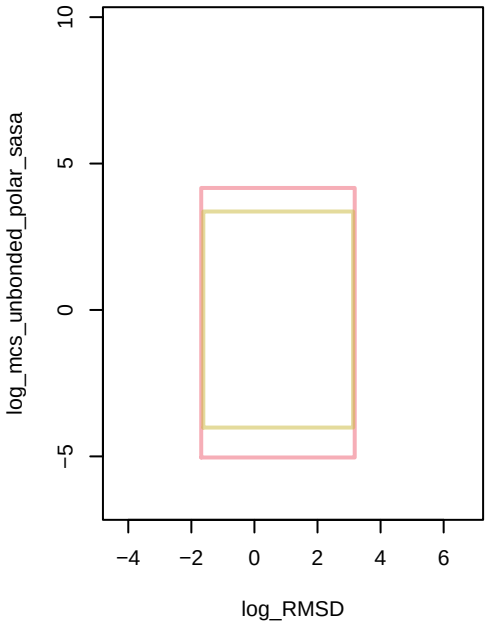
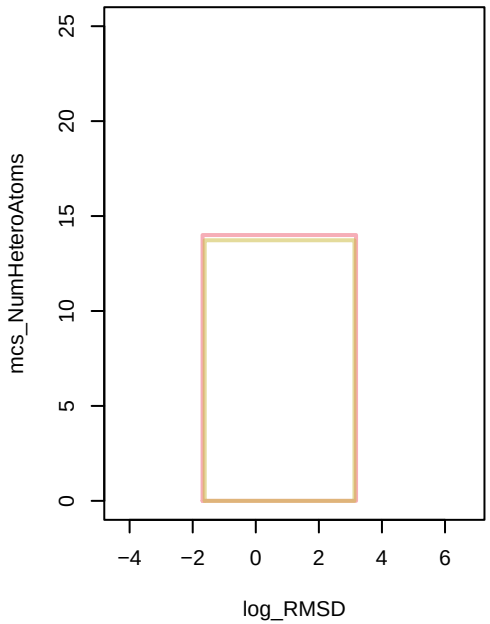
−− STATS maxD −−
min ESS = 134.759839775045
max BMK = 0.167314932613898
max MCSE = 7.47994902837165
all stationary: FALSE
burn: 0
max rel.err.: 2.01599558824284

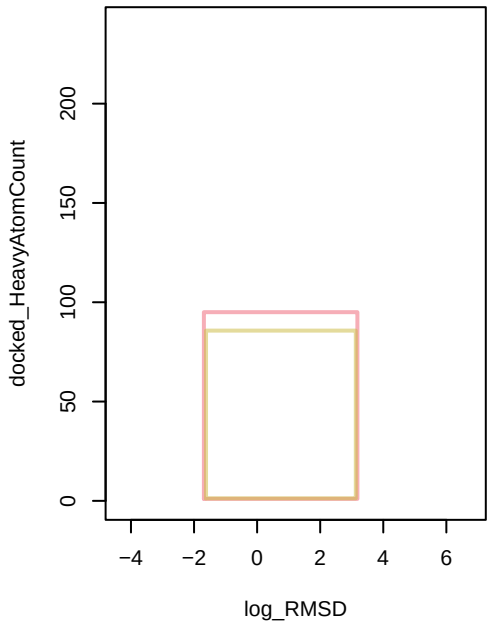
−− STATS 2D −−
min ESS = 1816.20039150839
max BMK = 0.047445835976675
max MCSE = 2.27191770727548
all stationary: TRUE
burn: 0
max rel.err.: 1.76720213788593

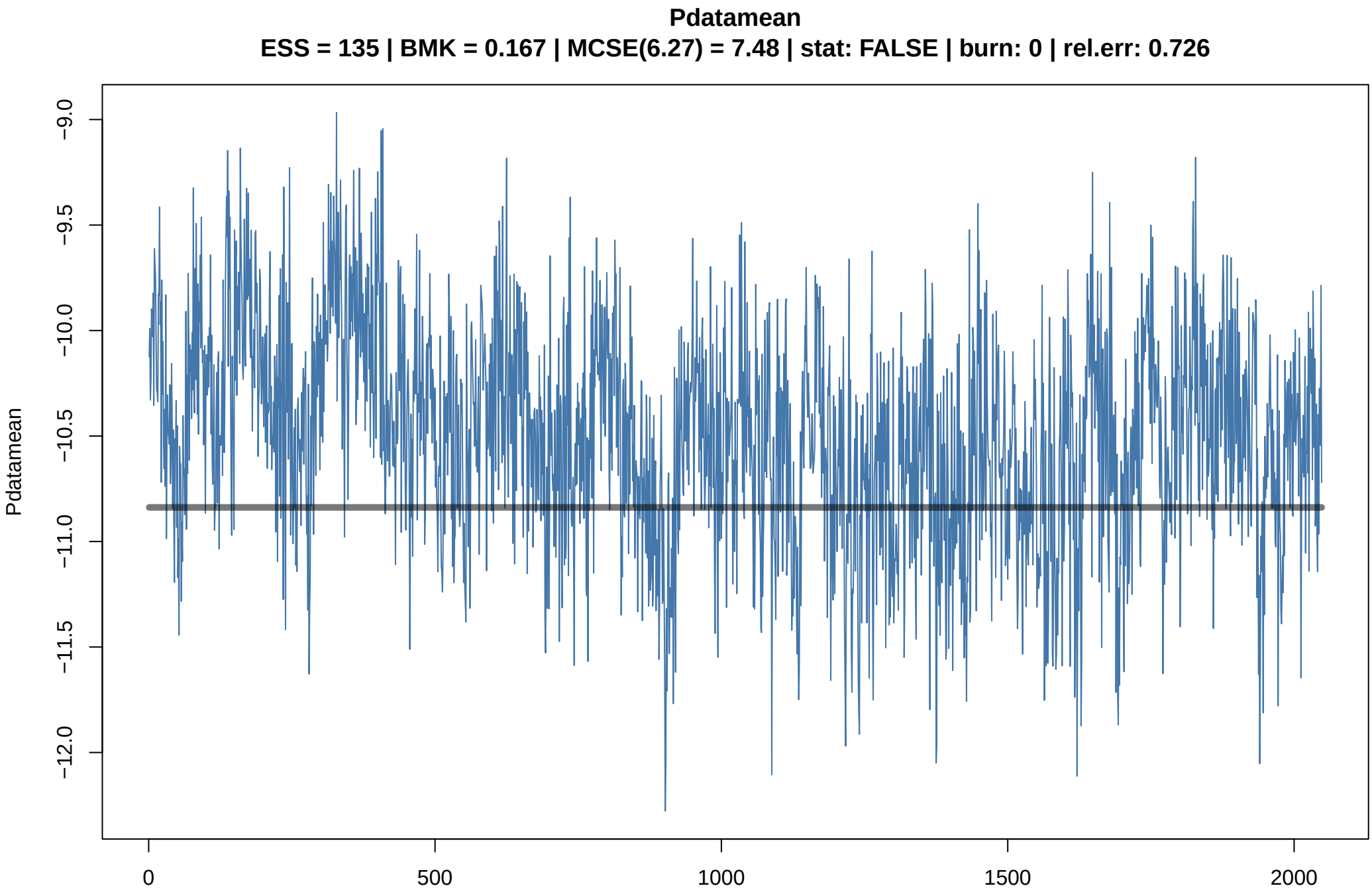
−− STATS 1D −−
min ESS = 1681.5405573915
max BMK = 0.064398734740048 9
max MCSE = 2.81418394666694
all stationary: TRUE
burn: 0
max rel.err.: 2.33350387093594

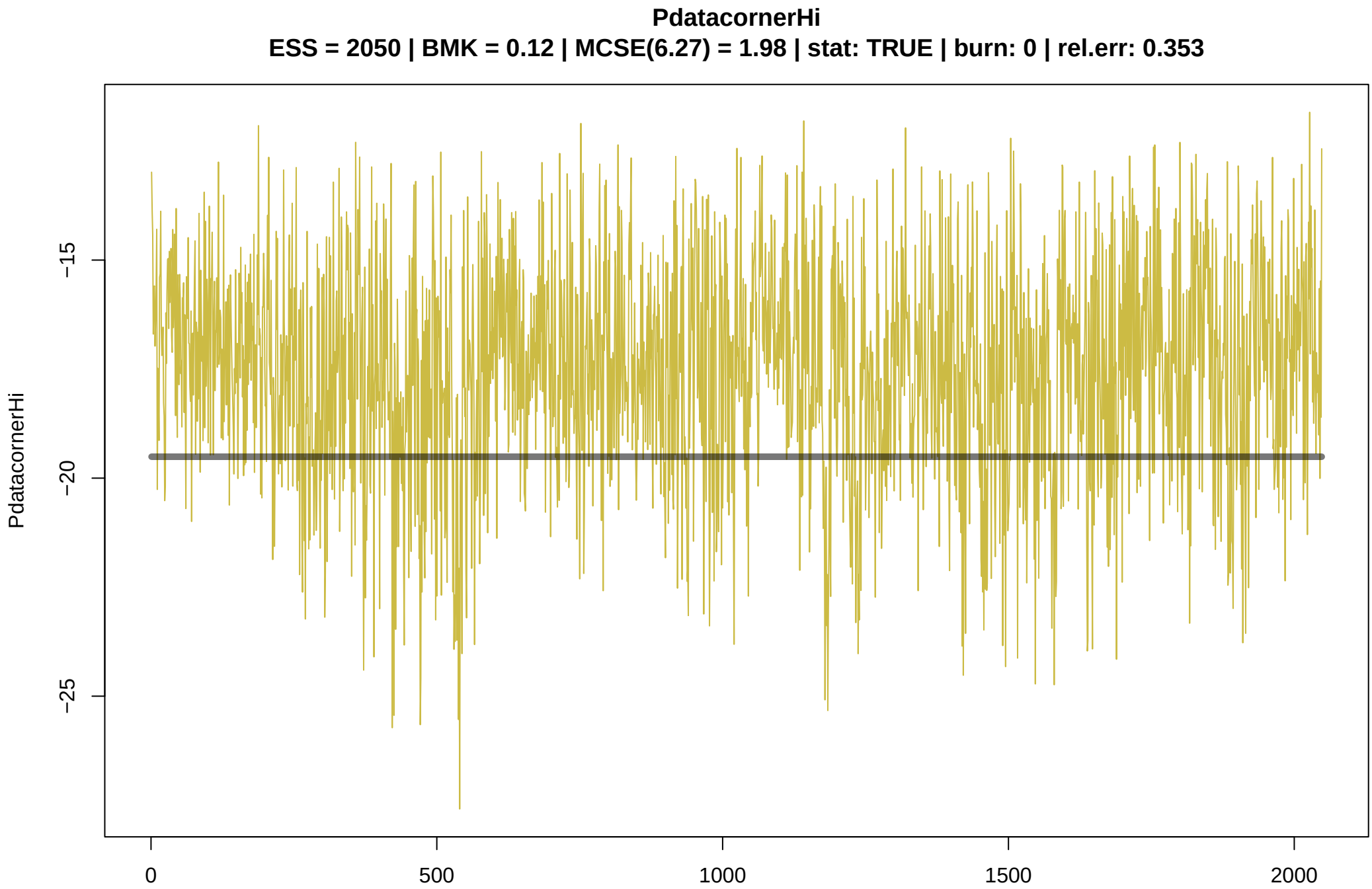
Occupied clusters: 9 of 16

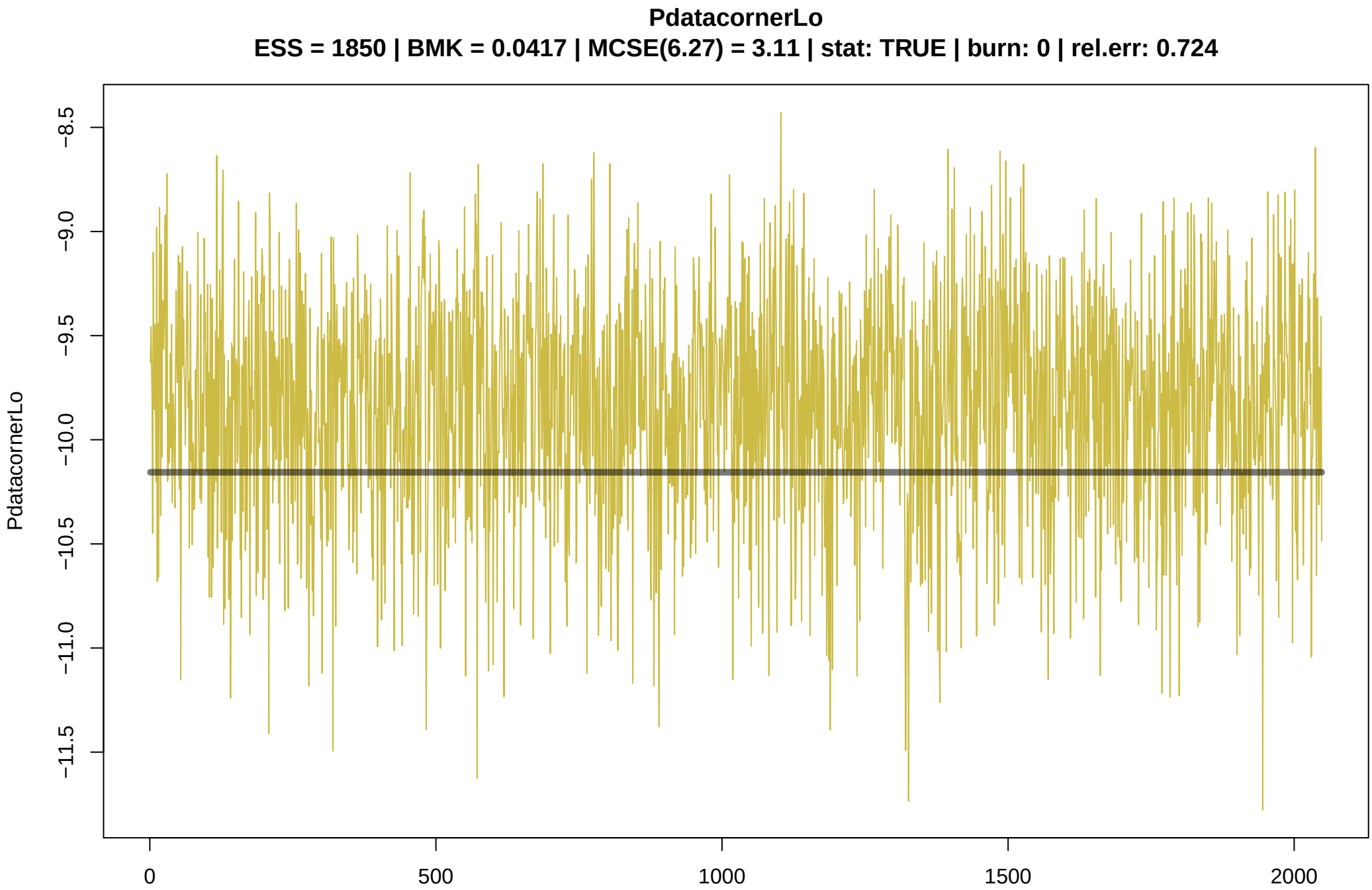

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

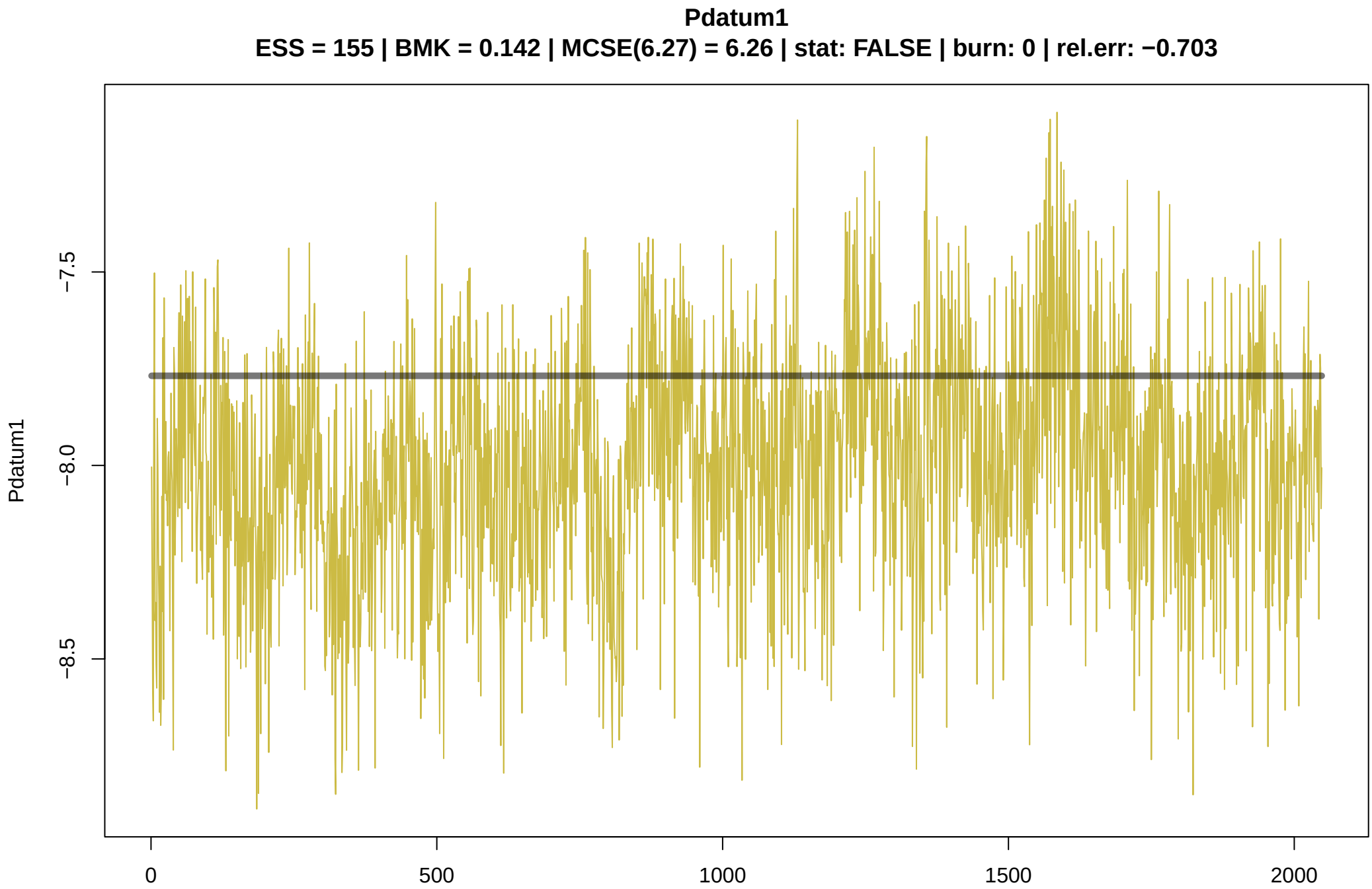

mcs_NumHeteroAtoms
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

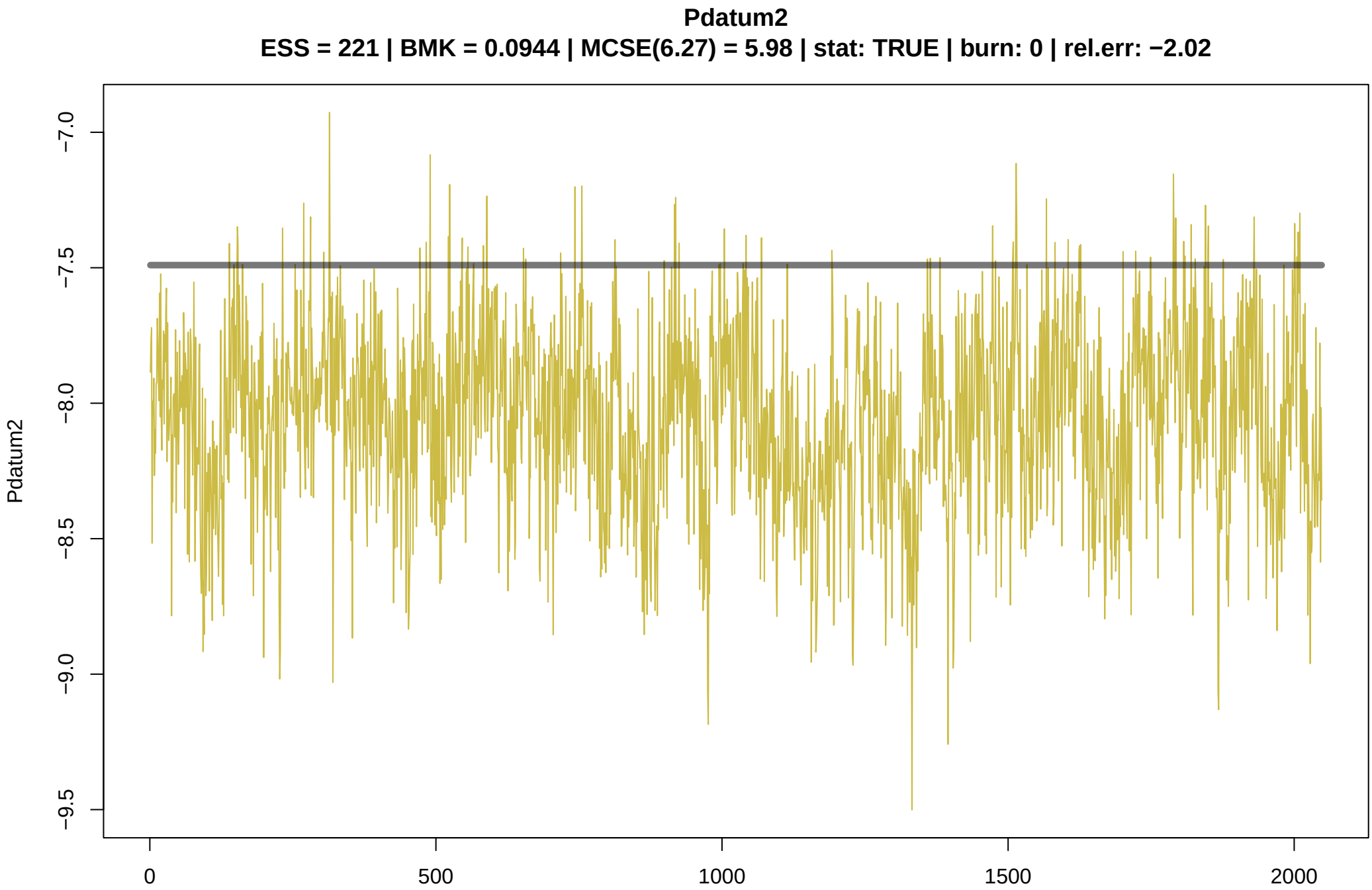

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

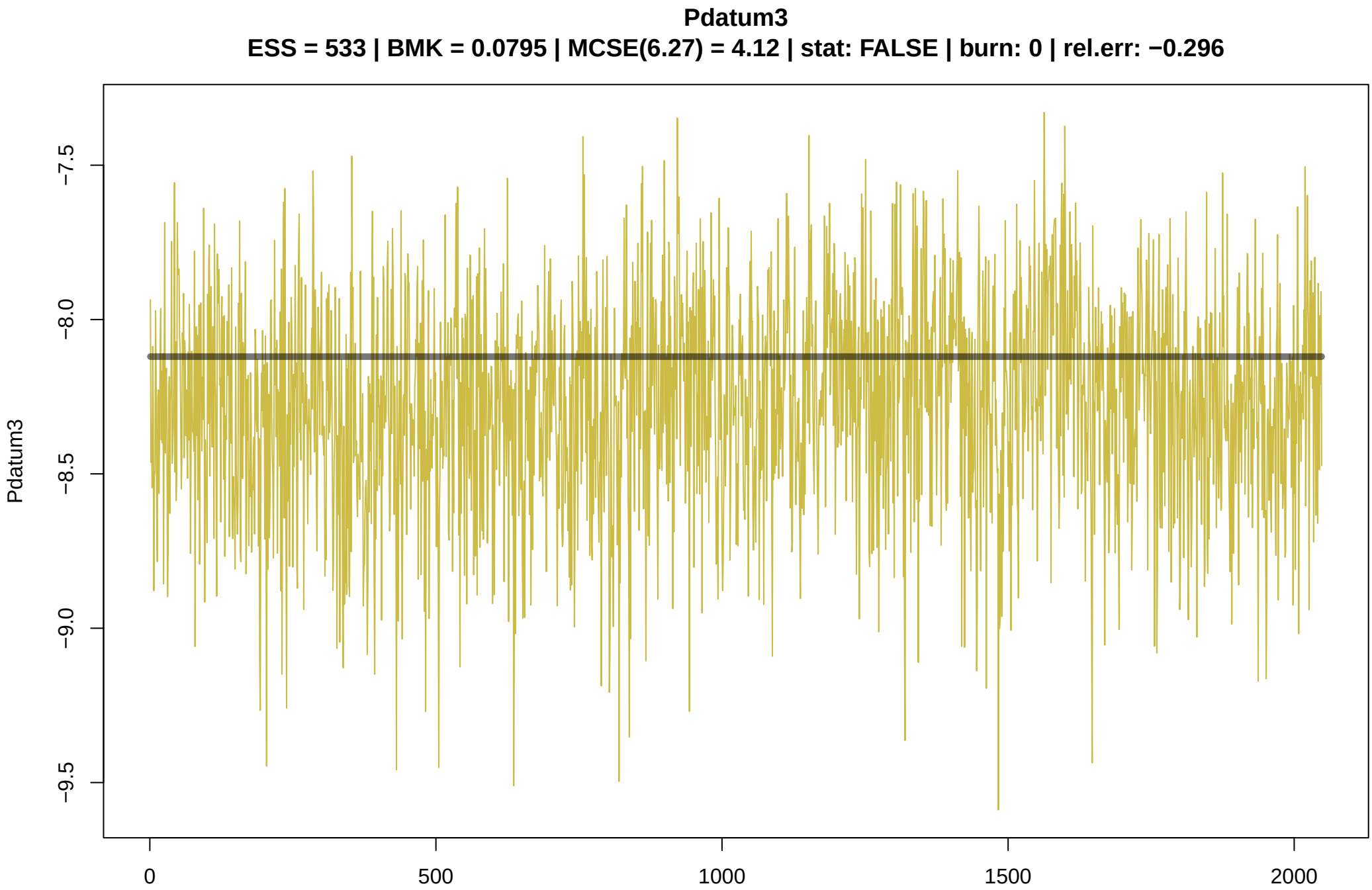

Pdatamean
ESS = 135 | BMK = 0.167 | MCSE(6.27) = 7.48 | stat: FALSE | burn: 0 | rel.err: 0.726
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

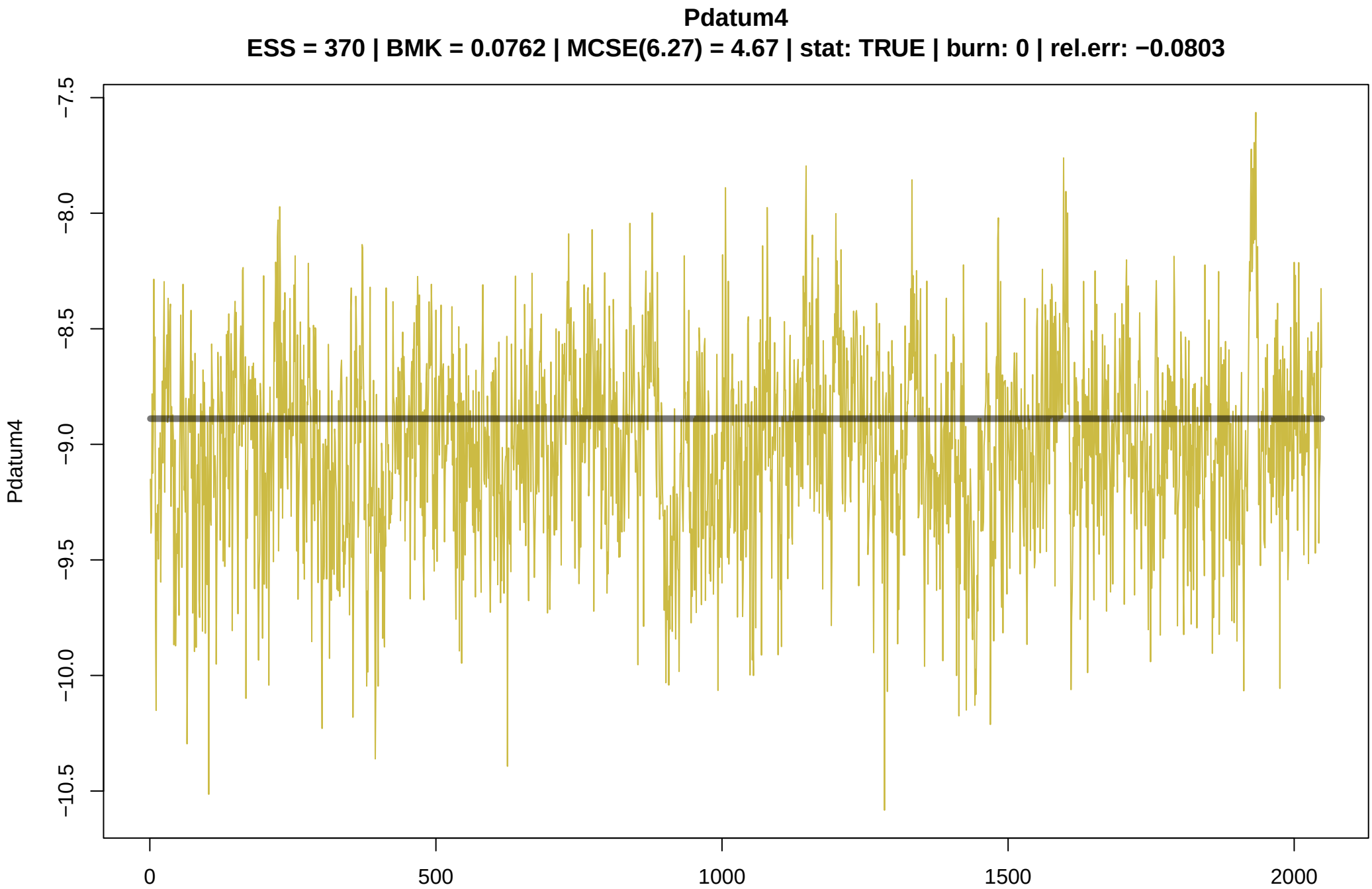

PdatacornerHi
ESS = 2050 | BMK = 0.12 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | rel.err: 0.353
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

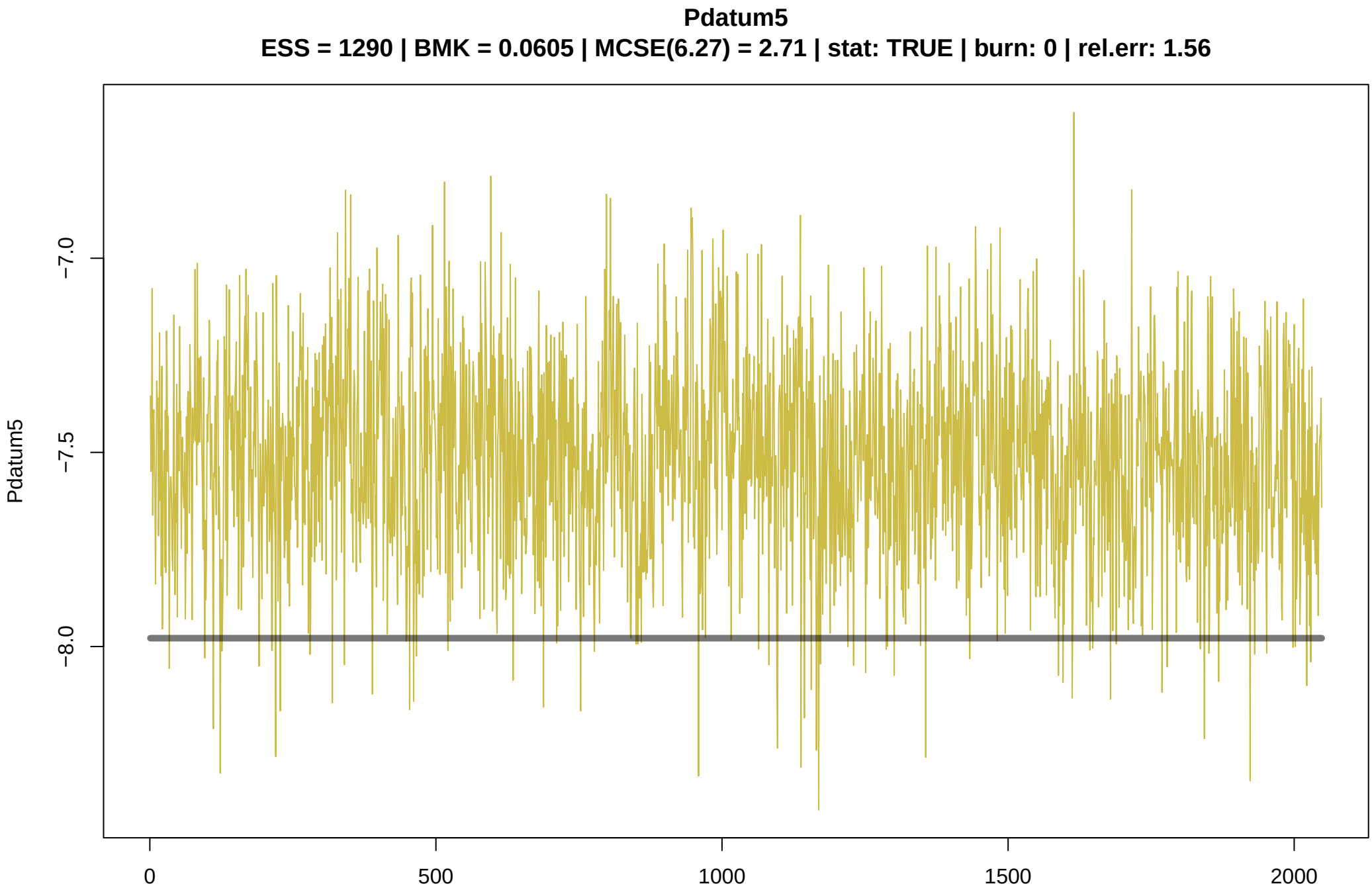

PdatacornerLo
ESS = 1850 | BMK = 0.0417 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: 0.724
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
0
500
1000
1500
2000

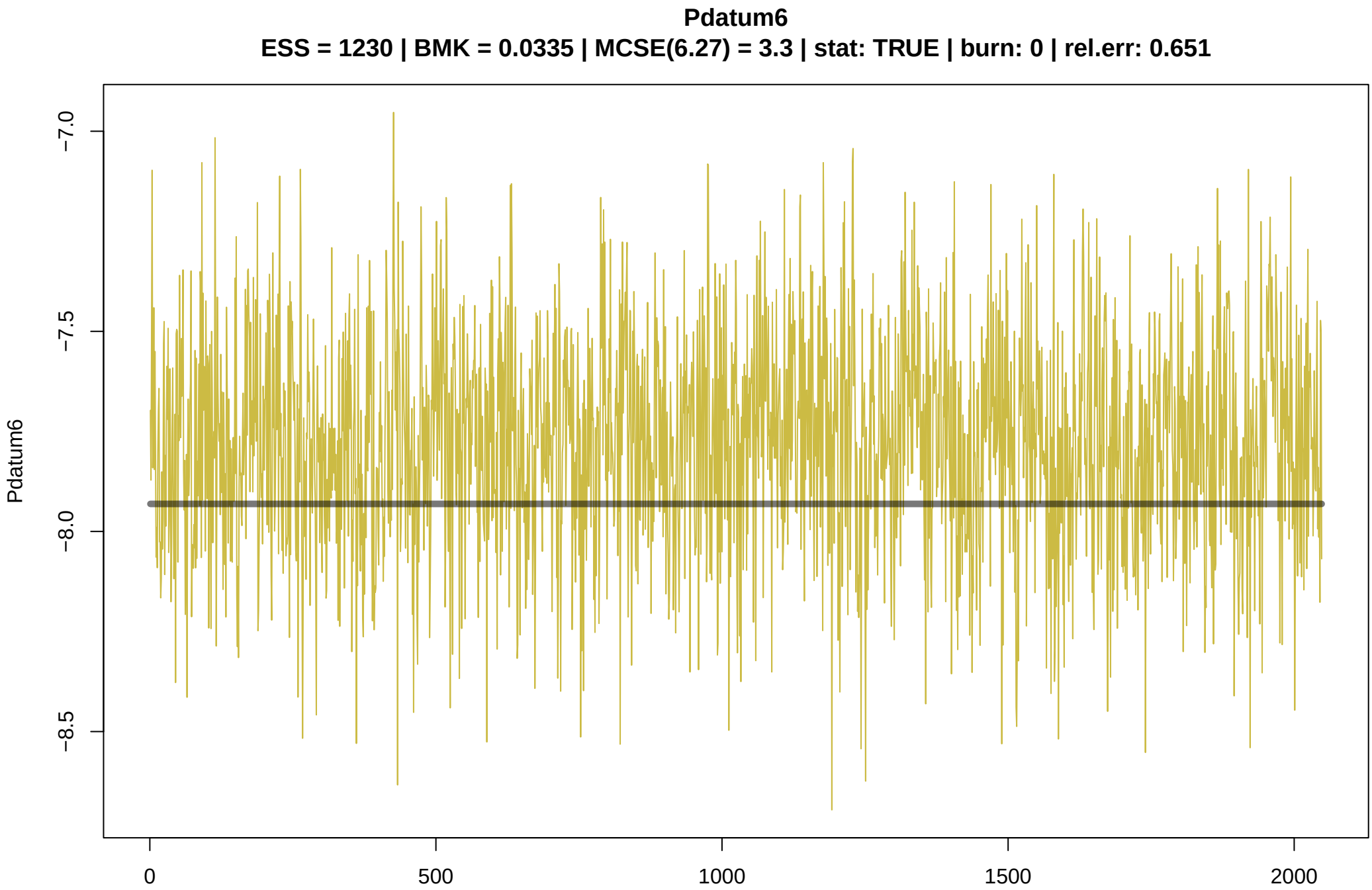

Pdatum1
ESS = 155 | BMK = 0.142 | MCSE(6.27) = 6.26 | stat: FALSE | burn: 0 | rel.err: −0.703
Pdatum1
−7.5
−8.0
−8.5
0
500
1000
1500
2000

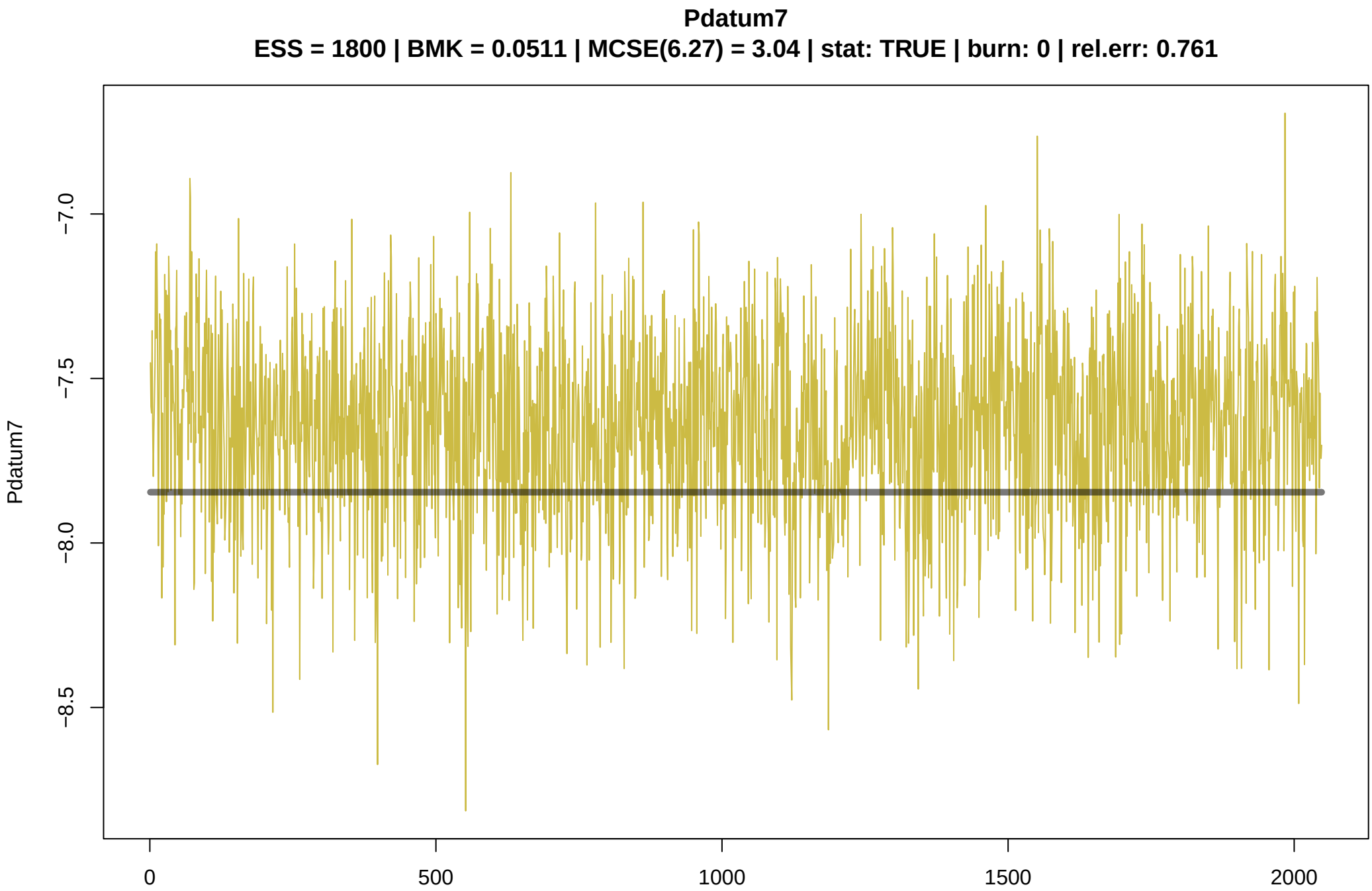

Pdatum2
ESS = 221 | BMK = 0.0944 | MCSE(6.27) = 5.98 | stat: TRUE | burn: 0 | rel.err: −2.02
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

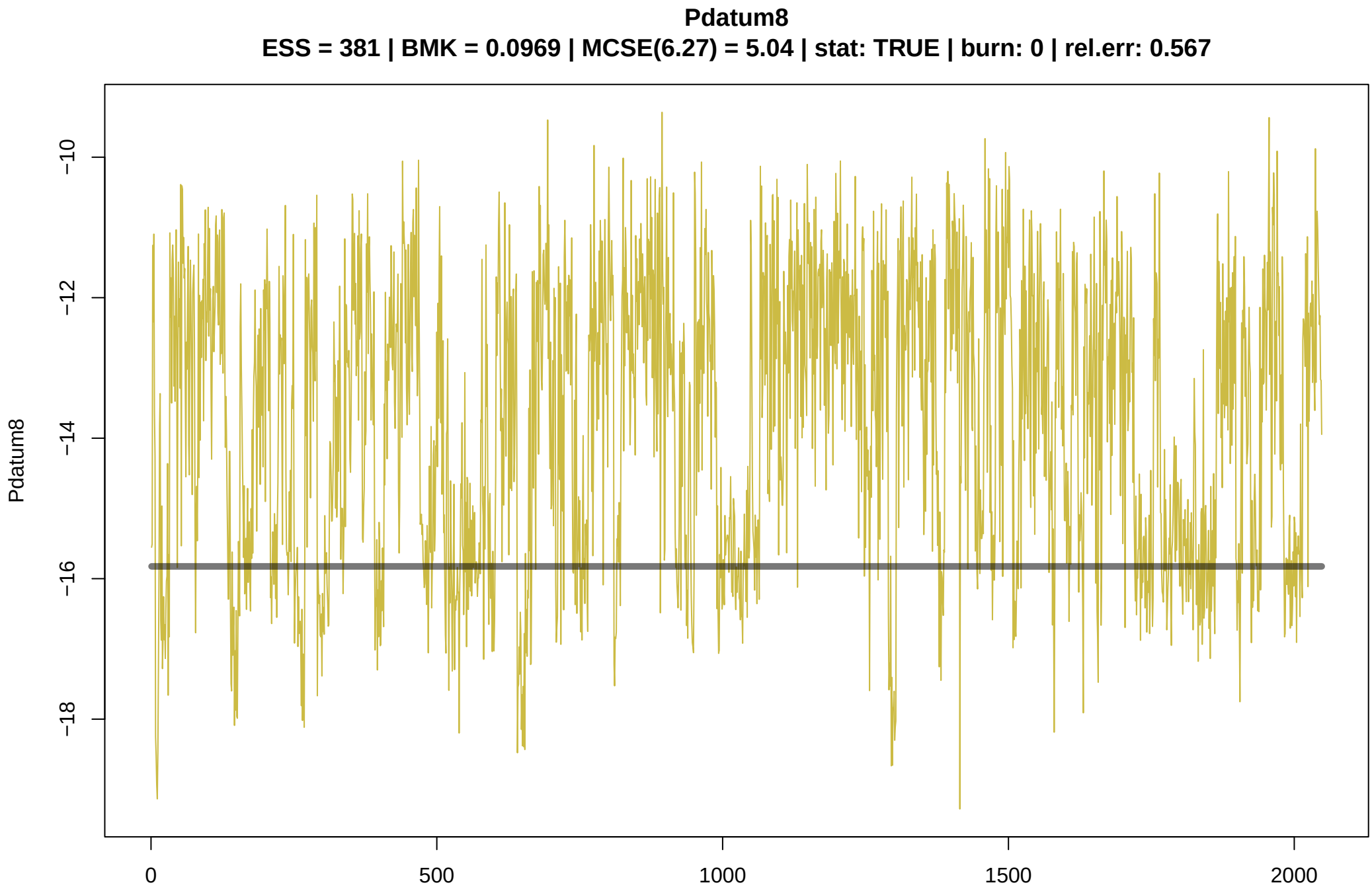

Pdatum3
ESS = 533 | BMK = 0.0795 | MCSE(6.27) = 4.12 | stat: FALSE | burn: 0 | rel.err: −0.296
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

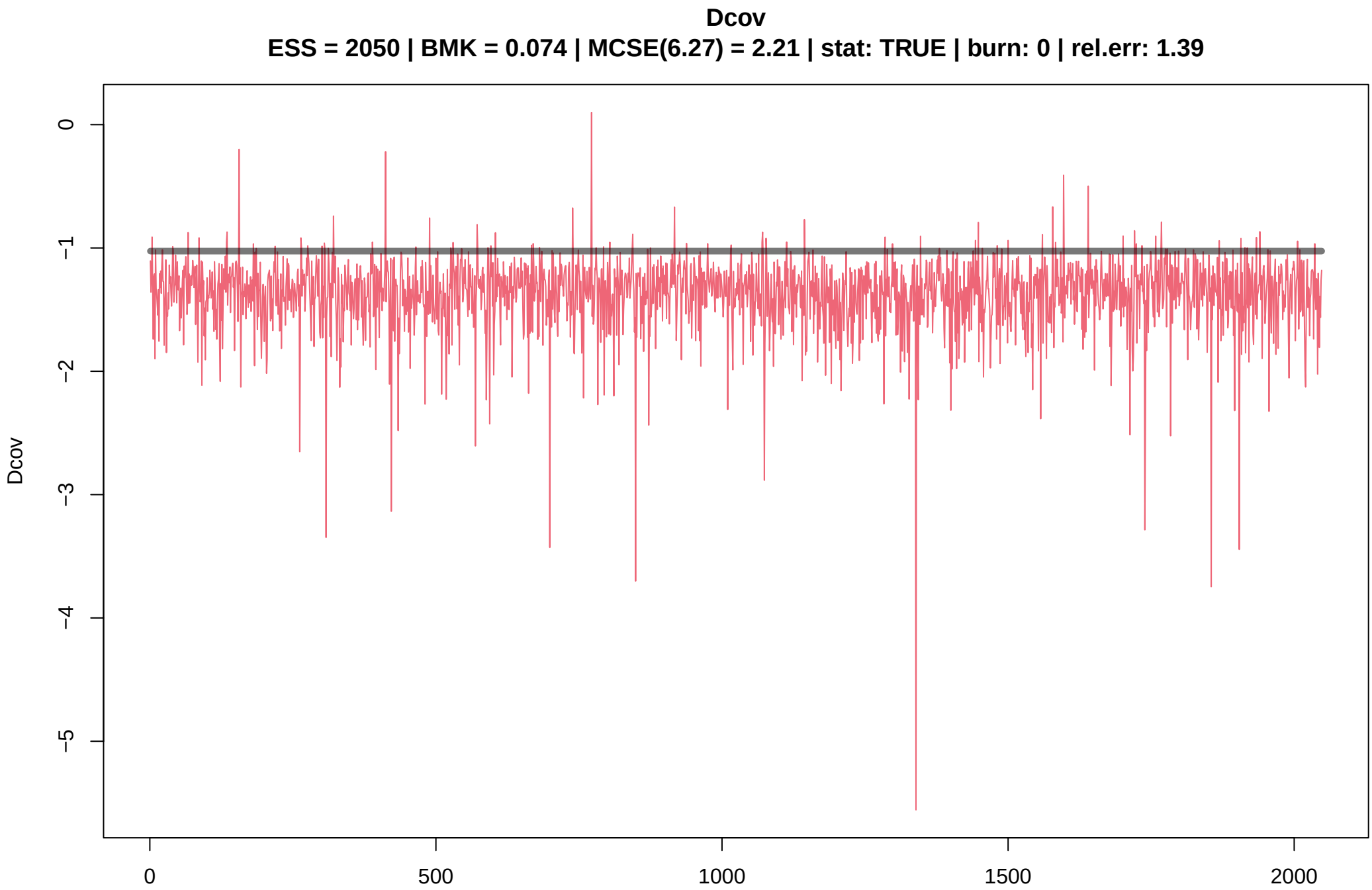

Pdatum4
ESS = 370 | BMK = 0.0762 | MCSE(6.27) = 4.67 | stat: TRUE | burn: 0 | rel.err: −0.0803
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

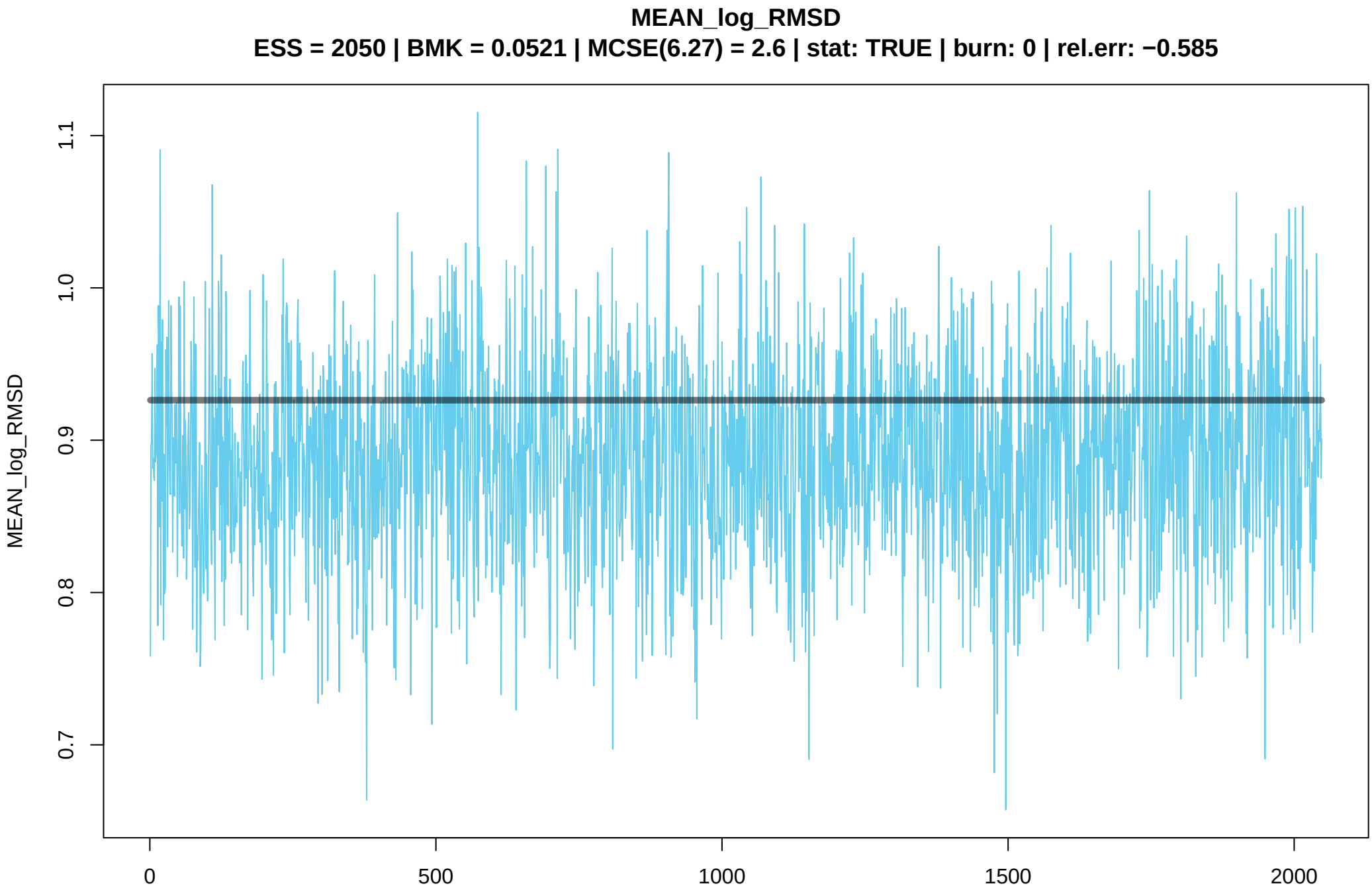

Pdatum5
ESS = 1290 | BMK = 0.0605 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0 | rel.err: 1.56
Pdatum5
−7.0
−7.5
−8.0
0
500
1000
1500
2000

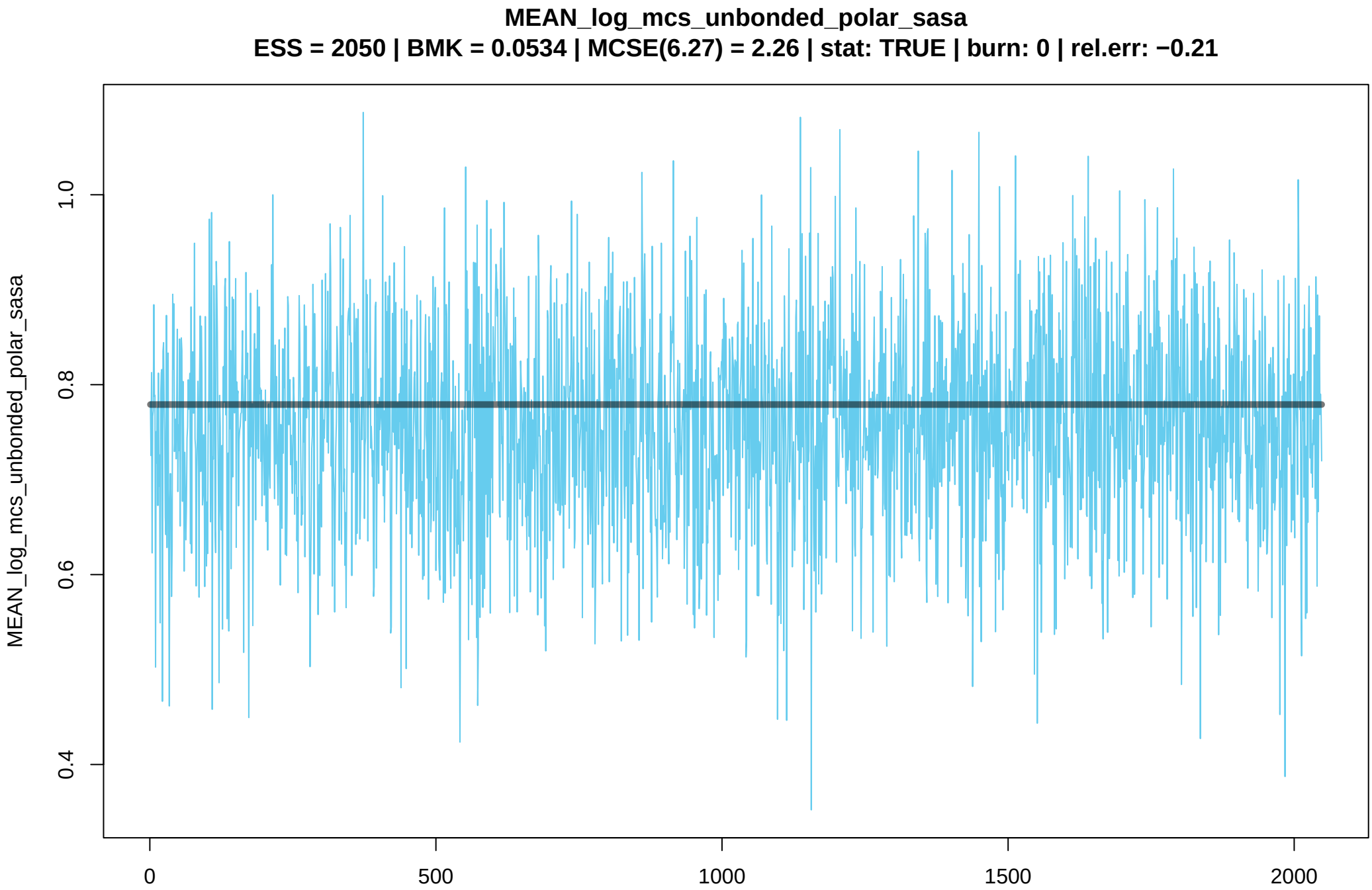

Pdatum6
ESS = 1230 | BMK = 0.0335 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: 0.651
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

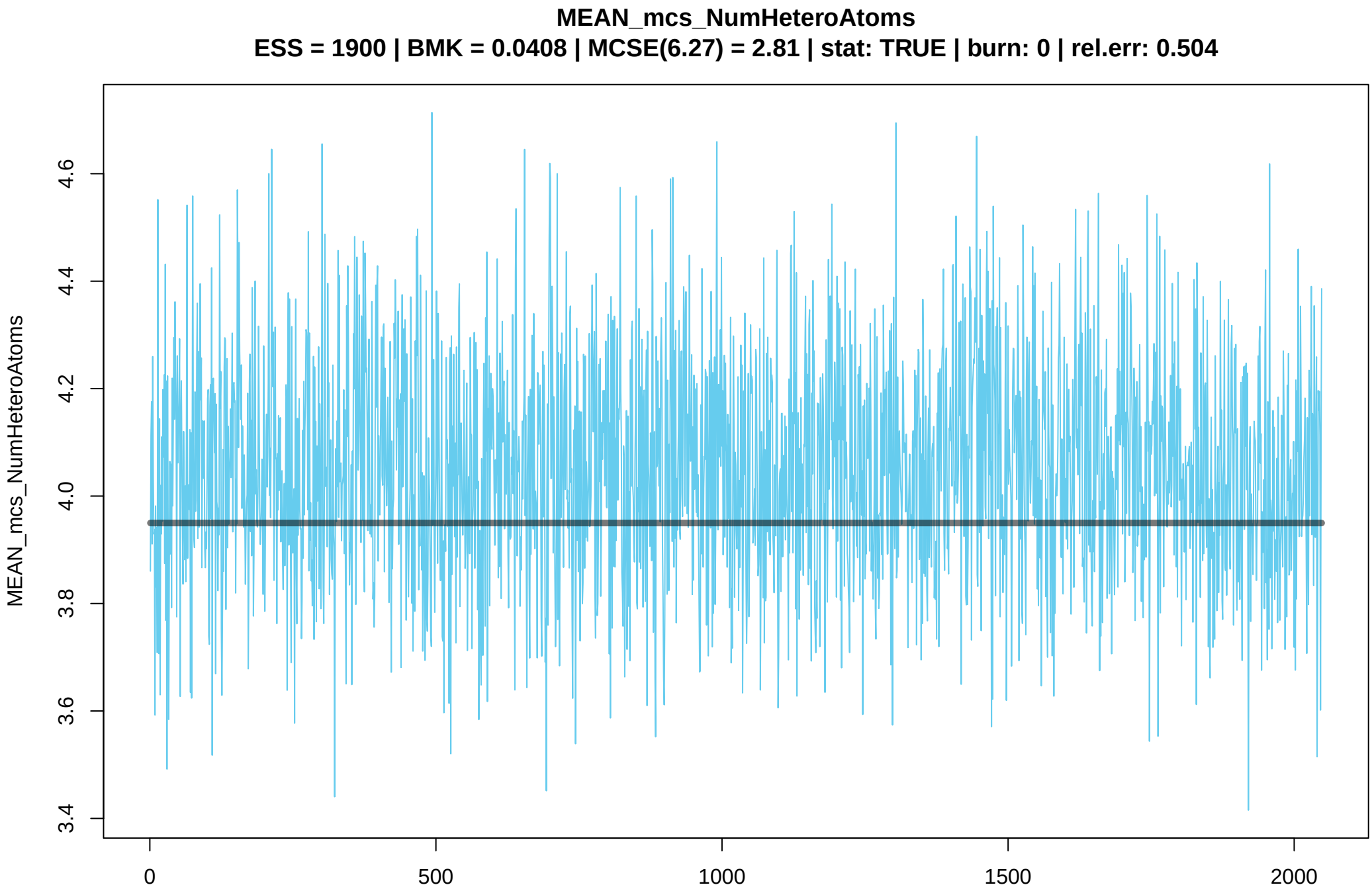

Pdatum7
ESS = 1800 | BMK = 0.0511 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 0.761
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

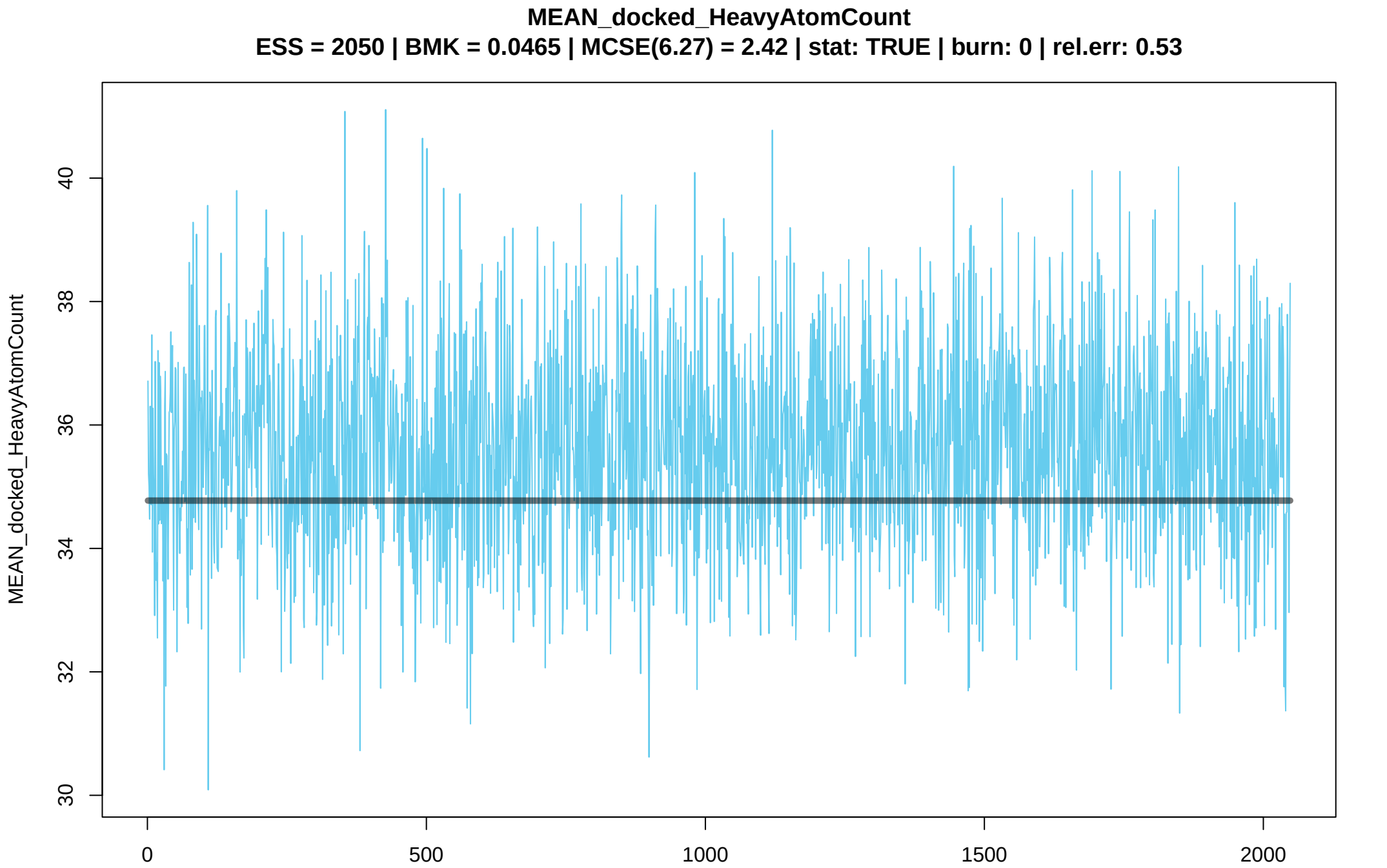

Pdatum8
ESS = 381 | BMK = 0.0969 | MCSE(6.27) = 5.04 | stat: TRUE | burn: 0 | rel.err: 0.567
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

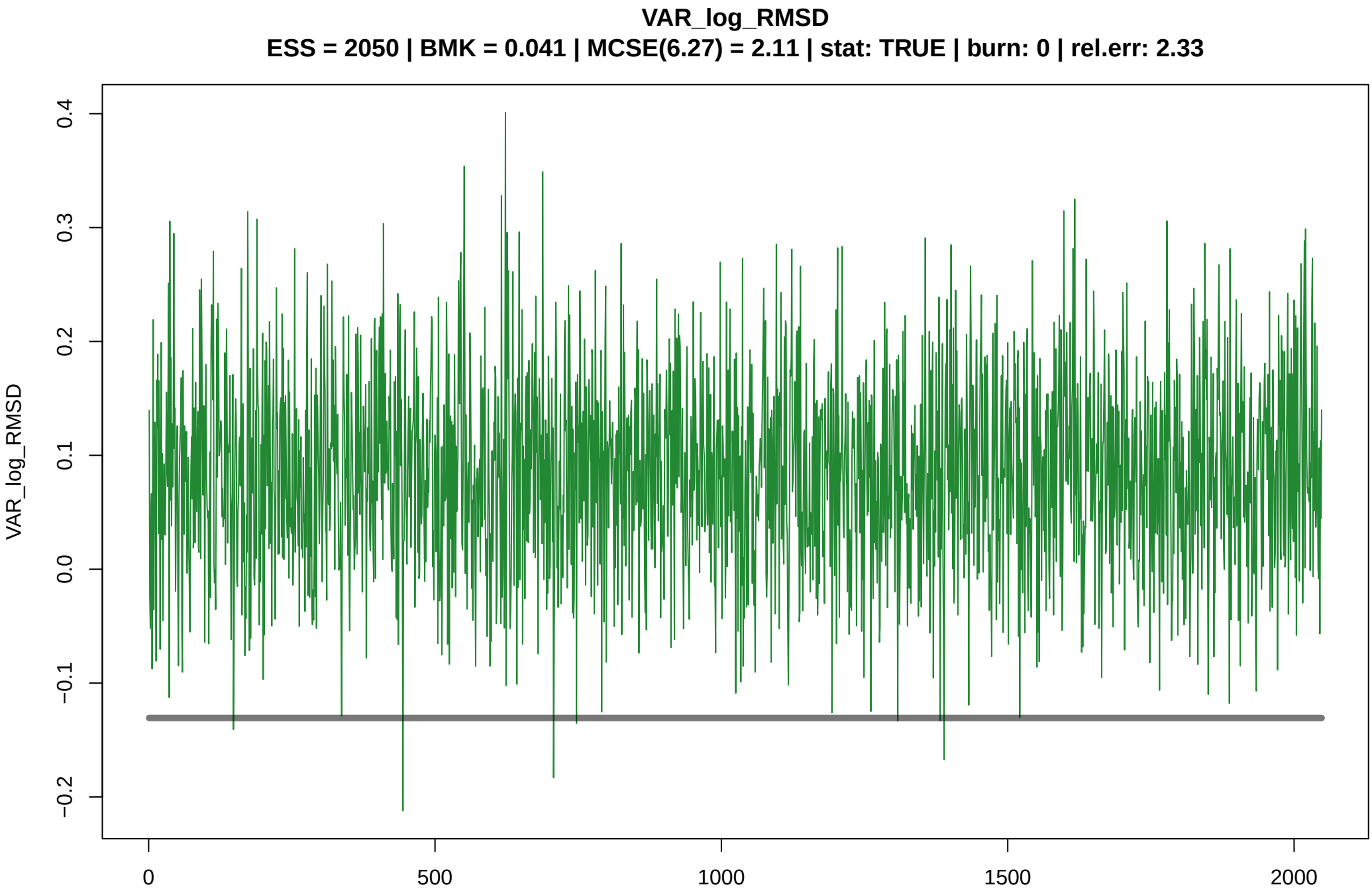

Dcov
ESS = 2050 | BMK = 0.074 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: 1.39
Dcov
0
−1
−2
−3
−4
−5
0
500
1000
1500
2000

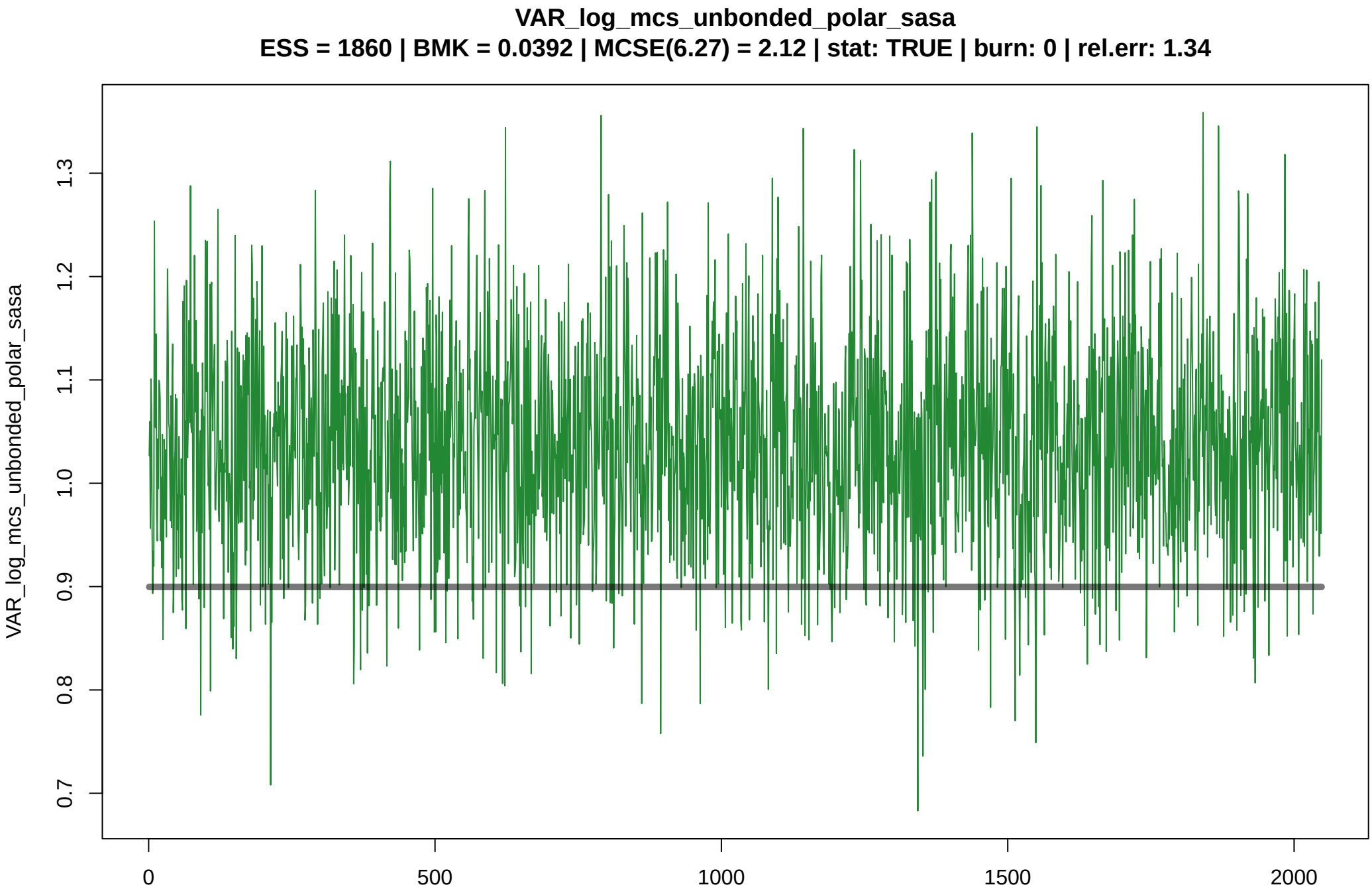

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0521 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: −0.585
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

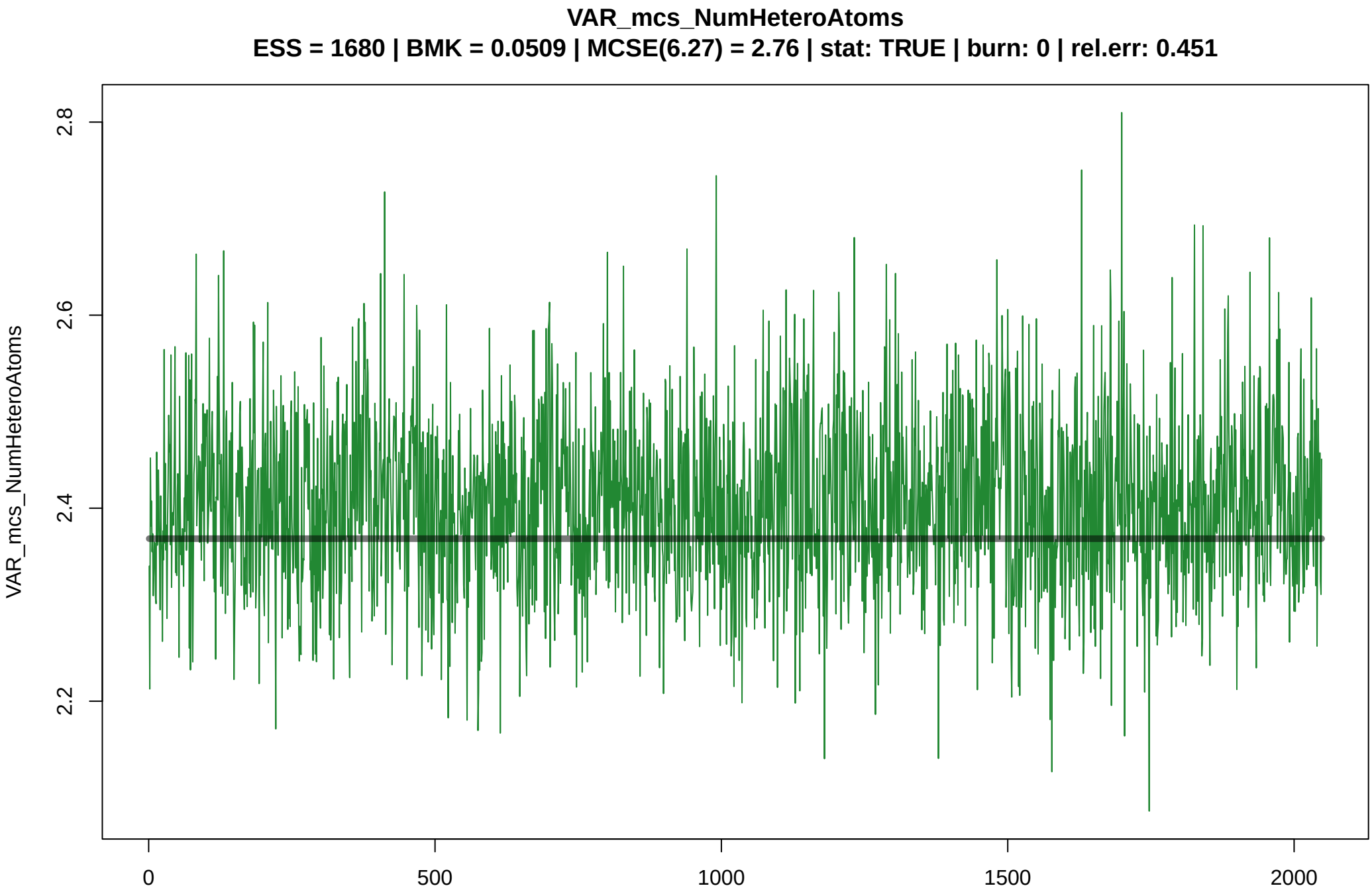

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0534 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: −0.21
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

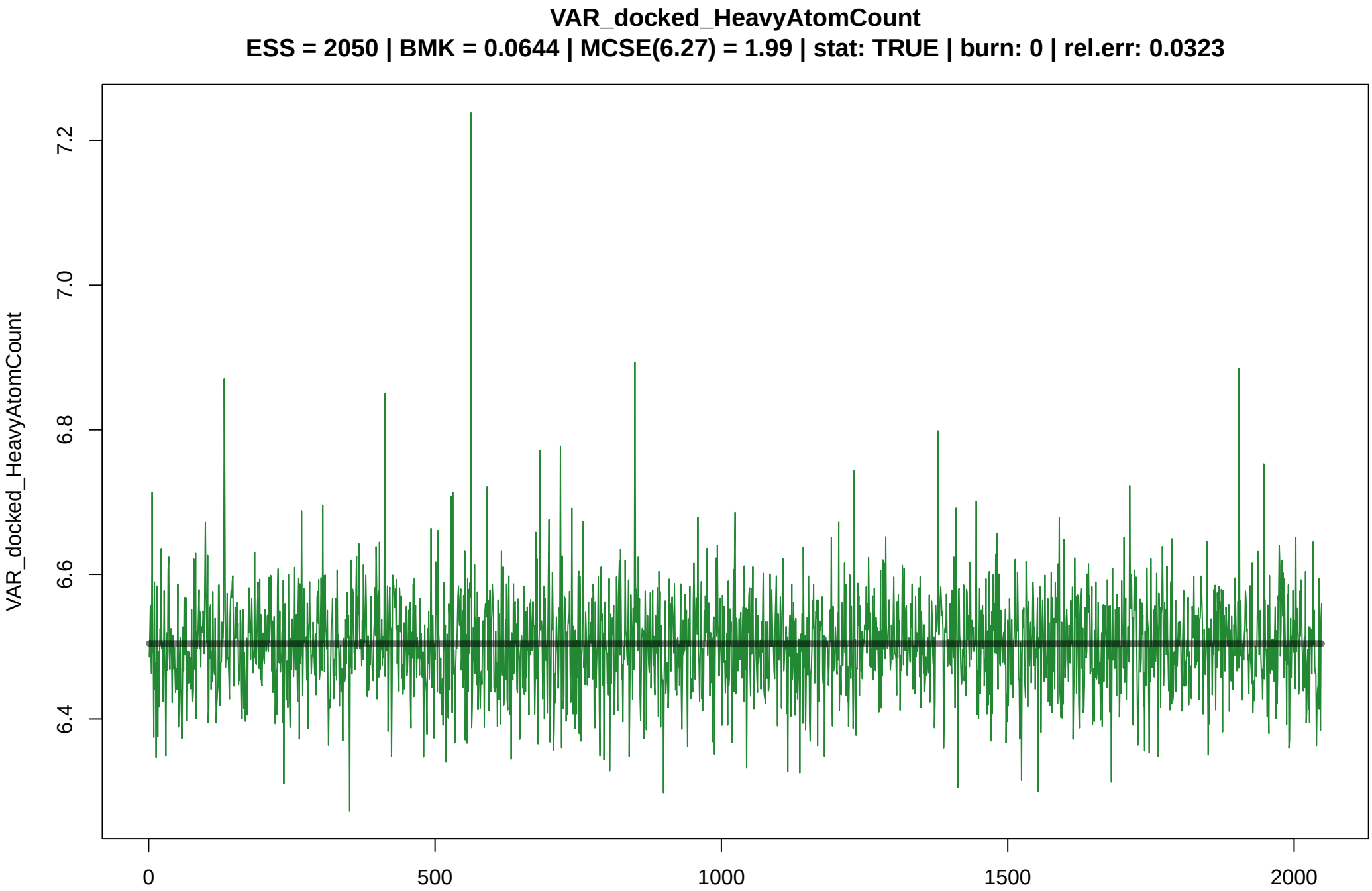

MEAN_mcs_NumHeteroAtoms
ESS = 1900 | BMK = 0.0408 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: 0.504
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
0
500
1000
1500
2000

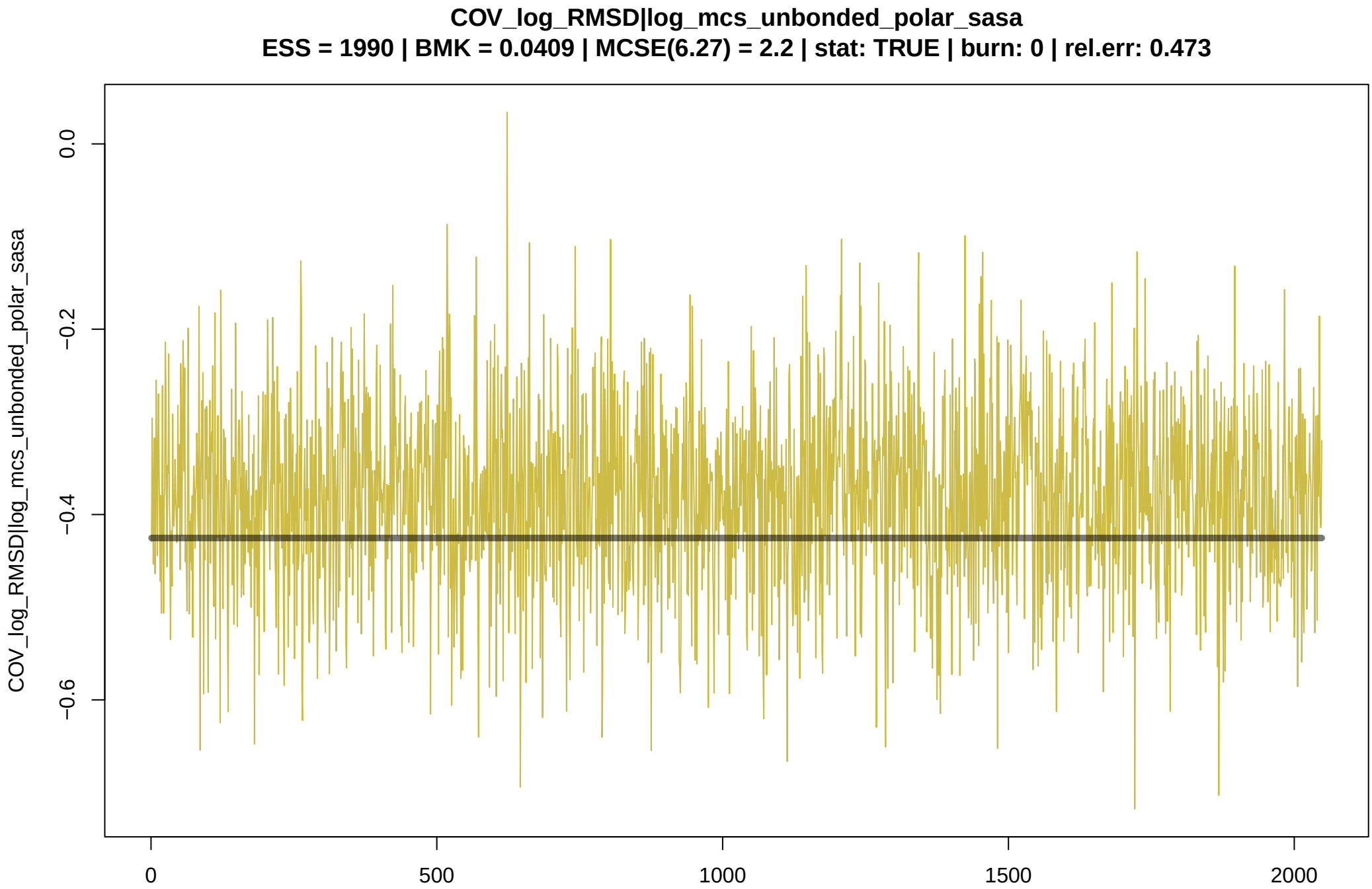

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0465 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.53
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

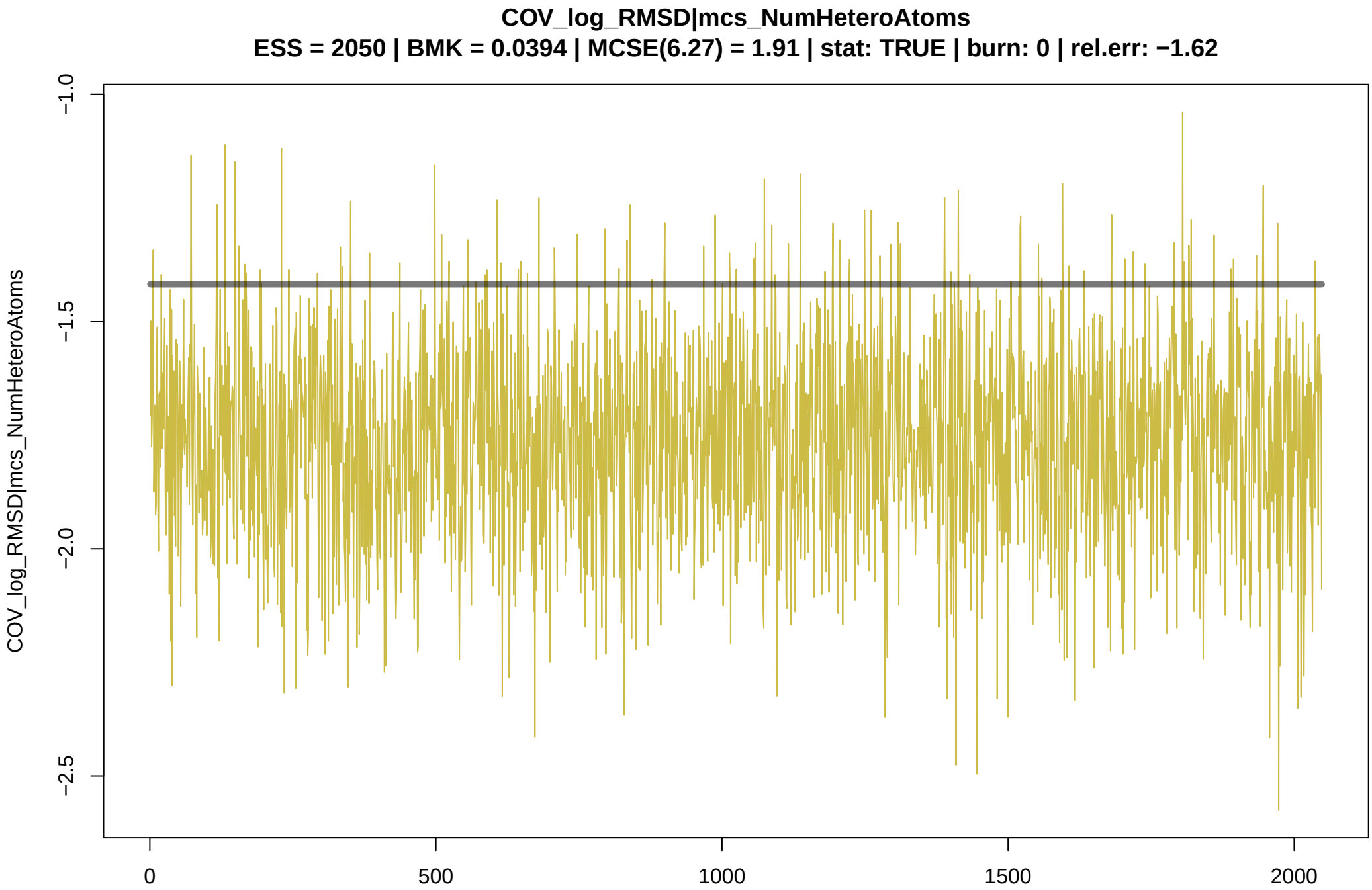

VAR_log_RMSD
ESS = 2050 | BMK = 0.041 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: 2.33
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

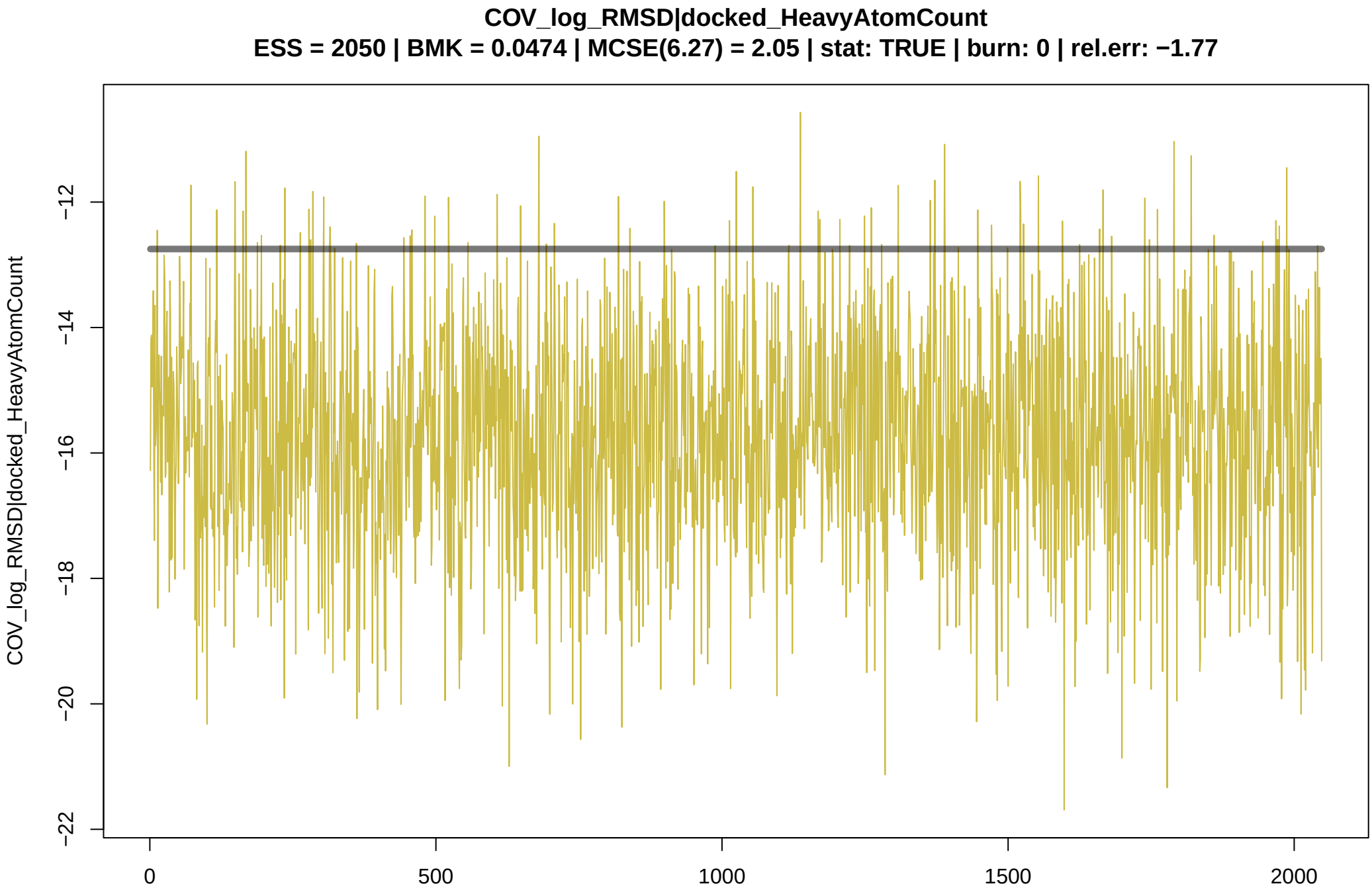

VAR_log_mcs_unbonded_polar_sasa
ESS = 1860 | BMK = 0.0392 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: 1.34
VAR_log_mcs_unbonded_polar_sasa
0.7
0.8
0.9
1.0
1.1
1.2
1.3
0
500
1000
1500
2000

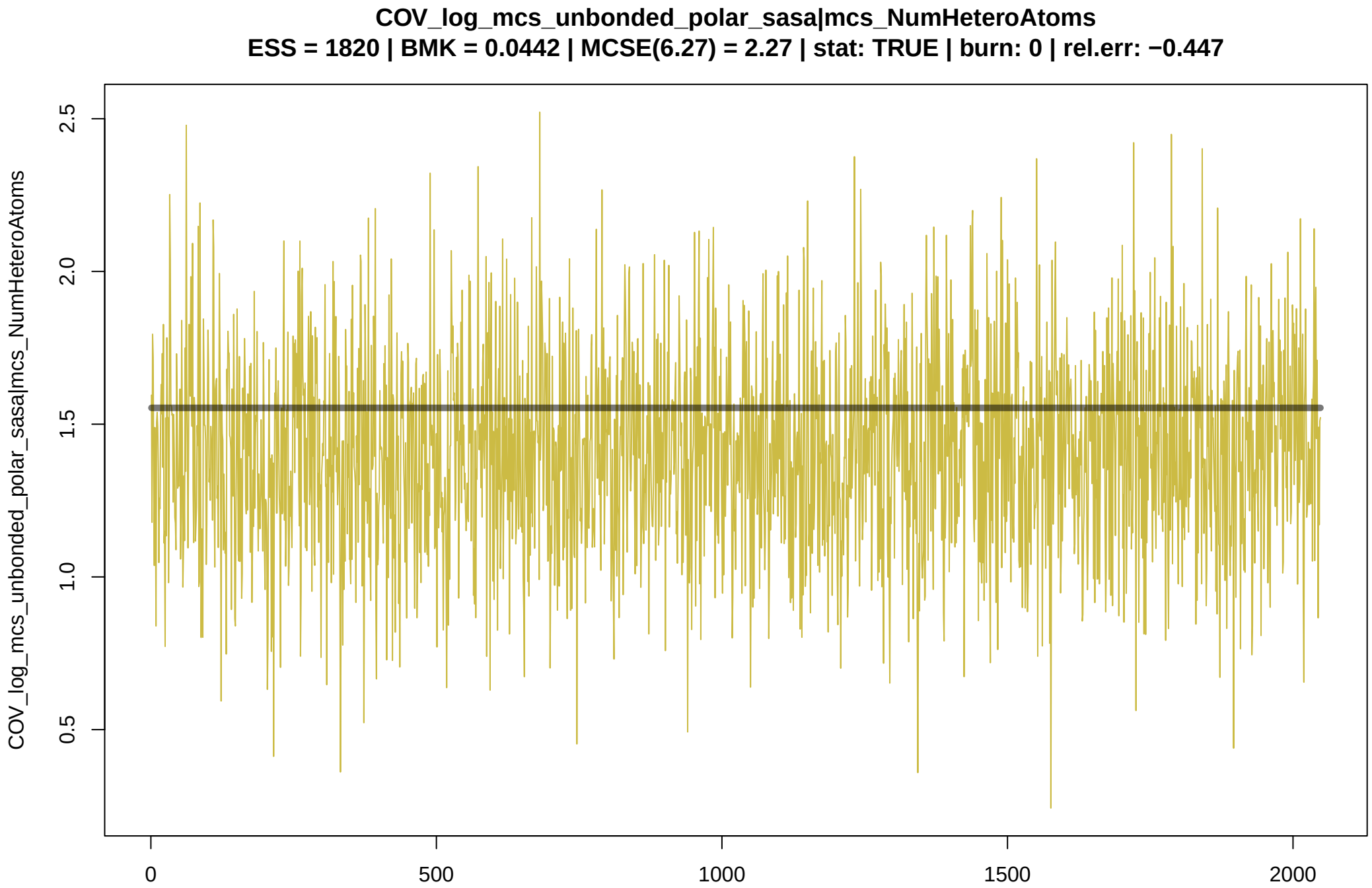

VAR_mcs_NumHeteroAtoms
ESS = 1680 | BMK = 0.0509 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: 0.451
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

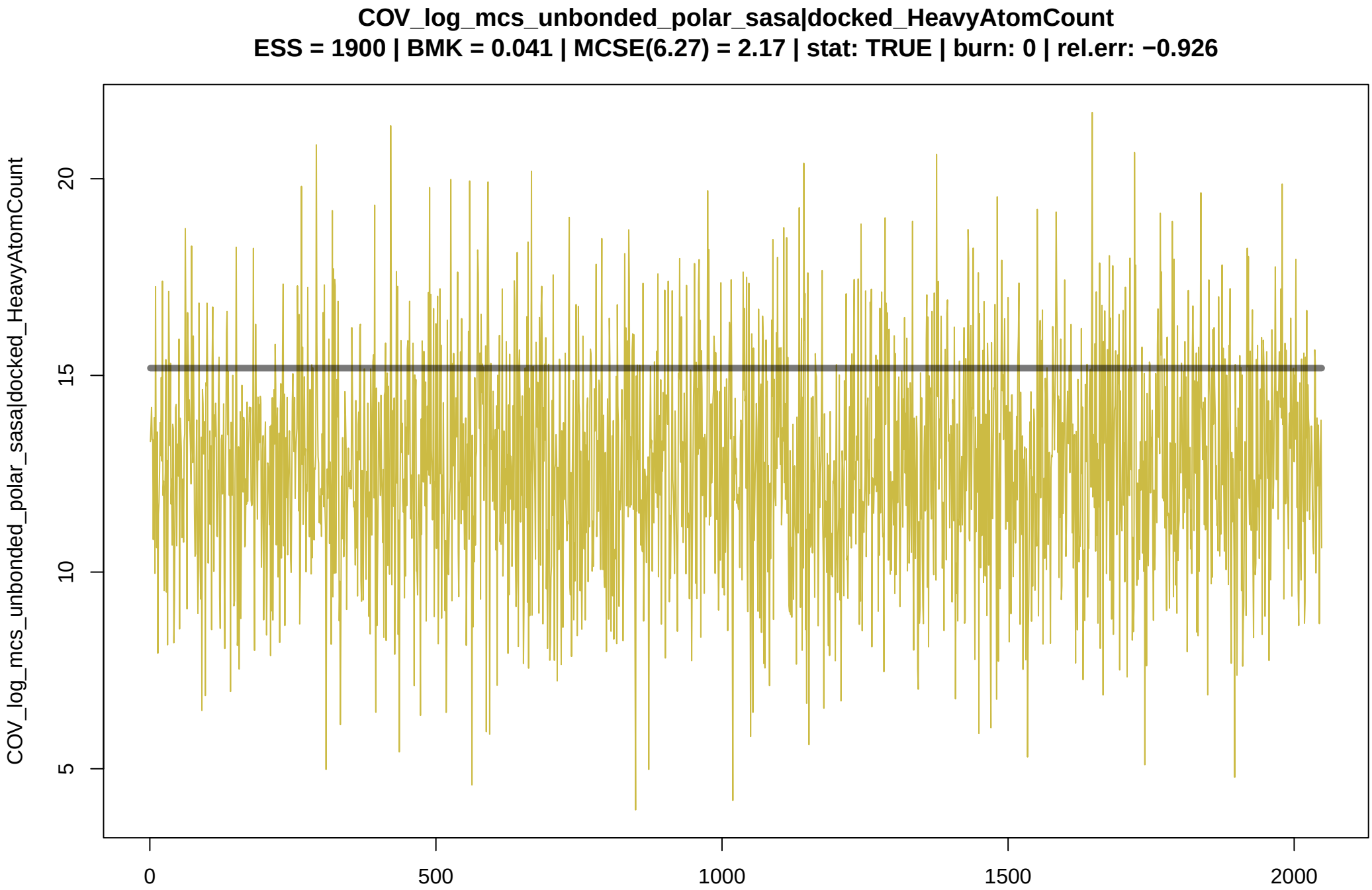

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0644 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 0.0323
VAR_docked_HeavyAtomCount
6.4
6.6
6.8
7.0
7.2
0
500
1000
1500
2000

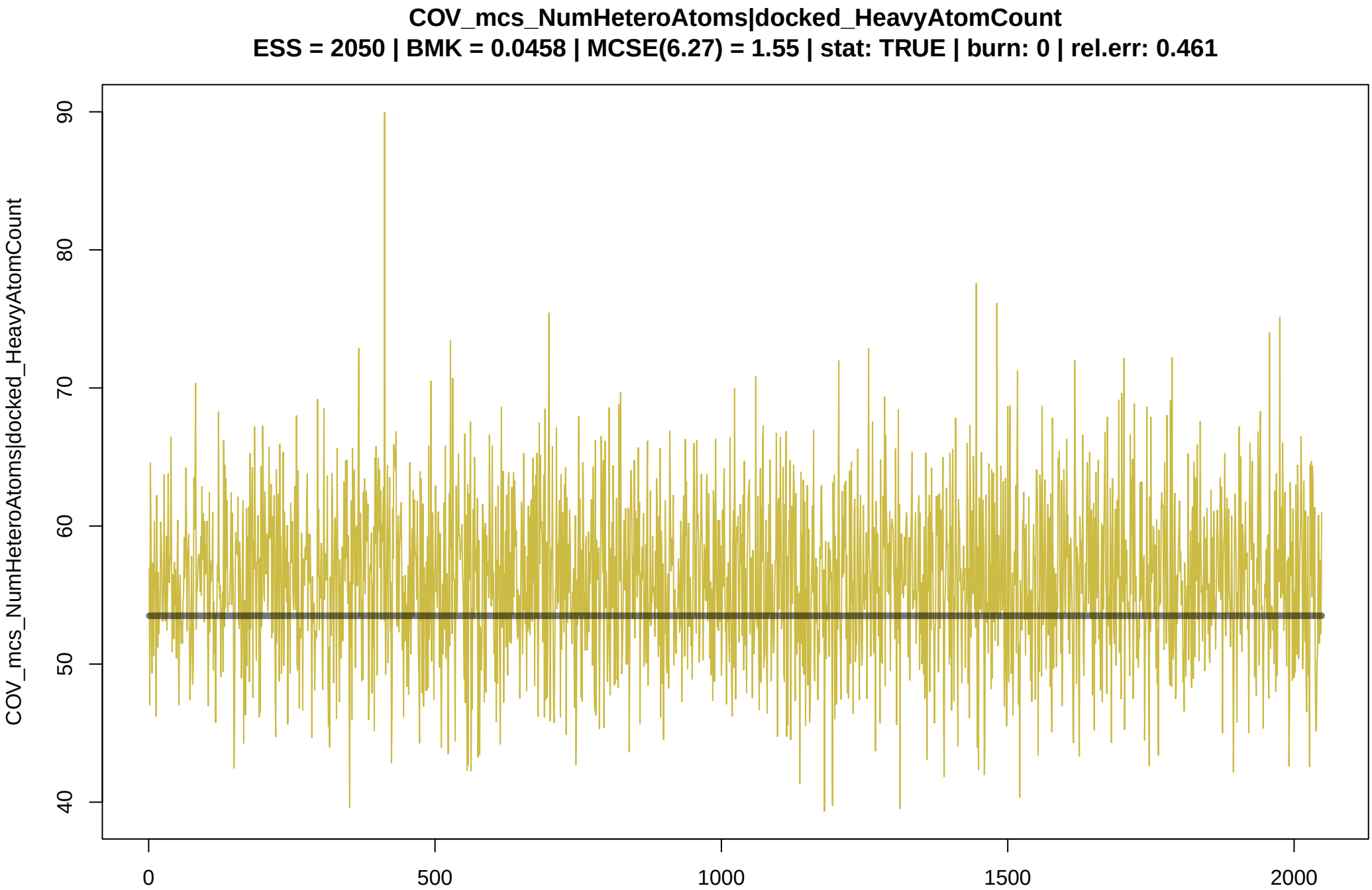

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1990 | BMK = 0.0409 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: 0.473
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0394 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0 | rel.err: −1.62
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.5
−2.0
−2.5
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0474 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: −1.77
COV_log_RMSD|docked_HeavyAtomCount
−12
−14
−16
−18
−20
−22
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1820 | BMK = 0.0442 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: −0.447
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1900 | BMK = 0.041 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: −0.926
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: 0.461
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
90
80
70
60
50
40
0
500
1000
1500
2000