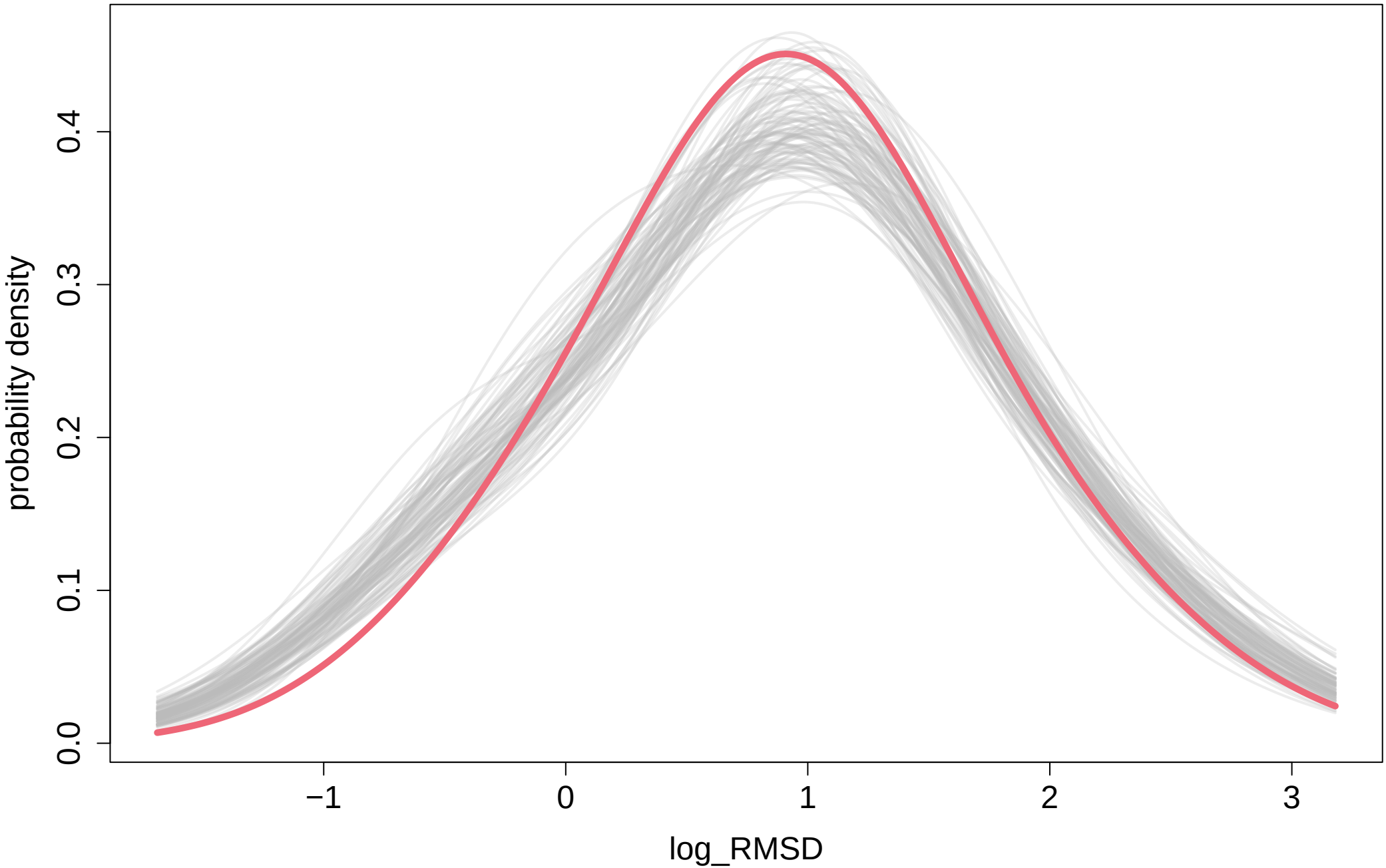
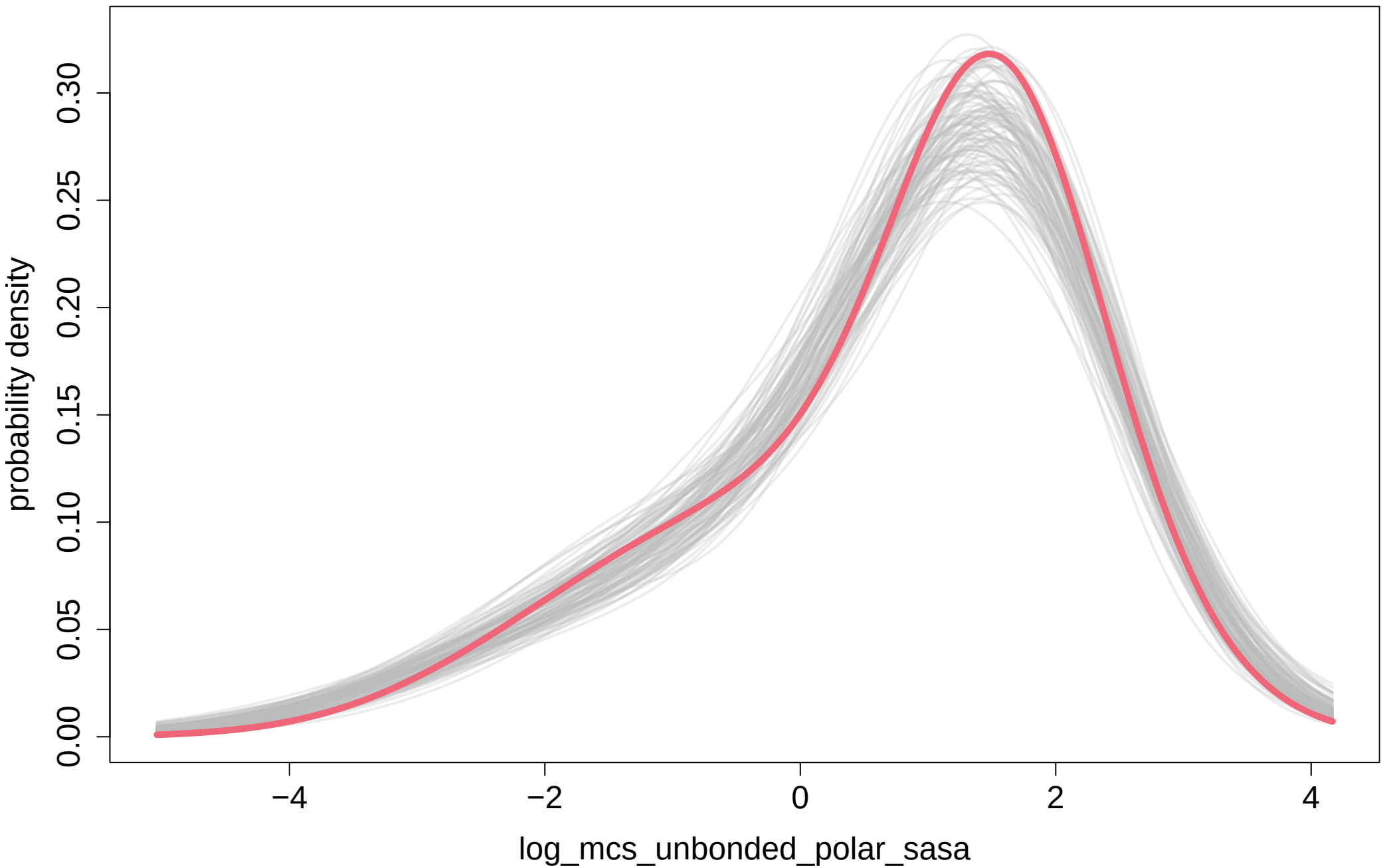
−− STATS maxD −−
min ESS = 193.071190031571
max BMK = 0.112618516388456
max MCSE = 5.76323969544954
all stationary: FALSE
burn: 0
max rel.err.: 2.00951807260667

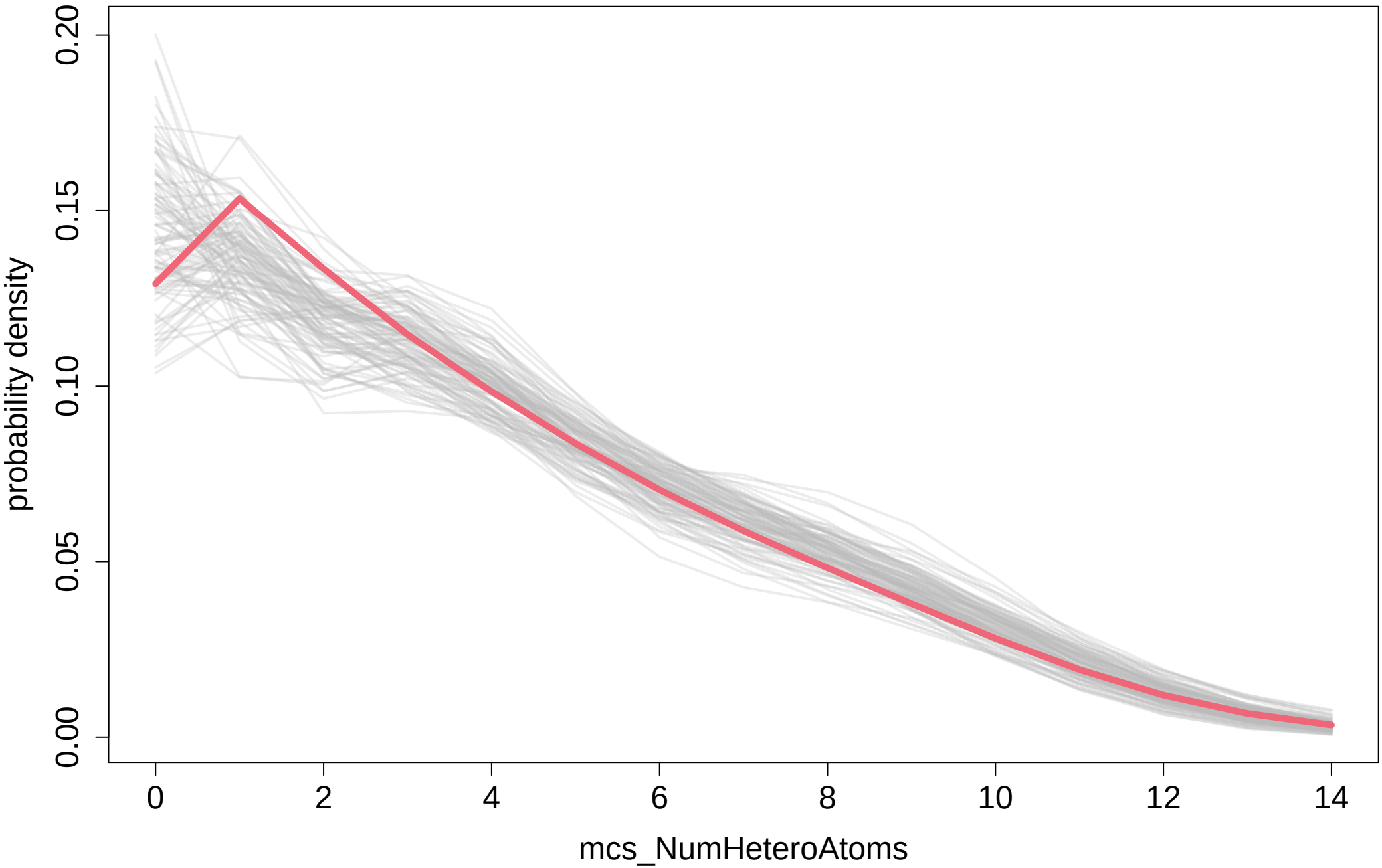
−− STATS 2D −−
min ESS = 3736.80122859402
max BMK = 0.042553772403939
max MCSE = 1.74923666173169
all stationary: TRUE
burn: 0
max rel.err.: 1.76430307818546

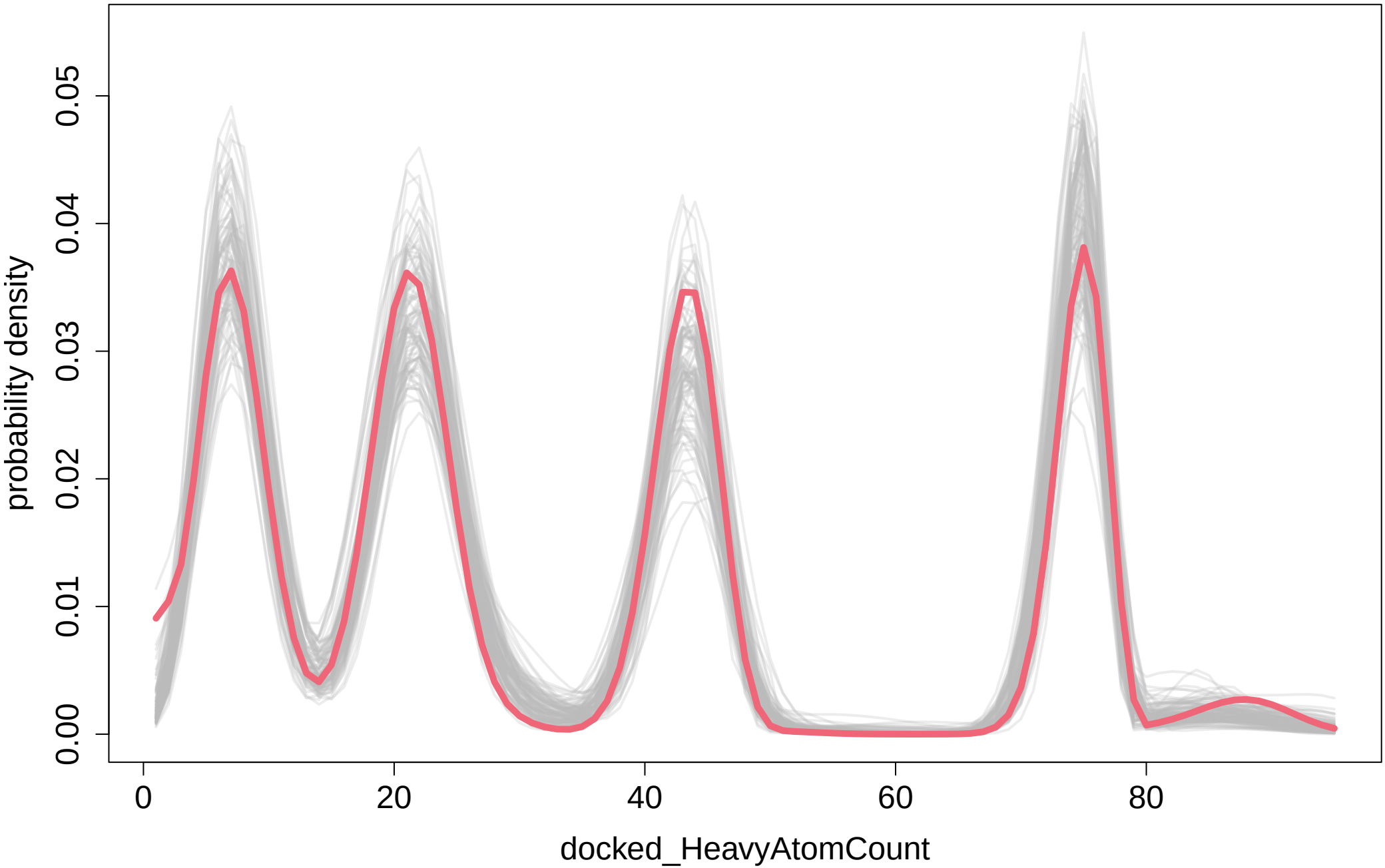
−− STATS 1D −−
min ESS = 2854.92837951306
max BMK = 0.060141879357057 3
max MCSE = 2.24781313763201
all stationary: FALSE
burn: 0
max rel.err.: 2.26275990591772

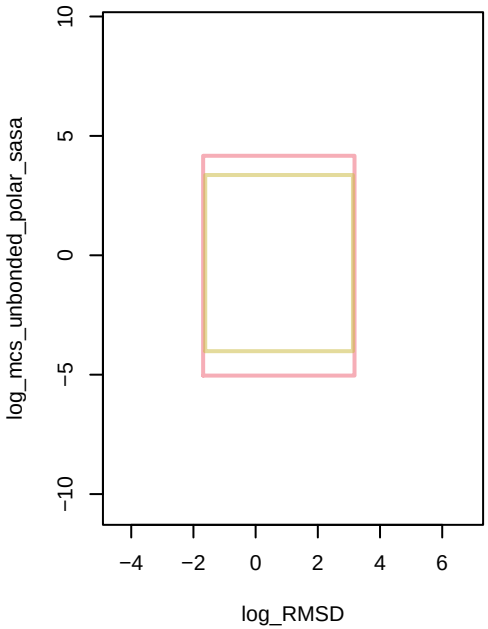
Occupied clusters: 10 of 16
LL: −2160 +− 6.61

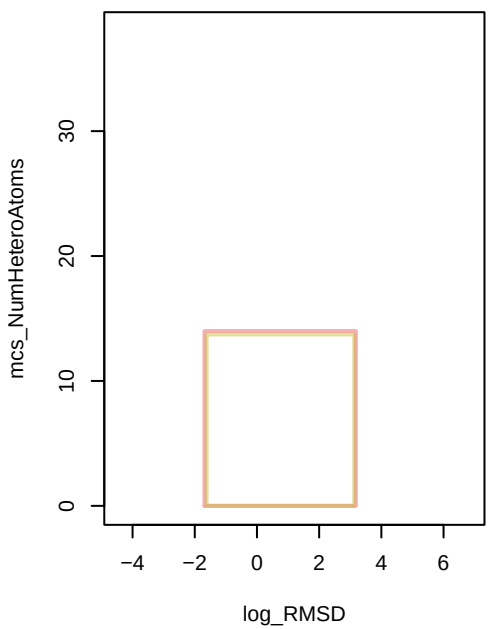

probability density
0.0
0.1
0.2
0.3
0.4
−1
0
1
2
3
log_RMSD

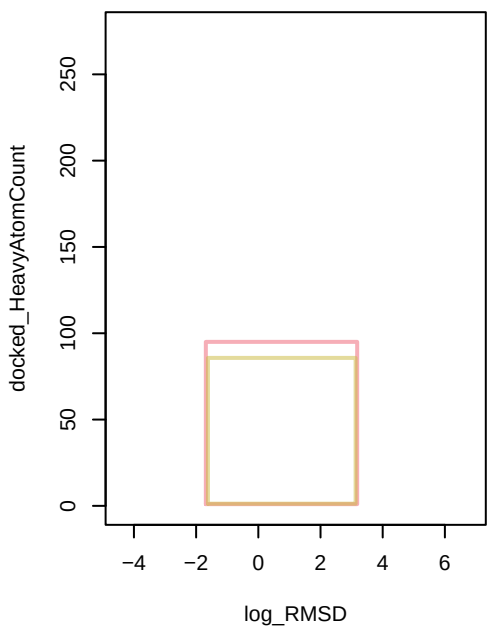

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

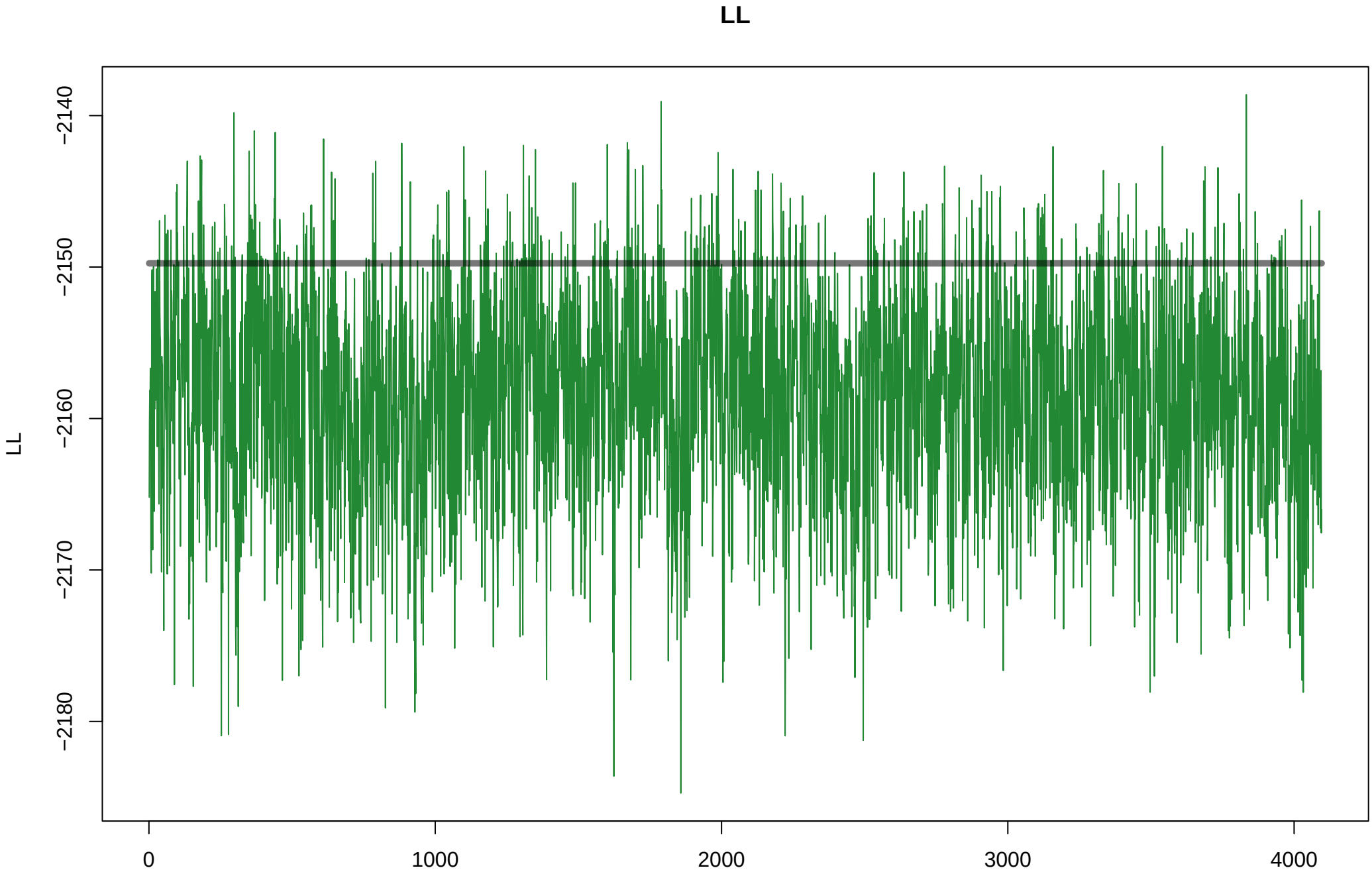

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

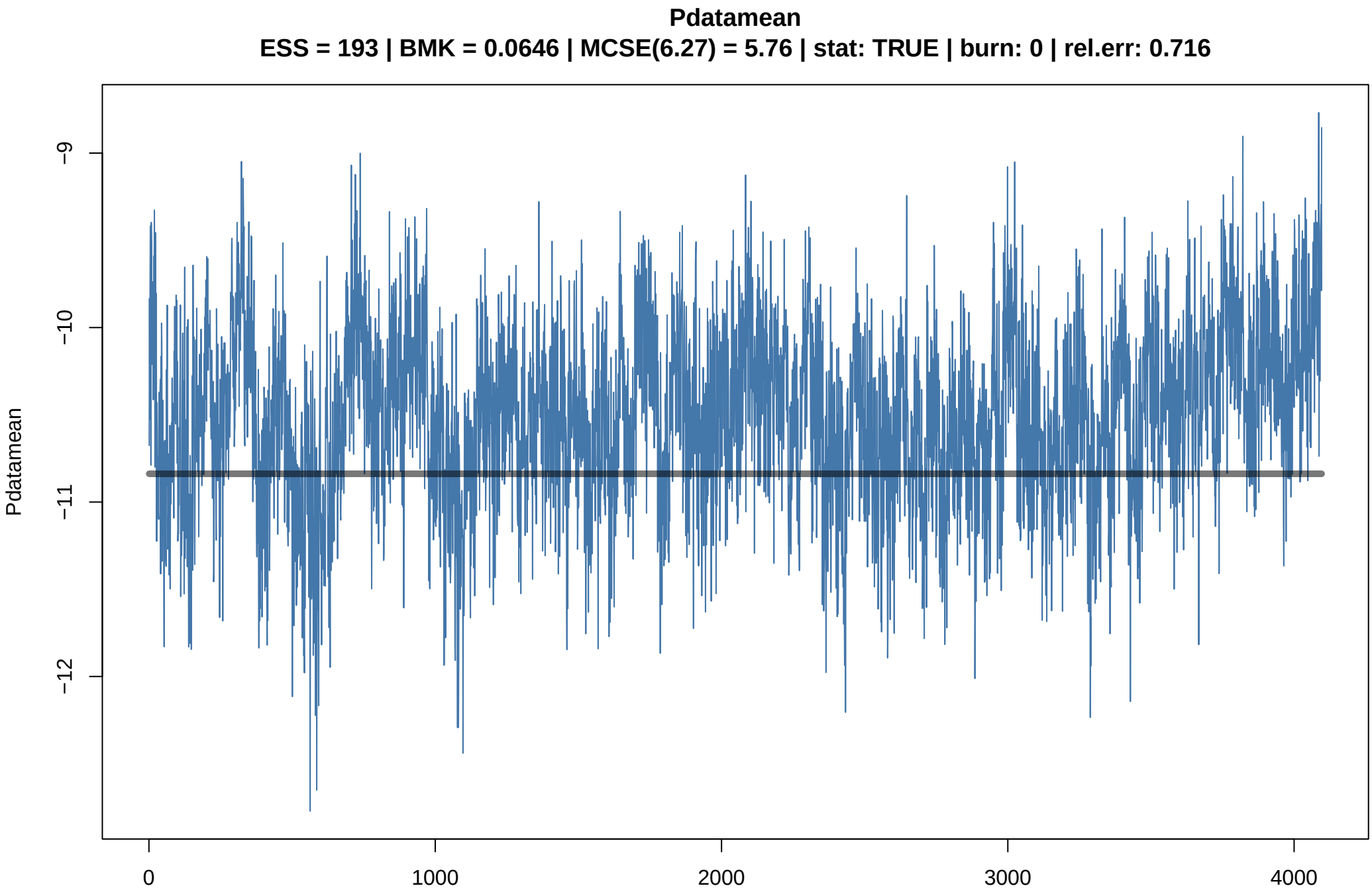

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
20
40
60
80
docked_HeavyAtomCount

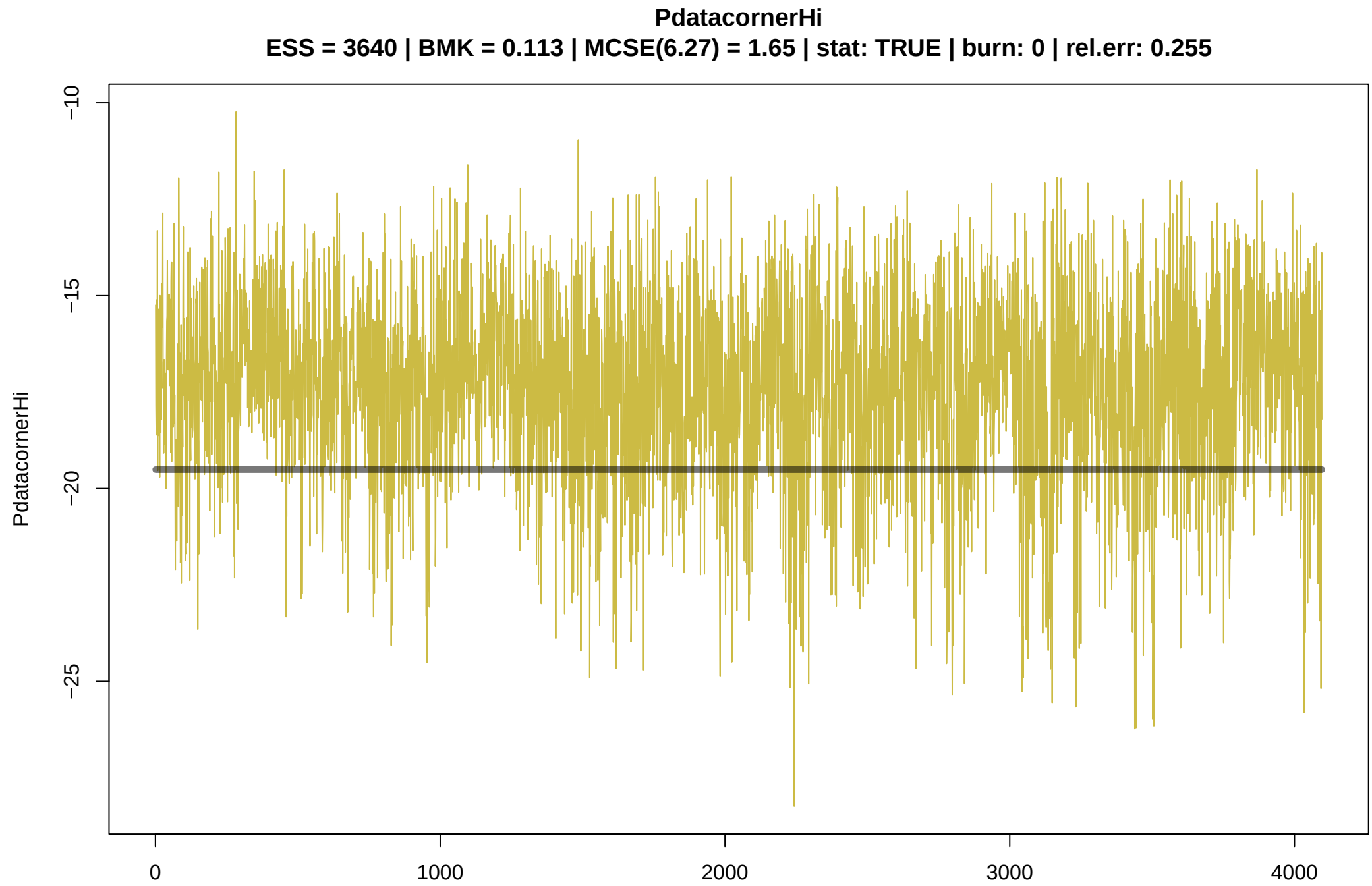

log_mcs_unbonded_polar_sasa
10
5
0
−5
−10
−4
−2
0
2
4
6
log_RMSD

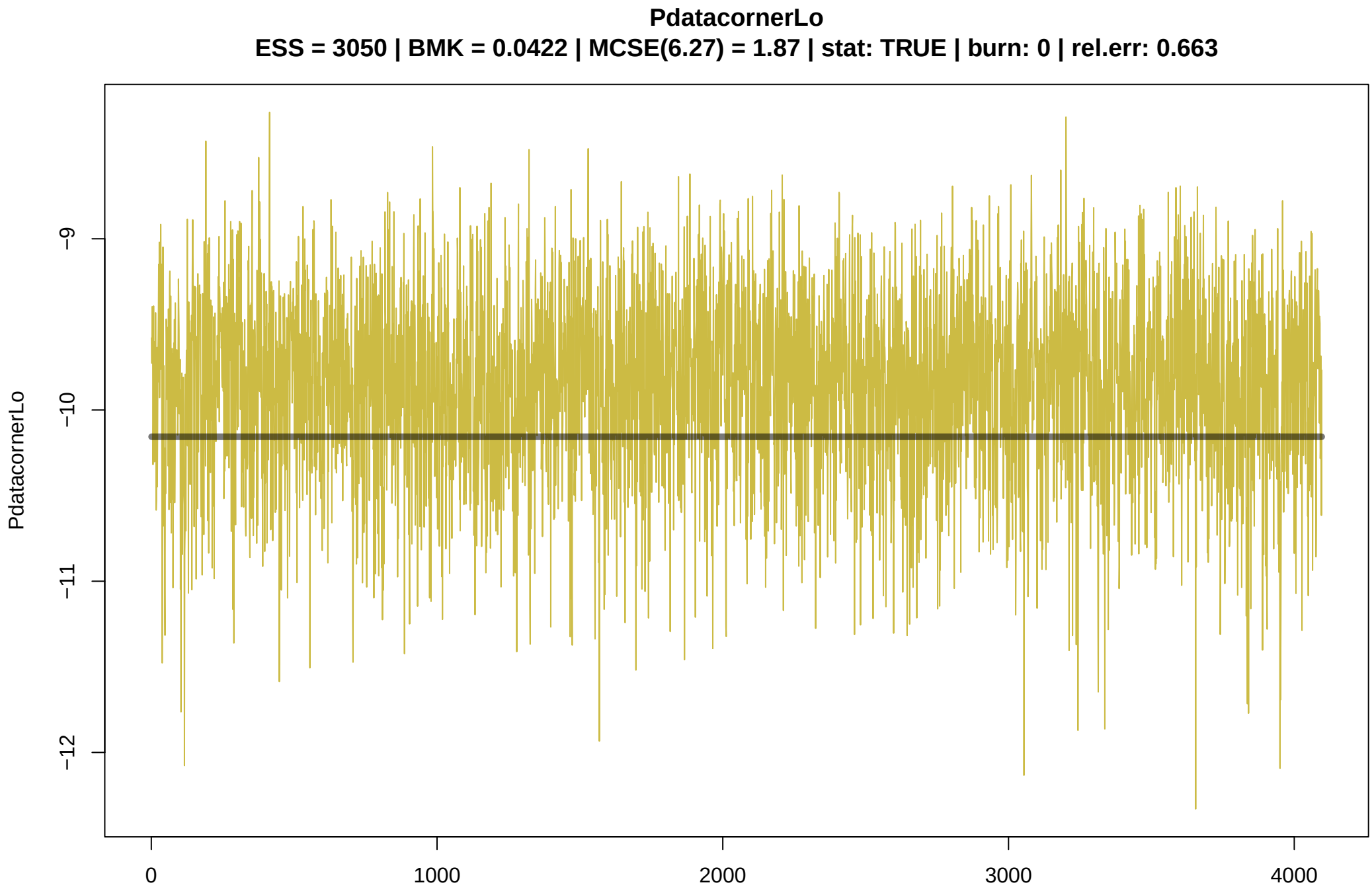

mcs_NumHeteroAtoms
30
20
10
0
−4
−2
0
2
4
6
log_RMSD

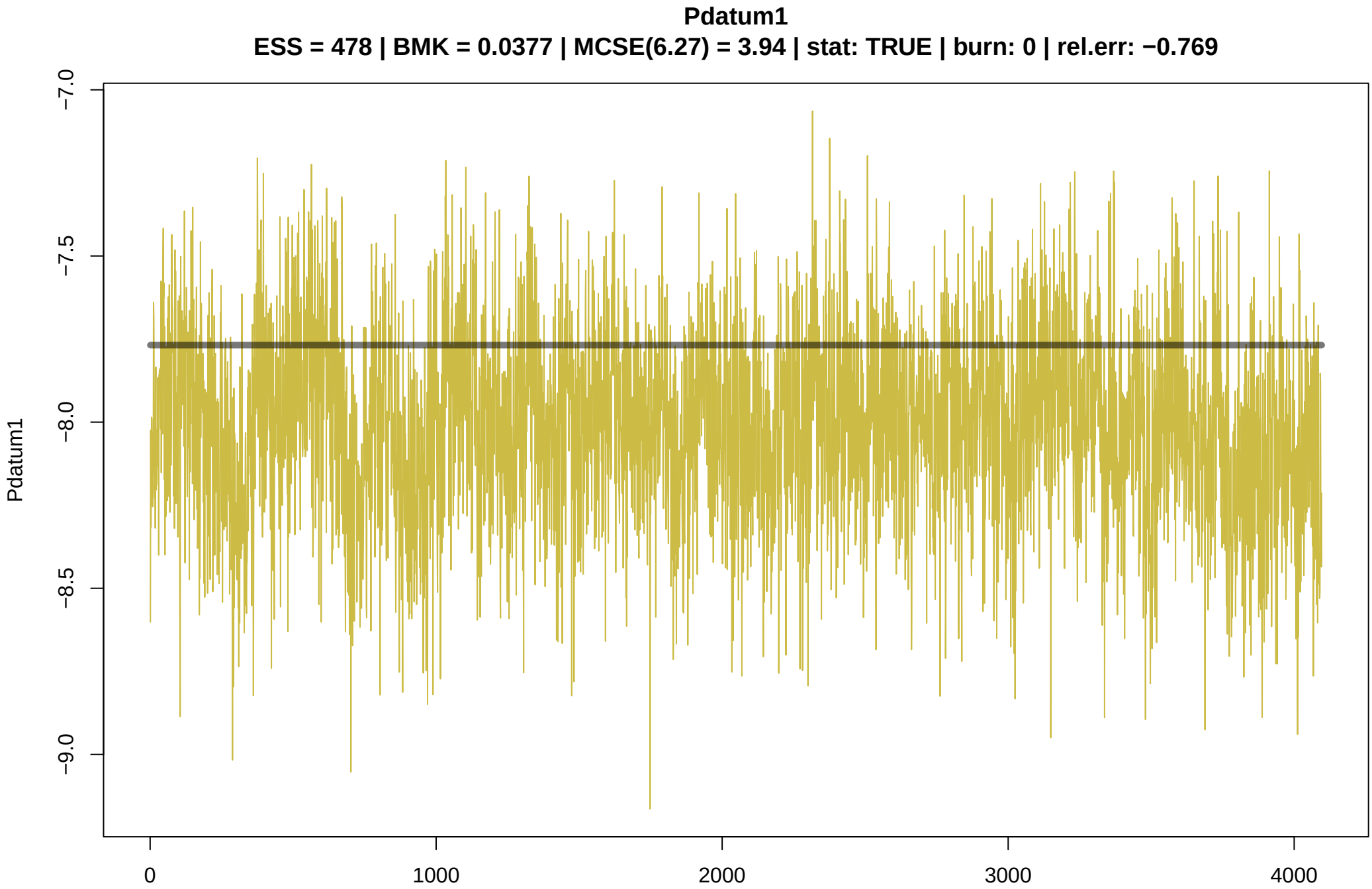

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

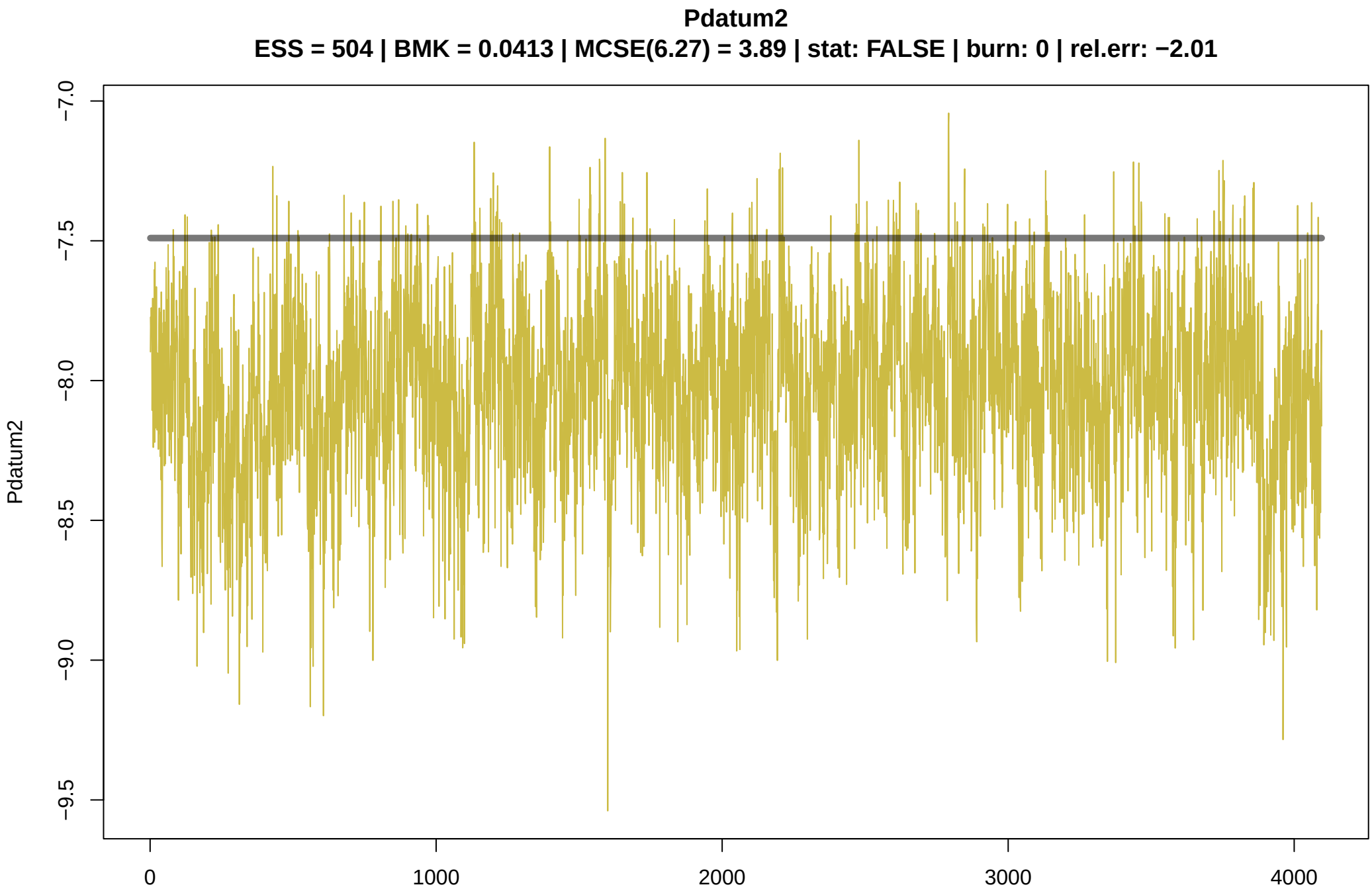

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

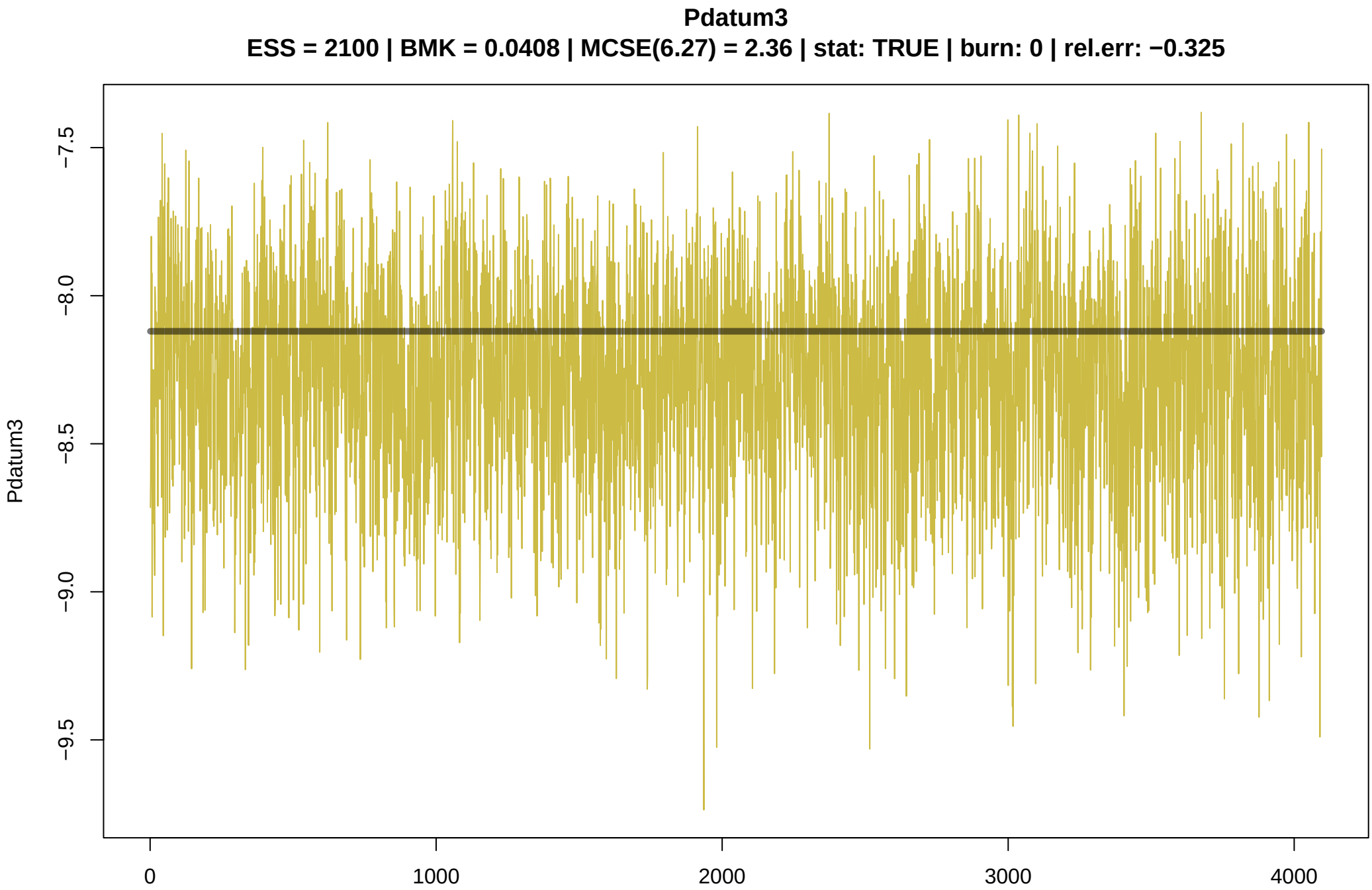

Pdatamean
ESS = 193 | BMK = 0.0646 | MCSE(6.27) = 5.76 | stat: TRUE | burn: 0 | rel.err: 0.716
Pdatamean
−9
−10
−11
−12
0
1000
2000
3000
4000

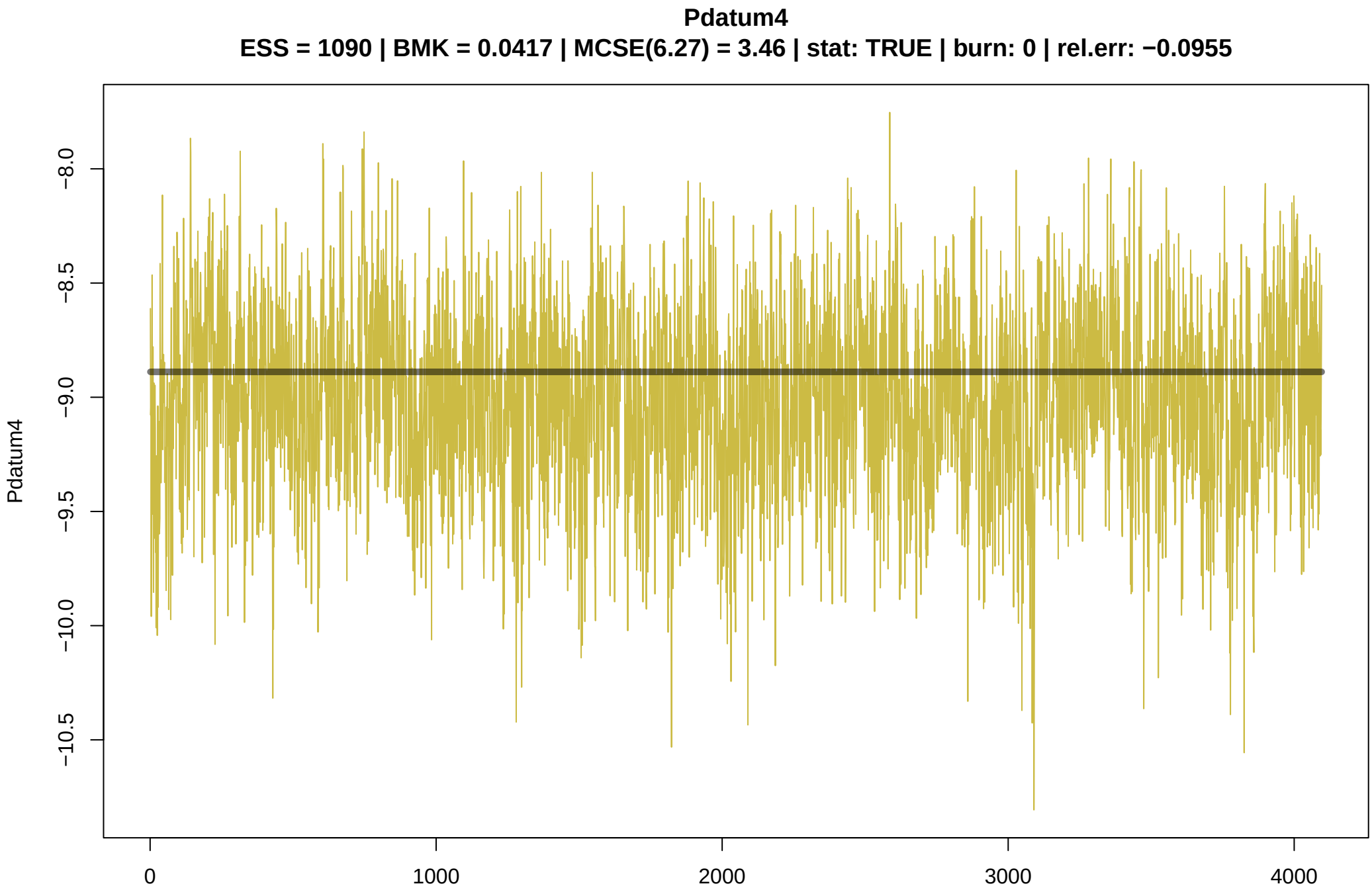

PdatacornerHi
ESS = 3640 | BMK = 0.113 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: 0.255
PdatacornerHi
−10
−15
−20
−25
0
1000
2000
3000
4000

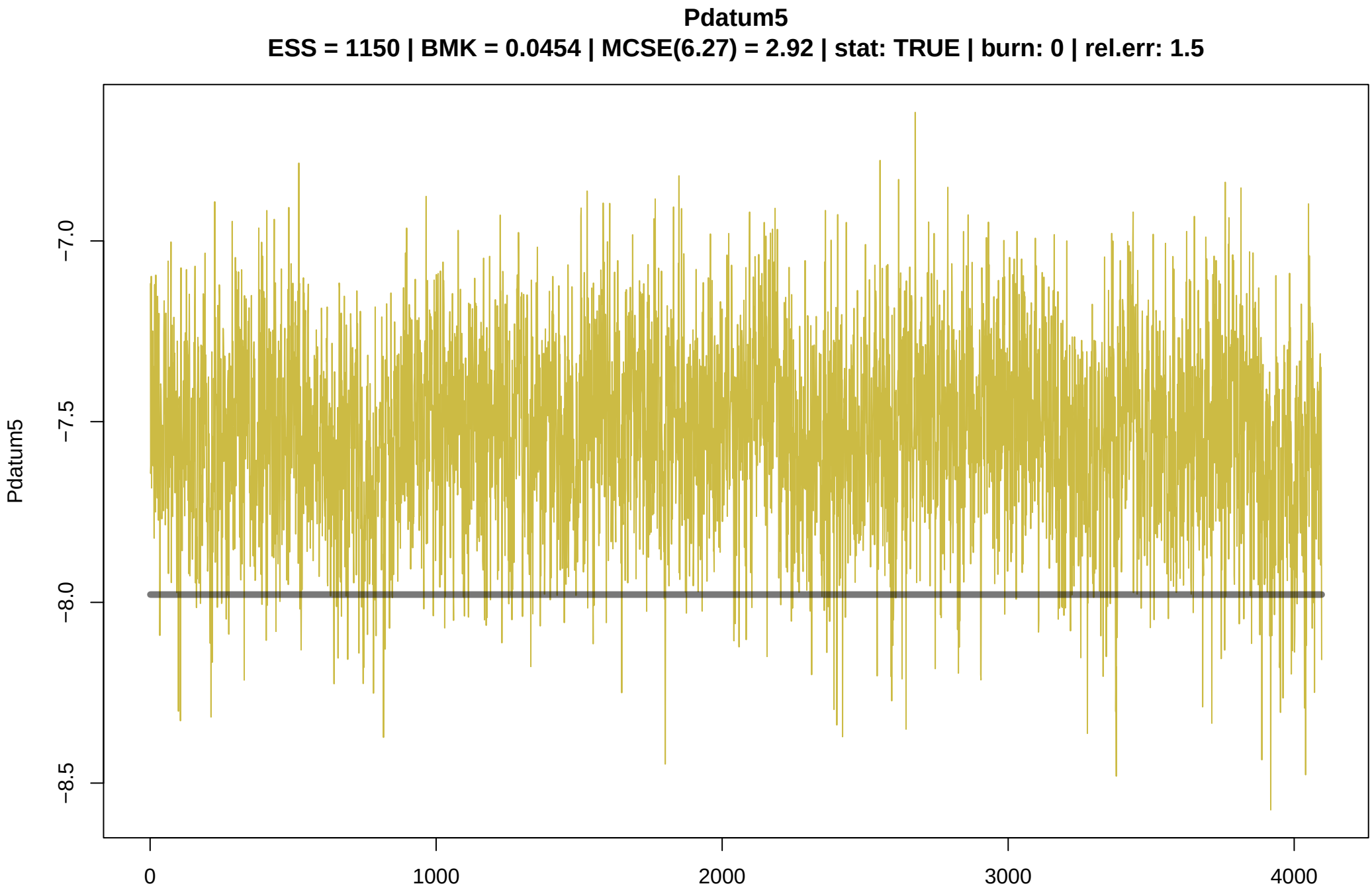

PdatacornerLo
ESS = 3050 | BMK = 0.0422 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0 | rel.err: 0.663
PdatacornerLo
−9
−10
−11
−12
0
1000
2000
3000
4000

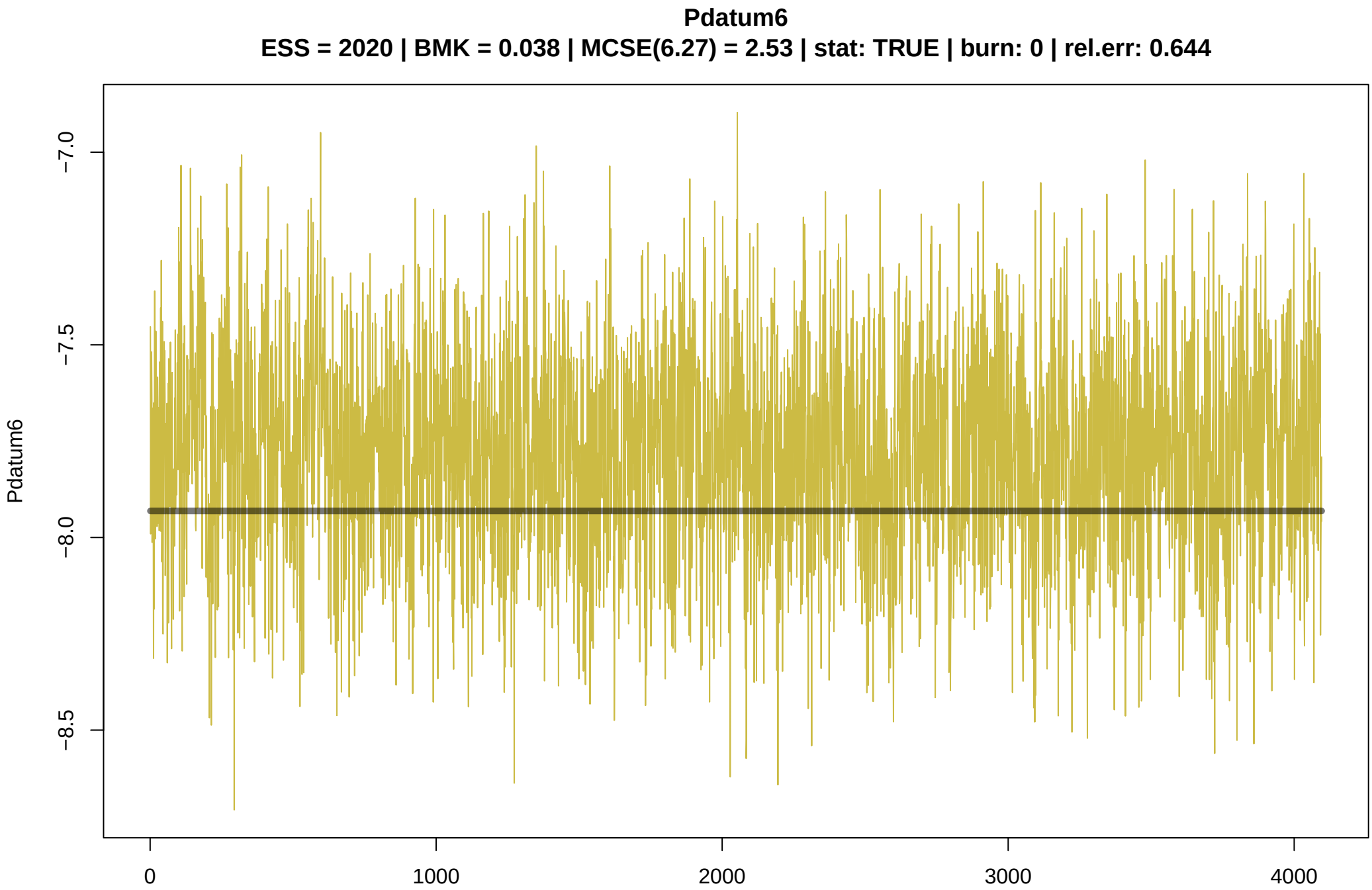

Pdatum1
ESS = 478 | BMK = 0.0377 | MCSE(6.27) = 3.94 | stat: TRUE | burn: 0 | rel.err: −0.769
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

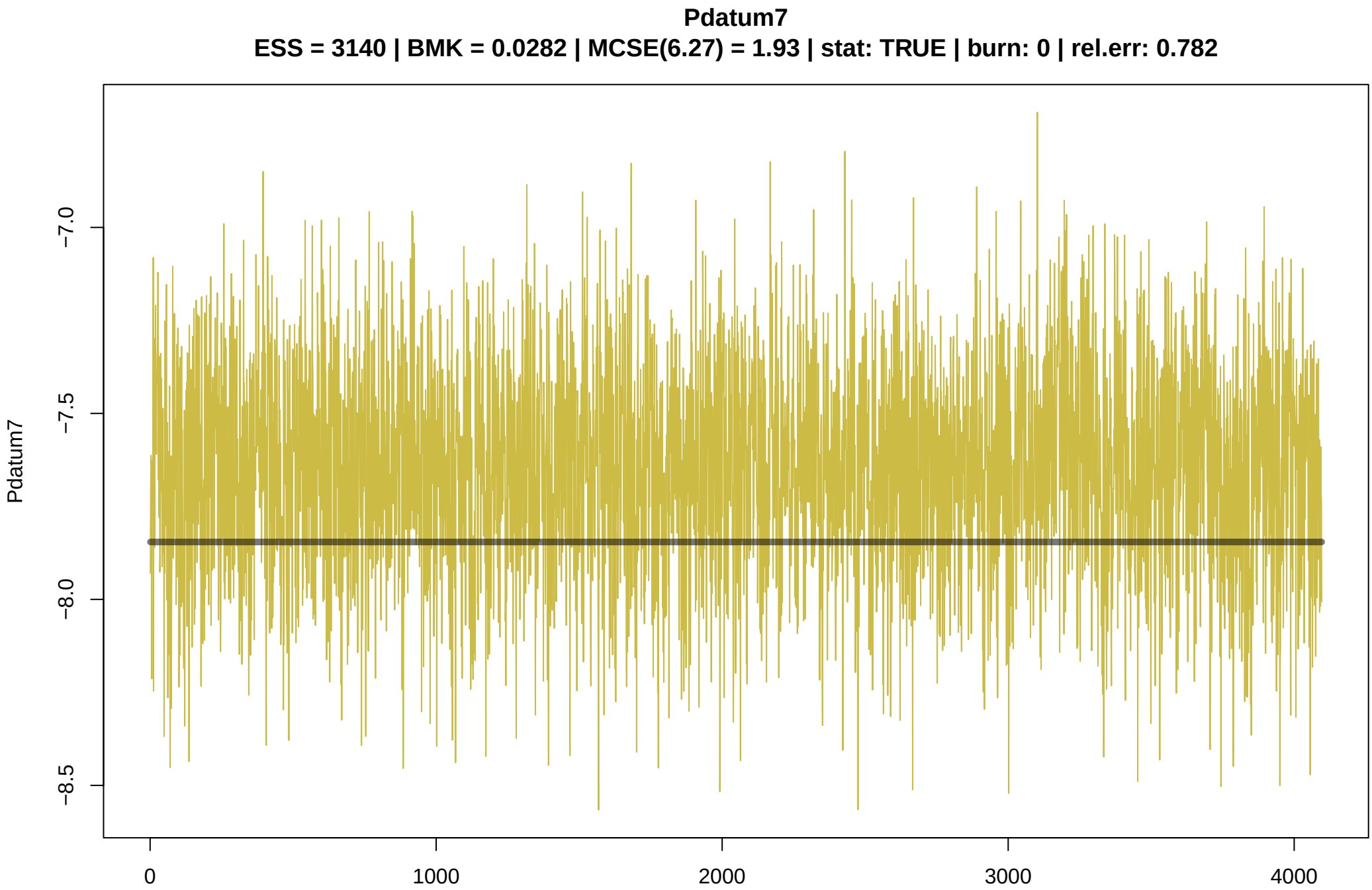

Pdatum2
ESS = 504 | BMK = 0.0413 | MCSE(6.27) = 3.89 | stat: FALSE | burn: 0 | rel.err: −2.01
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

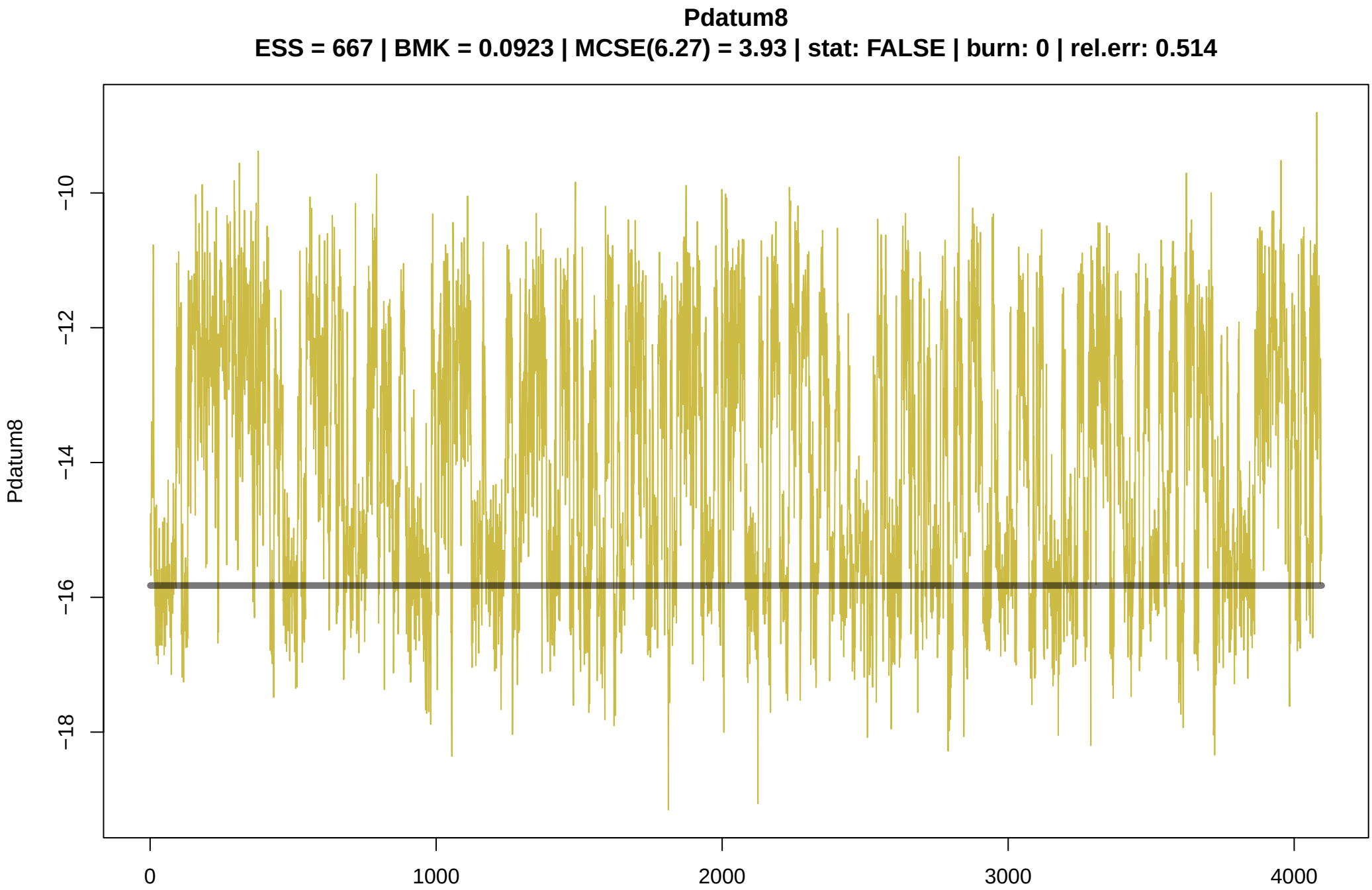

Pdatum3
ESS = 2100 | BMK = 0.0408 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0 | rel.err: −0.325
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

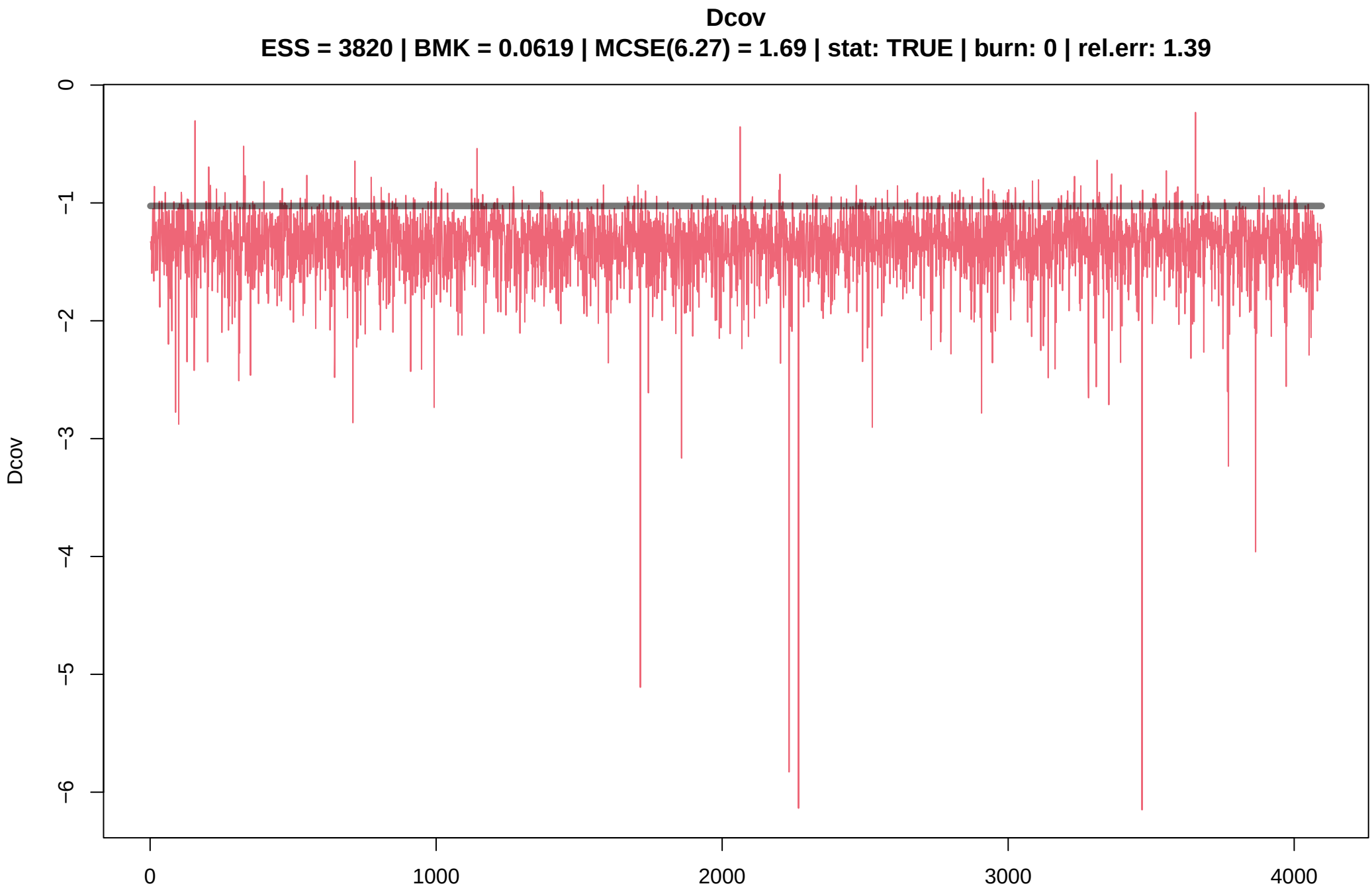

Pdatum4
ESS = 1090 | BMK = 0.0417 | MCSE(6.27) = 3.46 | stat: TRUE | burn: 0 | rel.err: −0.0955
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

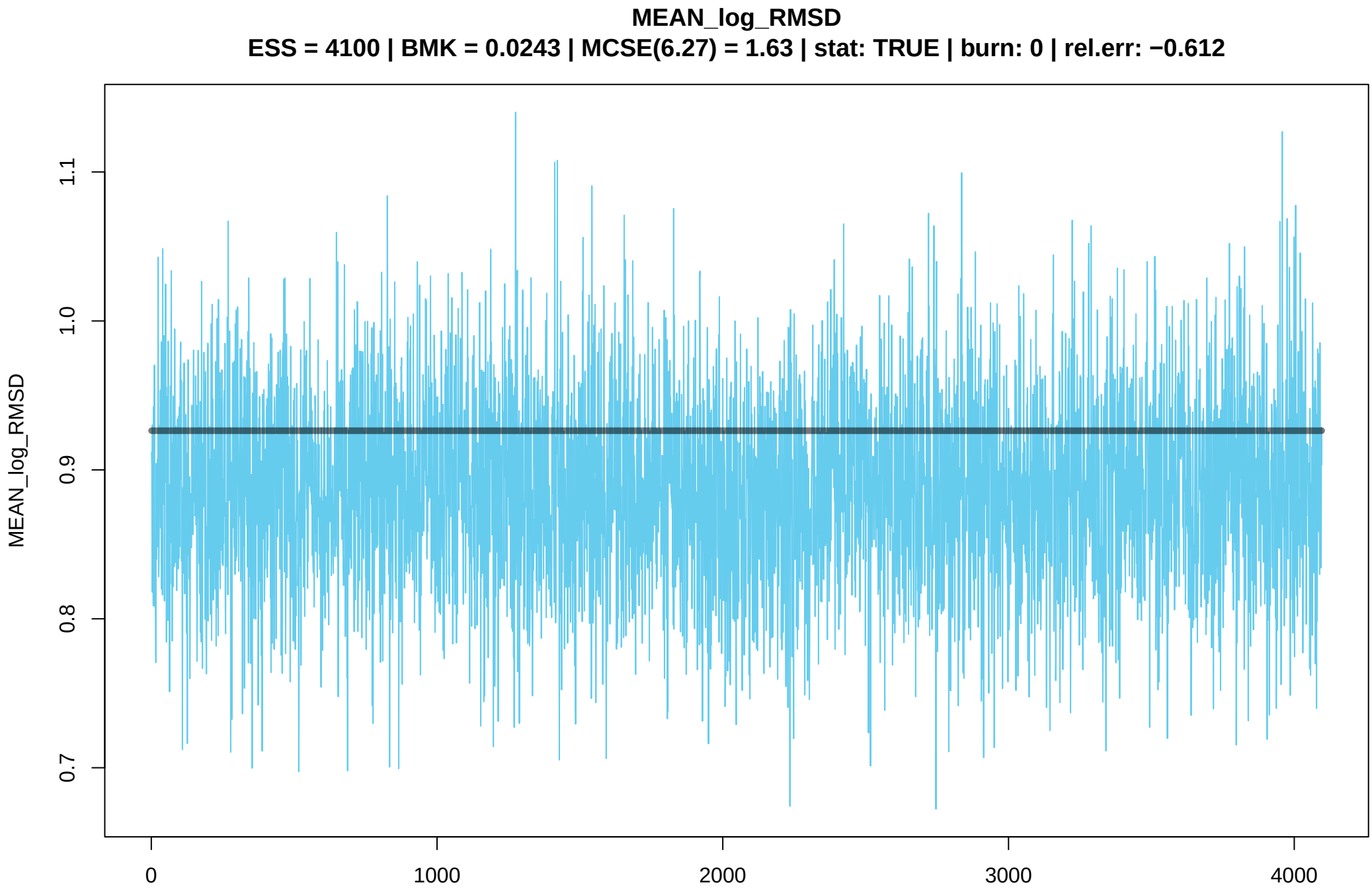

Pdatum5
ESS = 1150 | BMK = 0.0454 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | rel.err: 1.5
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

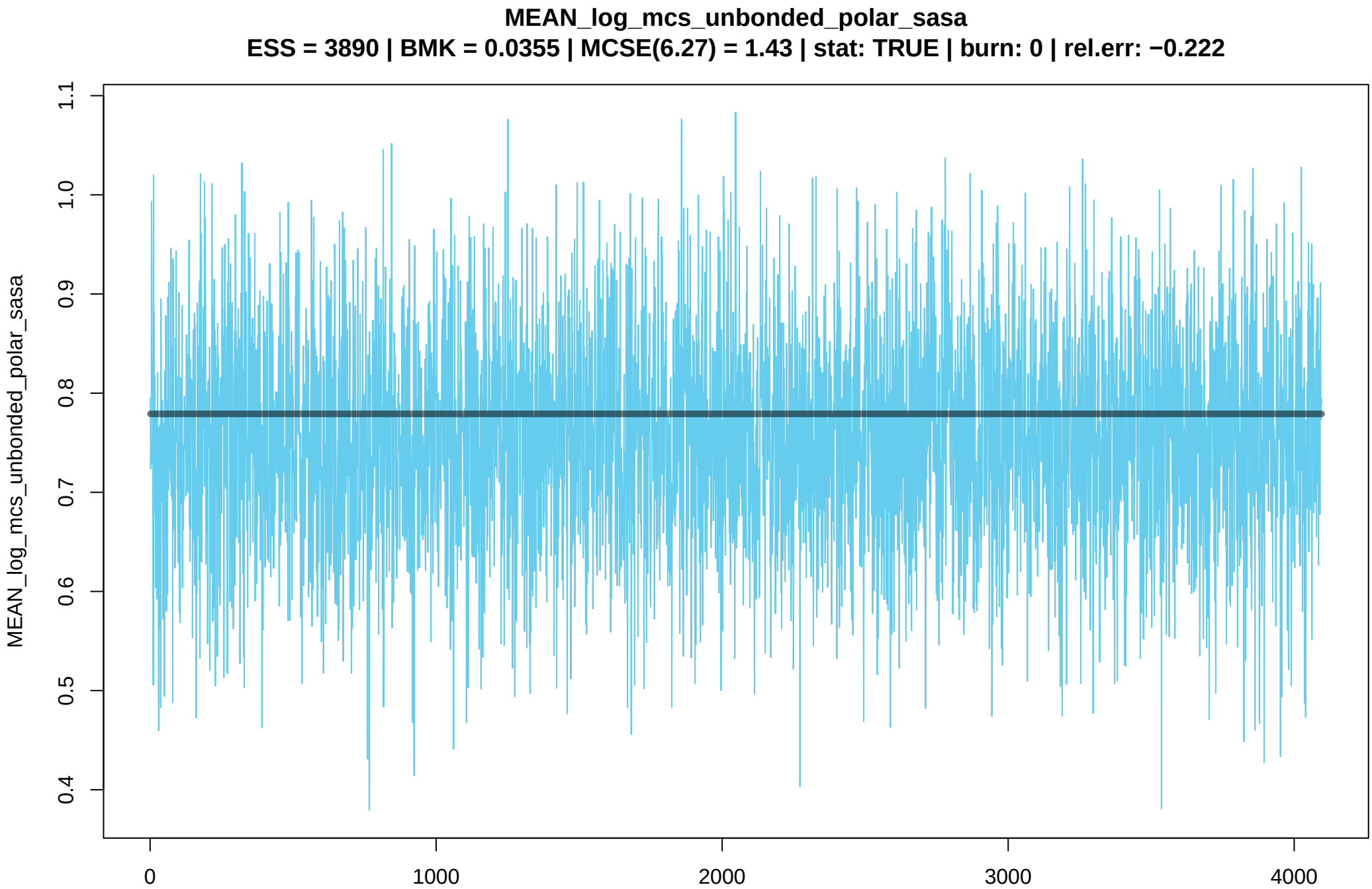

Pdatum6
ESS = 2020 | BMK = 0.038 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: 0.644
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

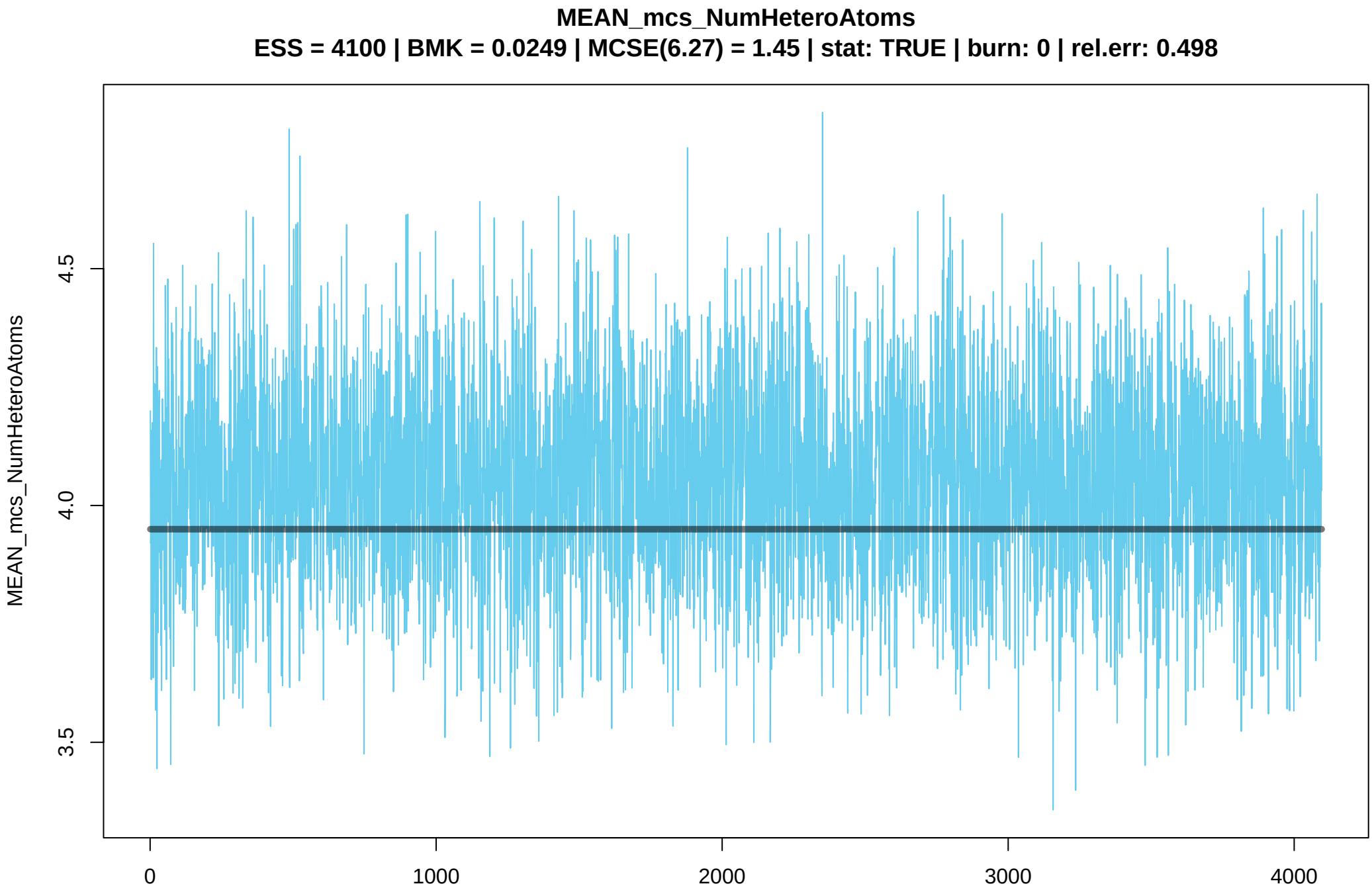

Pdatum7
ESS = 3140 | BMK = 0.0282 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: 0.782
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

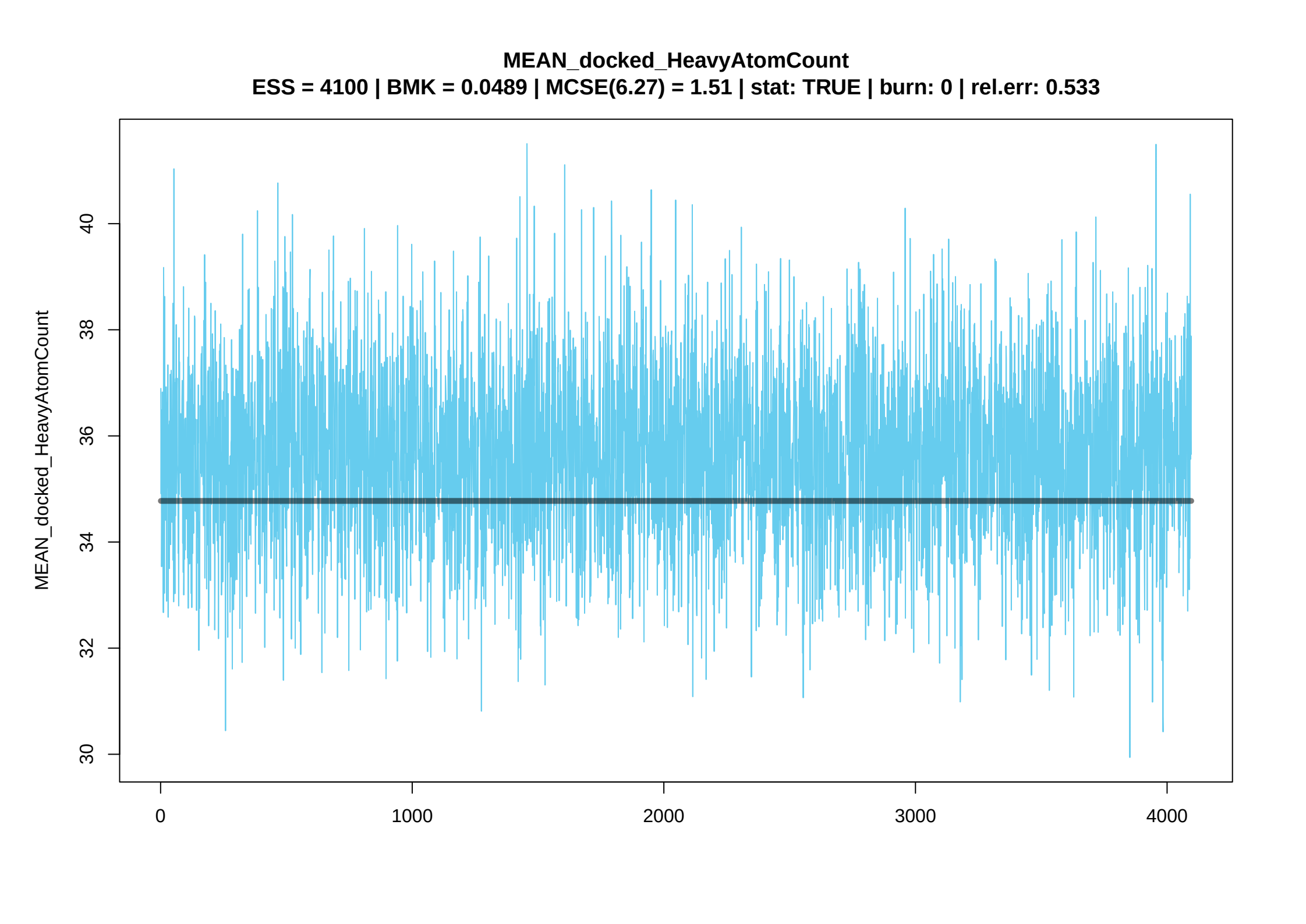

Pdatum8
ESS = 667 | BMK = 0.0923 | MCSE(6.27) = 3.93 | stat: FALSE | burn: 0 | rel.err: 0.514
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

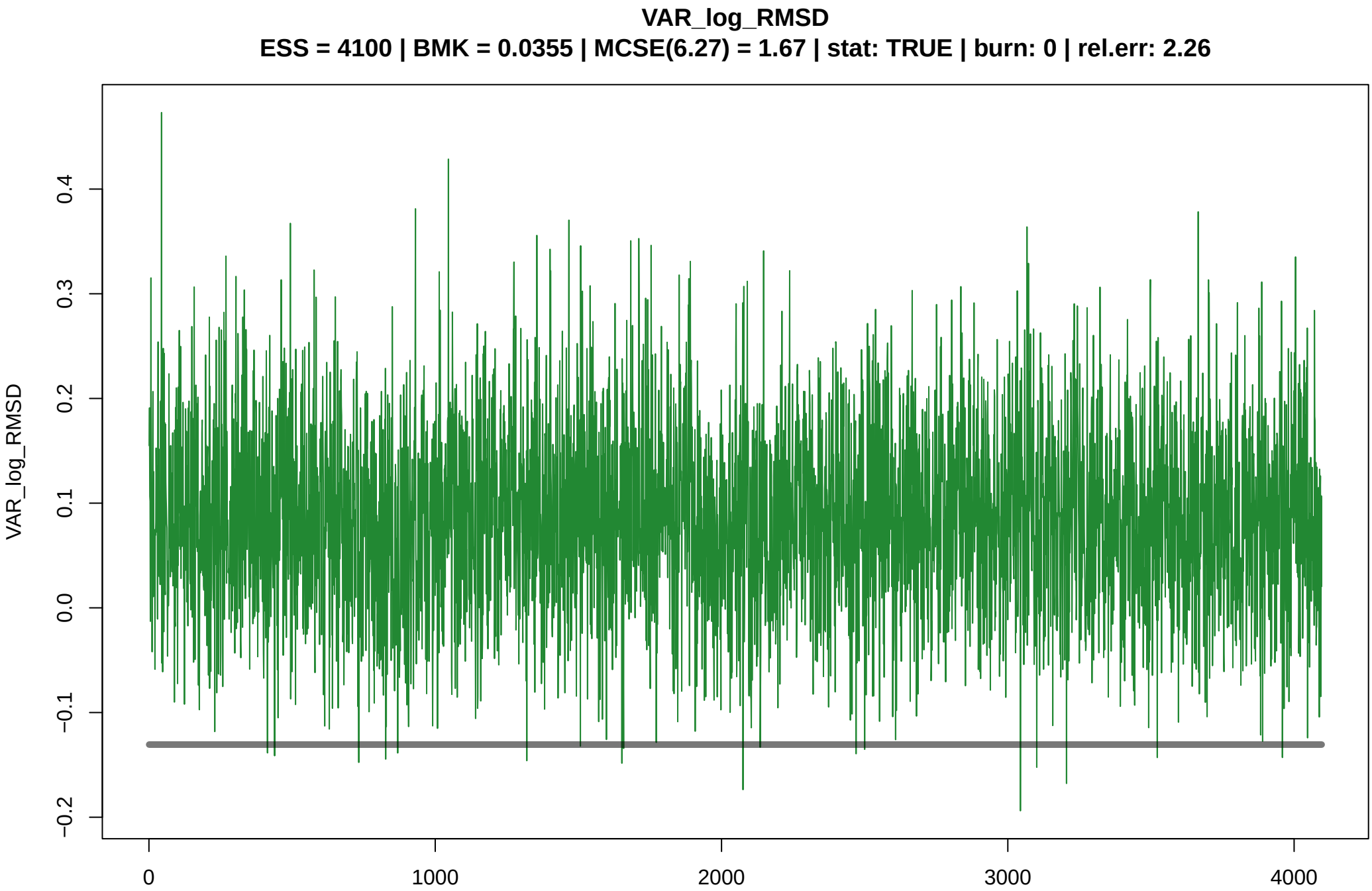

Dcov
ESS = 3820 | BMK = 0.0619 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 1.39
Dcov
0
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

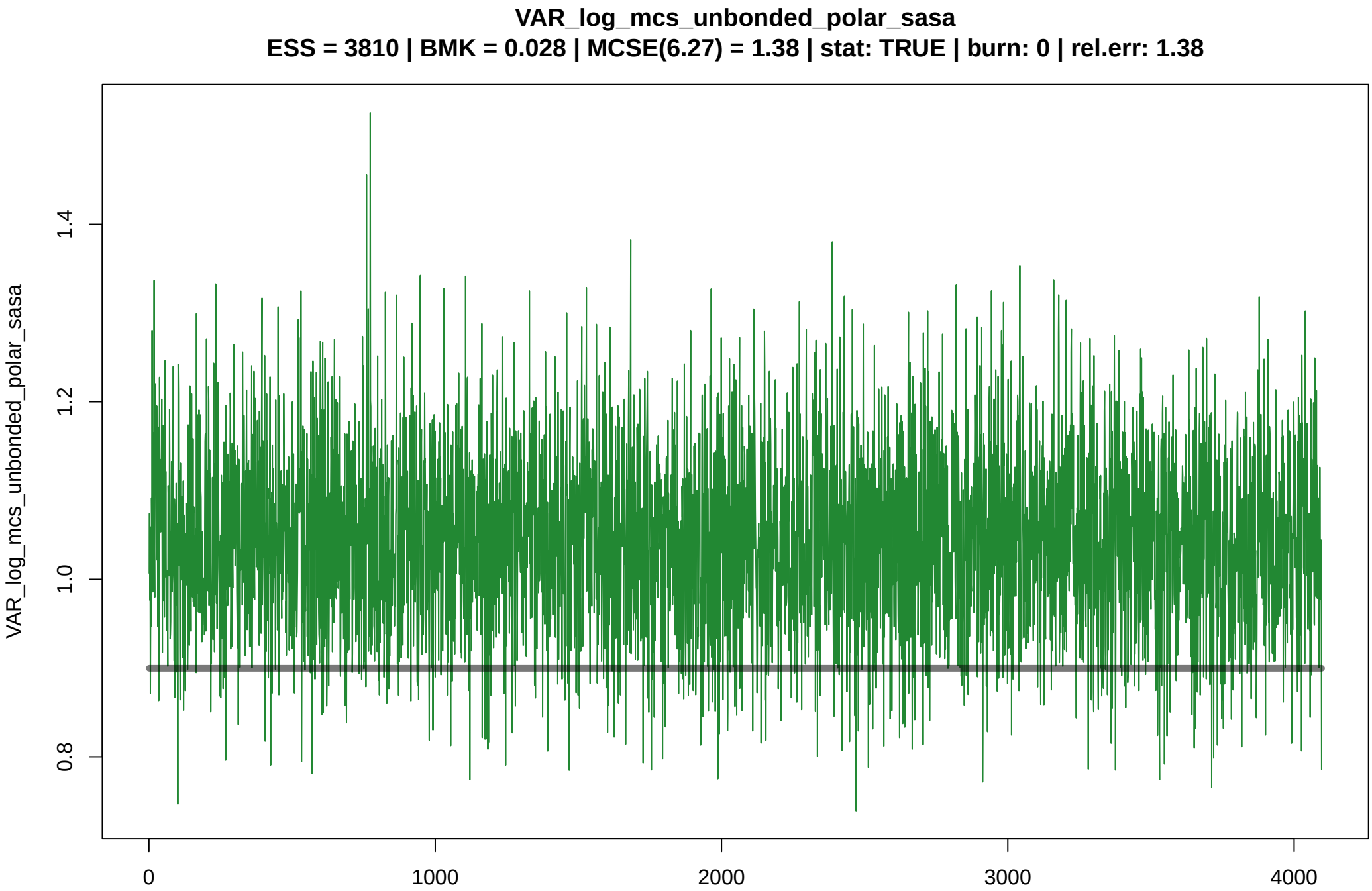

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0243 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: −0.612
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

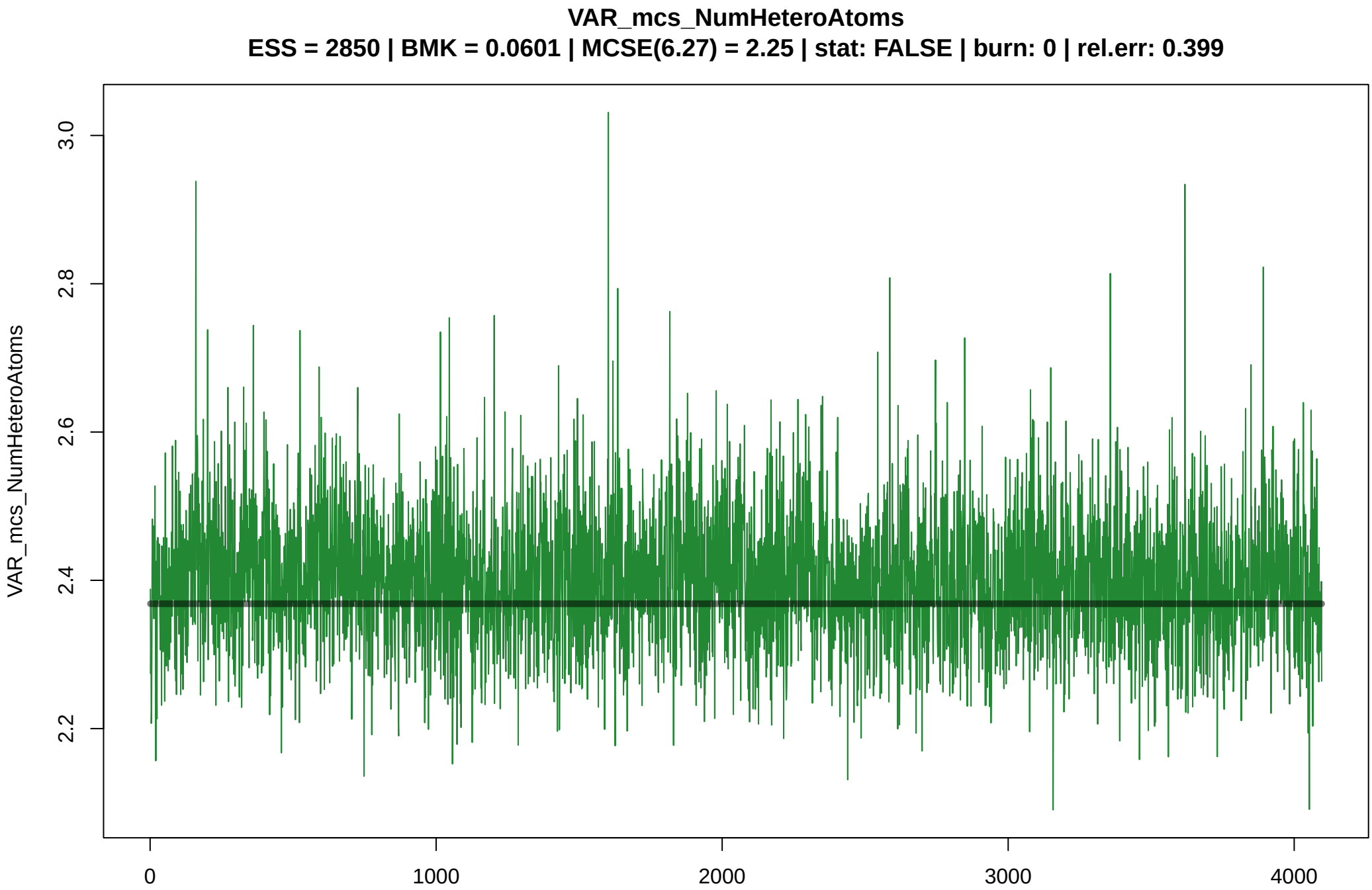

MEAN_log_mcs_unbonded_polar_sasa
ESS = 3890 | BMK = 0.0355 | MCSE(6.27) = 1.43 | stat: TRUE | burn: 0 | rel.err: −0.222
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

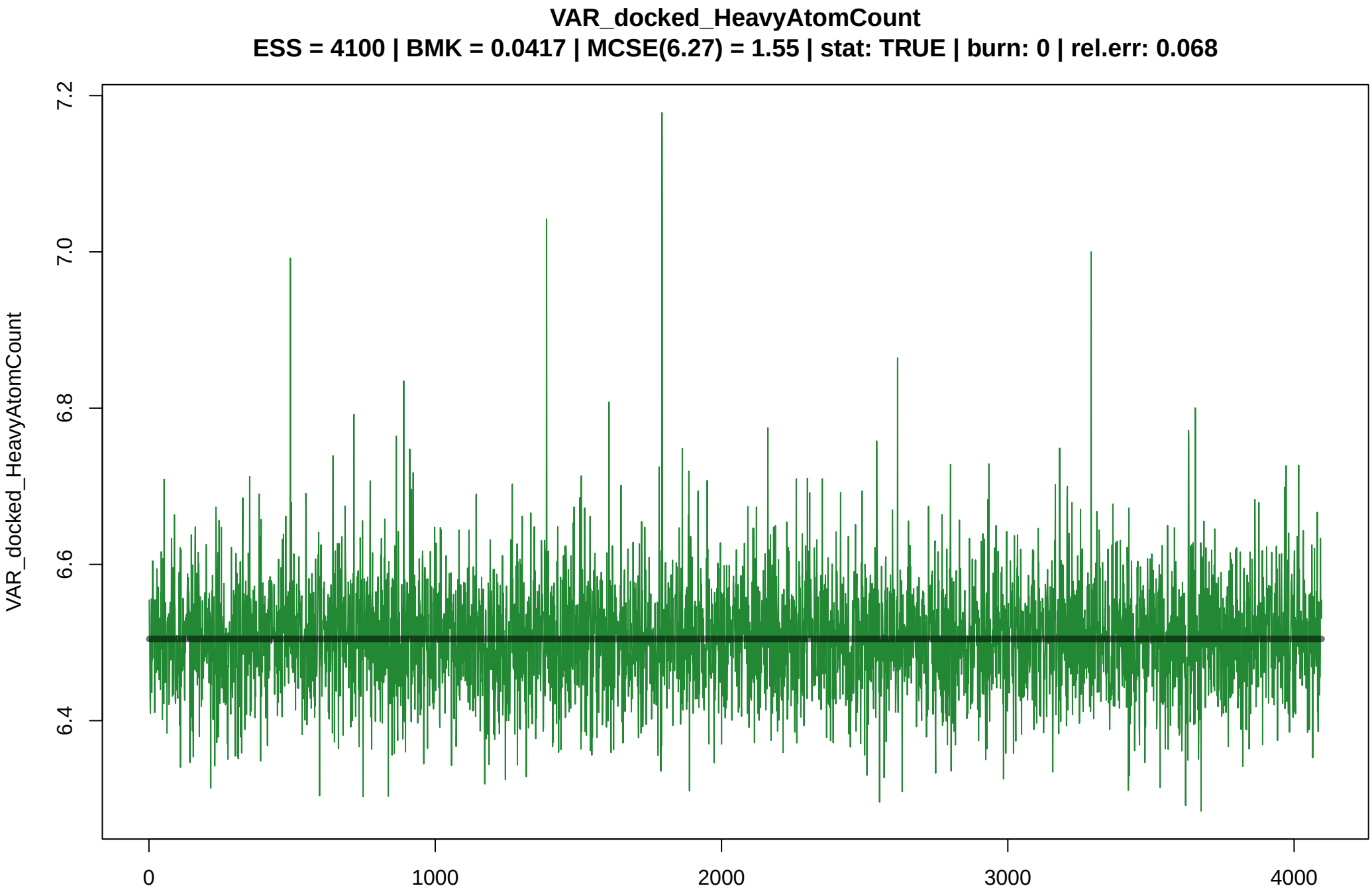

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0249 | MCSE(6.27) = 1.45 | stat: TRUE | burn: 0 | rel.err: 0.498
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

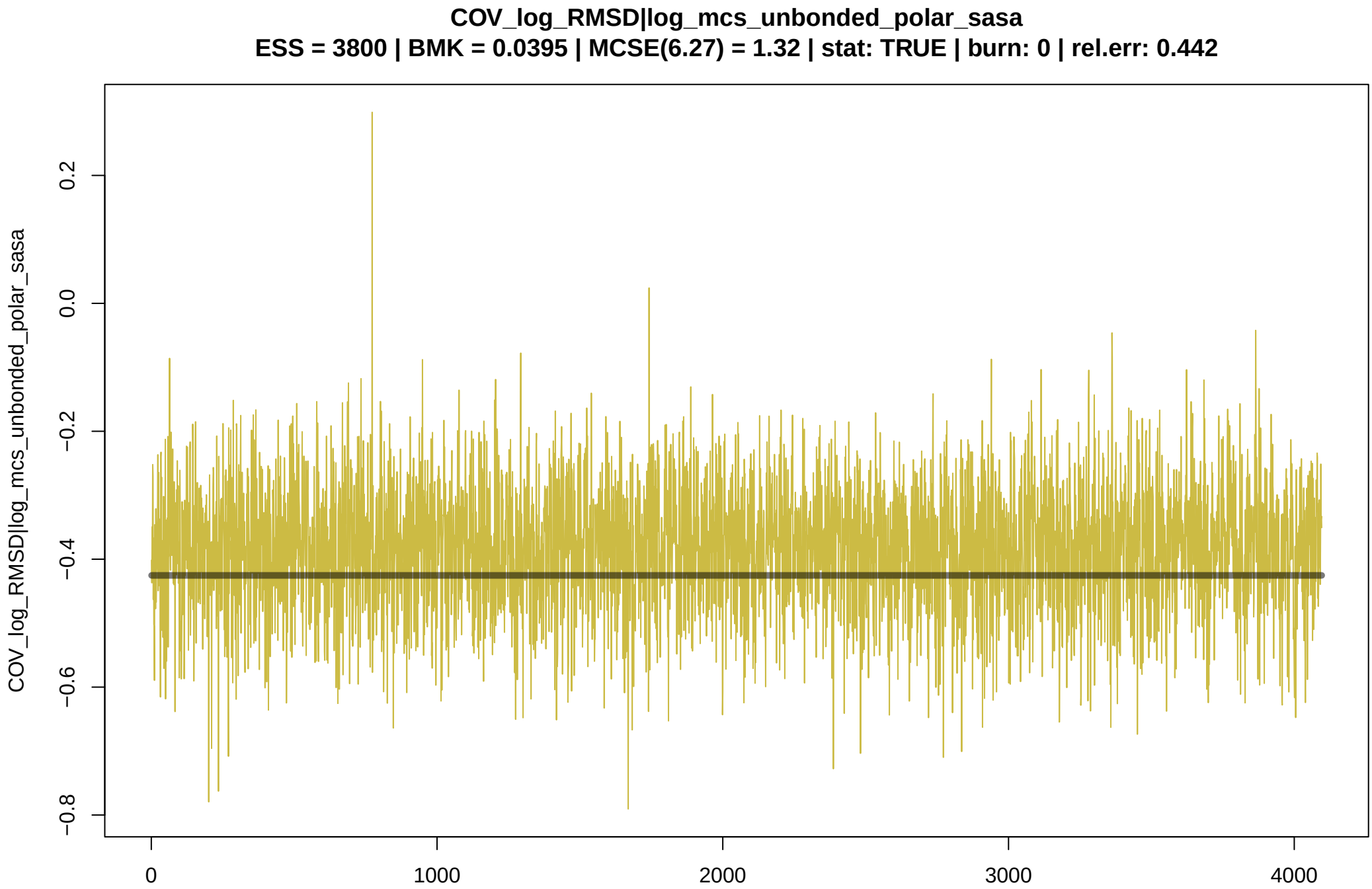

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0489 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0 | rel.err: 0.533
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
1000
2000
3000
4000

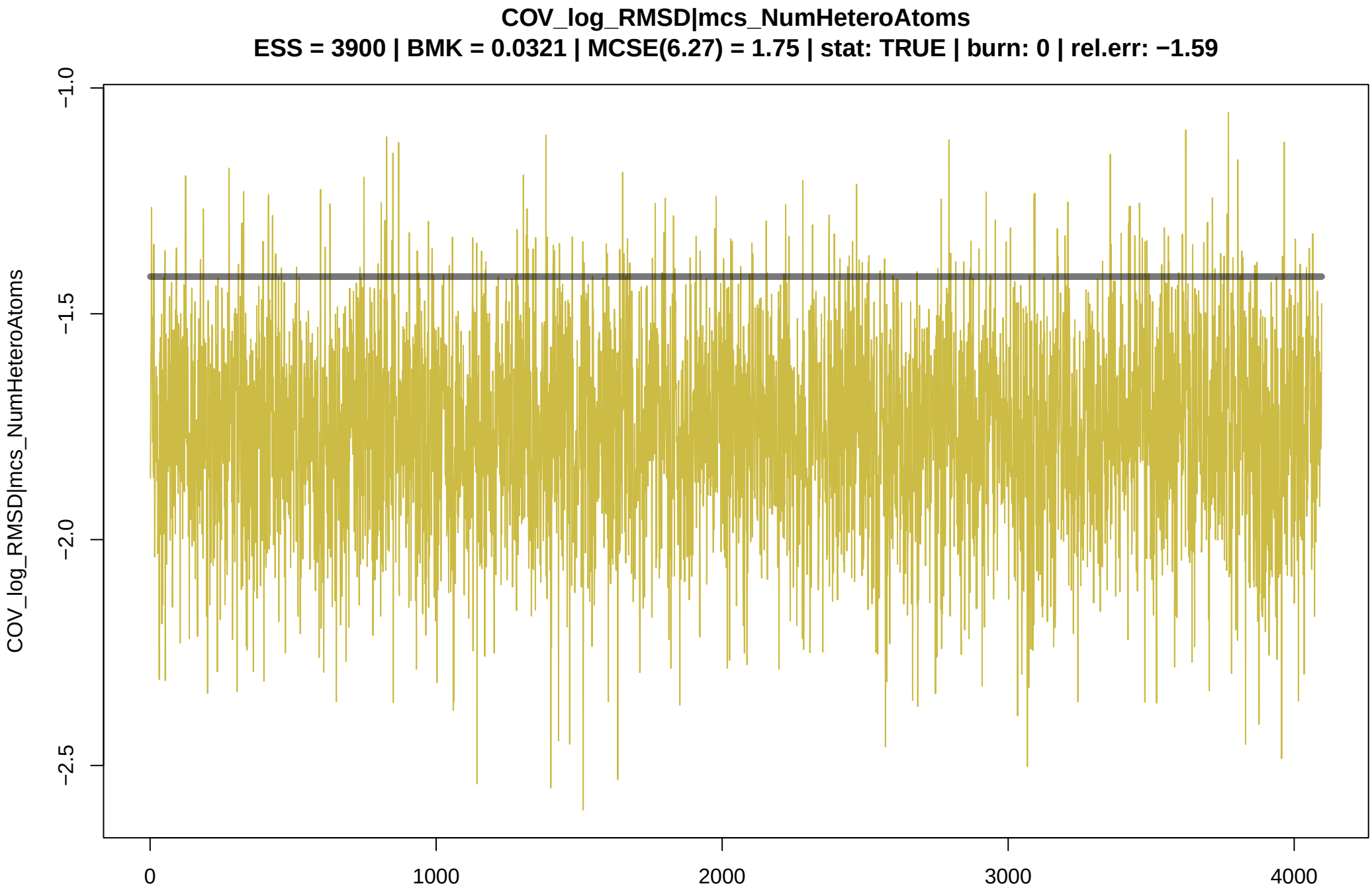

VAR_log_RMSD
ESS = 4100 | BMK = 0.0355 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: 2.26
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

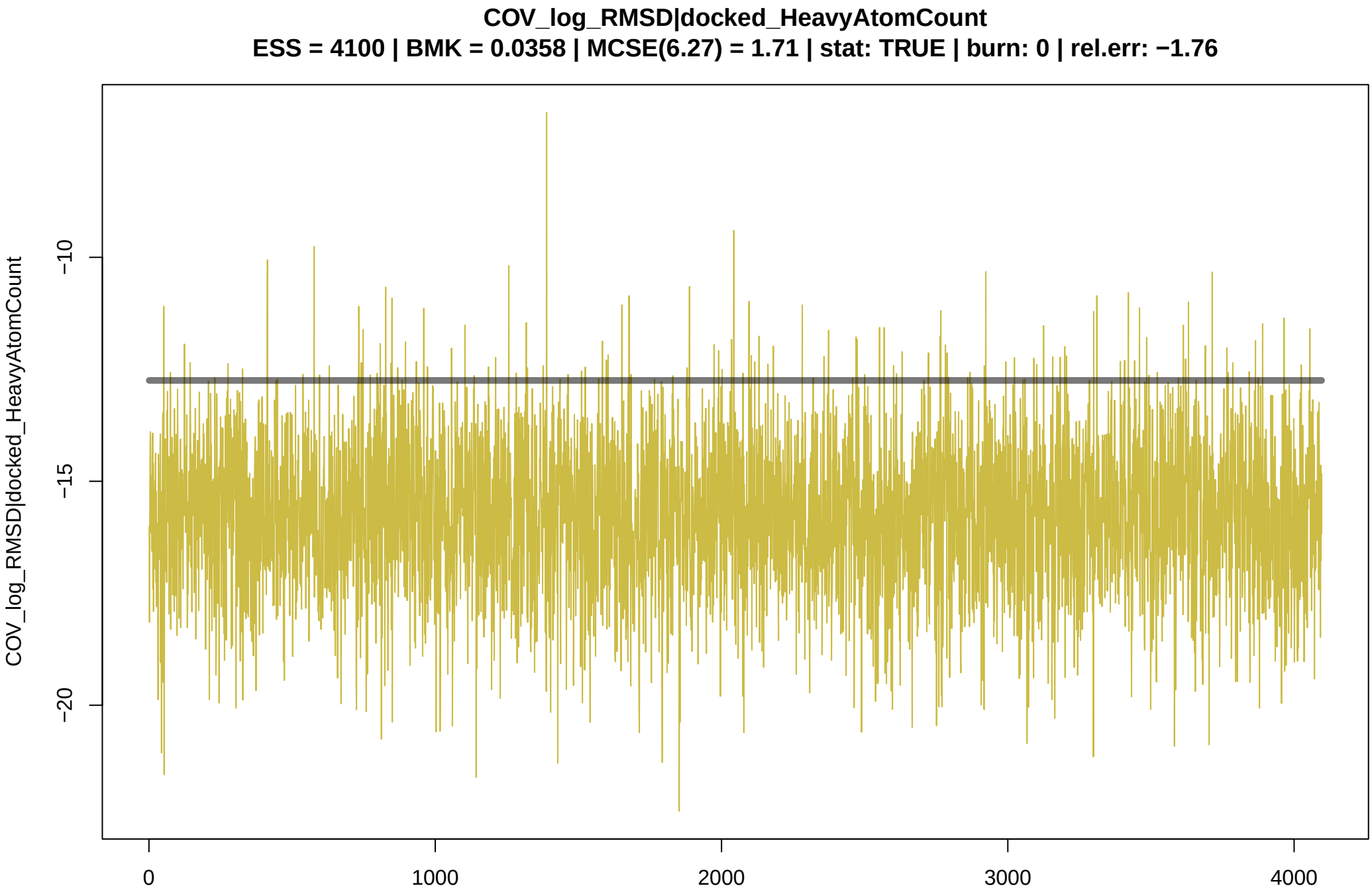

VAR_log_mcs_unbonded_polar_sasa
ESS = 3810 | BMK = 0.028 | MCSE(6.27) = 1.38 | stat: TRUE | burn: 0 | rel.err: 1.38
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
0
1000
2000
3000
4000

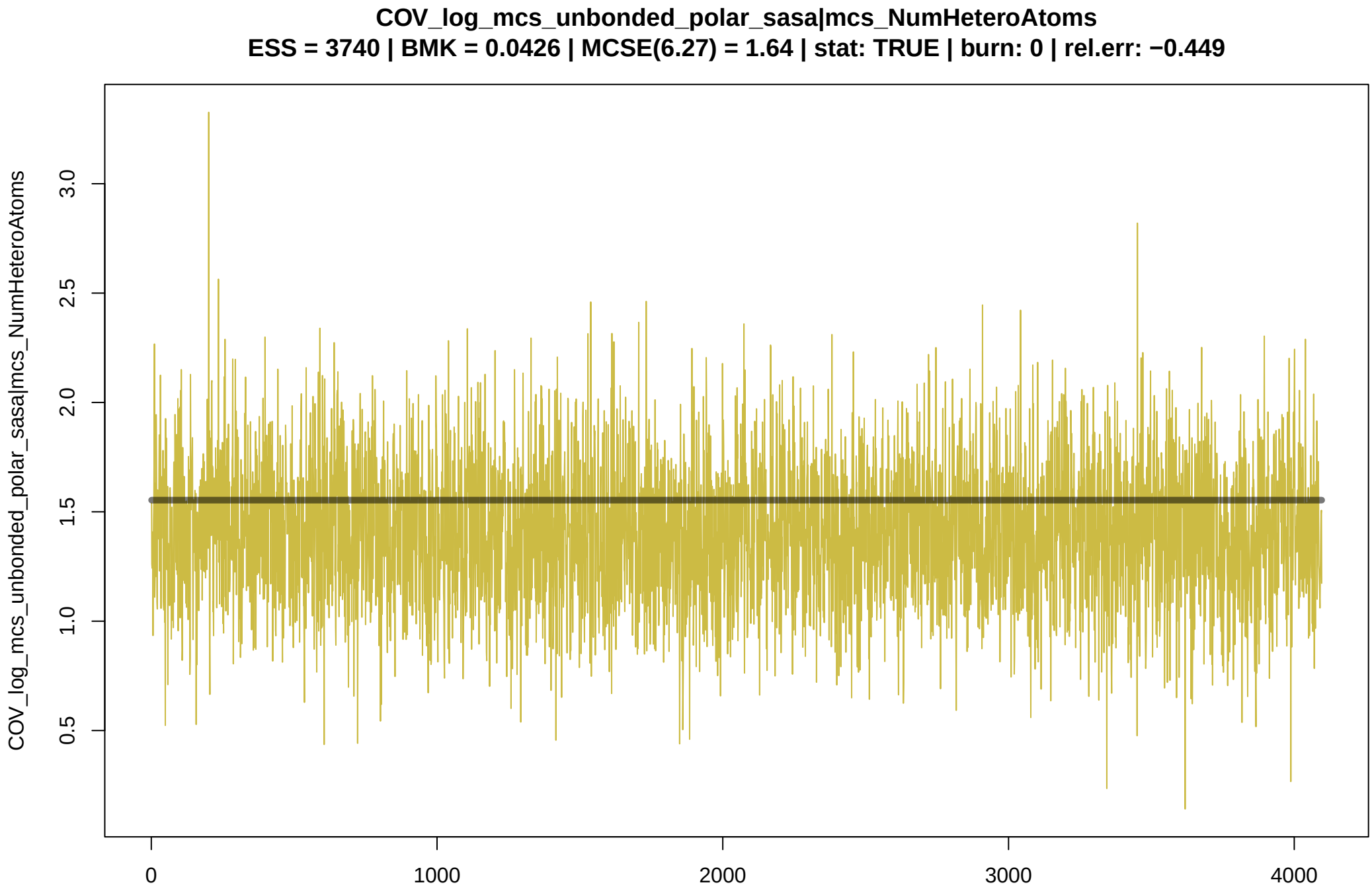

VAR_mcs_NumHeteroAtoms
ESS = 2850 | BMK = 0.0601 | MCSE(6.27) = 2.25 | stat: FALSE | burn: 0 | rel.err: 0.399
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
0
1000
2000
3000
4000

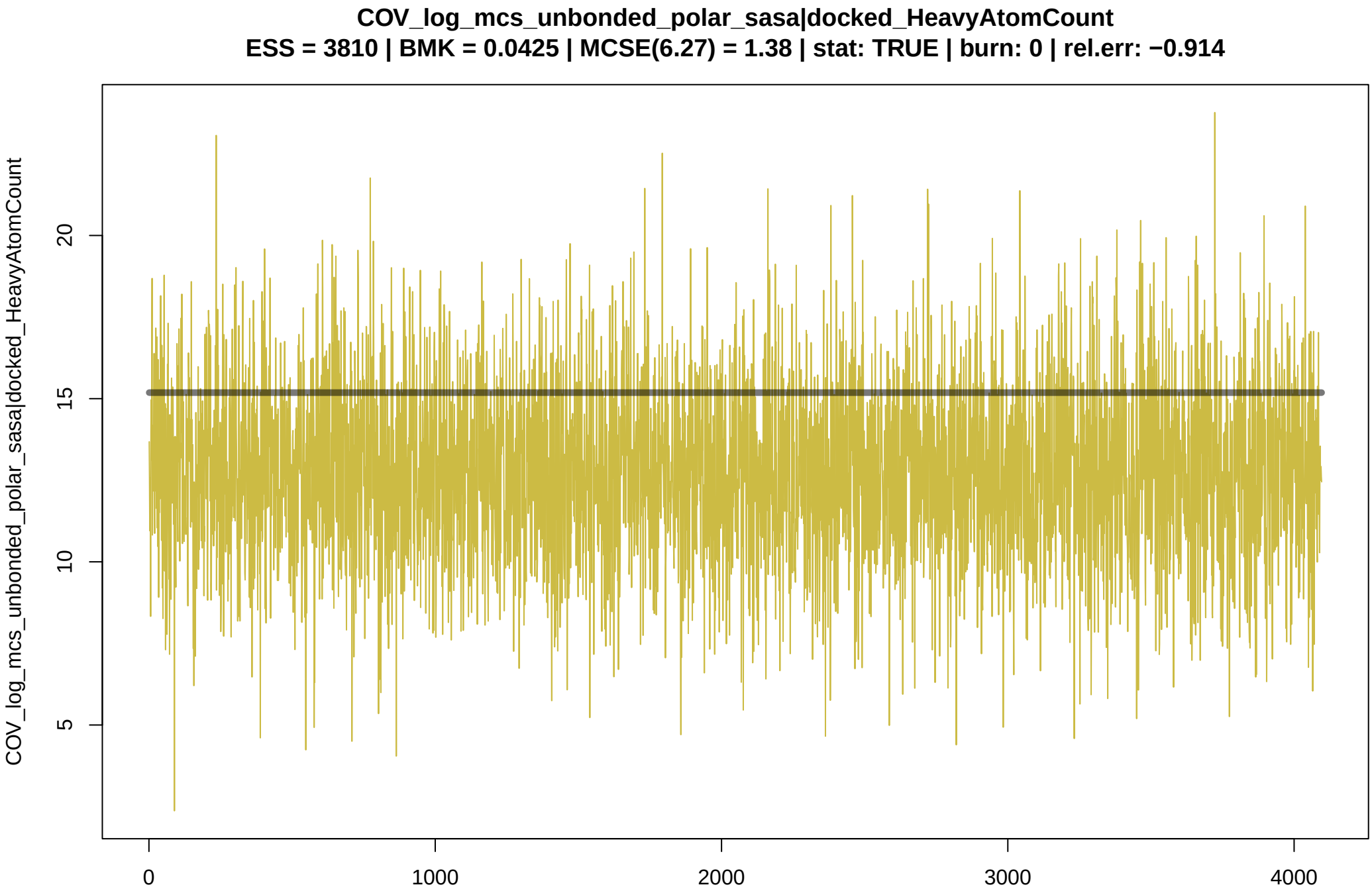

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0417 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: 0.068
VAR_docked_HeavyAtomCount
7.2
7.0
6.8
6.6
6.4
0
1000
2000
3000
4000

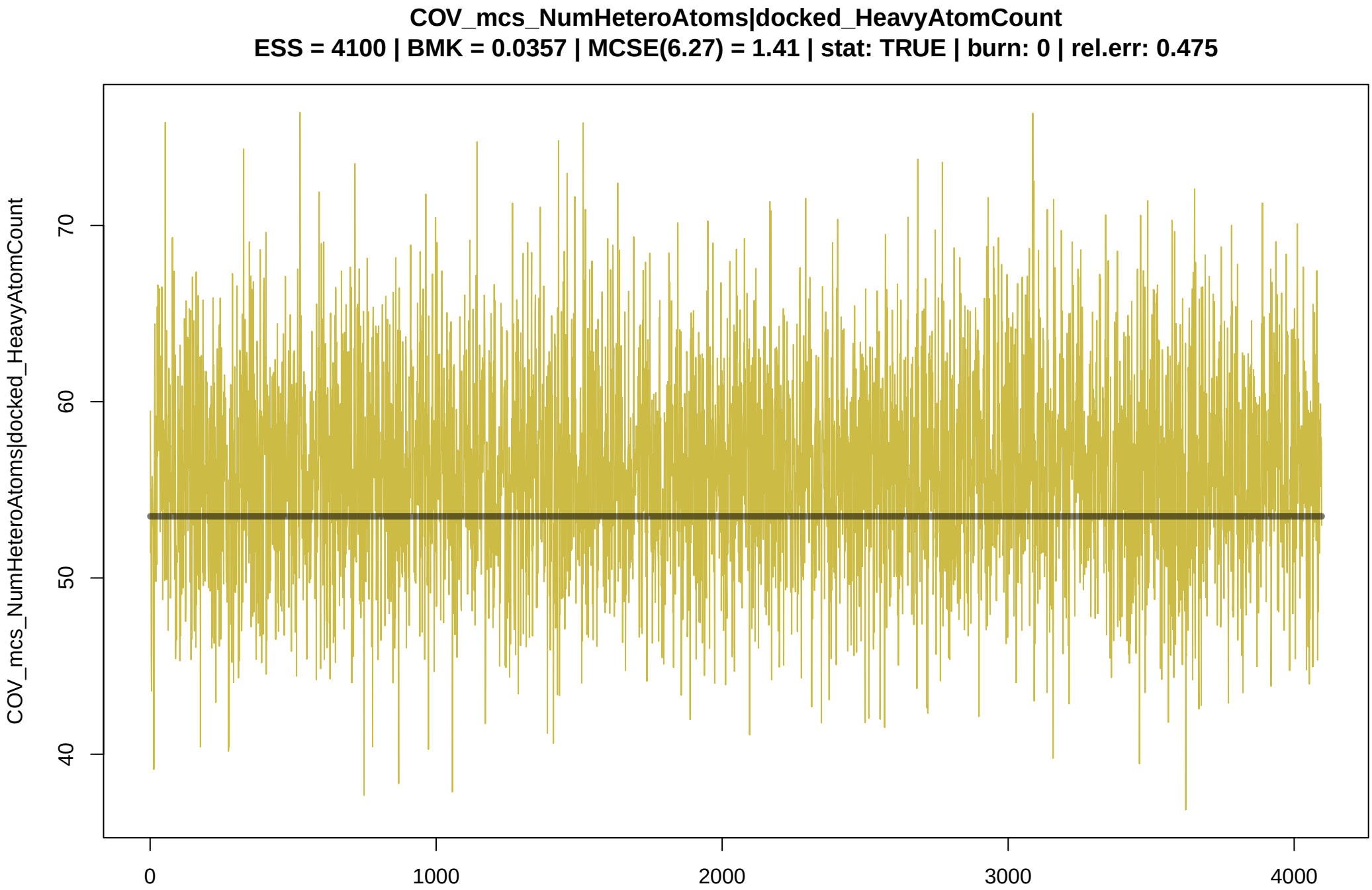

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3800 | BMK = 0.0395 | MCSE(6.27) = 1.32 | stat: TRUE | burn: 0 | rel.err: 0.442
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.2
0.0
−0.2
−0.4
−0.6
−0.8
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3900 | BMK = 0.0321 | MCSE(6.27) = 1.75 | 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 = 0.0358 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: −1.76
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3740 | BMK = 0.0426 | MCSE(6.27) = 1.64 | stat: TRUE | burn: 0 | rel.err: −0.449
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
3.0
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 3810 | BMK = 0.0425 | MCSE(6.27) = 1.38 | stat: TRUE | burn: 0 | rel.err: −0.914
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
0
1000
2000
3000
4000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0357 | MCSE(6.27) = 1.41 | stat: TRUE | burn: 0 | rel.err: 0.475
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
1000
2000
3000
4000