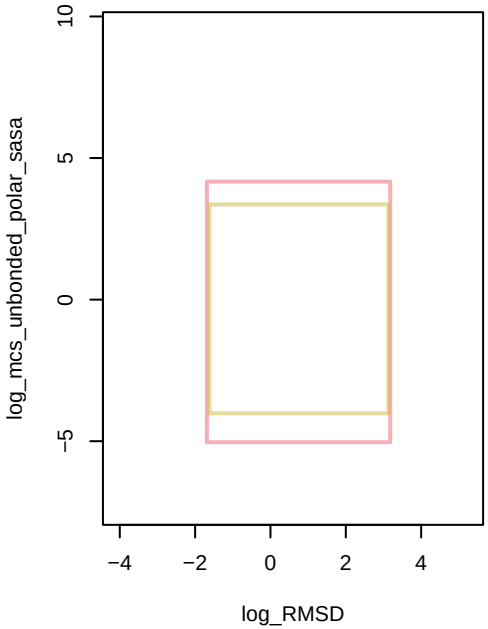
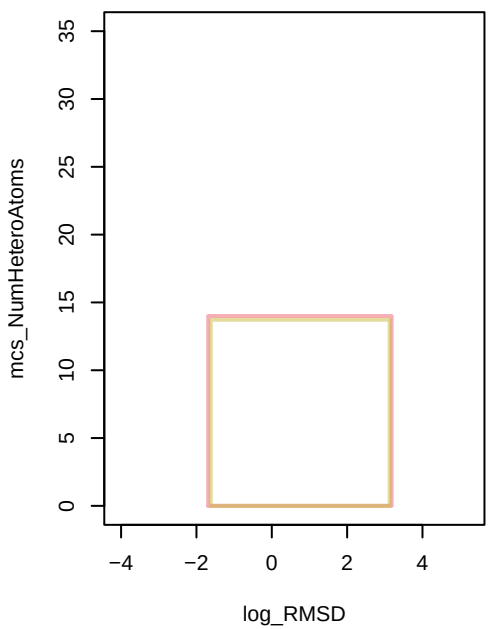
−− STATS maxD −−
min ESS = 63.6909016429014
max BMK = 0.138739970312971
max MCSE = 8.47586198892777
all stationary: FALSE
burn: 0
max rel.err.: 2.0669417344909

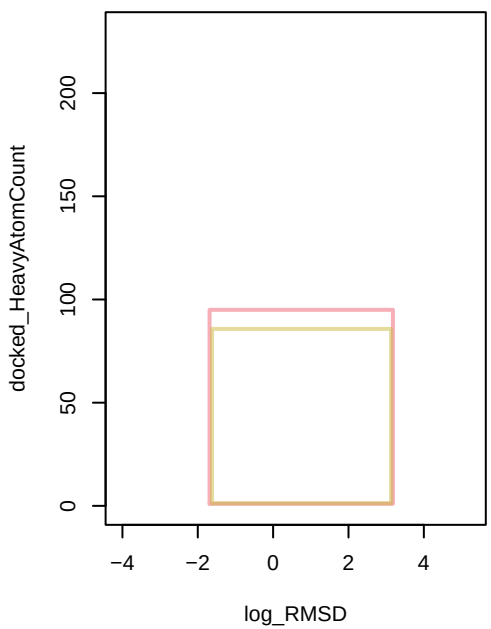
−− STATS 2D −−
min ESS = 1823.14009576795
max BMK = 0.048781591330 1106
max MCSE = 2.57509349440817
all stationary: FALSE
burn: 0
max rel.err.: 1.77754502973996

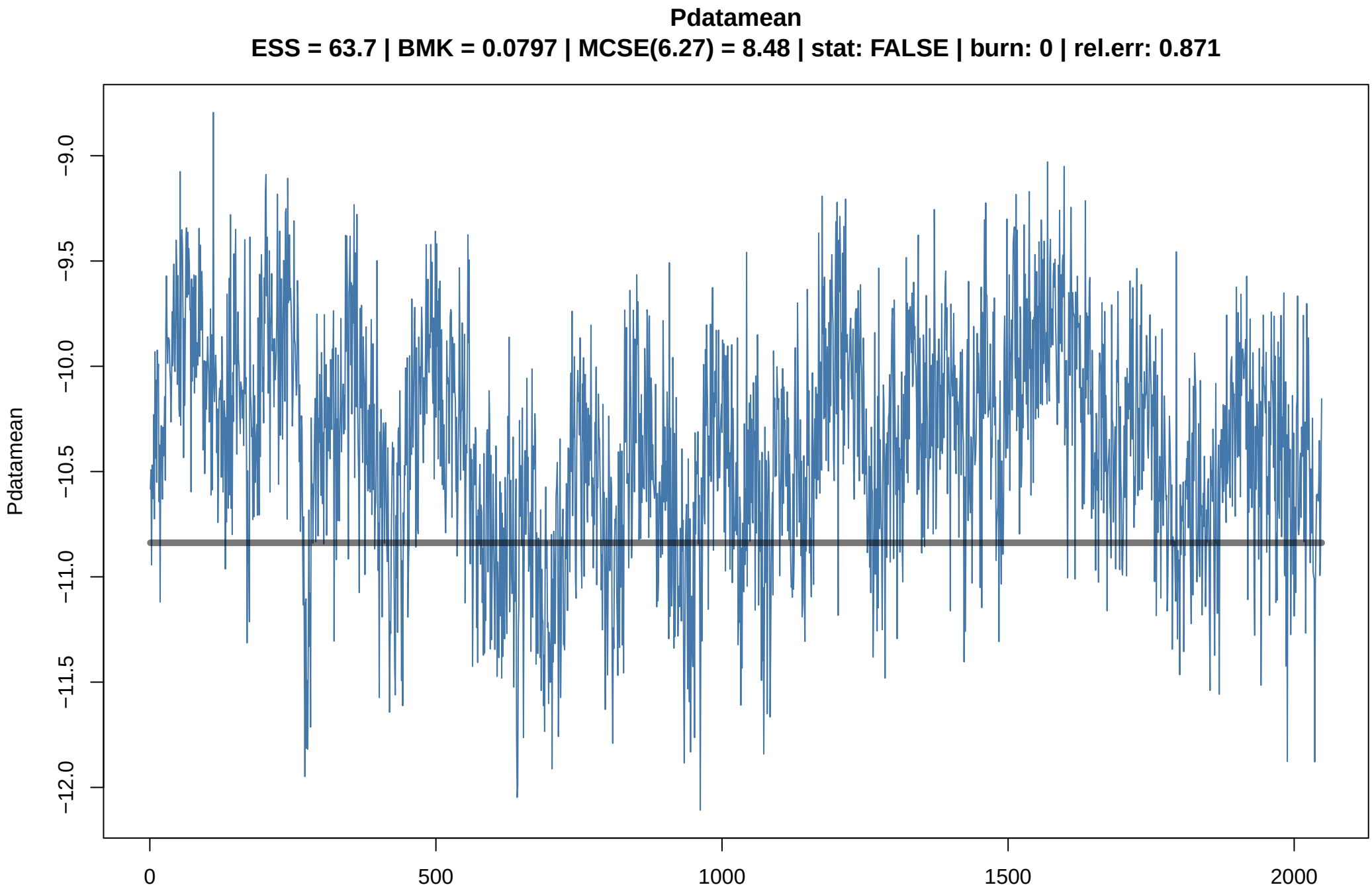
−− STATS 1D −−
min ESS = 1553.62266921442
max BMK = 0.059449153161 1276
max MCSE = 2.73504896257873
all stationary: TRUE
burn: 0
max rel.err.: 2.29113416386708

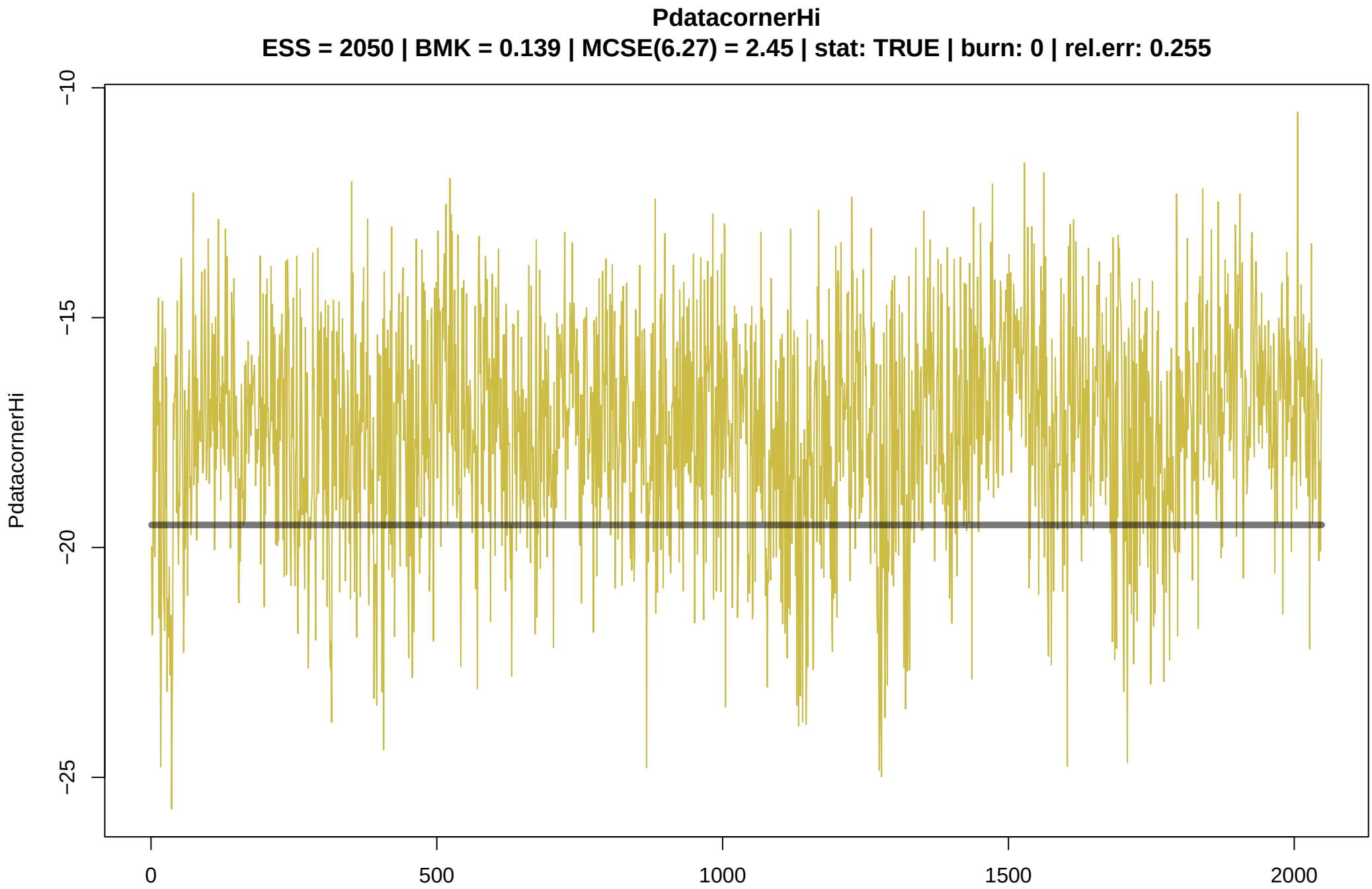
Occupied clusters: 11 of 16

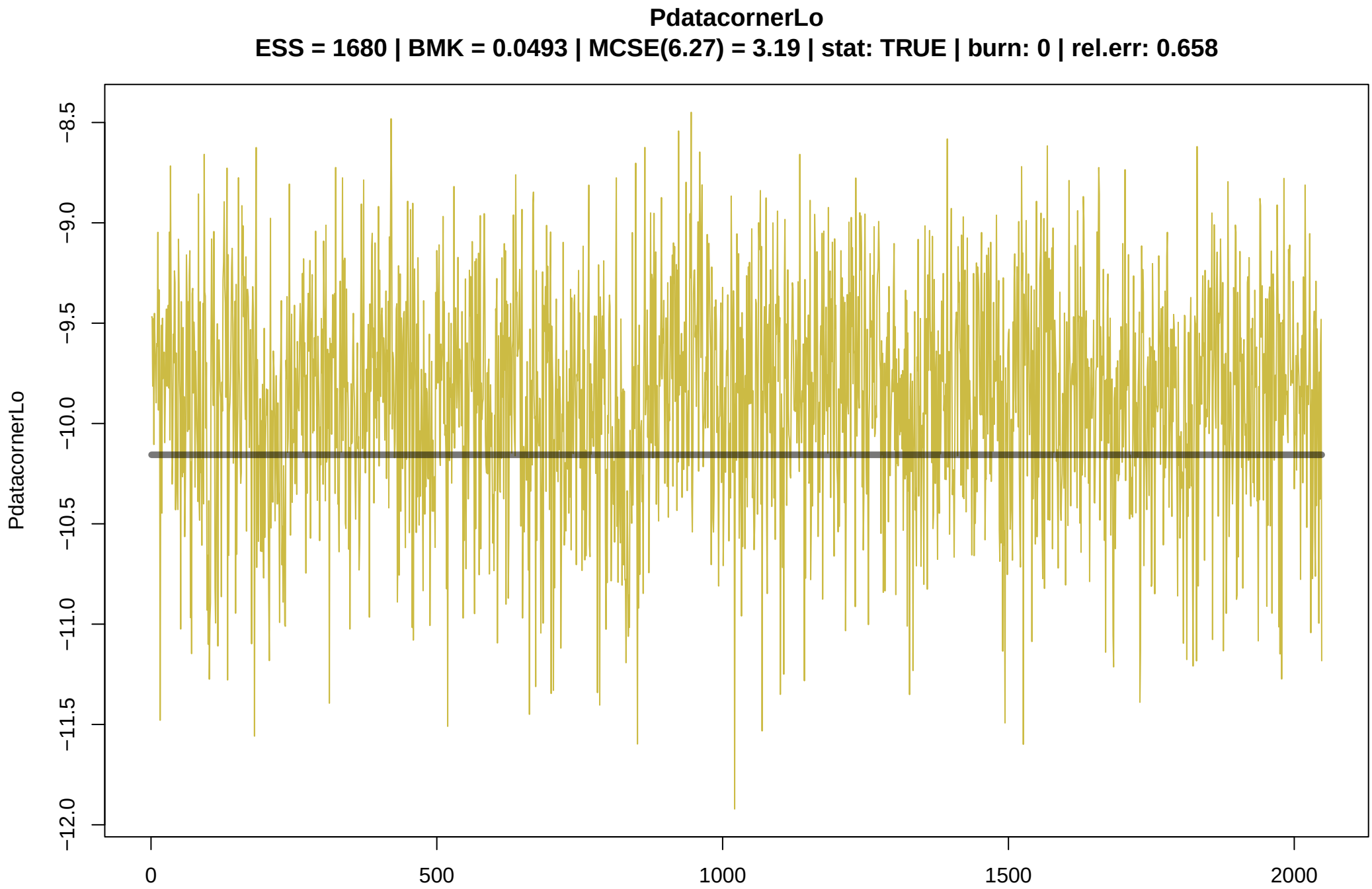

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
log_RMSD

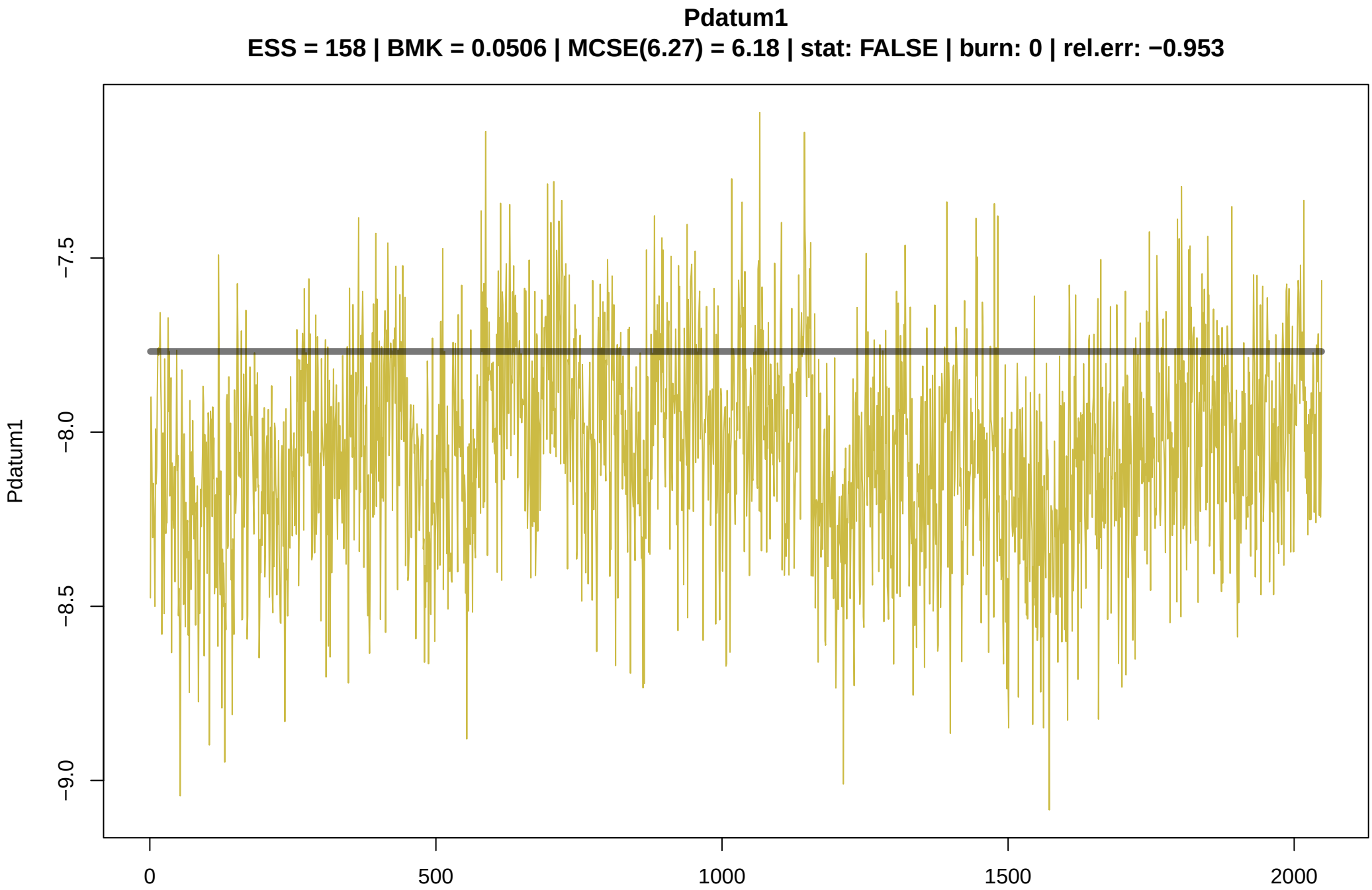

mcs_NumHeteroAtoms
35
30
25
20
15
10
5
0
−4
−2
0
2
4
log_RMSD

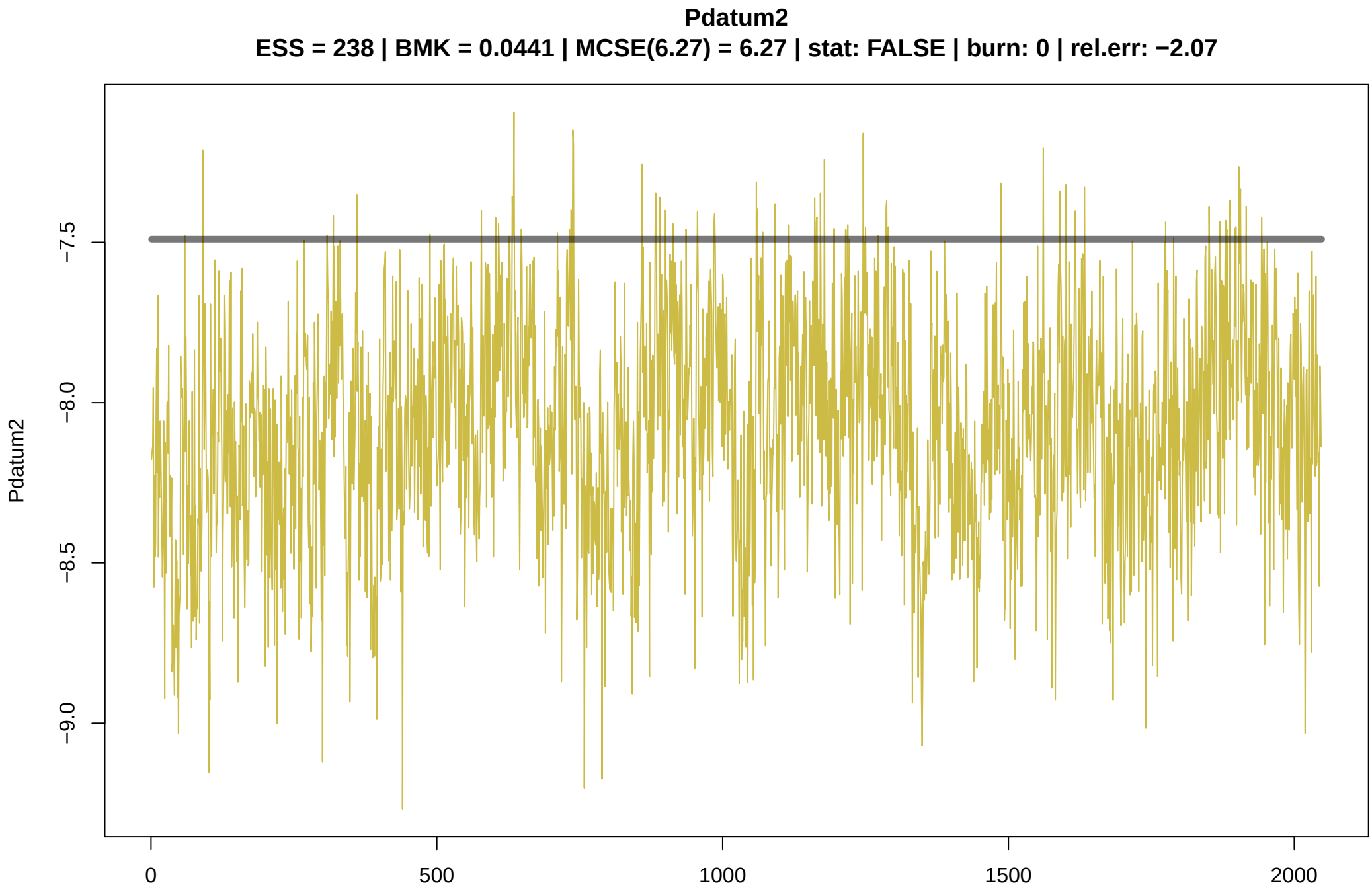

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
log_RMSD

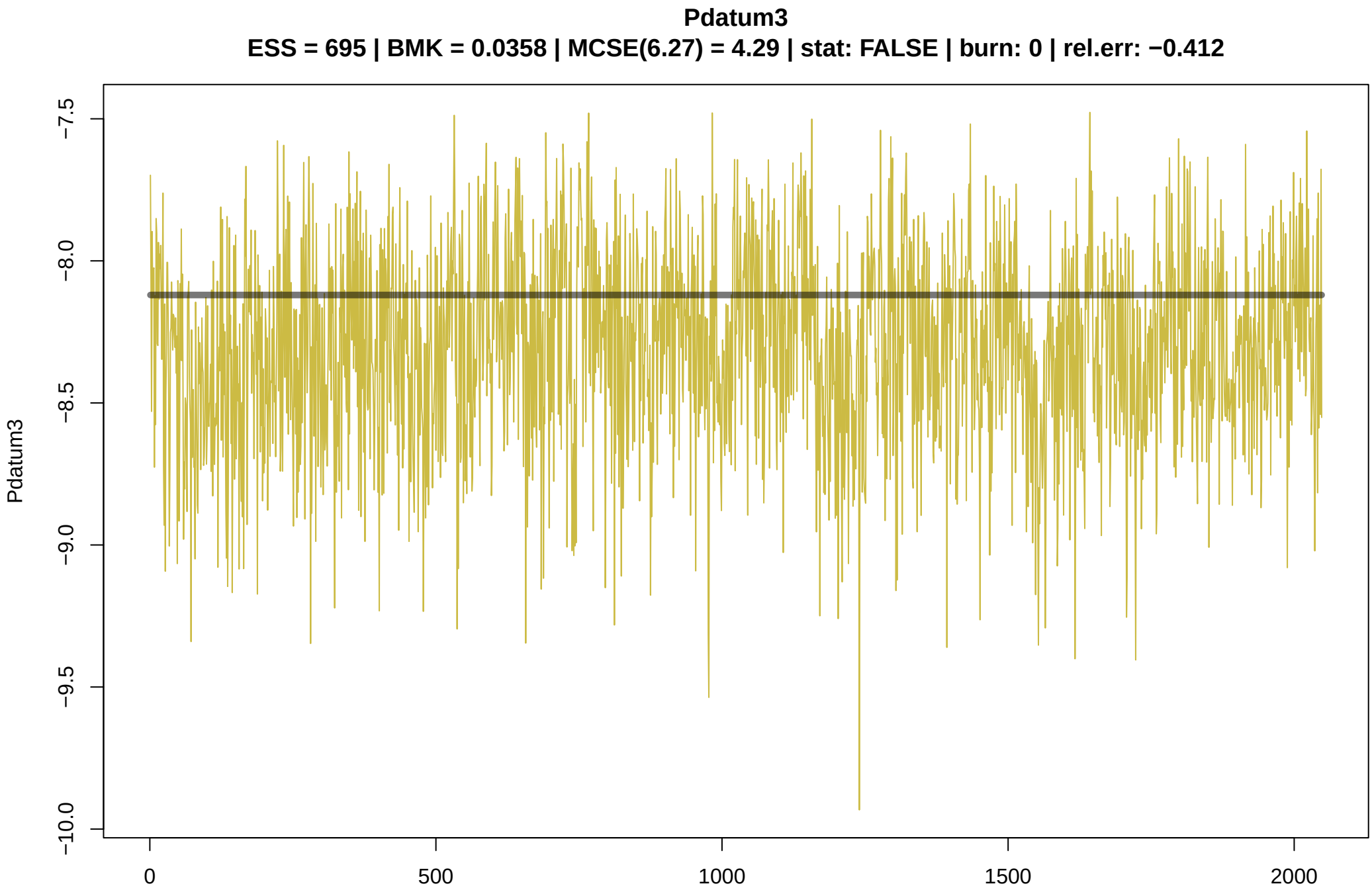

Pdatamean
ESS = 63.7 | BMK = 0.0797 | MCSE(6.27) = 8.48 | stat: FALSE | burn: 0 | rel.err: 0.871
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

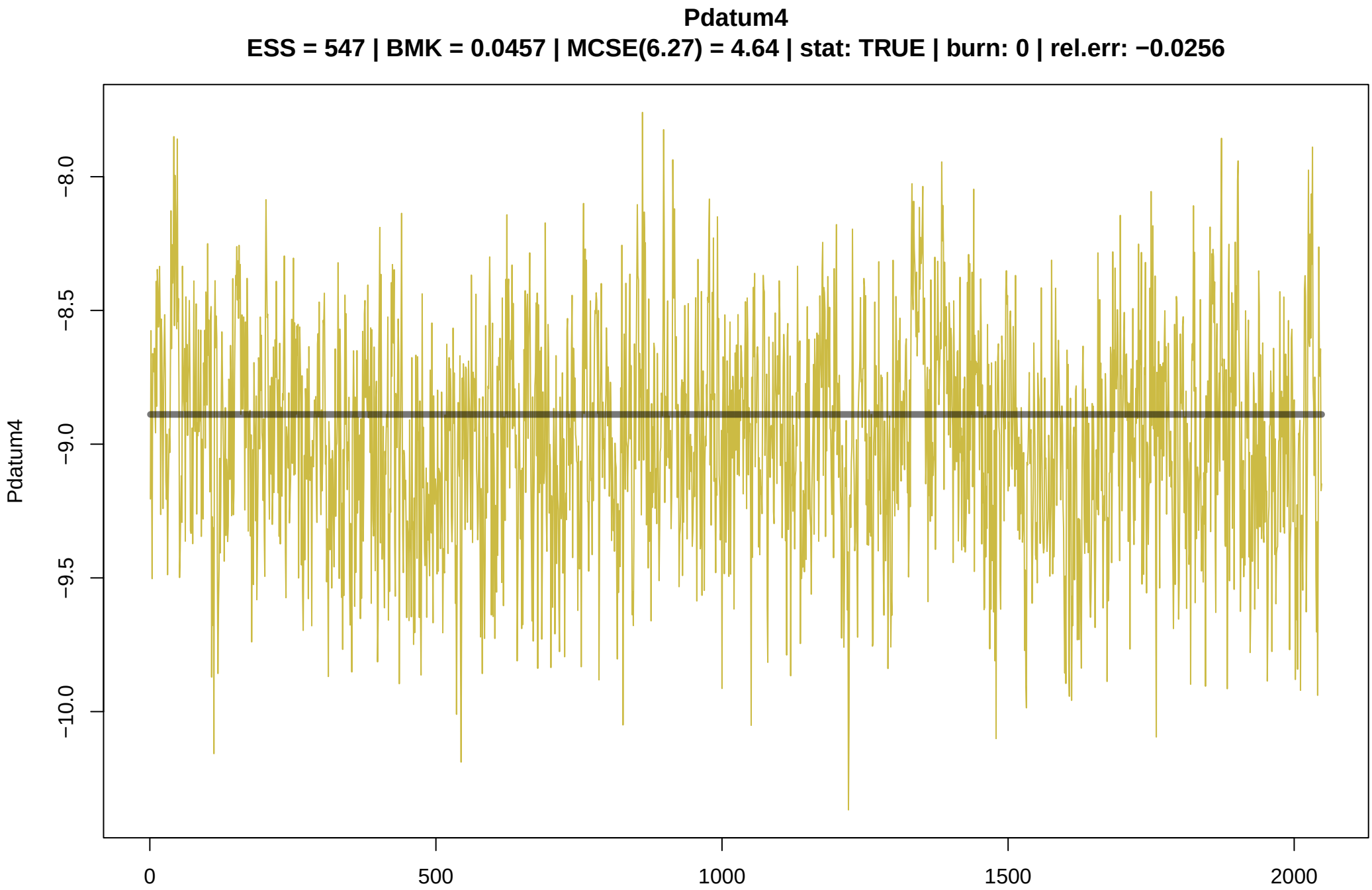

PdatacornerHi
ESS = 2050 | BMK = 0.139 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0 | rel.err: 0.255
PdatacornerHi
−10
−15
−20
−25
0
500
1000
1500
2000

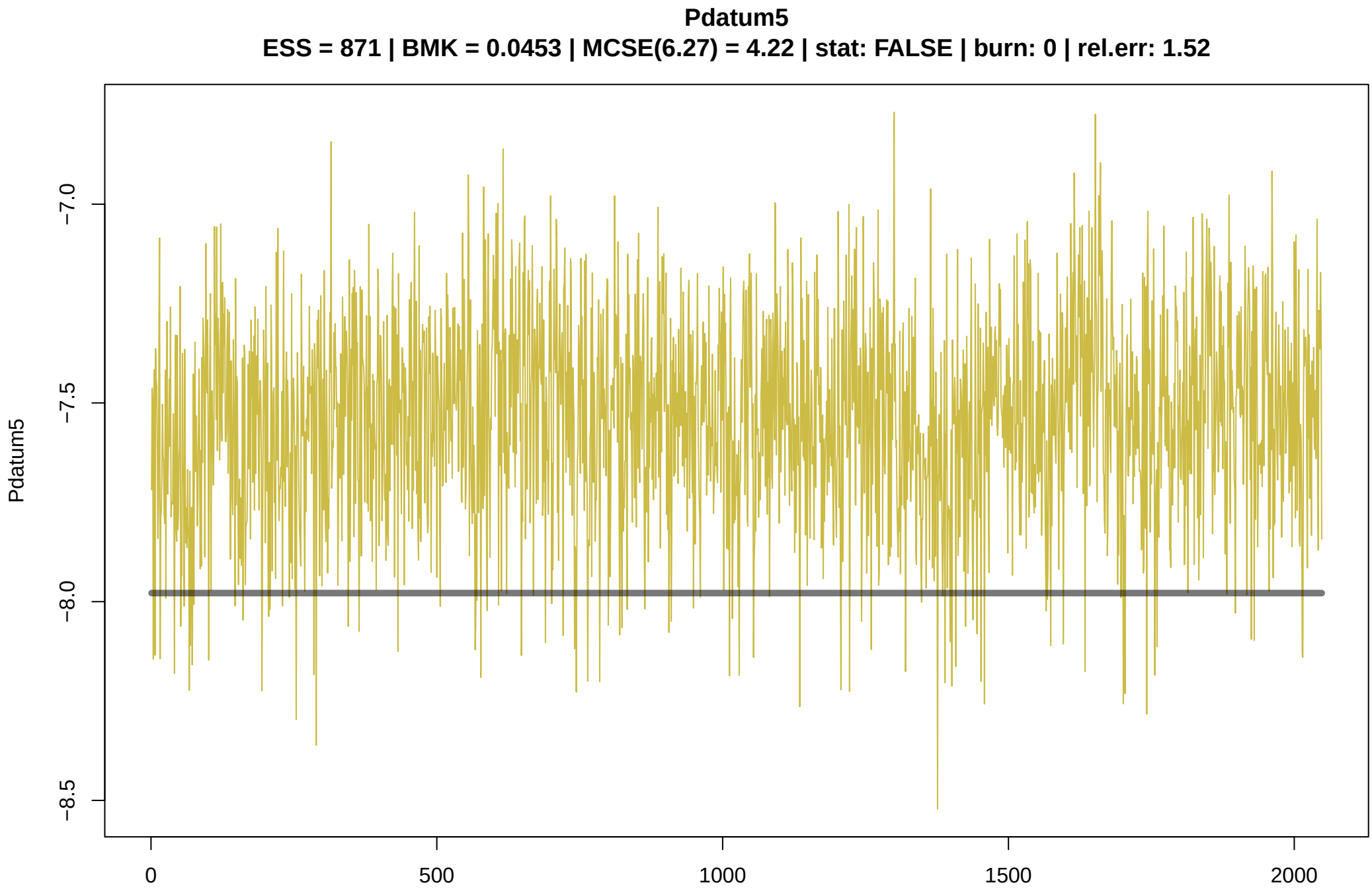

PdatacornerLo
ESS = 1680 | BMK = 0.0493 | MCSE(6.27) = 3.19 | stat: TRUE | burn: 0 | rel.err: 0.658
PdatacornerLo
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

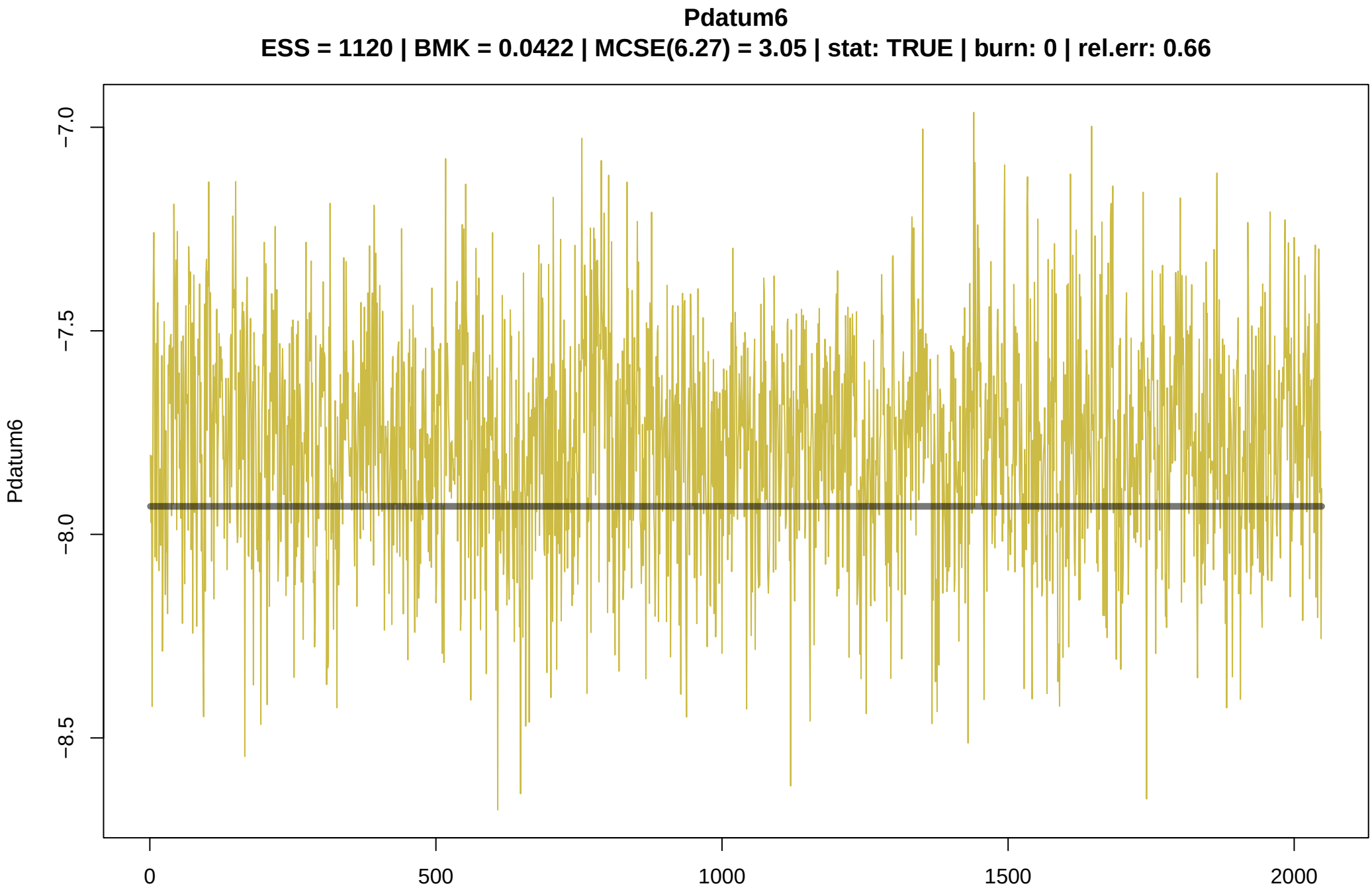

Pdatum1
ESS = 158 | BMK = 0.0506 | MCSE(6.27) = 6.18 | stat: FALSE | burn: 0 | rel.err: −0.953
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

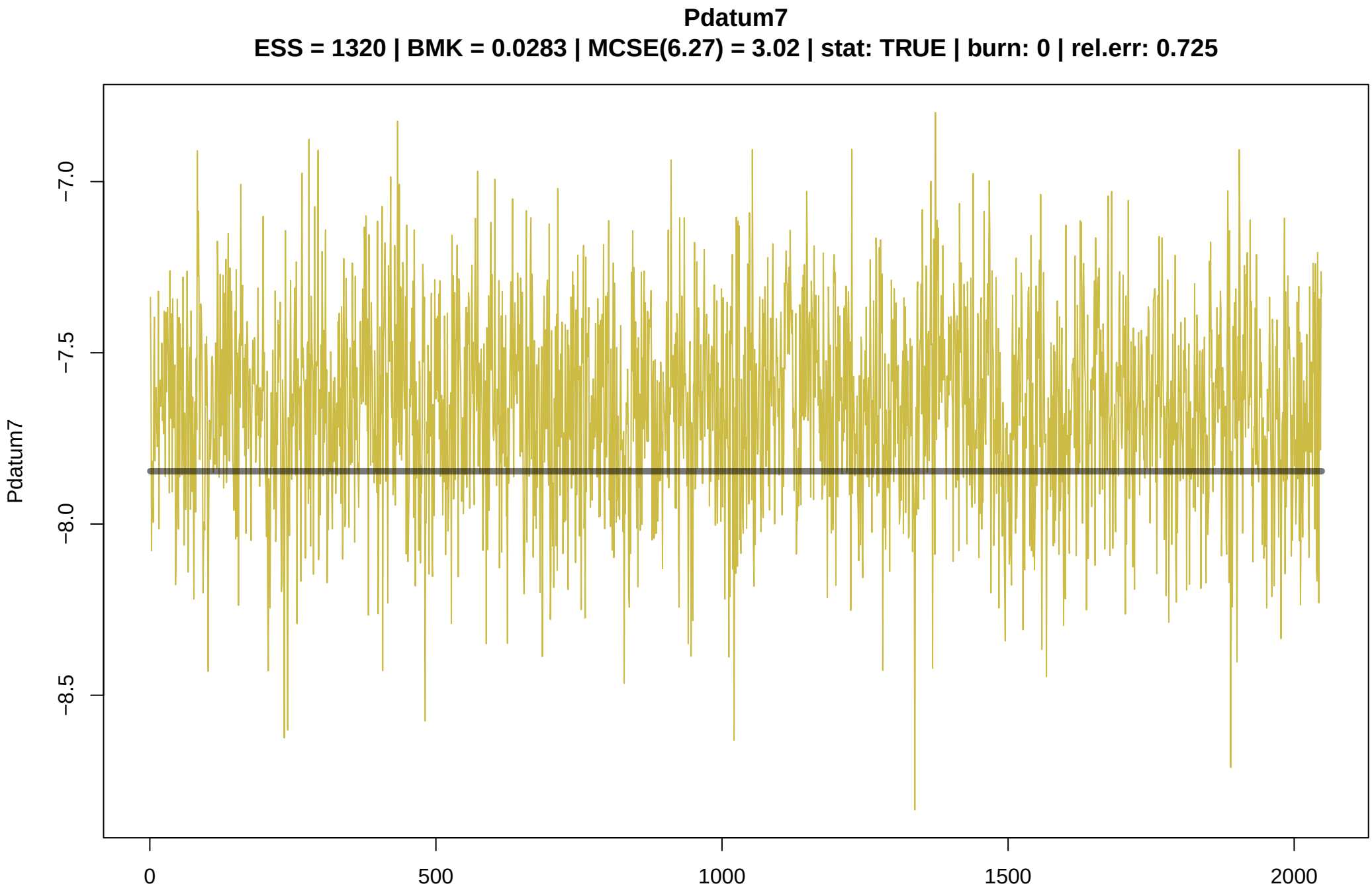

Pdatum2
ESS = 238 | BMK = 0.0441 | MCSE(6.27) = 6.27 | stat: FALSE | burn: 0 | rel.err: −2.07
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

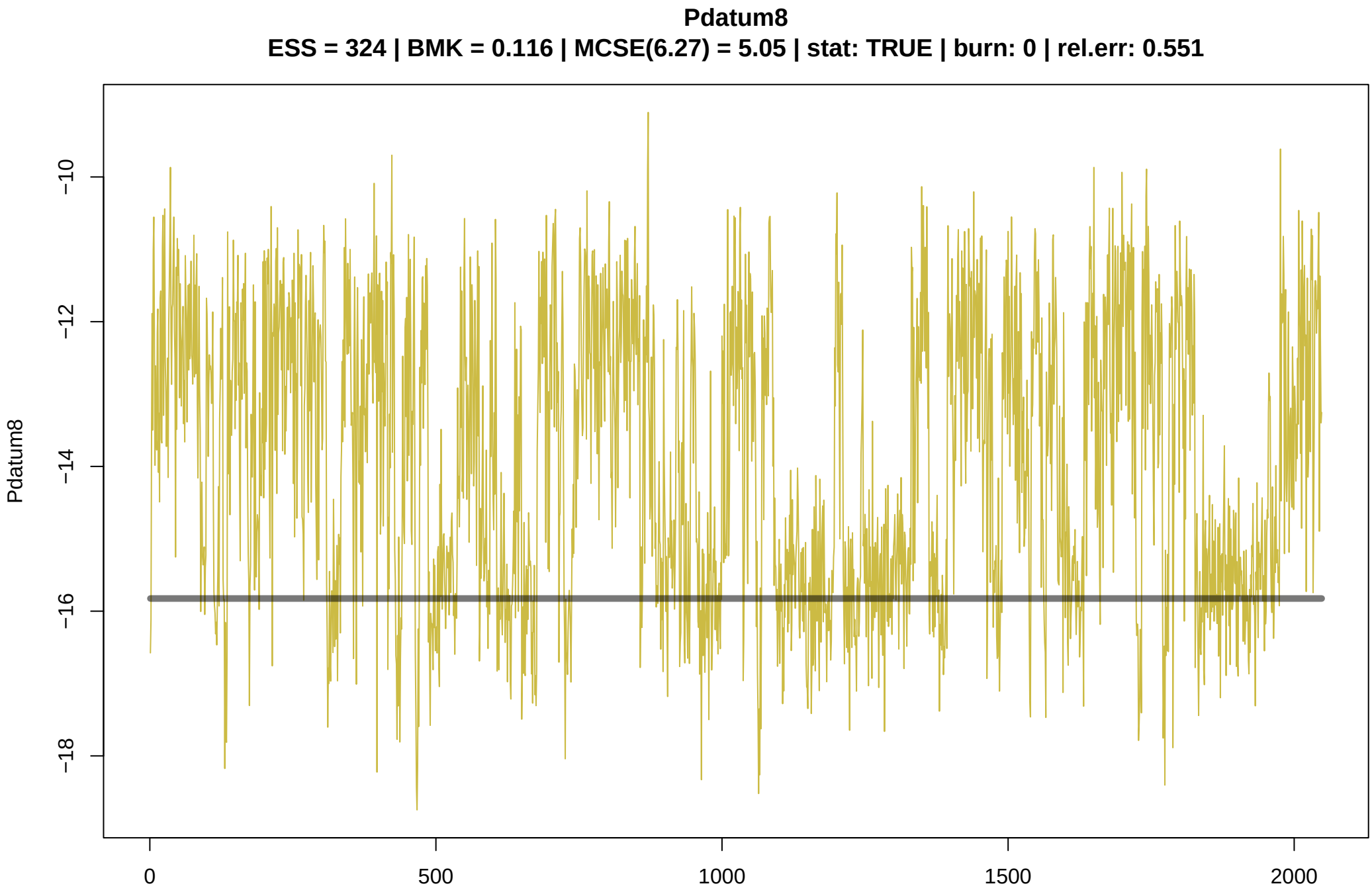

Pdatum3
ESS = 695 | BMK = 0.0358 | MCSE(6.27) = 4.29 | stat: FALSE | burn: 0 | rel.err: −0.412
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

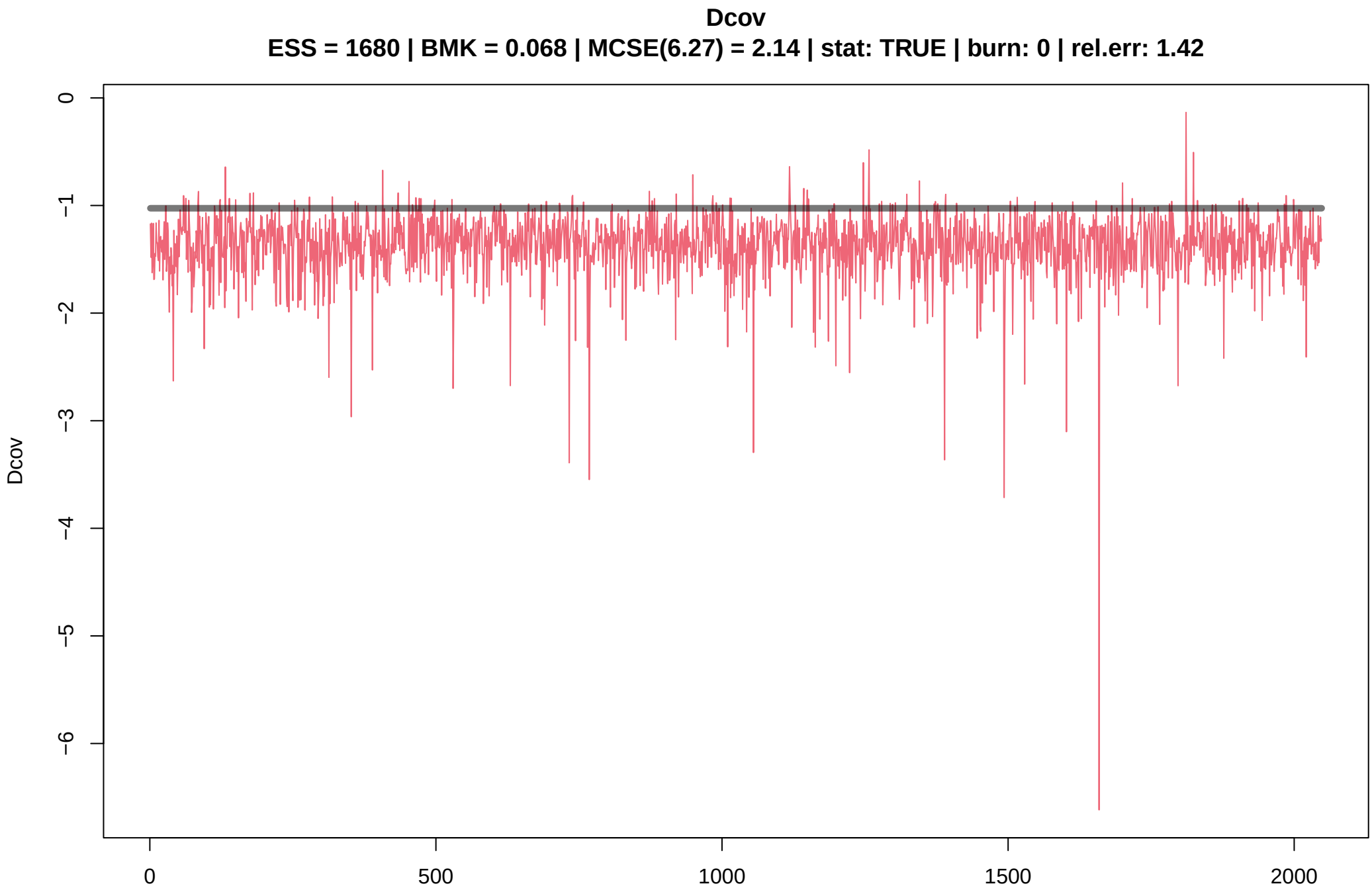

Pdatum4
ESS = 547 | BMK = 0.0457 | MCSE(6.27) = 4.64 | stat: TRUE | burn: 0 | rel.err: −0.0256
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

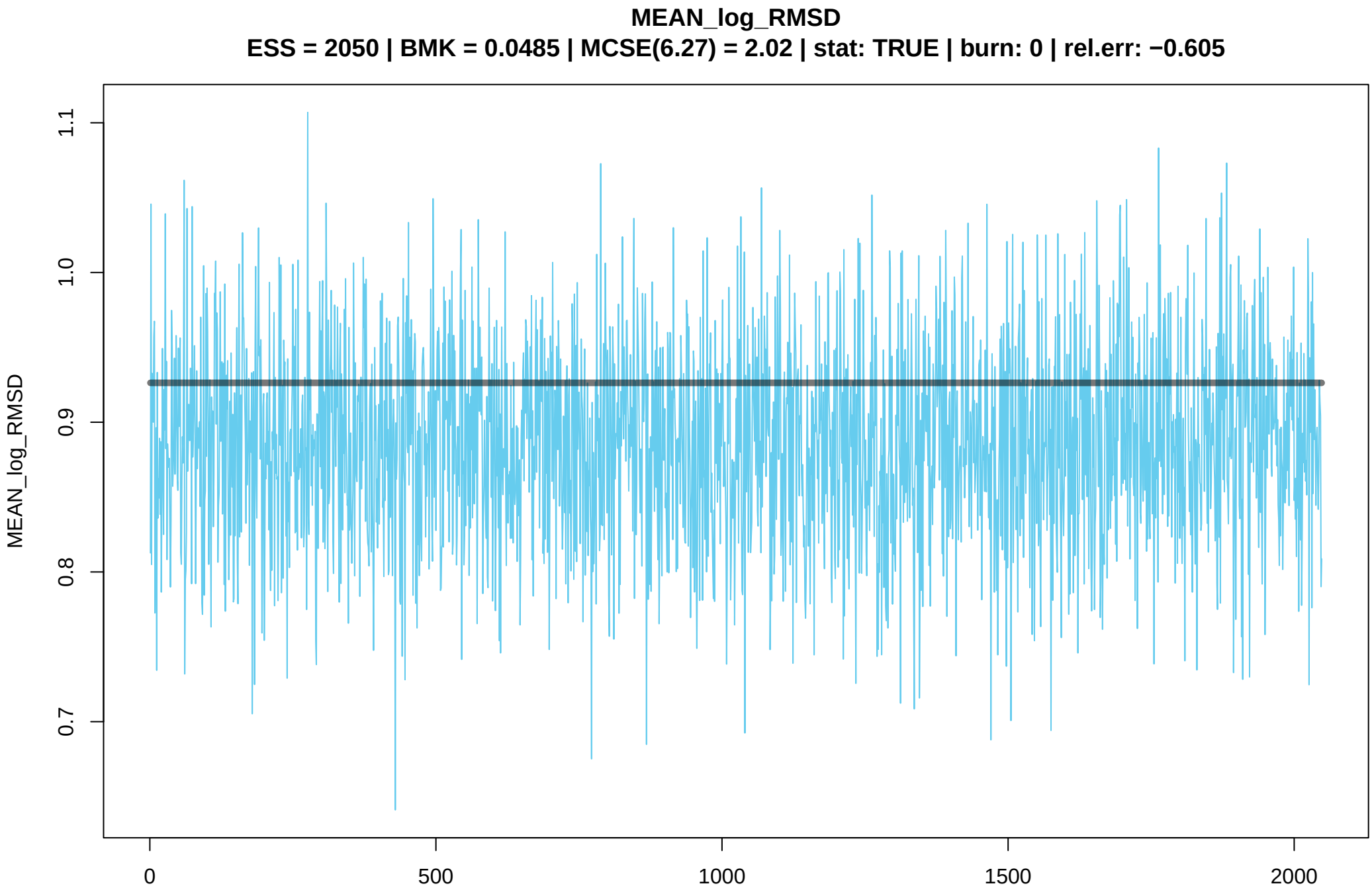

Pdatum5
ESS = 871 | BMK = 0.0453 | MCSE(6.27) = 4.22 | stat: FALSE | burn: 0 | rel.err: 1.52
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

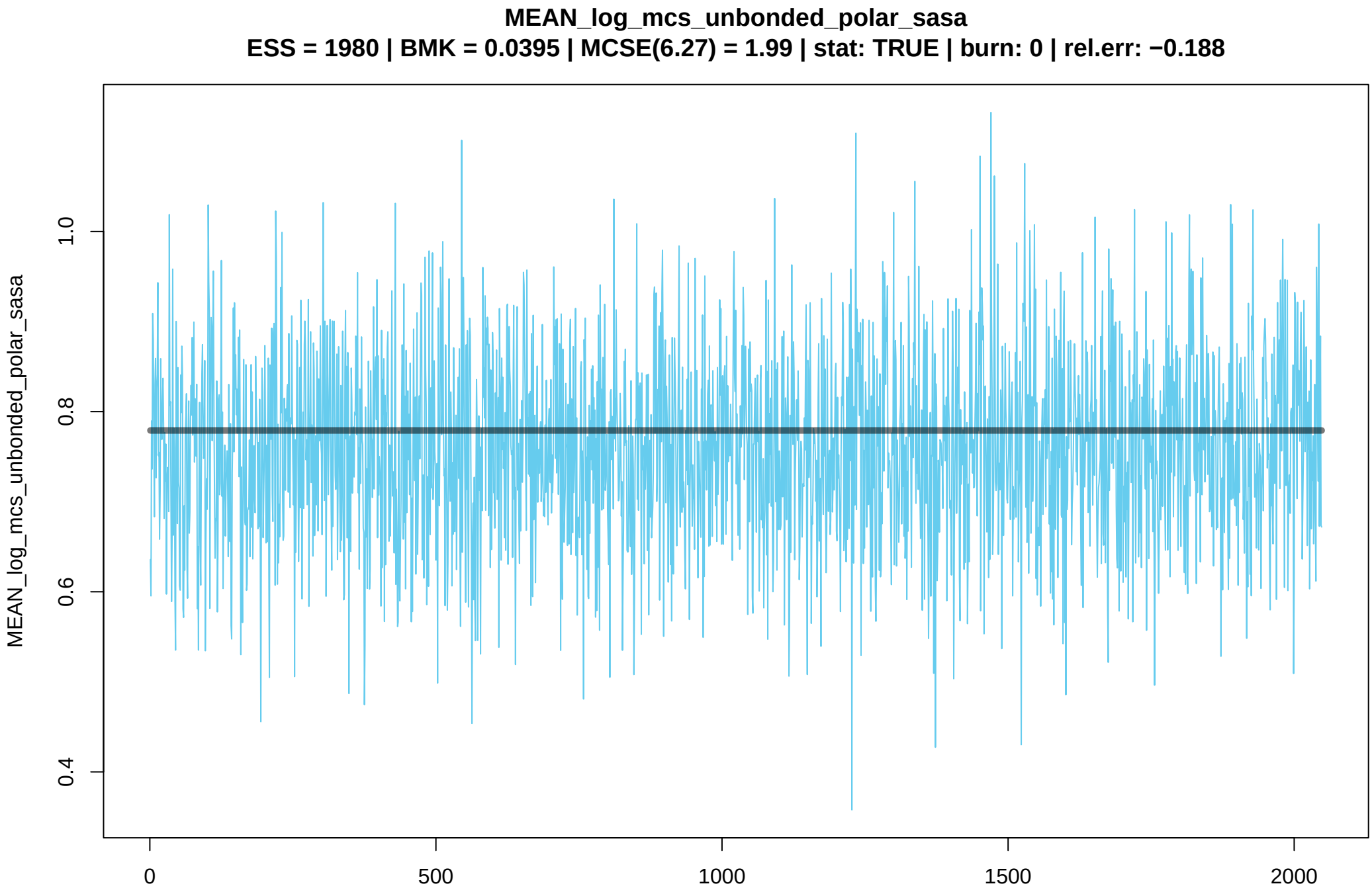

Pdatum6
ESS = 1120 | BMK = 0.0422 | MCSE(6.27) = 3.05 | stat: TRUE | burn: 0 | rel.err: 0.66
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

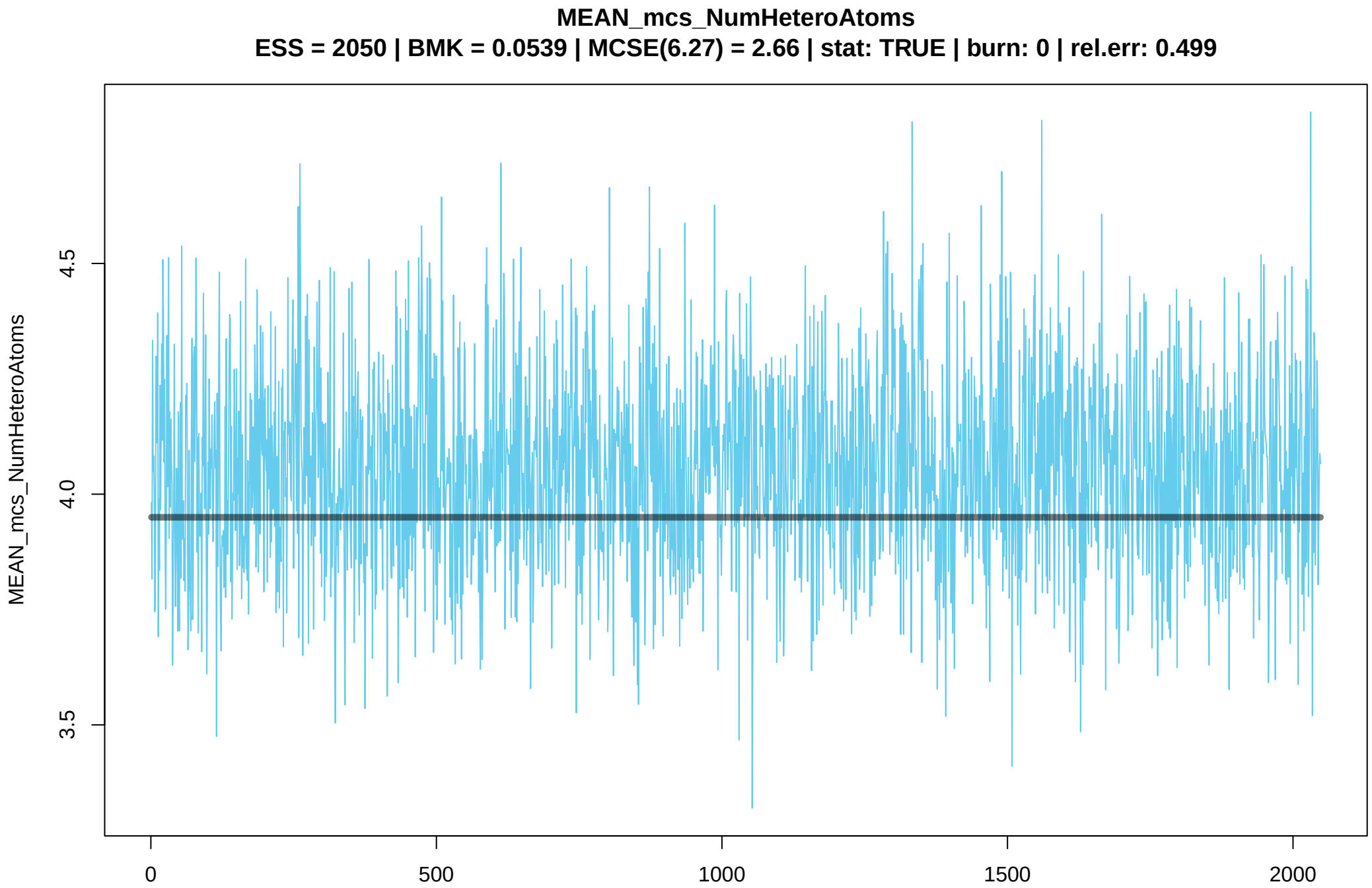

Pdatum7
ESS = 1320 | BMK = 0.0283 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0 | rel.err: 0.725
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

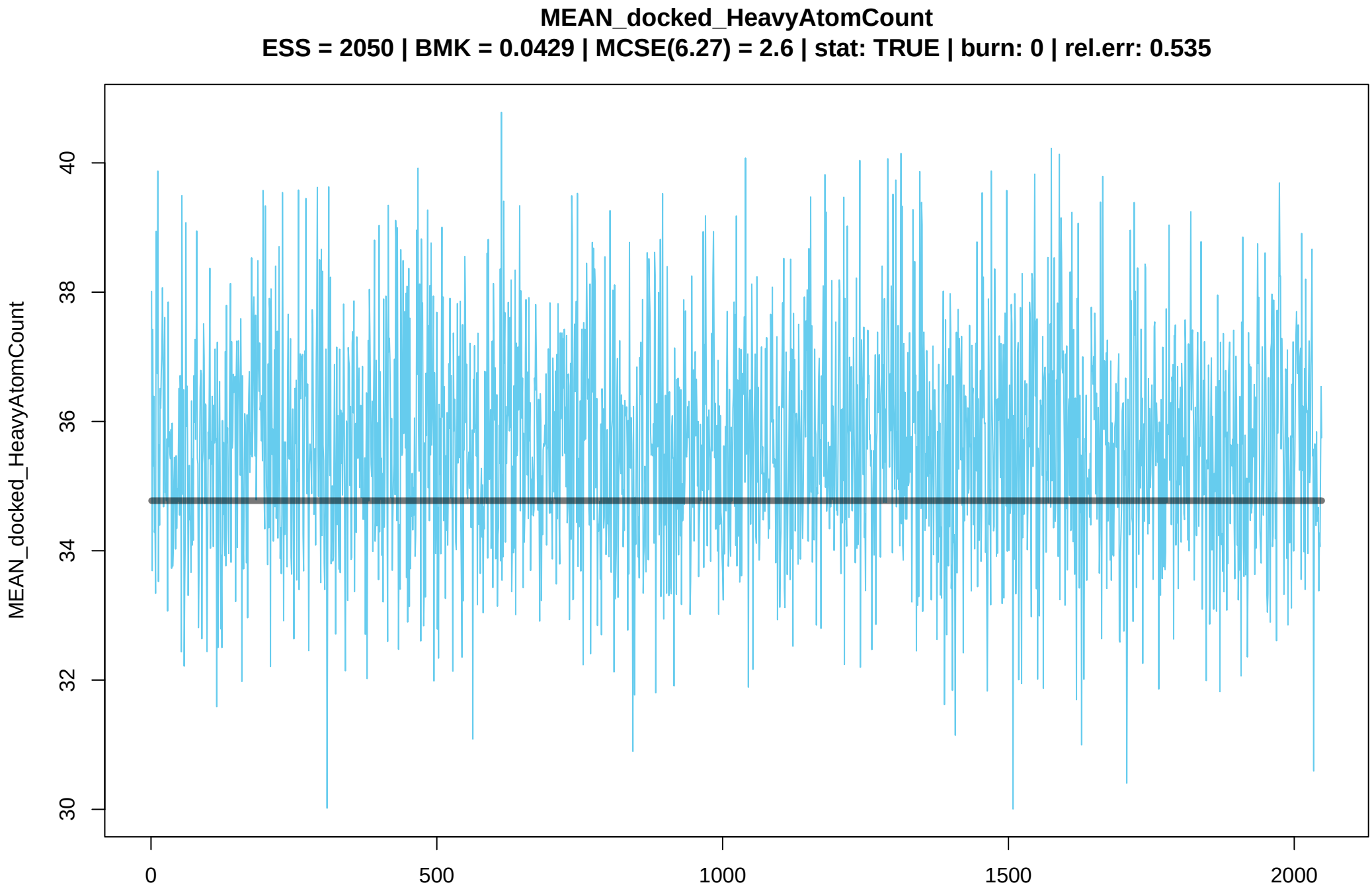

Pdatum8
ESS = 324 | BMK = 0.116 | MCSE(6.27) = 5.05 | stat: TRUE | burn: 0 | rel.err: 0.551
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

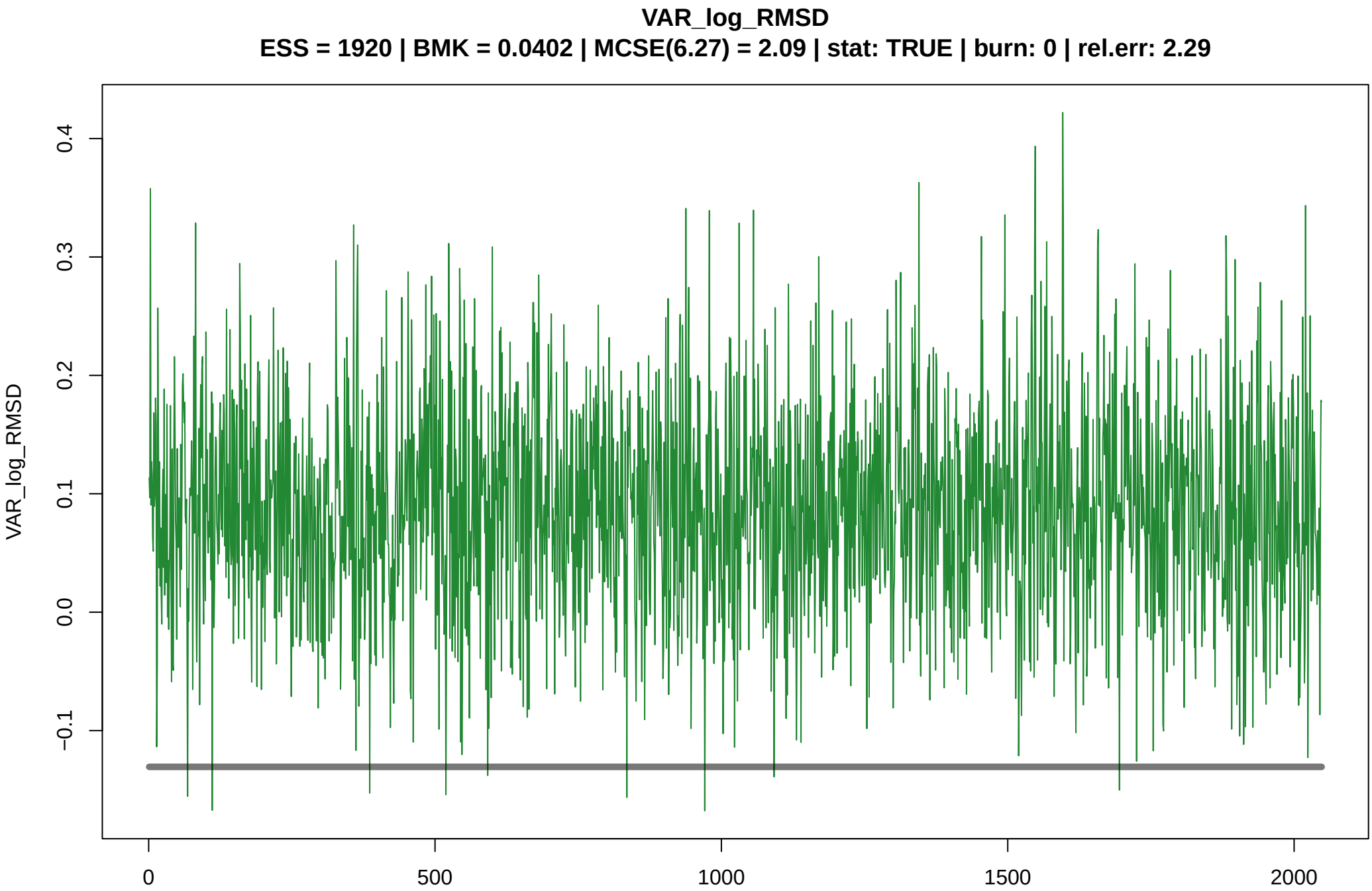

Dcov
ESS = 1680 | BMK = 0.068 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 1.42
Dcov
0
−1
−2
−3
−4
−5
−6
0
500
1000
1500
2000

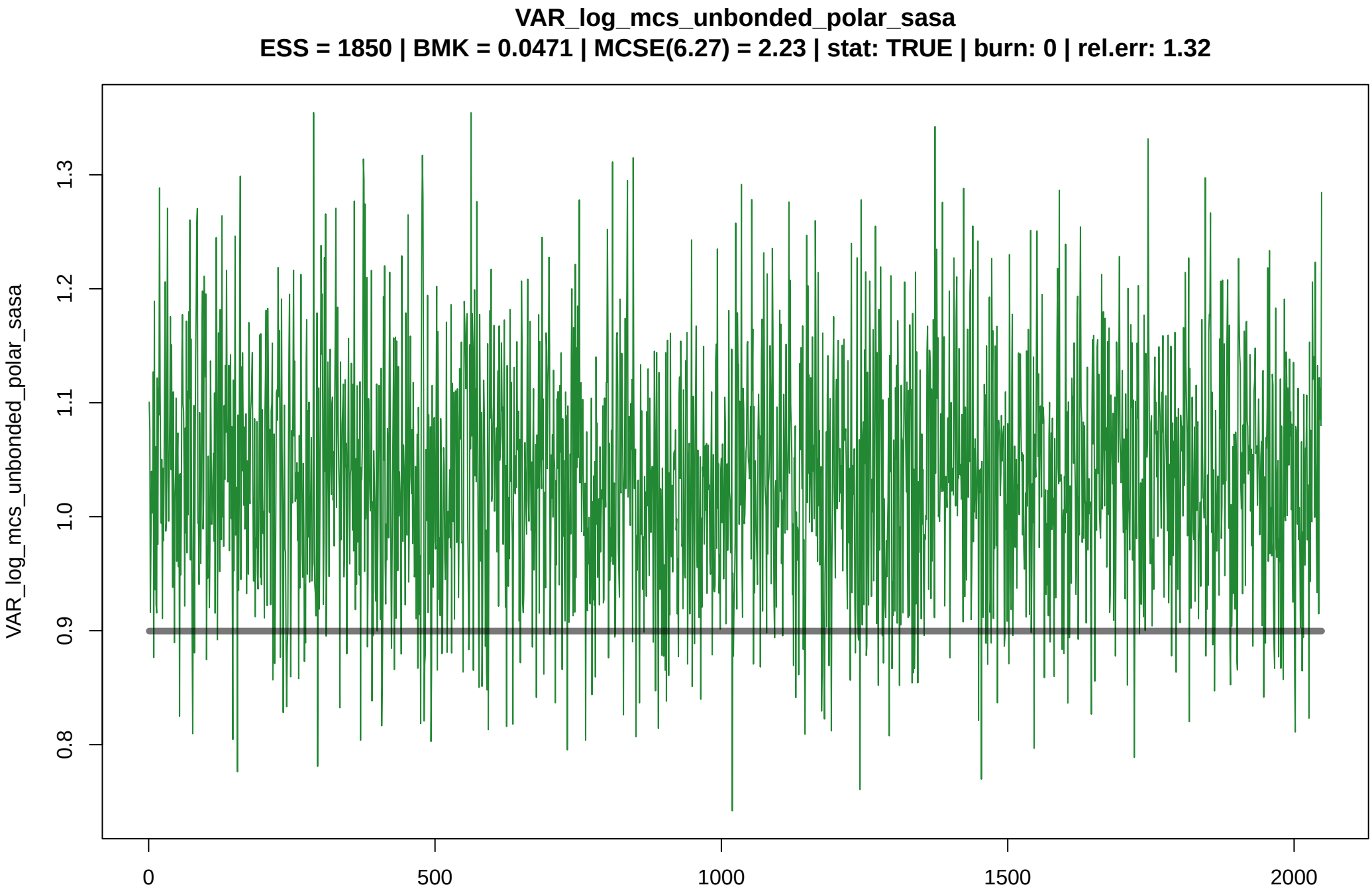

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0485 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0 | rel.err: −0.605
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

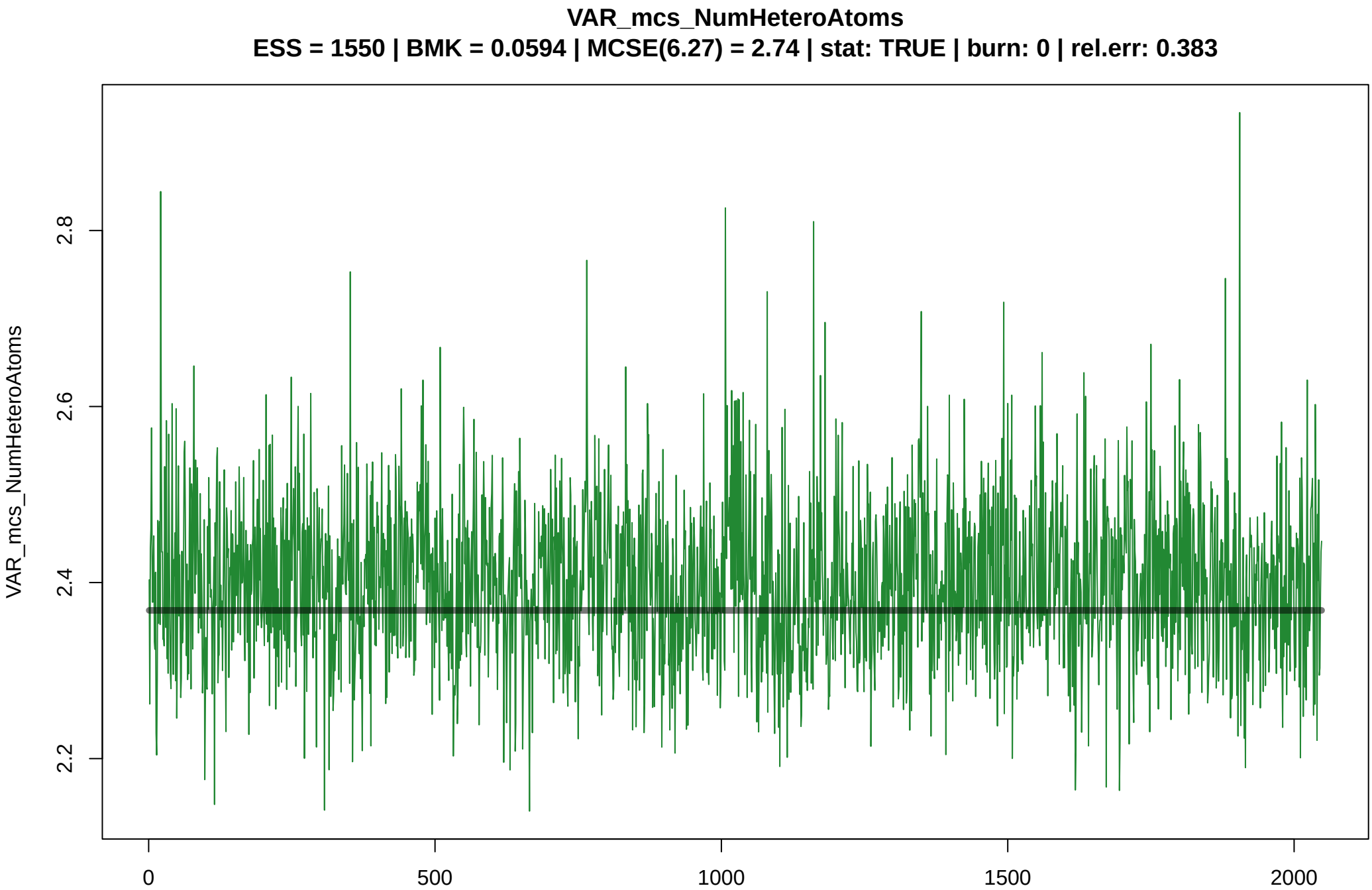

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1980 | BMK = 0.0395 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: −0.188
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

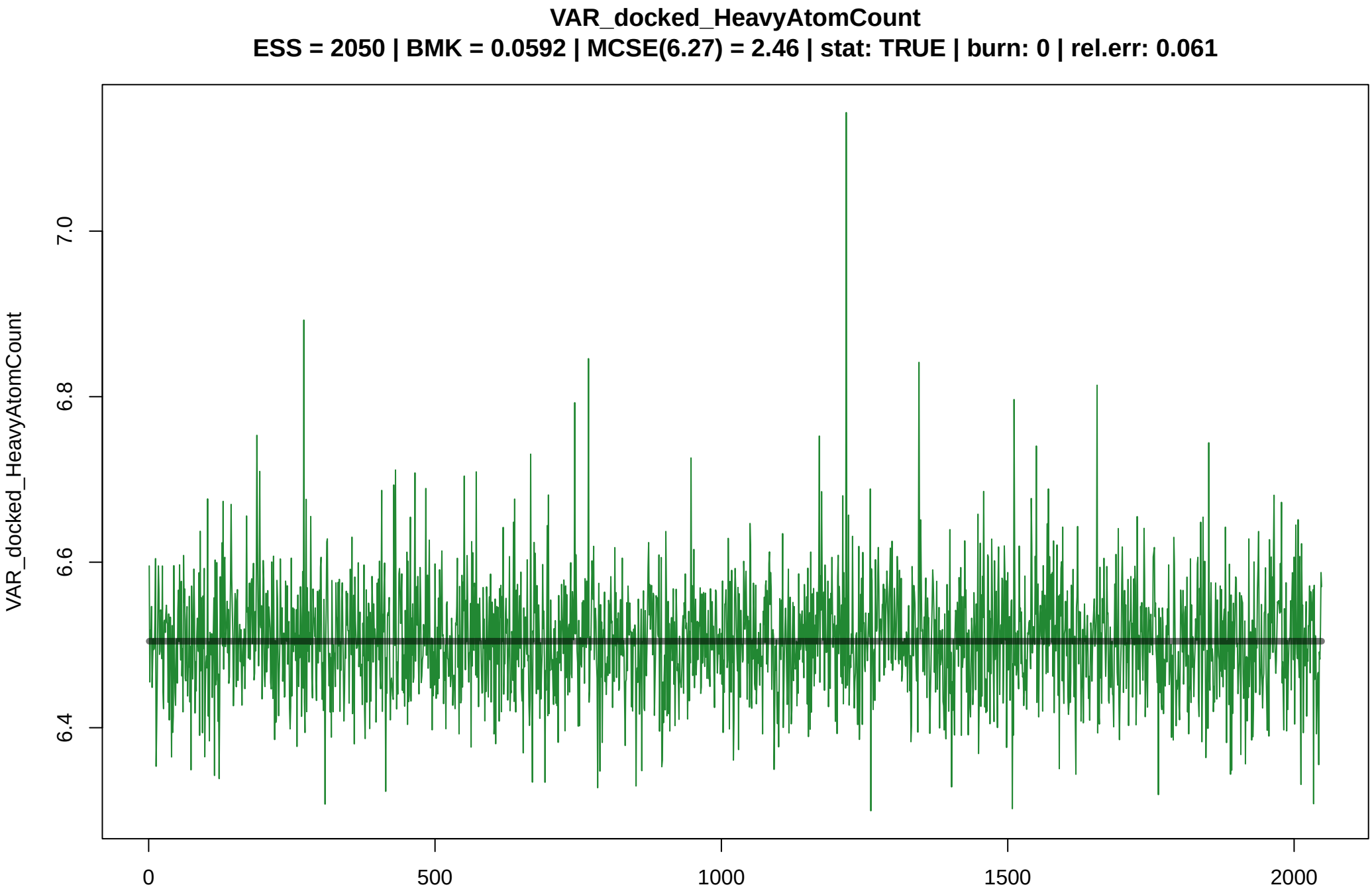

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0539 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | rel.err: 0.499
MEAN_mcs_NumHeteroAtoms
4.5
4.0
3.5
0
500
1000
1500
2000

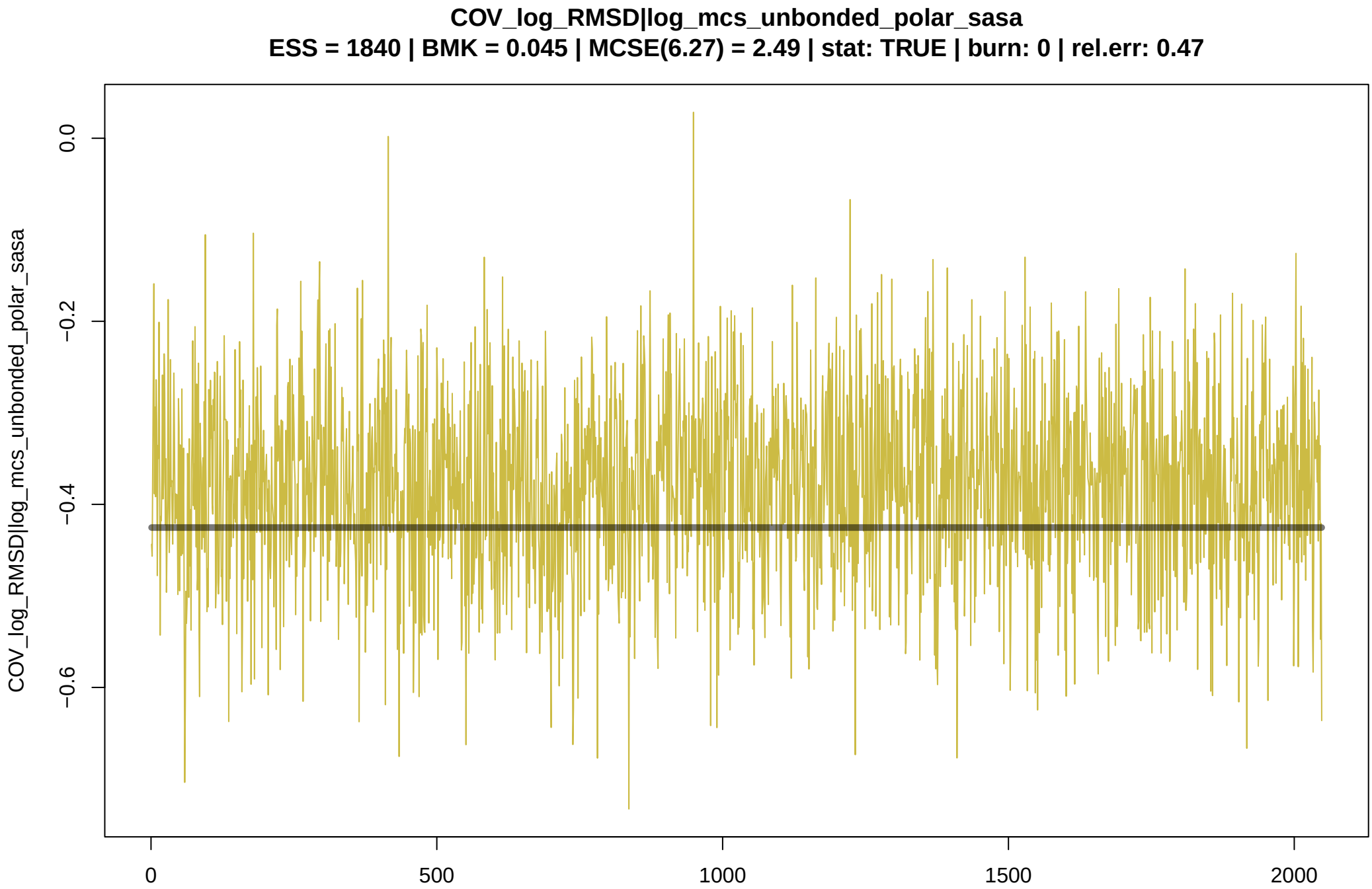

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0429 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 0.535
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

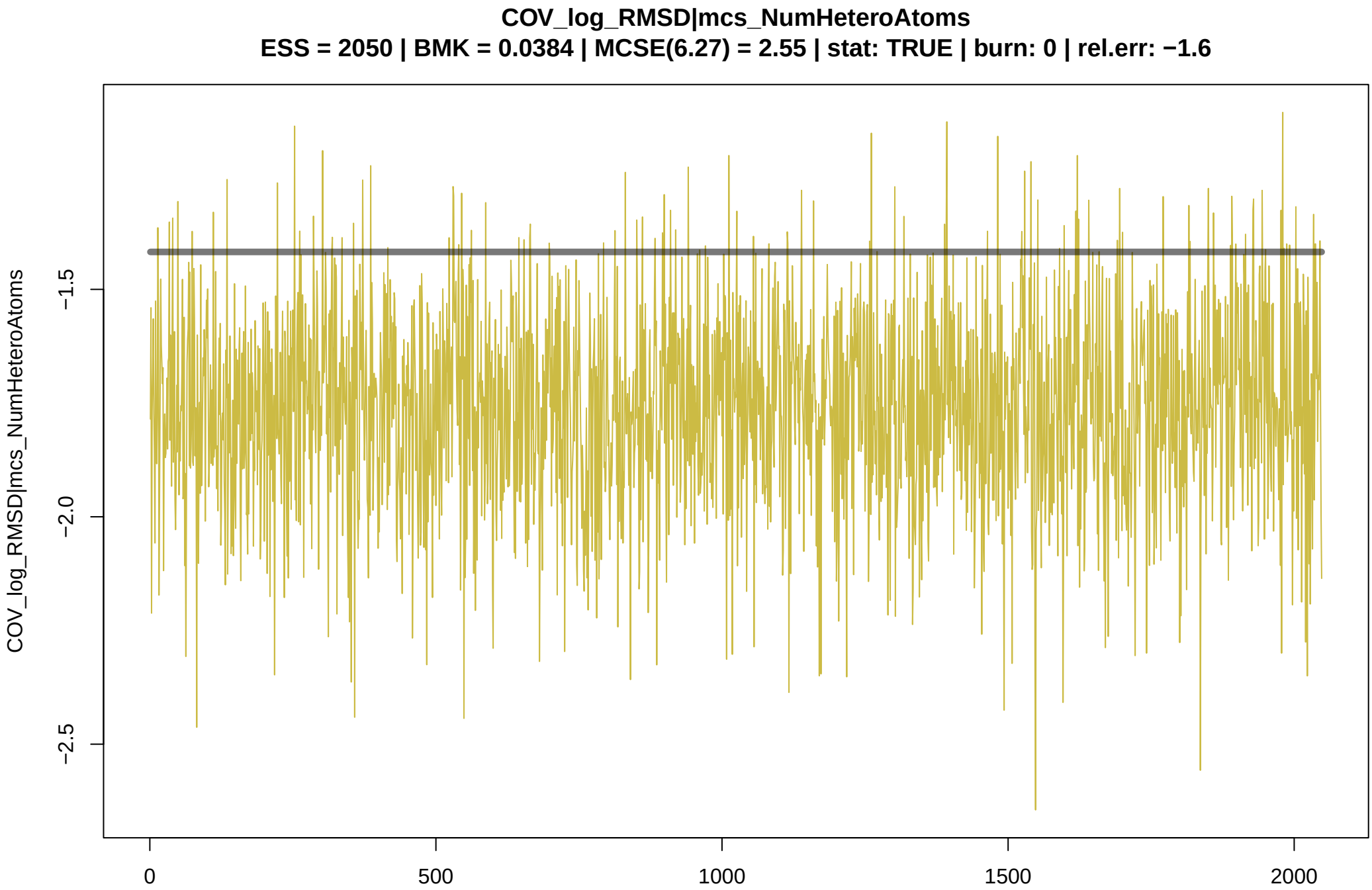

VAR_log_RMSD
ESS = 1920 | BMK = 0.0402 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 2.29
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000

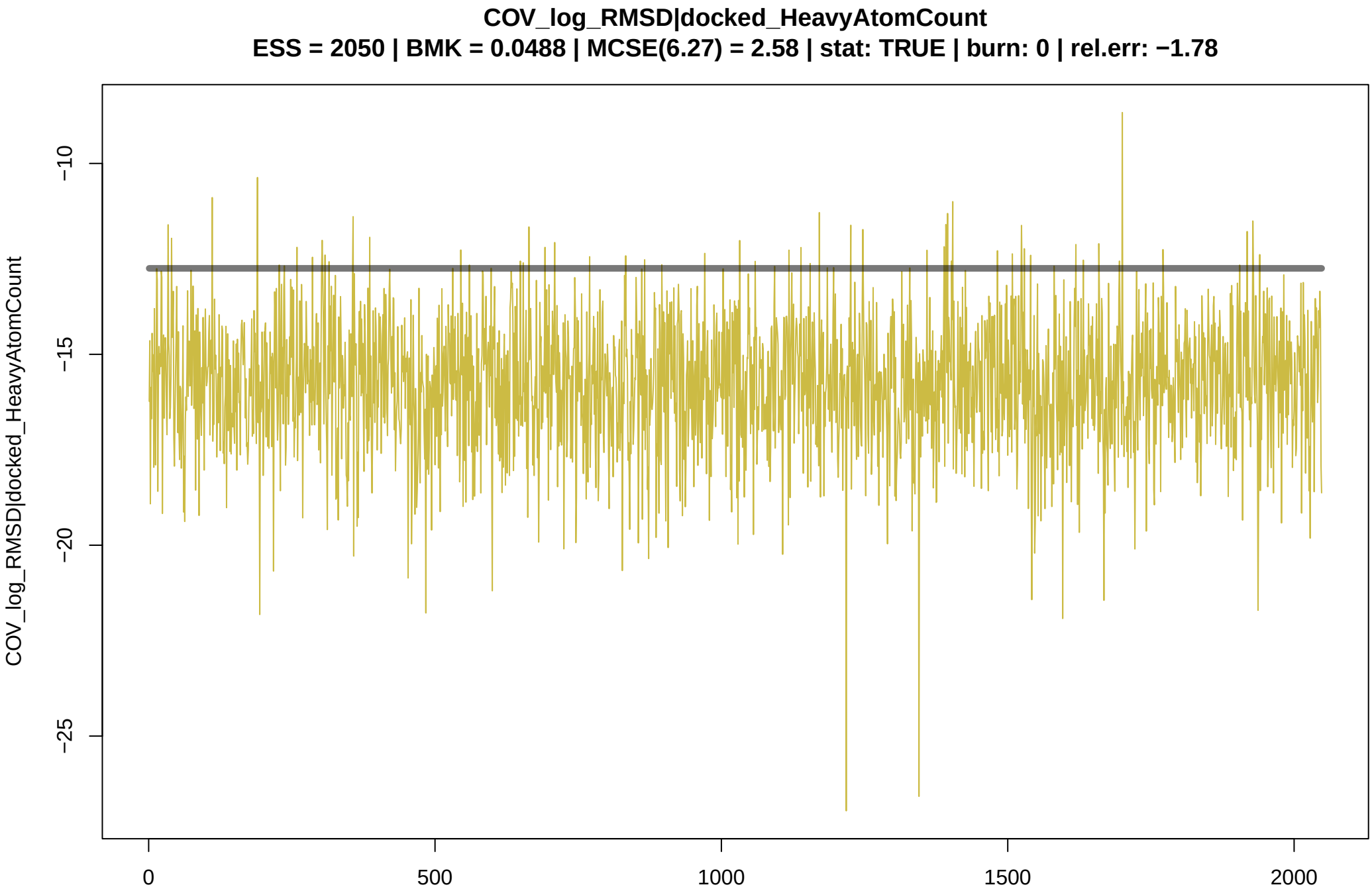

VAR_log_mcs_unbonded_polar_sasa
ESS = 1850 | BMK = 0.0471 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0 | rel.err: 1.32
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
0
500
1000
1500
2000

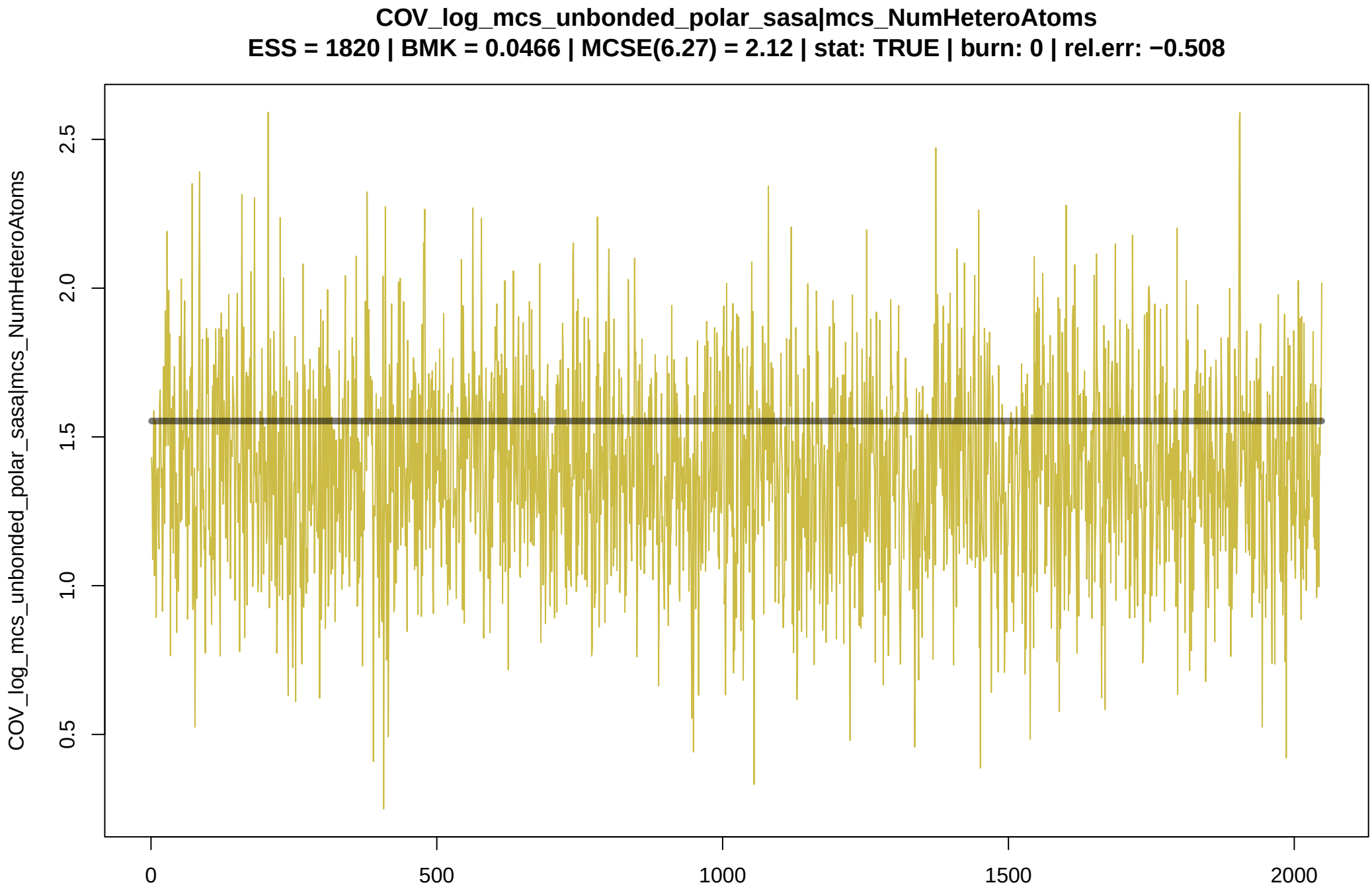

VAR_mcs_NumHeteroAtoms
ESS = 1550 | BMK = 0.0594 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0 | rel.err: 0.383
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

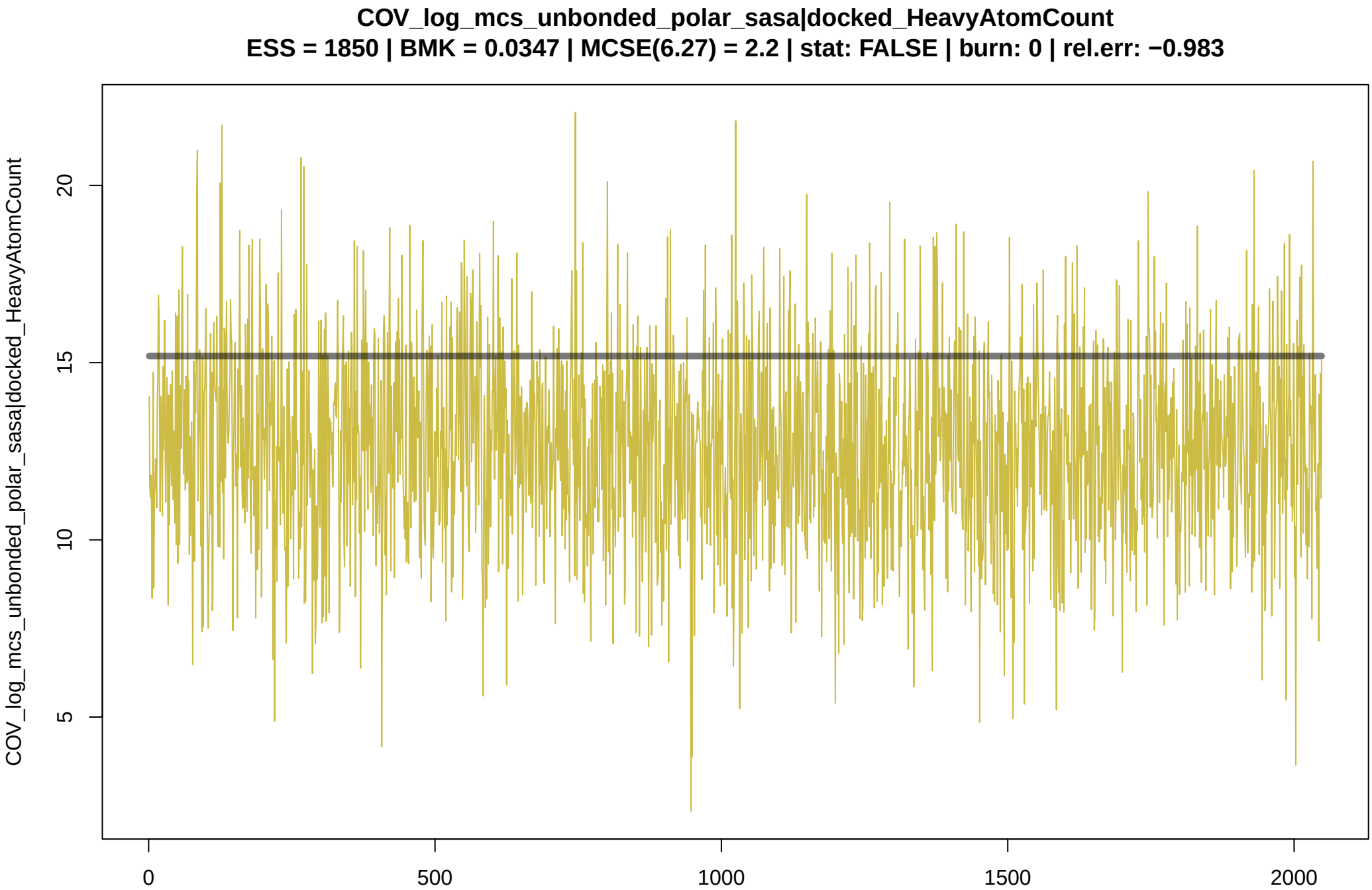

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0592 | MCSE(6.27) = 2.46 | stat: TRUE | burn: 0 | rel.err: 0.061
VAR_docked_HeavyAtomCount
6.4
6.6
6.8
7.0
0
500
1000
1500
2000

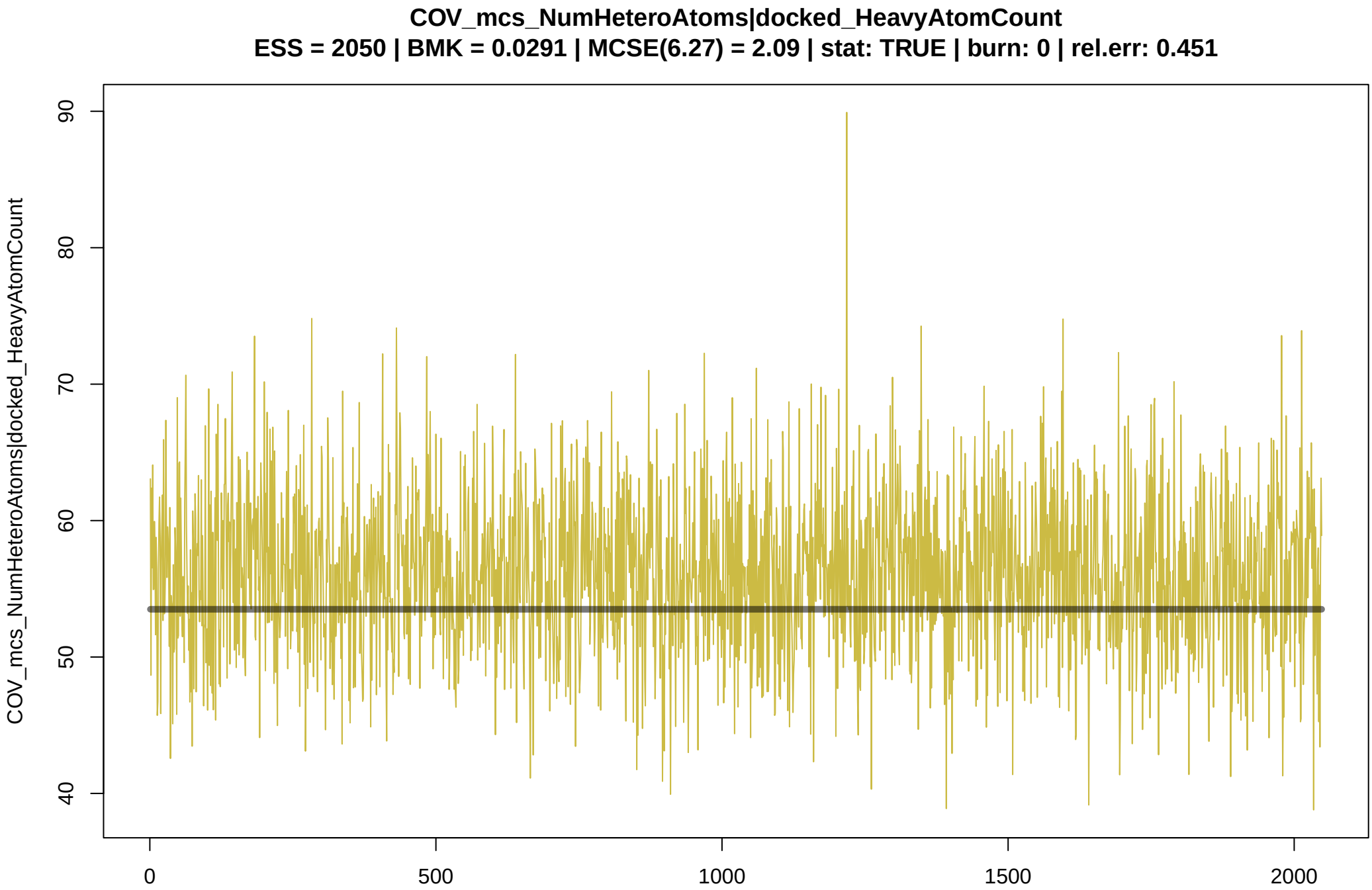

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1840 | BMK = 0.045 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0 | rel.err: 0.47
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0384 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: −1.6
COV_log_RMSD|mcs_NumHeteroAtoms
−1.5
−2.0
−2.5
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0488 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0 | rel.err: −1.78
COV_log_RMSD|docked_HeavyAtomCount
−10
−15
−20
−25
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 1820 | BMK = 0.0466 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: −0.508
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 = 1850 | BMK = 0.0347 | MCSE(6.27) = 2.2 | stat: FALSE | burn: 0 | rel.err: −0.983
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 = 0.0291 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.451
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
90
80
70
60
50
40
0
500
1000
1500
2000