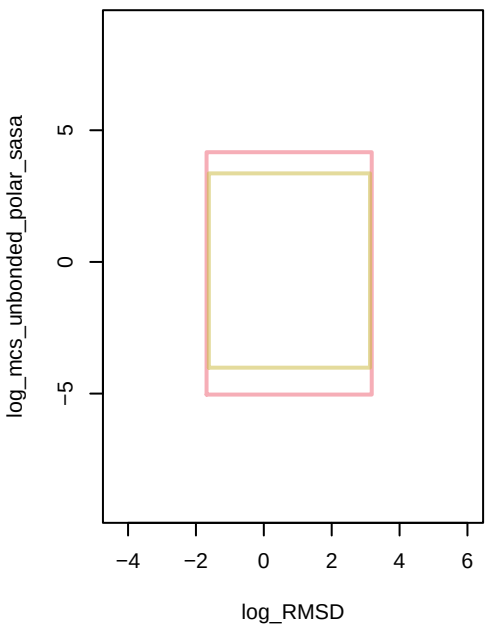
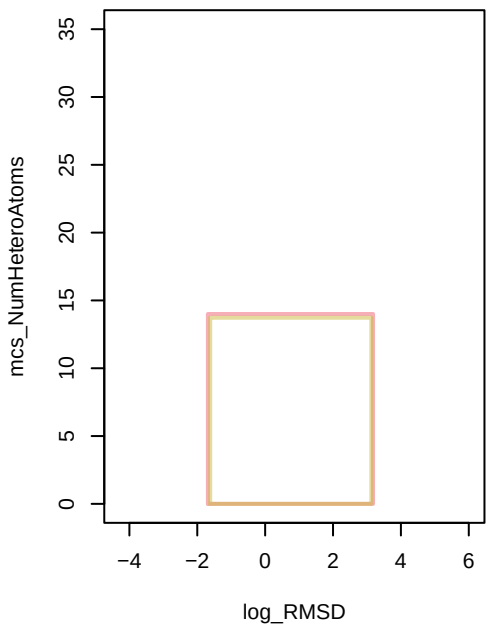
−− STATS maxD −−
min ESS = 94.4674444270459
max BMK = 0.150308827550978
max MCSE = 8.7841858670236
all stationary: FALSE
burn: 1428
max rel.err.: 2.10093132843498

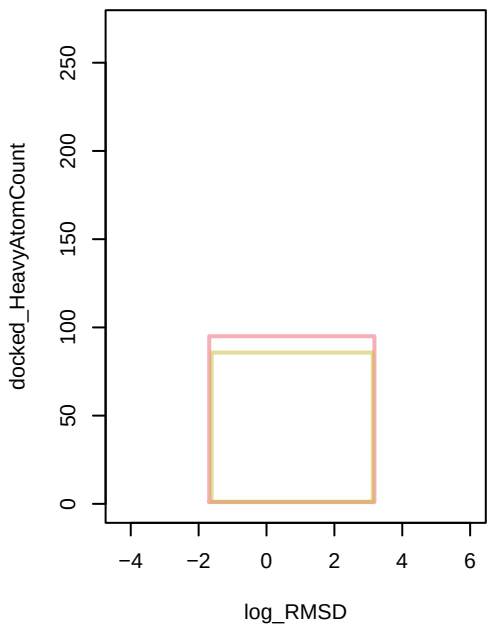
−− STATS 2D −−
min ESS = 2048
max BMK = 0.067902339435565 7
max MCSE = 2.65277777259647
all stationary: TRUE
burn: 0
max rel.err.: 1.73771122505691

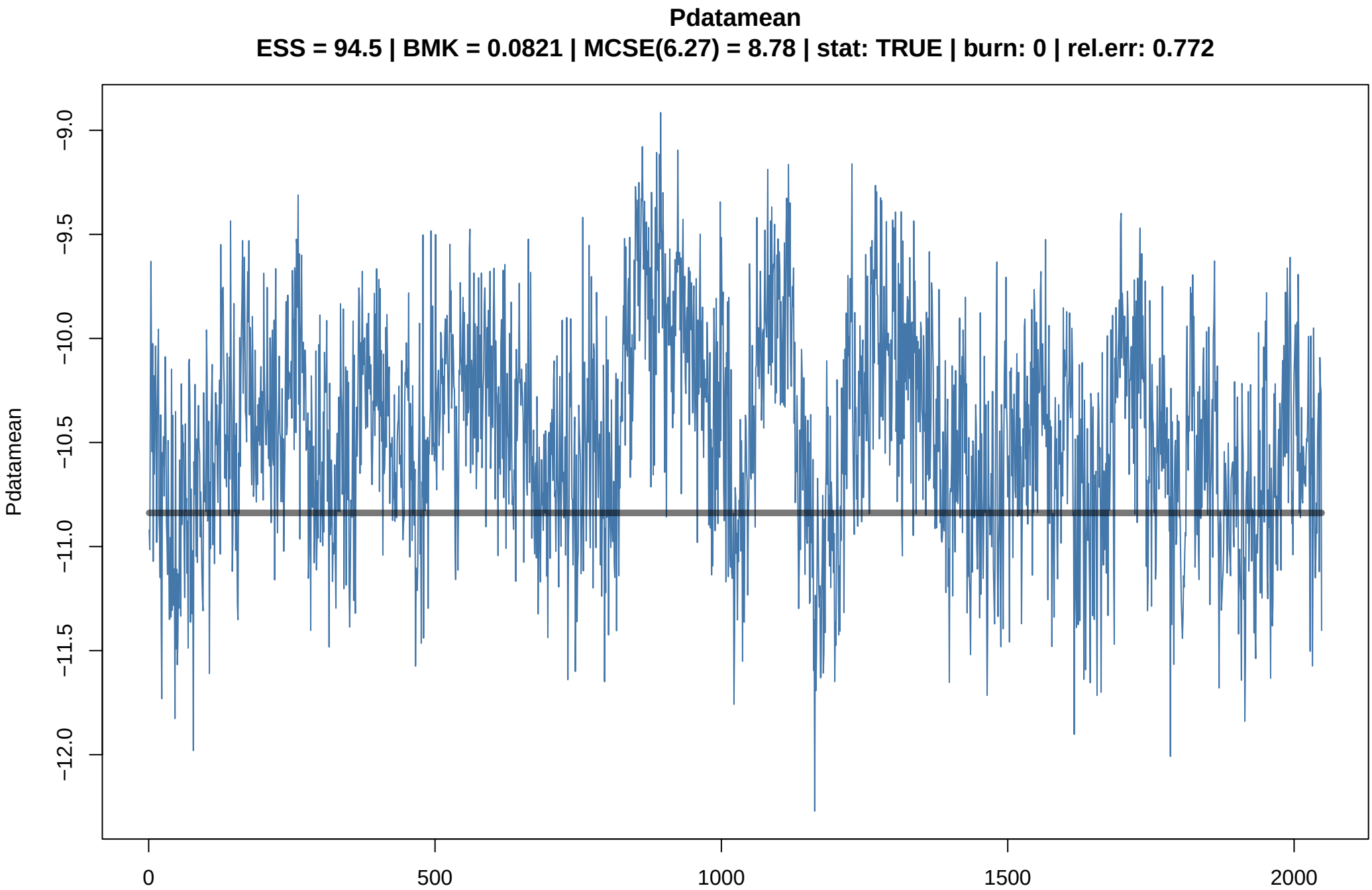
−− STATS 1D −−
min ESS = 1437.62489145666
max BMK = 0.0630777185515065
max MCSE = 3.2039063403484
all stationary: TRUE
burn: 0
max rel.err.: 2.27882169263241

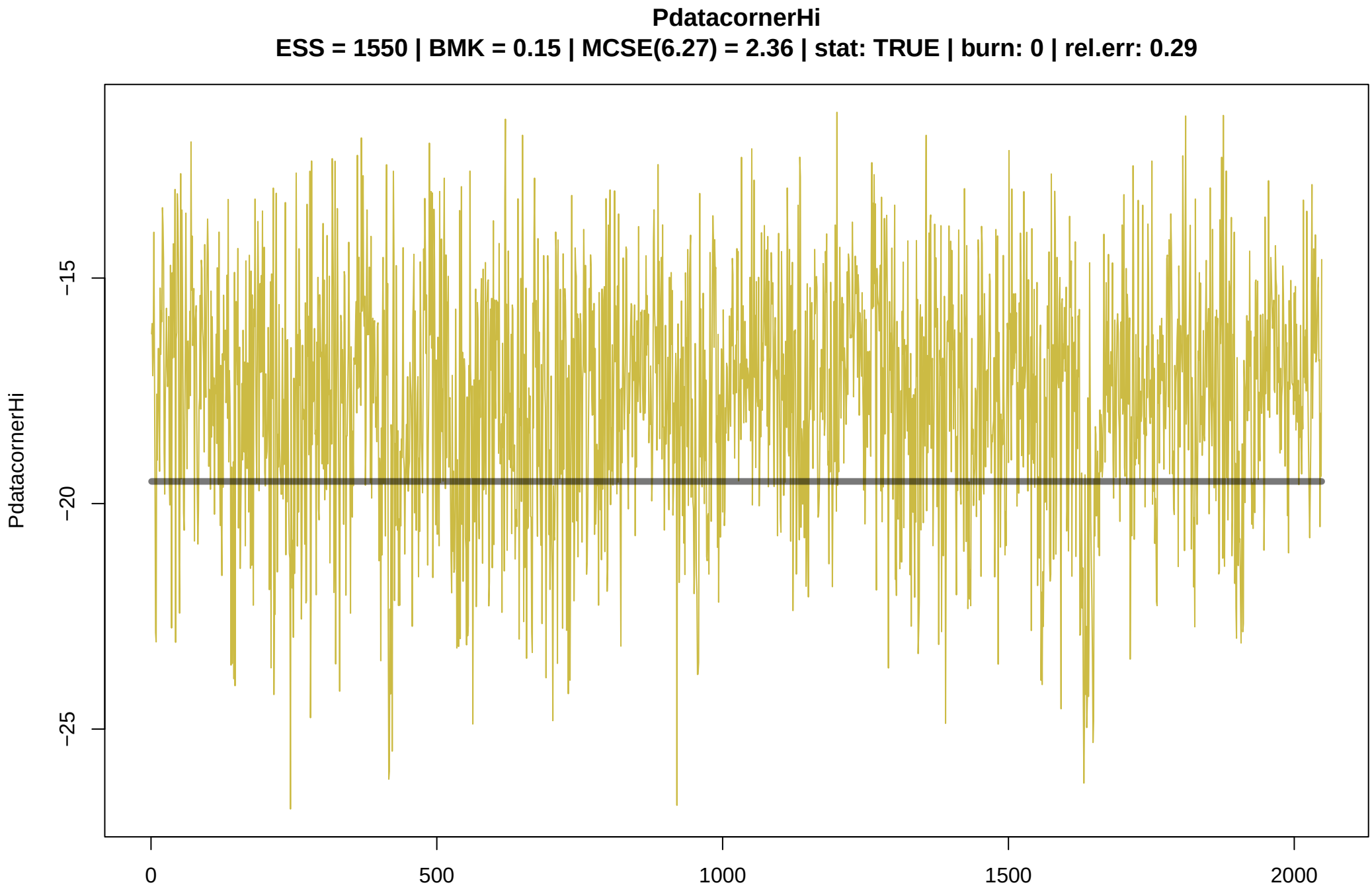
Occupied clusters: 9 of 16

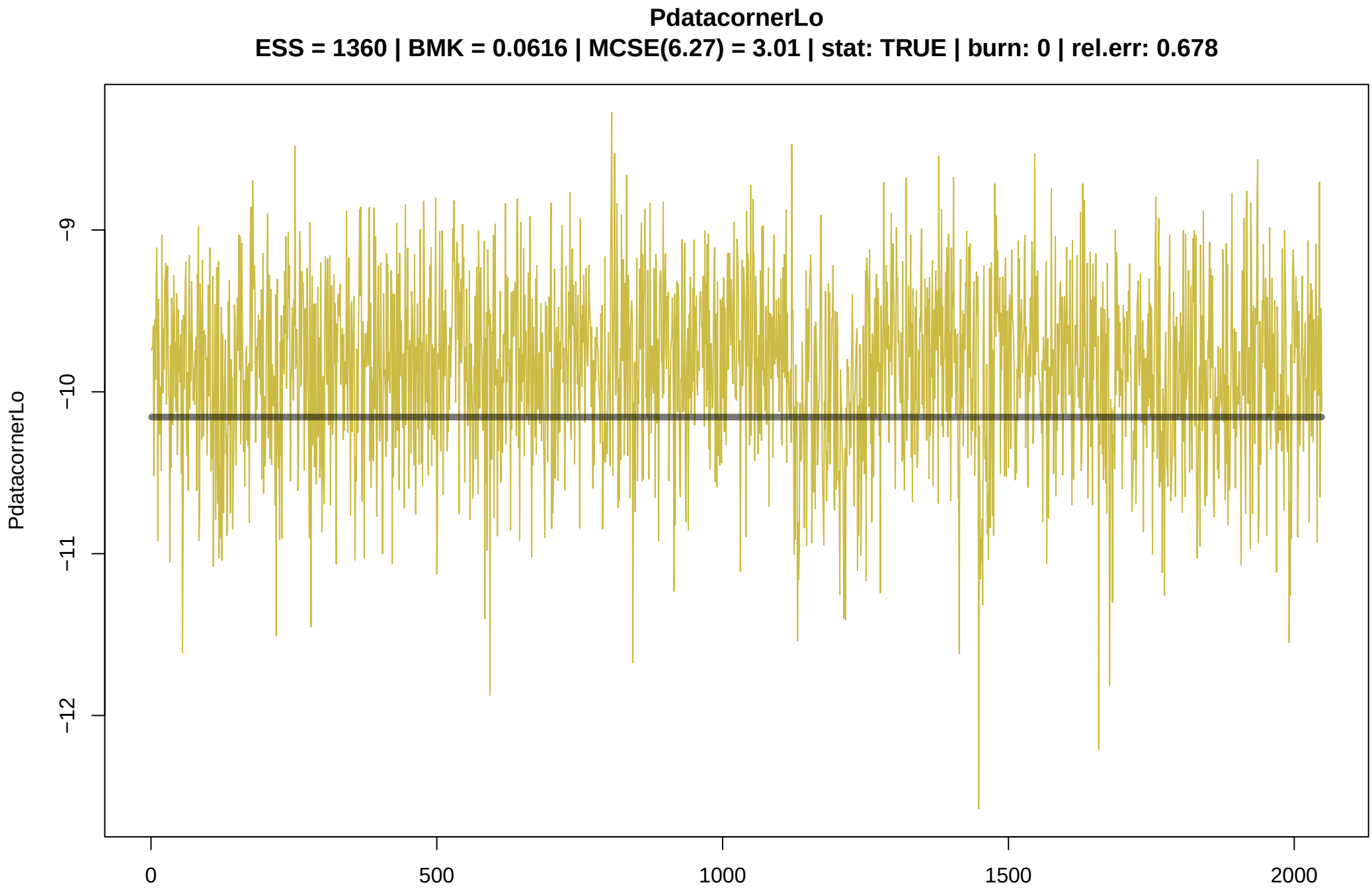

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

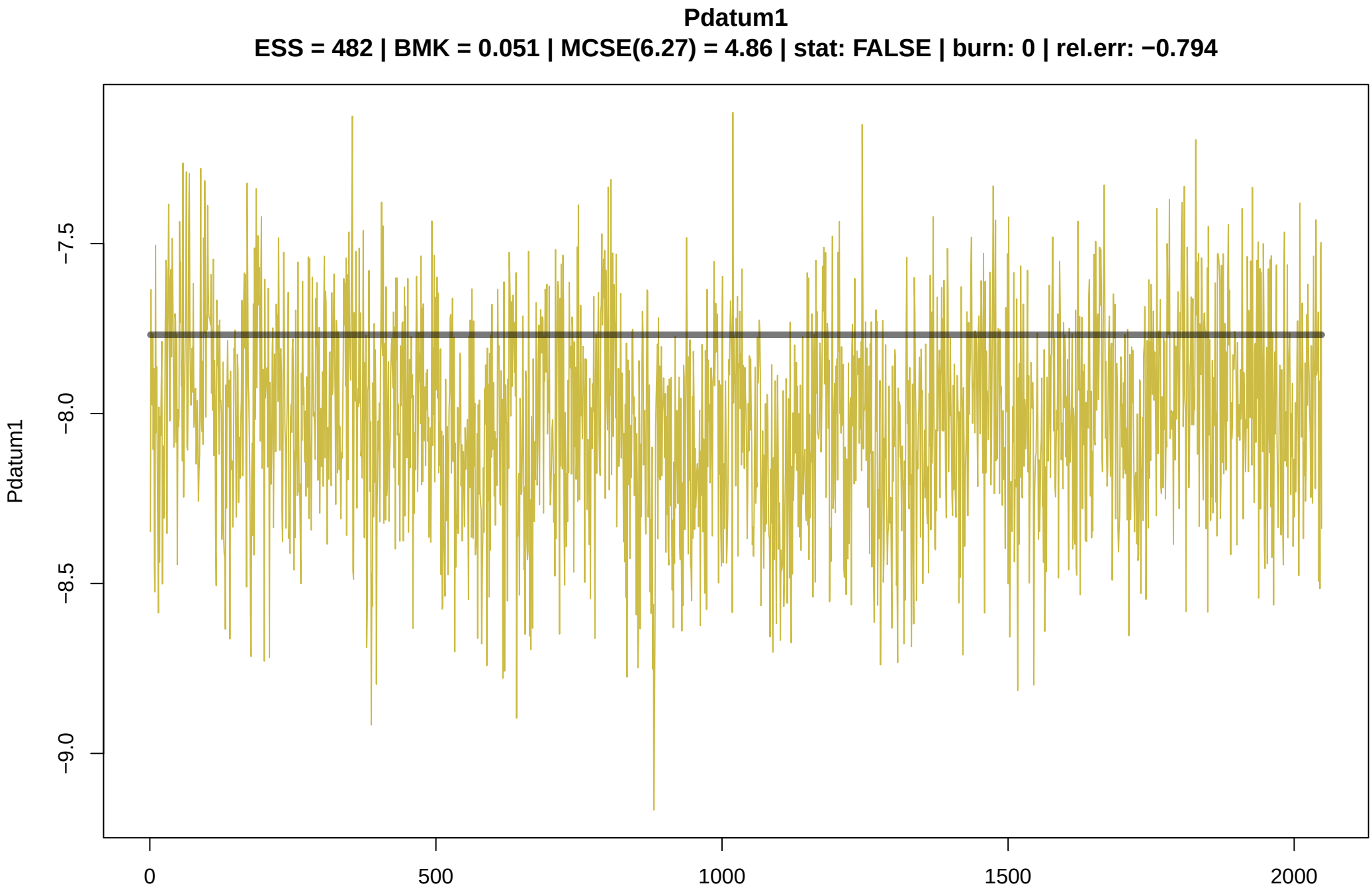

mcs_NumHeteroAtoms
35
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

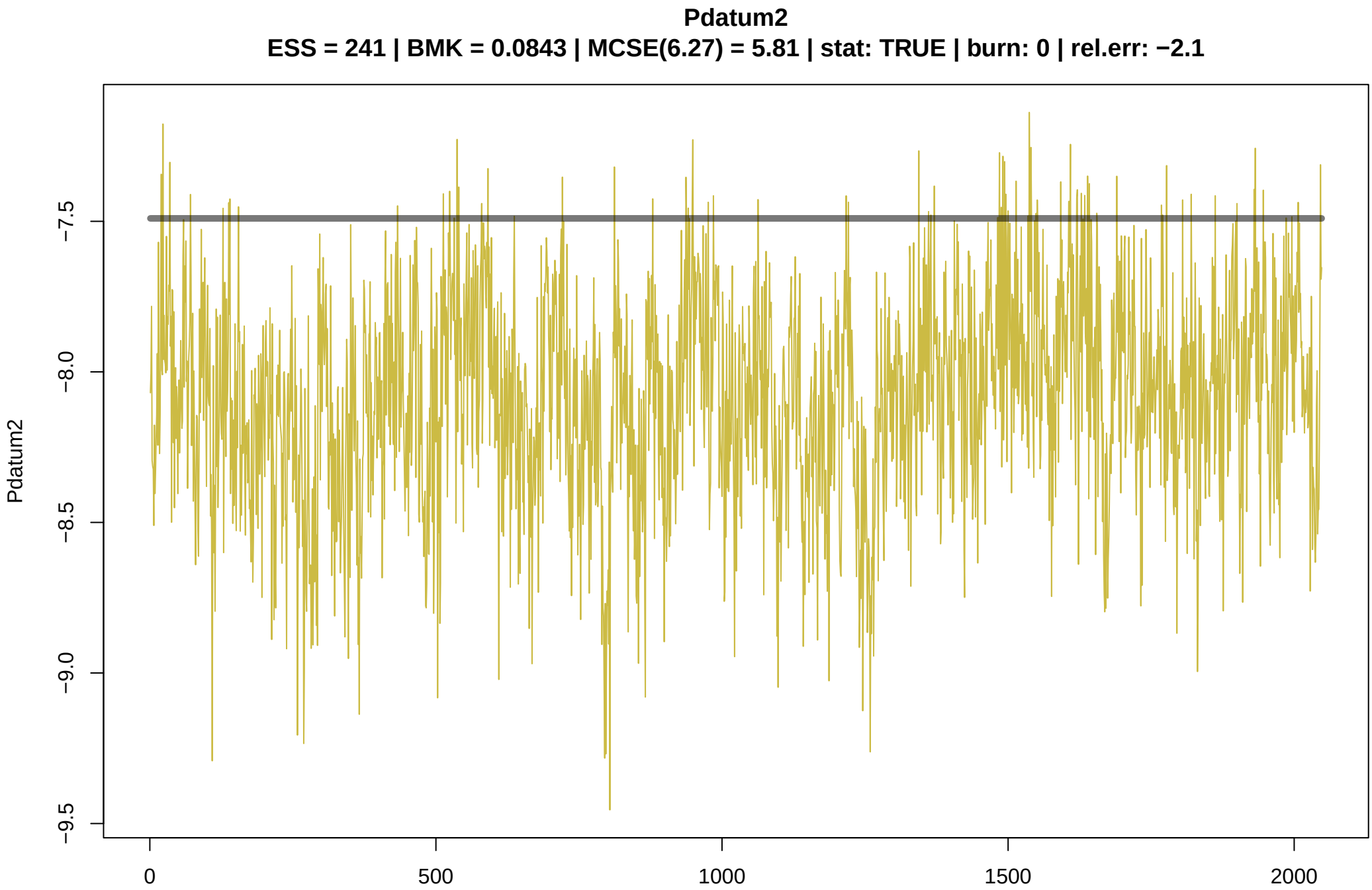

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

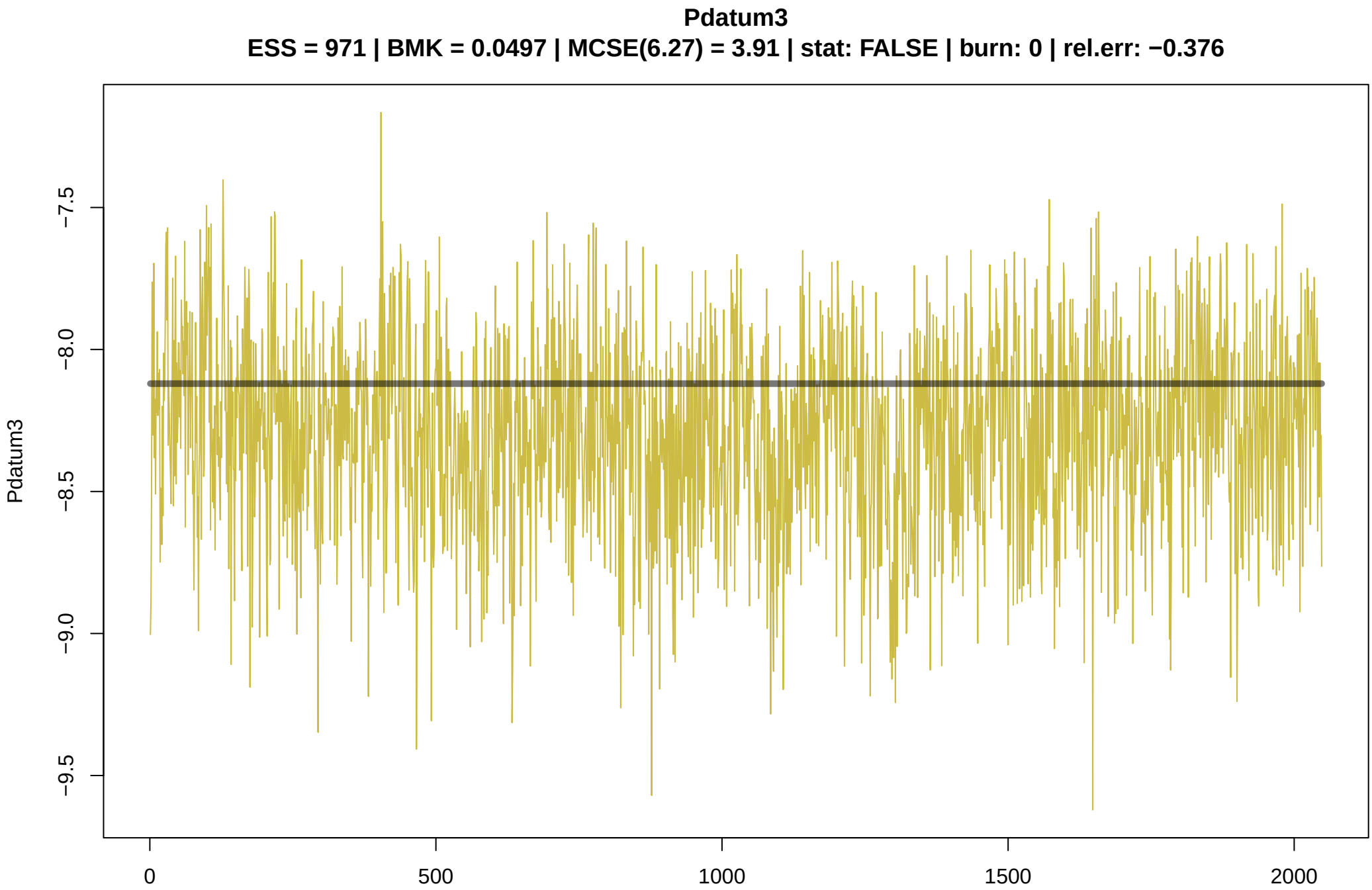

Pdatamean
ESS = 94.5 | BMK = 0.0821 | MCSE(6.27) = 8.78 | stat: TRUE | burn: 0 | rel.err: 0.772
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

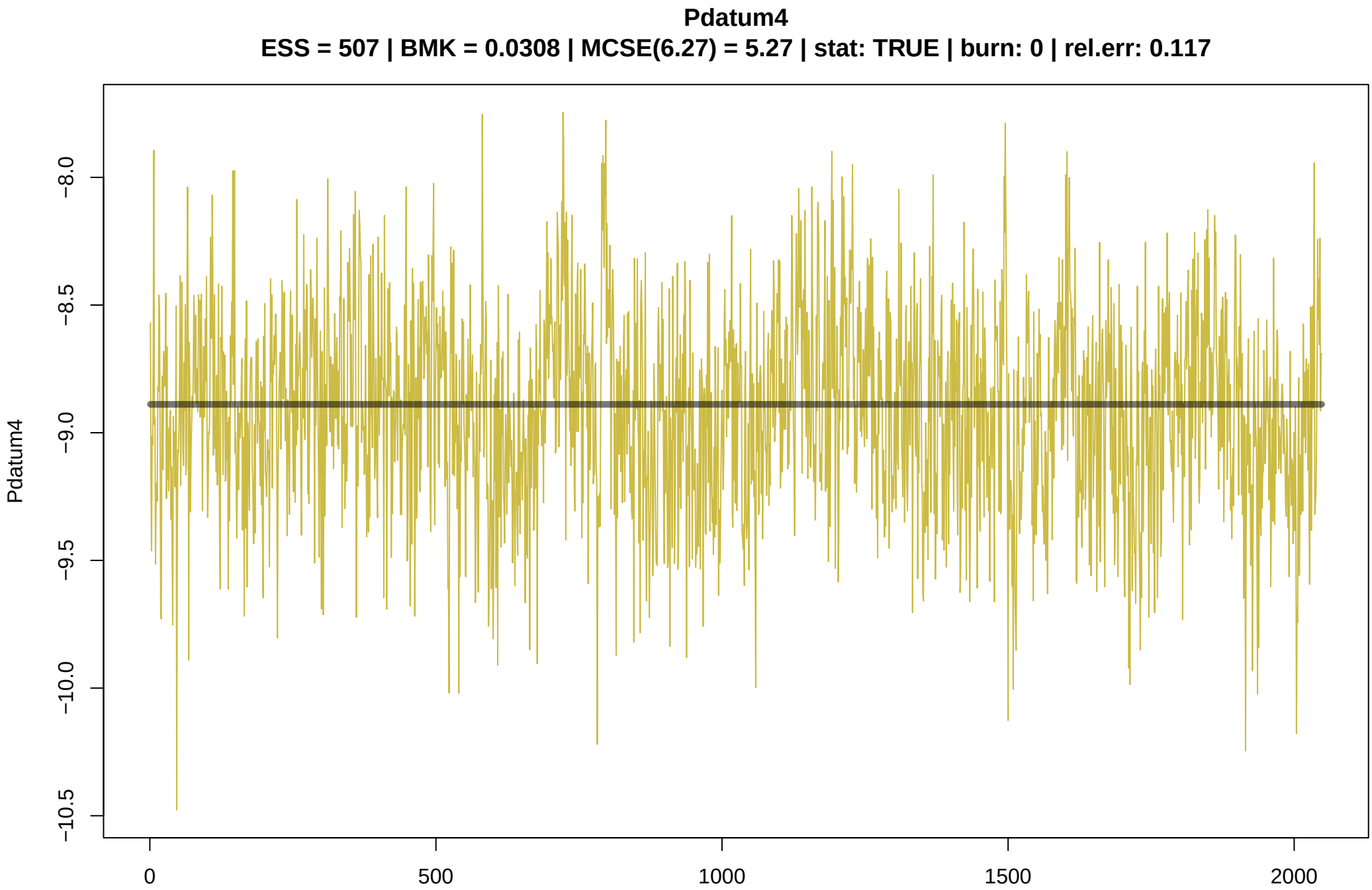

PdatacornerHi
ESS = 1550 | BMK = 0.15 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0 | rel.err: 0.29
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

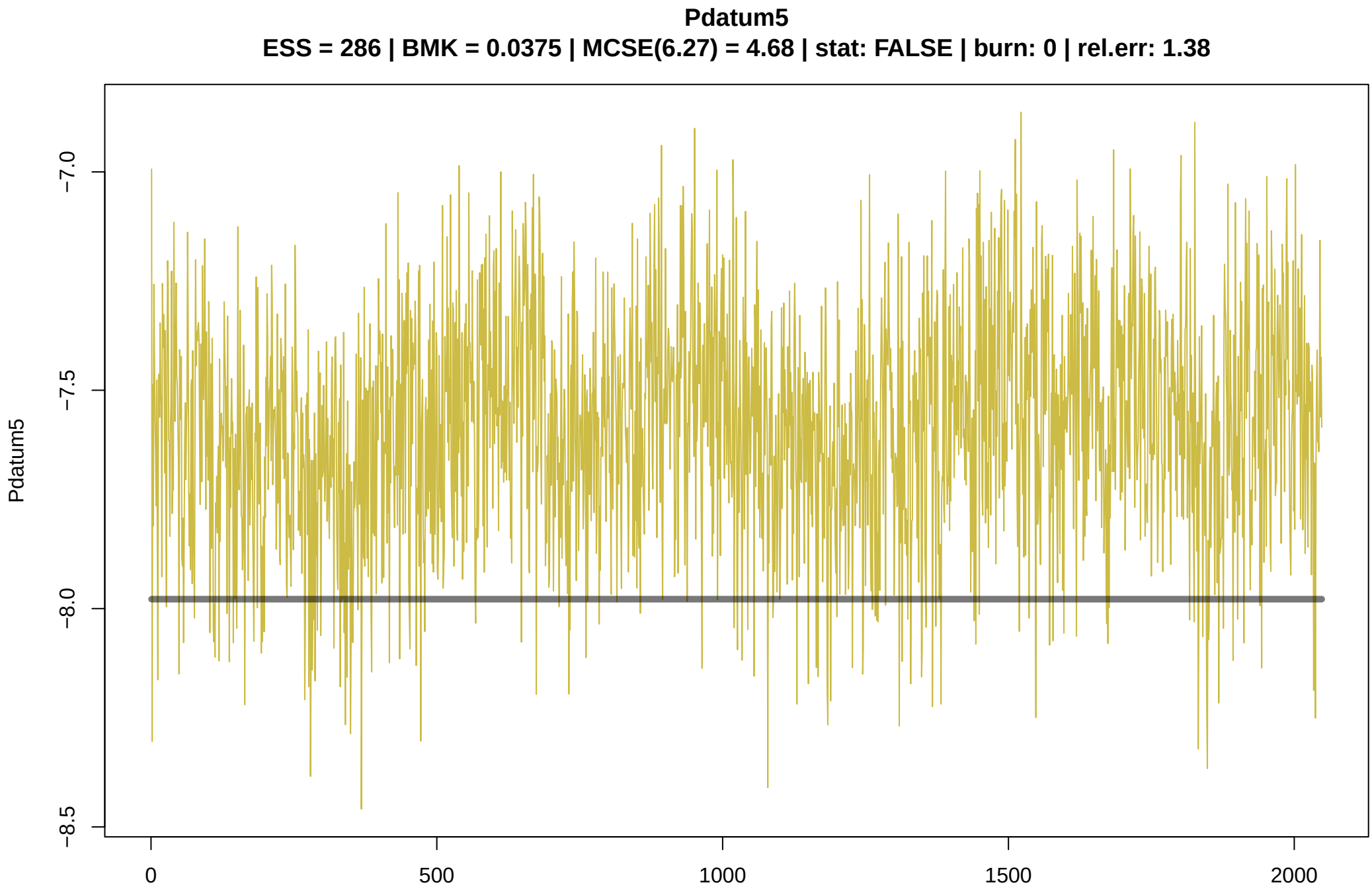

PdatacornerLo
ESS = 1360 | BMK = 0.0616 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0 | rel.err: 0.678
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

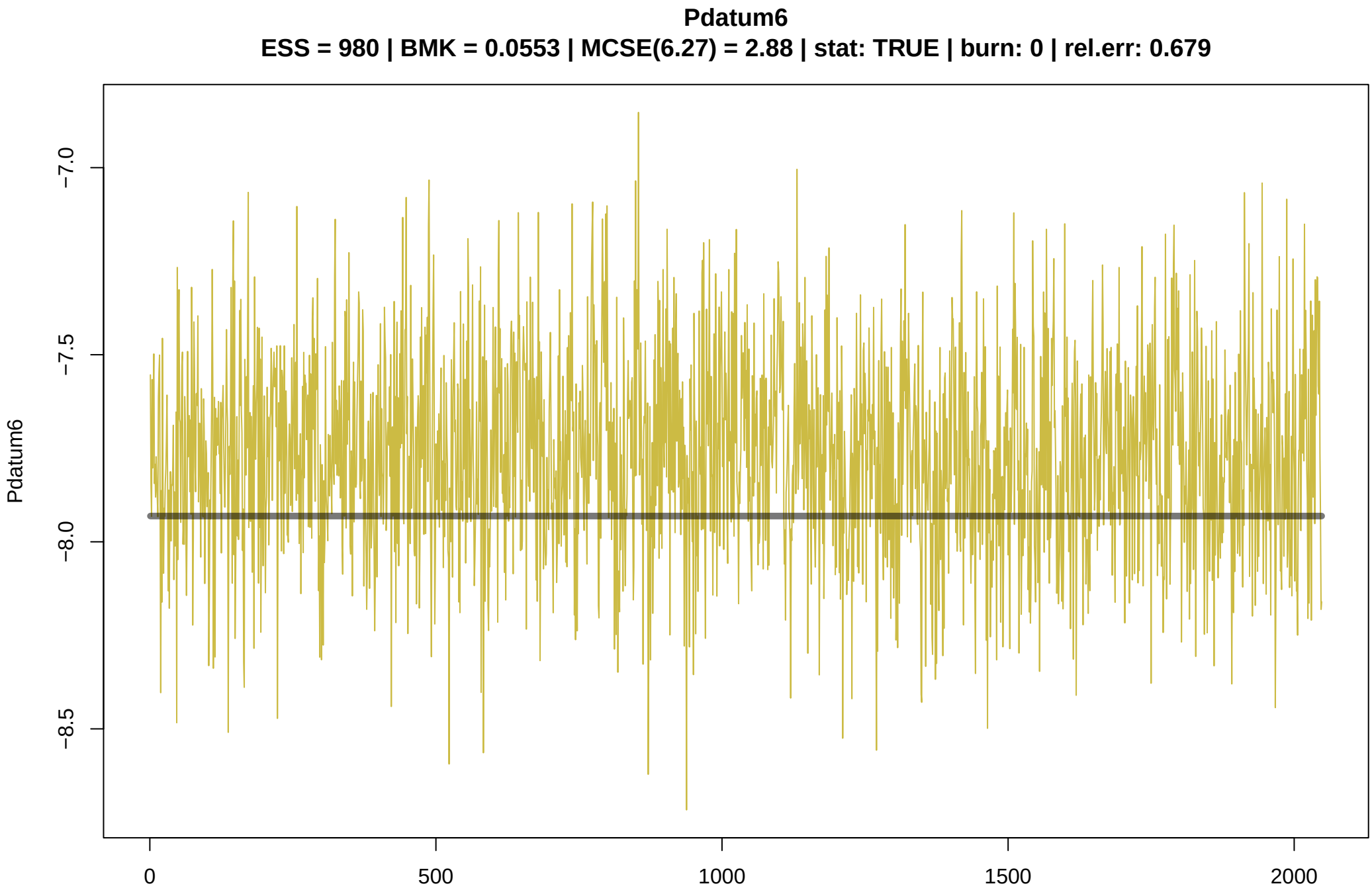

Pdatum1
ESS = 482 | BMK = 0.051 | MCSE(6.27) = 4.86 | stat: FALSE | burn: 0 | rel.err: −0.794
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

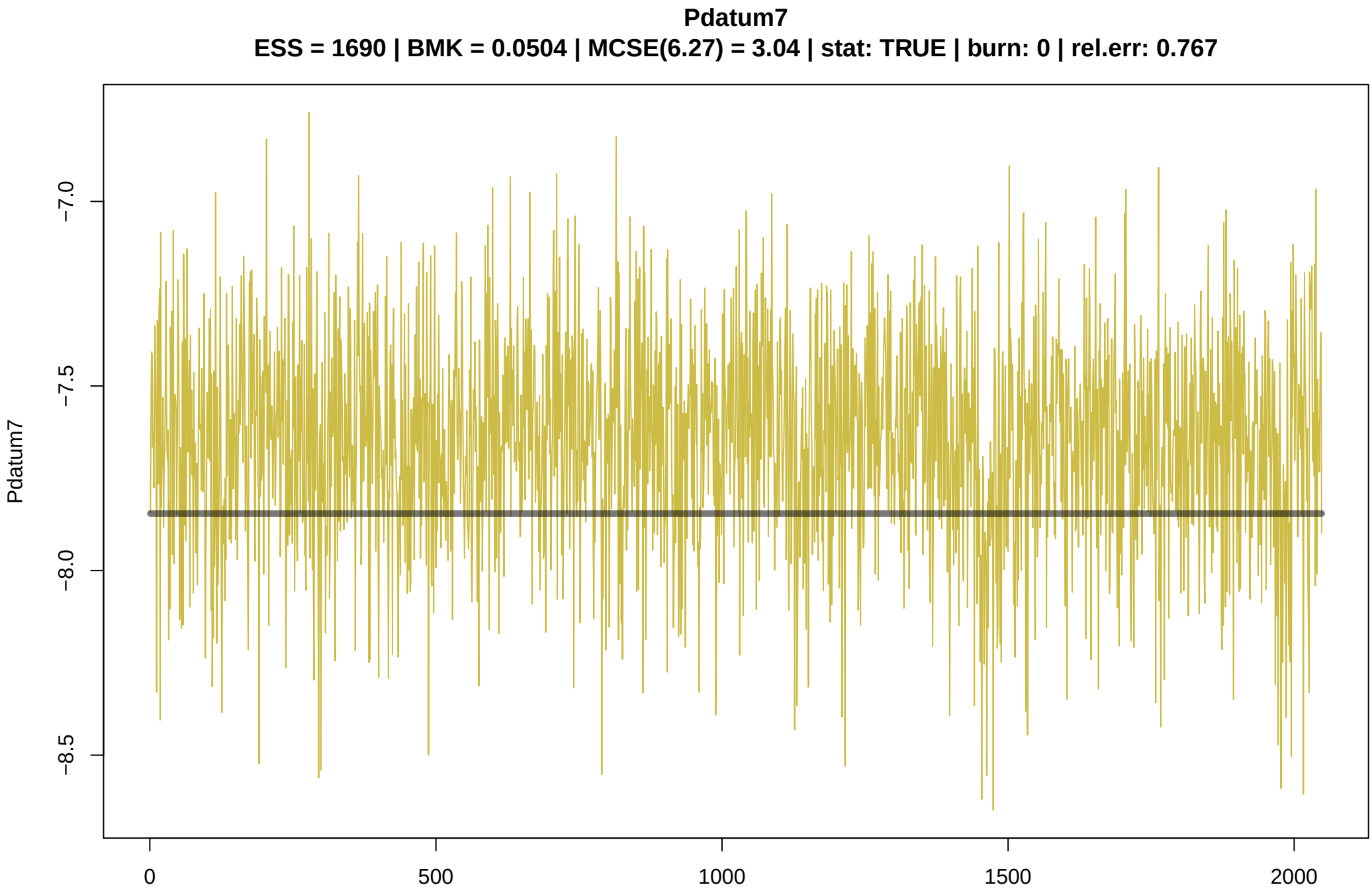

Pdatum2
ESS = 241 | BMK = 0.0843 | MCSE(6.27) = 5.81 | stat: TRUE | burn: 0 | rel.err: −2.1
Pdatum2
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

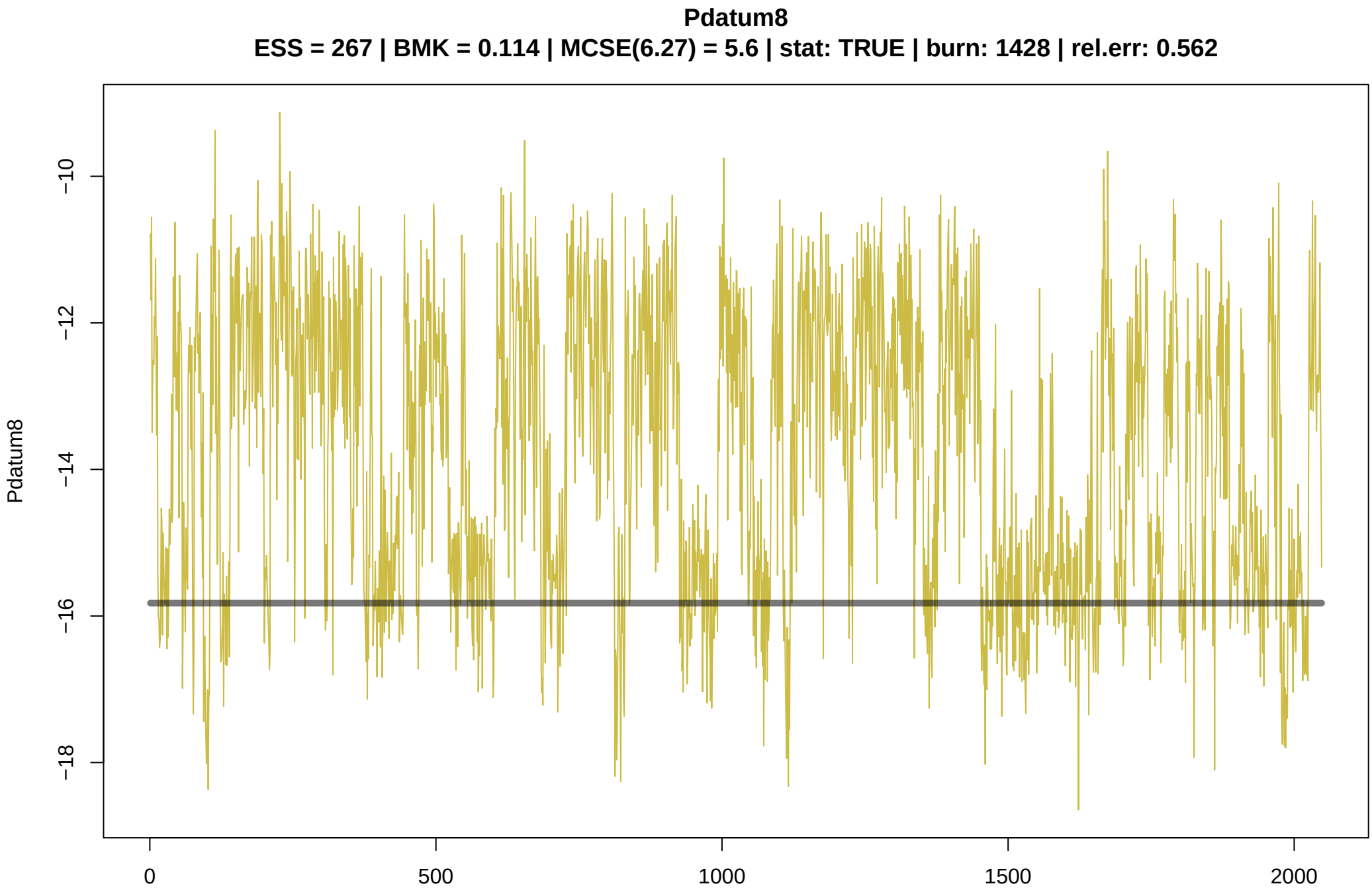

Pdatum3
ESS = 971 | BMK = 0.0497 | MCSE(6.27) = 3.91 | stat: FALSE | burn: 0 | rel.err: −0.376
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

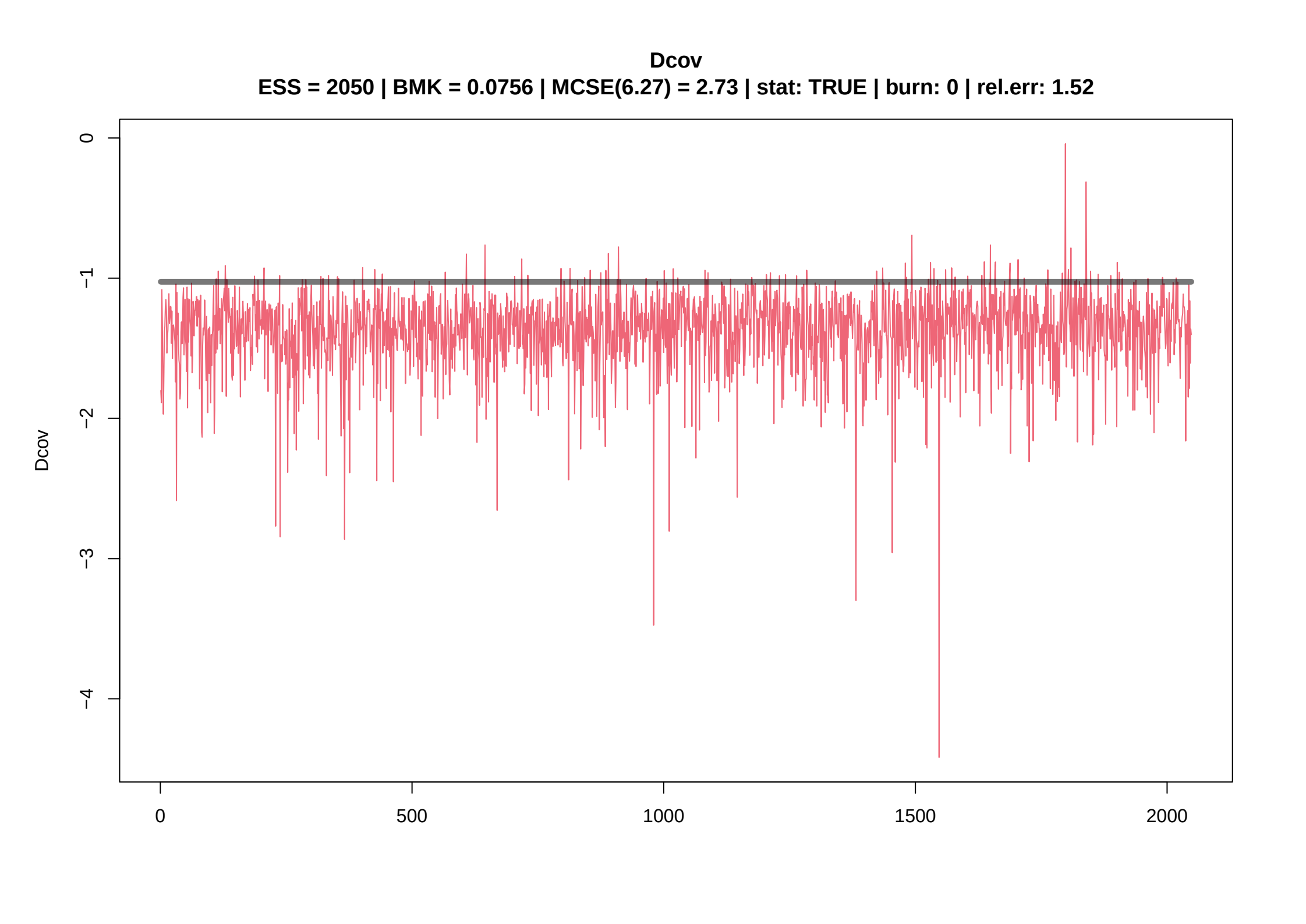

Pdatum4
ESS = 507 | BMK = 0.0308 | MCSE(6.27) = 5.27 | stat: TRUE | burn: 0 | rel.err: 0.117
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

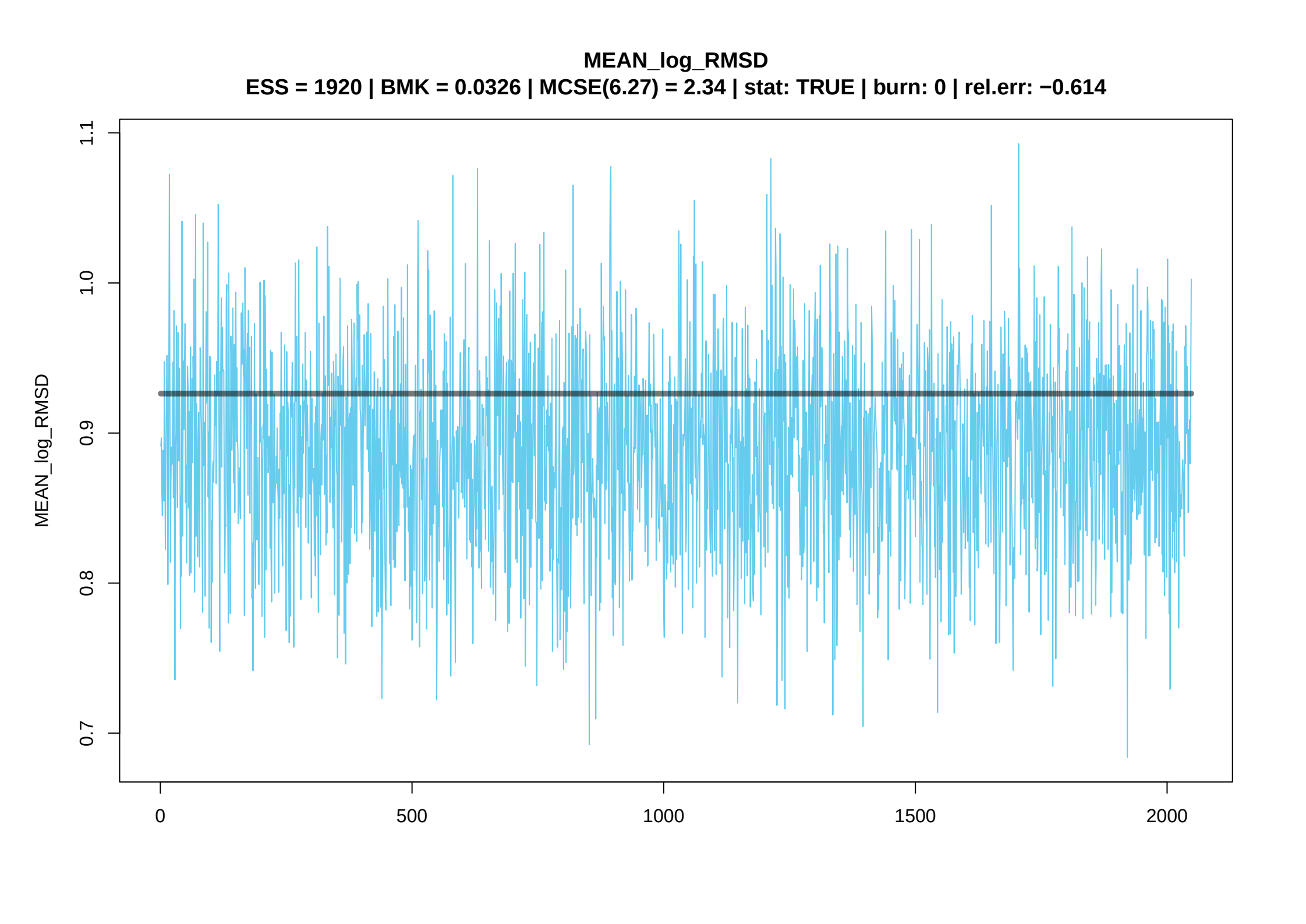

Pdatum5
ESS = 286 | BMK = 0.0375 | MCSE(6.27) = 4.68 | stat: FALSE | burn: 0 | rel.err: 1.38
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

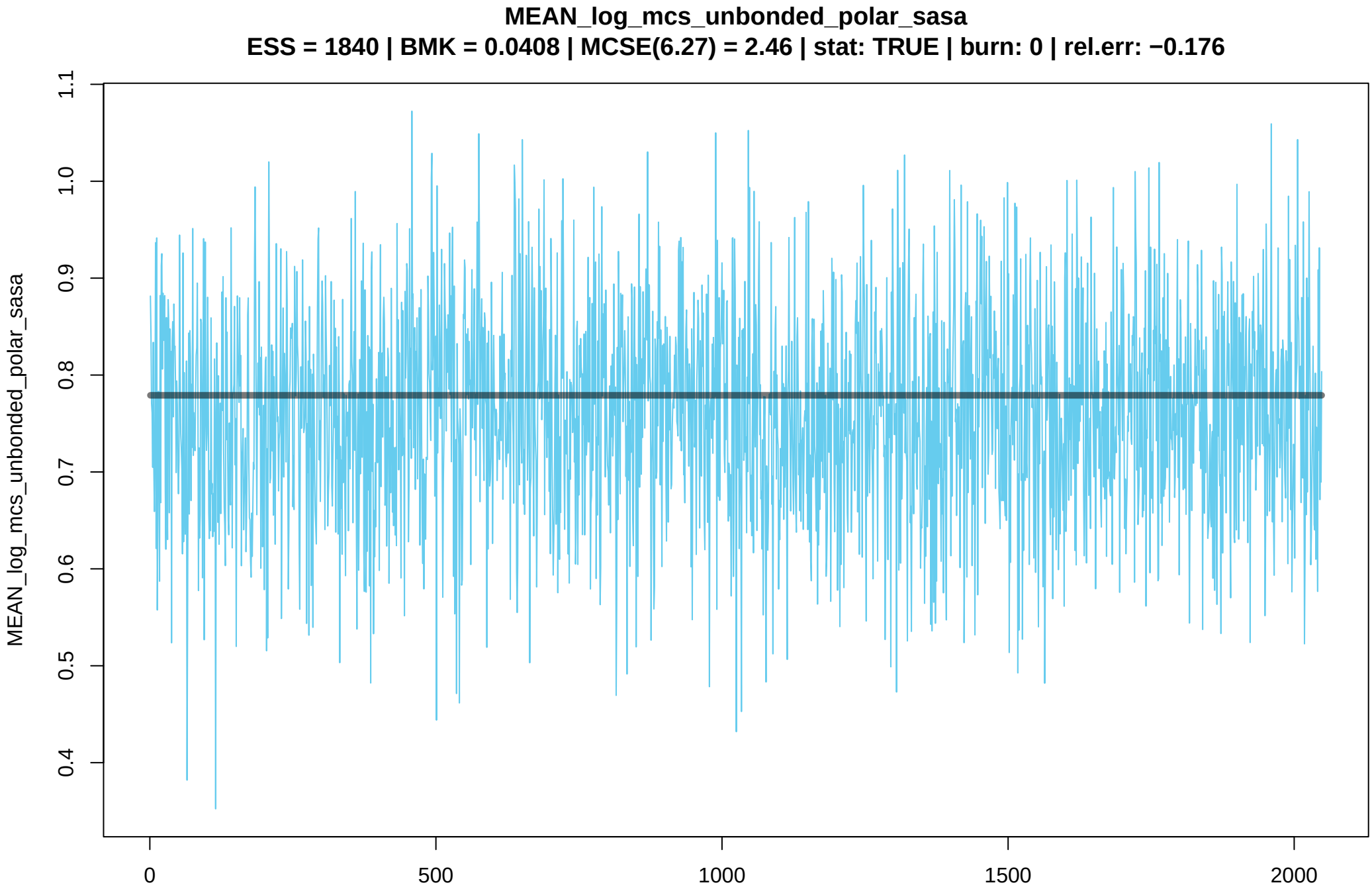

Pdatum6
ESS = 980 | BMK = 0.0553 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: 0.679
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

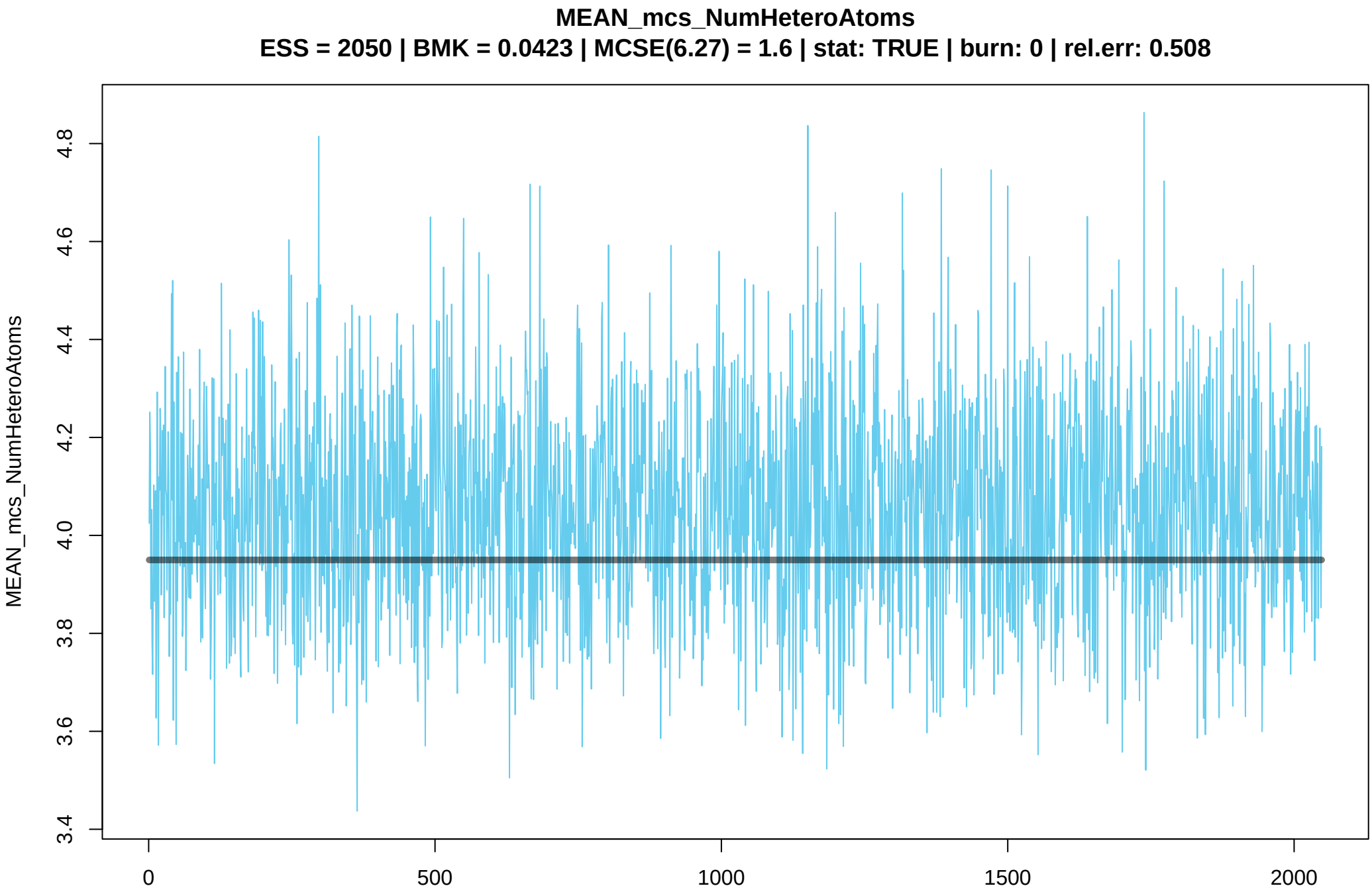

Pdatum7
ESS = 1690 | BMK = 0.0504 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 0.767
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

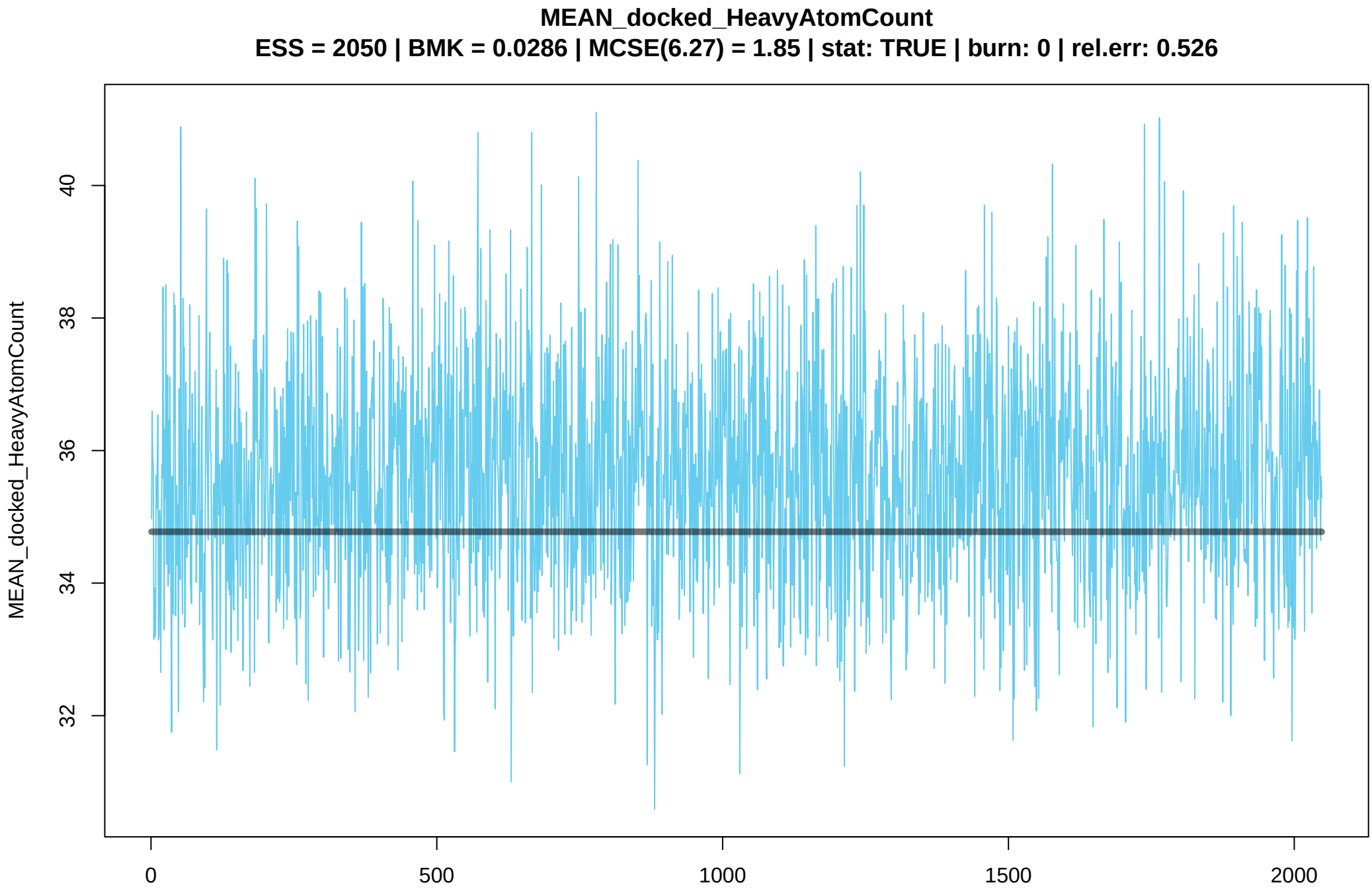

Pdatum8
ESS = 267 | BMK = 0.114 | MCSE(6.27) = 5.6 | stat: TRUE | burn: 1428 | rel.err: 0.562
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

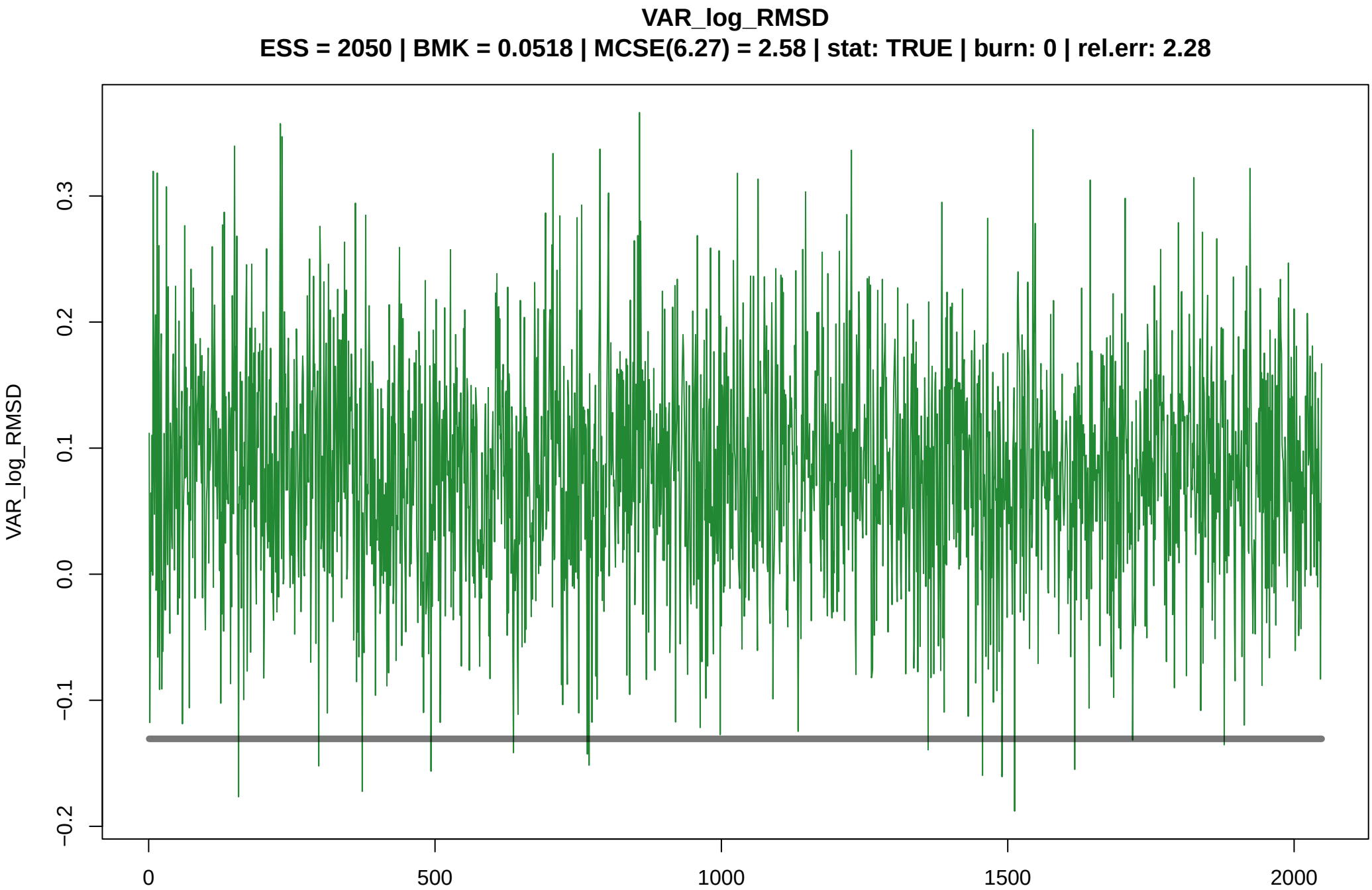

Dcov
ESS = 2050 | BMK = 0.0756 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0 | rel.err: 1.52
Dcov
0
−1
−2
−3
−4
0
500
1000
1500
2000

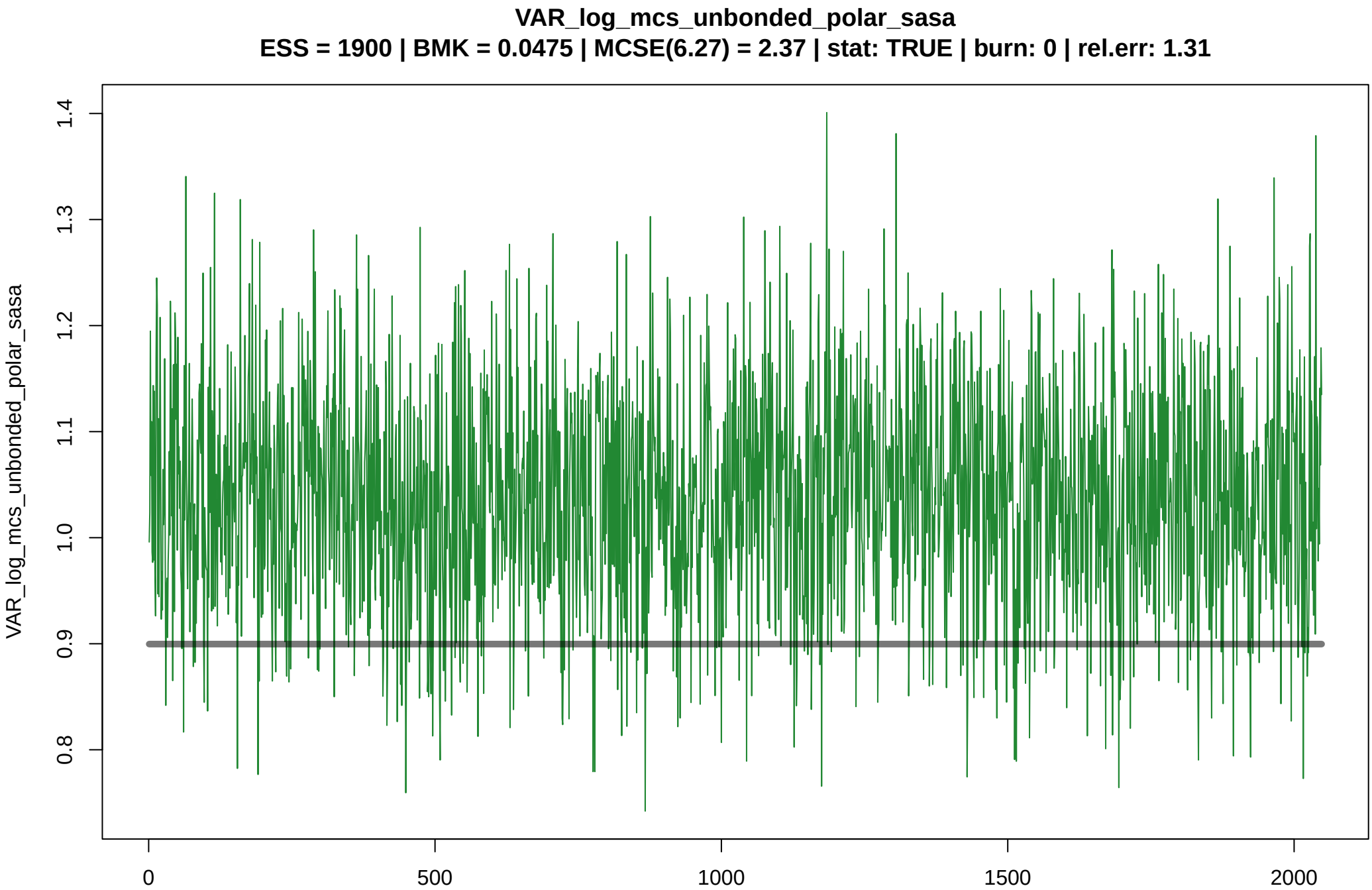

MEAN_log_RMSD
ESS = 1920 | BMK = 0.0326 | MCSE(6.27) = 2.34 | stat: TRUE | burn: 0 | rel.err: −0.614
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

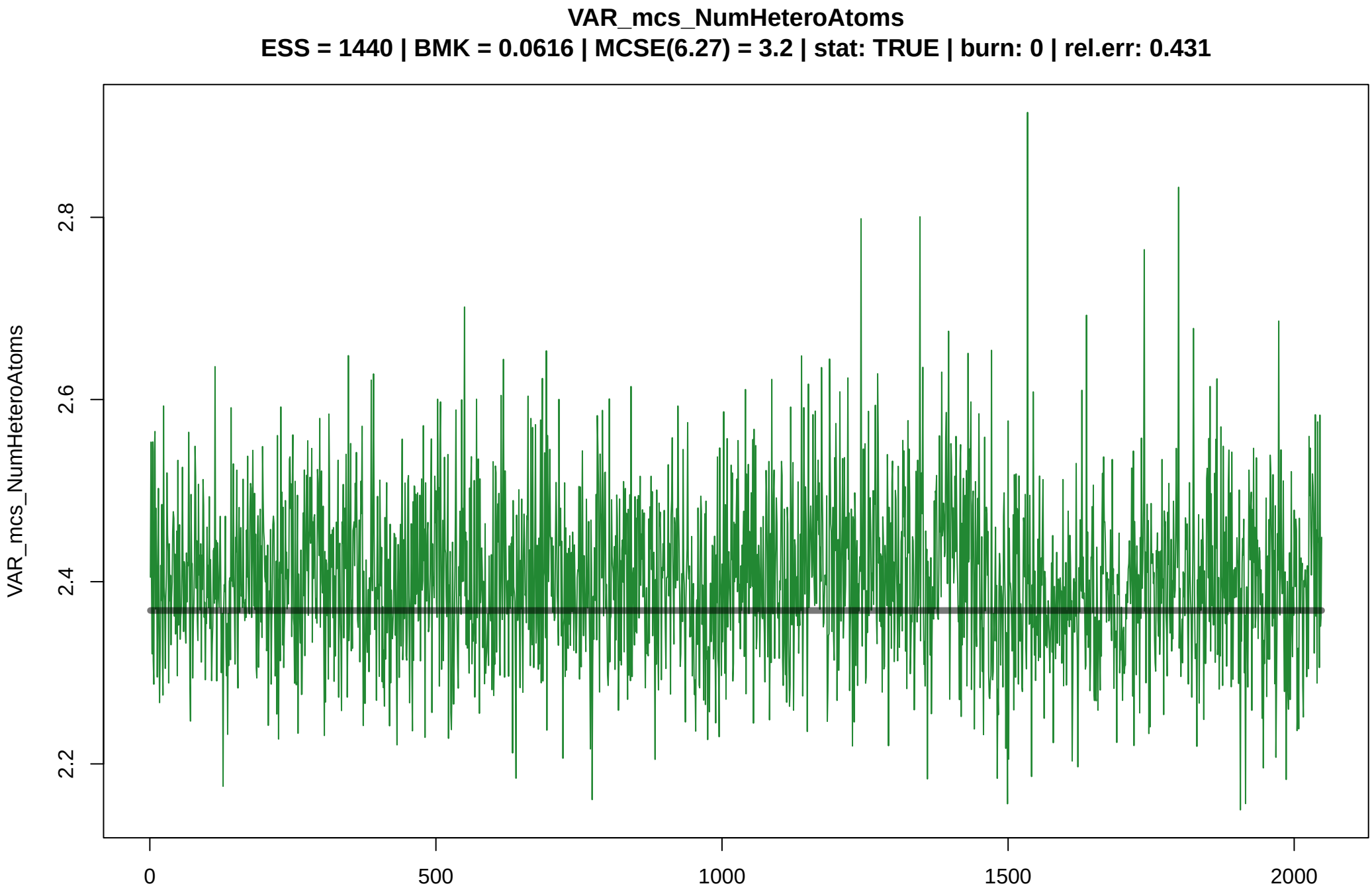

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1840 | BMK = 0.0408 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0 | rel.err: −0.176
MEAN_log_mcs_unbonded_polar_sasa
1.1
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0
500
1000
1500
2000

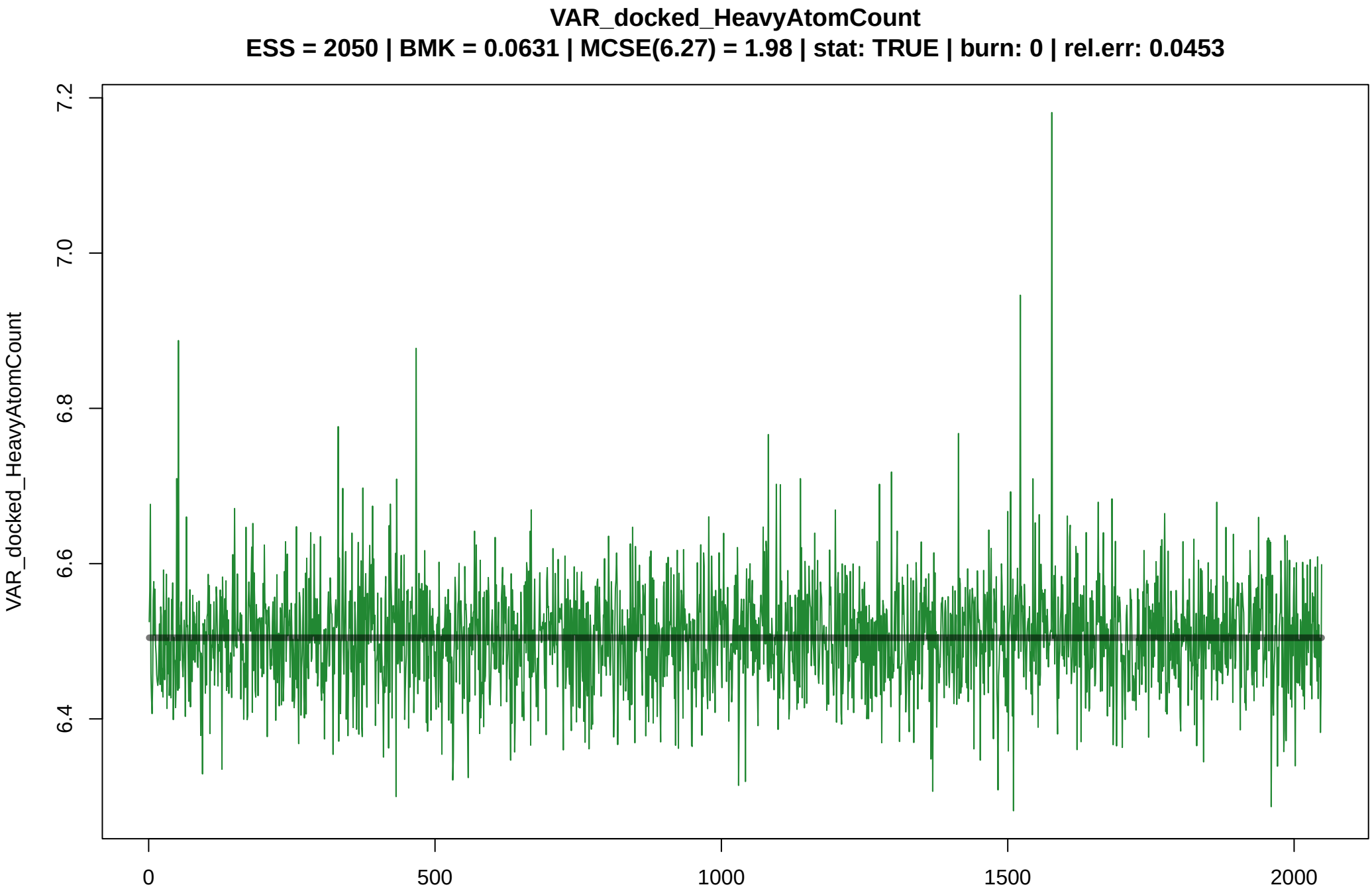

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0423 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 0.508
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

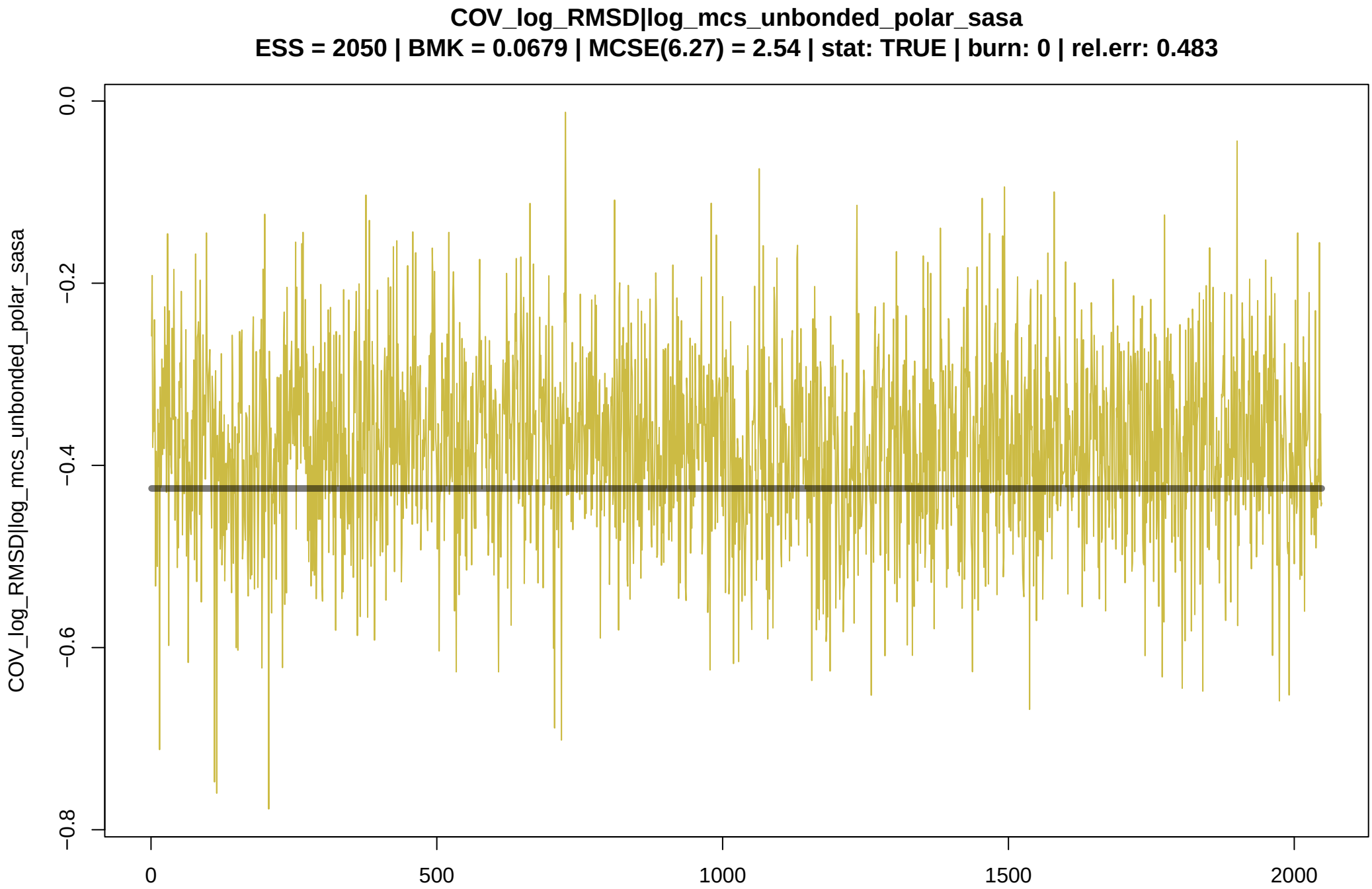

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0286 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: 0.526
MEAN_docked_HeavyAtomCount
32
34
36
38
40
0
500
1000
1500
2000

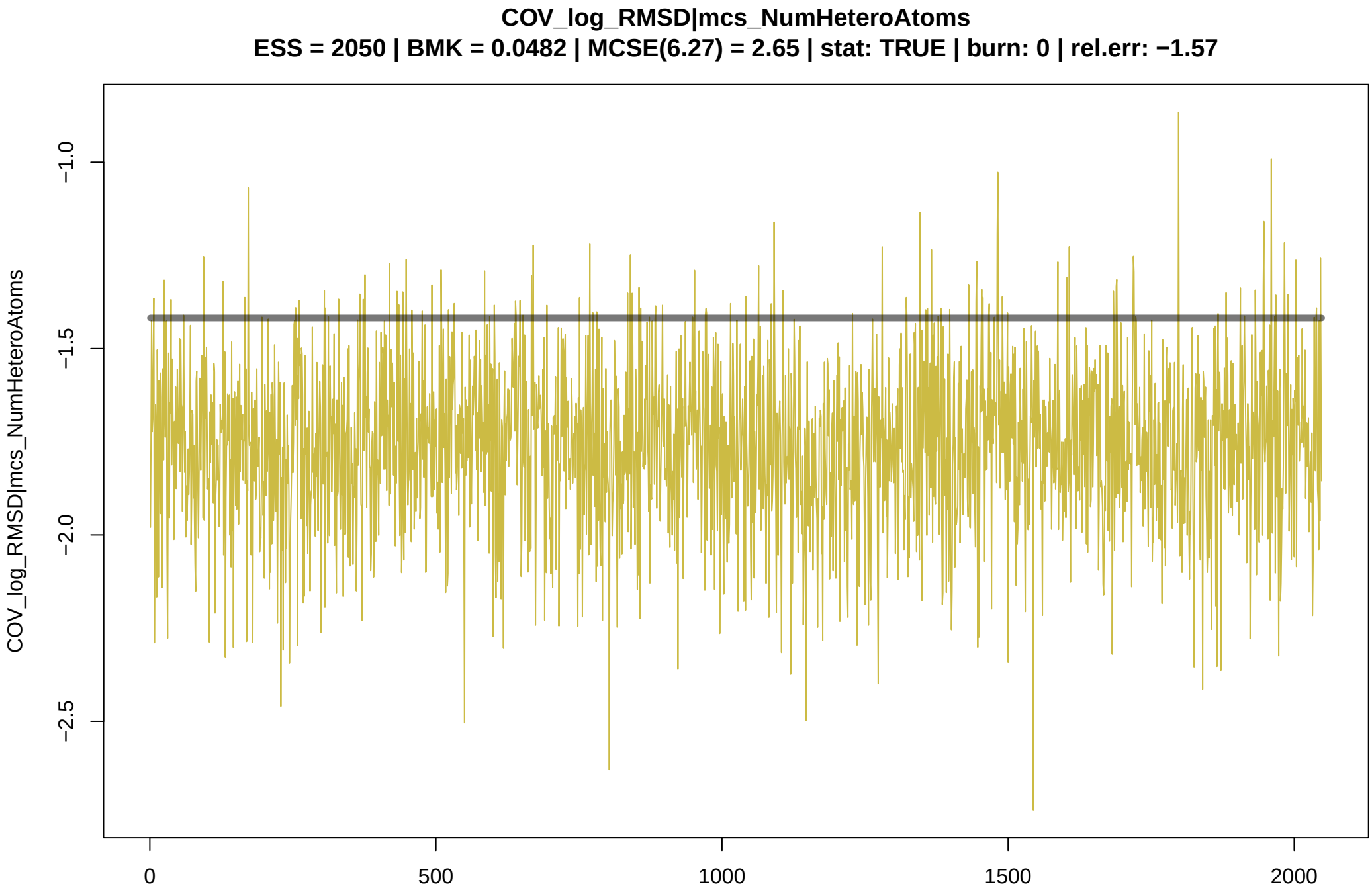

VAR_log_RMSD
ESS = 2050 | BMK = 0.0518 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: 2.28
VAR_log_RMSD
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

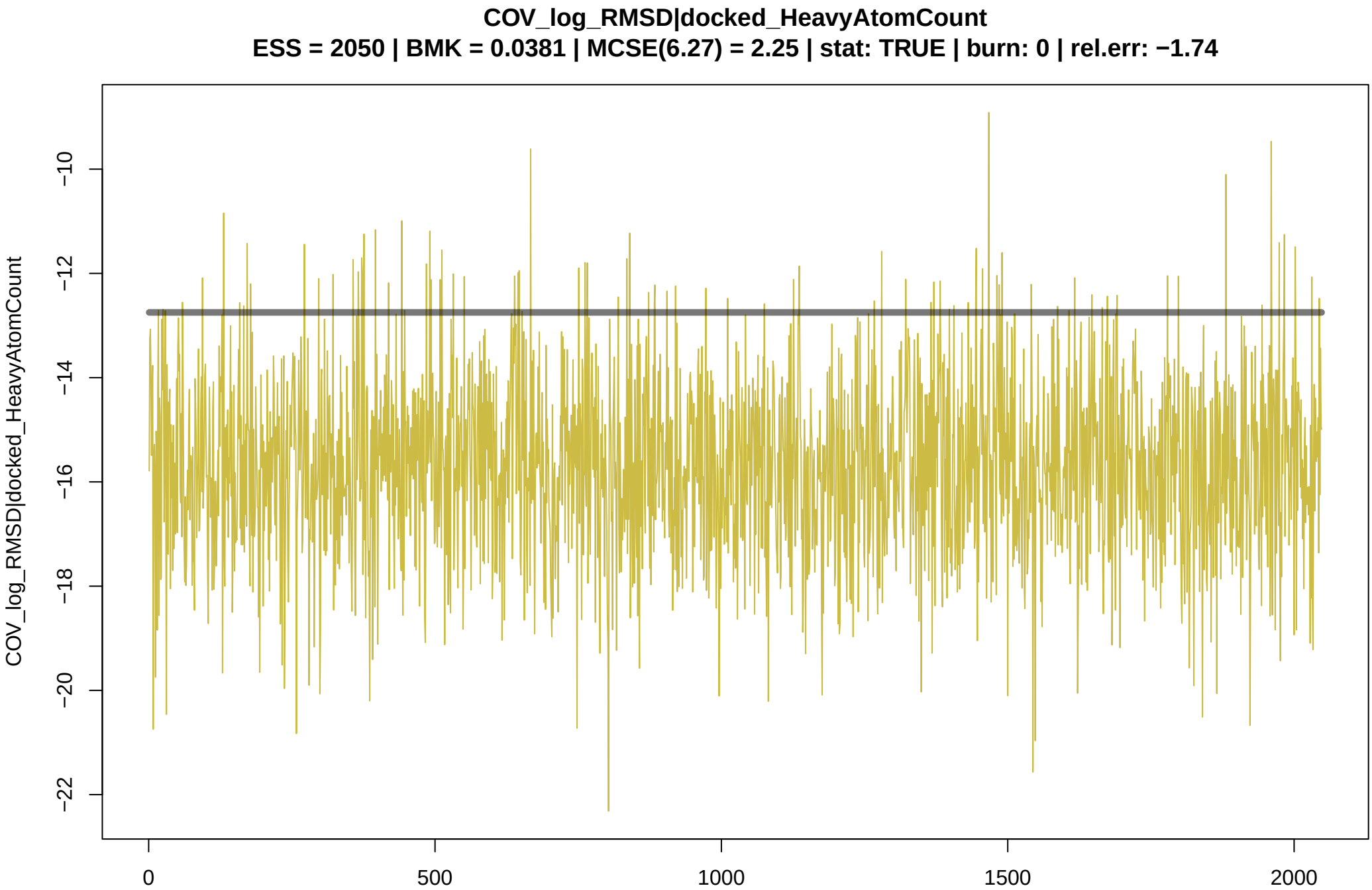

VAR_log_mcs_unbonded_polar_sasa
ESS = 1900 | BMK = 0.0475 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: 1.31
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

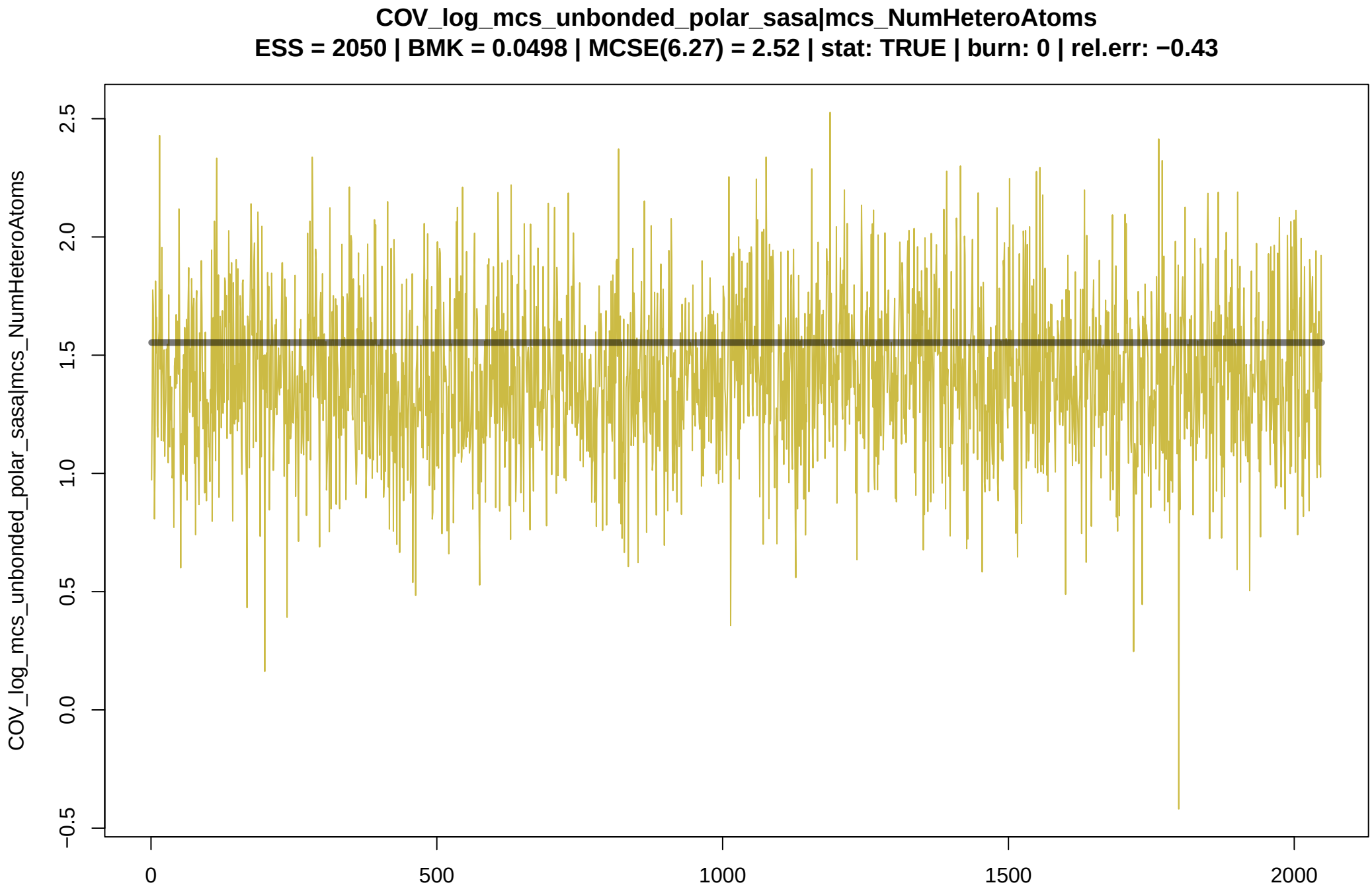

VAR_mcs_NumHeteroAtoms
ESS = 1440 | BMK = 0.0616 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: 0.431
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

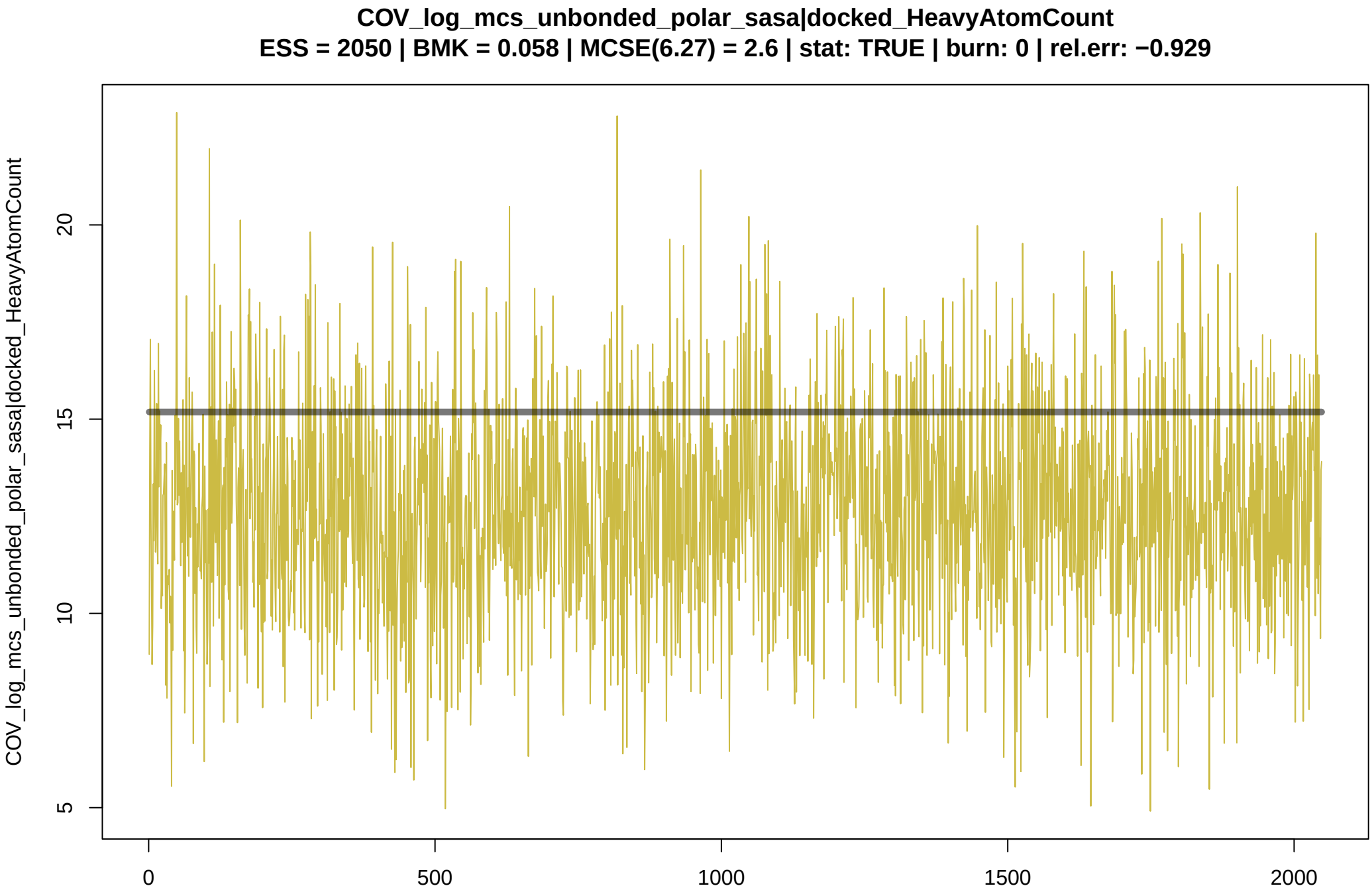

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0631 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | rel.err: 0.0453
VAR_docked_HeavyAtomCount
7.2
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

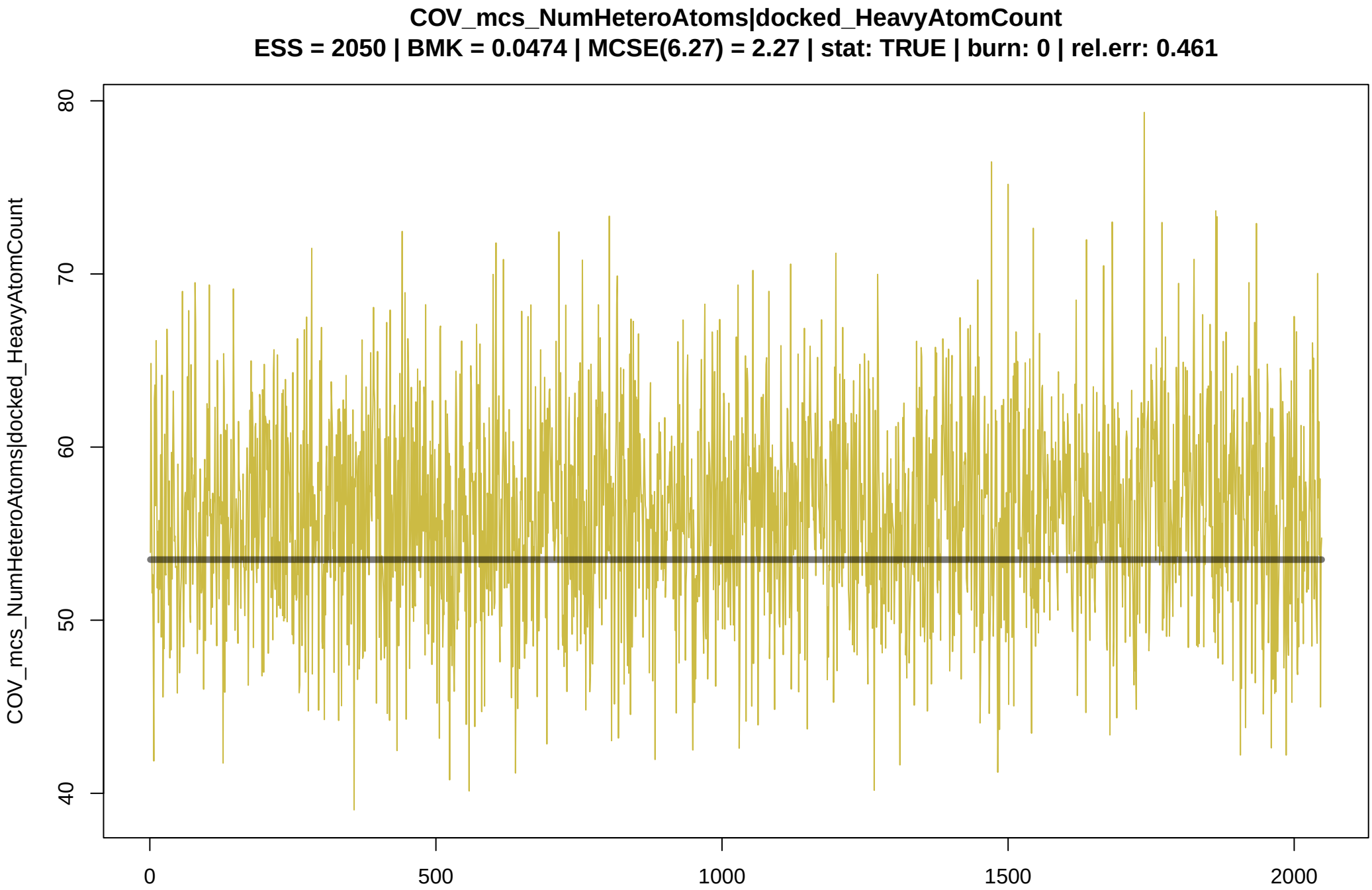

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0679 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: 0.483
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0482 | MCSE(6.27) = 2.65 | 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 = 0.0381 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: −1.74
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 = 0.0498 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: −0.43
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.058 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: −0.929
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 = 0.0474 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: 0.461
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
80
70
60
50
40
0
500
1000
1500
2000