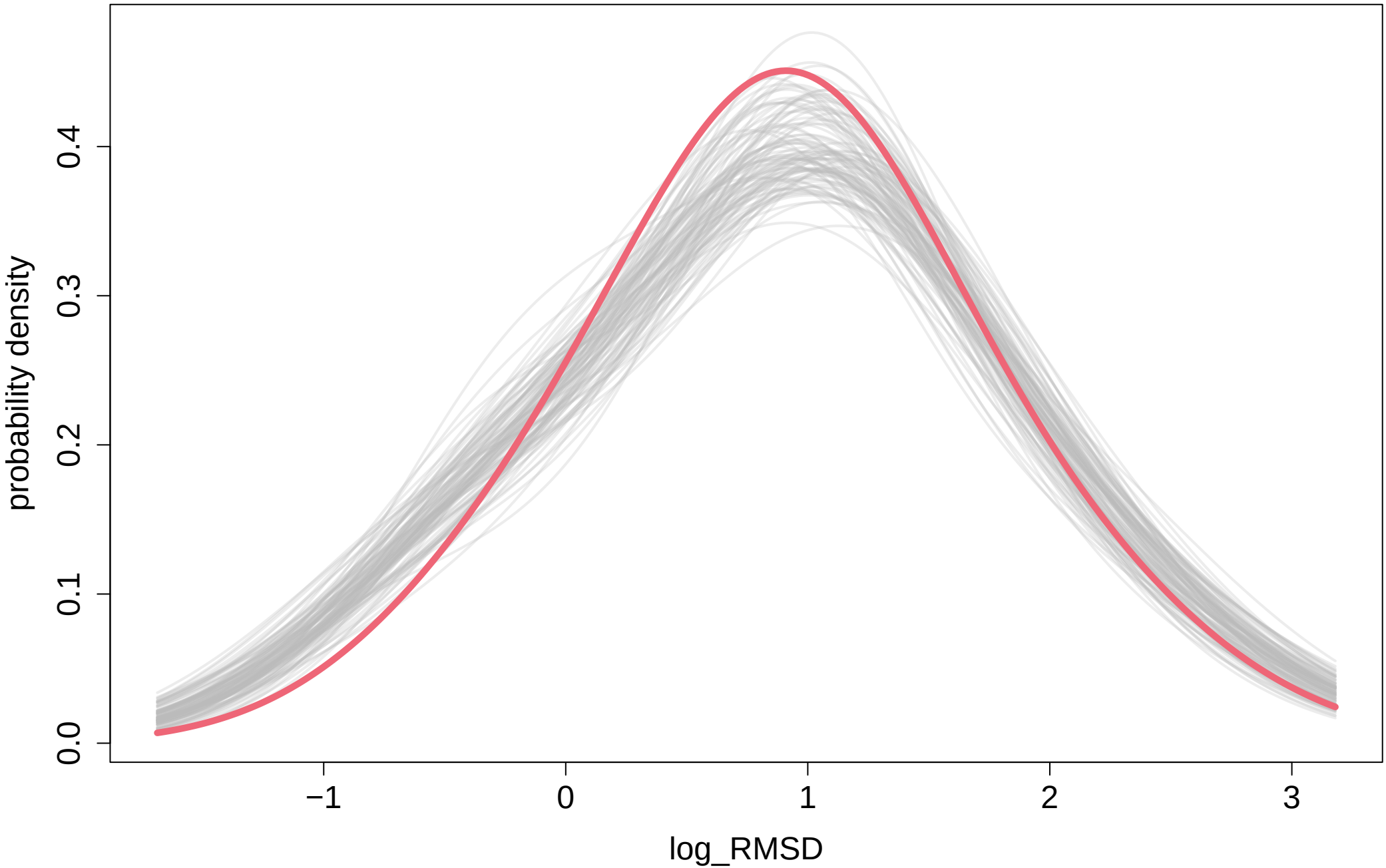
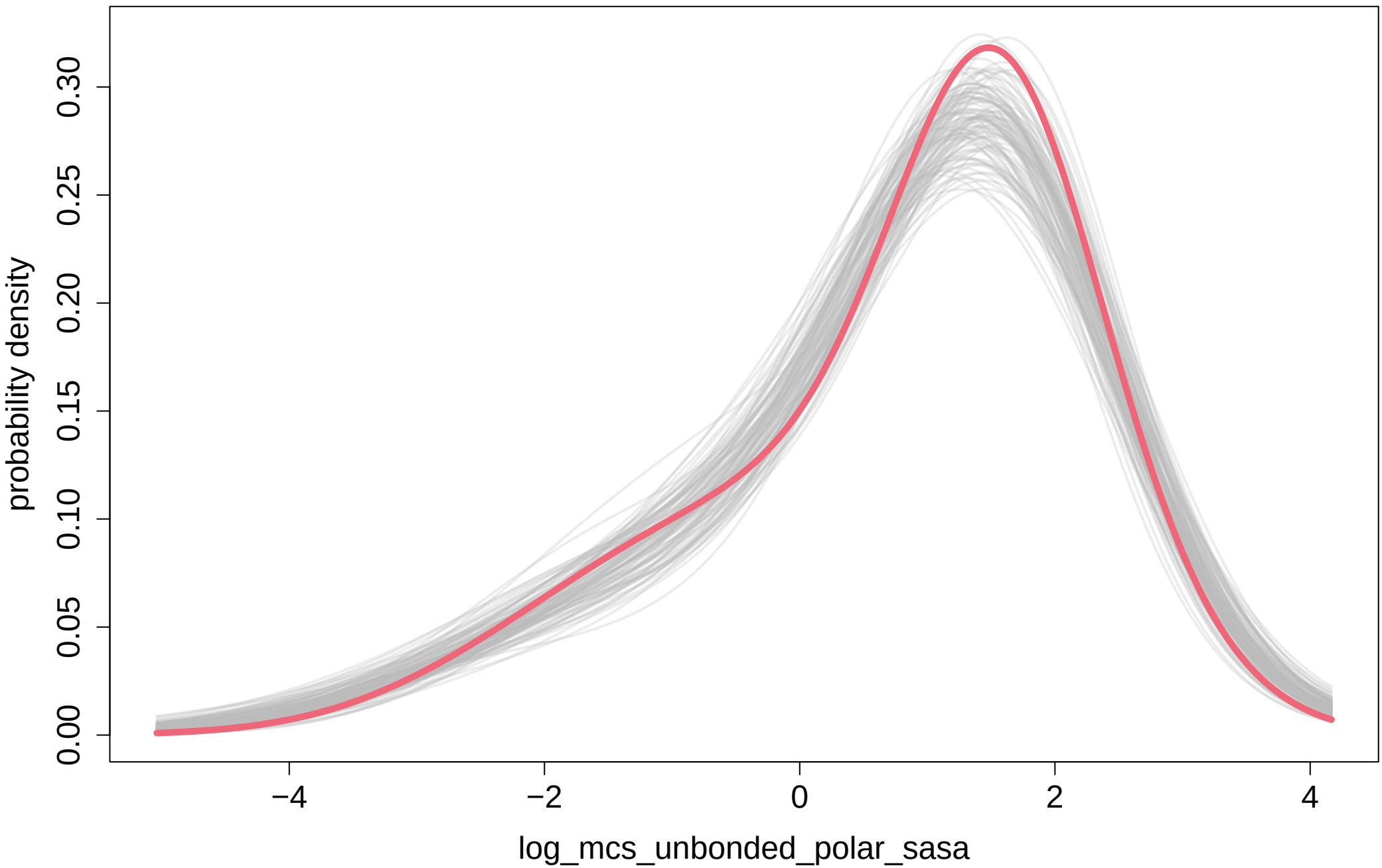
−− STATS maxD −−
min ESS = 136.612749101288
max BMK = 0.122507750279462
max MCSE = 6.90823537437204
all stationary: FALSE
burn: 0
max rel.err.: 2.19953880183993

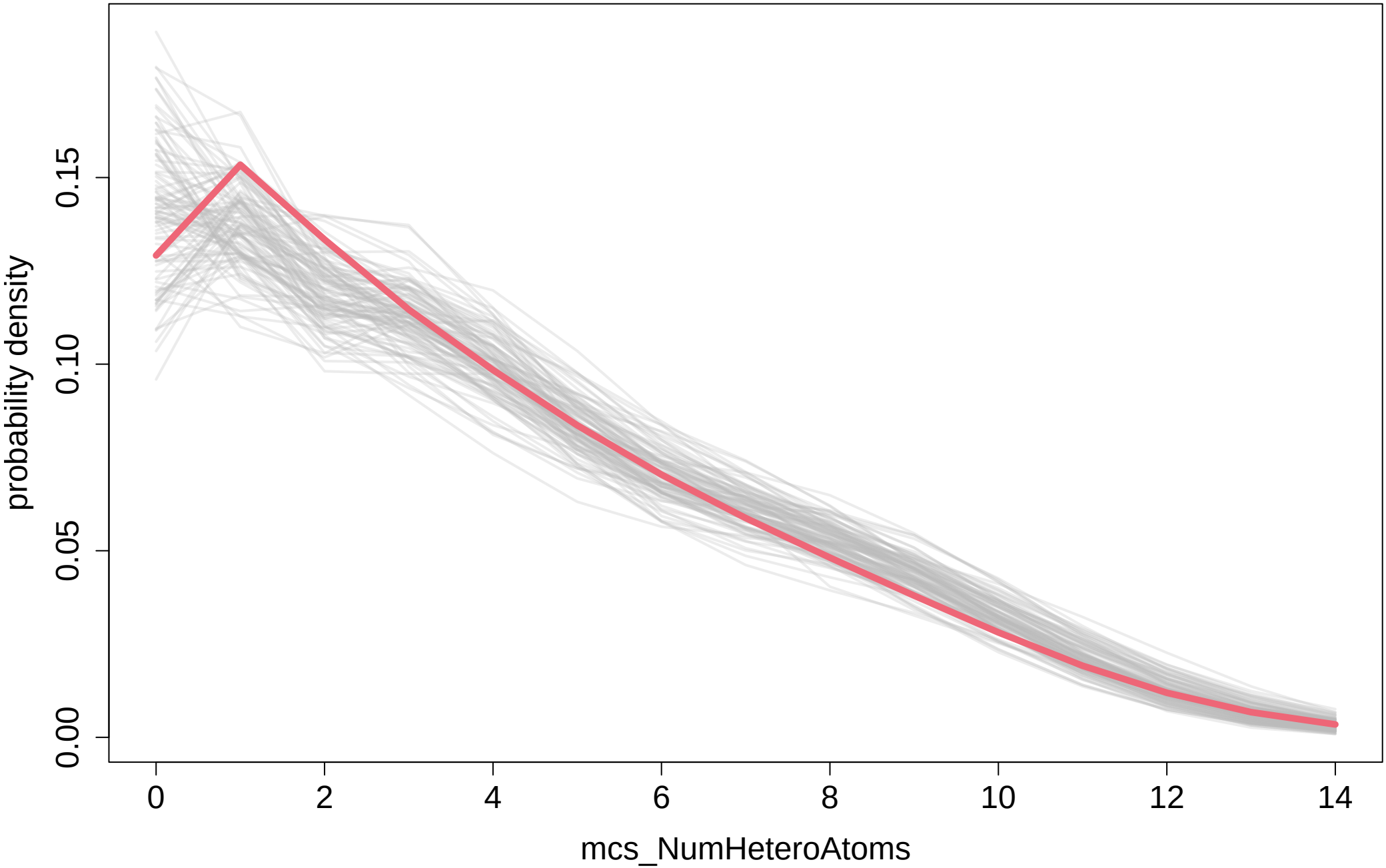
−− STATS 2D −−
min ESS = 2987.78912539936
max BMK = 0.039053026724131 1
max MCSE = 1.81526651383727
all stationary: TRUE
burn: 0
max rel.err.: 1.76995557119881

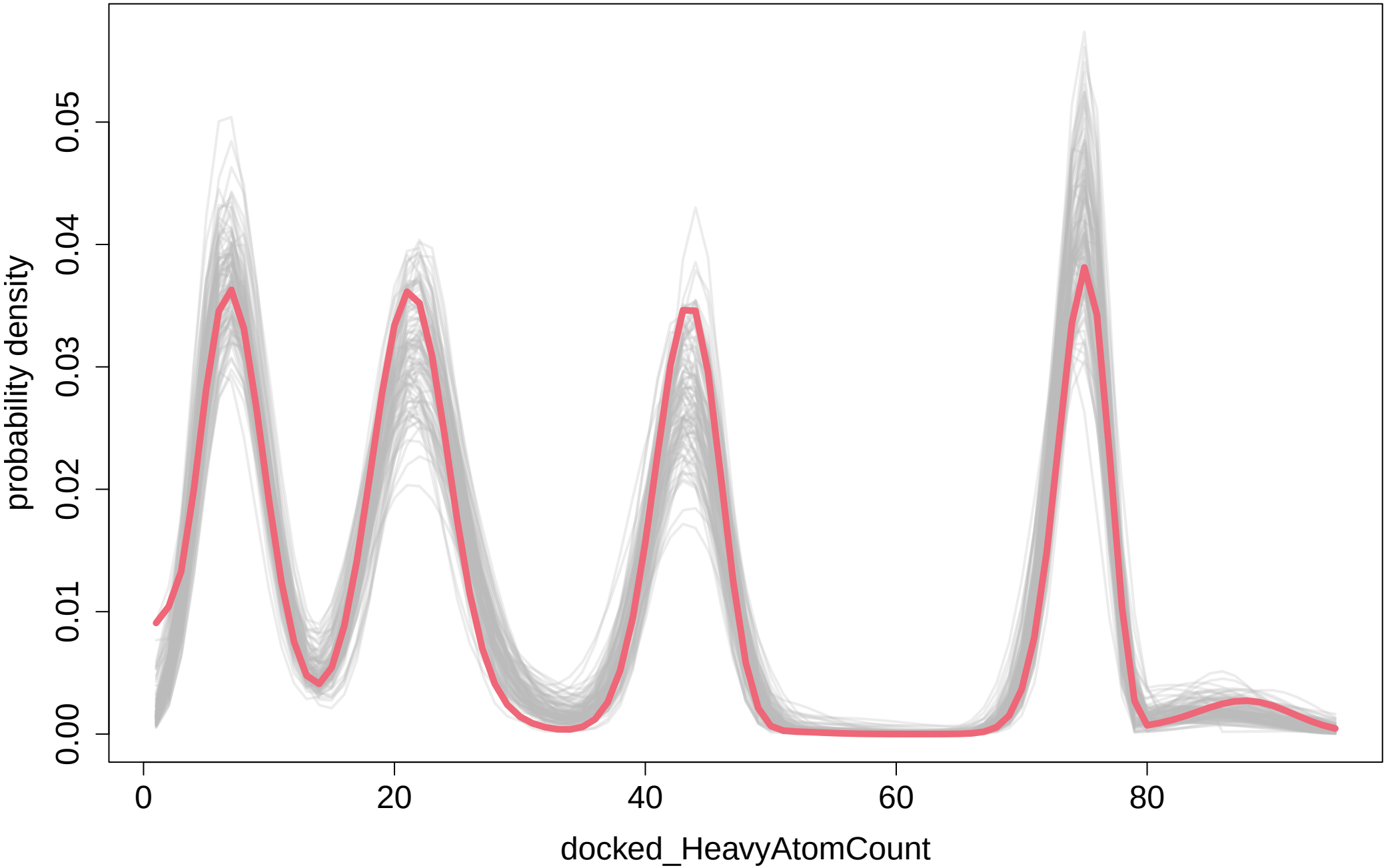
−− STATS 1D −−
min ESS = 2238.70540614654
max BMK = 0.047075320259440 4
max MCSE = 1.90035628208056
all stationary: TRUE
burn: 0
max rel.err.: 2.31341895307835

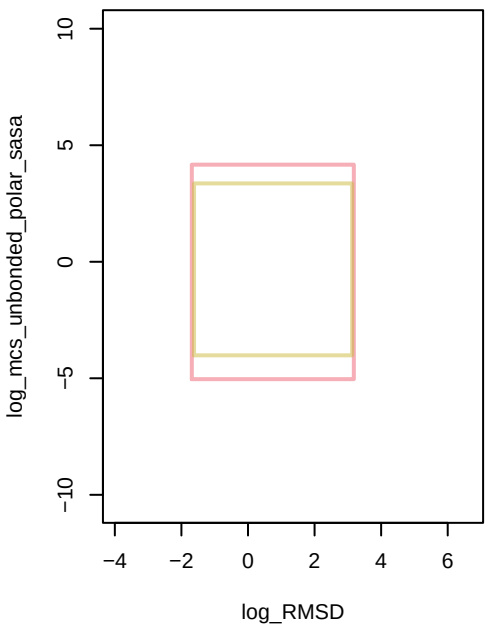
Occupied clusters: 10 of 16
LL: −2160 +− 6.66

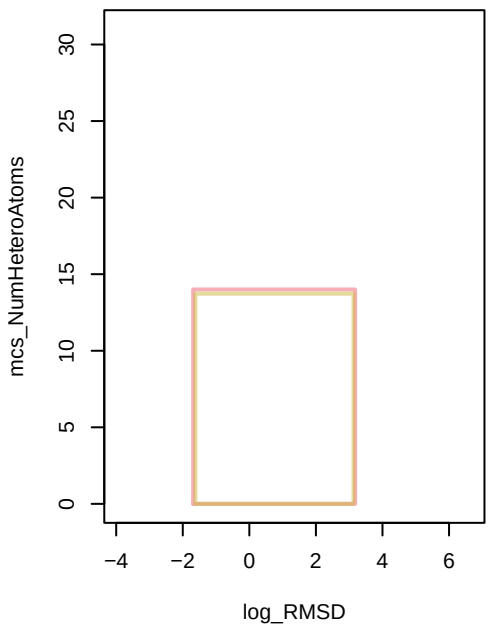

probability density
0.0
0.1
0.2
0.3
0.4
−1
0
1
2
3
log_RMSD

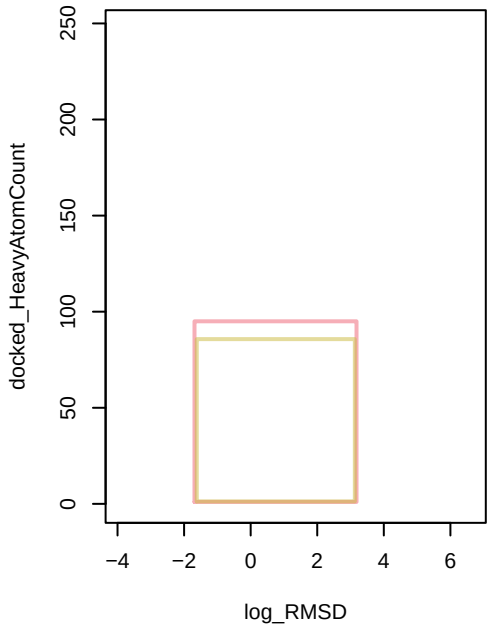

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

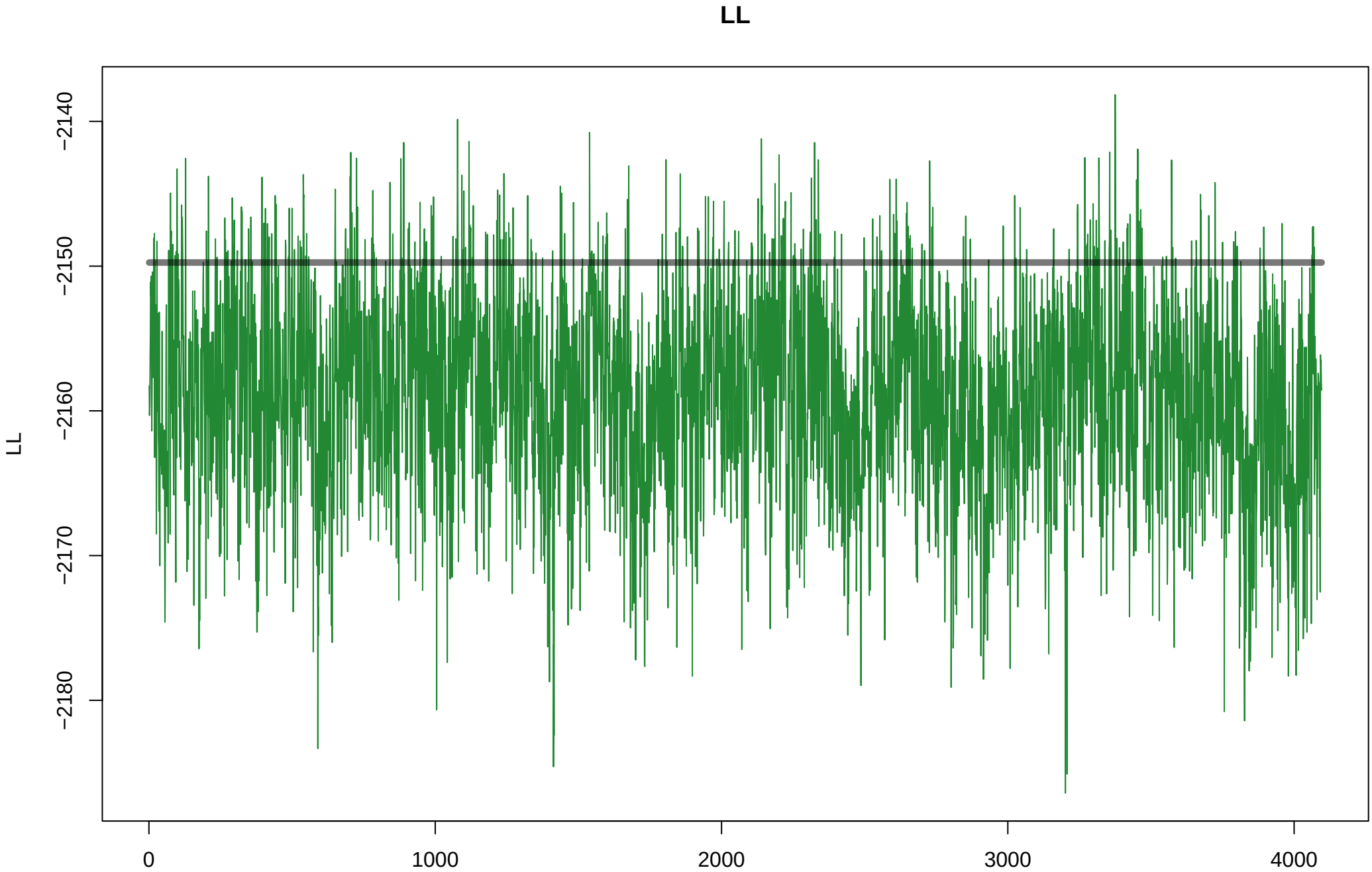

probability density
0.00
0.05
0.10
0.15
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

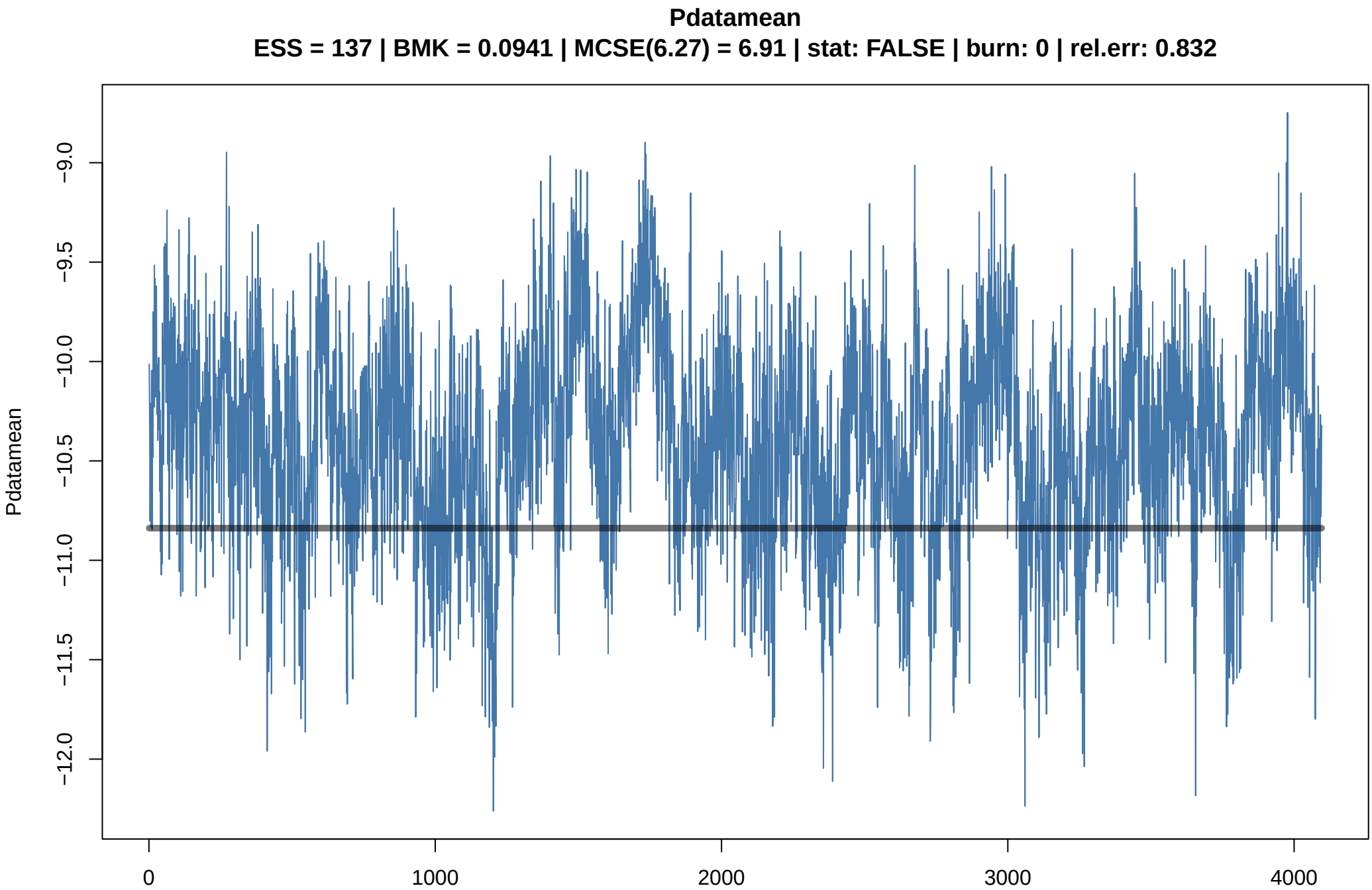

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
20
40
60
80
docked_HeavyAtomCount

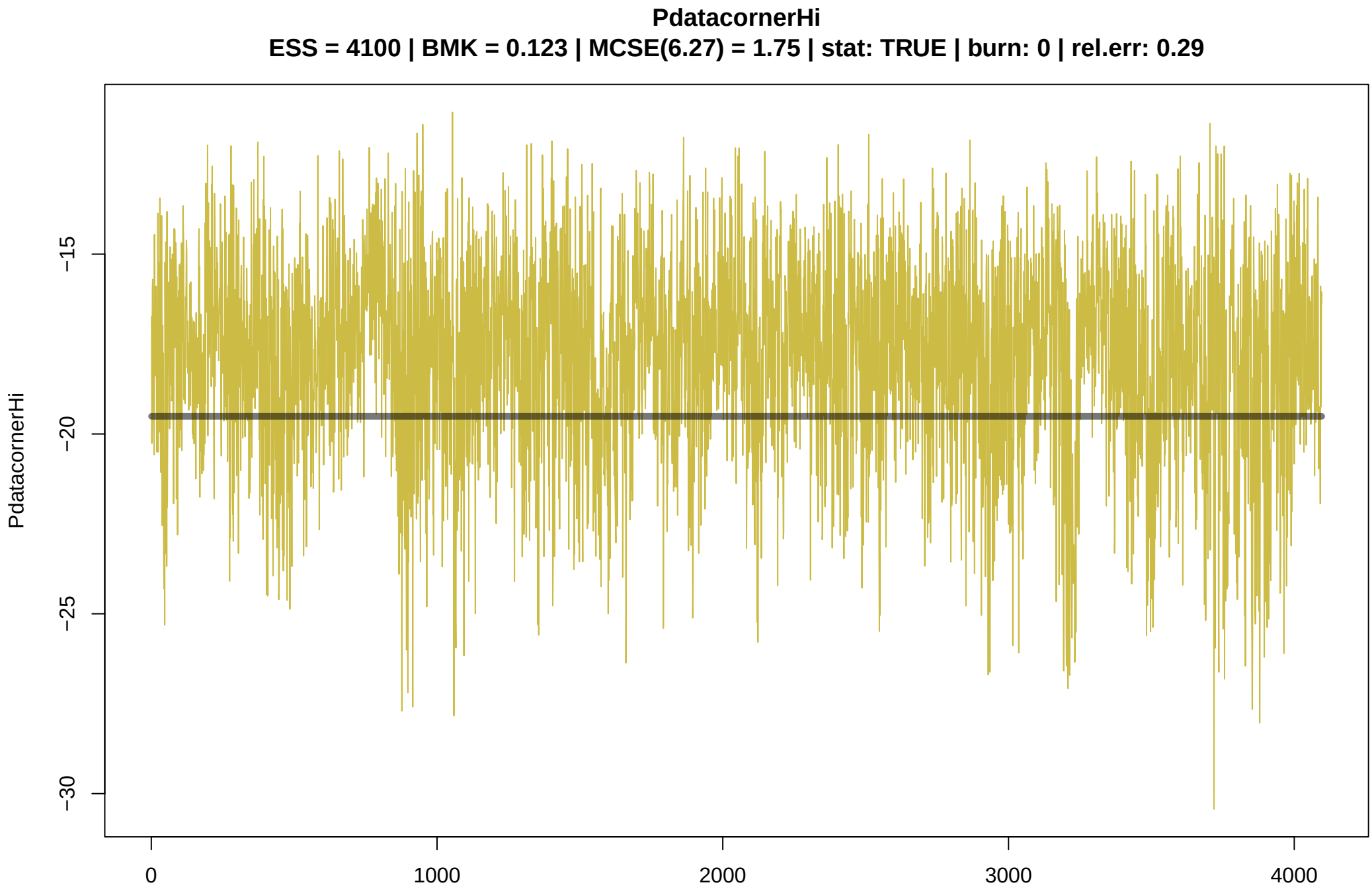

log_mcs_unbonded_polar_sasa
10
5
0
−5
−10
−4
−2
0
2
4
6
log_RMSD

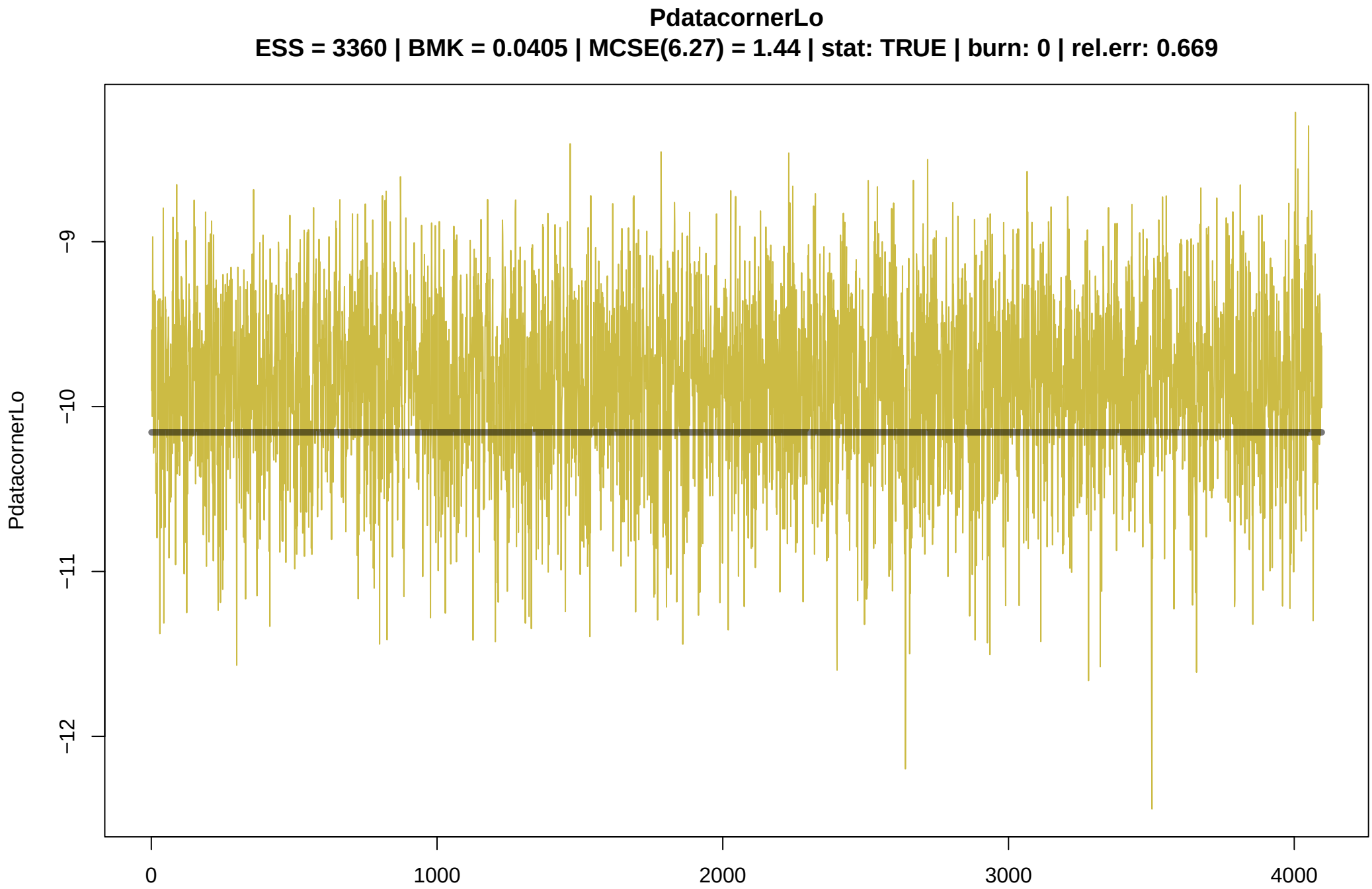

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

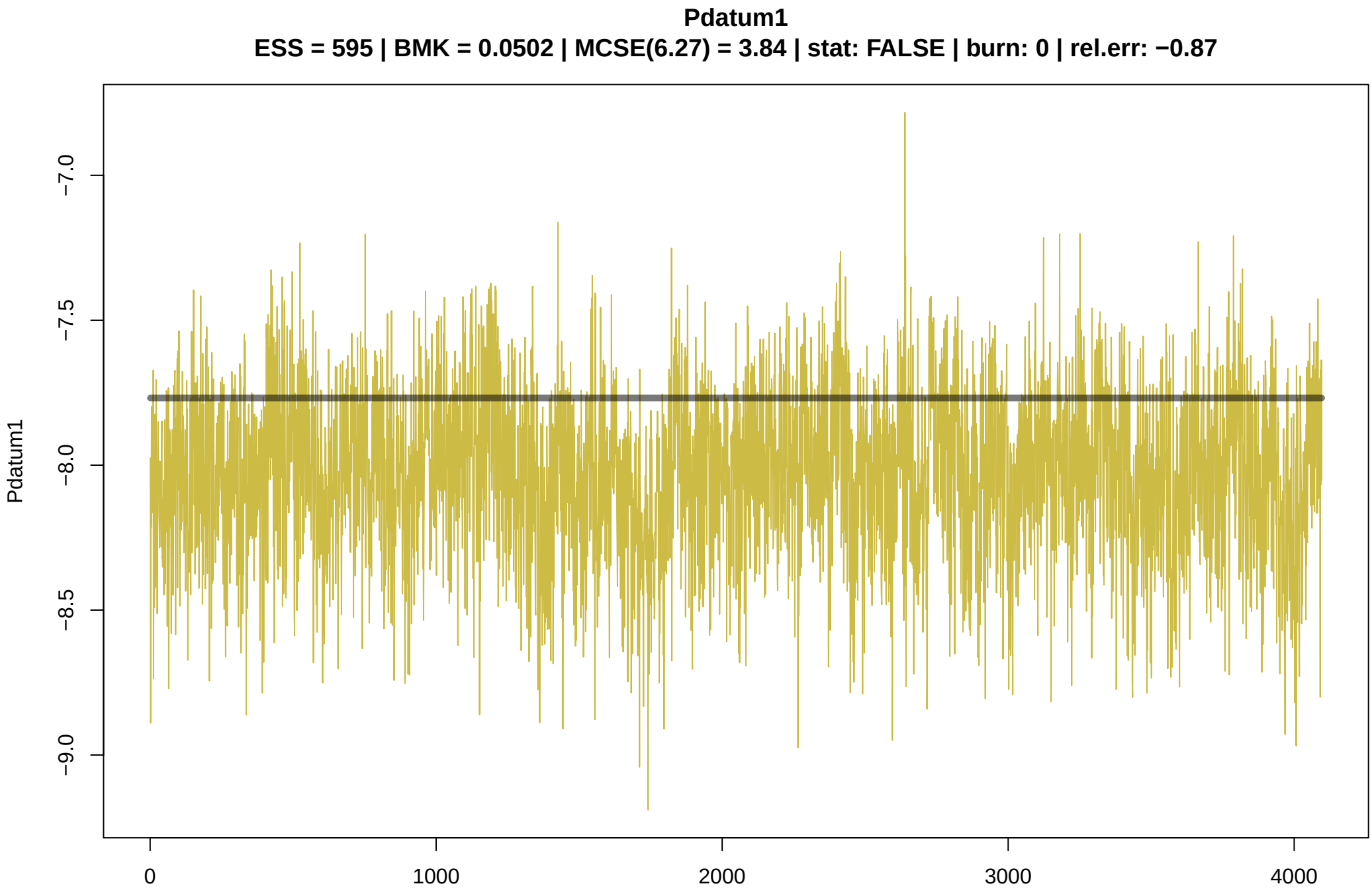

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

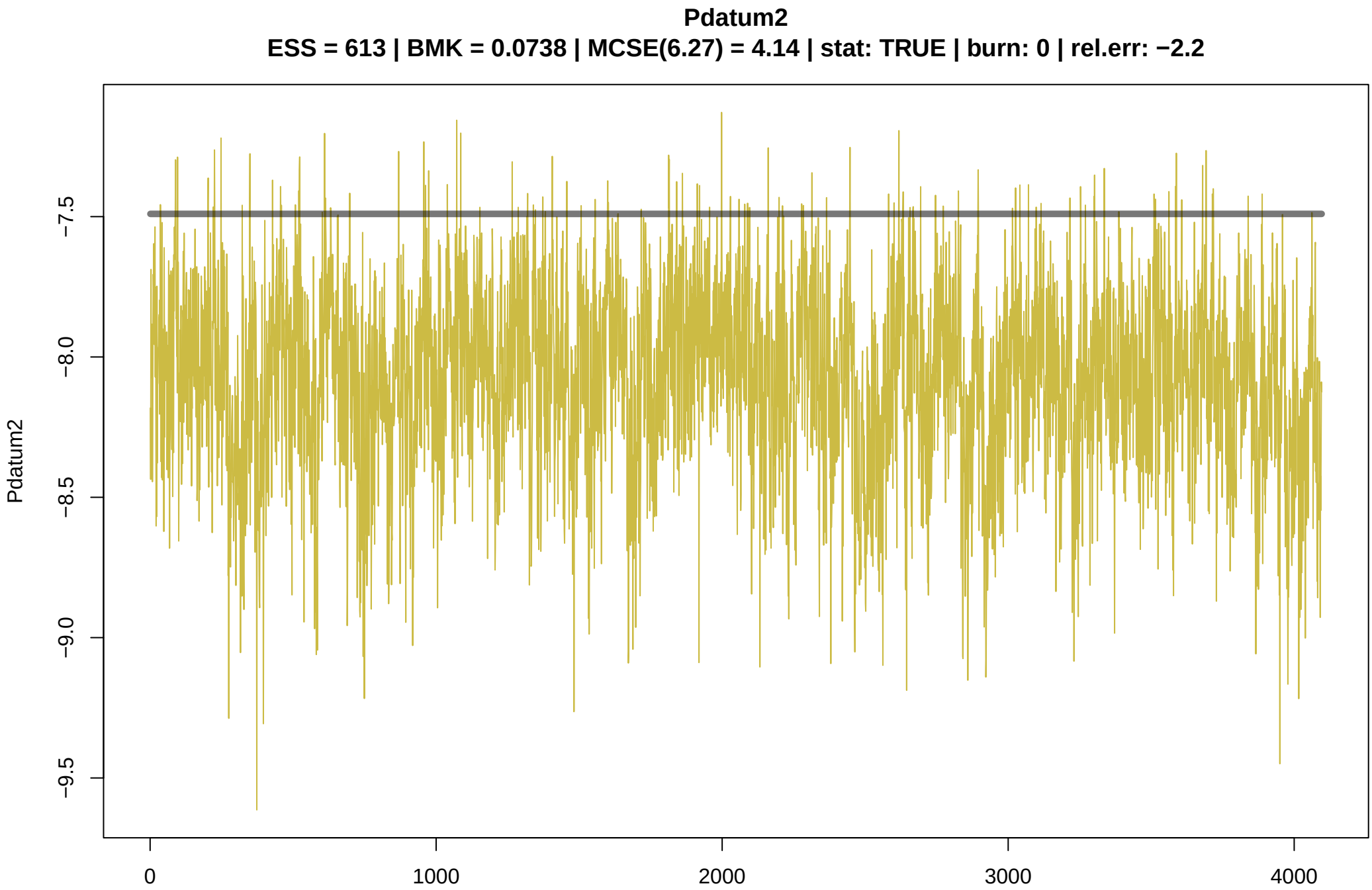

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

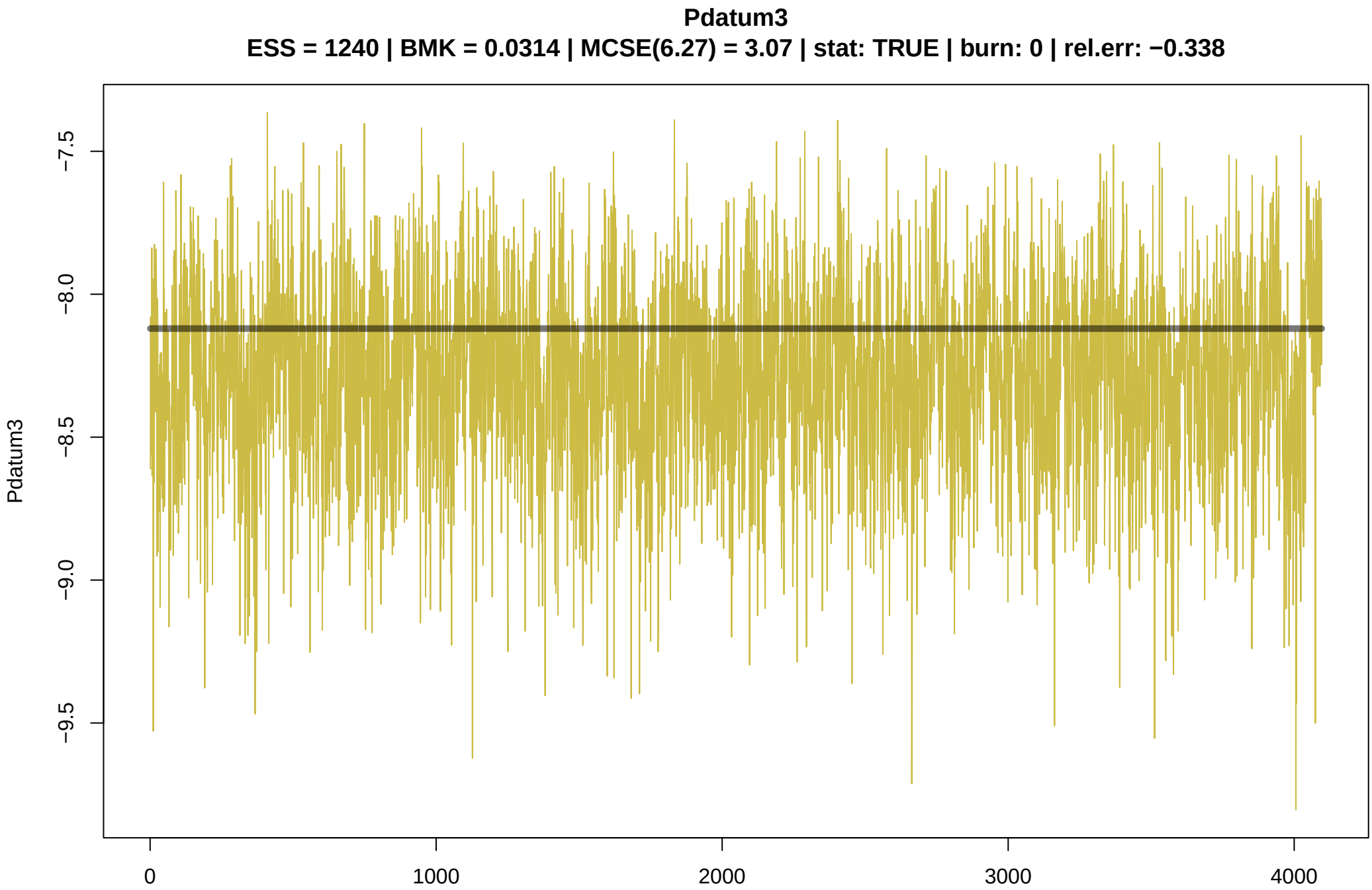

Pdatamean
ESS = 137 | BMK = 0.0941 | MCSE(6.27) = 6.91 | stat: FALSE | burn: 0 | rel.err: 0.832
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
1000
2000
3000
4000

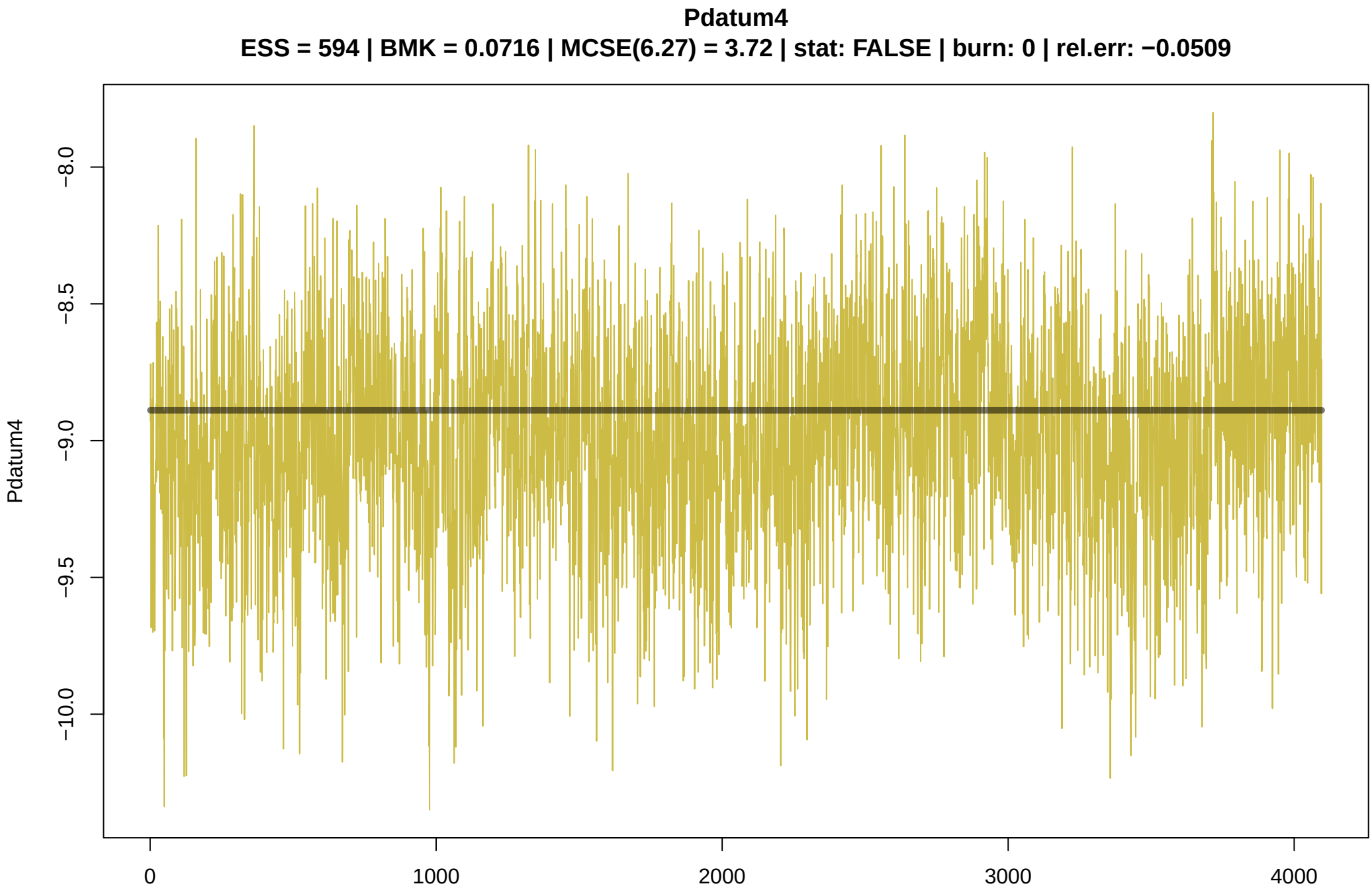

PdatacornerHi
ESS = 4100 | BMK = 0.123 | MCSE(6.27) = 1.75 | stat: TRUE | burn: 0 | rel.err: 0.29
PdatacornerHi
−15
−20
−25
−30
0
1000
2000
3000
4000

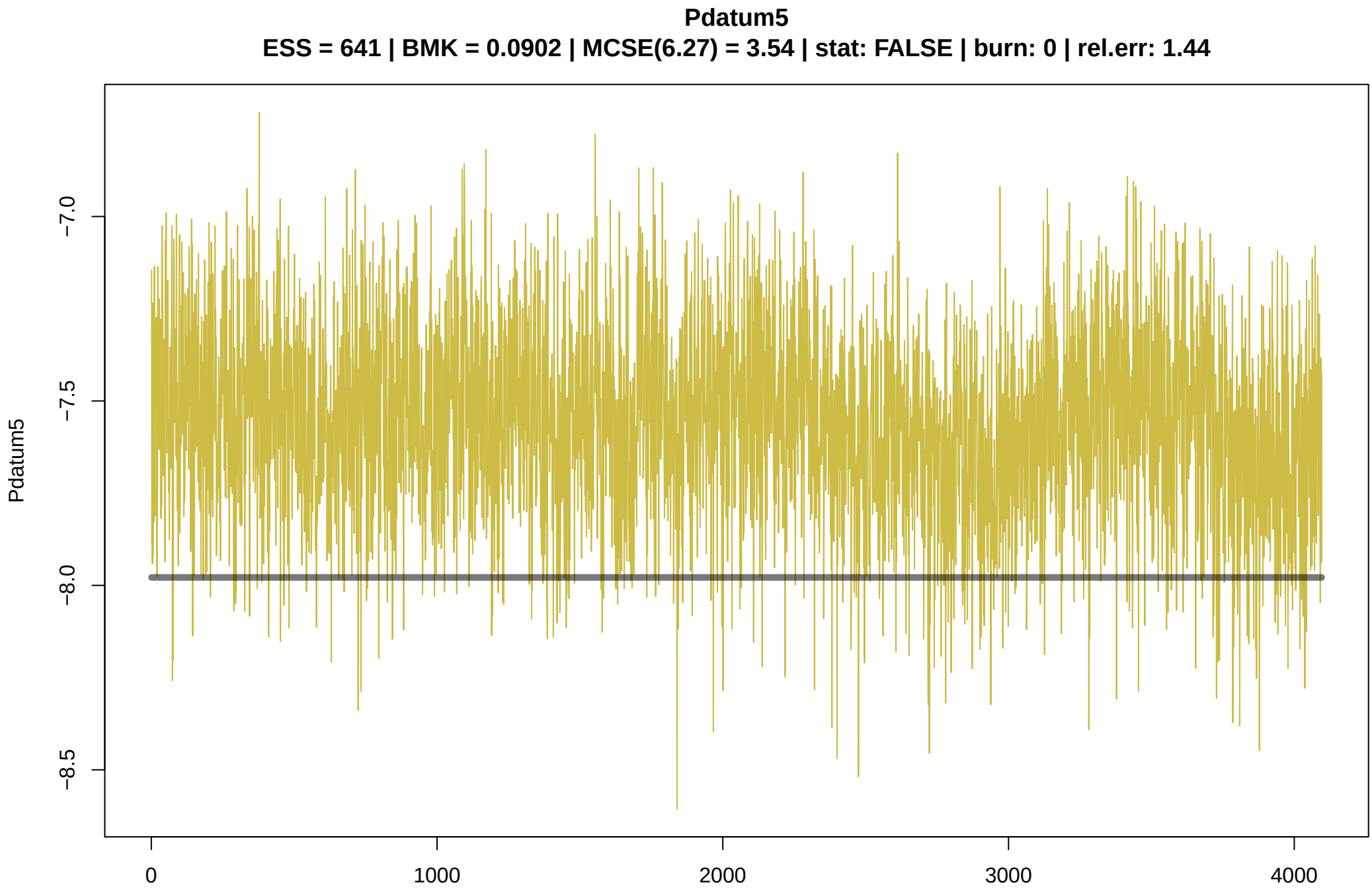

PdatacornerLo
ESS = 3360 | BMK = 0.0405 | MCSE(6.27) = 1.44 | stat: TRUE | burn: 0 | rel.err: 0.669
PdatacornerLo
−9
−10
−11
−12
0
1000
2000
3000
4000

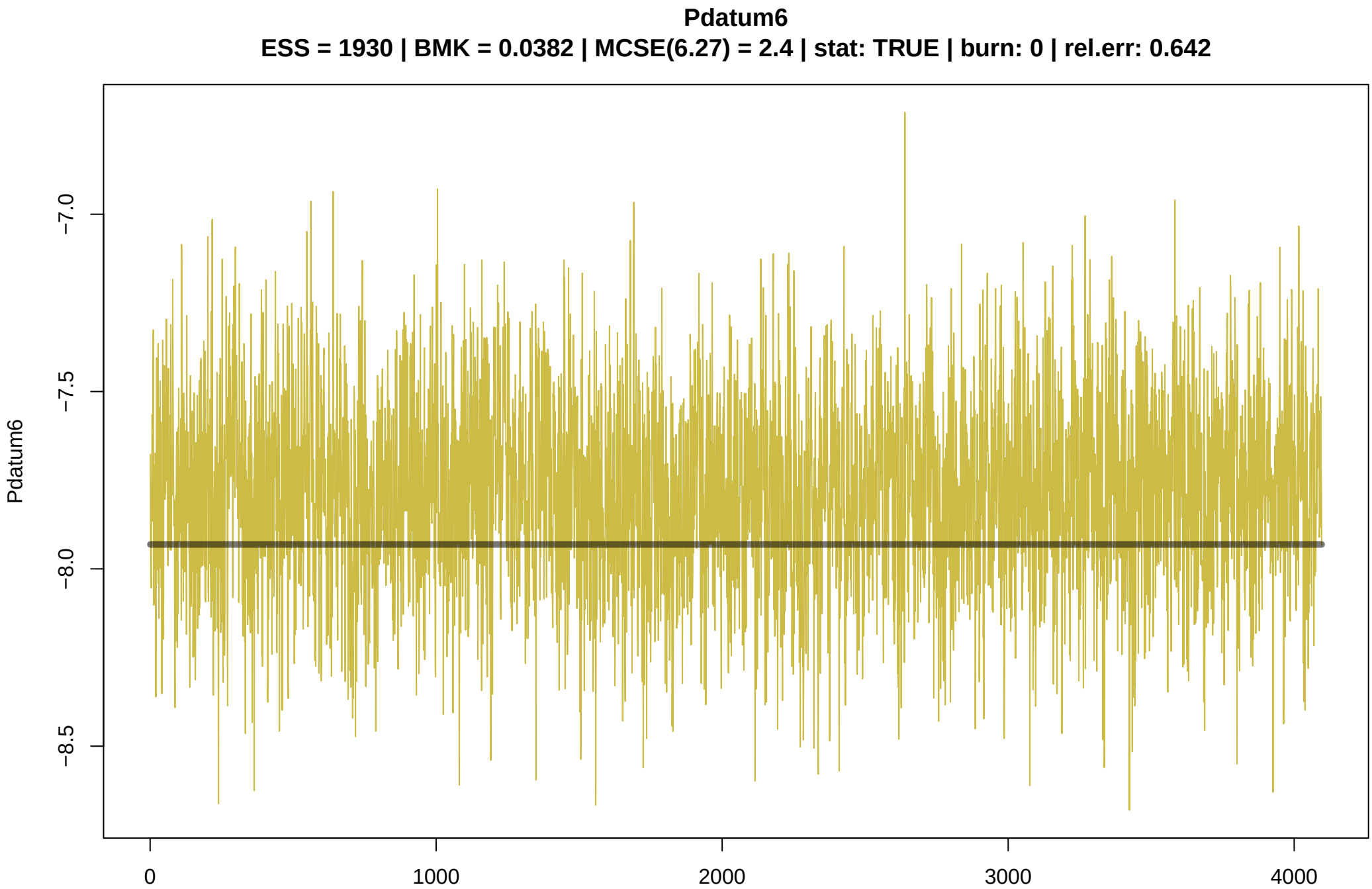

Pdatum1
ESS = 595 | BMK = 0.0502 | MCSE(6.27) = 3.84 | stat: FALSE | burn: 0 | rel.err: −0.87
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

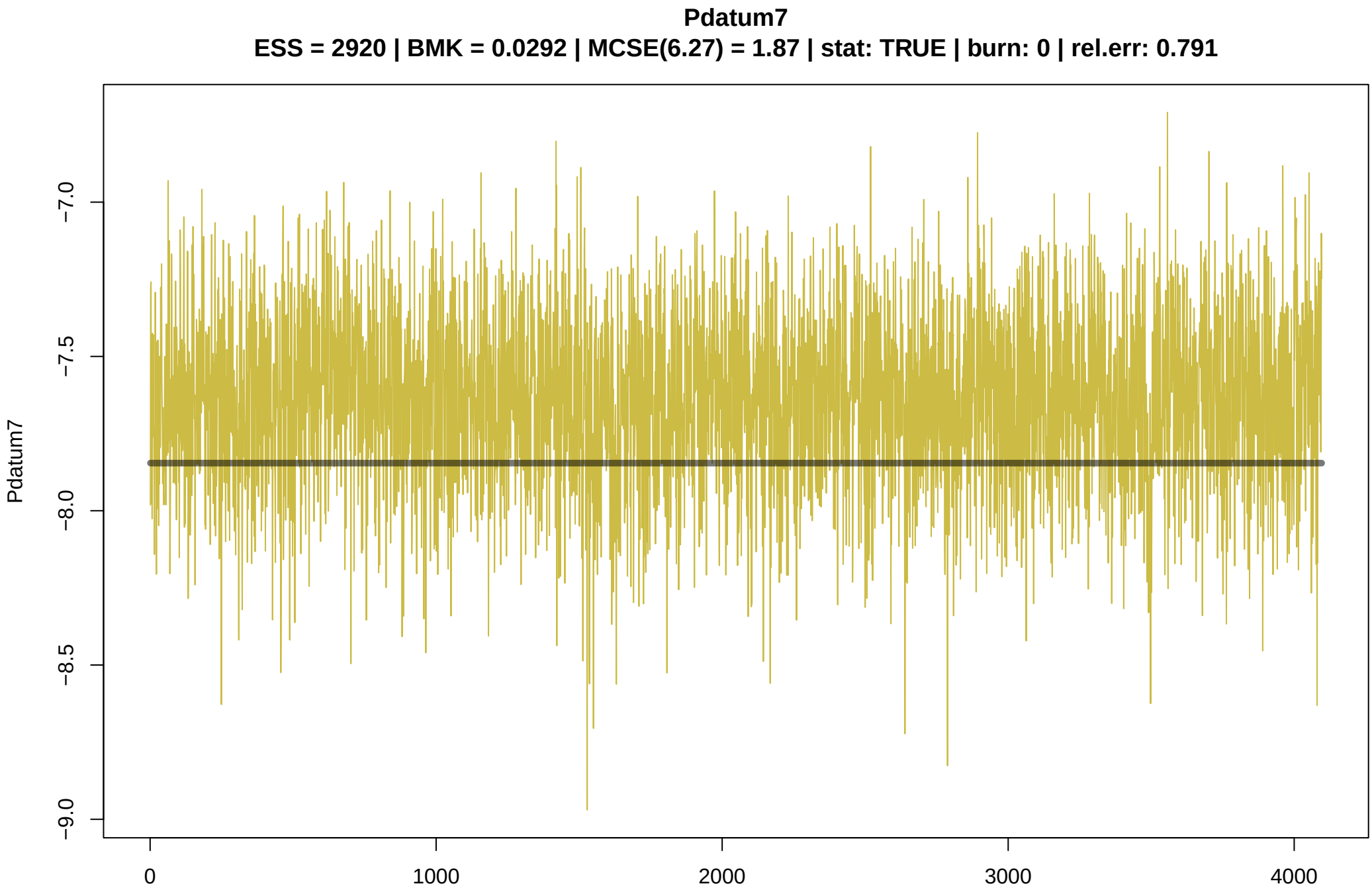

Pdatum2
ESS = 613 | BMK = 0.0738 | MCSE(6.27) = 4.14 | stat: TRUE | burn: 0 | rel.err: −2.2
Pdatum2
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

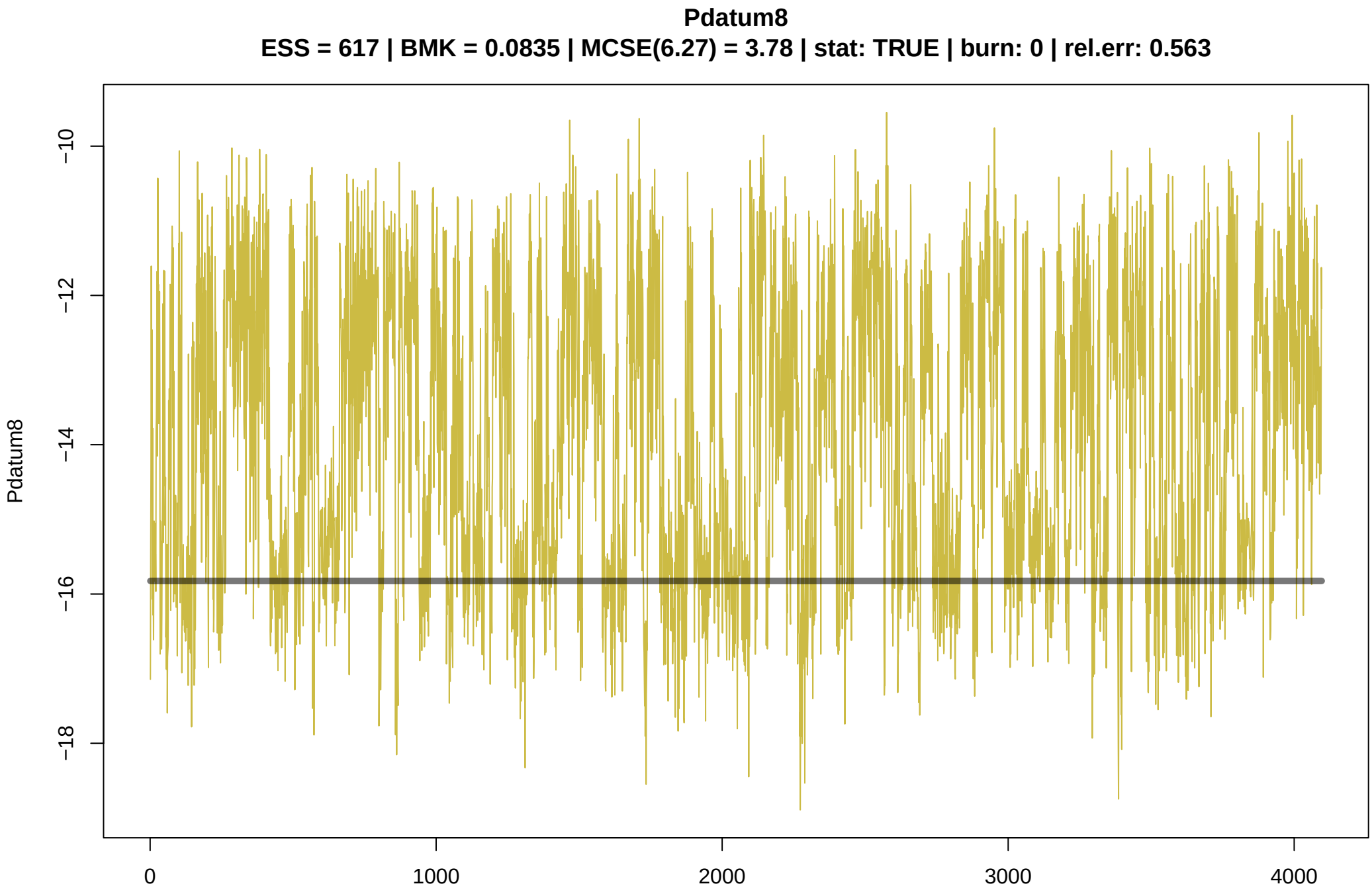

Pdatum3
ESS = 1240 | BMK = 0.0314 | MCSE(6.27) = 3.07 | stat: TRUE | burn: 0 | rel.err: −0.338
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

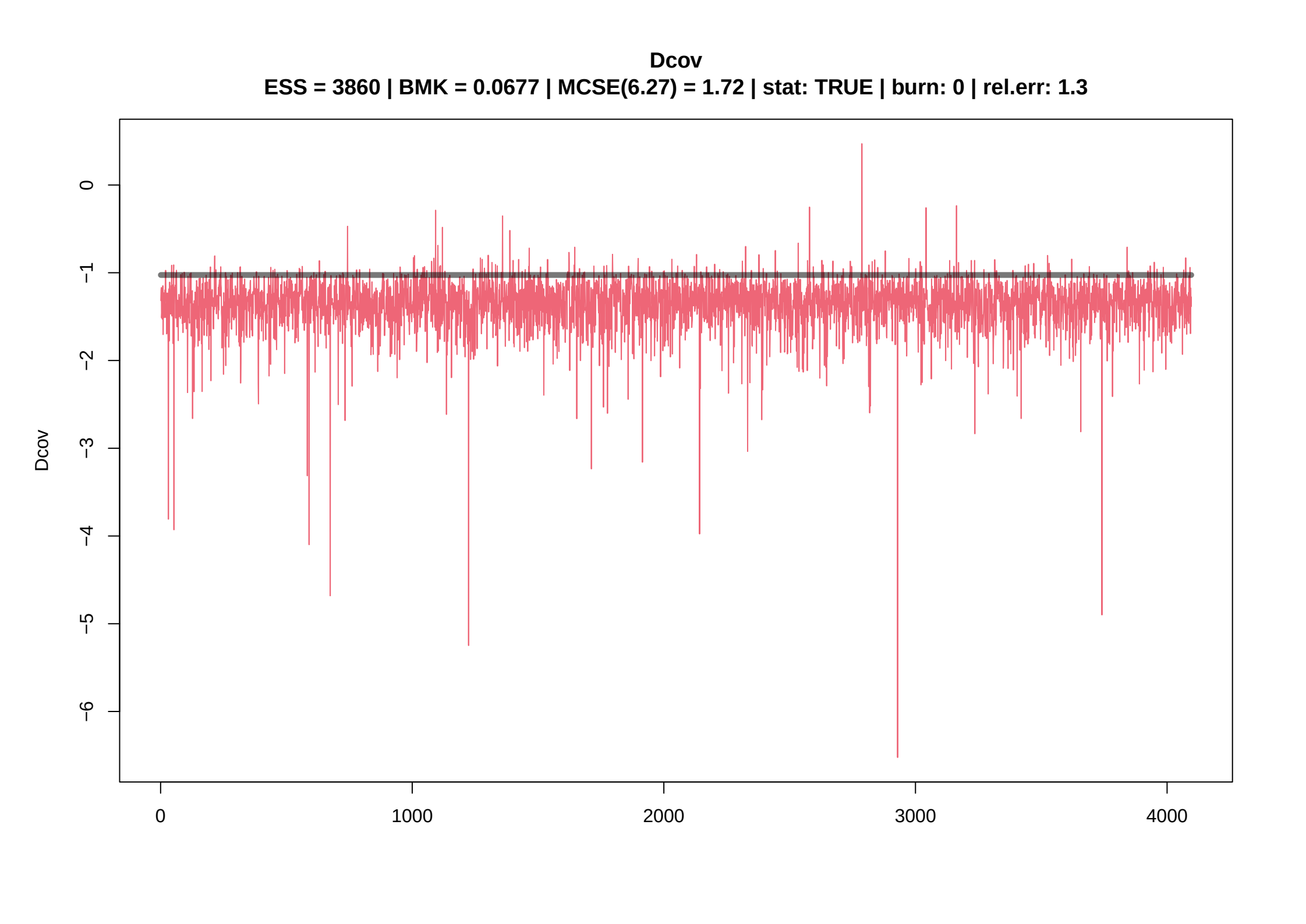

Pdatum4
ESS = 594 | BMK = 0.0716 | MCSE(6.27) = 3.72 | stat: FALSE | burn: 0 | rel.err: −0.0509
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
1000
2000
3000
4000

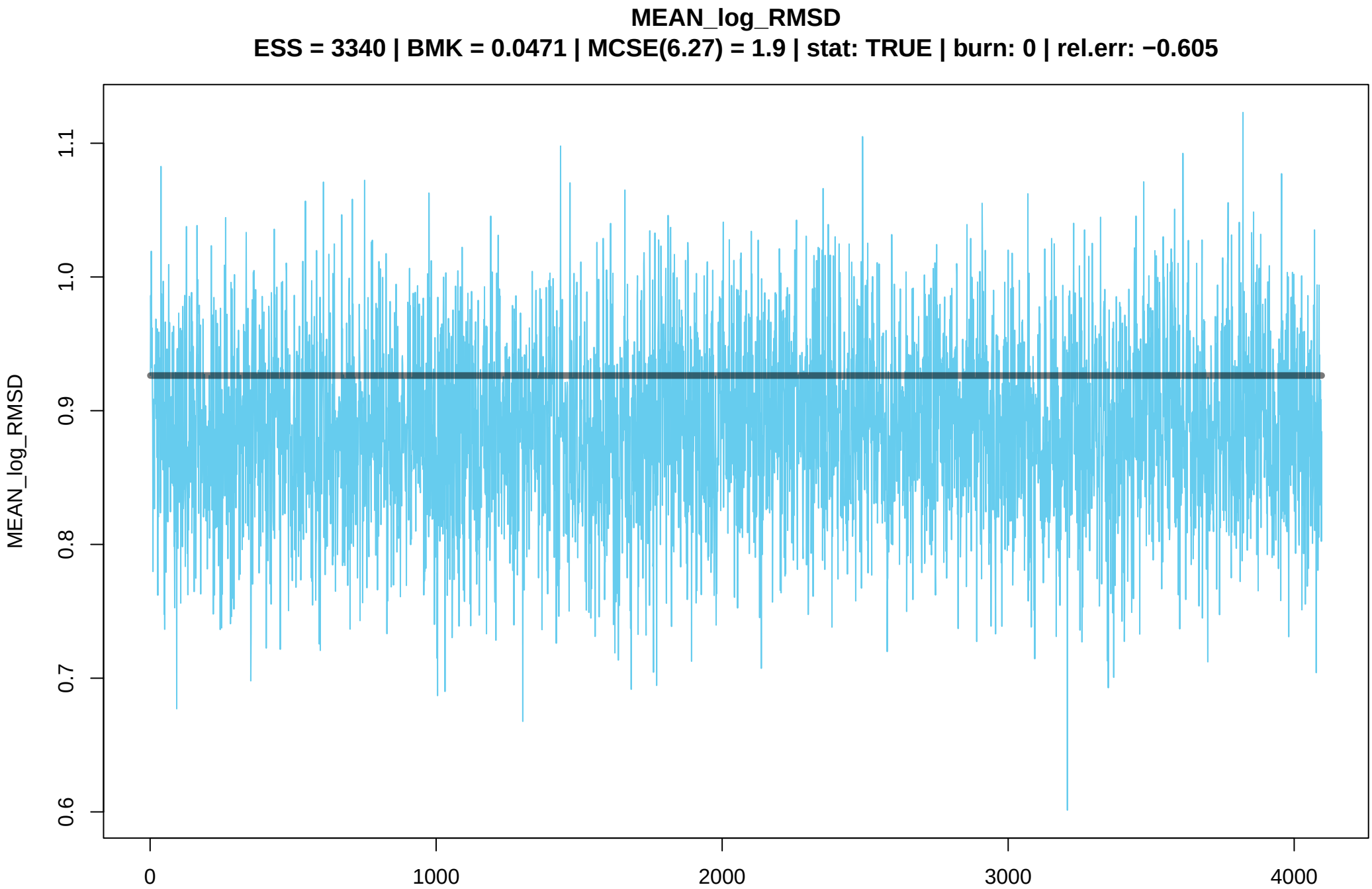

Pdatum5
ESS = 641 | BMK = 0.0902 | MCSE(6.27) = 3.54 | stat: FALSE | burn: 0 | rel.err: 1.44
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

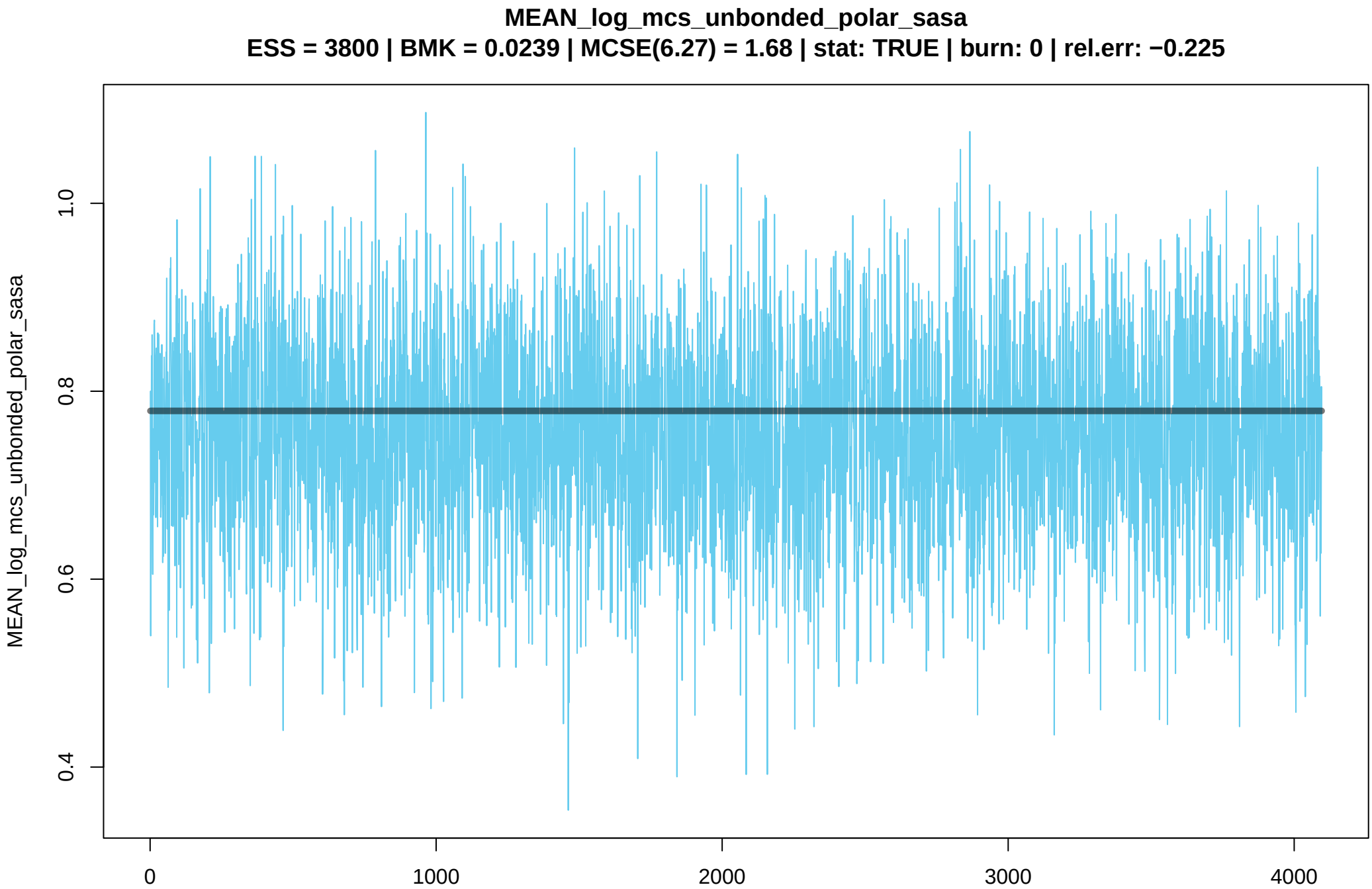

Pdatum6
ESS = 1930 | BMK = 0.0382 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: 0.642
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

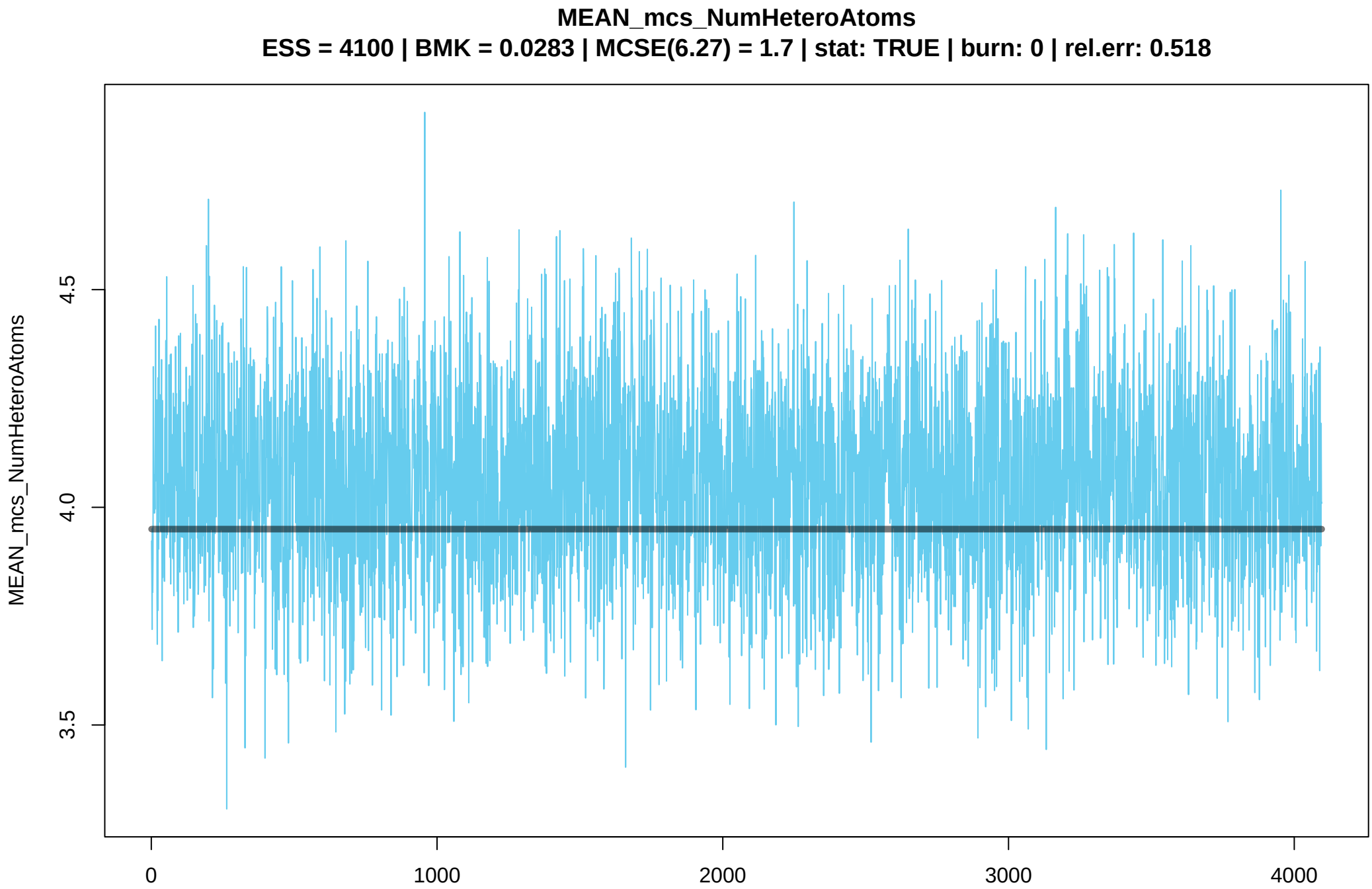

Pdatum7
ESS = 2920 | BMK = 0.0292 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0 | rel.err: 0.791
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

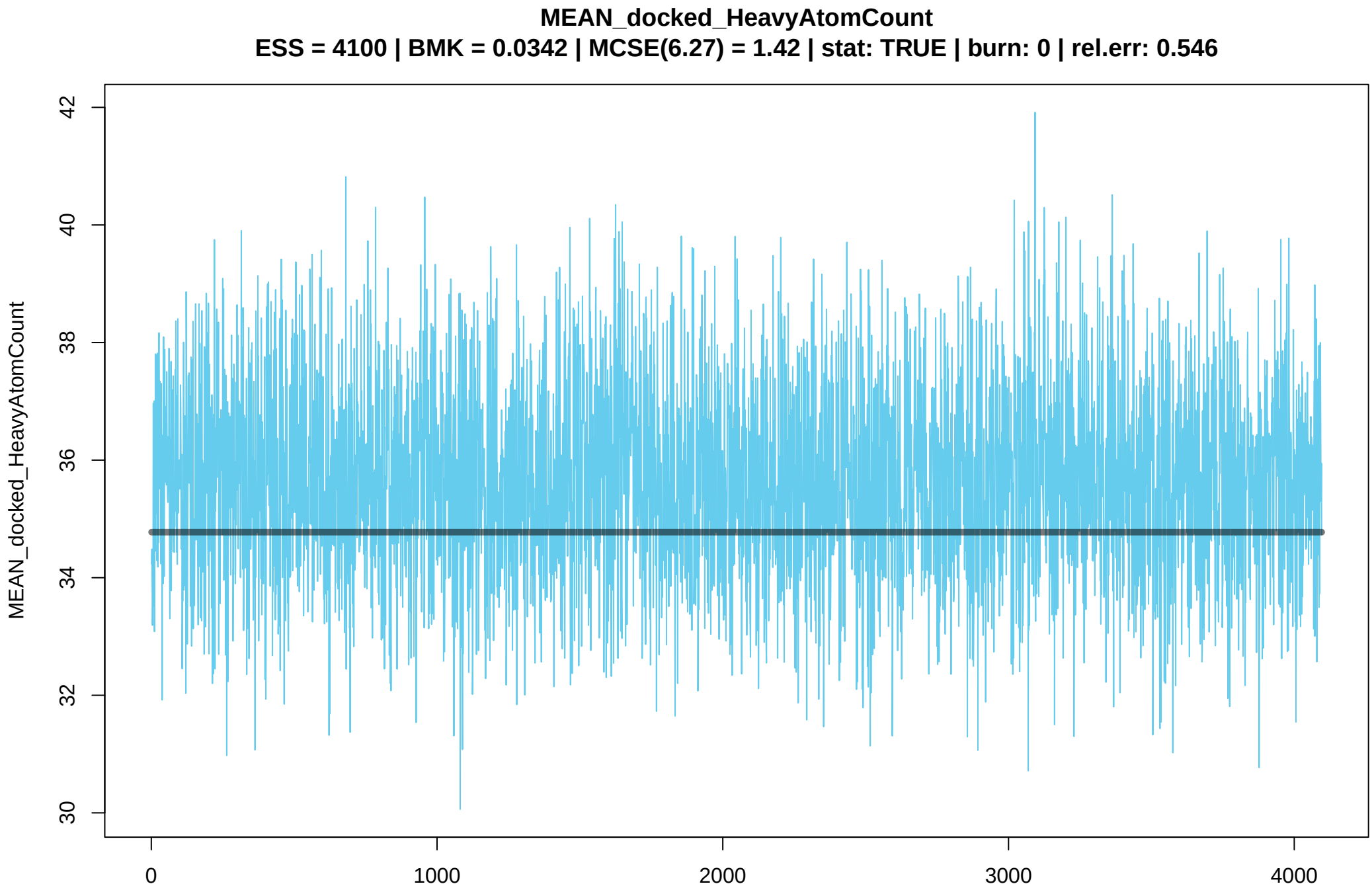

Pdatum8
ESS = 617 | BMK = 0.0835 | MCSE(6.27) = 3.78 | stat: TRUE | burn: 0 | rel.err: 0.563
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

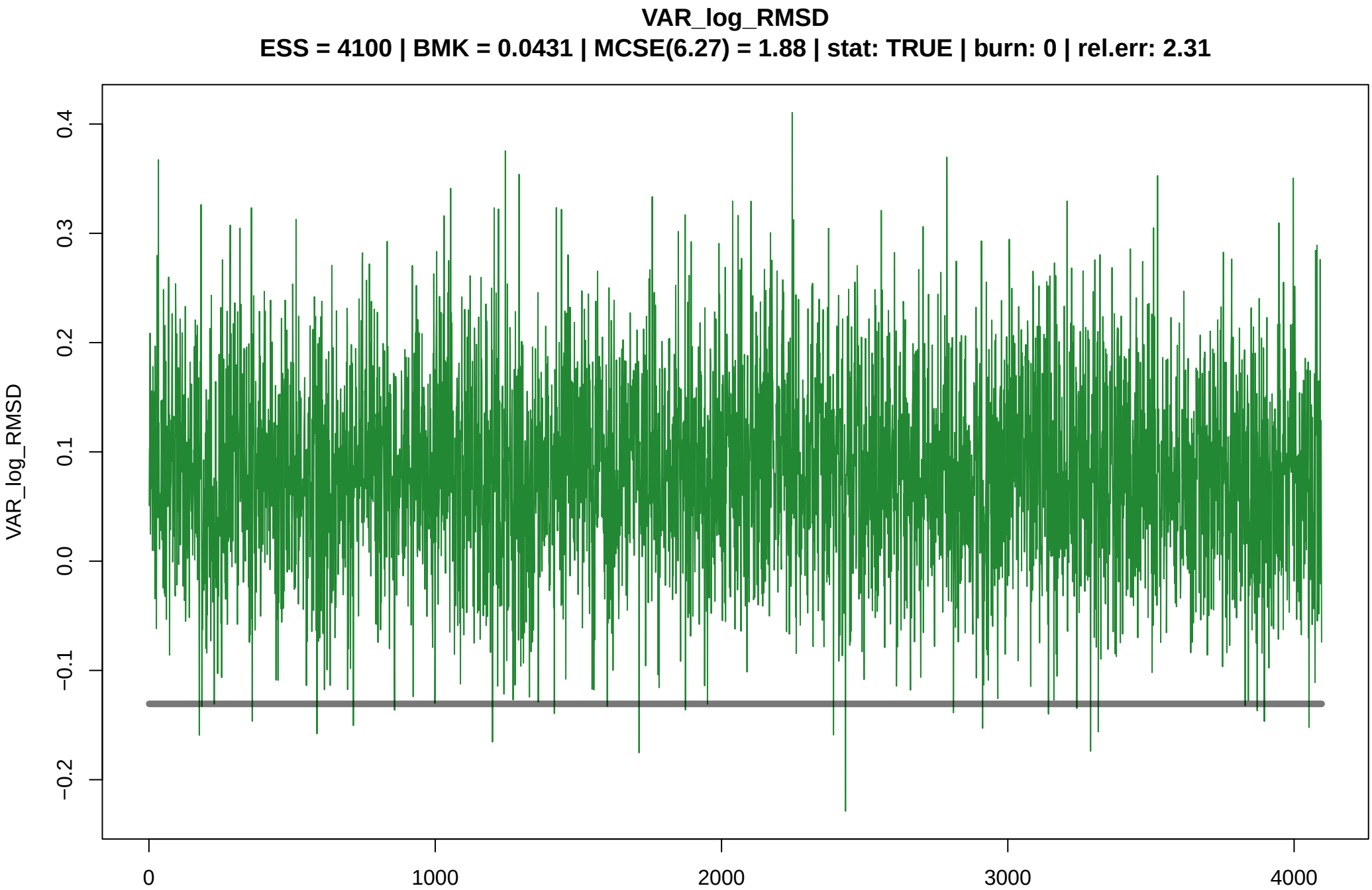

Dcov
ESS = 3860 | BMK = 0.0677 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0 | rel.err: 1.3
Dcov
0
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

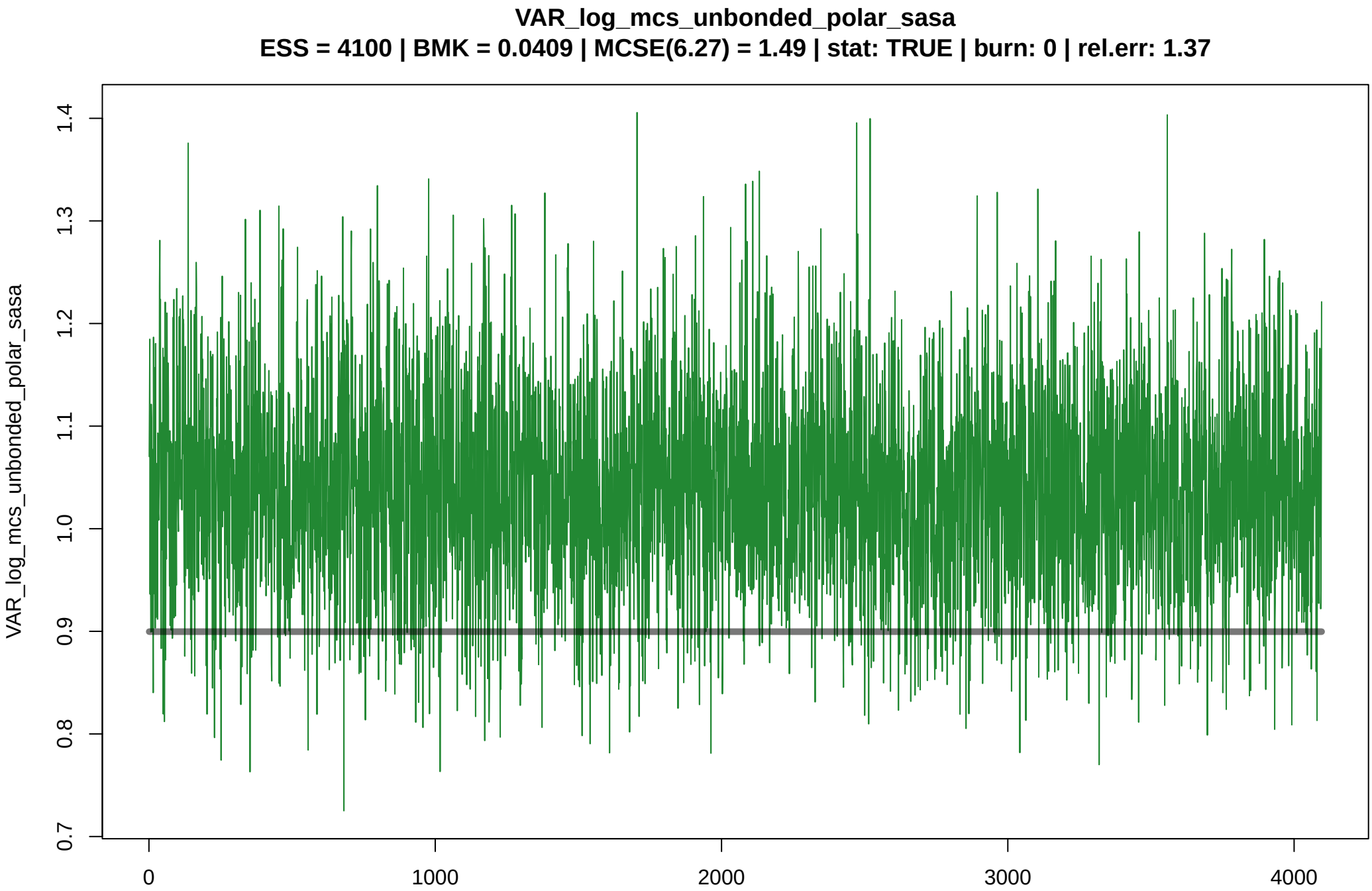

MEAN_log_RMSD
ESS = 3340 | BMK = 0.0471 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0 | rel.err: −0.605
MEAN_log_RMSD
0.6
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

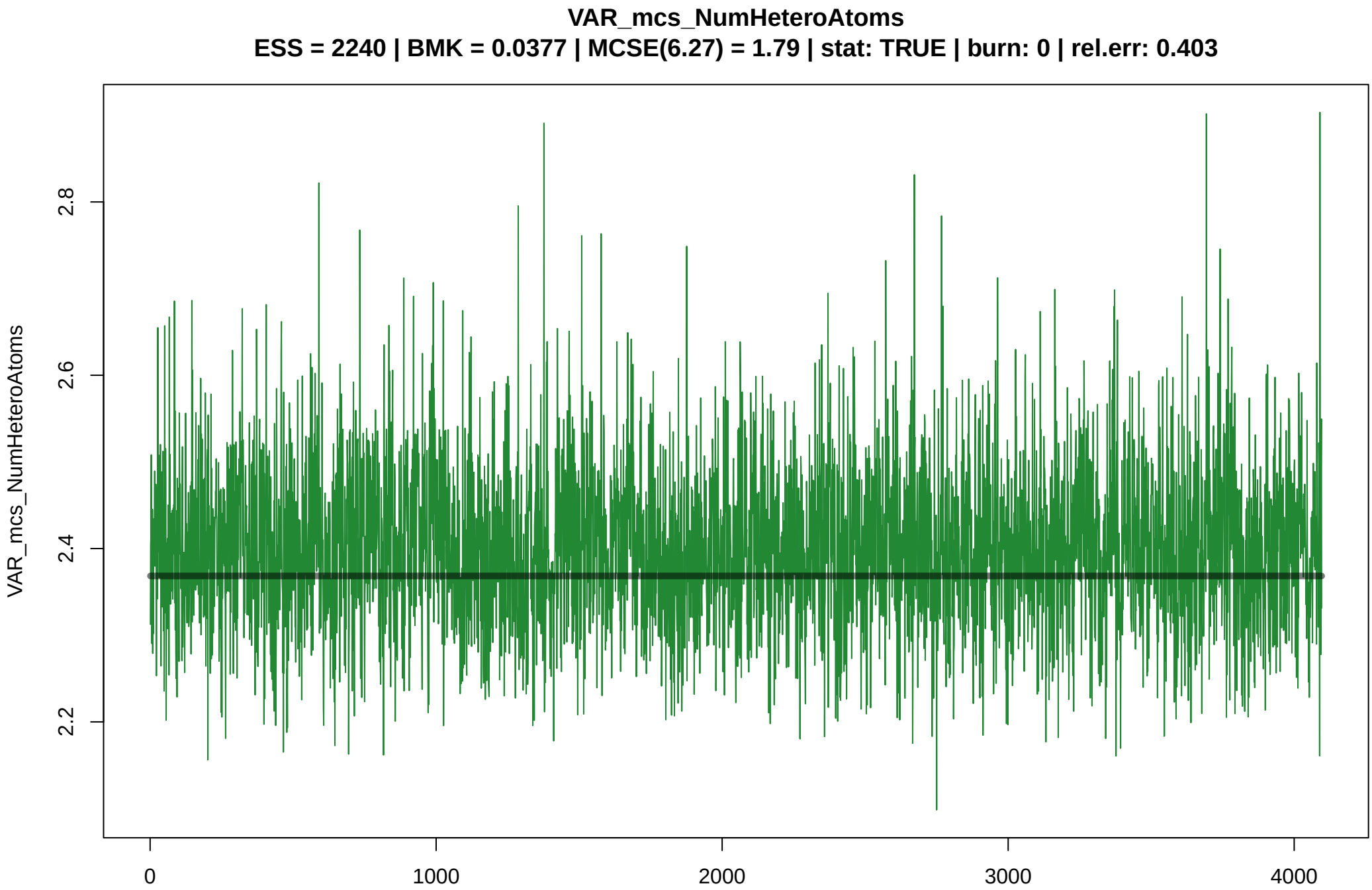

MEAN_log_mcs_unbonded_polar_sasa
ESS = 3800 | BMK = 0.0239 | MCSE(6.27) = 1.68 | stat: TRUE | burn: 0 | rel.err: −0.225
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

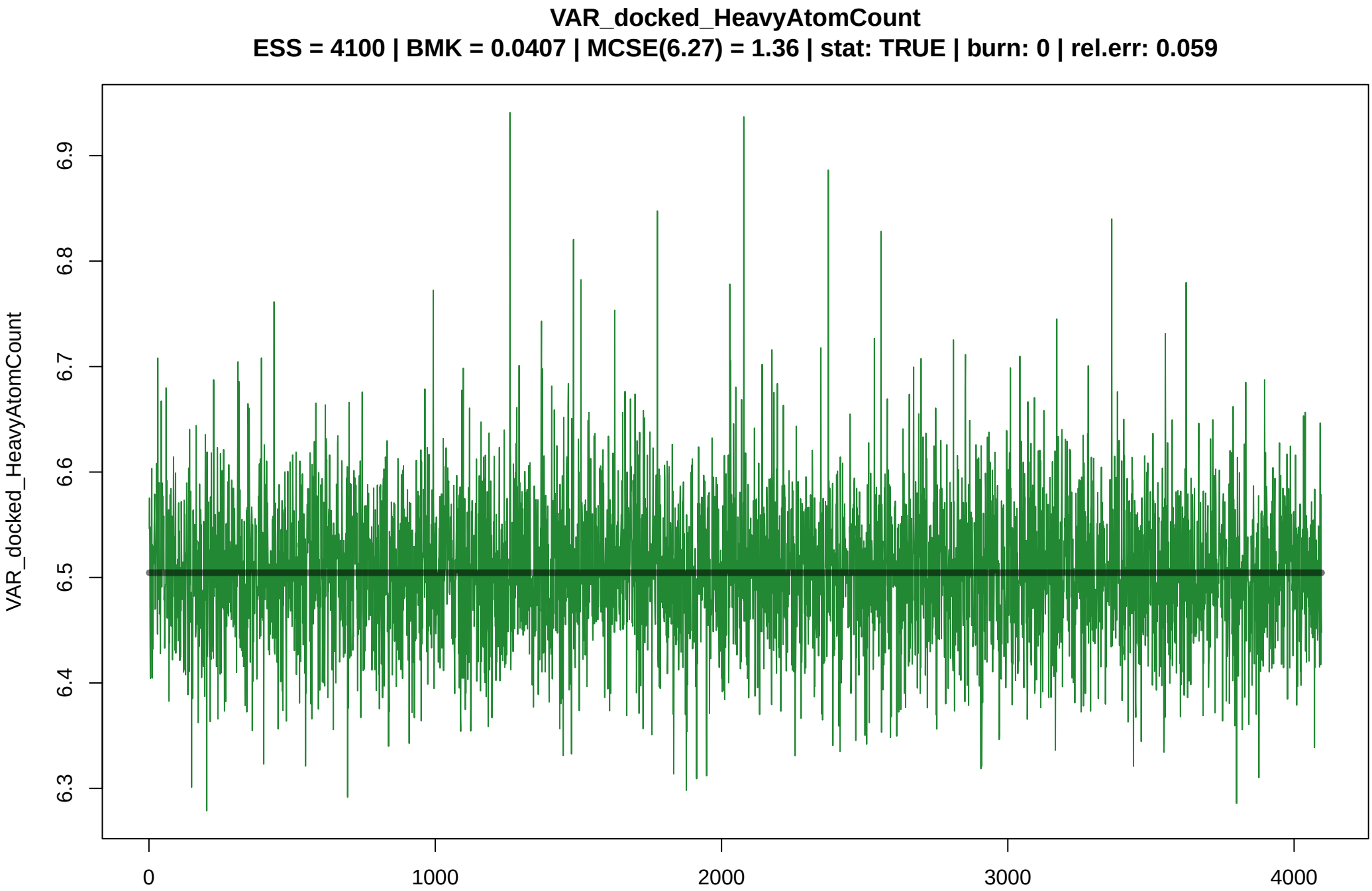

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0283 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0 | rel.err: 0.518
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

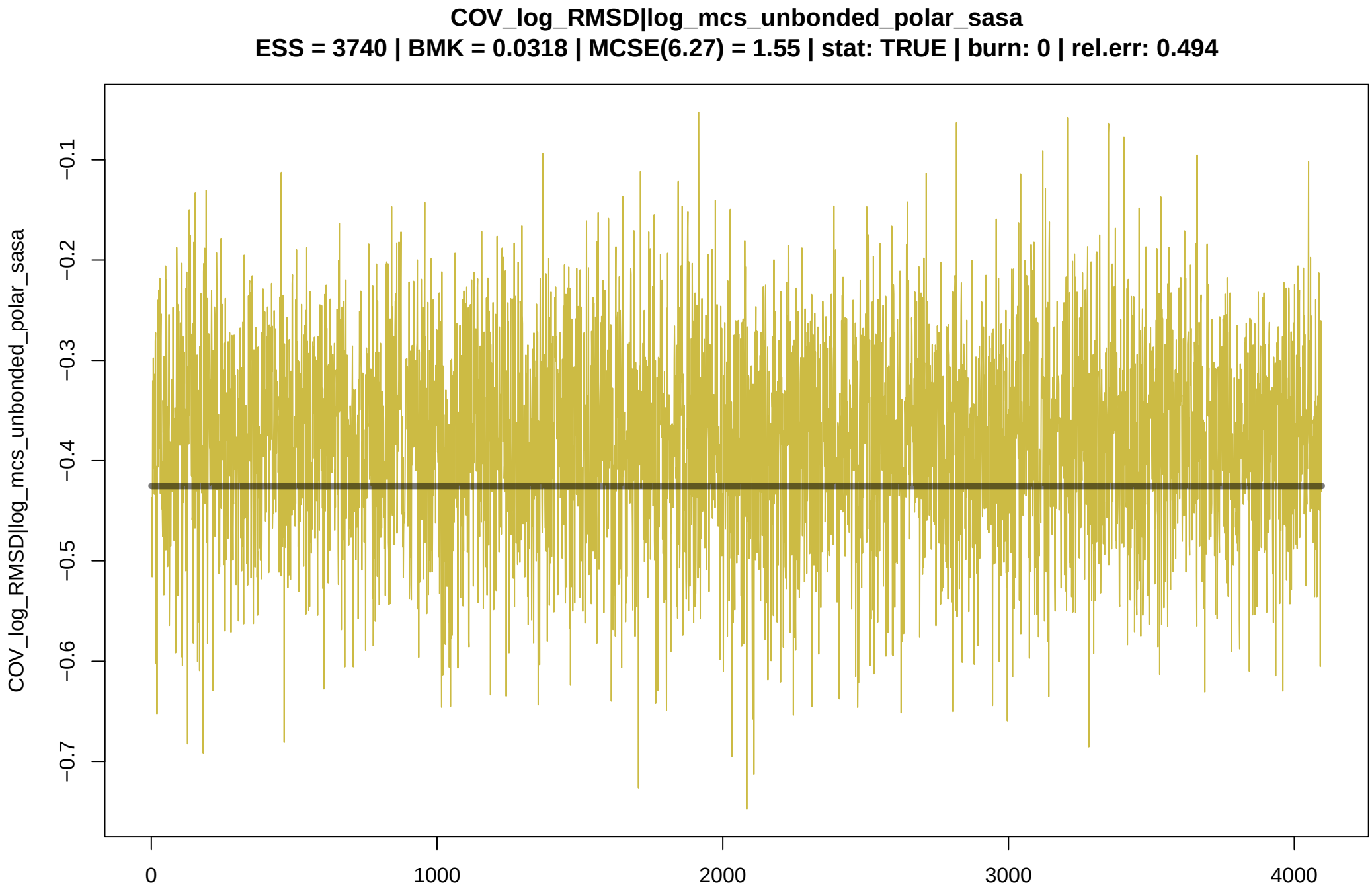

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0342 | MCSE(6.27) = 1.42 | stat: TRUE | burn: 0 | rel.err: 0.546
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
1000
2000
3000
4000

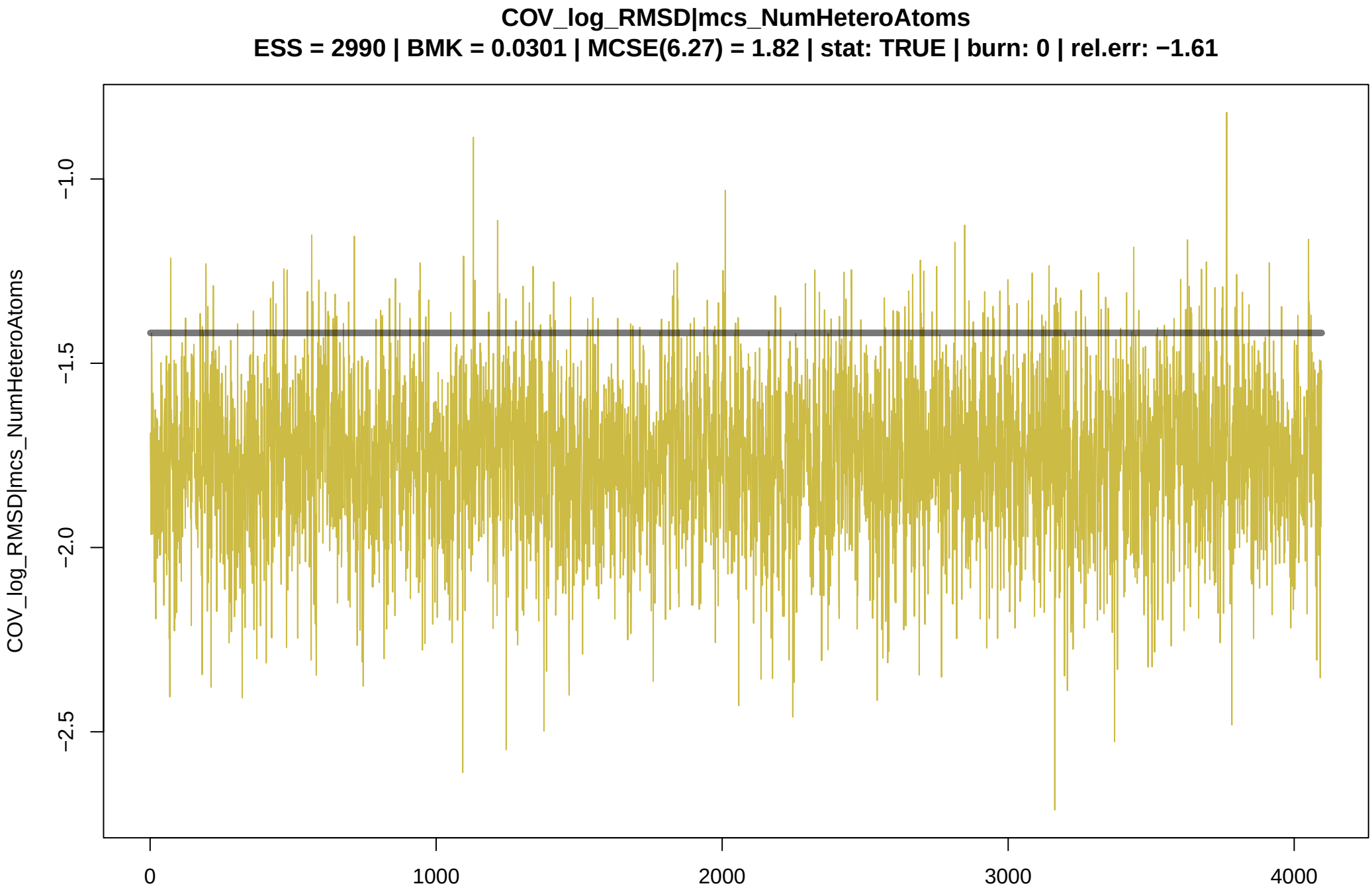

VAR_log_RMSD
ESS = 4100 | BMK = 0.0431 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 0 | rel.err: 2.31
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

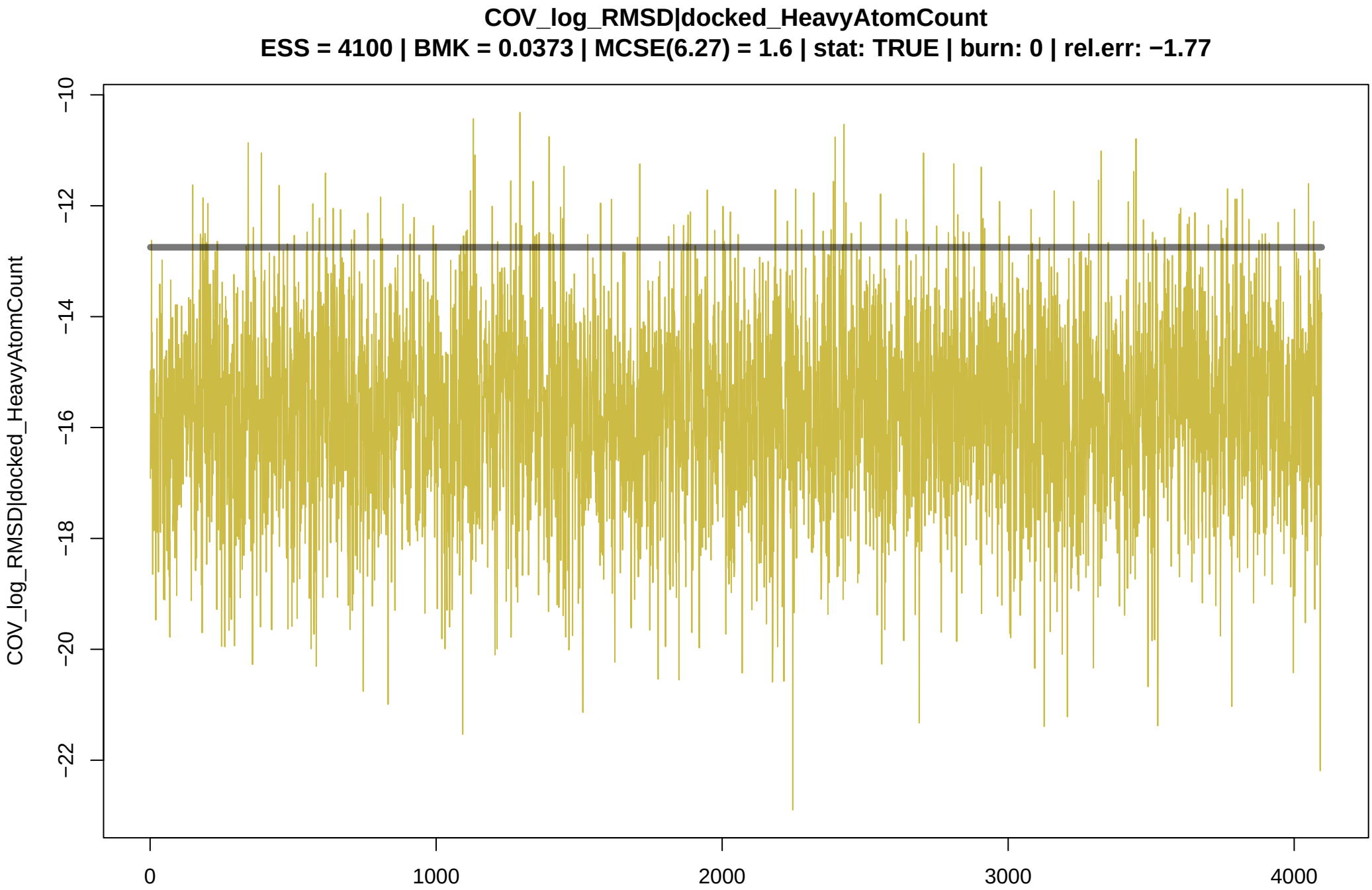

VAR_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0409 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0 | rel.err: 1.37
VAR_log_mcs_unbonded_polar_sasa
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
1000
2000
3000
4000

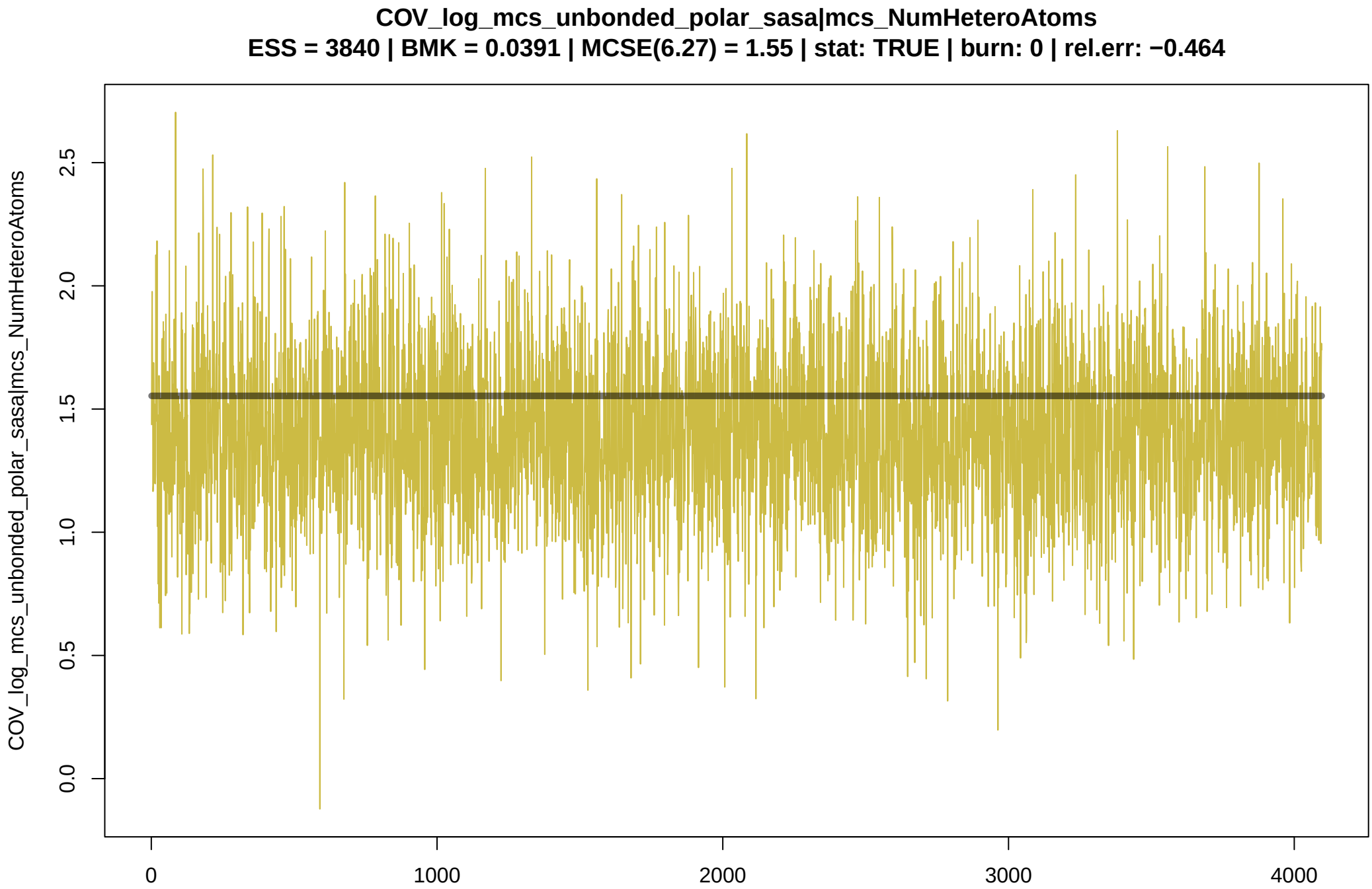

VAR_mcs_NumHeteroAtoms
ESS = 2240 | BMK = 0.0377 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.403
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
1000
2000
3000
4000

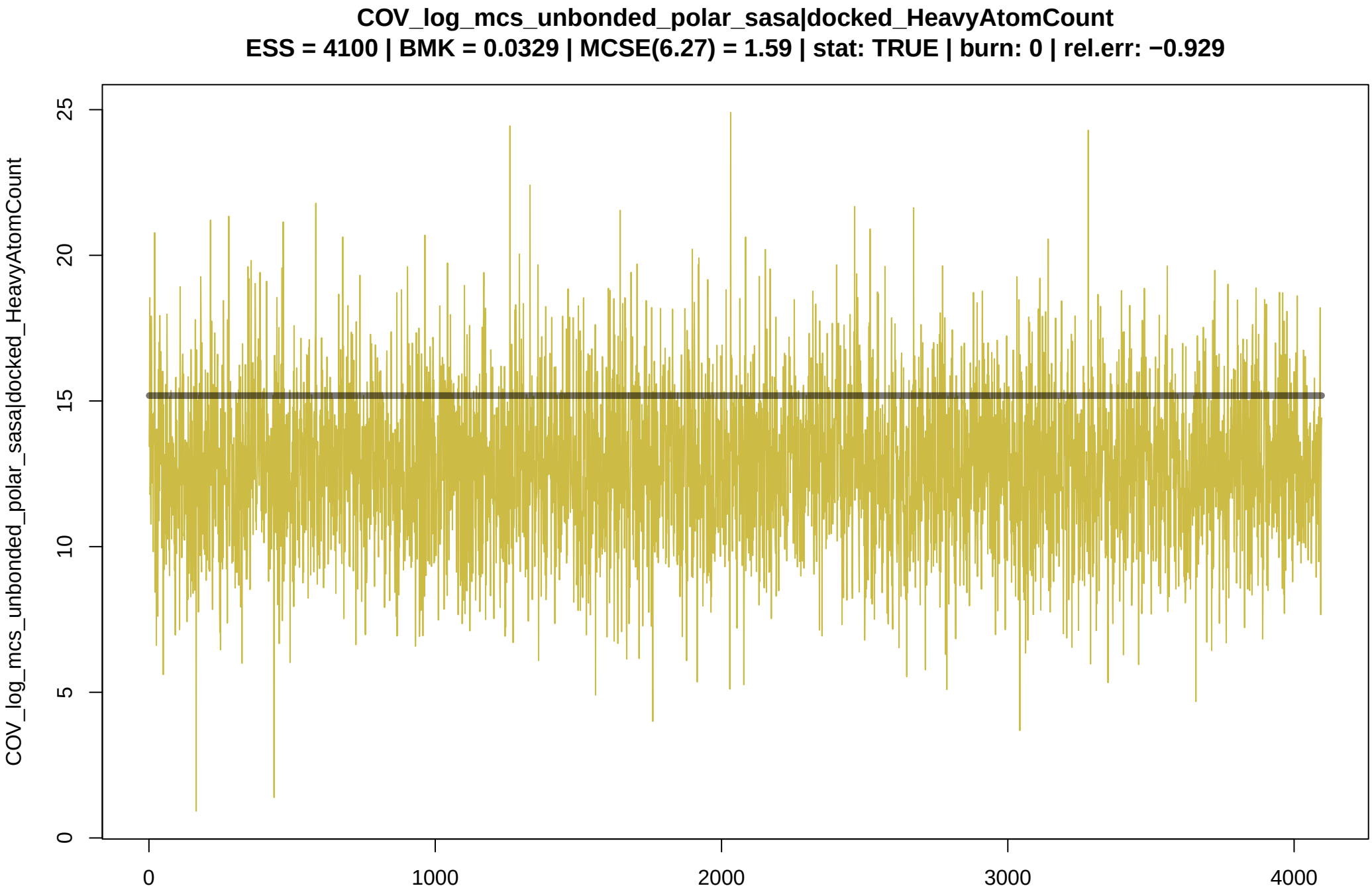

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0407 | MCSE(6.27) = 1.36 | stat: TRUE | burn: 0 | rel.err: 0.059
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
6.9
0
1000
2000
3000
4000

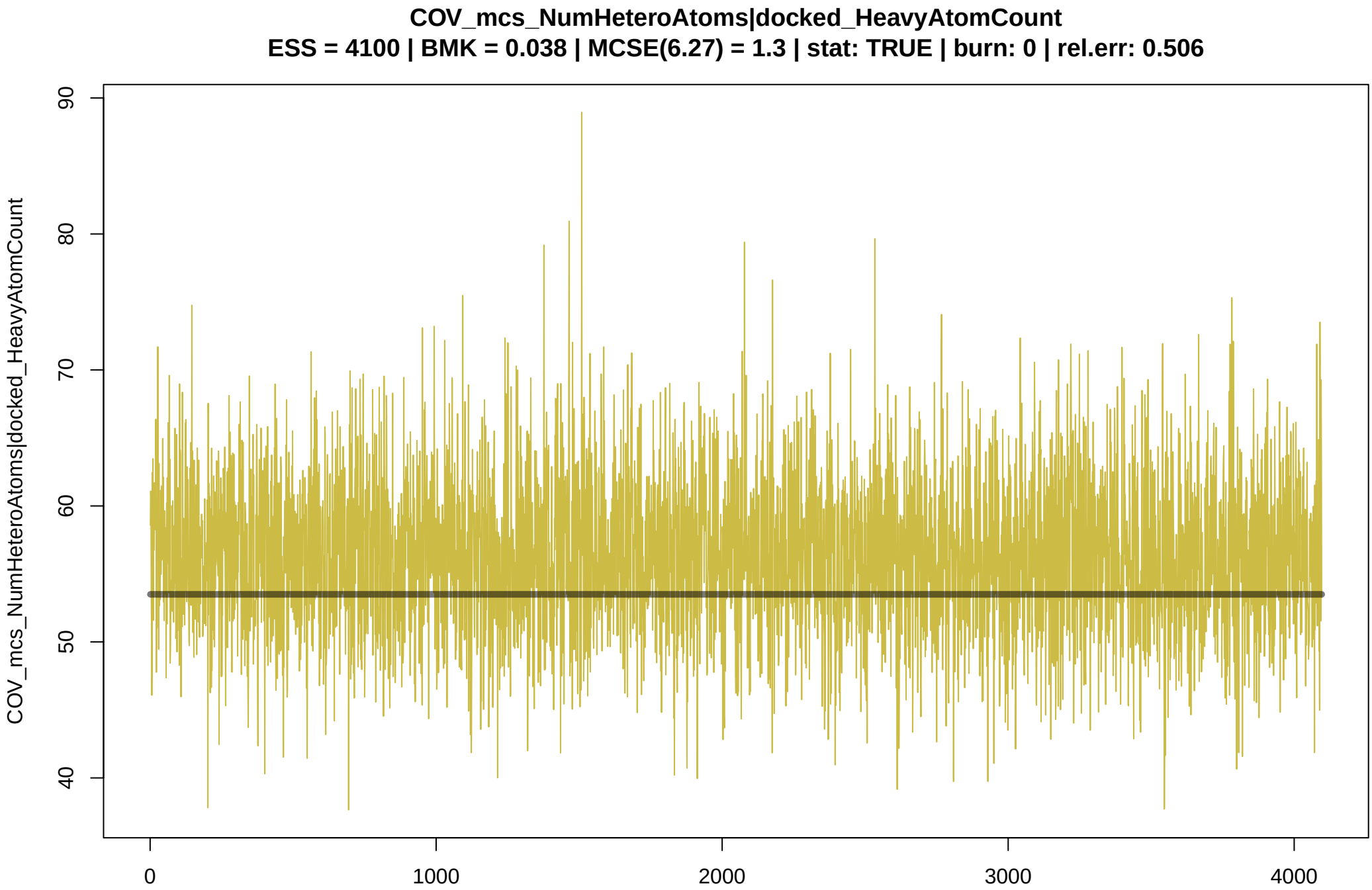

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3740 | BMK = 0.0318 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: 0.494
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2990 | BMK = 0.0301 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: −1.61
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.5
−2.0
−2.5
0
1000
2000
3000
4000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0373 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: −1.77
COV_log_RMSD|docked_HeavyAtomCount
−10
−12
−14
−16
−18
−20
−22
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3840 | BMK = 0.0391 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: −0.464
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.0
0.5
1.0
1.5
2.0
2.5
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0329 | MCSE(6.27) = 1.59 | stat: TRUE | burn: 0 | rel.err: −0.929
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0
5
10
15
20
25
0
1000
2000
3000
4000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.038 | MCSE(6.27) = 1.3 | stat: TRUE | burn: 0 | rel.err: 0.506
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
90
80
70
60
50
40
0
1000
2000
3000
4000