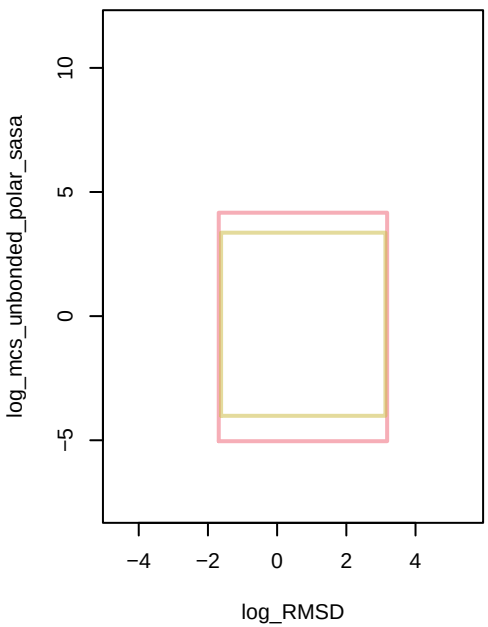
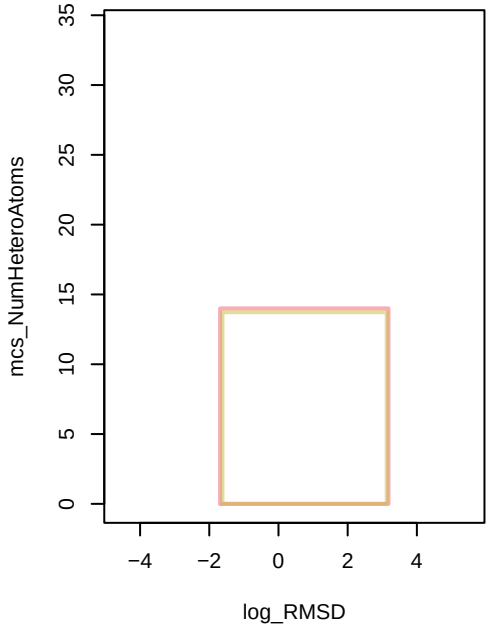
−− STATS maxD −−
min ESS = 109.930361703038
max BMK = 0.14453524781853
max MCSE = 7.86583005546839
all stationary: FALSE
burn: 0
max rel.err.: 2.00385829832637

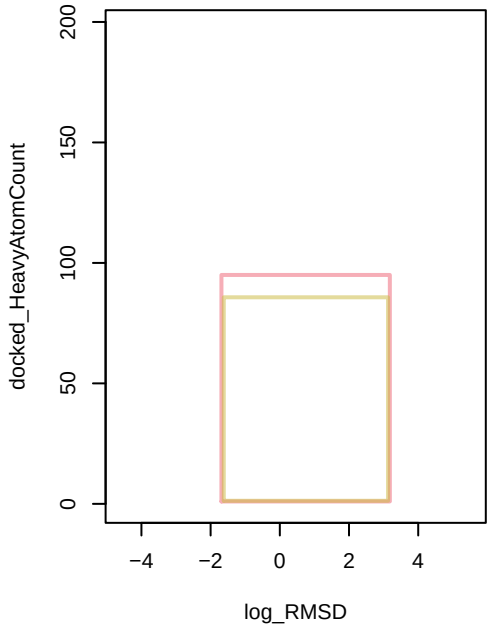
−− STATS 2D −−
min ESS = 1843.45155583632
max BMK = 0.048829575719282 6
max MCSE = 2.53734367712526
all stationary: TRUE
burn: 0
max rel.err.: 1.7808630562468

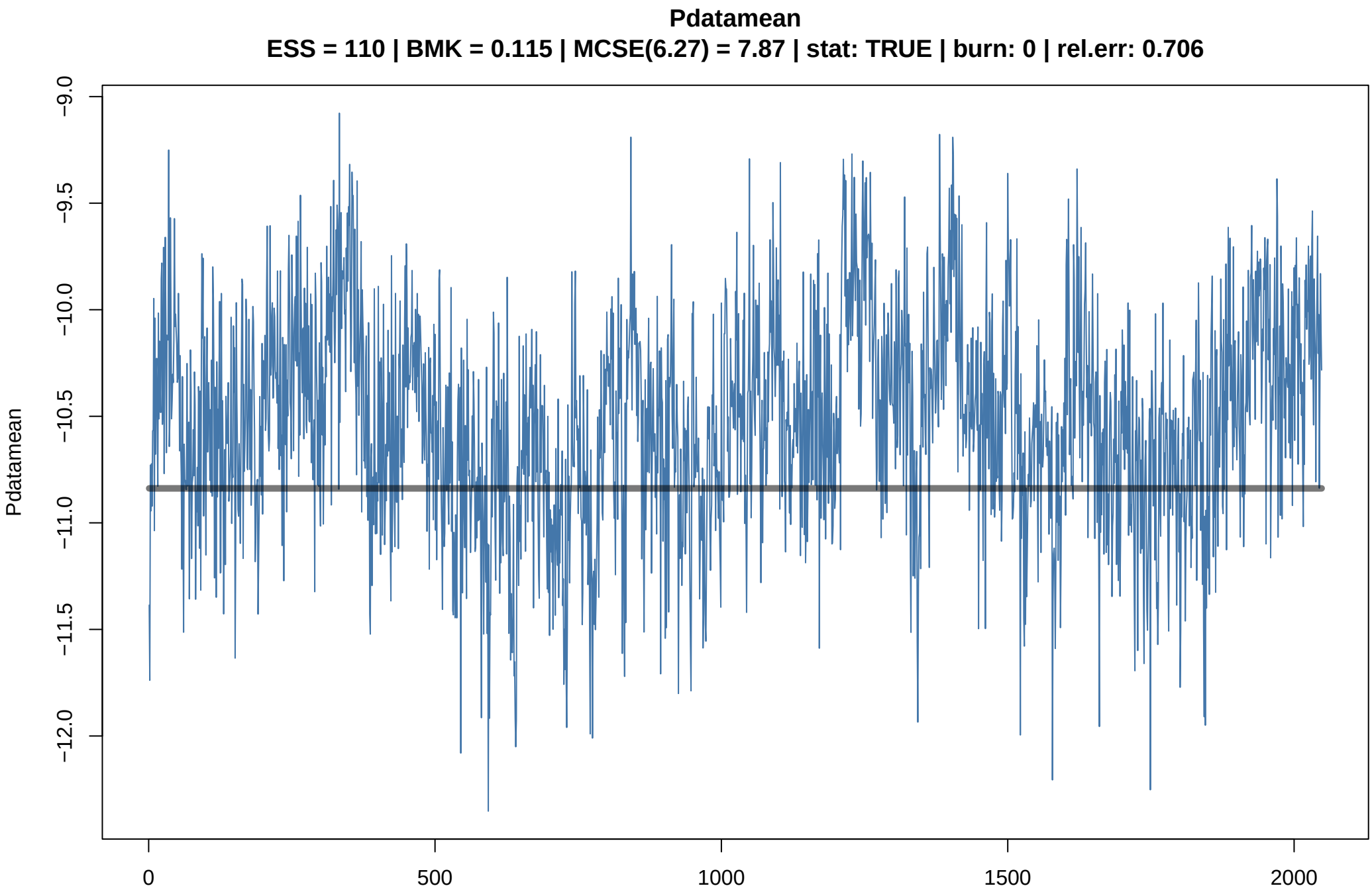
−− STATS 1D −−
min ESS = 1561.38157408103
max BMK = 0.064027834783043 1
max MCSE = 2.42438334245899
all stationary: TRUE
burn: 0
max rel.err.: 2.28525182684965

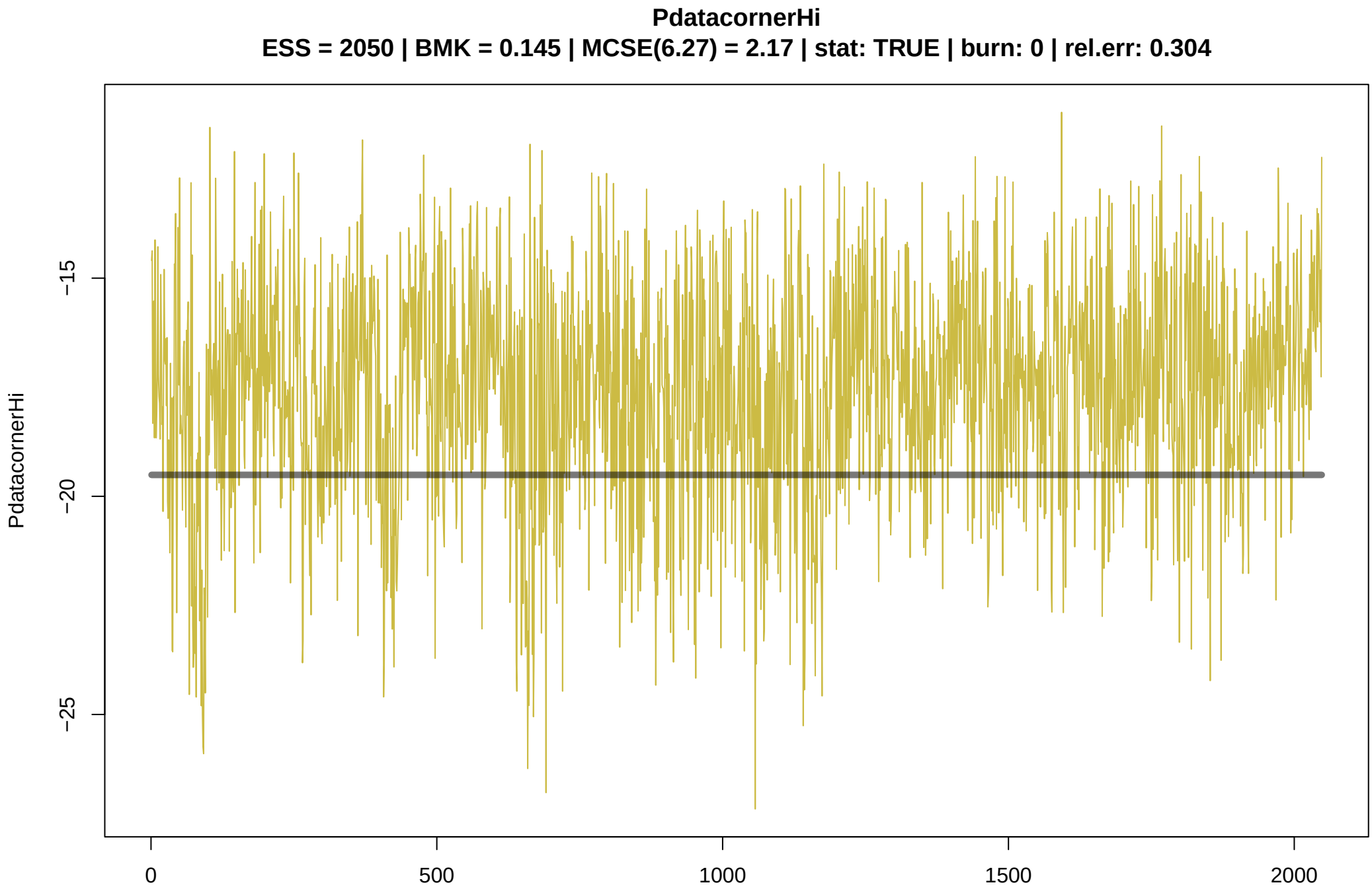
Occupied clusters: 10 of 16

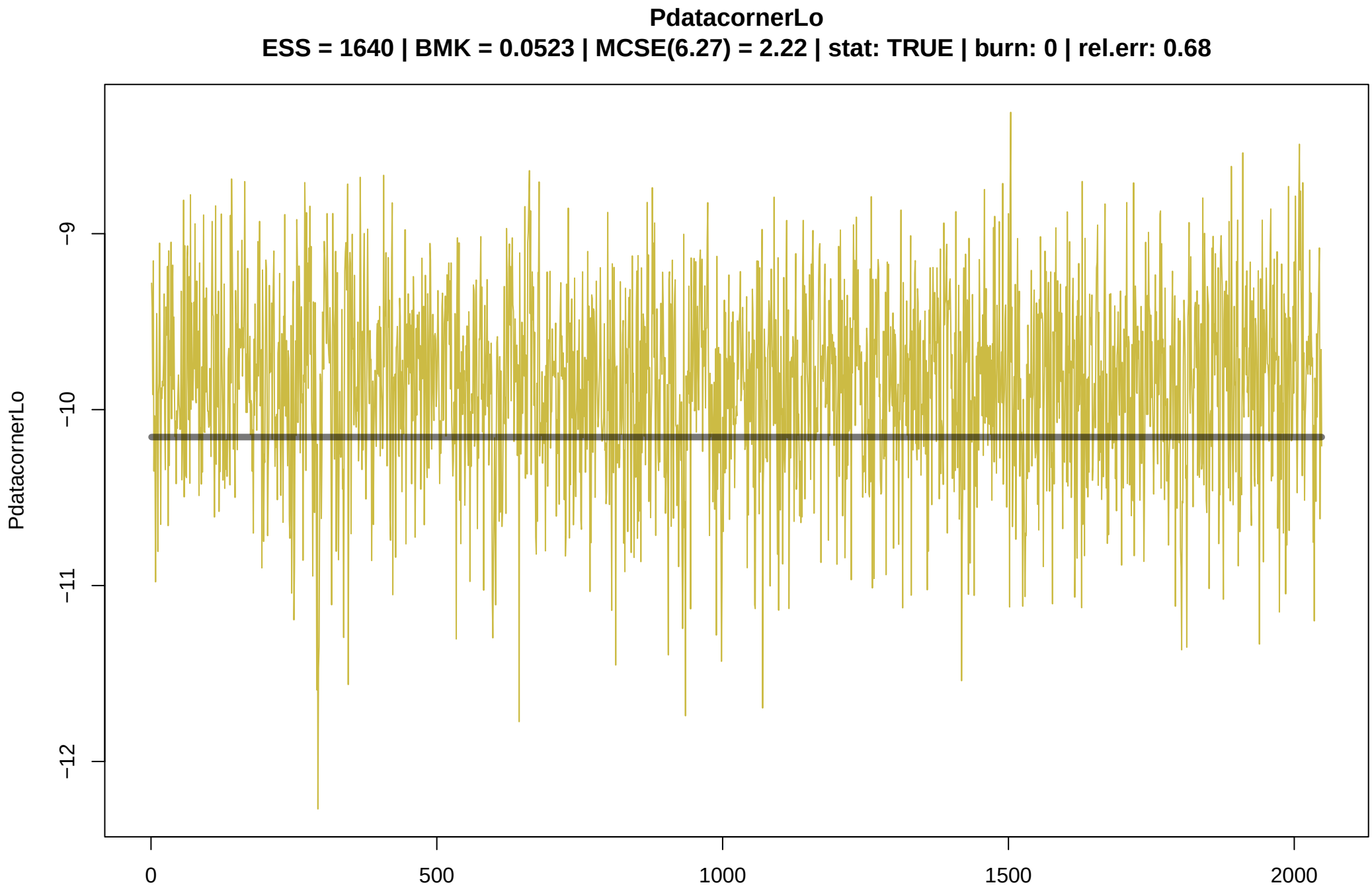

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
log_RMSD

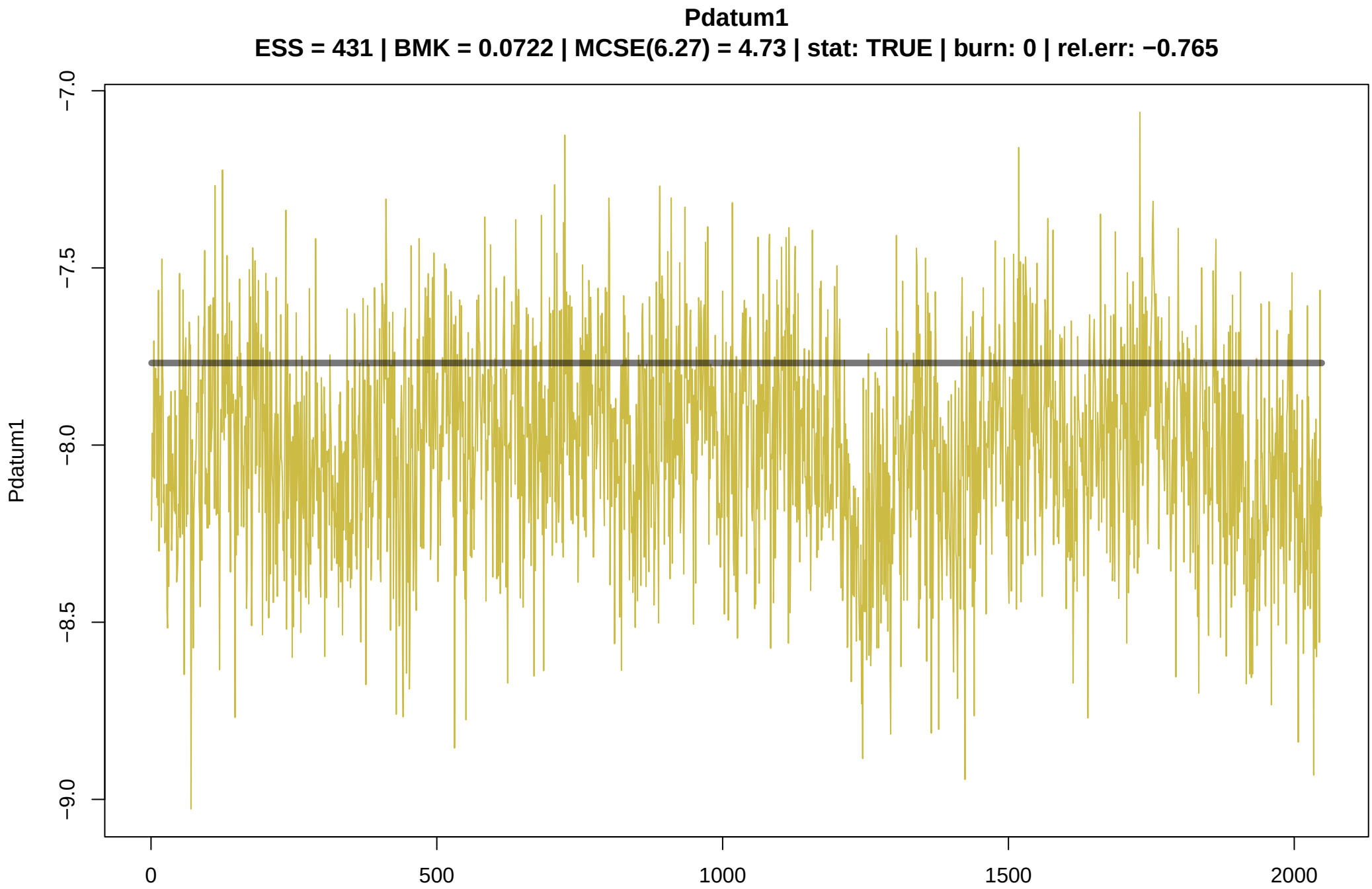

mcs_NumHeteroAtoms
35
30
25
20
15
10
5
0
−4
−2
0
2
4
log_RMSD

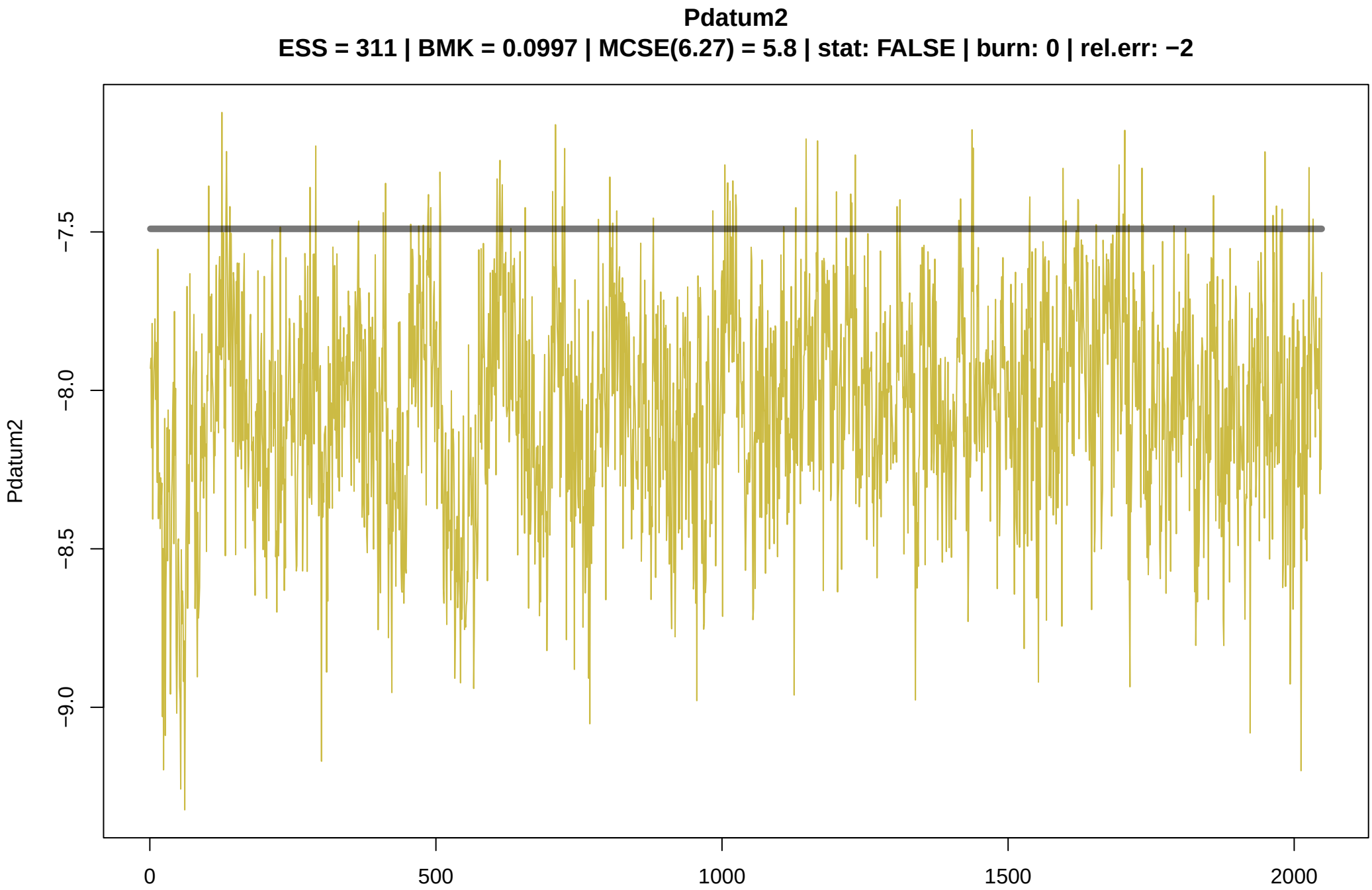

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
log_RMSD

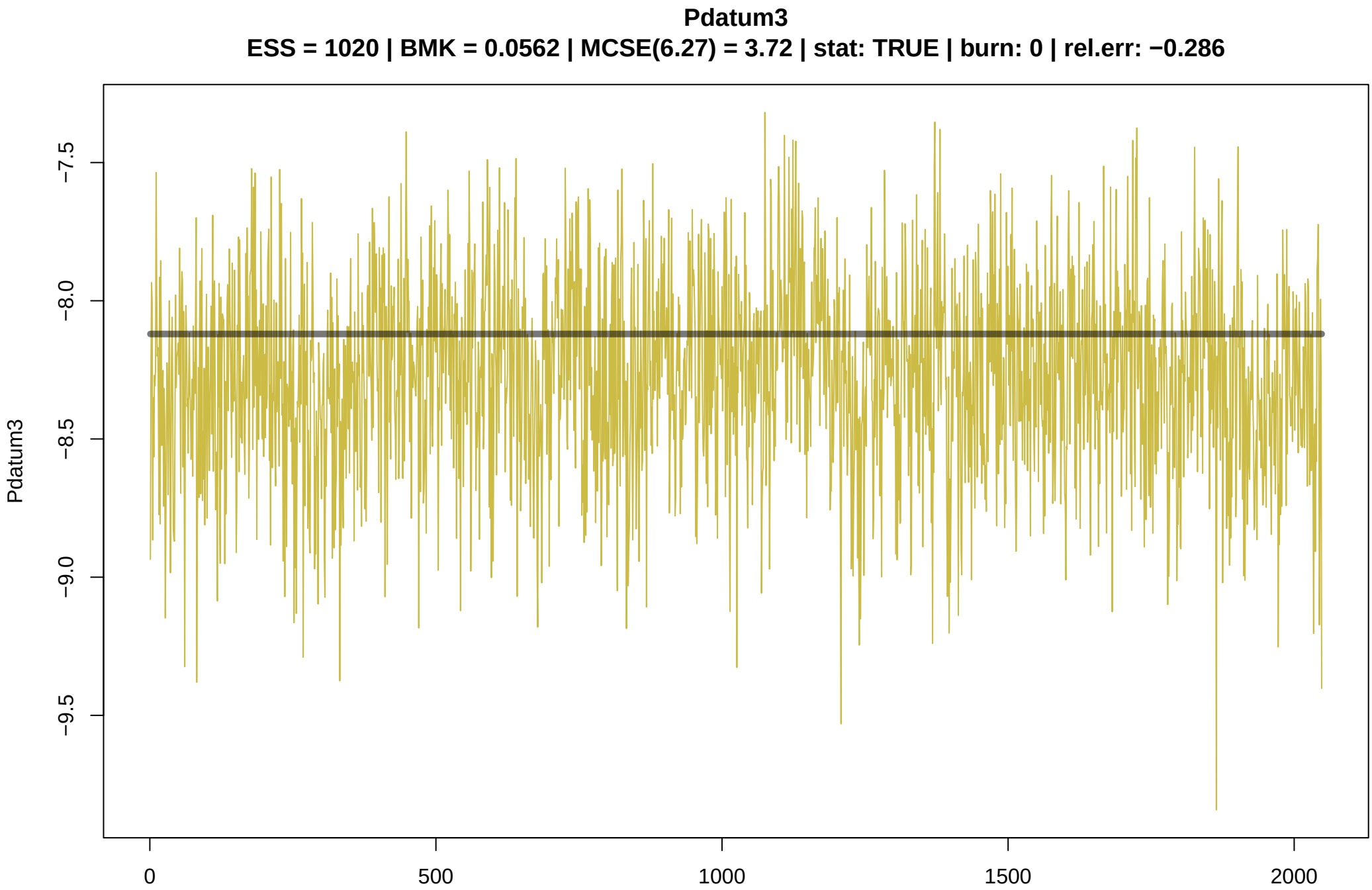

Pdatamean
ESS = 110 | BMK = 0.115 | MCSE(6.27) = 7.87 | stat: TRUE | burn: 0 | rel.err: 0.706
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

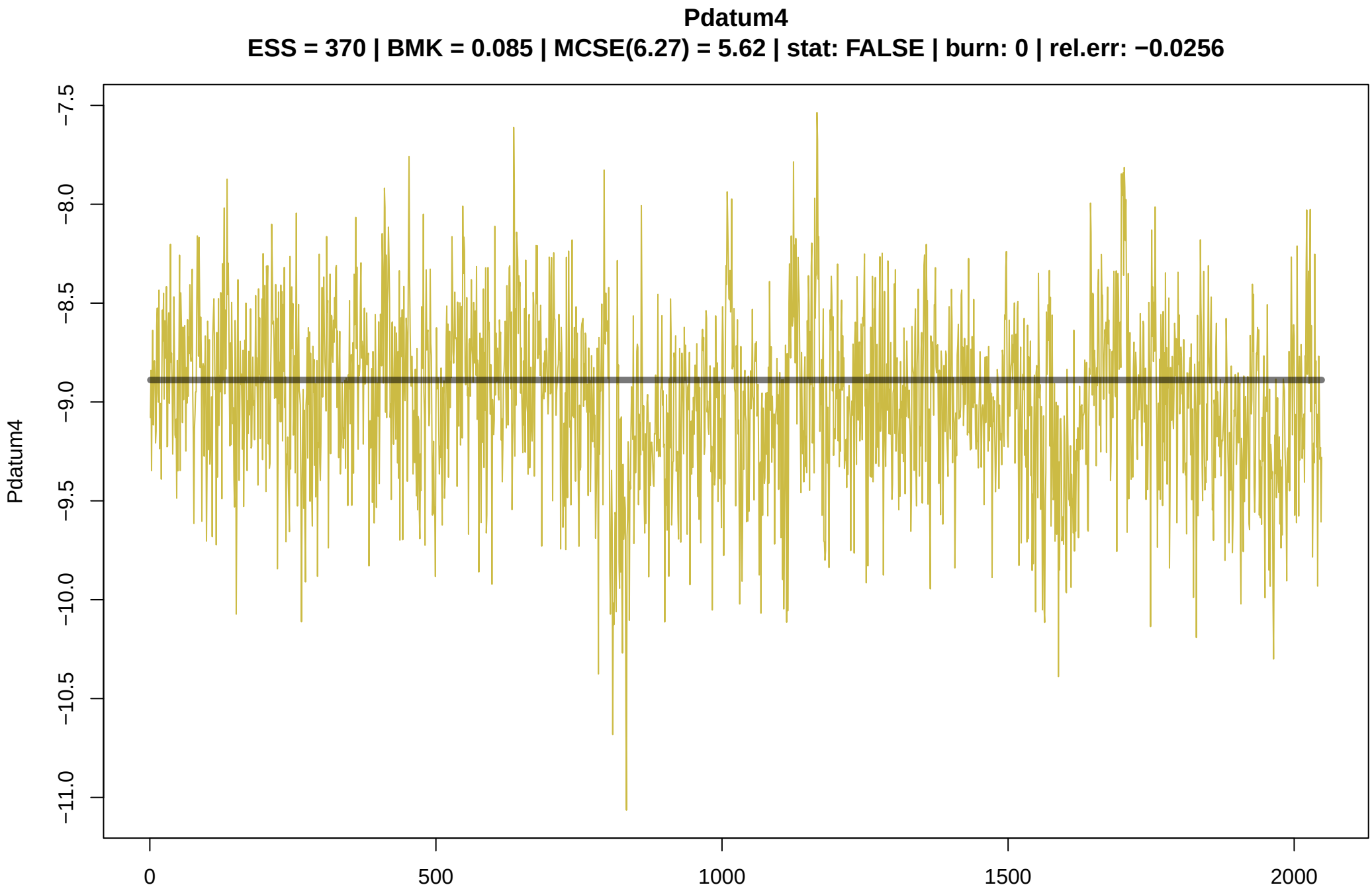

PdatacornerHi
ESS = 2050 | BMK = 0.145 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.304
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

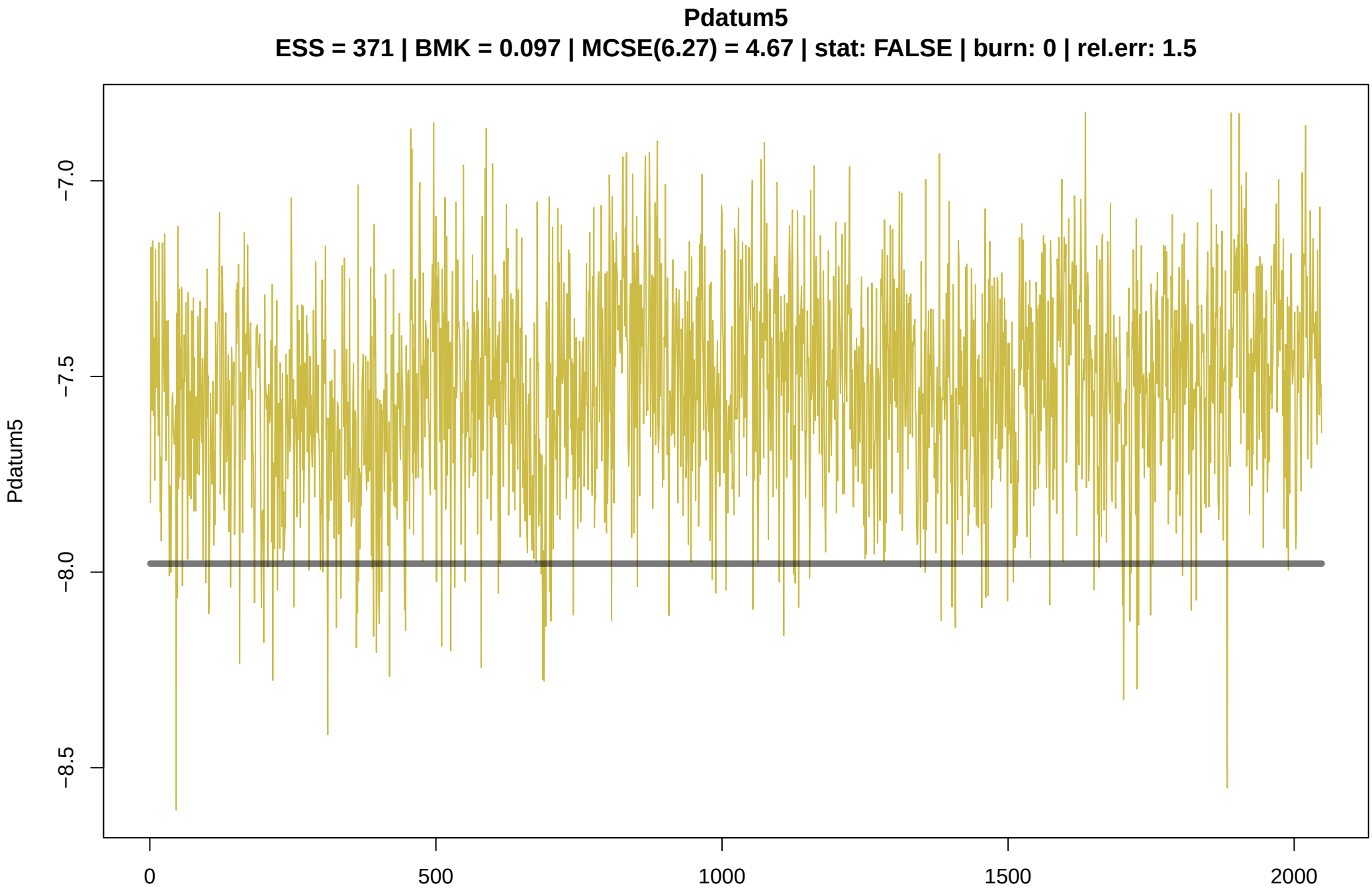

PdatacornerLo
ESS = 1640 | BMK = 0.0523 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0 | rel.err: 0.68
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

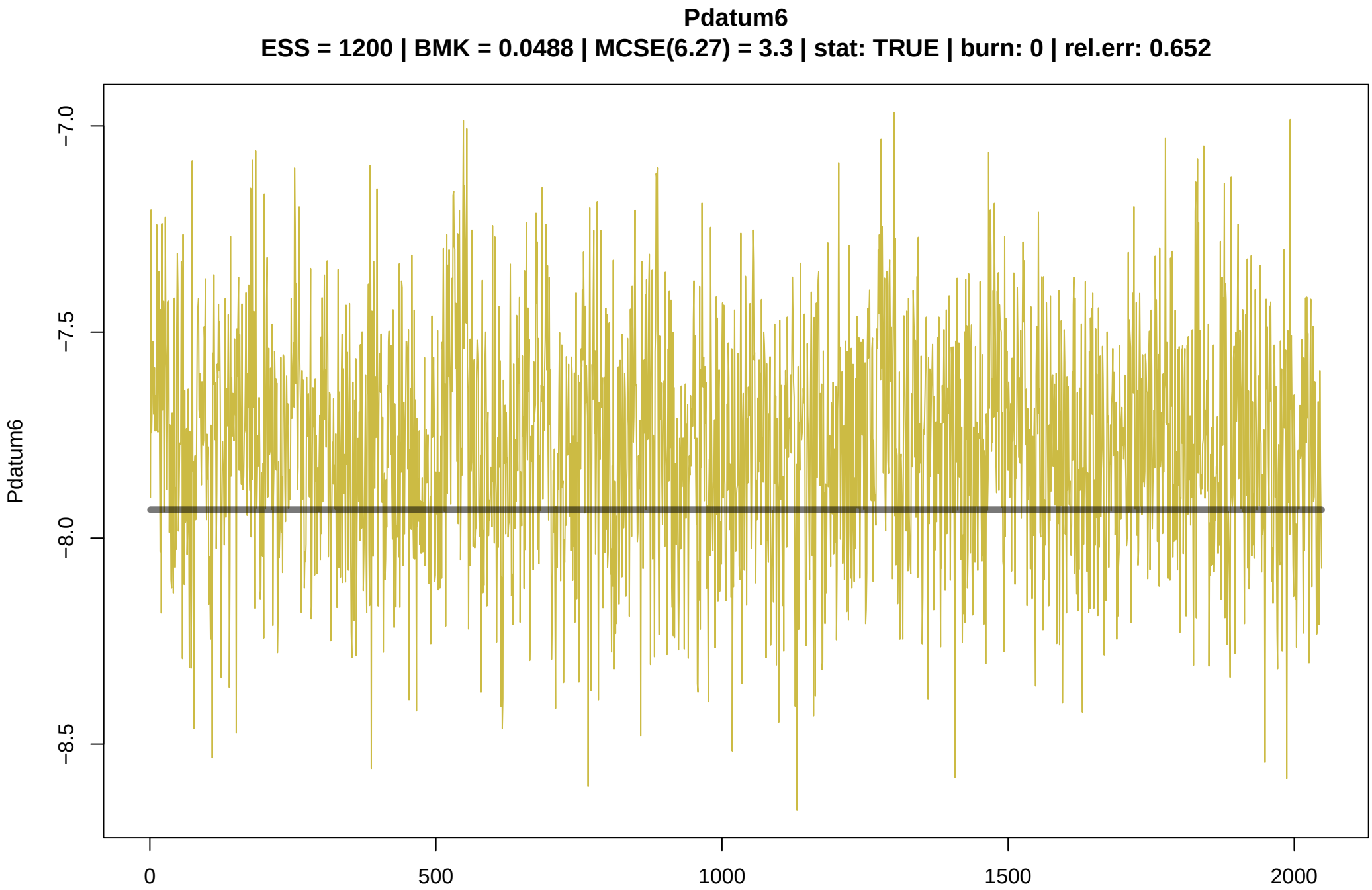

Pdatum1
ESS = 431 | BMK = 0.0722 | MCSE(6.27) = 4.73 | stat: TRUE | burn: 0 | rel.err: −0.765
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

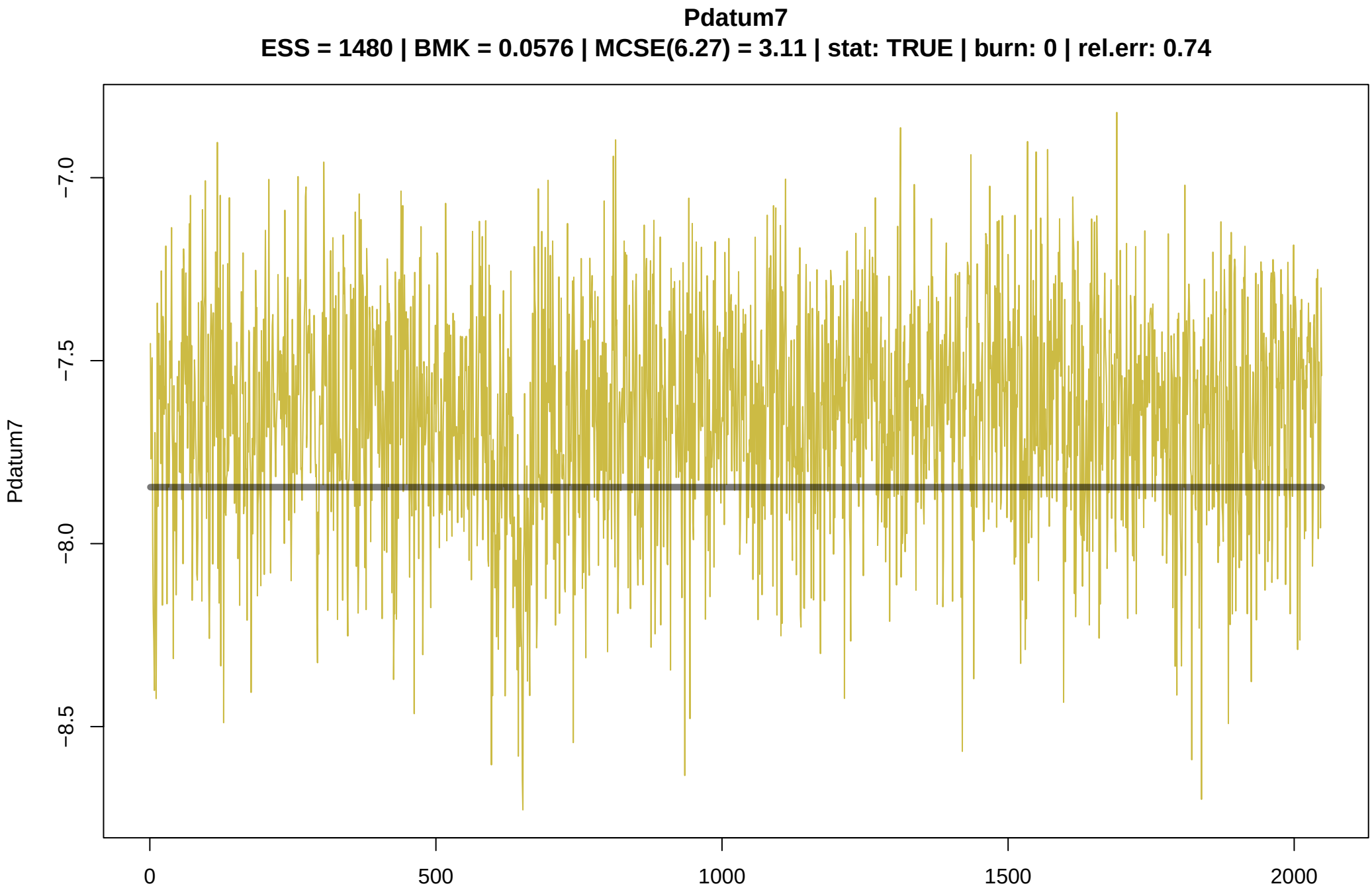

Pdatum2
ESS = 311 | BMK = 0.0997 | MCSE(6.27) = 5.8 | stat: FALSE | burn: 0 | rel.err: −2
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

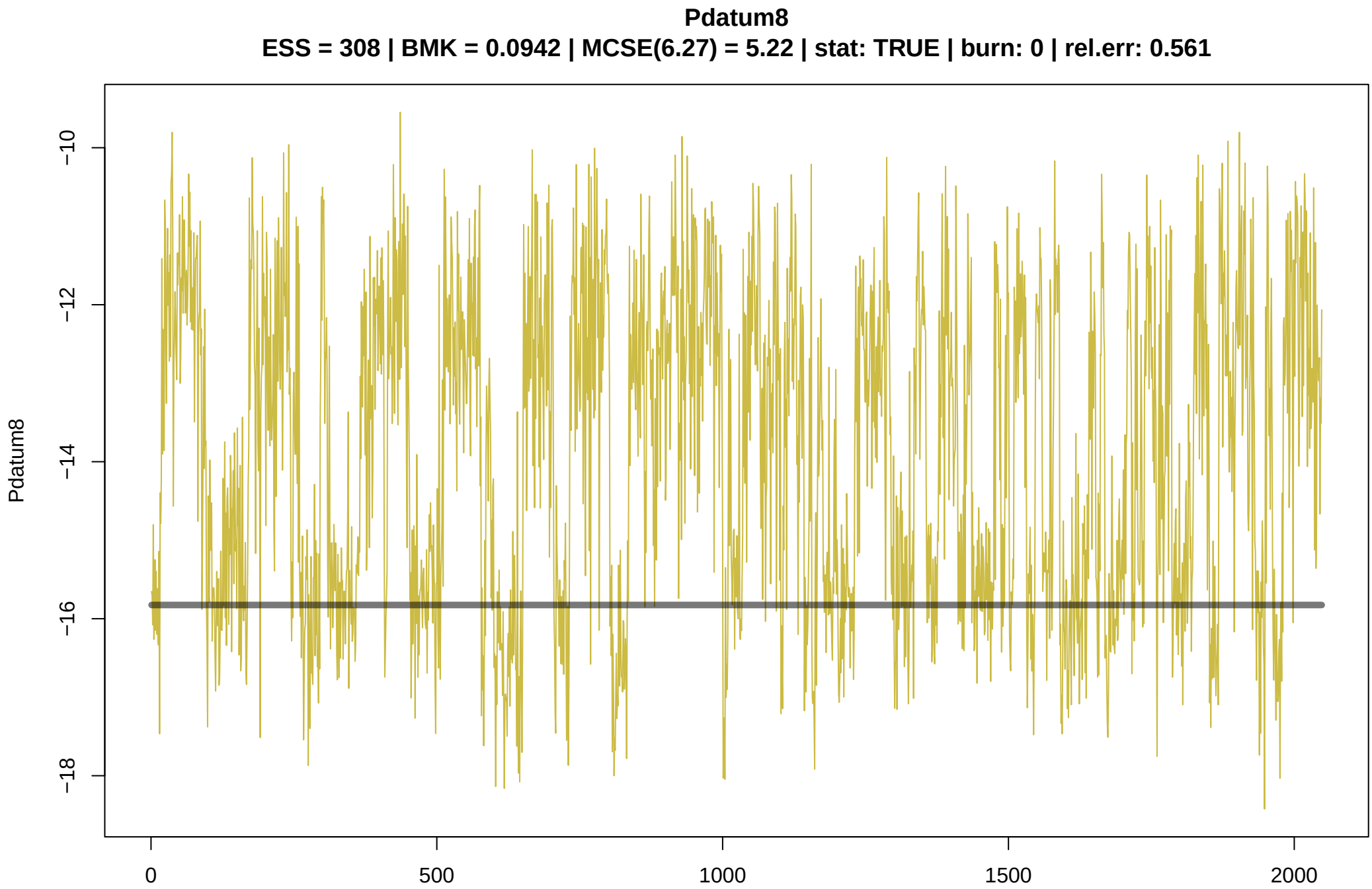

Pdatum3
ESS = 1020 | BMK = 0.0562 | MCSE(6.27) = 3.72 | stat: TRUE | burn: 0 | rel.err: −0.286
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

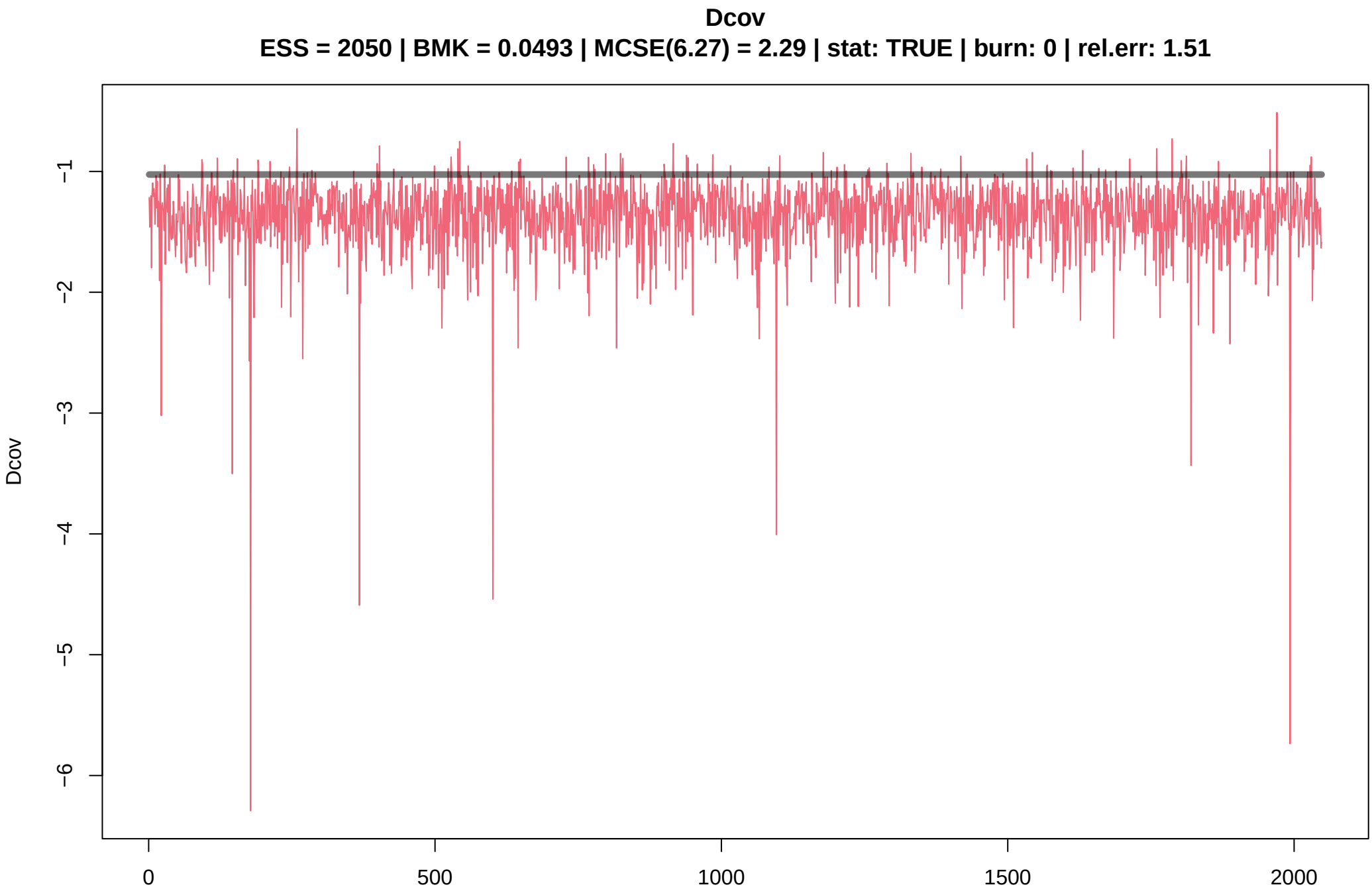

Pdatum4
ESS = 370 | BMK = 0.085 | MCSE(6.27) = 5.62 | stat: FALSE | burn: 0 | rel.err: −0.0256
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
0
500
1000
1500
2000

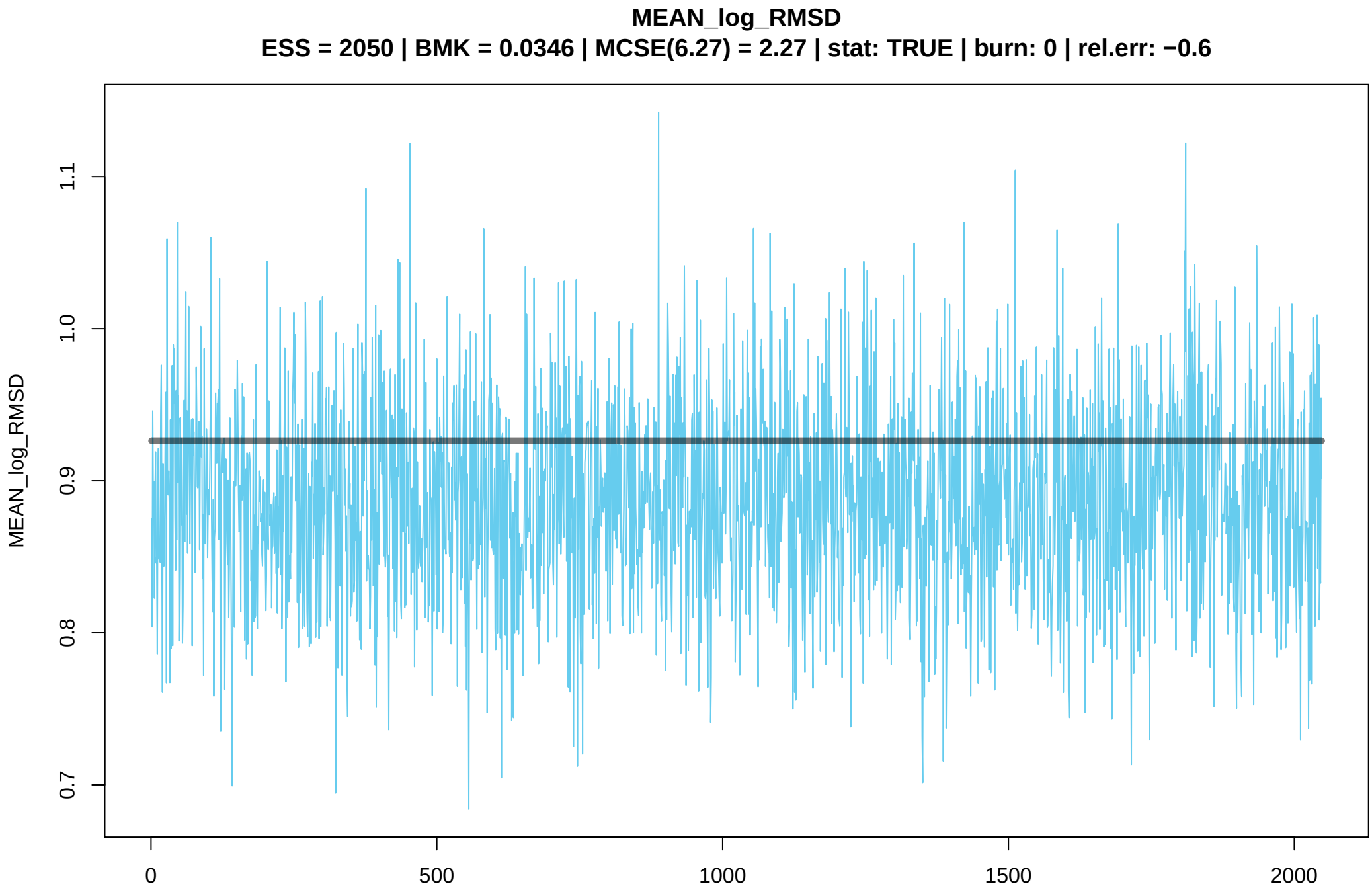

Pdatum5
ESS = 371 | BMK = 0.097 | MCSE(6.27) = 4.67 | stat: FALSE | burn: 0 | rel.err: 1.5
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

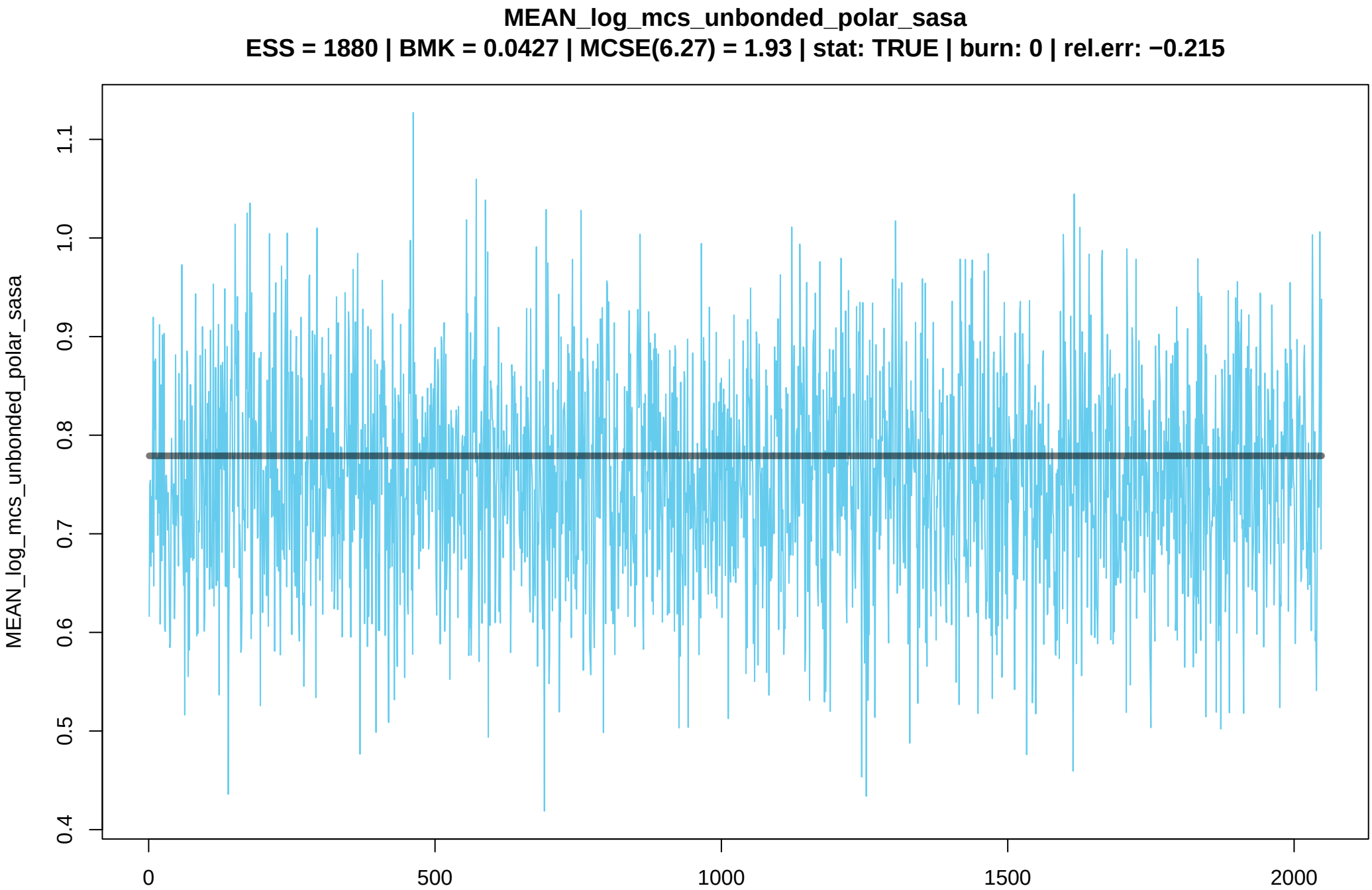

Pdatum6
ESS = 1200 | BMK = 0.0488 | MCSE(6.27) = 3.3 | stat: TRUE | burn: 0 | rel.err: 0.652
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

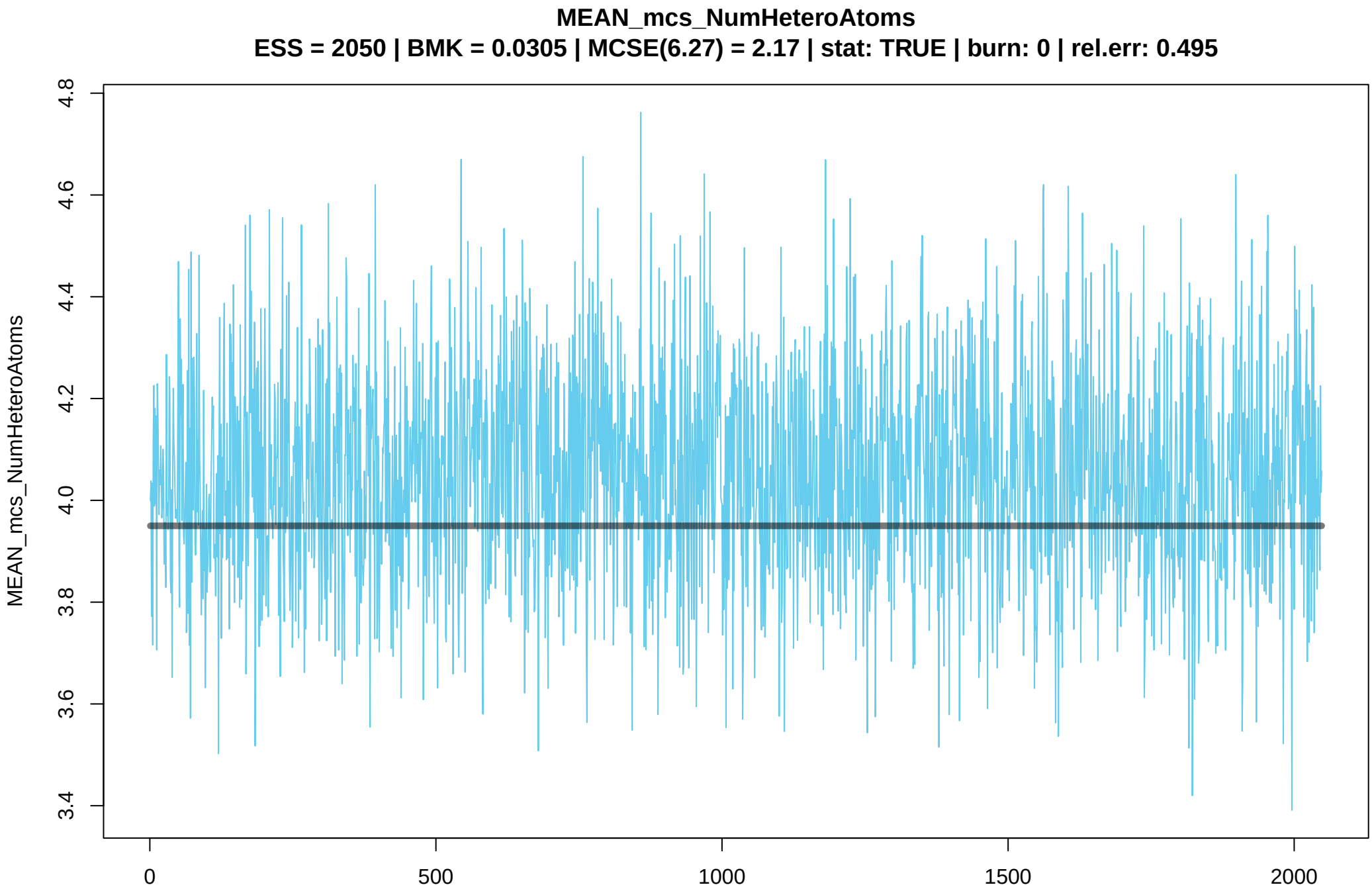

Pdatum7
ESS = 1480 | BMK = 0.0576 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: 0.74
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

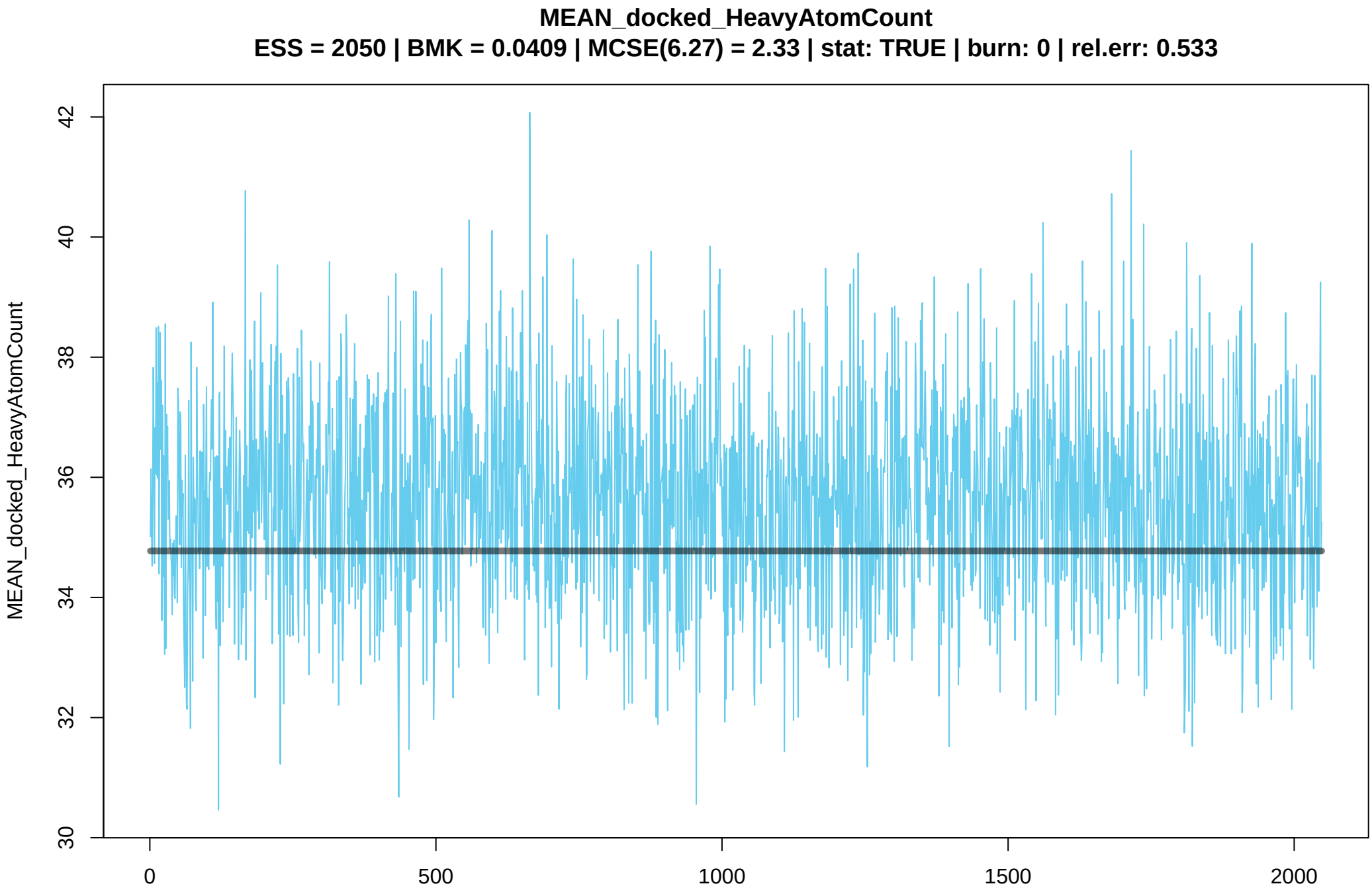

Pdatum8
ESS = 308 | BMK = 0.0942 | MCSE(6.27) = 5.22 | stat: TRUE | burn: 0 | rel.err: 0.561
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

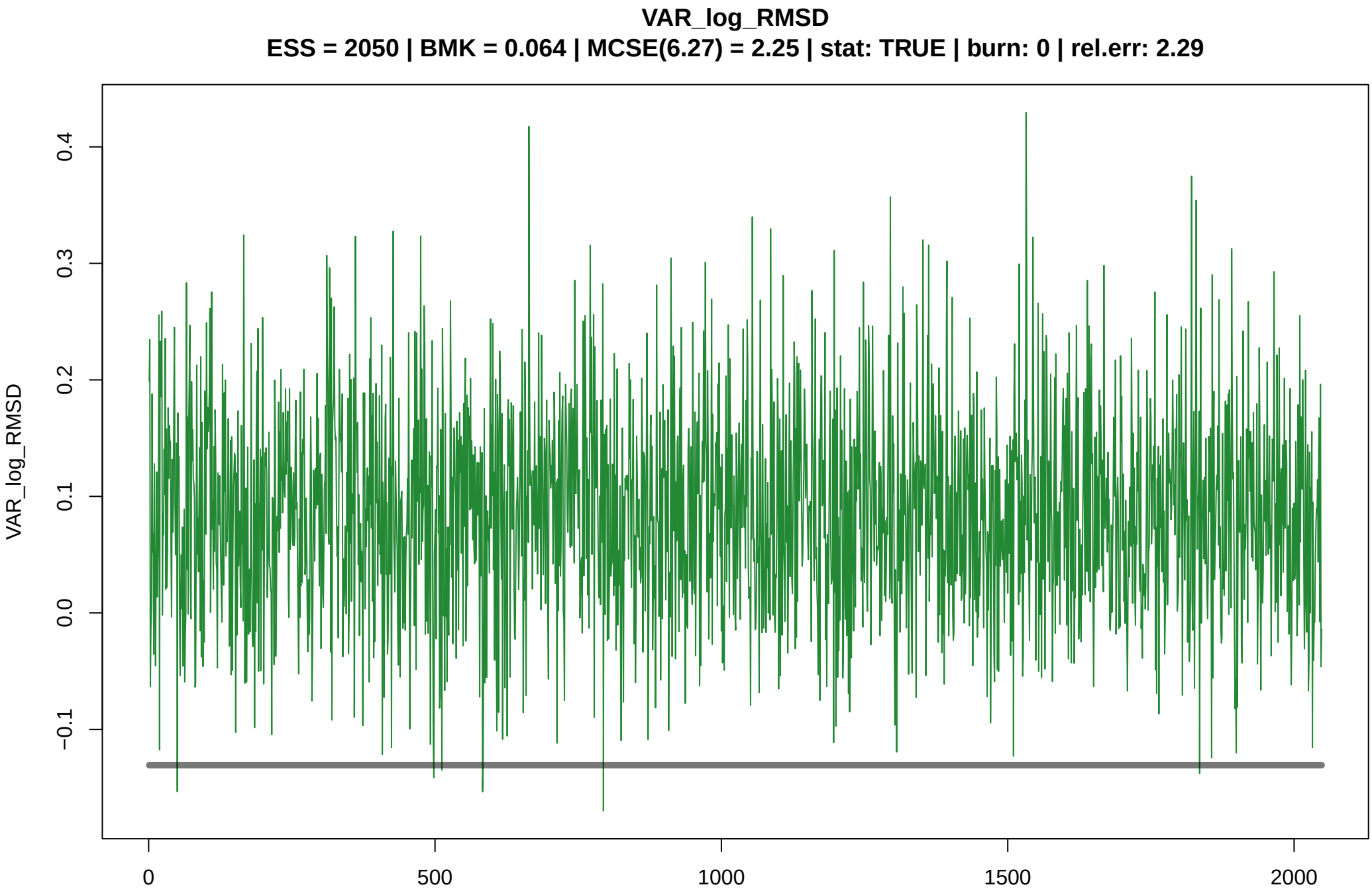

Dcov
ESS = 2050 | BMK = 0.0493 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0 | rel.err: 1.51
Dcov
−1
−2
−3
−4
−5
−6
0
500
1000
1500
2000

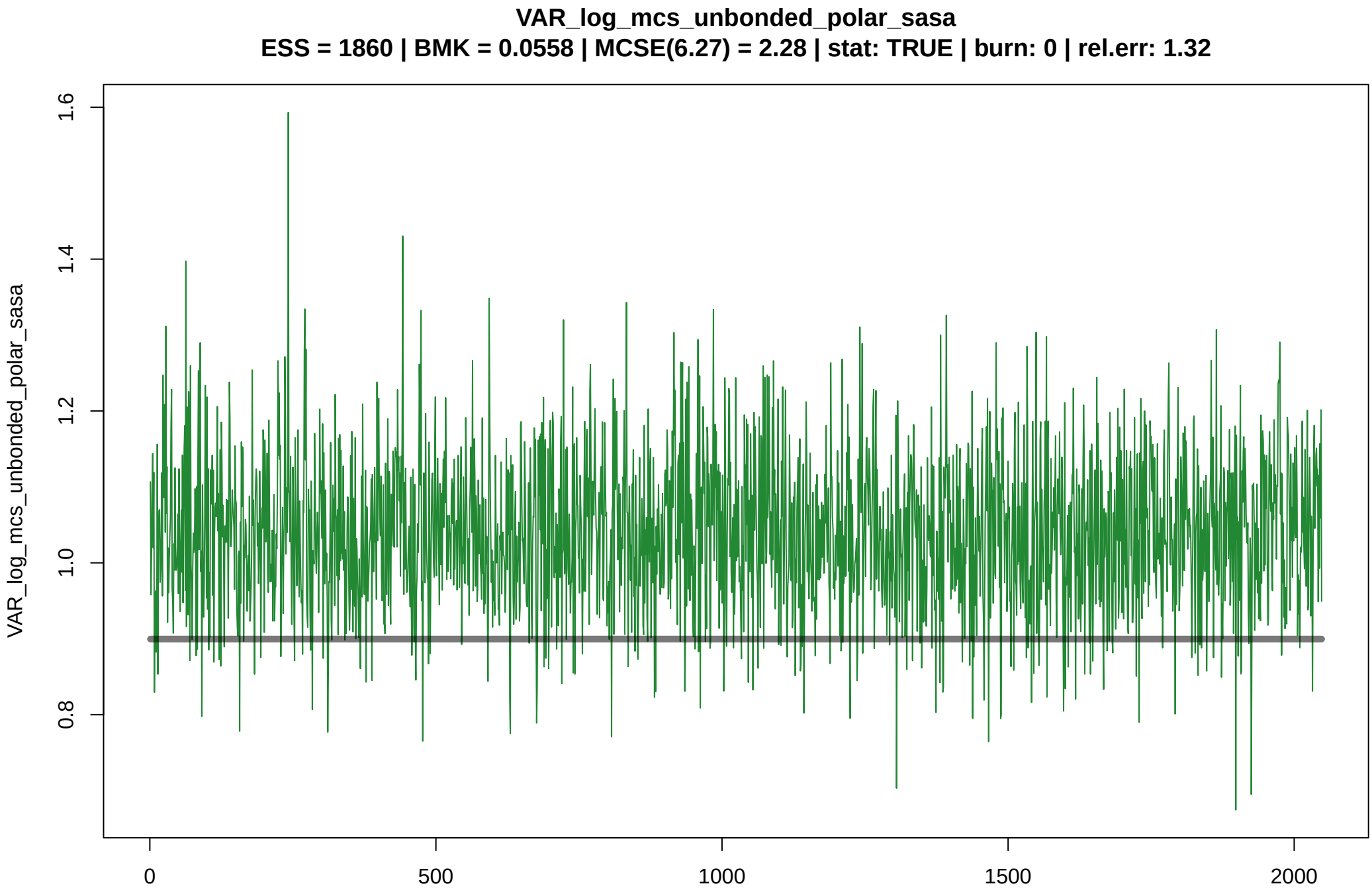

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0346 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0 | rel.err: −0.6
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

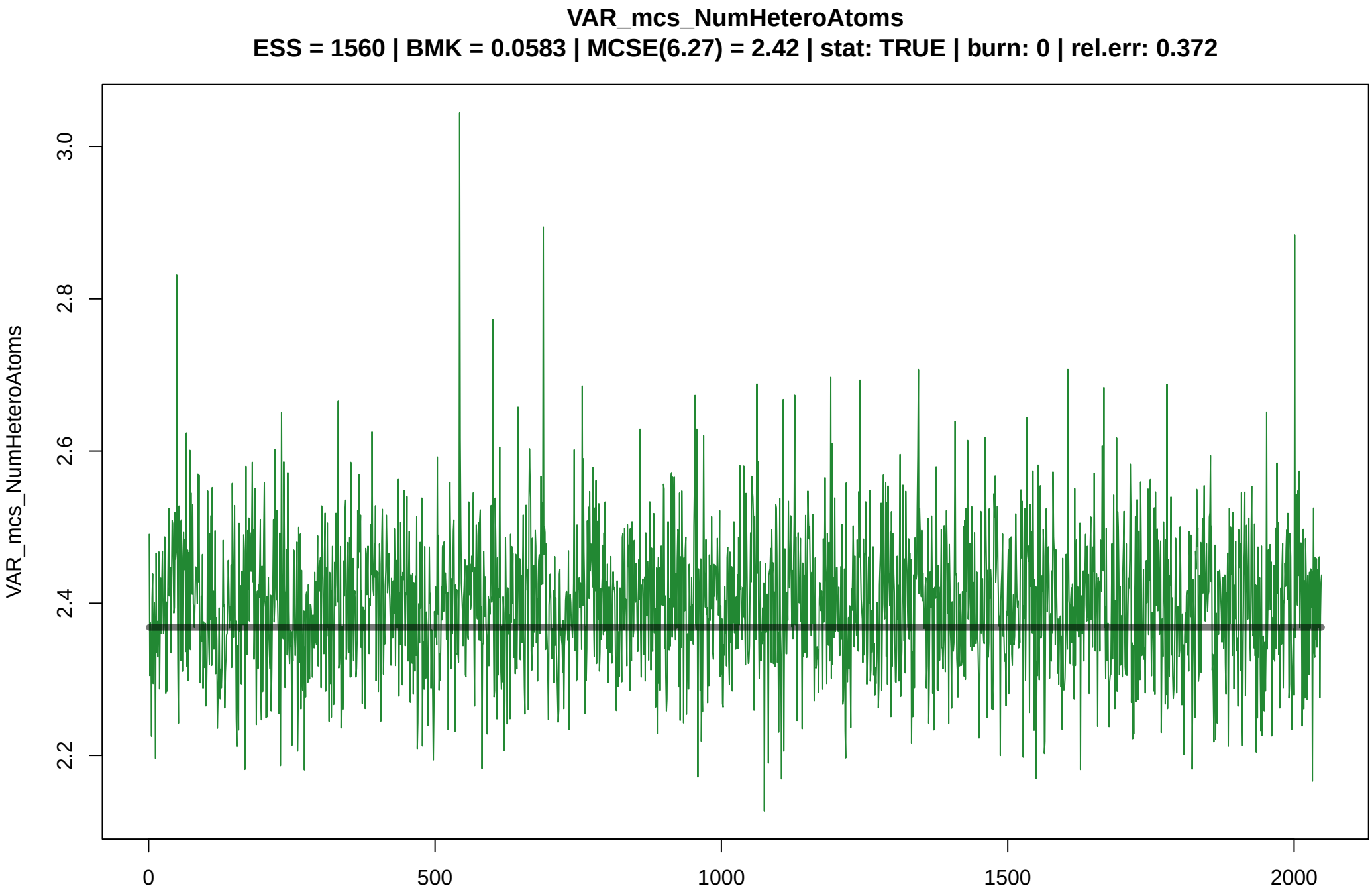

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1880 | BMK = 0.0427 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: −0.215
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

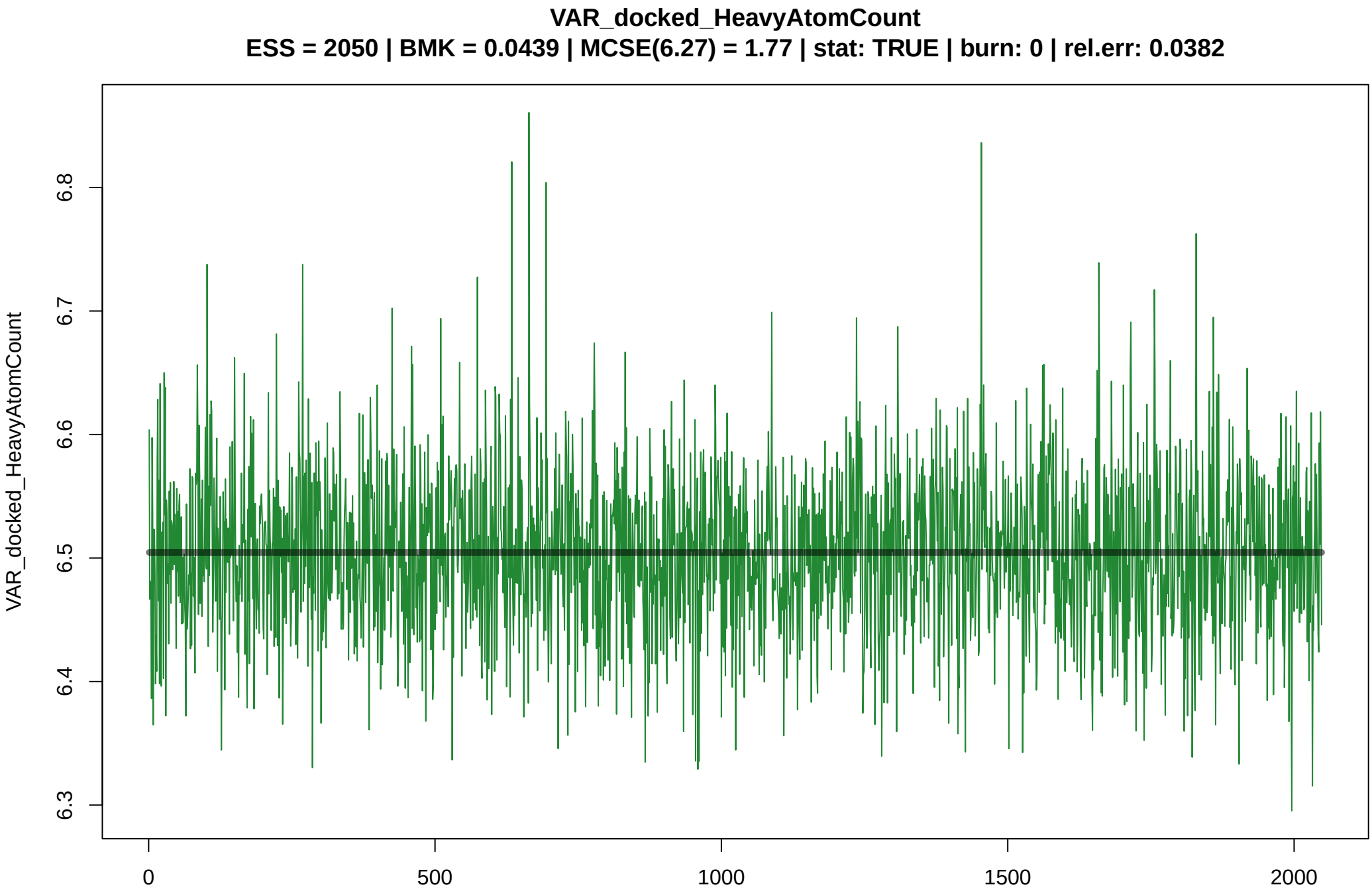

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0305 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.495
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

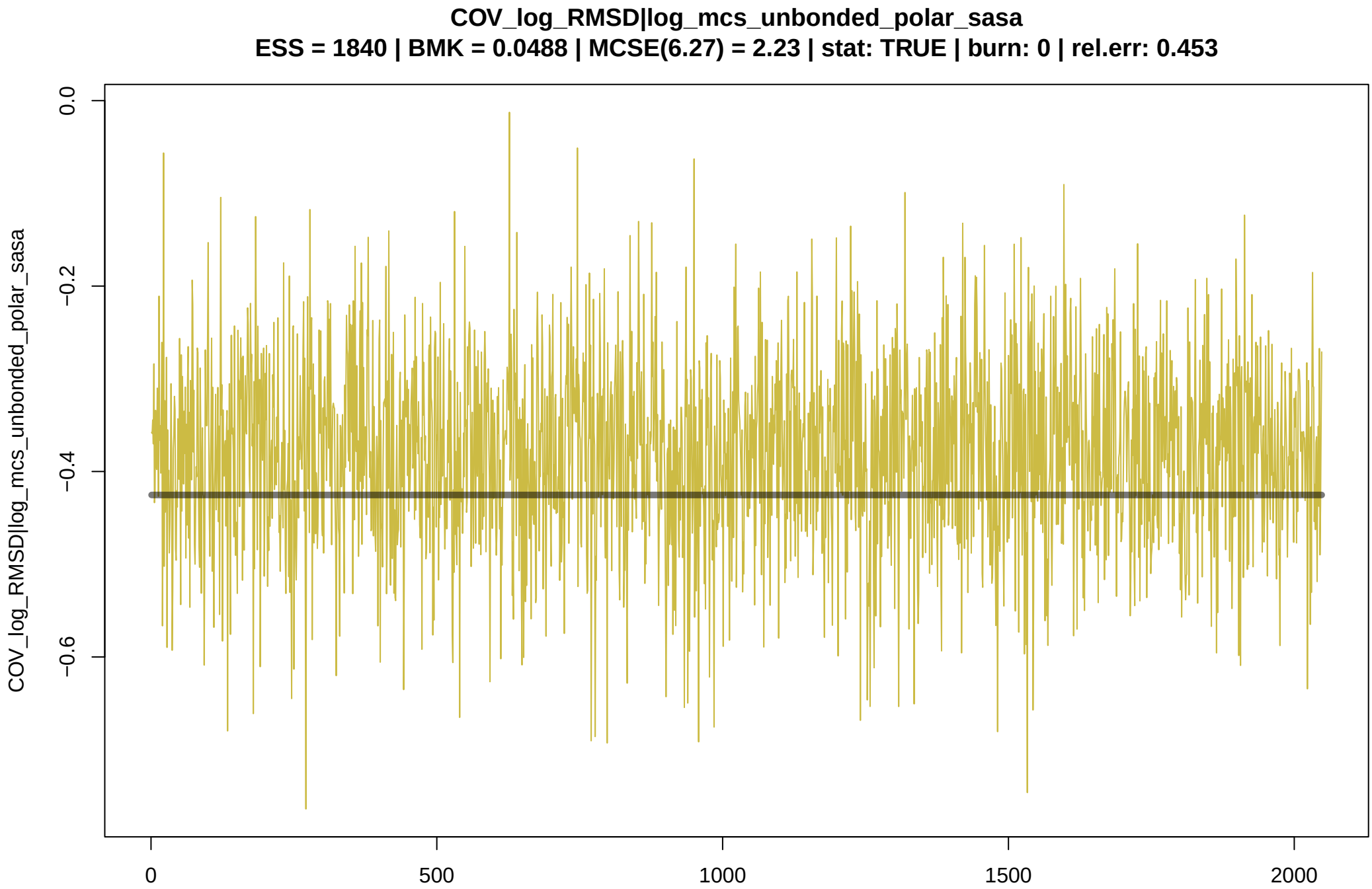

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0409 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 0.533
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
500
1000
1500
2000

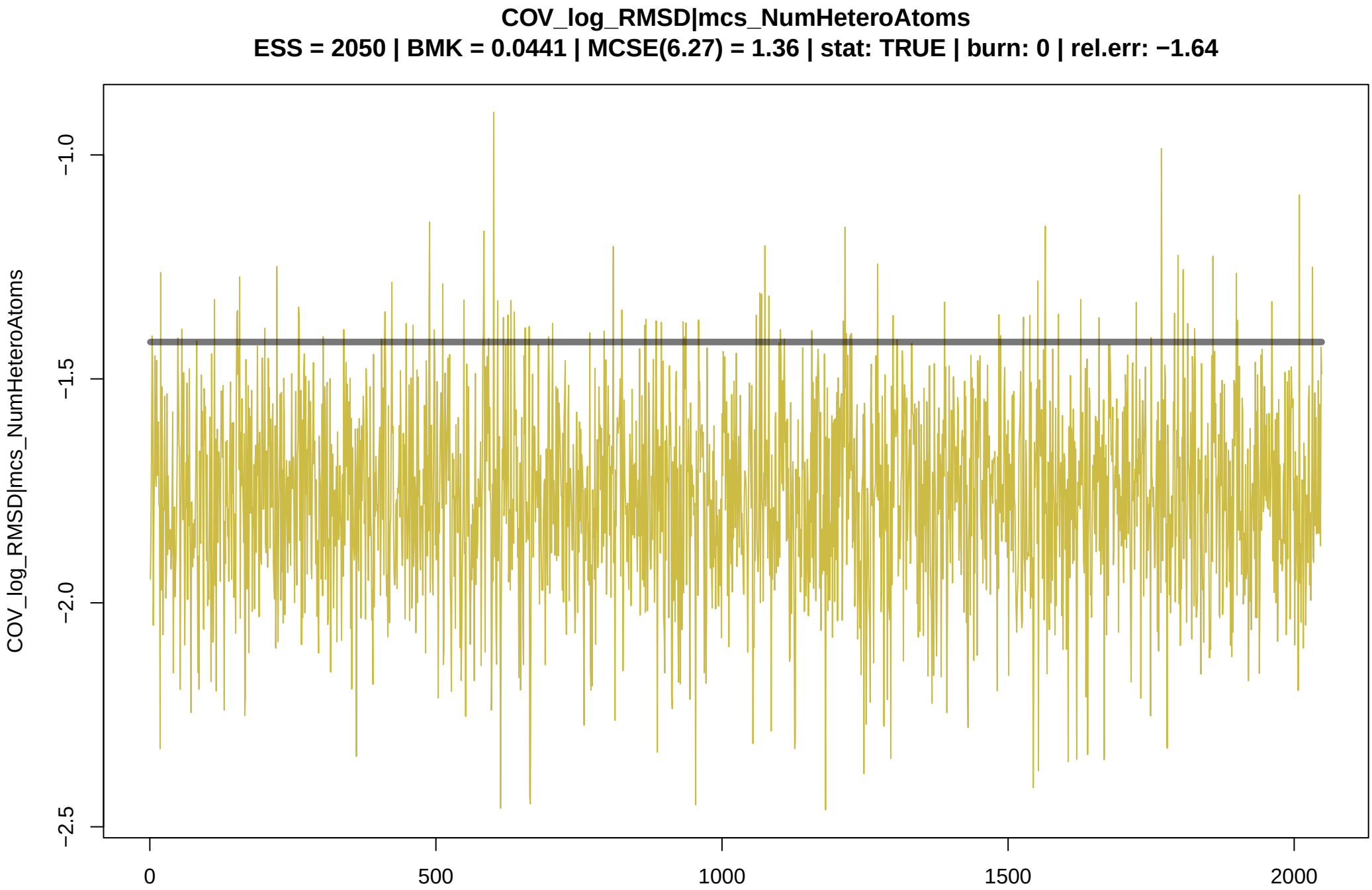

VAR_log_RMSD
ESS = 2050 | BMK = 0.064 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: 2.29
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000

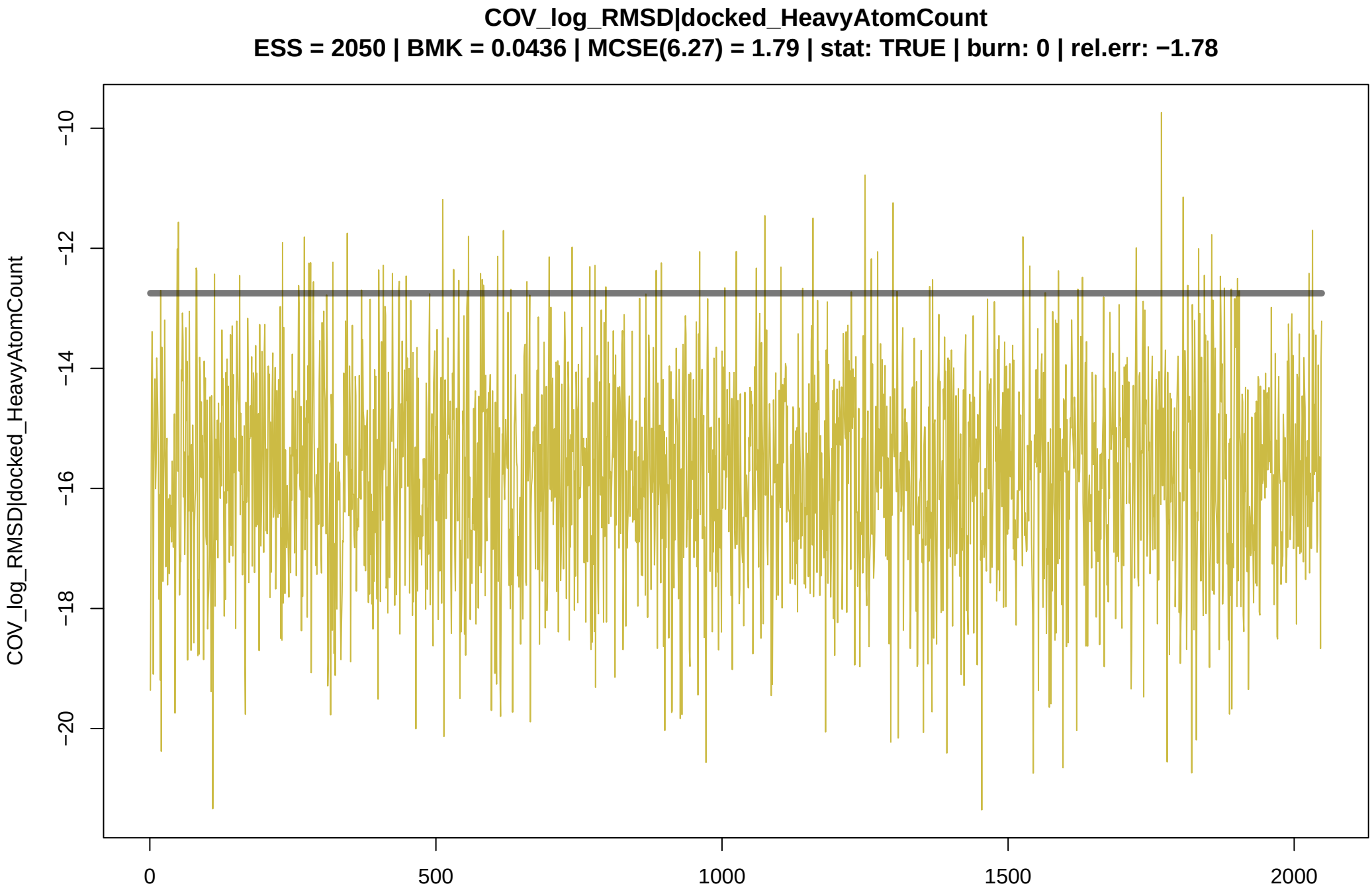

VAR_log_mcs_unbonded_polar_sasa
ESS = 1860 | BMK = 0.0558 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0 | rel.err: 1.32
VAR_log_mcs_unbonded_polar_sasa
0.8
1.0
1.2
1.4
1.6
0
500
1000
1500
2000

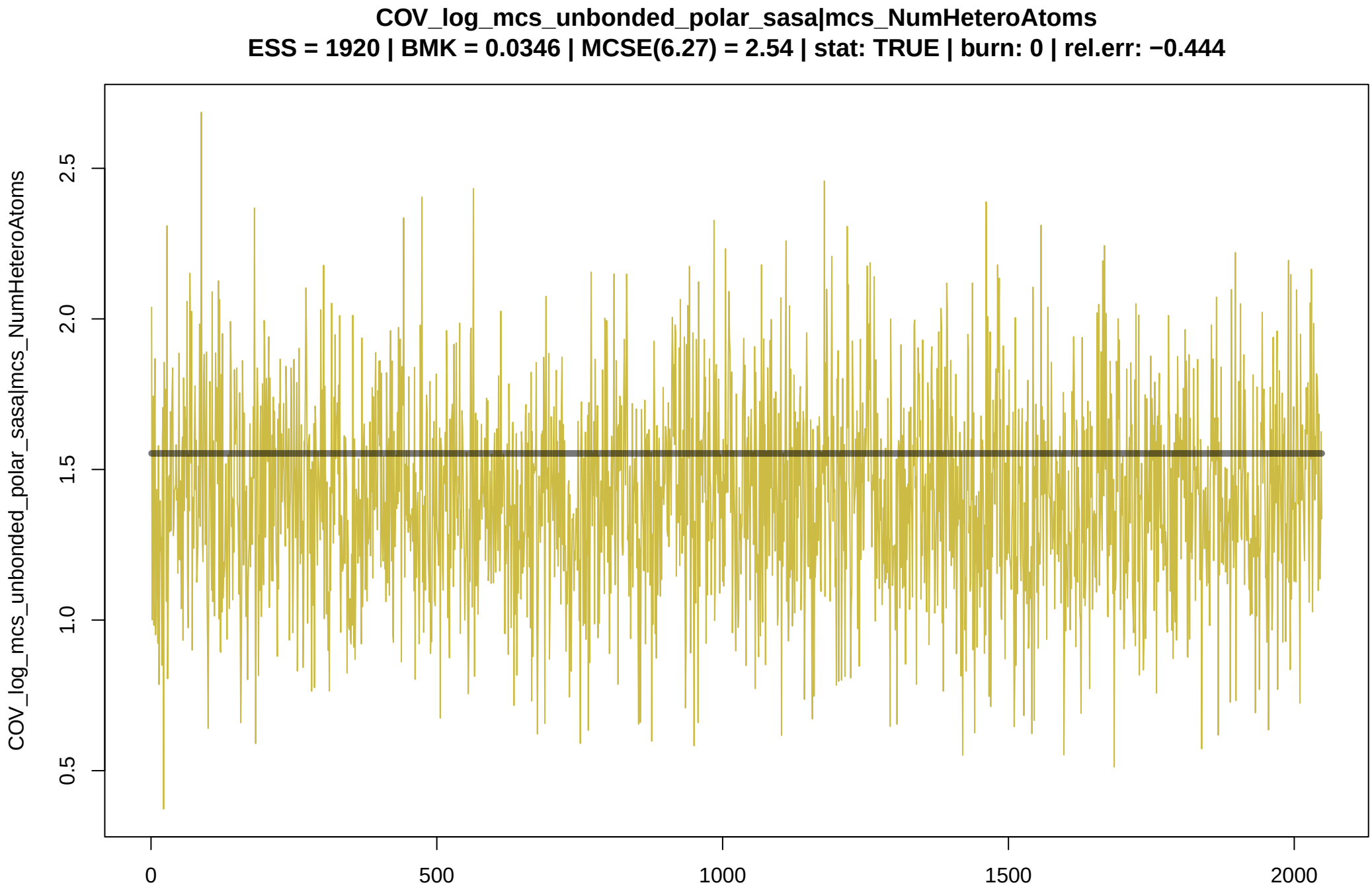

VAR_mcs_NumHeteroAtoms
ESS = 1560 | BMK = 0.0583 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: 0.372
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

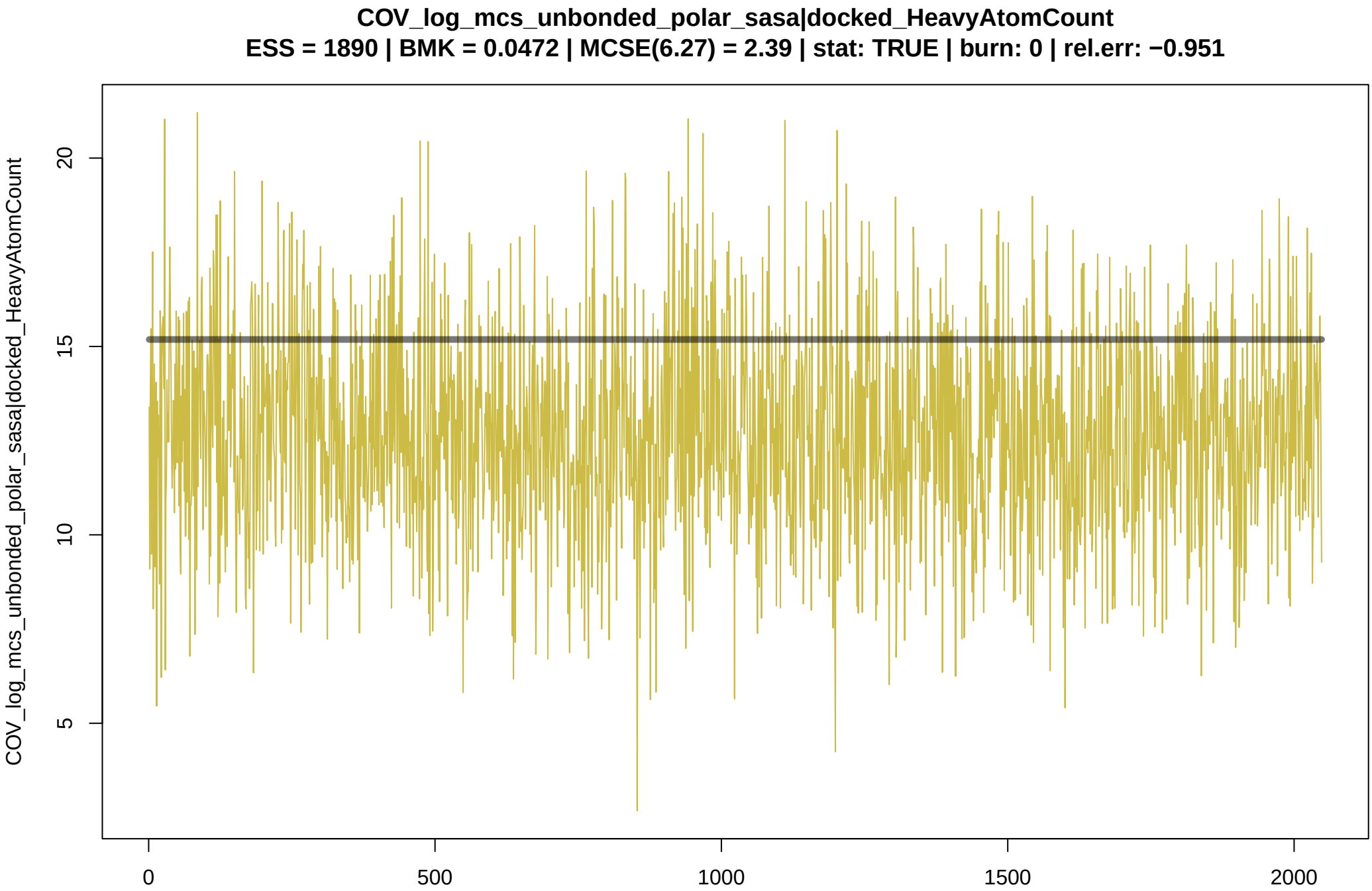

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0439 | MCSE(6.27) = 1.77 | stat: TRUE | burn: 0 | rel.err: 0.0382
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
0
500
1000
1500
2000

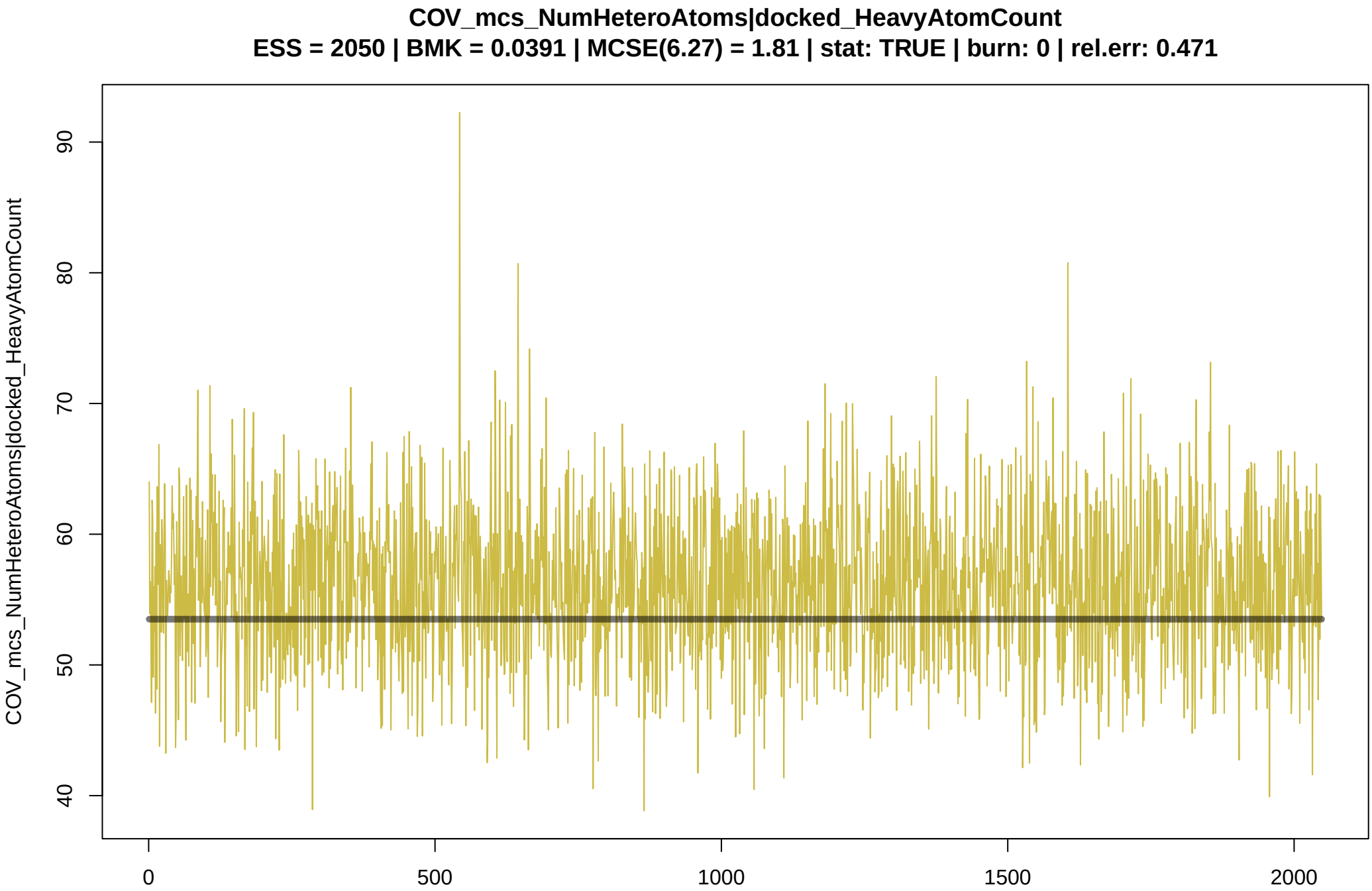

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1840 | BMK = 0.0488 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 0.453
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0441 | MCSE(6.27) = 1.36 | stat: TRUE | burn: 0 | rel.err: −1.64
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 = 0.0436 | MCSE(6.27) = 1.79 | stat: TRUE | burn: 0 | rel.err: −1.78
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 = 1920 | BMK = 0.0346 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0 | rel.err: −0.444
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 = 1890 | BMK = 0.0472 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 0 | rel.err: −0.951
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 = 0.0391 | MCSE(6.27) = 1.81 | stat: TRUE | burn: 0 | rel.err: 0.471
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
90
0
500
1000
1500
2000