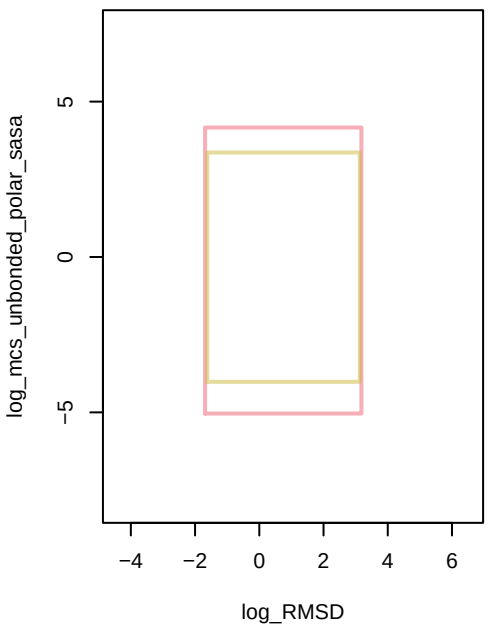
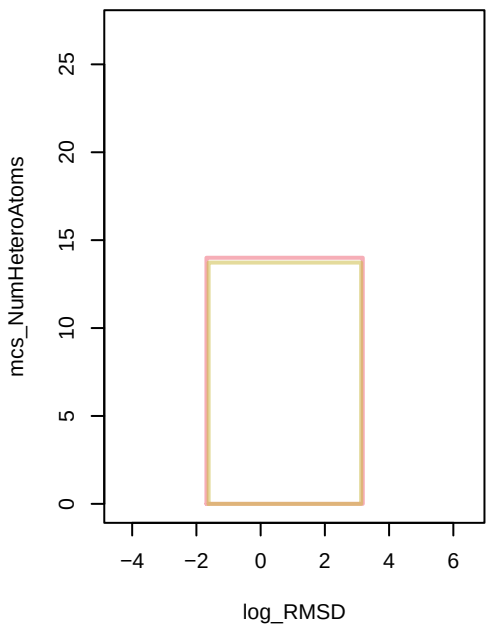
−− STATS maxD −−
min ESS = 61.9930418817095
max BMK = 0.138466722345846
max MCSE = 9.26587559948251
all stationary: FALSE
burn: 2040
max rel.err.: 2.1152793769053

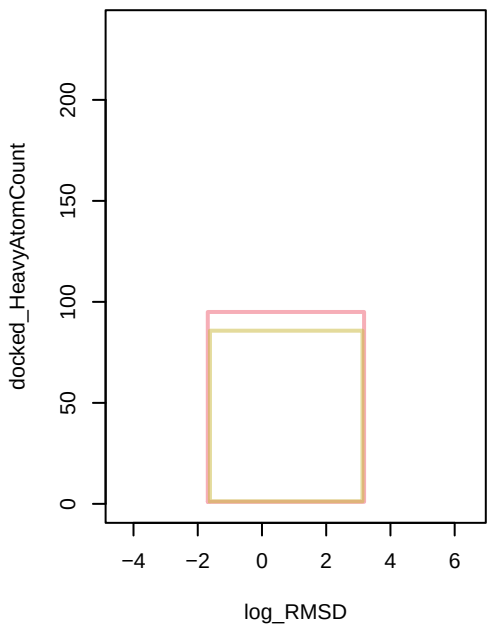
−− STATS 2D −−
min ESS = 2048
max BMK = 0.056964661448149
max MCSE = 2.23408079602859
all stationary: TRUE
burn: 0
max rel.err.: 1.75382312452745

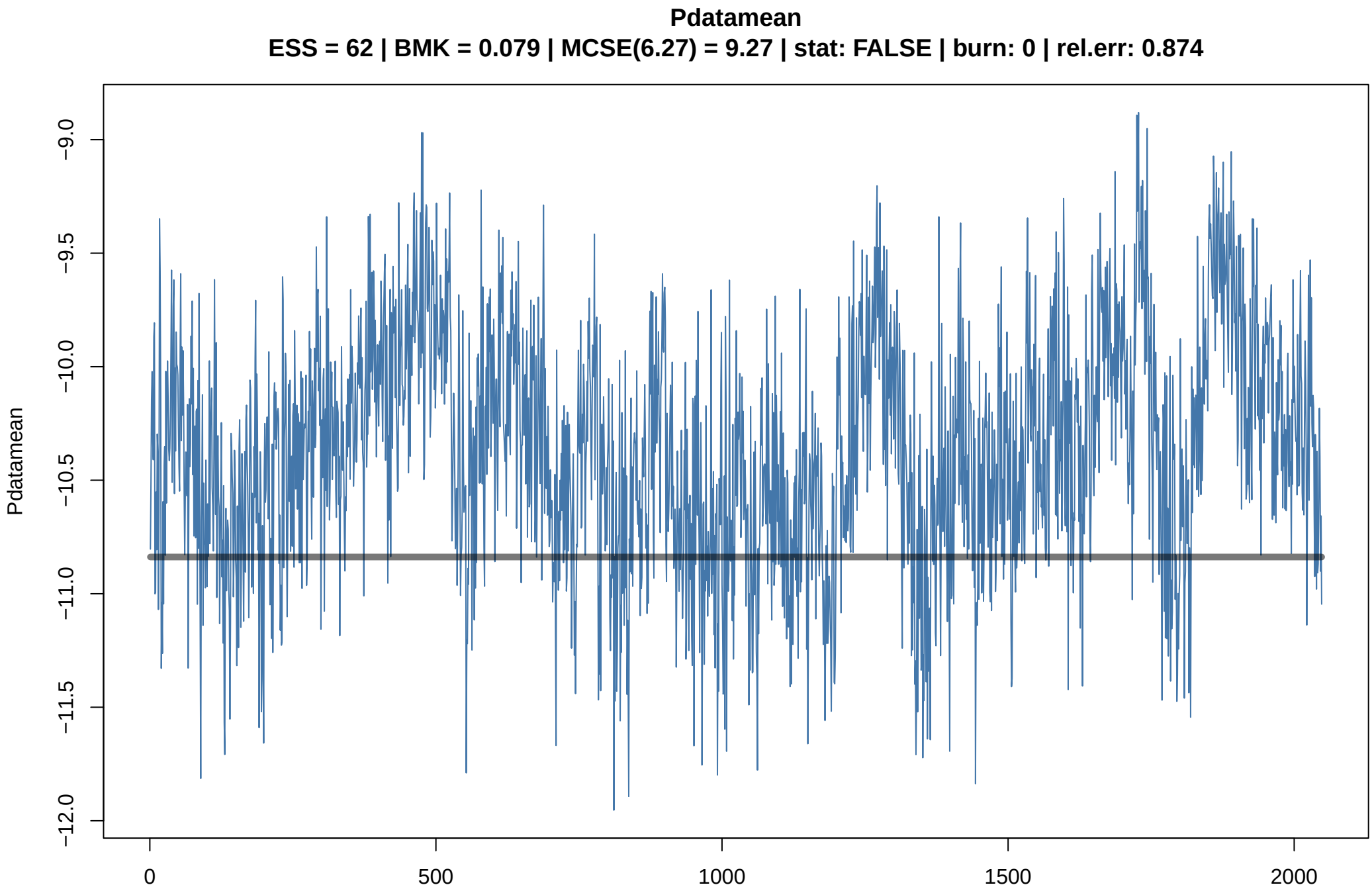
−− STATS 1D −−
min ESS = 1679.65663562796
max BMK = 0.058395309268181 6
max MCSE = 3.18566759141557
all stationary: TRUE
burn: 0
max rel.err.: 2.24762464840536

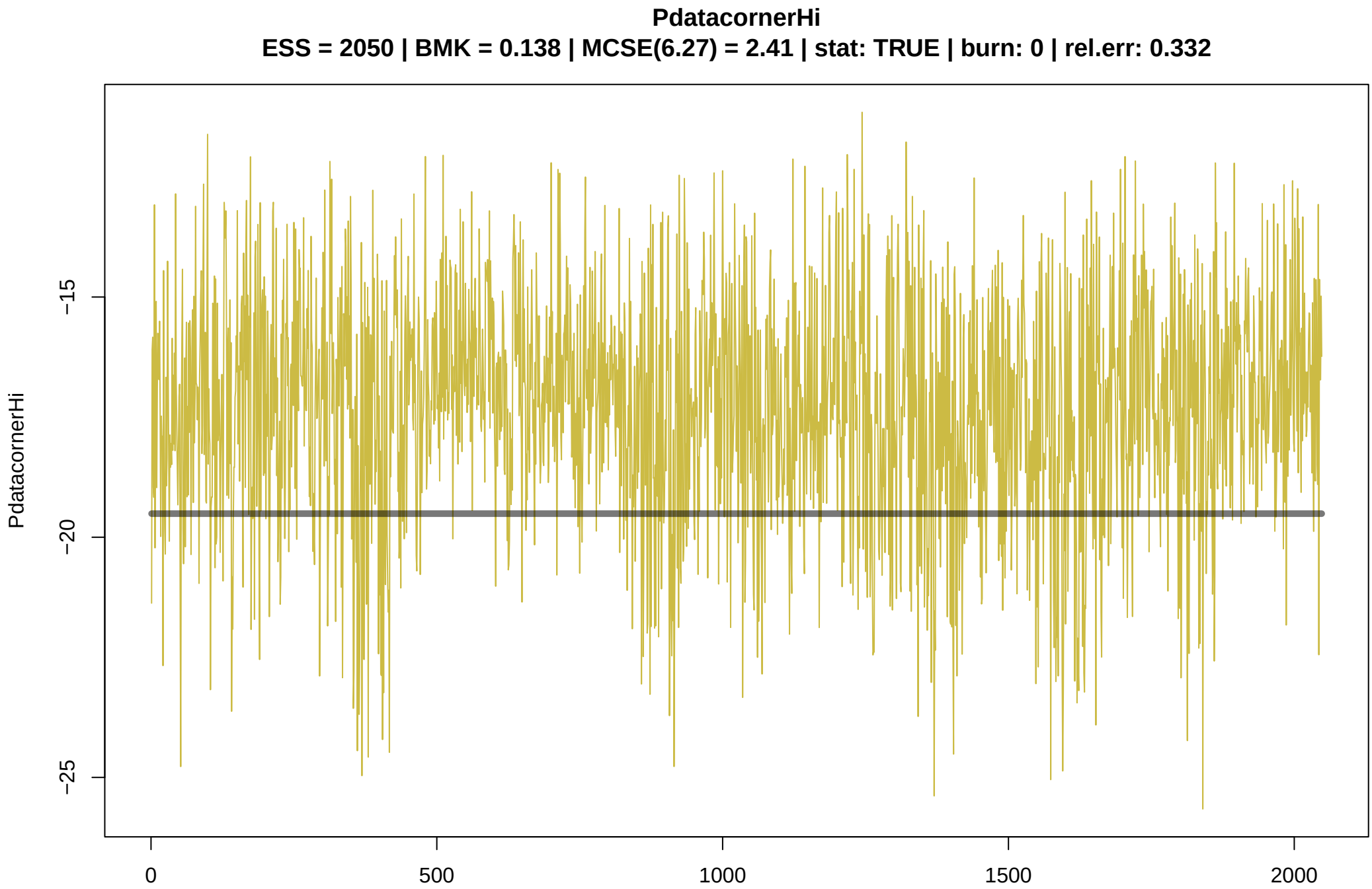
Occupied clusters: 10 of 16

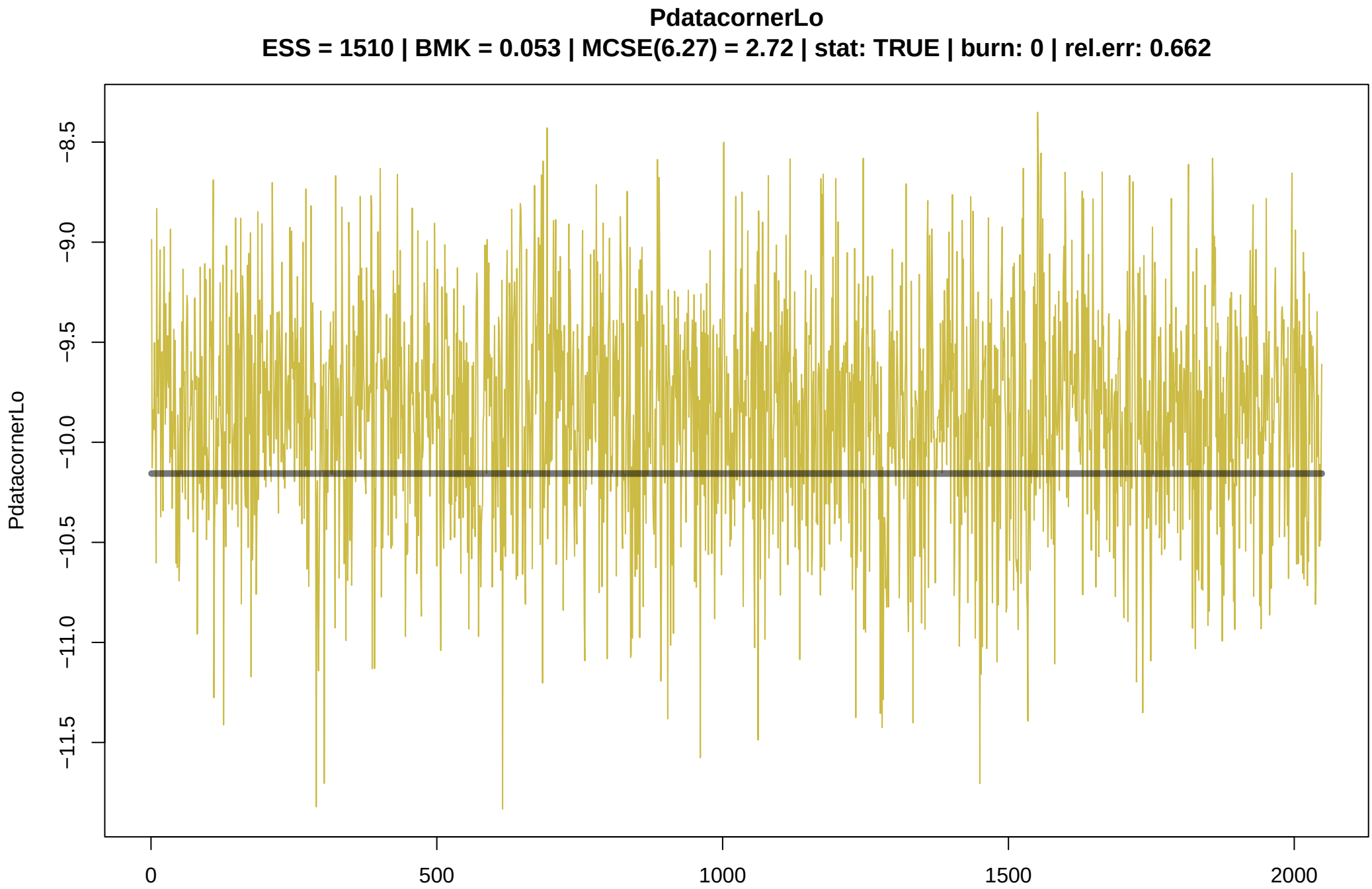

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

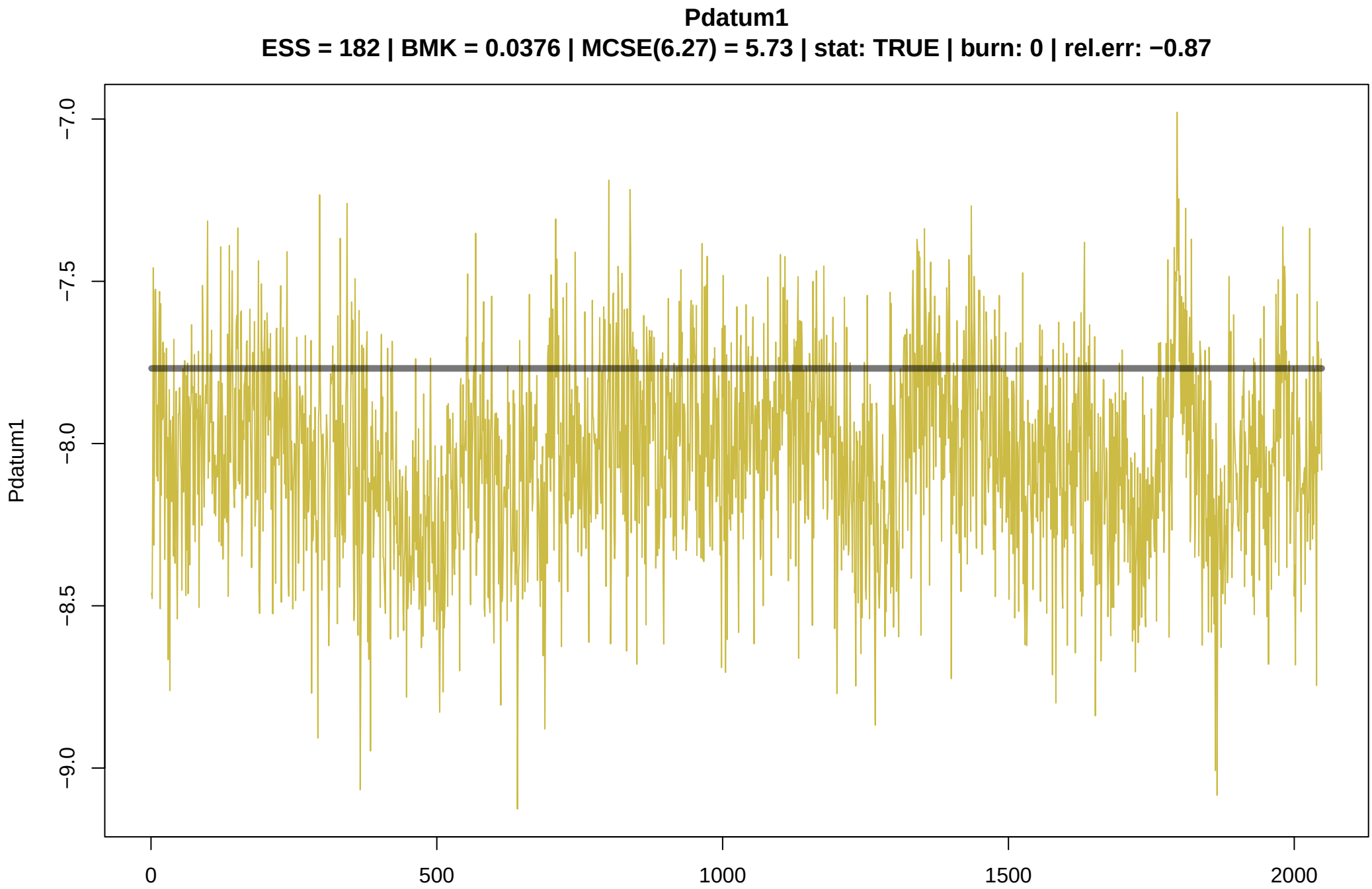

mcs_NumHeteroAtoms
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

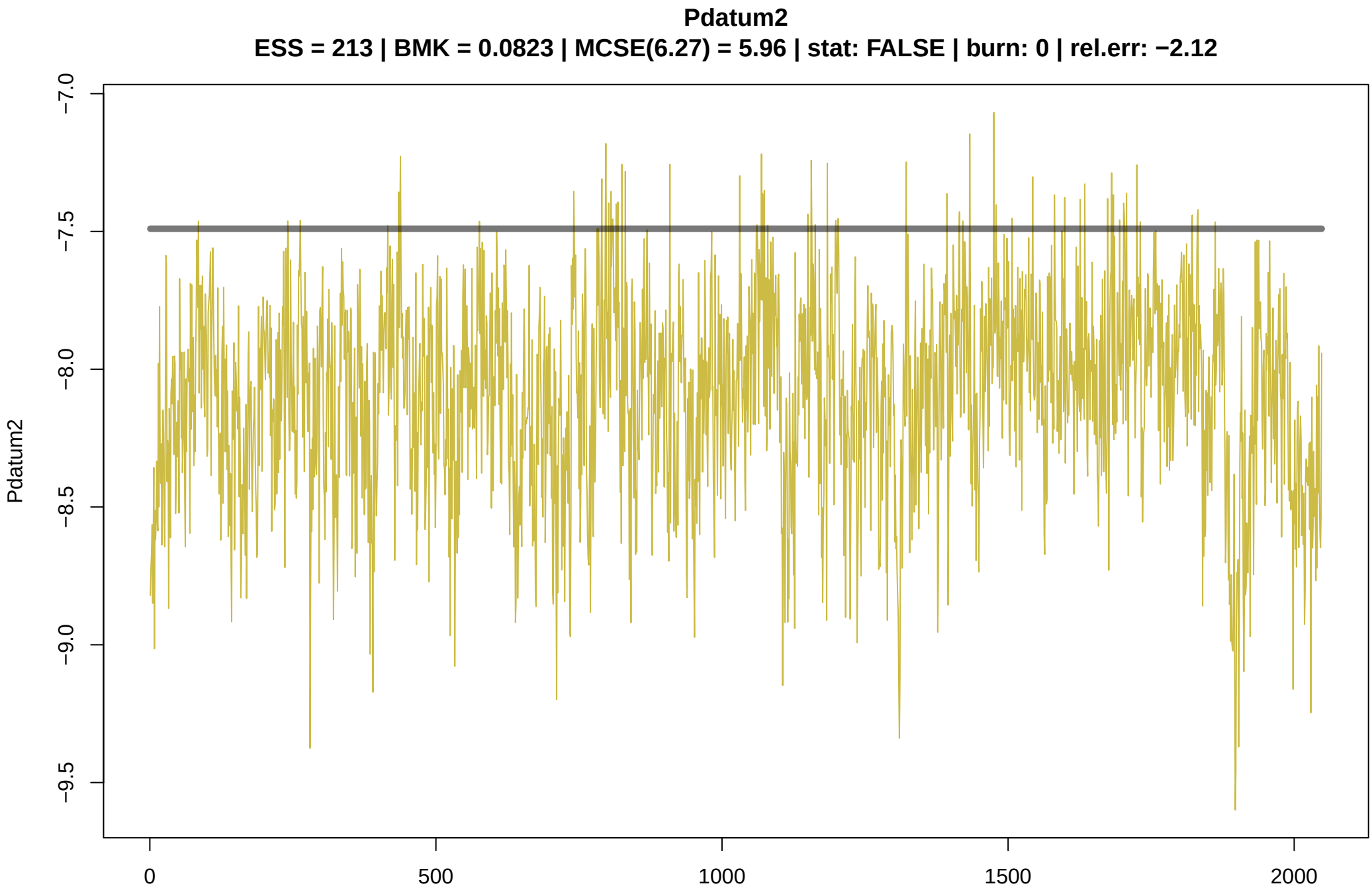

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

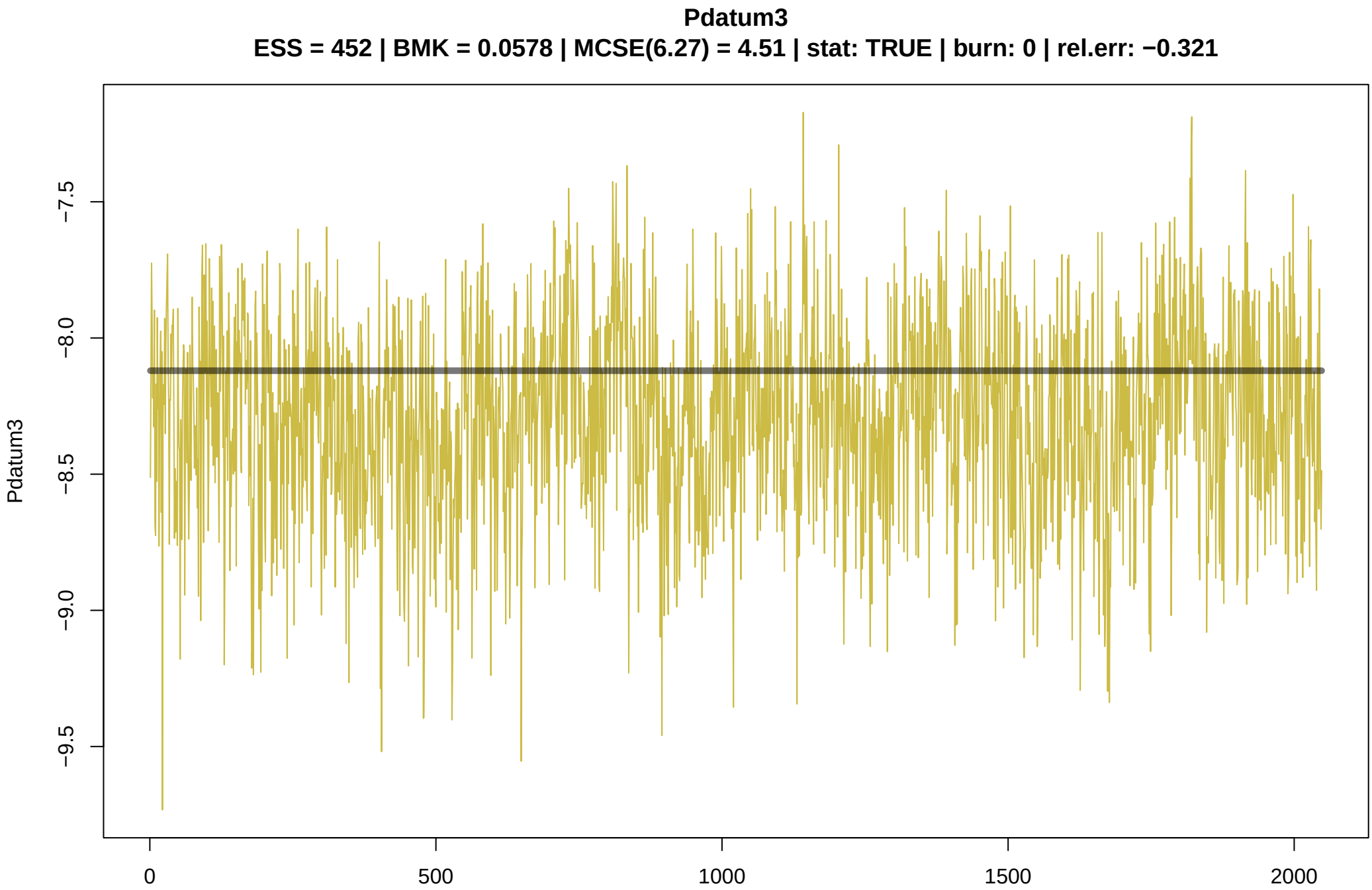

Pdatamean
ESS = 62 | BMK = 0.079 | MCSE(6.27) = 9.27 | stat: FALSE | burn: 0 | rel.err: 0.874
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

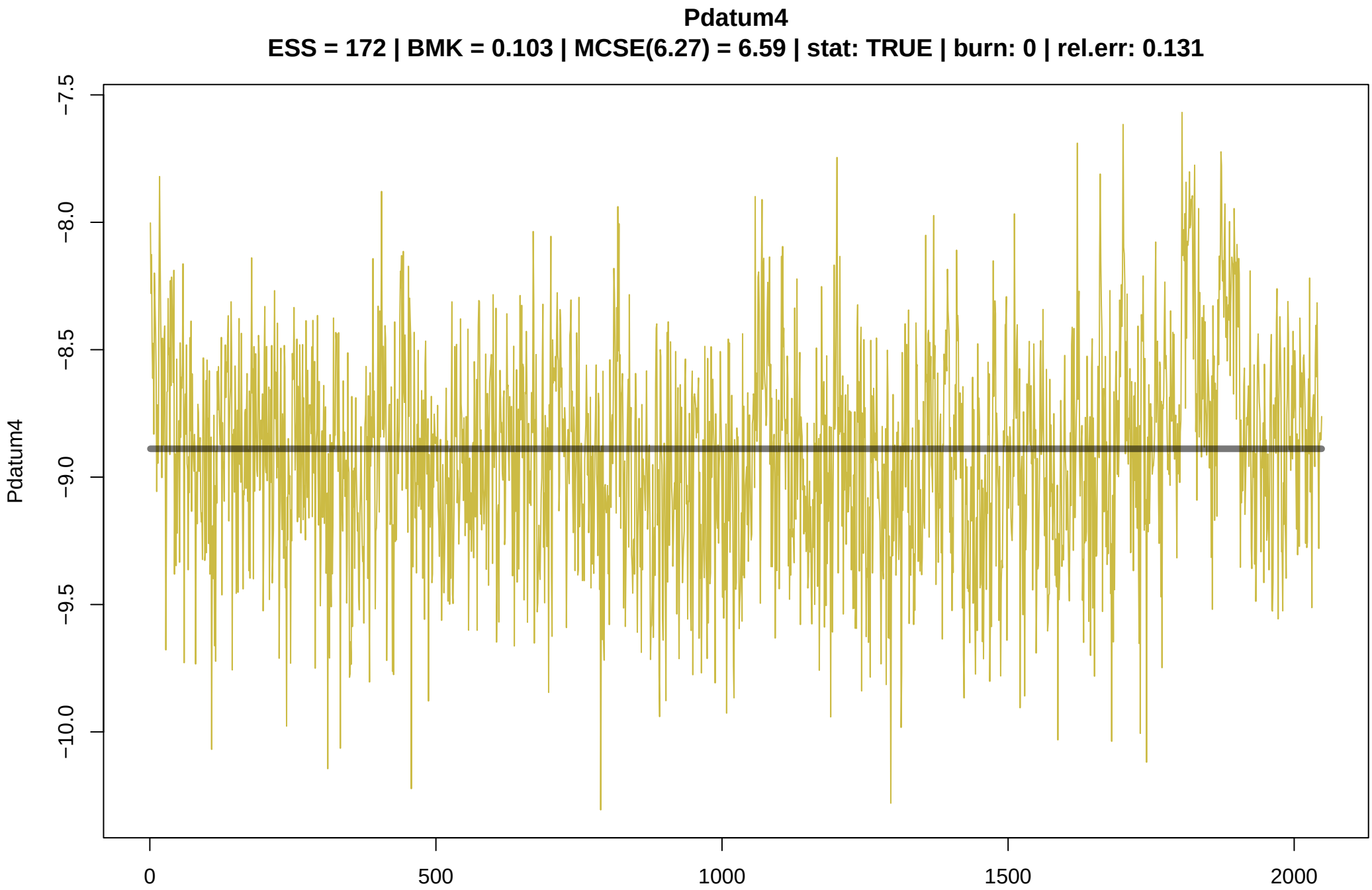

PdatacornerHi
ESS = 2050 | BMK = 0.138 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0 | rel.err: 0.332
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

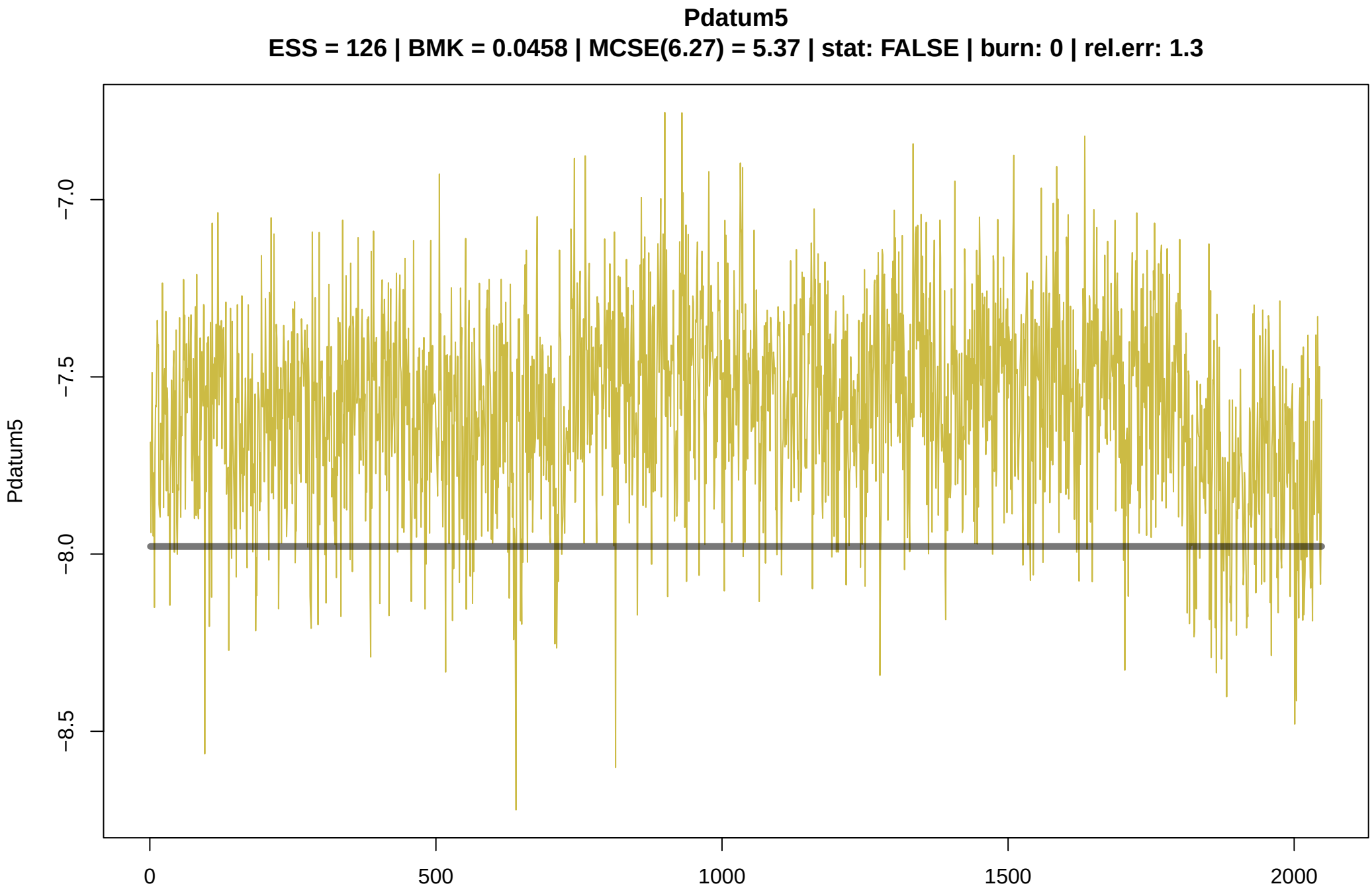

PdatacornerLo
ESS = 1510 | BMK = 0.053 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0 | rel.err: 0.662
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
0
500
1000
1500
2000

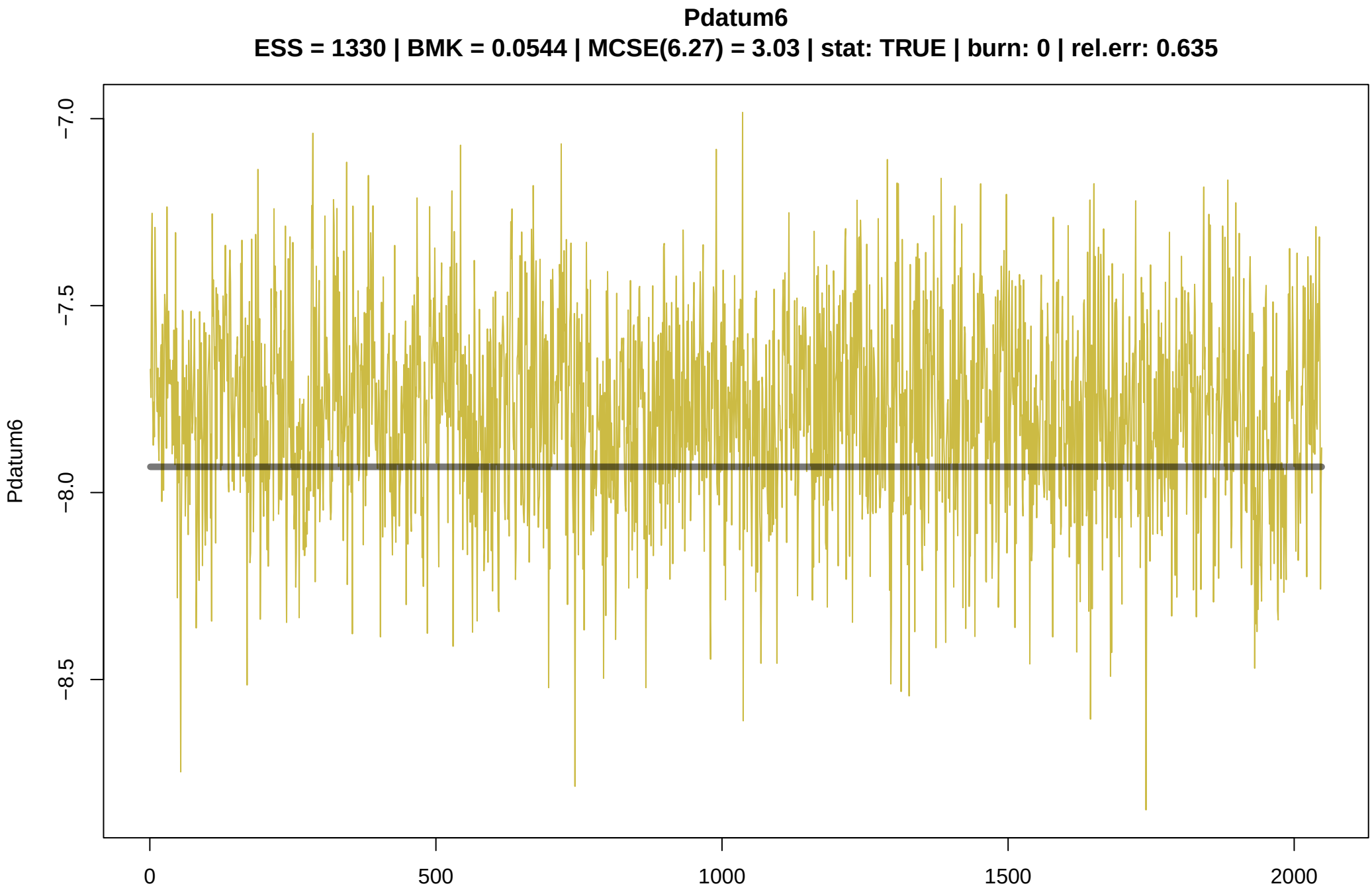

Pdatum1
ESS = 182 | BMK = 0.0376 | MCSE(6.27) = 5.73 | stat: TRUE | burn: 0 | rel.err: −0.87
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

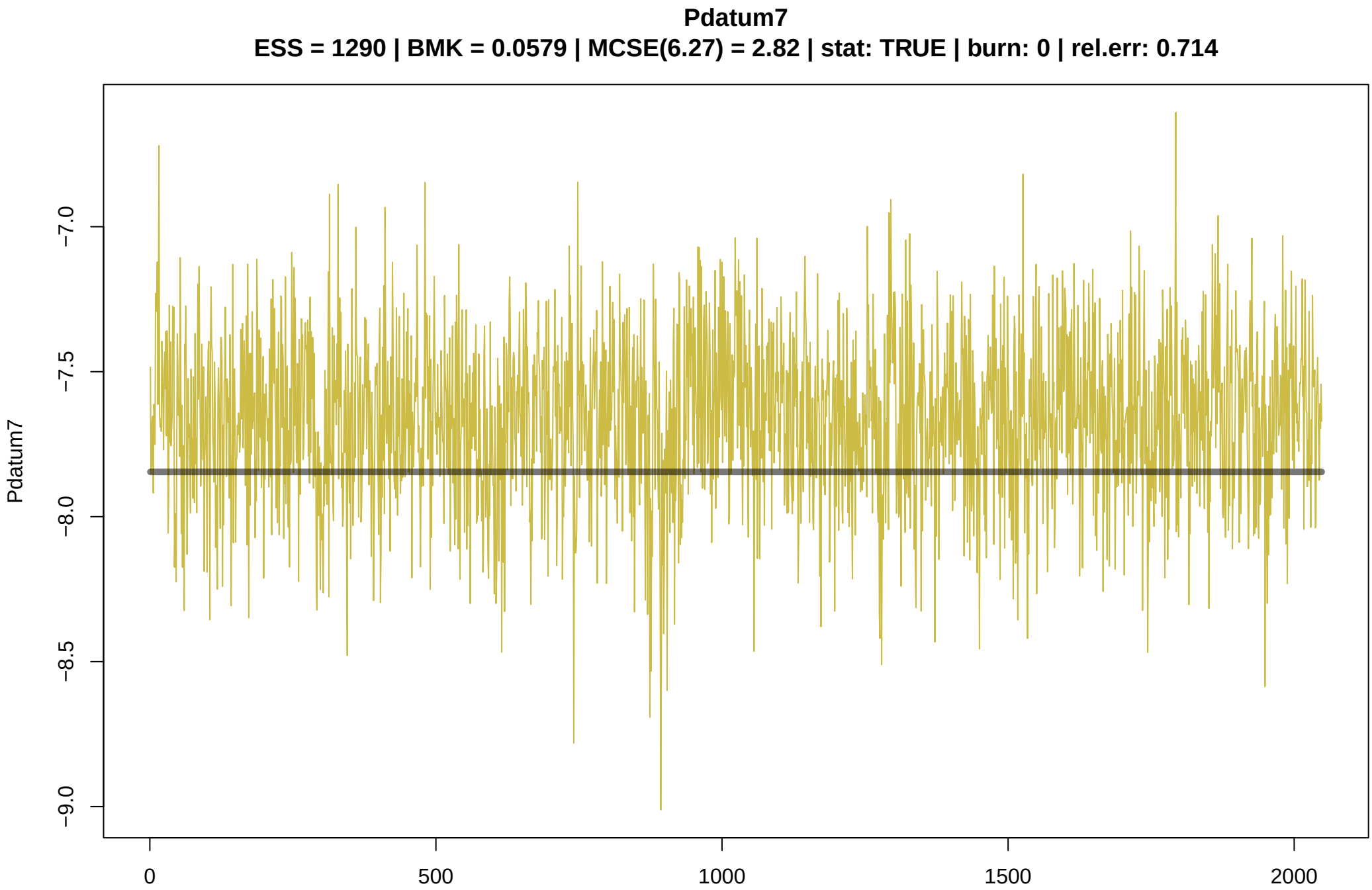

Pdatum2
ESS = 213 | BMK = 0.0823 | MCSE(6.27) = 5.96 | stat: FALSE | burn: 0 | rel.err: −2.12
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

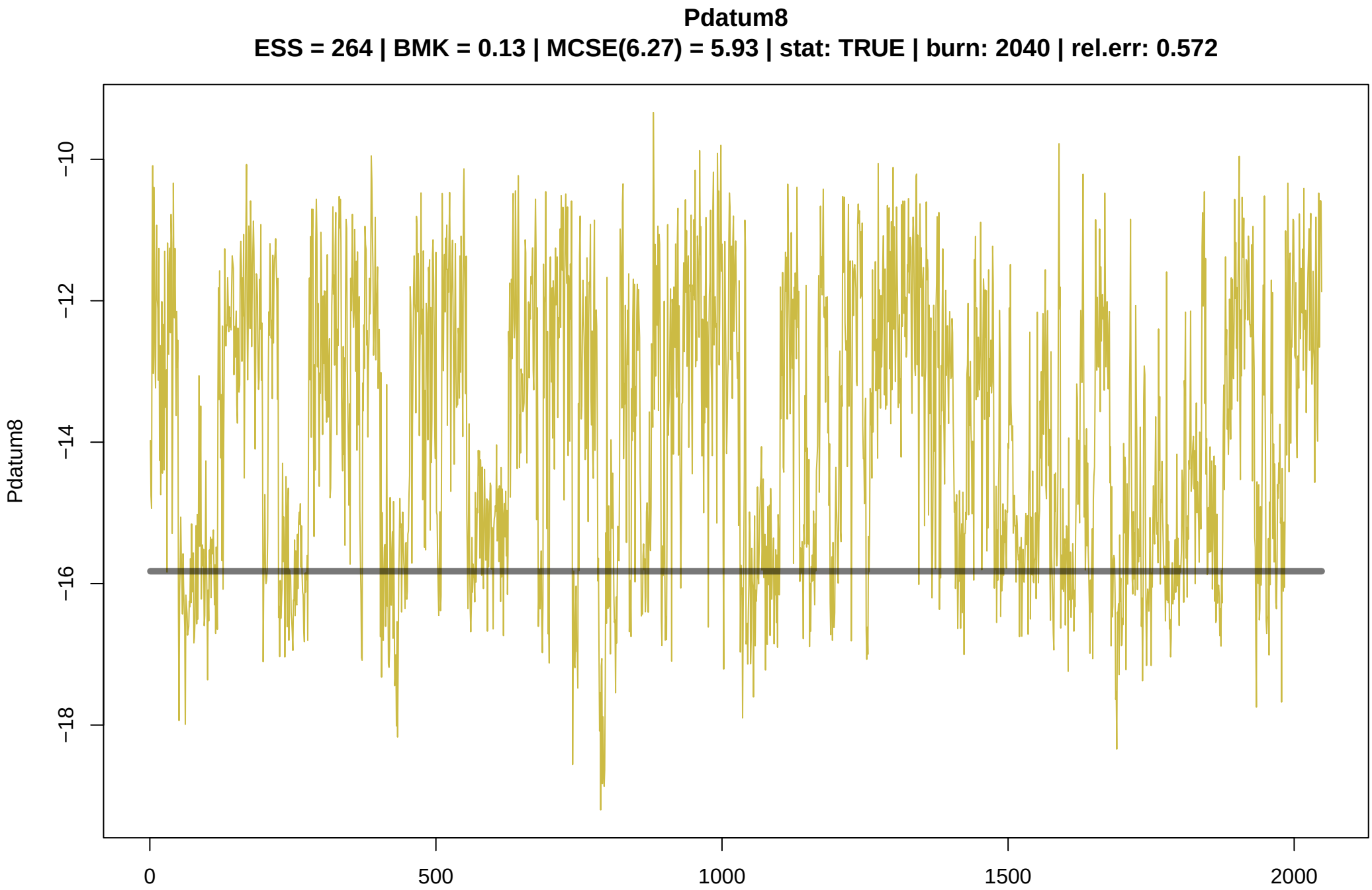

Pdatum3
ESS = 452 | BMK = 0.0578 | MCSE(6.27) = 4.51 | stat: TRUE | burn: 0 | rel.err: −0.321
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

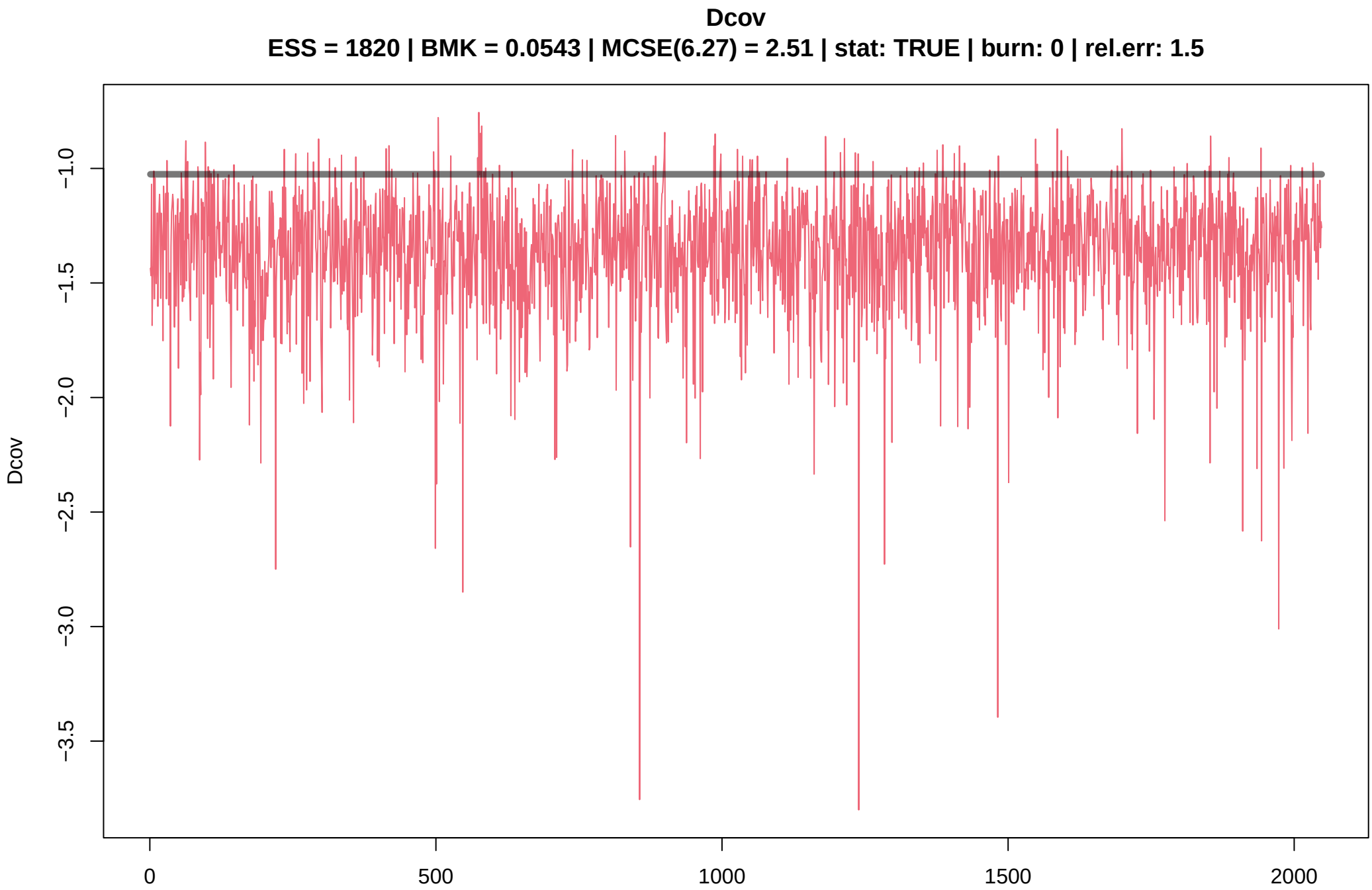

Pdatum4
ESS = 172 | BMK = 0.103 | MCSE(6.27) = 6.59 | stat: TRUE | burn: 0 | rel.err: 0.131
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

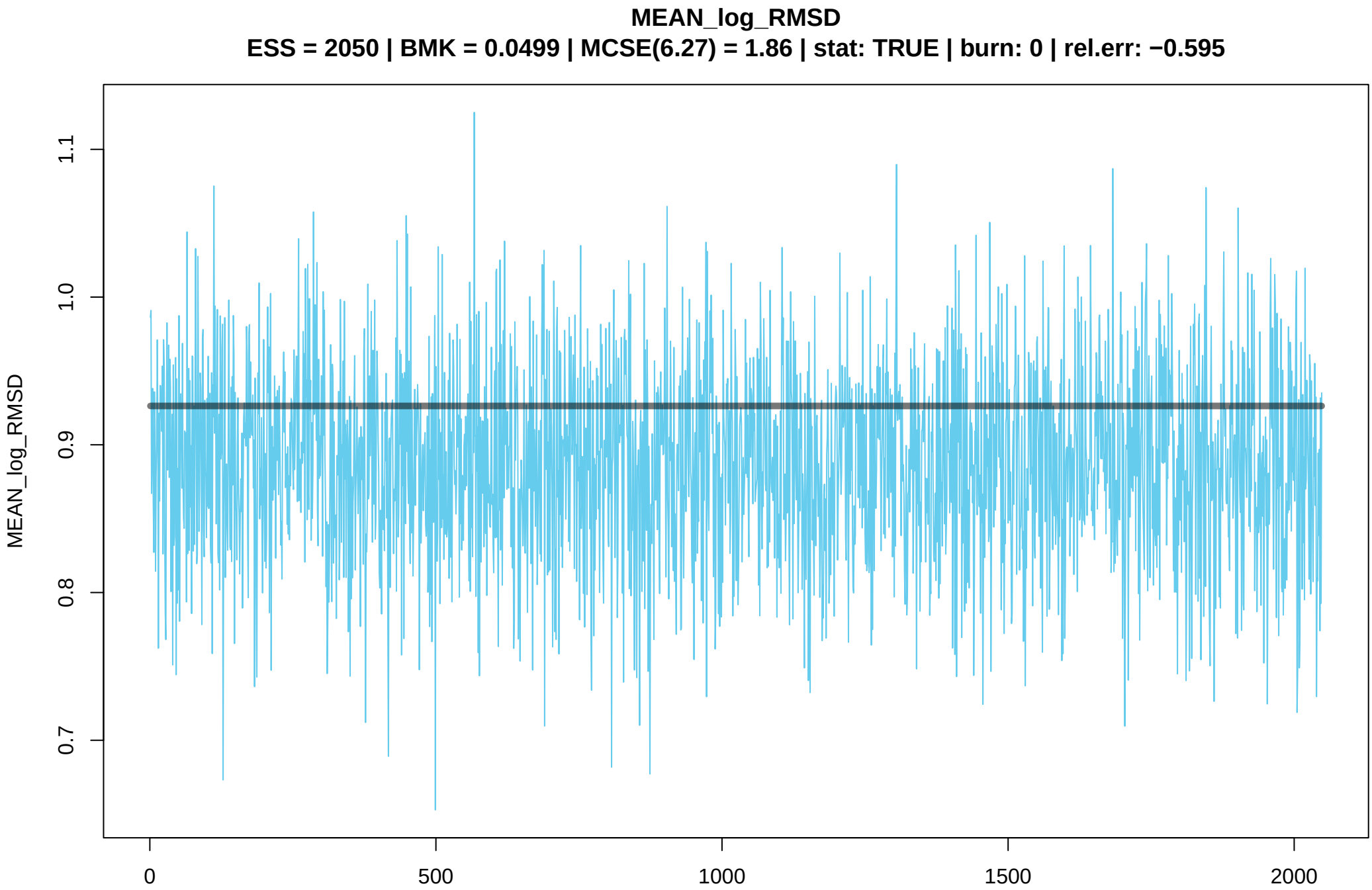

Pdatum5
ESS = 126 | BMK = 0.0458 | MCSE(6.27) = 5.37 | stat: FALSE | burn: 0 | rel.err: 1.3
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

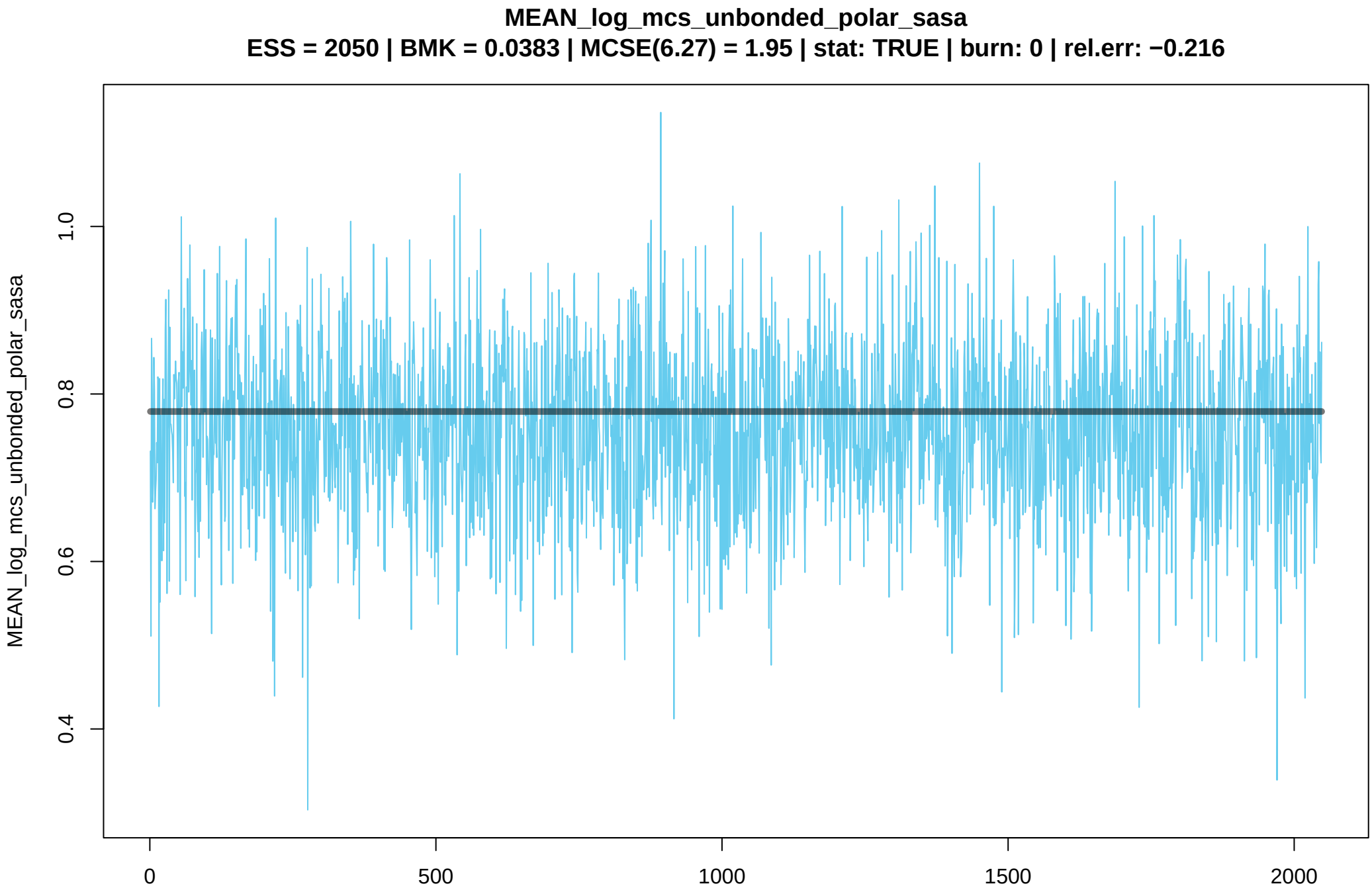

Pdatum6
ESS = 1330 | BMK = 0.0544 | MCSE(6.27) = 3.03 | stat: TRUE | burn: 0 | rel.err: 0.635
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

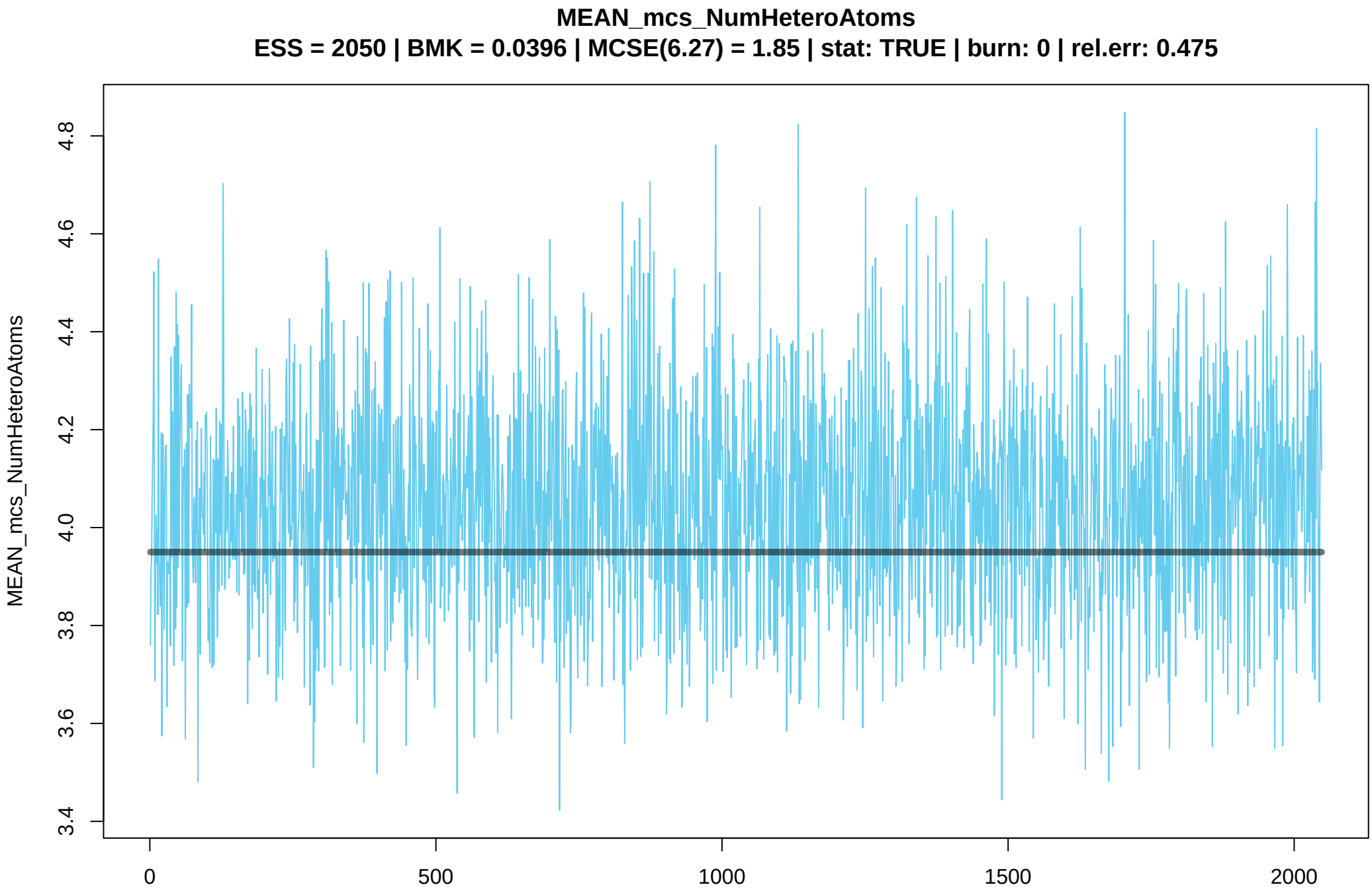

Pdatum7
ESS = 1290 | BMK = 0.0579 | MCSE(6.27) = 2.82 | stat: TRUE | burn: 0 | rel.err: 0.714
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

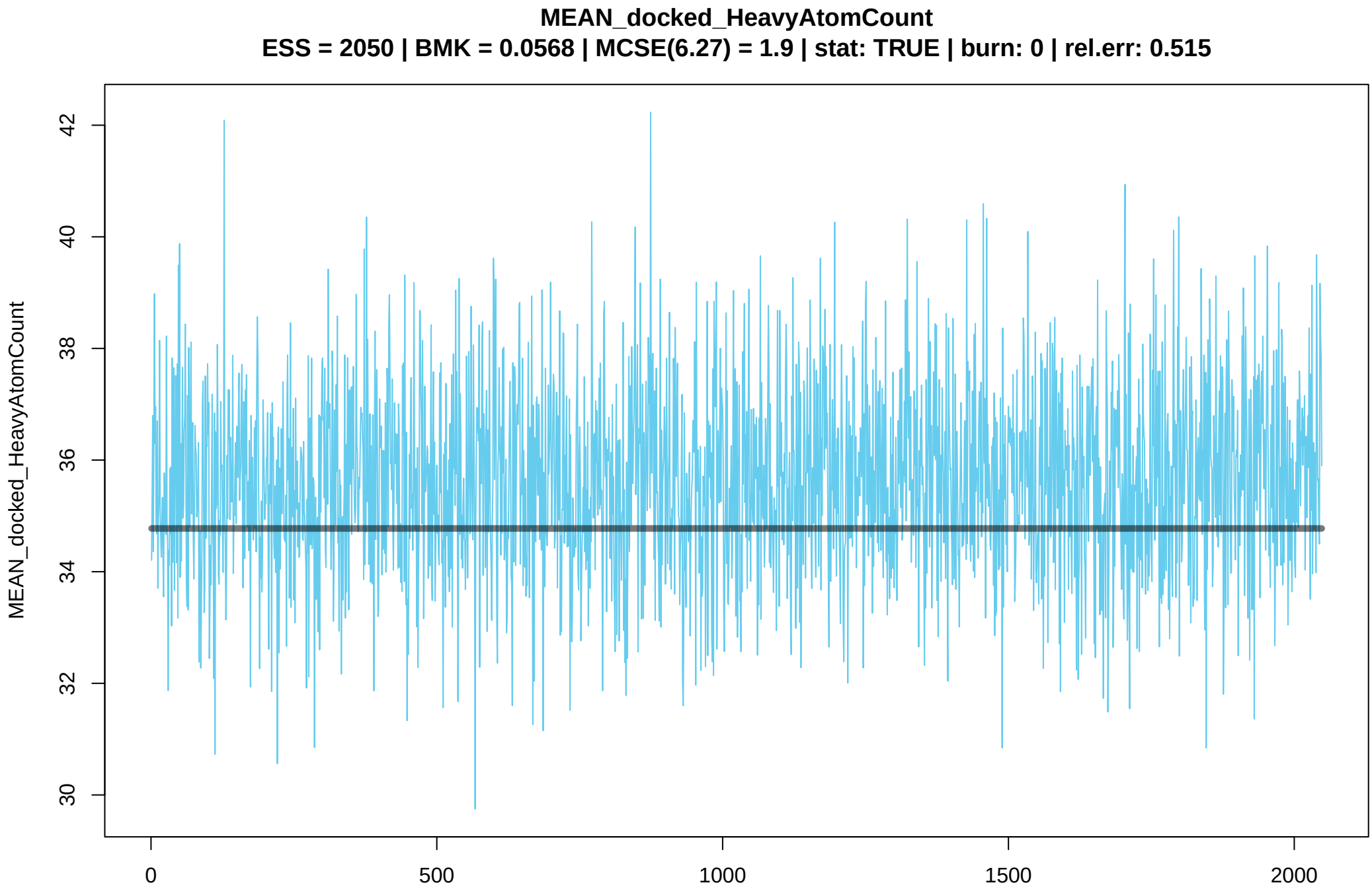

Pdatum8
ESS = 264 | BMK = 0.13 | MCSE(6.27) = 5.93 | stat: TRUE | burn: 2040 | rel.err: 0.572
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

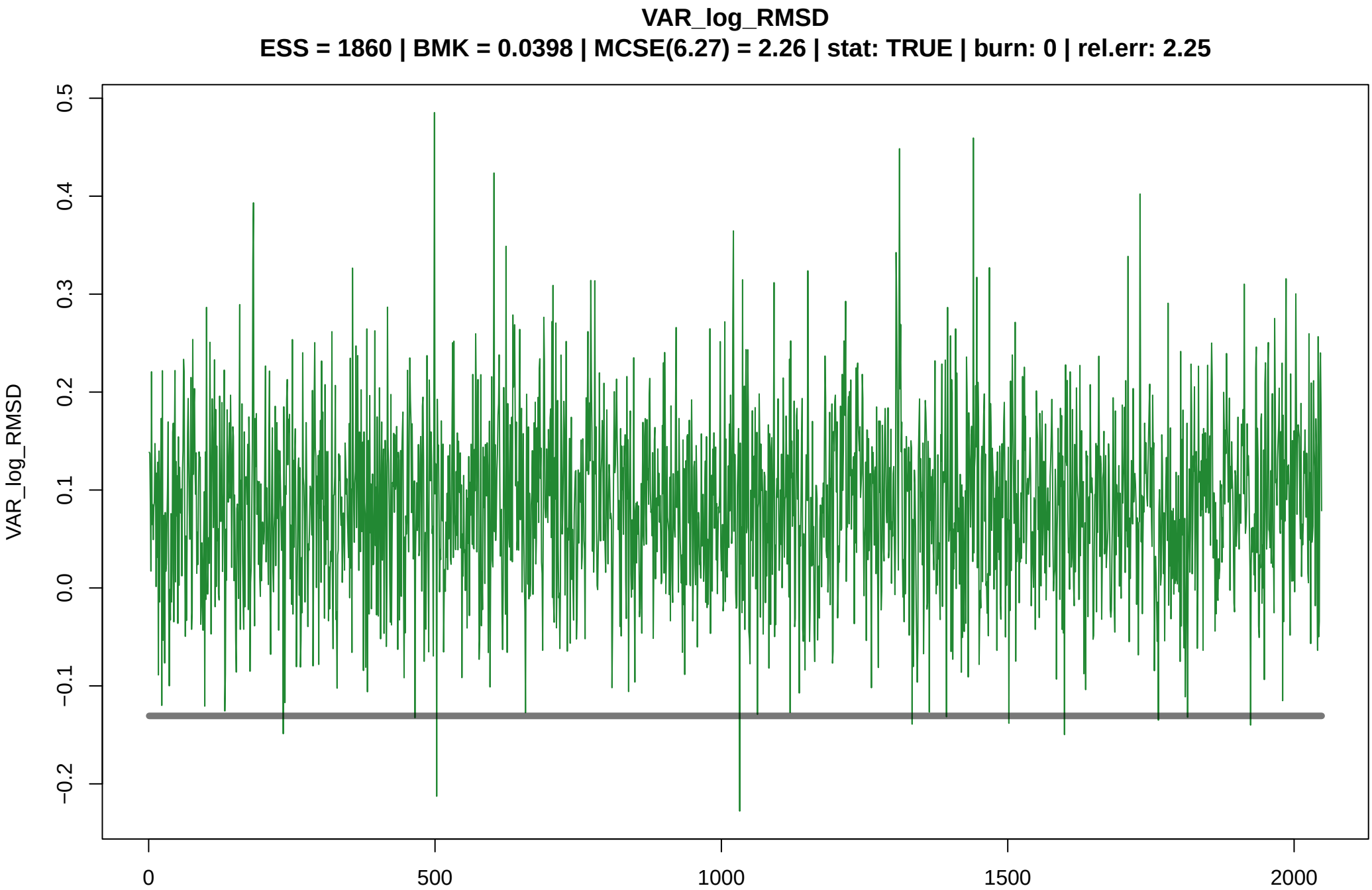

Dcov
ESS = 1820 | BMK = 0.0543 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0 | rel.err: 1.5
Dcov
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
0
500
1000
1500
2000

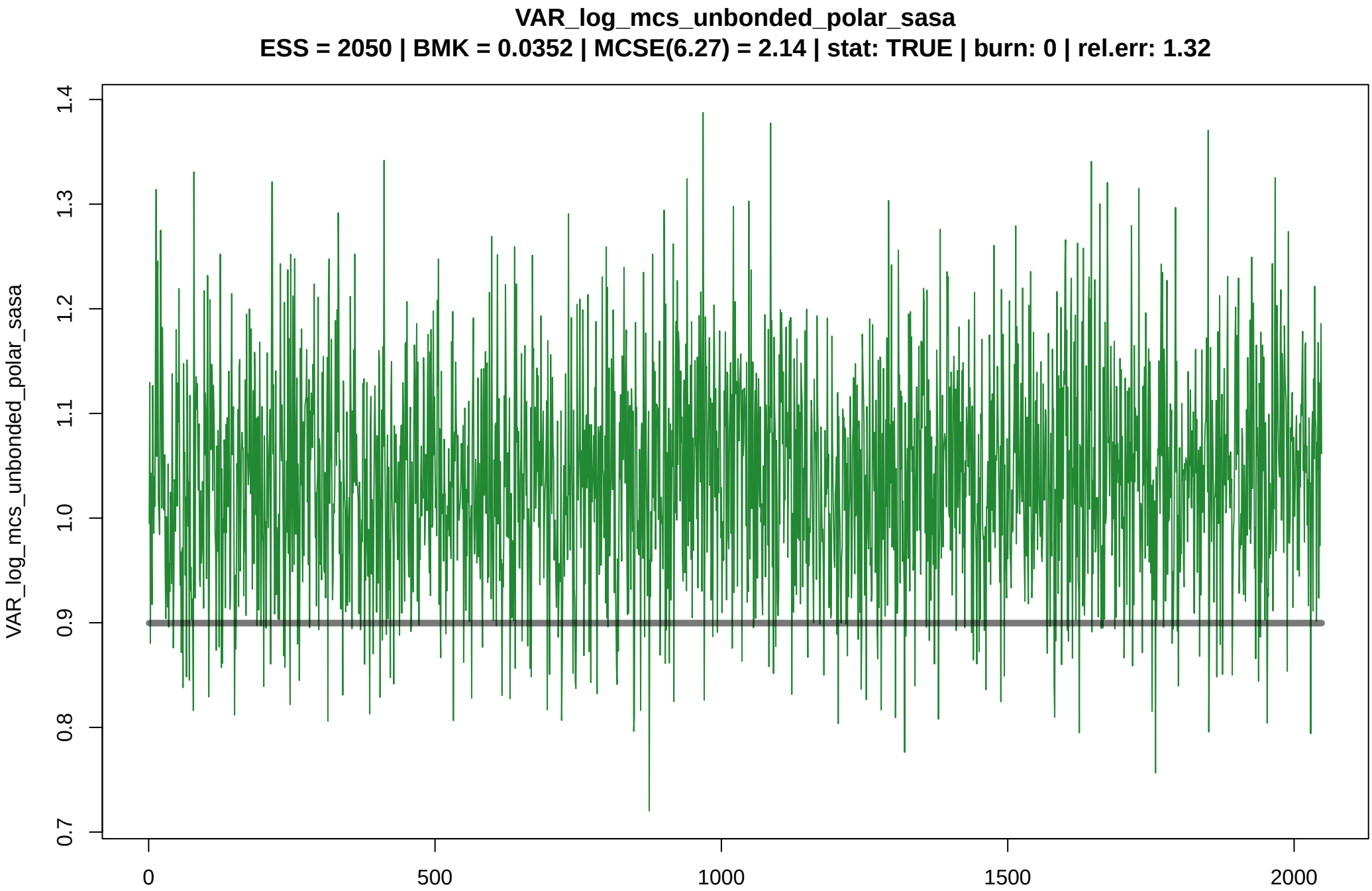

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0499 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0 | rel.err: −0.595
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

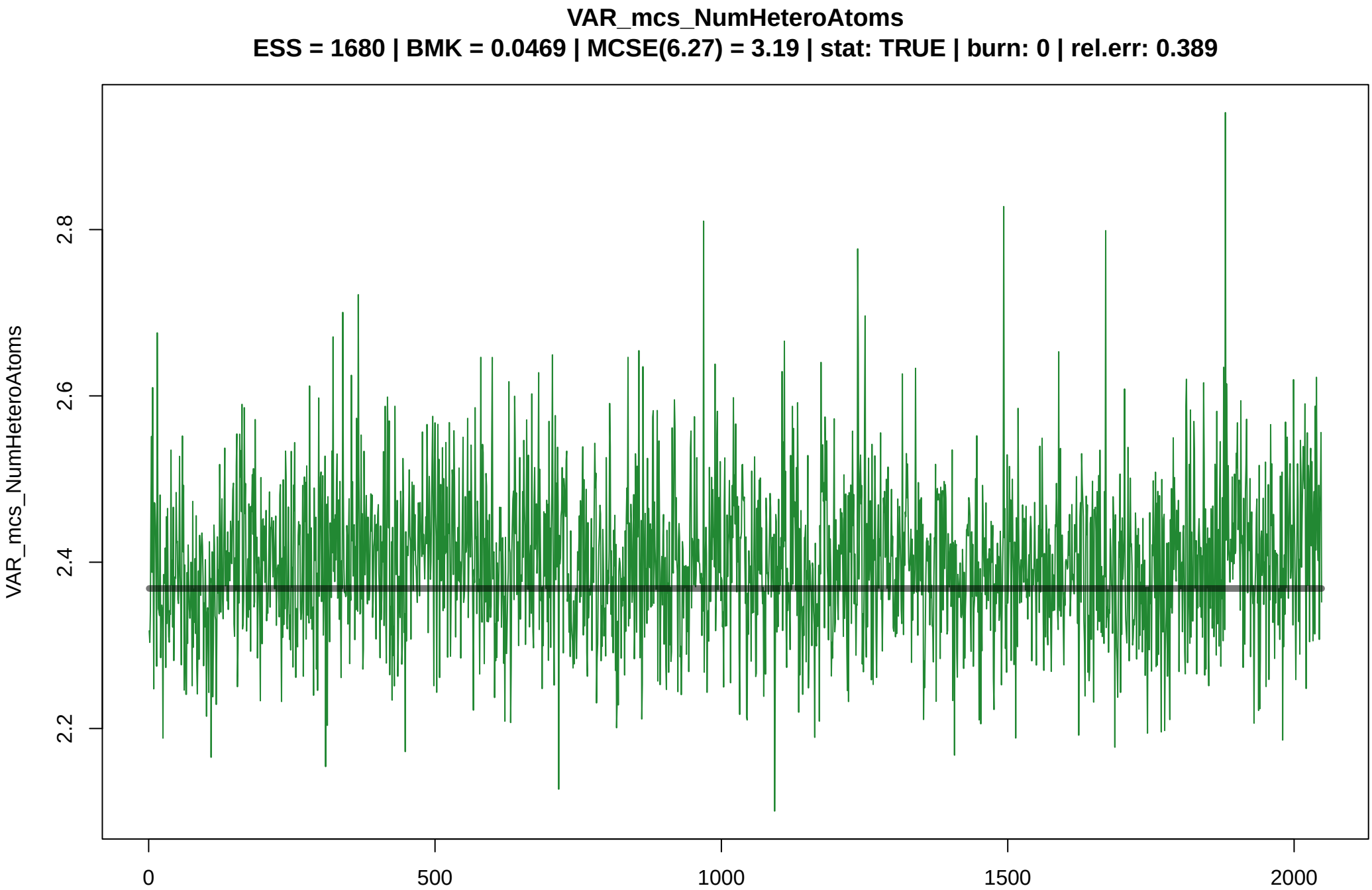

MEAN_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0383 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: −0.216
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

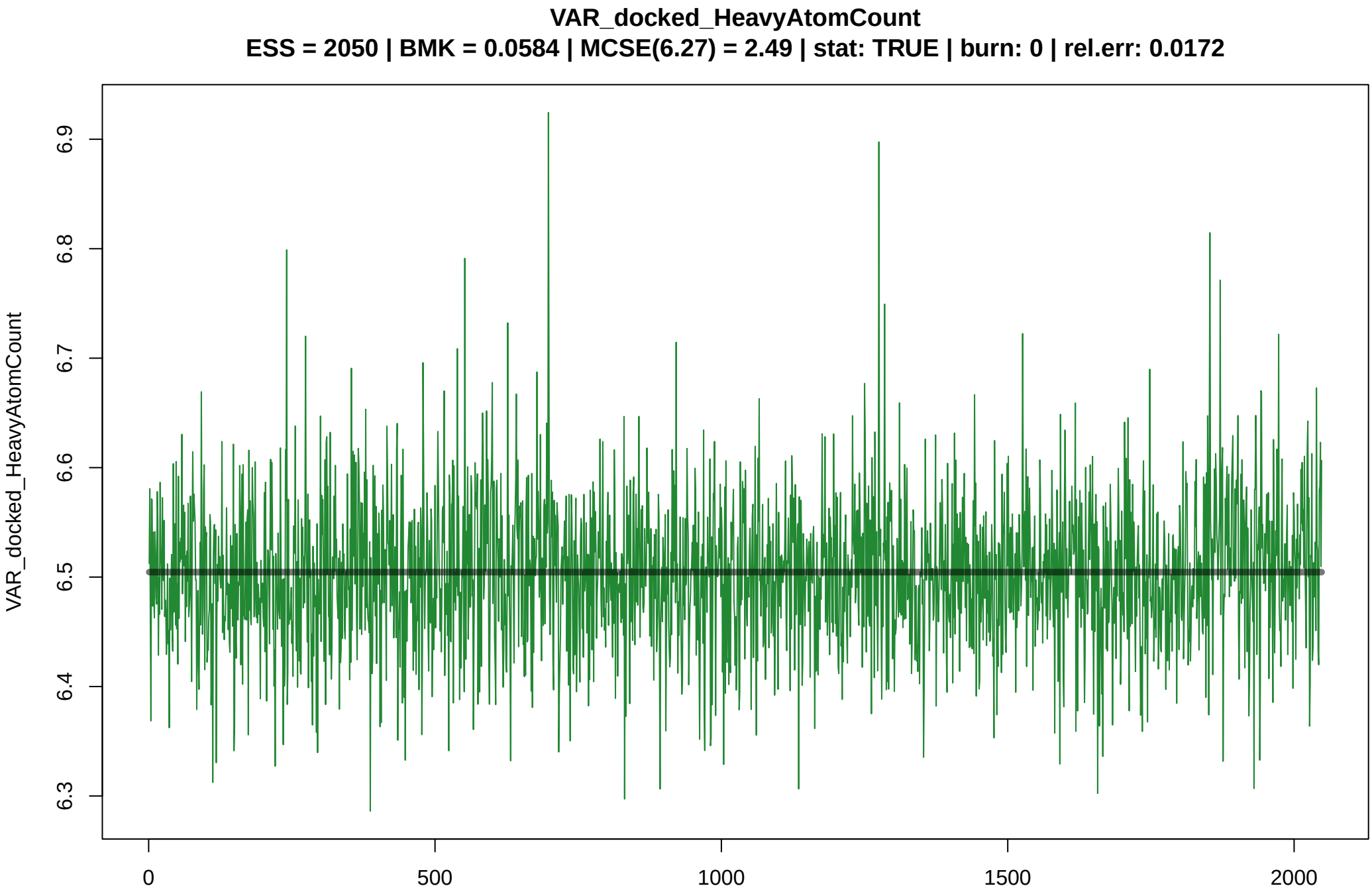

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0396 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: 0.475
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

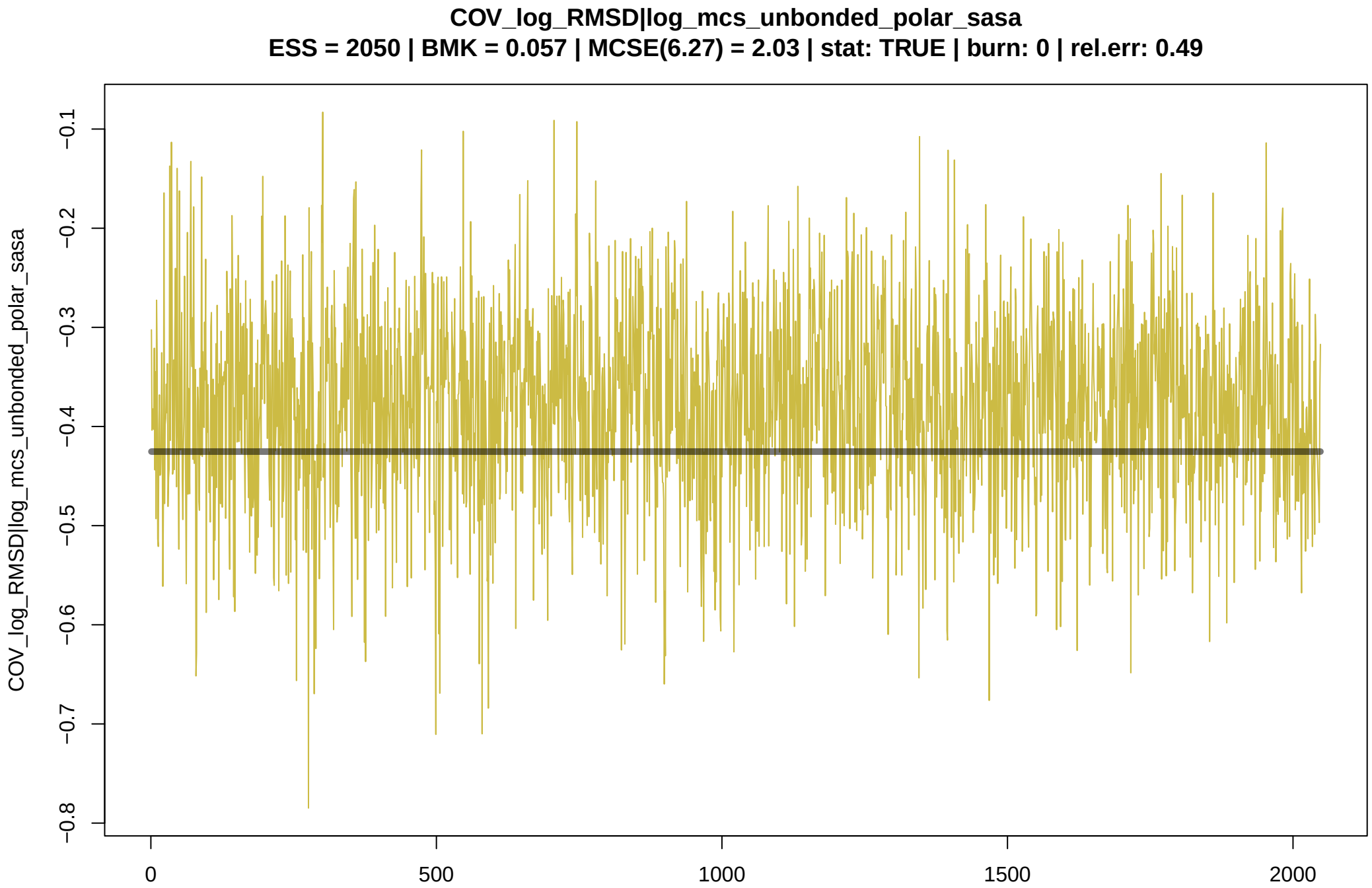

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0568 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0 | rel.err: 0.515
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
500
1000
1500
2000

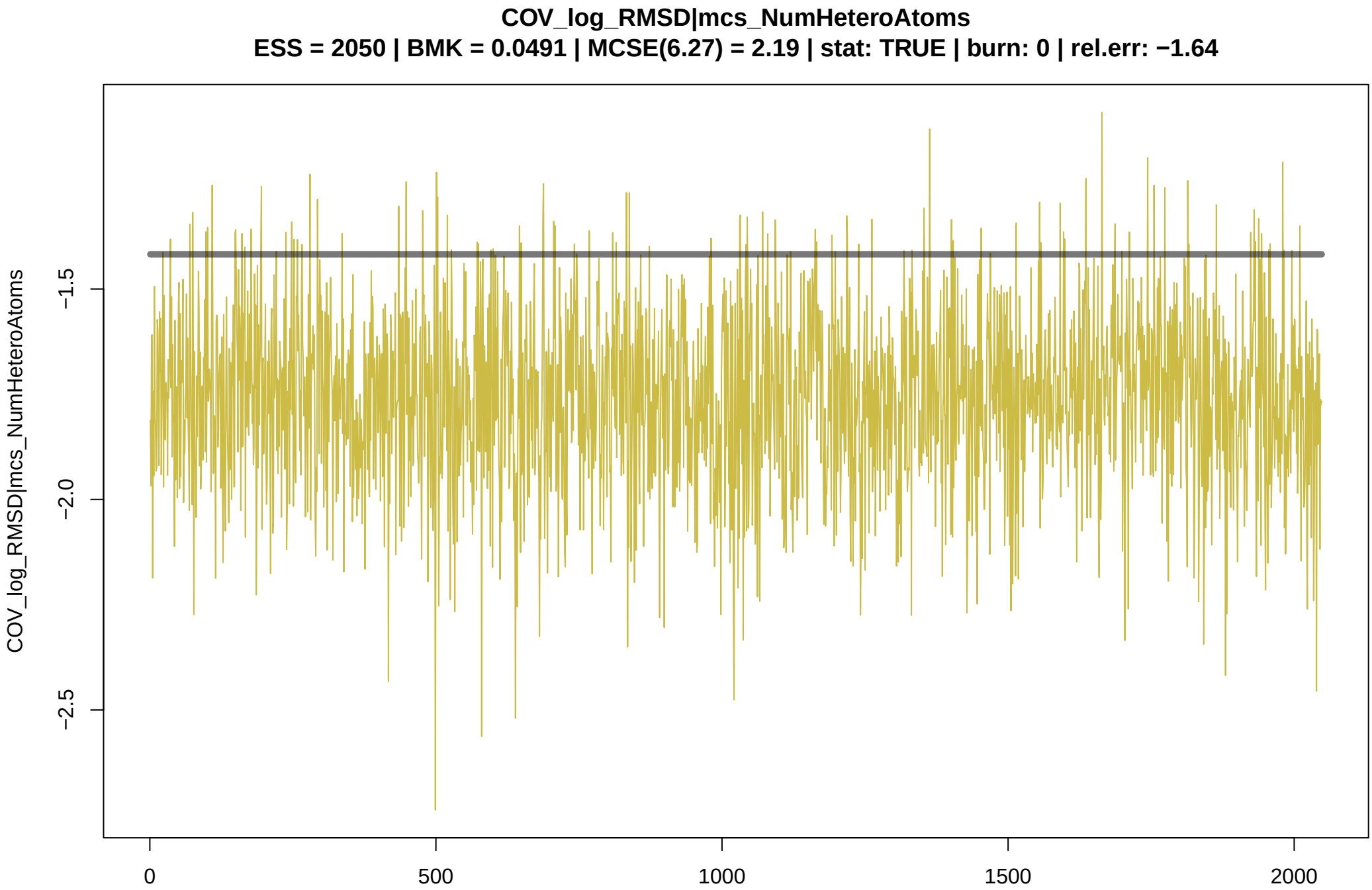

VAR_log_RMSD
ESS = 1860 | BMK = 0.0398 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: 2.25
VAR_log_RMSD
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

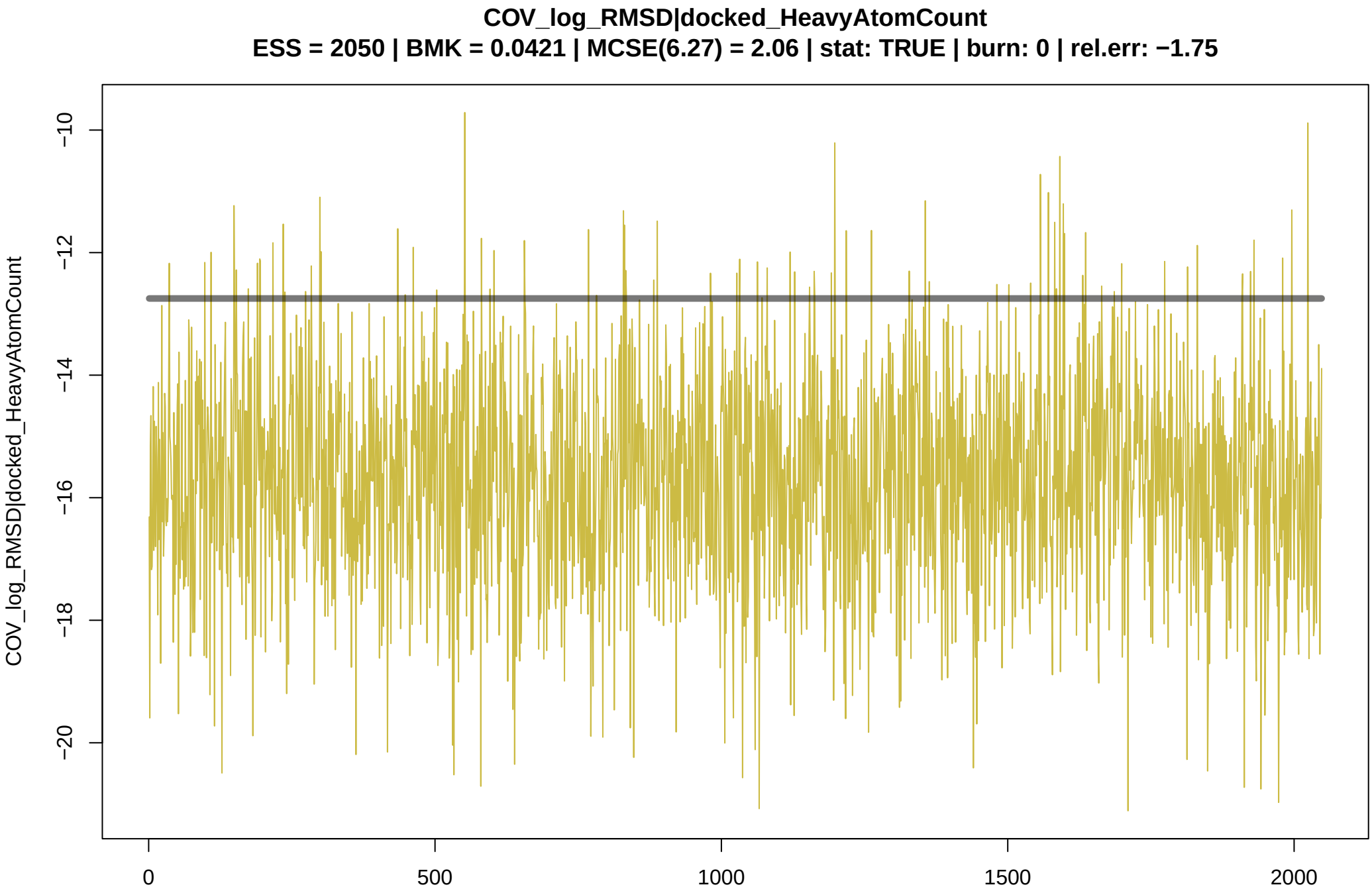

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 1.32
VAR_log_mcs_unbonded_polar_sasa
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

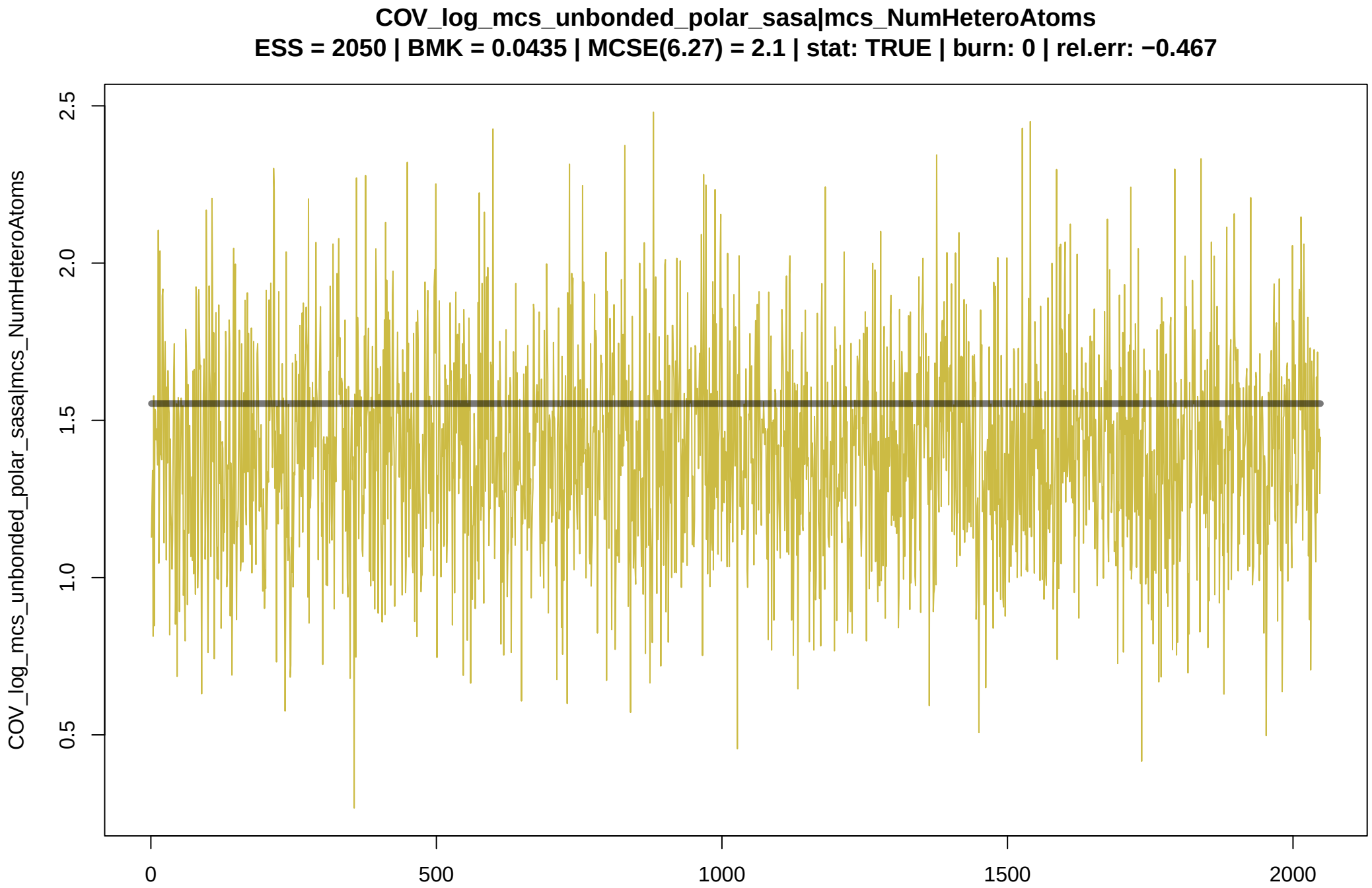

VAR_mcs_NumHeteroAtoms
ESS = 1680 | BMK = 0.0469 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | rel.err: 0.389
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

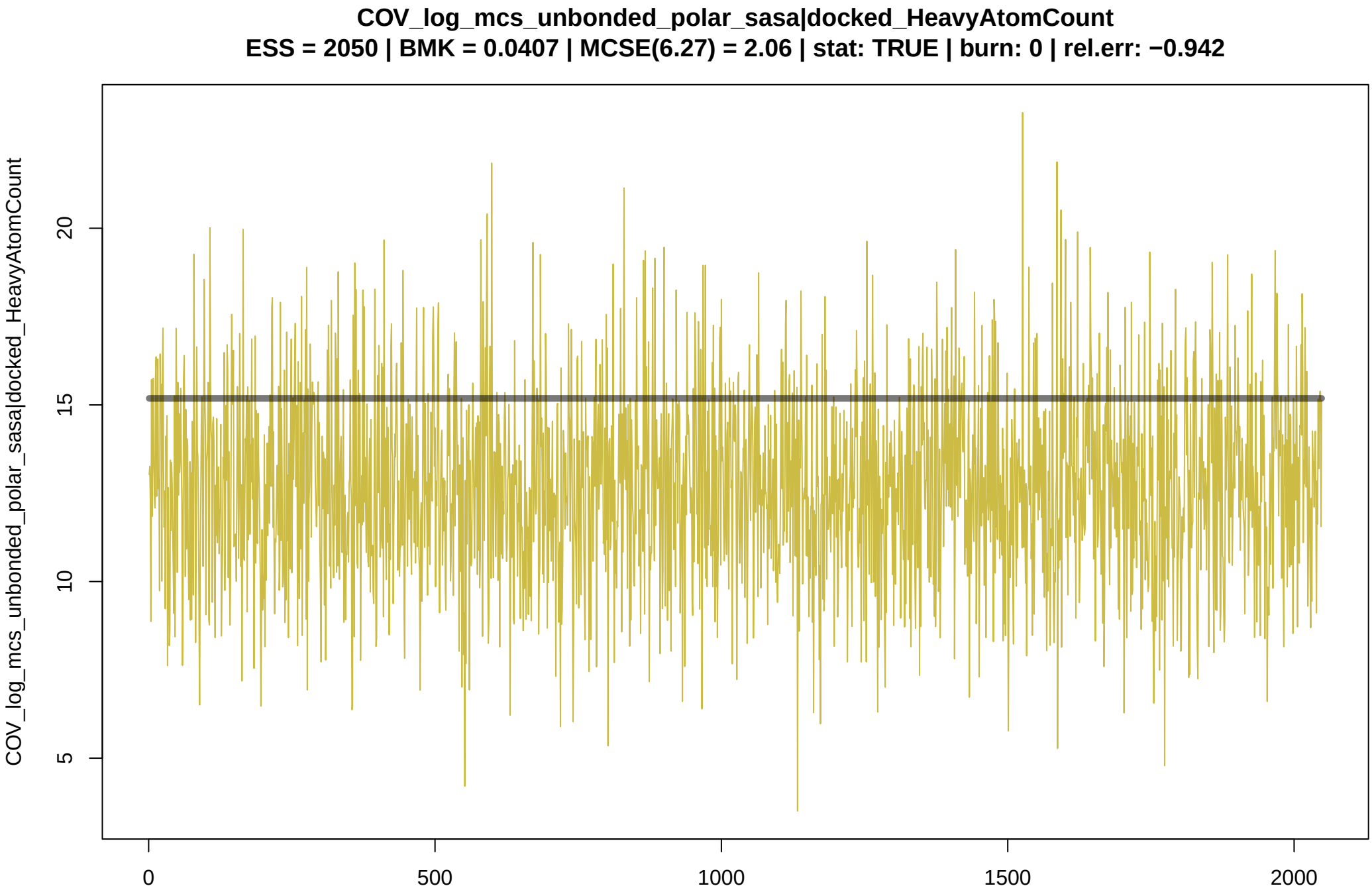

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0584 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | rel.err: 0.0172
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
6.9
0
500
1000
1500
2000

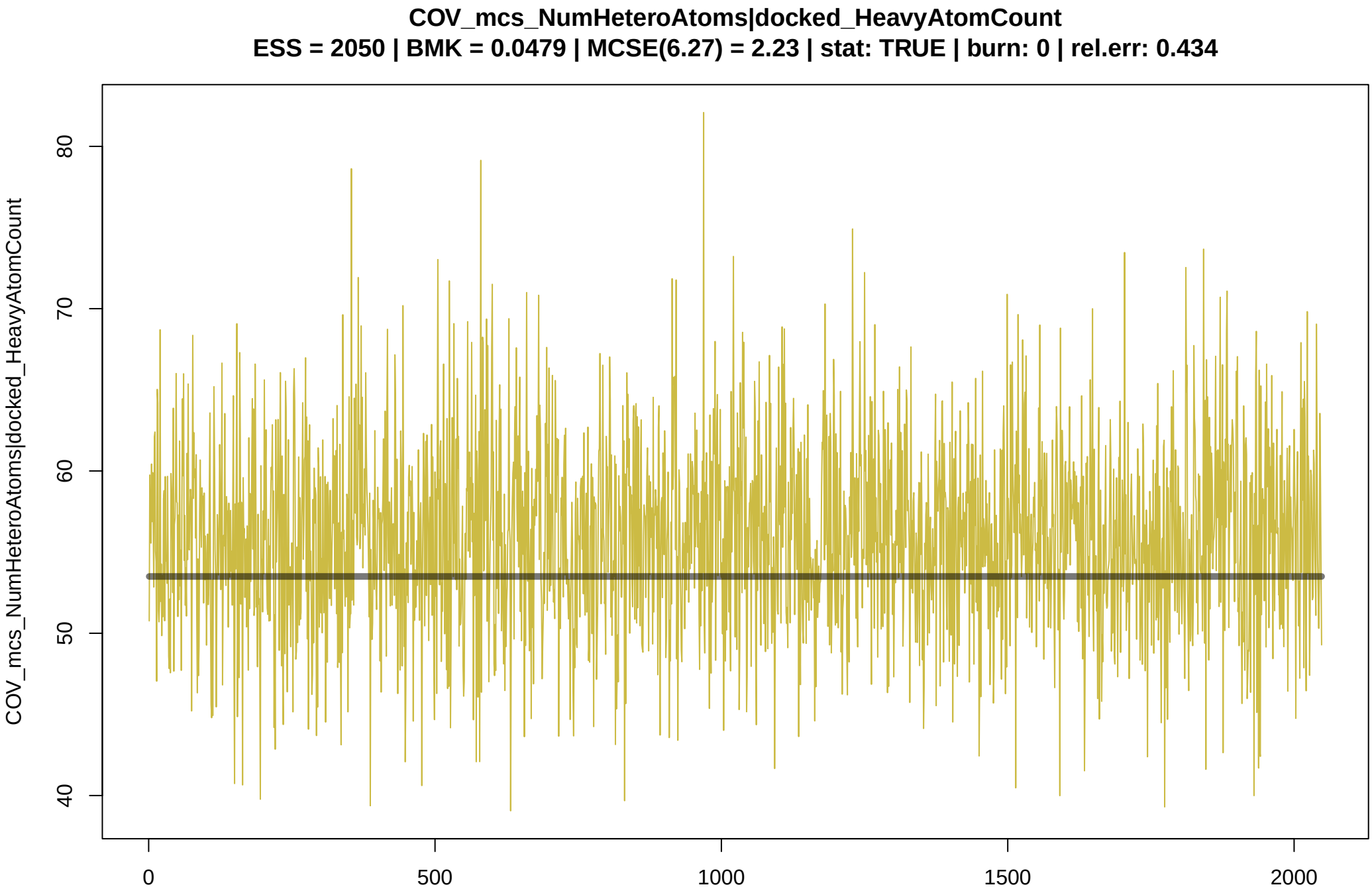

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.057 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0 | rel.err: 0.49
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0491 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: −1.64
COV_log_RMSD|mcs_NumHeteroAtoms
−1.5
−2.0
−2.5
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0421 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: −1.75
COV_log_RMSD|docked_HeavyAtomCount
−10
−12
−14
−16
−18
−20
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0435 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0 | rel.err: −0.467
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 = 2050 | BMK = 0.0407 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: −0.942
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0479 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.434
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000