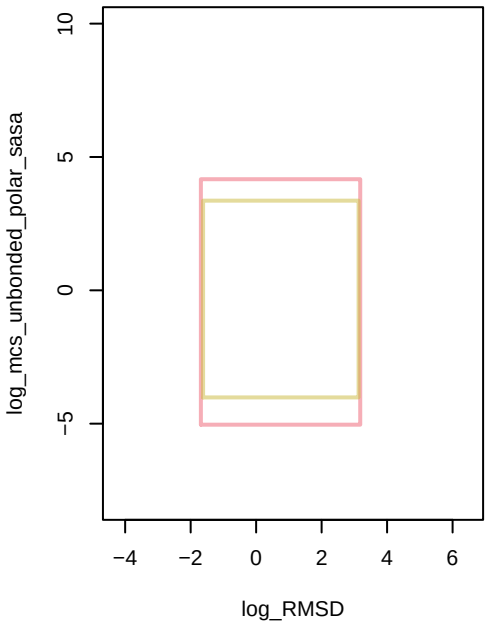
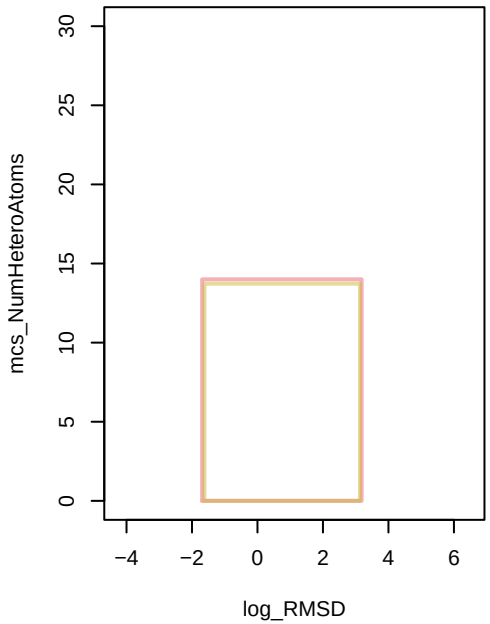
−− STATS maxD −−
min ESS = 7.9675063164854 7
max BMK = 0.407495007355625
max MCSE = 12.6017548492825
all stationary: FALSE
burn: 408
max rel.err.: 1.98580026807653

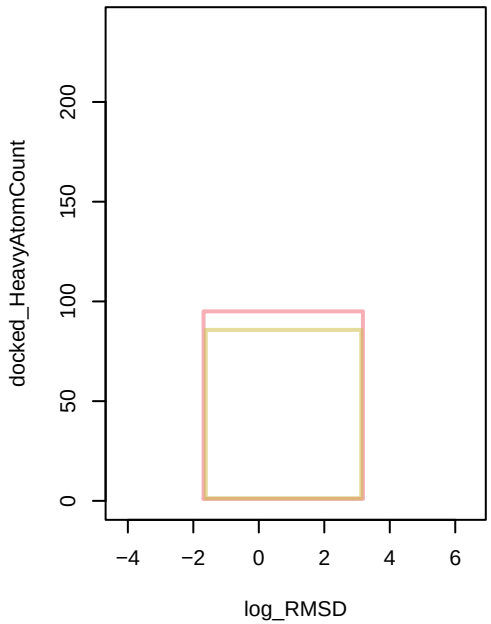
−− STATS 2D −−
min ESS = 1828.48602131803
max BMK = 0.061618522941411 5
max MCSE = 2.52473426695763
all stationary: TRUE
burn: 0
max rel.err.: 1.75853513037238

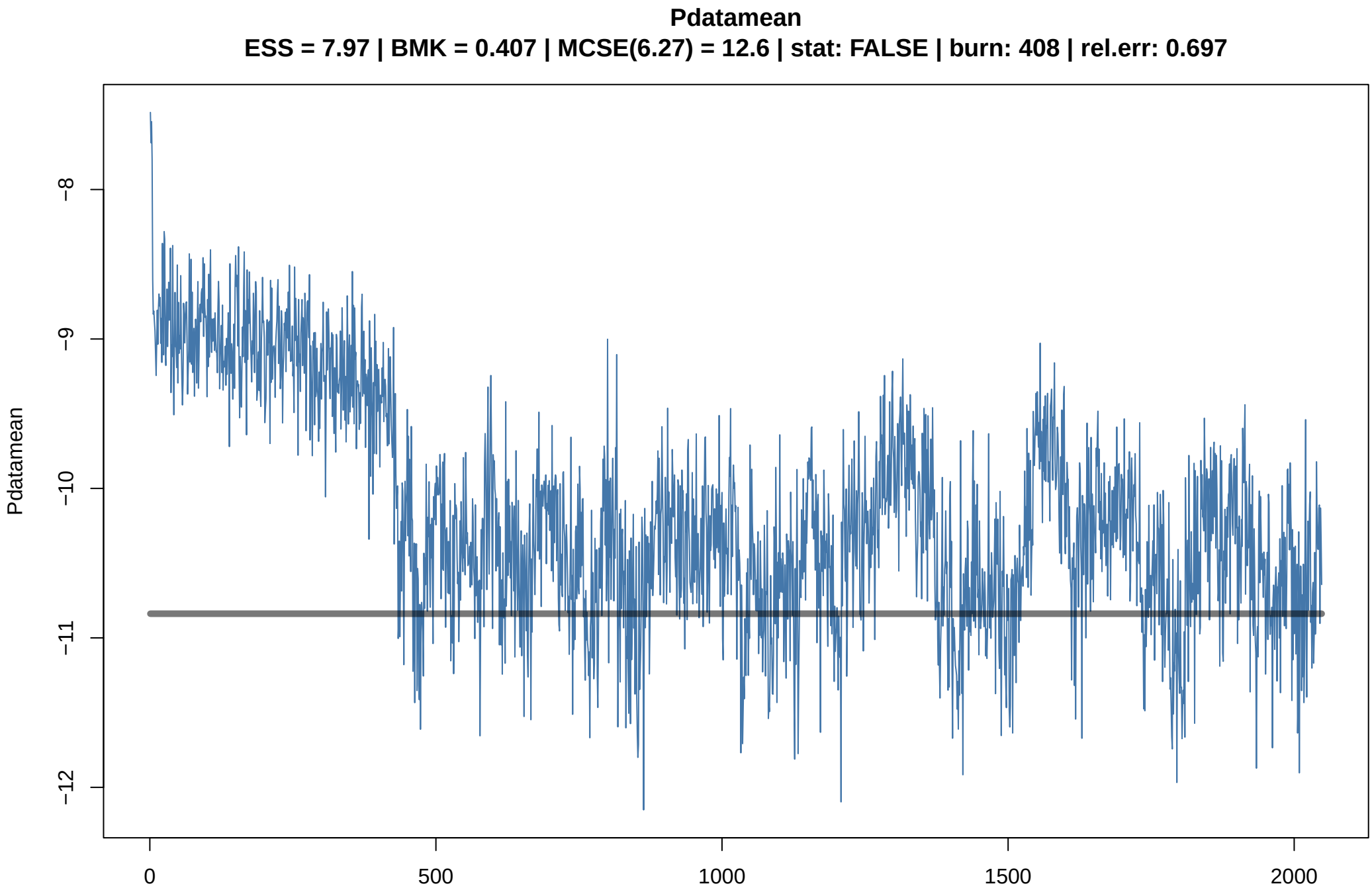
−− STATS 1D −−
min ESS = 1684.18202007565
max BMK = 0.0681739320802638
max MCSE = 2.67957160089949
all stationary: FALSE
burn: 0
max rel.err.: 2.23740189508801

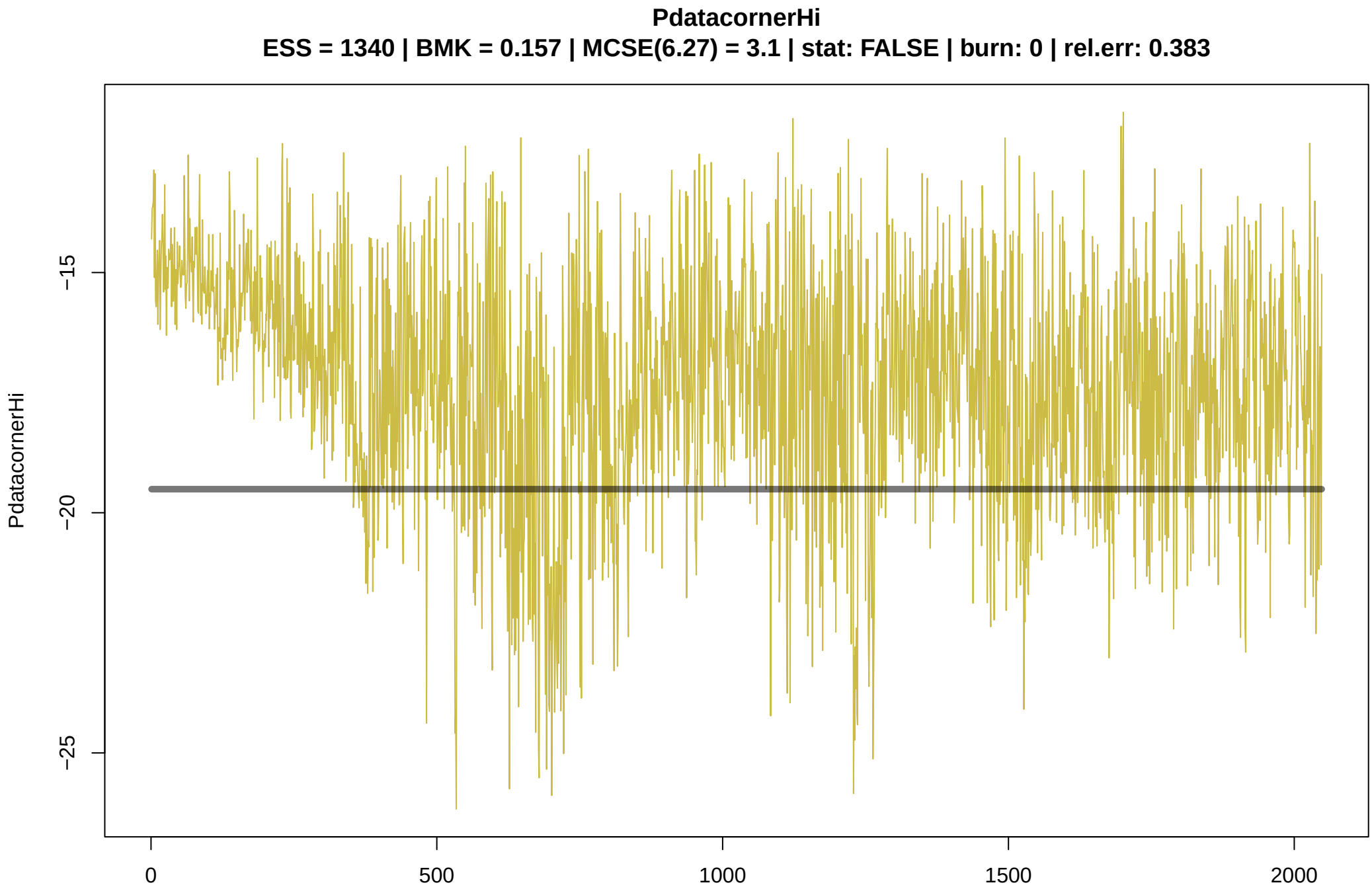
Occupied clusters: 11 of 16

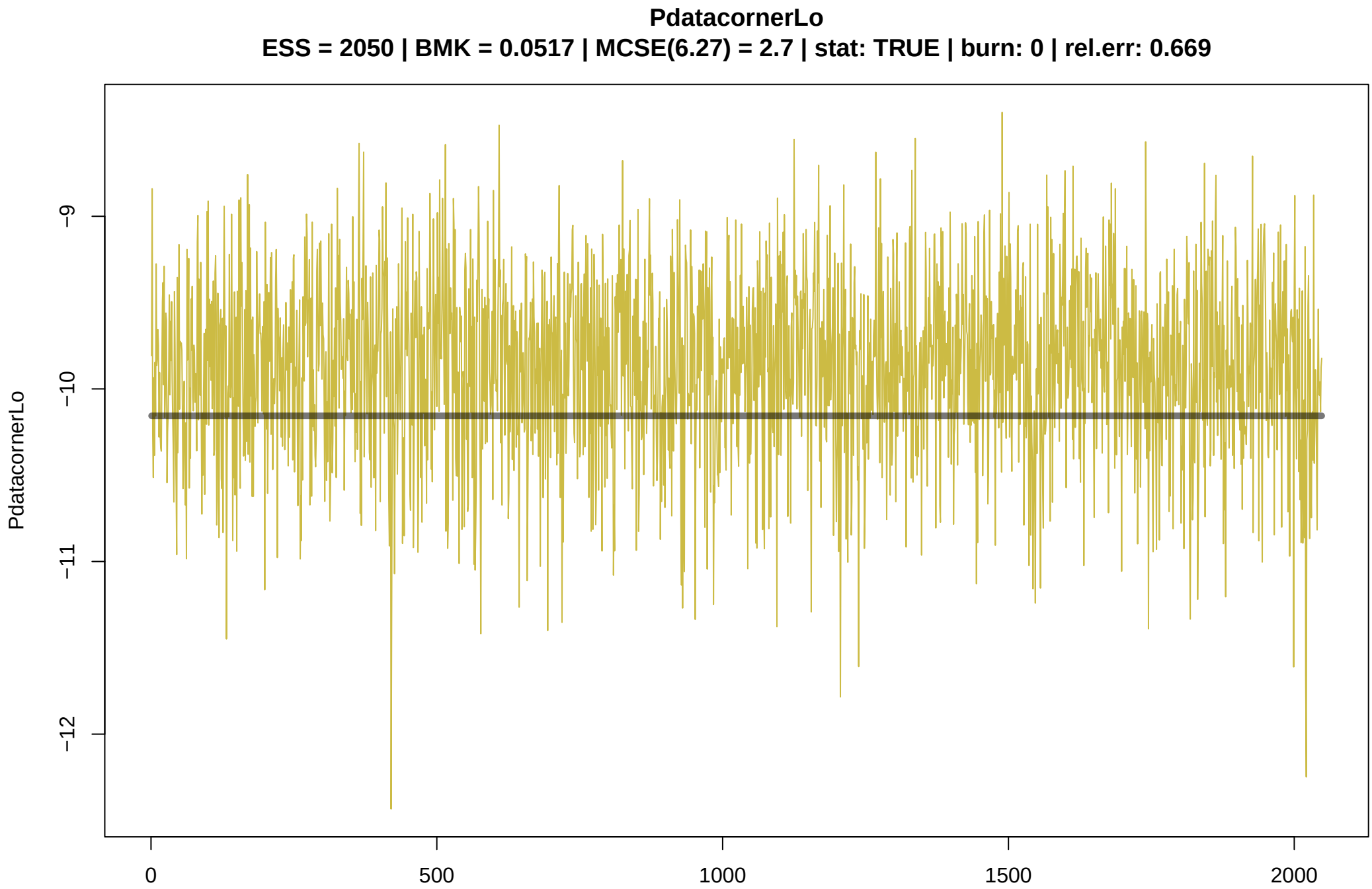

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

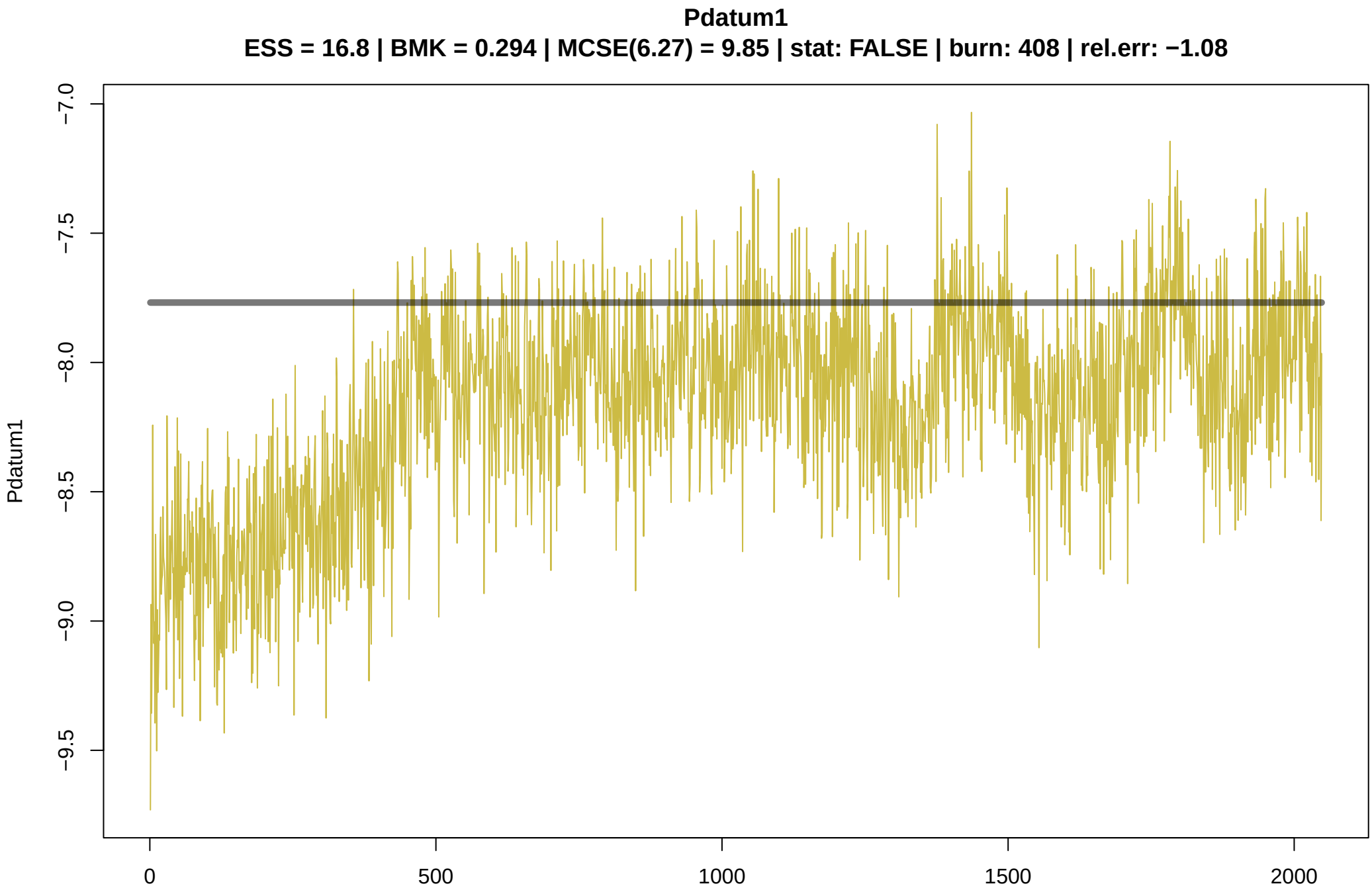

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

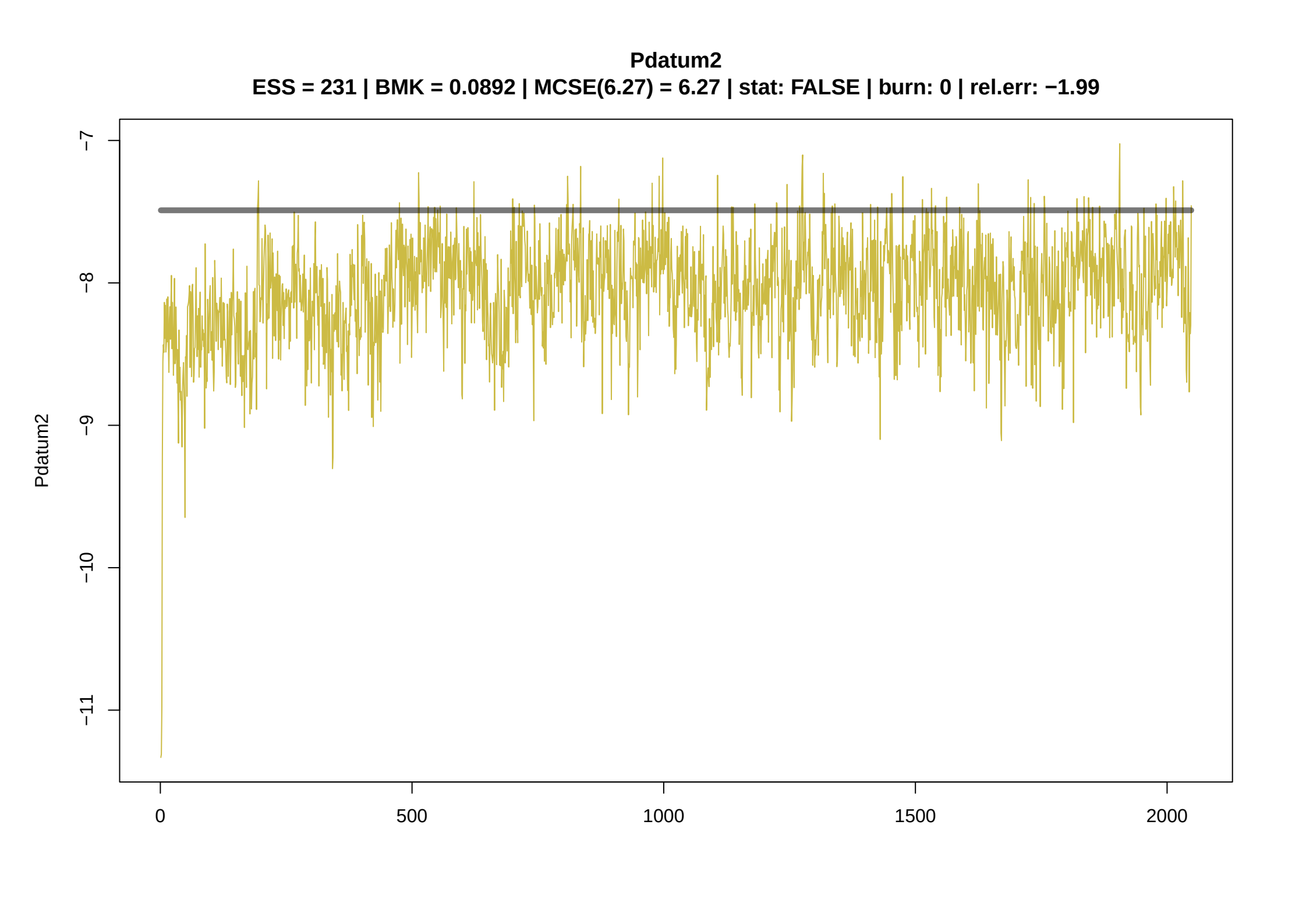

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

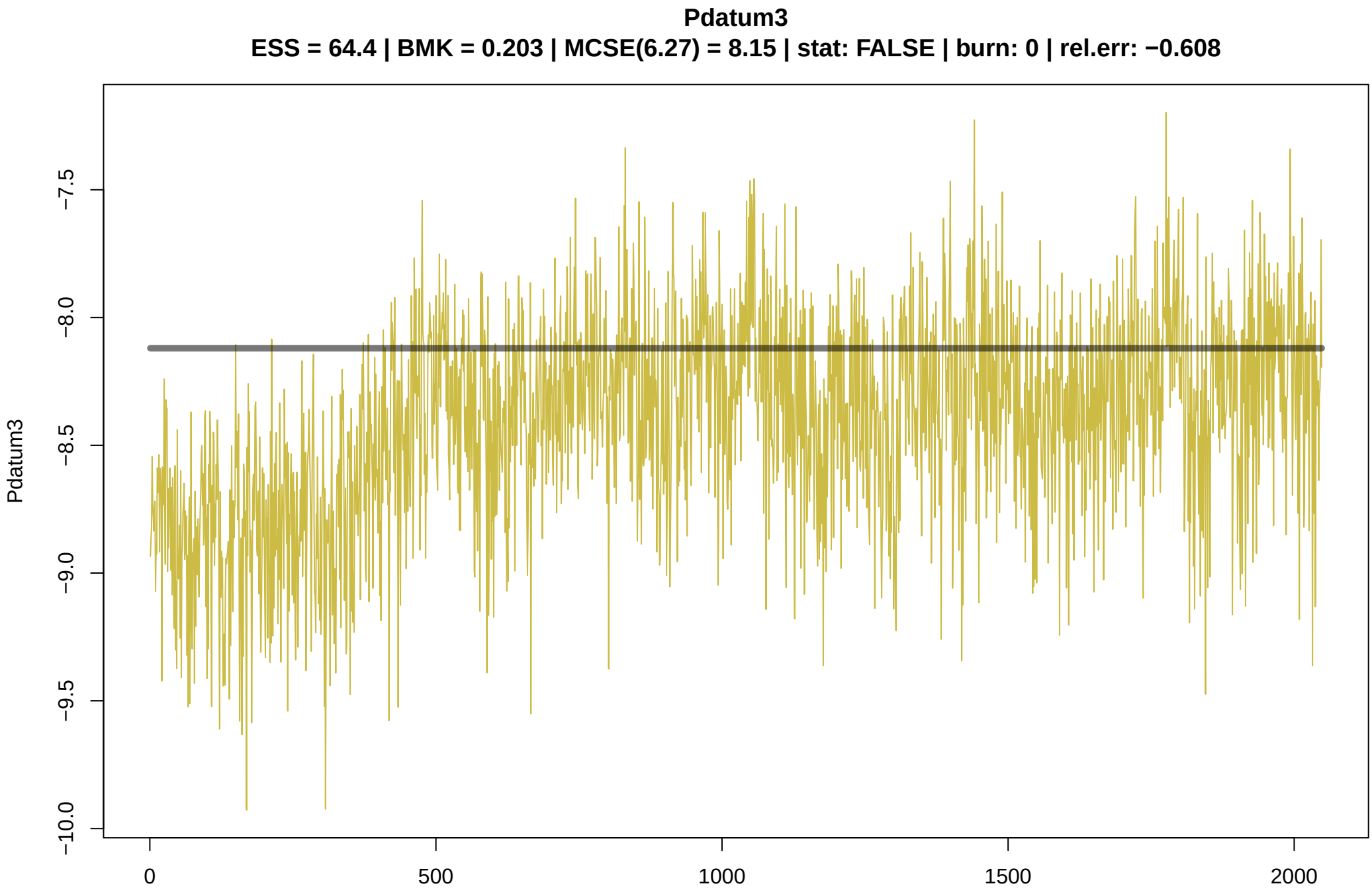

Pdatamean
ESS = 7.97 | BMK = 0.407 | MCSE(6.27) = 12.6 | stat: FALSE | burn: 408 | rel.err: 0.697
Pdatamean
−8
−9
−10
−11
−12
0
500
1000
1500
2000

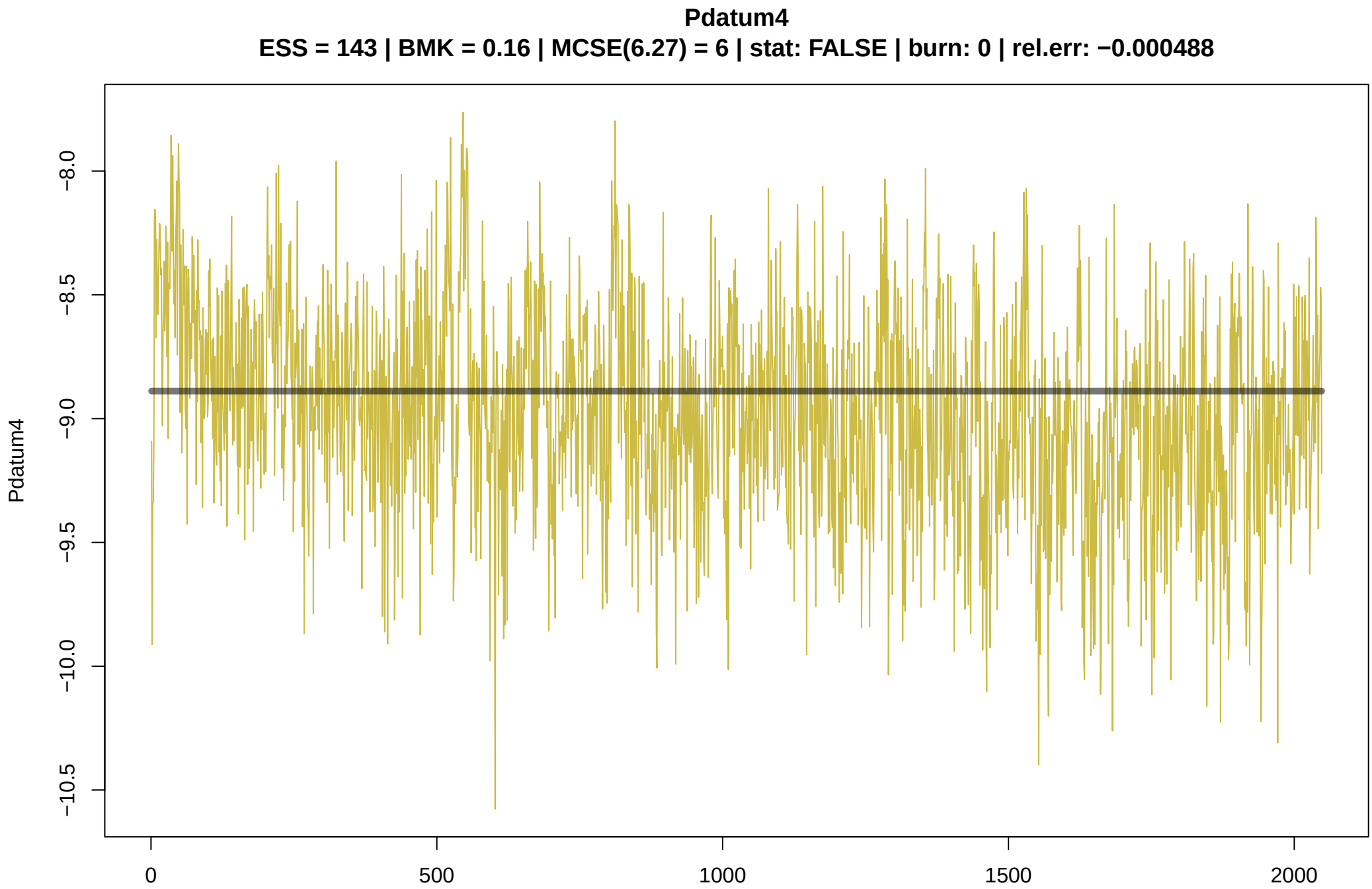

PdatacornerHi
ESS = 1340 | BMK = 0.157 | MCSE(6.27) = 3.1 | stat: FALSE | burn: 0 | rel.err: 0.383
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

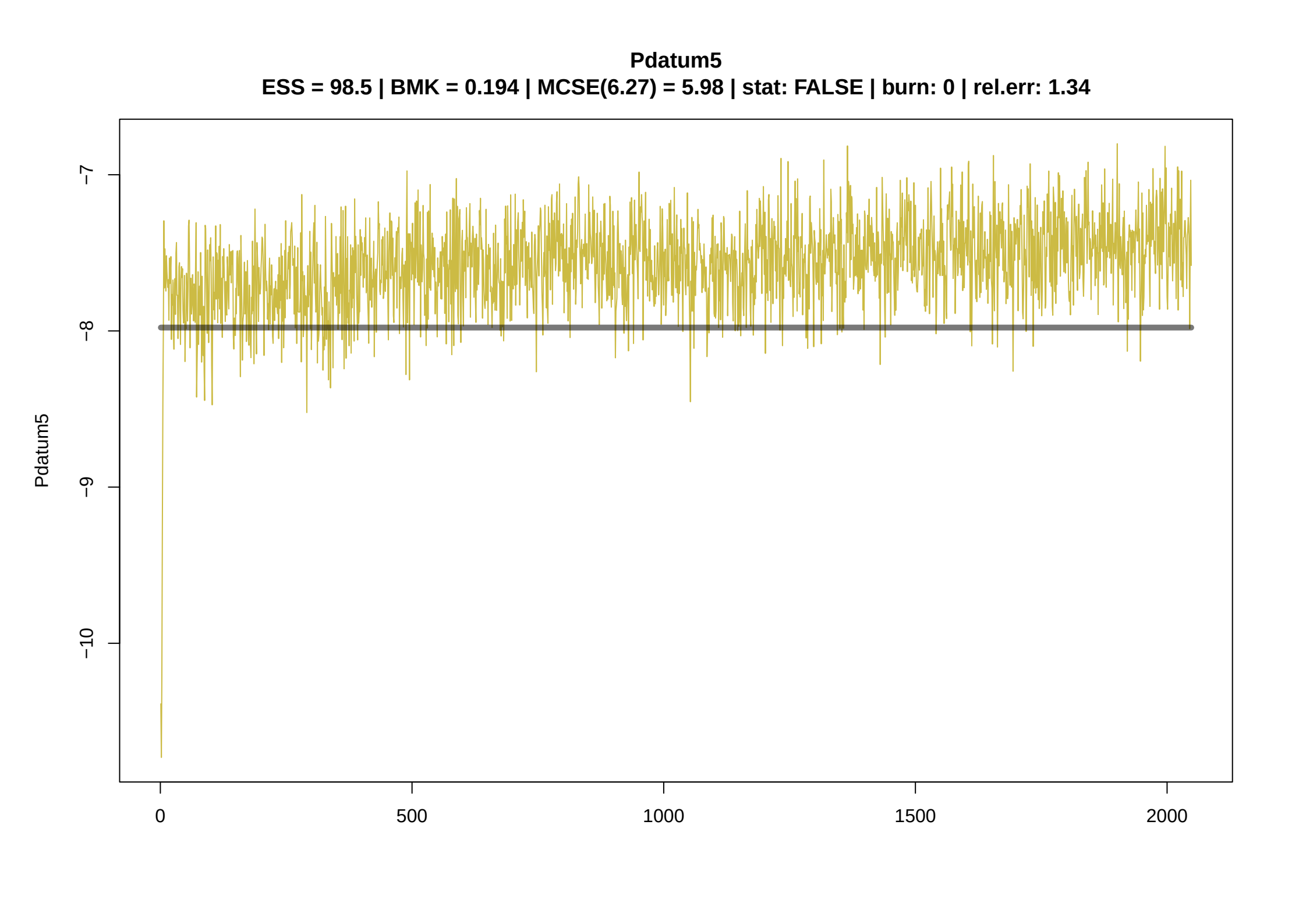

PdatacornerLo
ESS = 2050 | BMK = 0.0517 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0 | rel.err: 0.669
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

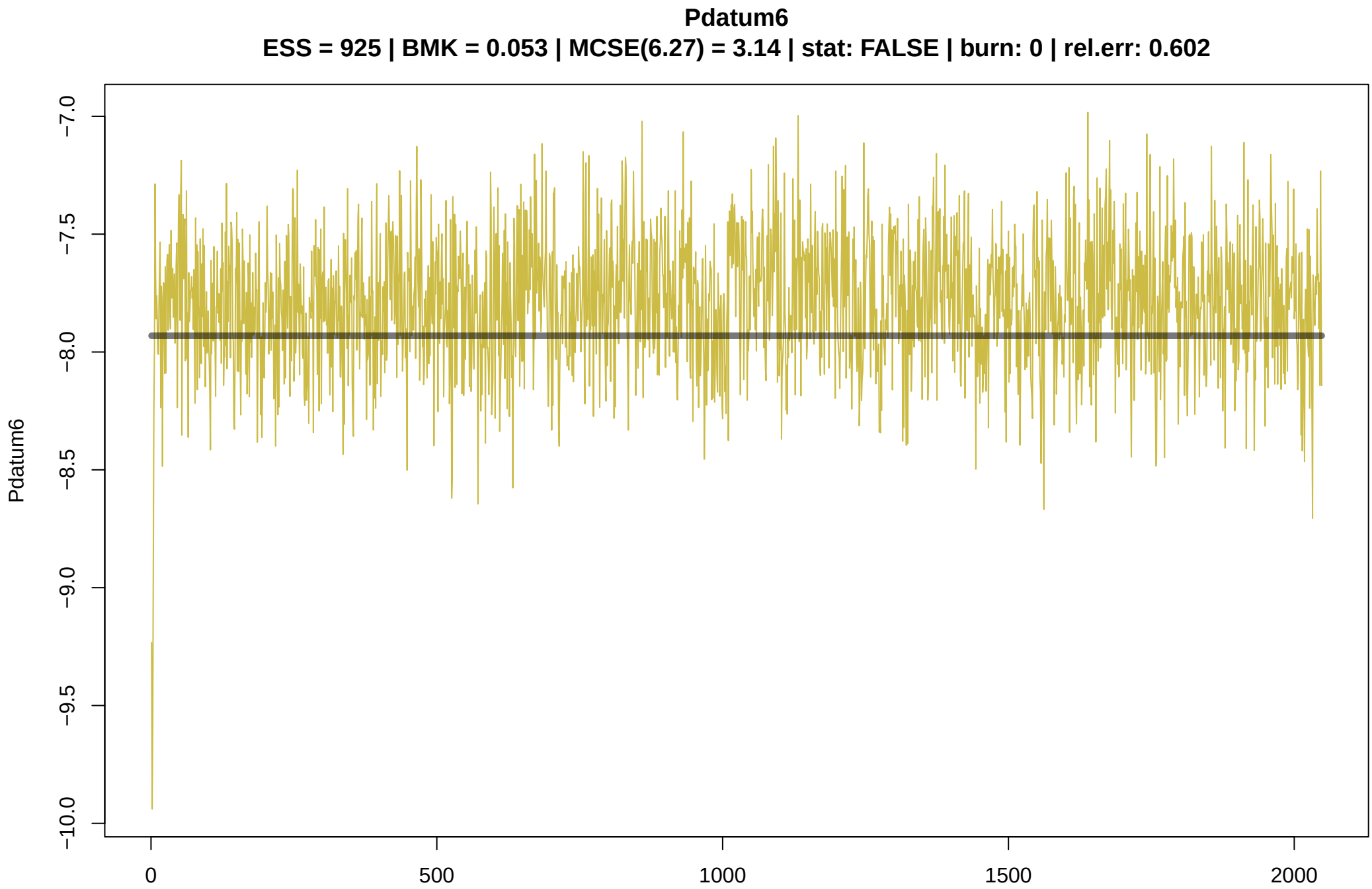

Pdatum1
ESS = 16.8 | BMK = 0.294 | MCSE(6.27) = 9.85 | stat: FALSE | burn: 408 | rel.err: −1.08
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

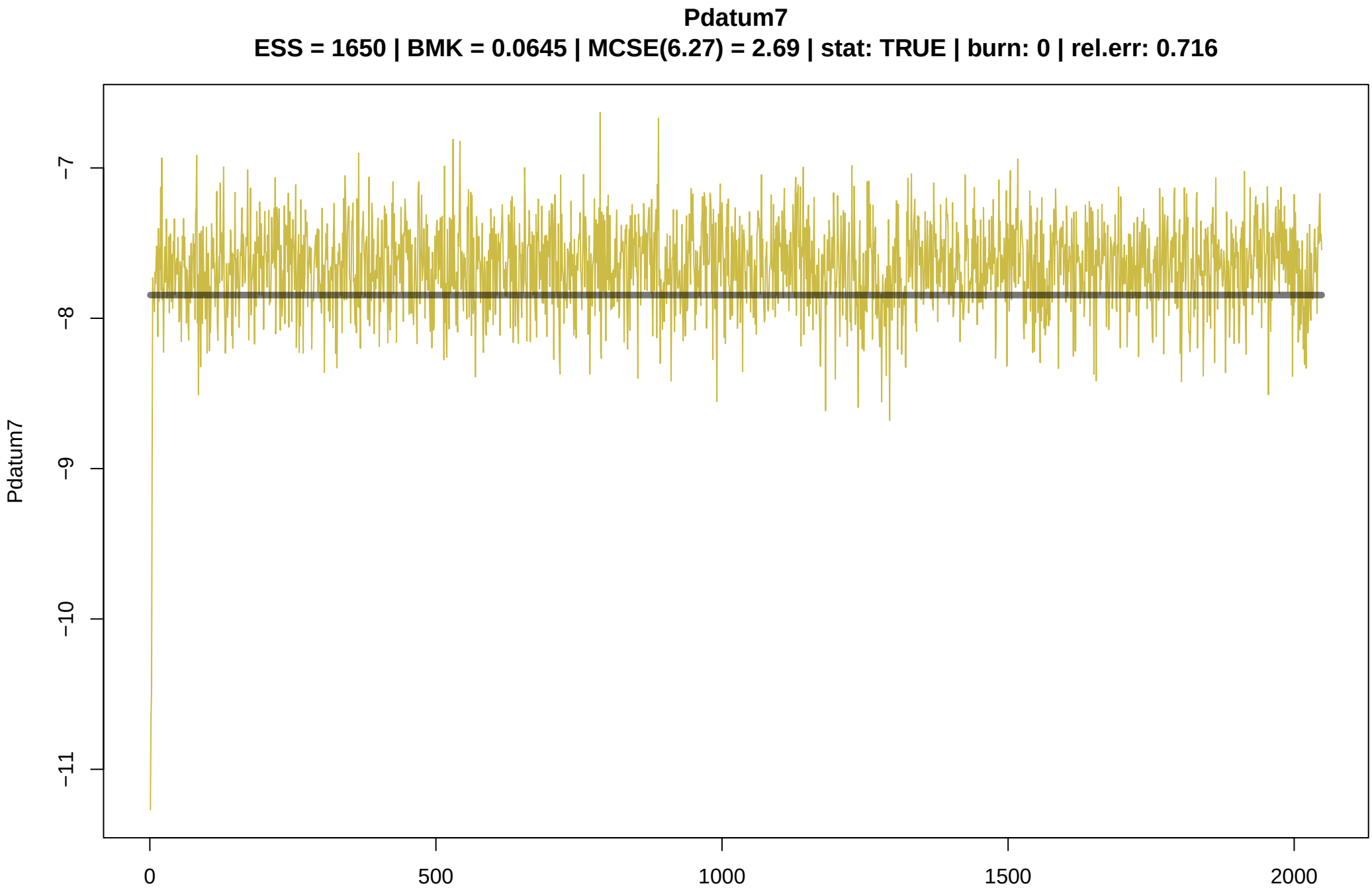

Pdatum2
ESS = 231 | BMK = 0.0892 | MCSE(6.27) = 6.27 | stat: FALSE | burn: 0 | rel.err: −1.99
Pdatum2
−7
−8
−9
−10
−11
0
500
1000
1500
2000

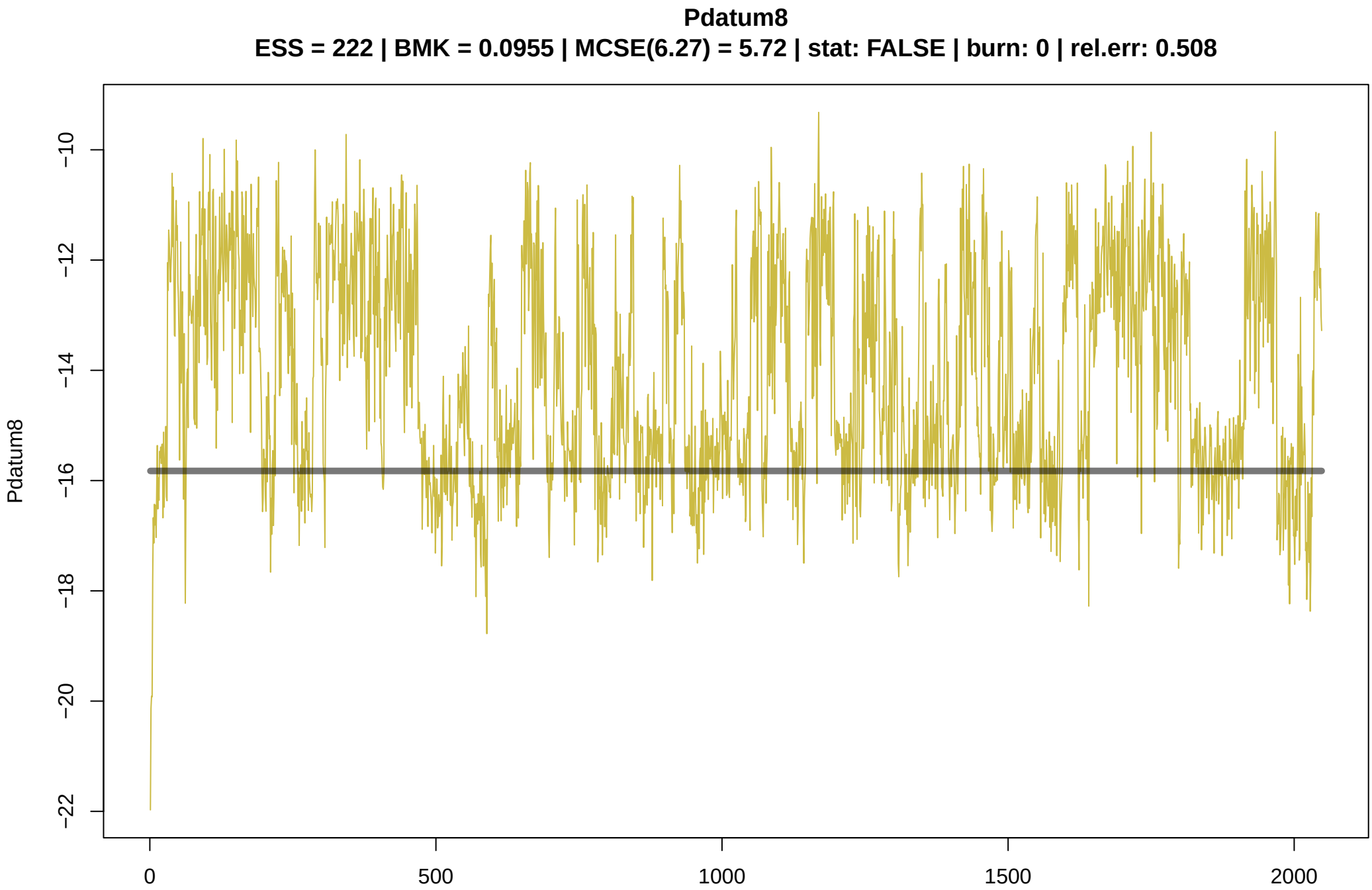

Pdatum3
ESS = 64.4 | BMK = 0.203 | MCSE(6.27) = 8.15 | stat: FALSE | burn: 0 | rel.err: −0.608
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

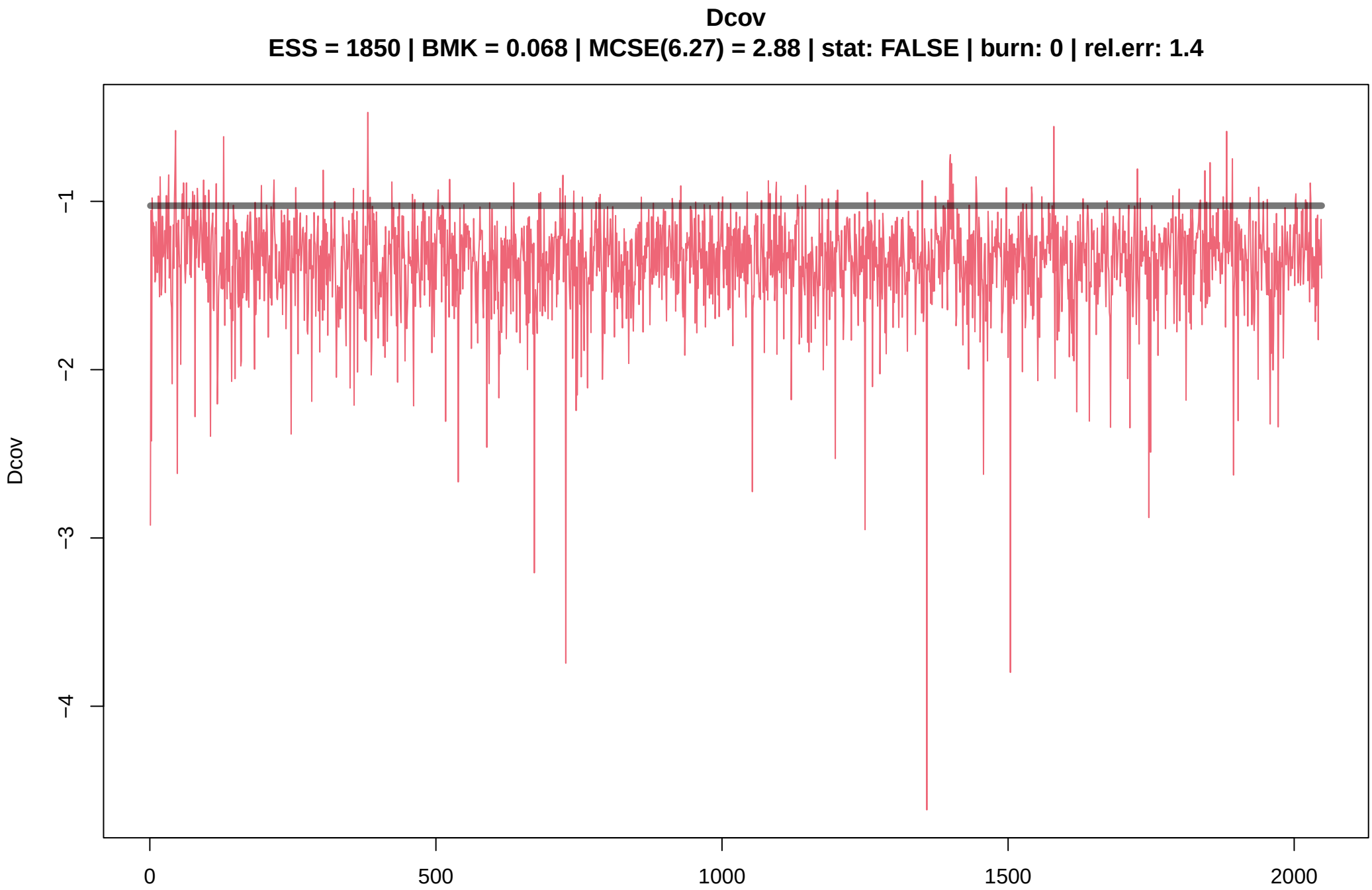

Pdatum4
ESS = 143 | BMK = 0.16 | MCSE(6.27) = 6 | stat: FALSE | burn: 0 | rel.err: −0.000488
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

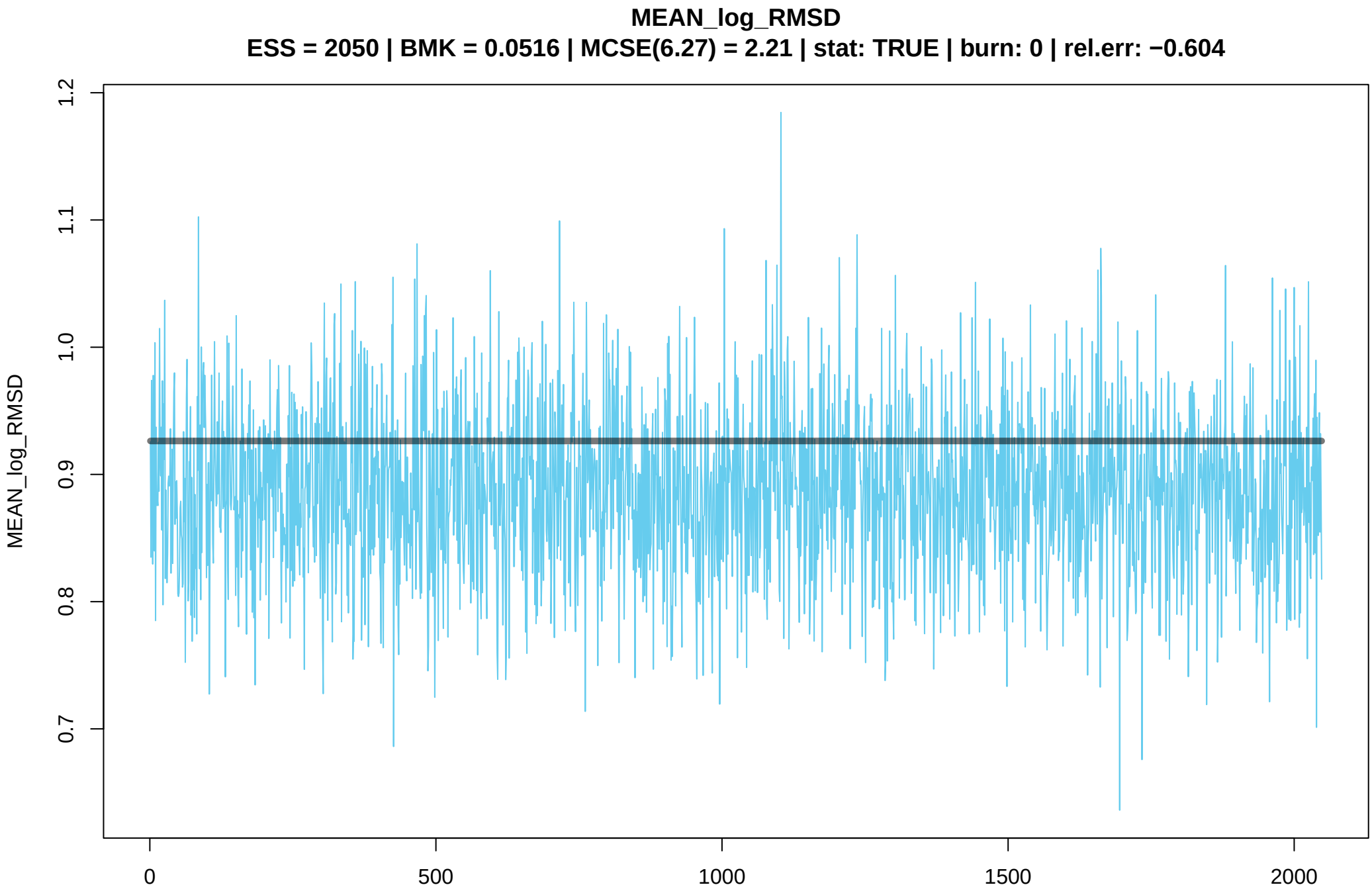

Pdatum5
ESS = 98.5 | BMK = 0.194 | MCSE(6.27) = 5.98 | stat: FALSE | burn: 0 | rel.err: 1.34
Pdatum5
−7
−8
−9
−10
0
500
1000
1500
2000

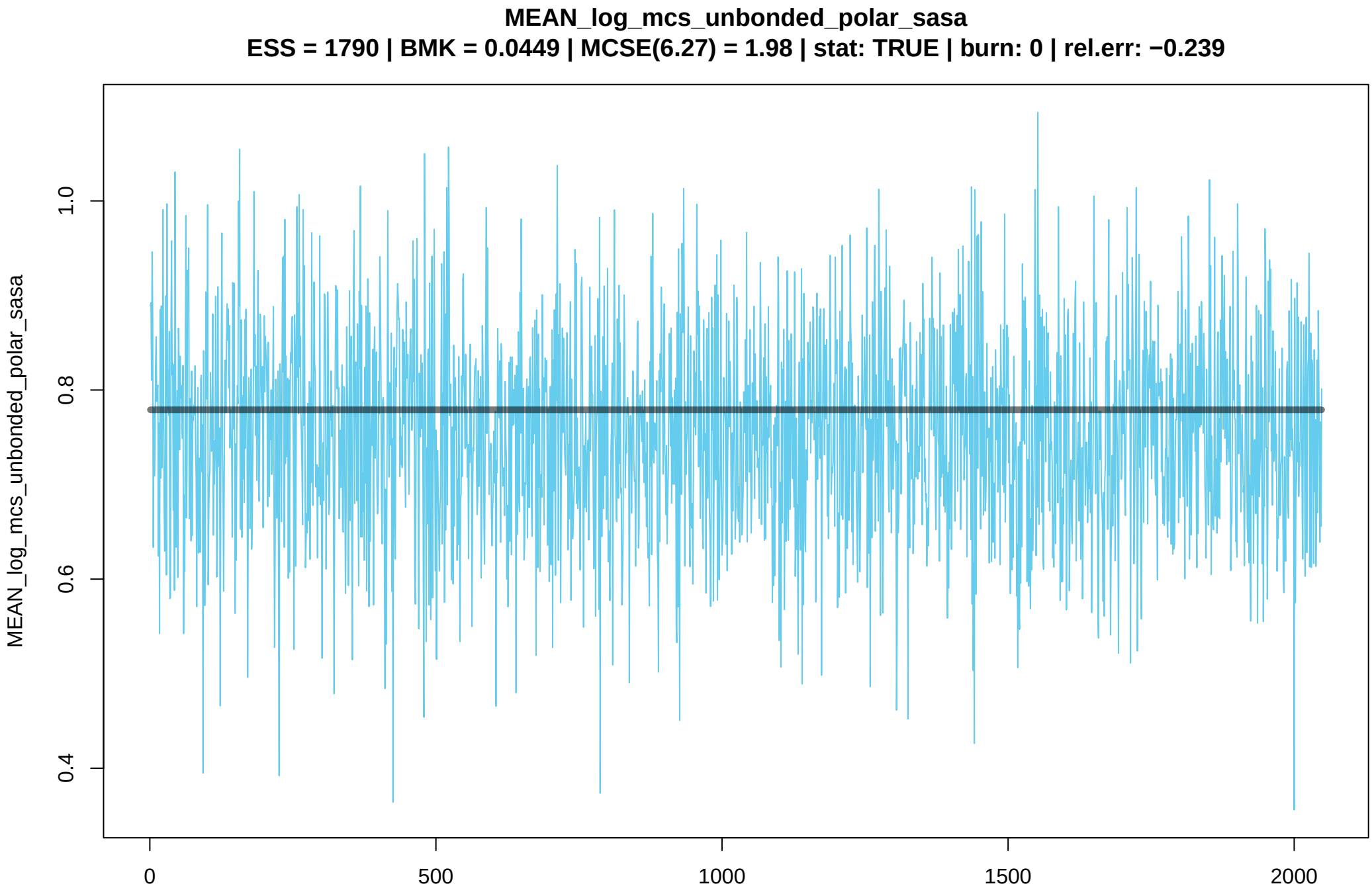

Pdatum6
ESS = 925 | BMK = 0.053 | MCSE(6.27) = 3.14 | stat: FALSE | burn: 0 | rel.err: 0.602
Pdatum6
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

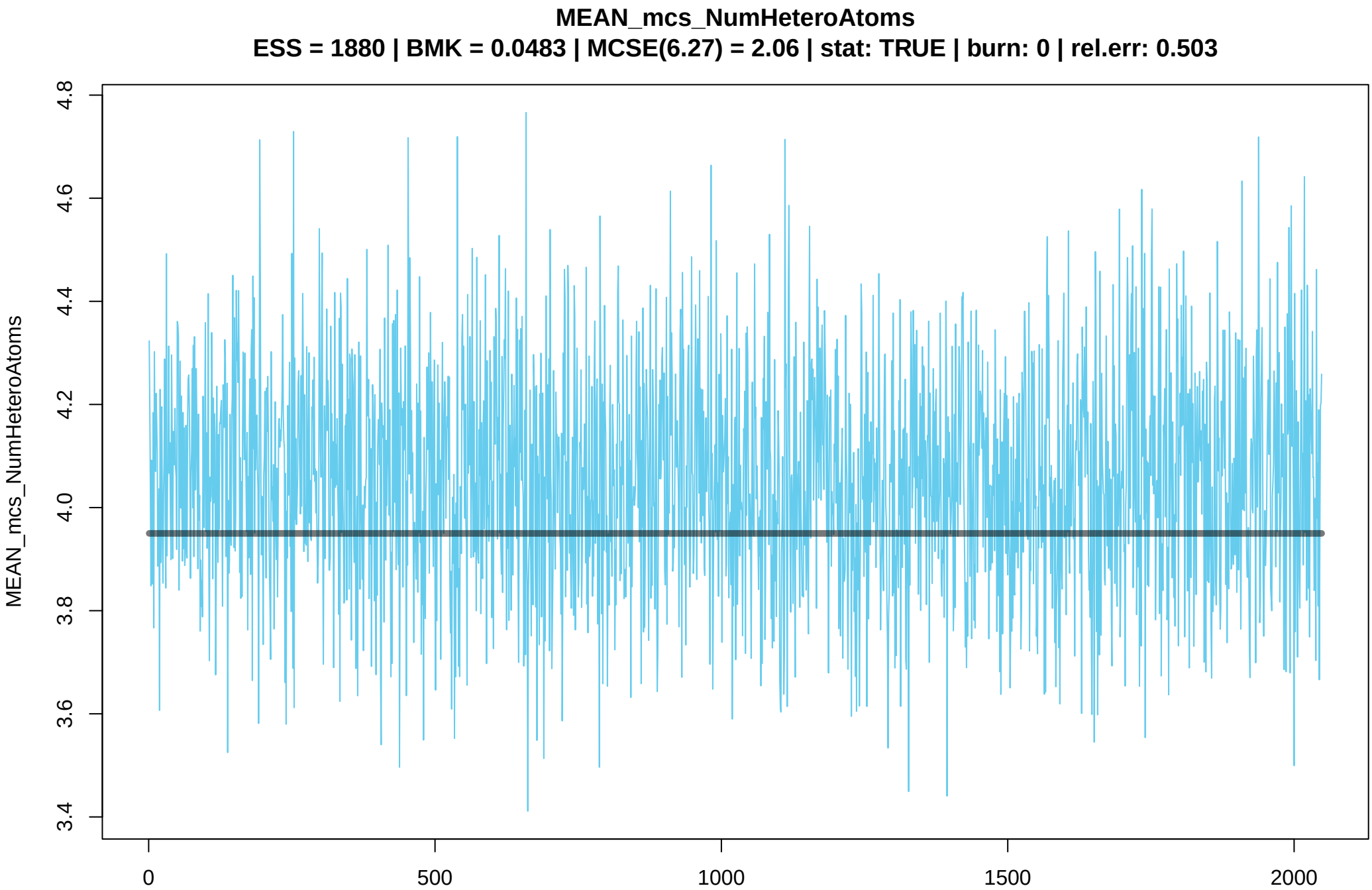

Pdatum7
ESS = 1650 | BMK = 0.0645 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0 | rel.err: 0.716
Pdatum7
−7
−8
−9
−10
−11
0
500
1000
1500
2000

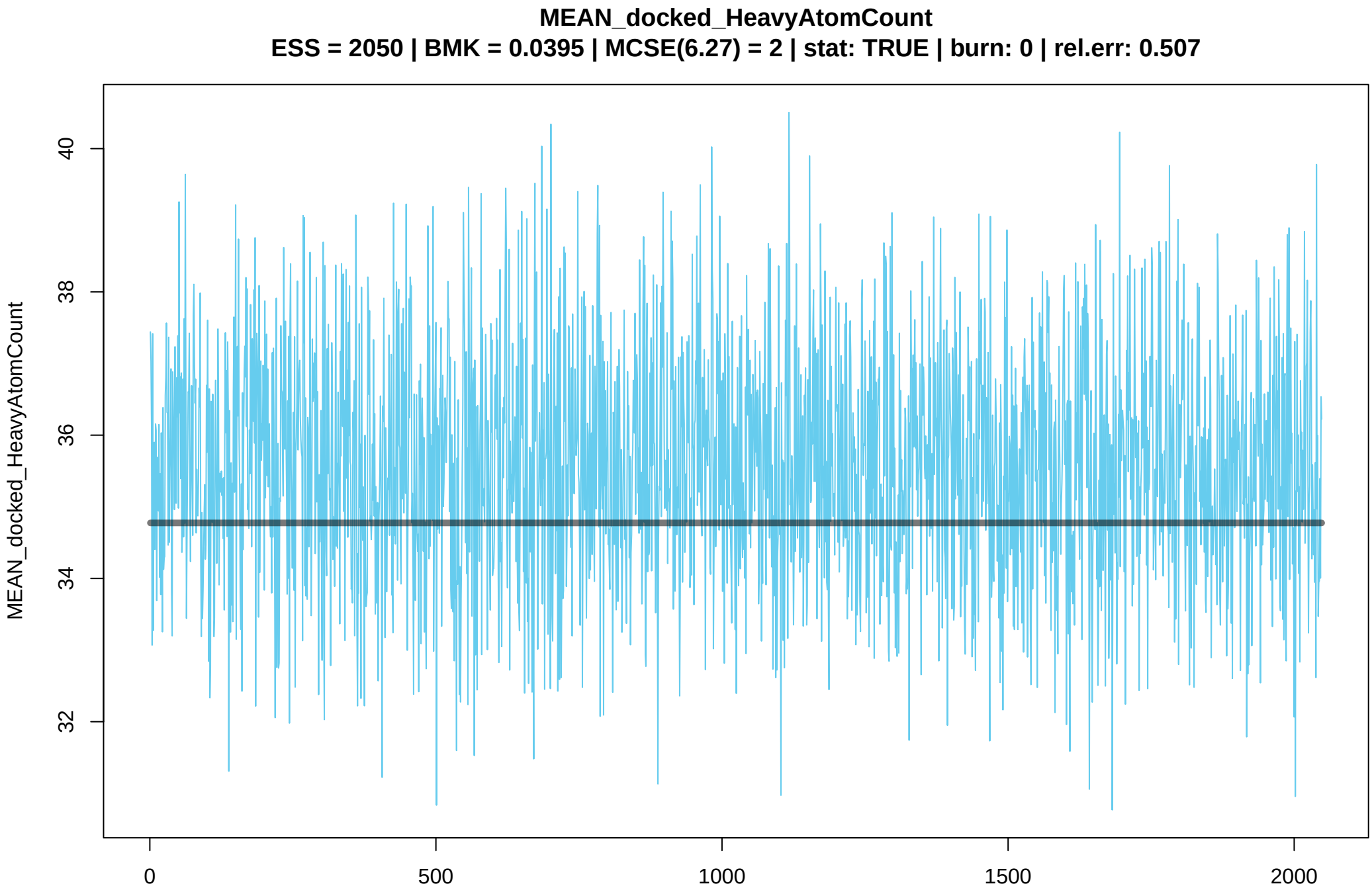

Pdatum8
ESS = 222 | BMK = 0.0955 | MCSE(6.27) = 5.72 | stat: FALSE | burn: 0 | rel.err: 0.508
Pdatum8
−10
−12
−14
−16
−18
−20
−22
0
500
1000
1500
2000

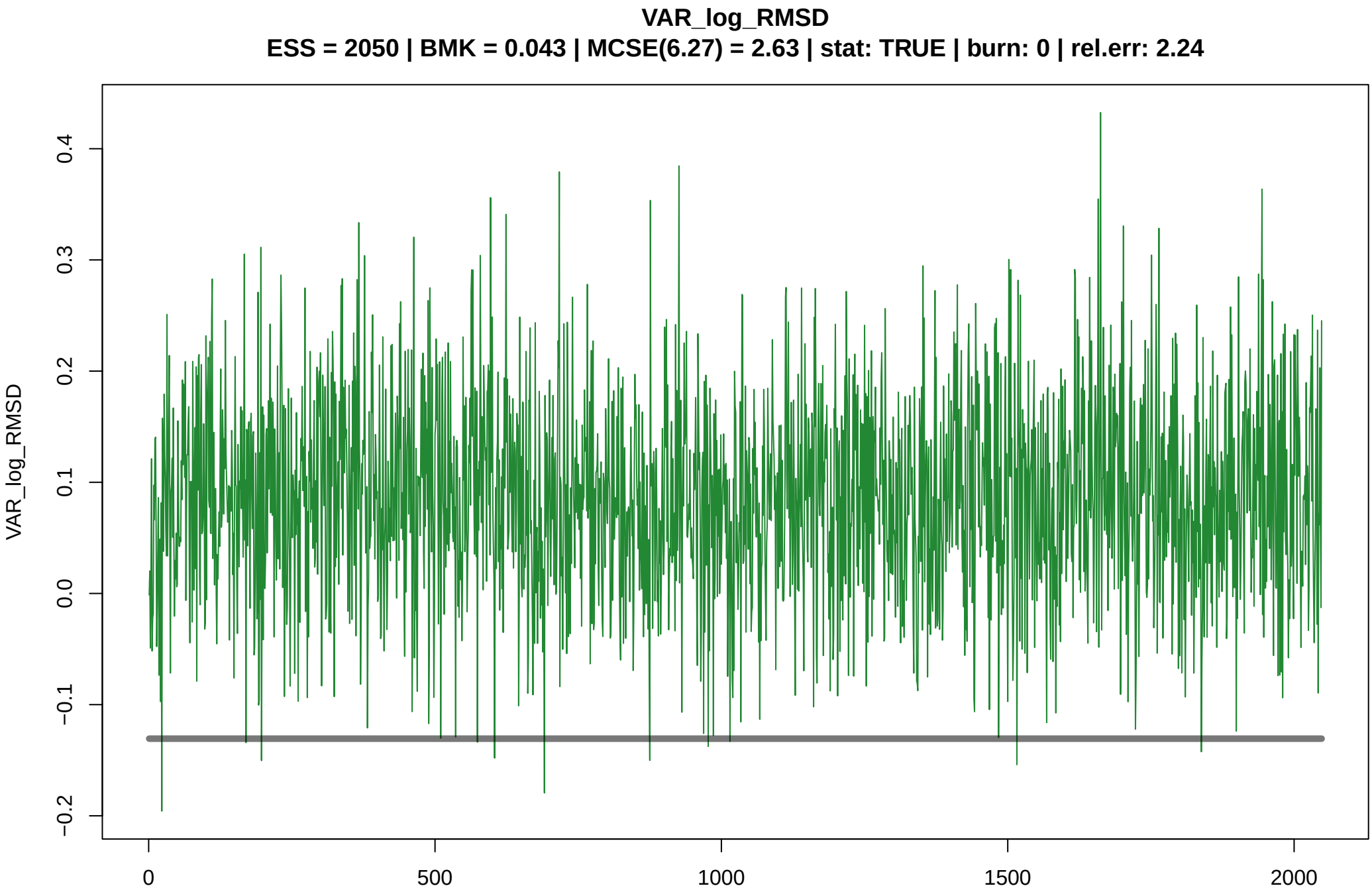

Dcov
ESS = 1850 | BMK = 0.068 | MCSE(6.27) = 2.88 | stat: FALSE | burn: 0 | rel.err: 1.4
Dcov
−1
−2
−3
−4
0
500
1000
1500
2000

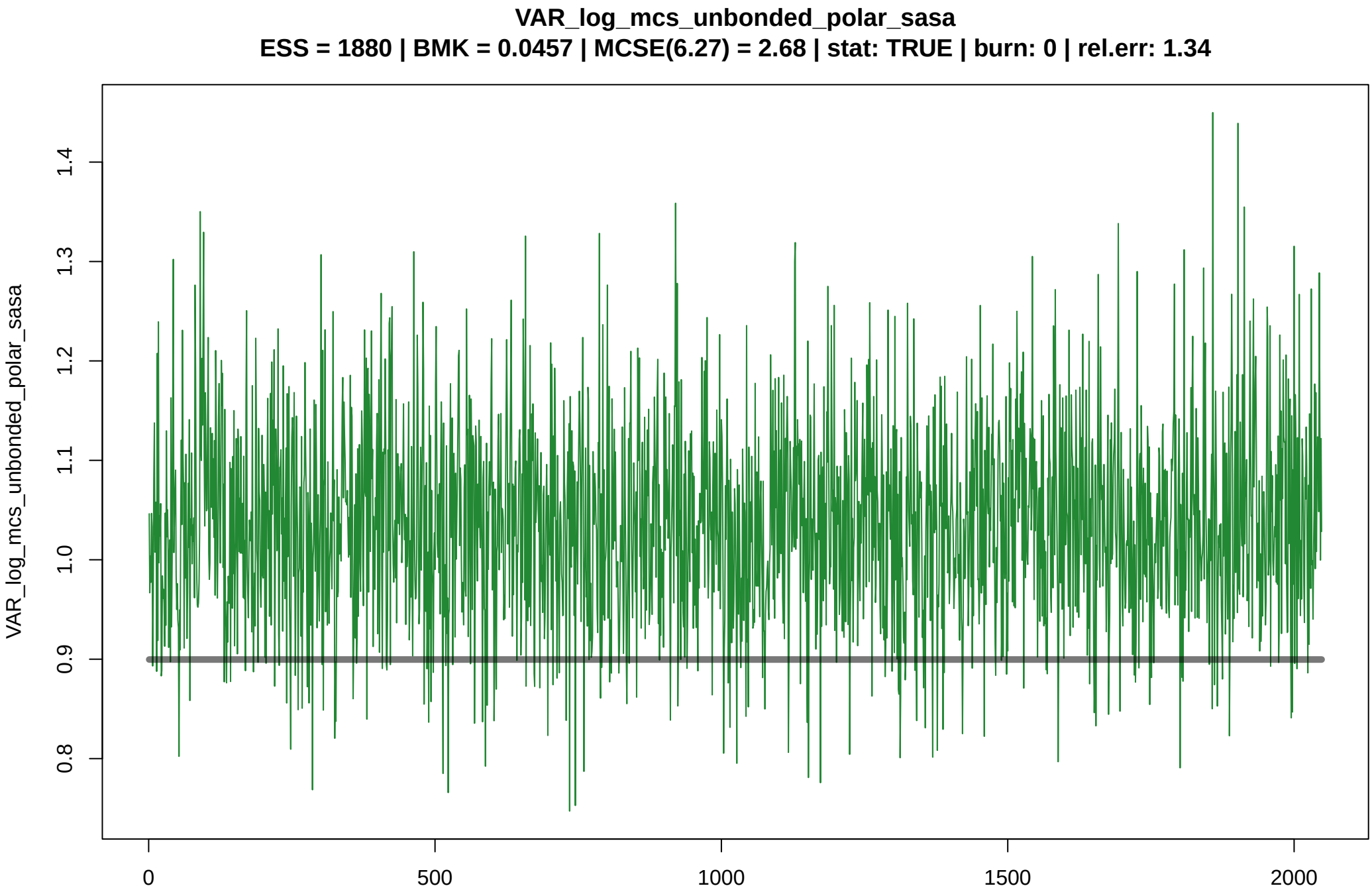

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0516 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0 | rel.err: −0.604
MEAN_log_RMSD
1.2
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

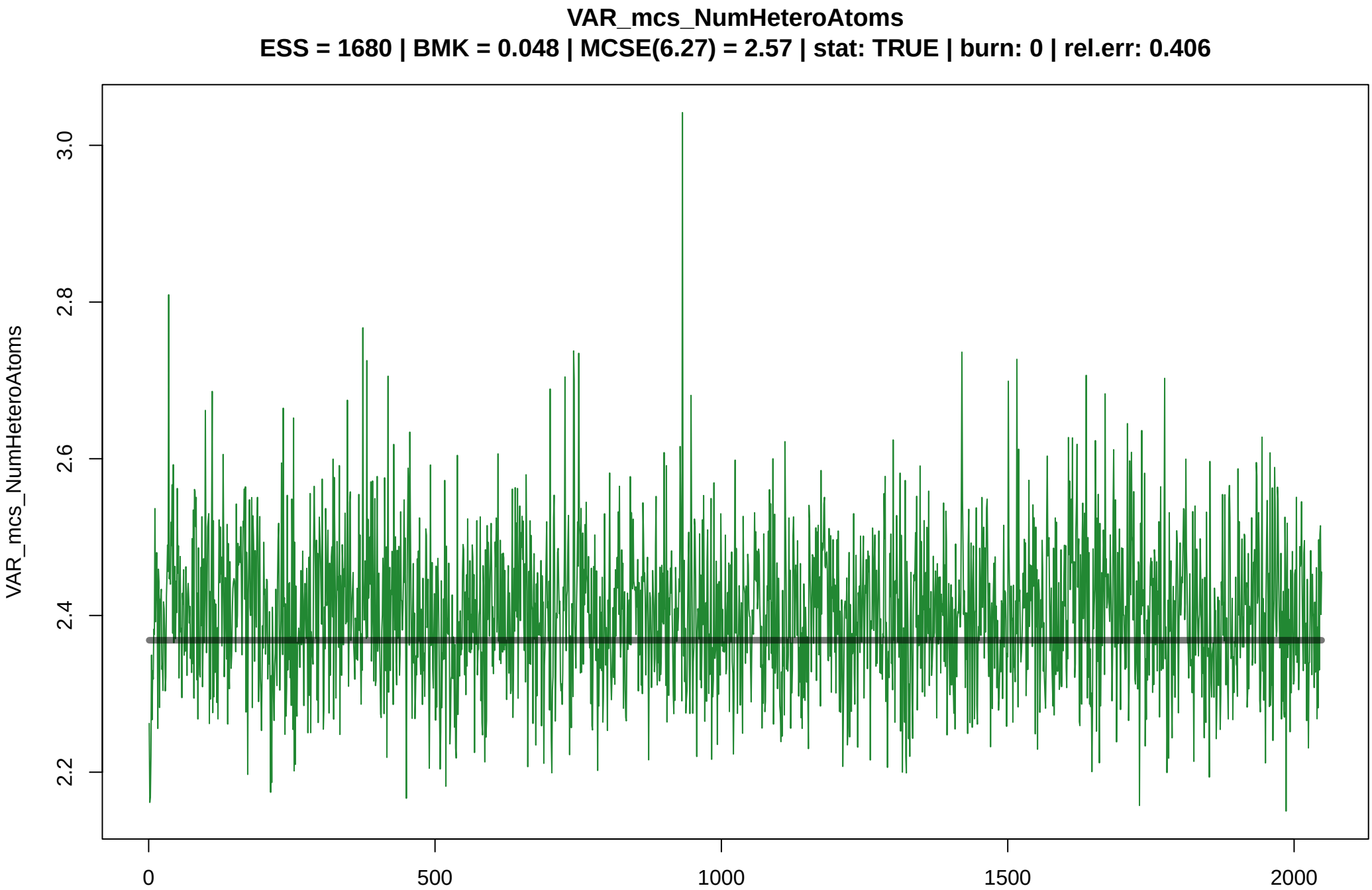

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1790 | BMK = 0.0449 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | rel.err: −0.239
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

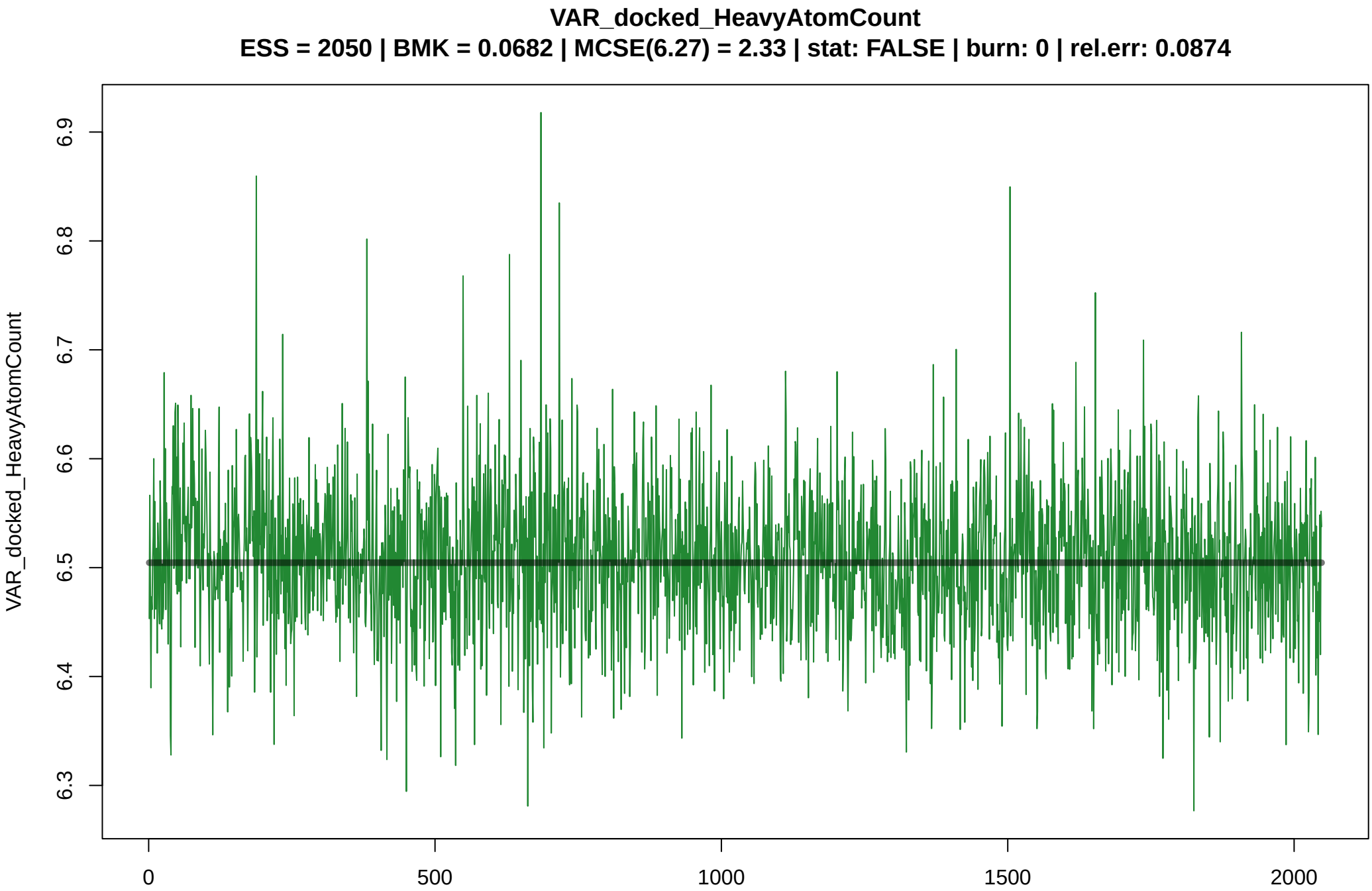

MEAN_mcs_NumHeteroAtoms
ESS = 1880 | BMK = 0.0483 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: 0.503
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

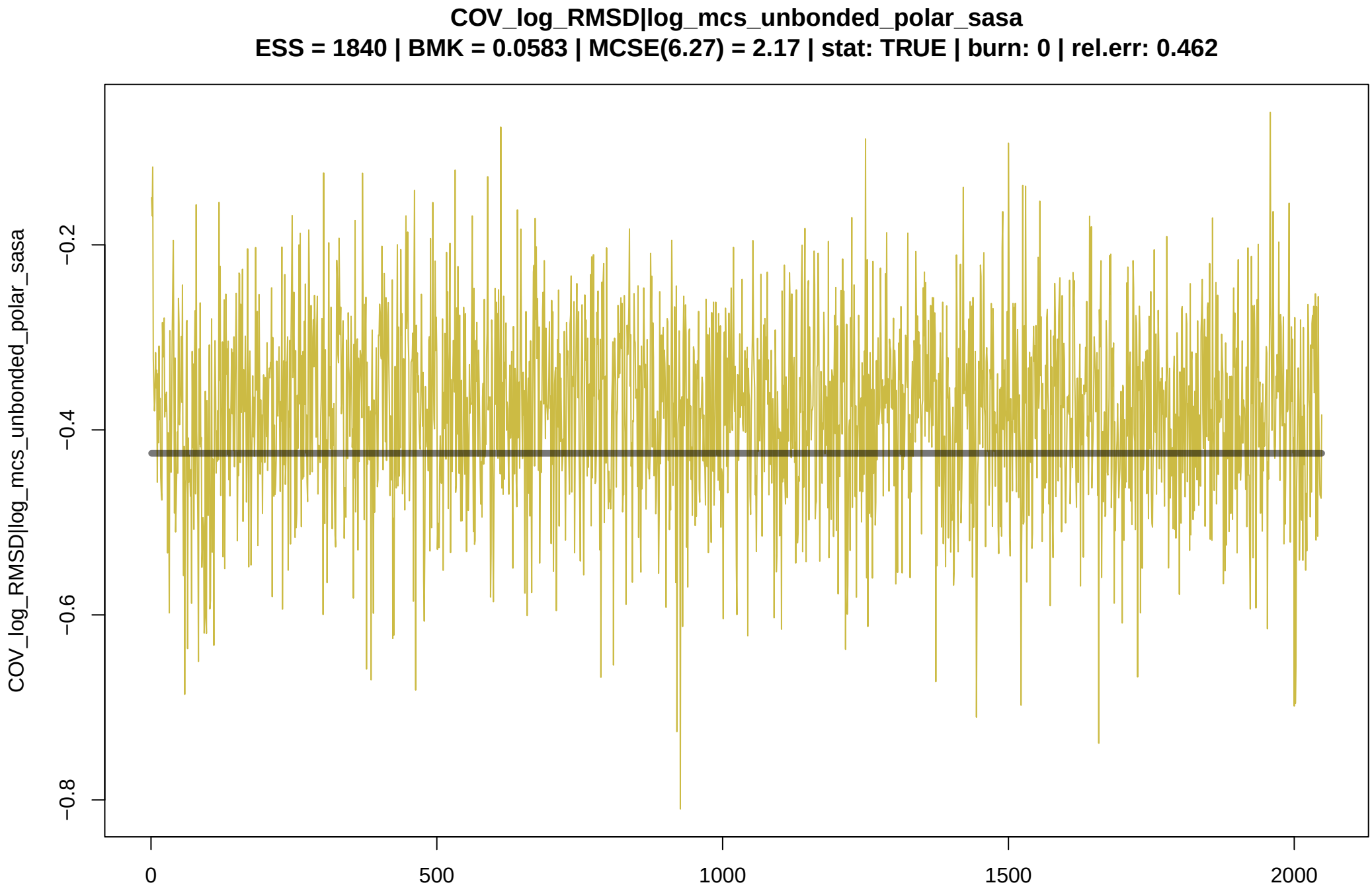

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0395 | MCSE(6.27) = 2 | stat: TRUE | burn: 0 | rel.err: 0.507
MEAN_docked_HeavyAtomCount
32
34
36
38
40
0
500
1000
1500
2000

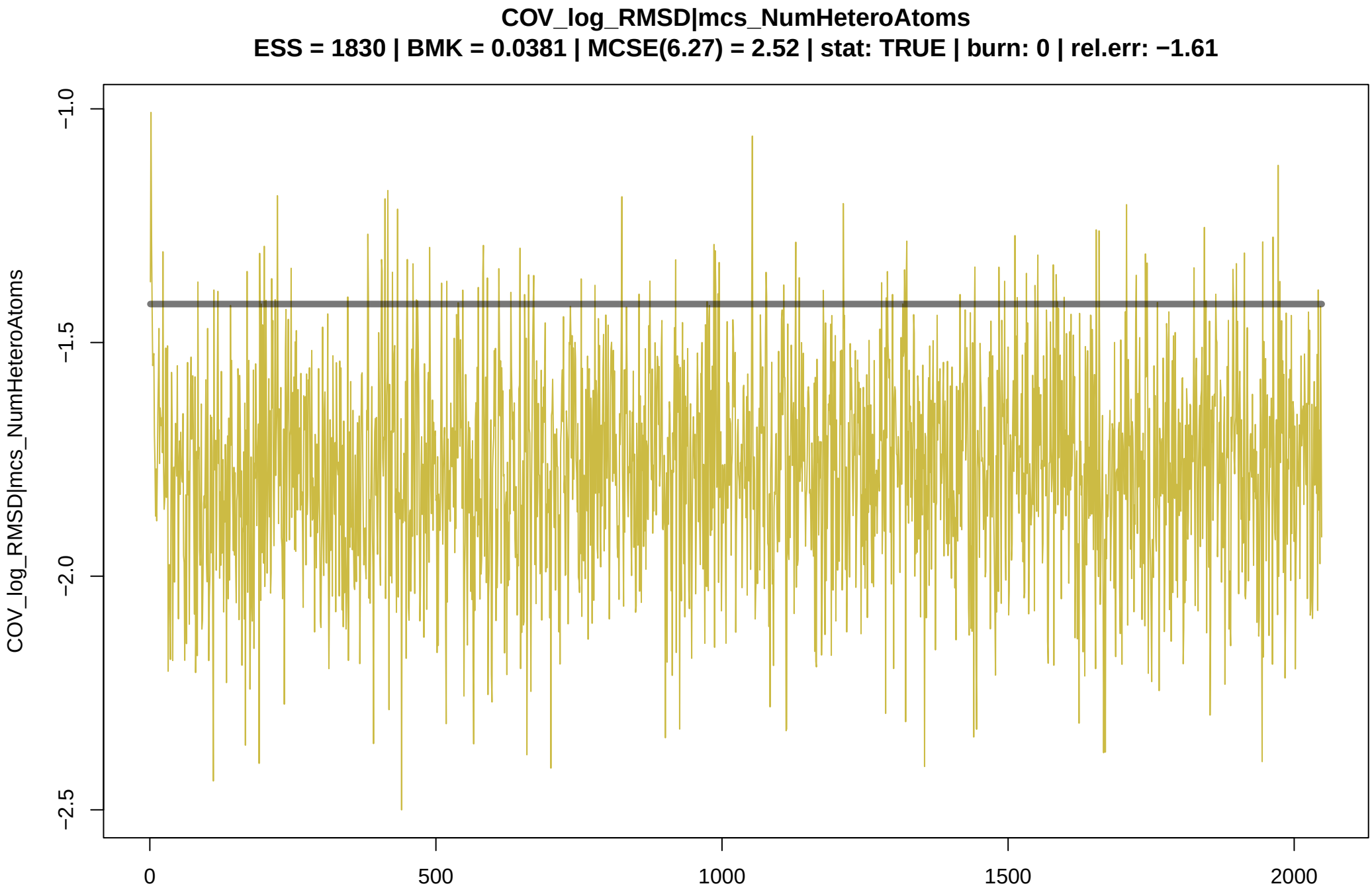

VAR_log_RMSD
ESS = 2050 | BMK = 0.043 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0 | rel.err: 2.24
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

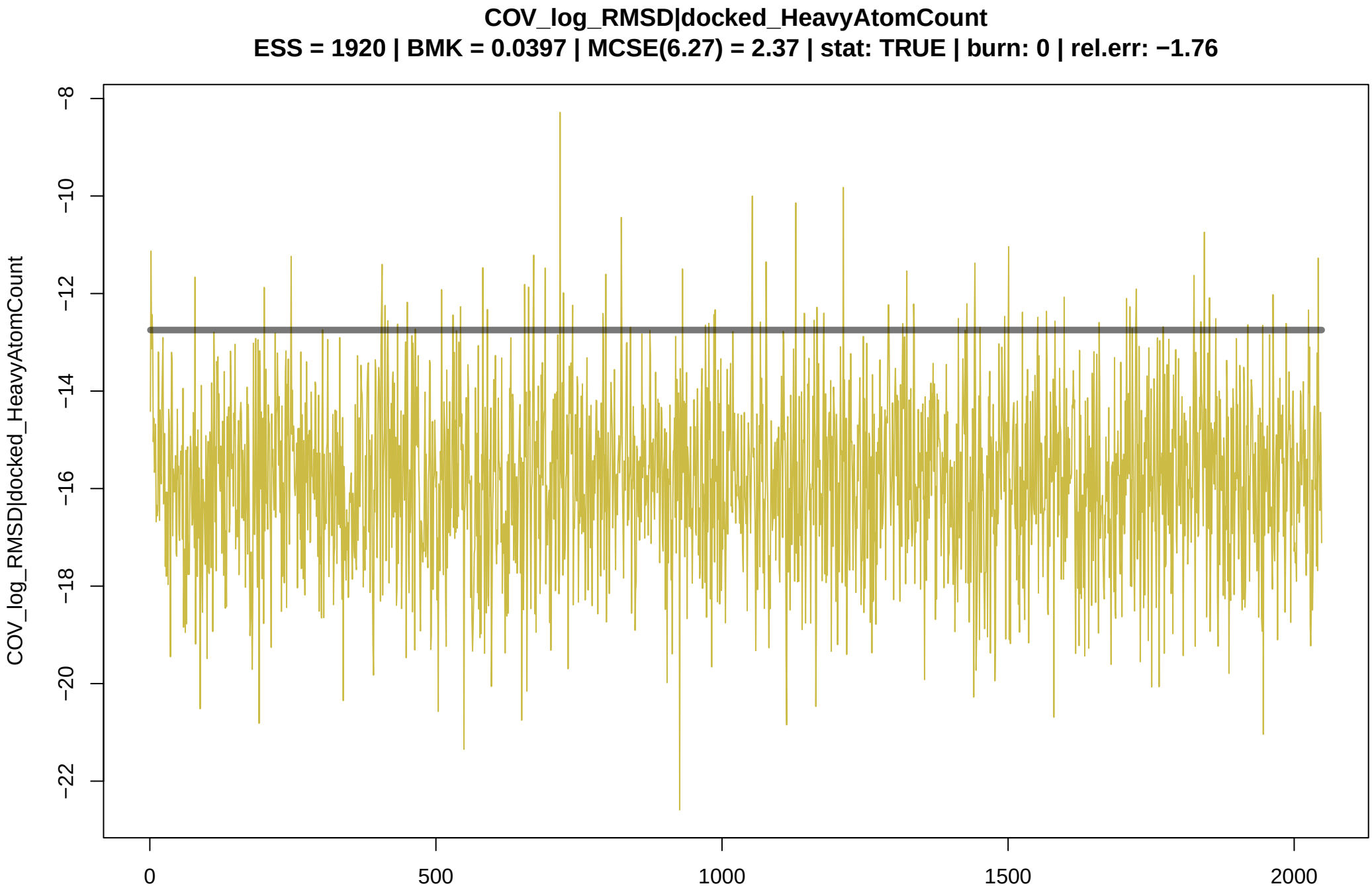

VAR_log_mcs_unbonded_polar_sasa
ESS = 1880 | BMK = 0.0457 | MCSE(6.27) = 2.68 | stat: TRUE | burn: 0 | rel.err: 1.34
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

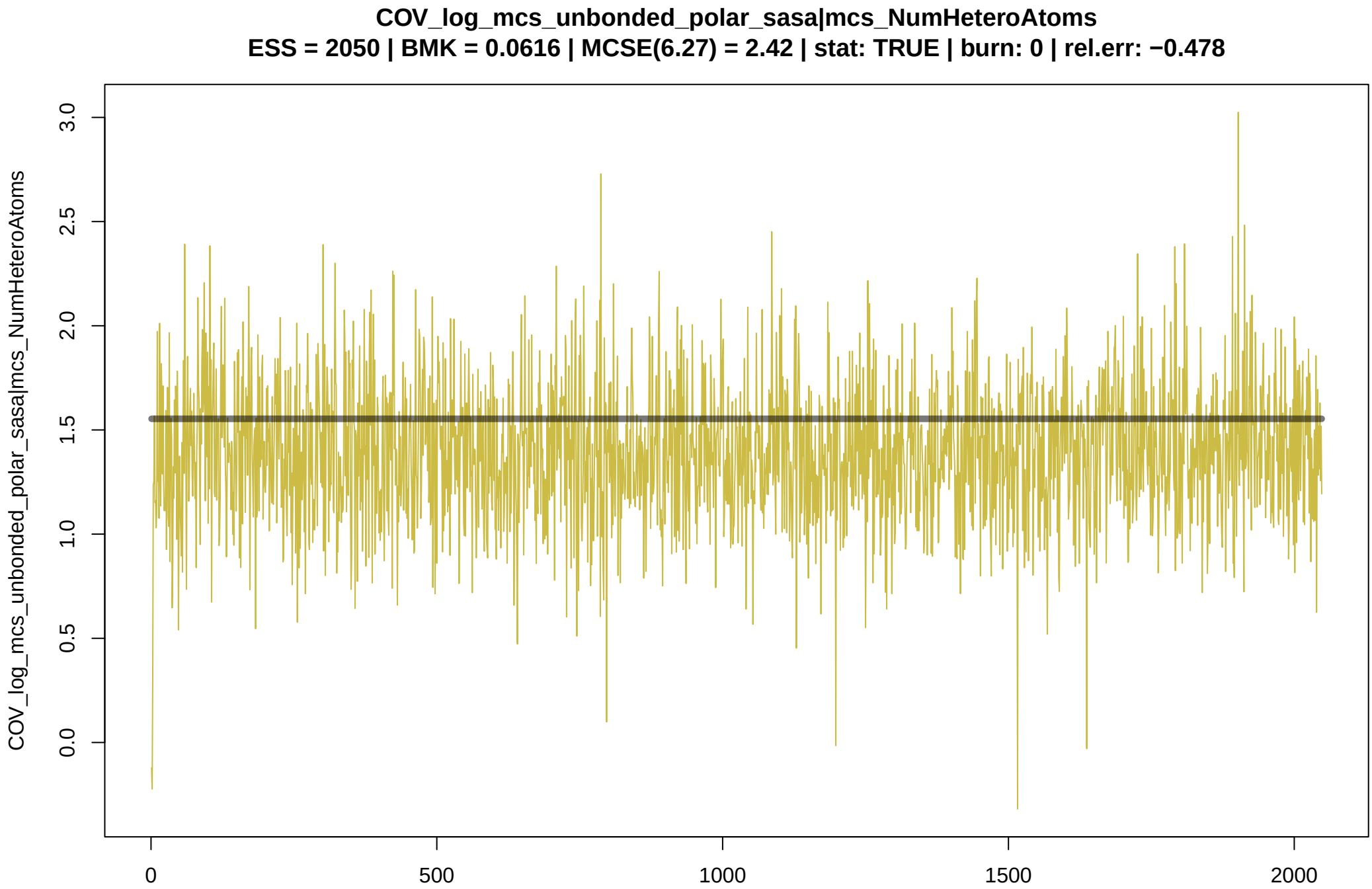

VAR_mcs_NumHeteroAtoms
ESS = 1680 | BMK = 0.048 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: 0.406
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

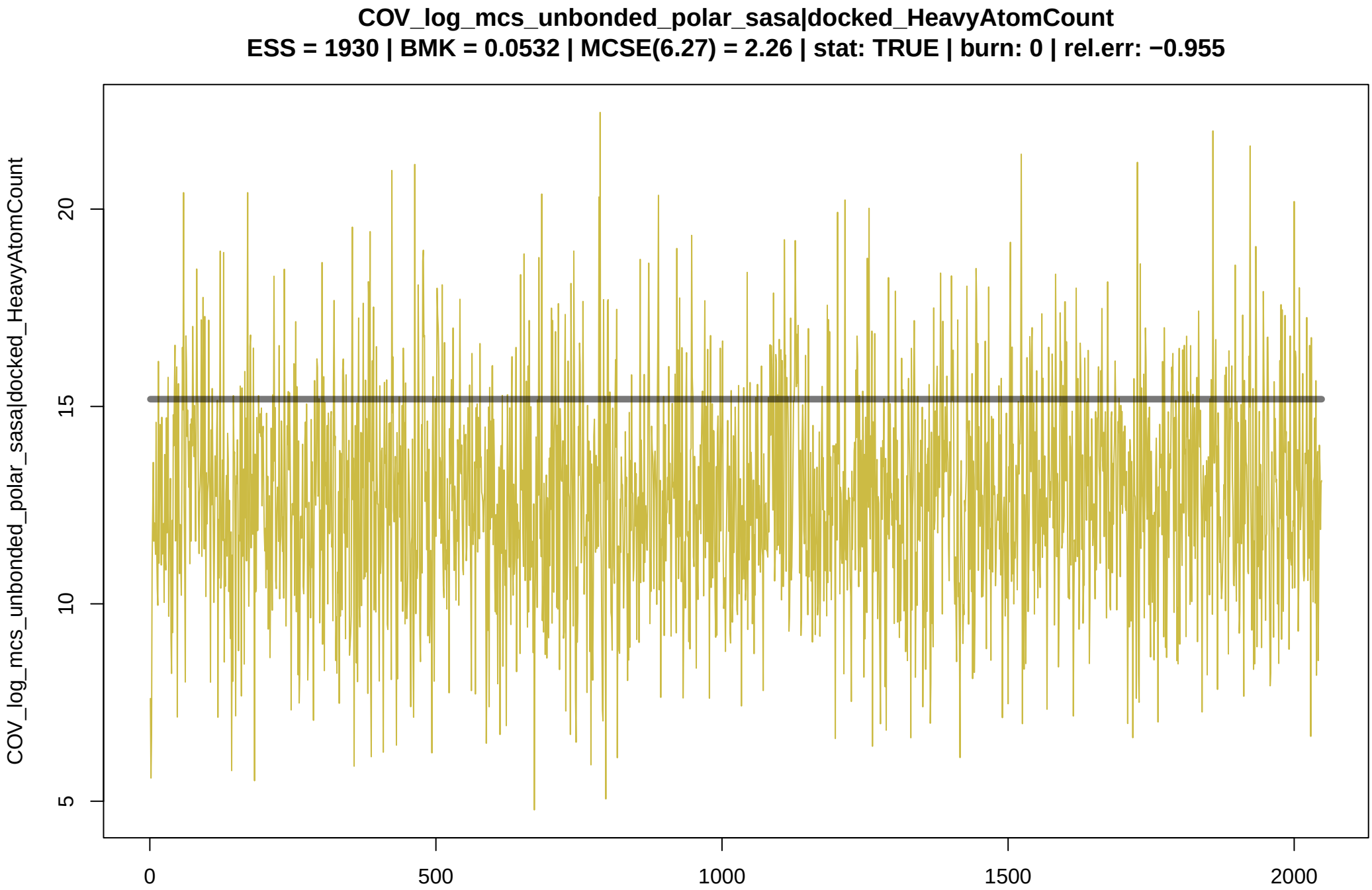

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0682 | MCSE(6.27) = 2.33 | stat: FALSE | burn: 0 | rel.err: 0.0874
VAR_docked_HeavyAtomCount
6.3
6.4
6.5
6.6
6.7
6.8
6.9
0
500
1000
1500
2000

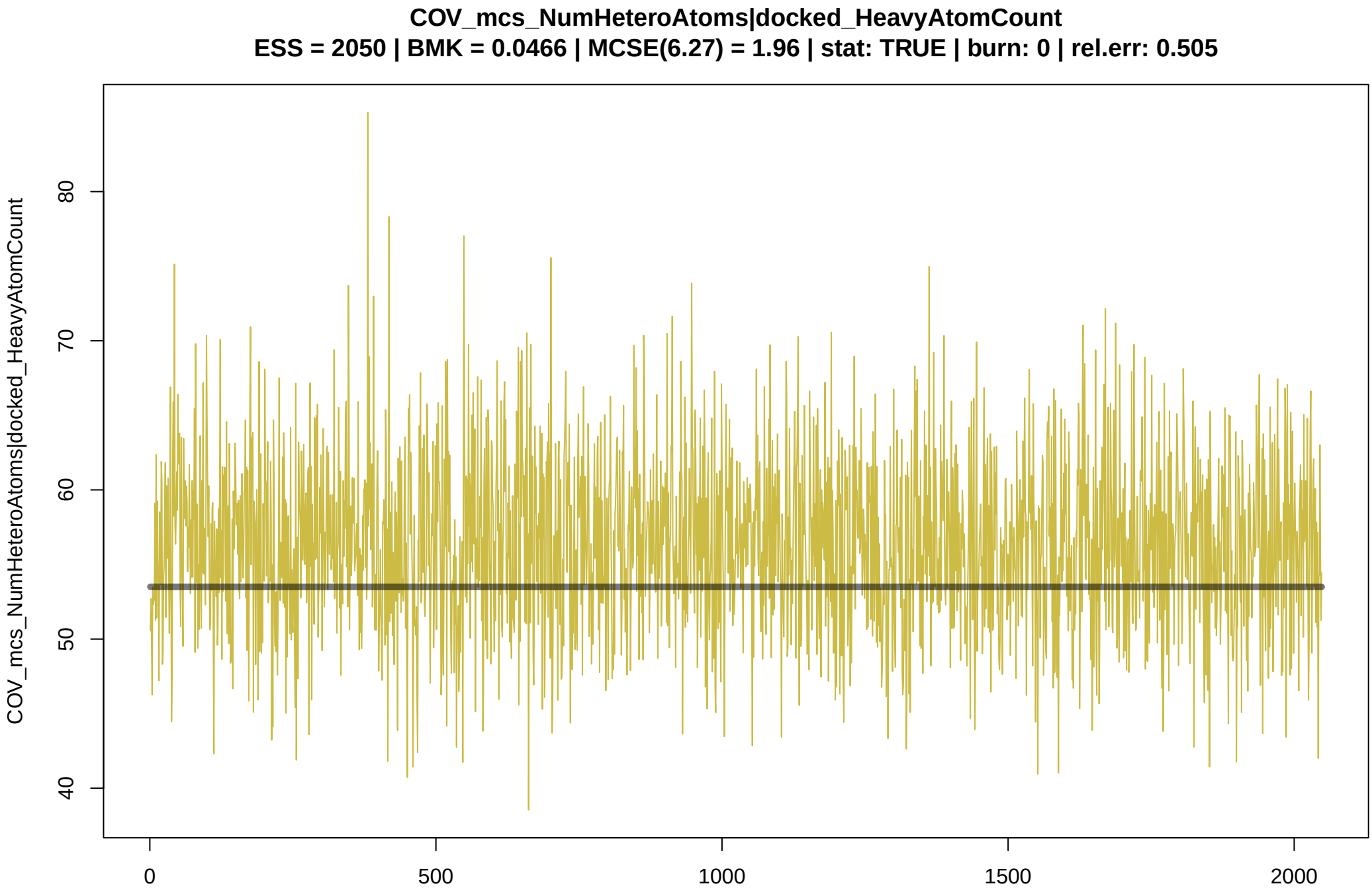

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1840 | BMK = 0.0583 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: 0.462
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.2
−0.4
−0.6
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1830 | BMK = 0.0381 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: −1.61
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.5
−2.0
−2.5
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0397 | MCSE(6.27) = 2.37 | stat: TRUE | burn: 0 | rel.err: −1.76
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 = 2050 | BMK = 0.0616 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0 | rel.err: −0.478
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.0
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 = 1930 | BMK = 0.0532 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: −0.955
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 = 0.0466 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0 | rel.err: 0.505
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
80
0
500
1000
1500
2000