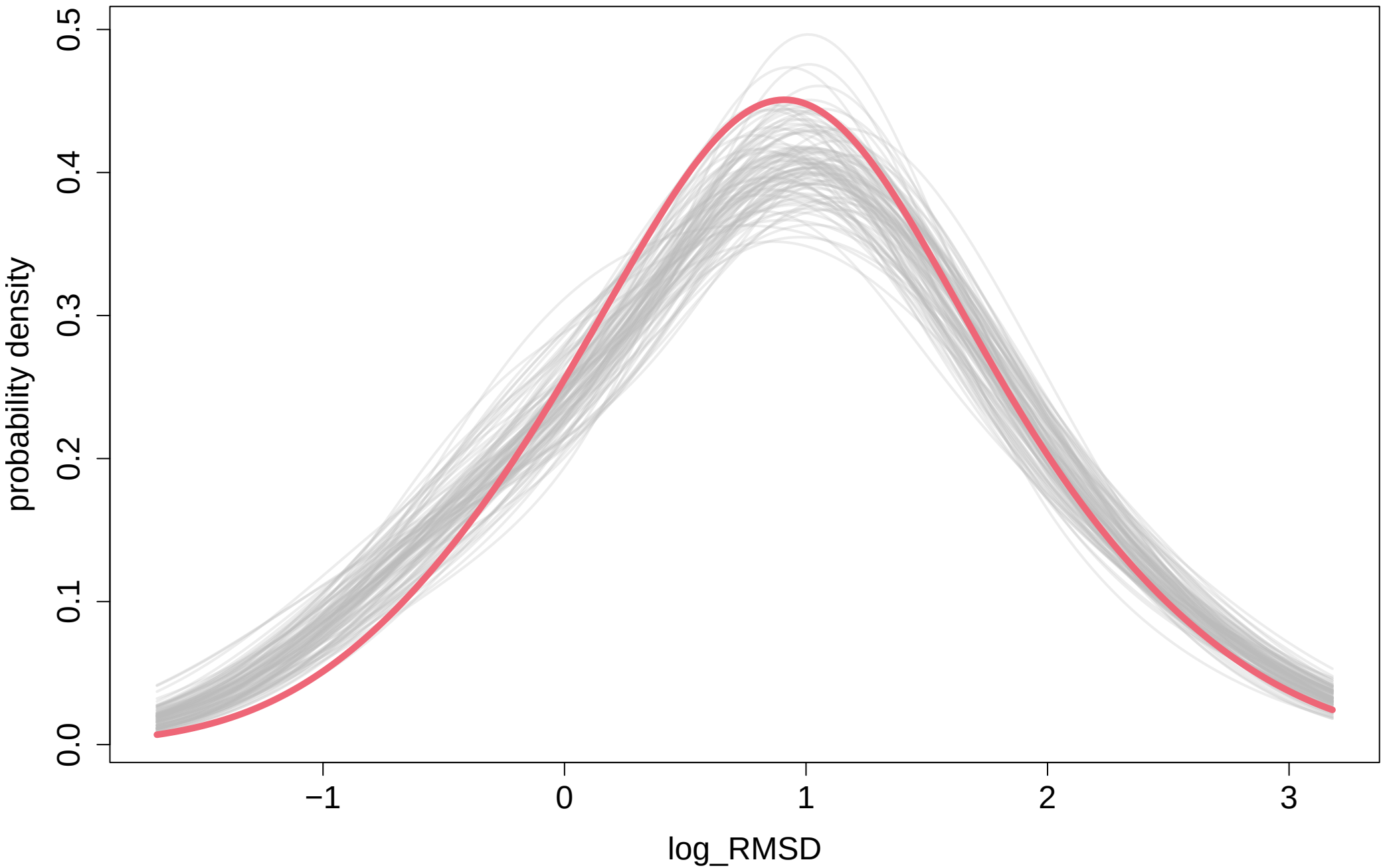
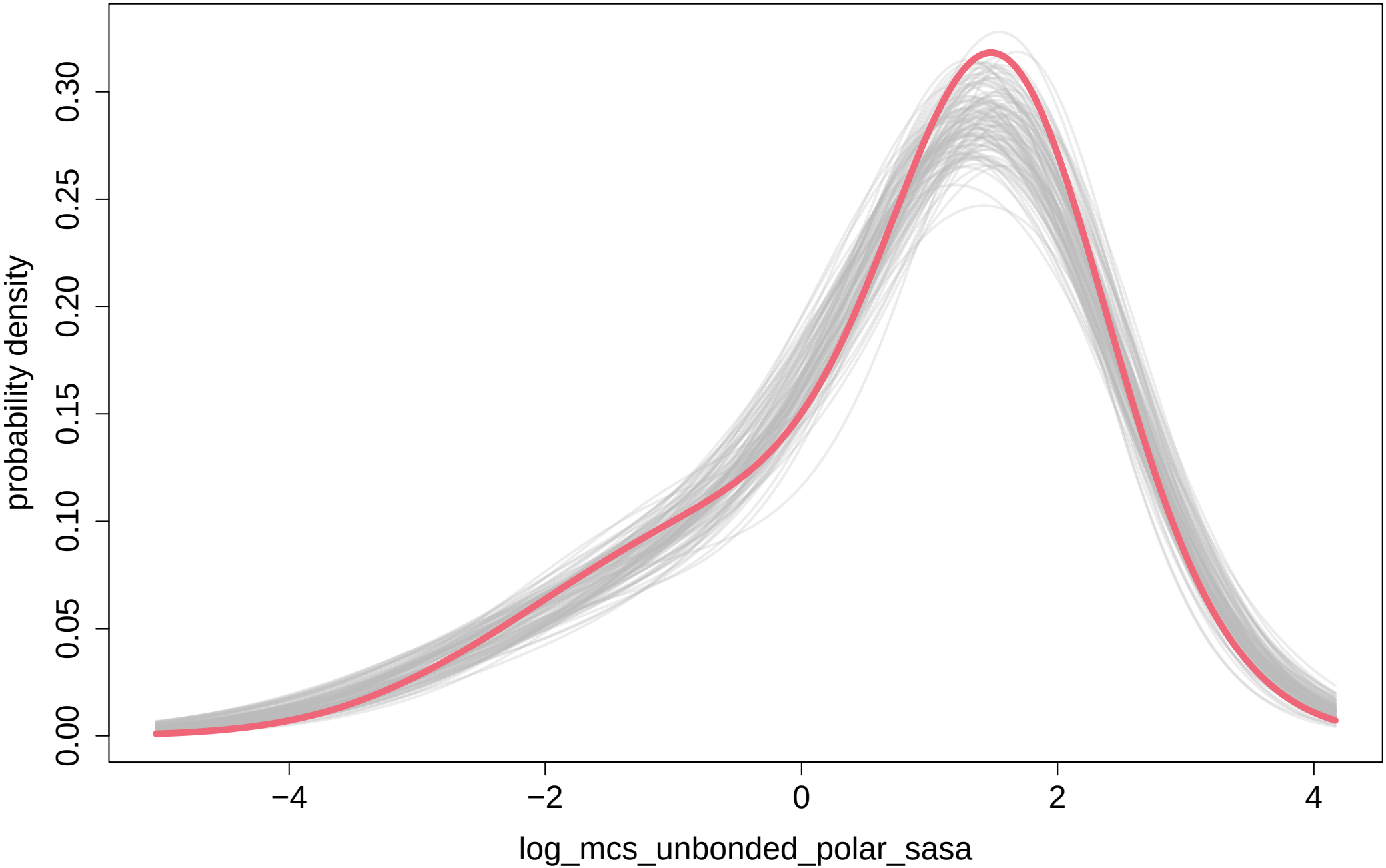
−− STATS maxD −−
min ESS = 183.211793275341
max BMK = 0.109666662837587
max MCSE = 6.10383258246047
all stationary: FALSE
burn: 4090
max rel.err.: 2.04854378543189

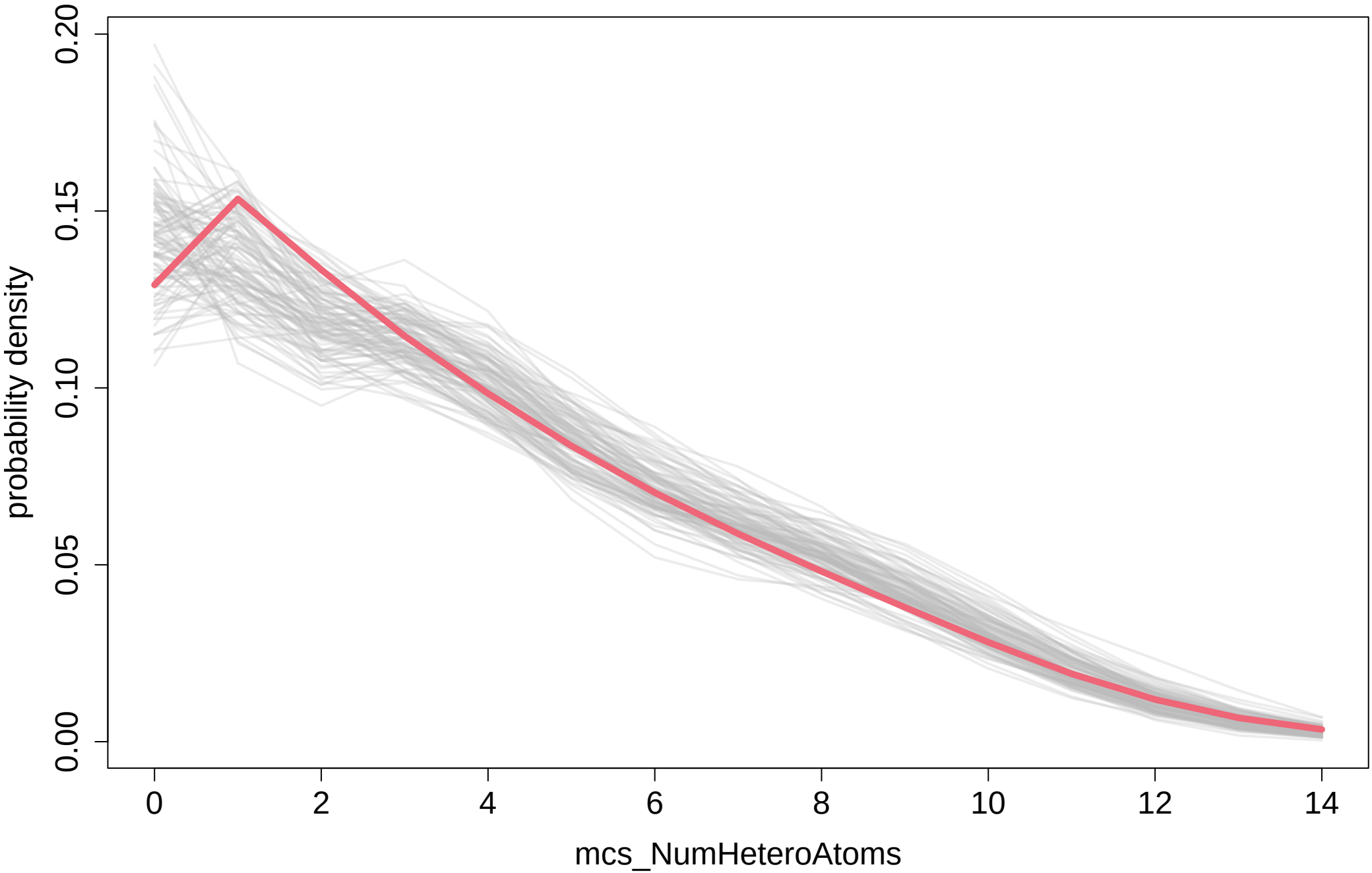
−− STATS 2D −−
min ESS = 3538.13915770878
max BMK = 0.0480581580687794
max MCSE = 1.85961126941863
all stationary: FALSE
burn: 0
max rel.err.: 1.78572412517052

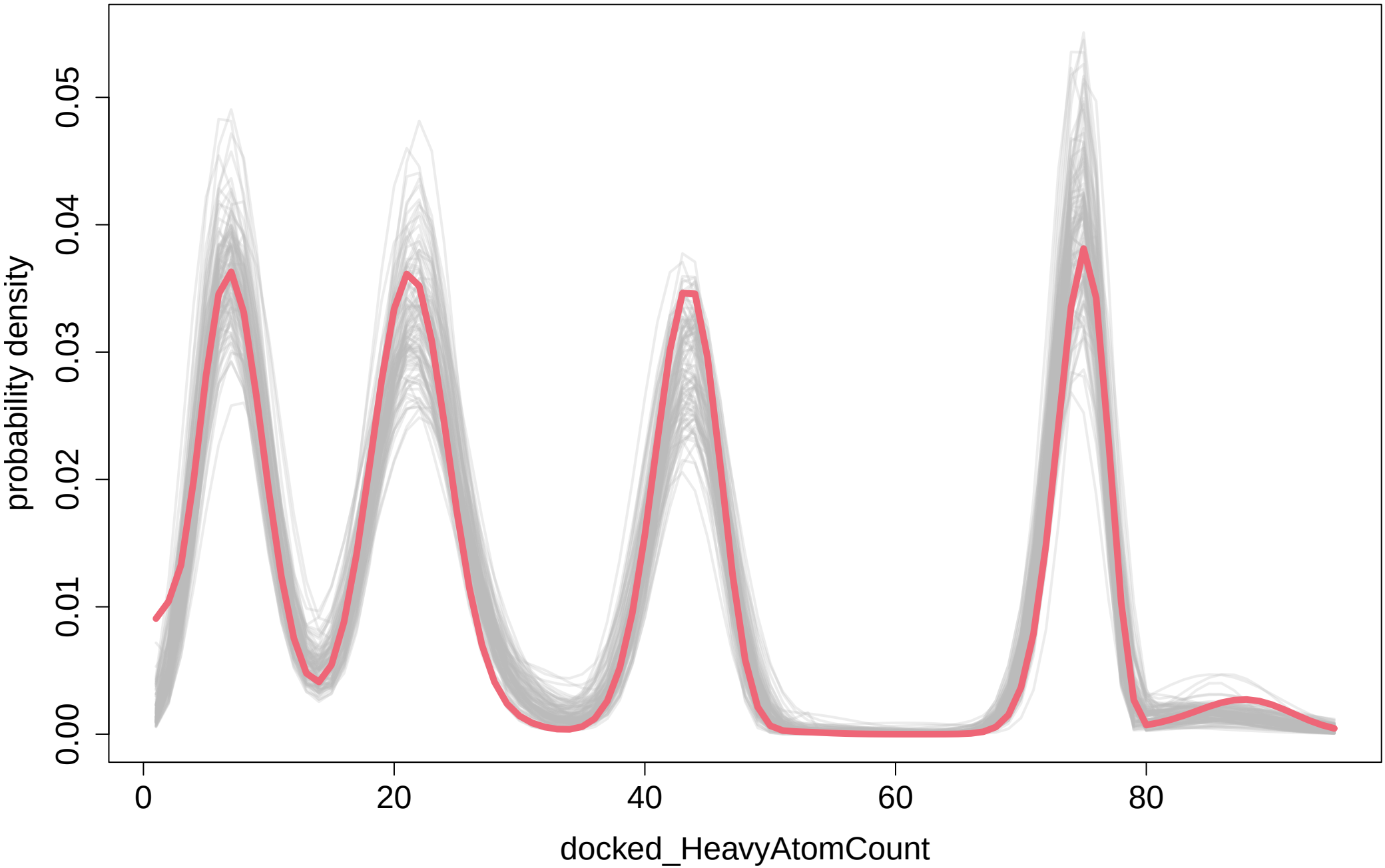
−− STATS 1D −−
min ESS = 3579.95397013962
max BMK = 0.050435912256034
max MCSE = 2.09196706319906
all stationary: FALSE
burn: 0
max rel.err.: 2.28060787031158

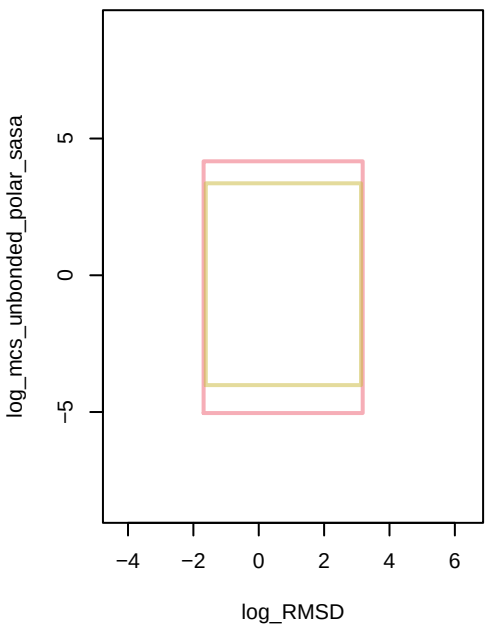
Occupied clusters: 8 of 16
LL: −2160 +− 6.51

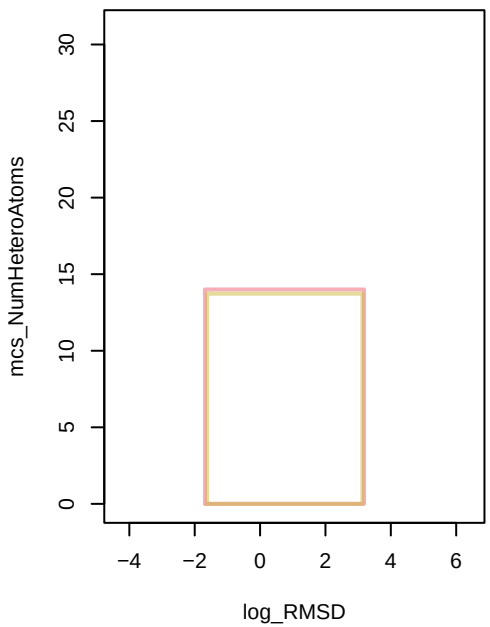

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−1
0
1
2
3
log_RMSD

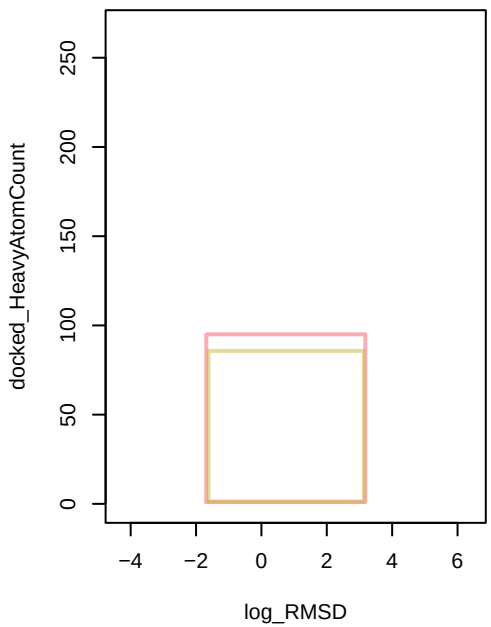

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

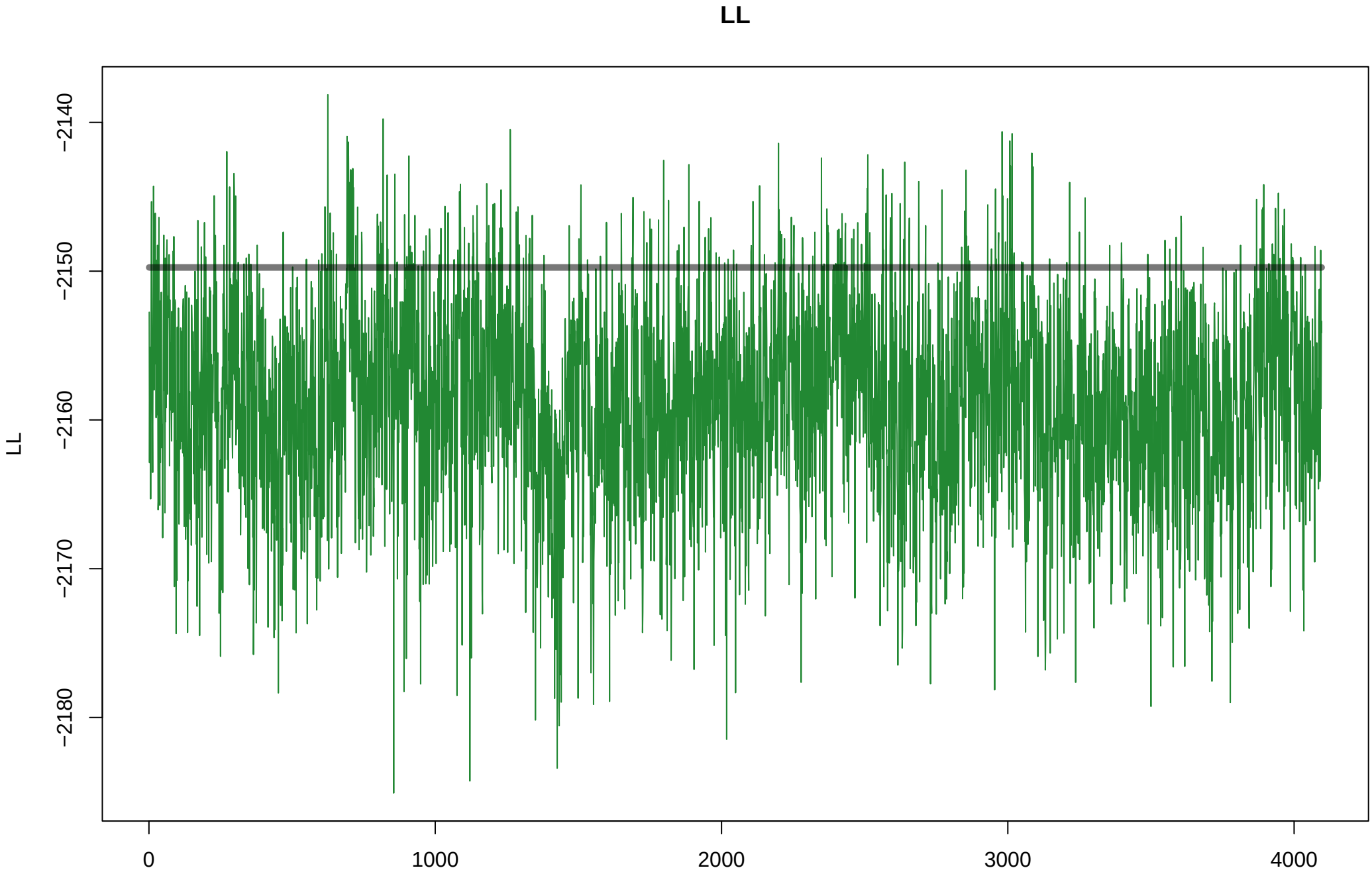

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

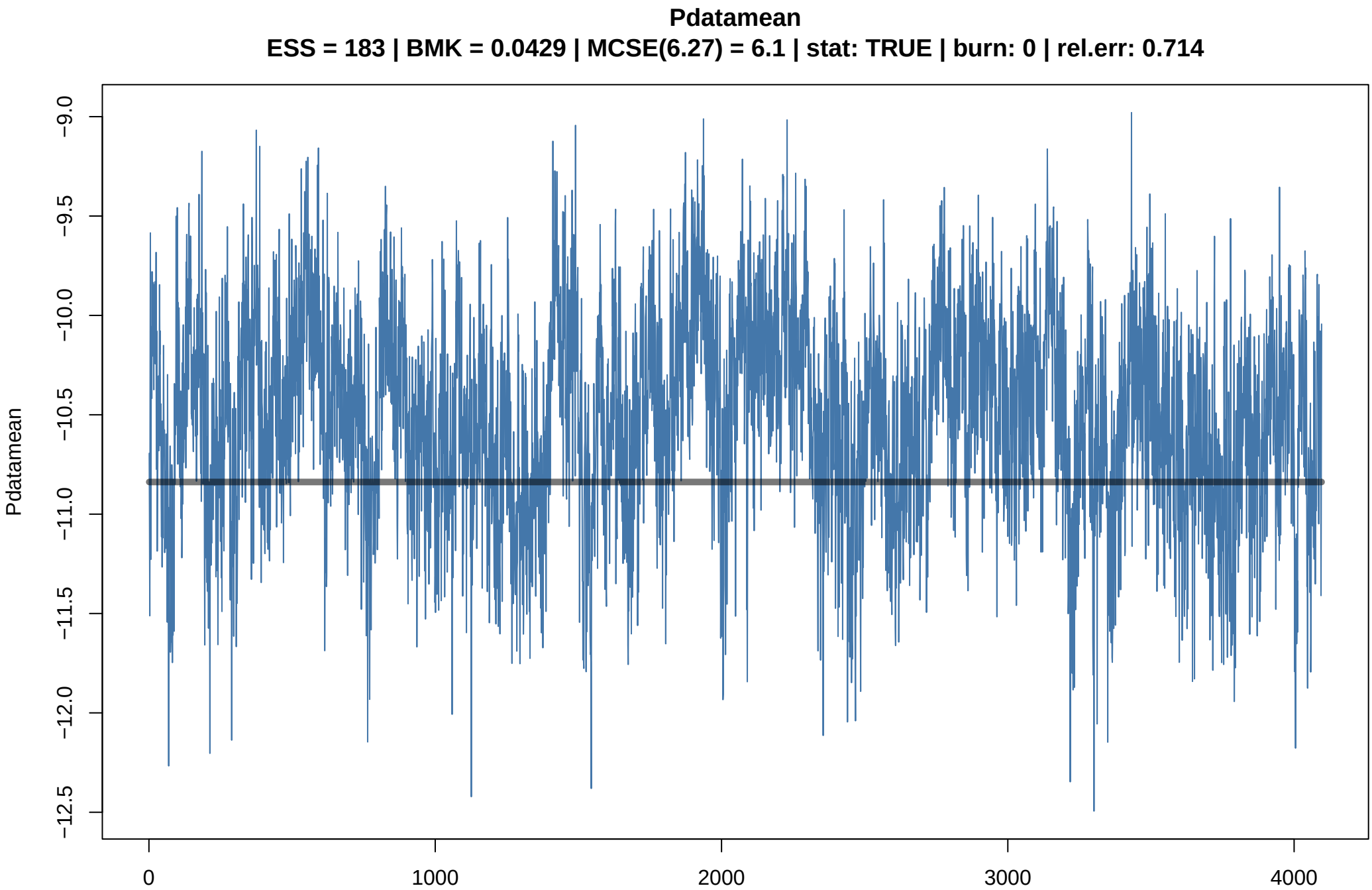

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
20
40
60
80
docked_HeavyAtomCount

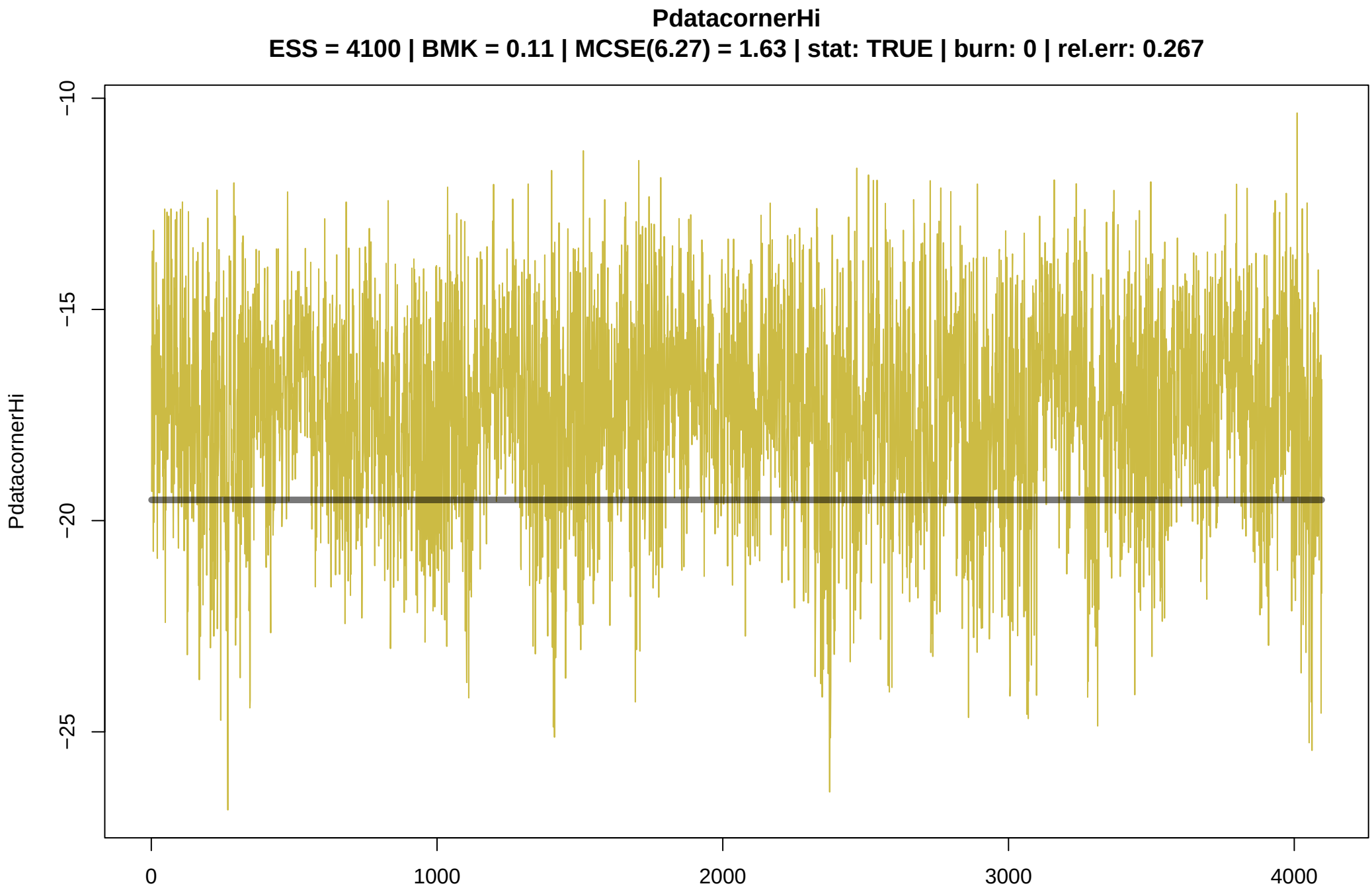

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

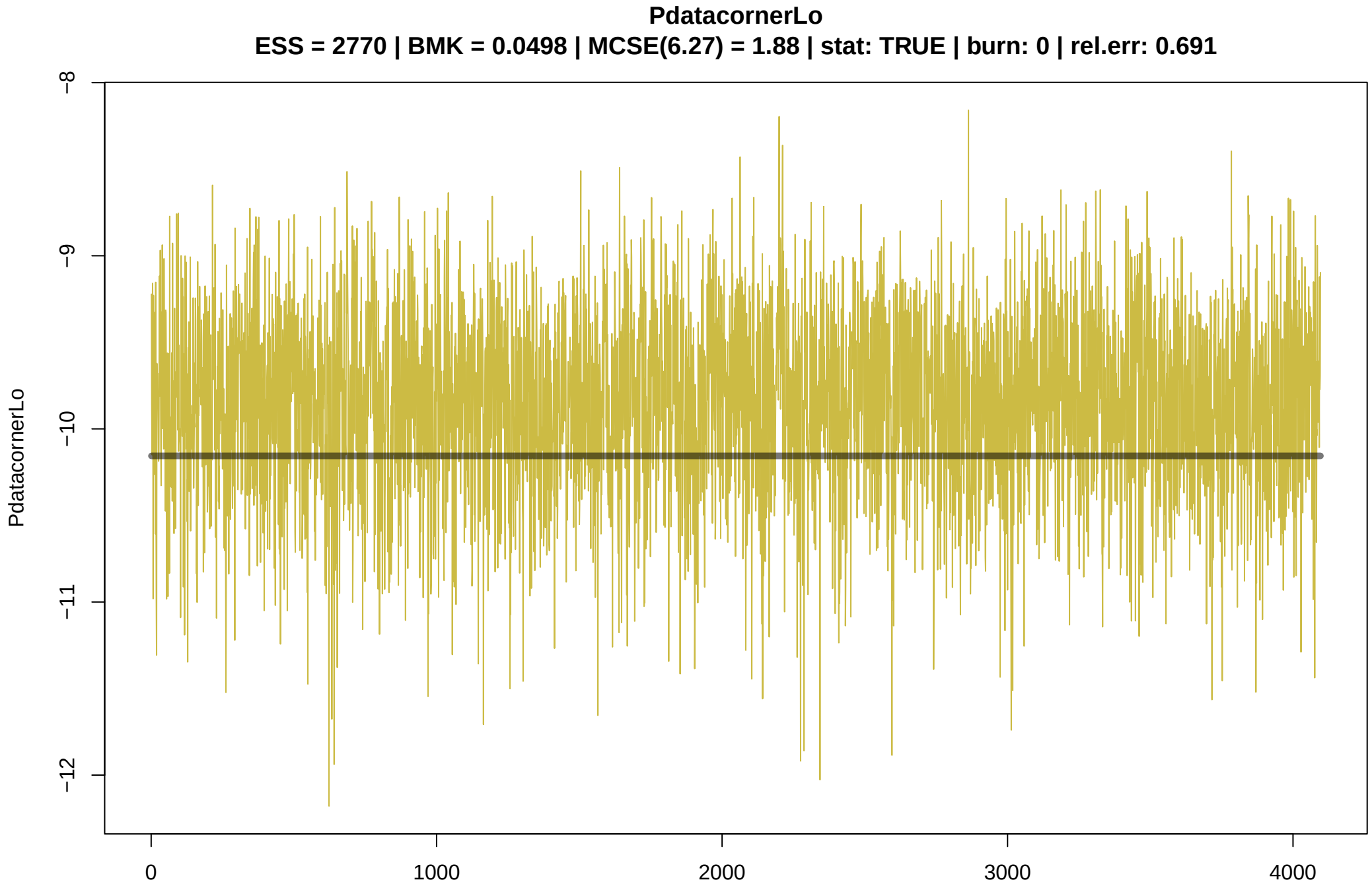

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

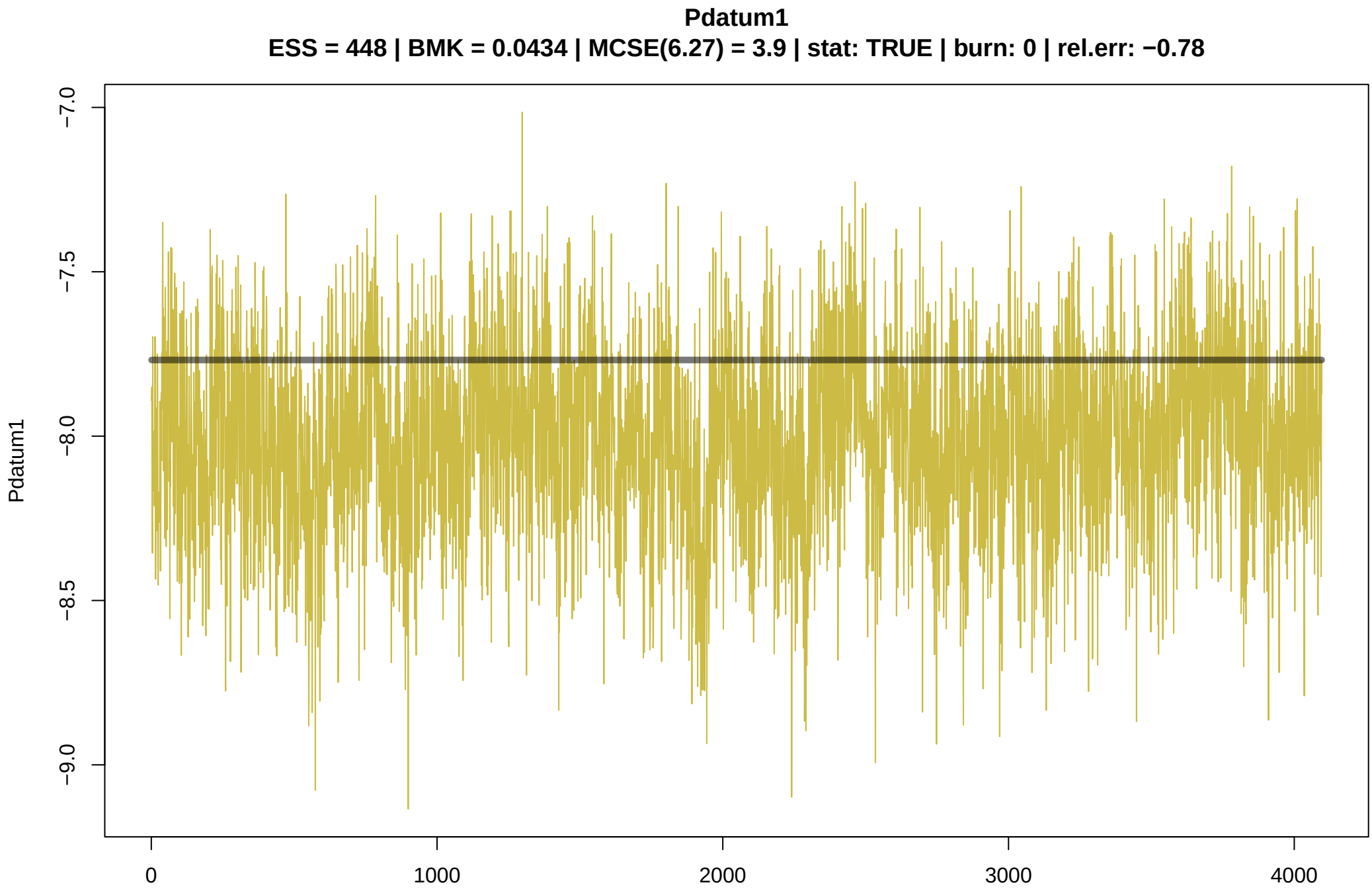

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

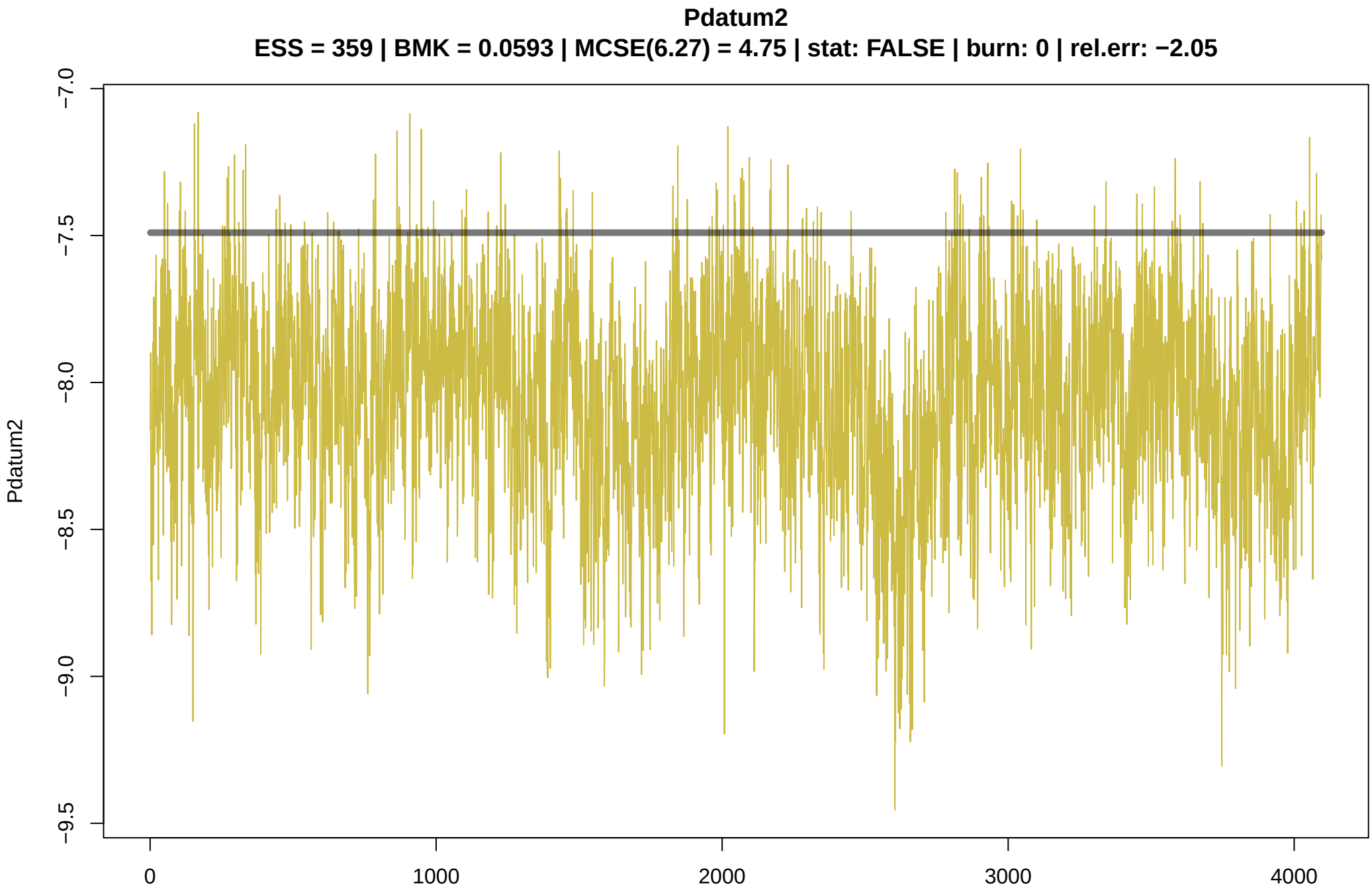

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

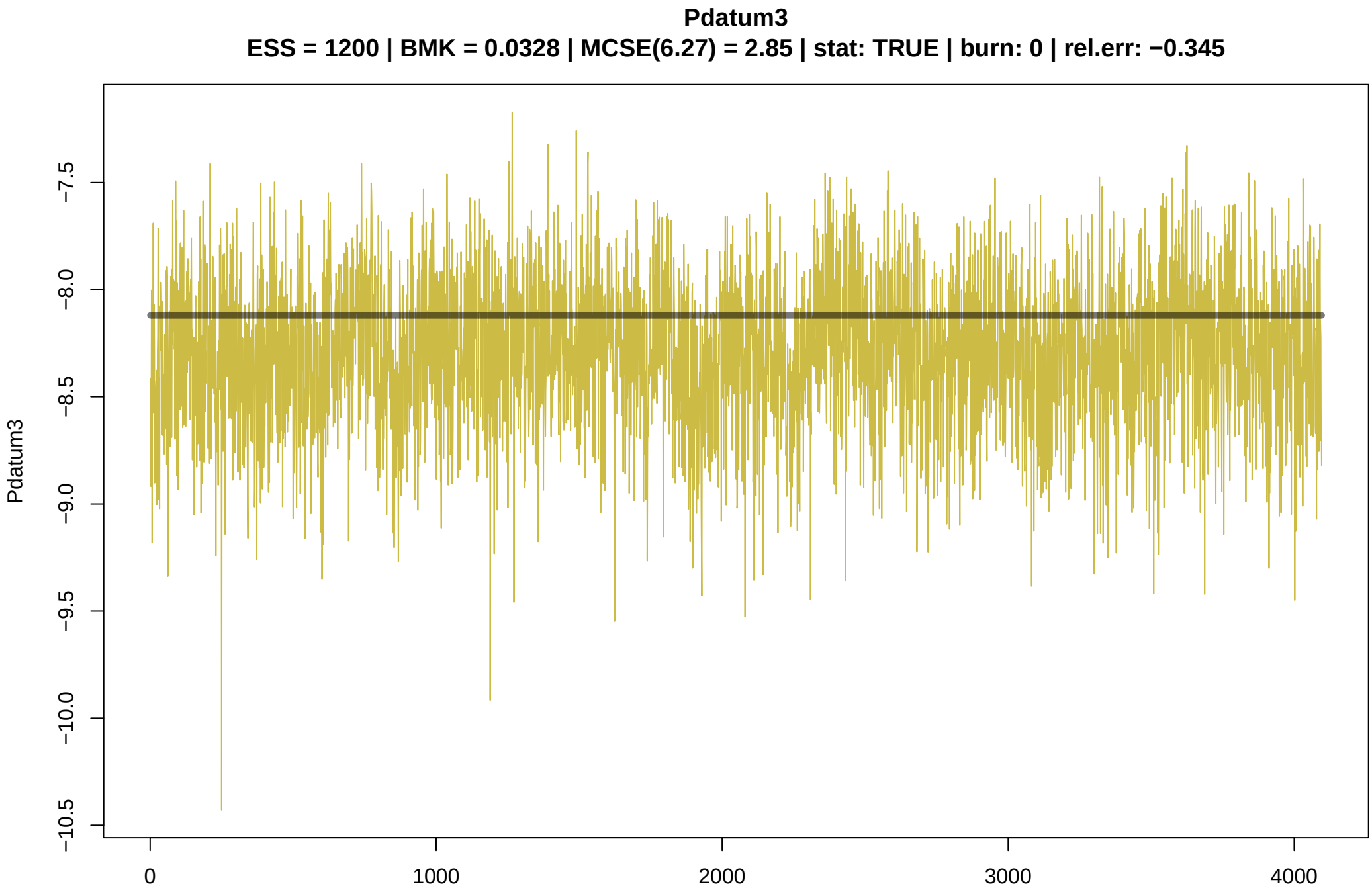

Pdatamean
ESS = 183 | BMK = 0.0429 | MCSE(6.27) = 6.1 | stat: TRUE | burn: 0 | rel.err: 0.714
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
−12.5
0
1000
2000
3000
4000

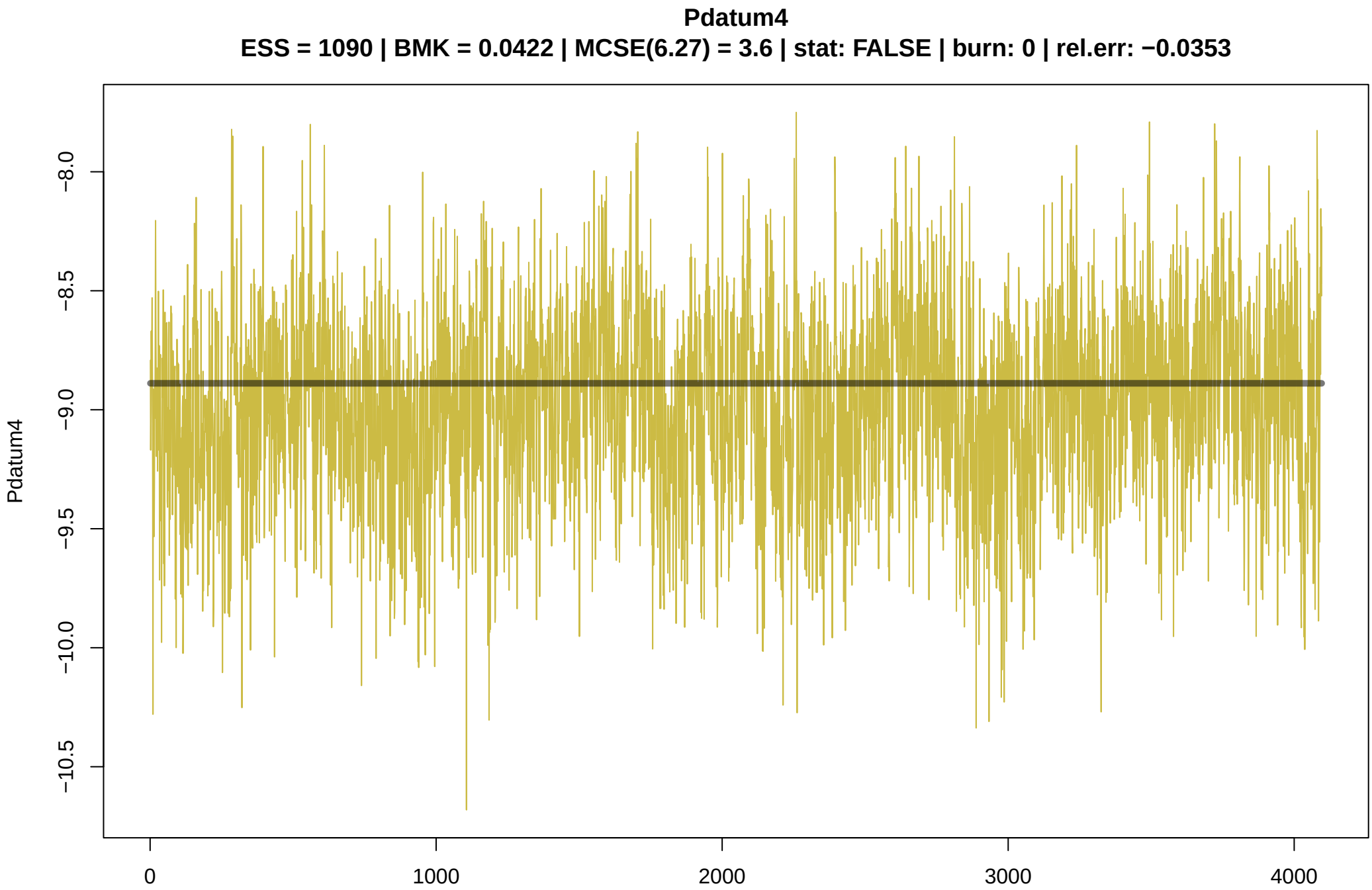

PdatacornerHi
ESS = 4100 | BMK = 0.11 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.267
PdatacornerHi
−10
−15
−20
−25
0
1000
2000
3000
4000

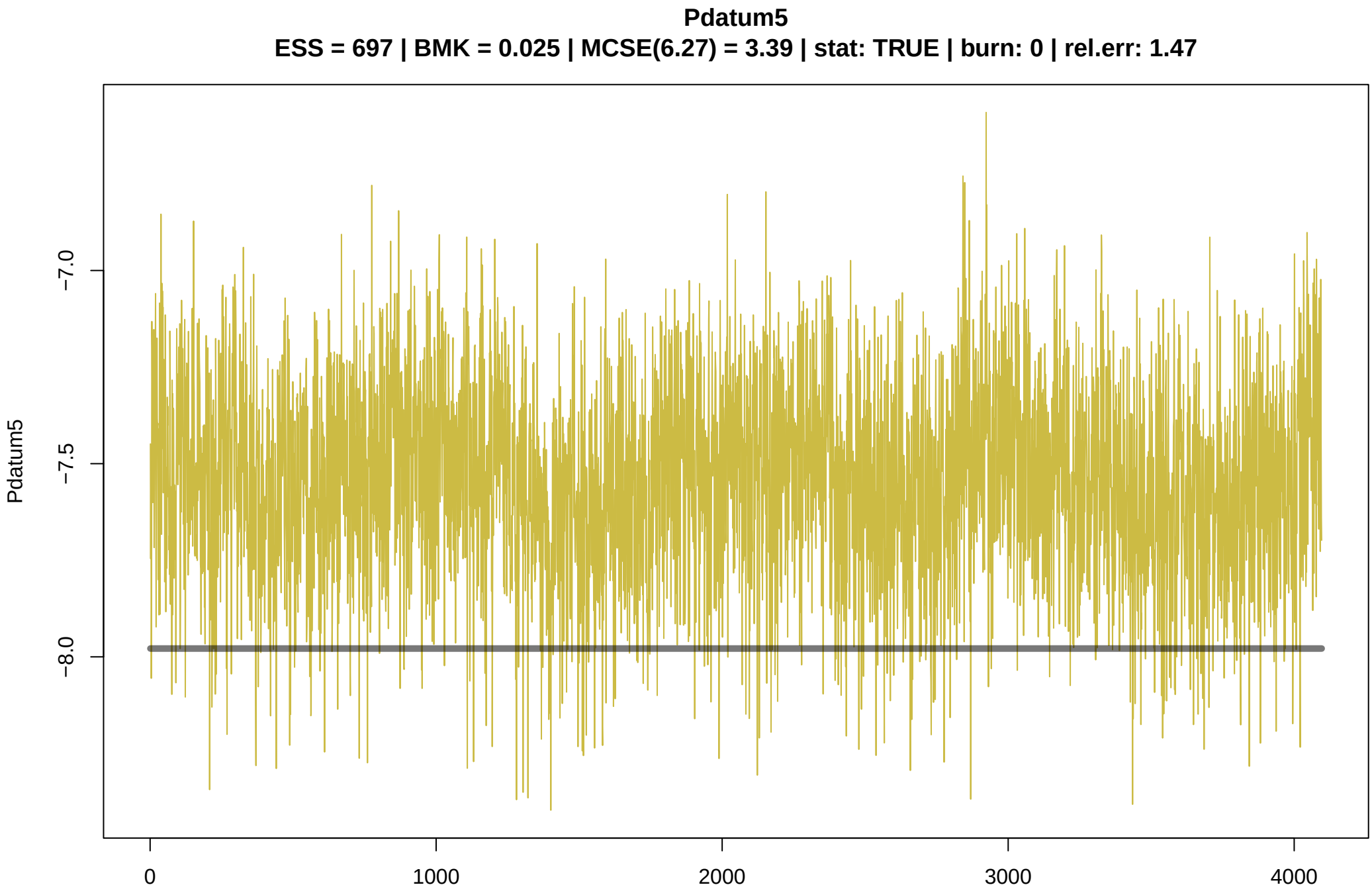

PdatacornerLo
ESS = 2770 | BMK = 0.0498 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 0 | rel.err: 0.691
PdatacornerLo
−8
−9
−10
−11
−12
0
1000
2000
3000
4000

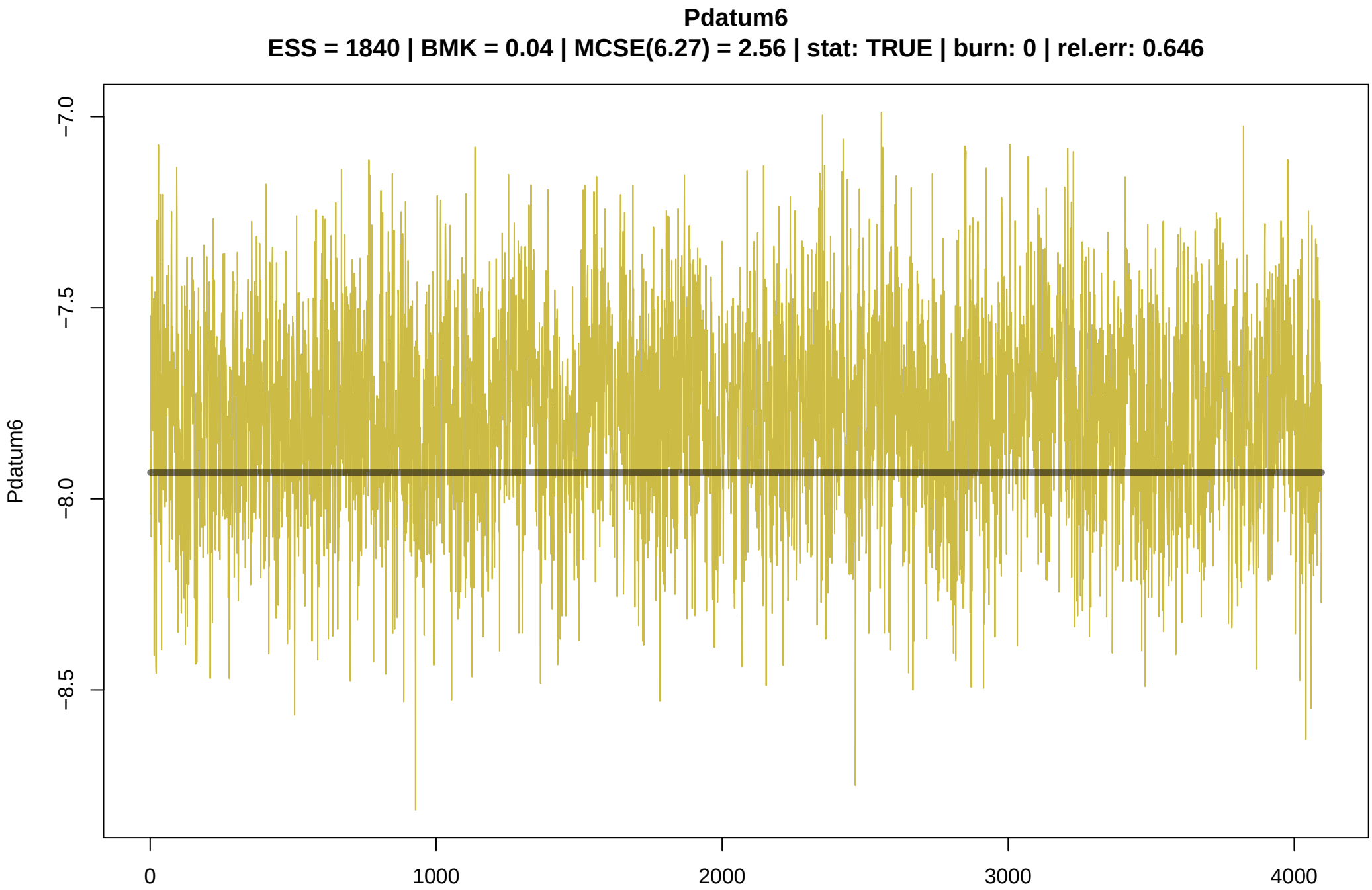

Pdatum1
ESS = 448 | BMK = 0.0434 | MCSE(6.27) = 3.9 | stat: TRUE | burn: 0 | rel.err: −0.78
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

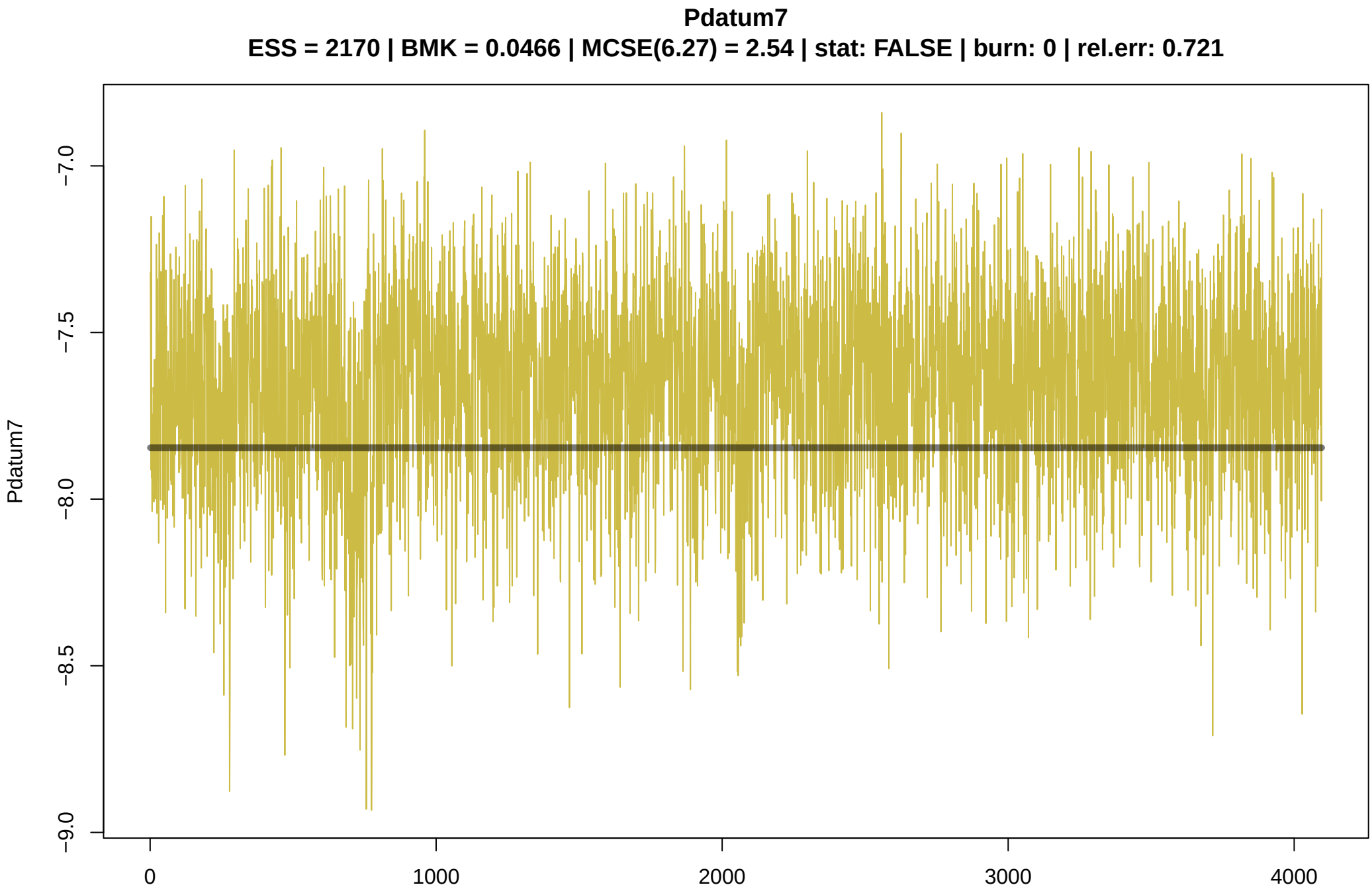

Pdatum2
ESS = 359 | BMK = 0.0593 | MCSE(6.27) = 4.75 | stat: FALSE | burn: 0 | rel.err: −2.05
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

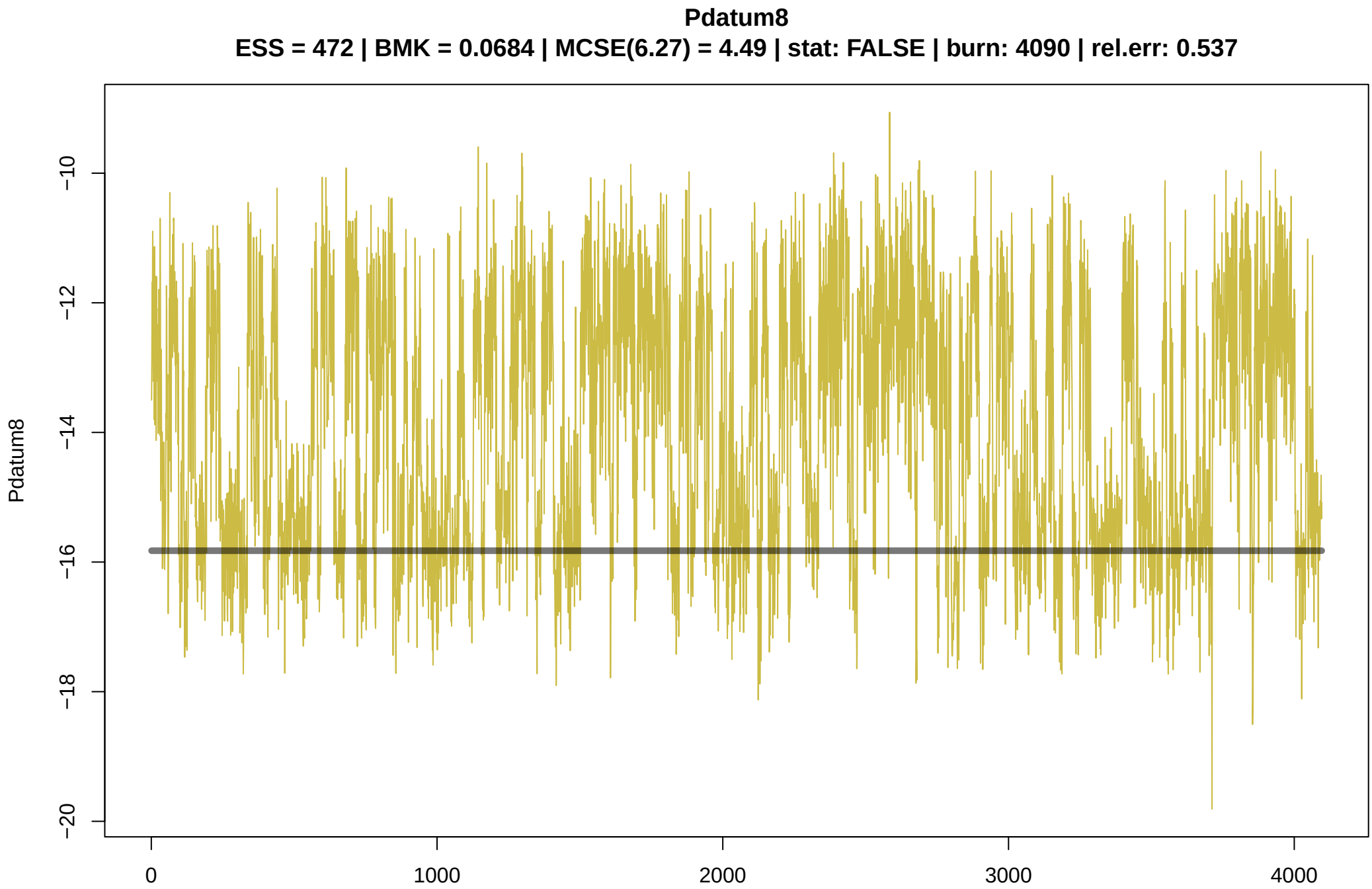

Pdatum3
ESS = 1200 | BMK = 0.0328 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0 | rel.err: −0.345
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

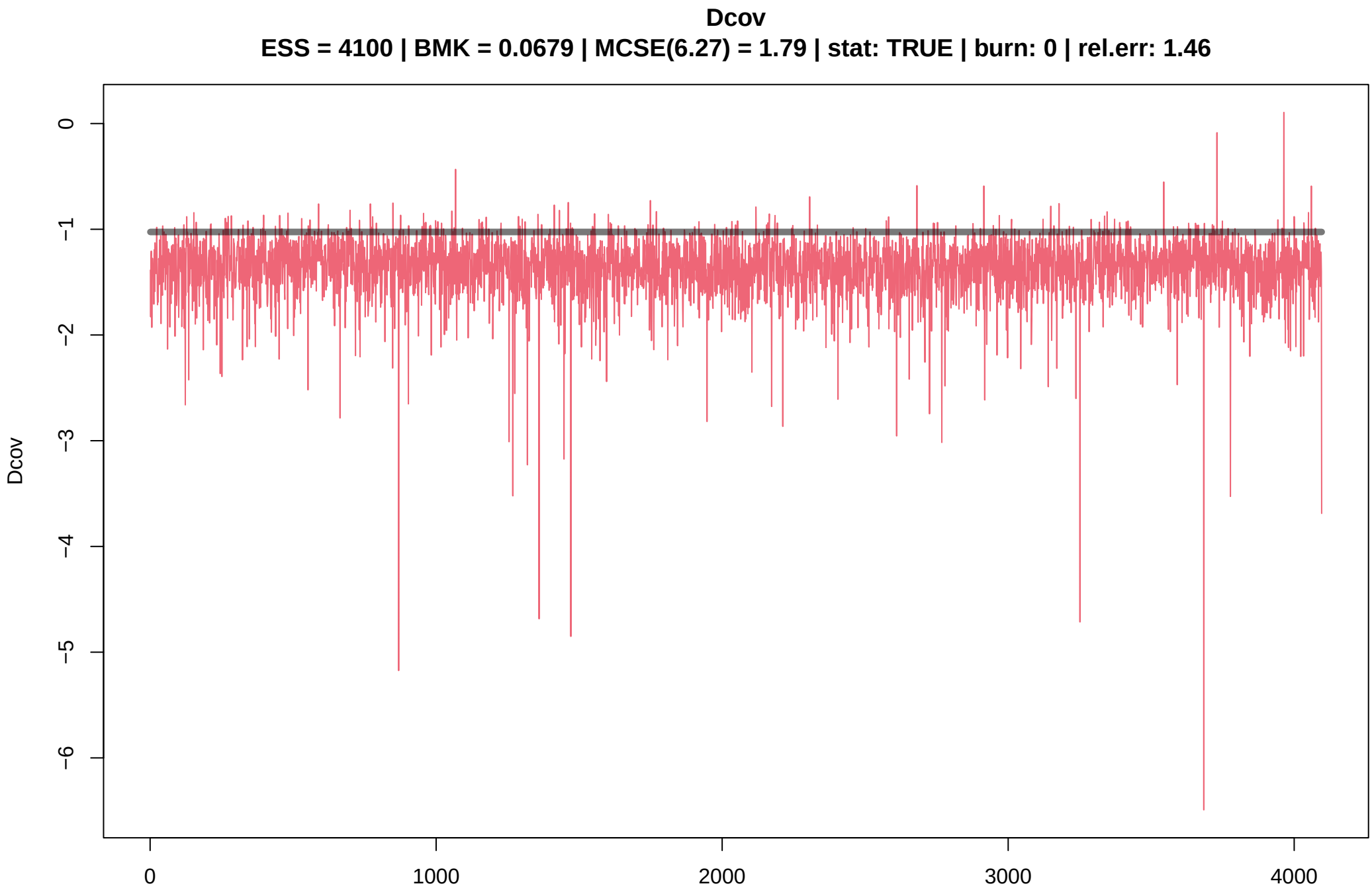

Pdatum4
ESS = 1090 | BMK = 0.0422 | MCSE(6.27) = 3.6 | stat: FALSE | burn: 0 | rel.err: −0.0353
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

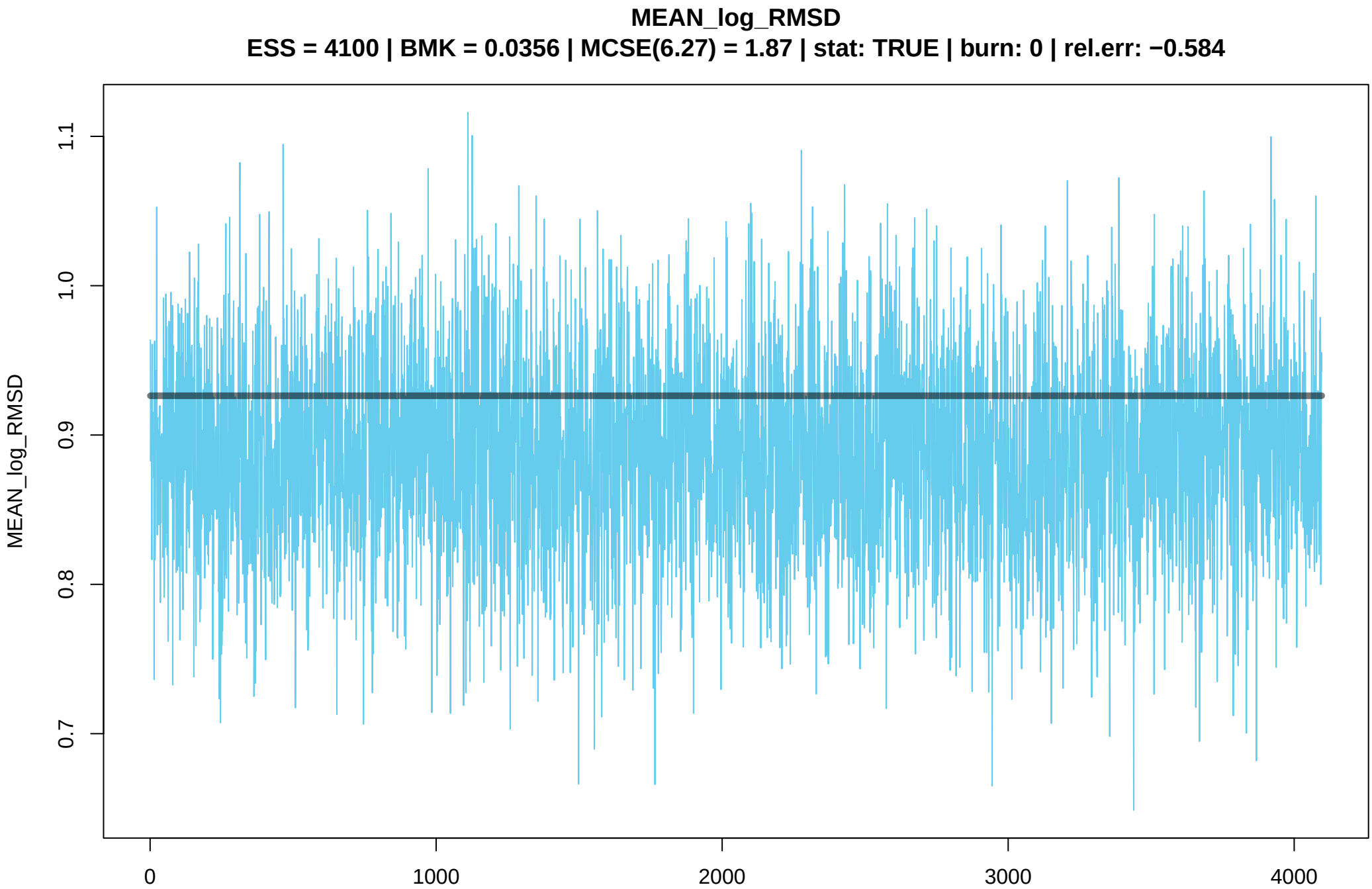

Pdatum5
ESS = 697 | BMK = 0.025 | MCSE(6.27) = 3.39 | stat: TRUE | burn: 0 | rel.err: 1.47
Pdatum5
−7.0
−7.5
−8.0
0
1000
2000
3000
4000

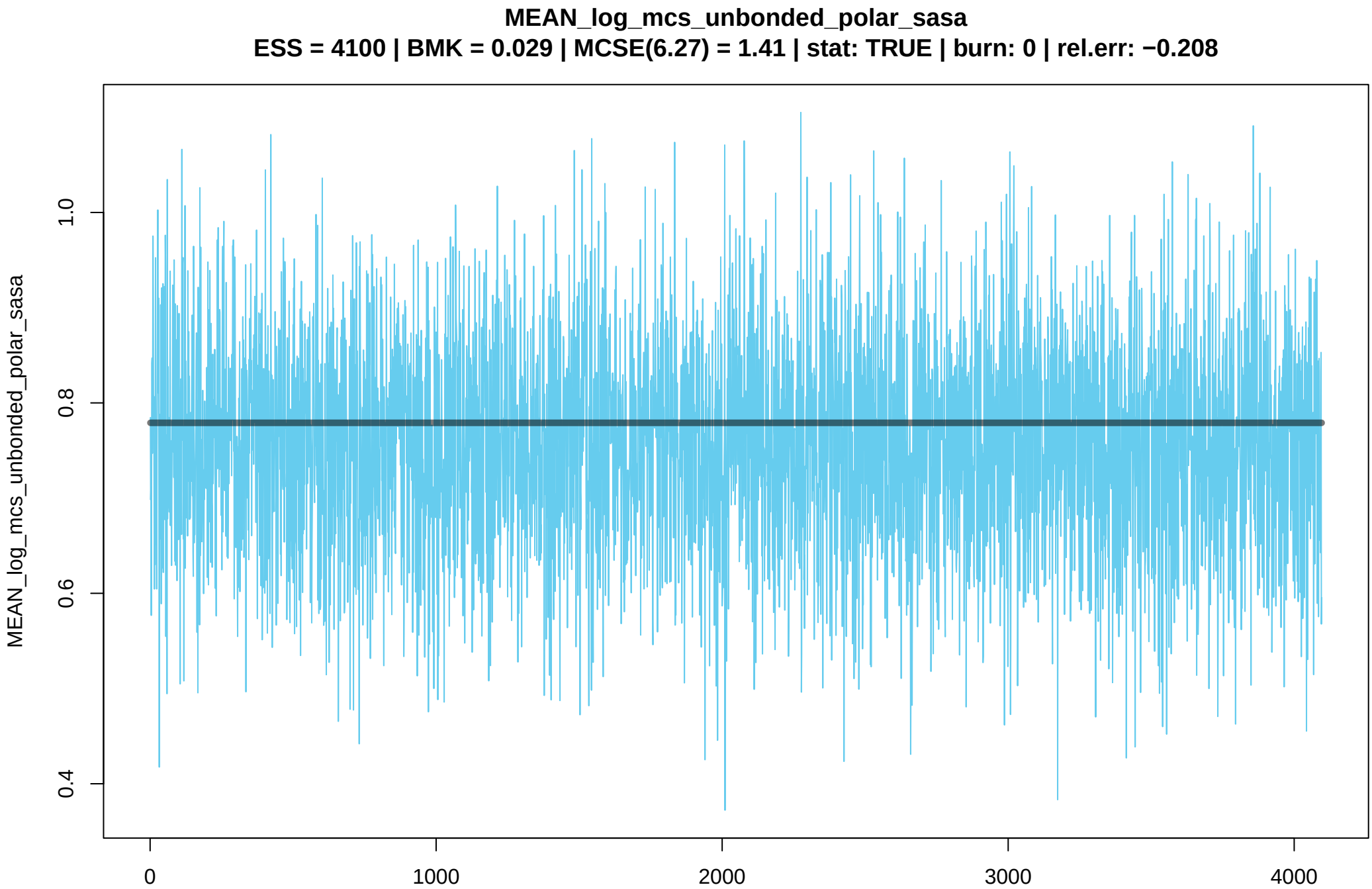

Pdatum6
ESS = 1840 | BMK = 0.04 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | rel.err: 0.646
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

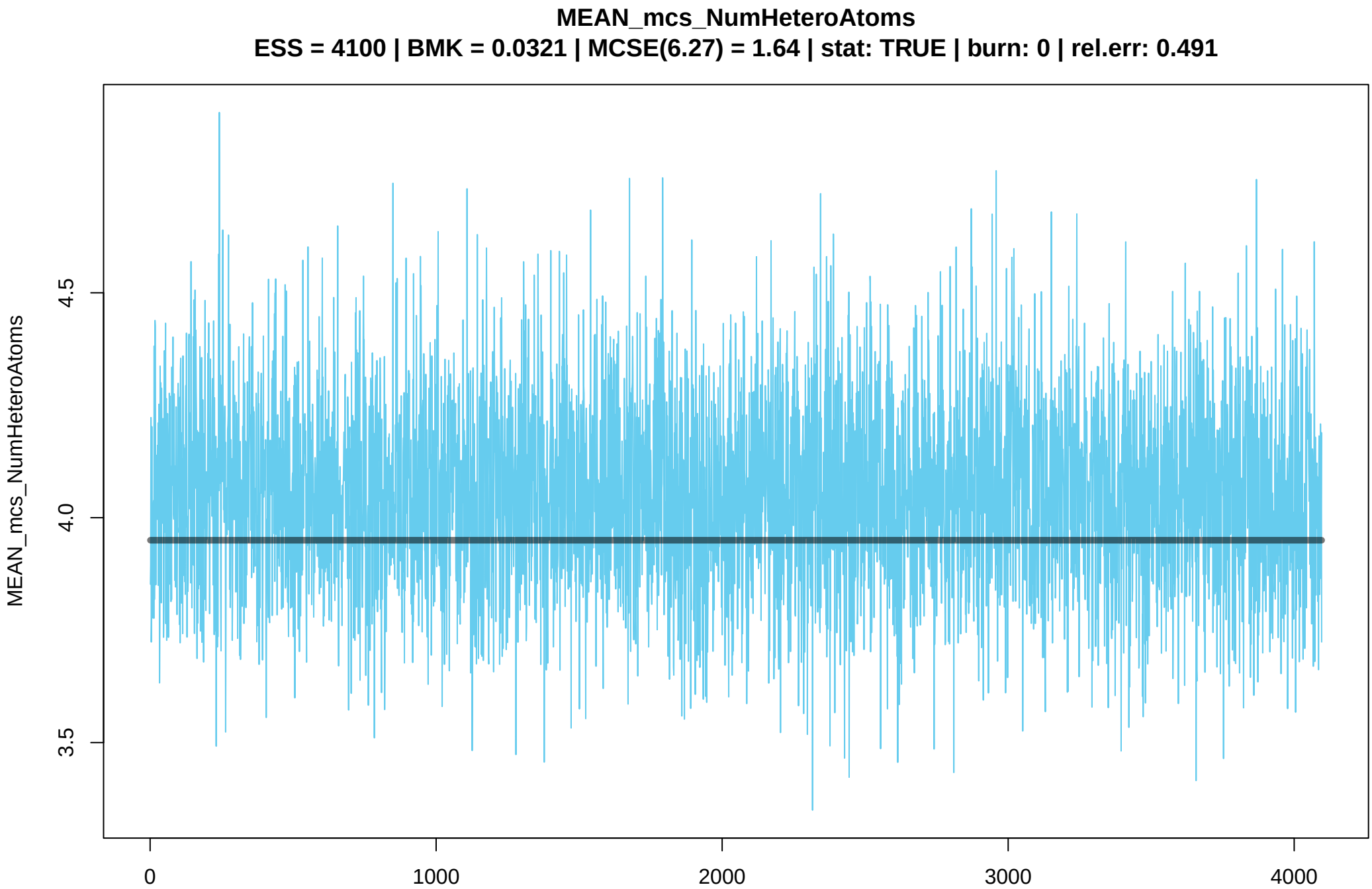

Pdatum7
ESS = 2170 | BMK = 0.0466 | MCSE(6.27) = 2.54 | stat: FALSE | burn: 0 | rel.err: 0.721
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

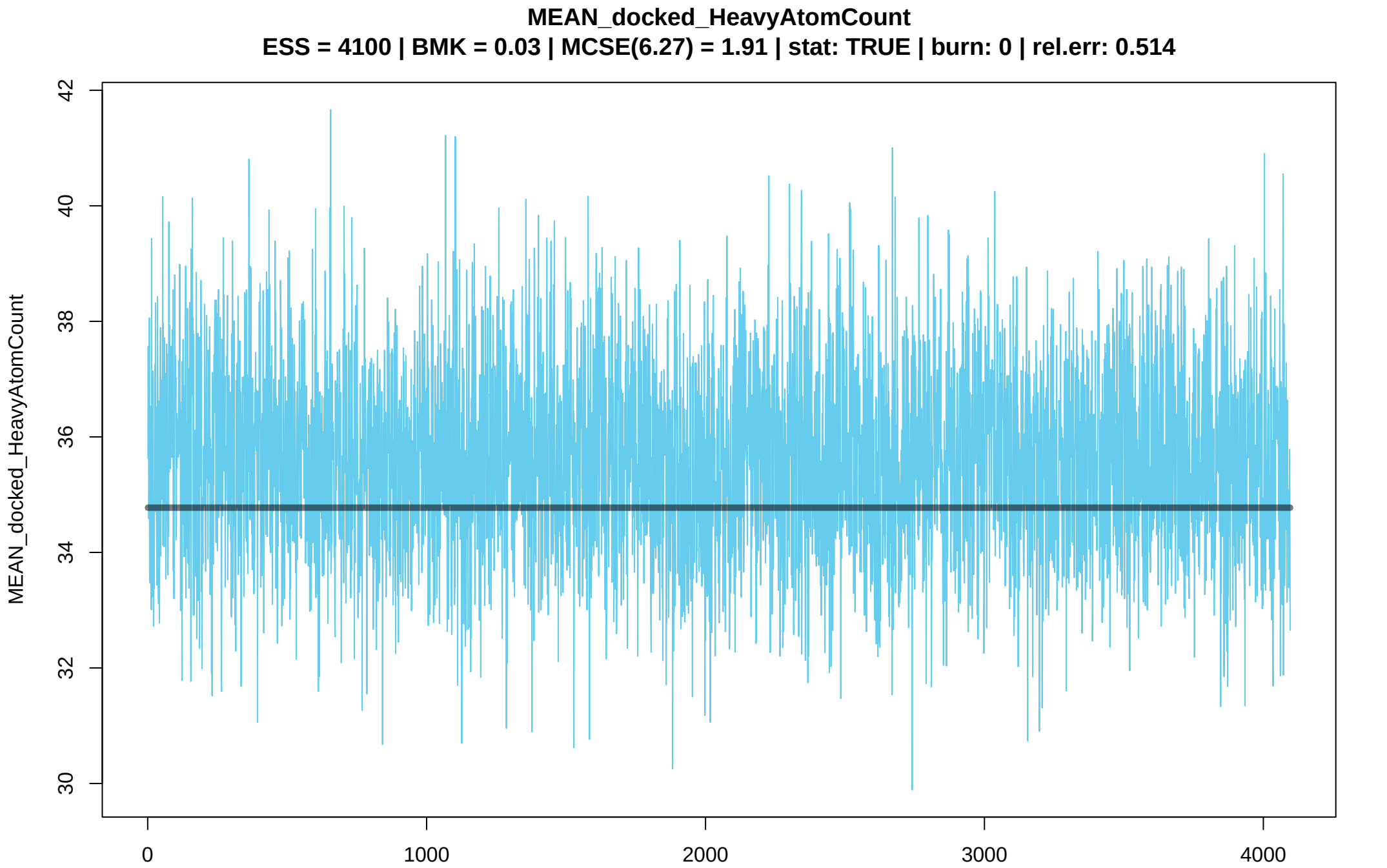

Pdatum8
ESS = 472 | BMK = 0.0684 | MCSE(6.27) = 4.49 | stat: FALSE | burn: 4090 | rel.err: 0.537
Pdatum8
−10
−12
−14
−16
−18
−20
0
1000
2000
3000
4000

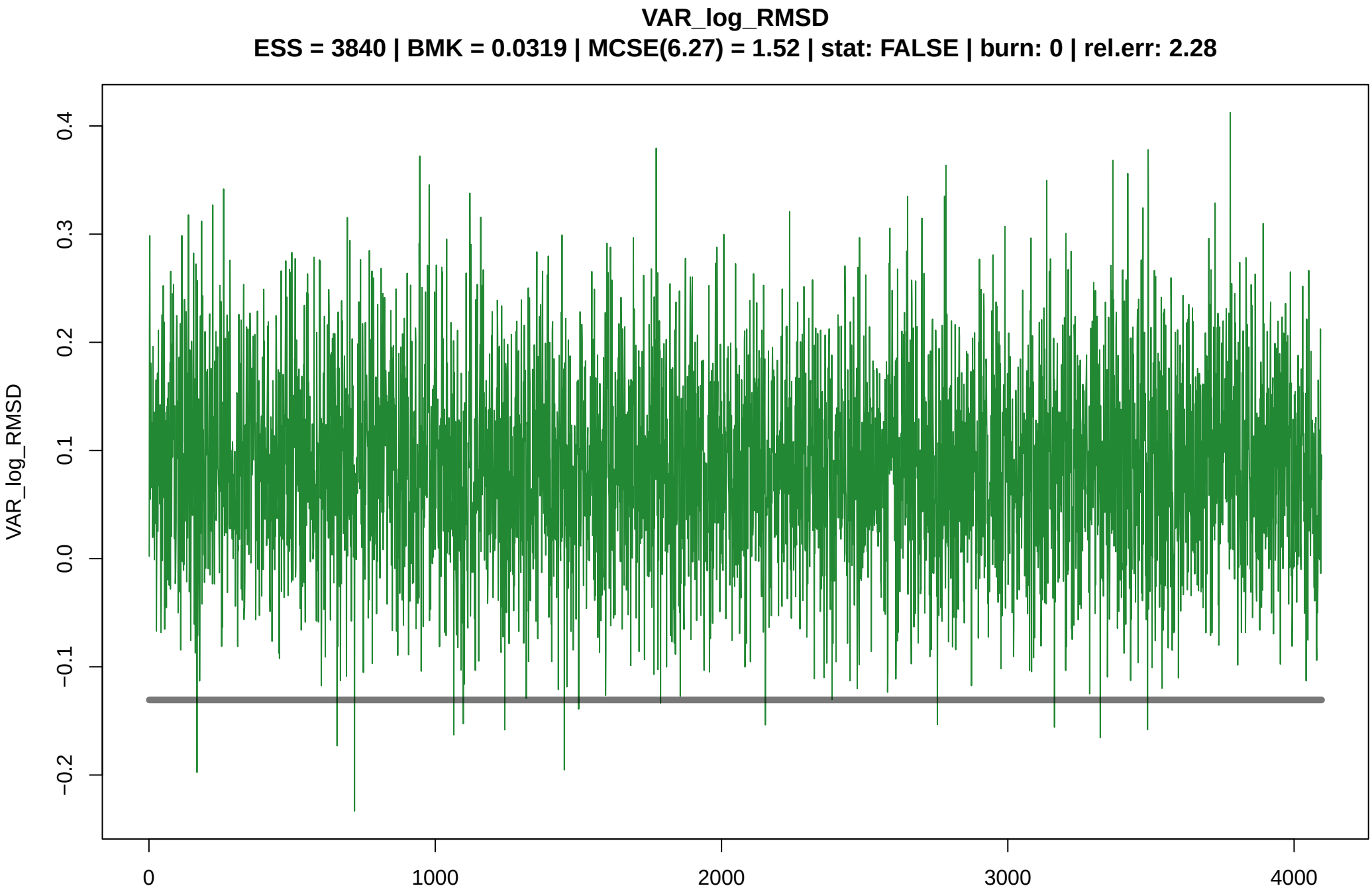

Dcov
ESS = 4100 | BMK = 0.0679 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 1.46
Dcov
0
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

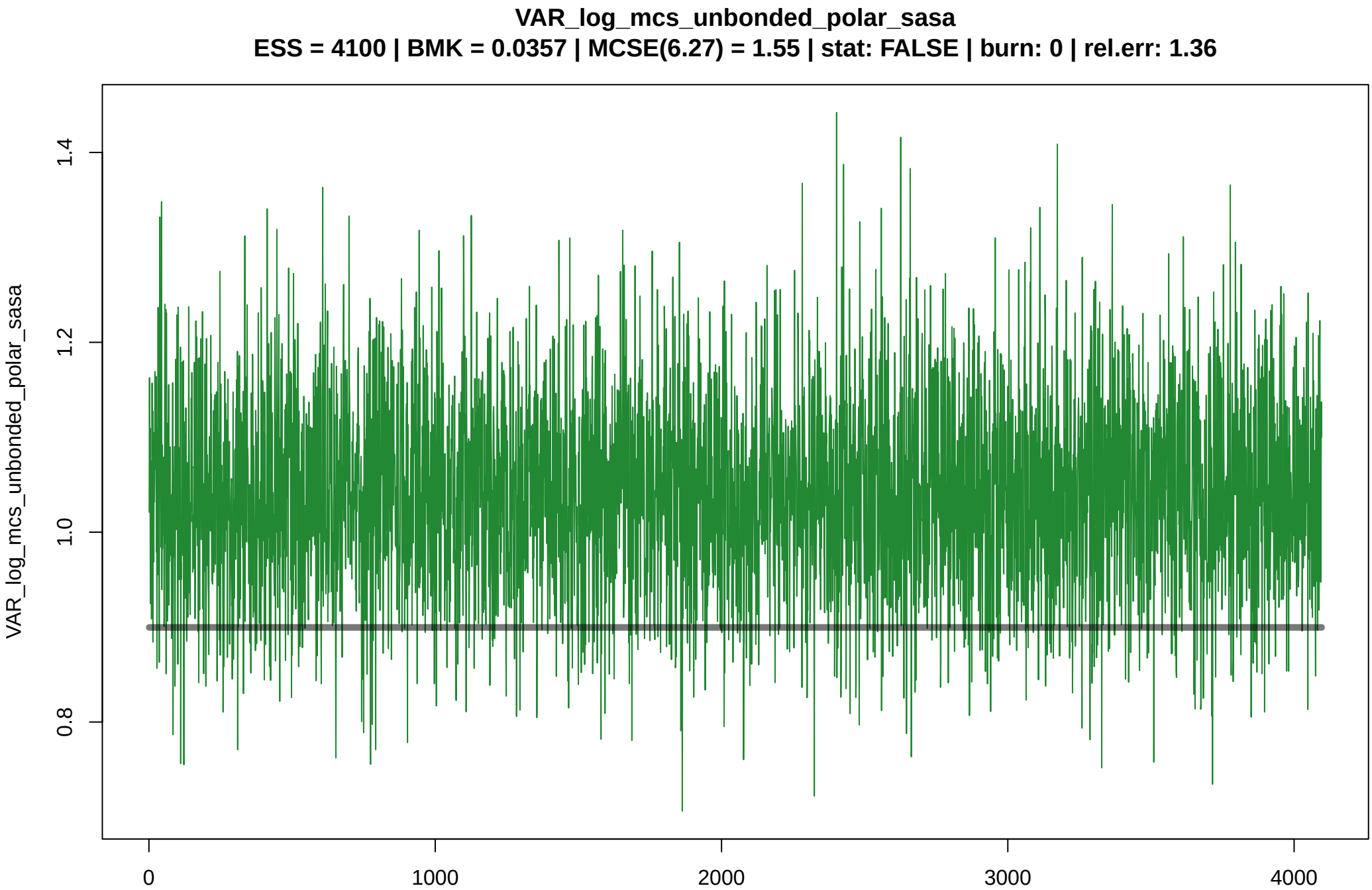

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0356 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0 | rel.err: −0.584
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

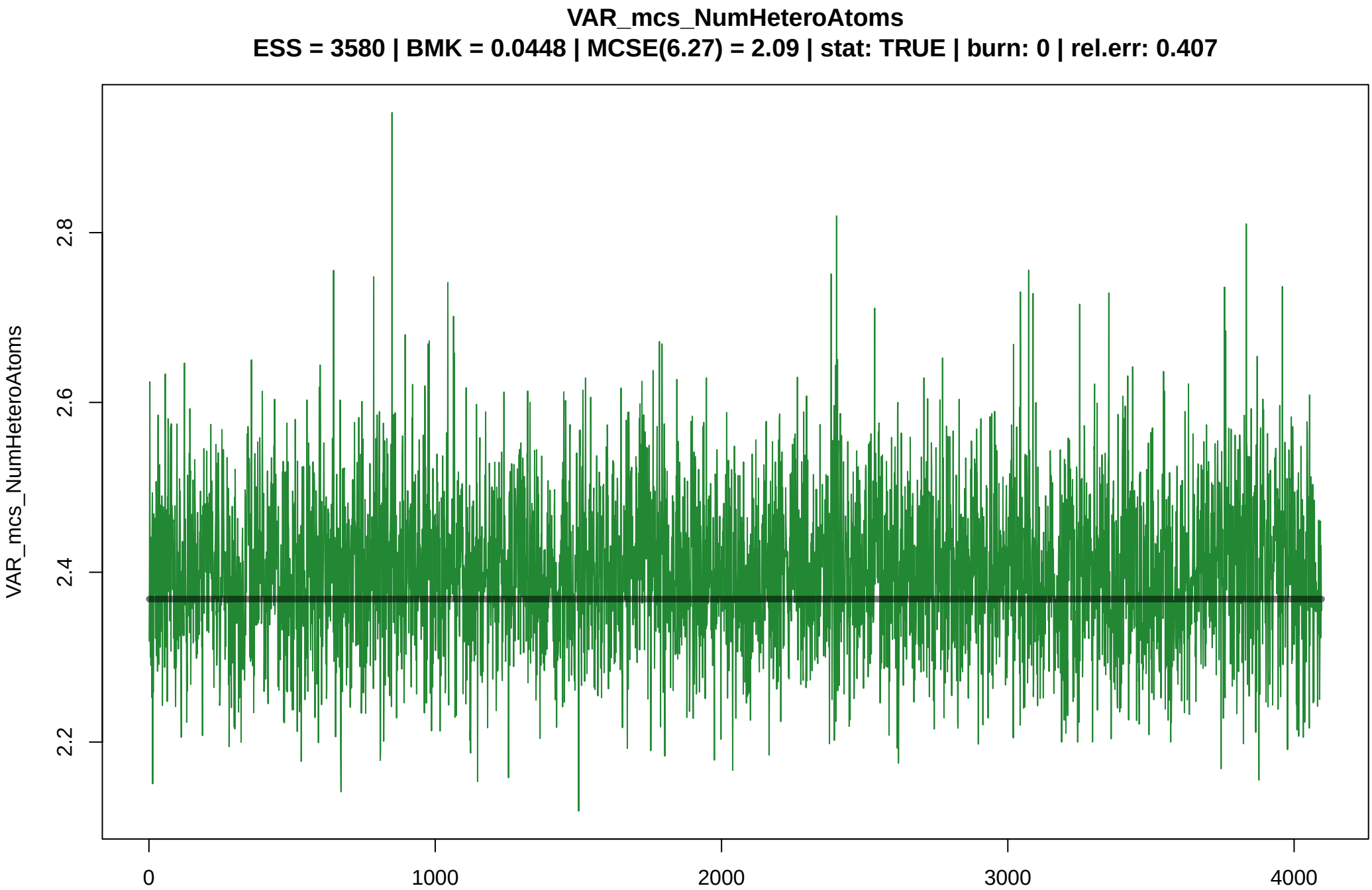

MEAN_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.029 | MCSE(6.27) = 1.41 | stat: TRUE | burn: 0 | rel.err: −0.208
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

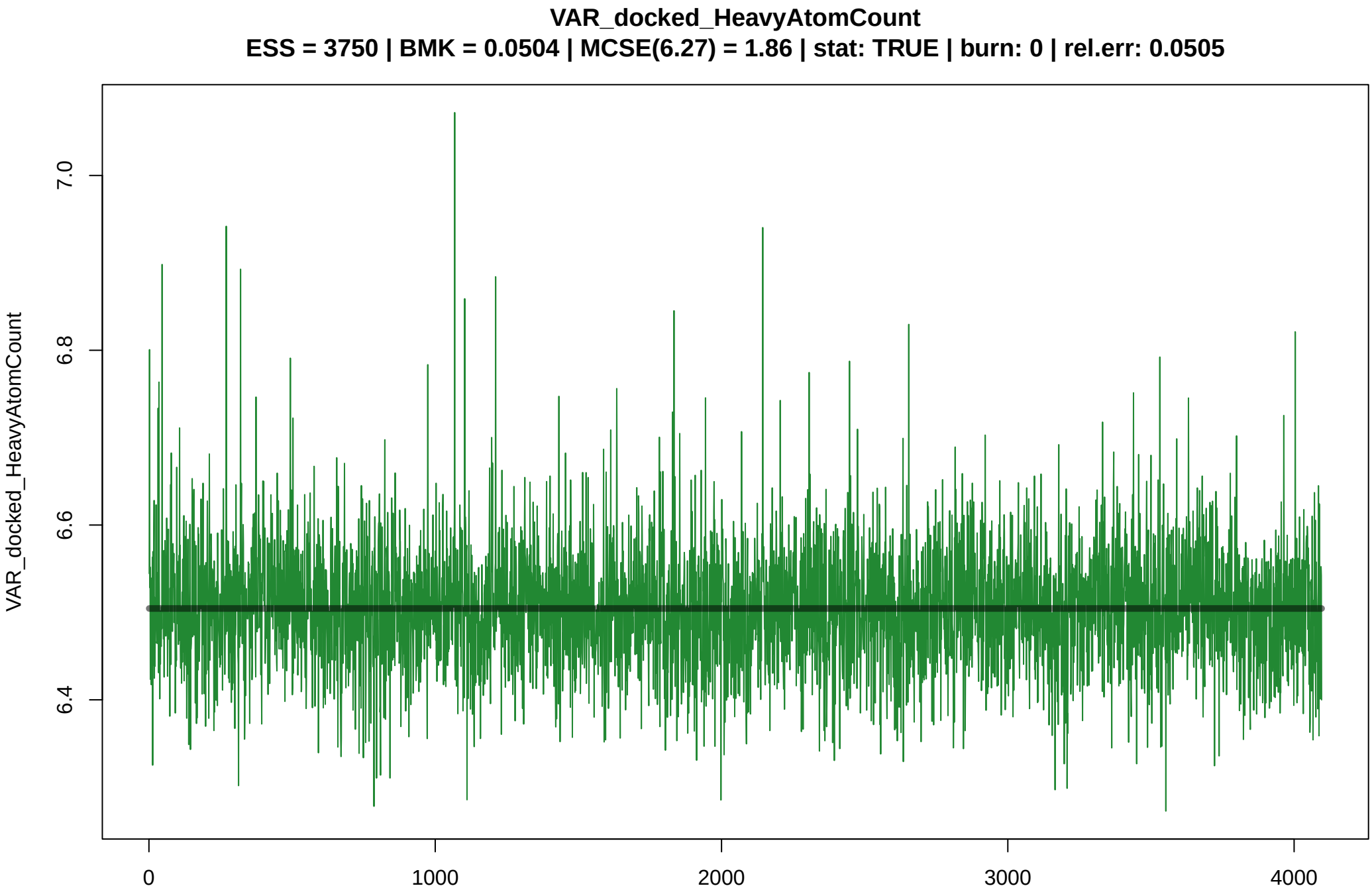

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0321 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: 0.491
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

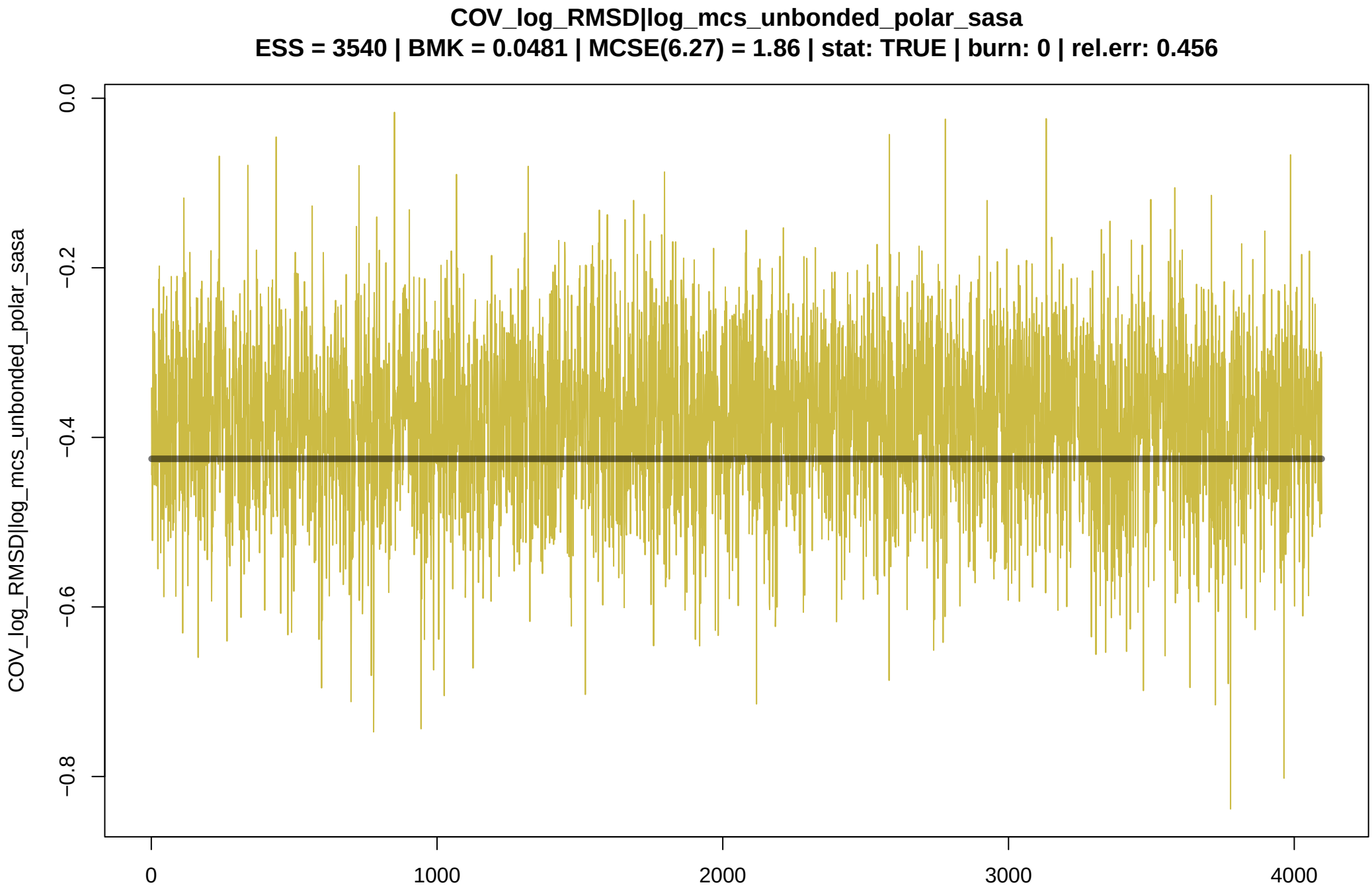

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.03 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0 | rel.err: 0.514
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
1000
2000
3000
4000

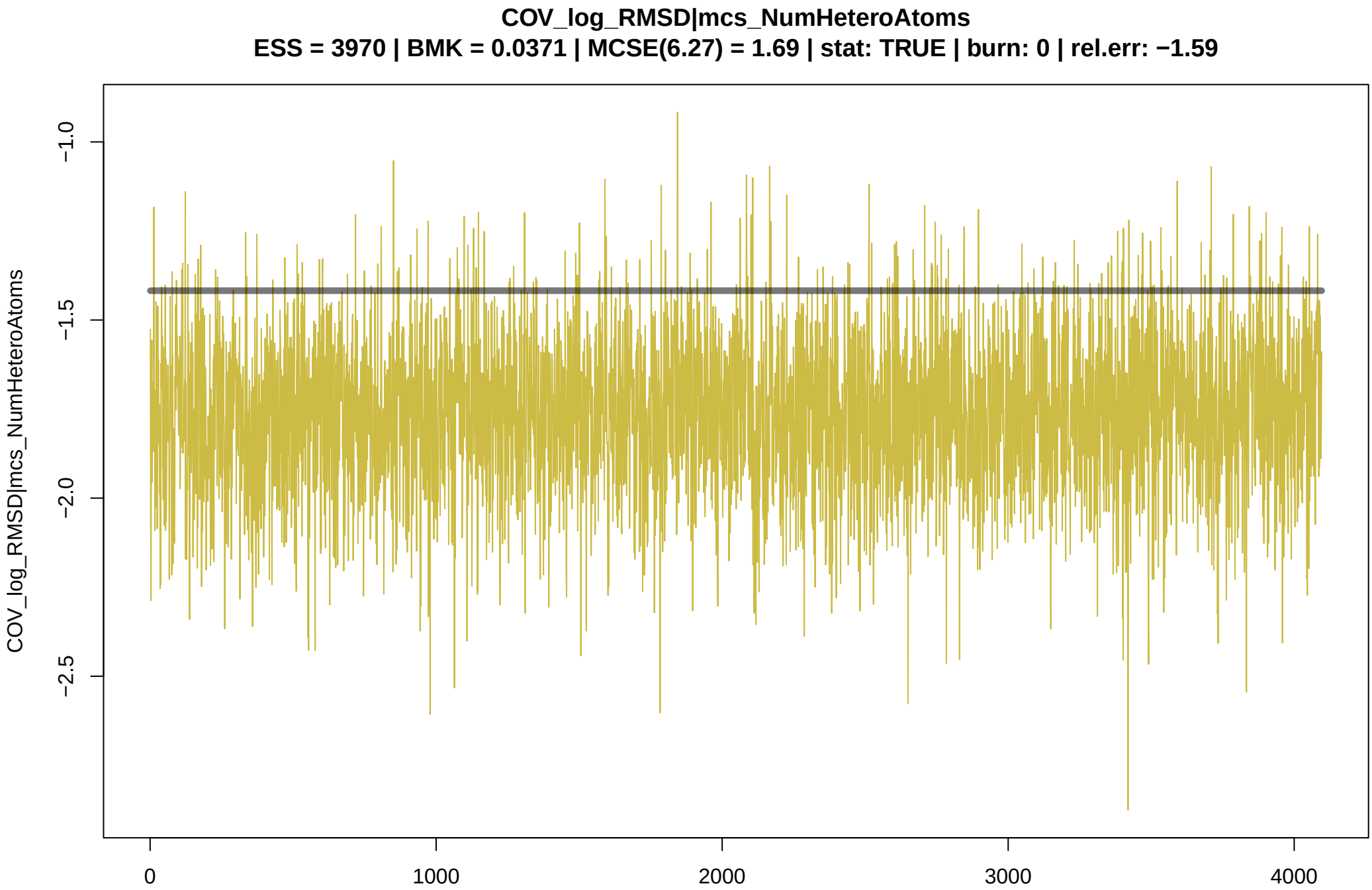

VAR_log_RMSD
ESS = 3840 | BMK = 0.0319 | MCSE(6.27) = 1.52 | stat: FALSE | burn: 0 | rel.err: 2.28
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

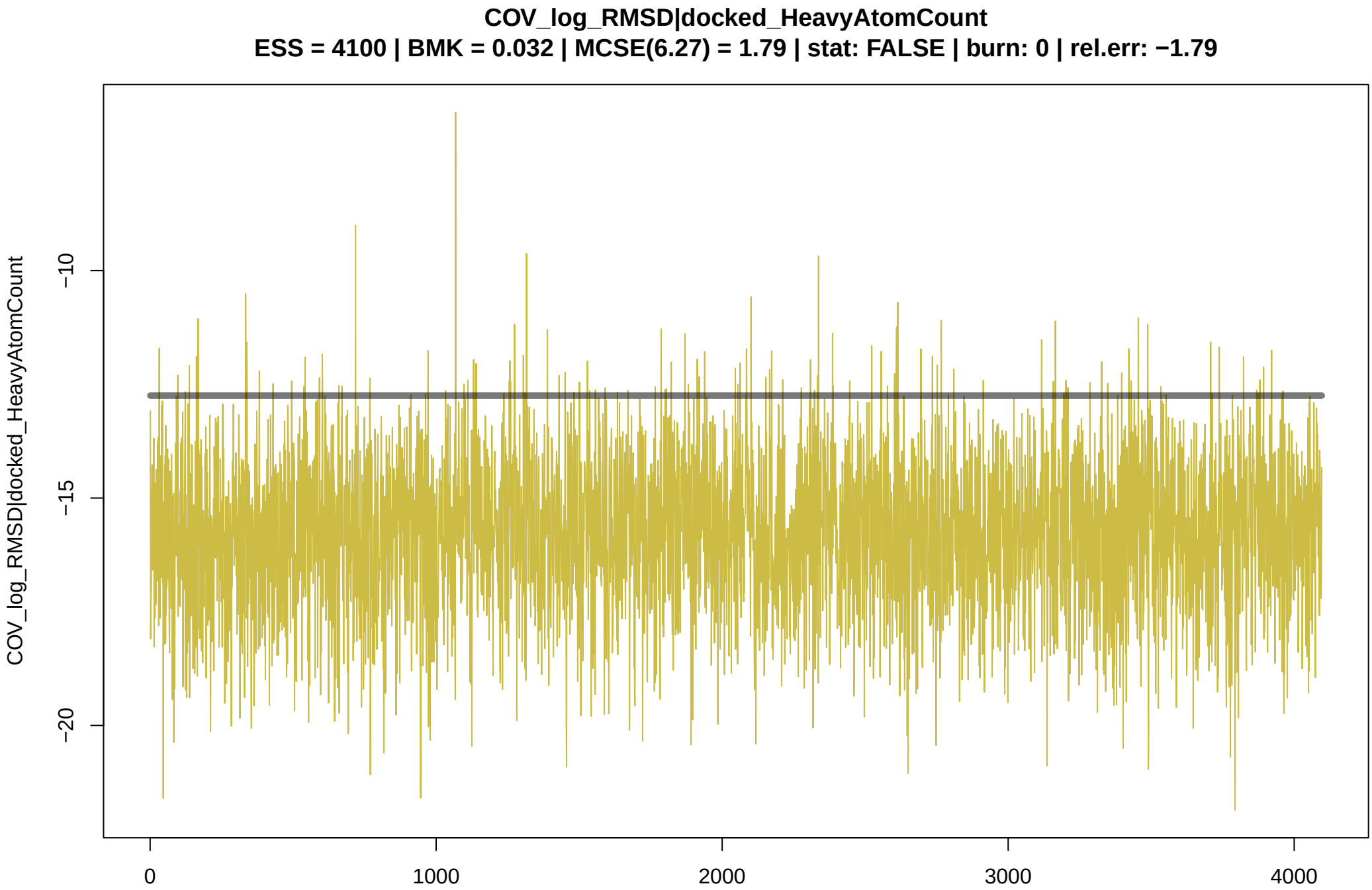

VAR_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0357 | MCSE(6.27) = 1.55 | stat: FALSE | burn: 0 | rel.err: 1.36
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
0
1000
2000
3000
4000

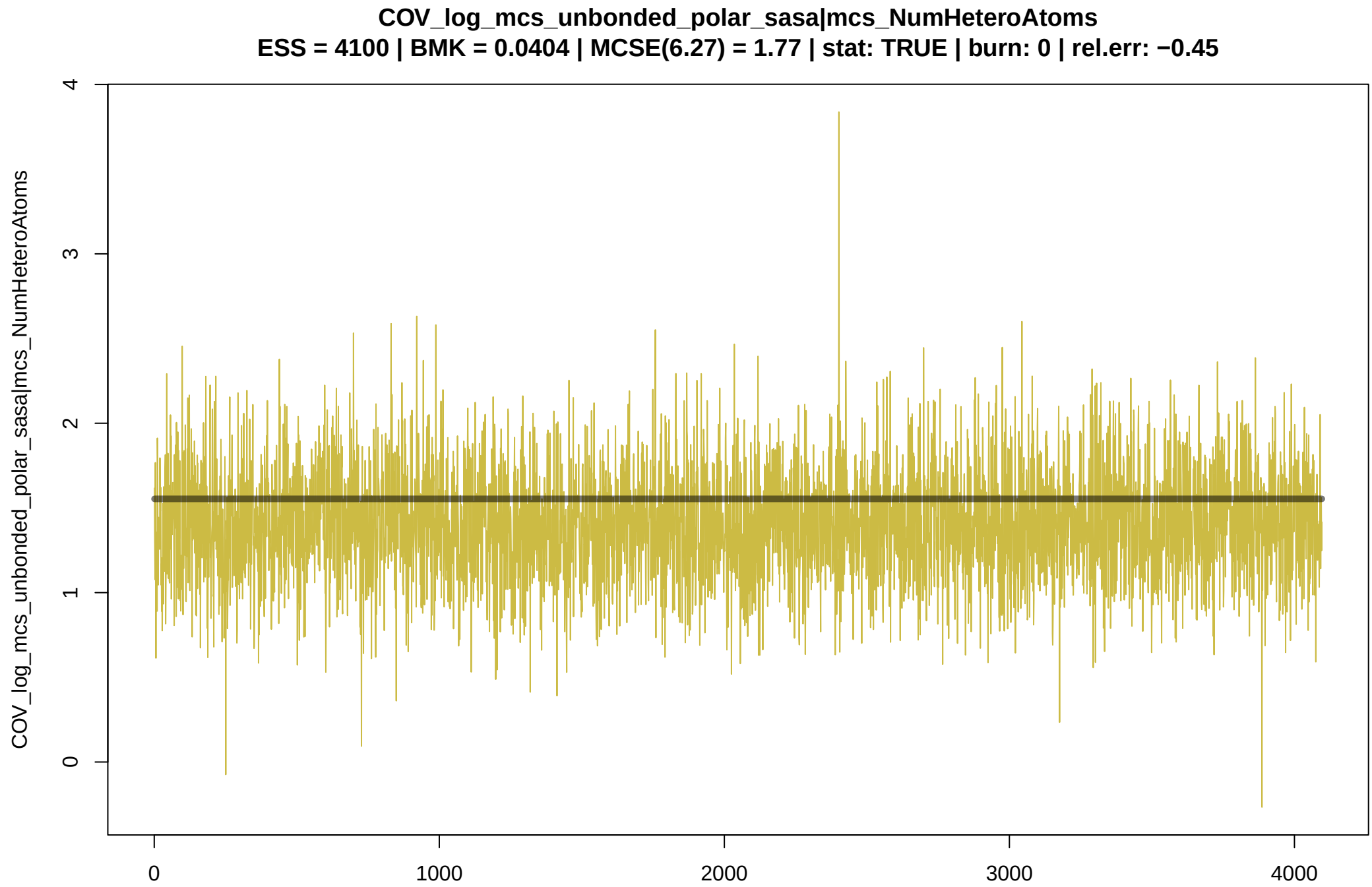

VAR_mcs_NumHeteroAtoms
ESS = 3580 | BMK = 0.0448 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.407
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
1000
2000
3000
4000

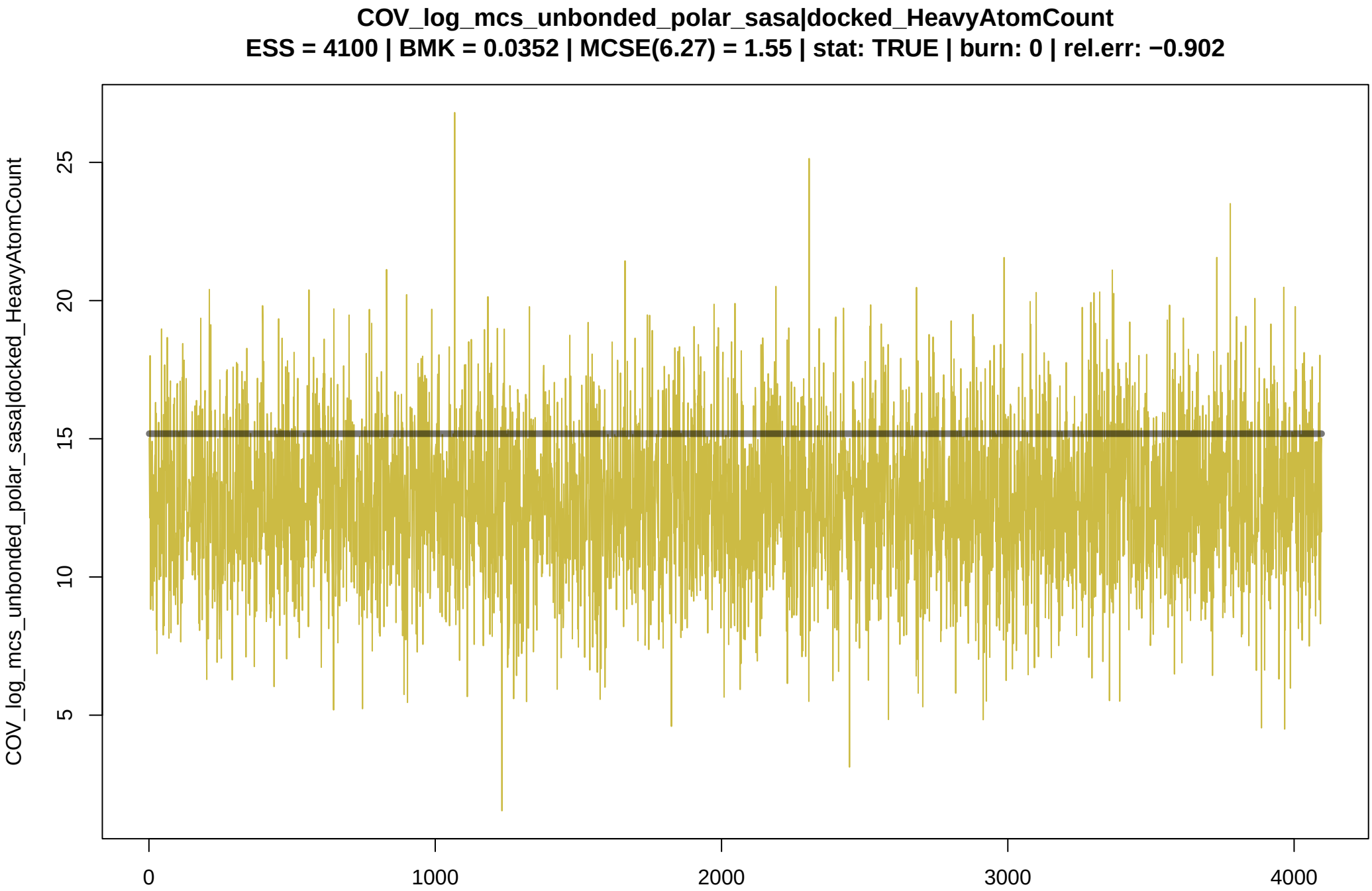

VAR_docked_HeavyAtomCount
ESS = 3750 | BMK = 0.0504 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0 | rel.err: 0.0505
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
1000
2000
3000
4000

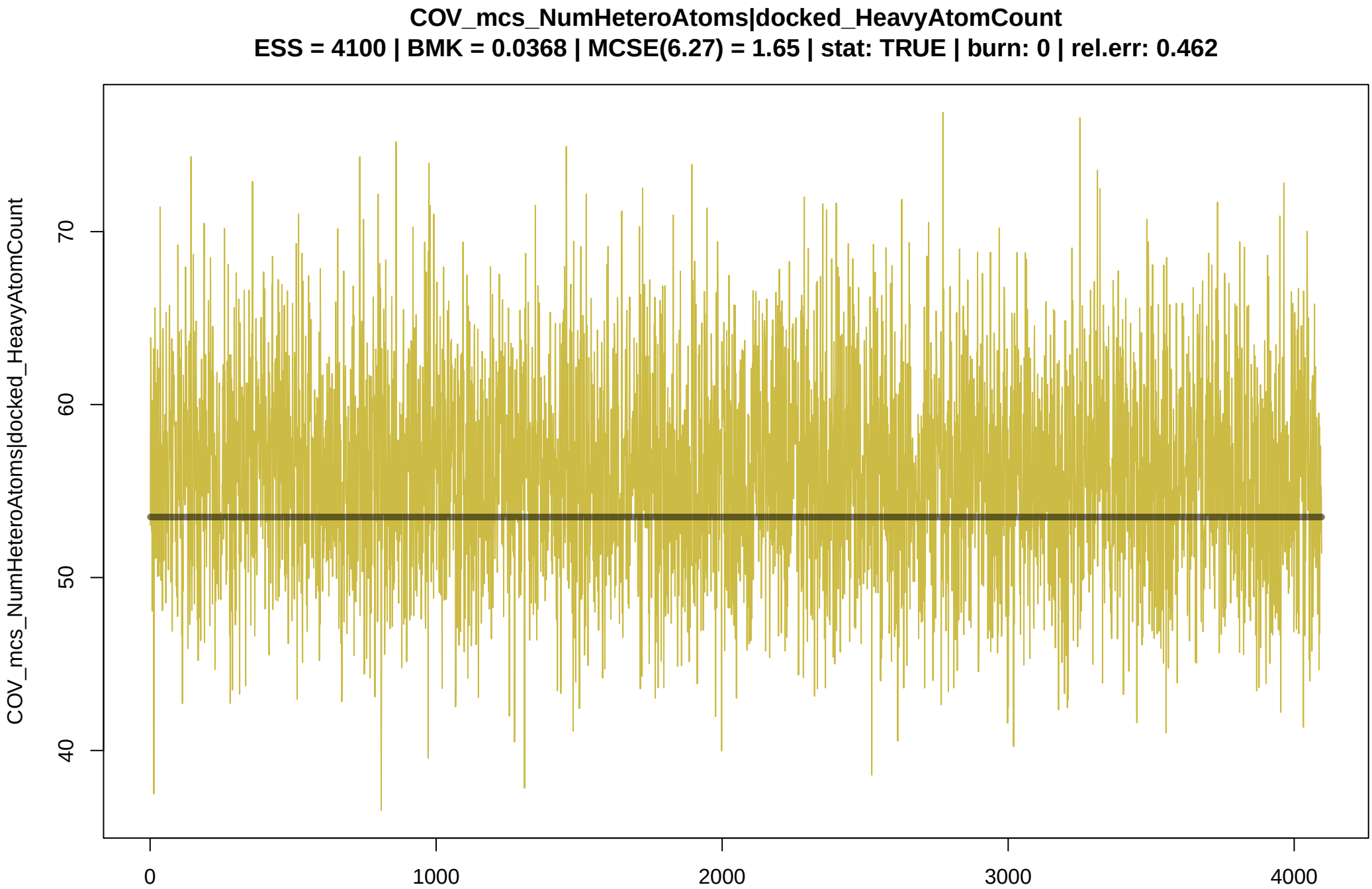

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3540 | BMK = 0.0481 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0 | rel.err: 0.456
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3970 | BMK = 0.0371 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: −1.59
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 = 0.032 | MCSE(6.27) = 1.79 | stat: FALSE | burn: 0 | rel.err: −1.79
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0404 | MCSE(6.27) = 1.77 | stat: TRUE | burn: 0 | rel.err: −0.45
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0
1
2
3
4
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0352 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: −0.902
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
25
0
1000
2000
3000
4000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0368 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: 0.462
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
1000
2000
3000
4000