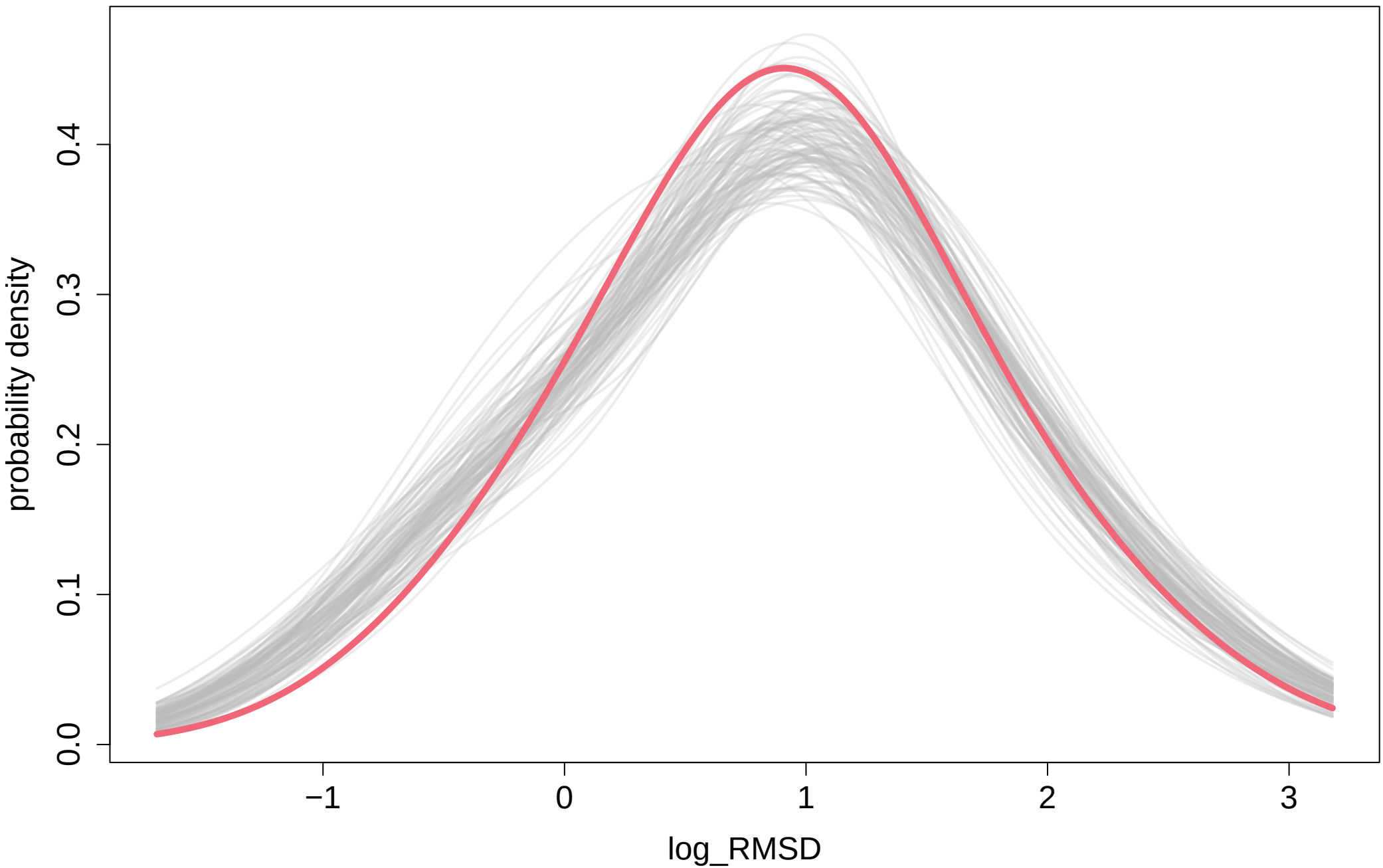
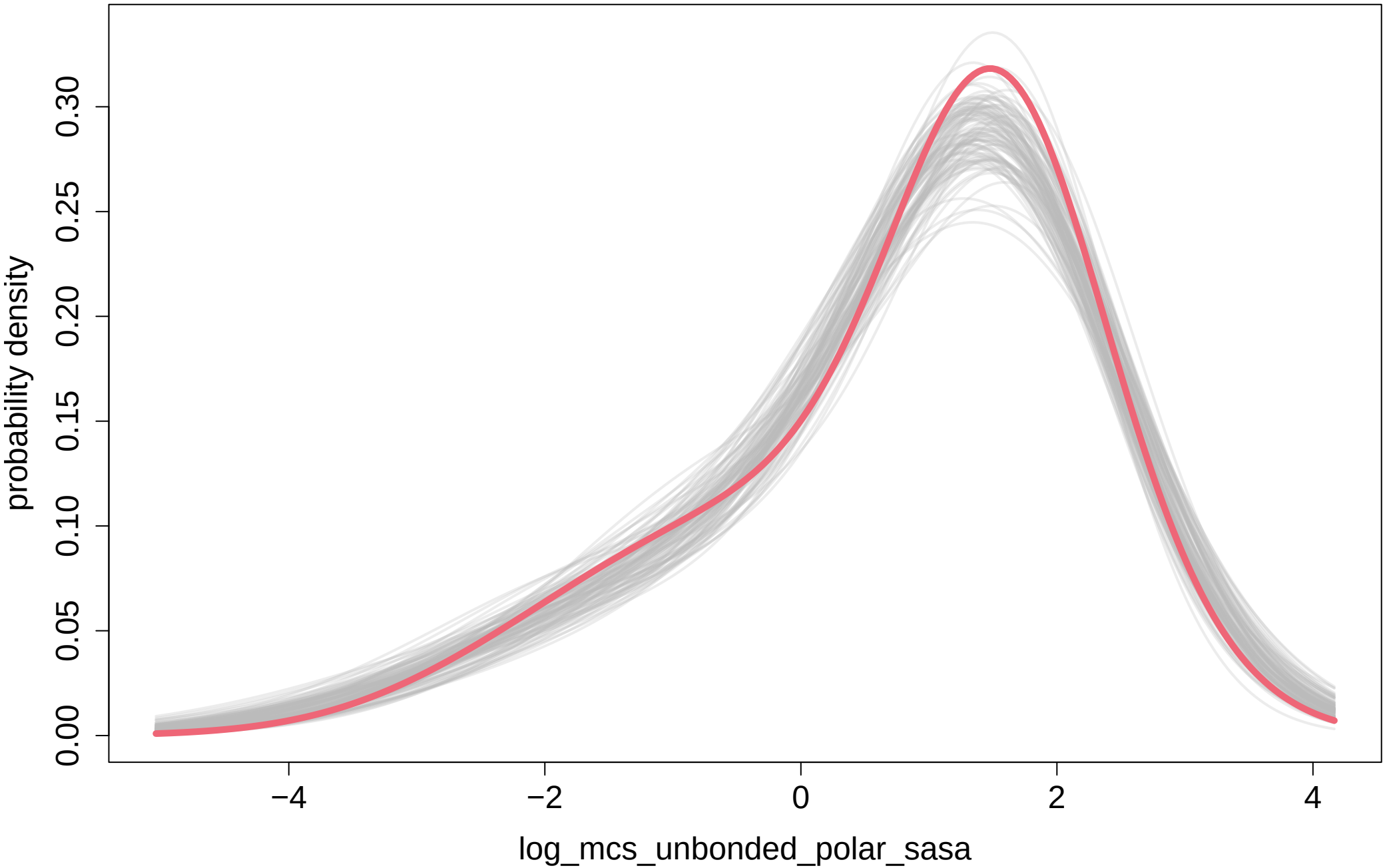
−− STATS maxD −−
min ESS = 302.592230892752
max BMK = 0.118494725641242
max MCSE = 5.44568843342439
all stationary: FALSE
burn: 0
max rel.err.: 1.97180711830812

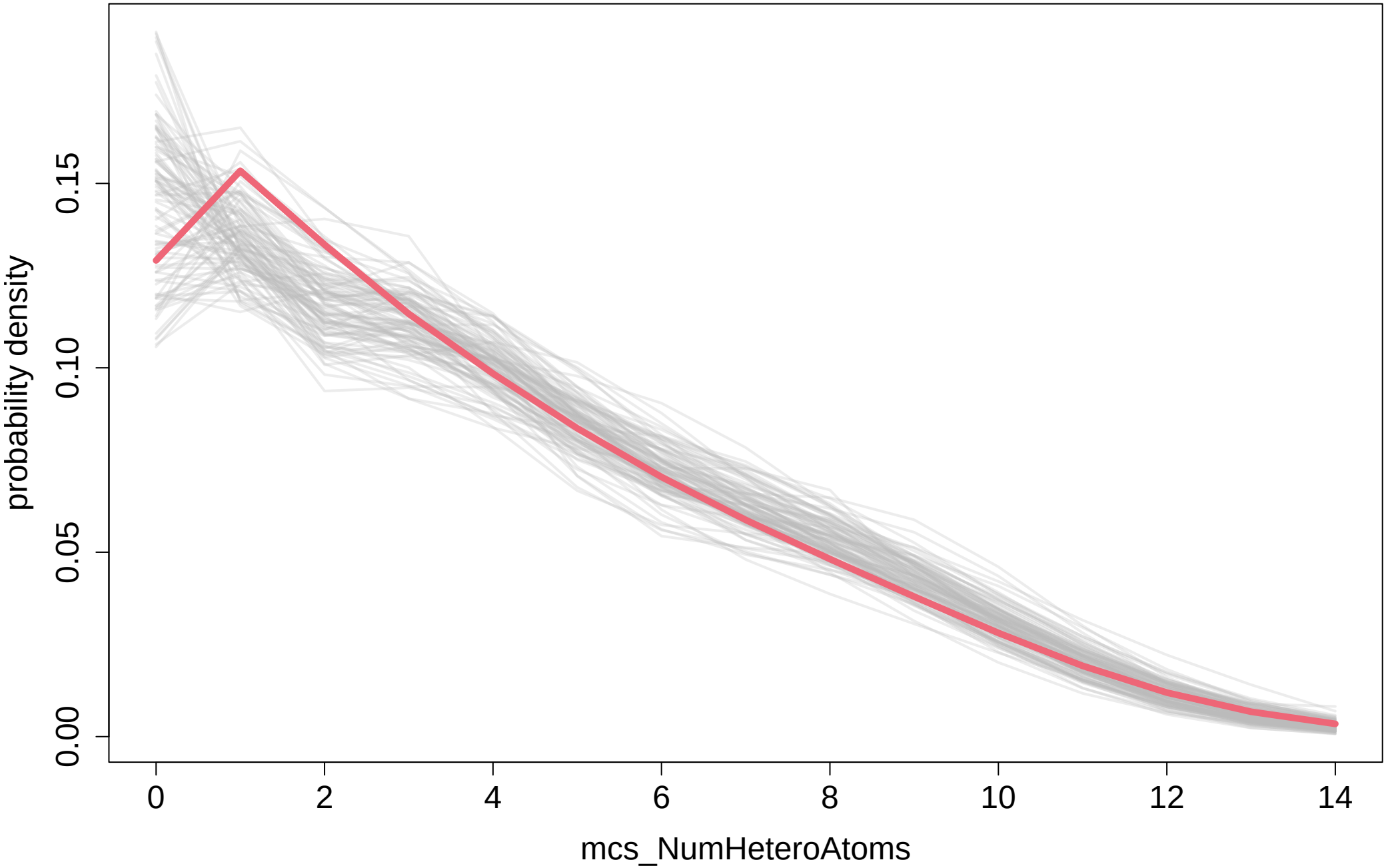
−− STATS 2D −−
min ESS = 3656.32488154547
max BMK = 0.052495446406915
max MCSE = 1.75913281633945
all stationary: TRUE
burn: 0
max rel.err.: 1.77979820165071

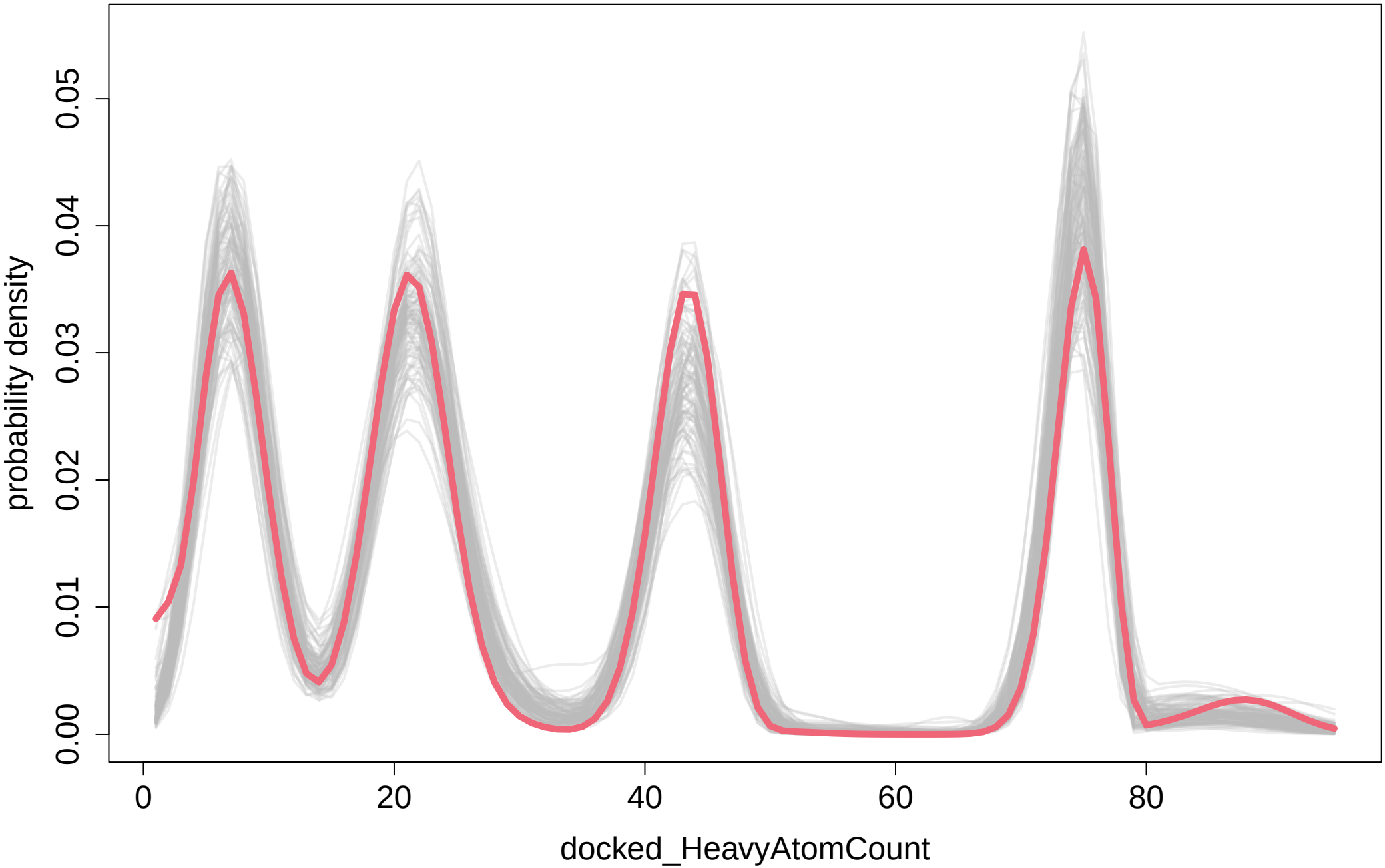
−− STATS 1D −−
min ESS = 2910.13425480568
max BMK = 0.061201891537352 6
max MCSE = 1.99469516775869
all stationary: TRUE
burn: 0
max rel.err.: 2.28089488346136

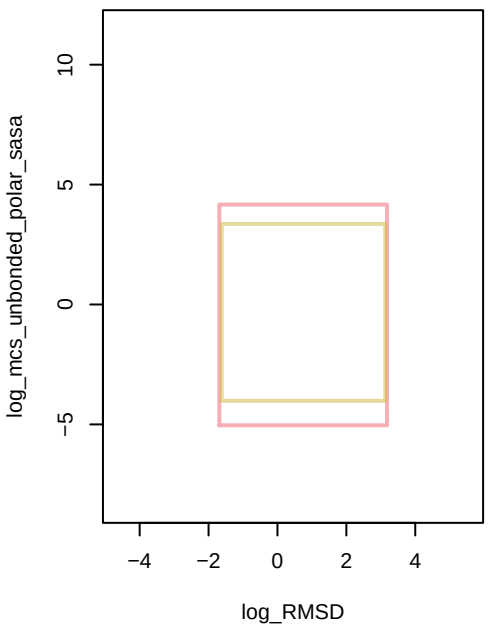
Occupied clusters: 10 of 16
LL: −2160 +− 6.59

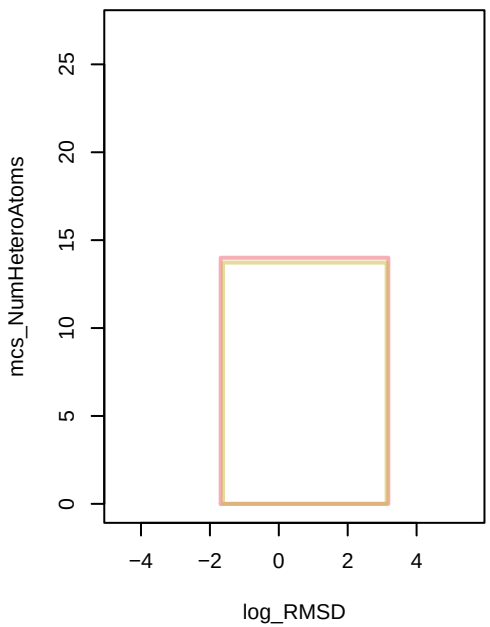

probability density
0.0
0.1
0.2
0.3
0.4
−1
0
1
2
3
log_RMSD

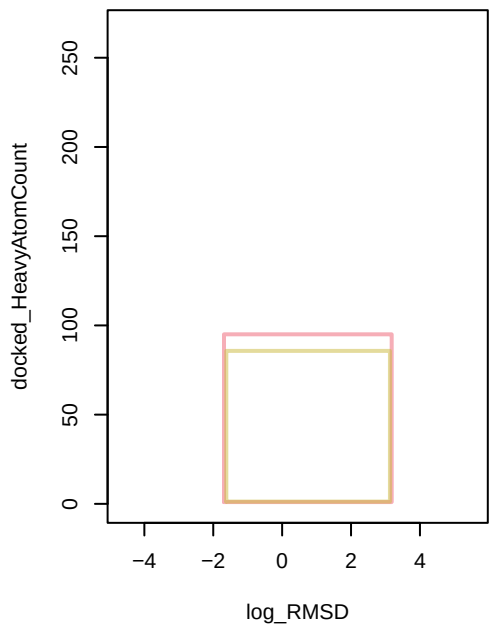

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

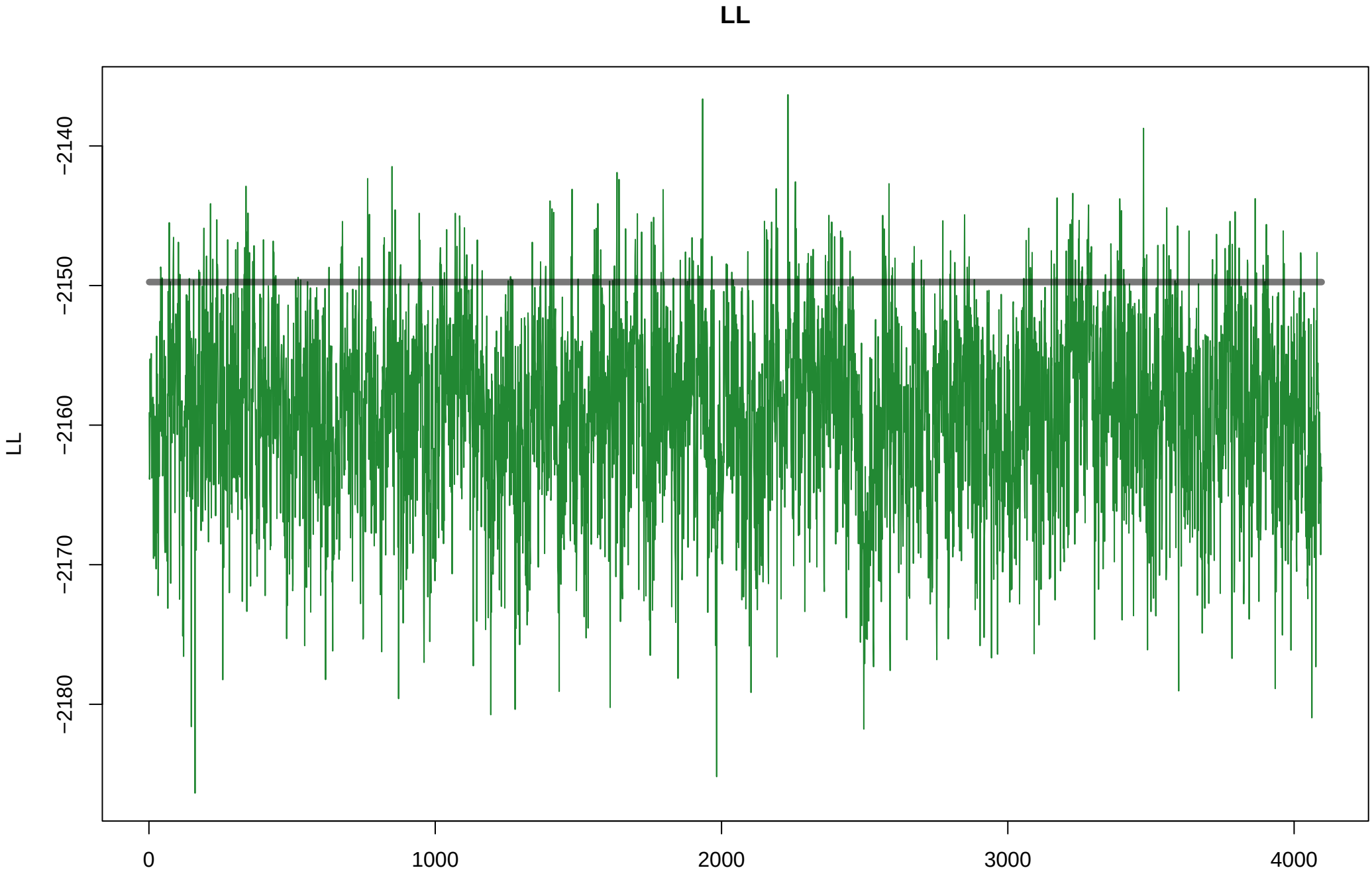

probability density
0.00
0.05
0.10
0.15
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

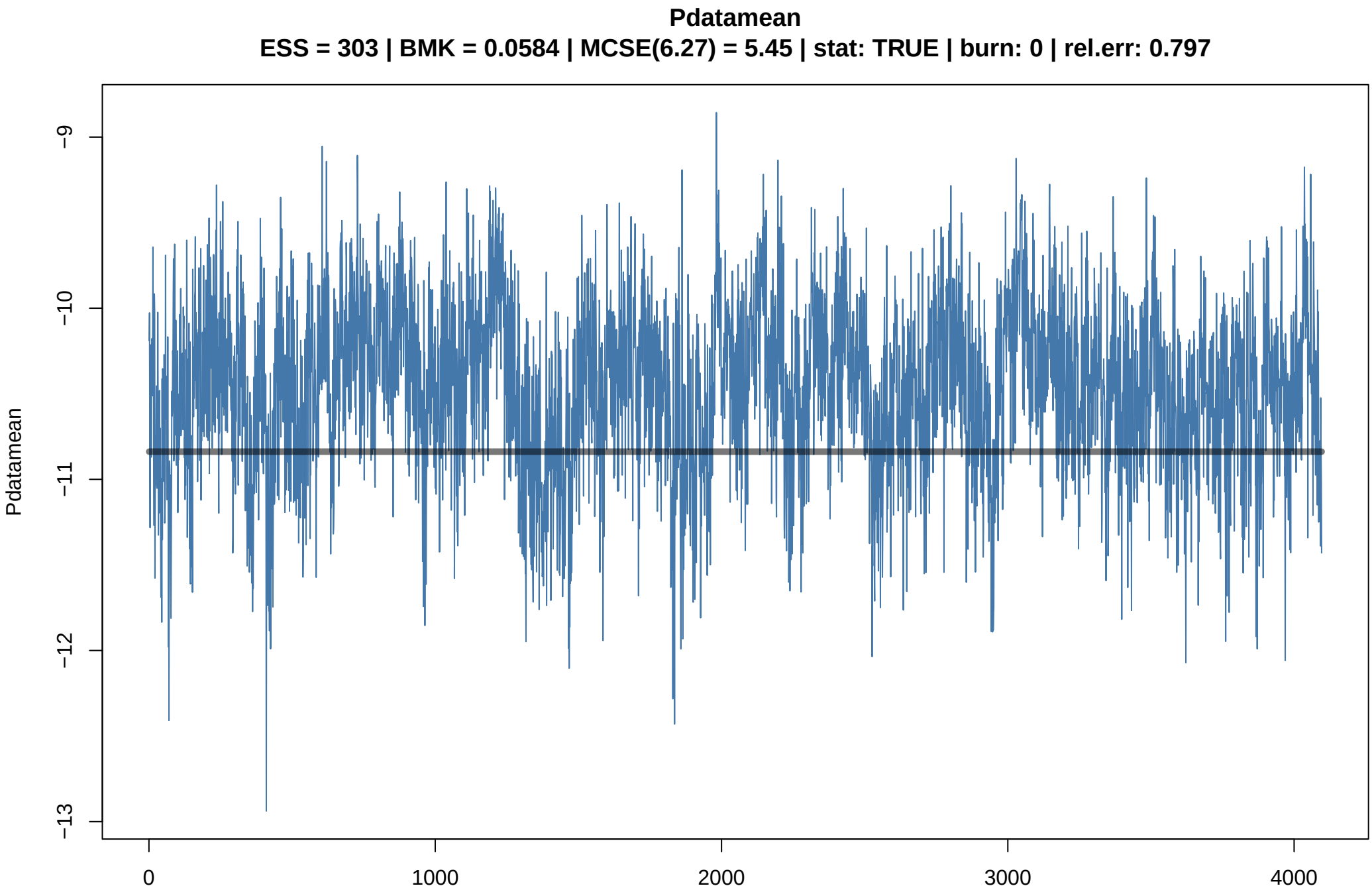

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
20
40
60
80
docked_HeavyAtomCount

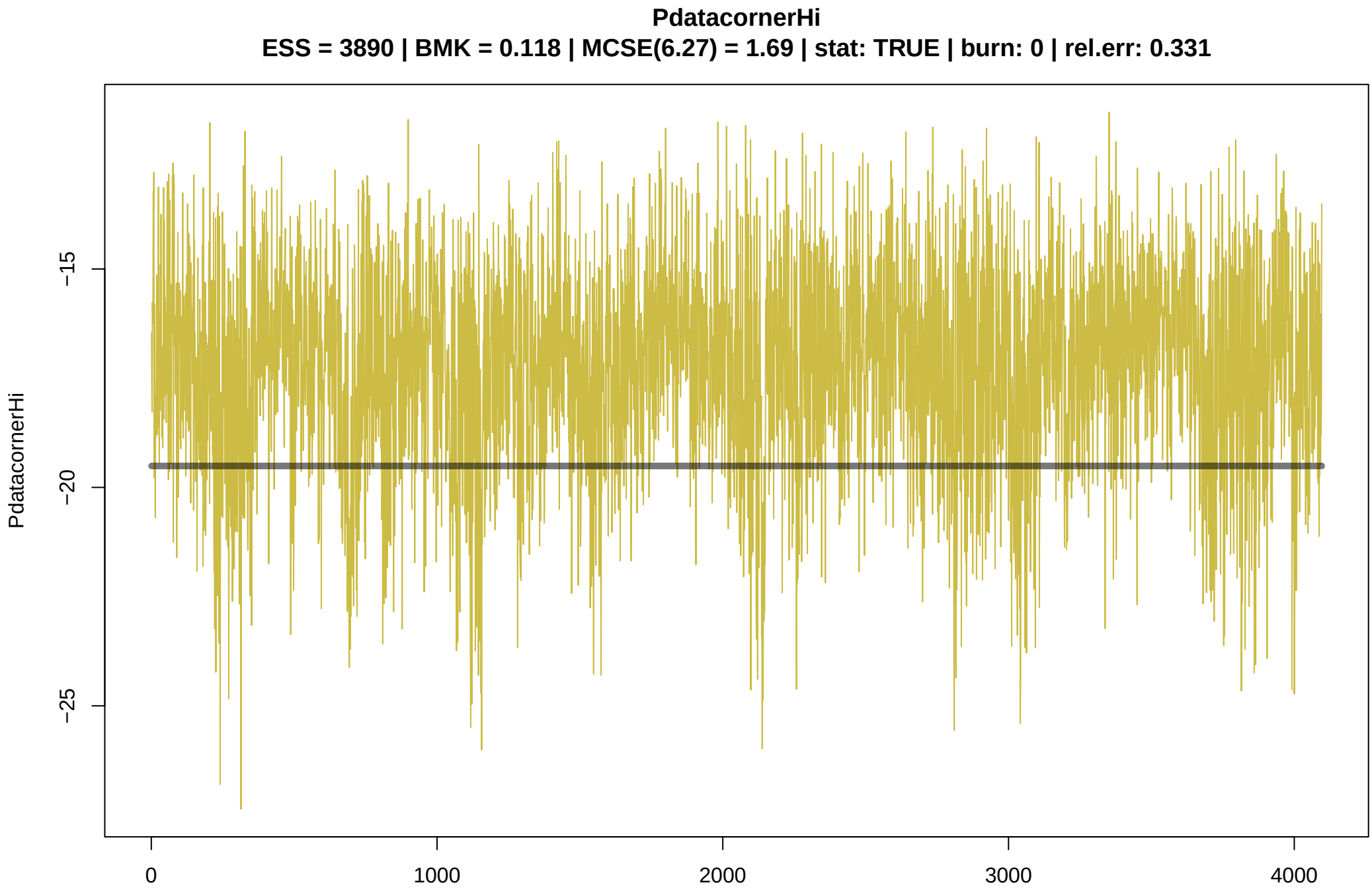

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
log_RMSD

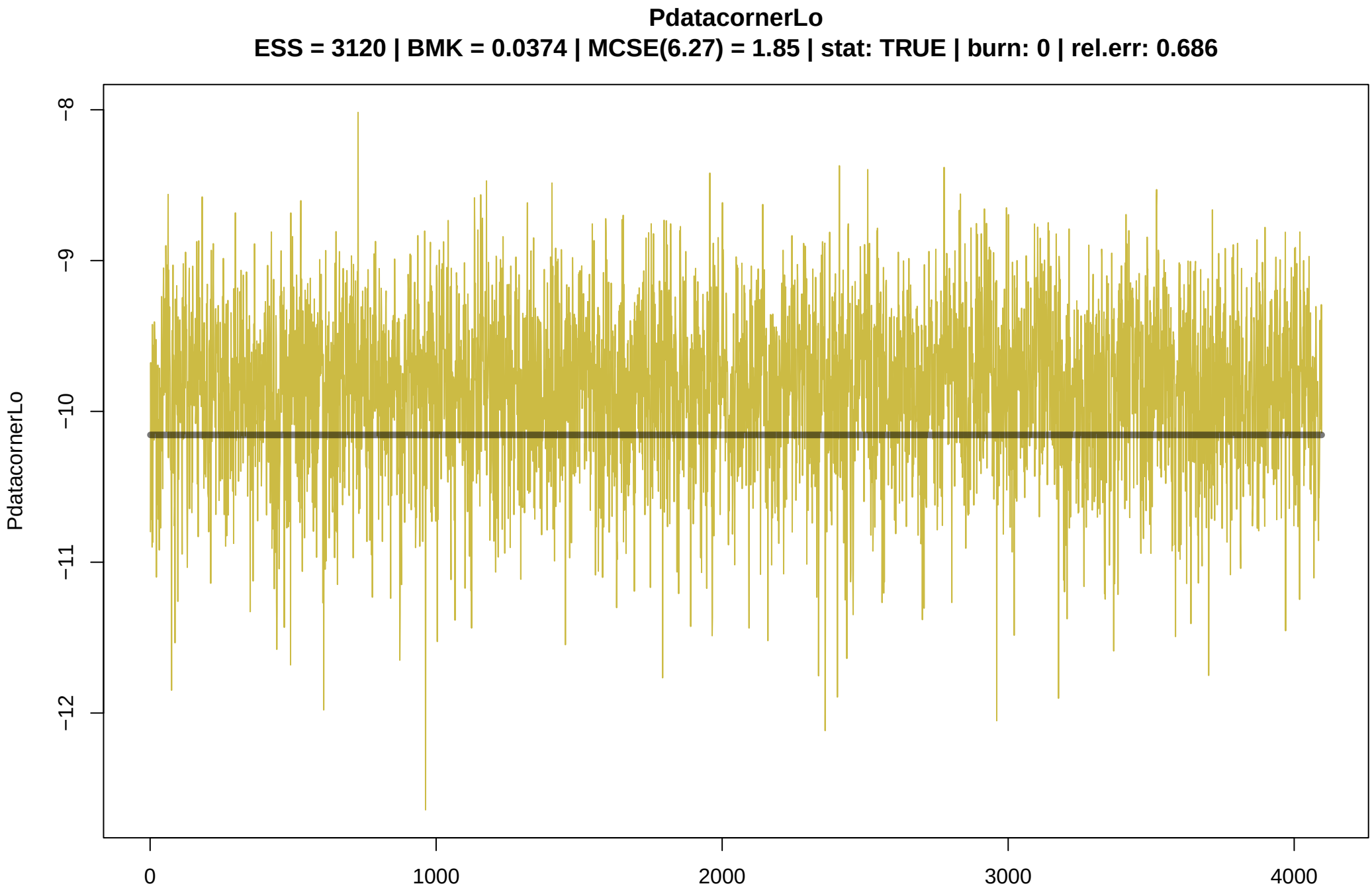

mcs_NumHeteroAtoms
25
20
15
10
5
0
−4
−2
0
2
4
log_RMSD

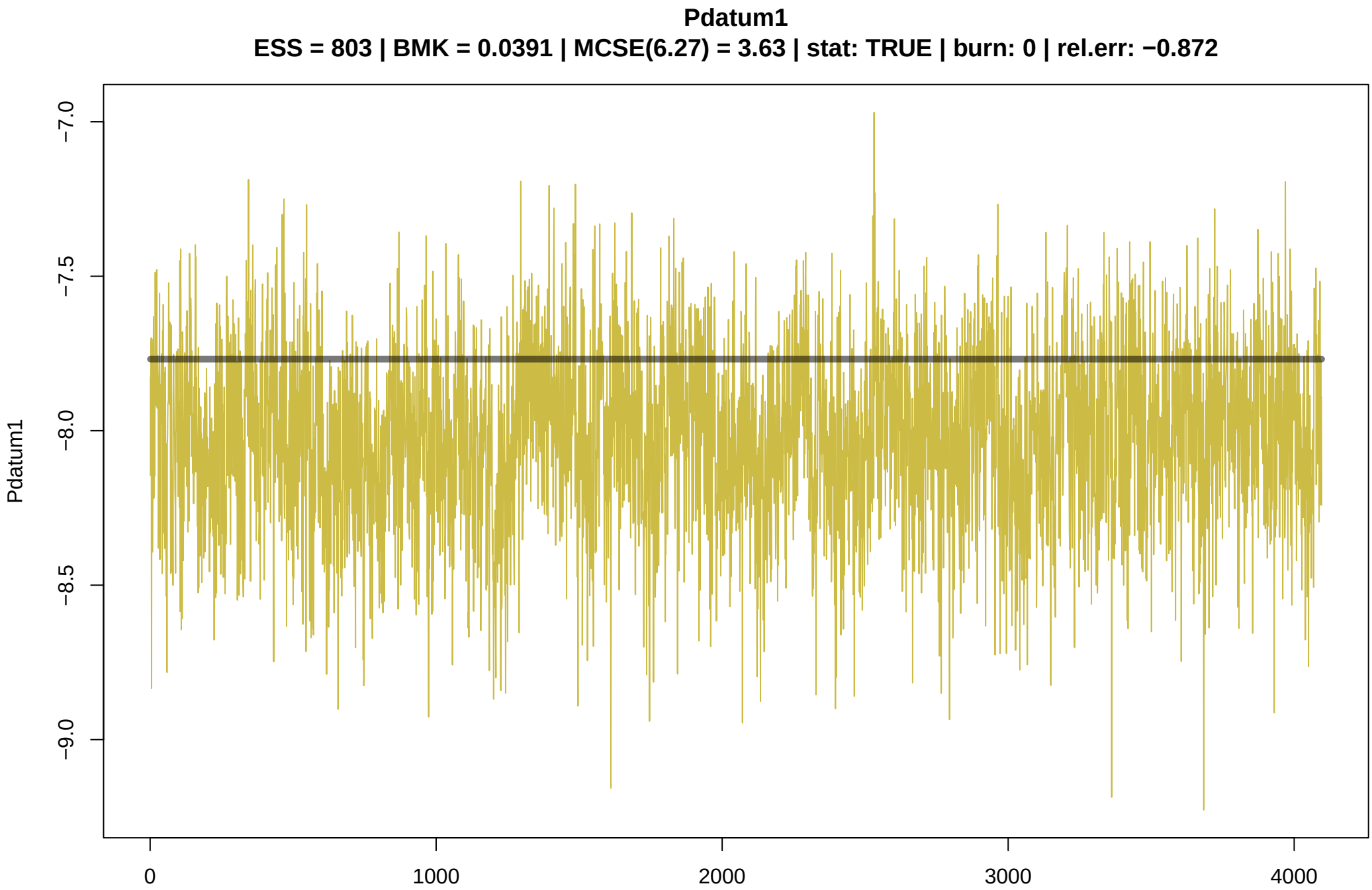

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
log_RMSD

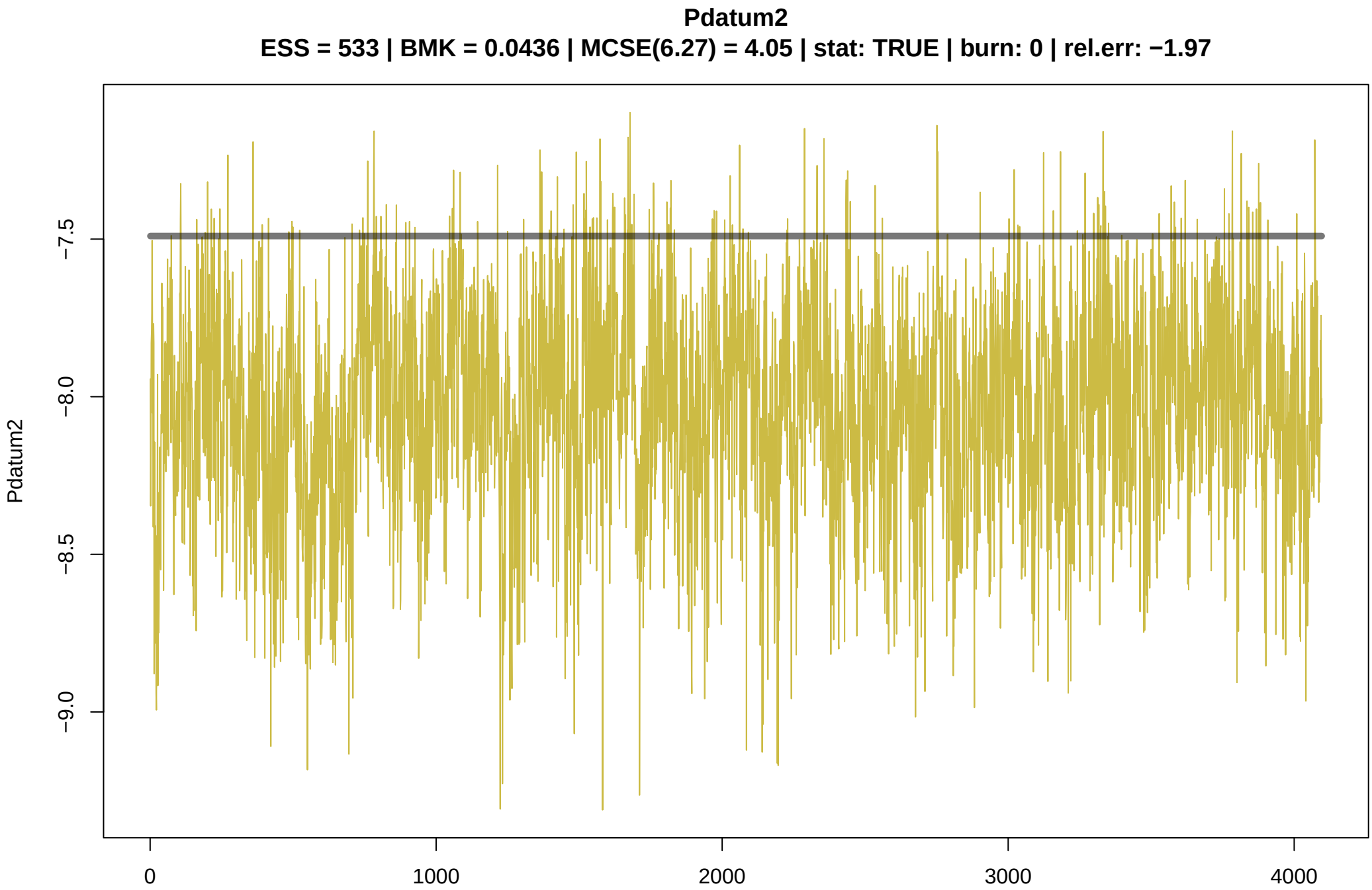

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

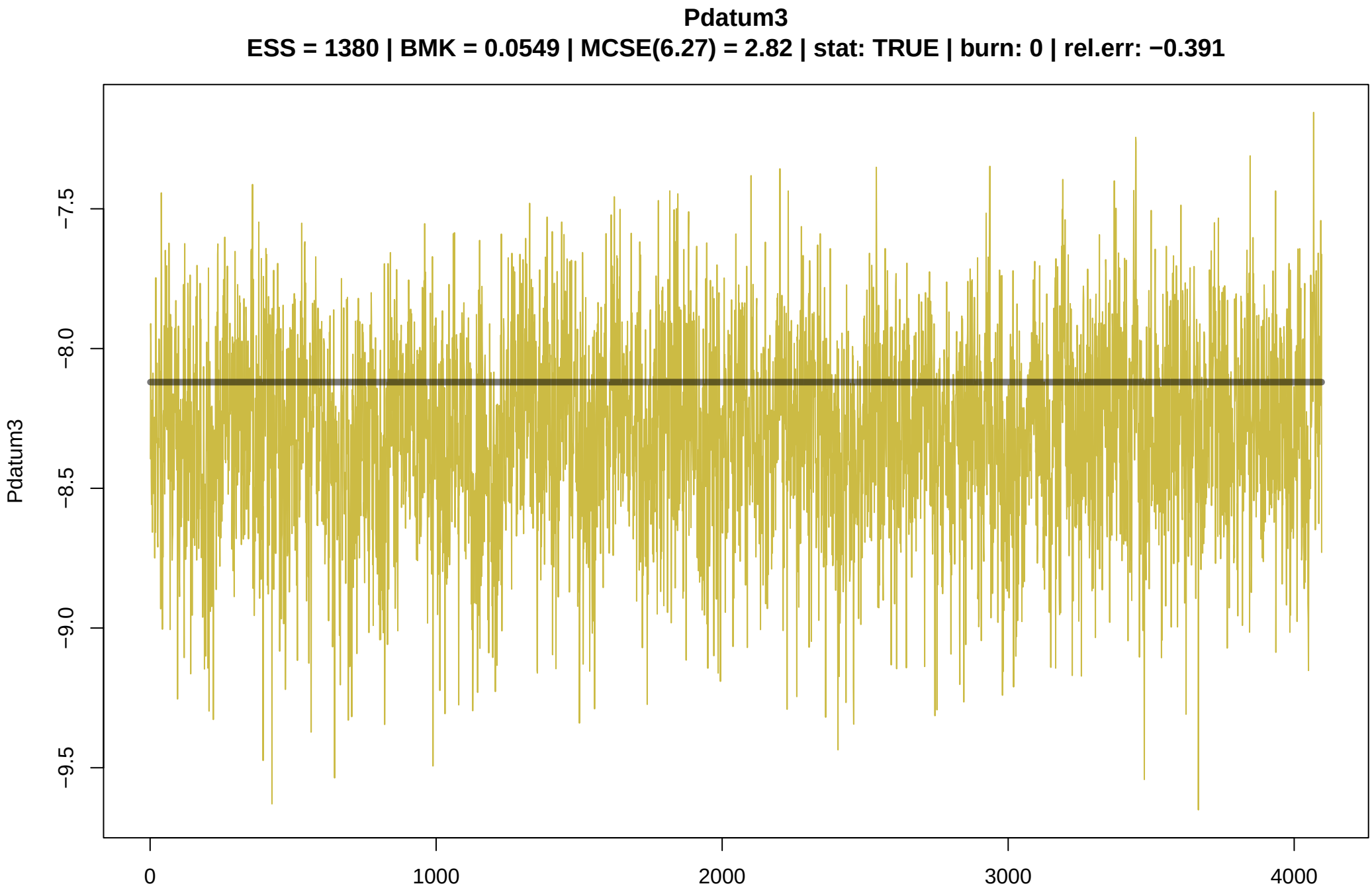

Pdatamean
ESS = 303 | BMK = 0.0584 | MCSE(6.27) = 5.45 | stat: TRUE | burn: 0 | rel.err: 0.797
Pdatamean
−9
−10
−11
−12
−13
0
1000
2000
3000
4000

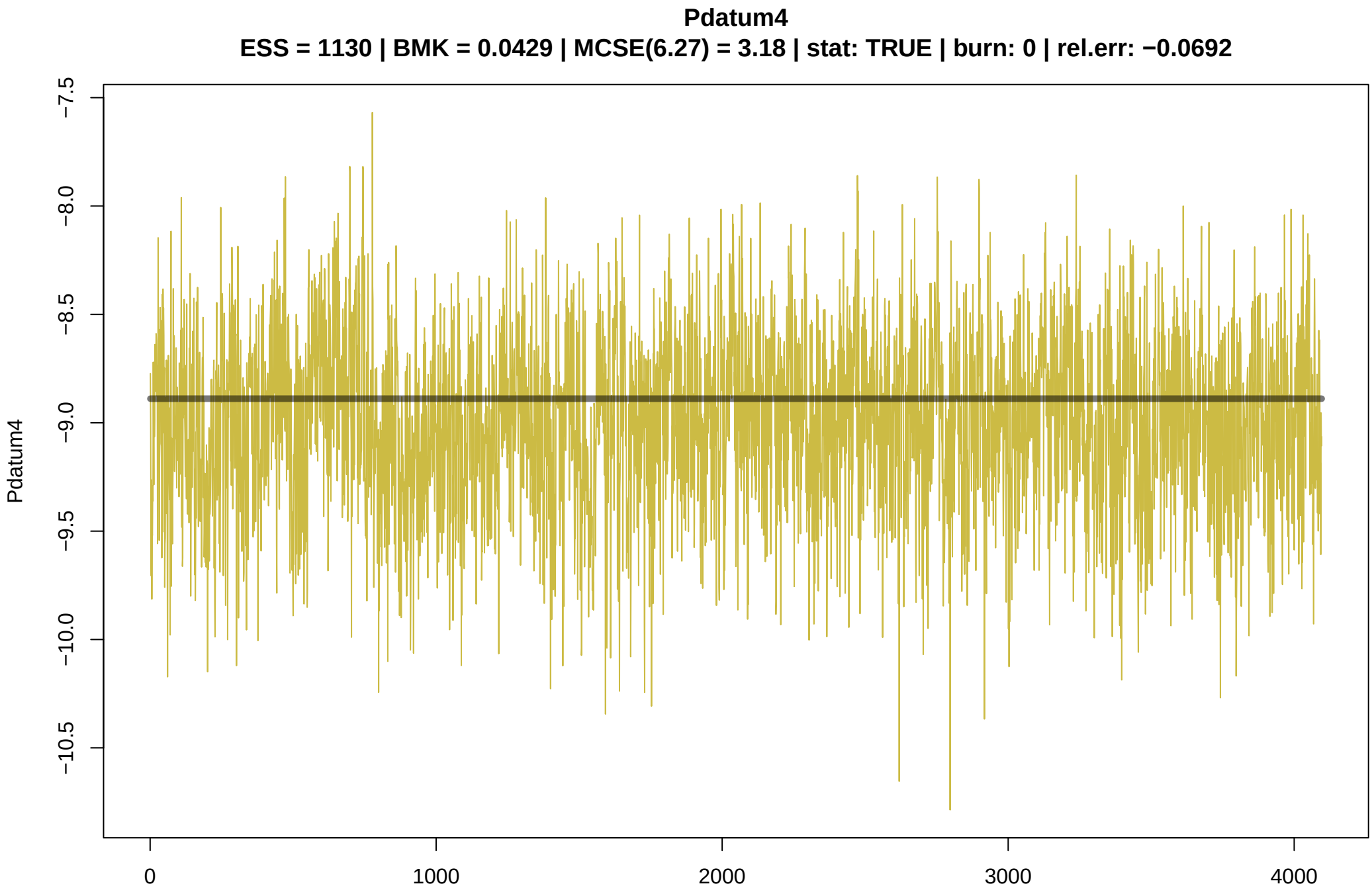

PdatacornerHi
ESS = 3890 | BMK = 0.118 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: 0.331
PdatacornerHi
−15
−20
−25
0
1000
2000
3000
4000

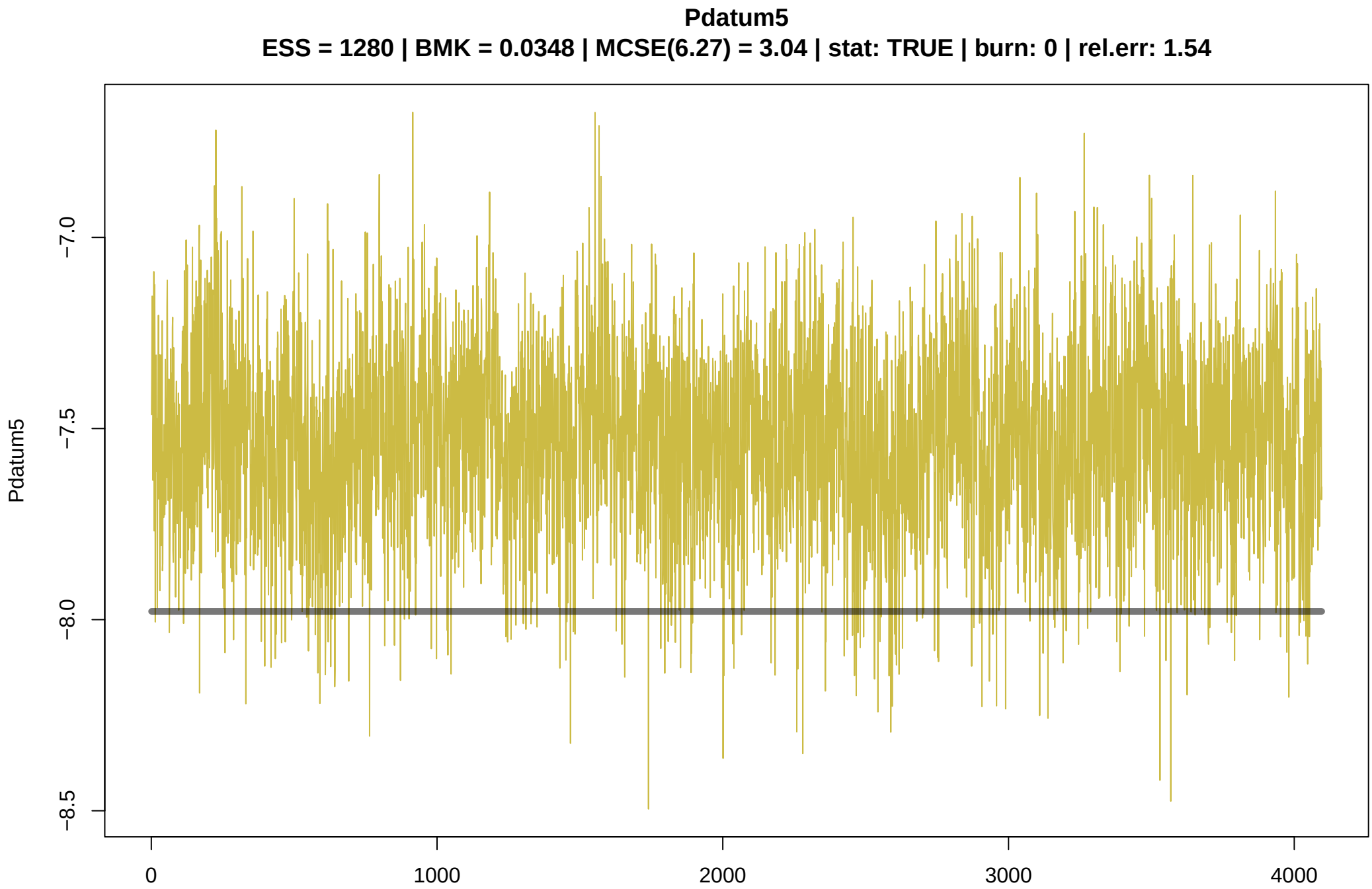

PdatacornerLo
ESS = 3120 | BMK = 0.0374 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: 0.686
PdatacornerLo
−8
−9
−10
−11
−12
0
1000
2000
3000
4000

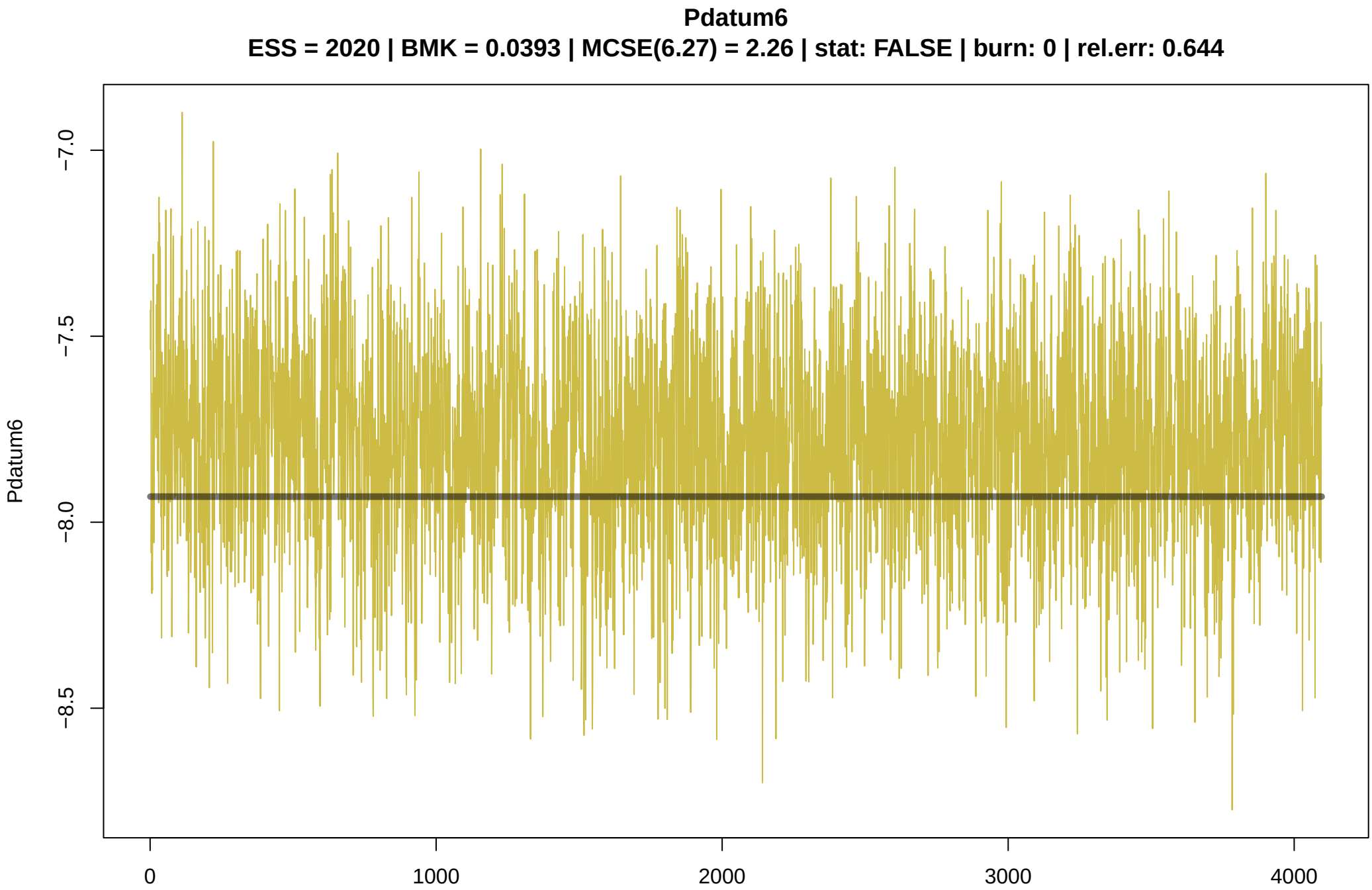

Pdatum1
ESS = 803 | BMK = 0.0391 | MCSE(6.27) = 3.63 | stat: TRUE | burn: 0 | rel.err: −0.872
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

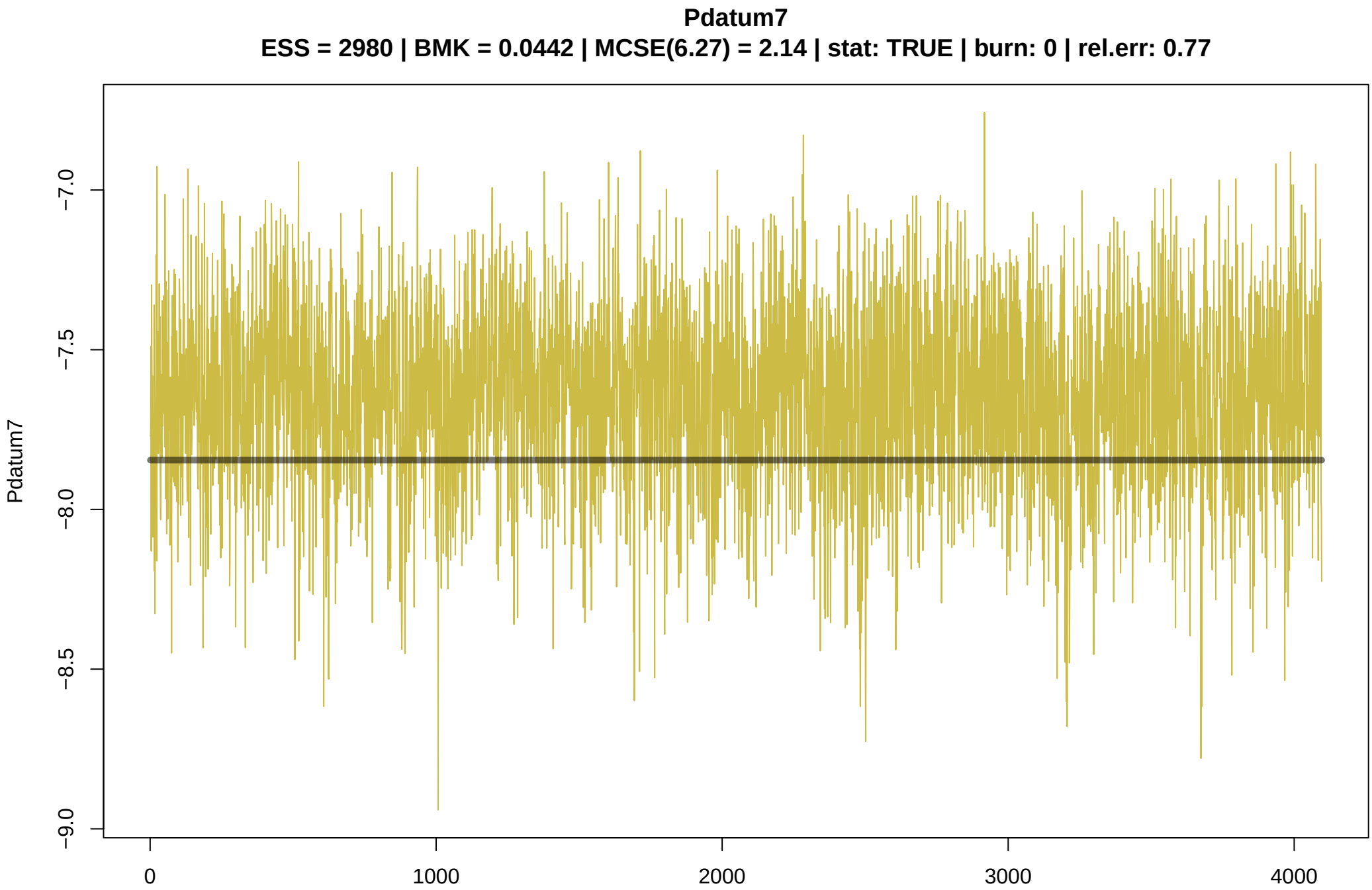

Pdatum2
ESS = 533 | BMK = 0.0436 | MCSE(6.27) = 4.05 | stat: TRUE | burn: 0 | rel.err: −1.97
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

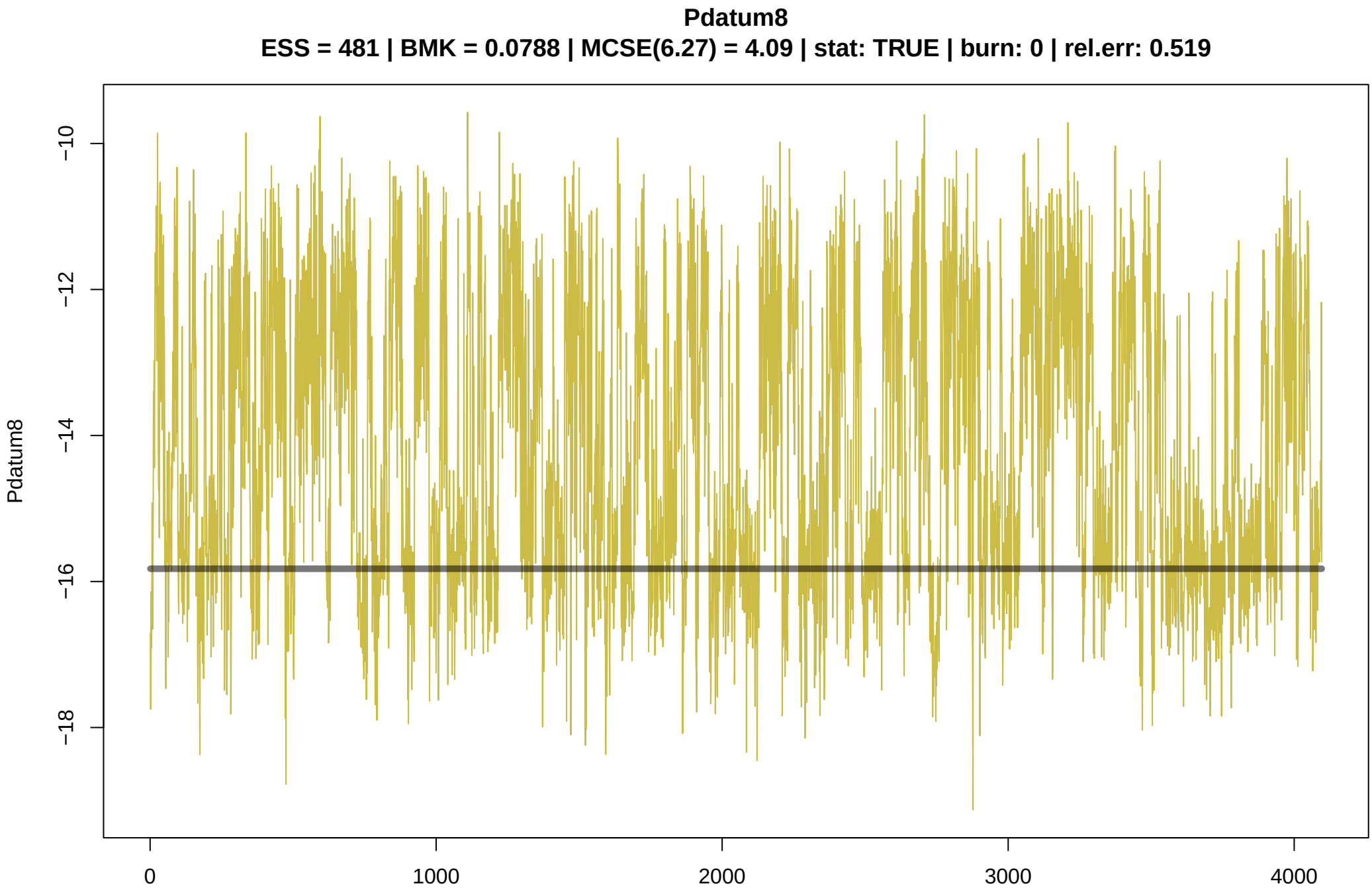

Pdatum3
ESS = 1380 | BMK = 0.0549 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: −0.391
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

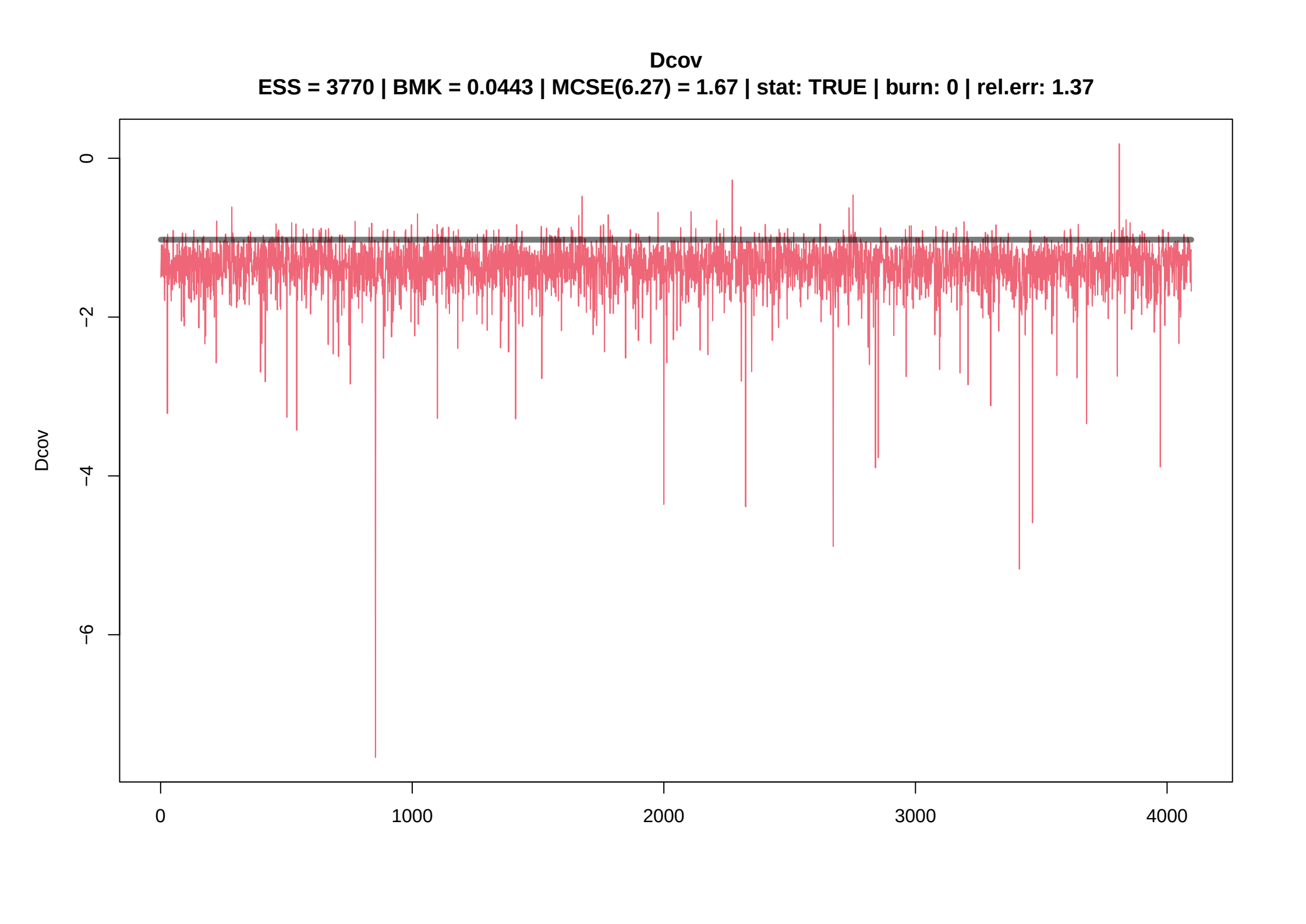

Pdatum4
ESS = 1130 | BMK = 0.0429 | MCSE(6.27) = 3.18 | stat: TRUE | burn: 0 | rel.err: −0.0692
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

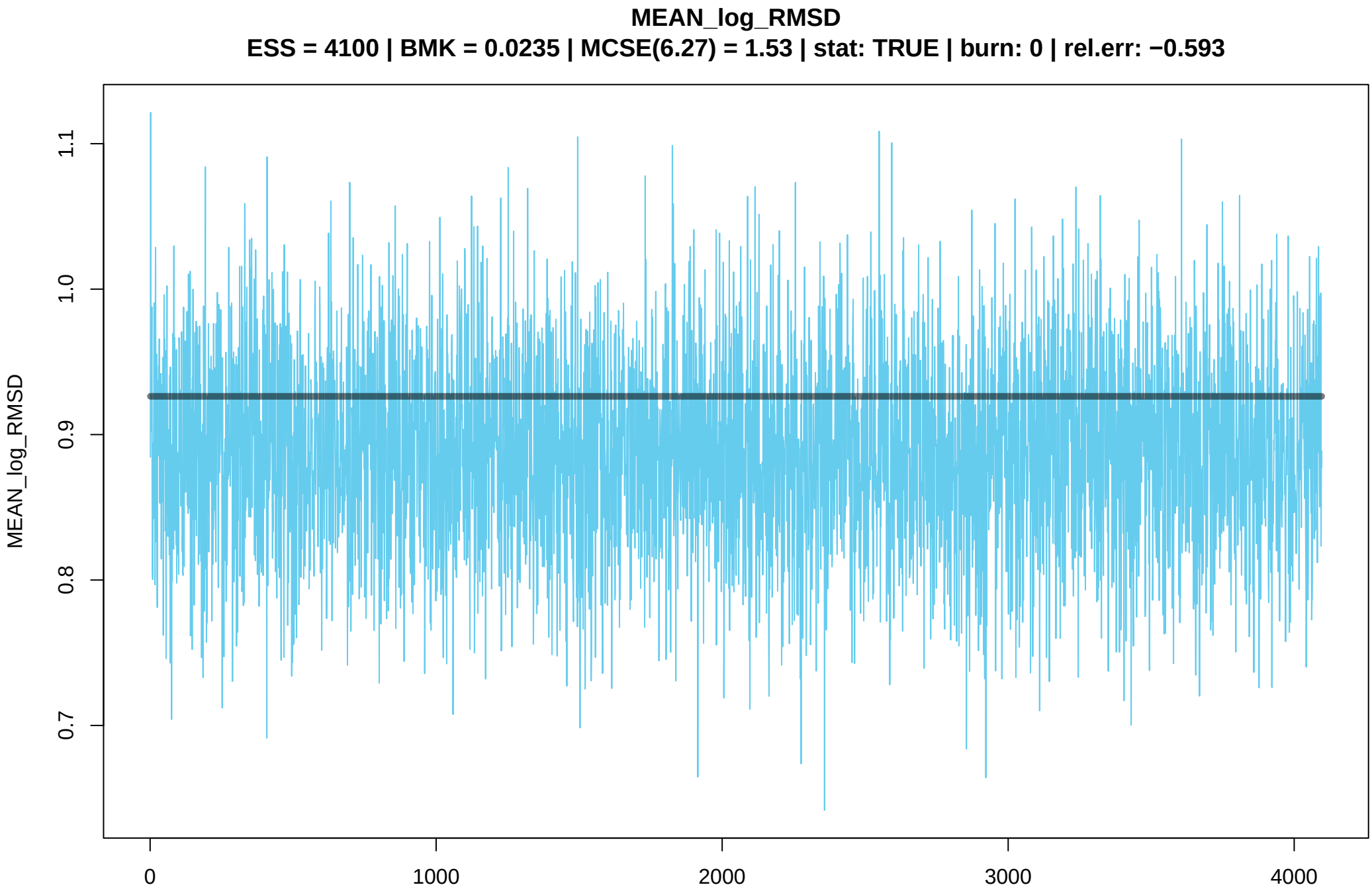

Pdatum5
ESS = 1280 | BMK = 0.0348 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: 1.54
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

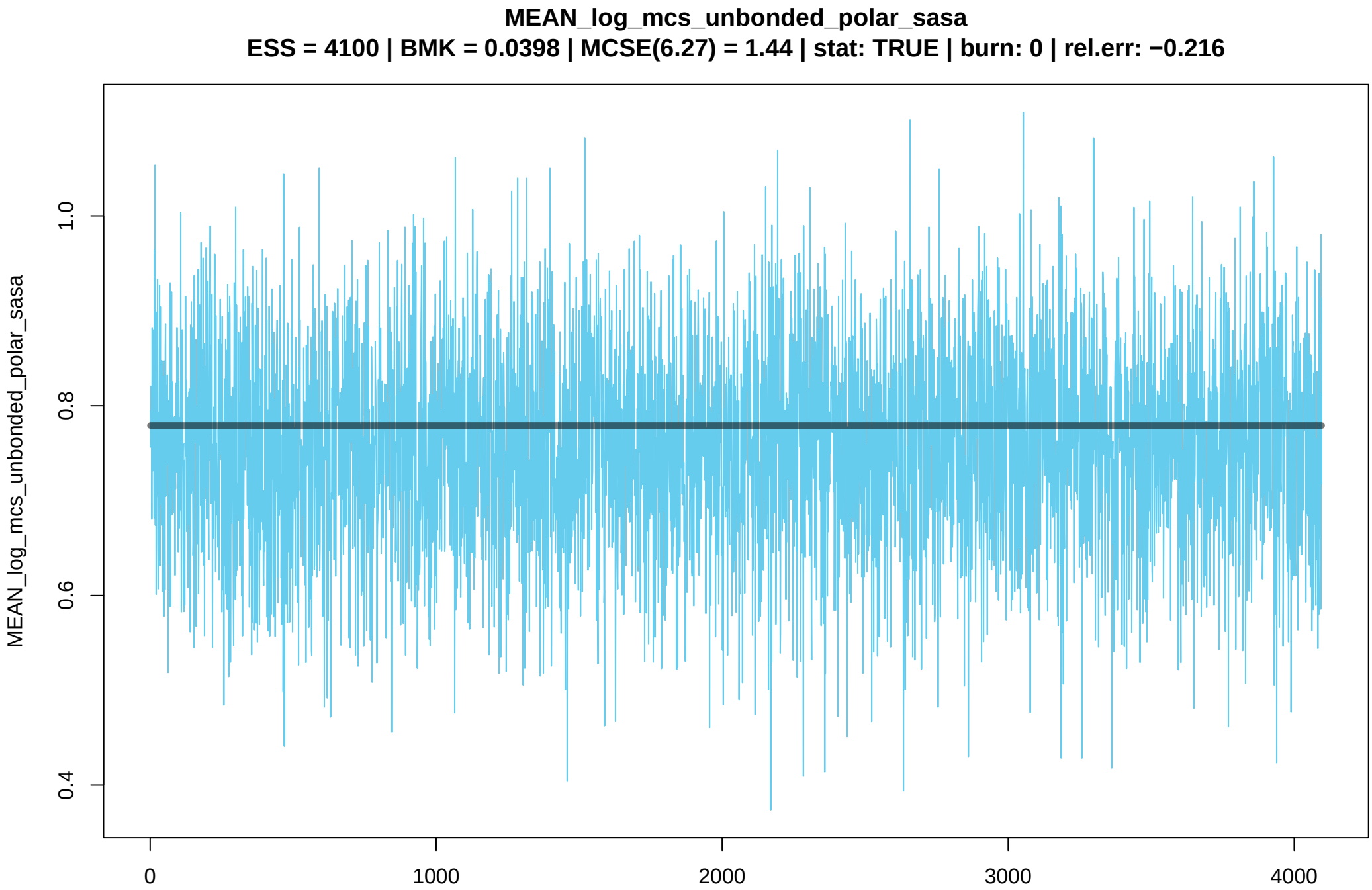

Pdatum6
ESS = 2020 | BMK = 0.0393 | MCSE(6.27) = 2.26 | stat: FALSE | burn: 0 | rel.err: 0.644
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

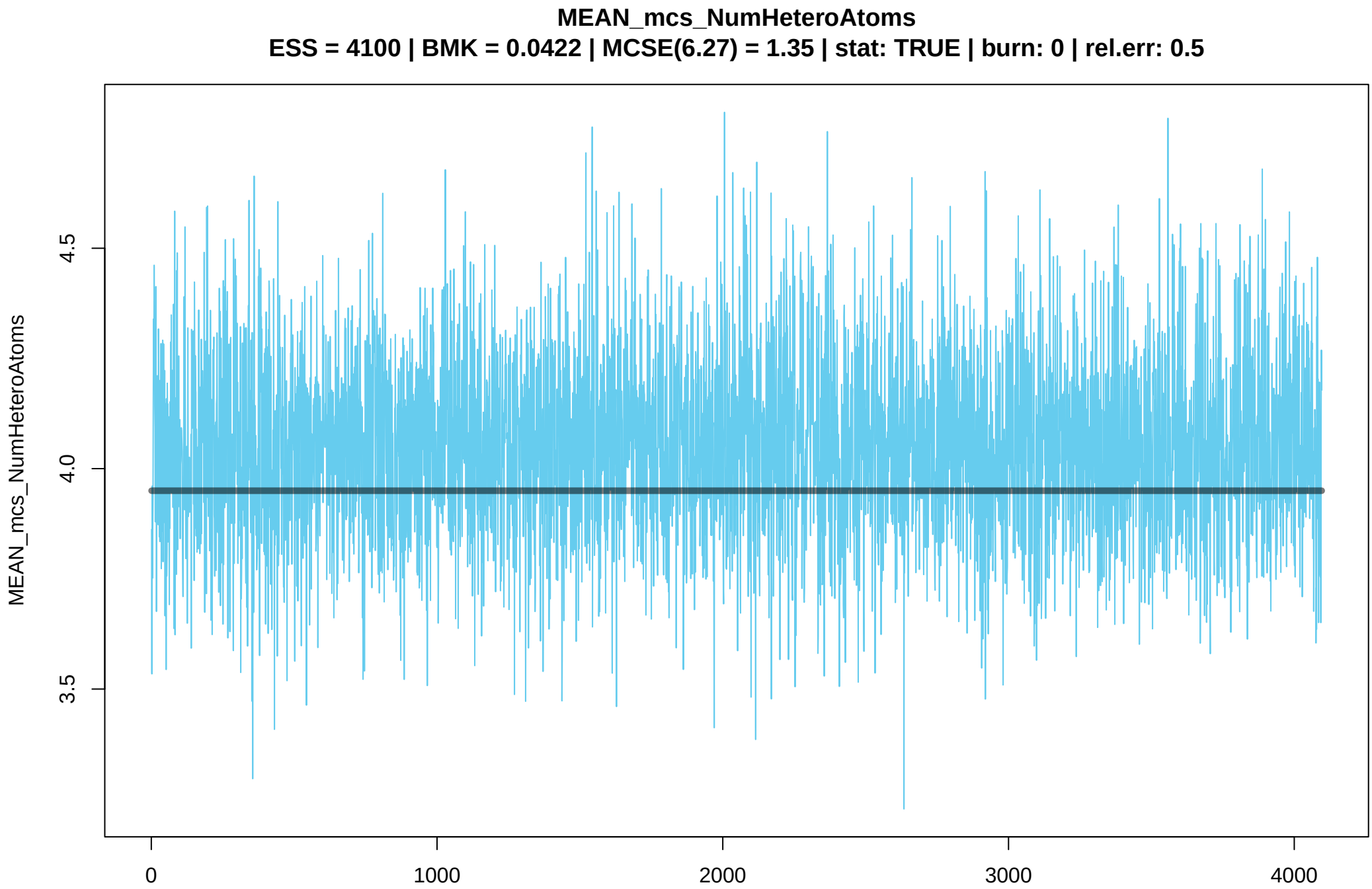

Pdatum7
ESS = 2980 | BMK = 0.0442 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.77
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

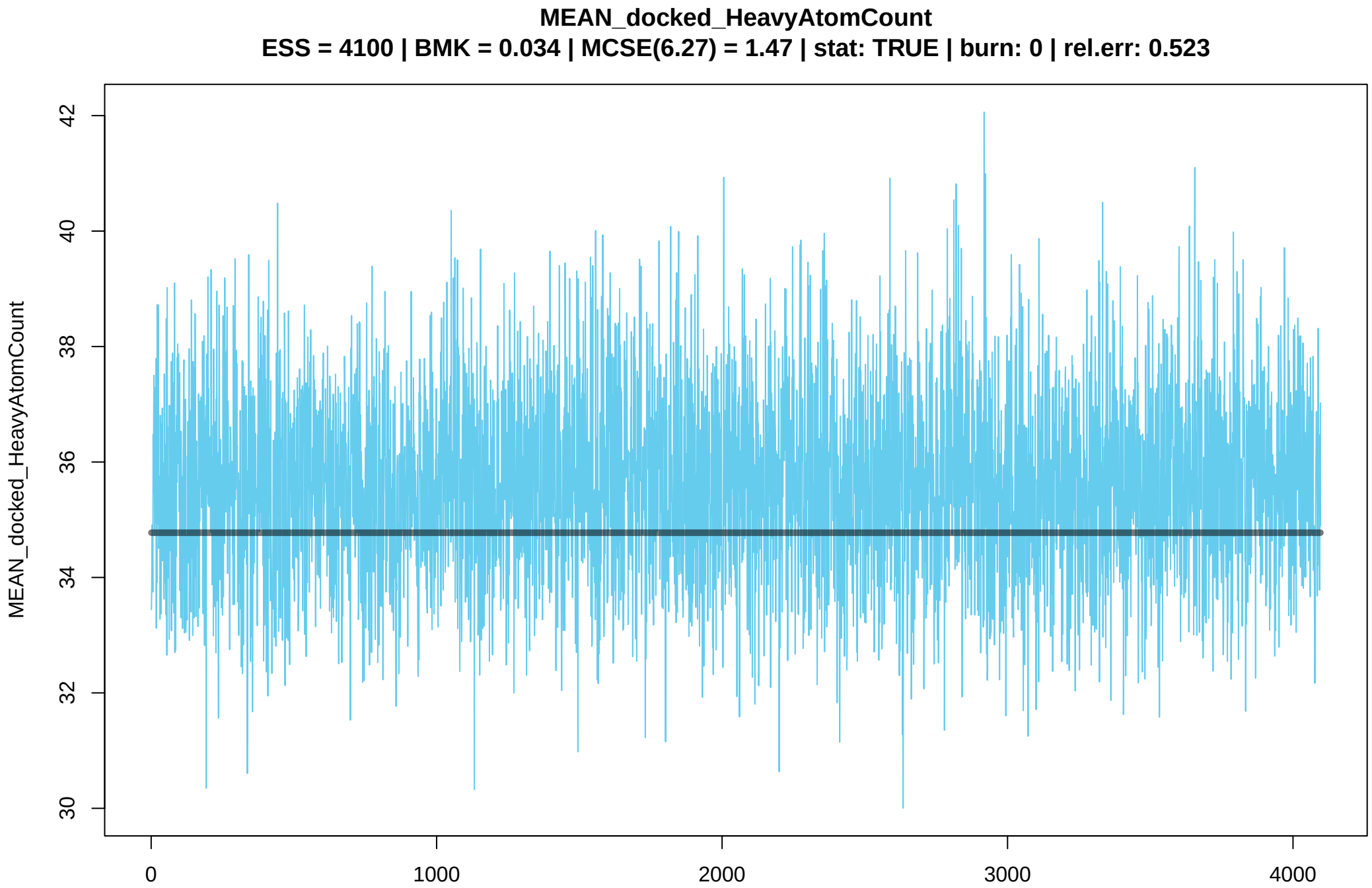

Pdatum8
ESS = 481 | BMK = 0.0788 | MCSE(6.27) = 4.09 | stat: TRUE | burn: 0 | rel.err: 0.519
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

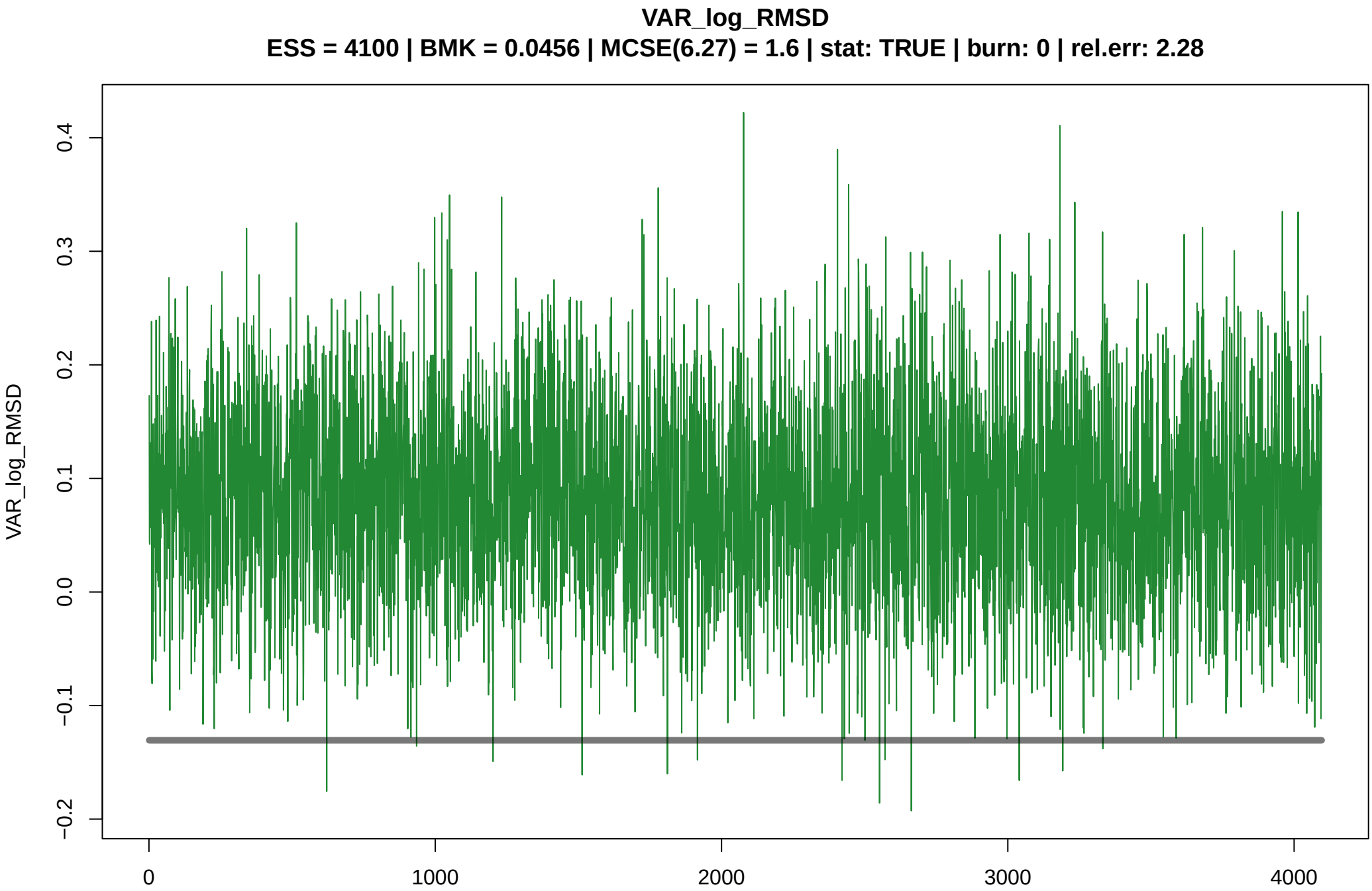

Dcov
ESS = 3770 | BMK = 0.0443 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: 1.37
Dcov
0
−2
−4
−6
0
1000
2000
3000
4000

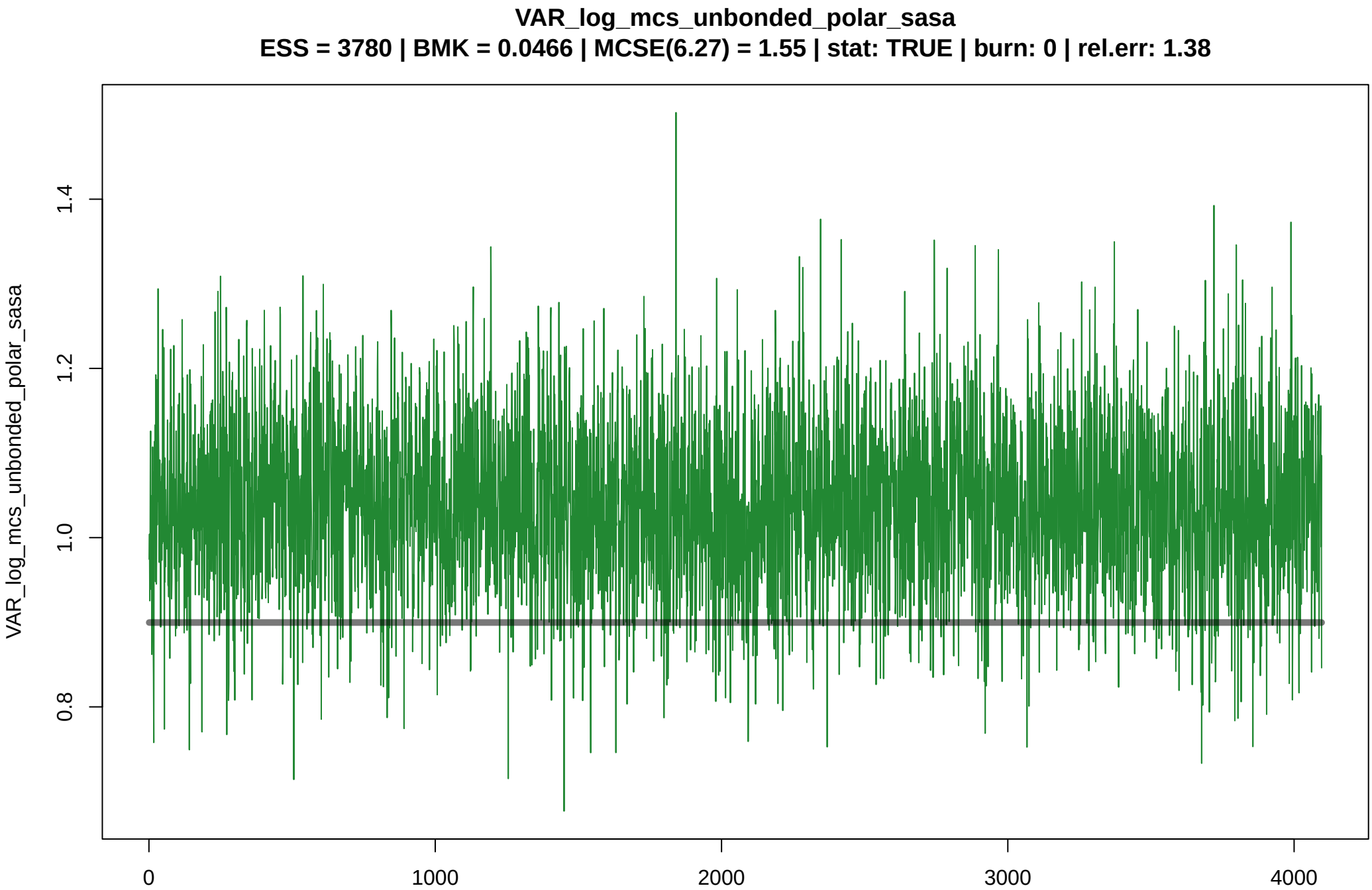

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0235 | MCSE(6.27) = 1.53 | stat: TRUE | burn: 0 | rel.err: −0.593
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

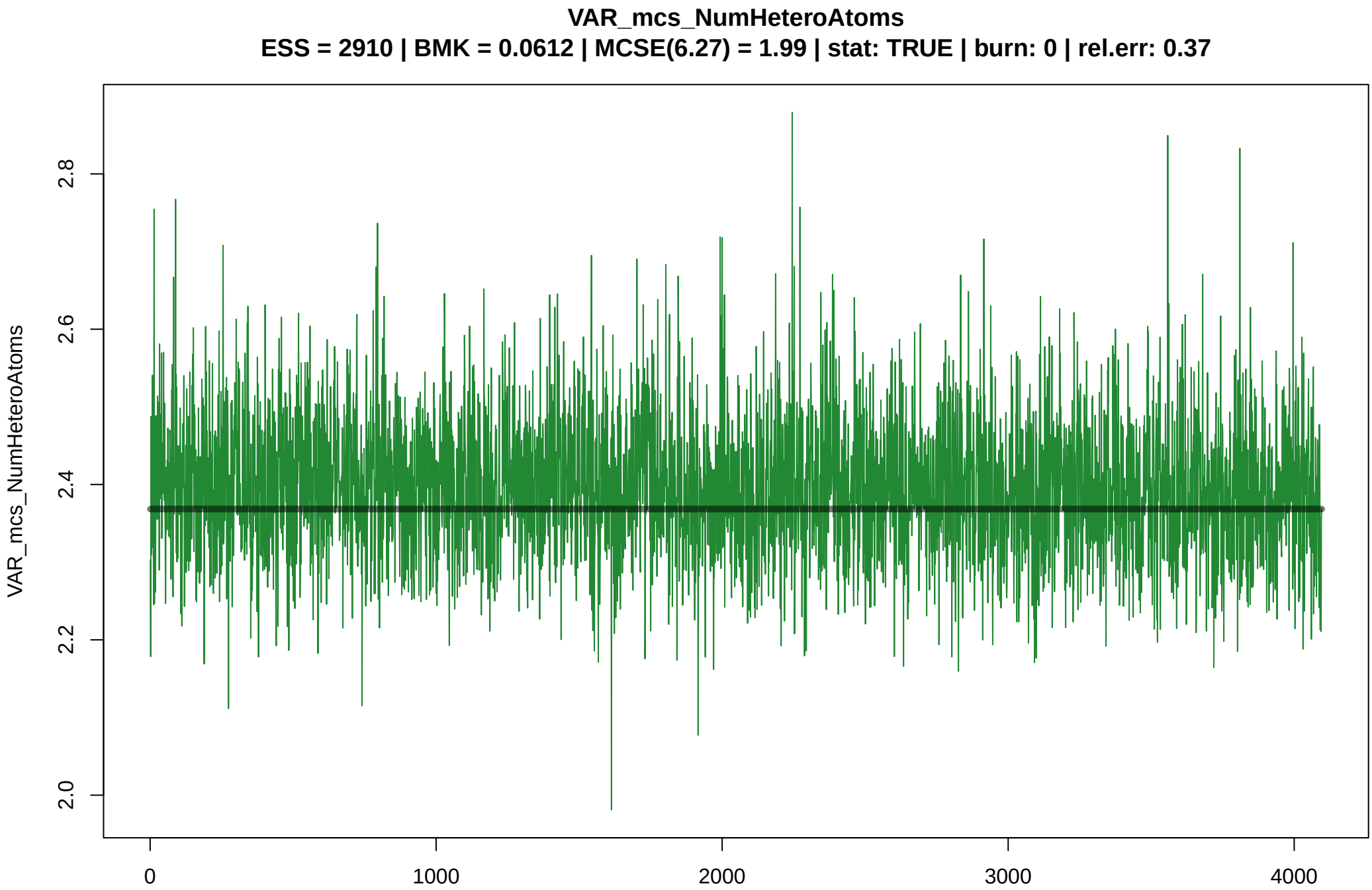

MEAN_log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0398 | MCSE(6.27) = 1.44 | stat: TRUE | burn: 0 | rel.err: −0.216
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

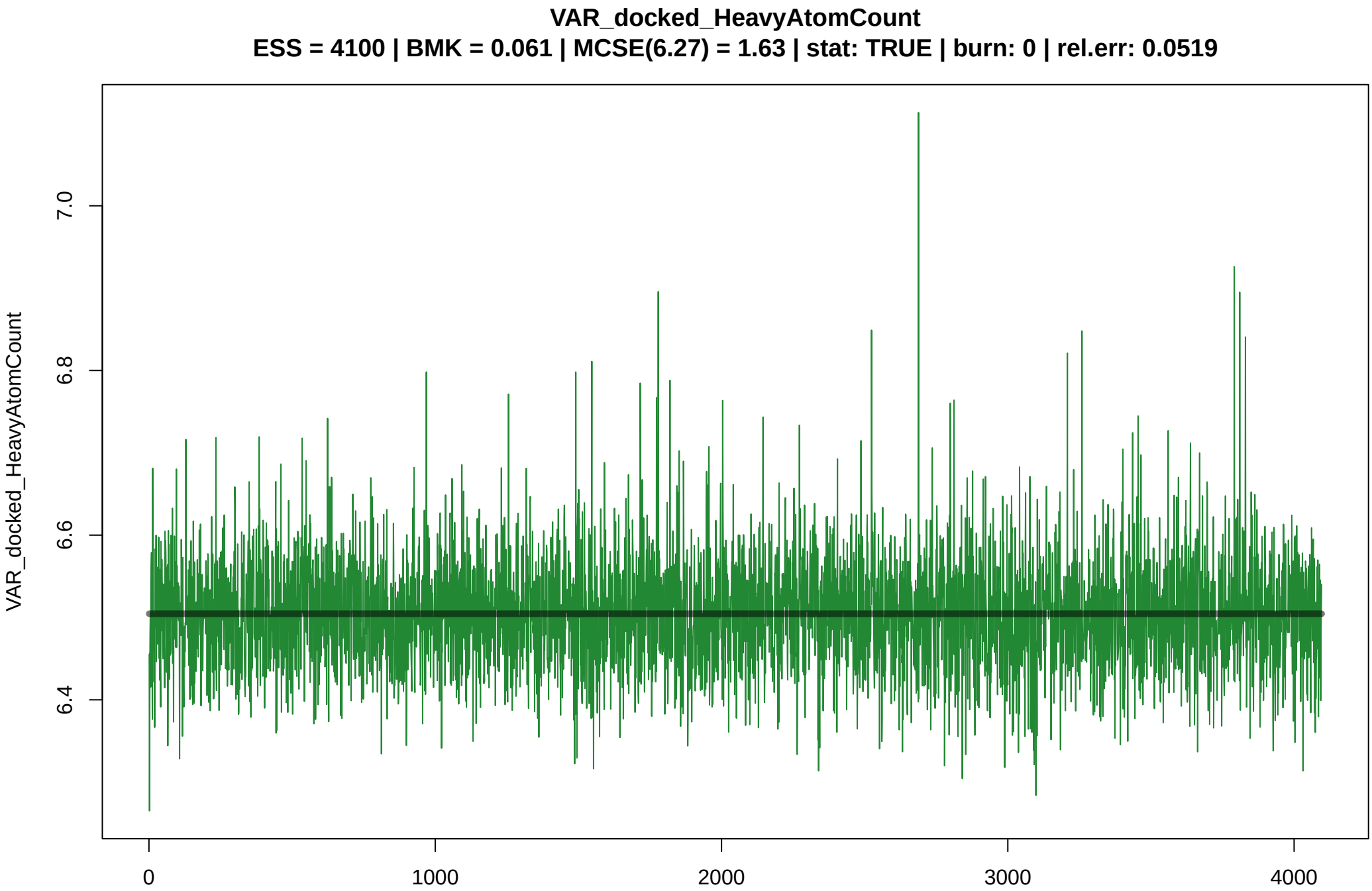

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0422 | MCSE(6.27) = 1.35 | stat: TRUE | burn: 0 | rel.err: 0.5
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

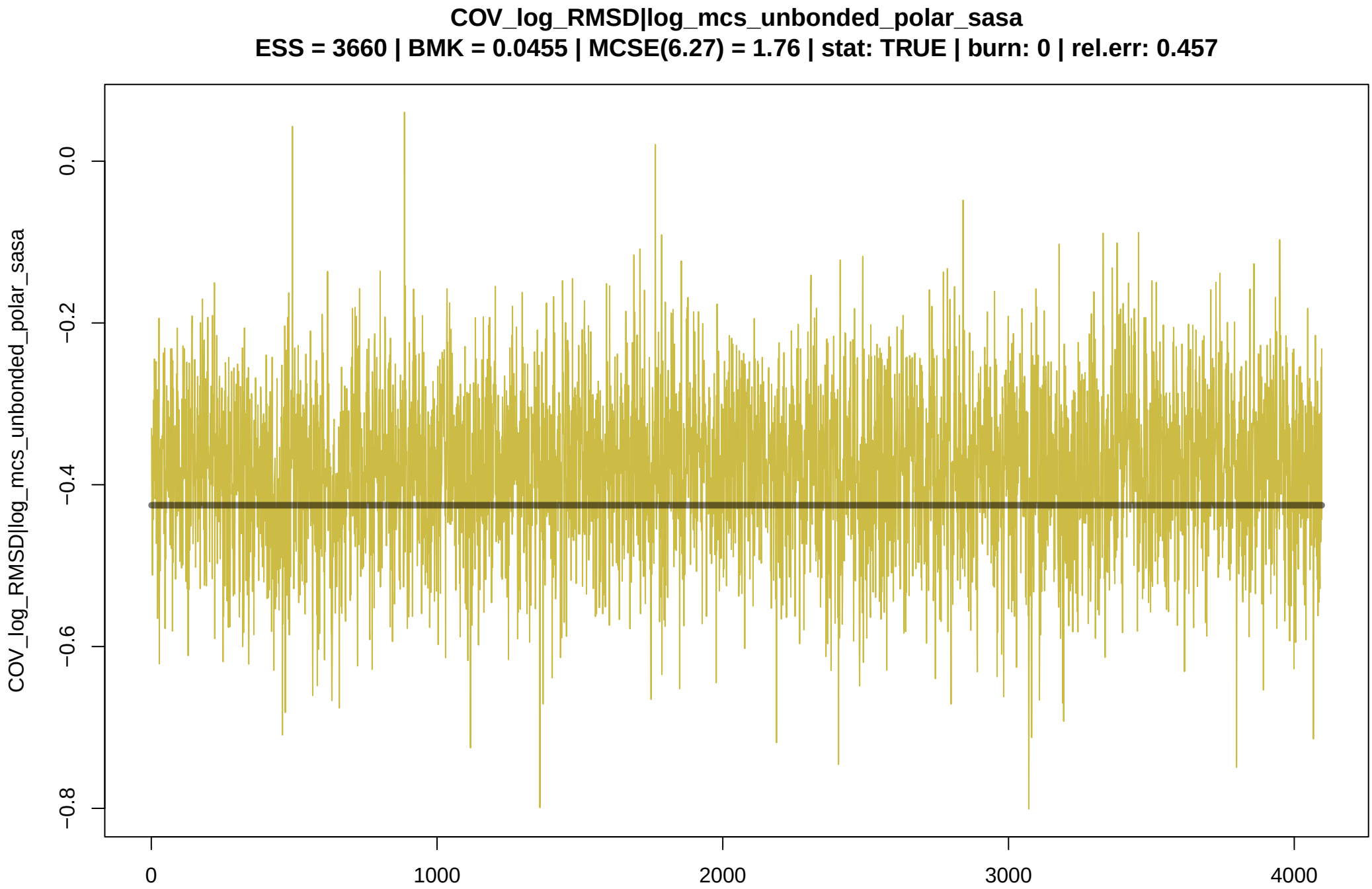

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.034 | MCSE(6.27) = 1.47 | stat: TRUE | burn: 0 | rel.err: 0.523
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
1000
2000
3000
4000

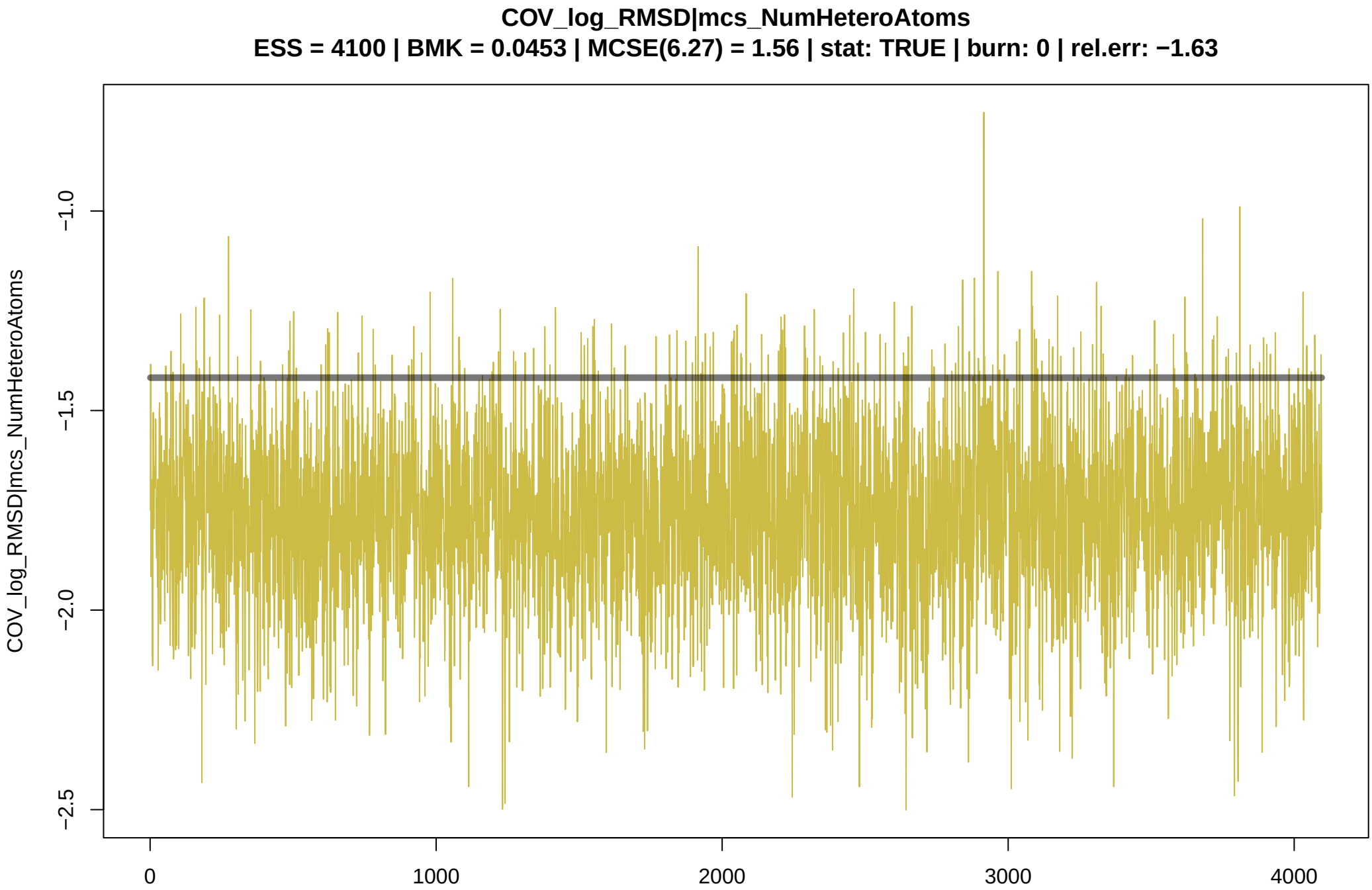

VAR_log_RMSD
ESS = 4100 | BMK = 0.0456 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 2.28
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

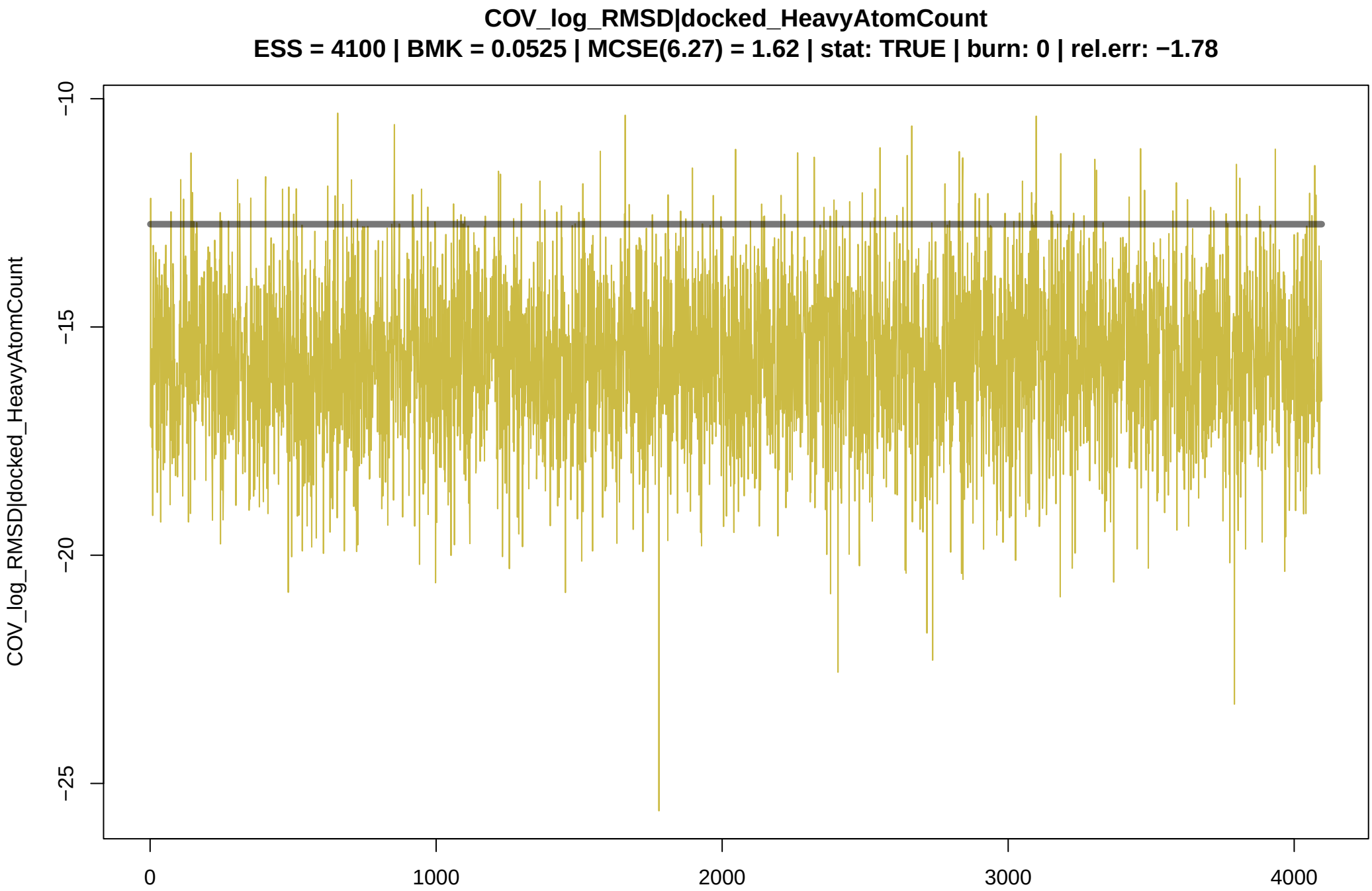

VAR_log_mcs_unbonded_polar_sasa
ESS = 3780 | BMK = 0.0466 | MCSE(6.27) = 1.55 | stat: TRUE | burn: 0 | rel.err: 1.38
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
0
1000
2000
3000
4000

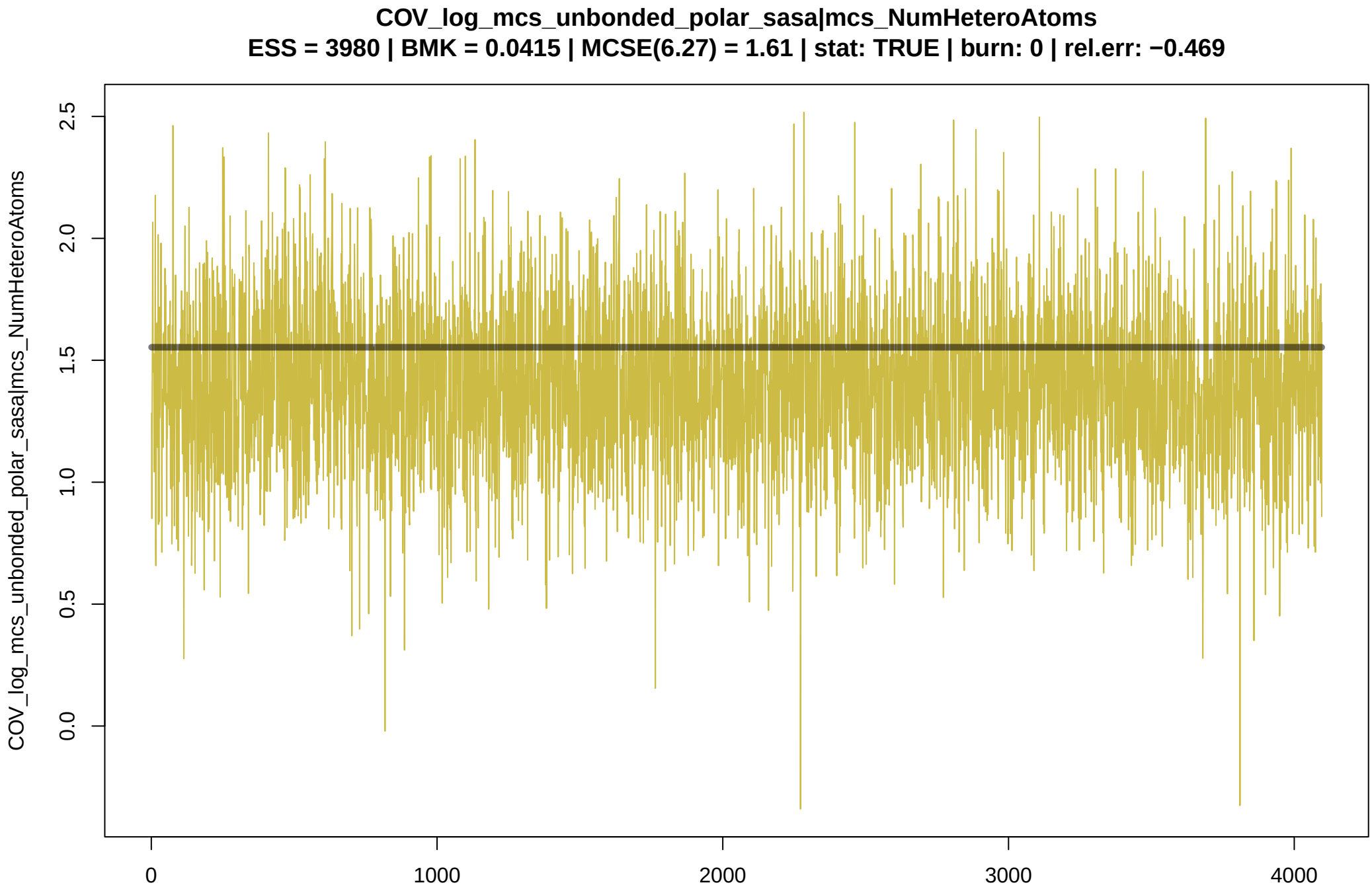

VAR_mcs_NumHeteroAtoms
ESS = 2910 | BMK = 0.0612 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 0.37
VAR_mcs_NumHeteroAtoms
2.0
2.2
2.4
2.6
2.8
0
1000
2000
3000
4000

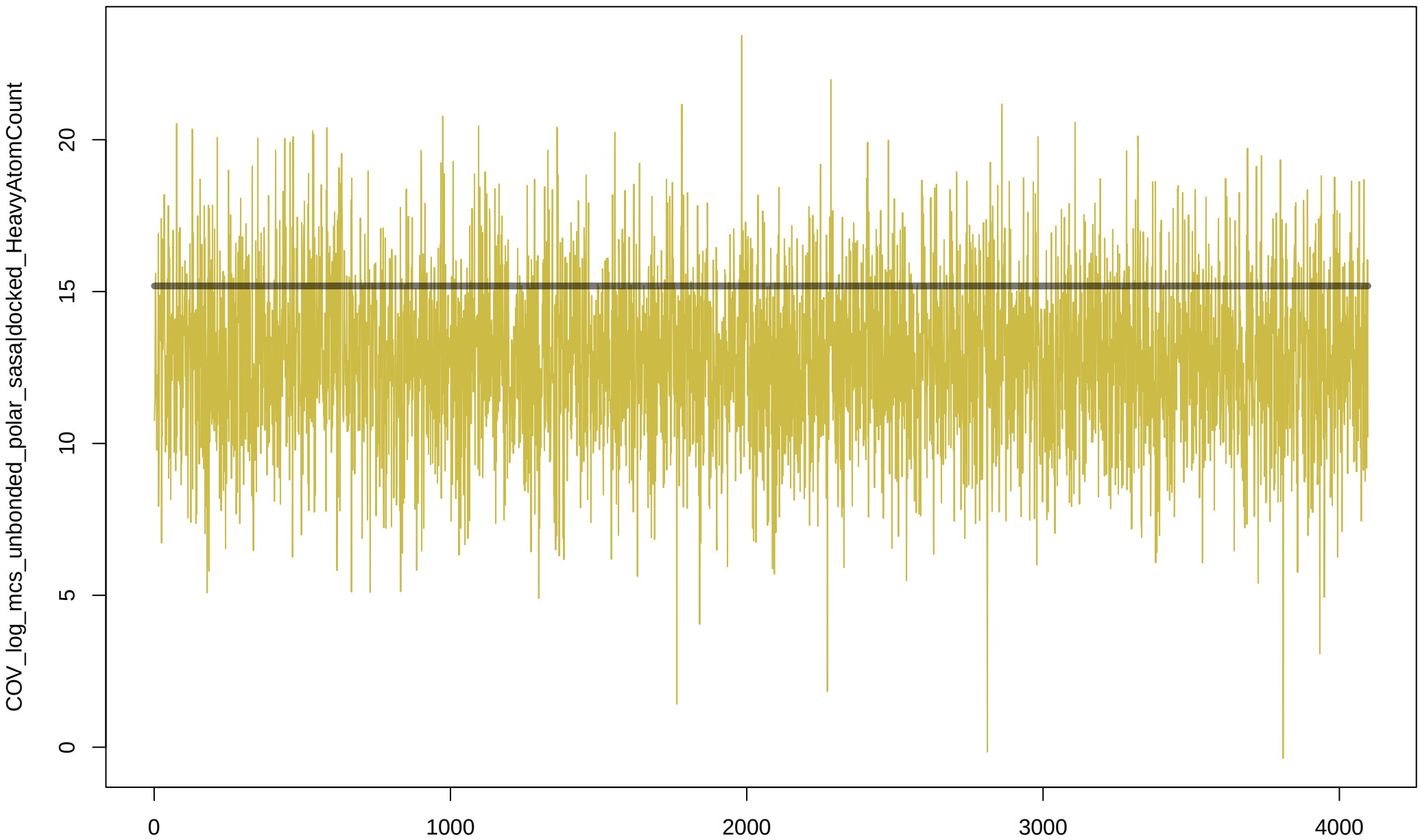

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.061 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.0519
VAR_docked_HeavyAtomCount
6.4
6.6
6.8
7.0
0
1000
2000
3000
4000

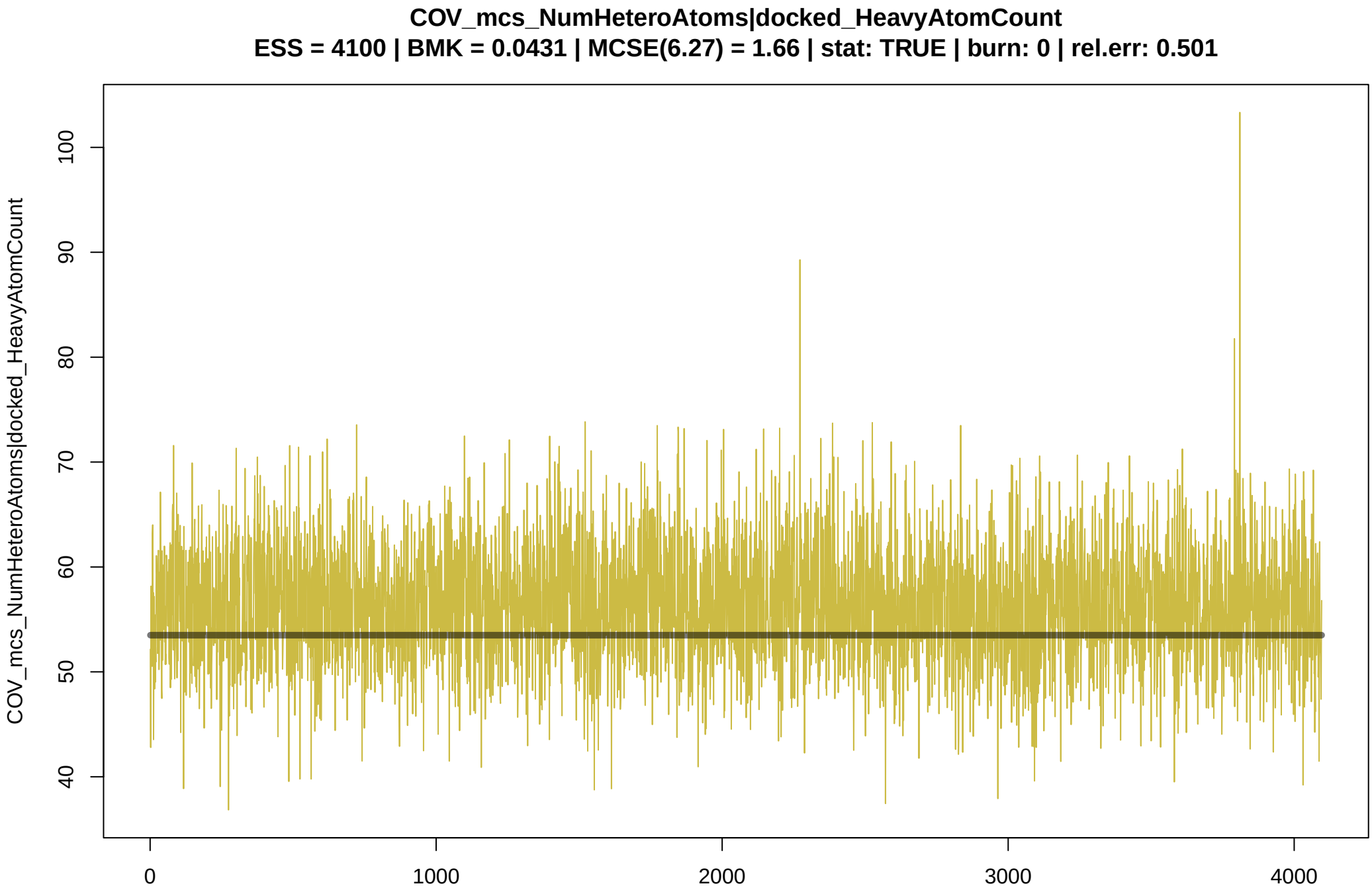

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3660 | BMK = 0.0455 | MCSE(6.27) = 1.76 | stat: TRUE | burn: 0 | rel.err: 0.457
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0453 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: −1.63
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 = 0.0525 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: −1.78
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
−25
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3980 | BMK = 0.0415 | MCSE(6.27) = 1.61 | stat: TRUE | burn: 0 | rel.err: −0.469
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 = 0.0444 | MCSE(6.27) = 1.56 | stat: TRUE | burn: 0 | rel.err: −0.905
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0
5
10
15
20
0
1000
2000
3000
4000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0431 | MCSE(6.27) = 1.66 | stat: TRUE | burn: 0 | rel.err: 0.501
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
90
100
0
1000
2000
3000
4000