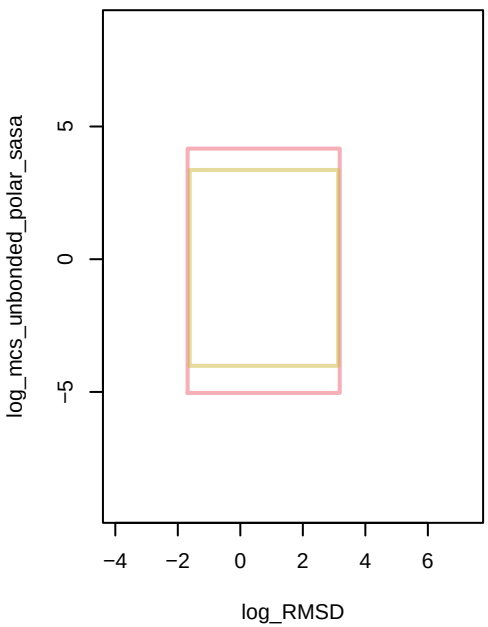
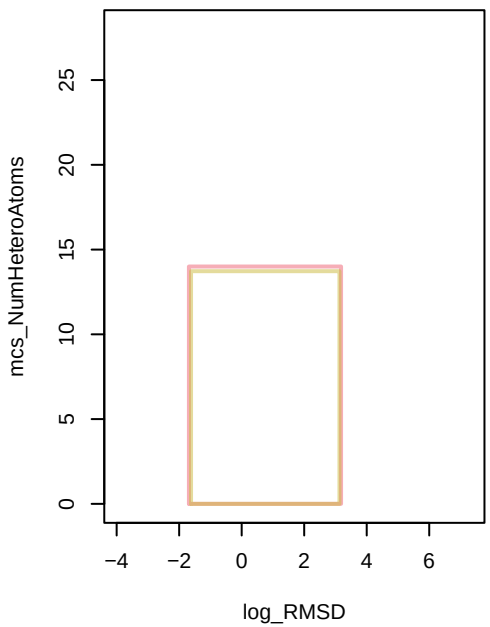
−− STATS maxD −−
min ESS = 100.720097315925
max BMK = 0.155462324488367
max MCSE = 7.71080045410512
all stationary: FALSE
burn: 612
max rel.err.: 1.94988483195452

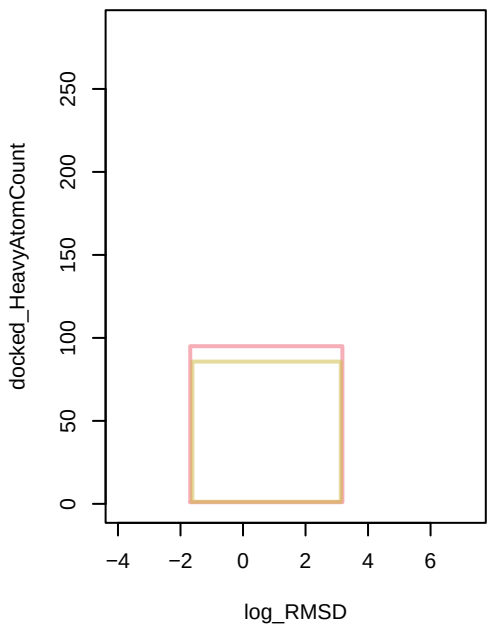
−− STATS 2D −−
min ESS = 1915.7391019545
max BMK = 0.044679414027757
max MCSE = 2.44493576857124
all stationary: TRUE
burn: 0
max rel.err.: 1.73576327512563

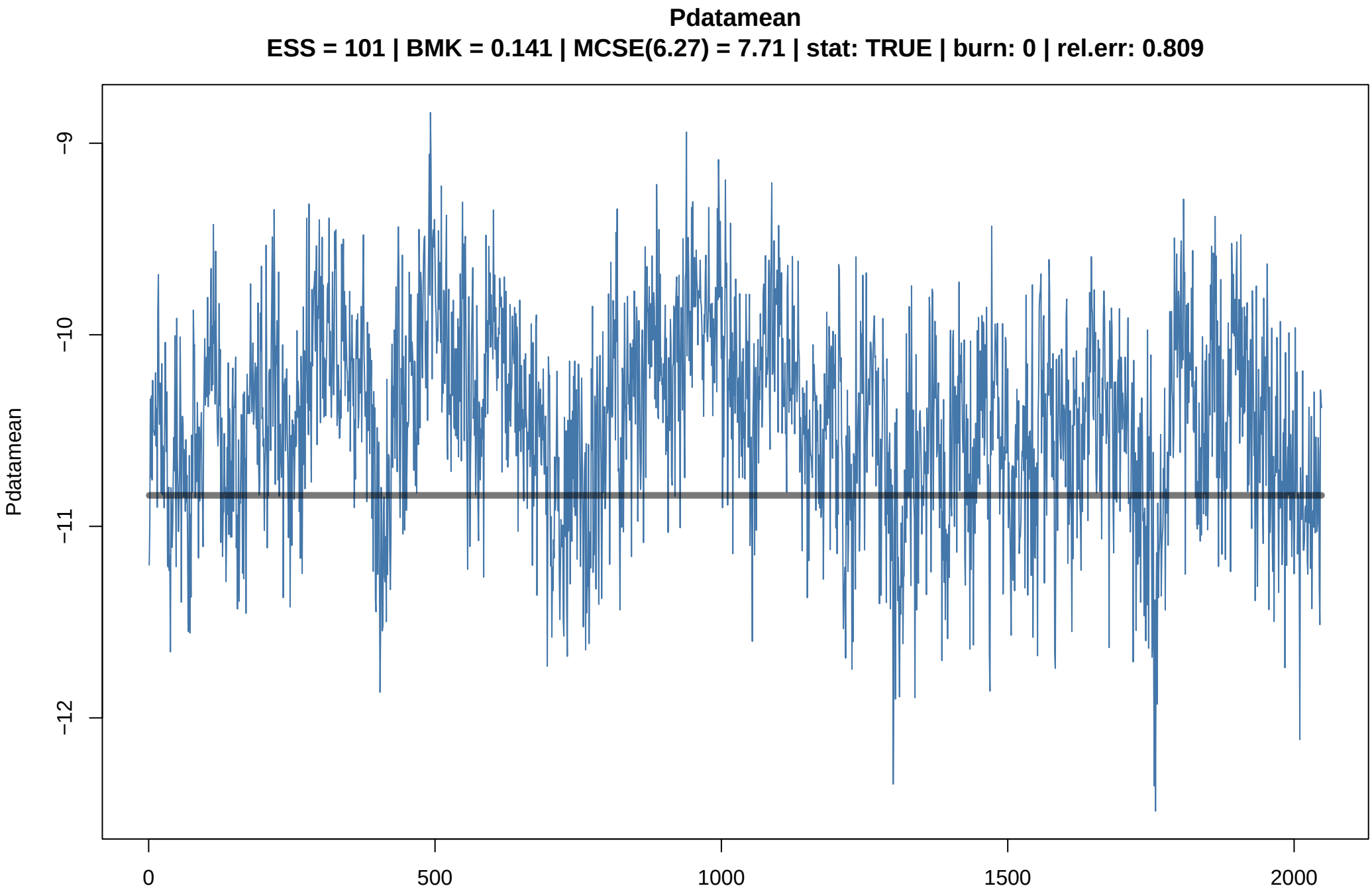
−− STATS 1D −−
min ESS = 1668.49591191927
max BMK = 0.054853897587829
max MCSE = 2.82351154982006
all stationary: TRUE
burn: 0
max rel.err.: 2.2324132569048

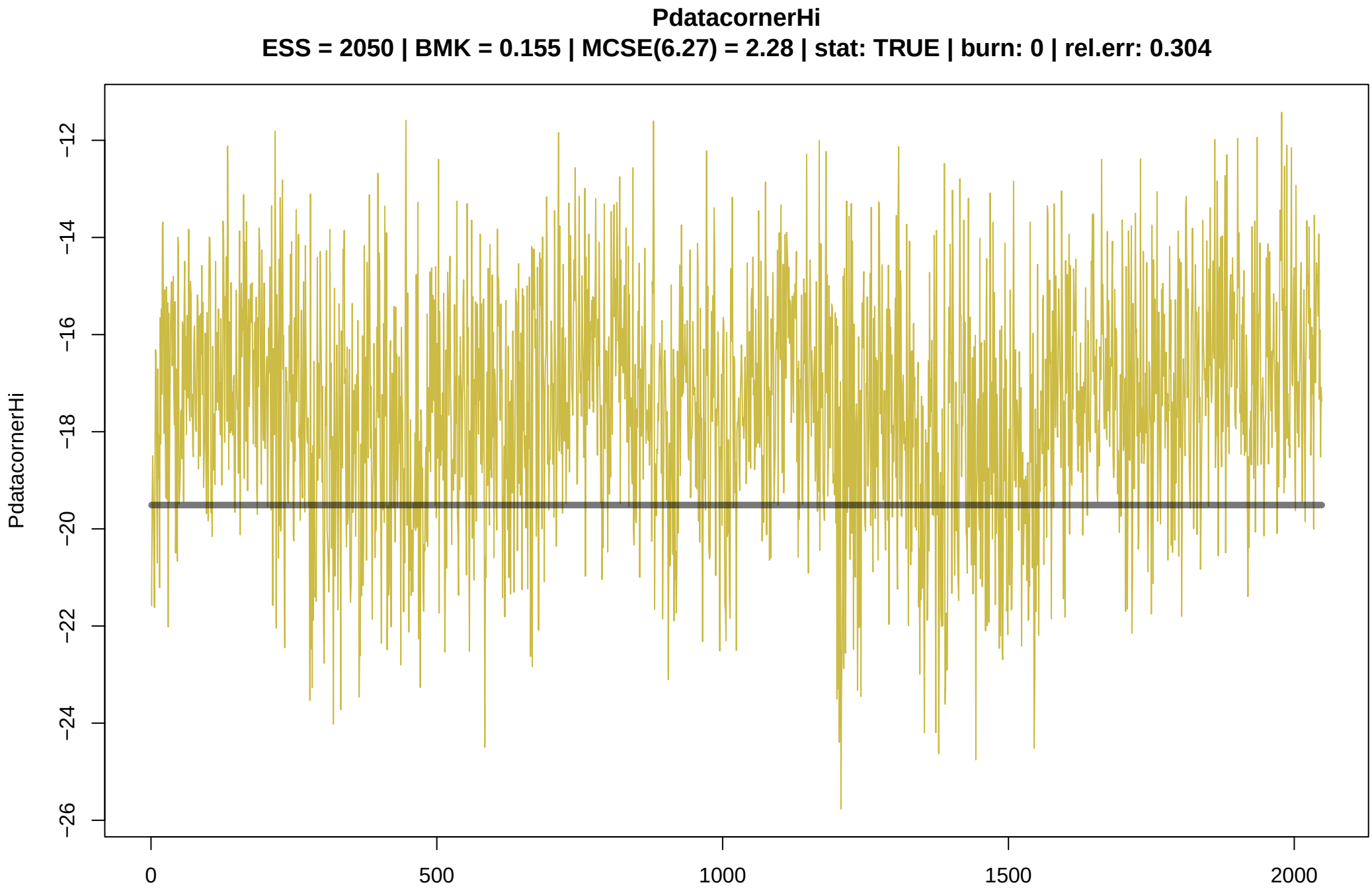
Occupied clusters: 8 of 16

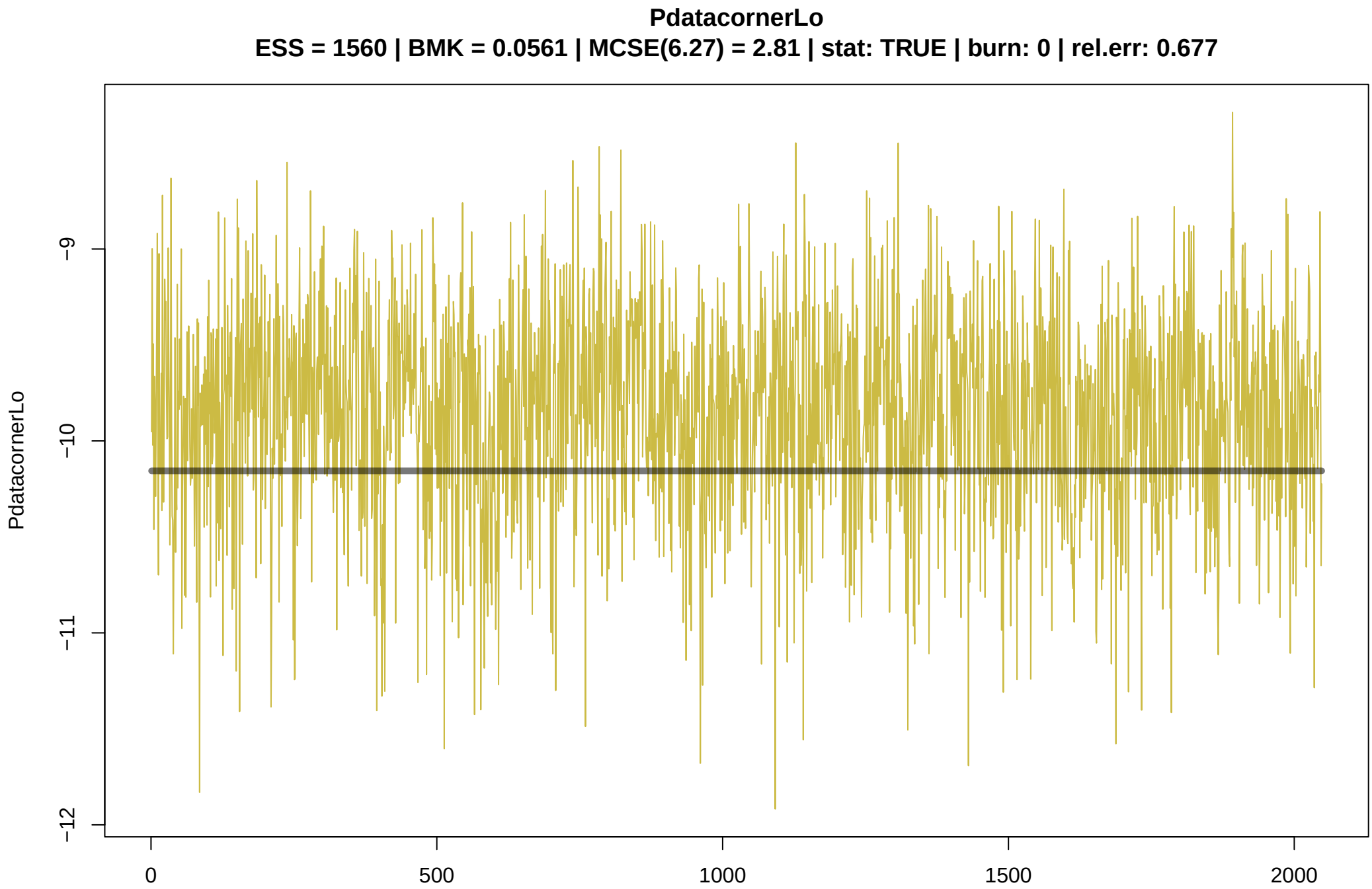

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

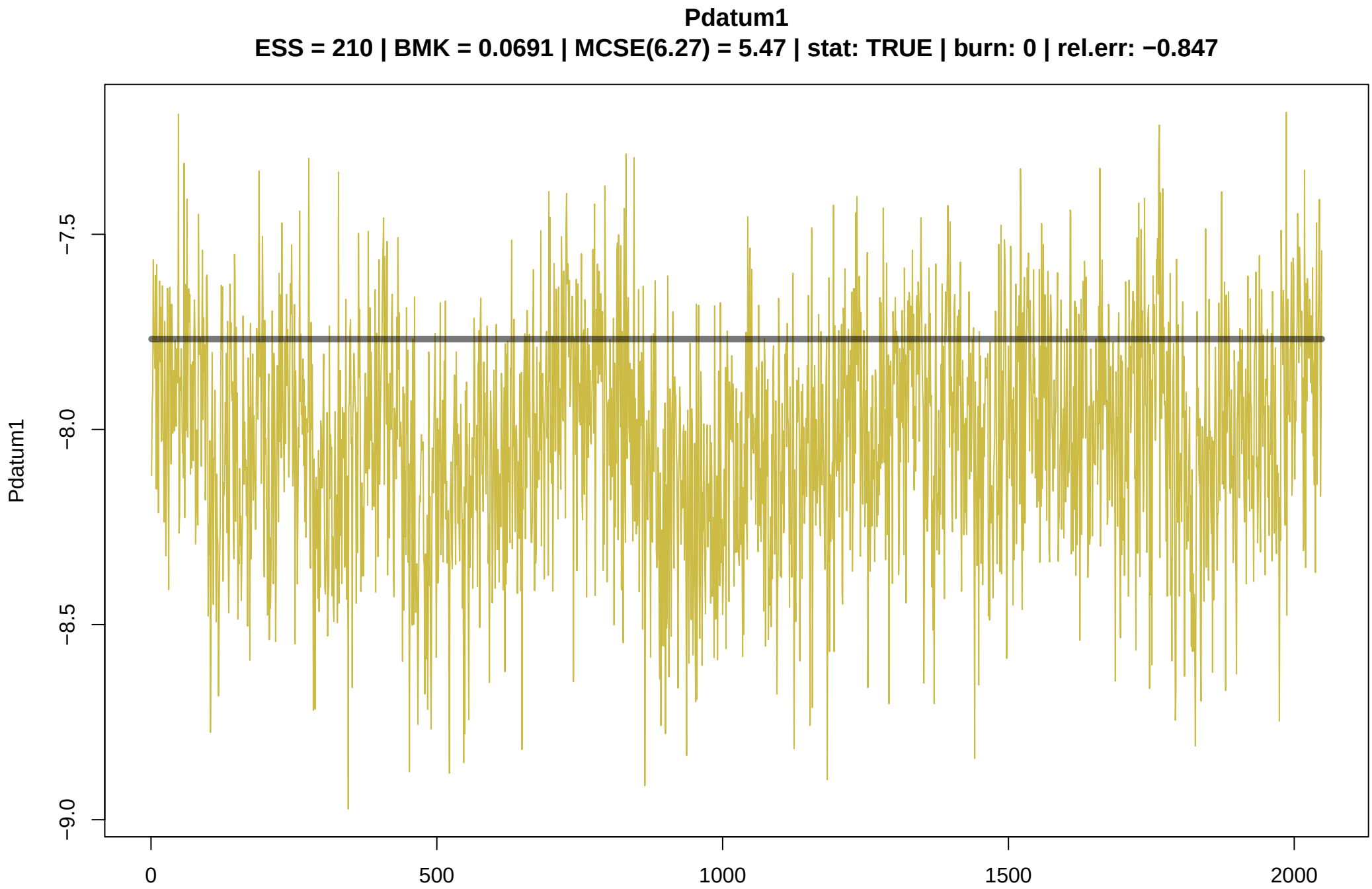

mcs_NumHeteroAtoms
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

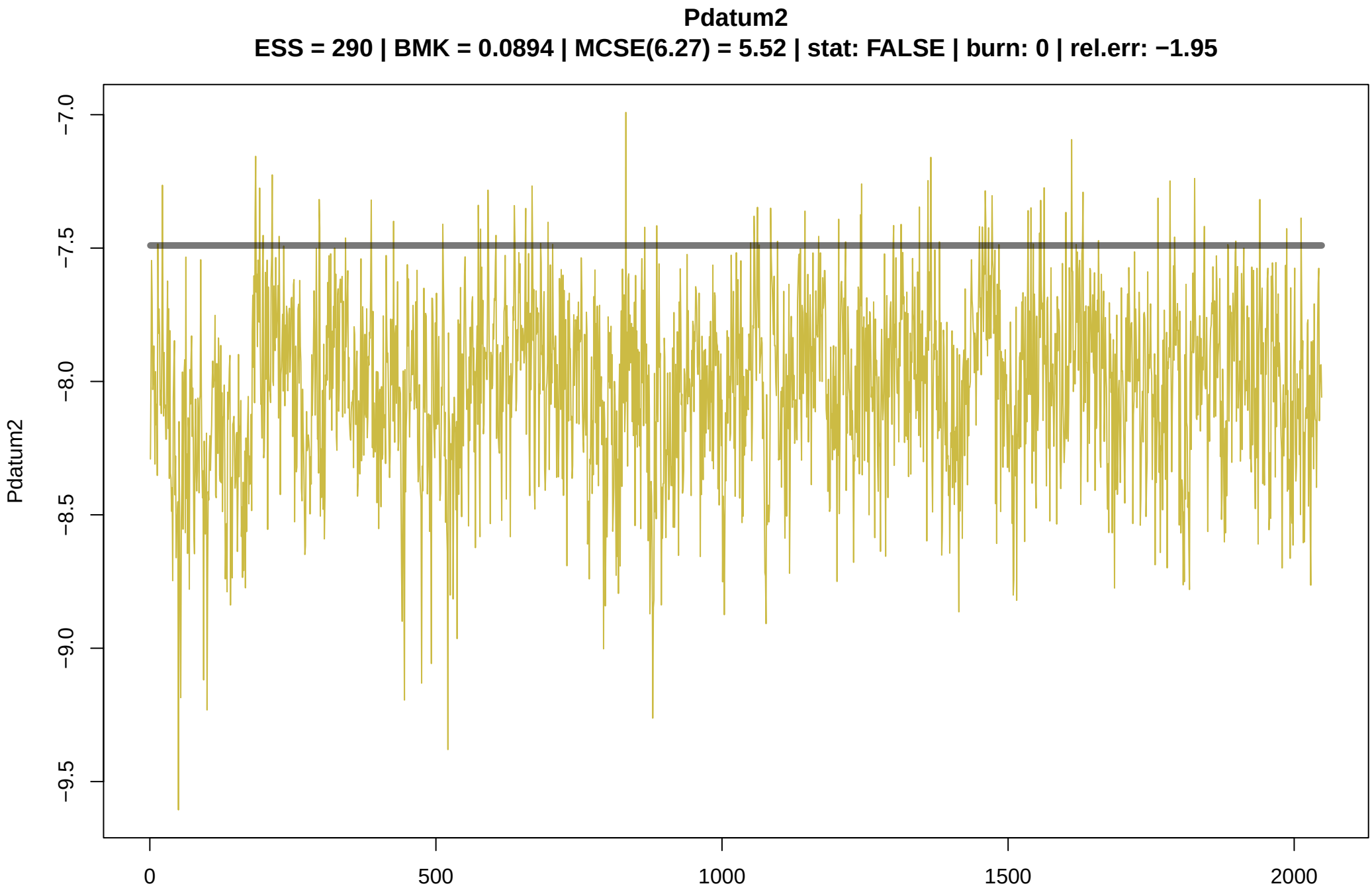

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

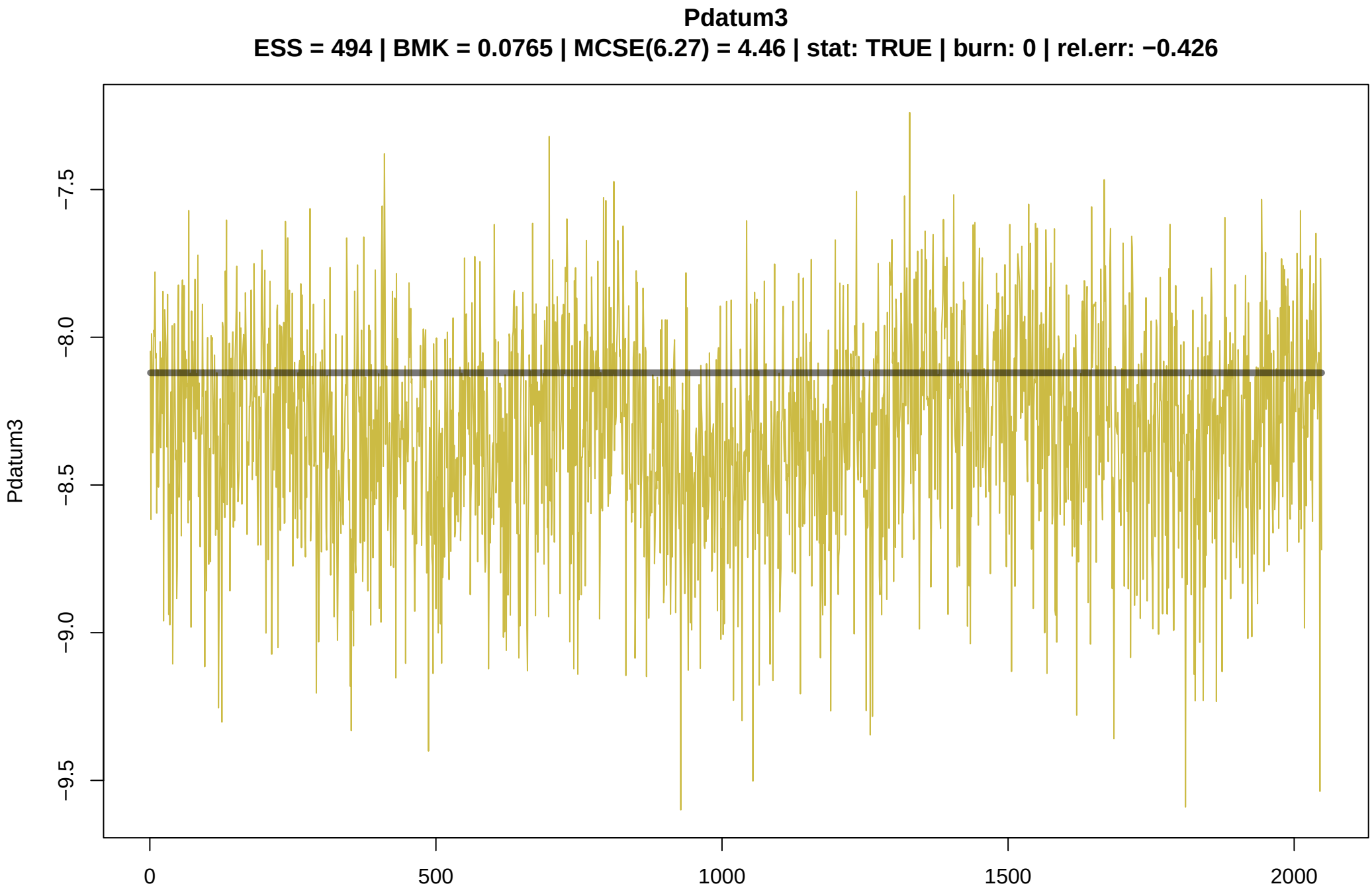

Pdatamean
ESS = 101 | BMK = 0.141 | MCSE(6.27) = 7.71 | stat: TRUE | burn: 0 | rel.err: 0.809
Pdatamean
−9
−10
−11
−12
0
500
1000
1500
2000

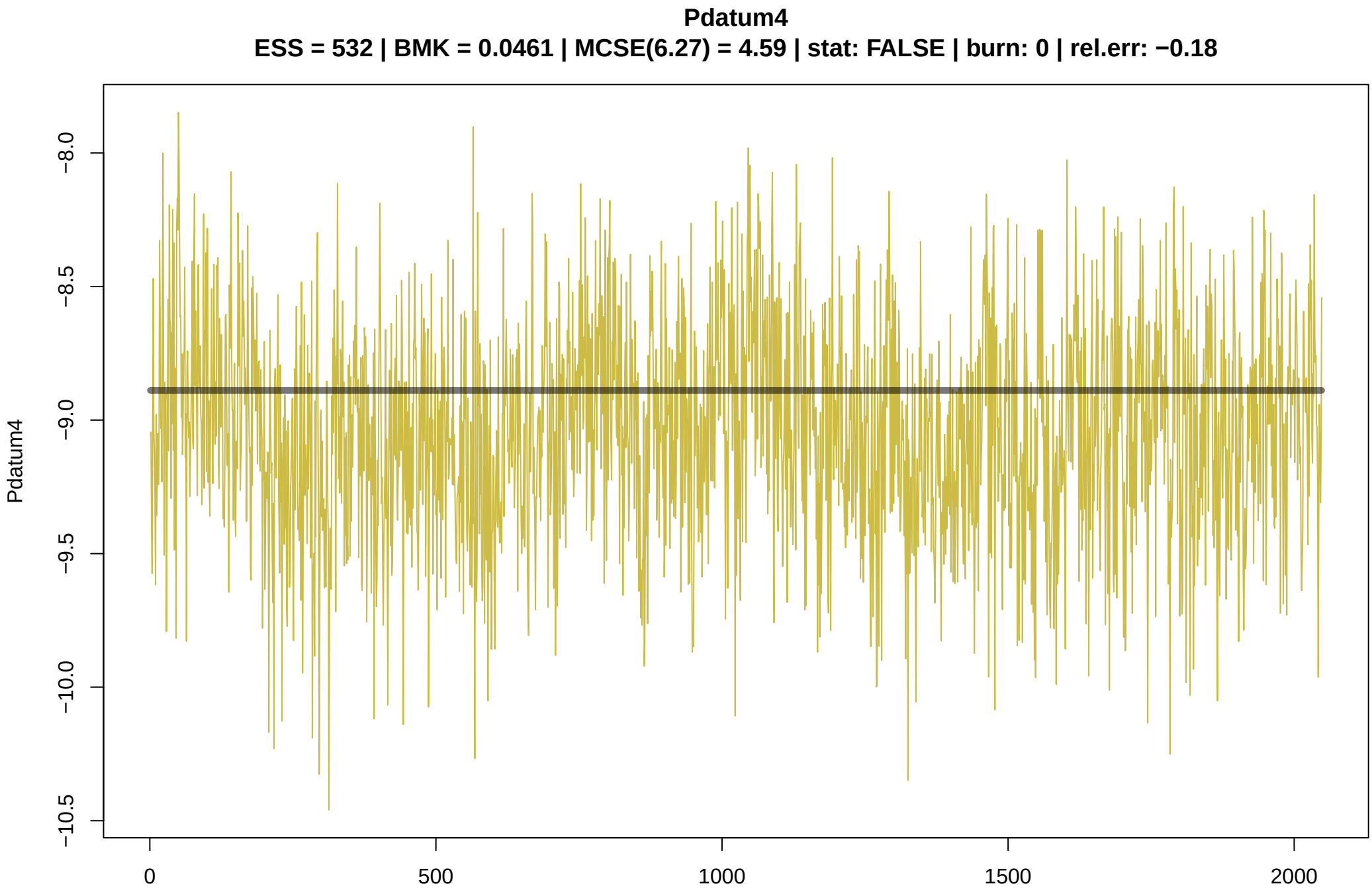

PdatacornerHi
ESS = 2050 | BMK = 0.155 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | rel.err: 0.304
PdatacornerHi
−12
−14
−16
−18
−20
−22
−24
−26
0
500
1000
1500
2000

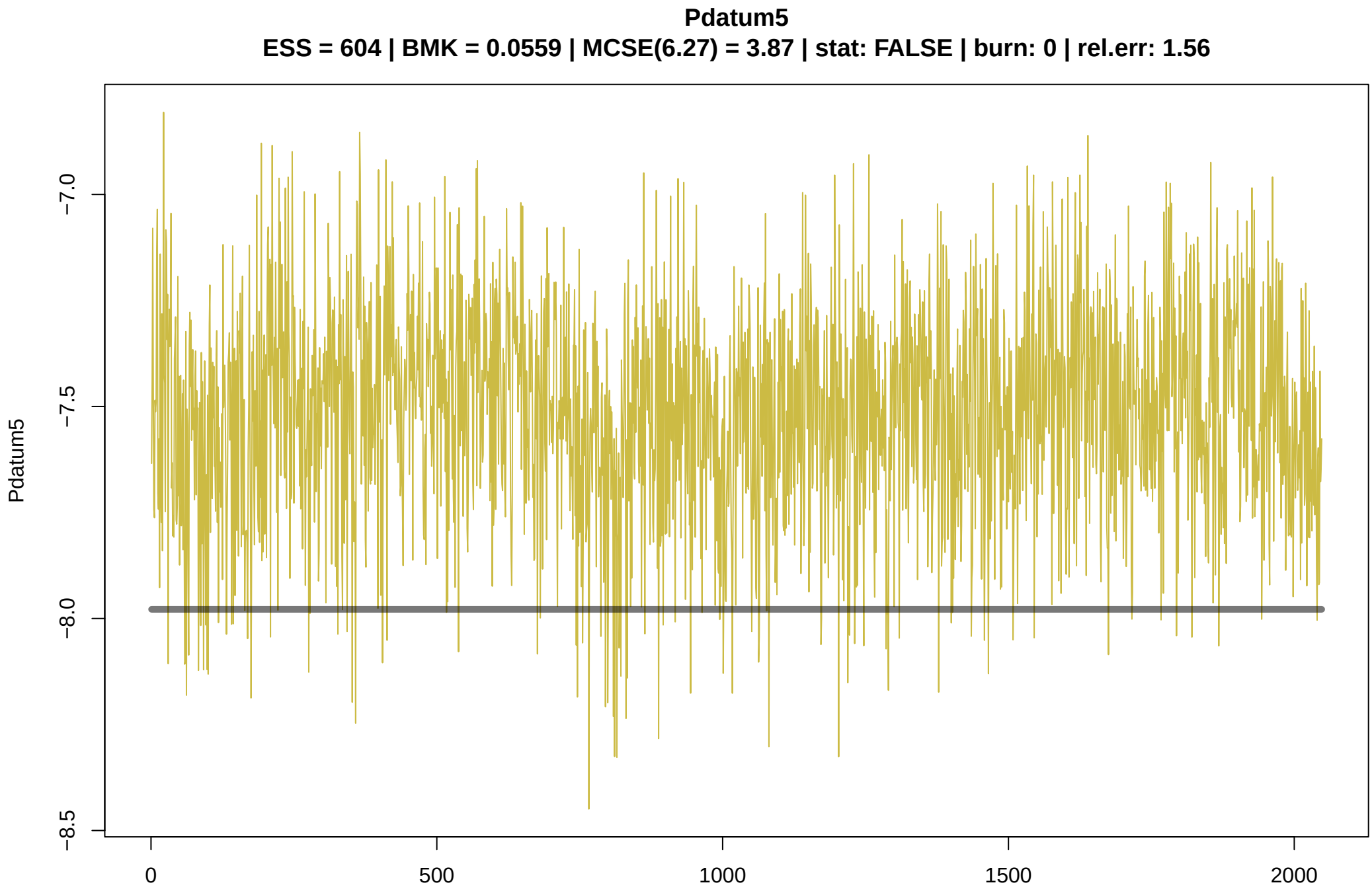

PdatacornerLo
ESS = 1560 | BMK = 0.0561 | MCSE(6.27) = 2.81 | stat: TRUE | burn: 0 | rel.err: 0.677
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

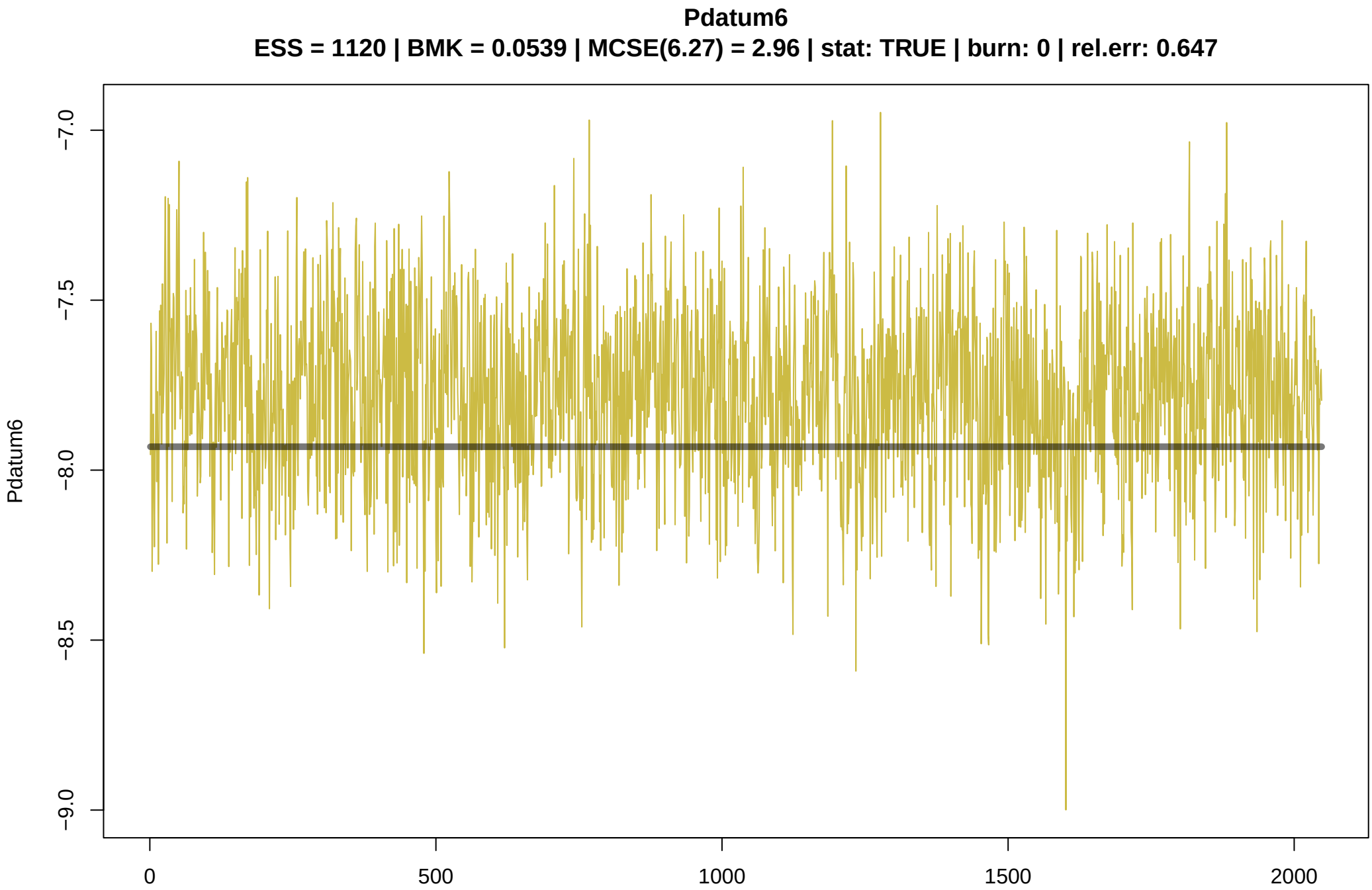

Pdatum1
ESS = 210 | BMK = 0.0691 | MCSE(6.27) = 5.47 | stat: TRUE | burn: 0 | rel.err: −0.847
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

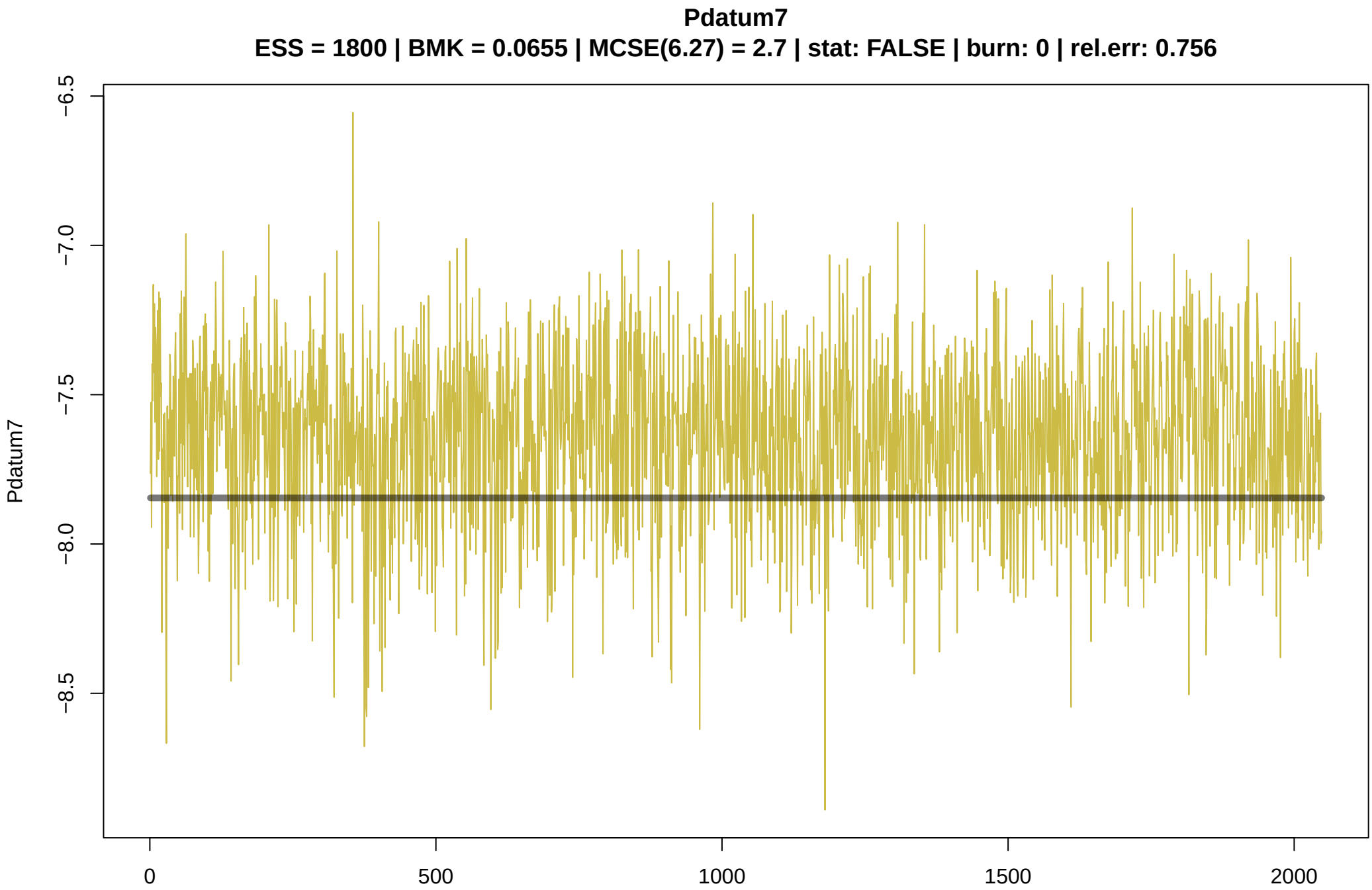

Pdatum2
ESS = 290 | BMK = 0.0894 | MCSE(6.27) = 5.52 | stat: FALSE | burn: 0 | rel.err: −1.95
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

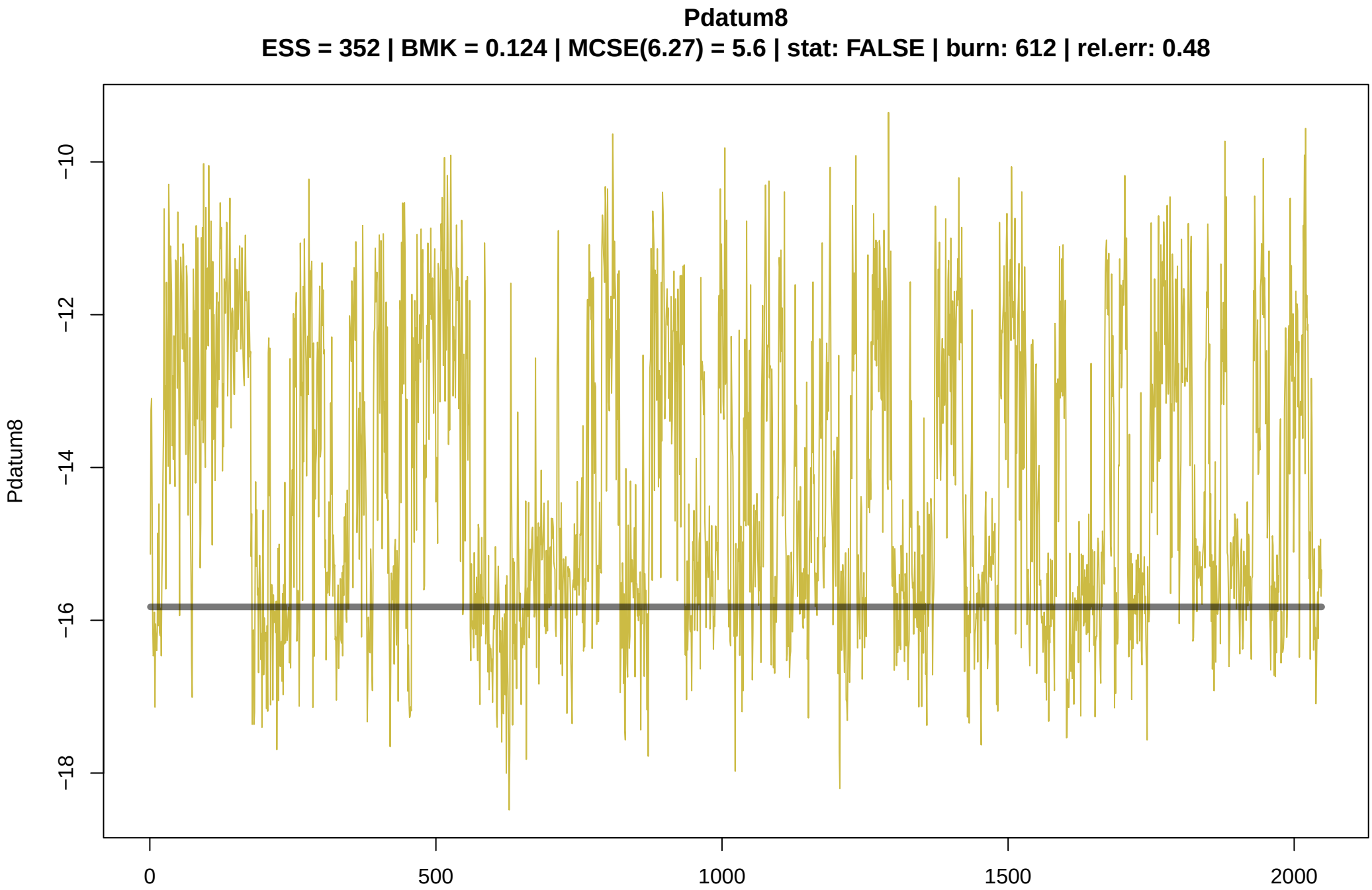

Pdatum3
ESS = 494 | BMK = 0.0765 | MCSE(6.27) = 4.46 | stat: TRUE | burn: 0 | rel.err: −0.426
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

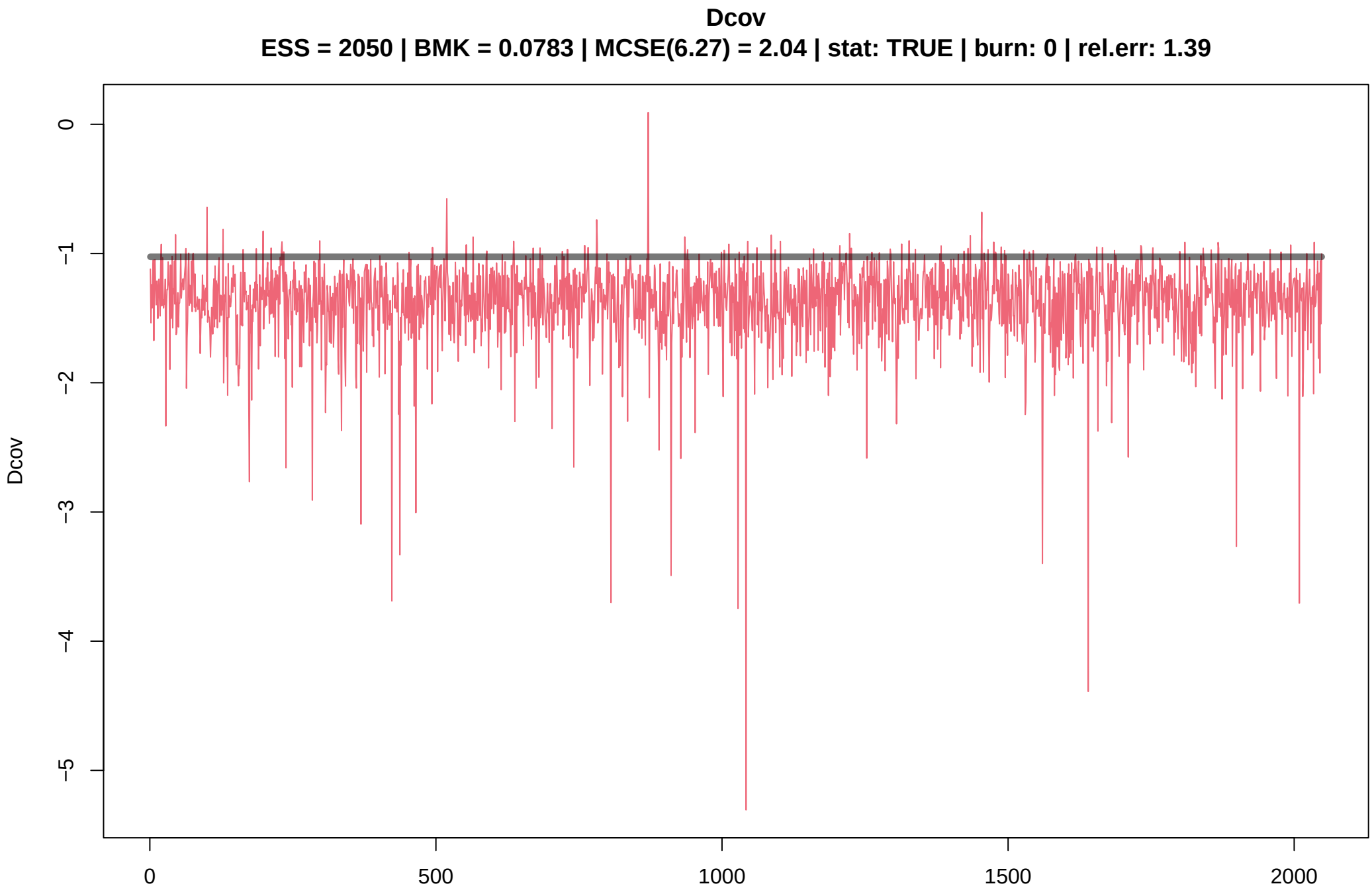

Pdatum4
ESS = 532 | BMK = 0.0461 | MCSE(6.27) = 4.59 | stat: FALSE | burn: 0 | rel.err: −0.18
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

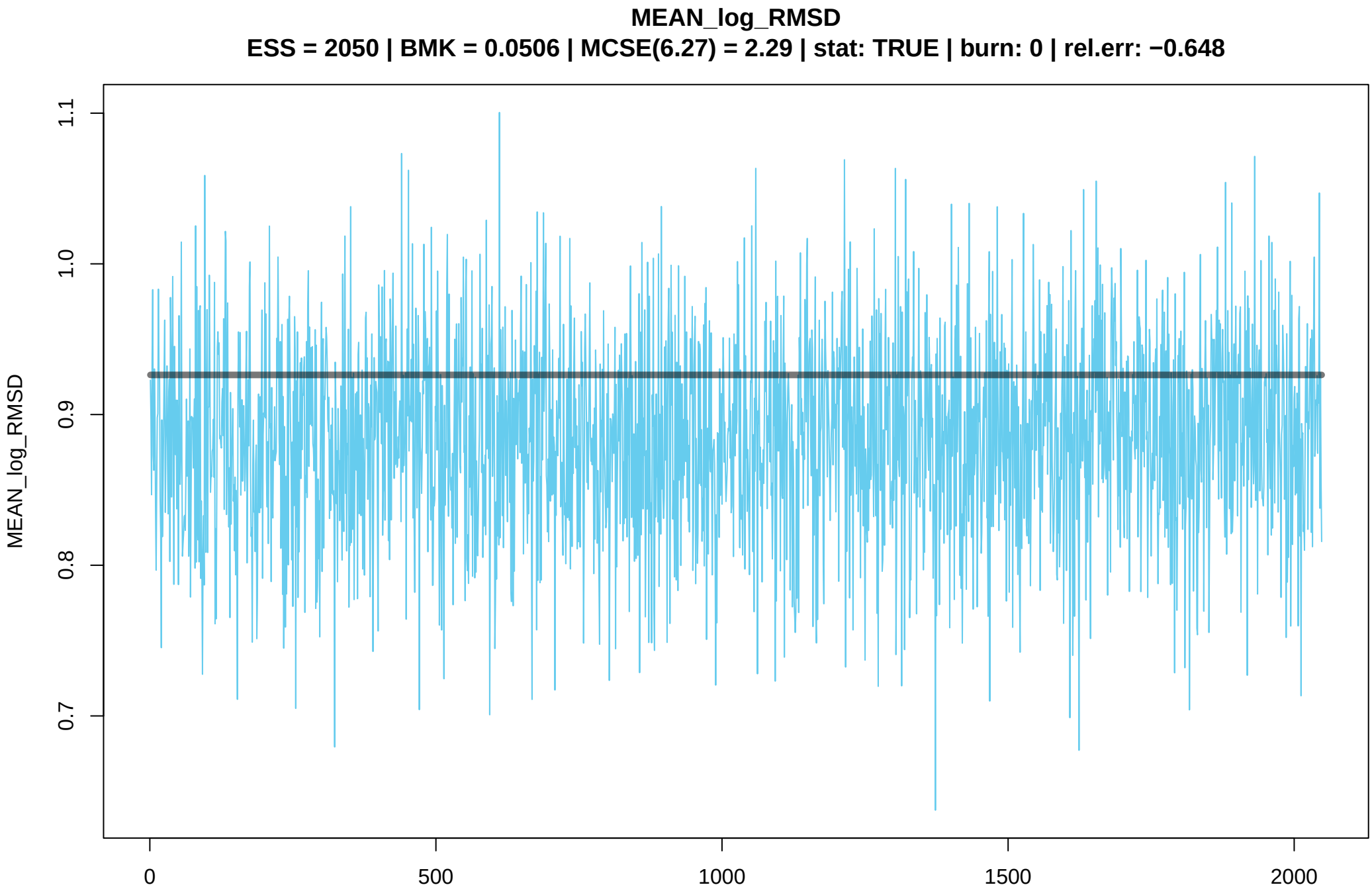

Pdatum5
ESS = 604 | BMK = 0.0559 | MCSE(6.27) = 3.87 | stat: FALSE | burn: 0 | rel.err: 1.56
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

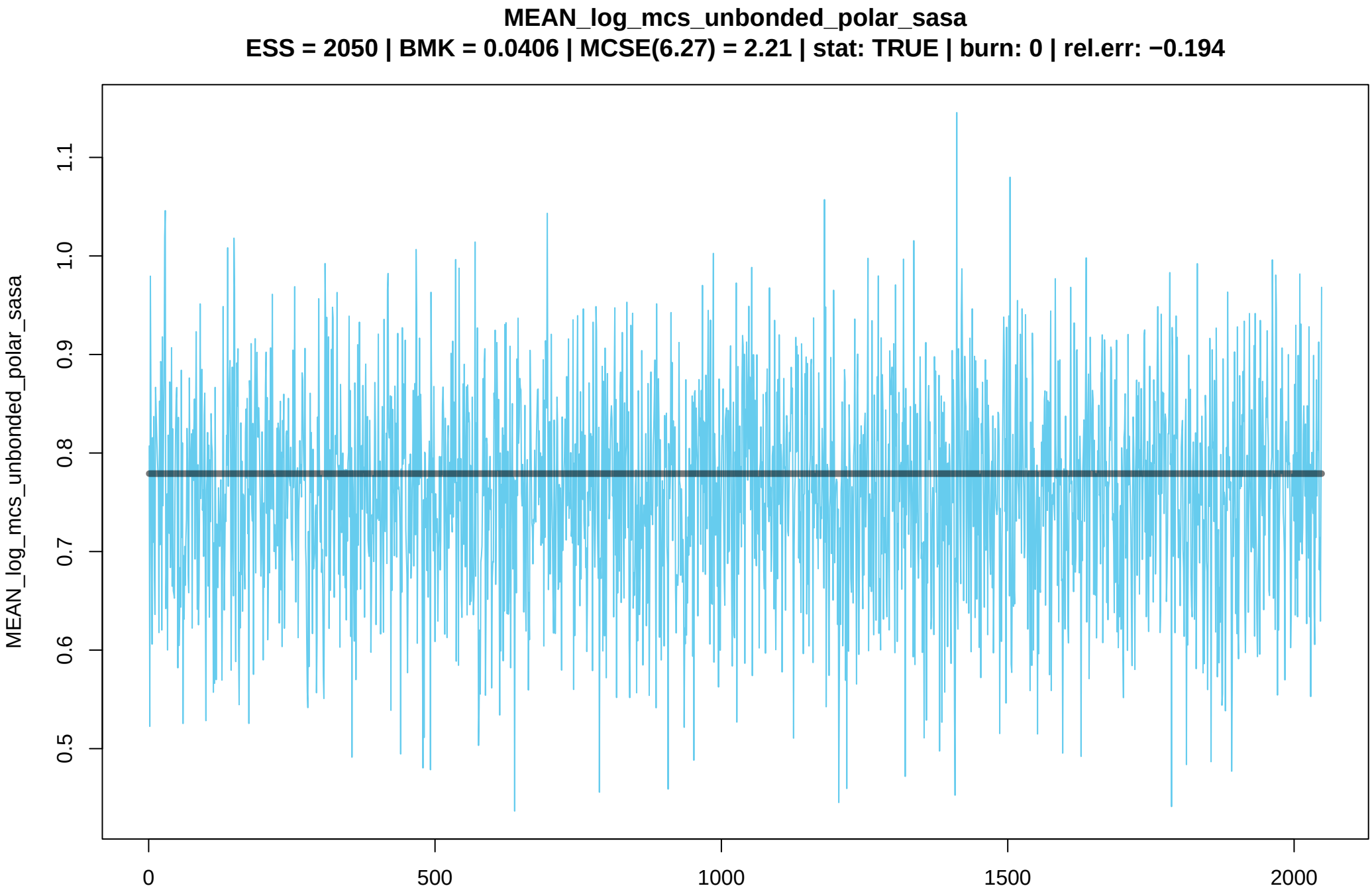

Pdatum6
ESS = 1120 | BMK = 0.0539 | MCSE(6.27) = 2.96 | stat: TRUE | burn: 0 | rel.err: 0.647
Pdatum6
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

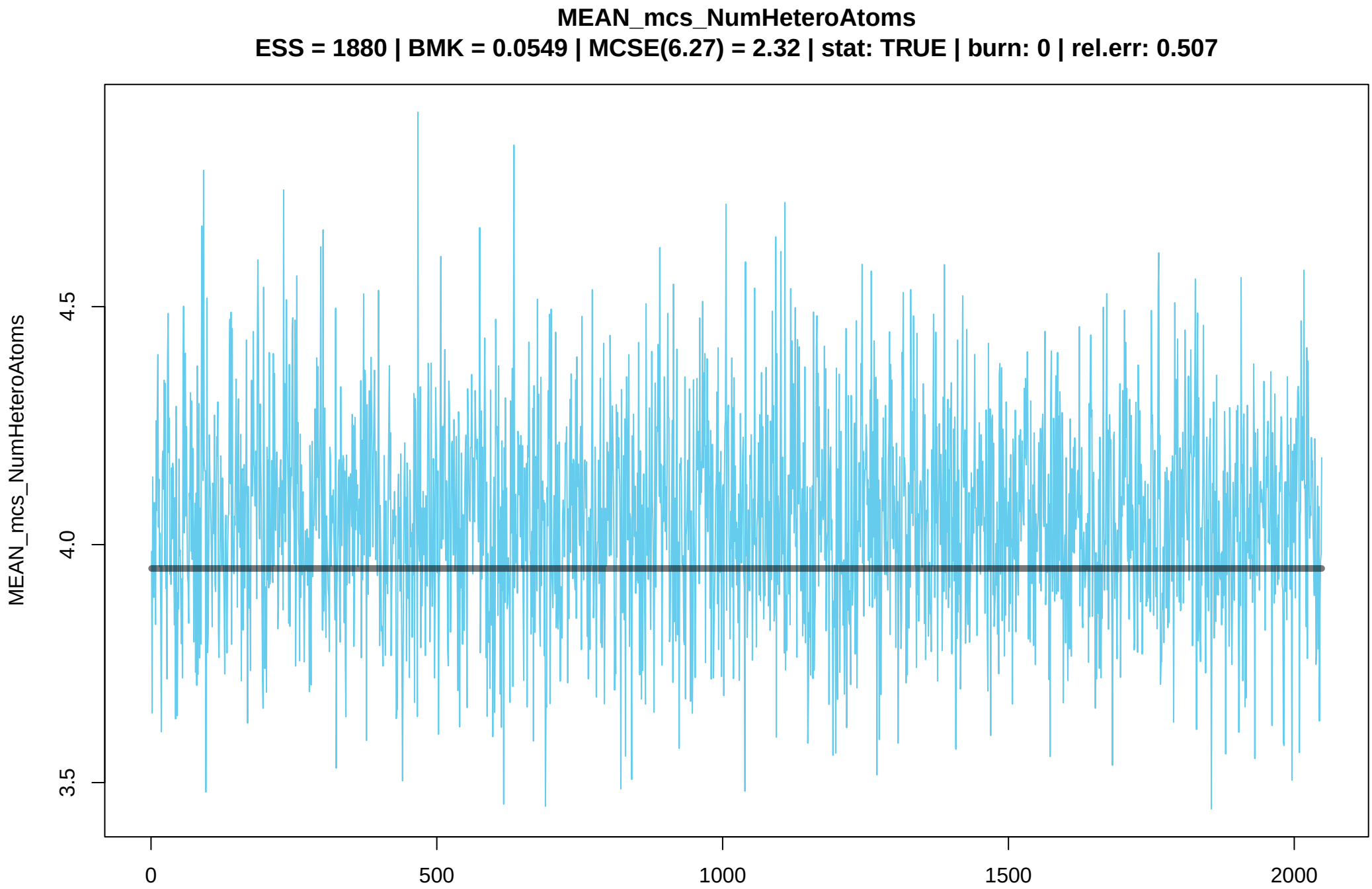

Pdatum7
ESS = 1800 | BMK = 0.0655 | MCSE(6.27) = 2.7 | stat: FALSE | burn: 0 | rel.err: 0.756
Pdatum7
−6.5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

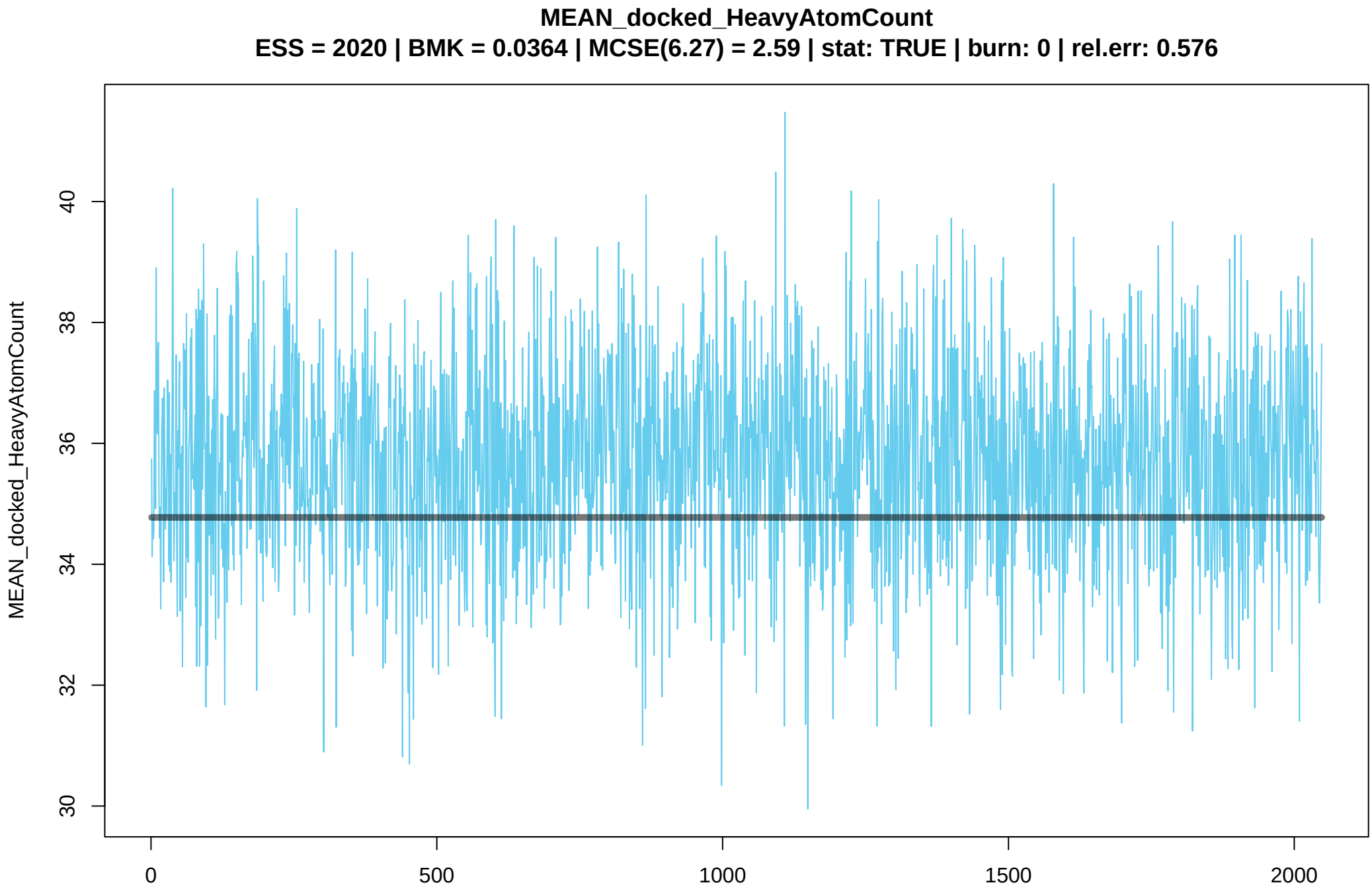

Pdatum8
ESS = 352 | BMK = 0.124 | MCSE(6.27) = 5.6 | stat: FALSE | burn: 612 | rel.err: 0.48
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

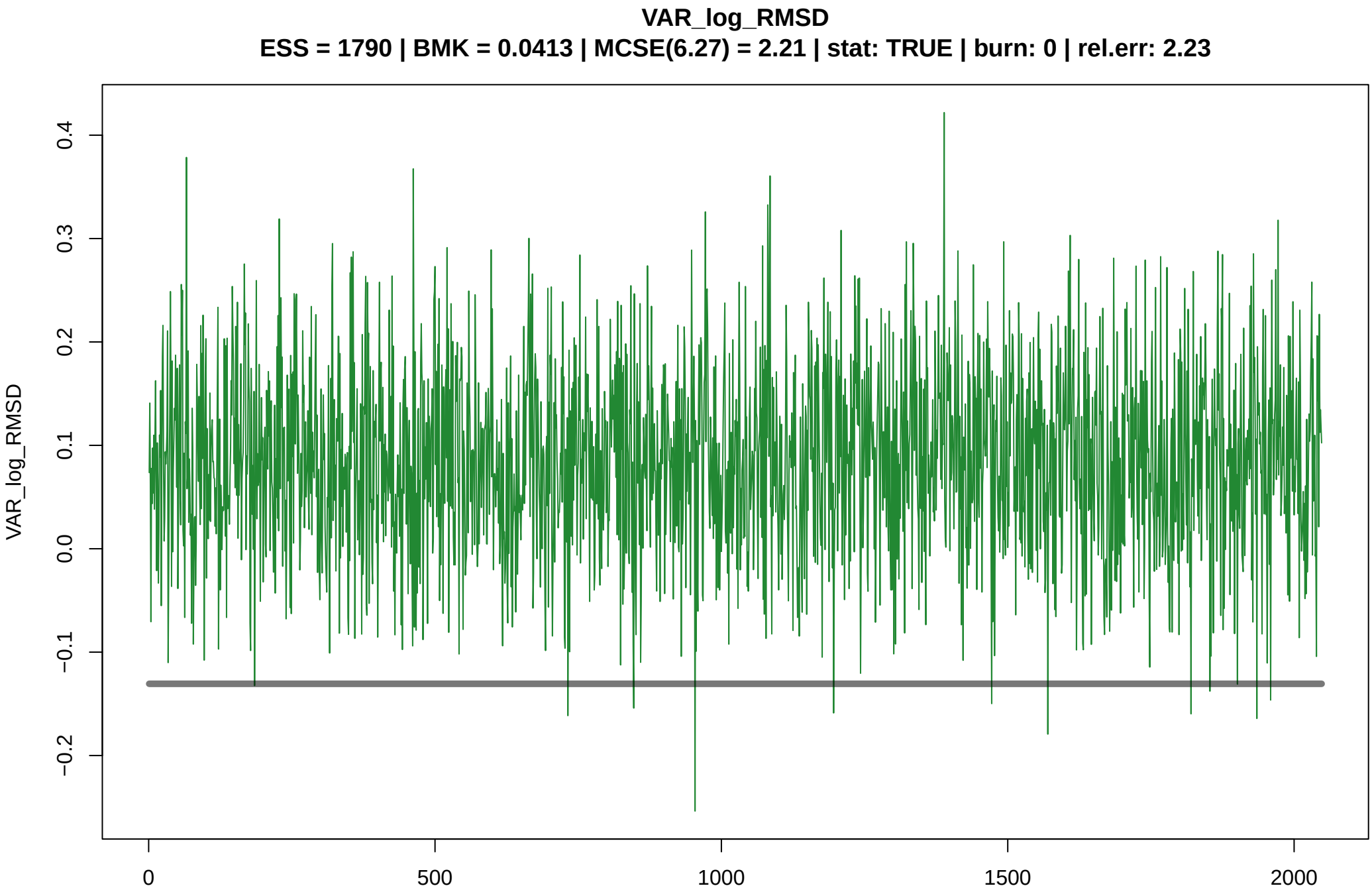

Dcov
ESS = 2050 | BMK = 0.0783 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: 1.39
Dcov
0
−1
−2
−3
−4
−5
0
500
1000
1500
2000

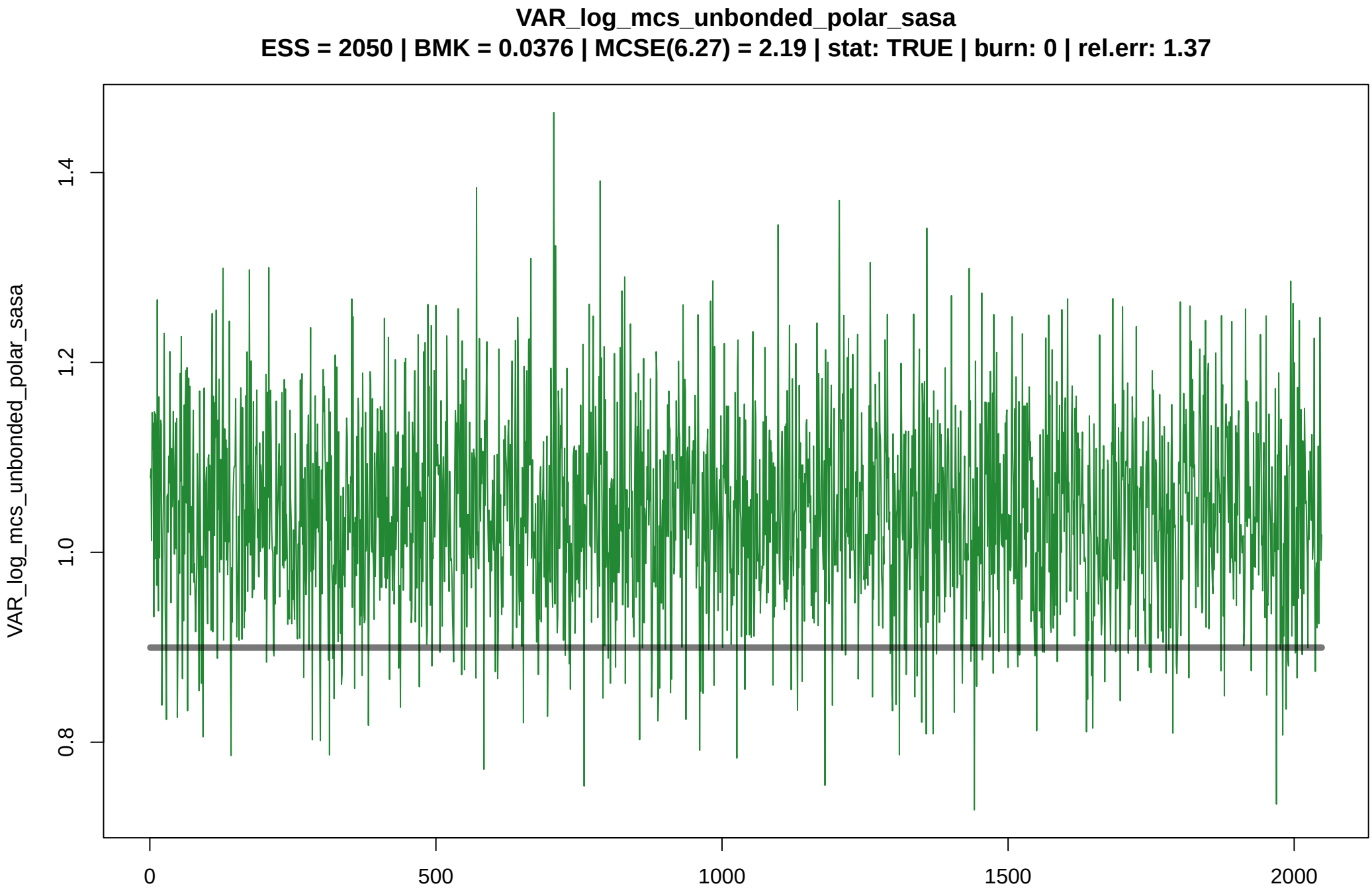

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0506 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: −0.648
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

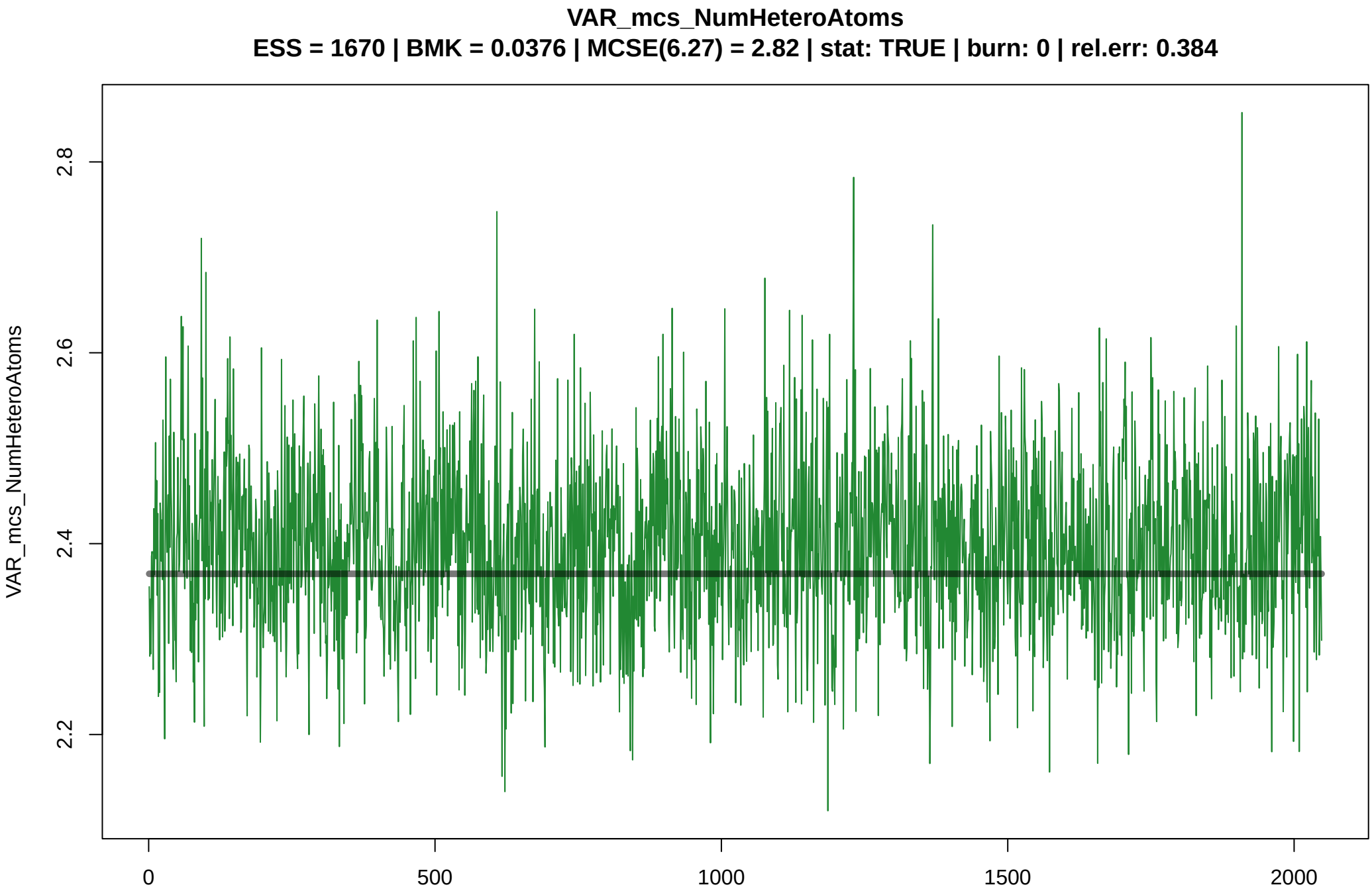

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0406 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: −0.194
MEAN_log_mcs_unbonded_polar_sasa
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

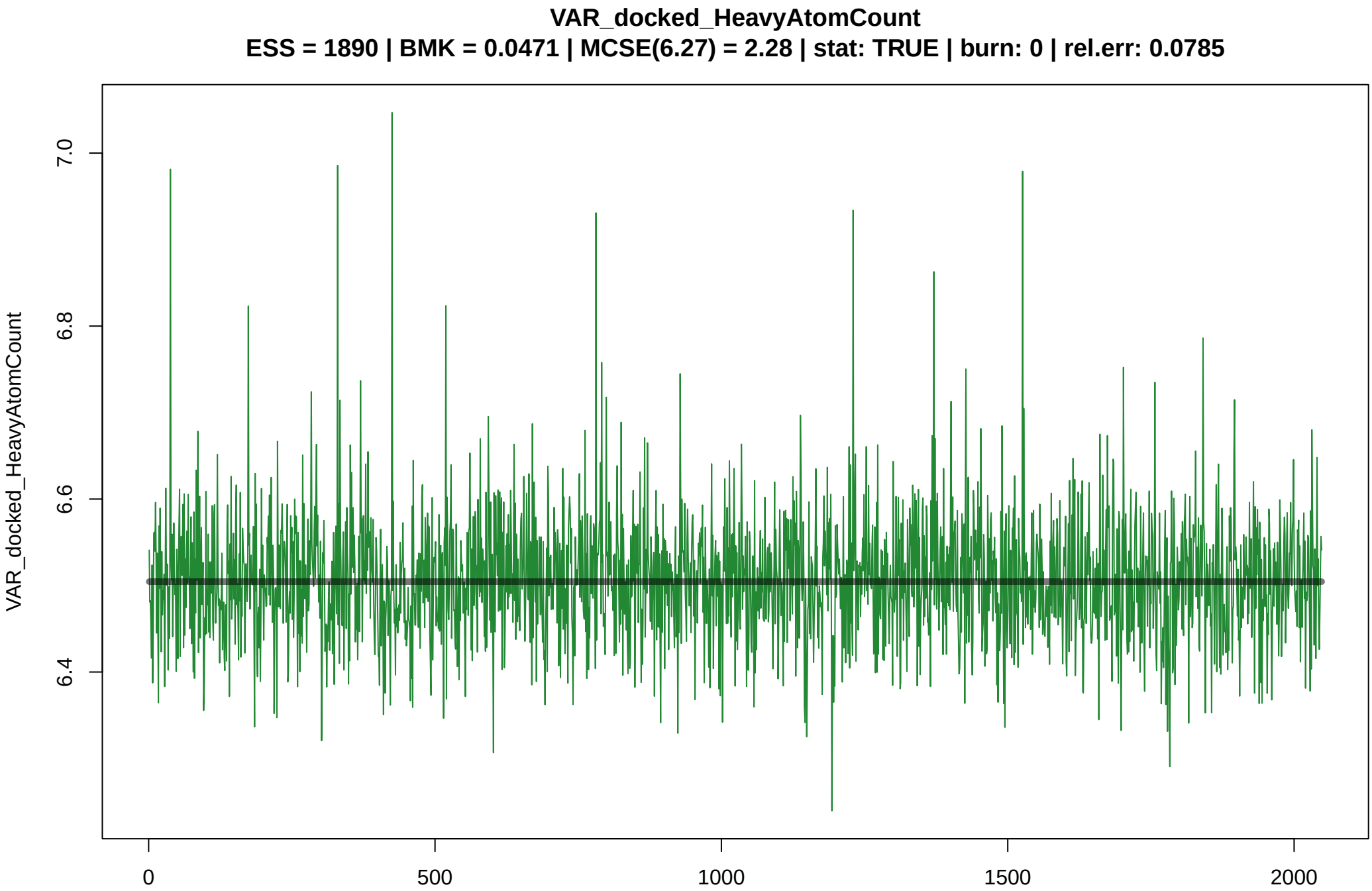

MEAN_mcs_NumHeteroAtoms
ESS = 1880 | BMK = 0.0549 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: 0.507
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
500
1000
1500
2000

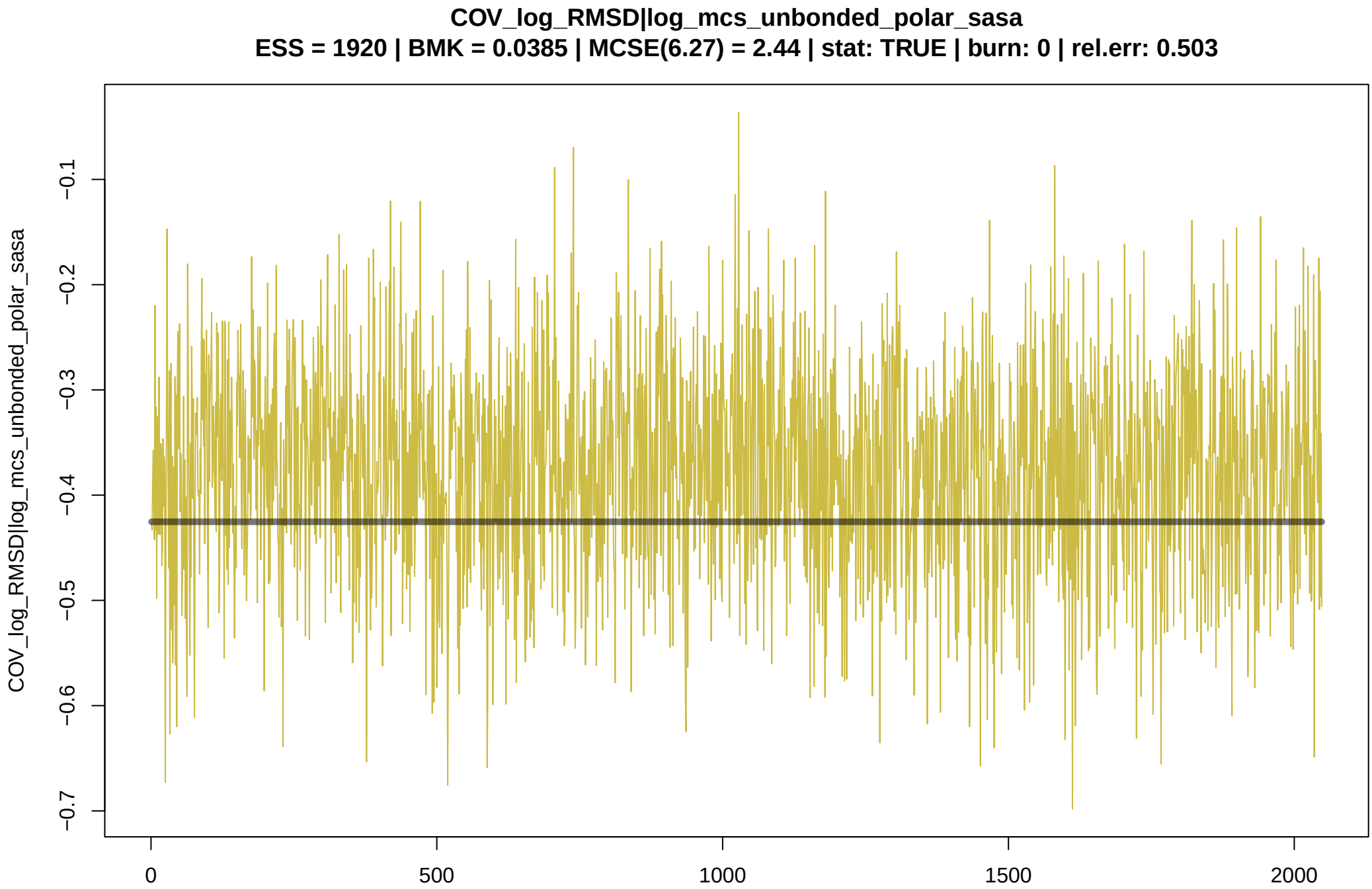

MEAN_docked_HeavyAtomCount
ESS = 2020 | BMK = 0.0364 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 0.576
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

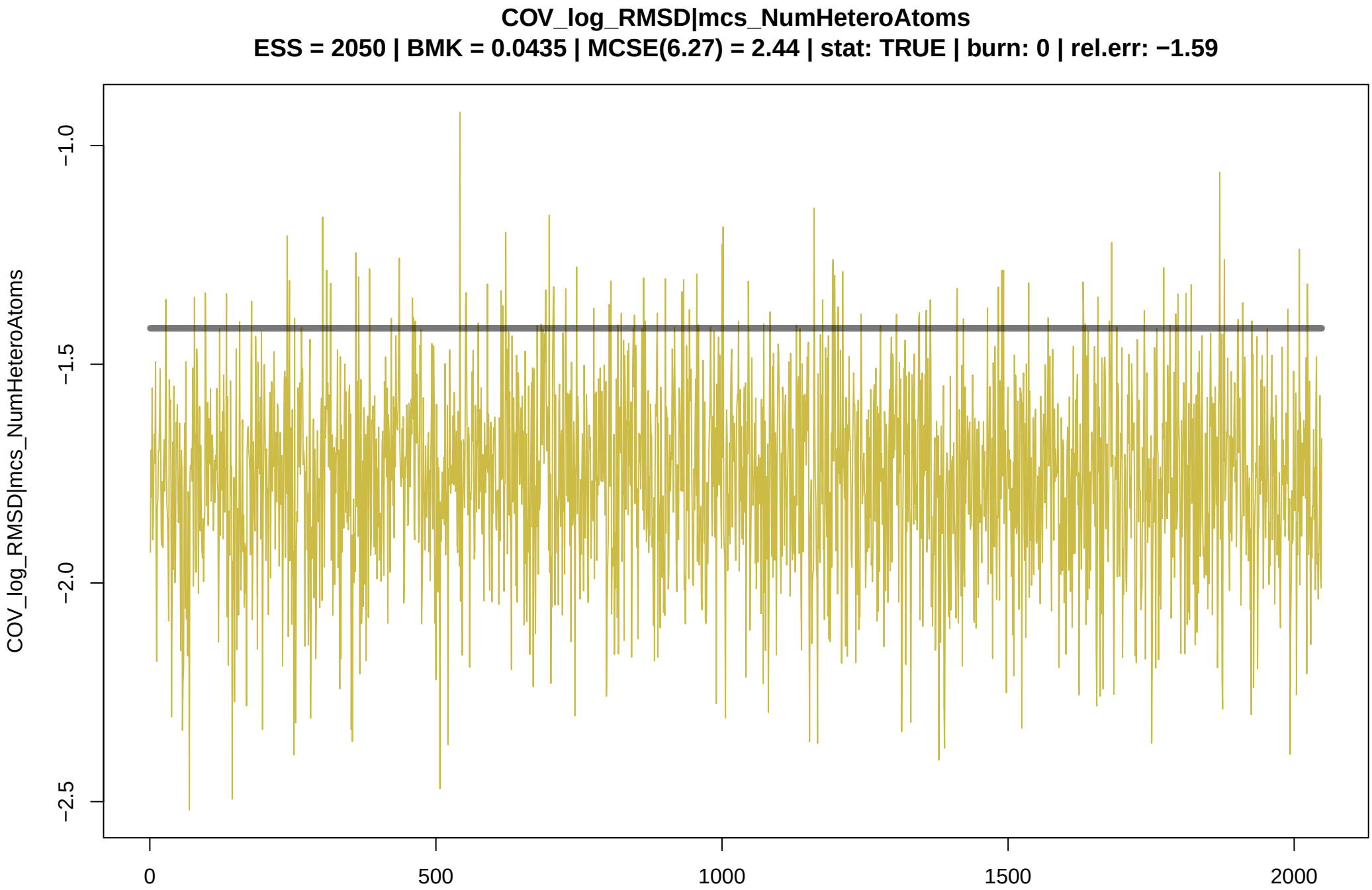

VAR_log_RMSD
ESS = 1790 | BMK = 0.0413 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: 2.23
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

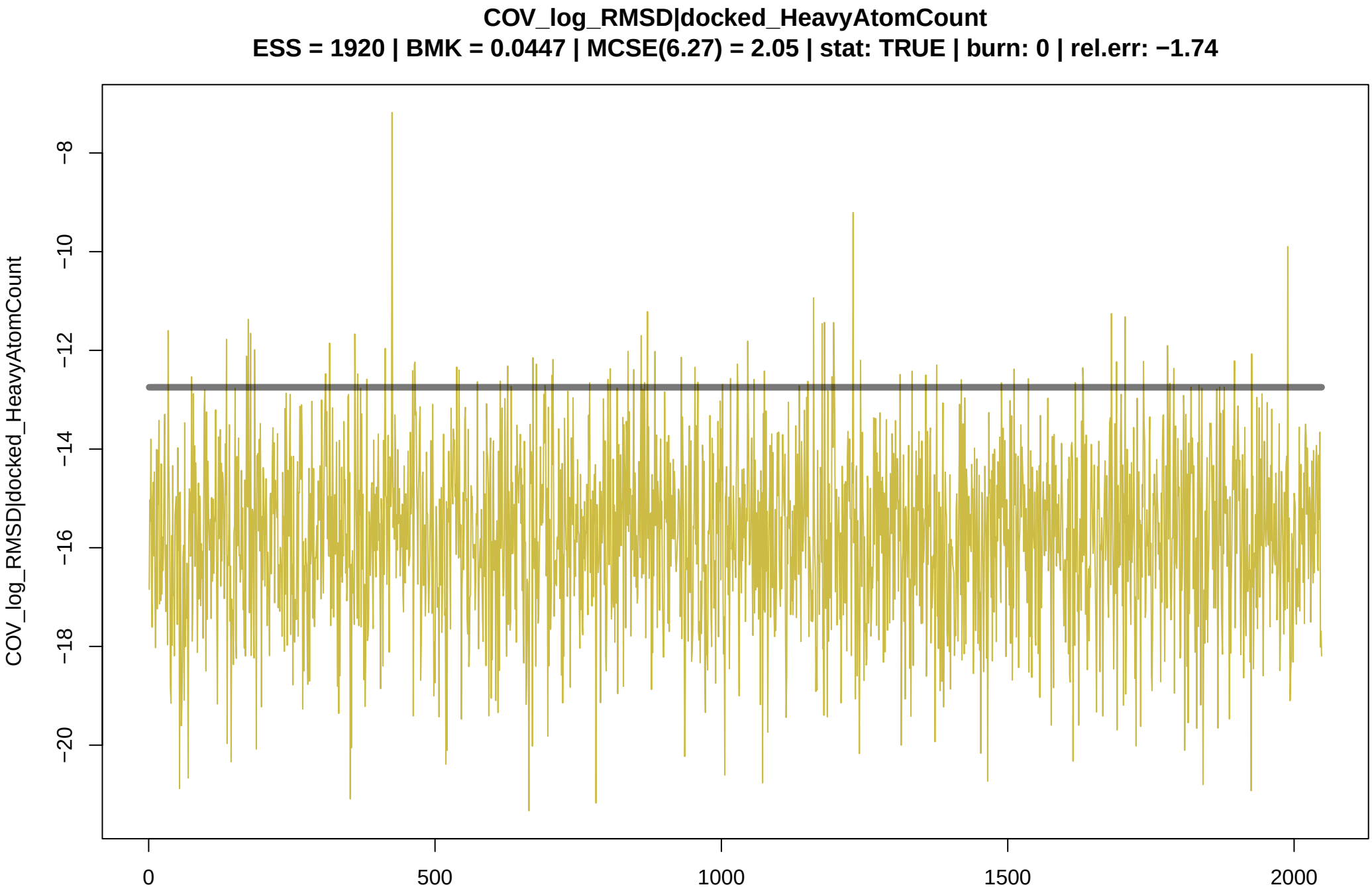

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0376 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: 1.37
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

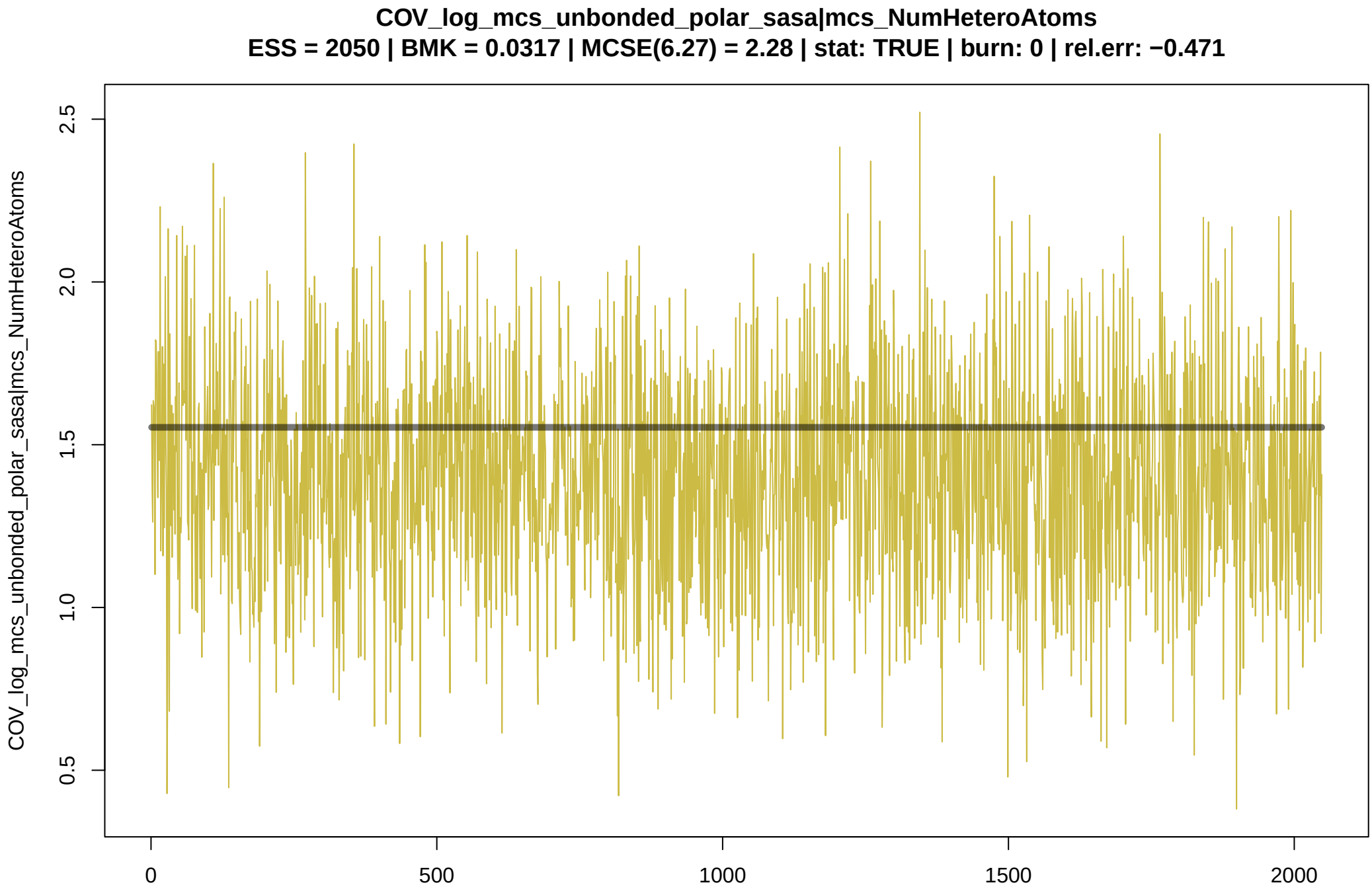

VAR_mcs_NumHeteroAtoms
ESS = 1670 | BMK = 0.0376 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: 0.384
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

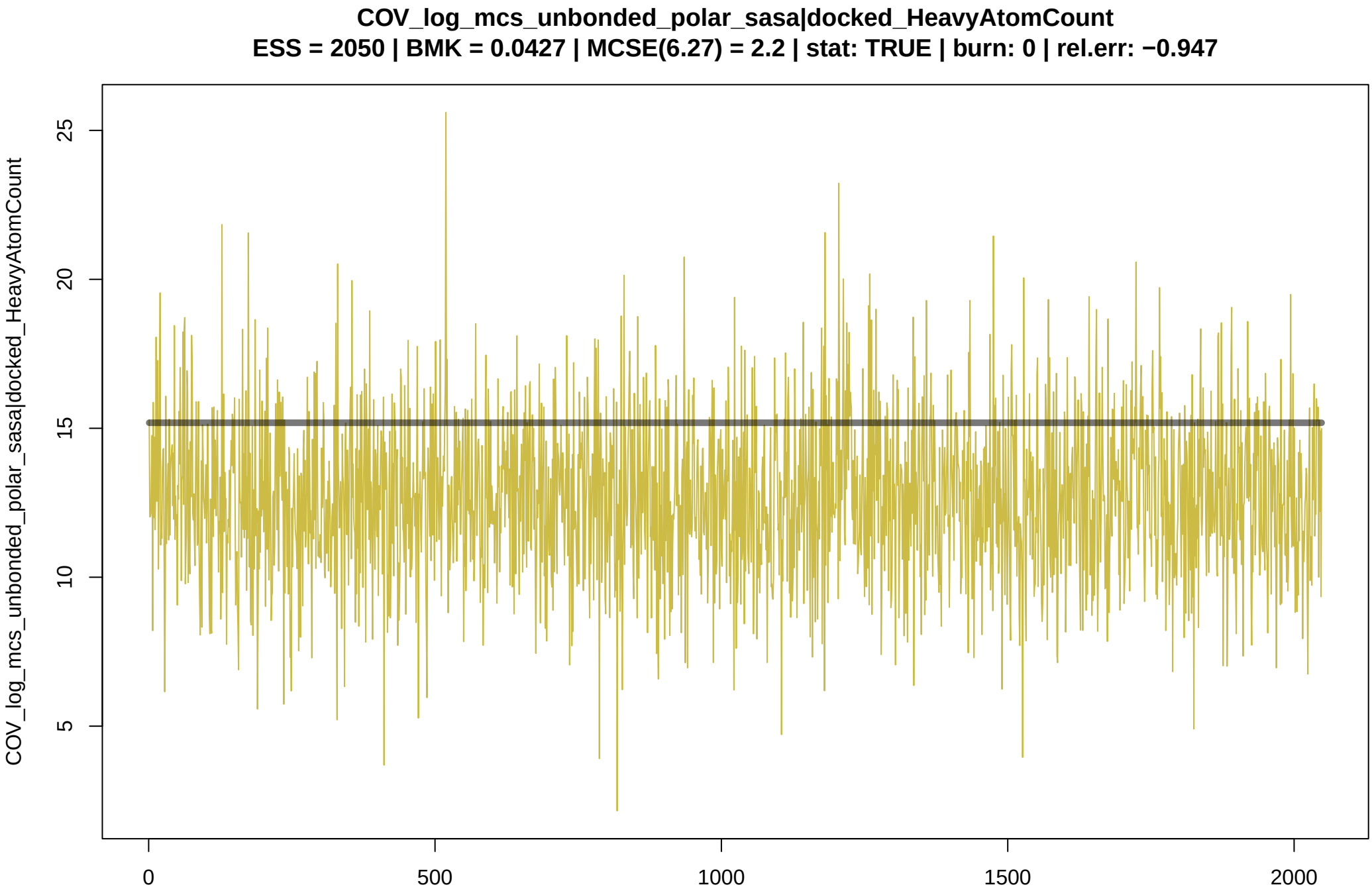

VAR_docked_HeavyAtomCount
ESS = 1890 | BMK = 0.0471 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | rel.err: 0.0785
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

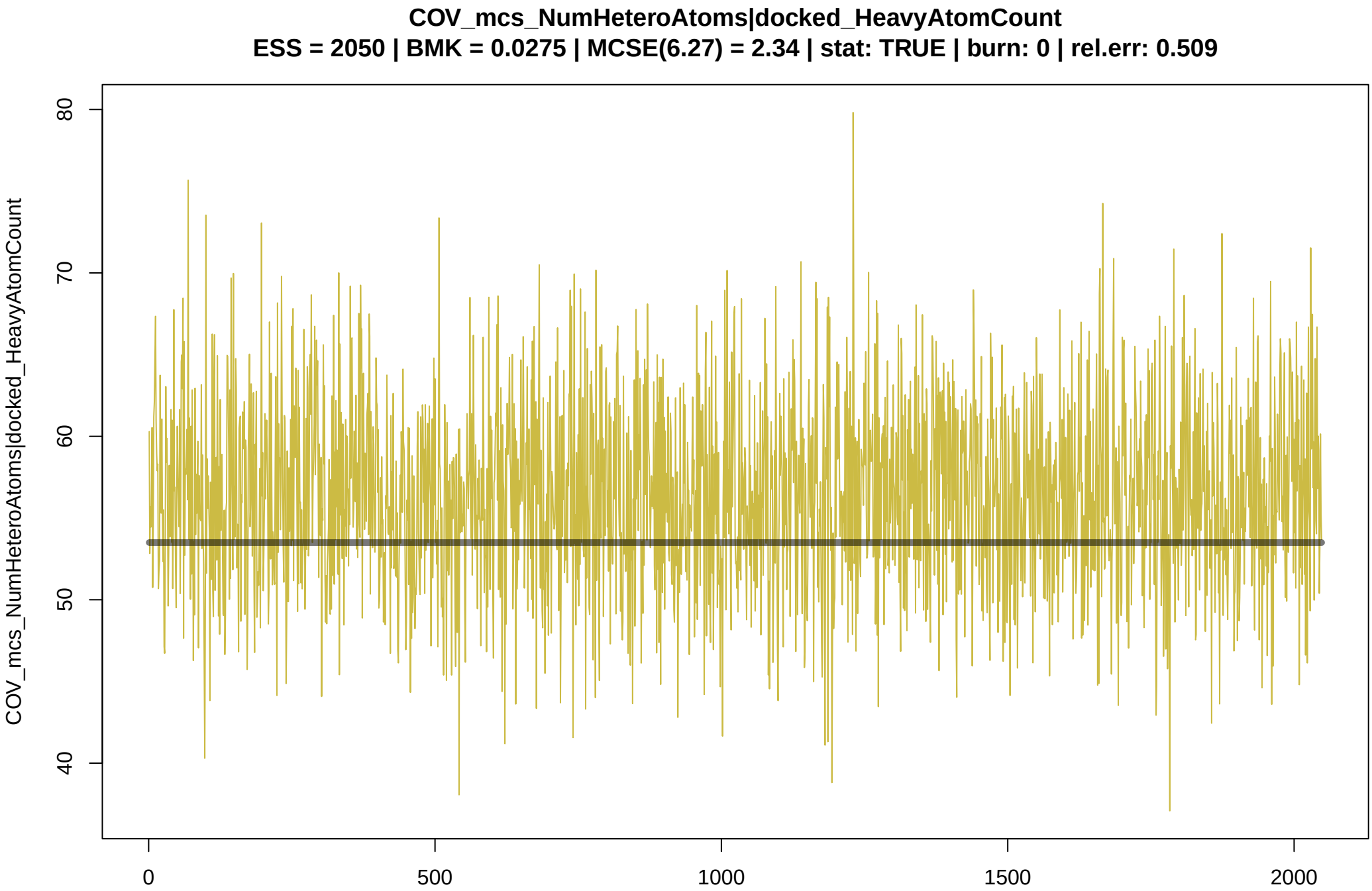

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1920 | BMK = 0.0385 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: 0.503
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0435 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: −1.59
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 = 0.0447 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: −1.74
COV_log_RMSD|docked_HeavyAtomCount
−8
−10
−12
−14
−16
−18
−20
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0317 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | rel.err: −0.471
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 = 2050 | BMK = 0.0427 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: −0.947
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
25
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0275 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: 0.509
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
80
70
60
50
40
0
500
1000
1500
2000