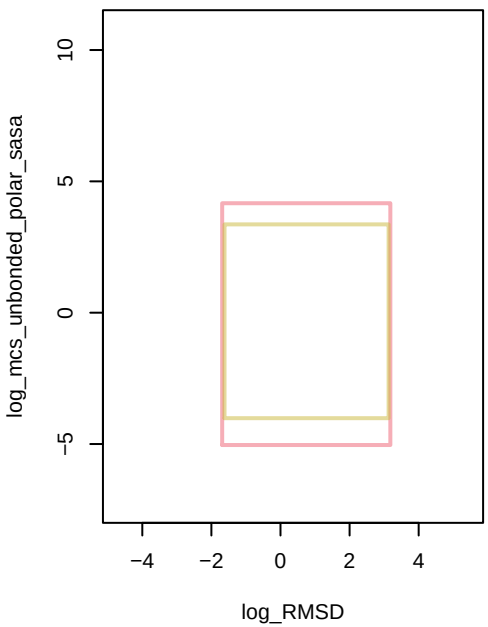
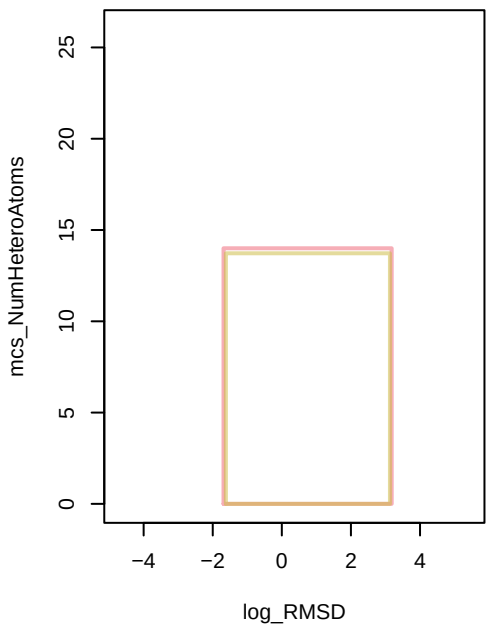
−− STATS maxD −−
min ESS = 31.6258389619106
max BMK = 0.14977917185479
max MCSE = 9.92980505063955
all stationary: FALSE
burn: 0
max rel.err.: 2.12113067058305

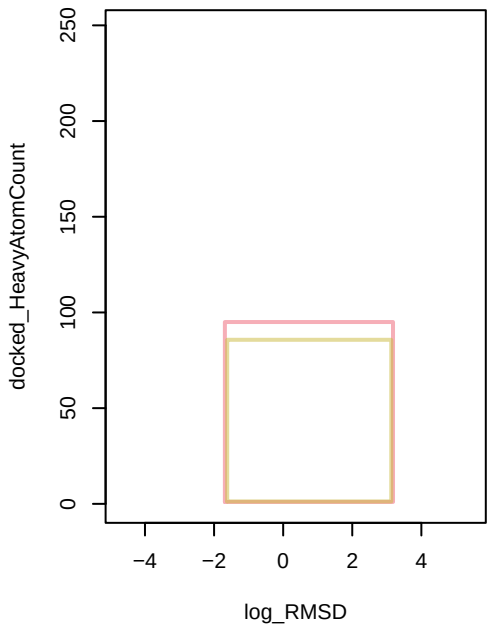
−− STATS 2D −−
min ESS = 1534.61864333729
max BMK = 0.056940229561376 1
max MCSE = 2.63130318891389
all stationary: TRUE
burn: 0
max rel.err.: 1.8249871968001

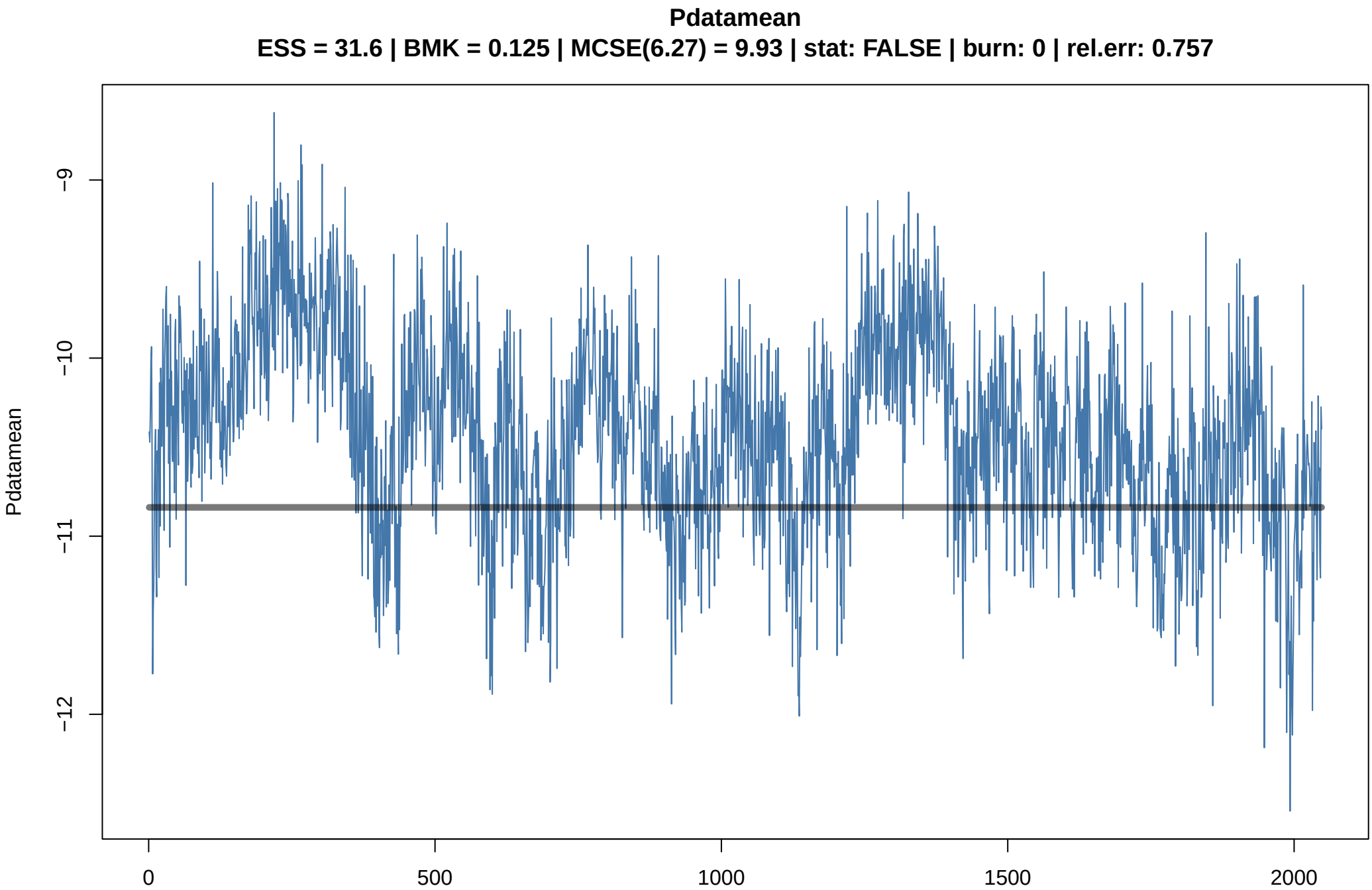
−− STATS 1D −−
min ESS = 1335.62810095053
max BMK = 0.062130702514807 4
max MCSE = 2.74579559237281
all stationary: TRUE
burn: 0
max rel.err.: 2.2971308194226

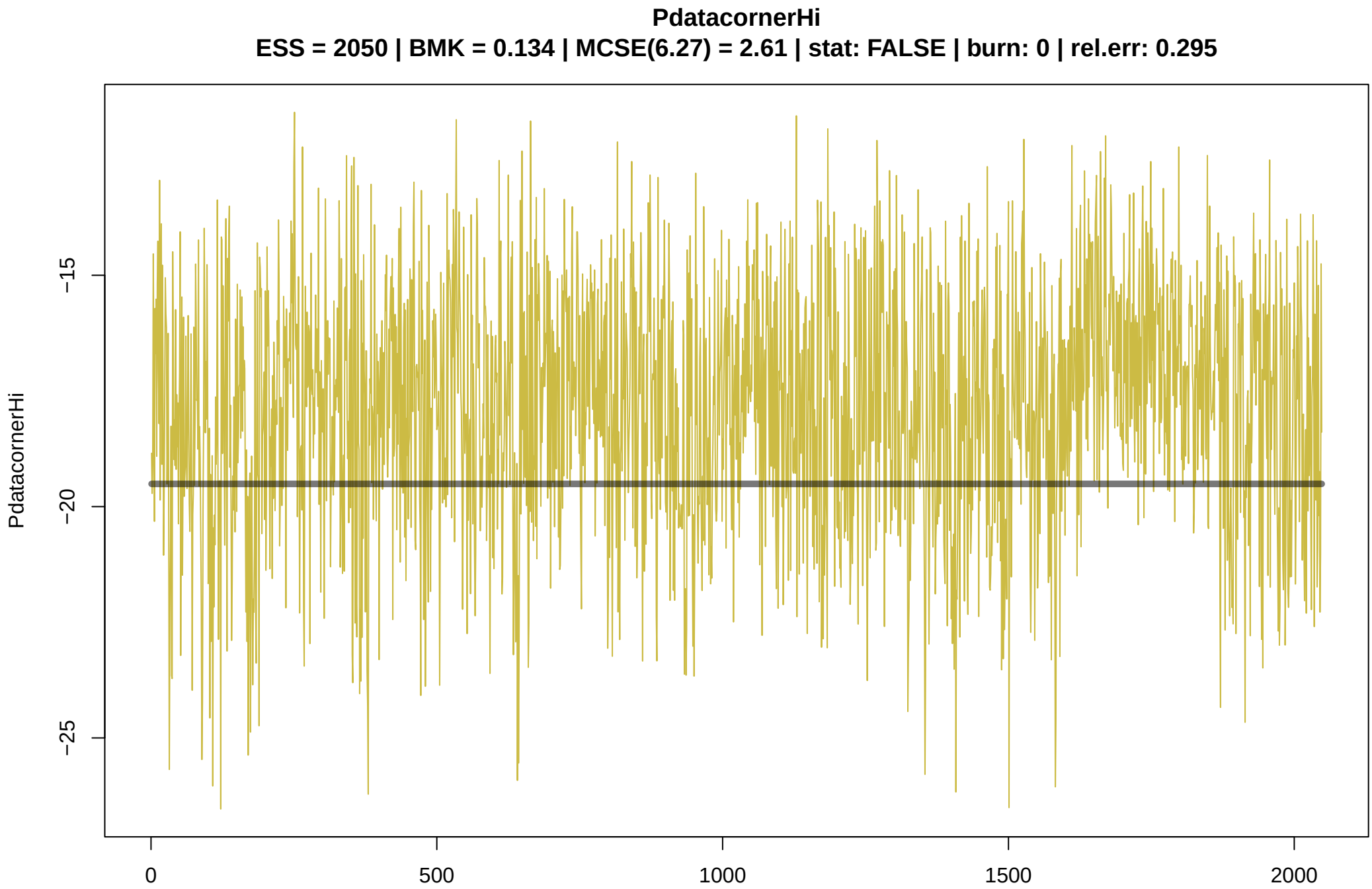
Occupied clusters: 9 of 16

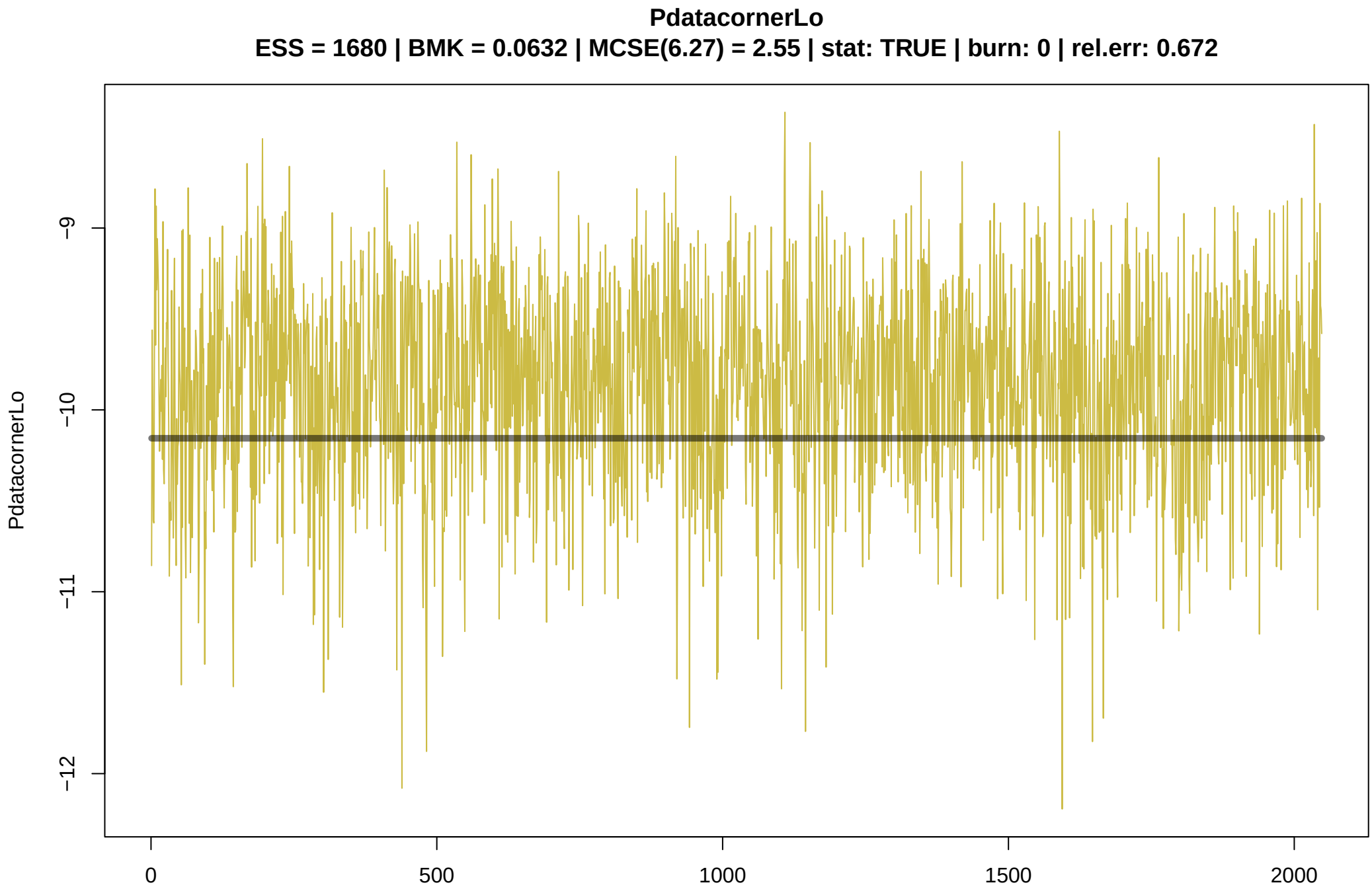

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
log_RMSD

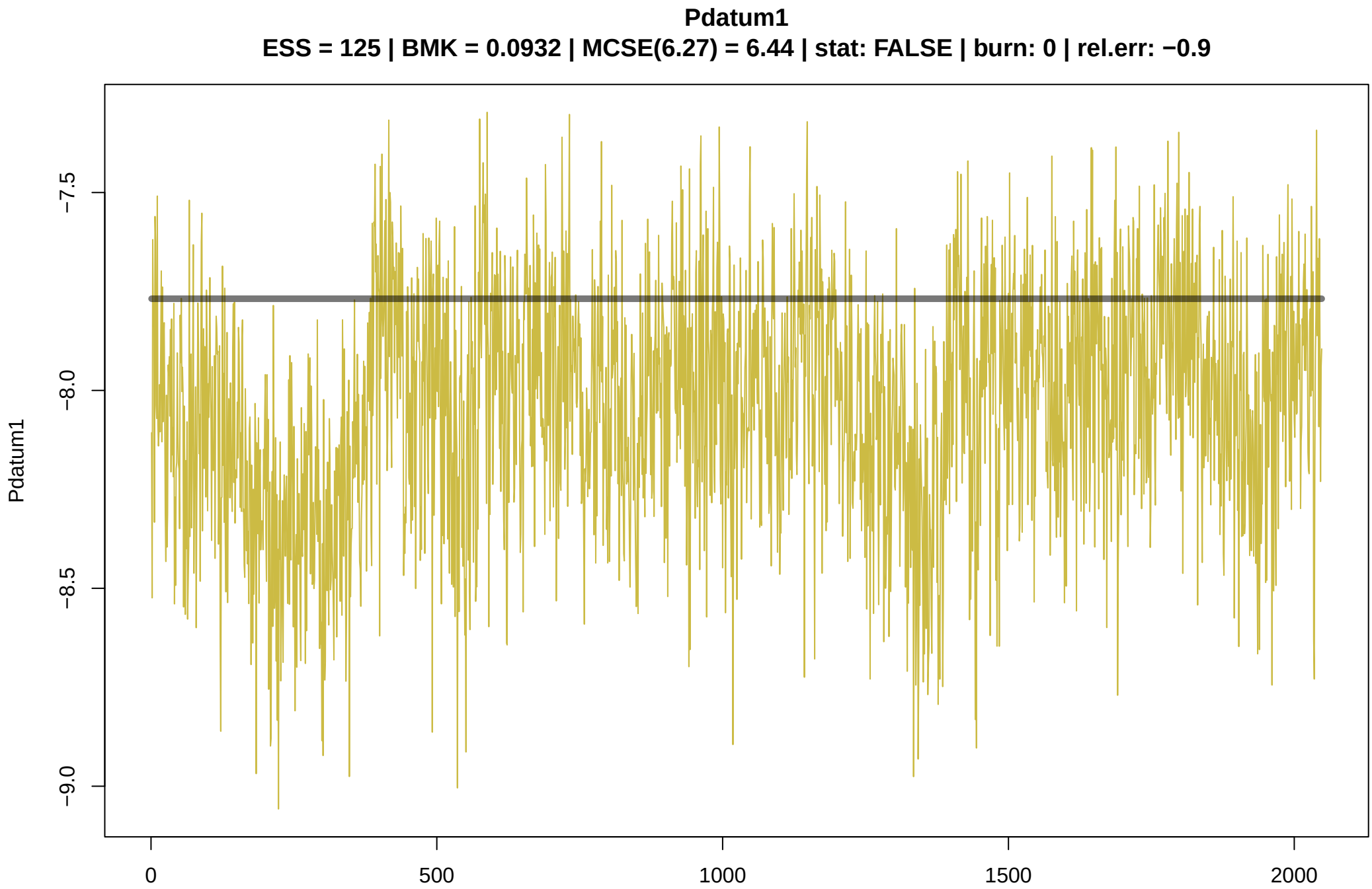

mcs_NumHeteroAtoms
25
20
15
10
5
0
−4
−2
0
2
4
log_RMSD

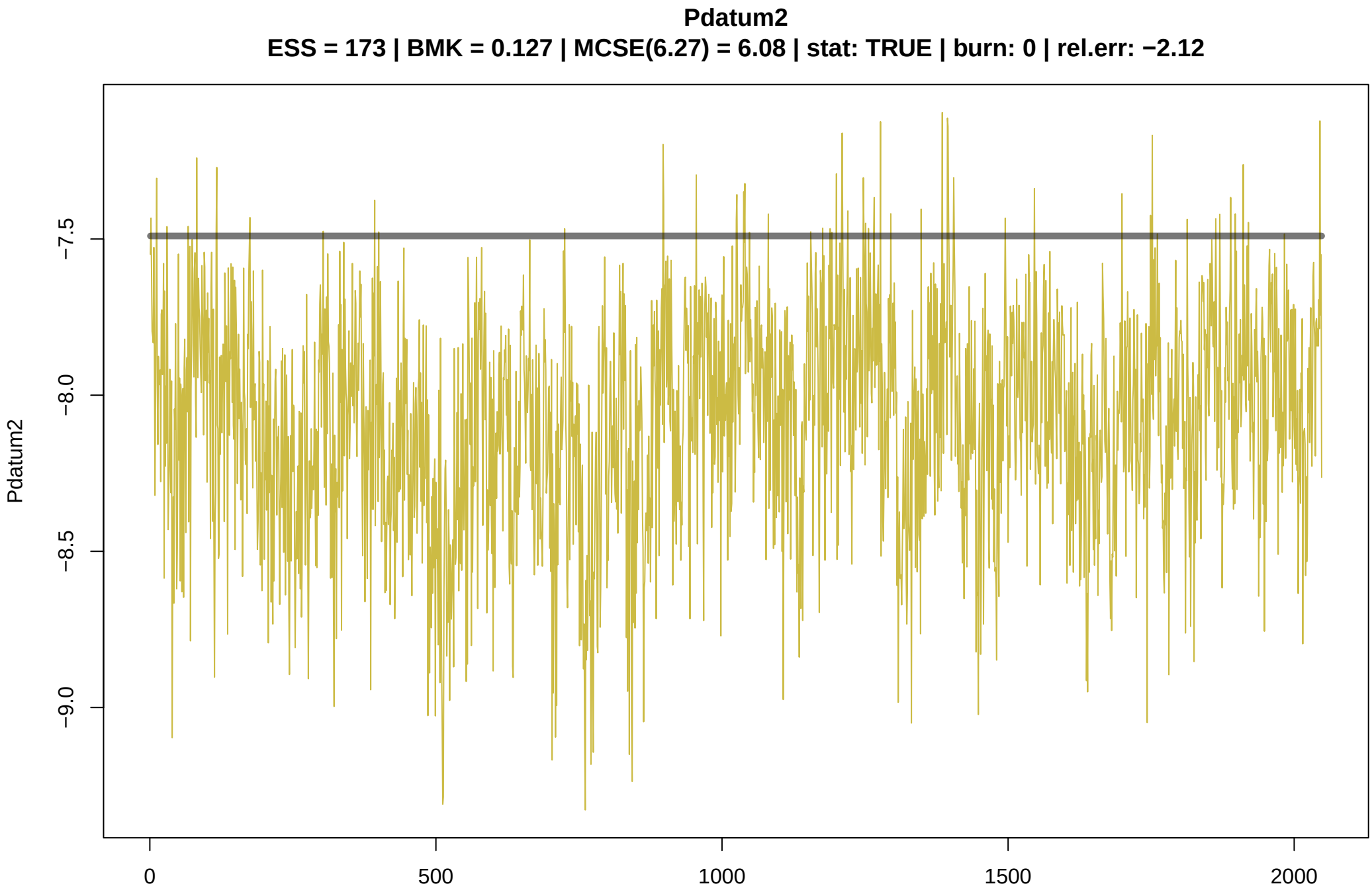

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
log_RMSD

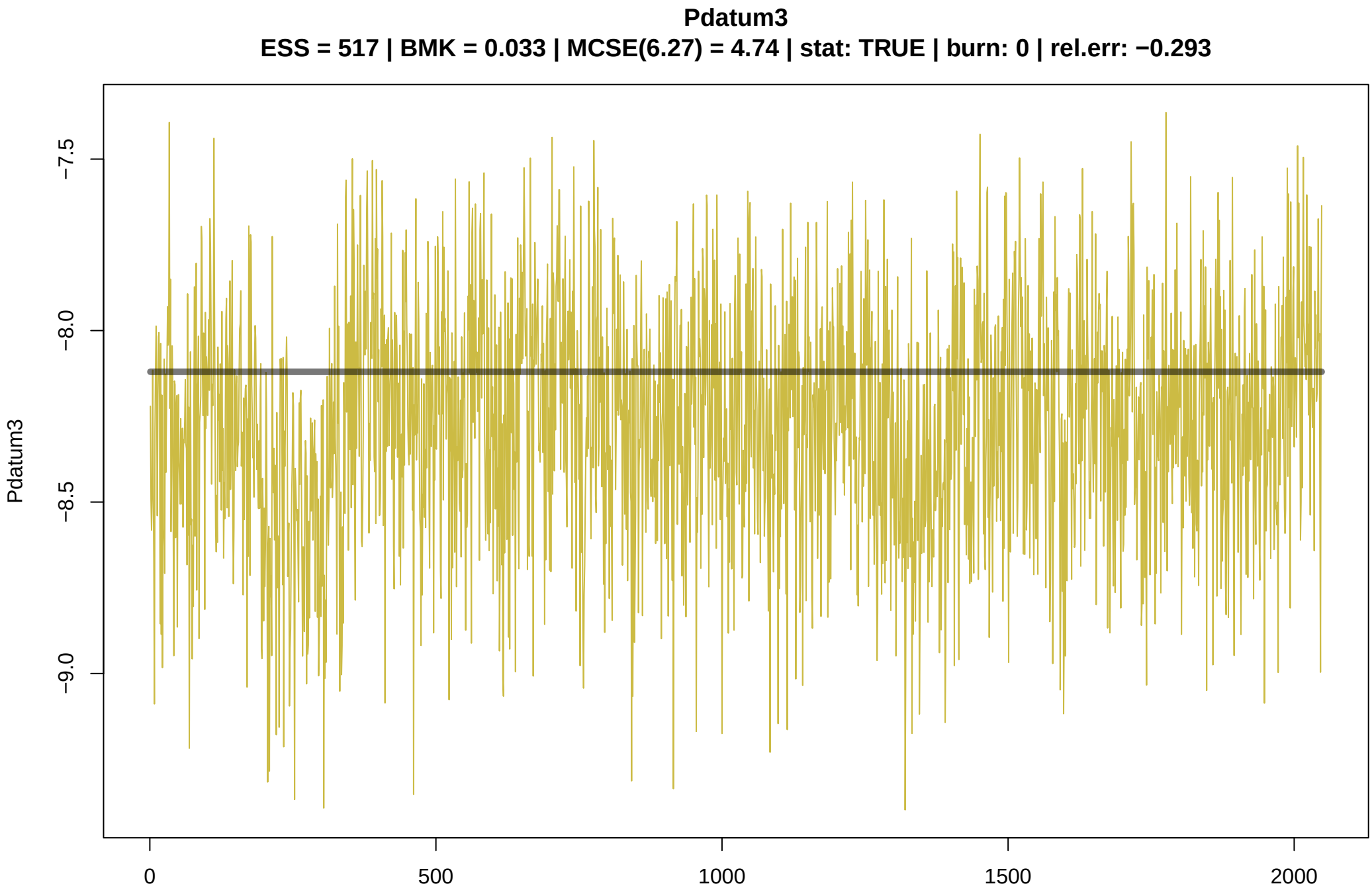

Pdatamean
ESS = 31.6 | BMK = 0.125 | MCSE(6.27) = 9.93 | stat: FALSE | burn: 0 | rel.err: 0.757
Pdatamean
−9
−10
−11
−12
0
500
1000
1500
2000

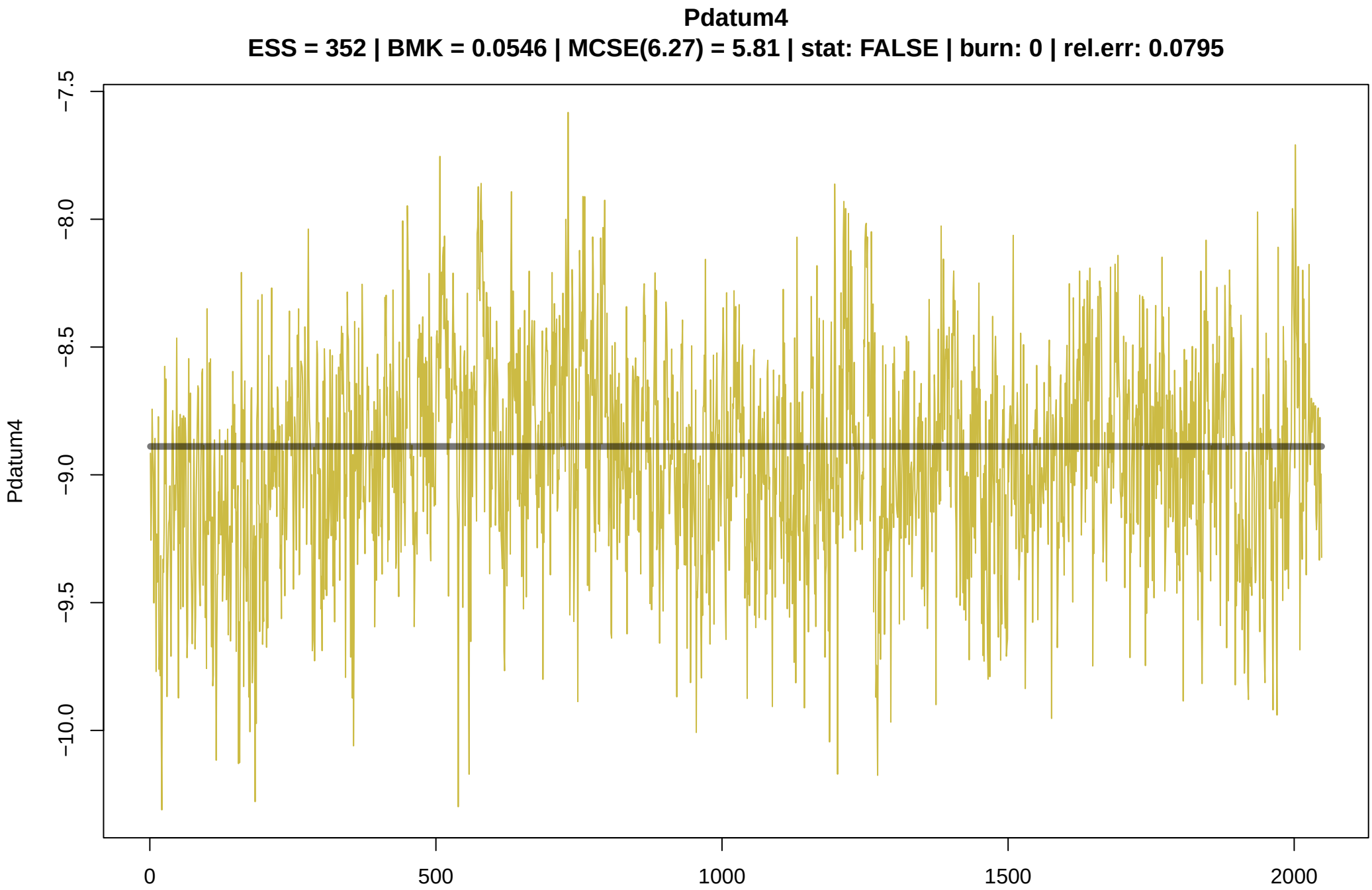

PdatacornerHi
ESS = 2050 | BMK = 0.134 | MCSE(6.27) = 2.61 | stat: FALSE | burn: 0 | rel.err: 0.295
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

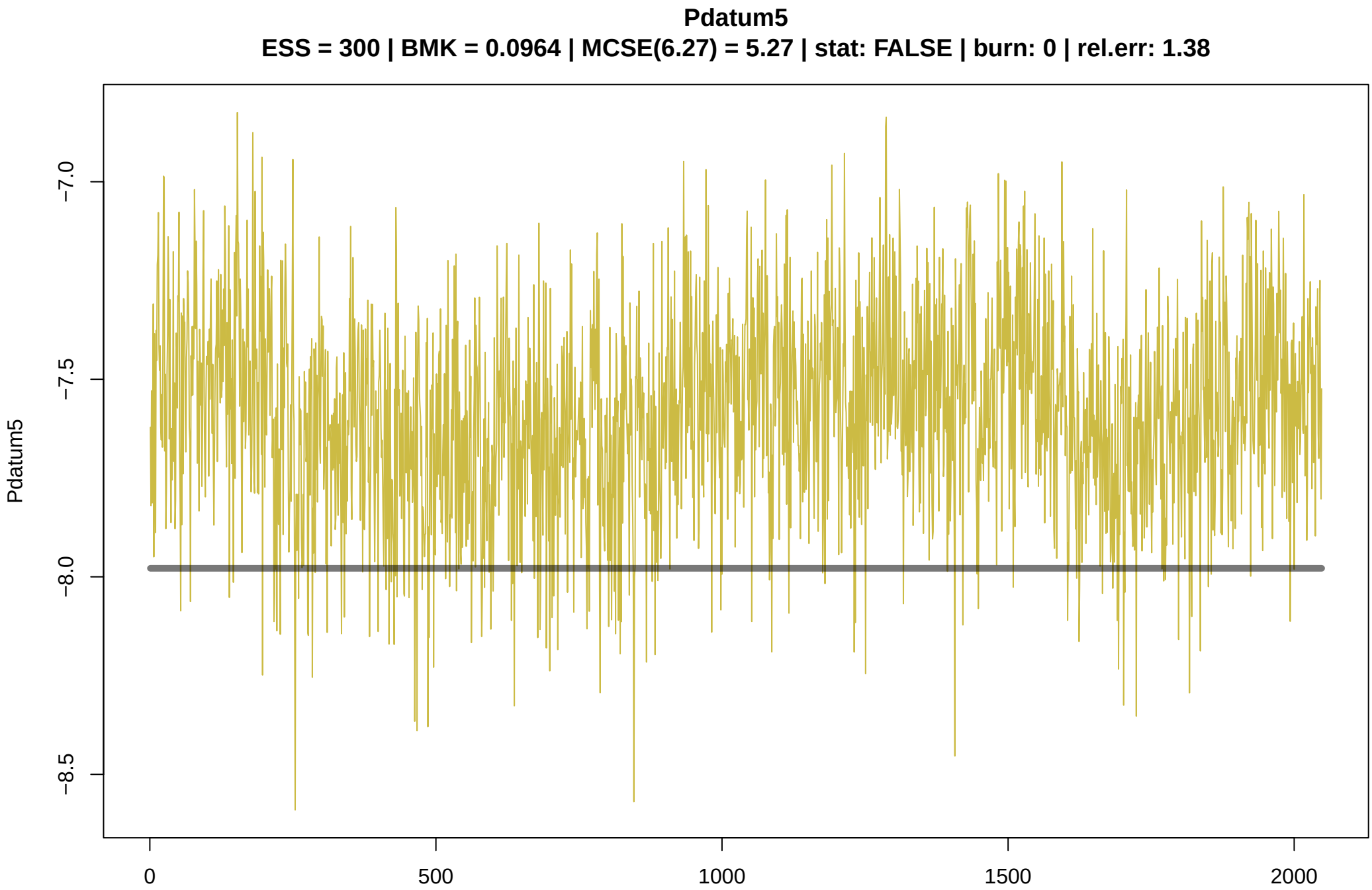

PdatacornerLo
ESS = 1680 | BMK = 0.0632 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 0.672
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

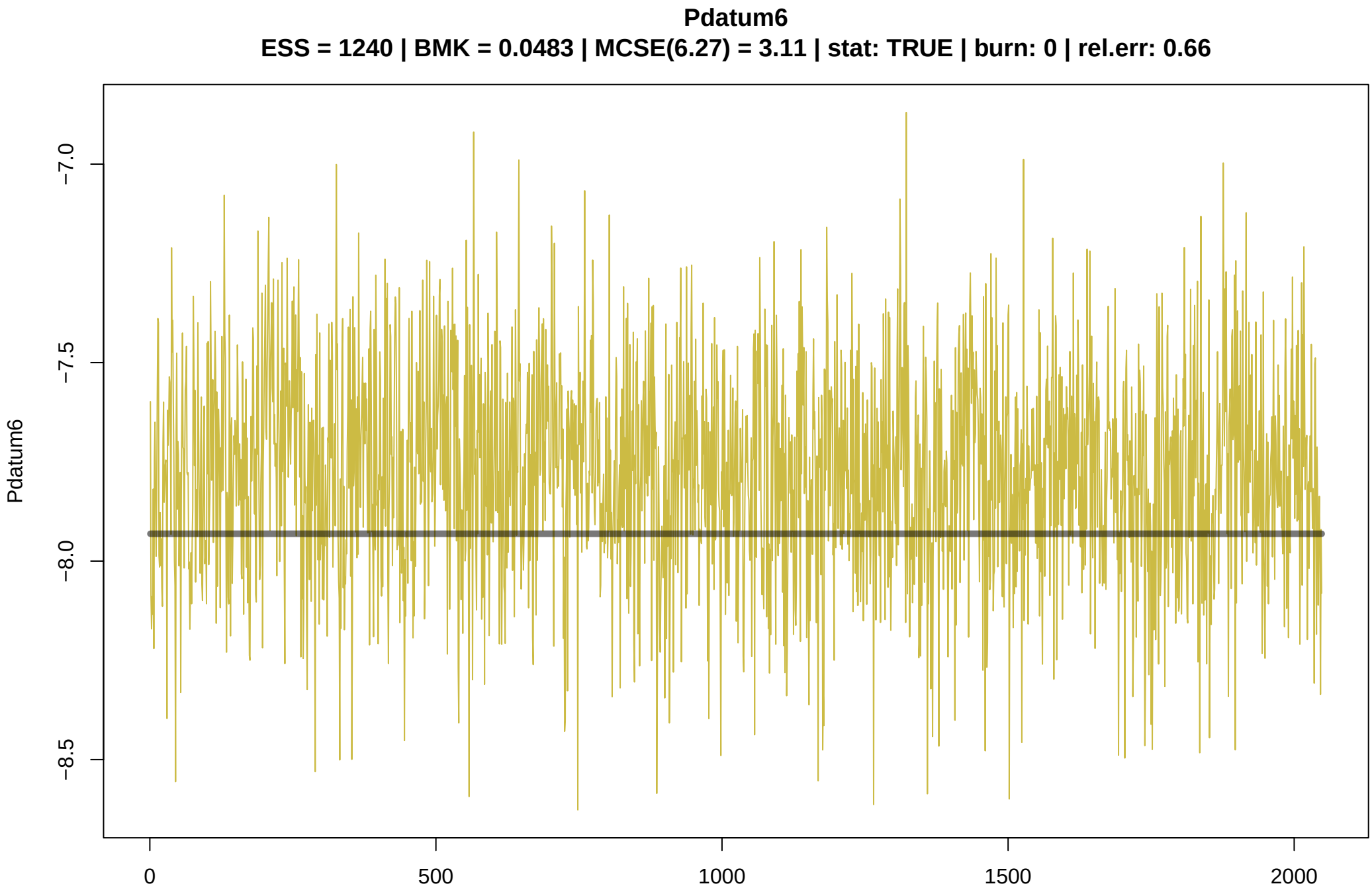

Pdatum1
ESS = 125 | BMK = 0.0932 | MCSE(6.27) = 6.44 | stat: FALSE | burn: 0 | rel.err: −0.9
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

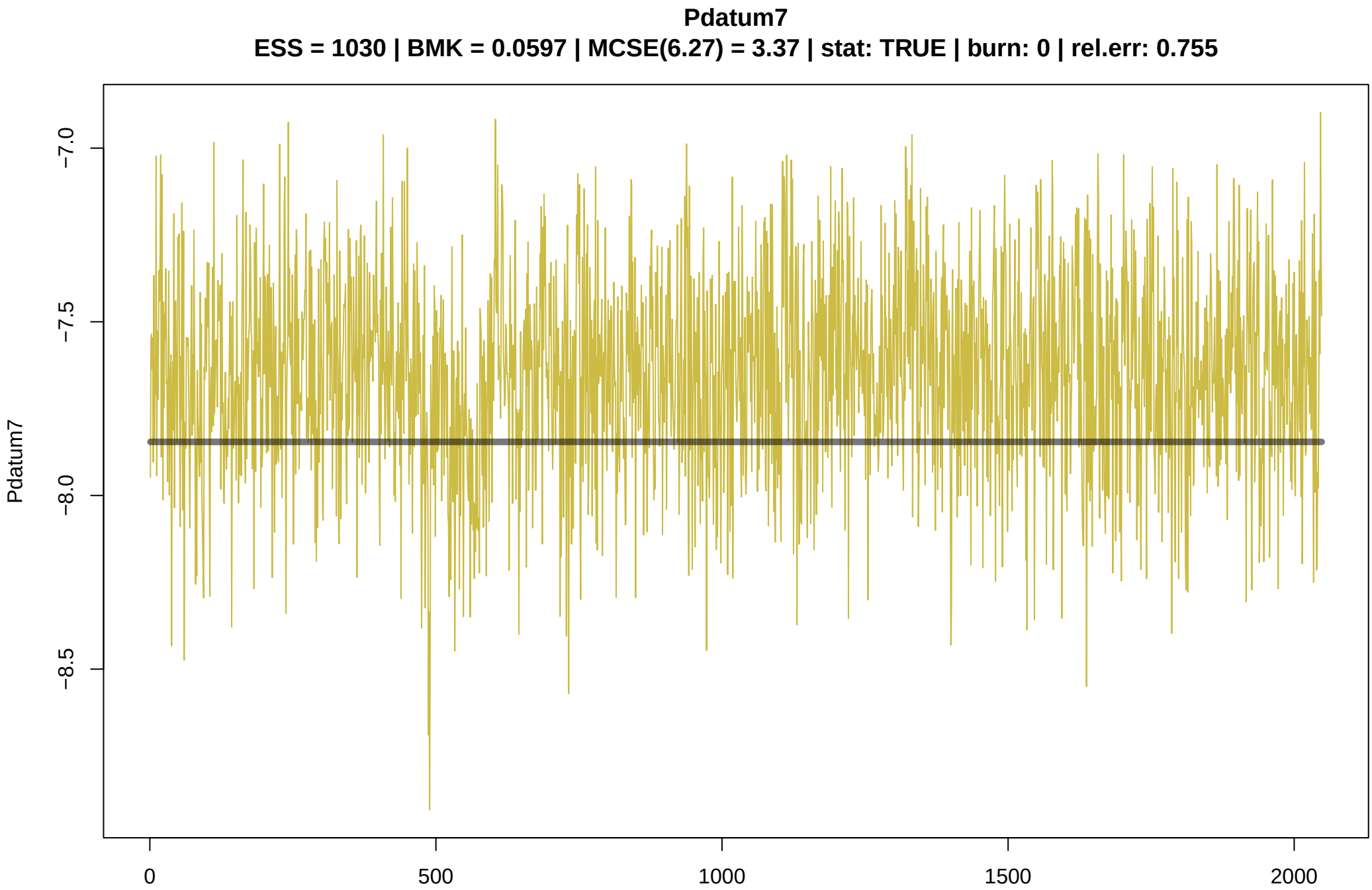

Pdatum2
ESS = 173 | BMK = 0.127 | MCSE(6.27) = 6.08 | stat: TRUE | burn: 0 | rel.err: −2.12
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

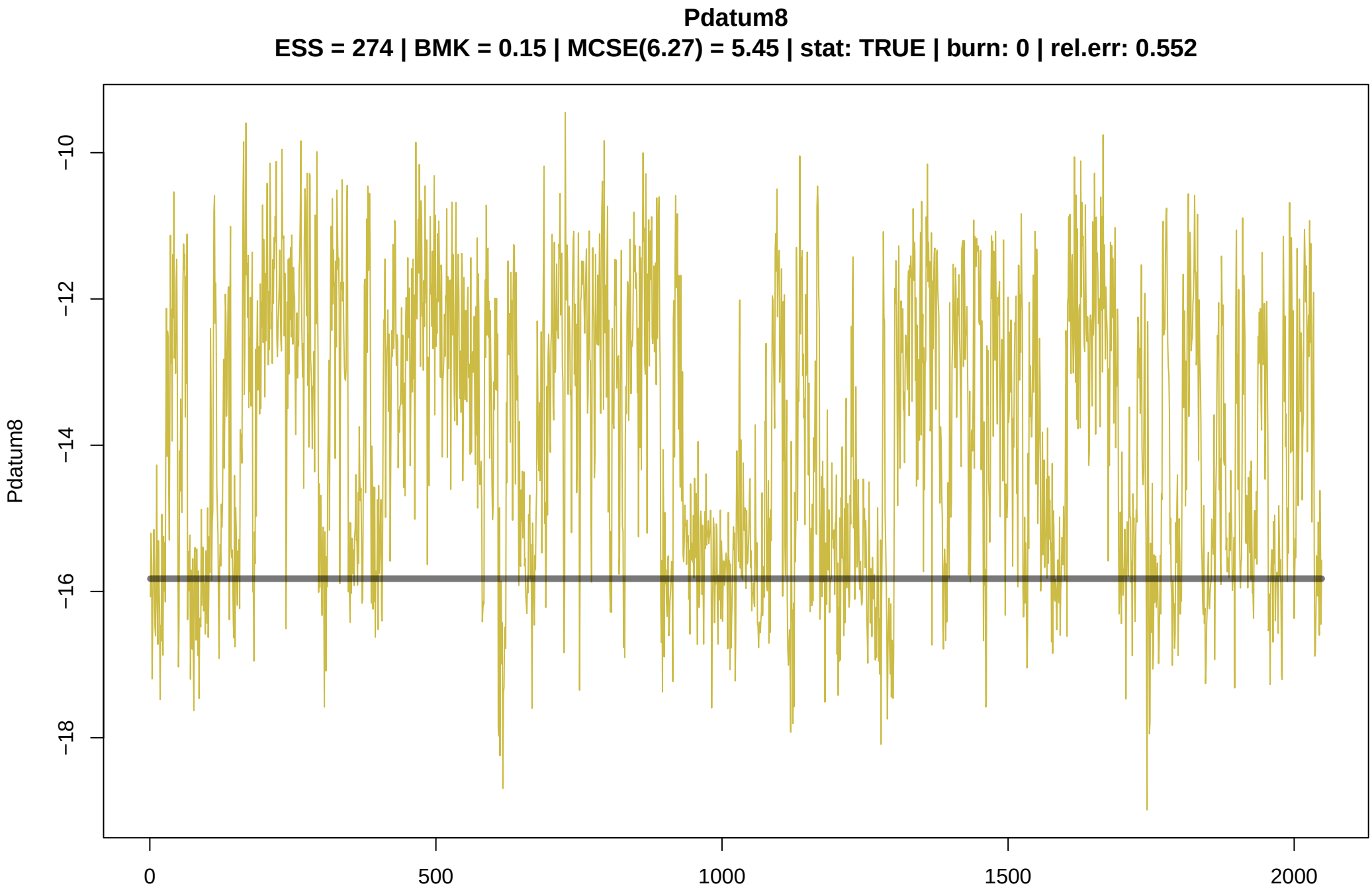

Pdatum3
ESS = 517 | BMK = 0.033 | MCSE(6.27) = 4.74 | stat: TRUE | burn: 0 | rel.err: −0.293
Pdatum3
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

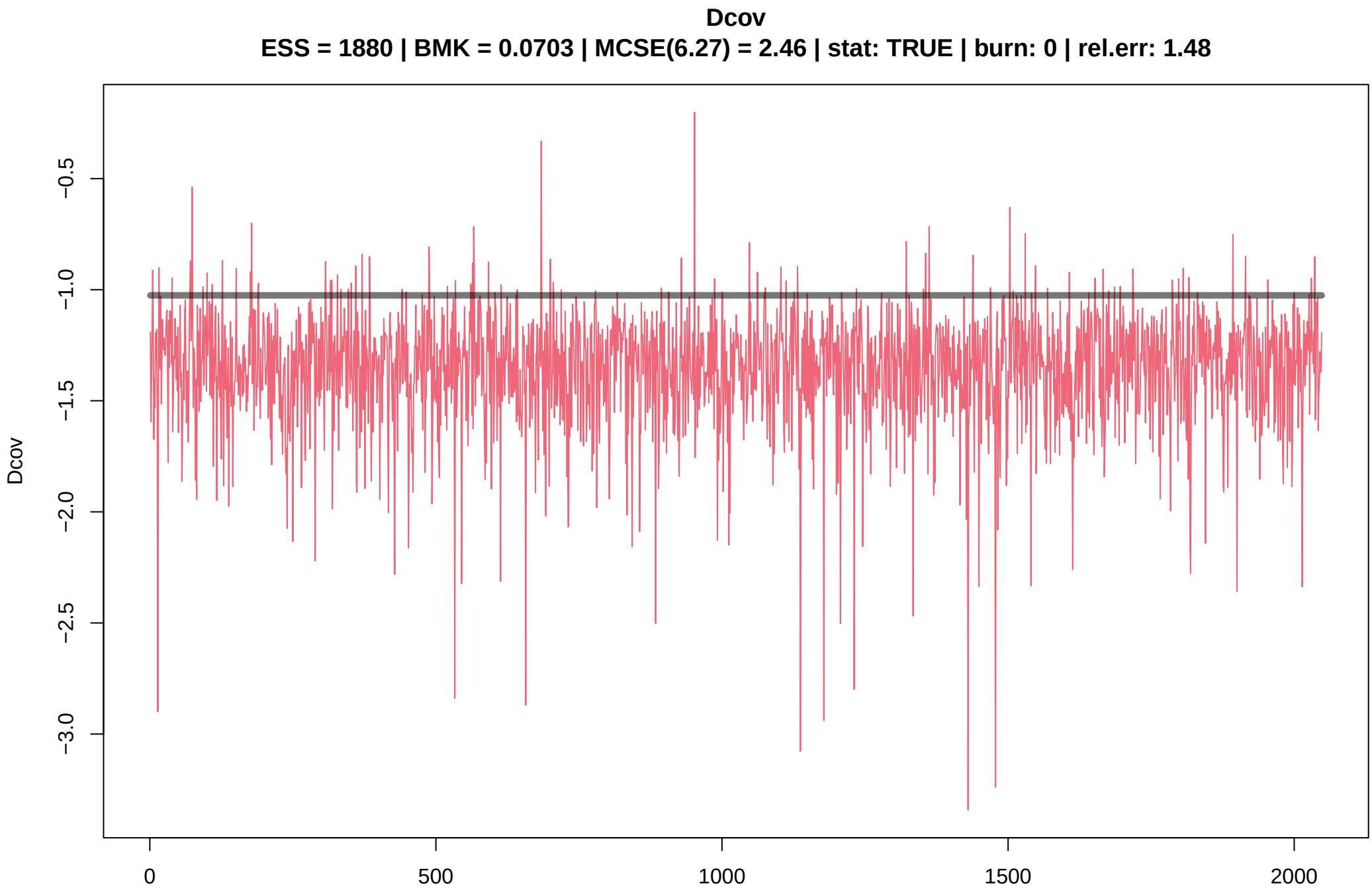

Pdatum4
ESS = 352 | BMK = 0.0546 | MCSE(6.27) = 5.81 | stat: FALSE | burn: 0 | rel.err: 0.0795
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

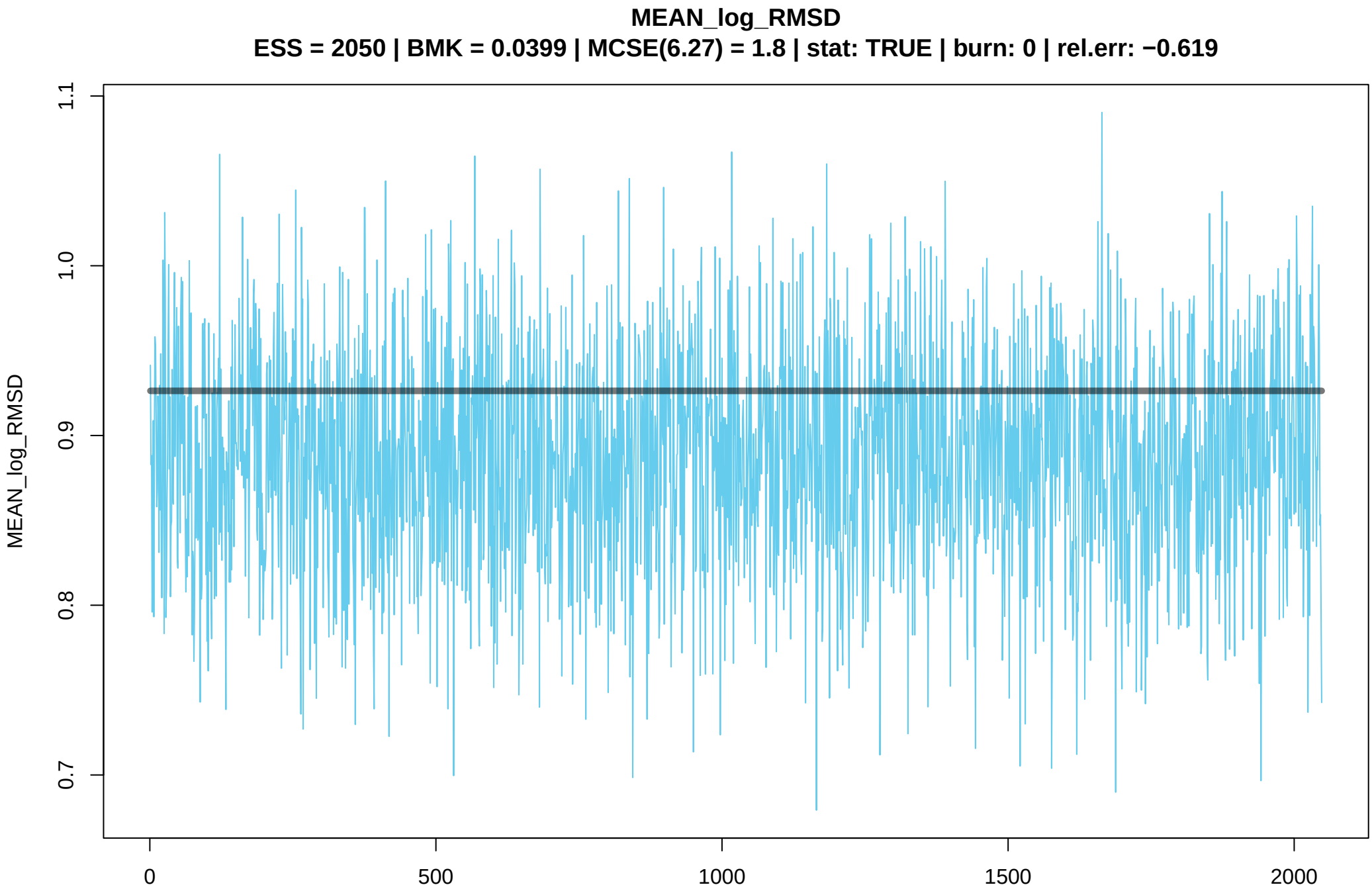

Pdatum5
ESS = 300 | BMK = 0.0964 | MCSE(6.27) = 5.27 | stat: FALSE | burn: 0 | rel.err: 1.38
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

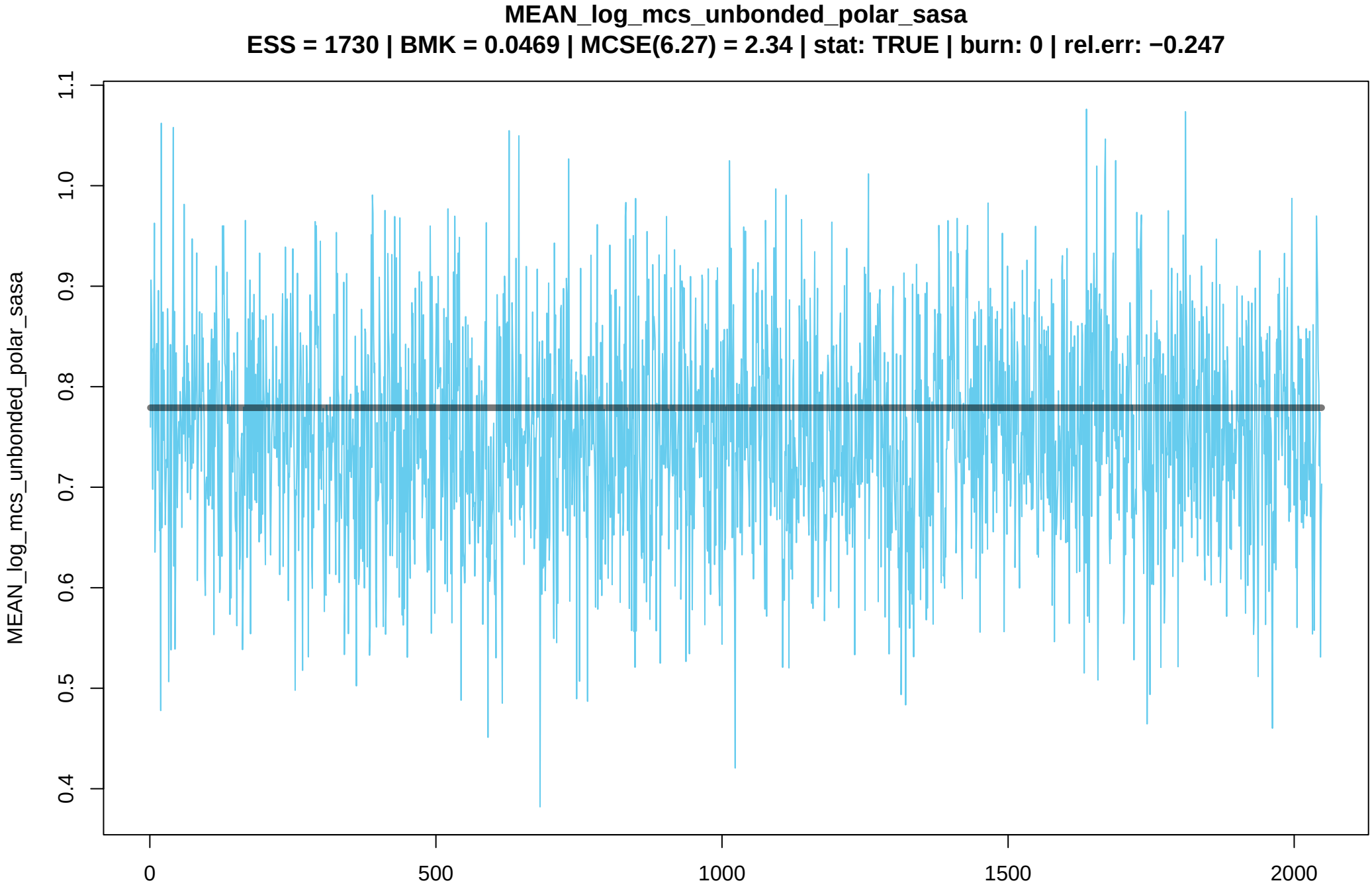

Pdatum6
ESS = 1240 | BMK = 0.0483 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: 0.66
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

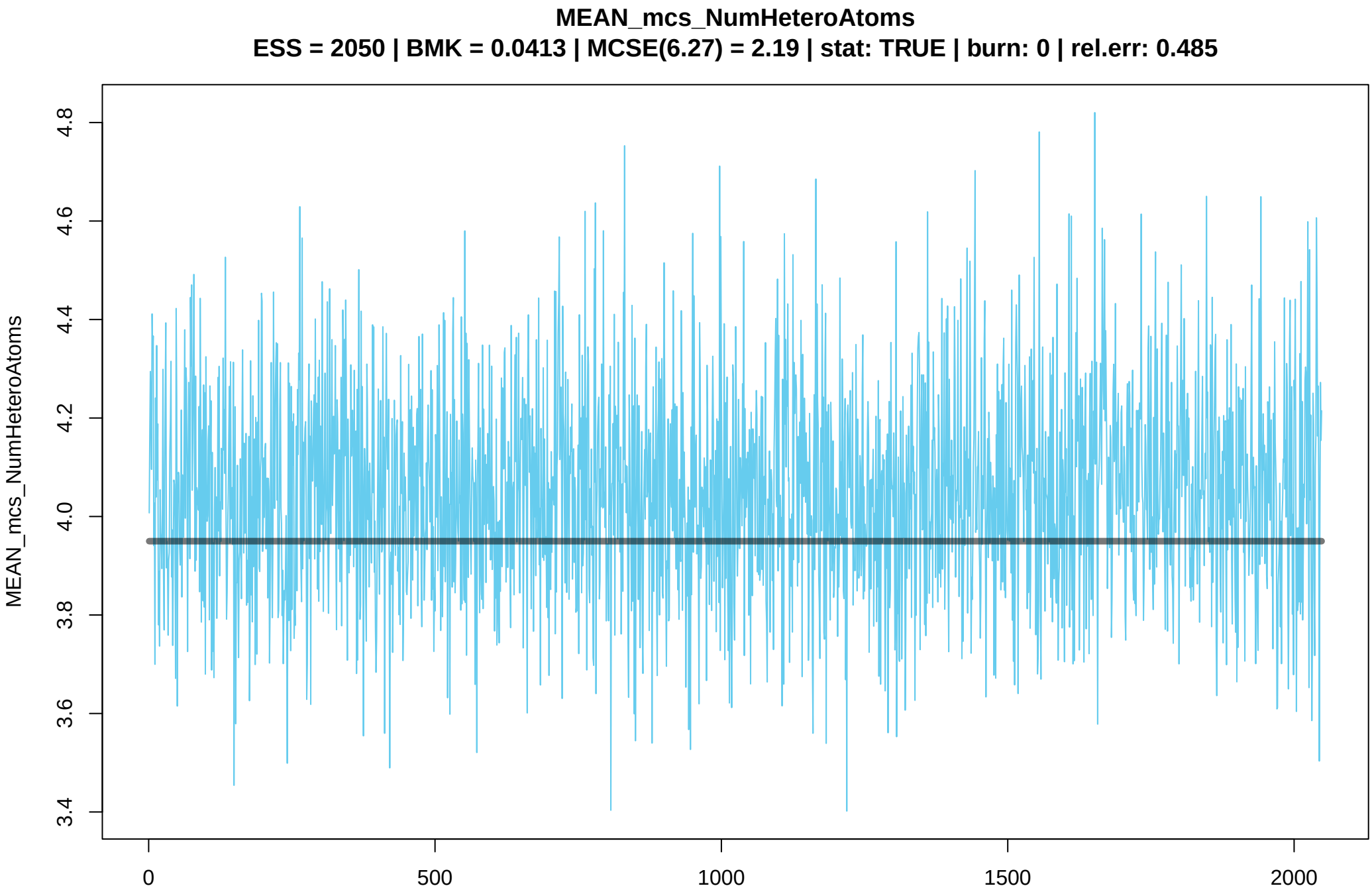

Pdatum7
ESS = 1030 | BMK = 0.0597 | MCSE(6.27) = 3.37 | stat: TRUE | burn: 0 | rel.err: 0.755
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

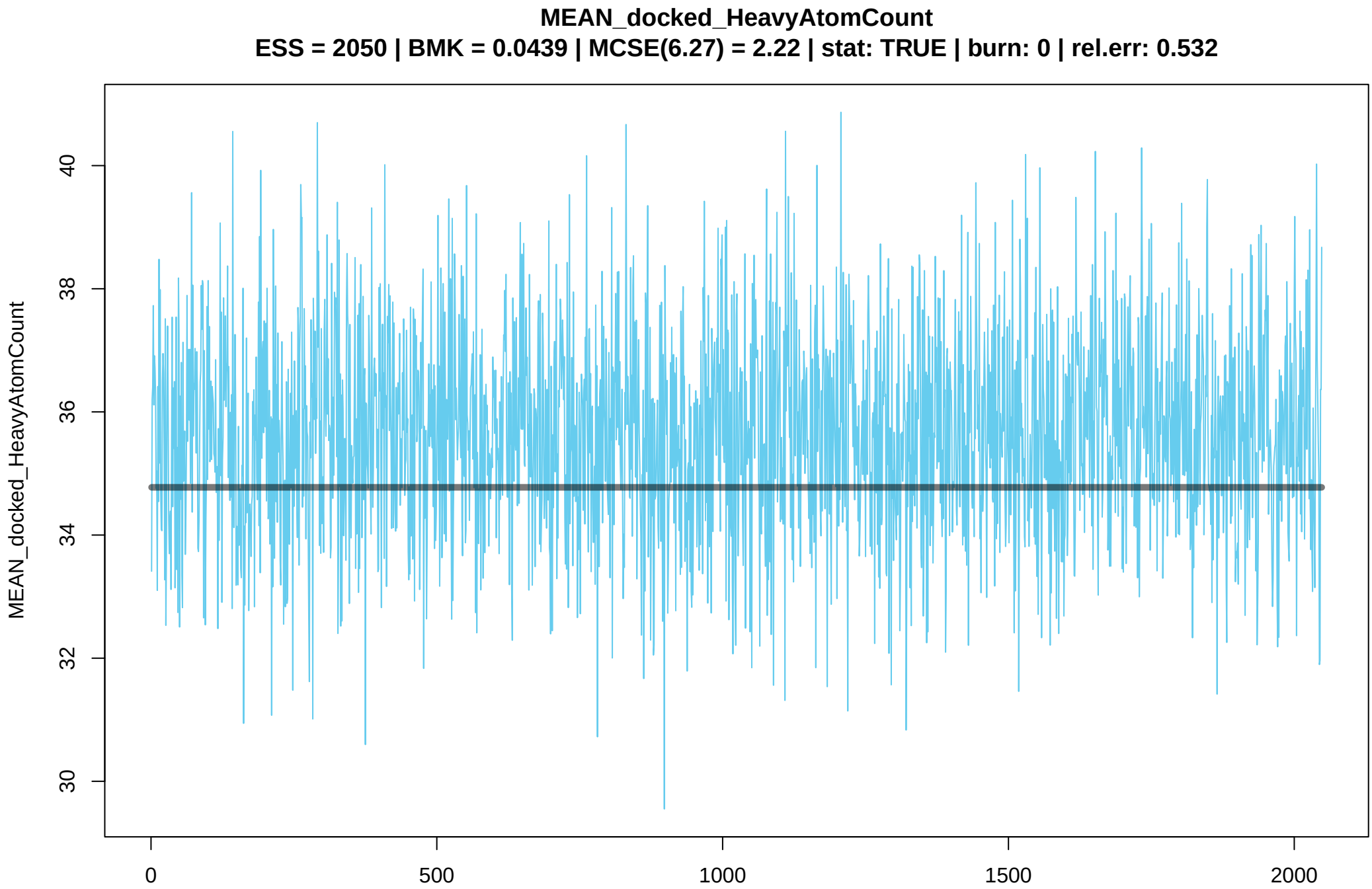

Pdatum8
ESS = 274 | BMK = 0.15 | MCSE(6.27) = 5.45 | stat: TRUE | burn: 0 | rel.err: 0.552
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

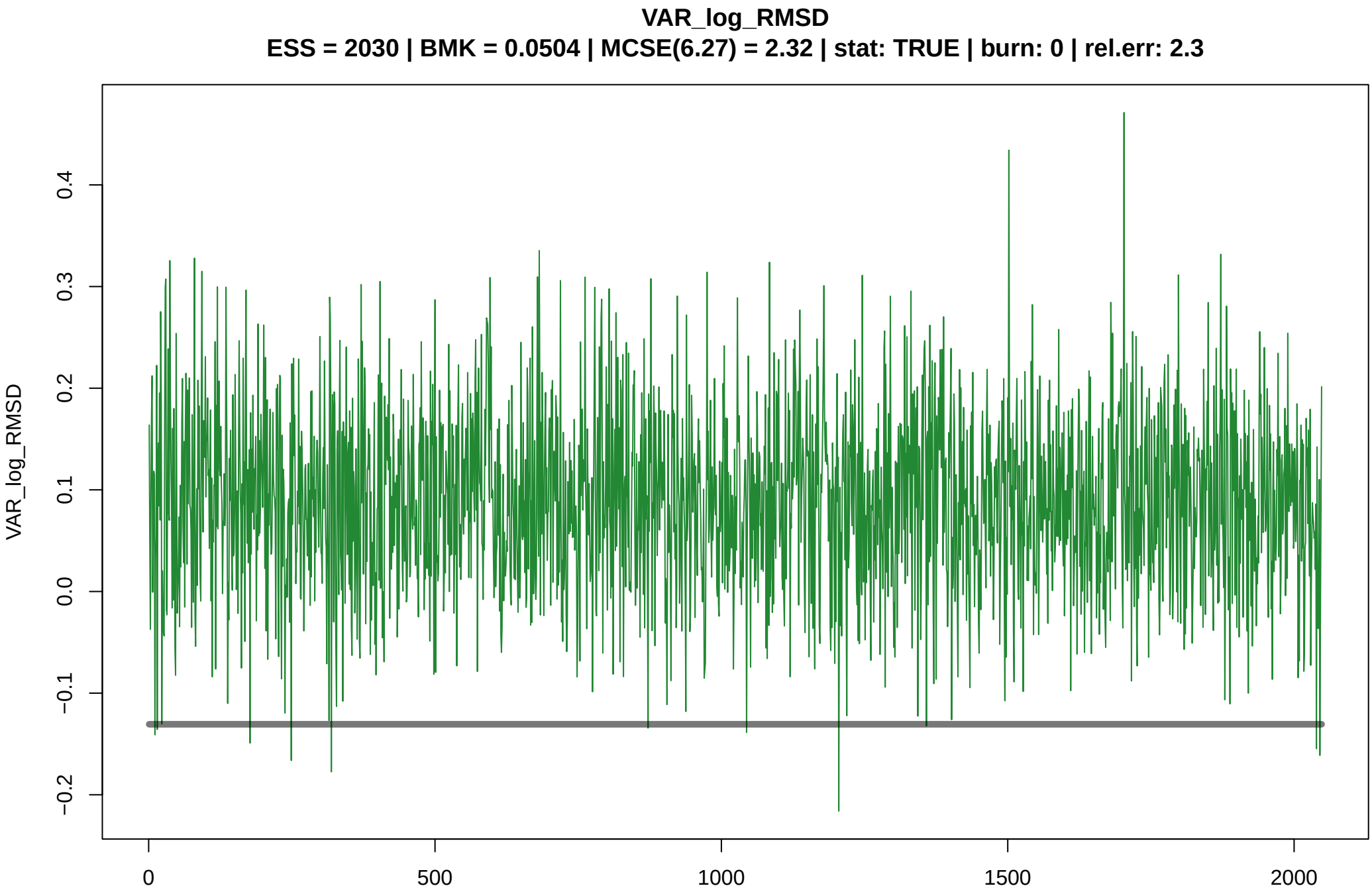

Dcov
ESS = 1880 | BMK = 0.0703 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0 | rel.err: 1.48
Dcov
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
0
500
1000
1500
2000

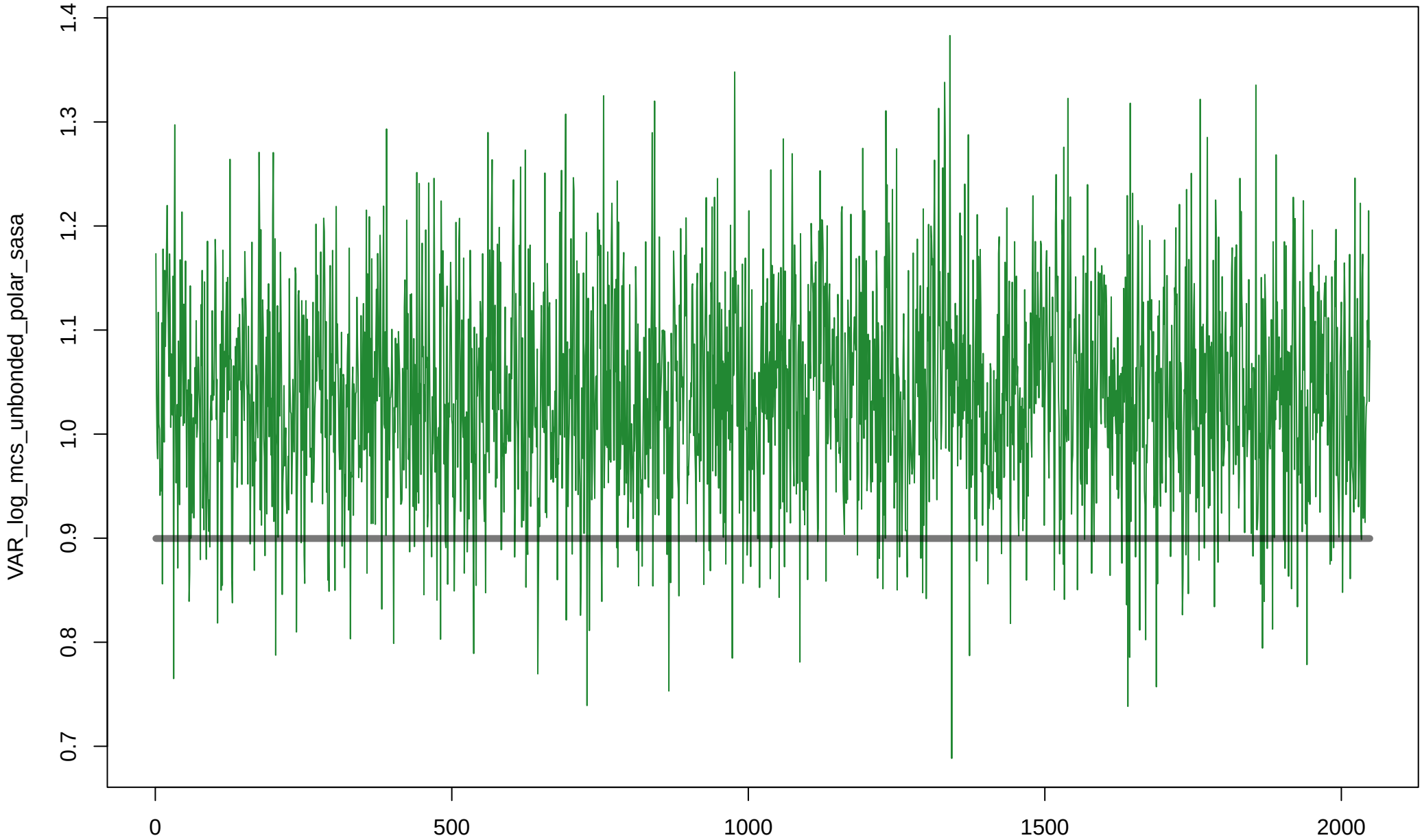

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0399 | MCSE(6.27) = 1.8 | stat: TRUE | burn: 0 | rel.err: −0.619
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

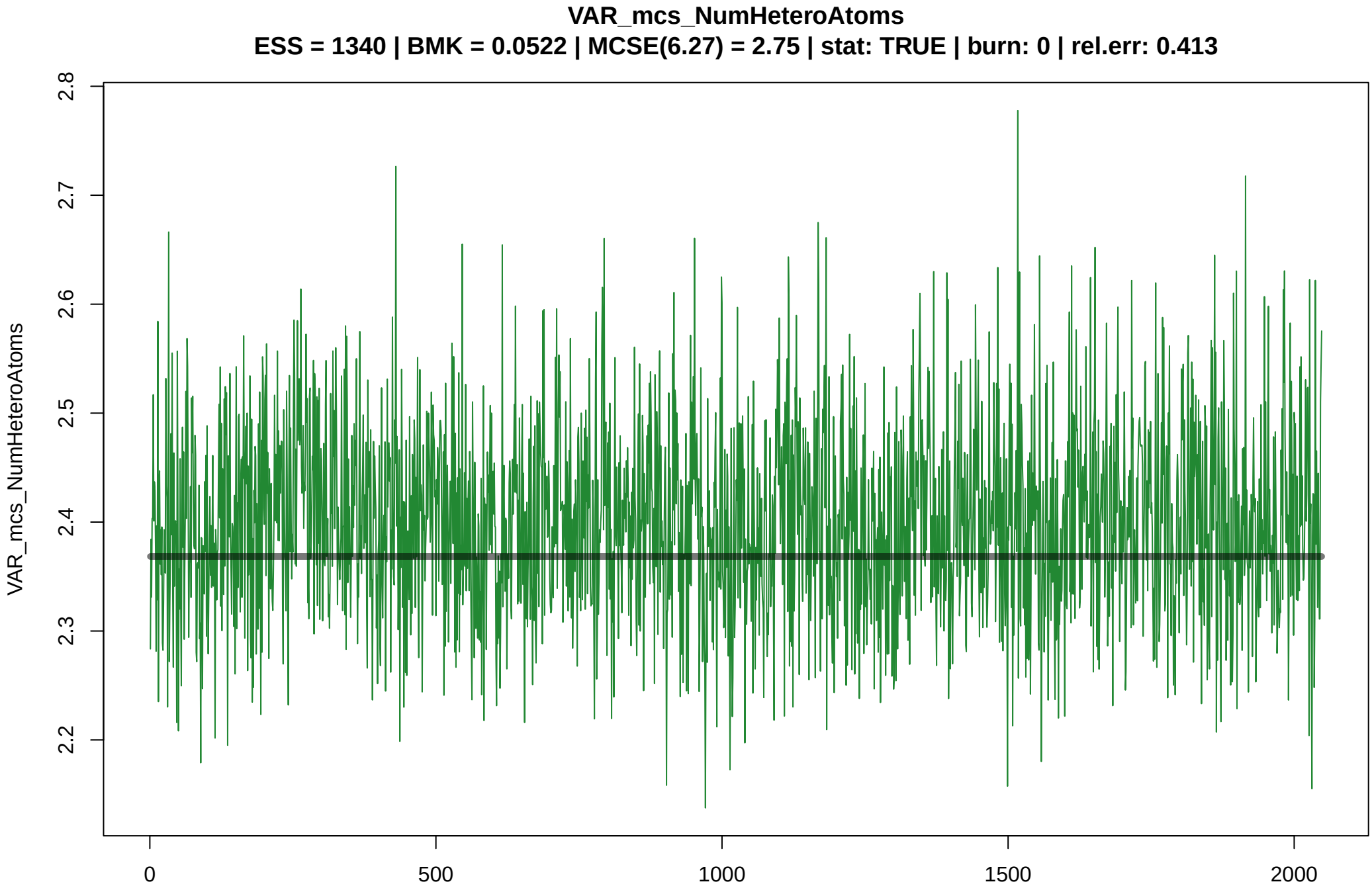

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1730 | BMK = 0.0469 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: −0.247
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

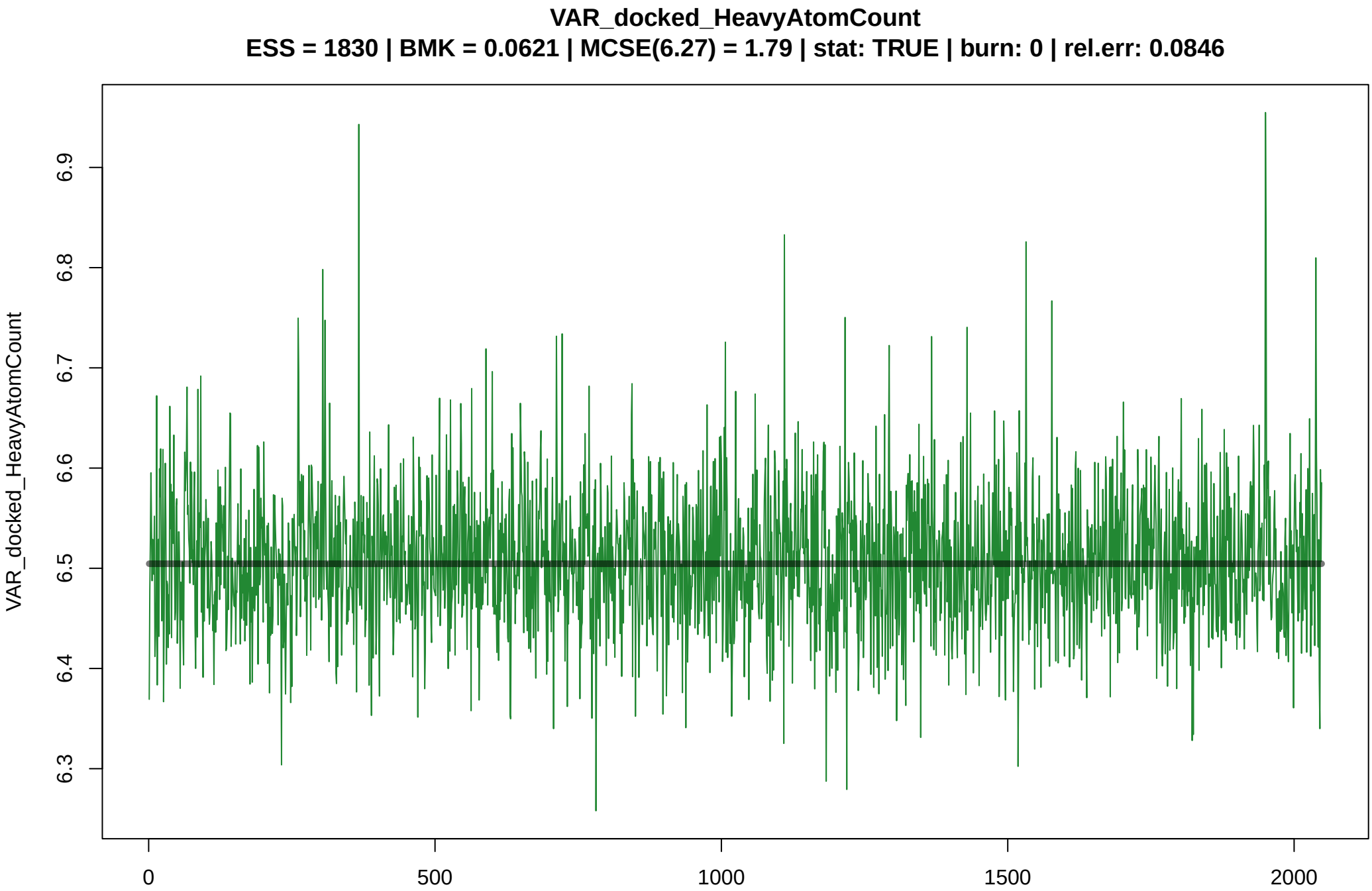

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: 0.485
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

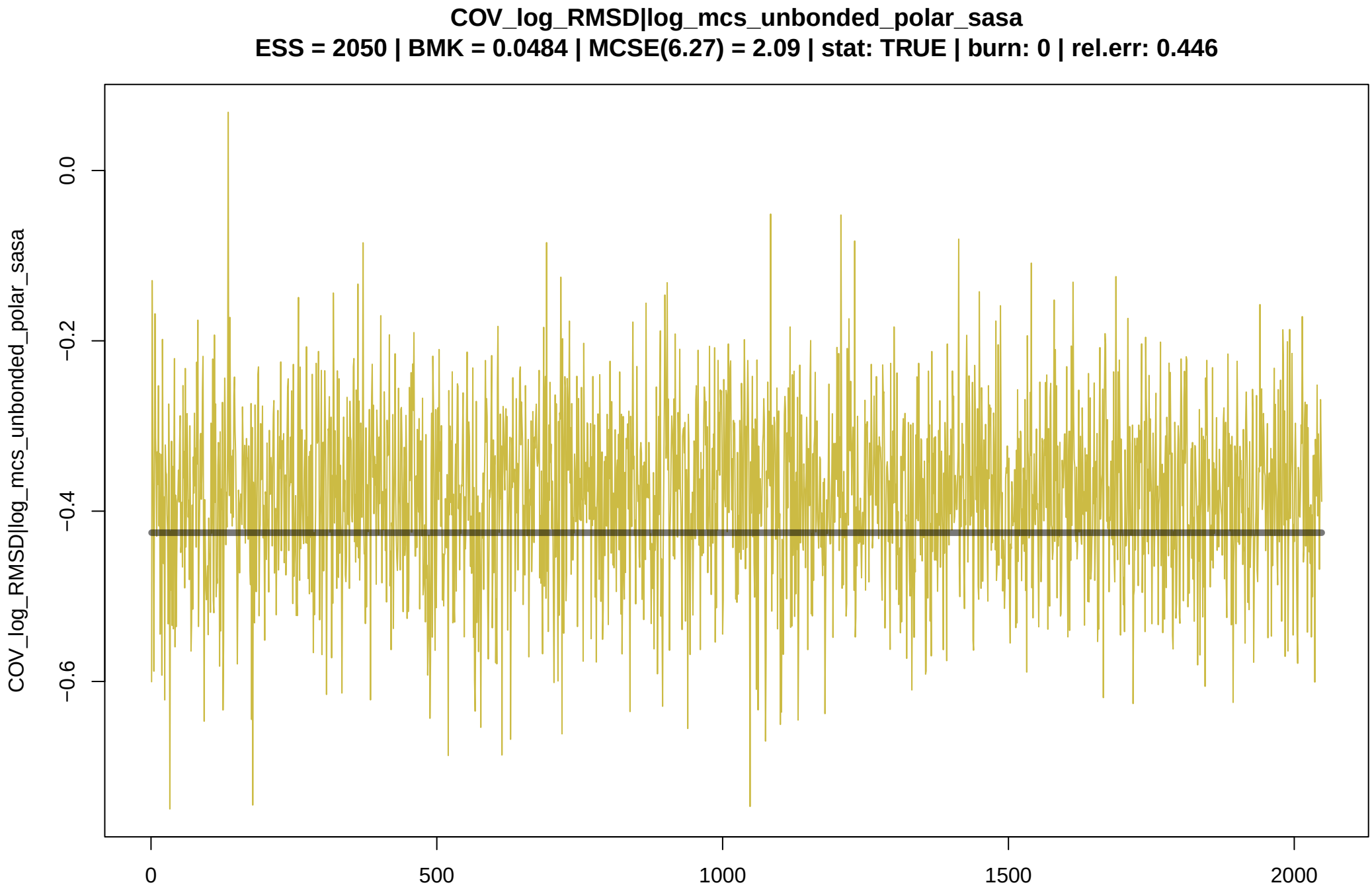

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0439 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0 | rel.err: 0.532
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

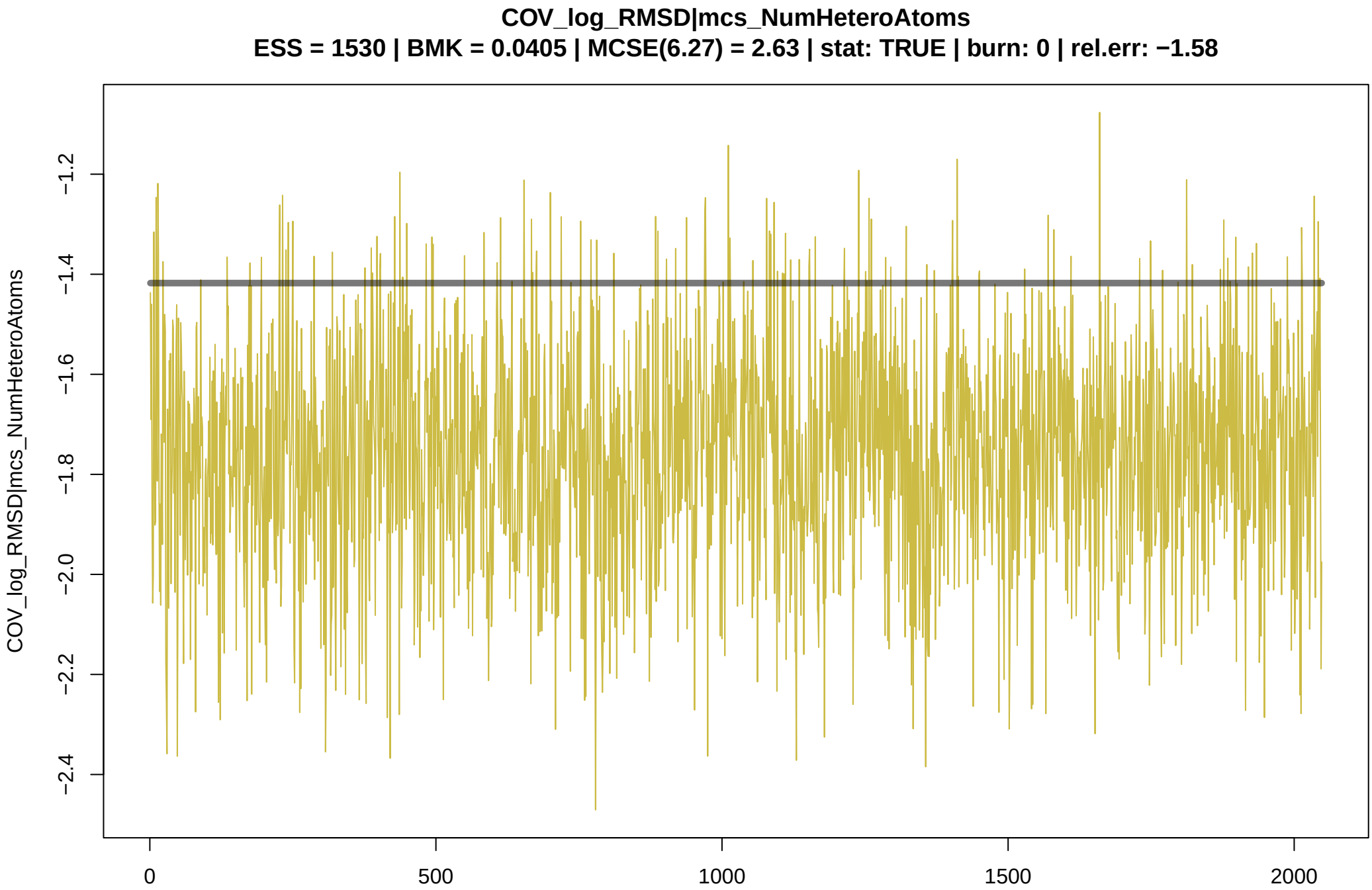

VAR_log_RMSD
ESS = 2030 | BMK = 0.0504 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: 2.3
VAR_log_RMSD
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

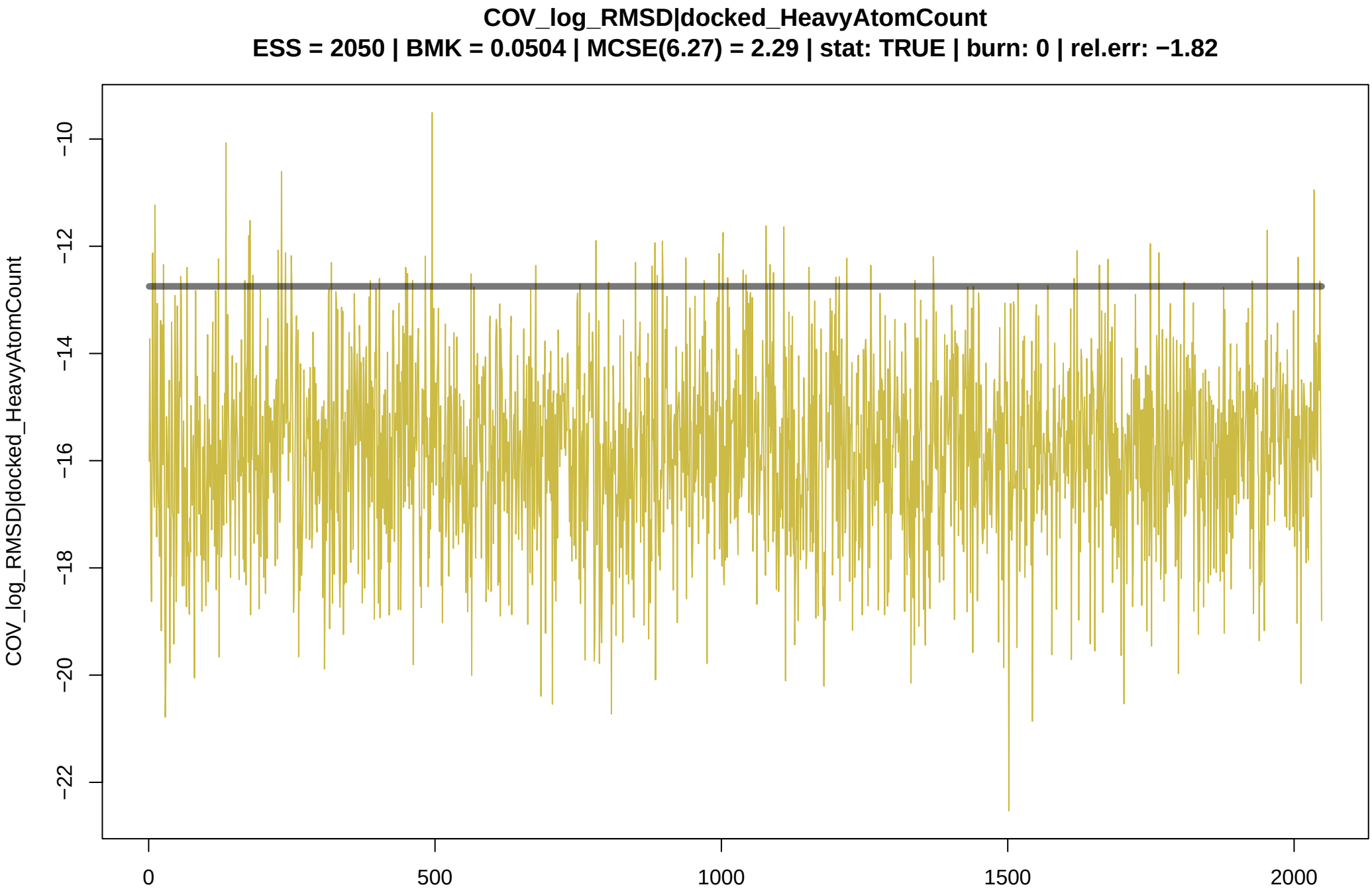

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0358 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | rel.err: 1.36
VAR_log_mcs_unbonded_polar_sasa
1.4
1.3
1.2
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

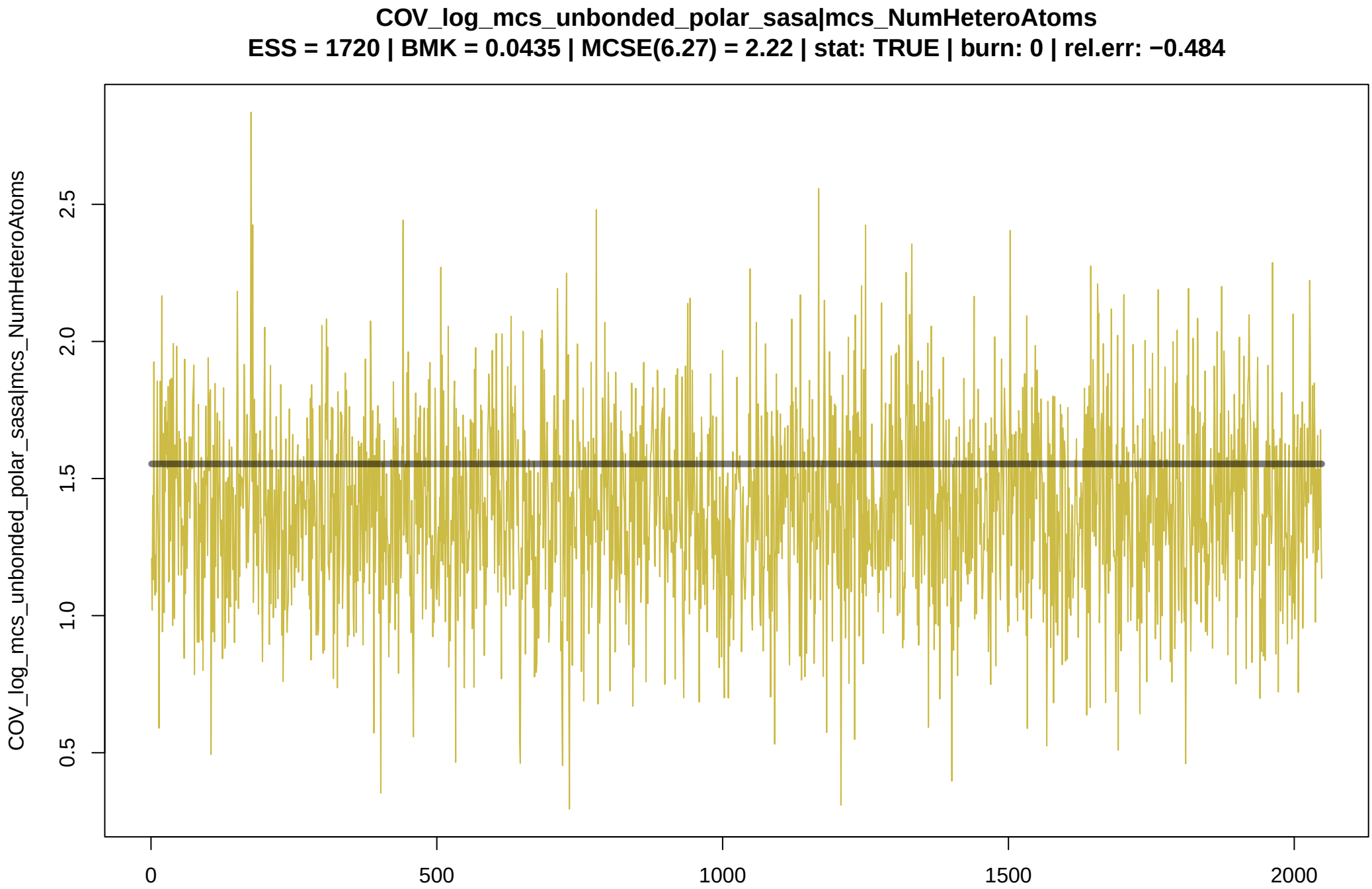

VAR_mcs_NumHeteroAtoms
ESS = 1340 | BMK = 0.0522 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0 | rel.err: 0.413
VAR_mcs_NumHeteroAtoms
2.2
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000

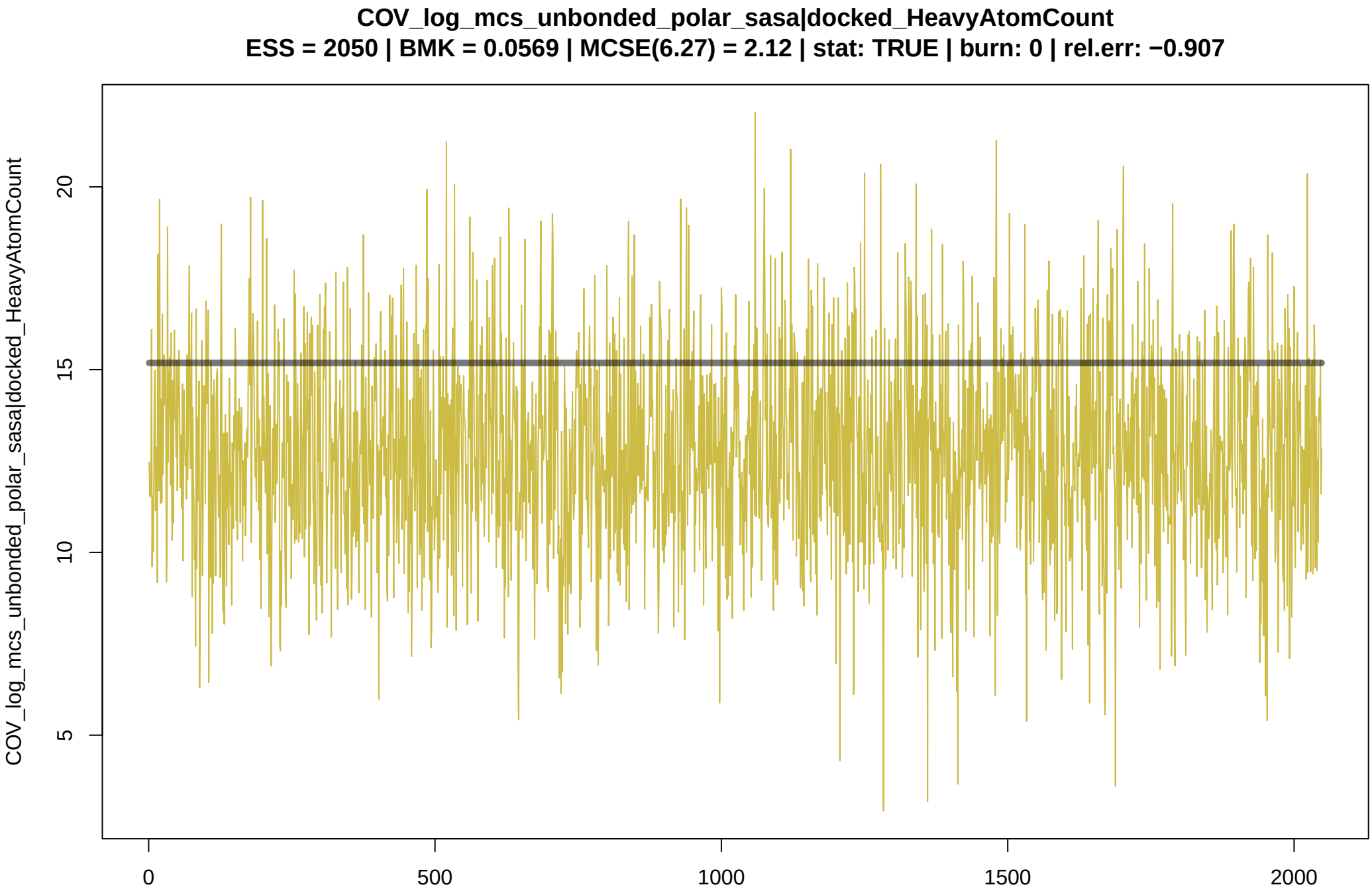

VAR_docked_HeavyAtomCount
ESS = 1830 | BMK = 0.0621 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.0846
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
6.9
0
500
1000
1500
2000

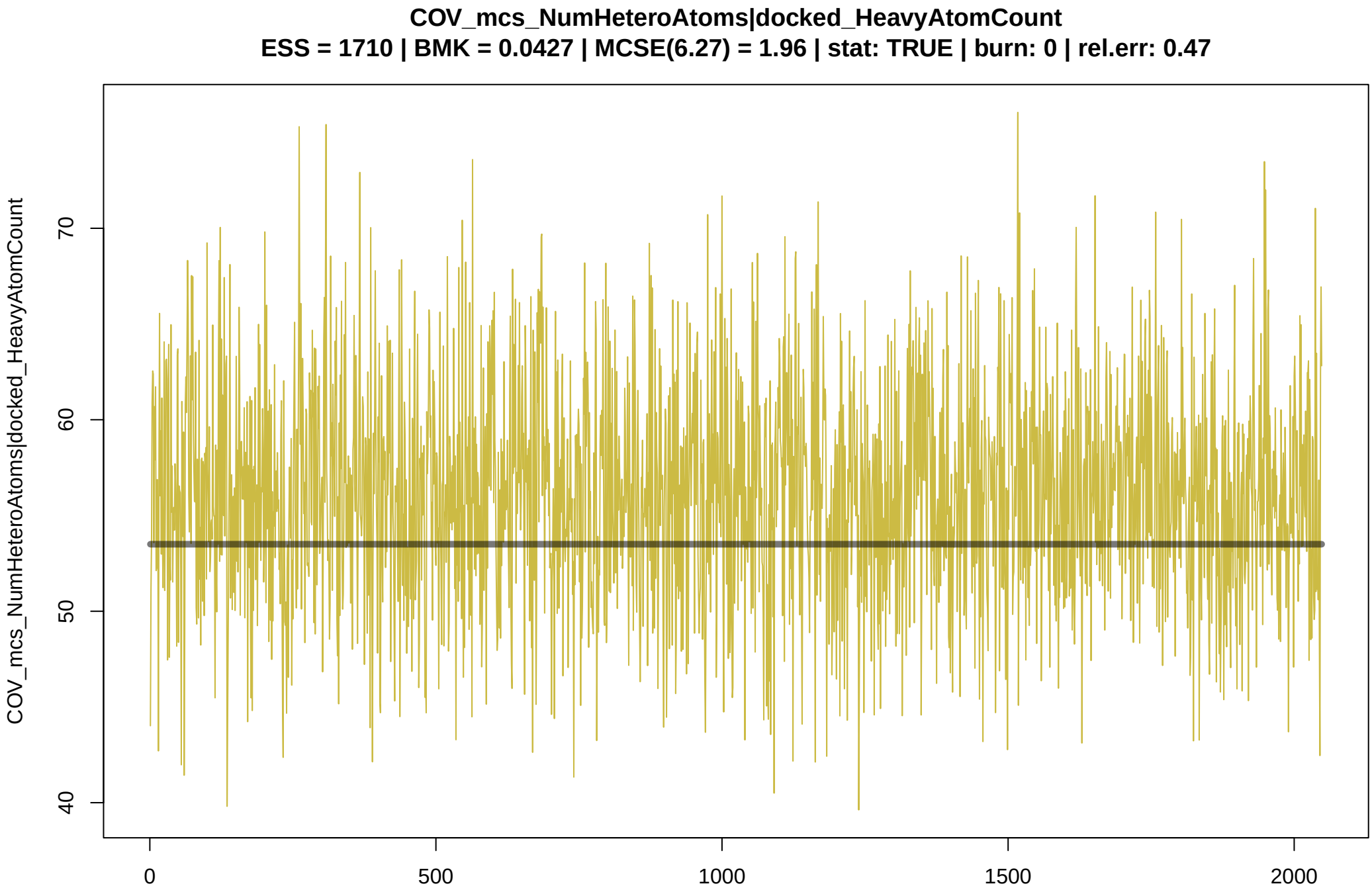

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0484 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.446
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1530 | BMK = 0.0405 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: −1.58
COV_log_RMSD|mcs_NumHeteroAtoms
−1.2
−1.4
−1.6
−1.8
−2.0
−2.2
−2.4
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0504 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: −1.82
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 = 1720 | BMK = 0.0435 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0 | rel.err: −0.484
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 = 0.0569 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: −0.907
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1710 | BMK = 0.0427 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0 | rel.err: 0.47
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
500
1000
1500
2000