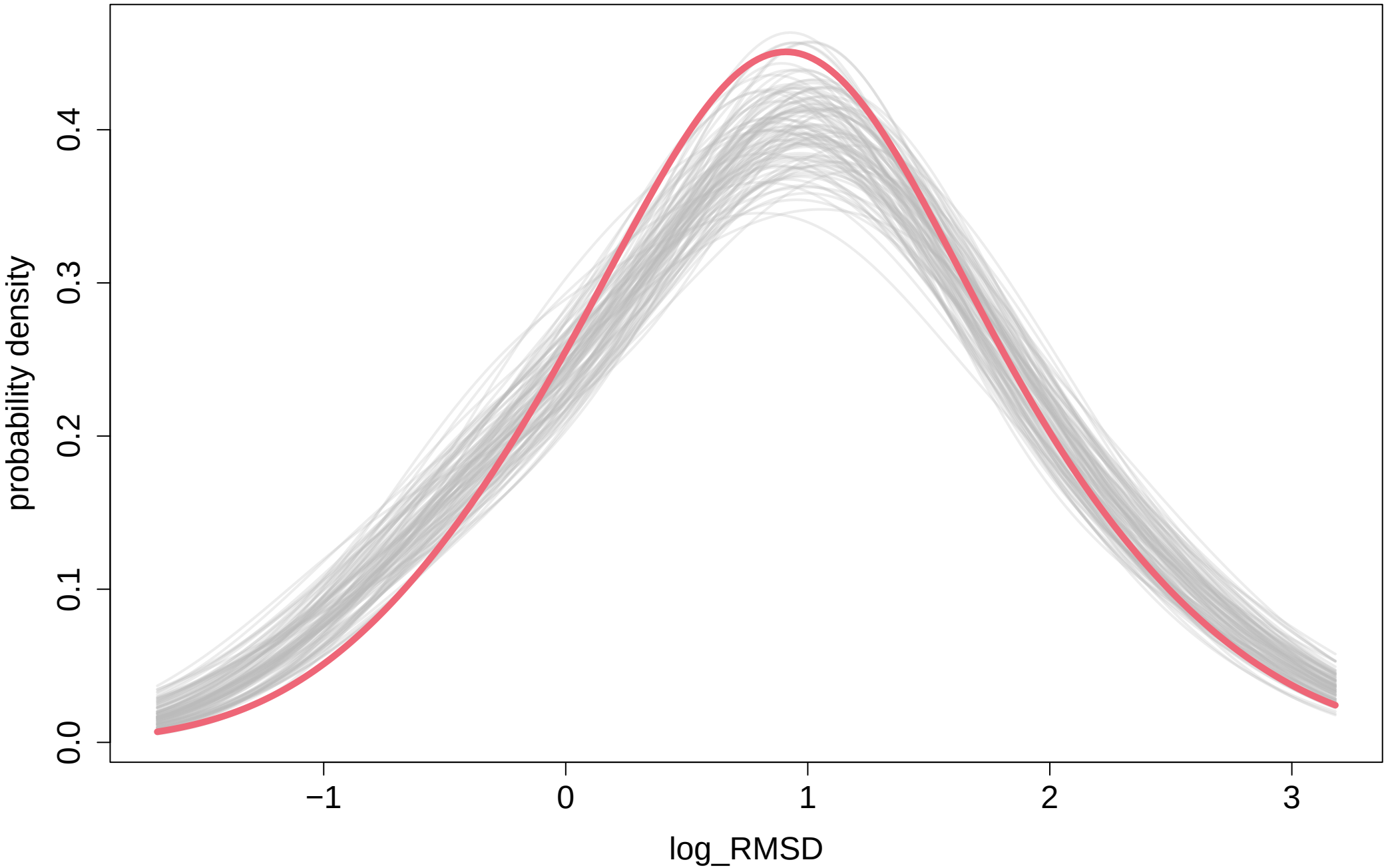
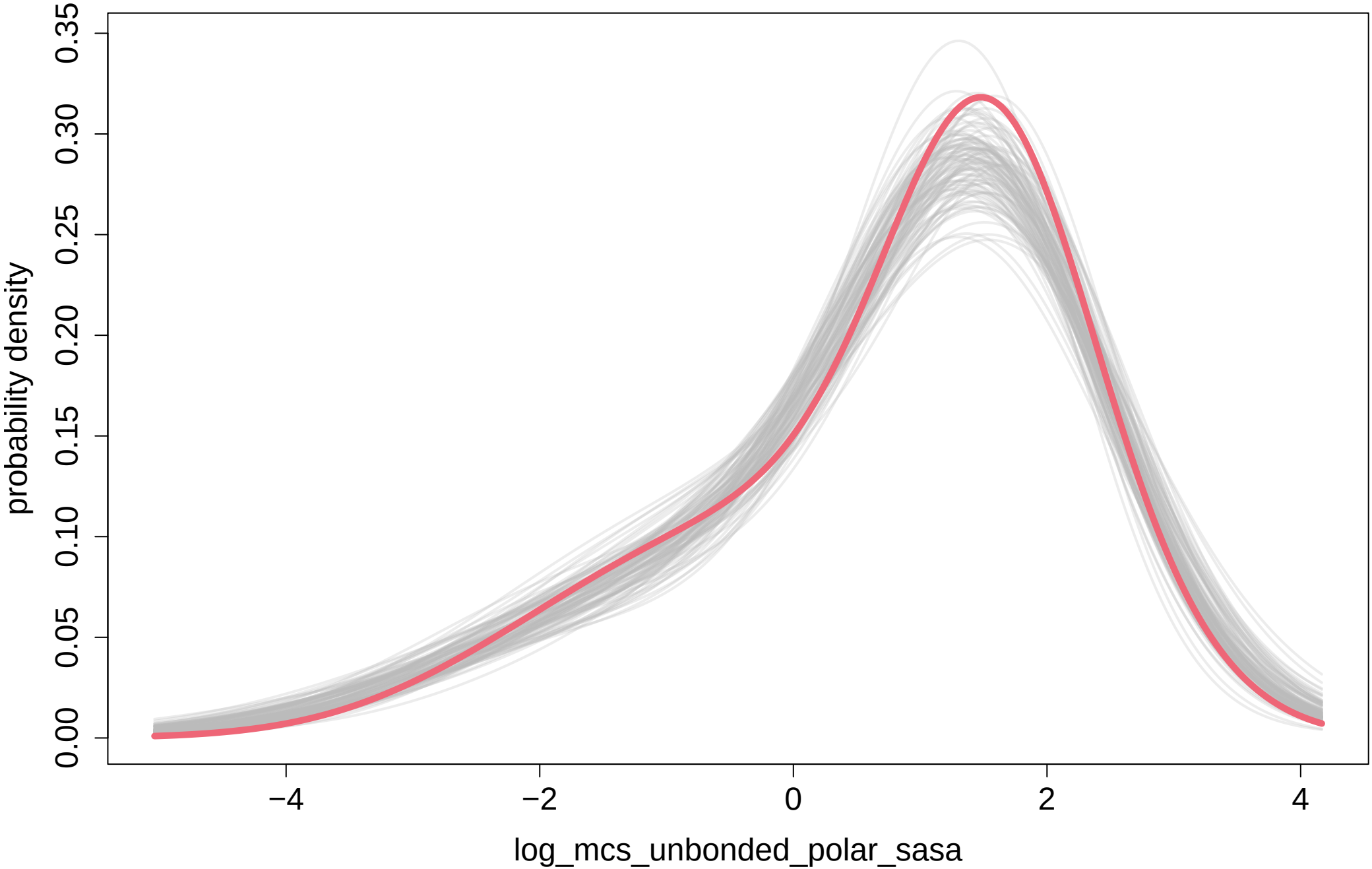
−− STATS maxD −−
min ESS = 121.264777781263
max BMK = 0.10789778353709
max MCSE = 6.98230310416748
all stationary: FALSE
burn: 0
max rel.err.: 2.10444542368886

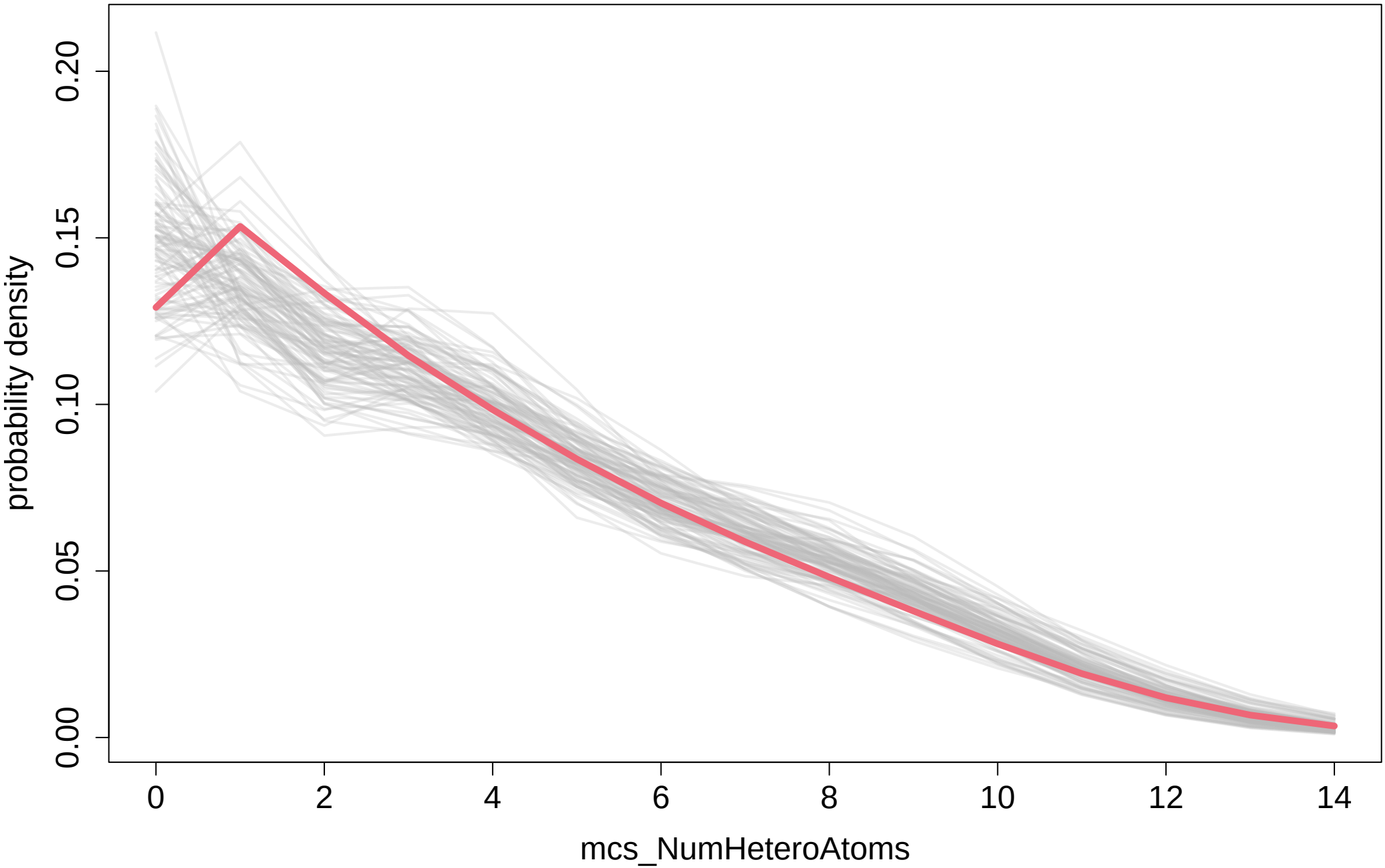
−− STATS 2D −−
min ESS = 3522.89096828321
max BMK = 0.045617114044011
max MCSE = 1.91593027091773
all stationary: TRUE
burn: 0
max rel.err.: 1.77185497902568

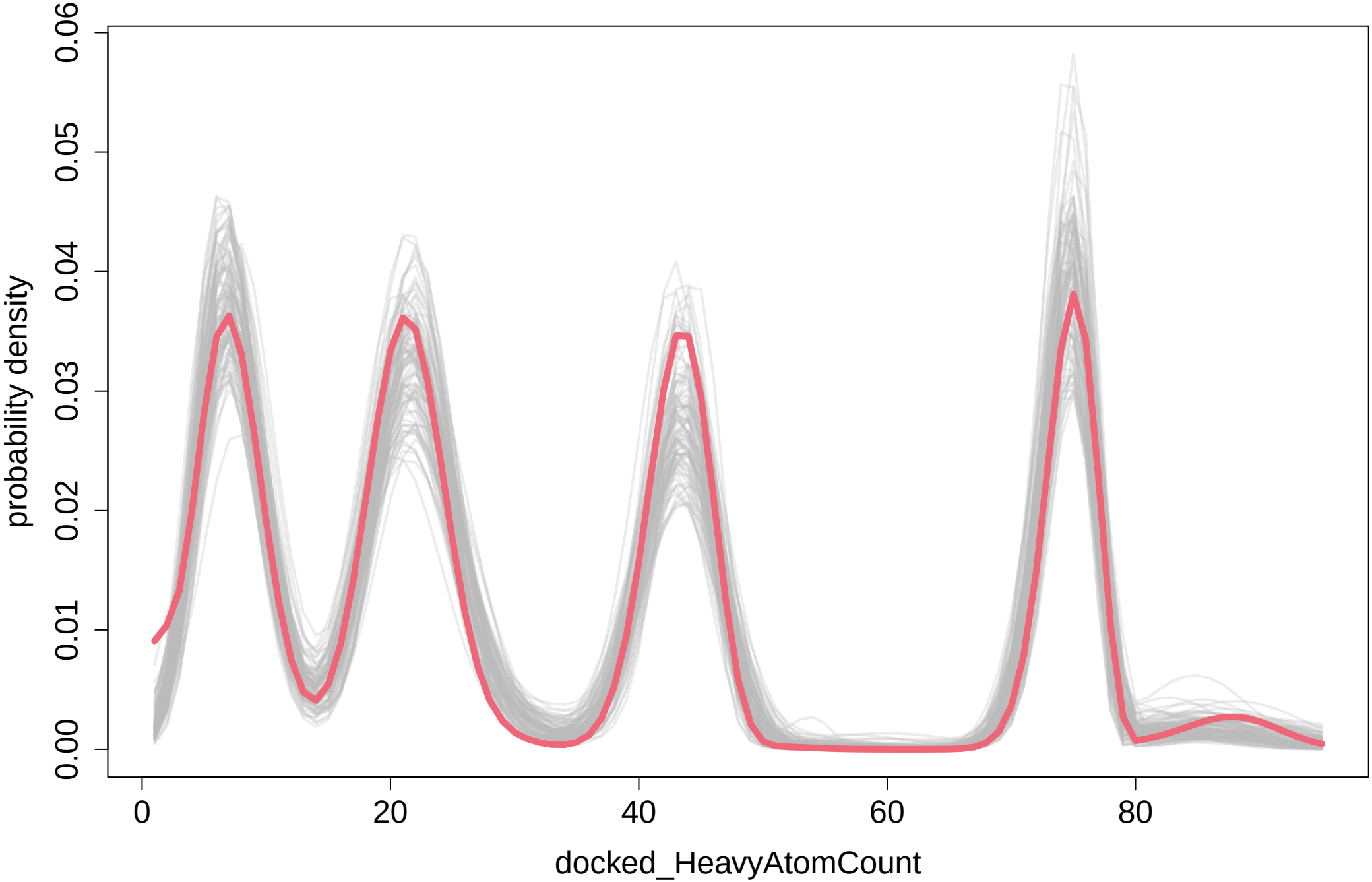
−− STATS 1D −−
min ESS = 2235.58347020747
max BMK = 0.045247203363670 5
max MCSE = 2.21295220687683
all stationary: TRUE
burn: 0
max rel.err.: 2.26378711647769

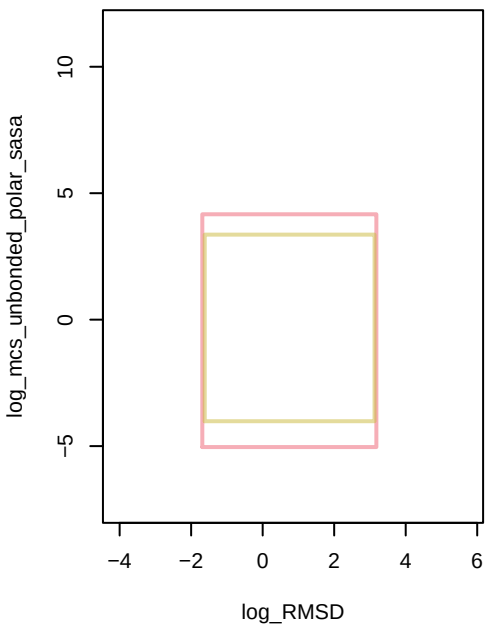
Occupied clusters: 10 of 16
LL: −2160 +− 6.91

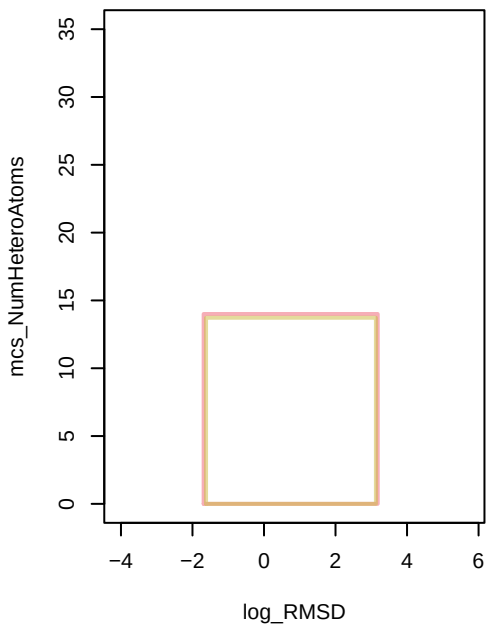

probability density
0.0
0.1
0.2
0.3
0.4
−1
0
1
2
3
log_RMSD

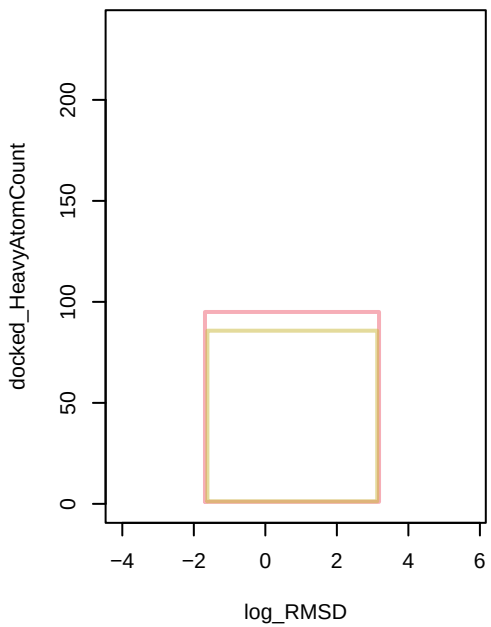

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

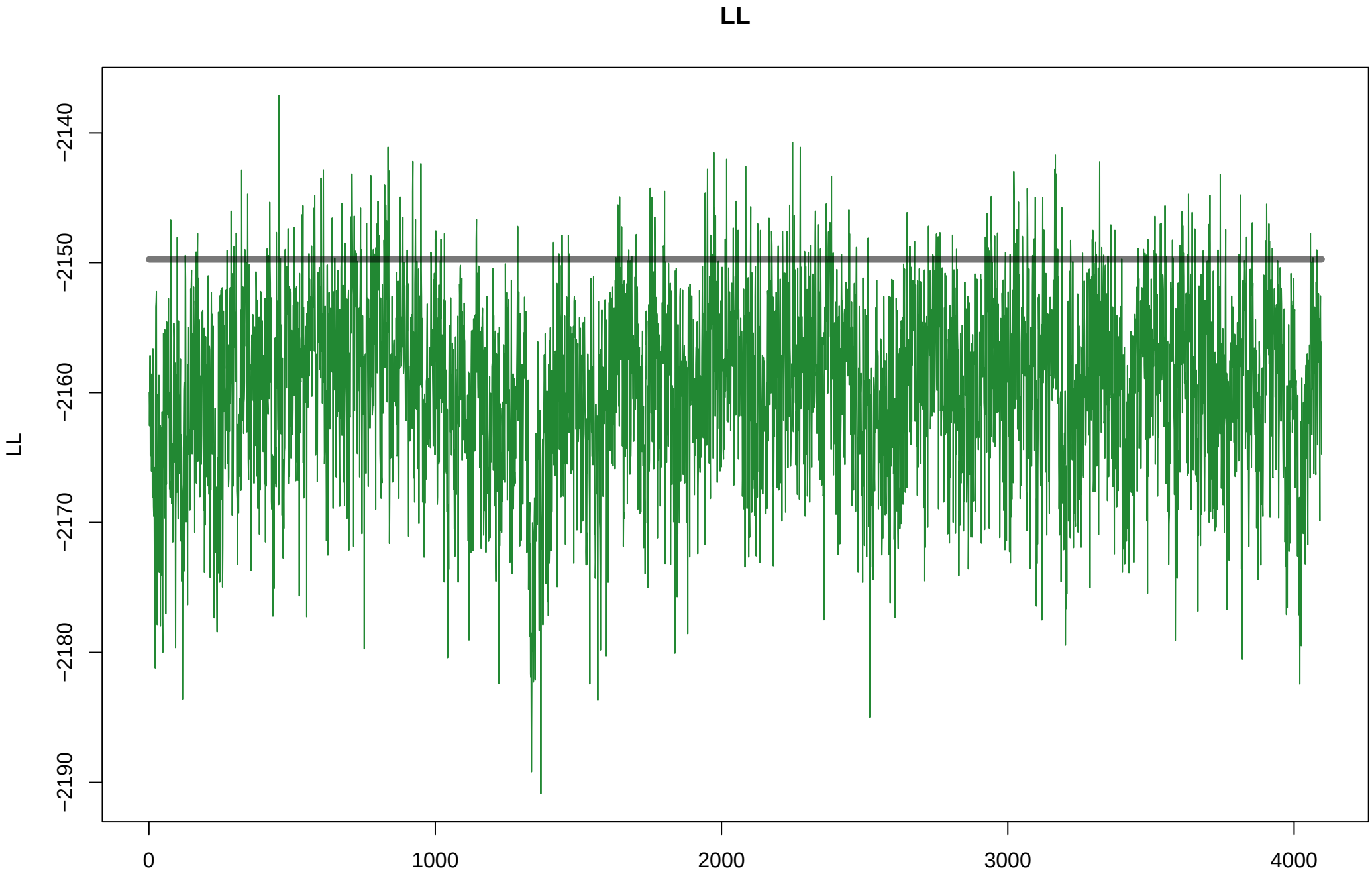

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

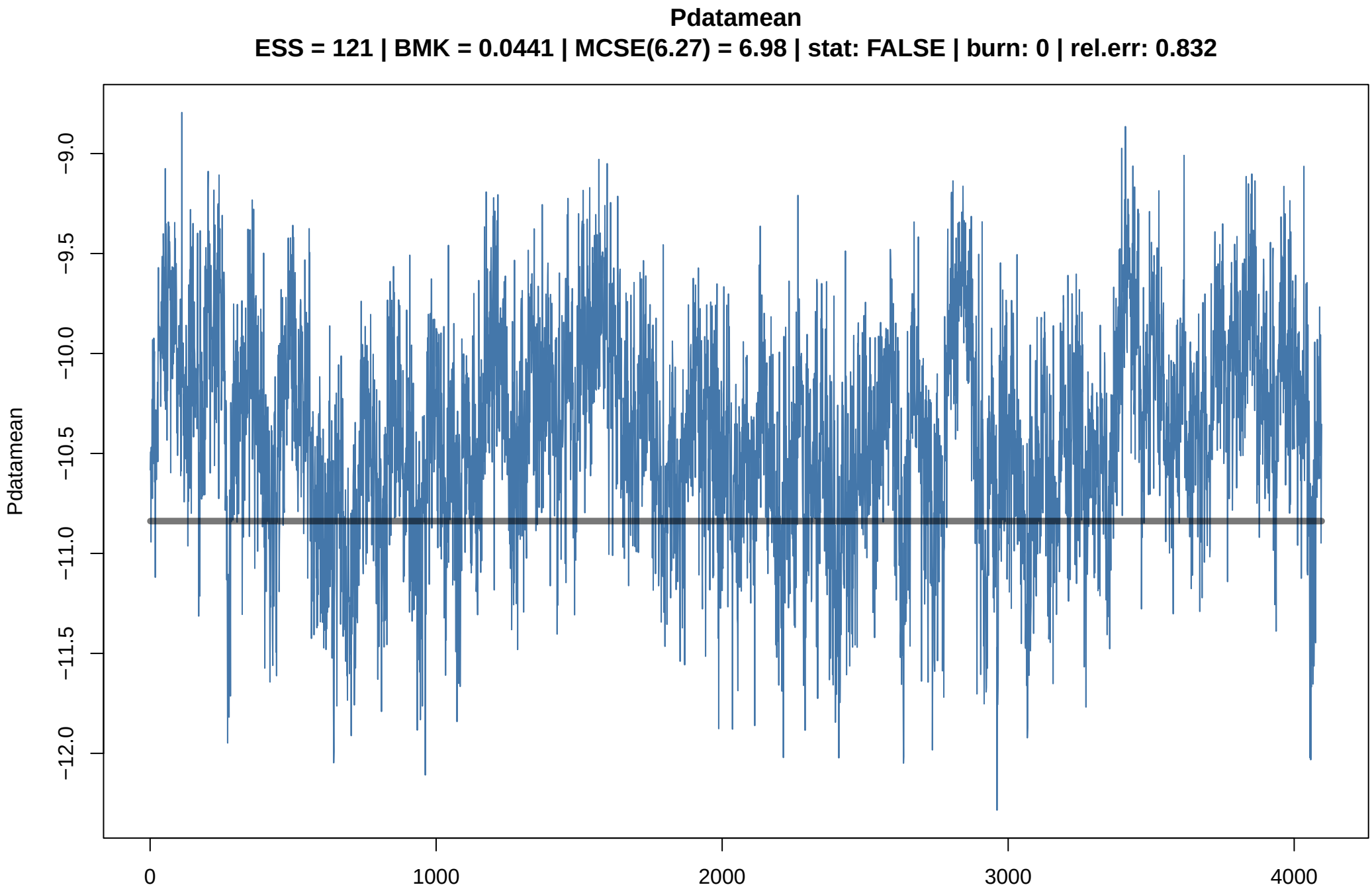

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0.06
0
20
40
60
80
docked_HeavyAtomCount

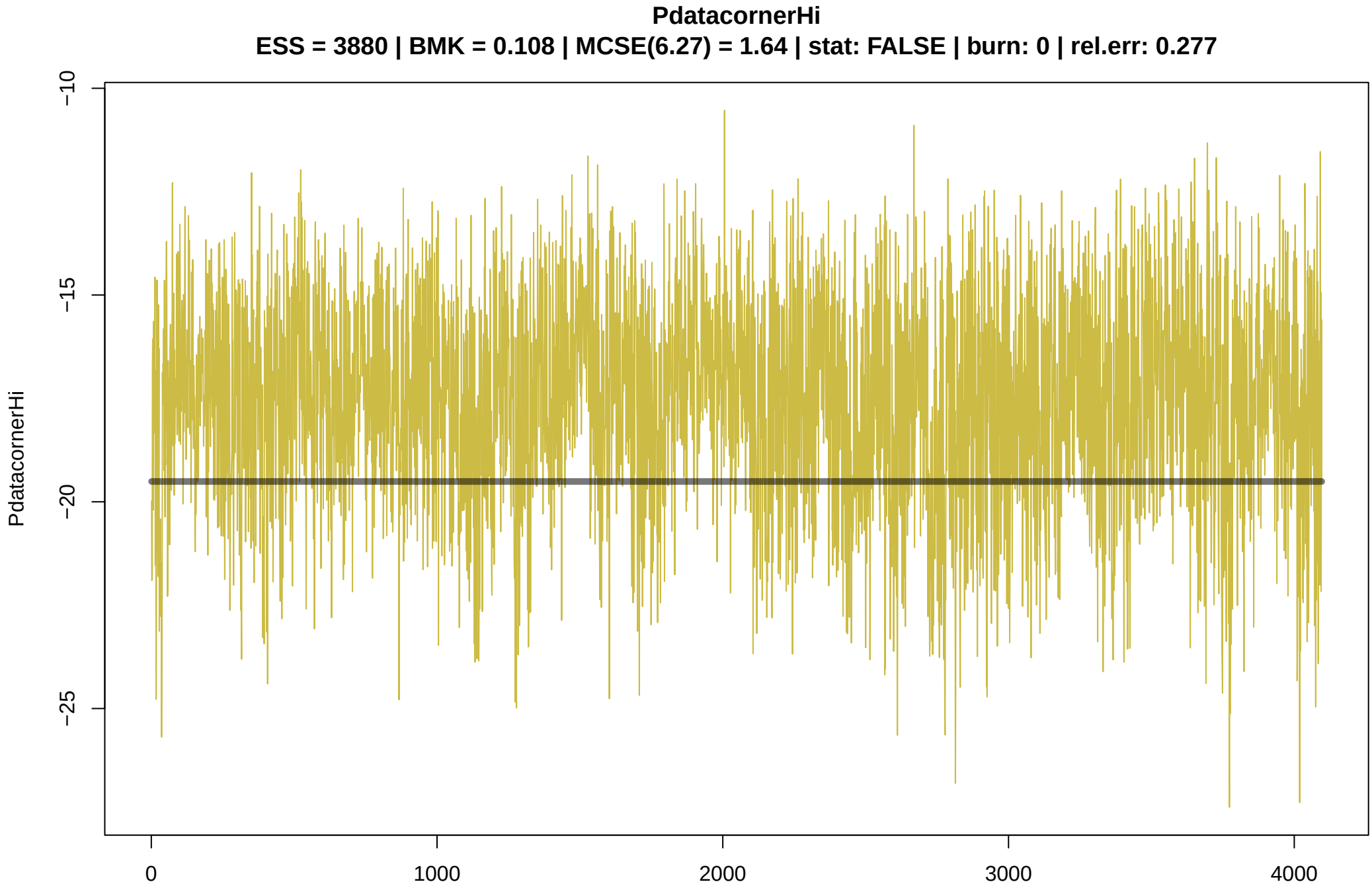

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

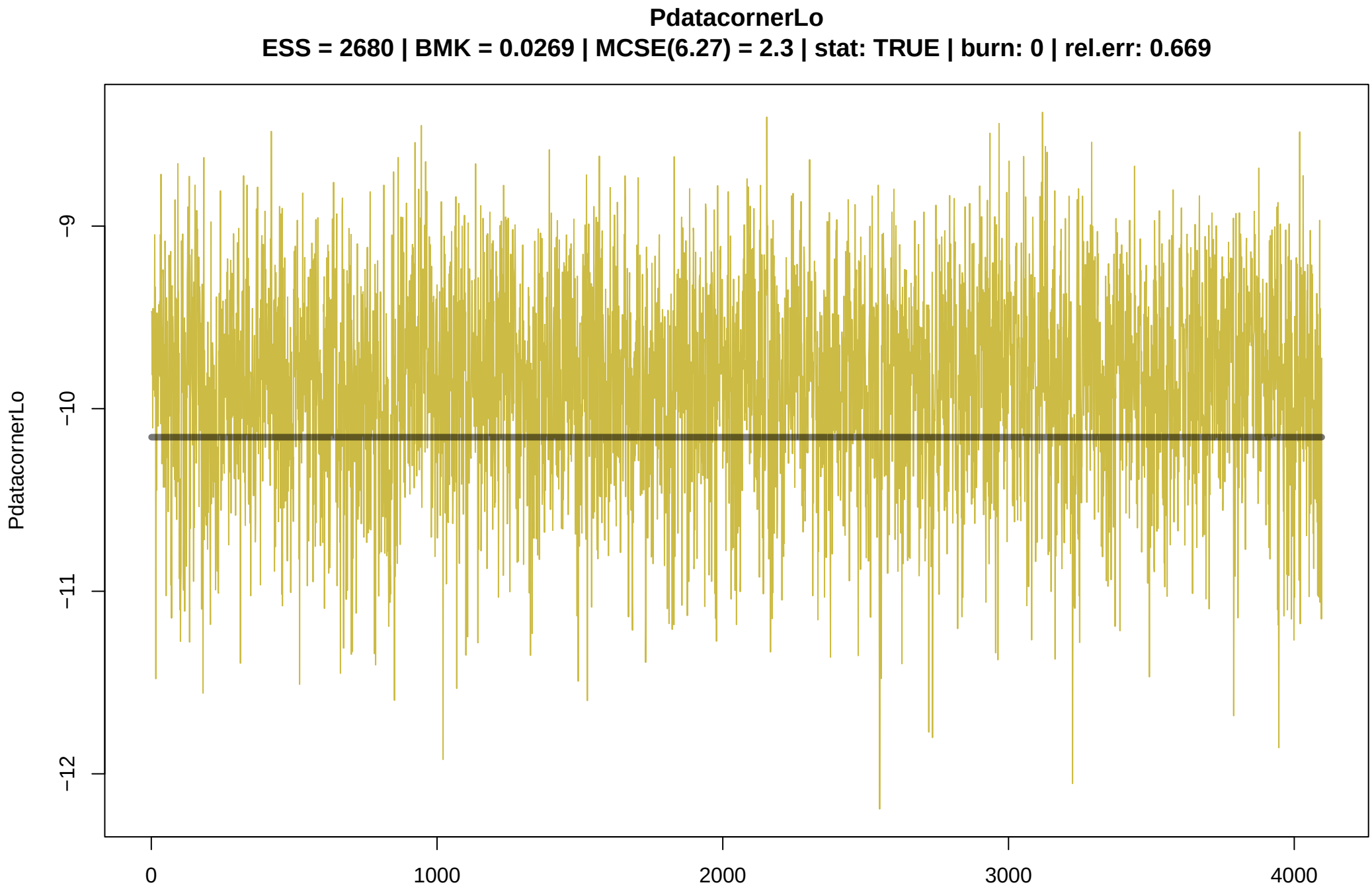

mcs_NumHeteroAtoms
35
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

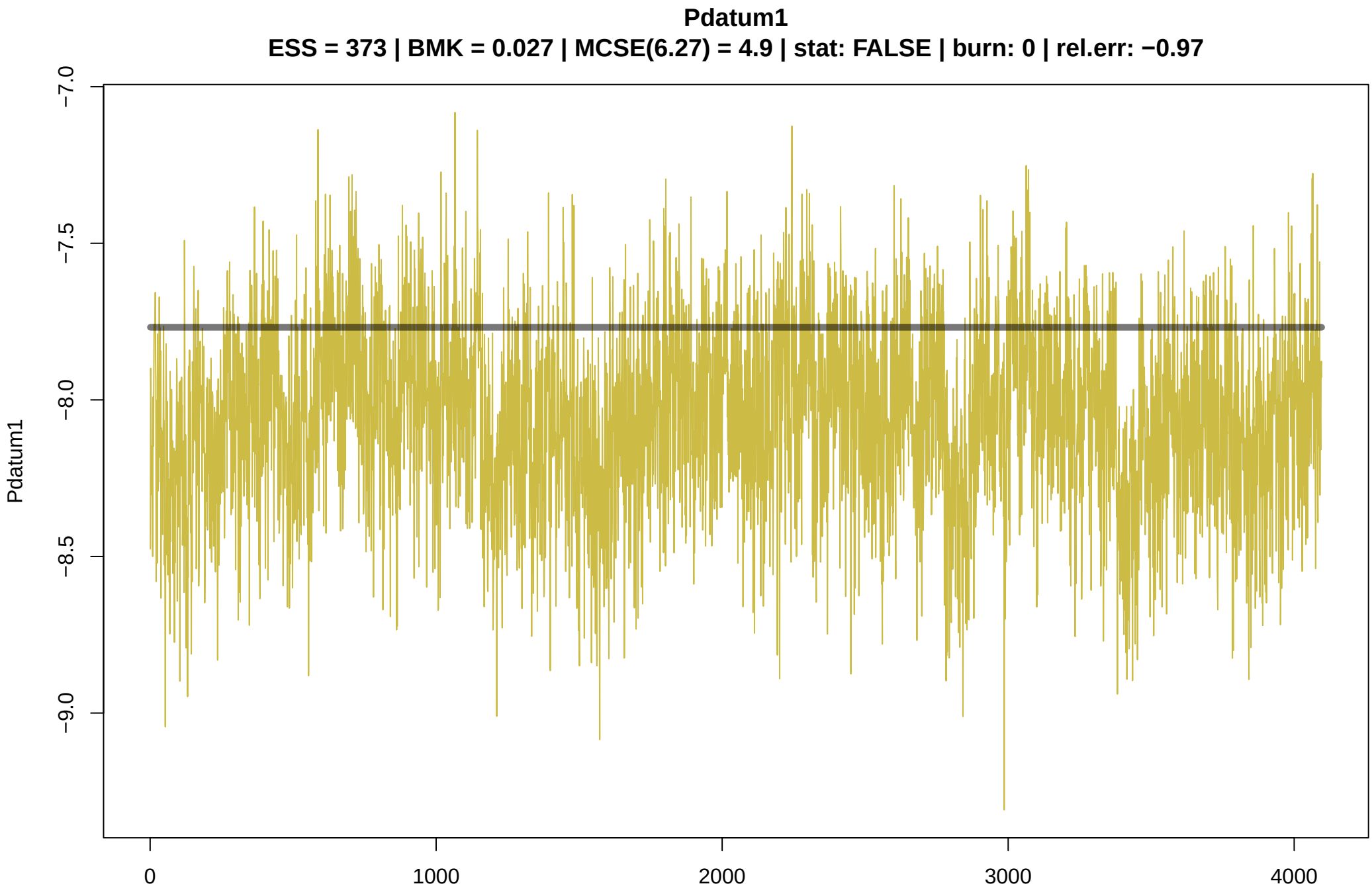

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

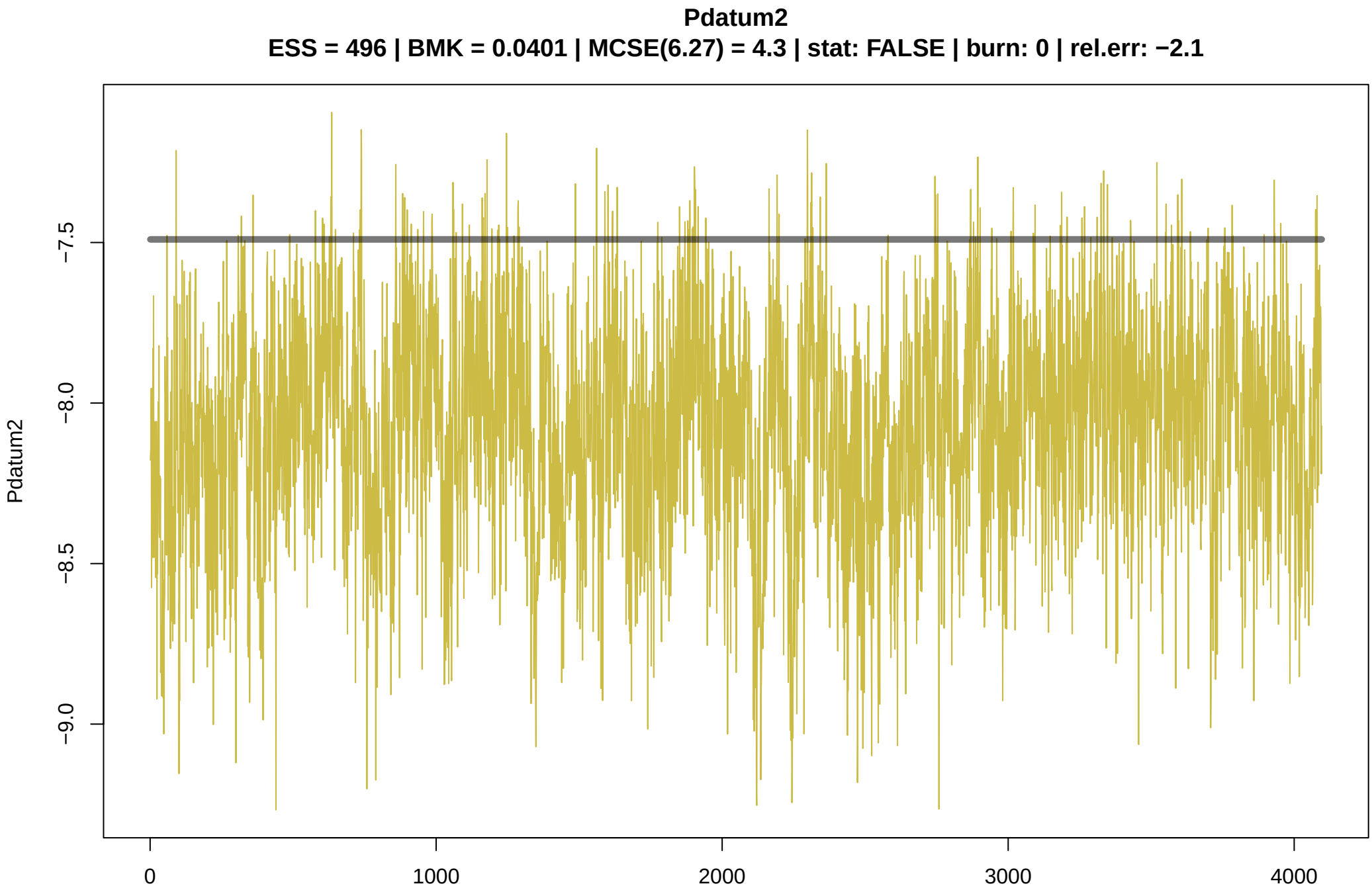

LL
LL
−2140
−2150
−2160
−2170
−2180
−2190
0
1000
2000
3000
4000

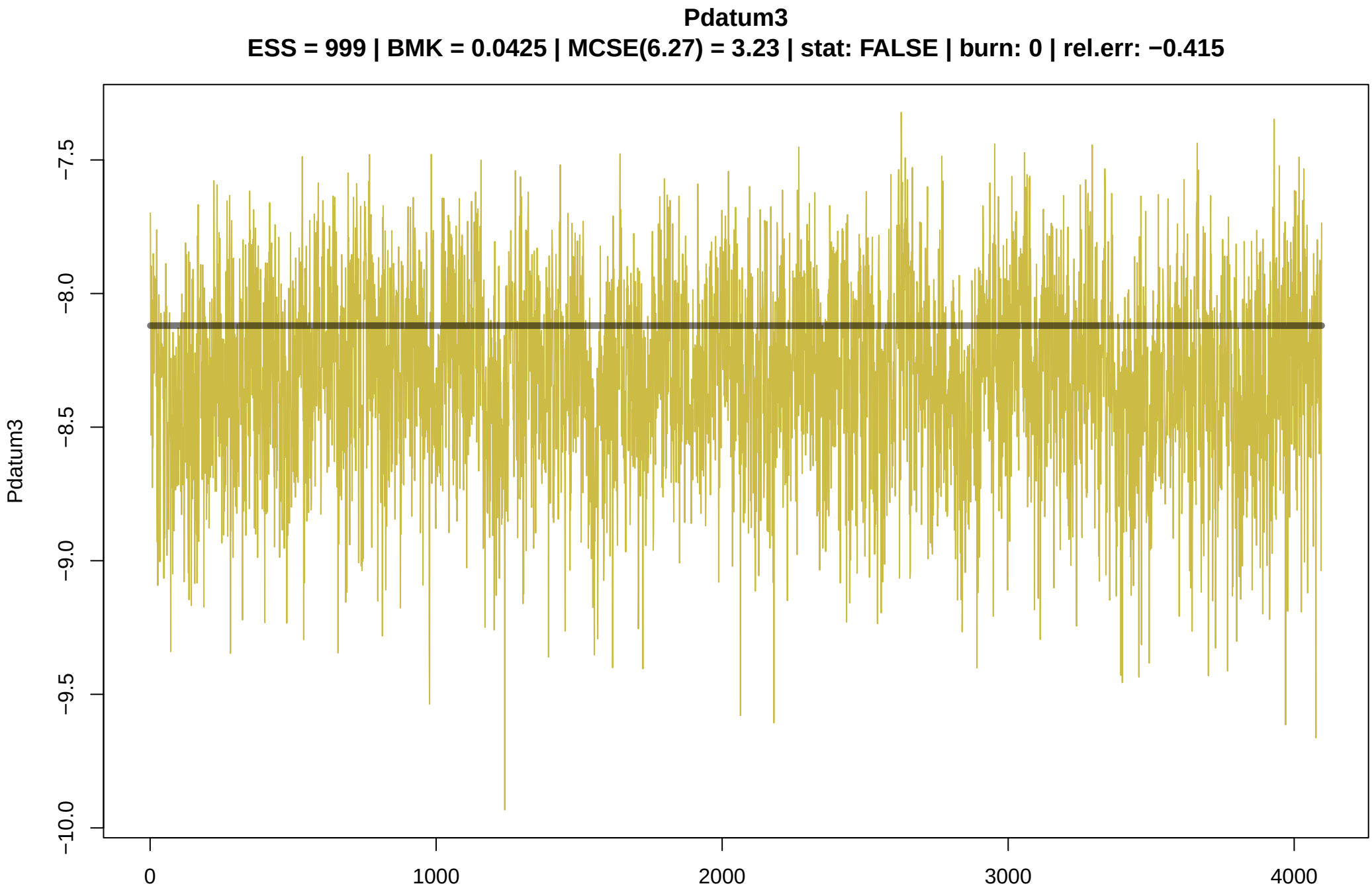

Pdatamean
ESS = 121 | BMK = 0.0441 | MCSE(6.27) = 6.98 | stat: FALSE | burn: 0 | rel.err: 0.832
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
1000
2000
3000
4000

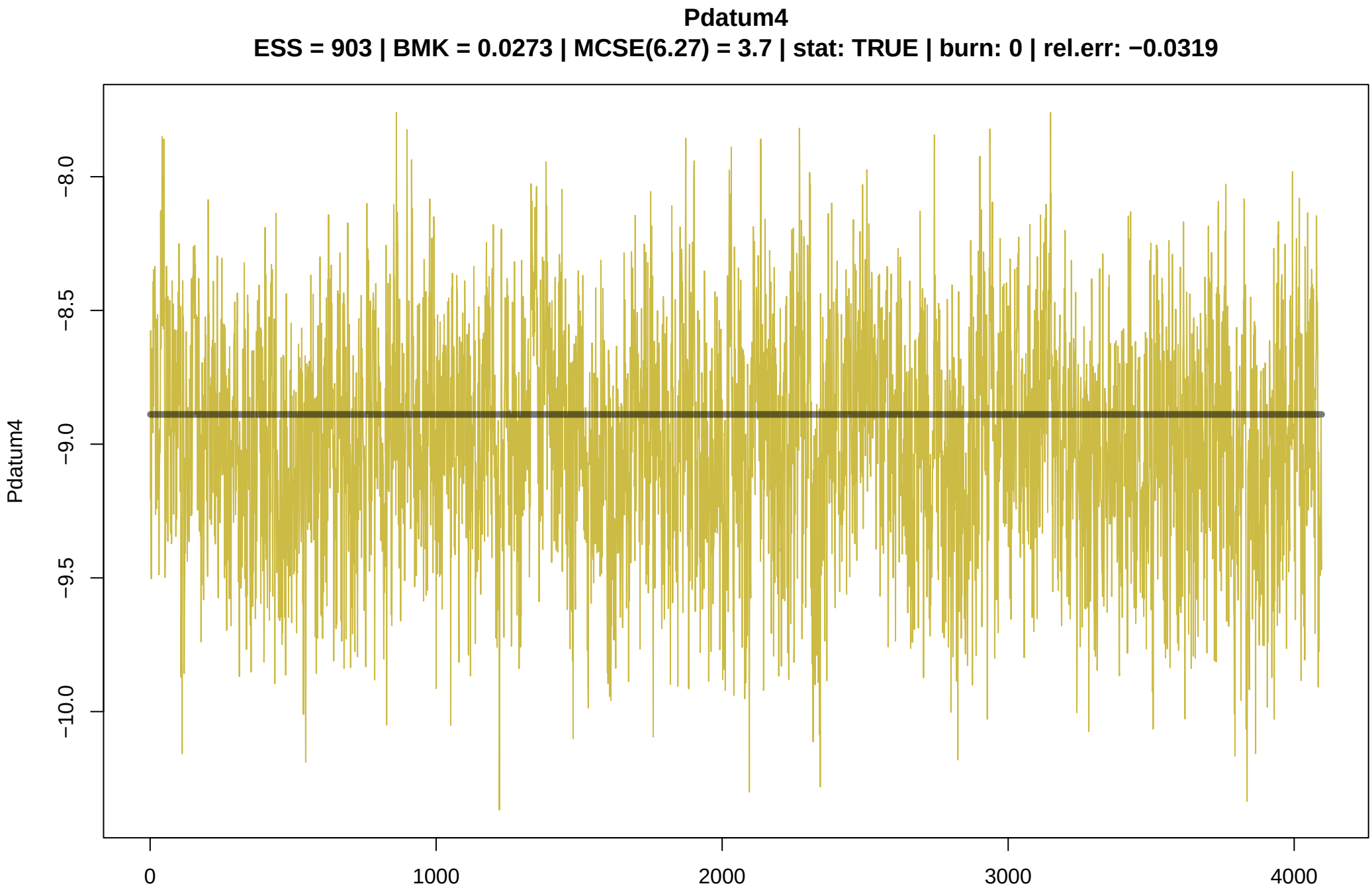

PdatacornerHi
ESS = 3880 | BMK = 0.108 | MCSE(6.27) = 1.64 | stat: FALSE | burn: 0 | rel.err: 0.277
PdatacornerHi
−10
−15
−20
−25
0
1000
2000
3000
4000

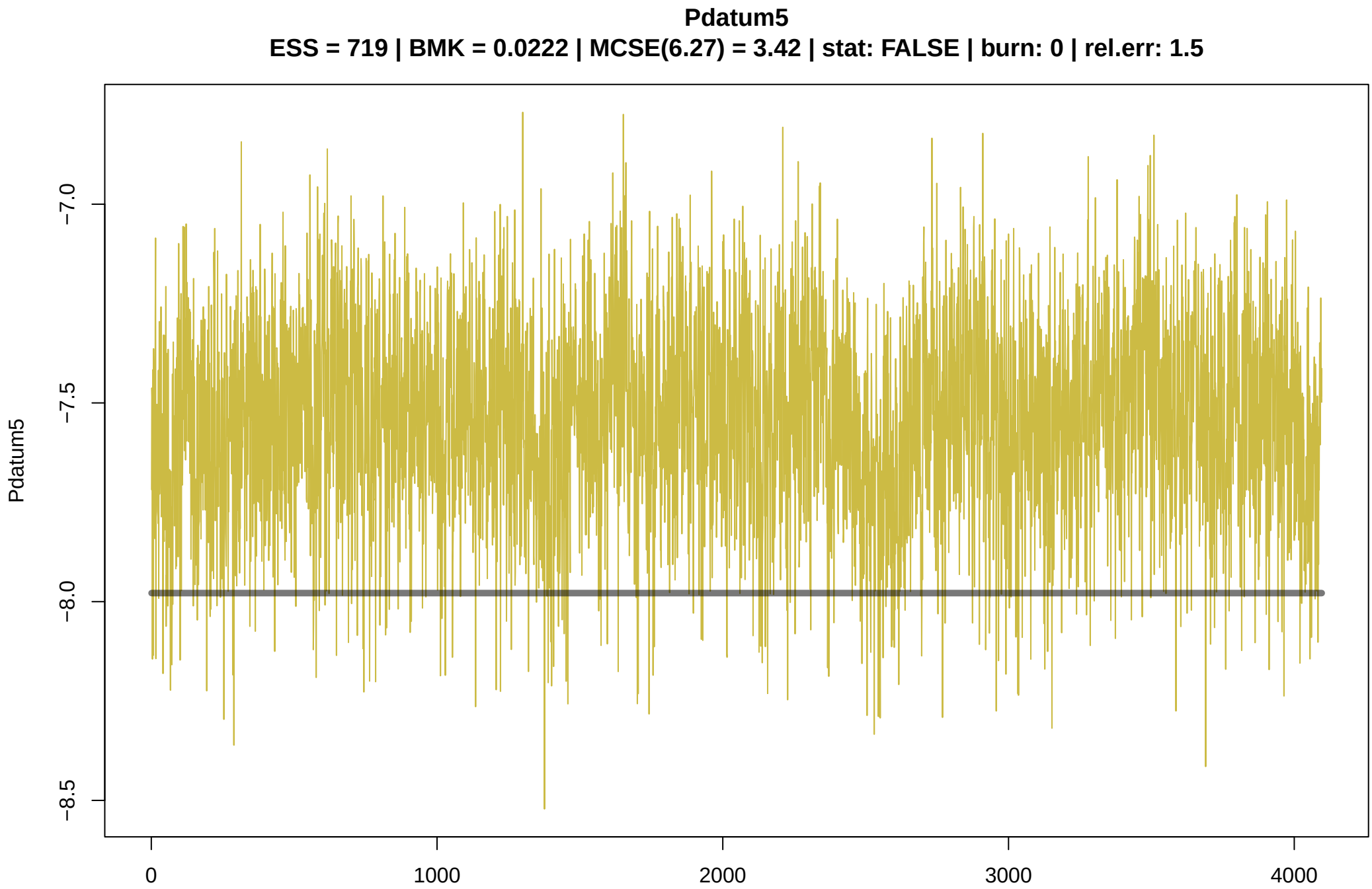

PdatacornerLo
ESS = 2680 | BMK = 0.0269 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: 0.669
PdatacornerLo
−9
−10
−11
−12
0
1000
2000
3000
4000

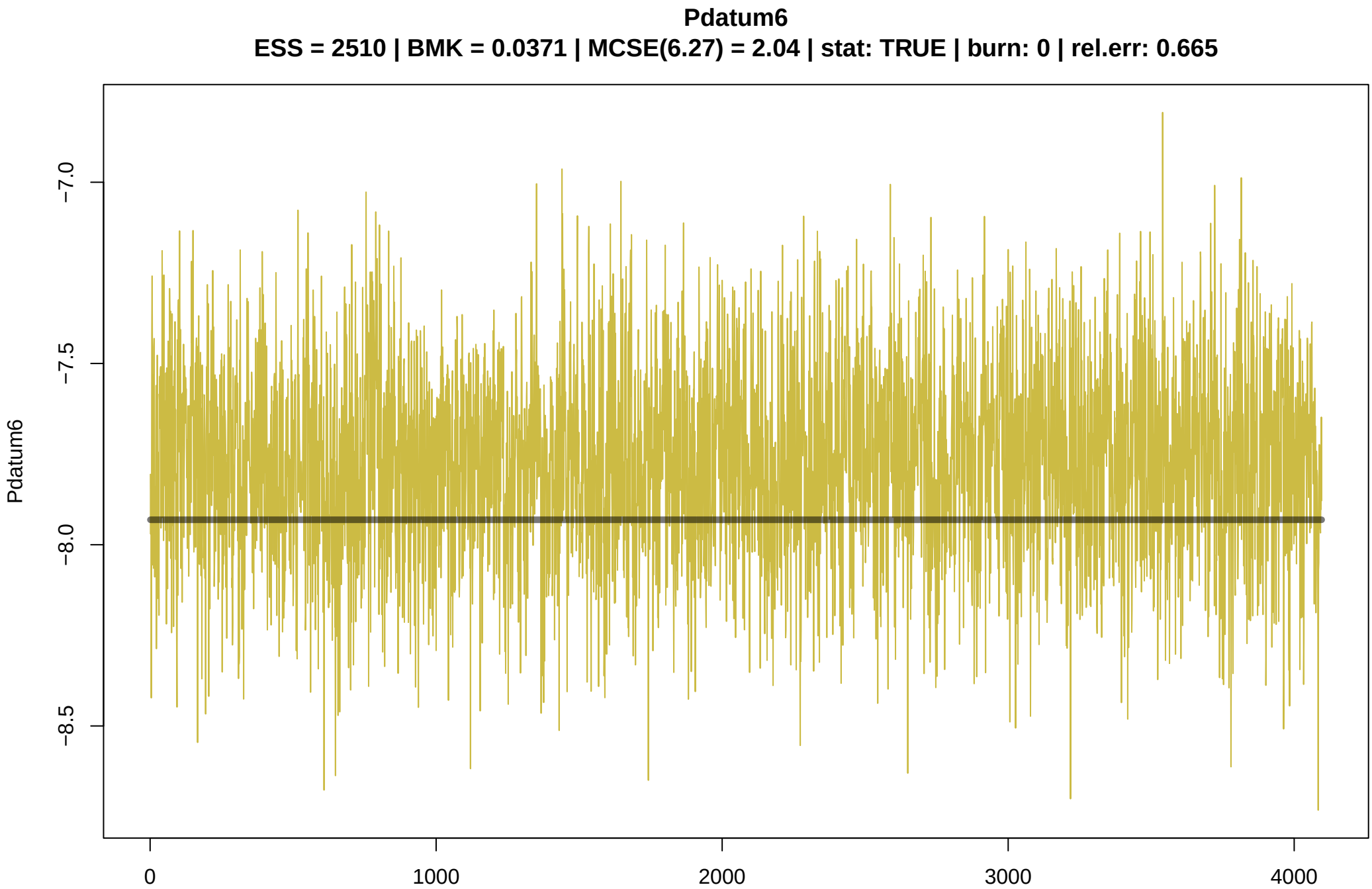

Pdatum1
ESS = 373 | BMK = 0.027 | MCSE(6.27) = 4.9 | stat: FALSE | burn: 0 | rel.err: −0.97
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

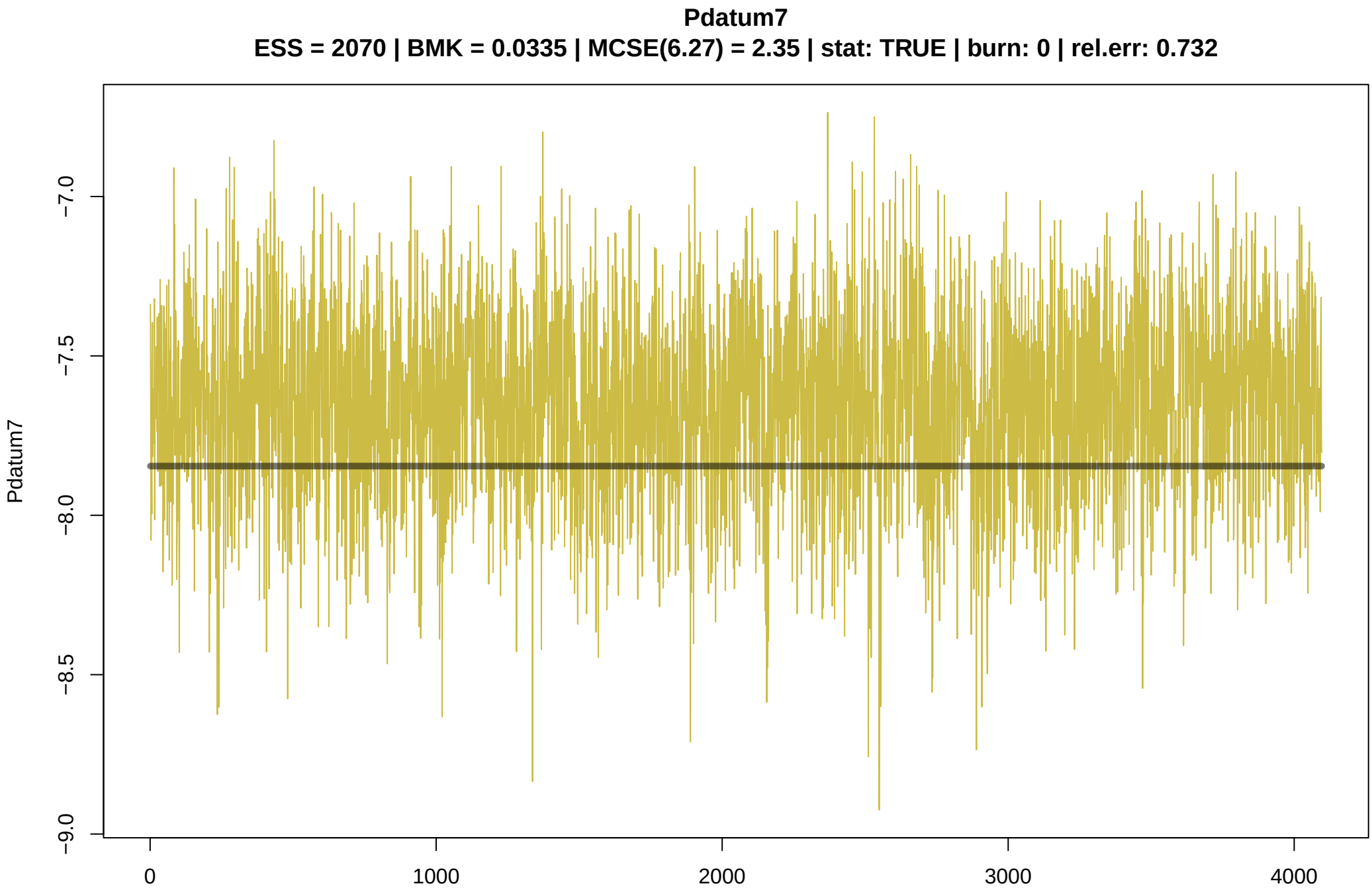

Pdatum2
ESS = 496 | BMK = 0.0401 | MCSE(6.27) = 4.3 | stat: FALSE | burn: 0 | rel.err: −2.1
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

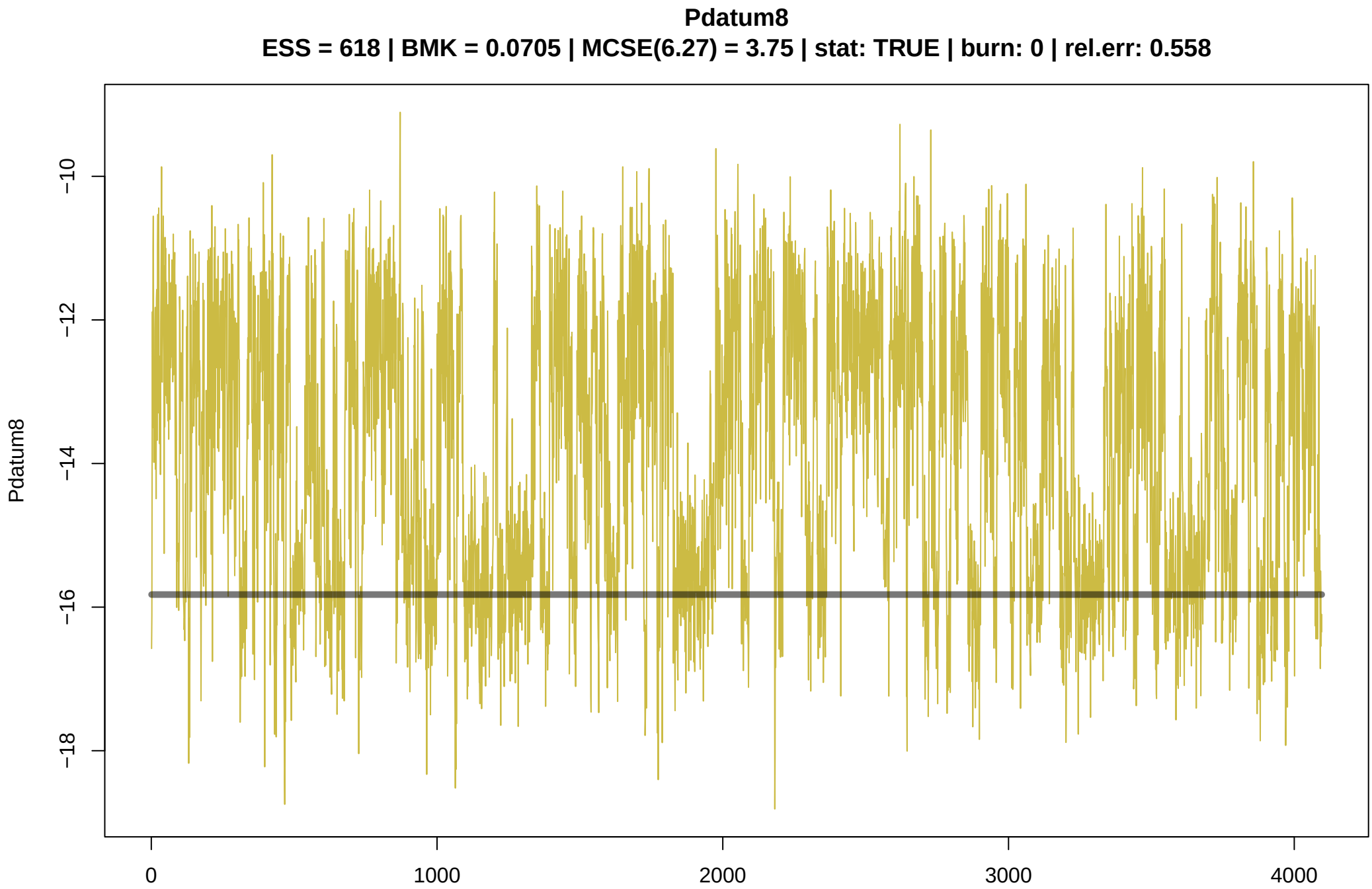

Pdatum3
ESS = 999 | BMK = 0.0425 | MCSE(6.27) = 3.23 | stat: FALSE | burn: 0 | rel.err: −0.415
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
1000
2000
3000
4000

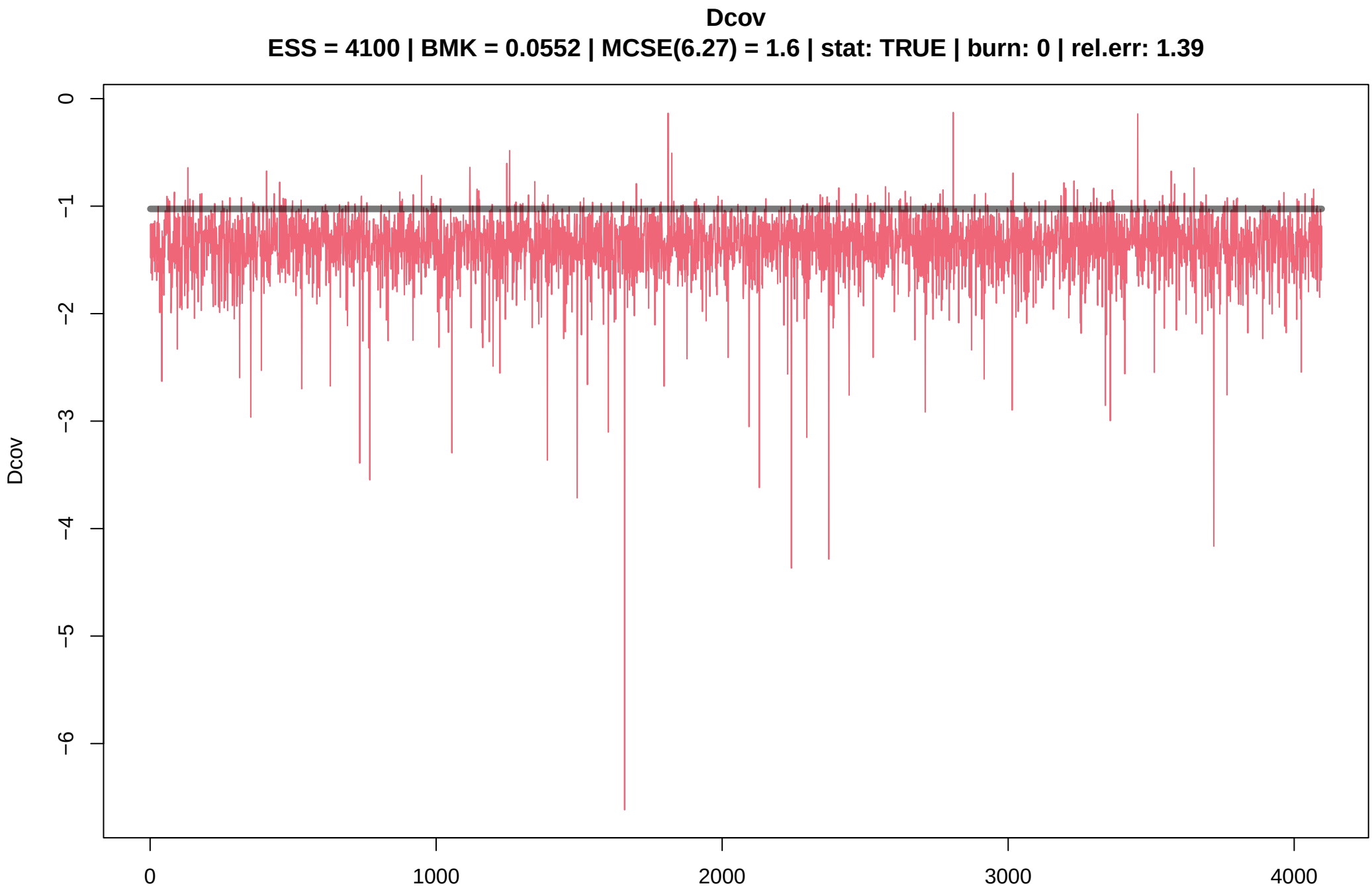

Pdatum4
ESS = 903 | BMK = 0.0273 | MCSE(6.27) = 3.7 | stat: TRUE | burn: 0 | rel.err: −0.0319
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
1000
2000
3000
4000

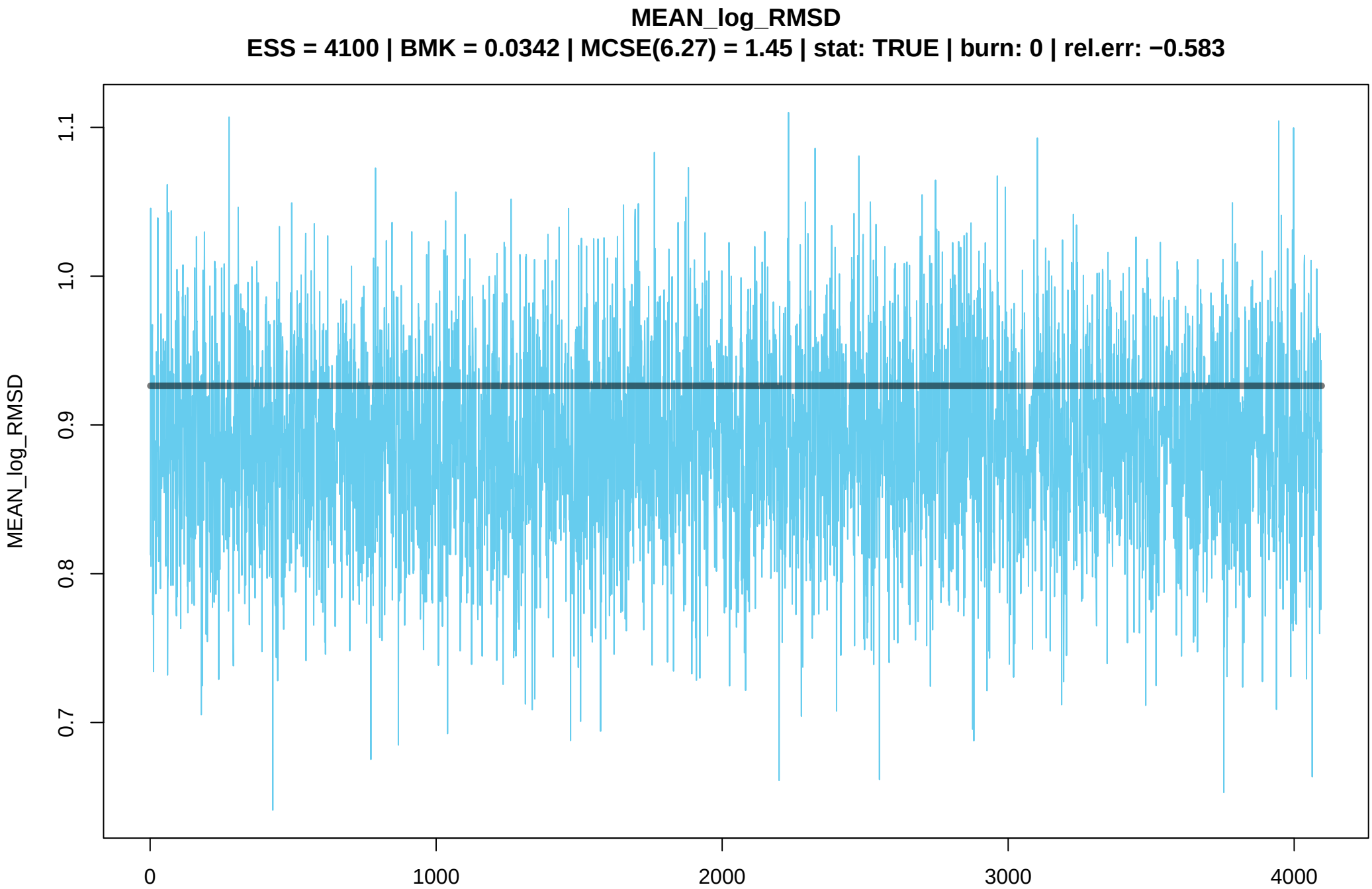

Pdatum5
ESS = 719 | BMK = 0.0222 | MCSE(6.27) = 3.42 | stat: FALSE | burn: 0 | rel.err: 1.5
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

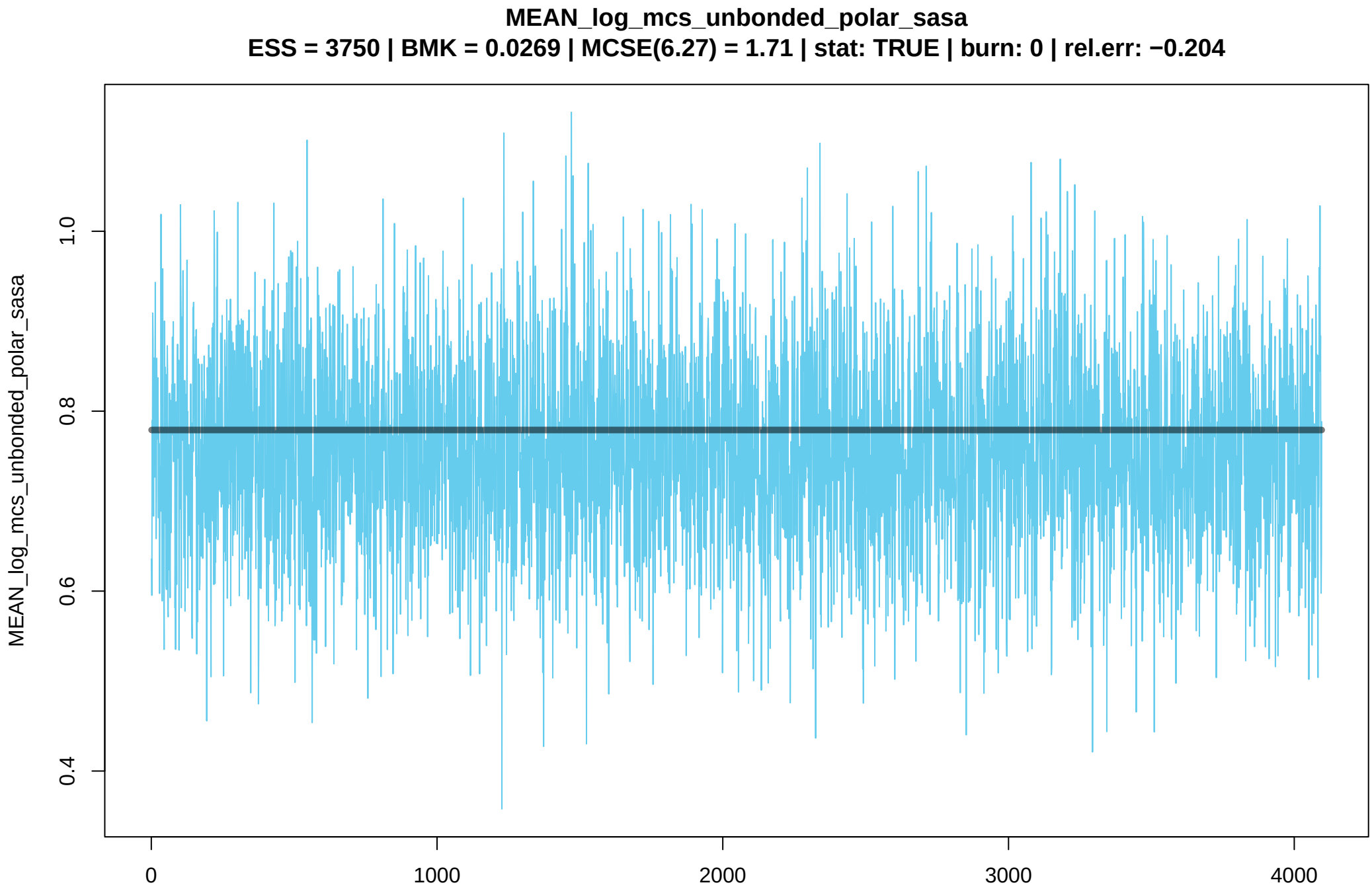

Pdatum6
ESS = 2510 | BMK = 0.0371 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0 | rel.err: 0.665
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
1000
2000
3000
4000

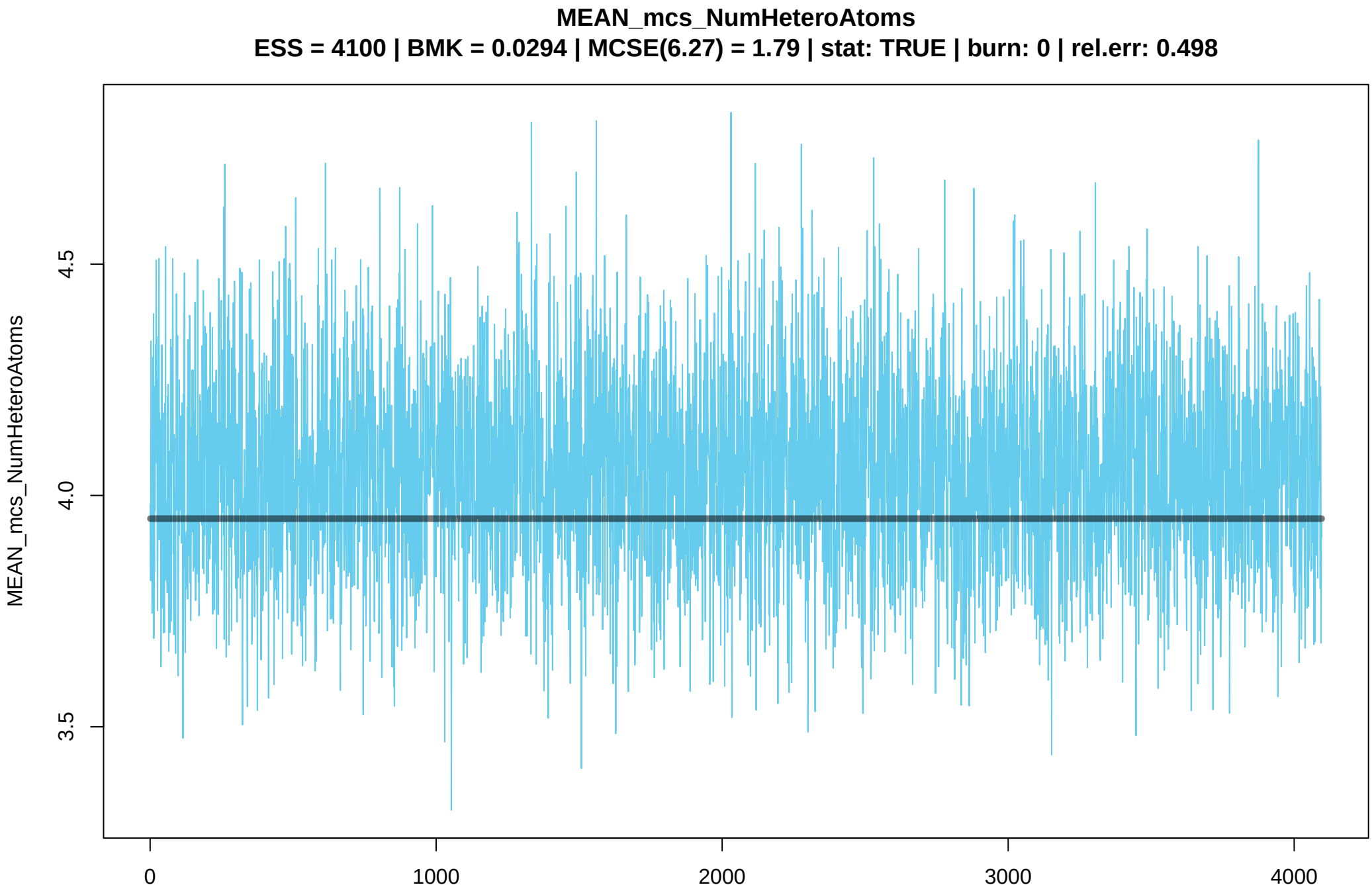

Pdatum7
ESS = 2070 | BMK = 0.0335 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 0.732
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
1000
2000
3000
4000

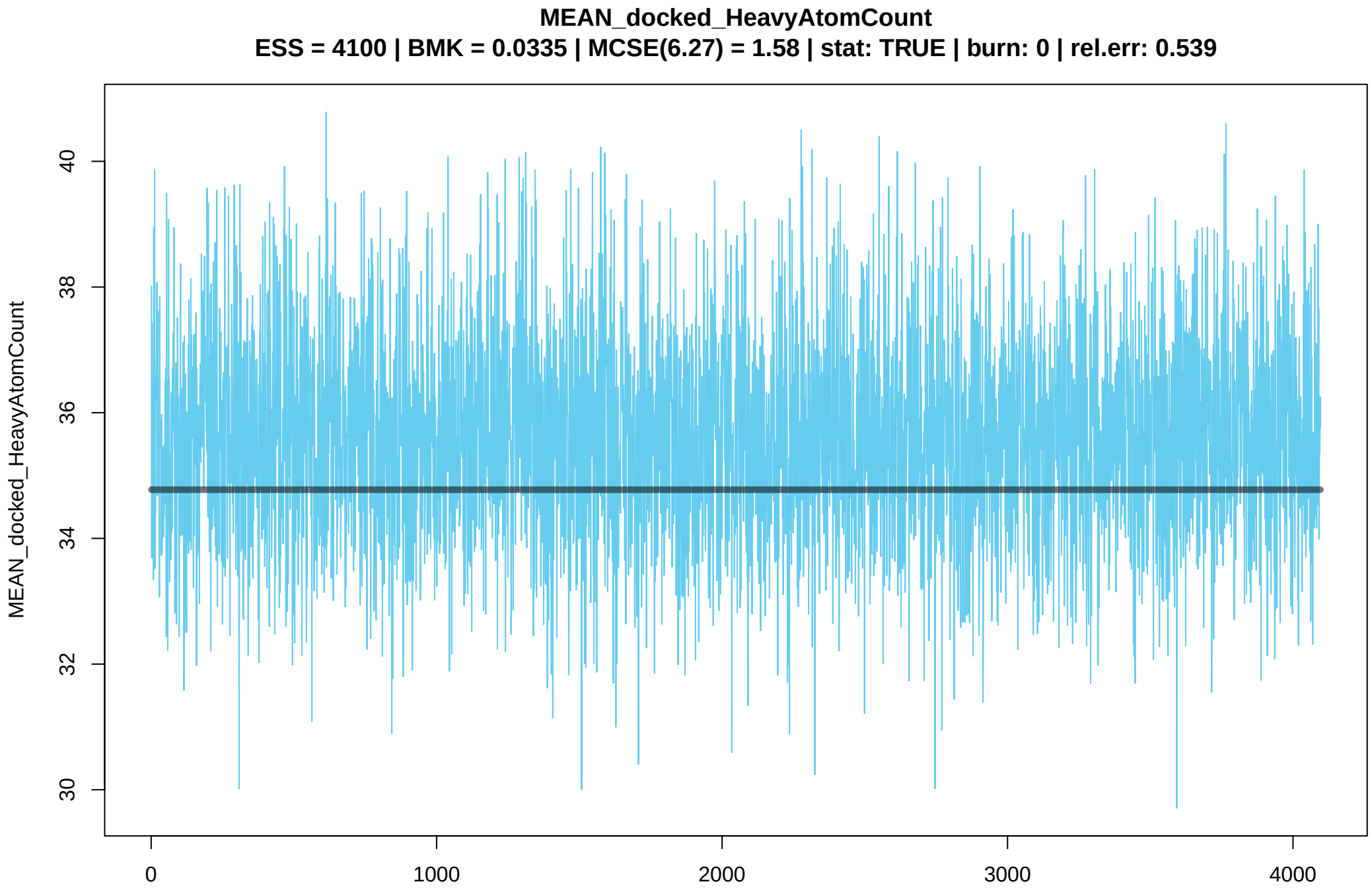

Pdatum8
ESS = 618 | BMK = 0.0705 | MCSE(6.27) = 3.75 | stat: TRUE | burn: 0 | rel.err: 0.558
Pdatum8
−10
−12
−14
−16
−18
0
1000
2000
3000
4000

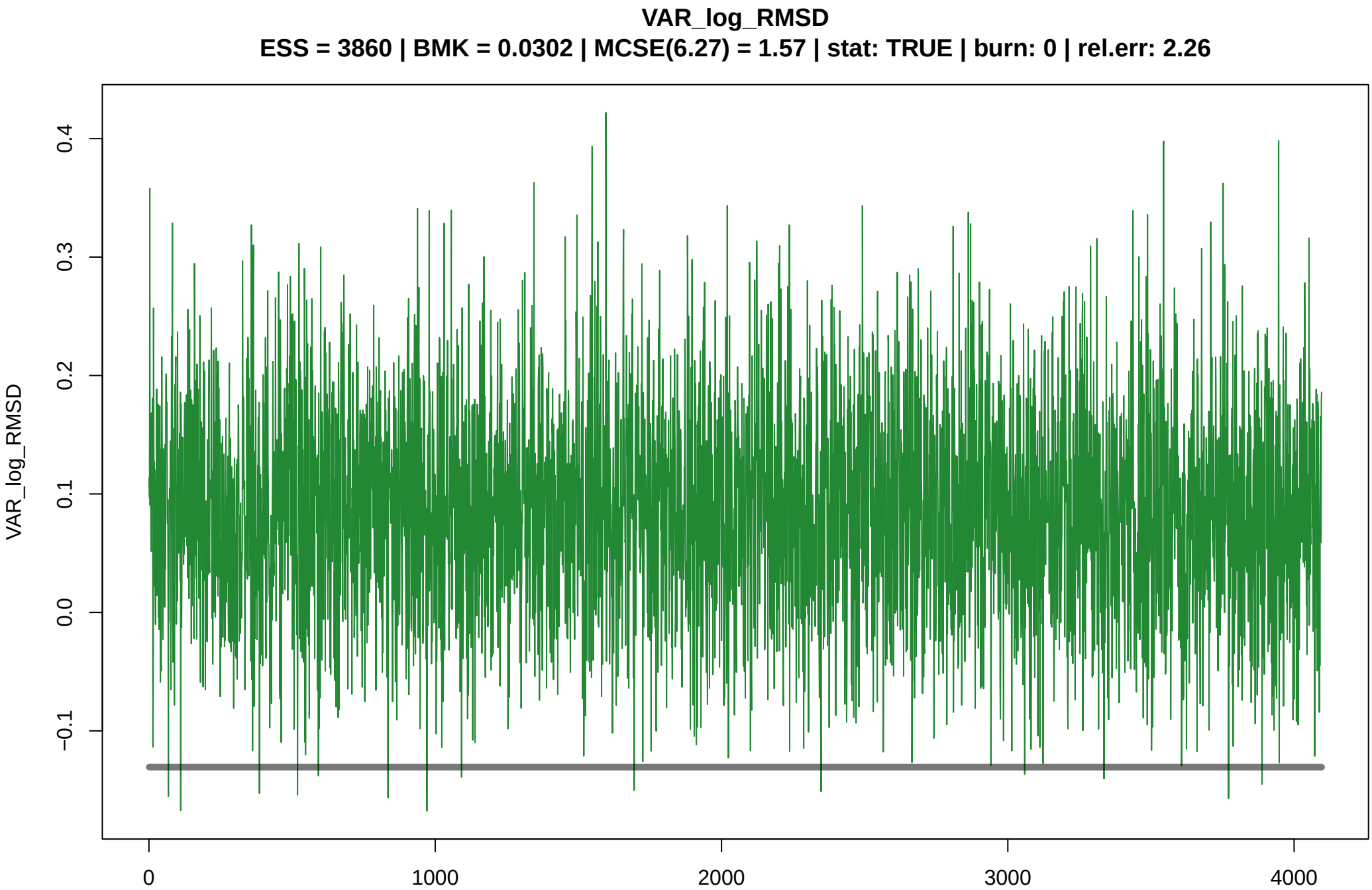

Dcov
ESS = 4100 | BMK = 0.0552 | MCSE(6.27) = 1.6 | stat: TRUE | burn: 0 | rel.err: 1.39
Dcov
0
−1
−2
−3
−4
−5
−6
0
1000
2000
3000
4000

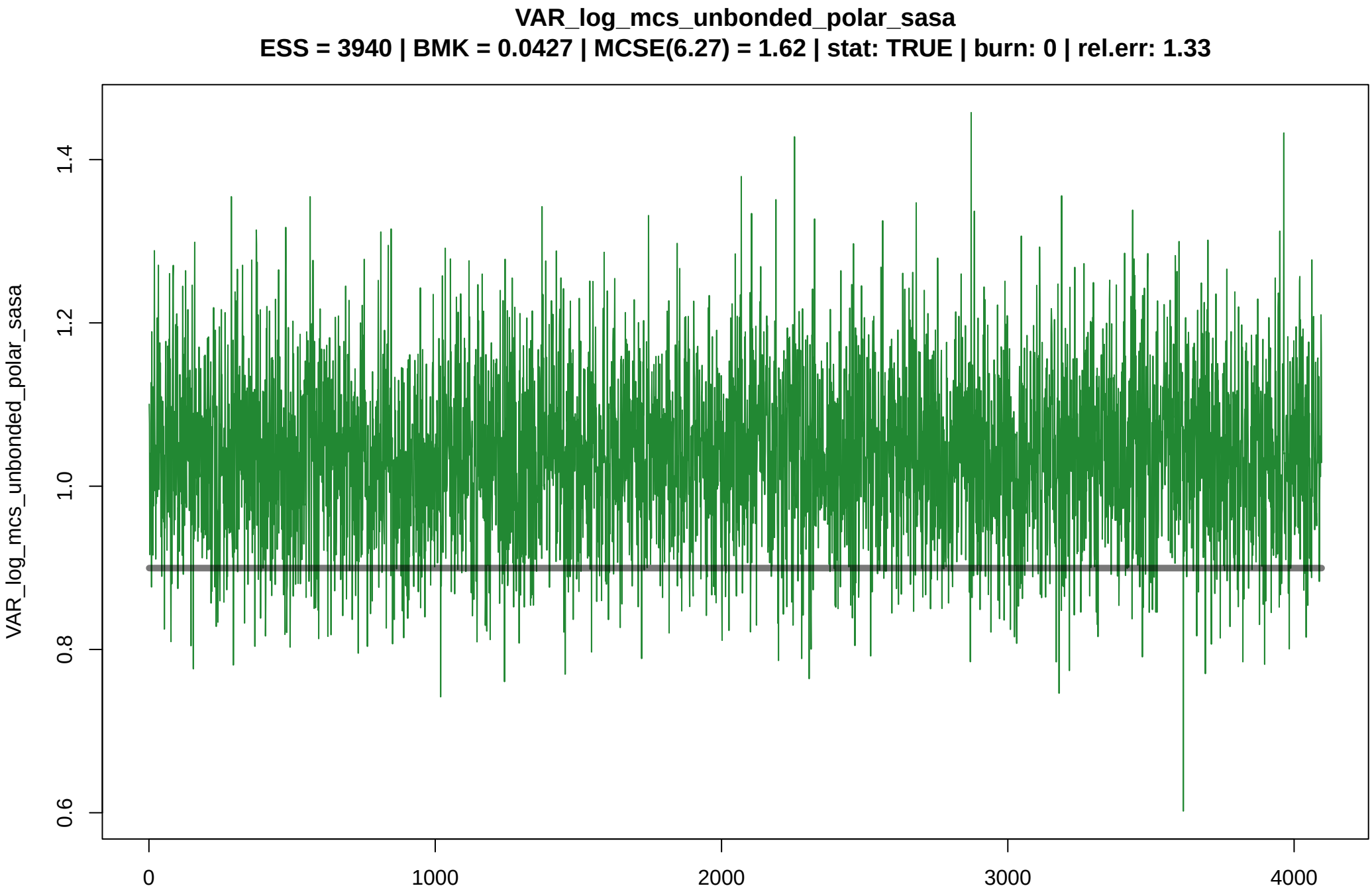

MEAN_log_RMSD
ESS = 4100 | BMK = 0.0342 | MCSE(6.27) = 1.45 | stat: TRUE | burn: 0 | rel.err: −0.583
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
1000
2000
3000
4000

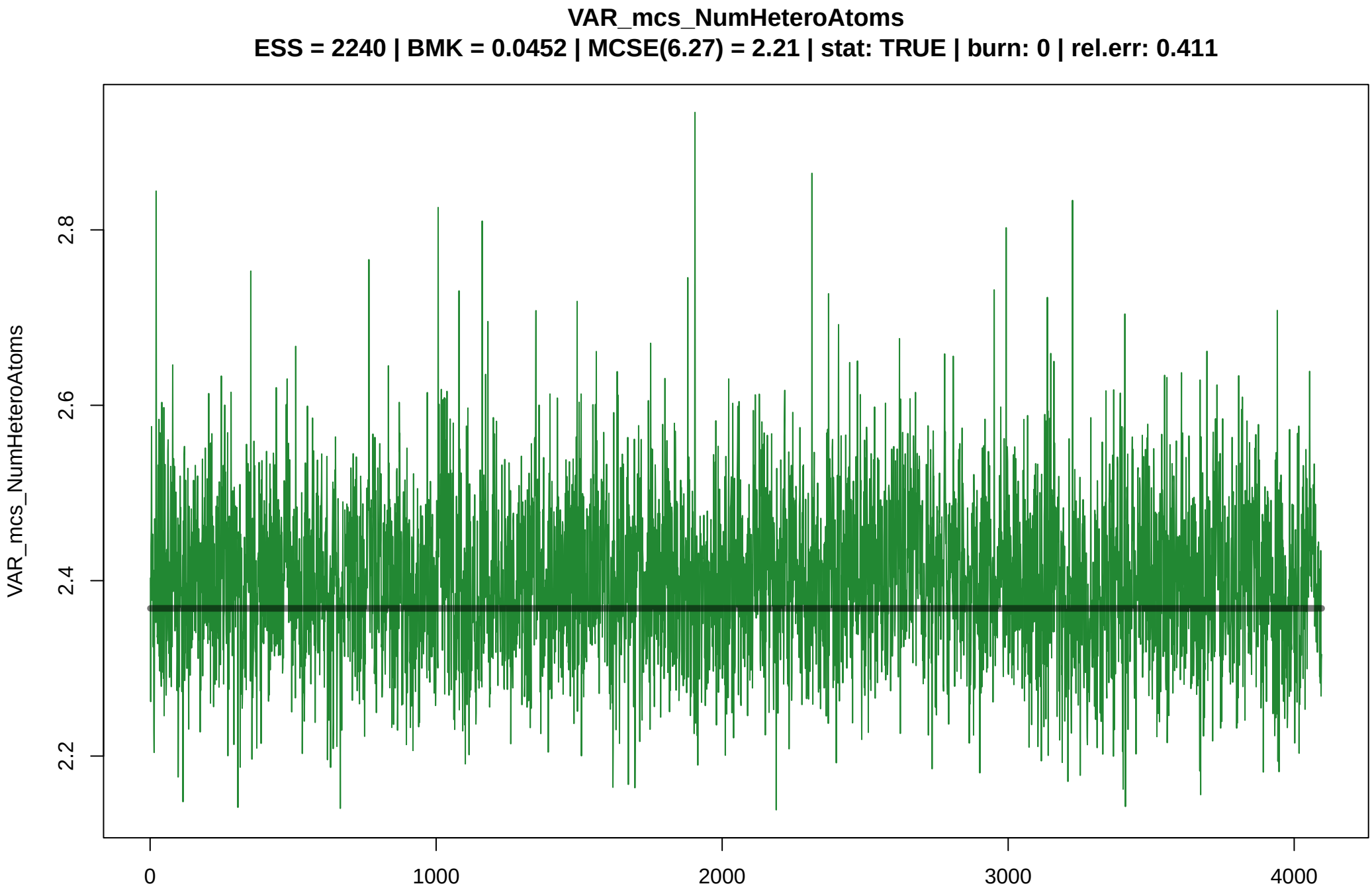

MEAN_log_mcs_unbonded_polar_sasa
ESS = 3750 | BMK = 0.0269 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0 | rel.err: −0.204
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
1000
2000
3000
4000

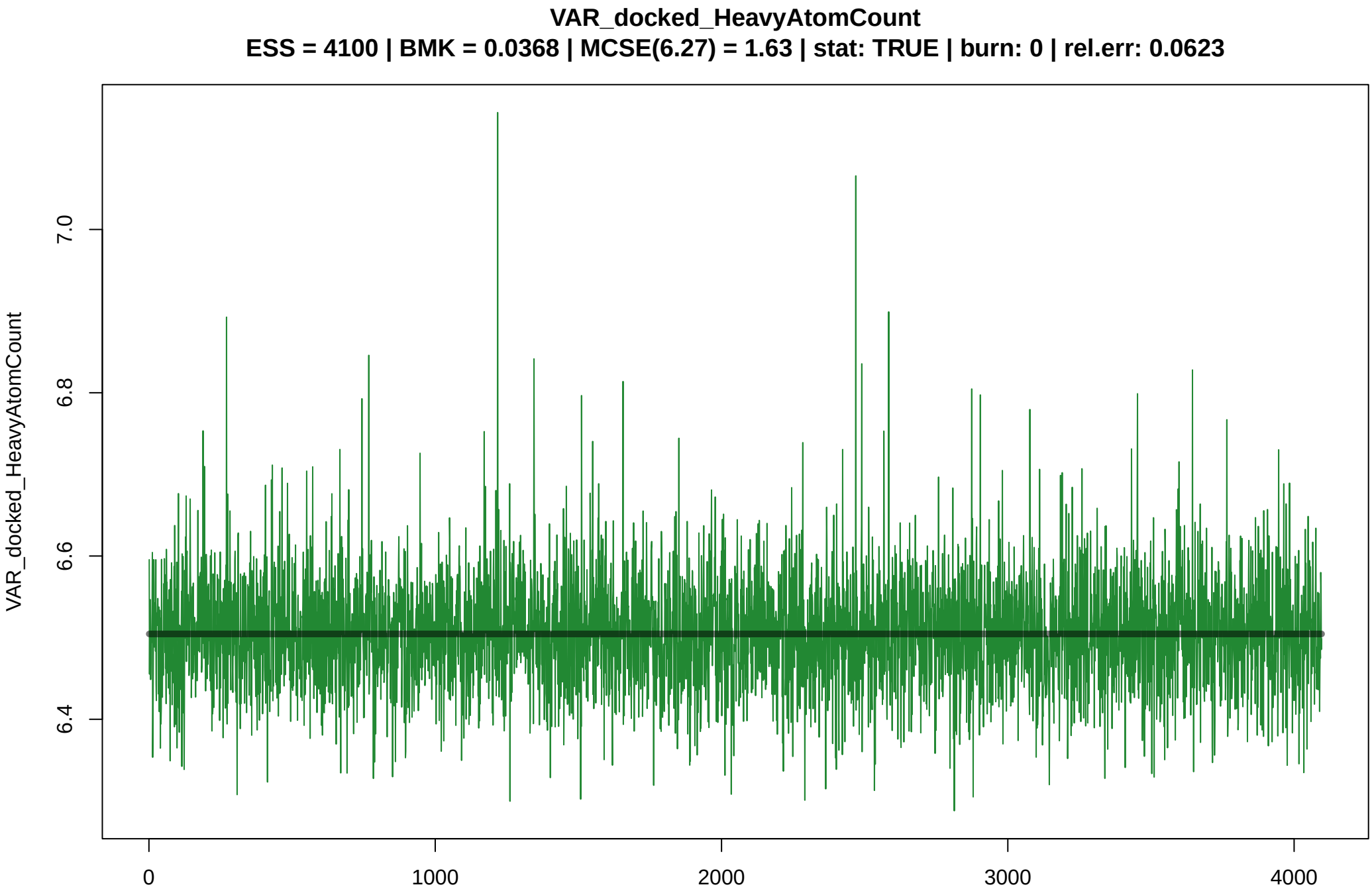

MEAN_mcs_NumHeteroAtoms
ESS = 4100 | BMK = 0.0294 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: 0.498
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
1000
2000
3000
4000

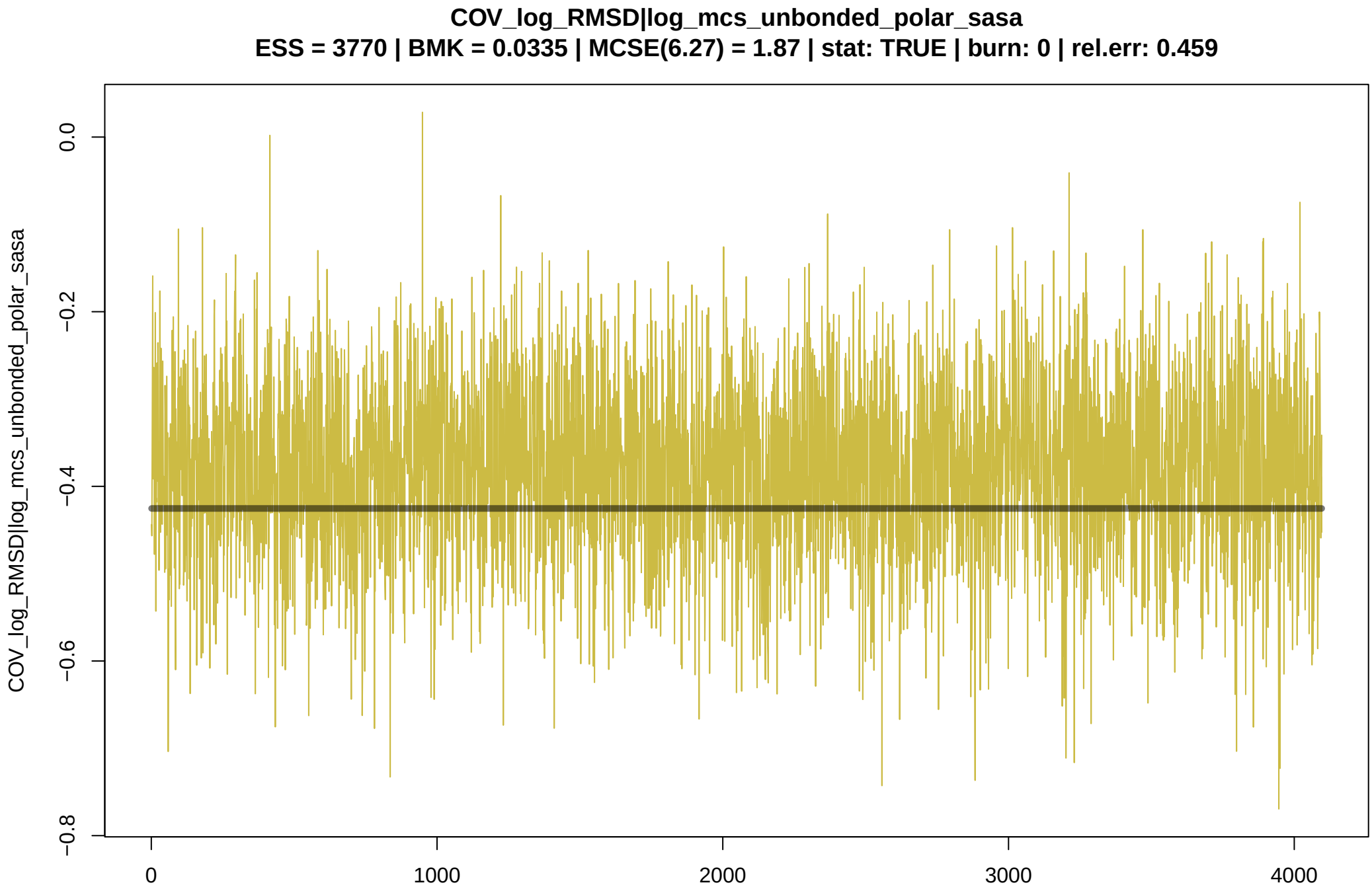

MEAN_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0335 | MCSE(6.27) = 1.58 | stat: TRUE | burn: 0 | rel.err: 0.539
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
1000
2000
3000
4000

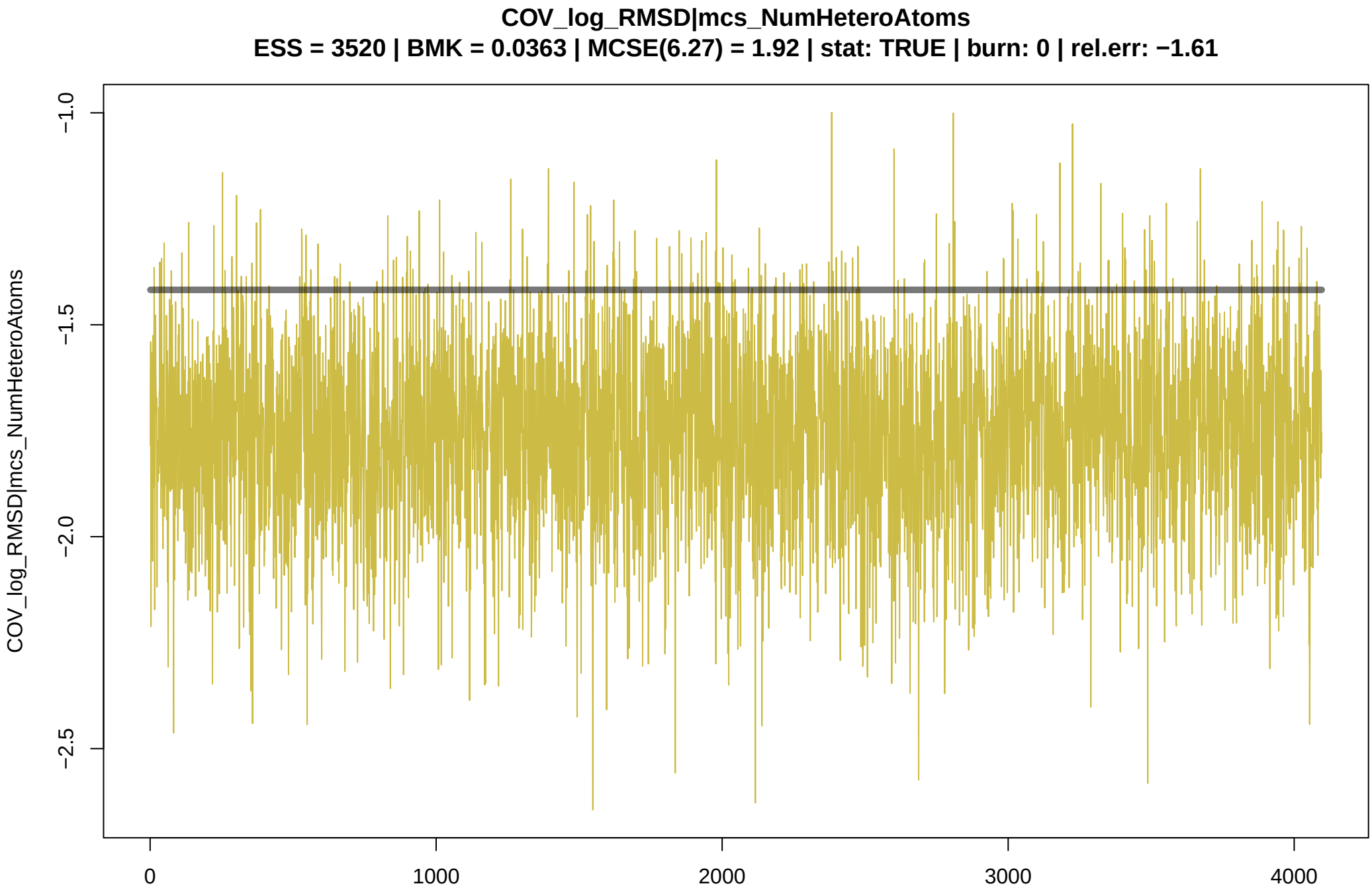

VAR_log_RMSD
ESS = 3860 | BMK = 0.0302 | MCSE(6.27) = 1.57 | stat: TRUE | burn: 0 | rel.err: 2.26
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
0
1000
2000
3000
4000

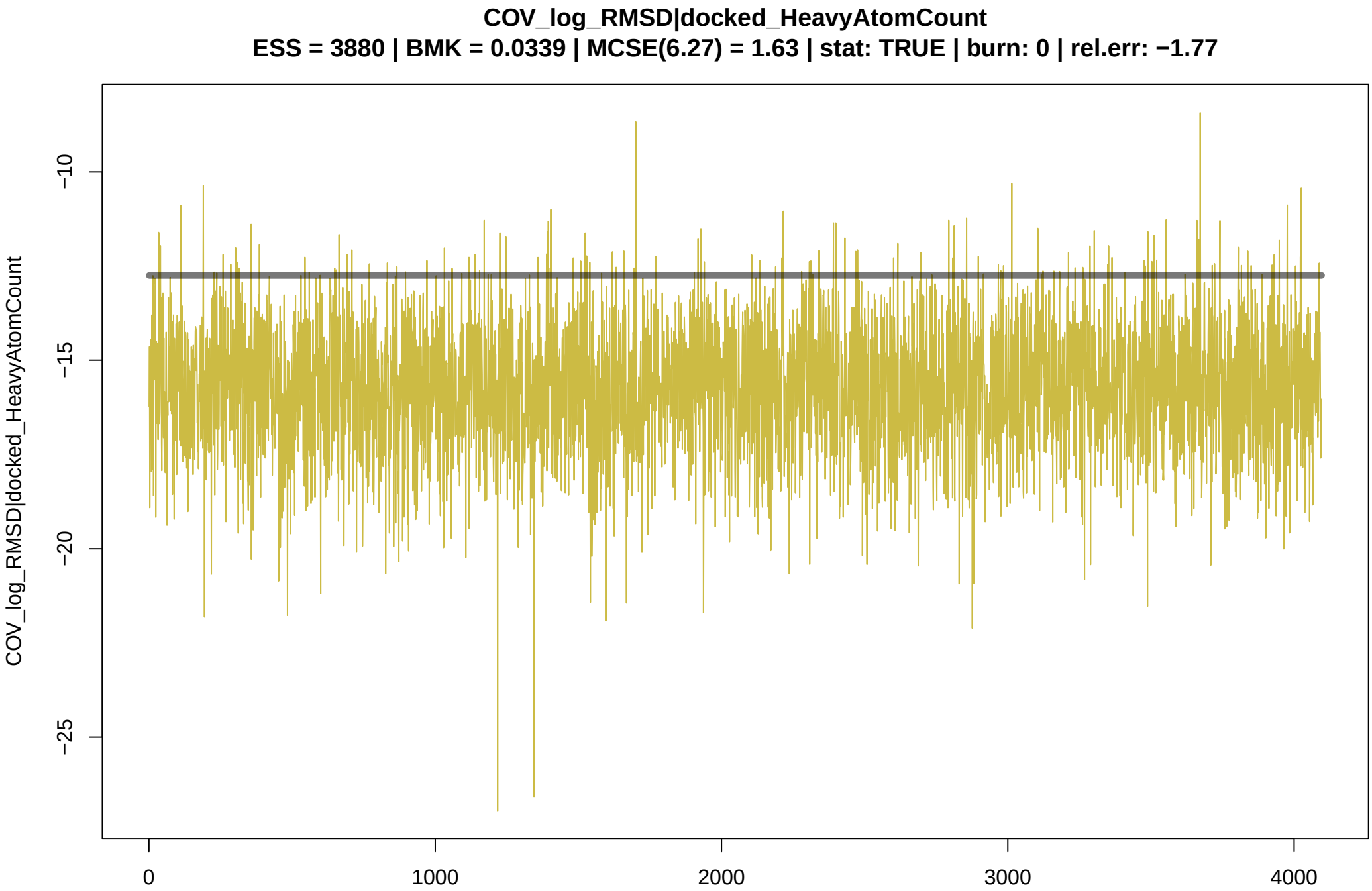

VAR_log_mcs_unbonded_polar_sasa
ESS = 3940 | BMK = 0.0427 | MCSE(6.27) = 1.62 | stat: TRUE | burn: 0 | rel.err: 1.33
VAR_log_mcs_unbonded_polar_sasa
0.6
0.8
1.0
1.2
1.4
0
1000
2000
3000
4000

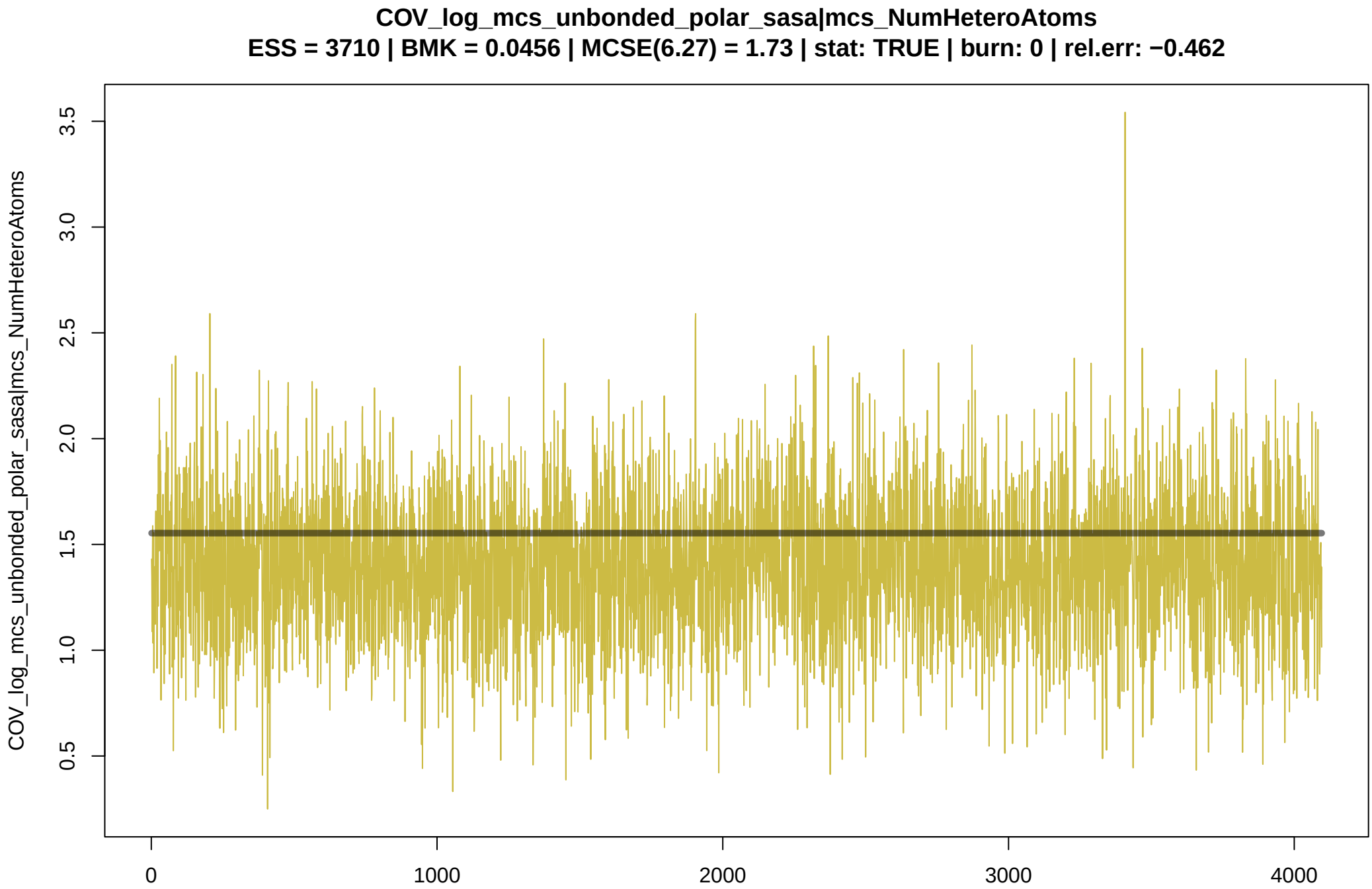

VAR_mcs_NumHeteroAtoms
ESS = 2240 | BMK = 0.0452 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: 0.411
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
1000
2000
3000
4000

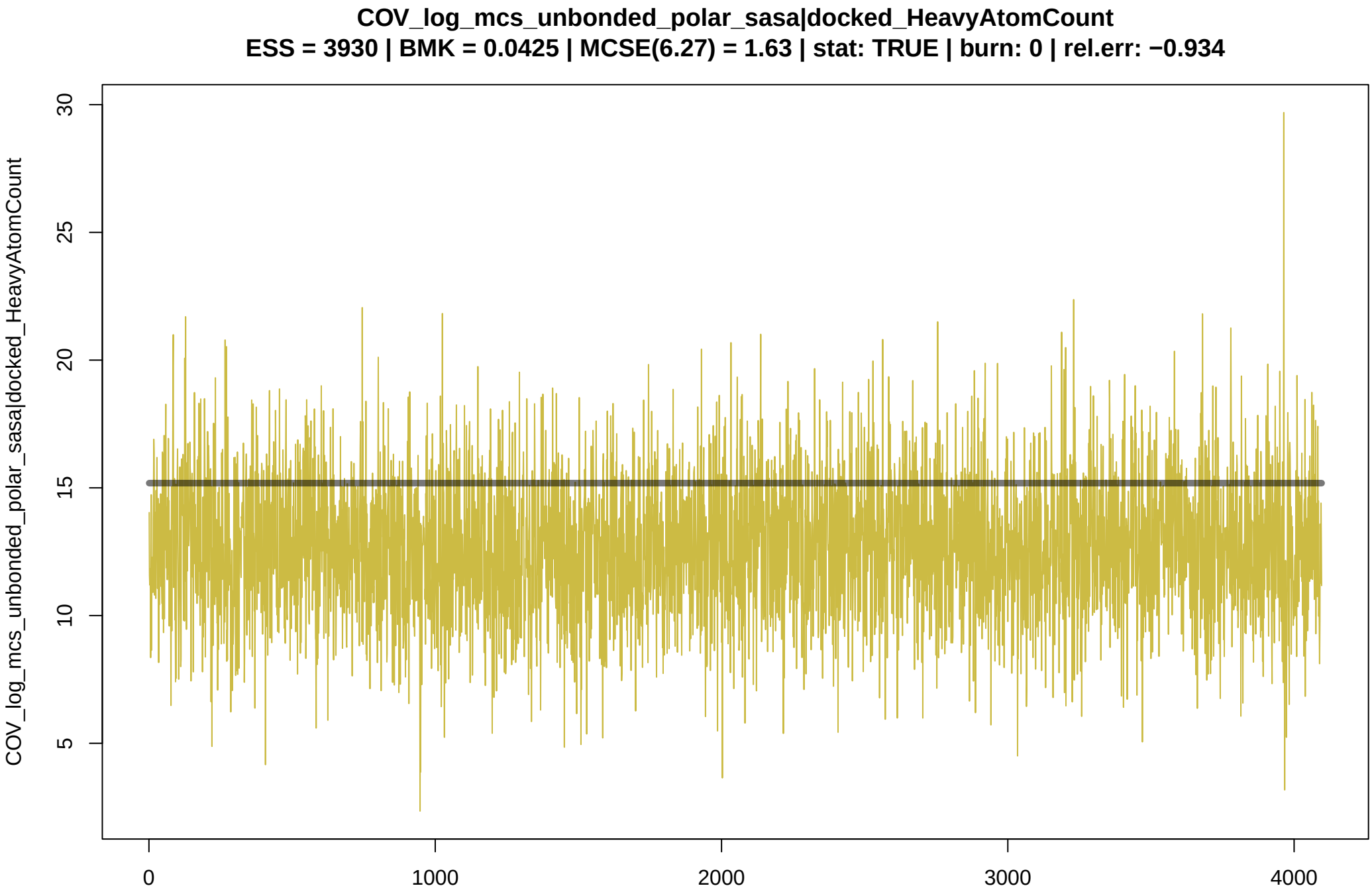

VAR_docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0368 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: 0.0623
VAR_docked_HeavyAtomCount
6.4
6.6
6.8
7.0
0
1000
2000
3000
4000

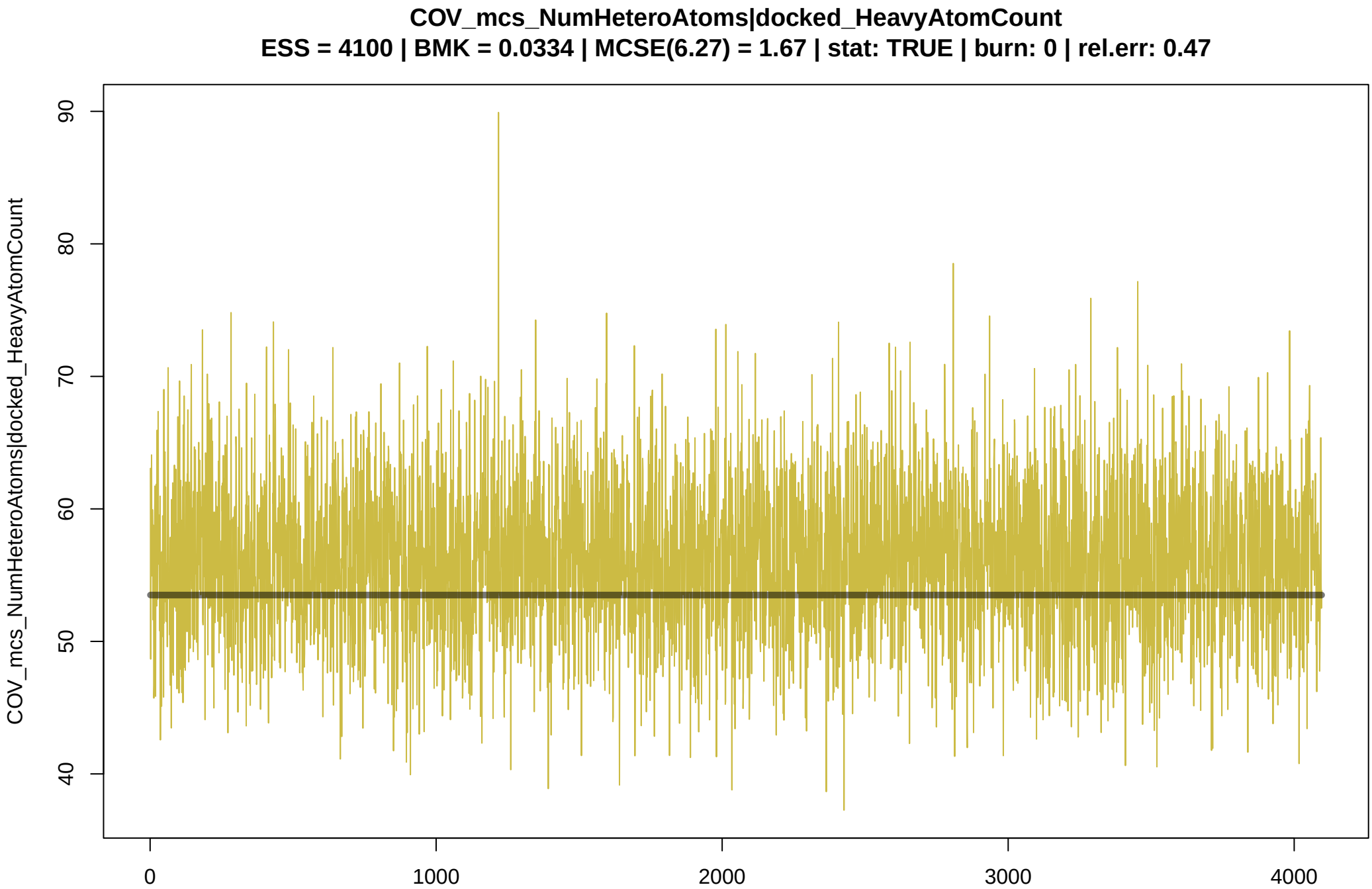

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 3770 | BMK = 0.0335 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0 | rel.err: 0.459
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
1000
2000
3000
4000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 3520 | BMK = 0.0363 | MCSE(6.27) = 1.92 | 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 = 3880 | BMK = 0.0339 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: −1.77
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
−25
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 3710 | BMK = 0.0456 | MCSE(6.27) = 1.73 | stat: TRUE | burn: 0 | rel.err: −0.462
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
1000
2000
3000
4000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 3930 | BMK = 0.0425 | MCSE(6.27) = 1.63 | stat: TRUE | burn: 0 | rel.err: −0.934
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
25
30
0
1000
2000
3000
4000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 4100 | BMK = 0.0334 | MCSE(6.27) = 1.67 | stat: TRUE | burn: 0 | rel.err: 0.47
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
90
80
70
60
50
40
0
1000
2000
3000
4000