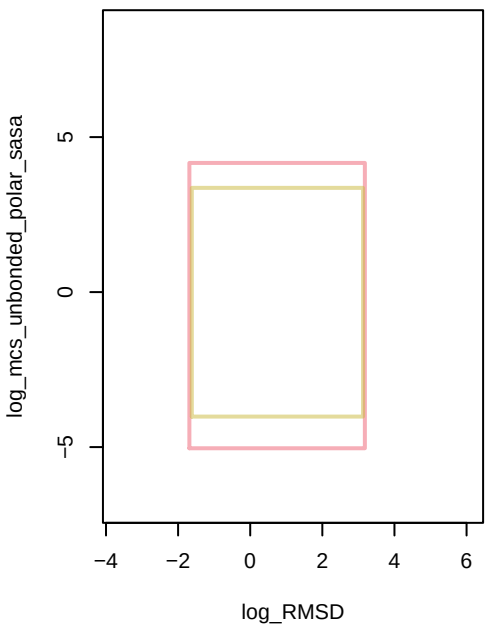
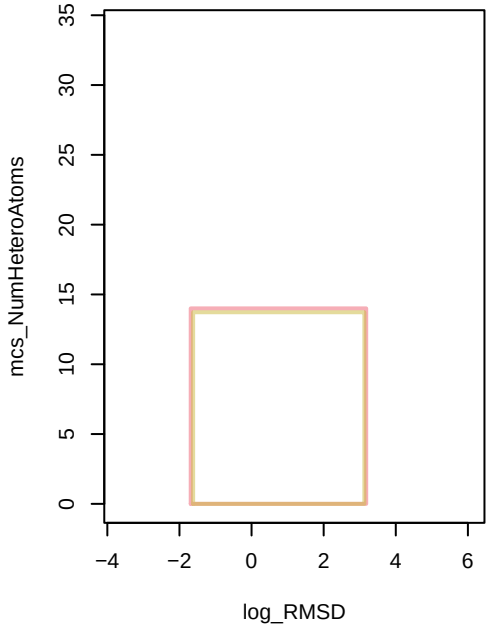
−− STATS maxD −−
min ESS = 116.42984690607 1
max BMK = 0.169587684691241
max MCSE = 8.25734920769785
all stationary: FALSE
burn: 0
max rel.err.: 2.13444516682626

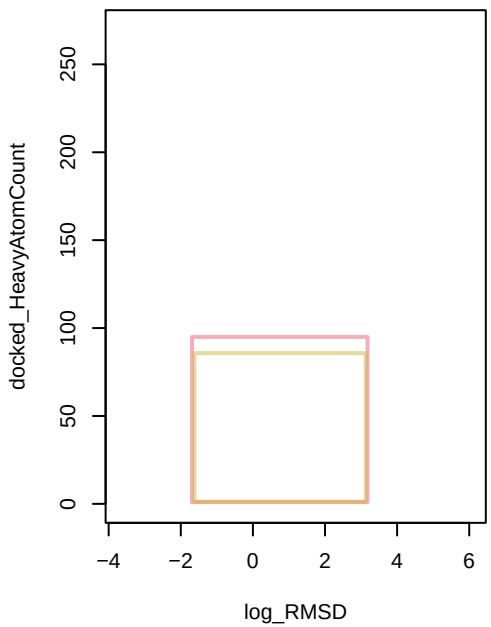
−− STATS 2D −−
min ESS = 1895.50993365077
max BMK = 0.059412372384 1349
max MCSE = 2.59235482760582
all stationary: TRUE
burn: 0
max rel.err.: 1.7886571252752

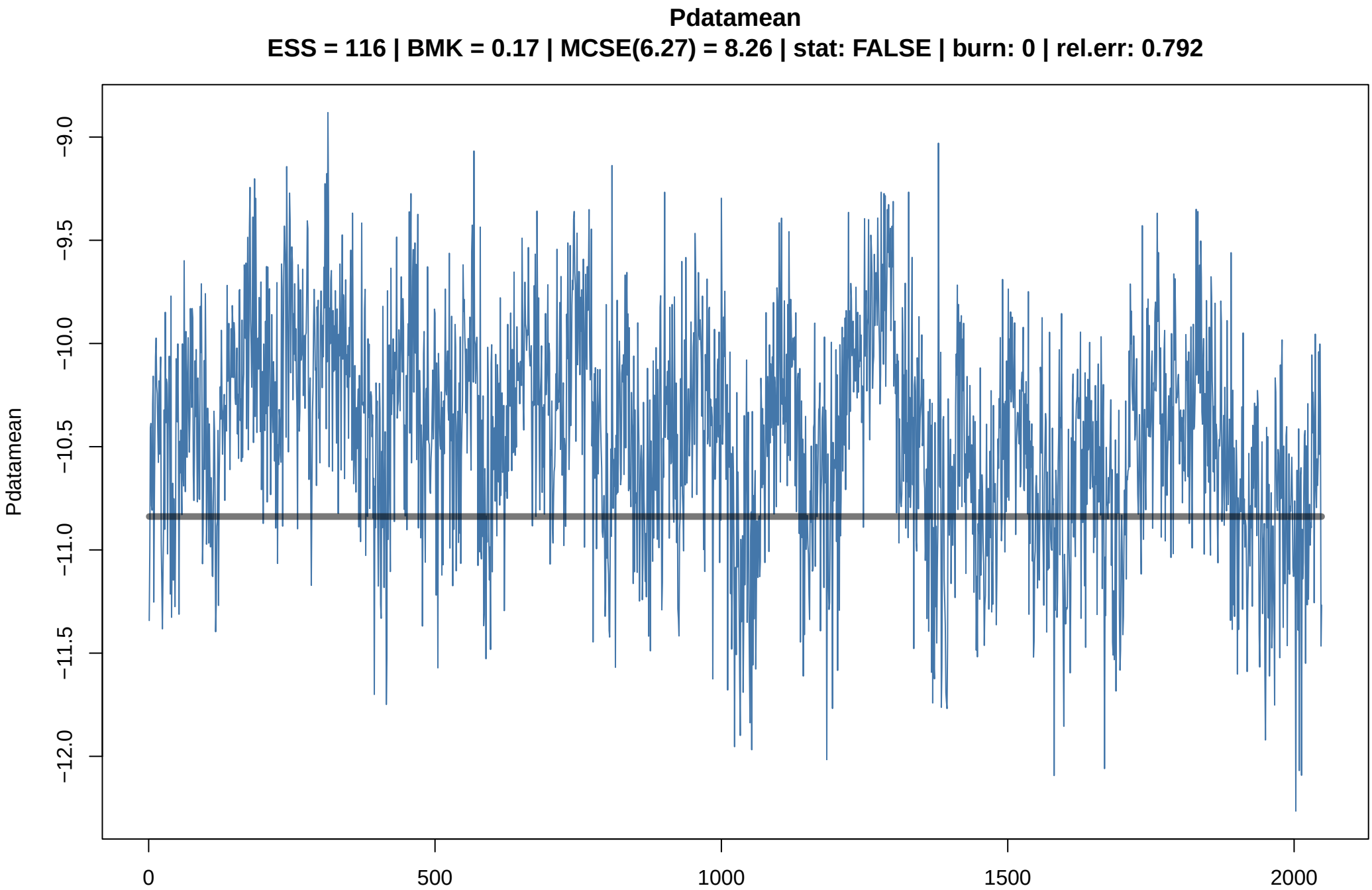
−− STATS 1D −−
min ESS = 1269.81687930201
max BMK = 0.069832332163 6036
max MCSE = 3.05320540171572
all stationary: TRUE
burn: 0
max rel.err.: 2.24831636901743

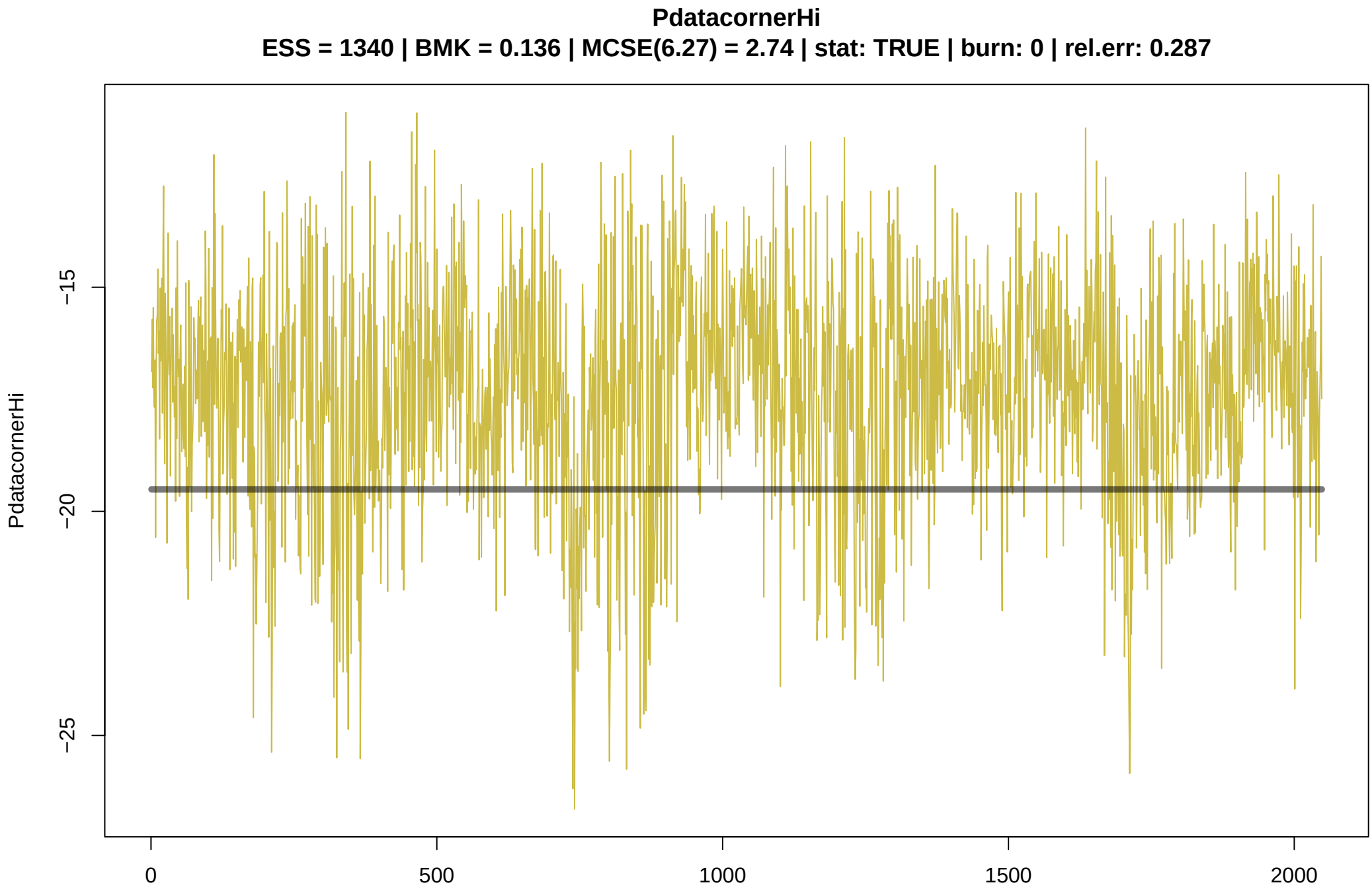
Occupied clusters: 11 of 16

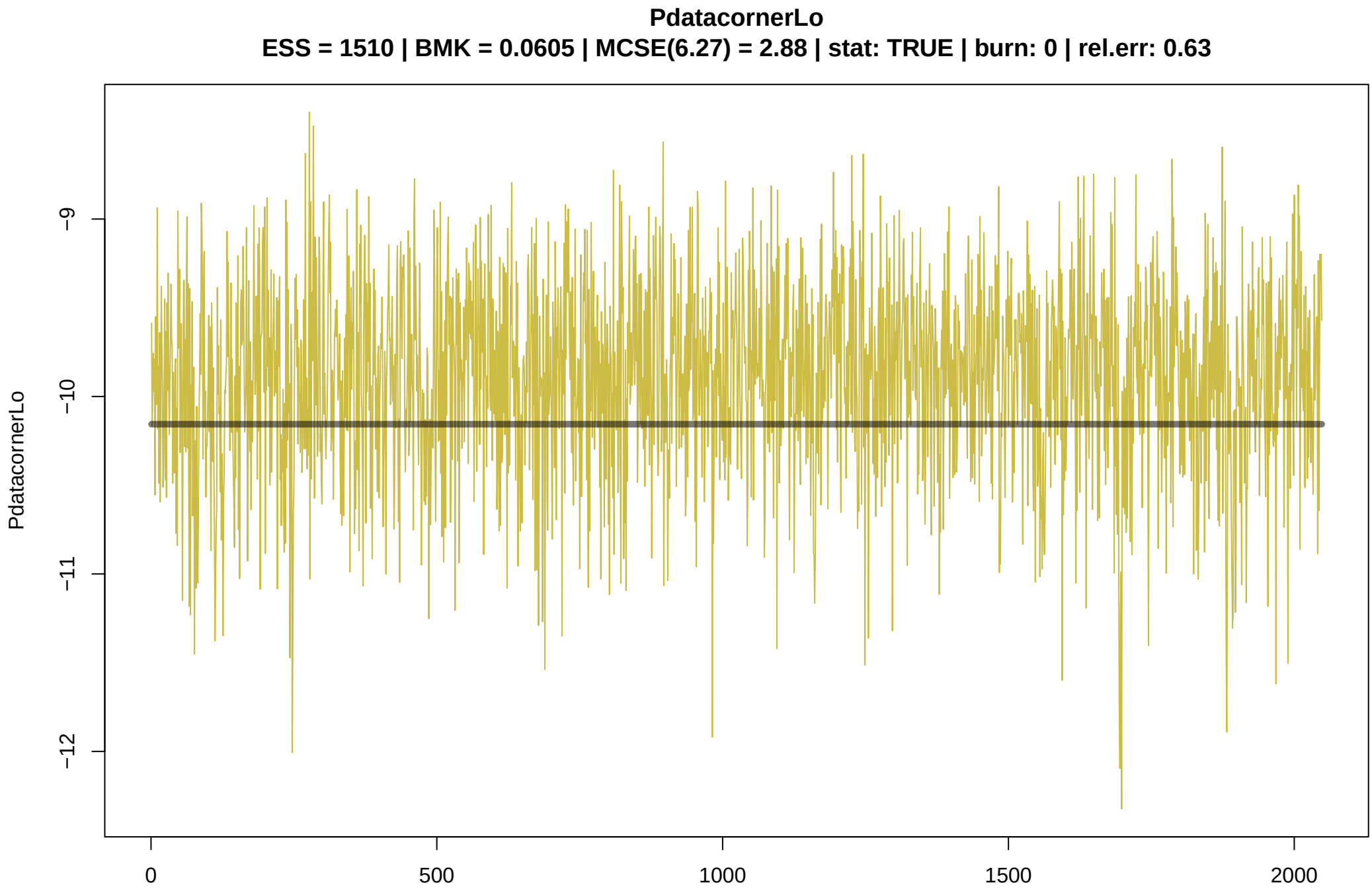

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

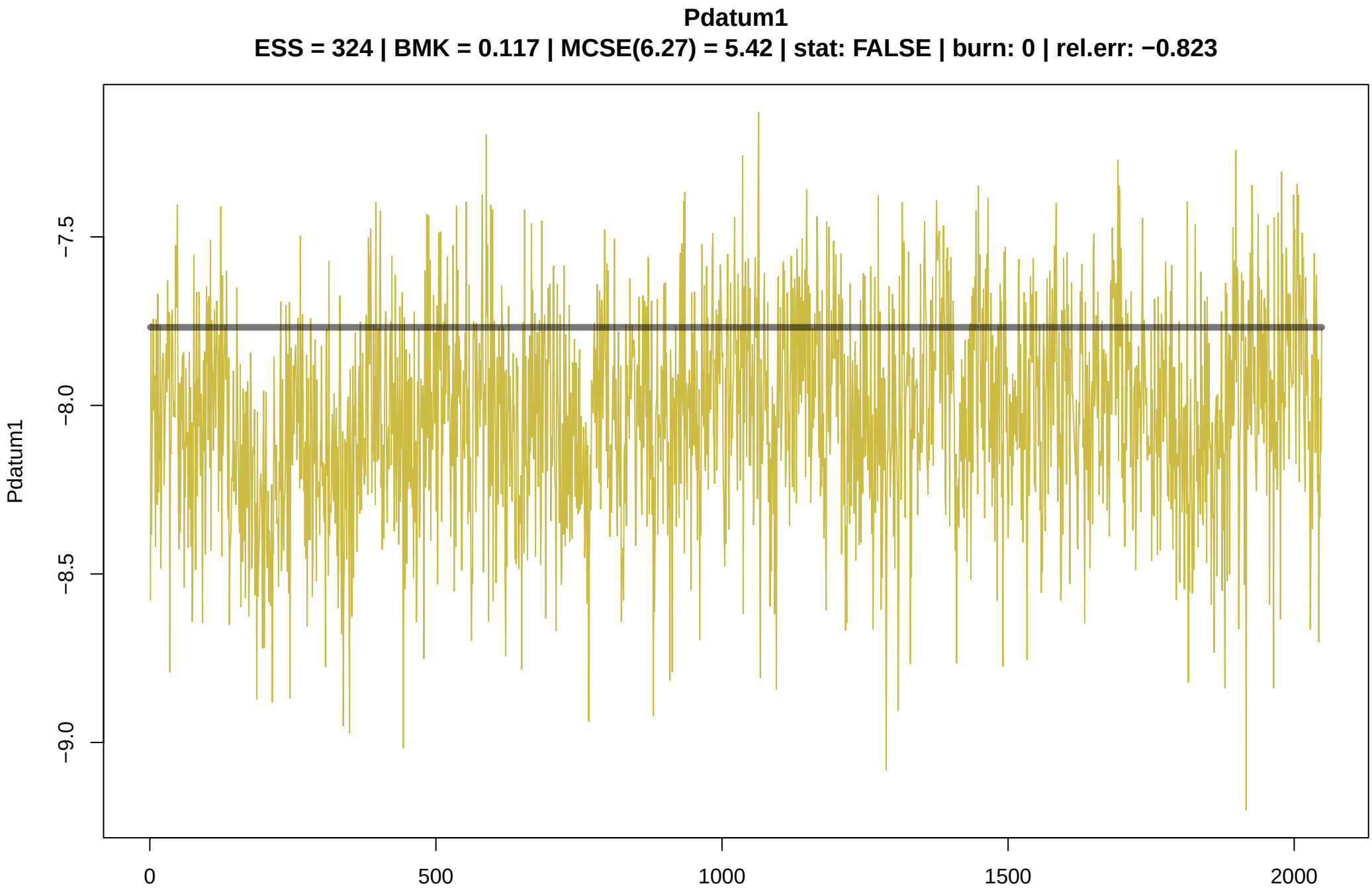

mcs_NumHeteroAtoms
35
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

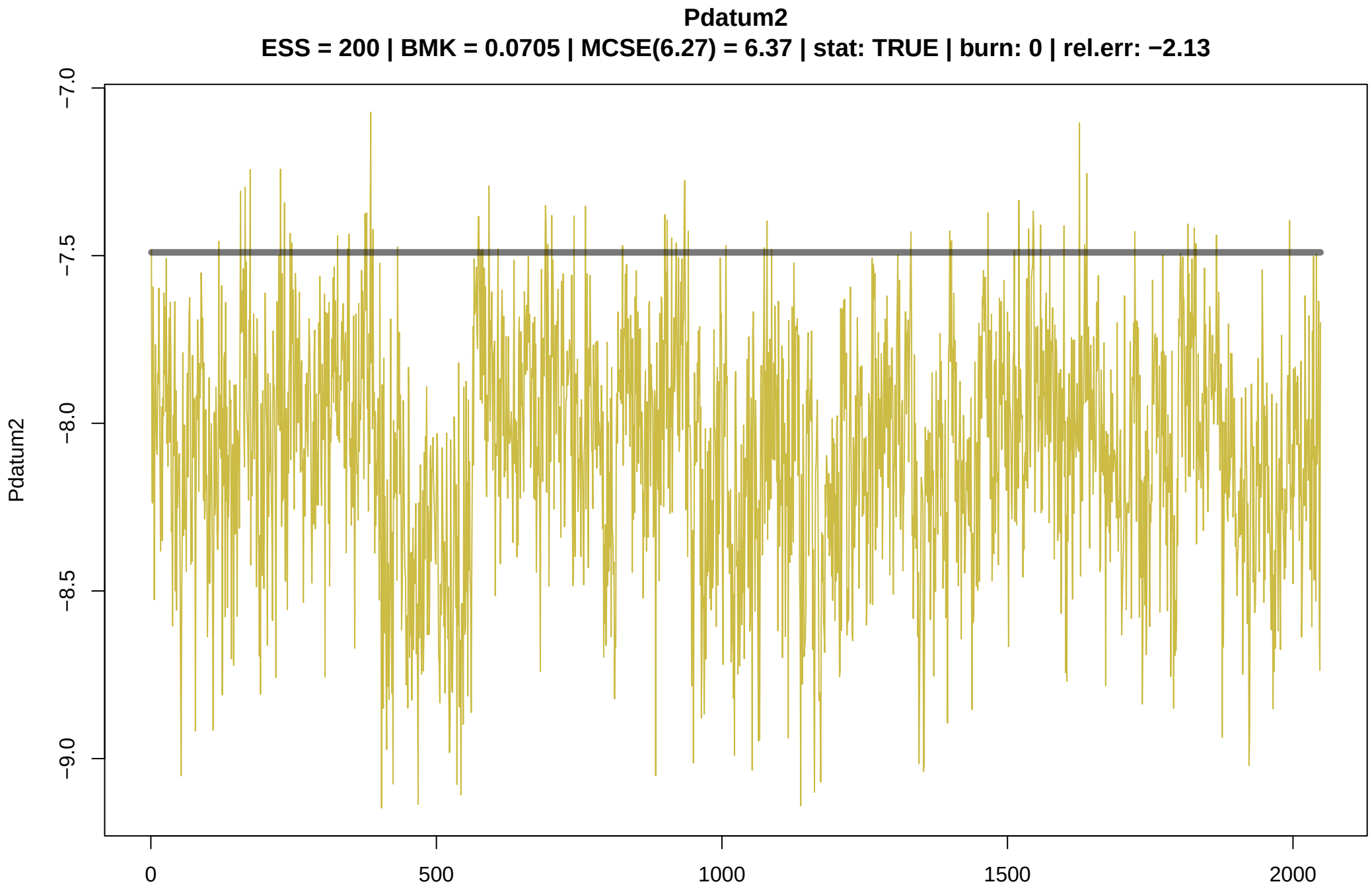

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

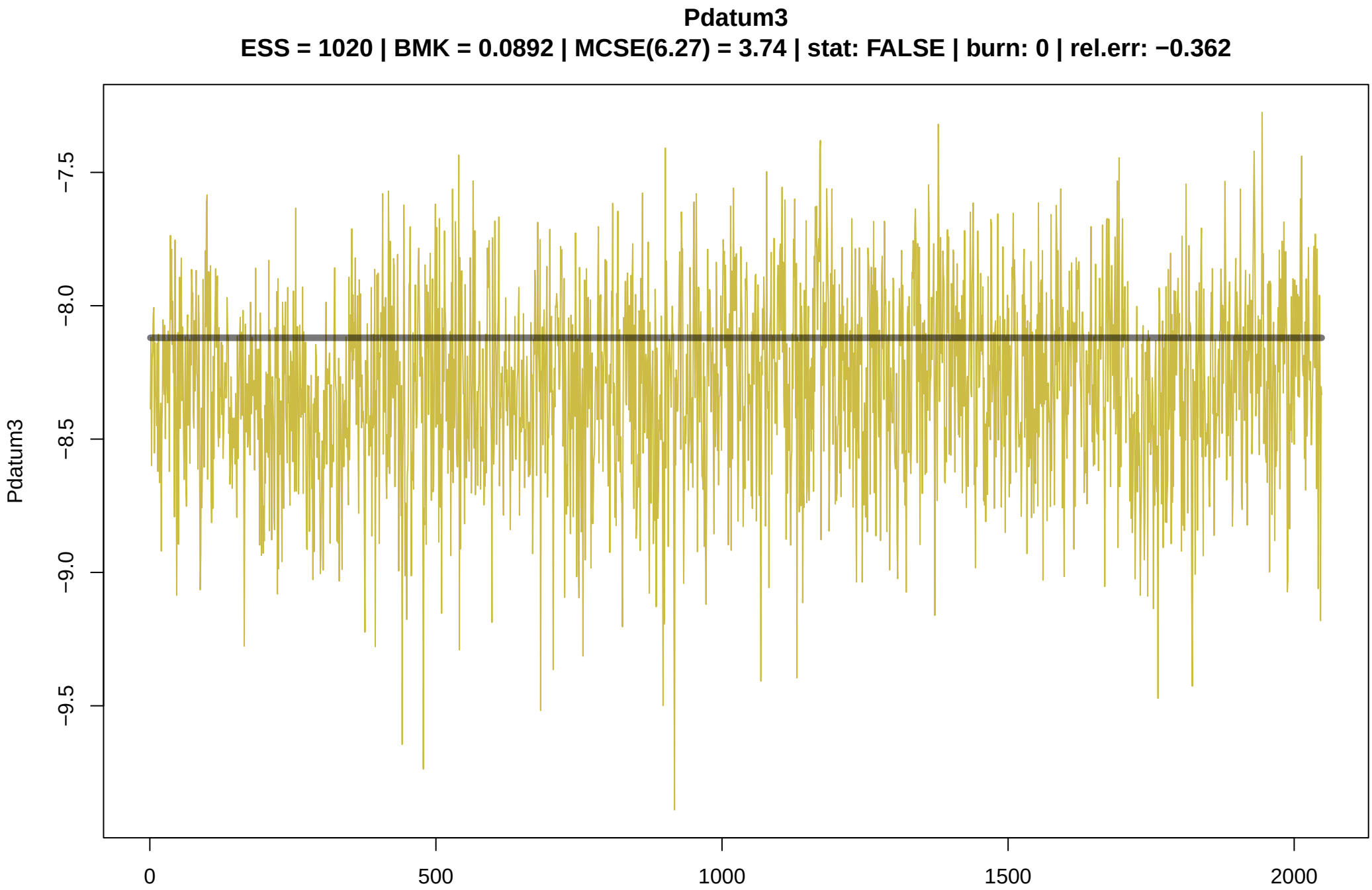

Pdatamean
ESS = 116 | BMK = 0.17 | MCSE(6.27) = 8.26 | stat: FALSE | burn: 0 | rel.err: 0.792
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

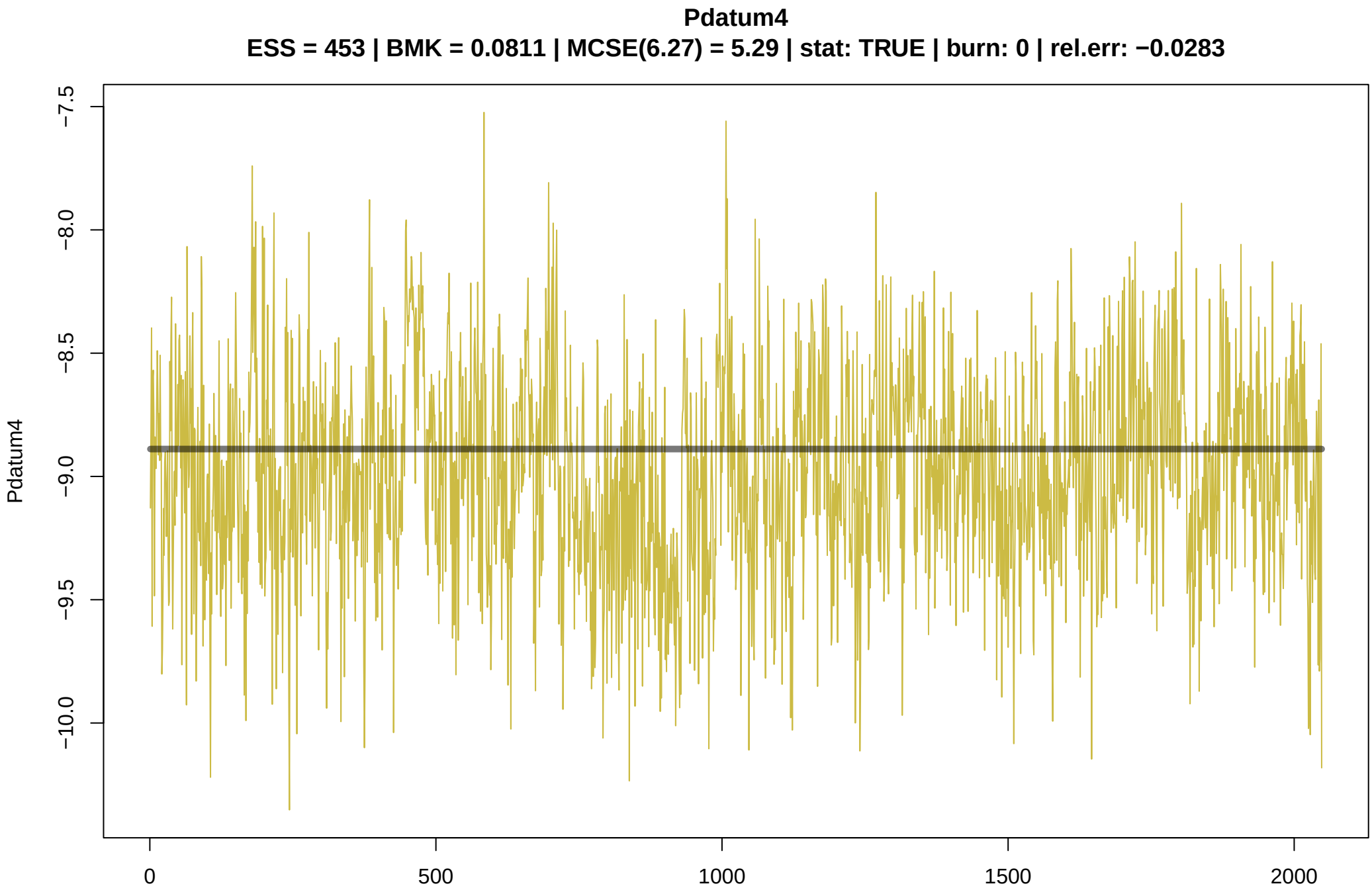

PdatacornerHi
ESS = 1340 | BMK = 0.136 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | rel.err: 0.287
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

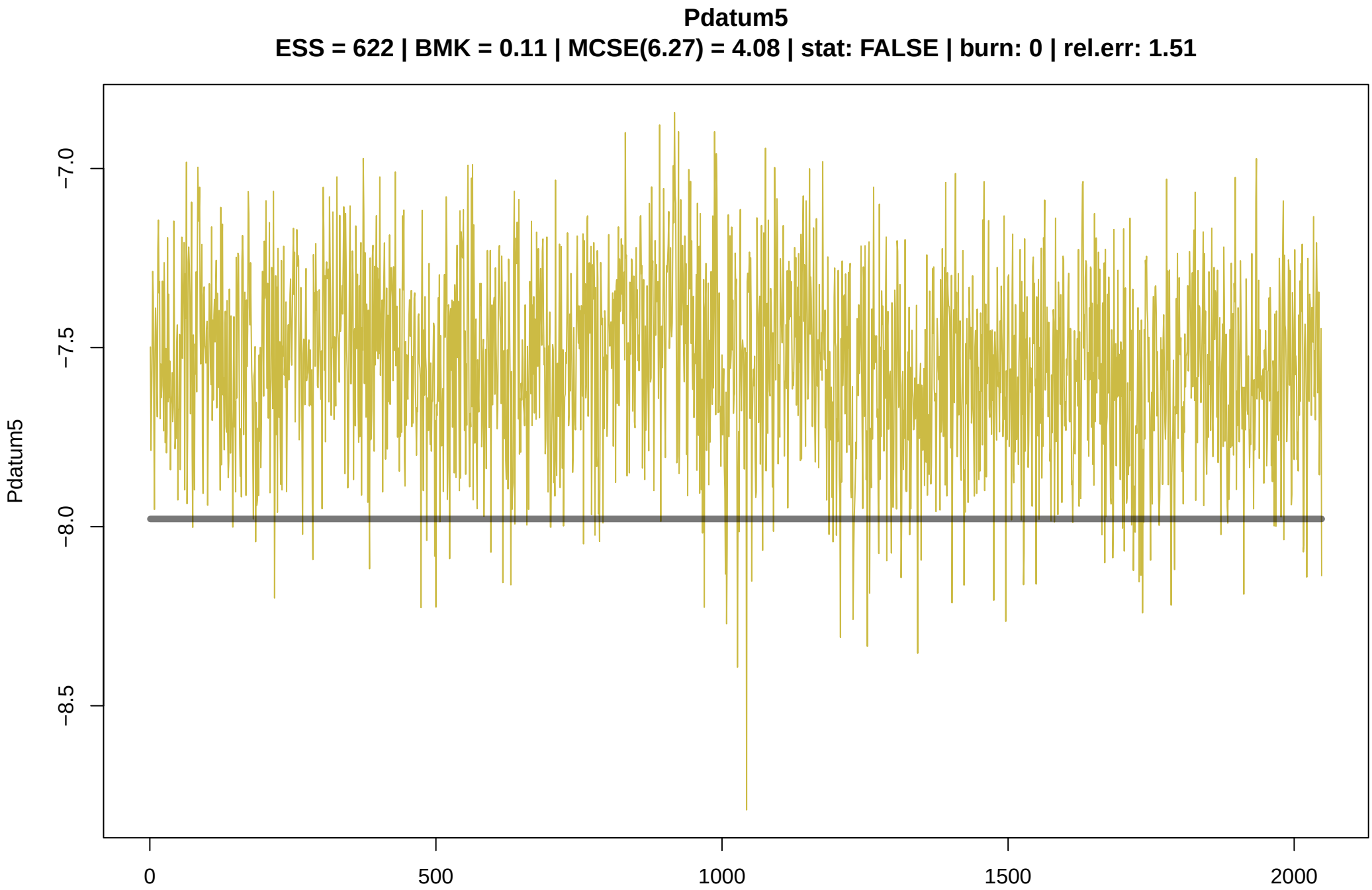

PdatacornerLo
ESS = 1510 | BMK = 0.0605 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: 0.63
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

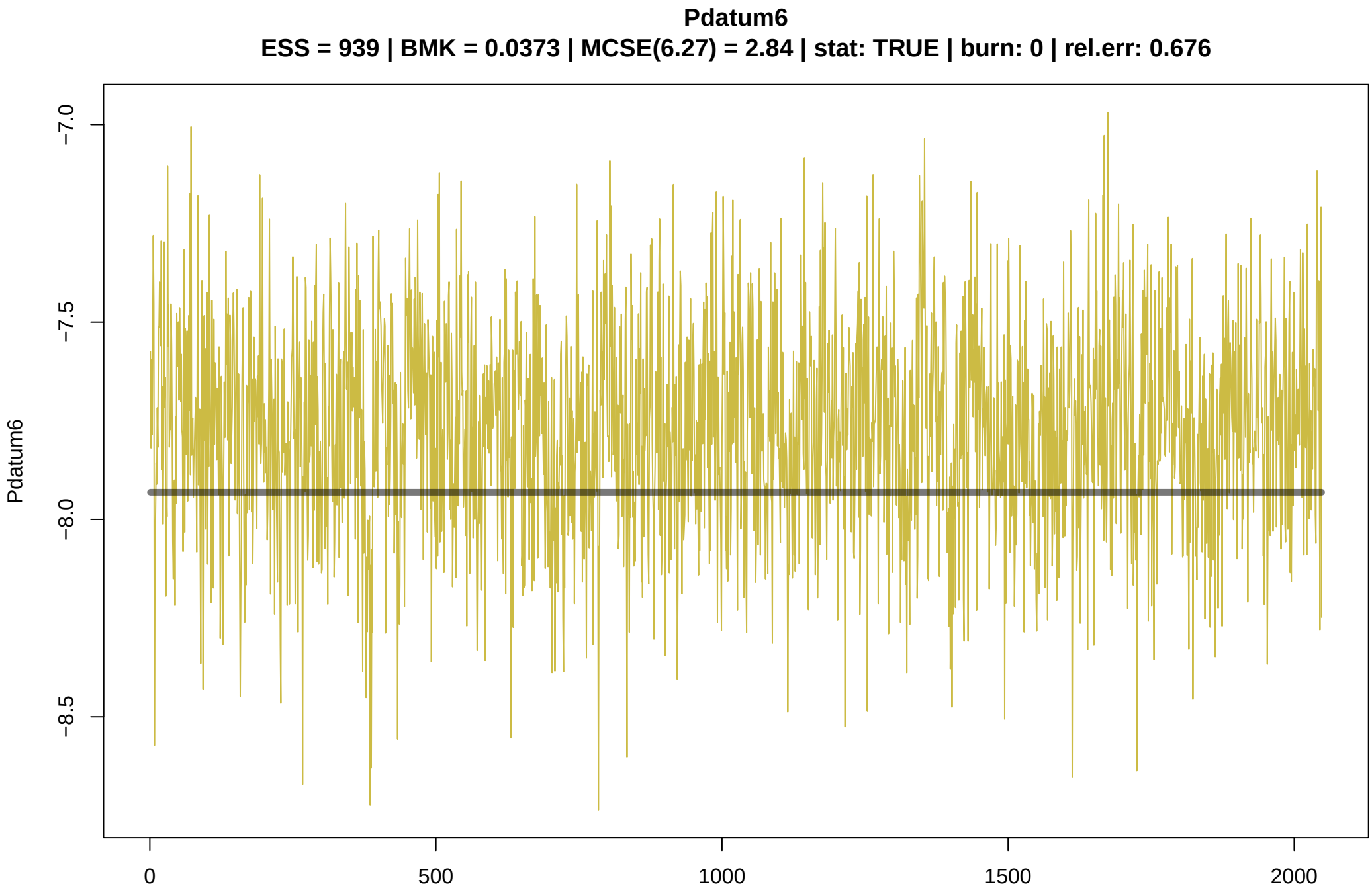

Pdatum1
ESS = 324 | BMK = 0.117 | MCSE(6.27) = 5.42 | stat: FALSE | burn: 0 | rel.err: −0.823
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

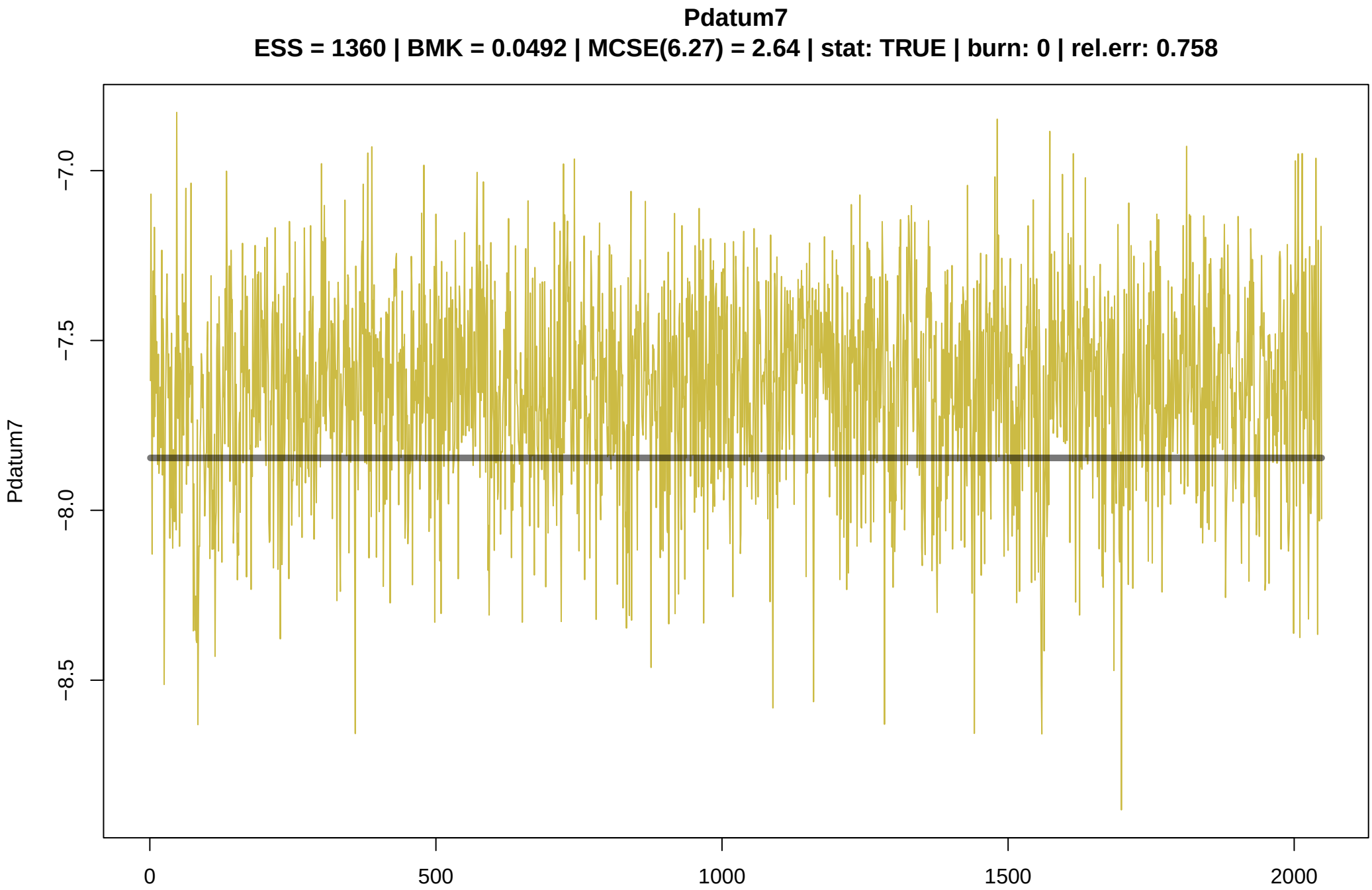

Pdatum2
ESS = 200 | BMK = 0.0705 | MCSE(6.27) = 6.37 | stat: TRUE | burn: 0 | rel.err: −2.13
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

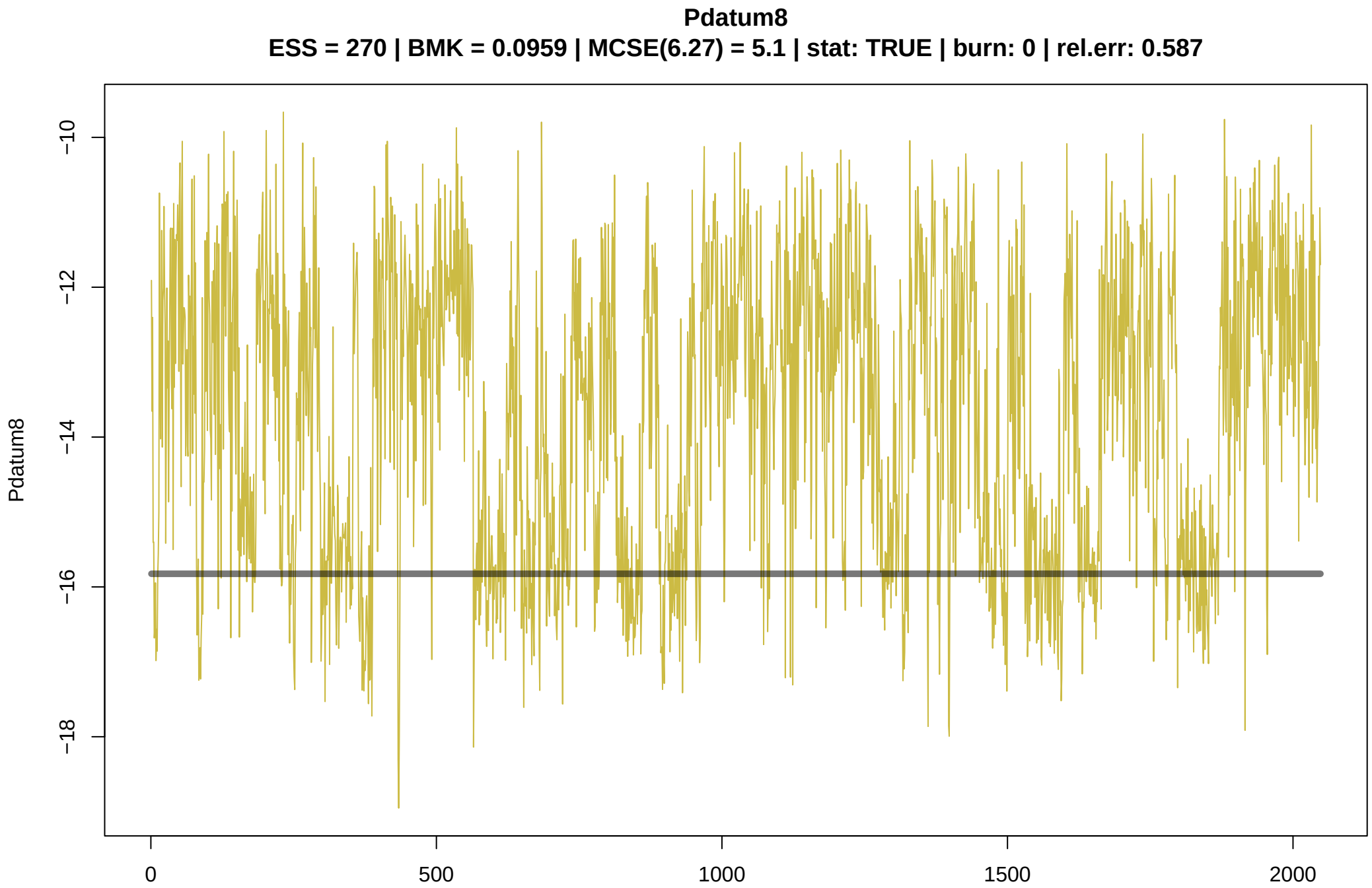

Pdatum3
ESS = 1020 | BMK = 0.0892 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0 | rel.err: −0.362
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

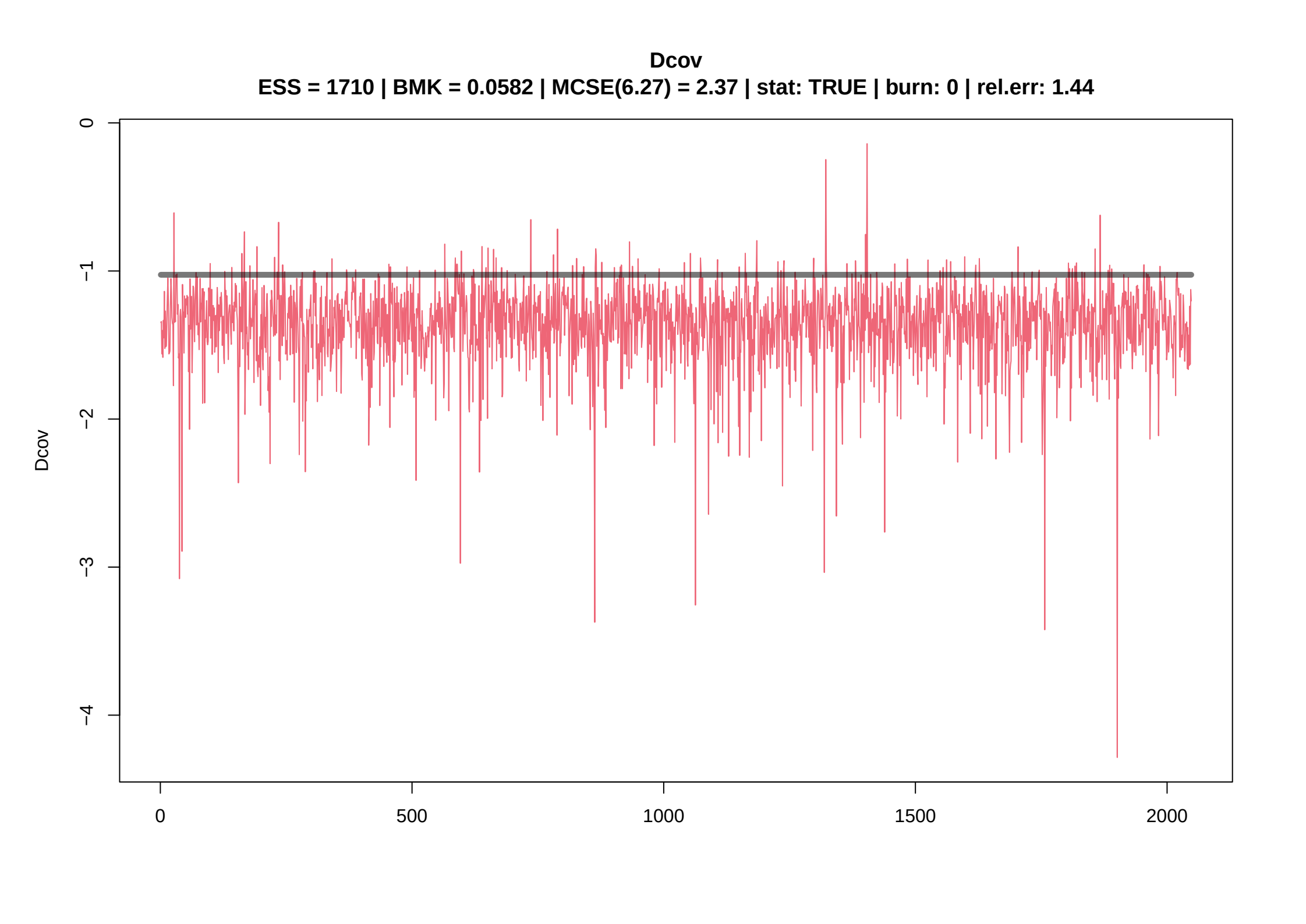

Pdatum4
ESS = 453 | BMK = 0.0811 | MCSE(6.27) = 5.29 | stat: TRUE | burn: 0 | rel.err: −0.0283
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

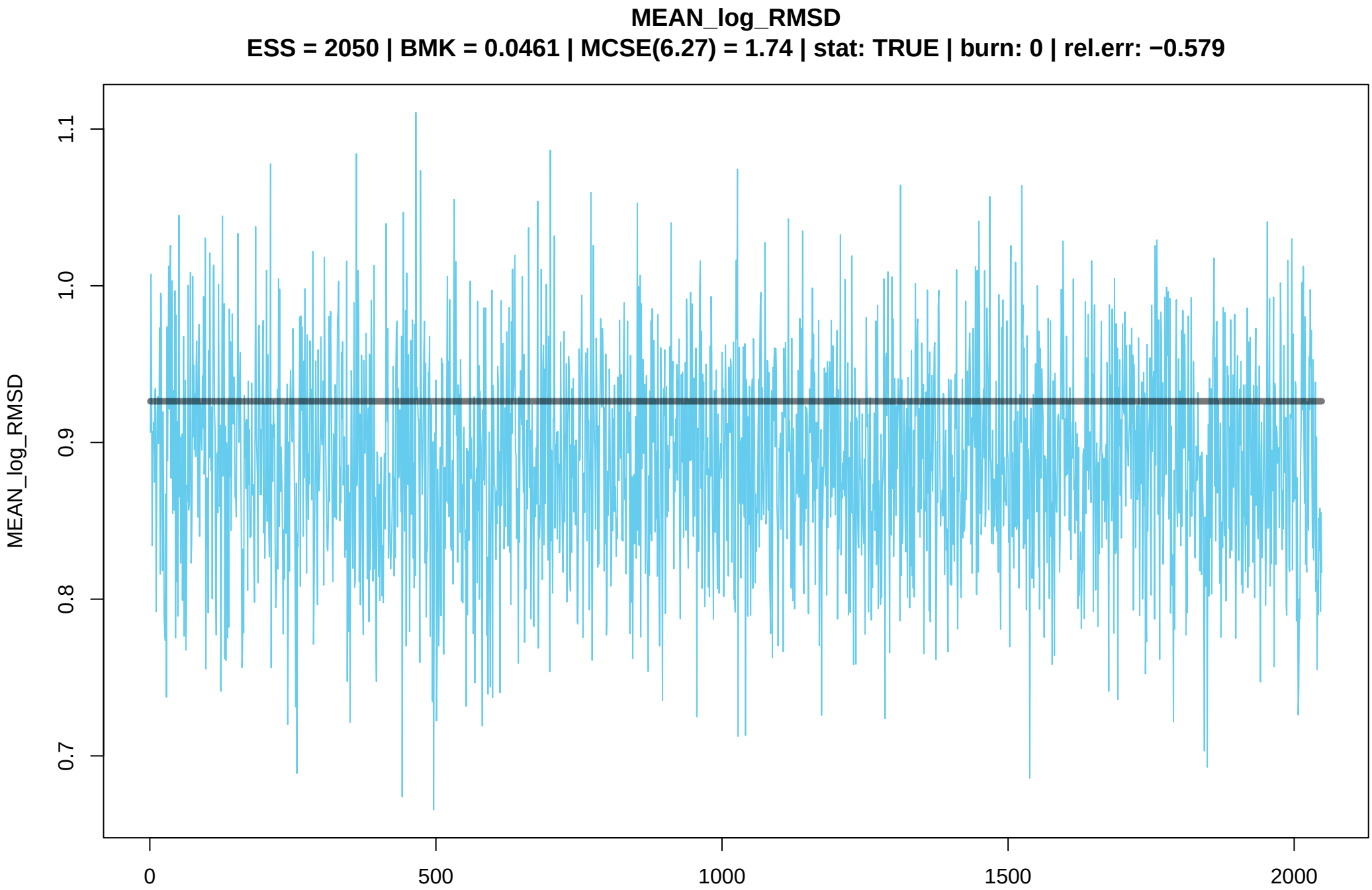

Pdatum5
ESS = 622 | BMK = 0.11 | MCSE(6.27) = 4.08 | stat: FALSE | burn: 0 | rel.err: 1.51
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

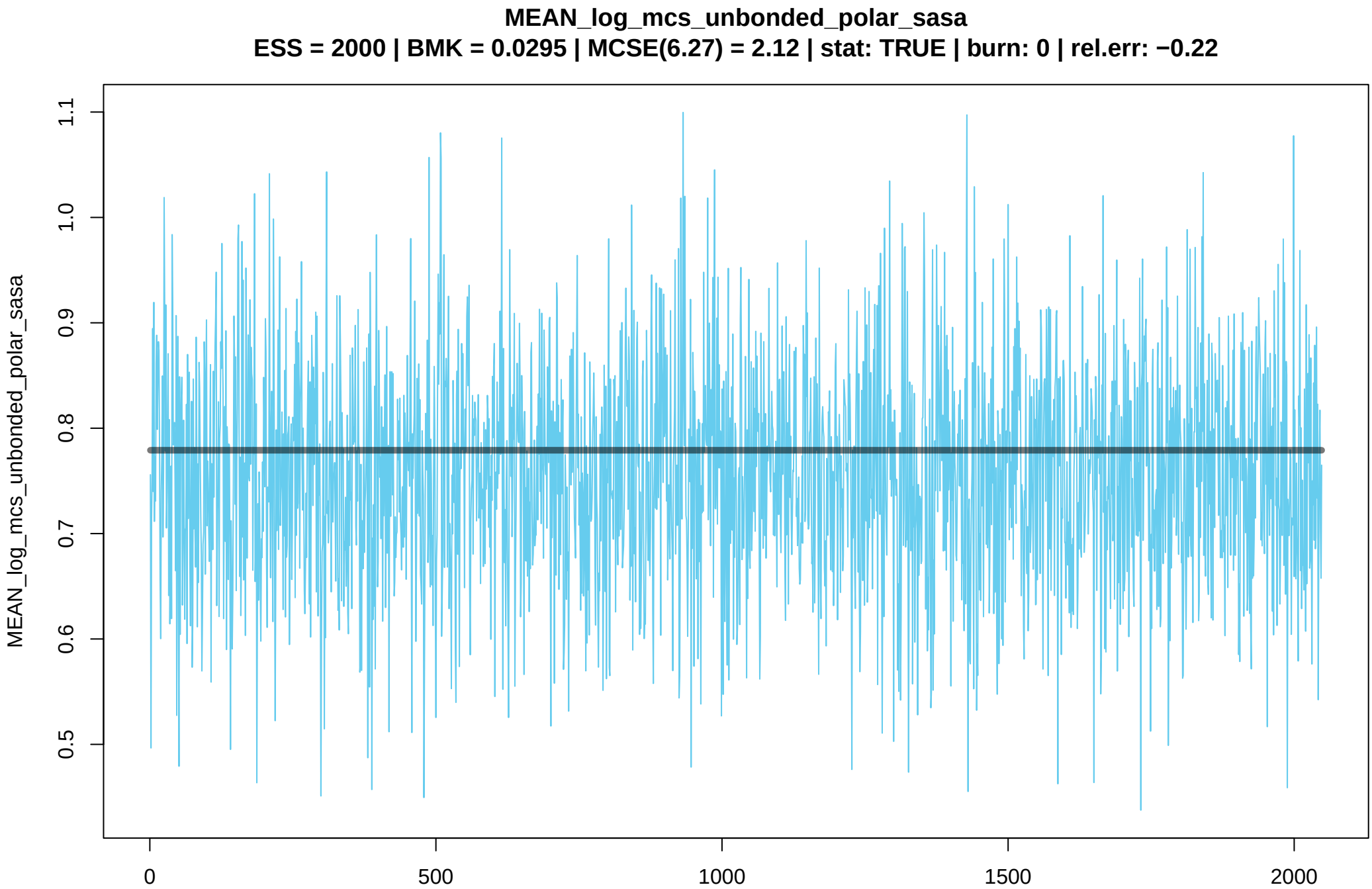

Pdatum6
ESS = 939 | BMK = 0.0373 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0 | rel.err: 0.676
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

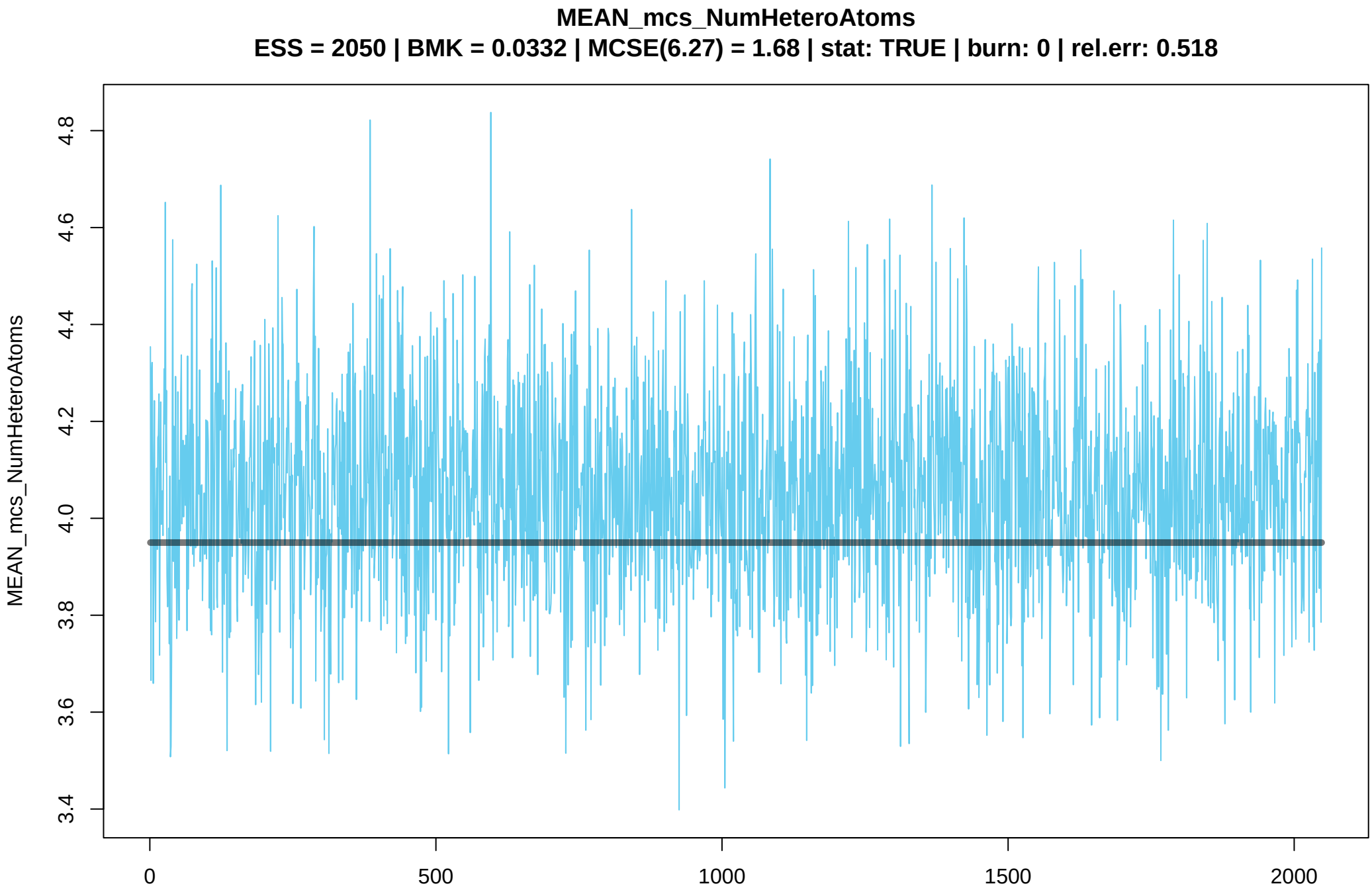

Pdatum7
ESS = 1360 | BMK = 0.0492 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: 0.758
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

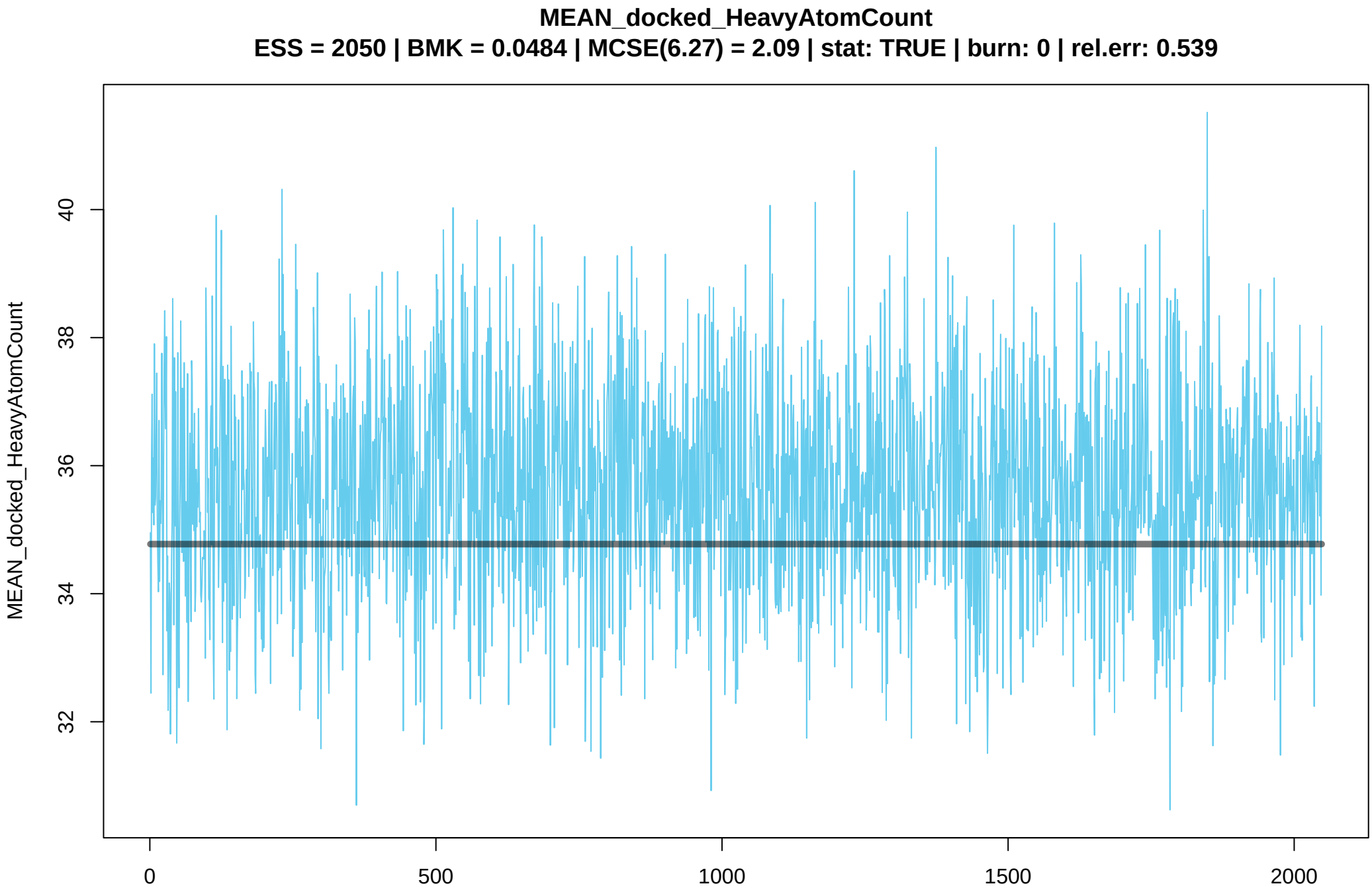

Pdatum8
ESS = 270 | BMK = 0.0959 | MCSE(6.27) = 5.1 | stat: TRUE | burn: 0 | rel.err: 0.587
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

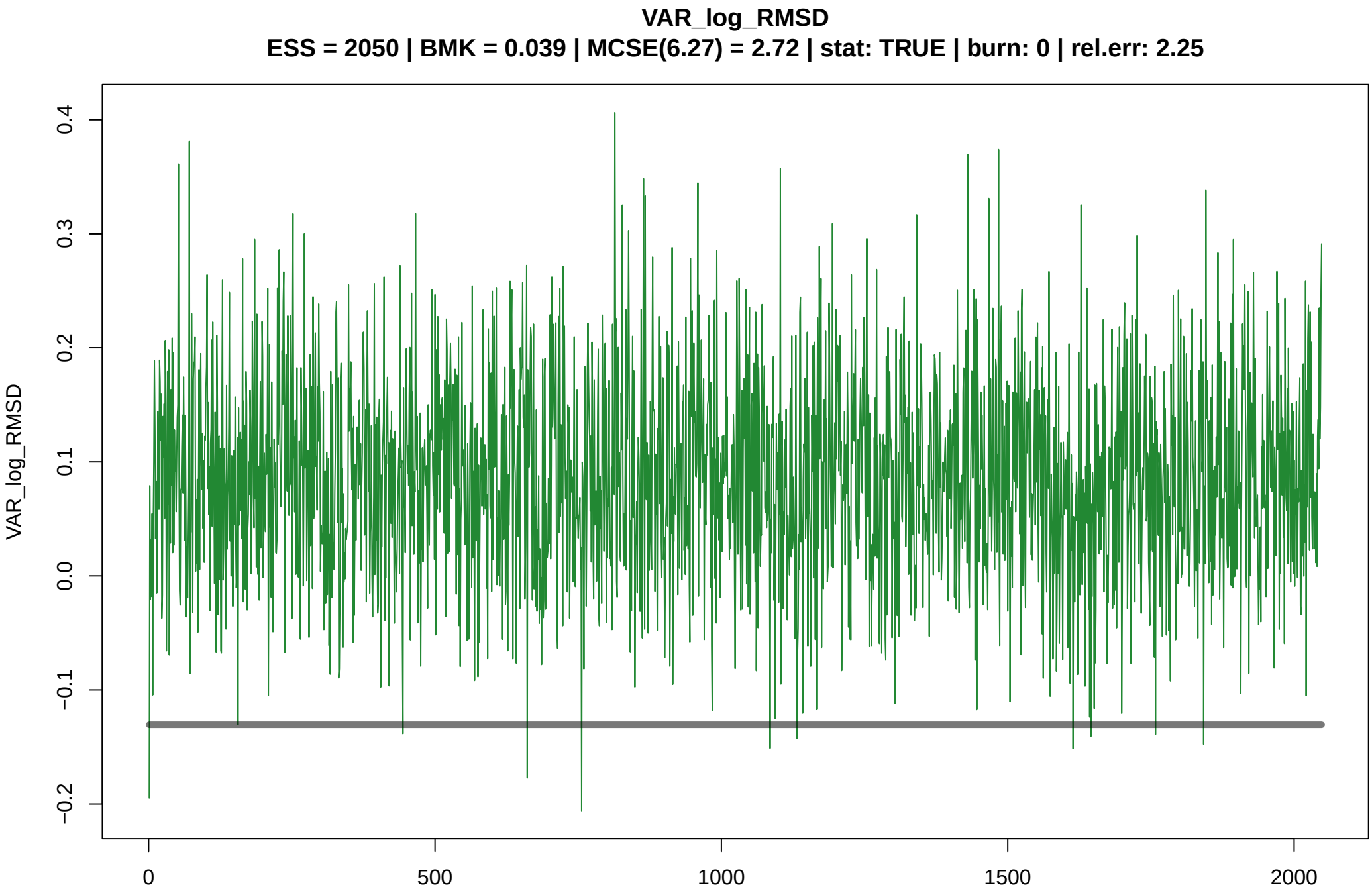

Dcov
ESS = 1710 | BMK = 0.0582 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 1.44
Dcov
0
−1
−2
−3
−4
0
500
1000
1500
2000

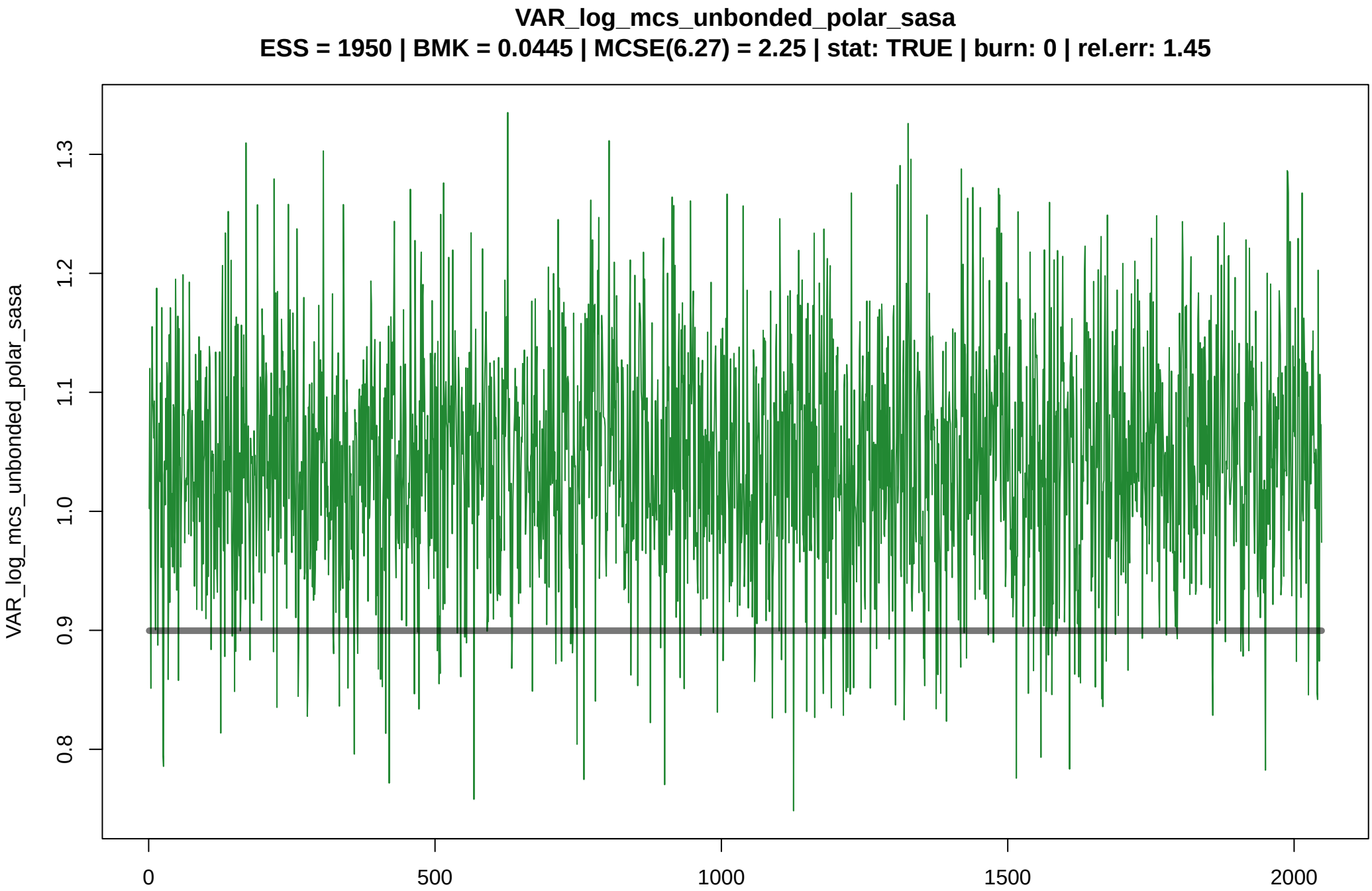

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0461 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0 | rel.err: −0.579
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

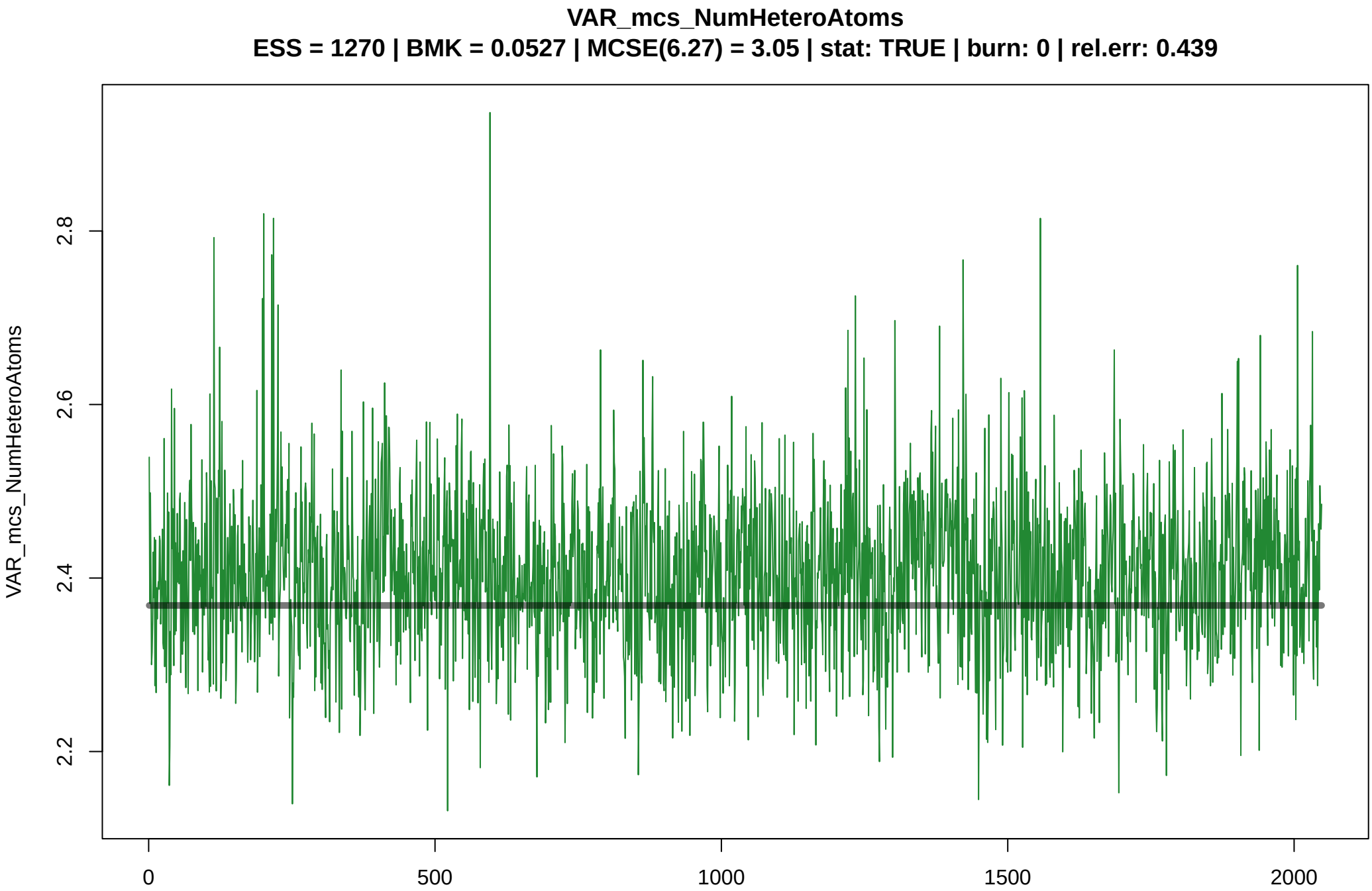

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2000 | BMK = 0.0295 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: −0.22
MEAN_log_mcs_unbonded_polar_sasa
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

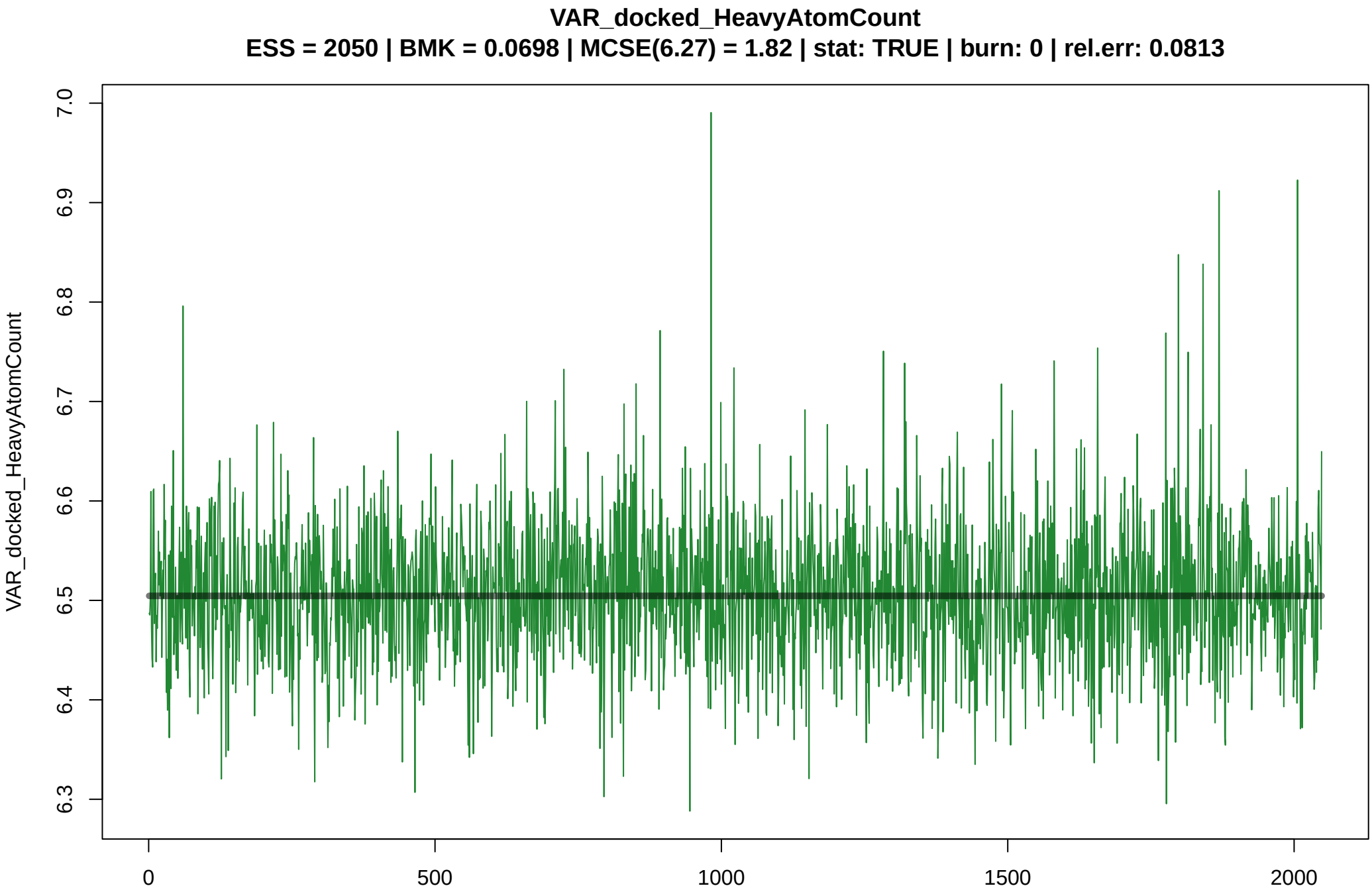

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0332 | MCSE(6.27) = 1.68 | stat: TRUE | burn: 0 | rel.err: 0.518
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

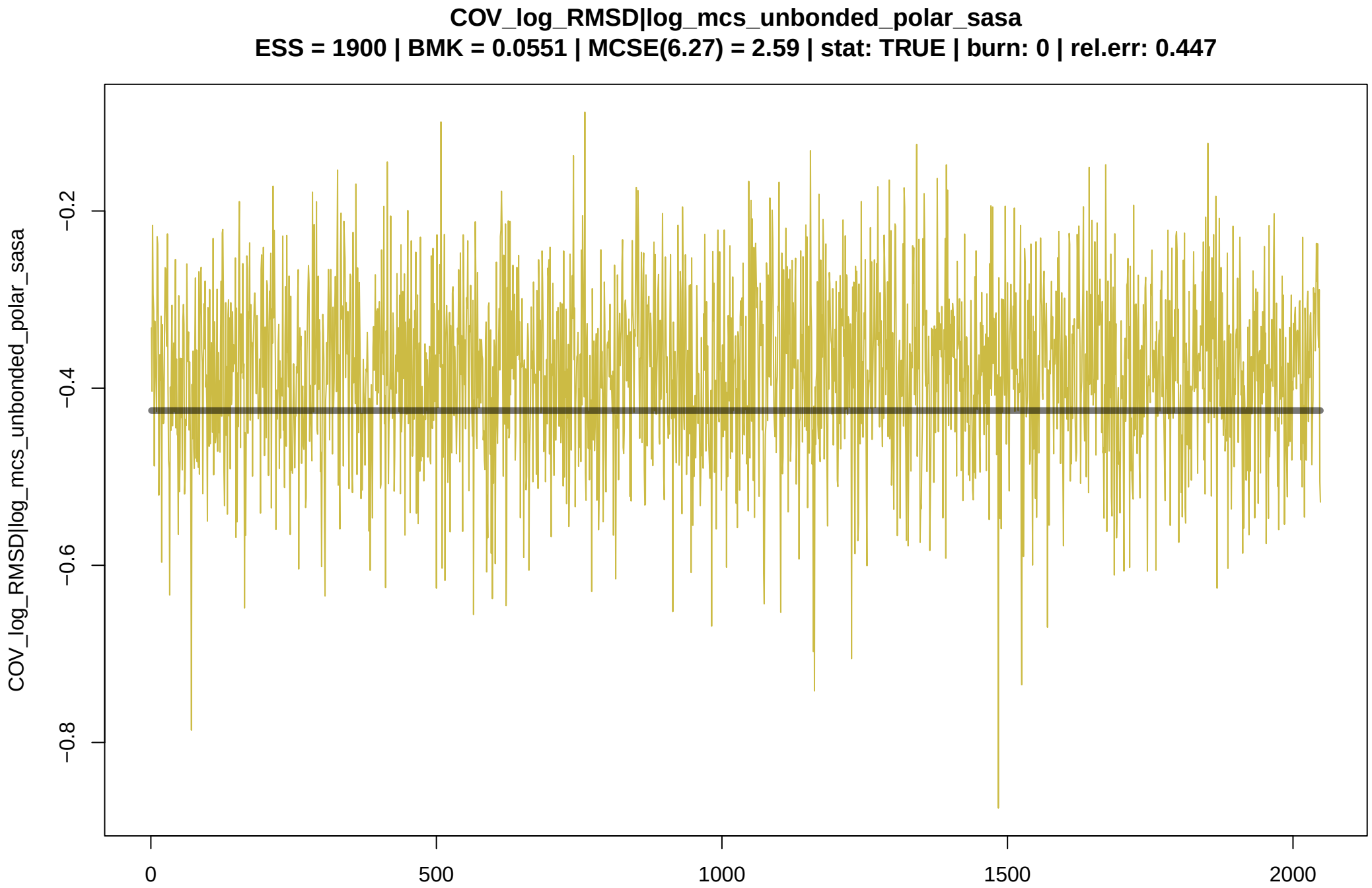

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0484 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.539
MEAN_docked_HeavyAtomCount
32
34
36
38
40
0
500
1000
1500
2000

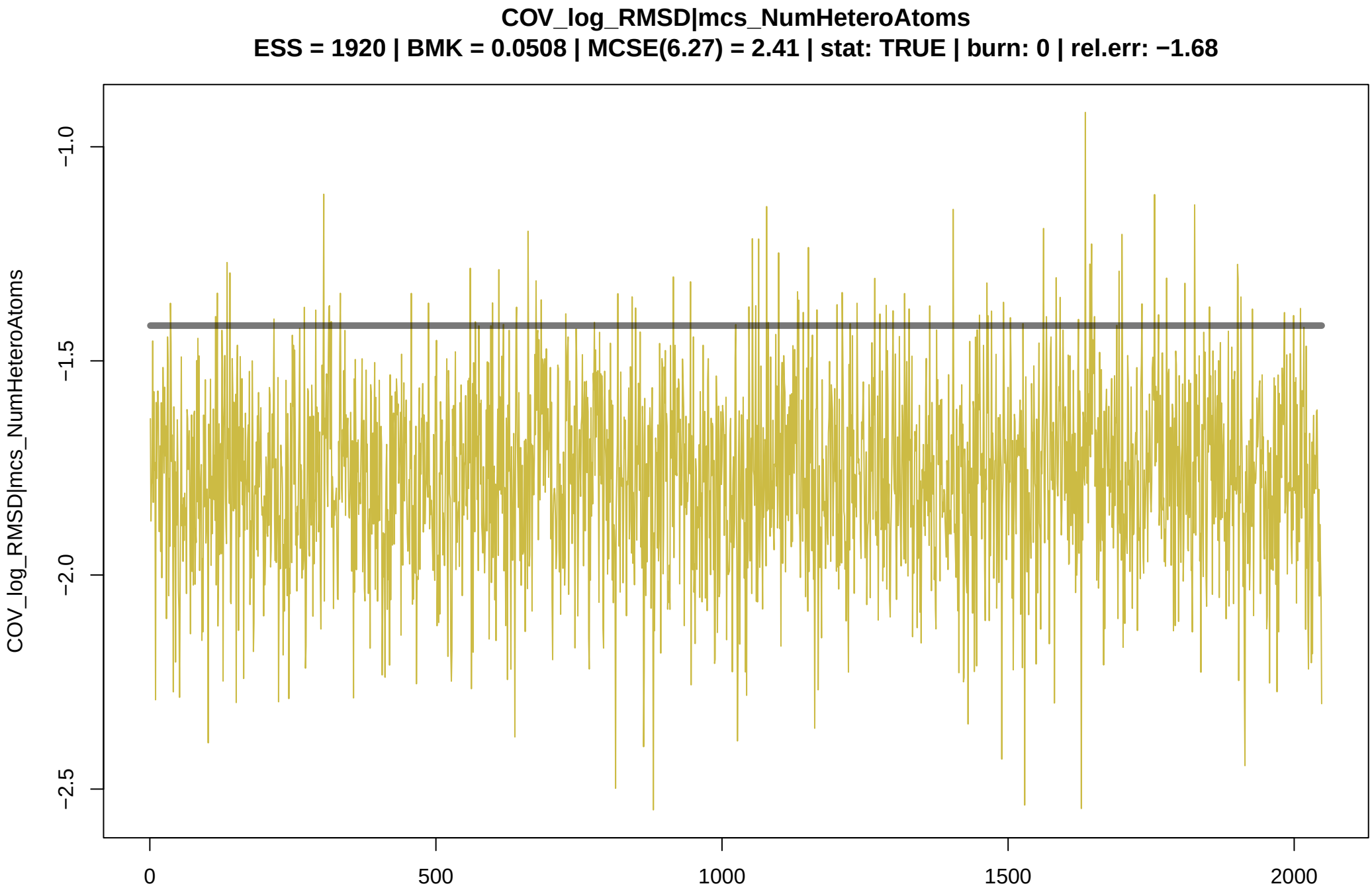

VAR_log_RMSD
ESS = 2050 | BMK = 0.039 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 2.25
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

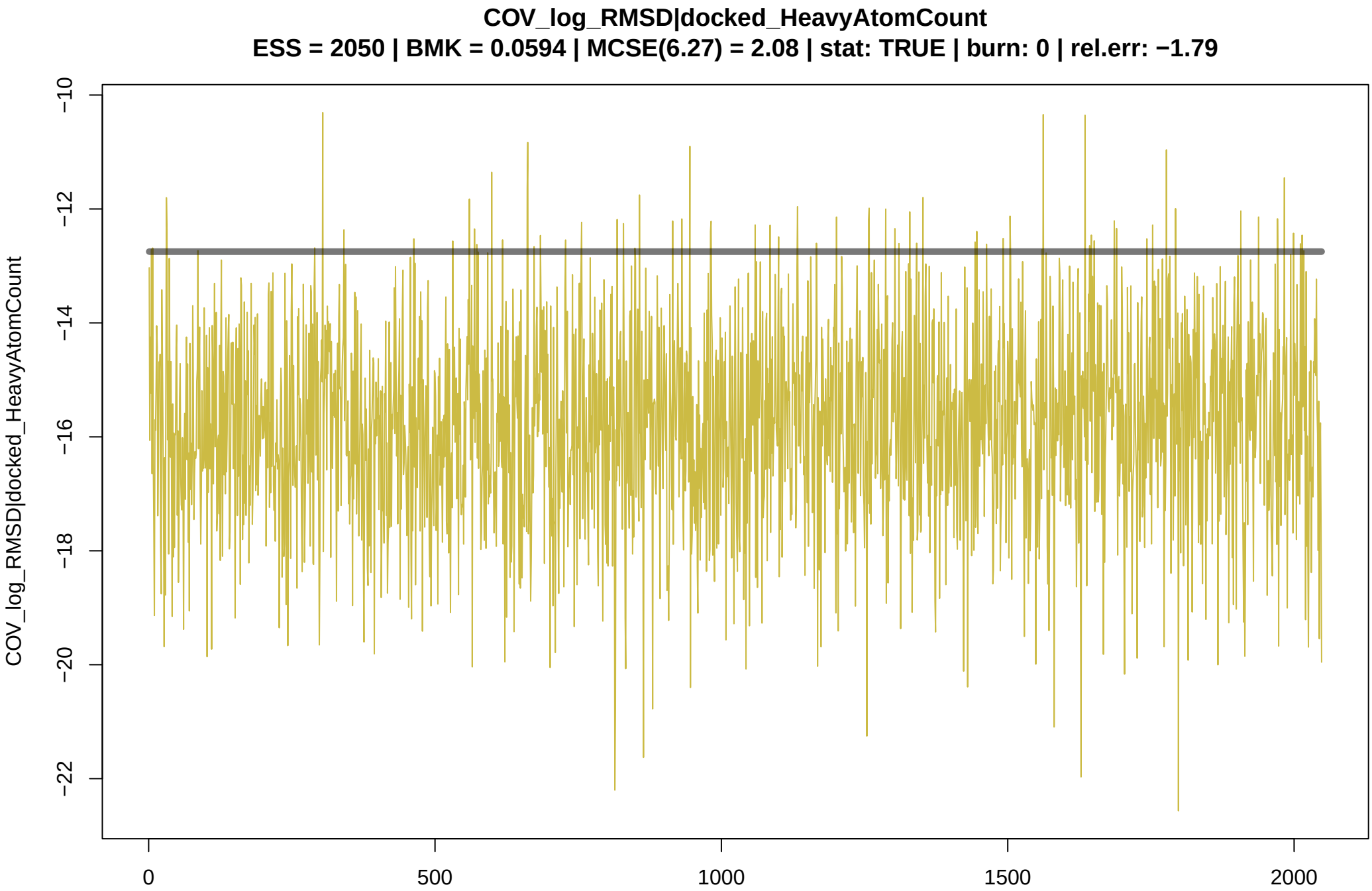

VAR_log_mcs_unbonded_polar_sasa
ESS = 1950 | BMK = 0.0445 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: 1.45
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
0
500
1000
1500
2000

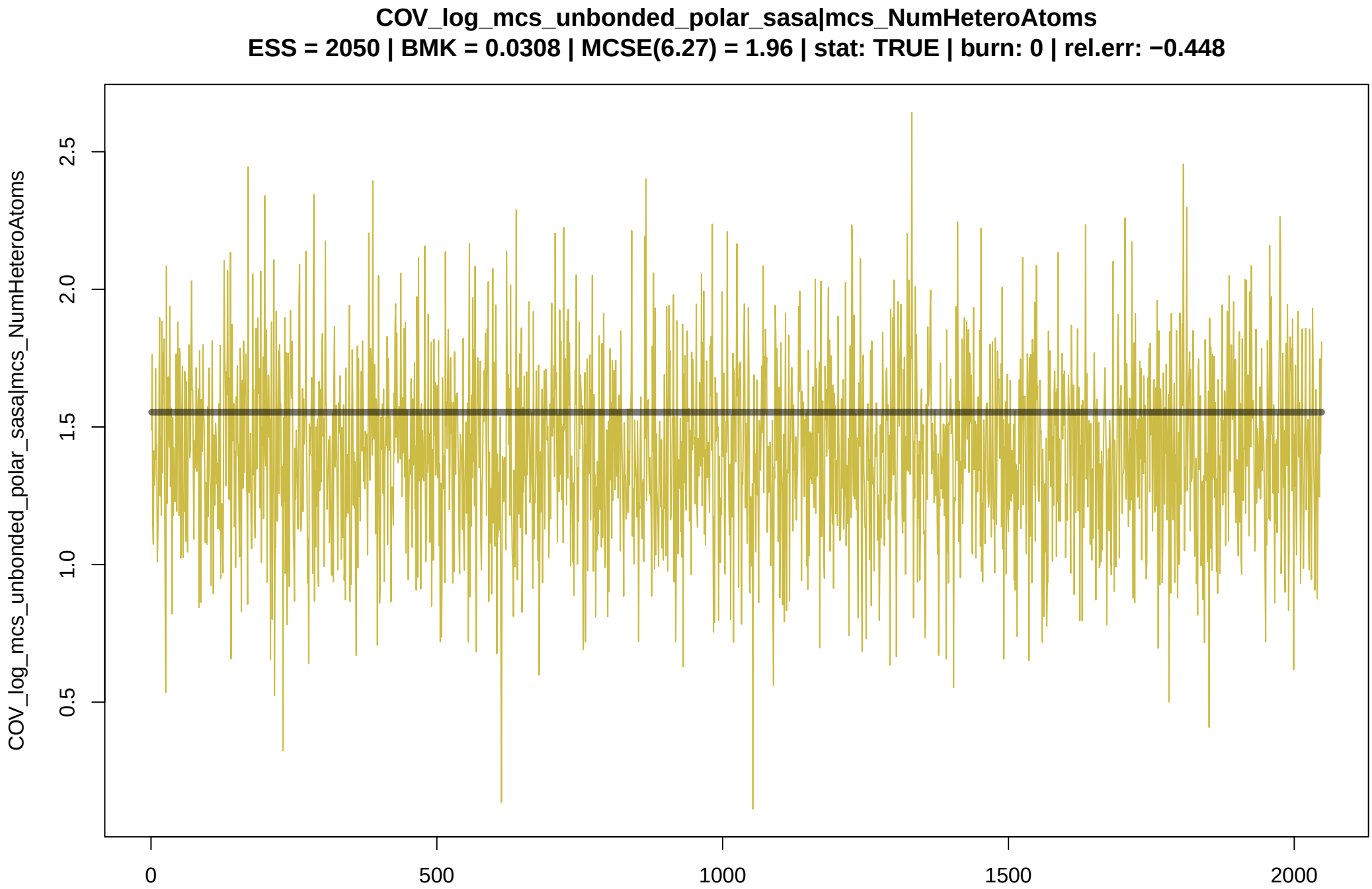

VAR_mcs_NumHeteroAtoms
ESS = 1270 | BMK = 0.0527 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | rel.err: 0.439
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

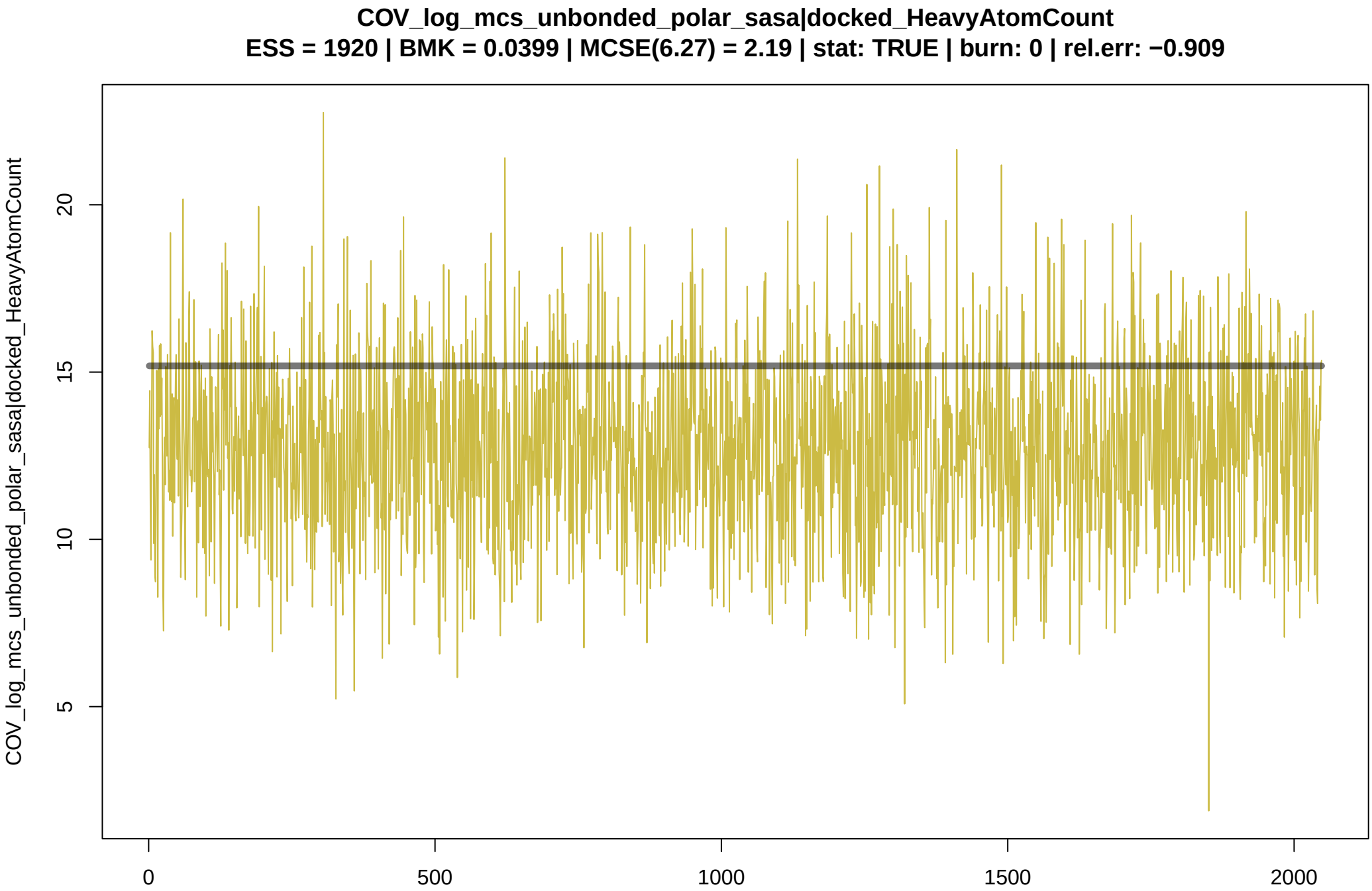

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0698 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: 0.0813
VAR_docked_HeavyAtomCount
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
0
500
1000
1500
2000

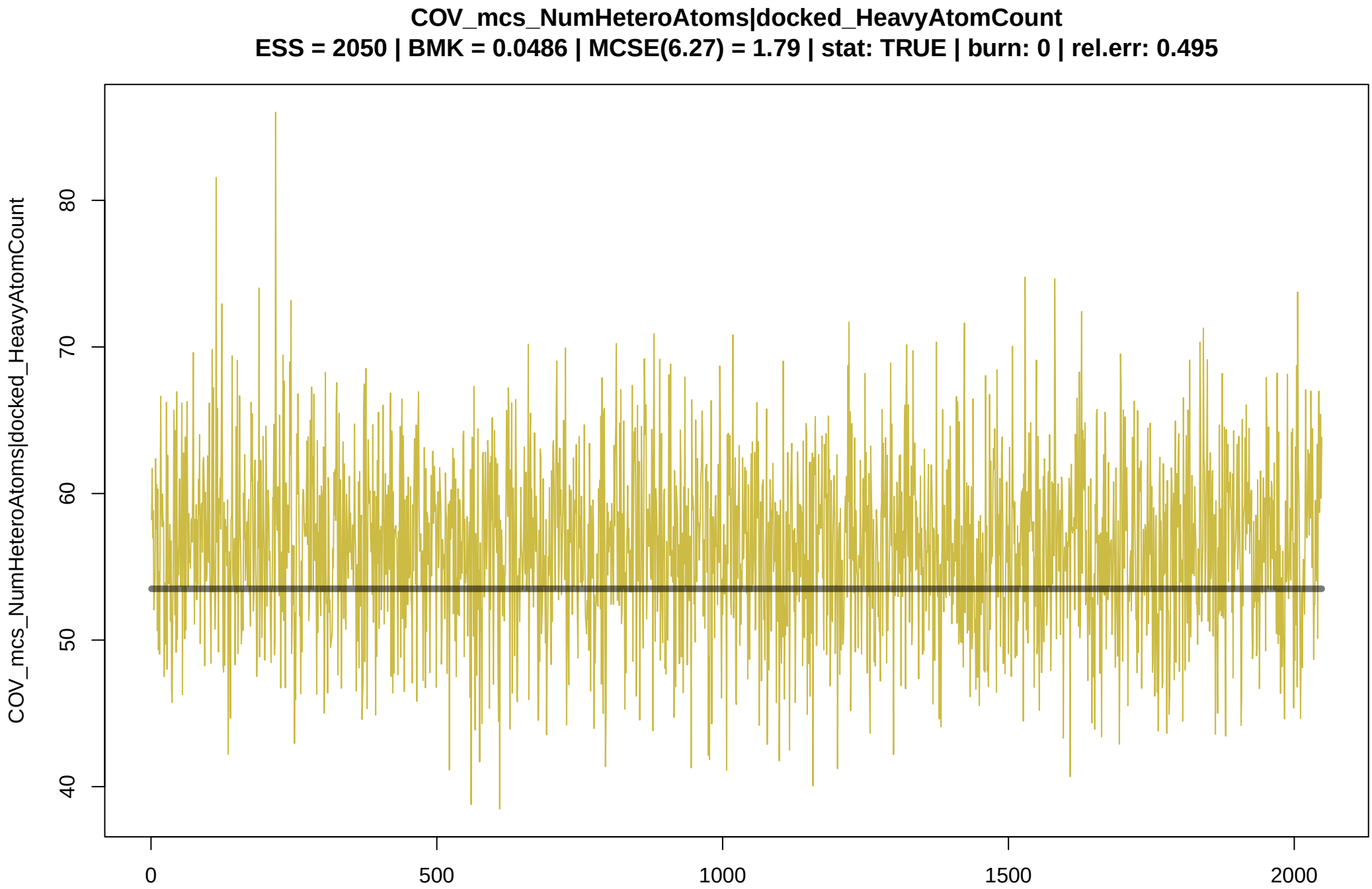

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1900 | BMK = 0.0551 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 0.447
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.2
−0.4
−0.6
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0508 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | rel.err: −1.68
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 = 0.0594 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: −1.79
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 = 0.0308 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0 | rel.err: −0.448
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 = 1920 | BMK = 0.0399 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: −0.909
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 = 0.0486 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.495
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000