

-- STATS maxD --

min ESS = 139.451416694591

max BMK = 0.189813494387631

max MCSE = 6.95583175449688

all stationary: FALSE

burn: 0

max rel.err.: 1.96148545684631

-- STATS 2D --

min ESS = 1871.69442723613

max BMK = 0.0549493831918659

max MCSE = 2.55407506736692

all stationary: TRUE

burn: 0

max rel.err.: 1.78033179331154

-- STATS 1D --

min ESS = 1900.52329155601

max BMK = 0.058897735380355

max MCSE = 3.01771736722943

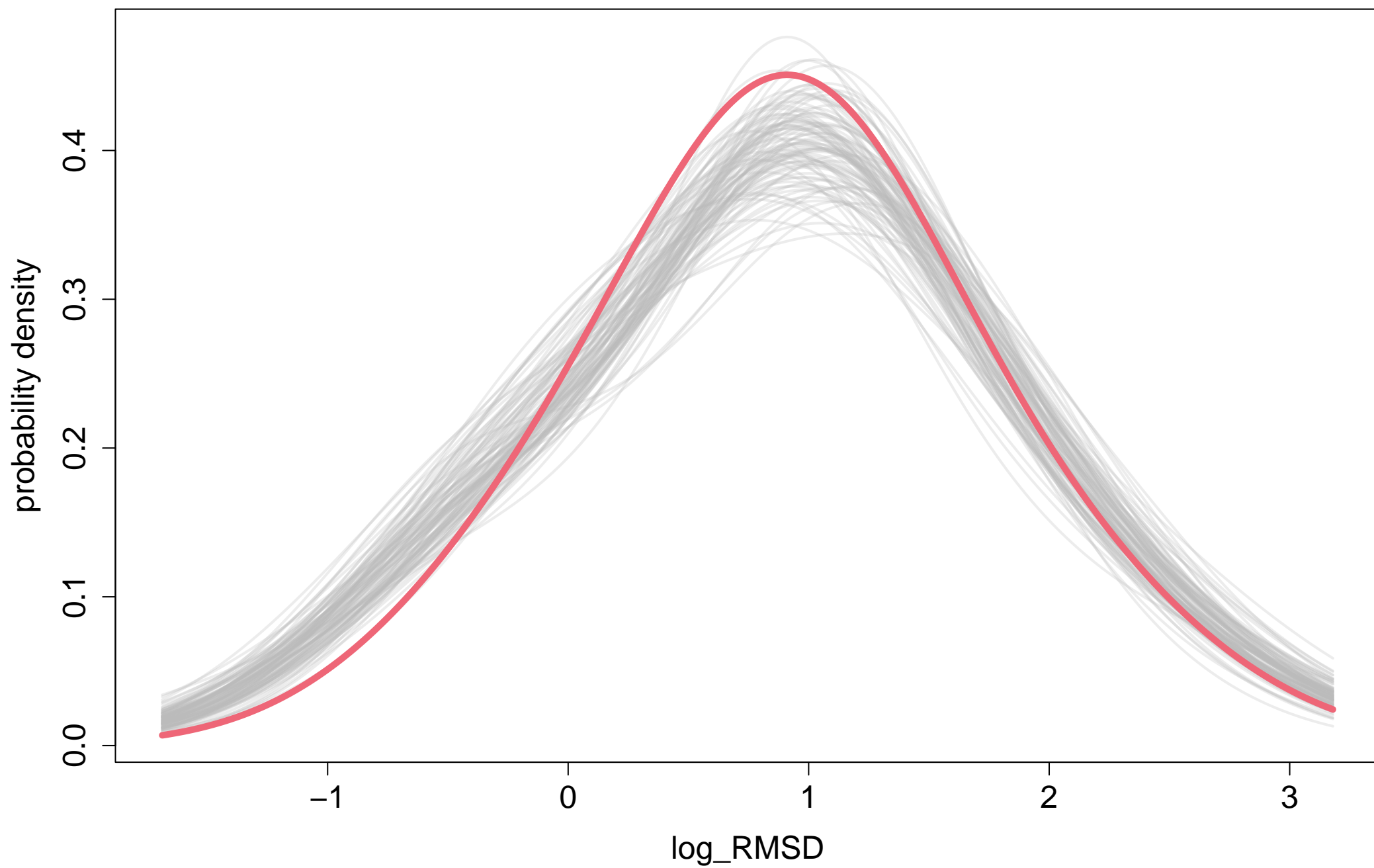
all stationary: FALSE

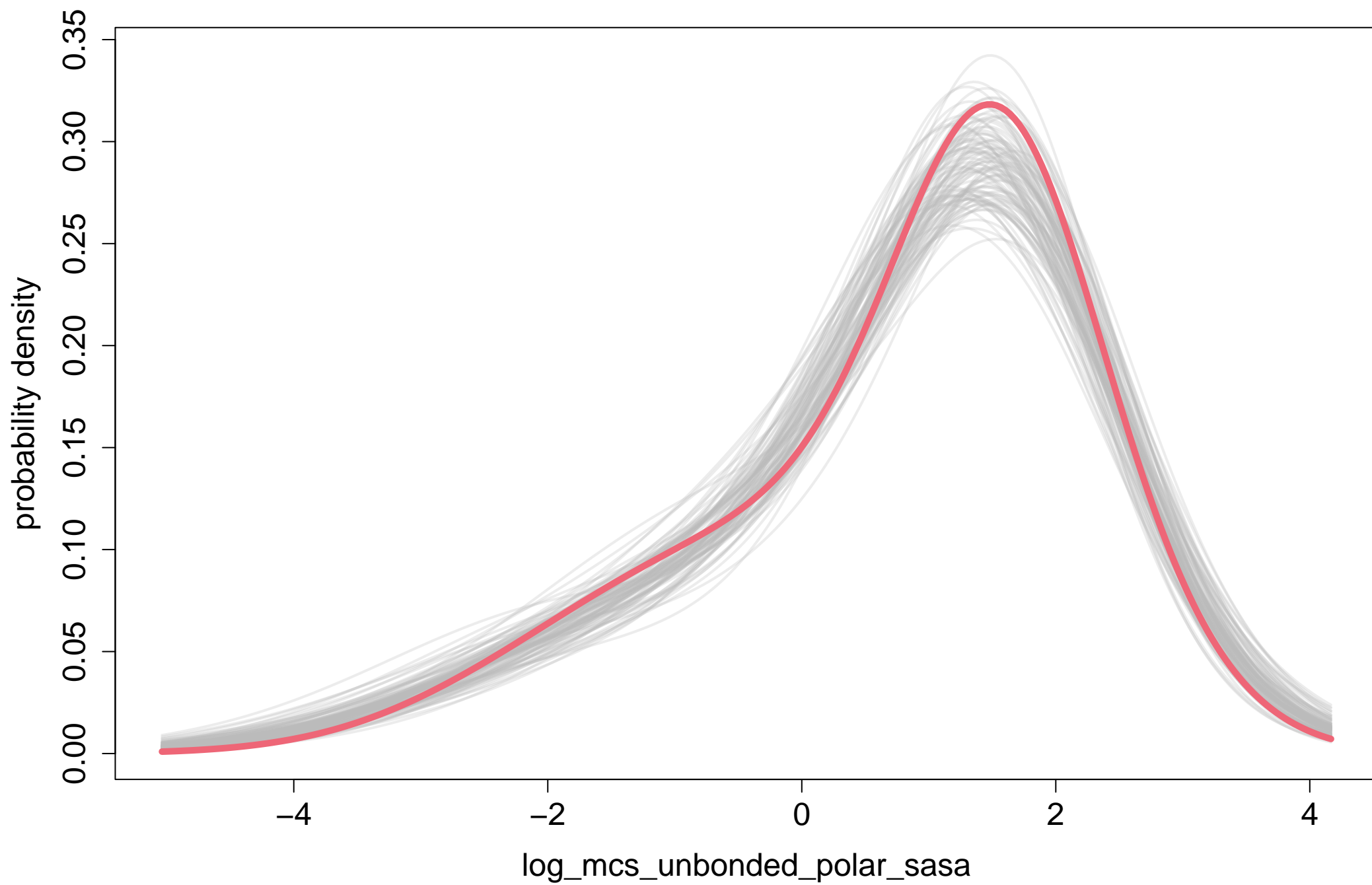
burn: 0

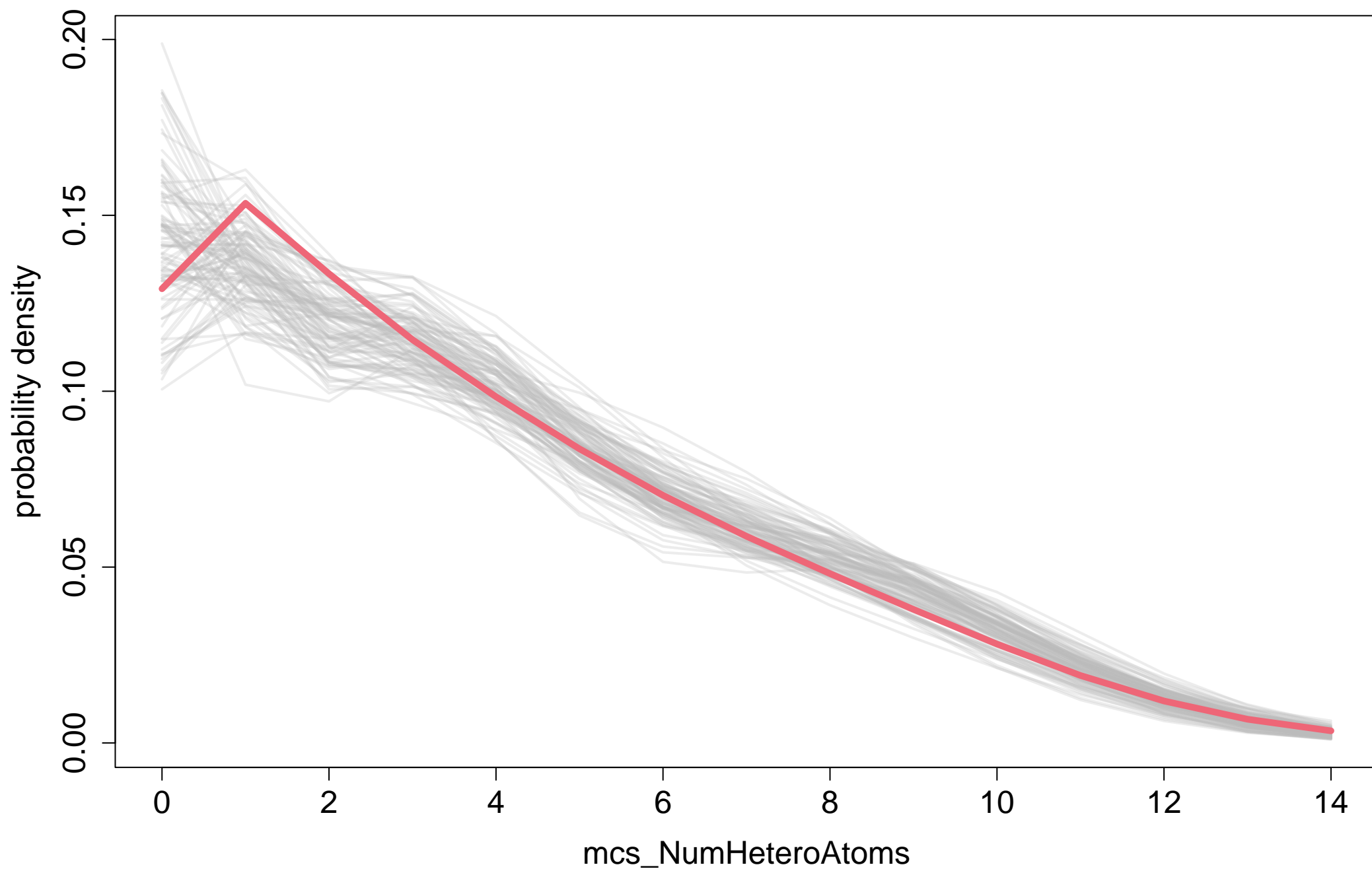
max rel.err.: 2.23211475104557

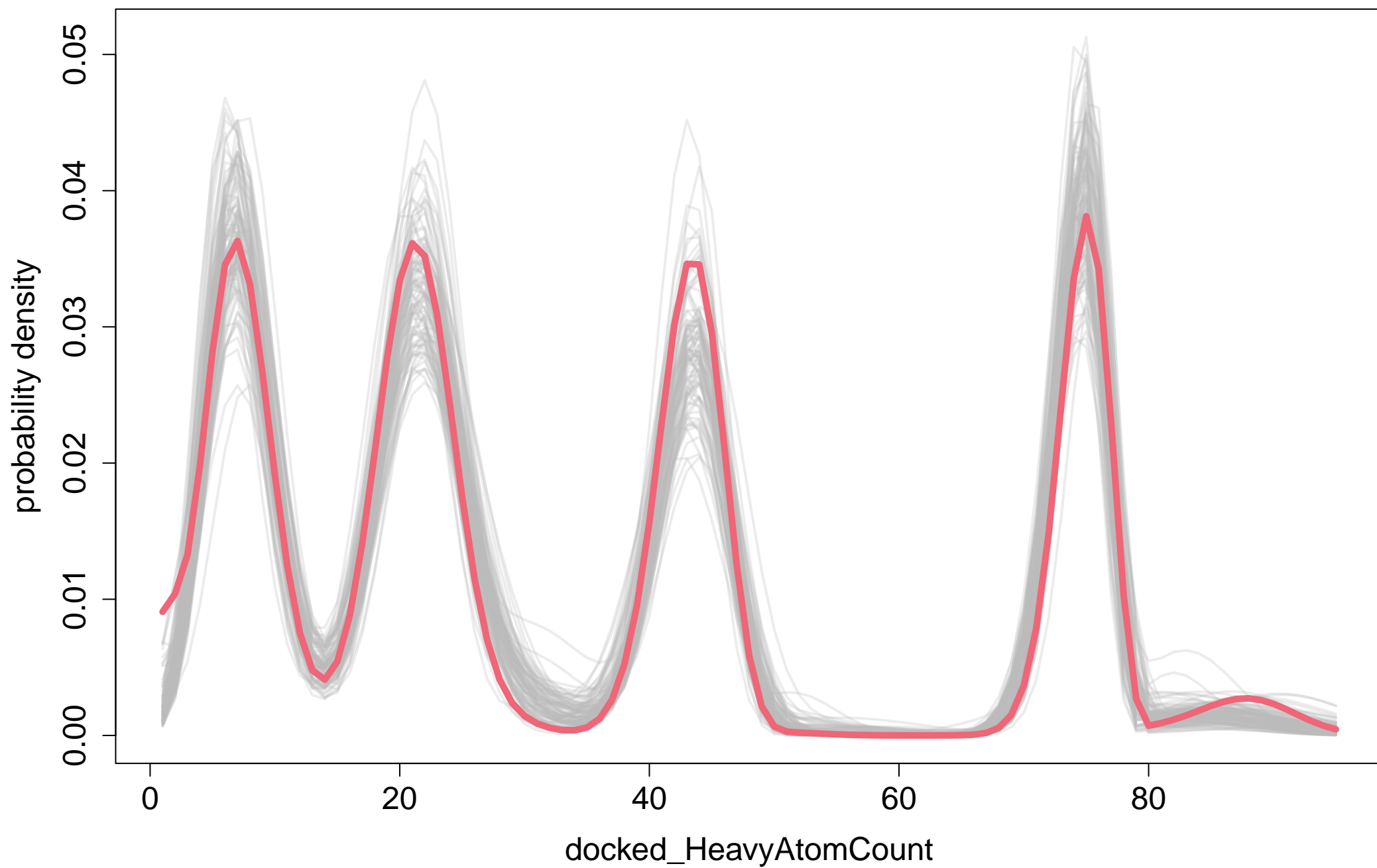
Occupied clusters: 9 of 16

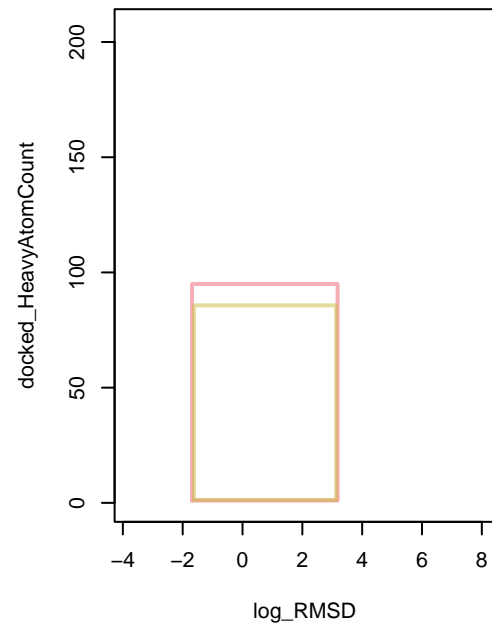
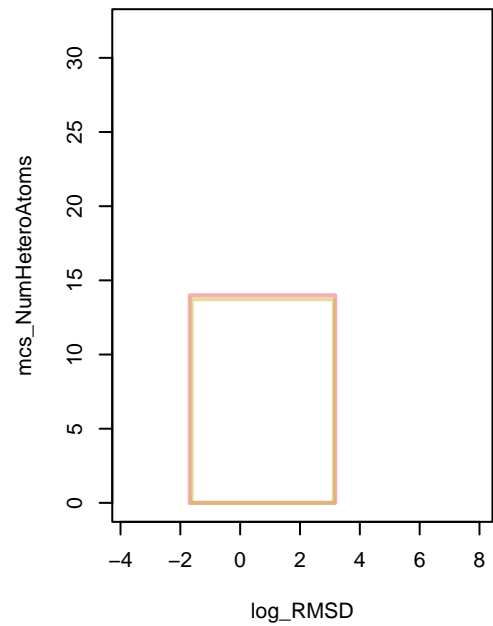
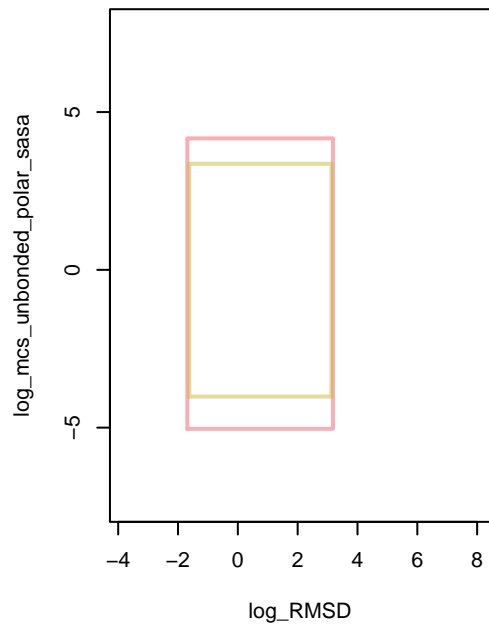
LL: -2159.00020569332 sd: 6.47819063160562





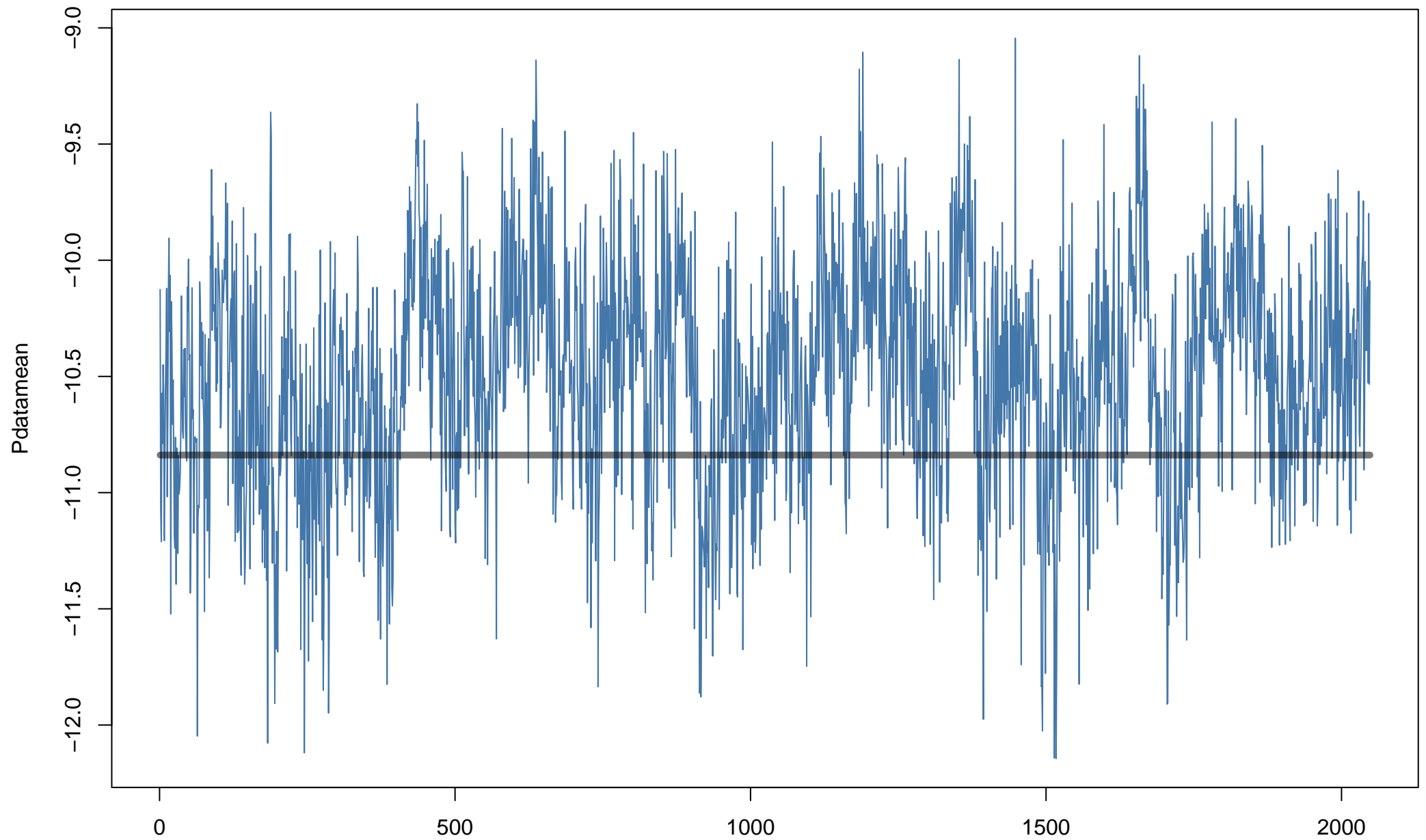




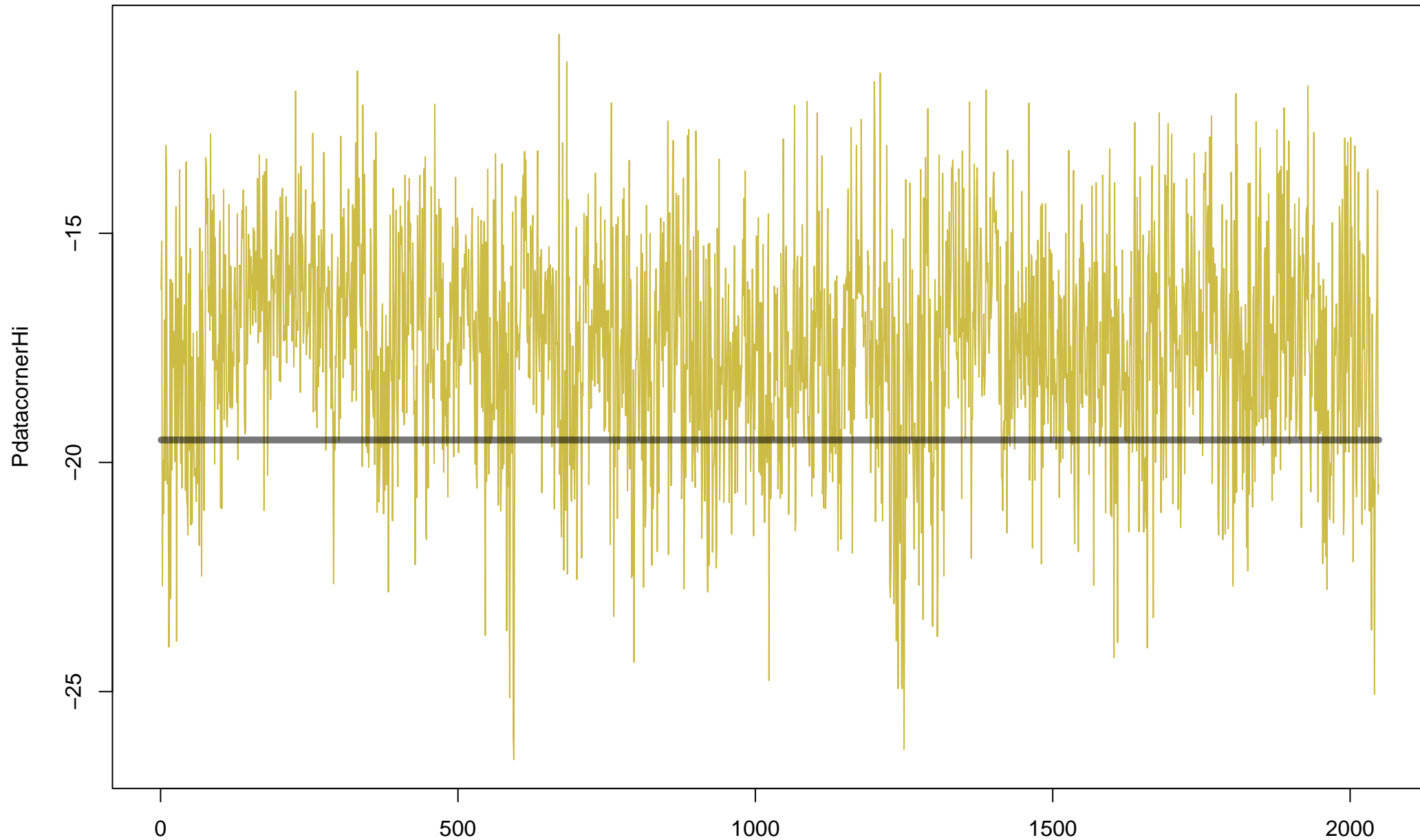


**Pdatamean**

**ESS = 139 | BMK = 0.0906 | MCSE(6.27) = 6.96 | stat: FALSE | burn: 0 | rel.err: 0.749**

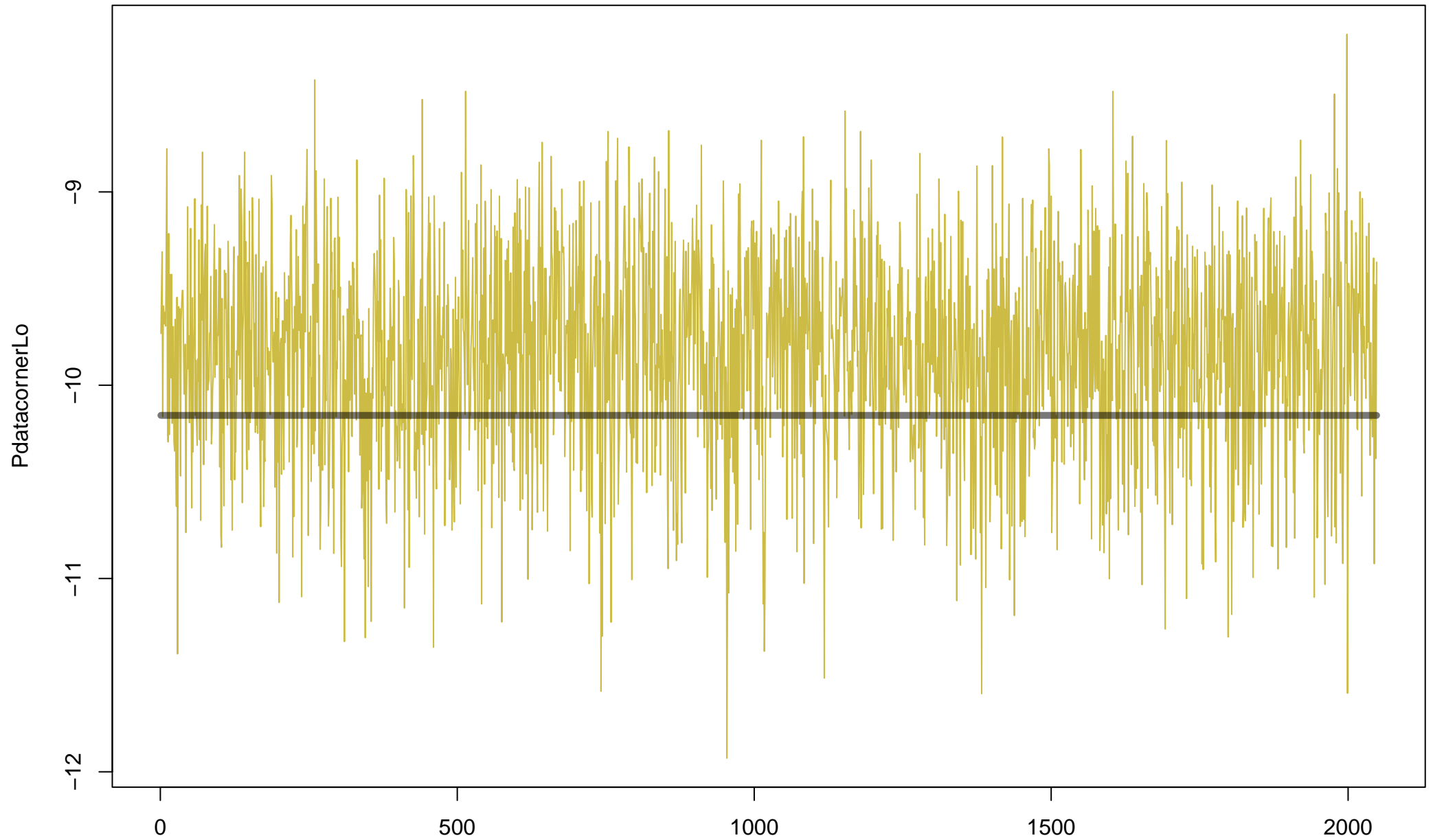


**PdatacornerHi**  
**ESS = 1290 | BMK = 0.16 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.264**

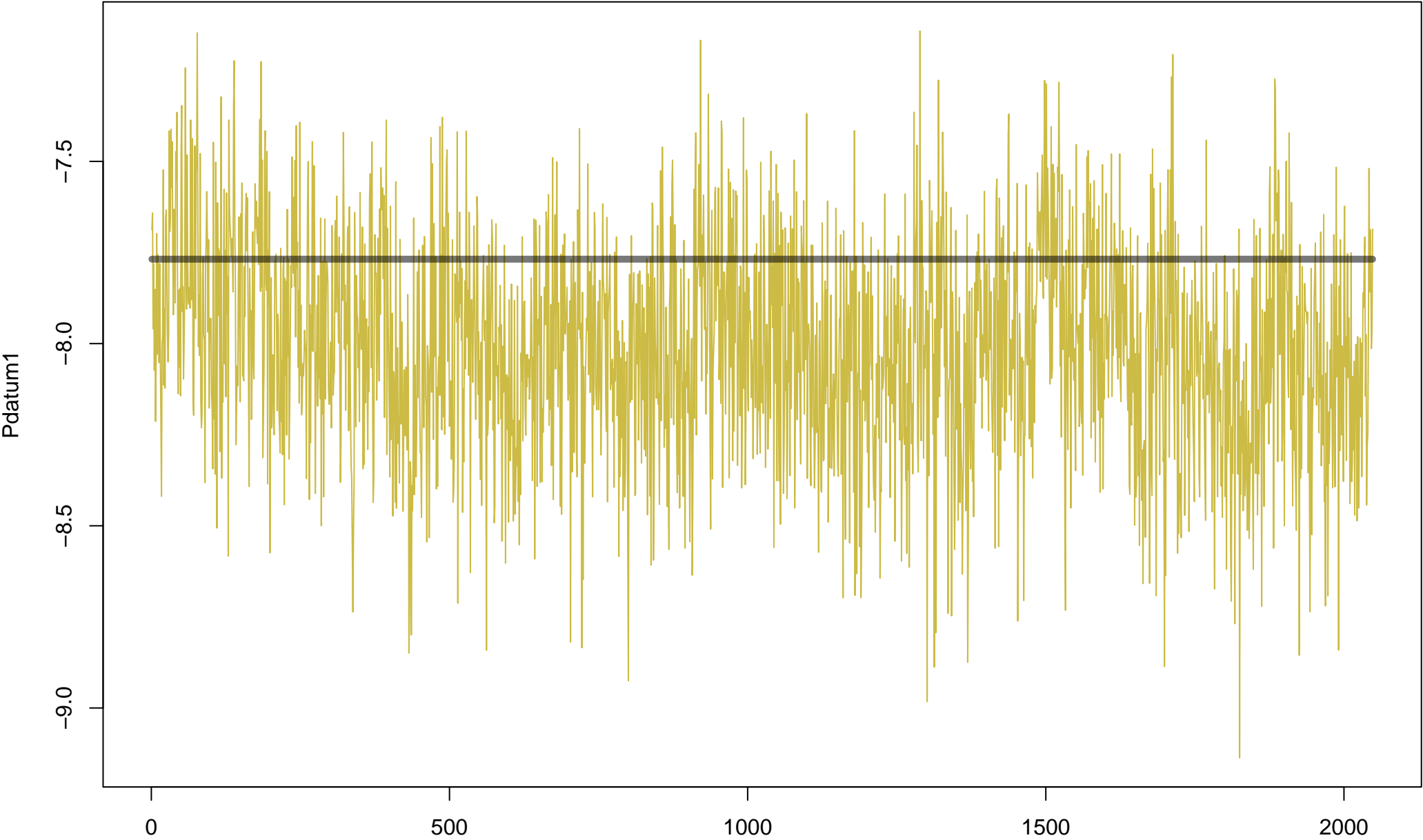




**PdatacornerLo**  
**ESS = 1900 | BMK = 0.0436 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 0.703**

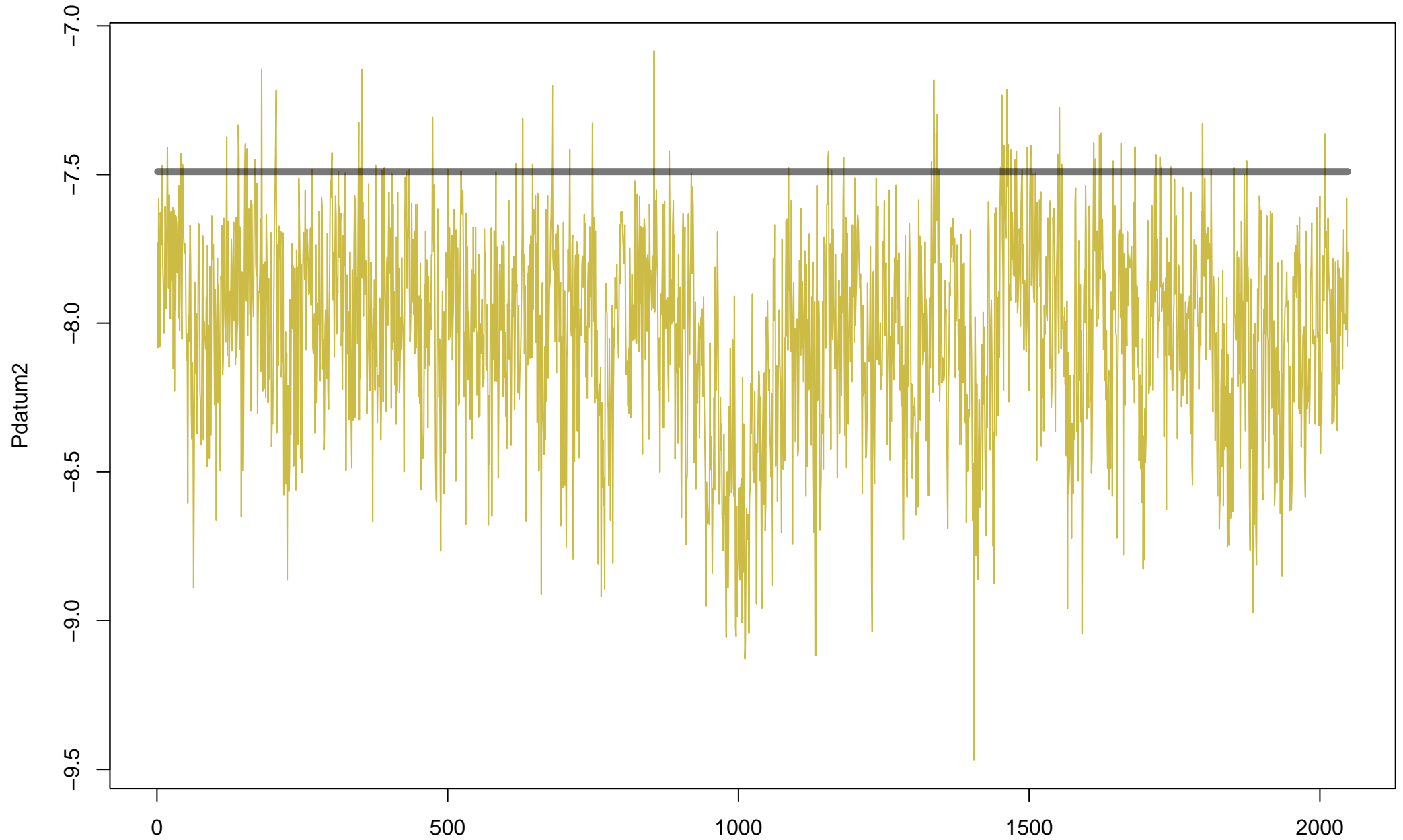


**Pdatum1**  
**ESS = 267 | BMK = 0.0796 | MCSE(6.27) = 5.26 | stat: FALSE | burn: 0 | rel.err: -0.743**



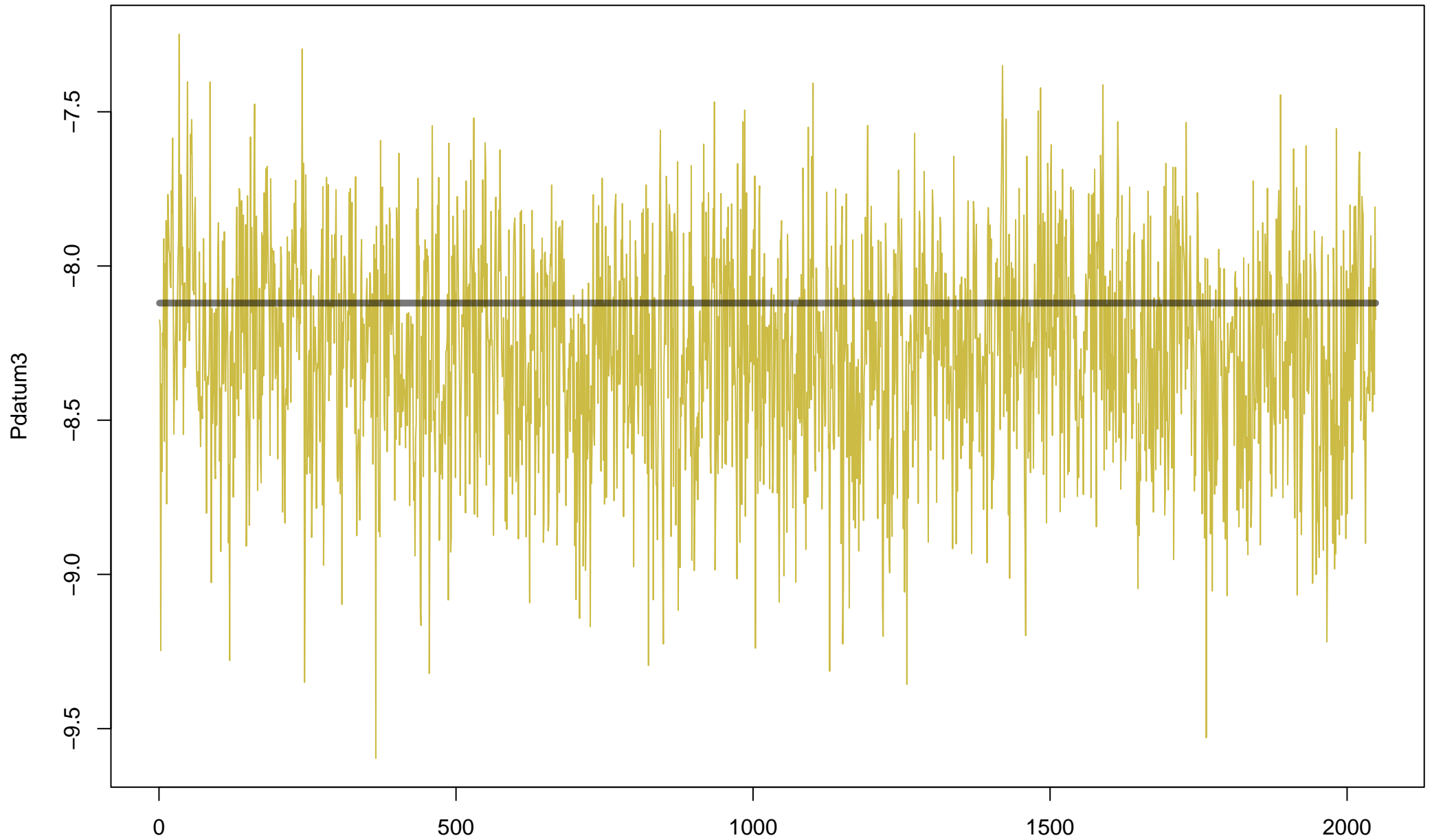
**Pdatum2**

**ESS = 237 | BMK = 0.0588 | MCSE(6.27) = 6.36 | stat: FALSE | burn: 0 | rel.err: -1.96**



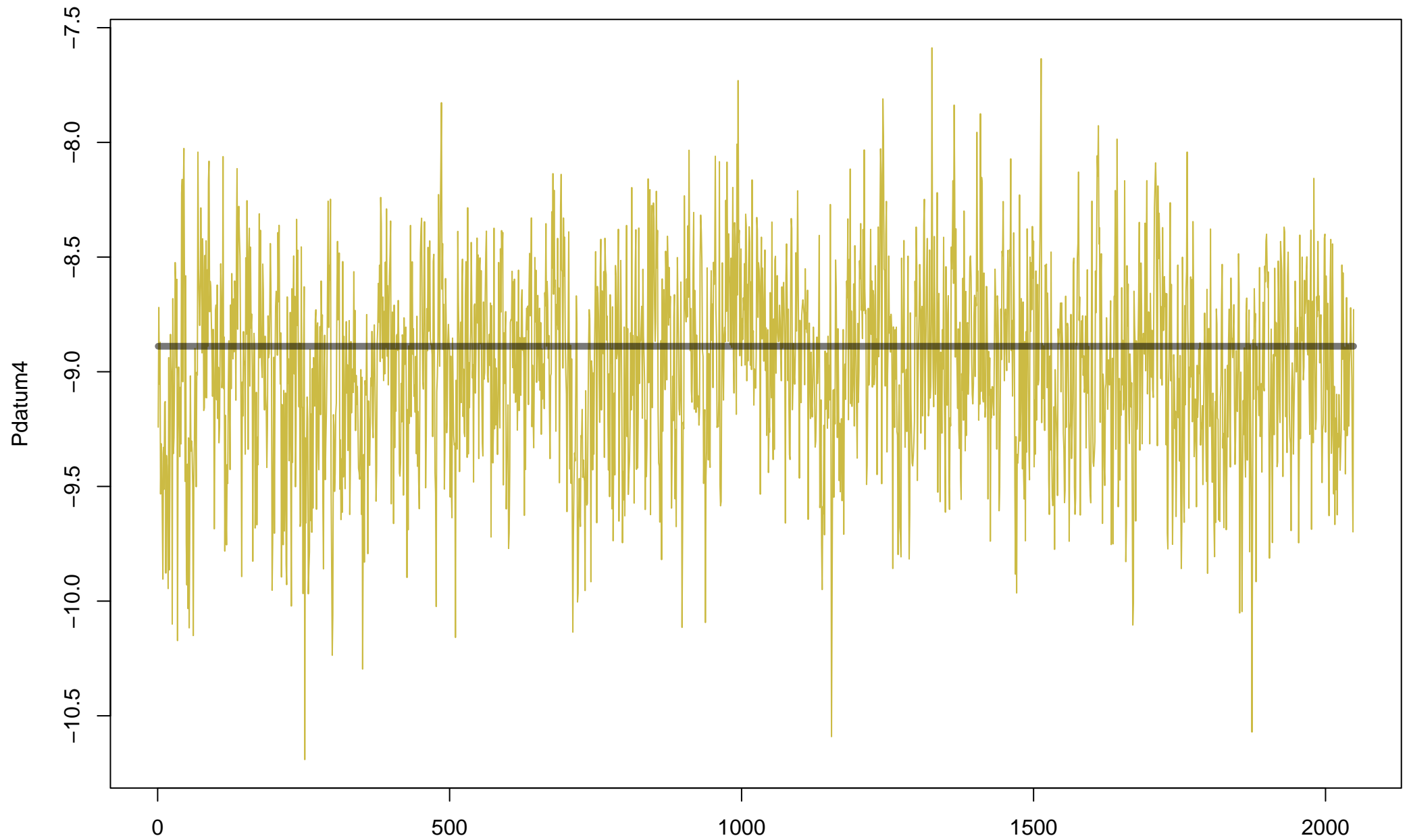
**Pdatum3**

**ESS = 781 | BMK = 0.036 | MCSE(6.27) = 3.63 | stat: FALSE | burn: 0 | rel.err: -0.321**



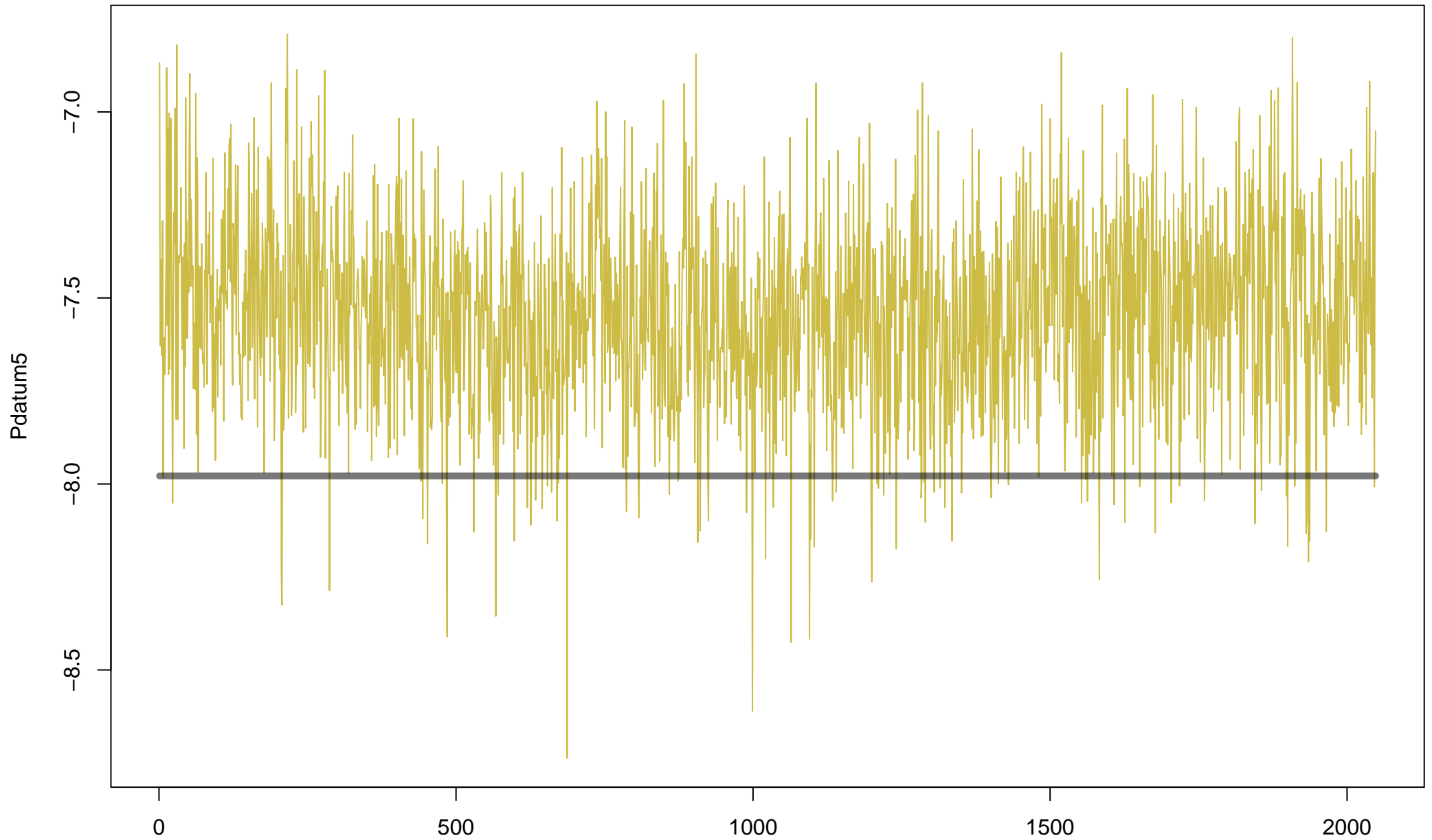
**Pdatum4**

**ESS = 454 | BMK = 0.0615 | MCSE(6.27) = 4.44 | stat: TRUE | burn: 0 | rel.err: -0.0147**



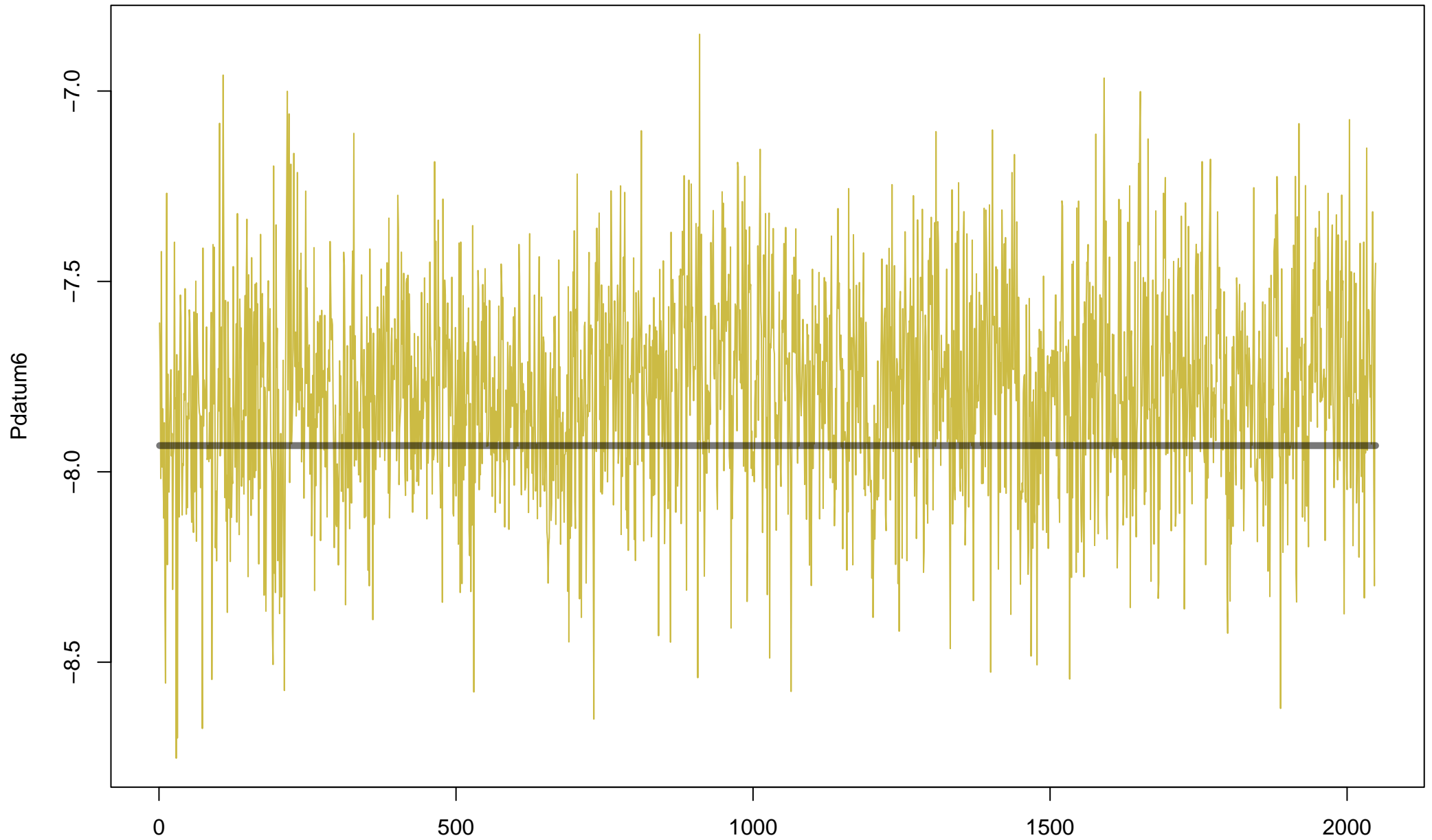
**Pdatum5**

**ESS = 901 | BMK = 0.0642 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0 | rel.err: 1.47**



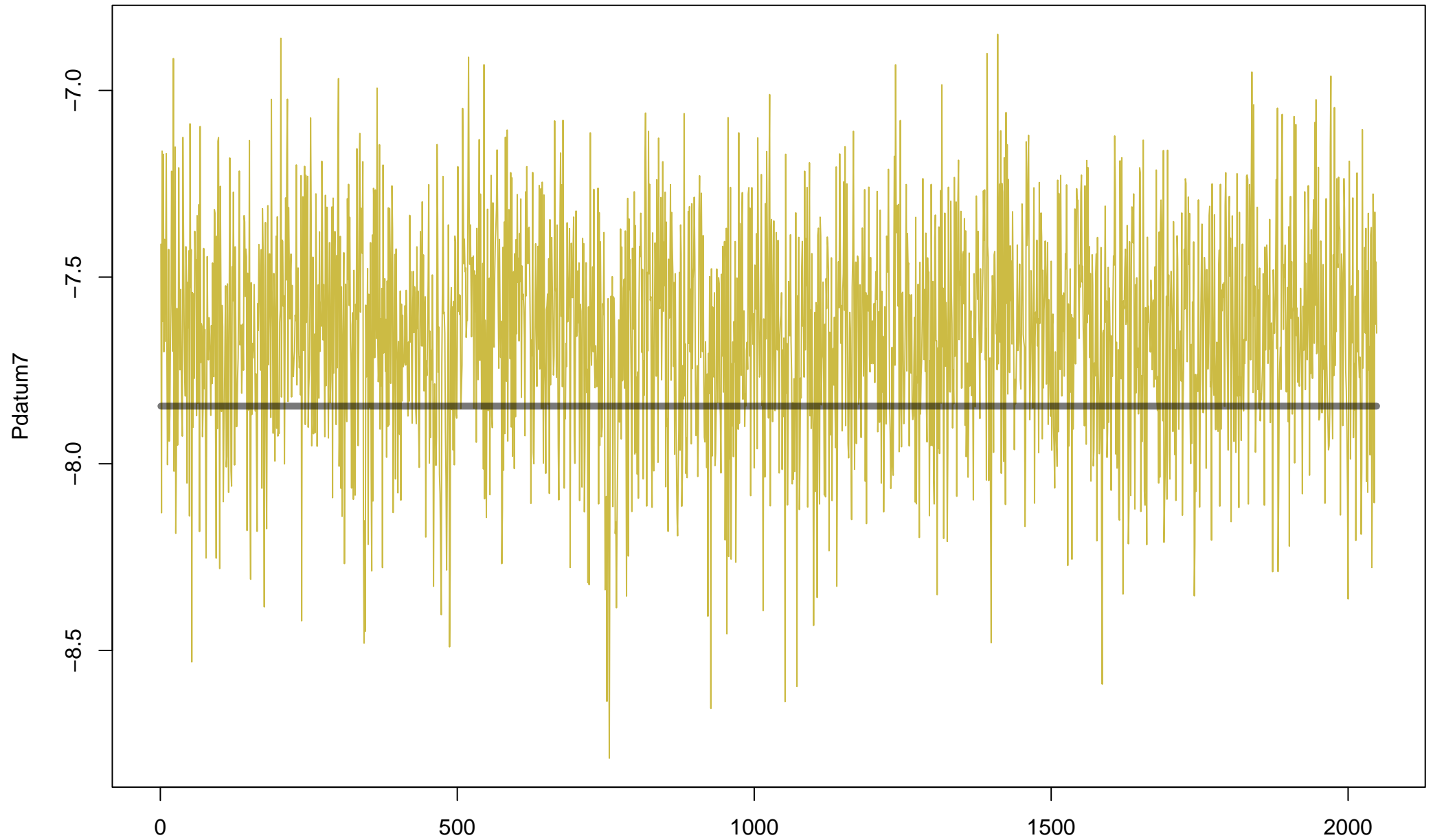
**Pdatum6**

**ESS = 966 | BMK = 0.0578 | MCSE(6.27) = 3.32 | stat: FALSE | burn: 0 | rel.err: 0.614**



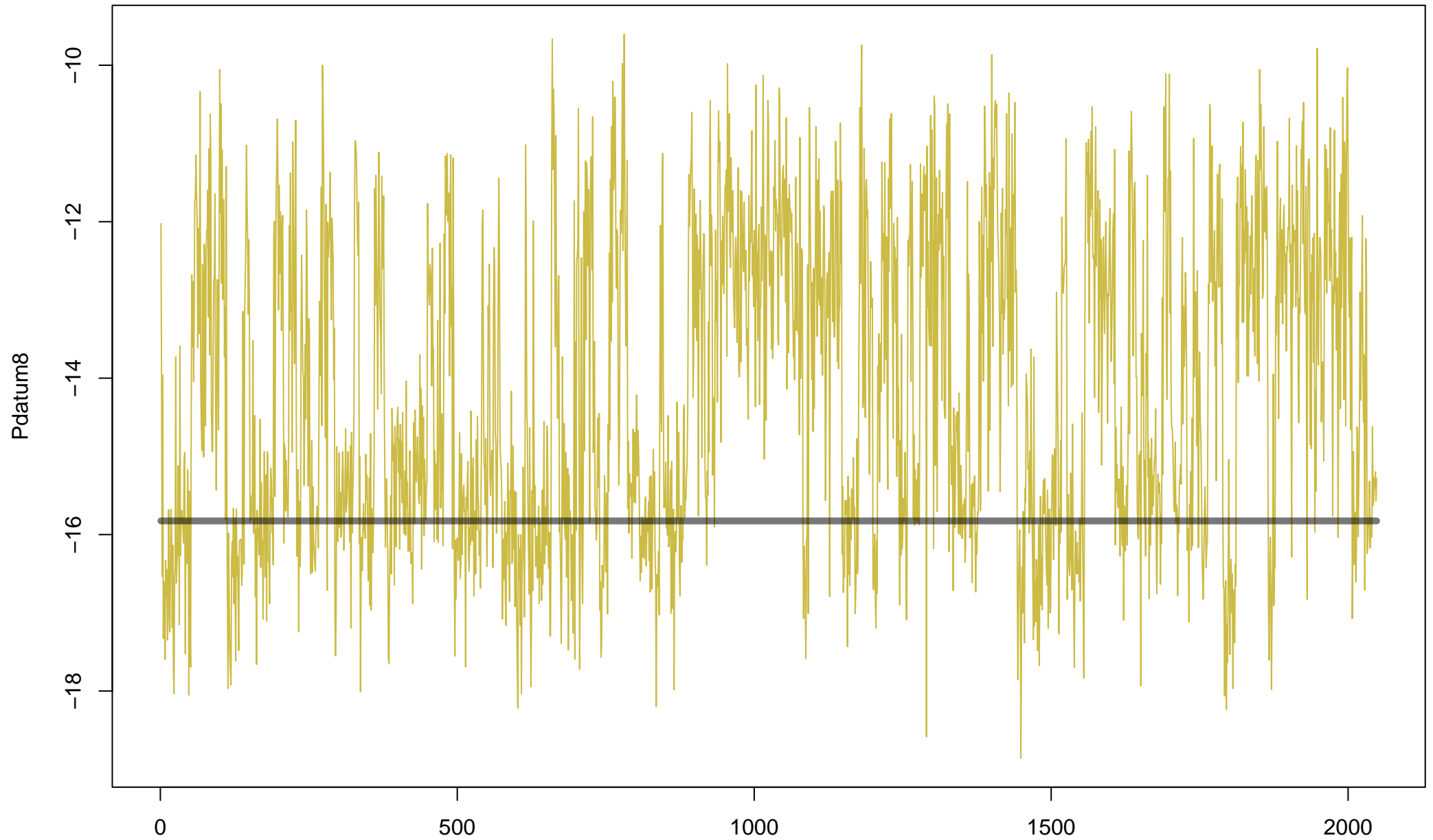
**Pdatum7**

**ESS = 1360 | BMK = 0.0396 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | rel.err: 0.743**



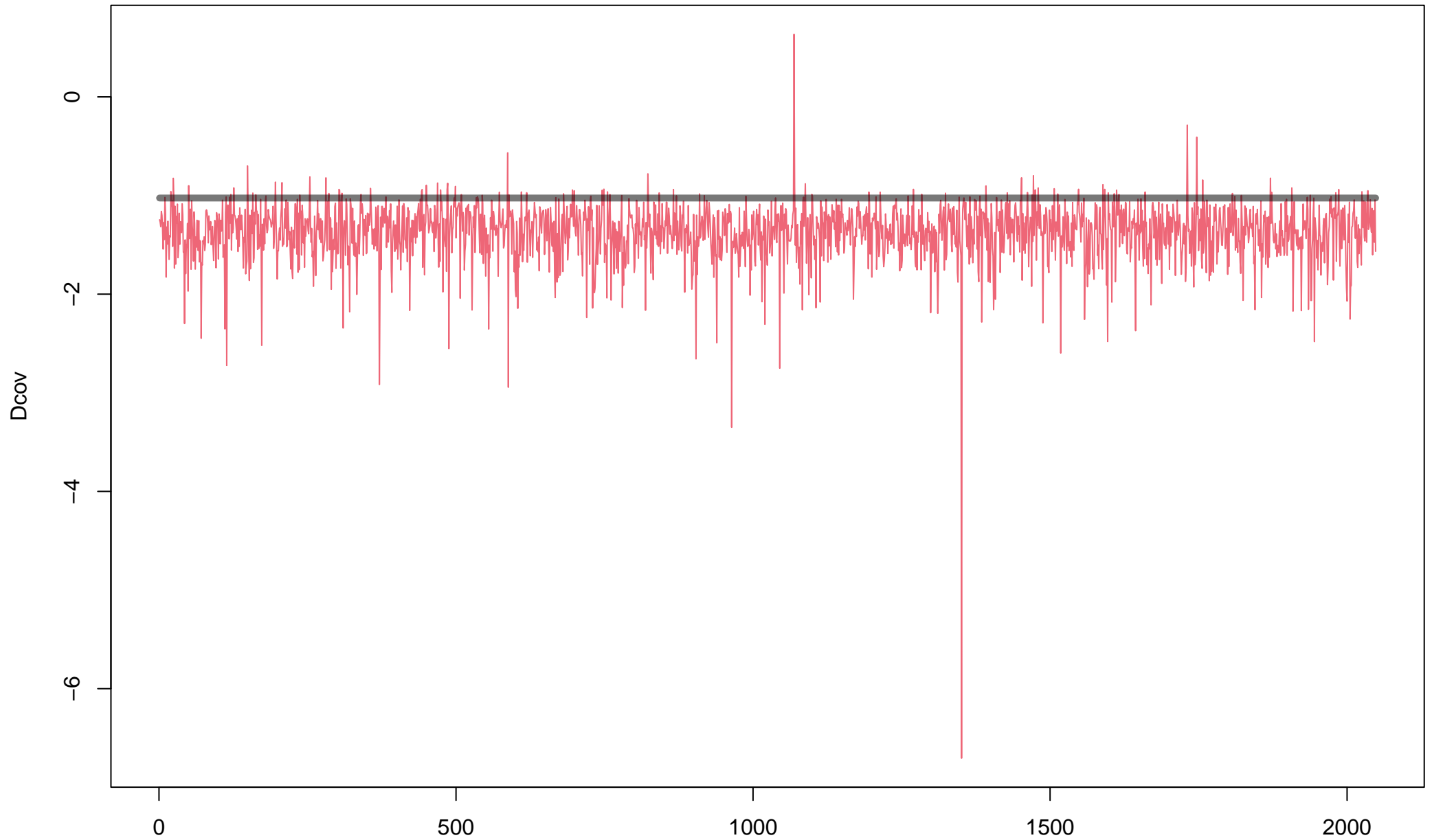


**Pdatum8**  
**ESS = 495 | BMK = 0.19 | MCSE(6.27) = 4.59 | stat: TRUE | burn: 0 | rel.err: 0.496**

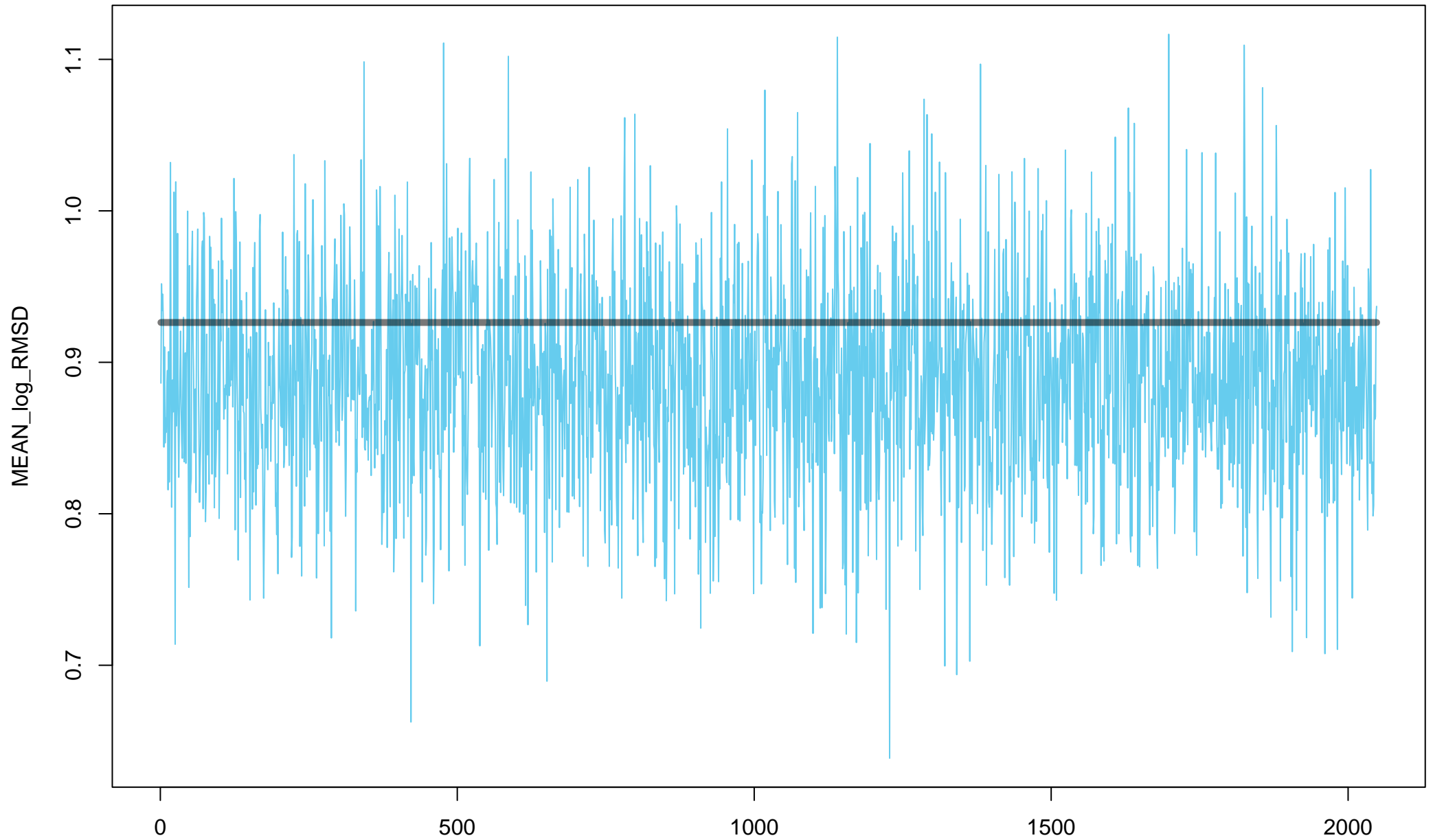


Dcov

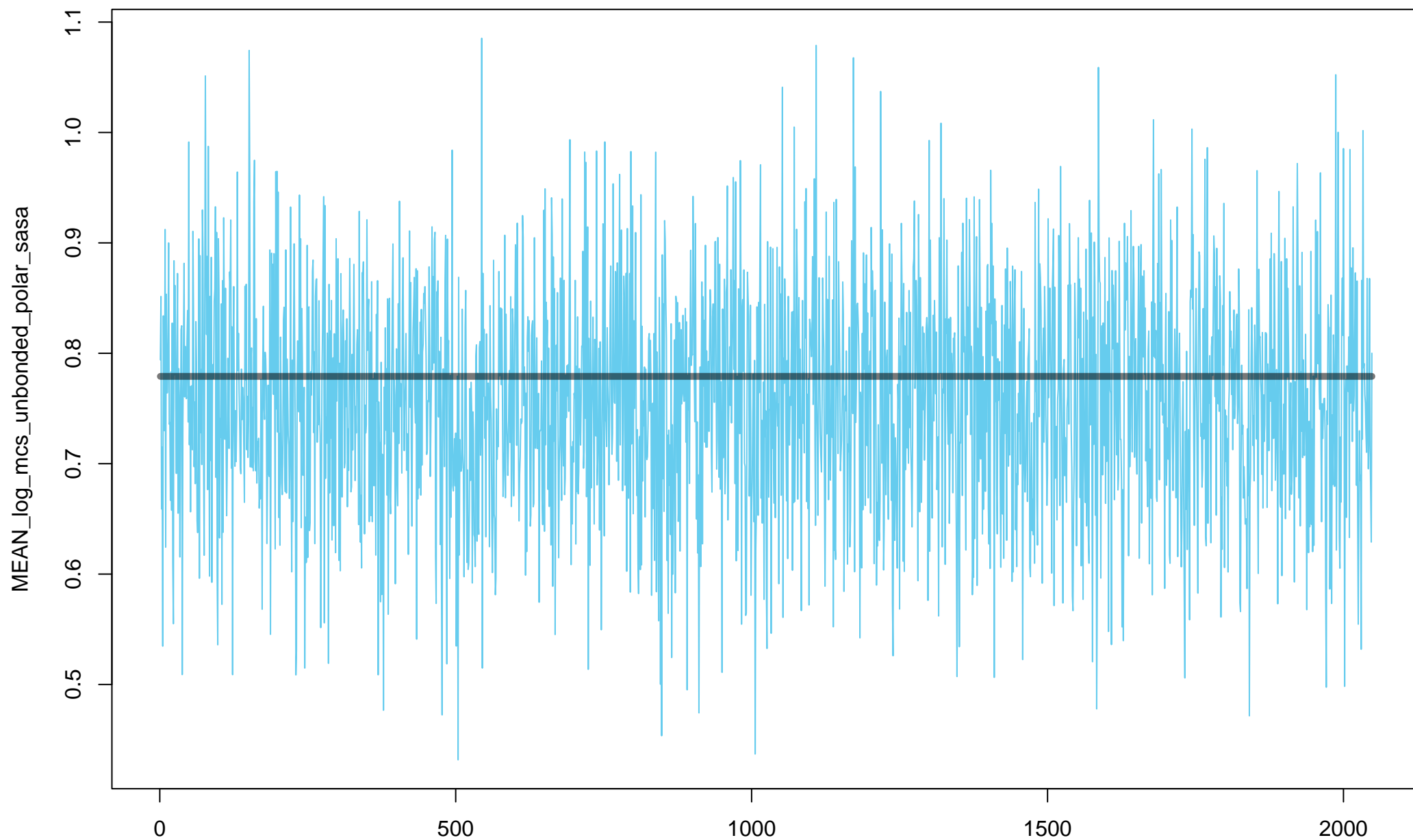
ESS = 1720 | BMK = 0.0658 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: 1.29



**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0487 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0 | rel.err: -0.58**

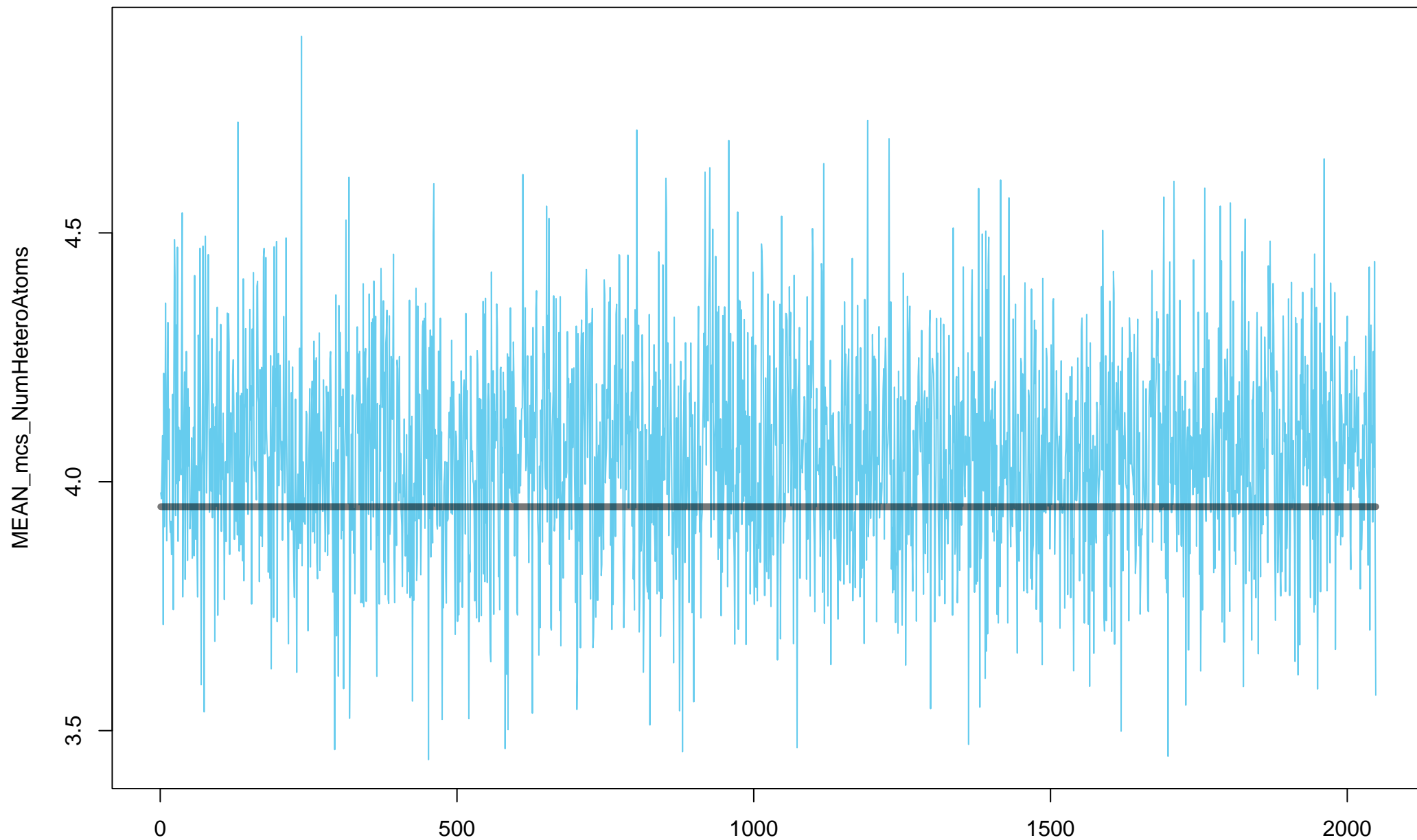


**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | rel.err: -0.22**

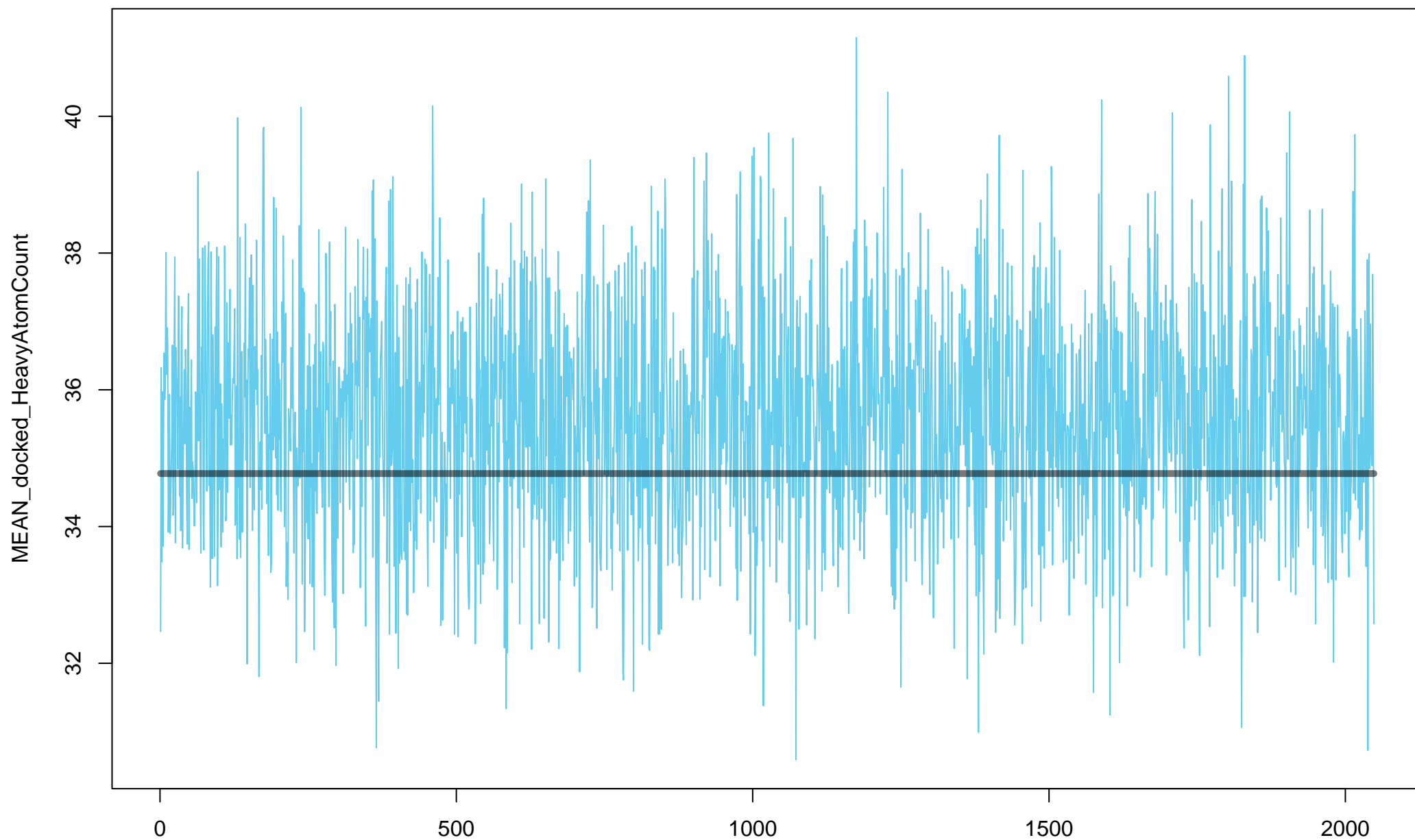


# MEAN\_mcs\_NumHeteroAtoms

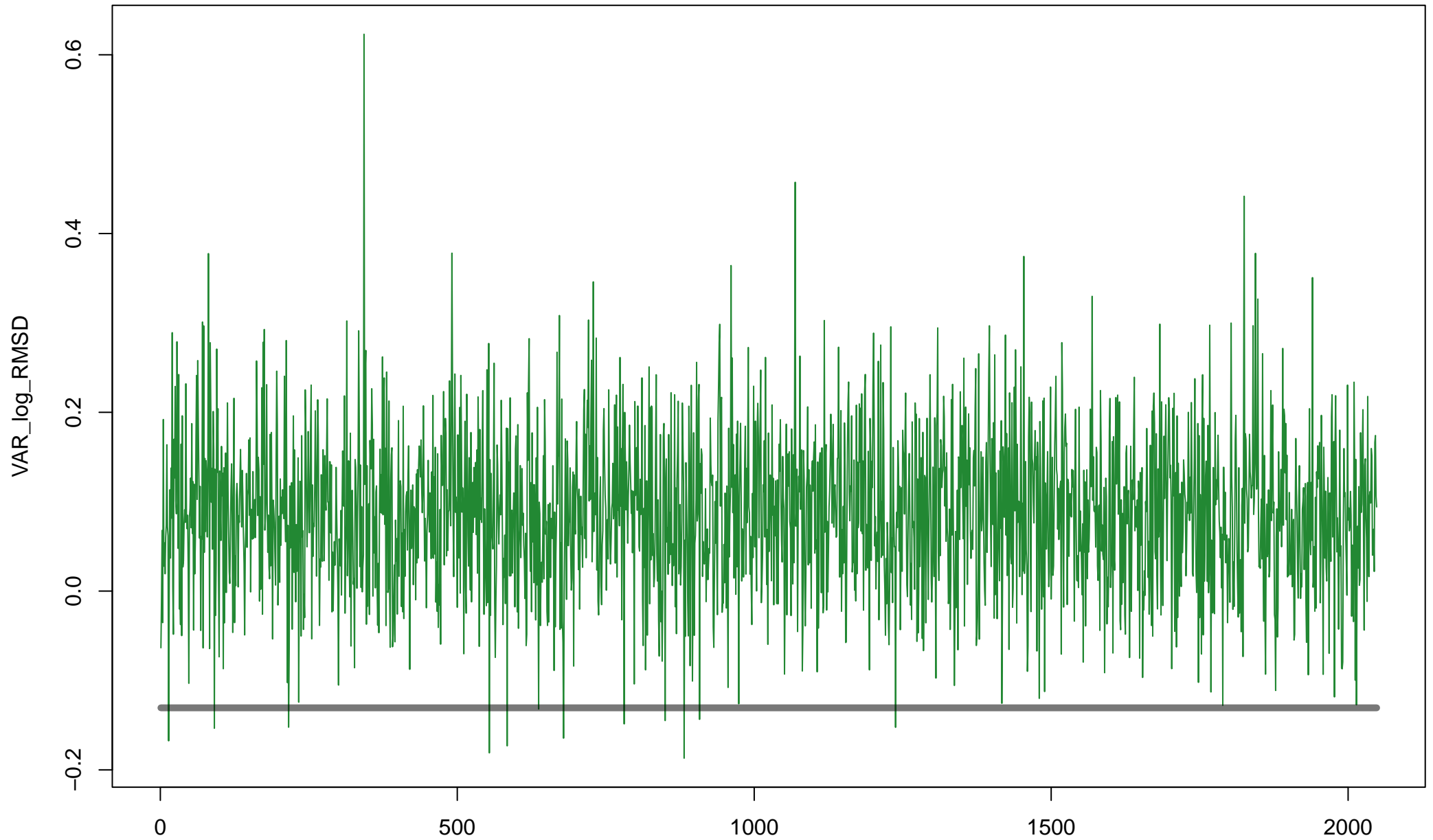
ESS = 2050 | BMK = 0.0346 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 0 | rel.err: 0.498



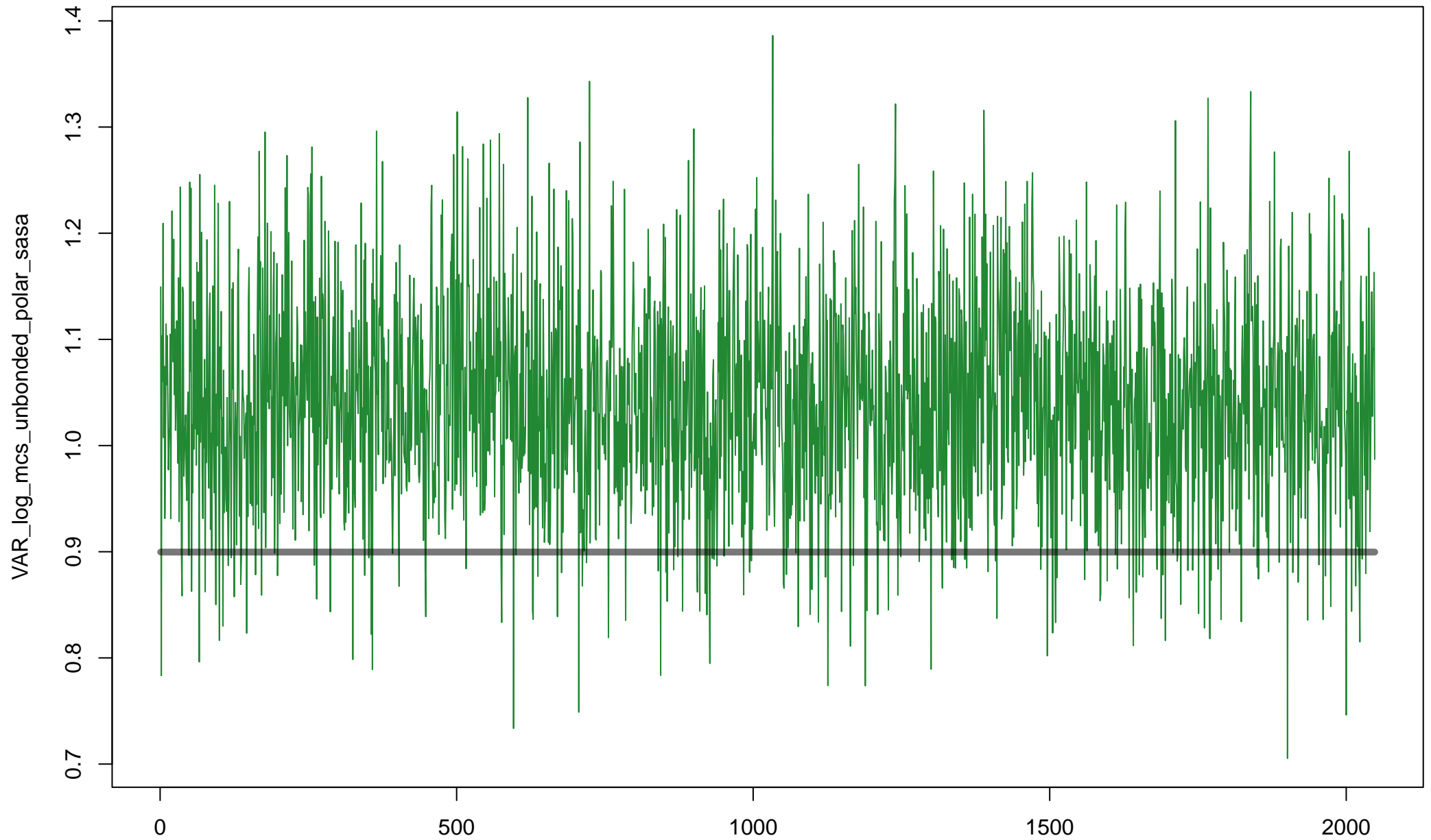
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0521 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 0.501**



**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0589 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0 | rel.err: 2.23**

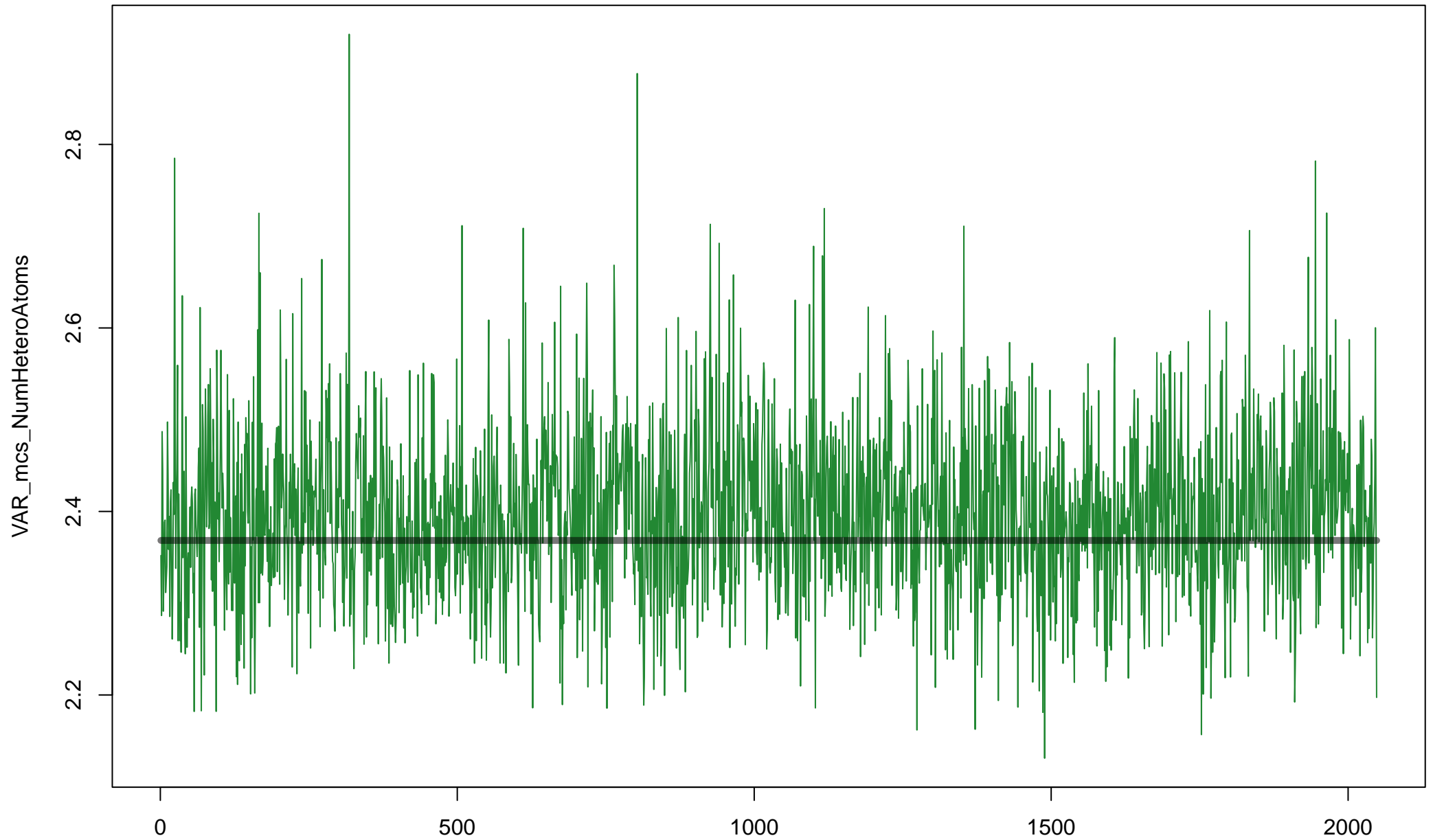


**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0471 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | rel.err: 1.37**

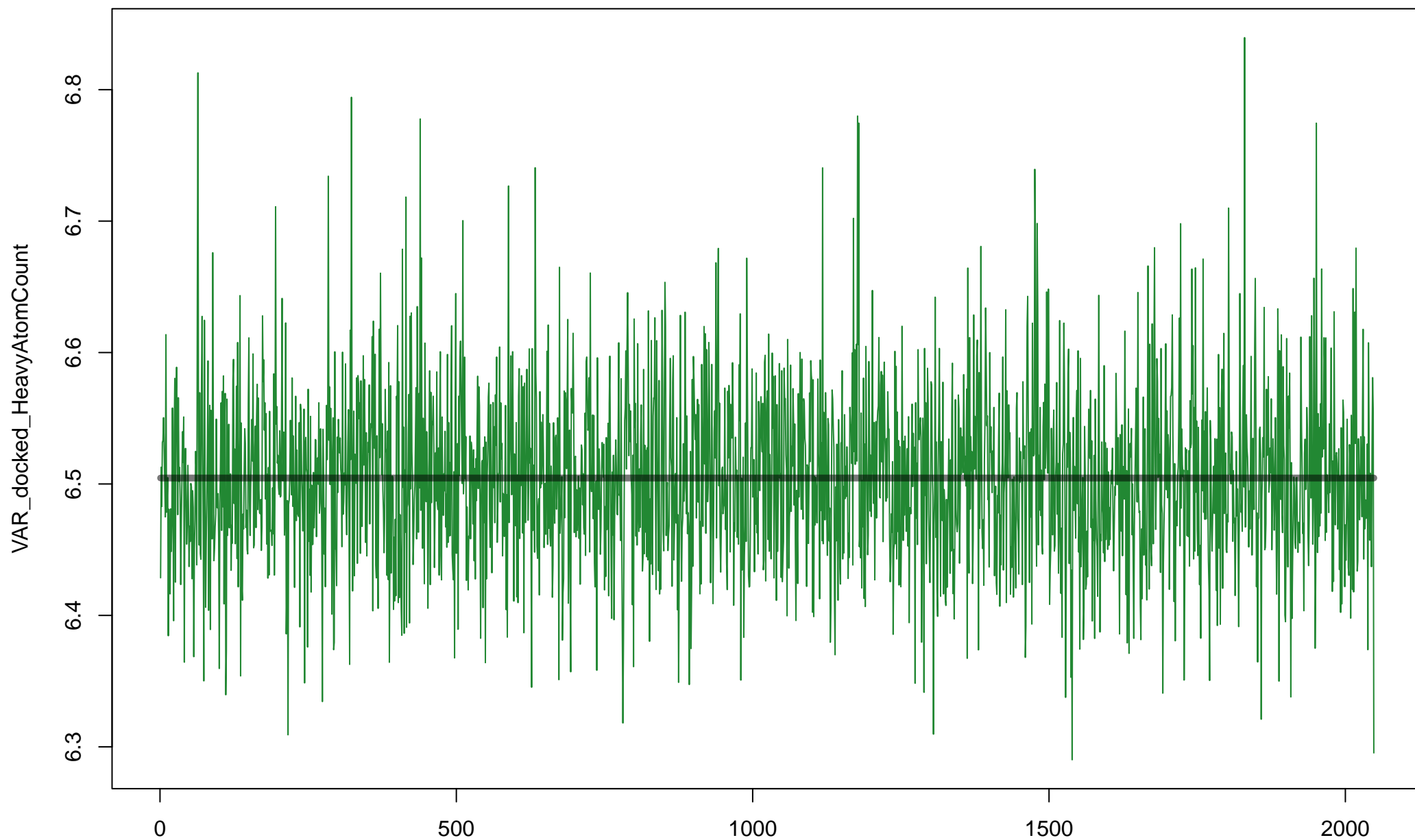




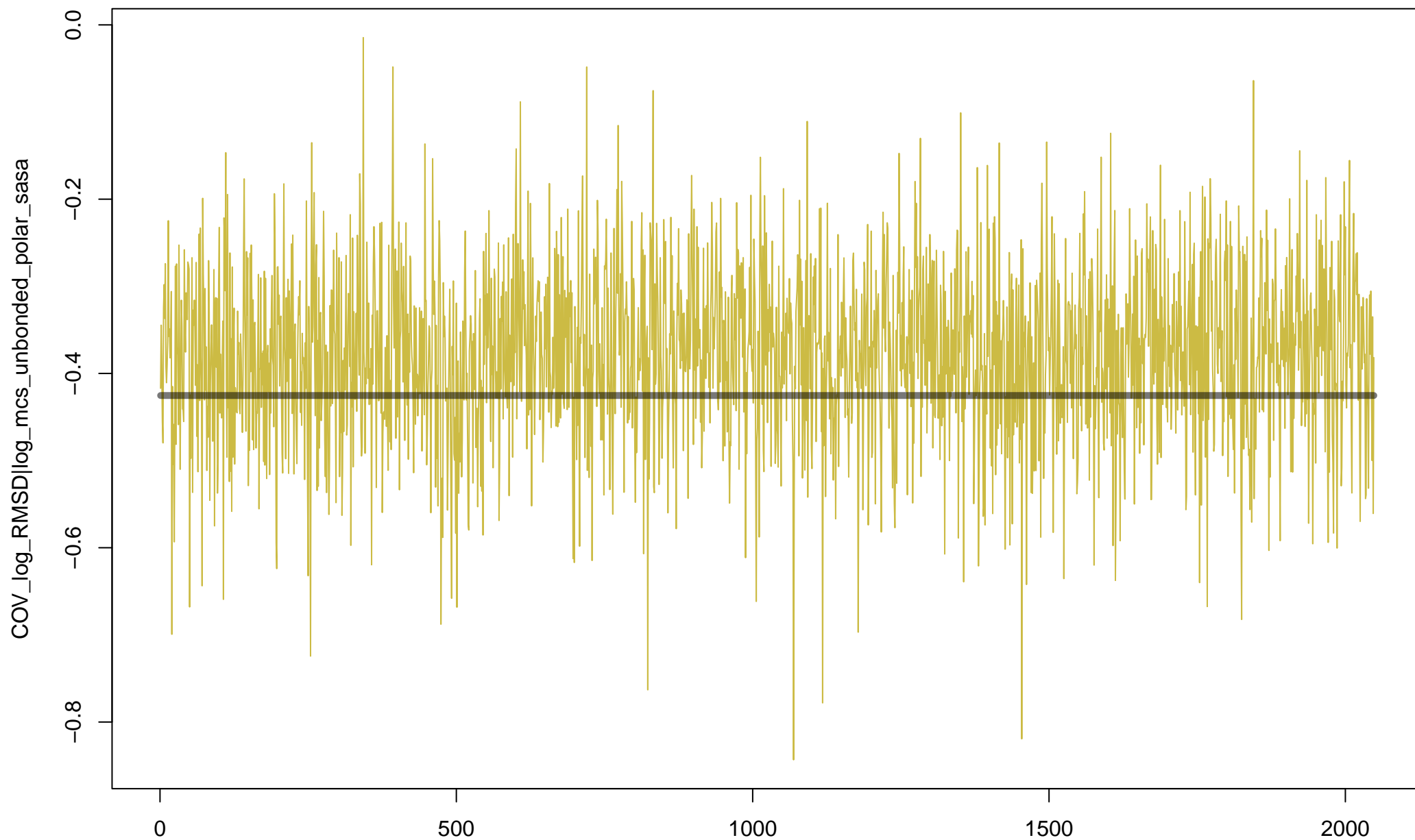
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1900 | BMK = 0.051 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | rel.err: 0.353**



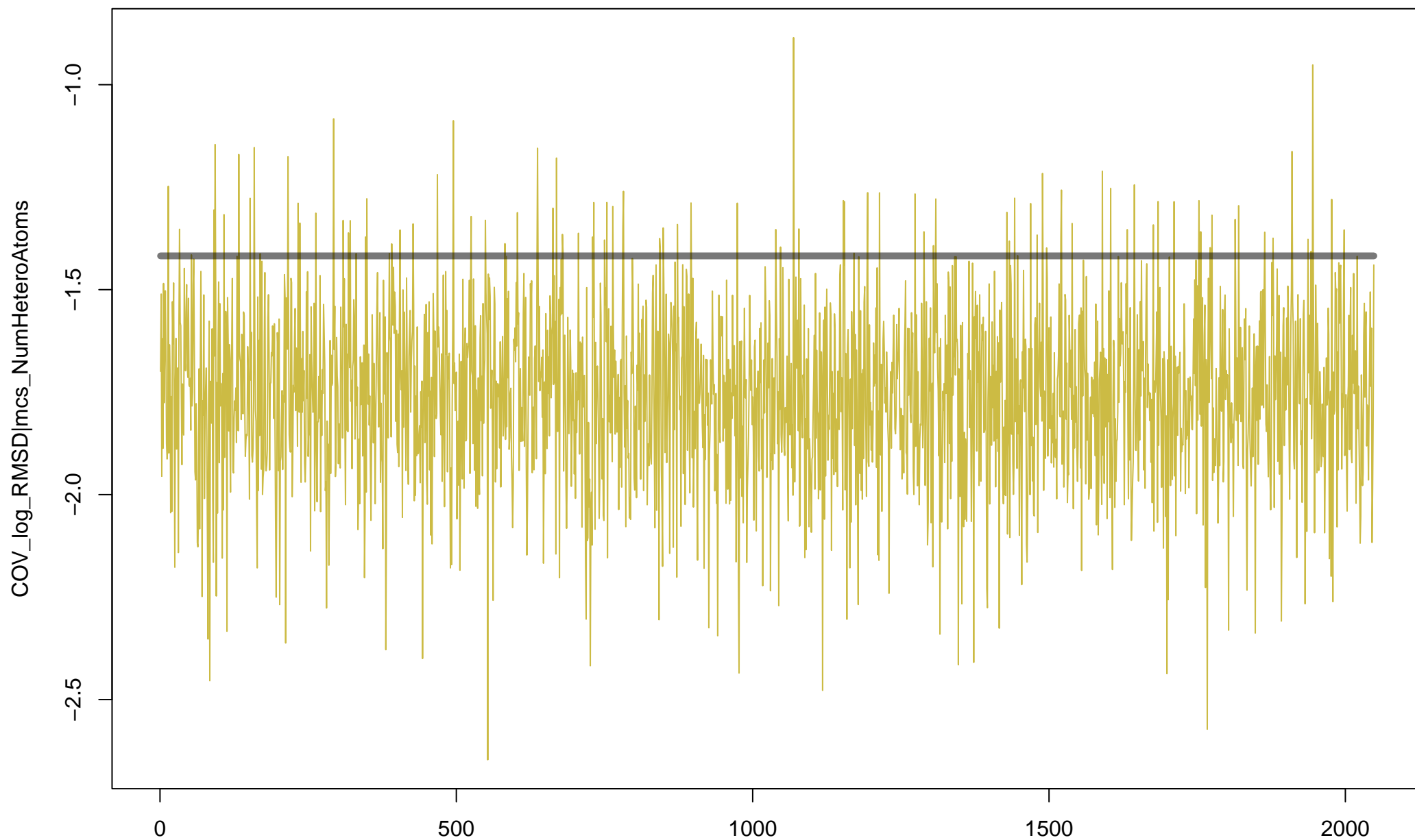
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0434 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: 0.0429**



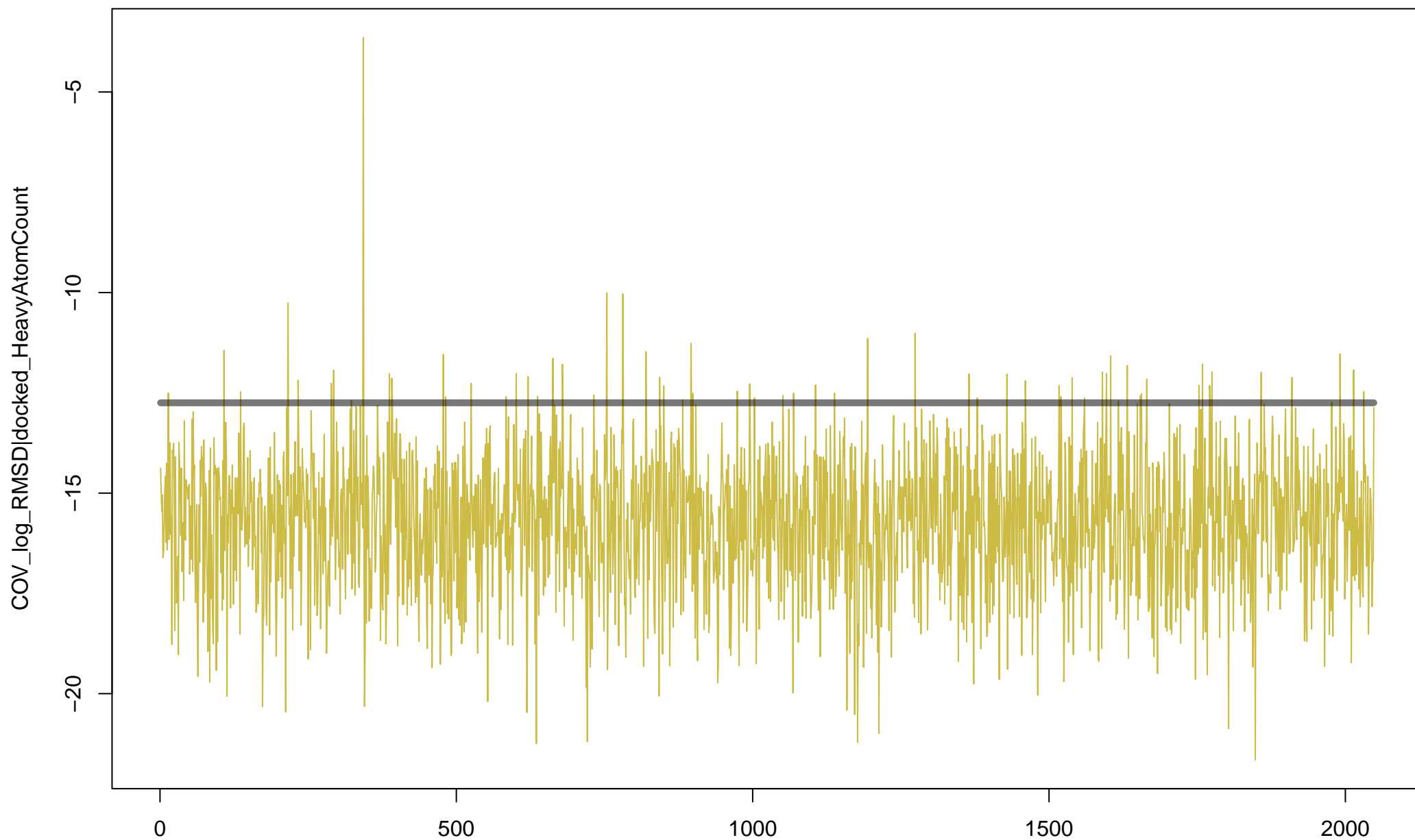
**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2030 | BMK = 0.0436 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: 0.477**



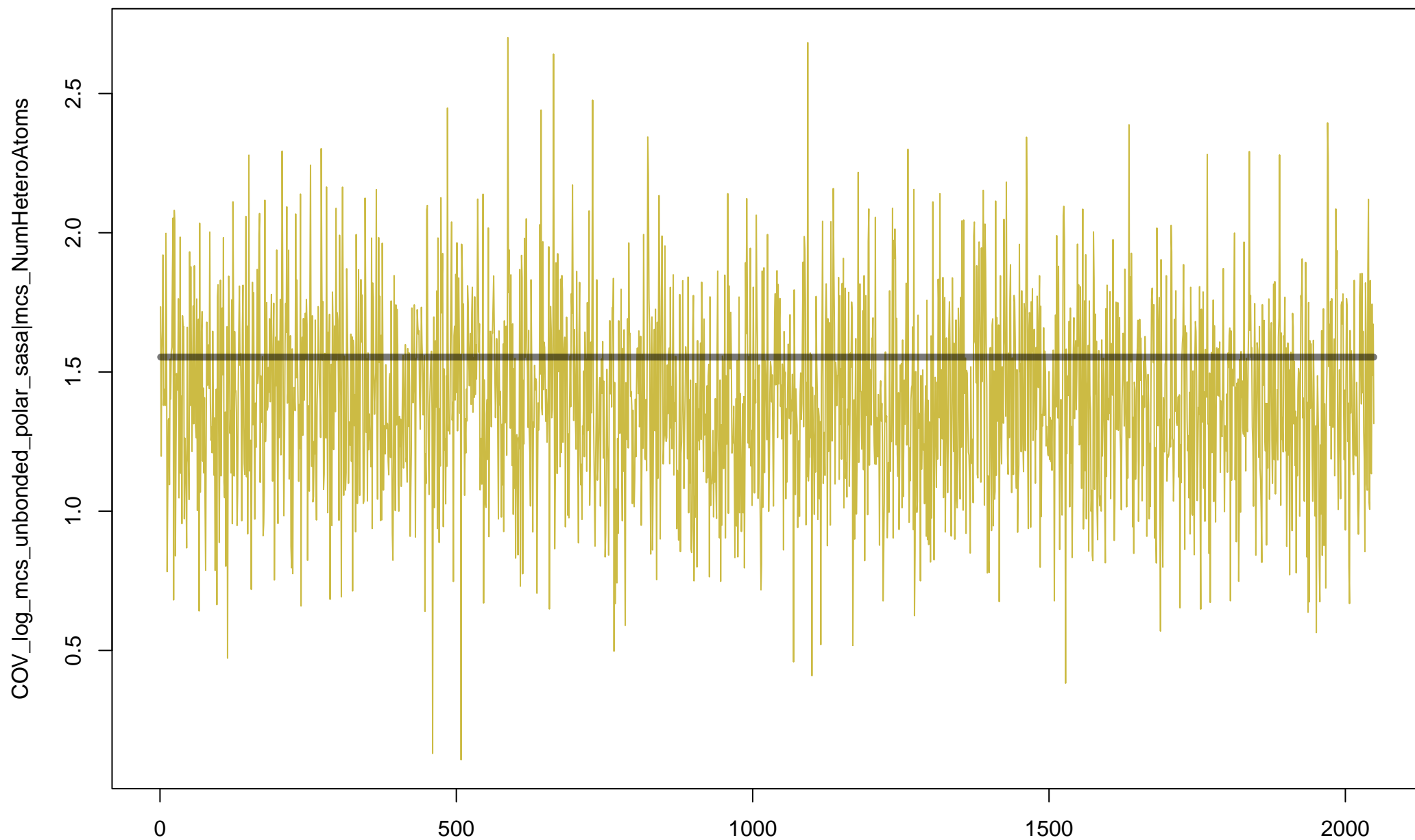
**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1900 | BMK = 0.0491 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: -1.6**



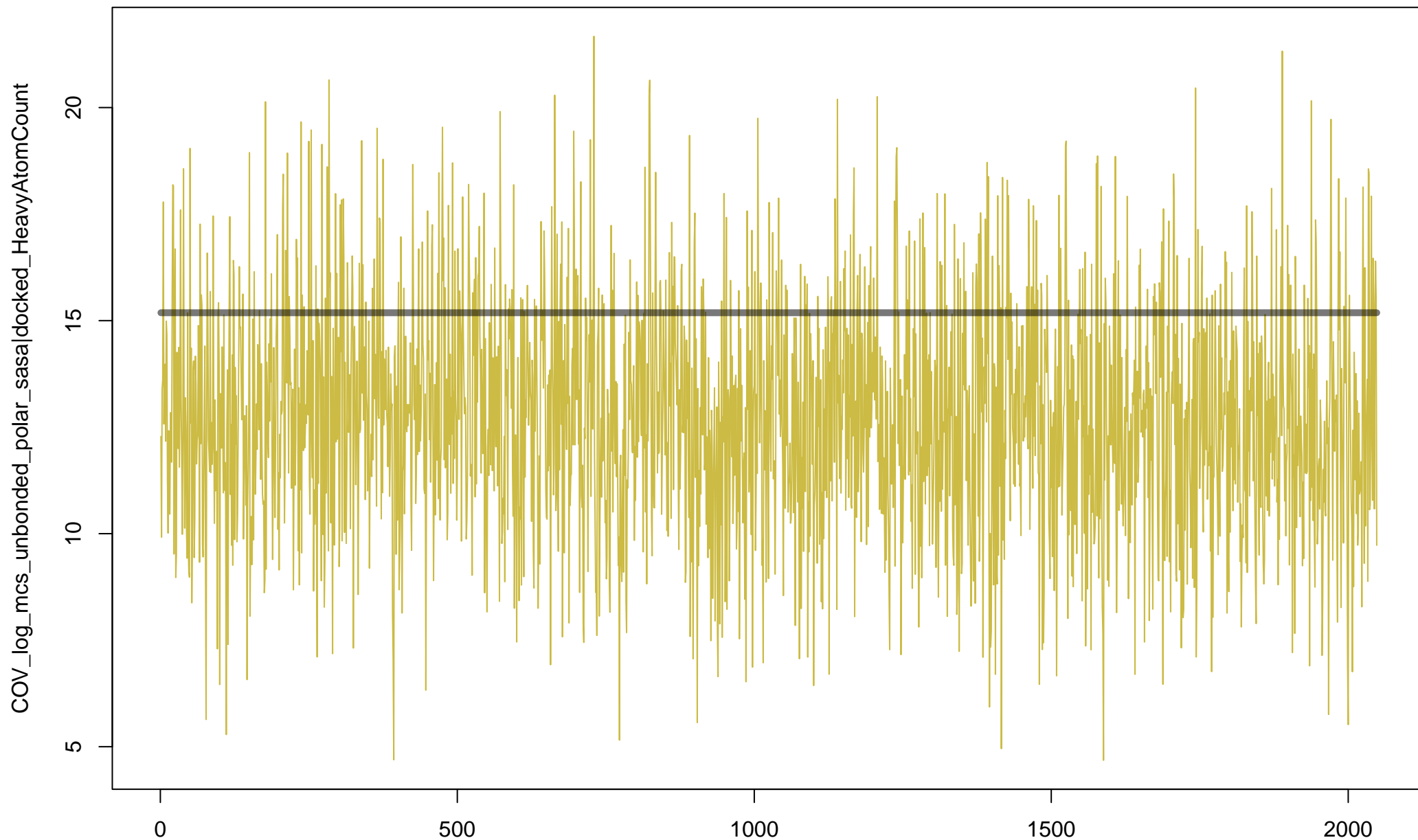
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0549 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: -1.78**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 1910 | BMK = 0.0401 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0 | rel.err: -0.457**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 1870 | BMK = 0.0404 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: -0.921**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0421 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: 0.477**

