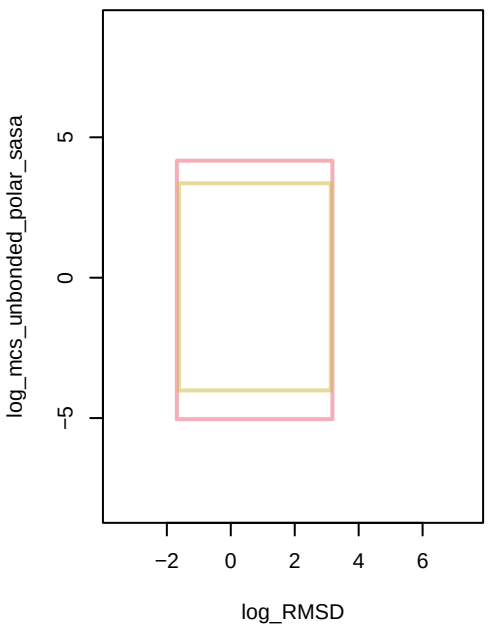
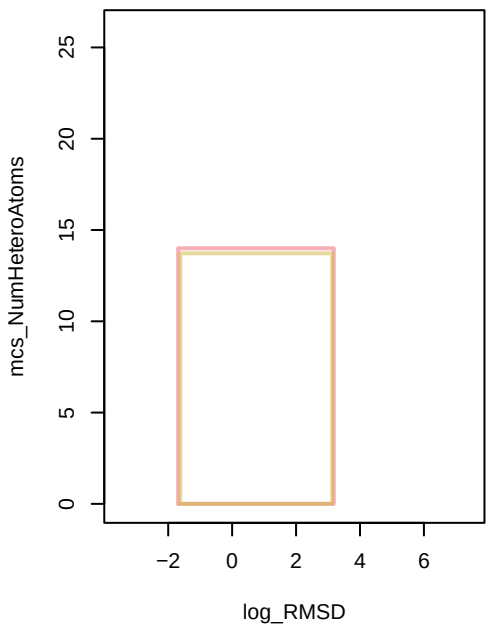
−− STATS maxD −−
min ESS = 26.4428537001257
max BMK = 0.140049221650041
max MCSE = 9.76601813730342
all stationary: FALSE
burn: 612
max rel.err.: 2.1000649323507

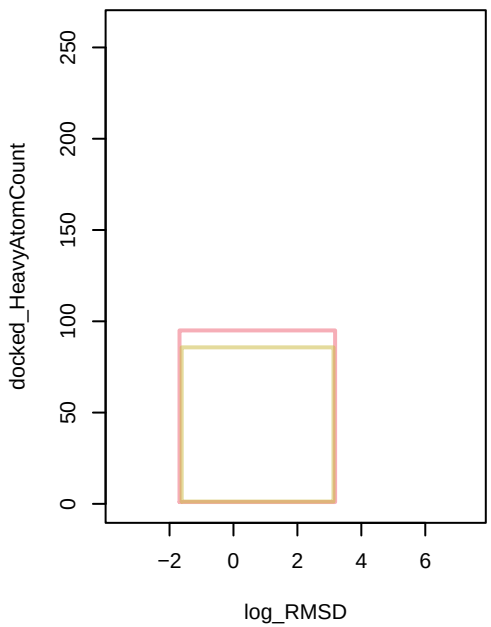
−− STATS 2D −−
min ESS = 1628.0325564804
max BMK = 0.056210308423385 7
max MCSE = 3.04270909051362
all stationary: TRUE
burn: 0
max rel.err.: 1.78435049177206

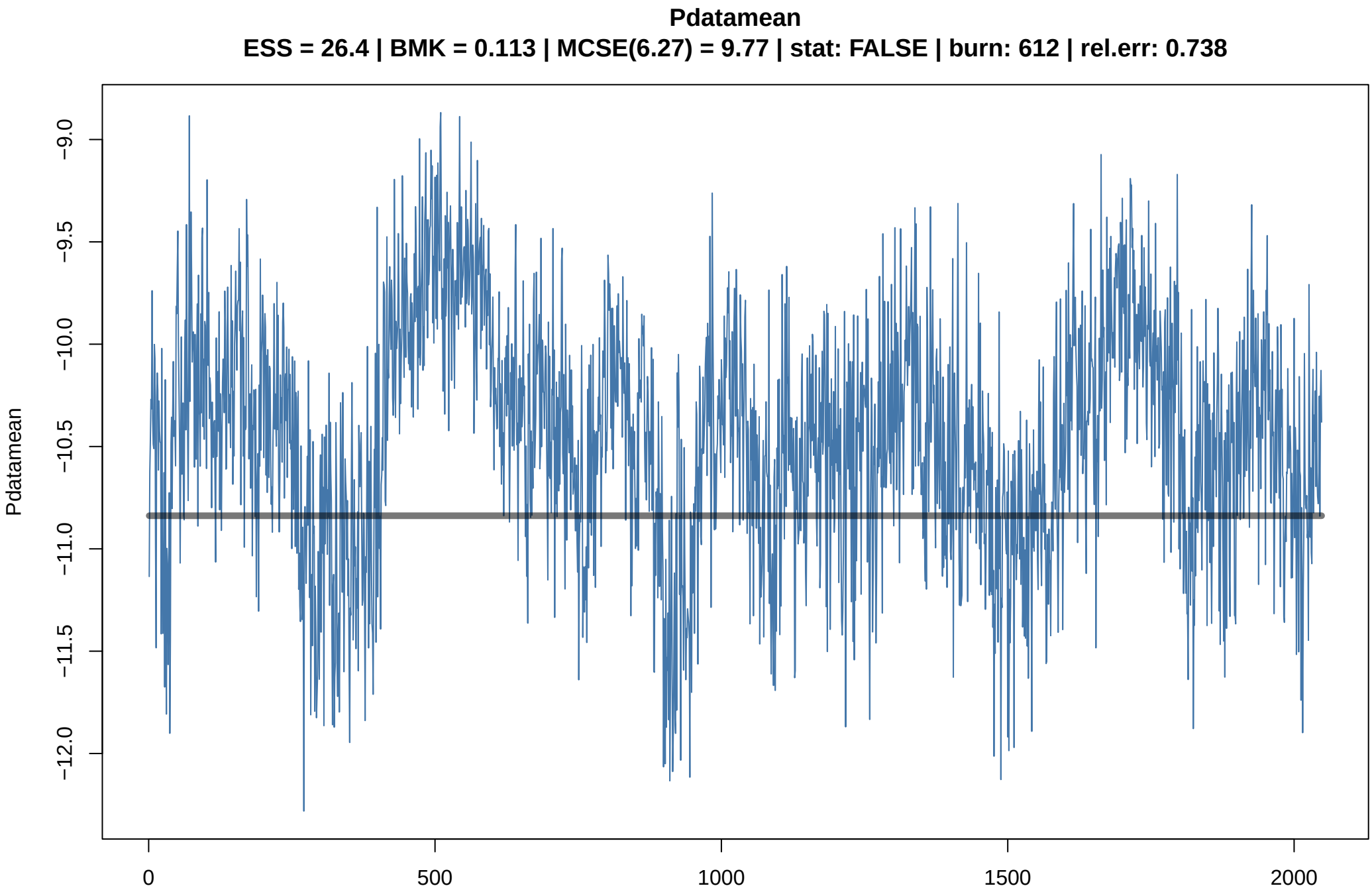
−− STATS 1D −−
min ESS = 1824.29141782669
max BMK = 0.062367736998486 7
max MCSE = 2.85804651842636
all stationary: FALSE
burn: 0
max rel.err.: 2.33290274961655

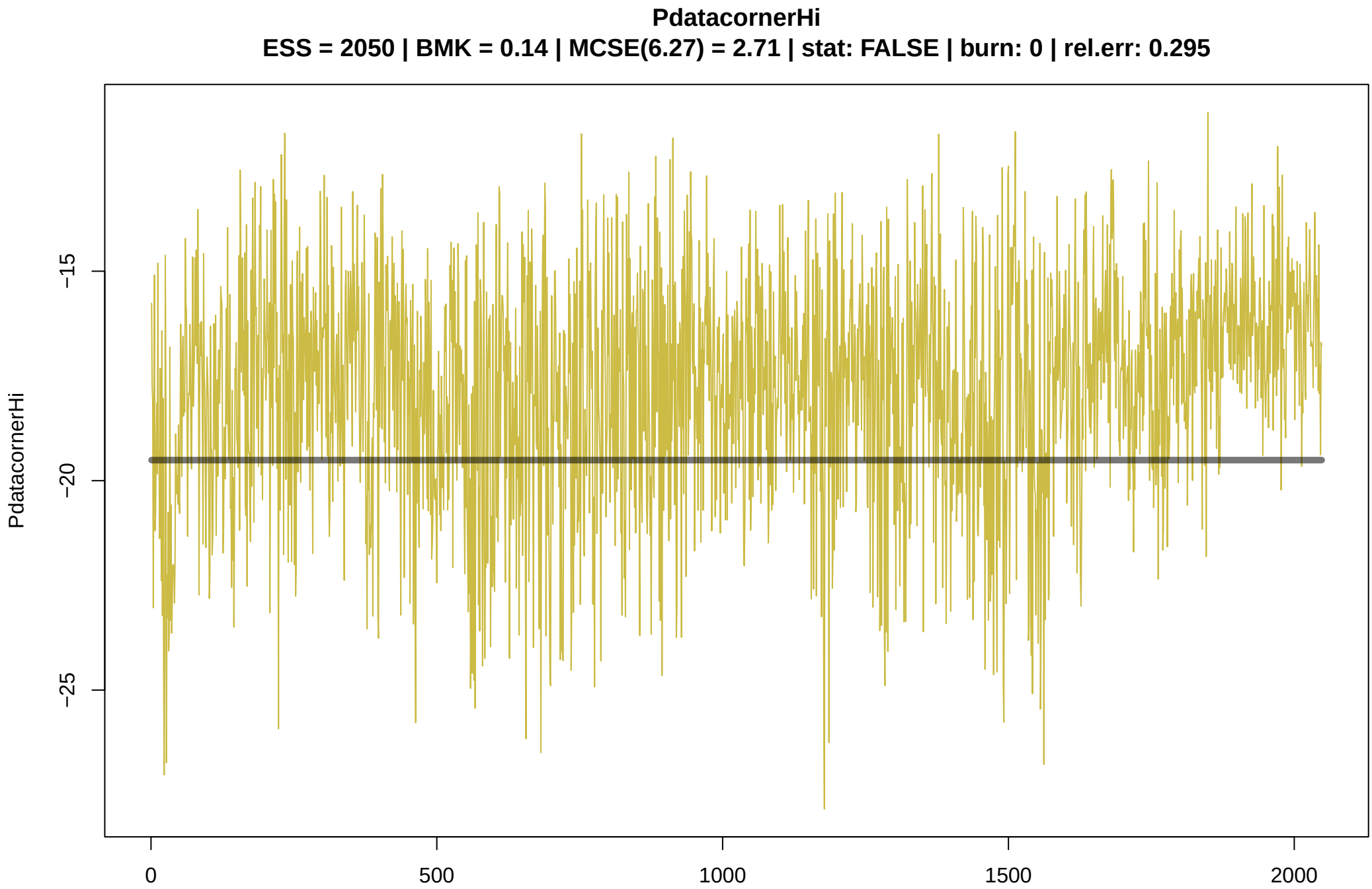
Occupied clusters: 9 of 16

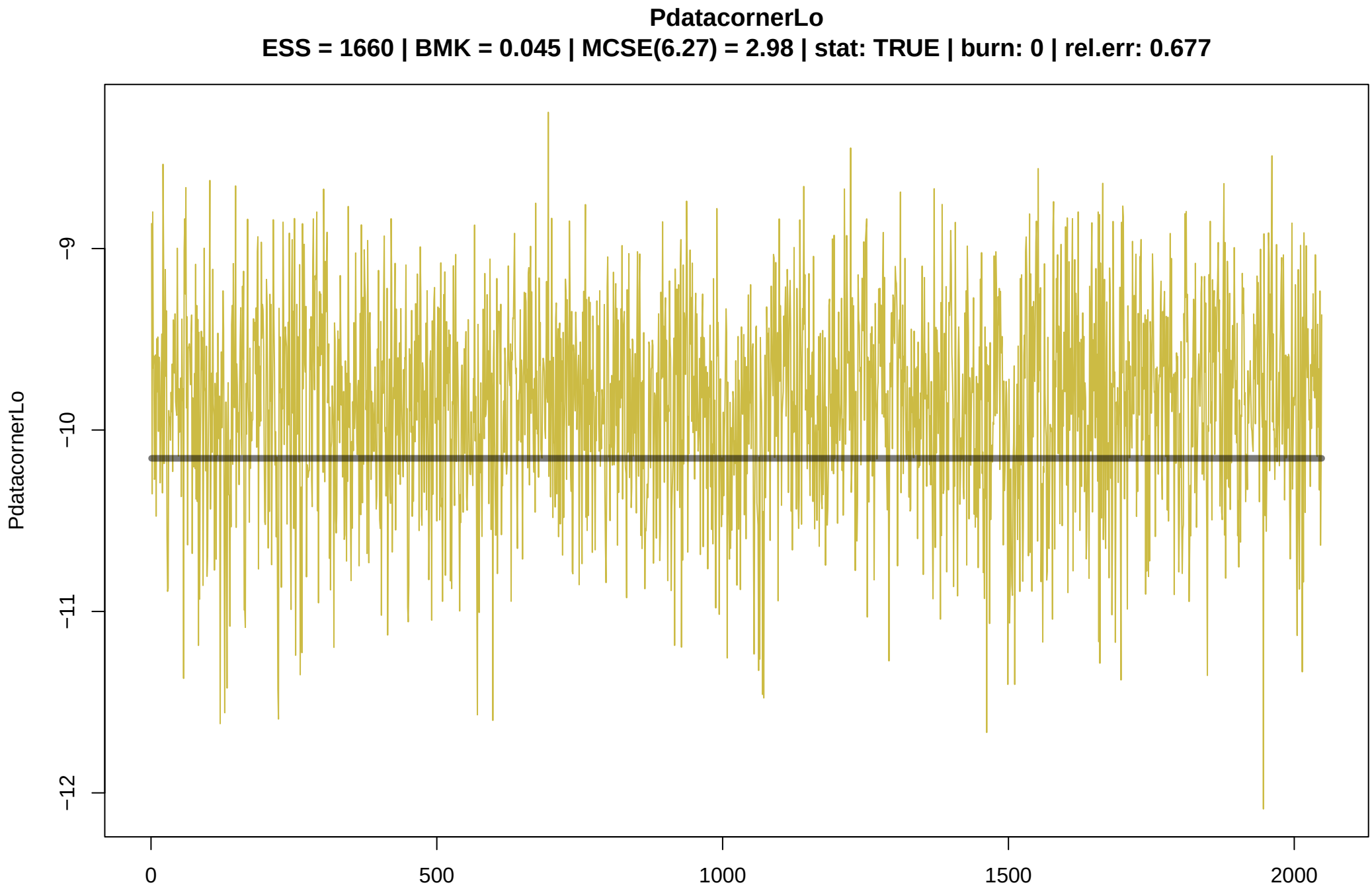

log_mcs_unbonded_polar_sasa
5
0
−5
−2
0
2
4
6
log_RMSD

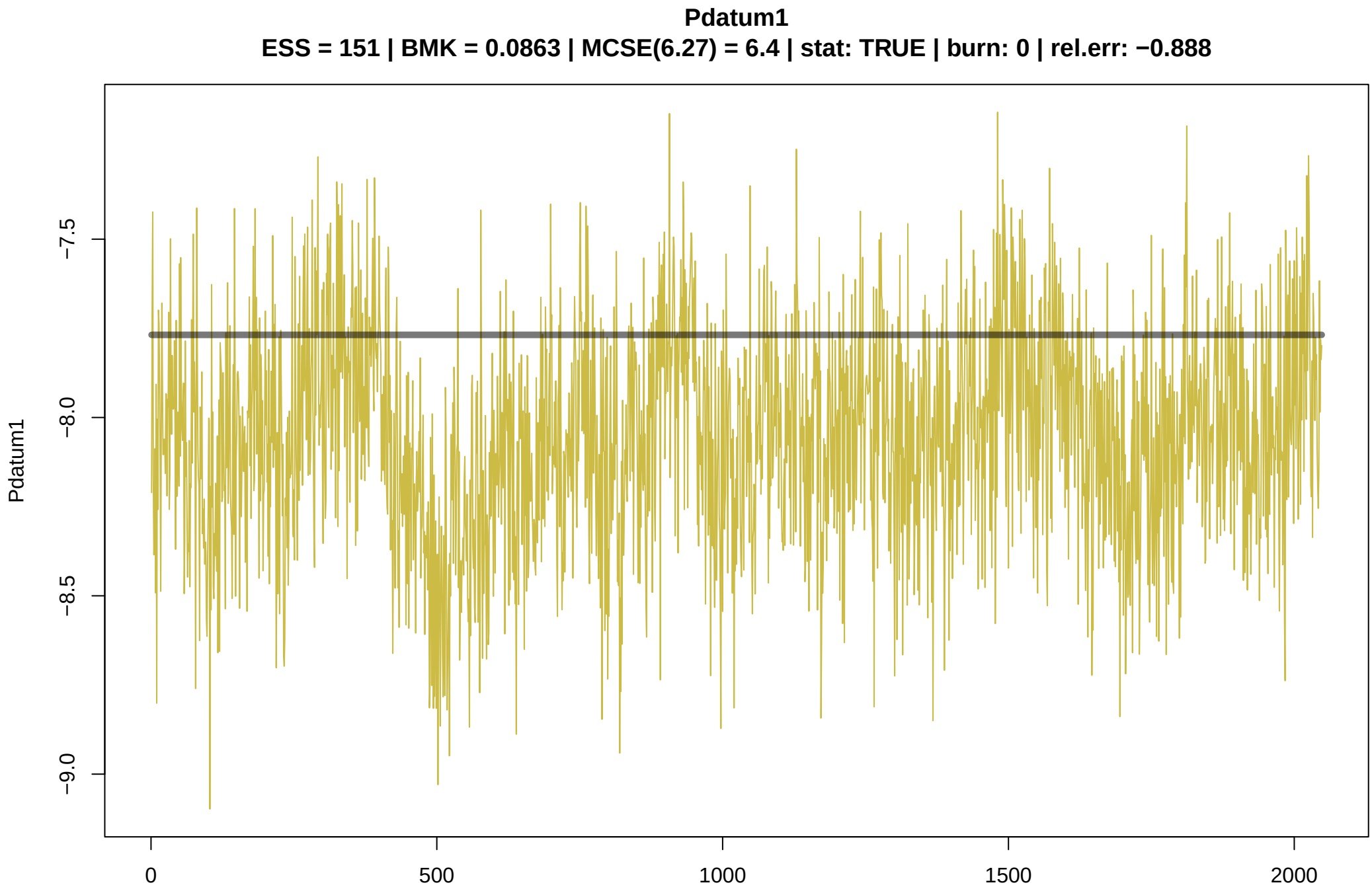

mcs_NumHeteroAtoms
25
20
15
10
5
0
−2
0
2
4
6
log_RMSD

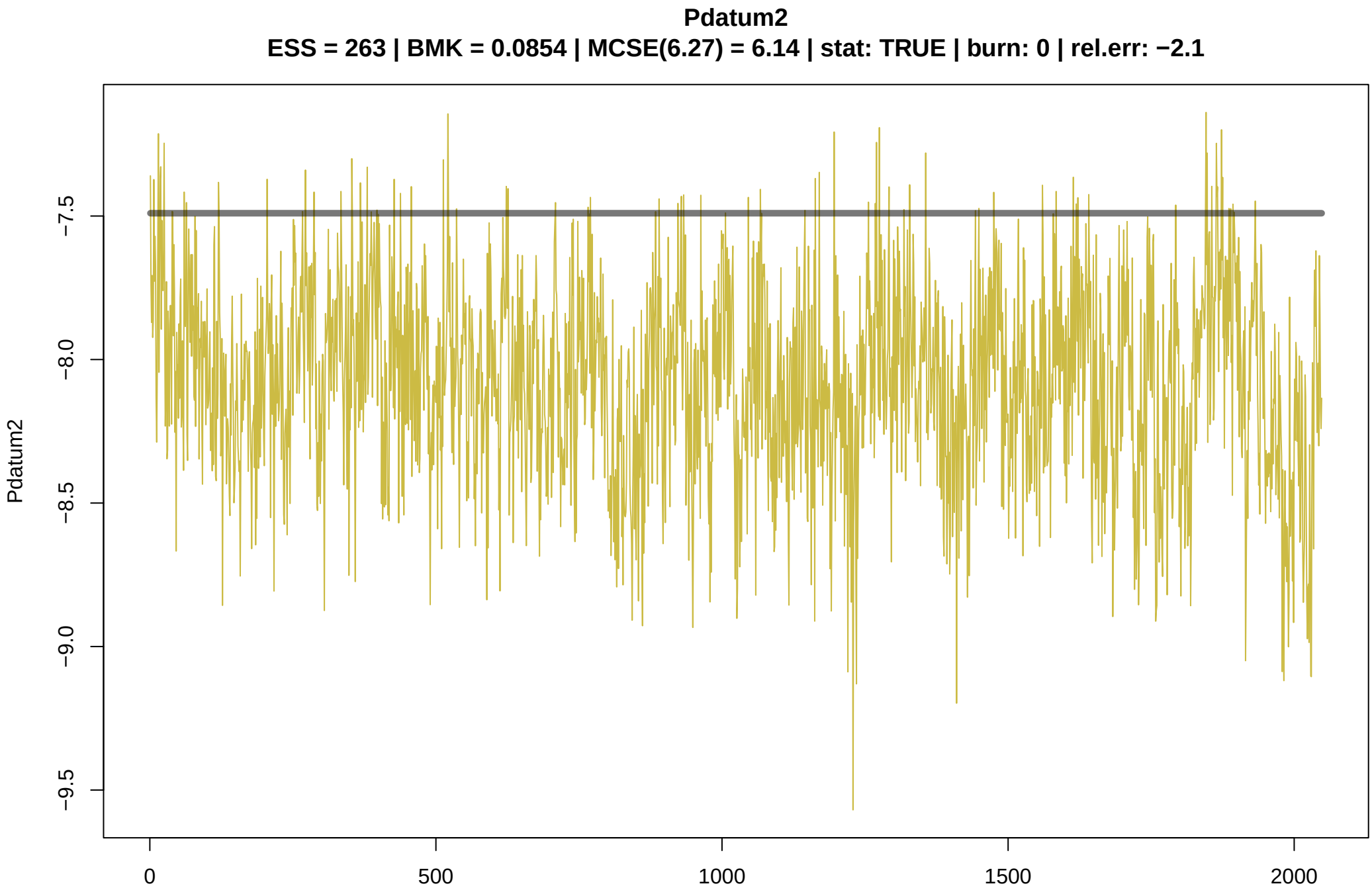

docked_HeavyAtomCount
250
200
150
100
50
0
−2
0
2
4
6
log_RMSD

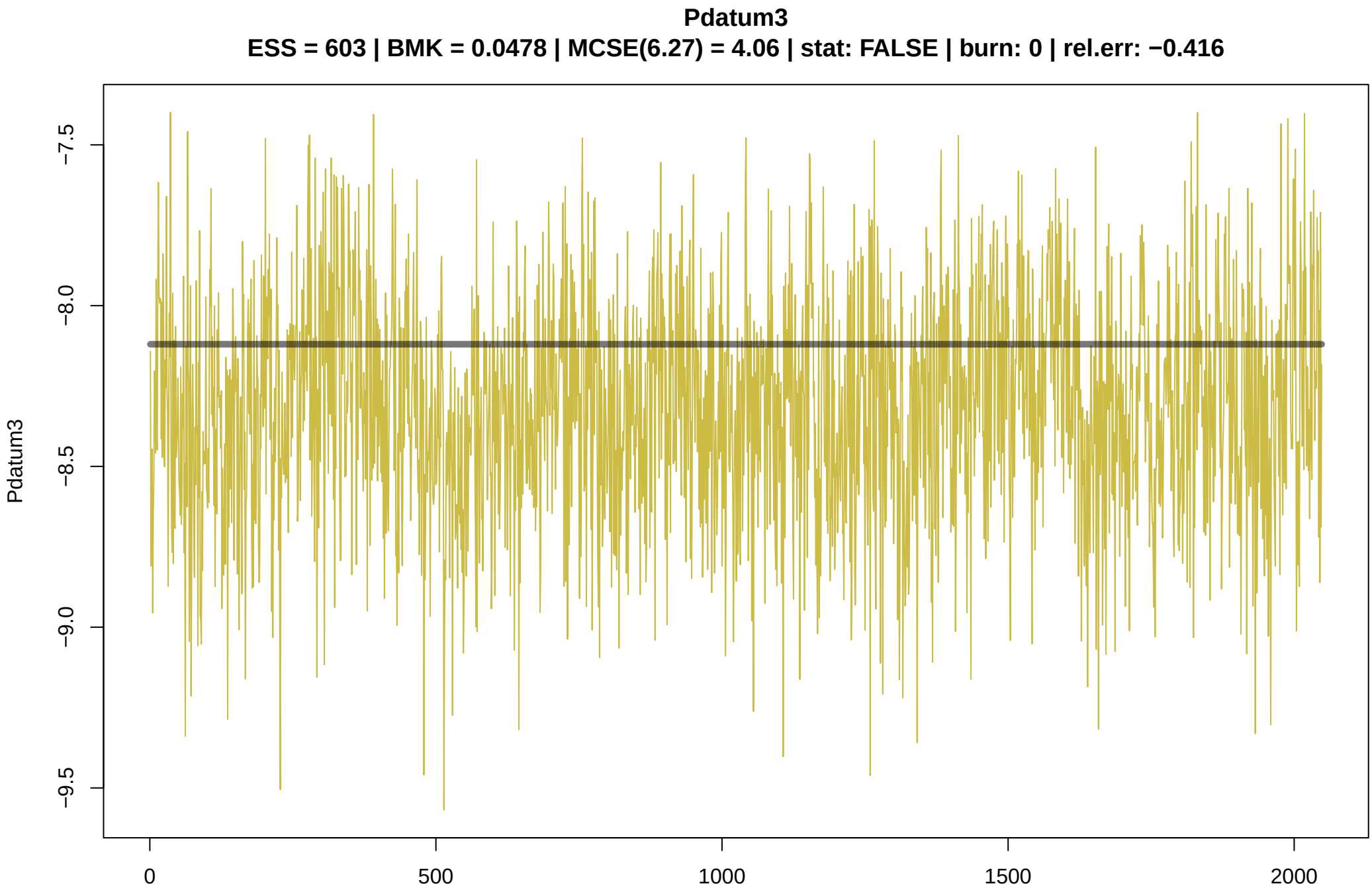

Pdatamean
ESS = 26.4 | BMK = 0.113 | MCSE(6.27) = 9.77 | stat: FALSE | burn: 612 | rel.err: 0.738
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

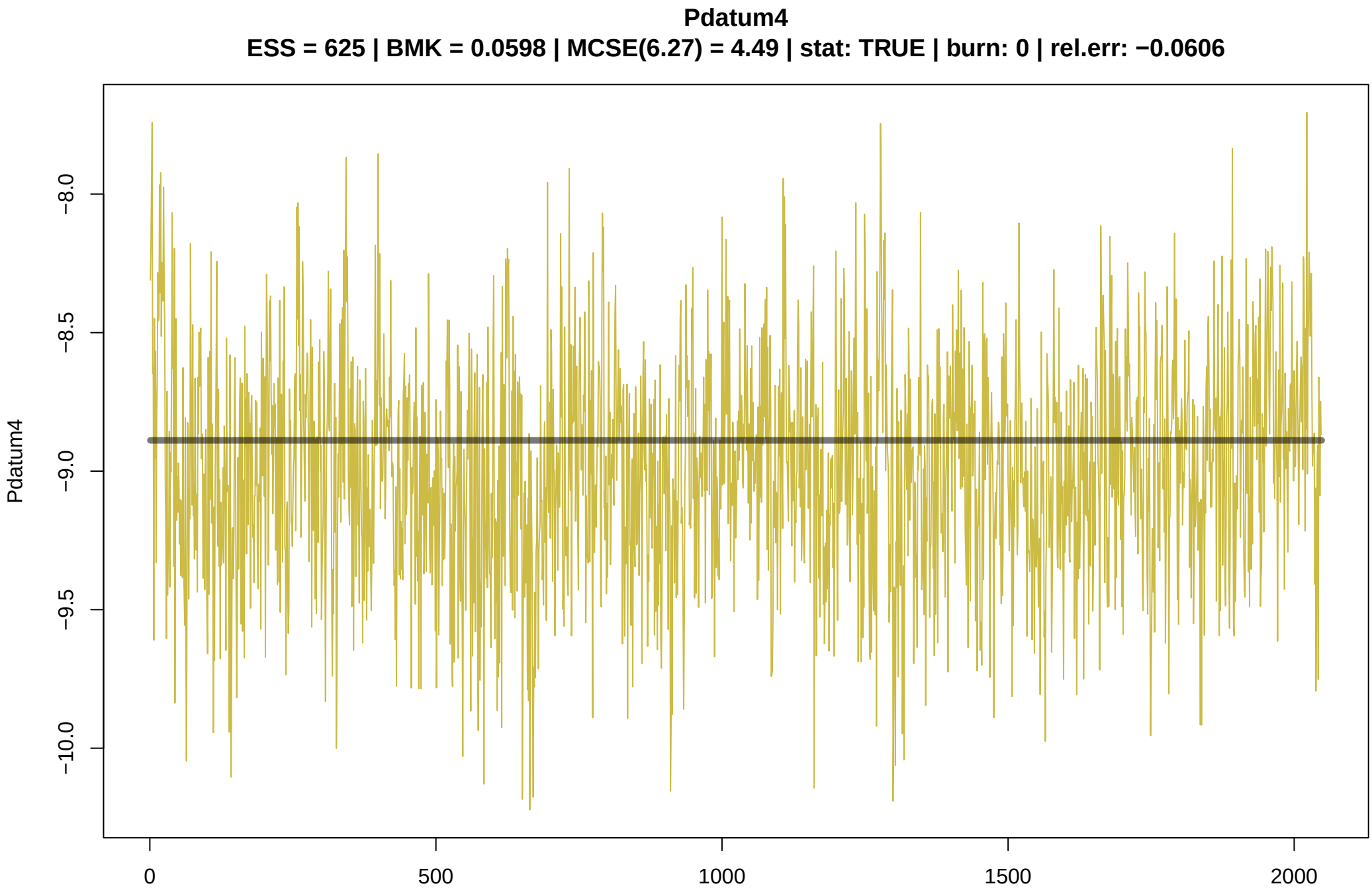

PdatacornerHi
ESS = 2050 | BMK = 0.14 | MCSE(6.27) = 2.71 | stat: FALSE | burn: 0 | rel.err: 0.295
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

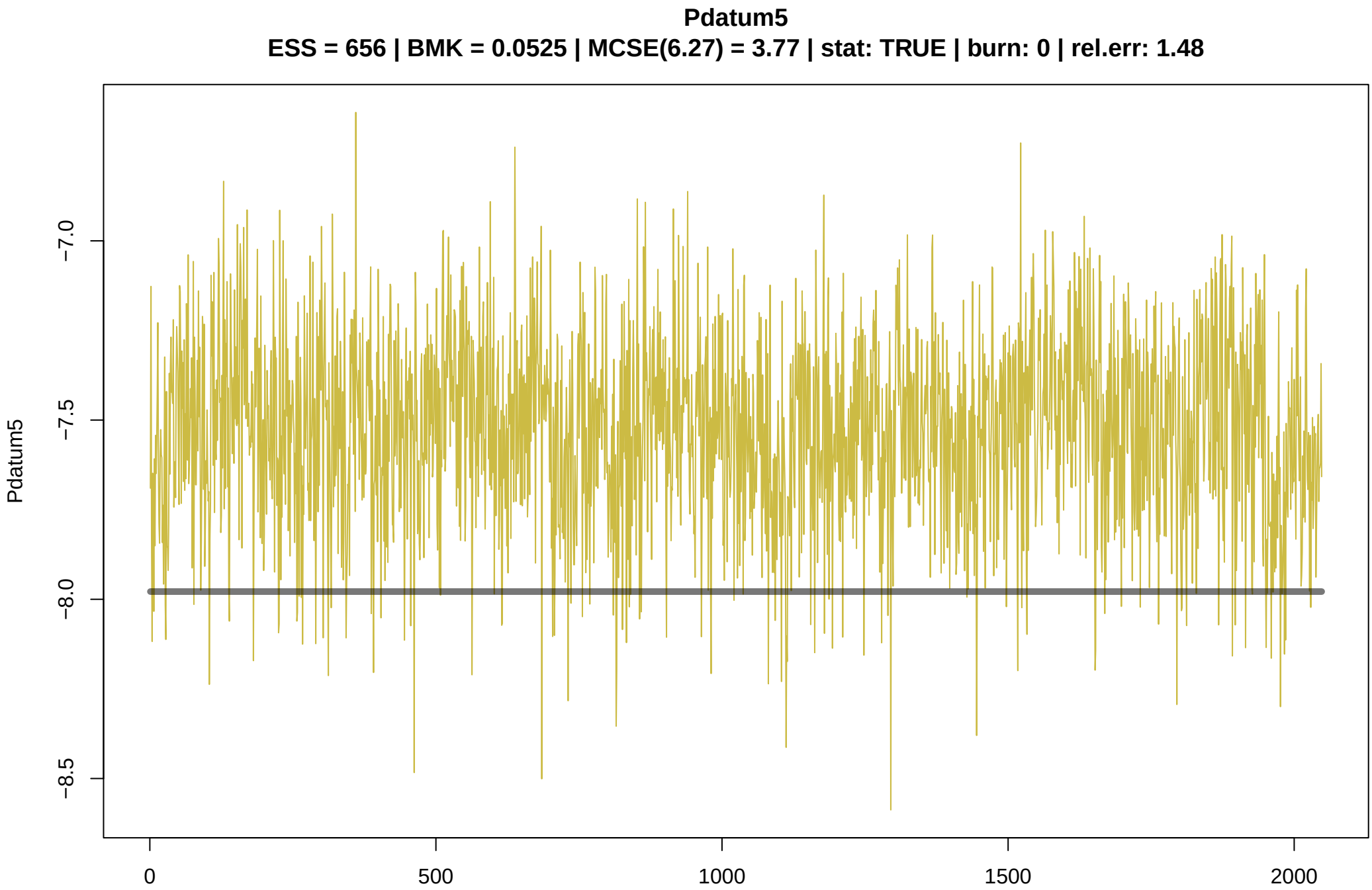

PdatacornerLo
ESS = 1660 | BMK = 0.045 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0 | rel.err: 0.677
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

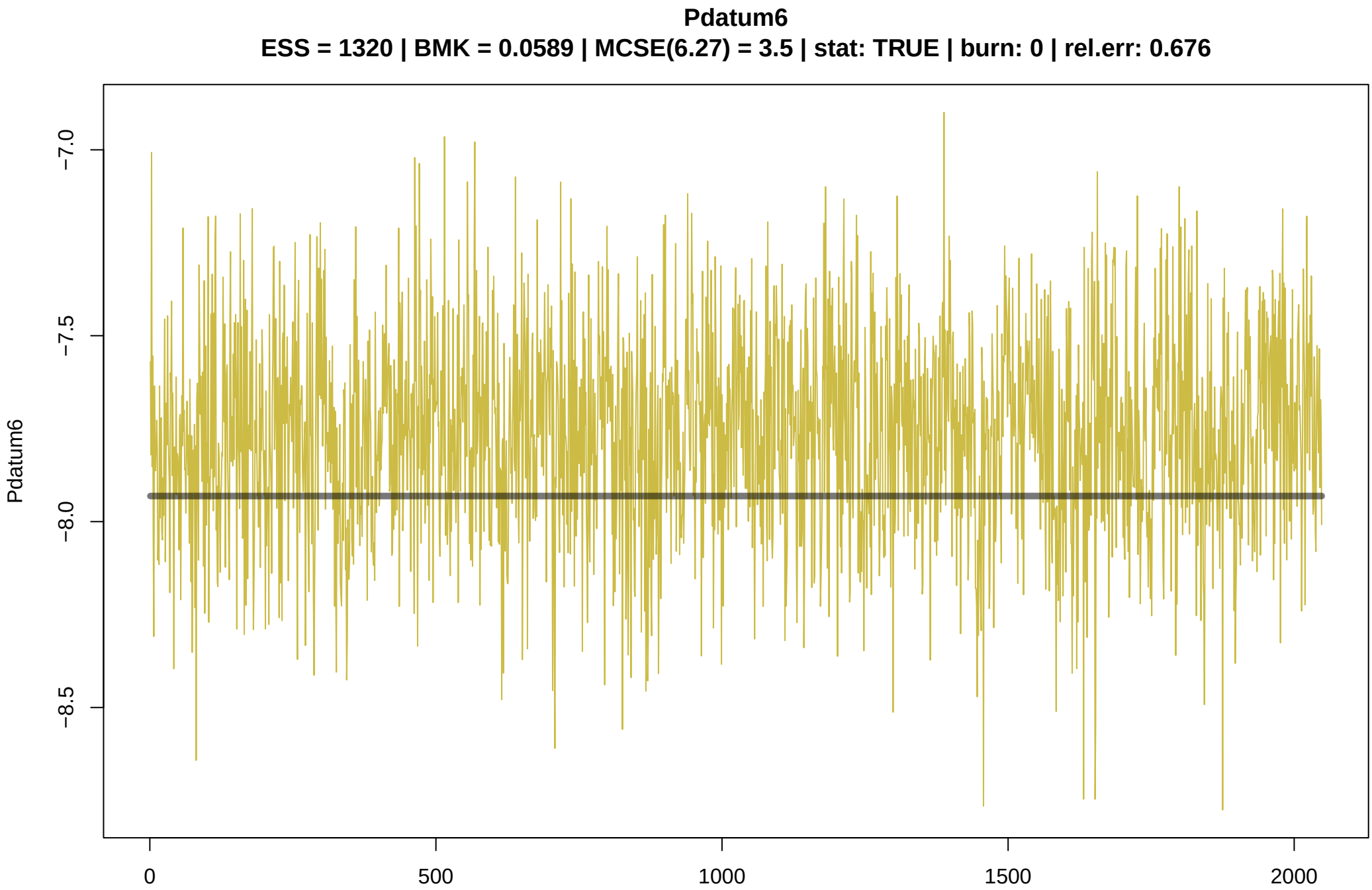

Pdatum1
ESS = 151 | BMK = 0.0863 | MCSE(6.27) = 6.4 | stat: TRUE | burn: 0 | rel.err: −0.888
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

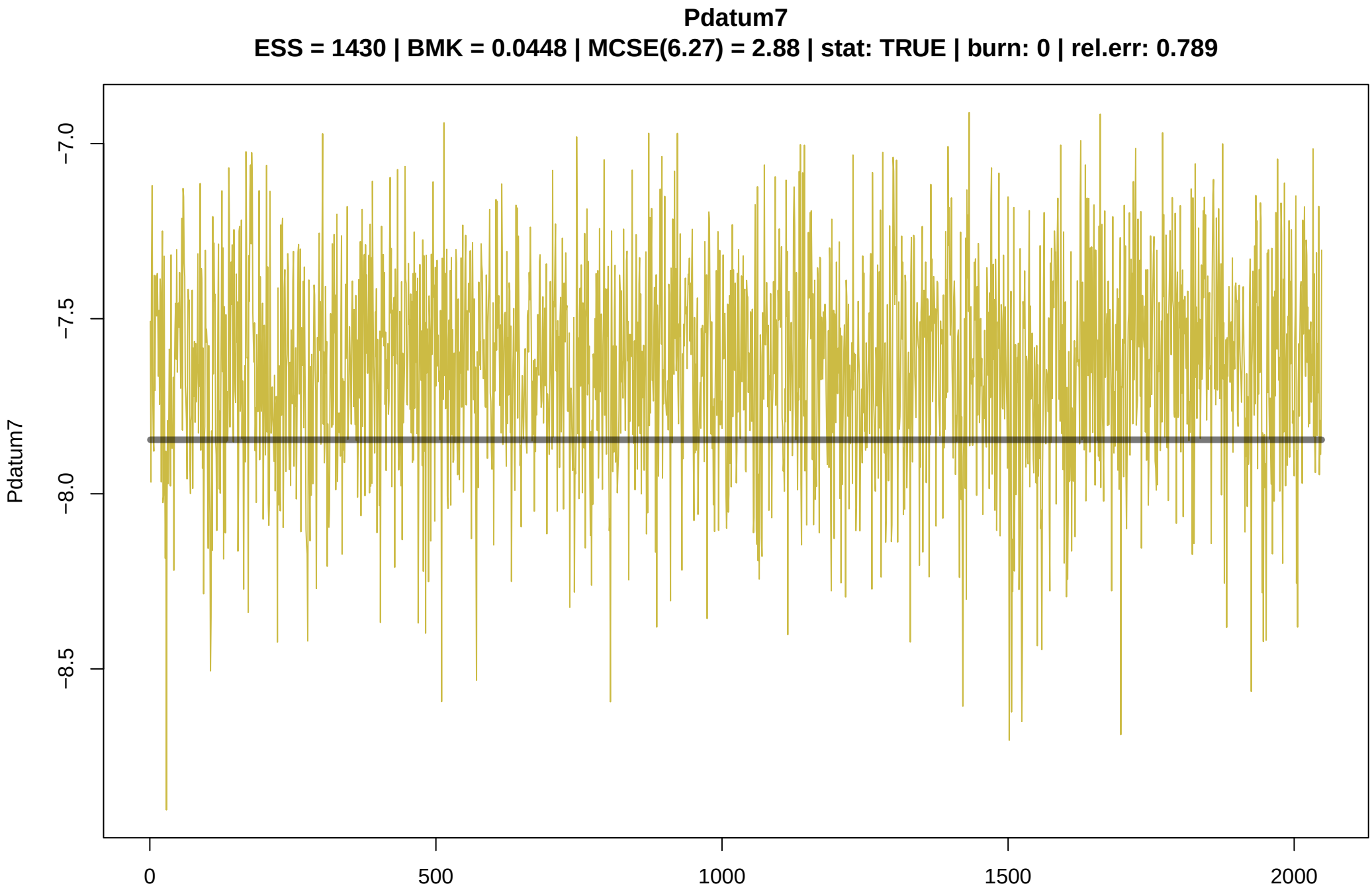

Pdatum2
ESS = 263 | BMK = 0.0854 | MCSE(6.27) = 6.14 | stat: TRUE | burn: 0 | rel.err: −2.1
Pdatum2
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

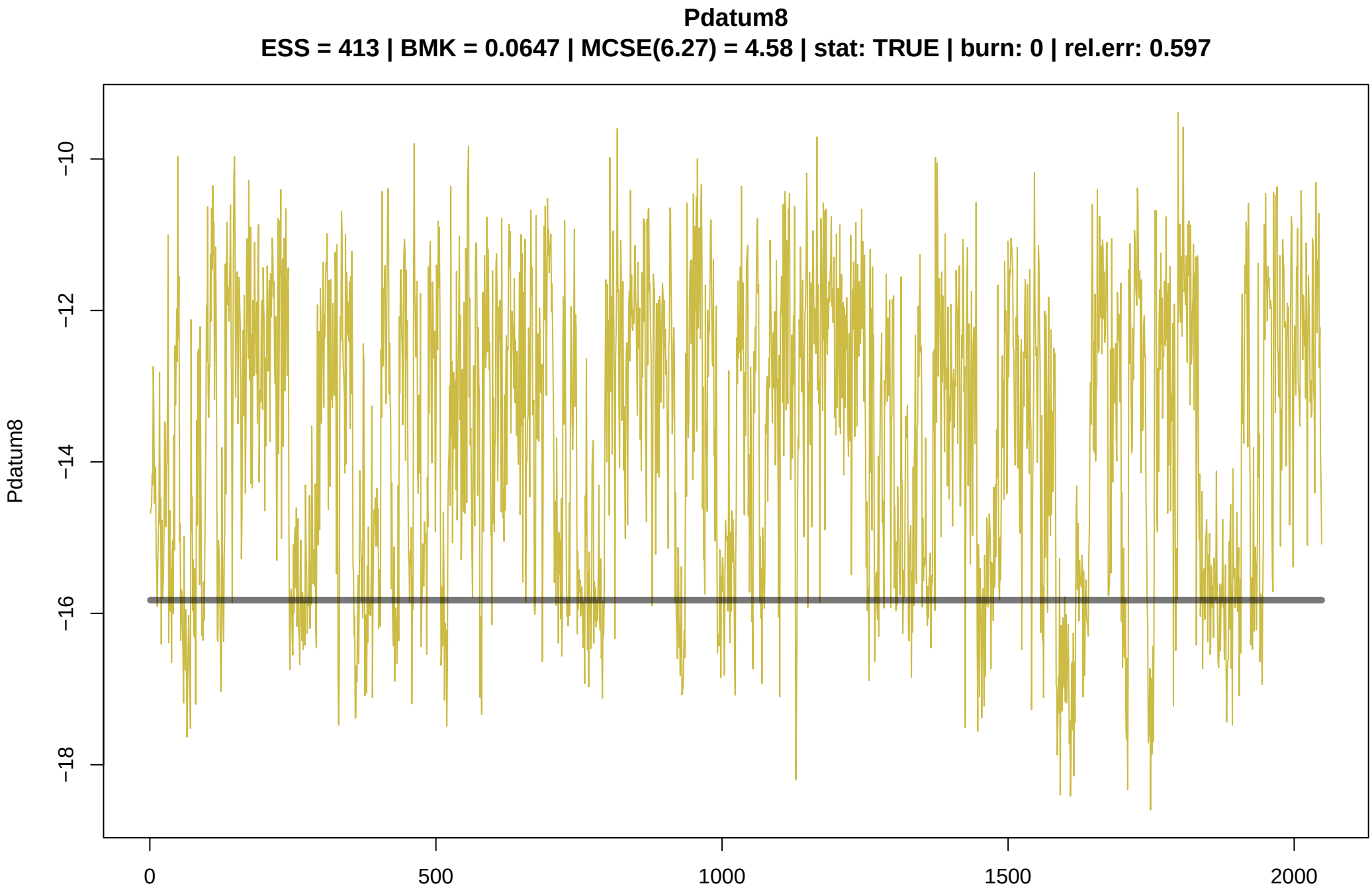

Pdatum3
ESS = 603 | BMK = 0.0478 | MCSE(6.27) = 4.06 | stat: FALSE | burn: 0 | rel.err: −0.416
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

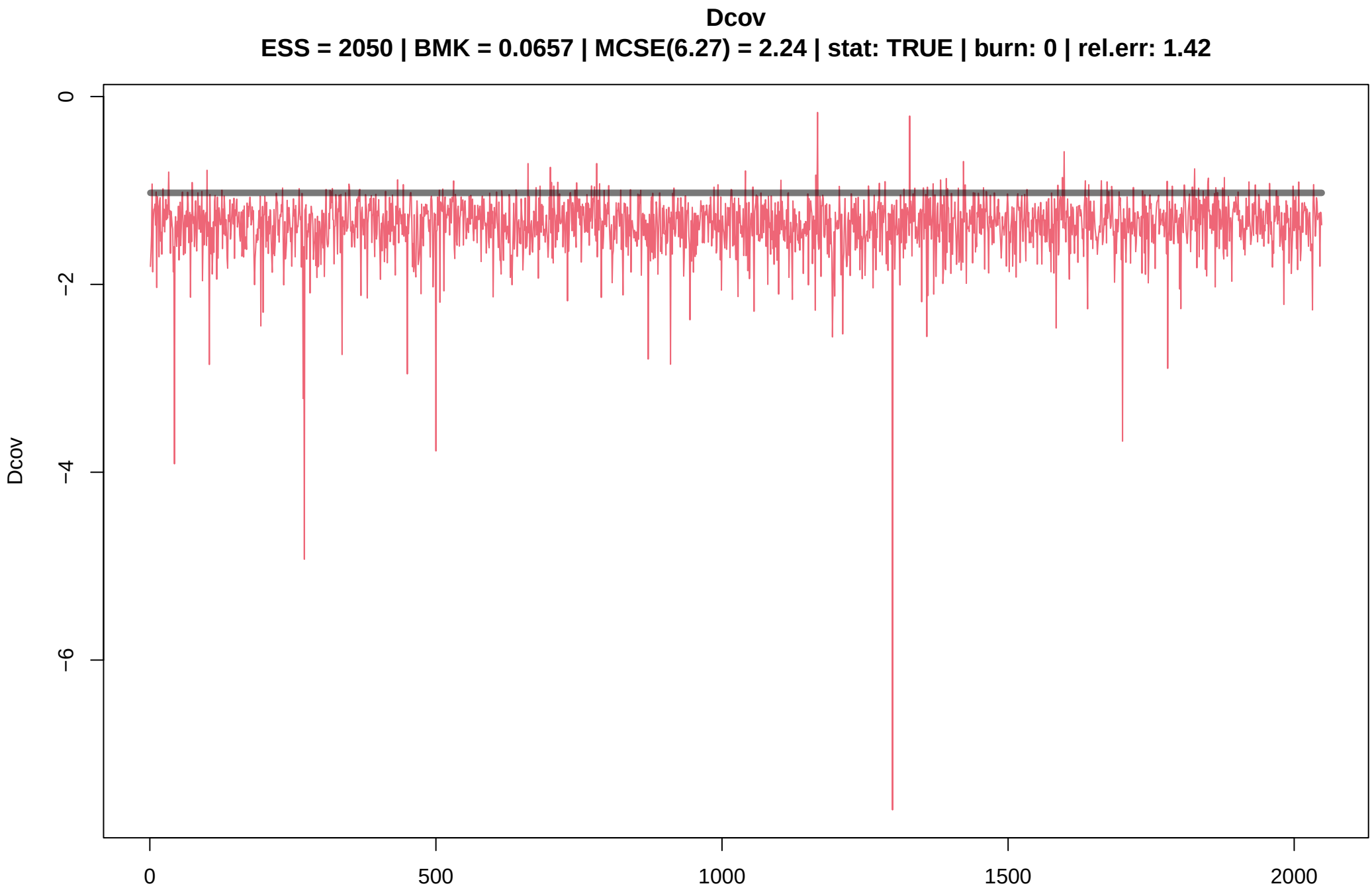

Pdatum4
ESS = 625 | BMK = 0.0598 | MCSE(6.27) = 4.49 | stat: TRUE | burn: 0 | rel.err: −0.0606
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

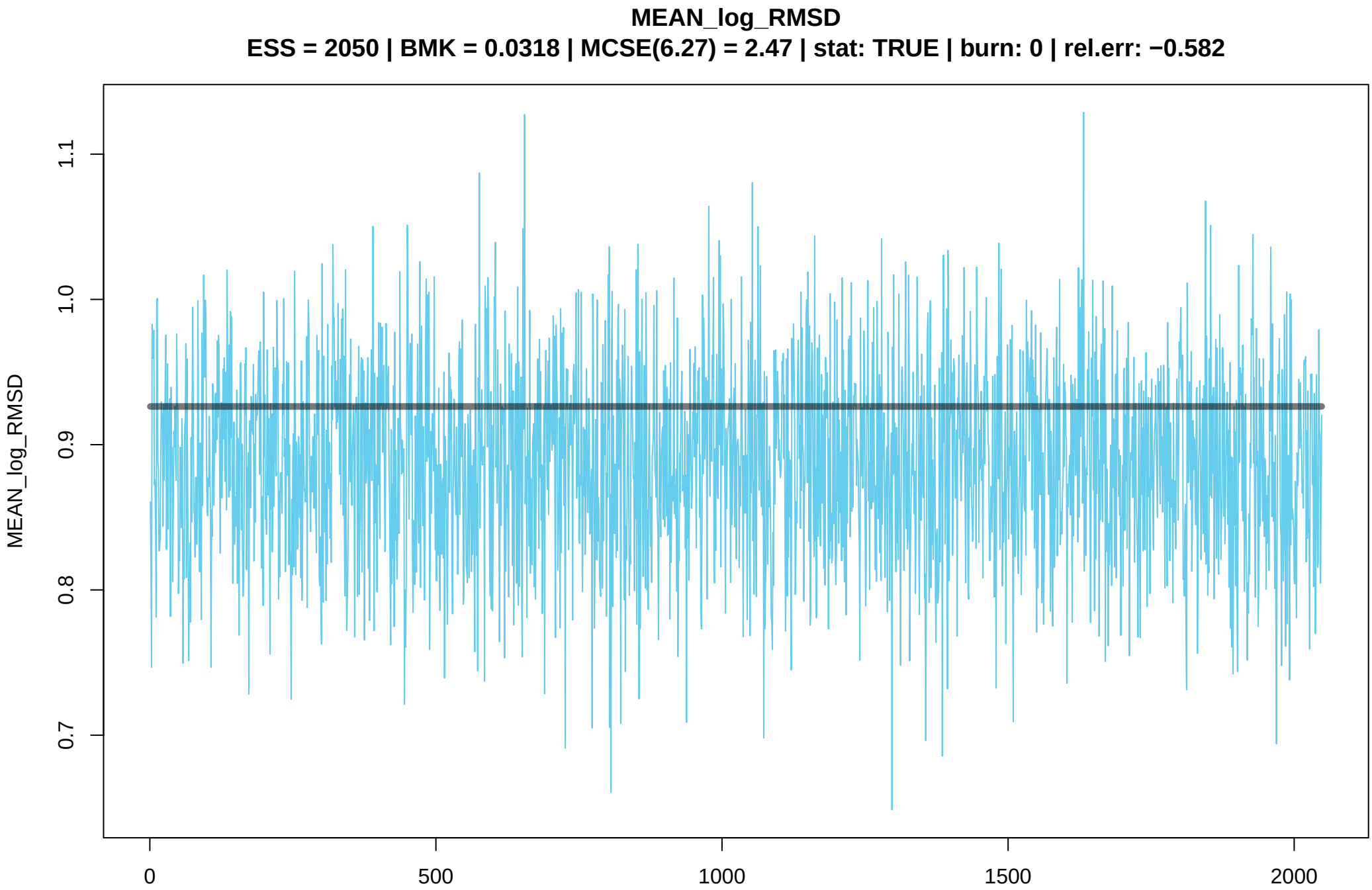

Pdatum5
ESS = 656 | BMK = 0.0525 | MCSE(6.27) = 3.77 | stat: TRUE | burn: 0 | rel.err: 1.48
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

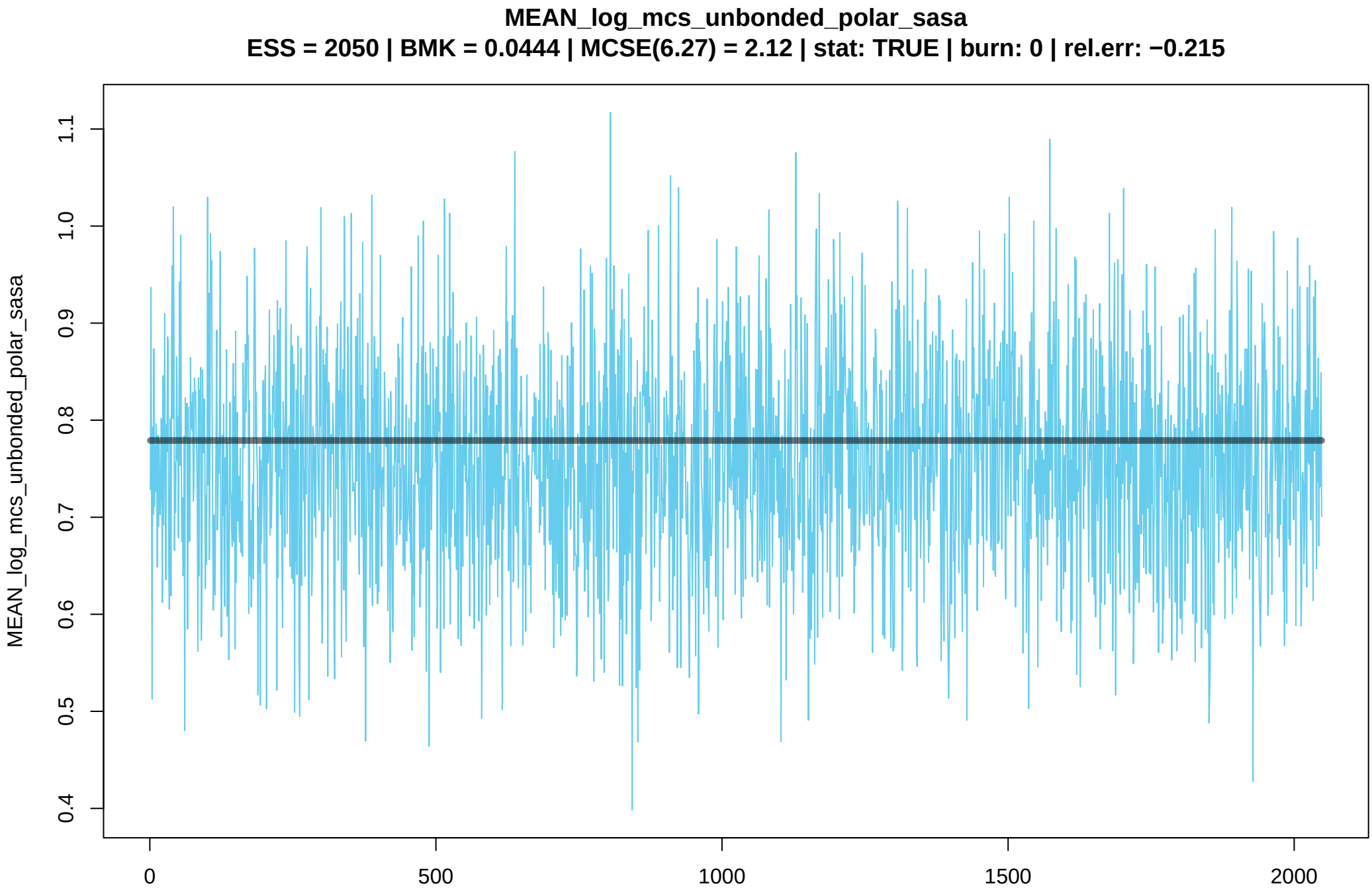

Pdatum6
ESS = 1320 | BMK = 0.0589 | MCSE(6.27) = 3.5 | stat: TRUE | burn: 0 | rel.err: 0.676
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

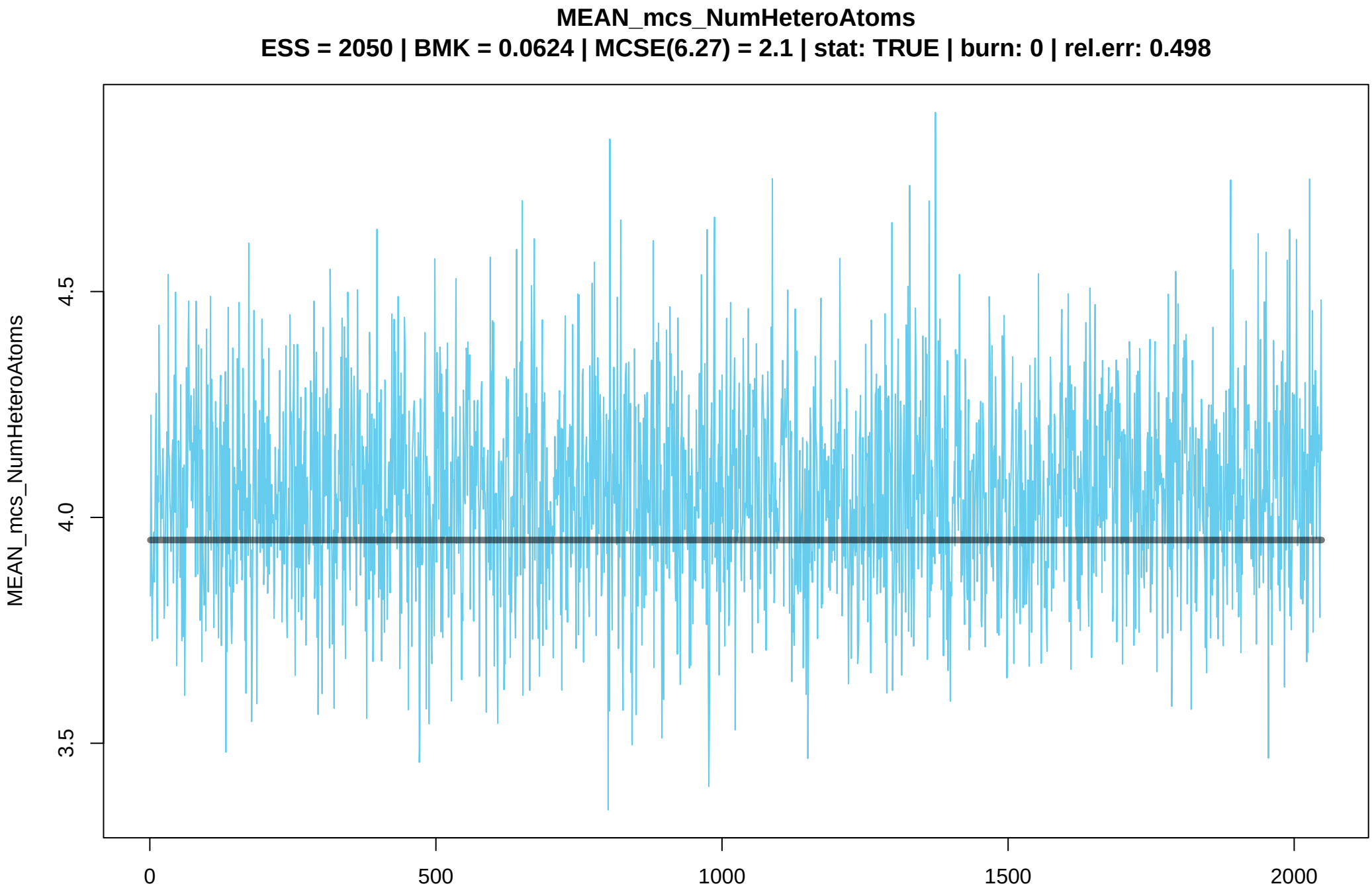

Pdatum7
ESS = 1430 | BMK = 0.0448 | MCSE(6.27) = 2.88 | stat: TRUE | burn: 0 | rel.err: 0.789
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

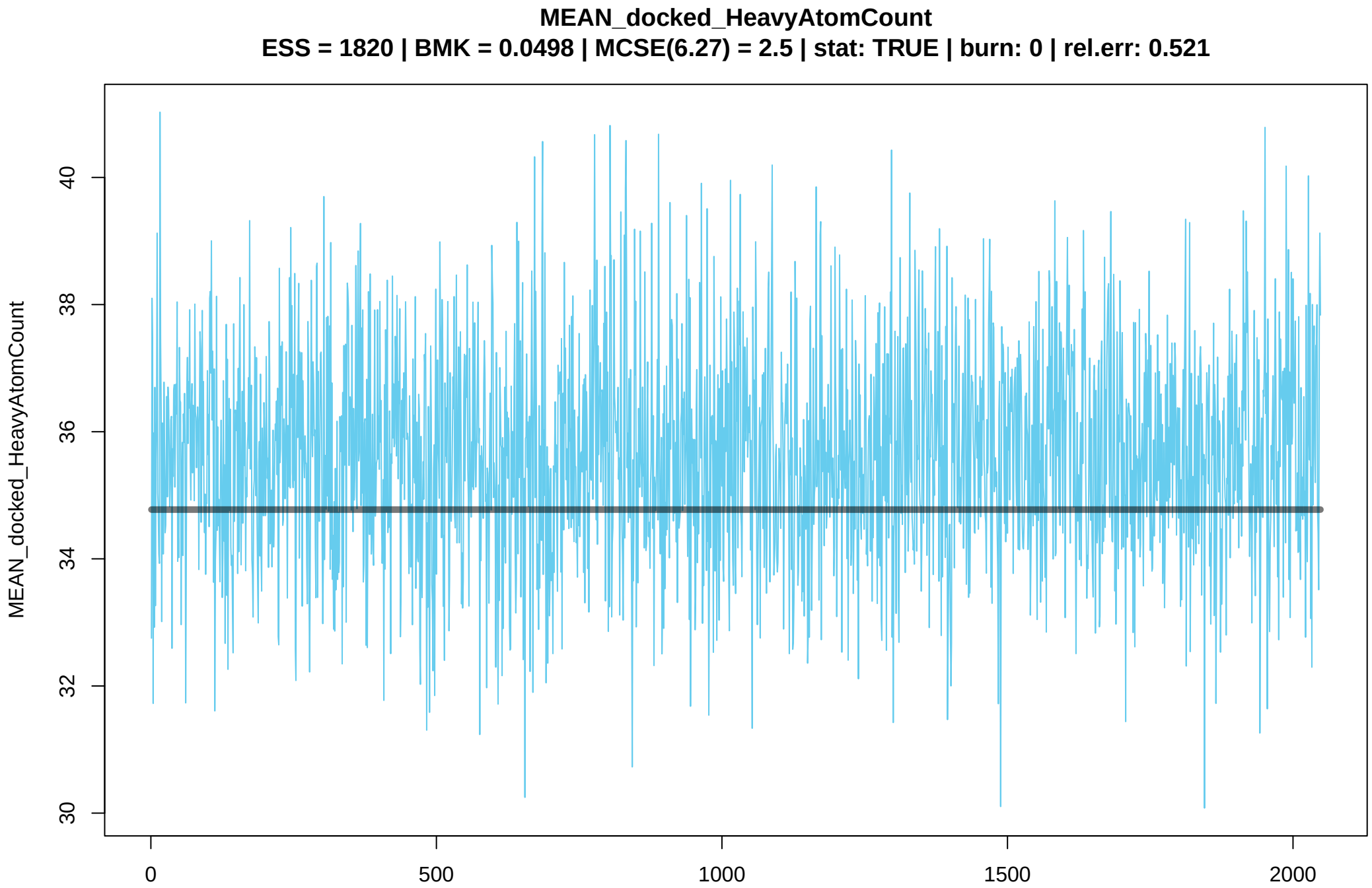

Pdatum8
ESS = 413 | BMK = 0.0647 | MCSE(6.27) = 4.58 | stat: TRUE | burn: 0 | rel.err: 0.597
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

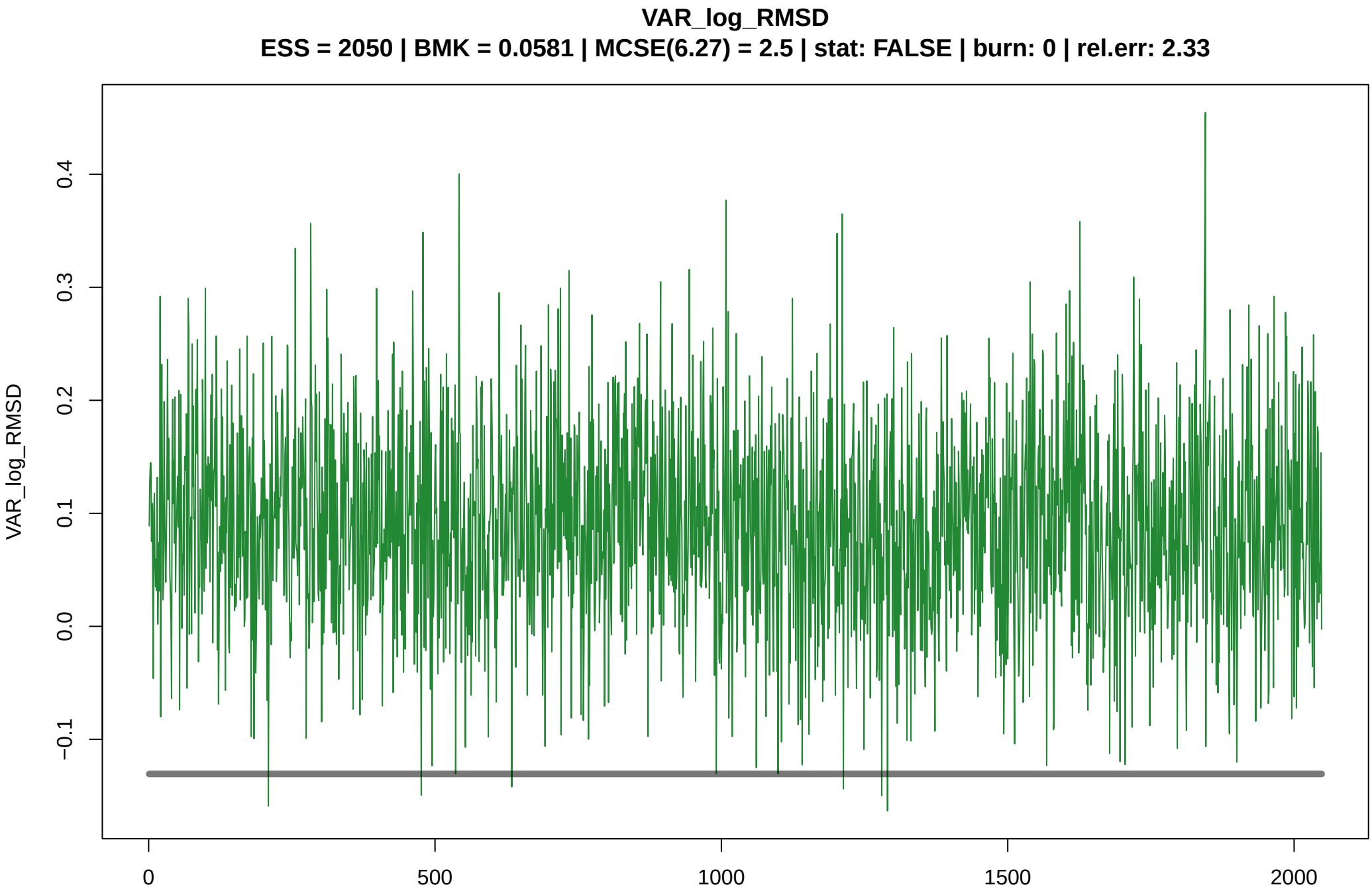

Dcov
ESS = 2050 | BMK = 0.0657 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | rel.err: 1.42
Dcov
0
−2
−4
−6
0
500
1000
1500
2000

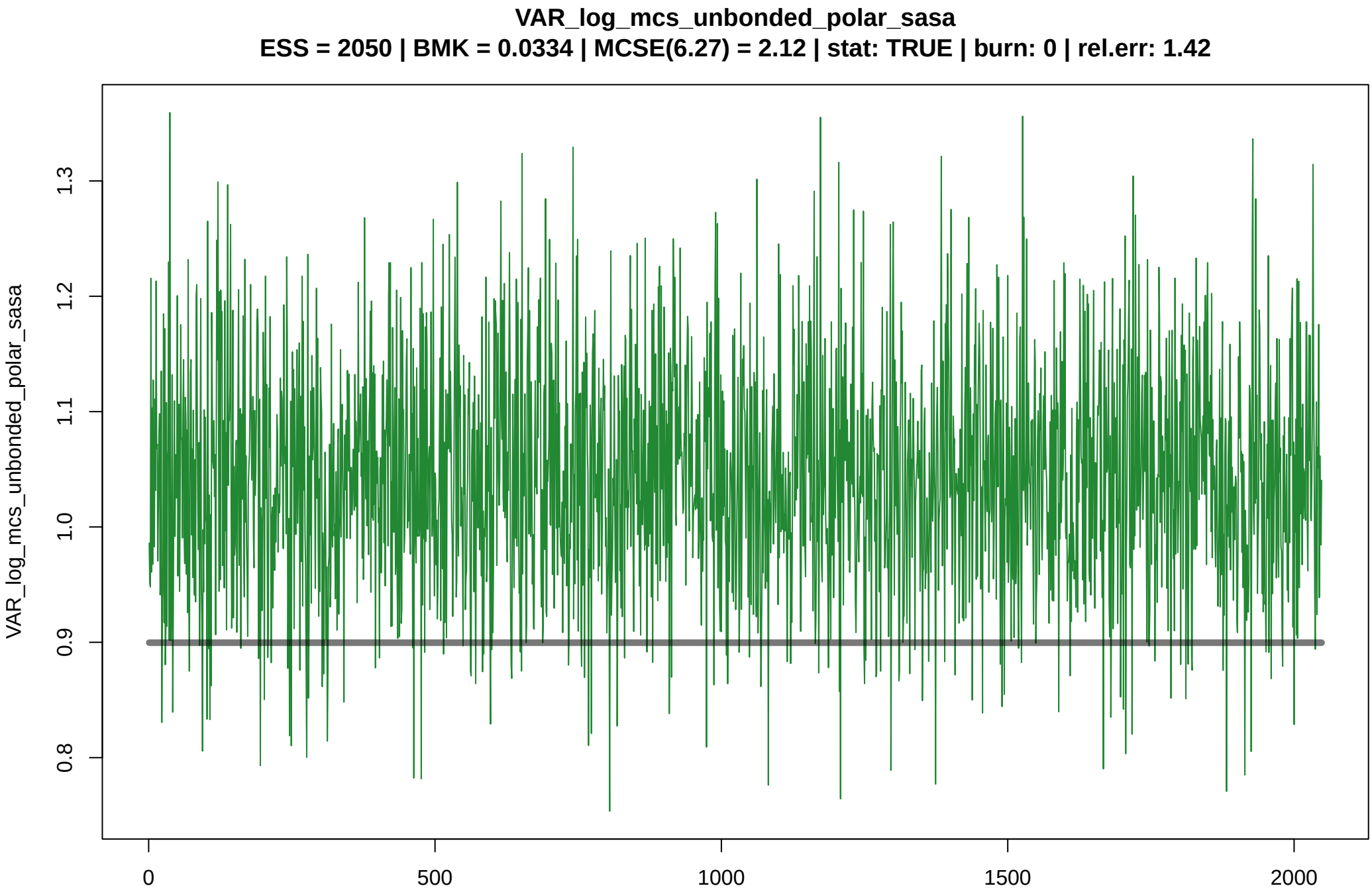

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0318 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | rel.err: −0.582
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

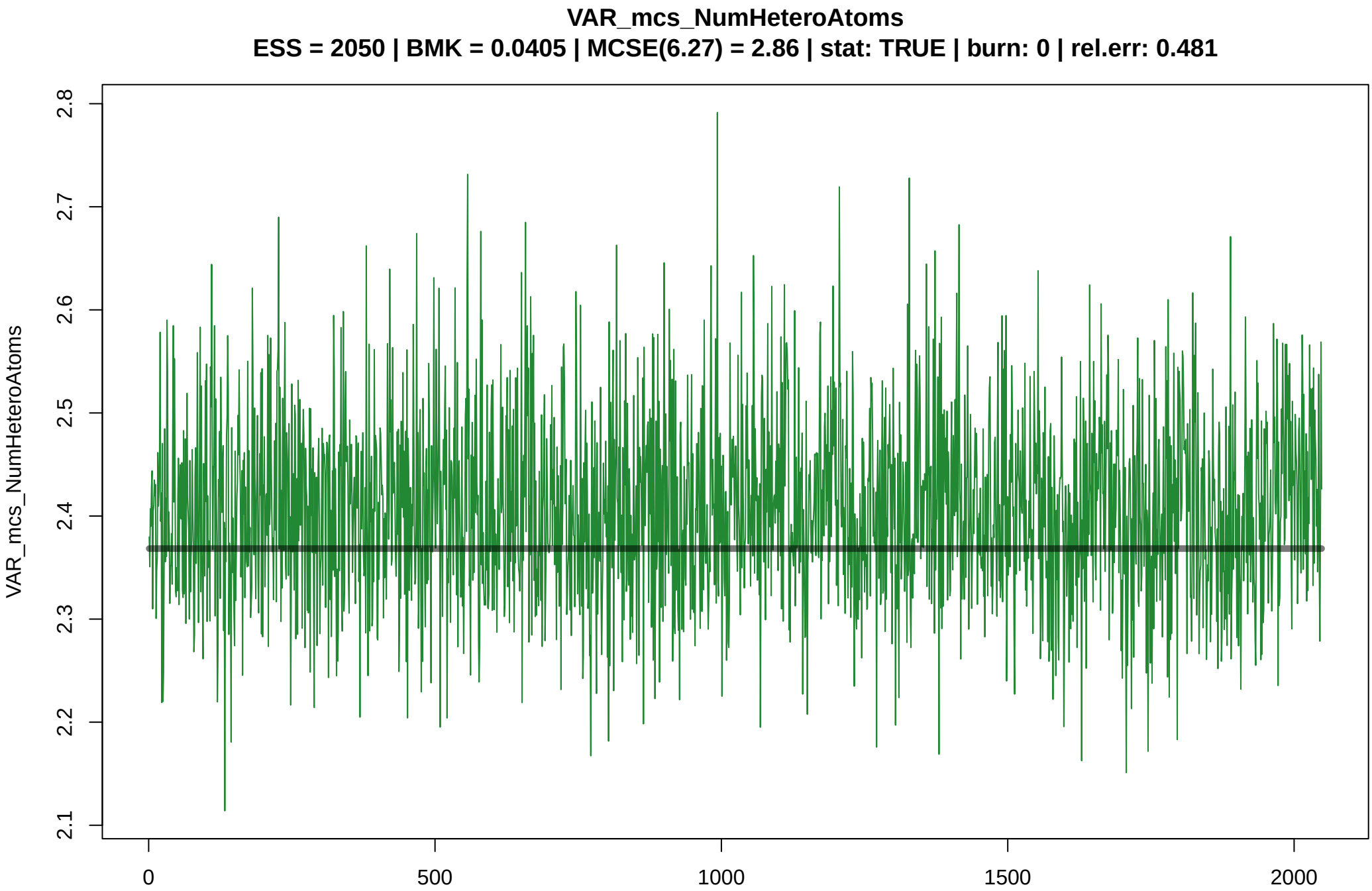

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0444 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: −0.215
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

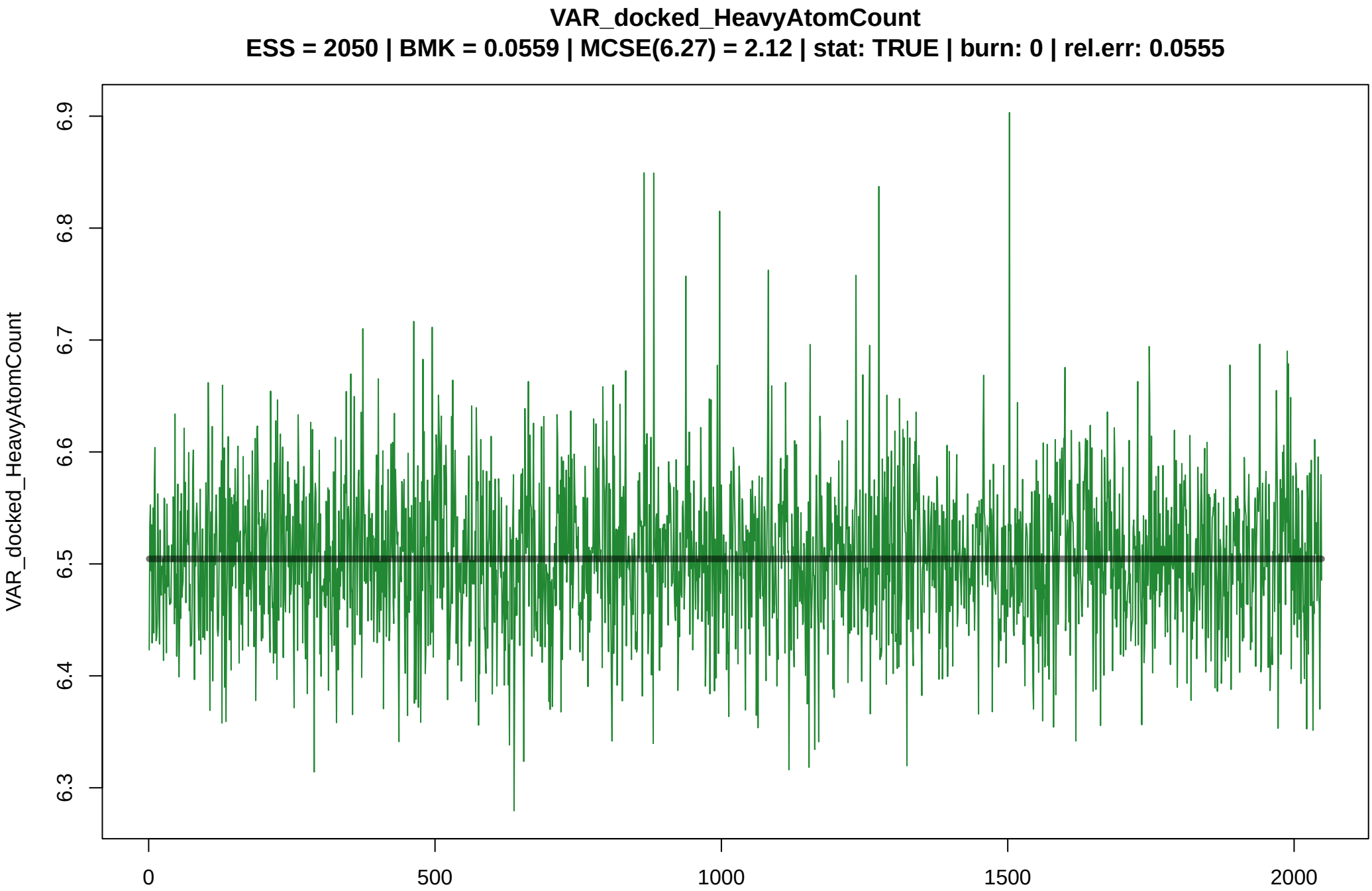

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0624 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0 | rel.err: 0.498
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
500
1000
1500
2000

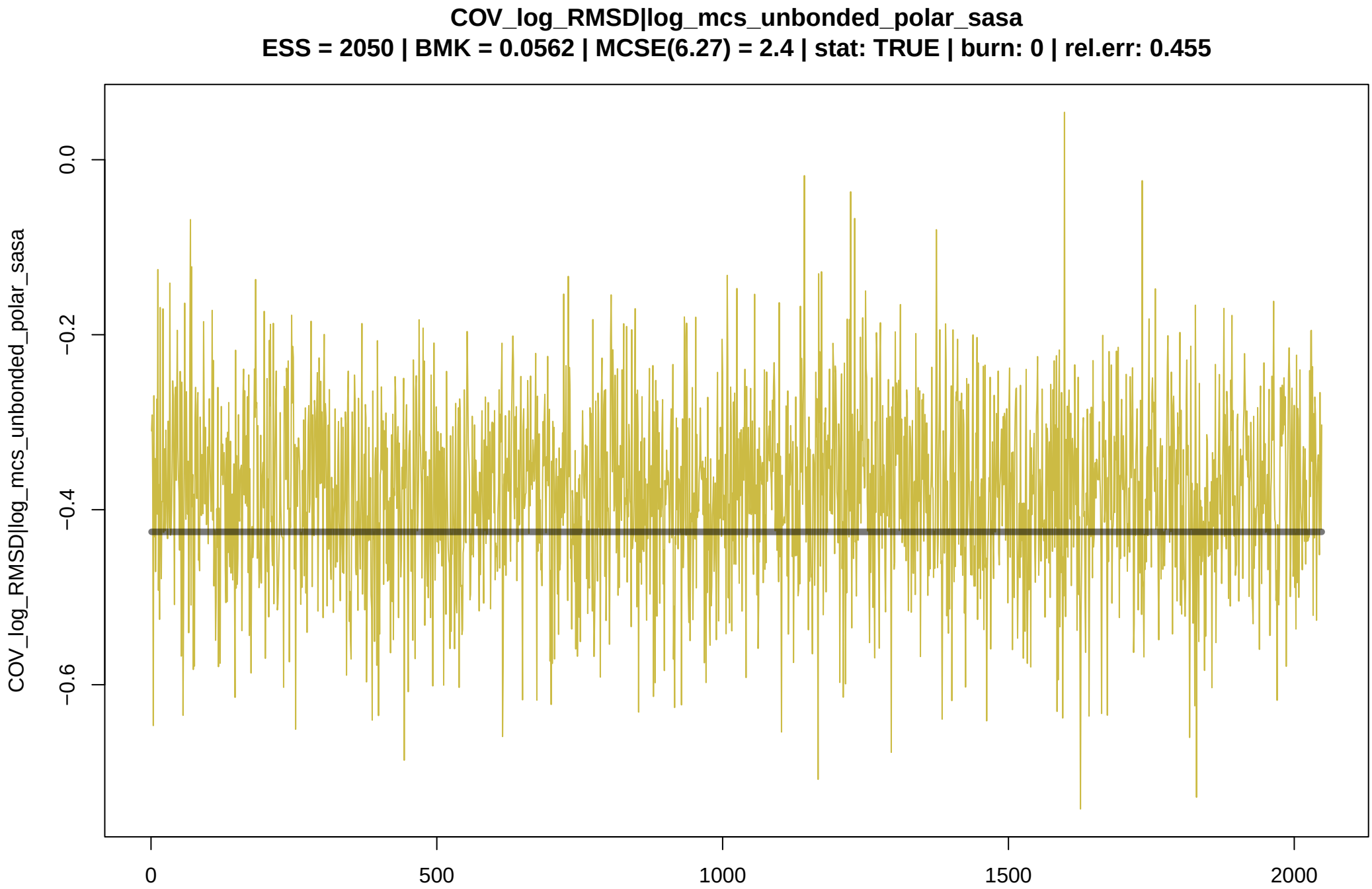

MEAN_docked_HeavyAtomCount
ESS = 1820 | BMK = 0.0498 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 0.521
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

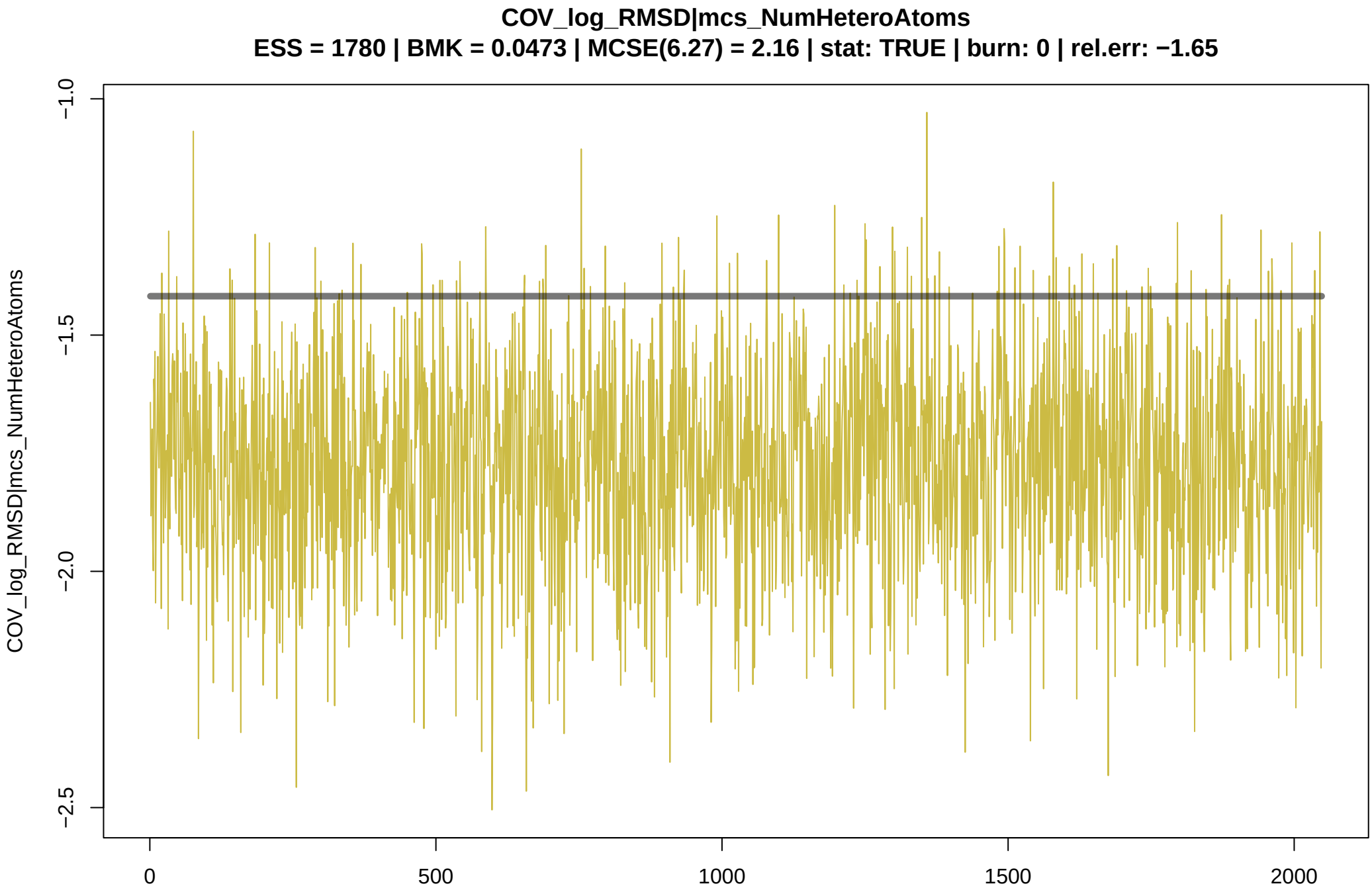

VAR_log_RMSD
ESS = 2050 | BMK = 0.0581 | MCSE(6.27) = 2.5 | stat: FALSE | burn: 0 | rel.err: 2.33
VAR_log_RMSD
−0.1
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

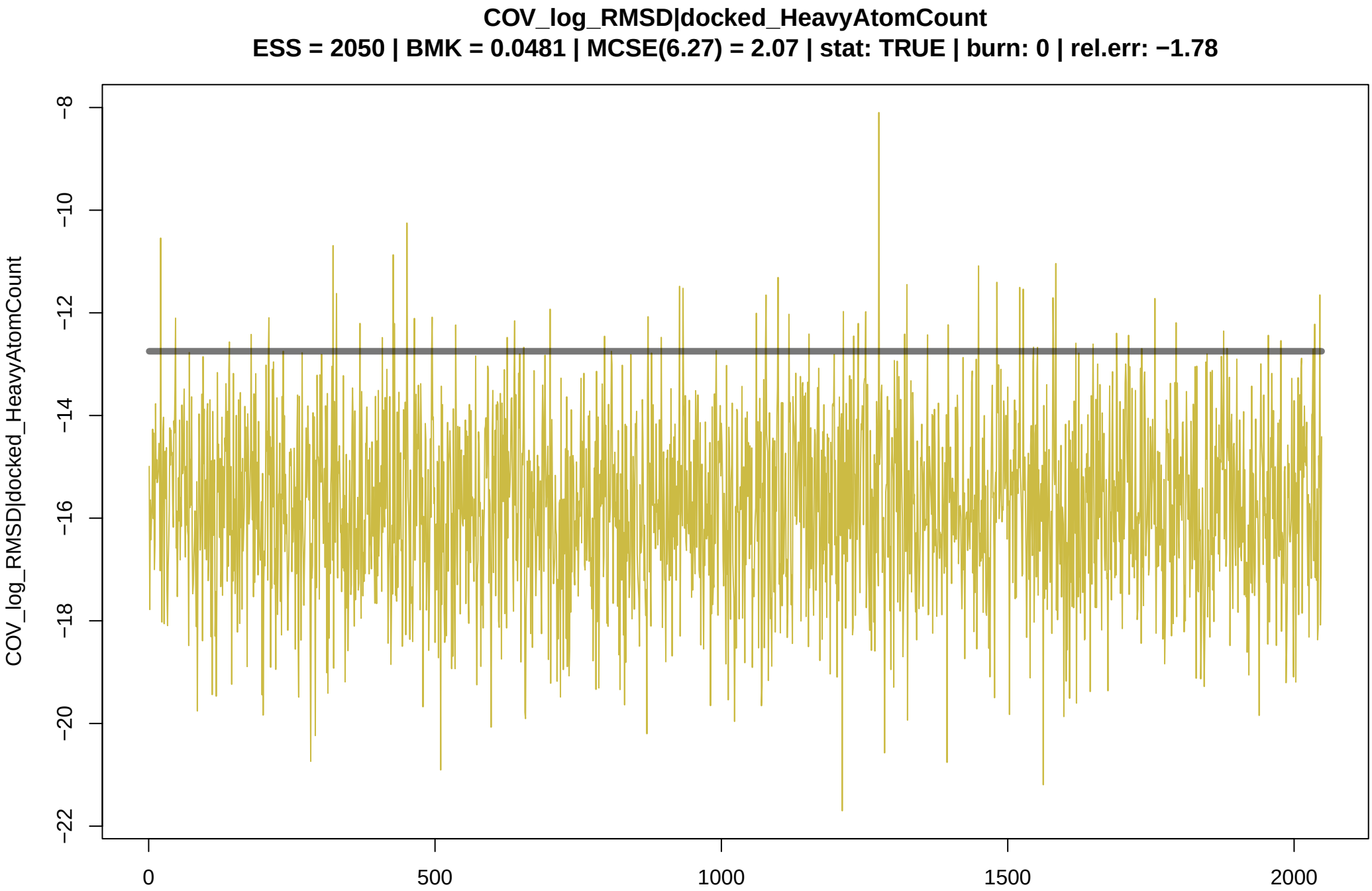

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0334 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: 1.42
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
0
500
1000
1500
2000

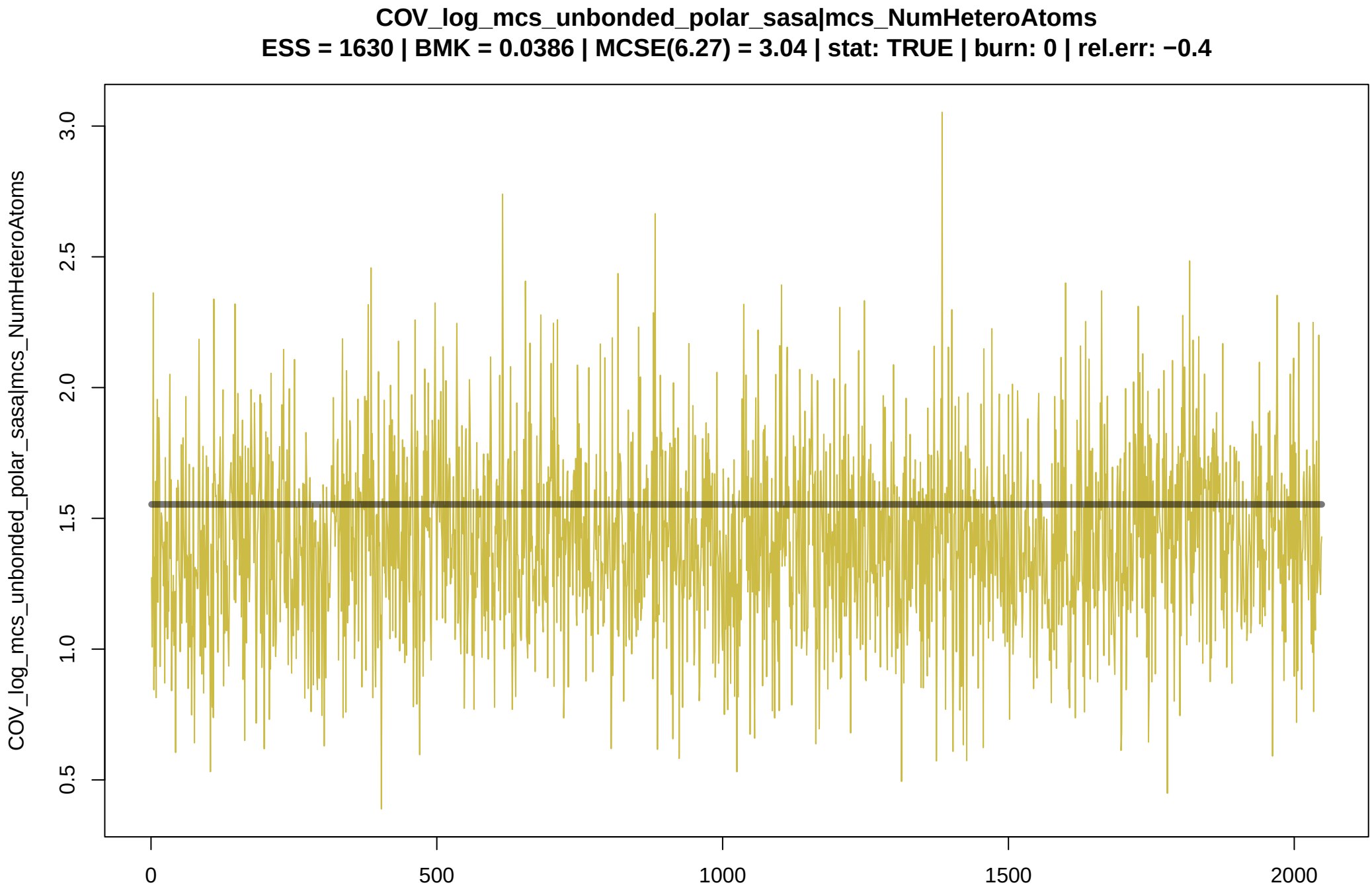

VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0405 | MCSE(6.27) = 2.86 | stat: TRUE | burn: 0 | rel.err: 0.481
VAR_mcs_NumHeteroAtoms
2.1
2.2
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000

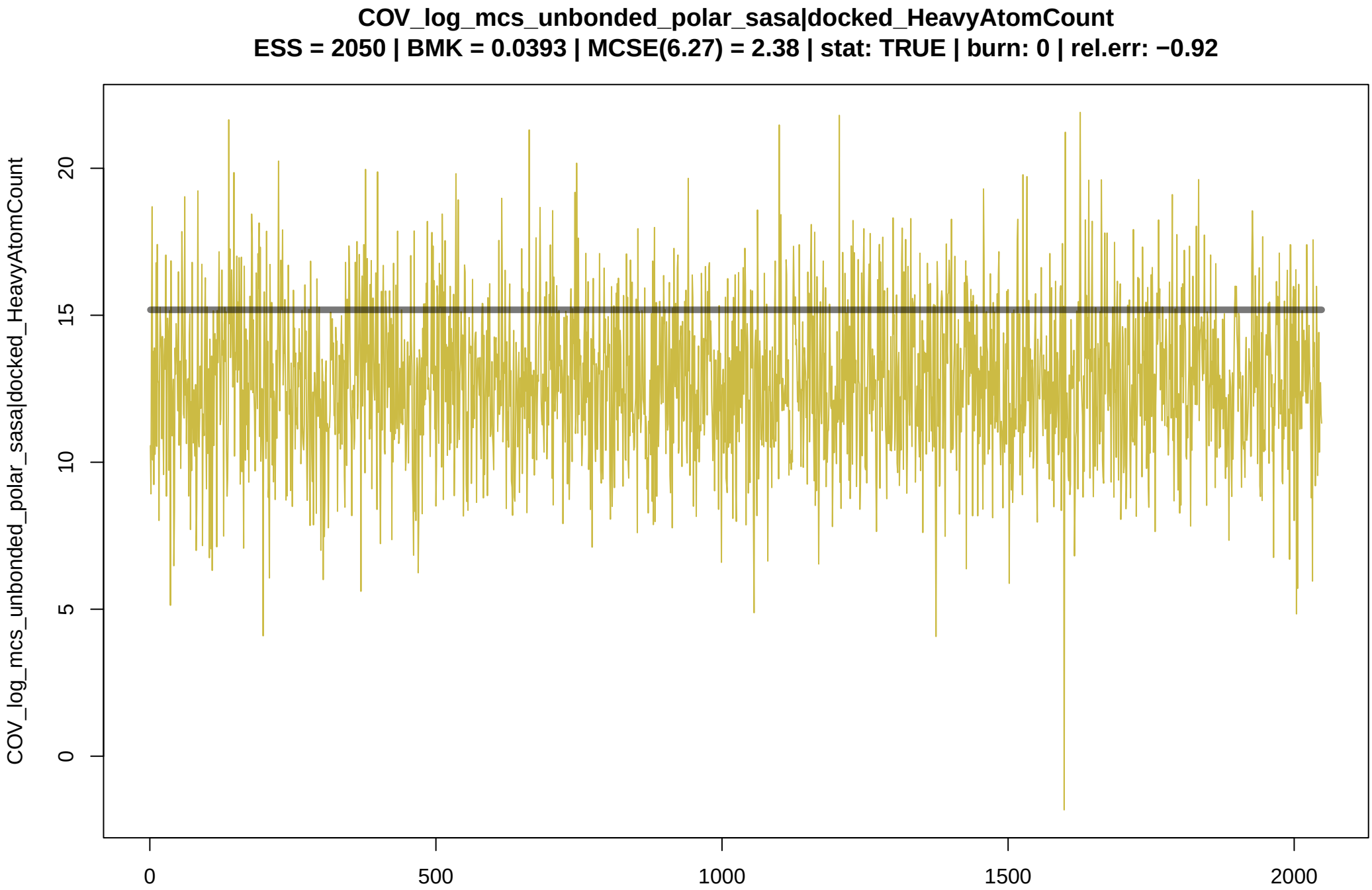

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0559 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: 0.0555
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
6.9
0
500
1000
1500
2000

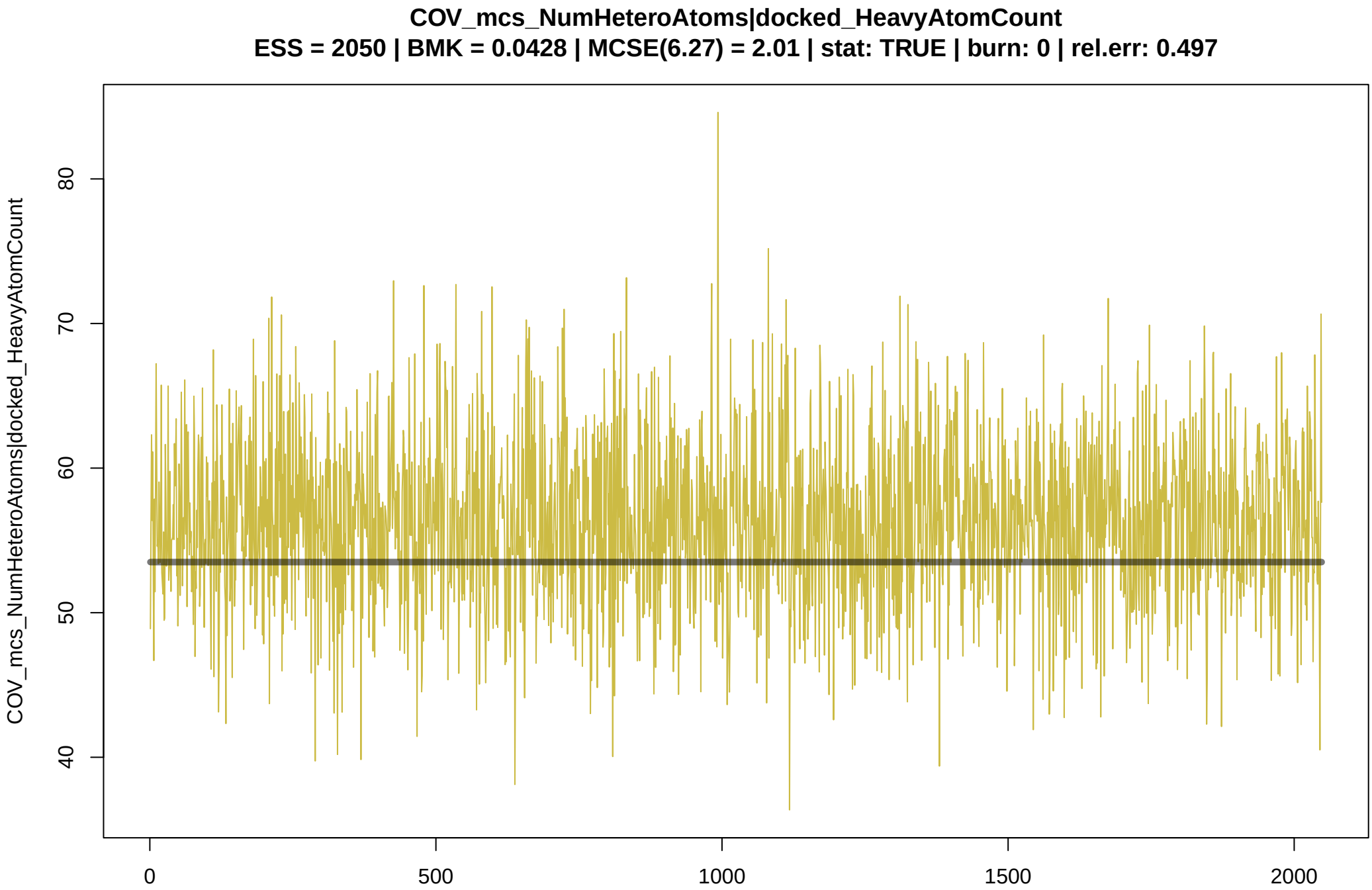

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0562 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0 | rel.err: 0.455
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1780 | BMK = 0.0473 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0 | rel.err: −1.65
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.5
−2.0
−2.5
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0481 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0 | rel.err: −1.78
COV_log_RMSD|docked_HeavyAtomCount
−8
−10
−12
−14
−16
−18
−20
−22
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1630 | BMK = 0.0386 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0 | rel.err: −0.4
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
3.0
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0393 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0 | rel.err: −0.92
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 = 0.0428 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: 0.497
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000