

-- STATS maxD --

min ESS = 108.765609775025

max BMK = 0.137512011001492

max MCSE = 8.03189022073936

all stationary: FALSE

burn: 1020

max rel.err.: 2.1136644911418

-- STATS 1D --

min ESS = 1790.69521715505

max BMK = 0.0695611541961601

max MCSE = 2.54128107372164

all stationary: TRUE

burn: 0

max rel.err.: 2.21123148977364

-- STATS 2D --

min ESS = 1916.72737103099

max BMK = 0.0581595464574121

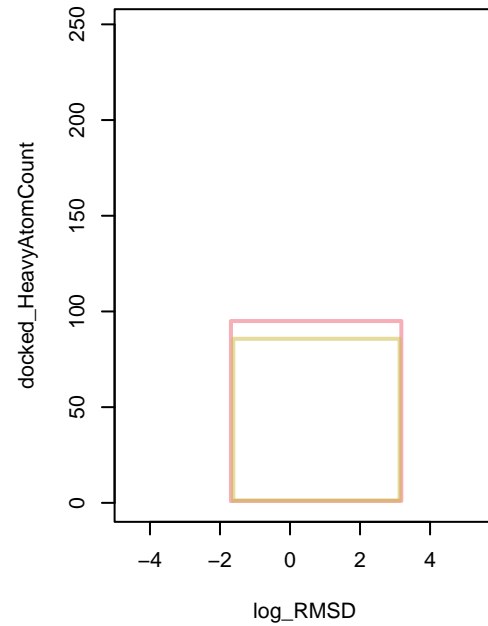
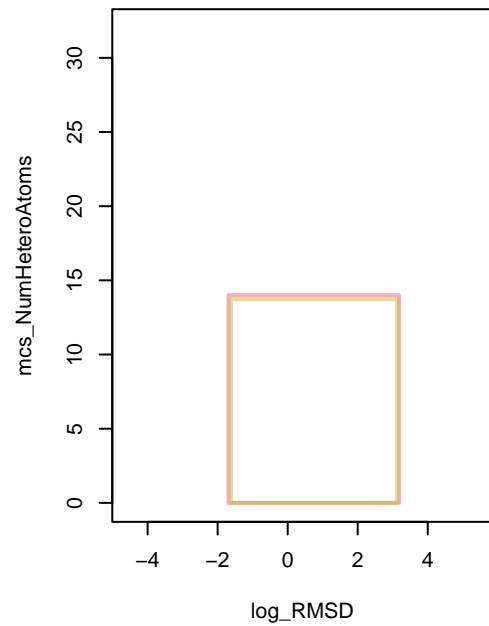
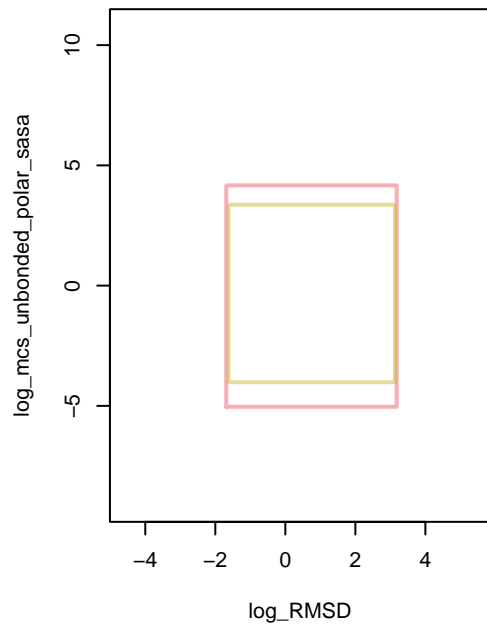
max MCSE = 2.61687902047623

all stationary: TRUE

burn: 0

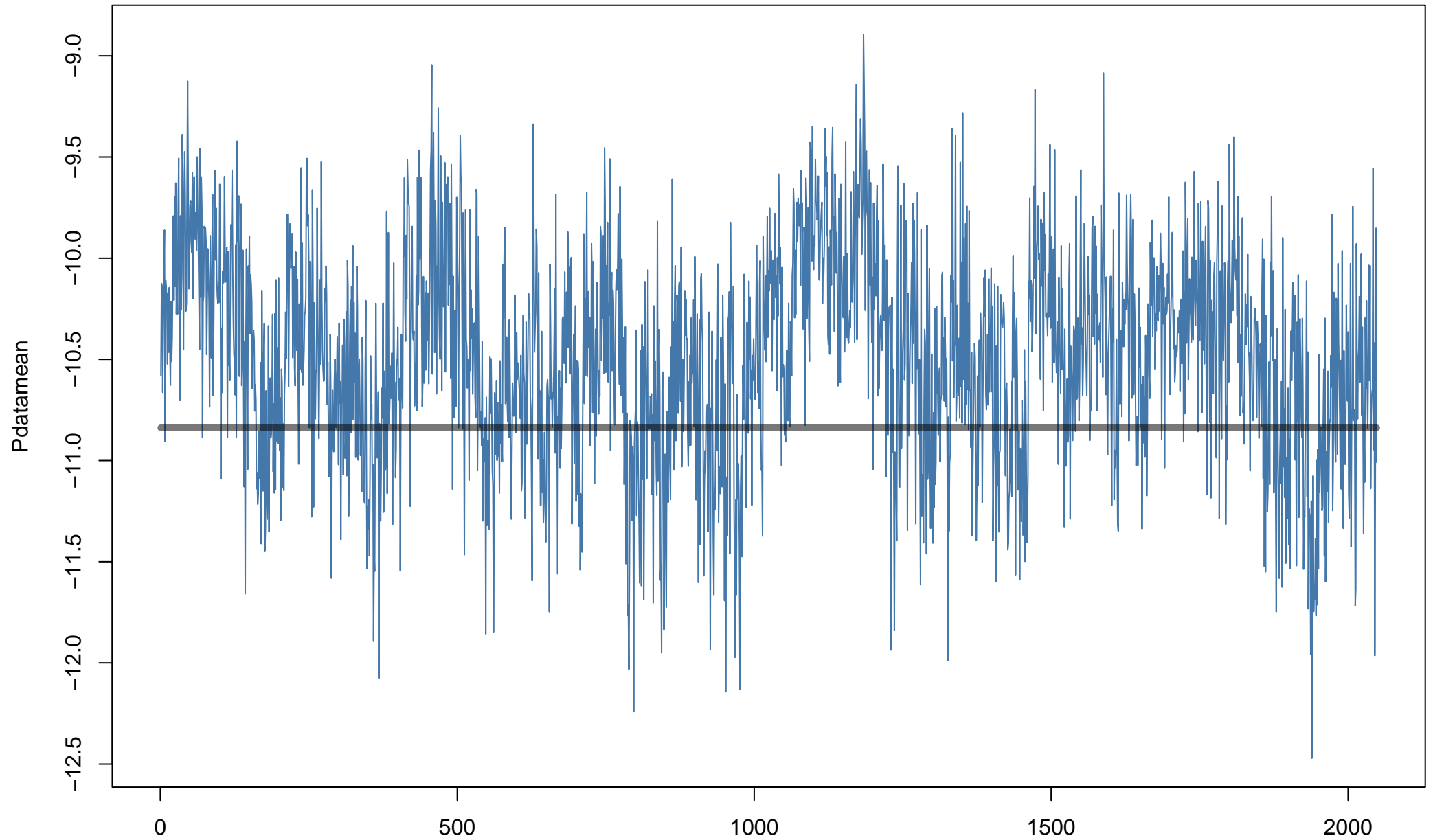
max rel.err.: 1.75695687850083

Occupied clusters: 9 of 16

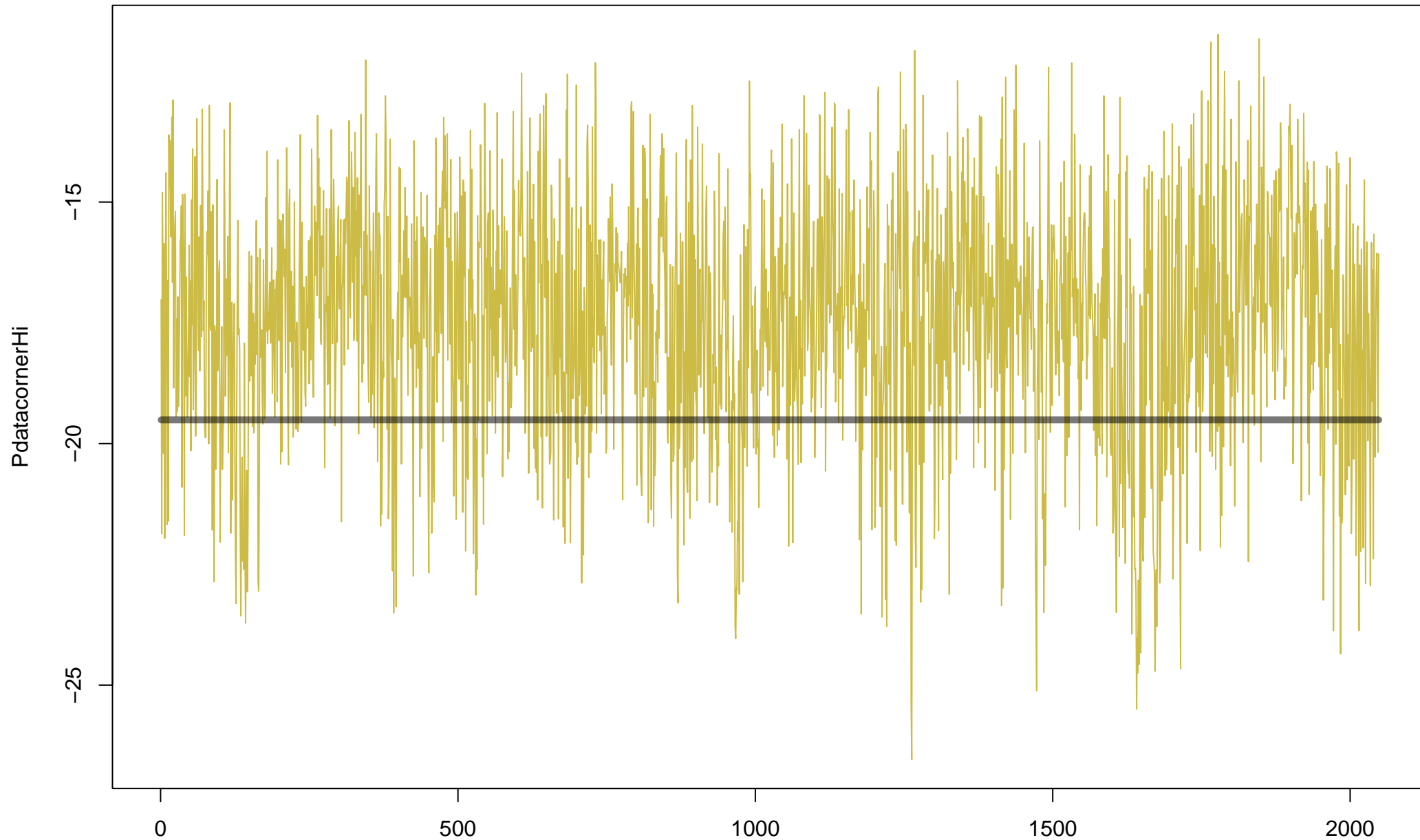


**Pdatamean**

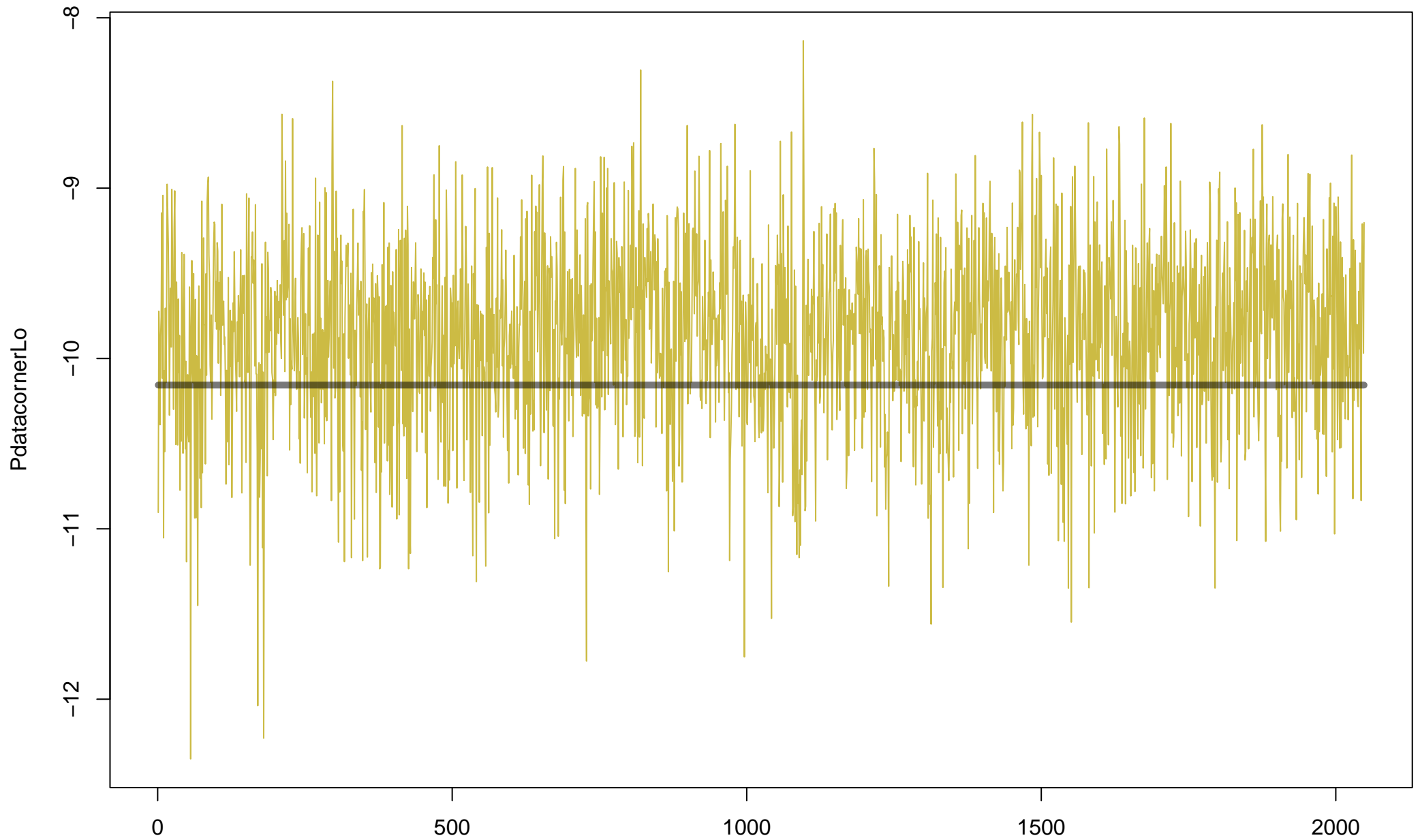
**ESS = 109 | BMK = 0.0769 | MCSE(6.27) = 8.03 | stat: TRUE | burn: 1020 | rel.err: 0.744**



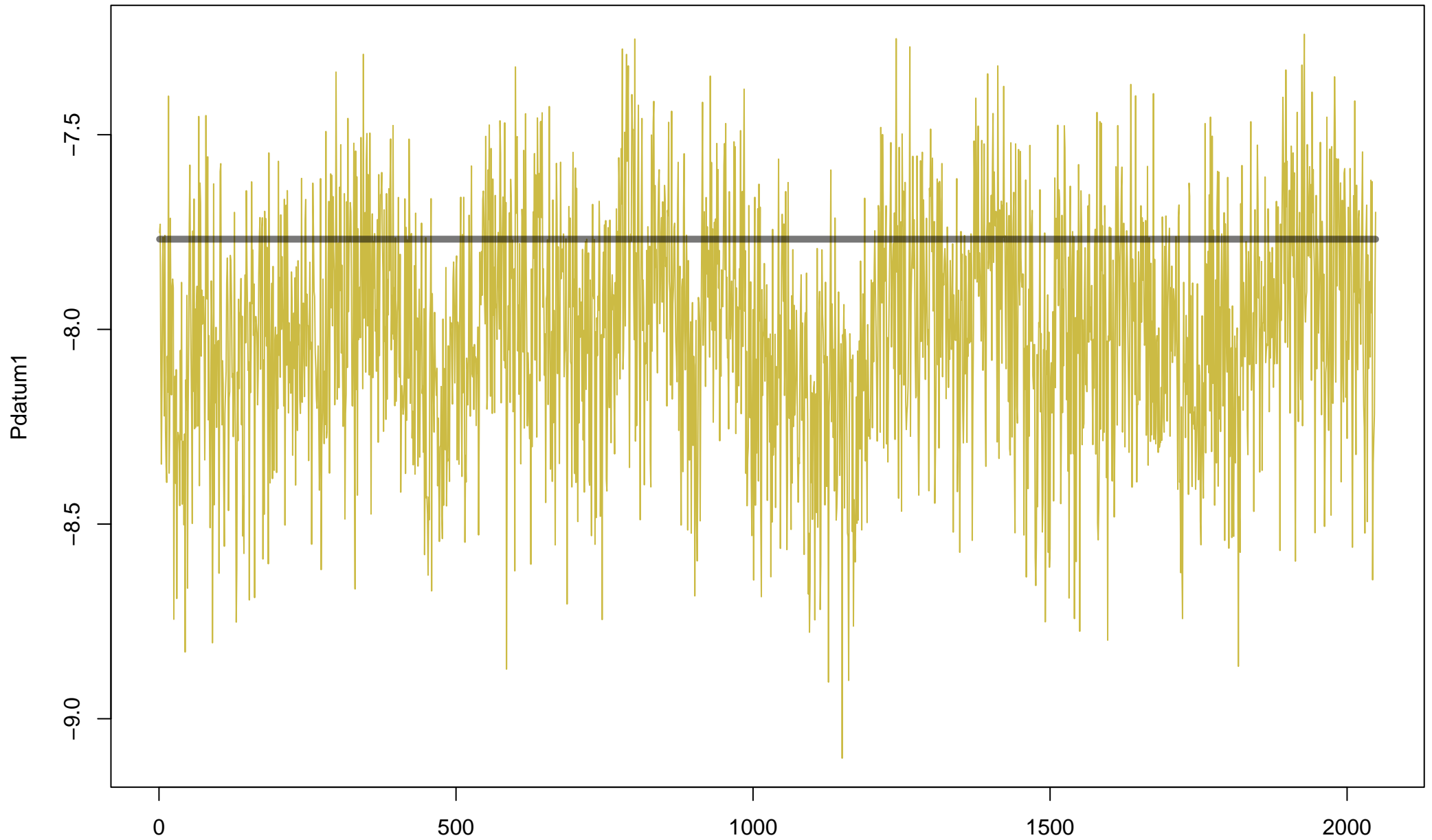
**PdatacornerHi**  
**ESS = 1400 | BMK = 0.138 | MCSE(6.27) = 2.66 | stat: FALSE | burn: 0 | rel.err: 0.333**



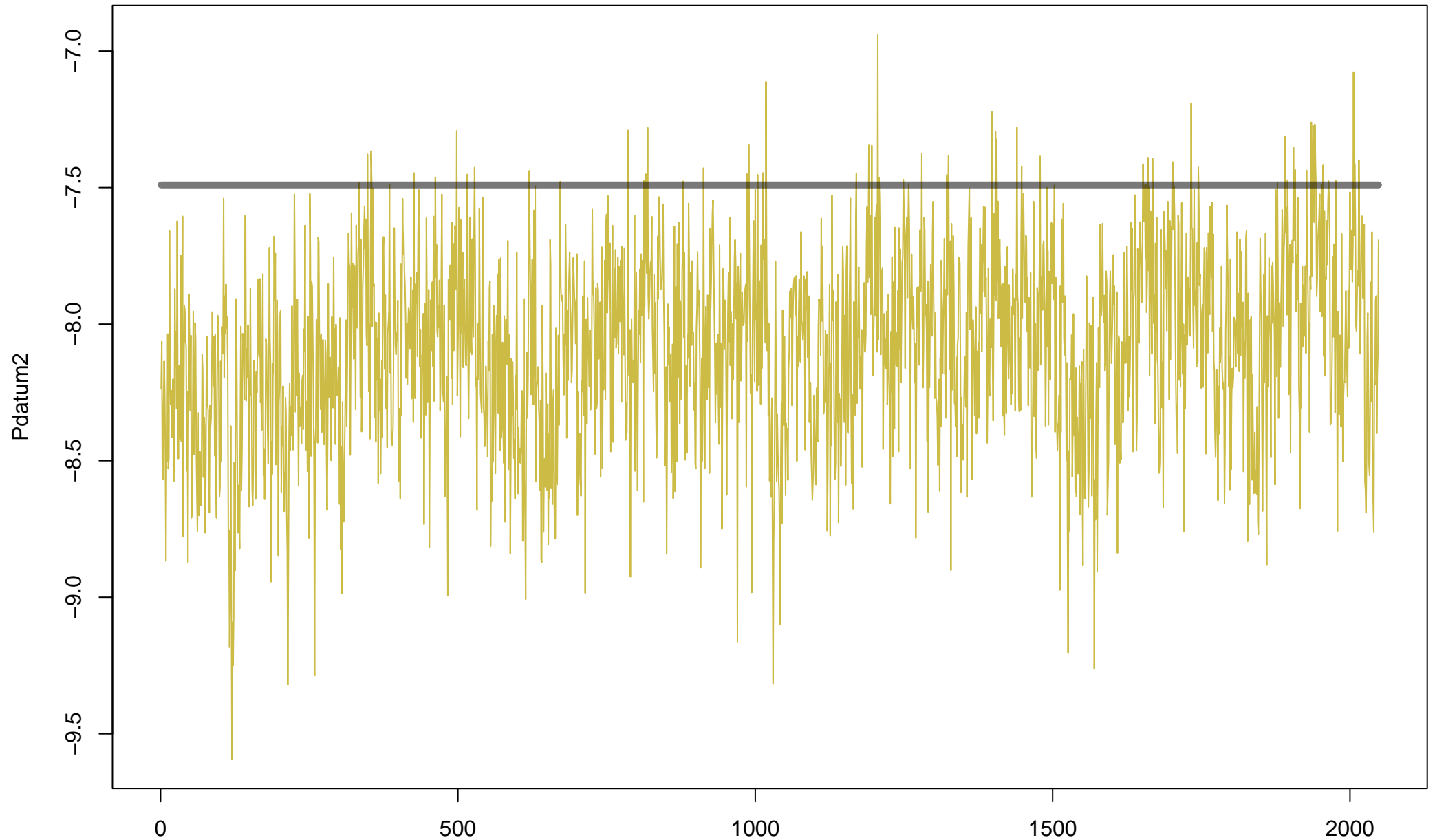
**PdatacornerLo**  
**ESS = 1680 | BMK = 0.0497 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: 0.656**



**Pdatum1**  
**ESS = 237 | BMK = 0.0322 | MCSE(6.27) = 5.68 | stat: FALSE | burn: 0 | rel.err: -0.734**

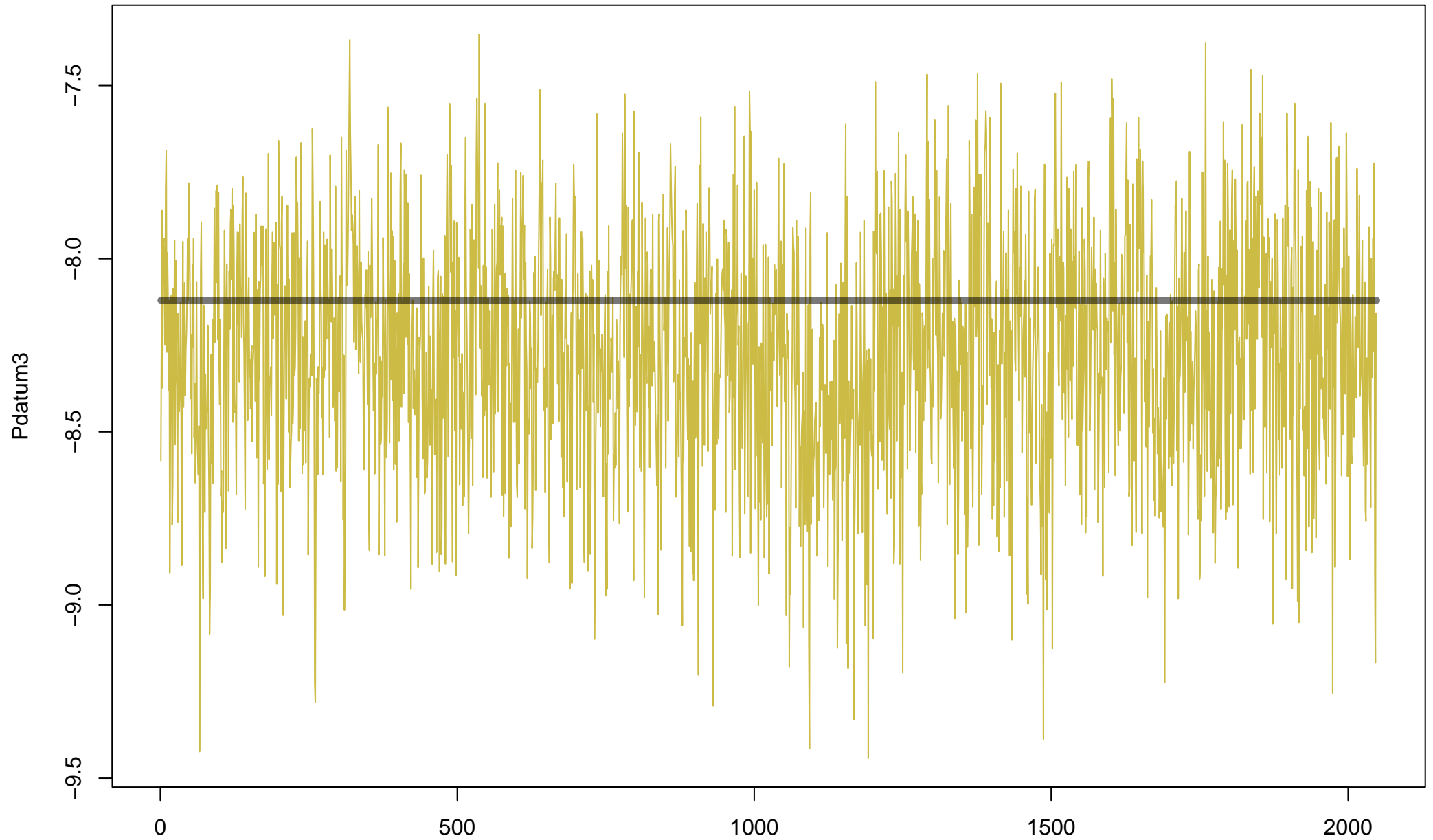


**Pdatum2**  
**ESS = 198 | BMK = 0.11 | MCSE(6.27) = 6.5 | stat: FALSE | burn: 0 | rel.err: -2.11**



**Pdatum3**

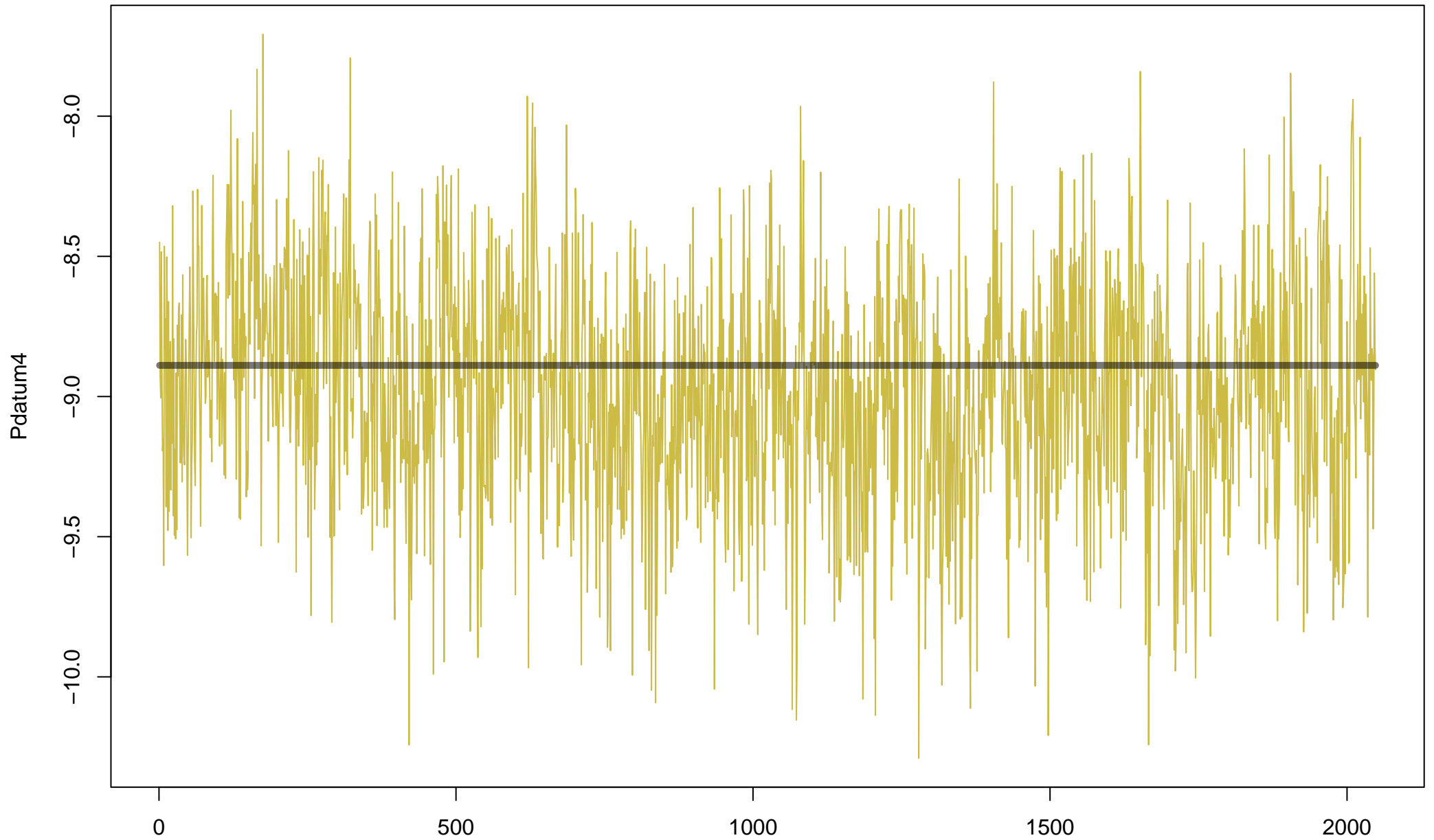
**ESS = 783 | BMK = 0.0583 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | rel.err: -0.297**





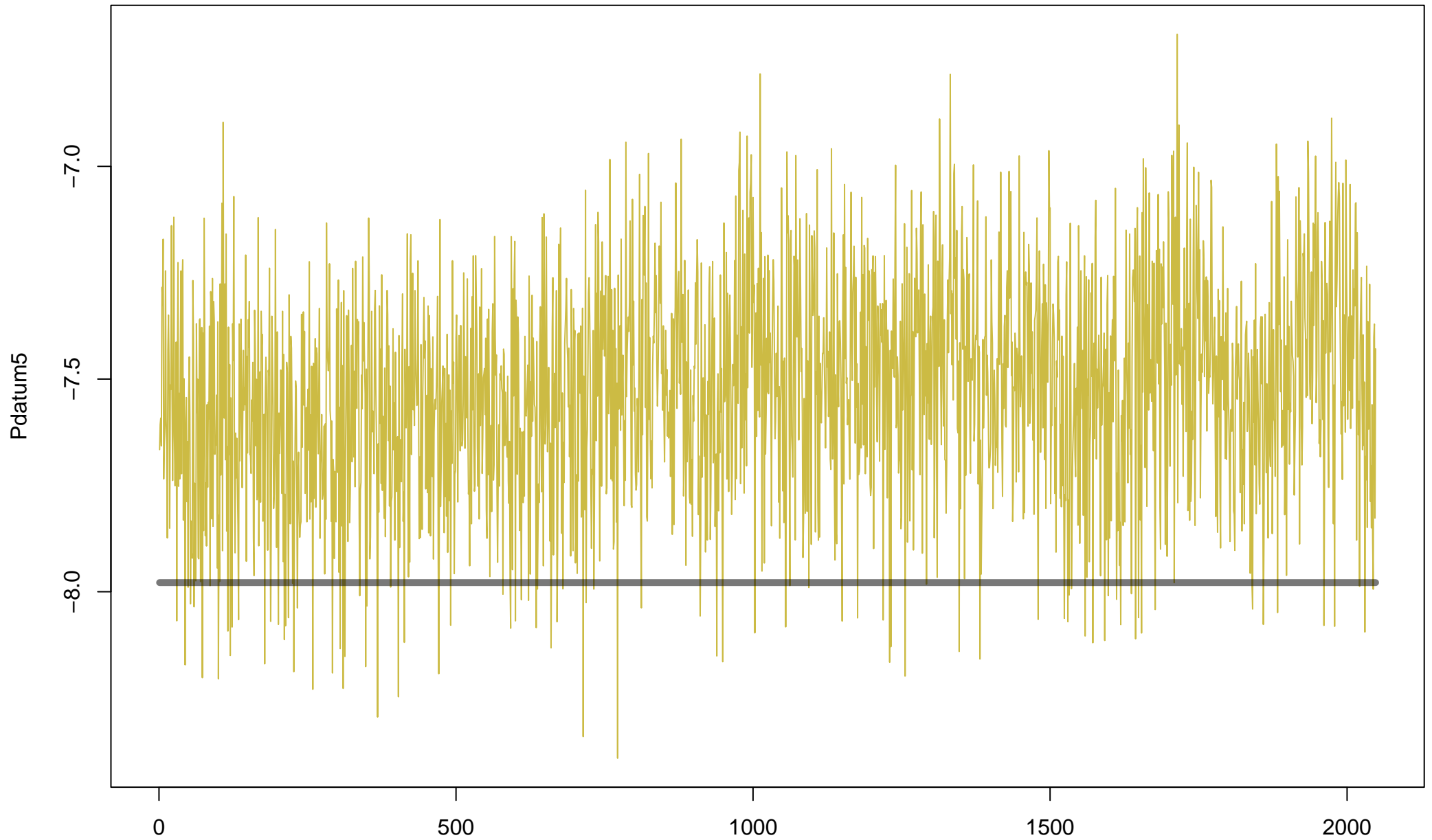
**Pdatum4**

**ESS = 539 | BMK = 0.072 | MCSE(6.27) = 4.78 | stat: FALSE | burn: 0 | rel.err: -0.0284**



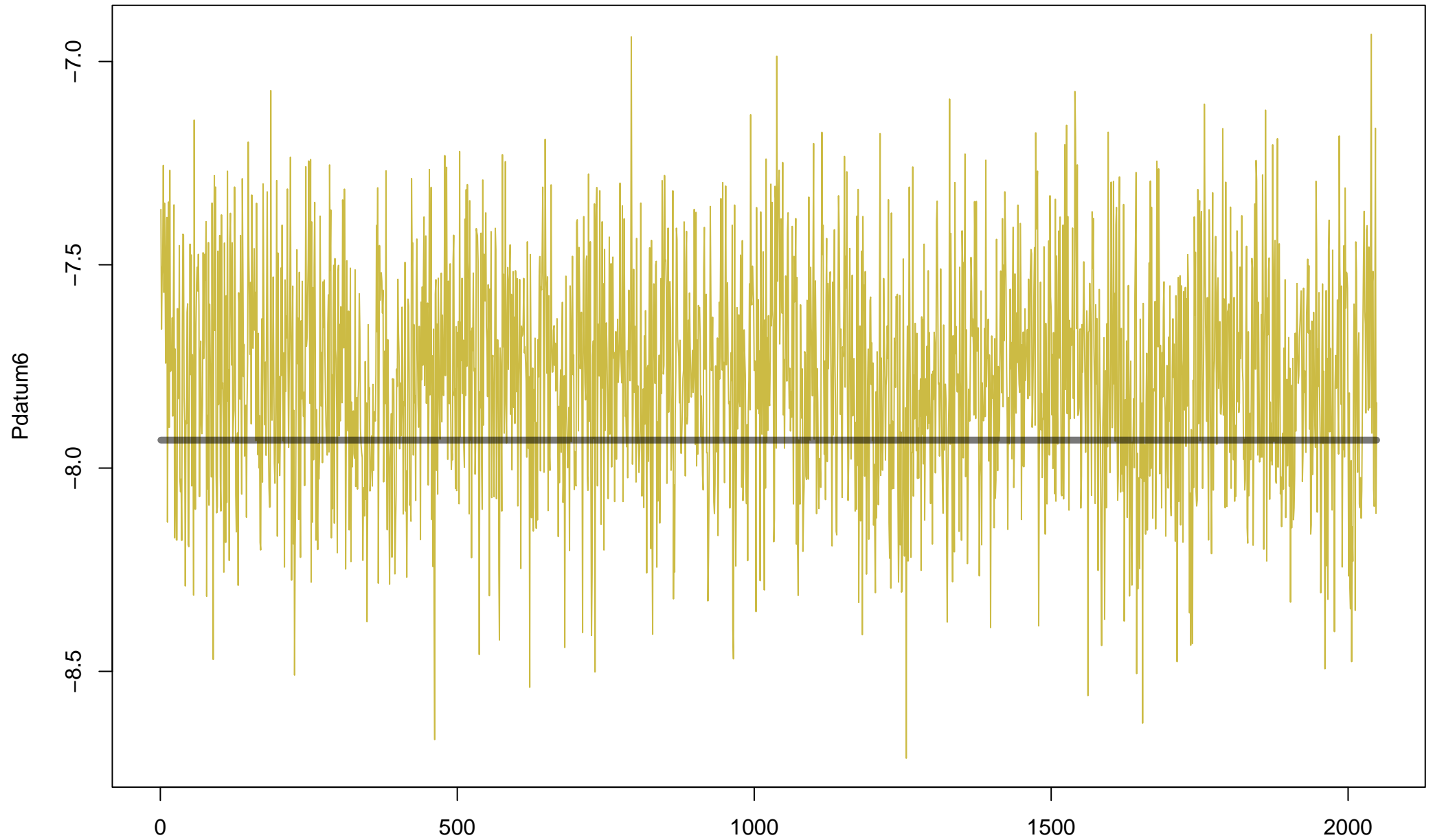
Pdatum5

ESS = 196 | BMK = 0.13 | MCSE(6.27) = 4.65 | stat: FALSE | burn: 0 | rel.err: 1.51



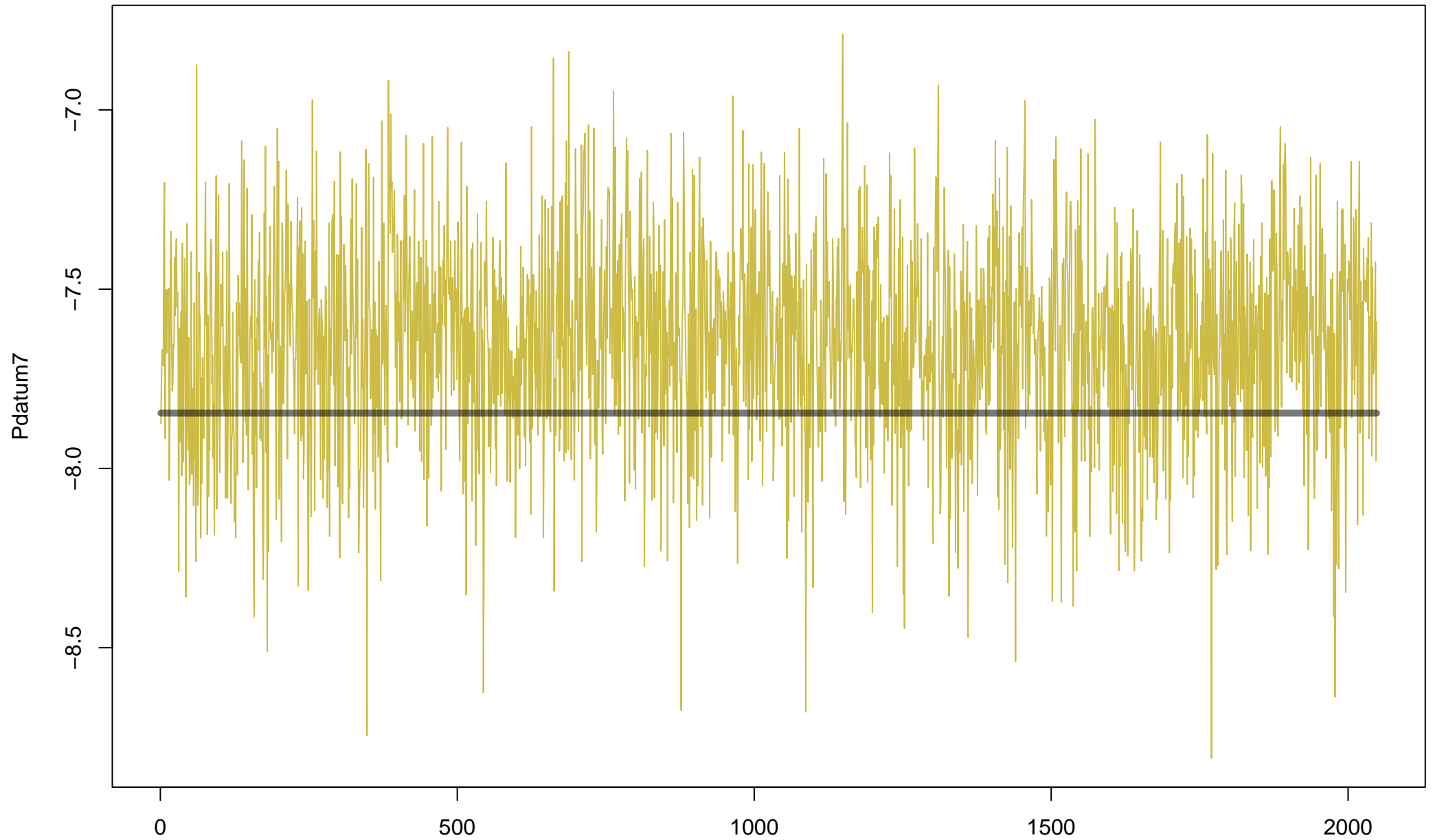
**Pdatum6**

**ESS = 1350 | BMK = 0.0499 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: 0.645**

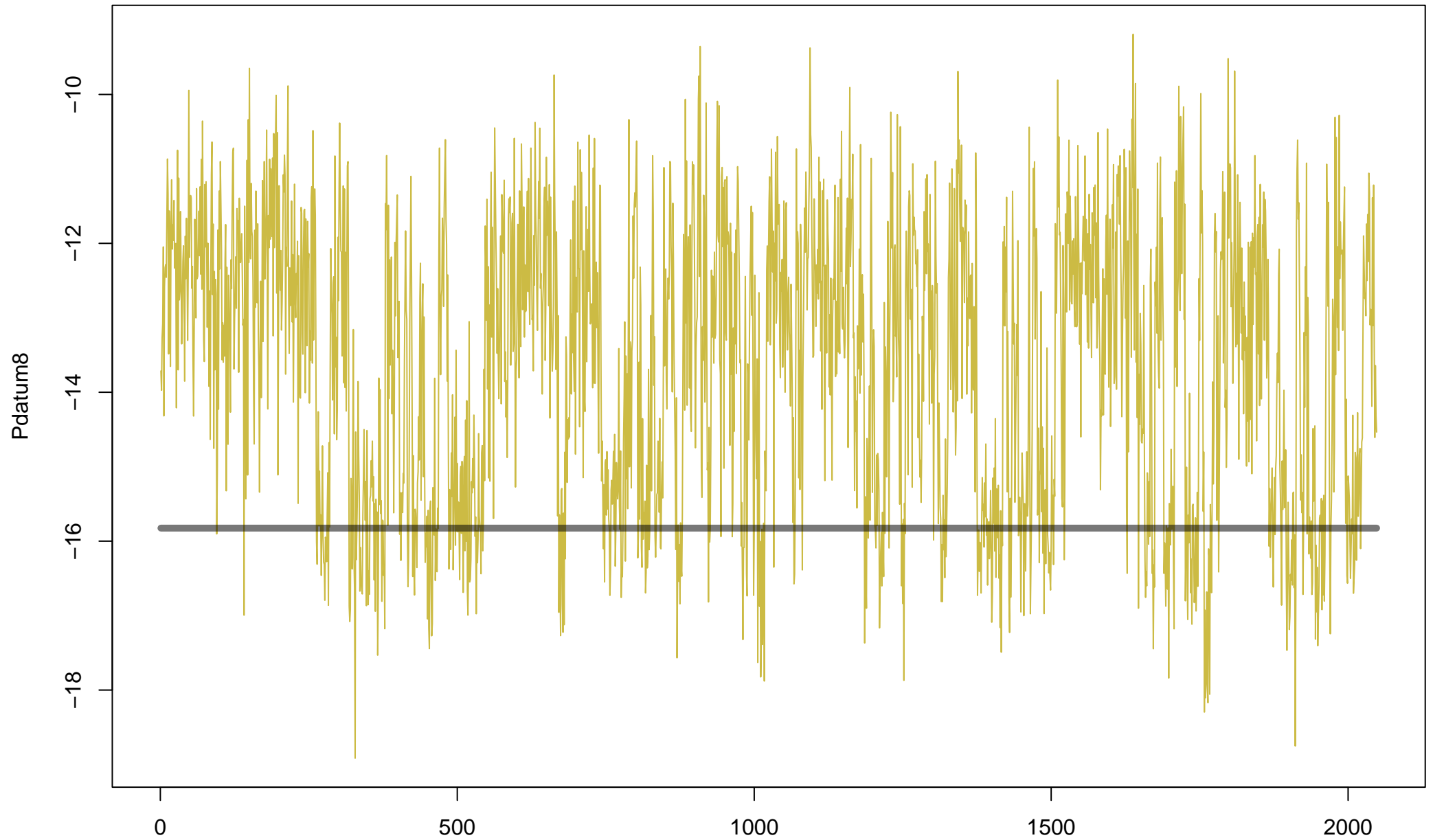


**Pdatum7**

**ESS = 1400 | BMK = 0.0494 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0 | rel.err: 0.748**

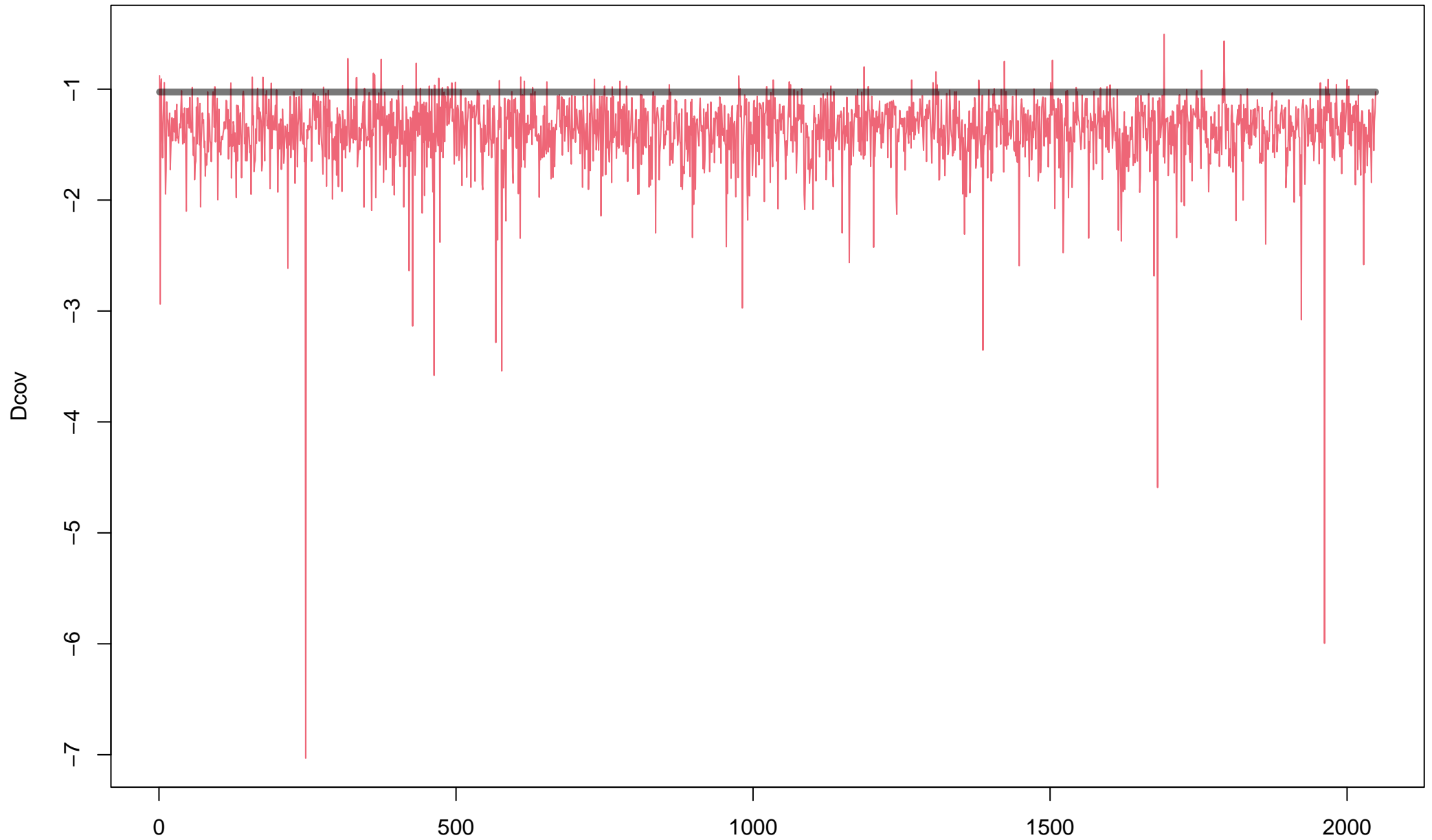


**Pdatum8**  
**ESS = 673 | BMK = 0.0872 | MCSE(6.27) = 4.3 | stat: FALSE | burn: 0 | rel.err: 0.542**

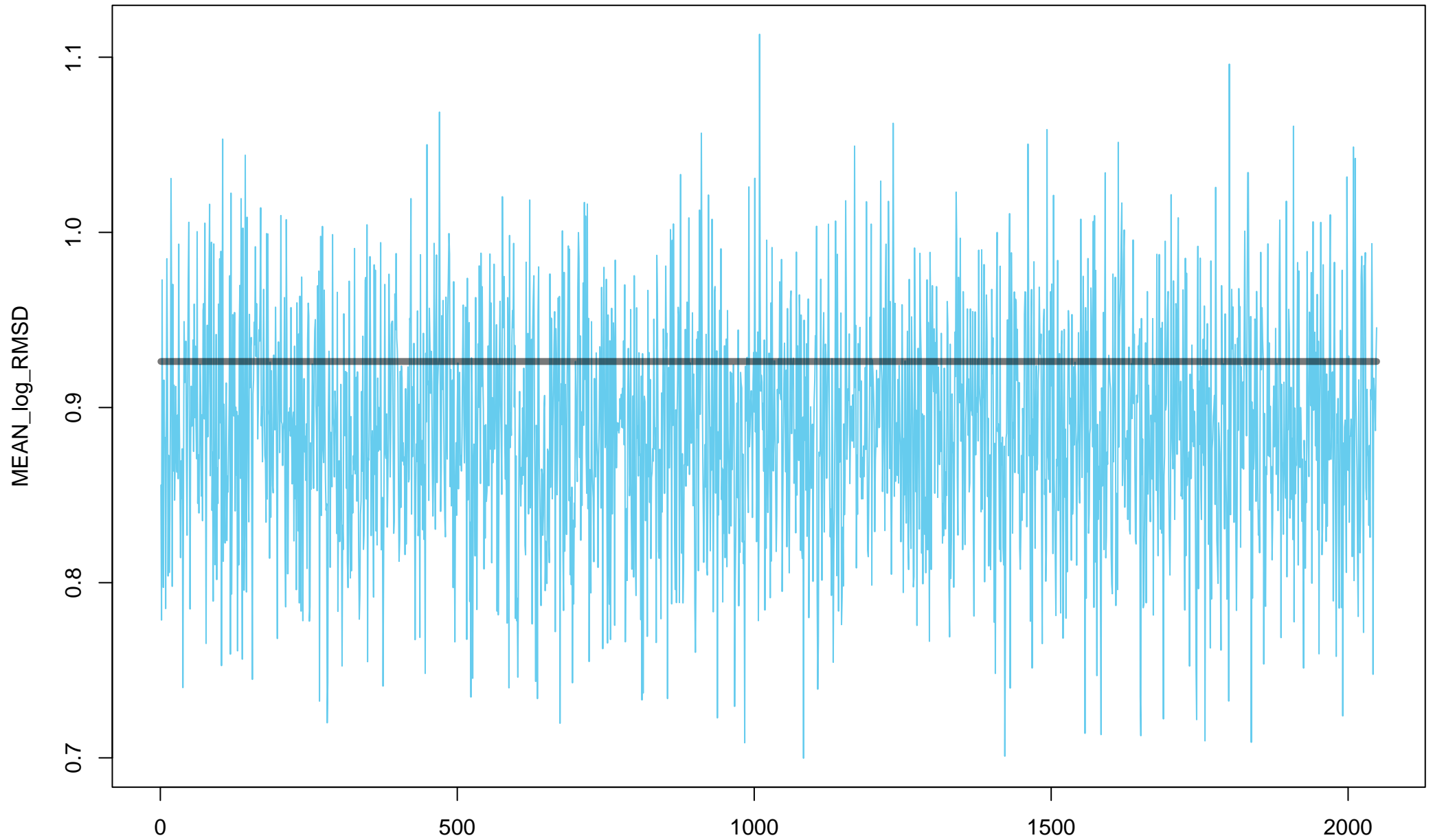


Dcov

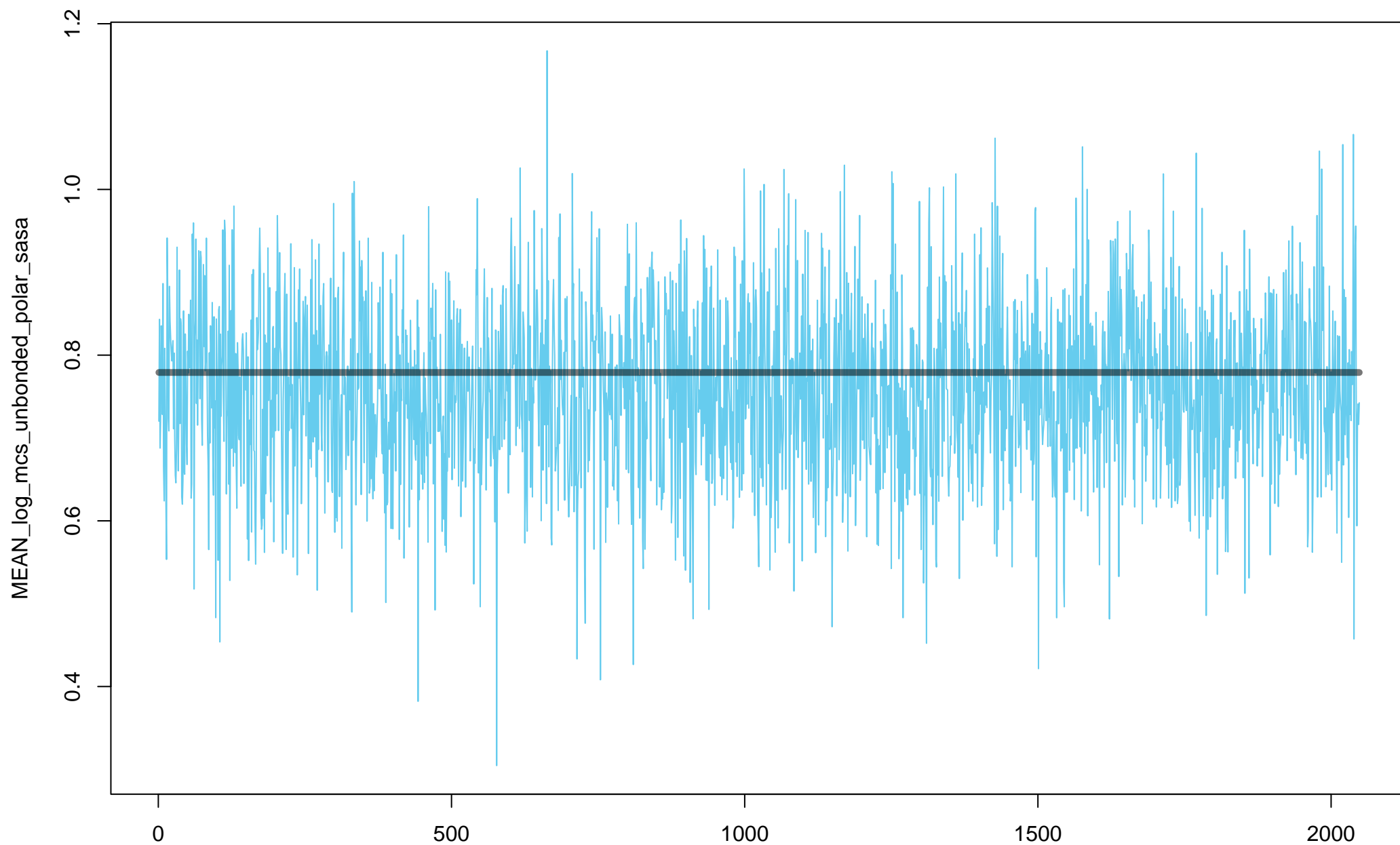
ESS = 1740 | BMK = 0.0662 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: 1.51



**MEAN\_log\_RMSD**  
**ESS = 2050 | BMK = 0.036 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: -0.616**



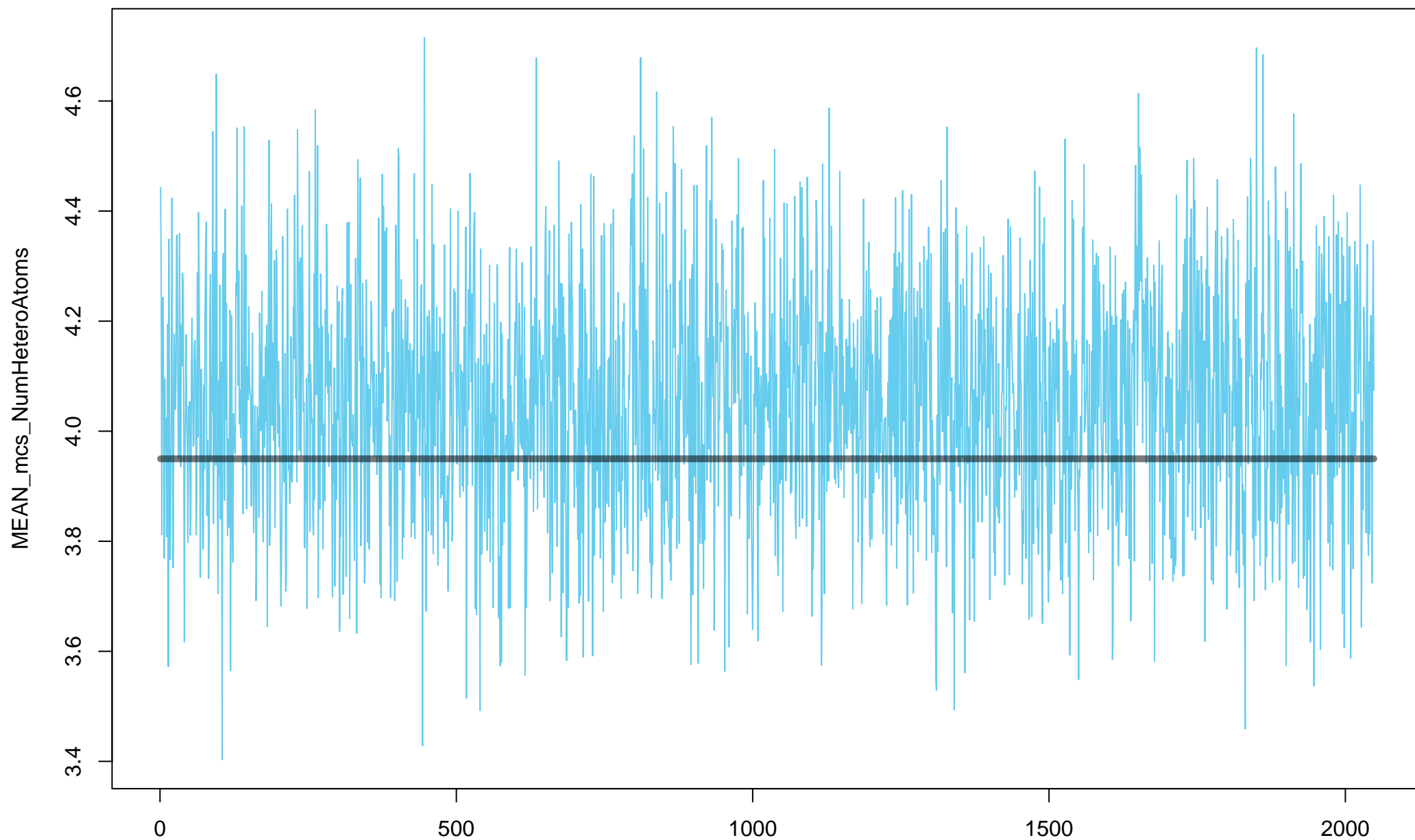
**MEAN\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0618 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: -0.206**



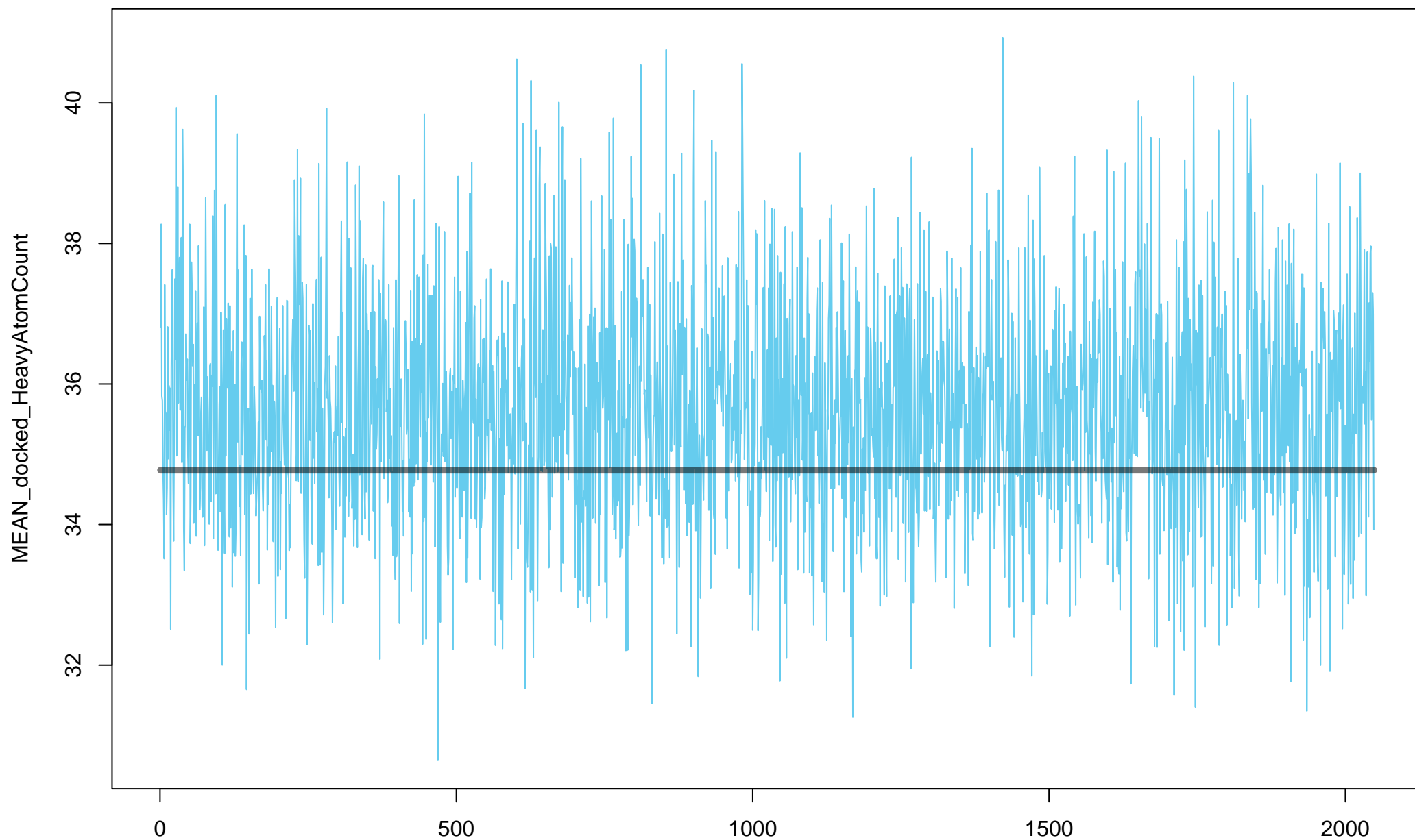


# MEAN\_mcs\_NumHeteroAtoms

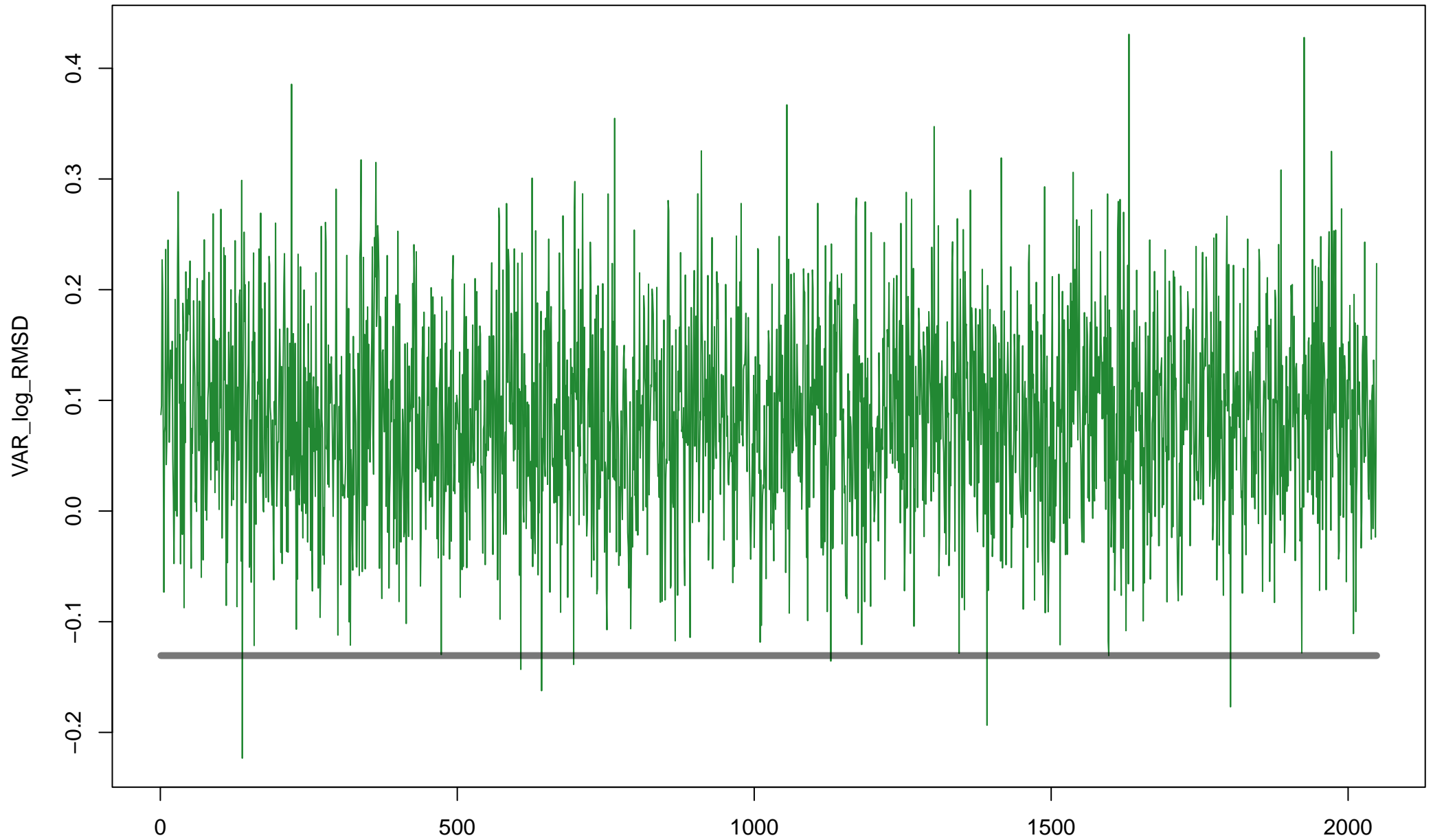
ESS = 1880 | BMK = 0.0431 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.489



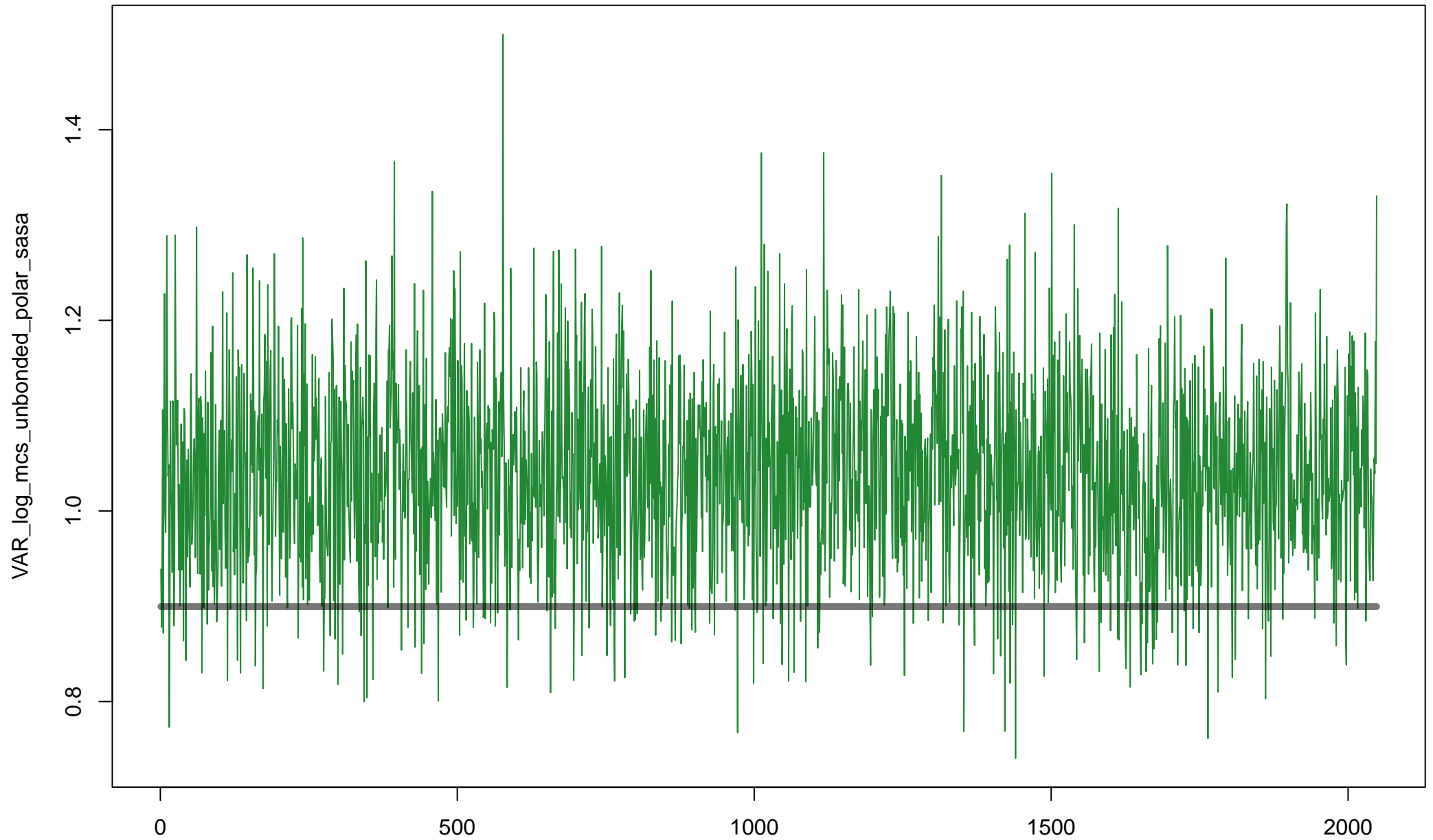
**MEAN\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0366 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0 | rel.err: 0.541**



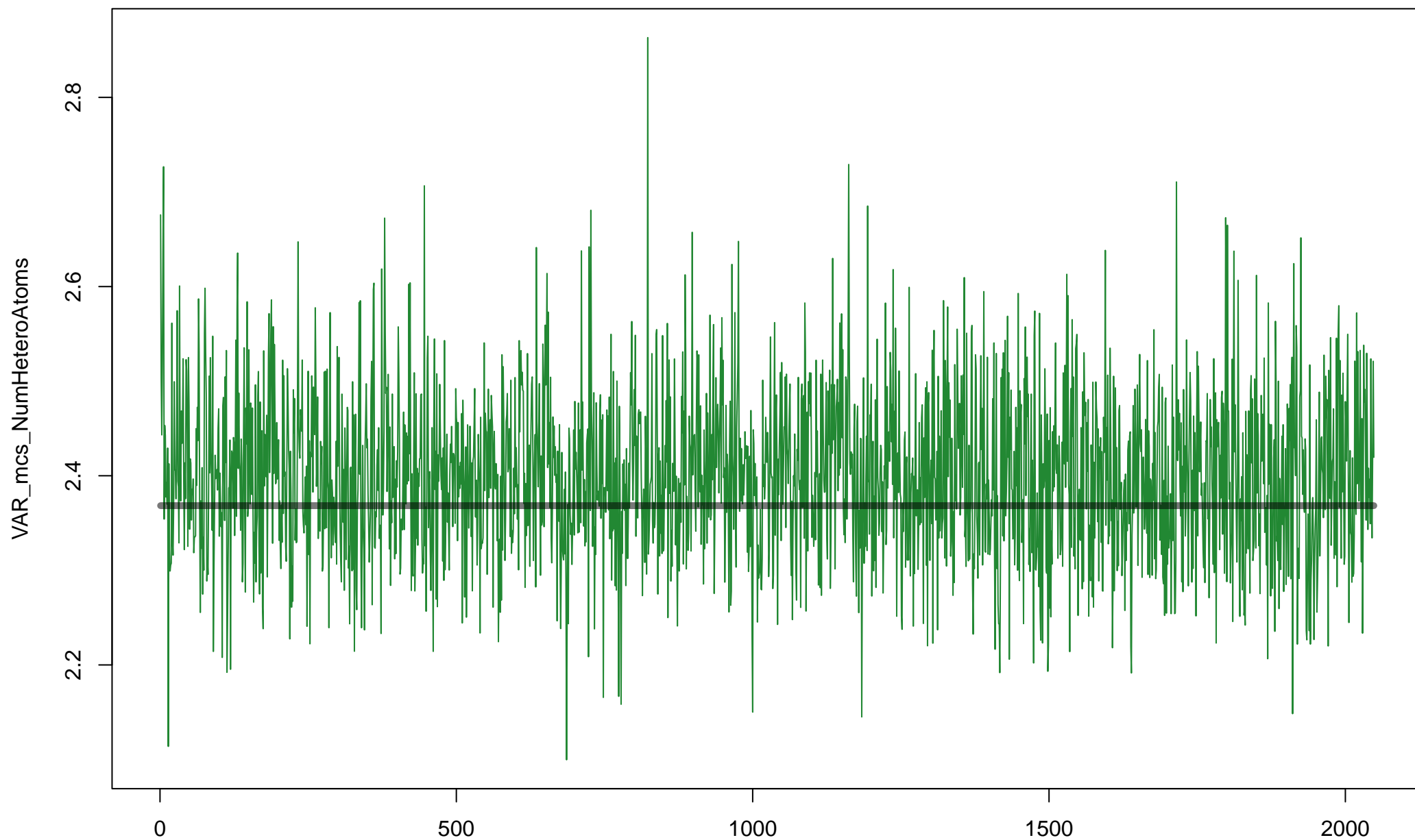
**VAR\_log\_RMSD**  
**ESS = 2050 | BMK = 0.0385 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 2.21**



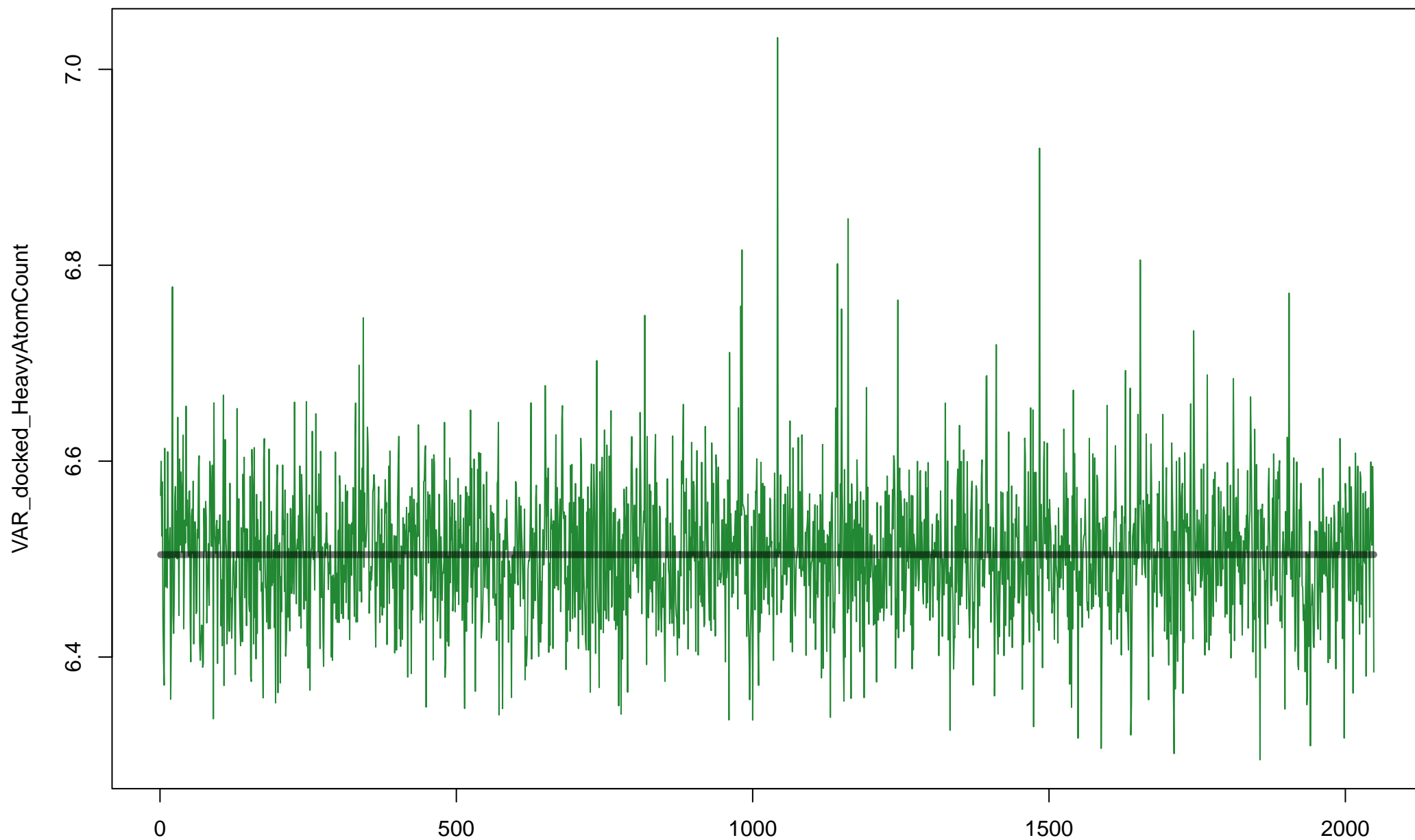
**VAR\_log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 2050 | BMK = 0.0435 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: 1.34**



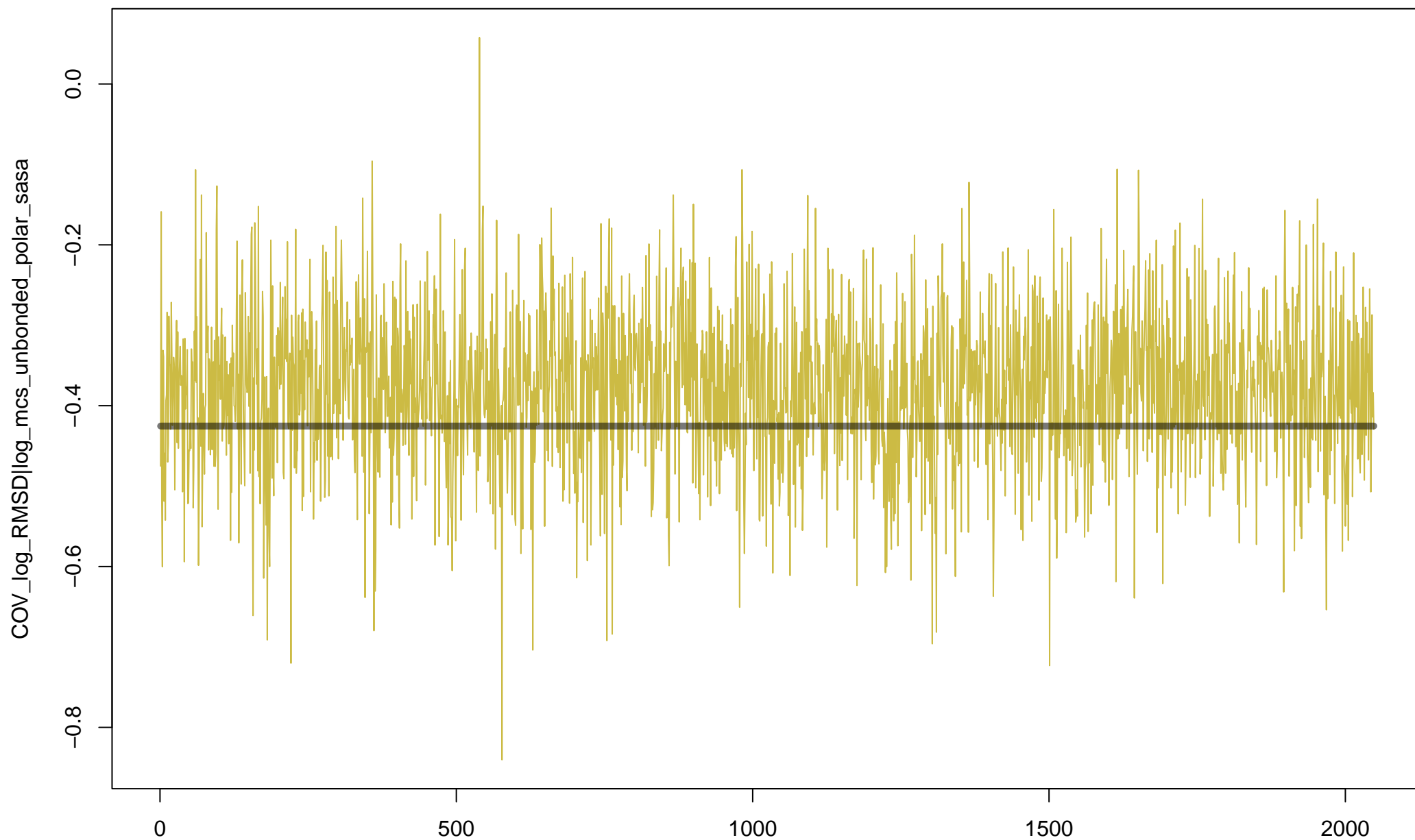
**VAR\_mcs\_NumHeteroAtoms**  
**ESS = 1790 | BMK = 0.0658 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: 0.391**



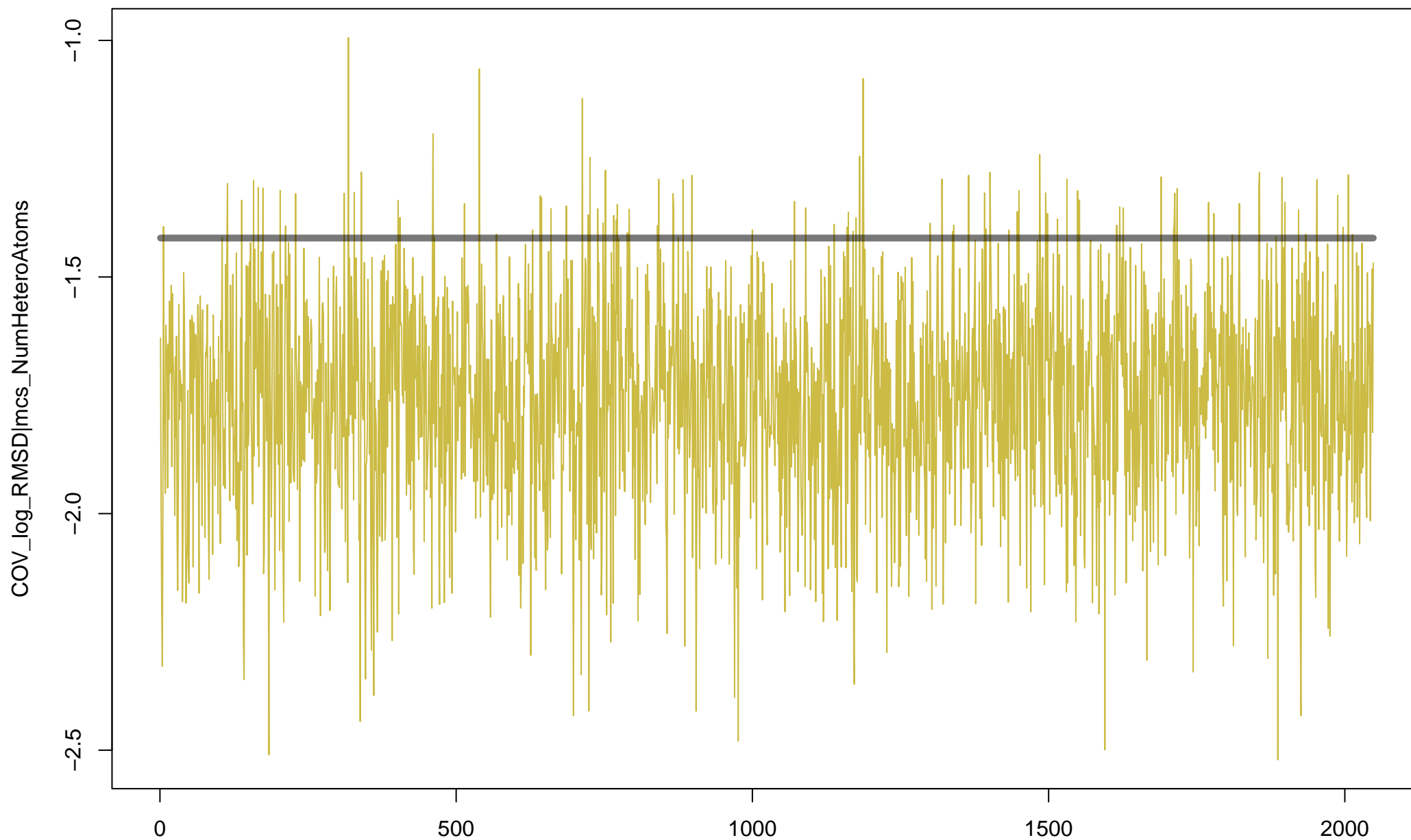
**VAR\_docked\_HeavyAtomCount**  
**ESS = 2050 | BMK = 0.0696 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: 0.0482**



**COV\_log\_RMSD|log\_mcs\_unbonded\_polar\_sasa**  
**ESS = 1920 | BMK = 0.0412 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: 0.478**

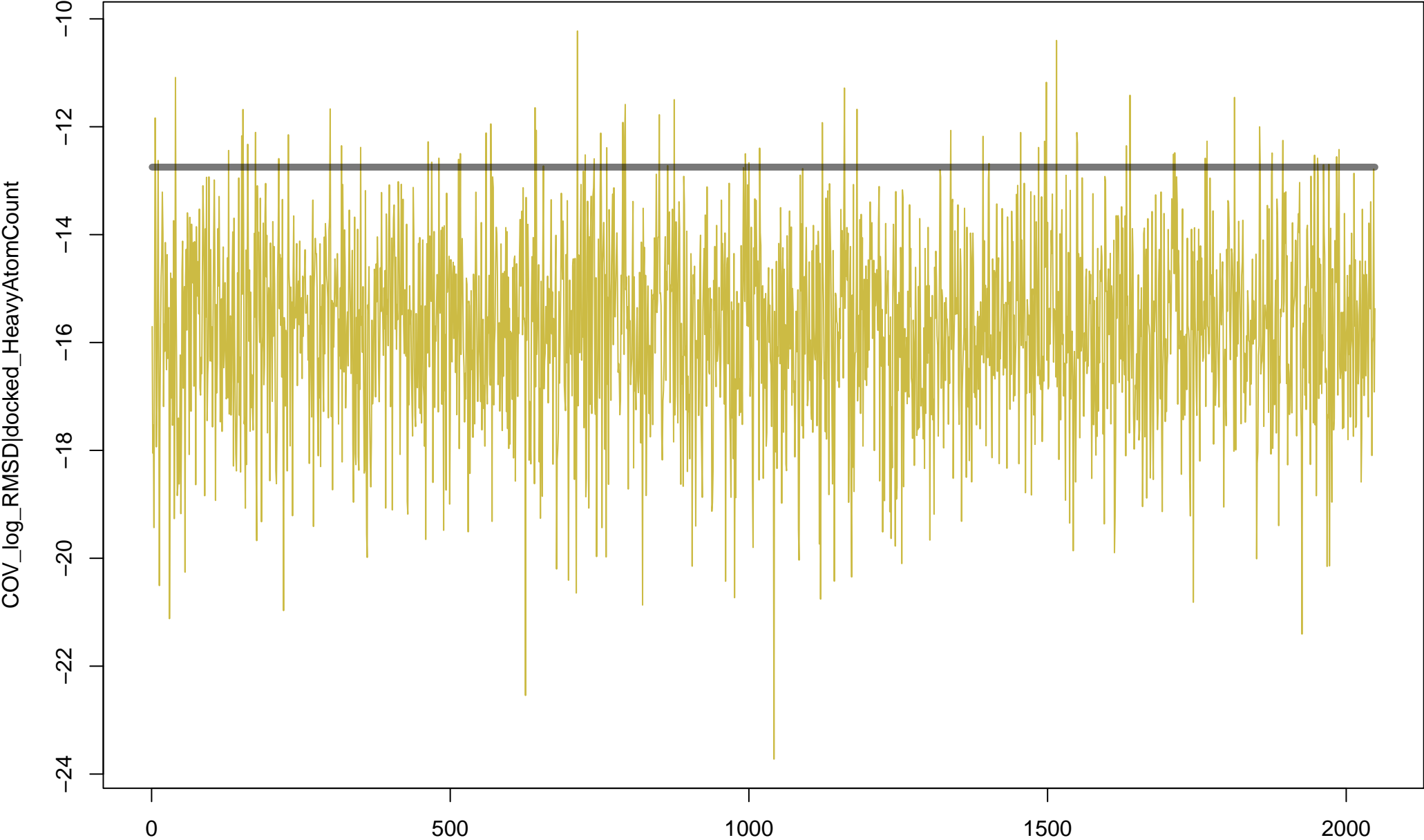


**COV\_log\_RMSD|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0414 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: -1.58**

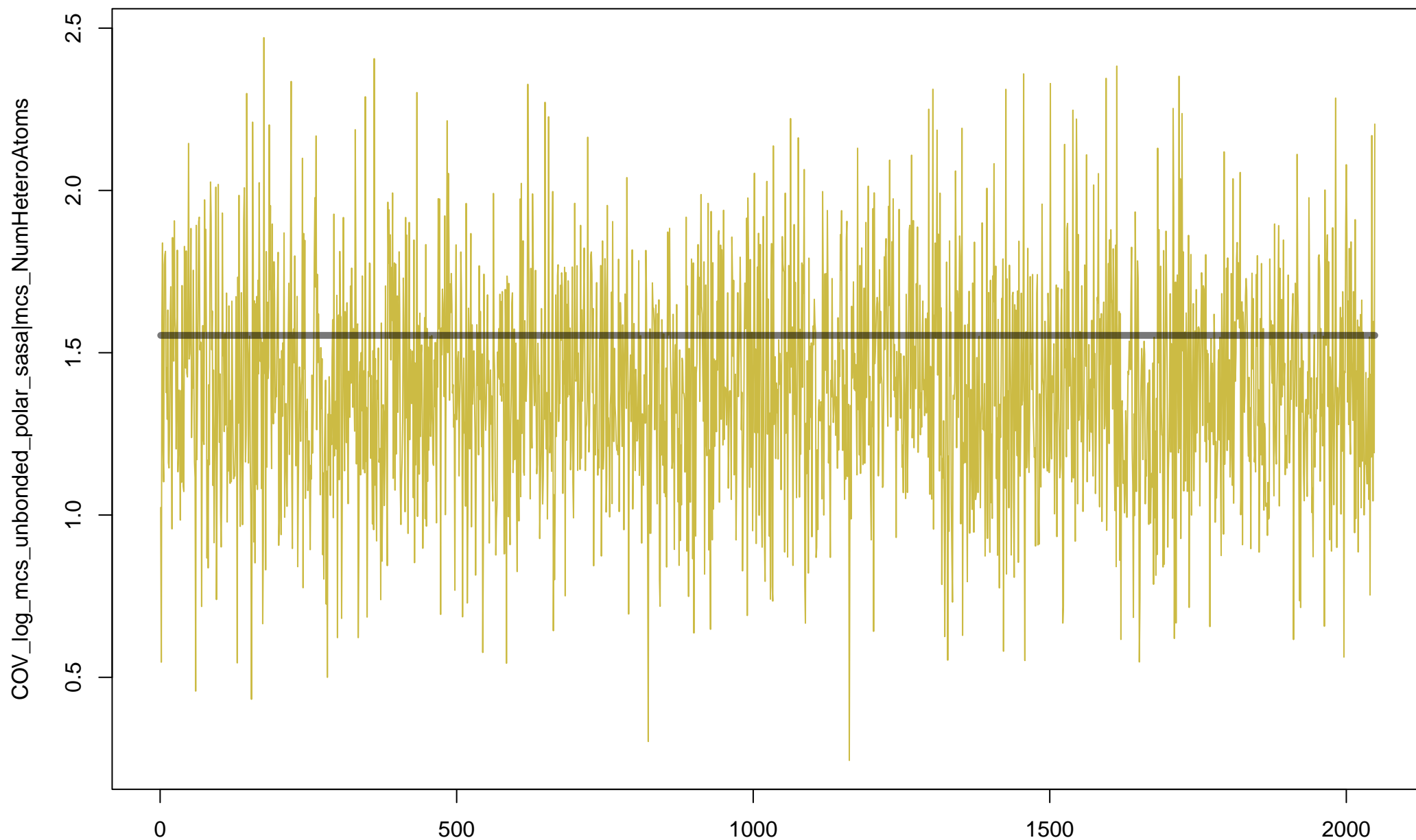




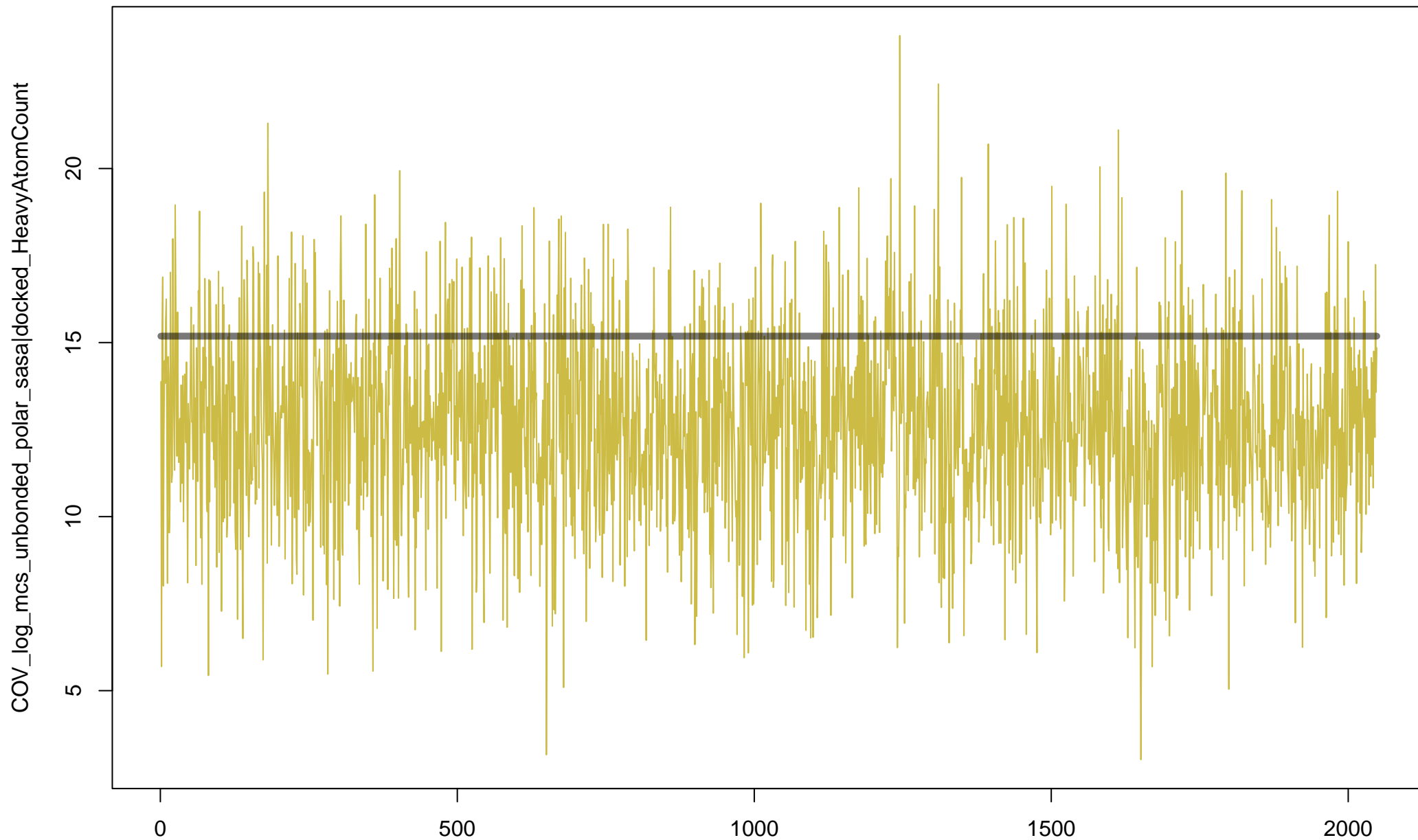
COV\_log\_RMSD|docked\_HeavyAtomCount  
ESS = 2050 | BMK = 0.0582 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: -1.76



**COV\_log\_mcs\_unbonded\_polar\_sasa|mcs\_NumHeteroAtoms**  
**ESS = 2050 | BMK = 0.0358 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: -0.481**



**COV\_log\_mcs\_unbonded\_polar\_sasa|docked\_HeavyAtomCount**  
**ESS = 2030 | BMK = 0.0512 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: -0.953**



**COV\_mcs\_NumHeteroAtoms|docked\_HeavyAtomCount**  
**ESS = 2030 | BMK = 0.0427 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | rel.err: 0.469**

