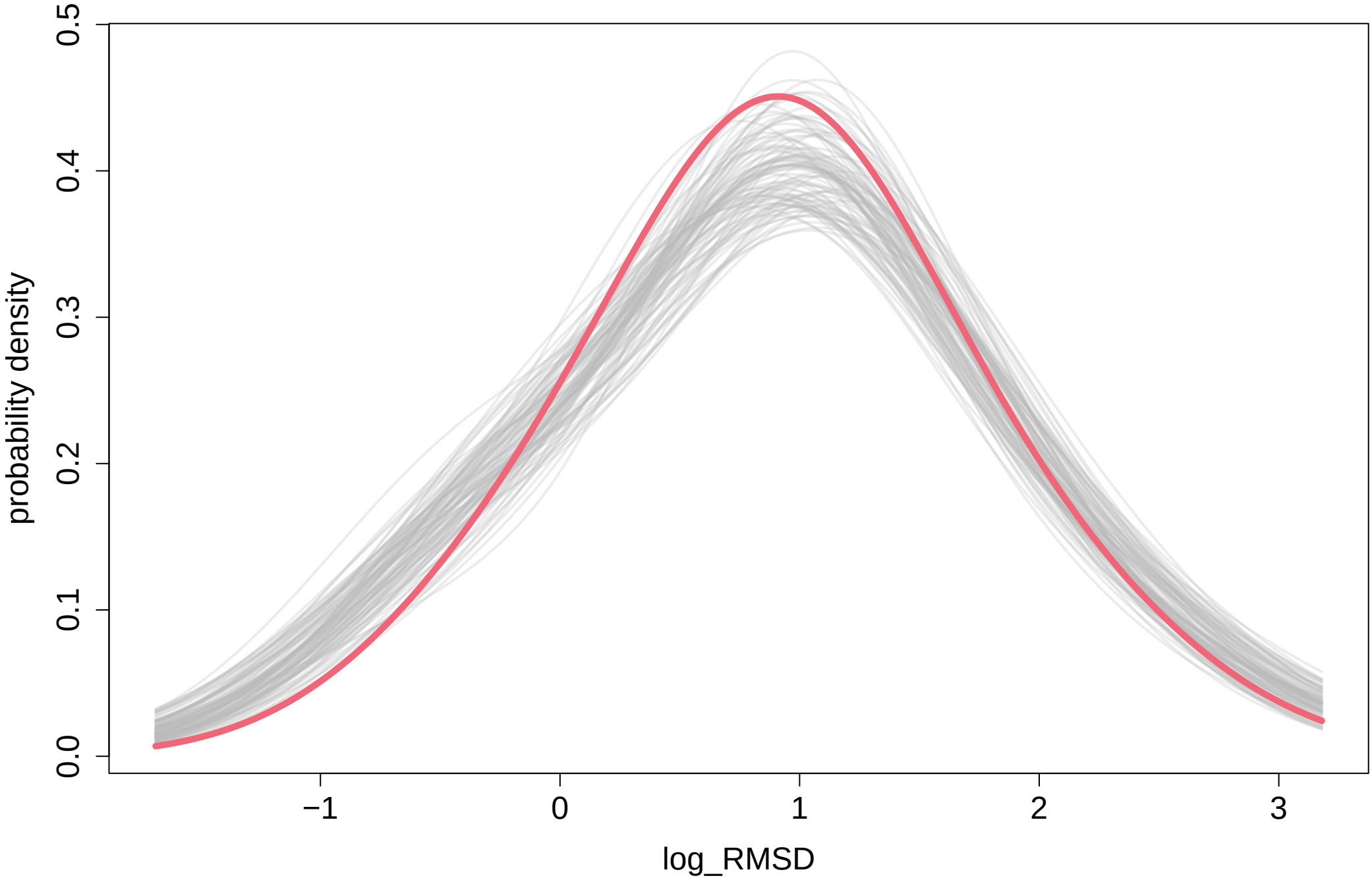
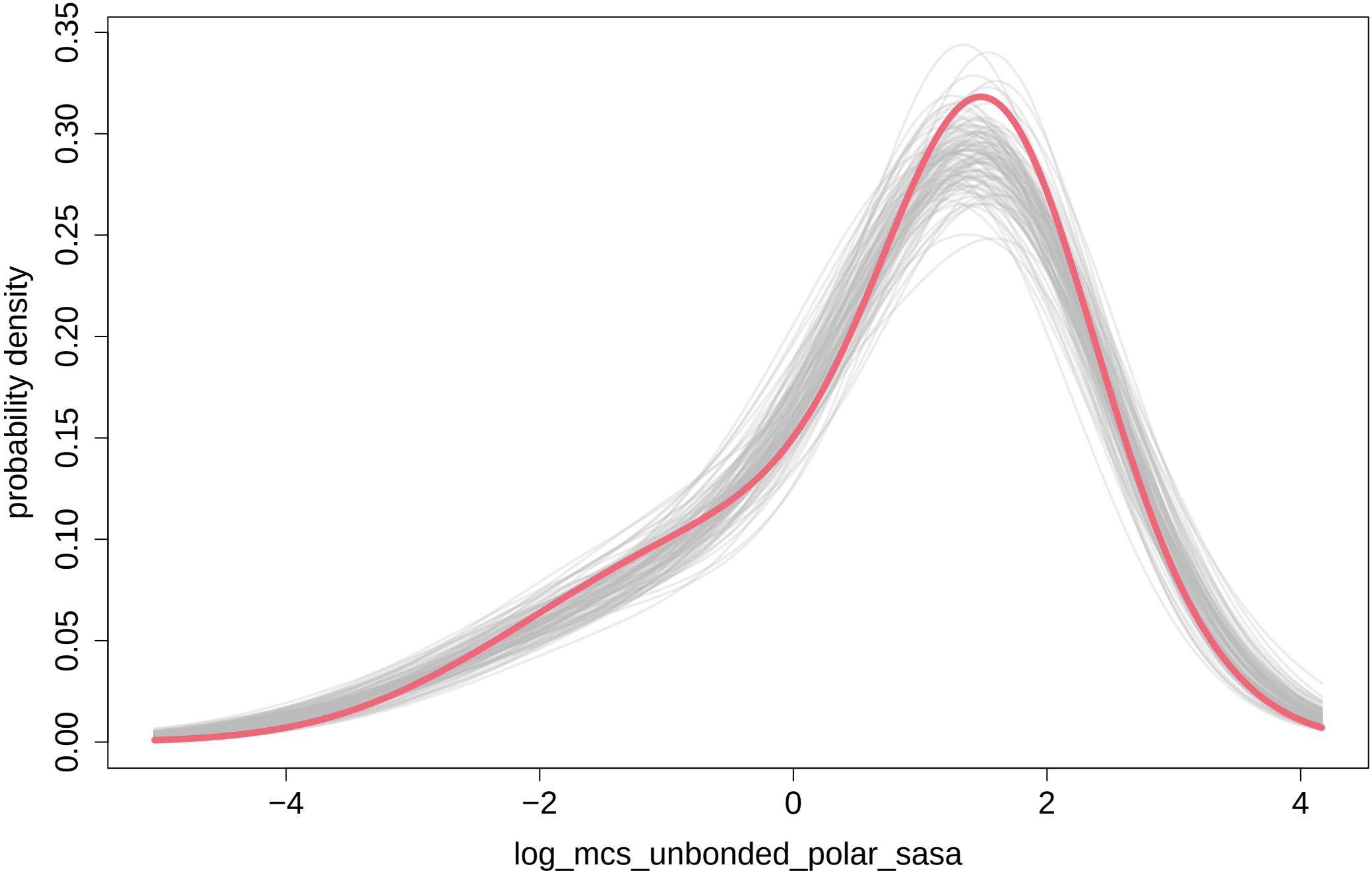
−− STATS maxD −−
min ESS = 141.659912967009
max BMK = 0.124541435746285
max MCSE = 7.11678914244484
all stationary: FALSE
burn: 0
max rel.err.: 2.05192941945213

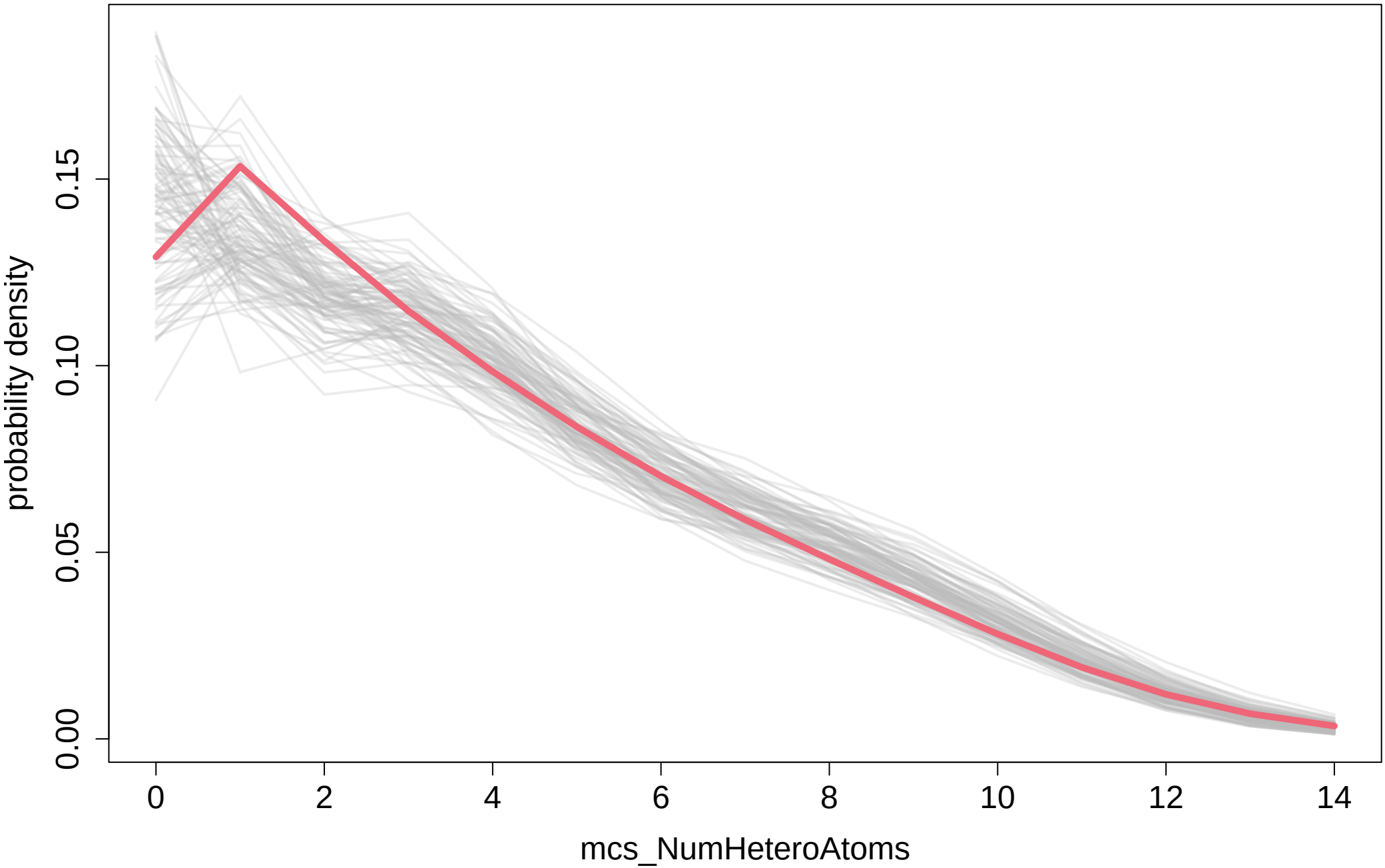
−− STATS 2D −−
min ESS = 3428.70685797961
max BMK = 0.041241154259285 5
max MCSE = 1.92370230925344
all stationary: FALSE
burn: 0
max rel.err.: 1.74612397085485

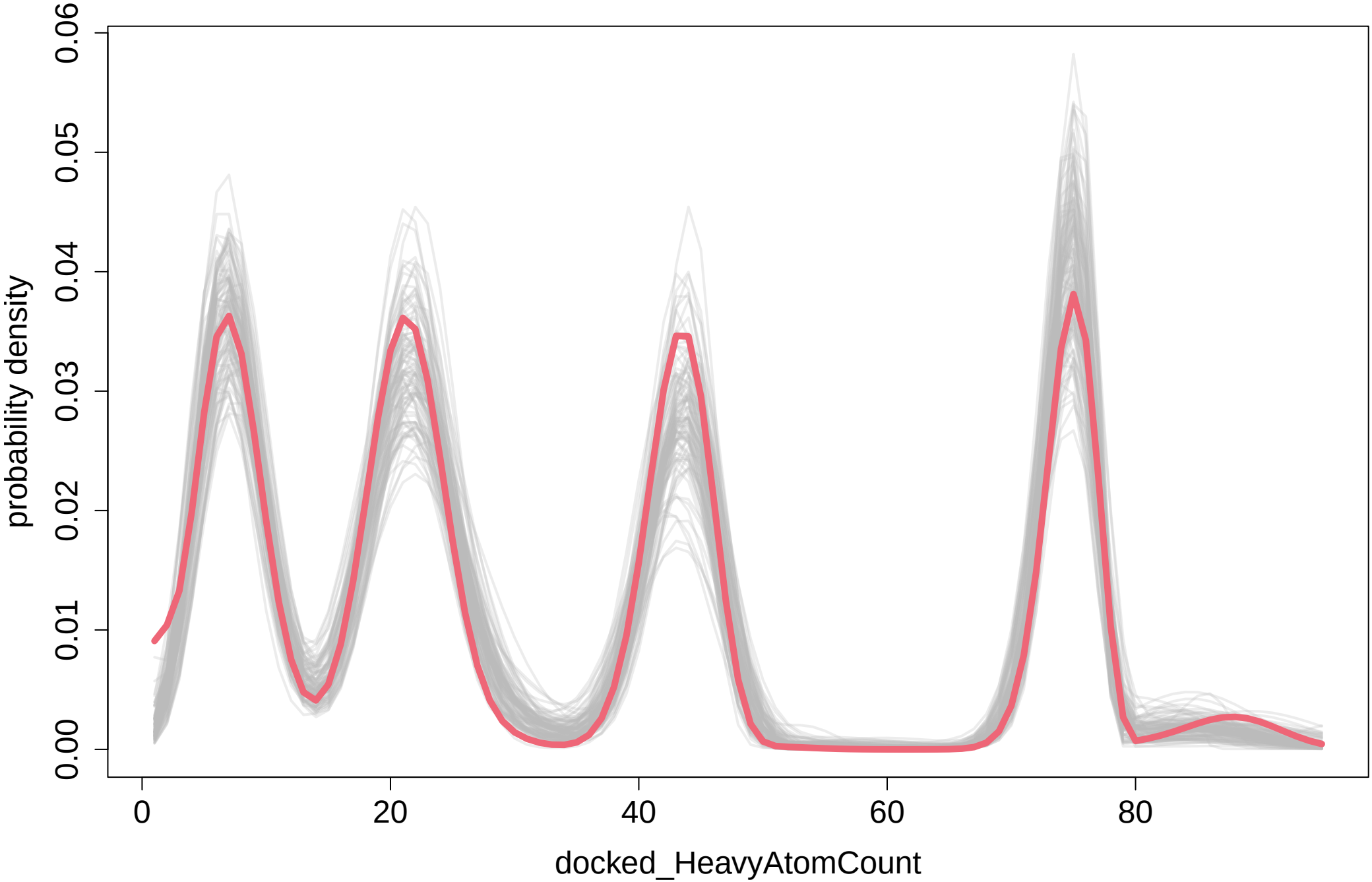
−− STATS 1D −−
min ESS = 3111.75710317174
max BMK = 0.057174675339676 2
max MCSE = 2.01402496838341
all stationary: FALSE
burn: 0
max rel.err.: 2.30795125674937

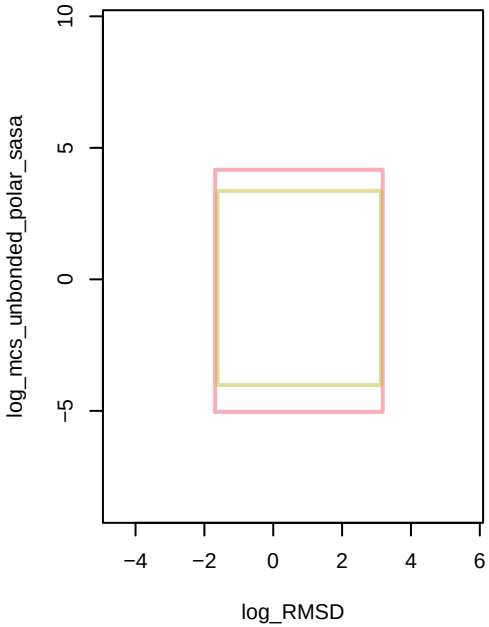
Occupied clusters: 10 of 16
LL: −2160 +− 6.86

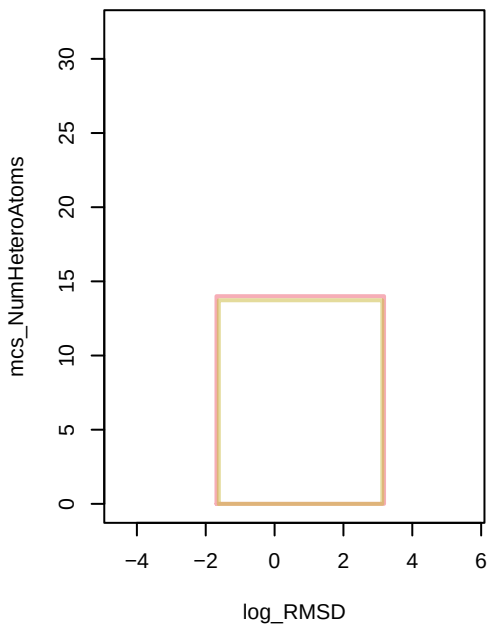

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−1
0
1
2
3
log_RMSD

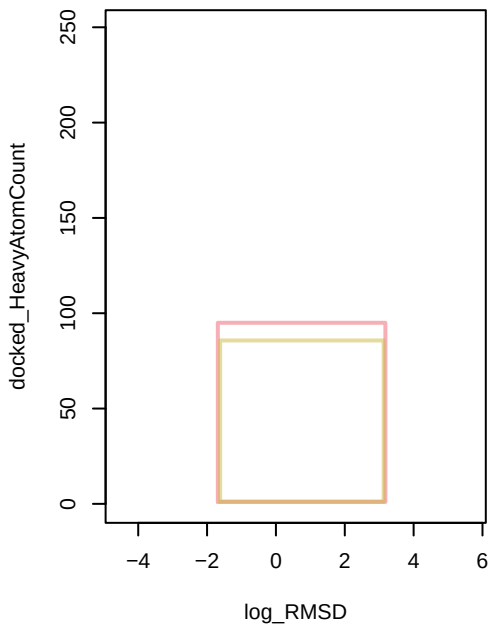

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

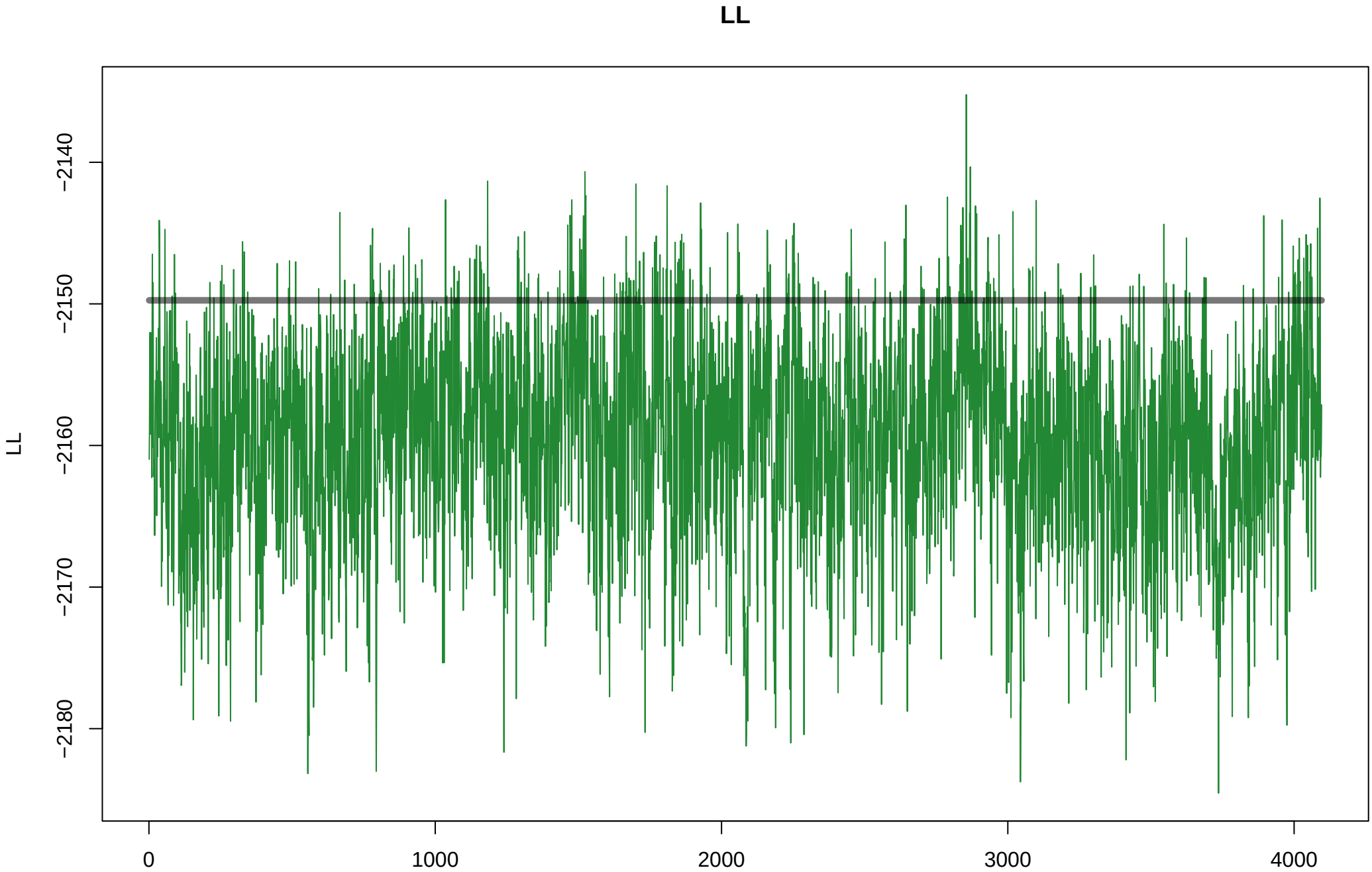

probability density
0.00
0.05
0.10
0.15
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

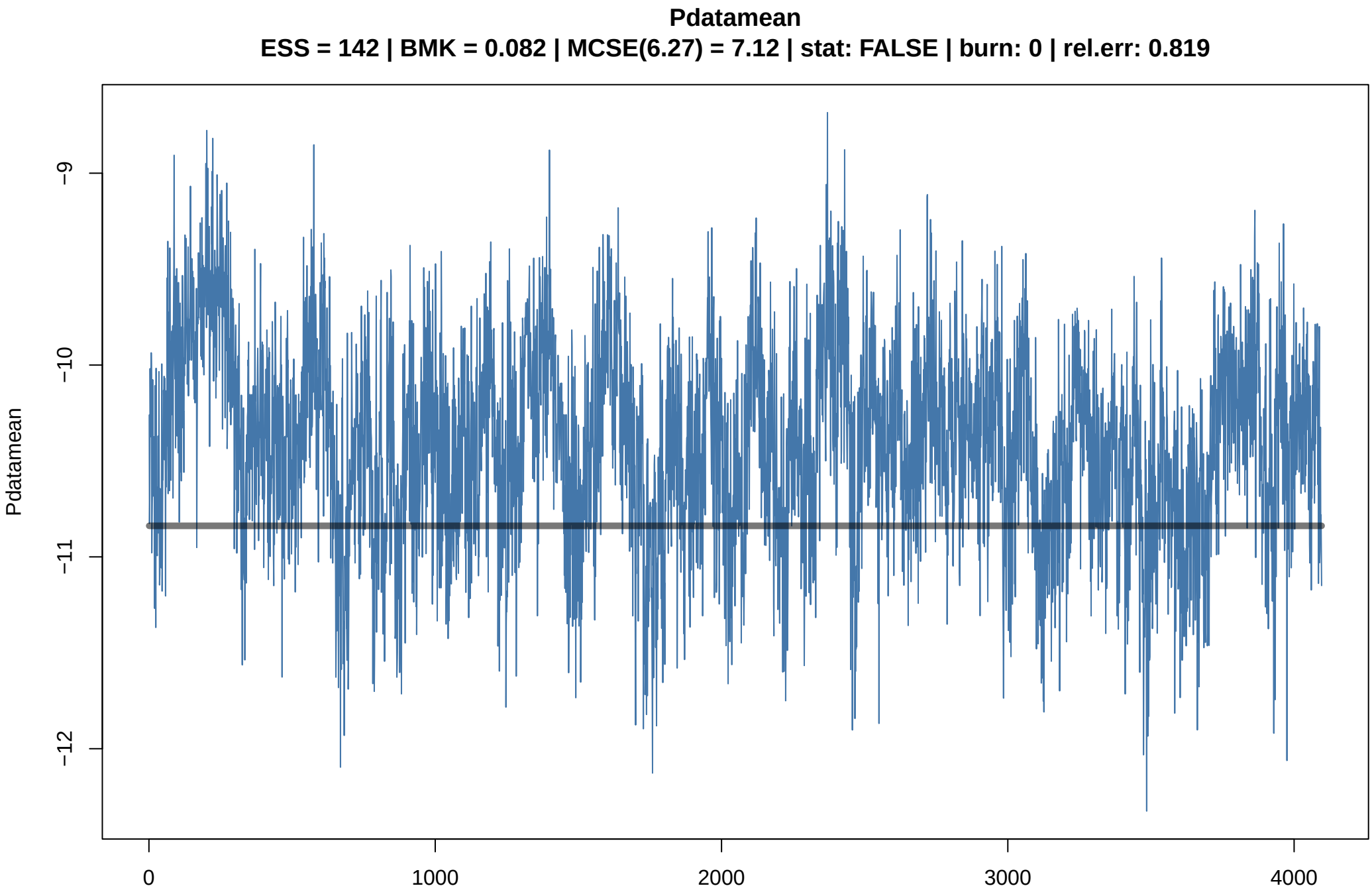

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0
20
40
60
80
docked_HeavyAtomCount

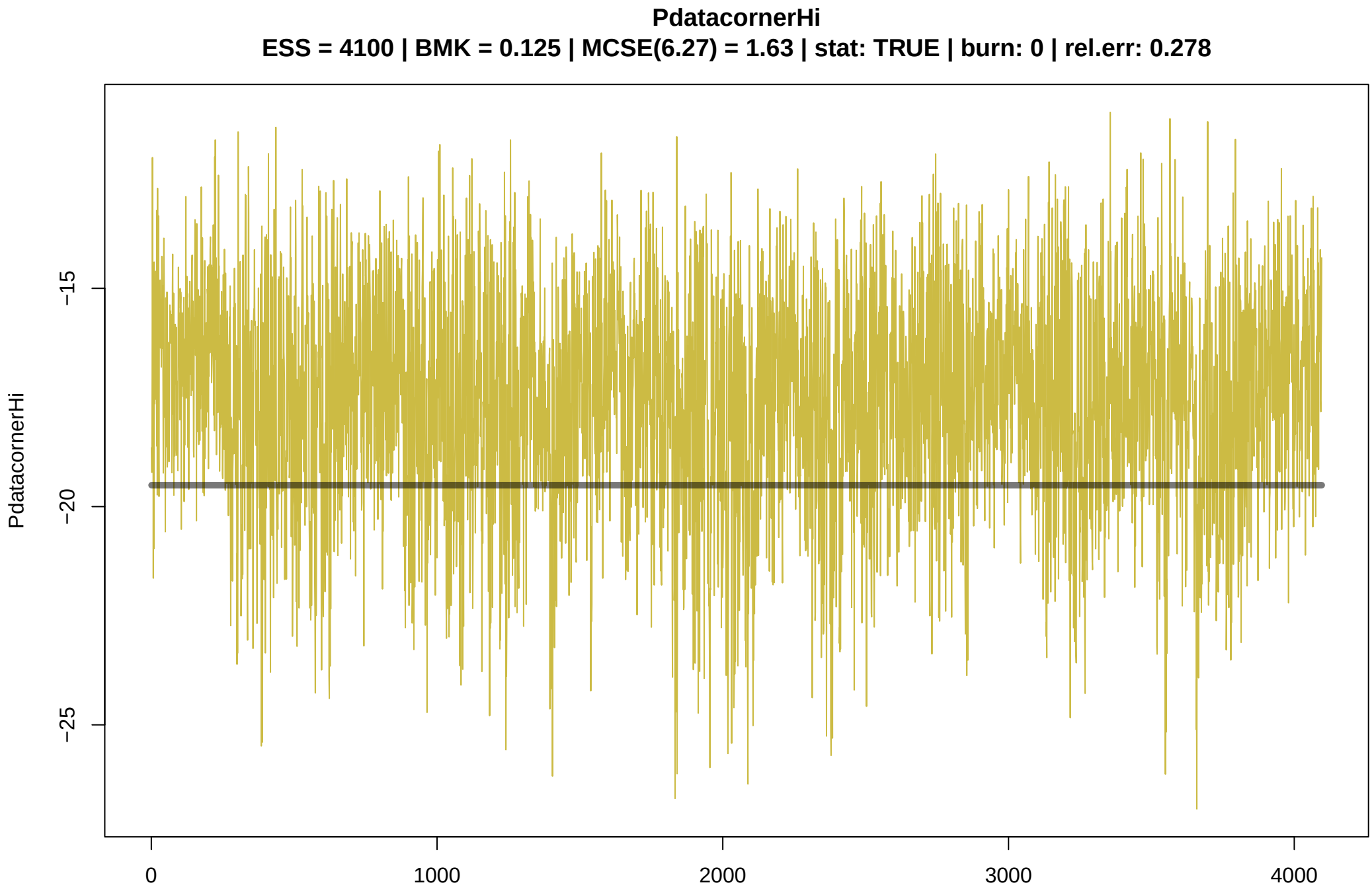

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

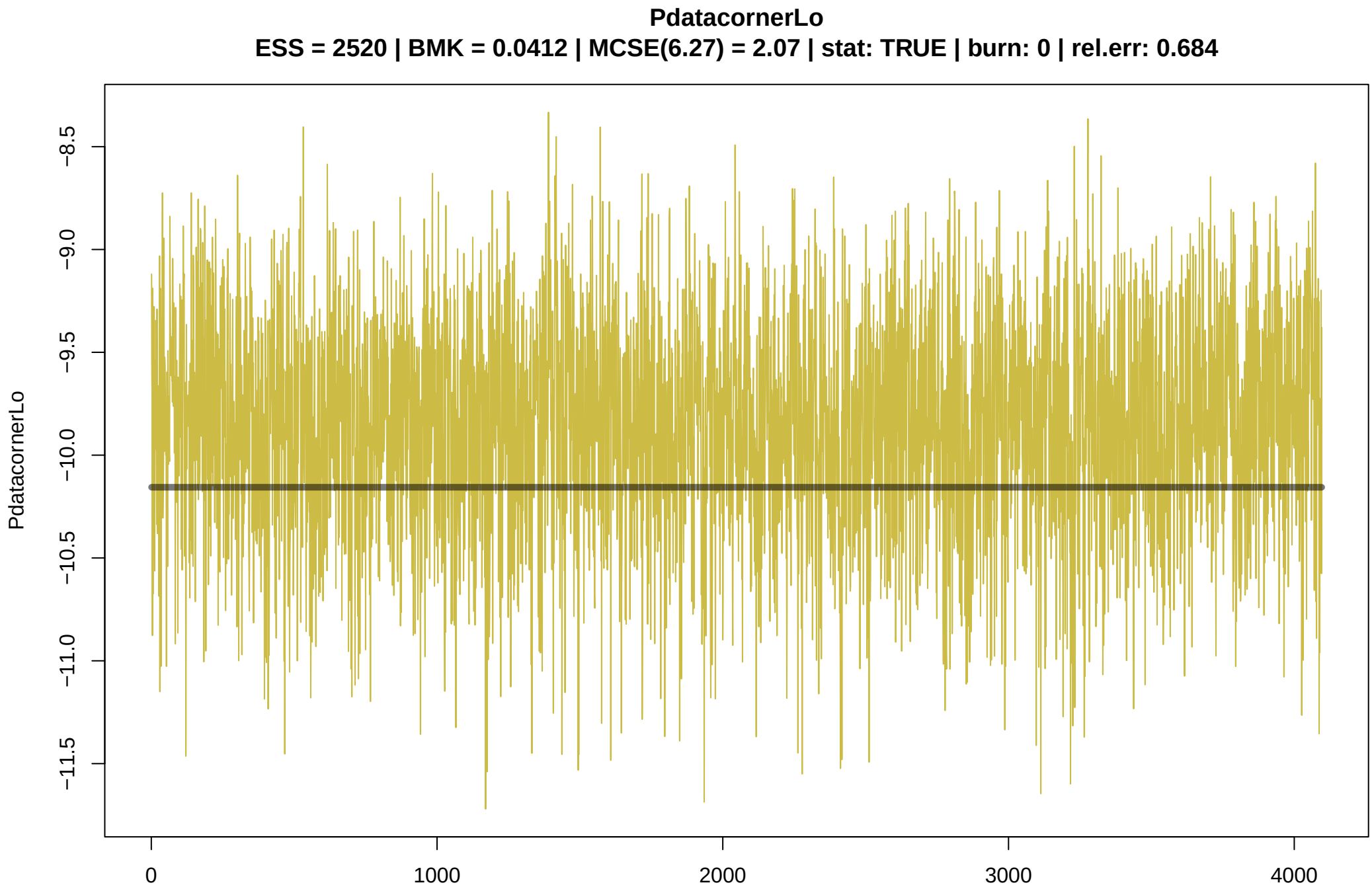

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

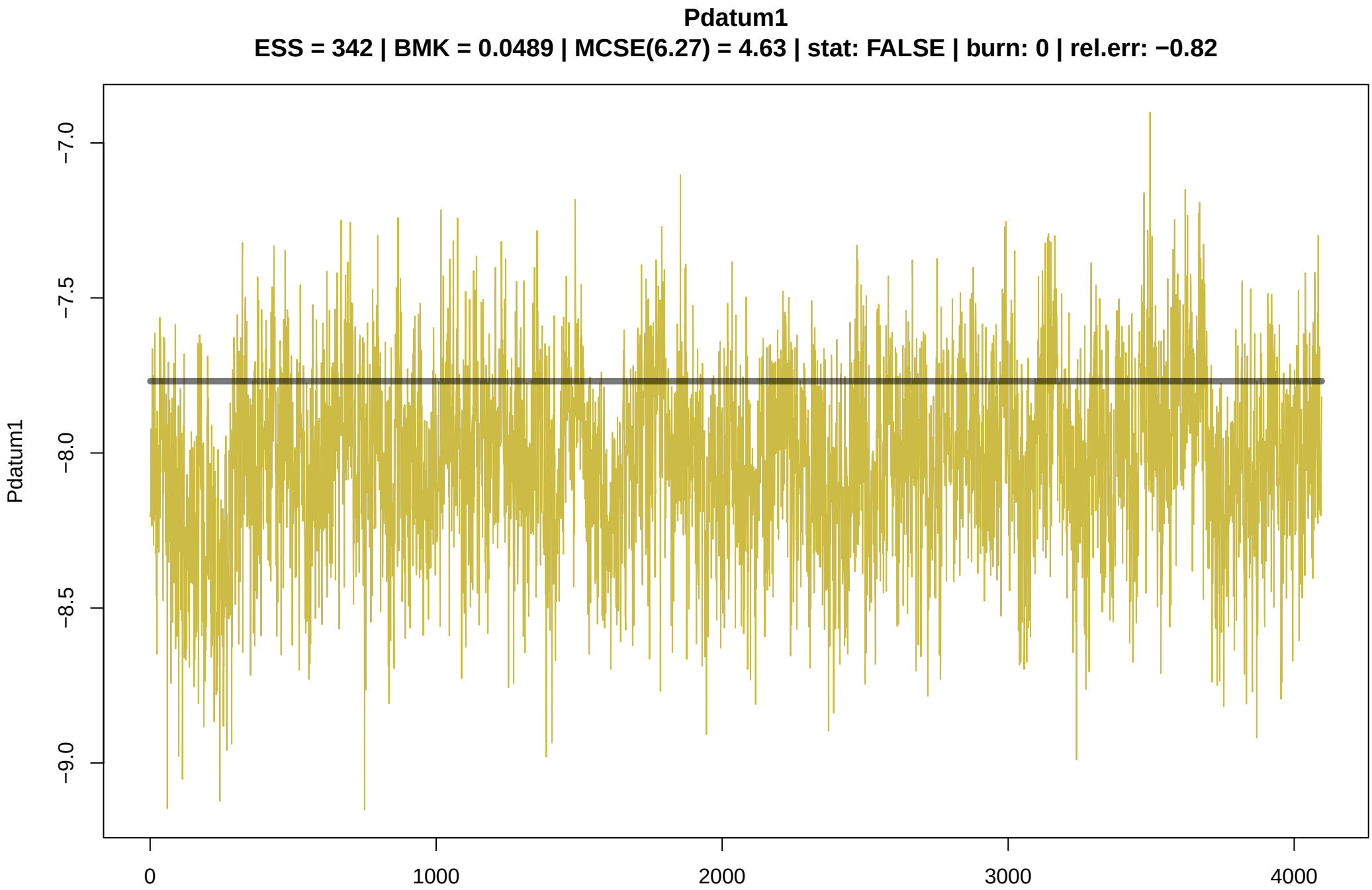

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

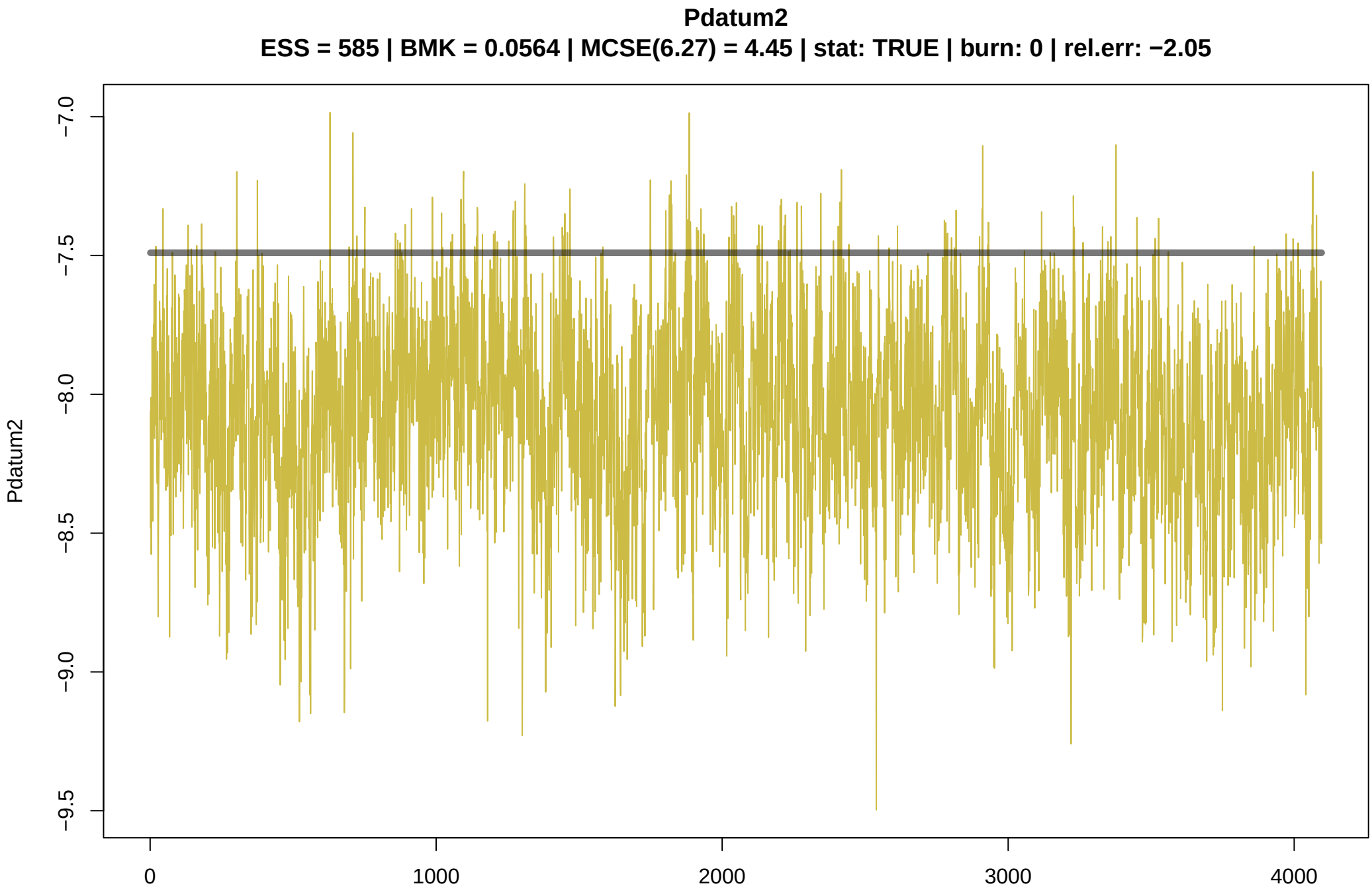

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

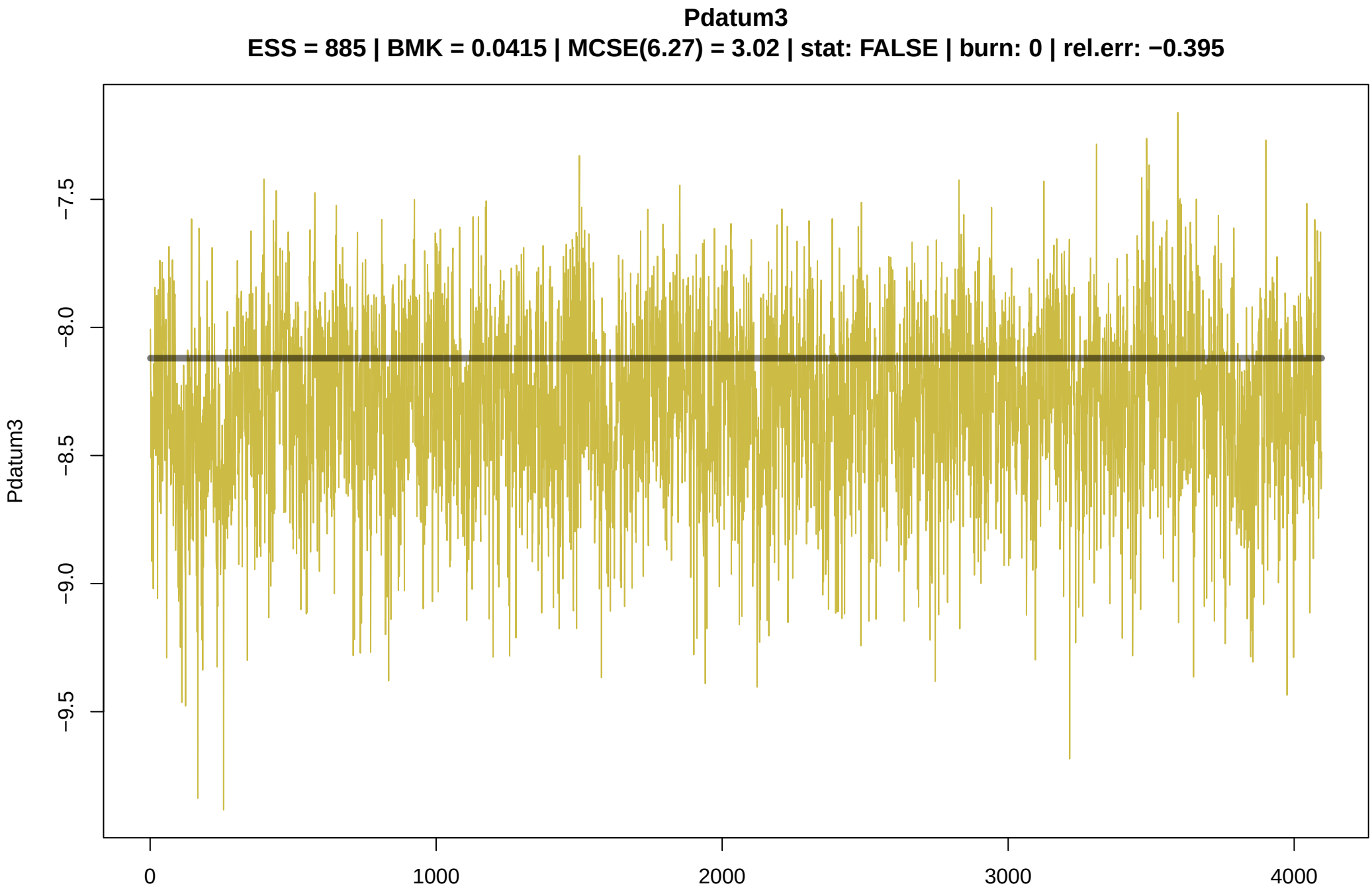

Pdatamean
ESS = 142 | BMK = 0.082 | MCSE(6.27) = 7.12 | stat: FALSE | burn: 0 | rel.err: 0.819
Pdatamean
−9
−10
−11
−12
0
1000
2000
3000
4000

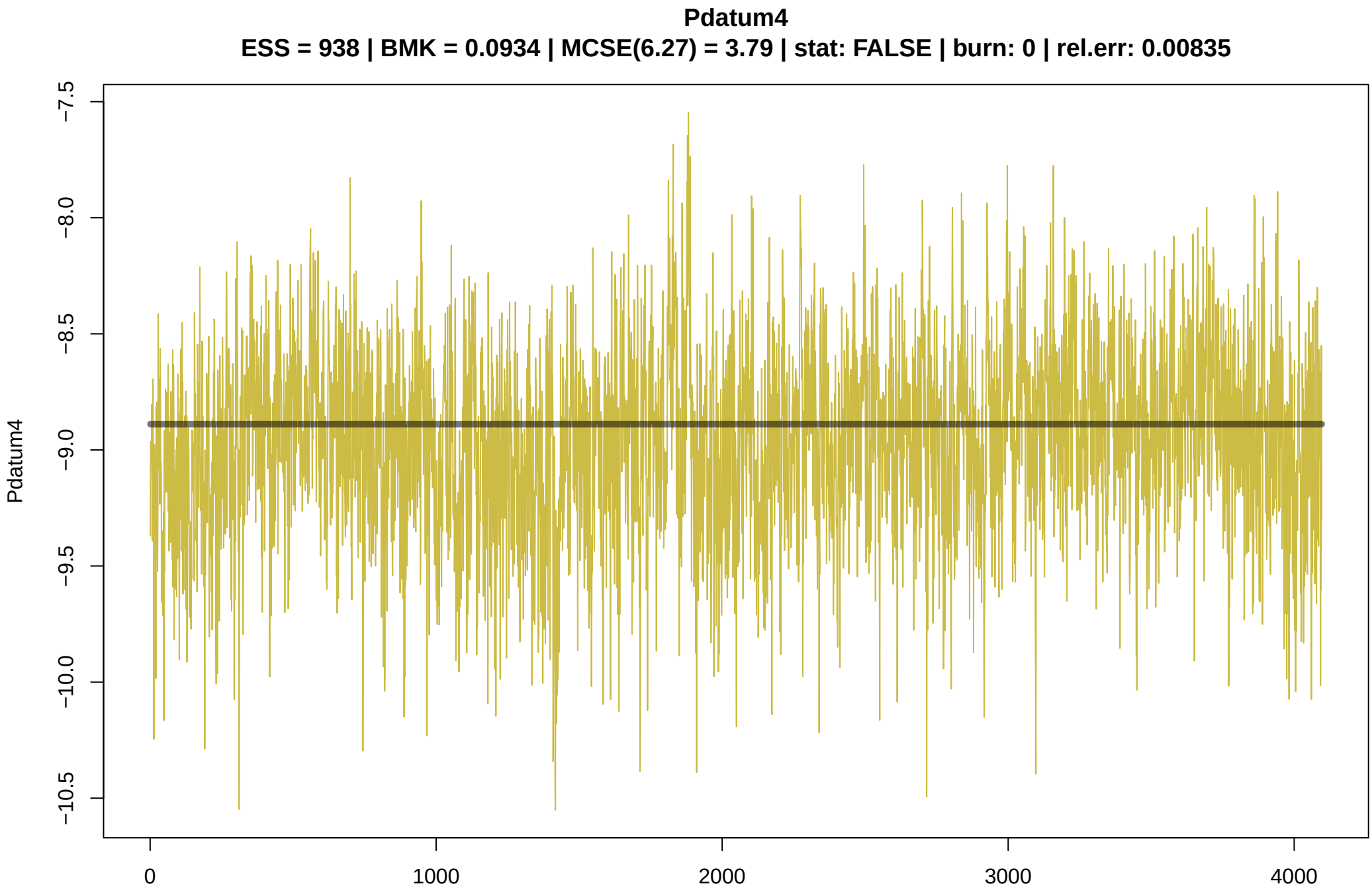

PdatacornerHi
ESS = 4100 | BMK = 0.125 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.278
PdatacornerHi
−15
−20
−25
0
1000
2000
3000
4000

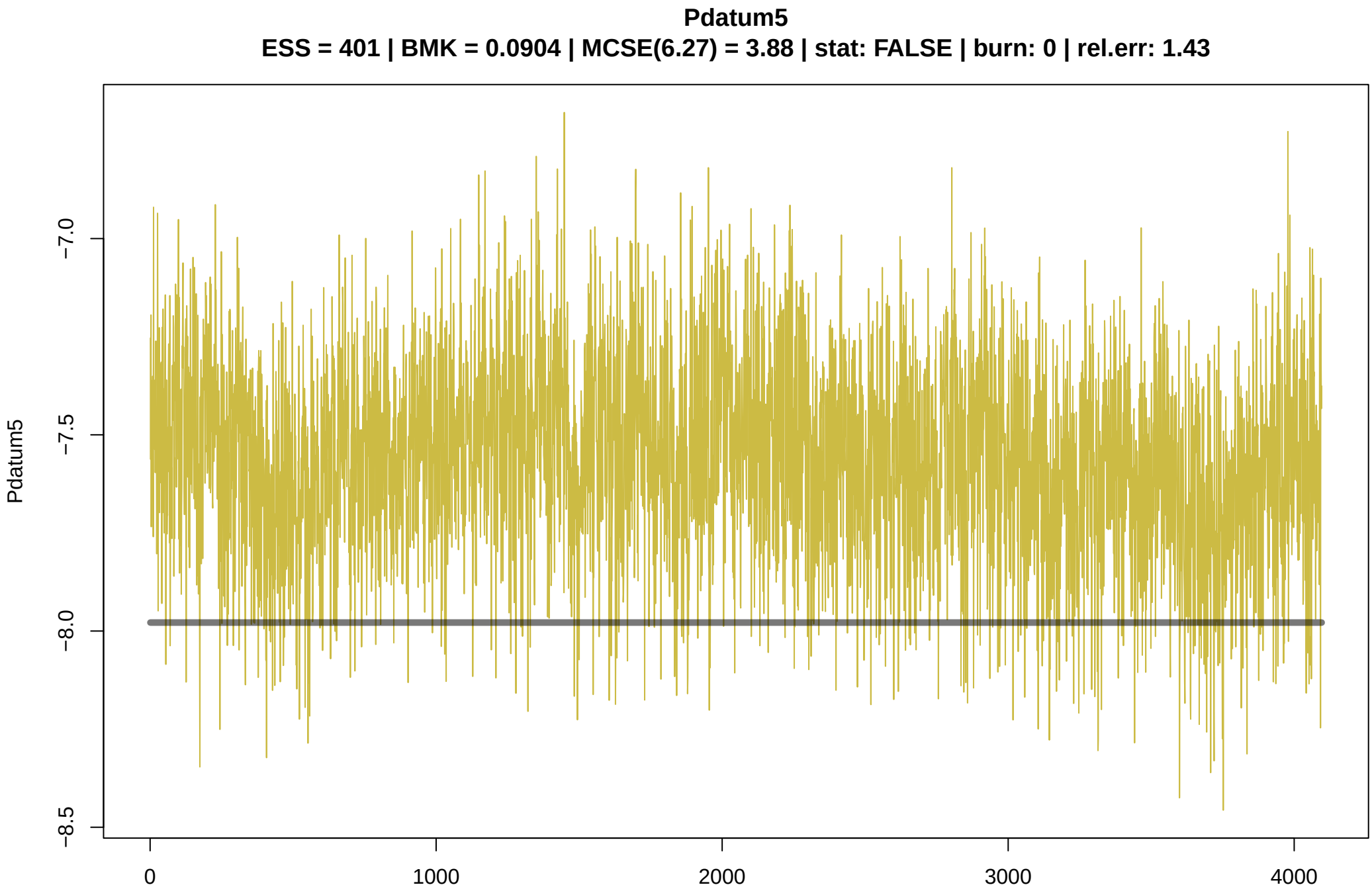

PdatacornerLo
ESS = 2520 | BMK = 0.0412 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: 0.684
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
0
1000
2000
3000
4000

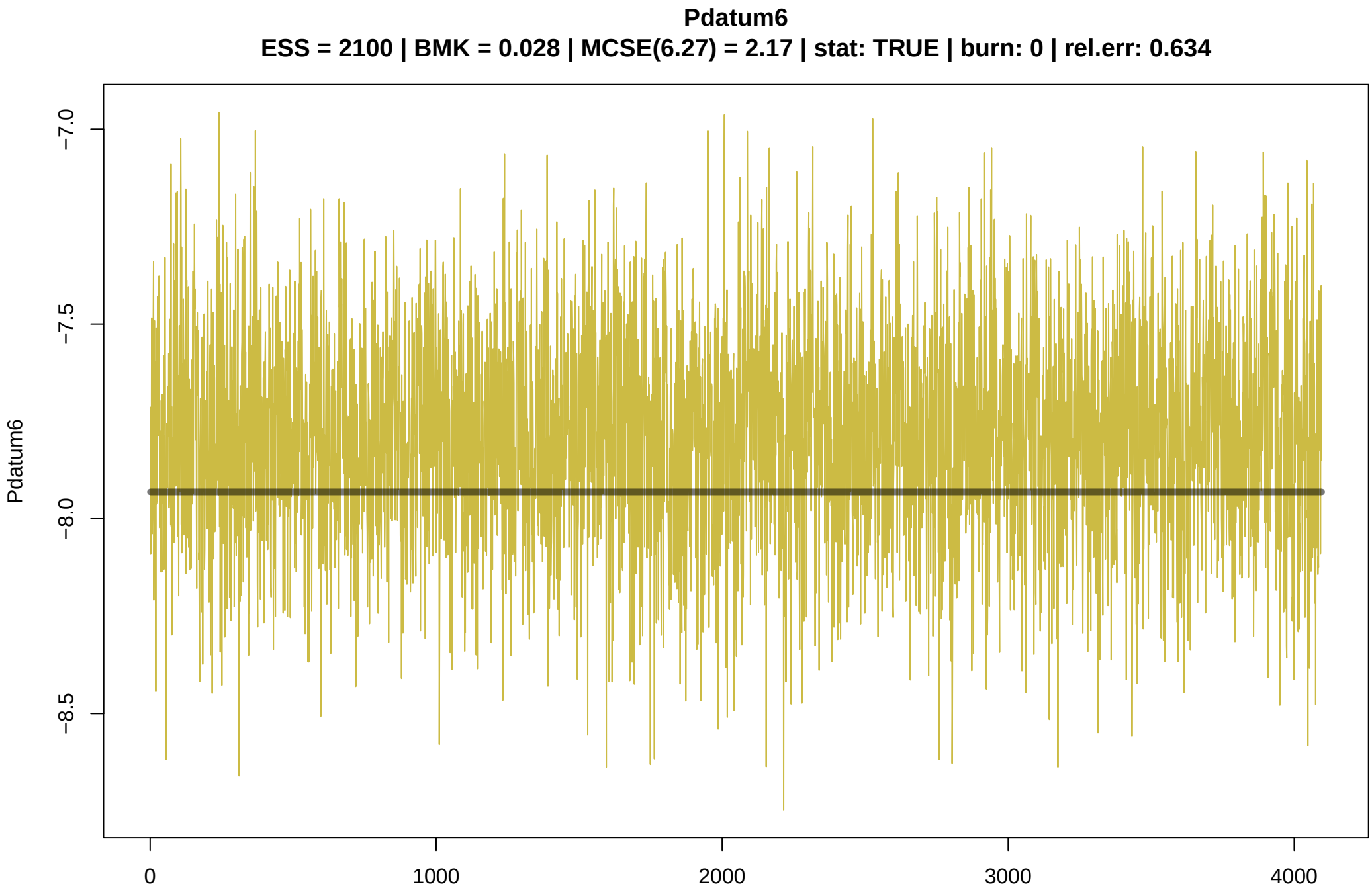

Pdatum1
ESS = 342 | BMK = 0.0489 | MCSE(6.27) = 4.63 | stat: FALSE | burn: 0 | rel.err: −0.82
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

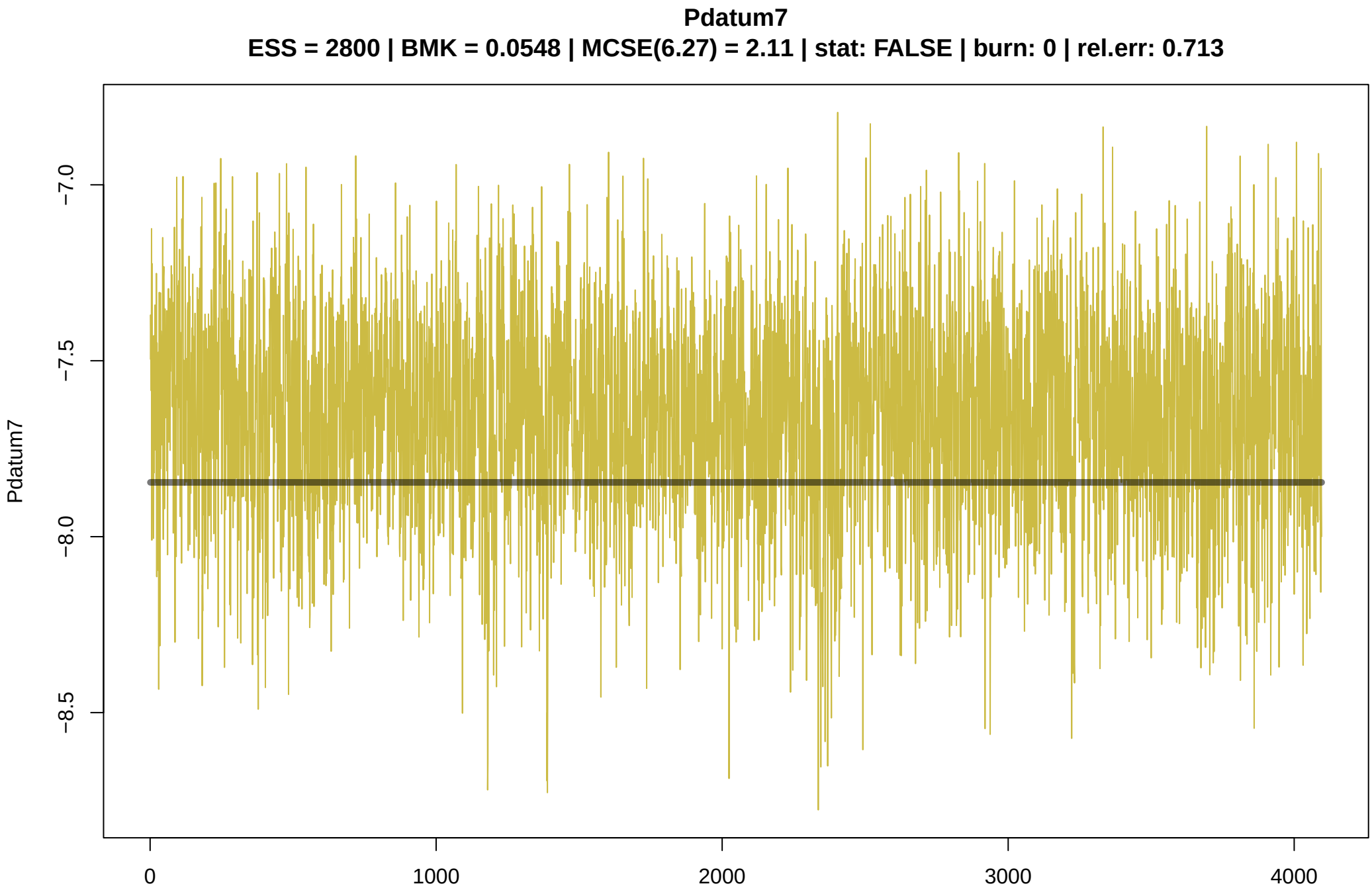

Pdatum2
ESS = 585 | BMK = 0.0564 | MCSE(6.27) = 4.45 | stat: TRUE | burn: 0 | rel.err: −2.05
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

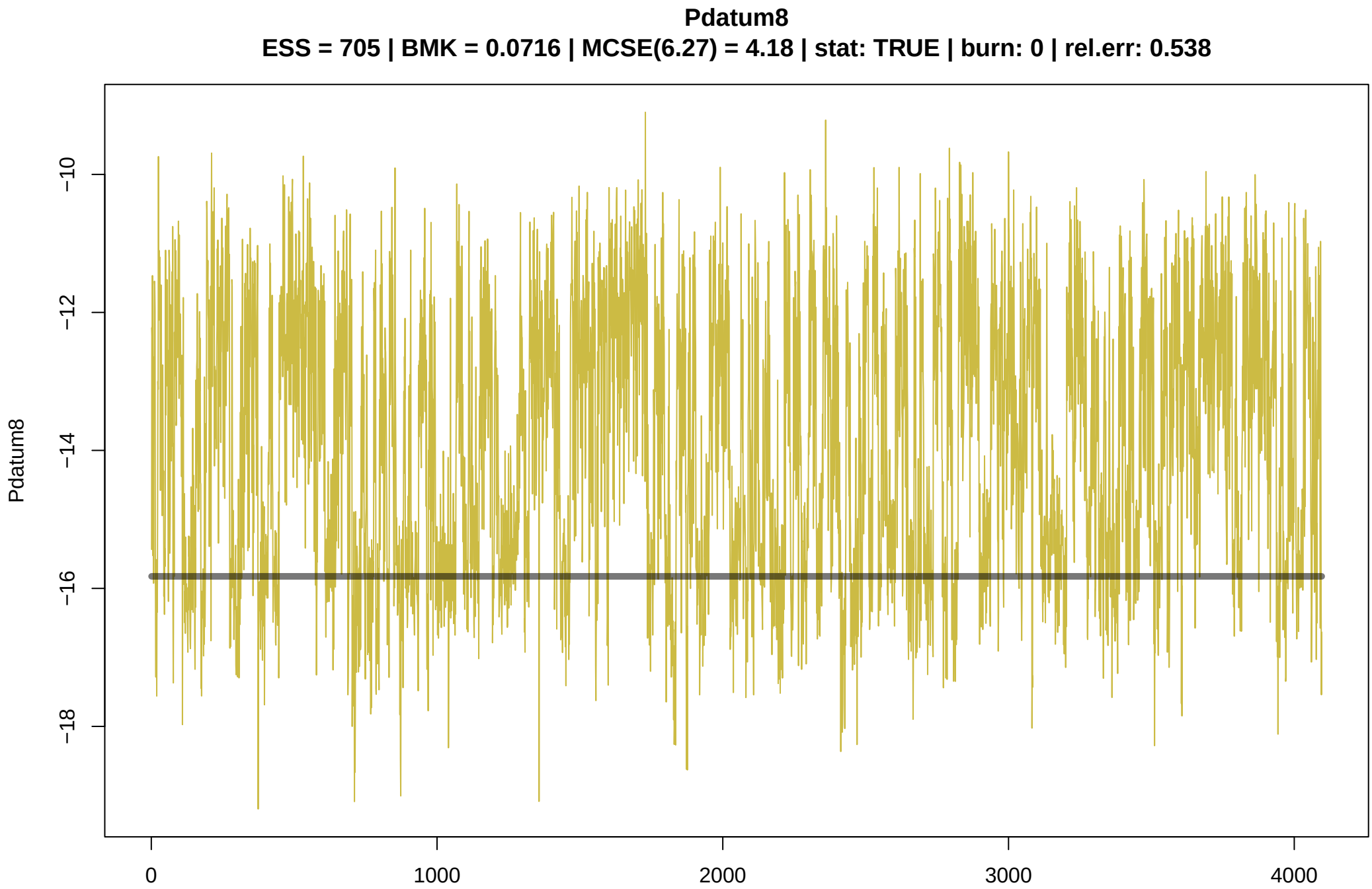

Pdatum3
ESS = 885 | BMK = 0.0415 | MCSE(6.27) = 3.02 | stat: FALSE | burn: 0 | rel.err: −0.395
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

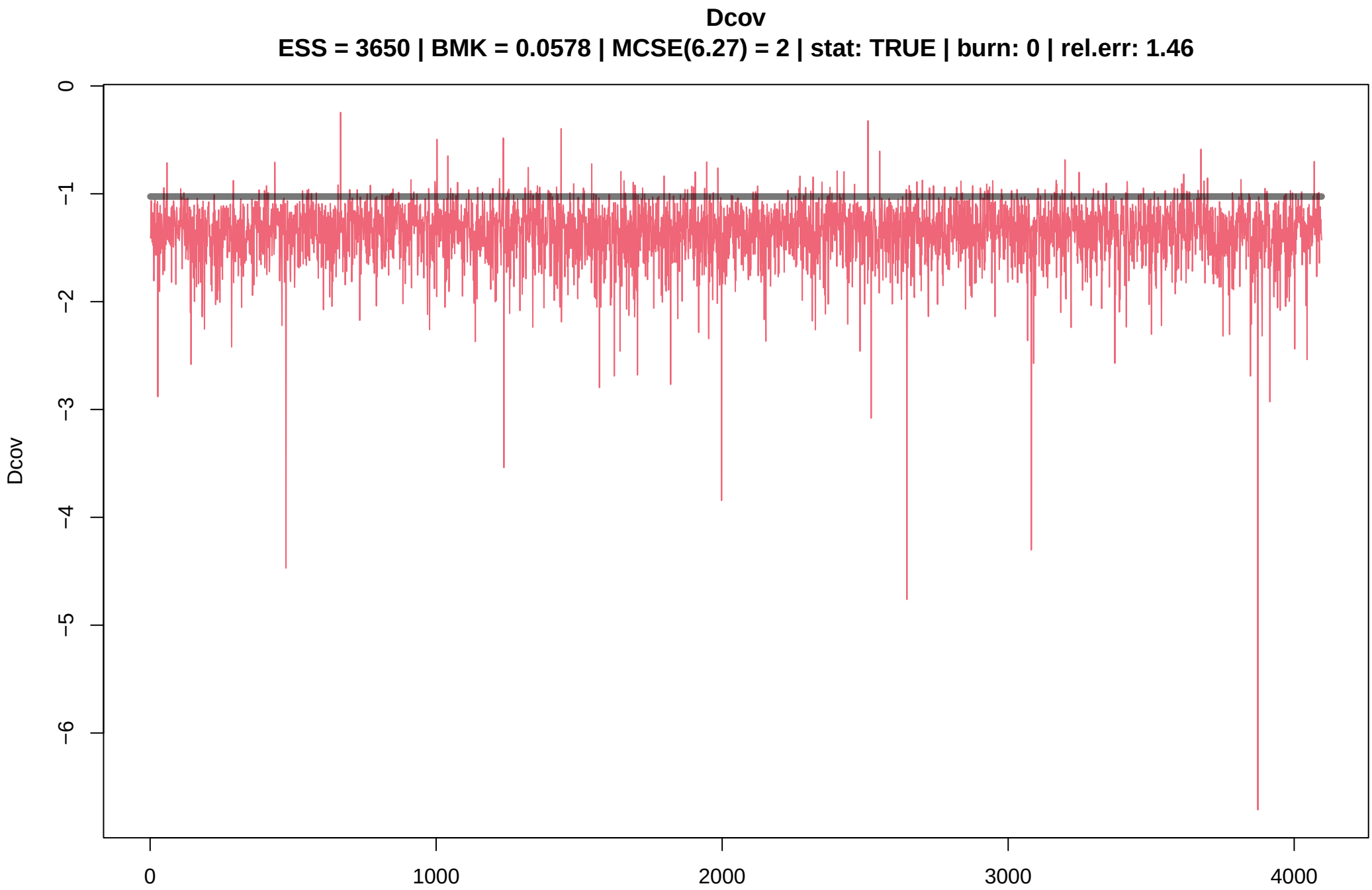

Pdatum4
ESS = 938 | BMK = 0.0934 | MCSE(6.27) = 3.79 | stat: FALSE | burn: 0 | rel.err: 0.00835
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

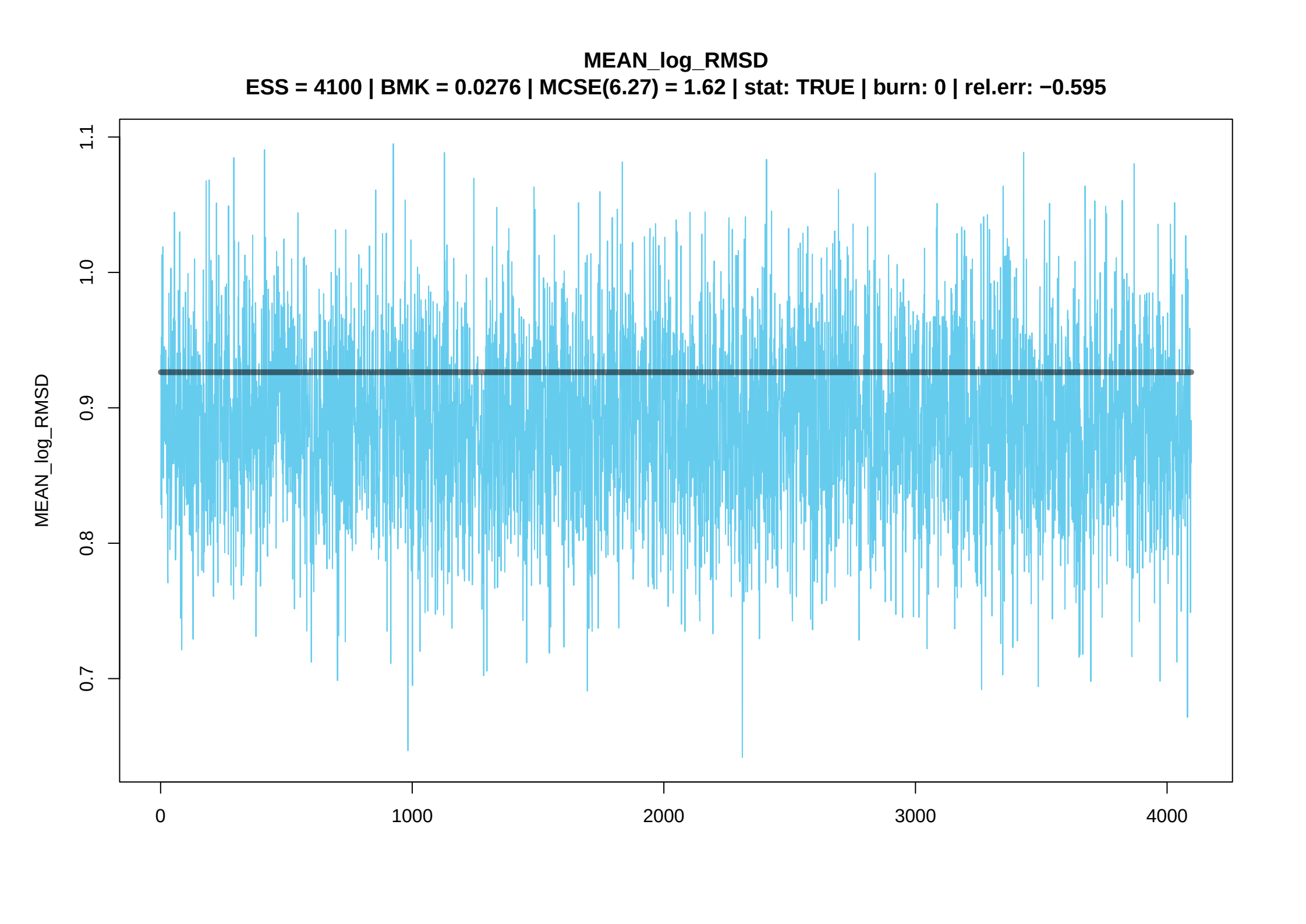

Pdatum5
ESS = 401 | BMK = 0.0904 | MCSE(6.27) = 3.88 | stat: FALSE | burn: 0 | rel.err: 1.43
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

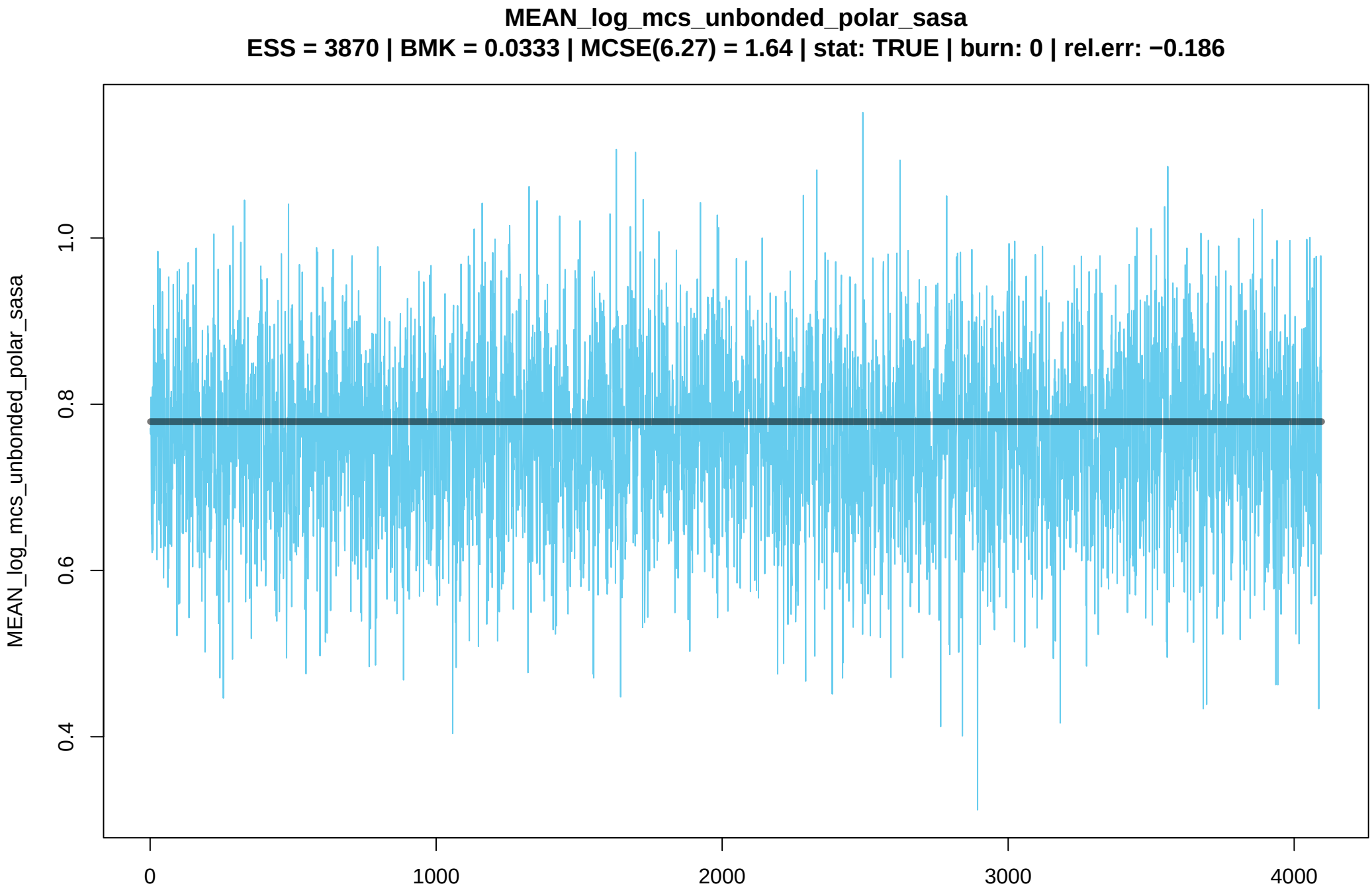

Pdatum6
ESS = 2100 | BMK = 0.028 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.634
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

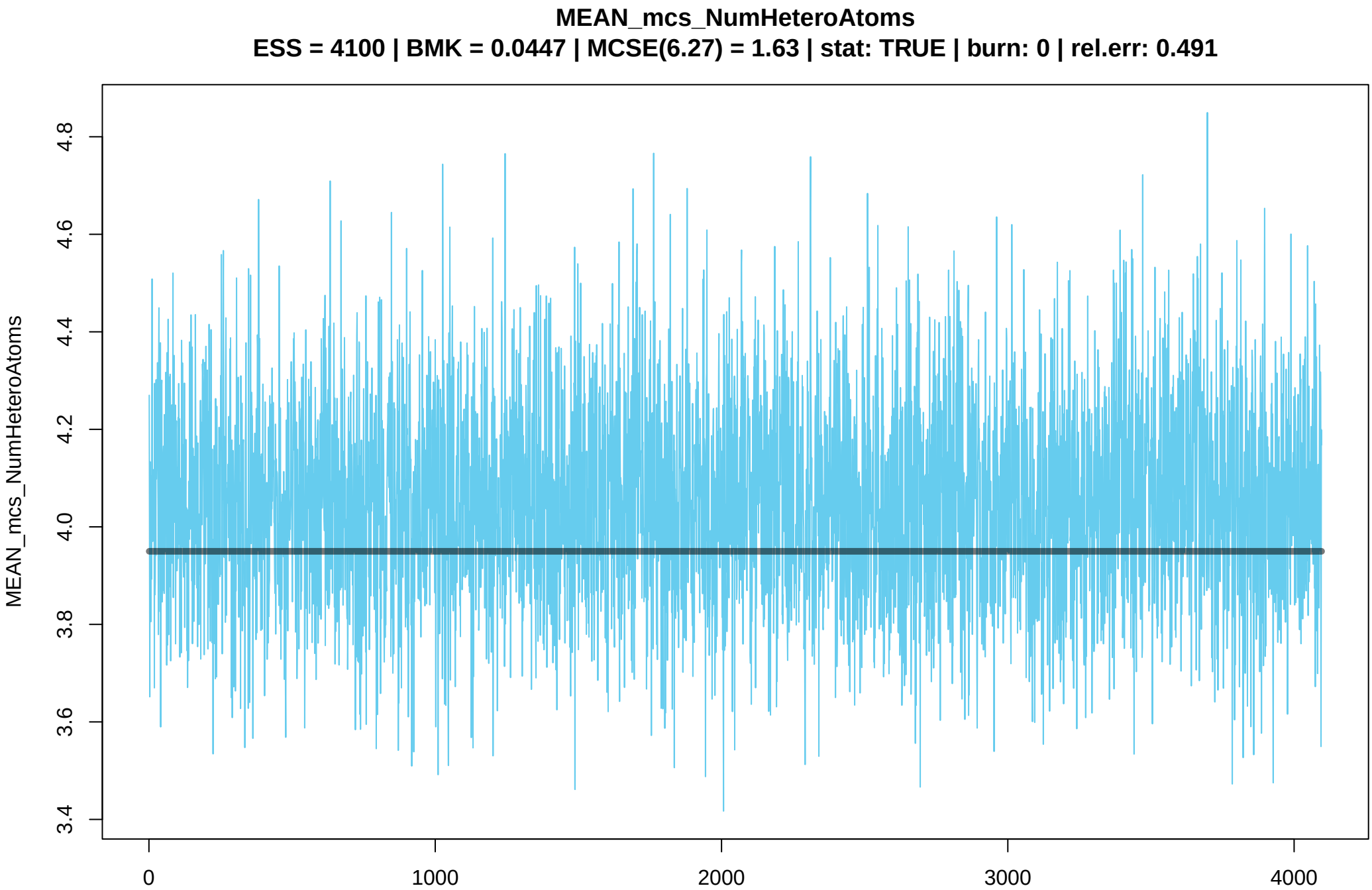

Pdatum7
ESS = 2800 | BMK = 0.0548 | MCSE(6.27) = 2.11 | stat: FALSE | burn: 0 | rel.err: 0.713
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

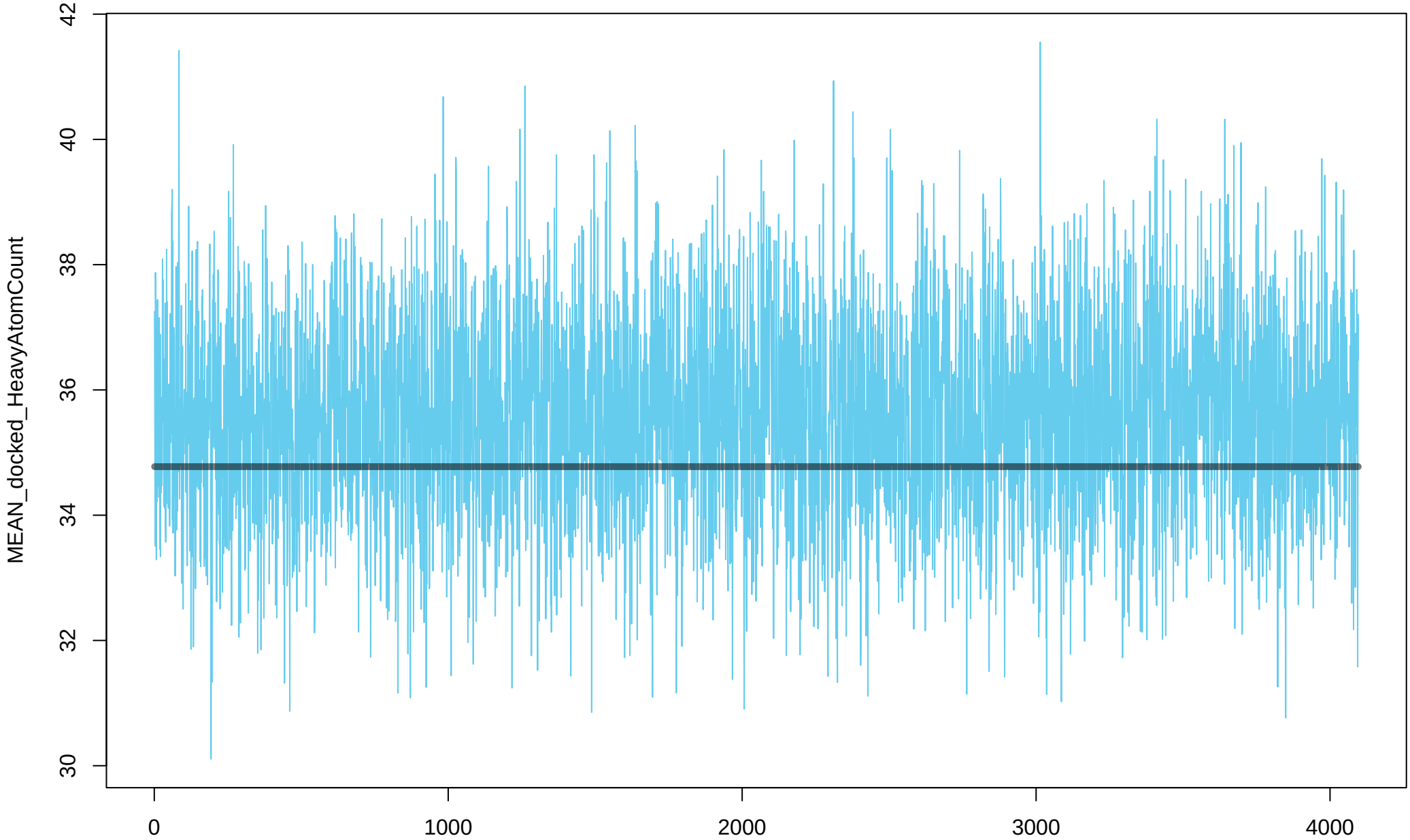

Pdatum8
ESS = 705 | BMK = 0.0716 | MCSE(6.27) = 4.18 | stat: TRUE | burn: 0 | rel.err: 0.538
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

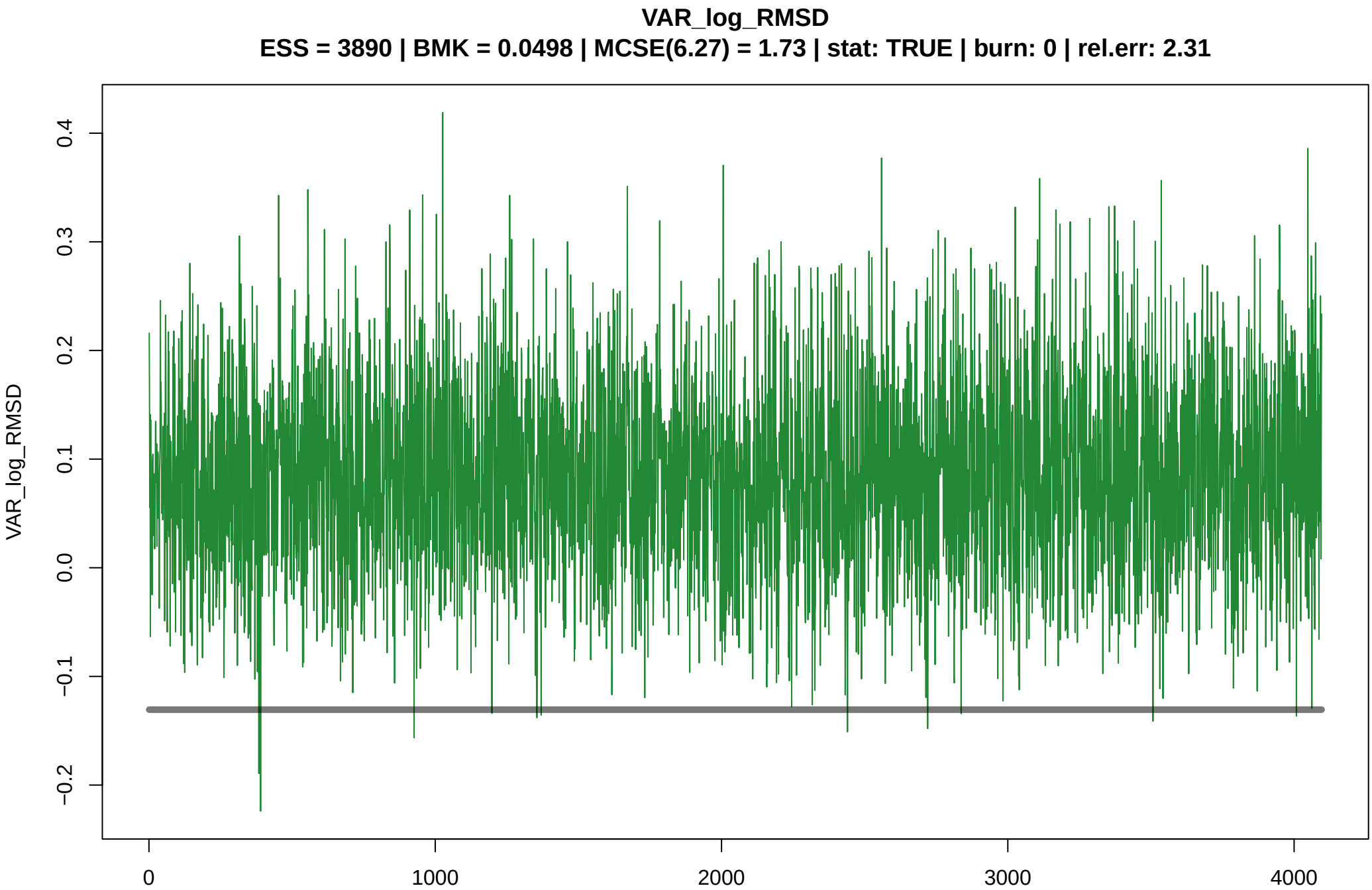

Dcov
ESS = 3650 | BMK = 0.0578 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: 1.46
Dcov
0
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

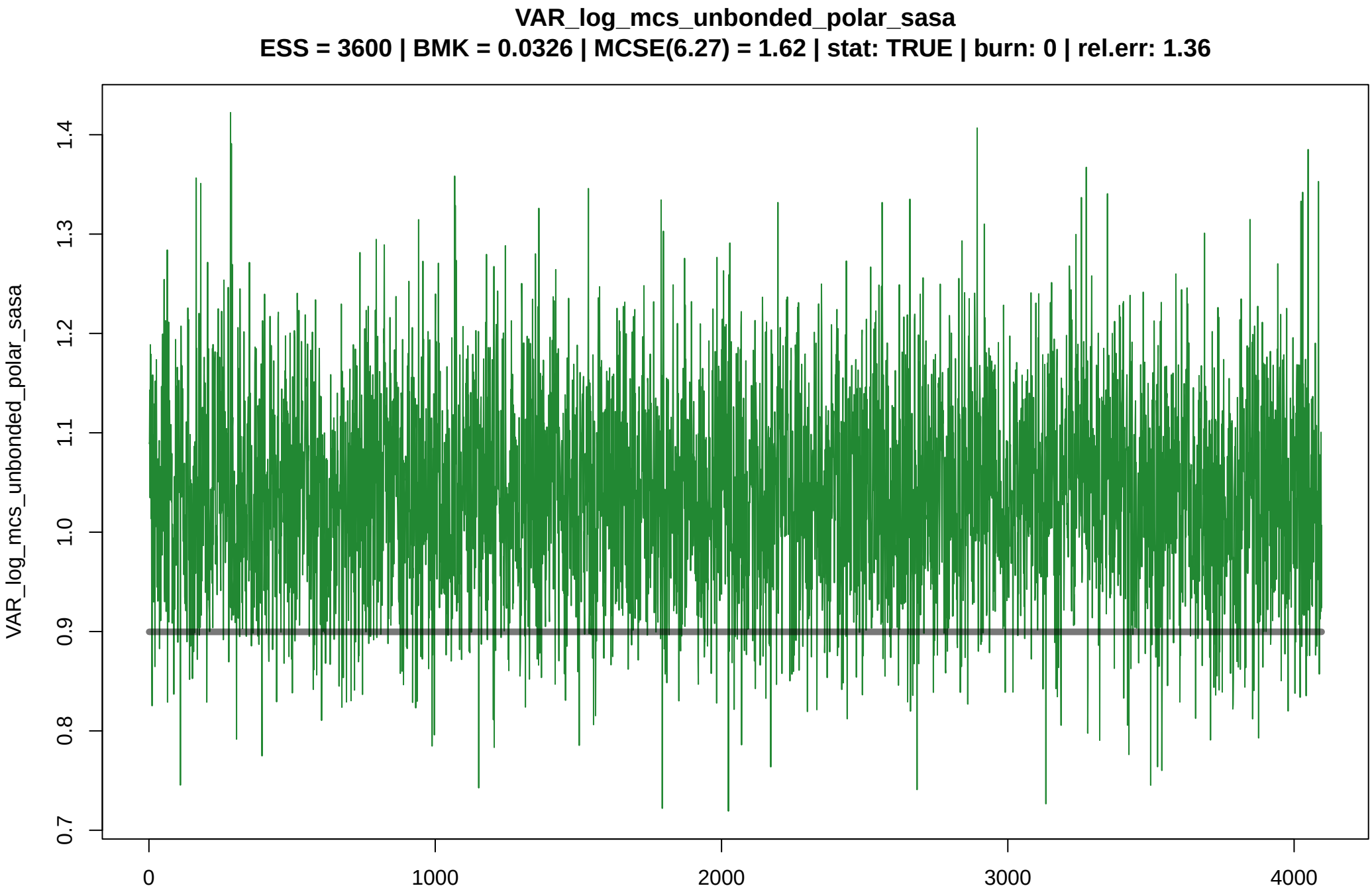

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0276 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: −0.595
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
1000
2000
3000
4000

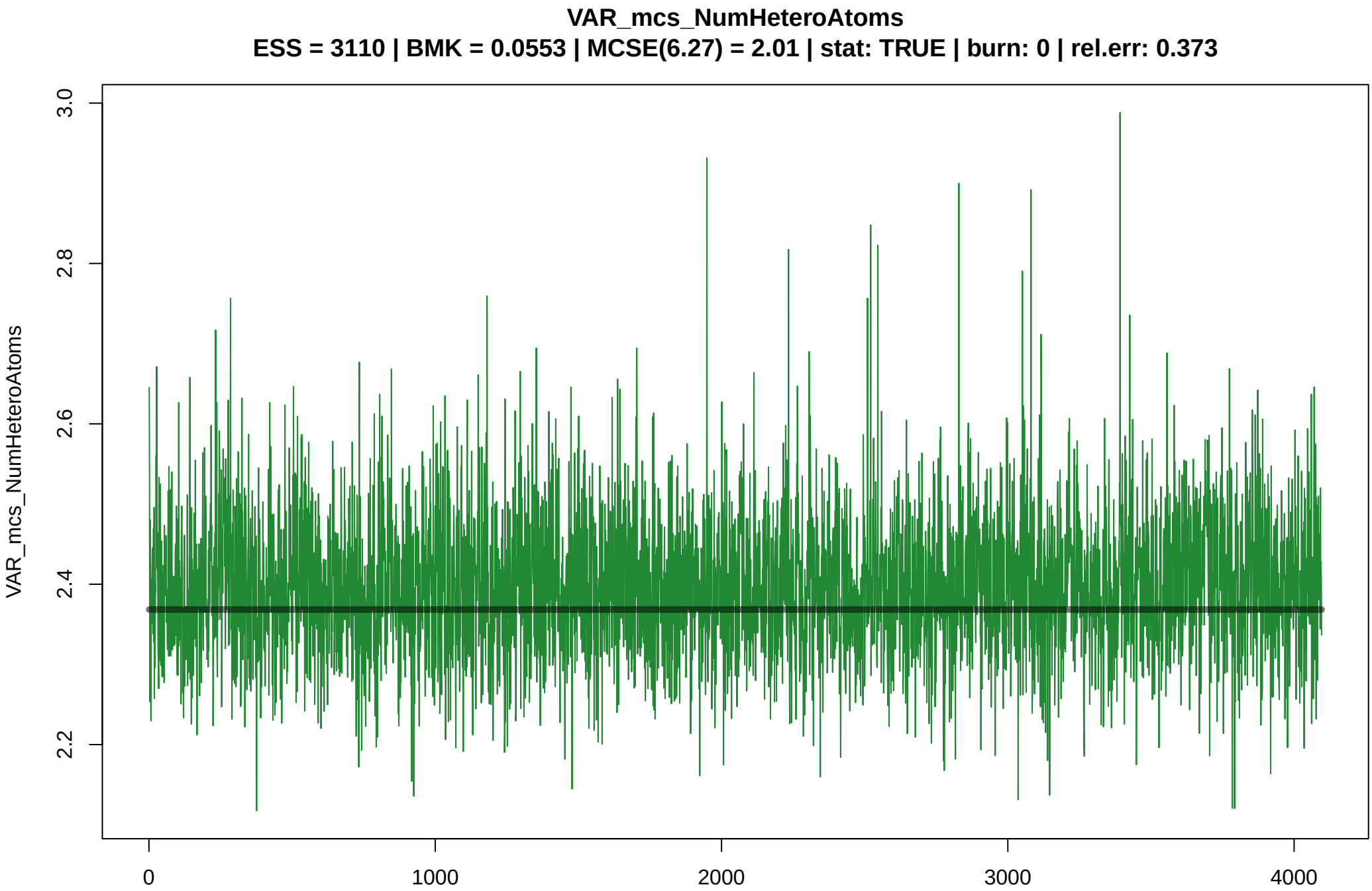

MEAN_log_mcs_unbonded_polar_sasa
ESS = 3870 | BMK = 0.0333 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: −0.186
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

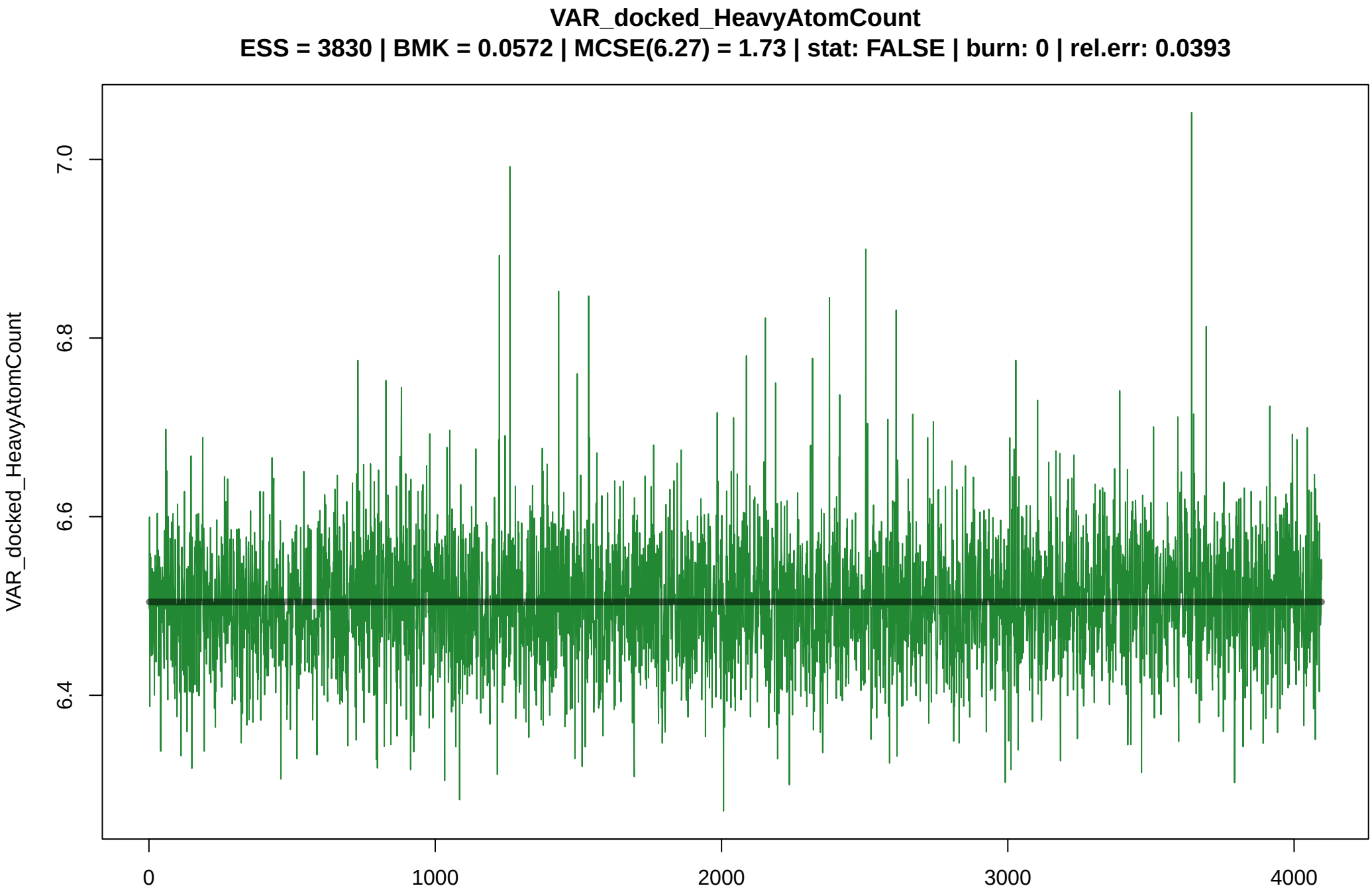

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0447 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.491
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
1000
2000
3000
4000

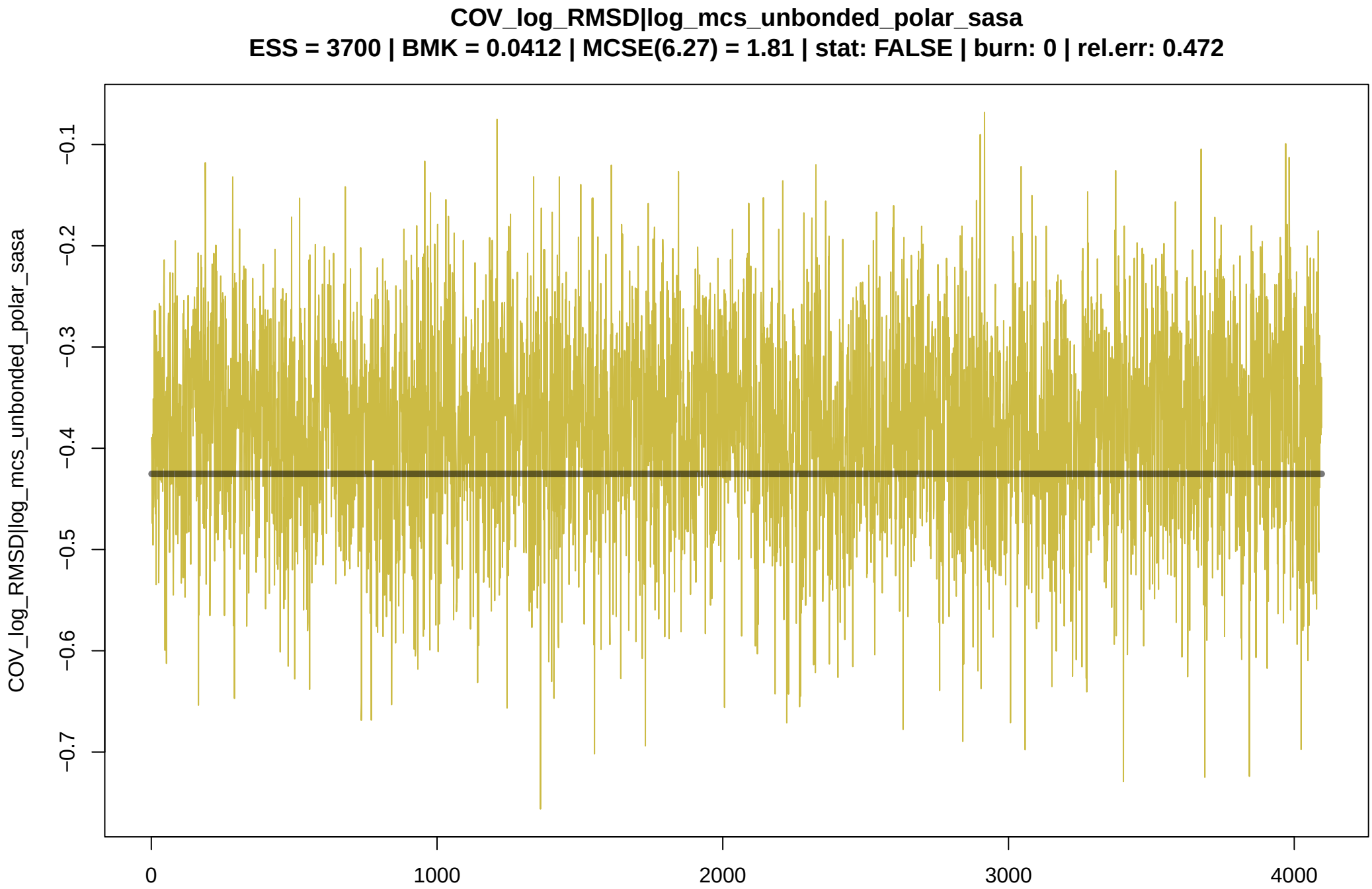

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0281 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 0.507
MEAN_docked_HeavyAtomCount
42
40
38
36
34
32
30
0
1000
2000
3000
4000

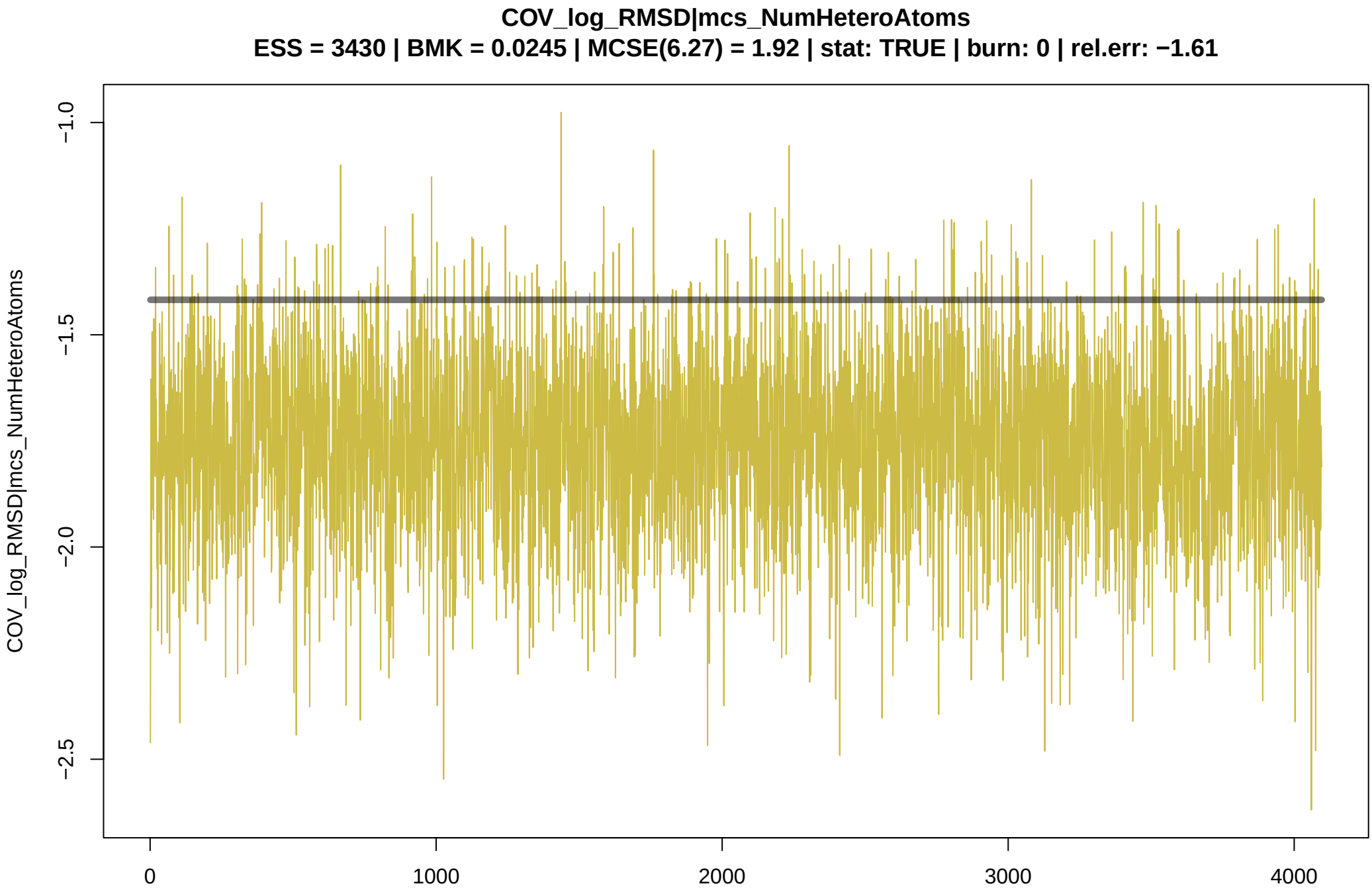

VAR_log_RMSD
ESS = 3890 | BMK = 0.0498 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: 2.31
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

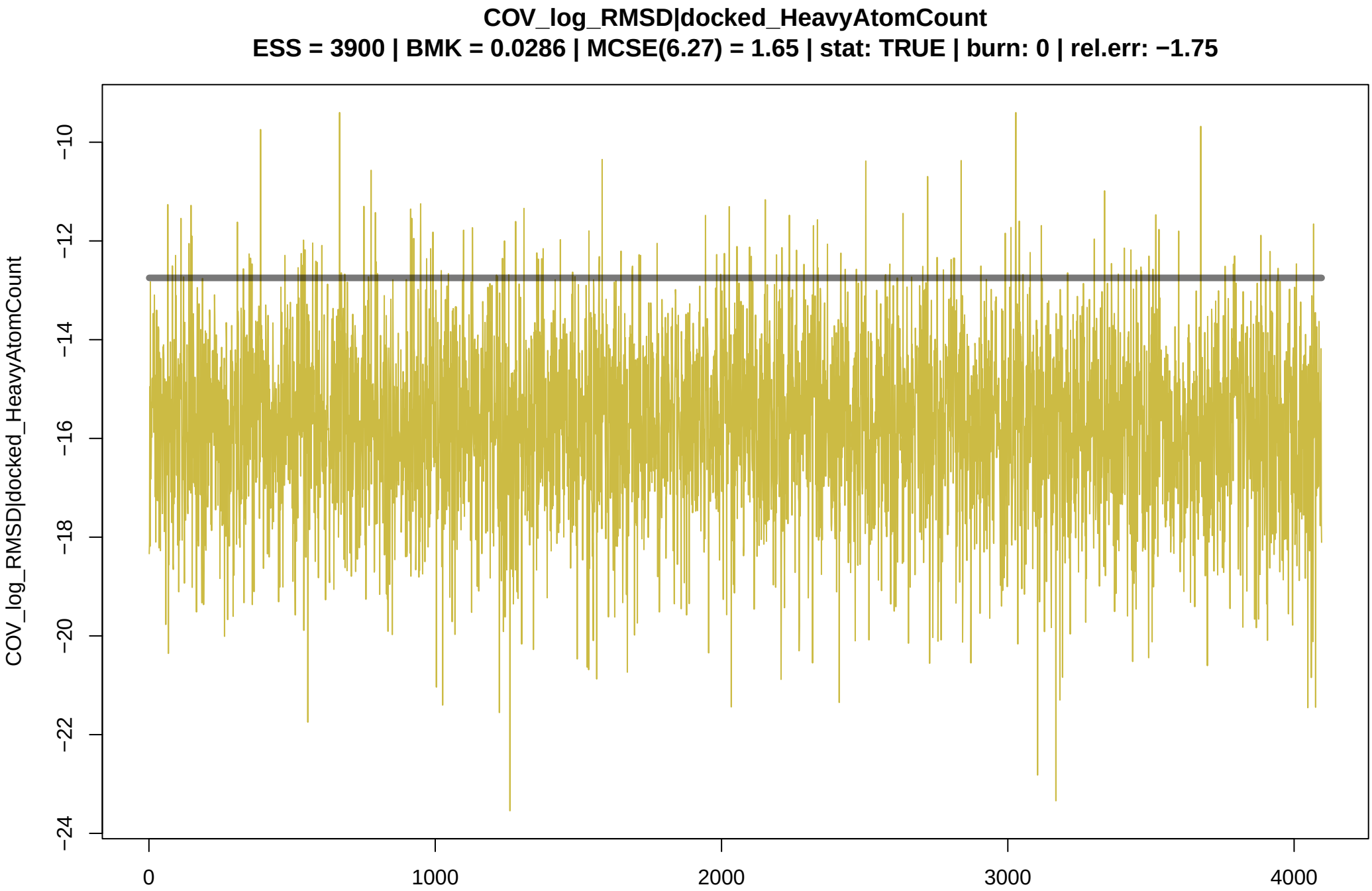

VAR_log_mcs_unbonded_polar_sasa
ESS = 3600 | BMK = 0.0326 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: 1.36
VAR_log_mcs_unbonded_polar_sasa
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
1000
2000
3000
4000

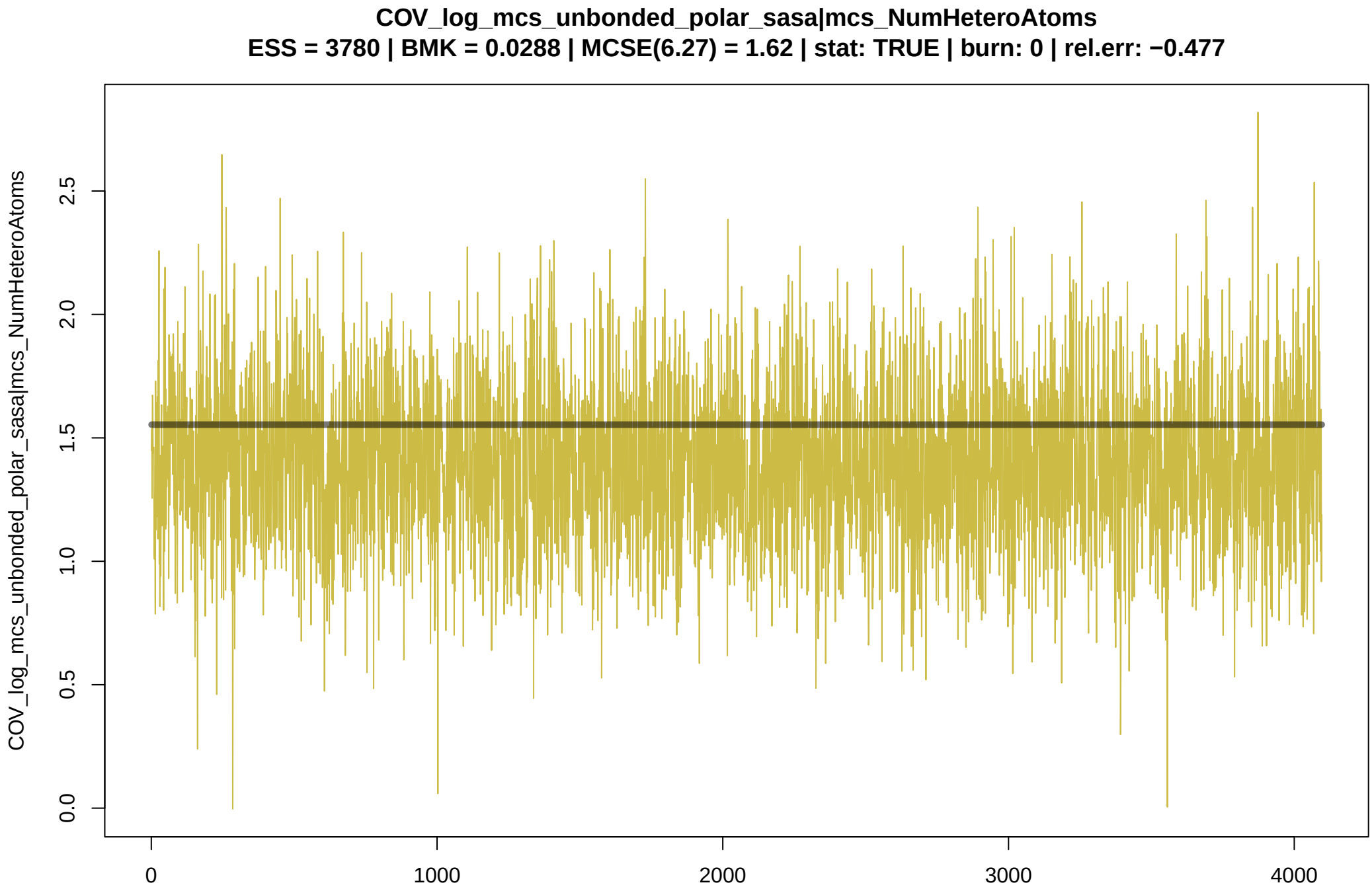

VAR_mcs_NumHeteroAtoms
ESS = 3110 | BMK = 0.0553 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: 0.373
VAR_mcs_NumHeteroAtoms
3.0
2.8
2.6
2.4
2.2
0
1000
2000
3000
4000

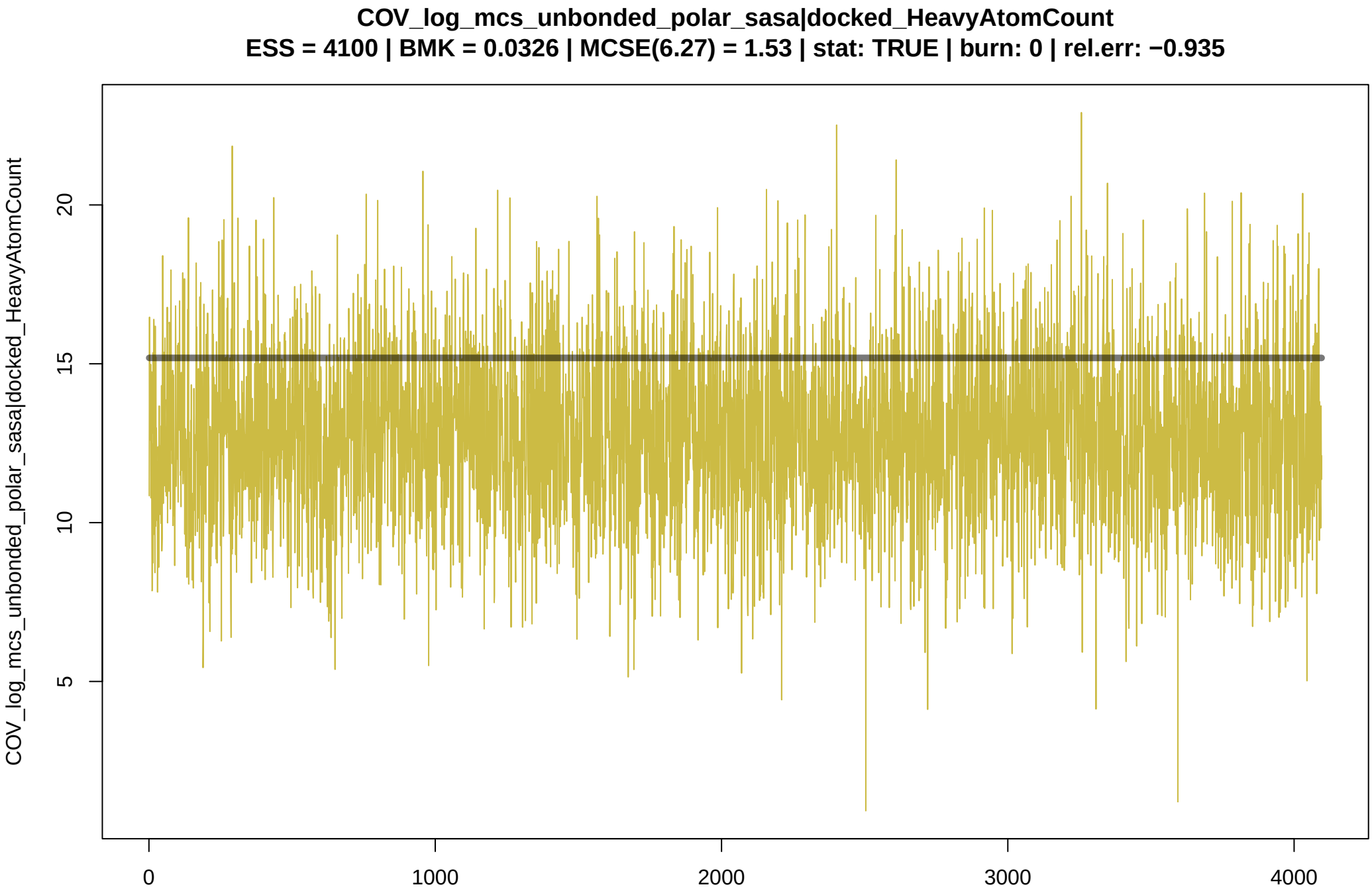

VAR_docked_HeavyAtomCount
ESS = 3830 | BMK = 0.0572 | MCSE(6.27) = 1.73 | stat: FALSE | burn: 0 | rel.err: 0.0393
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
1000
2000
3000
4000

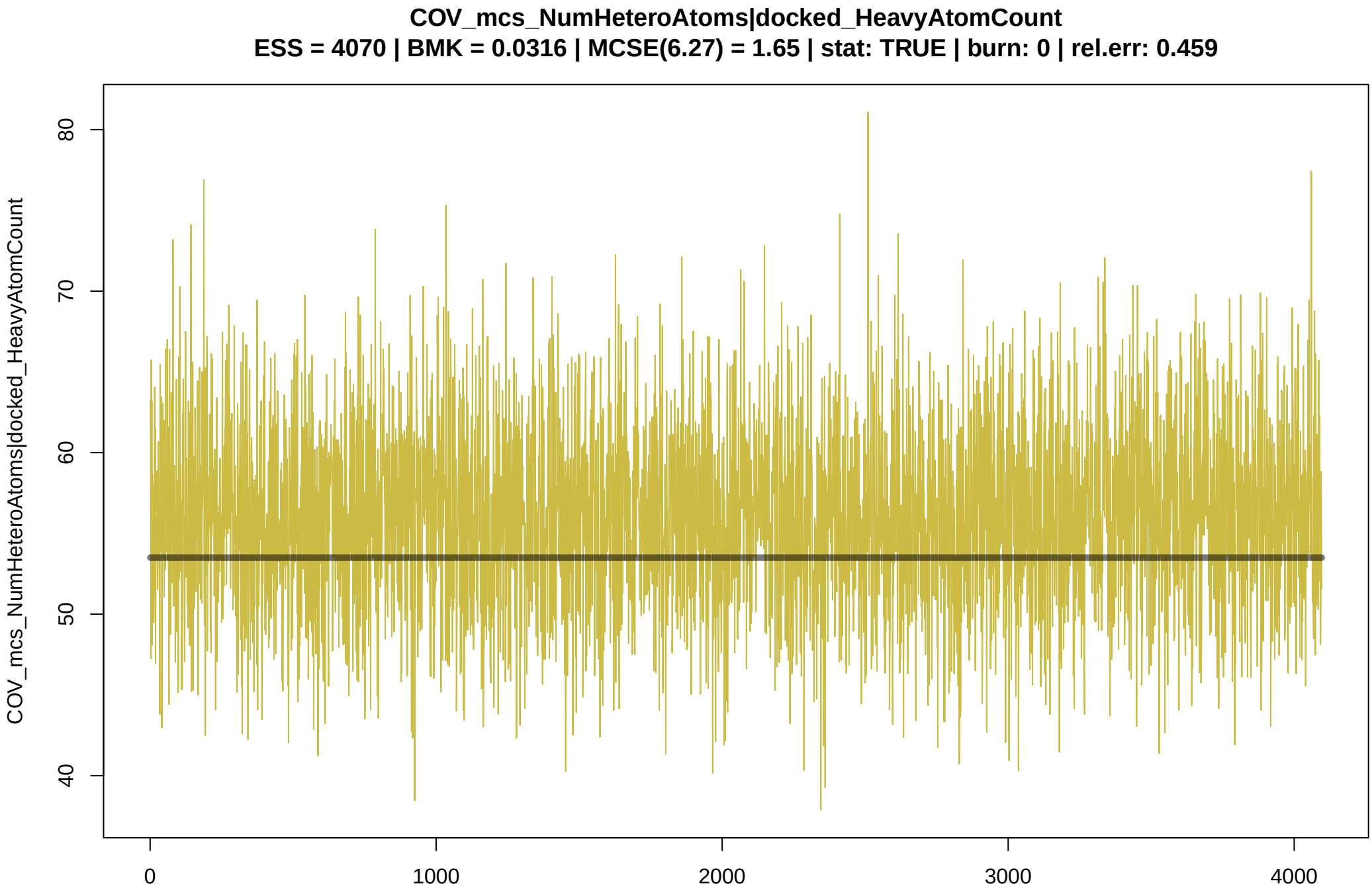

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3700 | BMK = 0.0412 | MCSE(6.27) = 1.81 | stat: FALSE | burn: 0 | rel.err: 0.472
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3430 | BMK = 0.0245 | MCSE(6.27) = 1.92 | 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 = 3900 | BMK = 0.0286 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: −1.75
COV_log_RMSD|docked_HeavyAtomCount
−10
−12
−14
−16
−18
−20
−22
−24
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3780 | BMK = 0.0288 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: −0.477
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 = 0.0326 | MCSE(6.27) = 1.53 | stat: TRUE | burn: 0 | rel.err: −0.935
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
0
1000
2000
3000
4000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4070 | BMK = 0.0316 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: 0.459
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
80
70
60
50
40
0
1000
2000
3000
4000