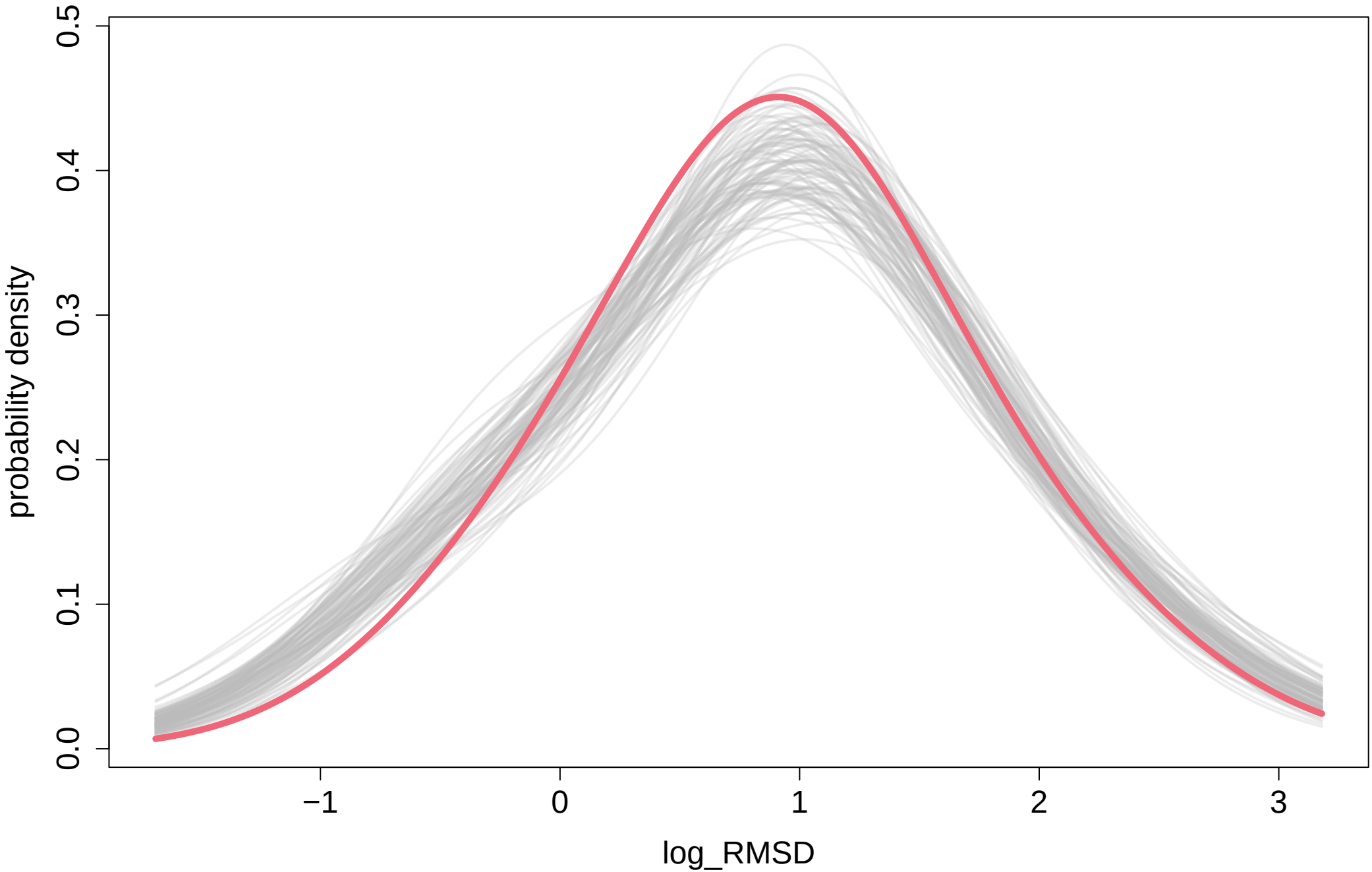
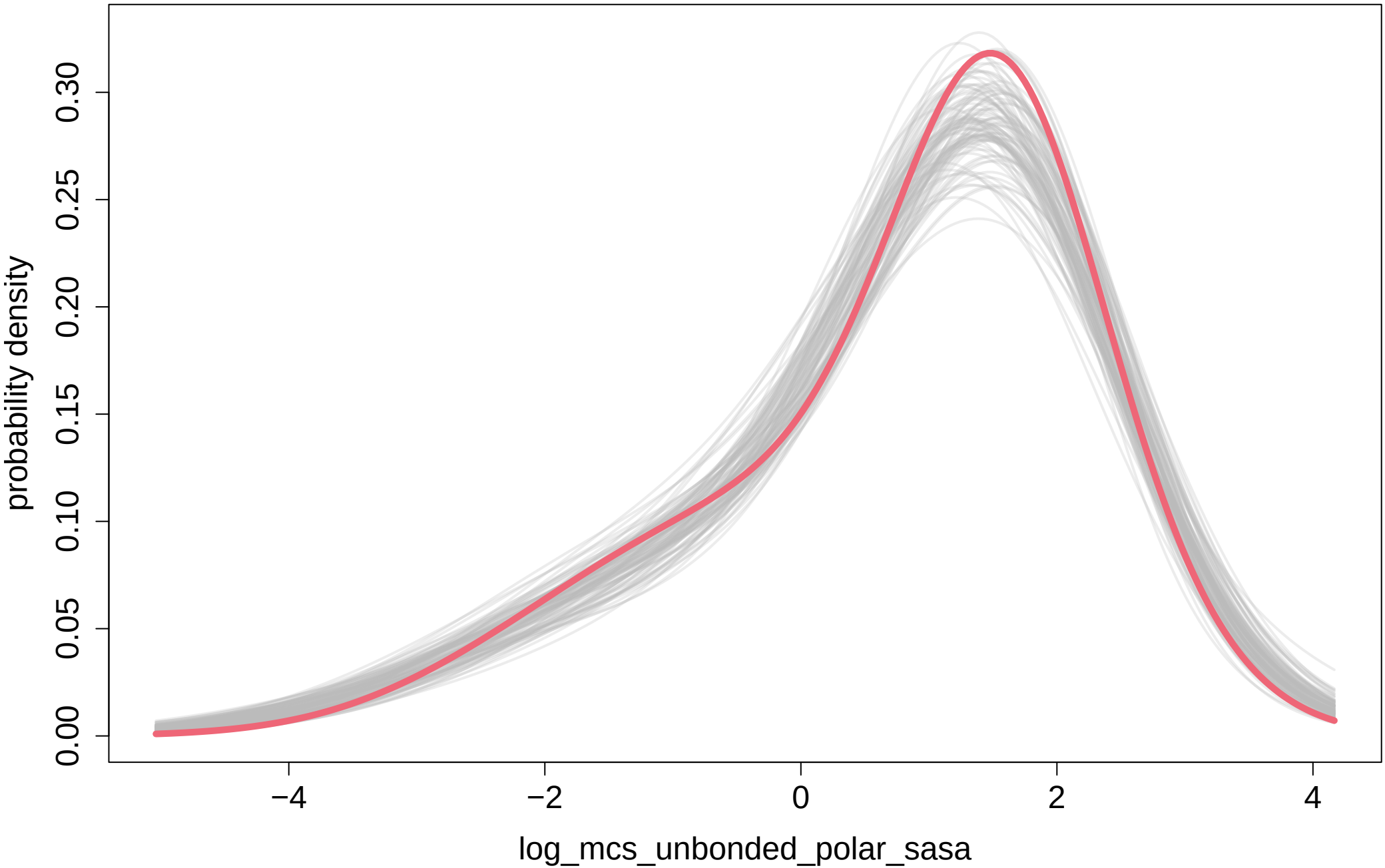
−− STATS maxD −−
min ESS = 77.4619216685008
max BMK = 0.19711070740612
max MCSE = 7.30208925808224
all stationary: FALSE
burn: 0
max rel.err.: 2.13482123429098

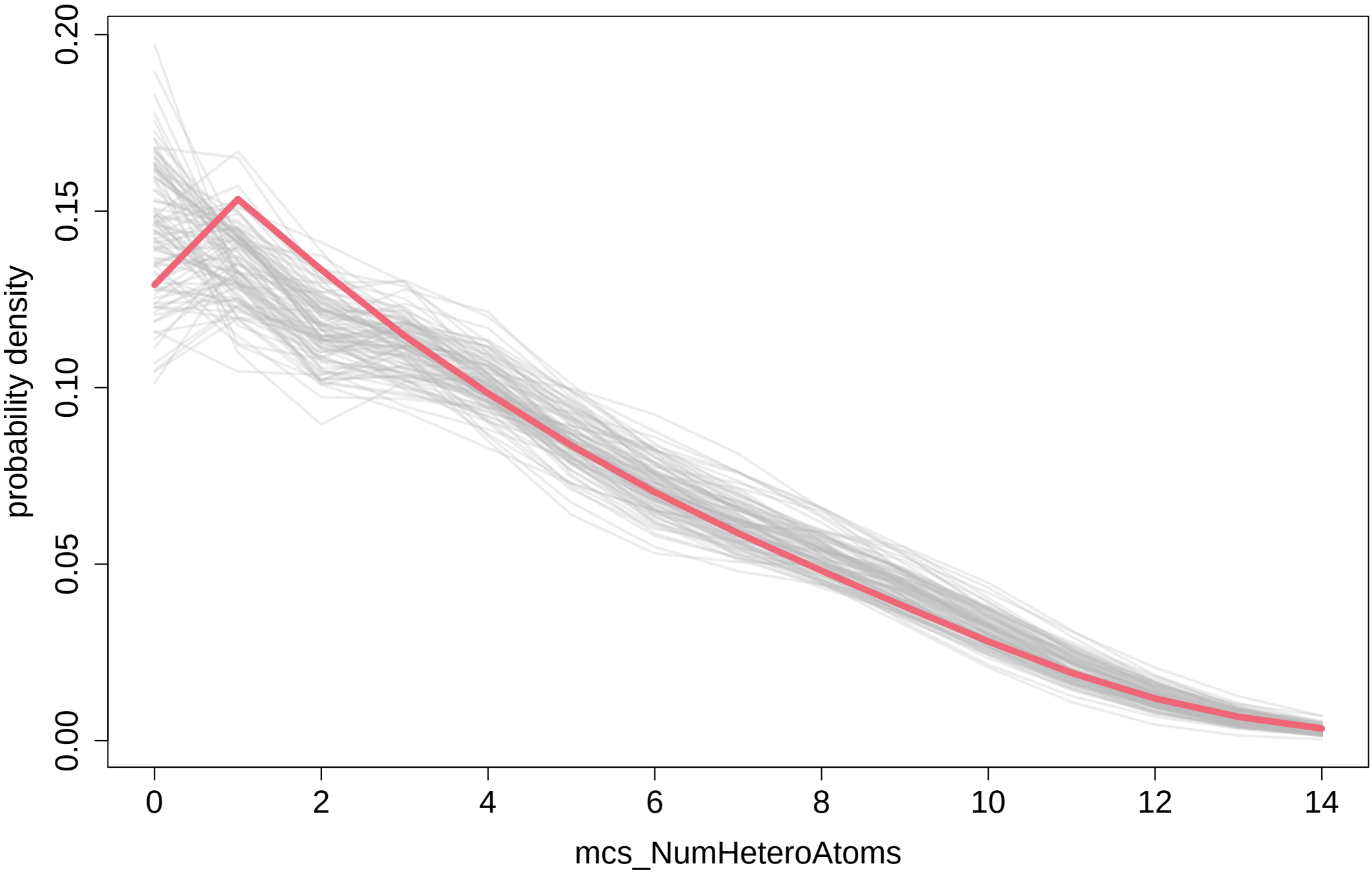
−− STATS 2D −−
min ESS = 4095.99999999999
max BMK = 0.037891781120975
max MCSE = 1.81558128266687
all stationary: FALSE
burn: 0
max rel.err.: 1.81402547739758

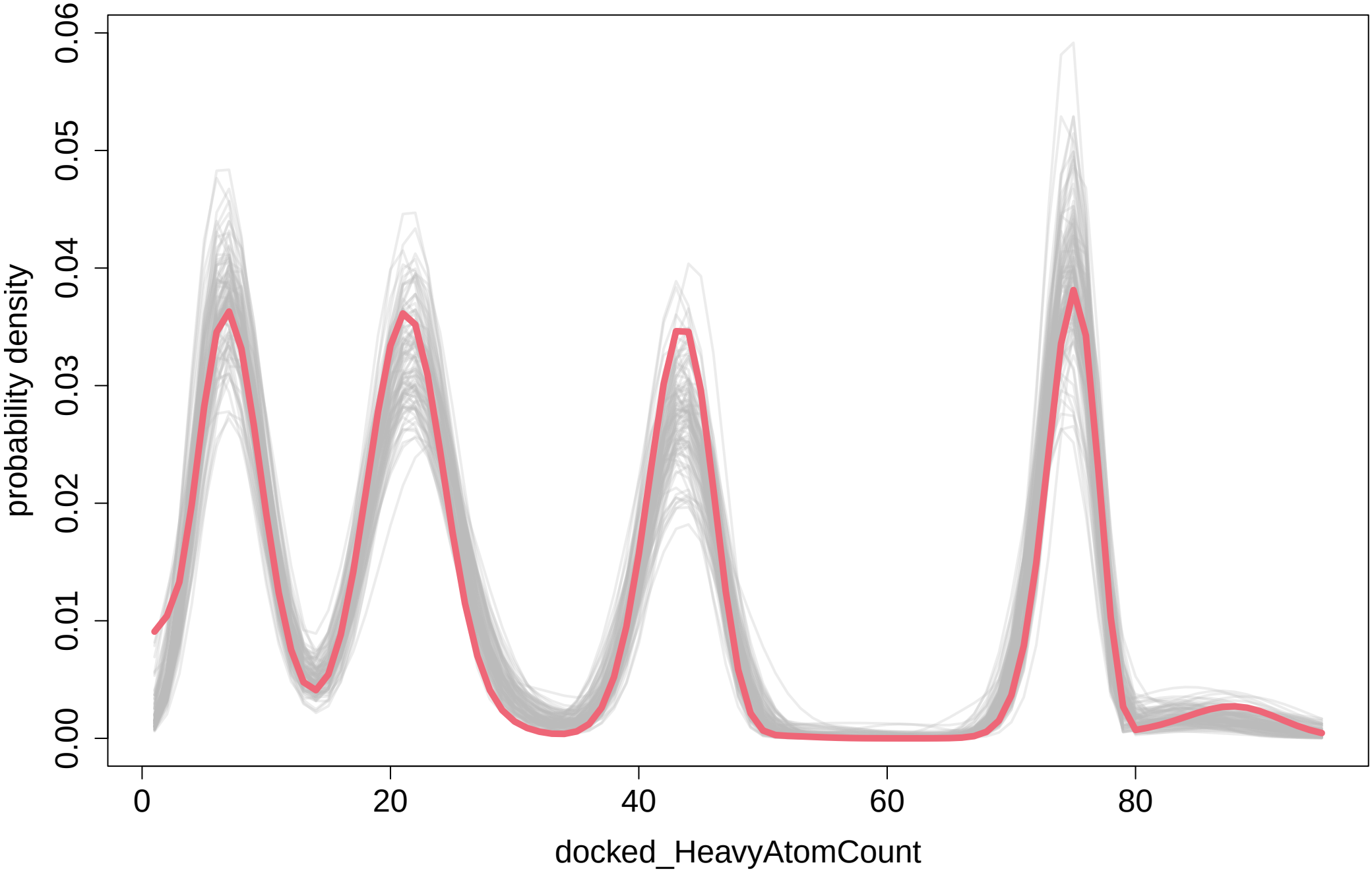
−− STATS 1D −−
min ESS = 3286.7148888631
max BMK = 0.055740628884309 9
max MCSE = 1.80260874136294
all stationary: TRUE
burn: 0
max rel.err.: 2.28780050809299

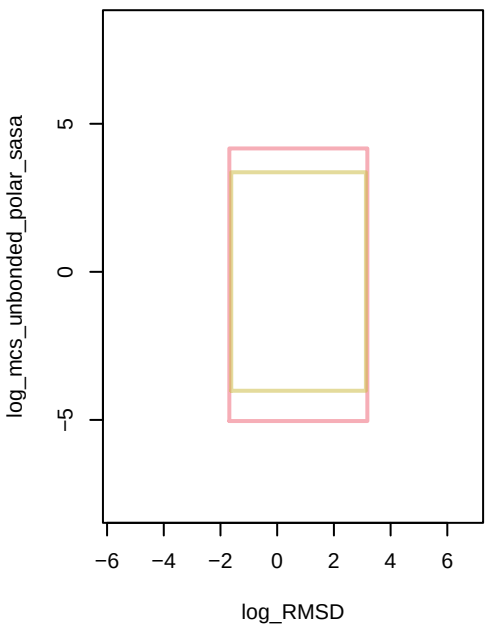
Occupied clusters: 10 of 16
LL: −2160 +− 6.98

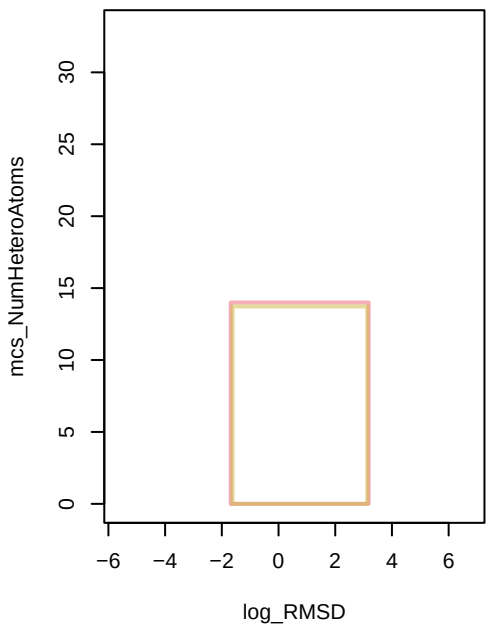

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−1
0
1
2
3
log_RMSD

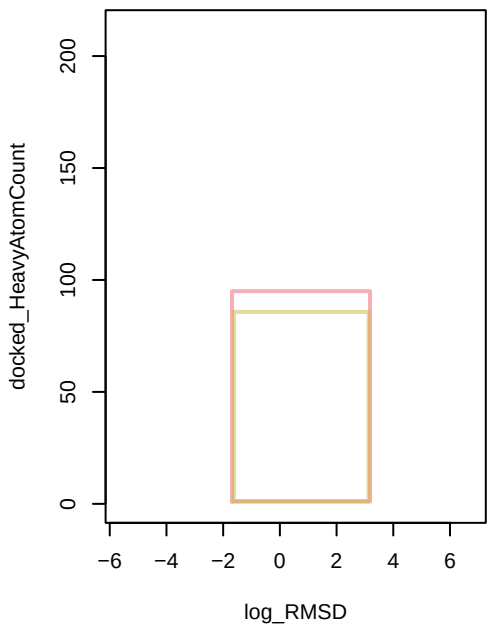

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

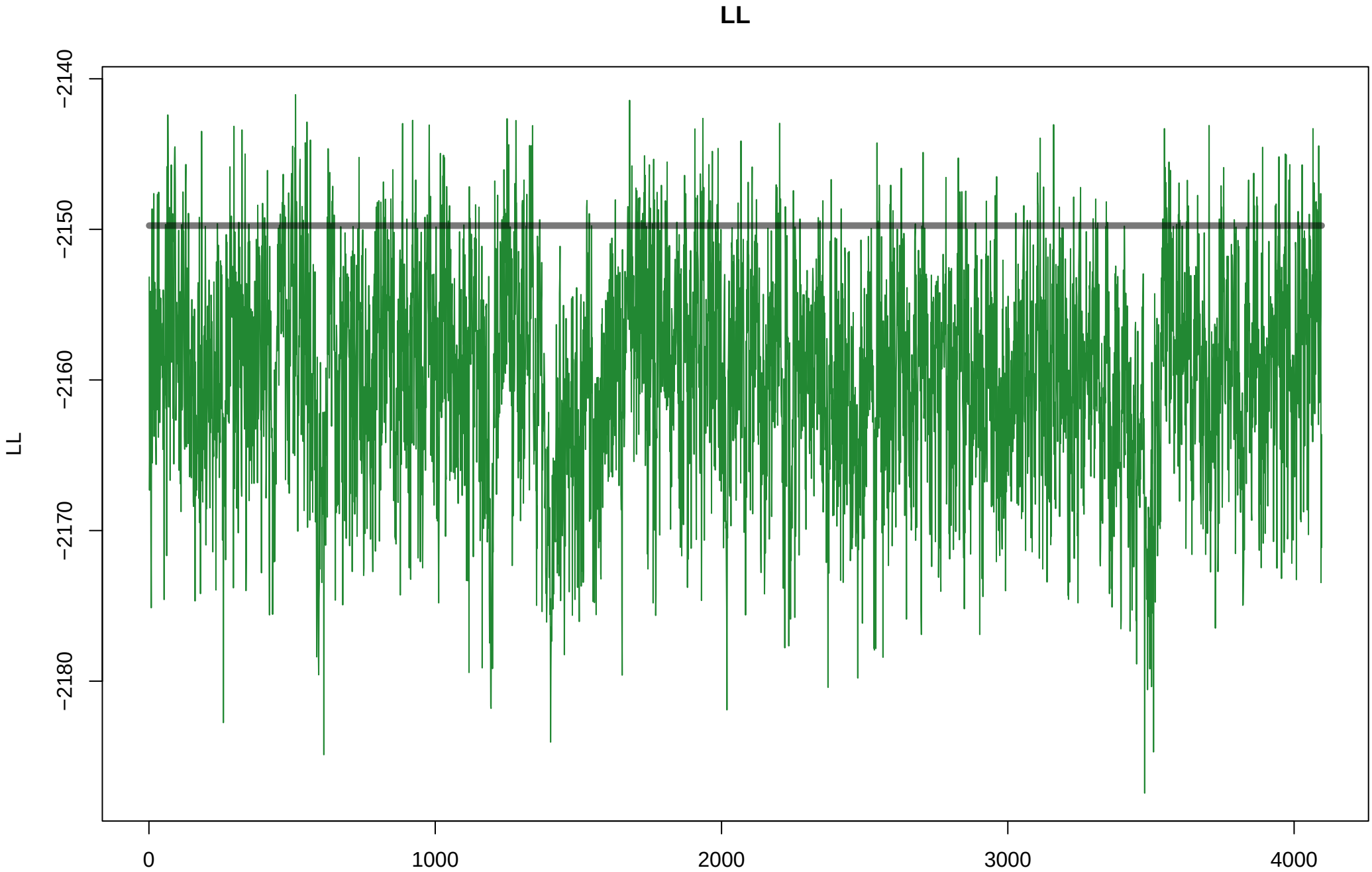

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

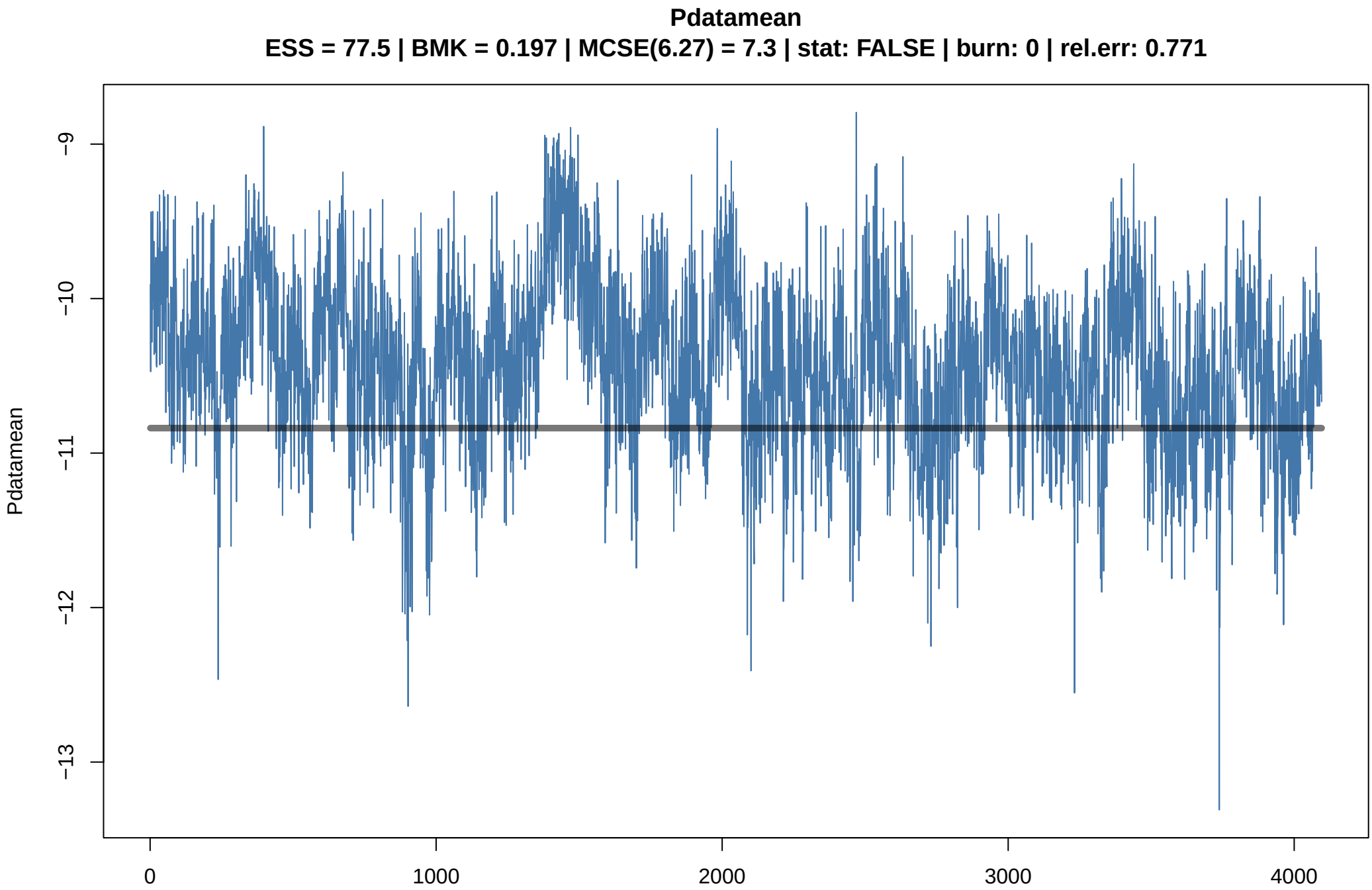

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0
20
40
60
80
docked_HeavyAtomCount

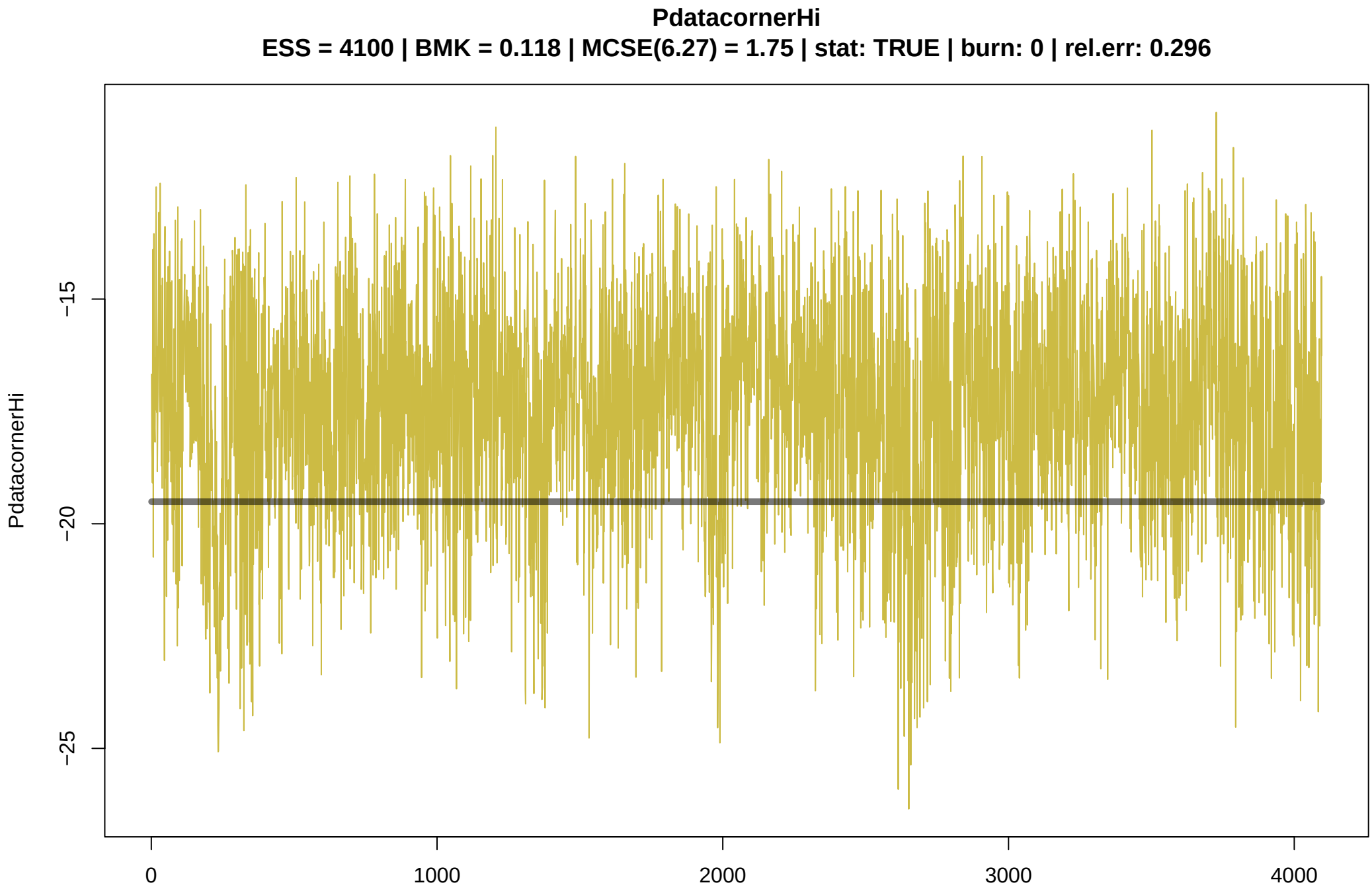

log_mcs_unbonded_polar_sasa
5
0
−5
−6
−4
−2
0
2
4
6
log_RMSD

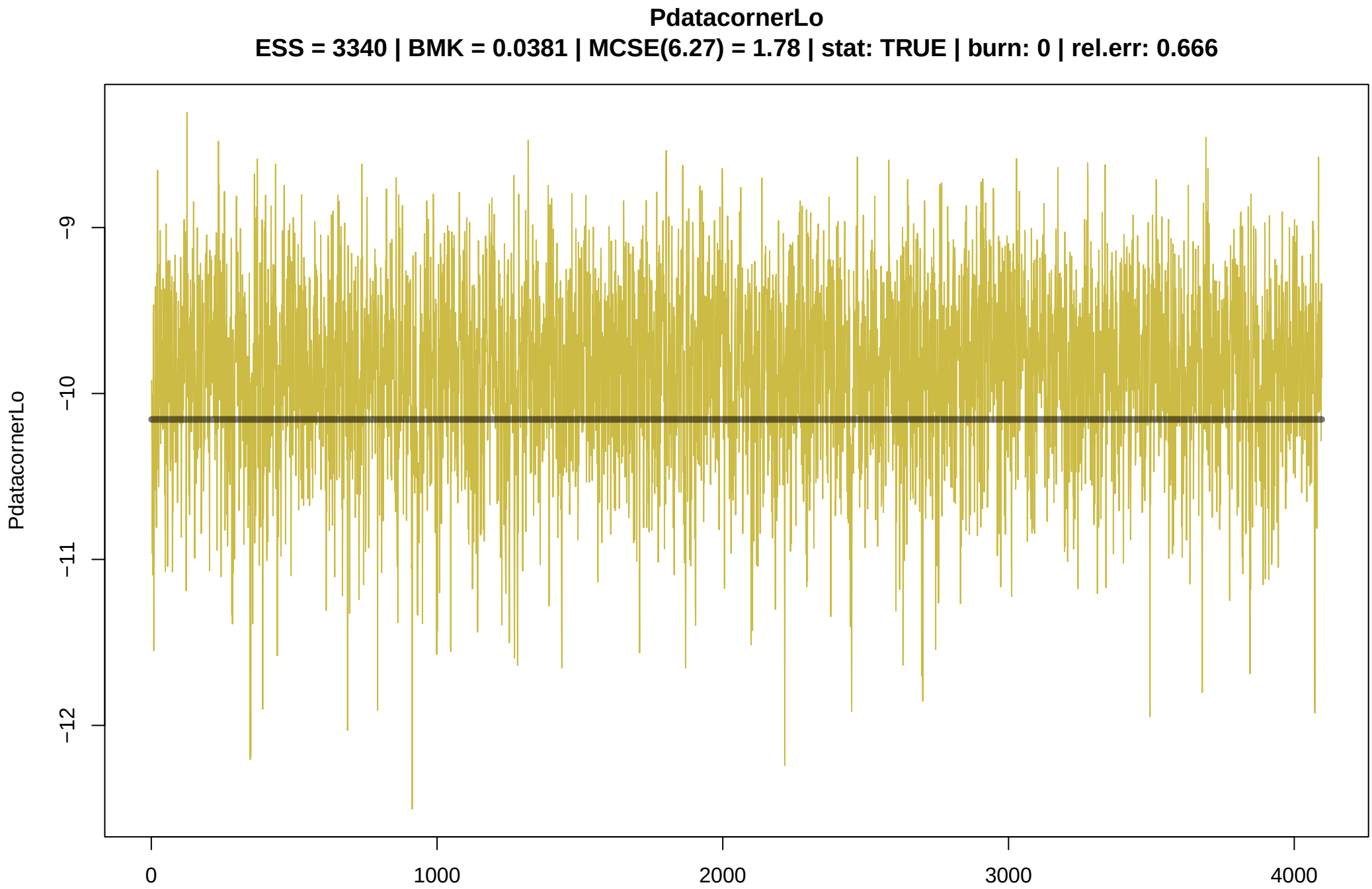

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−6
−4
−2
0
2
4
6
log_RMSD

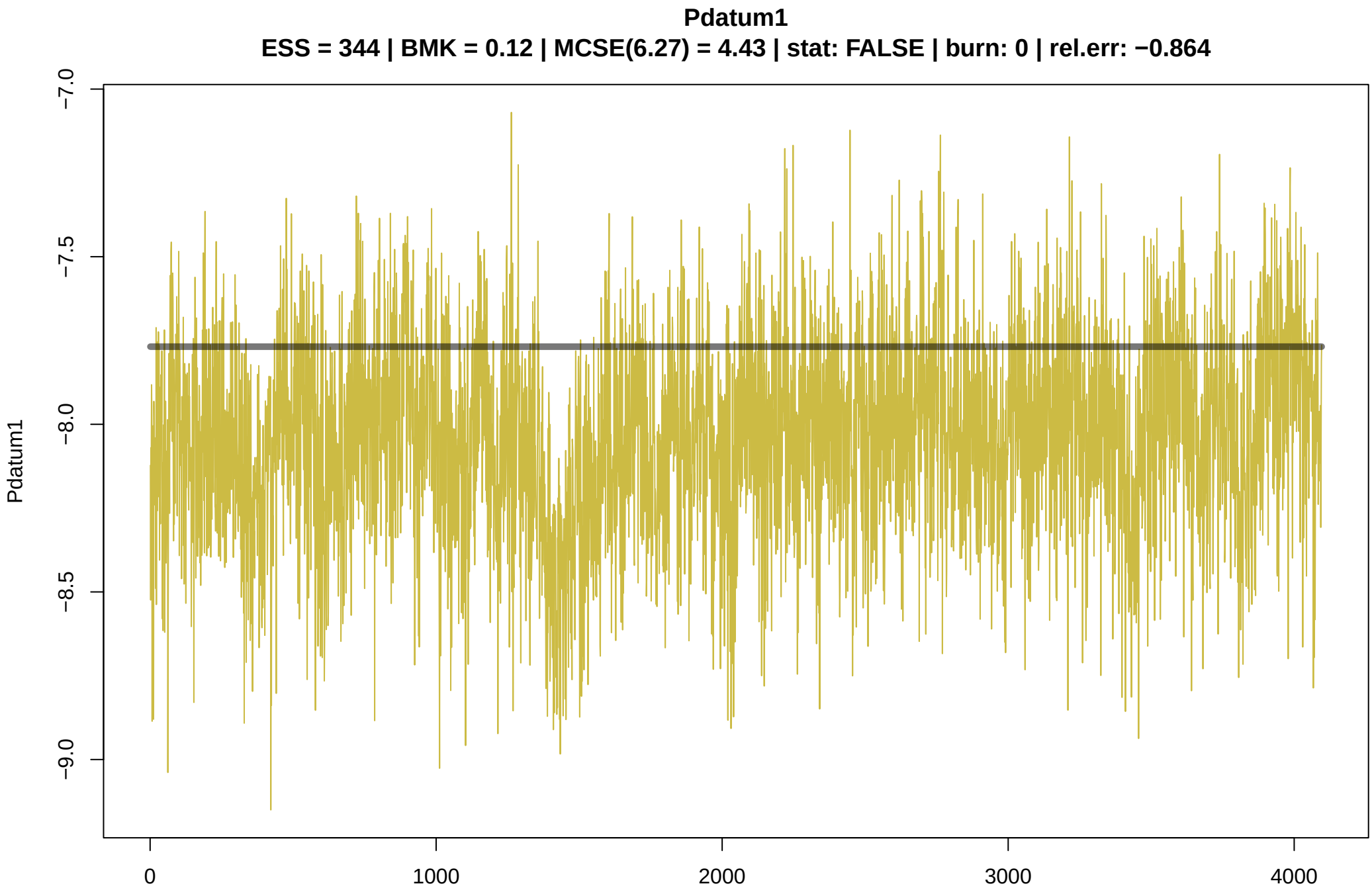

docked_HeavyAtomCount
200
150
100
50
0
−6
−4
−2
0
2
4
6
log_RMSD

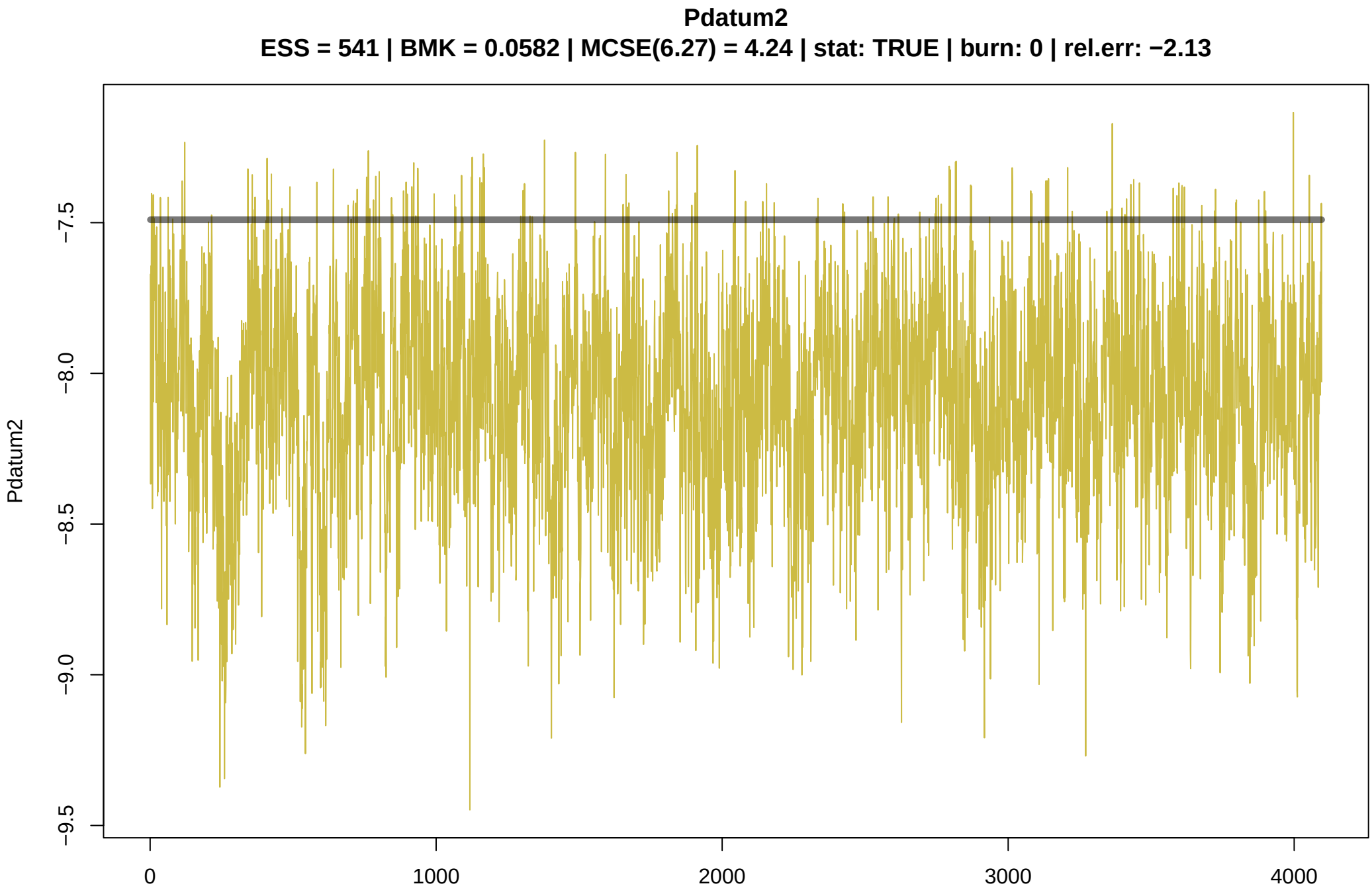

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

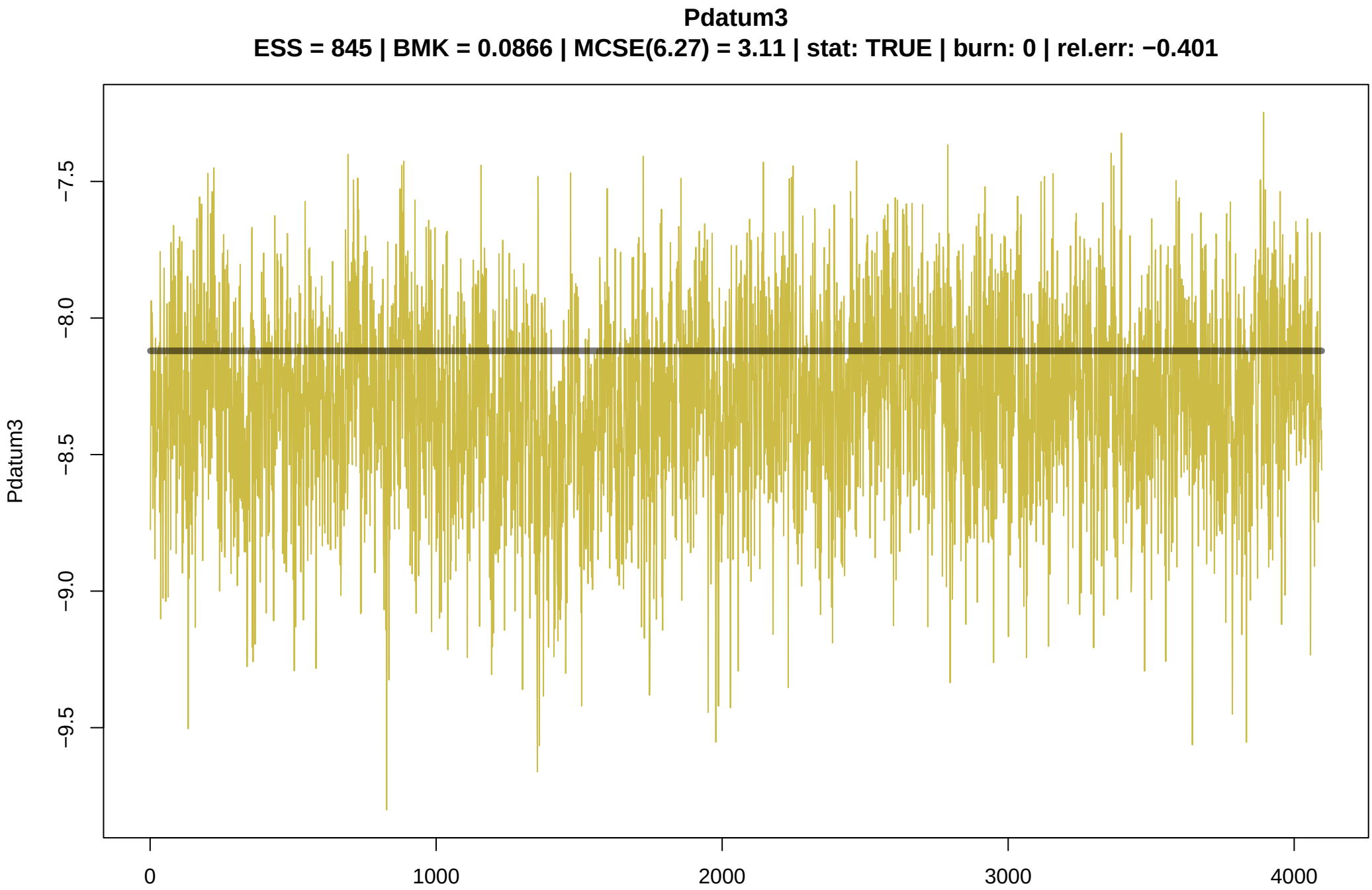

Pdatamean
ESS = 77.5 | BMK = 0.197 | MCSE(6.27) = 7.3 | stat: FALSE | burn: 0 | rel.err: 0.771
Pdatamean
−9
−10
−11
−12
−13
0
1000
2000
3000
4000

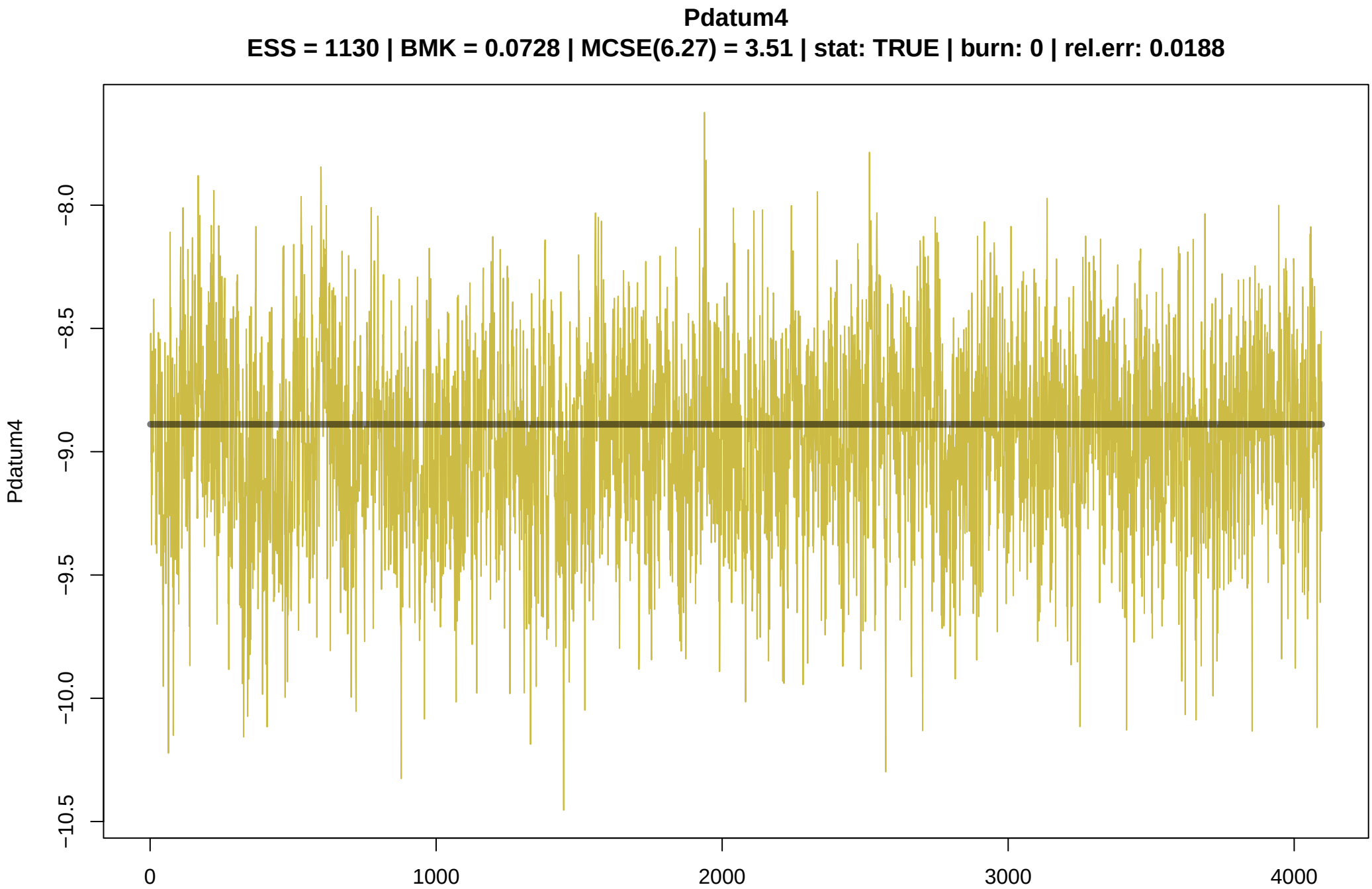

PdatacornerHi
ESS = 4100 | BMK = 0.118 | MCSE(6.27) = 1.75 | stat: TRUE | burn: 0 | rel.err: 0.296
PdatacornerHi
−15
−20
−25
0
1000
2000
3000
4000

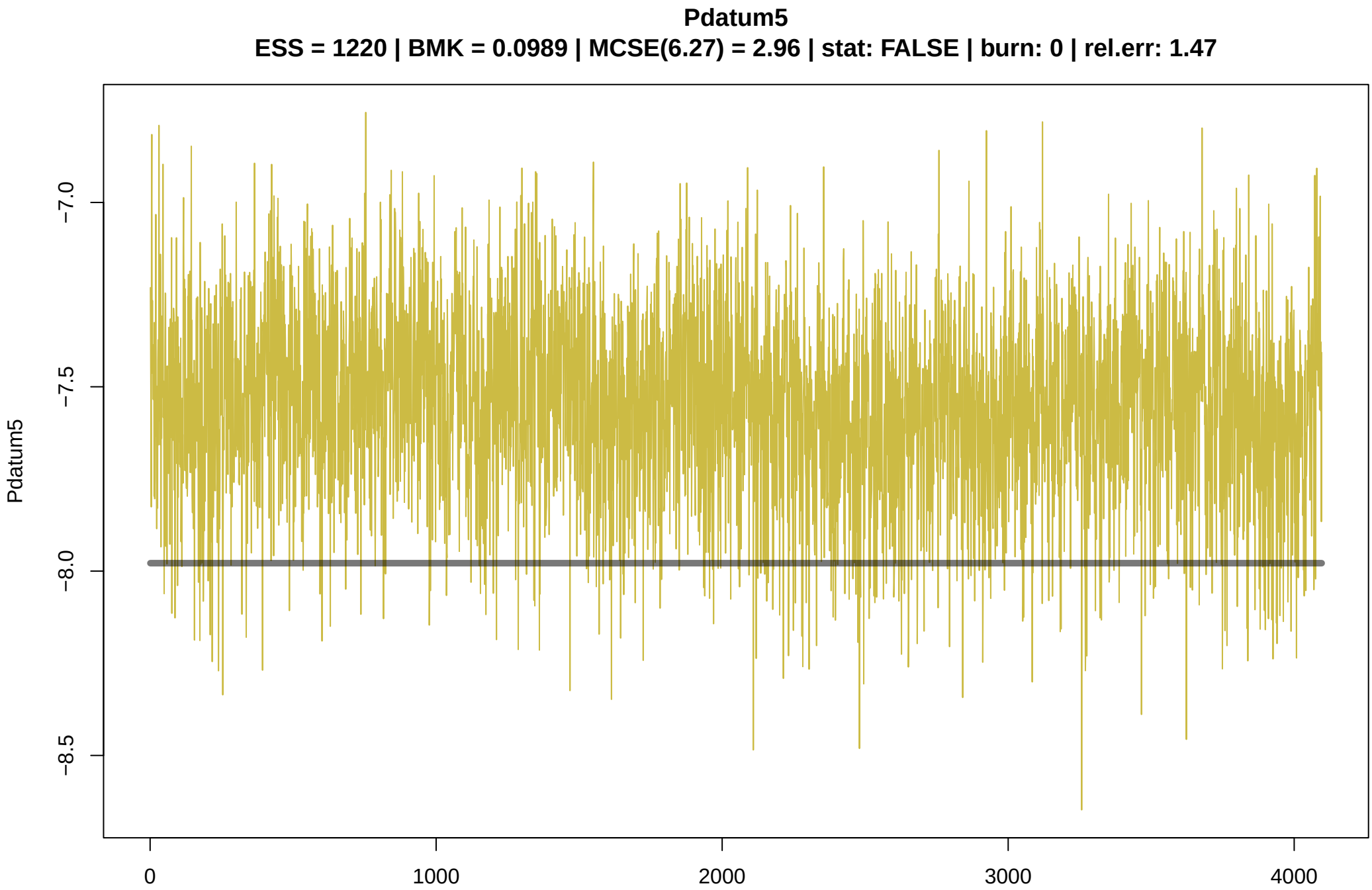

PdatacornerLo
ESS = 3340 | BMK = 0.0381 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0 | rel.err: 0.666
PdatacornerLo
−9
−10
−11
−12
0
1000
2000
3000
4000

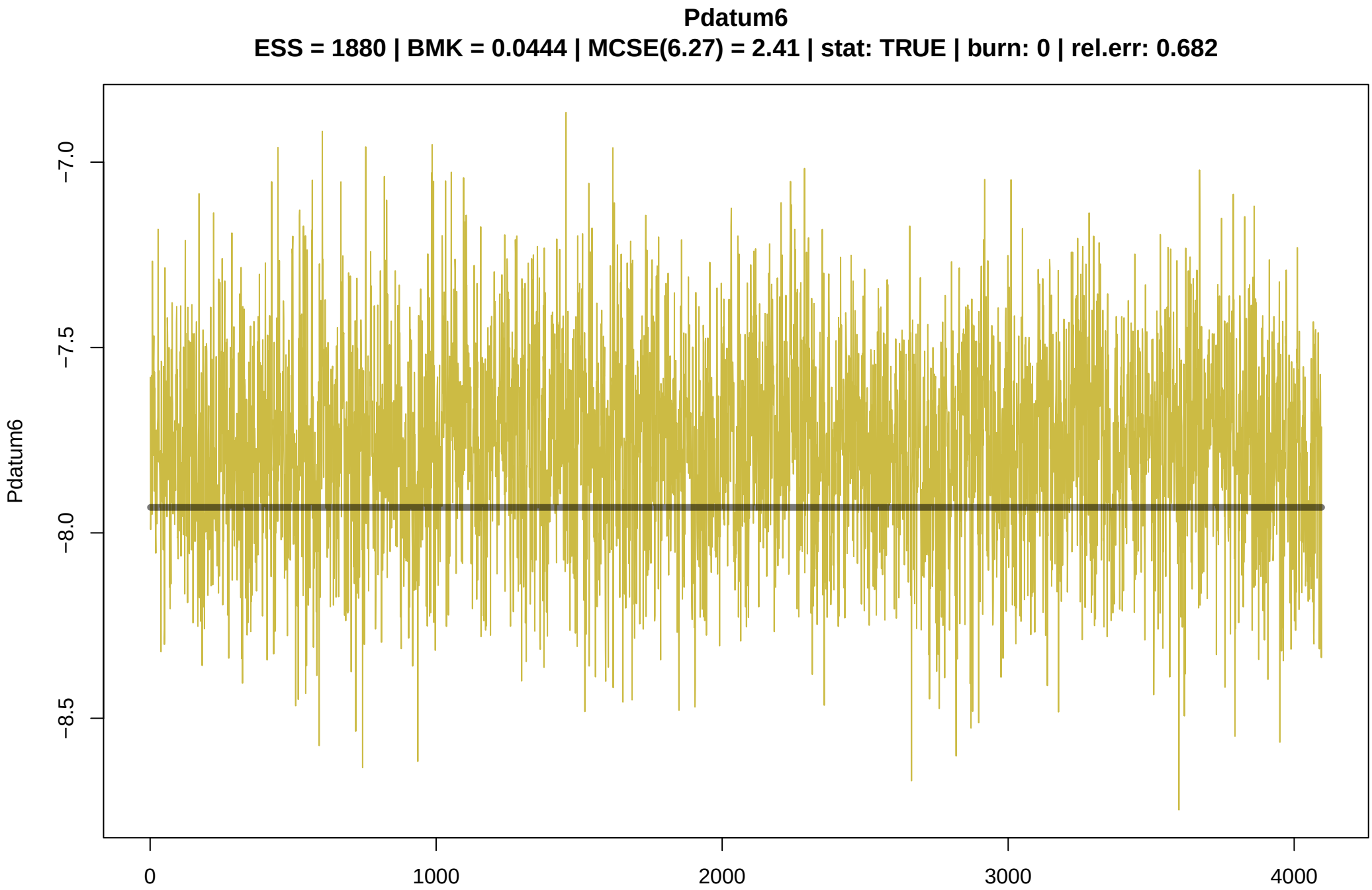

Pdatum1
ESS = 344 | BMK = 0.12 | MCSE(6.27) = 4.43 | stat: FALSE | burn: 0 | rel.err: −0.864
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

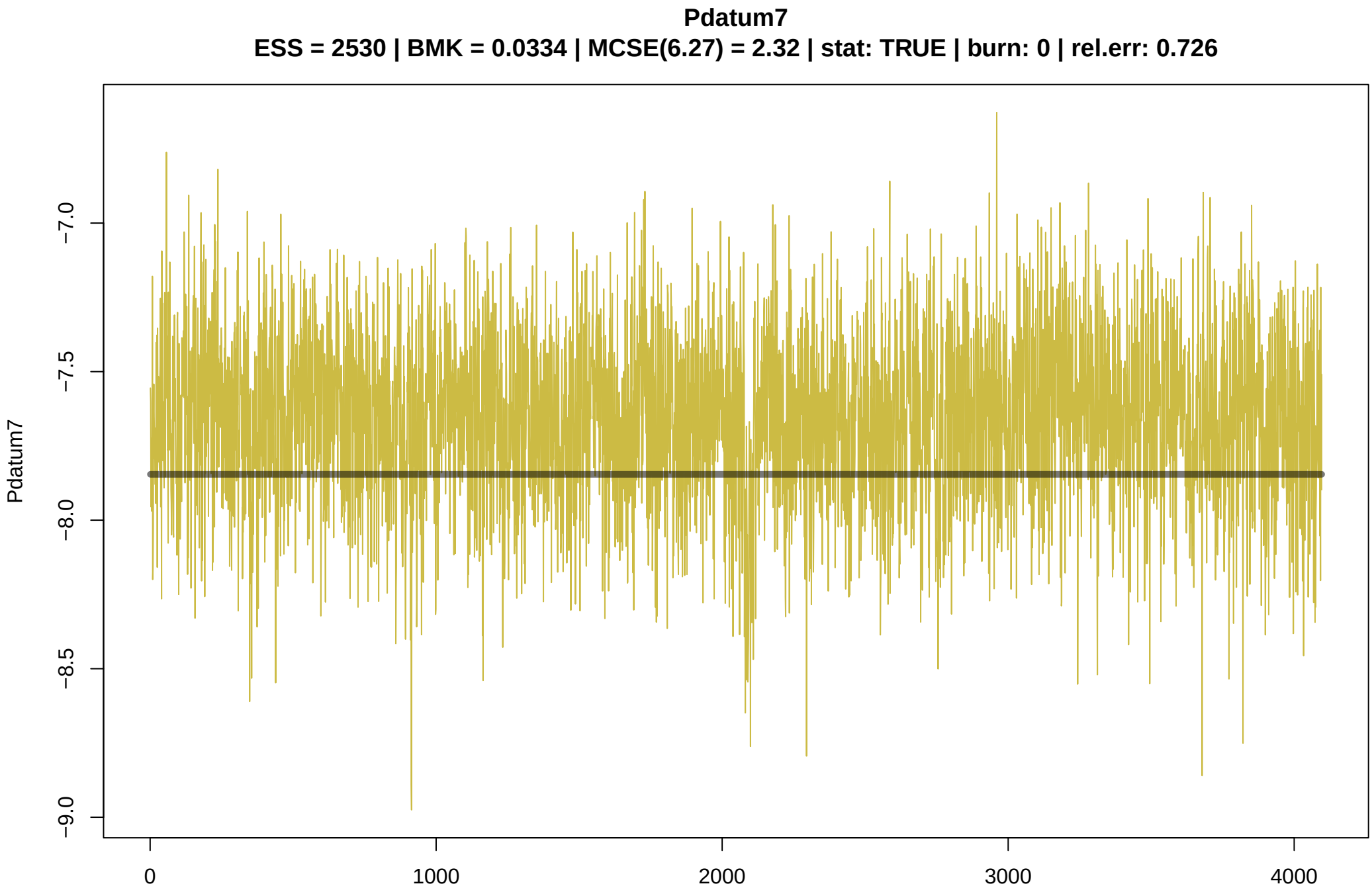

Pdatum2
ESS = 541 | BMK = 0.0582 | MCSE(6.27) = 4.24 | stat: TRUE | burn: 0 | rel.err: −2.13
Pdatum2
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

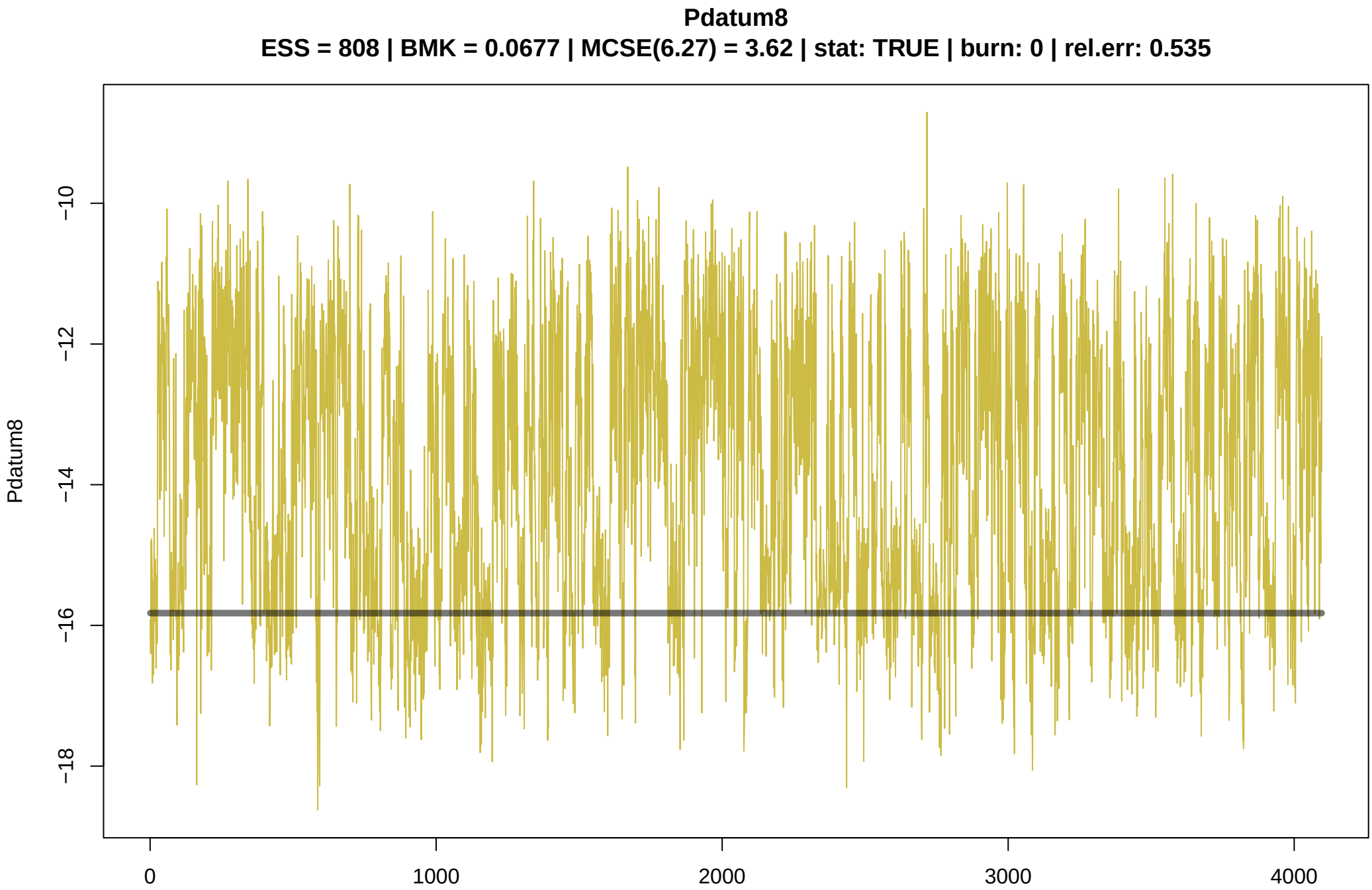

Pdatum3
ESS = 845 | BMK = 0.0866 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: −0.401
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

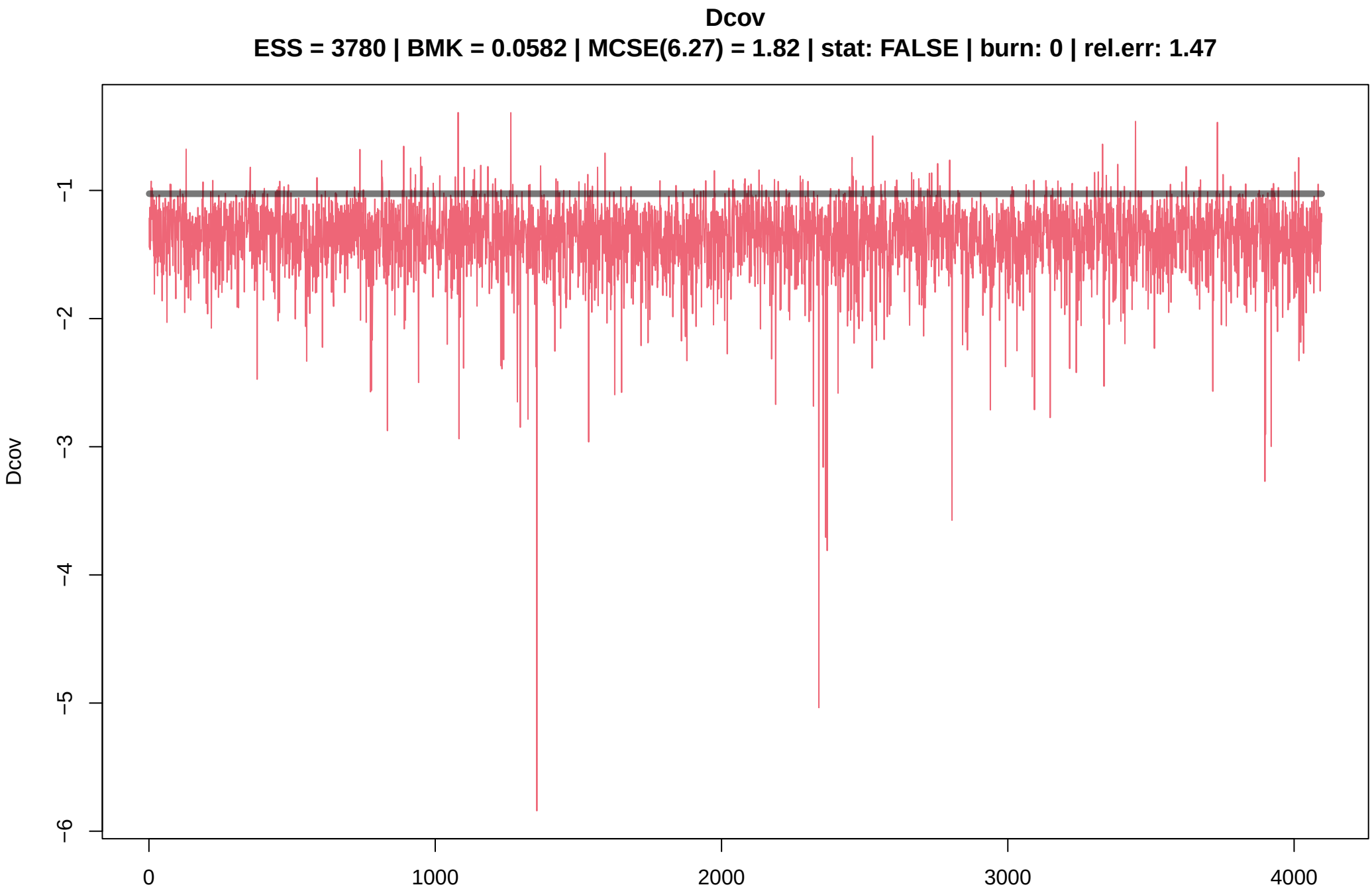

Pdatum4
ESS = 1130 | BMK = 0.0728 | MCSE(6.27) = 3.51 | stat: TRUE | burn: 0 | rel.err: 0.0188
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

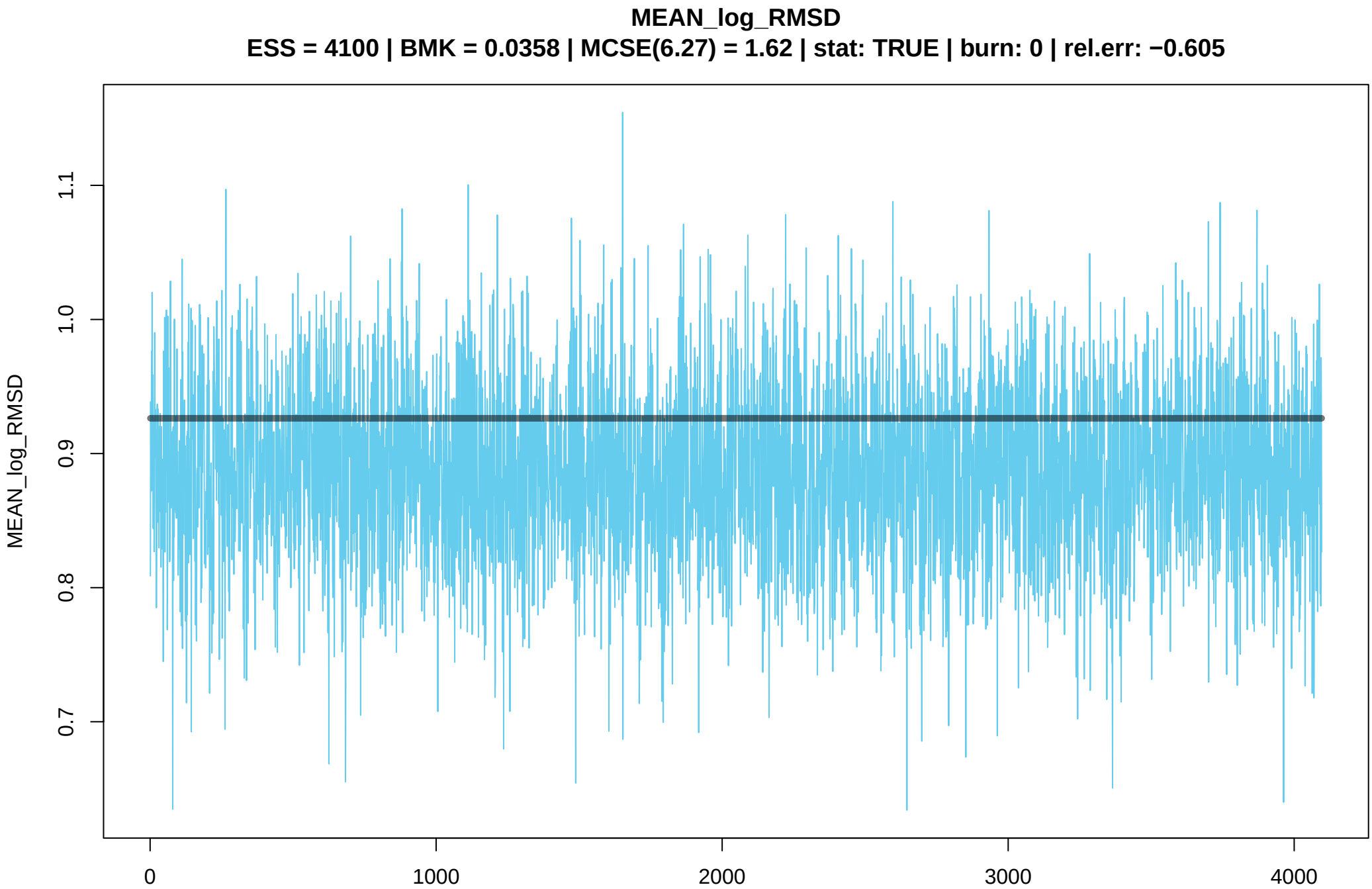

Pdatum5
ESS = 1220 | BMK = 0.0989 | MCSE(6.27) = 2.96 | stat: FALSE | burn: 0 | rel.err: 1.47
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

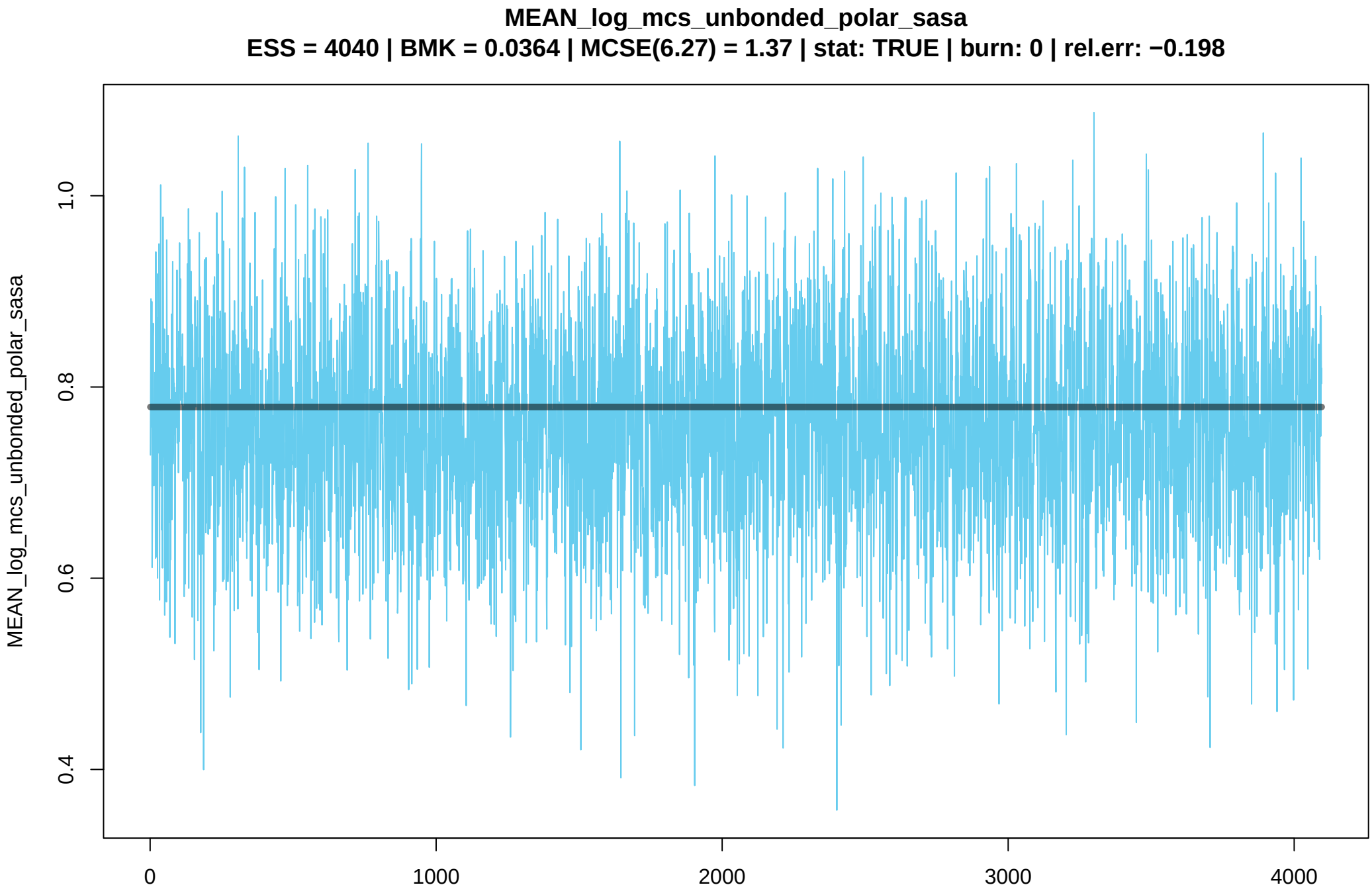

Pdatum6
ESS = 1880 | BMK = 0.0444 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | rel.err: 0.682
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

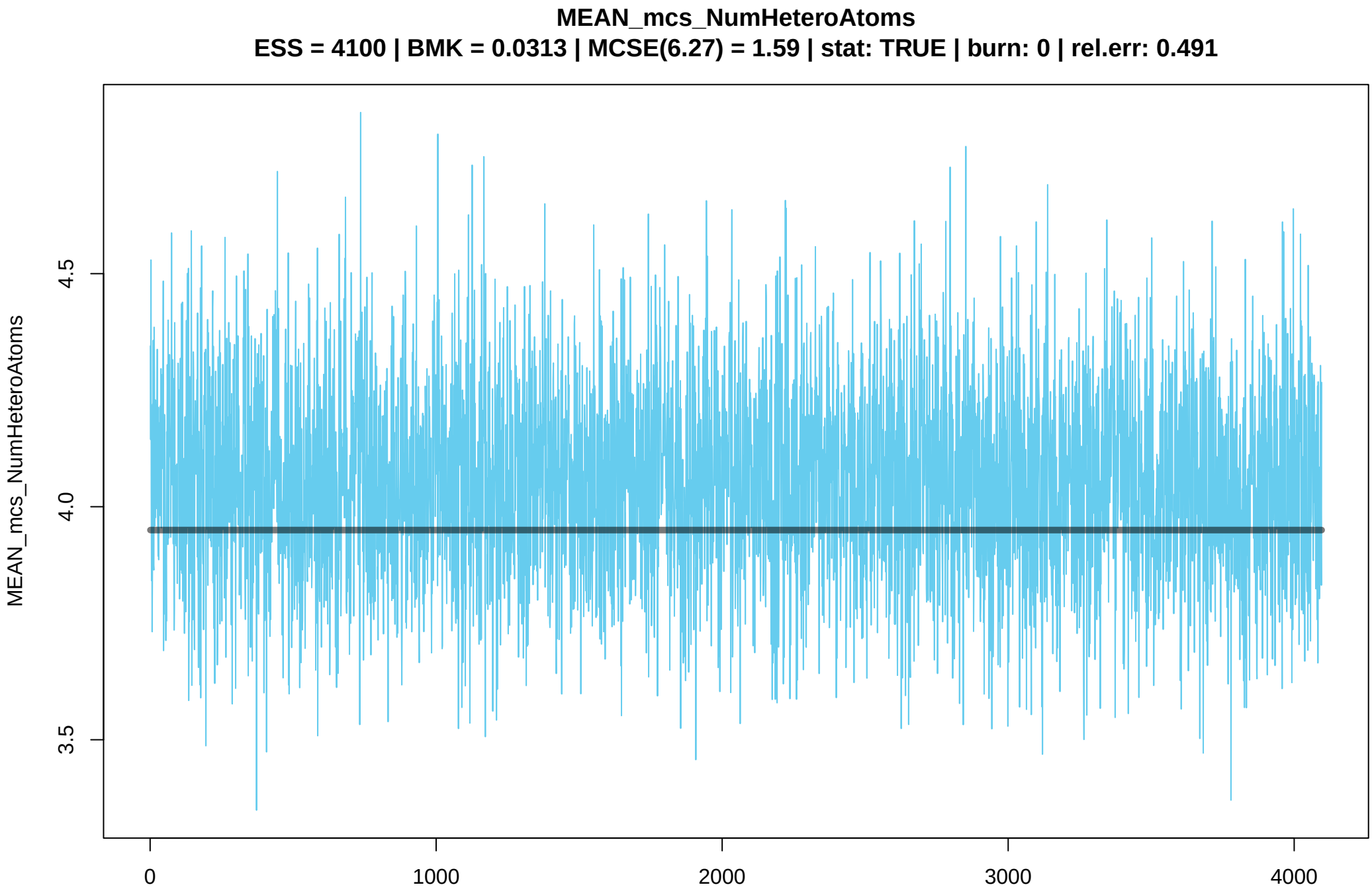

Pdatum7
ESS = 2530 | BMK = 0.0334 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: 0.726
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

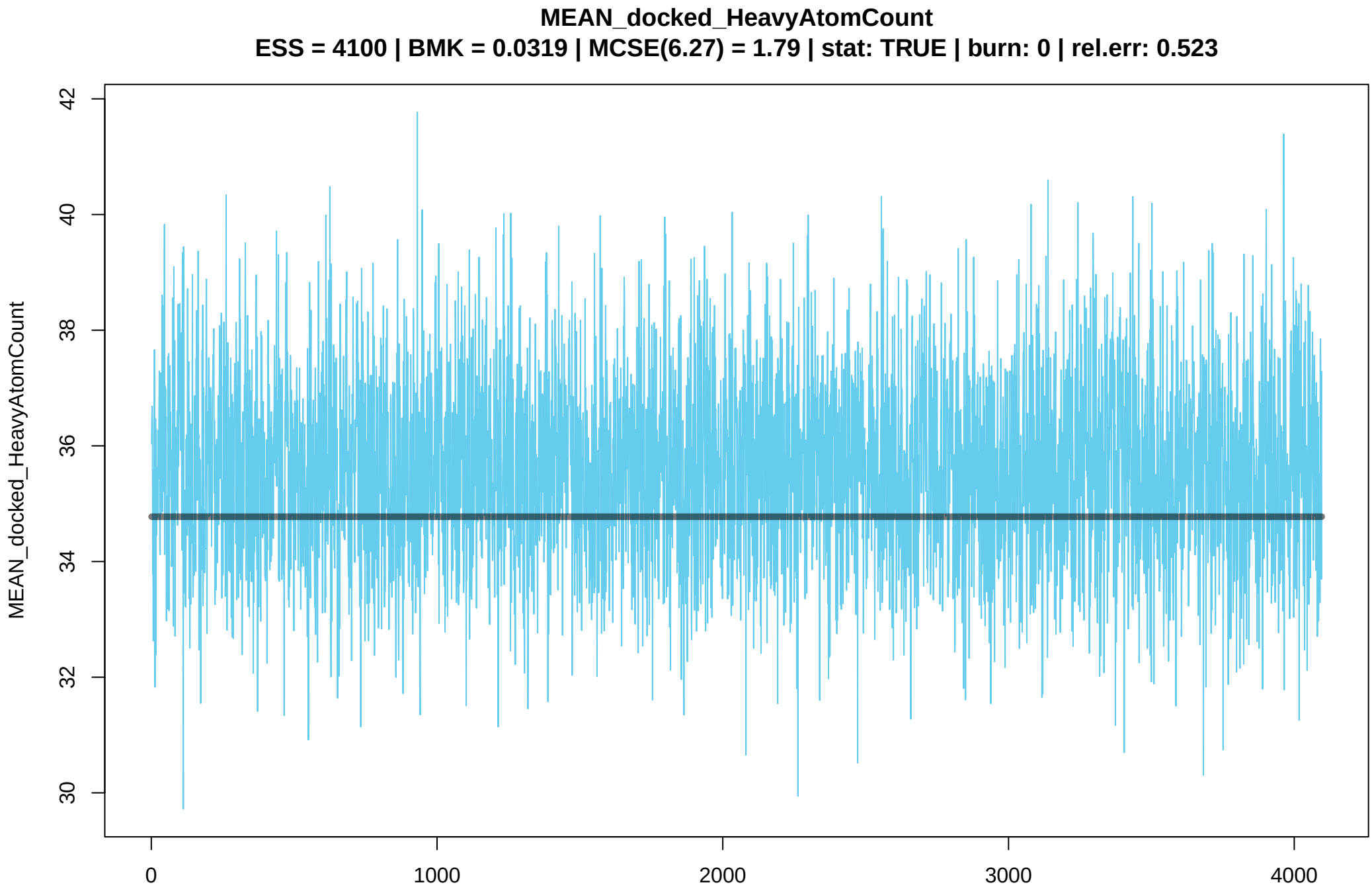

Pdatum8
ESS = 808 | BMK = 0.0677 | MCSE(6.27) = 3.62 | stat: TRUE | burn: 0 | rel.err: 0.535
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

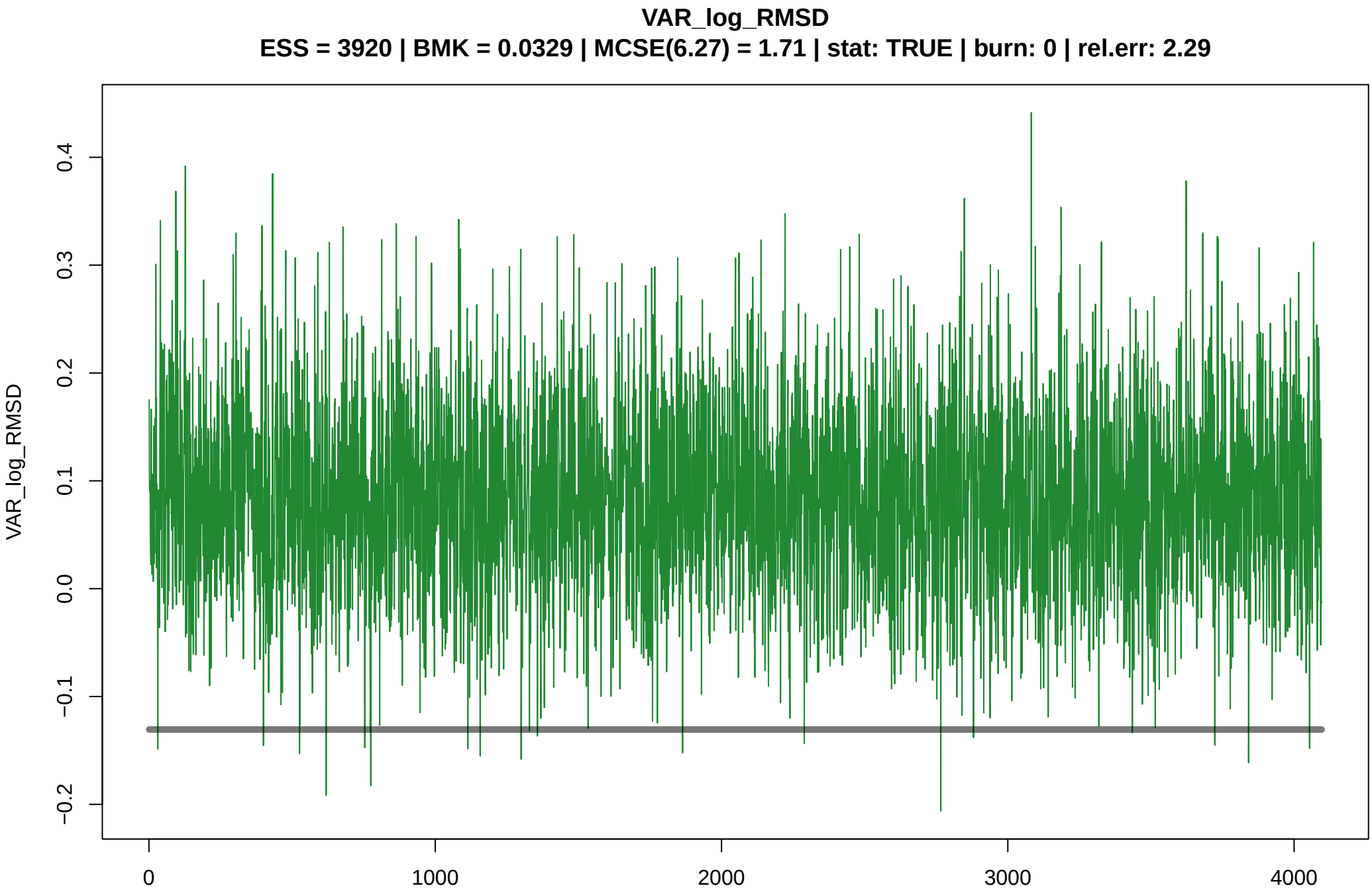

Dcov
ESS = 3780 | BMK = 0.0582 | MCSE(6.27) = 1.82 | stat: FALSE | burn: 0 | rel.err: 1.47
Dcov
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

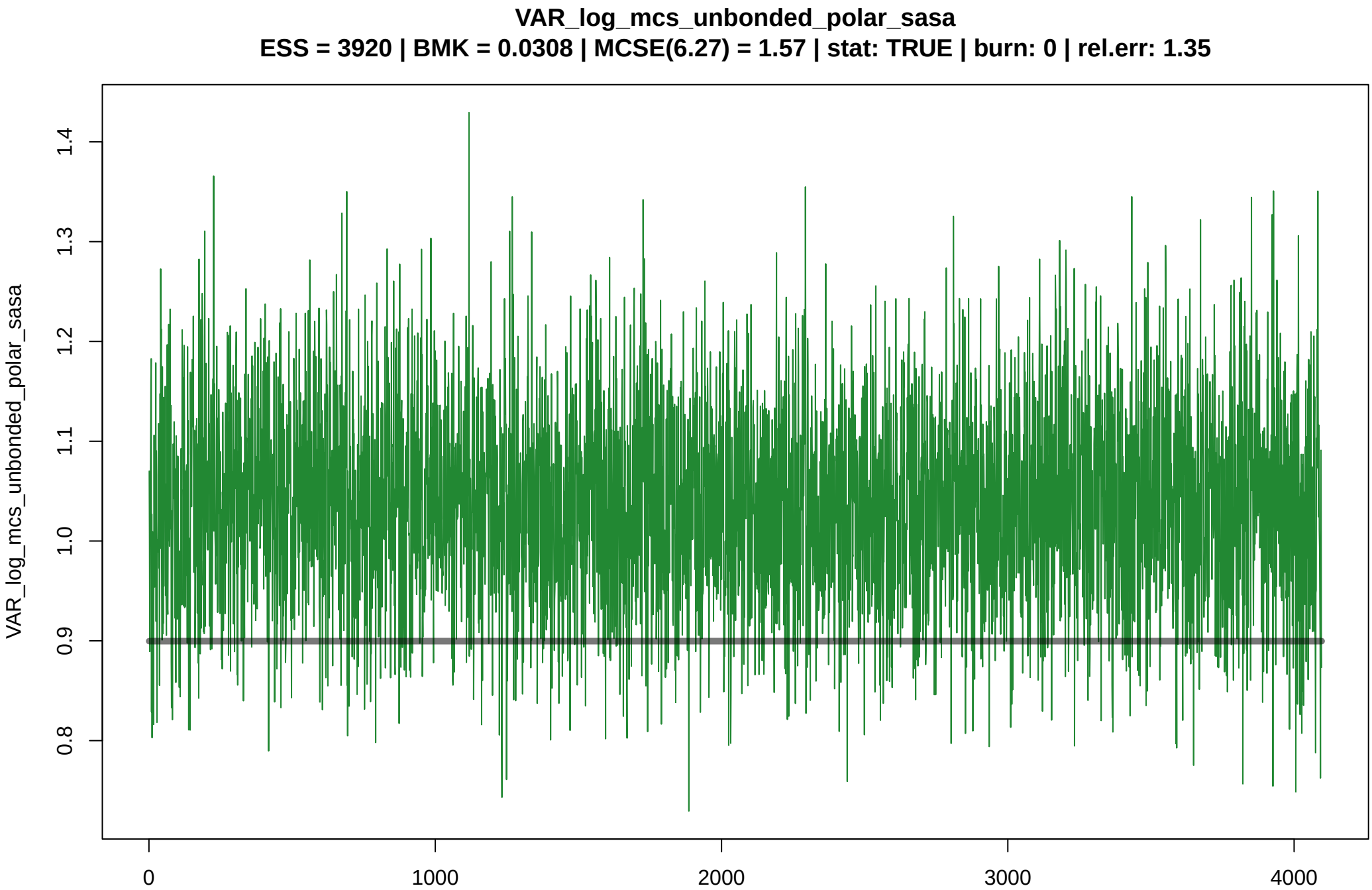

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0358 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: −0.605
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

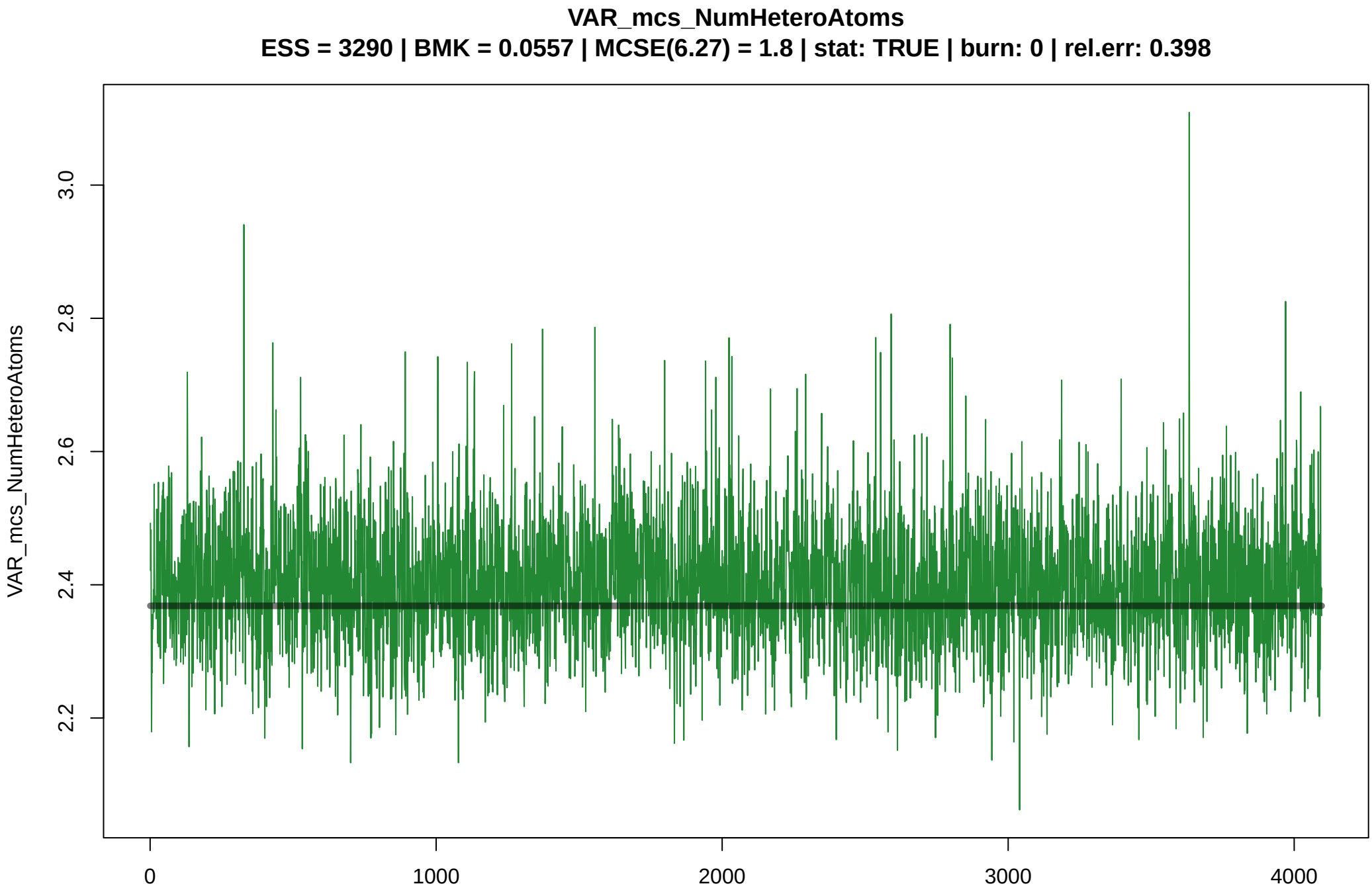

MEAN_log_mcs_unbonded_polar_sasa
ESS = 4040 | BMK = 0.0364 | MCSE(6.27) = 1.37 | stat: TRUE | burn: 0 | rel.err: −0.198
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

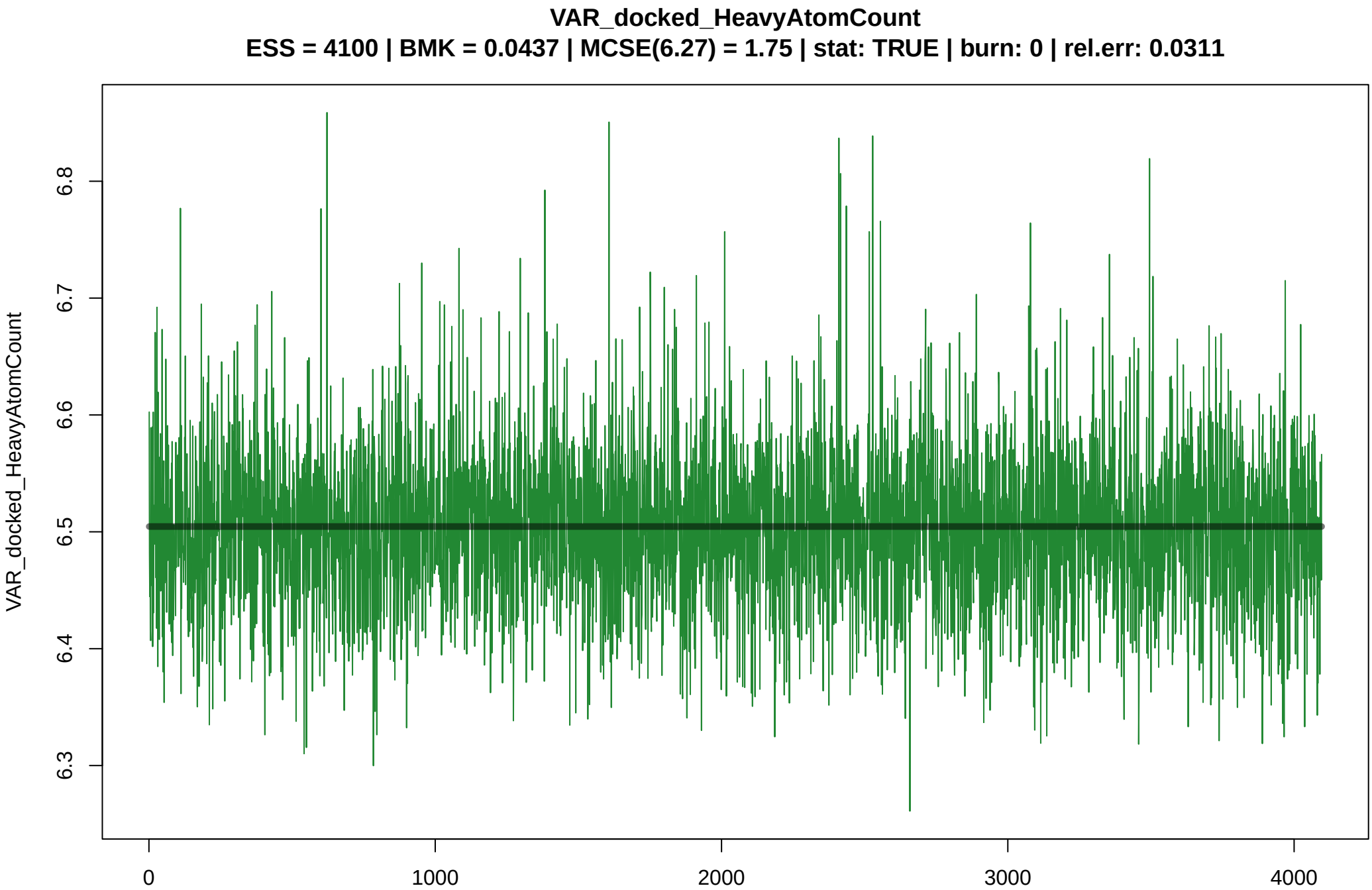

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0313 | MCSE(6.27) = 1.59 | stat: TRUE | burn: 0 | rel.err: 0.491
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

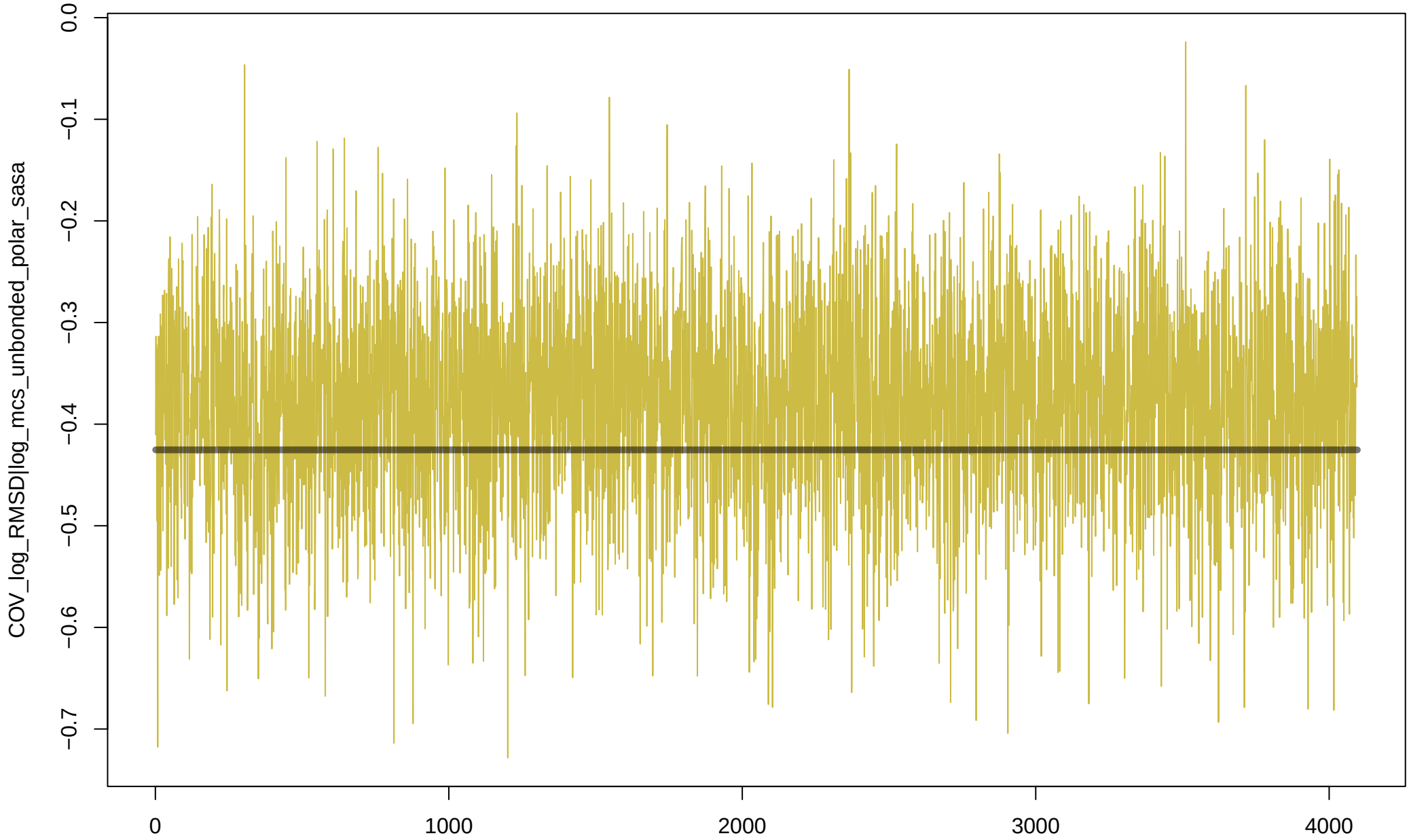

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0319 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.523
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
1000
2000
3000
4000

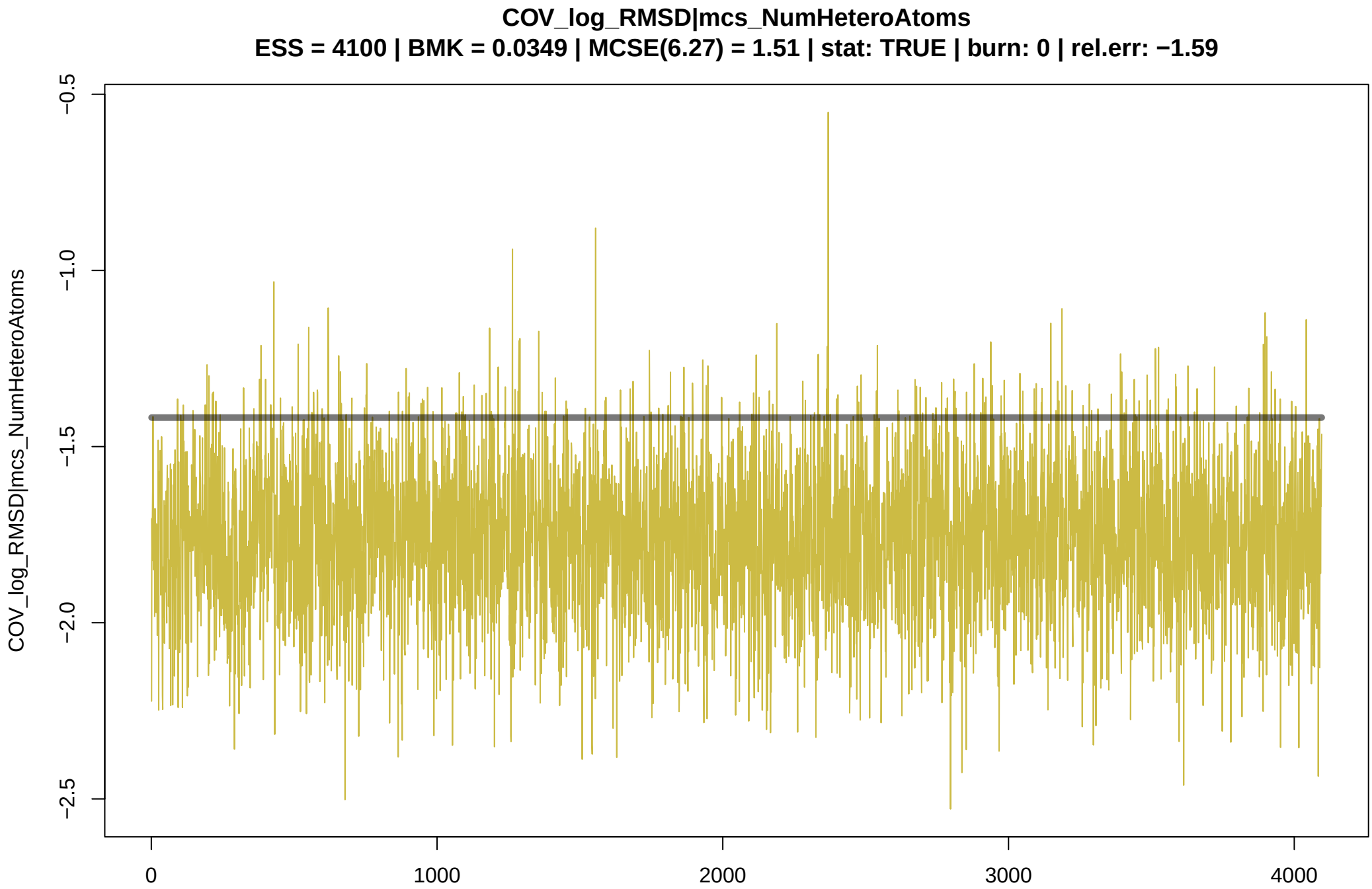

VAR_log_RMSD
ESS = 3920 | BMK = 0.0329 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: 2.29
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

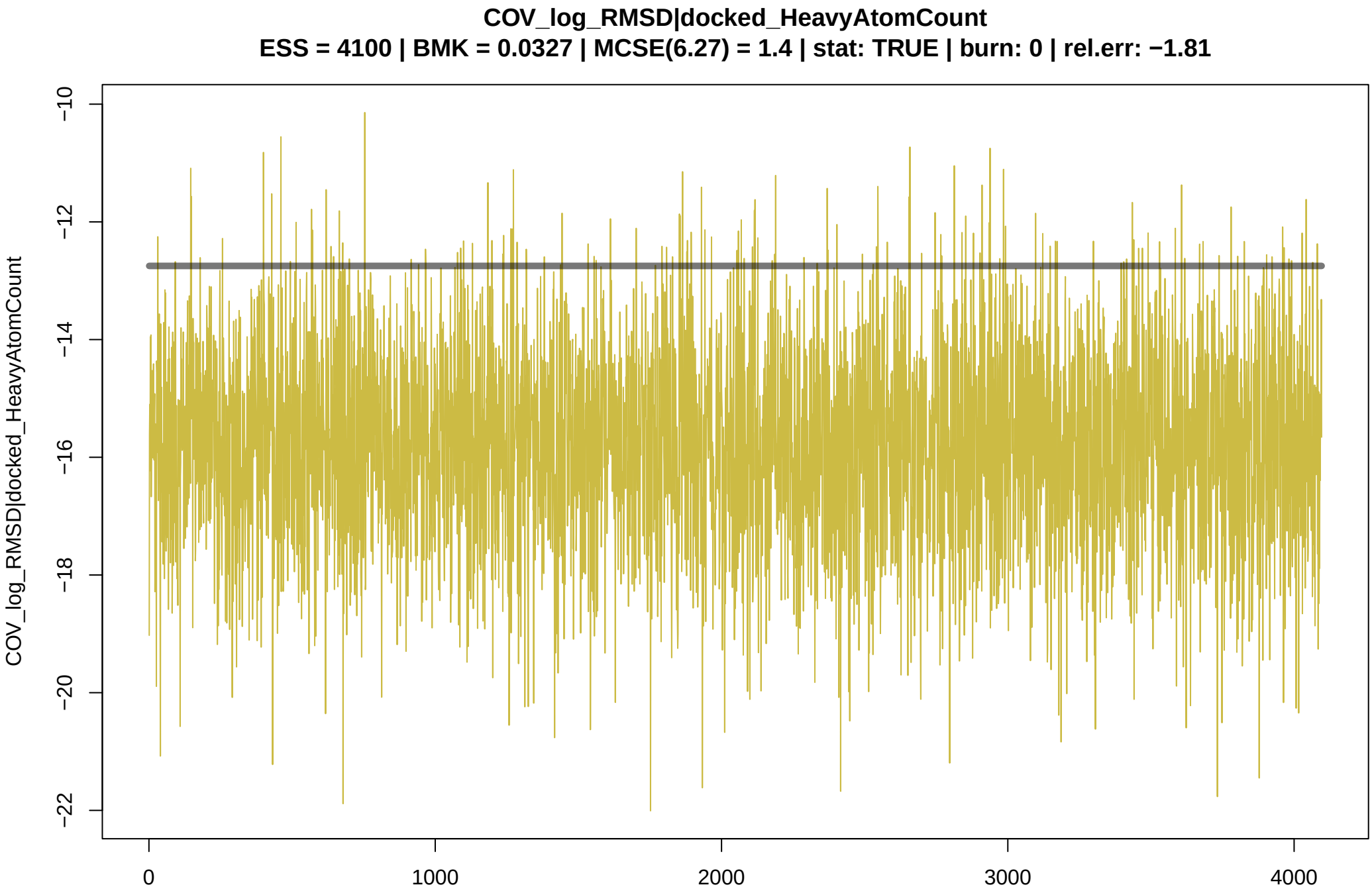

VAR_log_mcs_unbonded_polar_sasa
ESS = 3920 | BMK = 0.0308 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0 | rel.err: 1.35
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
1000
2000
3000
4000

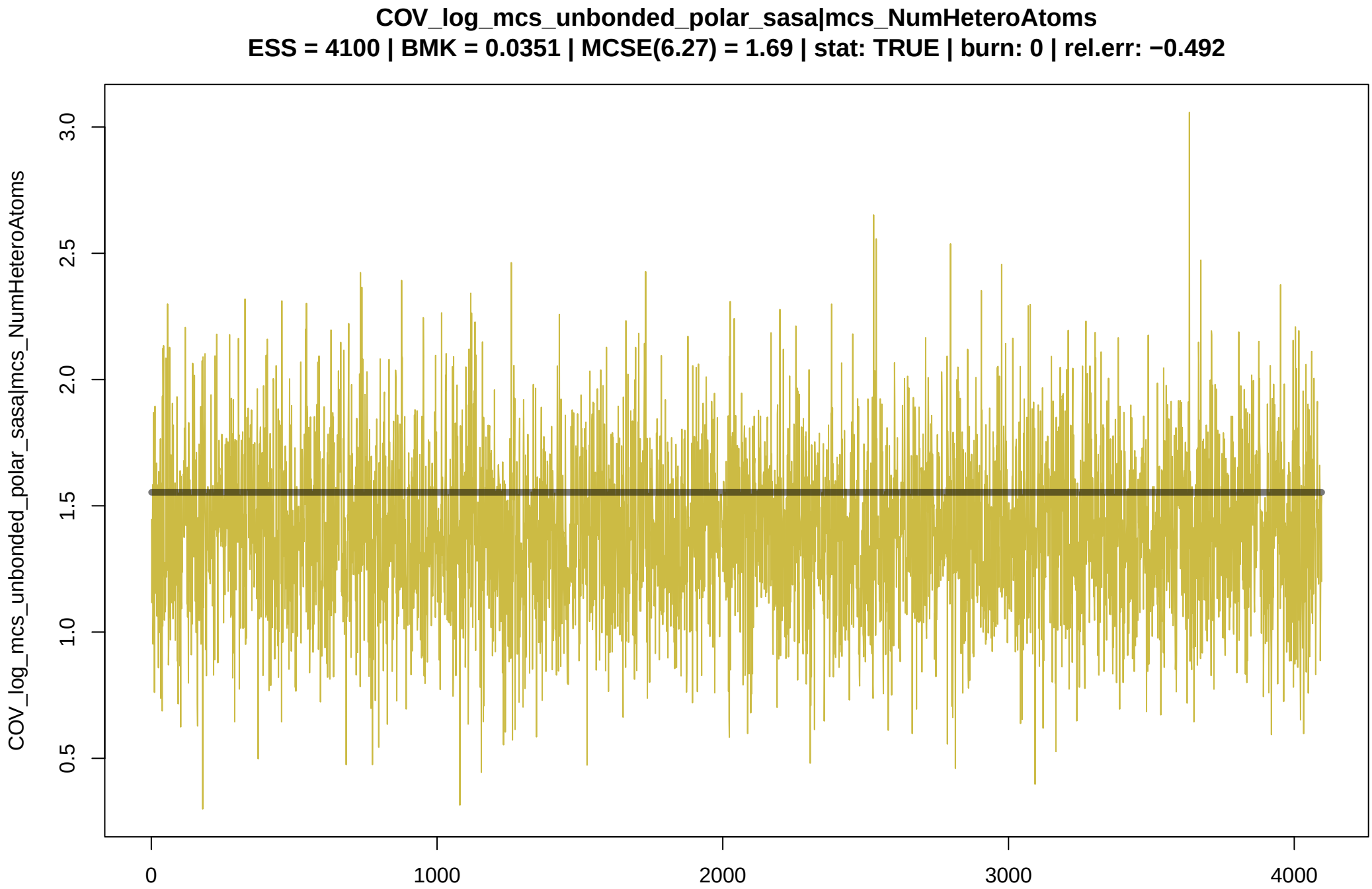

VAR_mcs_NumHeteroAtoms
ESS = 3290 | BMK = 0.0557 | MCSE(6.27) = 1.8 | stat: TRUE | burn: 0 | rel.err: 0.398
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
0
1000
2000
3000
4000

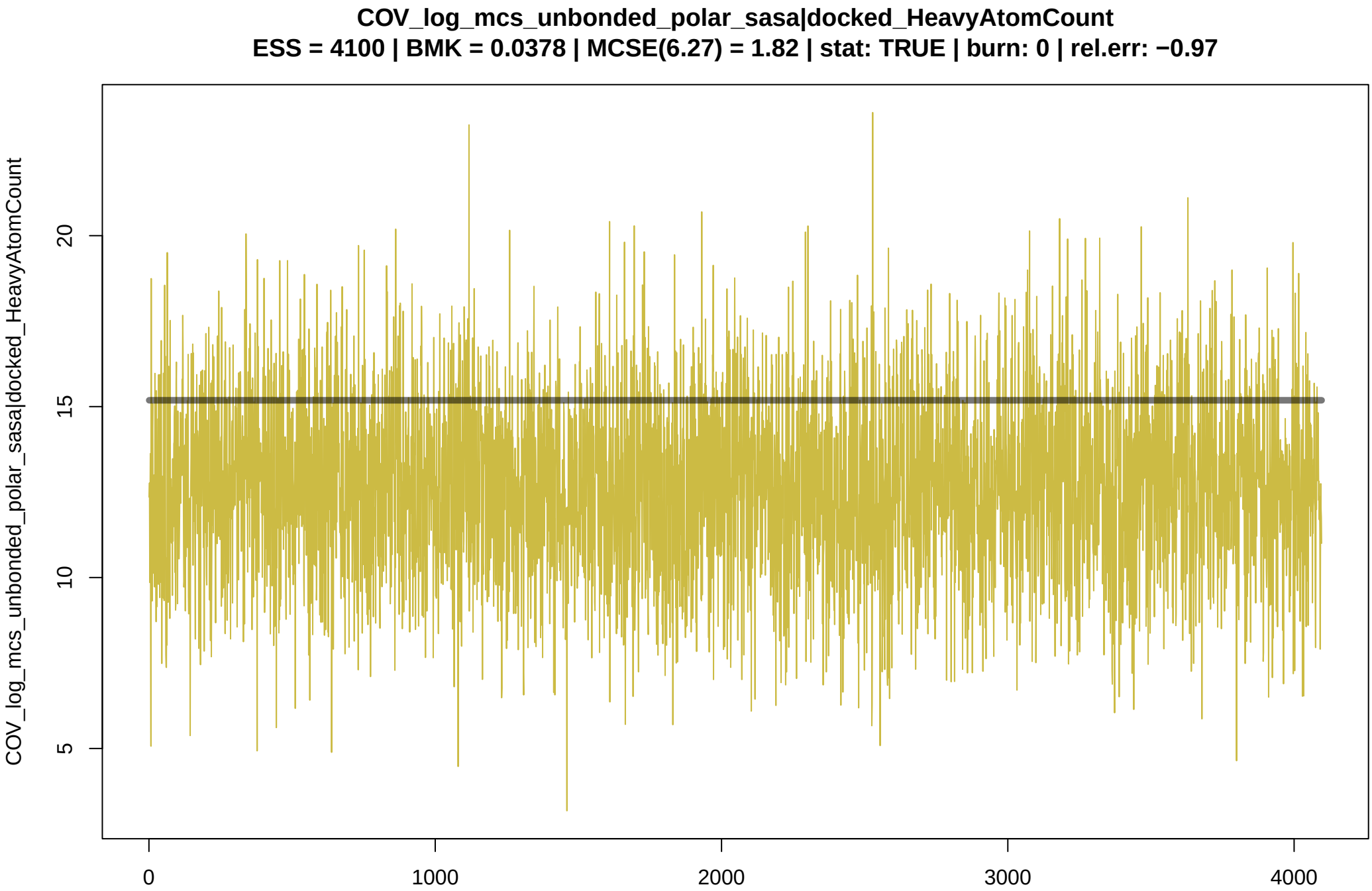

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0437 | MCSE(6.27) = 1.75 | stat: TRUE | burn: 0 | rel.err: 0.0311
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
0
1000
2000
3000
4000

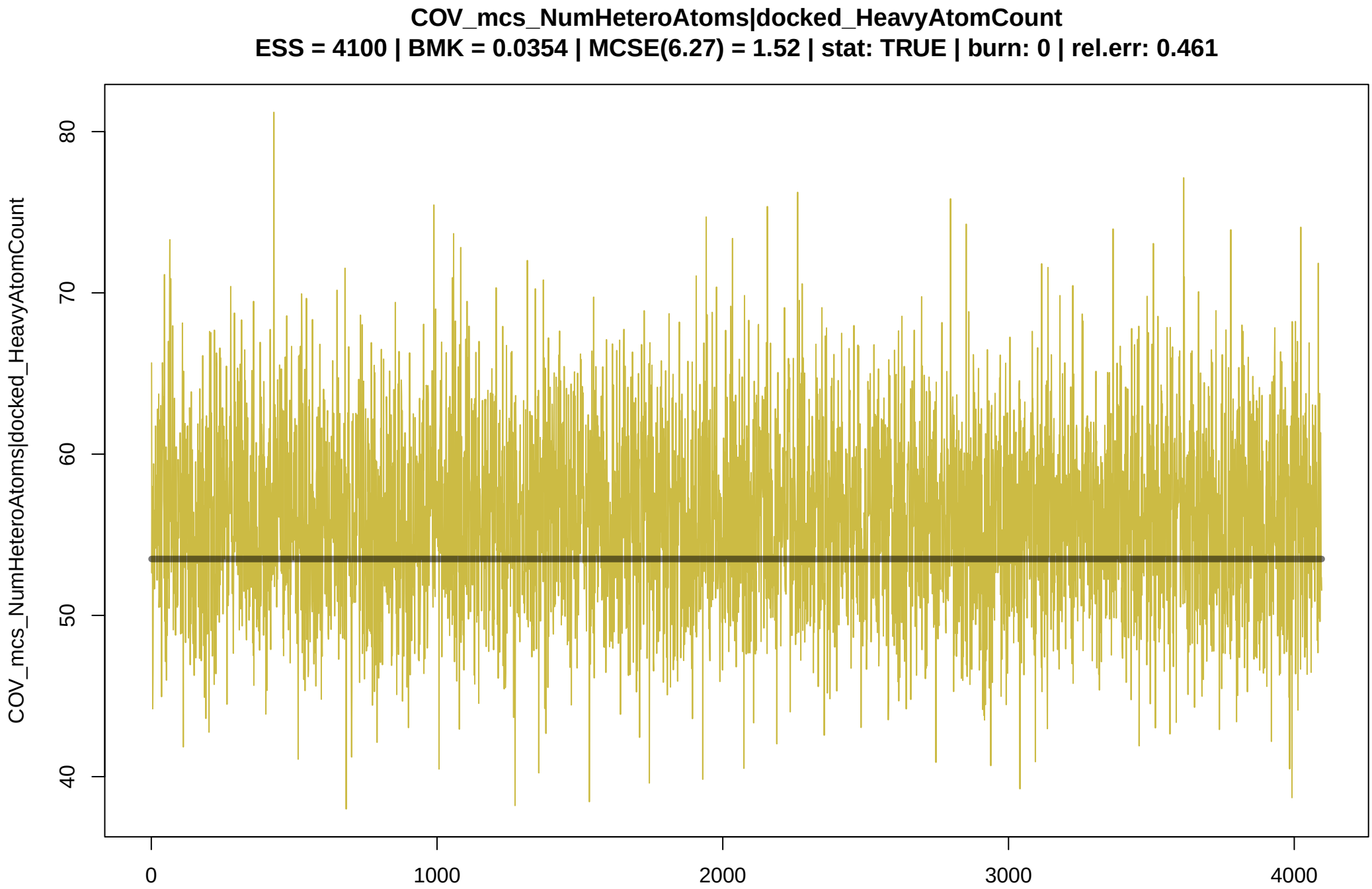

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 4100 | BMK = 0.0348 | MCSE(6.27) = 1.7 | stat: FALSE | burn: 0 | rel.err: 0.493
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0349 | MCSE(6.27) = 1.51 | stat: TRUE | burn: 0 | rel.err: −1.59
COV_log_RMSD|mcs_NumHeteroAtoms
−0.5
−1.0
−1.5
−2.0
−2.5
0
1000
2000
3000
4000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0327 | MCSE(6.27) = 1.4 | stat: TRUE | burn: 0 | rel.err: −1.81
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 = 0.0351 | MCSE(6.27) = 1.69 | stat: TRUE | burn: 0 | rel.err: −0.492
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 = 4100 | BMK = 0.0378 | MCSE(6.27) = 1.82 | stat: TRUE | burn: 0 | rel.err: −0.97
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 = 0.0354 | MCSE(6.27) = 1.52 | stat: TRUE | burn: 0 | rel.err: 0.461
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
1000
2000
3000
4000