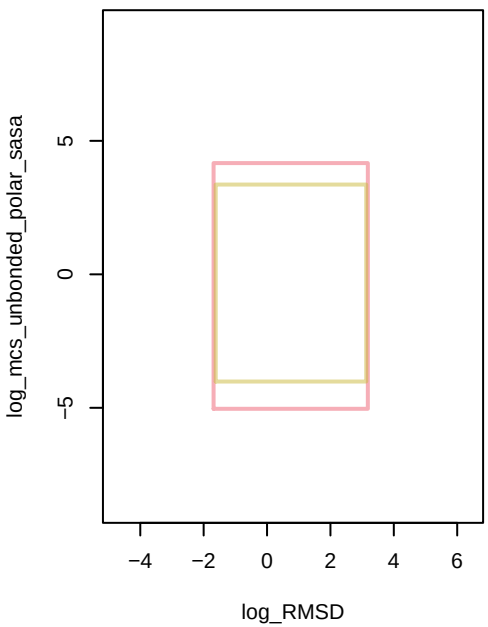
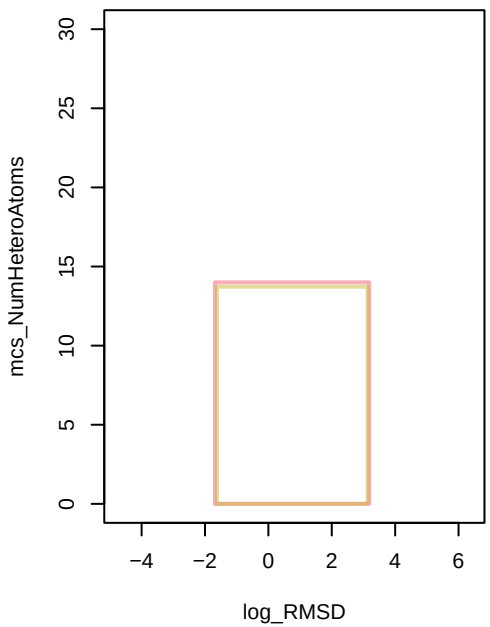
−− STATS maxD −−
min ESS = 83.6258357567131
max BMK = 0.146453417455258
max MCSE = 7.61398661539827
all stationary: FALSE
burn: 0
max rel.err.: 2.1624966805217

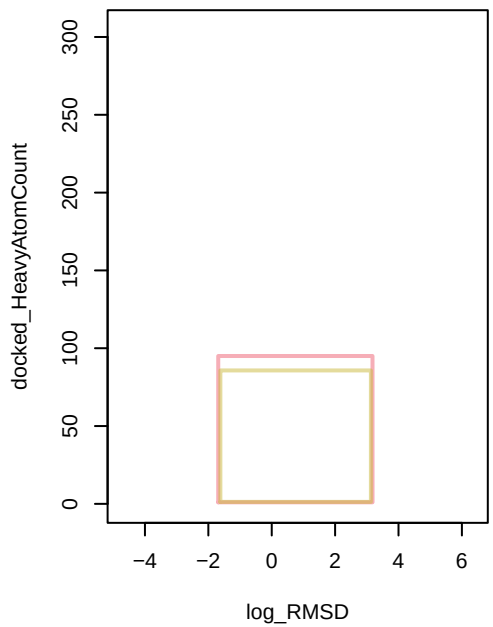
−− STATS 2D −−
min ESS = 2048
max BMK = 0.071872223366808 8
max MCSE = 2.71937638078883
all stationary: TRUE
burn: 0
max rel.err.: 1.71356329802567

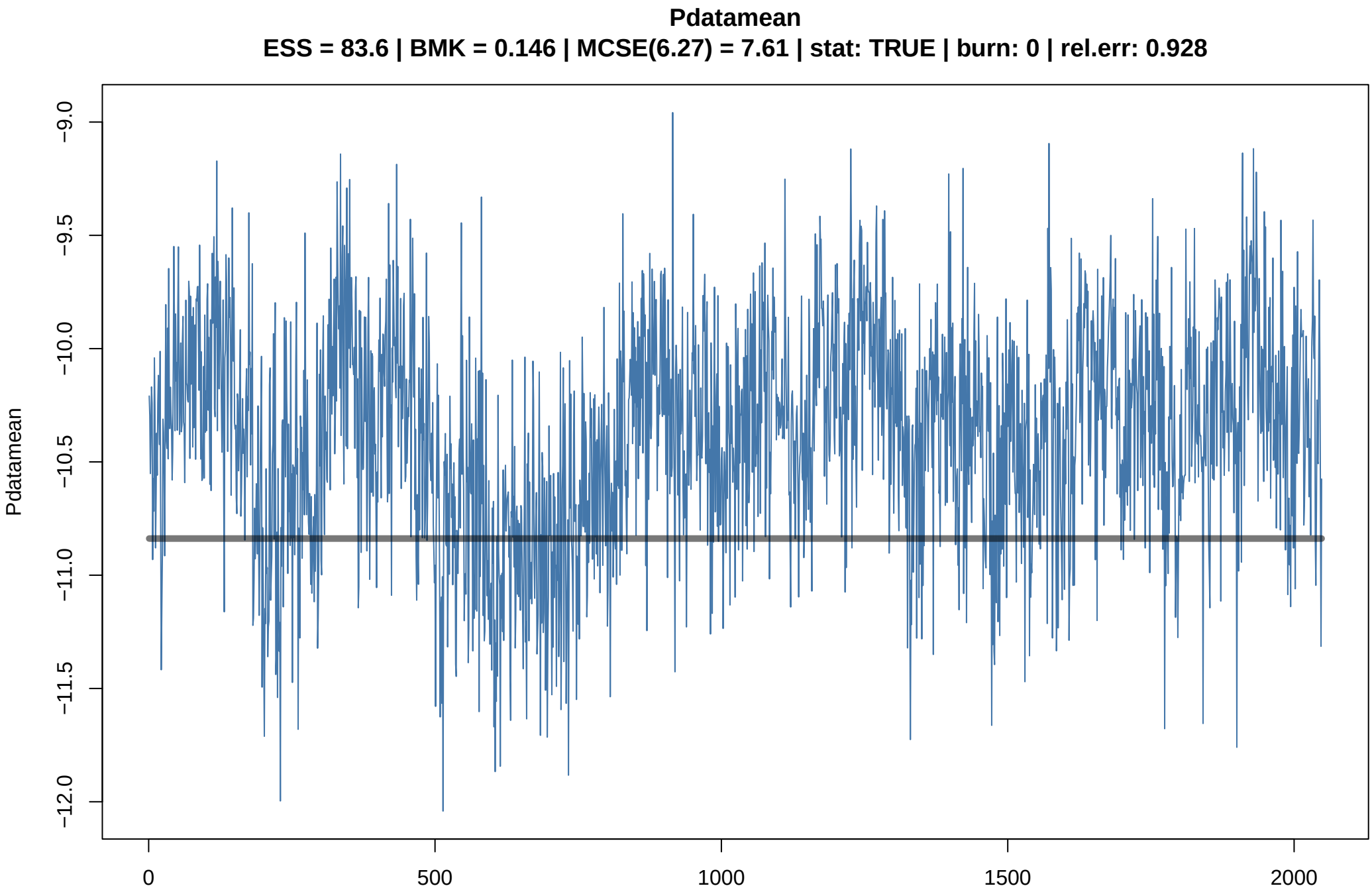
−− STATS 1D −−
min ESS = 886.830982576754
max BMK = 0.056954097967624 2
max MCSE = 3.39671627235942
all stationary: TRUE
burn: 0
max rel.err.: 2.26419106133066

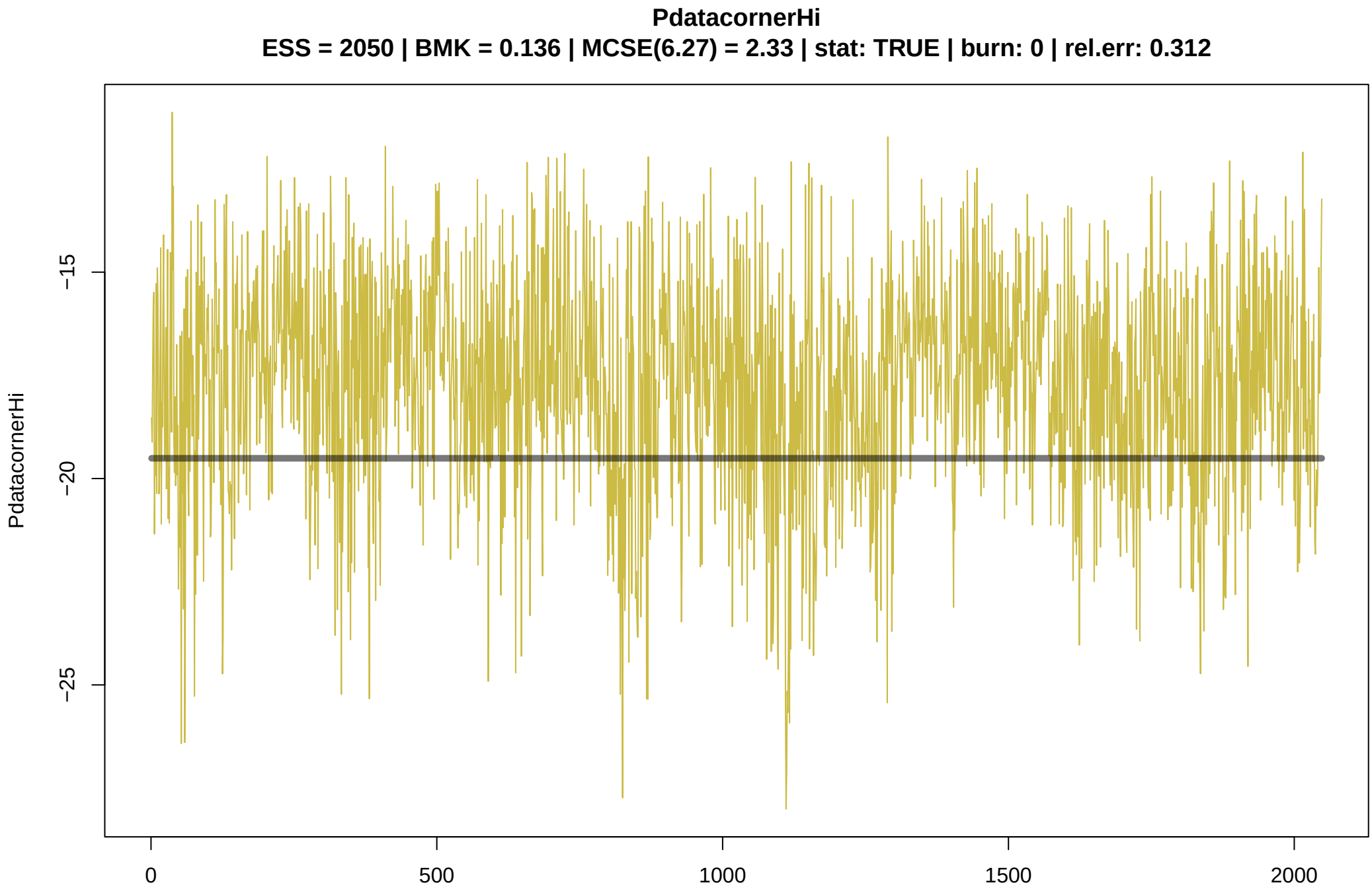
Occupied clusters: 9 of 16

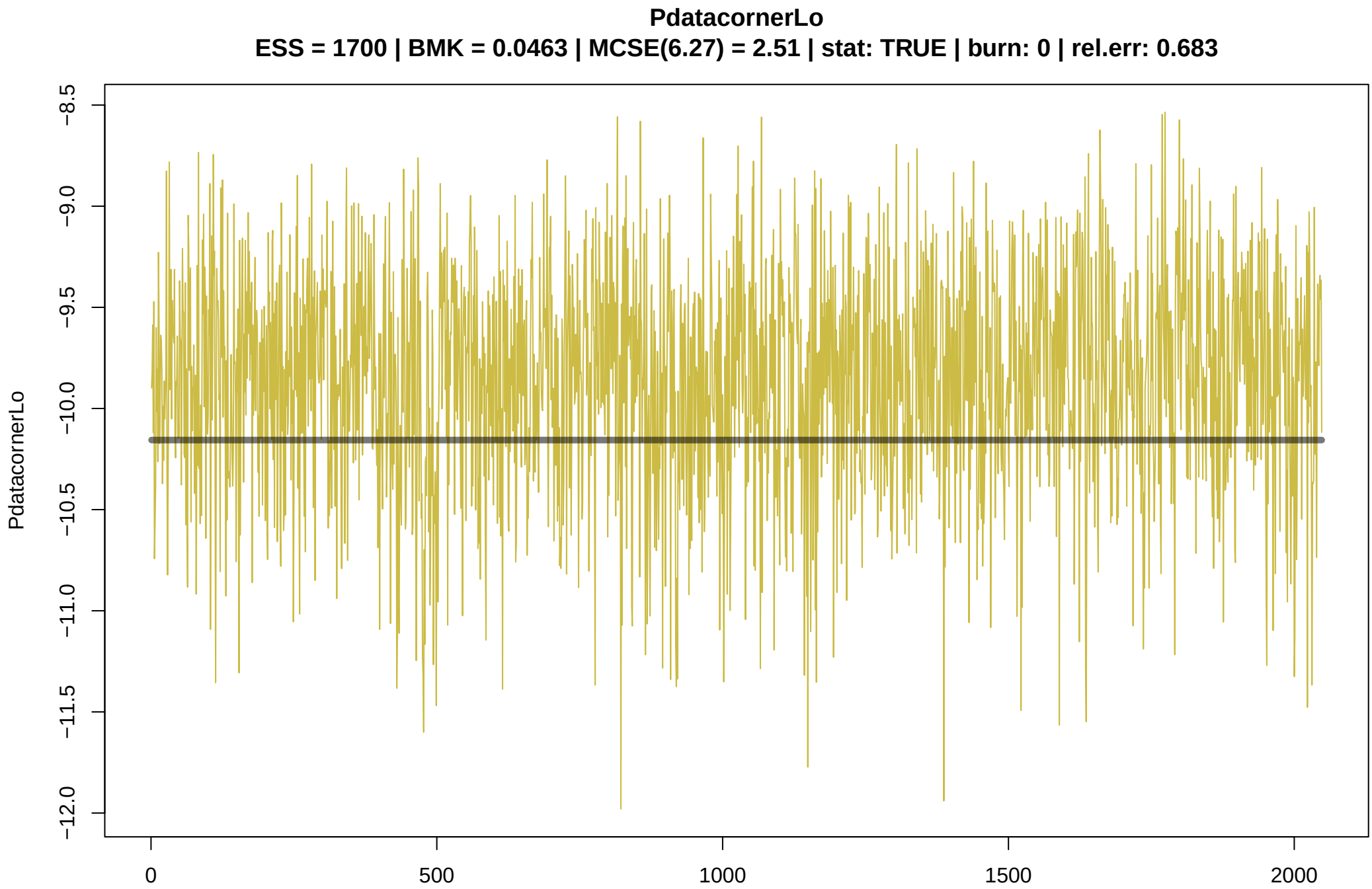

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

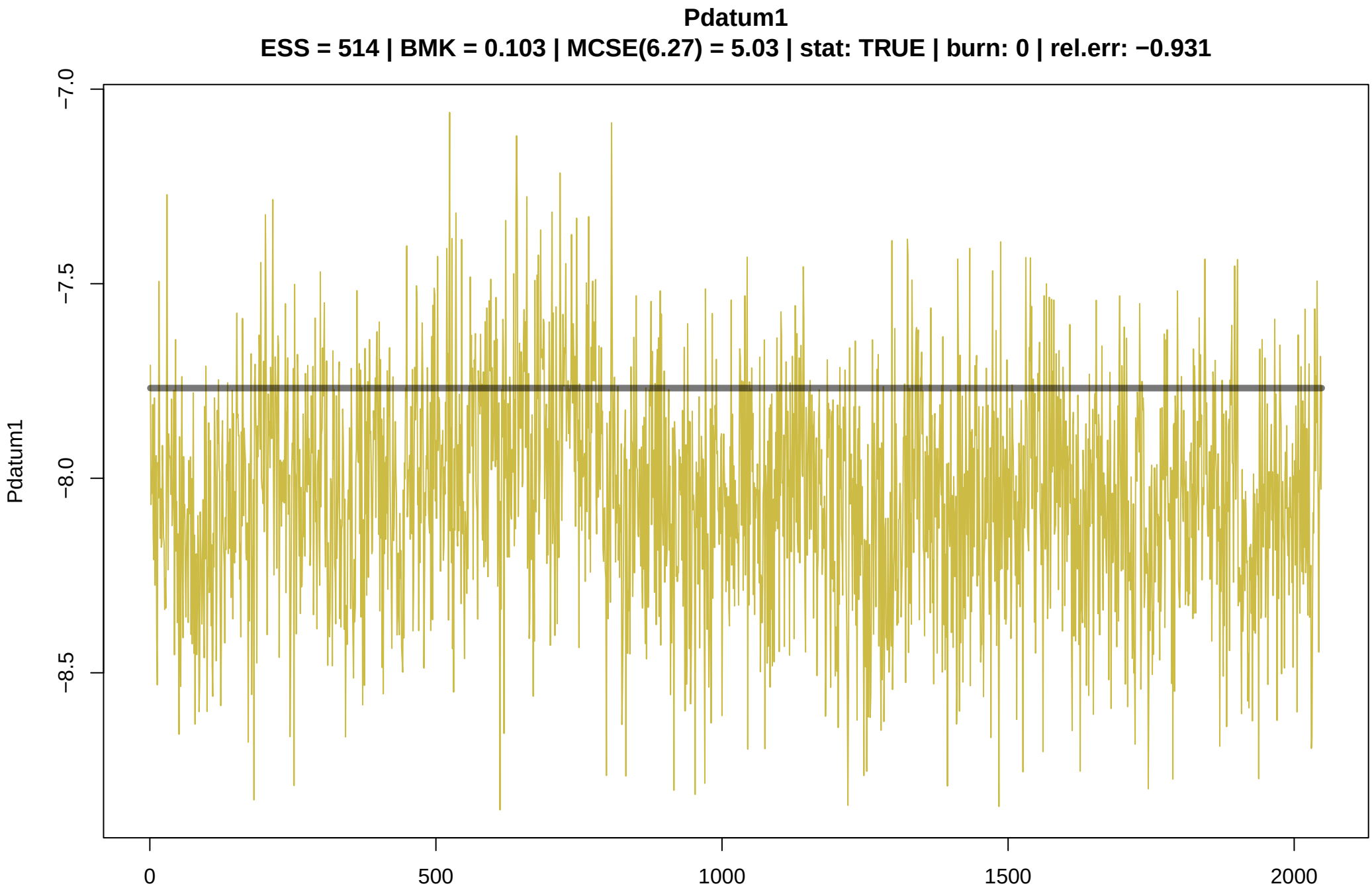

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

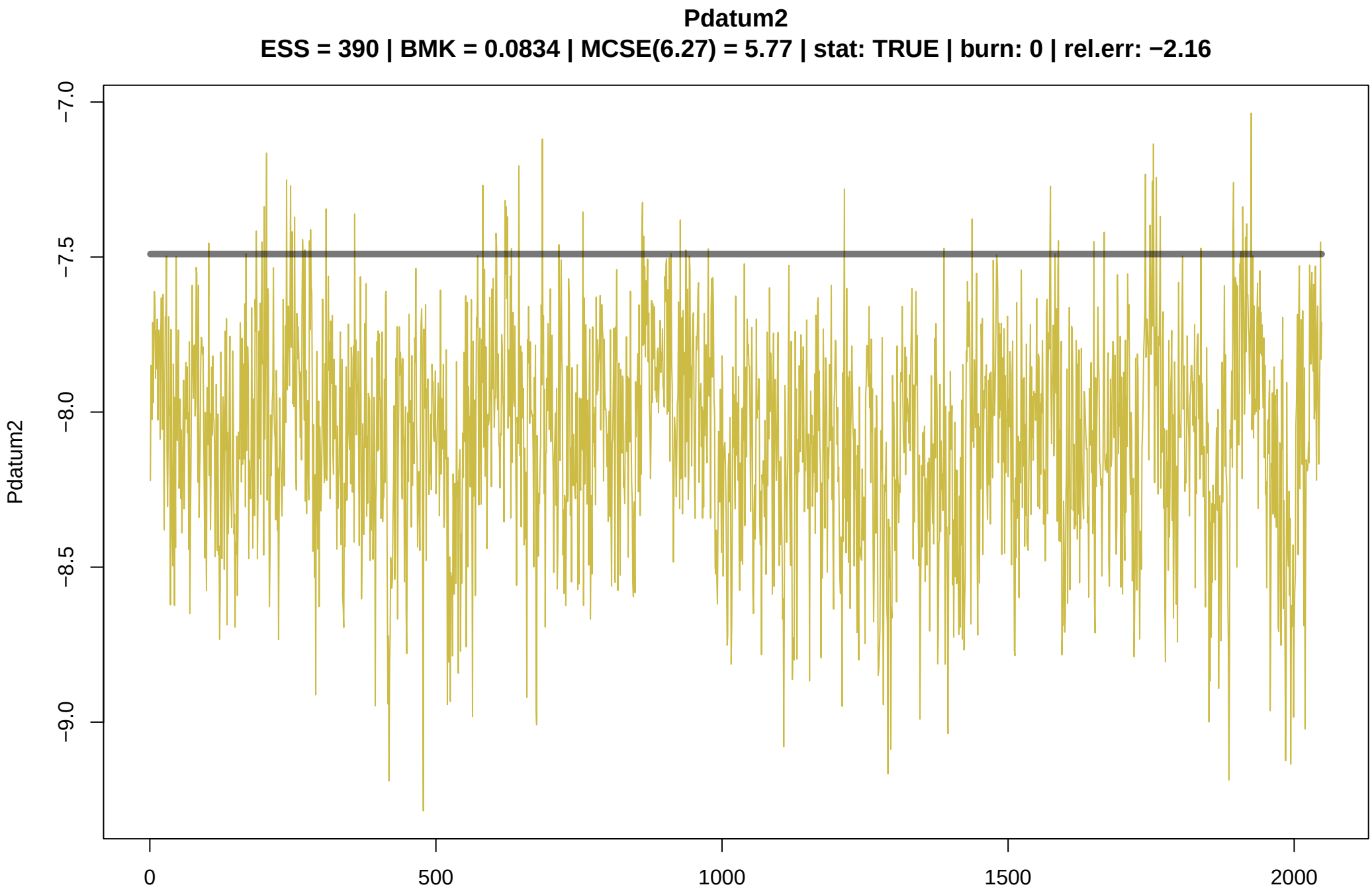

docked_HeavyAtomCount
300
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

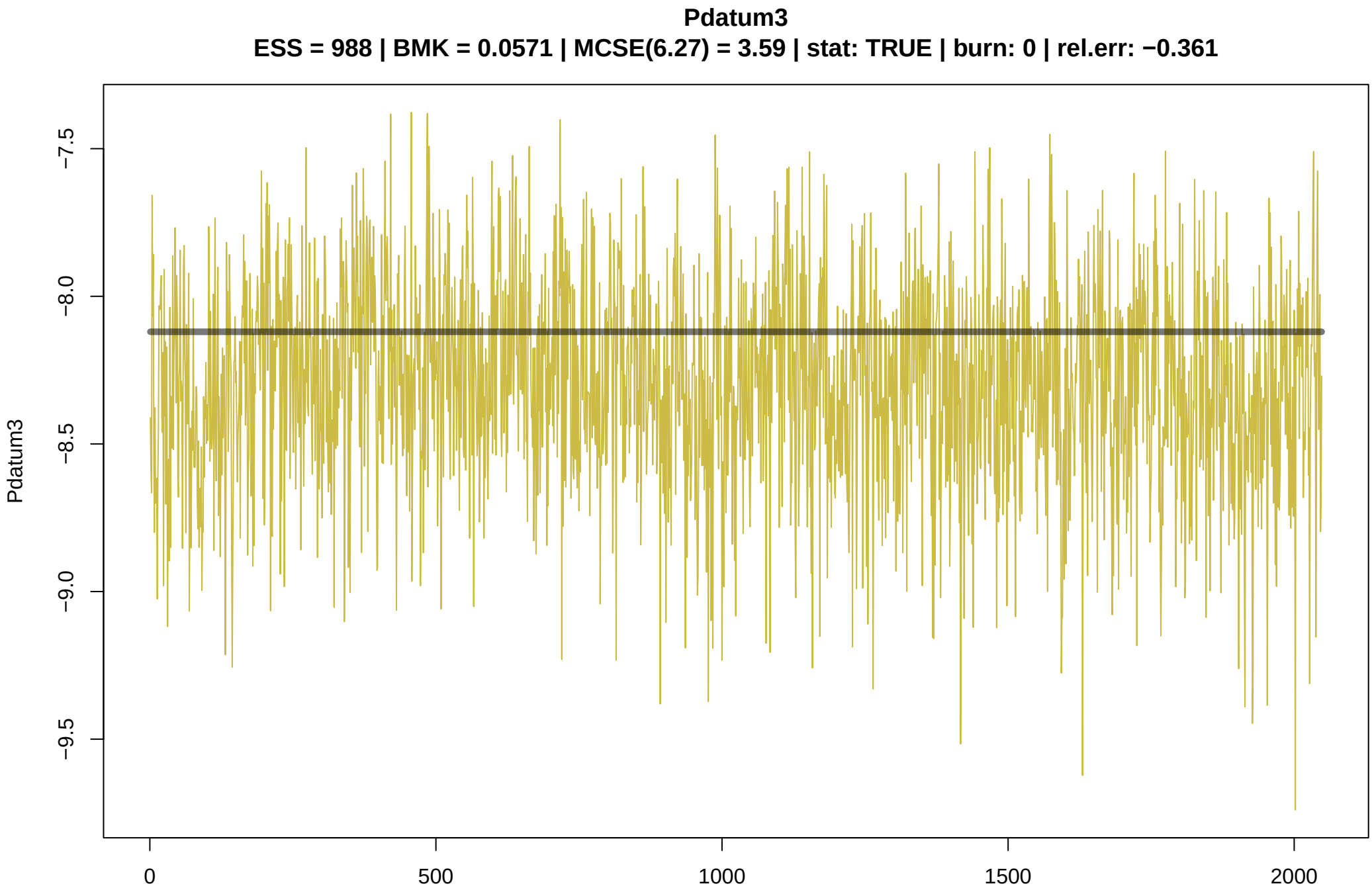

Pdatamean
ESS = 83.6 | BMK = 0.146 | MCSE(6.27) = 7.61 | stat: TRUE | burn: 0 | rel.err: 0.928
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

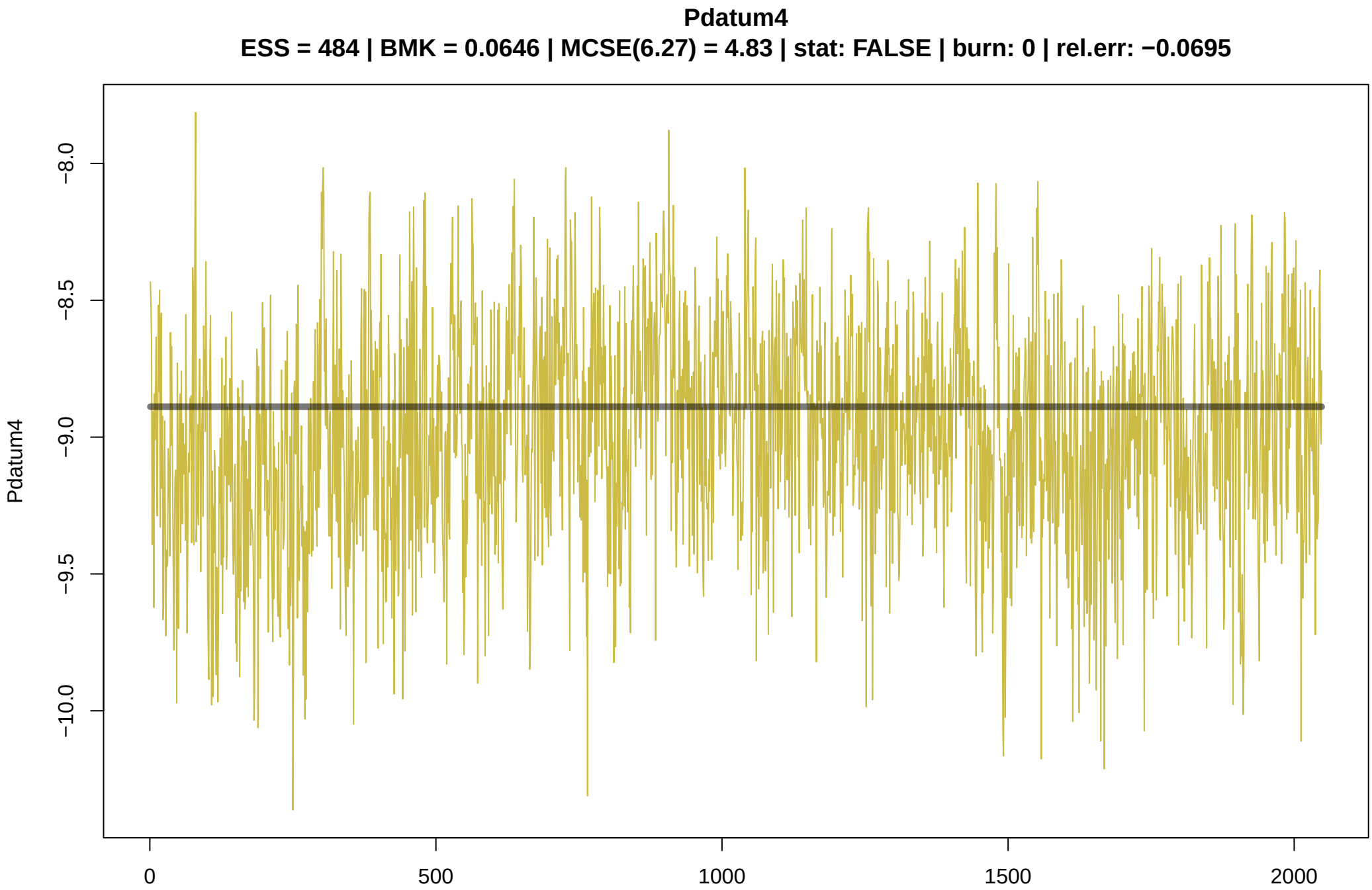

PdatacornerHi
ESS = 2050 | BMK = 0.136 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 0.312
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

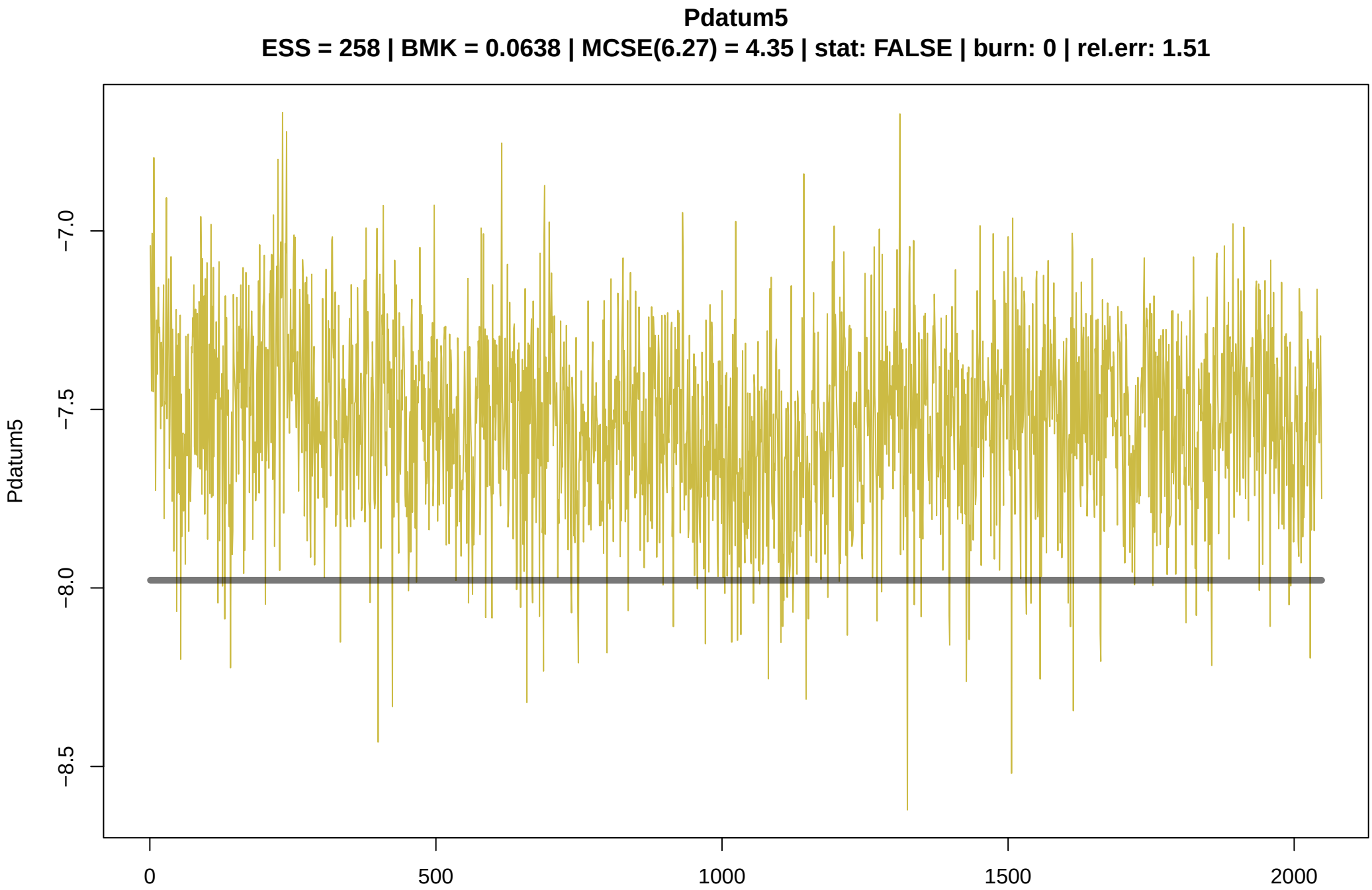

PdatacornerLo
ESS = 1700 | BMK = 0.0463 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: 0.683
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

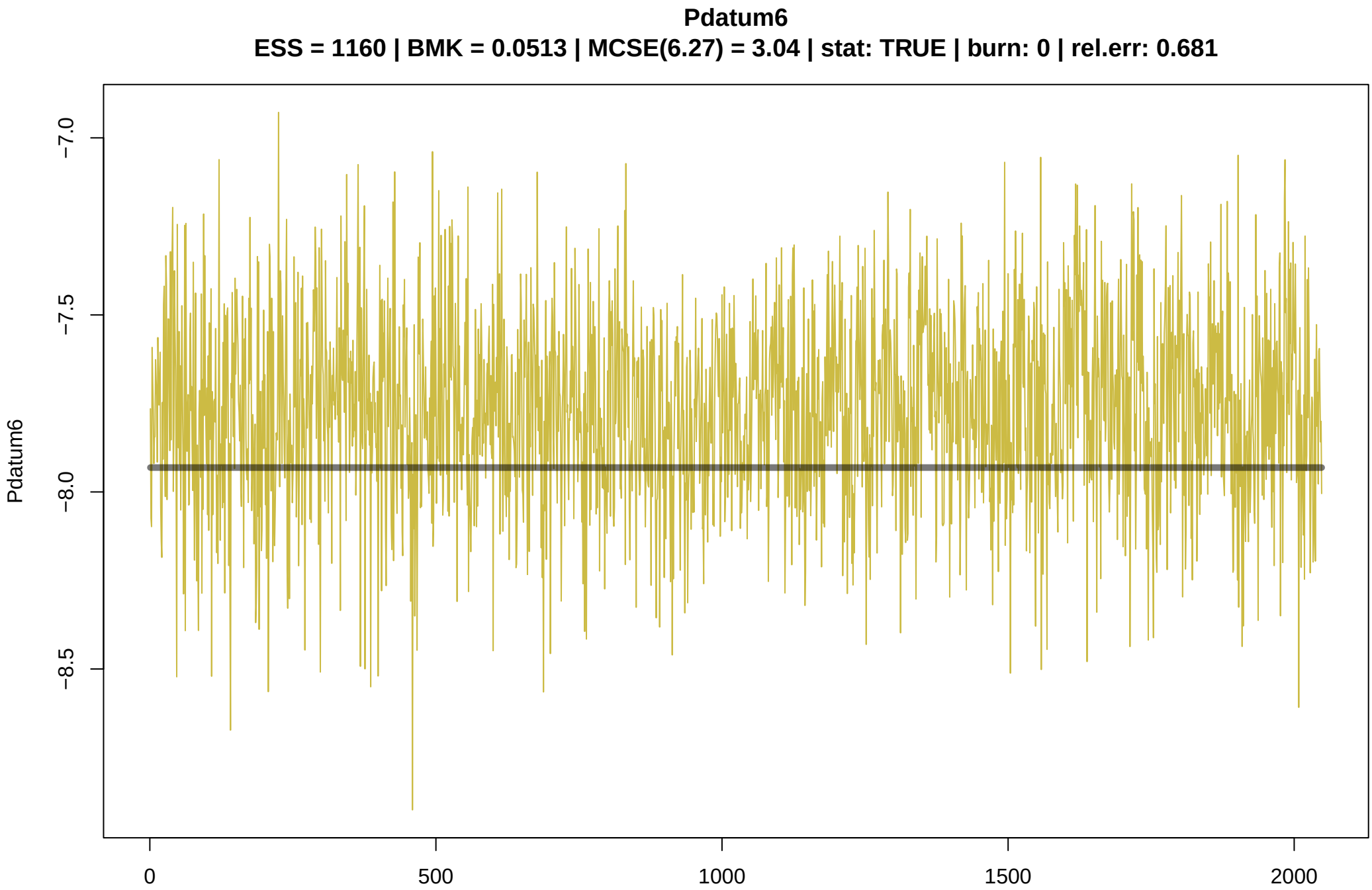

Pdatum1
ESS = 514 | BMK = 0.103 | MCSE(6.27) = 5.03 | stat: TRUE | burn: 0 | rel.err: −0.931
Pdatum1
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

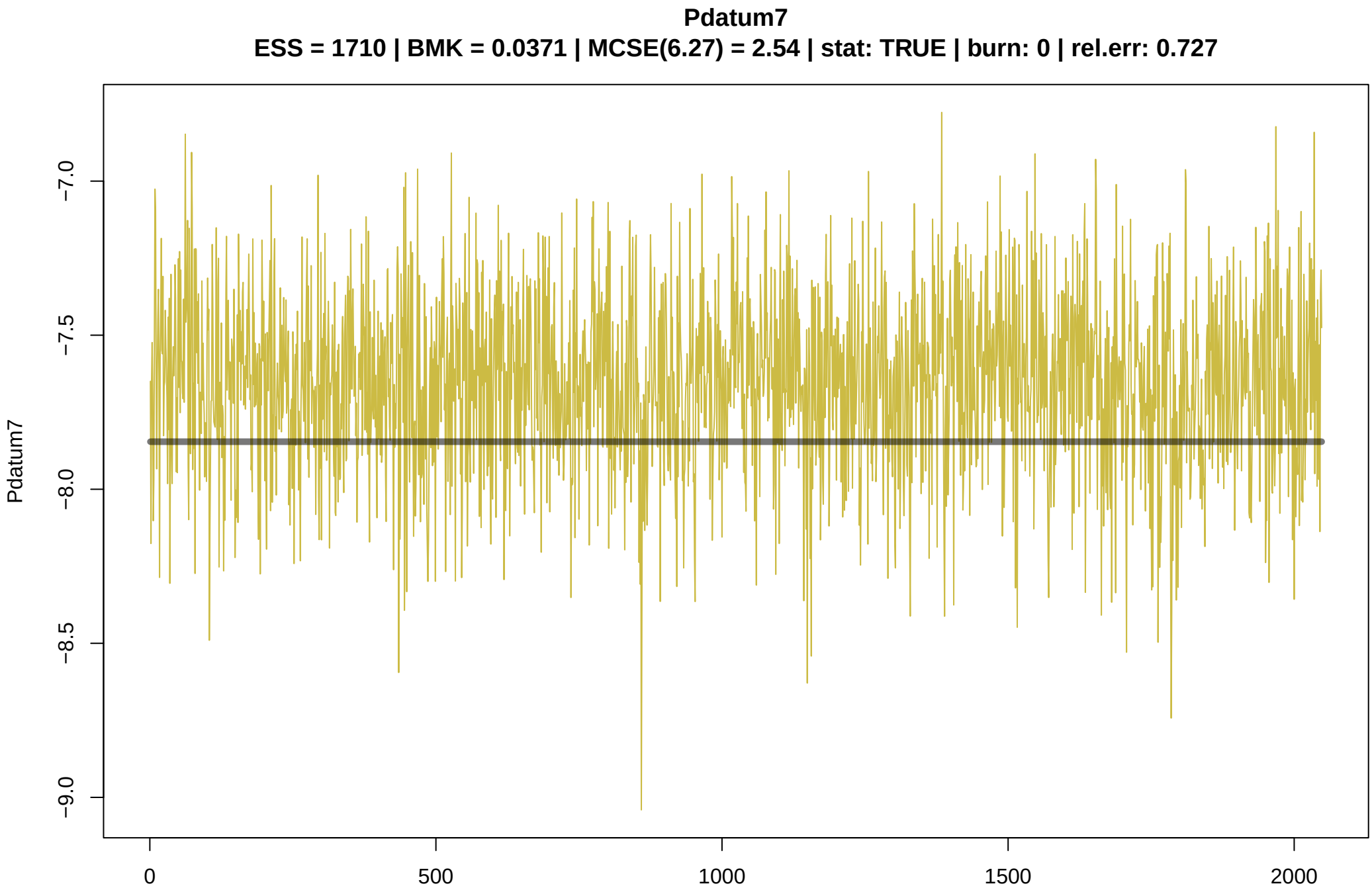

Pdatum2
ESS = 390 | BMK = 0.0834 | MCSE(6.27) = 5.77 | stat: TRUE | burn: 0 | rel.err: −2.16
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

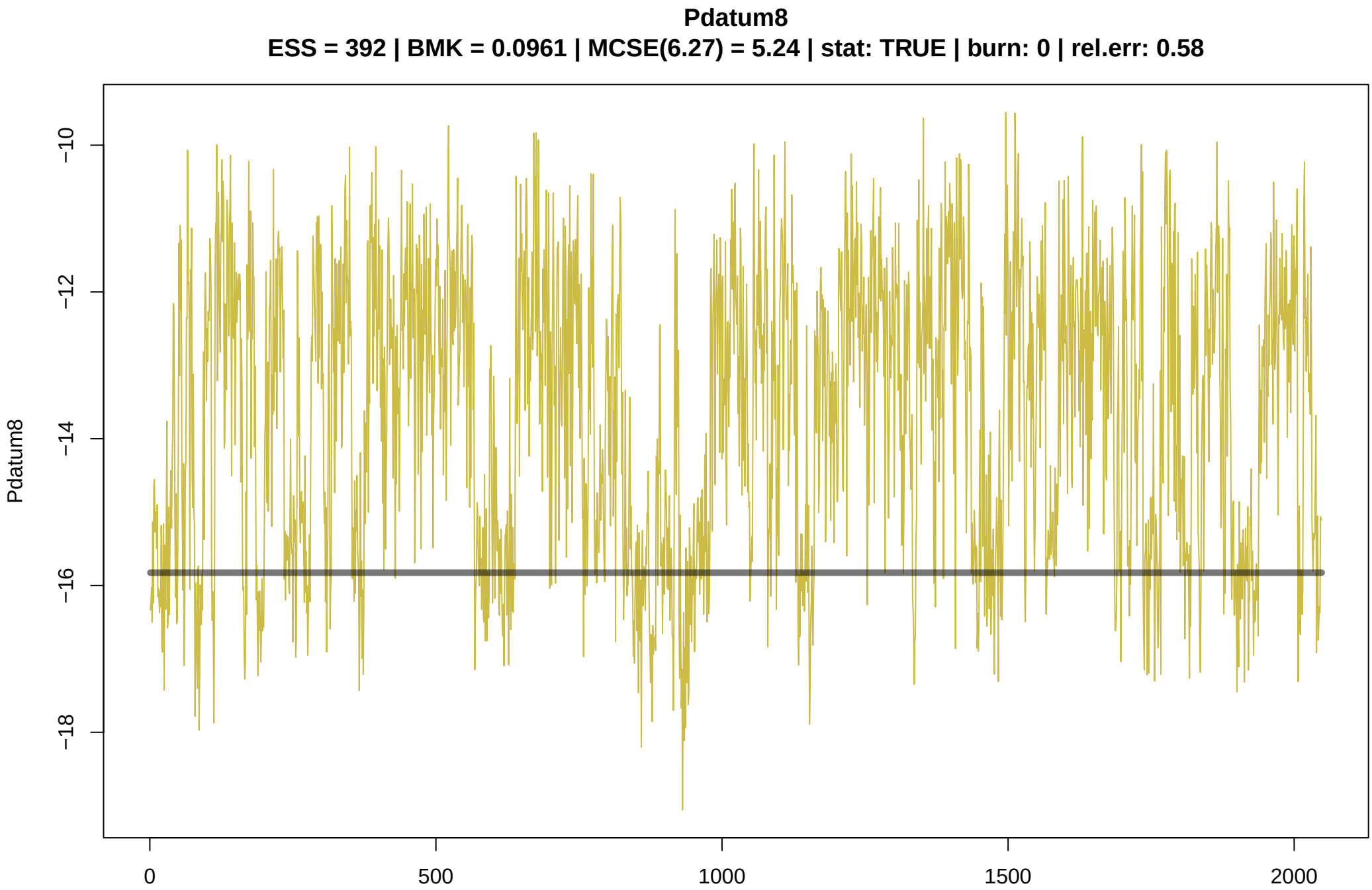

Pdatum3
ESS = 988 | BMK = 0.0571 | MCSE(6.27) = 3.59 | stat: TRUE | burn: 0 | rel.err: −0.361
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

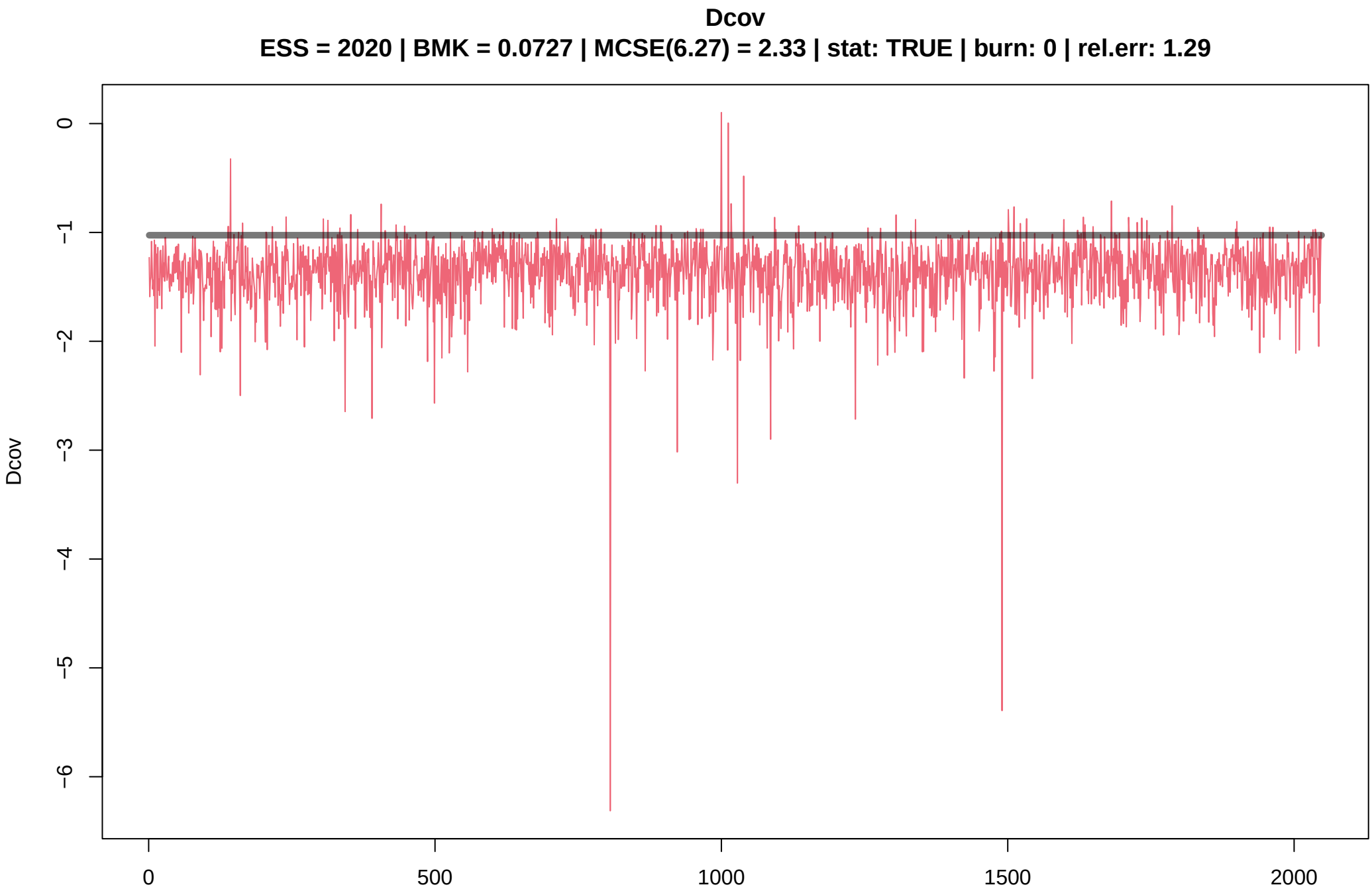

Pdatum4
ESS = 484 | BMK = 0.0646 | MCSE(6.27) = 4.83 | stat: FALSE | burn: 0 | rel.err: −0.0695
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

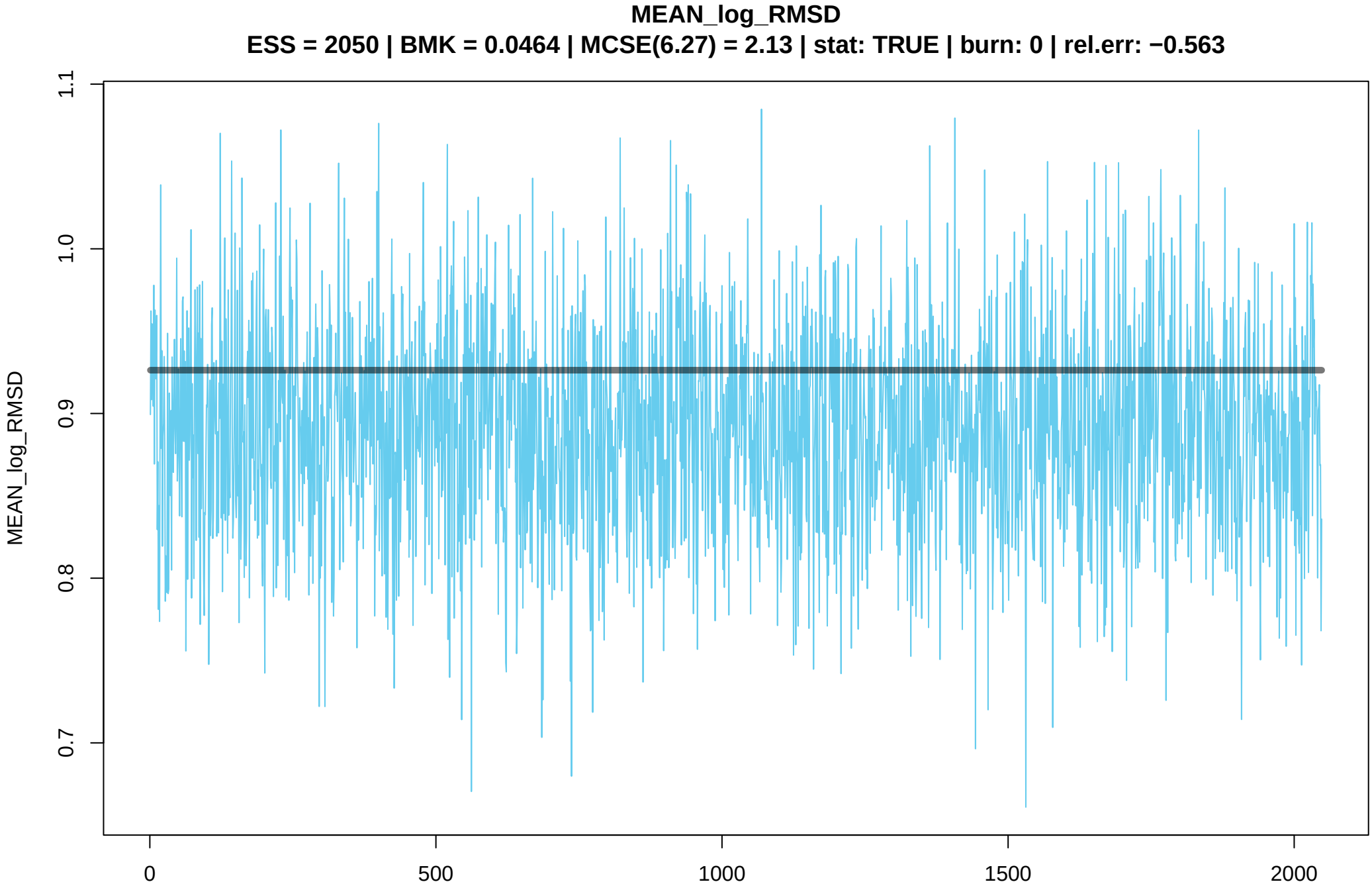

Pdatum5
ESS = 258 | BMK = 0.0638 | MCSE(6.27) = 4.35 | stat: FALSE | burn: 0 | rel.err: 1.51
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

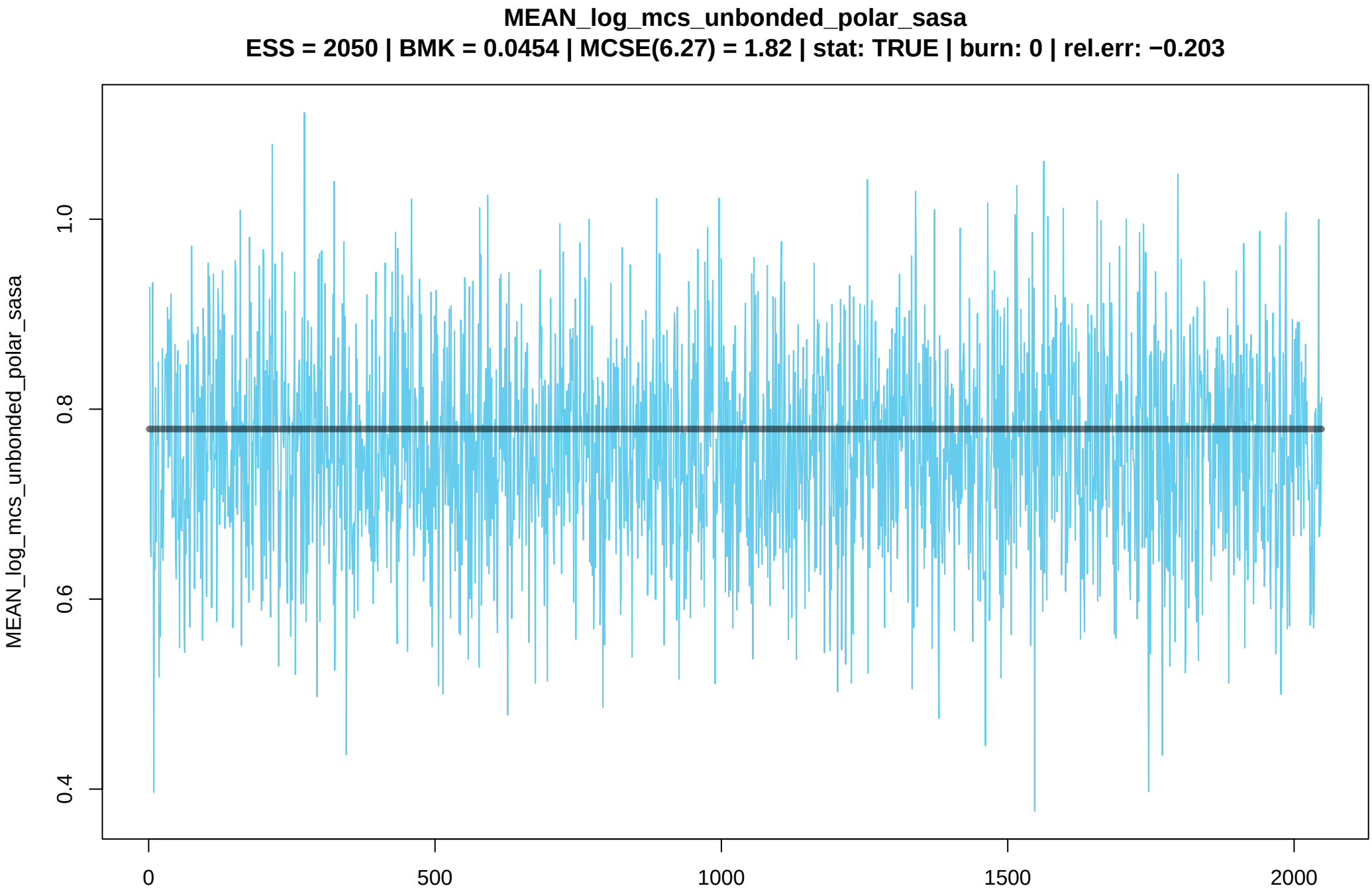

Pdatum6
ESS = 1160 | BMK = 0.0513 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 0.681
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

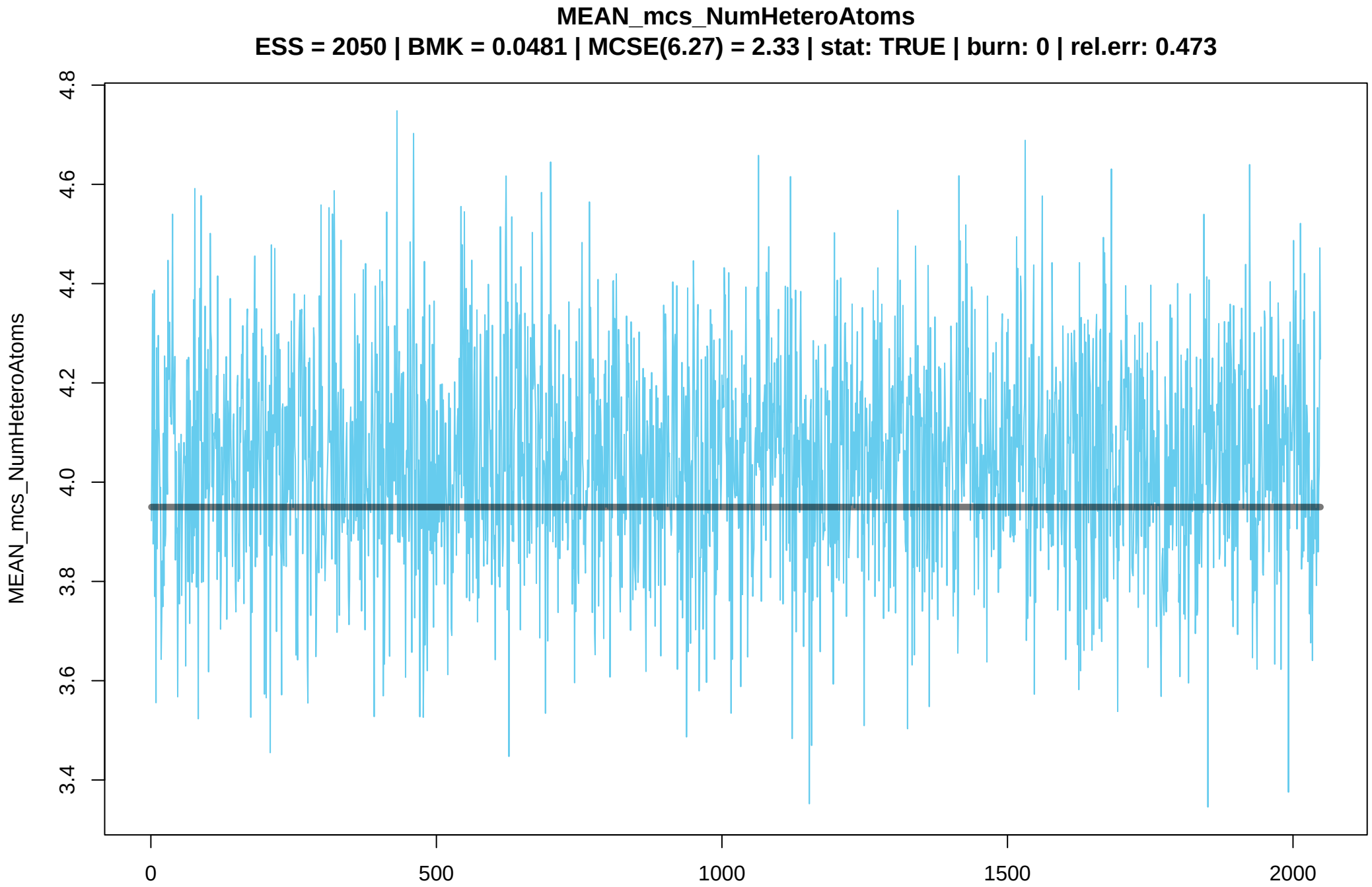

Pdatum7
ESS = 1710 | BMK = 0.0371 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: 0.727
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

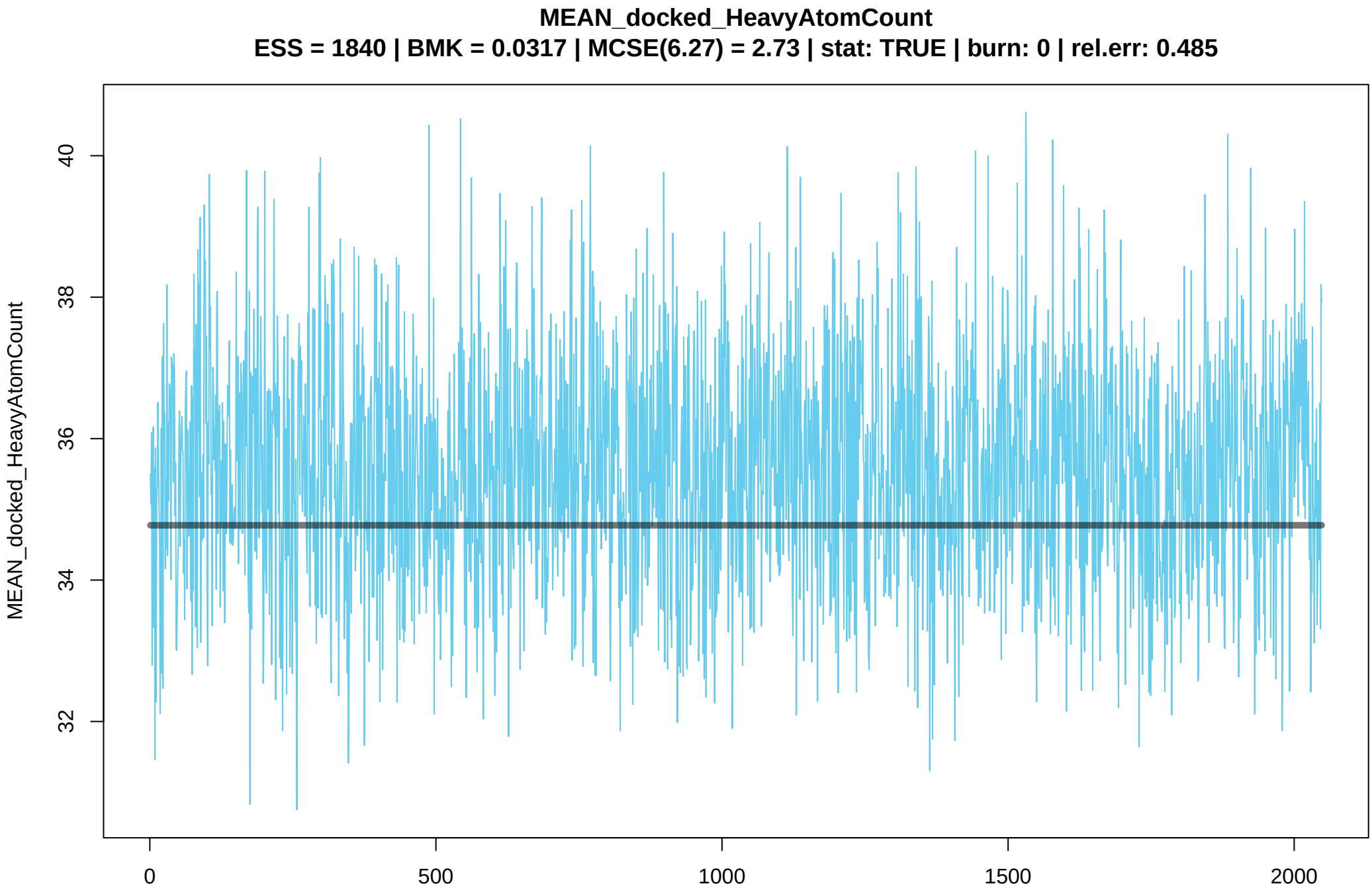

Pdatum8
ESS = 392 | BMK = 0.0961 | MCSE(6.27) = 5.24 | stat: TRUE | burn: 0 | rel.err: 0.58
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

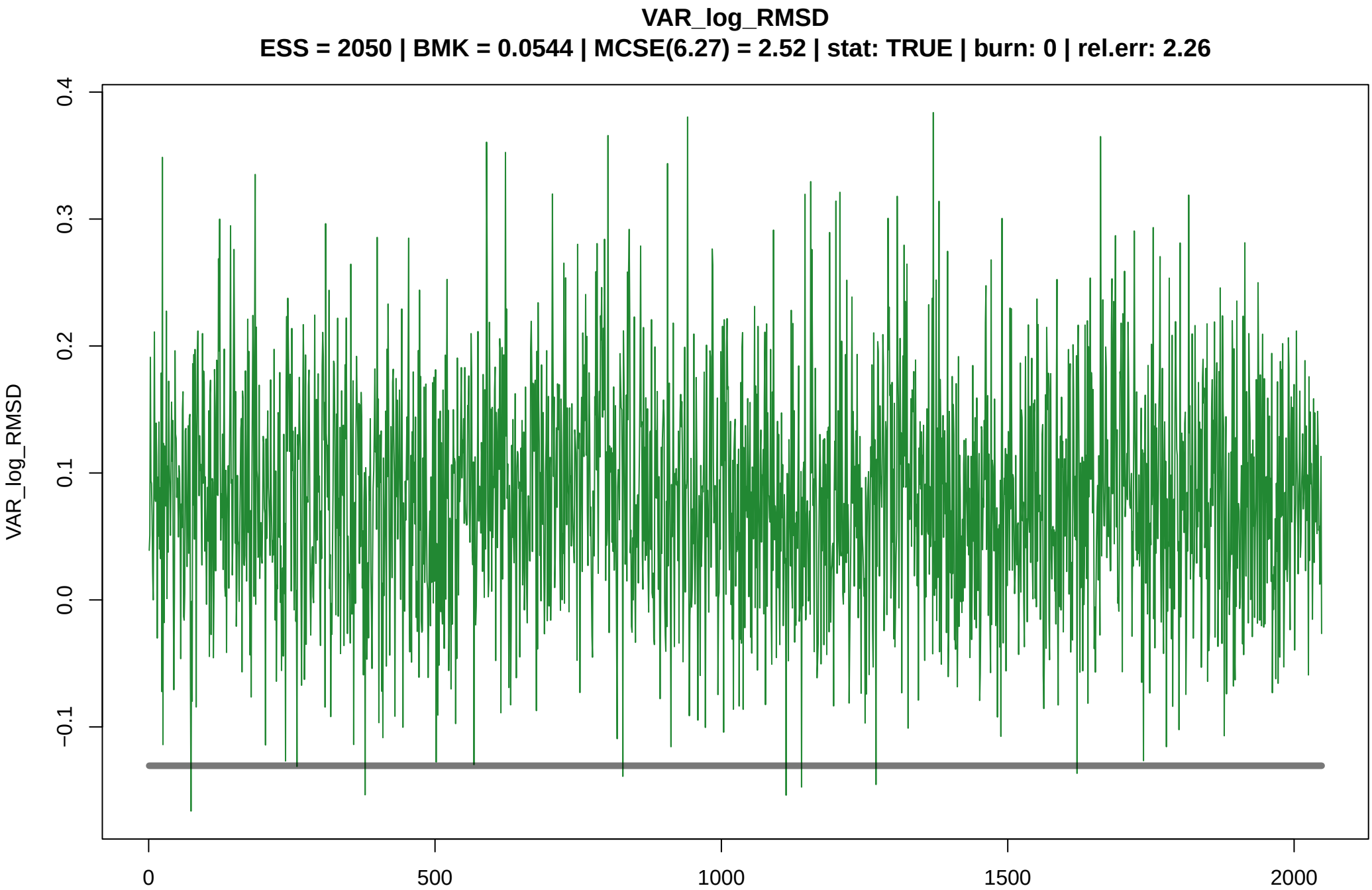

Dcov
ESS = 2020 | BMK = 0.0727 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 1.29
Dcov
0
−1
−2
−3
−4
−5
−6
0
500
1000
1500
2000

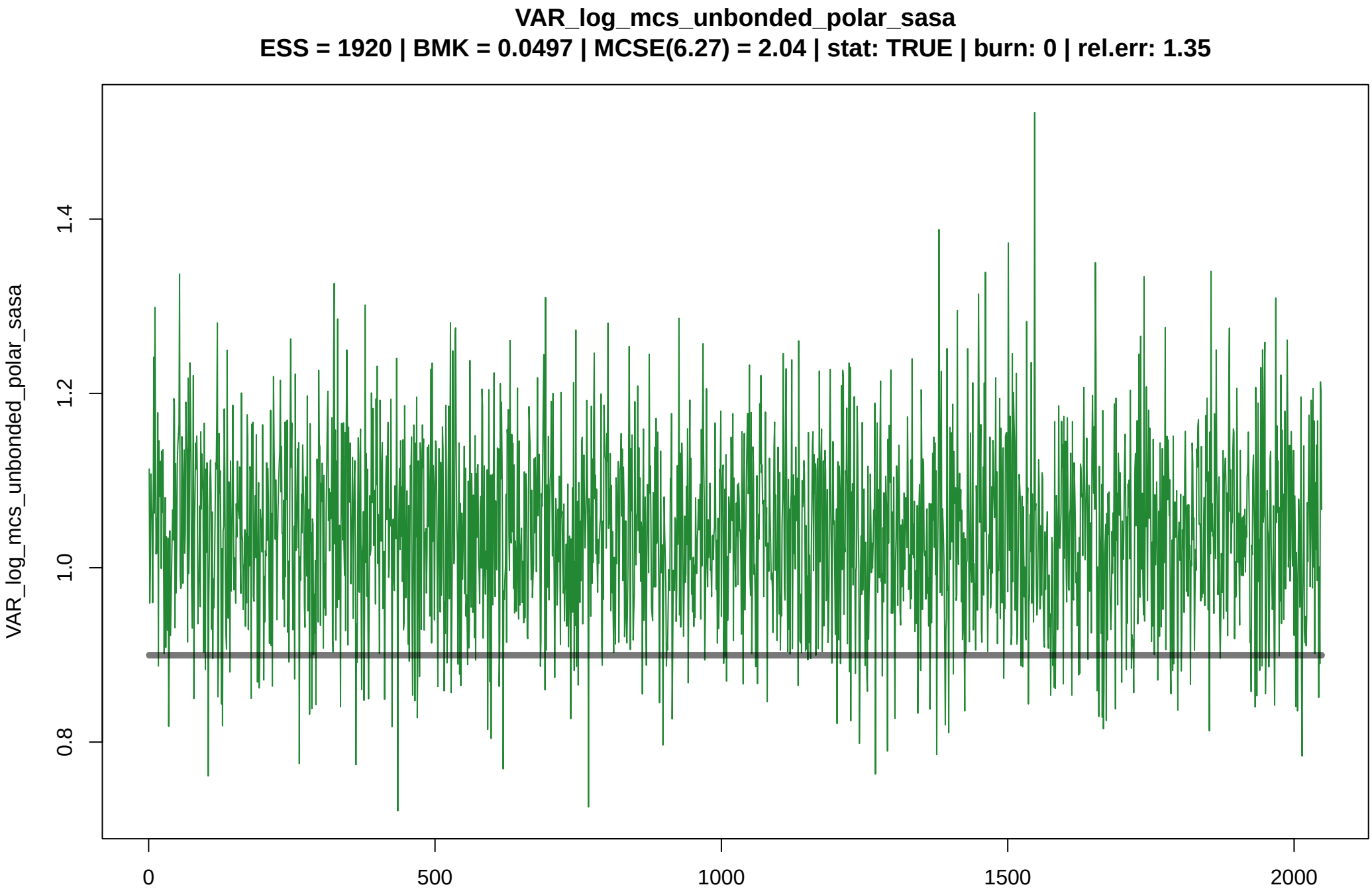

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0464 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0 | rel.err: −0.563
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

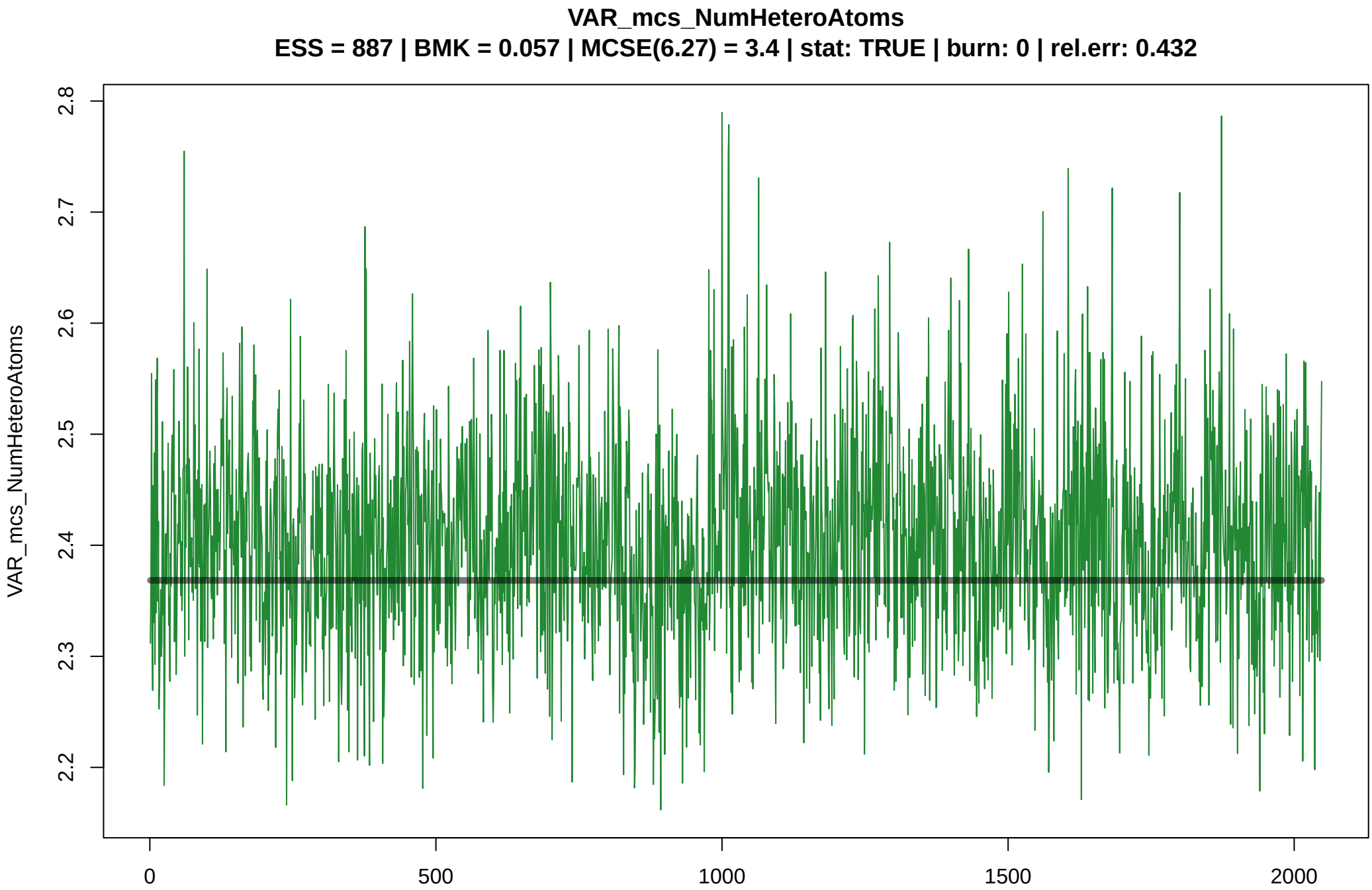

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0454 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: −0.203
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

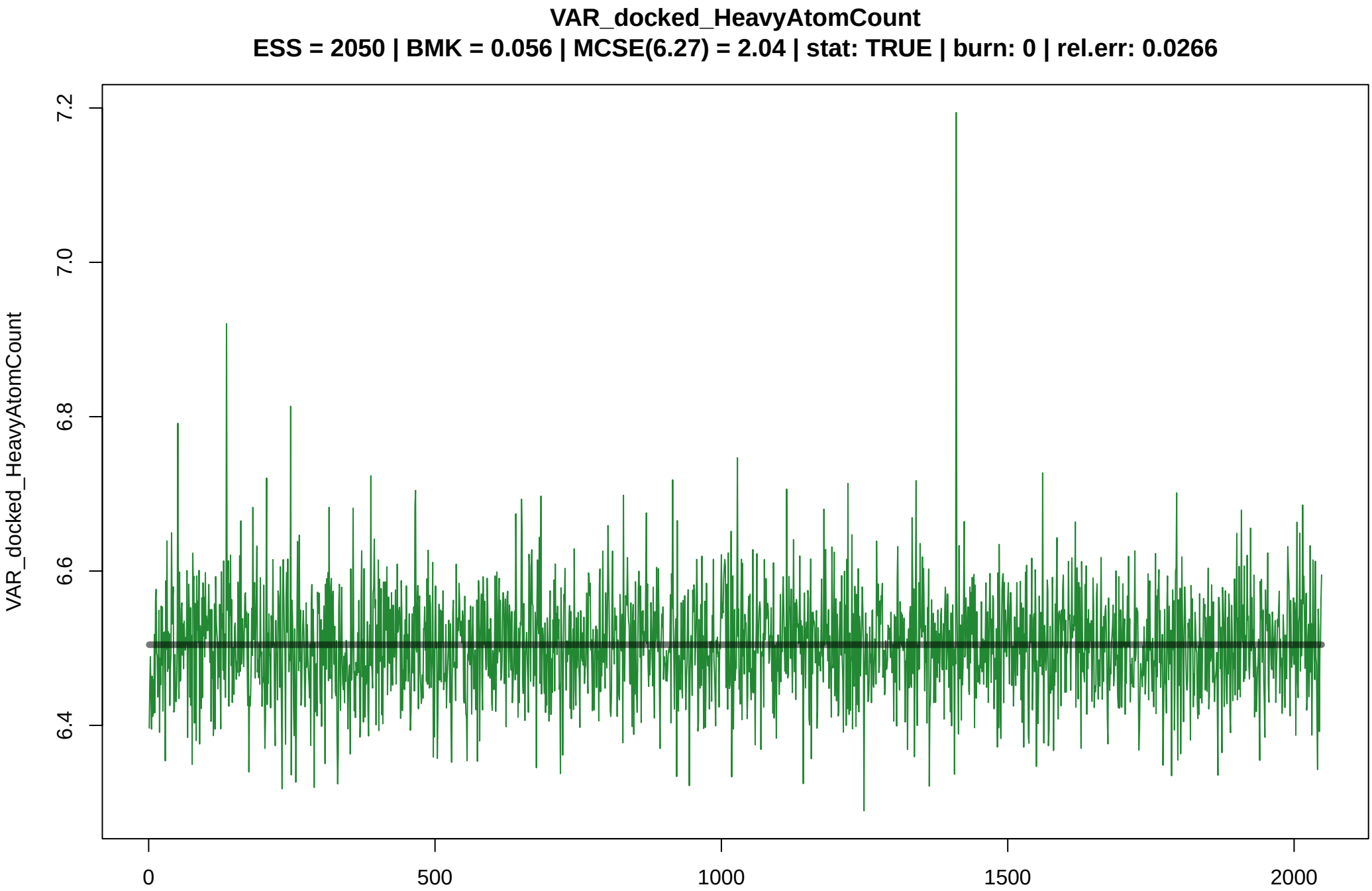

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 0.473
MEAN_mcs_NumHeteroAtoms
4.8
4.6
4.4
4.2
4.0
3.8
3.6
3.4
0
500
1000
1500
2000

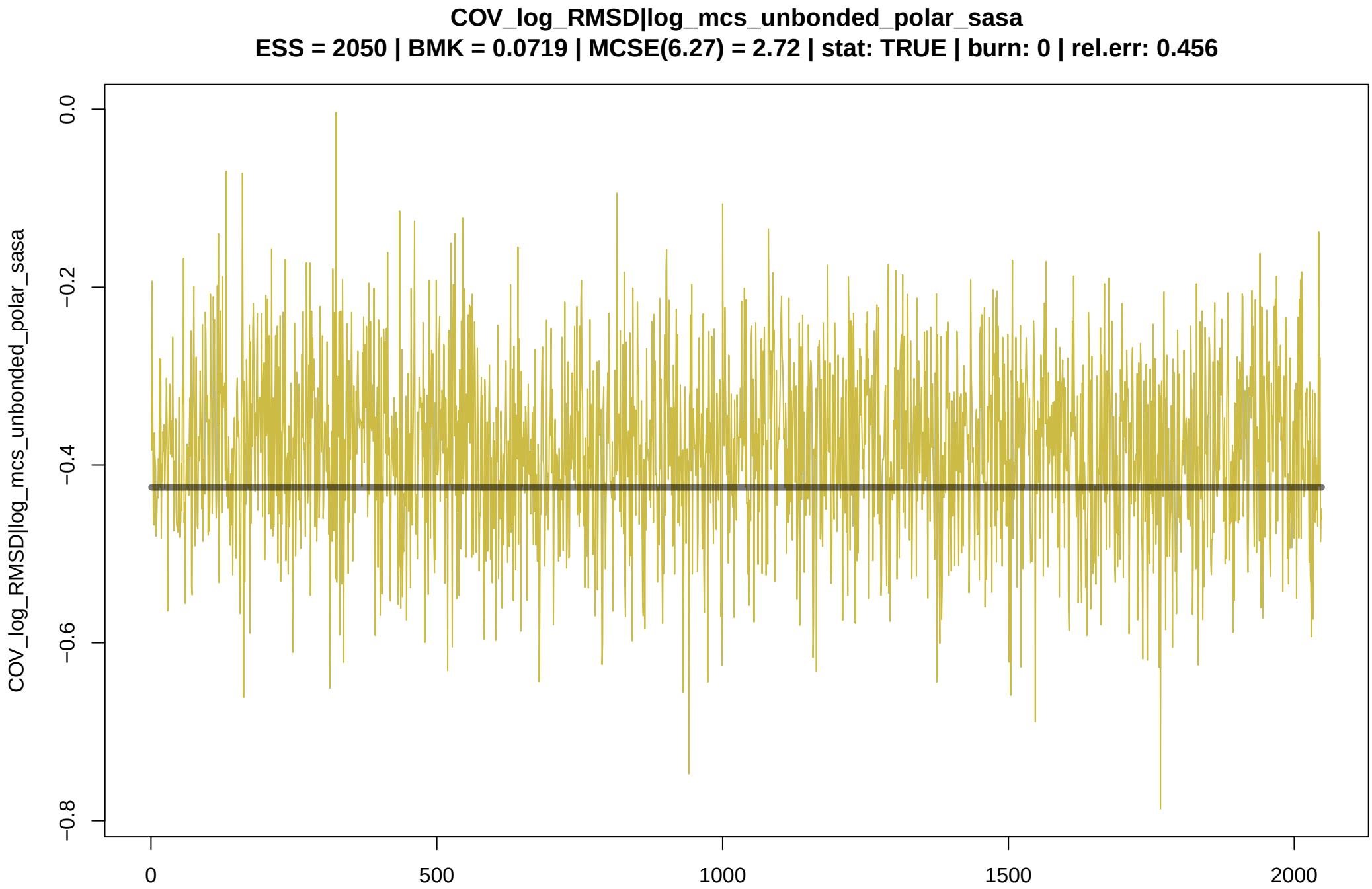

MEAN_docked_HeavyAtomCount
ESS = 1840 | BMK = 0.0317 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | rel.err: 0.485
MEAN_docked_HeavyAtomCount
32
34
36
38
40
0
500
1000
1500
2000

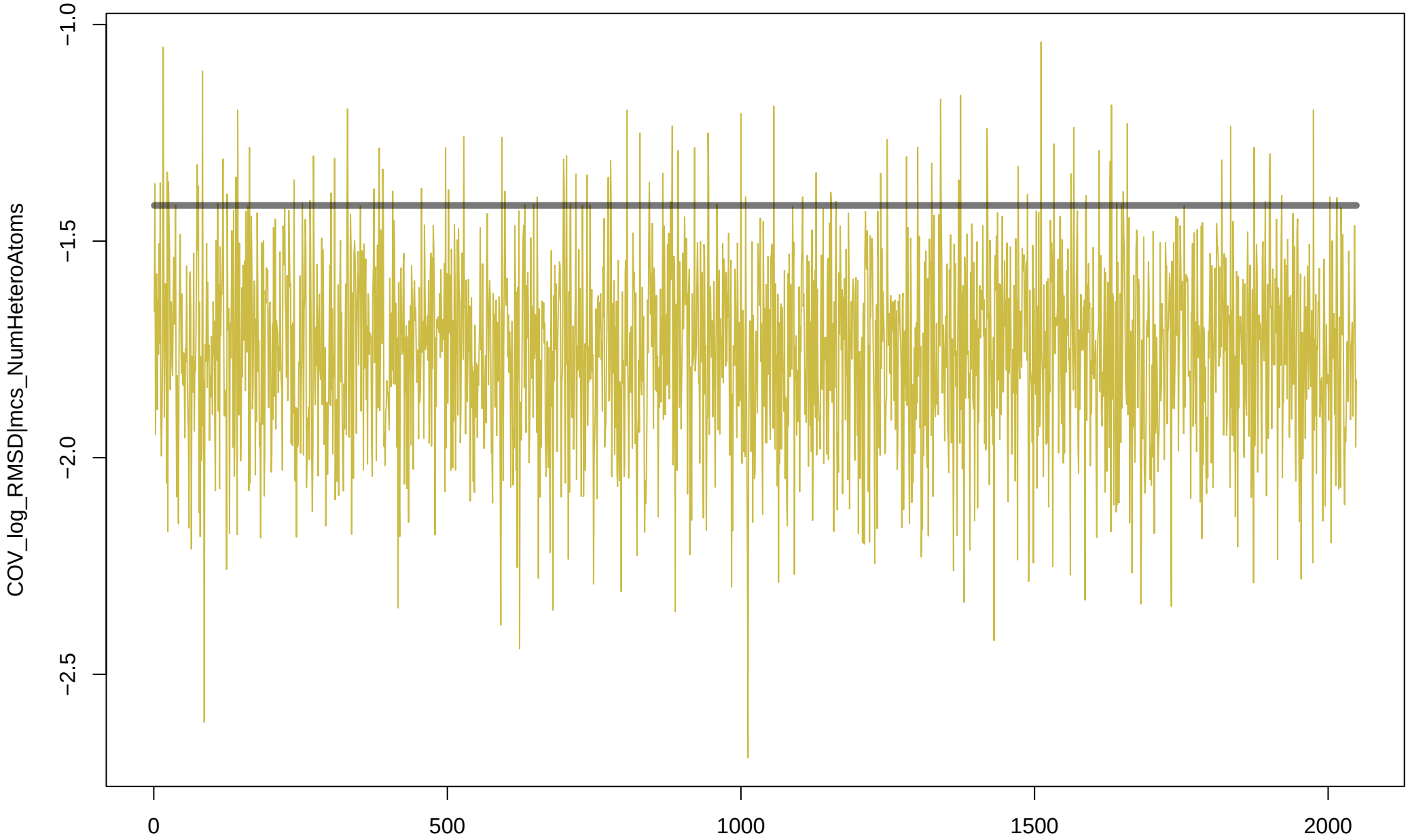

VAR_log_RMSD
ESS = 2050 | BMK = 0.0544 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: 2.26
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000

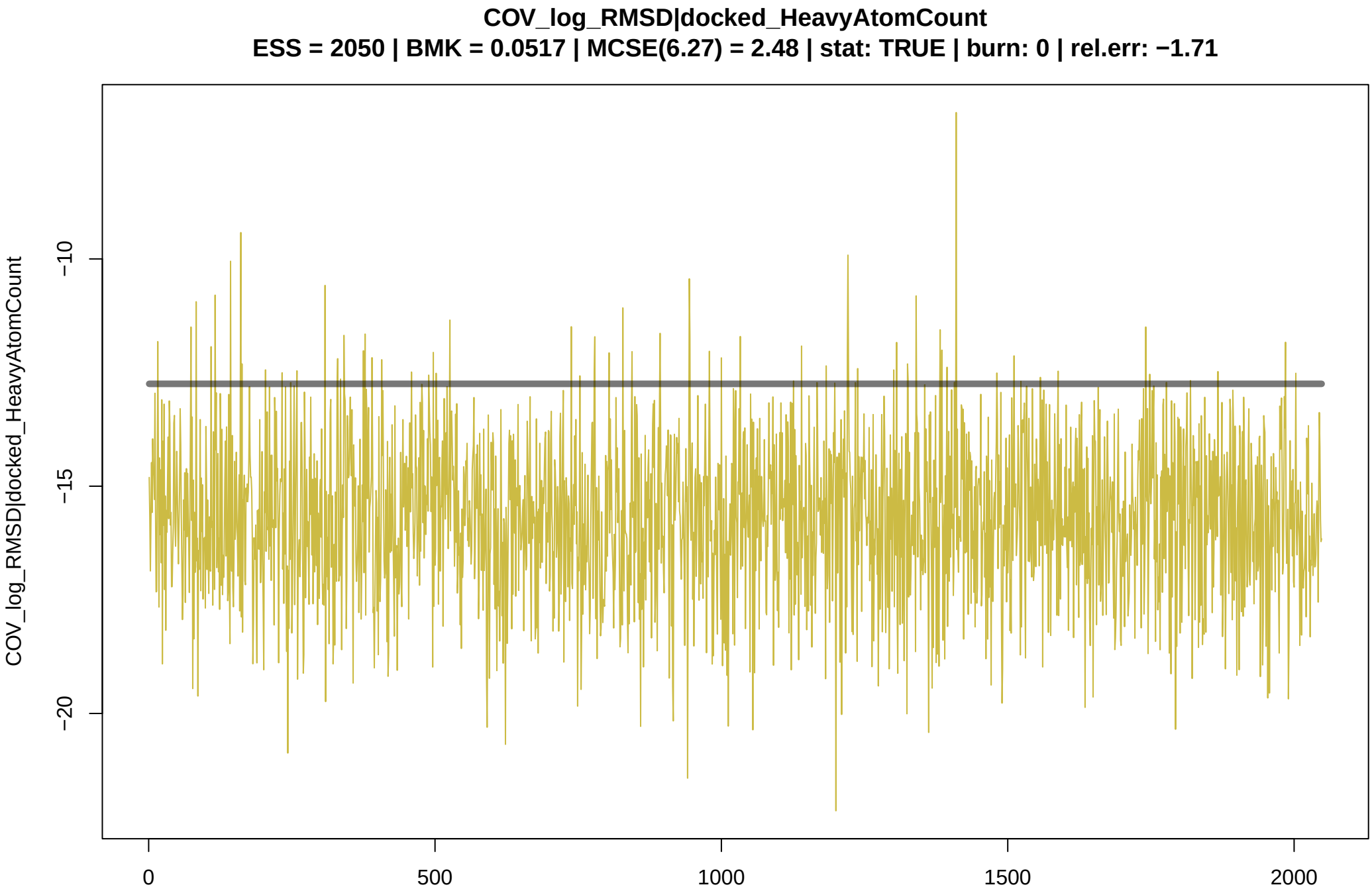

VAR_log_mcs_unbonded_polar_sasa
ESS = 1920 | BMK = 0.0497 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: 1.35
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

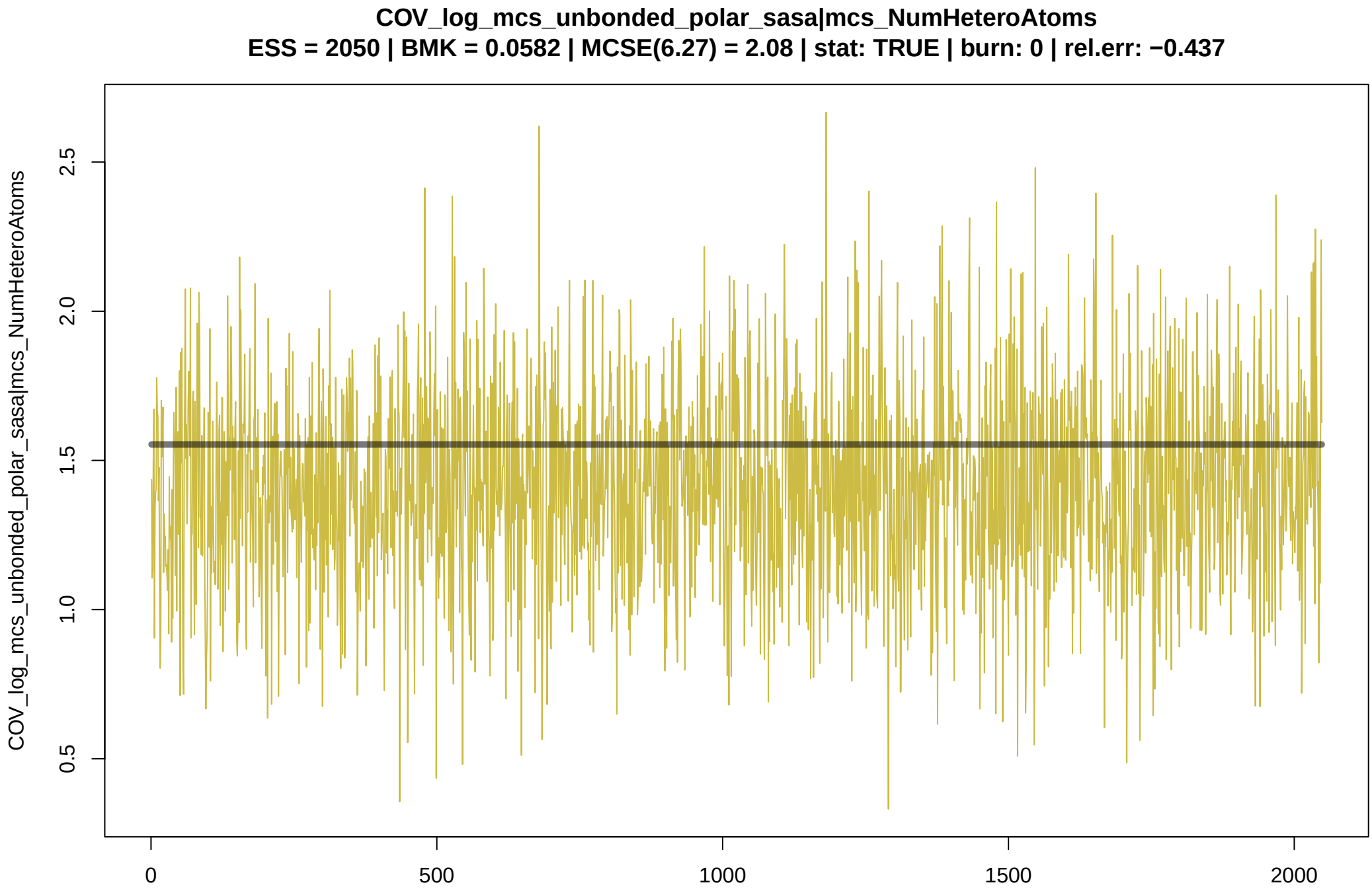

VAR_mcs_NumHeteroAtoms
ESS = 887 | BMK = 0.057 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0 | rel.err: 0.432
VAR_mcs_NumHeteroAtoms
2.2
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000

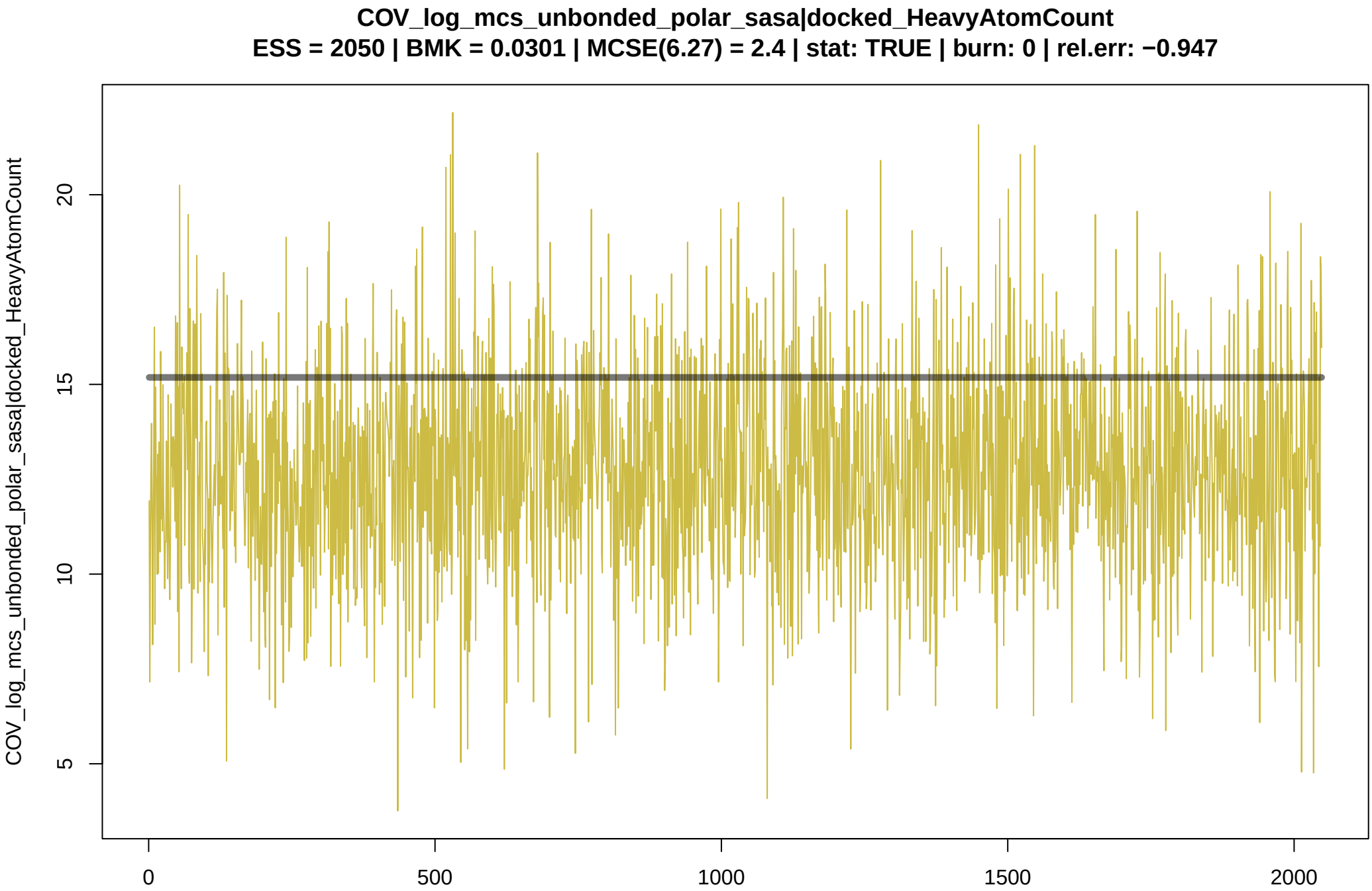

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.056 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: 0.0266
VAR_docked_HeavyAtomCount
7.2
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

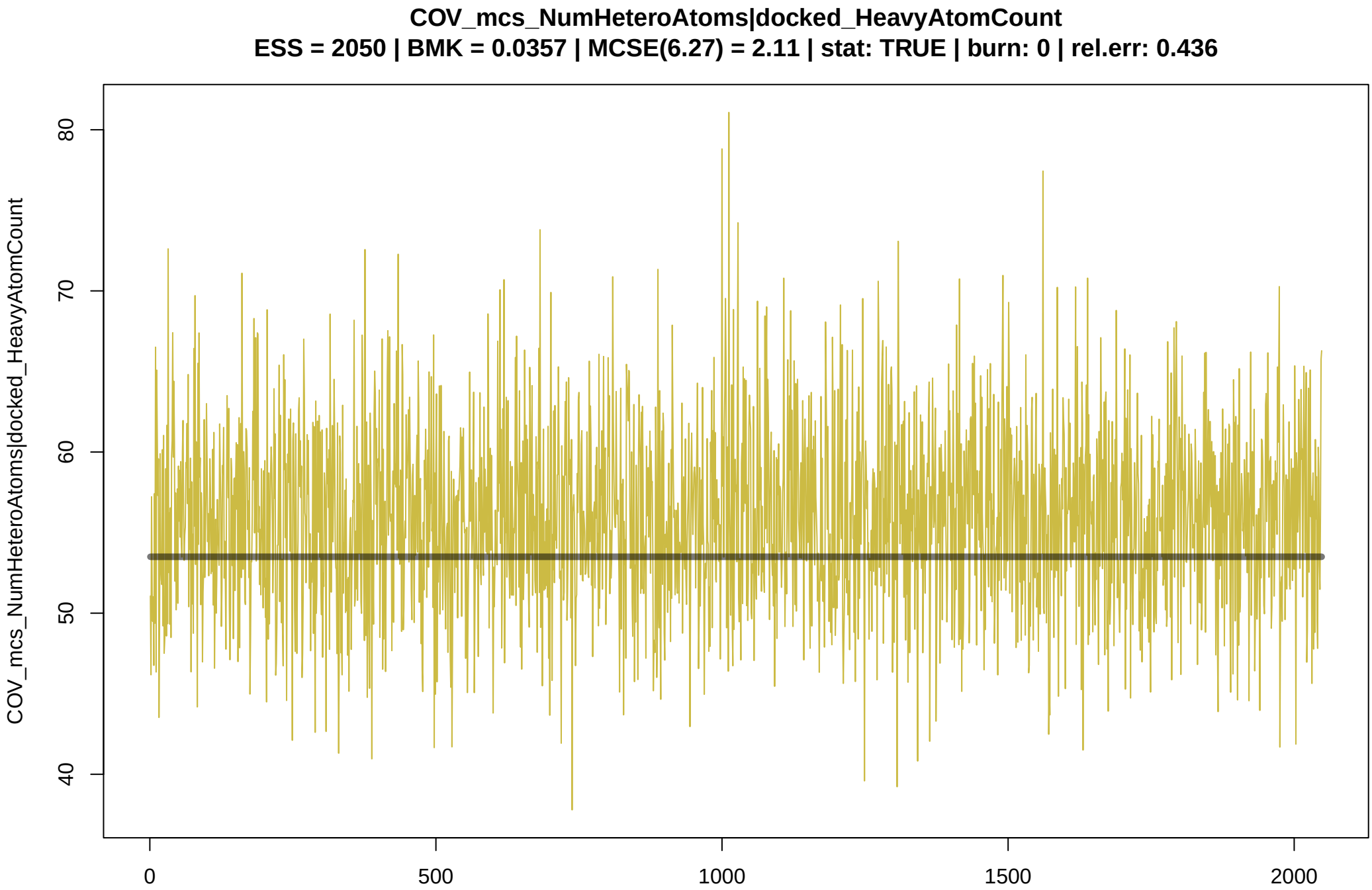

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0719 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 0.456
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0 | rel.err: −1.57
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 = 0.0517 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0 | rel.err: −1.71
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0582 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: −0.437
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 = 0.0301 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: −0.947
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 = 0.0357 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: 0.436
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000