

-- STATS maxD --

min ESS = 169.741319004492

max BMK = 0.123814716623891

max MCSE = 6.53708805712395

all stationary: FALSE

burn: 0

max rel.err.: 2.51520349472418

-- STATS 1D --

min ESS = 3142.12368696742

max BMK = 0.0604961565714755

max MCSE = 1.84632446017346

all stationary: TRUE

burn: 0

max rel.err.: 2.29901638661118

-- STATS 2D --

min ESS = 3573.5647196565

max BMK = 0.0402558406190933

max MCSE = 1.79429188764255

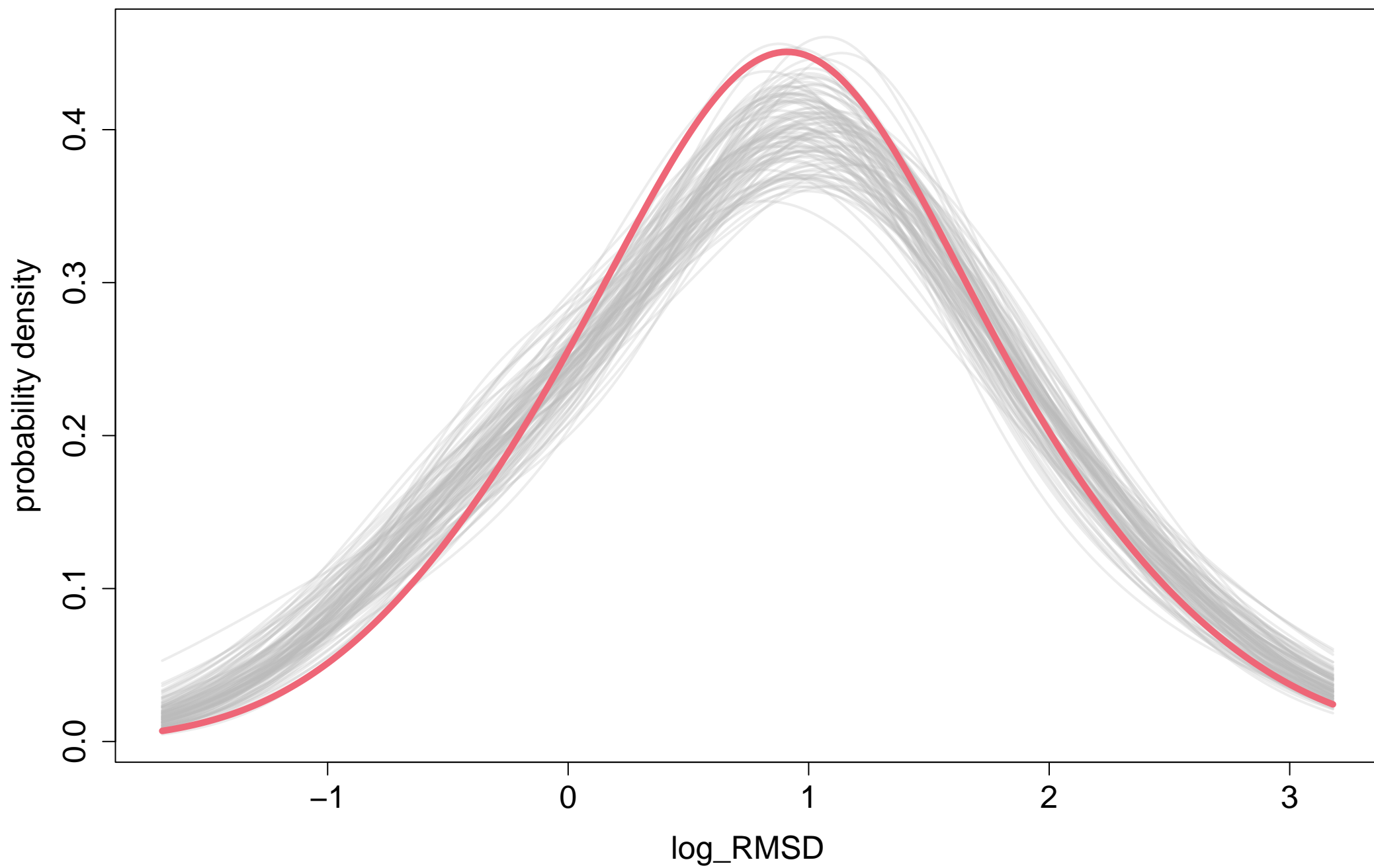
all stationary: TRUE

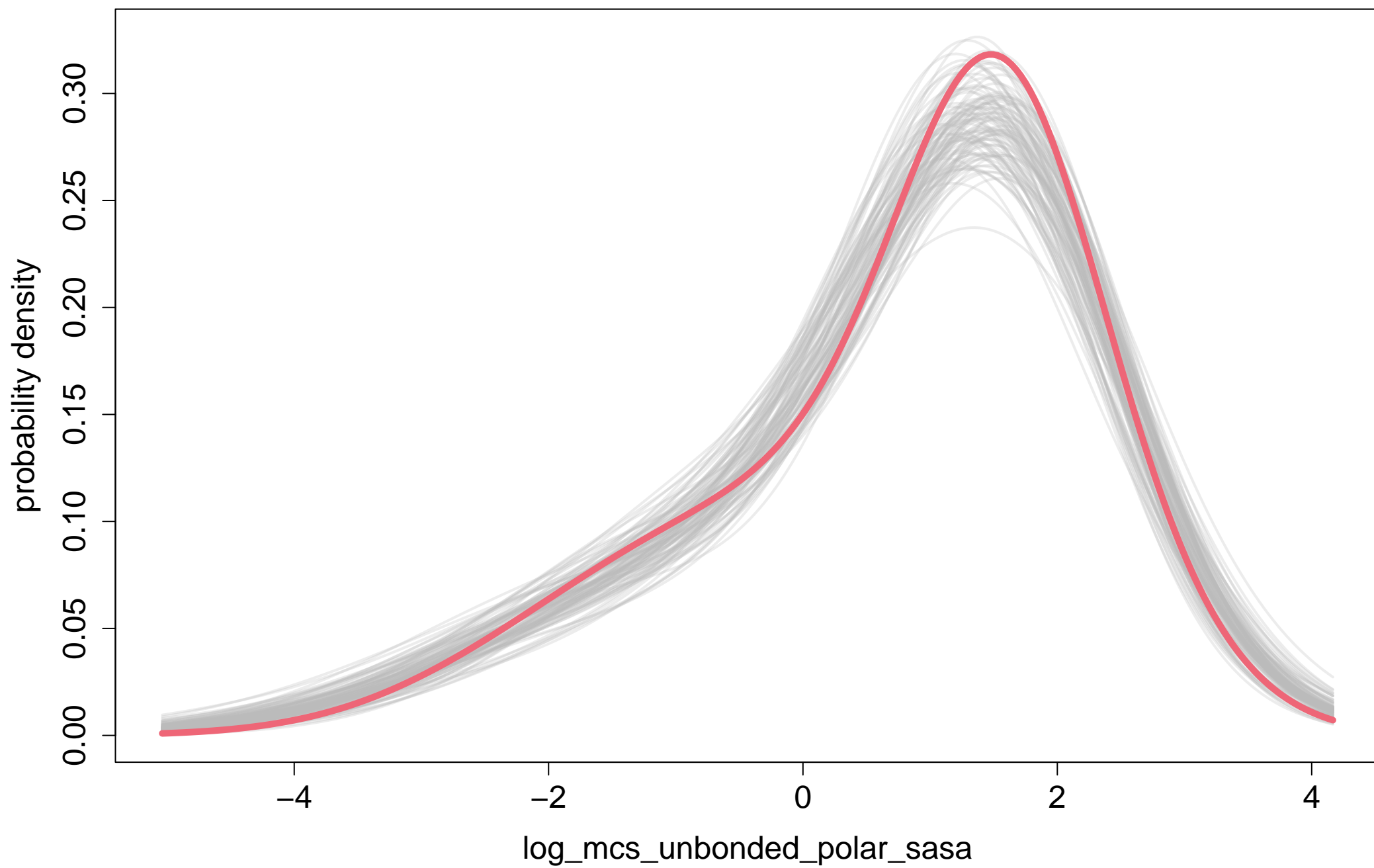
burn: 0

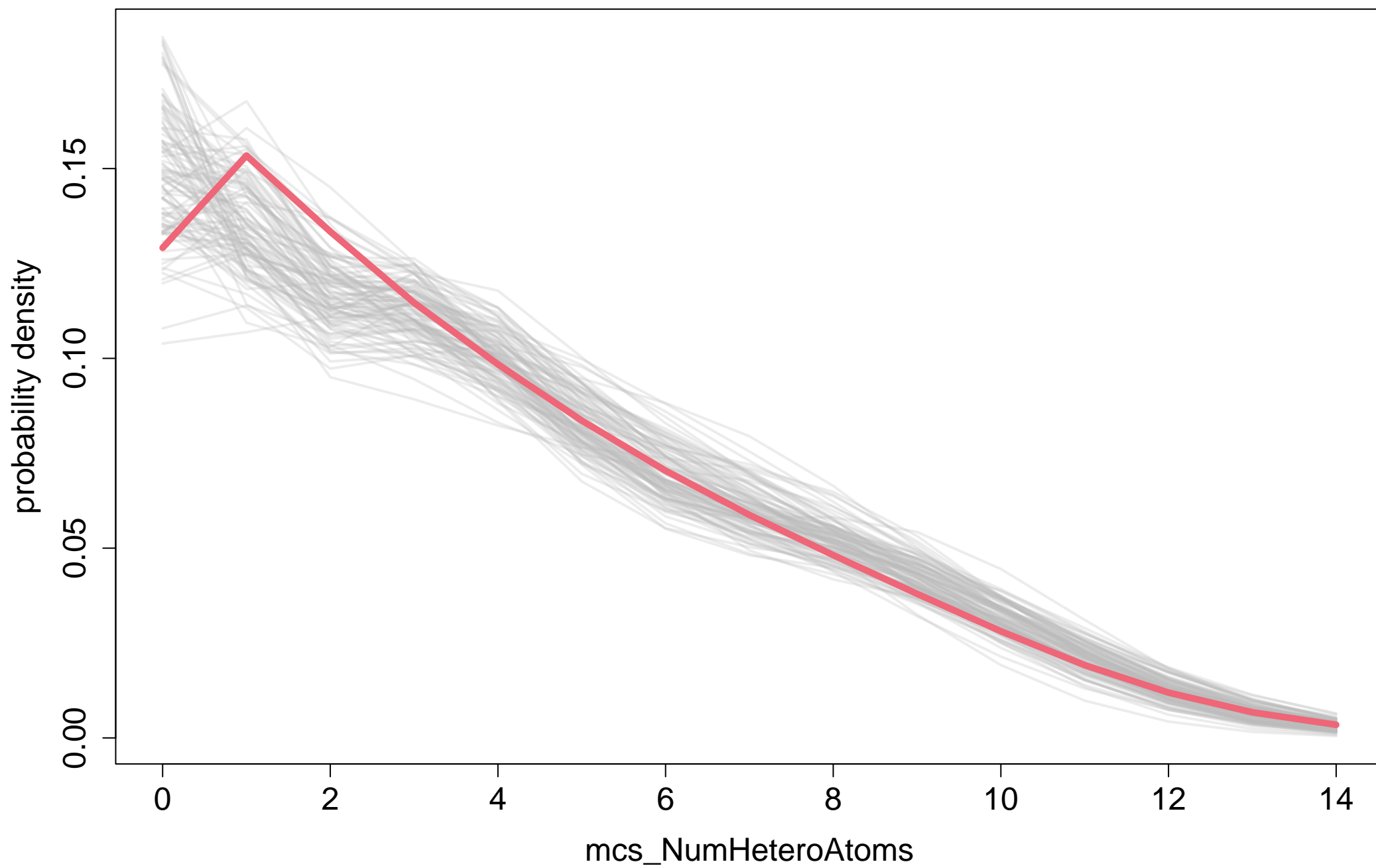
max rel.err.: 1.77801398947813

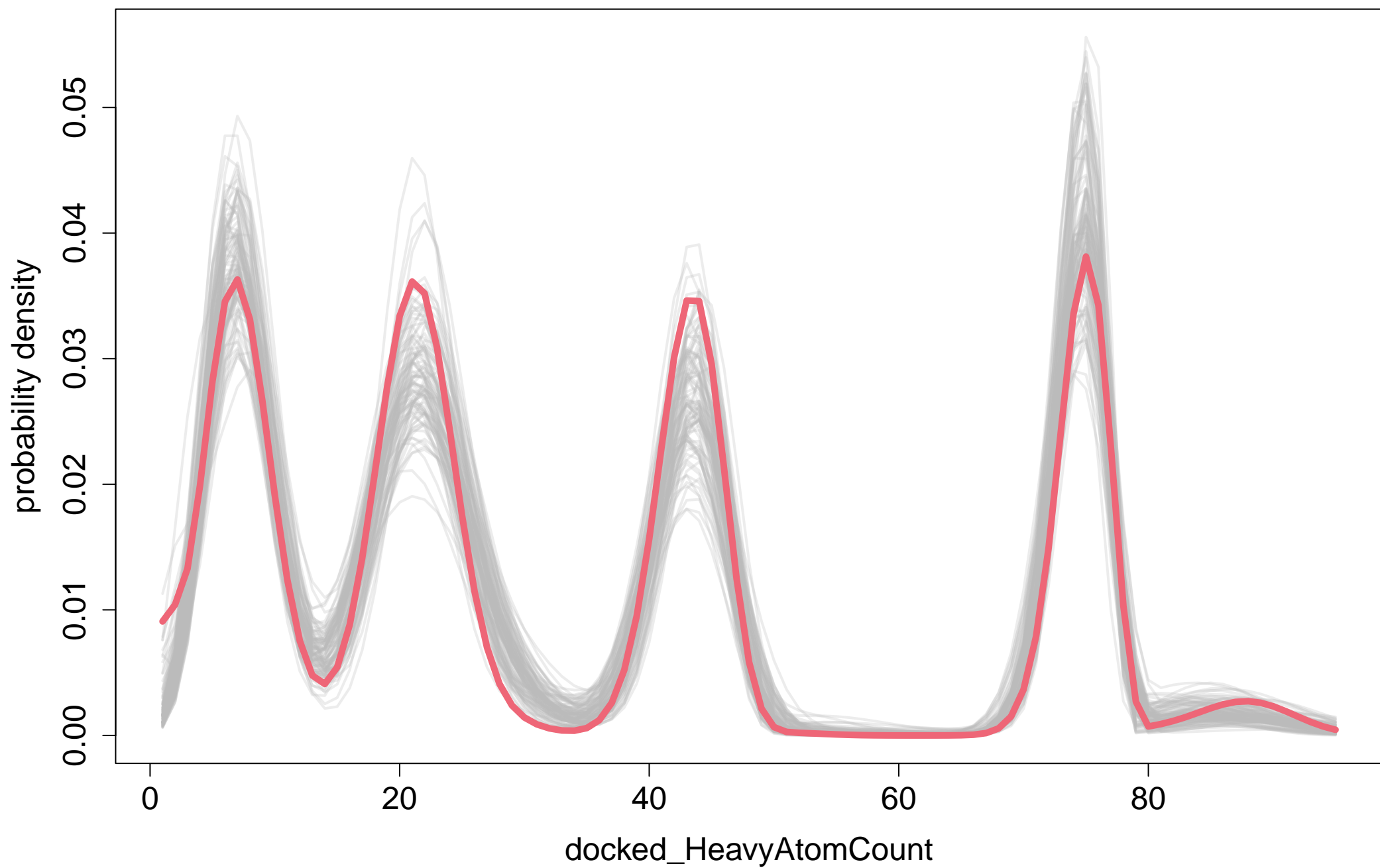
Occupied clusters: 13 of 16

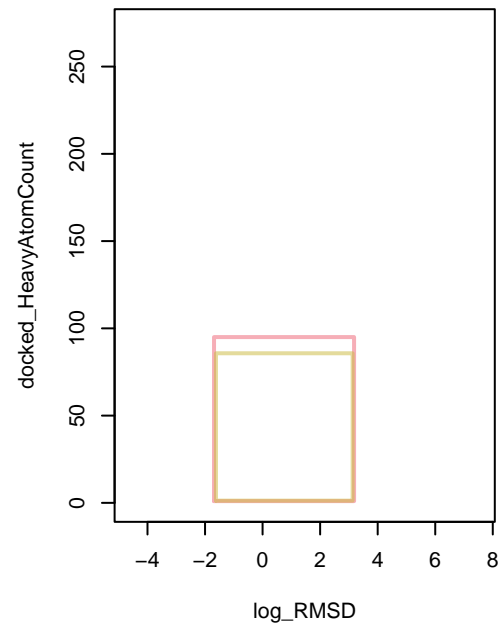
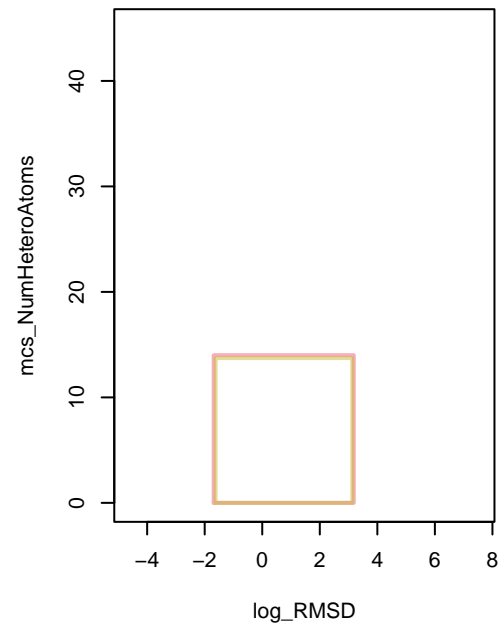
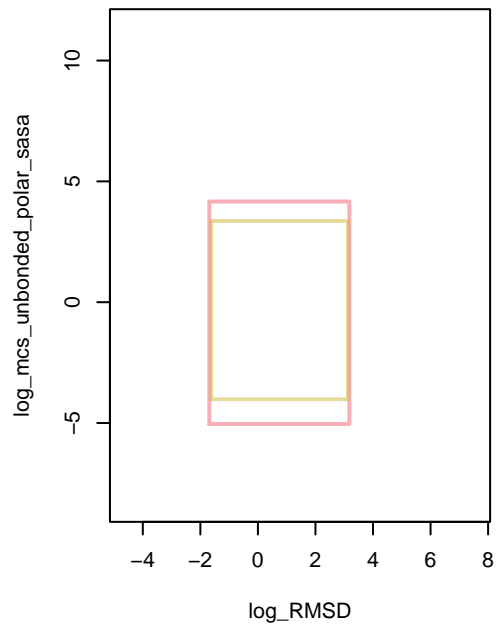
LL: -2160 +- 6.99



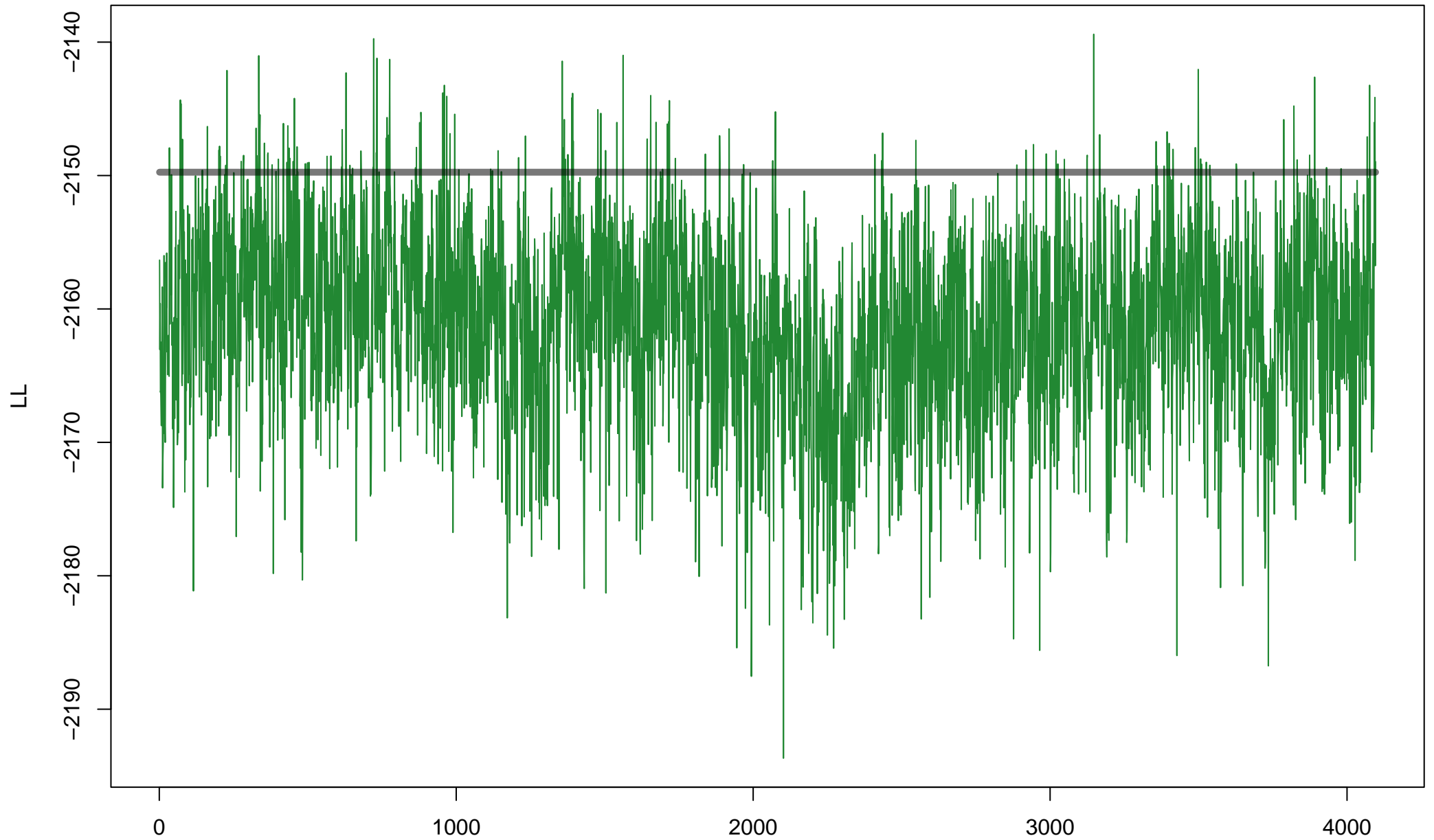




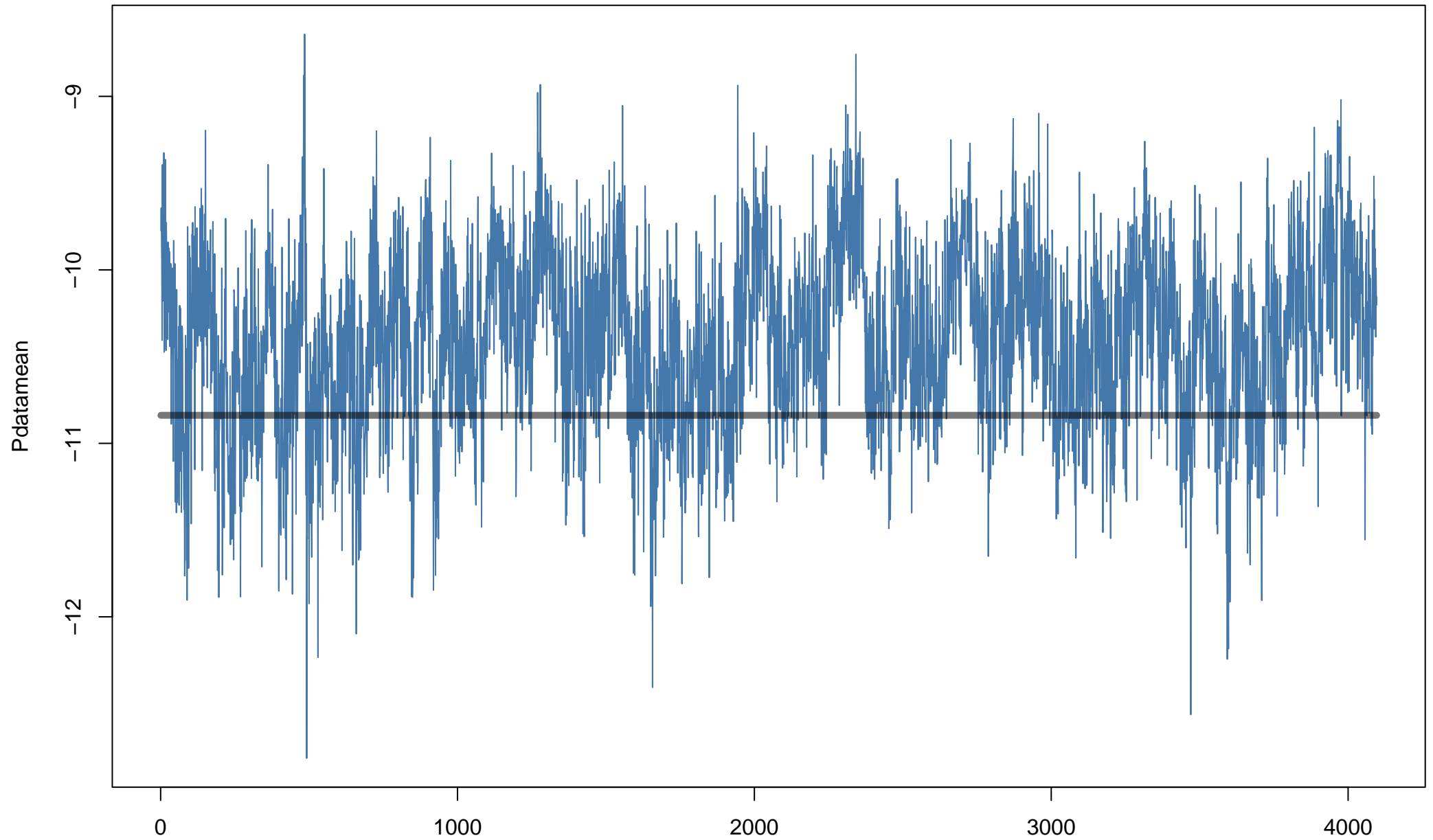




LL

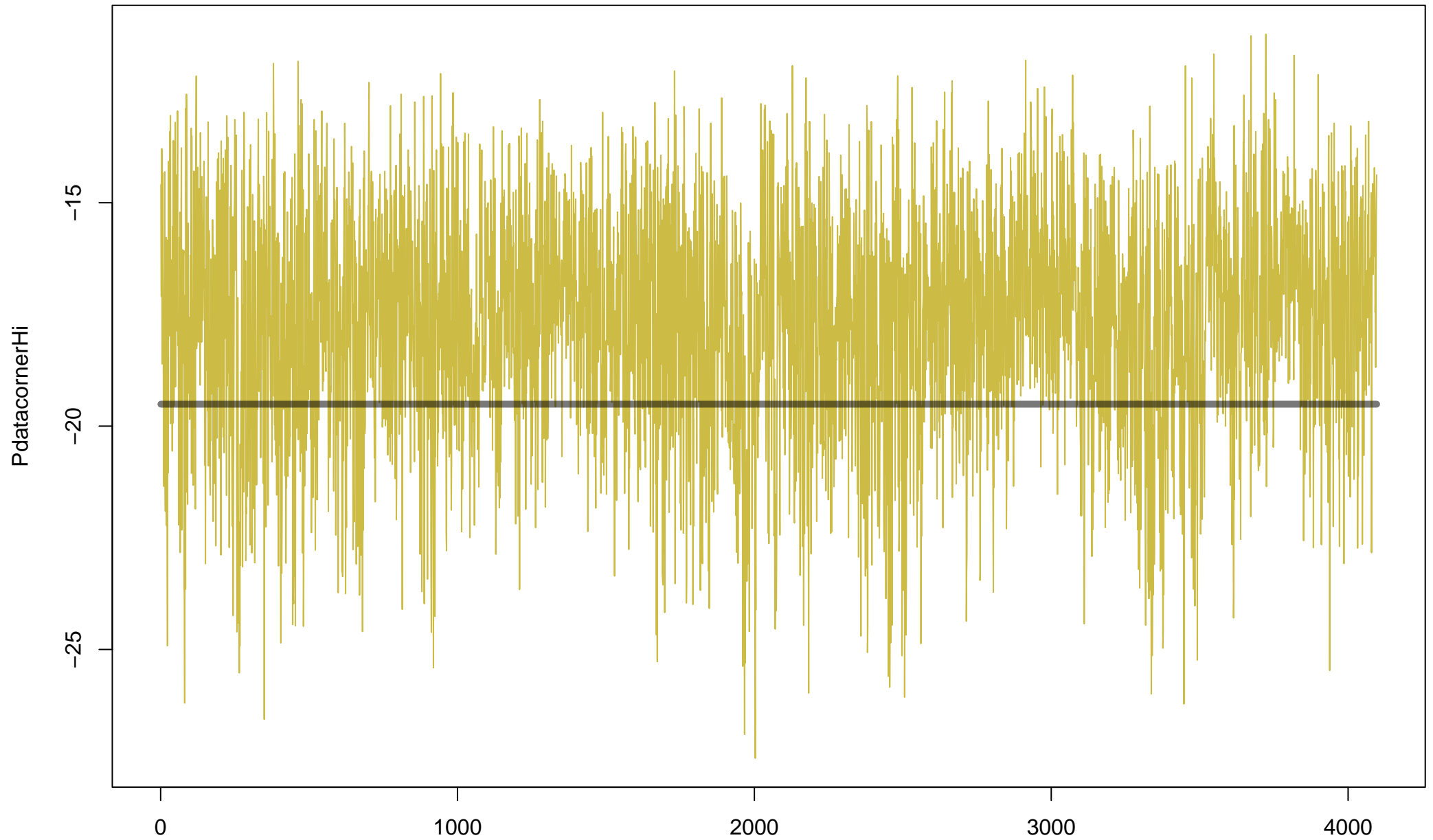


**Pdatamean**  
**ESS = 170 | BMK = 0.102 | MCSE(6.27) = 6.54 | stat: FALSE | burn: 0 | rel.err: 0.838**

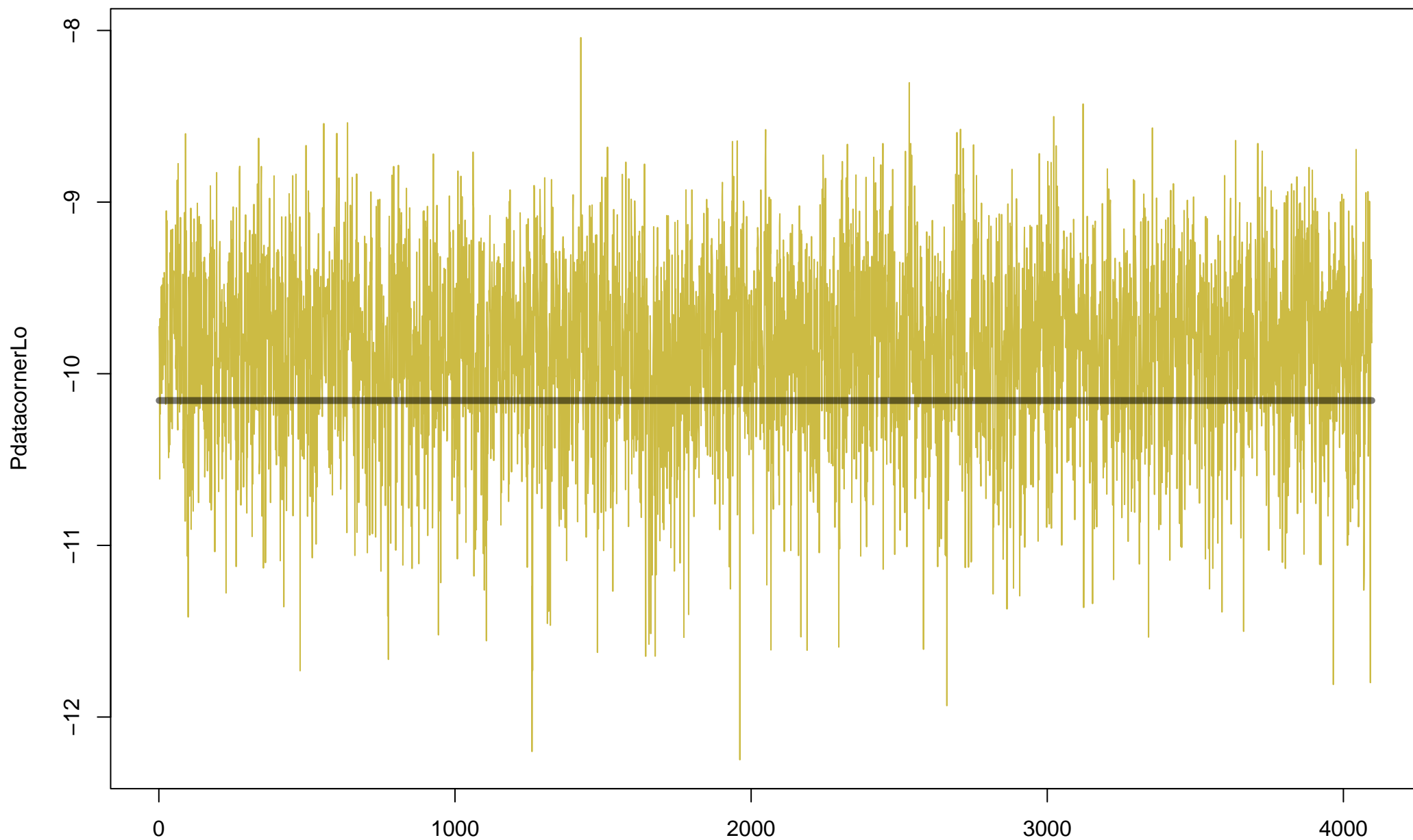




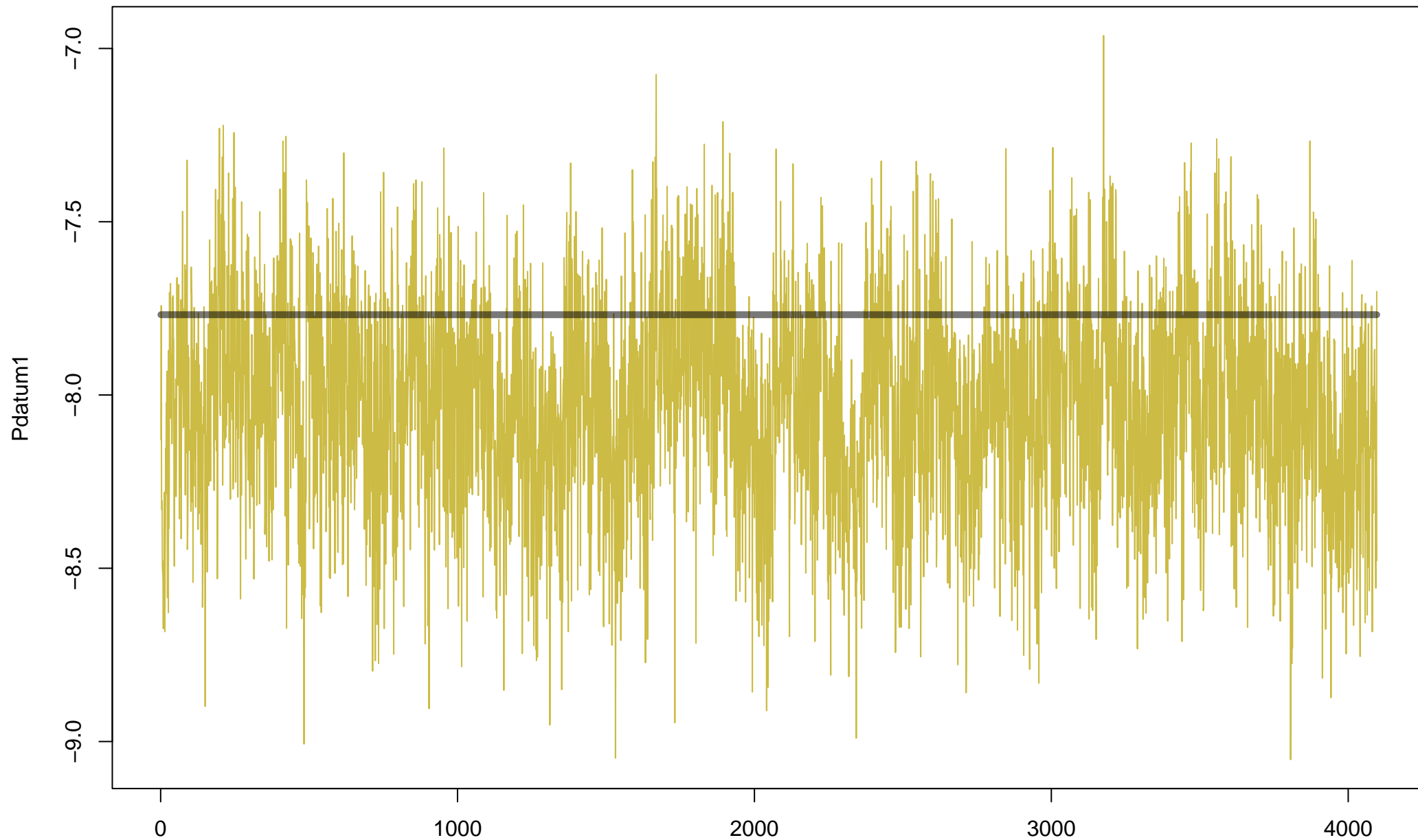
**PdatacornerHi**  
**ESS = 4100 | BMK = 0.117 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: 0.302**



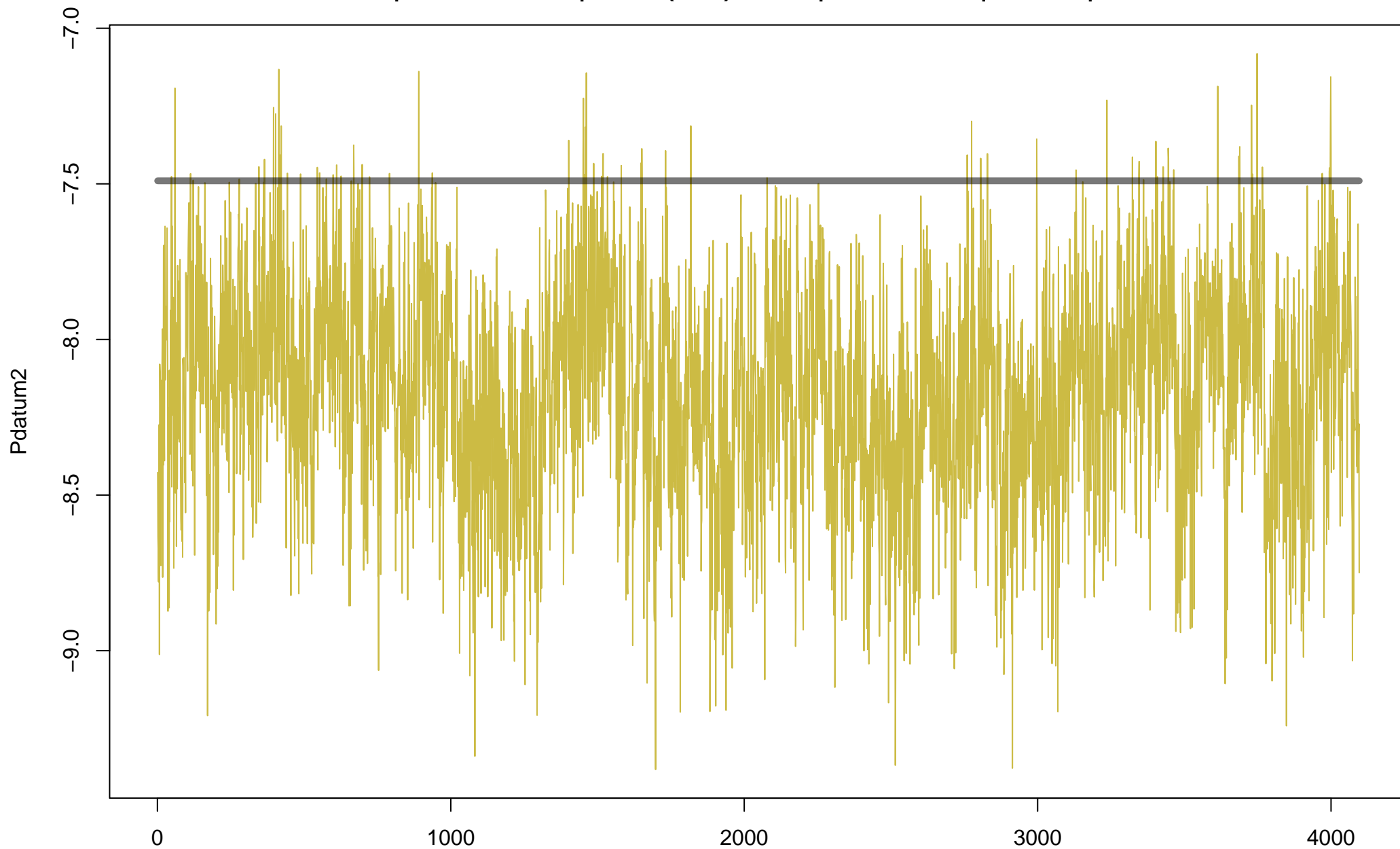
**PdatacornerLo**  
**ESS = 2970 | BMK = 0.0359 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: 0.663**



**Pdatum1**  
**ESS = 386 | BMK = 0.0497 | MCSE(6.27) = 4.45 | stat: TRUE | burn: 0 | rel.err: -0.836**

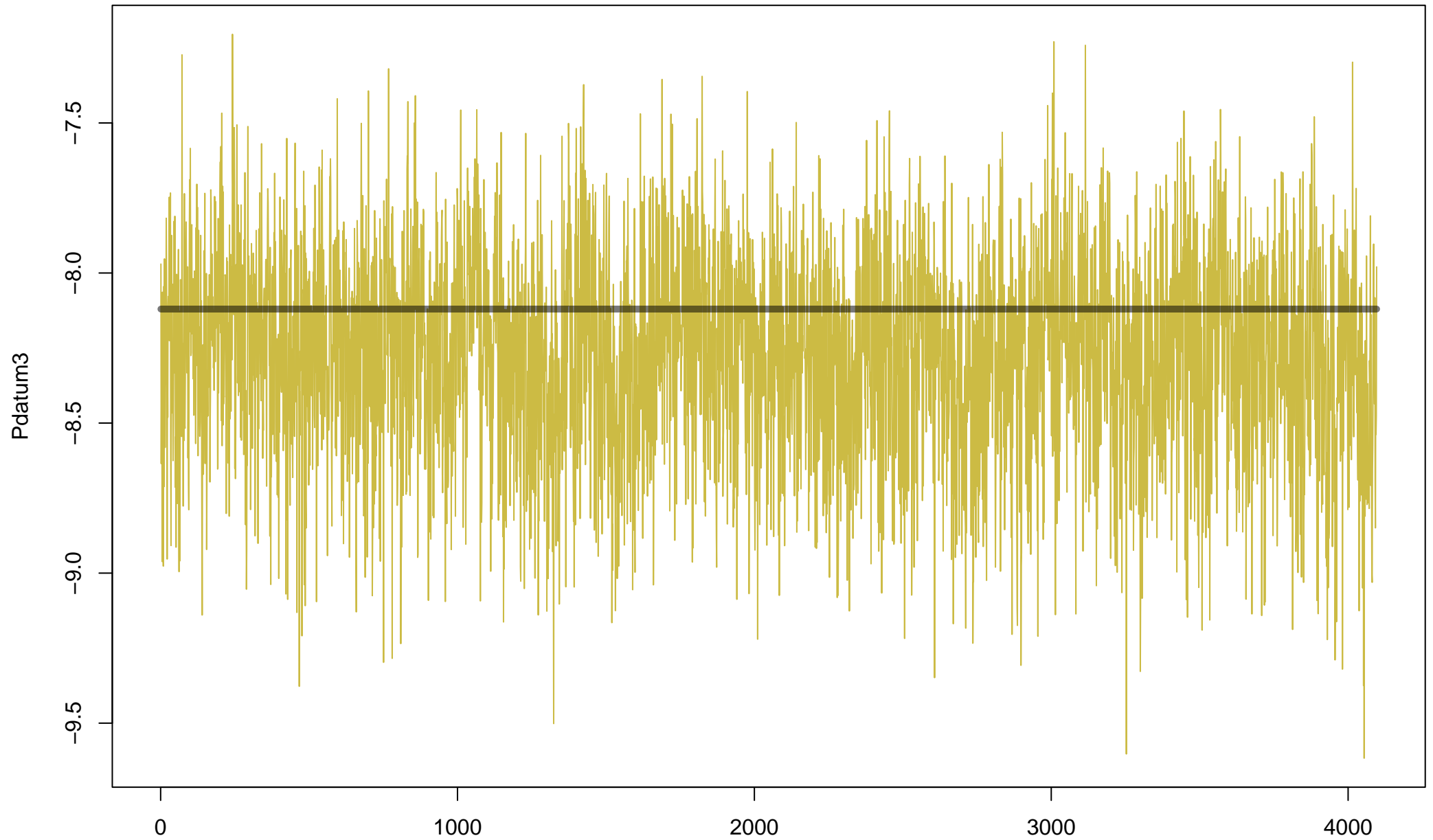


**Pdatum2**  
**ESS = 249 | BMK = 0.0451 | MCSE(6.27) = 5.19 | stat: FALSE | burn: 0 | rel.err: -2.52**

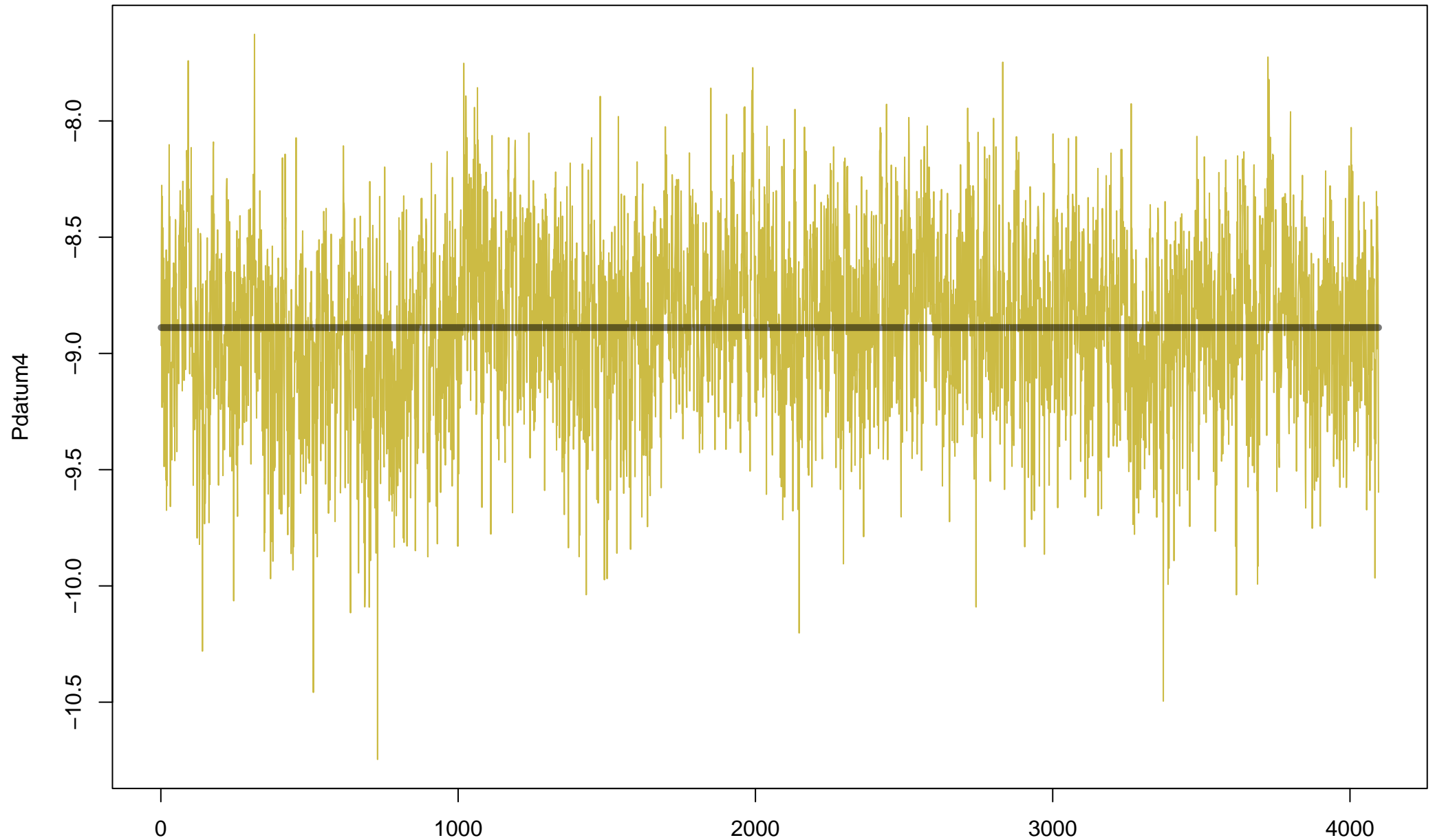


**Pdatum3**

**ESS = 888 | BMK = 0.0477 | MCSE(6.27) = 3.1 | stat: FALSE | burn: 0 | rel.err: -0.323**

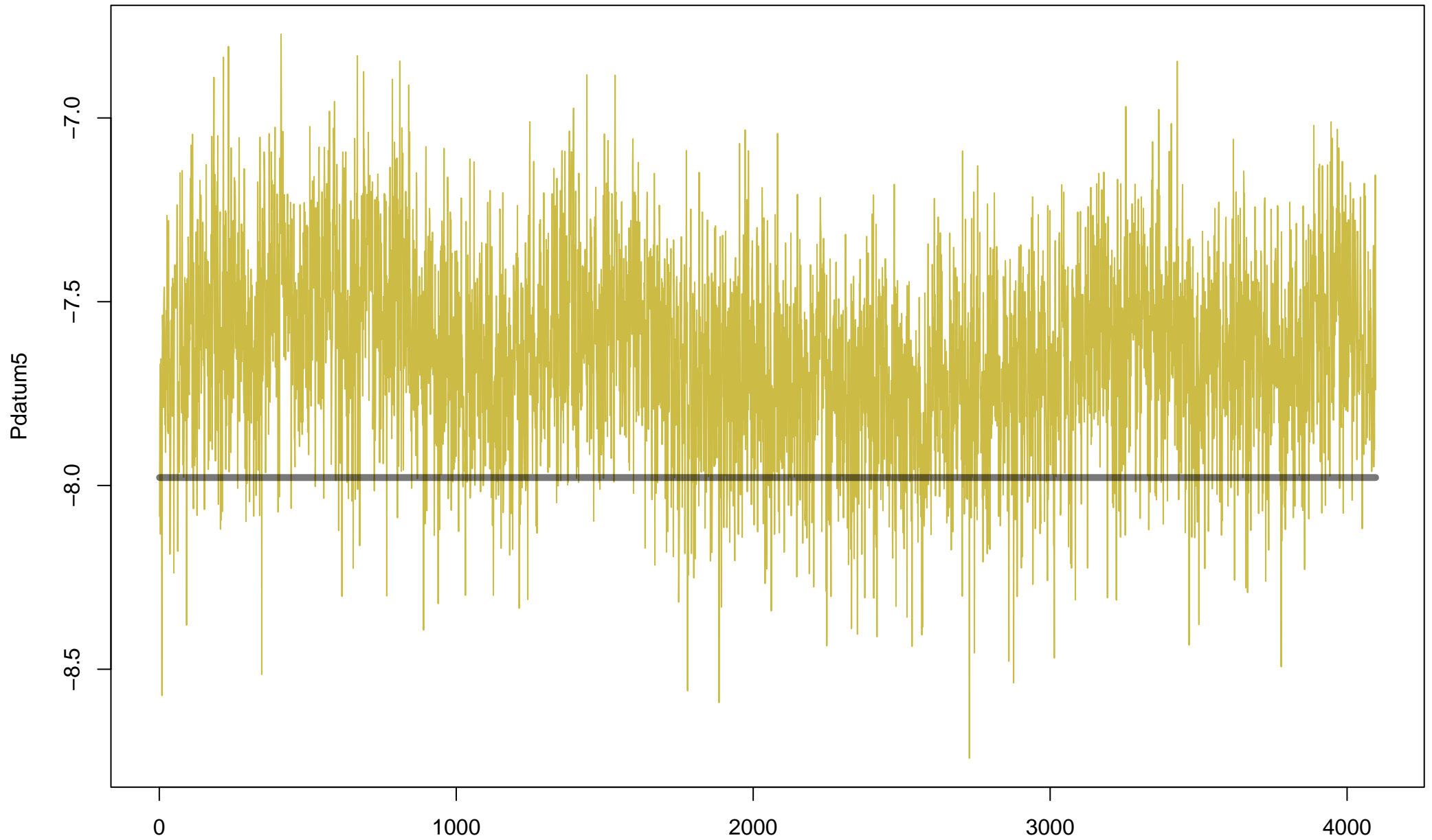


**Pdatum4**  
**ESS = 978 | BMK = 0.0493 | MCSE(6.27) = 3.97 | stat: TRUE | burn: 0 | rel.err: 0.2**



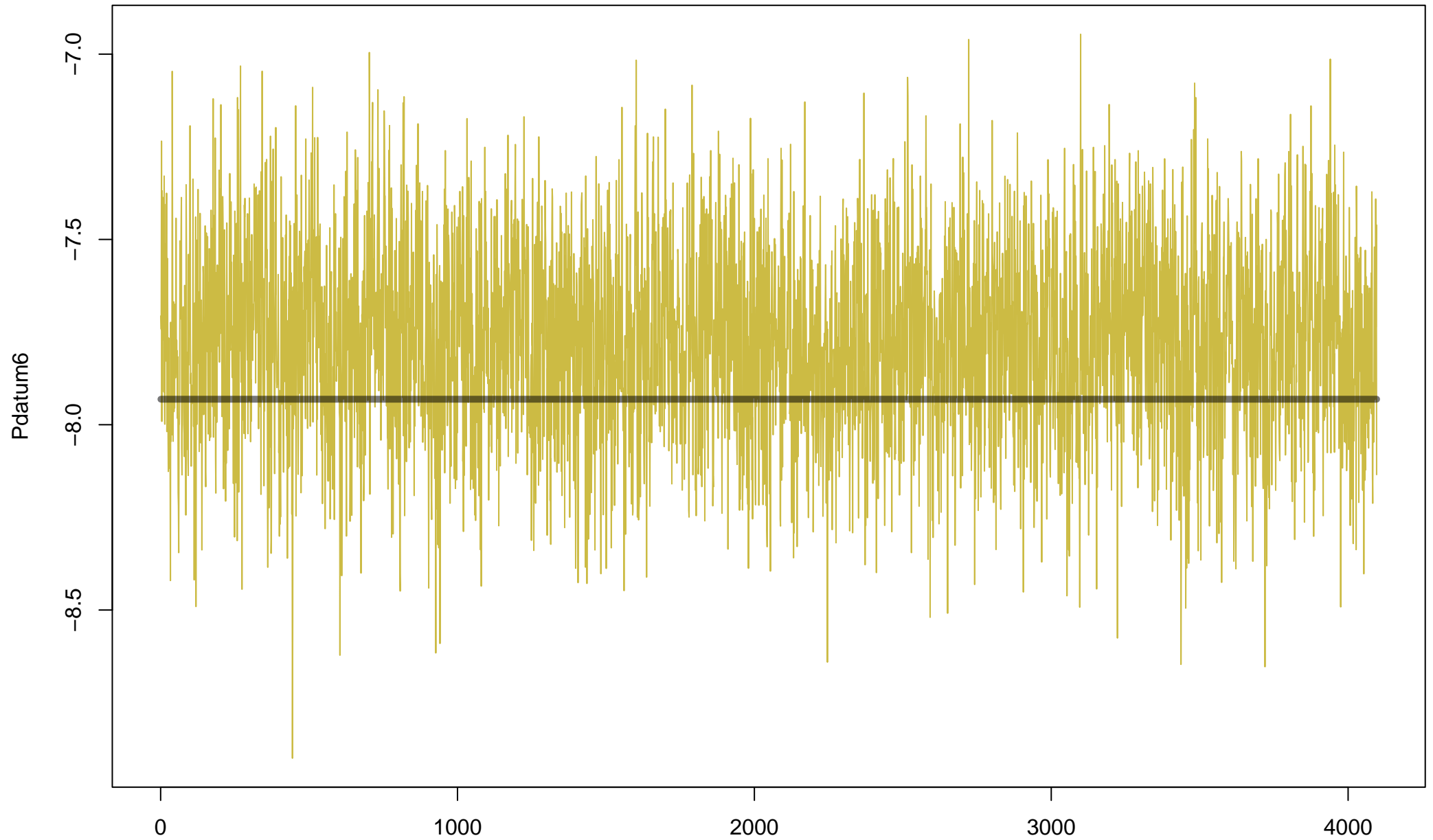
**Pdatum5**

**ESS = 170 | BMK = 0.124 | MCSE(6.27) = 4.68 | stat: FALSE | burn: 0 | rel.err: 1.19**



**Pdatum6**

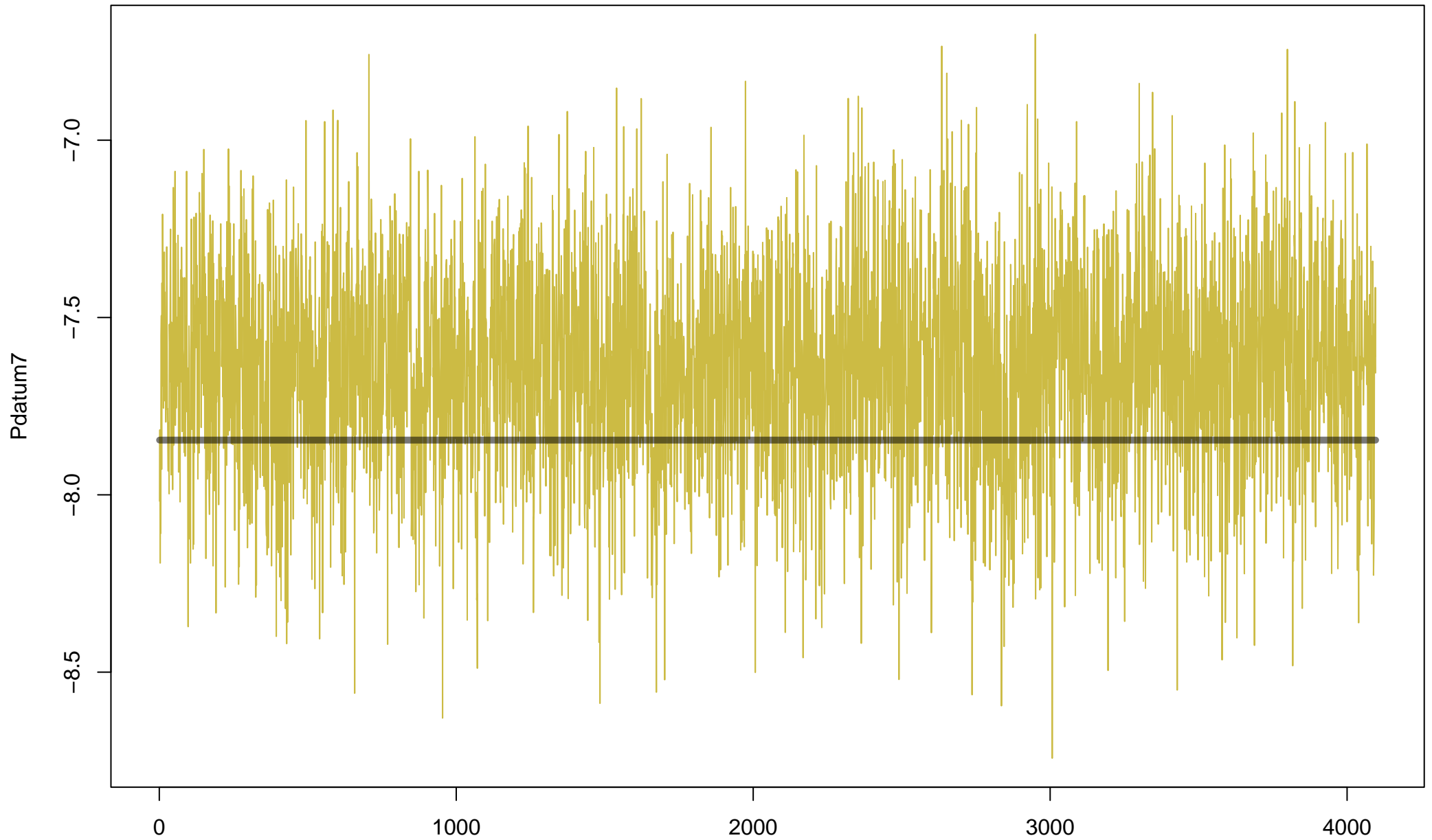
**ESS = 2270 | BMK = 0.0409 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.667**





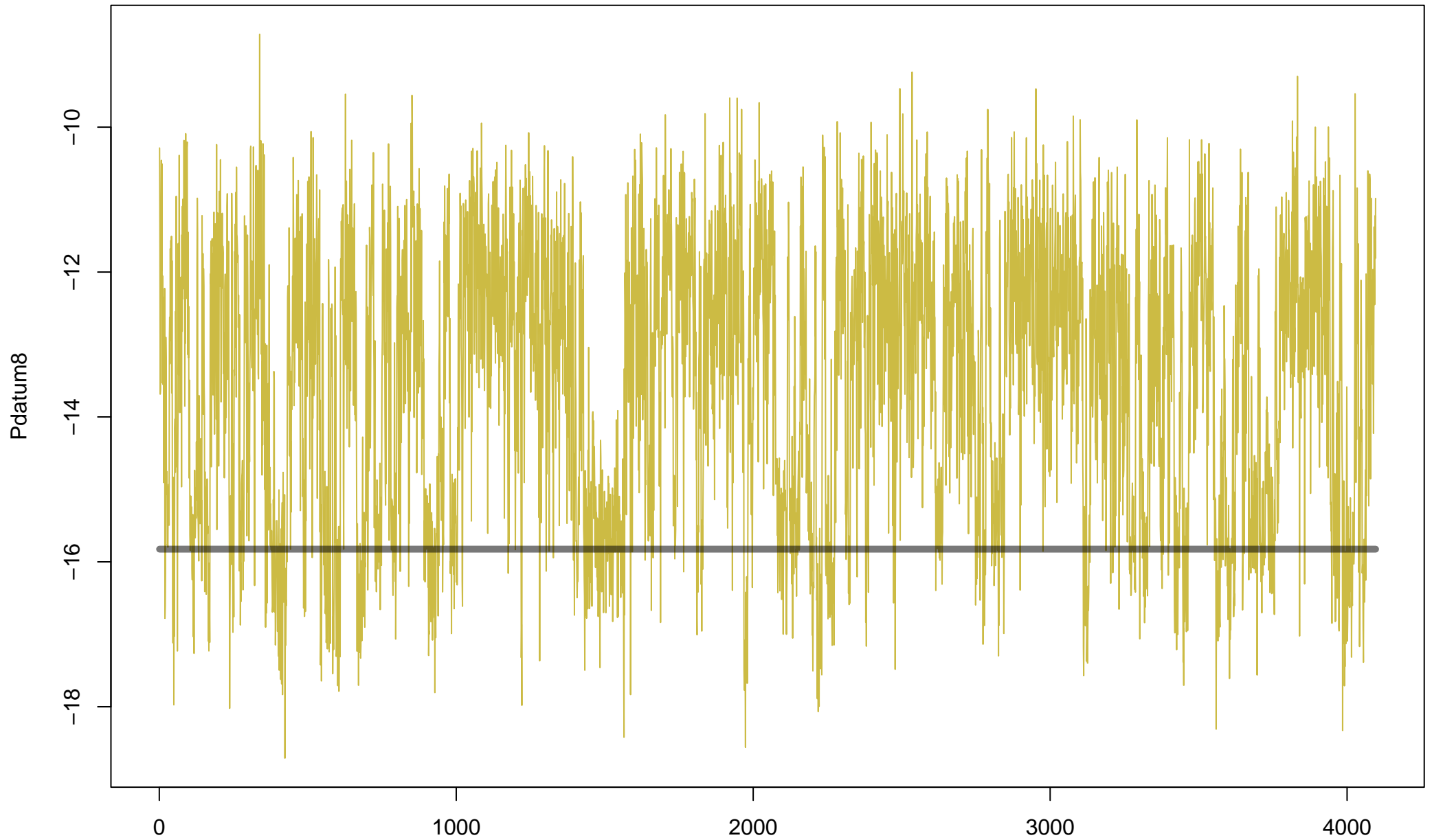
**Pdatum7**

**ESS = 2570 | BMK = 0.0389 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | rel.err: 0.758**



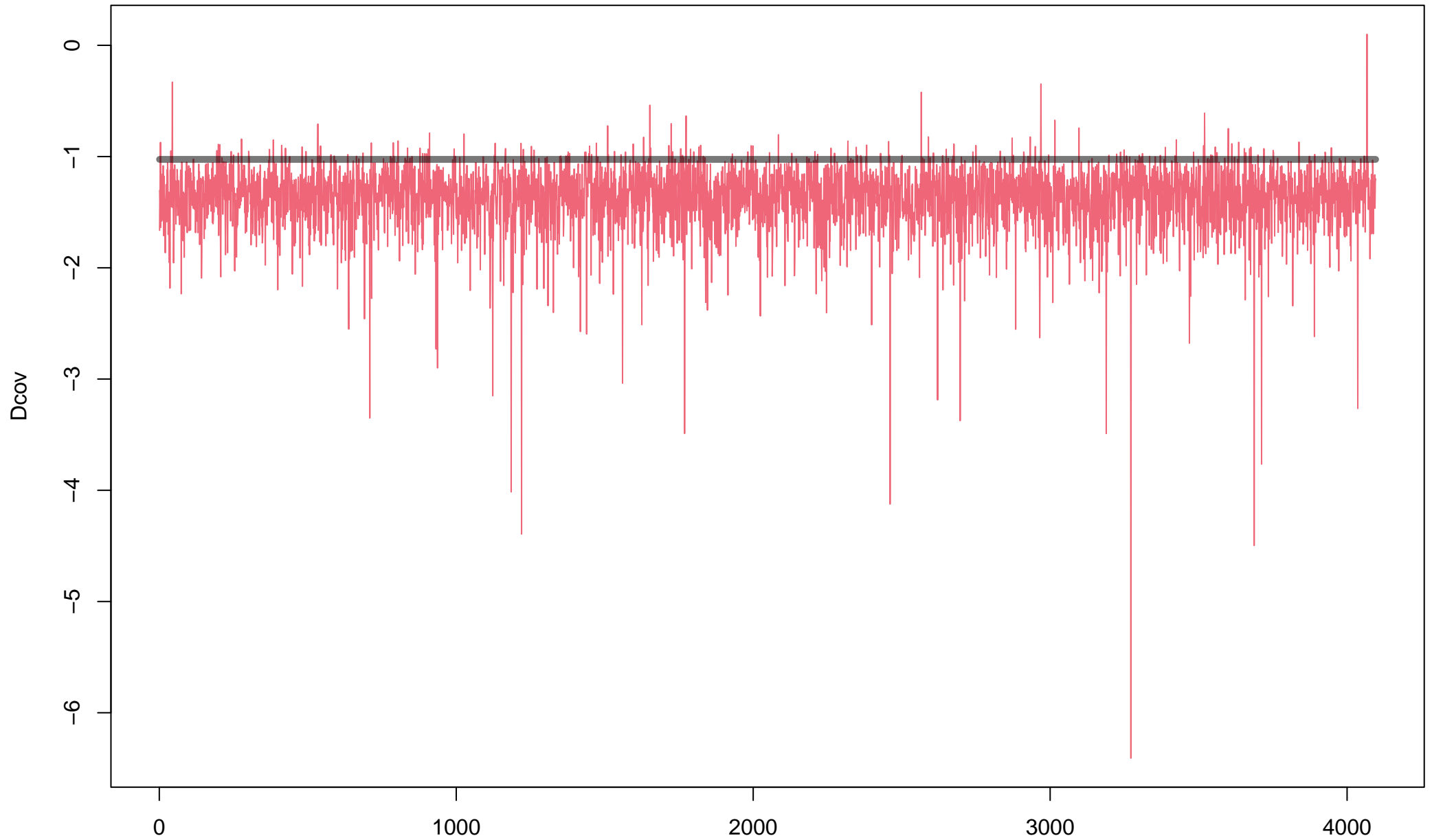
**Pdatum8**

**ESS = 768 | BMK = 0.0629 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0 | rel.err: 0.581**



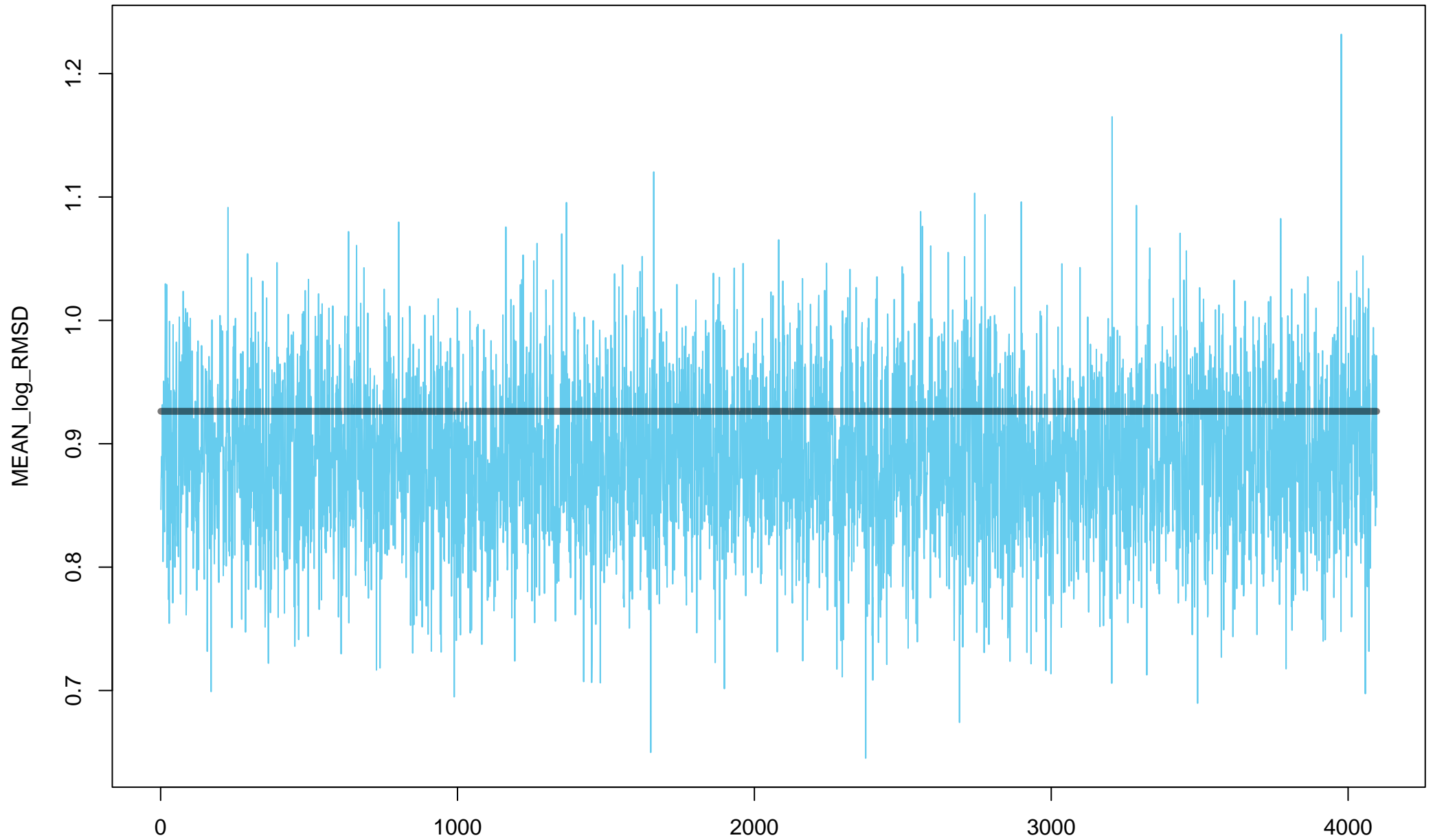
Dcov

ESS = 3460 | BMK = 0.0461 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: 1.47

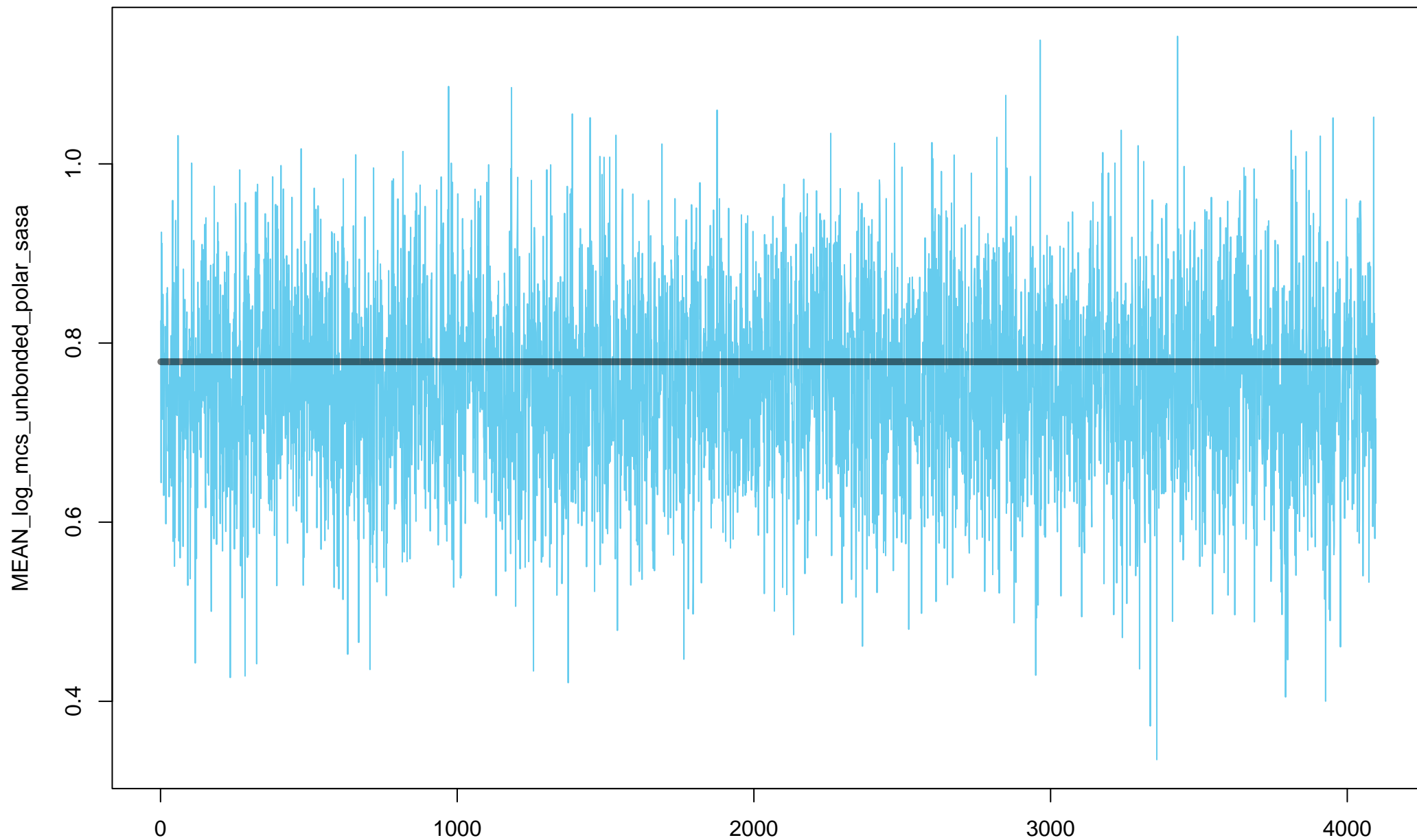


# MEAN\_log\_RMSD

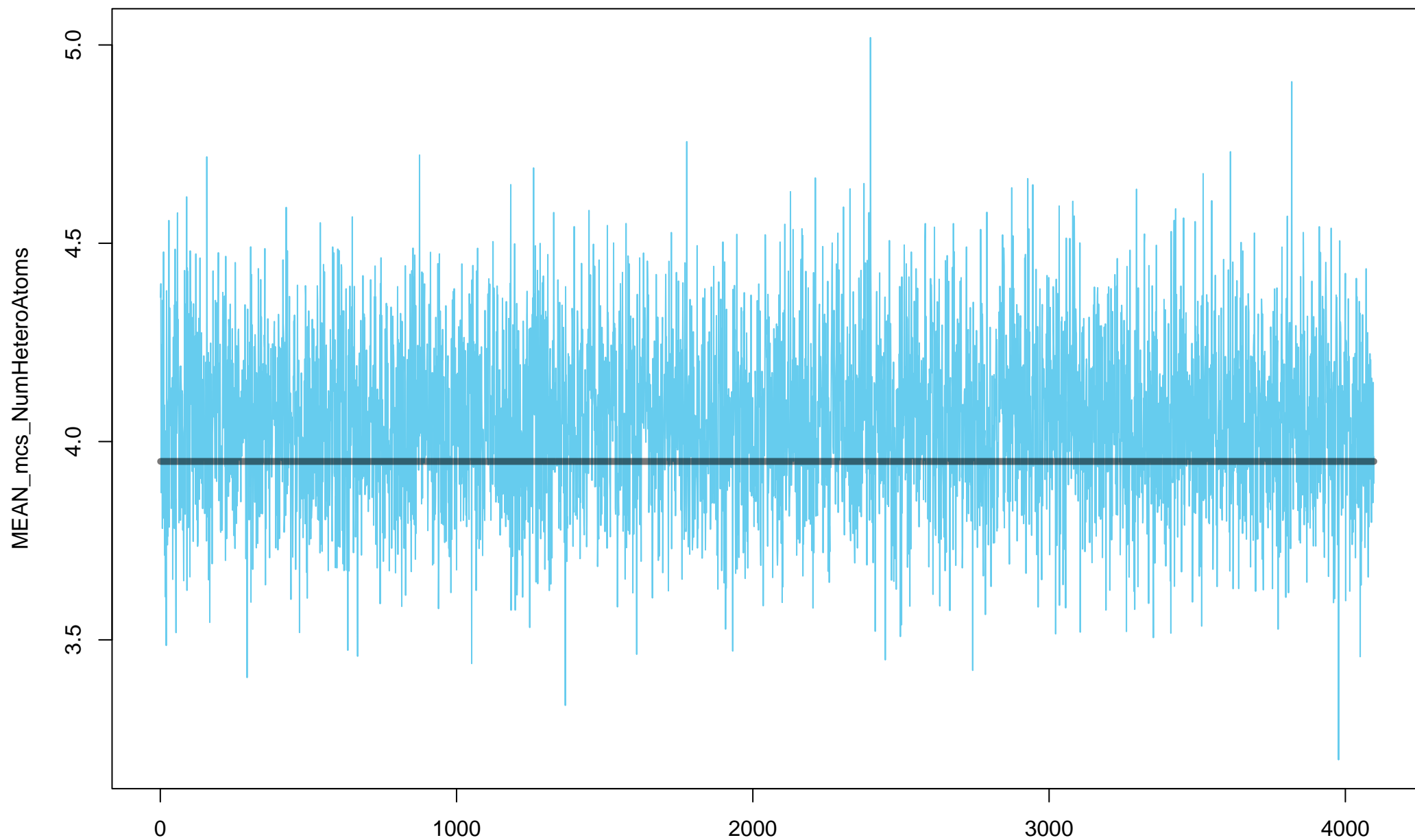
ESS = 4100 | BMK = 0.0298 | MCSE(6.27) = 1.66 | stat: TRUE | burn: 0 | rel.err: -0.579



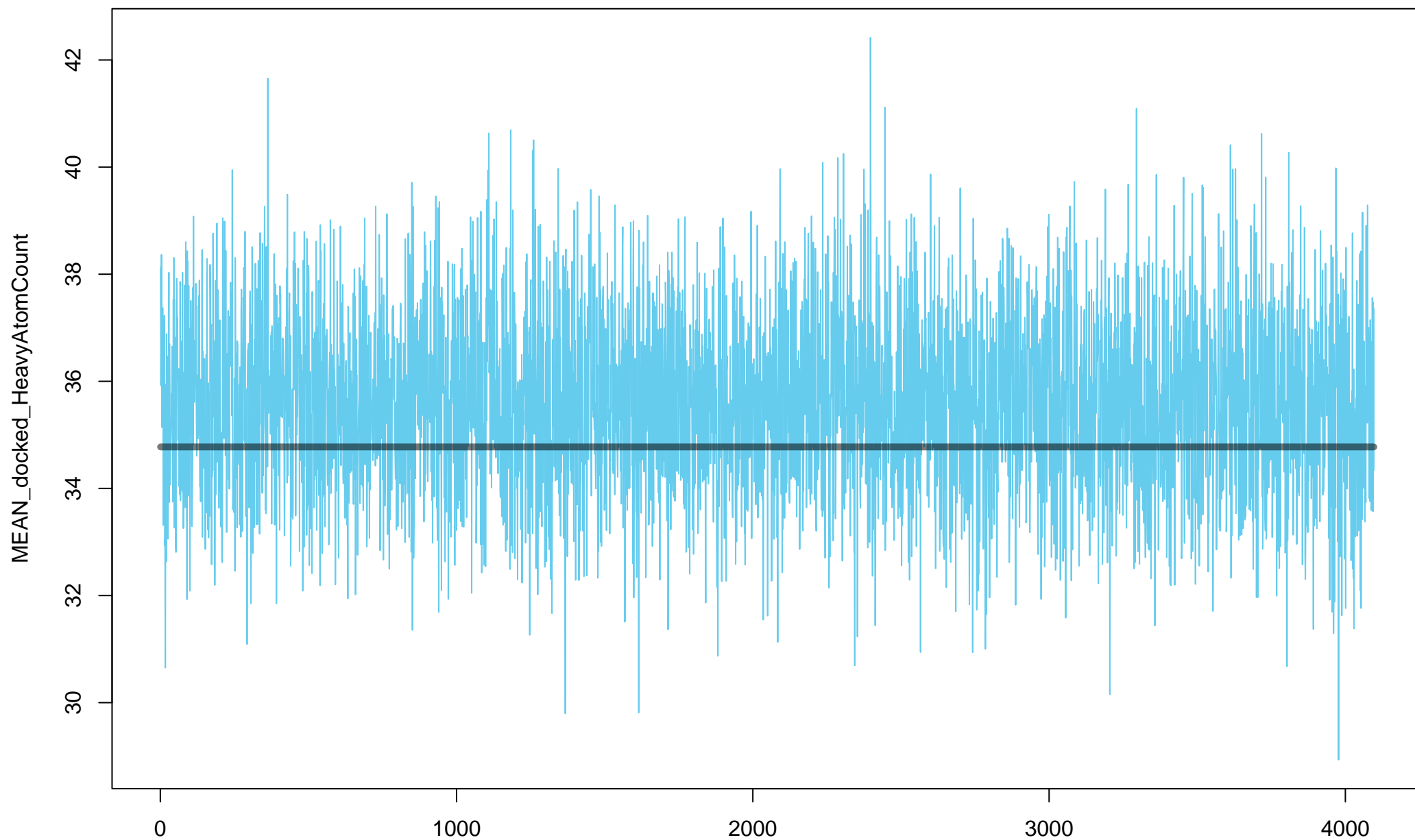
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 3820 | BMK = 0.0359 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: -0.222**



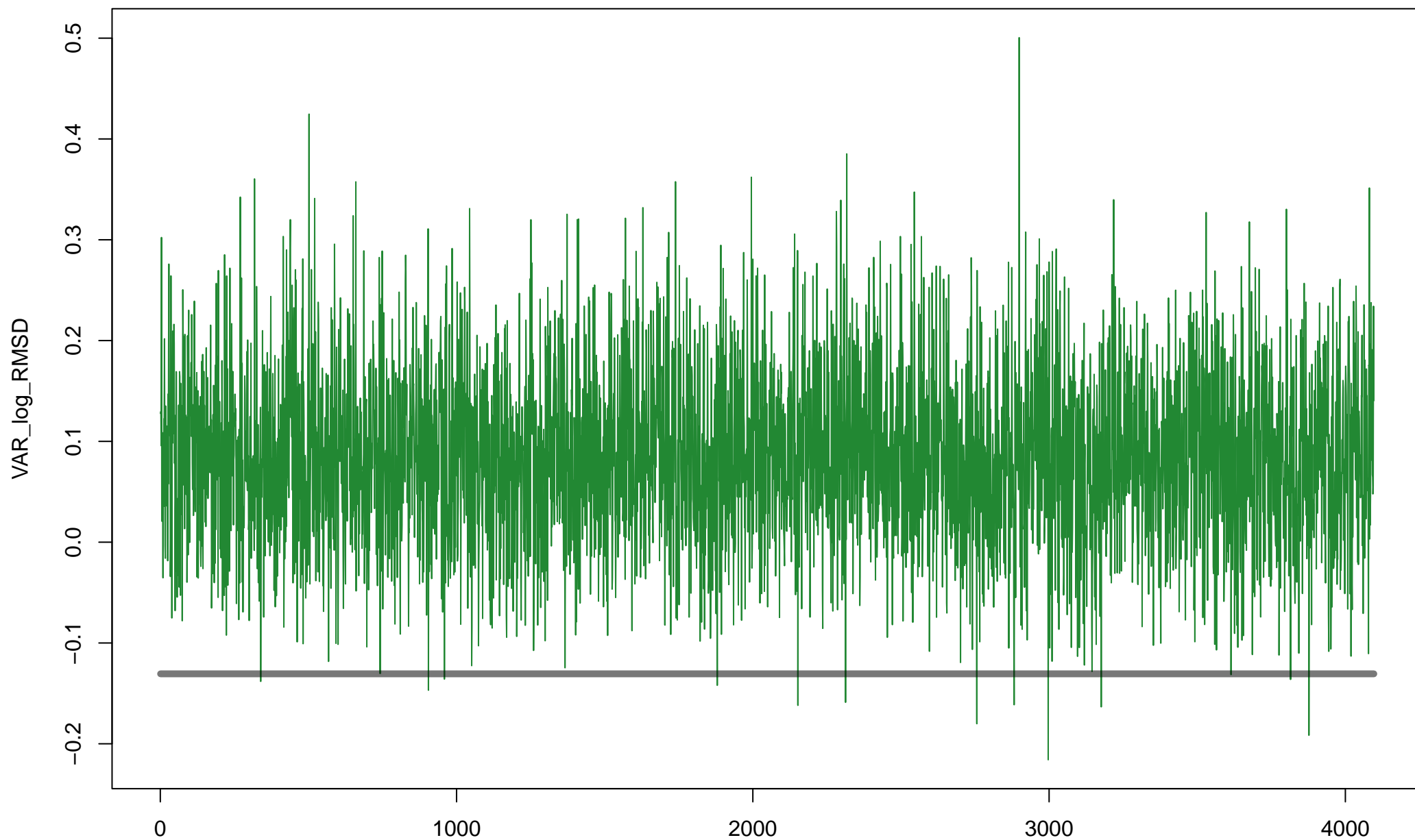
**MEAN\_mcs\_NumHeteroAtoms**  
**ESS = 4100 | BMK = 0.046 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0 | rel.err: 0.49**



**MEAN\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0409 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0 | rel.err: 0.496**

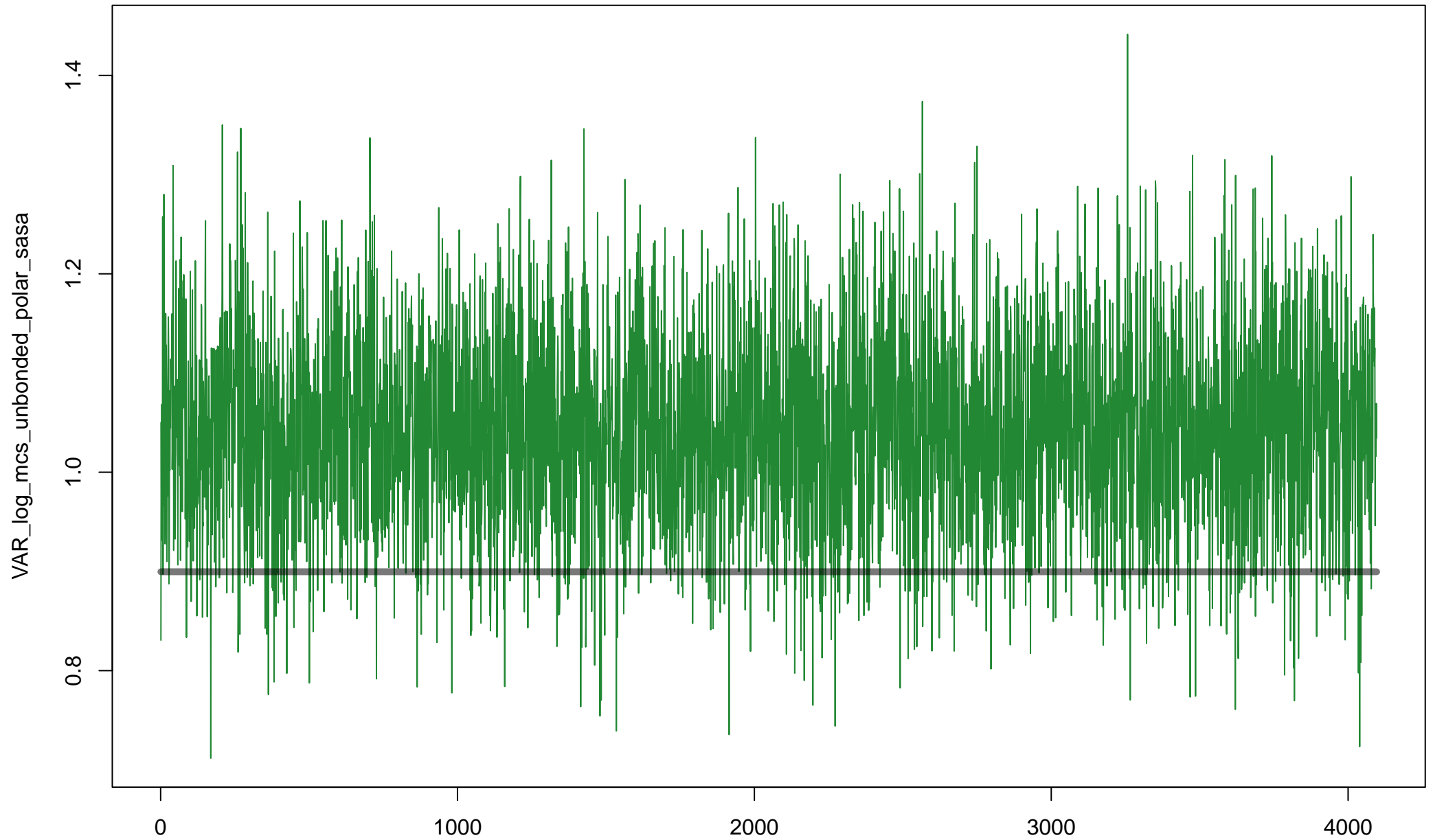


**VAR\_log\_RMSD**  
**ESS = 3790 | BMK = 0.0415 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: 2.3**

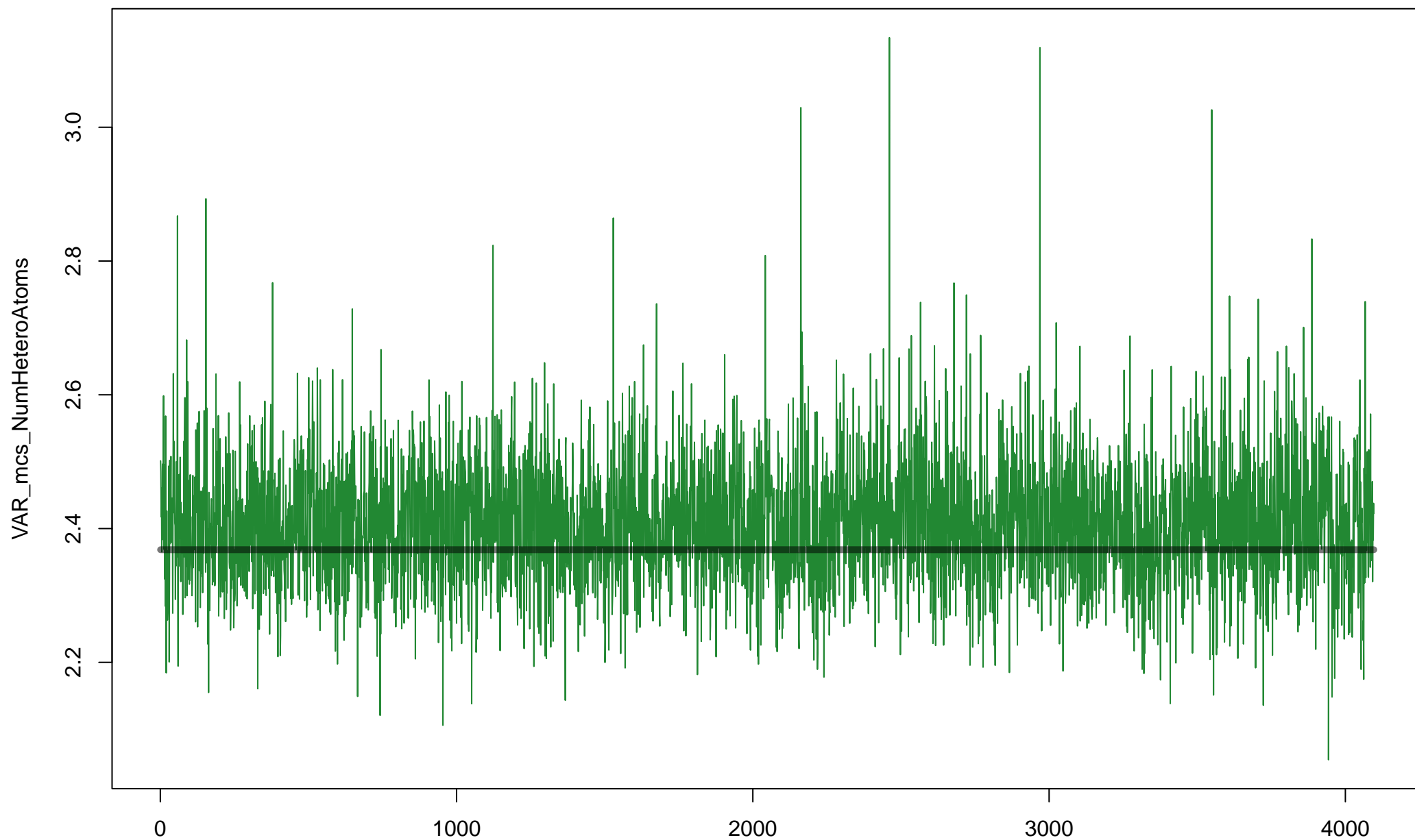




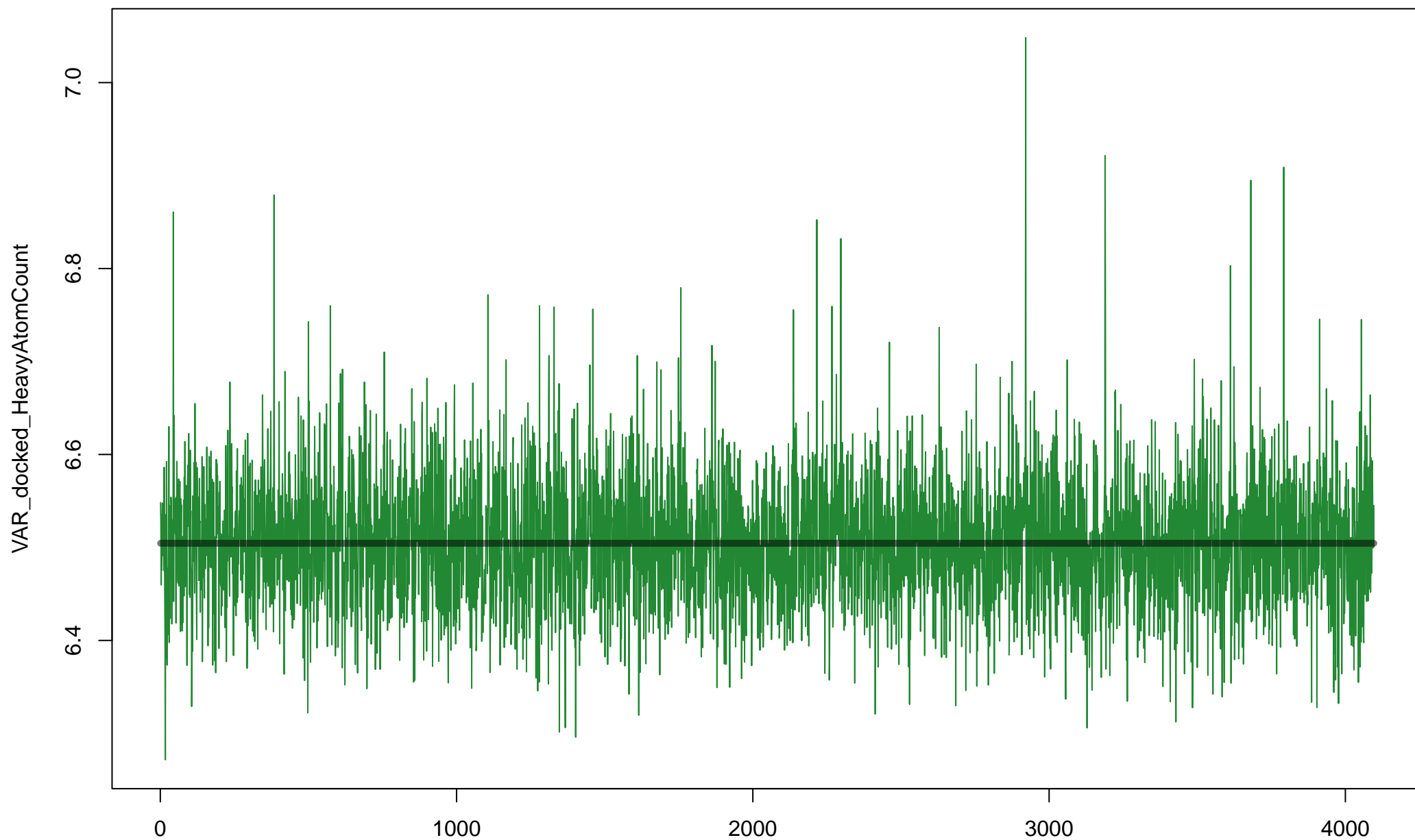
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 4100 | BMK = 0.0449 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0 | rel.err: 1.39**



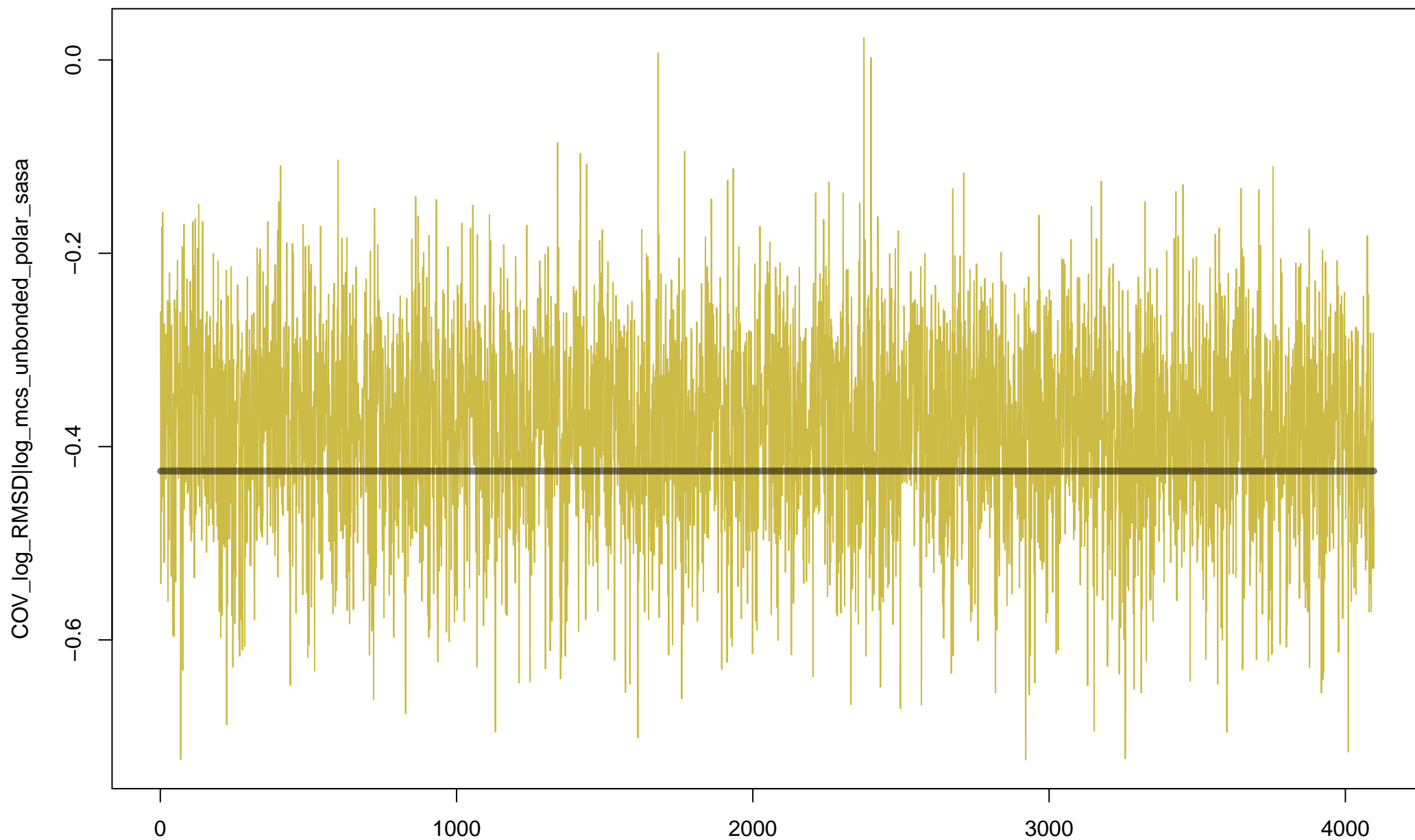
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 3140 | BMK = 0.0605 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: 0.437**



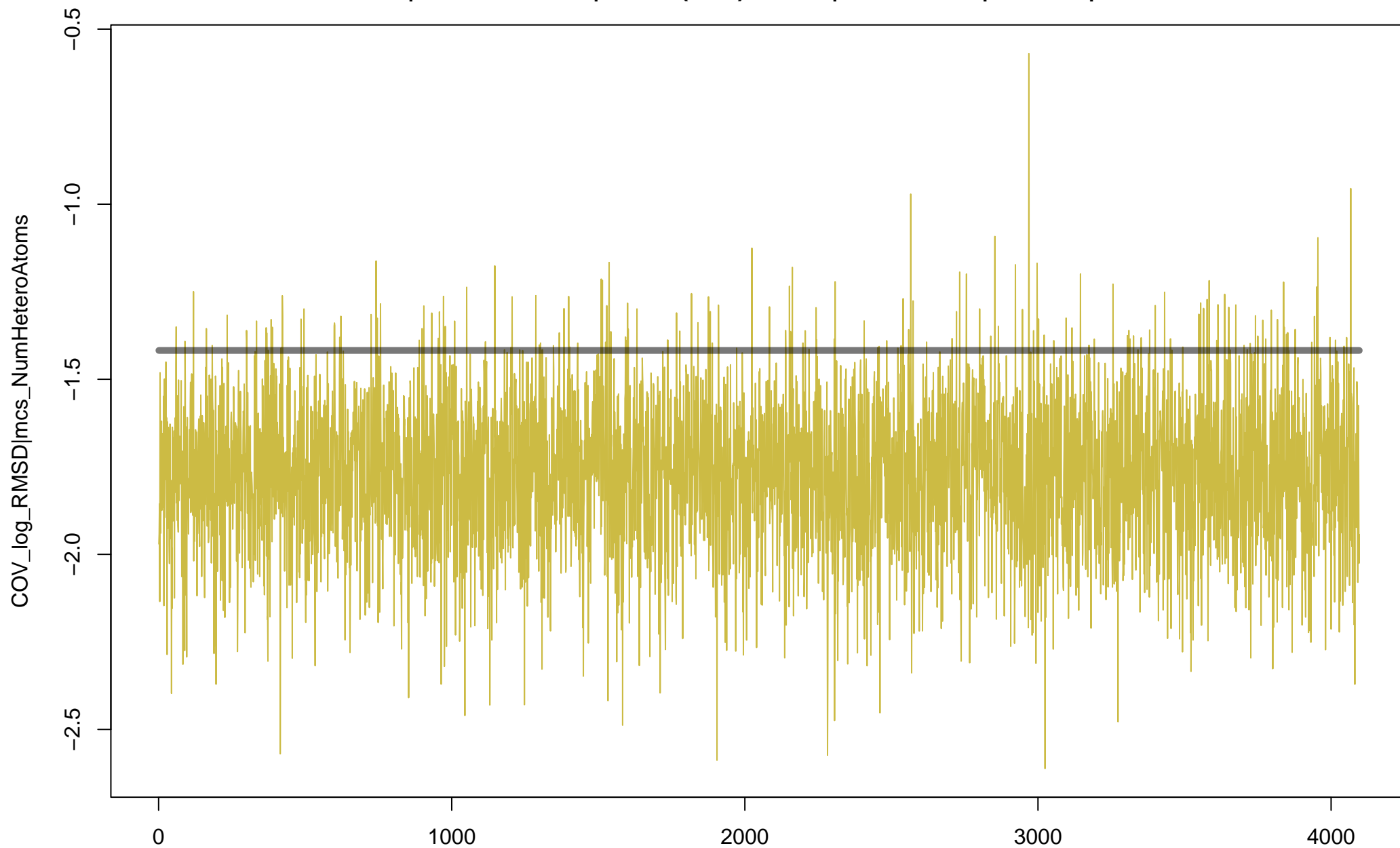
**VAR\_docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0482 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0 | rel.err: 0.0695**



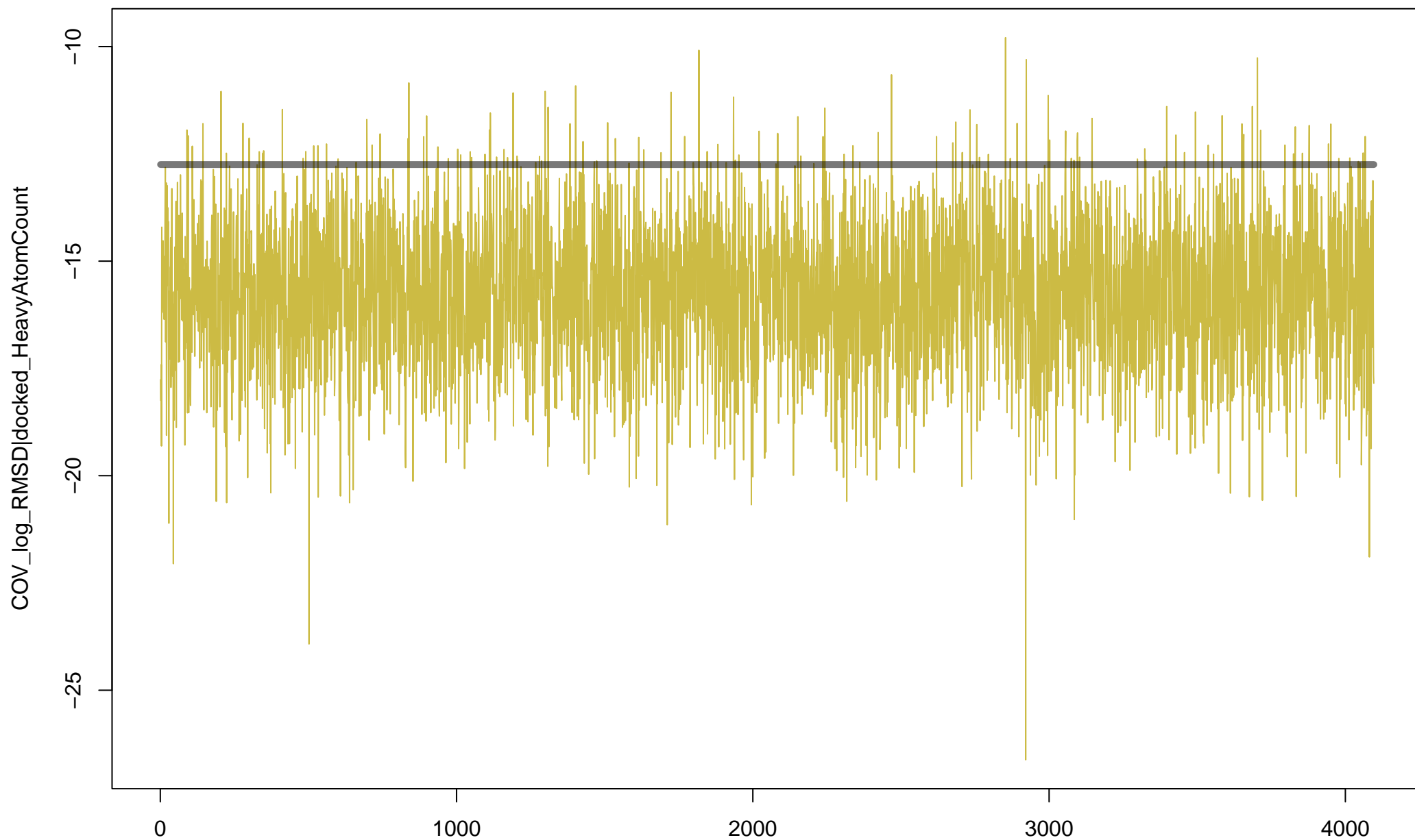
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 3570 | BMK = 0.0403 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.443**



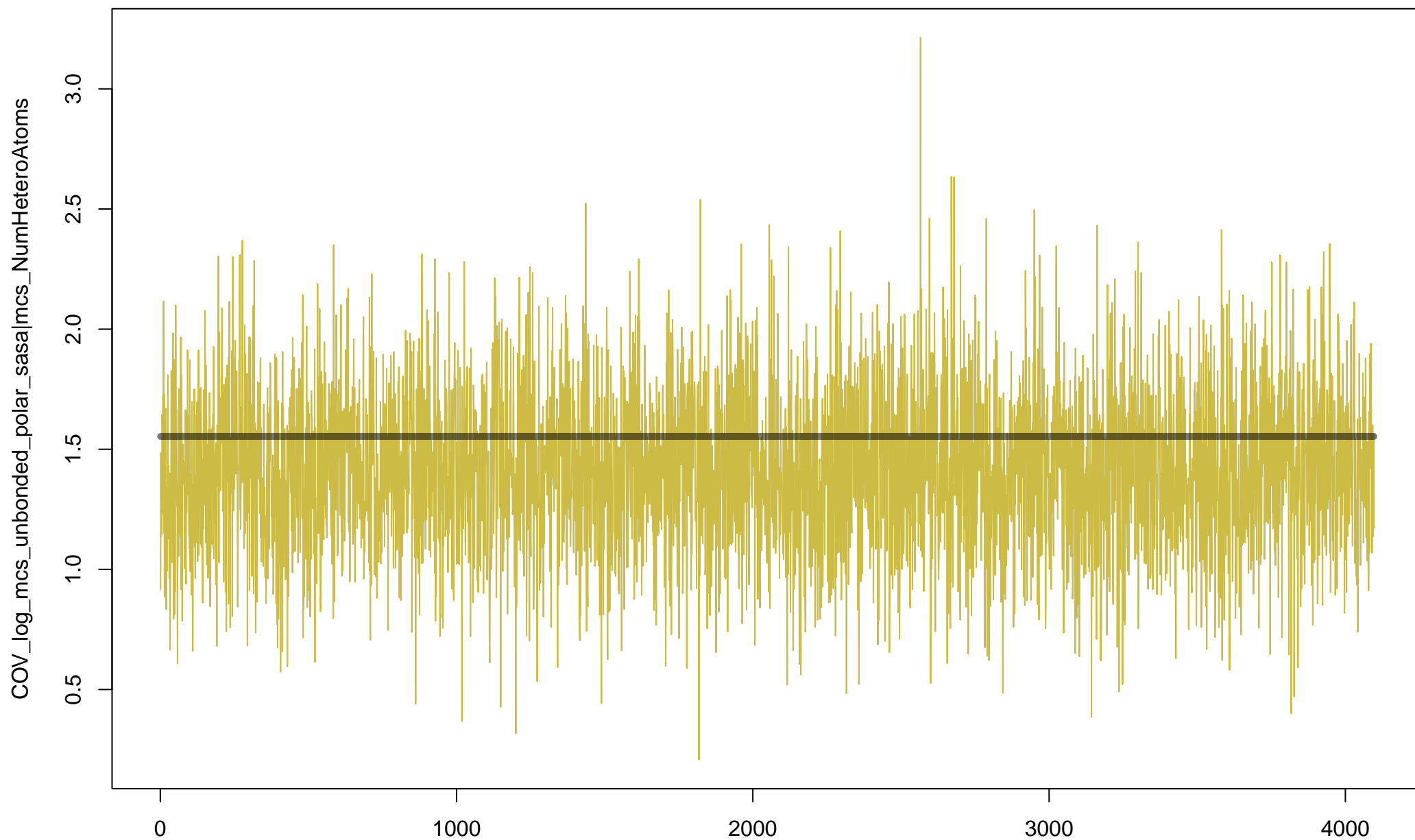
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 3730 | BMK = 0.0389 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: -1.65**



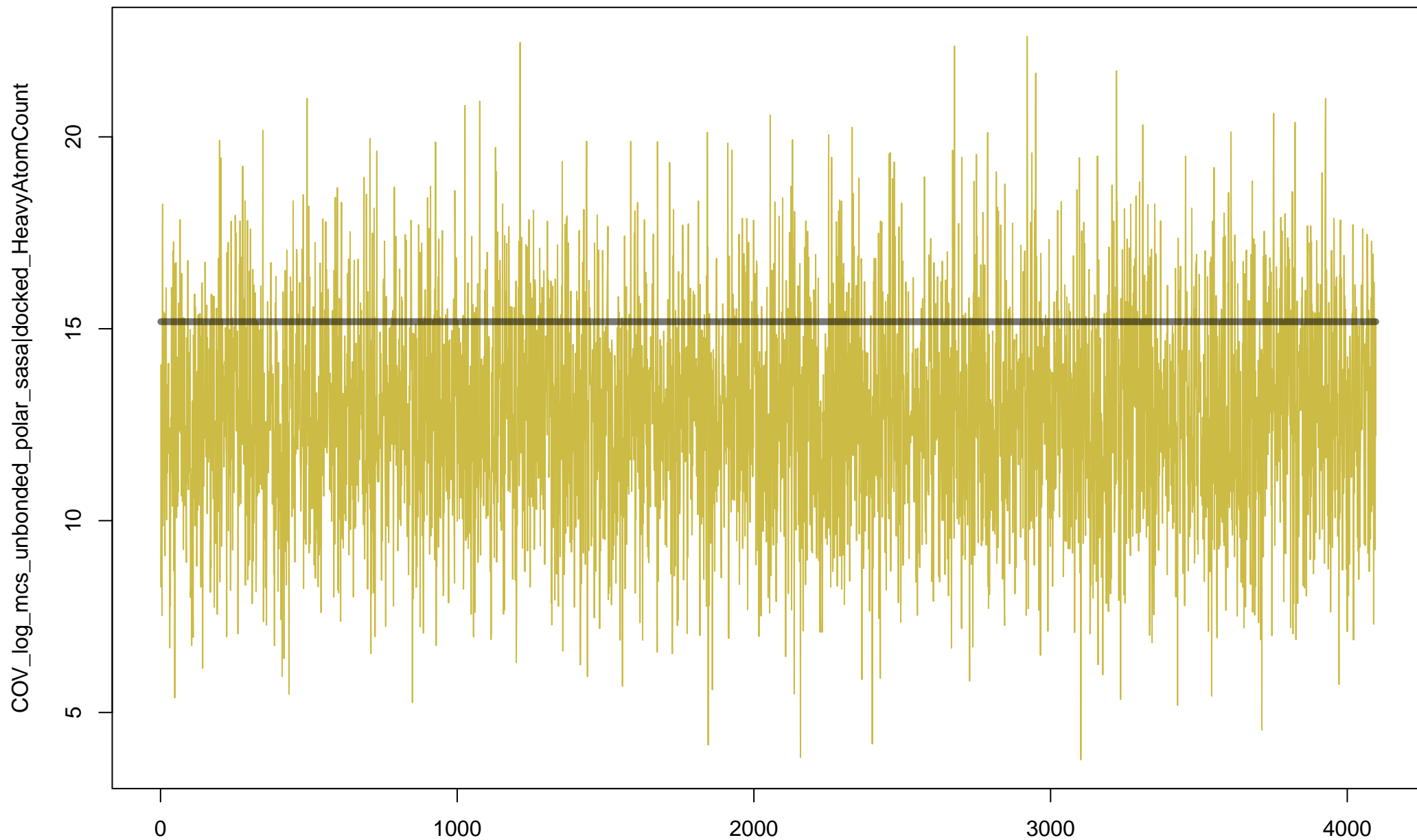
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0296 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0 | rel.err: -1.78**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 3800 | BMK = 0.0337 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: -0.419**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.0368 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: -0.903**





**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 4100 | BMK = 0.028 | MCSE(6.27) = 1.38 | stat: TRUE | burn: 0 | rel.err: 0.484**

