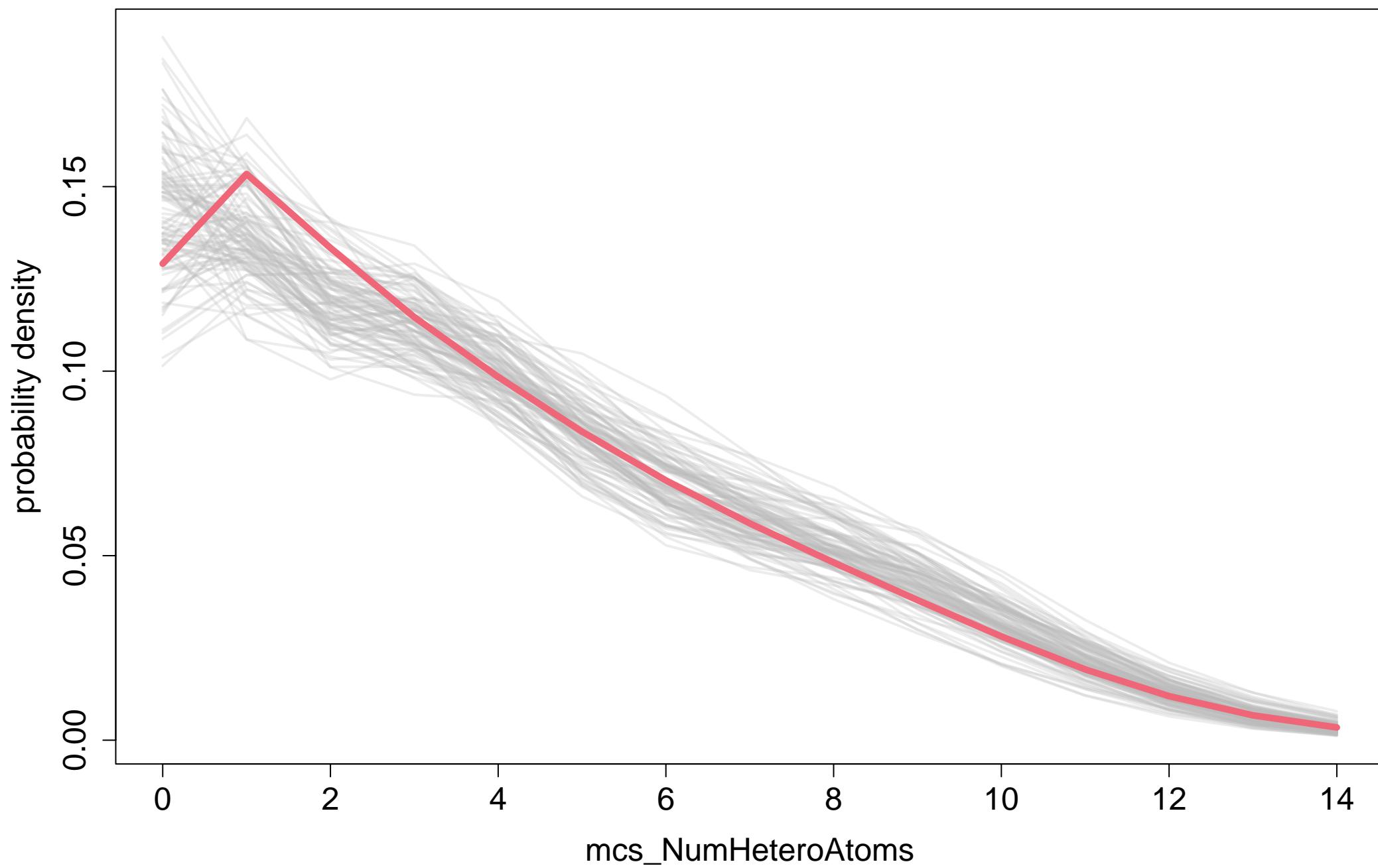
max rel.err.: 1.78726919455887

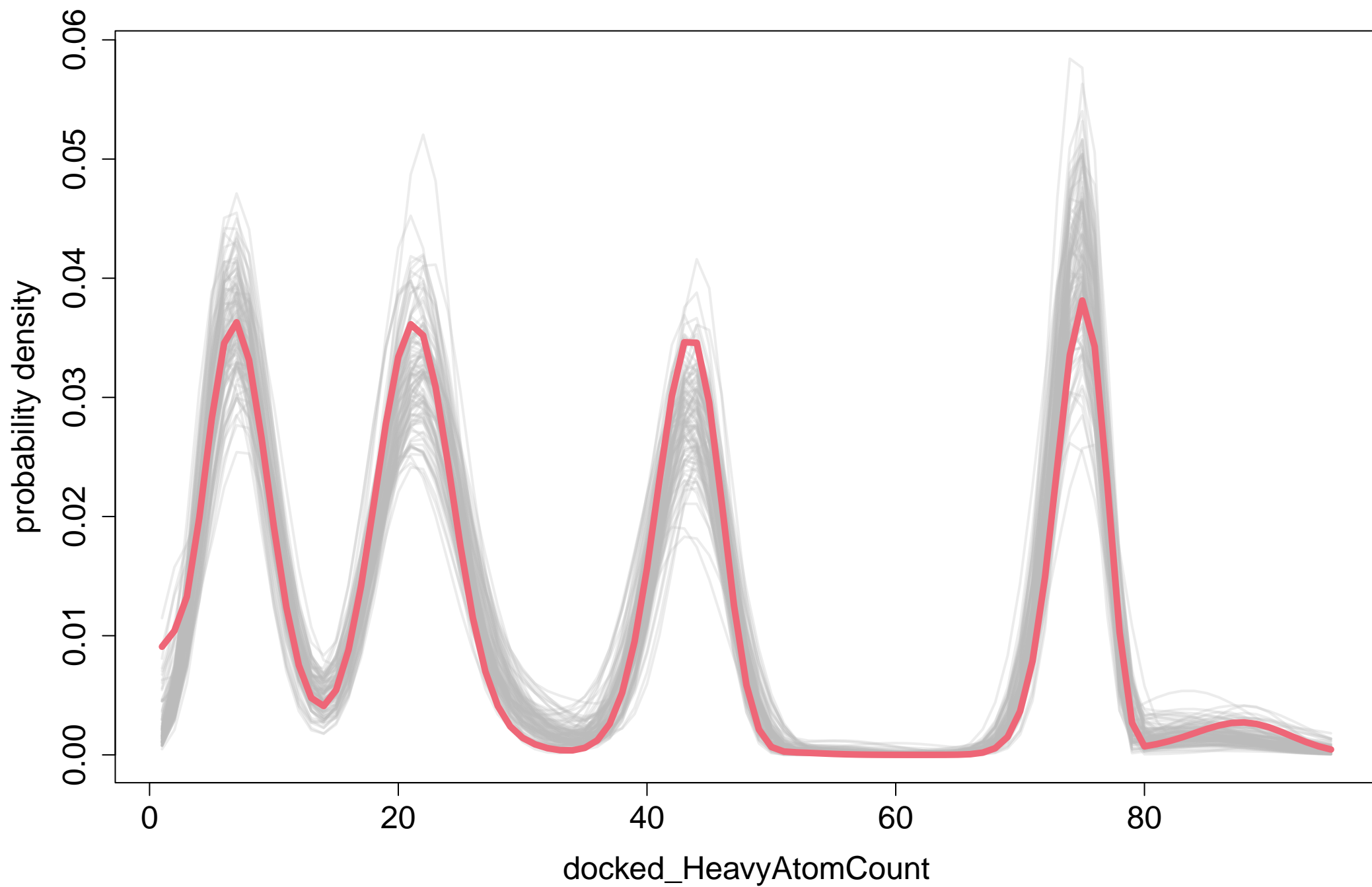
Occupied clusters: 9 of 16

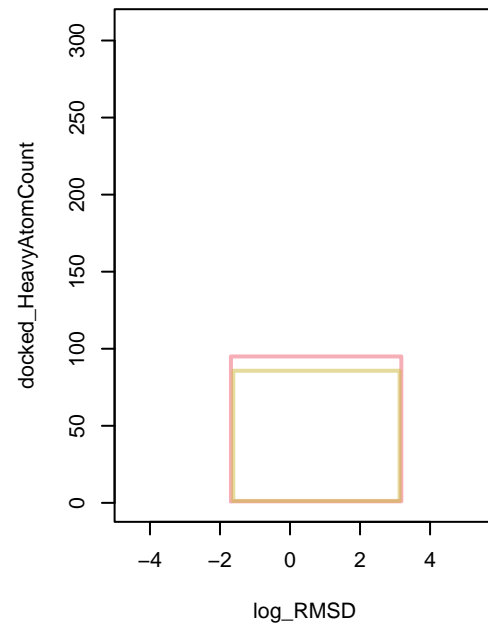
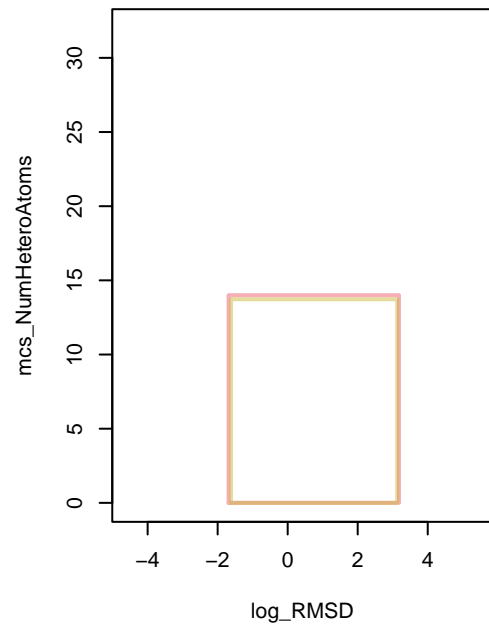
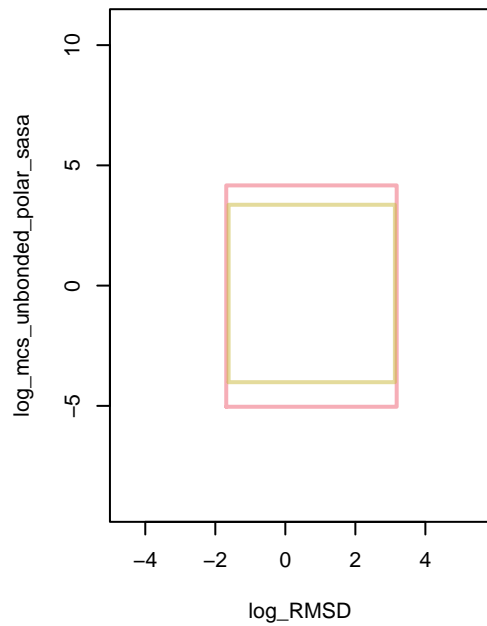
LL: -2160 +- 6.6



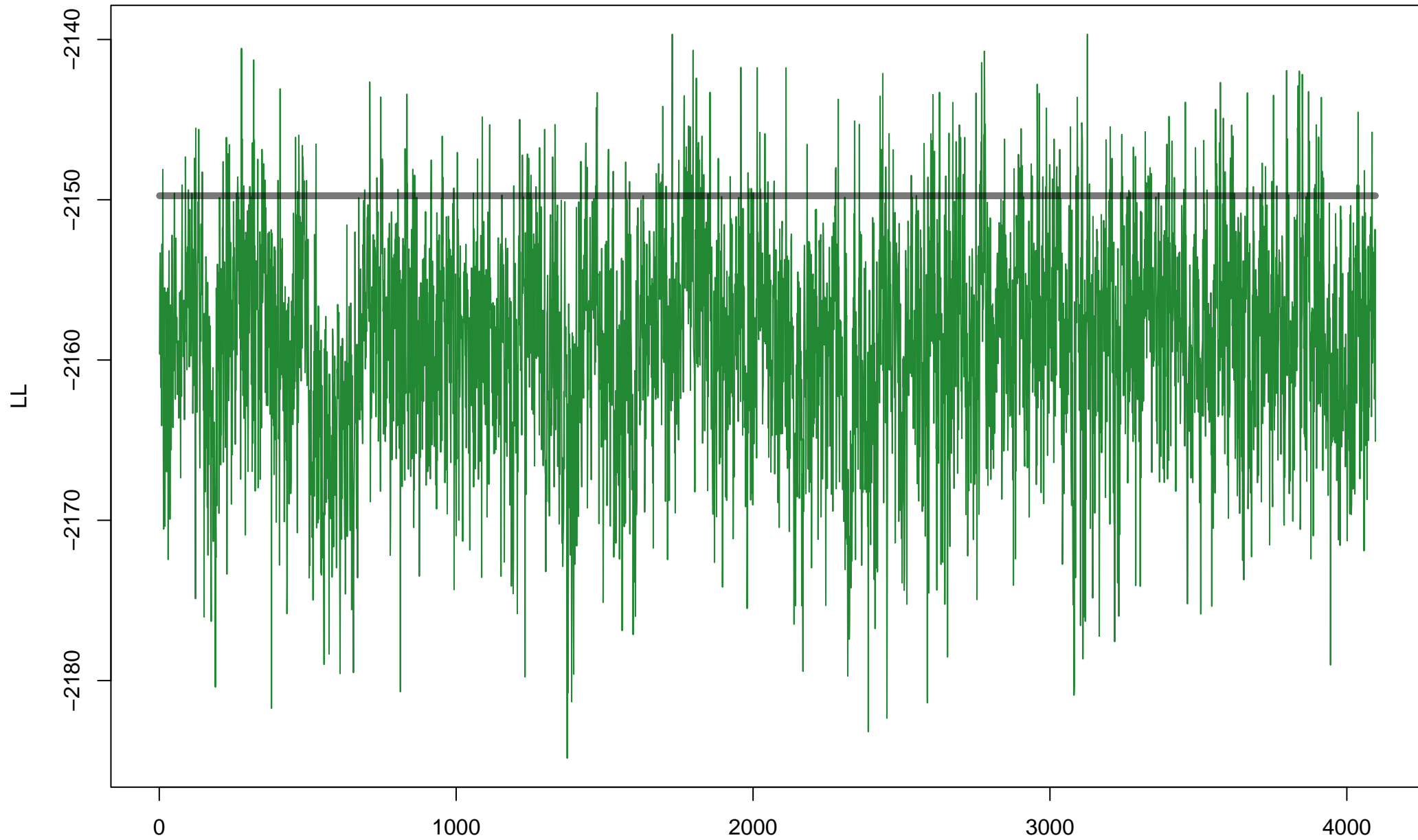




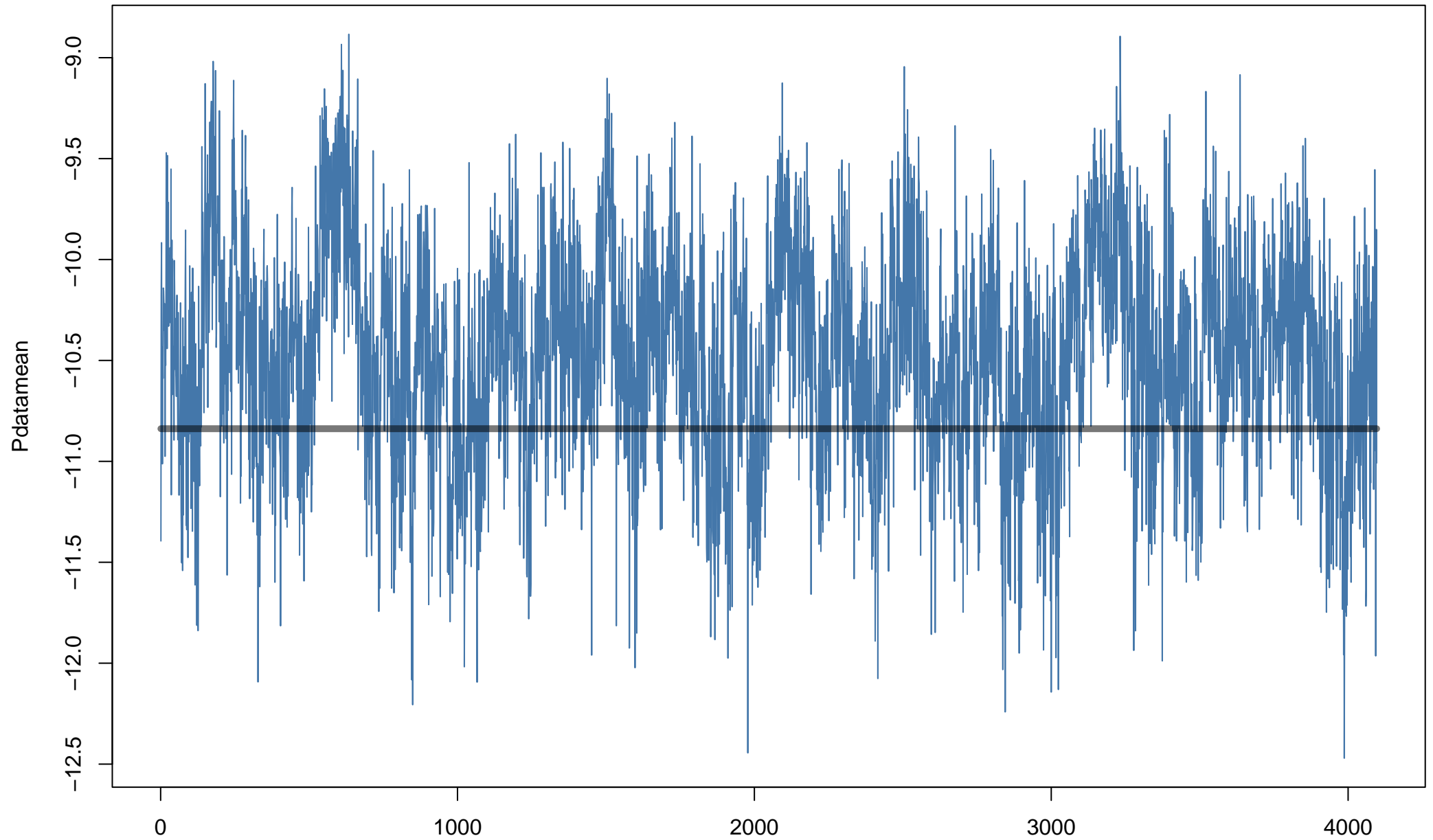




LL

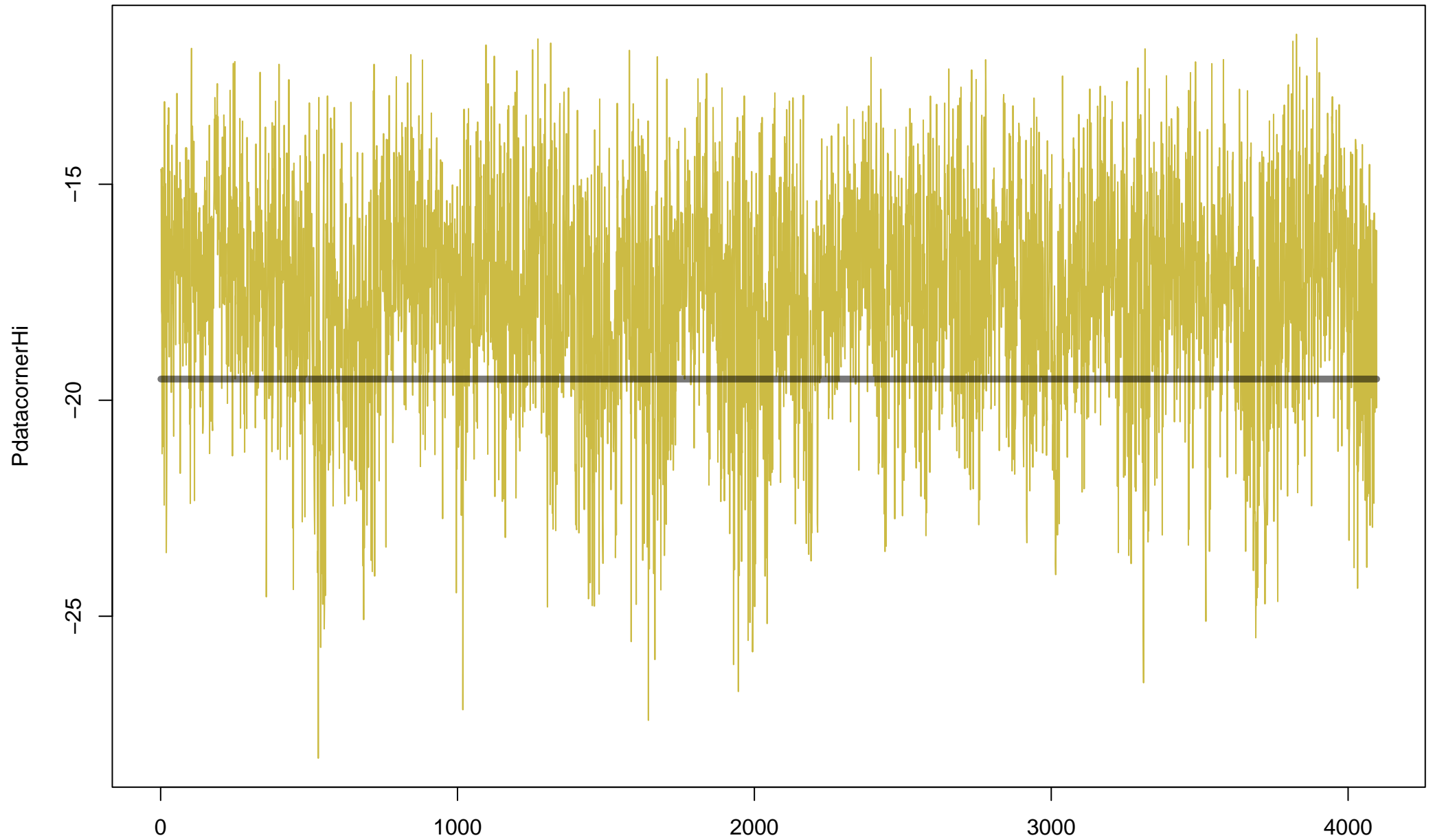


**Pdatamean**  
**ESS = 142 | BMK = 0.0468 | MCSE(6.27) = 6.89 | stat: TRUE | burn: 0 | rel.err: 0.723**

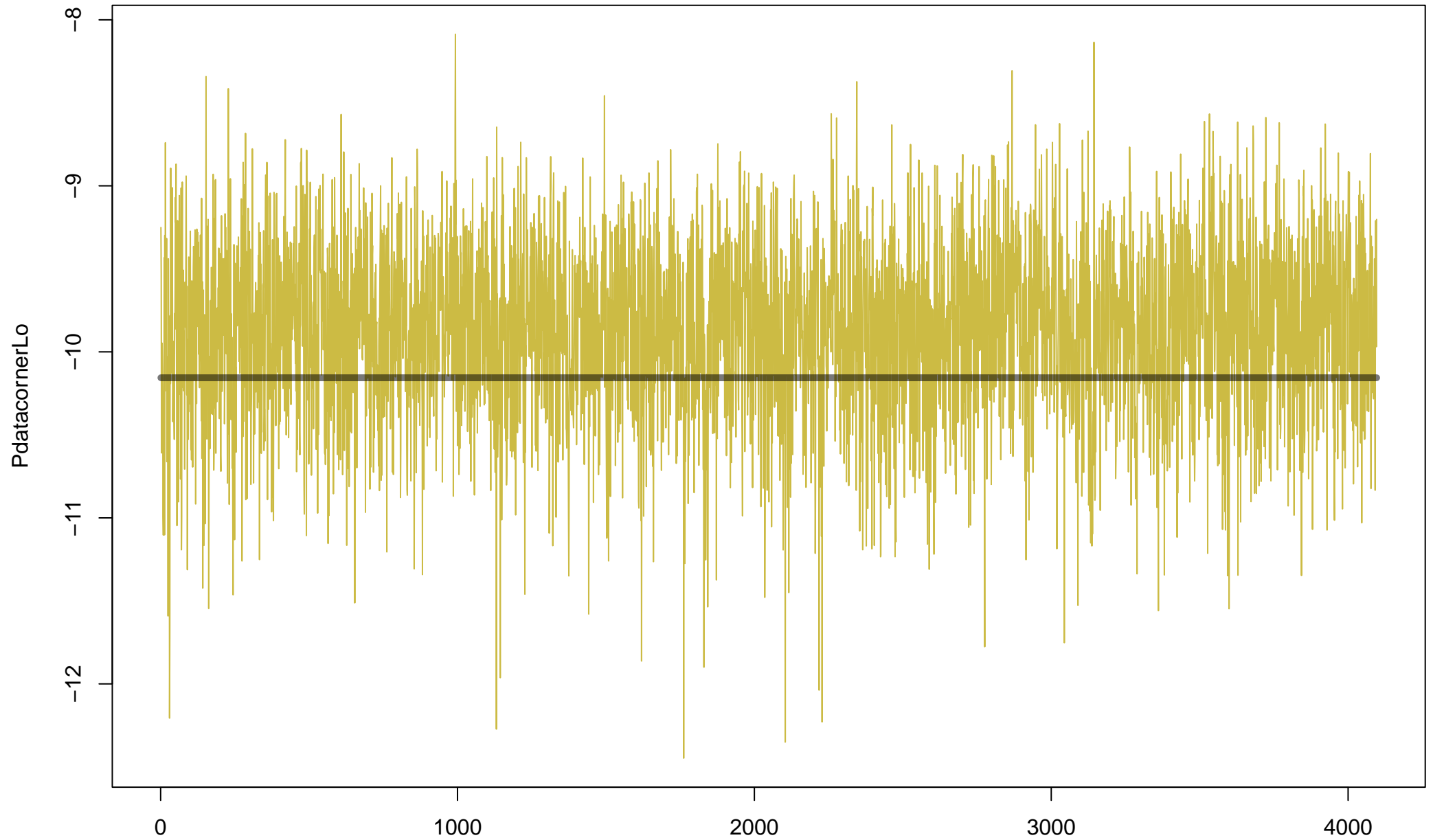




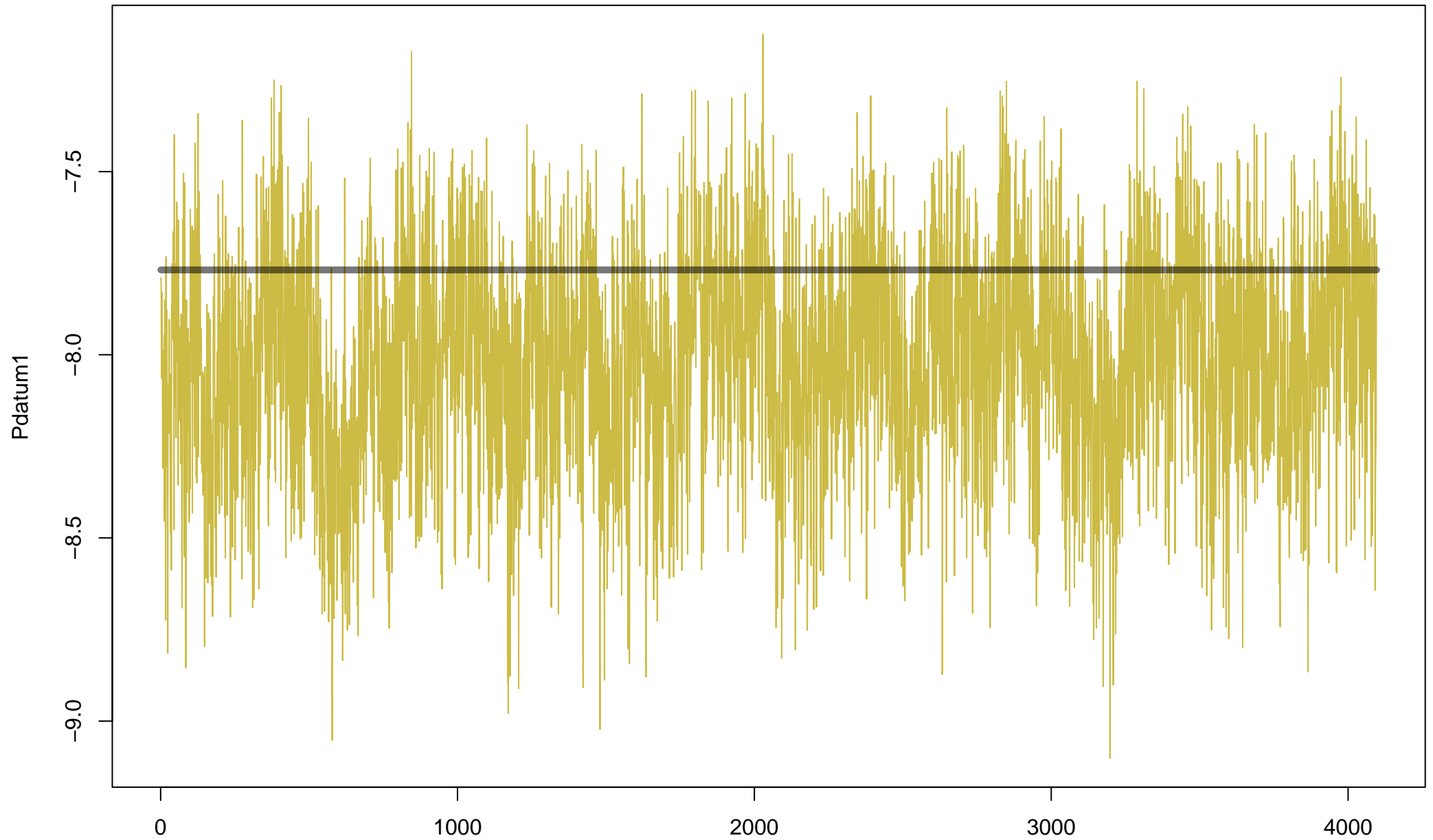
**PdatacornerHi**  
**ESS = 3920 | BMK = 0.118 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: 0.323**



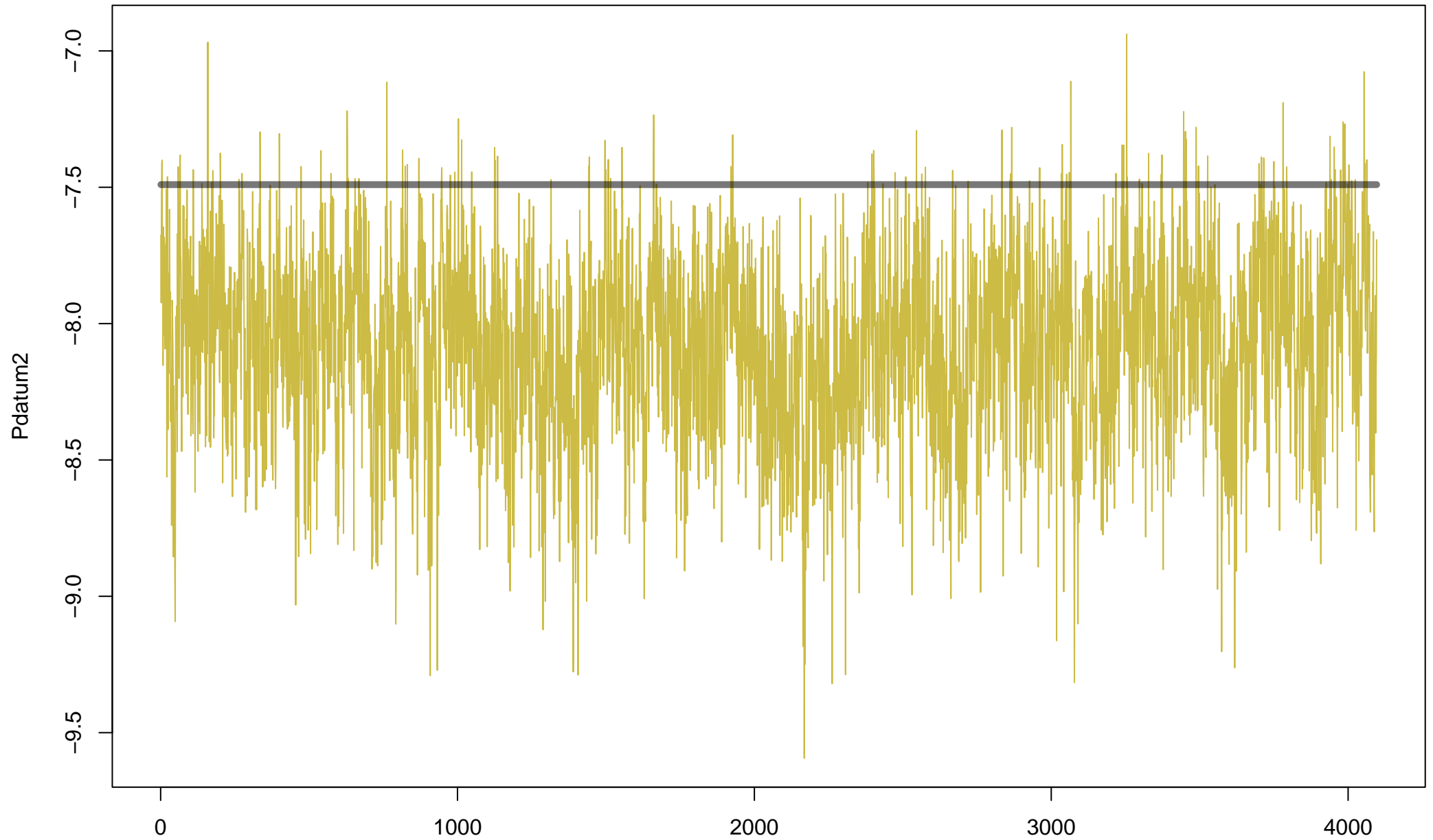
**PdatacornerLo**  
**ESS = 3440 | BMK = 0.041 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0 | rel.err: 0.649**



**Pdatum1**  
**ESS = 345 | BMK = 0.0455 | MCSE(6.27) = 4.56 | stat: TRUE | burn: 0 | rel.err: -0.769**

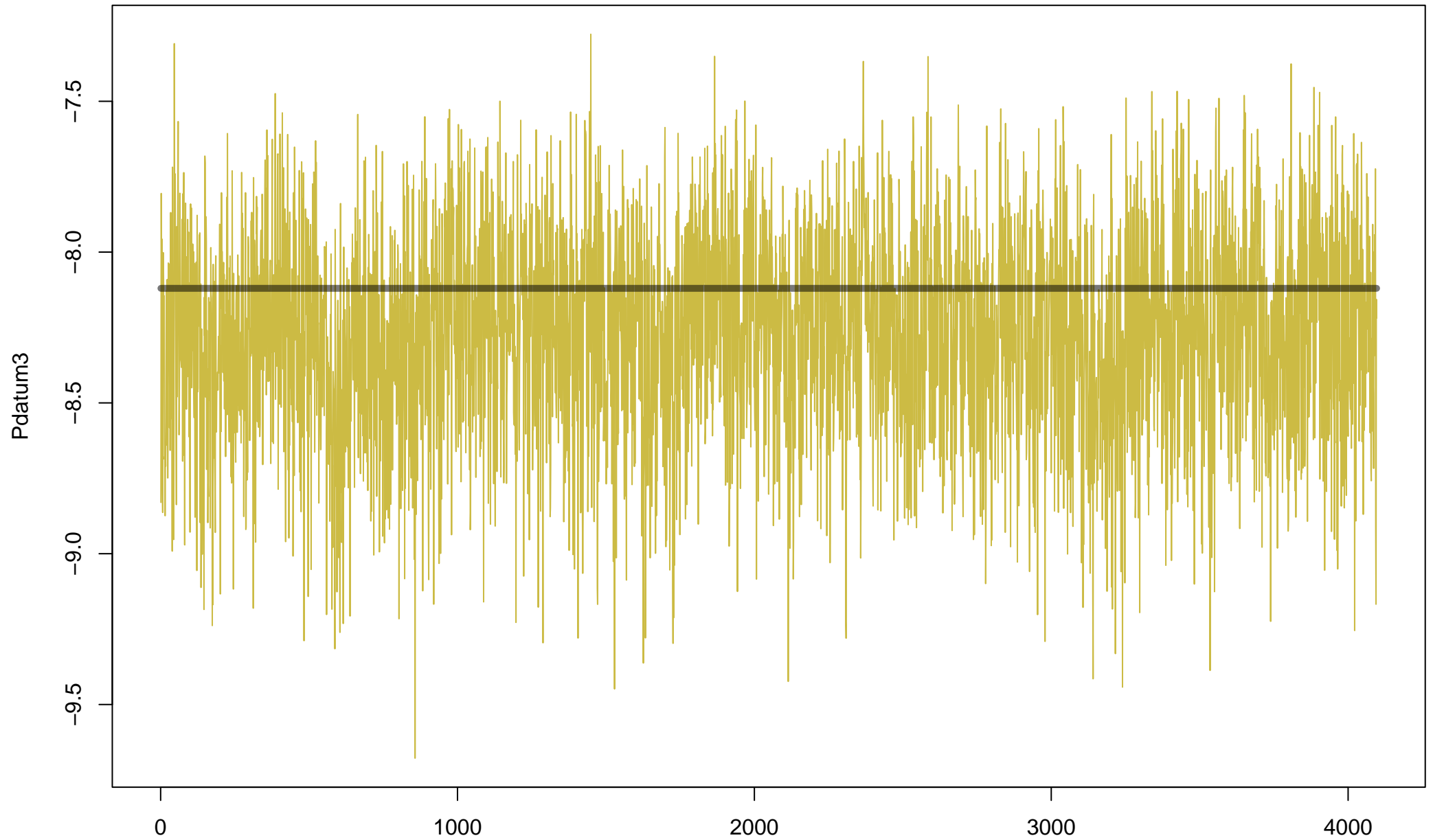


**Pdatum2**  
**ESS = 465 | BMK = 0.0421 | MCSE(6.27) = 4.33 | stat: TRUE | burn: 0 | rel.err: -2.17**



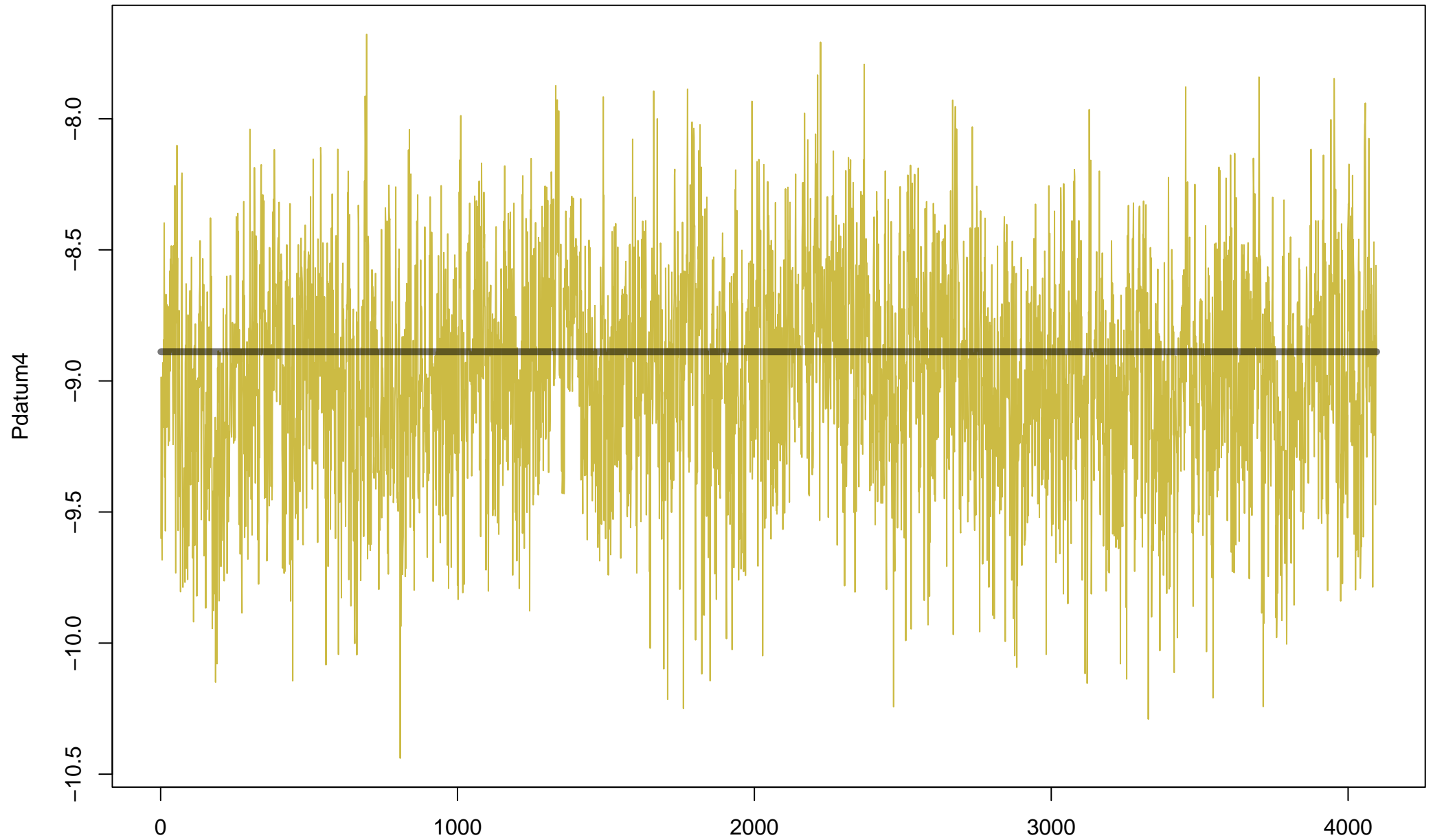
**Pdatum3**

**ESS = 1900 | BMK = 0.0362 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: -0.314**



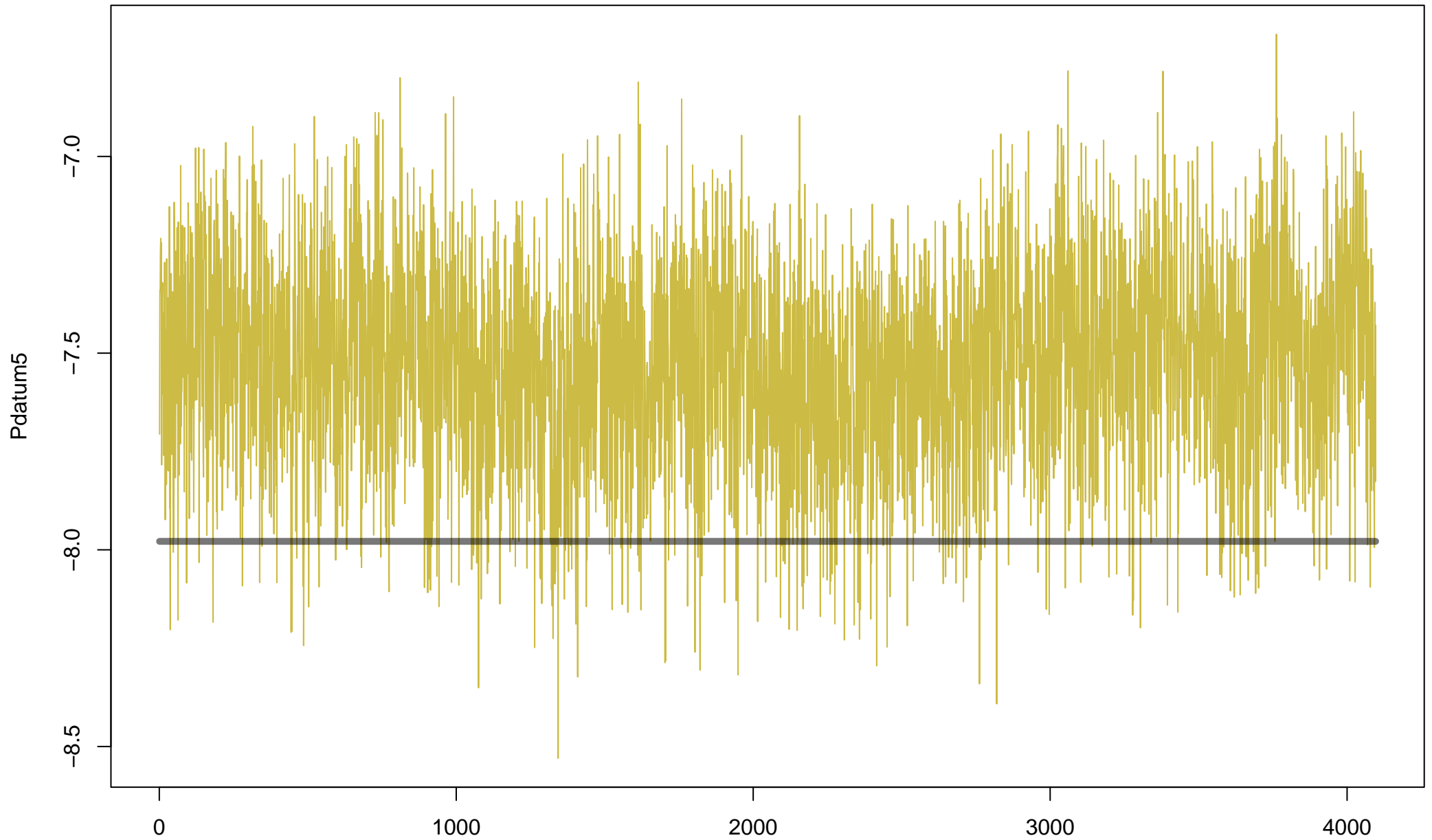
**Pdatum4**

**ESS = 1060 | BMK = 0.032 | MCSE(6.27) = 3.67 | stat: TRUE | burn: 0 | rel.err: -0.0343**



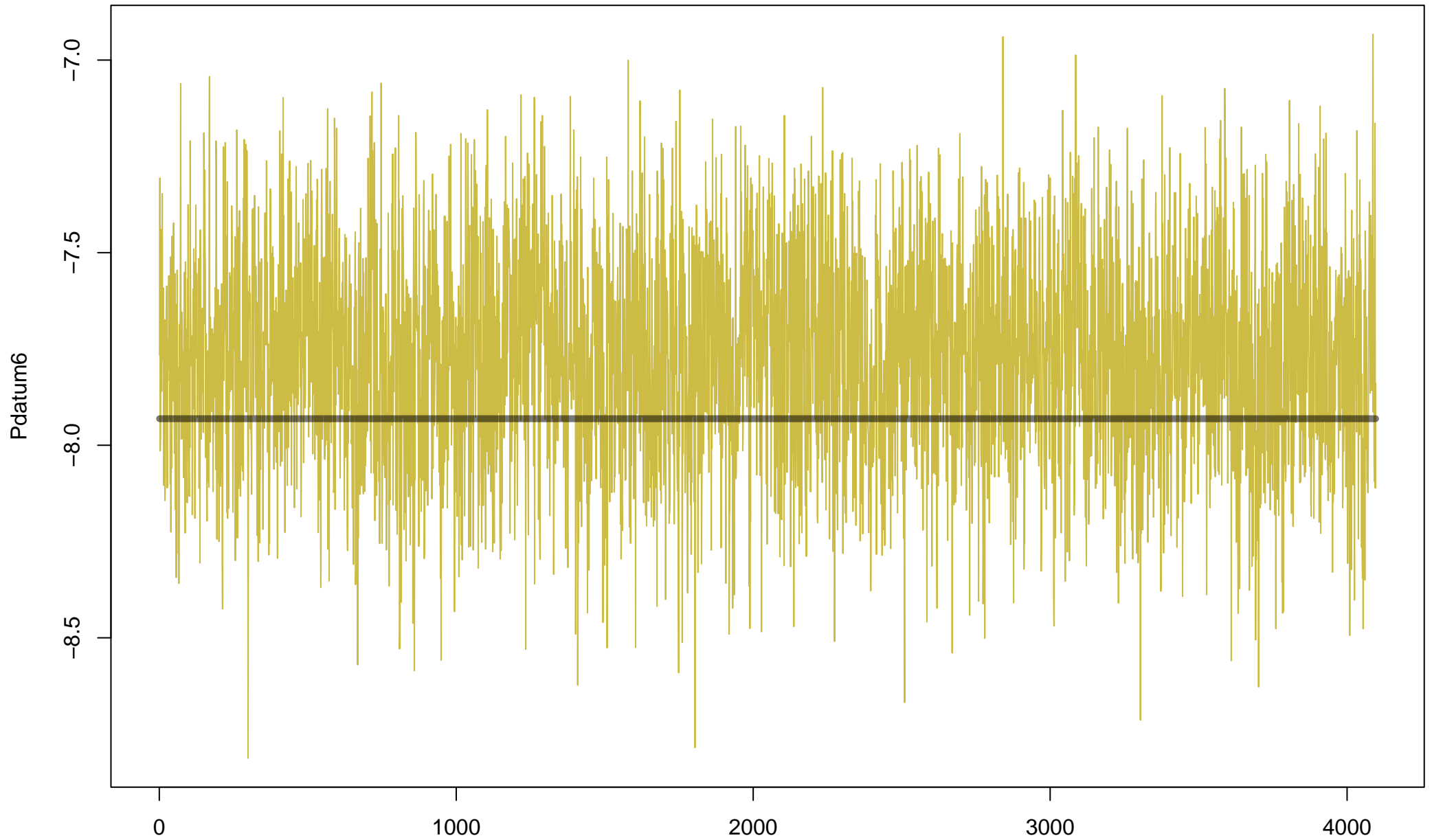
**Pdatum5**

**ESS = 696 | BMK = 0.0269 | MCSE(6.27) = 3.34 | stat: TRUE | burn: 0 | rel.err: 1.51**



**Pdatum6**

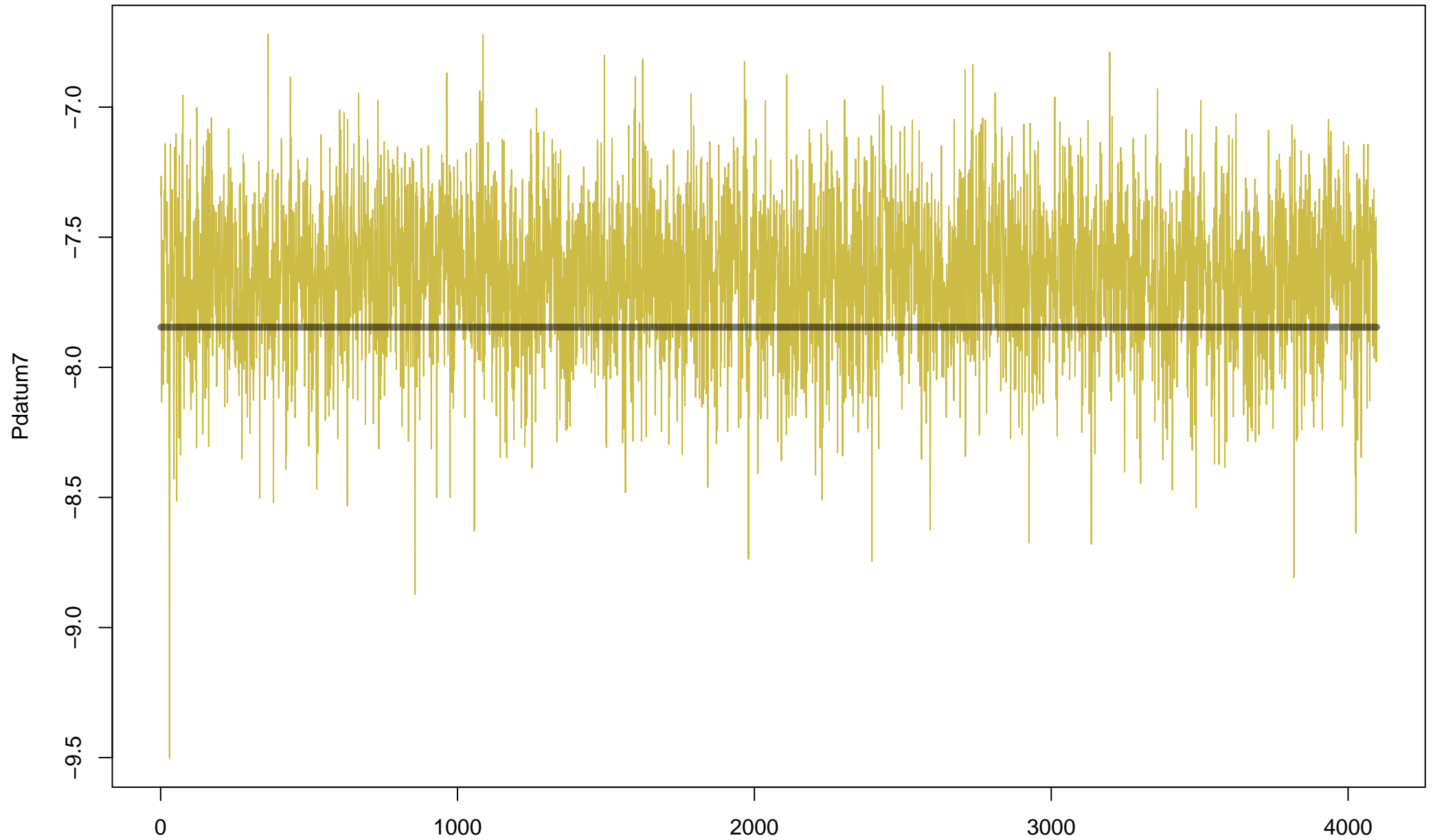
**ESS = 2420 | BMK = 0.0388 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.65**





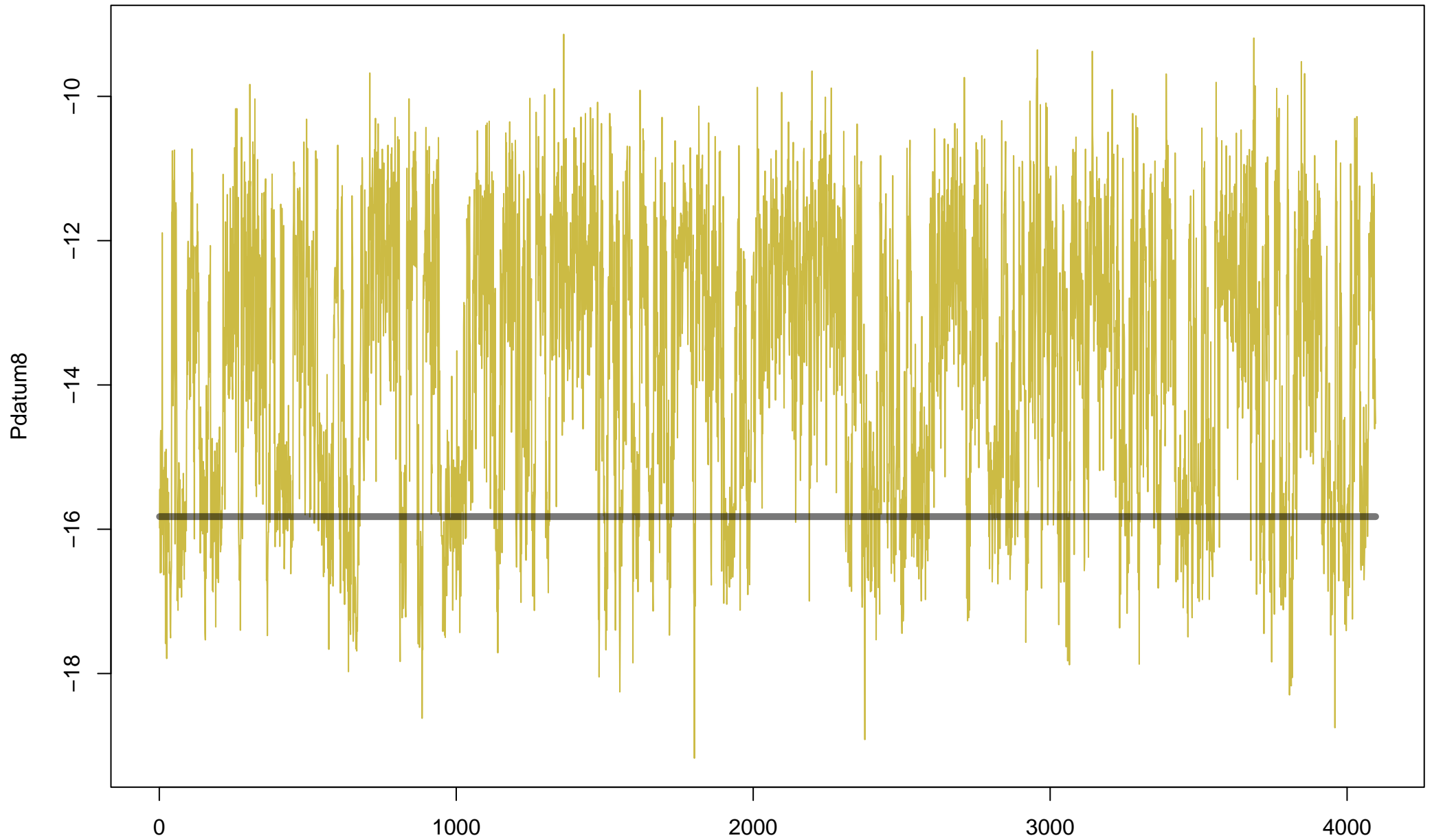
**Pdatum7**

**ESS = 3280 | BMK = 0.0358 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0 | rel.err: 0.747**



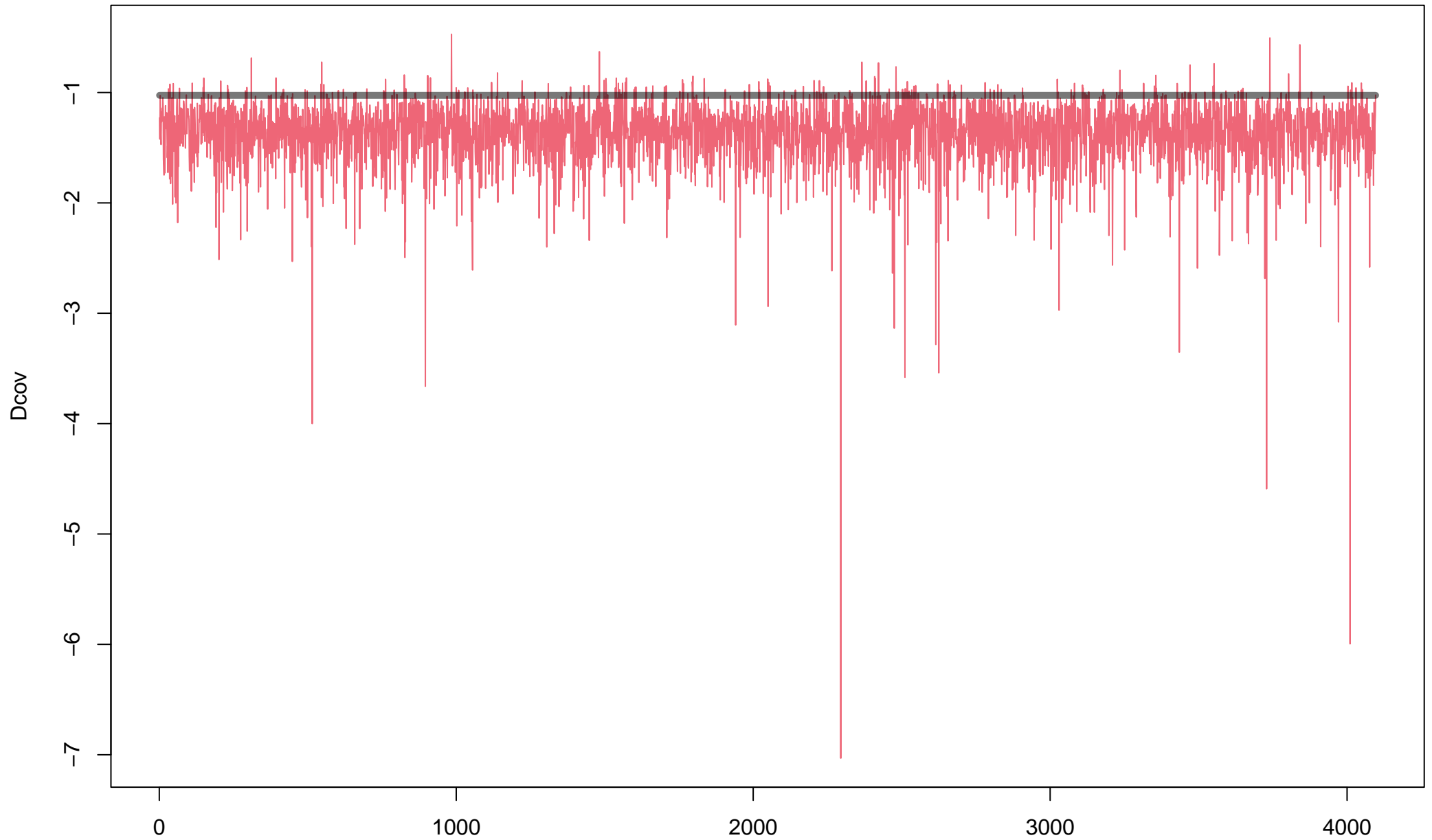
**Pdatum8**

**ESS = 881 | BMK = 0.0573 | MCSE(6.27) = 3.52 | stat: FALSE | burn: 0 | rel.err: 0.563**

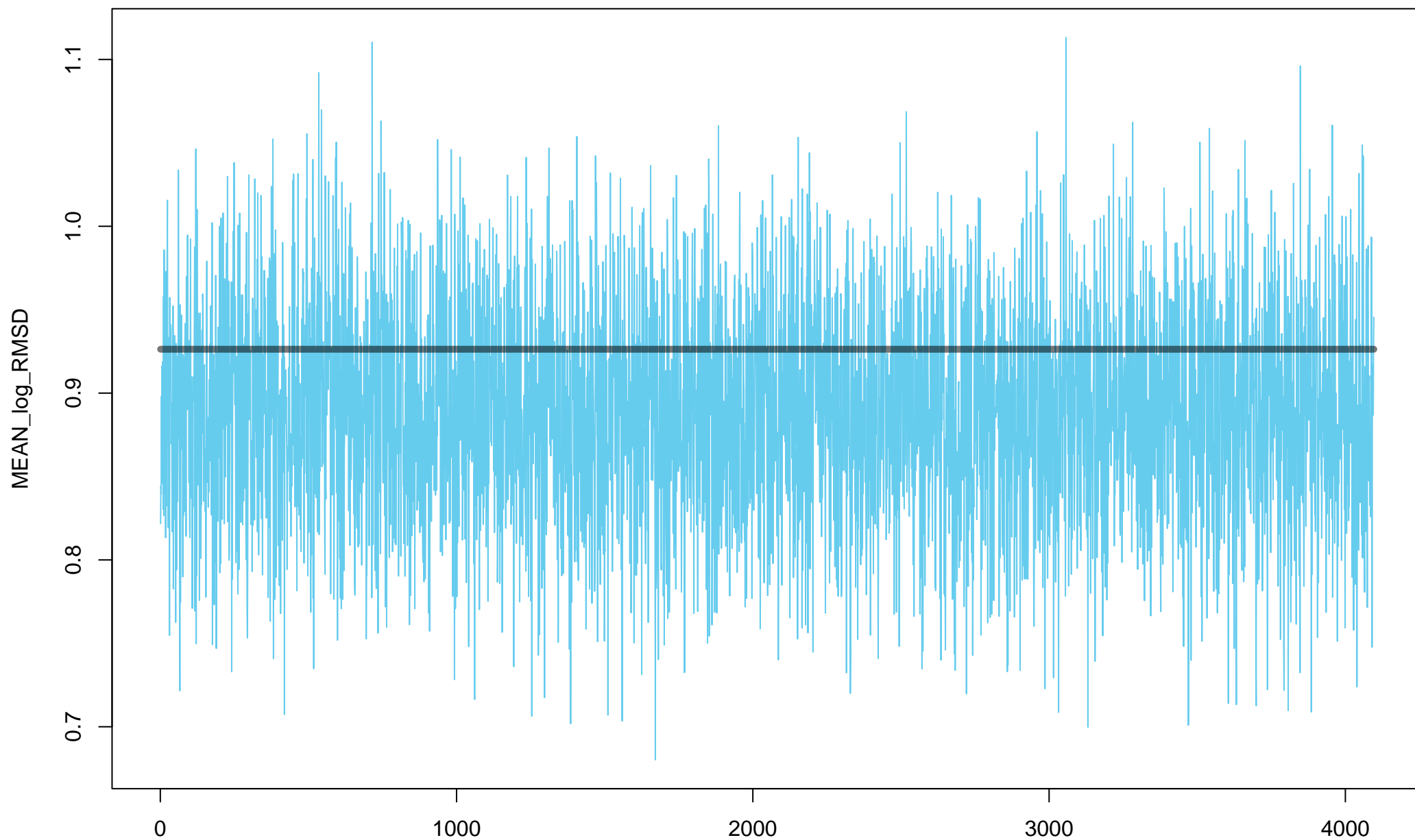


Dcov

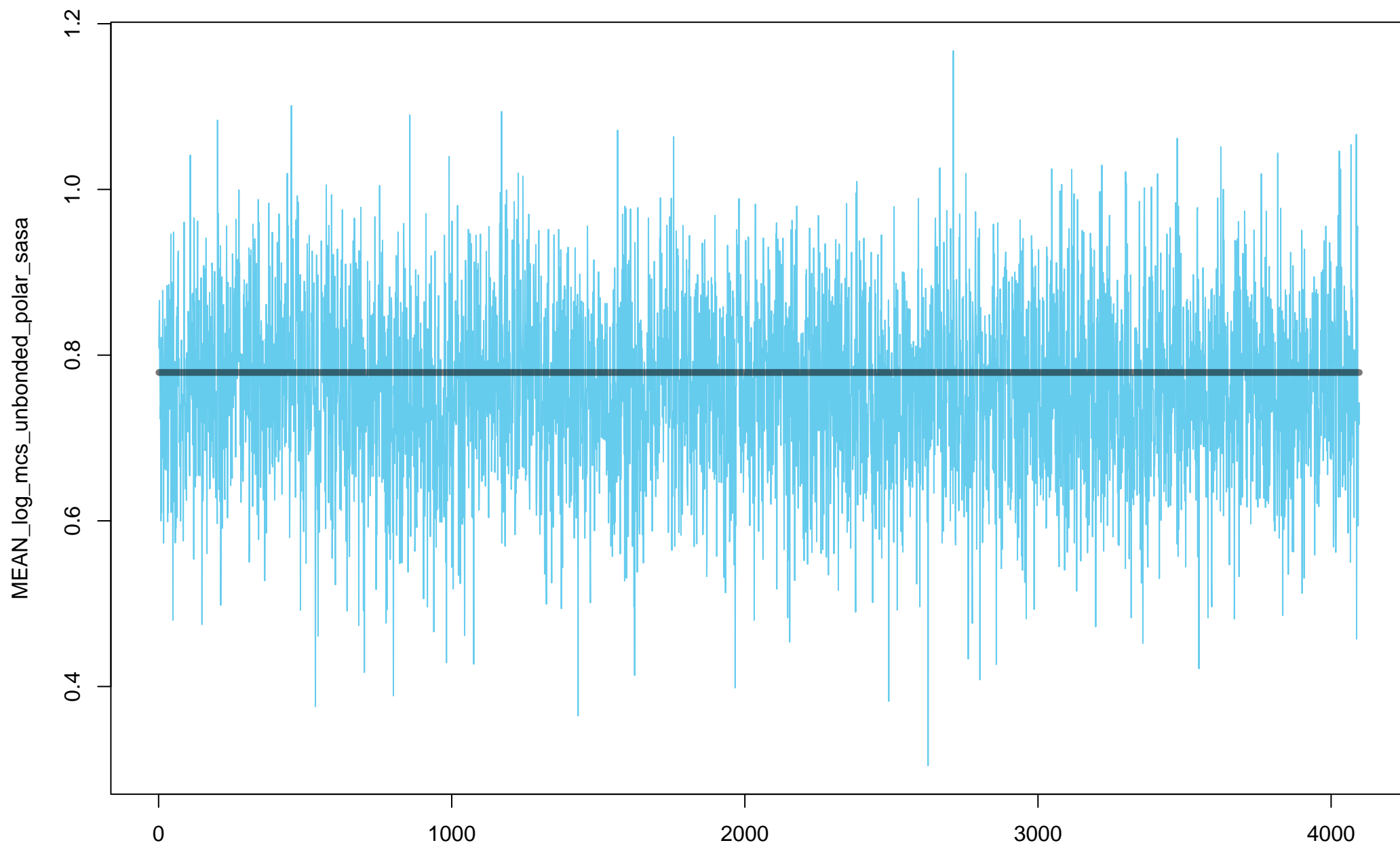
ESS = 4100 | BMK = 0.0591 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0 | rel.err: 1.53



**MEAN\_log\_RMSD**  
**ESS = 4100 | BMK = 0.0324 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: -0.591**

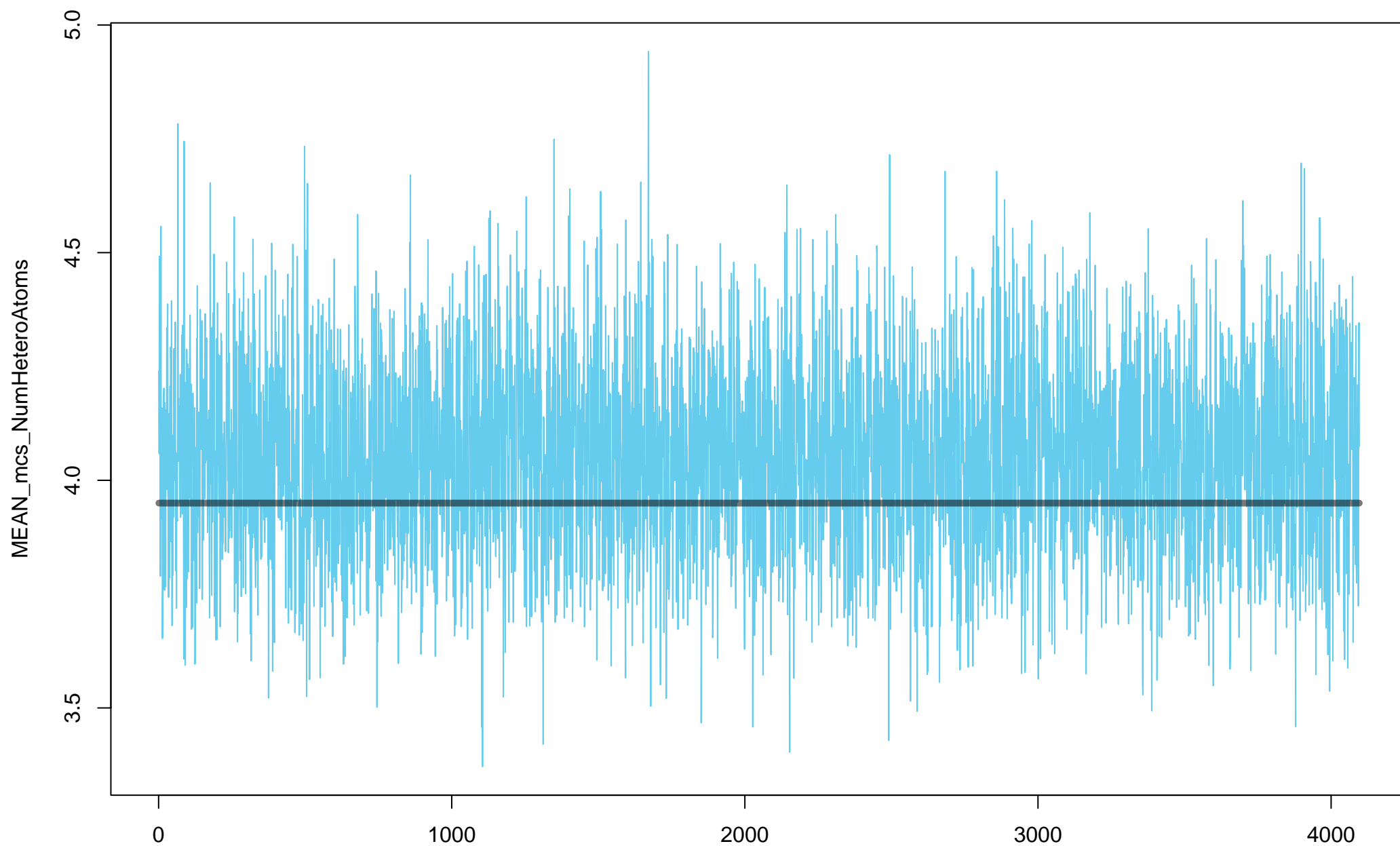


**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 3850 | BMK = 0.0387 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: -0.202**

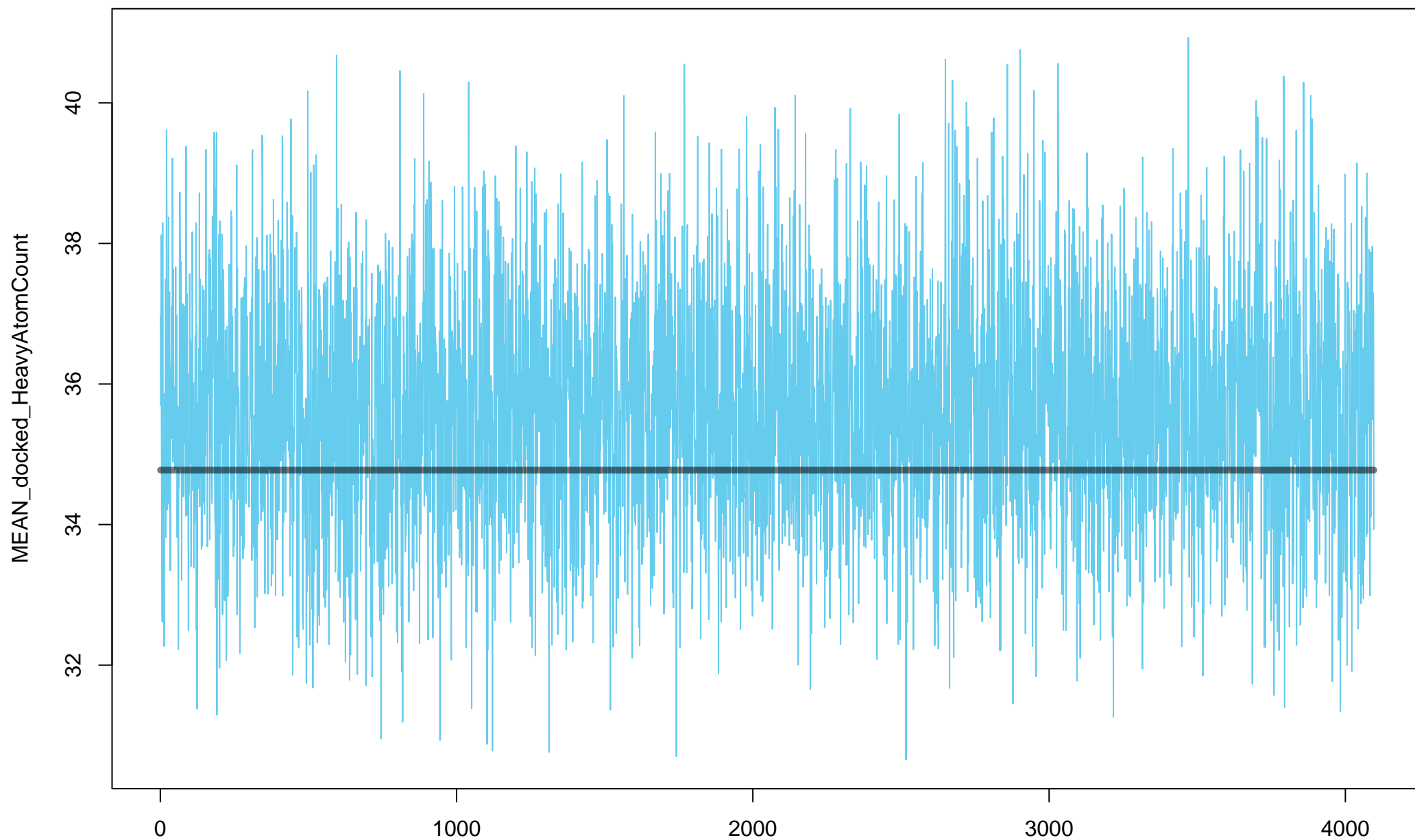


# MEAN\_mcs\_NumHeteroAtoms

ESS = 4100 | BMK = 0.0325 | MCSE(6.27) = 1.34 | stat: TRUE | burn: 0 | rel.err: 0.486

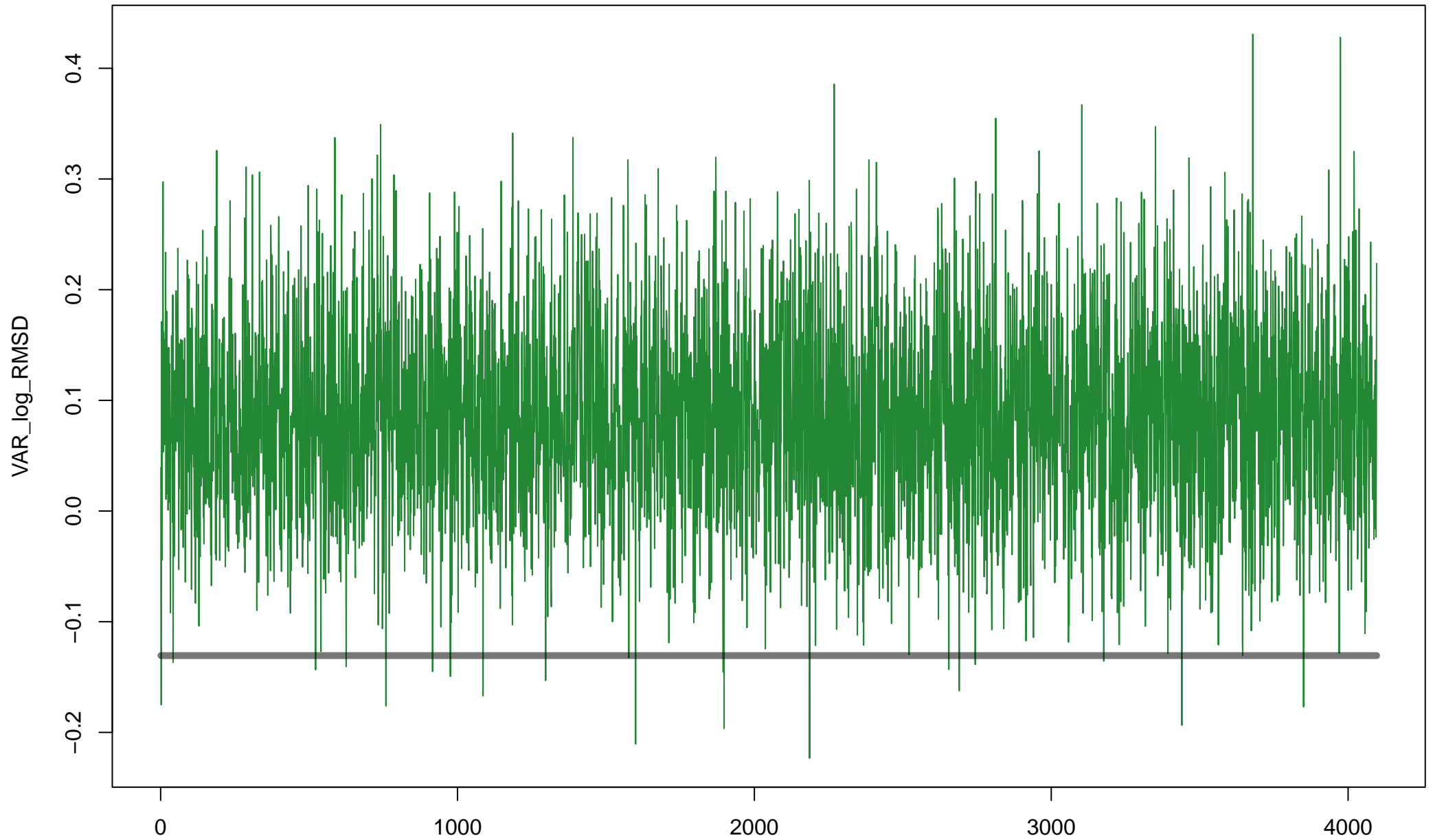


**MEAN\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0327 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 0.521**



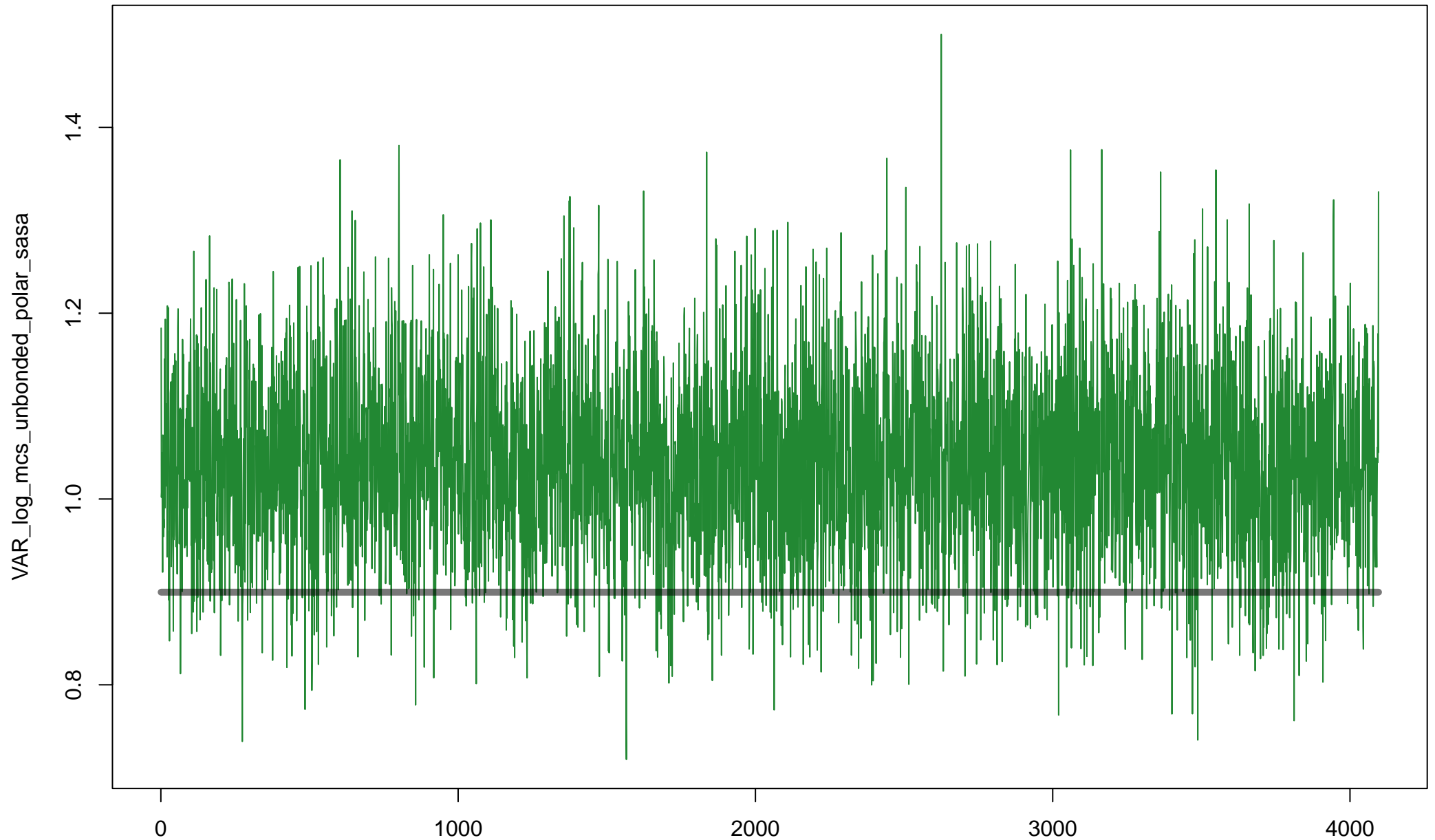
# VAR\_log\_RMSD

ESS = 4100 | BMK = 0.0471 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0 | rel.err: 2.27

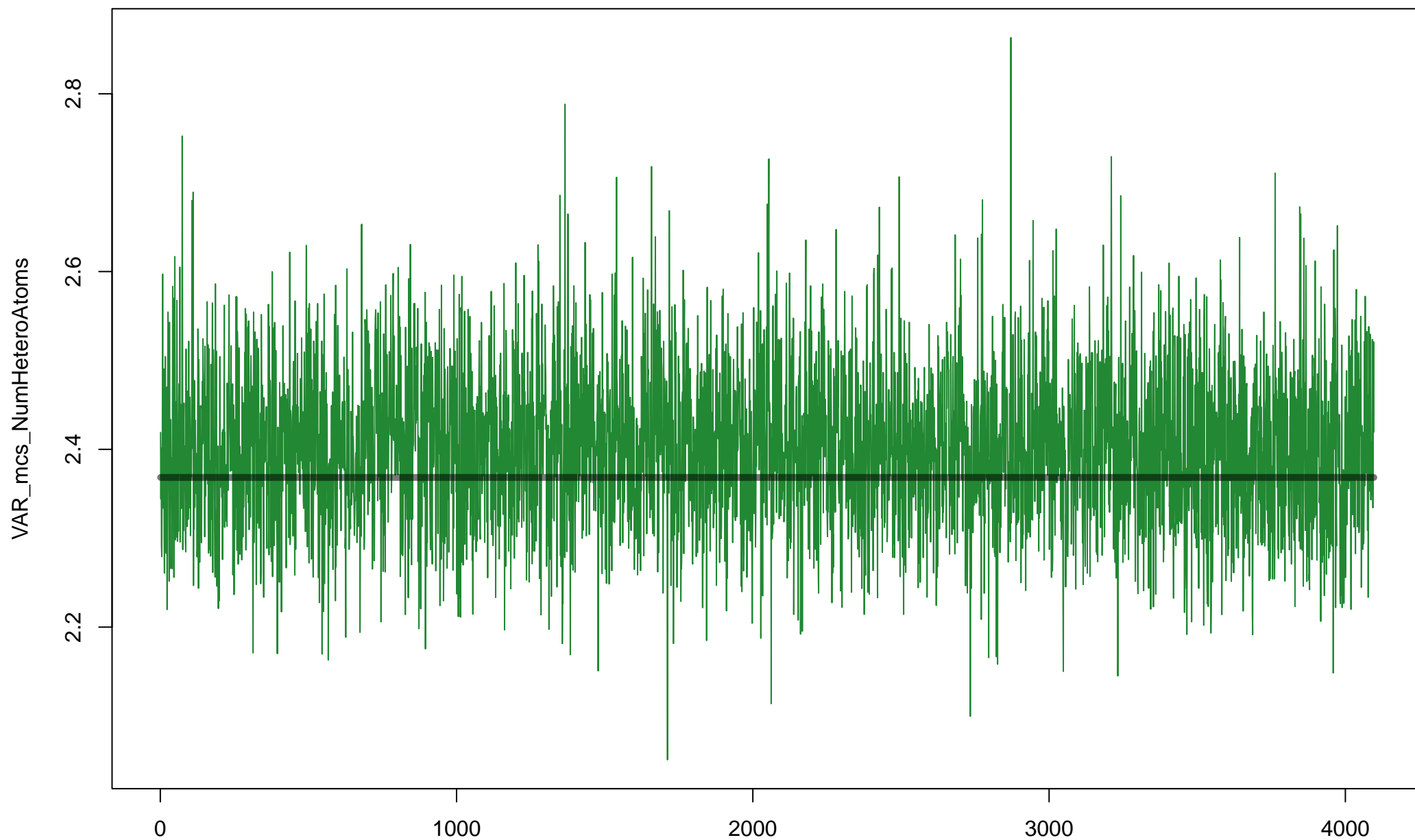




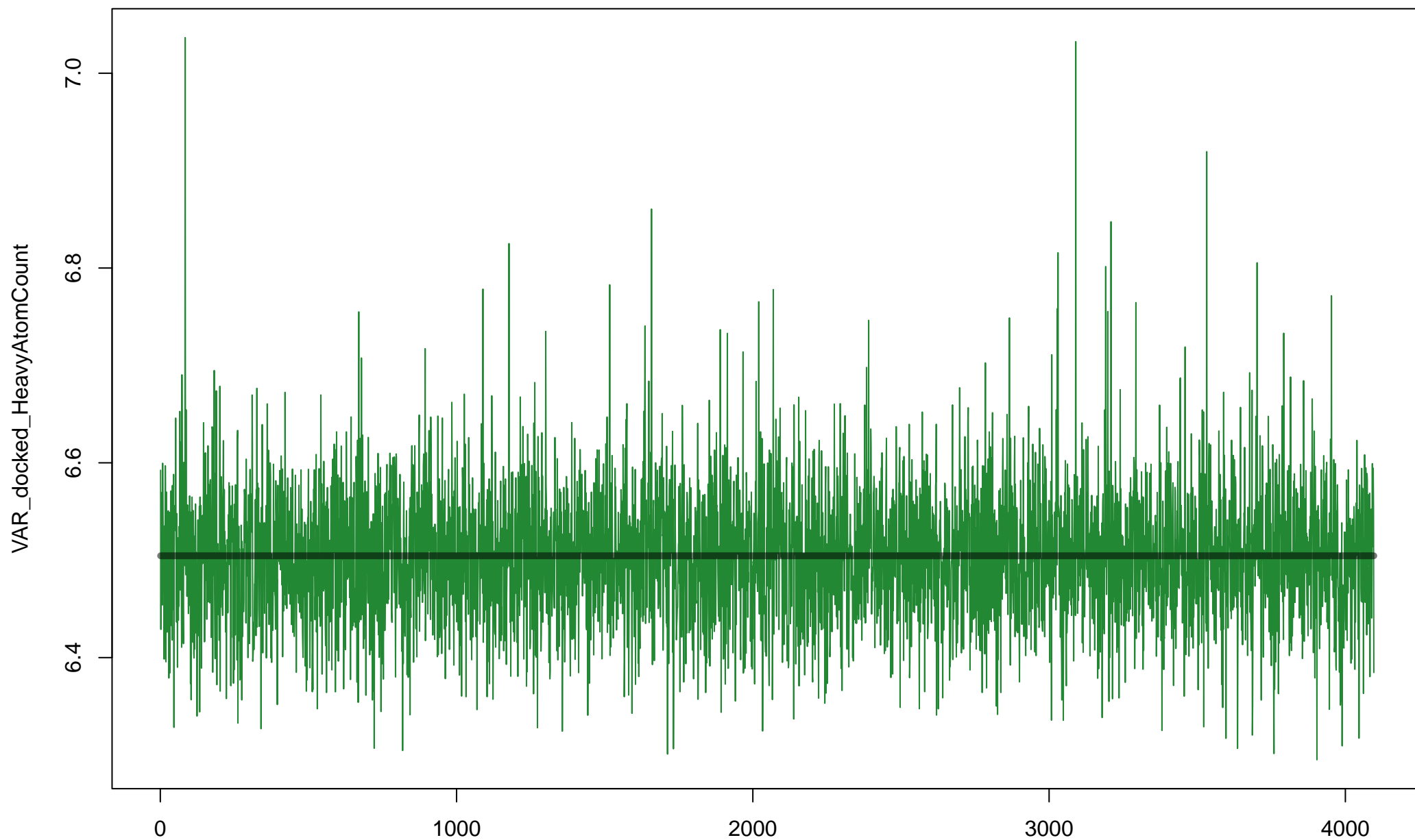
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 3690 | BMK = 0.0336 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0 | rel.err: 1.36**



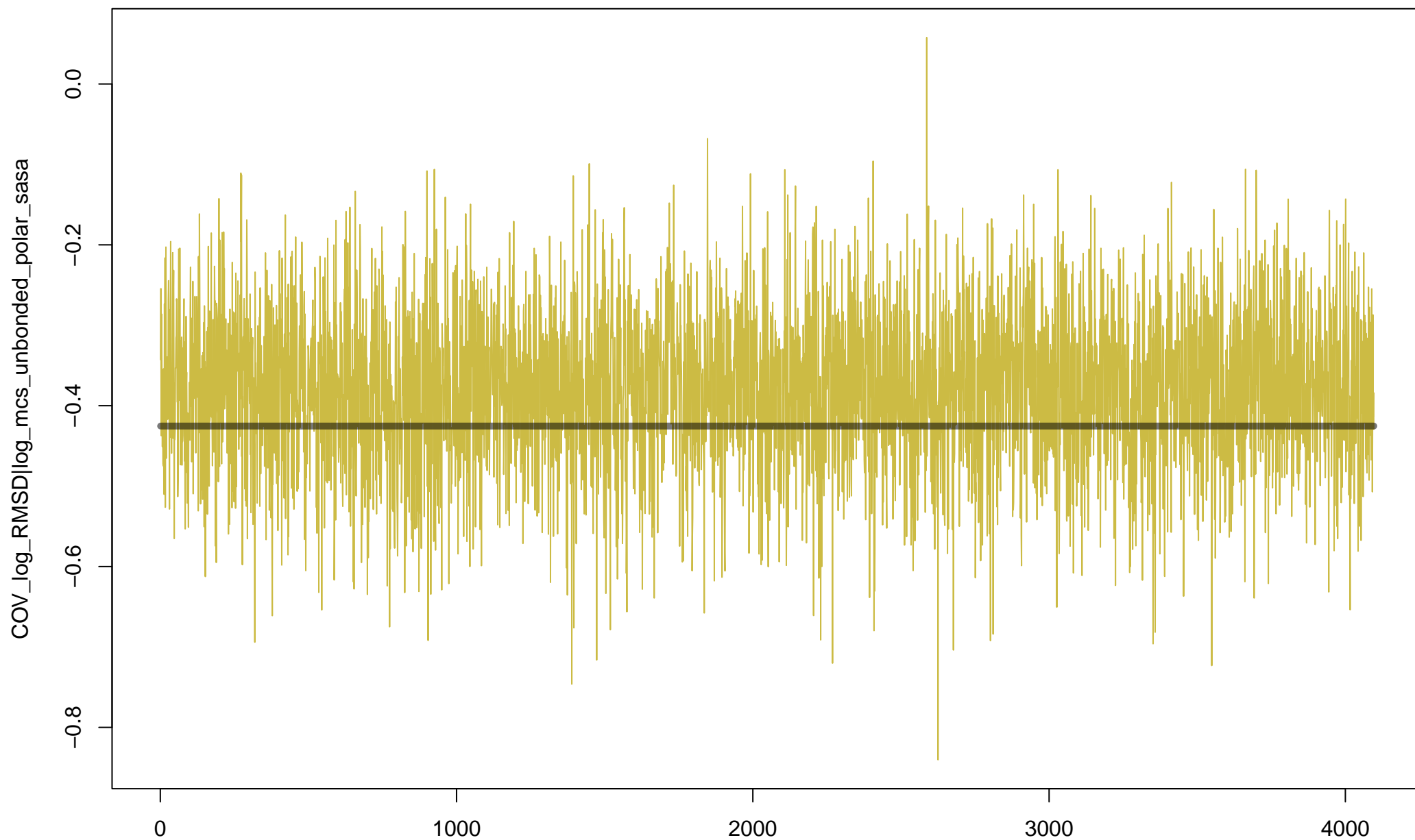
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 2980 | BMK = 0.0463 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: 0.415**



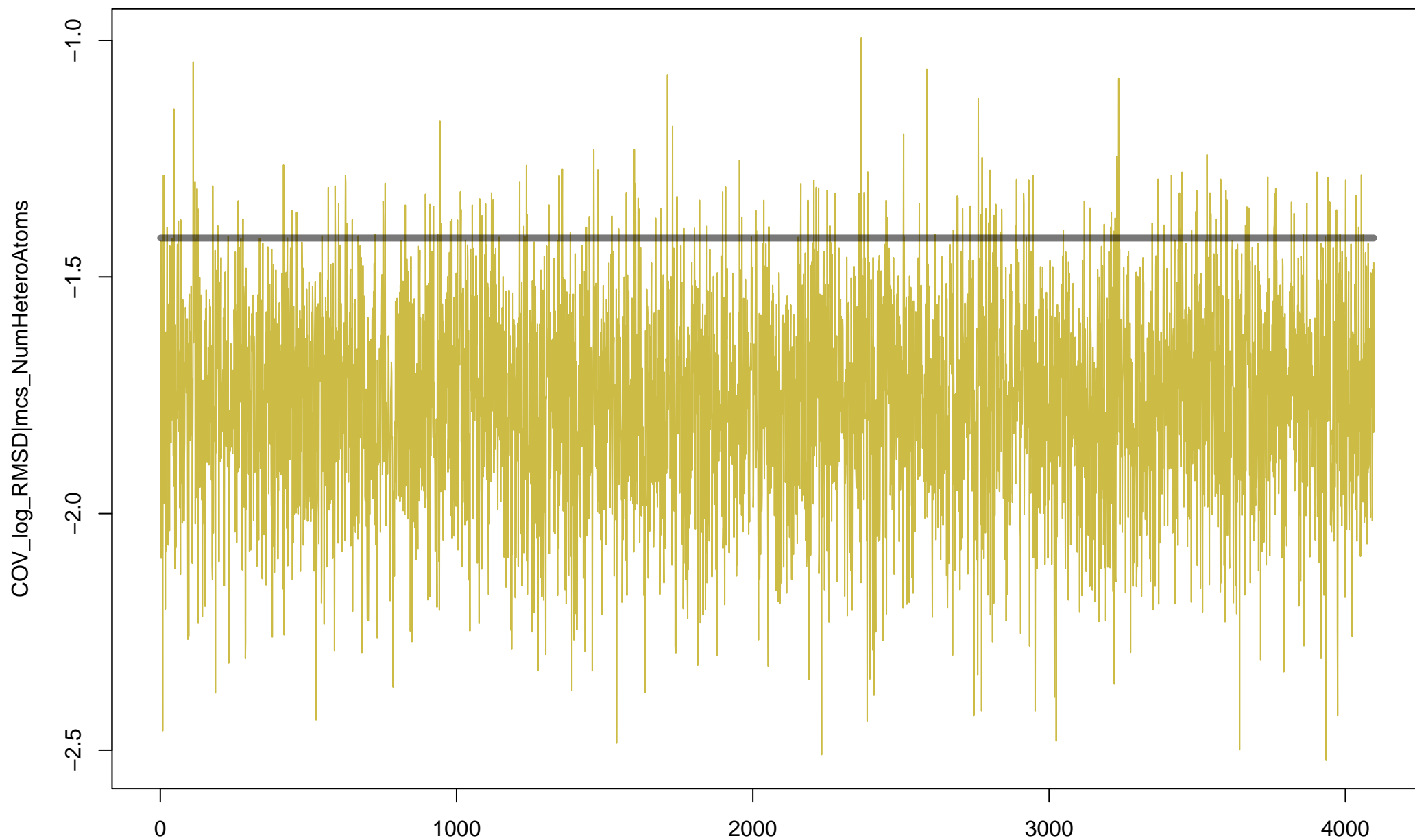
**VAR\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0408 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.0334**



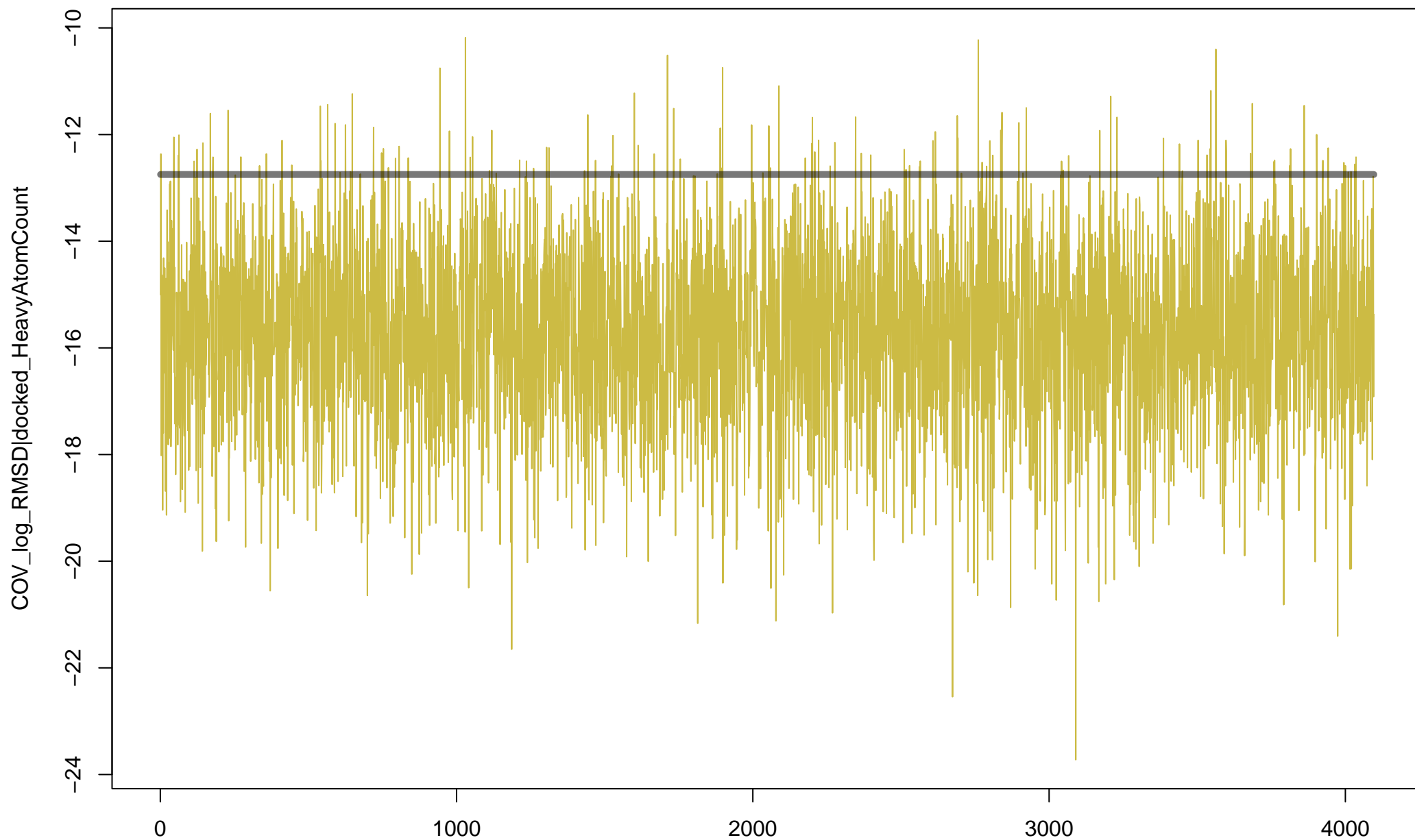
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 3790 | BMK = 0.0304 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0 | rel.err: 0.464**



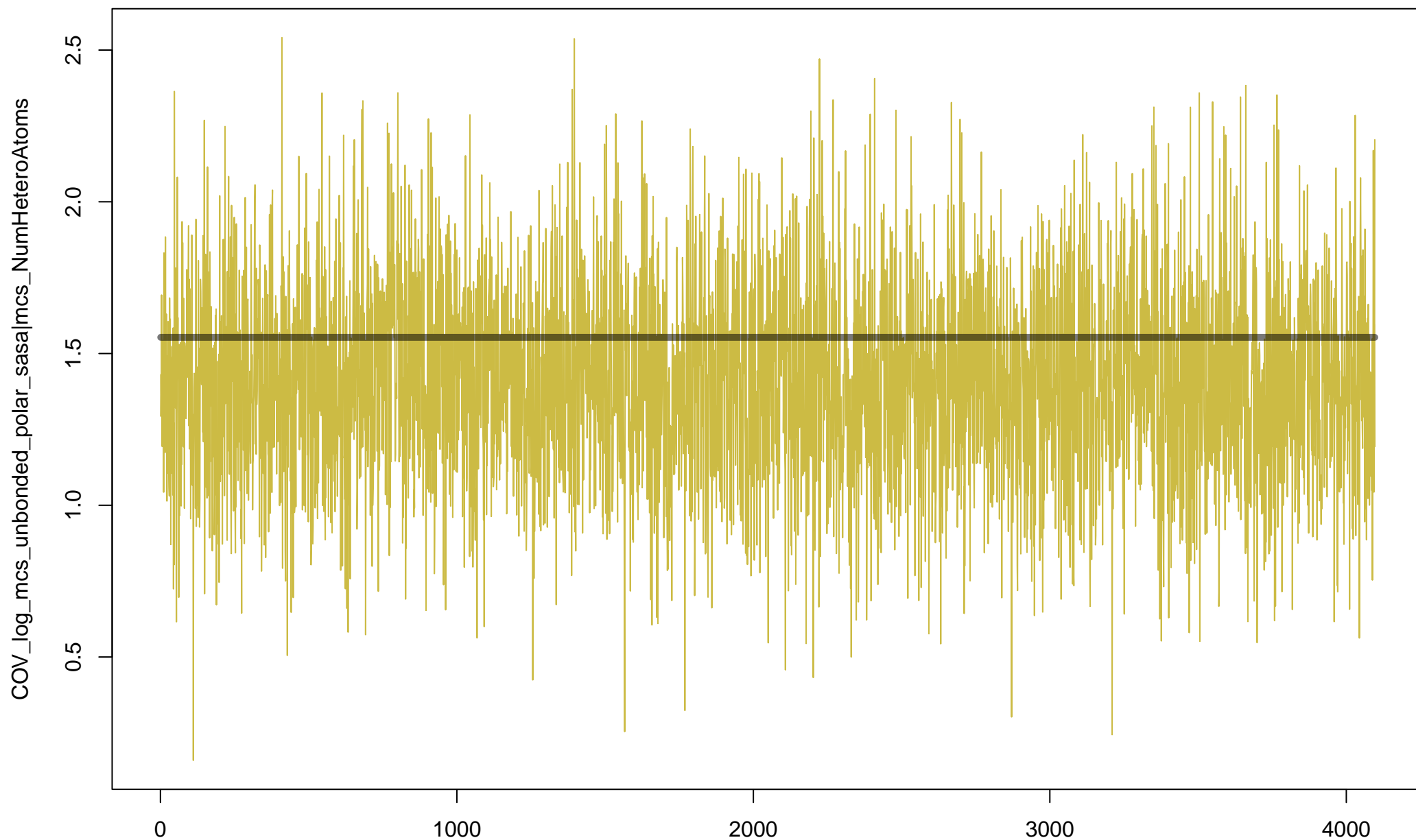
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 3900 | BMK = 0.0303 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: -1.62**



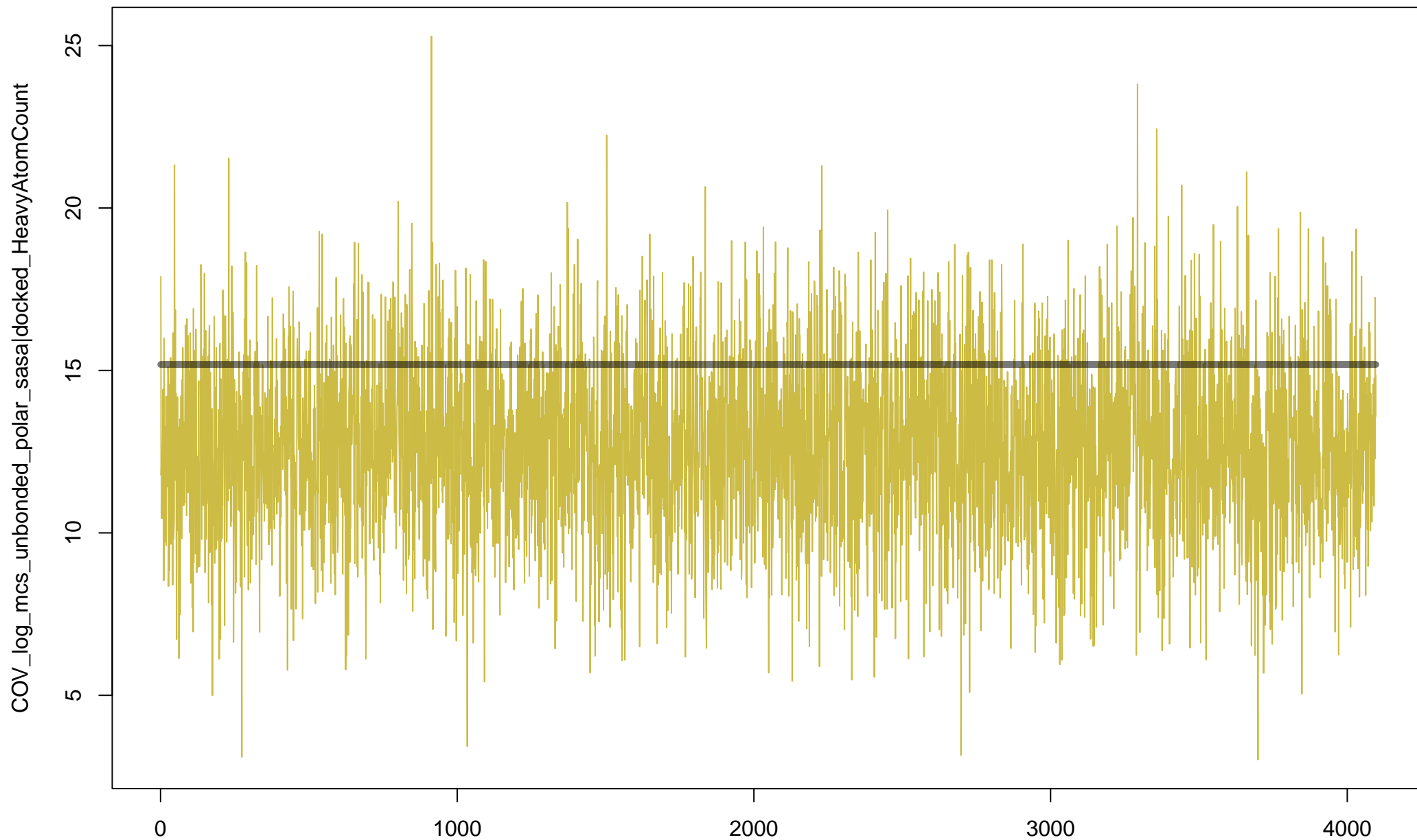
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 3810 | BMK = 0.0383 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: -1.79**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 3890 | BMK = 0.036 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0 | rel.err: -0.467**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0327 | MCSE(6.27) = 1.61 | stat: TRUE | burn: 0 | rel.err: -0.965**





**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0405 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0 | rel.err: 0.451**

