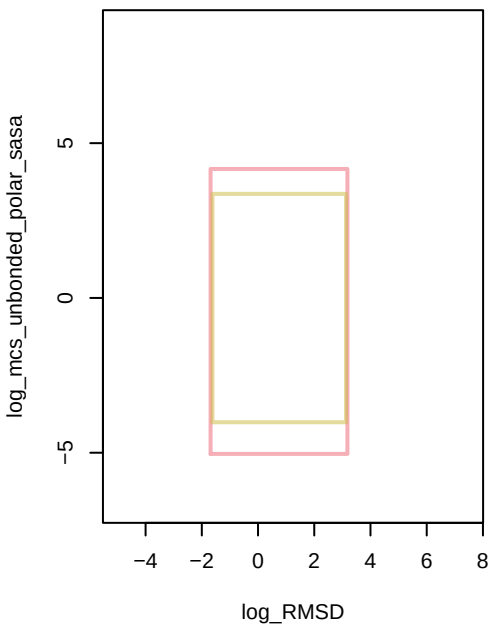
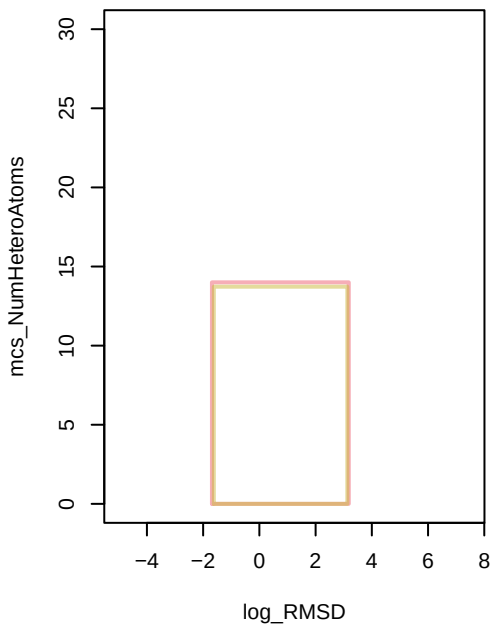
−− STATS maxD −−
min ESS = 103.555191982763
max BMK = 0.143103223144629
max MCSE = 7.21991065716993
all stationary: FALSE
burn: 0
max rel.err.: 2.14597445849199

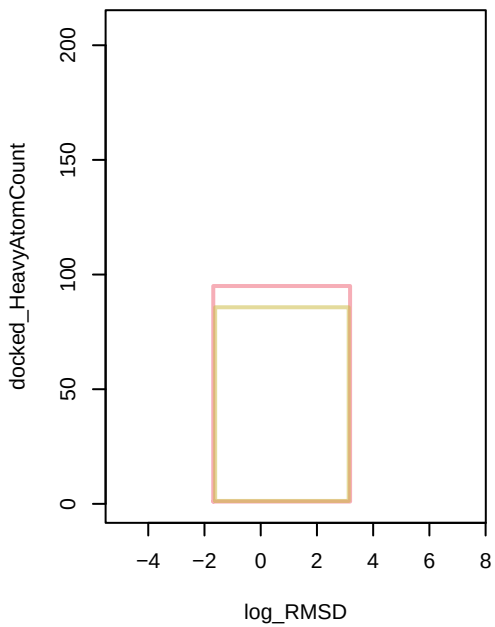
−− STATS 2D −−
min ESS = 1856.22438590447
max BMK = 0.05740871196212
max MCSE = 2.73501944291976
all stationary: TRUE
burn: 0
max rel.err.: 1.72006956971392

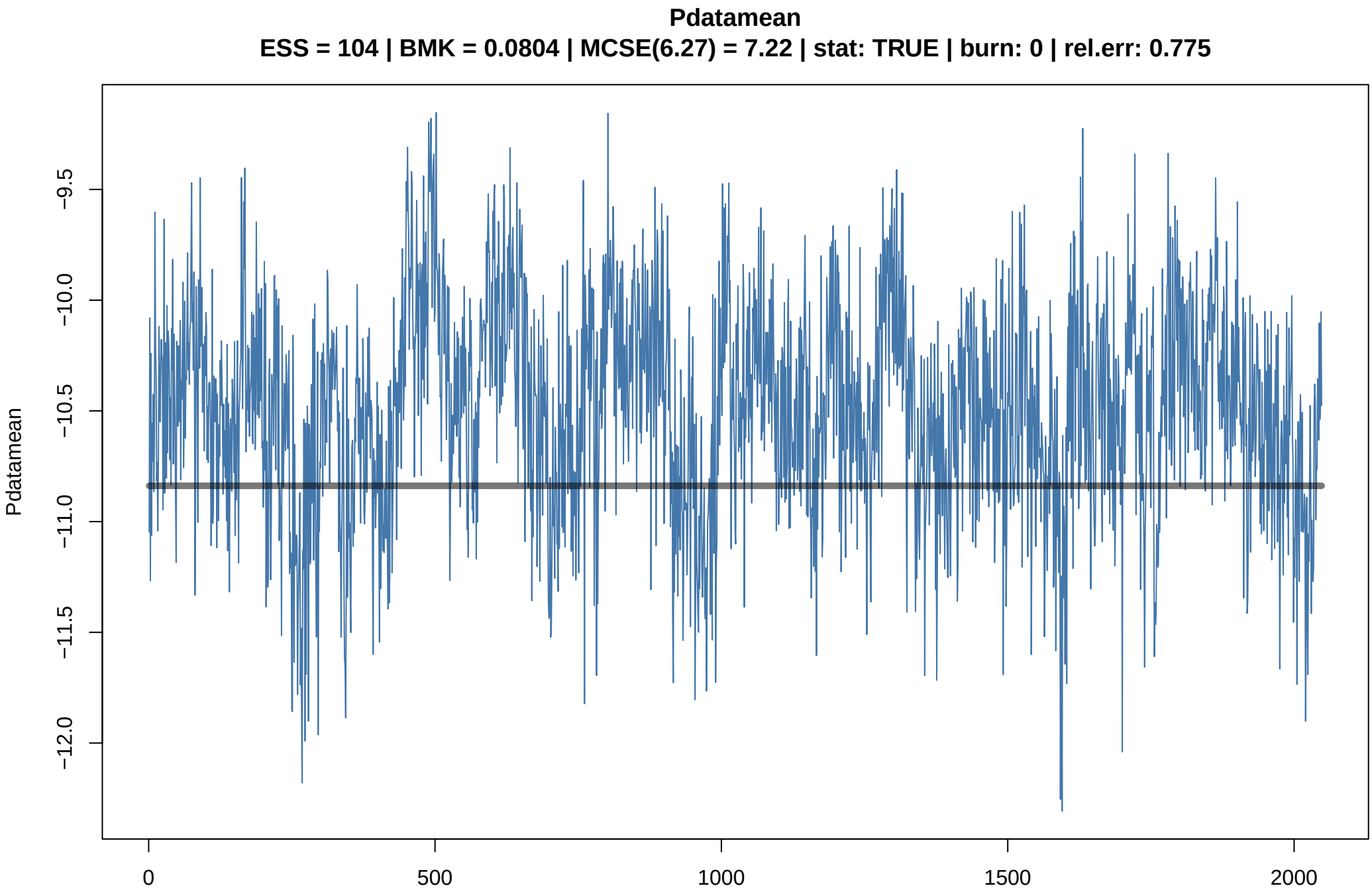
−− STATS 1D −−
min ESS = 1290.61520553023
max BMK = 0.0674710187112221
max MCSE = 3.02092580658758
all stationary: TRUE
burn: 0
max rel.err.: 2.21393511509494

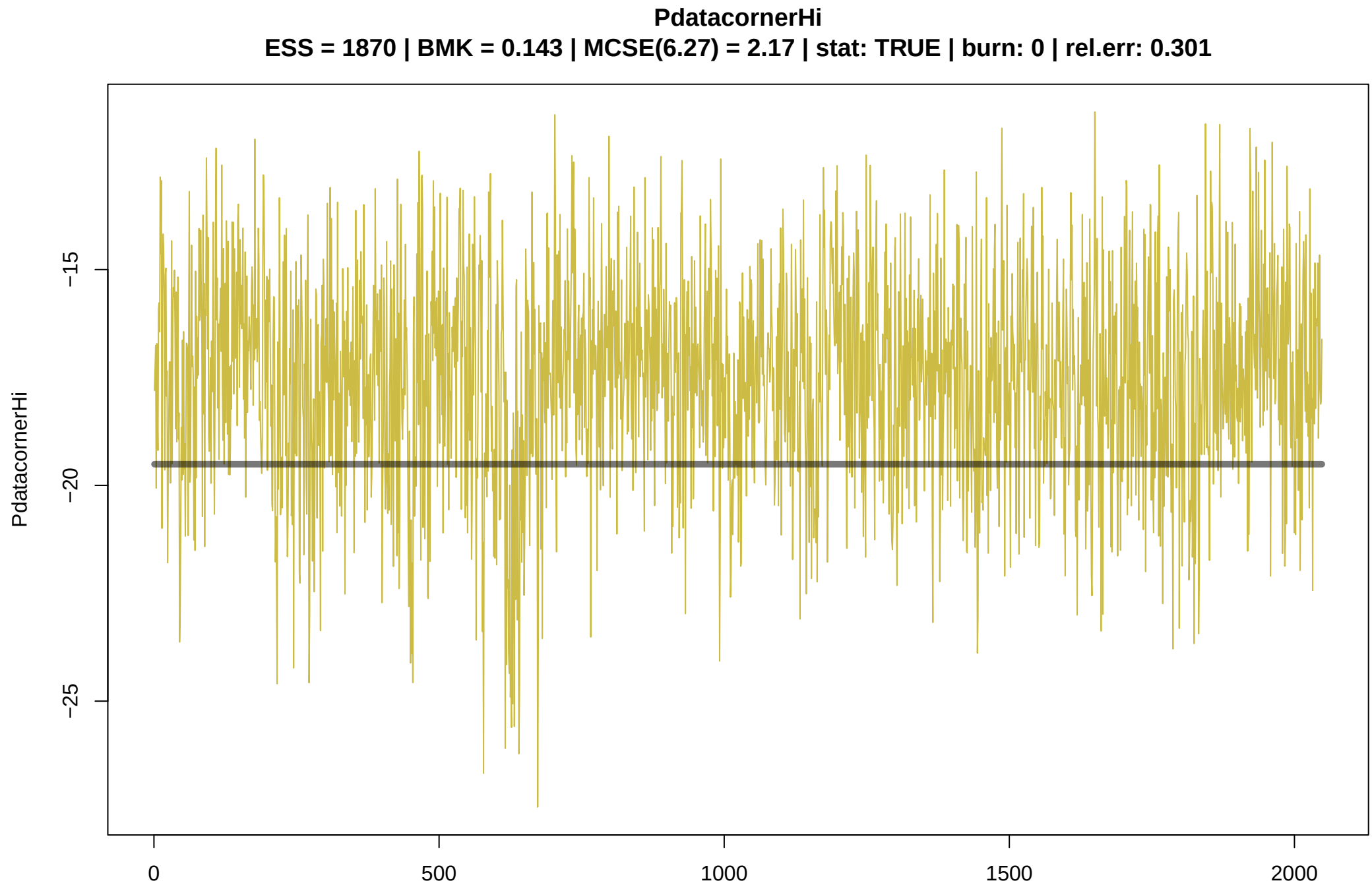
Occupied clusters: 8 of 16

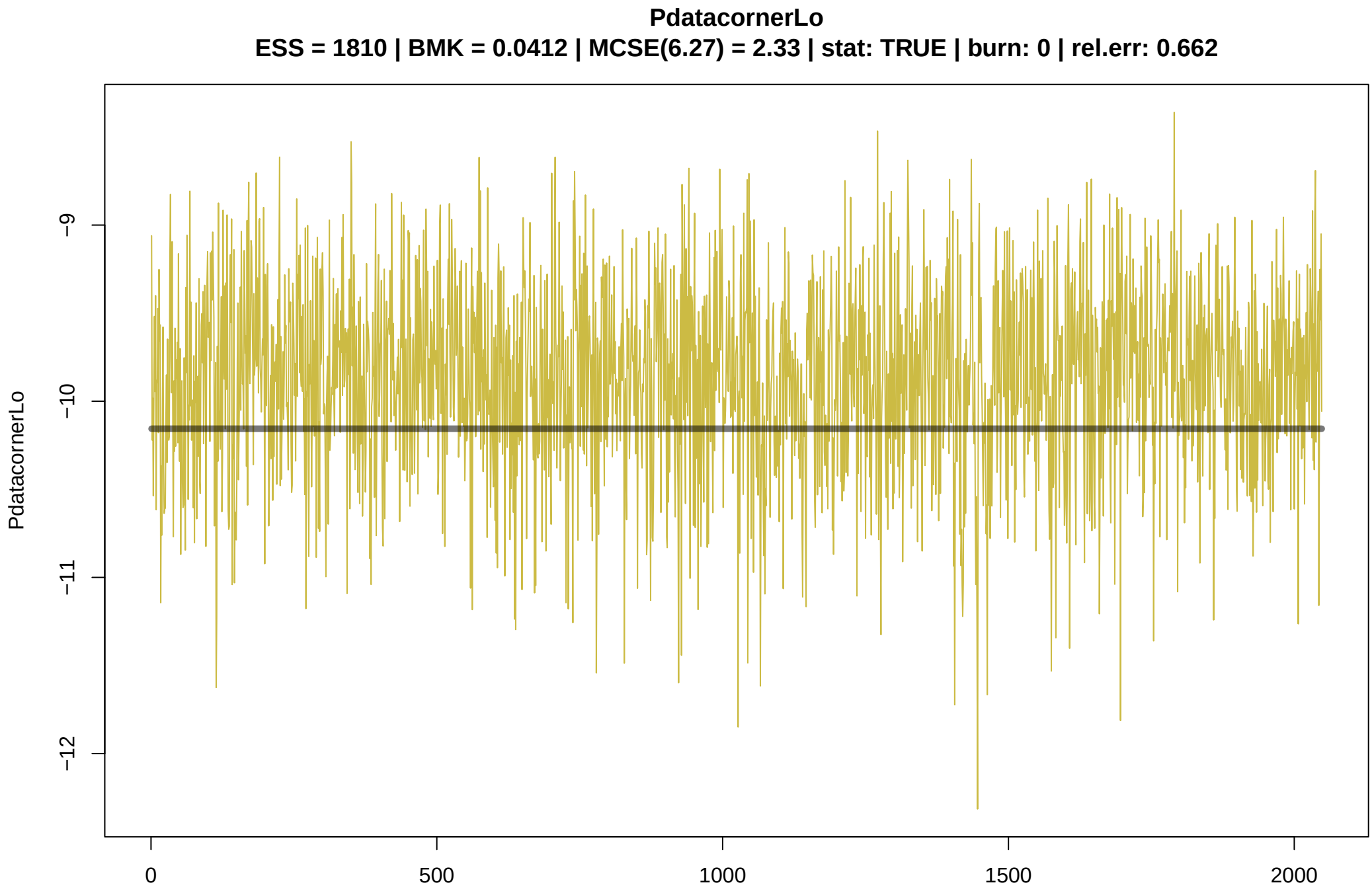

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
8
log_RMSD

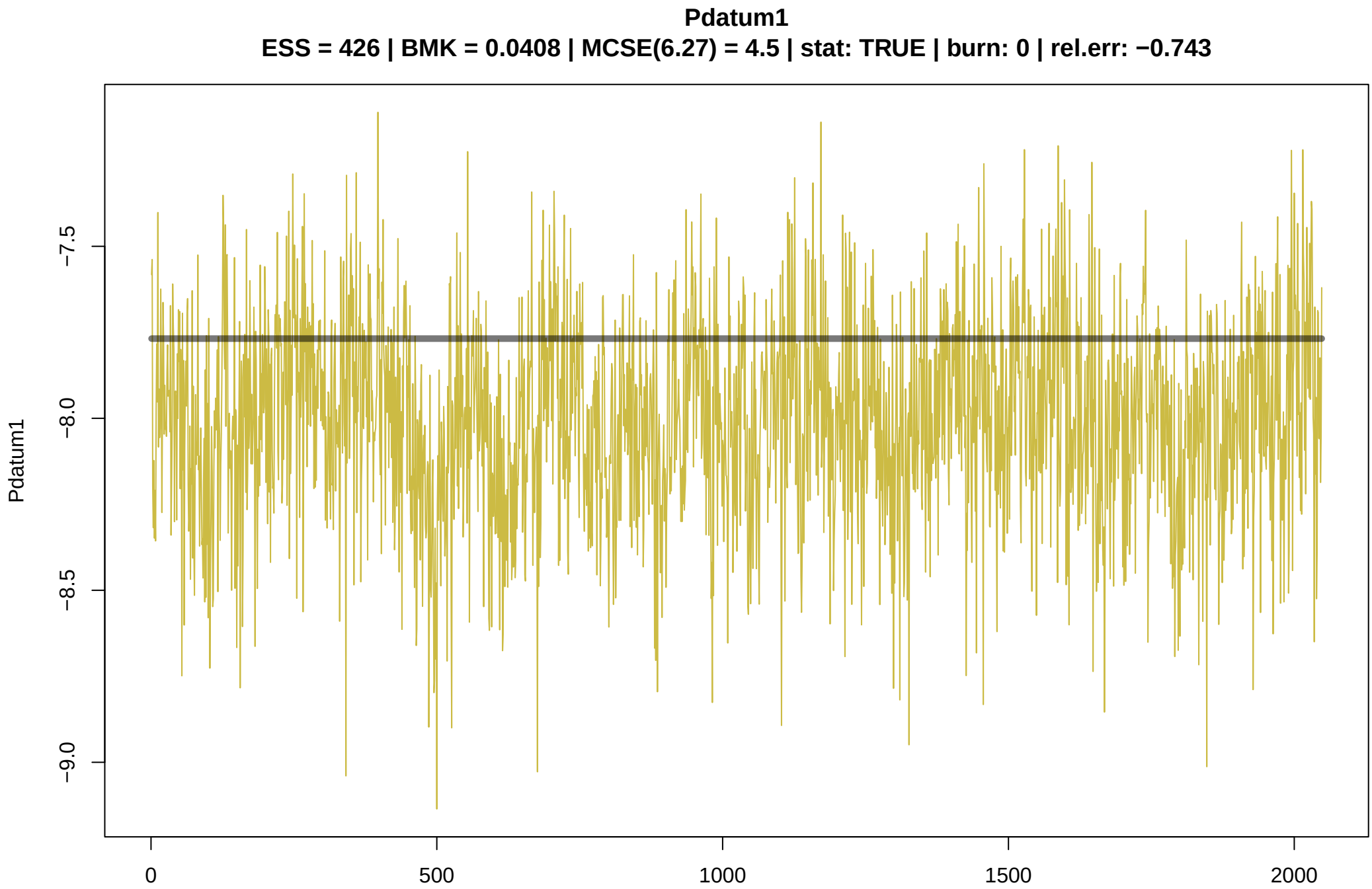

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
8
log_RMSD

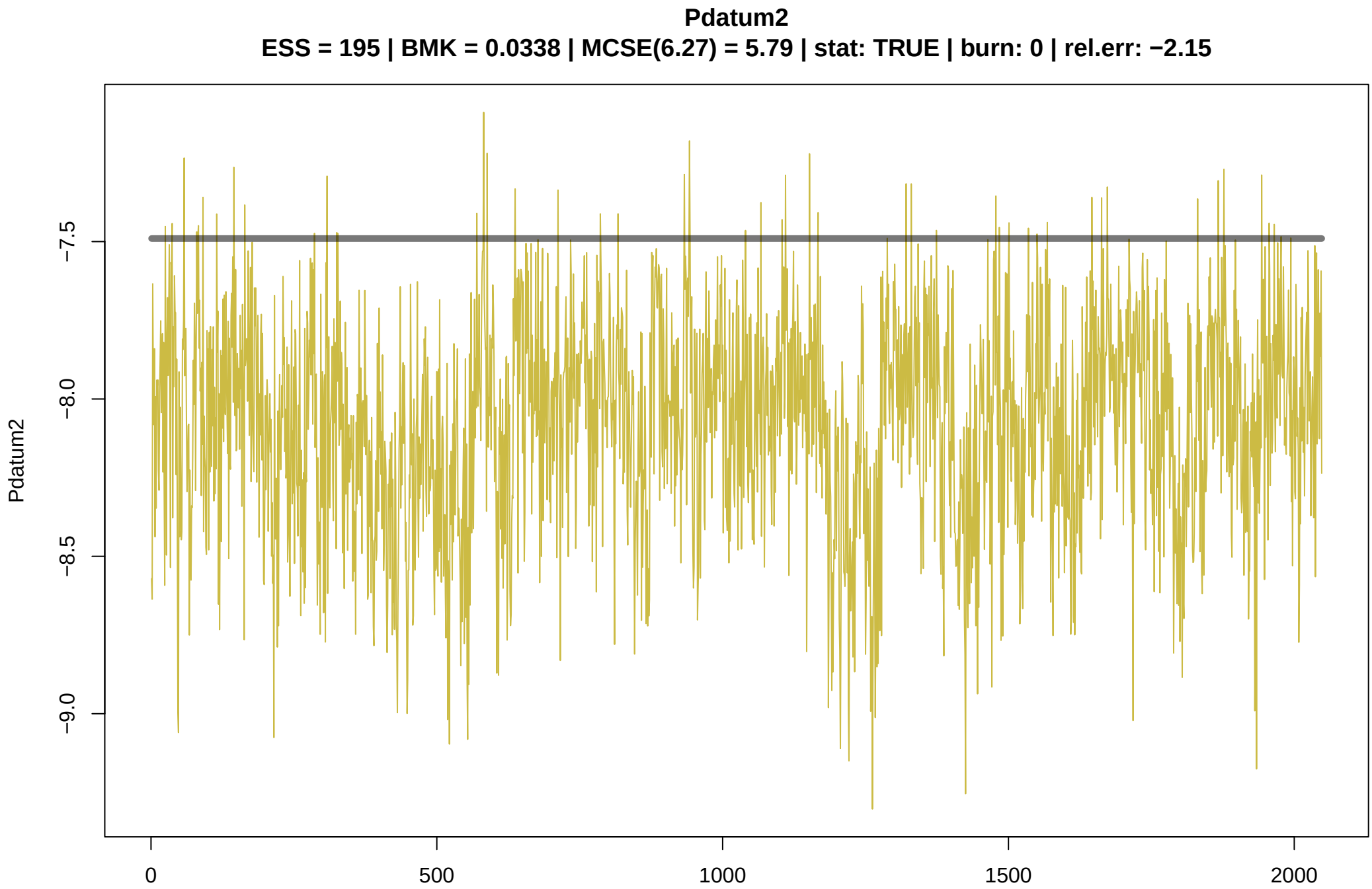

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
8
log_RMSD

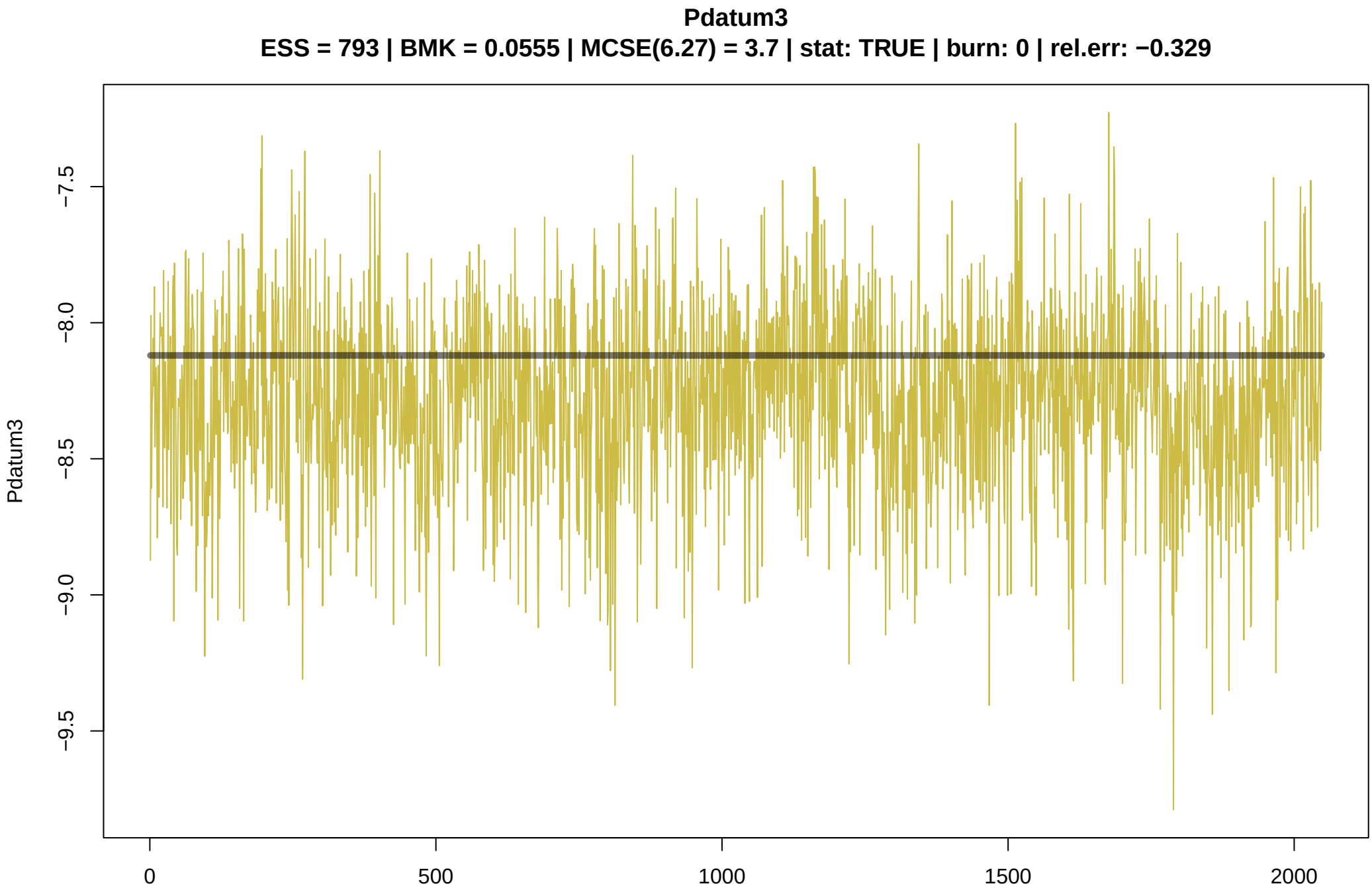

Pdatamean
ESS = 104 | BMK = 0.0804 | MCSE(6.27) = 7.22 | stat: TRUE | burn: 0 | rel.err: 0.775
Pdatamean
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

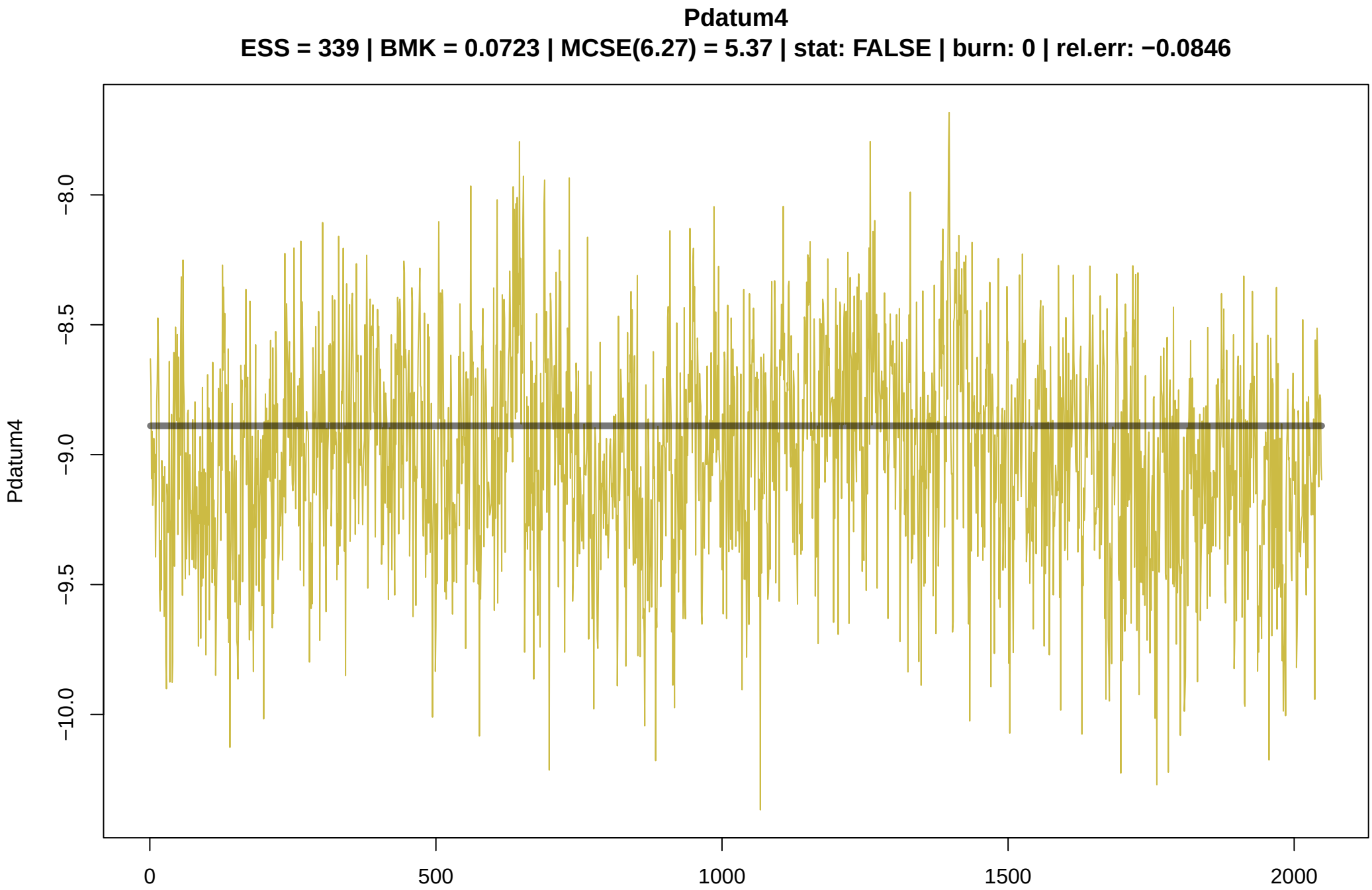

PdatacornerHi
ESS = 1870 | BMK = 0.143 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.301
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

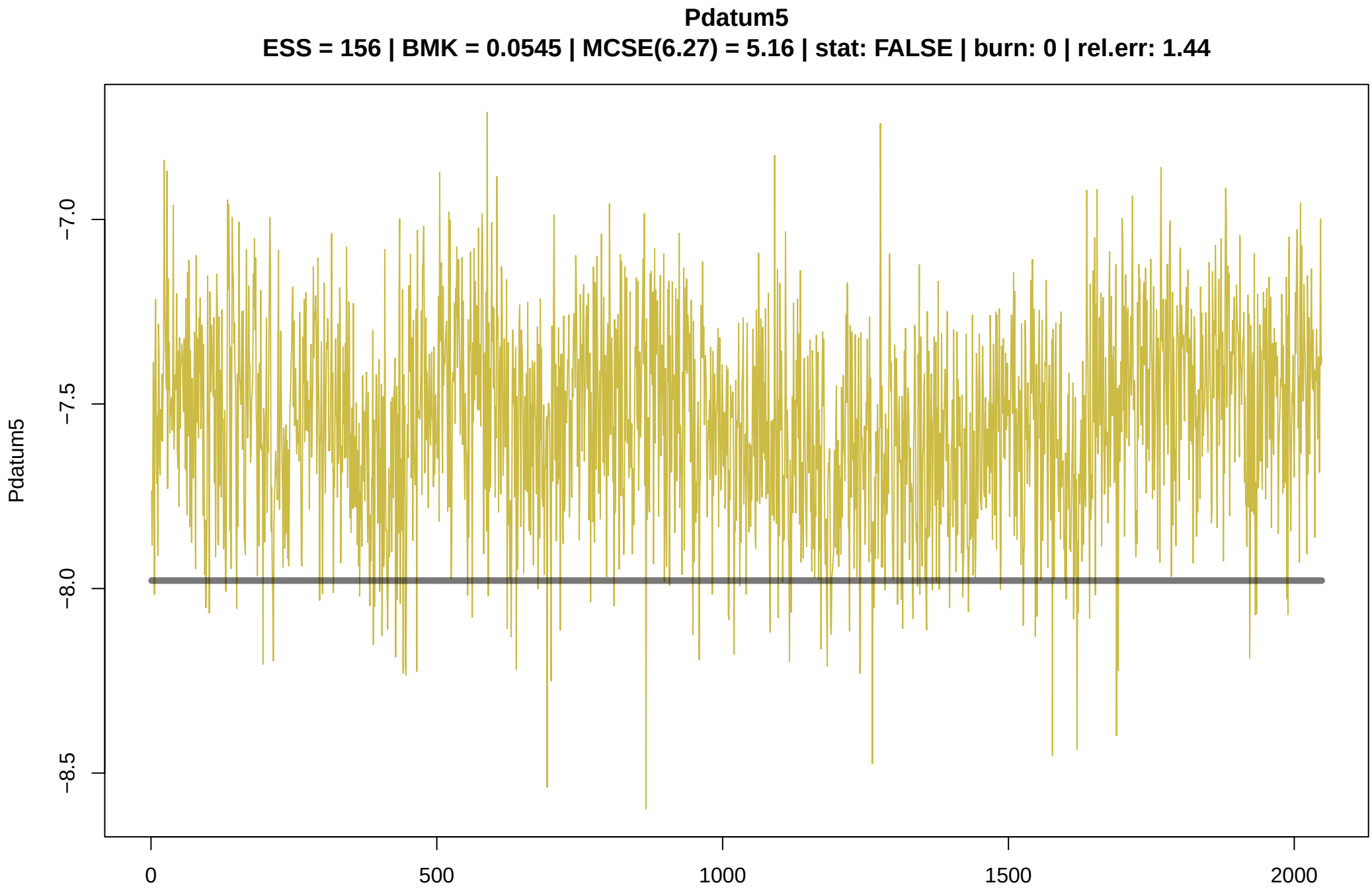

PdatacornerLo
ESS = 1810 | BMK = 0.0412 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 0.662
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

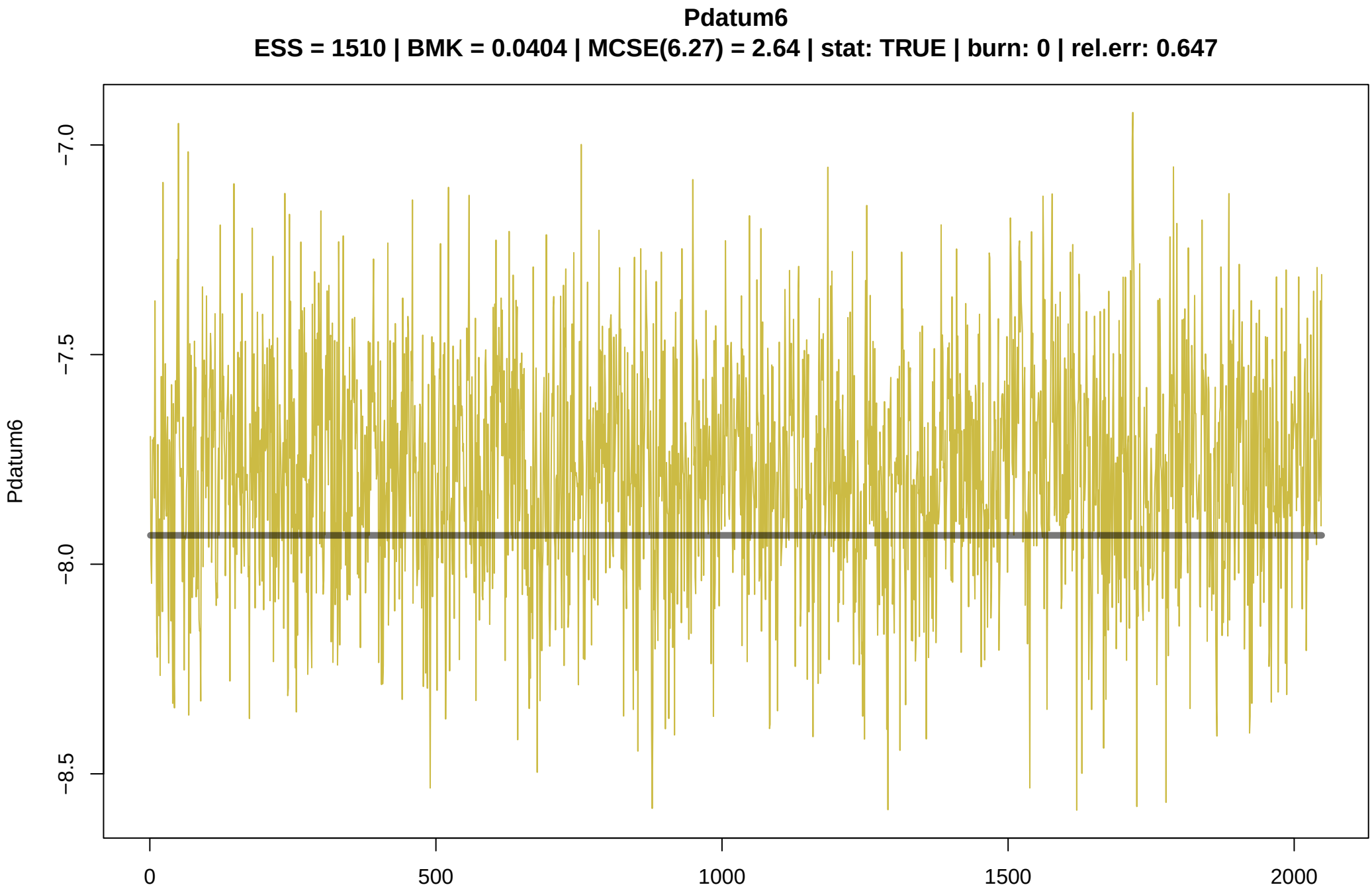

Pdatum1
ESS = 426 | BMK = 0.0408 | MCSE(6.27) = 4.5 | stat: TRUE | burn: 0 | rel.err: −0.743
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

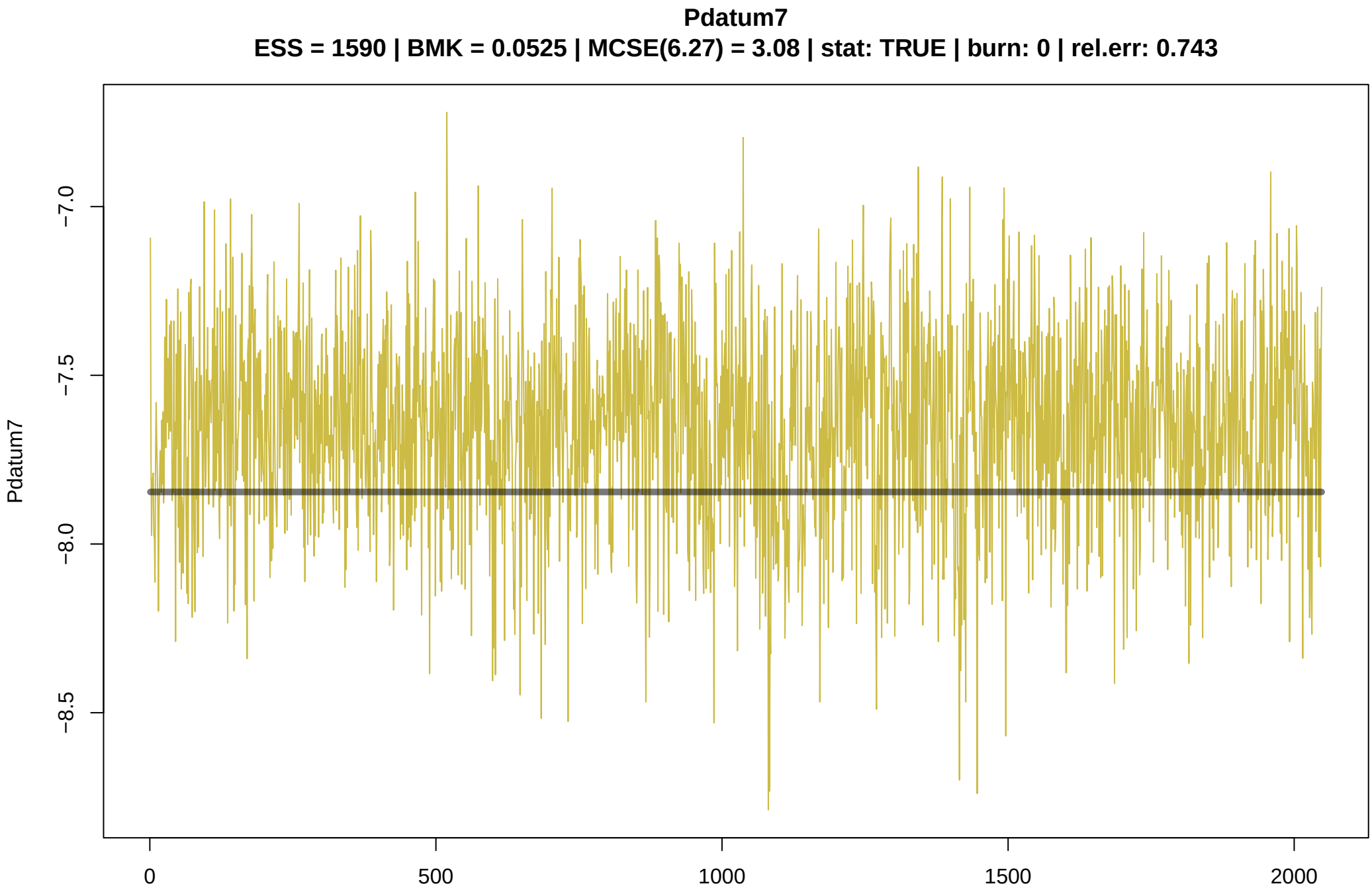

Pdatum2
ESS = 195 | BMK = 0.0338 | MCSE(6.27) = 5.79 | stat: TRUE | burn: 0 | rel.err: −2.15
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

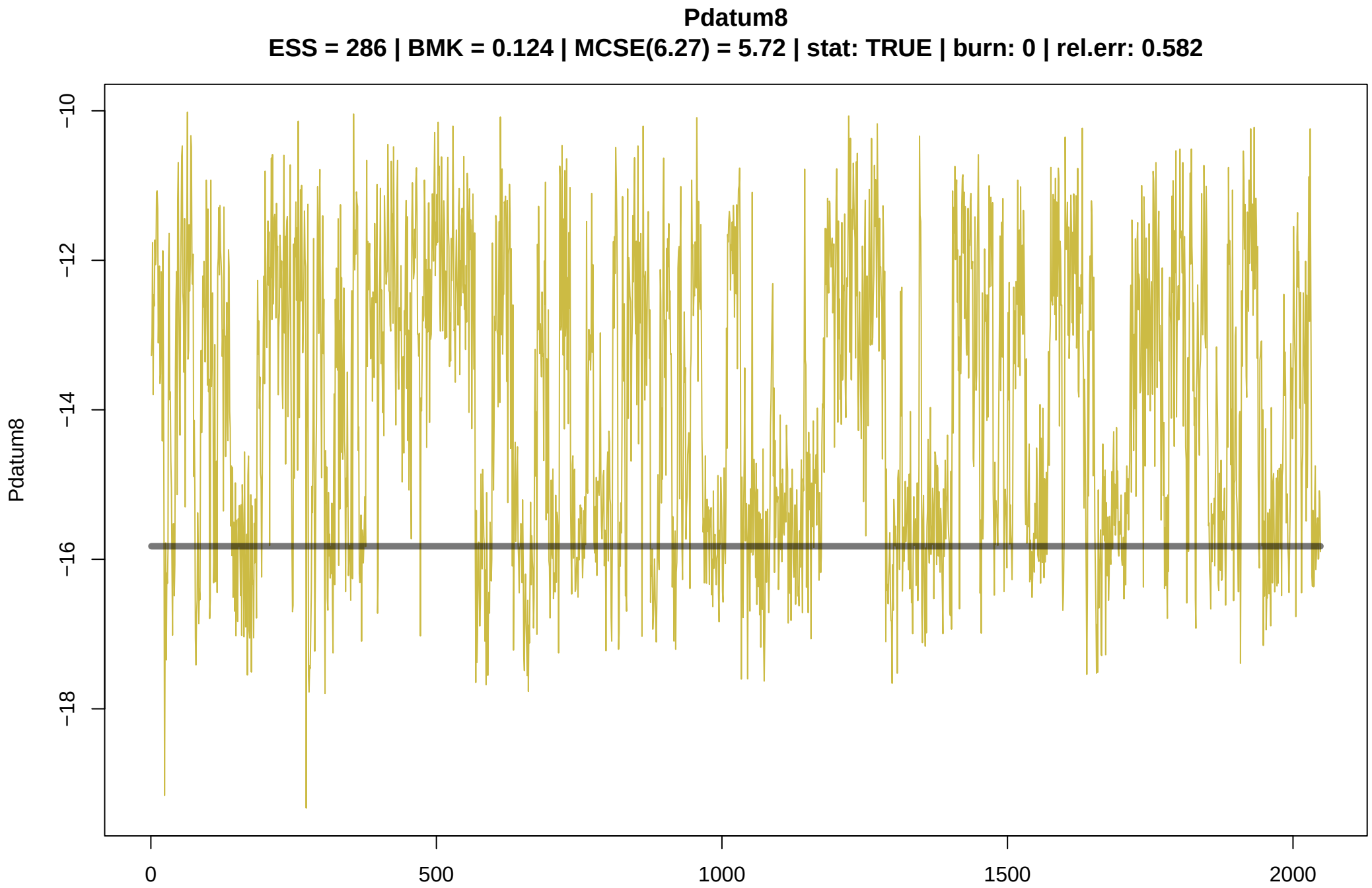

Pdatum3
ESS = 793 | BMK = 0.0555 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | rel.err: −0.329
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

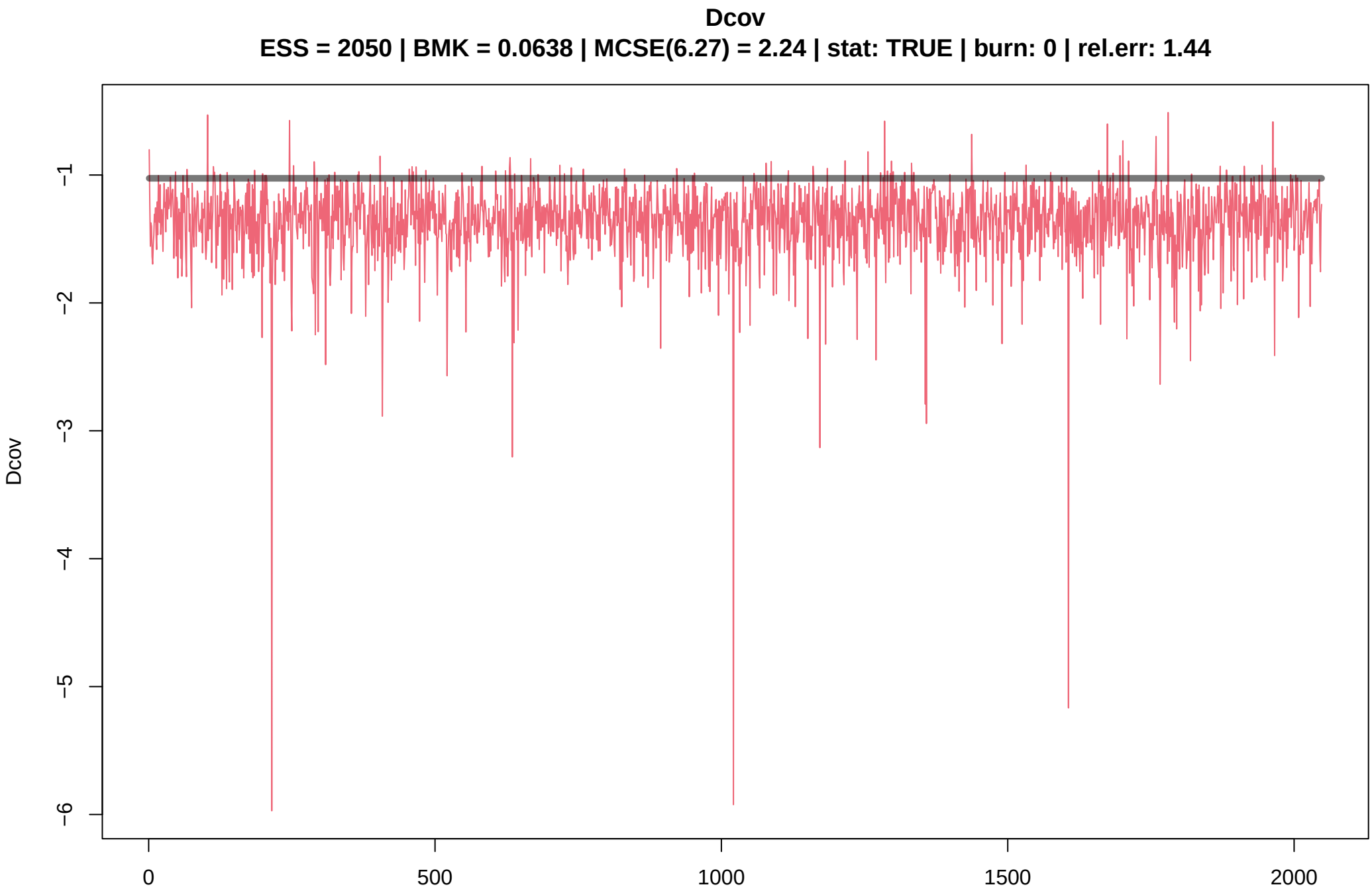

Pdatum4
ESS = 339 | BMK = 0.0723 | MCSE(6.27) = 5.37 | stat: FALSE | burn: 0 | rel.err: −0.0846
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

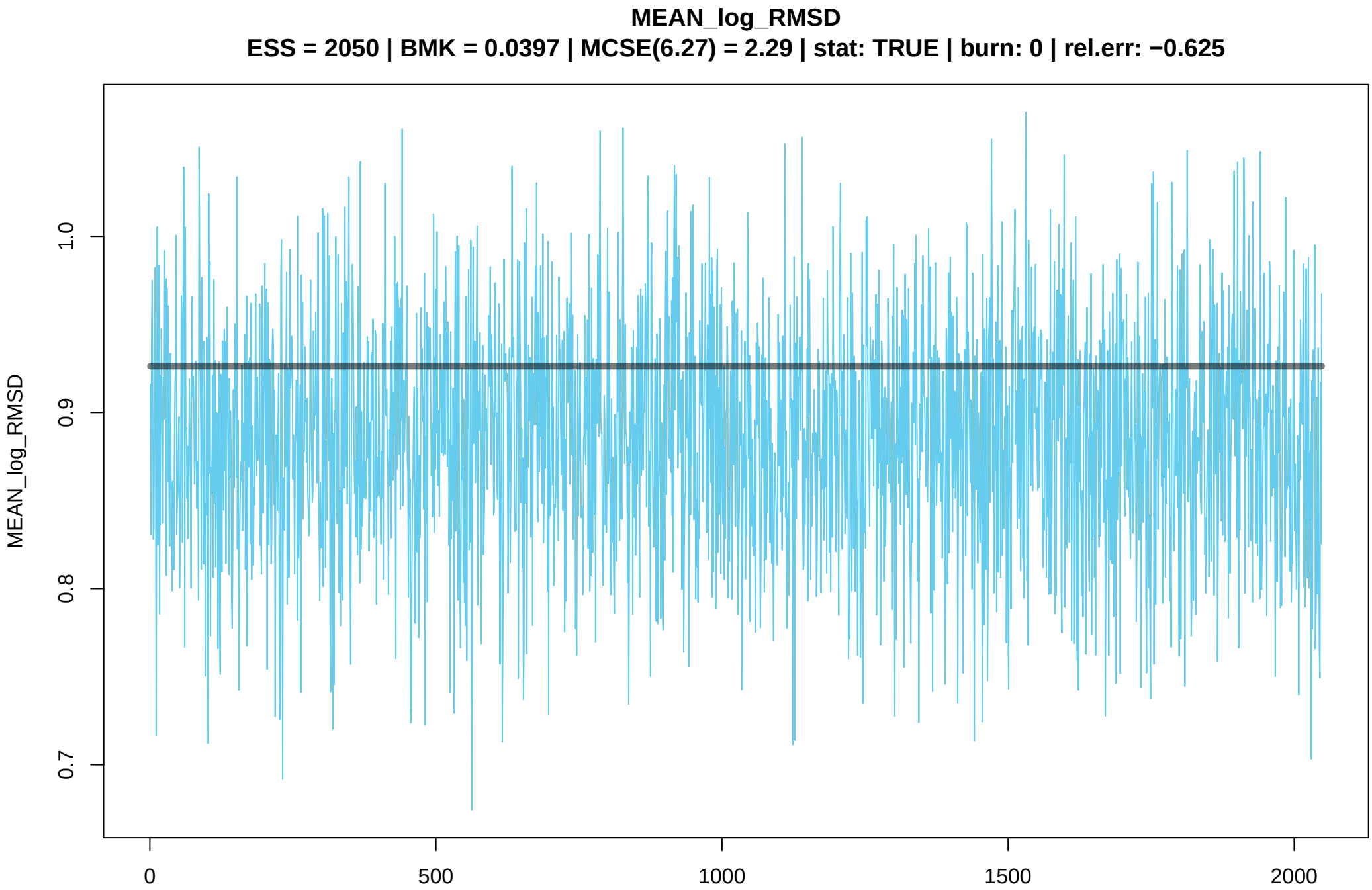

Pdatum5
ESS = 156 | BMK = 0.0545 | MCSE(6.27) = 5.16 | stat: FALSE | burn: 0 | rel.err: 1.44
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

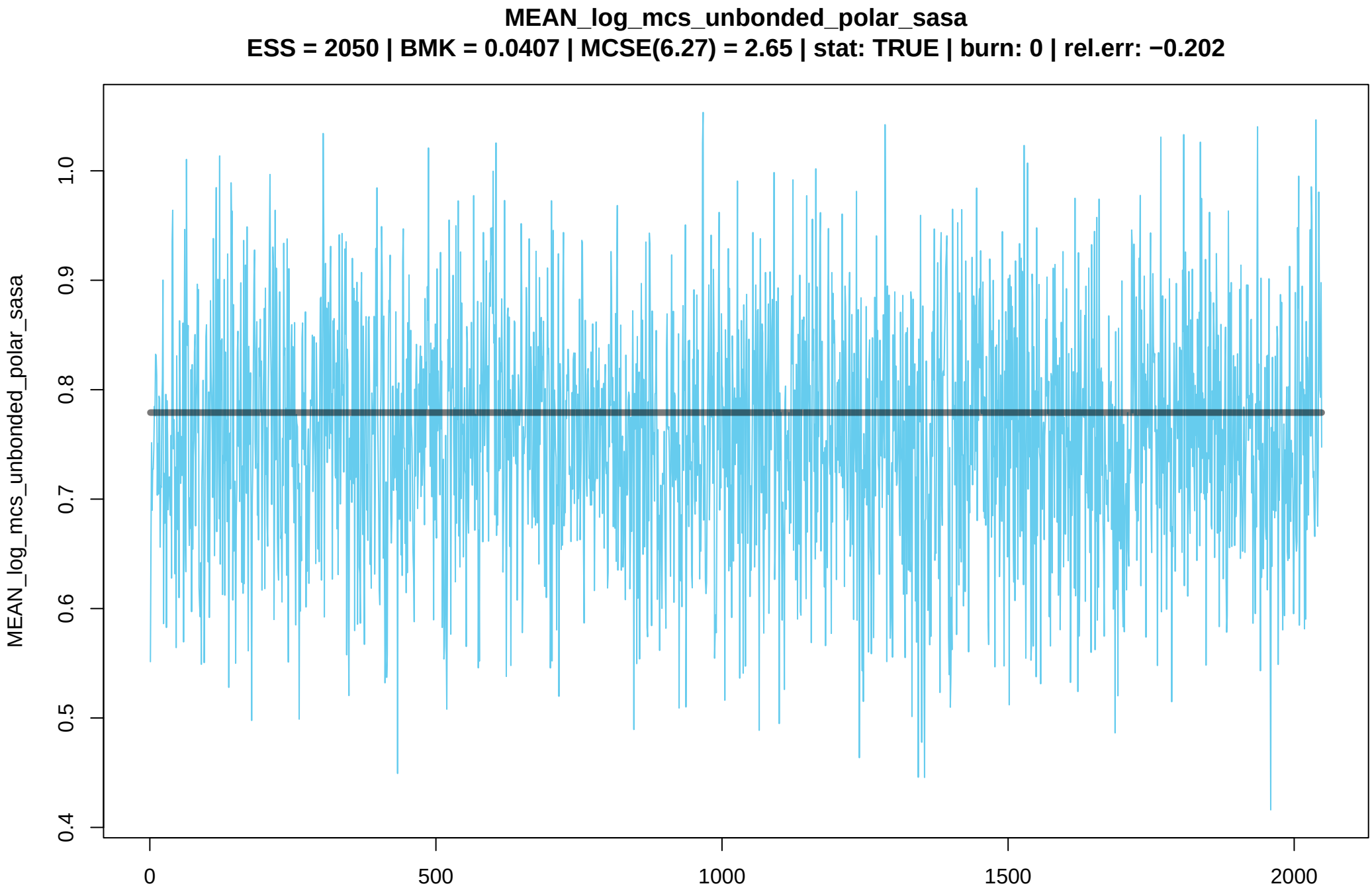

Pdatum6
ESS = 1510 | BMK = 0.0404 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: 0.647
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

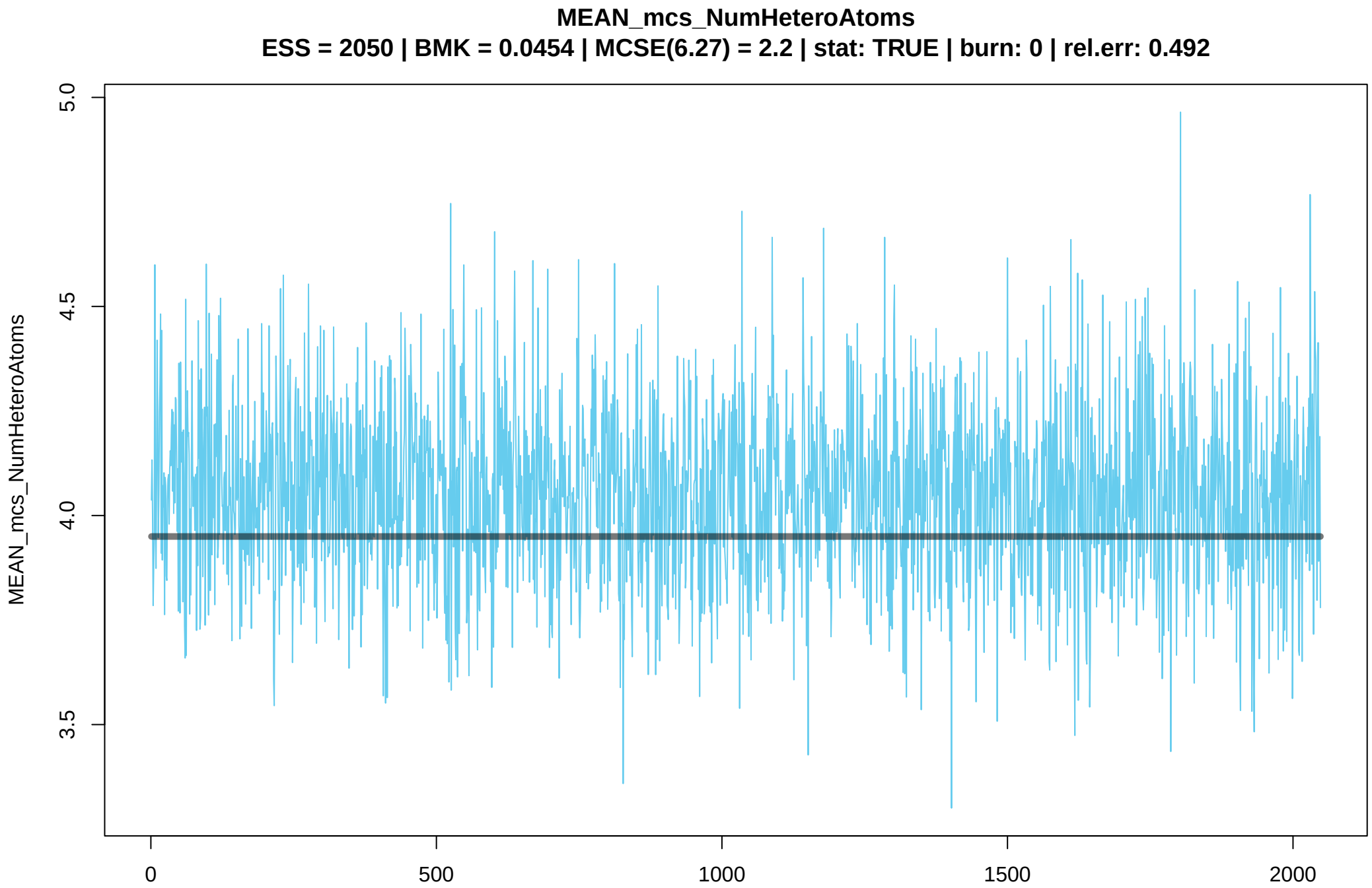

Pdatum7
ESS = 1590 | BMK = 0.0525 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0 | rel.err: 0.743
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

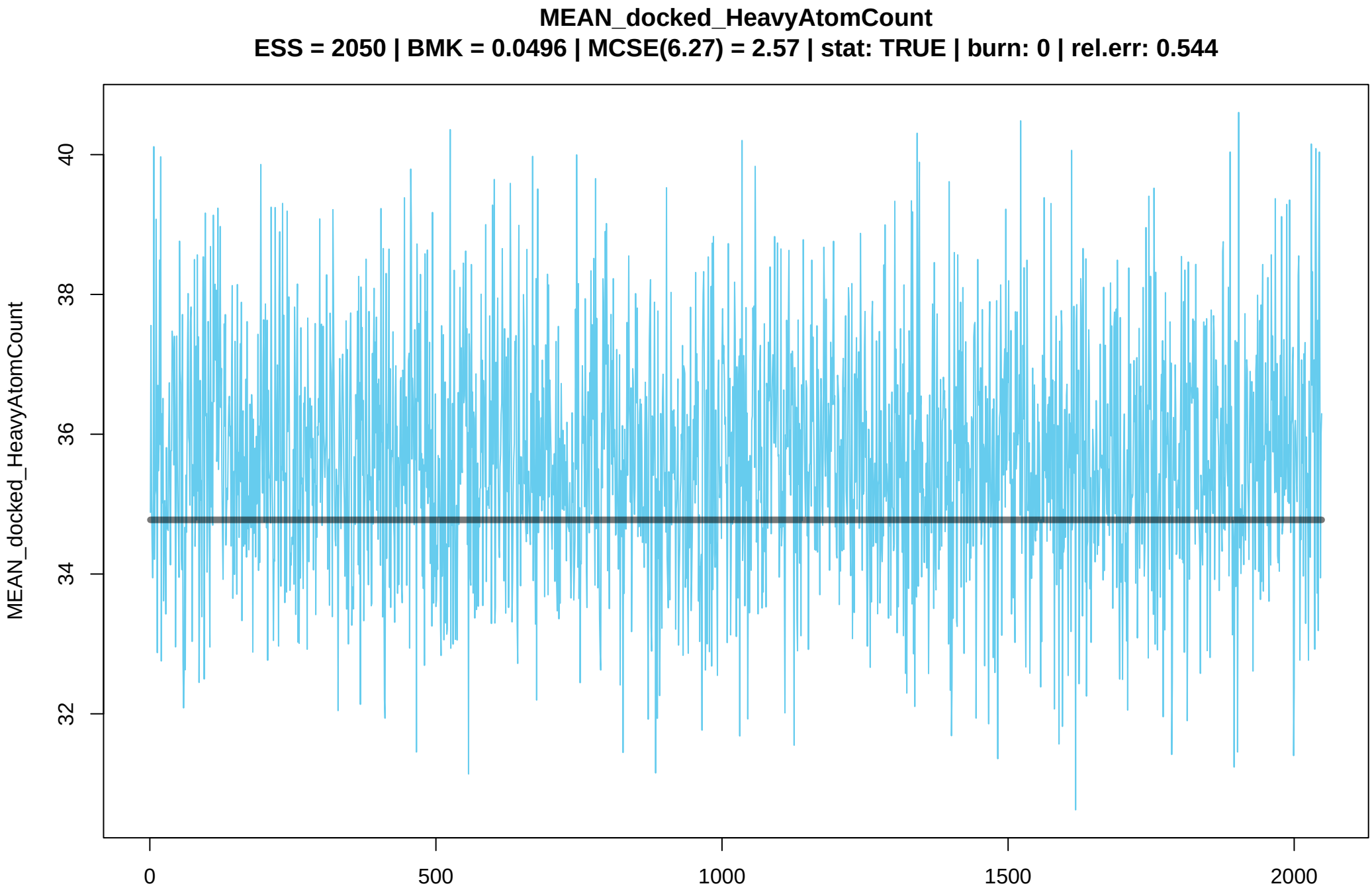

Pdatum8
ESS = 286 | BMK = 0.124 | MCSE(6.27) = 5.72 | stat: TRUE | burn: 0 | rel.err: 0.582
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

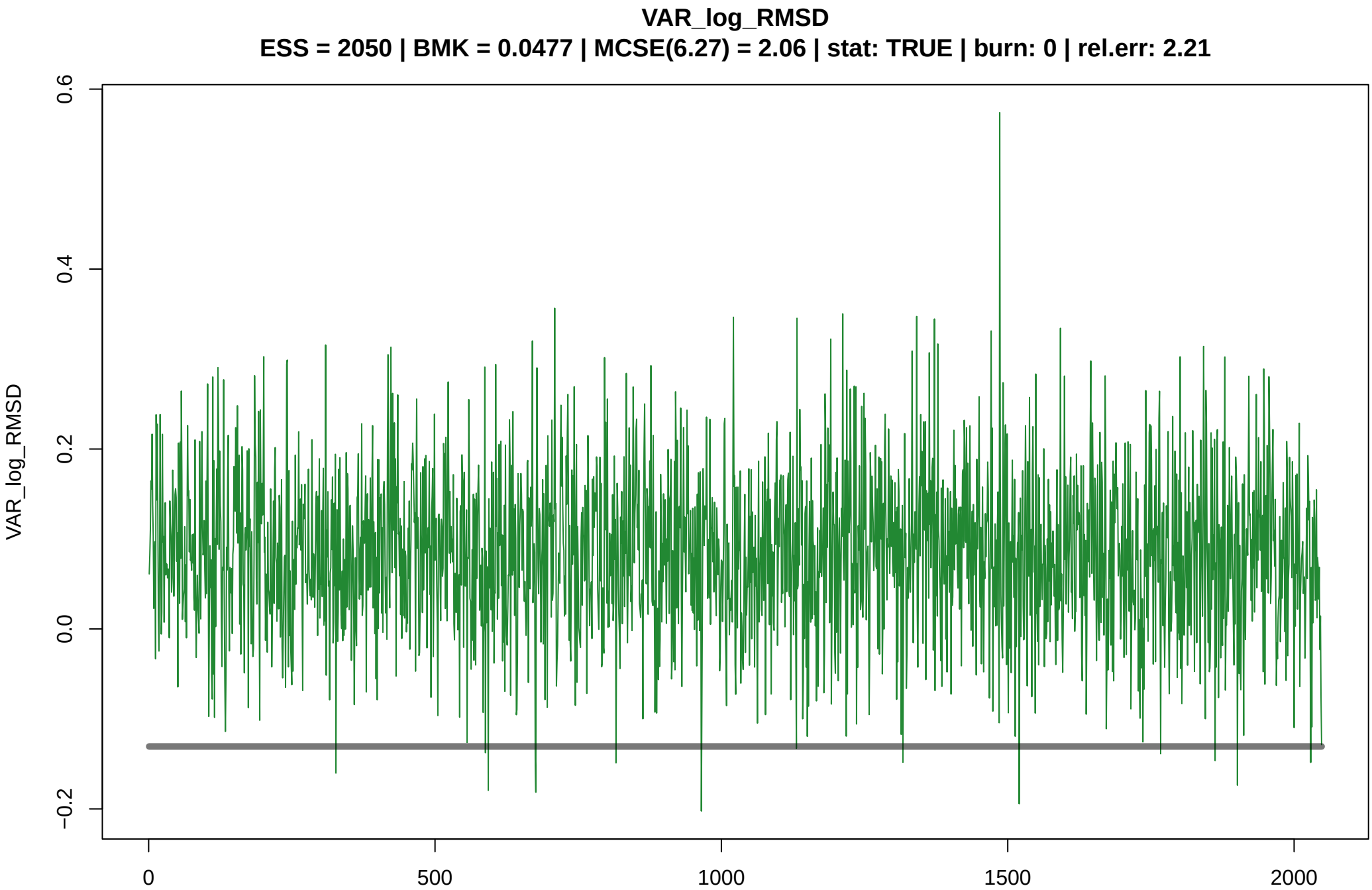

Dcov
ESS = 2050 | BMK = 0.0638 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | rel.err: 1.44
Dcov
−1
−2
−3
−4
−5
−6
0
500
1000
1500
2000

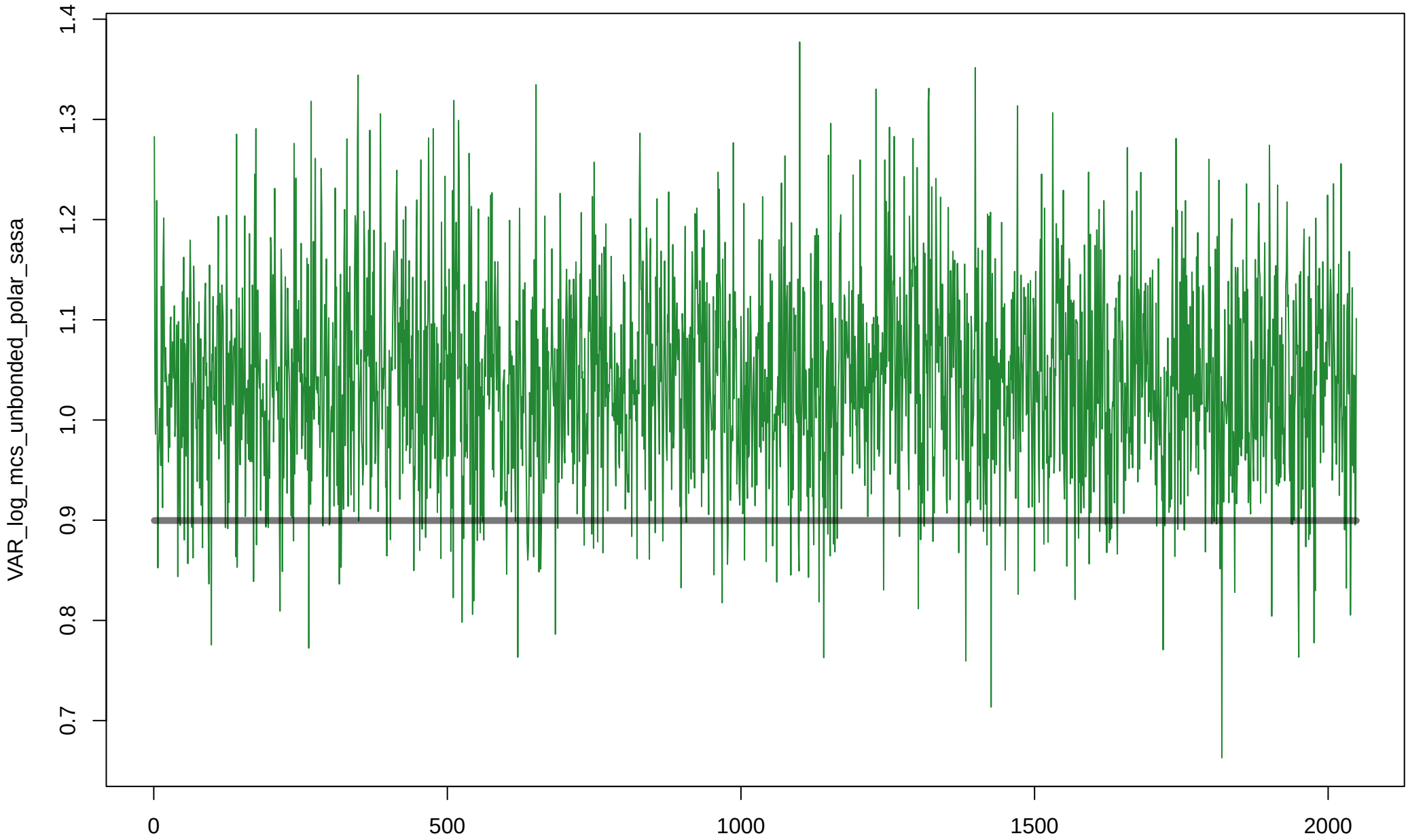

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0397 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: −0.625
MEAN_log_RMSD
0.7
0.8
0.9
1.0
0
500
1000
1500
2000

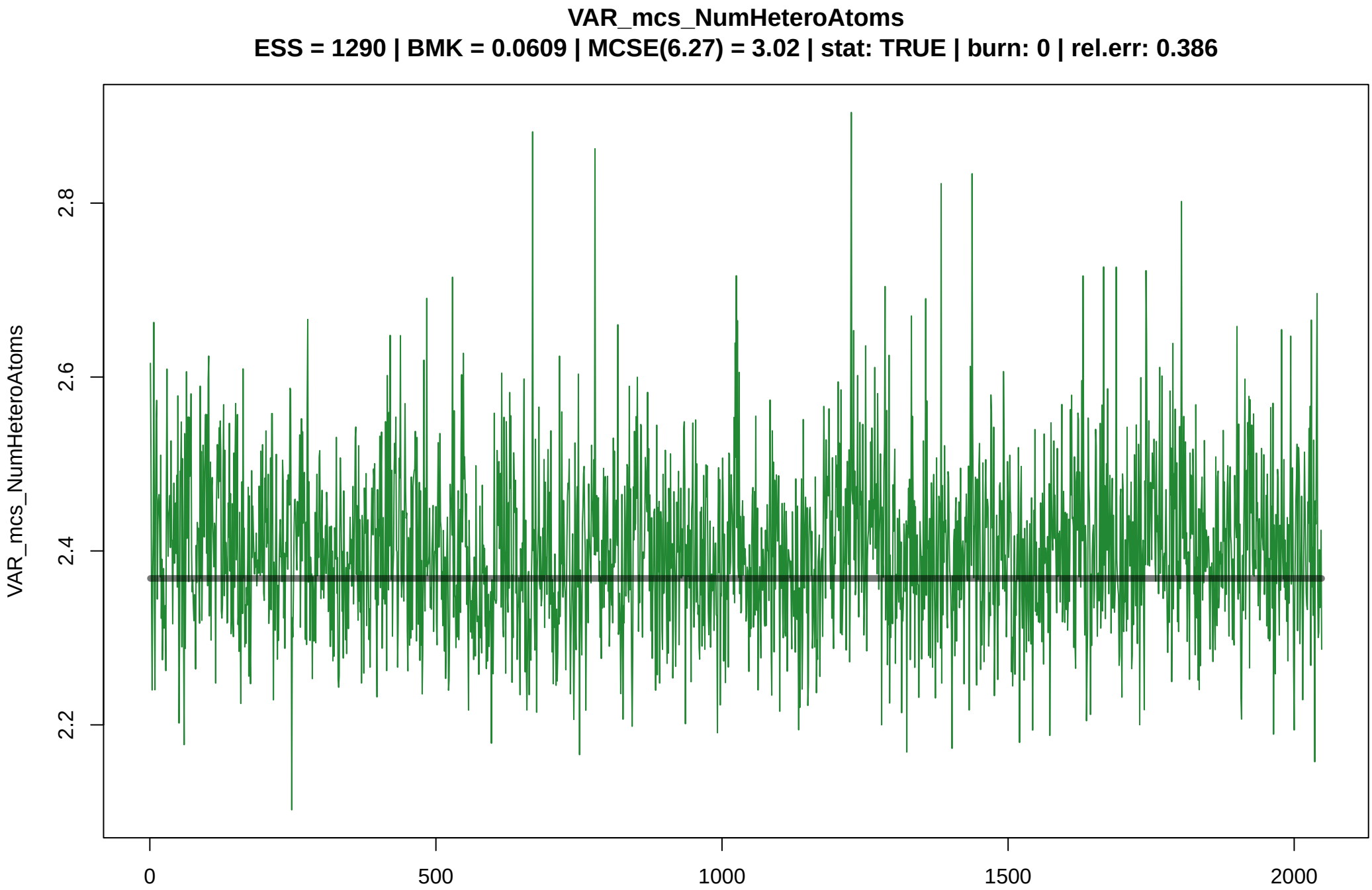

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: −0.202
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
0
500
1000
1500
2000

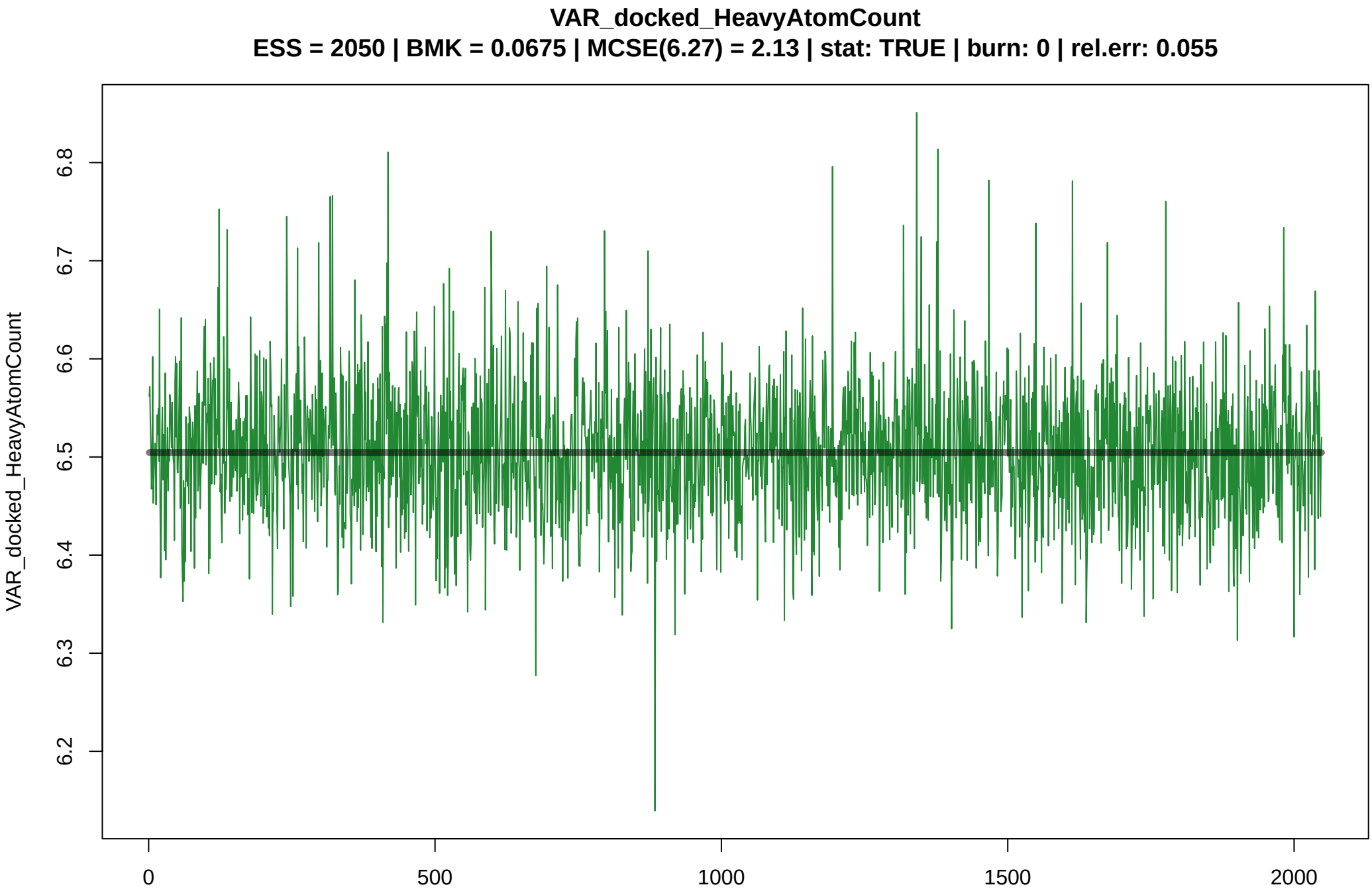

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0454 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: 0.492
MEAN_mcs_NumHeteroAtoms
5.0
4.5
4.0
3.5
0
500
1000
1500
2000

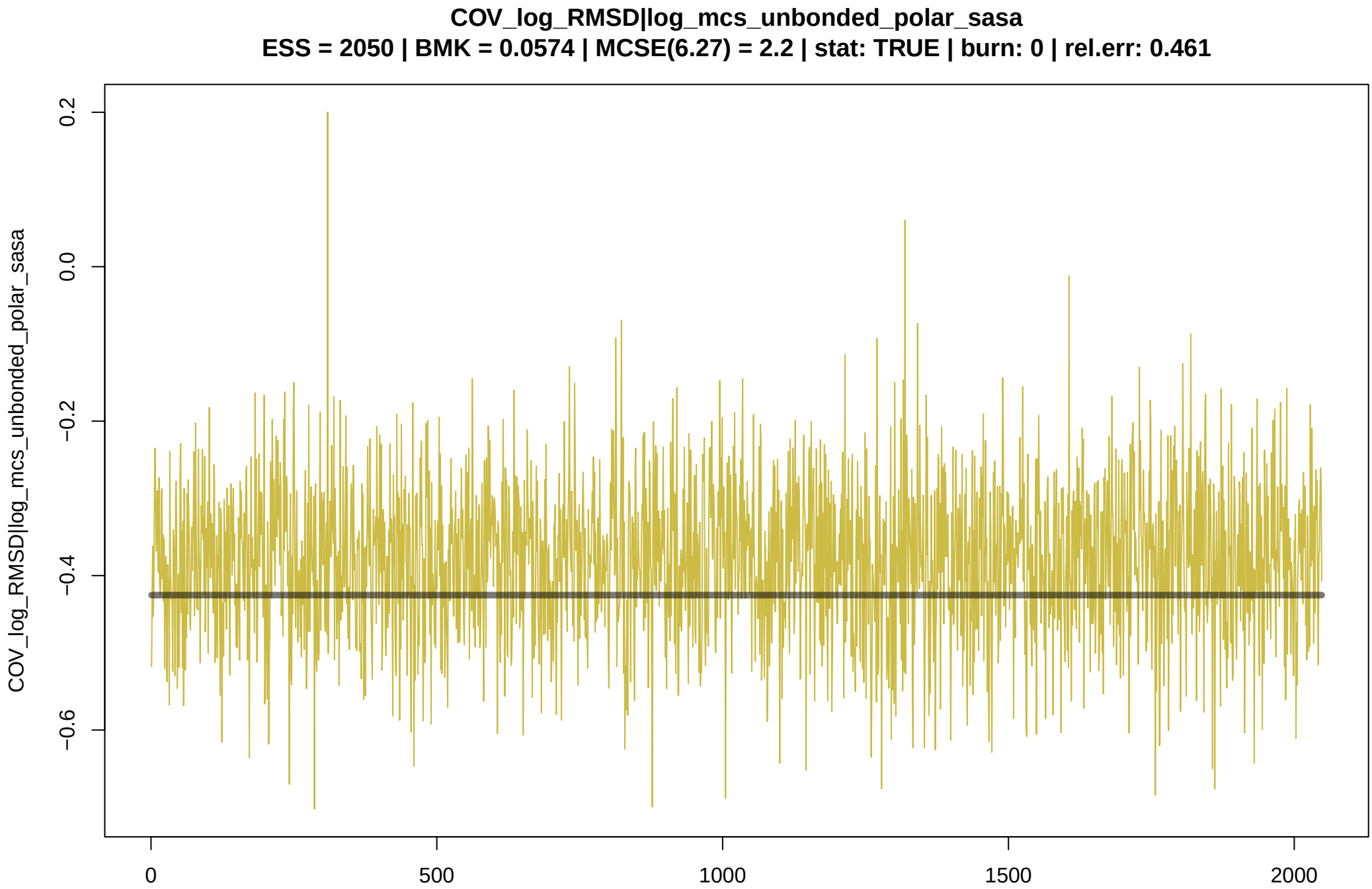

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0496 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: 0.544
MEAN_docked_HeavyAtomCount
32
34
36
38
40
0
500
1000
1500
2000

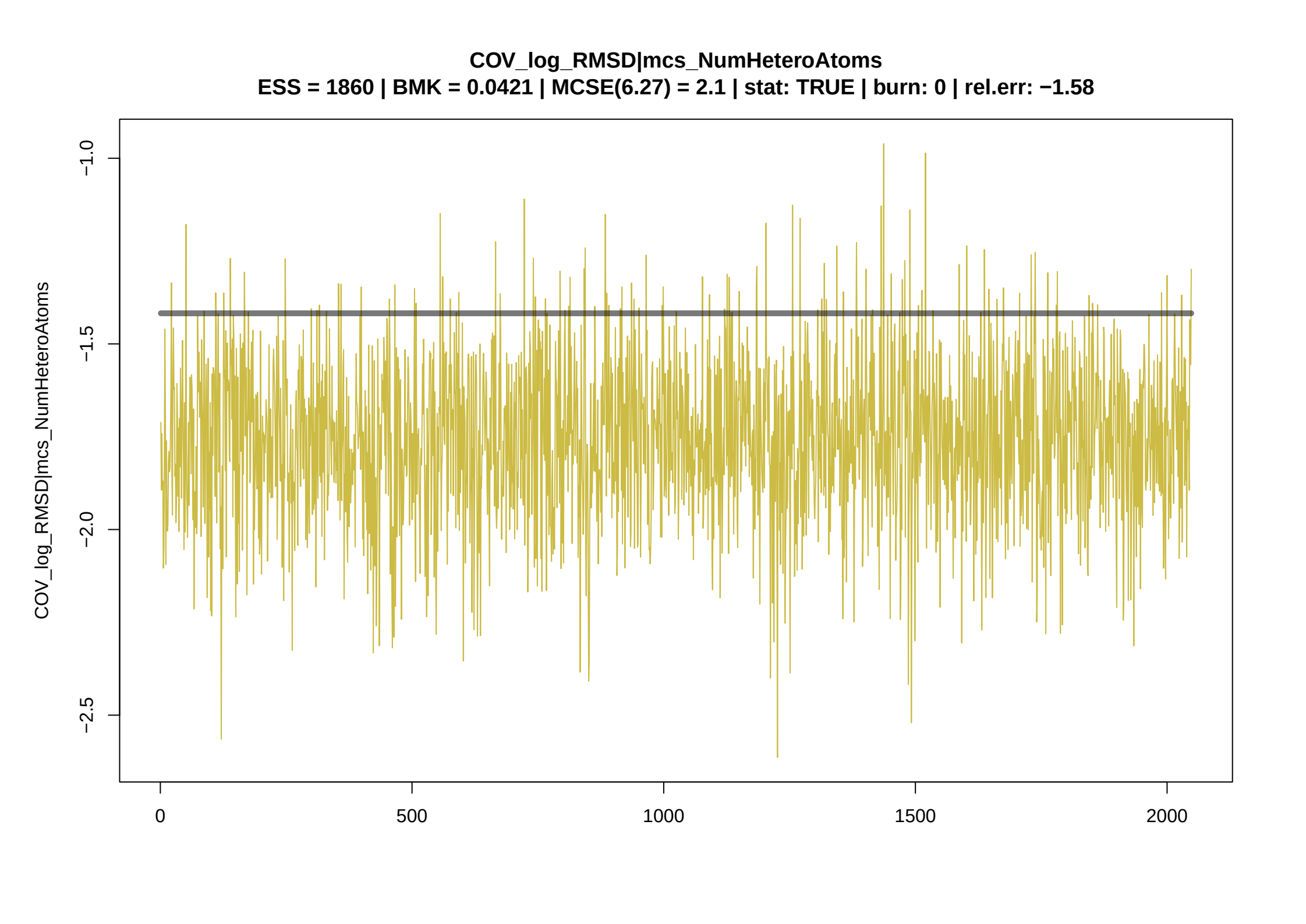

VAR_log_RMSD
ESS = 2050 | BMK = 0.0477 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: 2.21
VAR_log_RMSD
0.6
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

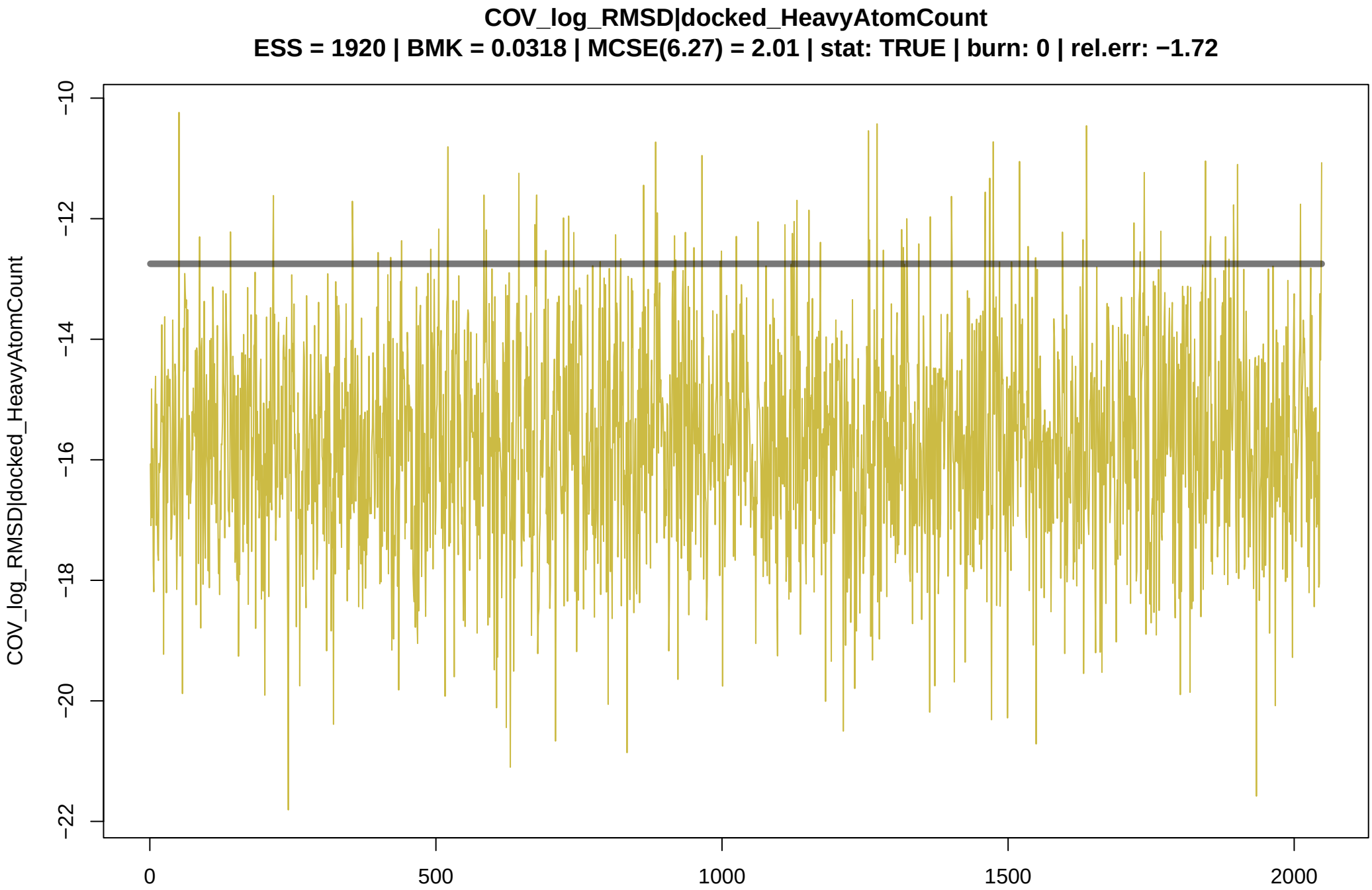

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0448 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 1.36
VAR_log_mcs_unbonded_polar_sasa
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

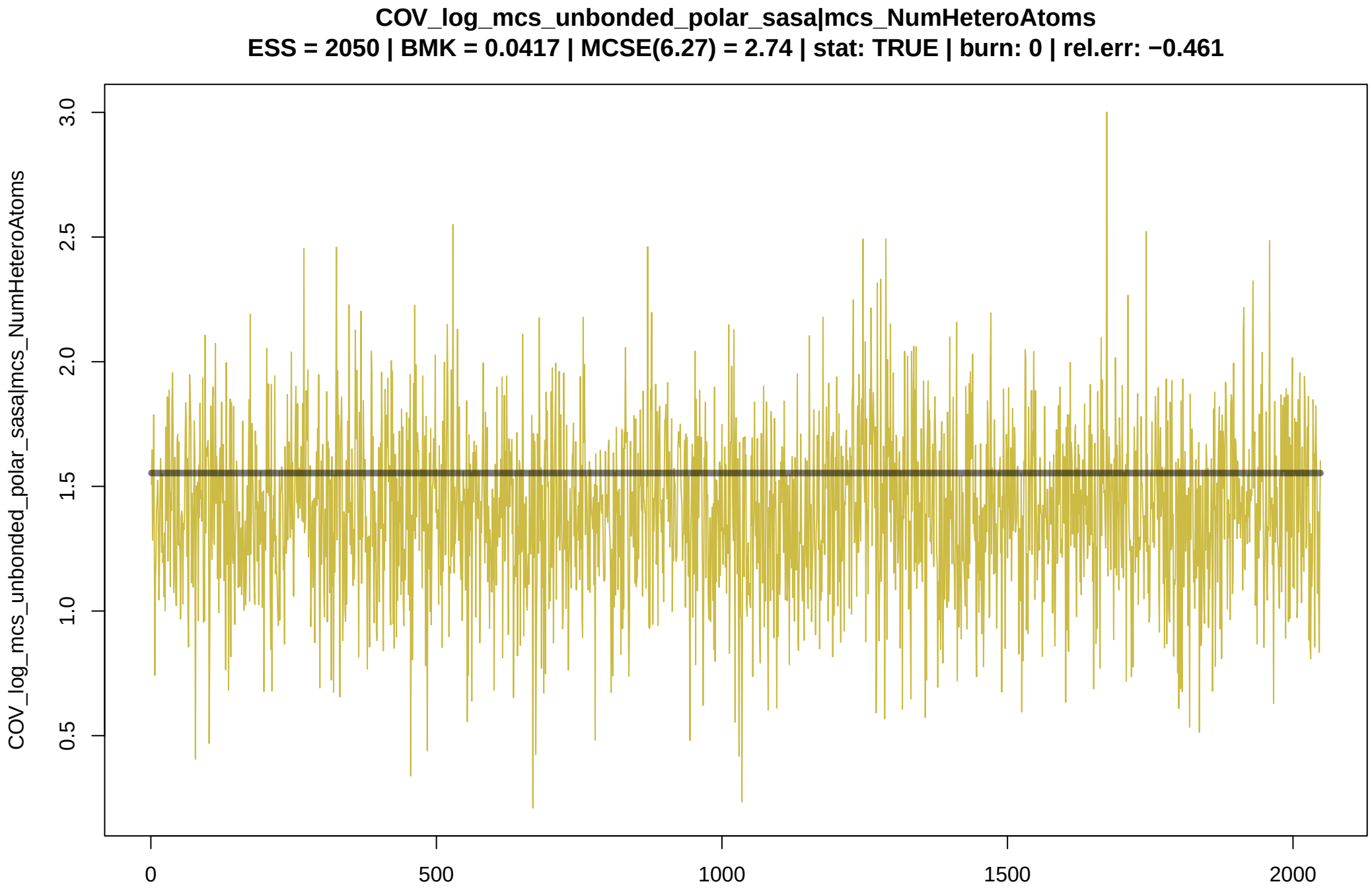

VAR_mcs_NumHeteroAtoms
ESS = 1290 | BMK = 0.0609 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | rel.err: 0.386
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

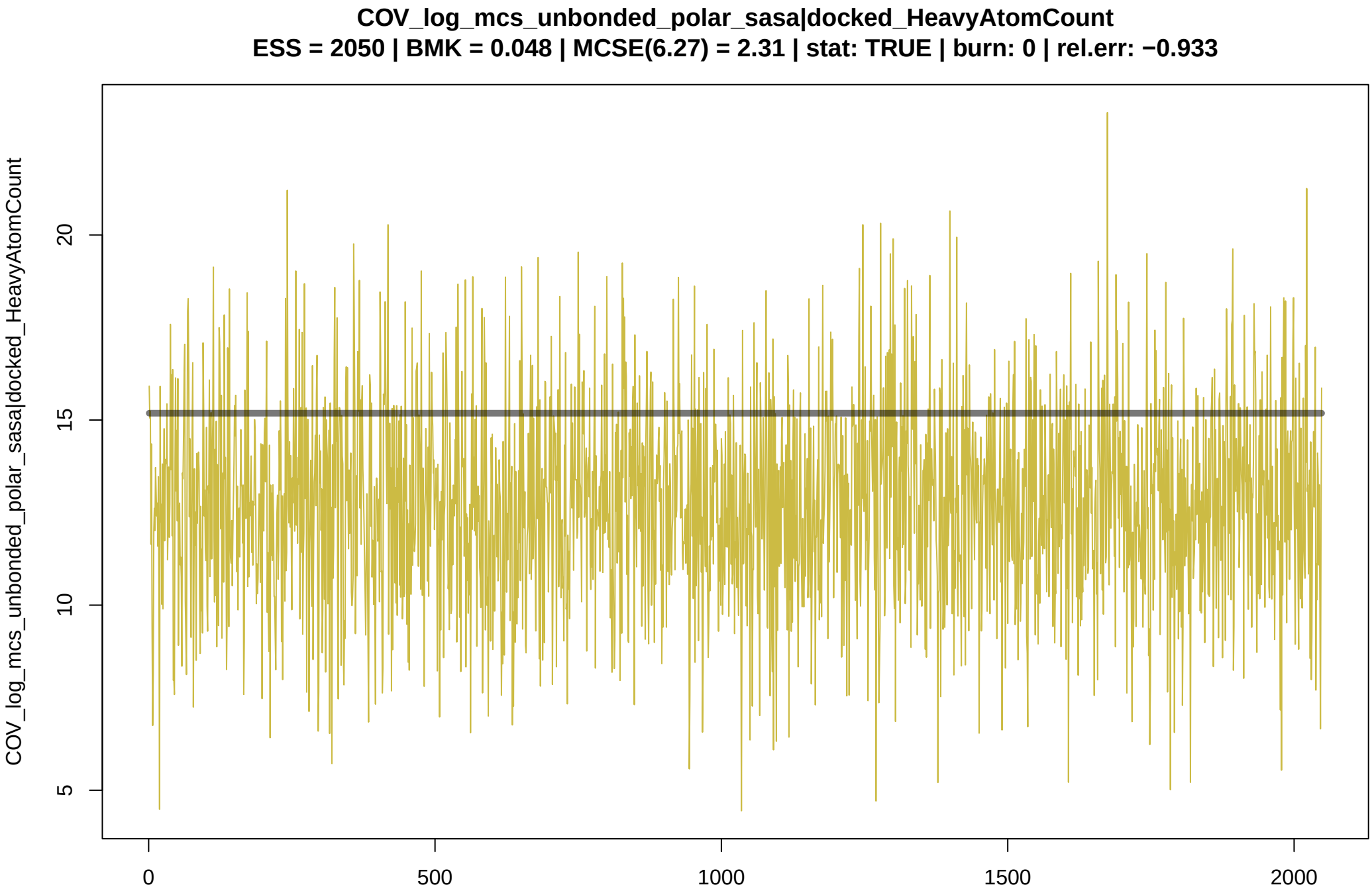

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0675 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: 0.055
VAR_docked_HeavyAtomCount
6.2
6.3
6.4
6.5
6.6
6.7
6.8
0
500
1000
1500
2000

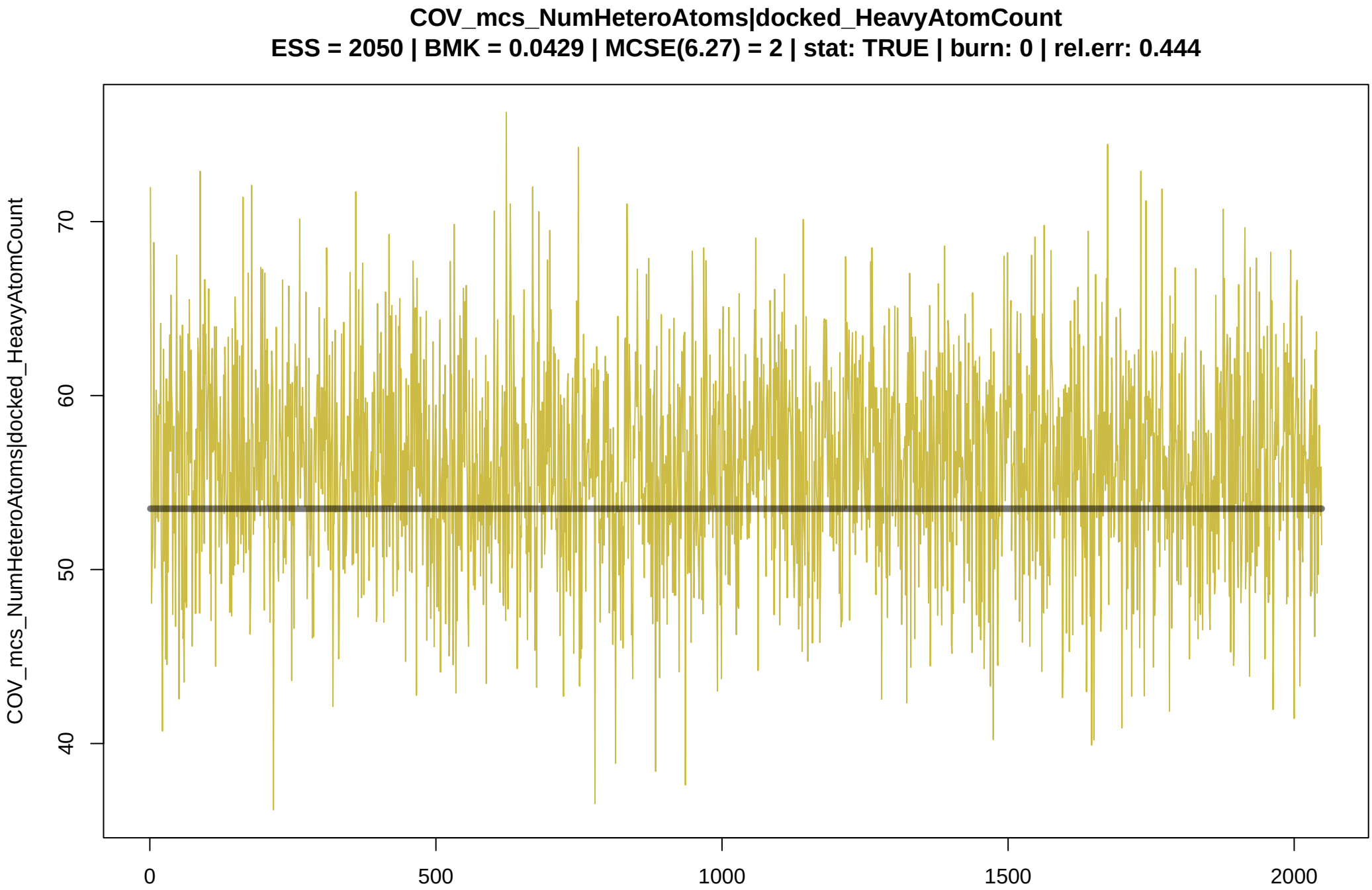

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0574 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: 0.461
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.2
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1860 | BMK = 0.0421 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0 | rel.err: −1.58
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.5
−2.0
−2.5
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0318 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: −1.72
COV_log_RMSD|docked_HeavyAtomCount
−10
−12
−14
−16
−18
−20
−22
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0417 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | rel.err: −0.461
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
3.0
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.048 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: −0.933
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 = 0.0429 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: 0.444
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
500
1000
1500
2000