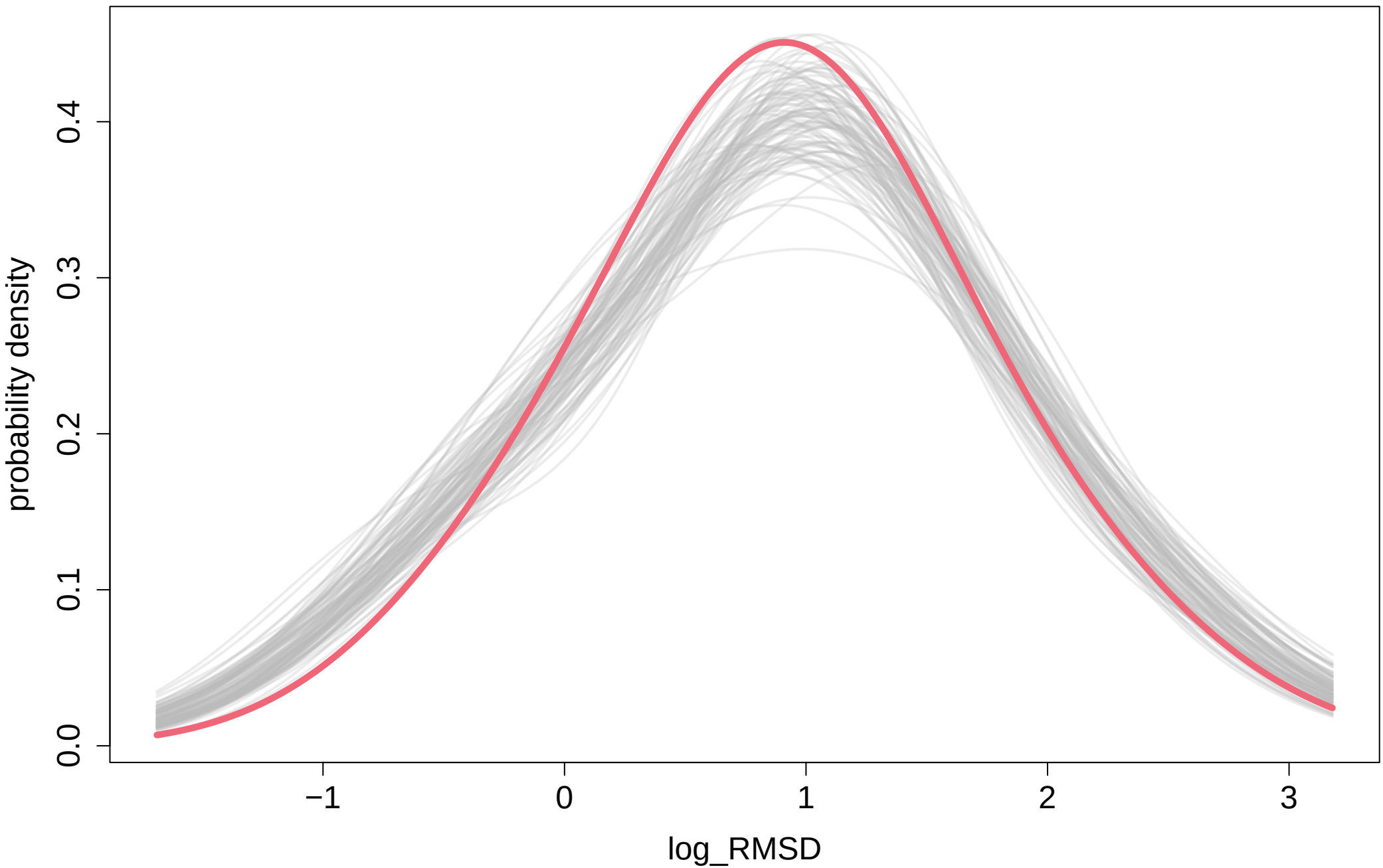
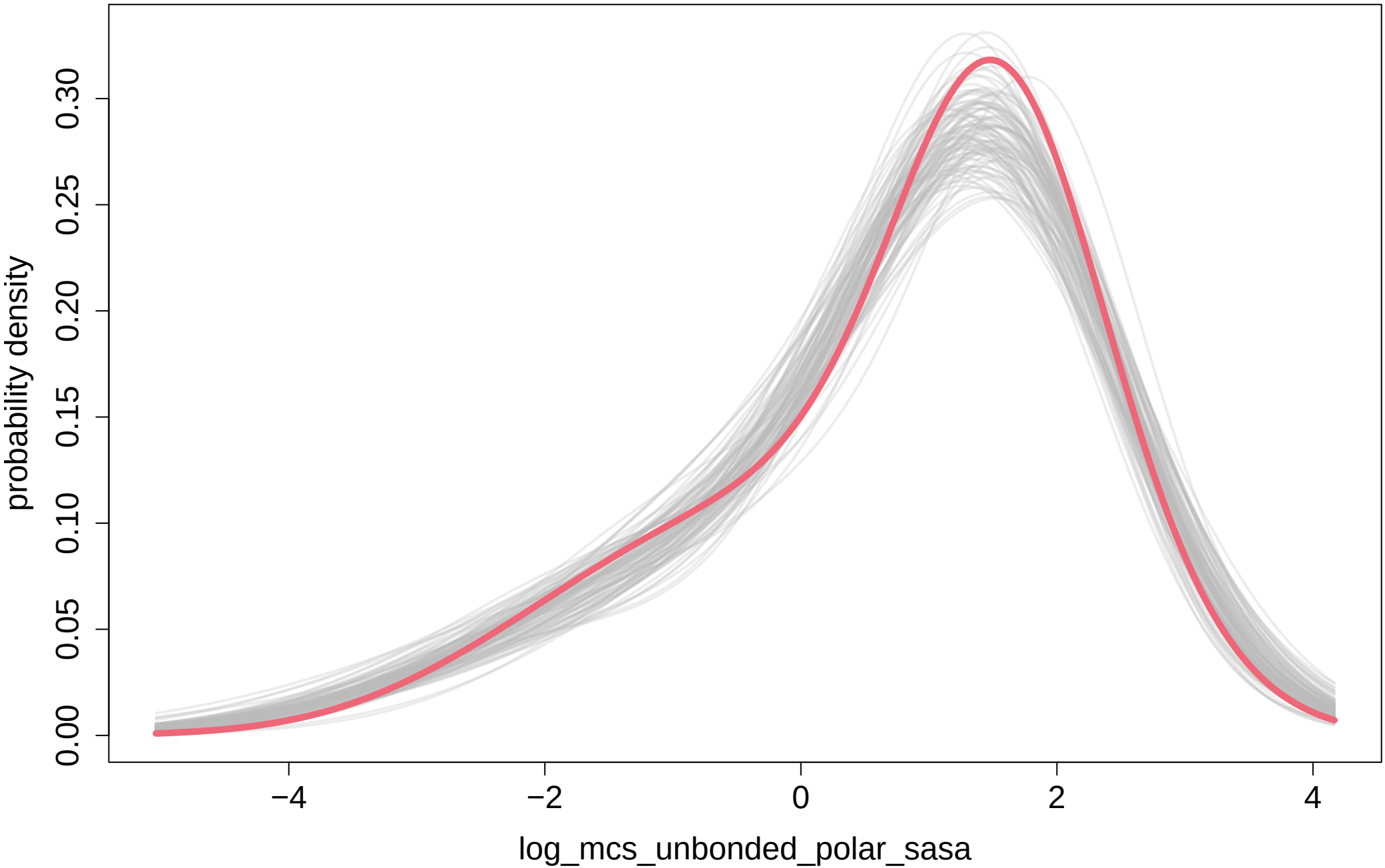
−− STATS maxD −−
min ESS = 158.692400082134
max BMK = 0.120624128728581
max MCSE = 6.4484408475662
all stationary: FALSE
burn: 0
max rel.err.: 2.27895390653437

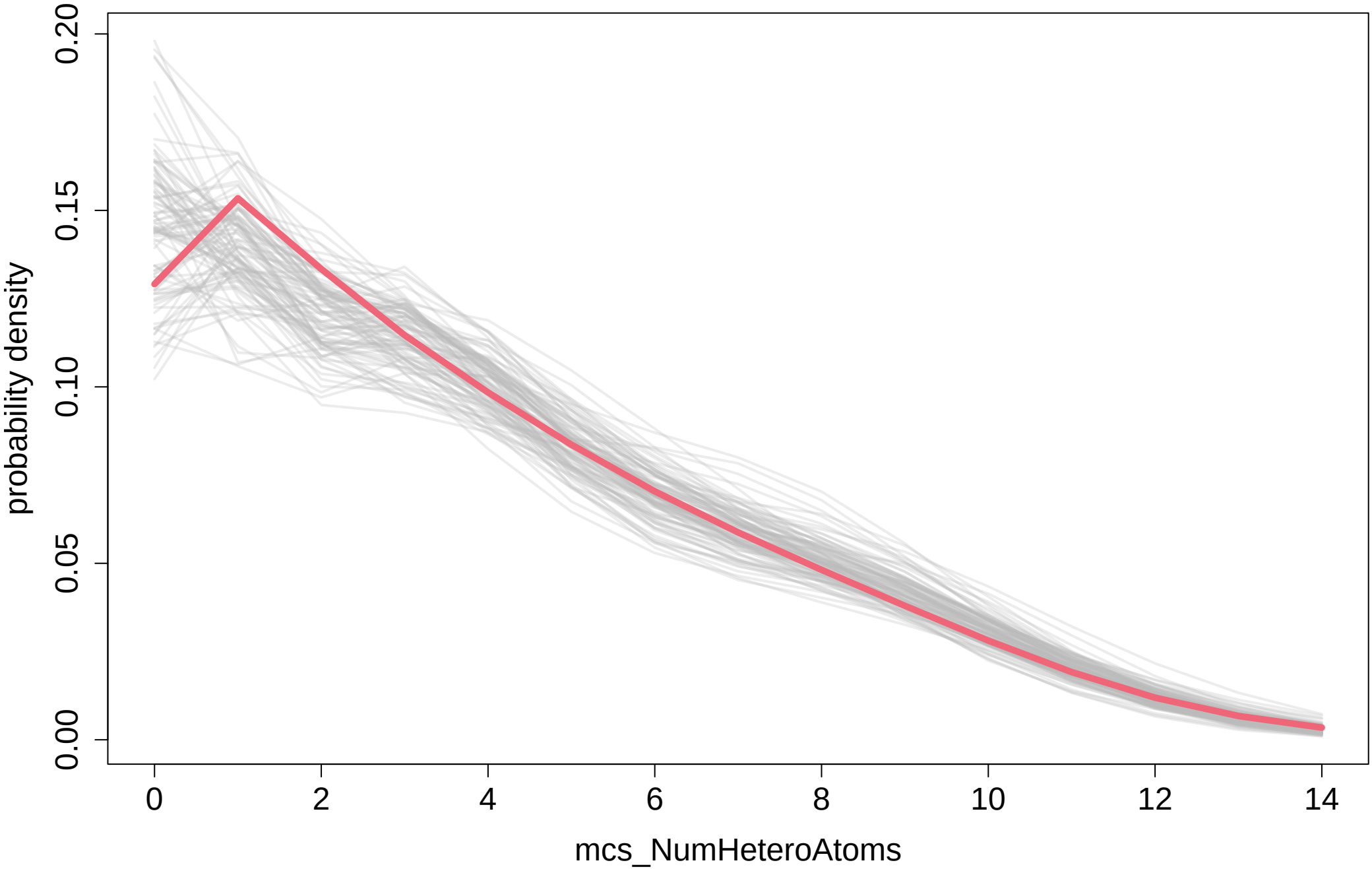
−− STATS 2D −−
min ESS = 2590.38211860916
max BMK = 0.046819258363329 1
max MCSE = 2.04008847144259
all stationary: TRUE
burn: 0
max rel.err.: 1.77680467325578

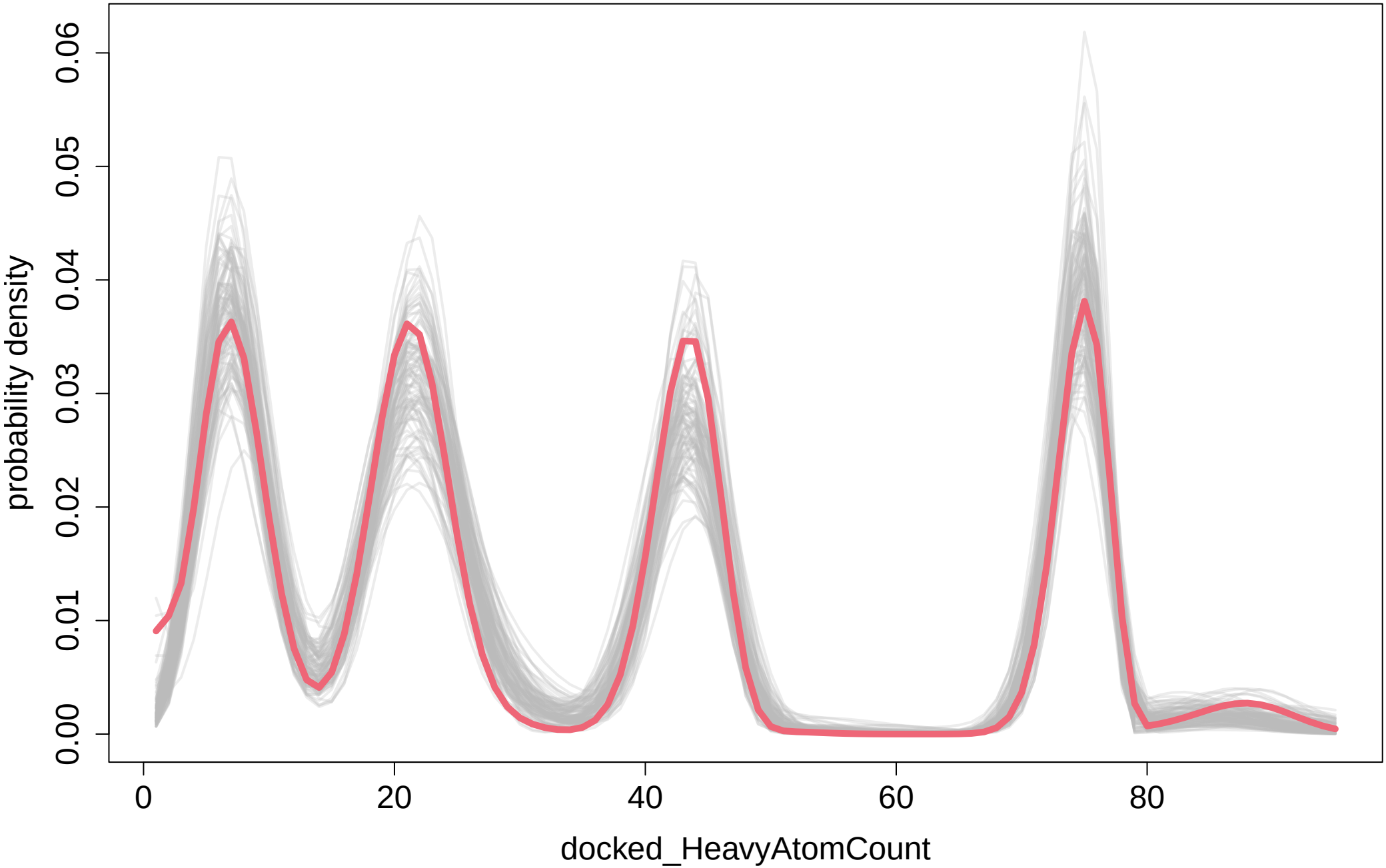
−− STATS 1D −−
min ESS = 2250.38034457948
max BMK = 0.055742392626090 1
max MCSE = 2.19267161244169
all stationary: TRUE
burn: 0
max rel.err.: 2.27982037973484

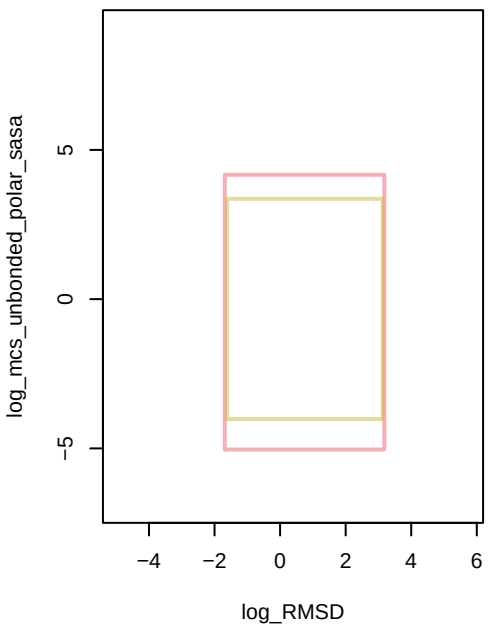
Occupied clusters: 10 of 16
LL: −2160 +− 6.85

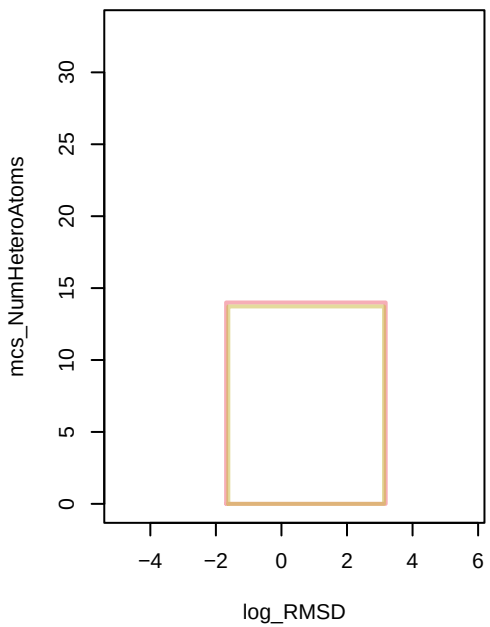

probability density
0.0
0.1
0.2
0.3
0.4
−1
0
1
2
3
log_RMSD

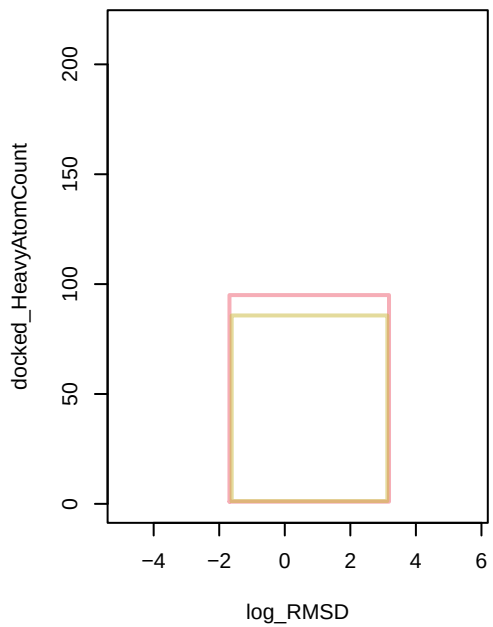

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

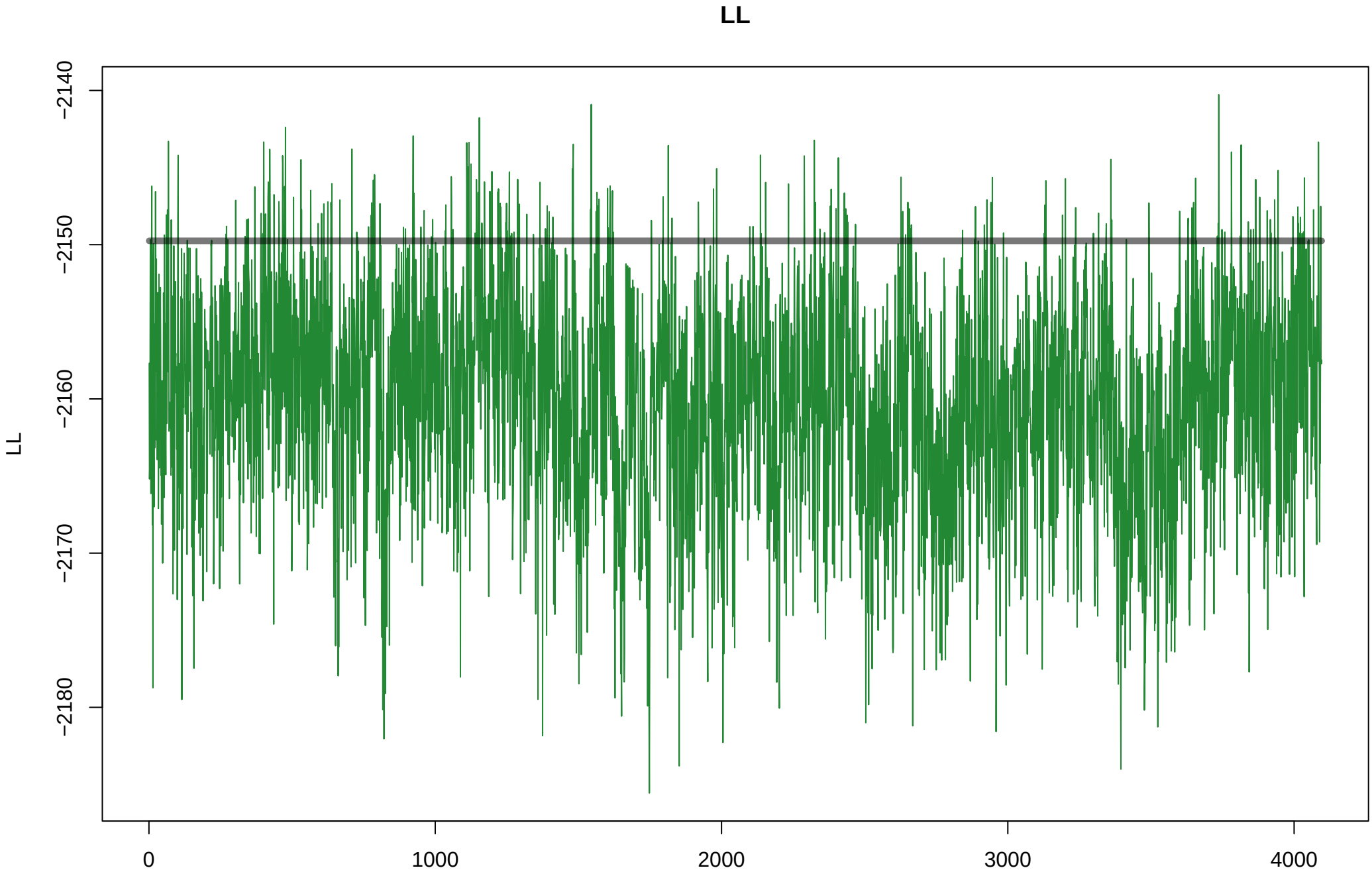

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

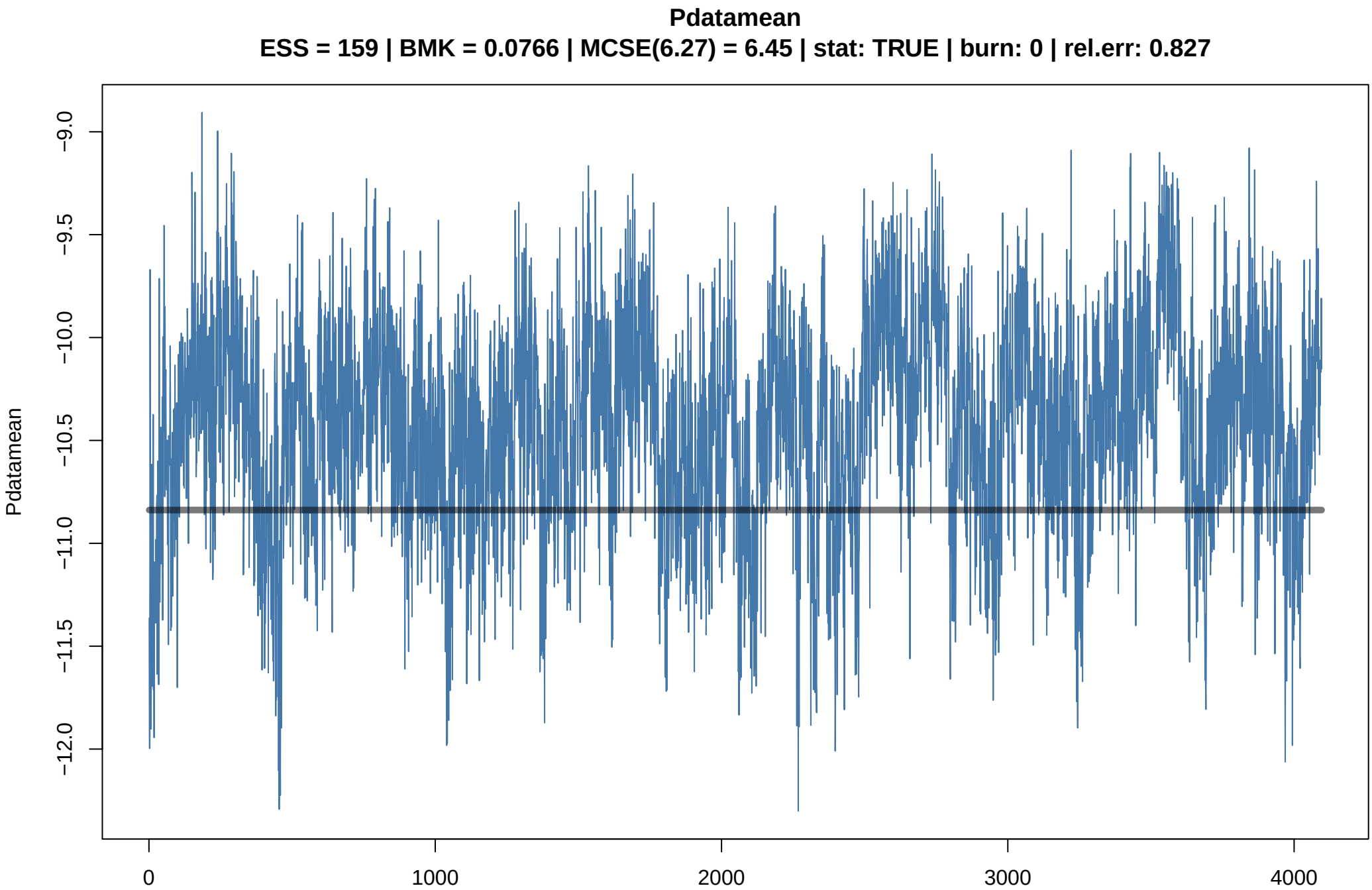

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0
20
40
60
80
docked_HeavyAtomCount

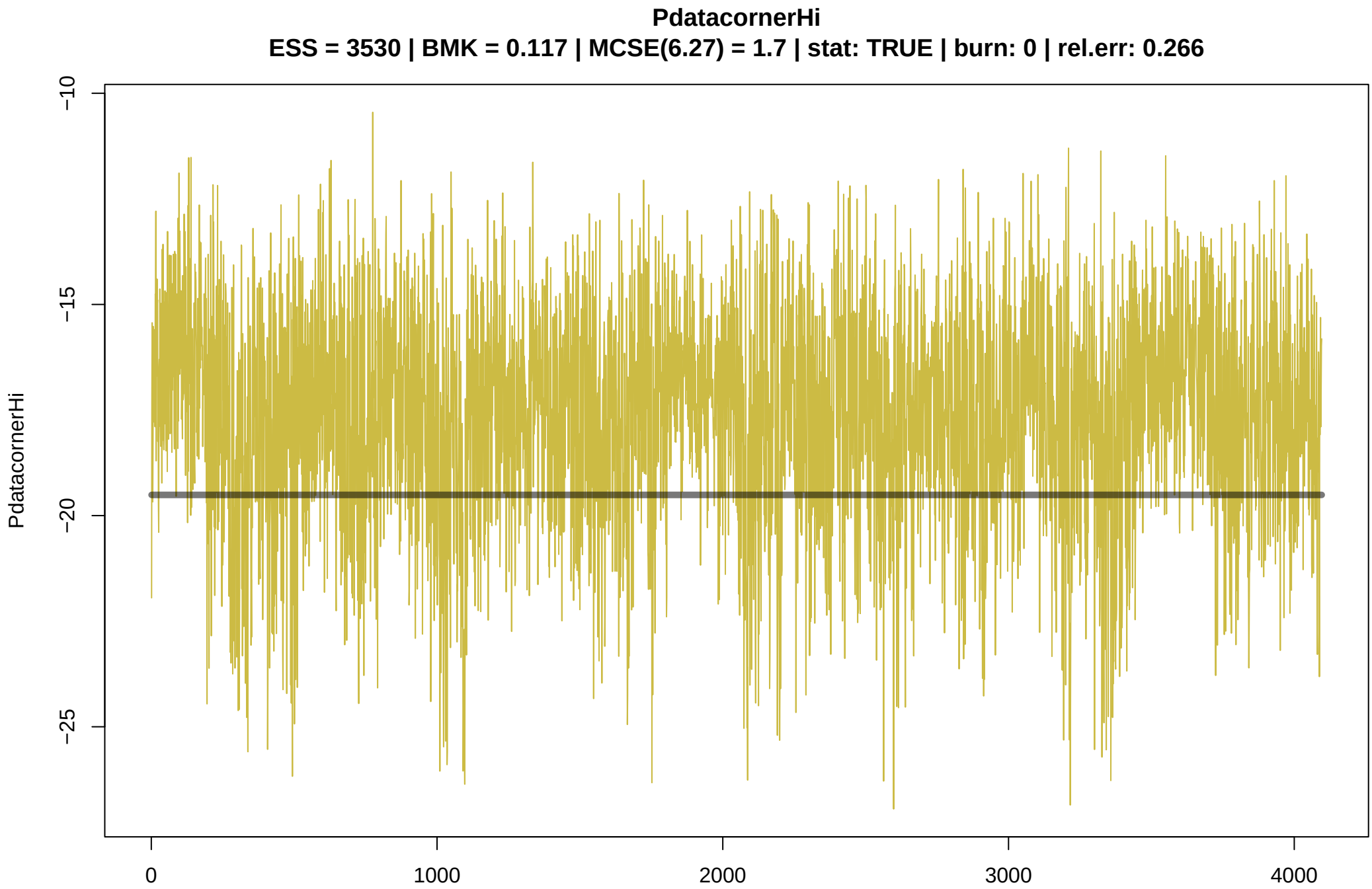

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

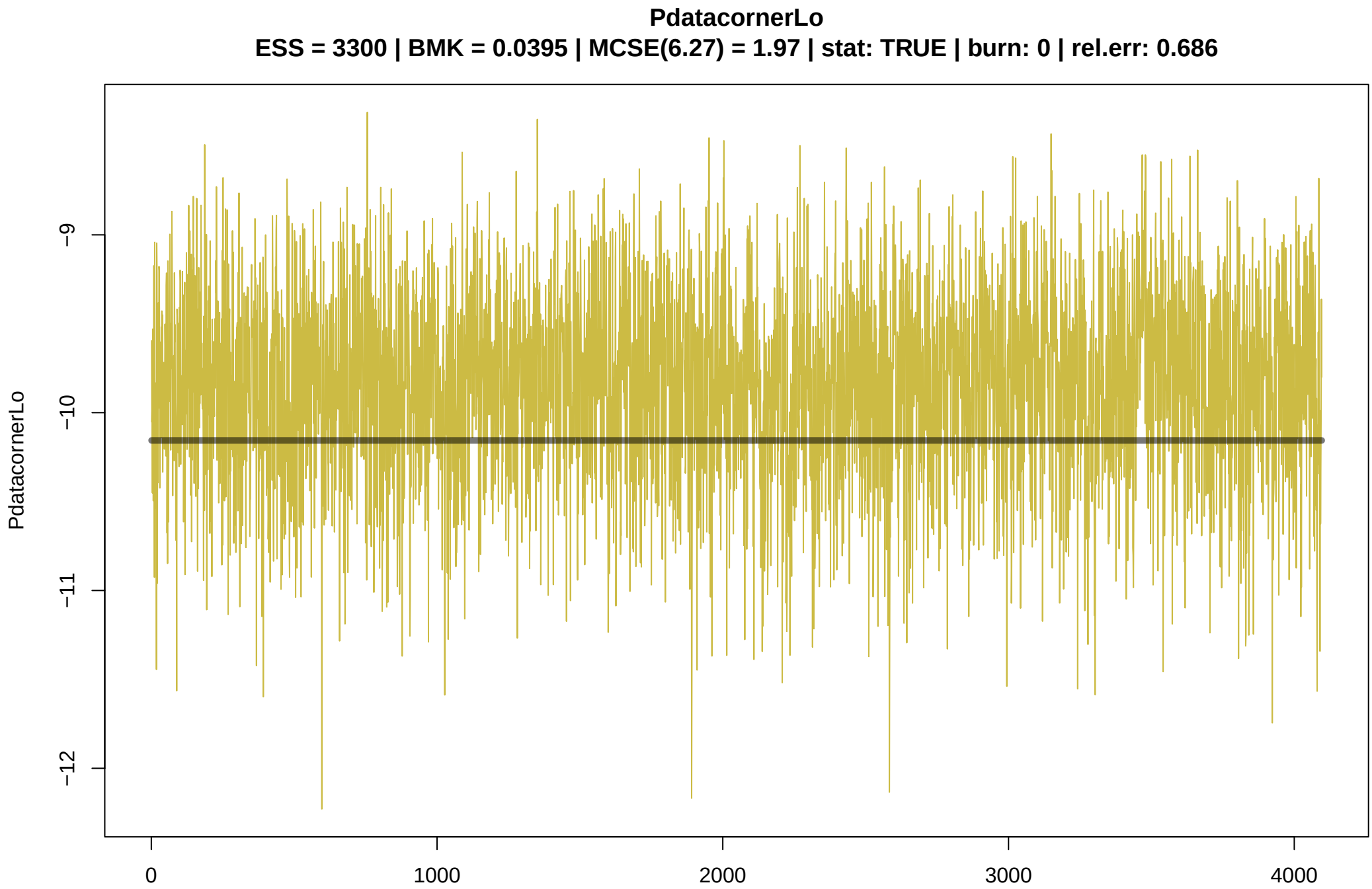

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

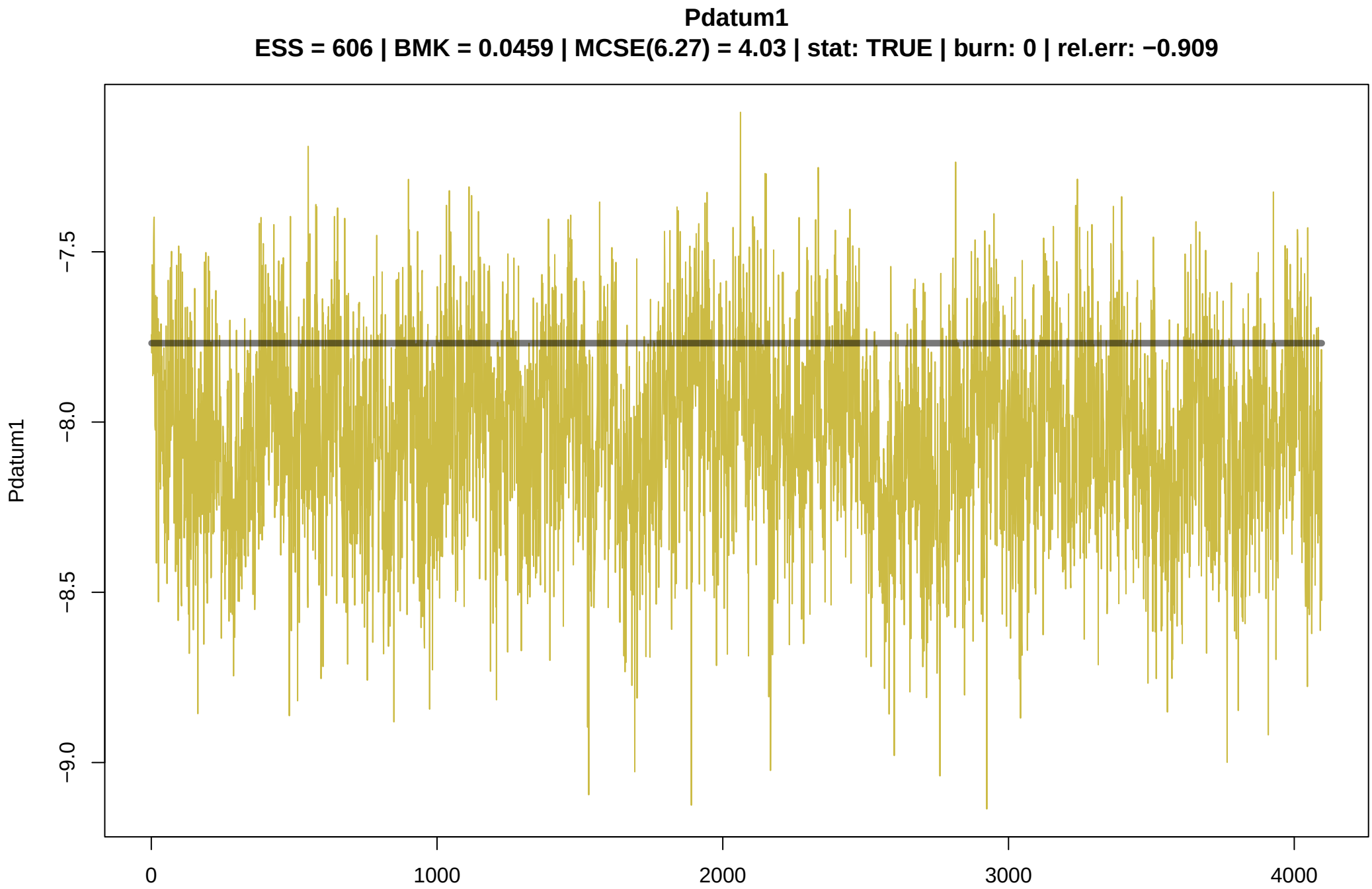

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

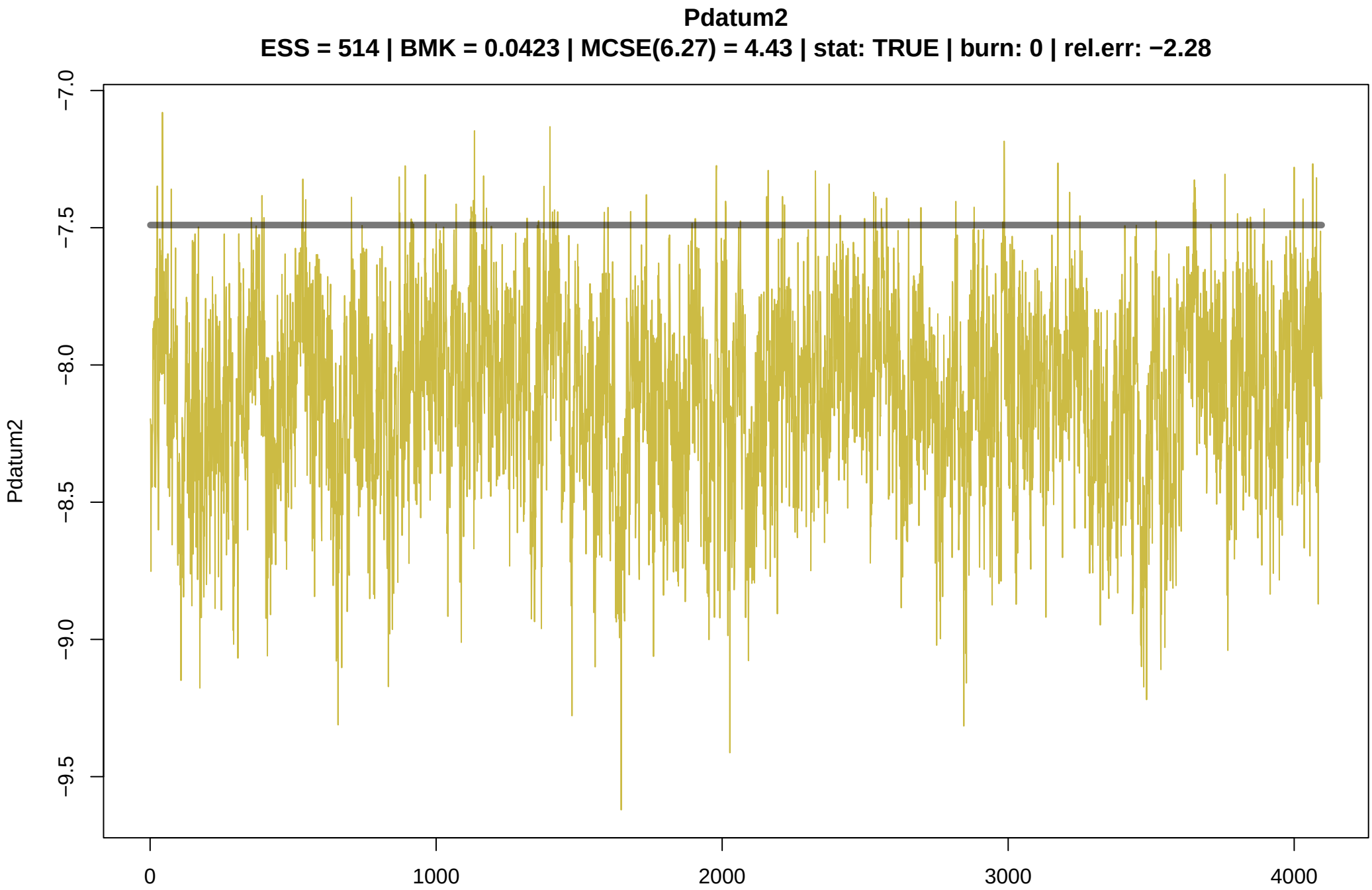

LL
LL
−2140
−2150
−2160
−2170
−2180
0
1000
2000
3000
4000

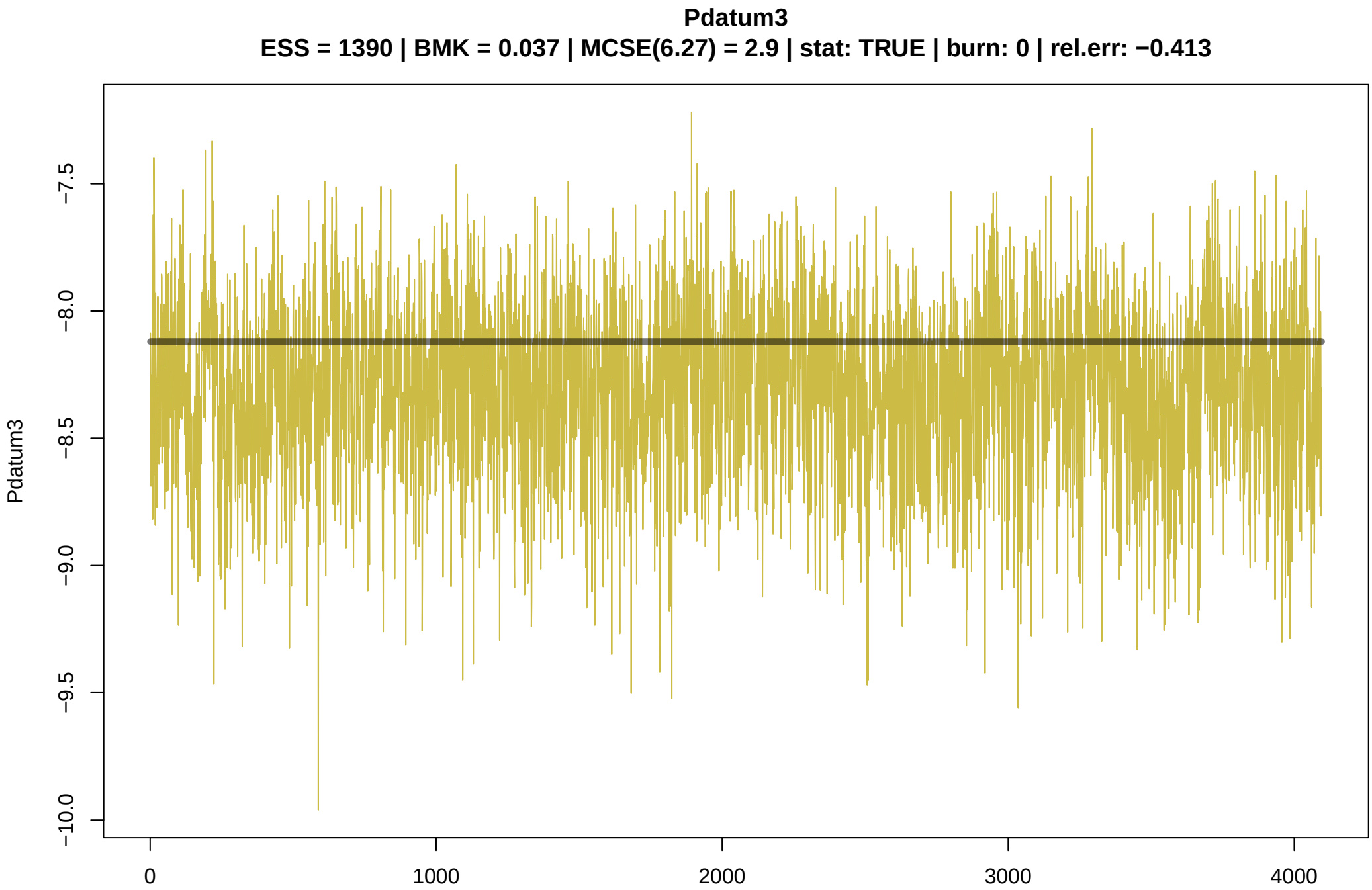

Pdatamean
ESS = 159 | BMK = 0.0766 | MCSE(6.27) = 6.45 | stat: TRUE | burn: 0 | rel.err: 0.827
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
1000
2000
3000
4000

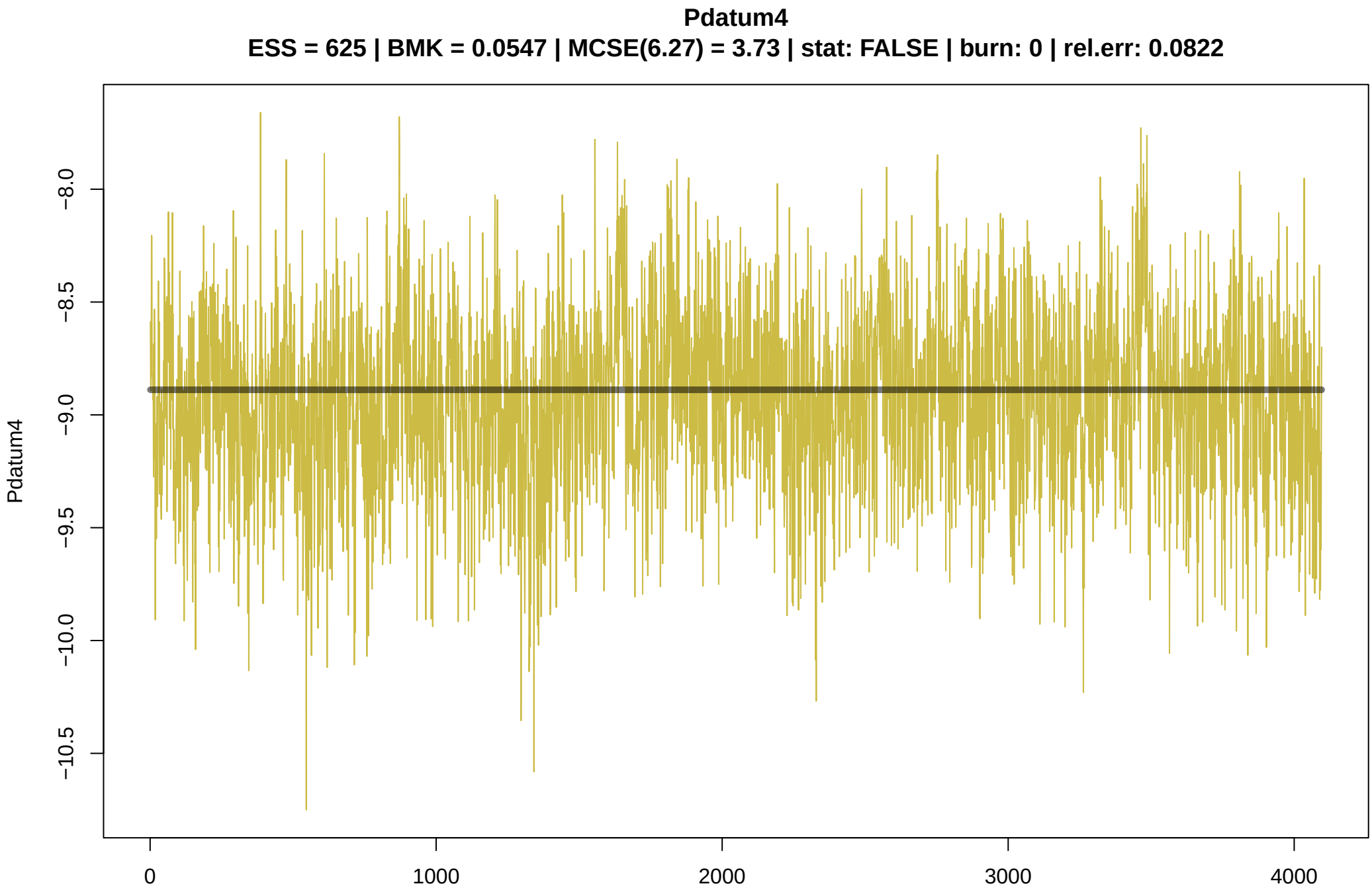

PdatacornerHi
ESS = 3530 | BMK = 0.117 | MCSE(6.27) = 1.7 | stat: TRUE | burn: 0 | rel.err: 0.266
PdatacornerHi
−10
−15
−20
−25
0
1000
2000
3000
4000

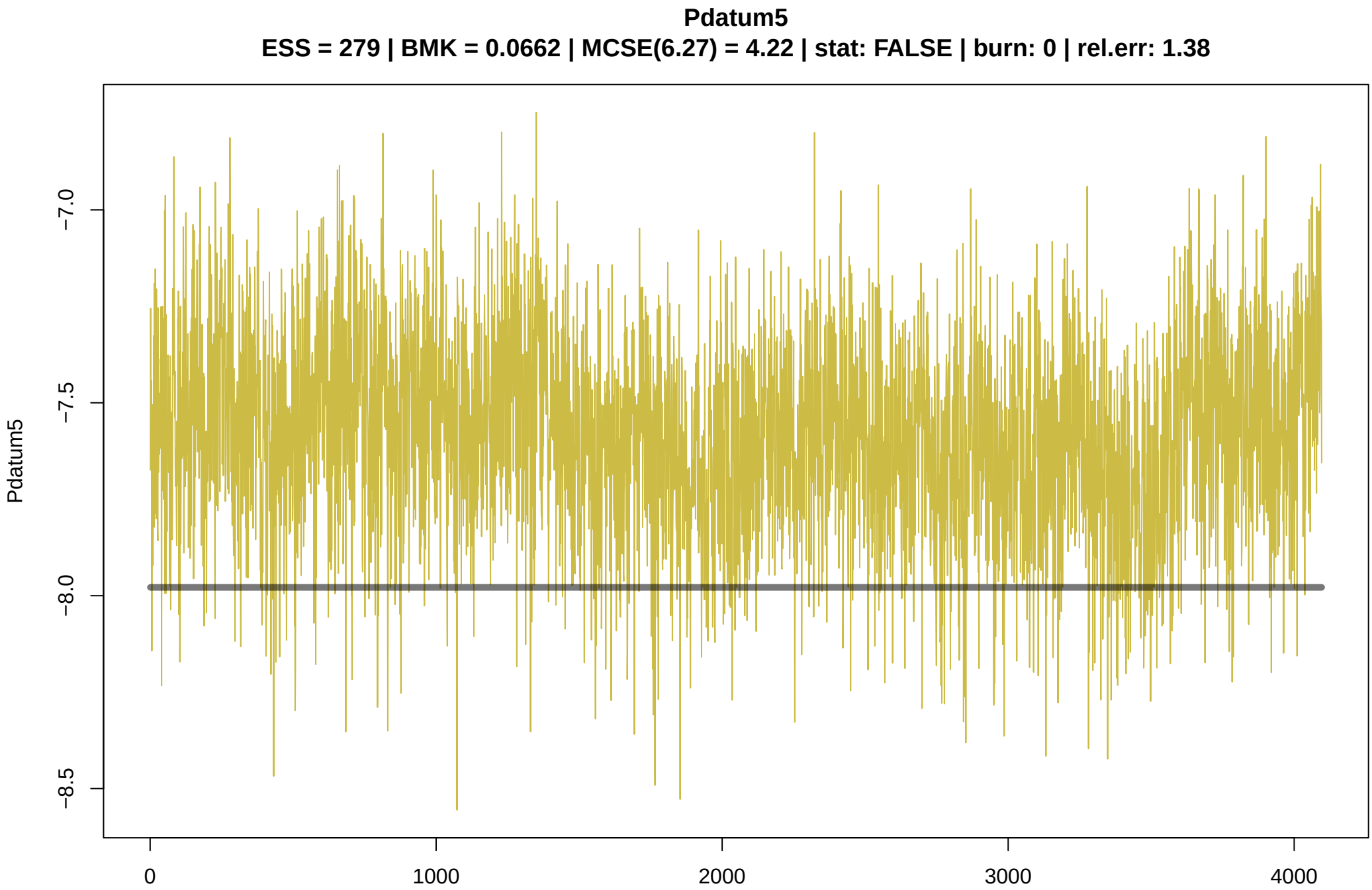

PdatacornerLo
ESS = 3300 | BMK = 0.0395 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0 | rel.err: 0.686
PdatacornerLo
−9
−10
−11
−12
0
1000
2000
3000
4000

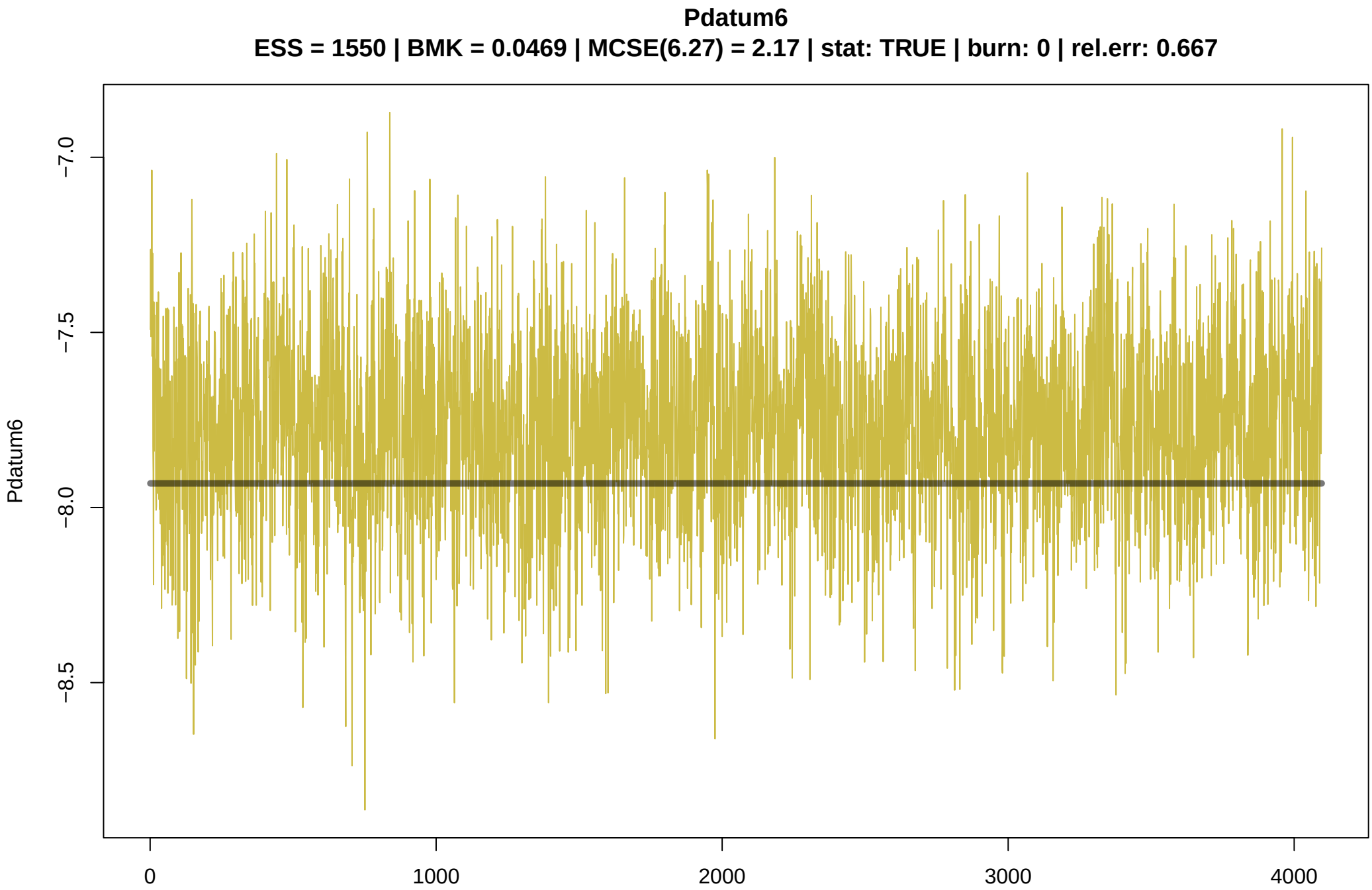

Pdatum1
ESS = 606 | BMK = 0.0459 | MCSE(6.27) = 4.03 | stat: TRUE | burn: 0 | rel.err: −0.909
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

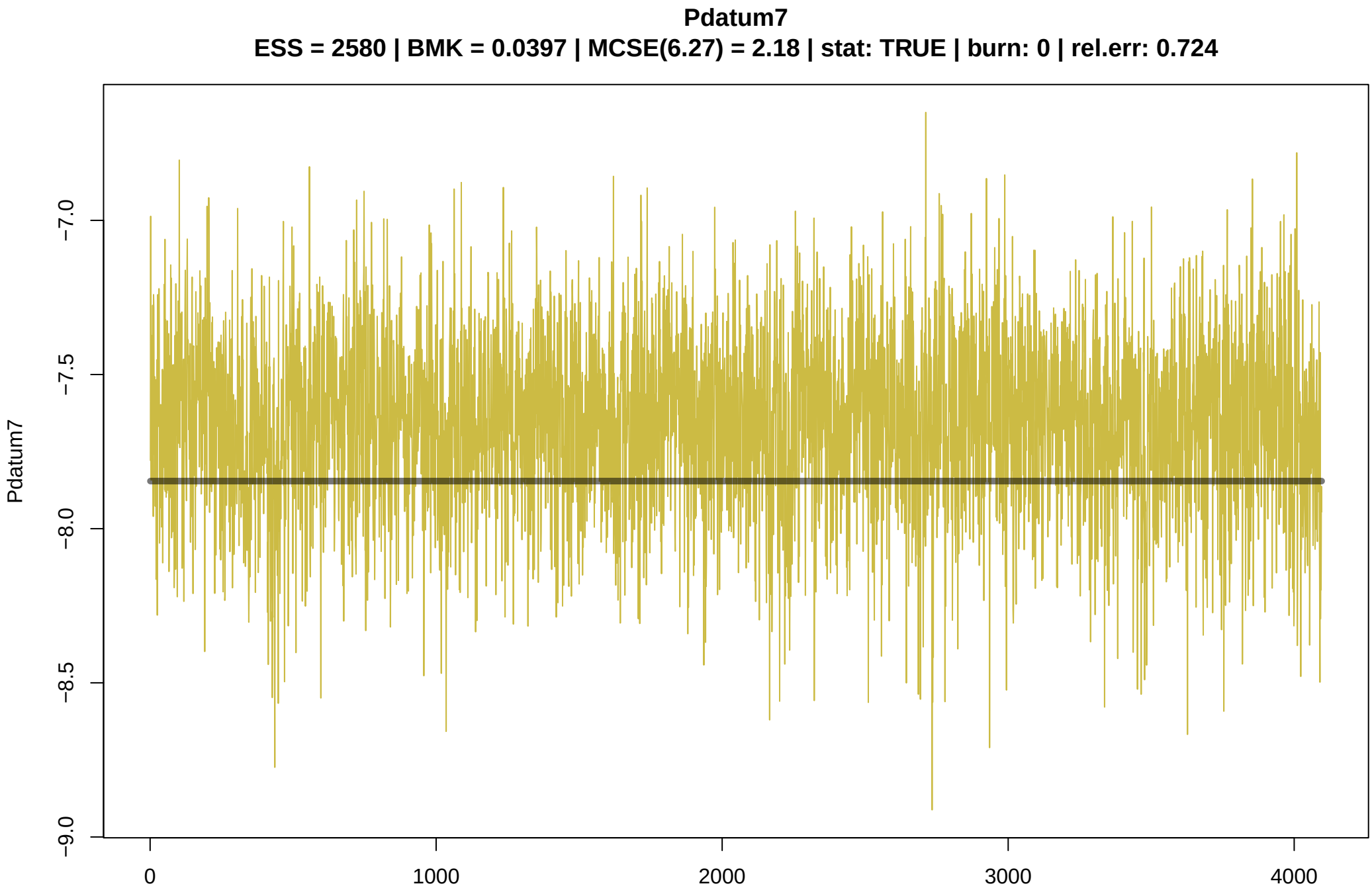

Pdatum2
ESS = 514 | BMK = 0.0423 | MCSE(6.27) = 4.43 | stat: TRUE | burn: 0 | rel.err: −2.28
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
1000
2000
3000
4000

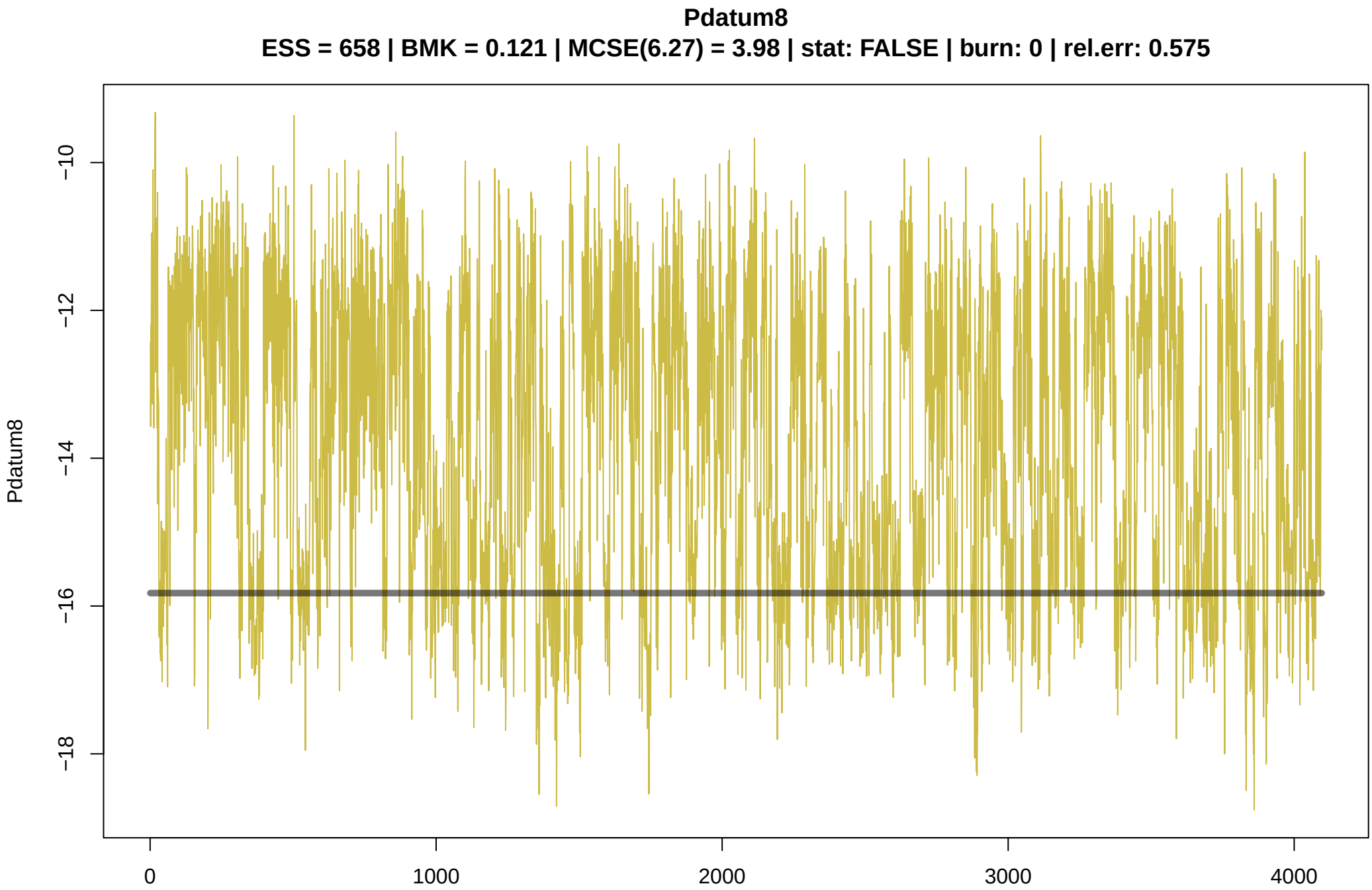

Pdatum3
ESS = 1390 | BMK = 0.037 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | rel.err: −0.413
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
1000
2000
3000
4000

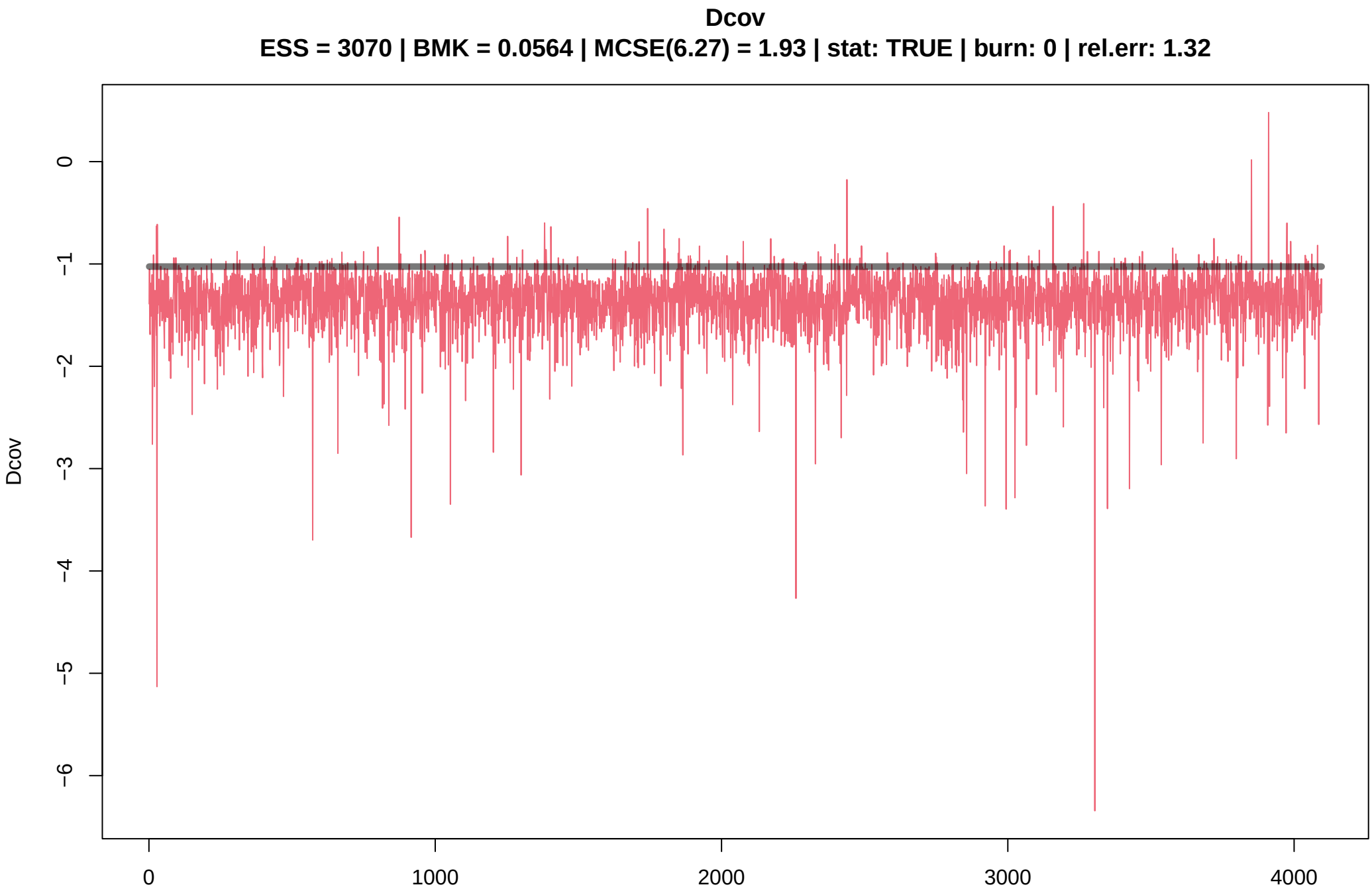

Pdatum4
ESS = 625 | BMK = 0.0547 | MCSE(6.27) = 3.73 | stat: FALSE | burn: 0 | rel.err: 0.0822
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
1000
2000
3000
4000

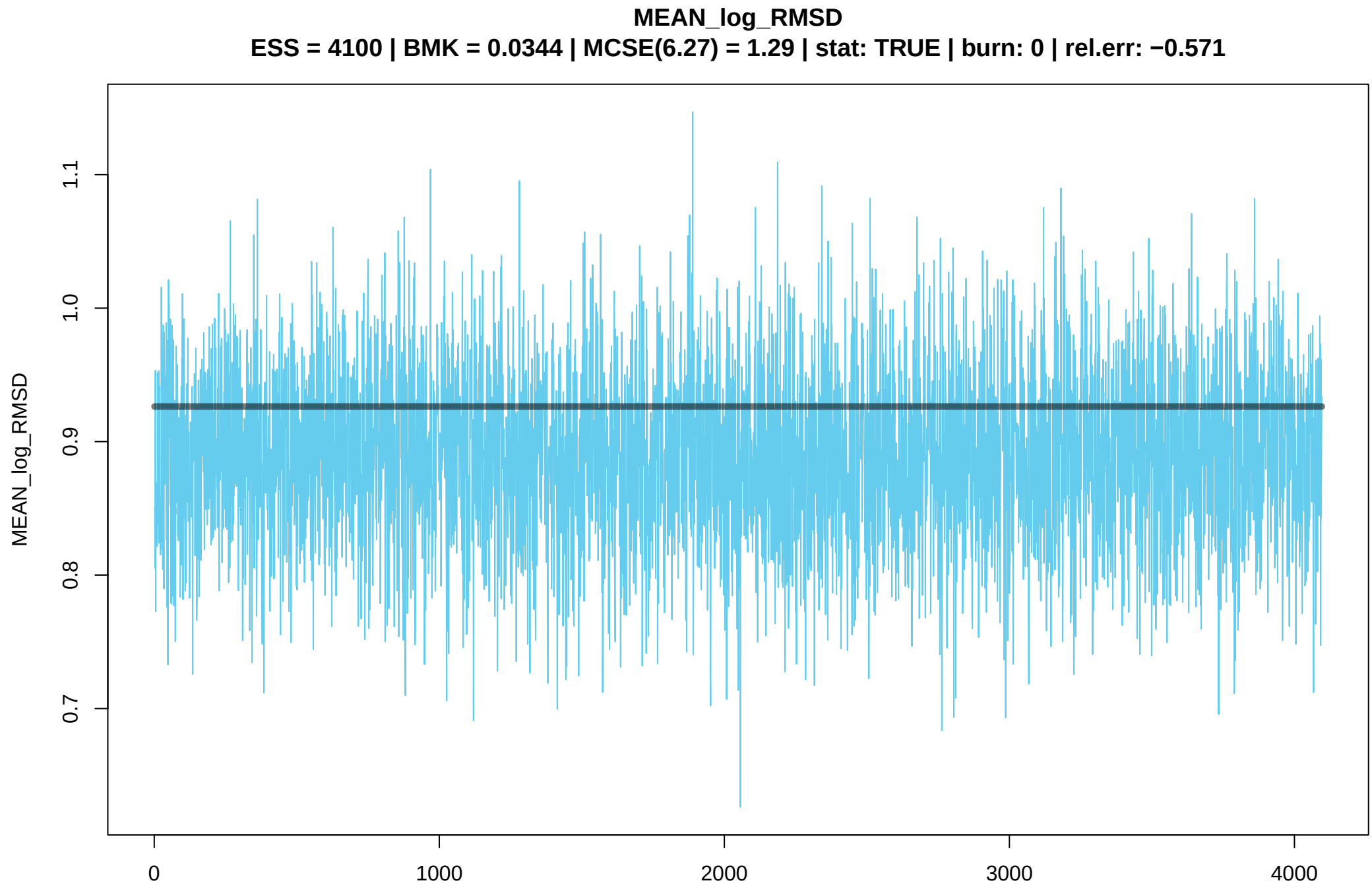

Pdatum5
ESS = 279 | BMK = 0.0662 | MCSE(6.27) = 4.22 | stat: FALSE | burn: 0 | rel.err: 1.38
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

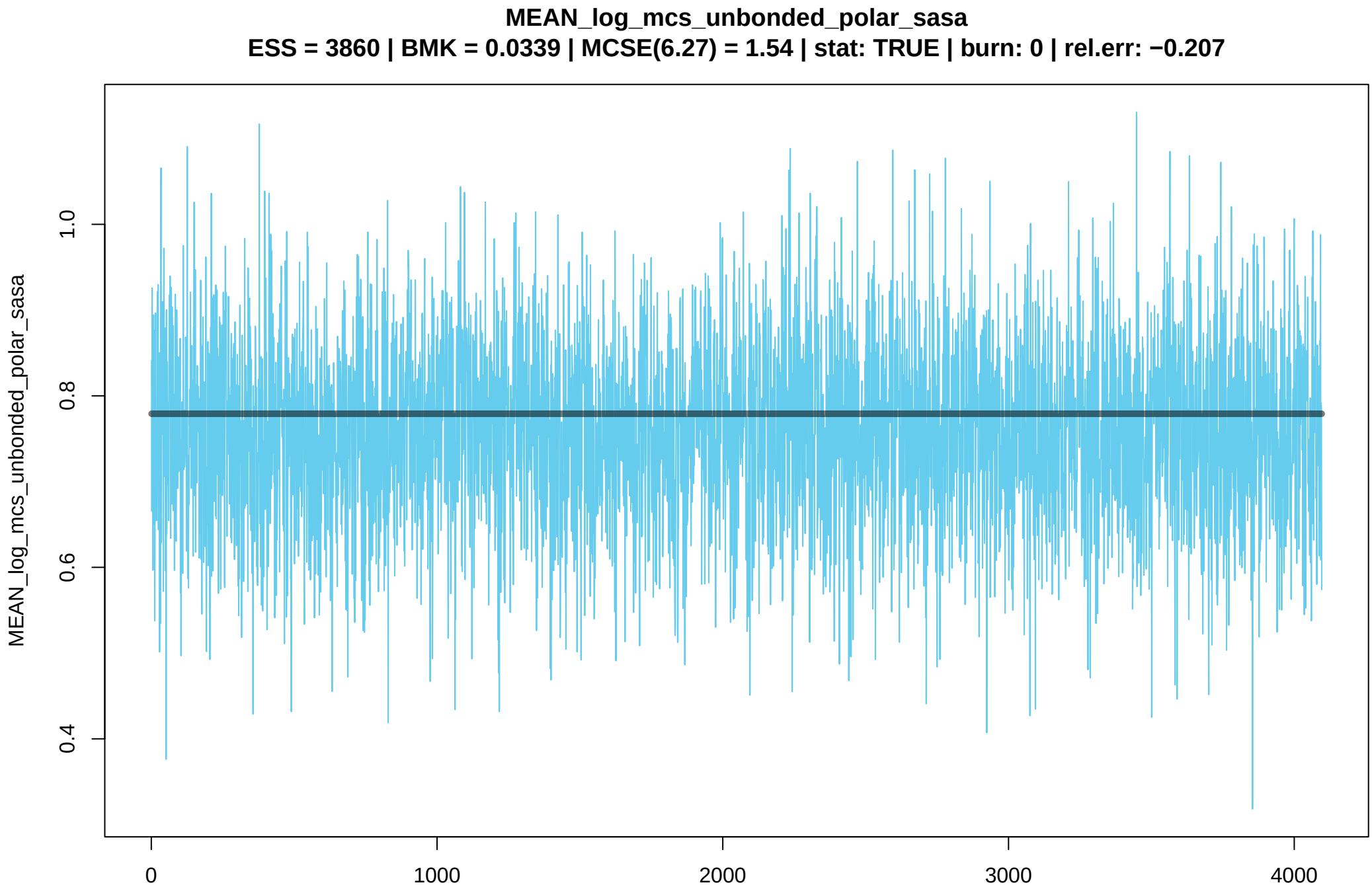

Pdatum6
ESS = 1550 | BMK = 0.0469 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.667
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

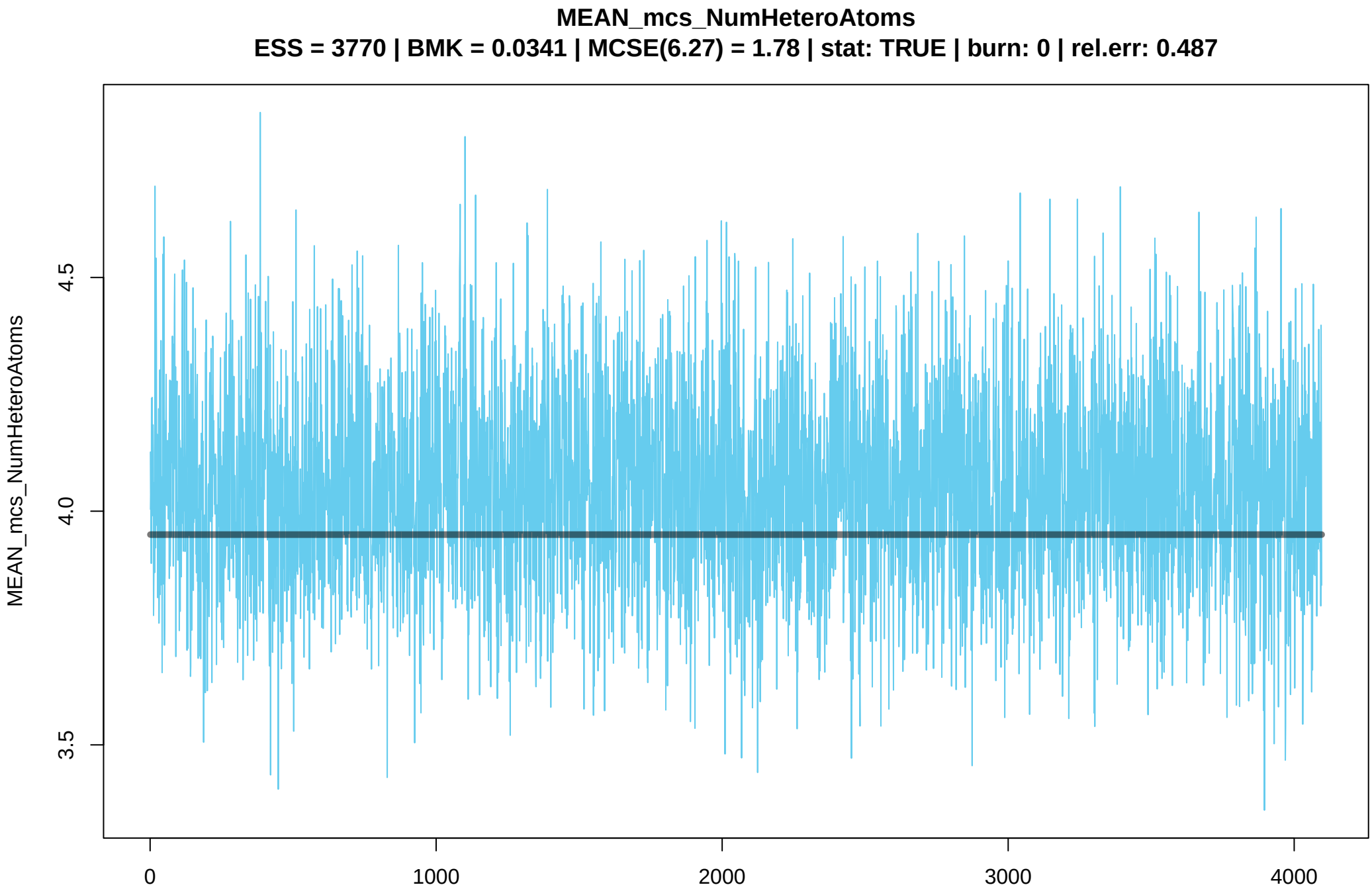

Pdatum7
ESS = 2580 | BMK = 0.0397 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0 | rel.err: 0.724
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

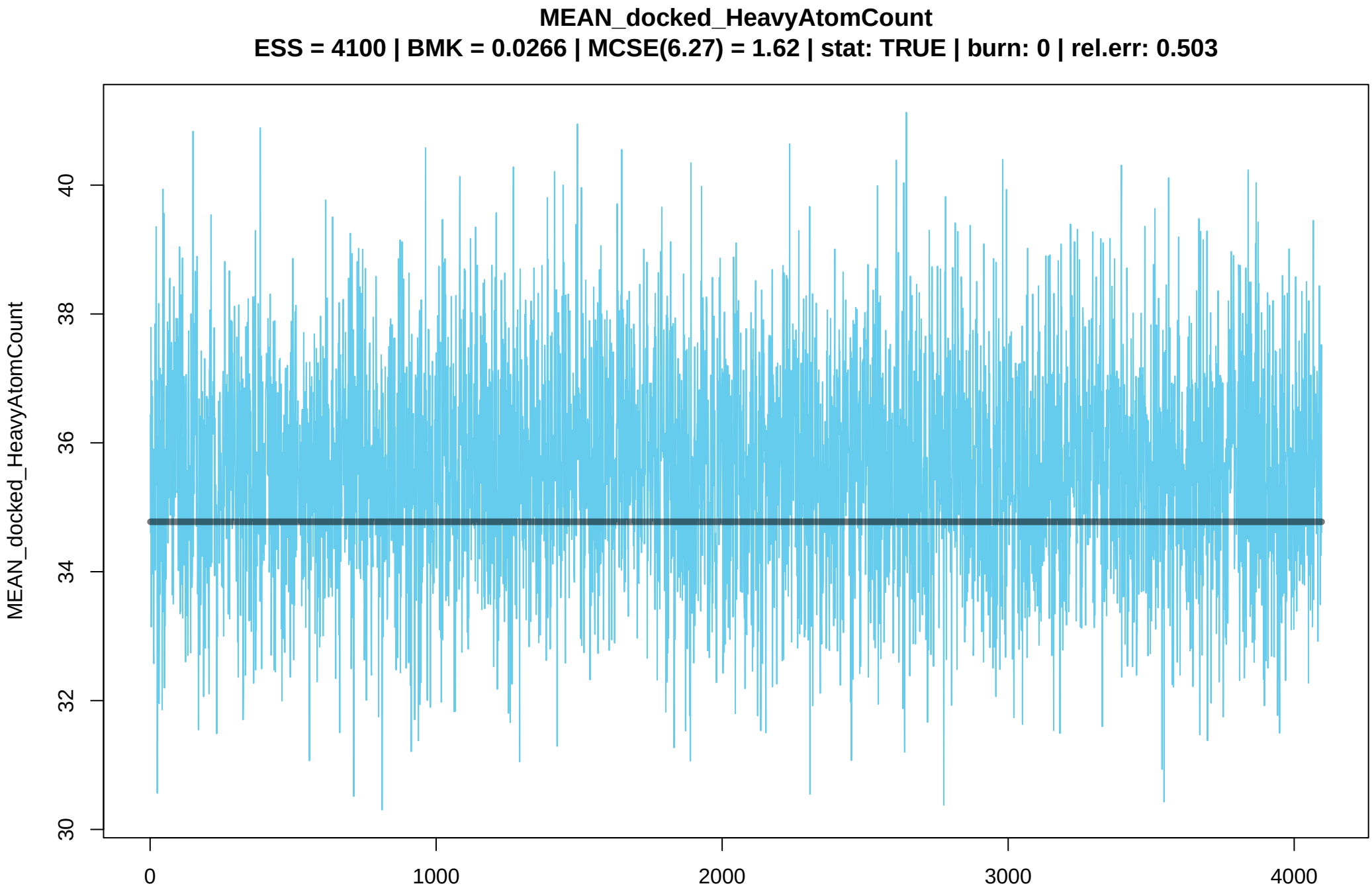

Pdatum8
ESS = 658 | BMK = 0.121 | MCSE(6.27) = 3.98 | stat: FALSE | burn: 0 | rel.err: 0.575
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

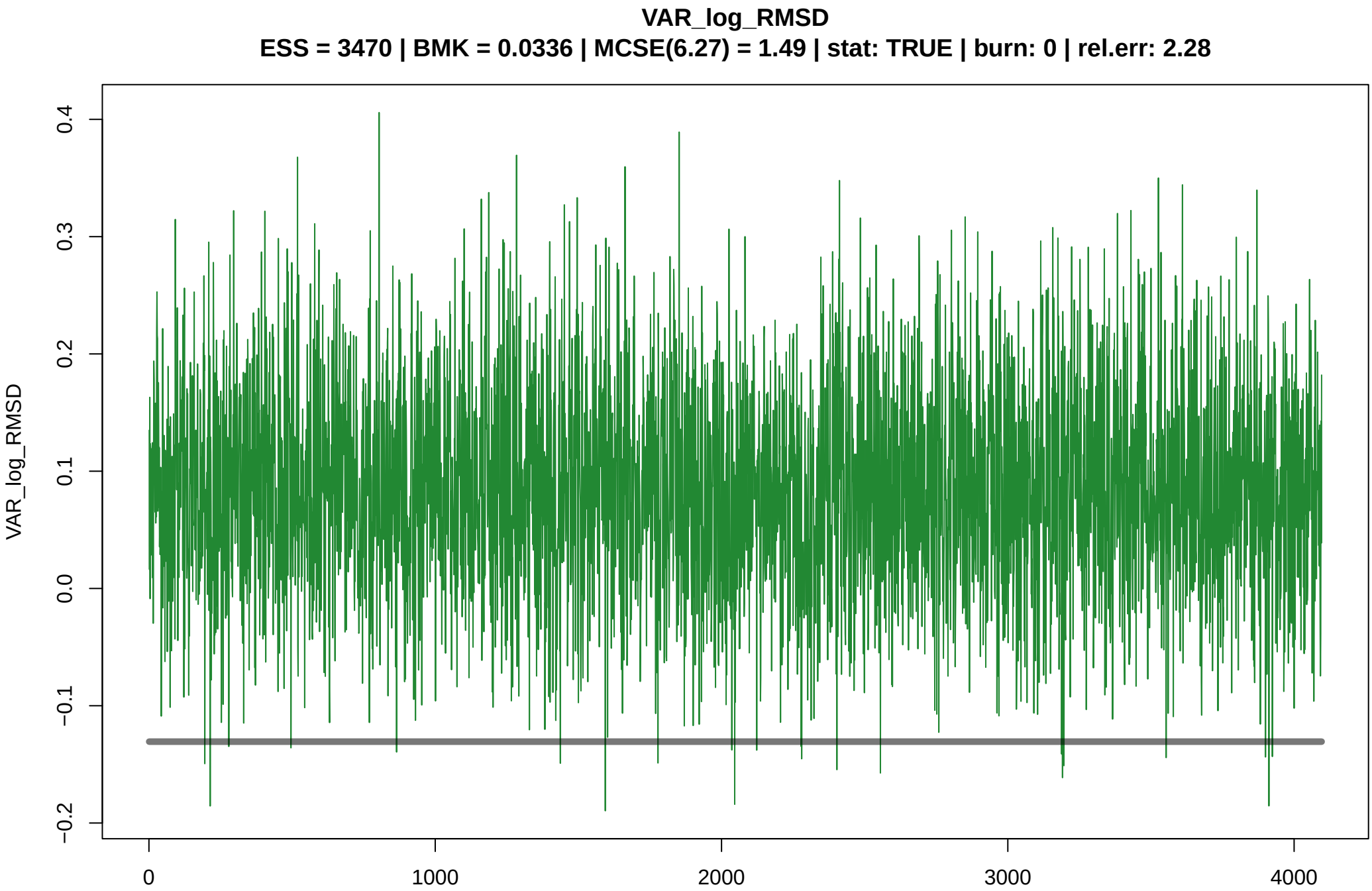

Dcov
ESS = 3070 | BMK = 0.0564 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: 1.32
Dcov
0
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

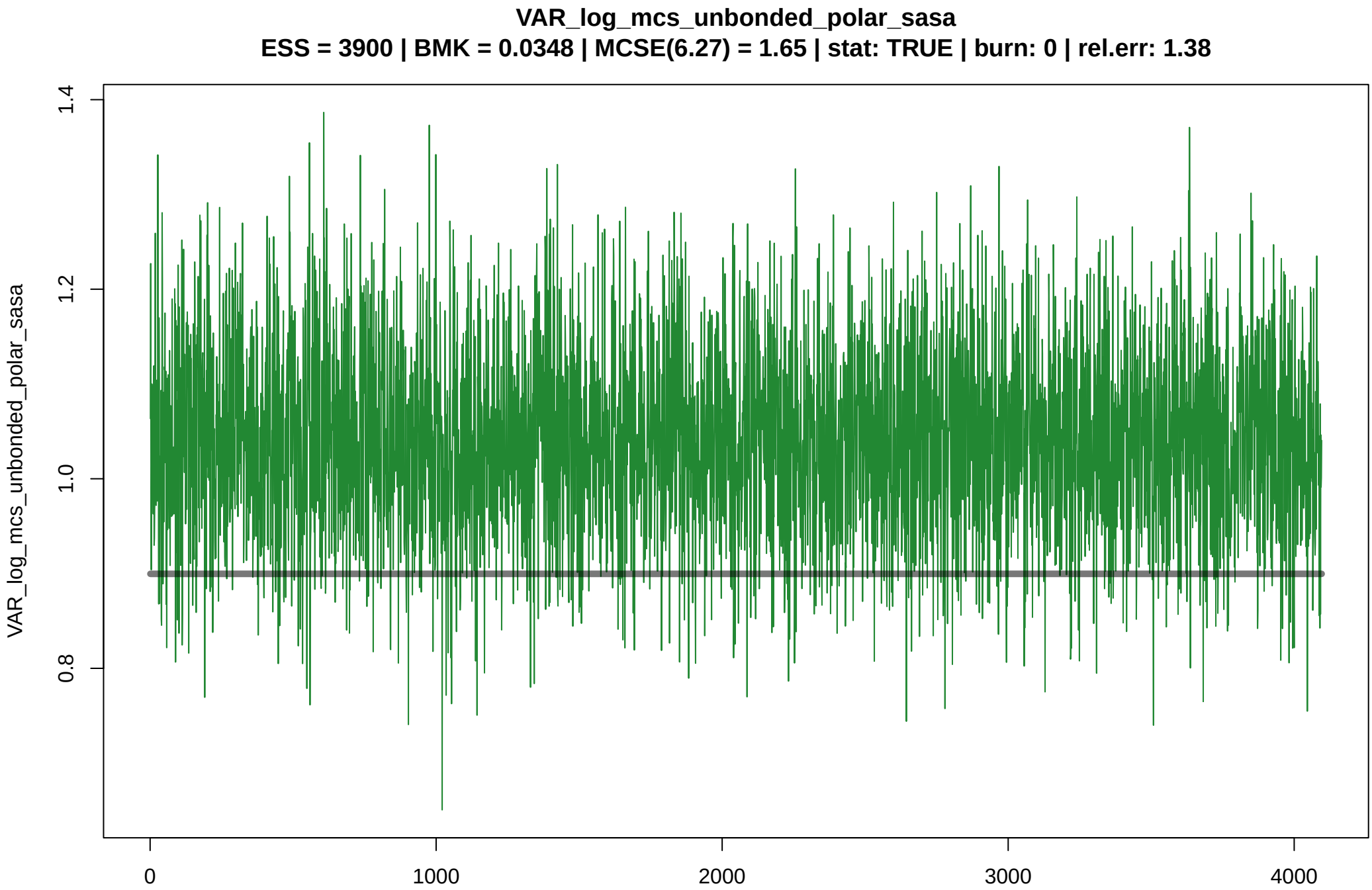

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0344 | MCSE(6.27) = 1.29 | stat: TRUE | burn: 0 | rel.err: −0.571
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

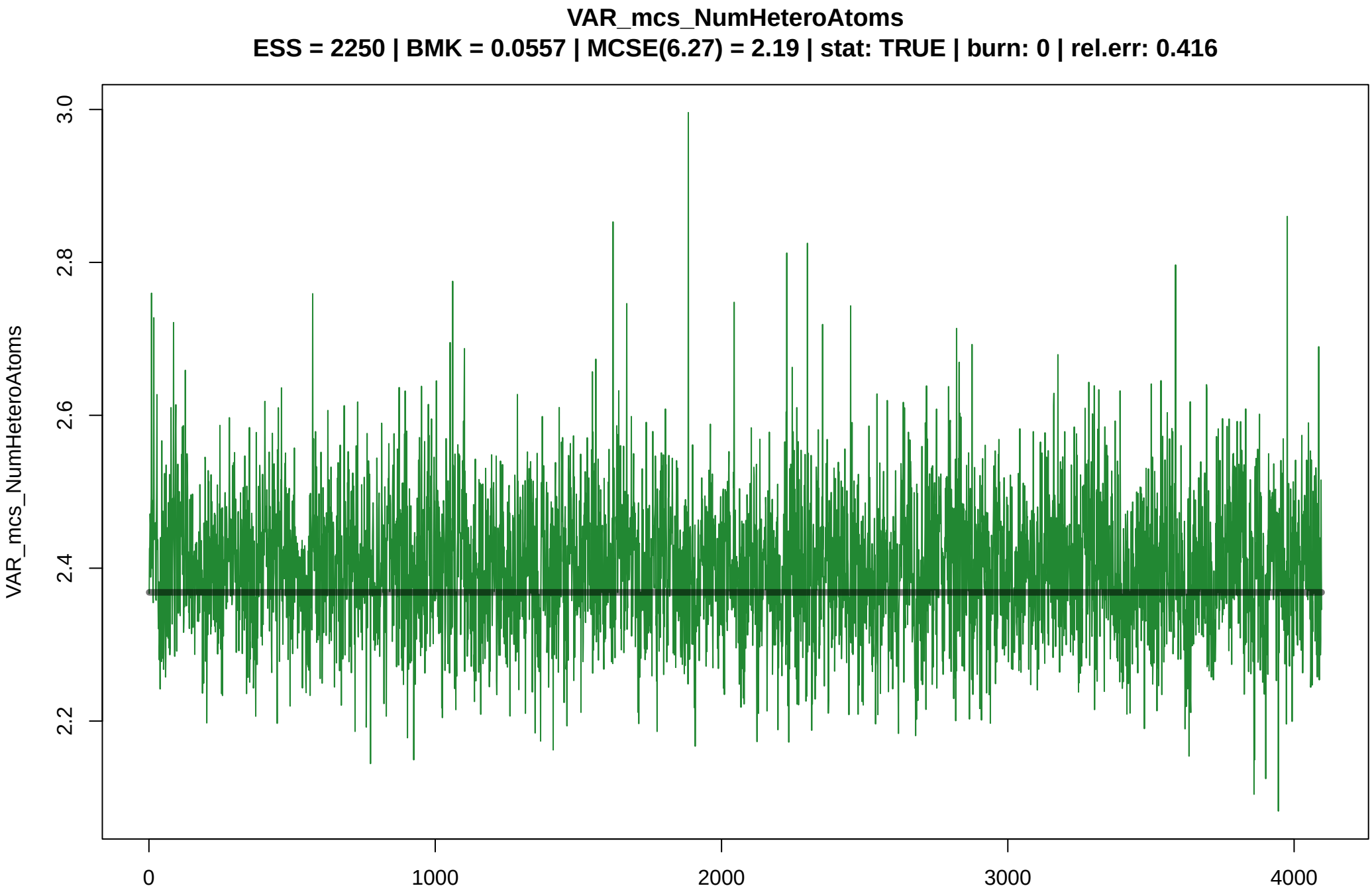

MEAN_log_mcs_unbonded_polar_sasa
ESS = 3860 | BMK = 0.0339 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0 | rel.err: −0.207
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

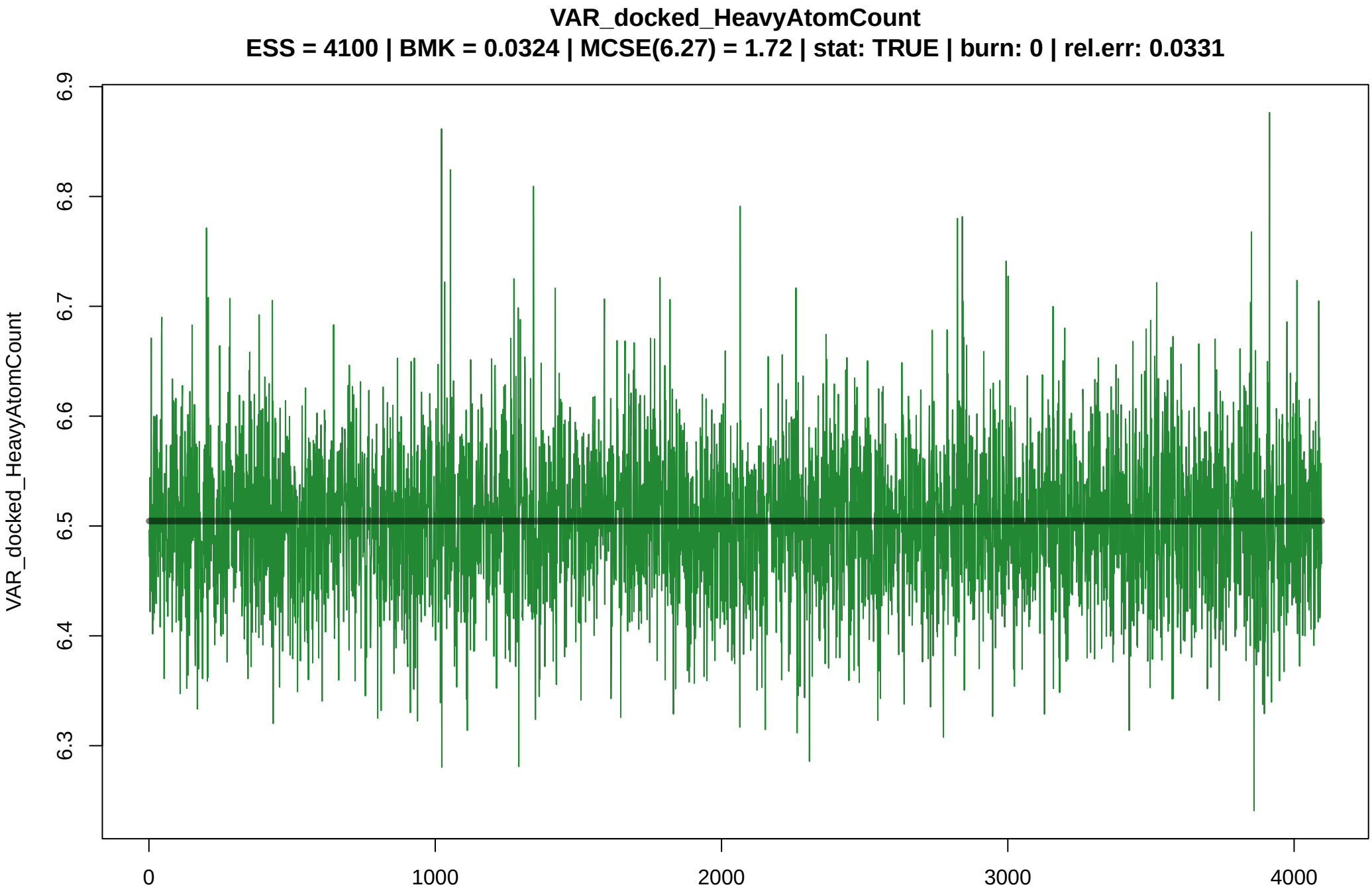

MEAN_mcs_NumHeteroAtoms
ESS = 3770 | BMK = 0.0341 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0 | rel.err: 0.487
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

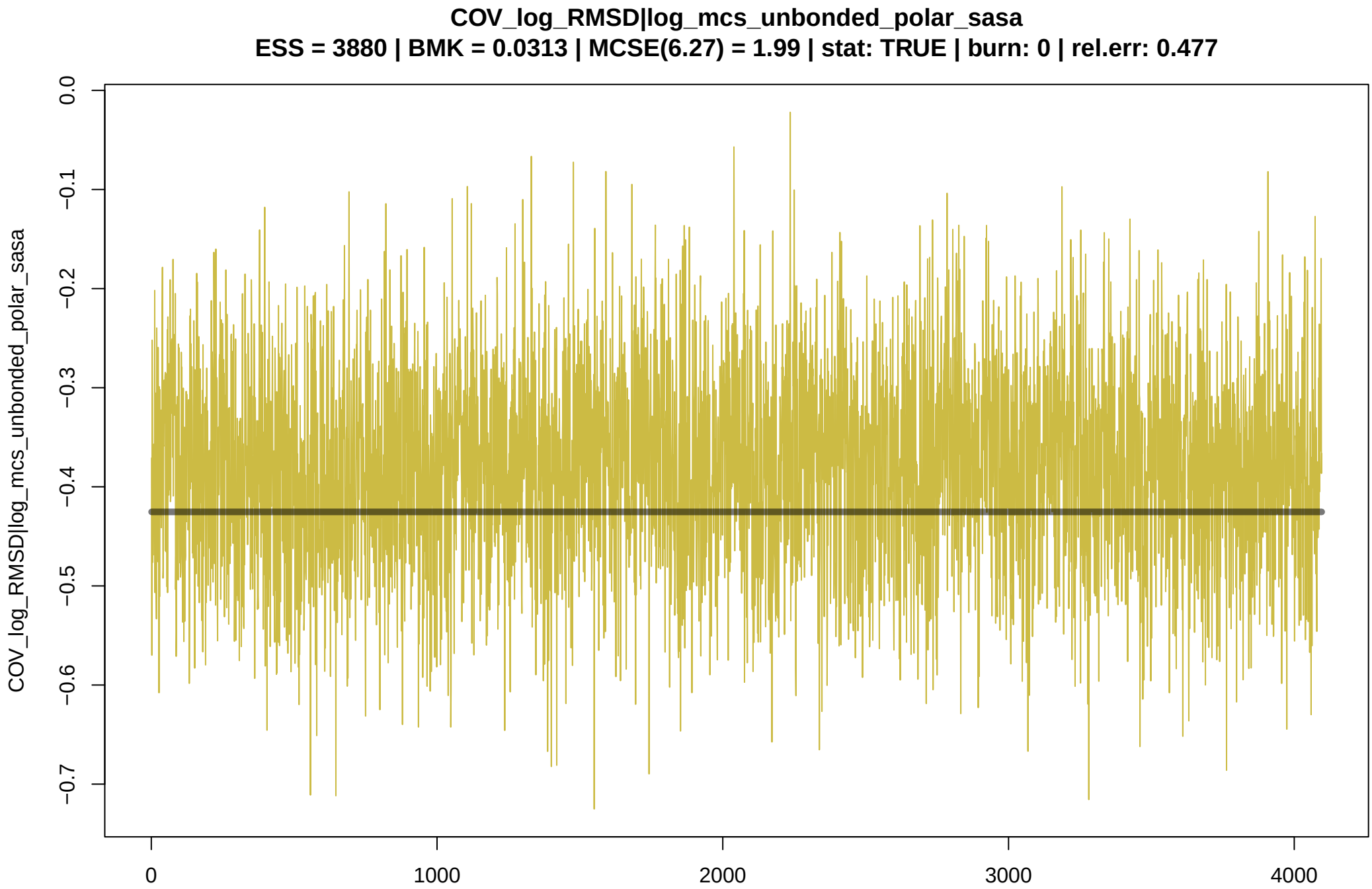

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0266 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: 0.503
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
1000
2000
3000
4000

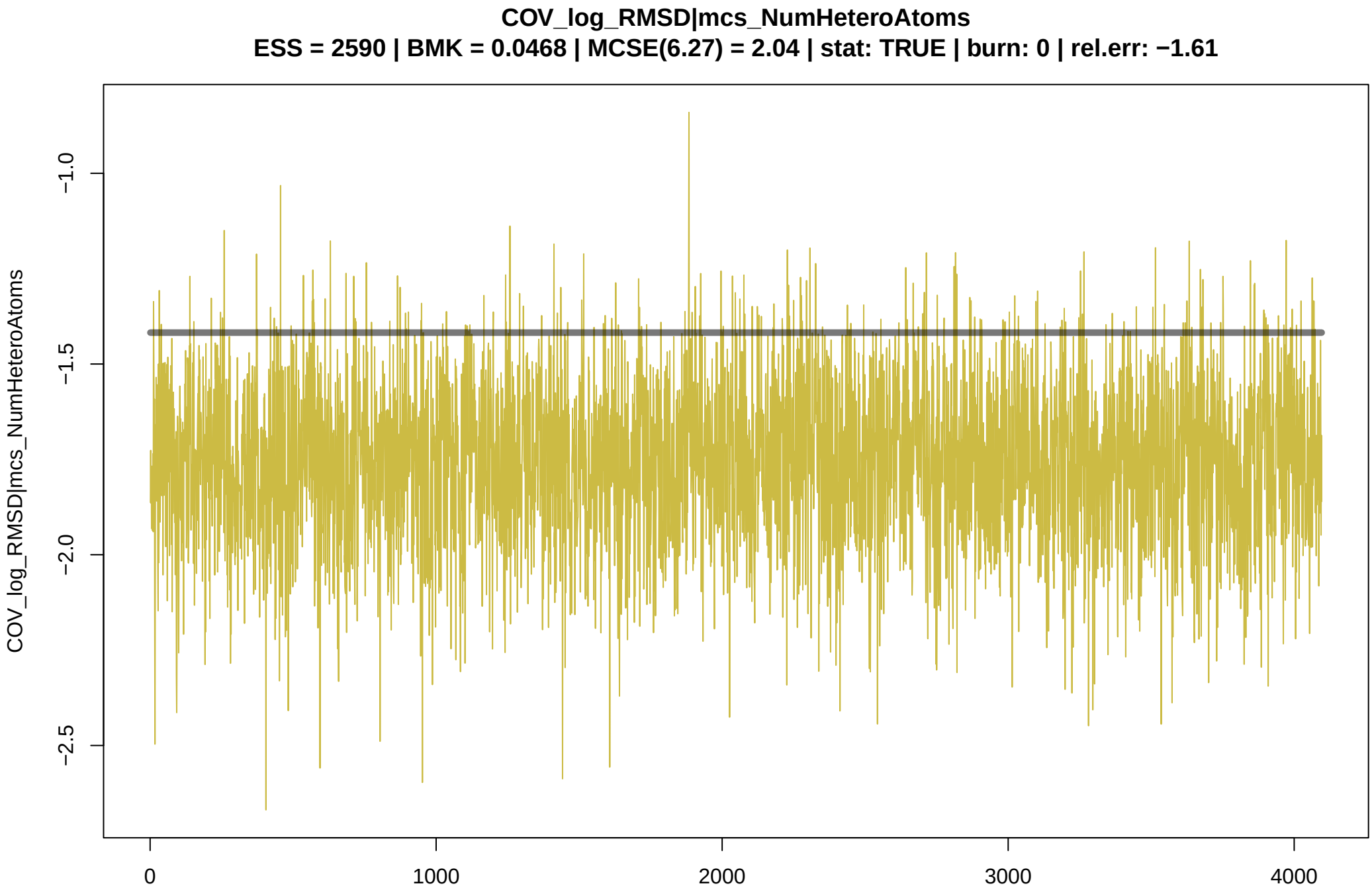

VAR_log_RMSD
ESS = 3470 | BMK = 0.0336 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0 | rel.err: 2.28
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
1000
2000
3000
4000

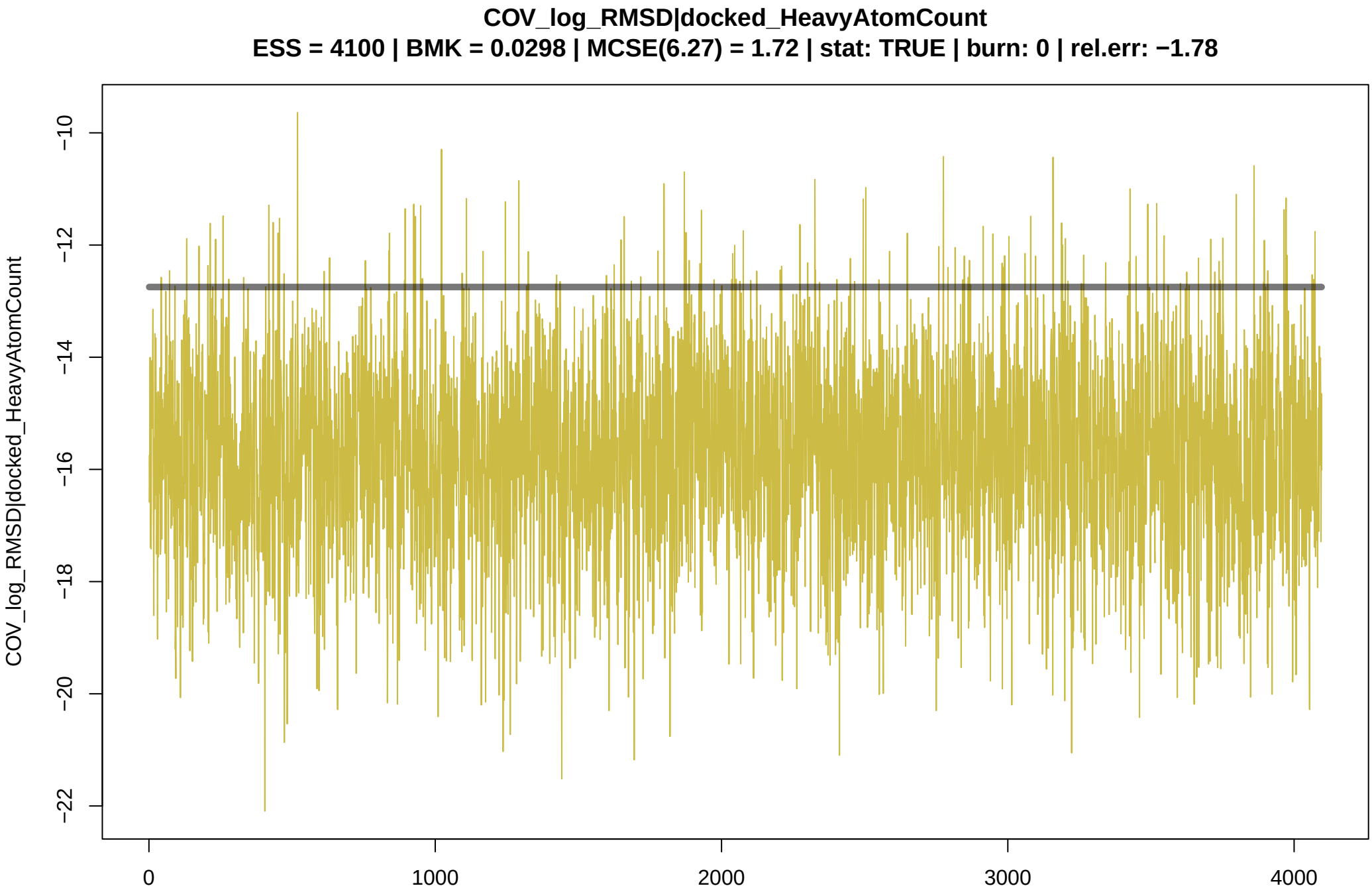

VAR_log_mcs_unbonded_polar_sasa
ESS = 3900 | BMK = 0.0348 | MCSE(6.27) = 1.65 | stat: TRUE | burn: 0 | rel.err: 1.38
VAR_log_mcs_unbonded_polar_sasa
1.4
1.2
1.0
0.8
0
1000
2000
3000
4000

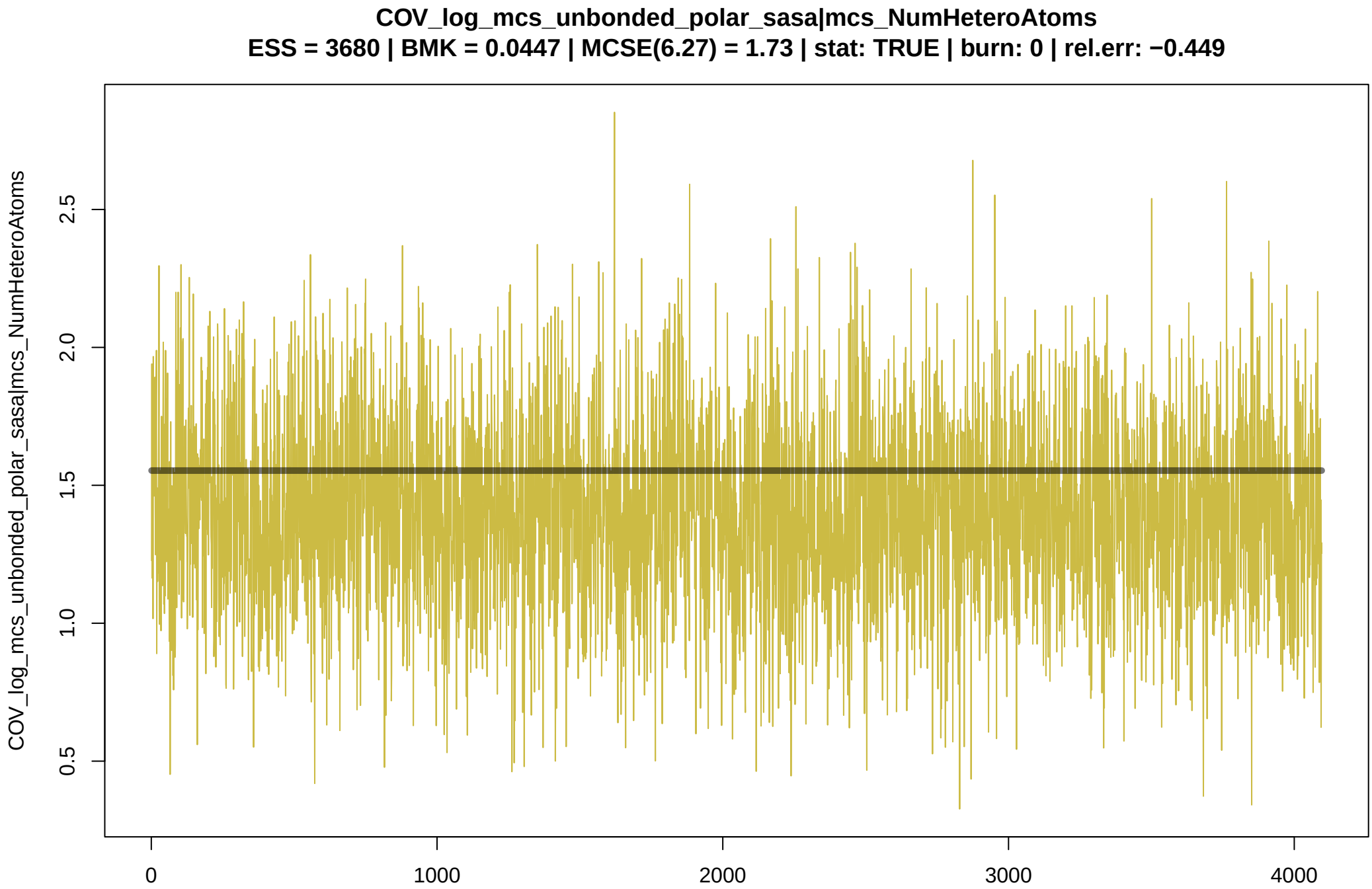

VAR_mcs_NumHeteroAtoms
ESS = 2250 | BMK = 0.0557 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: 0.416
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
0
1000
2000
3000
4000

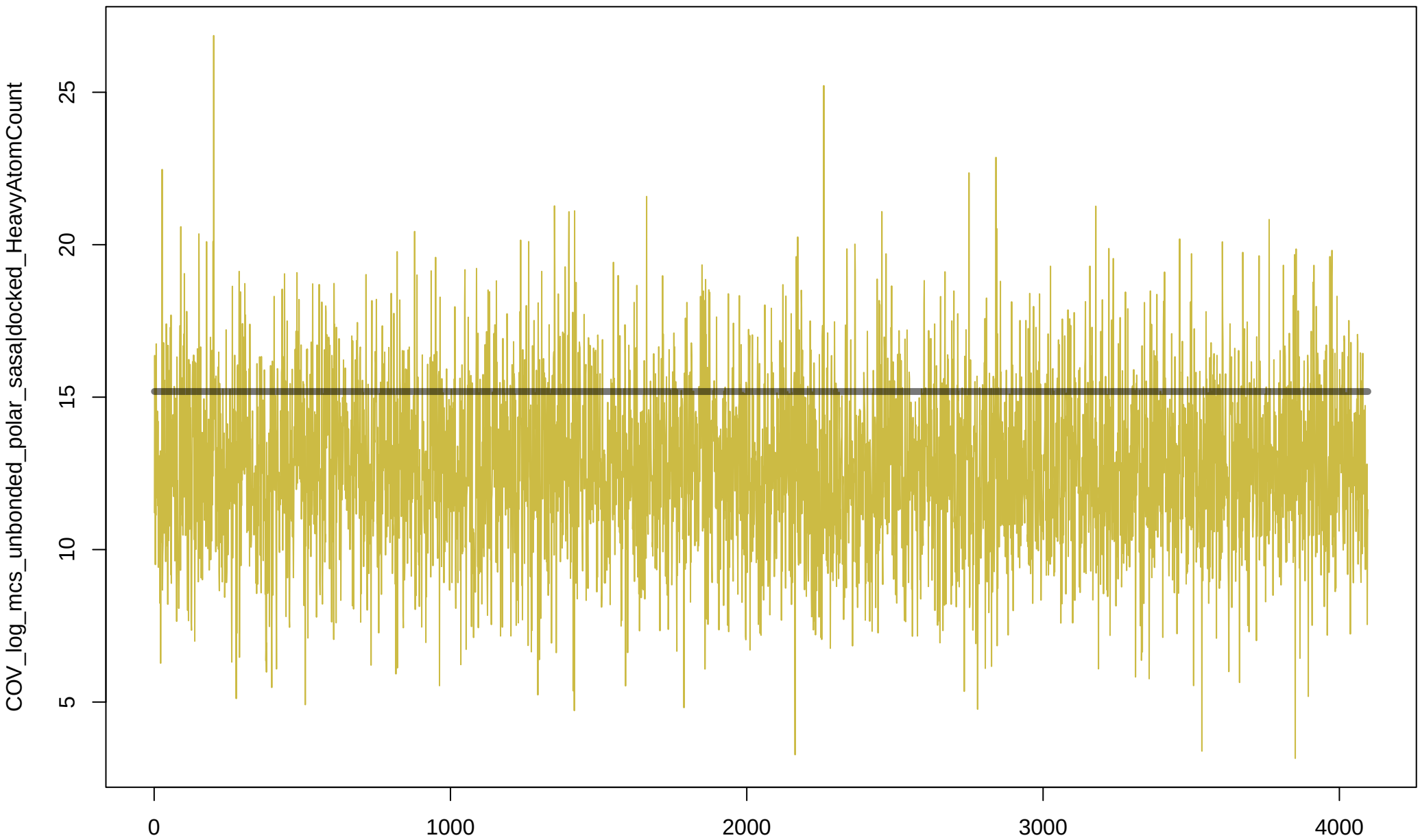

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0324 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0 | rel.err: 0.0331
VAR_docked_HeavyAtomCount
6.9
6.8
6.7
6.6
6.5
6.4
6.3
0
1000
2000
3000
4000

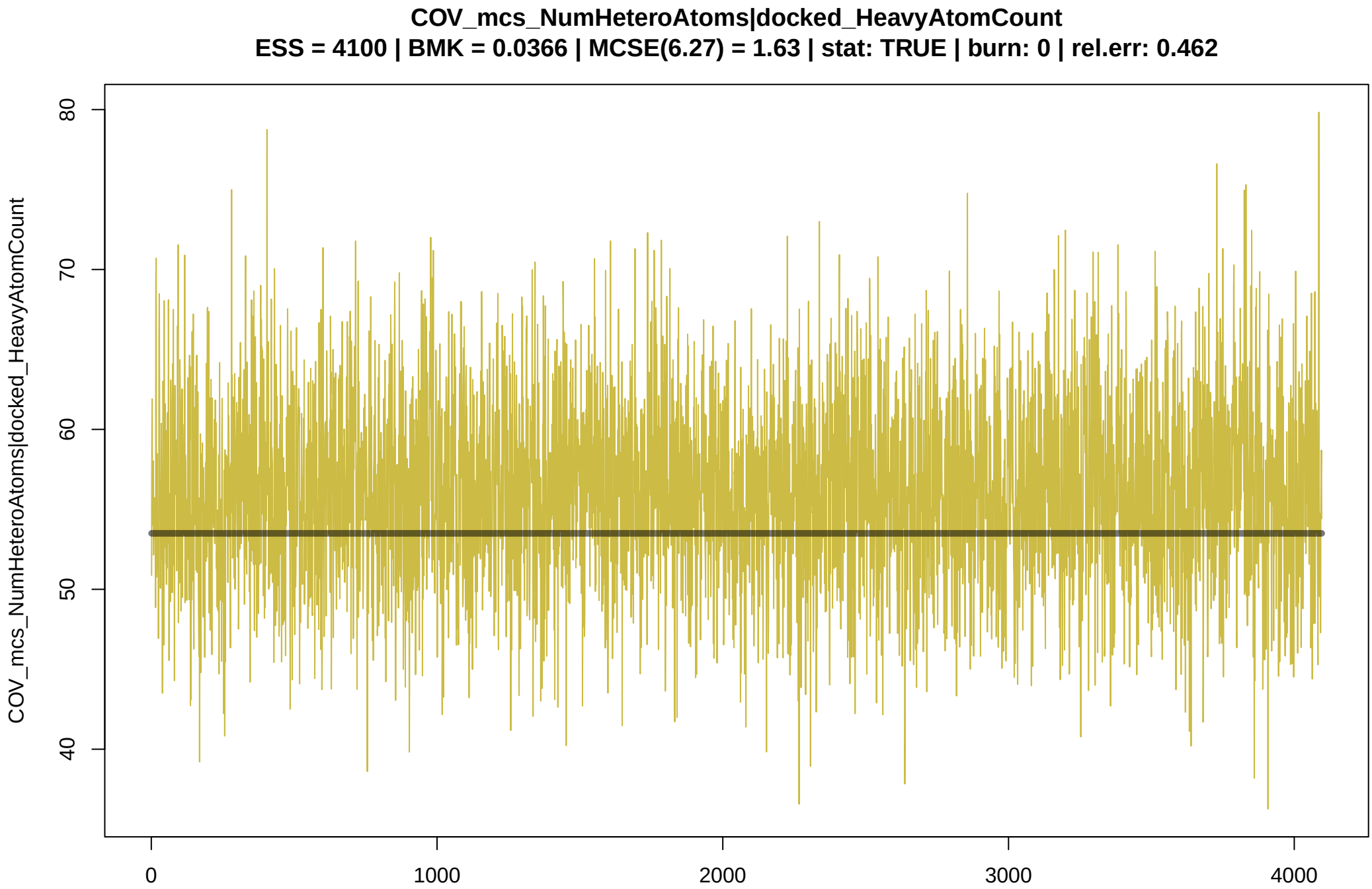

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3880 | BMK = 0.0313 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 0.477
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2590 | BMK = 0.0468 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: −1.61
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 = 0.0298 | MCSE(6.27) = 1.72 | stat: TRUE | burn: 0 | rel.err: −1.78
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 = 3680 | BMK = 0.0447 | MCSE(6.27) = 1.73 | 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
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 3420 | BMK = 0.0415 | MCSE(6.27) = 1.54 | stat: TRUE | burn: 0 | rel.err: −0.918
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 = 0.0366 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.462
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
80
70
60
50
40
0
1000
2000
3000
4000