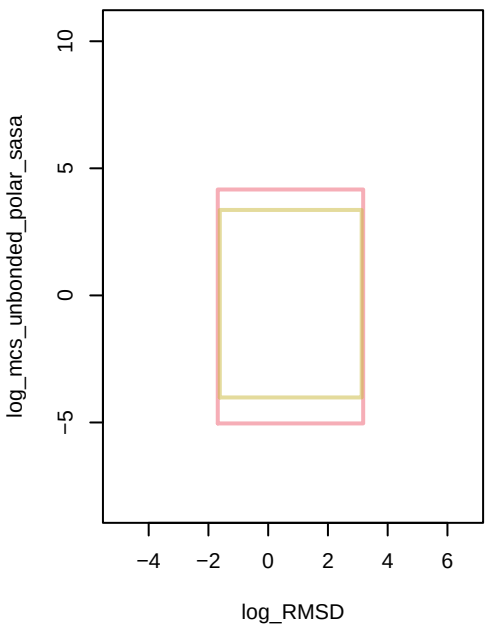
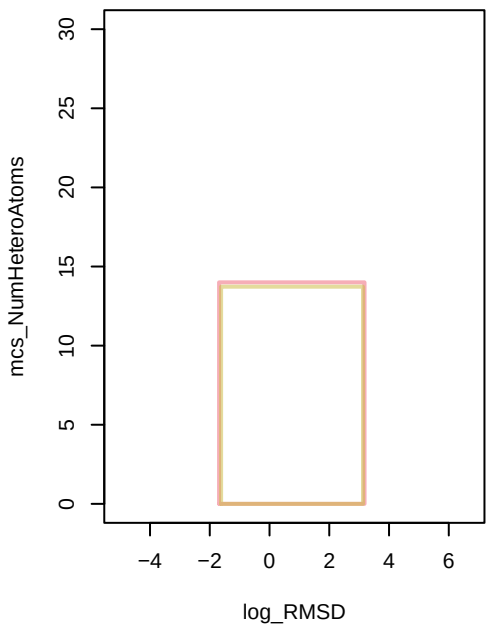
−− STATS maxD −−
min ESS = 104.691287215867
max BMK = 0.145194365904629
max MCSE = 8.41593729887374
all stationary: TRUE
burn: 0
max rel.err.: 2.12768573717581

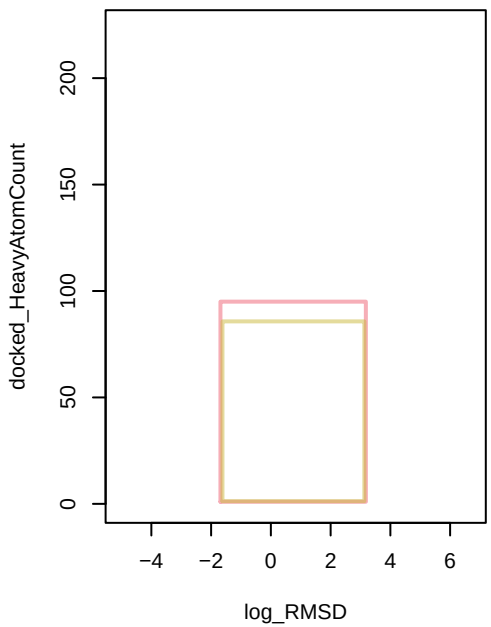
−− STATS 2D −−
min ESS = 1613.42374266216
max BMK = 0.061134083392721 6
max MCSE = 2.46681101867883
all stationary: TRUE
burn: 0
max rel.err.: 1.77726479076856

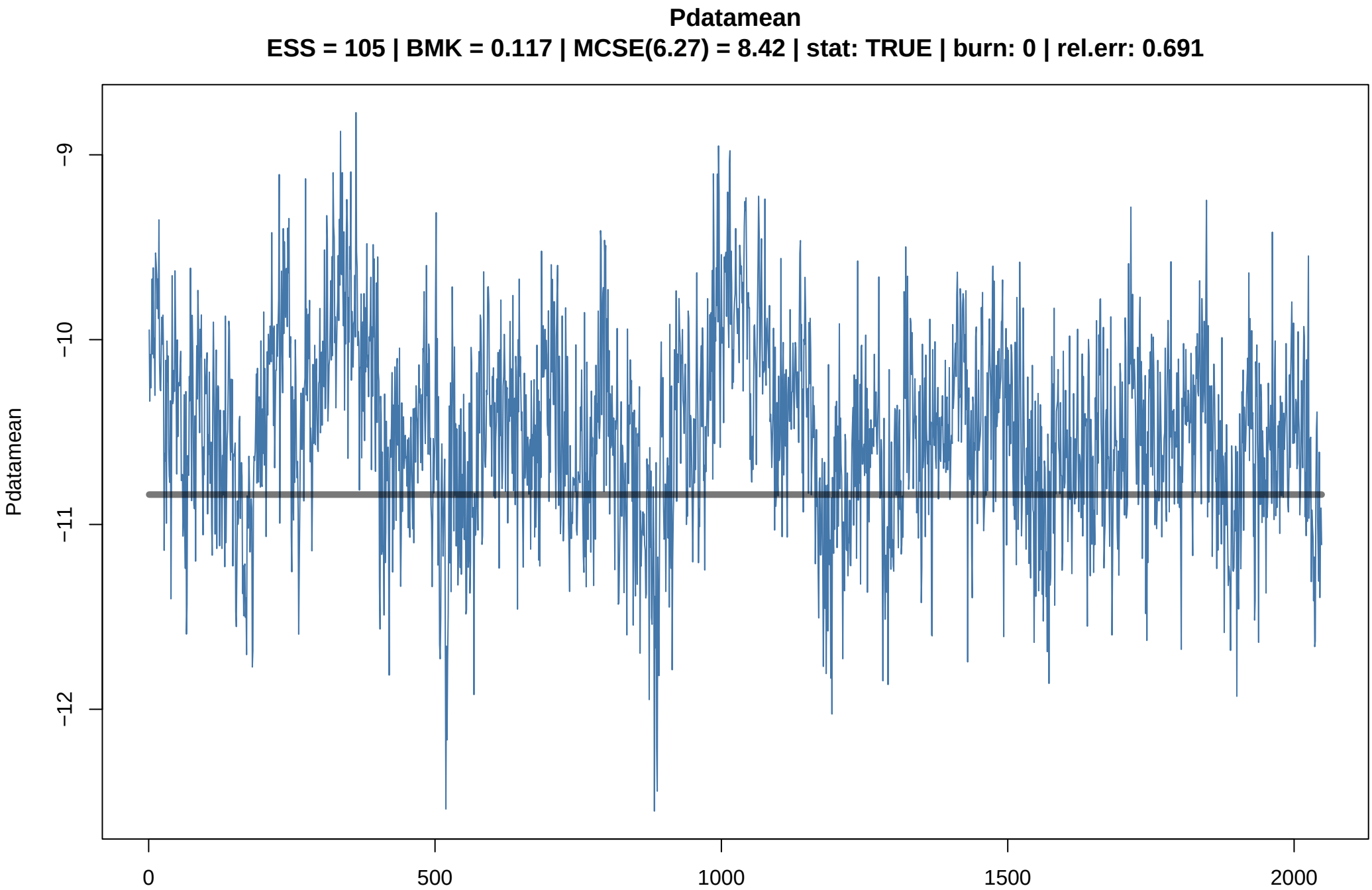
−− STATS 1D −−
min ESS = 1772.73538981322
max BMK = 0.069586370997616 8
max MCSE = 2.5134779662317
all stationary: TRUE
burn: 0
max rel.err.: 2.273523569532

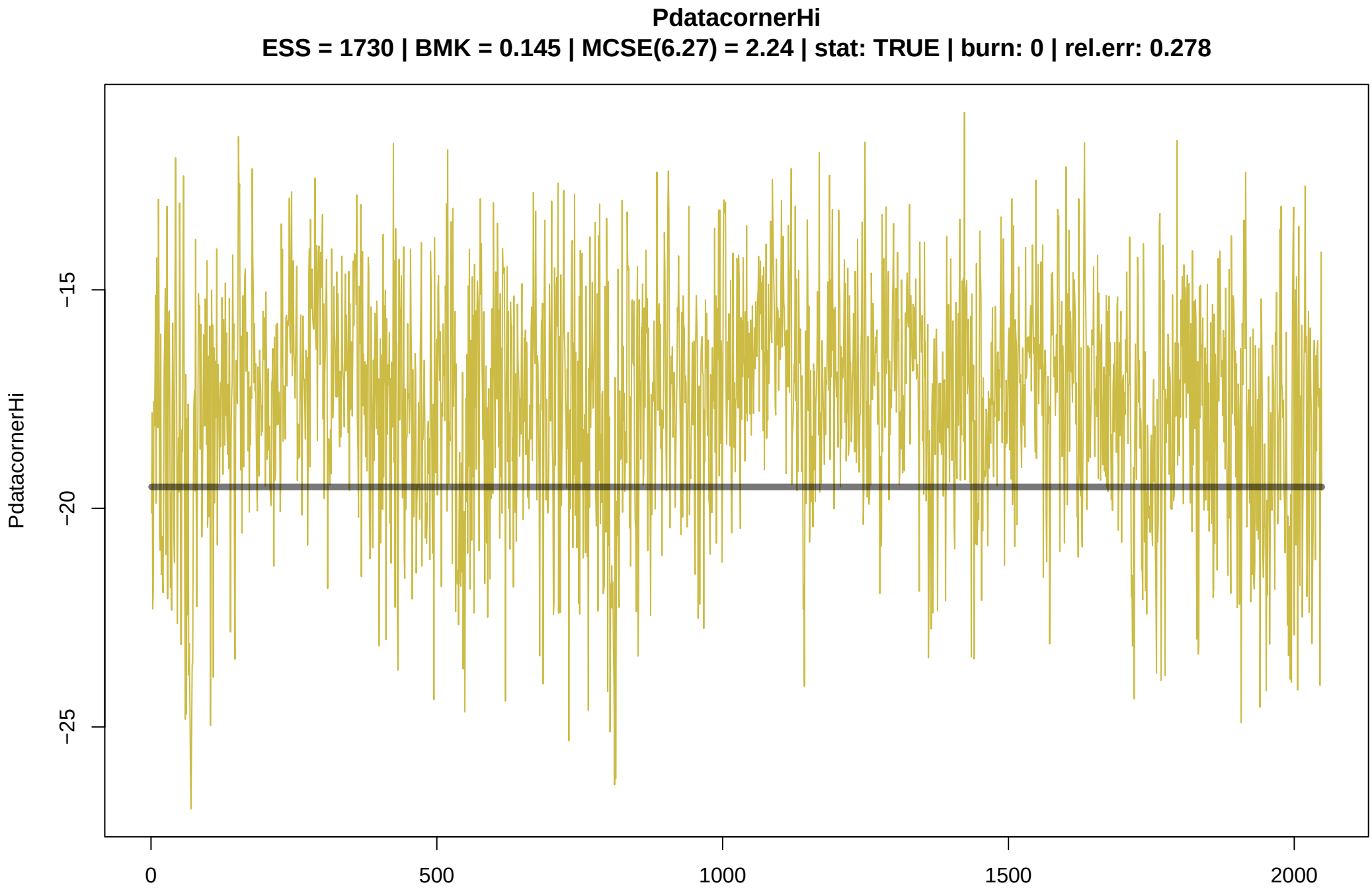
Occupied clusters: 9 of 16

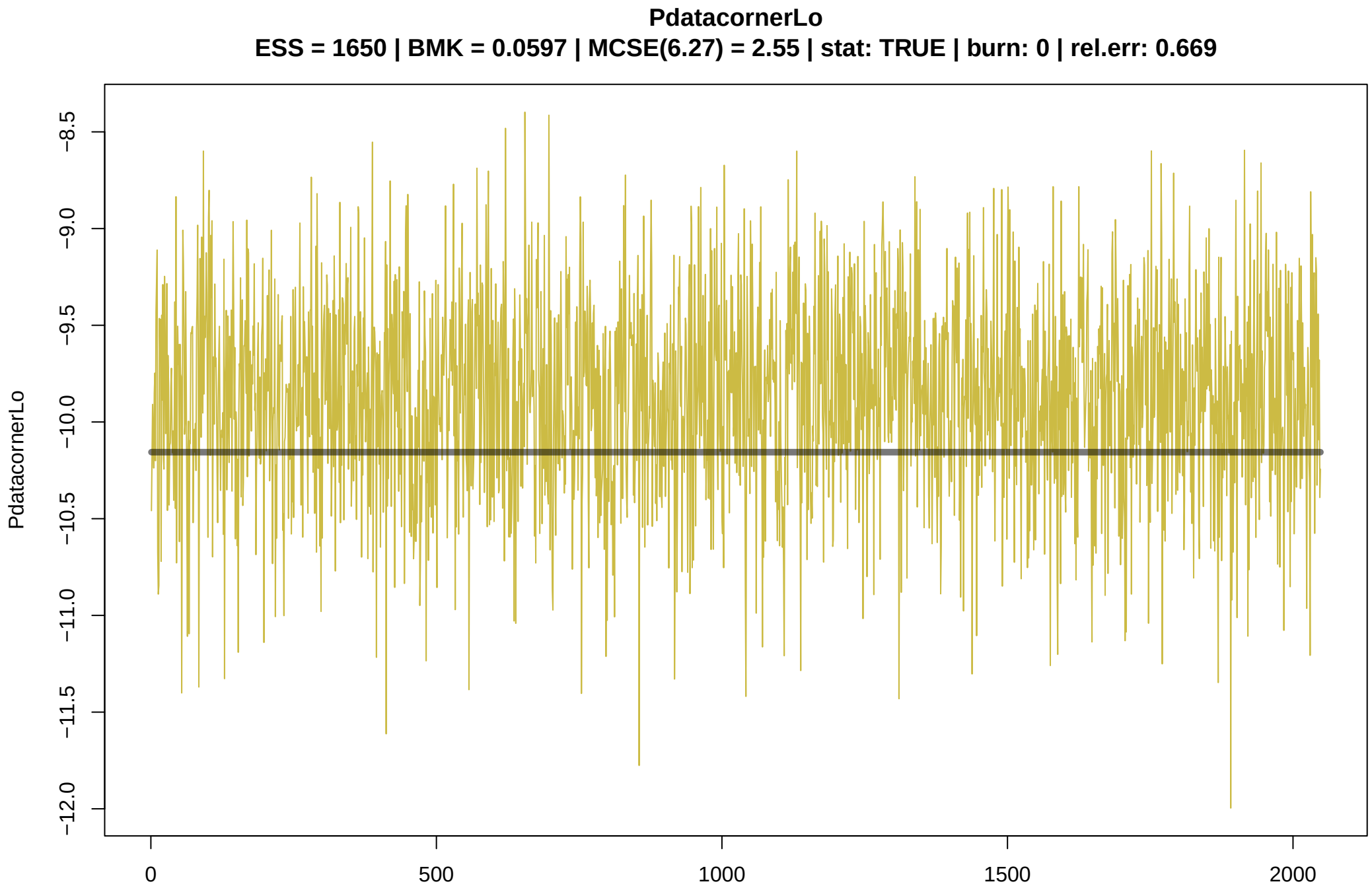

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

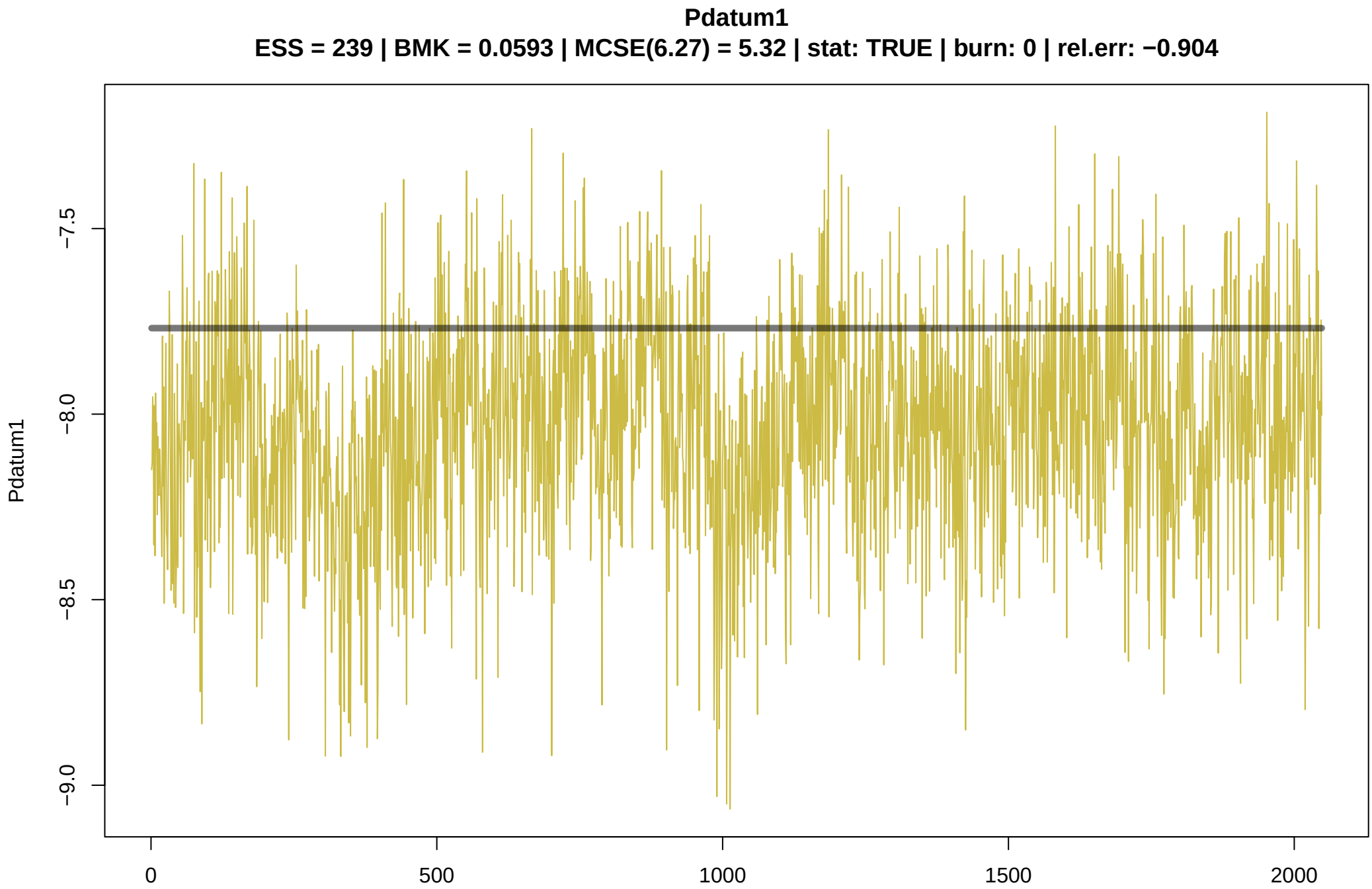

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

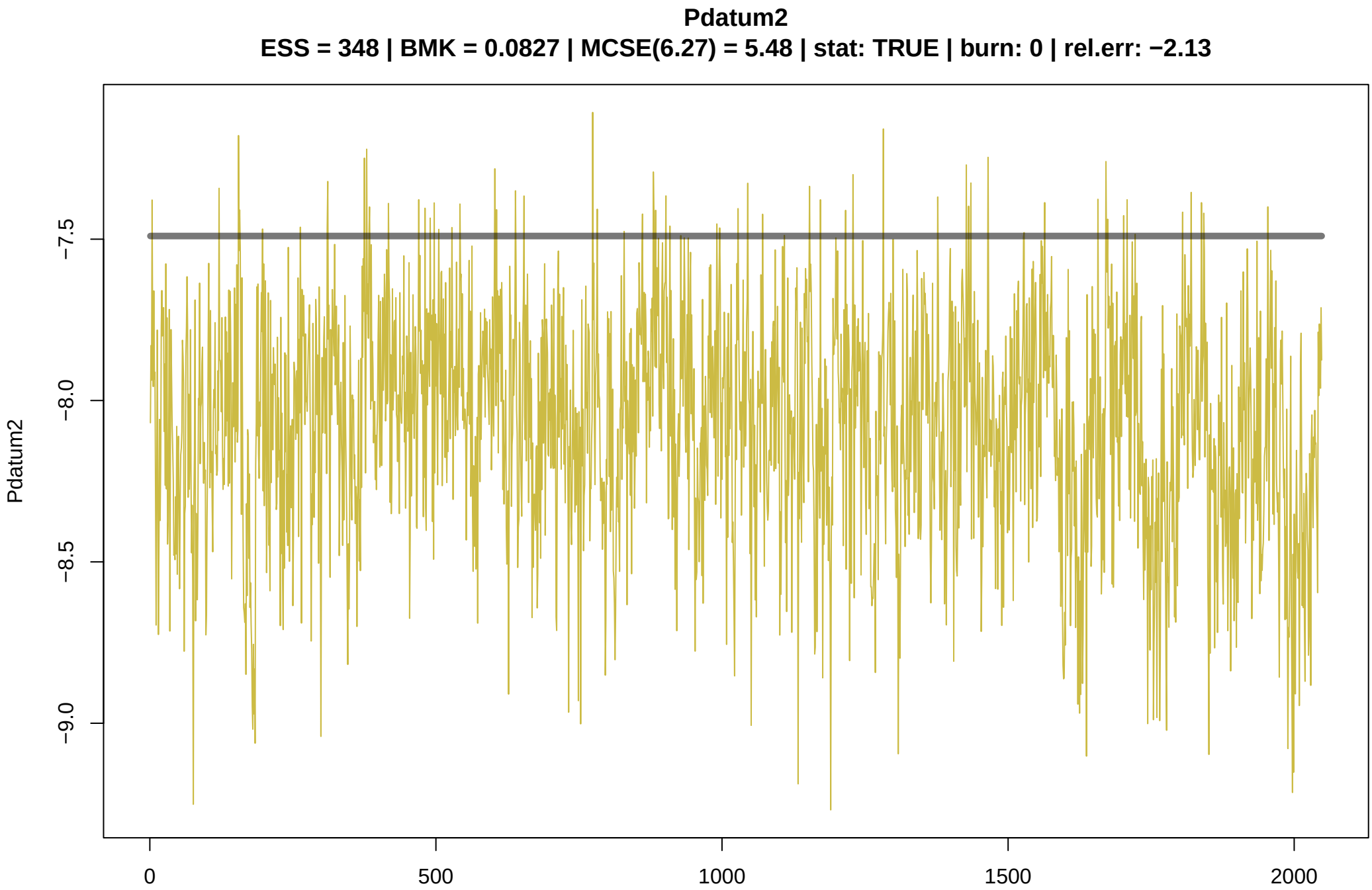

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

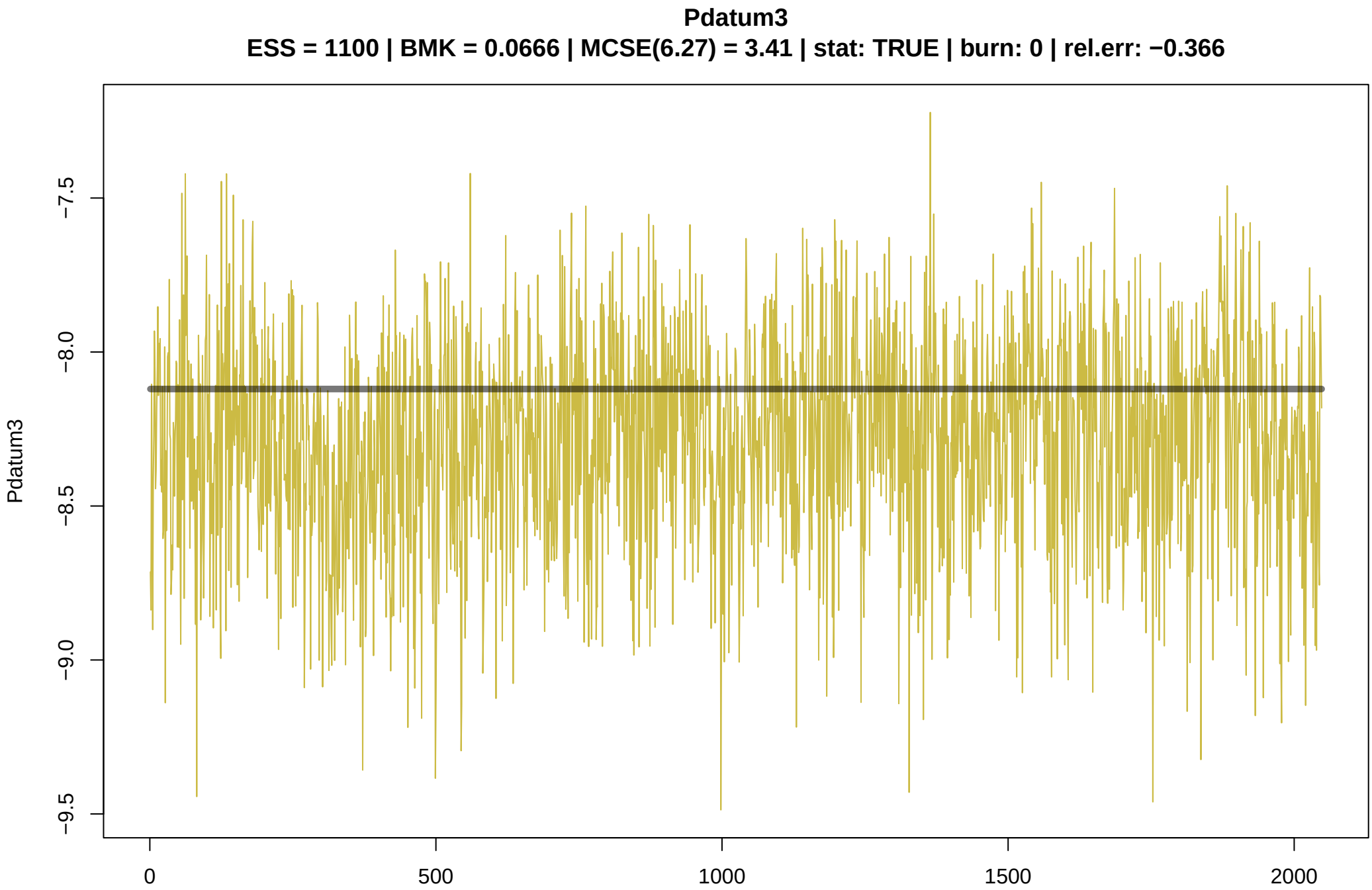

Pdatamean
ESS = 105 | BMK = 0.117 | MCSE(6.27) = 8.42 | stat: TRUE | burn: 0 | rel.err: 0.691
Pdatamean
−9
−10
−11
−12
0
500
1000
1500
2000

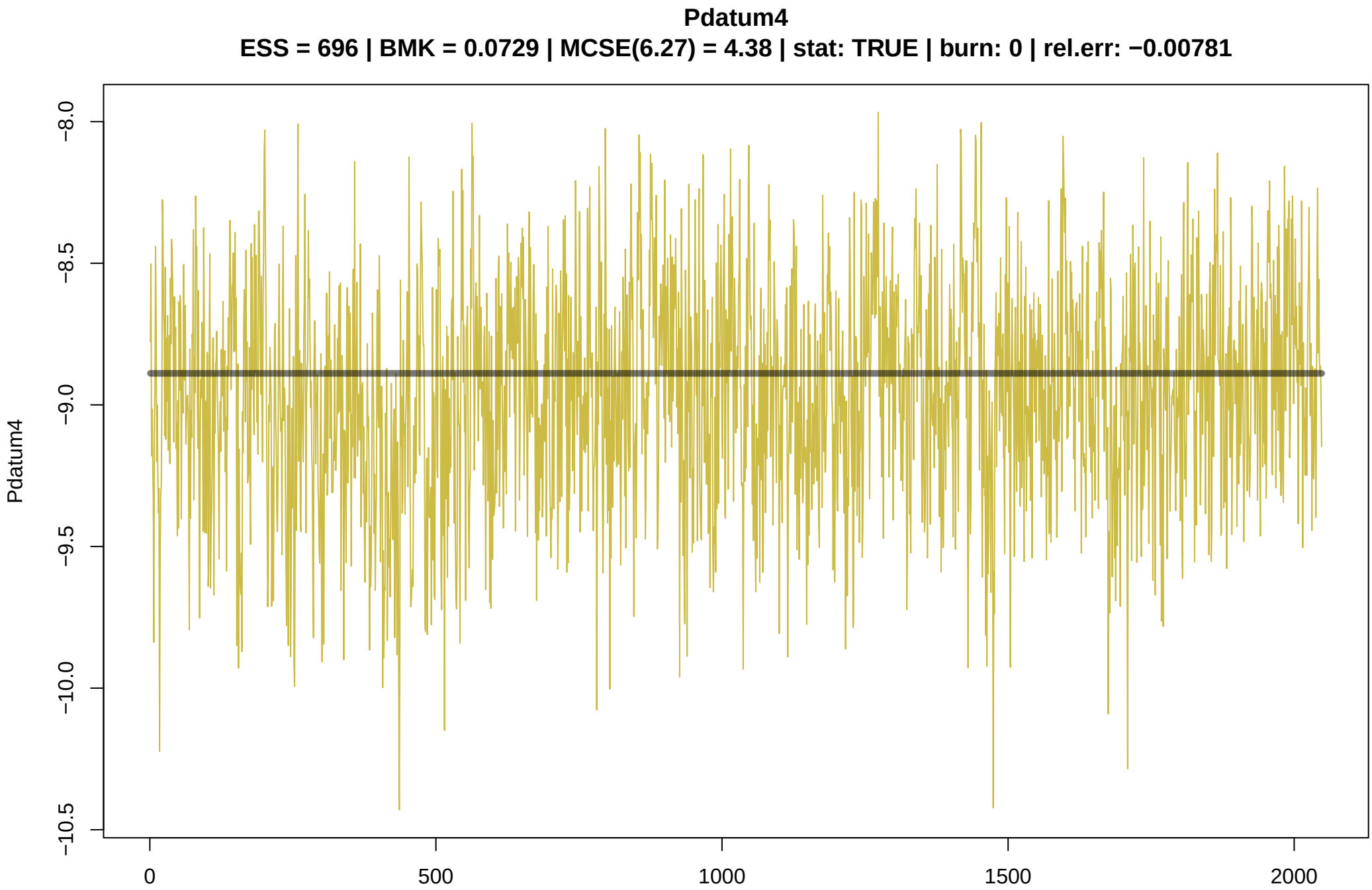

PdatacornerHi
ESS = 1730 | BMK = 0.145 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | rel.err: 0.278
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

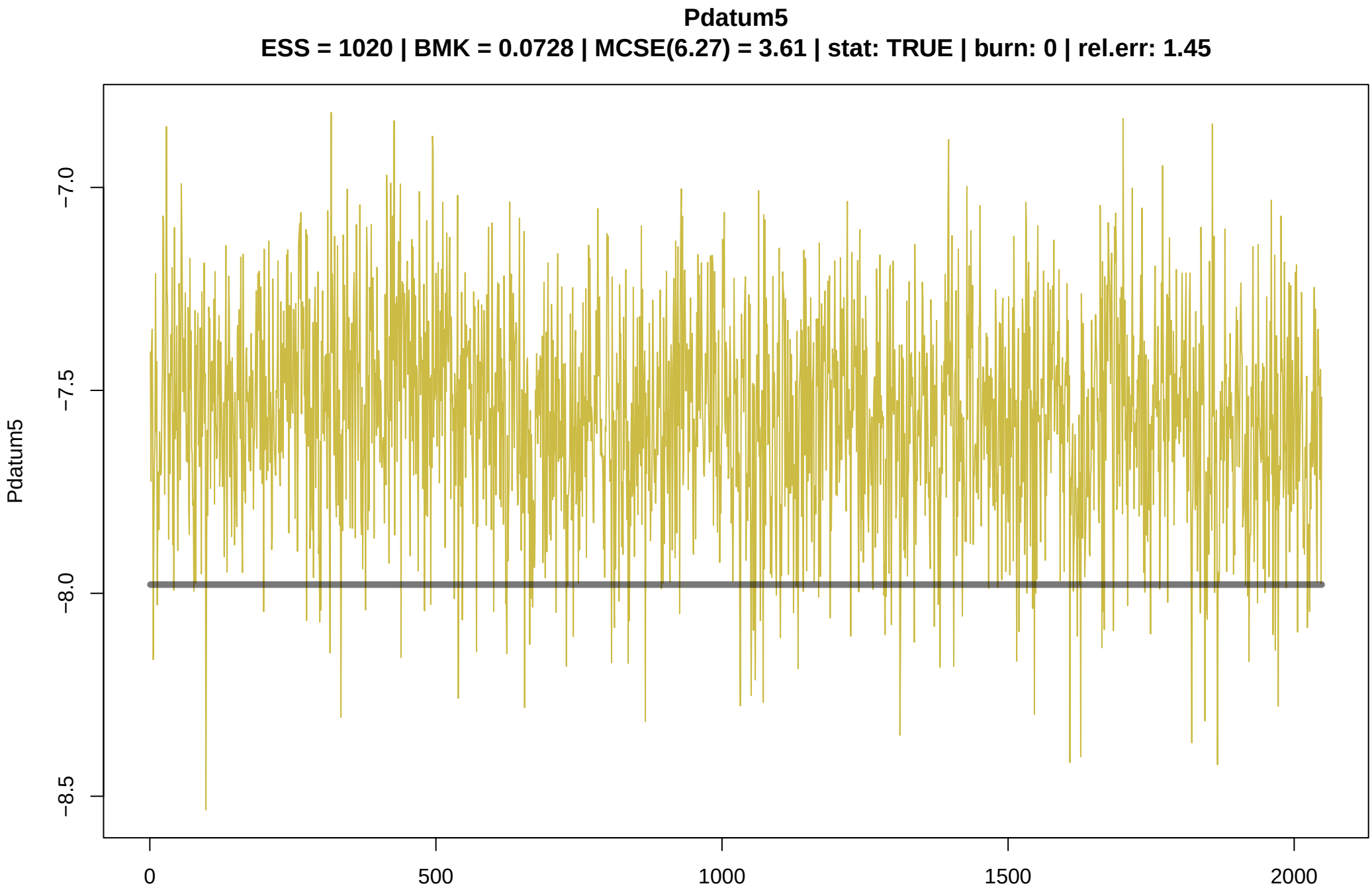

PdatacornerLo
ESS = 1650 | BMK = 0.0597 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 0.669
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

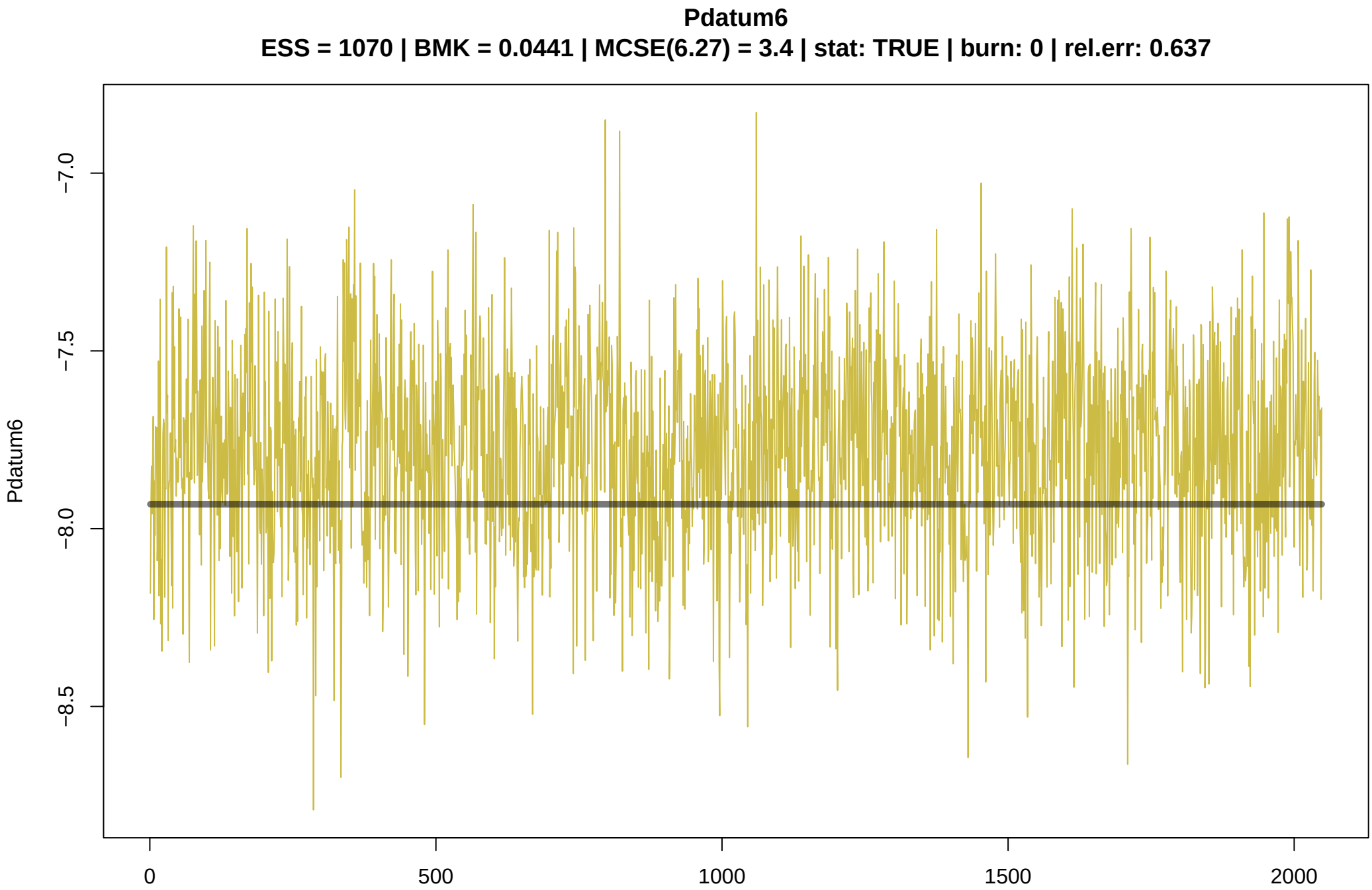

Pdatum1
ESS = 239 | BMK = 0.0593 | MCSE(6.27) = 5.32 | stat: TRUE | burn: 0 | rel.err: −0.904
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

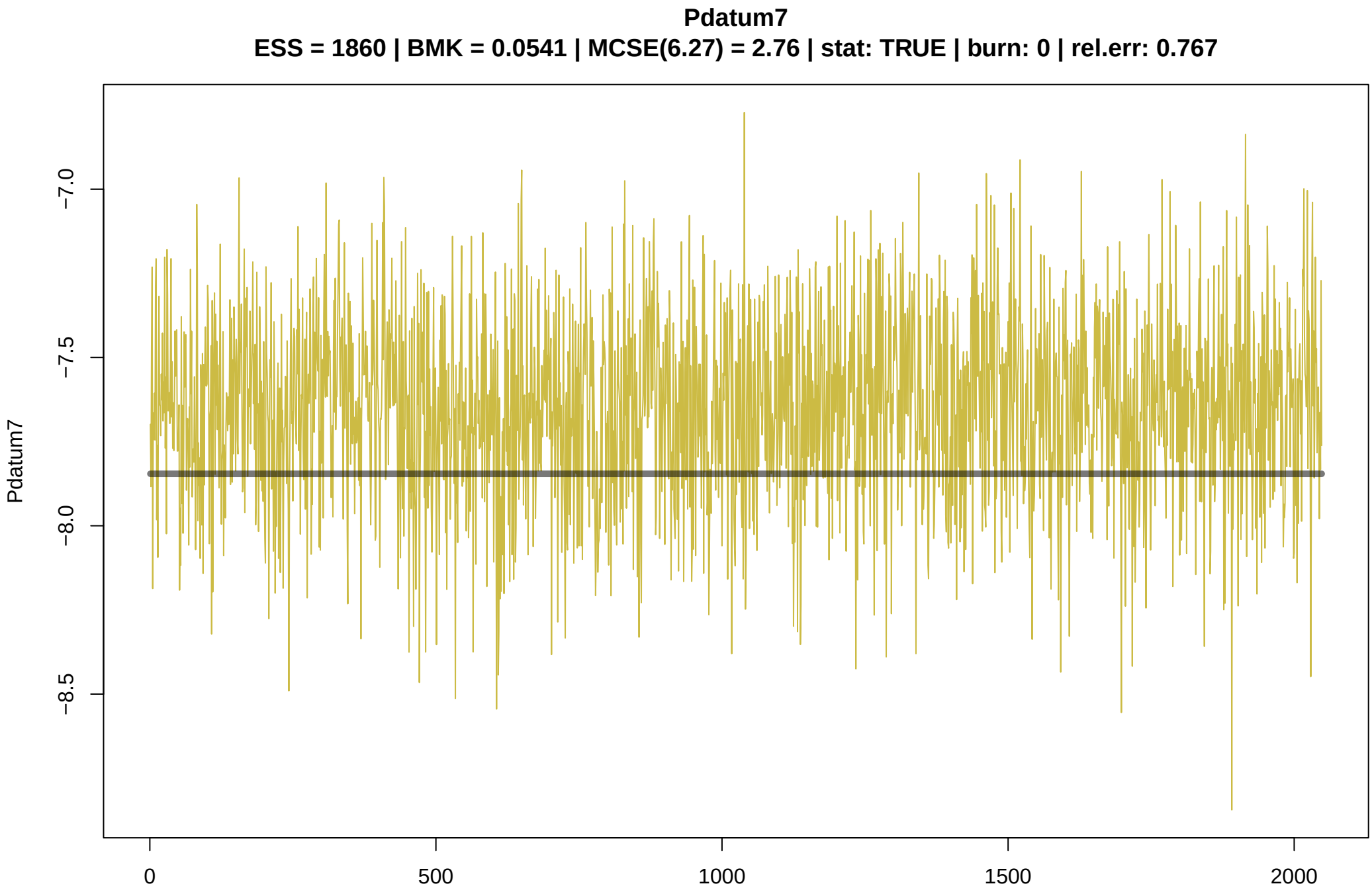

Pdatum2
ESS = 348 | BMK = 0.0827 | MCSE(6.27) = 5.48 | stat: TRUE | burn: 0 | rel.err: −2.13
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

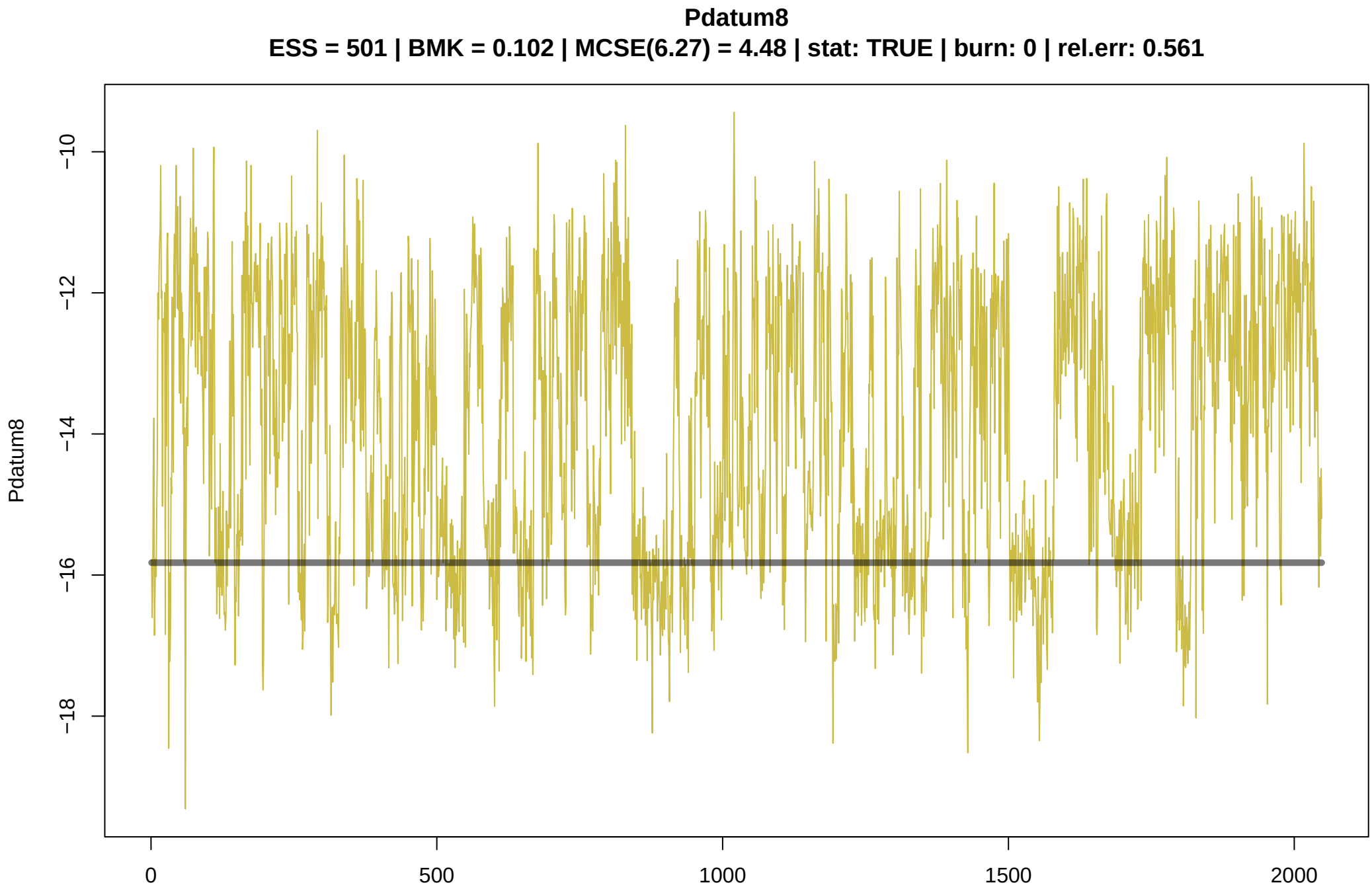

Pdatum3
ESS = 1100 | BMK = 0.0666 | MCSE(6.27) = 3.41 | stat: TRUE | burn: 0 | rel.err: −0.366
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

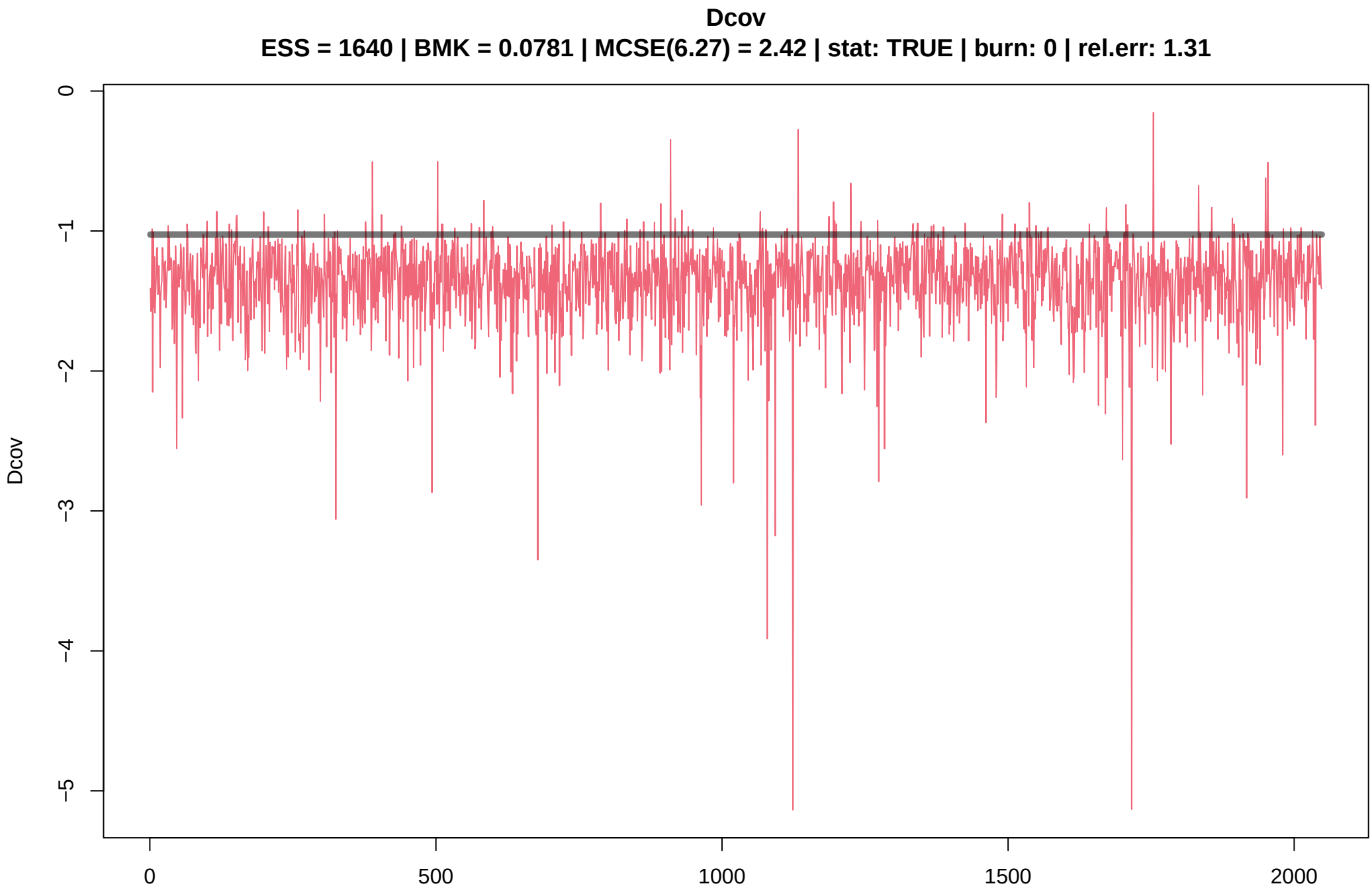

Pdatum4
ESS = 696 | BMK = 0.0729 | MCSE(6.27) = 4.38 | stat: TRUE | burn: 0 | rel.err: −0.00781
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

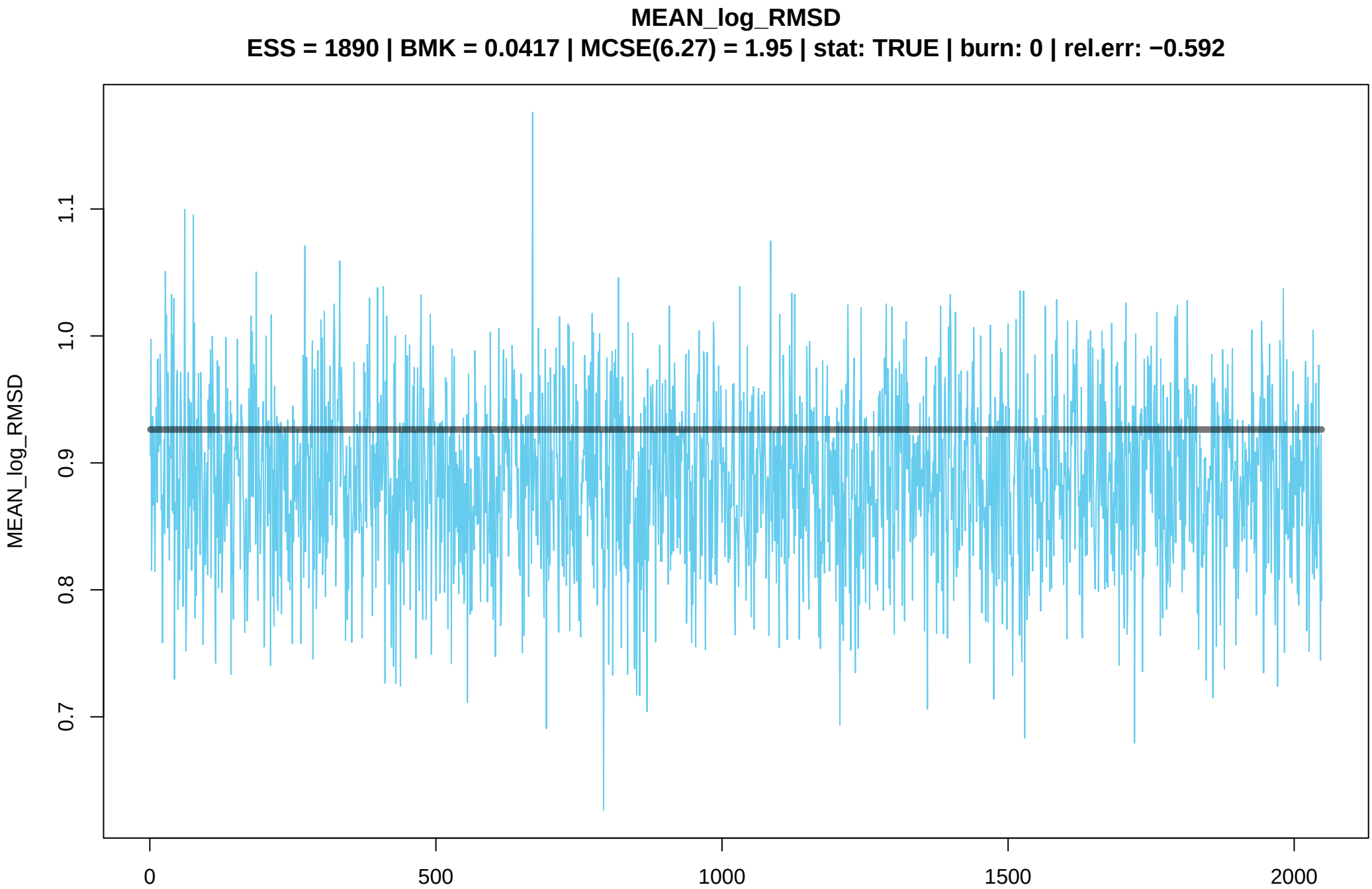

Pdatum5
ESS = 1020 | BMK = 0.0728 | MCSE(6.27) = 3.61 | stat: TRUE | burn: 0 | rel.err: 1.45
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

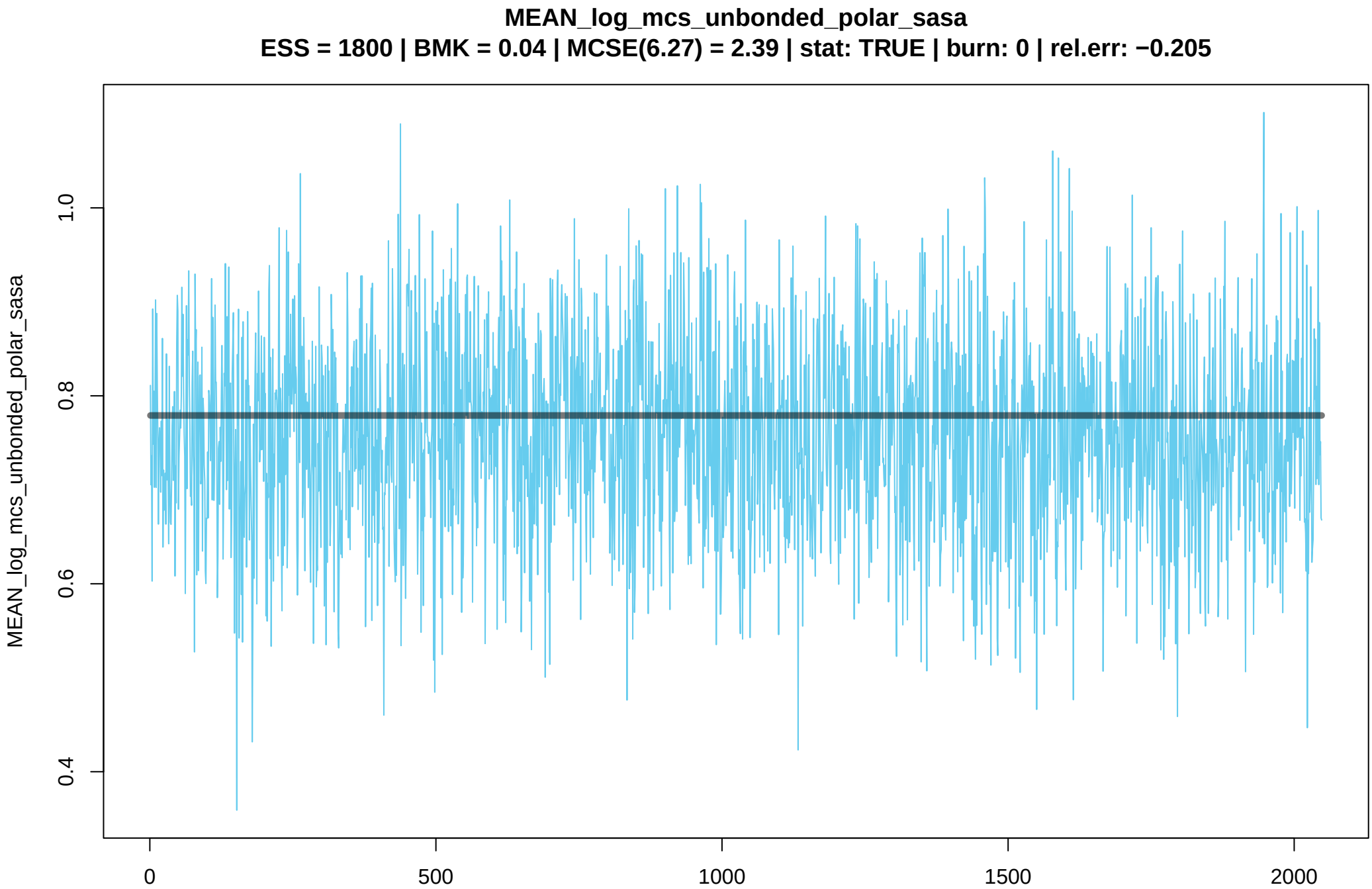

Pdatum6
ESS = 1070 | BMK = 0.0441 | MCSE(6.27) = 3.4 | stat: TRUE | burn: 0 | rel.err: 0.637
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

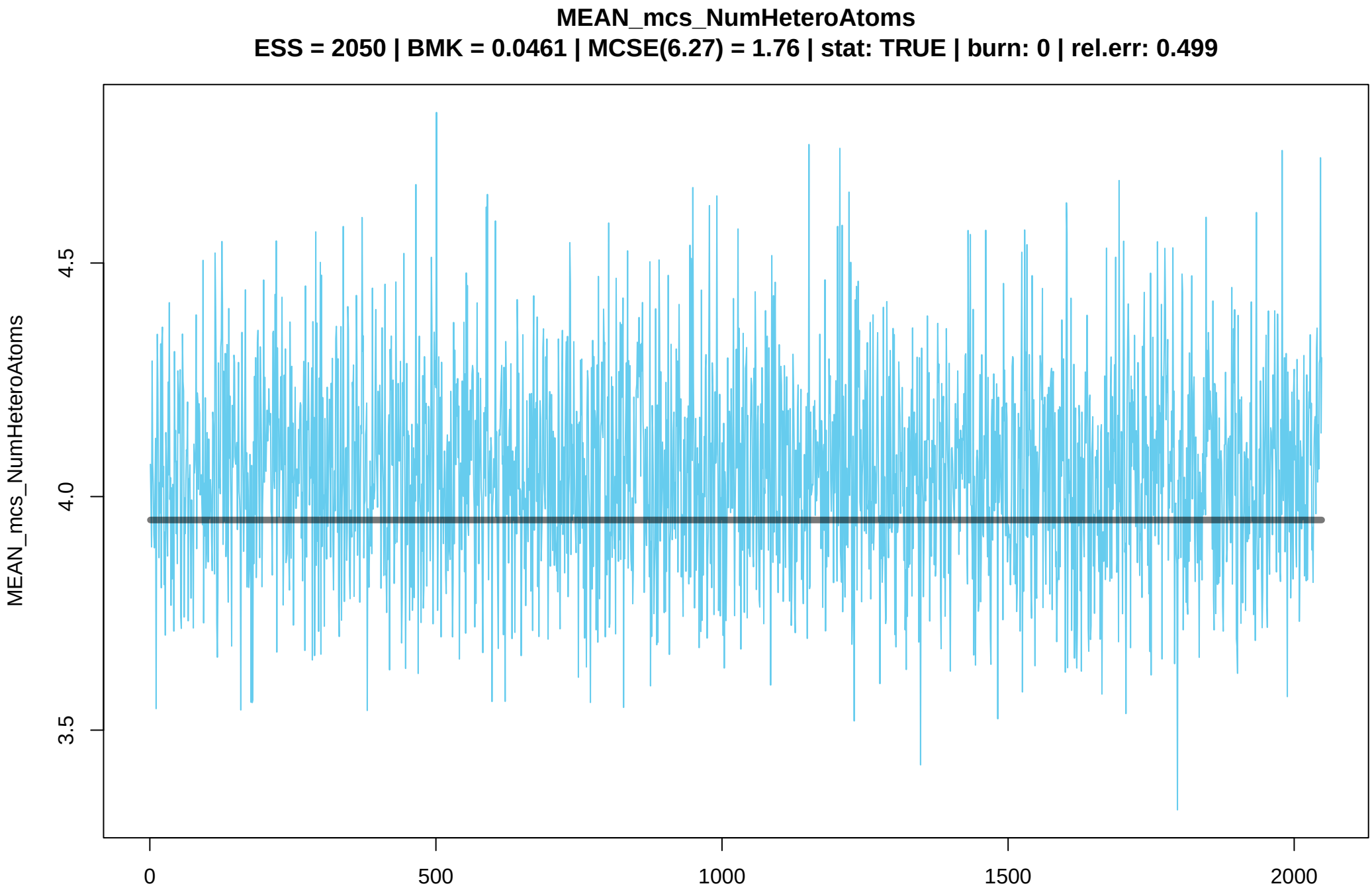

Pdatum7
ESS = 1860 | BMK = 0.0541 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0 | rel.err: 0.767
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

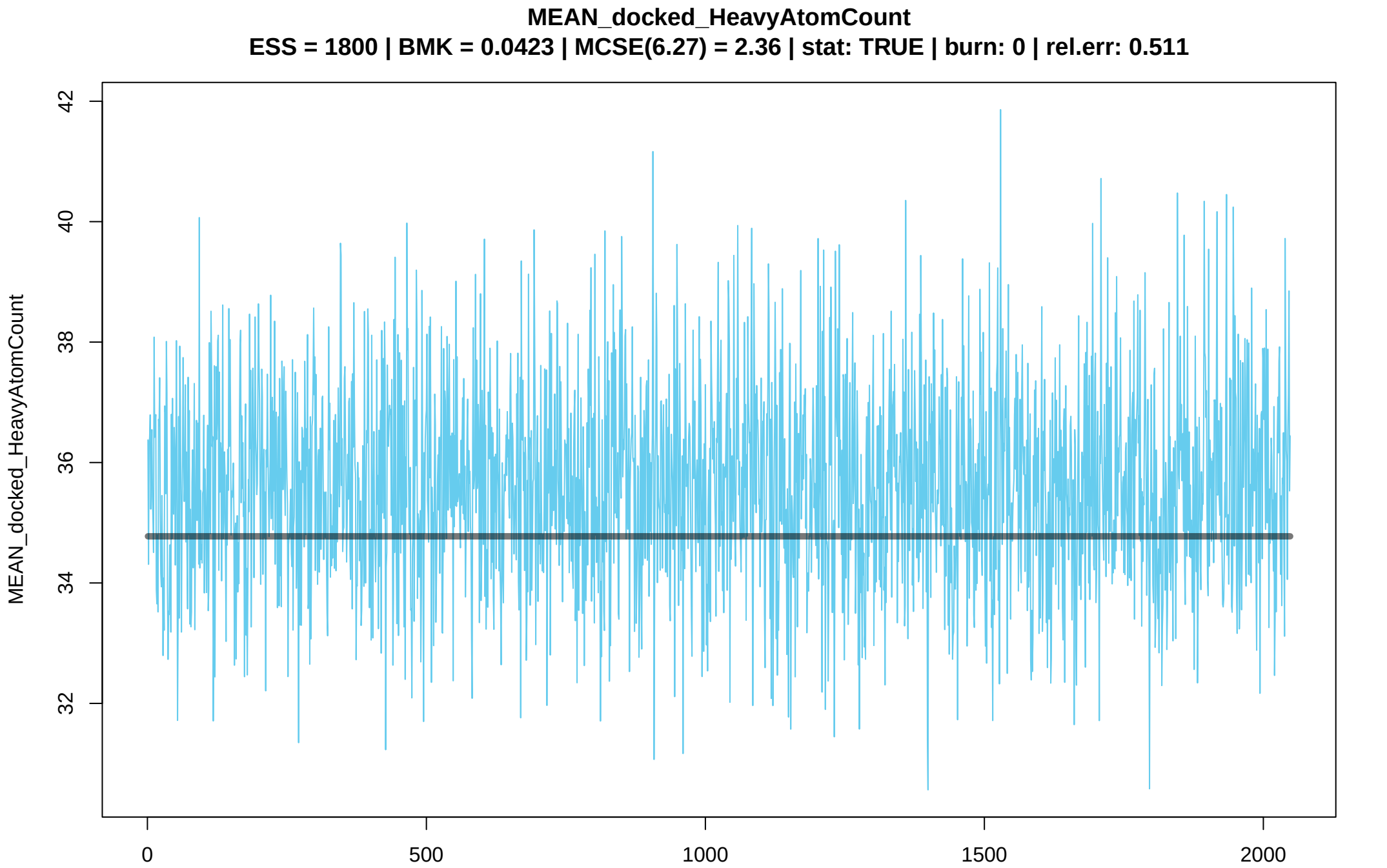

Pdatum8
ESS = 501 | BMK = 0.102 | MCSE(6.27) = 4.48 | stat: TRUE | burn: 0 | rel.err: 0.561
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

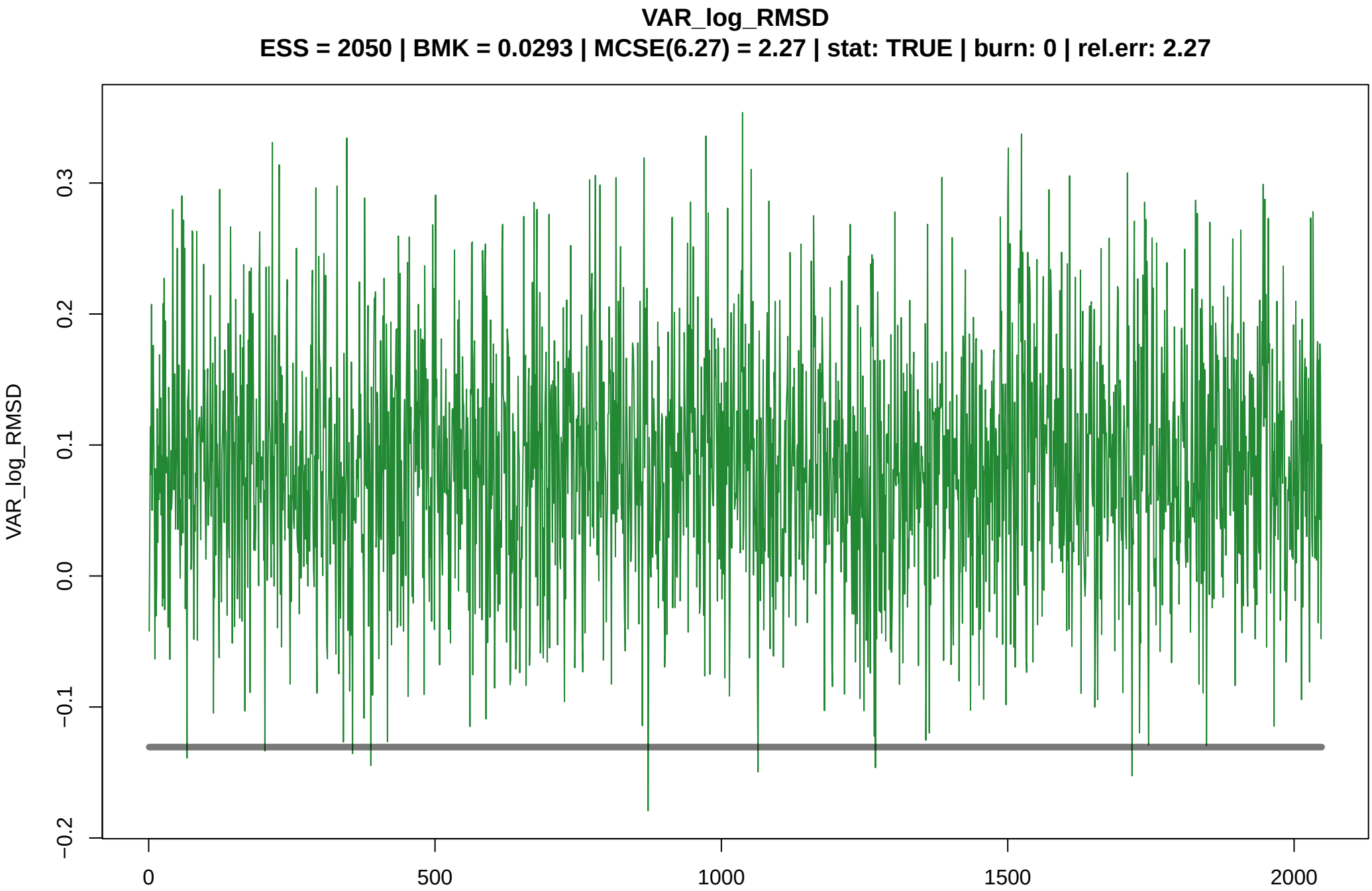

Dcov
ESS = 1640 | BMK = 0.0781 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 1.31
Dcov
0
−1
−2
−3
−4
−5
0
500
1000
1500
2000

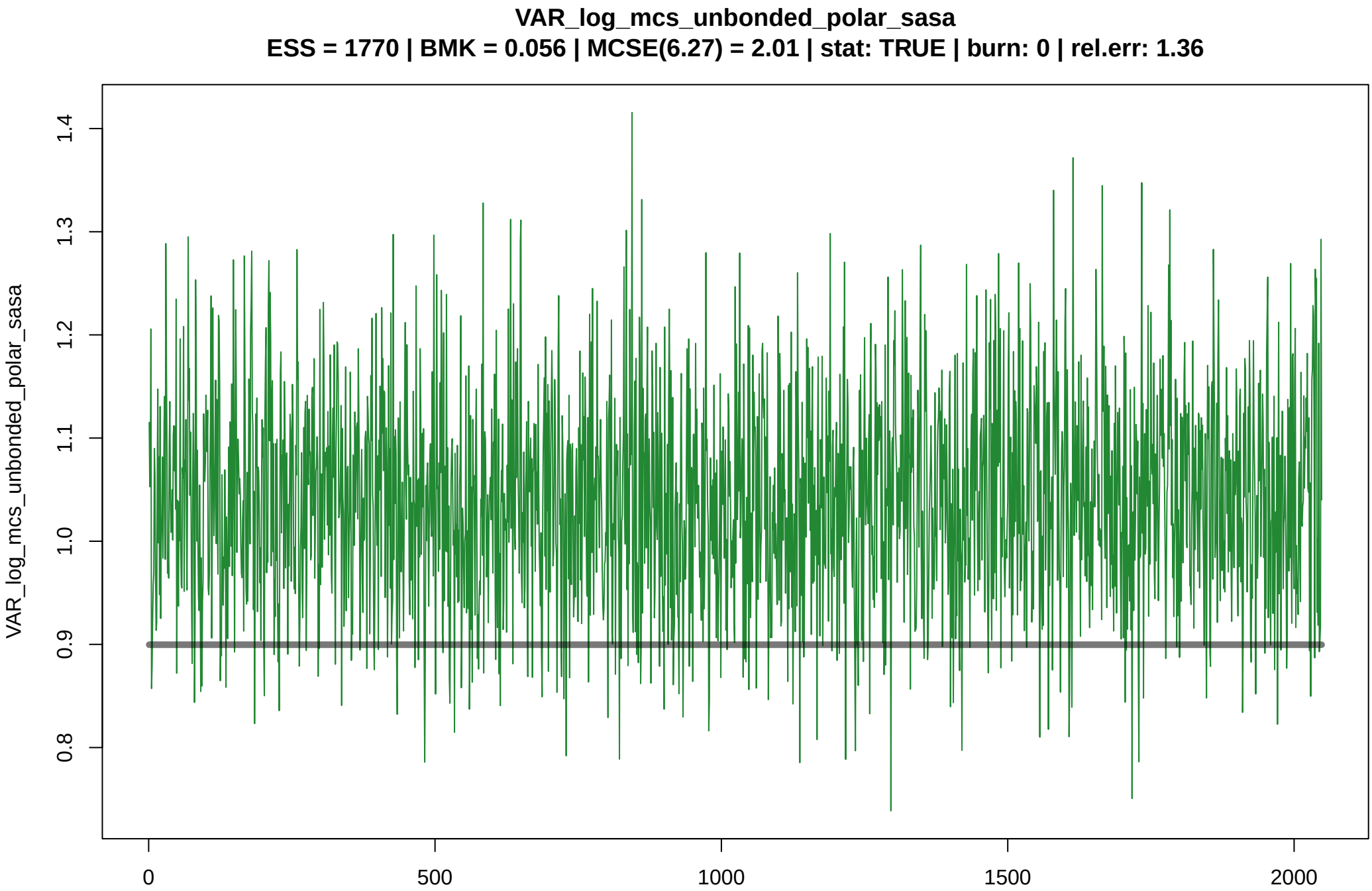

MEAN_log_RMSD
ESS = 1890 | BMK = 0.0417 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: −0.592
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

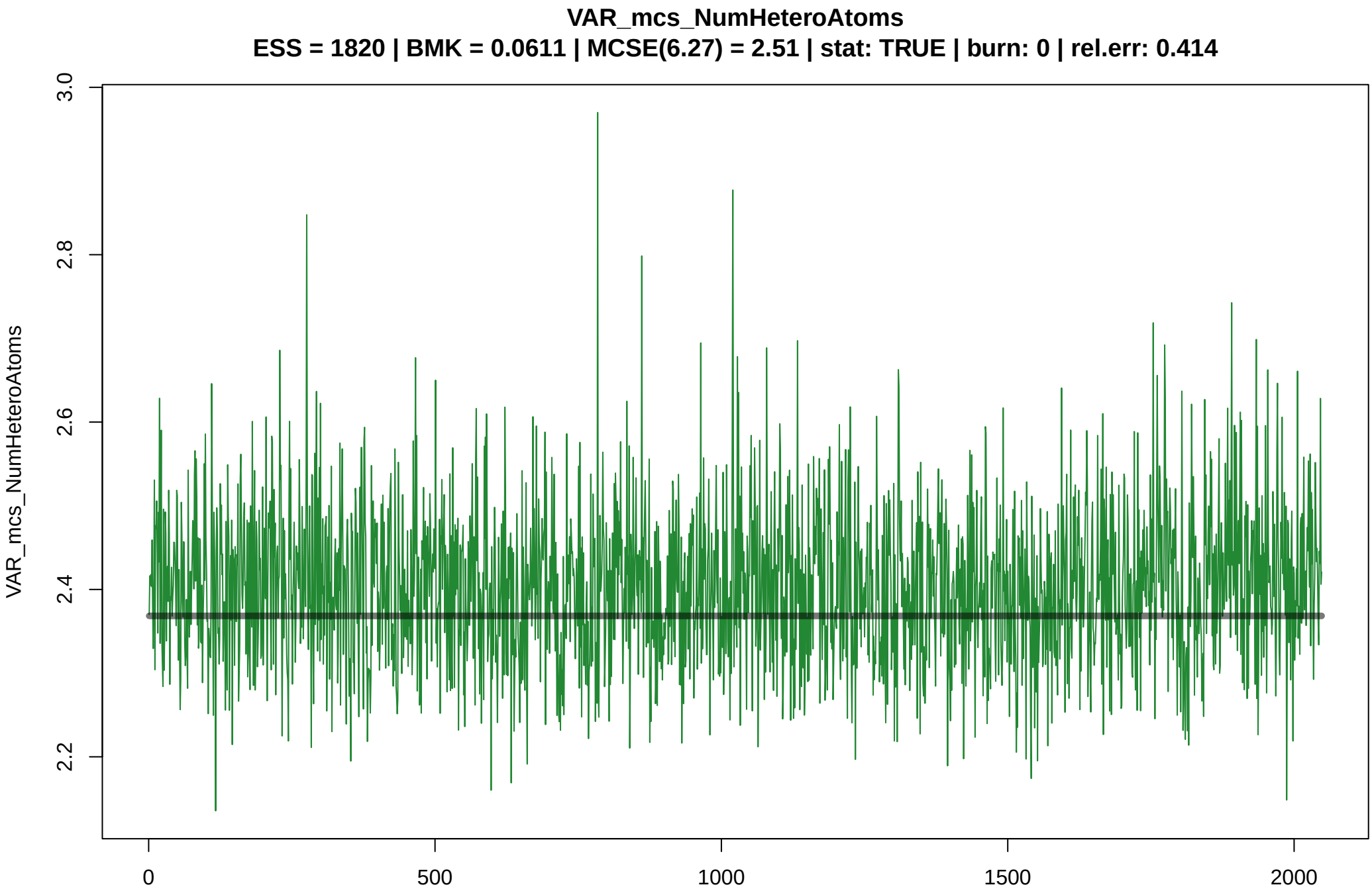

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1800 | BMK = 0.04 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: −0.205
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

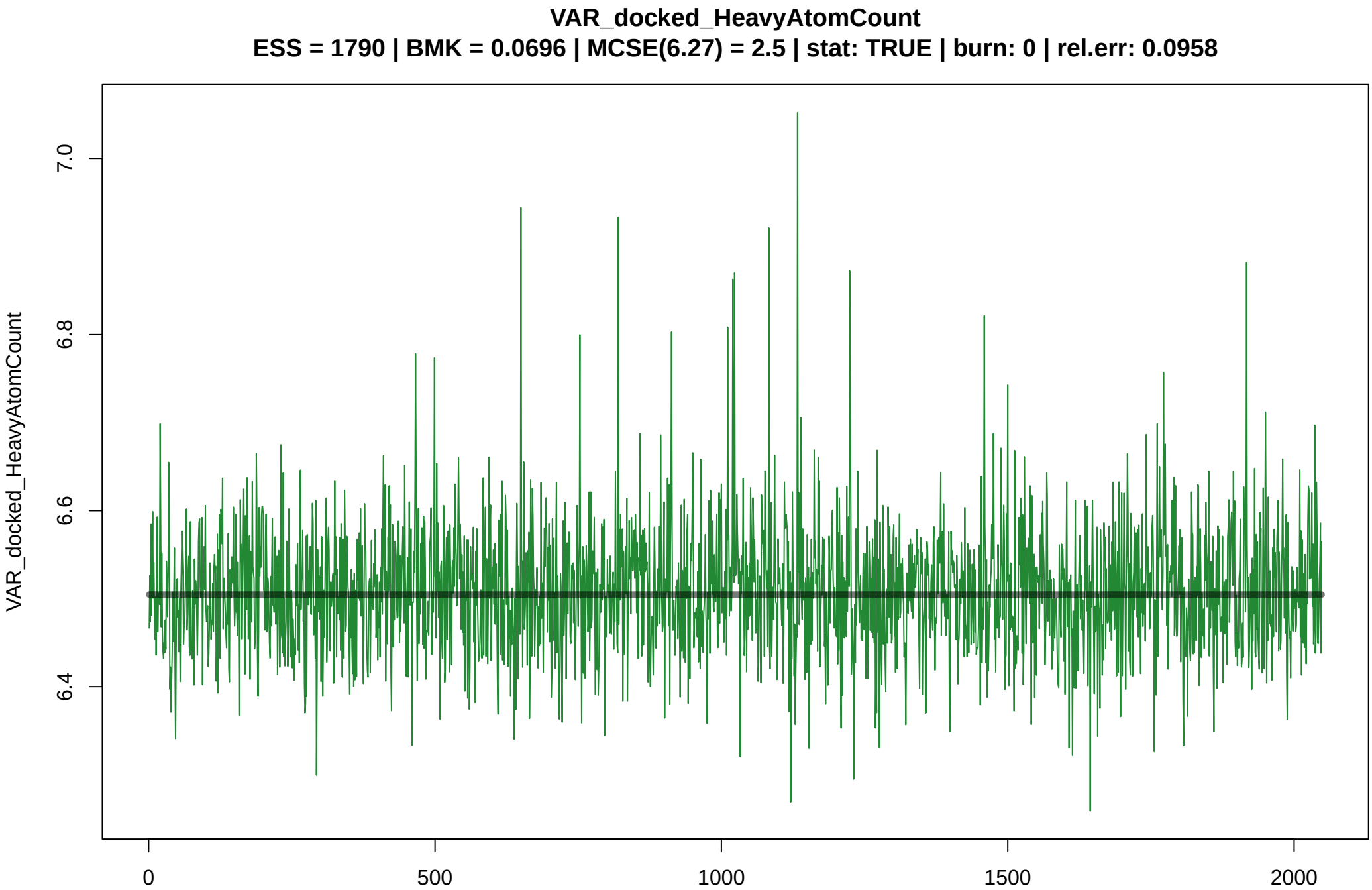

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0461 | MCSE(6.27) = 1.76 | stat: TRUE | burn: 0 | rel.err: 0.499
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
500
1000
1500
2000

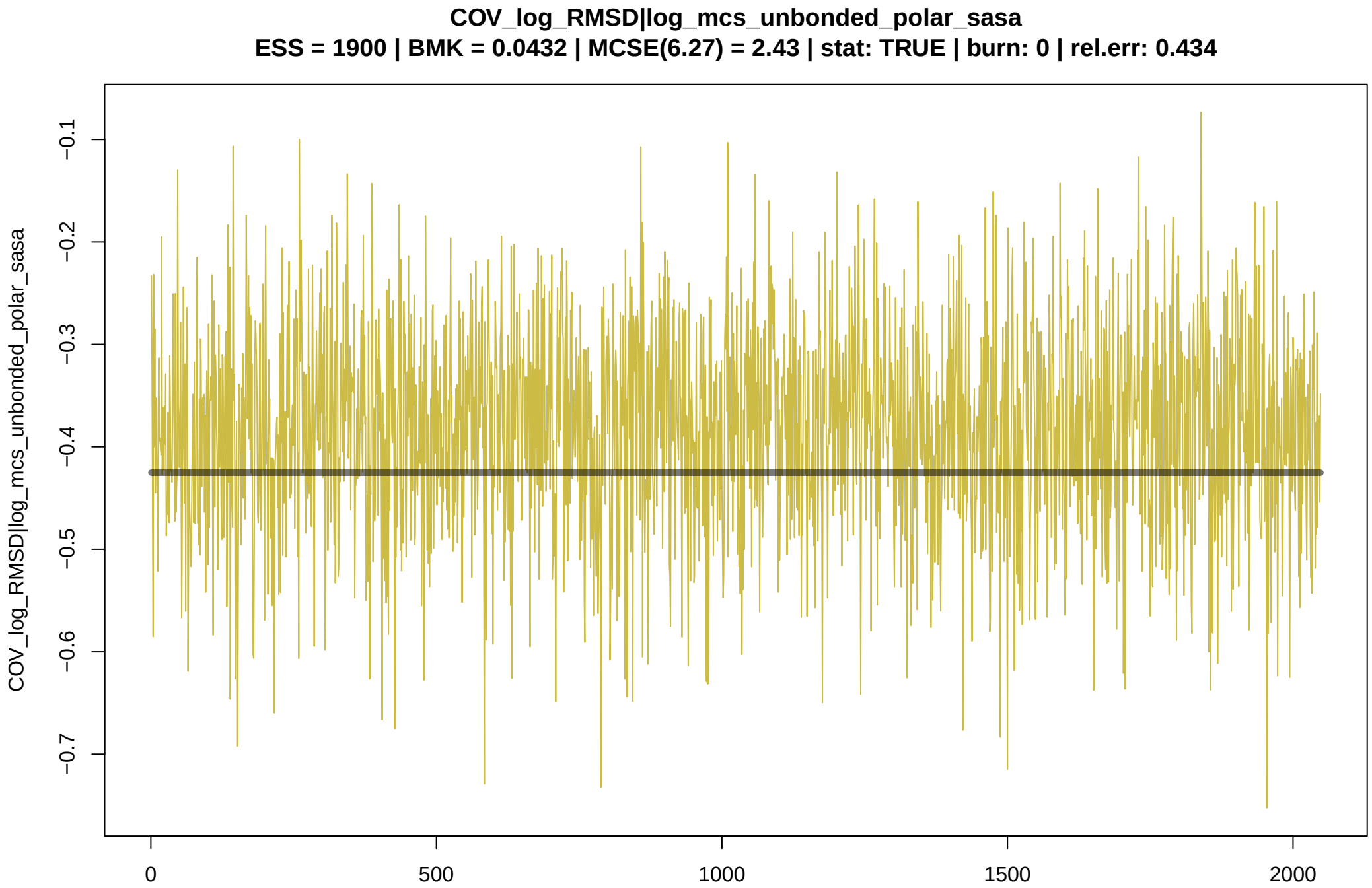

MEAN_docked_HeavyAtomCount
ESS = 1800 | BMK = 0.0423 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0 | rel.err: 0.511
MEAN_docked_HeavyAtomCount
32
34
36
38
40
42
0
500
1000
1500
2000

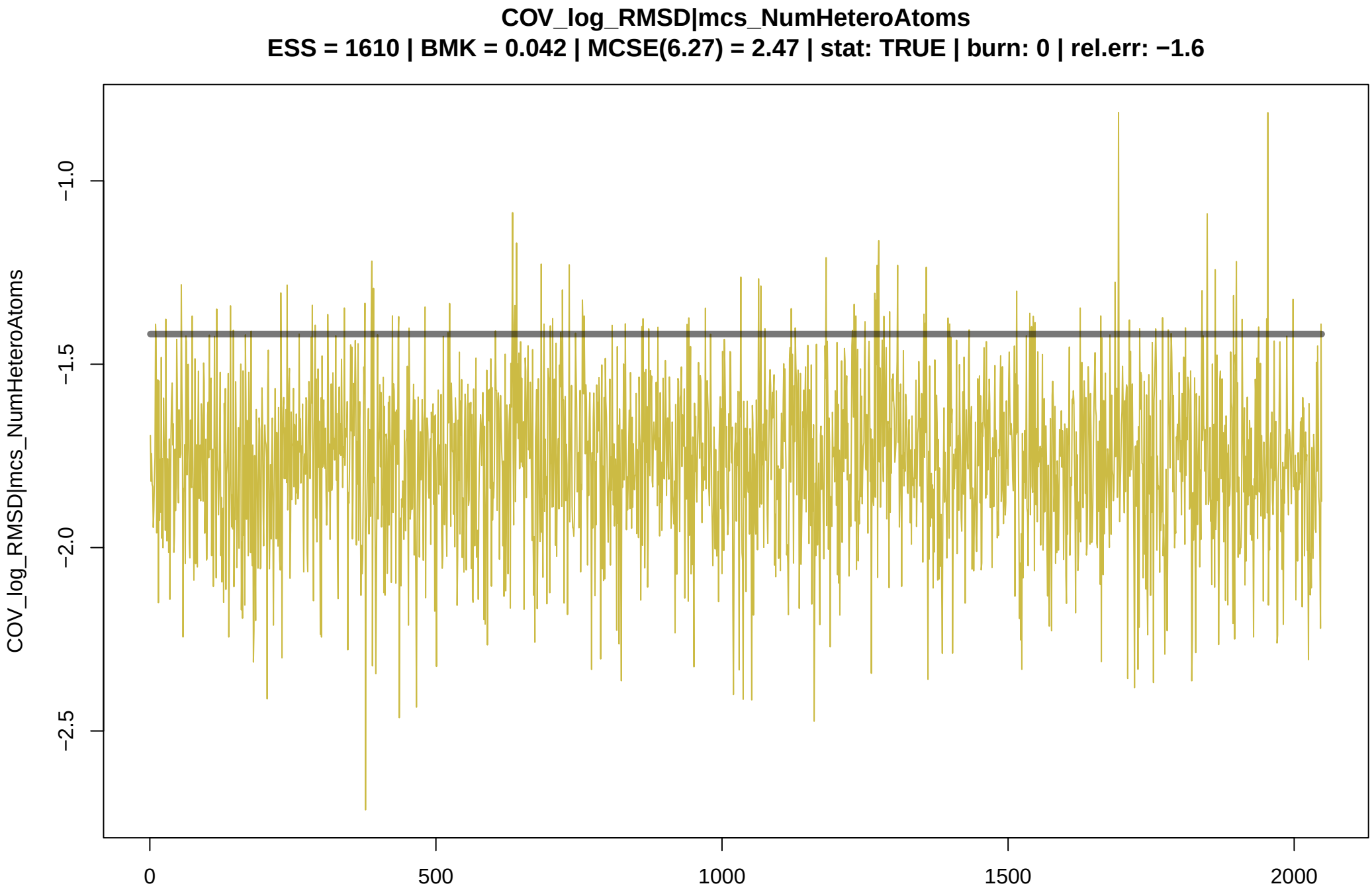

VAR_log_RMSD
ESS = 2050 | BMK = 0.0293 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: 2.27
VAR_log_RMSD
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

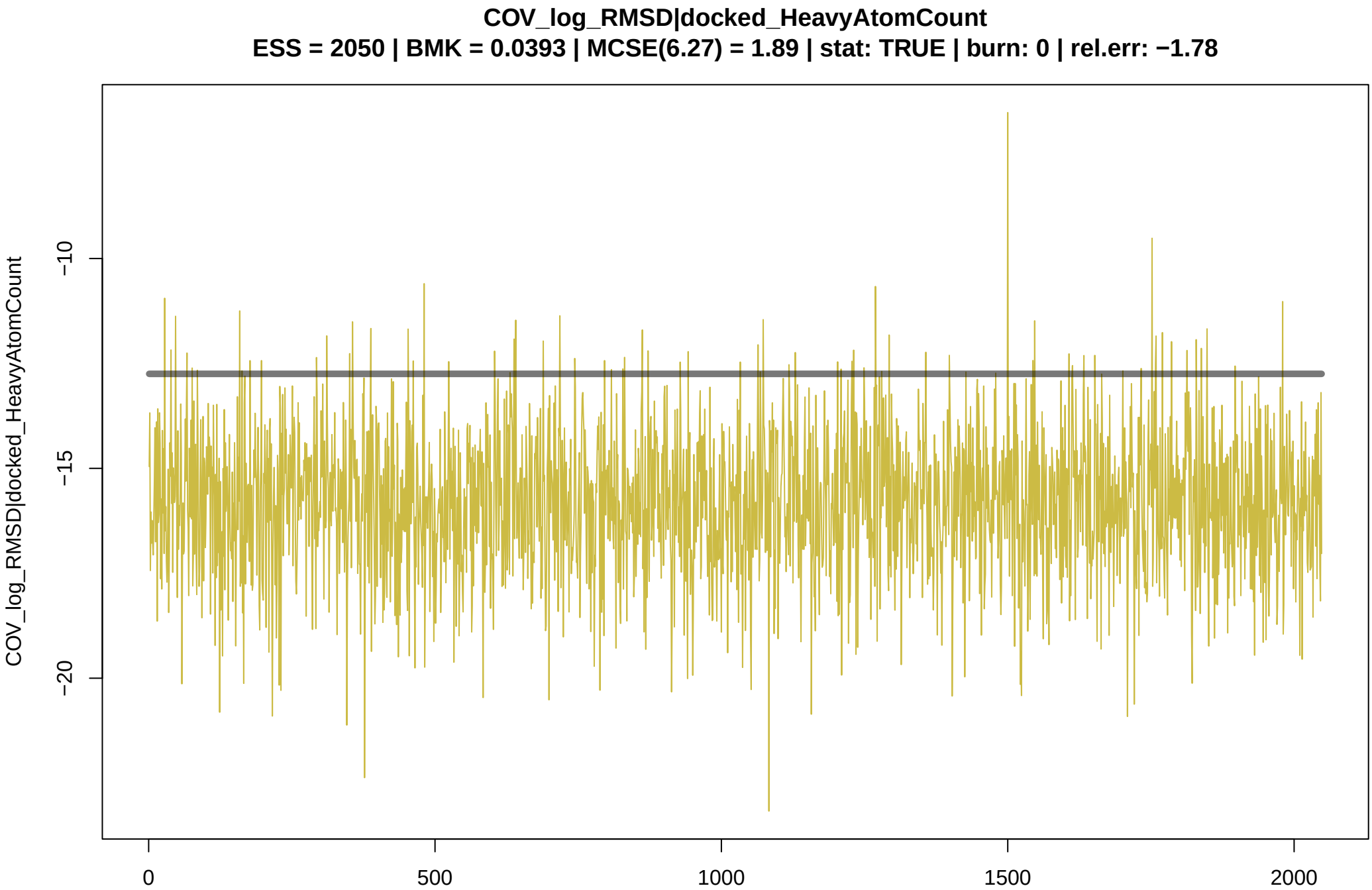

VAR_log_mcs_unbonded_polar_sasa
ESS = 1770 | BMK = 0.056 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: 1.36
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

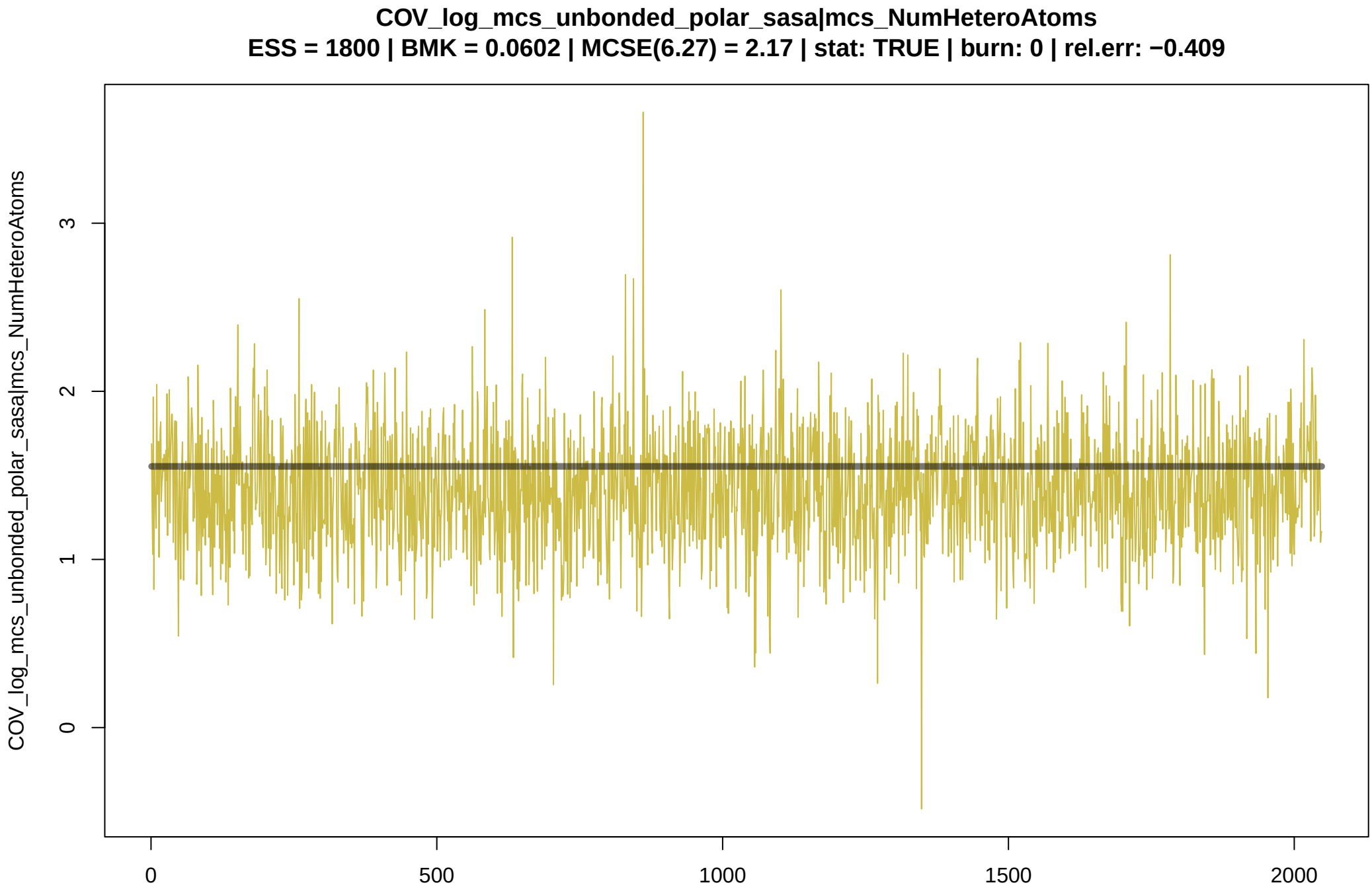

VAR_mcs_NumHeteroAtoms
ESS = 1820 | BMK = 0.0611 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: 0.414
VAR_mcs_NumHeteroAtoms
3.0
2.8
2.6
2.4
2.2
0
500
1000
1500
2000

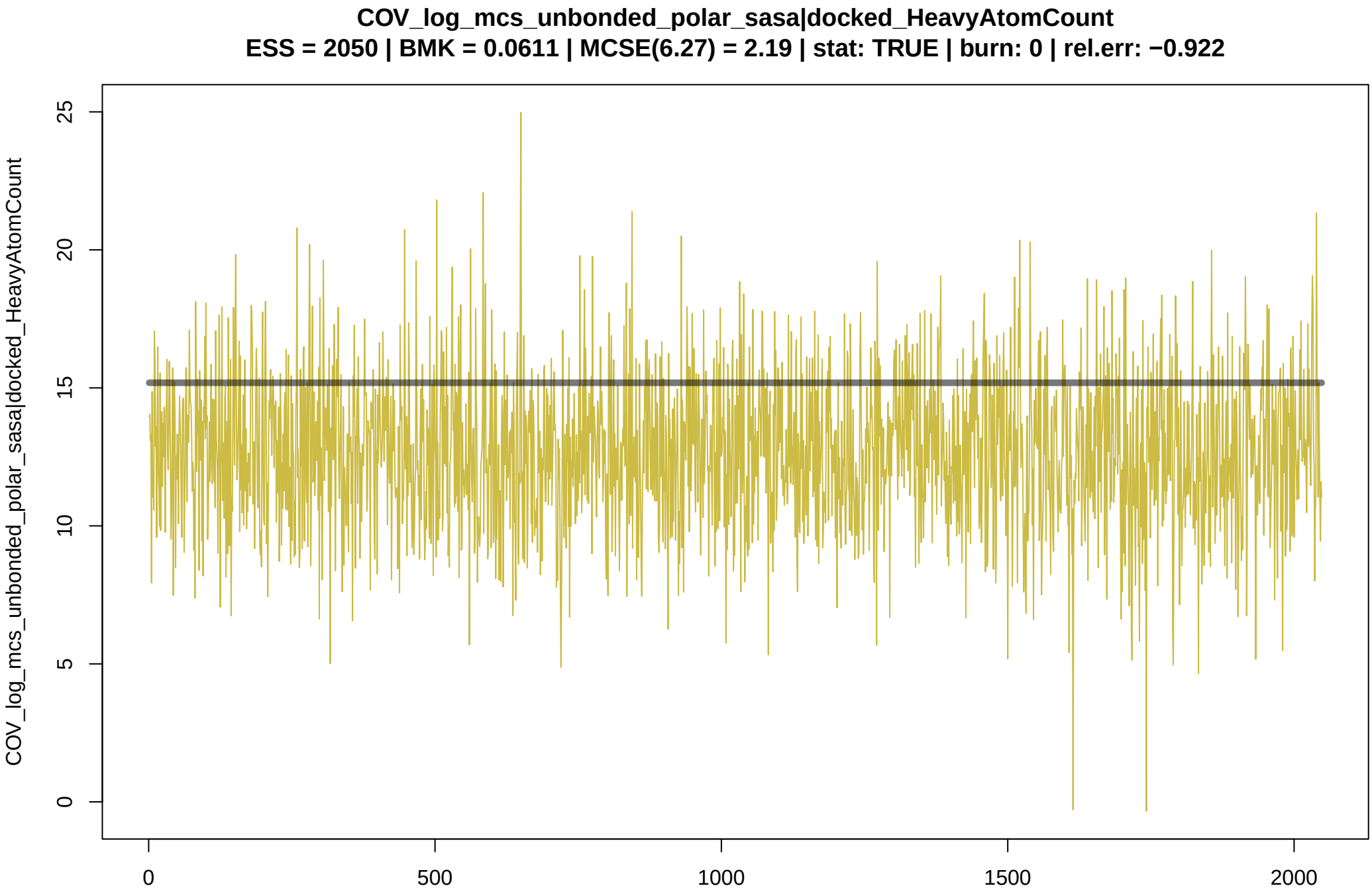

VAR_docked_HeavyAtomCount
ESS = 1790 | BMK = 0.0696 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 0.0958
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

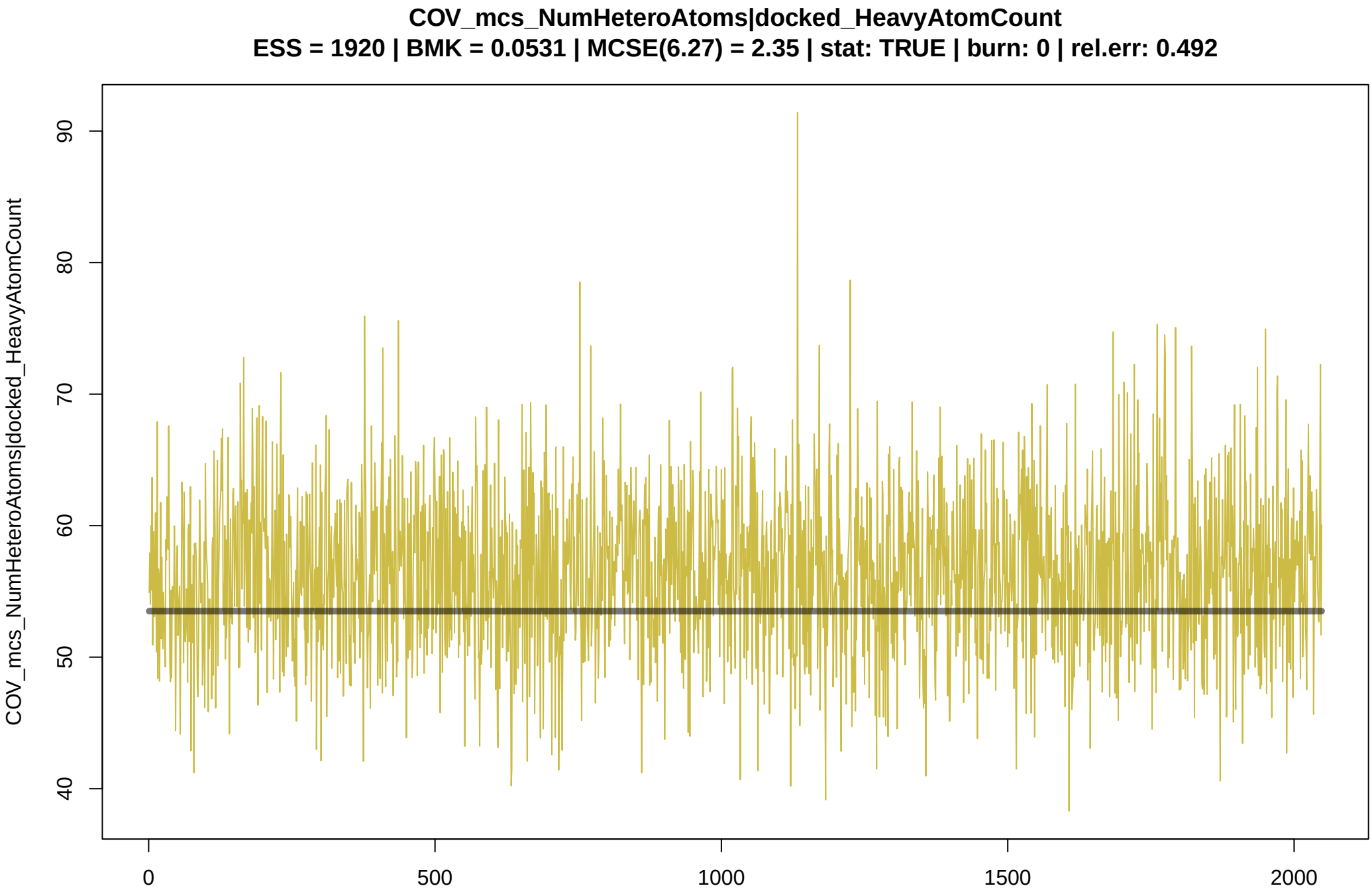

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1900 | BMK = 0.0432 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0 | rel.err: 0.434
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1610 | BMK = 0.042 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | rel.err: −1.6
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 = 0.0393 | MCSE(6.27) = 1.89 | stat: TRUE | burn: 0 | rel.err: −1.78
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1800 | BMK = 0.0602 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: −0.409
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0
1
2
3
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0611 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: −0.922
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0
5
10
15
20
25
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0531 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 0.492
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
90
0
500
1000
1500
2000