

-- STATS maxD --

min ESS = 86.0221147575997

max BMK = 0.139986662190434

max MCSE = 8.08471263084366

all stationary: TRUE

burn: 0

max rel.err.: 2.20020726187788

-- STATS 1D --

min ESS = 1692.35601899538

max BMK = 0.0673295720463373

max MCSE = 2.74488492605211

all stationary: TRUE

burn: 0

max rel.err.: 2.25180864667938

-- STATS 2D --

min ESS = 1785.58446483707

max BMK = 0.0573894307874708

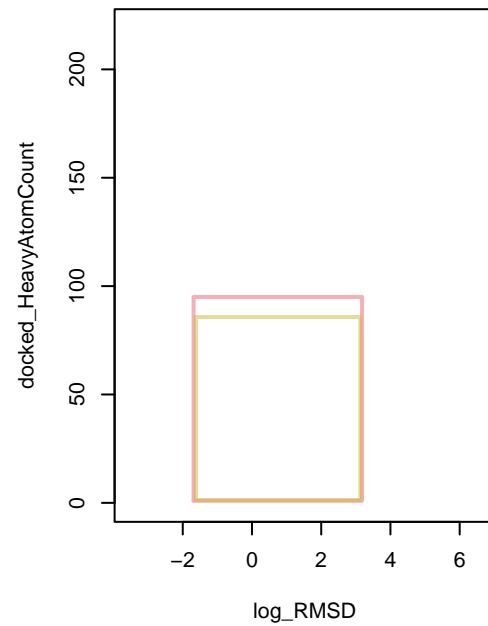
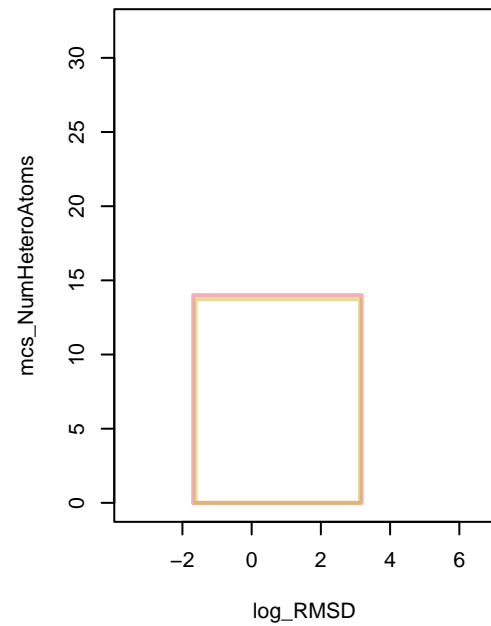
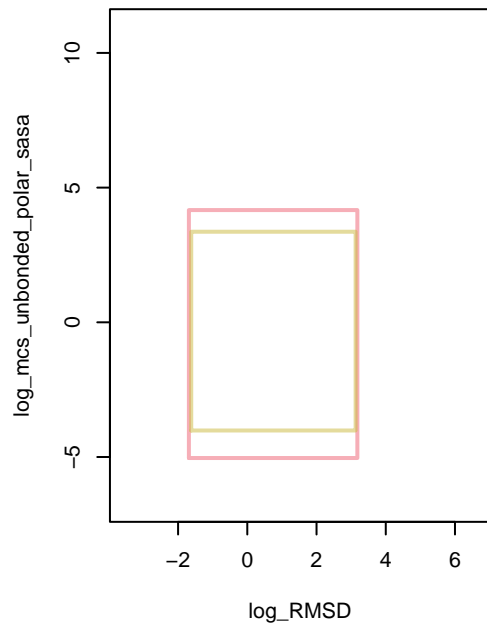
max MCSE = 2.78498209925673

all stationary: TRUE

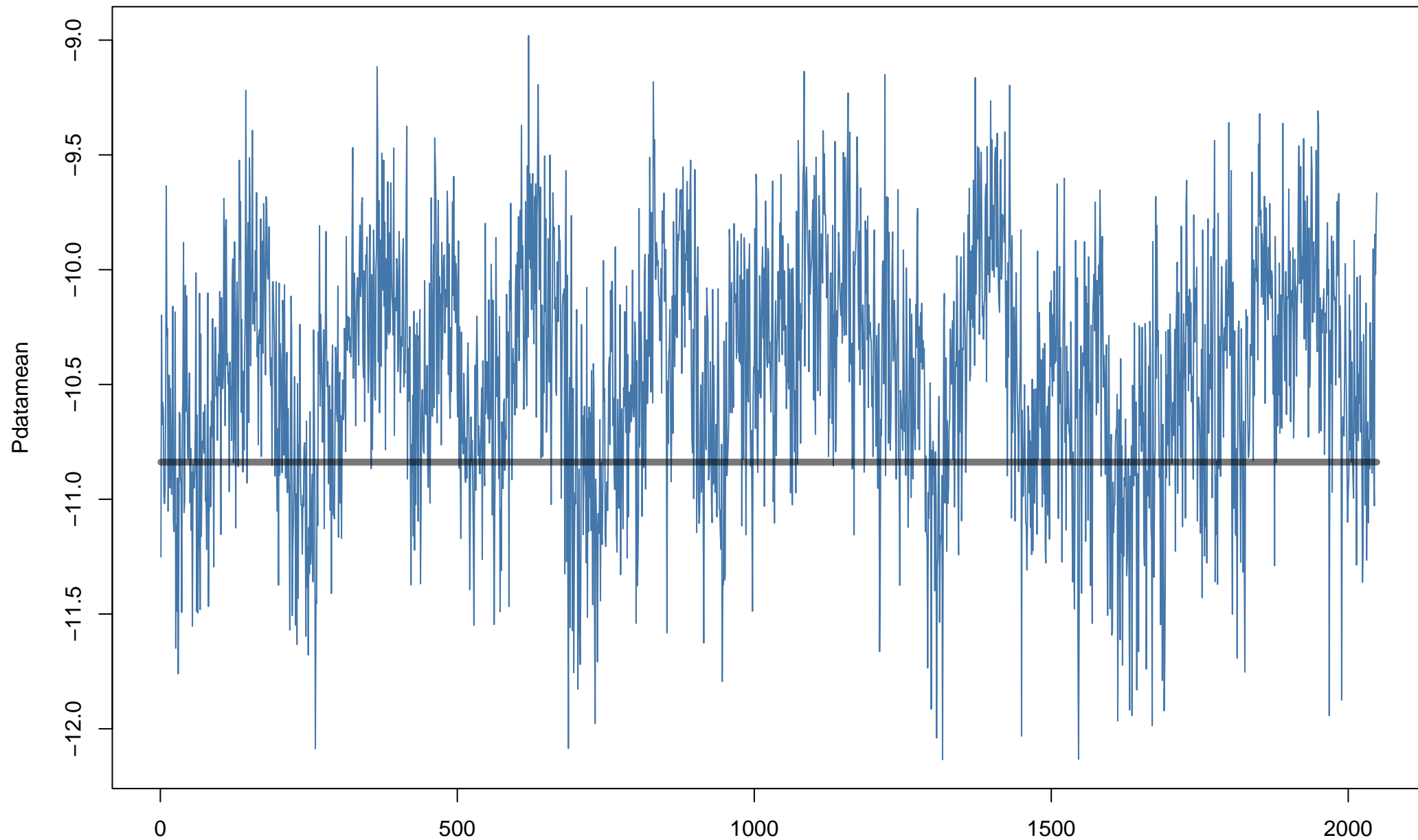
burn: 0

max rel.err.: 1.70997539950496

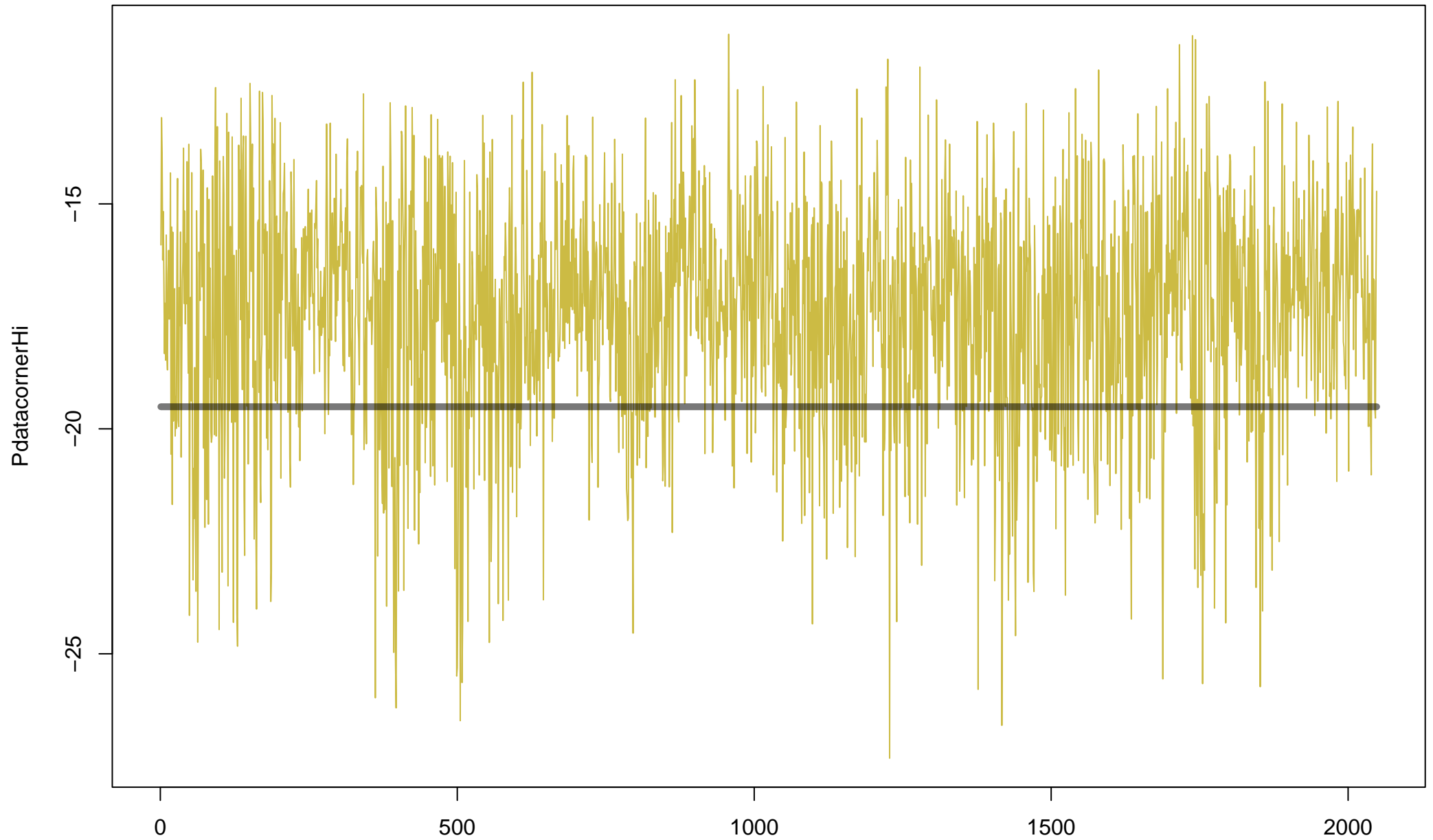
Occupied clusters: 8 of 16



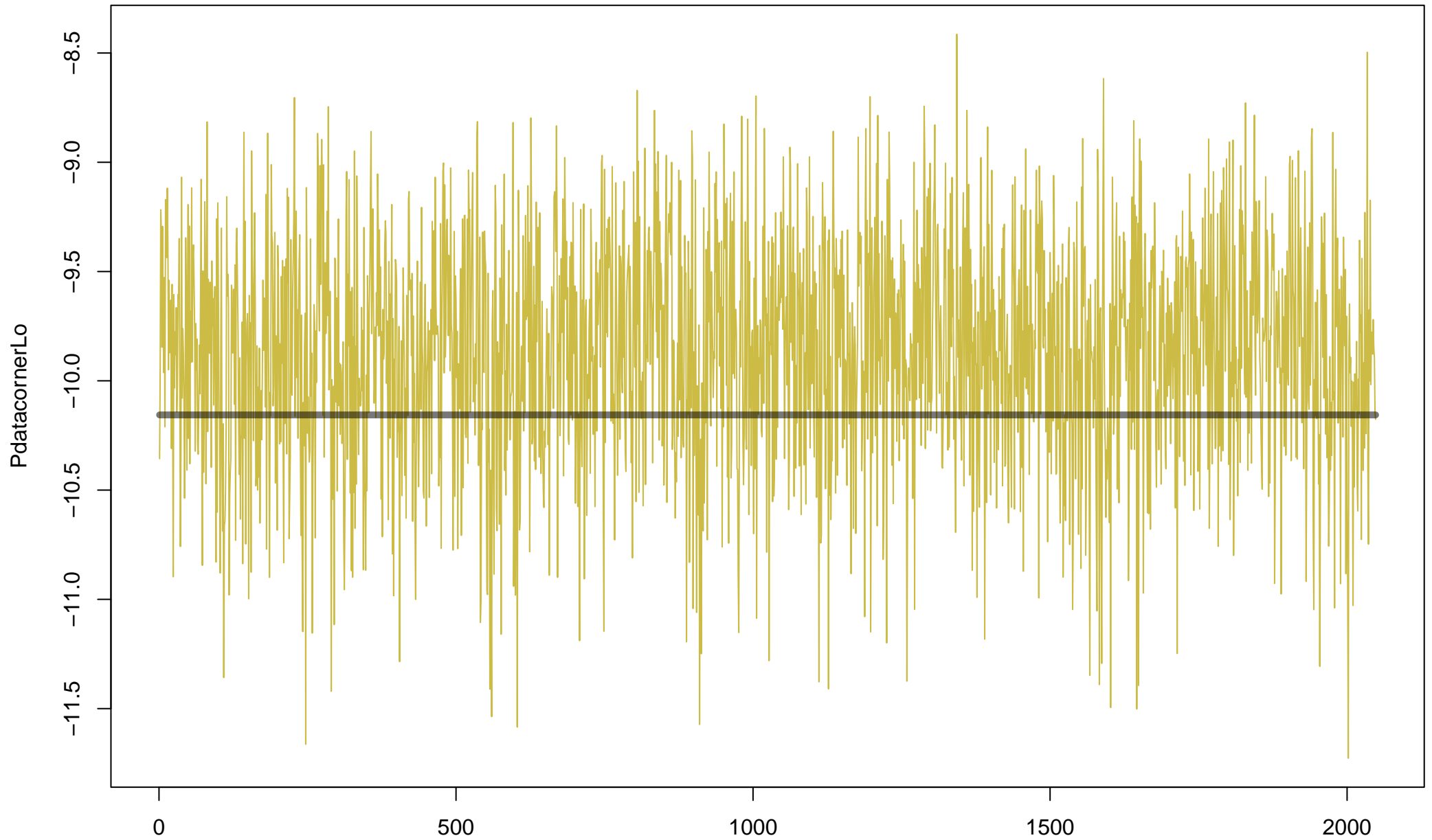
**Pdatamean**  
**ESS = 86 | BMK = 0.0607 | MCSE(6.27) = 8.08 | stat: TRUE | burn: 0 | rel.err: 0.795**



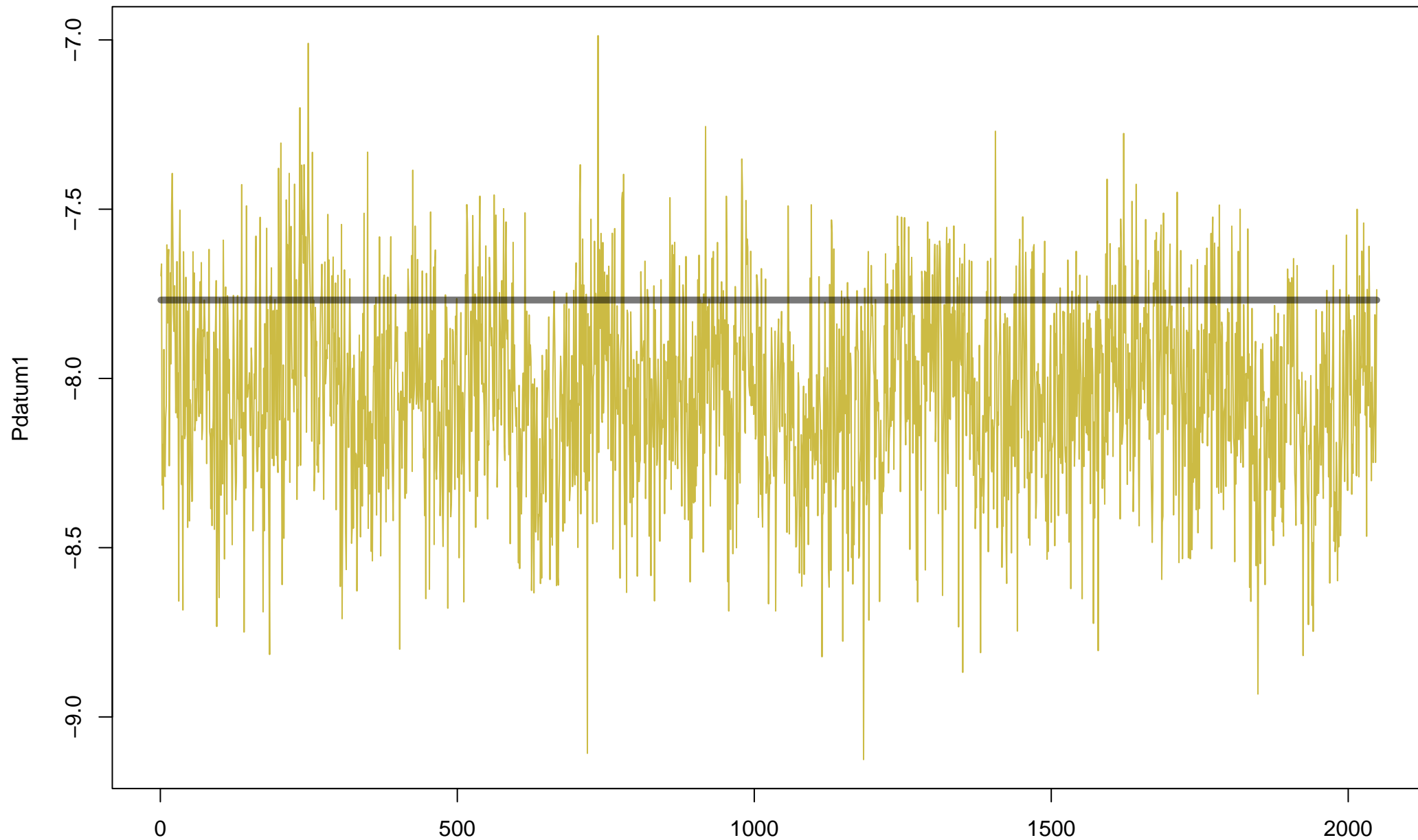
**PdatacornerHi**  
**ESS = 977 | BMK = 0.14 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: 0.304**



**PdatacornerLo**  
**ESS = 1760 | BMK = 0.0506 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.685**

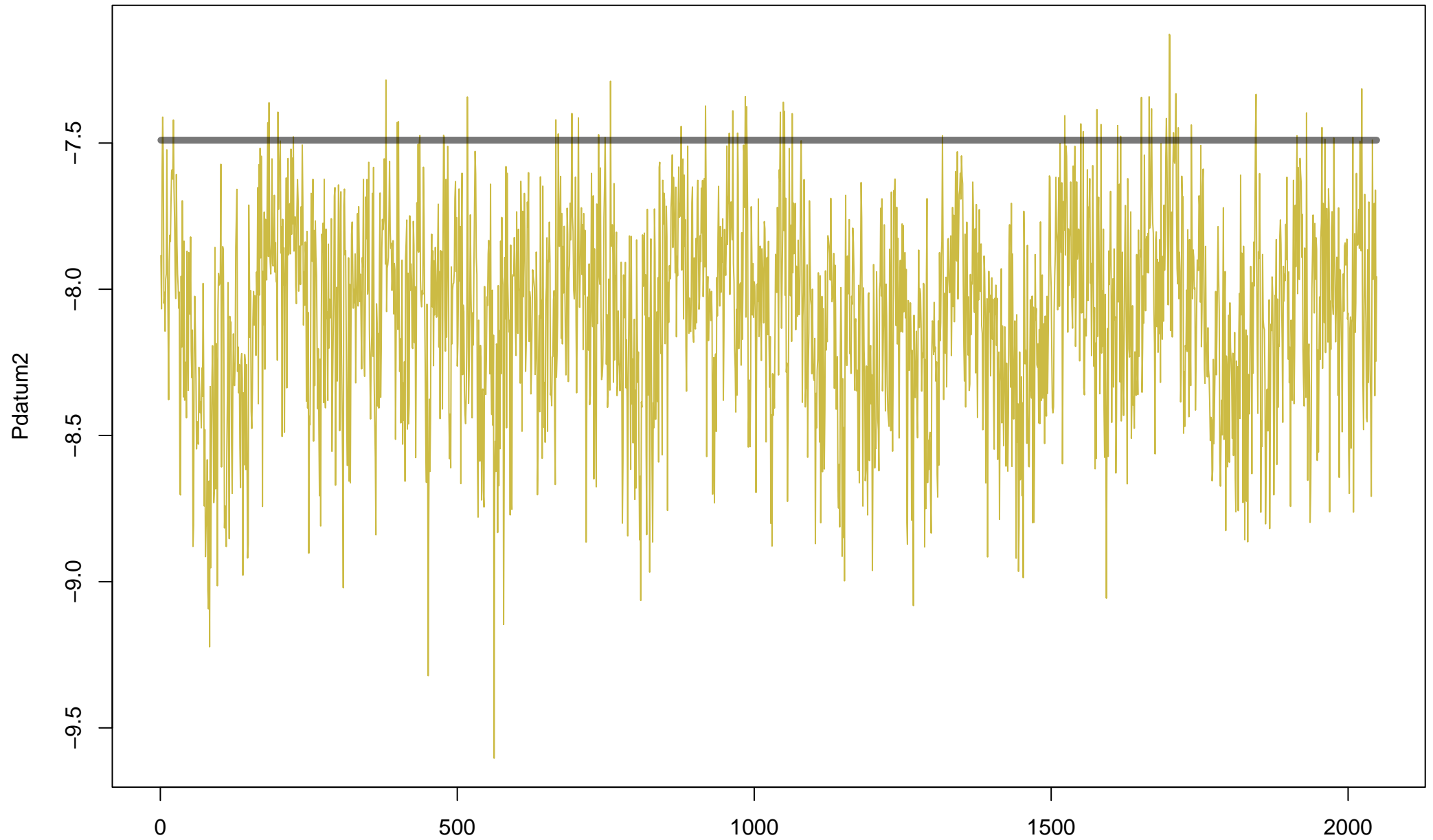


**Pdatum1**  
**ESS = 408 | BMK = 0.0719 | MCSE(6.27) = 4.51 | stat: TRUE | burn: 0 | rel.err: -0.935**



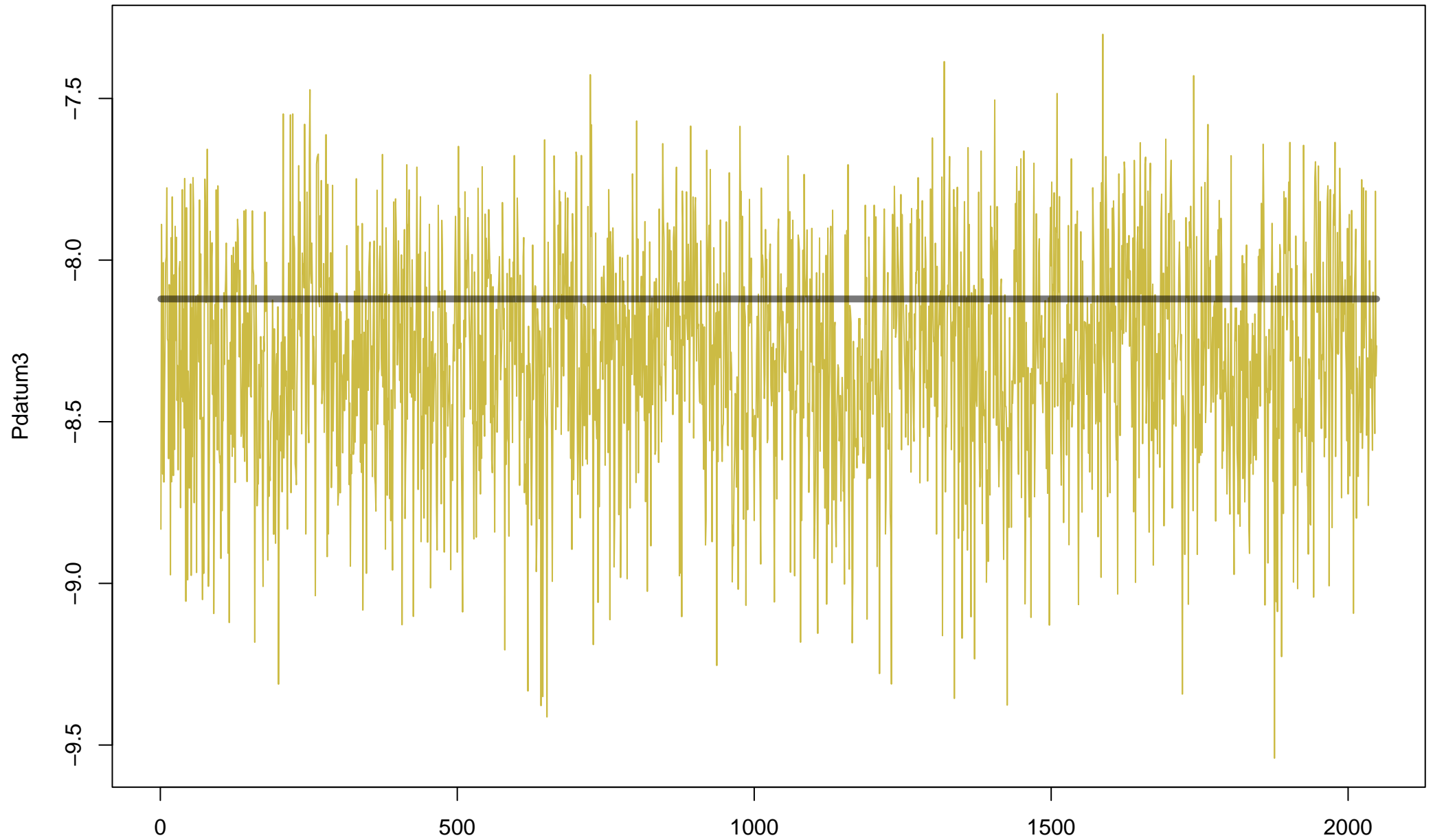
**Pdatum2**

**ESS = 262 | BMK = 0.0656 | MCSE(6.27) = 6.32 | stat: TRUE | burn: 0 | rel.err: -2.2**



**Pdatum3**

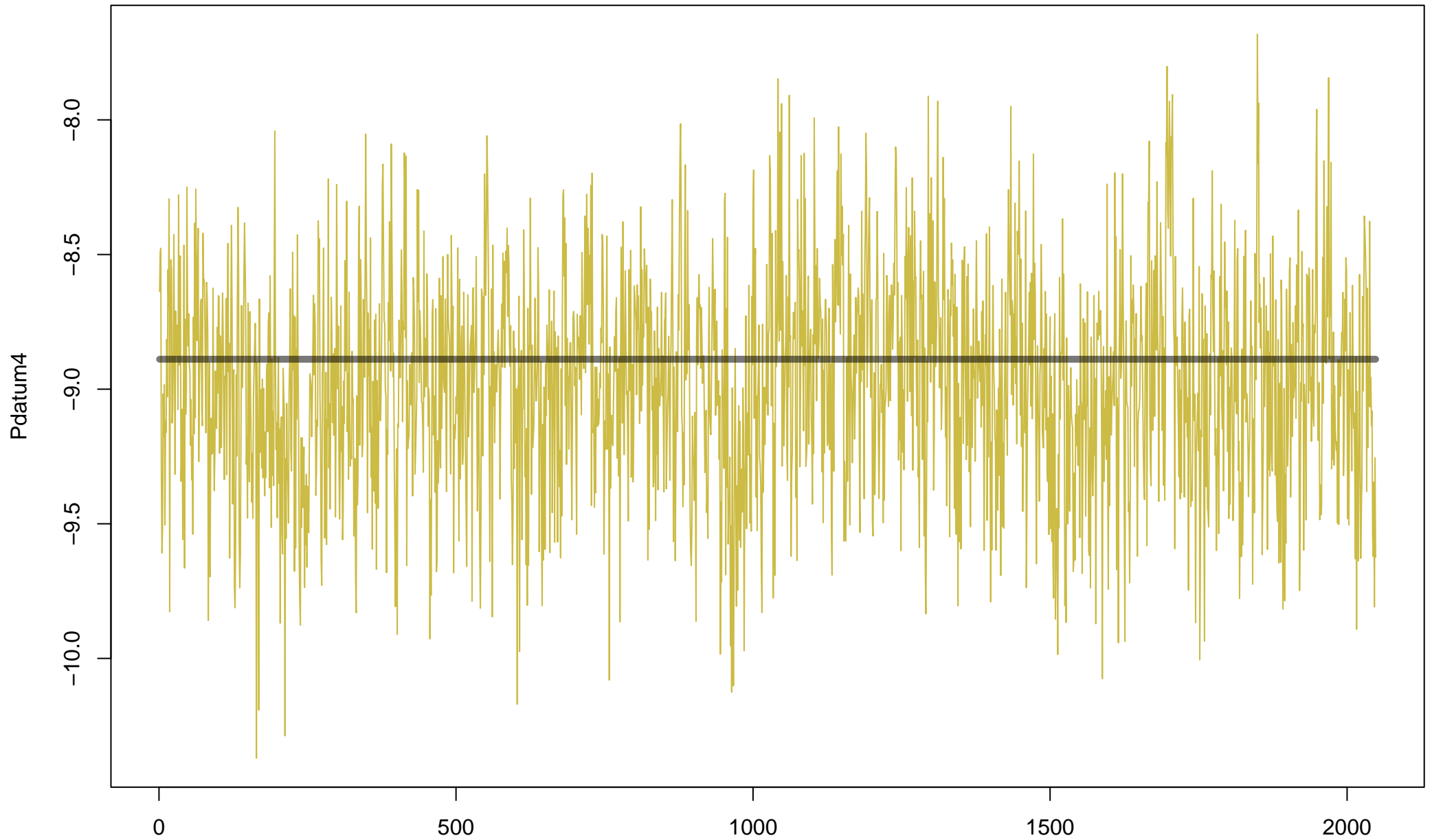
**ESS = 1160 | BMK = 0.0445 | MCSE(6.27) = 3.16 | stat: TRUE | burn: 0 | rel.err: -0.398**





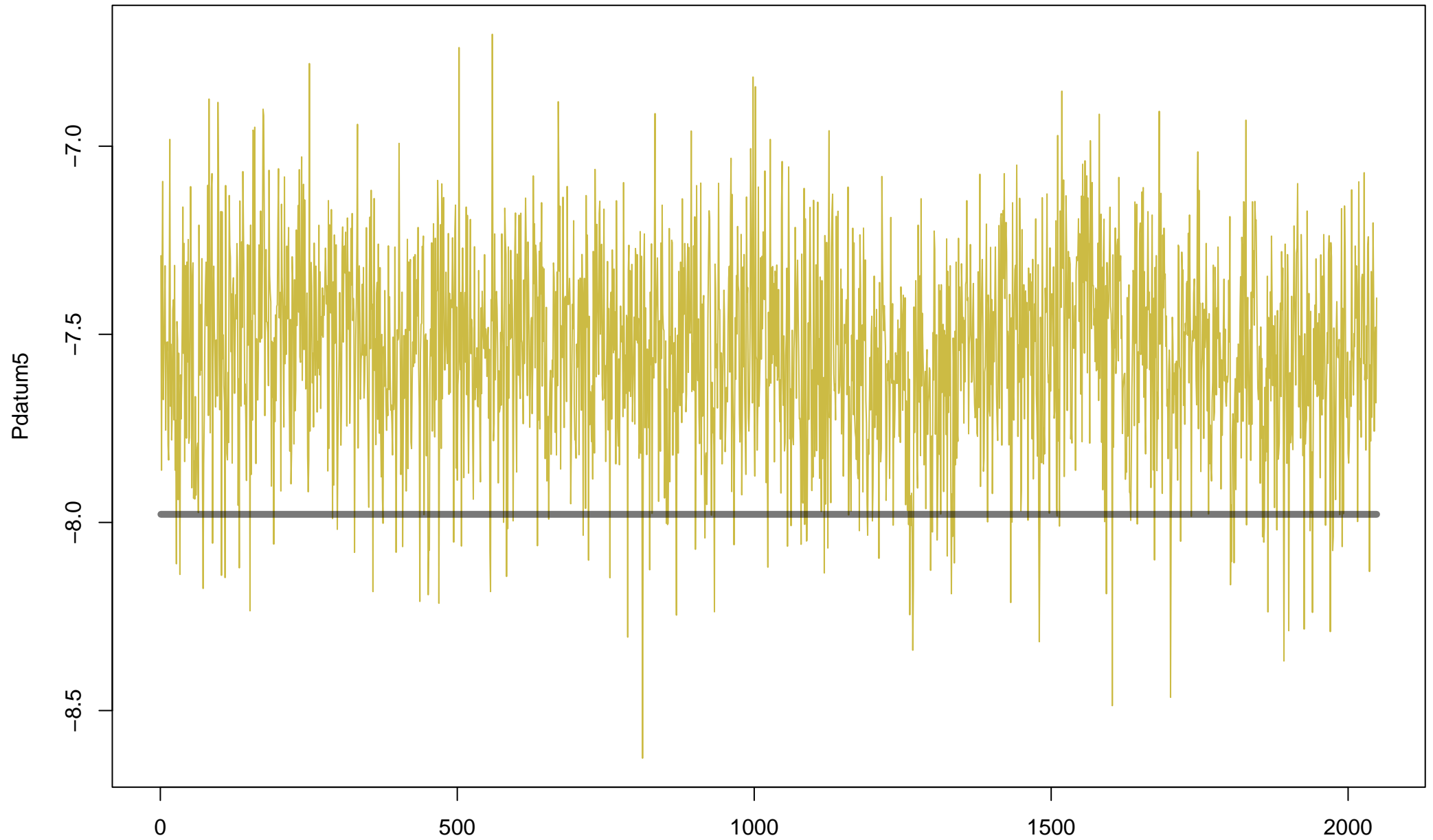
**Pdatum4**

**ESS = 621 | BMK = 0.0917 | MCSE(6.27) = 4.58 | stat: TRUE | burn: 0 | rel.err: -0.0399**

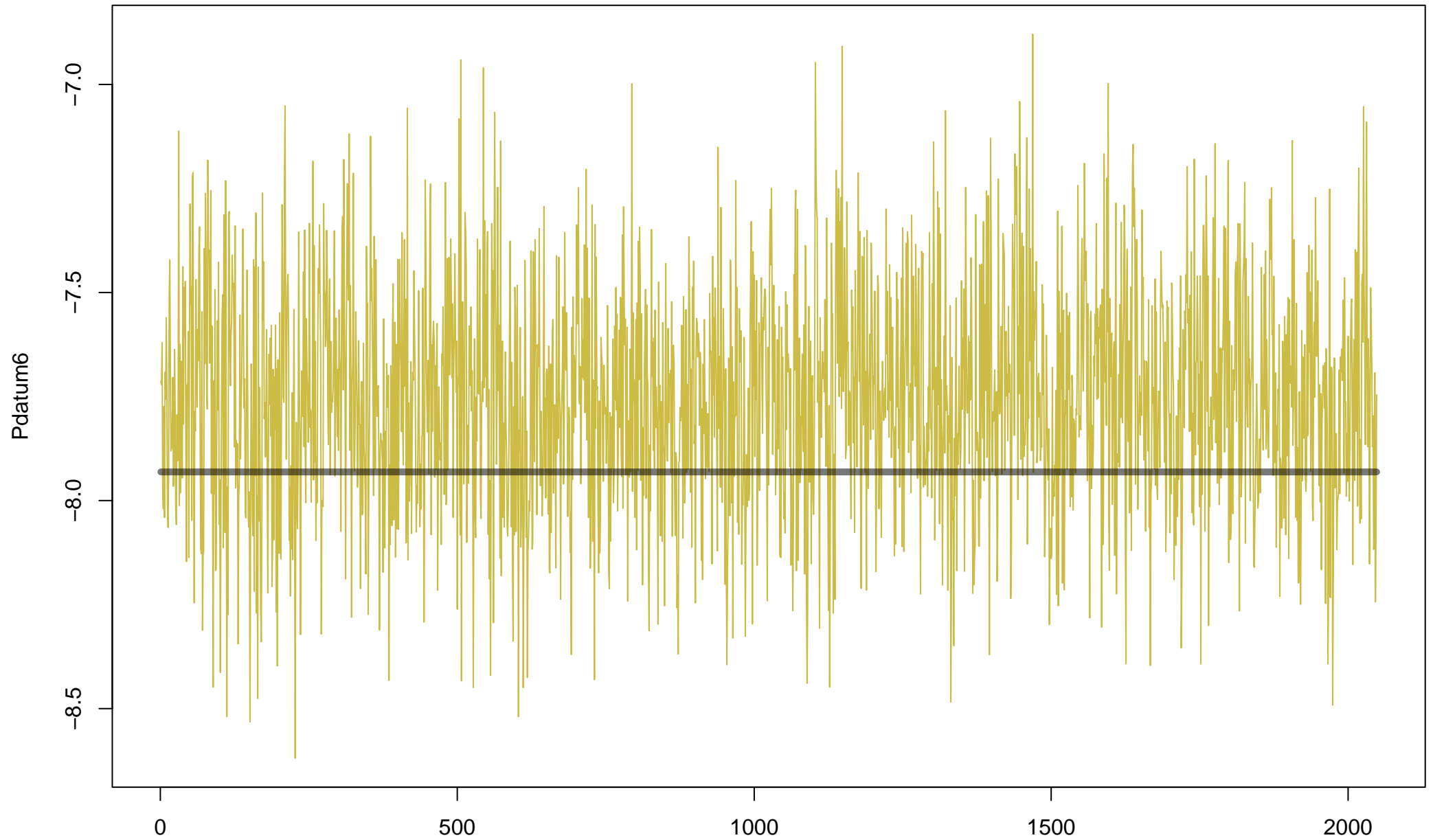


**Pdatum5**

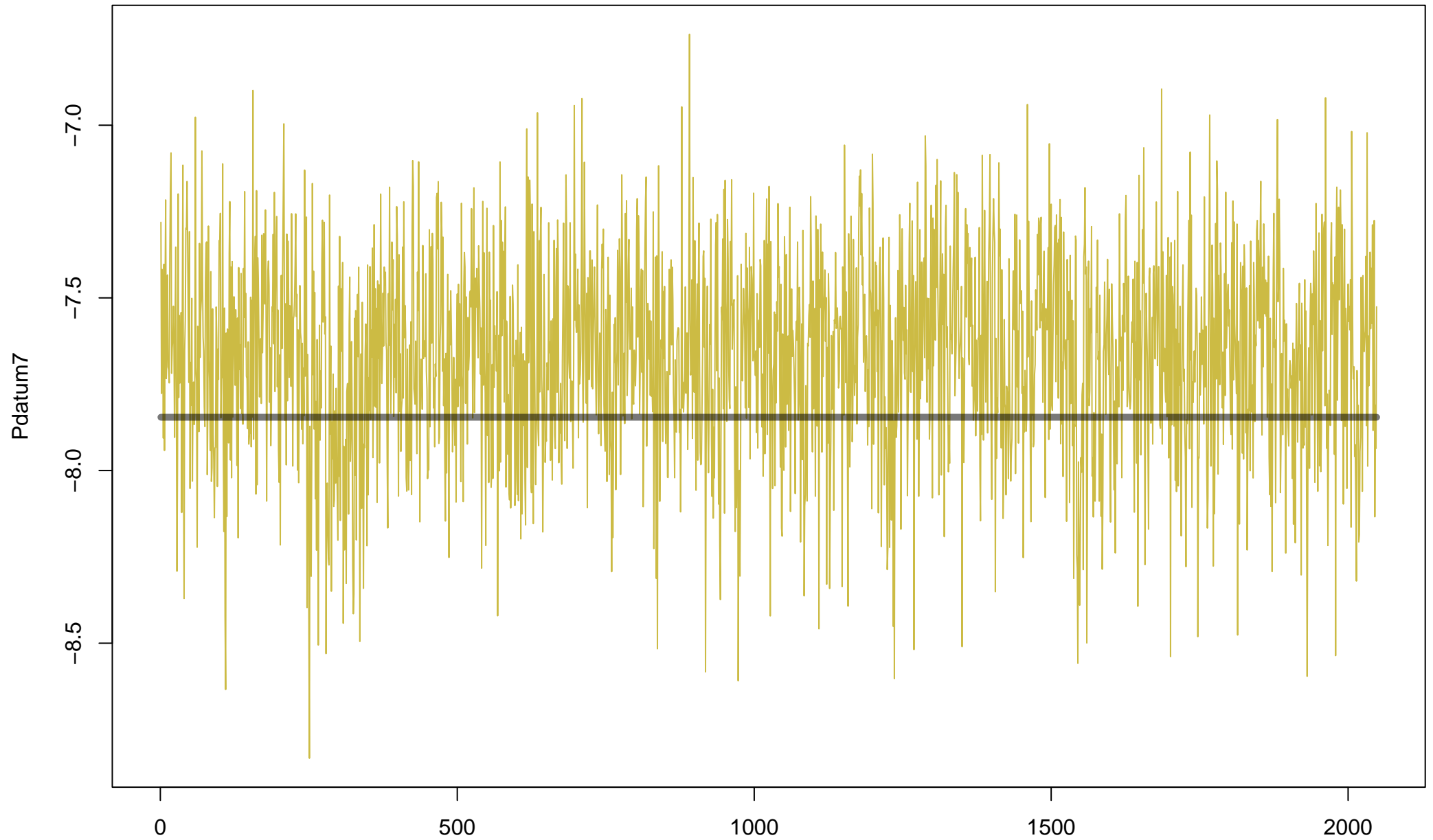
**ESS = 1350 | BMK = 0.0648 | MCSE(6.27) = 3.57 | stat: TRUE | burn: 0 | rel.err: 1.46**



**Pdatum6**  
**ESS = 1140 | BMK = 0.054 | MCSE(6.27) = 3.28 | stat: TRUE | burn: 0 | rel.err: 0.703**

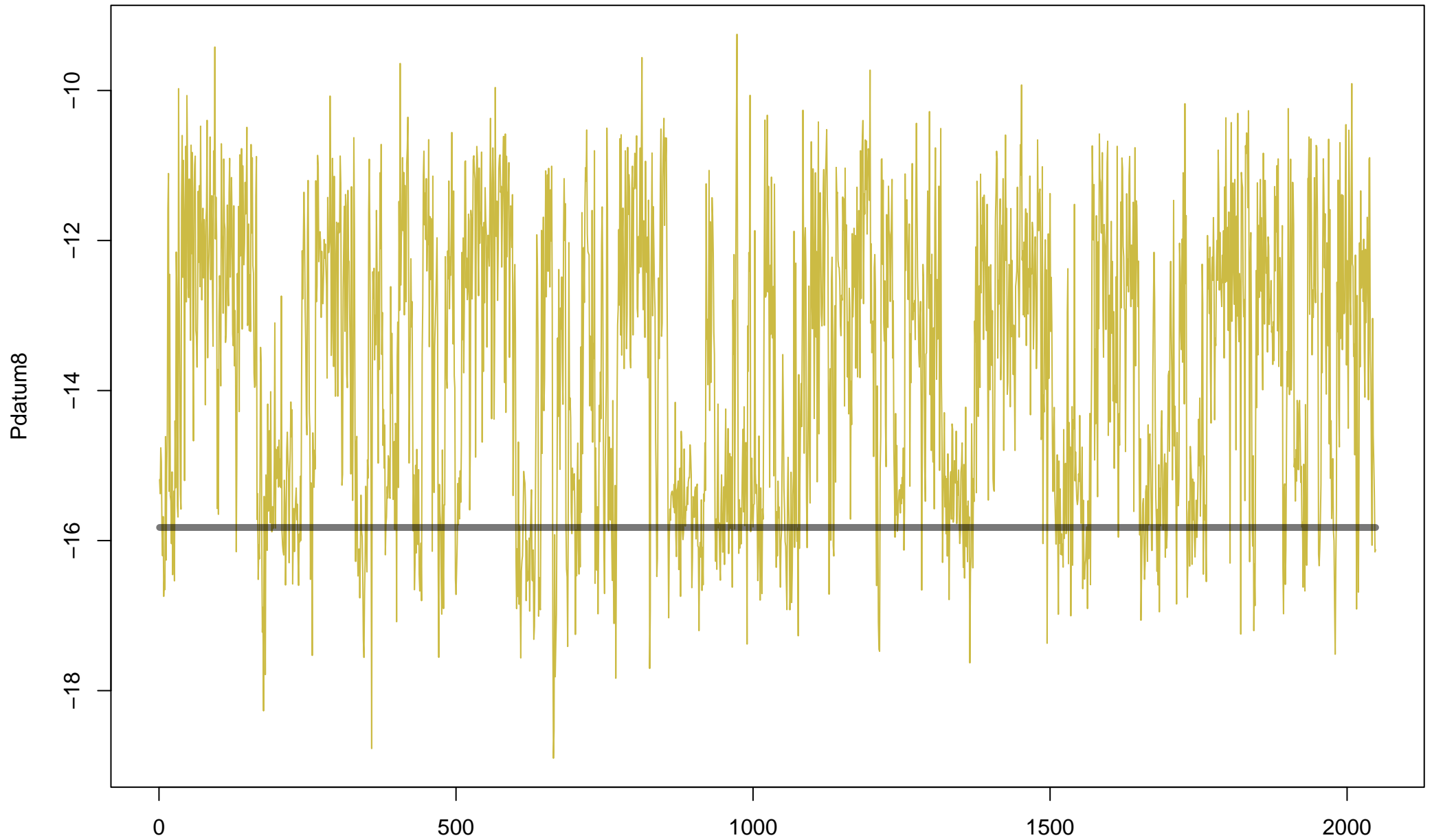


**Pdatum7**  
**ESS = 925 | BMK = 0.0439 | MCSE(6.27) = 3.49 | stat: TRUE | burn: 0 | rel.err: 0.687**



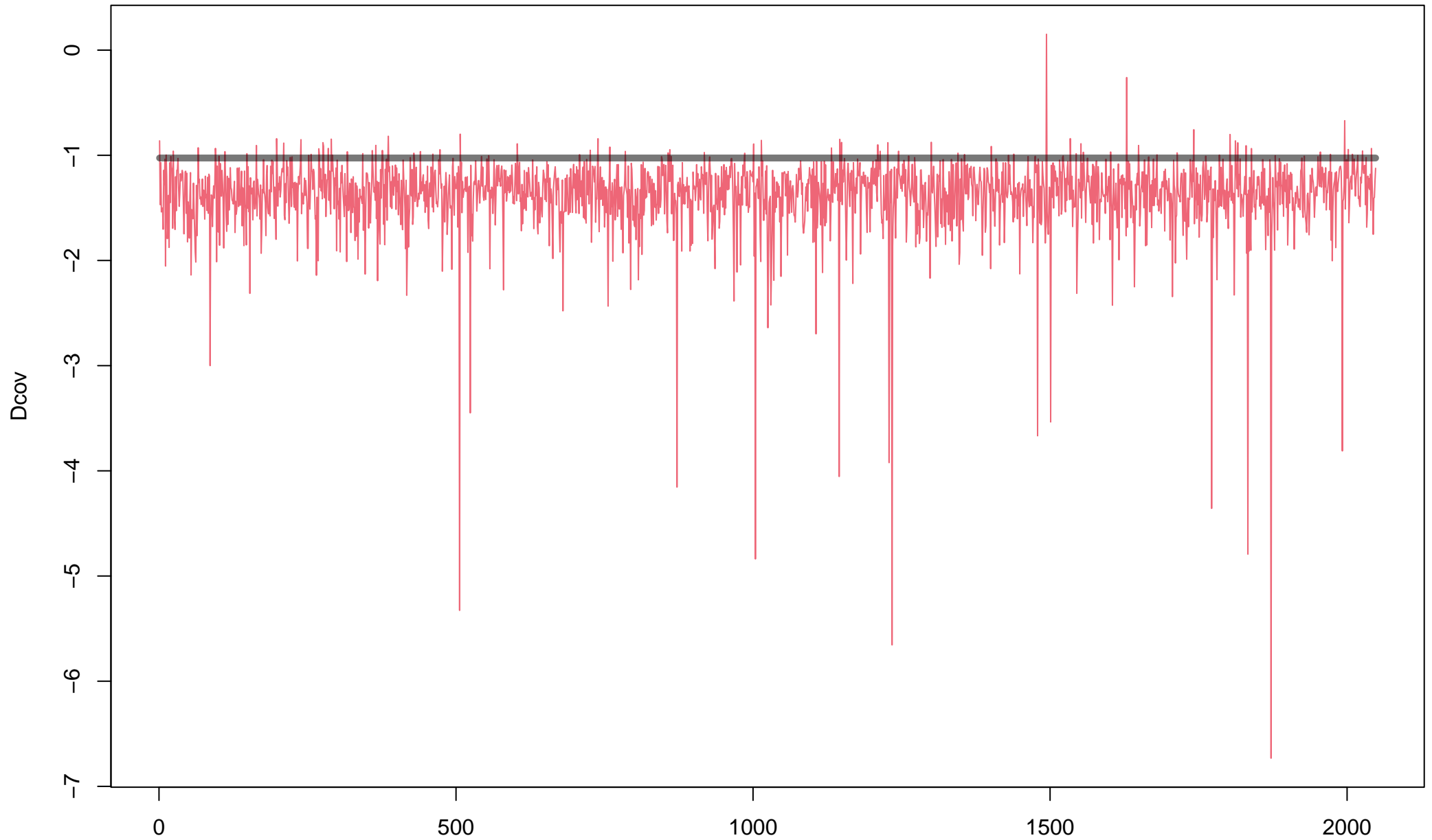
**Pdatum8**

**ESS = 407 | BMK = 0.102 | MCSE(6.27) = 4.99 | stat: TRUE | burn: 0 | rel.err: 0.578**

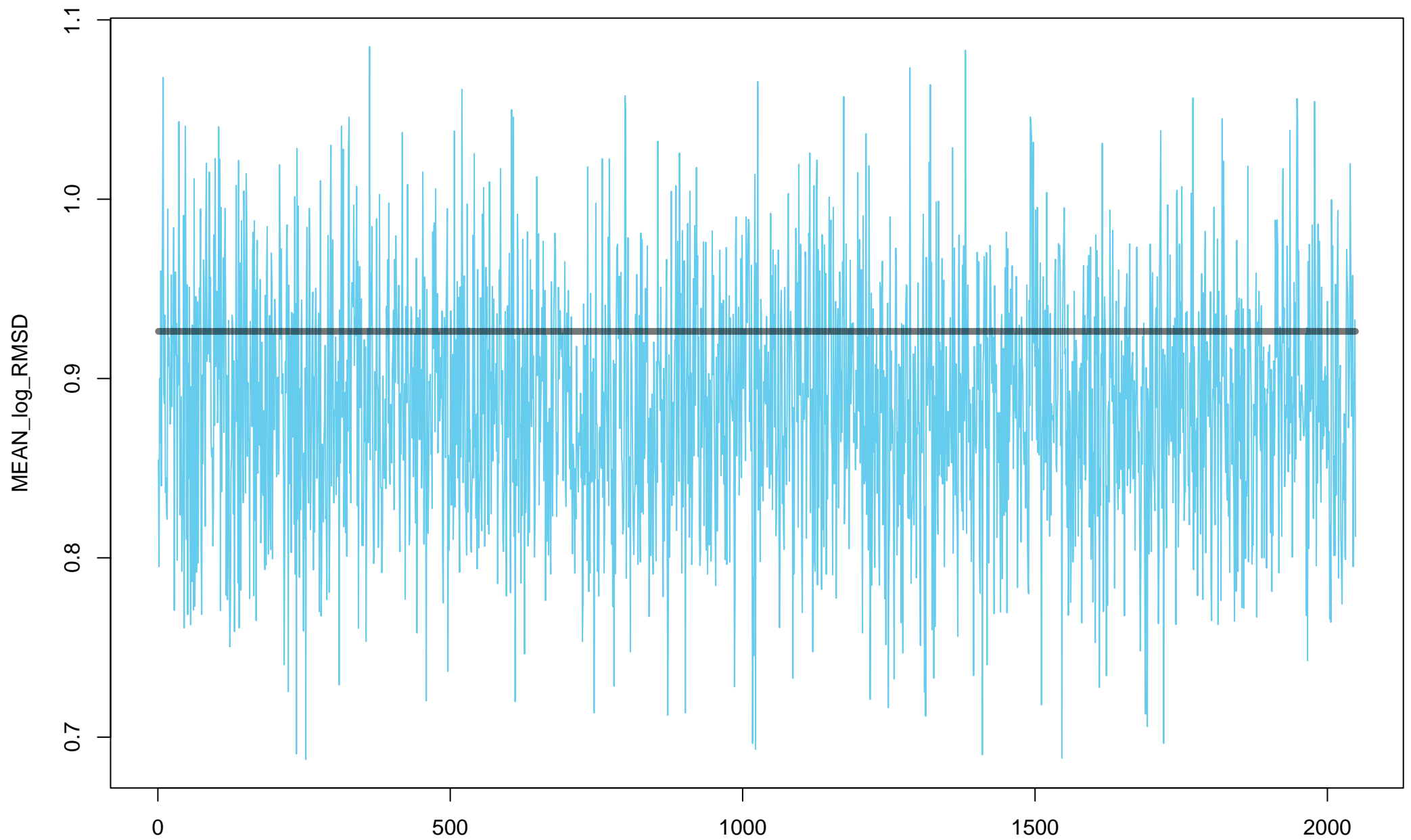


Dcov

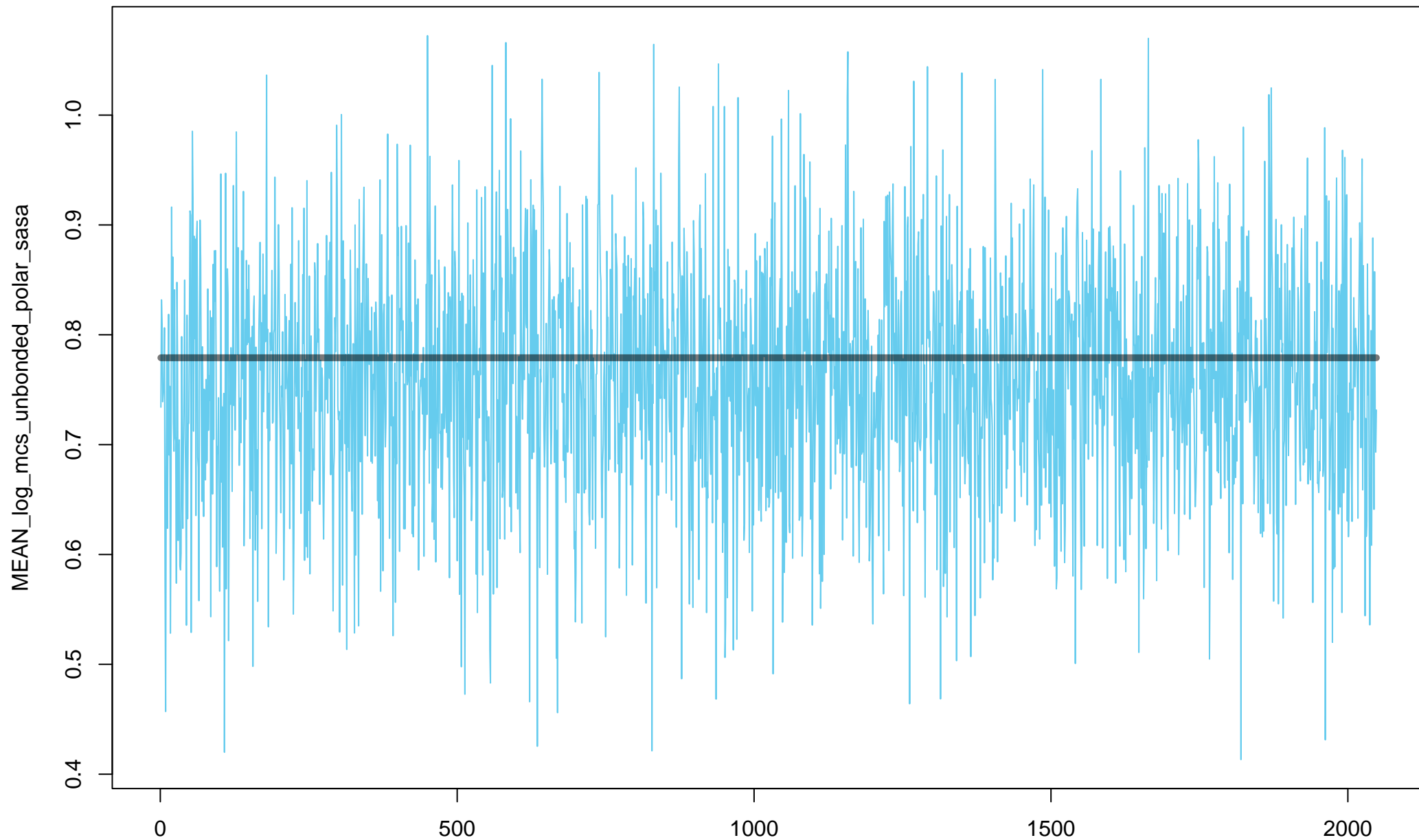
ESS = 1770 | BMK = 0.0579 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 1.33



**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0535 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: -0.604**



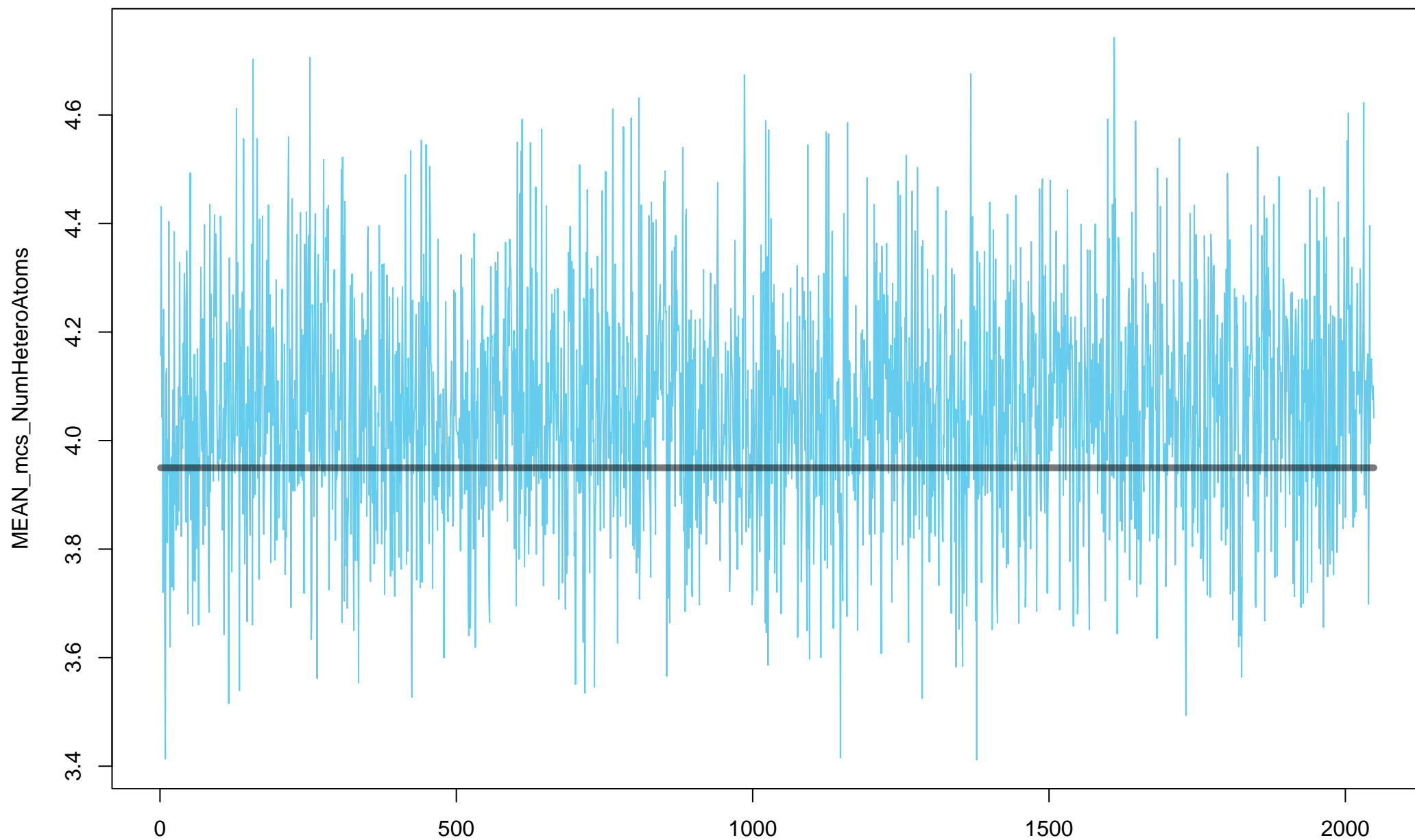
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: -0.197**



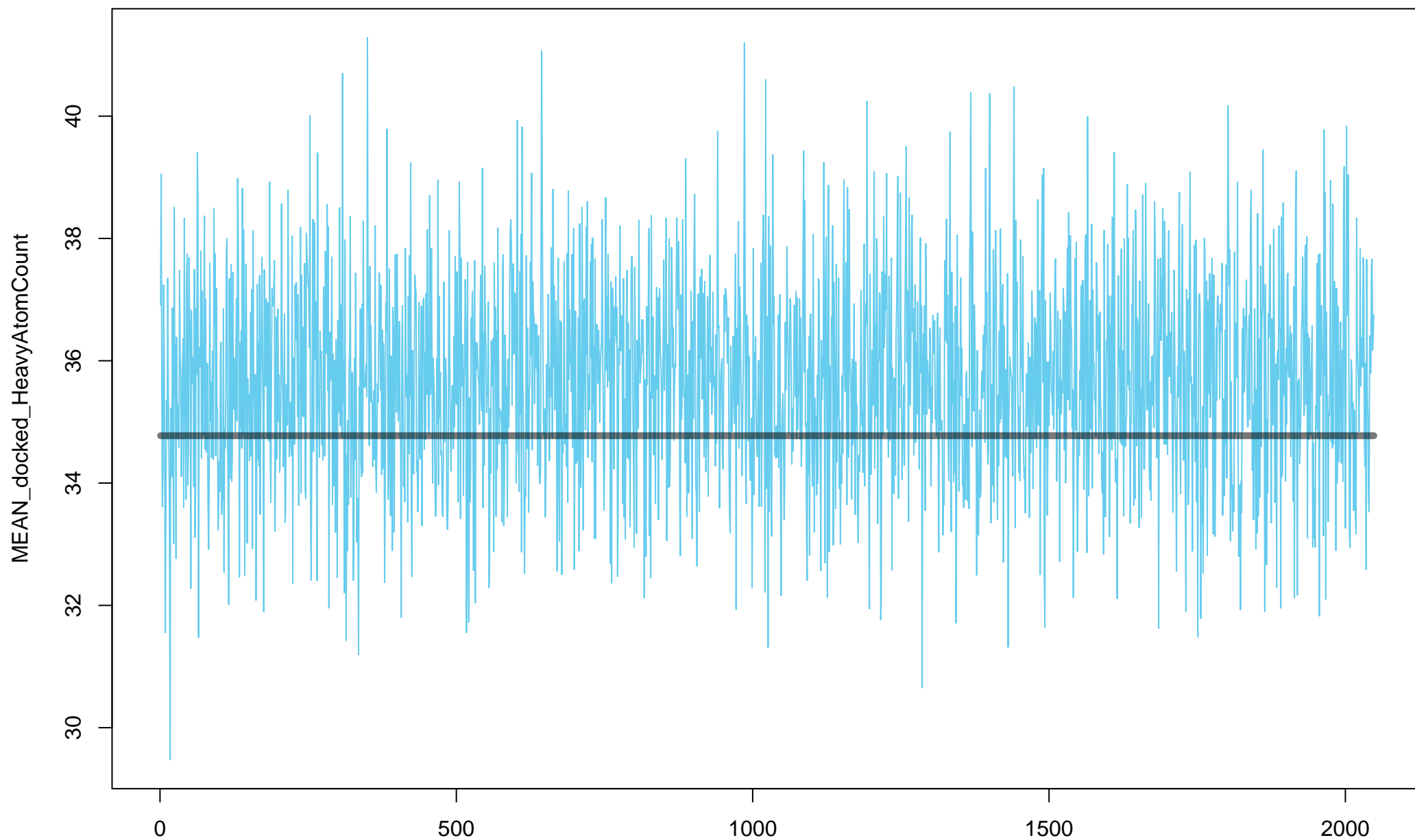


# MEAN\_mcs\_NumHeteroAtoms

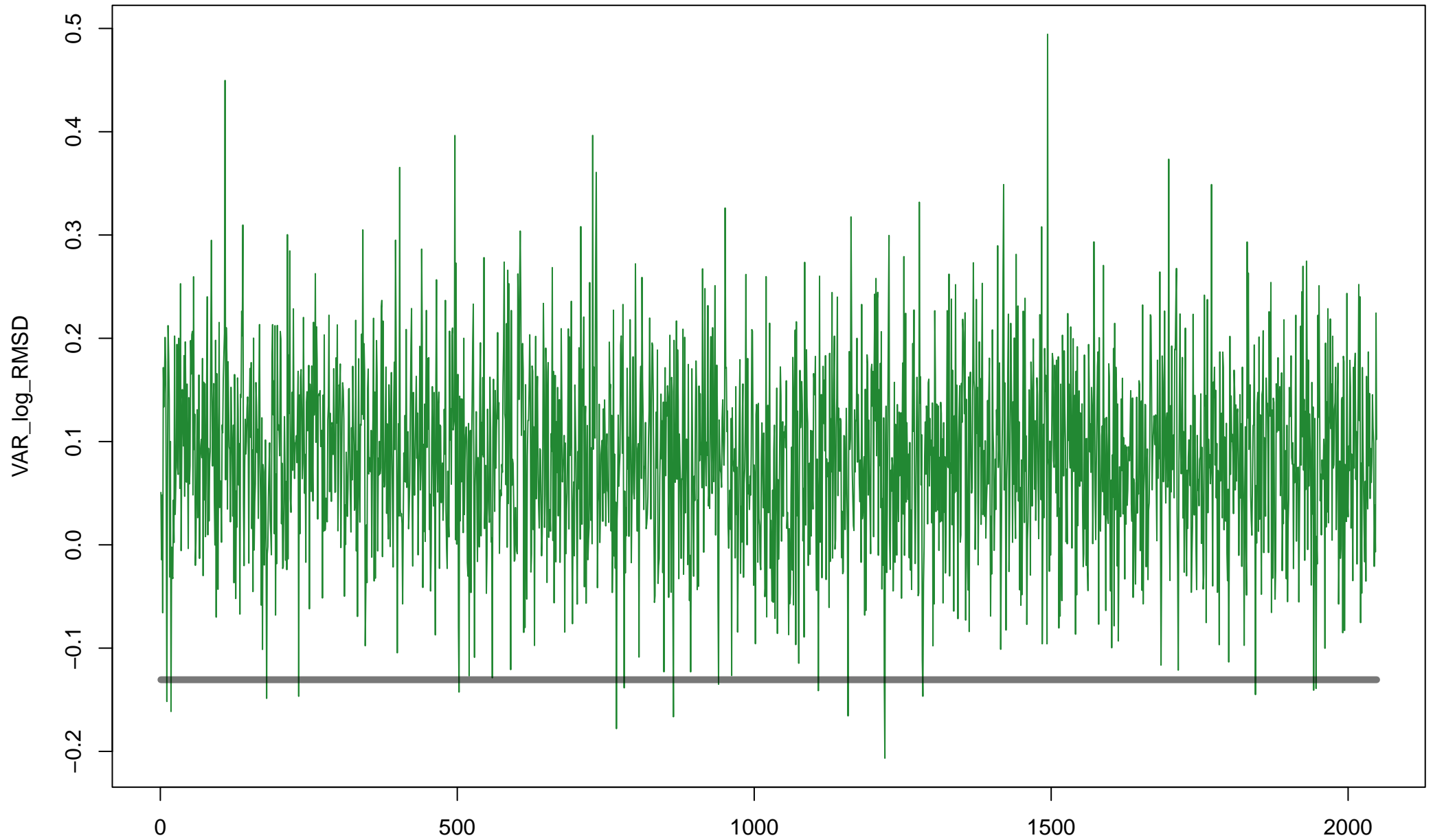
ESS = 2050 | BMK = 0.0412 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | rel.err: 0.521



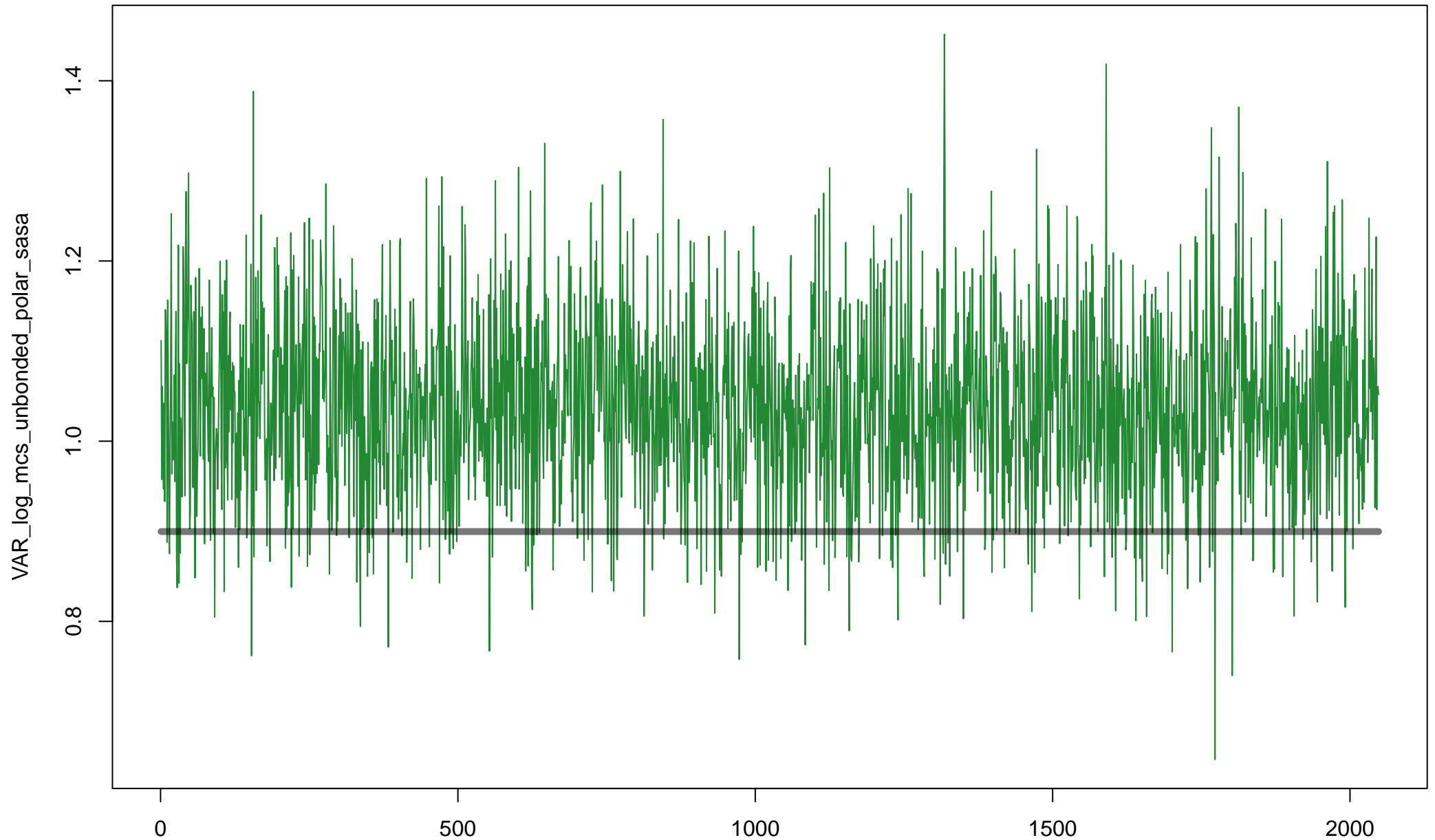
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0422 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: 0.542**



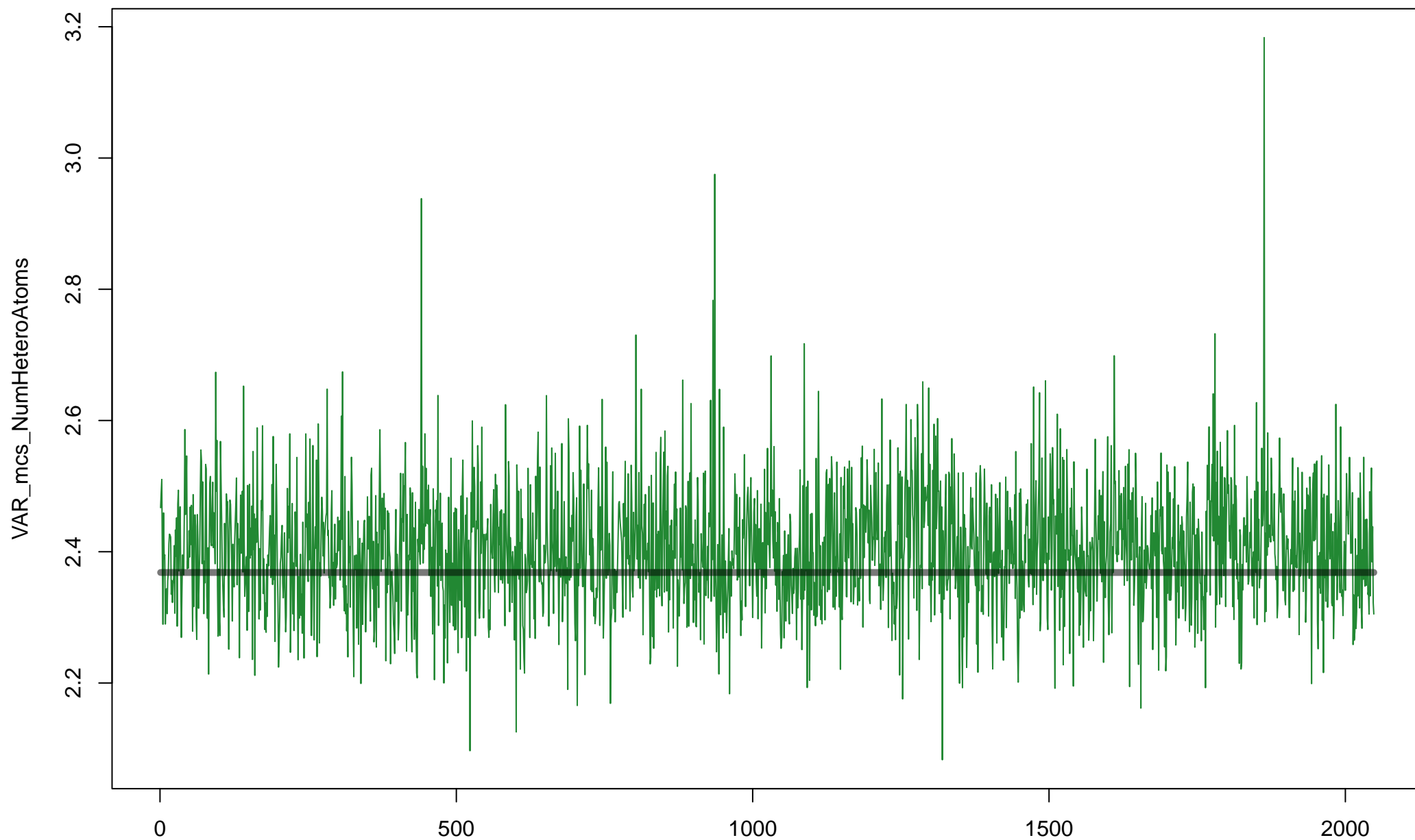
**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: 2.25**



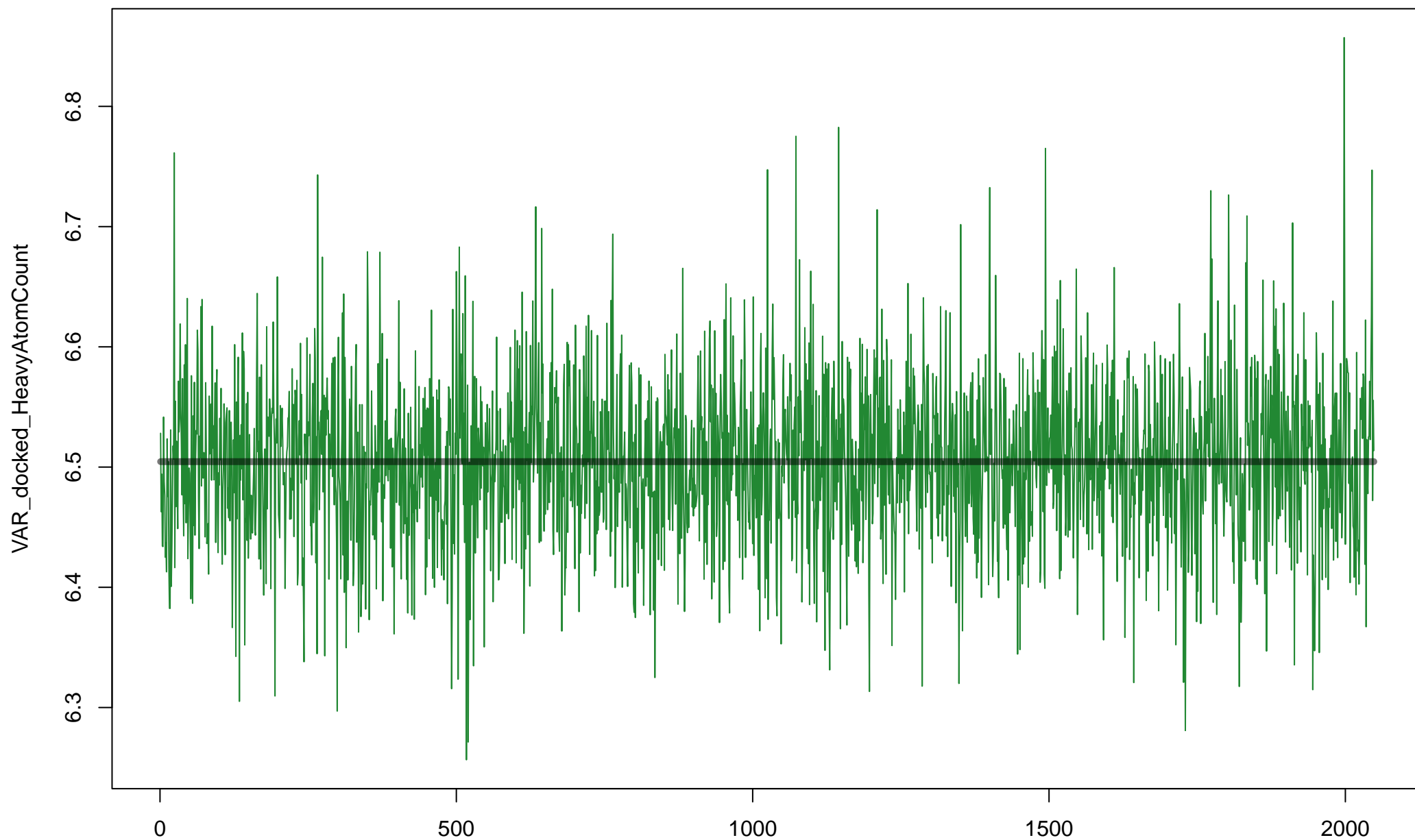
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: 1.31**



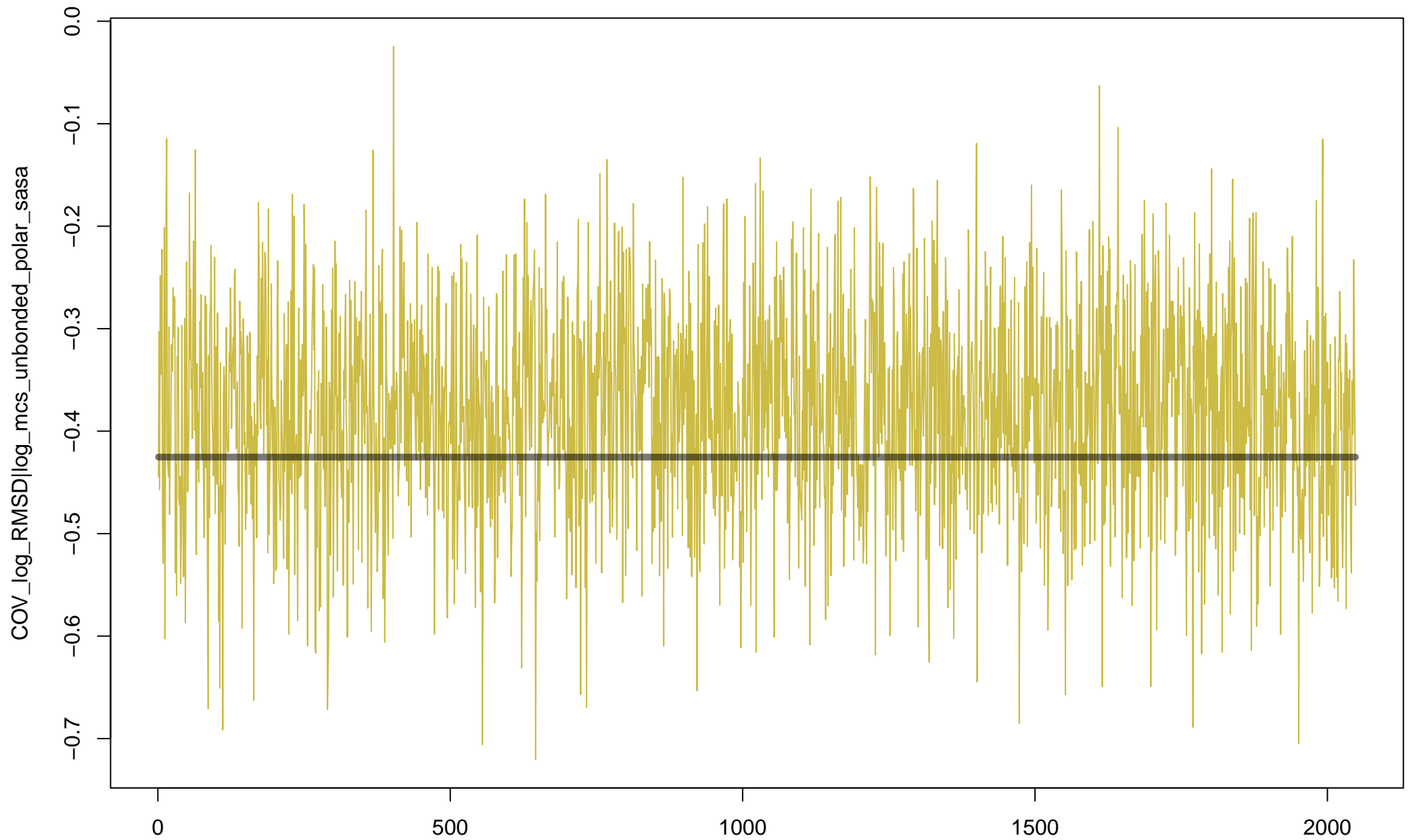
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1690 | BMK = 0.0673 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | rel.err: 0.403**



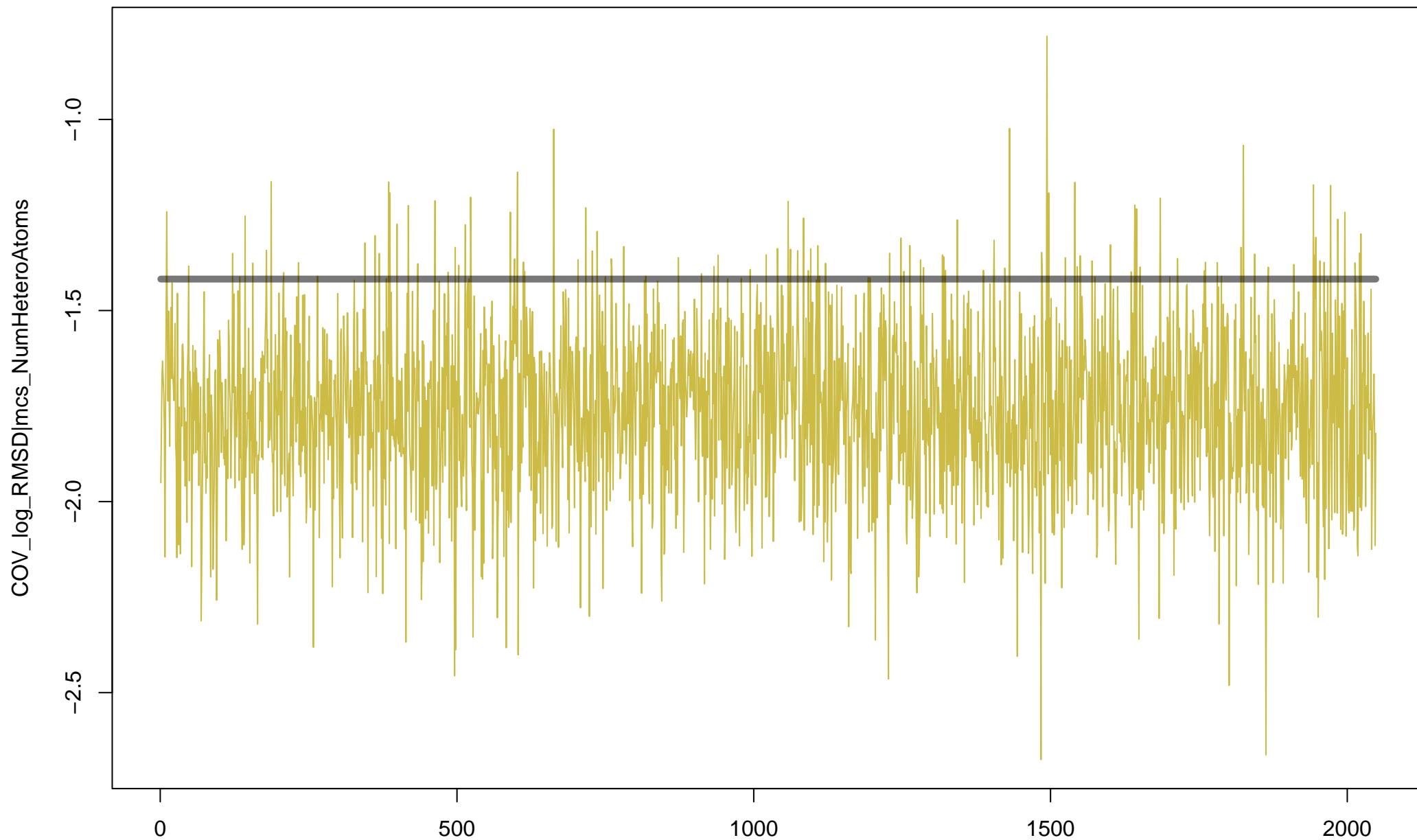
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0589 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.0354**



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1790 | BMK = 0.0319 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 0.45**

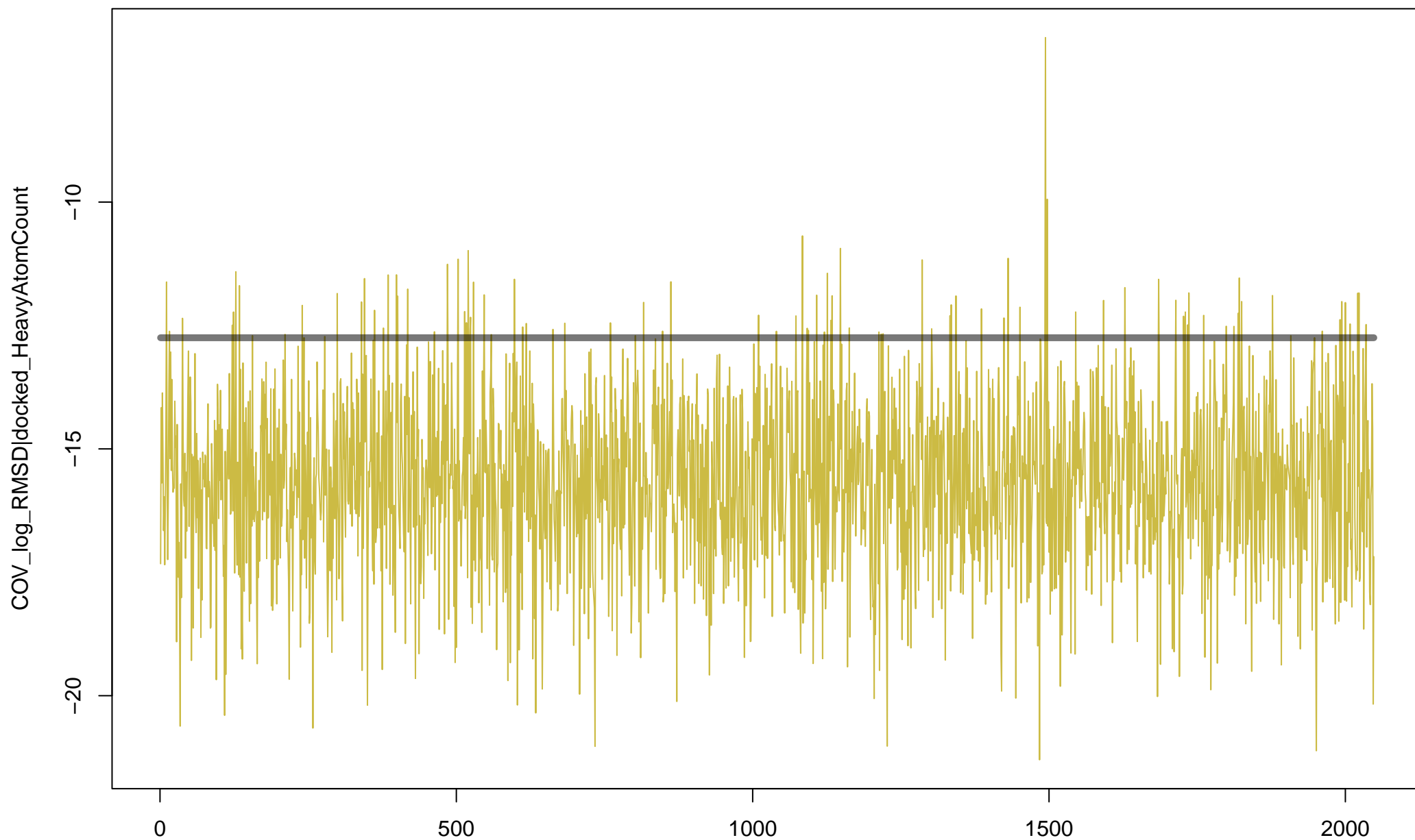


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 1920 | BMK = 0.0574 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: -1.57**

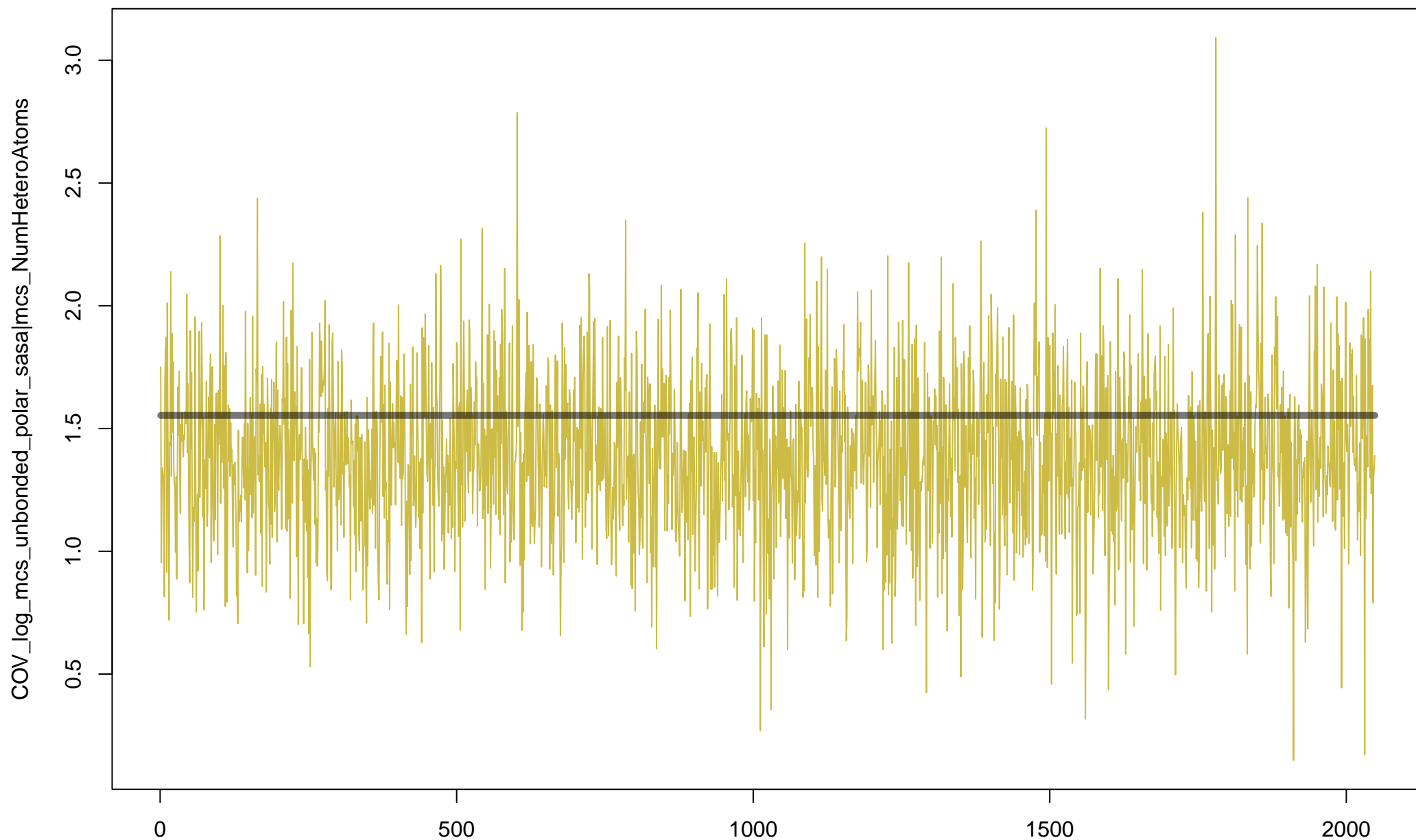




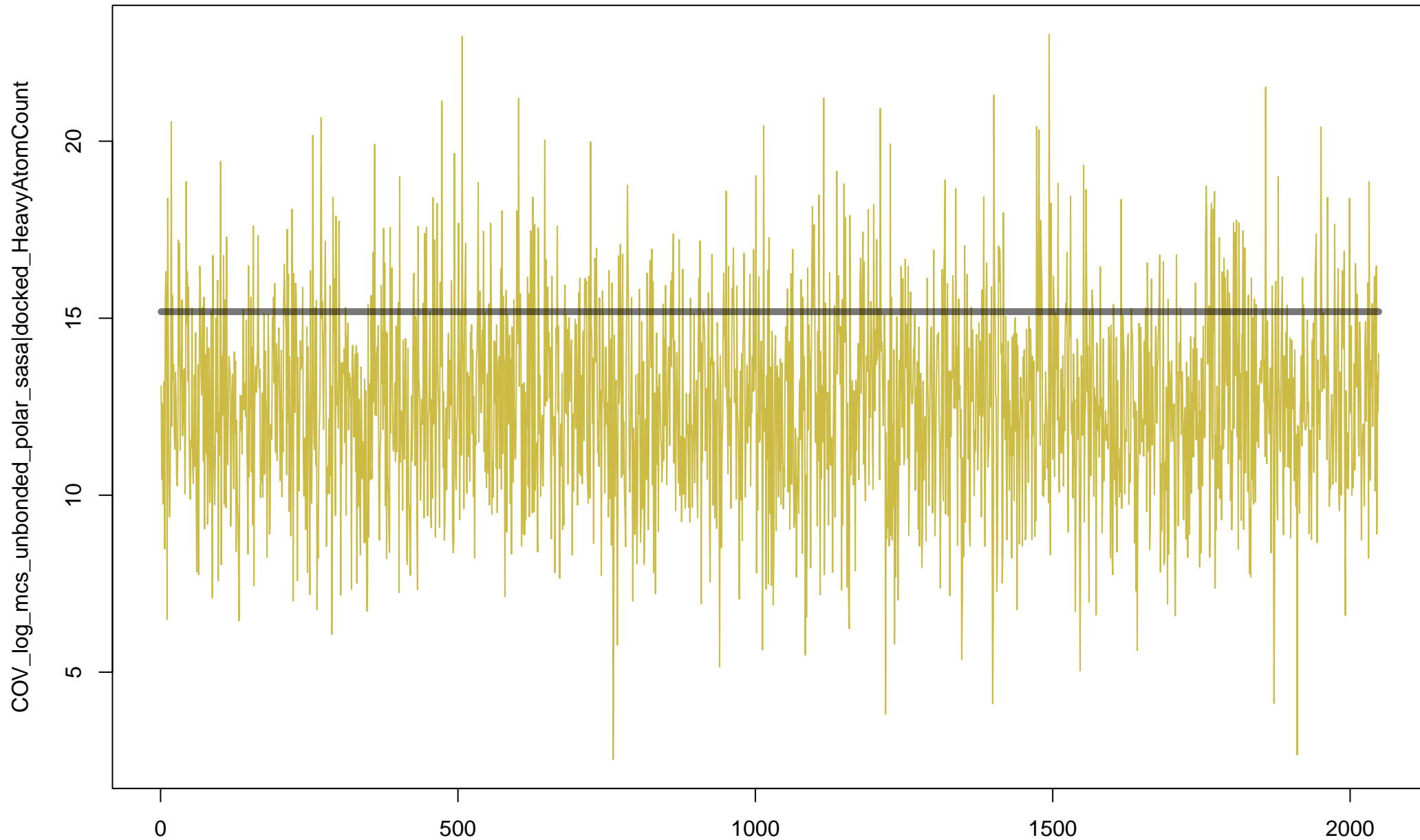
**COV\_log\_RMSD|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.04 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: -1.71**



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 1890 | BMK = 0.0554 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: -0.498**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 1890 | BMK = 0.0405 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: -0.941**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0561 | MCSE(6.27) = 1.84 | stat: TRUE | burn: 0 | rel.err: 0.482**

