

-- STATS maxD --

min ESS = 32.6777567574303

max BMK = 0.142015728431028

max MCSE = 9.53123931156102

all stationary: FALSE

burn: 0

max rel.err.: 2.0828620694634

-- STATS 1D --

min ESS = 1723.10656182148

max BMK = 0.0543845527140145

max MCSE = 2.75065109557334

all stationary: TRUE

burn: 0

max rel.err.: 2.29931156305789

-- STATS 2D --

min ESS = 1858.32062554992

max BMK = 0.0621872587253959

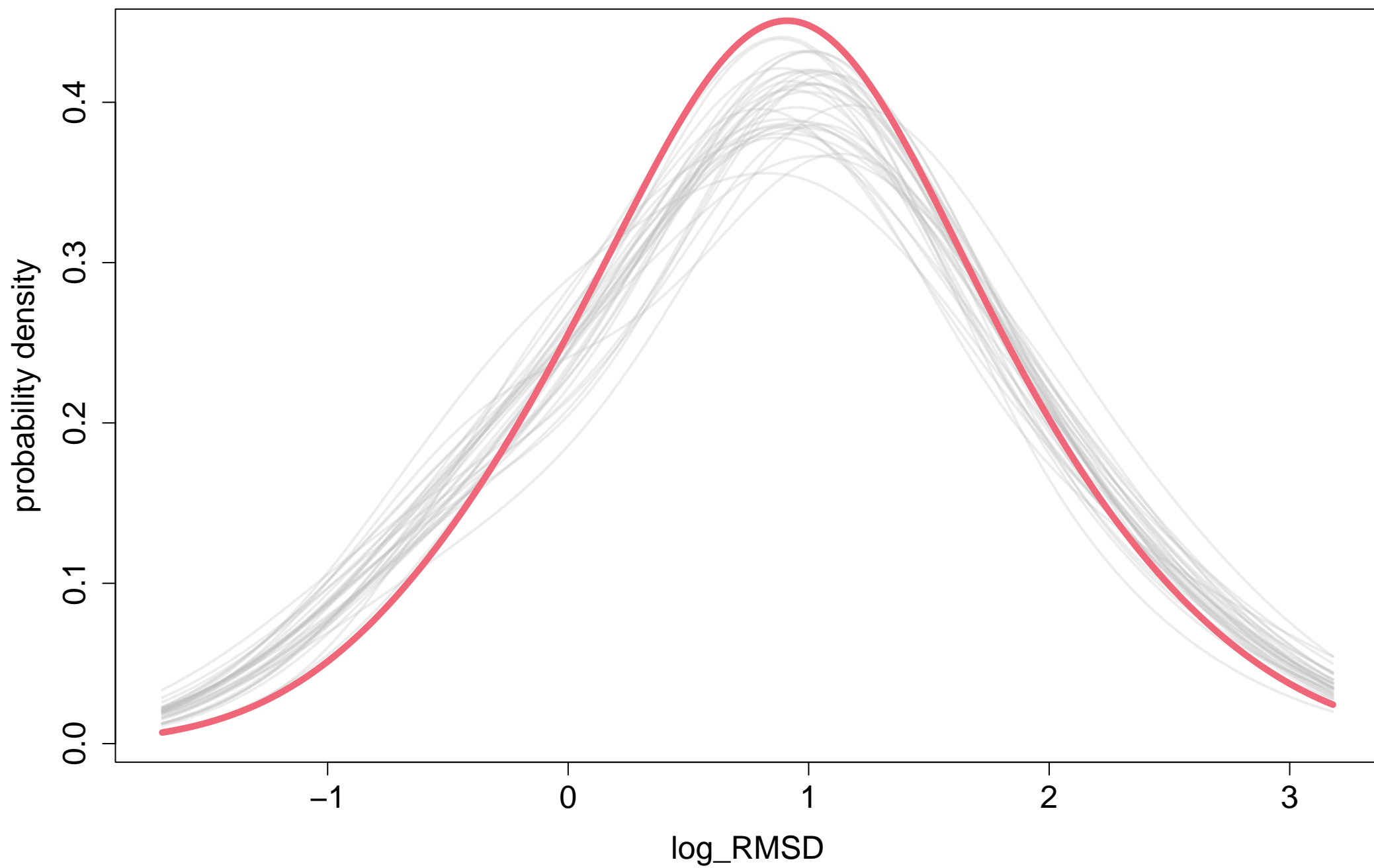
max MCSE = 2.62261780362333

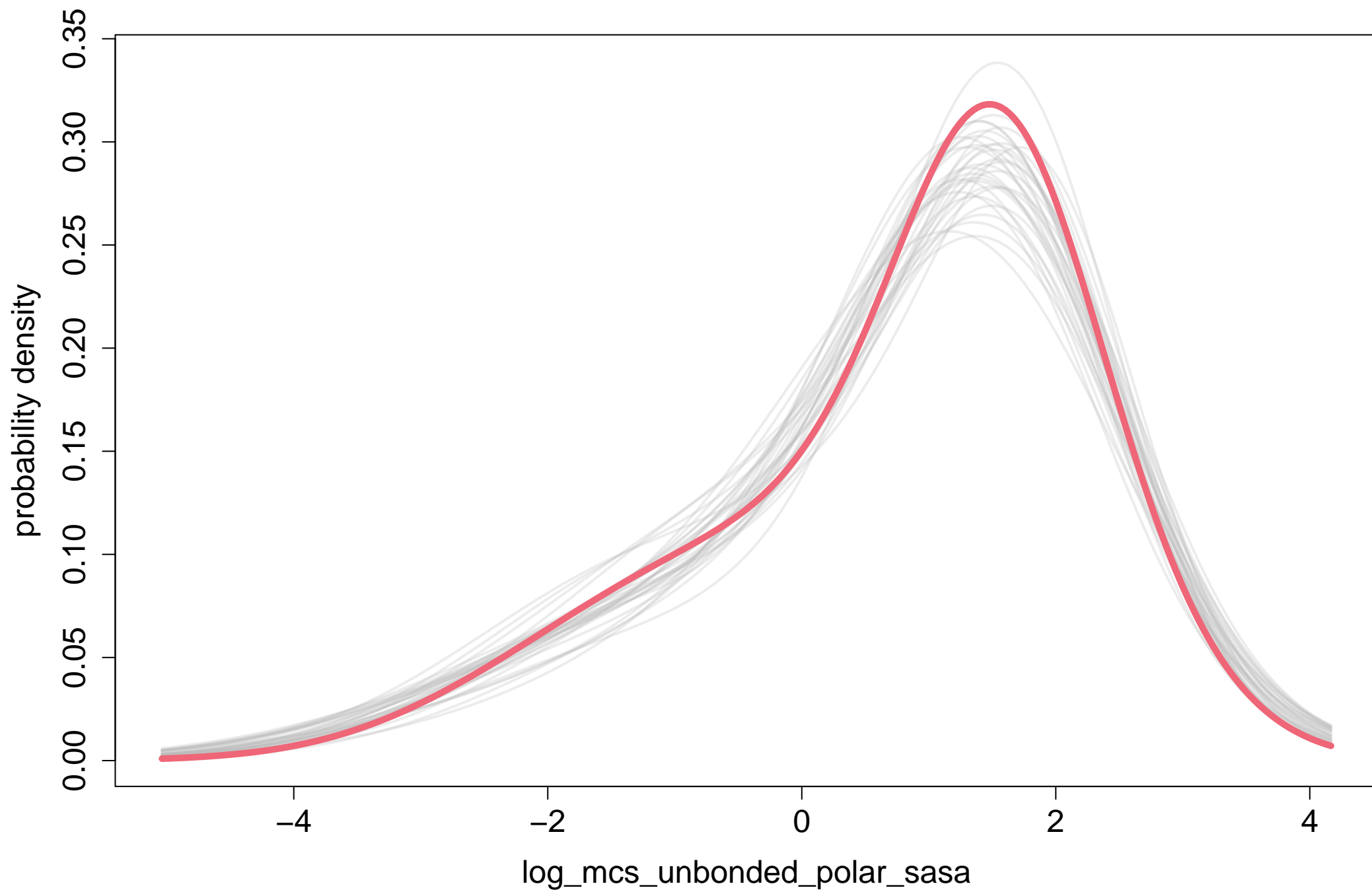
all stationary: TRUE

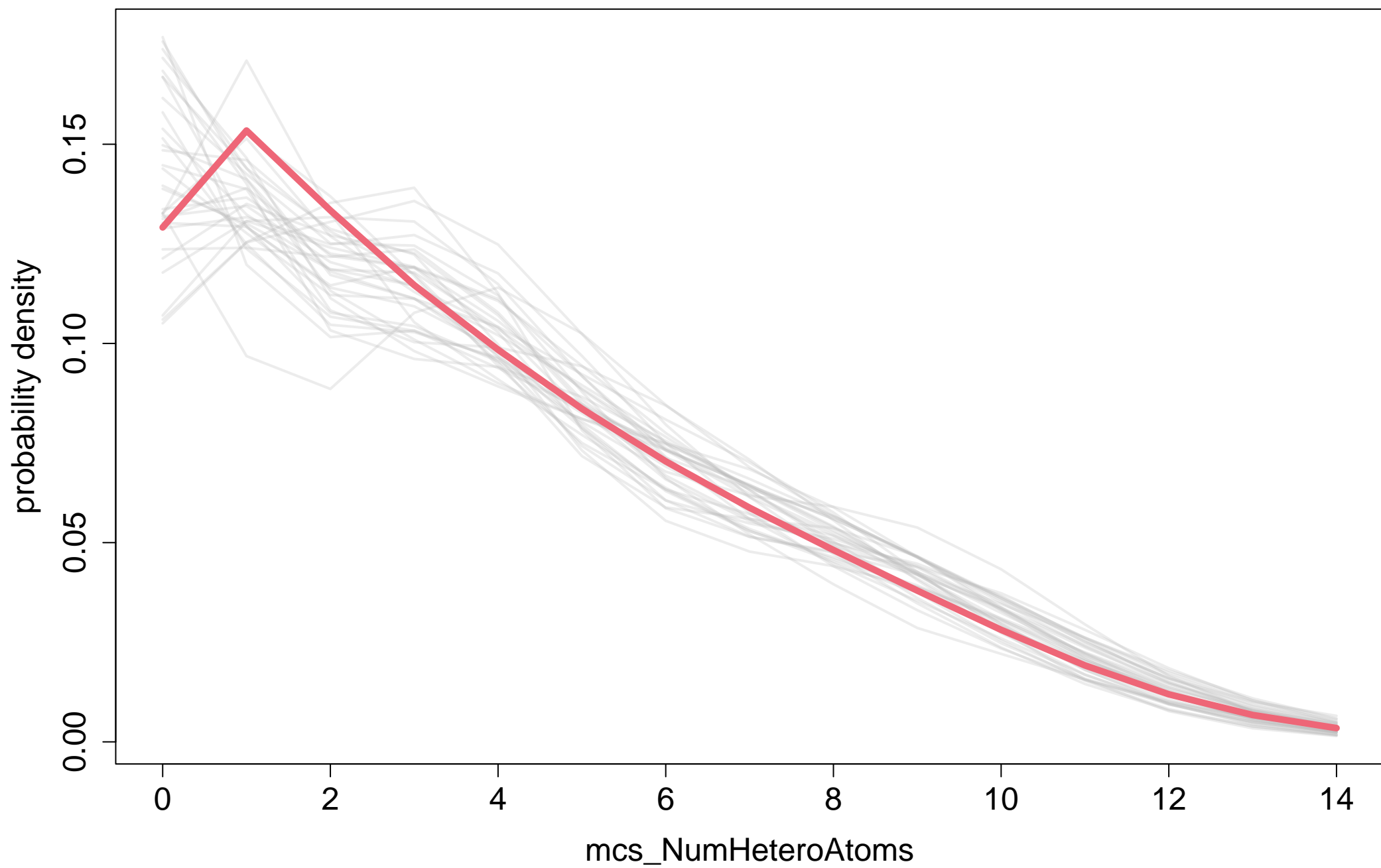
burn: 0

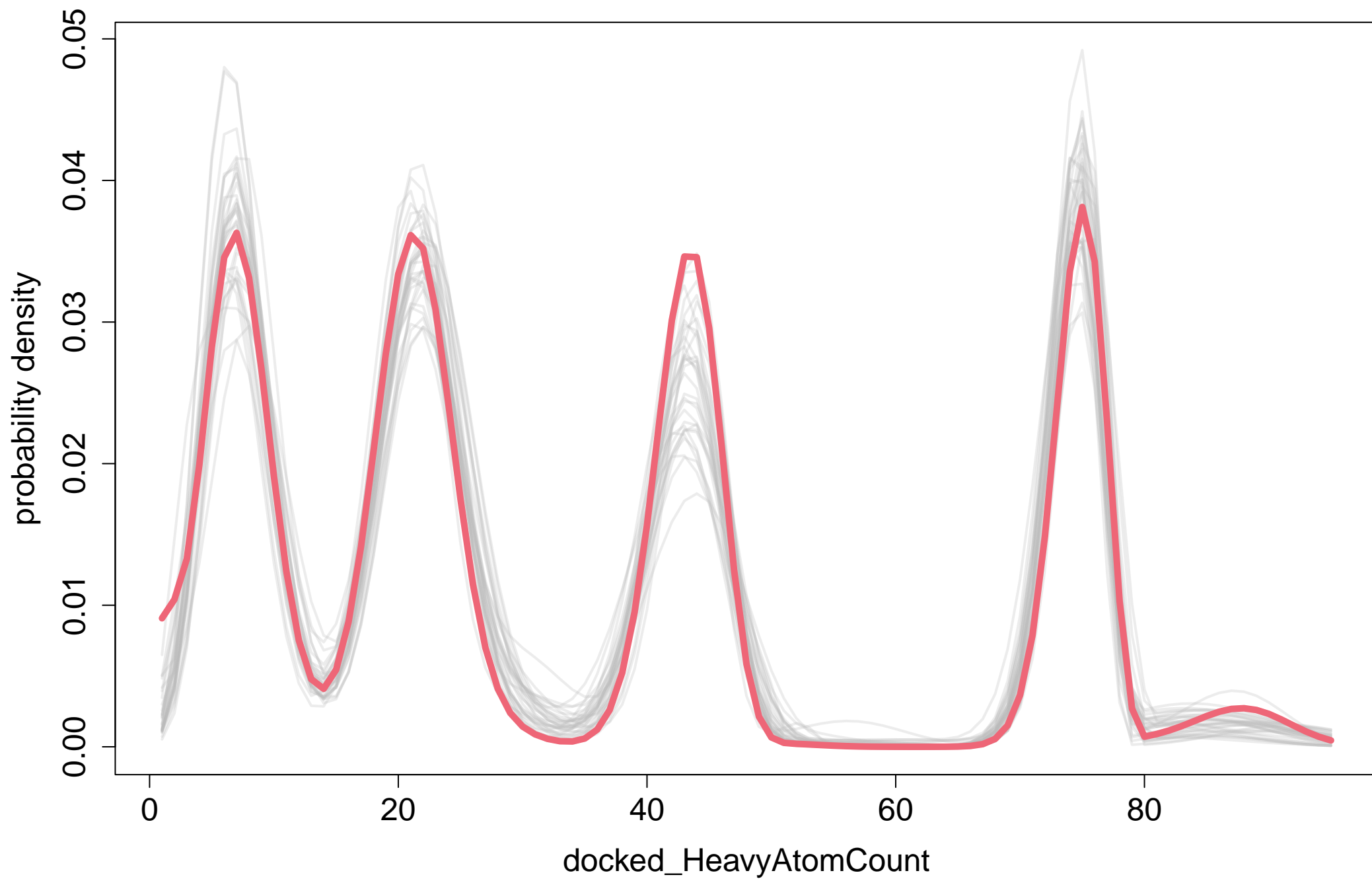
max rel.err.: 1.85331677745946

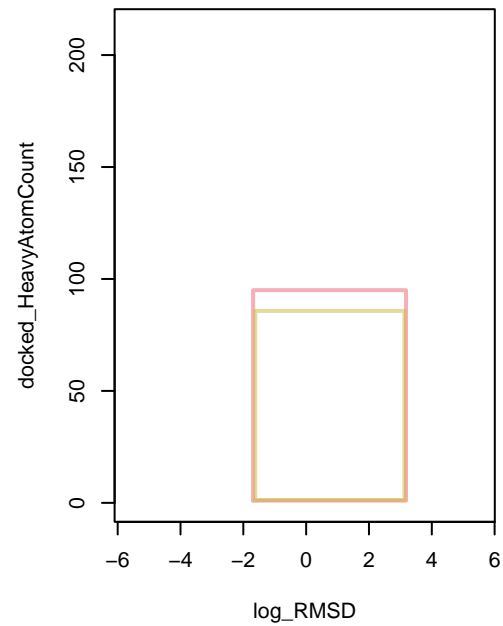
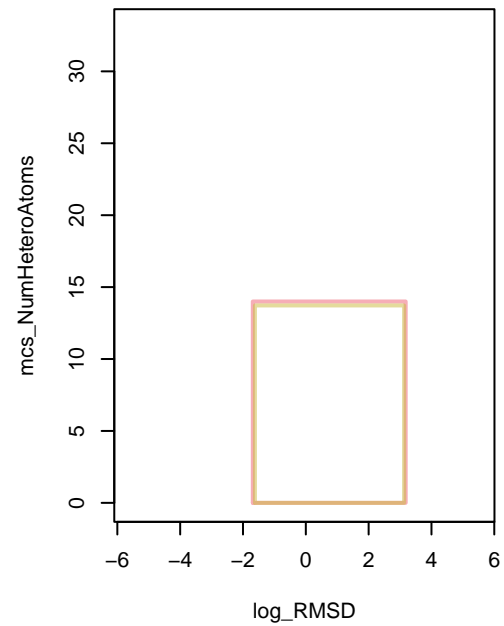
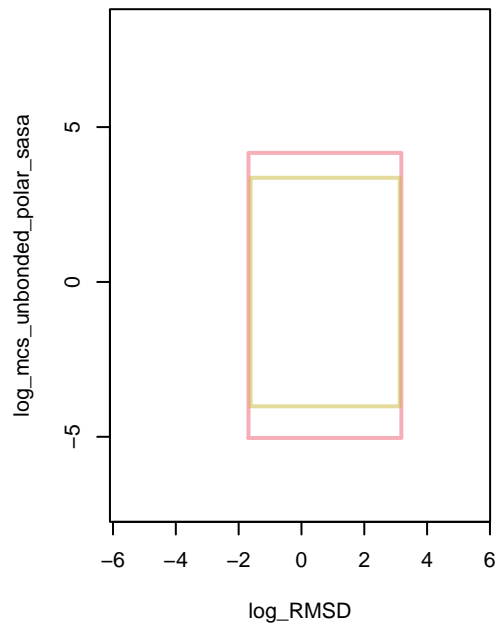
Occupied clusters: 9 of 16



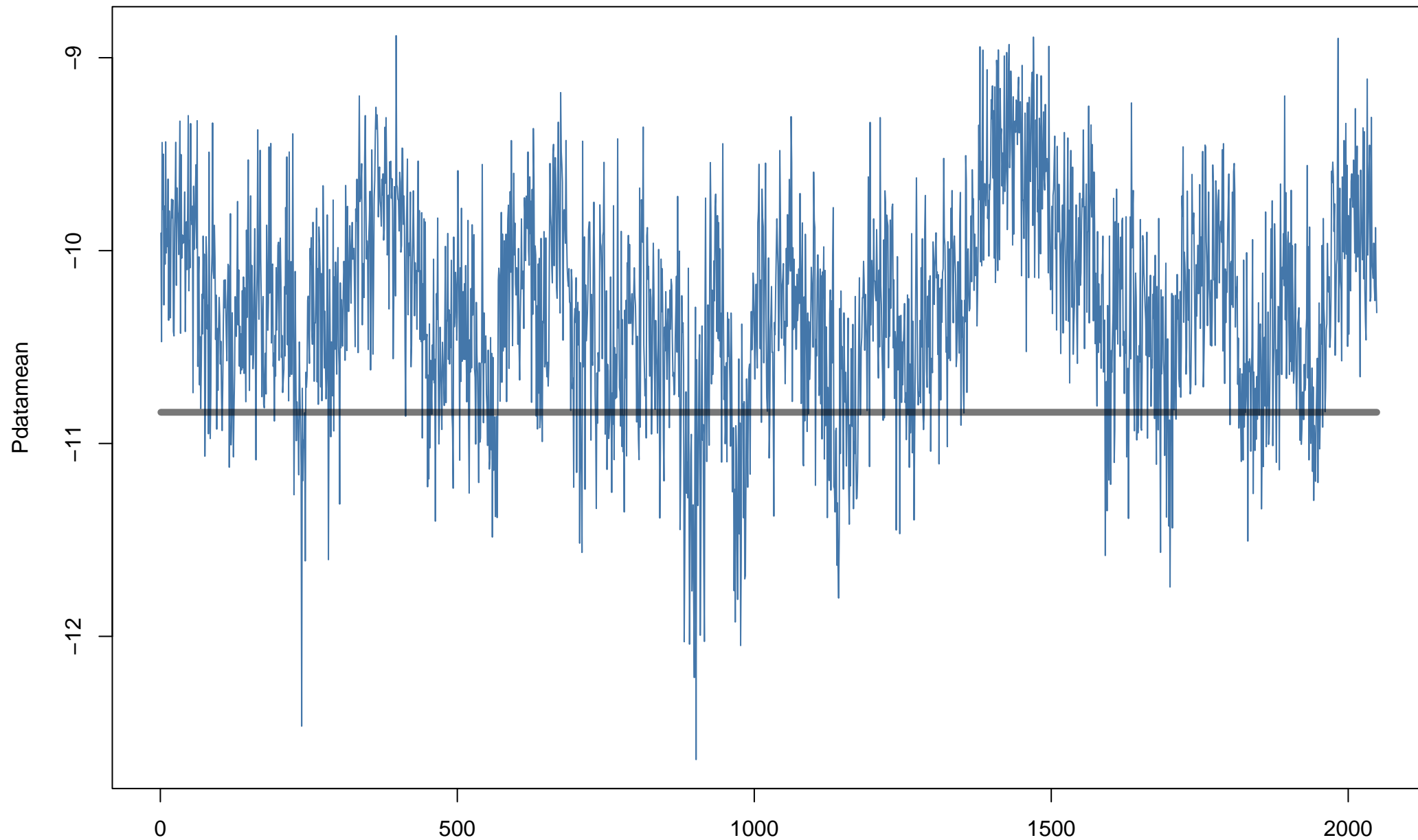




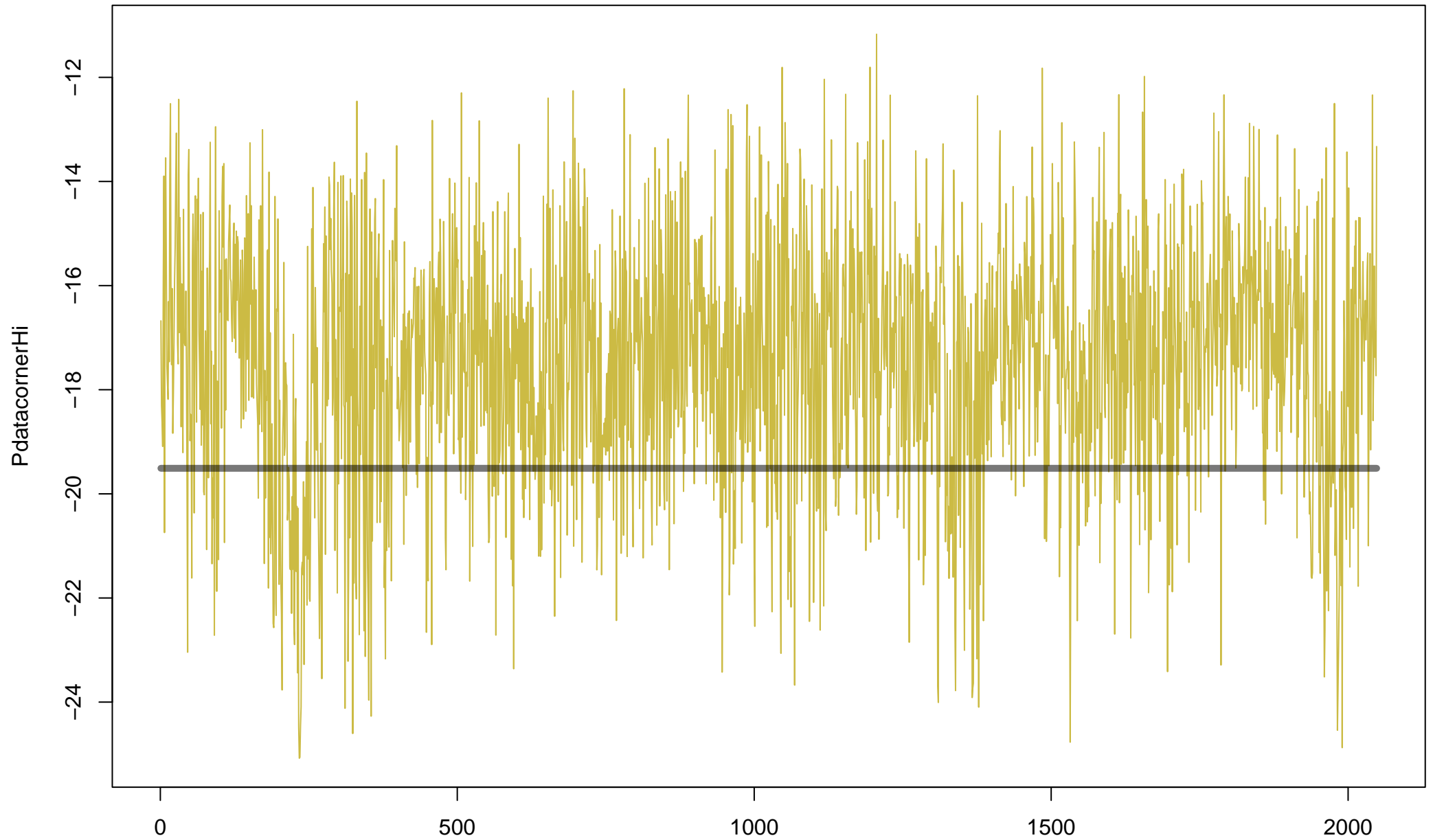




Pdatamean
ESS = 32.7 | BMK = 0.117 | MCSE(6.27) = 9.53 | stat: TRUE | burn: 0 | rel.err: 0.929

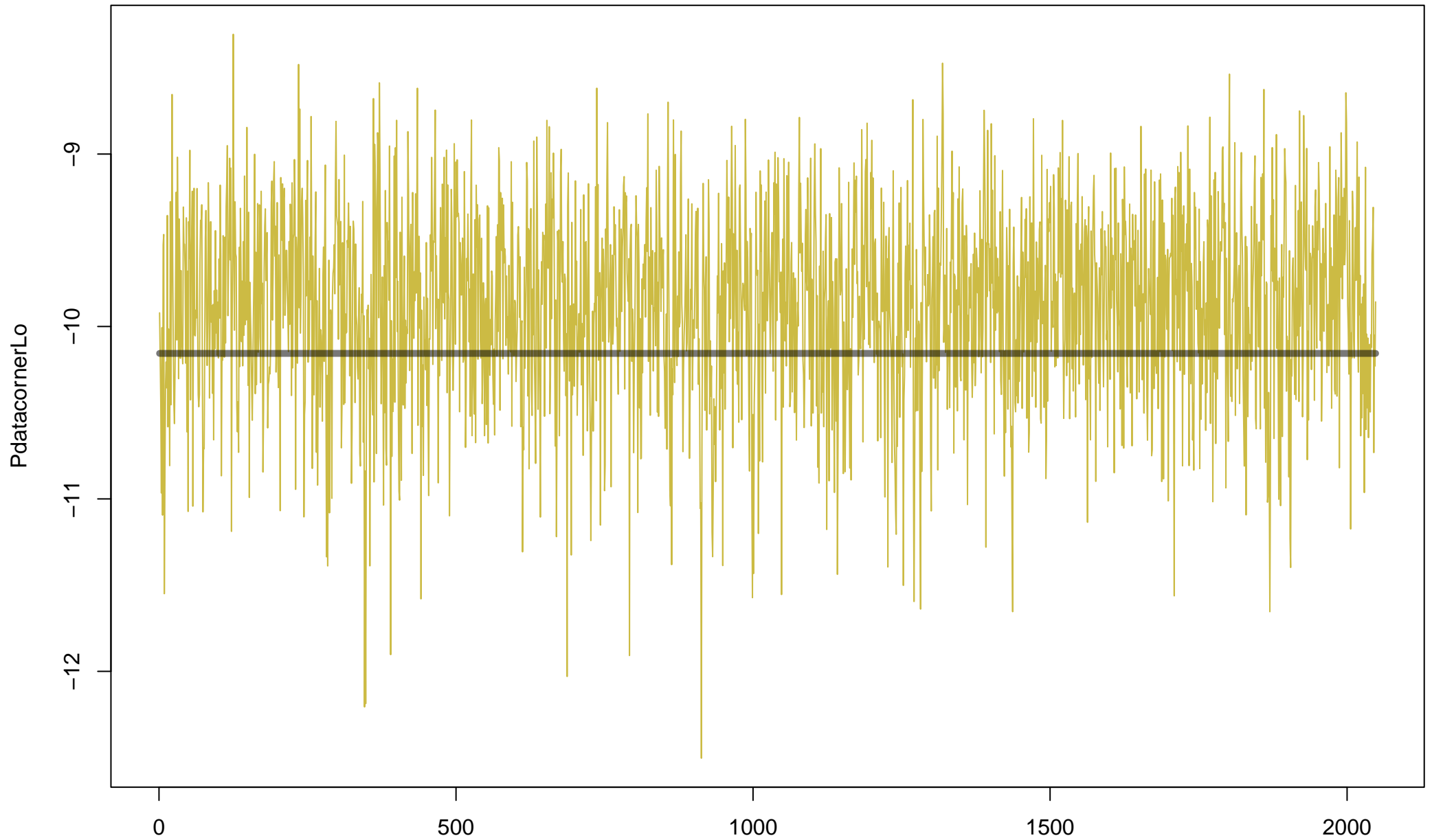


PdatacornerHi
ESS = 1630 | BMK = 0.142 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: 0.304

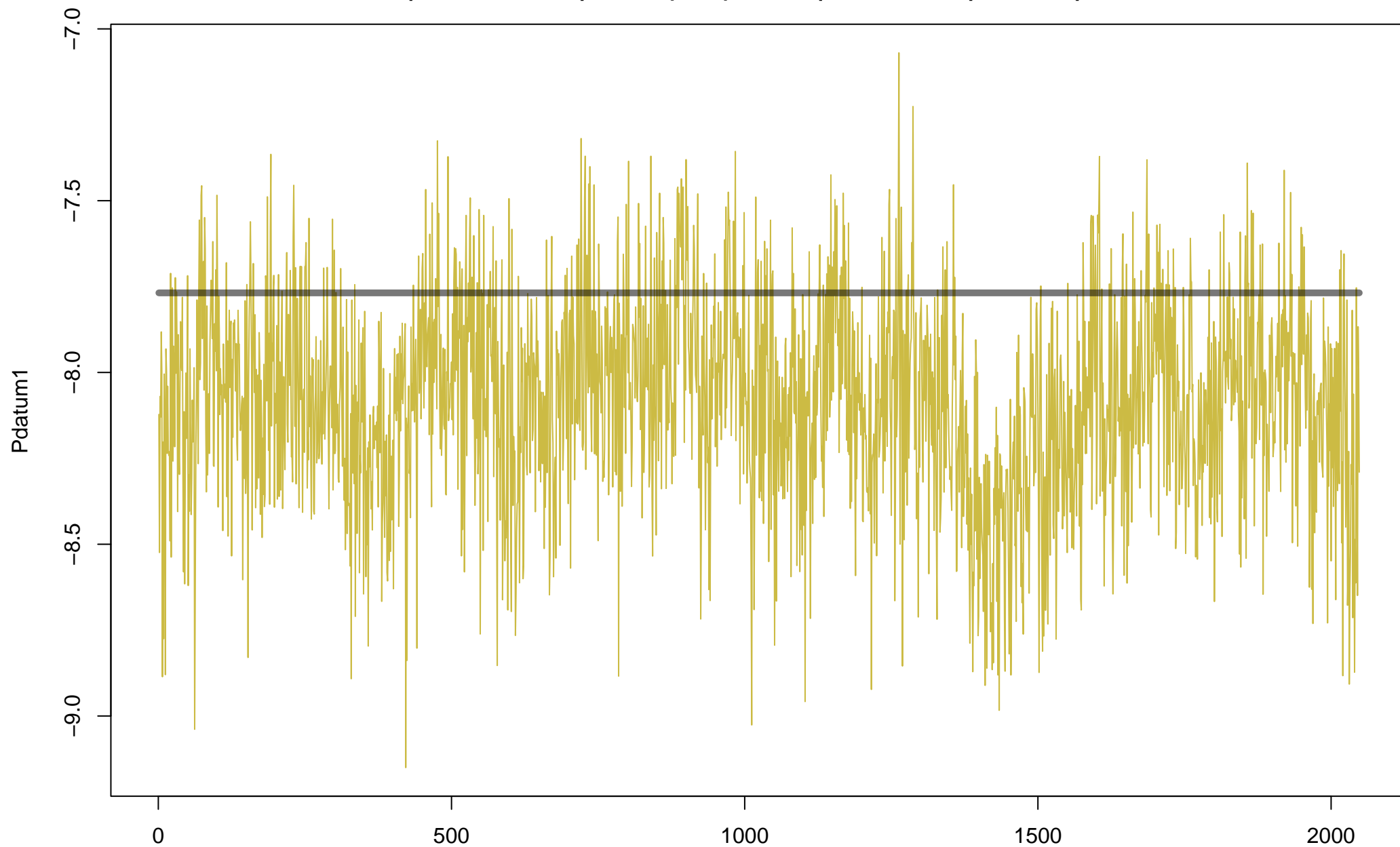


PdatacornerLo

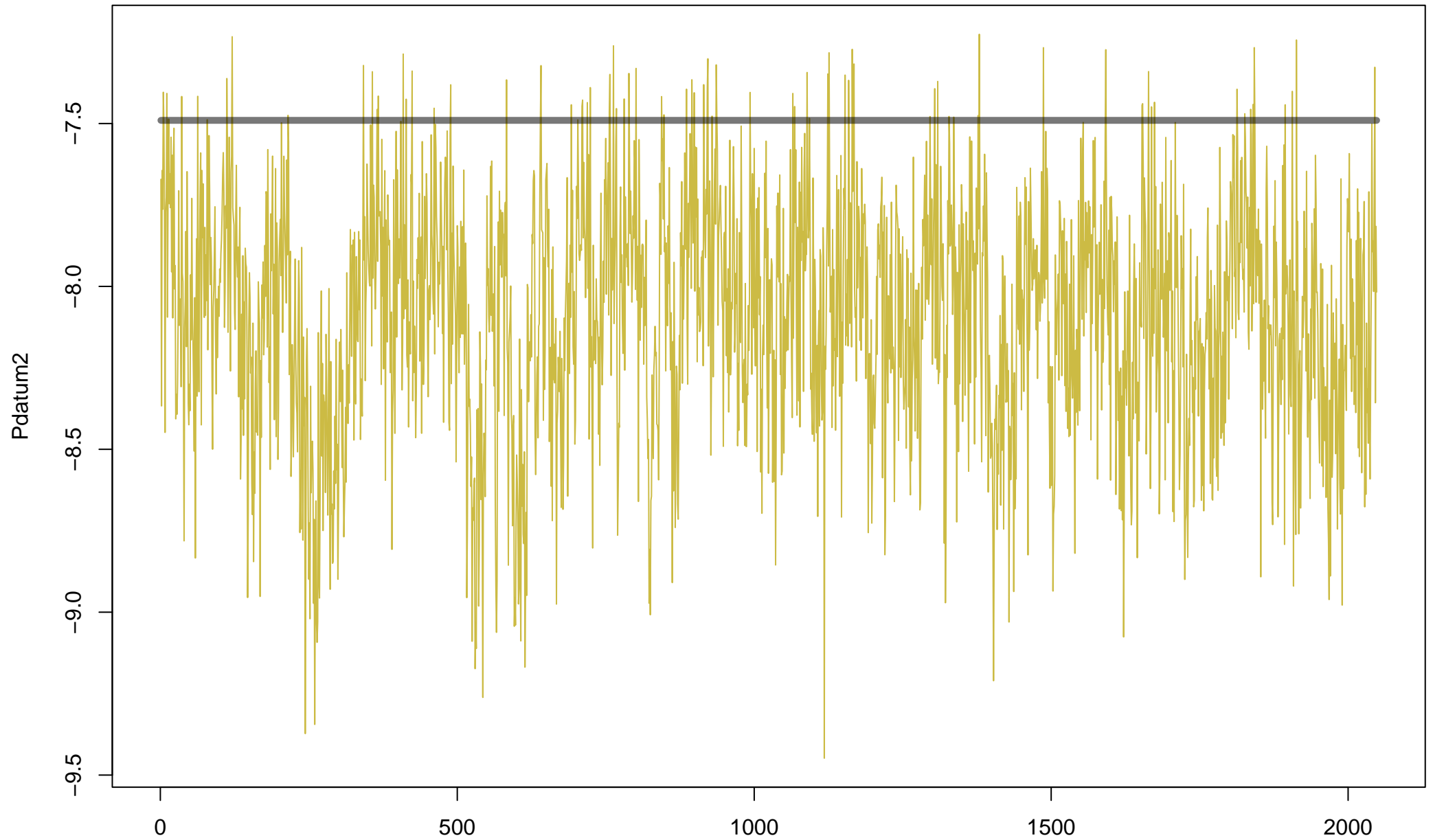
ESS = 1510 | BMK = 0.0408 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0 | rel.err: 0.644



Pdatum1
ESS = 154 | BMK = 0.104 | MCSE(6.27) = 6.03 | stat: TRUE | burn: 0 | rel.err: -1.07

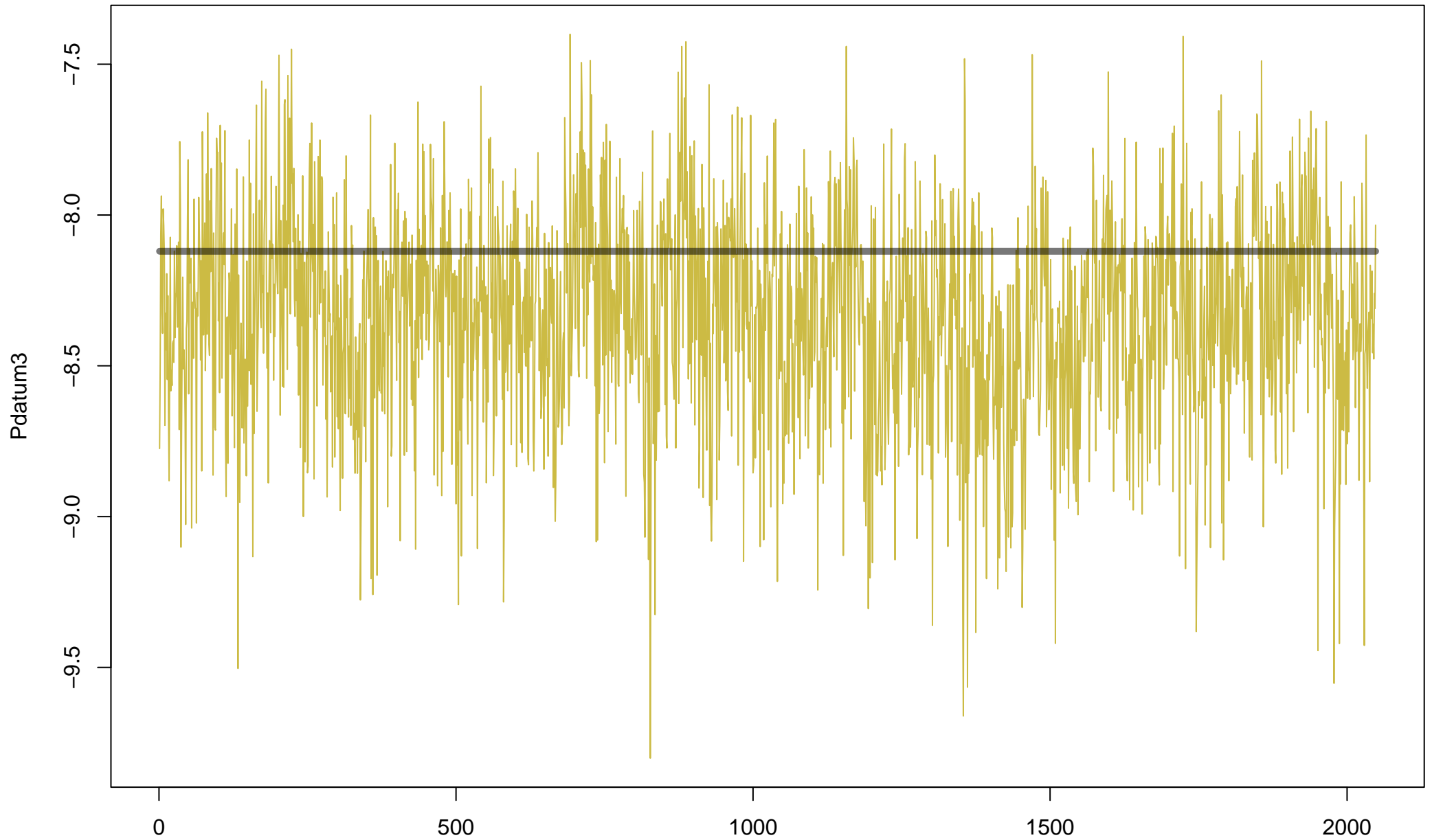


Pdatum2
ESS = 192 | BMK = 0.0682 | MCSE(6.27) = 6.48 | stat: TRUE | burn: 0 | rel.err: -2.08



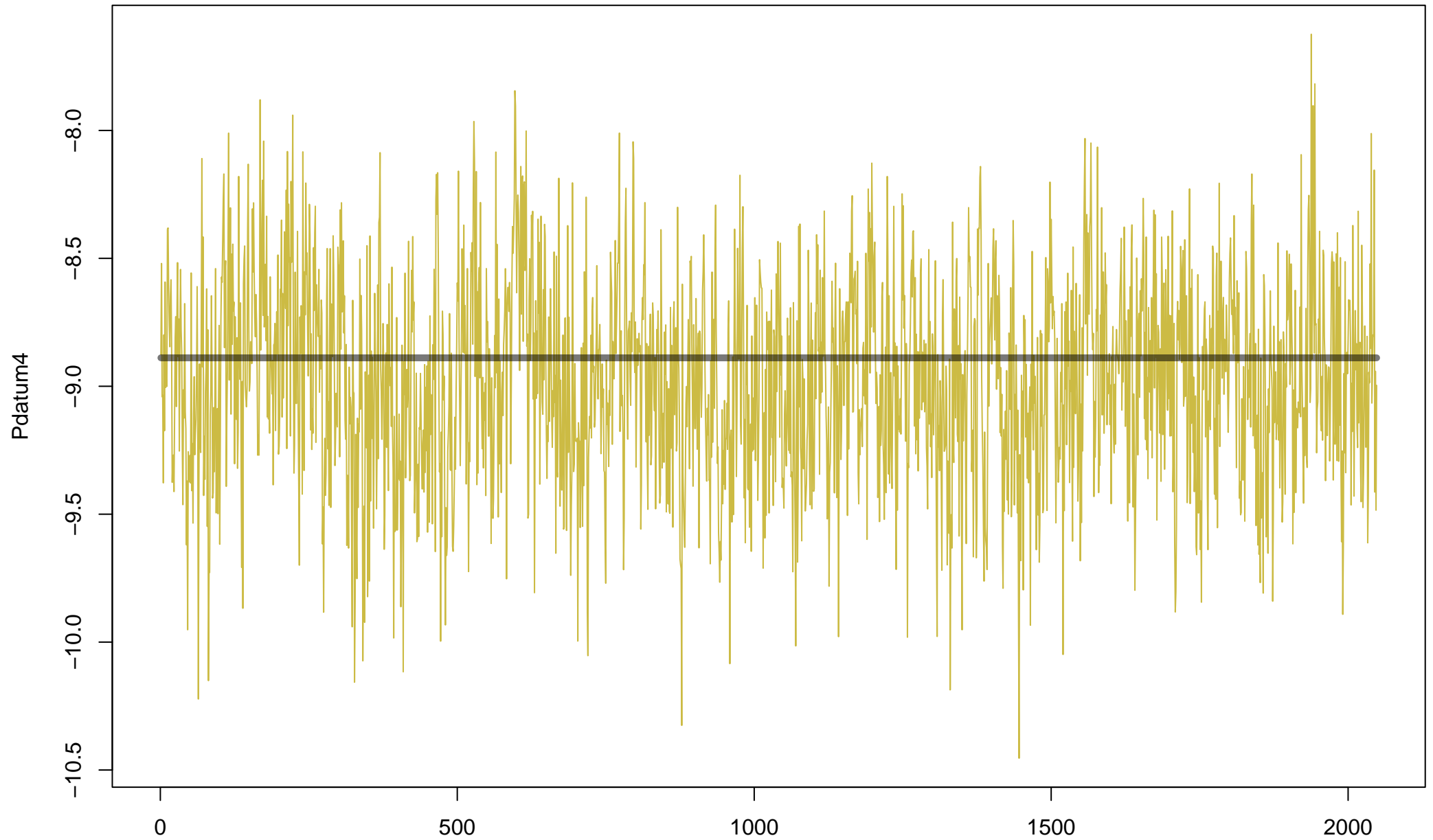
Pdatum3

ESS = 337 | BMK = 0.0799 | MCSE(6.27) = 4.81 | stat: FALSE | burn: 0 | rel.err: -0.533



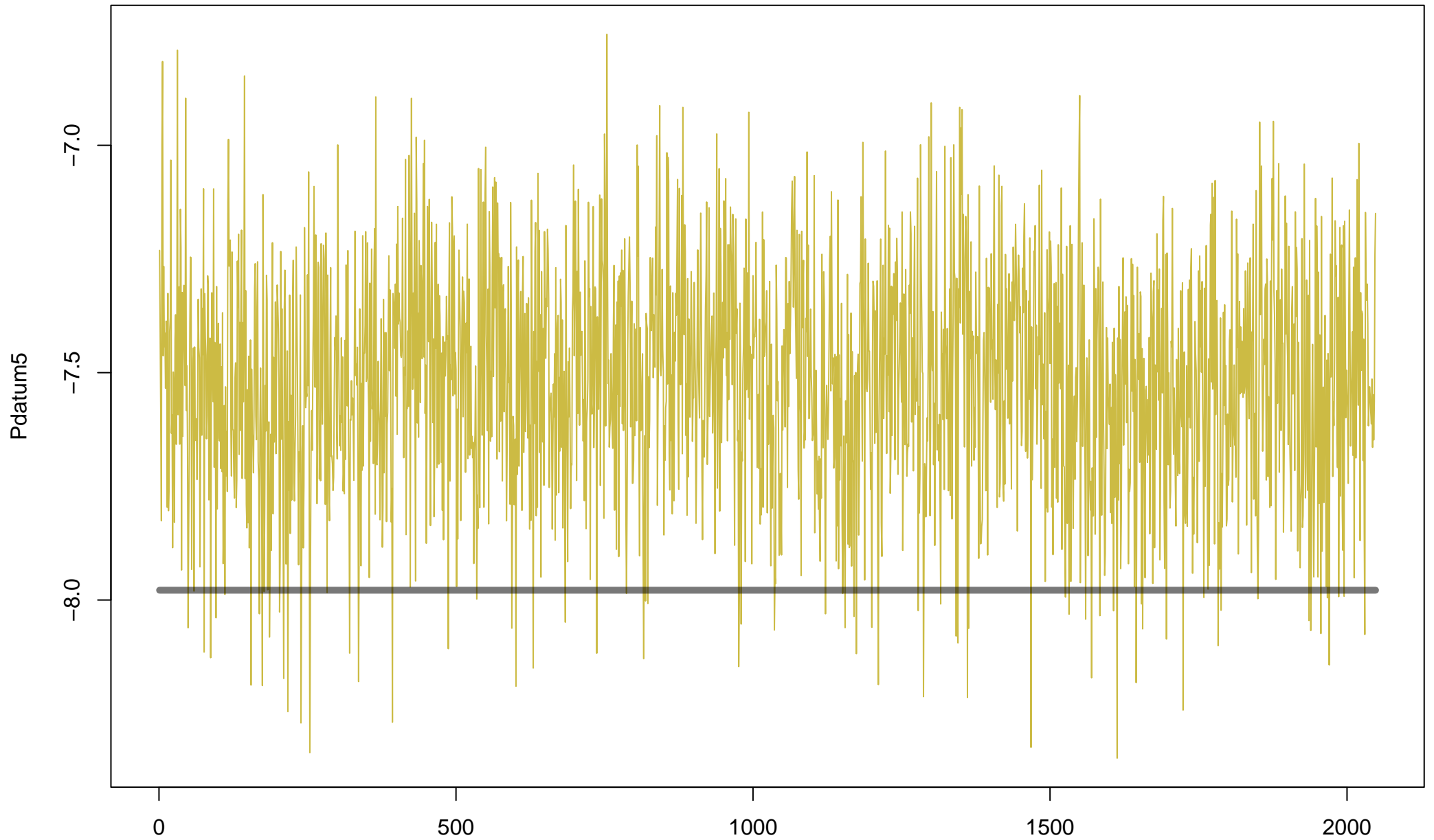
Pdatum4

ESS = 496 | BMK = 0.0557 | MCSE(6.27) = 5.15 | stat: TRUE | burn: 0 | rel.err: -0.0343



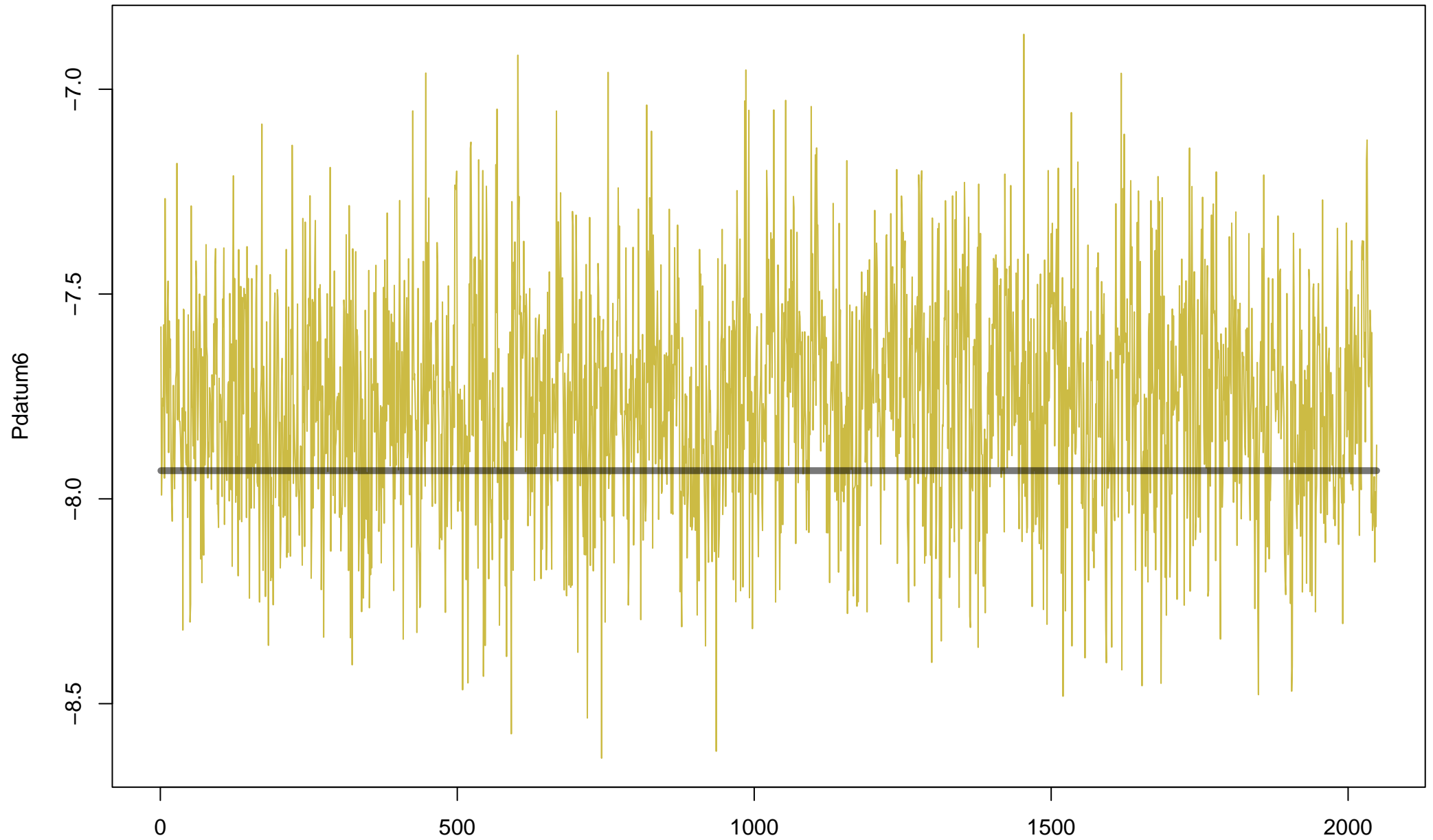
Pdatum5

ESS = 1190 | BMK = 0.0529 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: 1.57



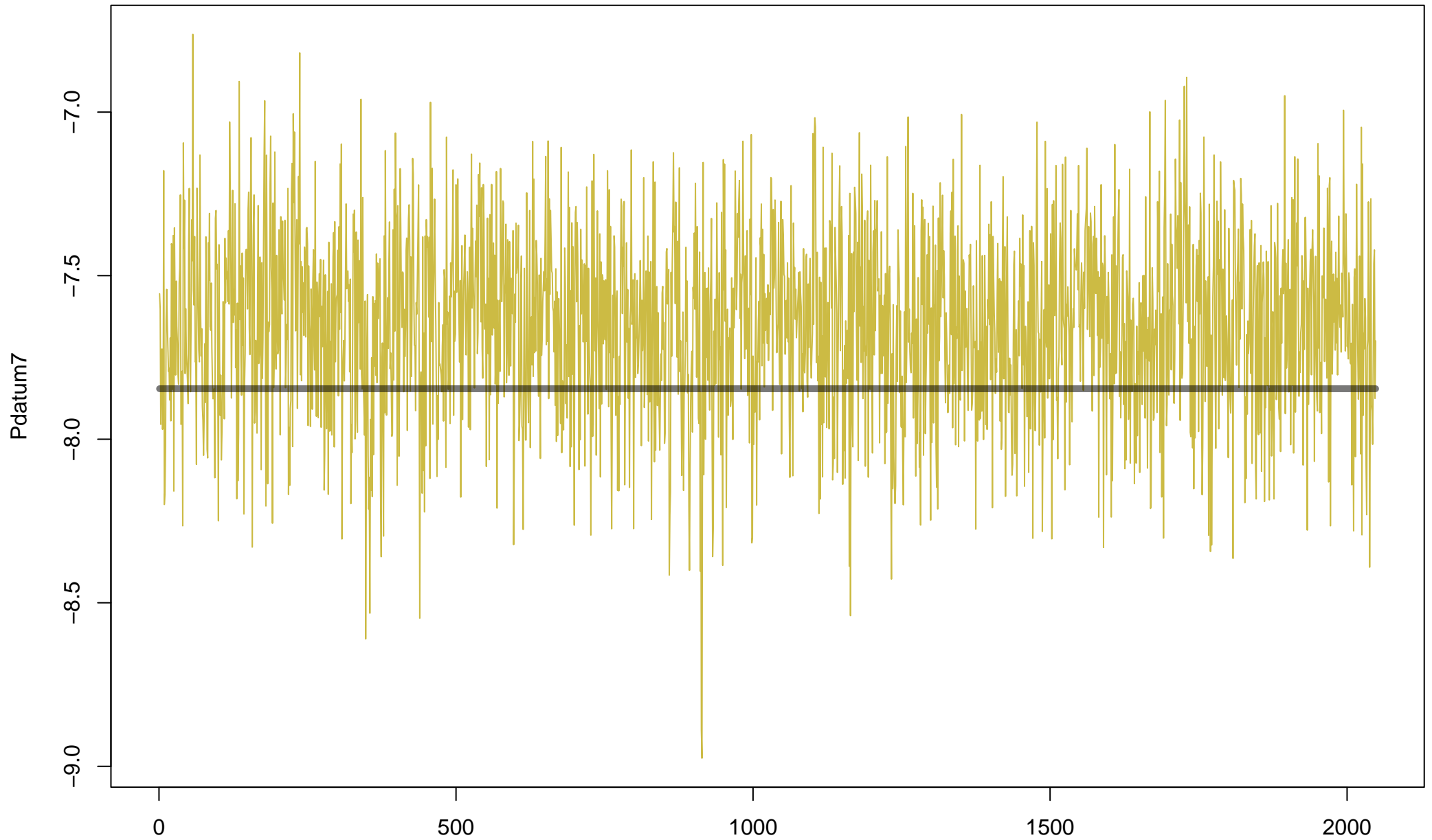
Pdatum6

ESS = 1110 | BMK = 0.0674 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: 0.673

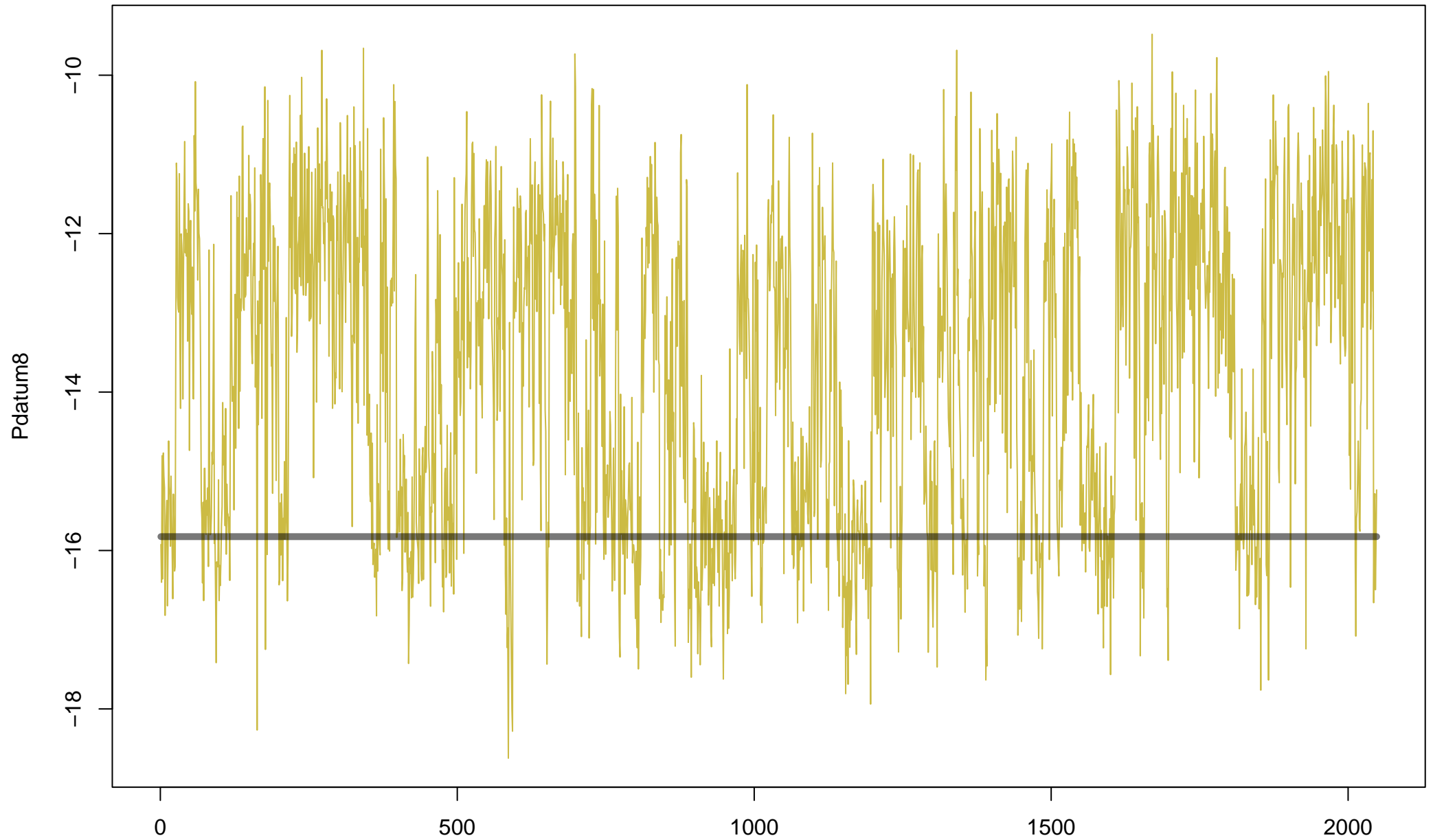


Pdatum7

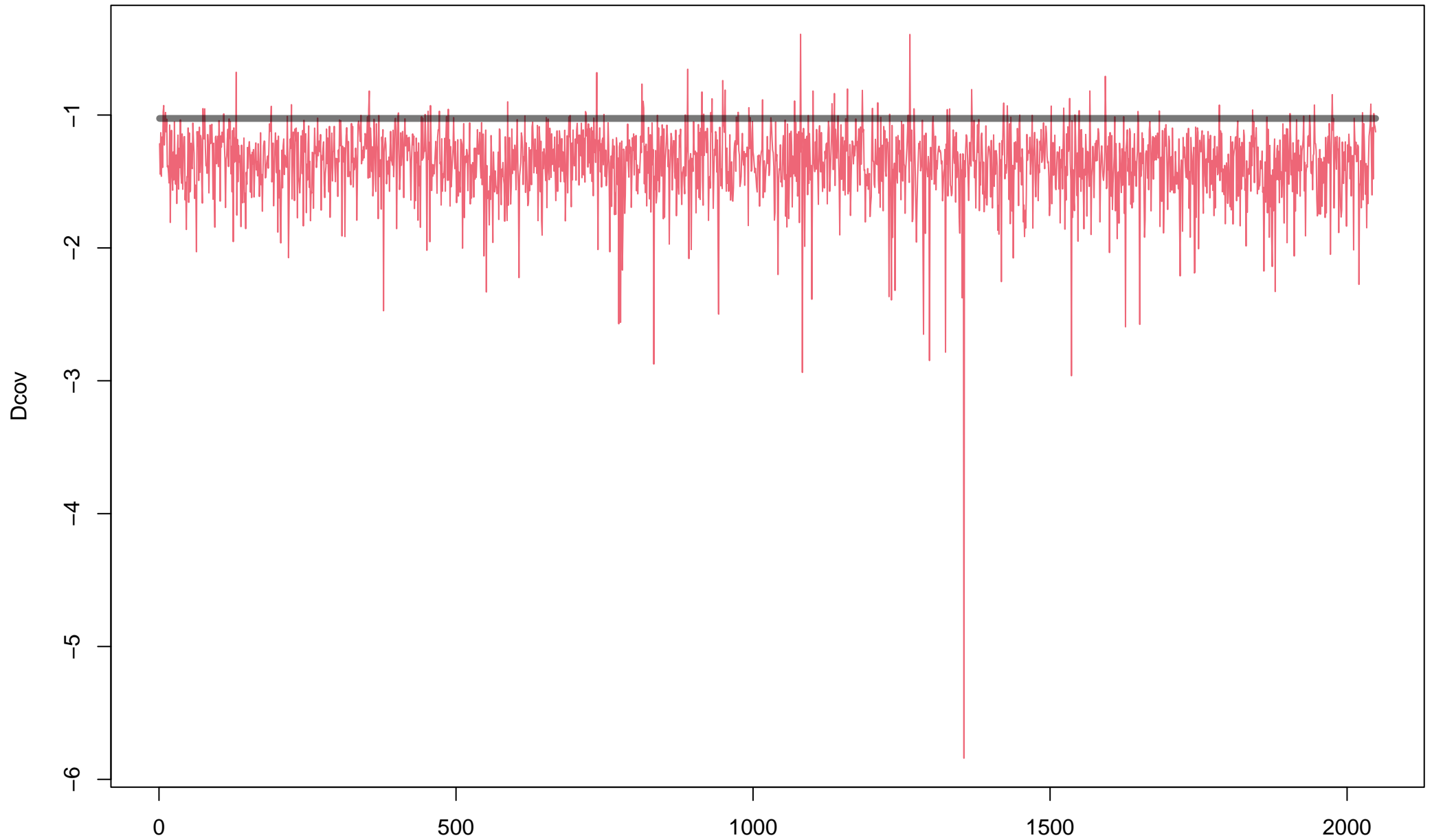
ESS = 1510 | BMK = 0.0414 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: 0.746



Pdatum8
ESS = 375 | BMK = 0.0874 | MCSE(6.27) = 5.3 | stat: TRUE | burn: 0 | rel.err: 0.574

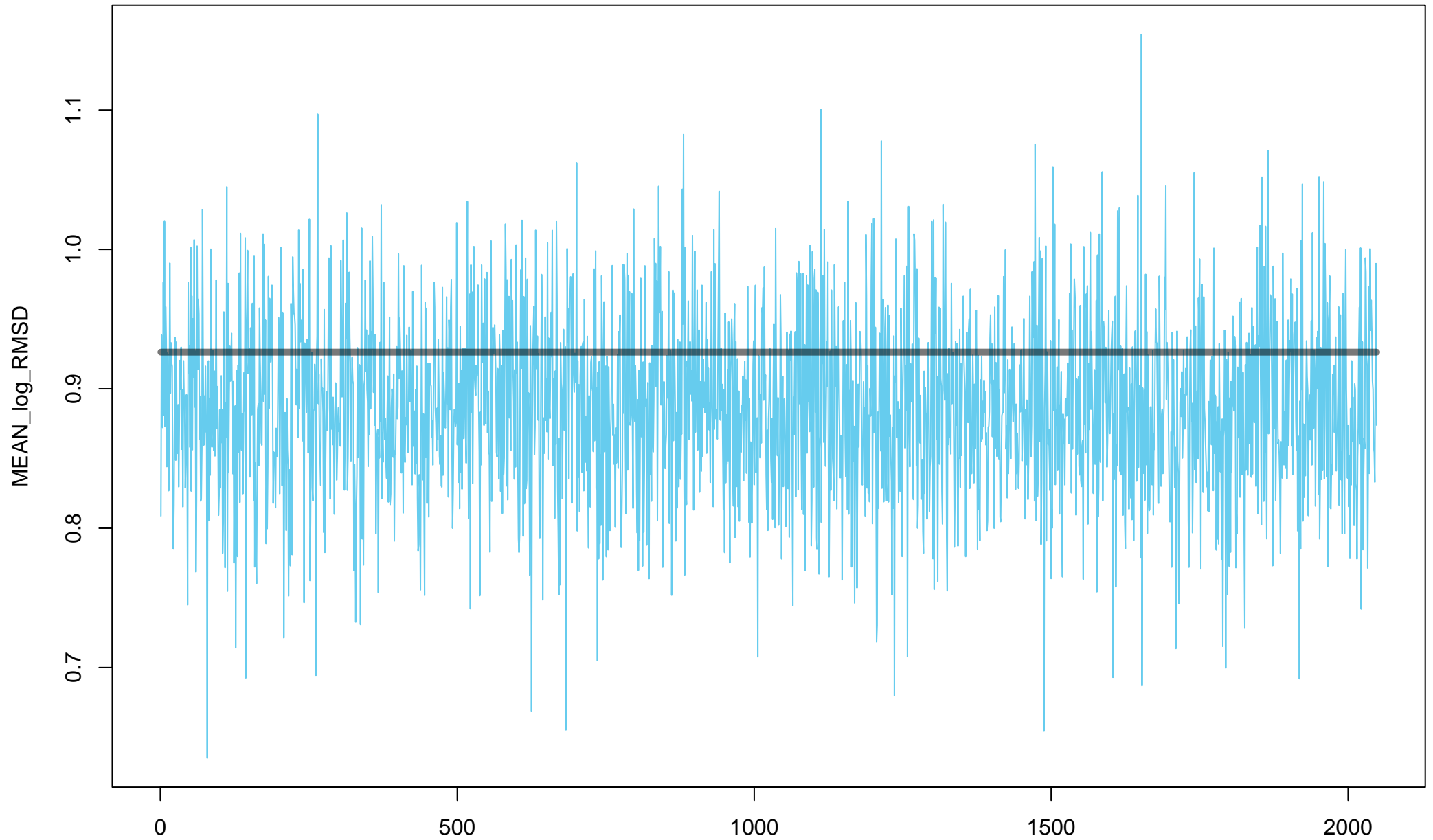


Dcov
ESS = 2050 | BMK = 0.0826 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0 | rel.err: 1.48

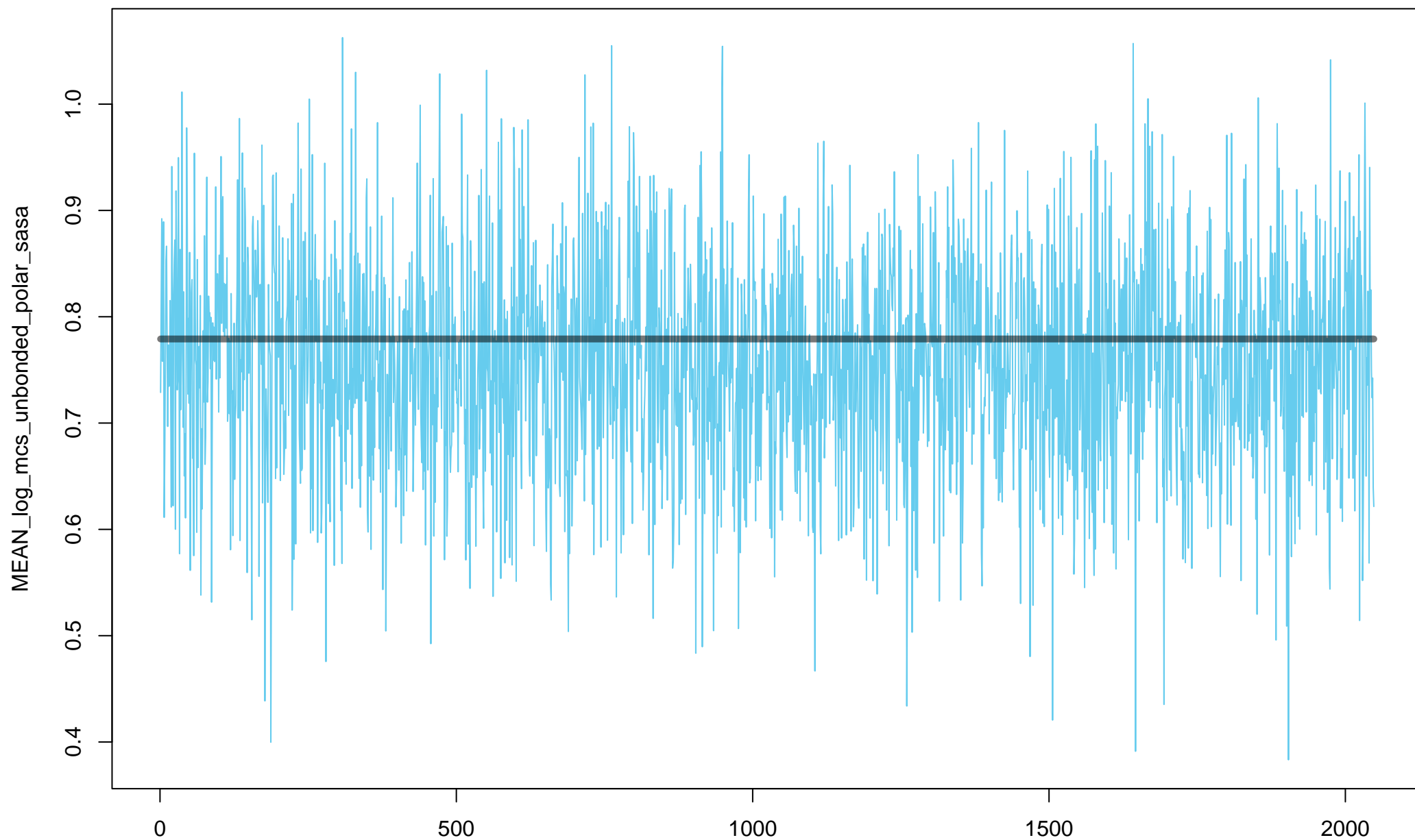


MEAN_log_RMSD

ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: -0.605

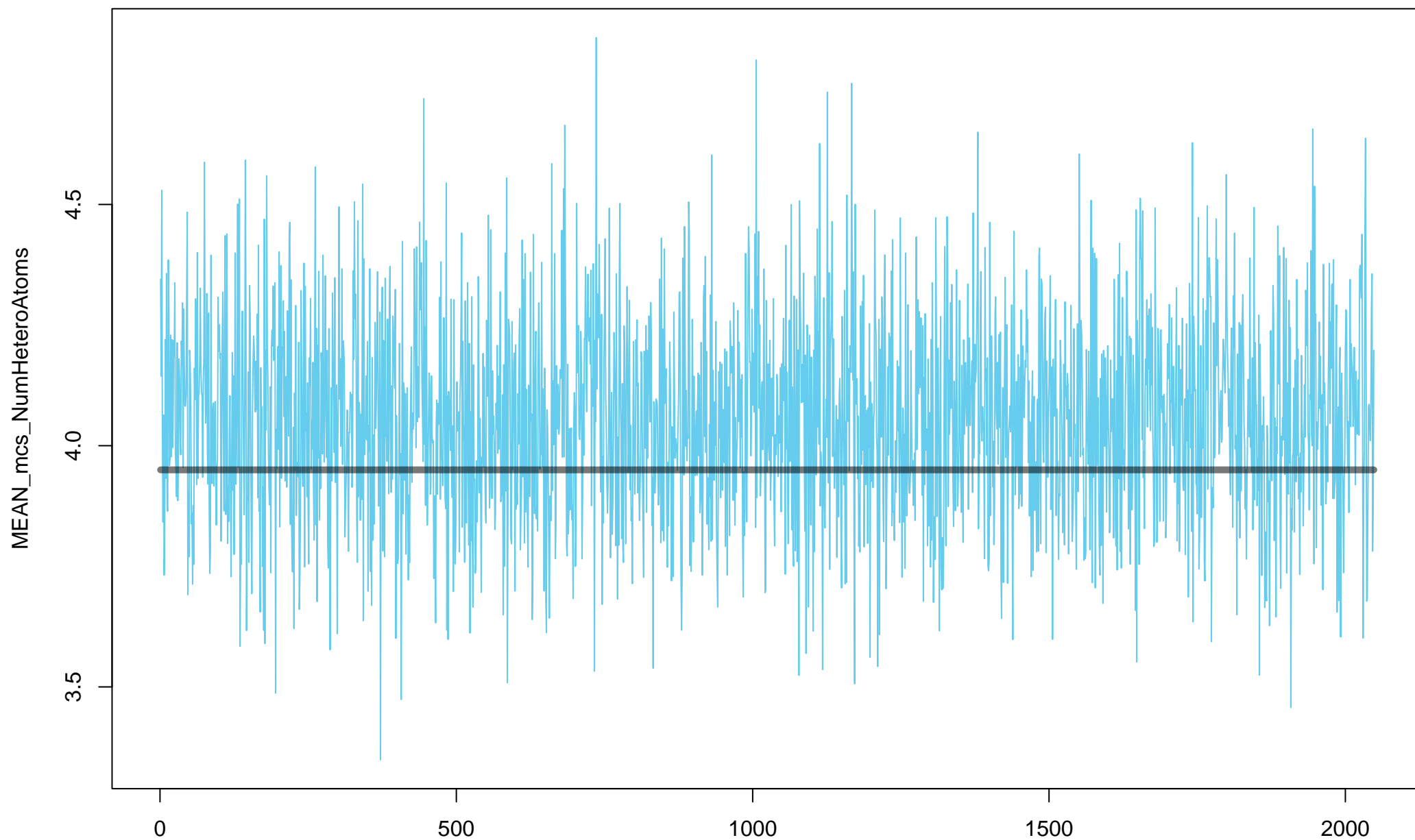


MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0363 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0 | rel.err: -0.222

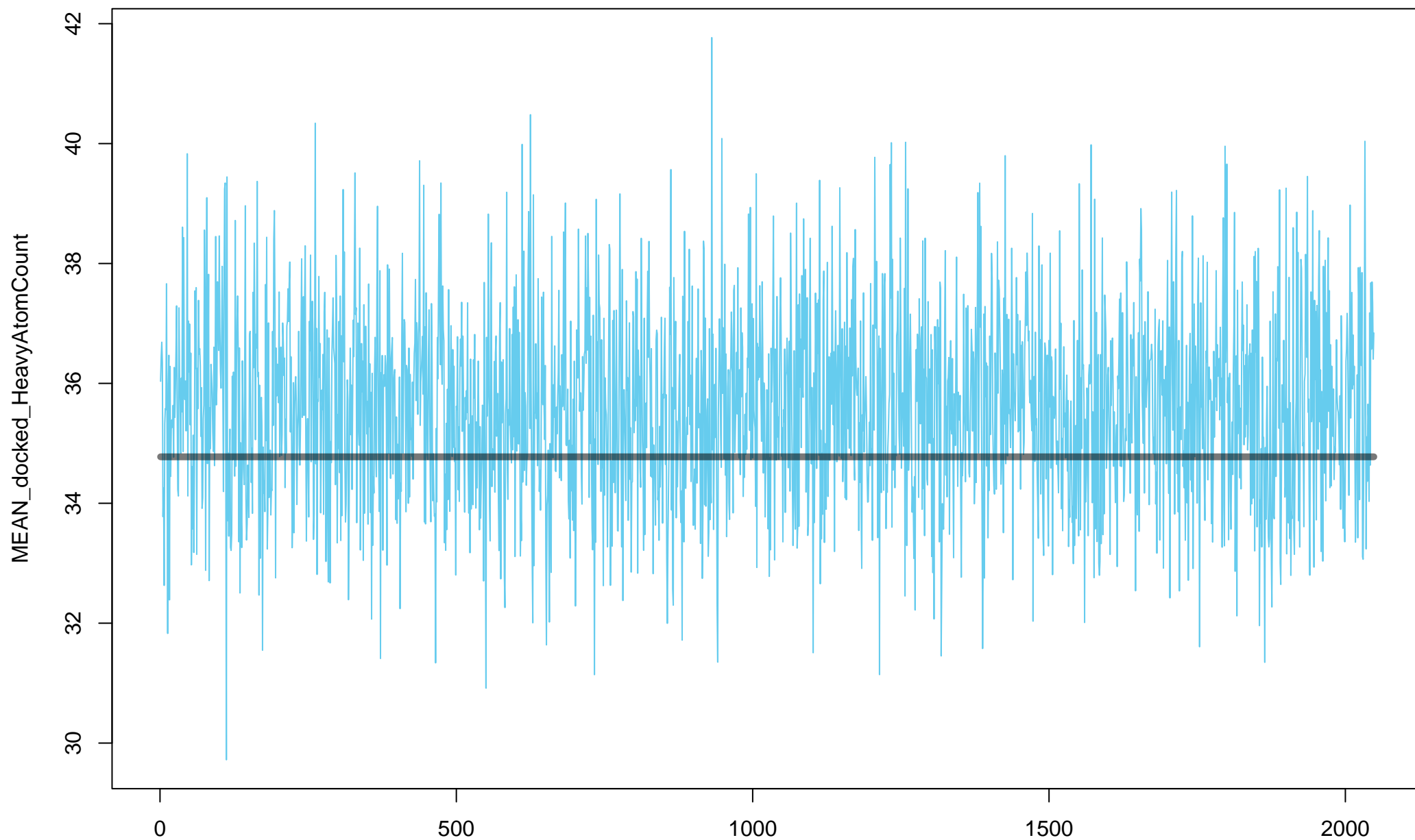


MEAN_mcs_NumHeteroAtoms

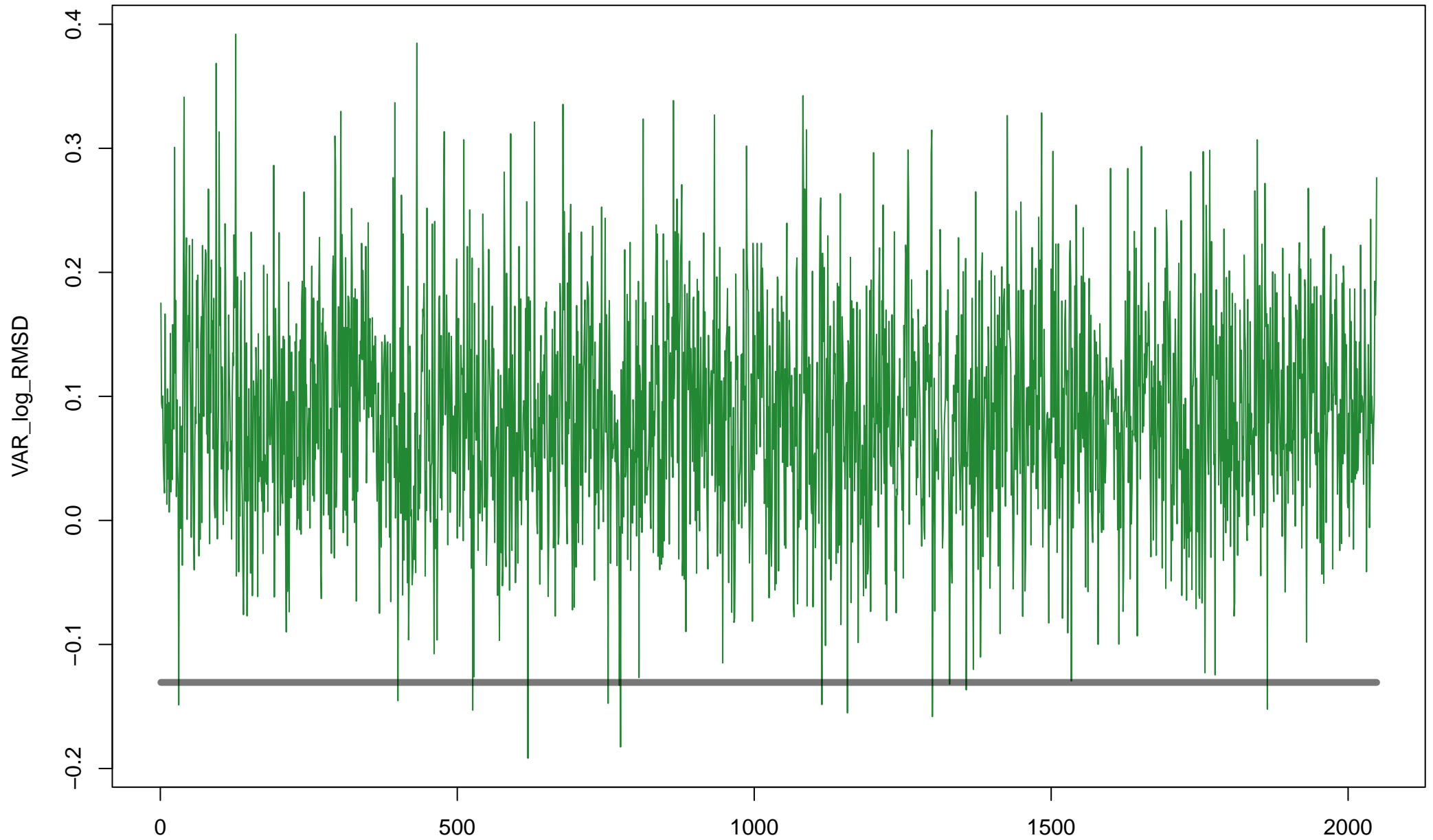
ESS = 2050 | BMK = 0.0368 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: 0.506



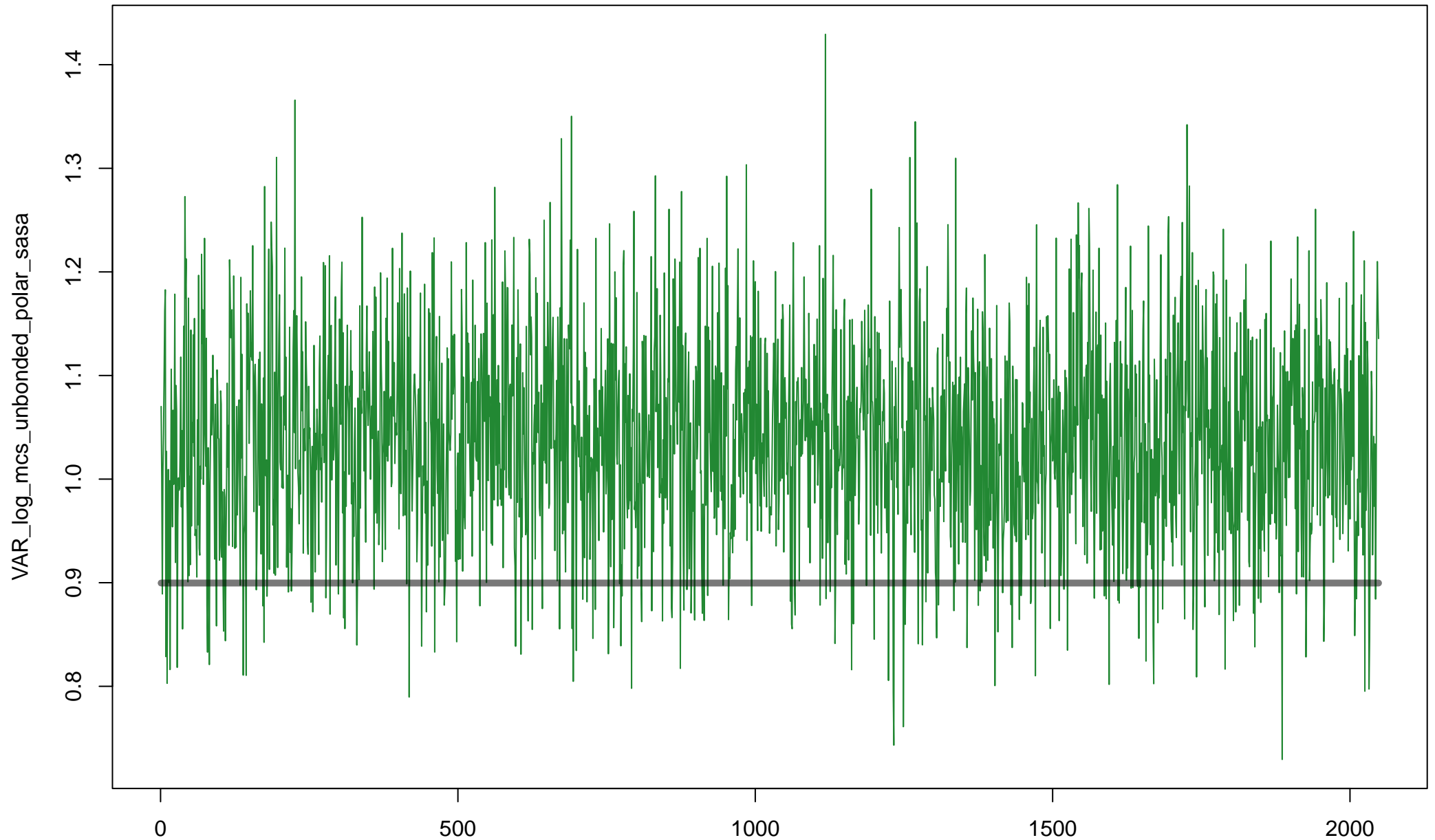
MEAN_docked_HeavyAtomCount
ESS = 1750 | BMK = 0.036 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: 0.525



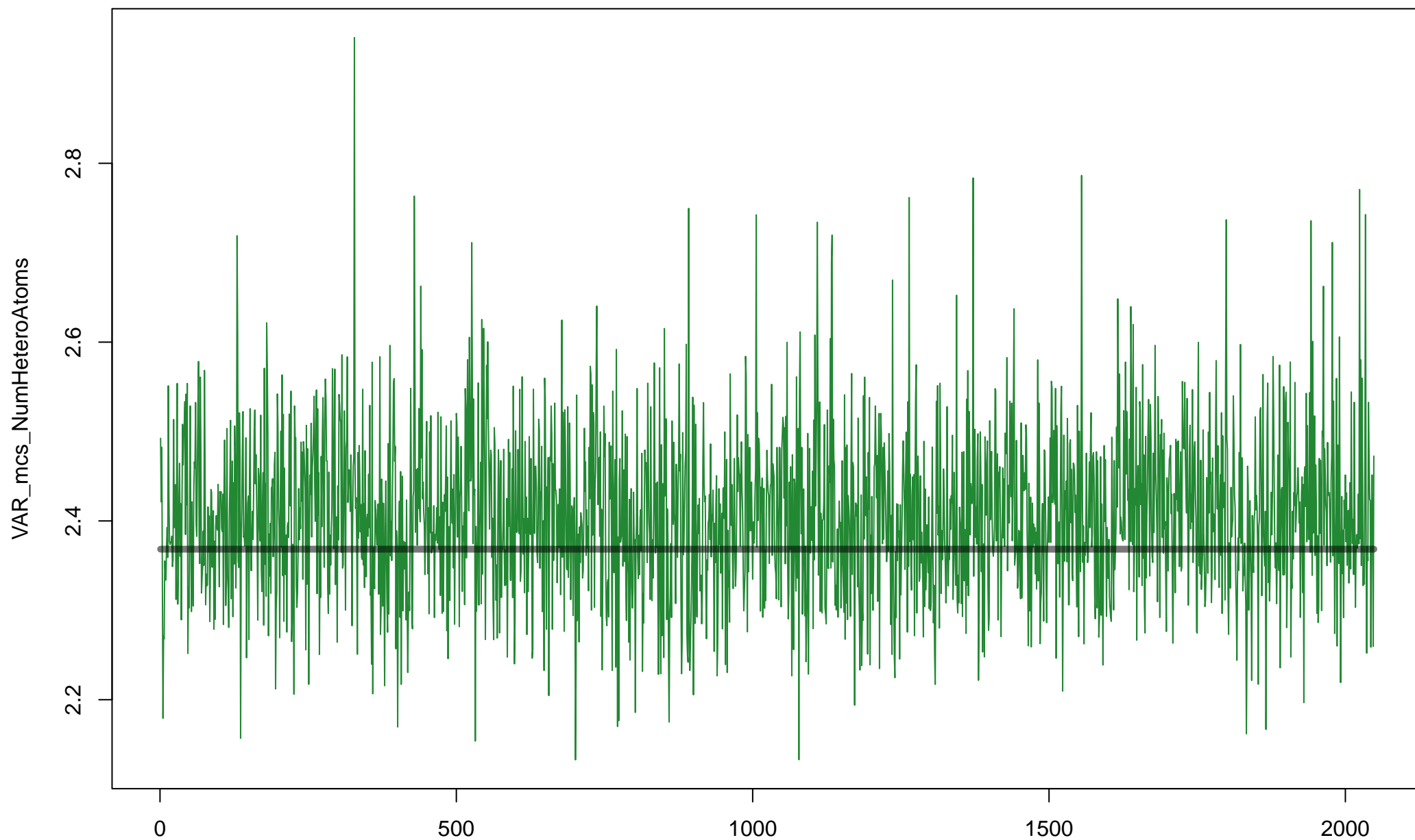
VAR_log_RMSD
ESS = 1720 | BMK = 0.0544 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | rel.err: 2.3



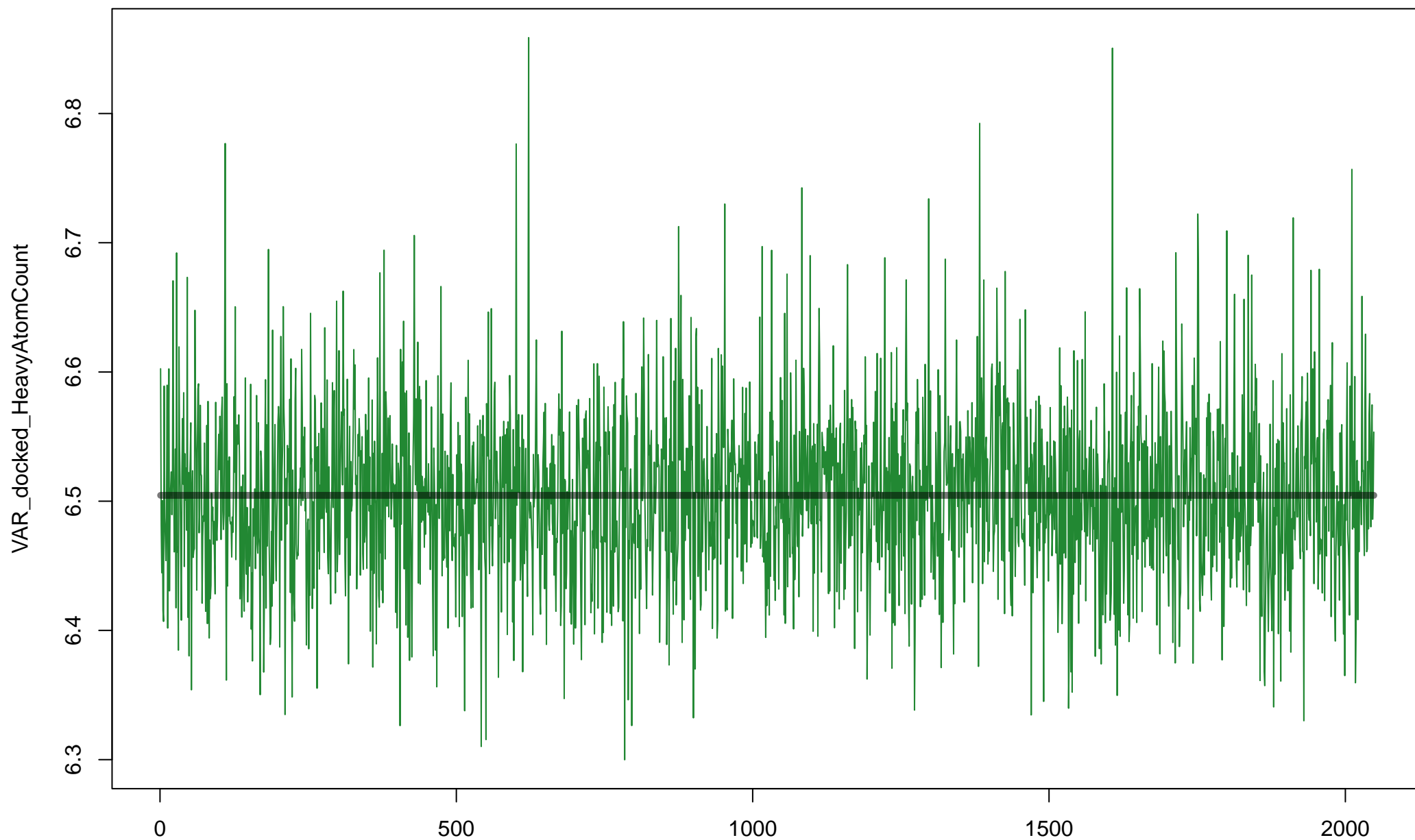
VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0408 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: 1.36



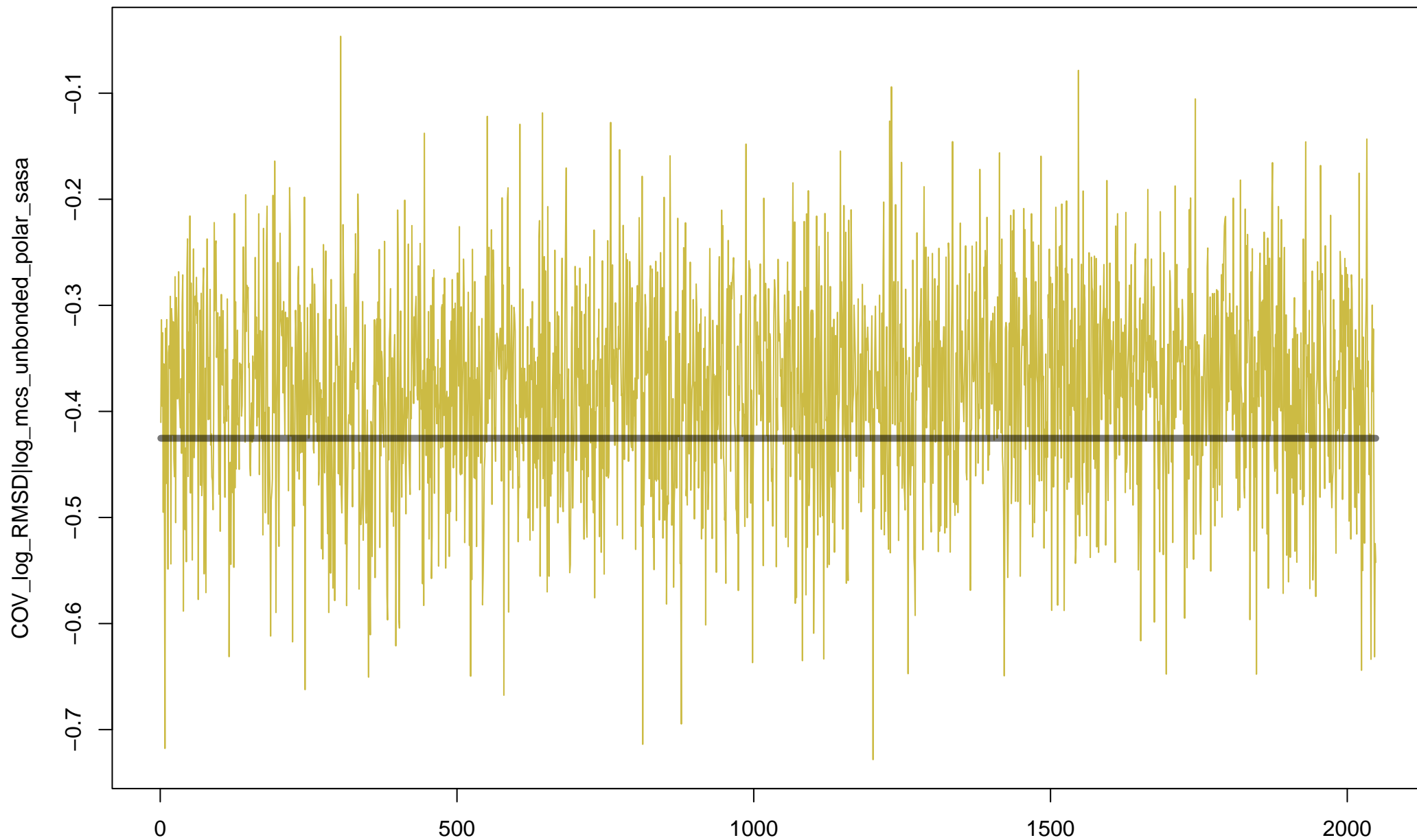
VAR_mcs_NumHeteroAtoms
ESS = 1770 | BMK = 0.0534 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: 0.444



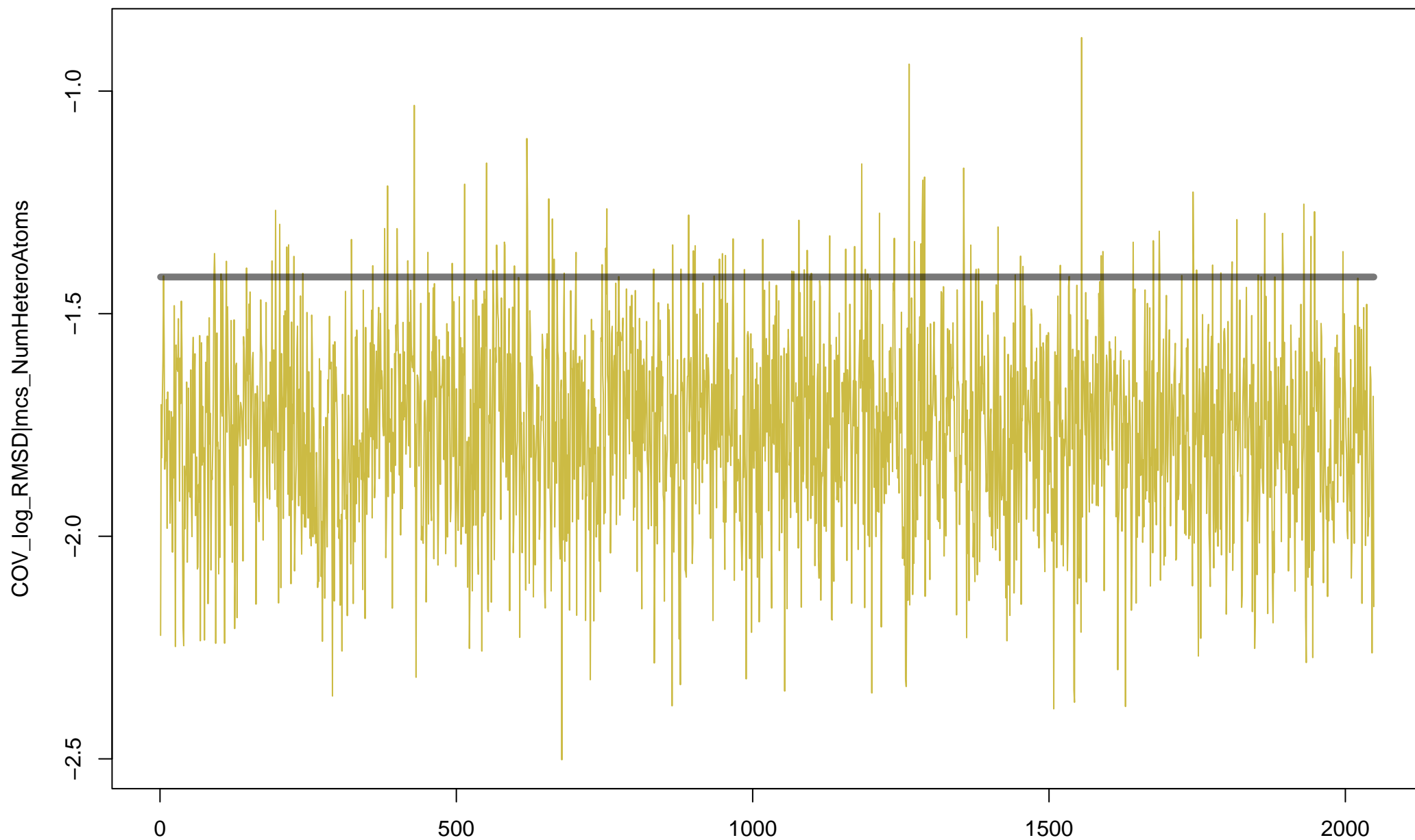
VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0508 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 0.0442



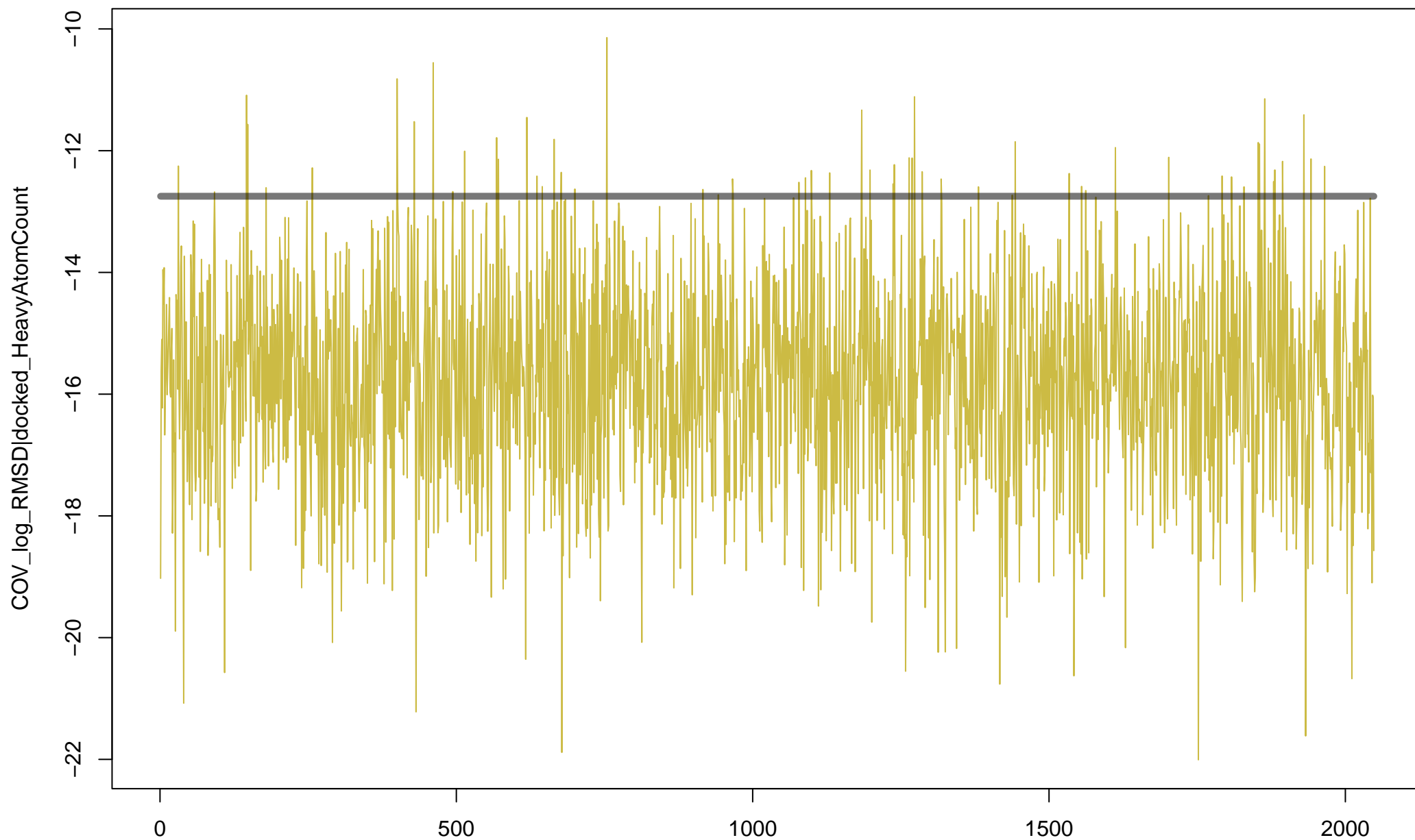
COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0477 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: 0.471



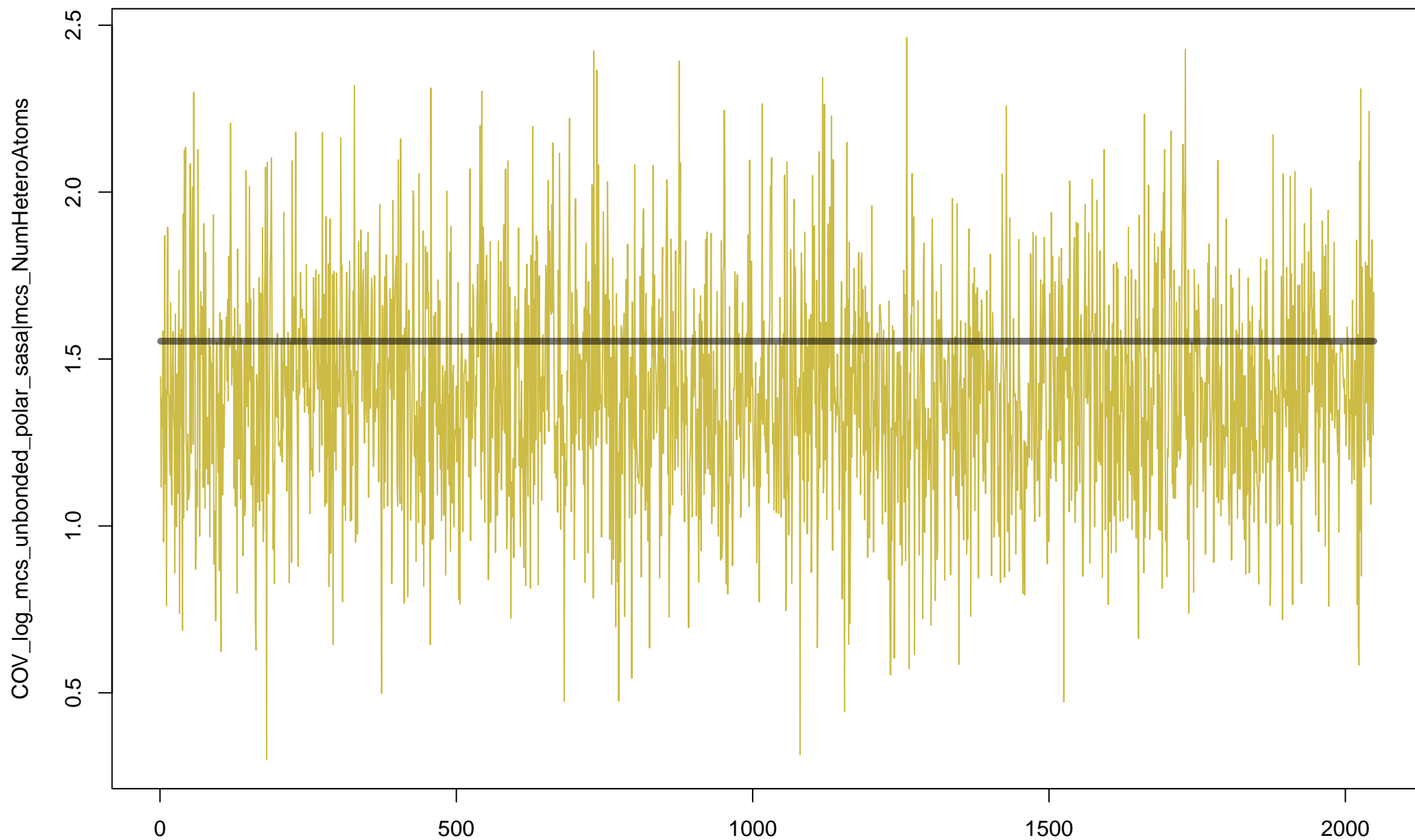
COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1860 | BMK = 0.0409 | MCSE(6.27) = 2.62 | stat: TRUE | burn: 0 | rel.err: -1.6



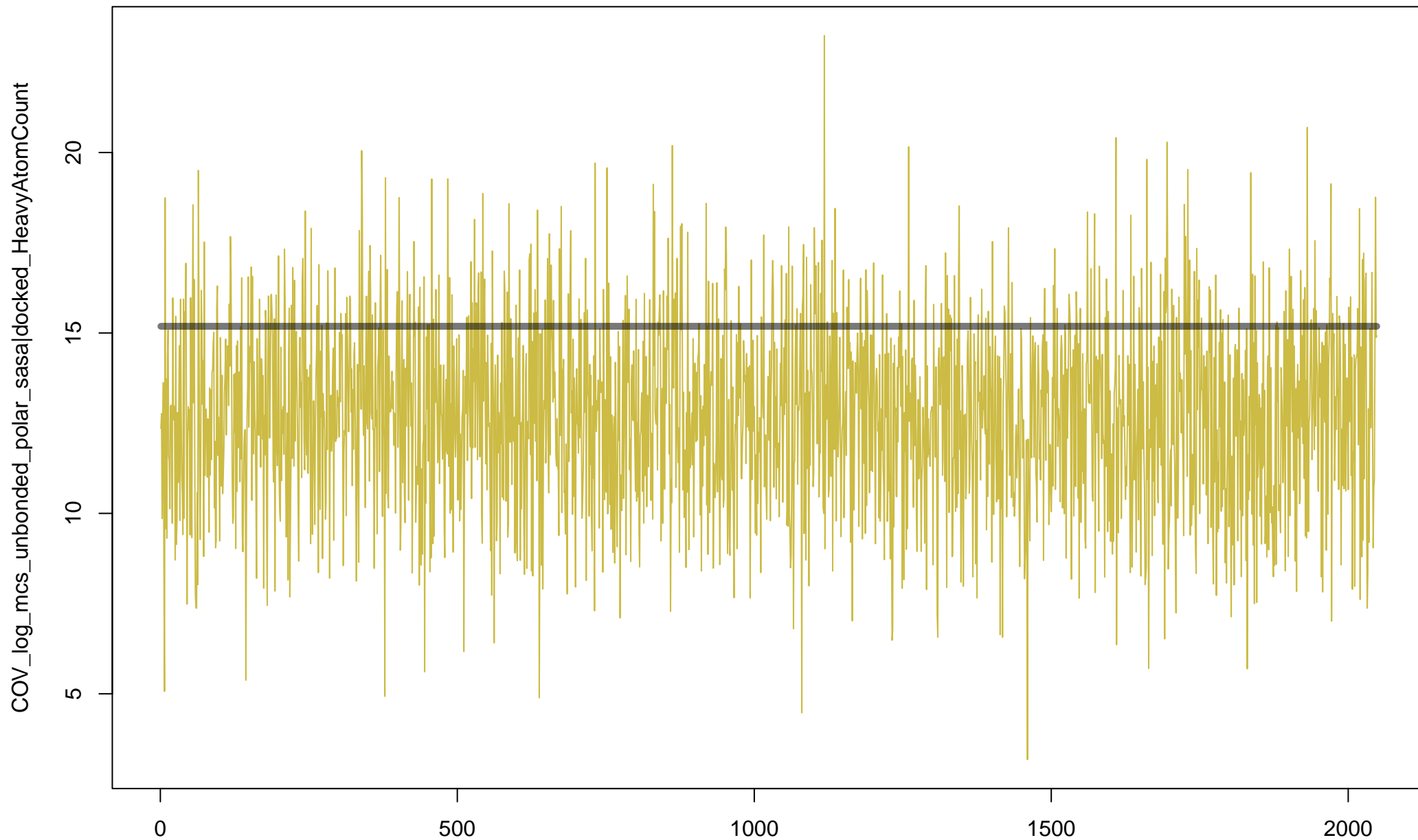
COV_log_RMSD|docked_HeavyAtomCount
ESS = 1950 | BMK = 0.0459 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: -1.85



COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1960 | BMK = 0.0362 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: -0.484



COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0622 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0 | rel.err: -0.966



COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0378 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: 0.467

