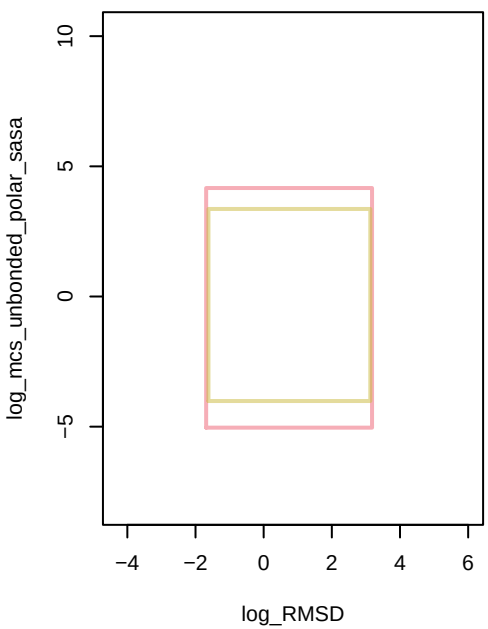
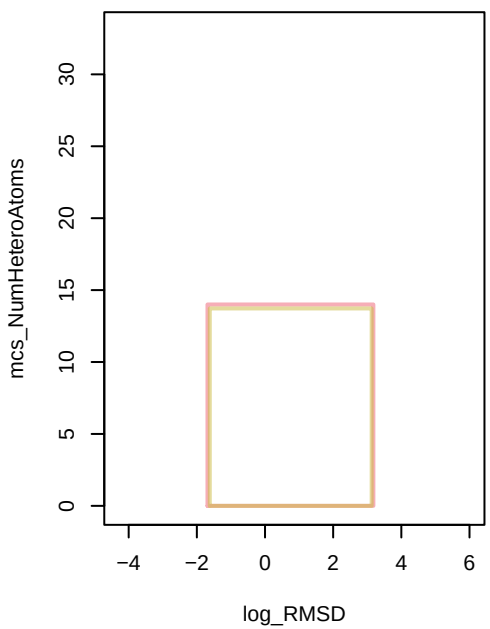
−− STATS maxD −−
min ESS = 104.375236159272
max BMK = 0.21303897065458
max MCSE = 7.09059719562736
all stationary: FALSE
burn: 0
max rel.err.: 2.0548080953758 7

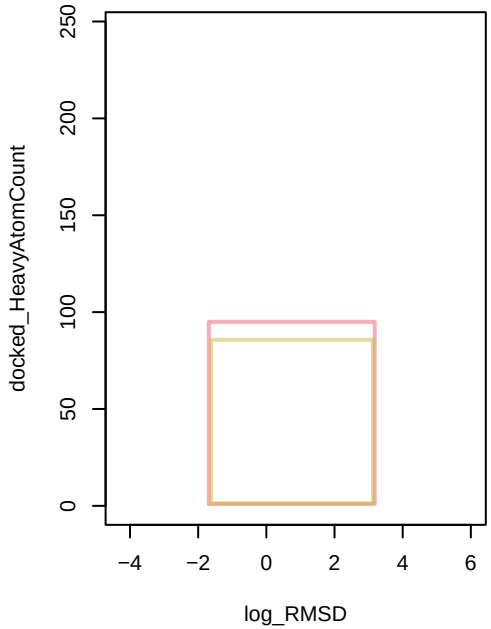
−− STATS 2D −−
min ESS = 1618.59370610936
max BMK = 0.052536436449655 8
max MCSE = 2.46891652451312
all stationary: FALSE
burn: 0
max rel.err.: 1.79156828579069

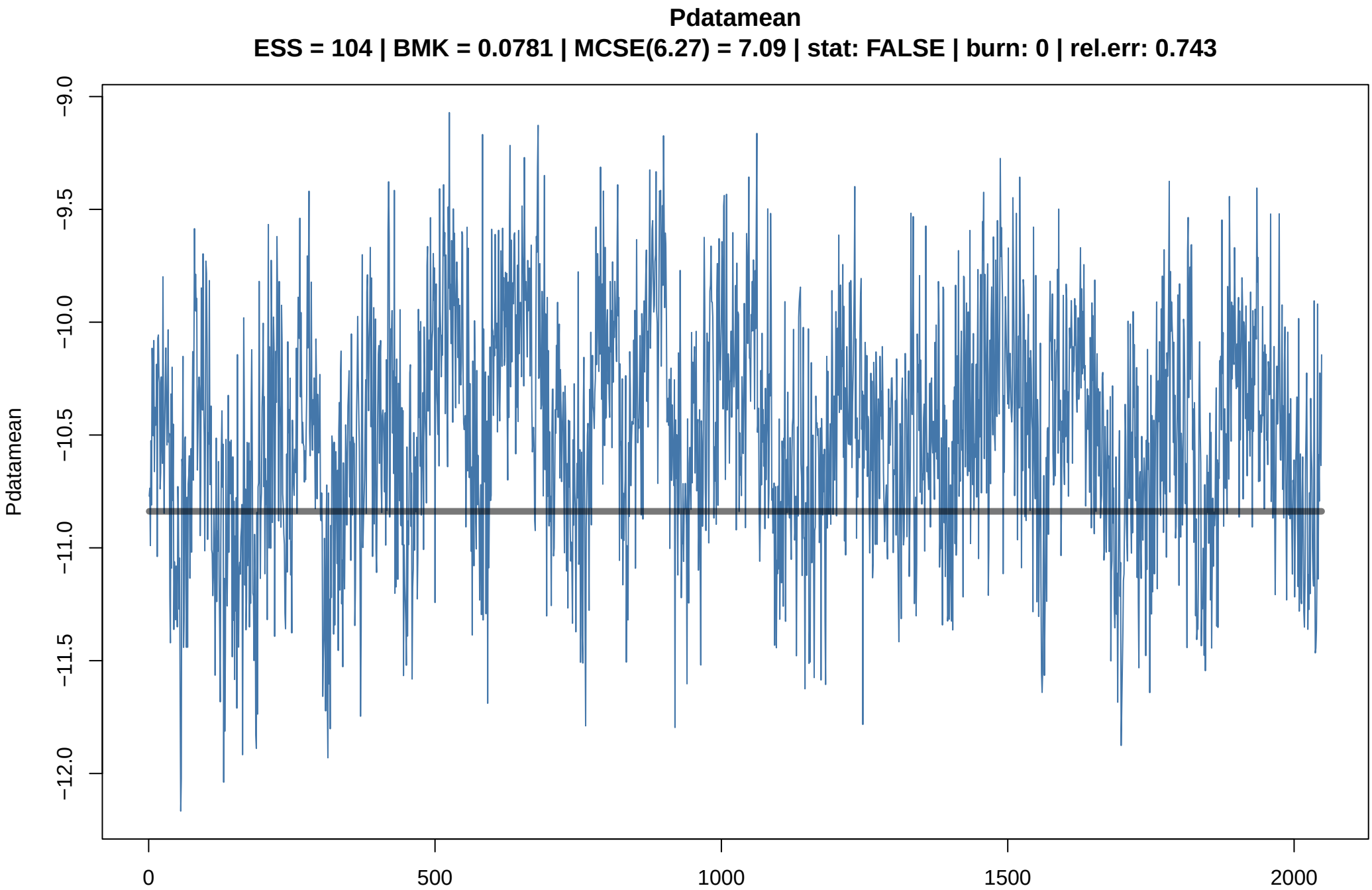
−− STATS 1D −−
min ESS = 1447.45564557472
max BMK = 0.067201101656586
max MCSE = 3.00273748861345
all stationary: TRUE
burn: 0
max rel.err.: 2.34763334131652

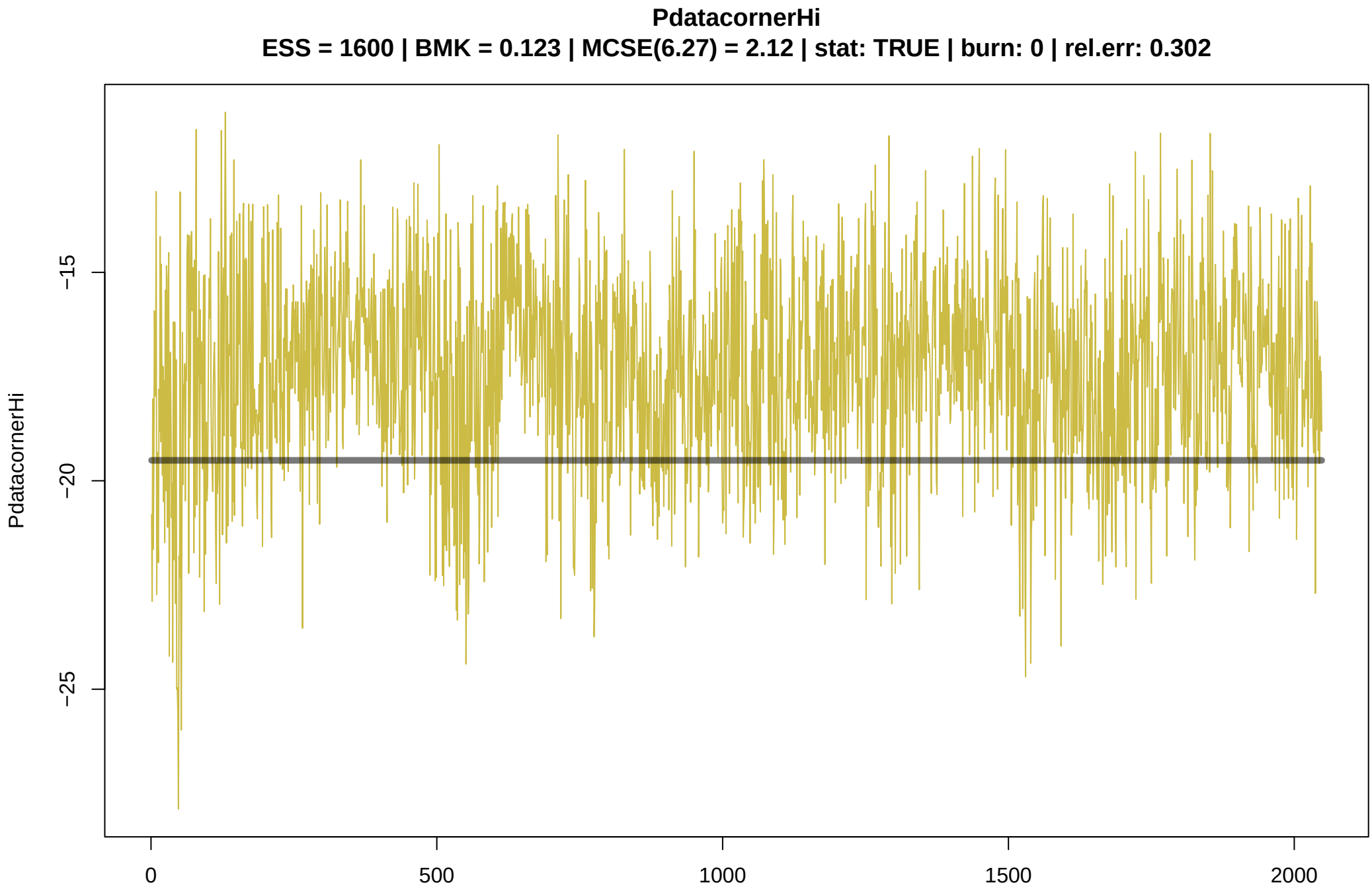
Occupied clusters: 10 of 16

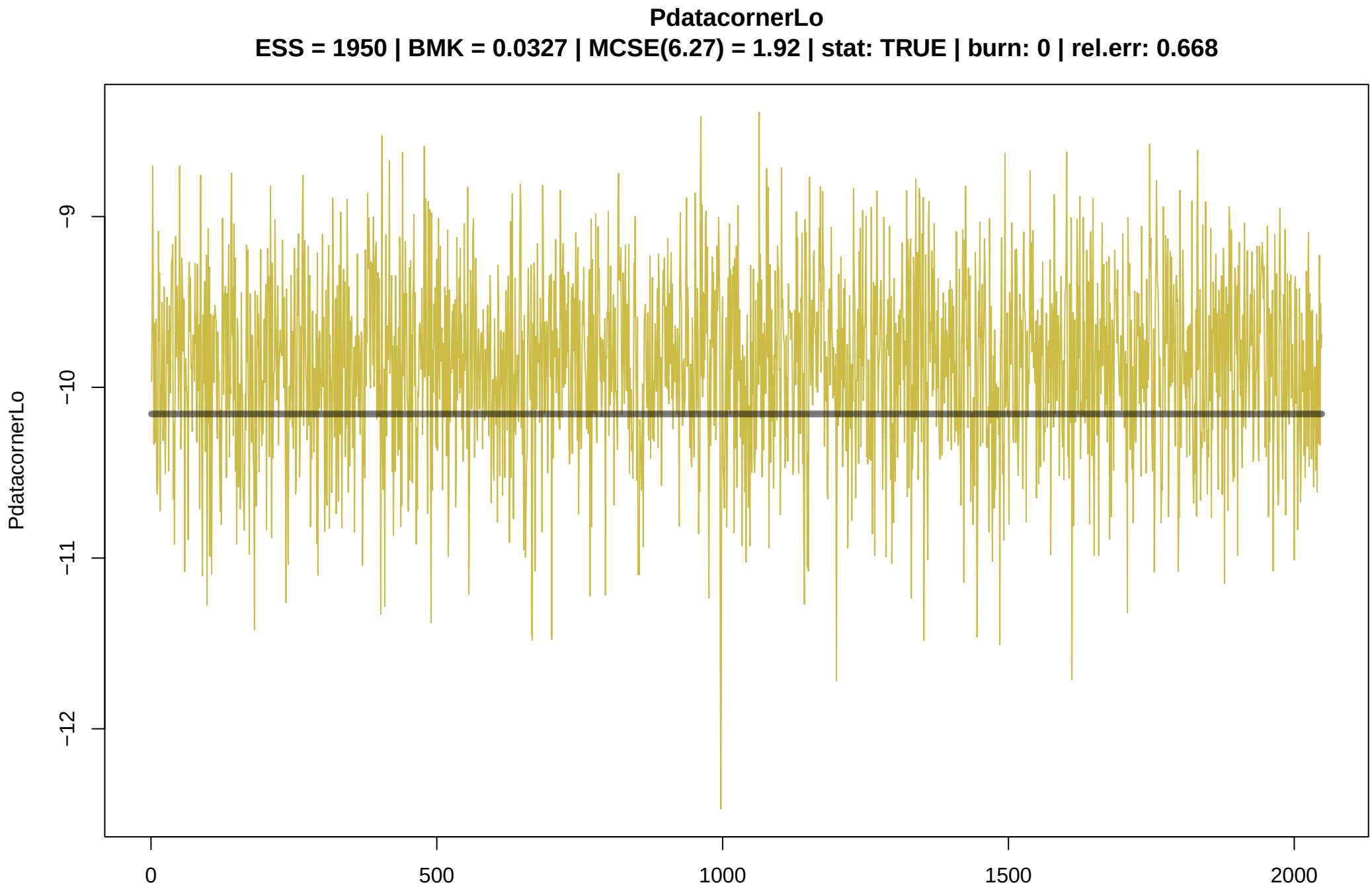

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

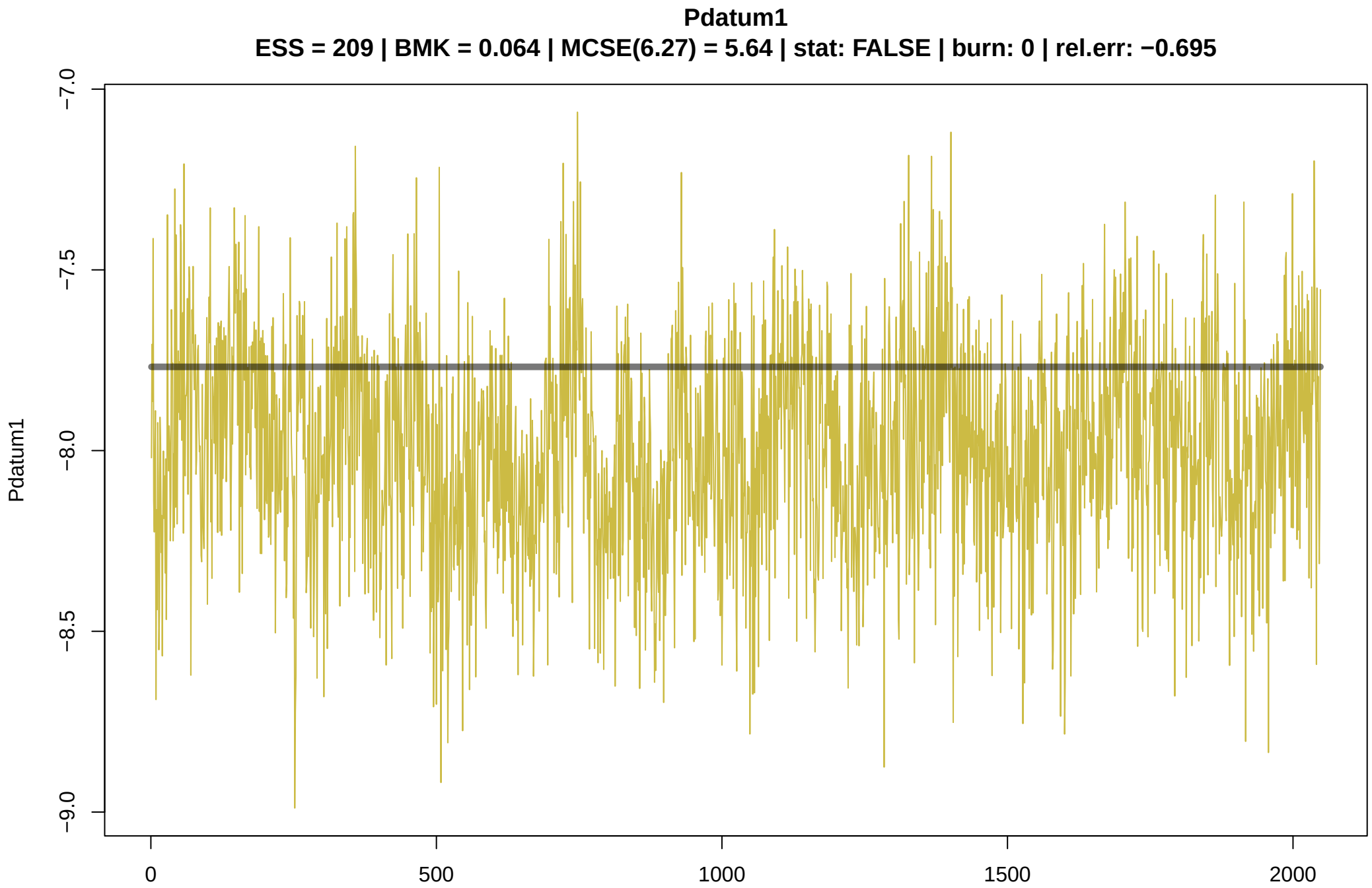

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

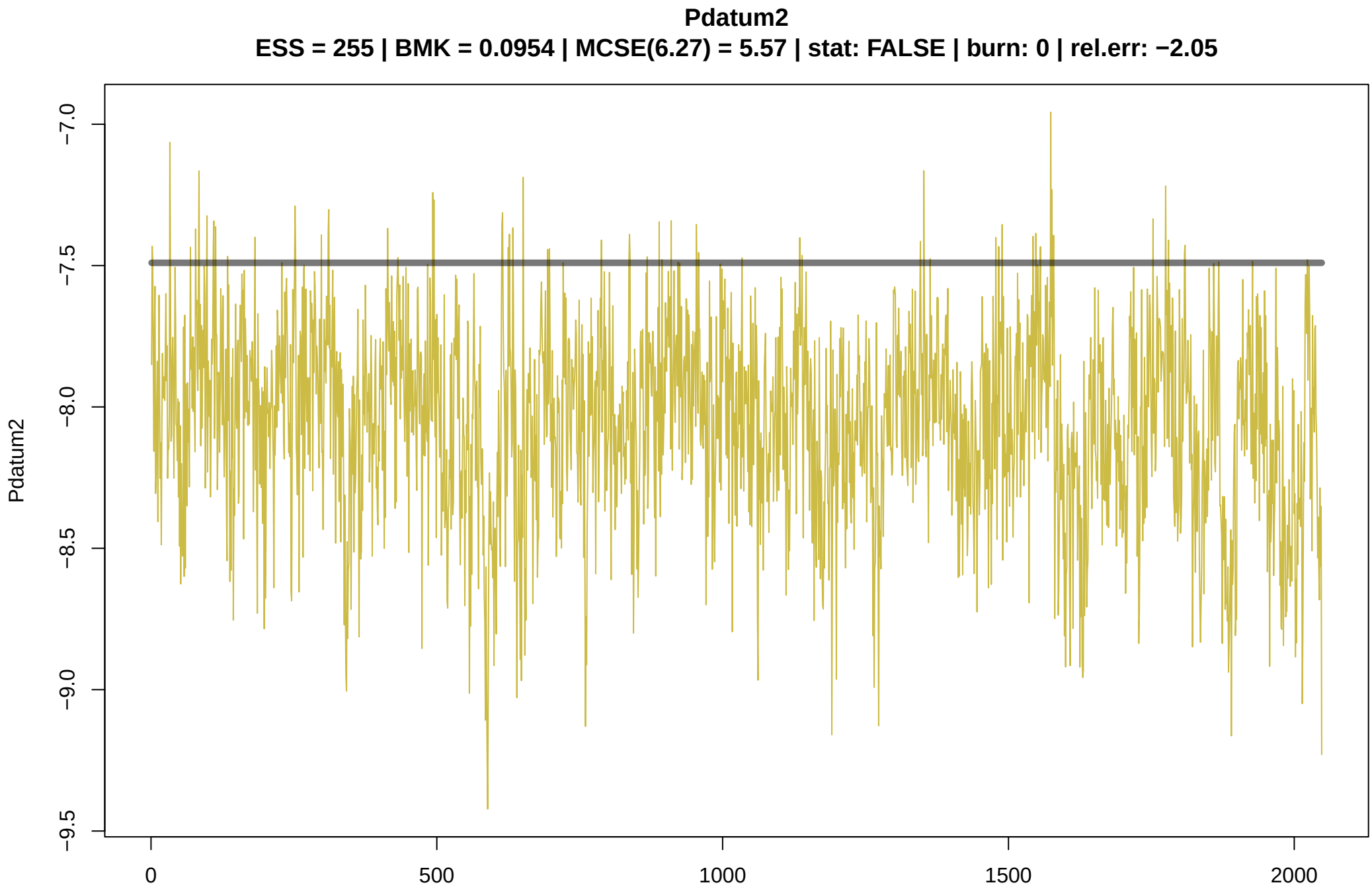

docked_HeavyAtomCount
250
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

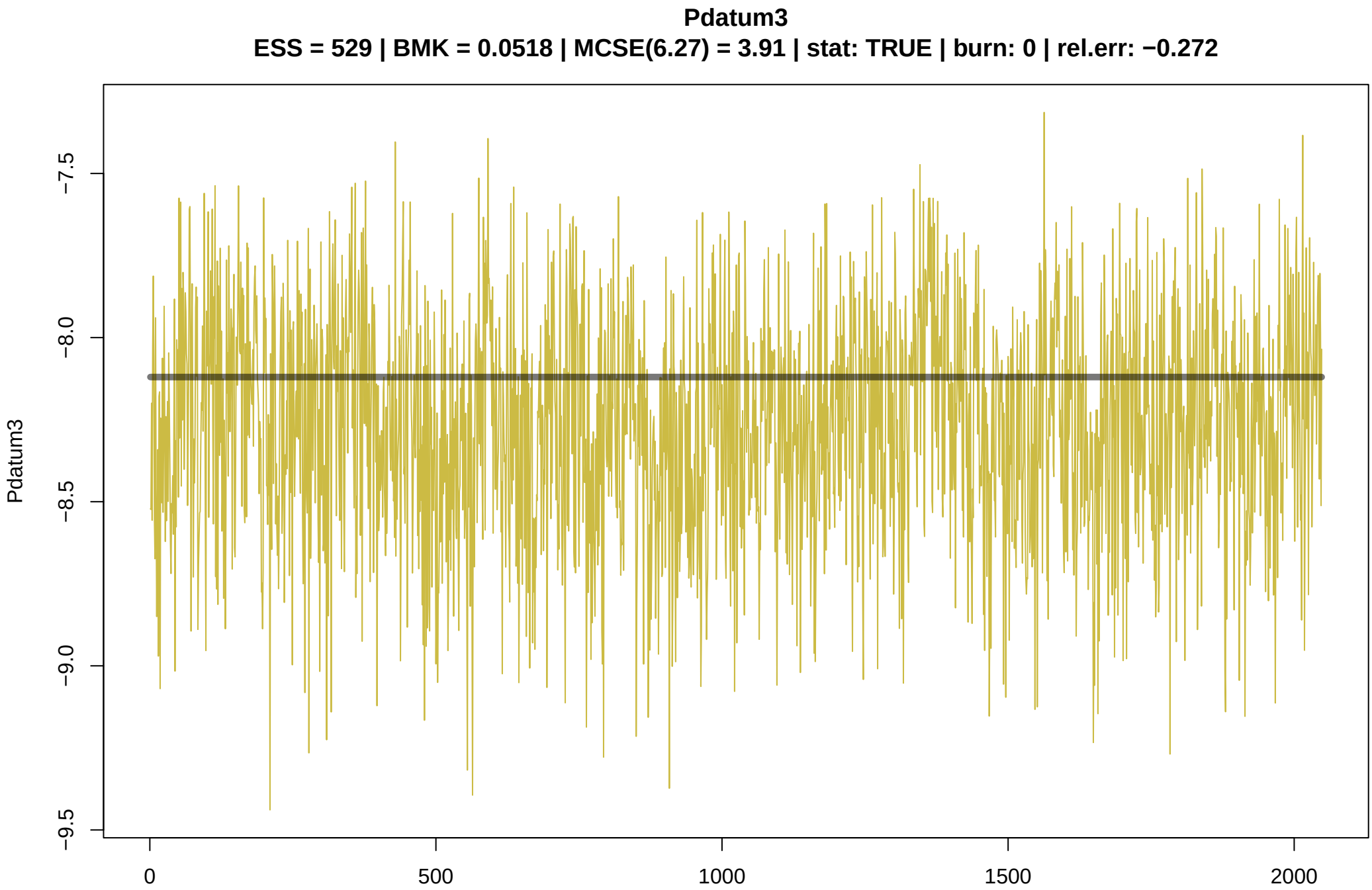

Pdatamean
ESS = 104 | BMK = 0.0781 | MCSE(6.27) = 7.09 | stat: FALSE | burn: 0 | rel.err: 0.743
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

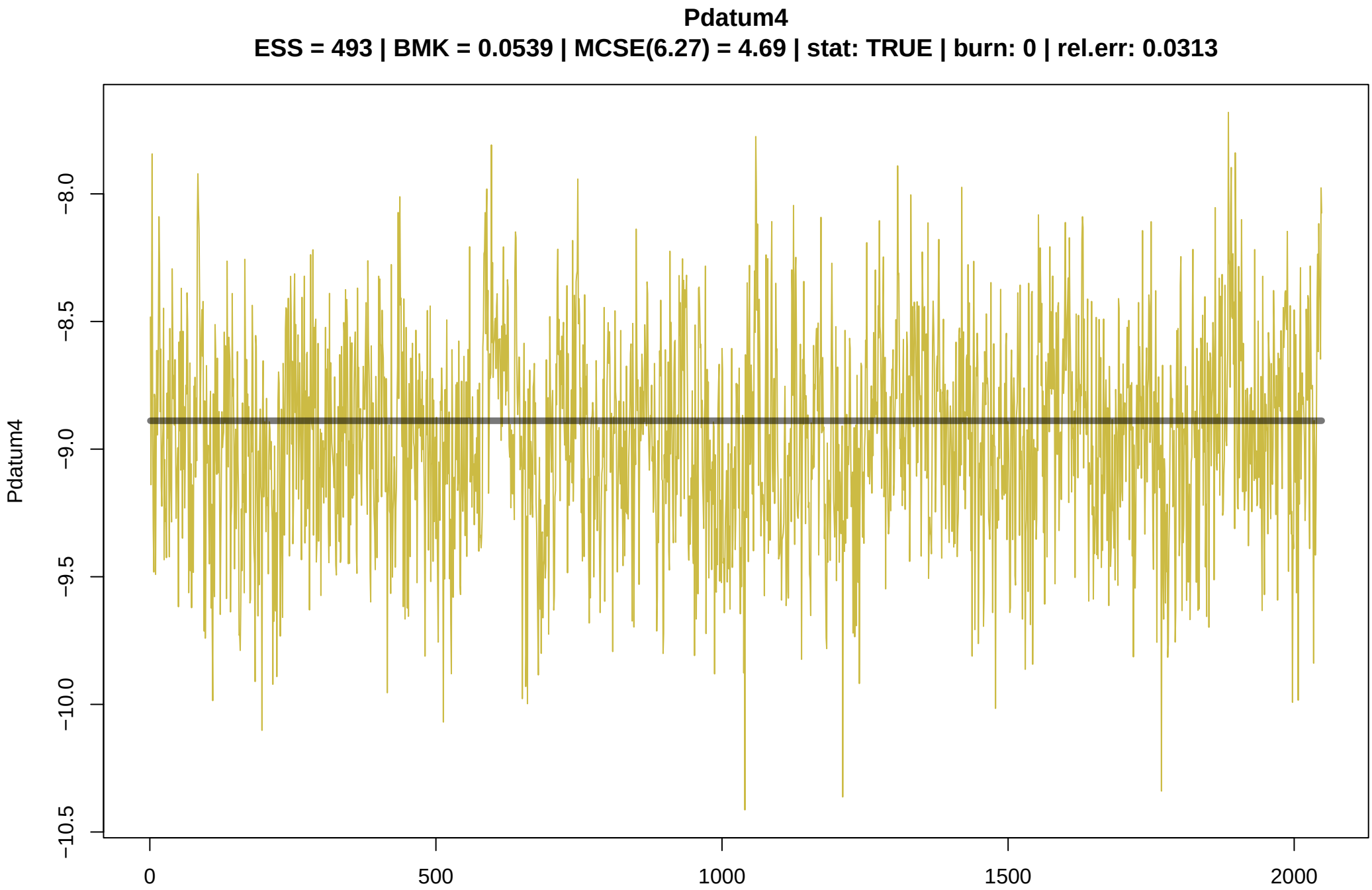

PdatacornerHi
ESS = 1600 | BMK = 0.123 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: 0.302
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

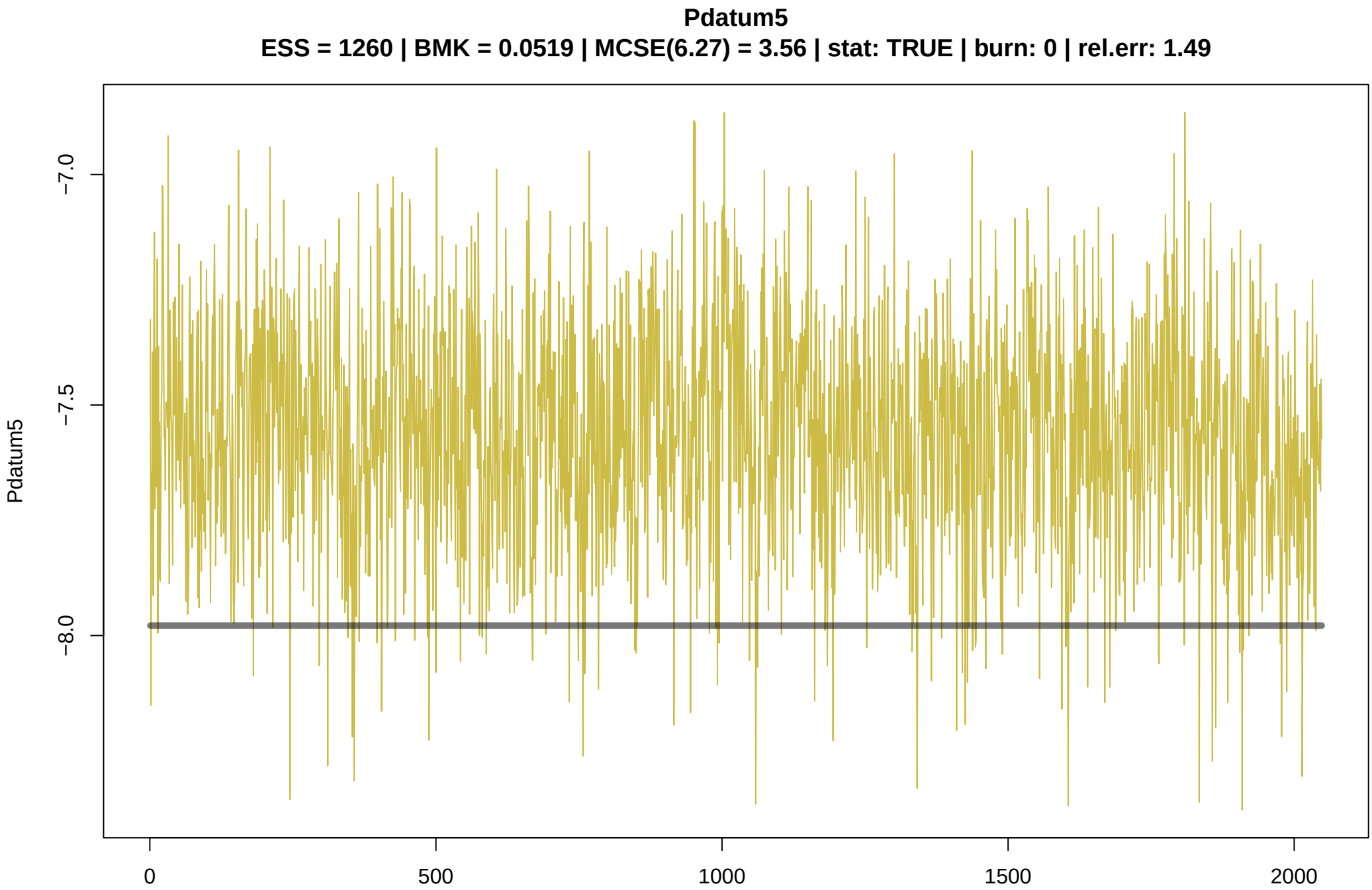

PdatacornerLo
ESS = 1950 | BMK = 0.0327 | MCSE(6.27) = 1.92 | stat: TRUE | burn: 0 | rel.err: 0.668
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

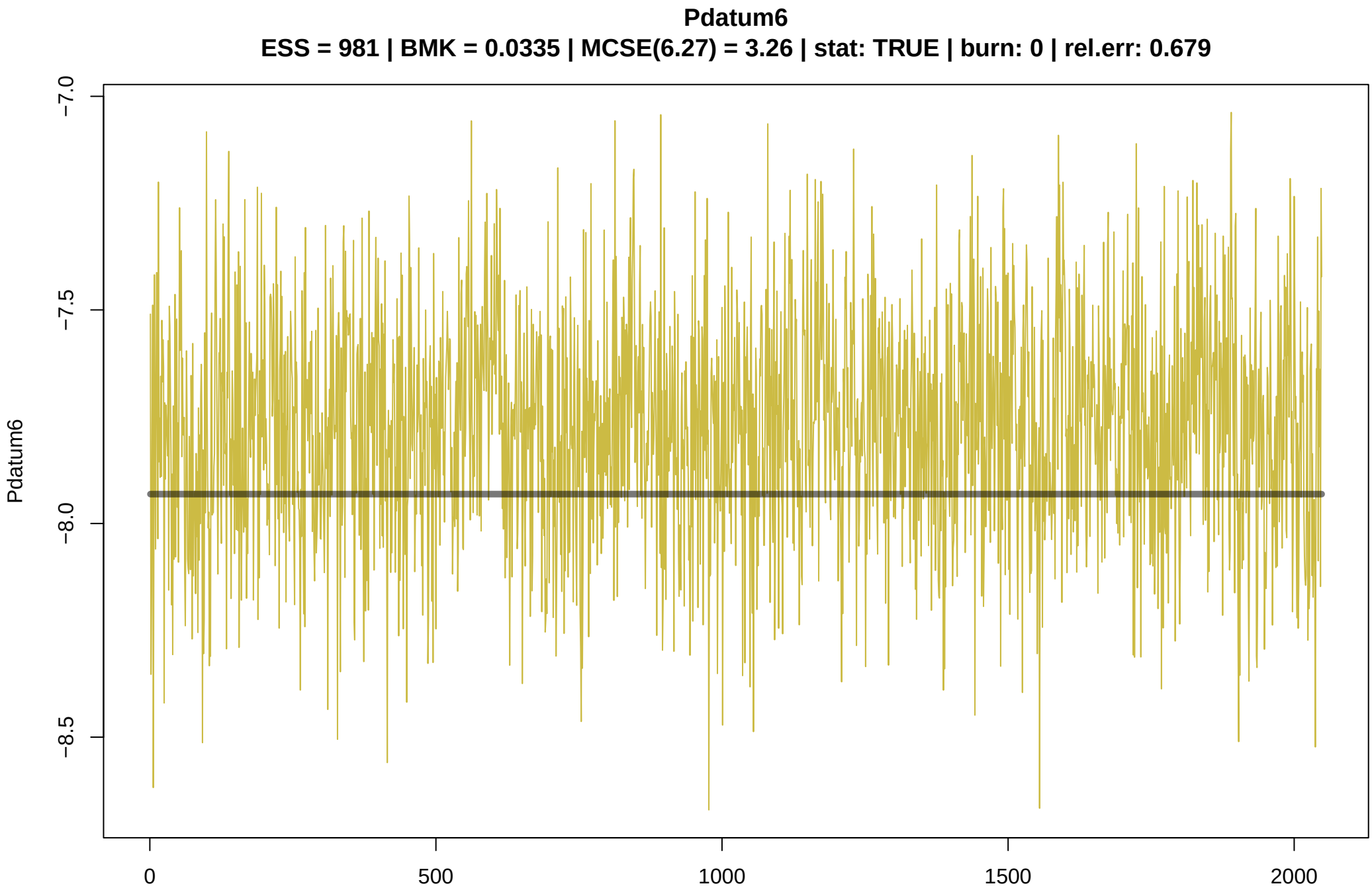

Pdatum1
ESS = 209 | BMK = 0.064 | MCSE(6.27) = 5.64 | stat: FALSE | burn: 0 | rel.err: −0.695
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

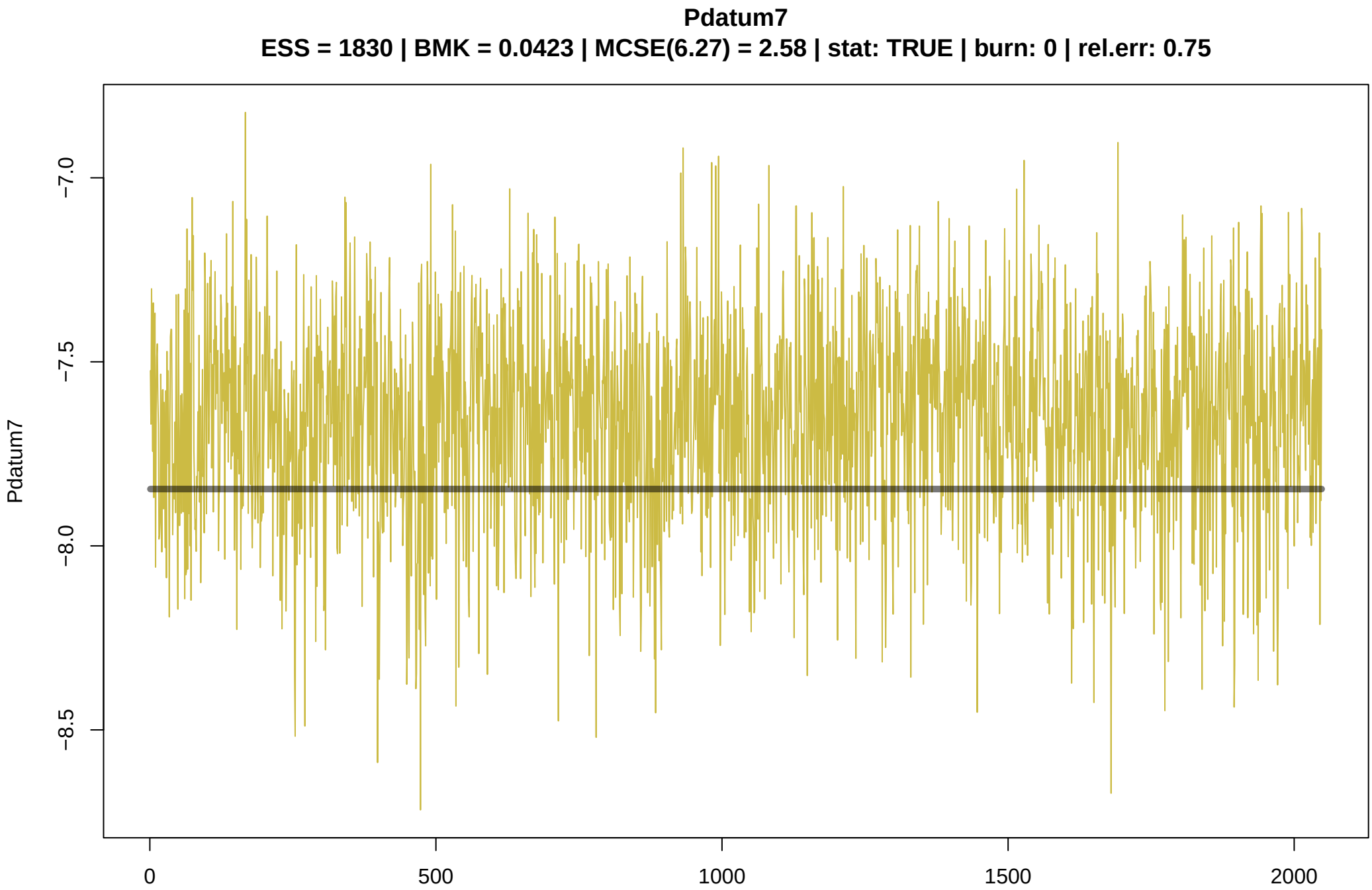

Pdatum2
ESS = 255 | BMK = 0.0954 | MCSE(6.27) = 5.57 | stat: FALSE | burn: 0 | rel.err: −2.05
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

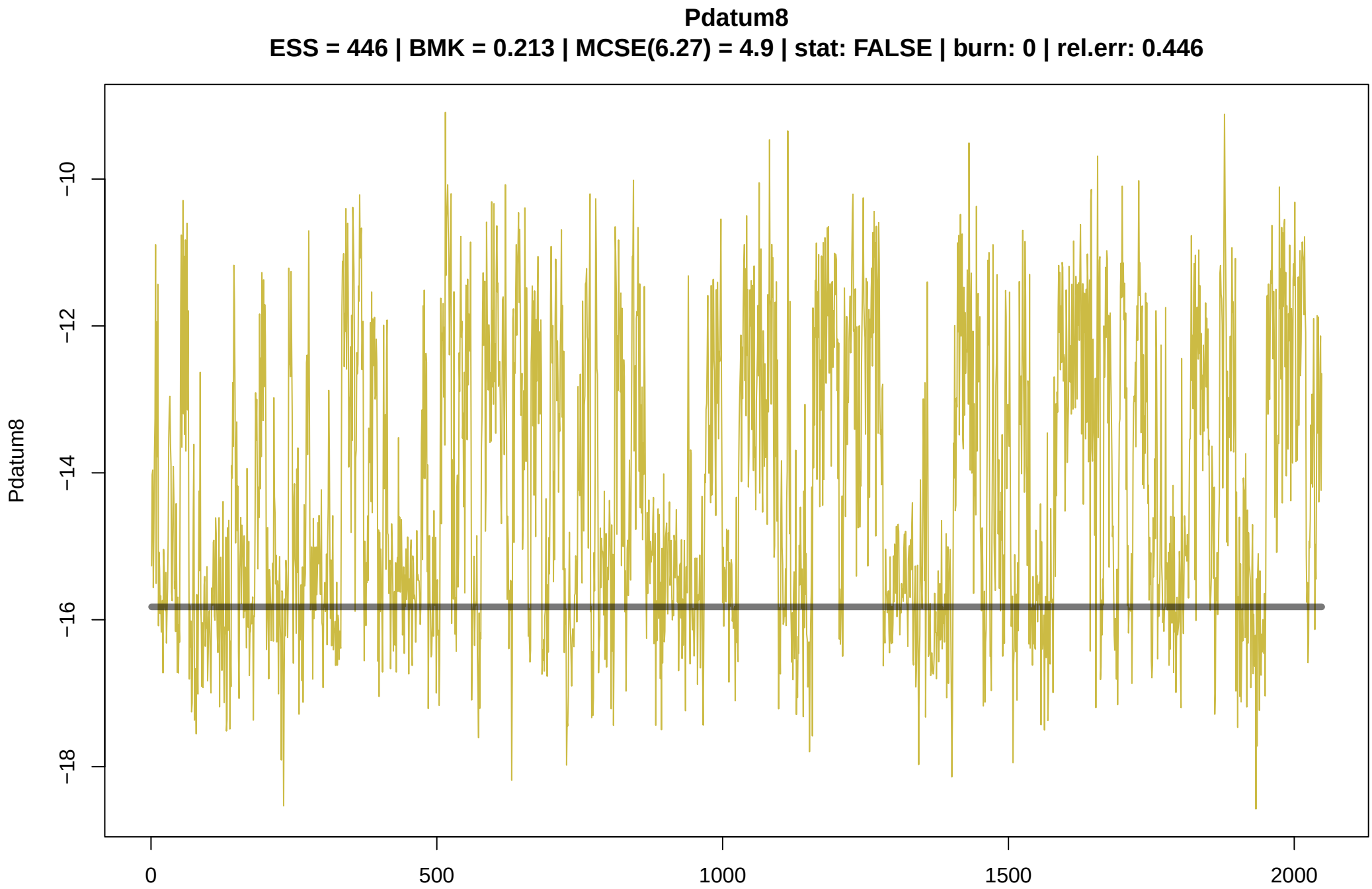

Pdatum3
ESS = 529 | BMK = 0.0518 | MCSE(6.27) = 3.91 | stat: TRUE | burn: 0 | rel.err: −0.272
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

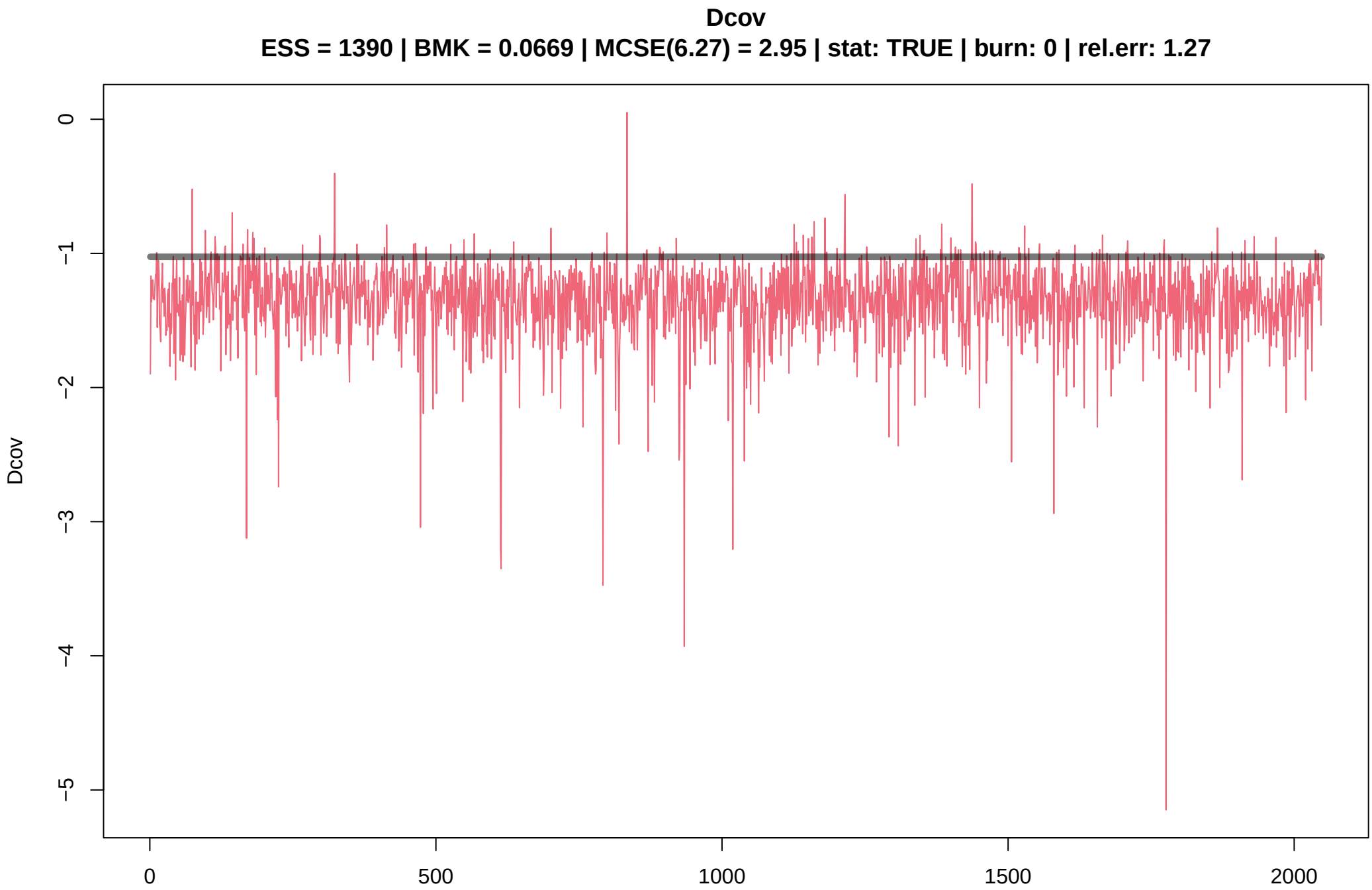

Pdatum4
ESS = 493 | BMK = 0.0539 | MCSE(6.27) = 4.69 | stat: TRUE | burn: 0 | rel.err: 0.0313
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

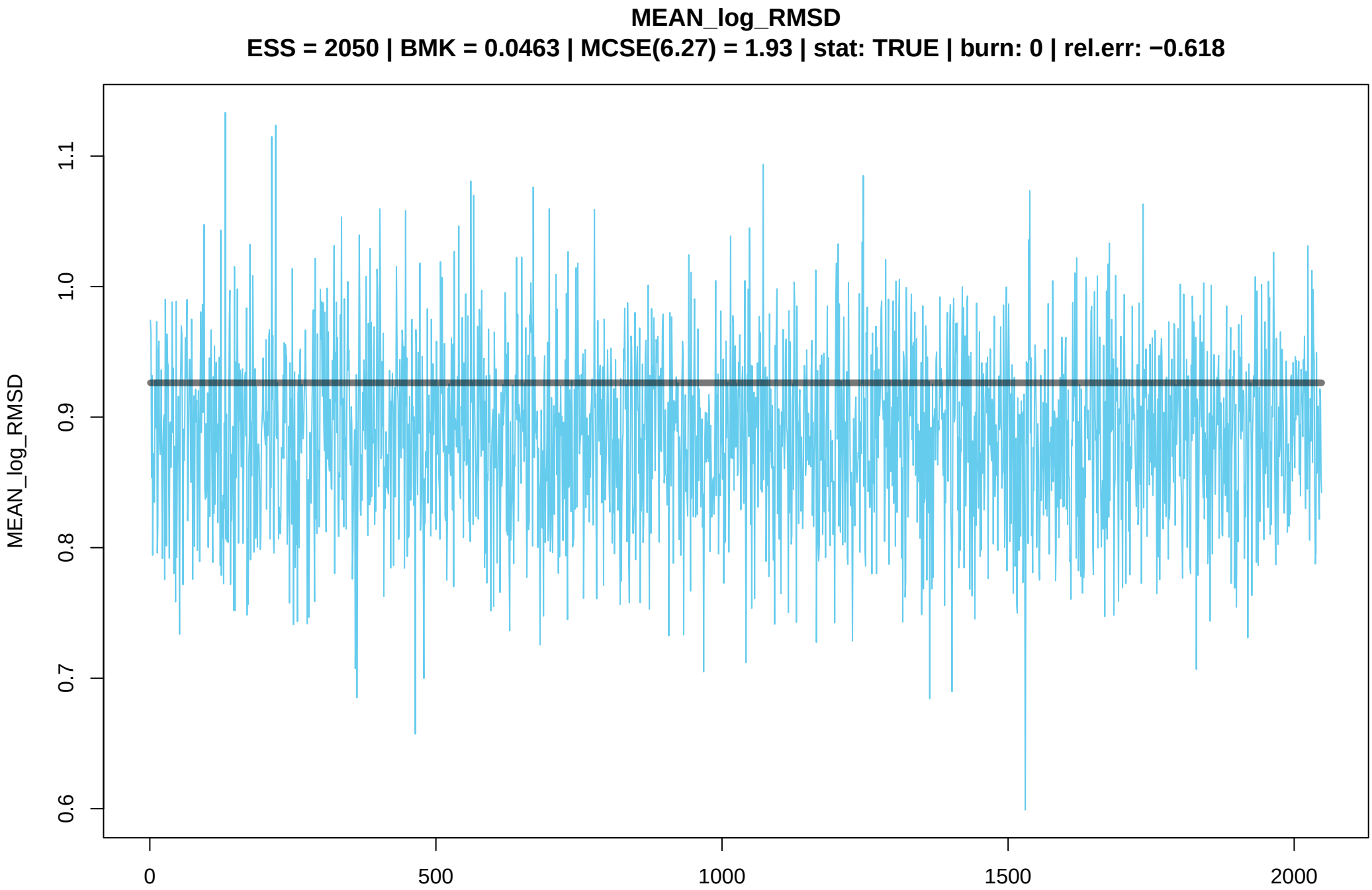

Pdatum5
ESS = 1260 | BMK = 0.0519 | MCSE(6.27) = 3.56 | stat: TRUE | burn: 0 | rel.err: 1.49
Pdatum5
−7.0
−7.5
−8.0
0
500
1000
1500
2000

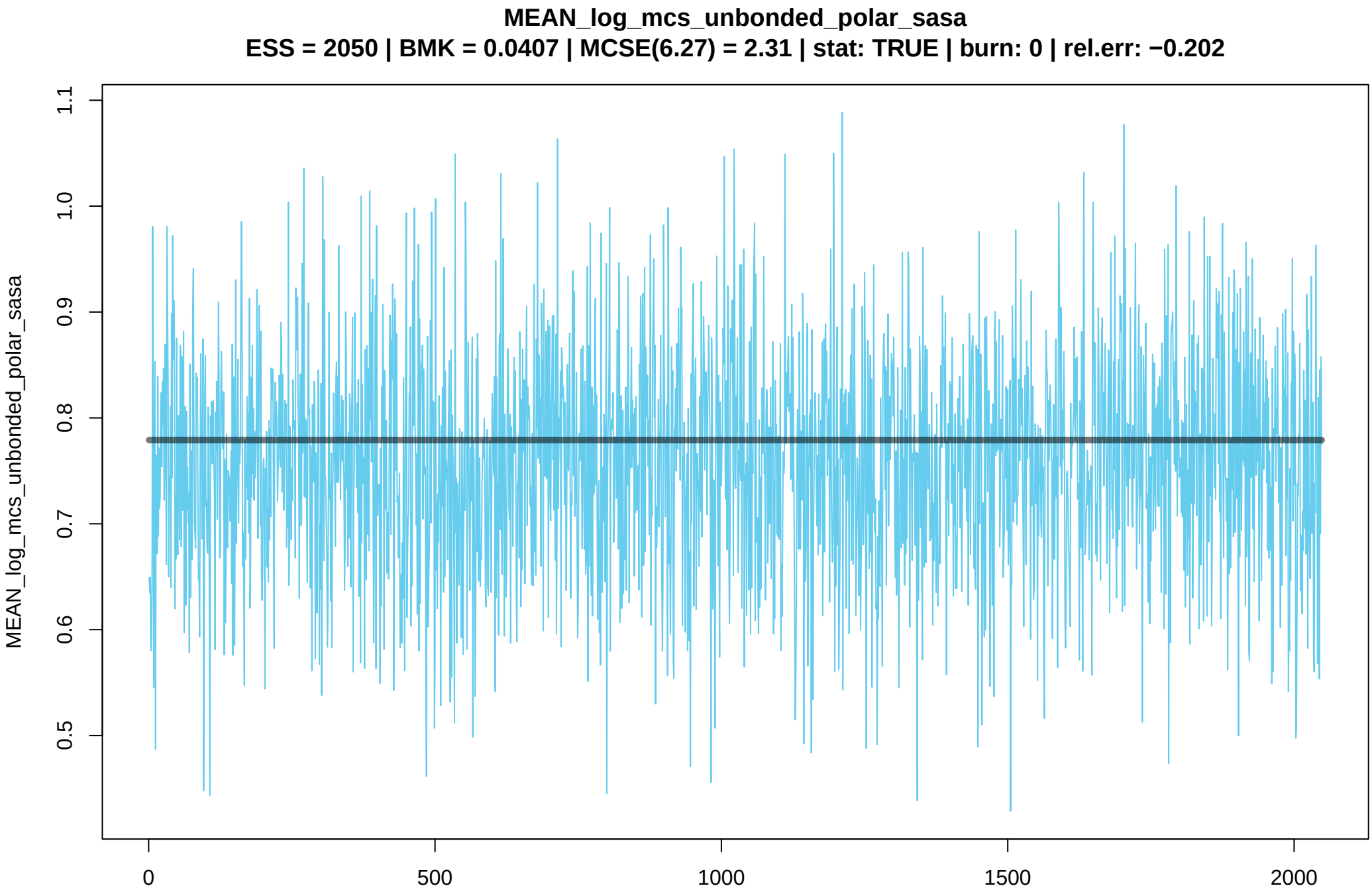

Pdatum6
ESS = 981 | BMK = 0.0335 | MCSE(6.27) = 3.26 | stat: TRUE | burn: 0 | rel.err: 0.679
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

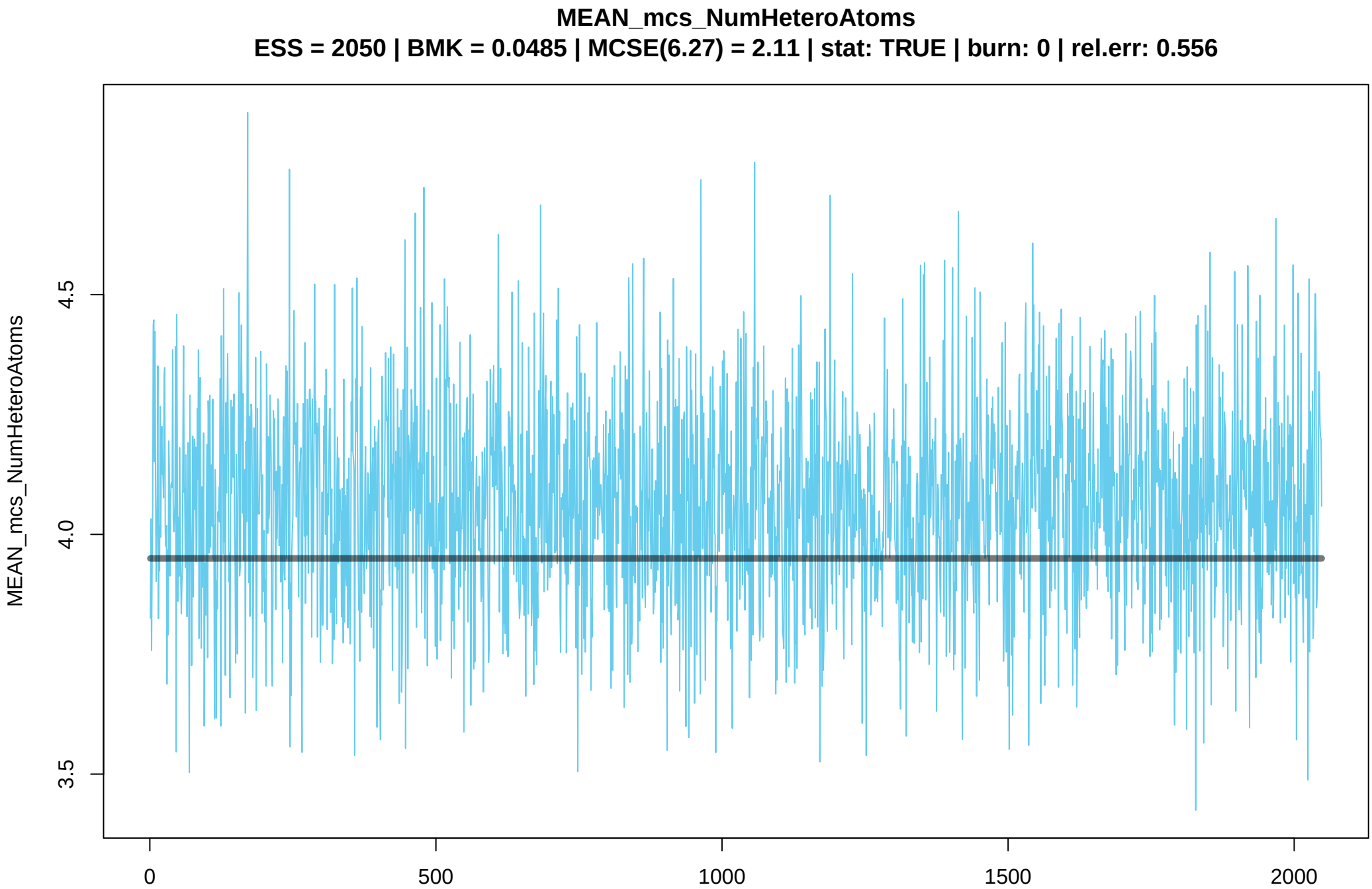

Pdatum7
ESS = 1830 | BMK = 0.0423 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: 0.75
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

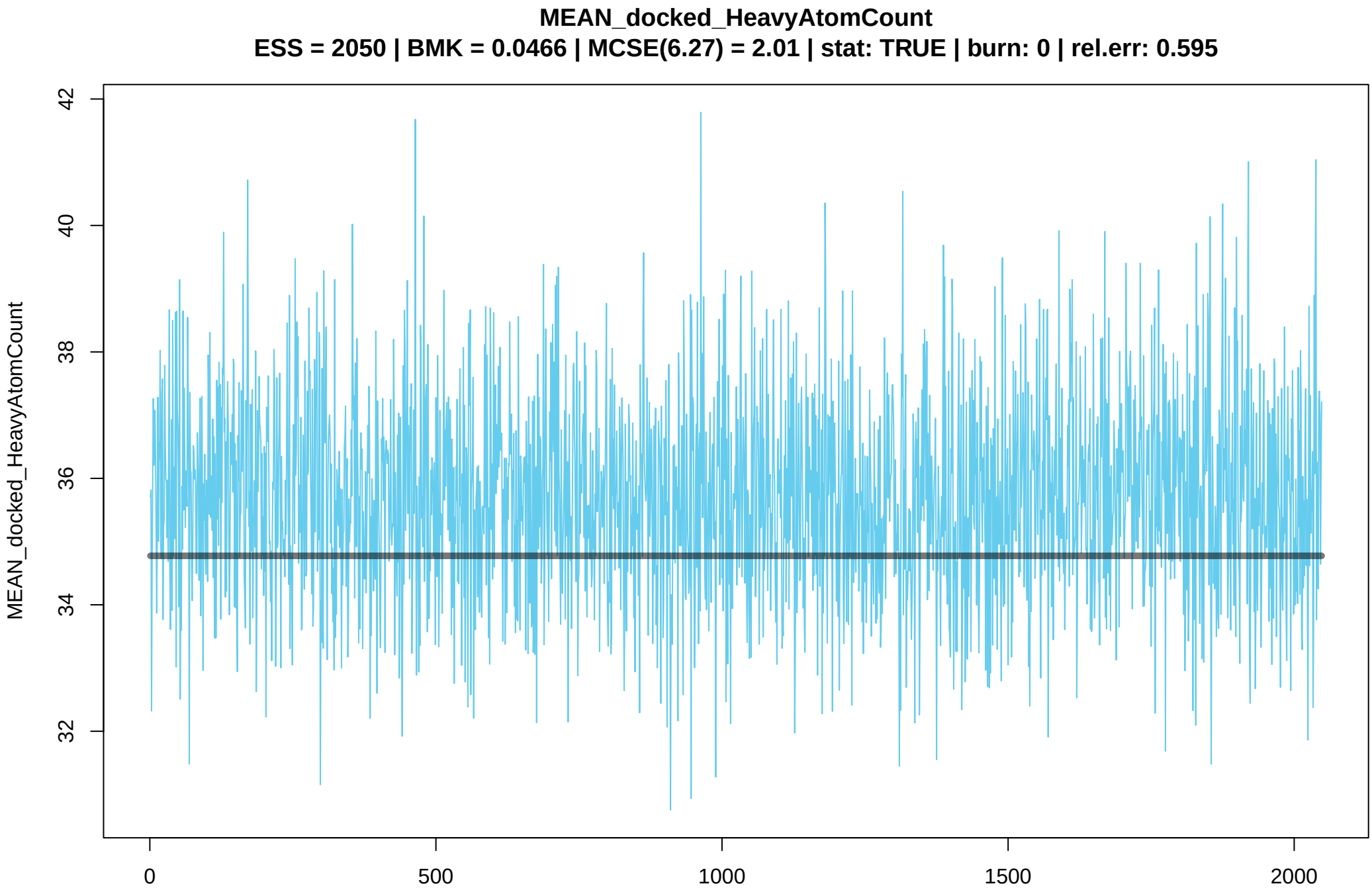

Pdatum8
ESS = 446 | BMK = 0.213 | MCSE(6.27) = 4.9 | stat: FALSE | burn: 0 | rel.err: 0.446
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

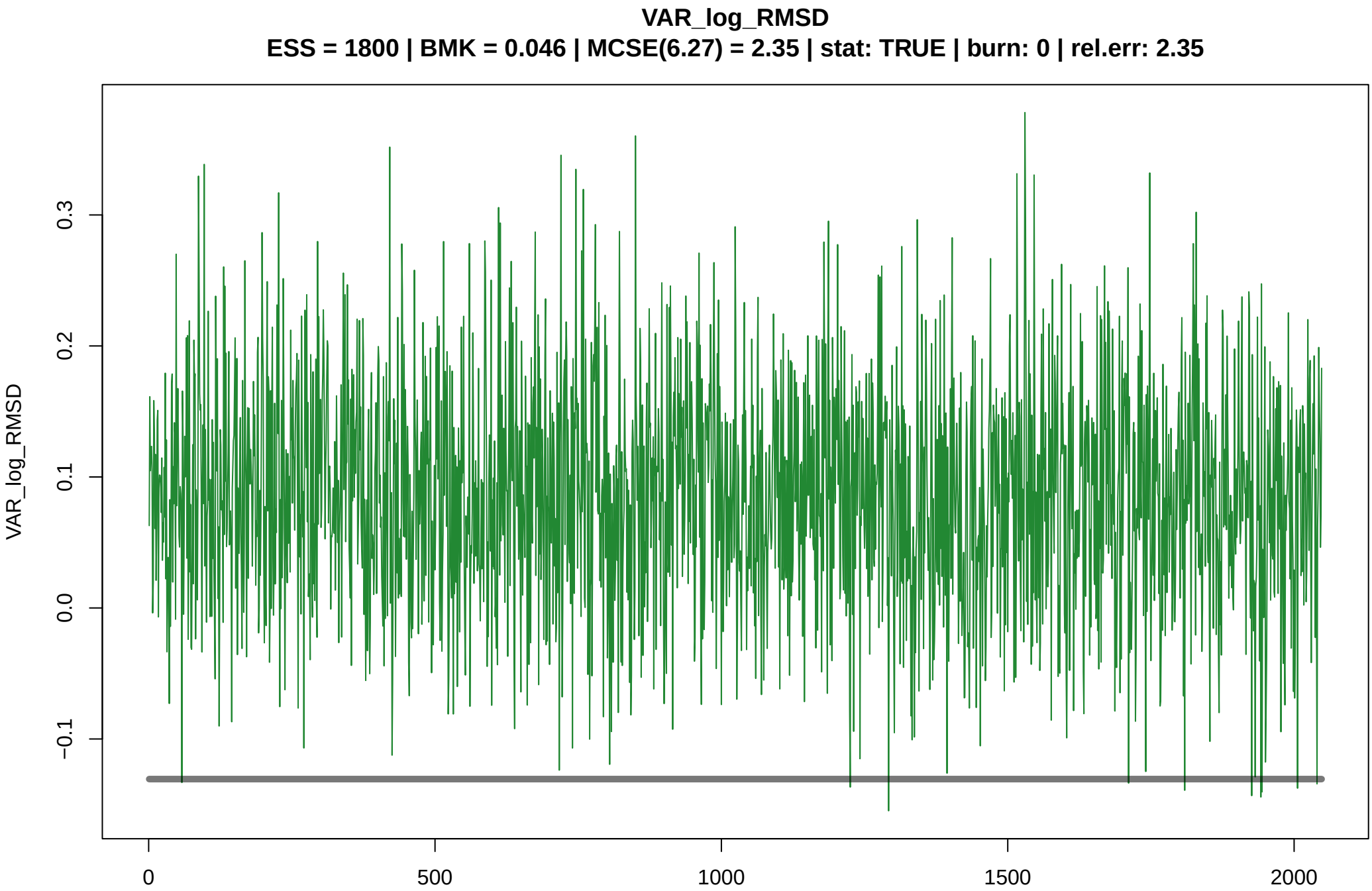

Dcov
ESS = 1390 | BMK = 0.0669 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: 1.27
Dcov
0
−1
−2
−3
−4
−5
0
500
1000
1500
2000

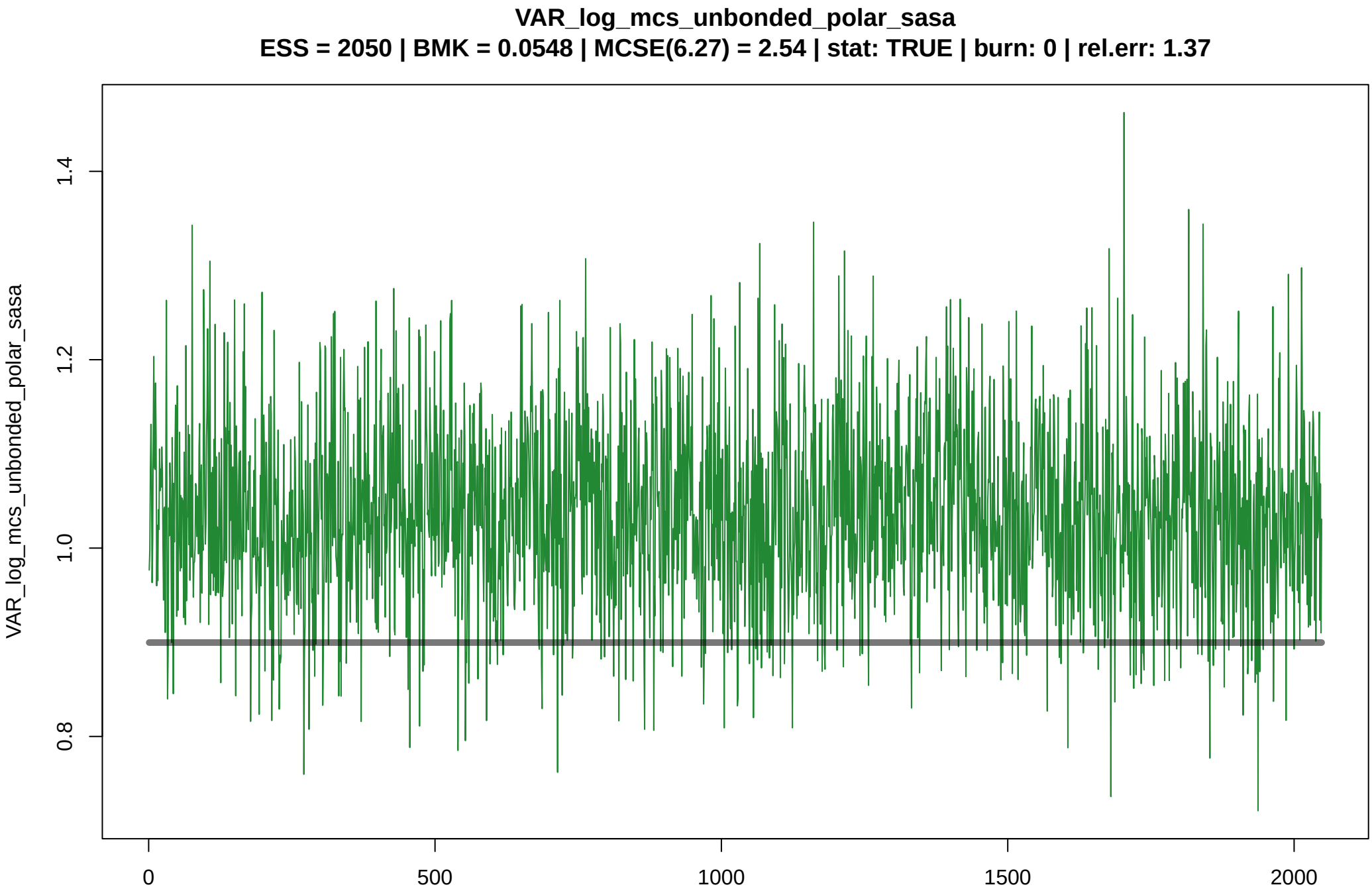

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0463 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: −0.618
MEAN_log_RMSD
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

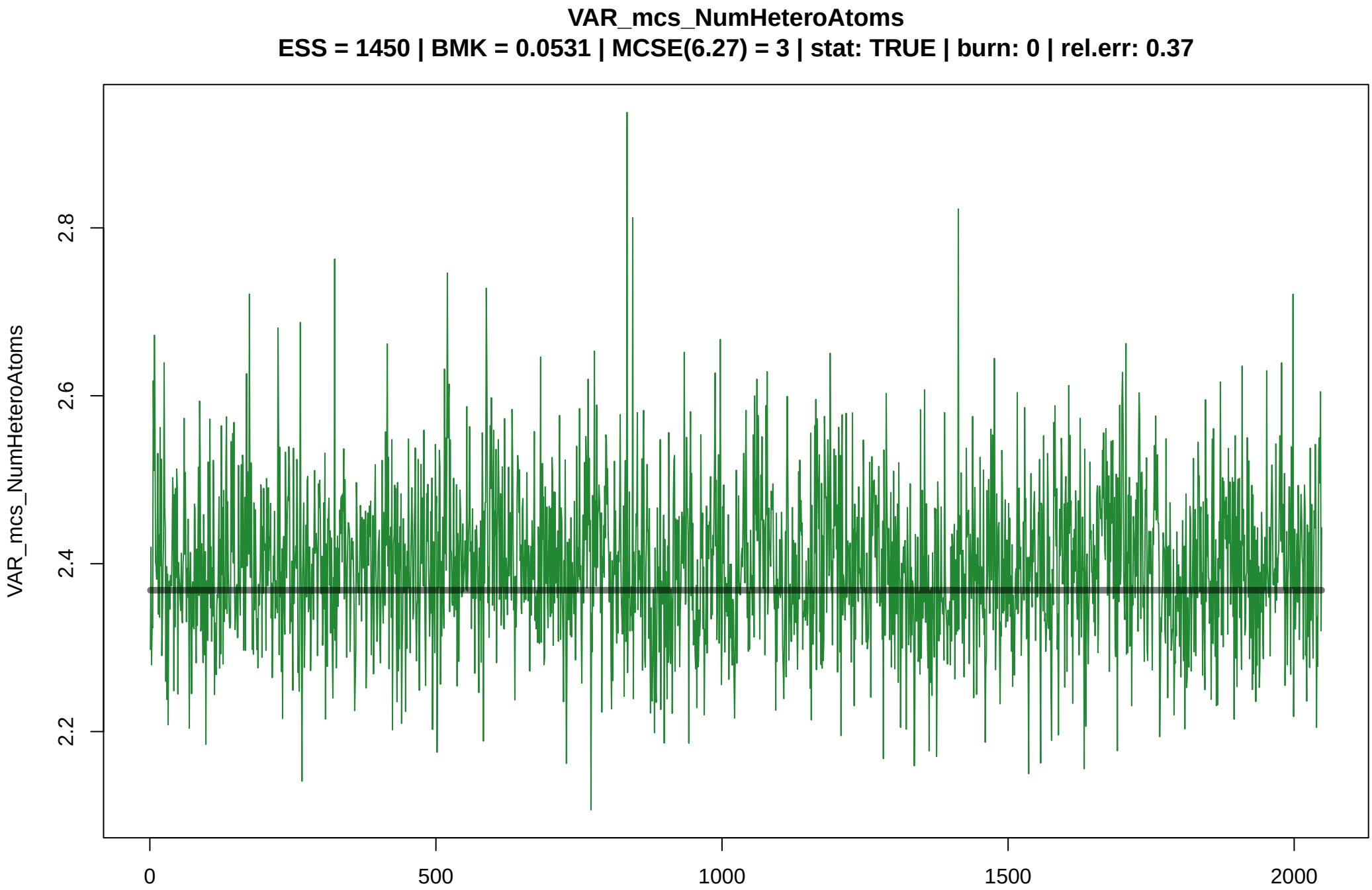

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: −0.202
MEAN_log_mcs_unbonded_polar_sasa
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

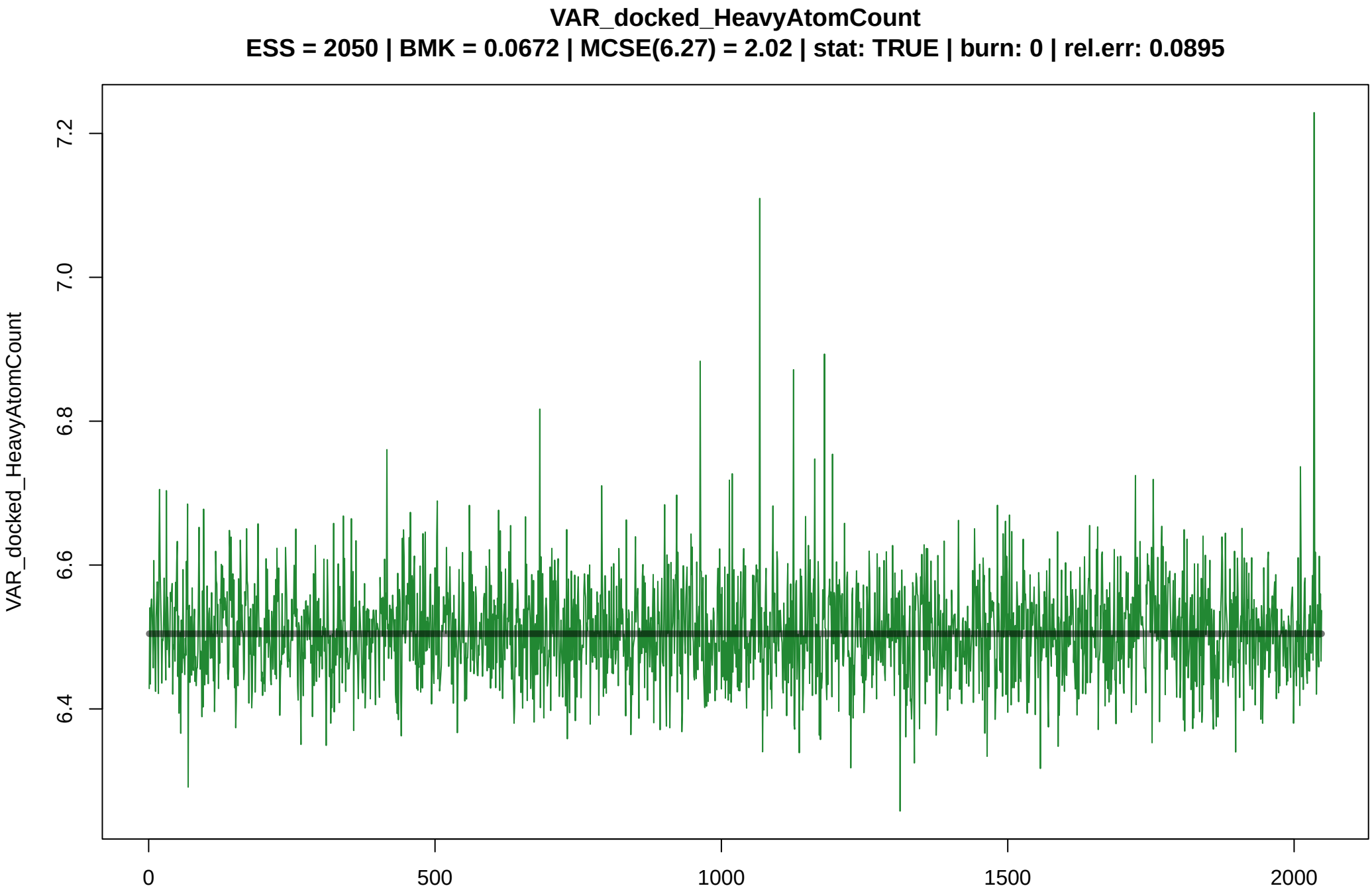

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0485 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: 0.556
MEAN_mcs_NumHeteroAtoms
3.5
4.0
4.5
0
500
1000
1500
2000

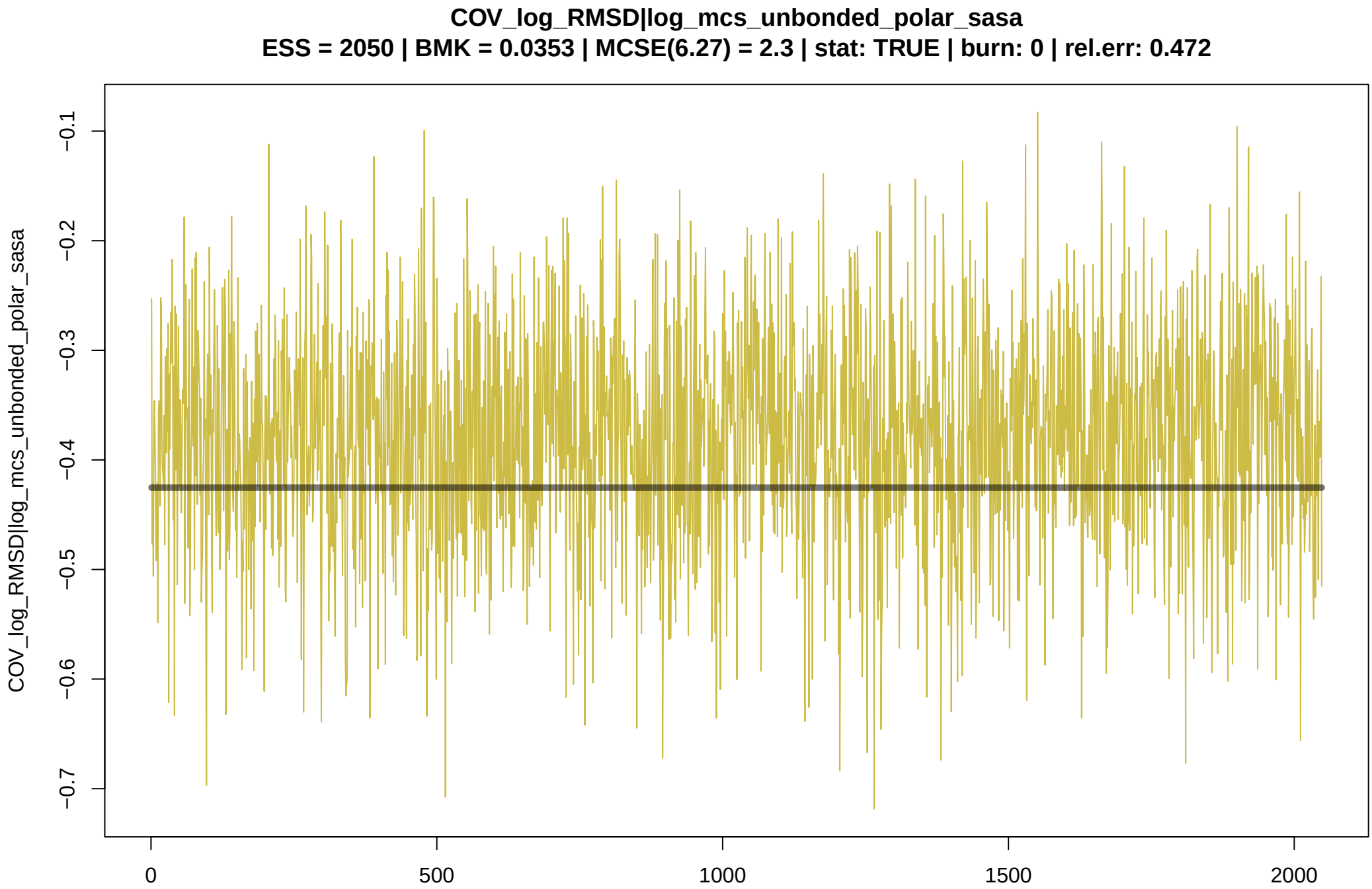

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0466 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0 | rel.err: 0.595
MEAN_docked_HeavyAtomCount
32
34
36
38
40
42
0
500
1000
1500
2000

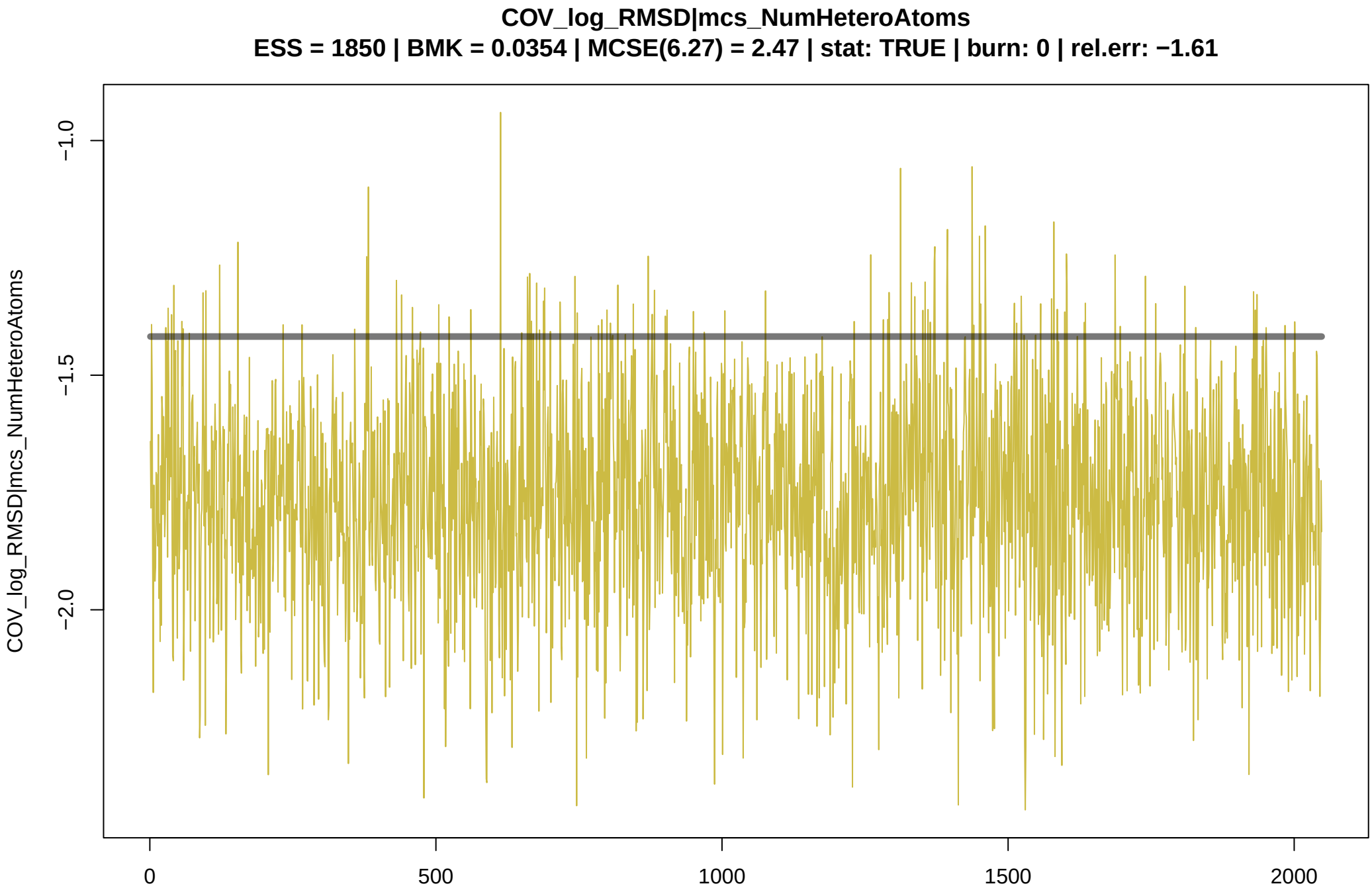

VAR_log_RMSD
ESS = 1800 | BMK = 0.046 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0 | rel.err: 2.35
VAR_log_RMSD
−0.1
0.0
0.1
0.2
0.3
0
500
1000
1500
2000

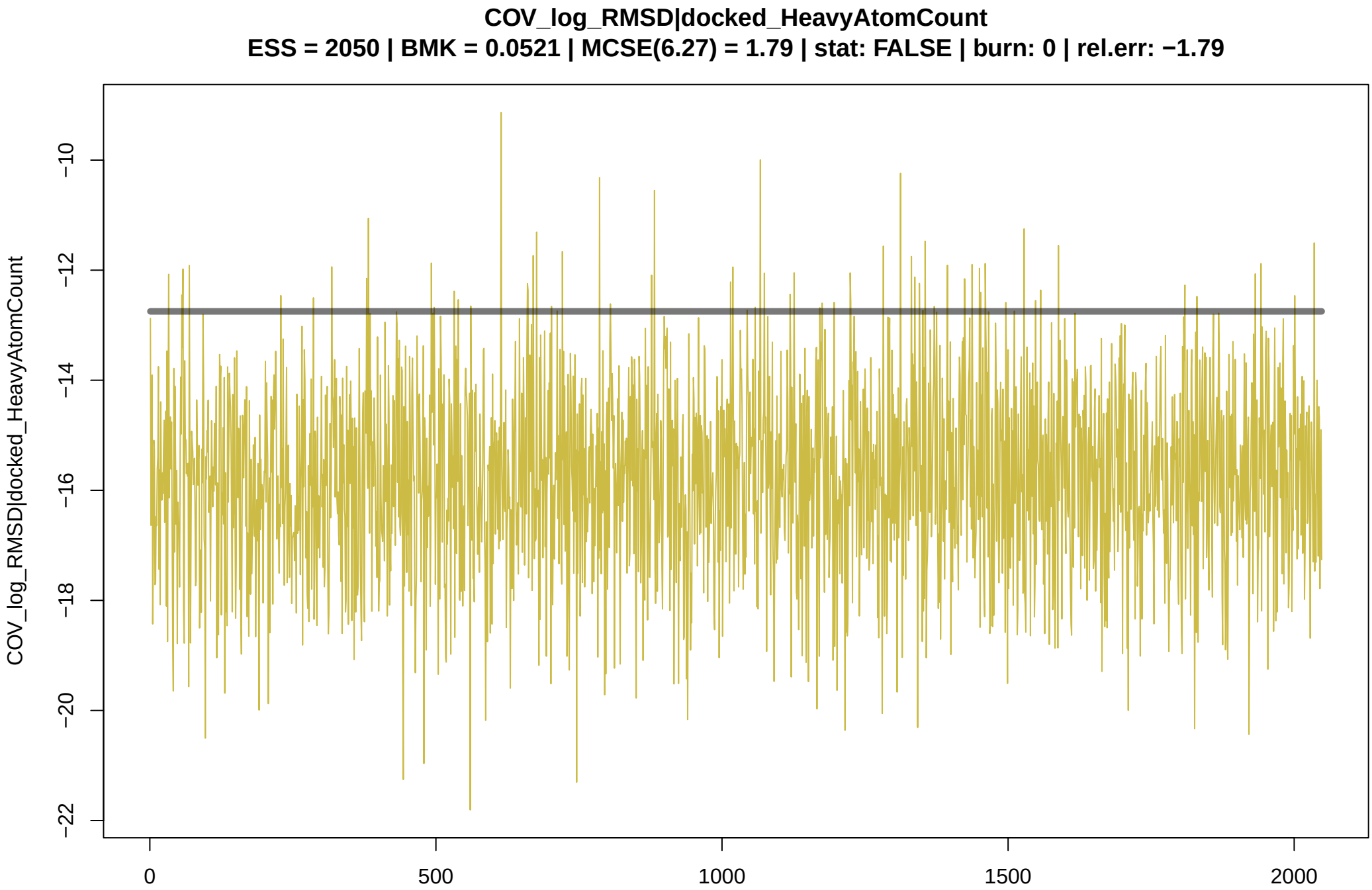

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0548 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: 1.37
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

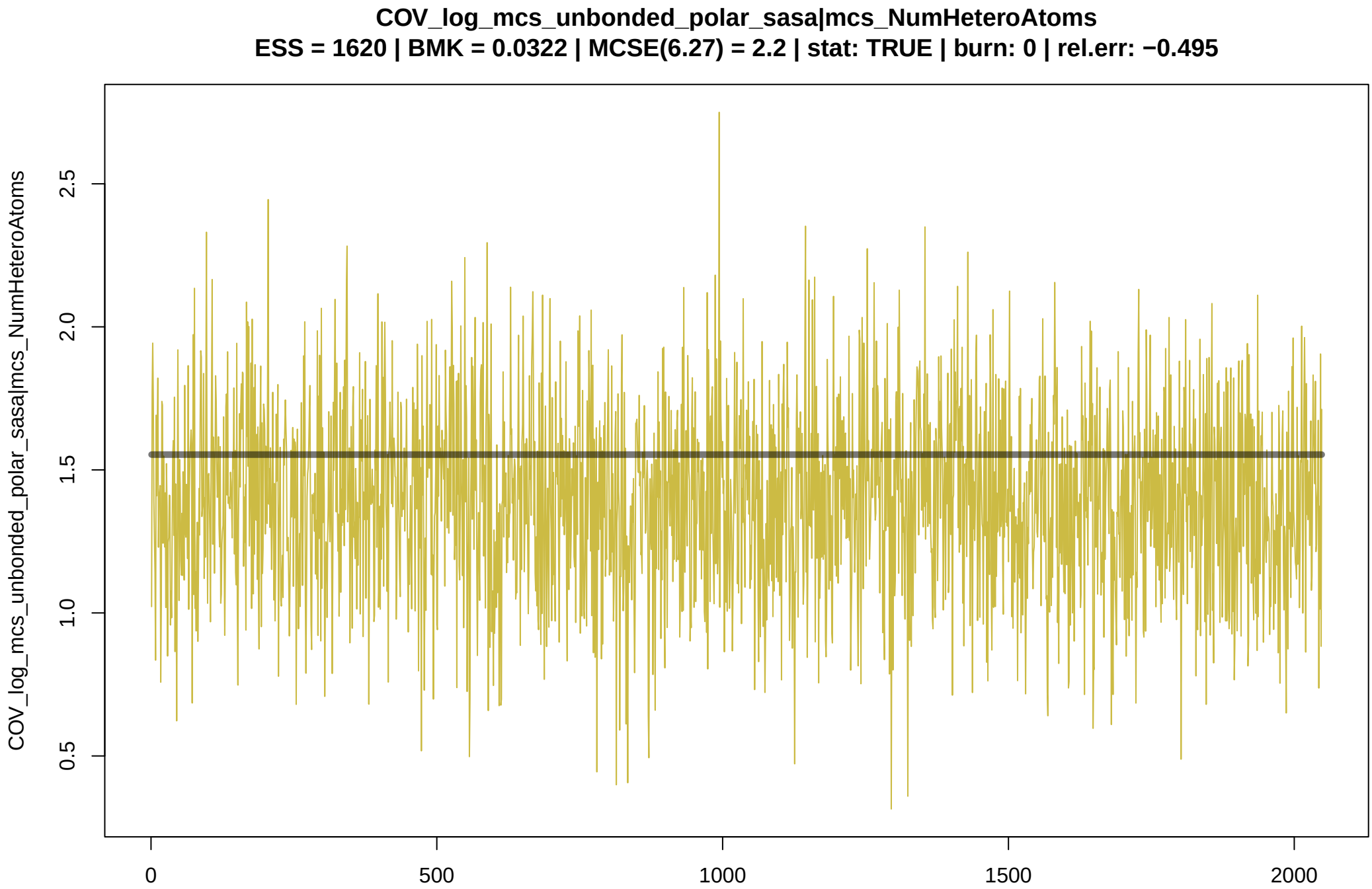

VAR_mcs_NumHeteroAtoms
ESS = 1450 | BMK = 0.0531 | MCSE(6.27) = 3 | stat: TRUE | burn: 0 | rel.err: 0.37
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

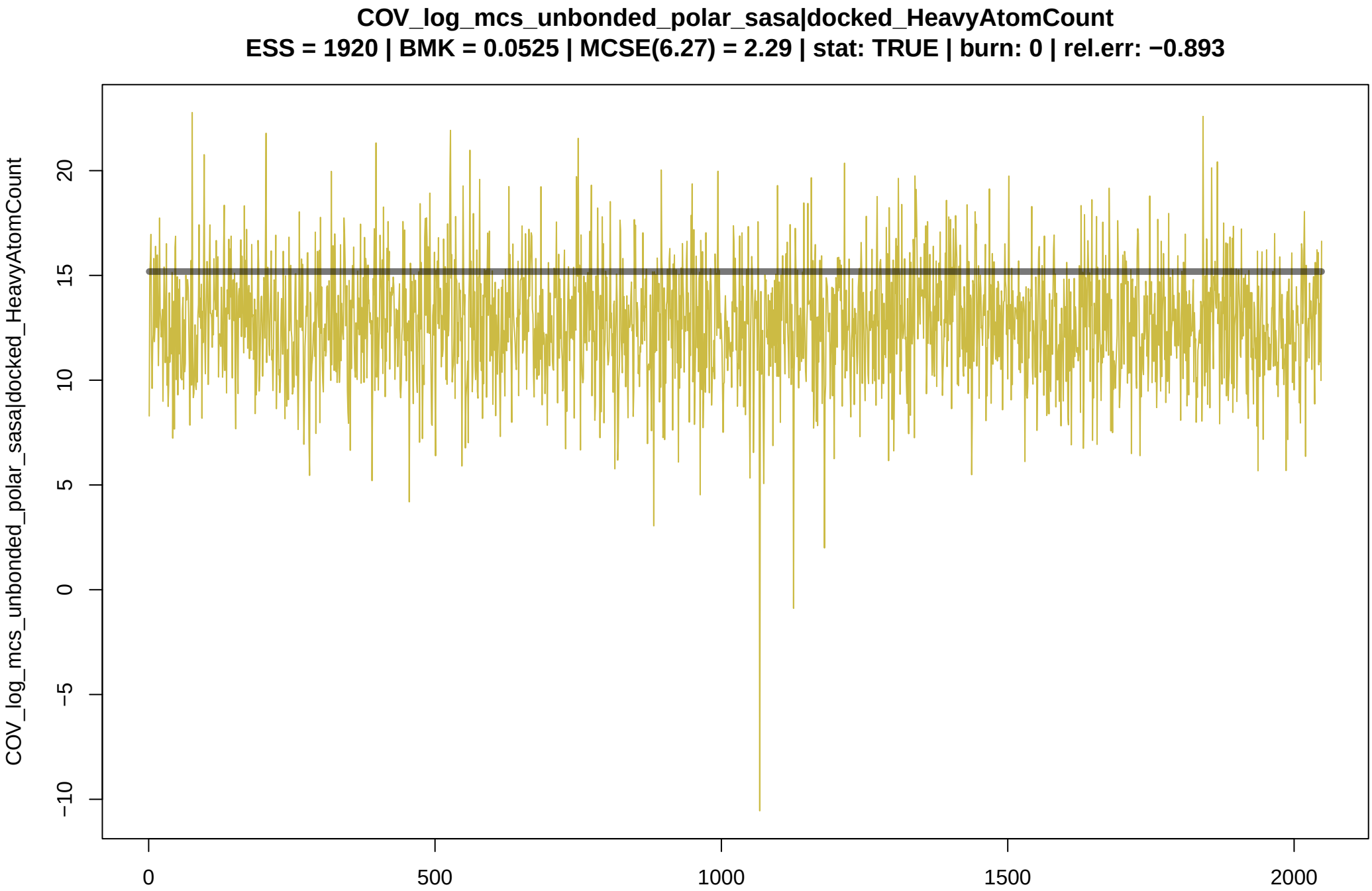

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0672 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0 | rel.err: 0.0895
VAR_docked_HeavyAtomCount
6.4
6.6
6.8
7.0
7.2
0
500
1000
1500
2000

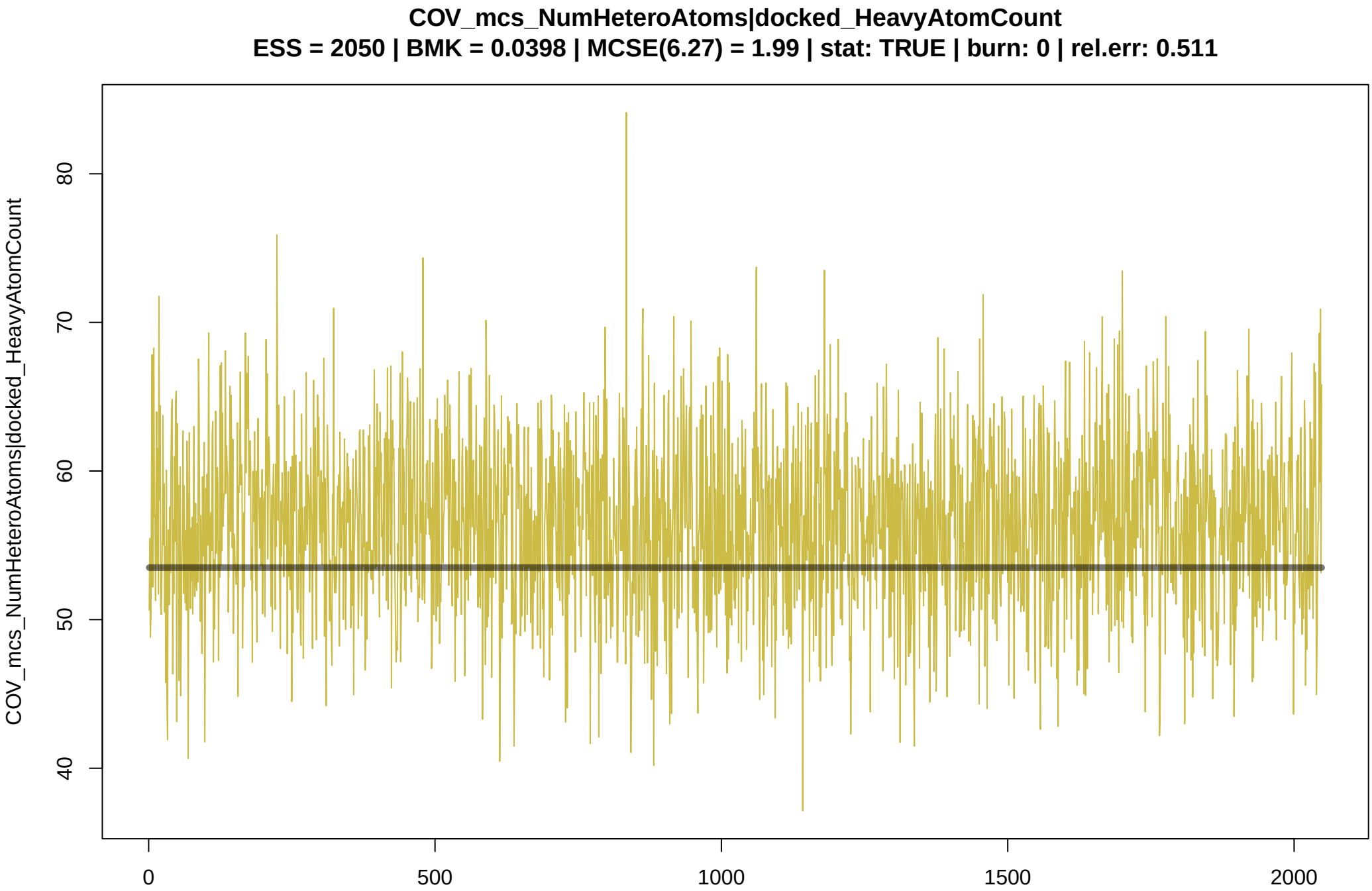

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0353 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: 0.472
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1850 | BMK = 0.0354 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0 | rel.err: −1.61
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.5
−2.0
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0521 | MCSE(6.27) = 1.79 | stat: FALSE | burn: 0 | rel.err: −1.79
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 = 1620 | BMK = 0.0322 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0 | rel.err: −0.495
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 = 0.0525 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: −0.893
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
20
15
10
5
0
−5
−10
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0398 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 0.511
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000