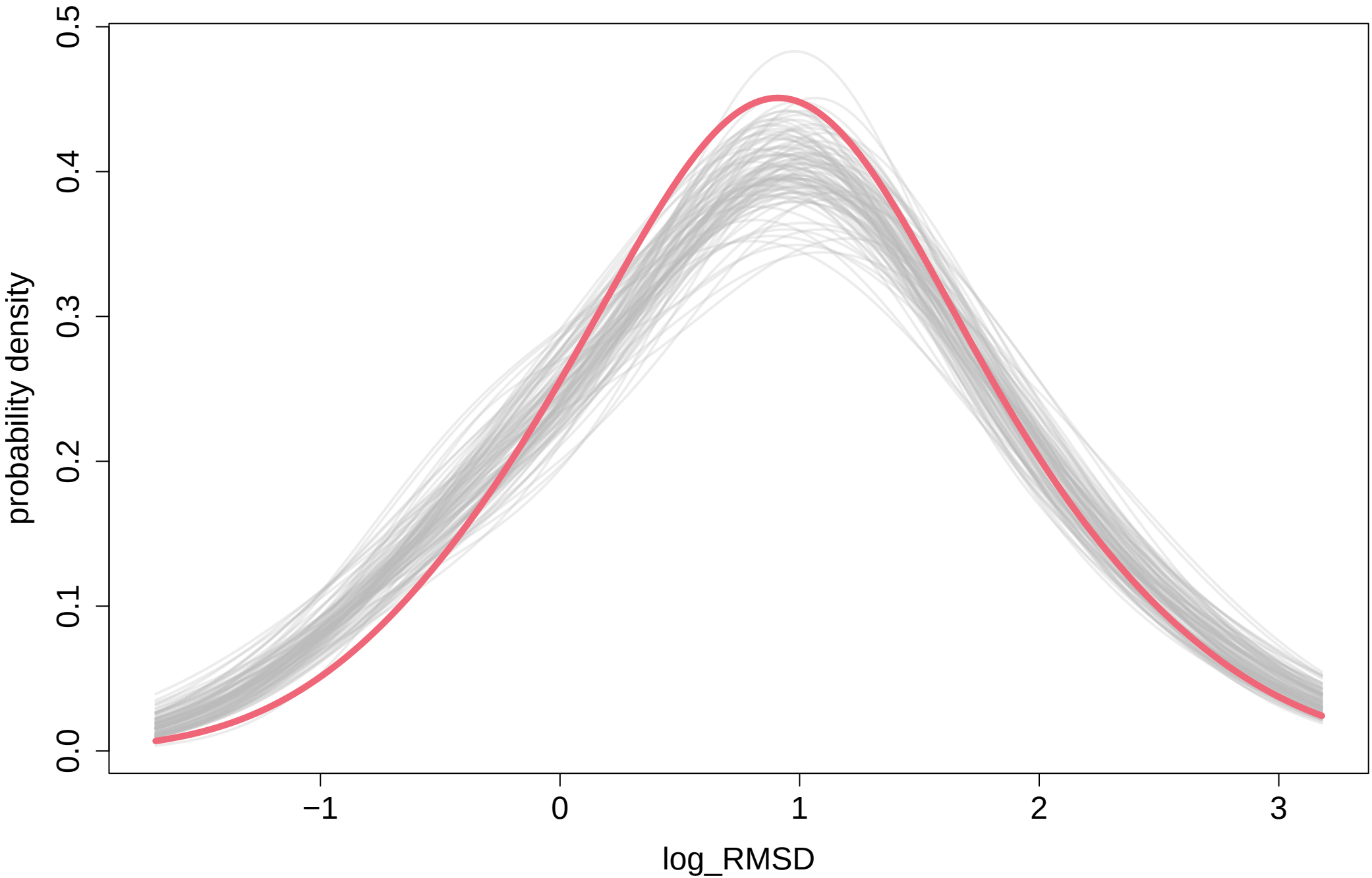
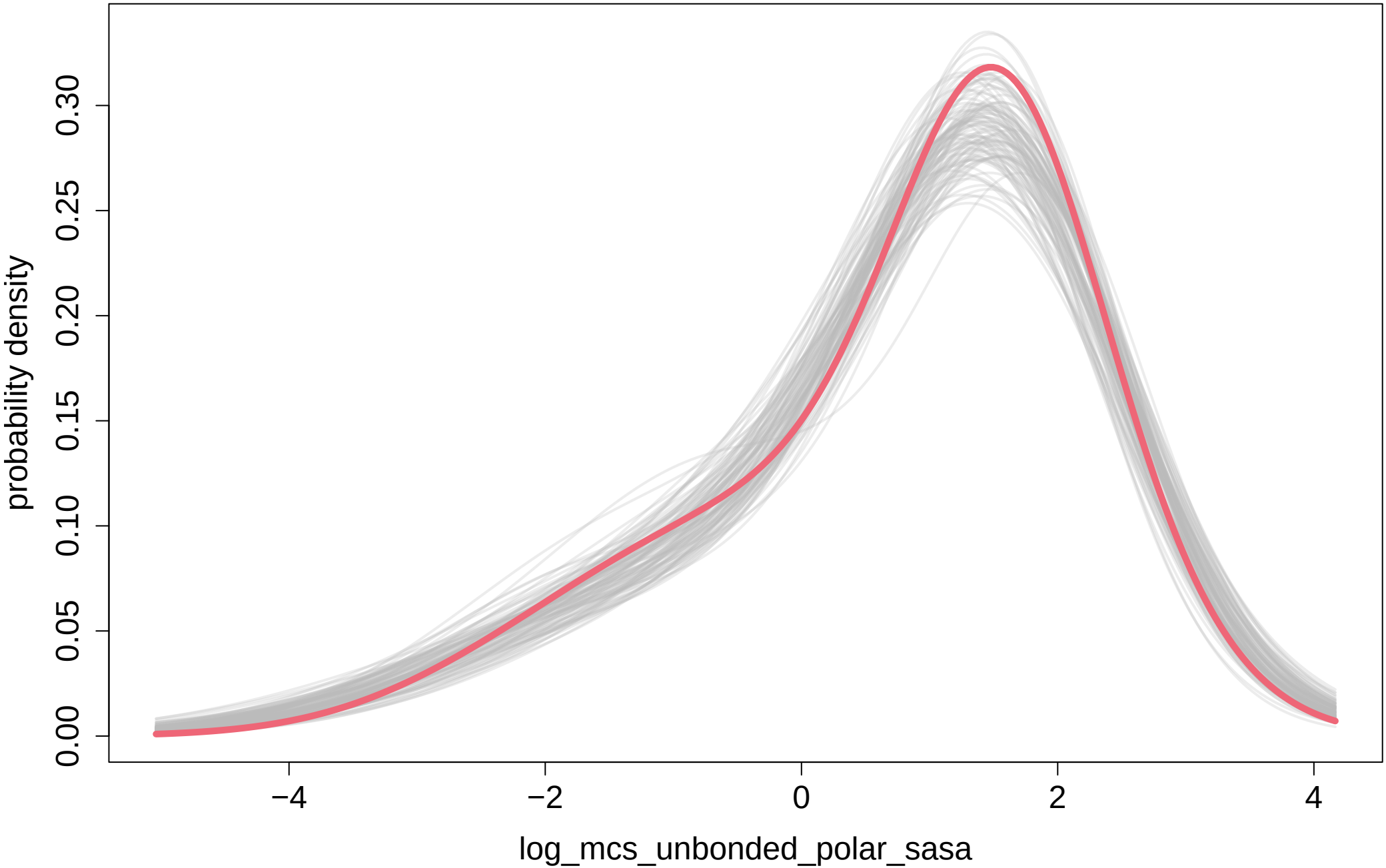
−− STATS maxD −−
min ESS = 89.6990708555492
max BMK = 0.200202958664143
max MCSE = 7.53735477798681
all stationary: FALSE
burn: 0
max rel.err.: 1.97506187737163

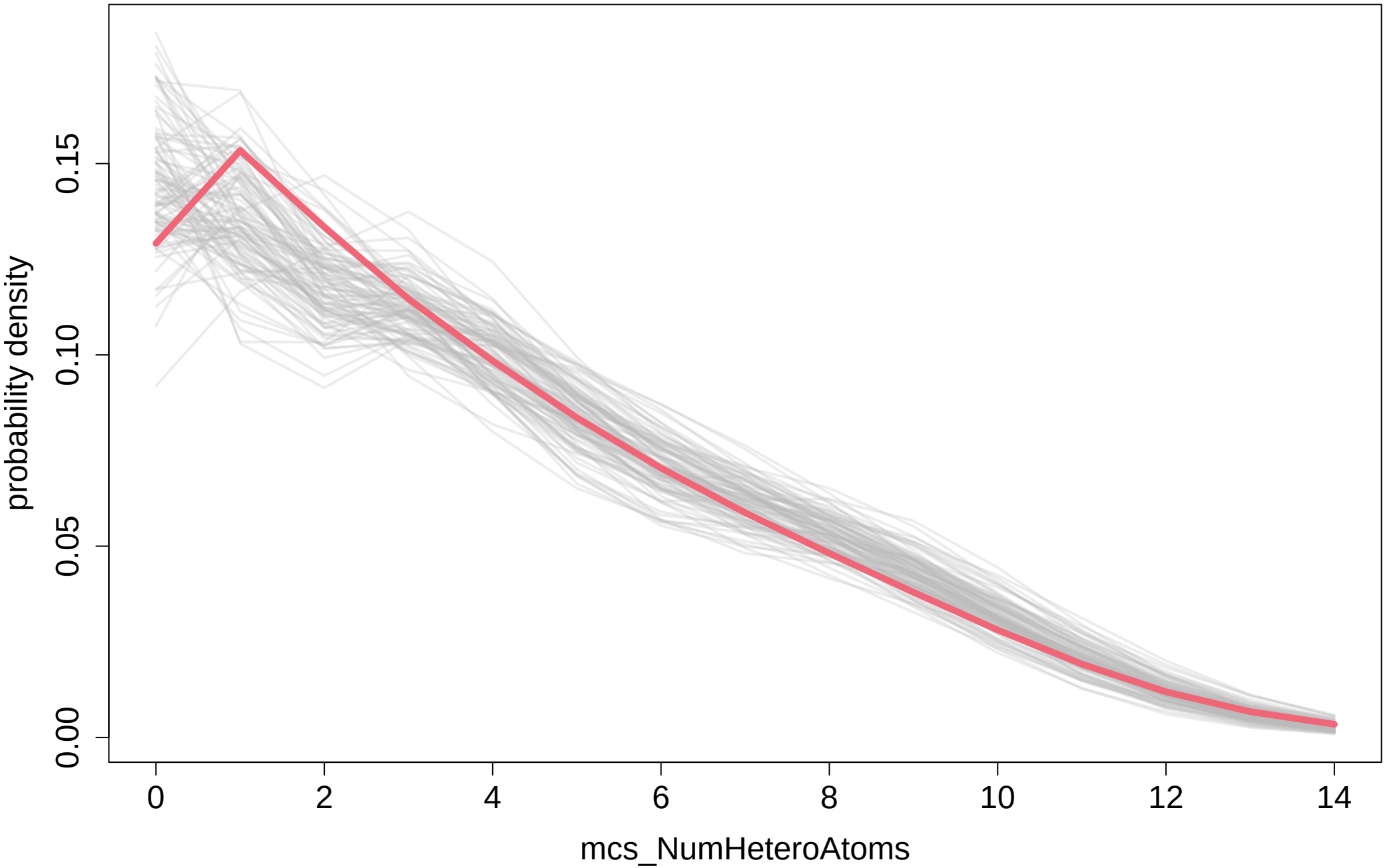
−− STATS 2D −−
min ESS = 1916.20998852591
max BMK = 0.057997553898631 9
max MCSE = 2.35780368374424
all stationary: TRUE
burn: 0
max rel.err.: 1.75389247527219

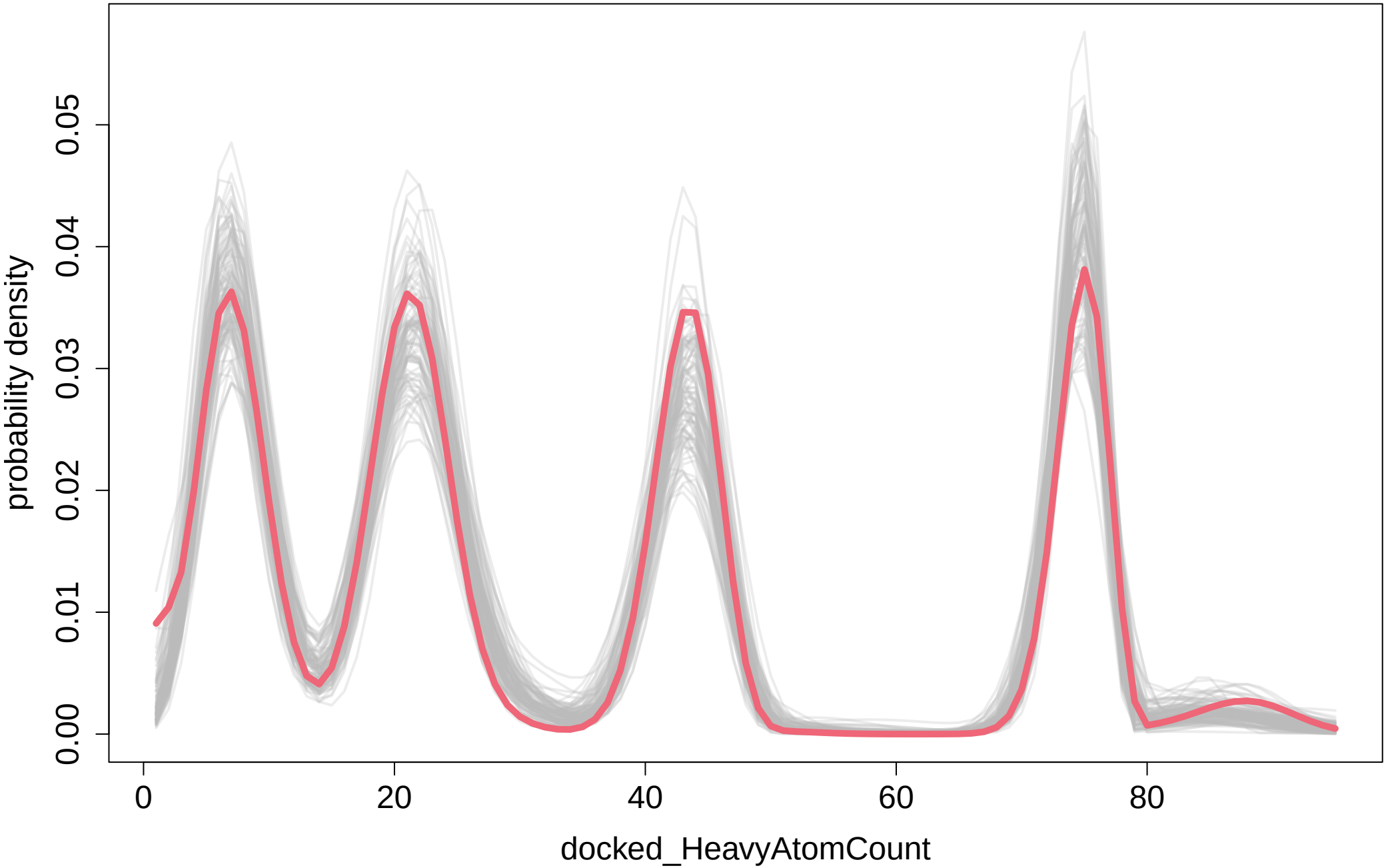
−− STATS 1D −−
min ESS = 1449.75257549958
max BMK = 0.0642273980405469
max MCSE = 2.57837260423432
all stationary: TRUE
burn: 0
max rel.err.: 2.2449346860115

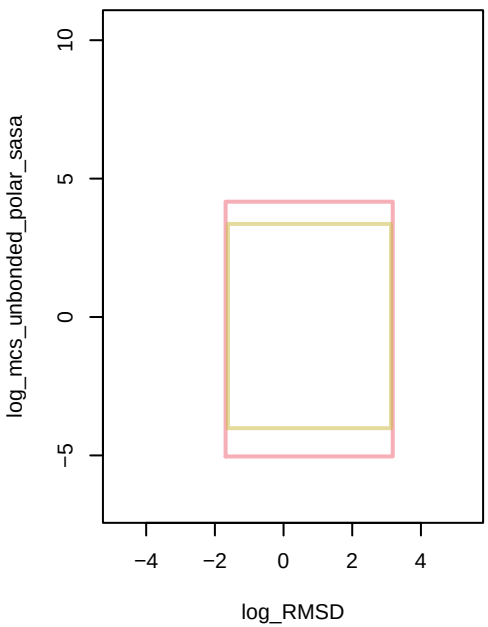
Occupied clusters: 9 of 16
LL: −2158.85943952113 sd: 6.63087563089868

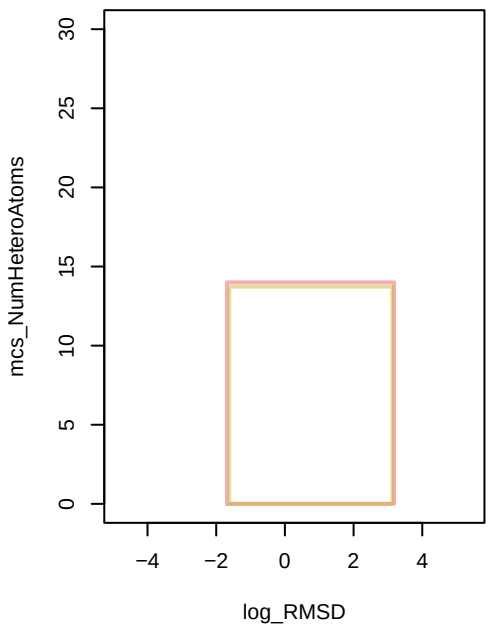

probability density
0.0
0.1
0.2
0.3
0.4
0.5
−1
0
1
2
3
log_RMSD

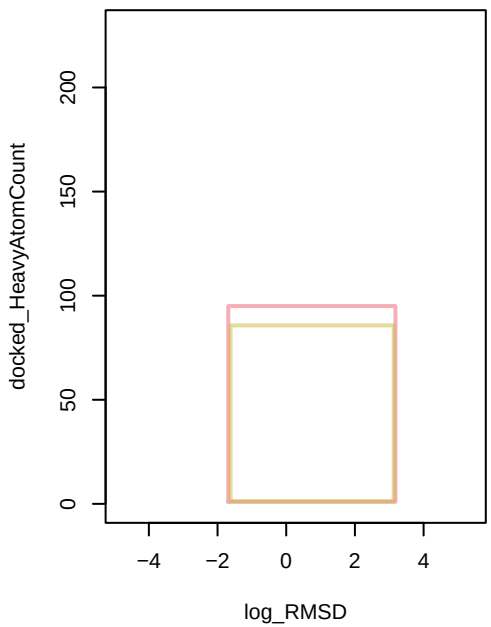

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
−4
−2
0
2
4
log_mcs_unbonded_polar_sasa

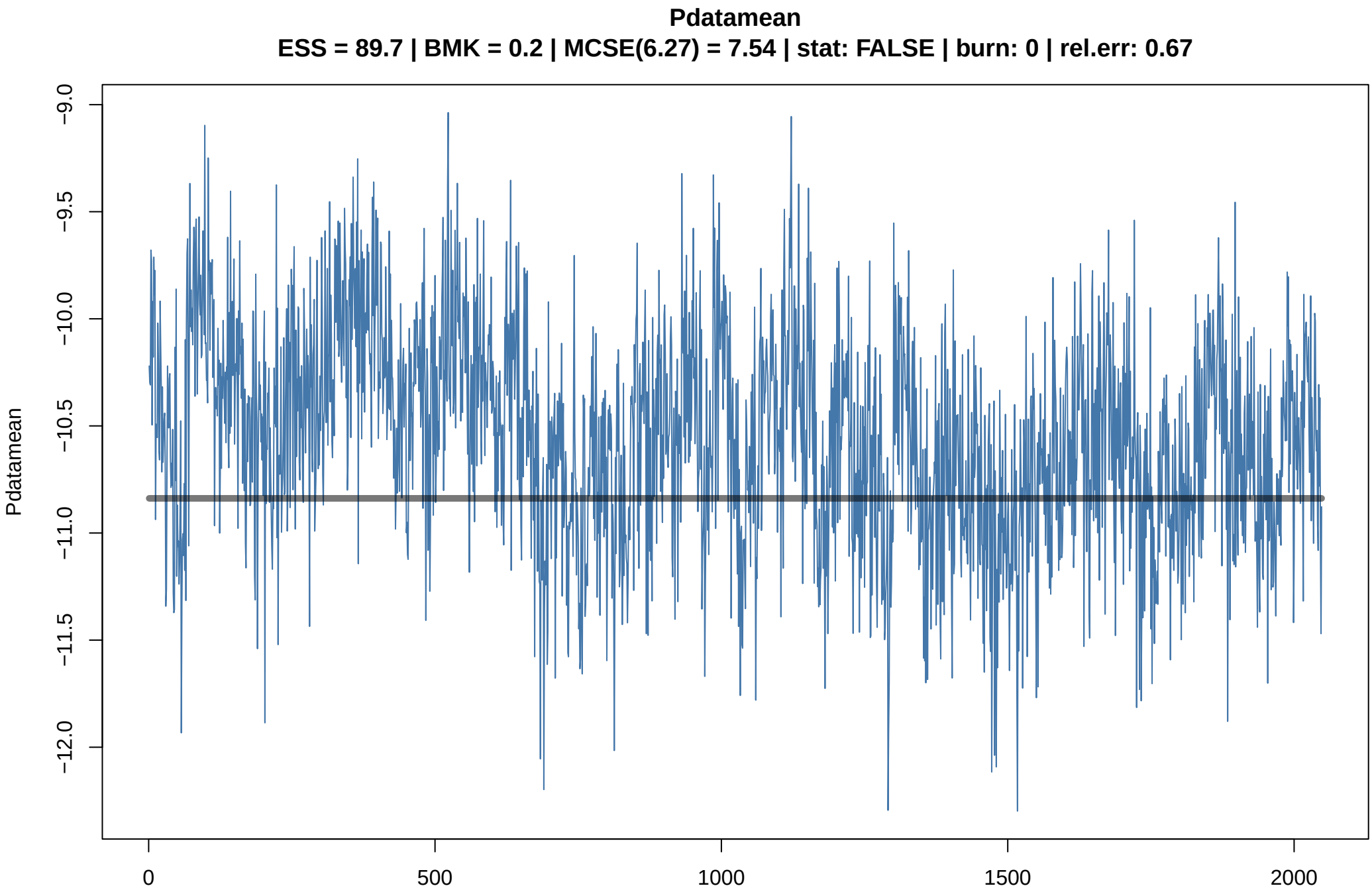

probability density
0.00
0.05
0.10
0.15
0
2
4
6
8
10
12
14
mcs_NumHeteroAtoms

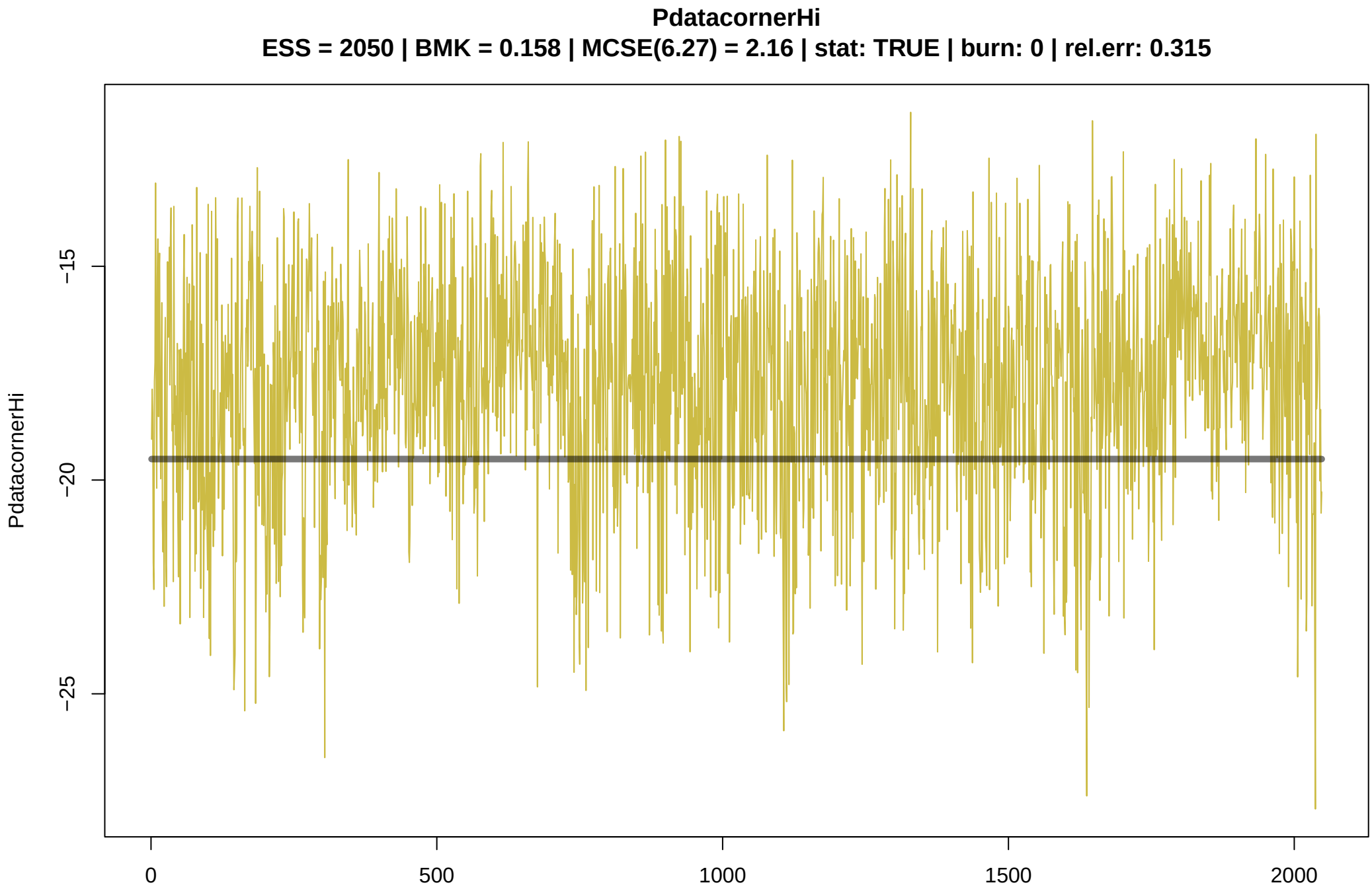

probability density
0.00
0.01
0.02
0.03
0.04
0.05
0
20
40
60
80
docked_HeavyAtomCount

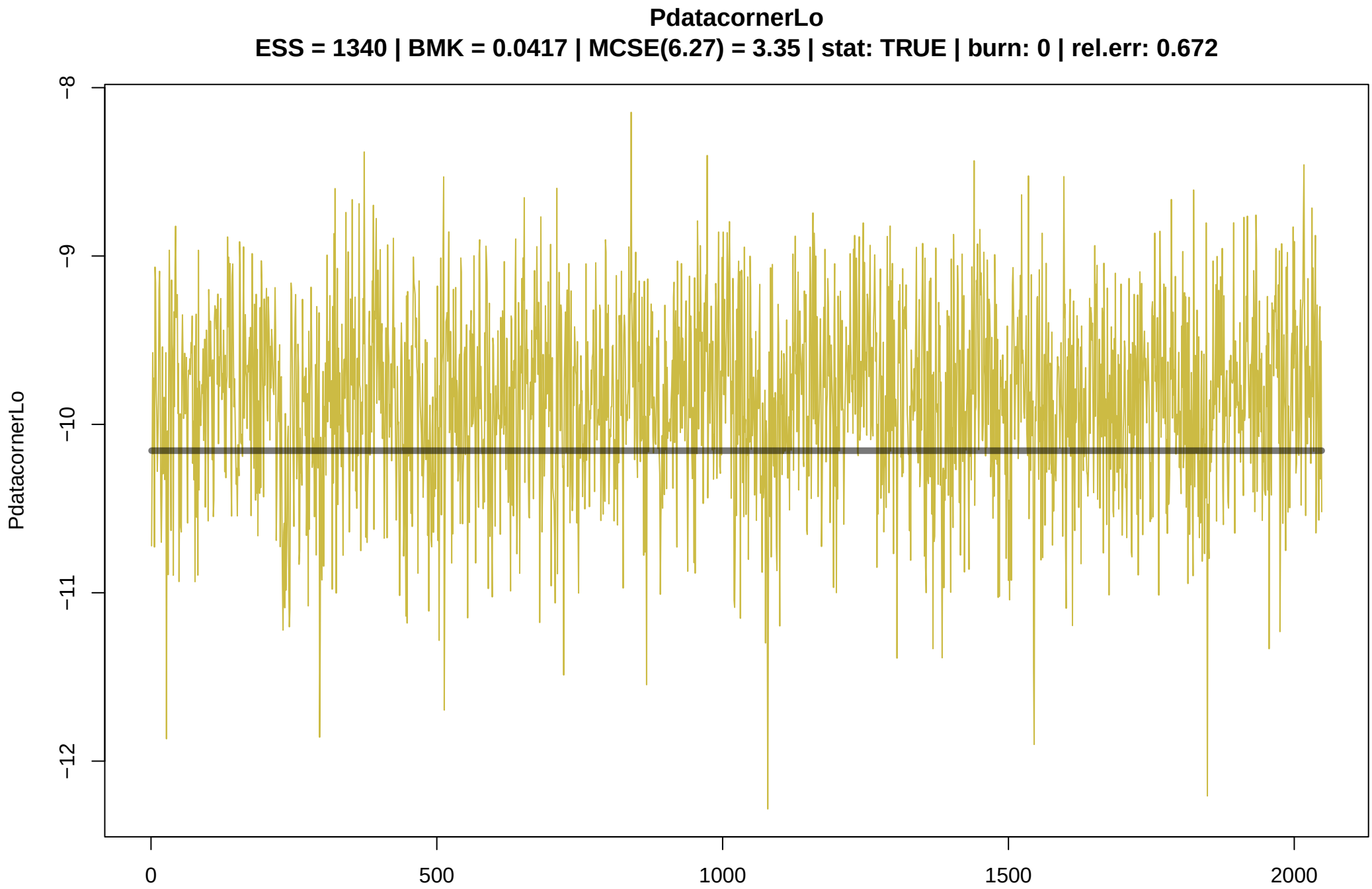

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
log_RMSD

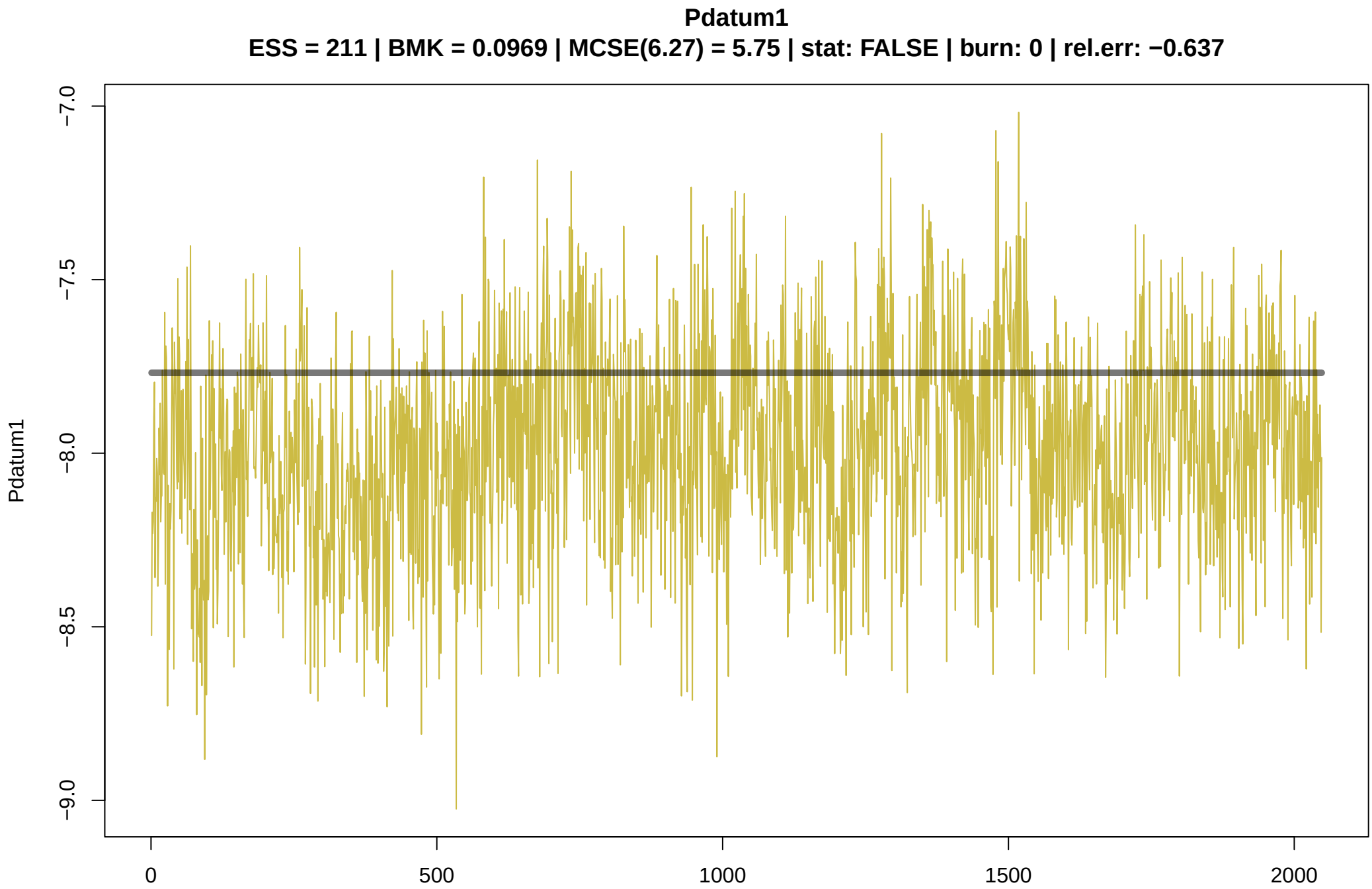

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
log_RMSD

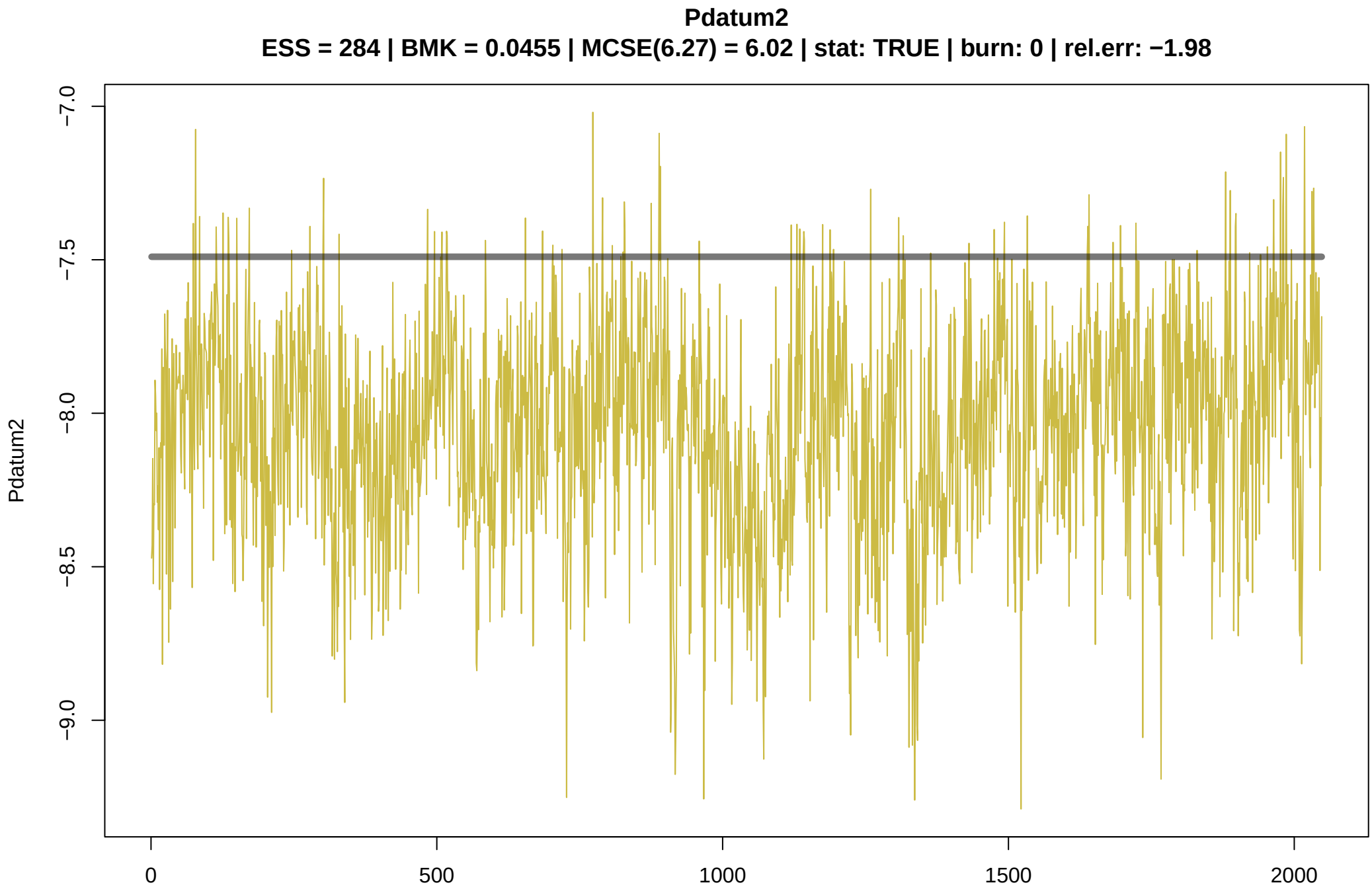

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
log_RMSD

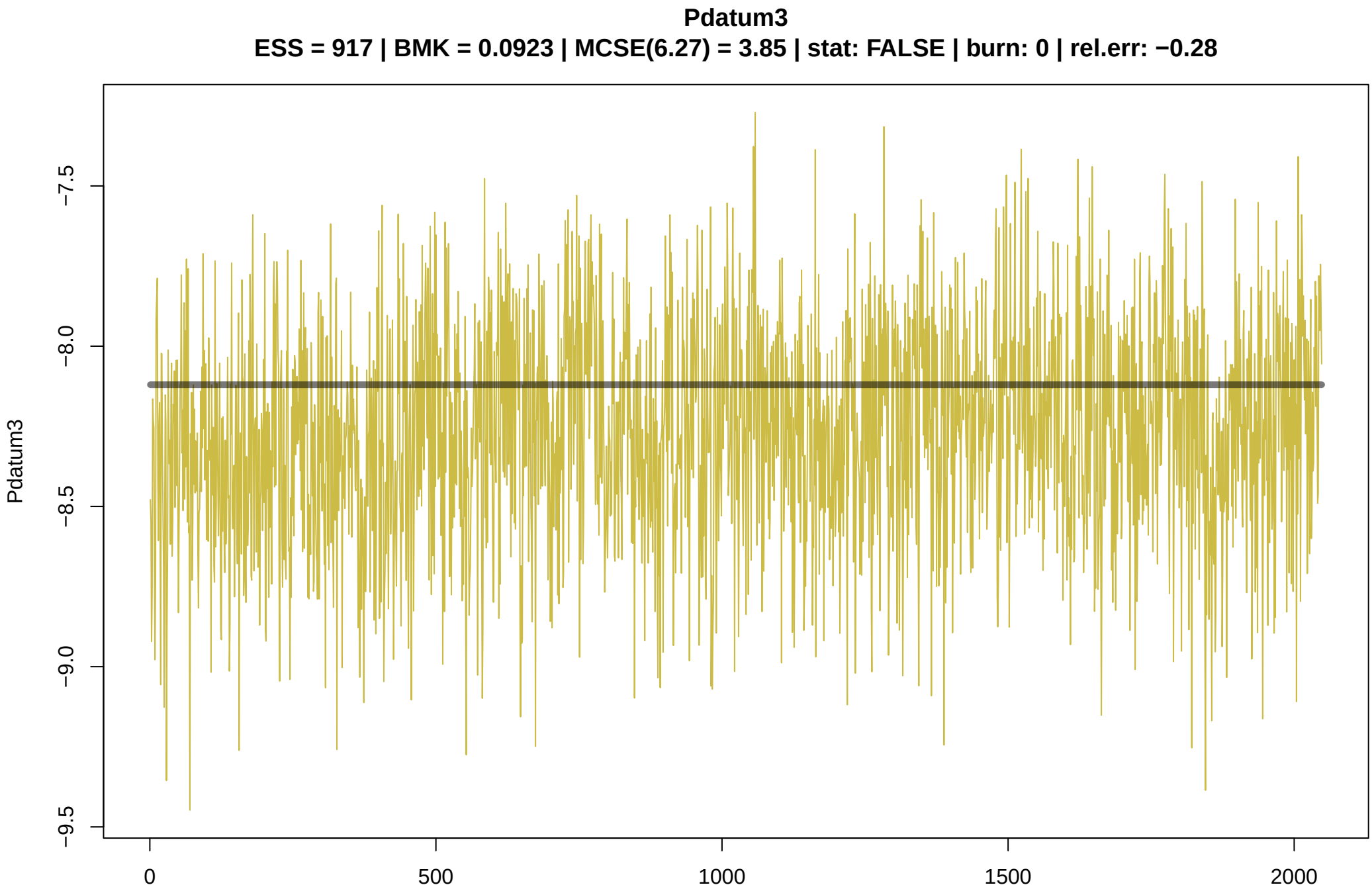

Pdatamean
ESS = 89.7 | BMK = 0.2 | MCSE(6.27) = 7.54 | stat: FALSE | burn: 0 | rel.err: 0.67
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

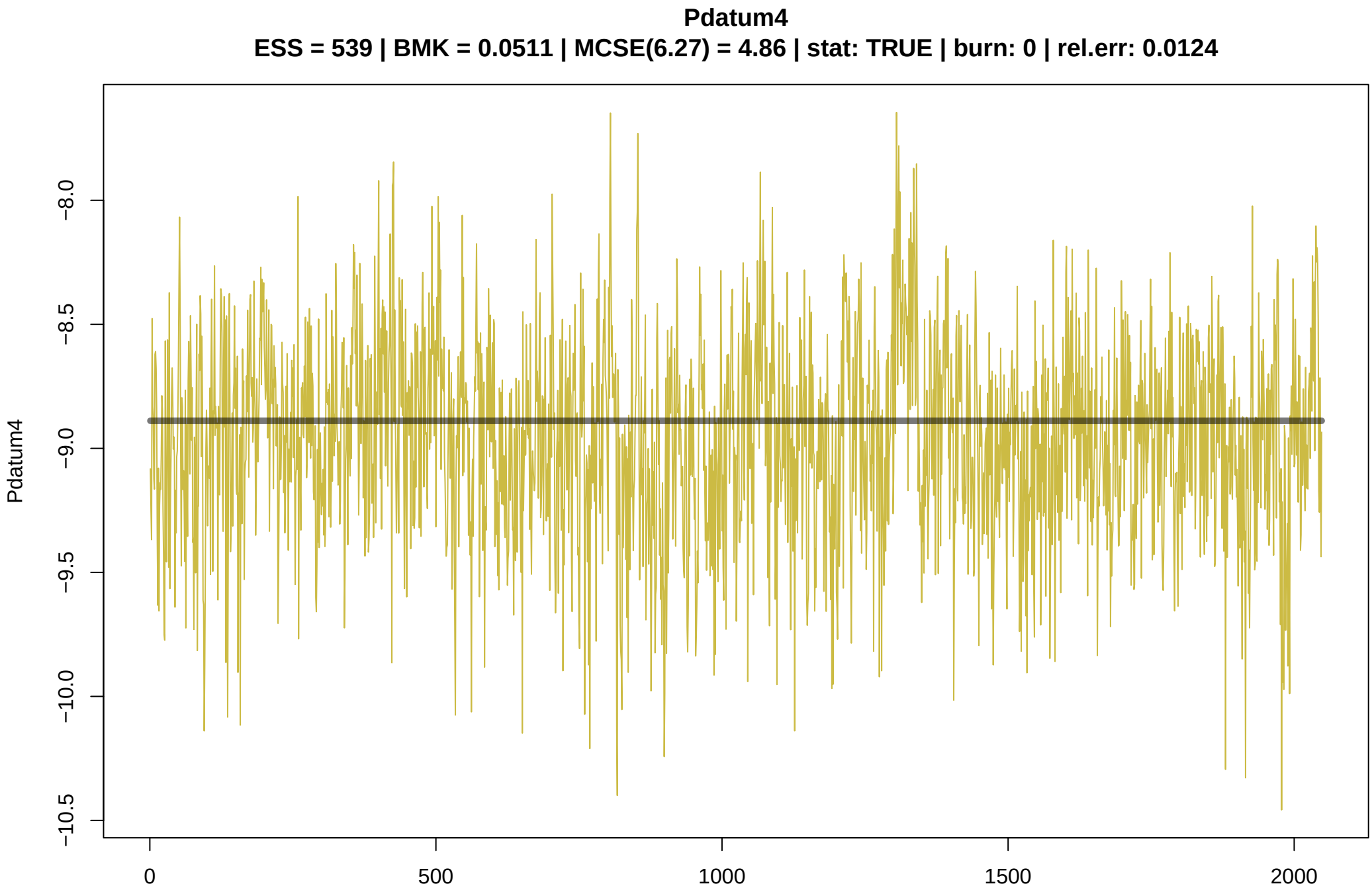

PdatacornerHi
ESS = 2050 | BMK = 0.158 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | rel.err: 0.315
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

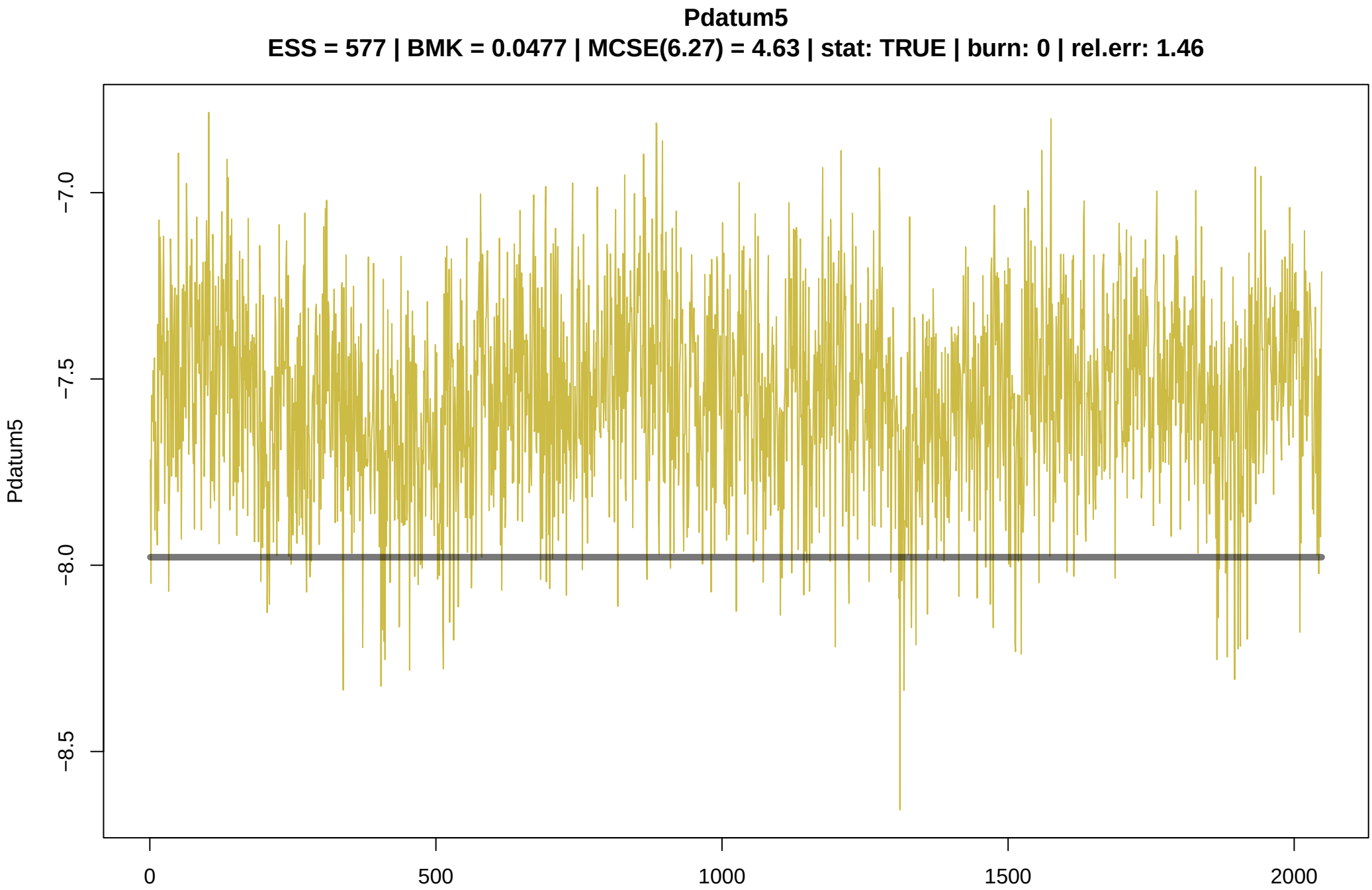

PdatacornerLo
ESS = 1340 | BMK = 0.0417 | MCSE(6.27) = 3.35 | stat: TRUE | burn: 0 | rel.err: 0.672
PdatacornerLo
−8
−9
−10
−11
−12
0
500
1000
1500
2000

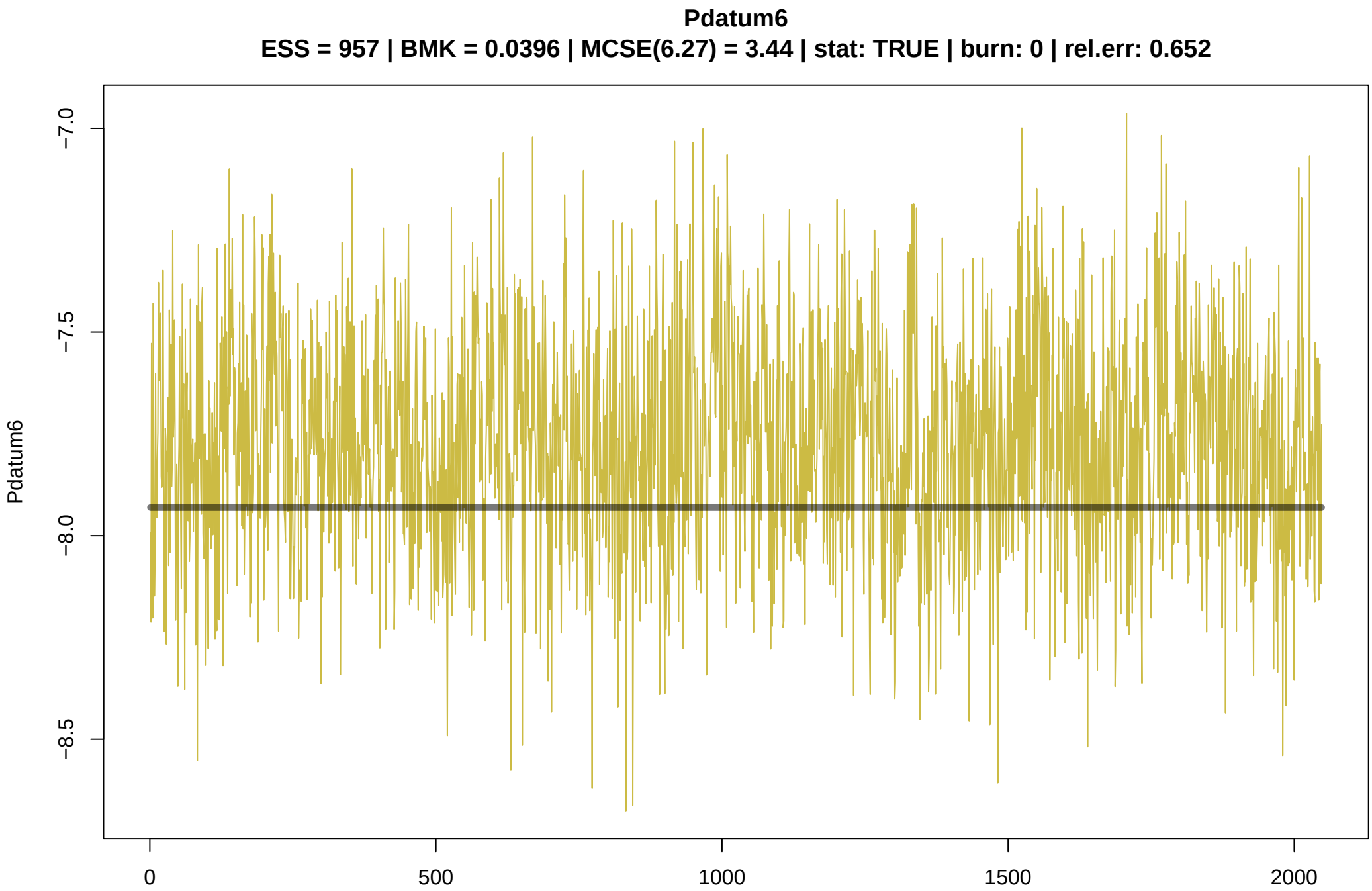

Pdatum1
ESS = 211 | BMK = 0.0969 | MCSE(6.27) = 5.75 | stat: FALSE | burn: 0 | rel.err: −0.637
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

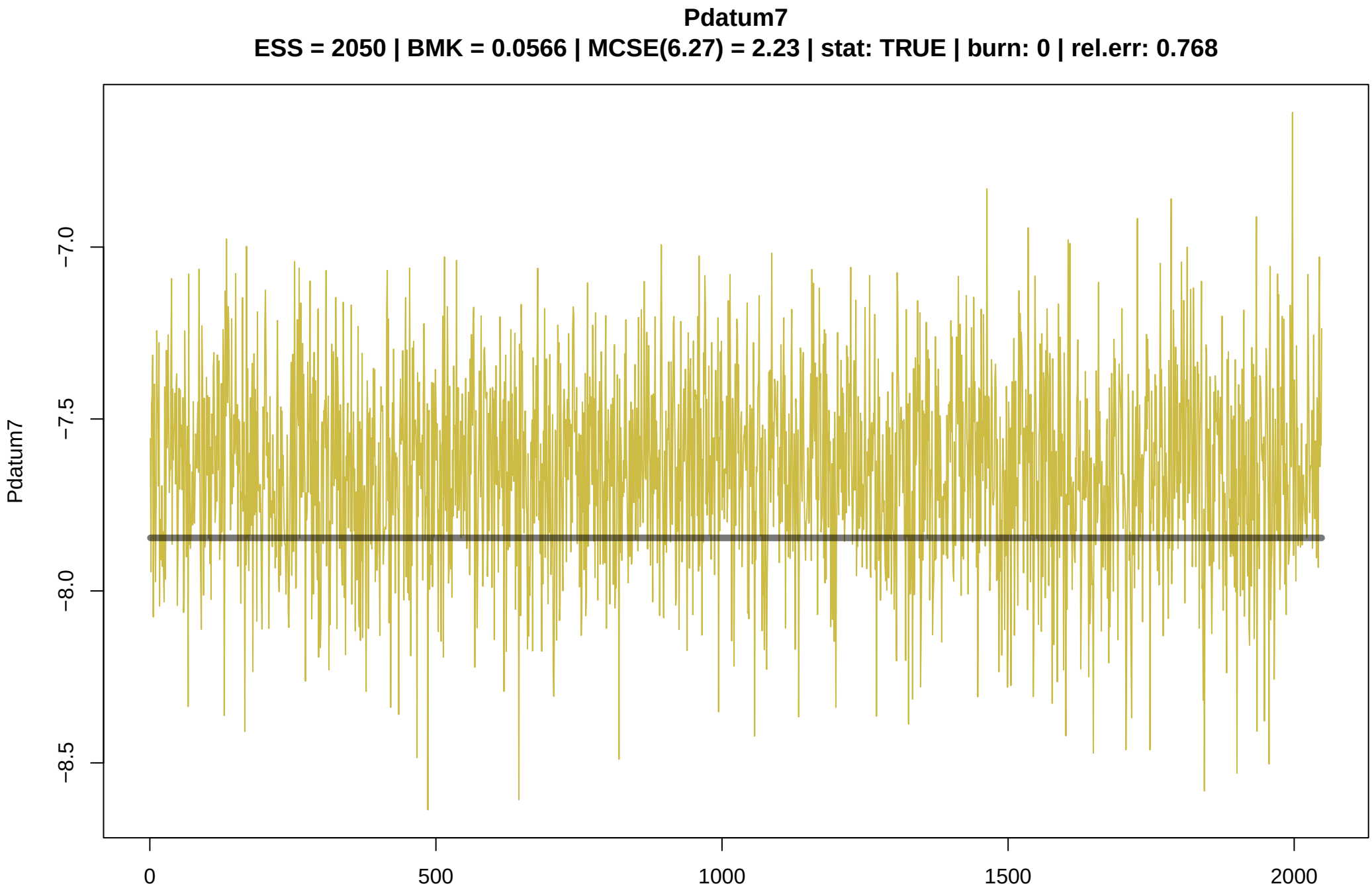

Pdatum2
ESS = 284 | BMK = 0.0455 | MCSE(6.27) = 6.02 | stat: TRUE | burn: 0 | rel.err: −1.98
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

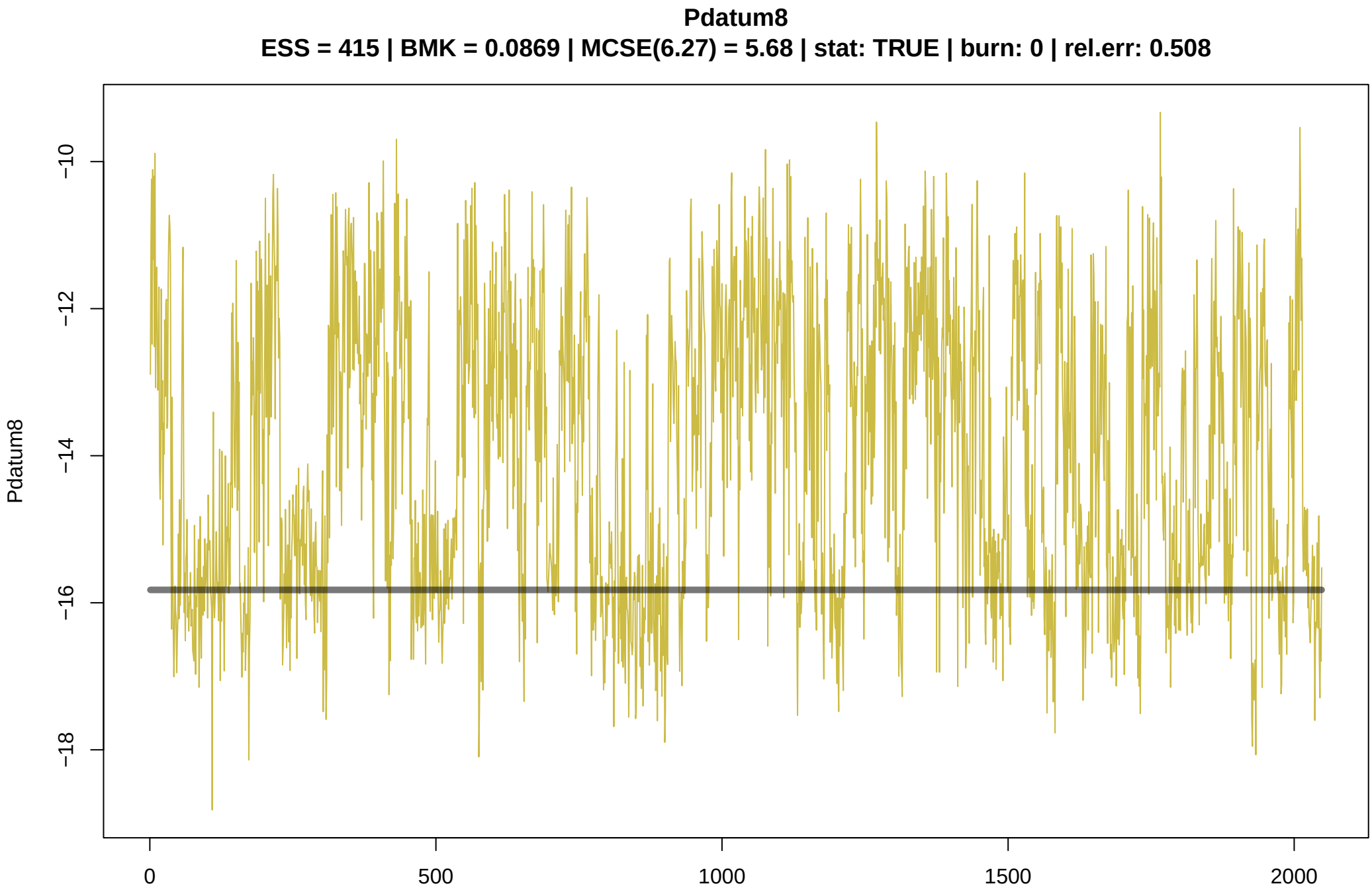

Pdatum3
ESS = 917 | BMK = 0.0923 | MCSE(6.27) = 3.85 | stat: FALSE | burn: 0 | rel.err: −0.28
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

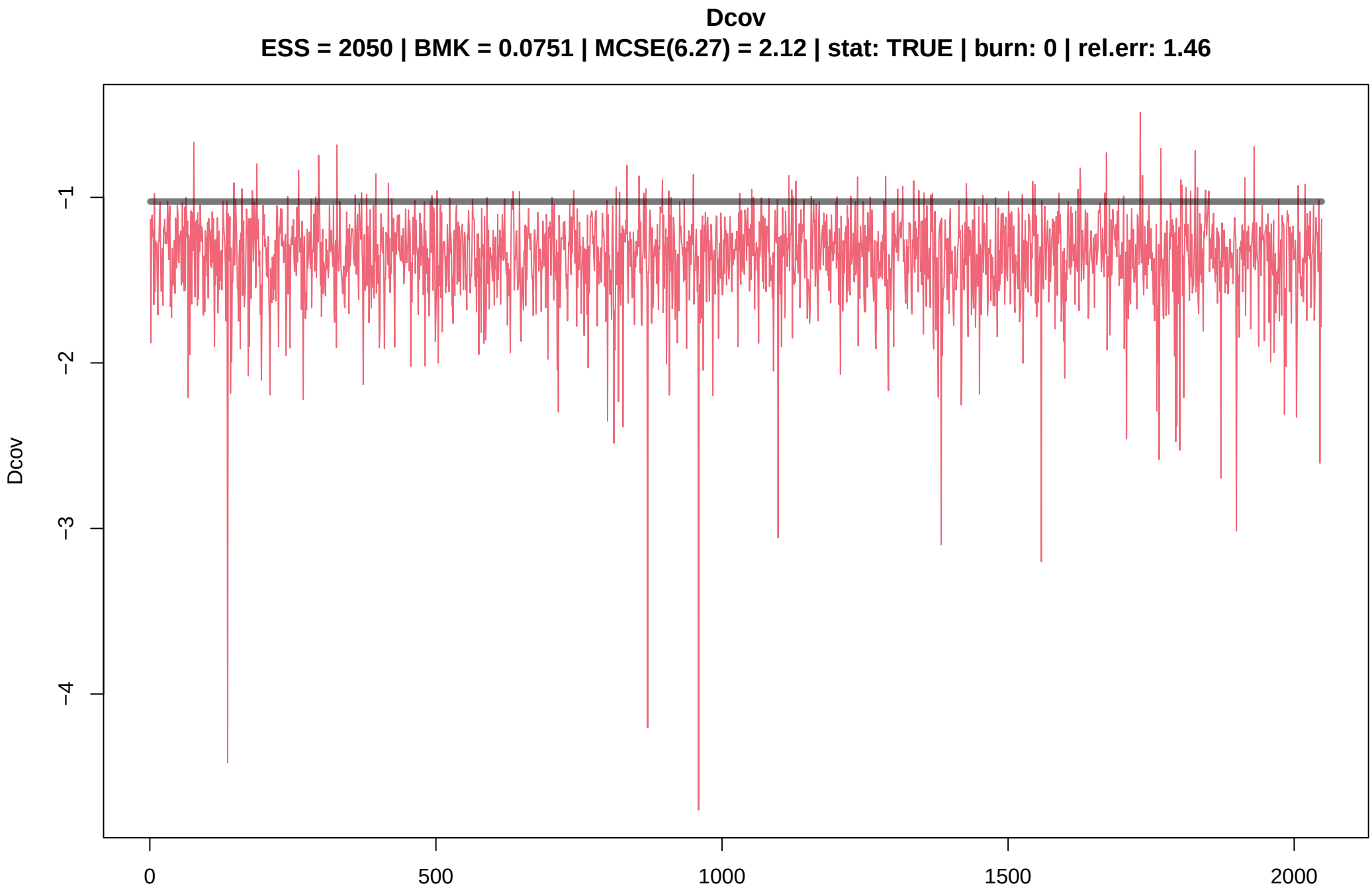

Pdatum4
ESS = 539 | BMK = 0.0511 | MCSE(6.27) = 4.86 | stat: TRUE | burn: 0 | rel.err: 0.0124
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

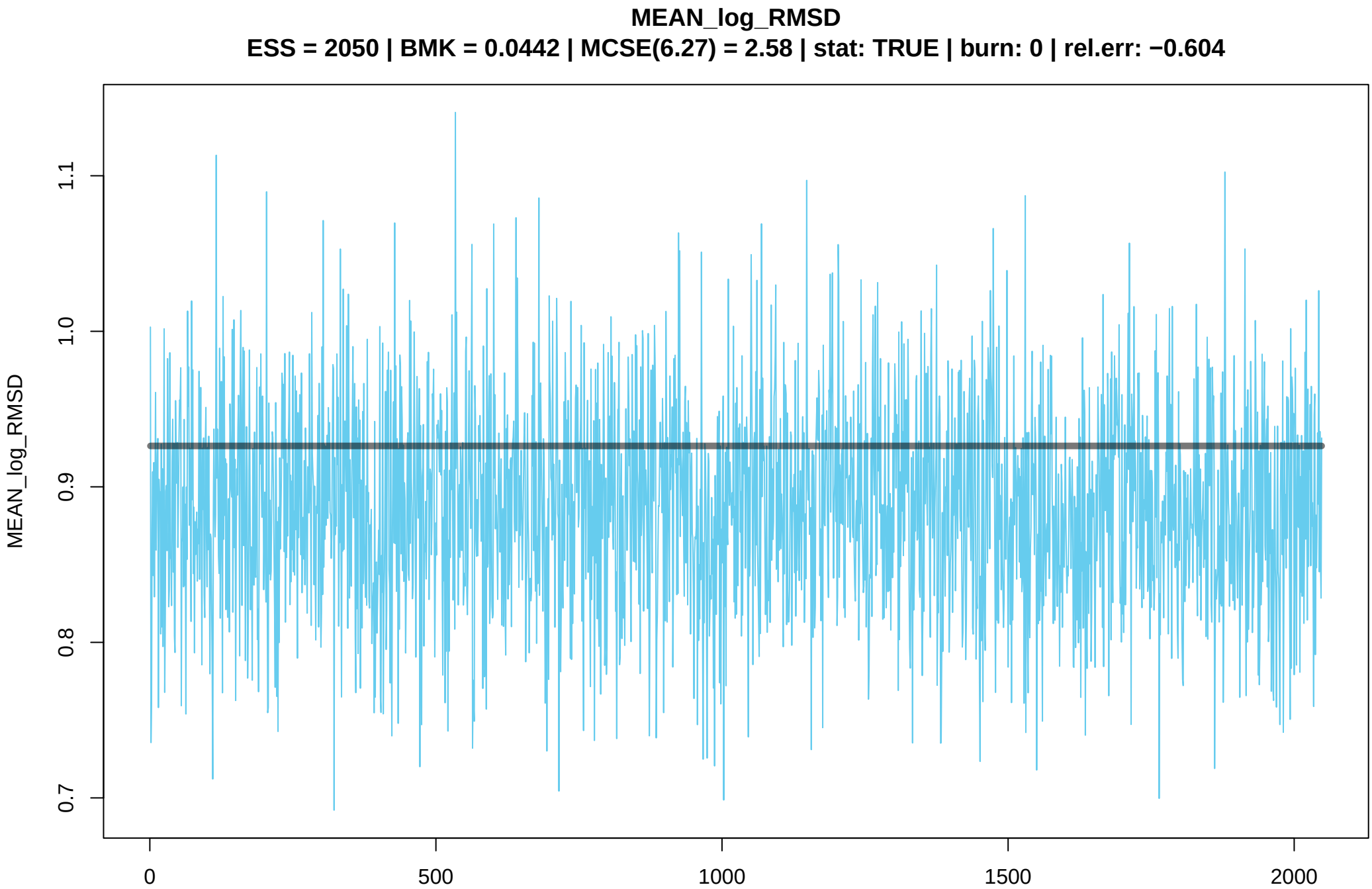

Pdatum5
ESS = 577 | BMK = 0.0477 | MCSE(6.27) = 4.63 | stat: TRUE | burn: 0 | rel.err: 1.46
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

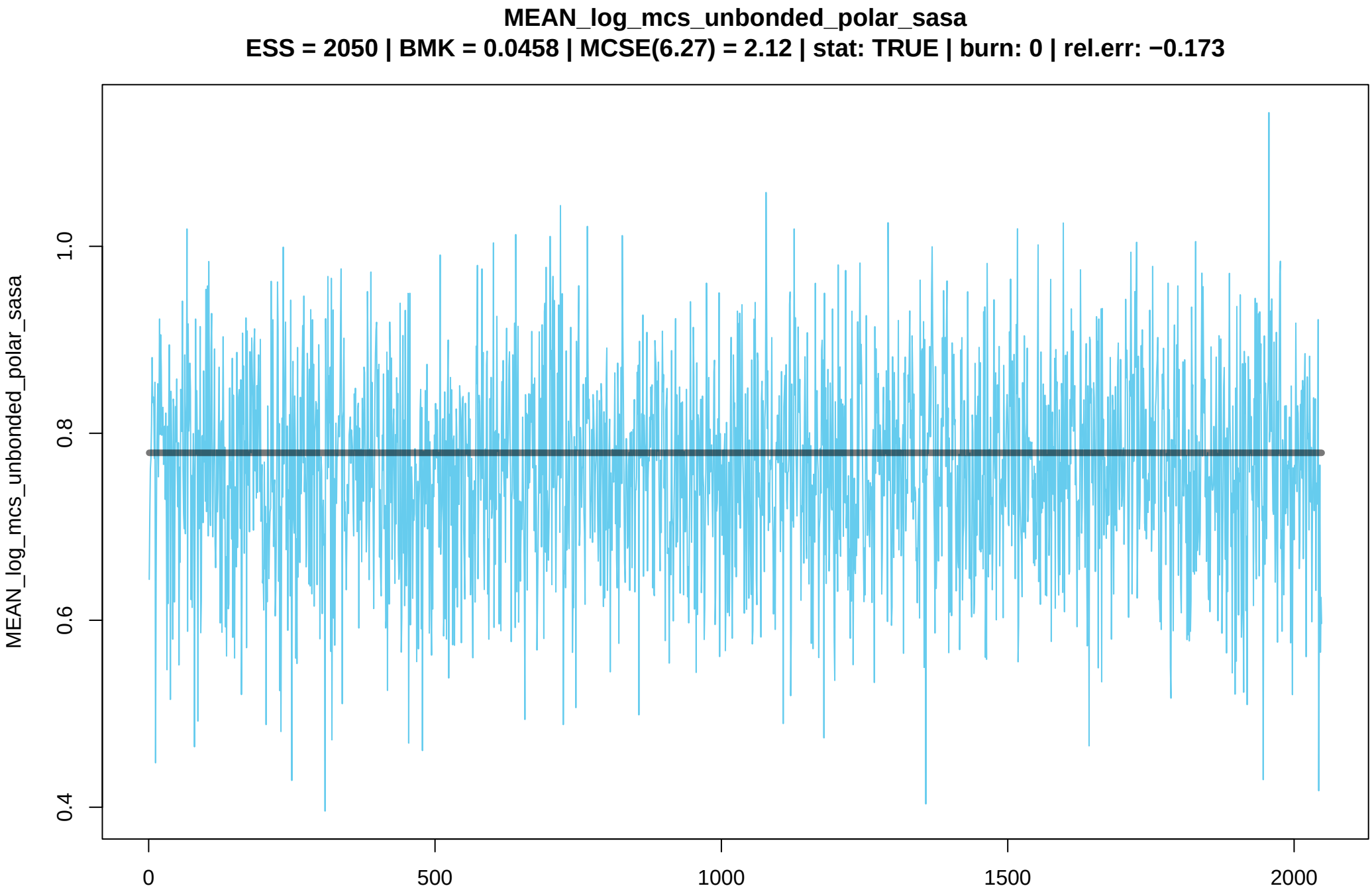

Pdatum6
ESS = 957 | BMK = 0.0396 | MCSE(6.27) = 3.44 | stat: TRUE | burn: 0 | rel.err: 0.652
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

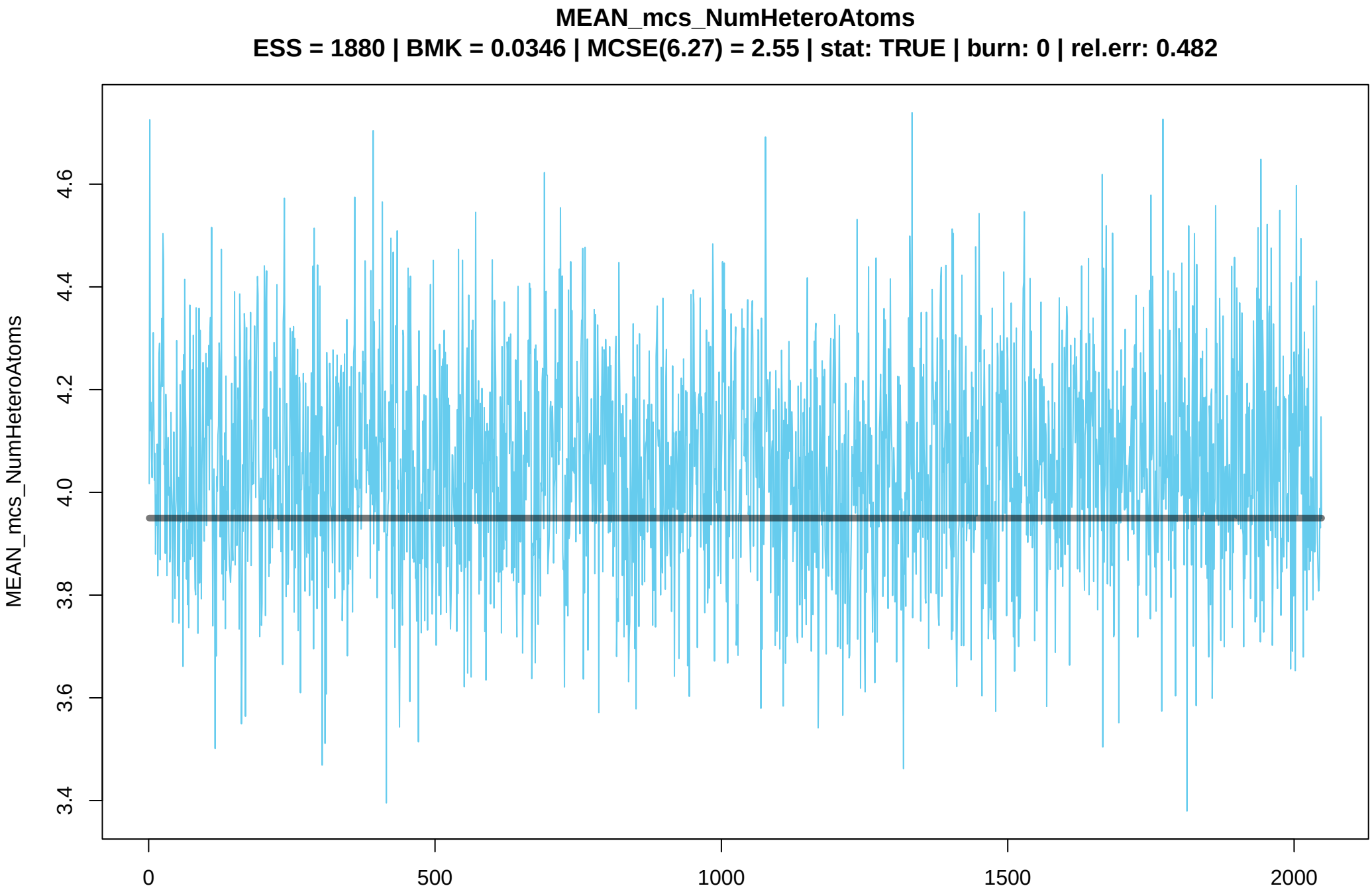

Pdatum7
ESS = 2050 | BMK = 0.0566 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.768
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

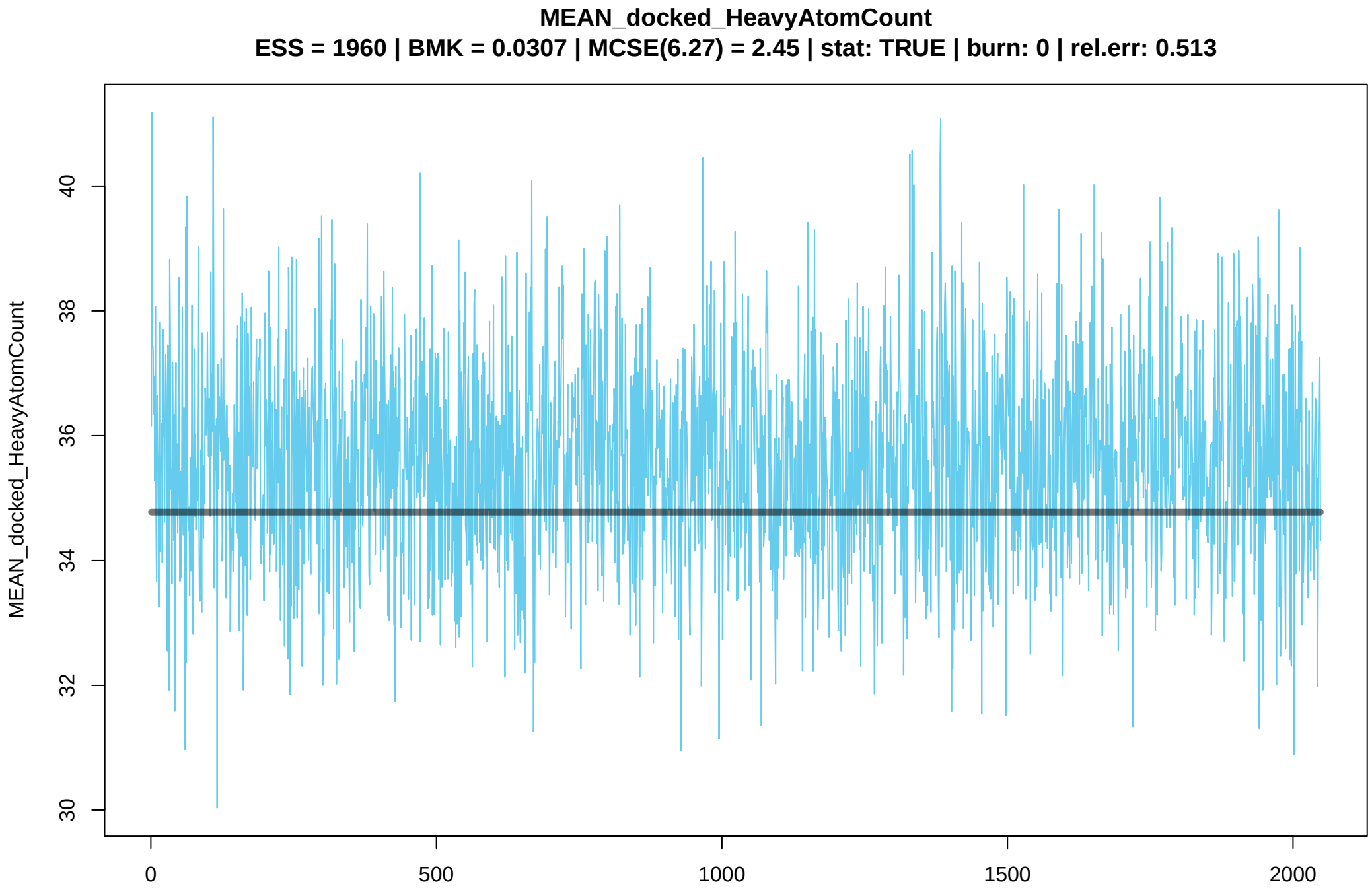

Pdatum8
ESS = 415 | BMK = 0.0869 | MCSE(6.27) = 5.68 | stat: TRUE | burn: 0 | rel.err: 0.508
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

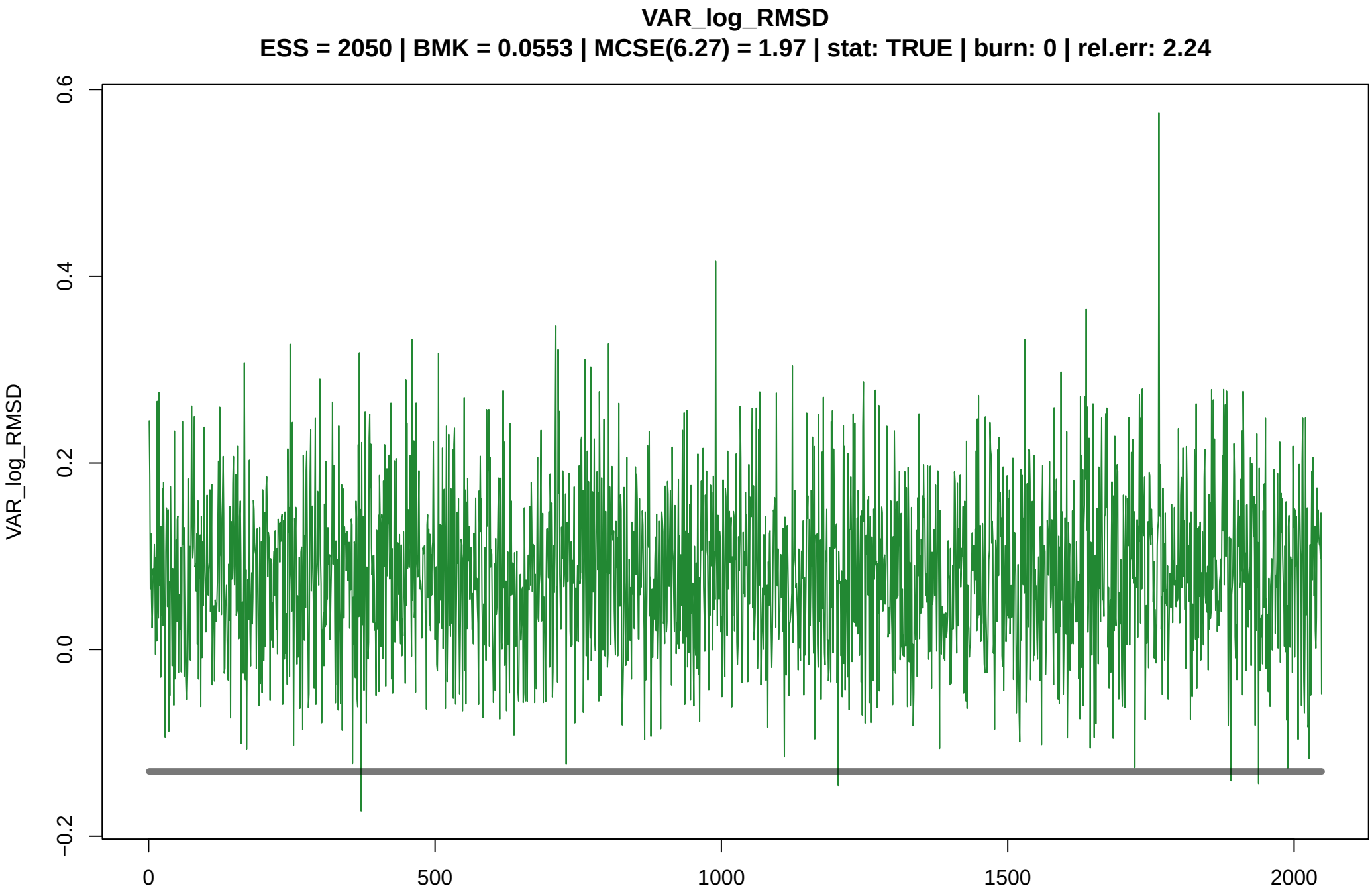

Dcov
ESS = 2050 | BMK = 0.0751 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: 1.46
Dcov
−1
−2
−3
−4
0
500
1000
1500
2000

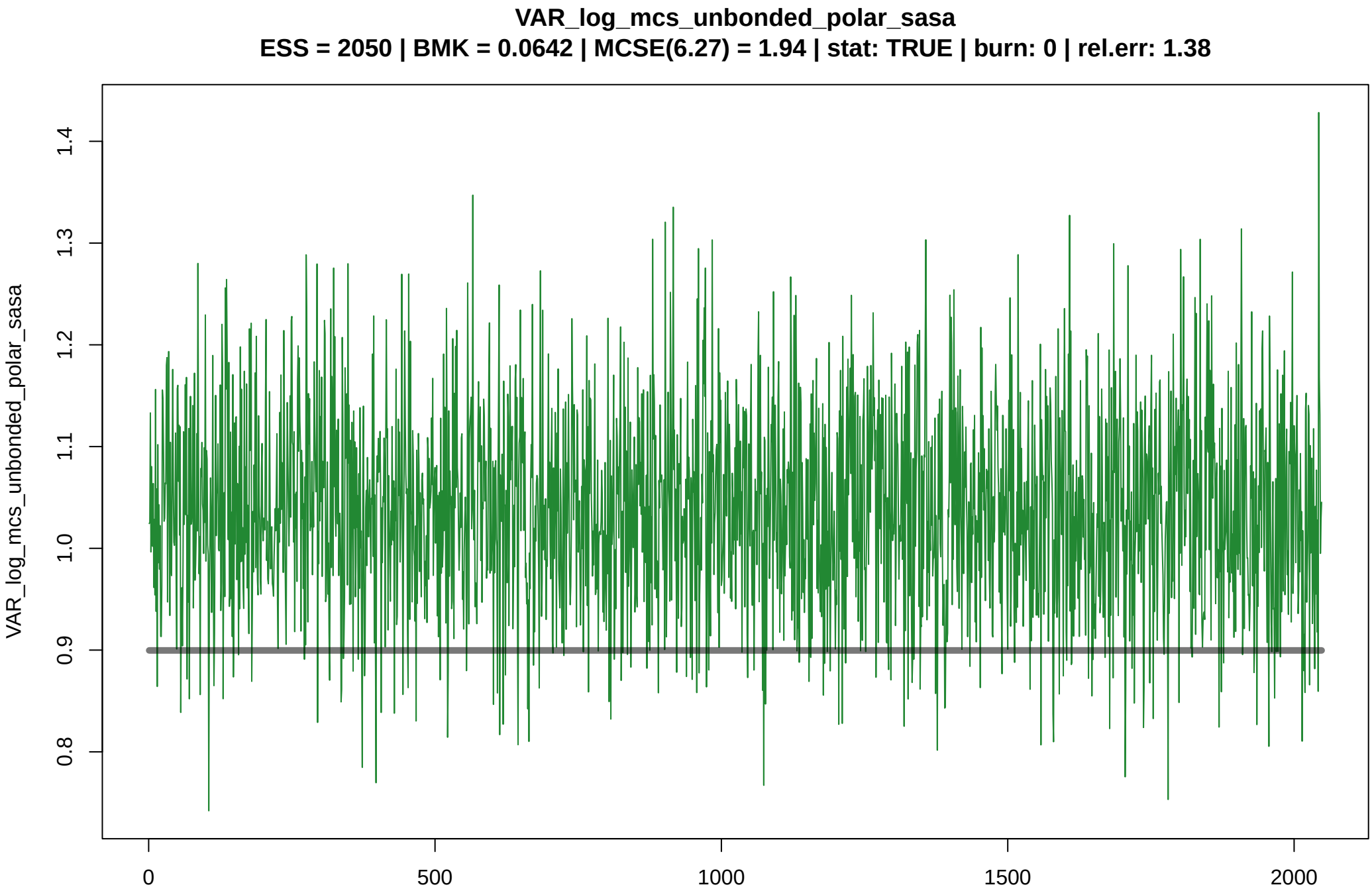

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0442 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: −0.604
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

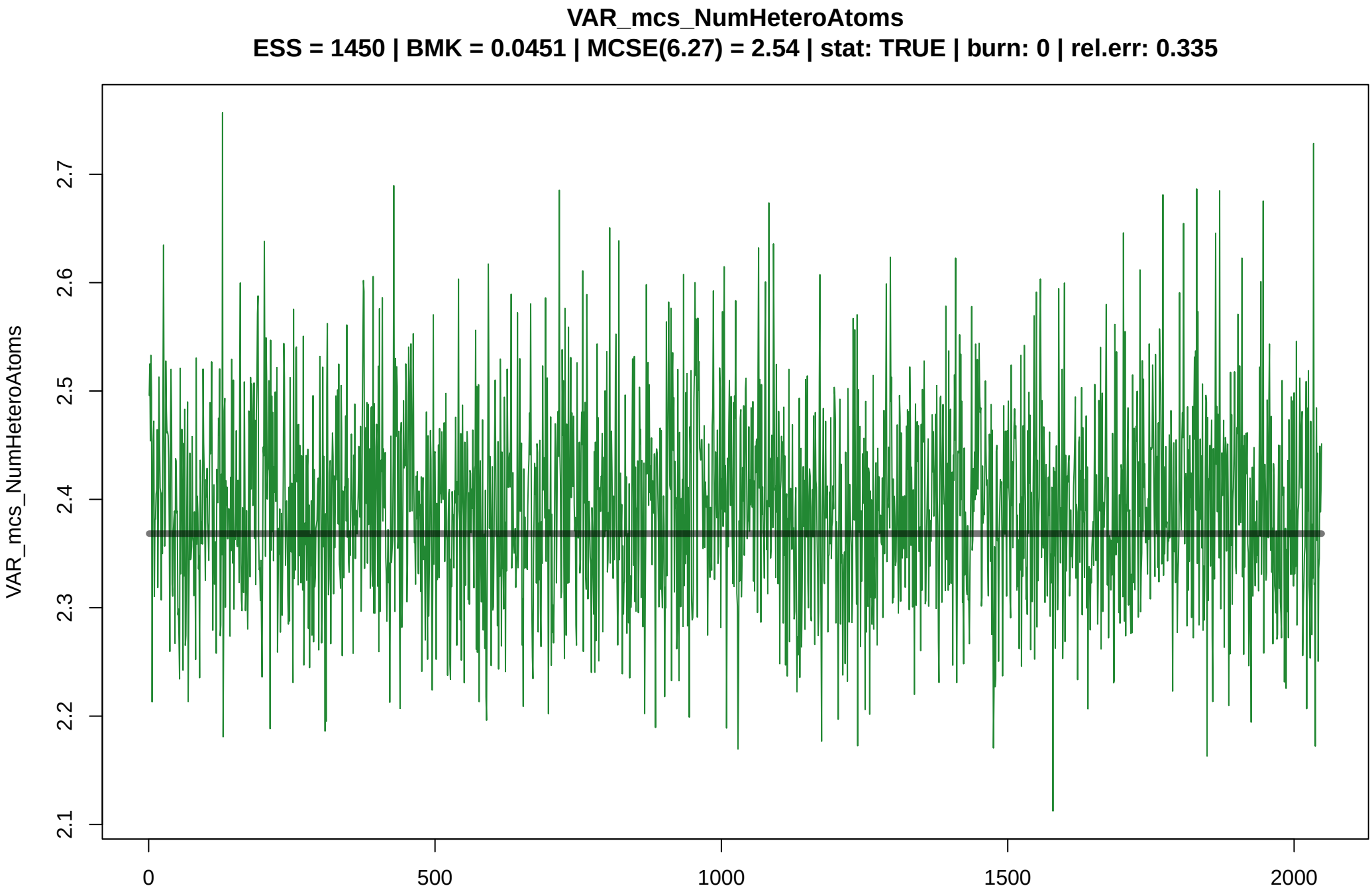

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: −0.173
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

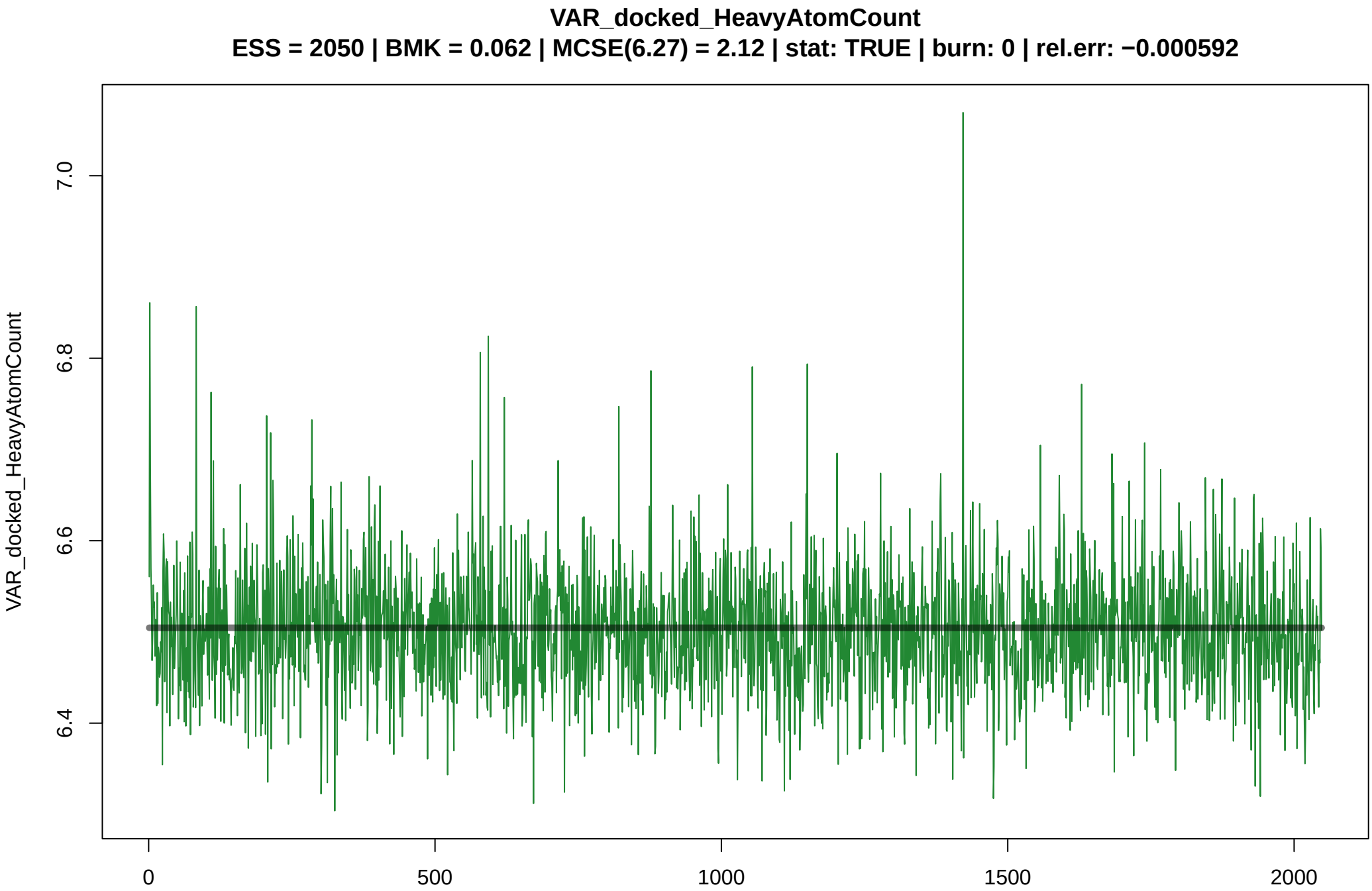

MEAN_mcs_NumHeteroAtoms
ESS = 1880 | BMK = 0.0346 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 0.482
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
0
500
1000
1500
2000

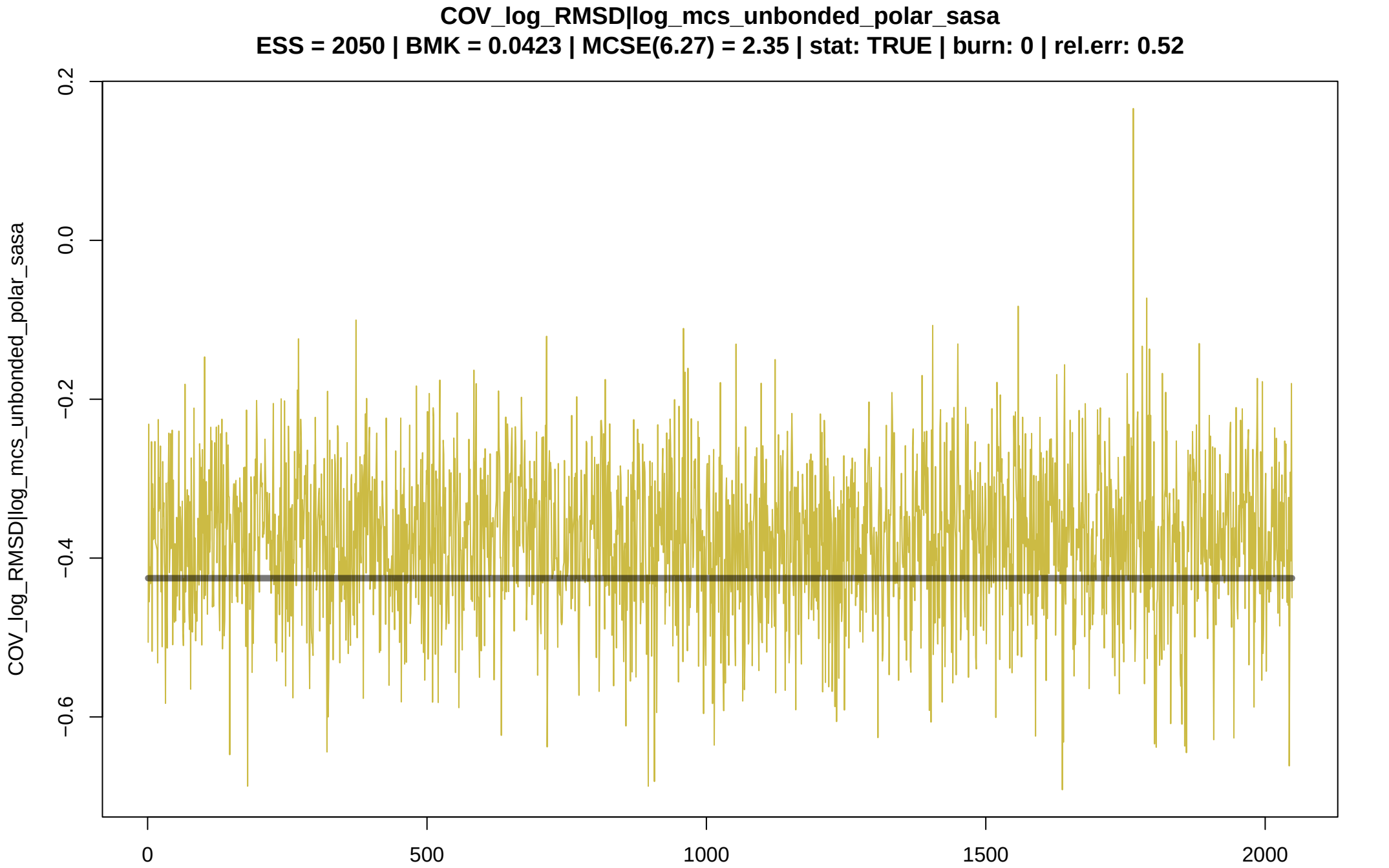

MEAN_docked_HeavyAtomCount
ESS = 1960 | BMK = 0.0307 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0 | rel.err: 0.513
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

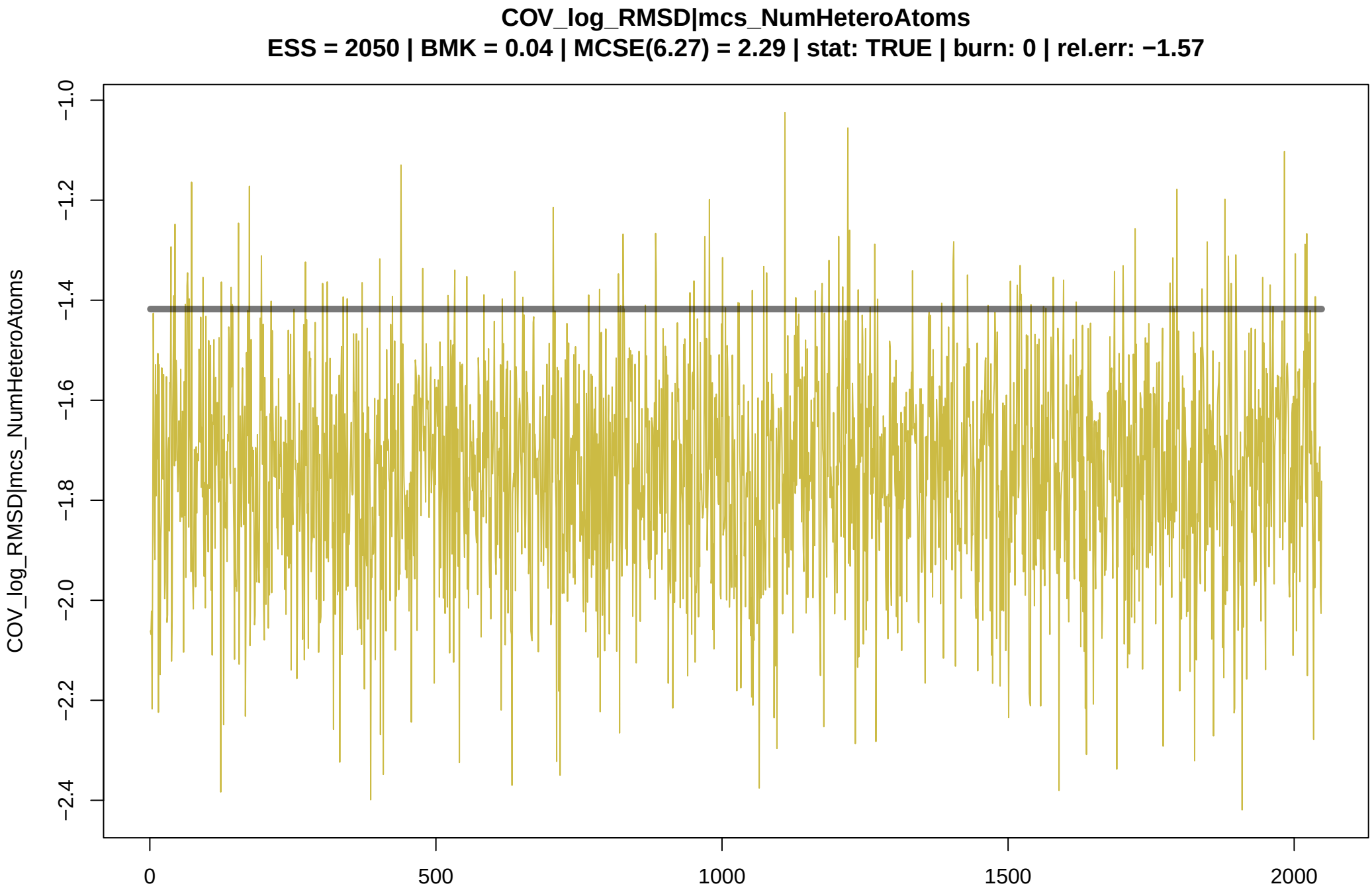

VAR_log_RMSD
ESS = 2050 | BMK = 0.0553 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0 | rel.err: 2.24
VAR_log_RMSD
0.6
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

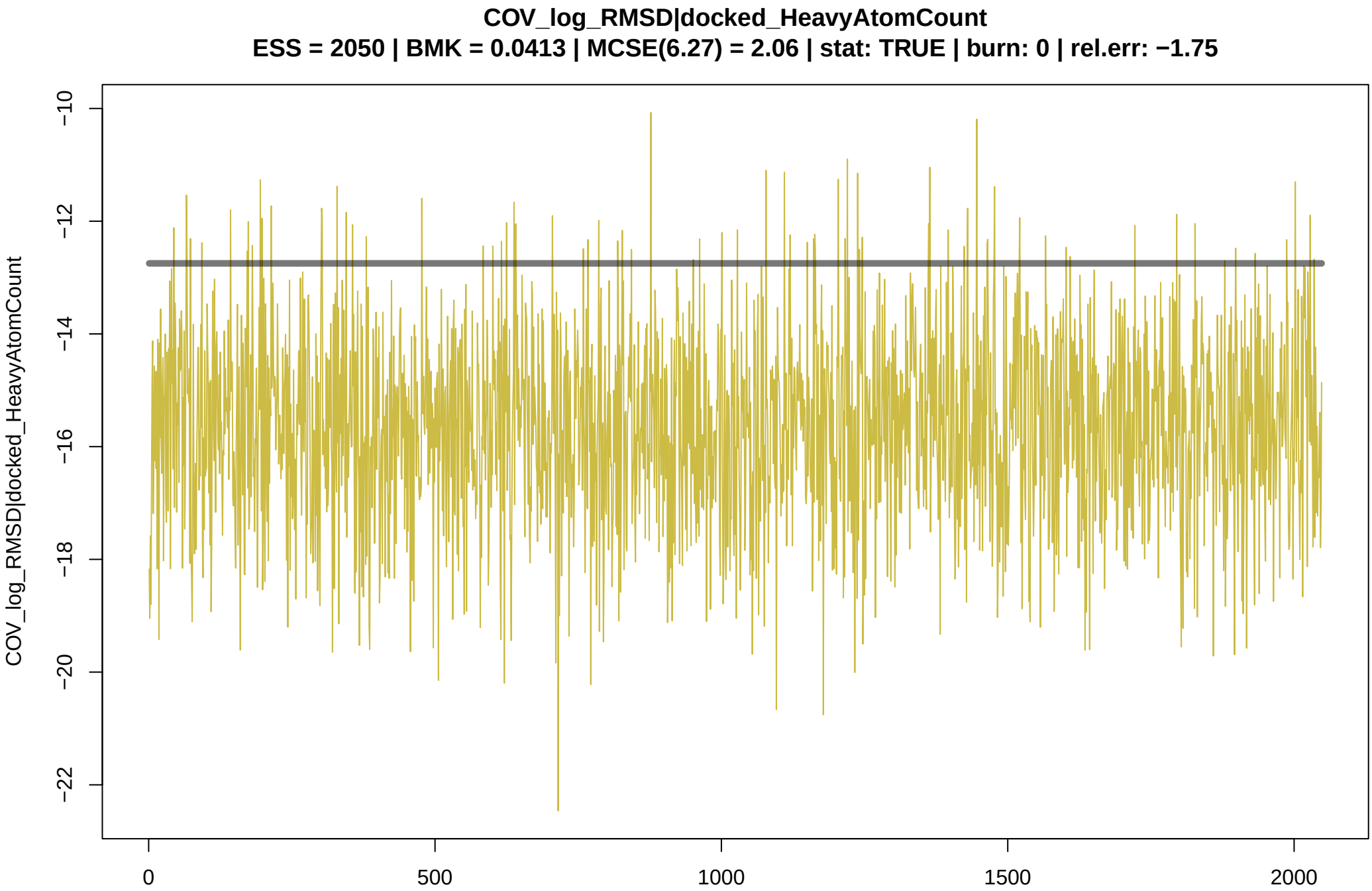

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0642 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0 | rel.err: 1.38
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

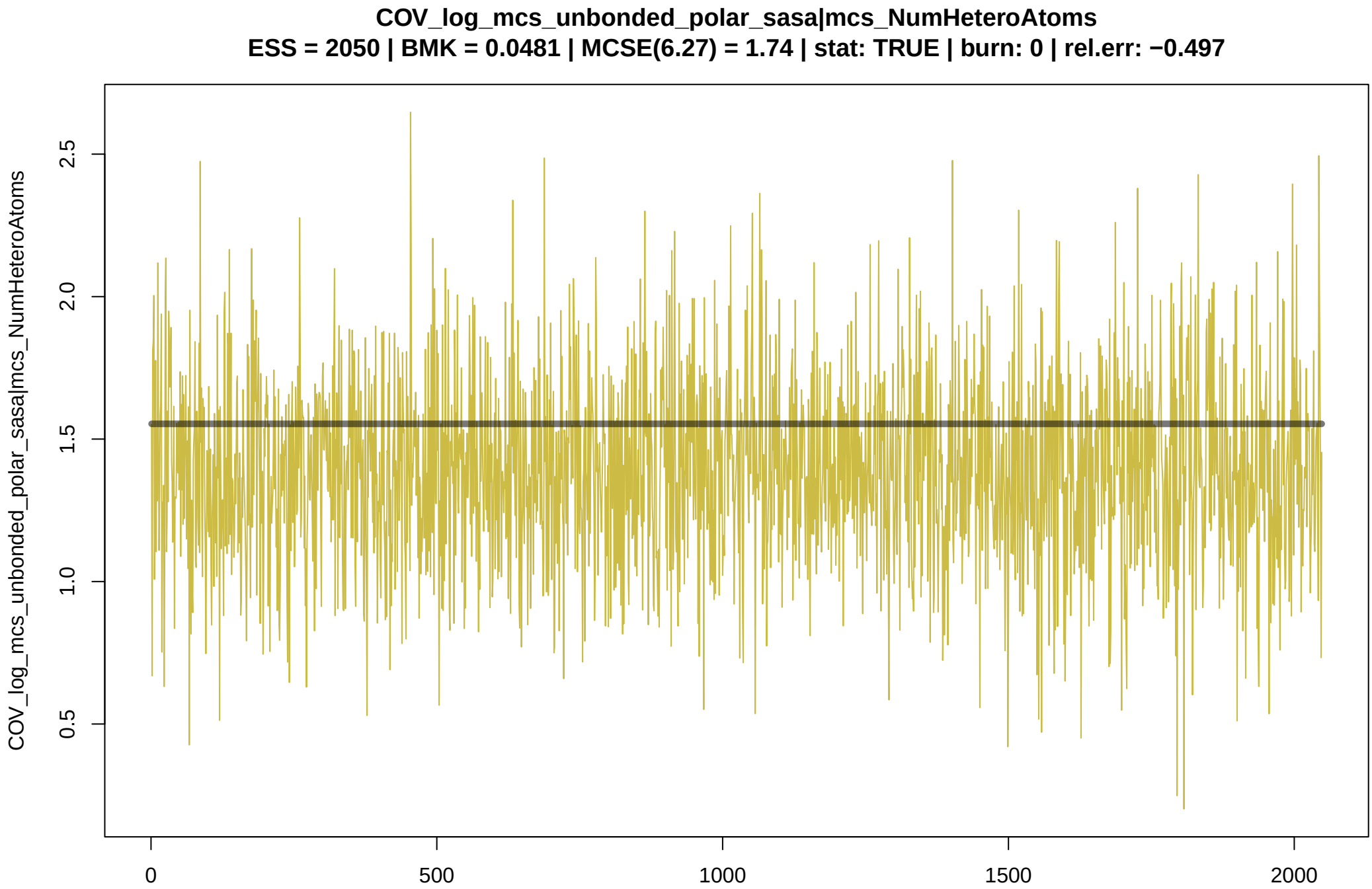

VAR_mcs_NumHeteroAtoms
ESS = 1450 | BMK = 0.0451 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: 0.335
VAR_mcs_NumHeteroAtoms
2.1
2.2
2.3
2.4
2.5
2.6
2.7
0
500
1000
1500
2000

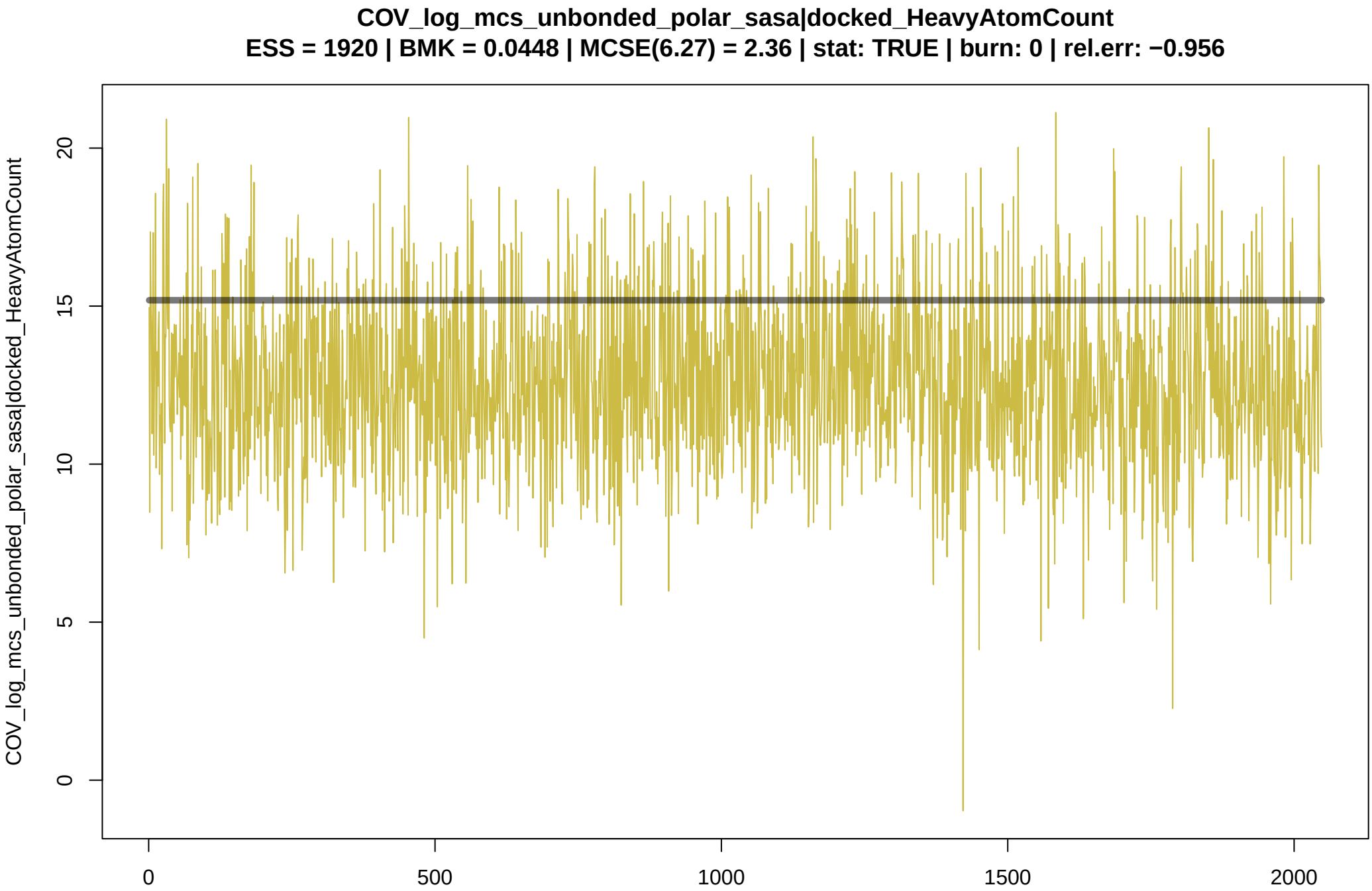

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.062 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: −0.000592
VAR_docked_HeavyAtomCount
6.4
6.6
6.8
7.0
0
500
1000
1500
2000

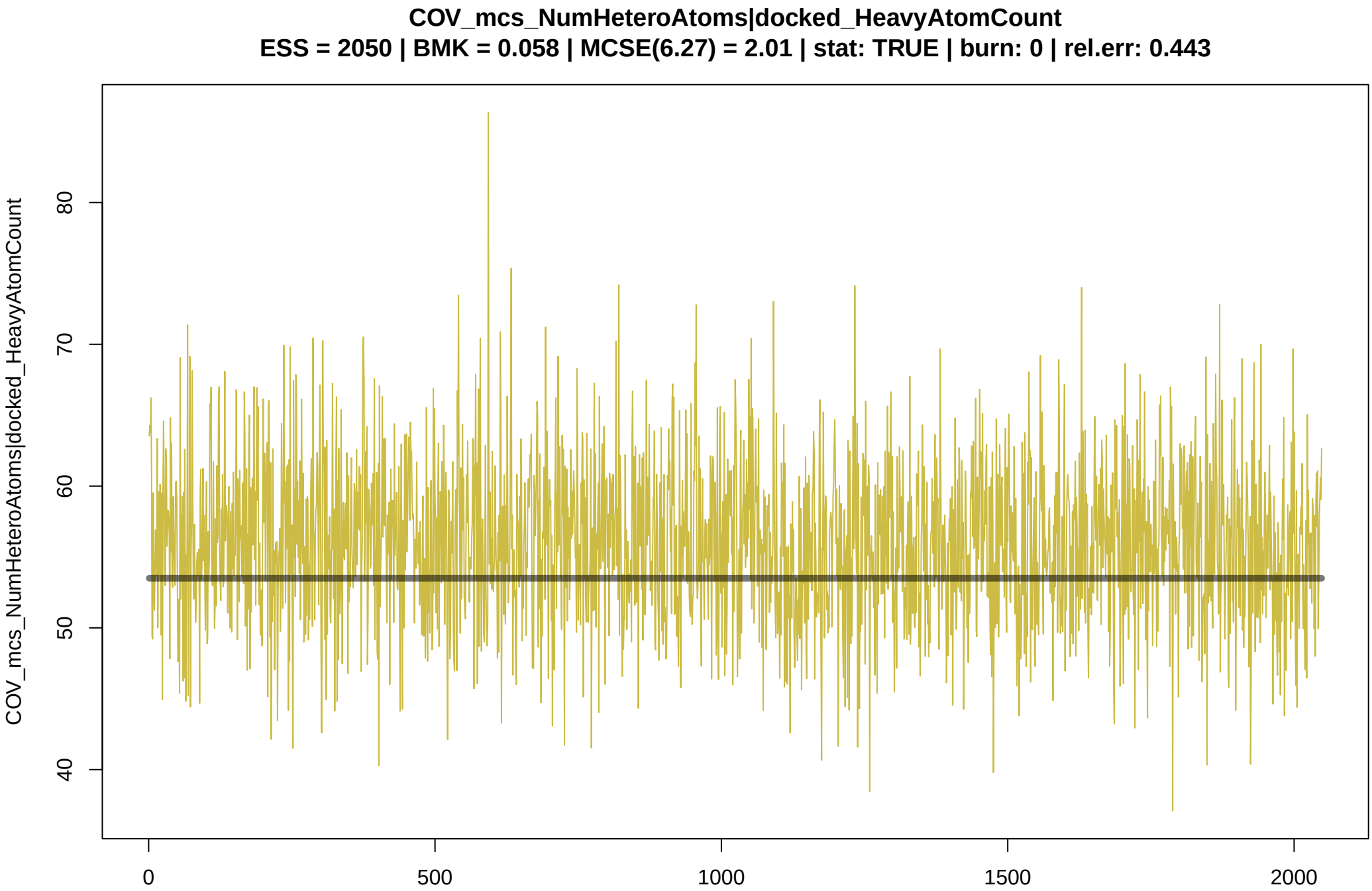

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0423 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 0.52
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.2
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.04 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: −1.57
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.2
−1.4
−1.6
−1.8
−2.0
−2.2
−2.4
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0413 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: −1.75
COV_log_RMSD|docked_HeavyAtomCount
−10
−12
−14
−16
−18
−20
−22
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 1.74 | stat: TRUE | burn: 0 | rel.err: −0.497
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0448 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0 | rel.err: −0.956
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
0
5
10
15
20
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.058 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: 0.443
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000