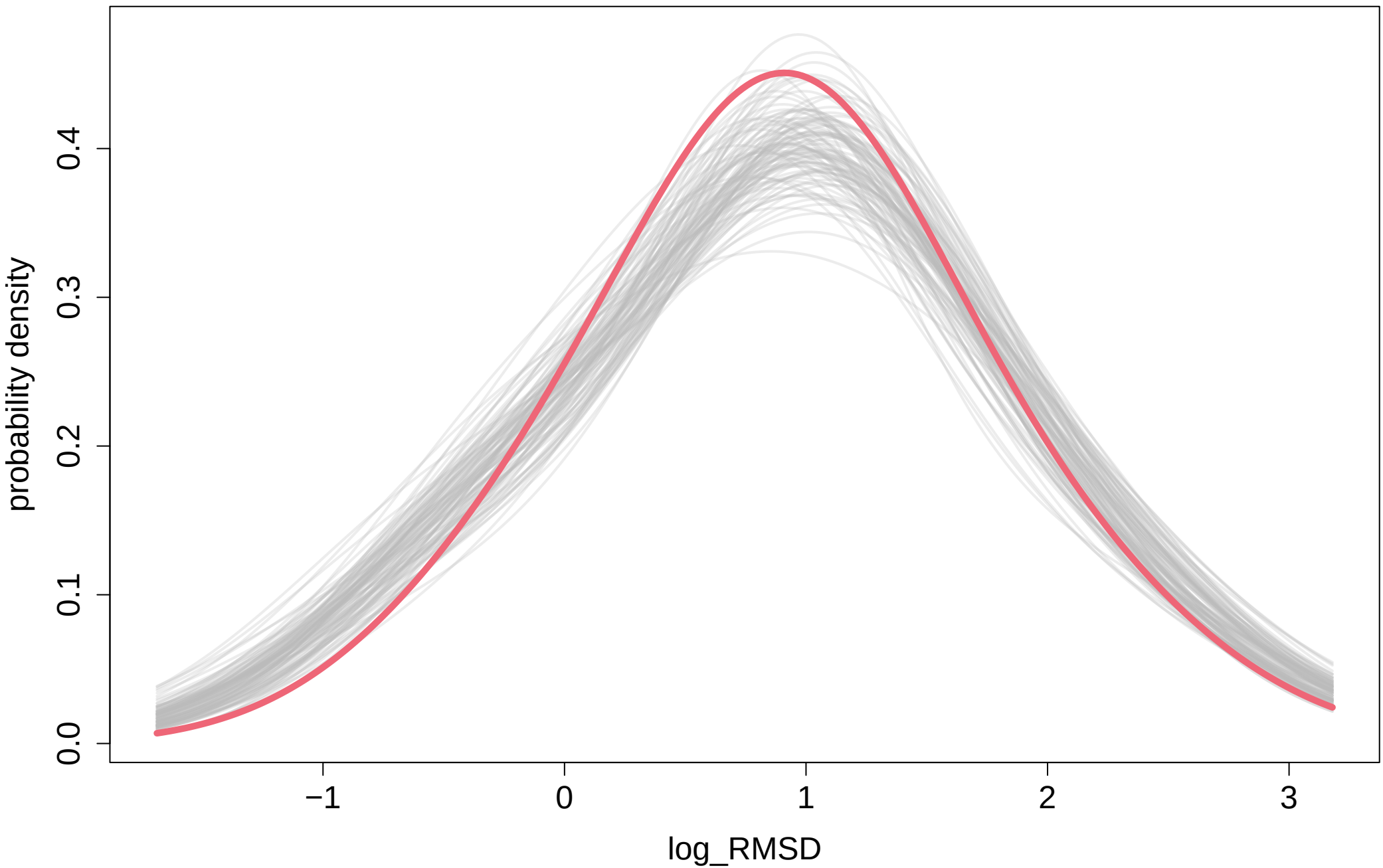
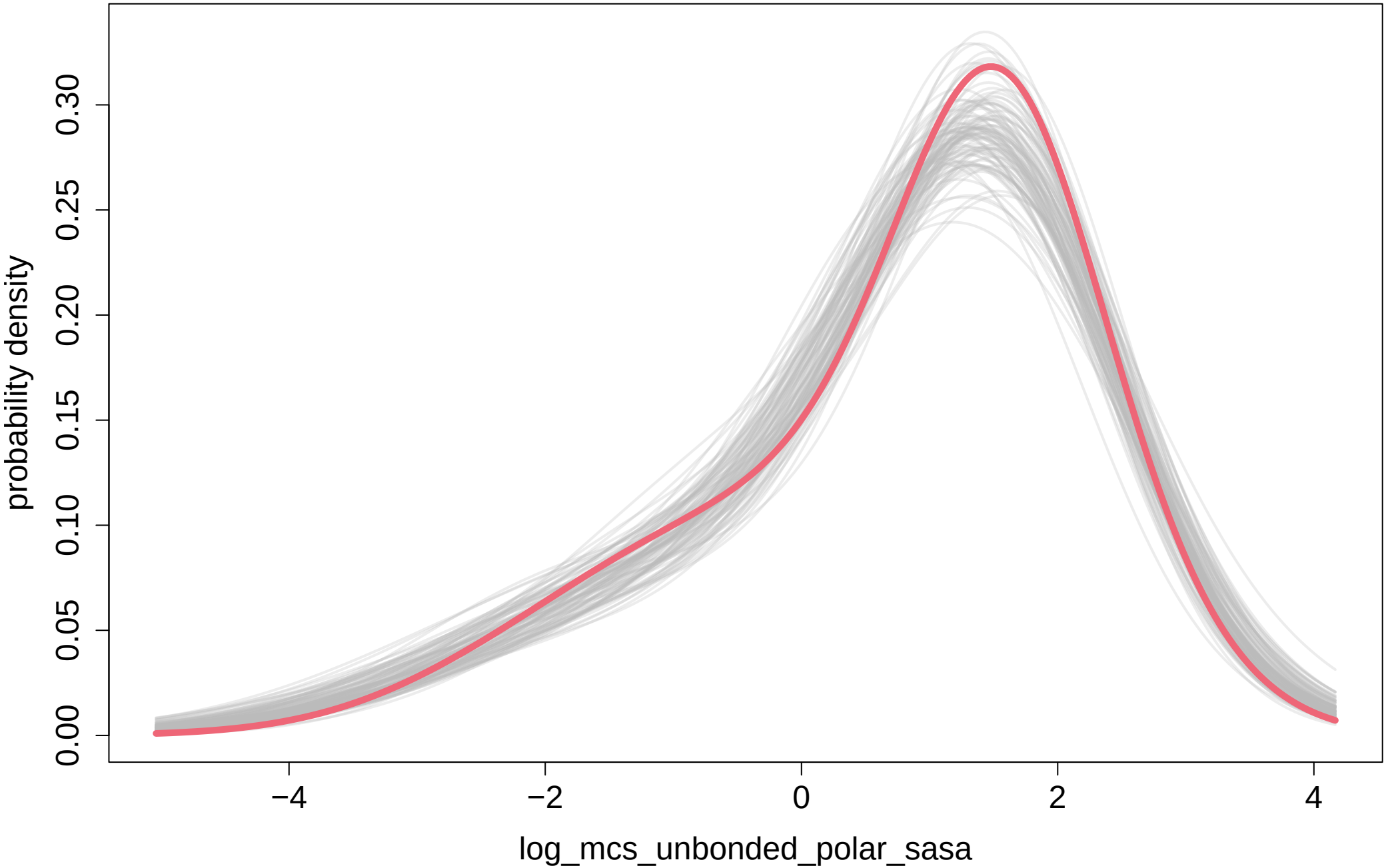
−− STATS maxD −−
min ESS = 293.92865993253
max BMK = 0.106299900815731
max MCSE = 5.63167798152898
all stationary: FALSE
burn: 0
max rel.err.: 2.06844247708268

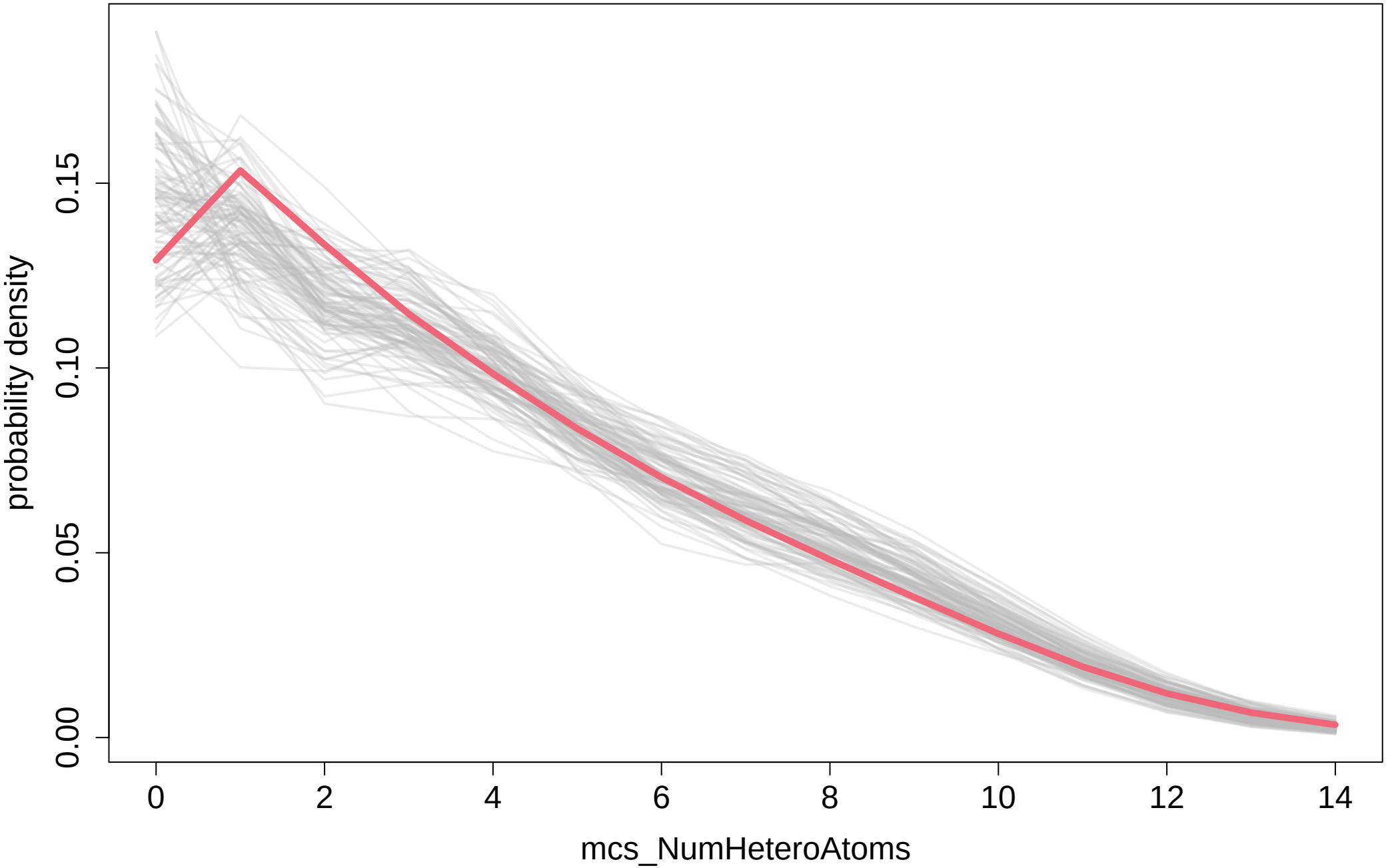
−− STATS 2D −−
min ESS = 3271.59258949955
max BMK = 0.042898245107940 3
max MCSE = 1.94442968738214
all stationary: FALSE
burn: 0
max rel.err.: 1.8003770630301

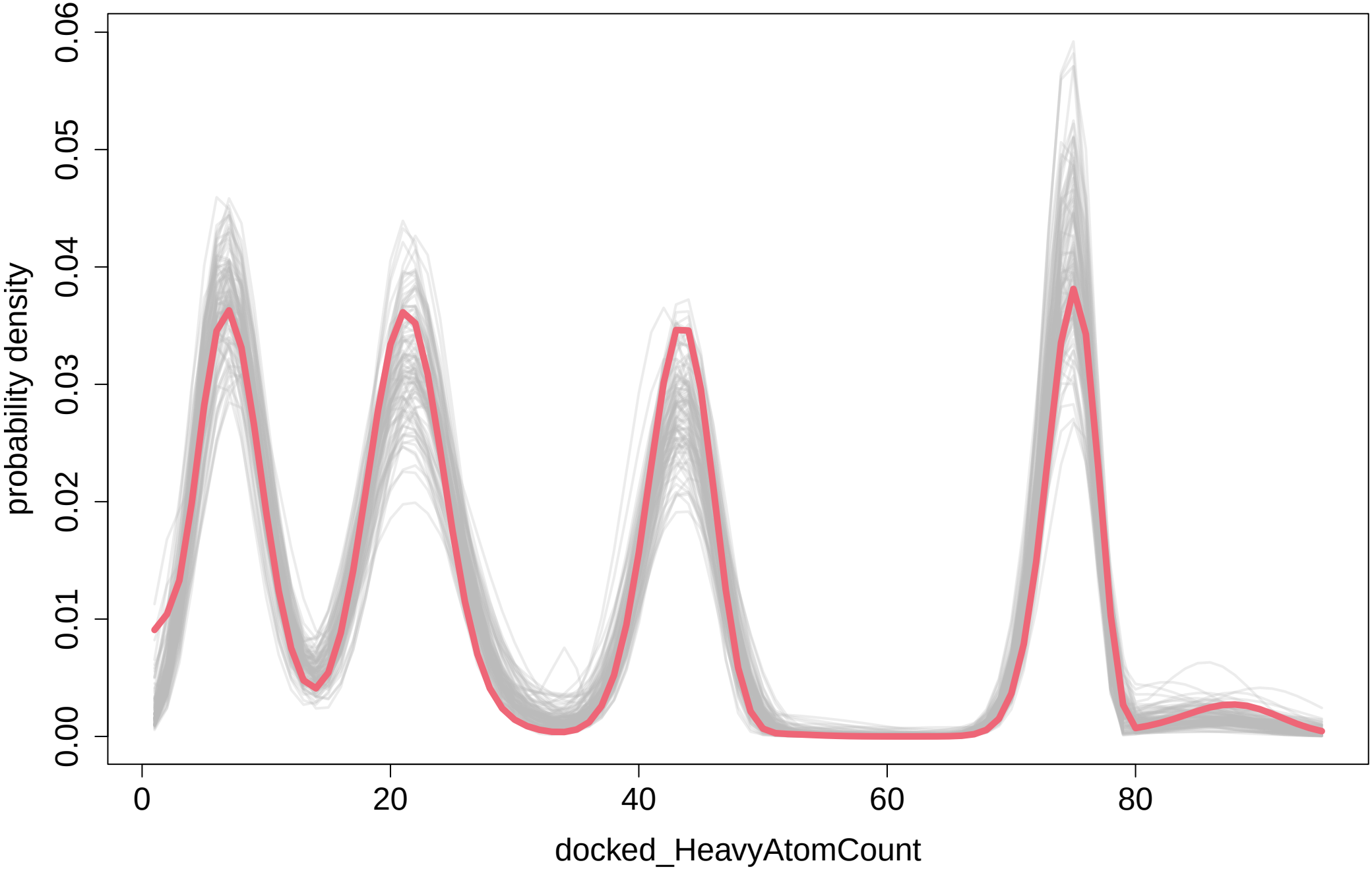
−− STATS 1D −−
min ESS = 2556.9356698031
max BMK = 0.049956233149830 5
max MCSE = 2.49966659633085
all stationary: TRUE
burn: 0
max rel.err.: 2.28806109791897

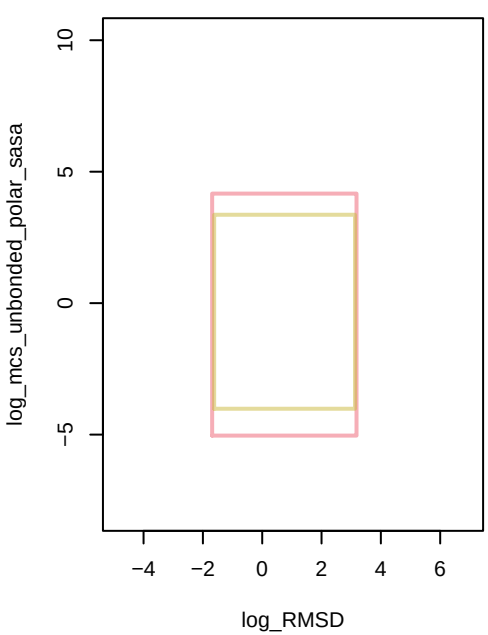
Occupied clusters: 9 of 16
LL: −2160 +− 6.74

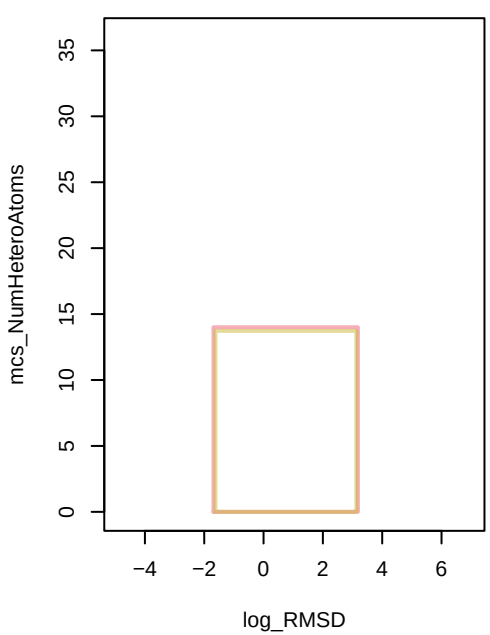

probability density
0.0
0.1
0.2
0.3
0.4
−1
0
1
2
3
log_RMSD

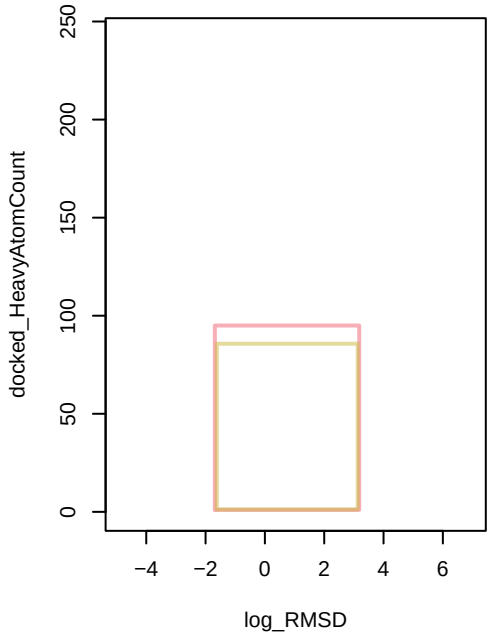

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

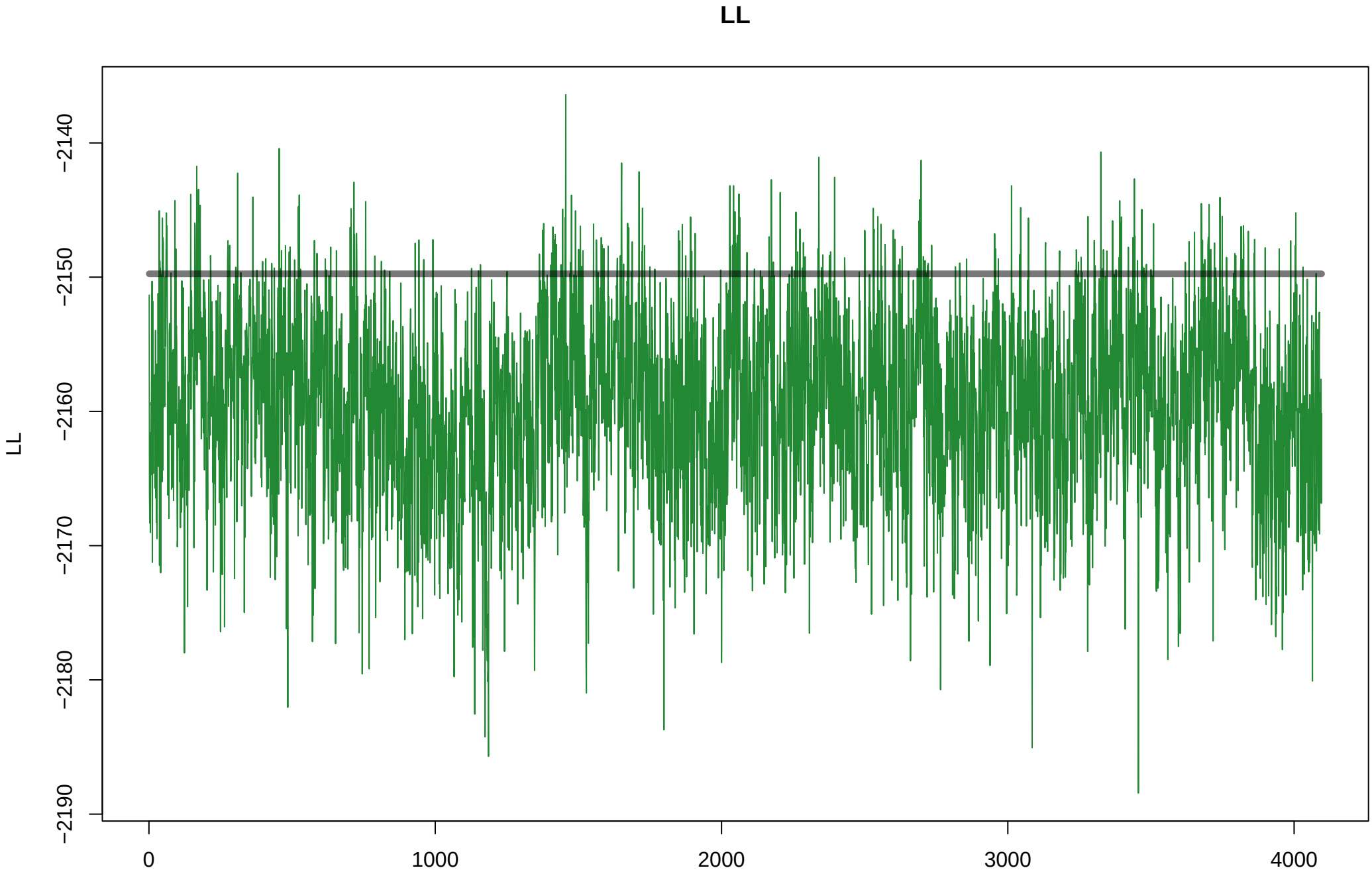

probability density
0.00
0.05
0.10
0.15
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

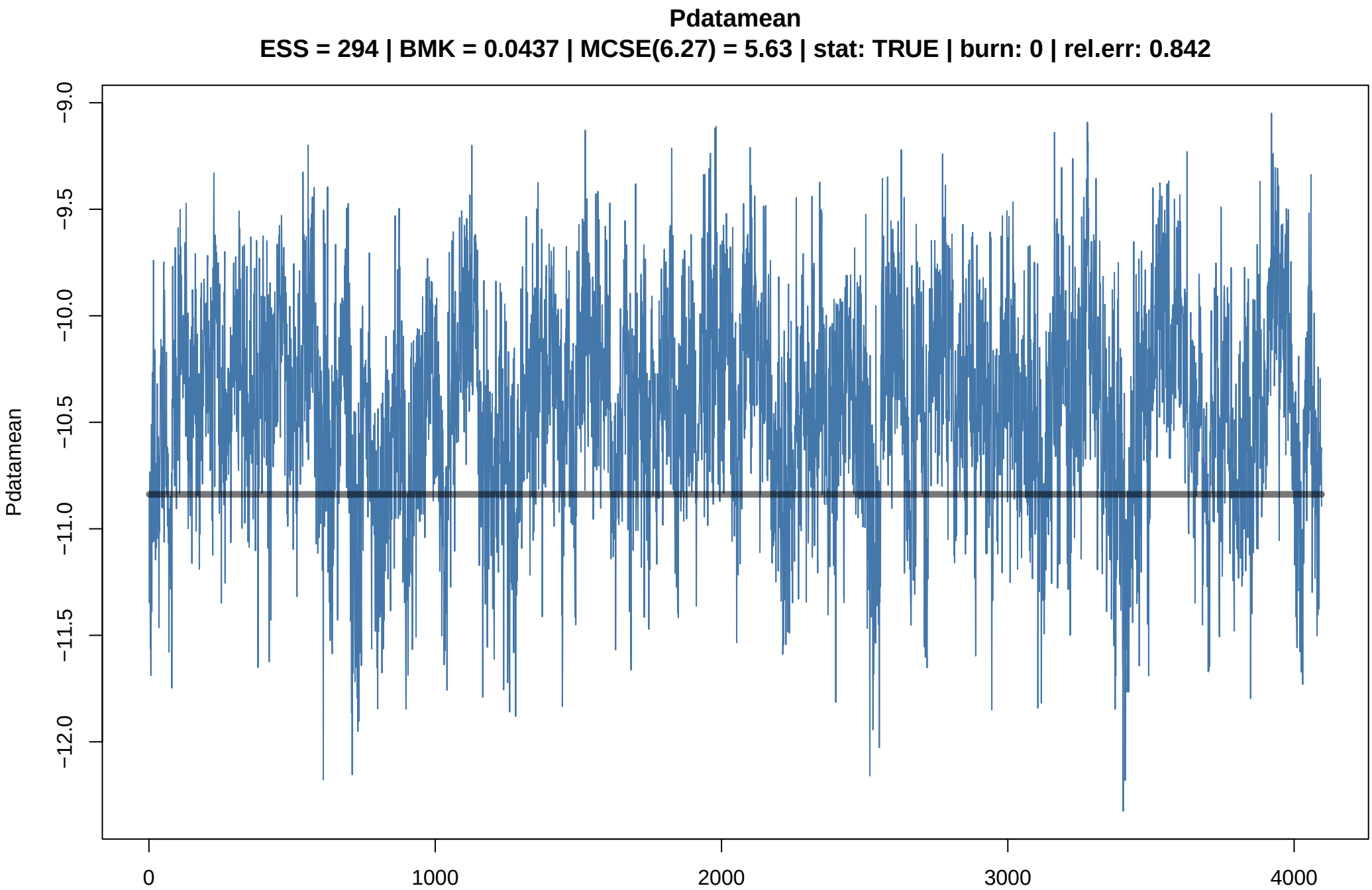

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0
20
40
60
80
docked_HeavyAtomCount

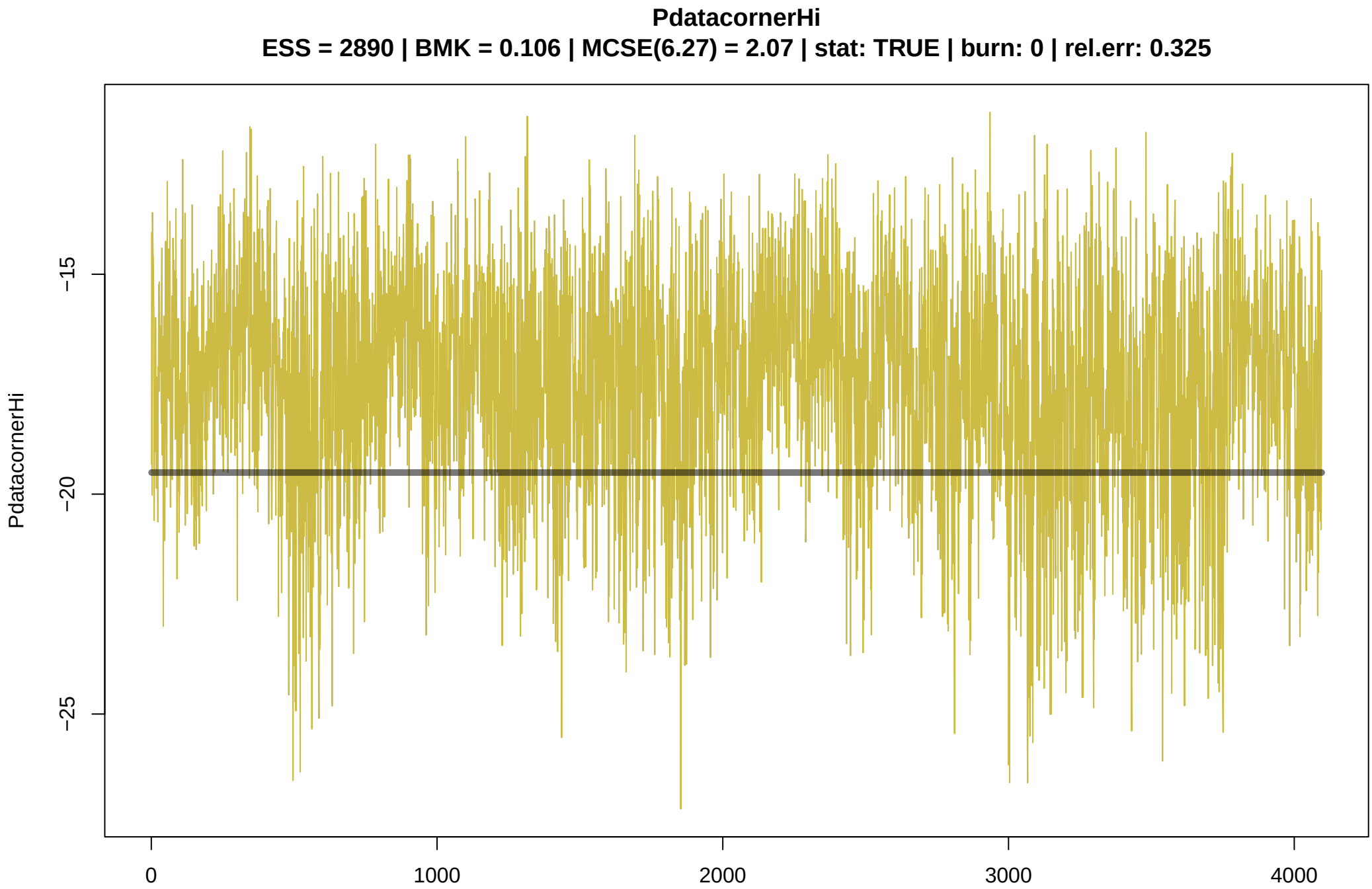

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

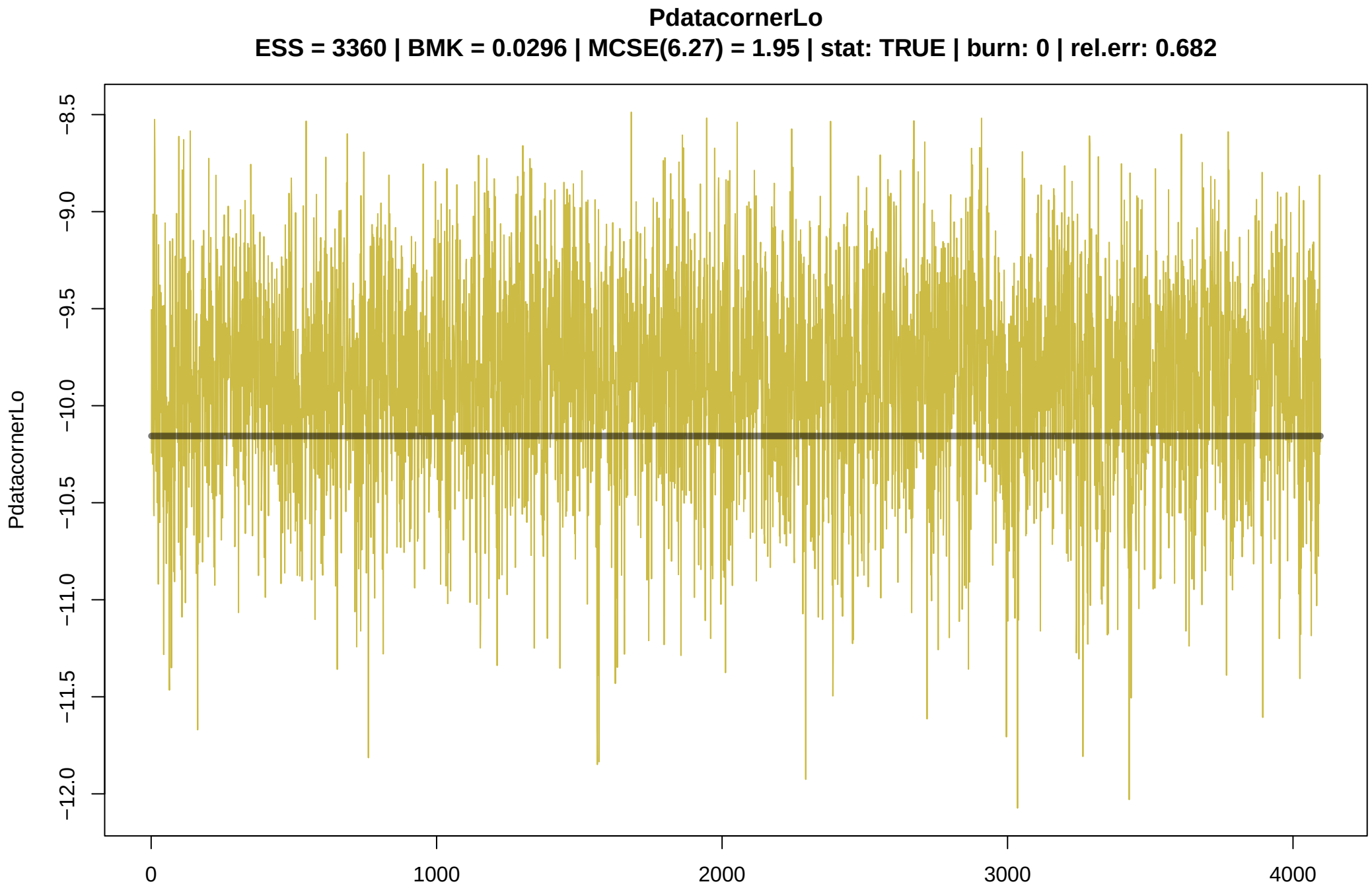

mcs_NumHeteroAtoms
35
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

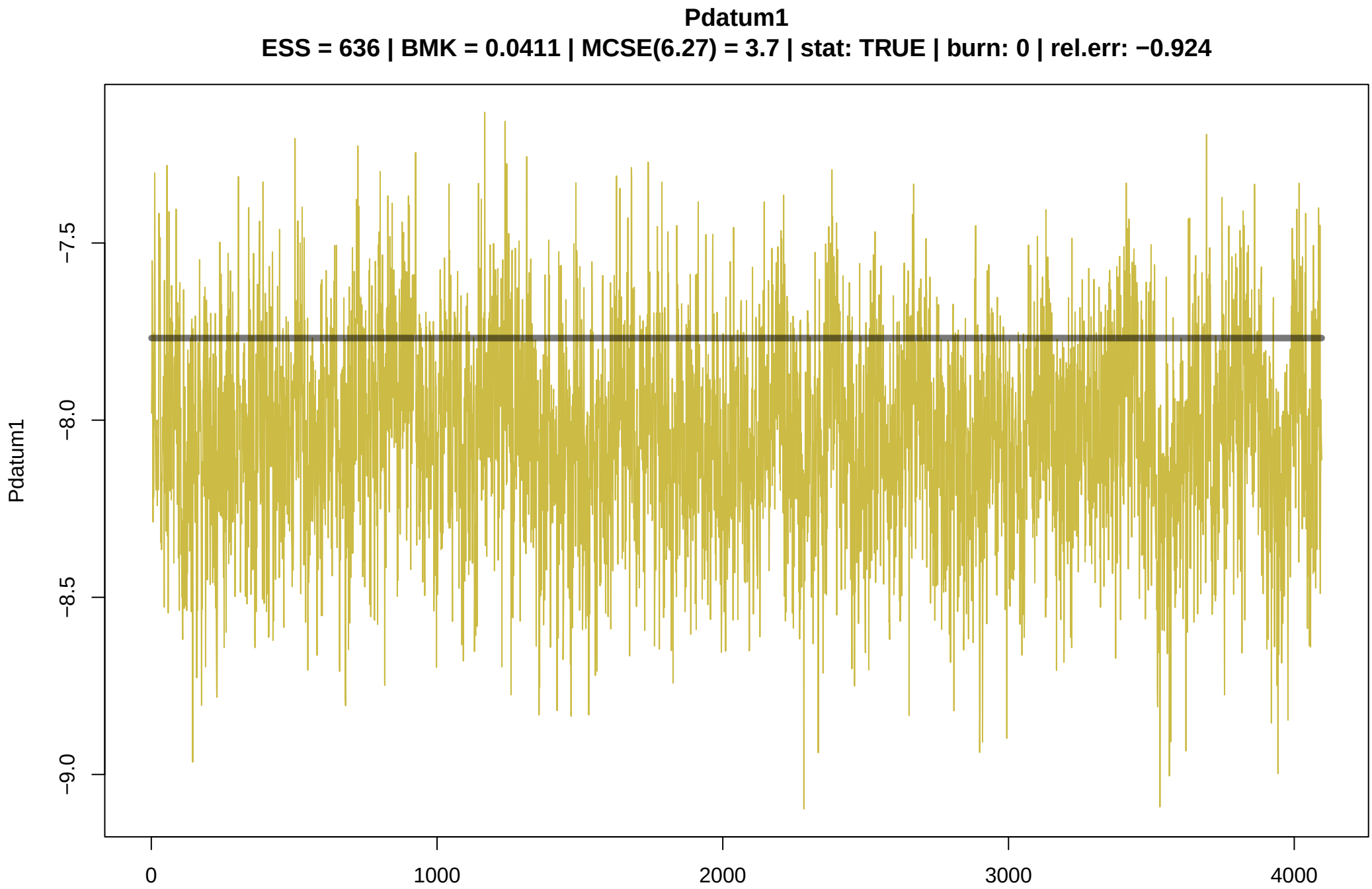

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

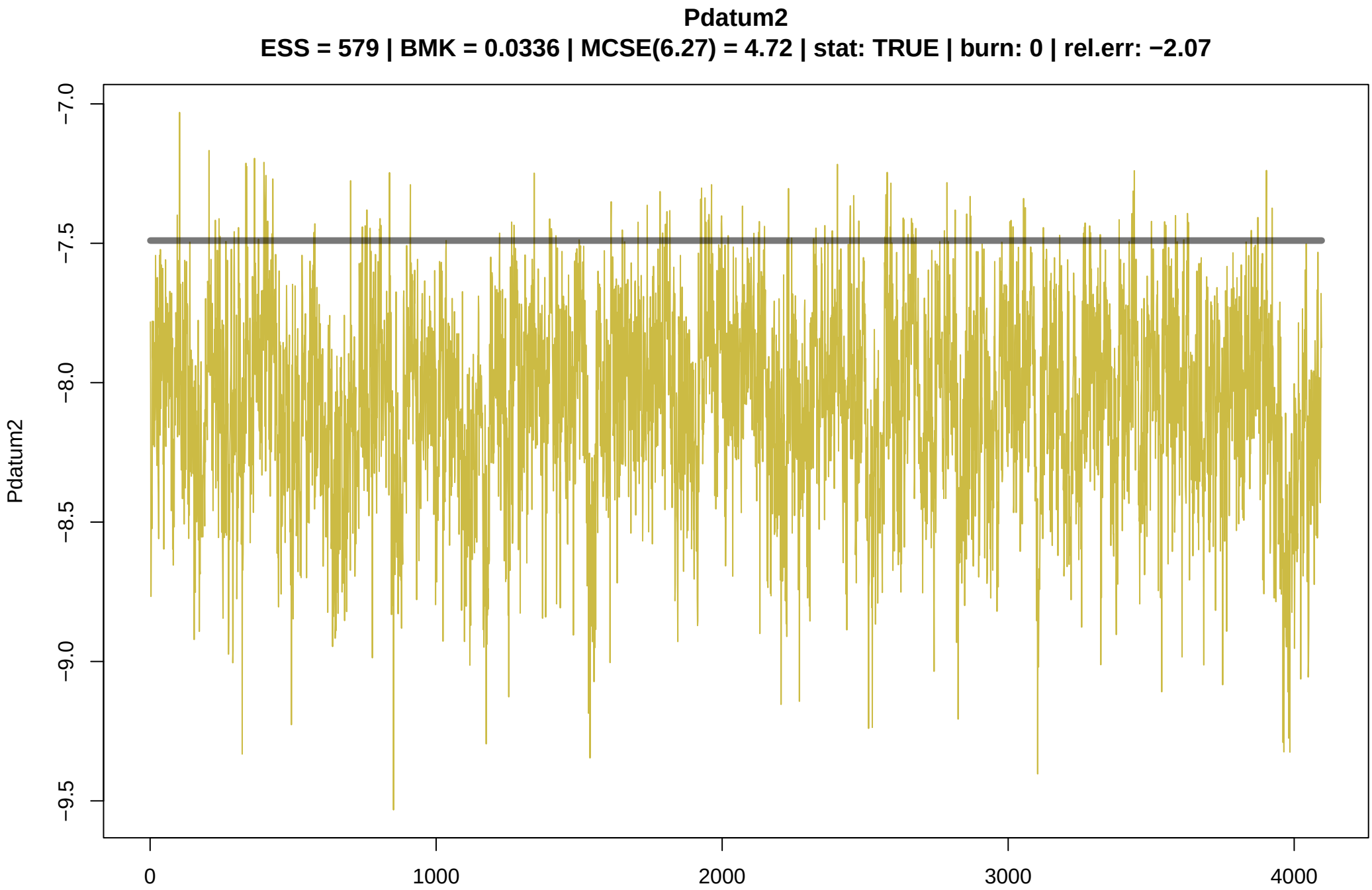

LL
LL
−2140
−2150
−2160
−2170
−2180
−2190
0
1000
2000
3000
4000

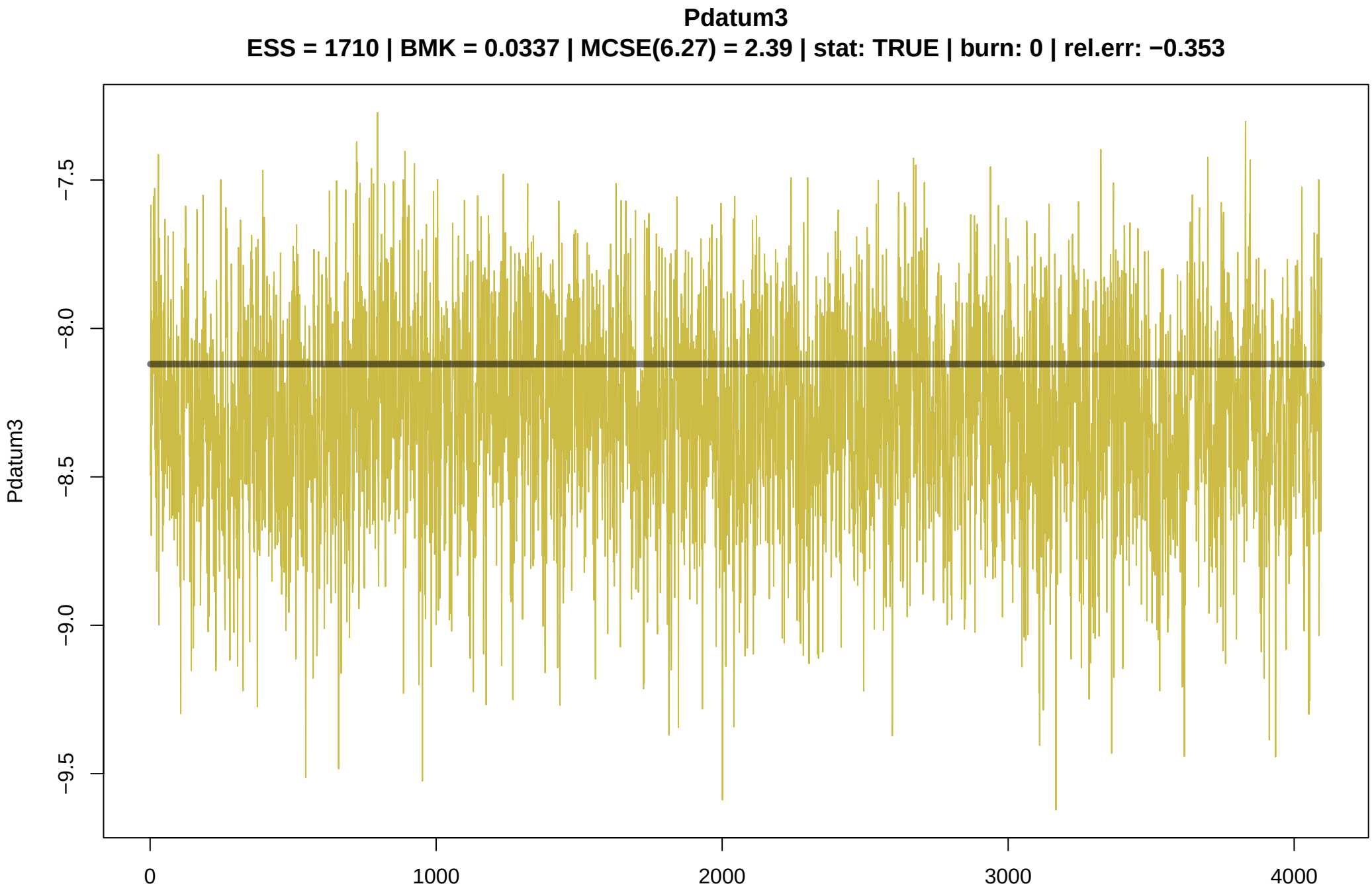

Pdatamean
ESS = 294 | BMK = 0.0437 | MCSE(6.27) = 5.63 | stat: TRUE | burn: 0 | rel.err: 0.842
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
1000
2000
3000
4000

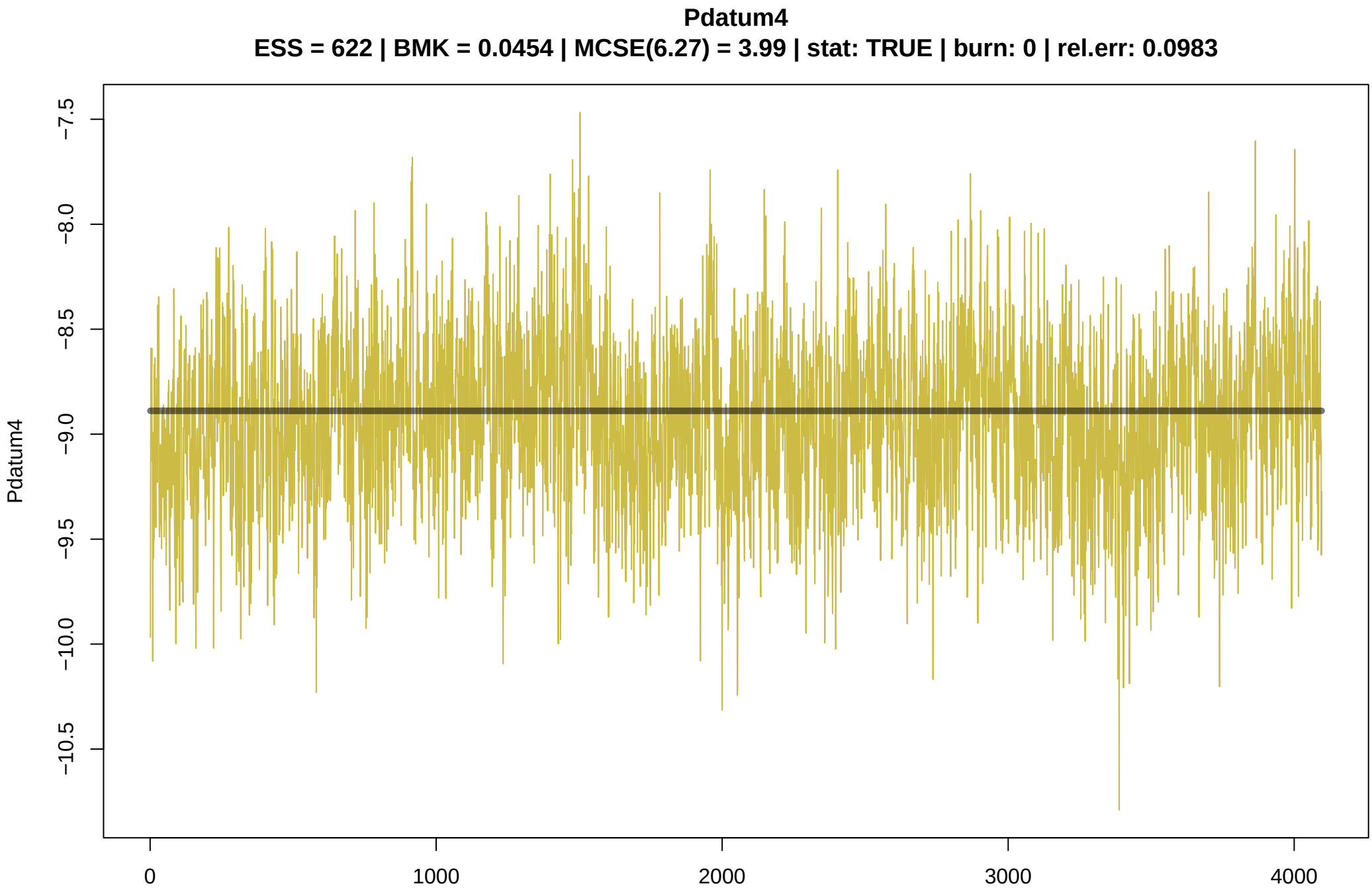

PdatacornerHi
ESS = 2890 | BMK = 0.106 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: 0.325
PdatacornerHi
−15
−20
−25
0
1000
2000
3000
4000

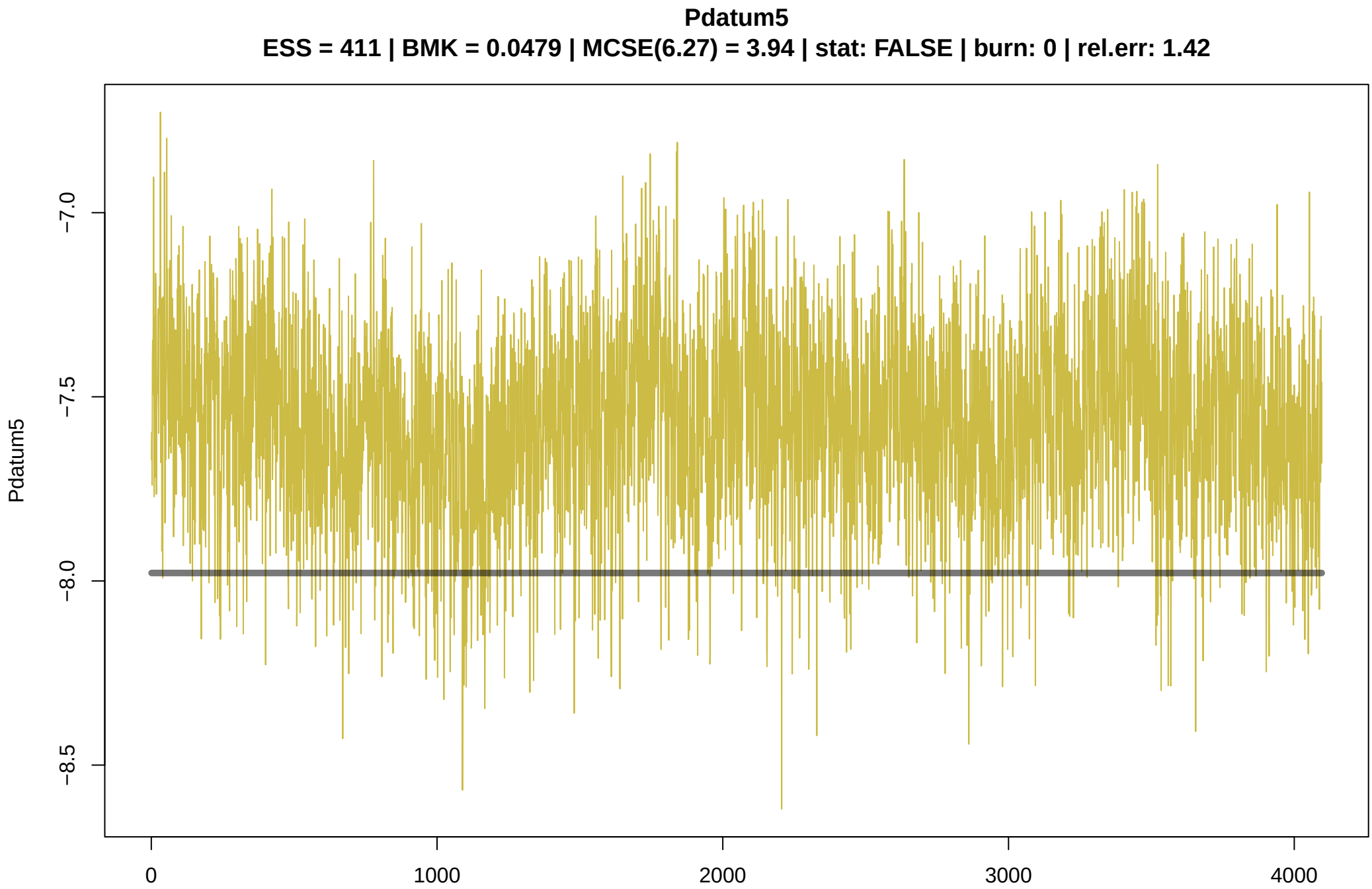

PdatacornerLo
ESS = 3360 | BMK = 0.0296 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: 0.682
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
1000
2000
3000
4000

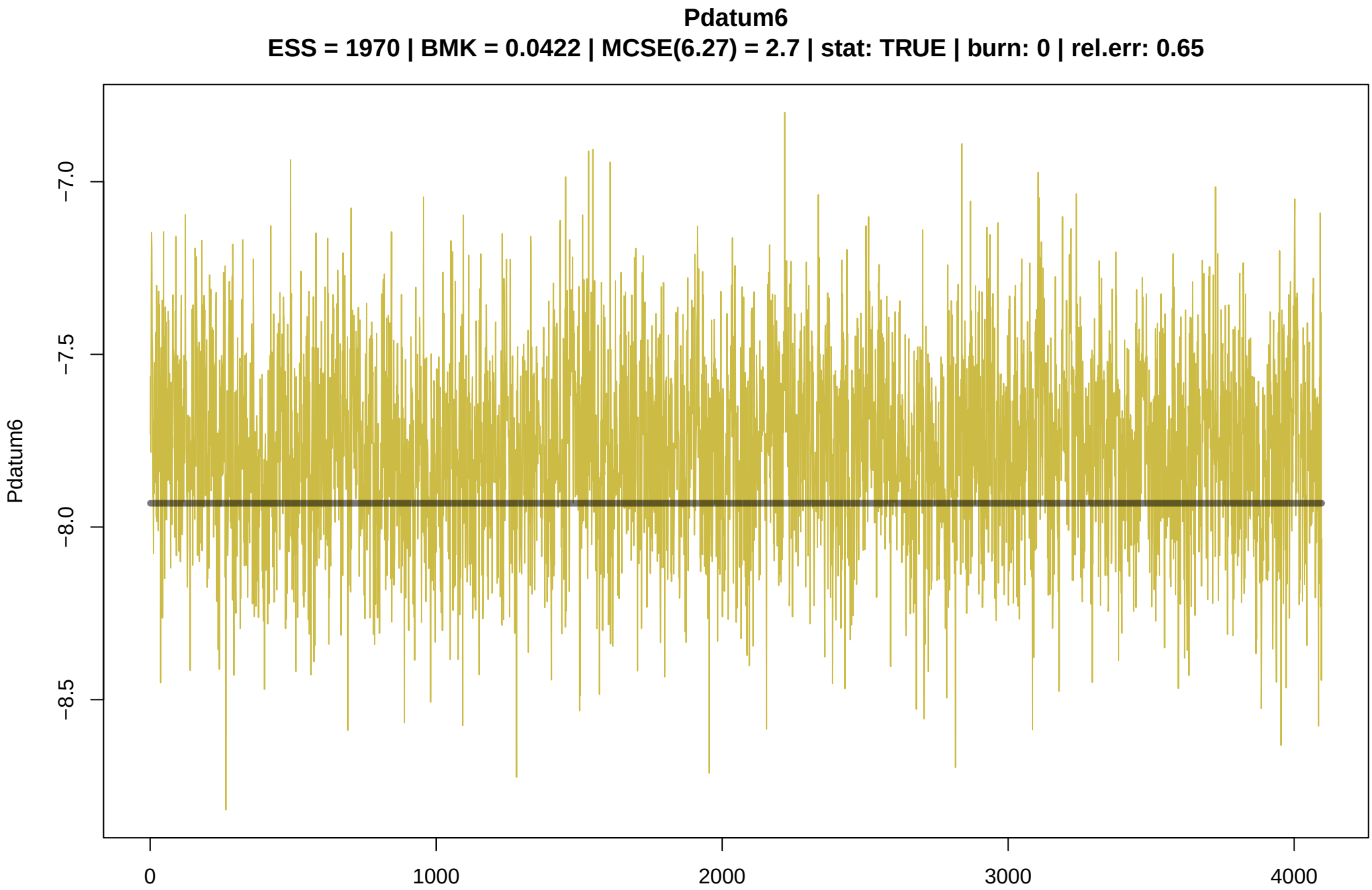

Pdatum1
ESS = 636 | BMK = 0.0411 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | rel.err: −0.924
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

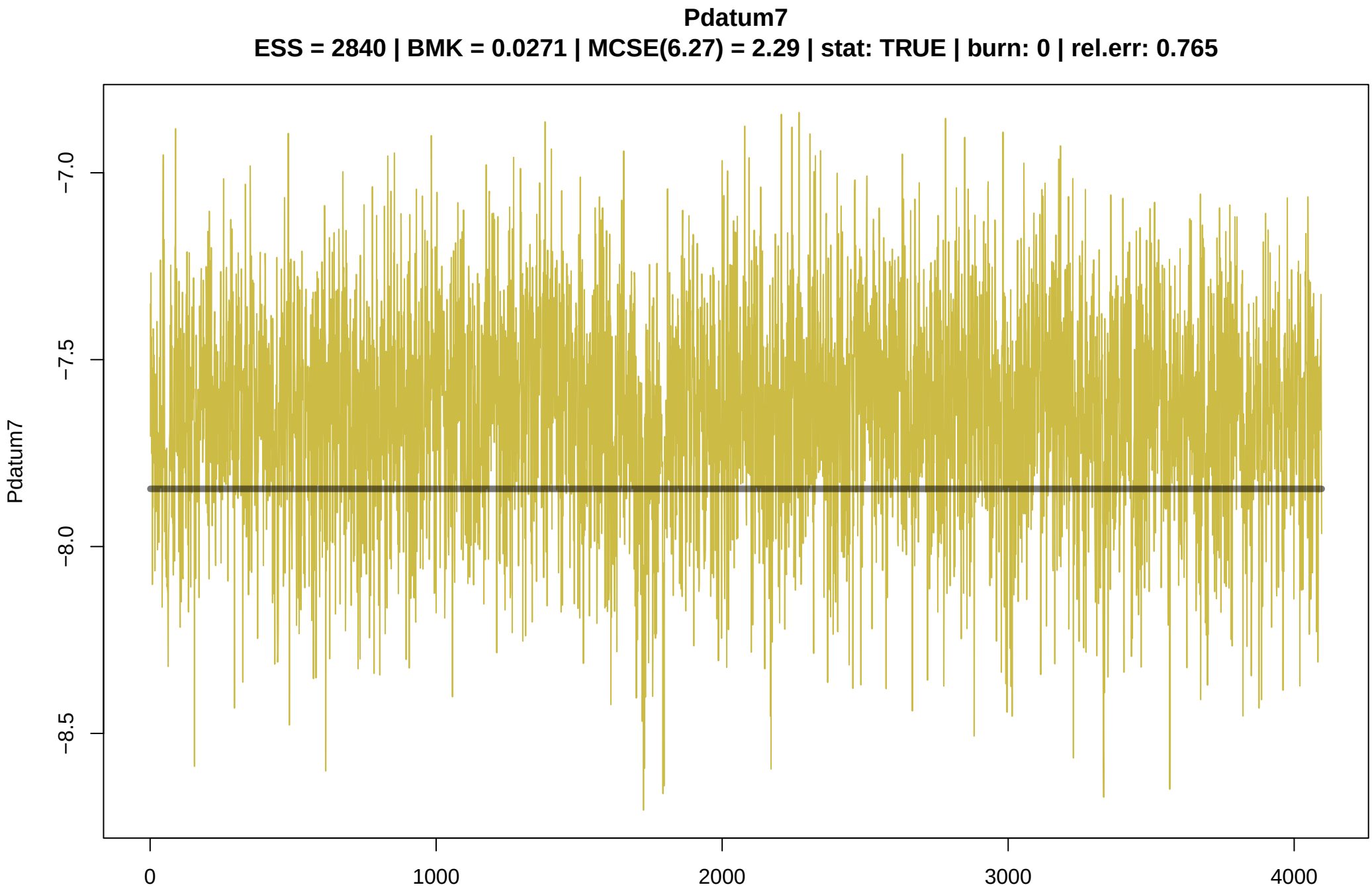

Pdatum2
ESS = 579 | BMK = 0.0336 | MCSE(6.27) = 4.72 | stat: TRUE | burn: 0 | rel.err: −2.07
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

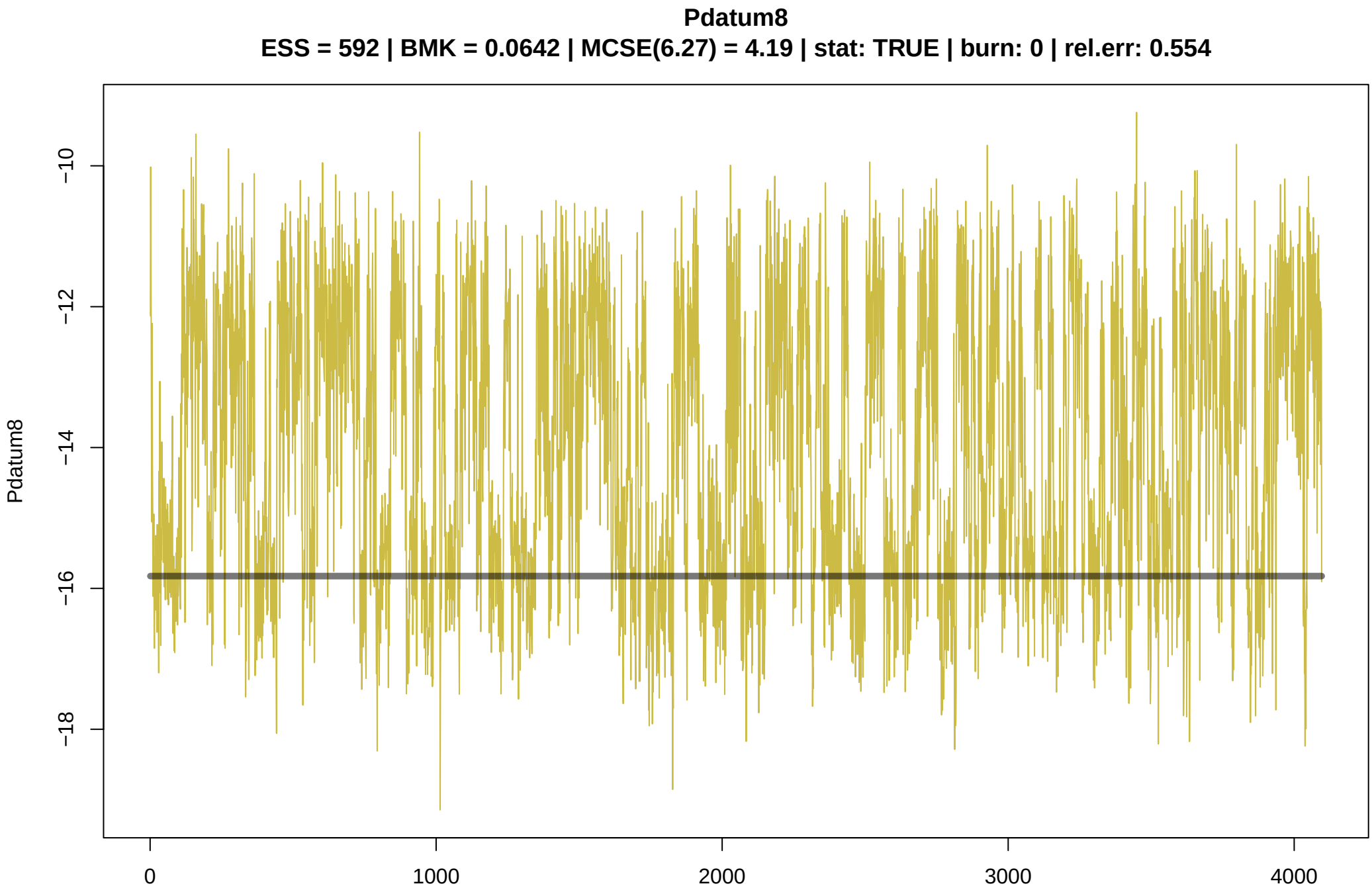

Pdatum3
ESS = 1710 | BMK = 0.0337 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: −0.353
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

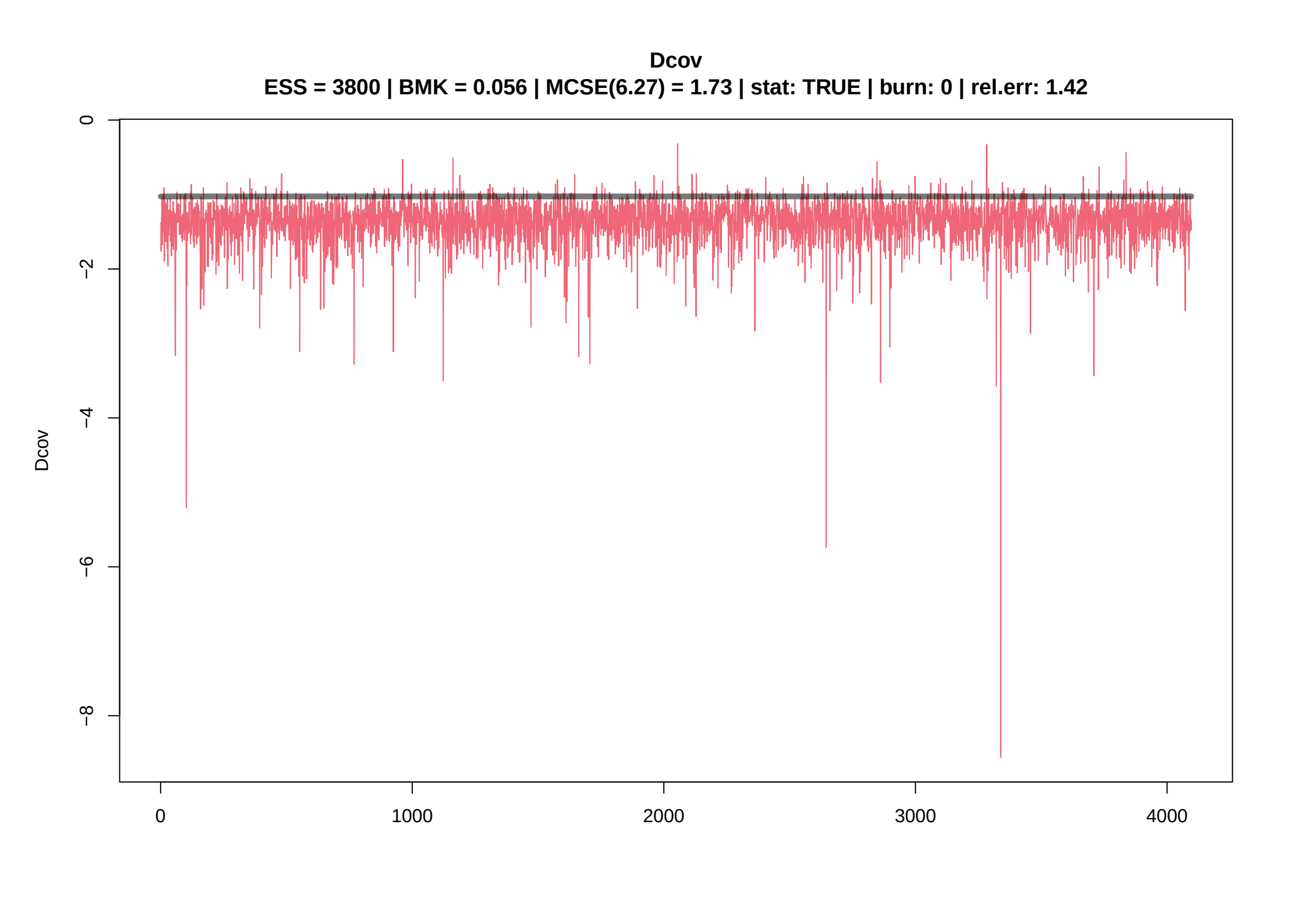

Pdatum4
ESS = 622 | BMK = 0.0454 | MCSE(6.27) = 3.99 | stat: TRUE | burn: 0 | rel.err: 0.0983
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

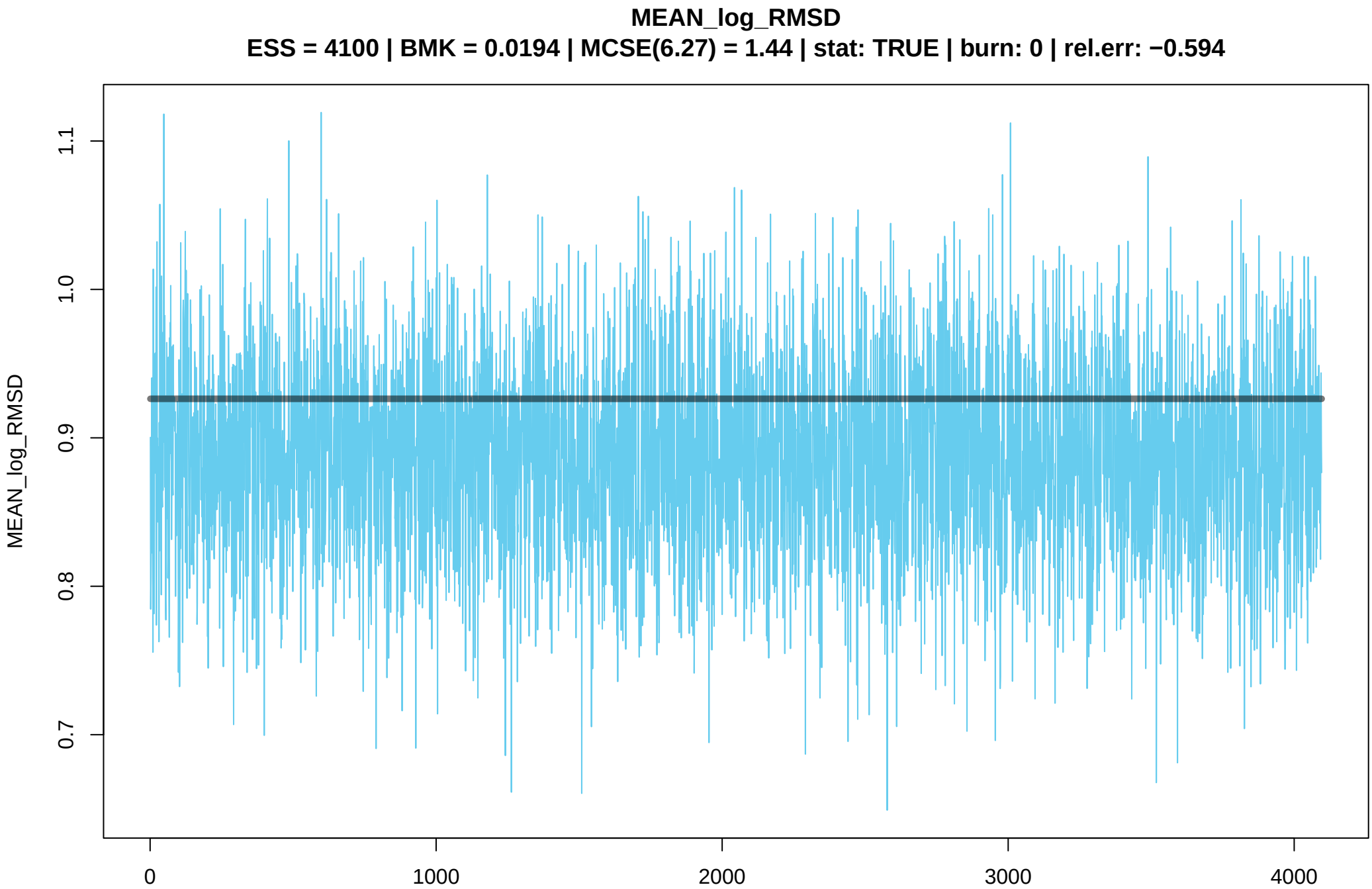

Pdatum5
ESS = 411 | BMK = 0.0479 | MCSE(6.27) = 3.94 | stat: FALSE | burn: 0 | rel.err: 1.42
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

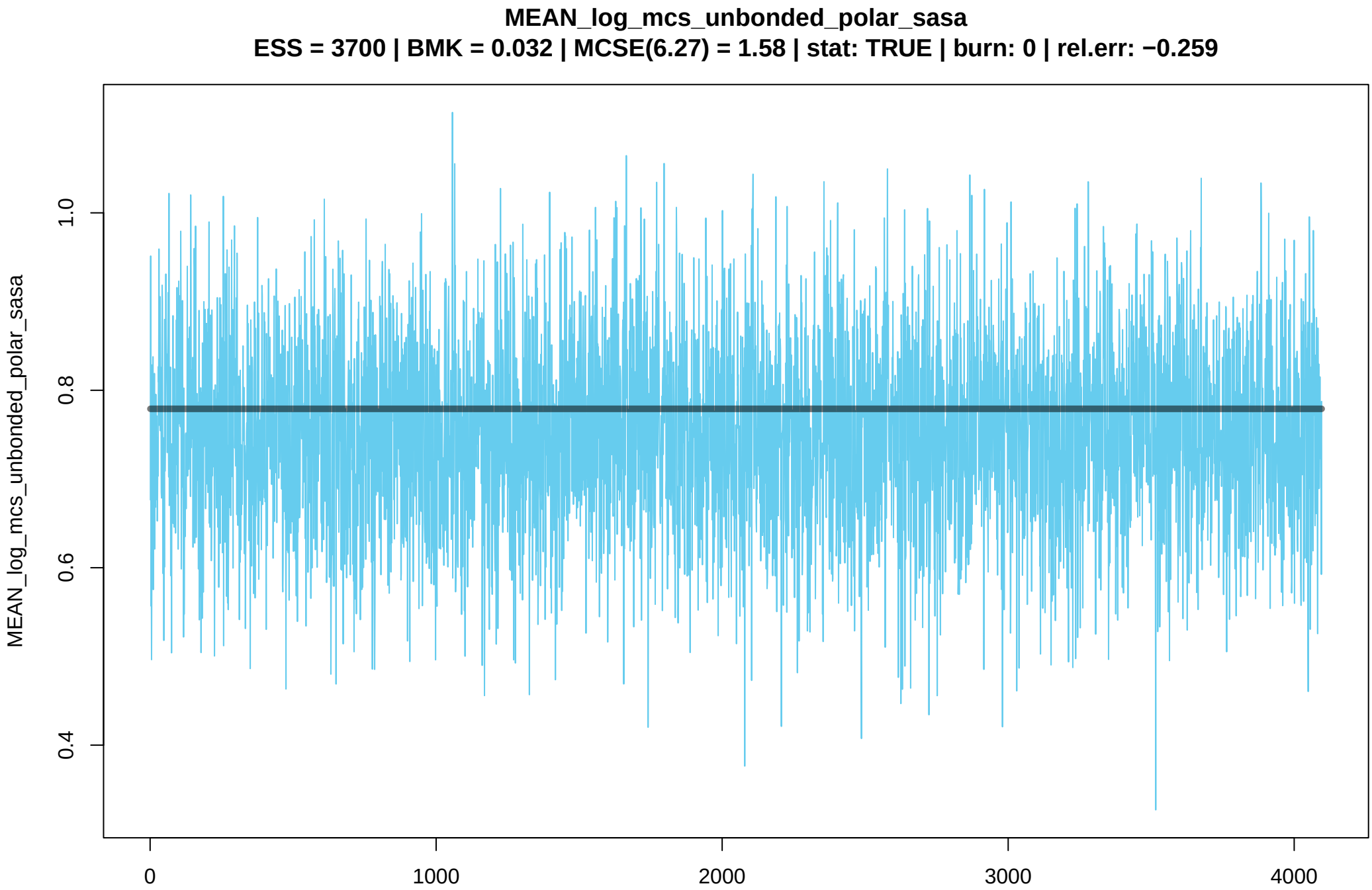

Pdatum6
ESS = 1970 | BMK = 0.0422 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: 0.65
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

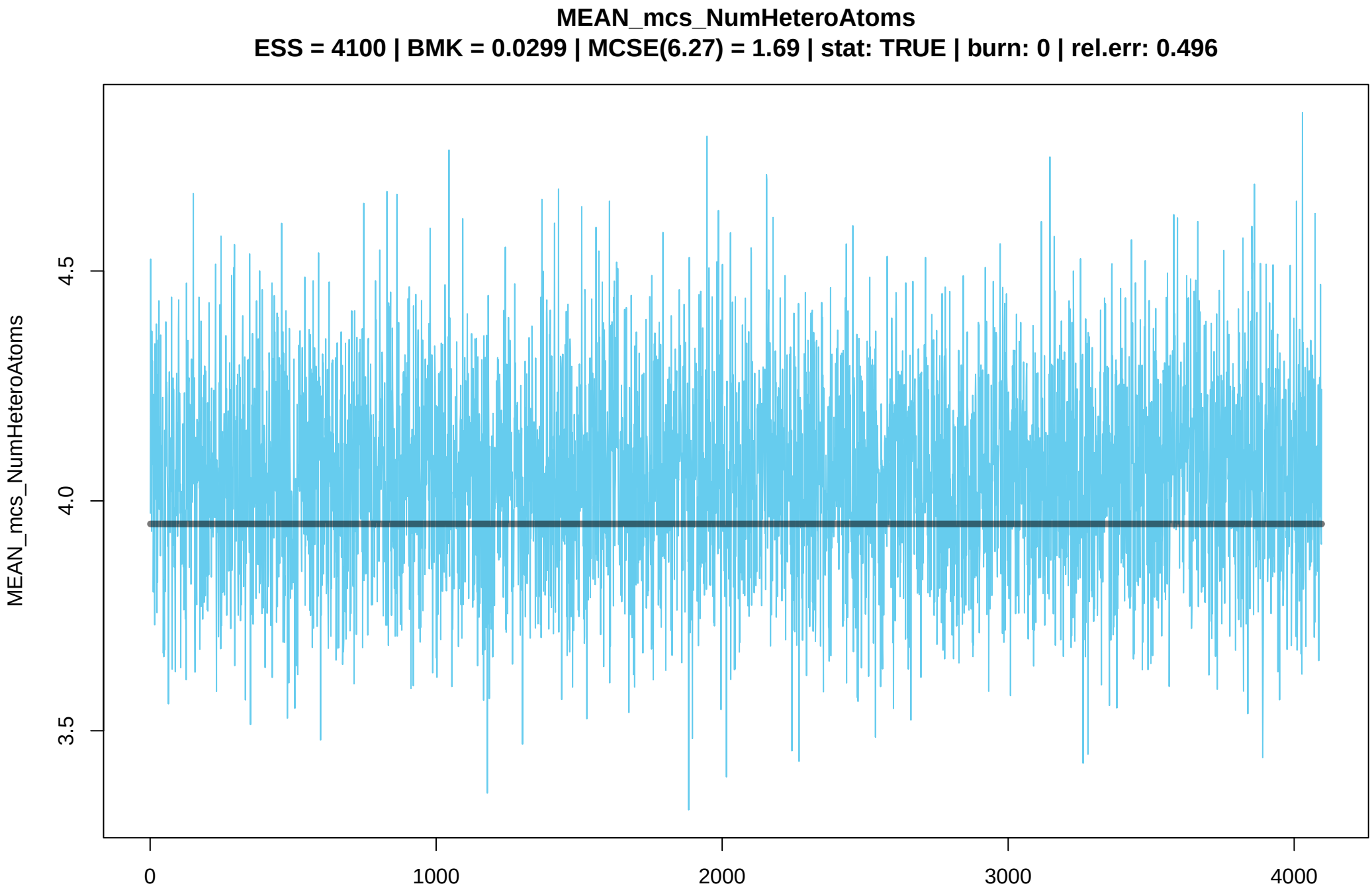

Pdatum7
ESS = 2840 | BMK = 0.0271 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: 0.765
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

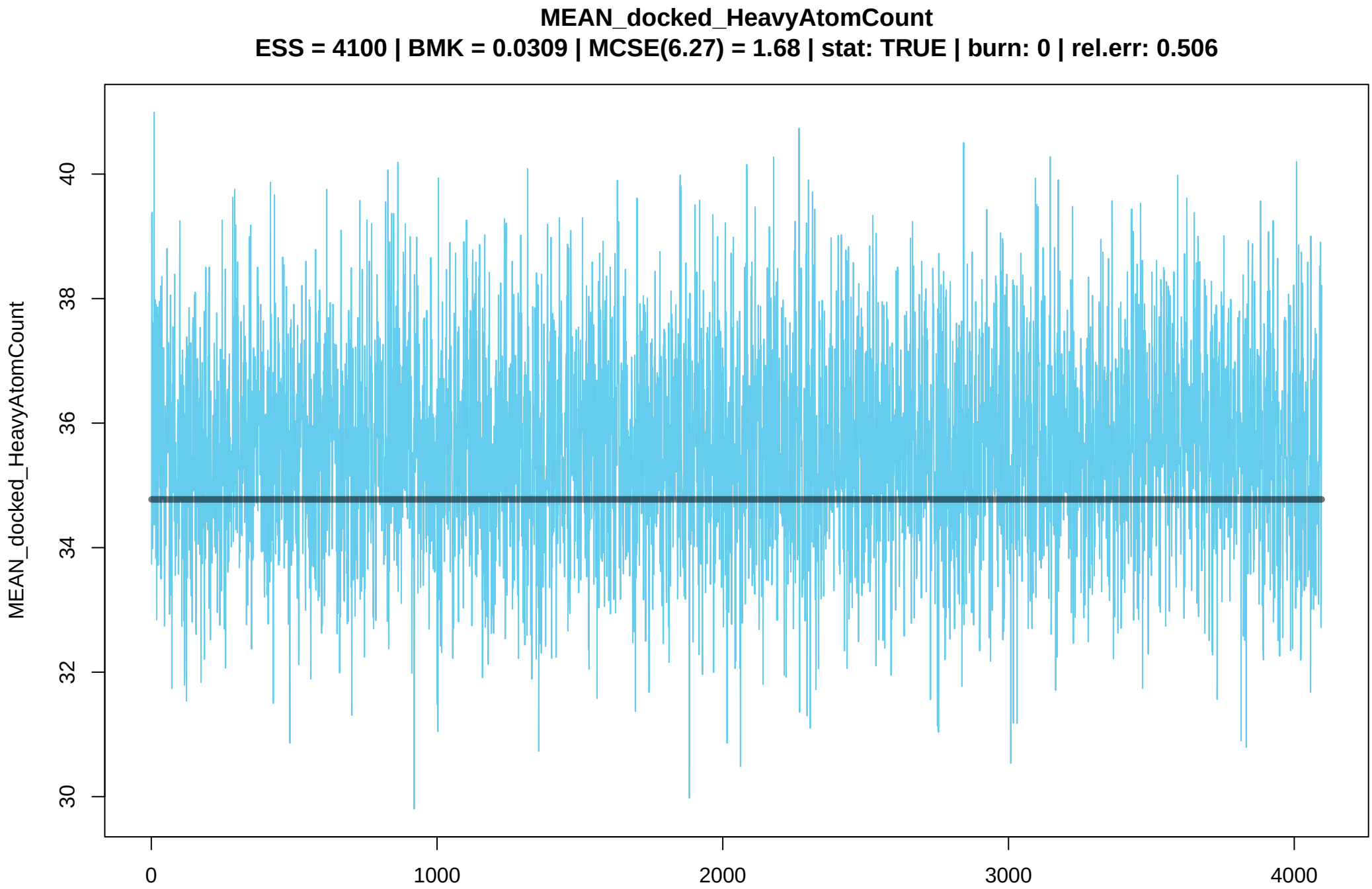

Pdatum8
ESS = 592 | BMK = 0.0642 | MCSE(6.27) = 4.19 | stat: TRUE | burn: 0 | rel.err: 0.554
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

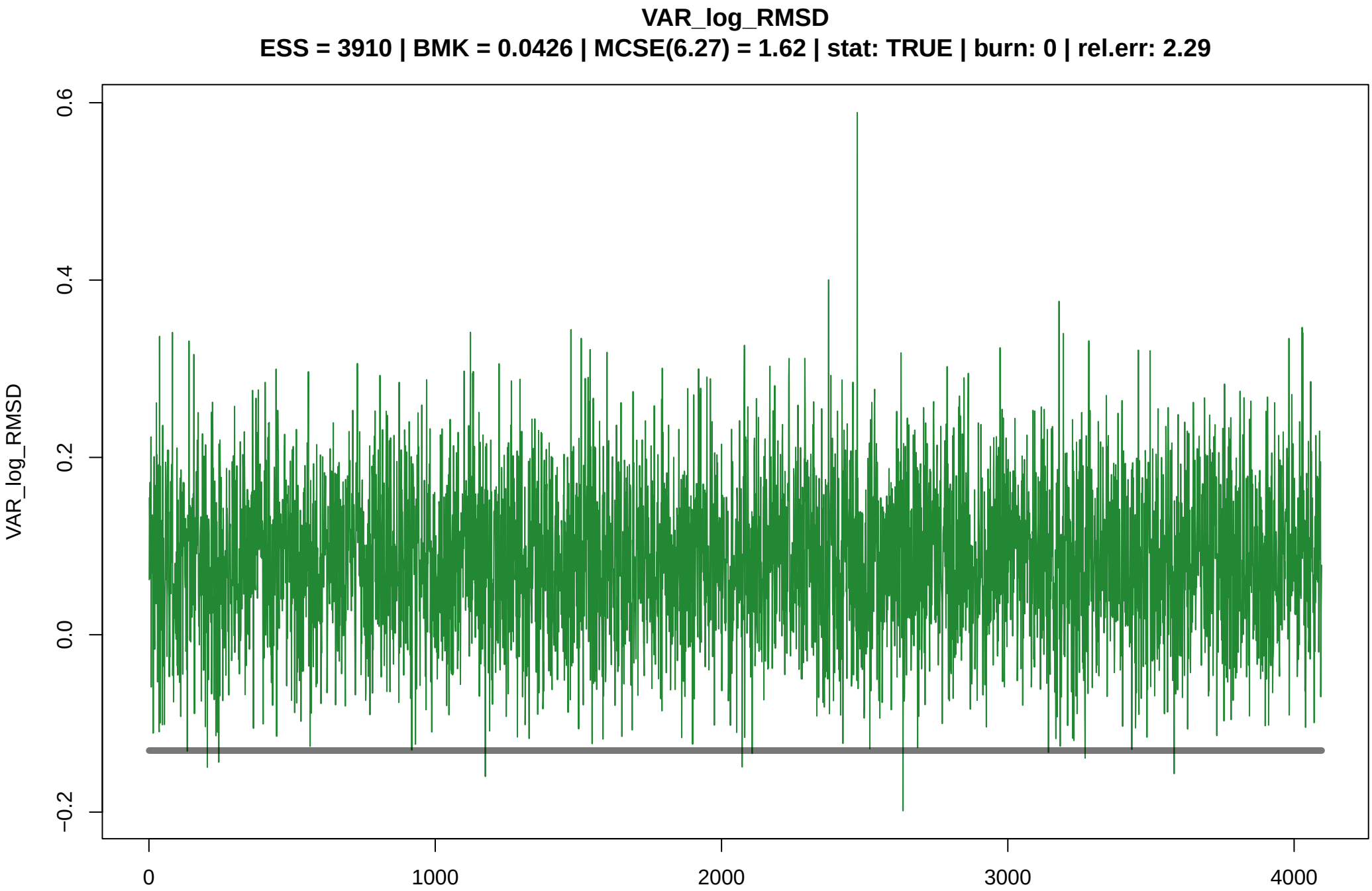

Dcov
ESS = 3800 | BMK = 0.056 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: 1.42
Dcov
0
−2
−4
−6
−8
0
1000
2000
3000
4000

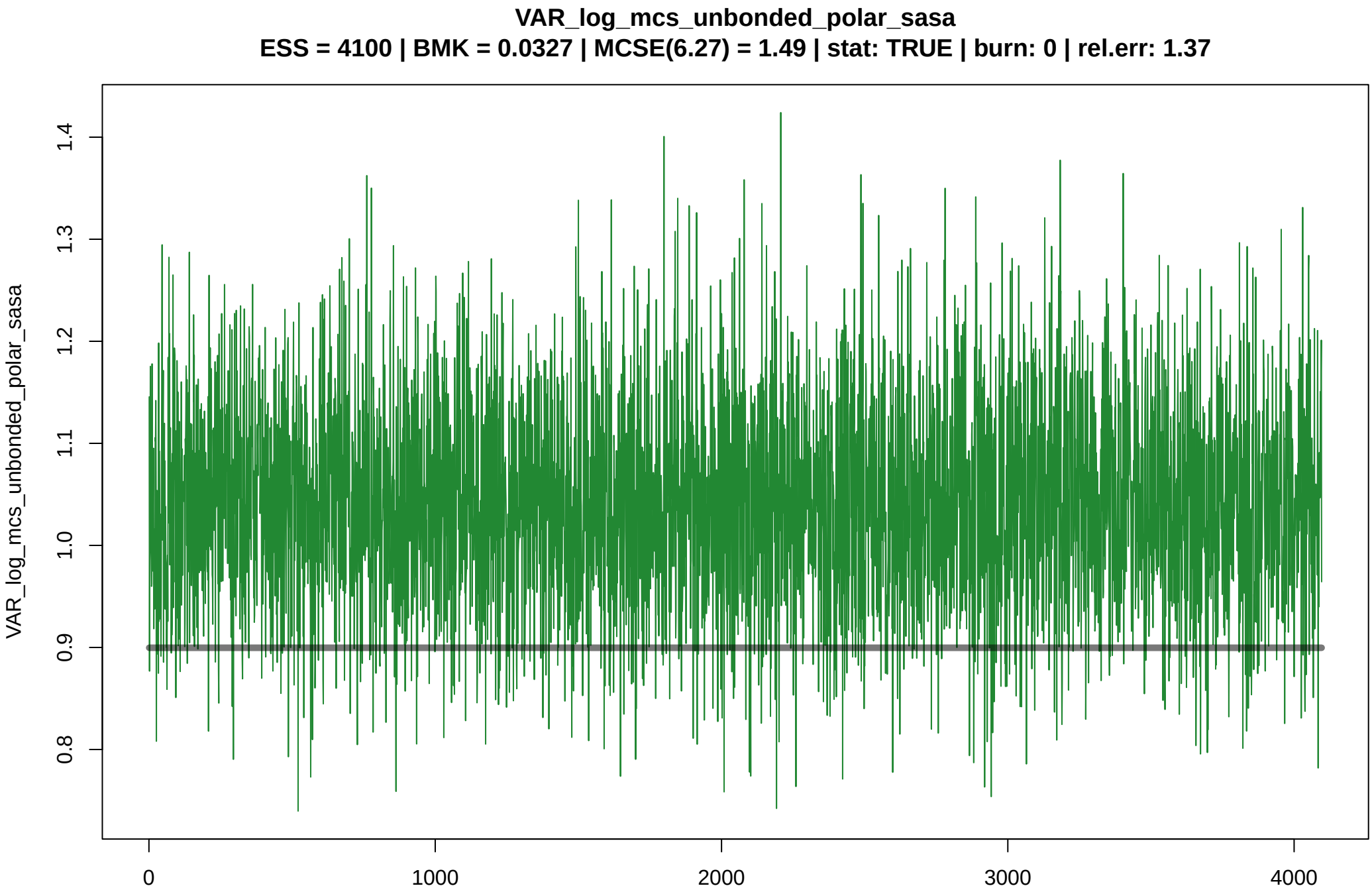

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0194 | MCSE(6.27) = 1.44 | stat: TRUE | burn: 0 | rel.err: −0.594
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

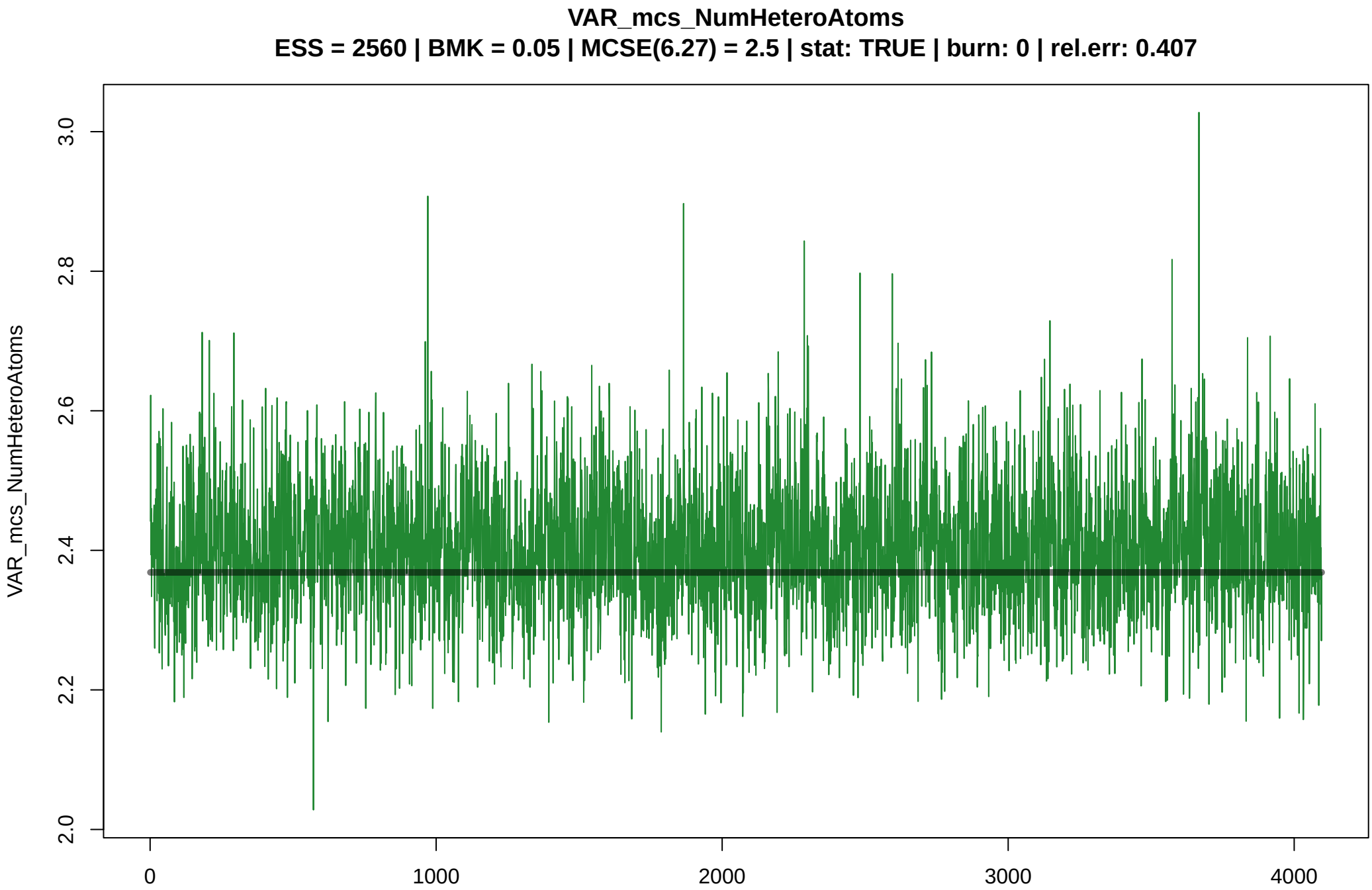

MEAN_log_mcs_unbonded_polar_sasa
ESS = 3700 | BMK = 0.032 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: −0.259
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

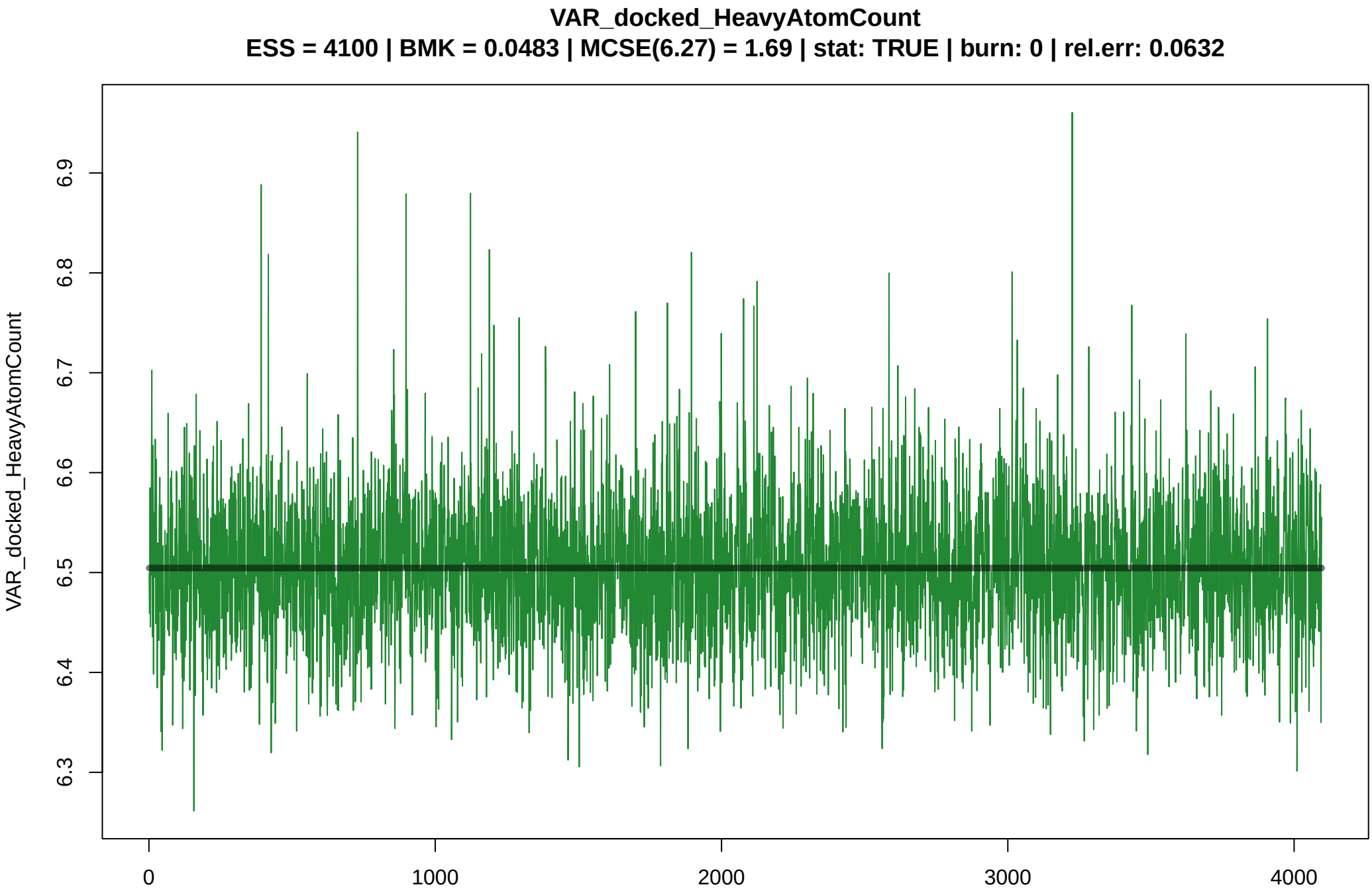

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0299 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.496
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

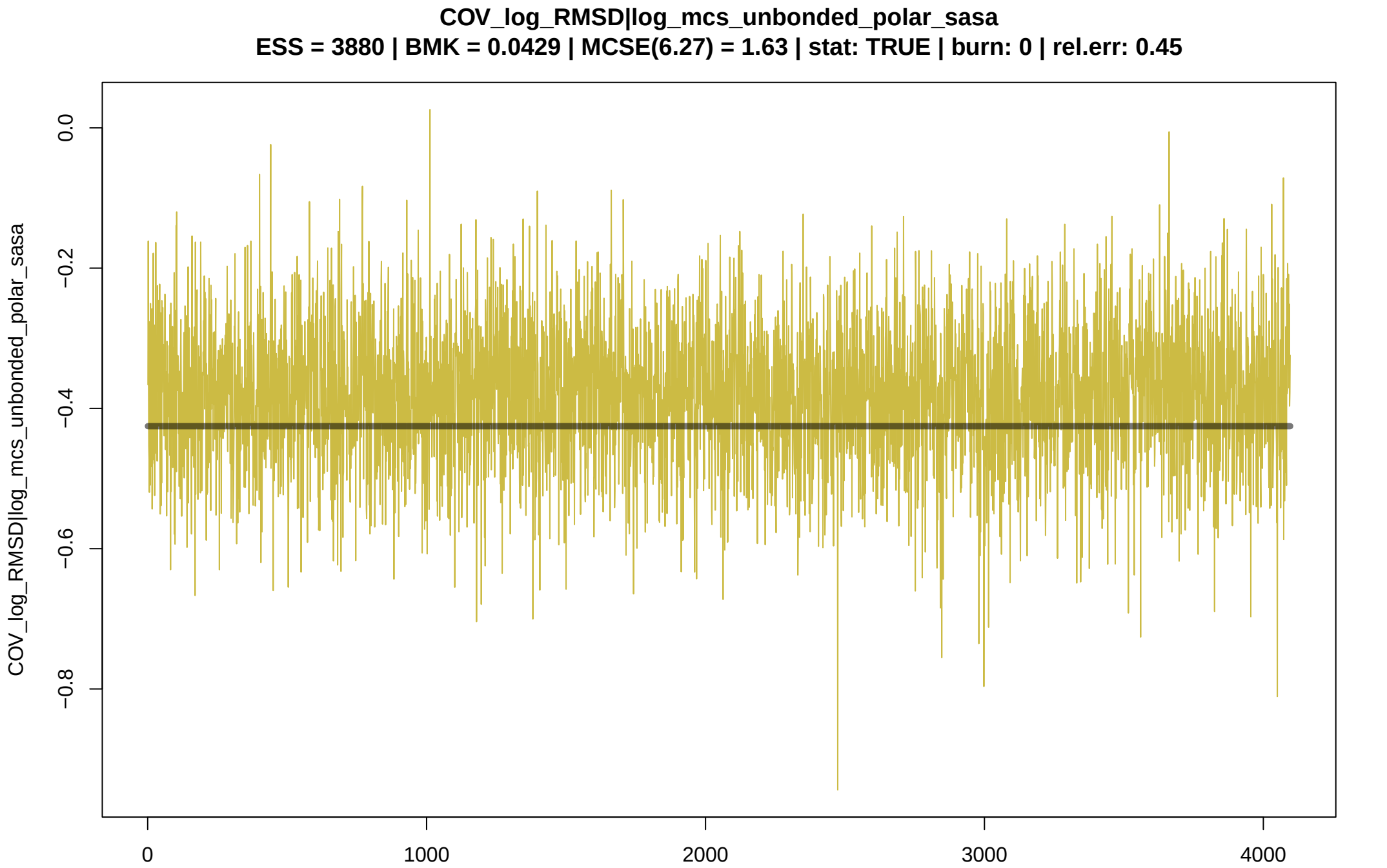

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0309 | MCSE(6.27) = 1.68 | stat: TRUE | burn: 0 | rel.err: 0.506
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
1000
2000
3000
4000

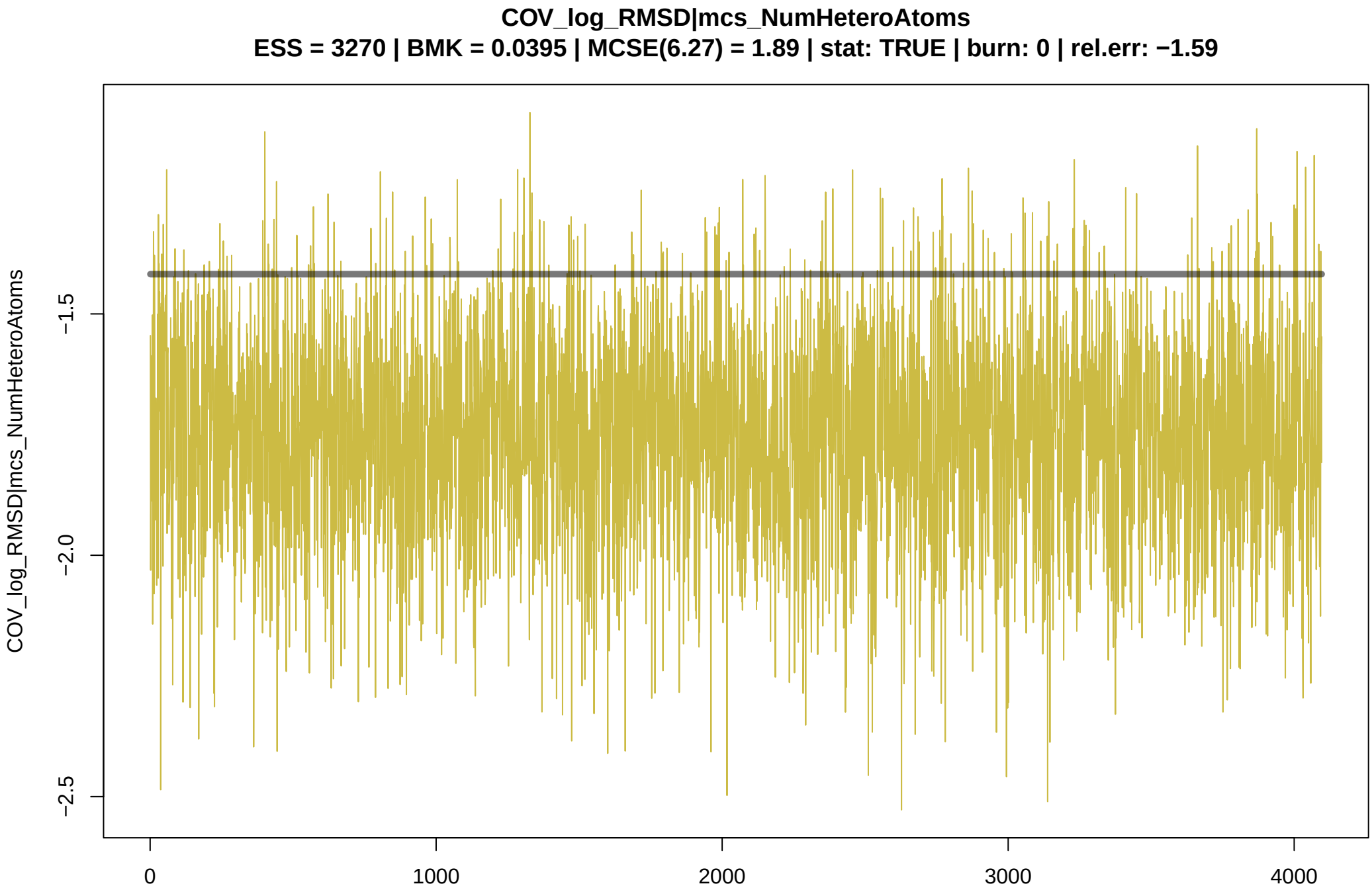

VAR_log_RMSD
ESS = 3910 | BMK = 0.0426 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: 2.29
VAR_log_RMSD
0.6
0.4
0.2
0.0
−0.2
0
1000
2000
3000
4000

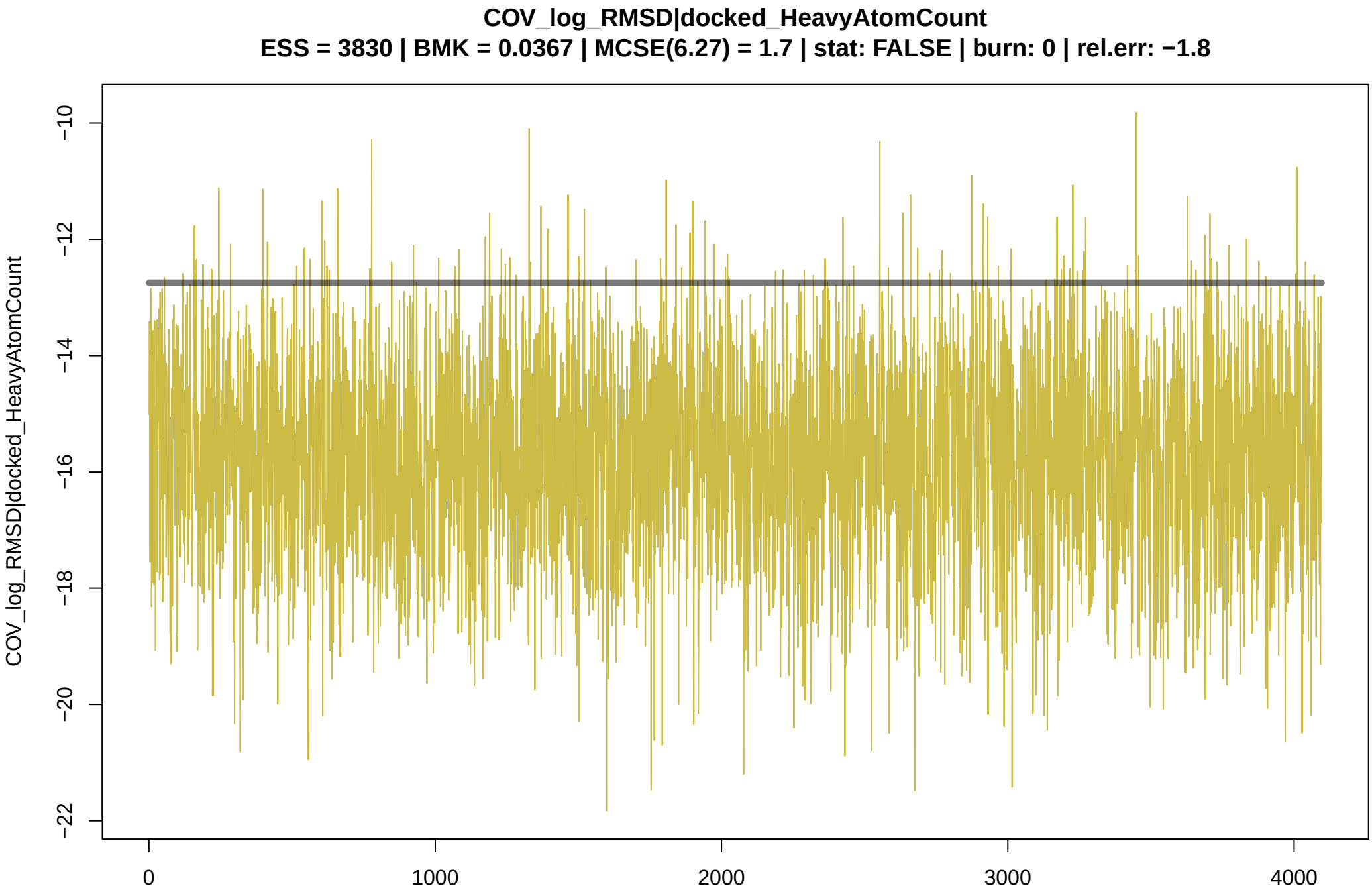

VAR_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0327 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0 | rel.err: 1.37
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
1000
2000
3000
4000

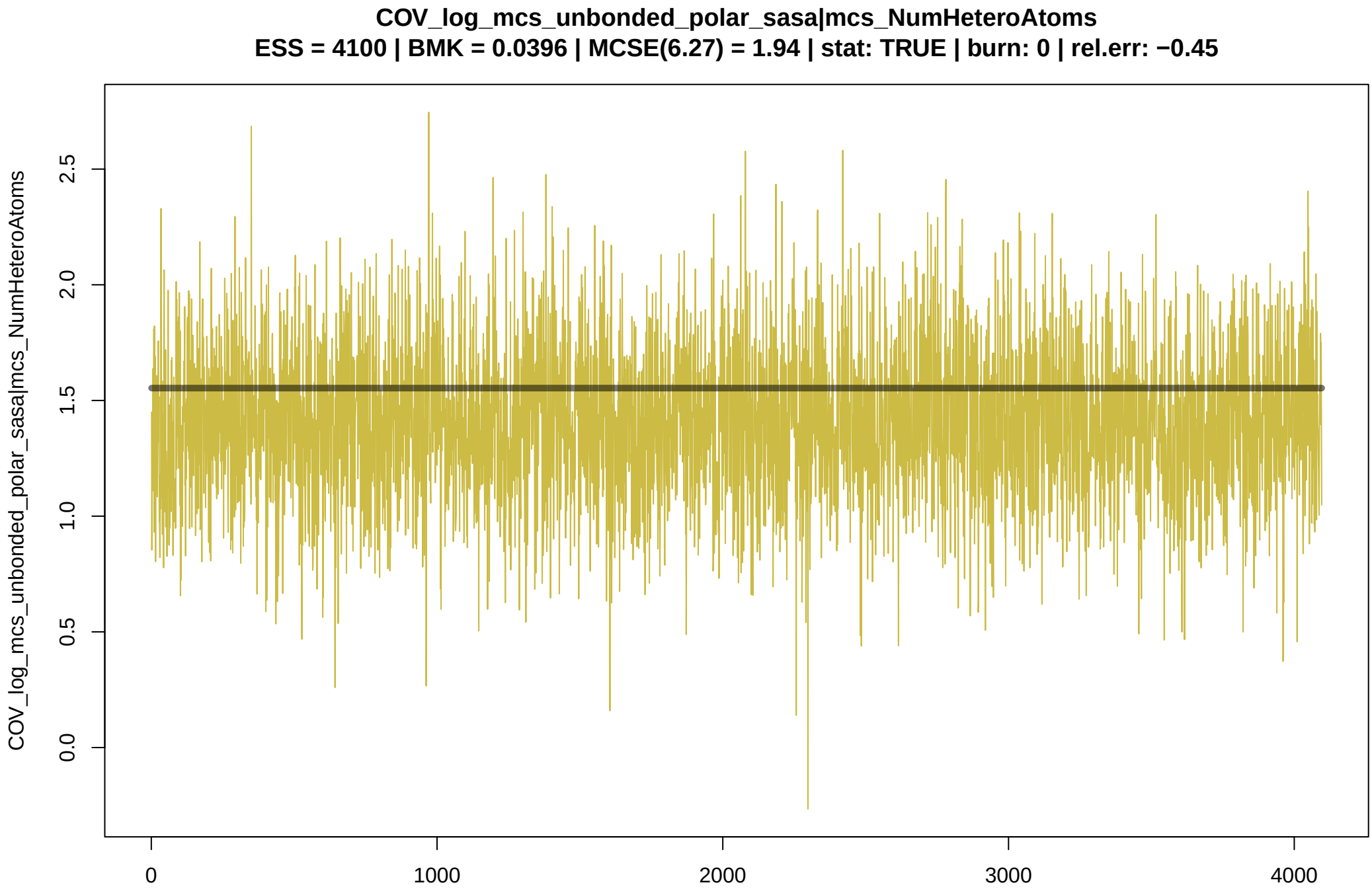

VAR_mcs_NumHeteroAtoms
ESS = 2560 | BMK = 0.05 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 0.407
VAR_mcs_NumHeteroAtoms
2.0
2.2
2.4
2.6
2.8
3.0
0
1000
2000
3000
4000

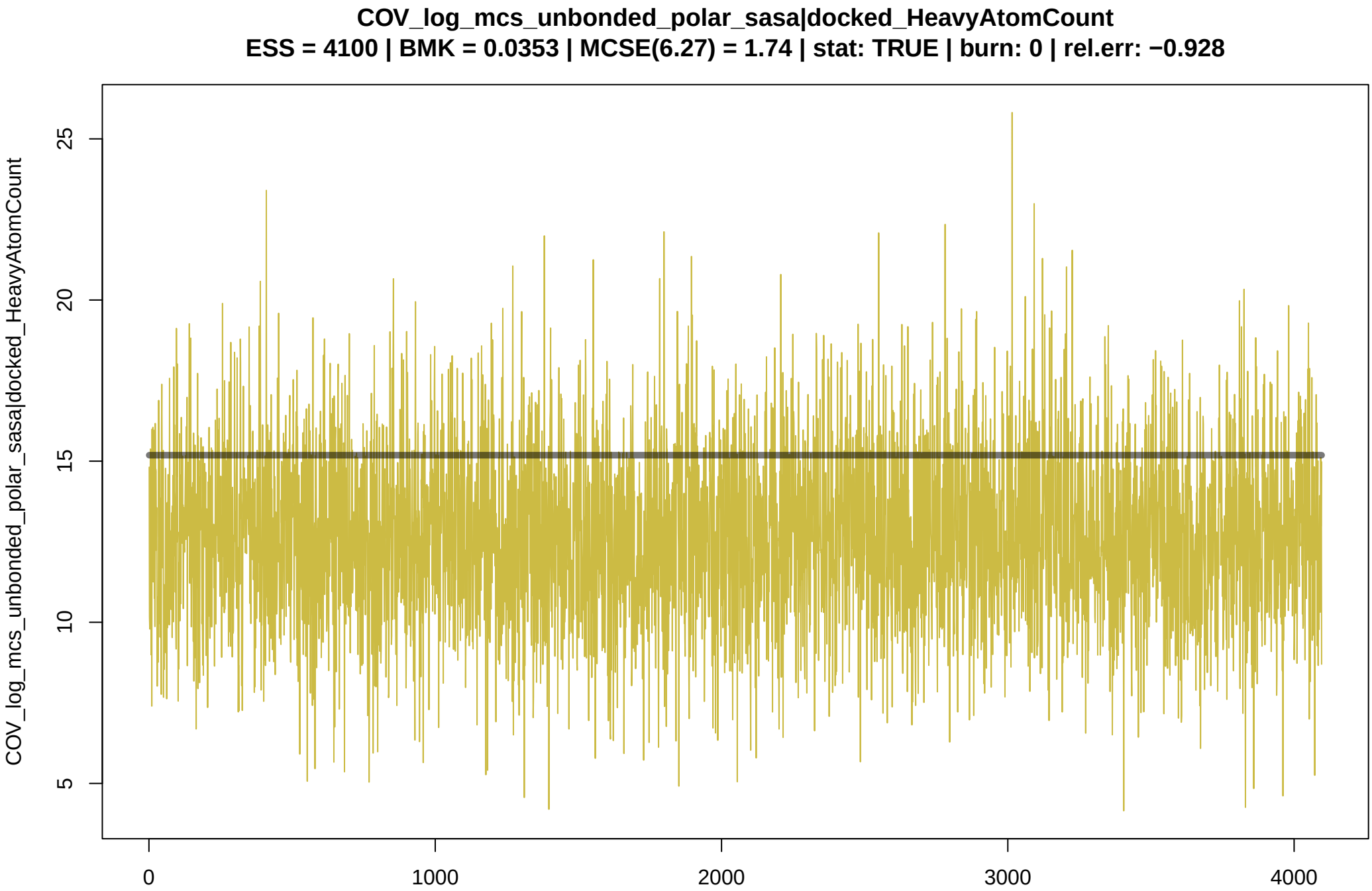

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0483 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.0632
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
6.9
0
1000
2000
3000
4000

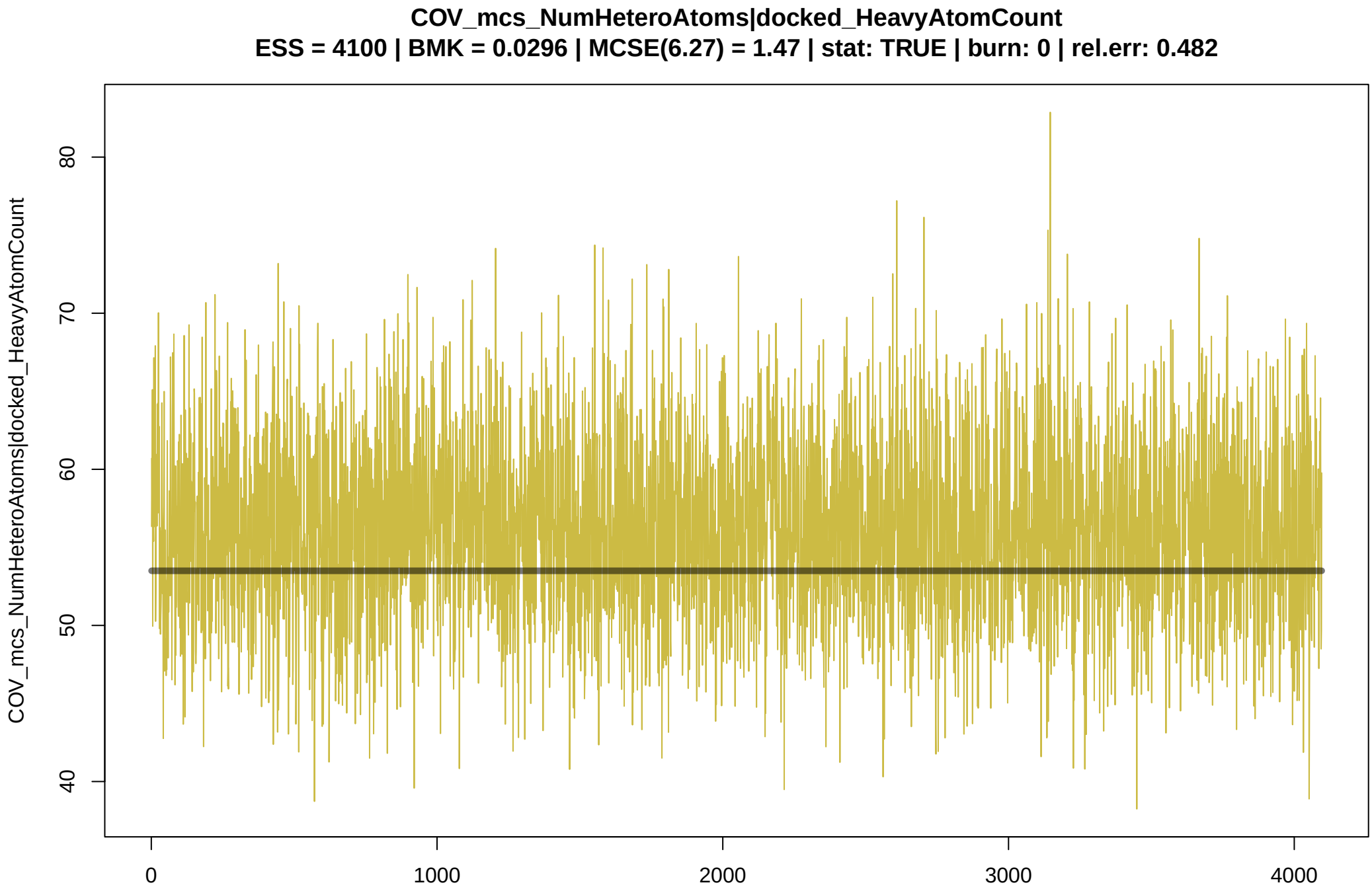

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3880 | BMK = 0.0429 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.45
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3270 | BMK = 0.0395 | MCSE(6.27) = 1.89 | stat: TRUE | burn: 0 | rel.err: −1.59
COV_log_RMSD|mcs_NumHeteroAtoms
−1.5
−2.0
−2.5
0
1000
2000
3000
4000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 3830 | BMK = 0.0367 | MCSE(6.27) = 1.7 | stat: FALSE | burn: 0 | rel.err: −1.8
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 = 4100 | BMK = 0.0396 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0 | rel.err: −0.45
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 = 0.0353 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0 | rel.err: −0.928
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 = 0.0296 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0 | rel.err: 0.482
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
1000
2000
3000
4000