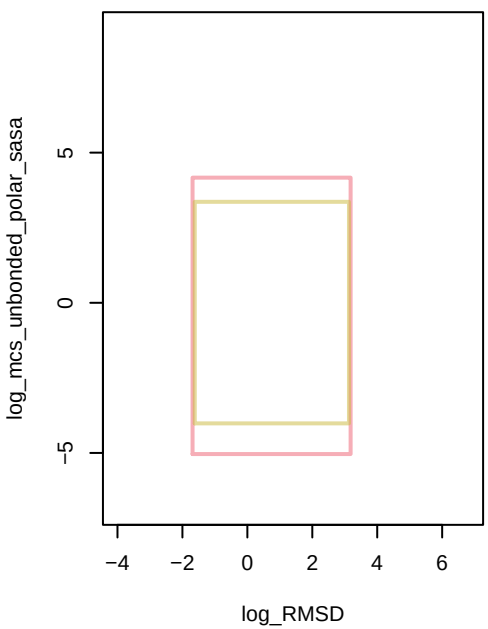
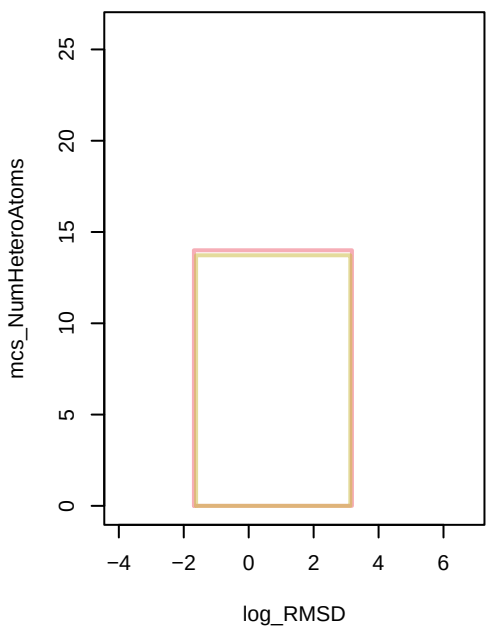
−− STATS maxD −−
min ESS = 11.1085510260915
max BMK = 0.153865027876761
max MCSE = 11.4474738439154
all stationary: FALSE
burn: 1224
max rel.err.: 2.20561736352057

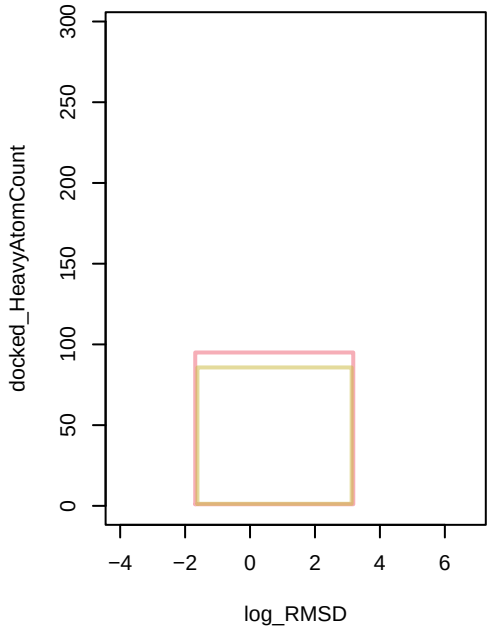
−− STATS 2D −−
min ESS = 1853.60873362588
max BMK = 0.059726092613605 8
max MCSE = 2.16301692889408
all stationary: TRUE
burn: 0
max rel.err.: 1.79449129337665

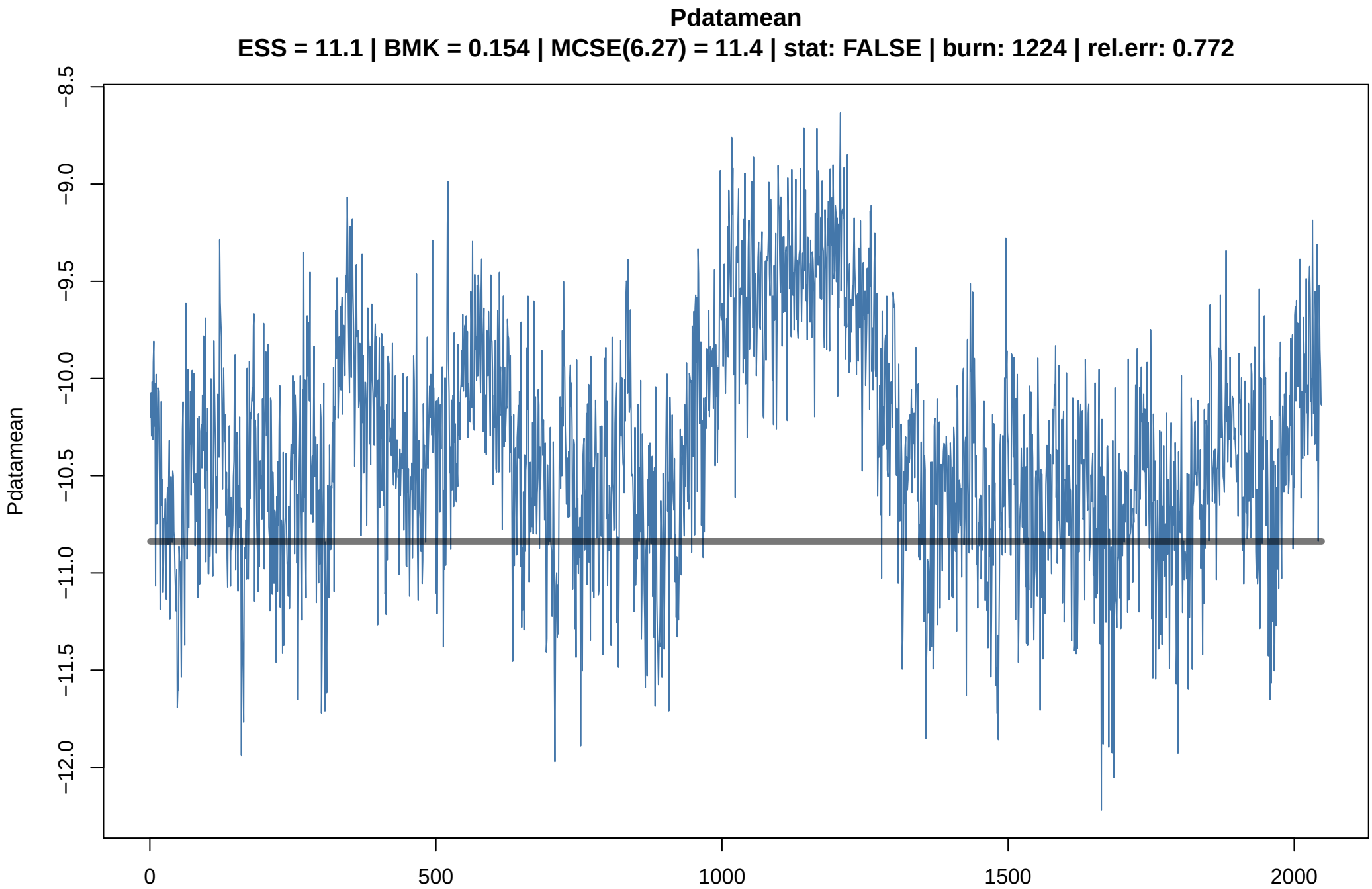
−− STATS 1D −−
min ESS = 1473.75670374703
max BMK = 0.073037705405224 4
max MCSE = 2.95418513193719
all stationary: TRUE
burn: 0
max rel.err.: 2.29589729728636

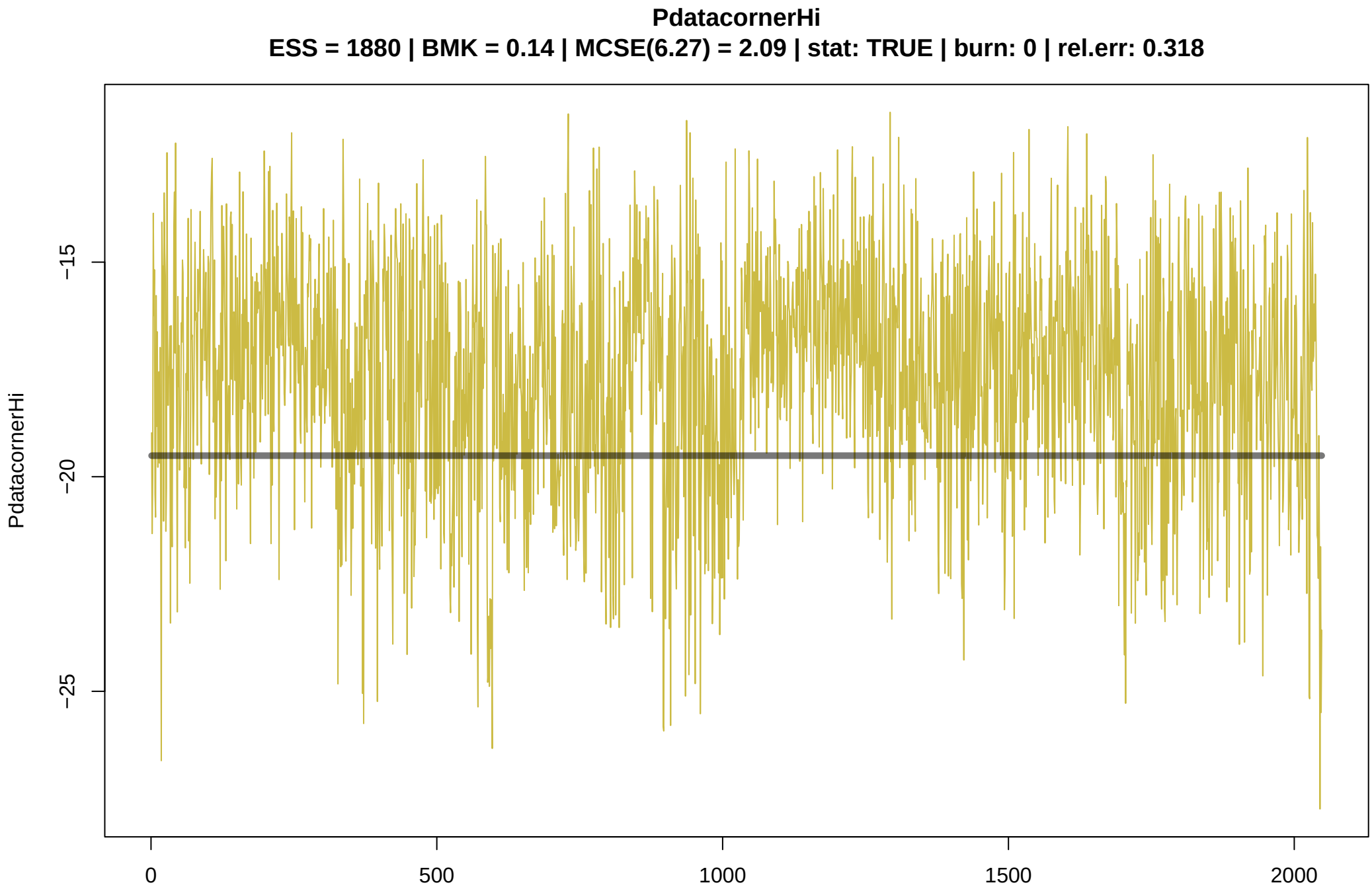
Occupied clusters: 8 of 16

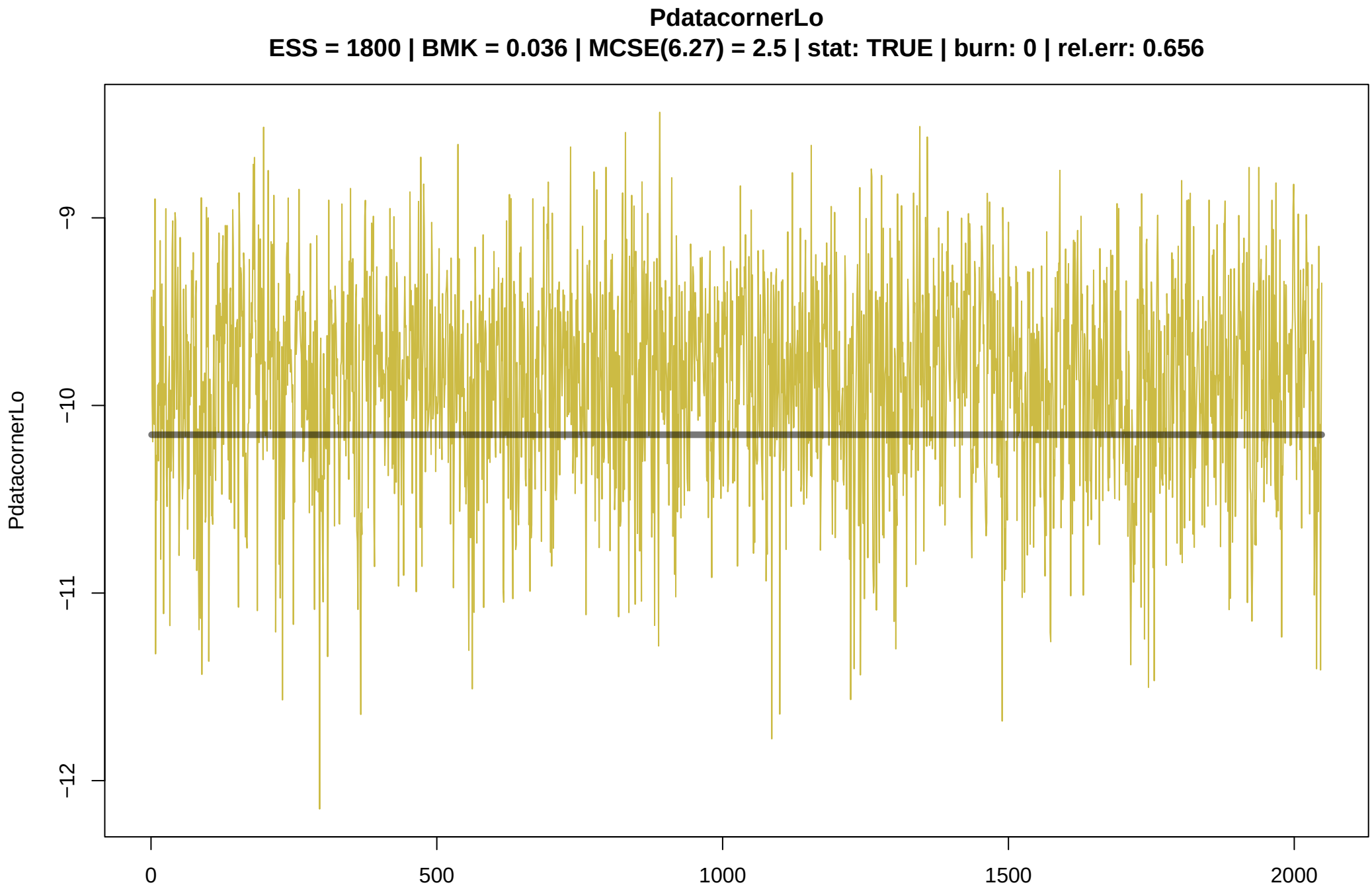

log_mcs_unbonded_polar_sasa
−5
0
5
−4
−2
0
2
4
6
log_RMSD

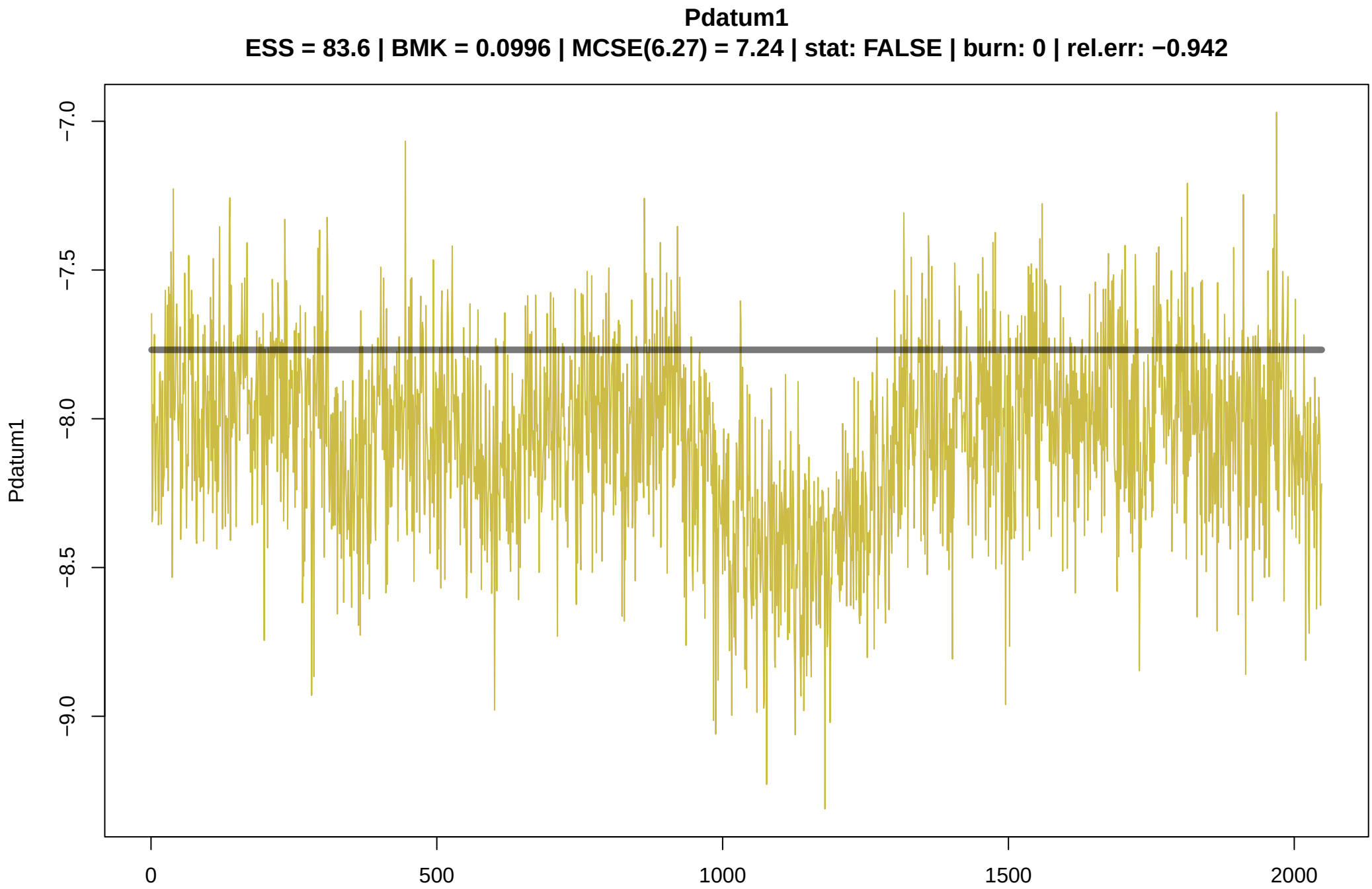

mcs_NumHeteroAtoms
0
5
10
15
20
25
−4
−2
0
2
4
6
log_RMSD

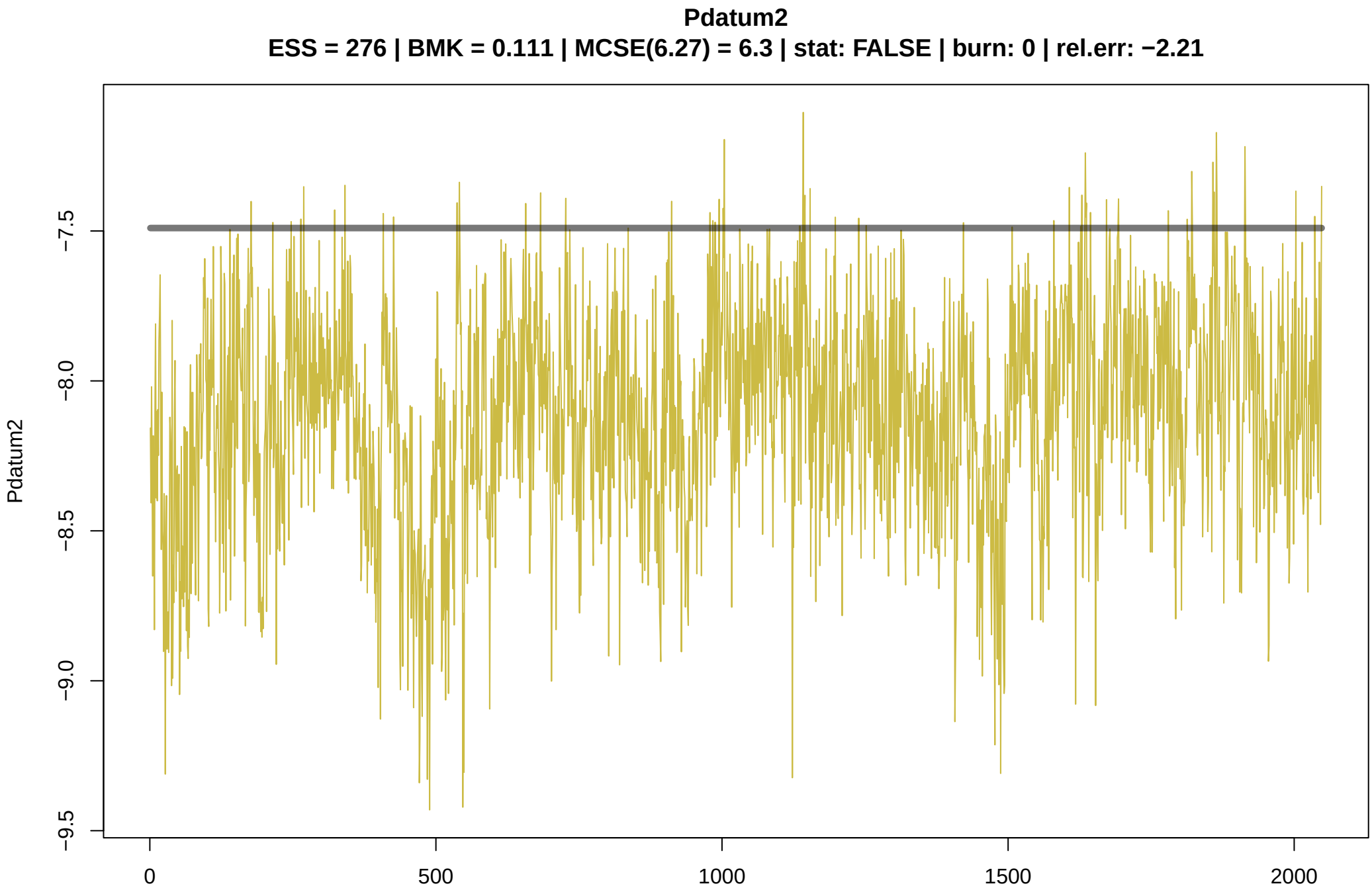

docked_HeavyAtomCount
0
50
100
150
200
250
300
−4
−2
0
2
4
6
log_RMSD

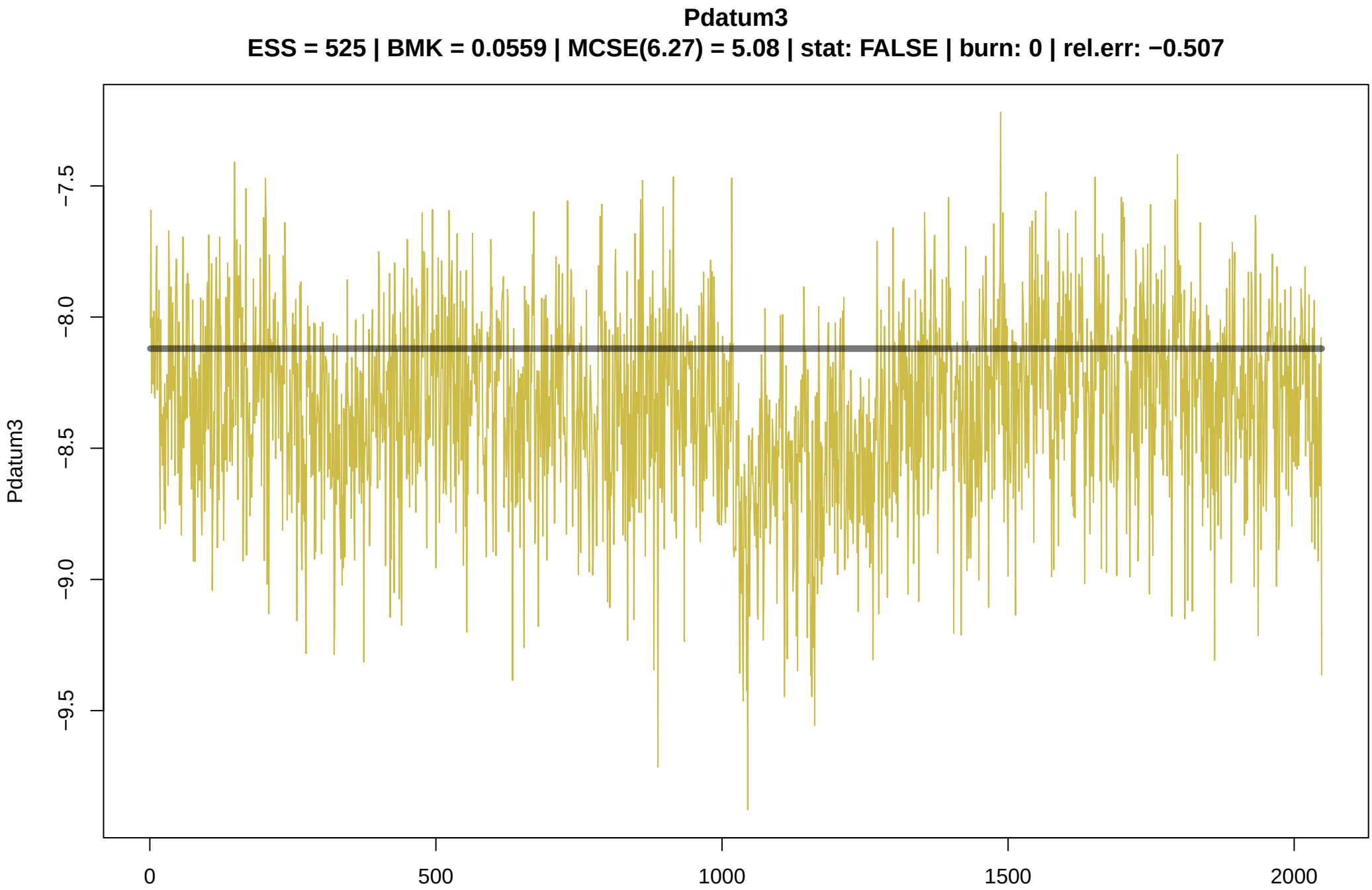

Pdatamean
ESS = 11.1 | BMK = 0.154 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 1224 | rel.err: 0.772
Pdatamean
−8.5
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

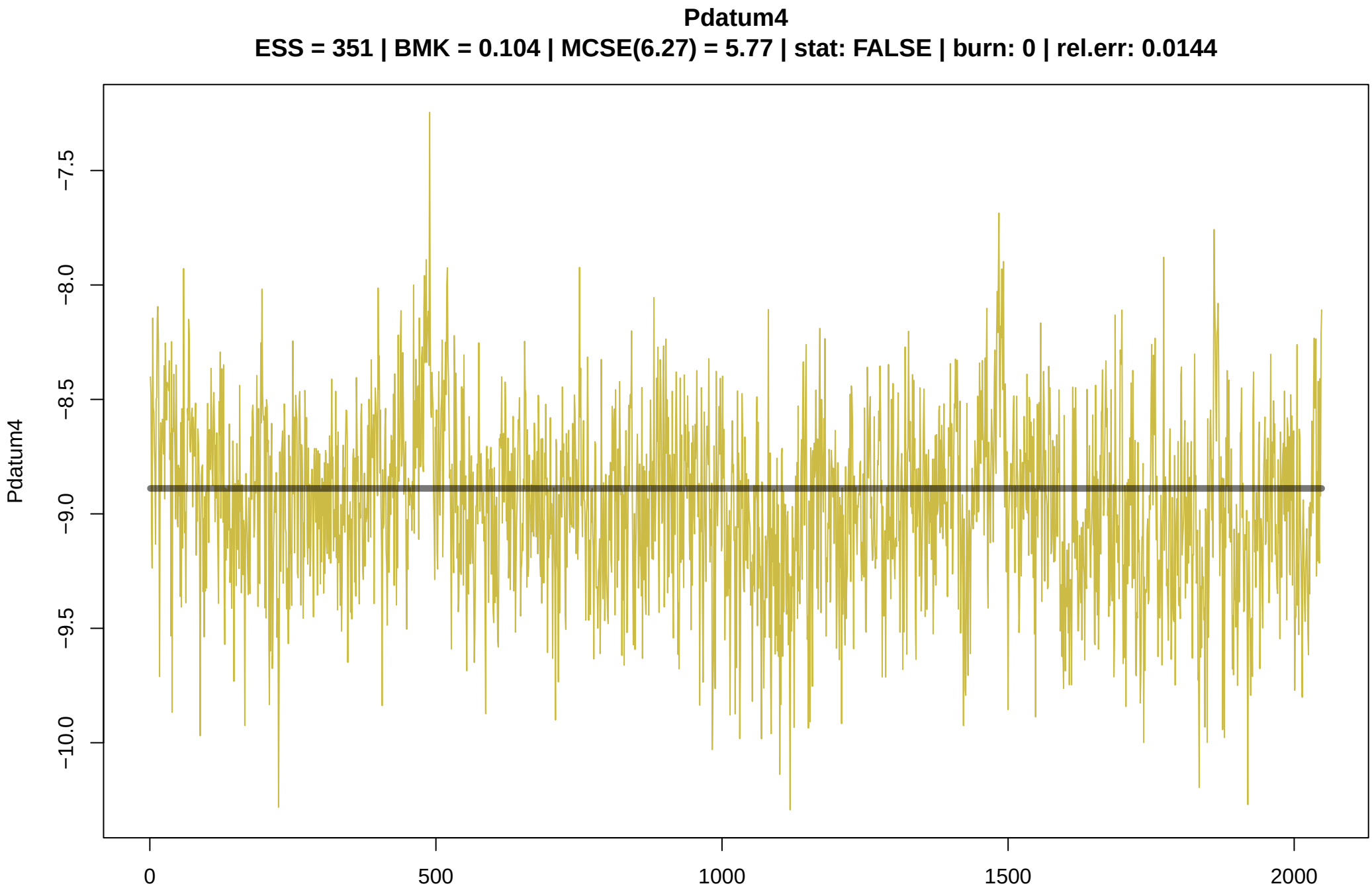

PdatacornerHi
ESS = 1880 | BMK = 0.14 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.318
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

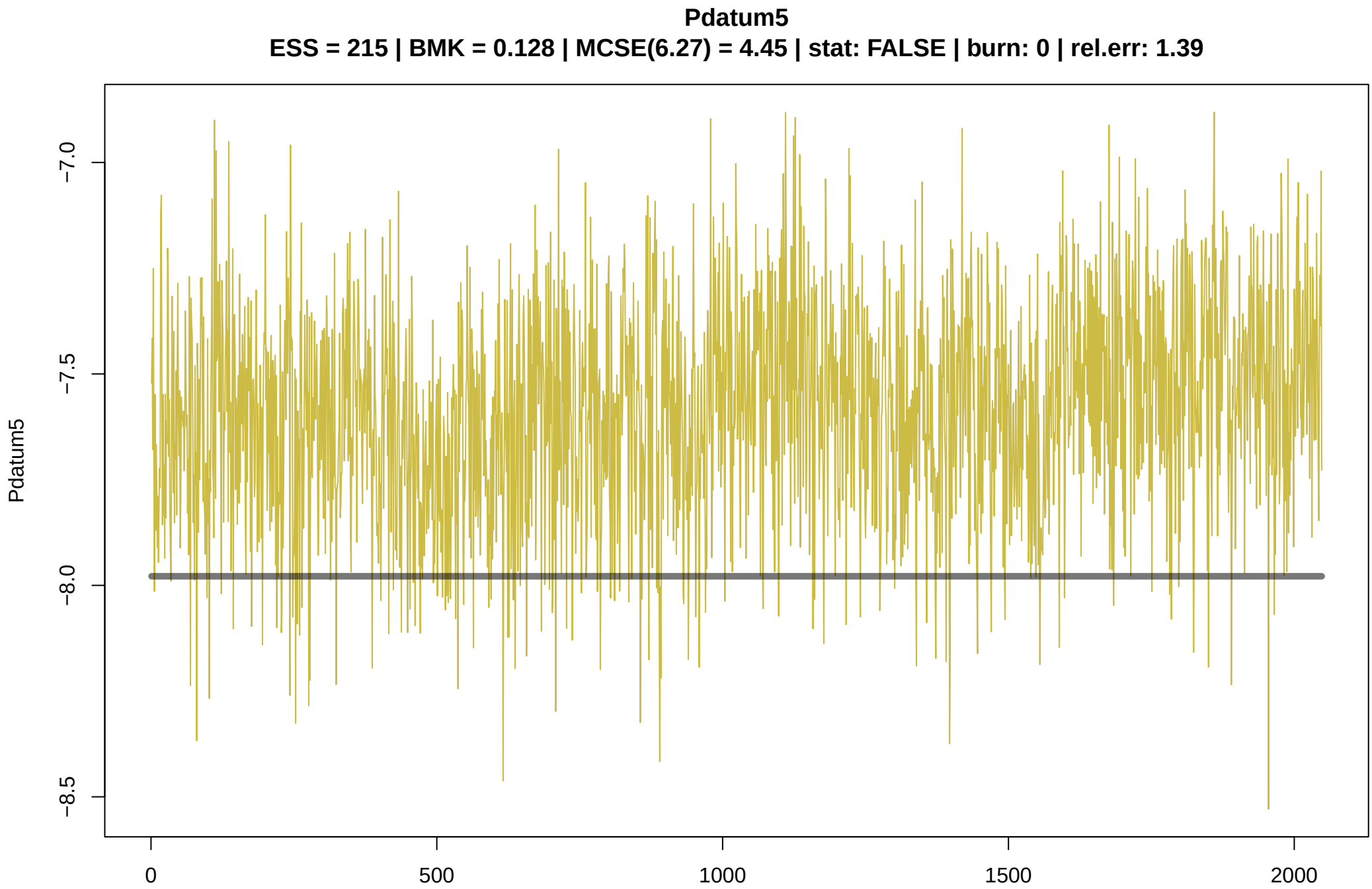

PdatacornerLo
ESS = 1800 | BMK = 0.036 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 0.656
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

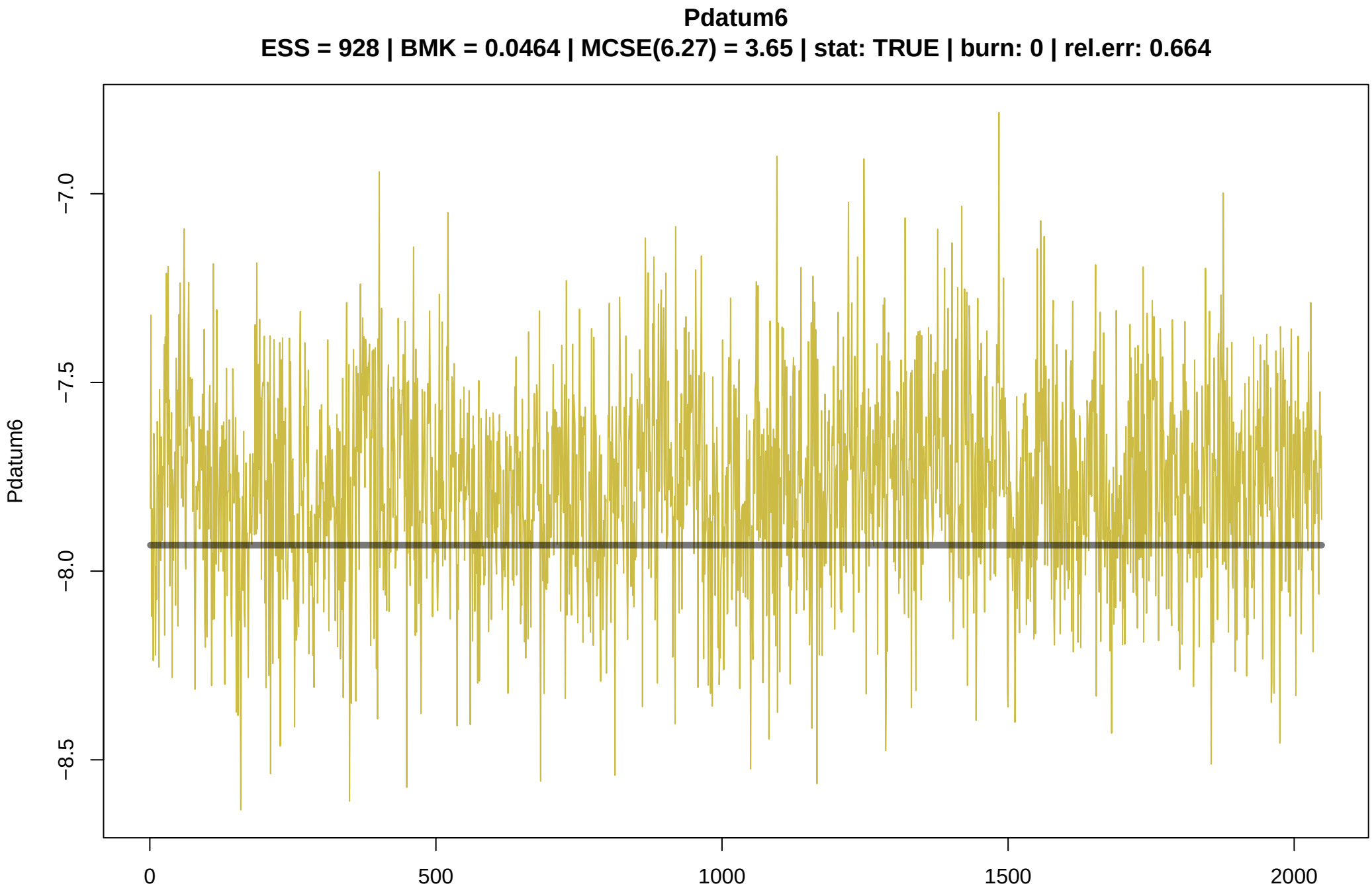

Pdatum1
ESS = 83.6 | BMK = 0.0996 | MCSE(6.27) = 7.24 | stat: FALSE | burn: 0 | rel.err: −0.942
Pdatum1
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

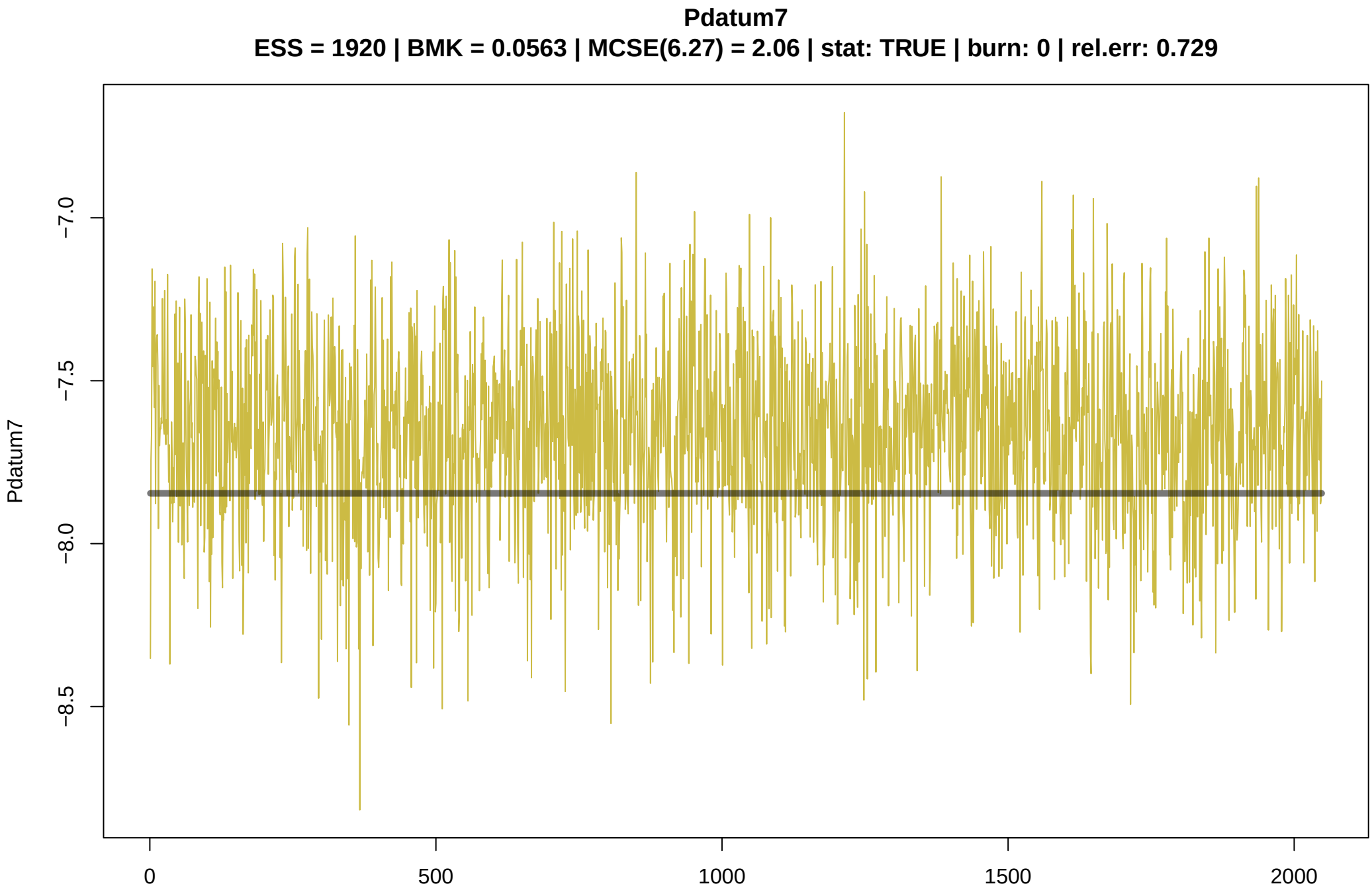

Pdatum2
ESS = 276 | BMK = 0.111 | MCSE(6.27) = 6.3 | stat: FALSE | burn: 0 | rel.err: −2.21
Pdatum2
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

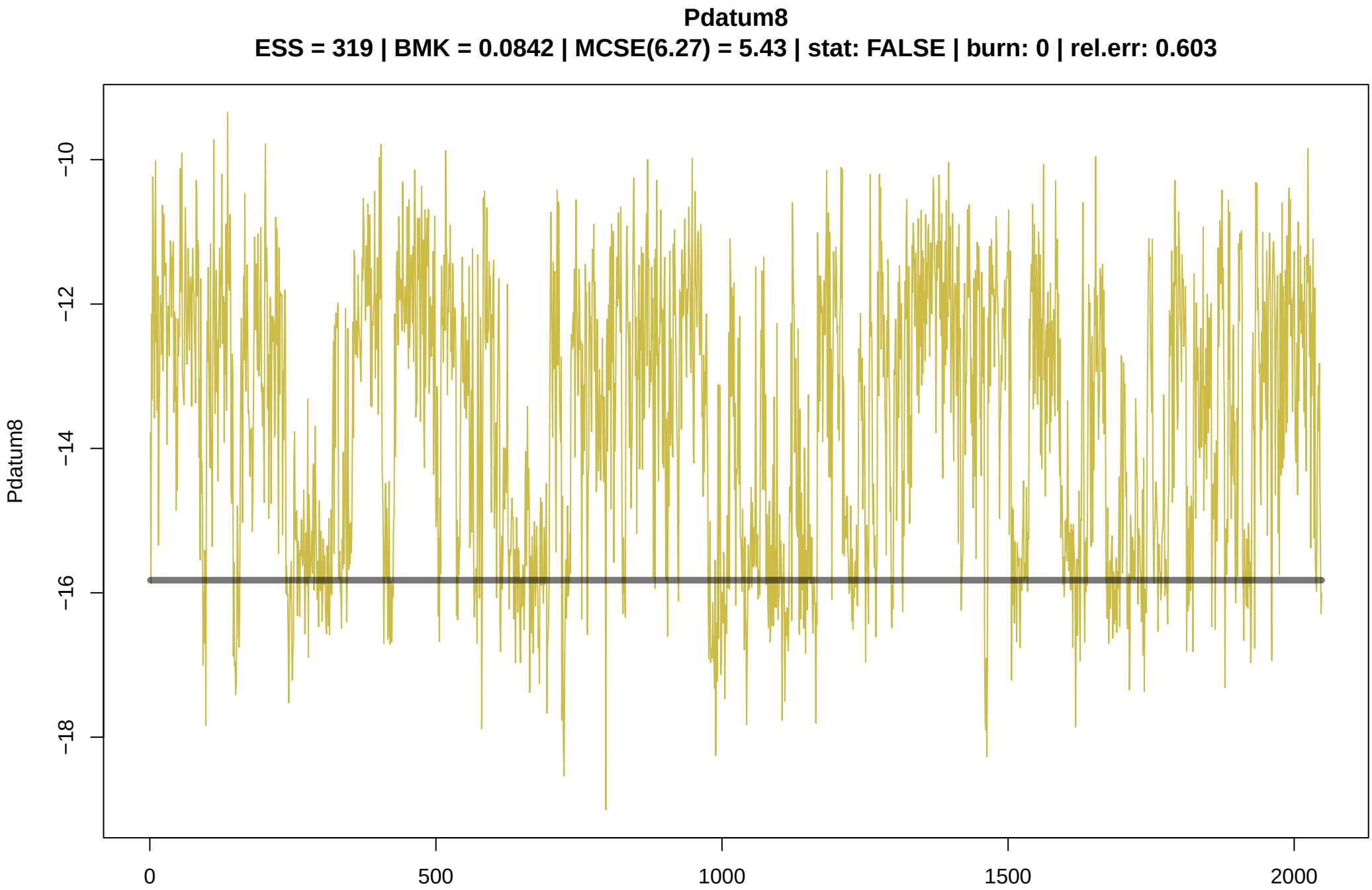

Pdatum3
ESS = 525 | BMK = 0.0559 | MCSE(6.27) = 5.08 | stat: FALSE | burn: 0 | rel.err: −0.507
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

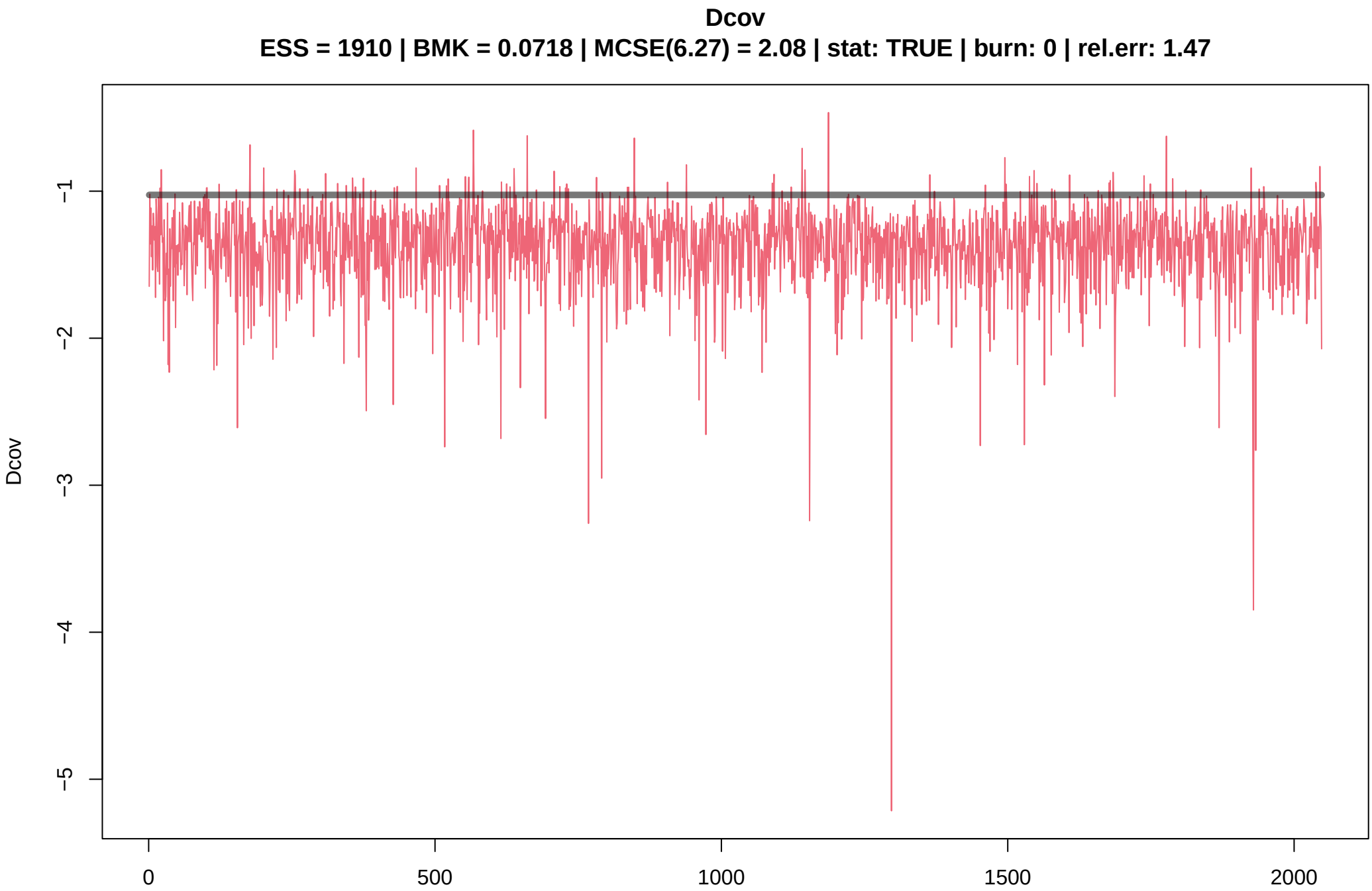

Pdatum4
ESS = 351 | BMK = 0.104 | MCSE(6.27) = 5.77 | stat: FALSE | burn: 0 | rel.err: 0.0144
Pdatum4
−7.5
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

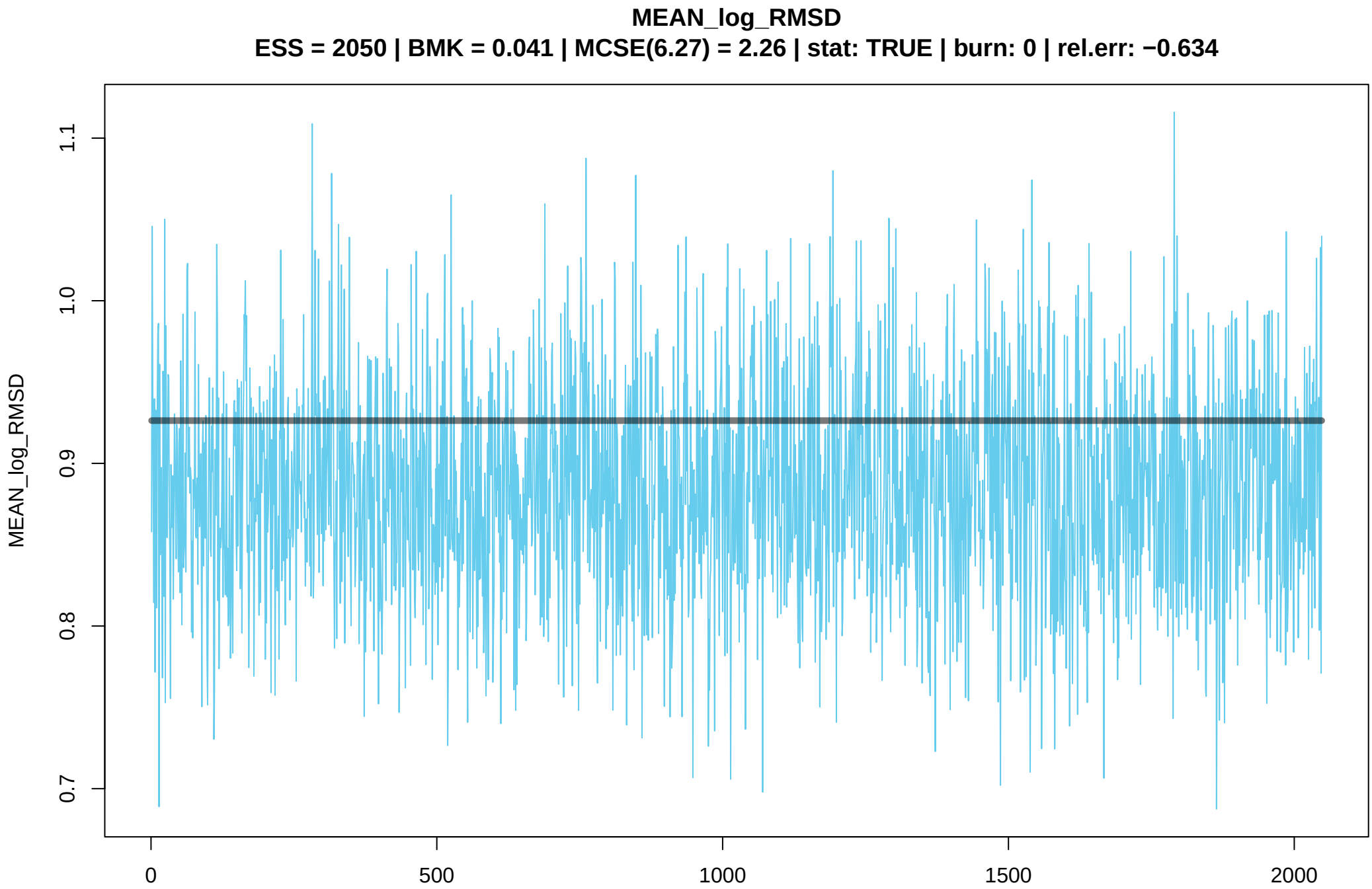

Pdatum5
ESS = 215 | BMK = 0.128 | MCSE(6.27) = 4.45 | stat: FALSE | burn: 0 | rel.err: 1.39
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

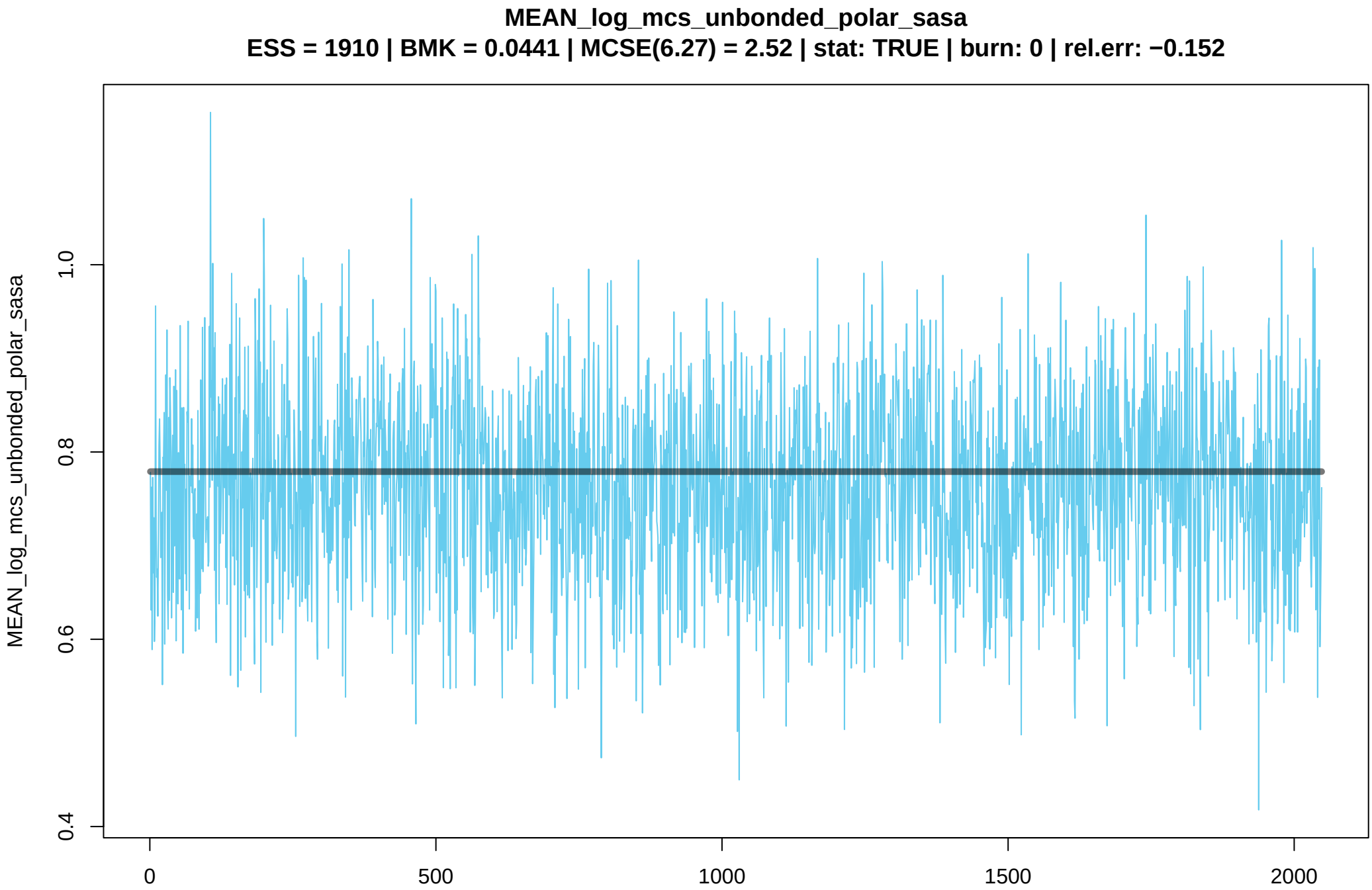

Pdatum6
ESS = 928 | BMK = 0.0464 | MCSE(6.27) = 3.65 | stat: TRUE | burn: 0 | rel.err: 0.664
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

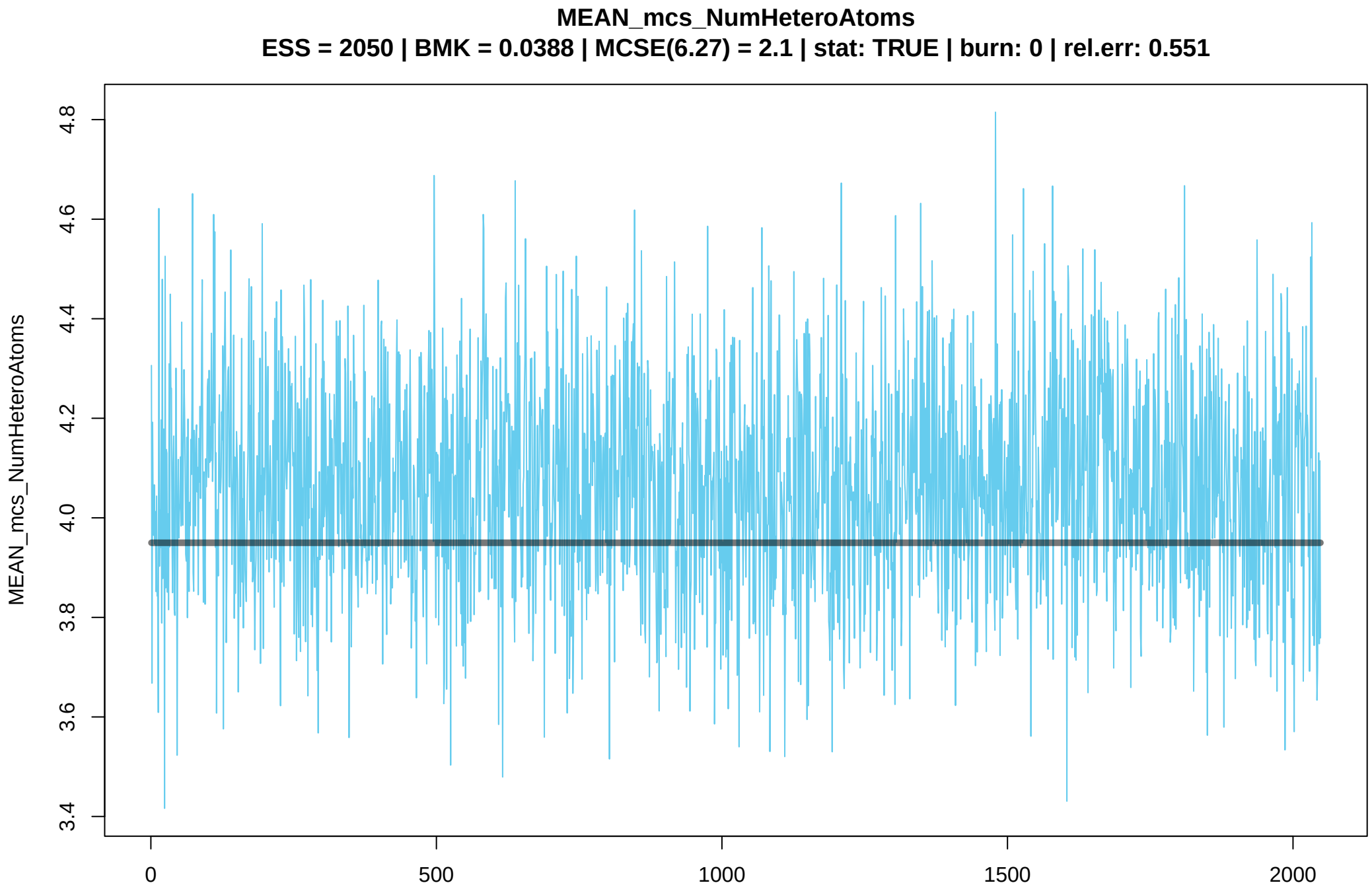

Pdatum7
ESS = 1920 | BMK = 0.0563 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0 | rel.err: 0.729
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

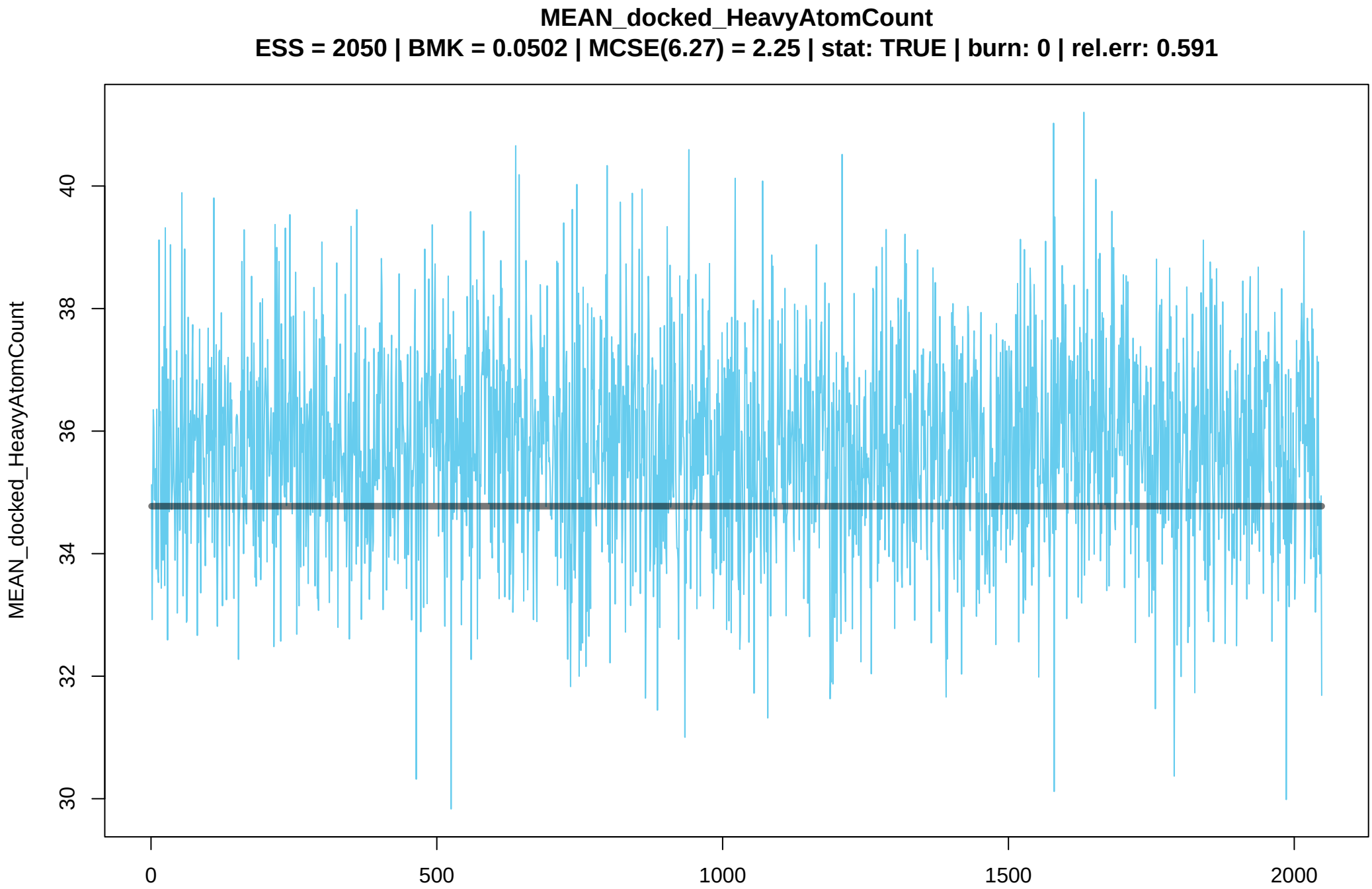

Pdatum8
ESS = 319 | BMK = 0.0842 | MCSE(6.27) = 5.43 | stat: FALSE | burn: 0 | rel.err: 0.603
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

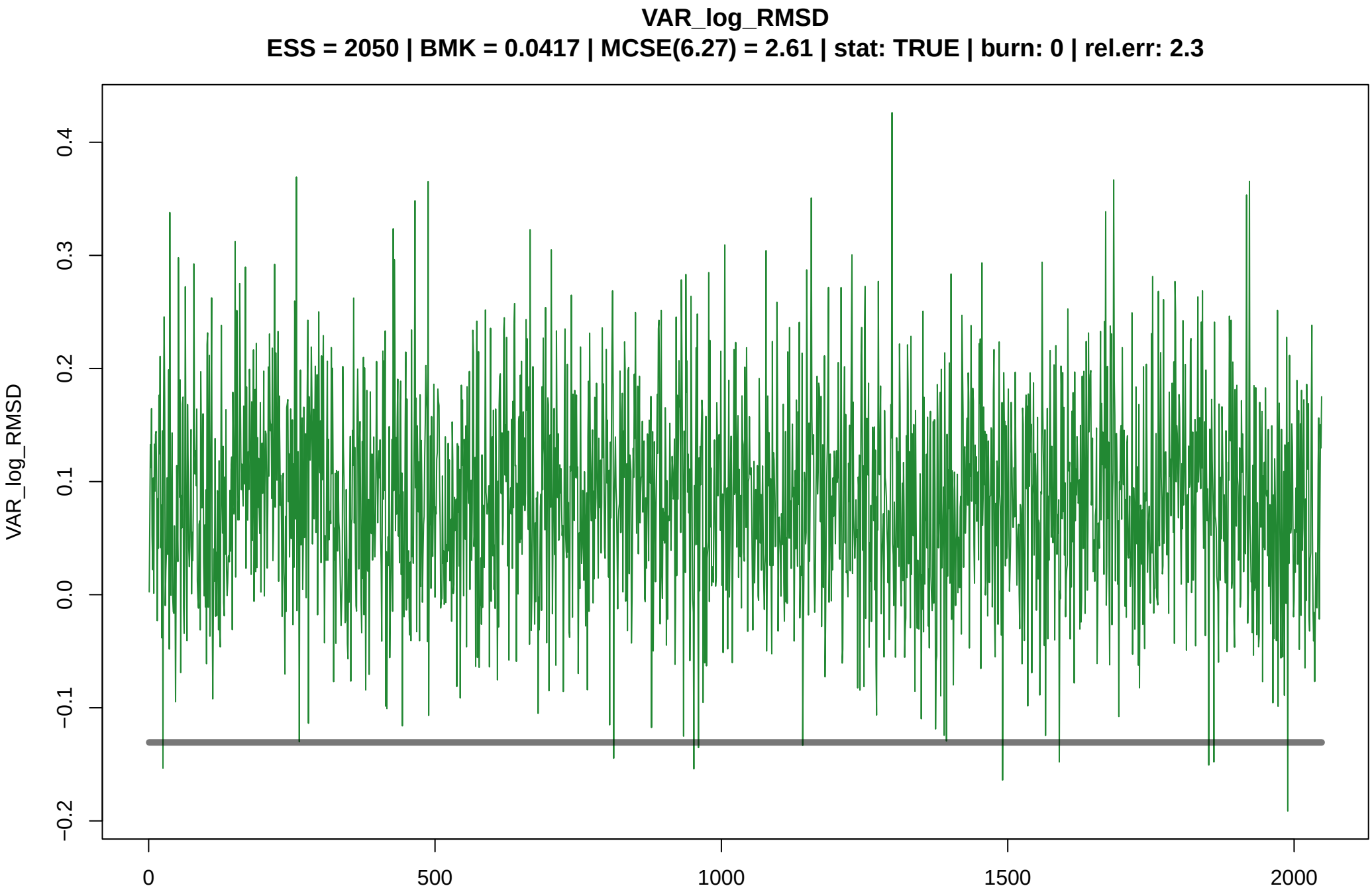

Dcov
ESS = 1910 | BMK = 0.0718 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: 1.47
Dcov
−1
−2
−3
−4
−5
0
500
1000
1500
2000

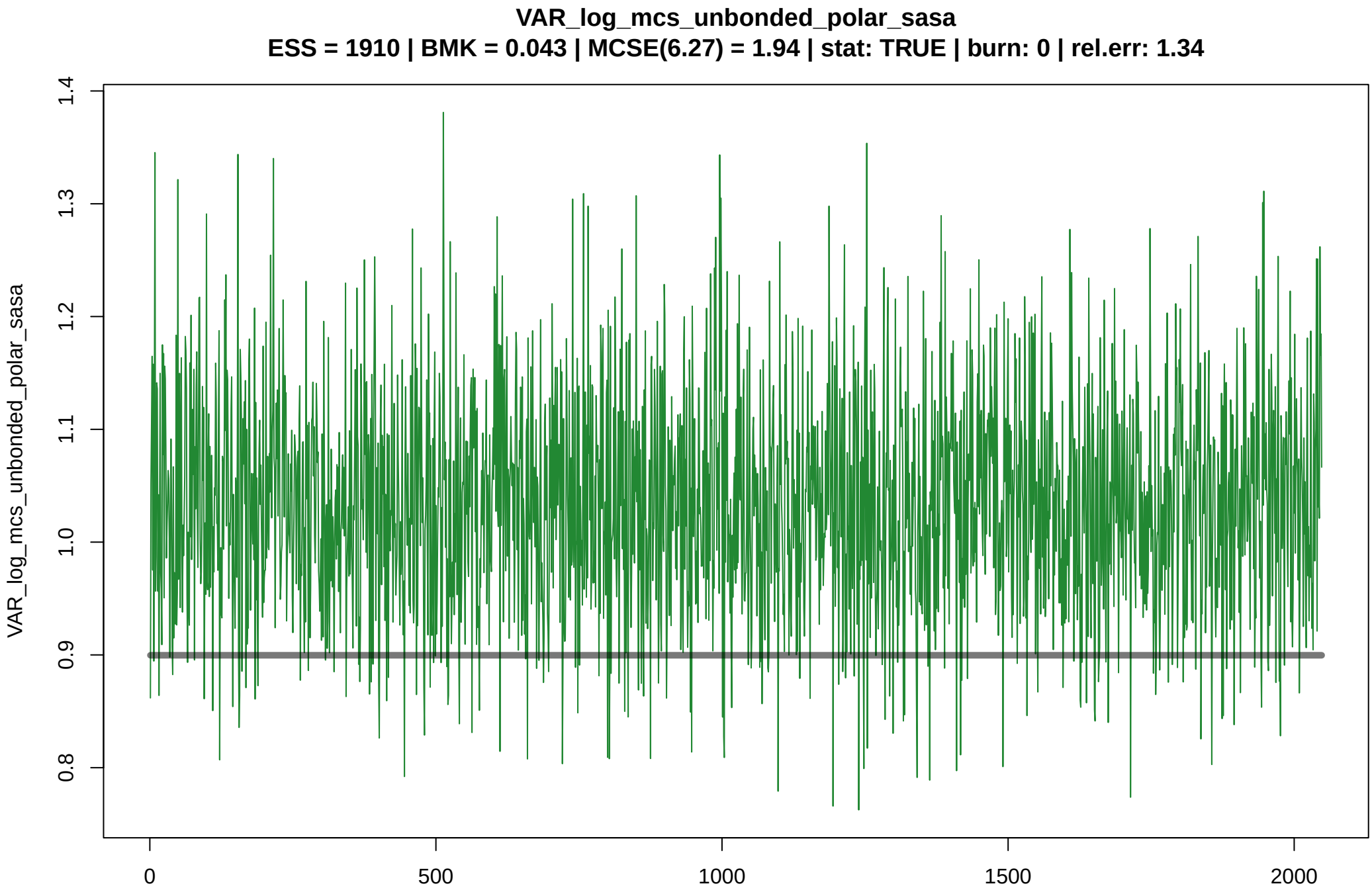

MEAN_log_RMSD
ESS = 2050 | BMK = 0.041 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0 | rel.err: −0.634
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

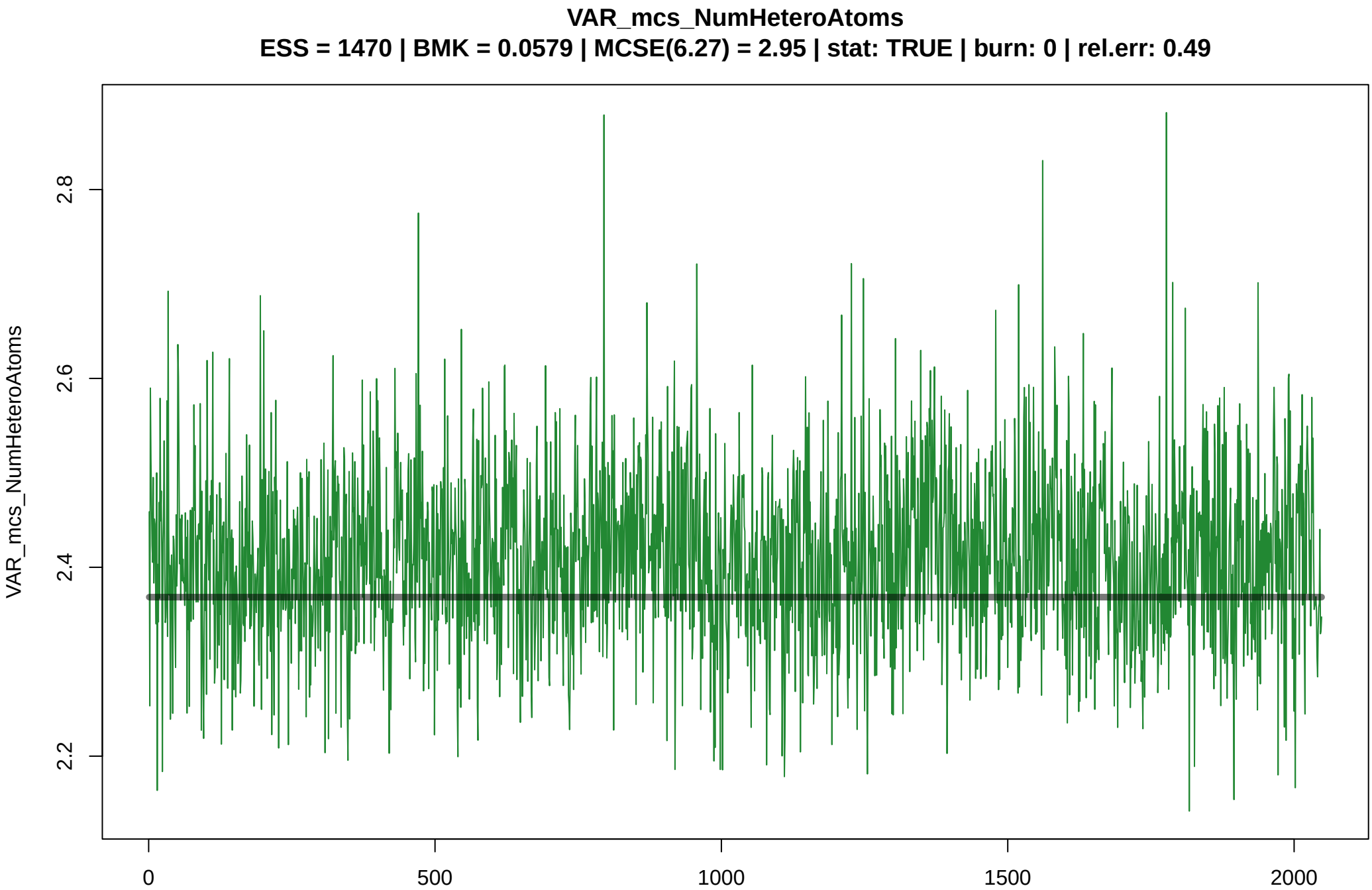

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1910 | BMK = 0.0441 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0 | rel.err: −0.152
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

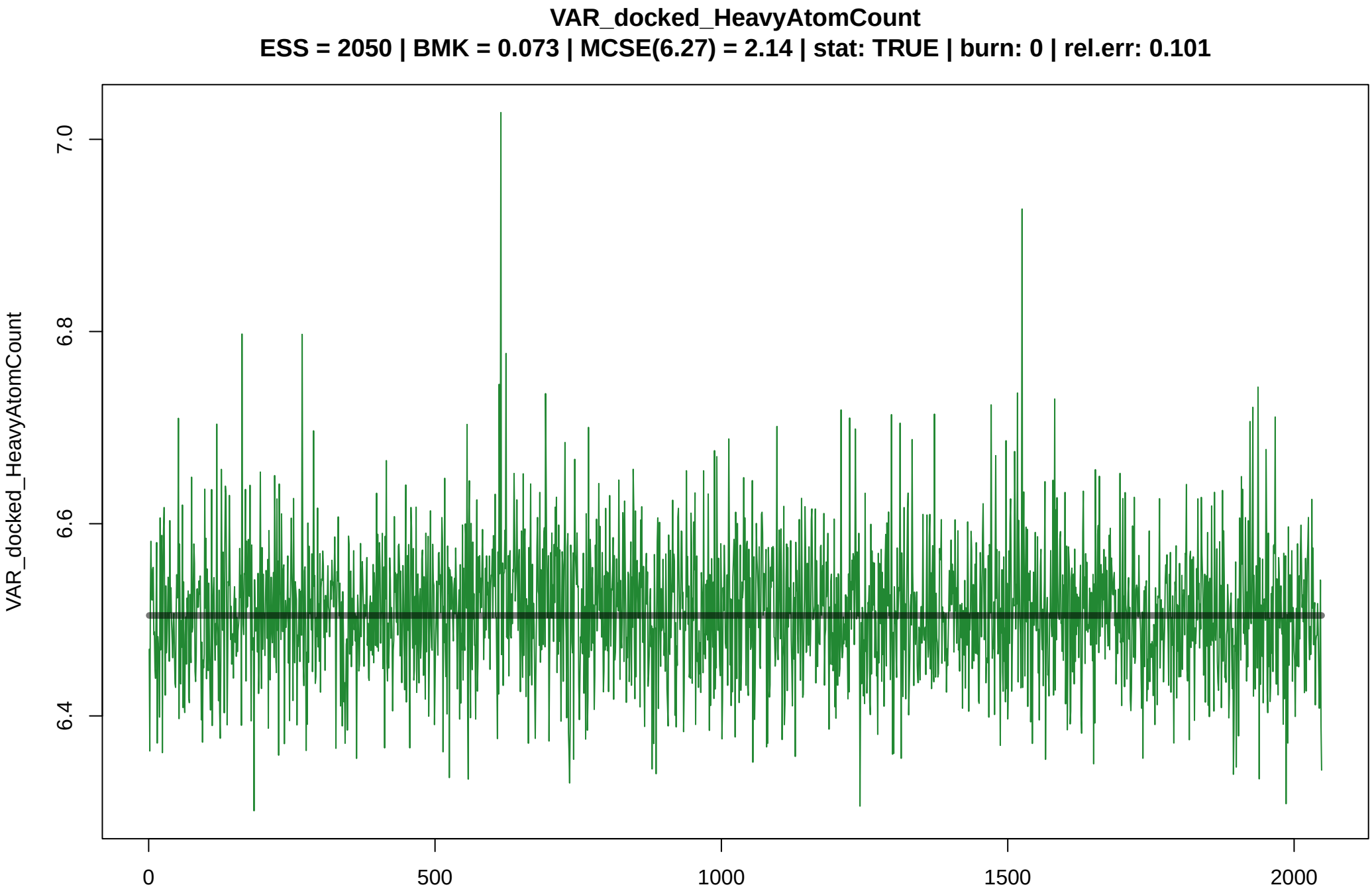

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0388 | MCSE(6.27) = 2.1 | stat: TRUE | burn: 0 | rel.err: 0.551
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

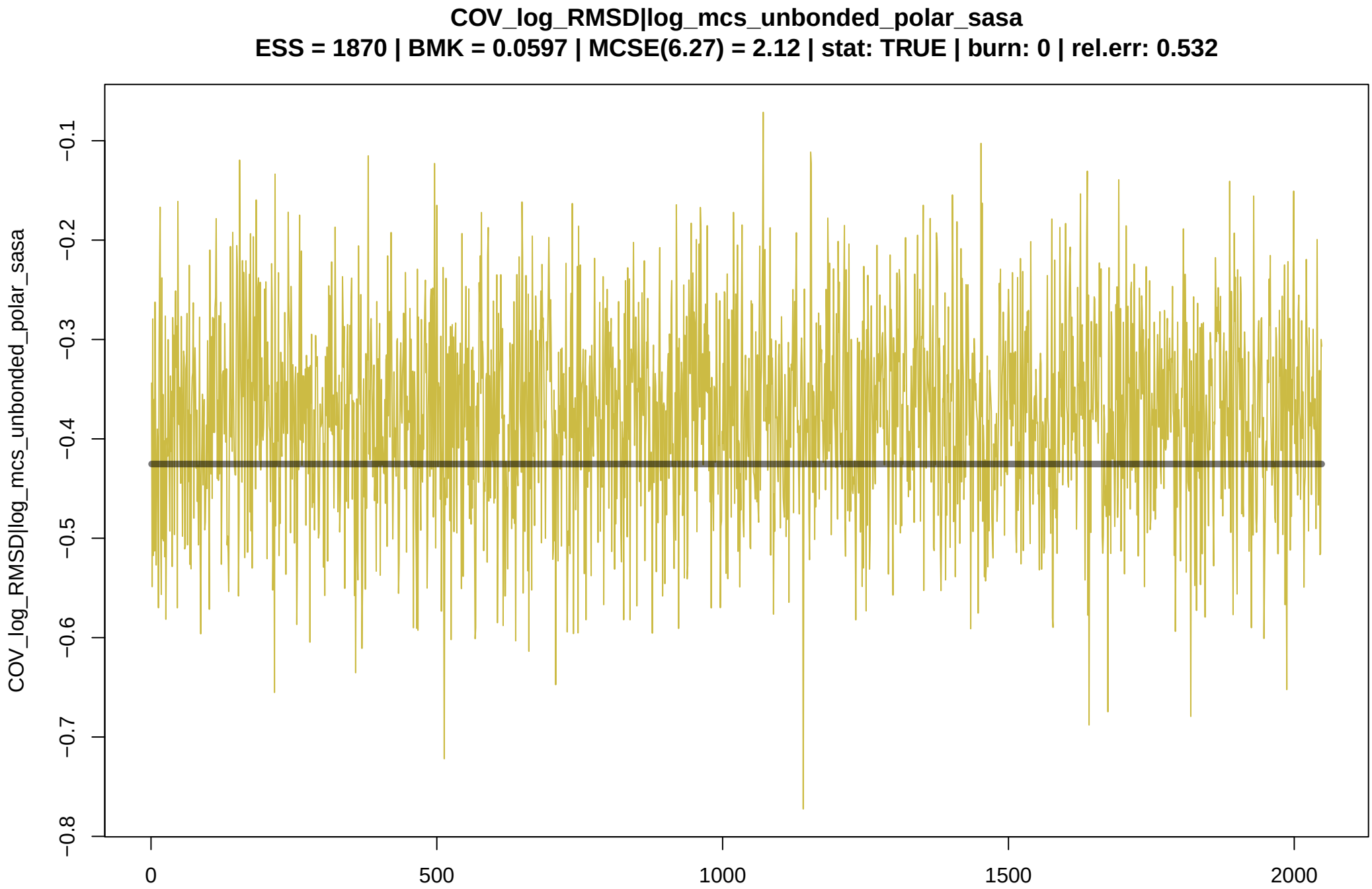

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0 | rel.err: 0.591
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

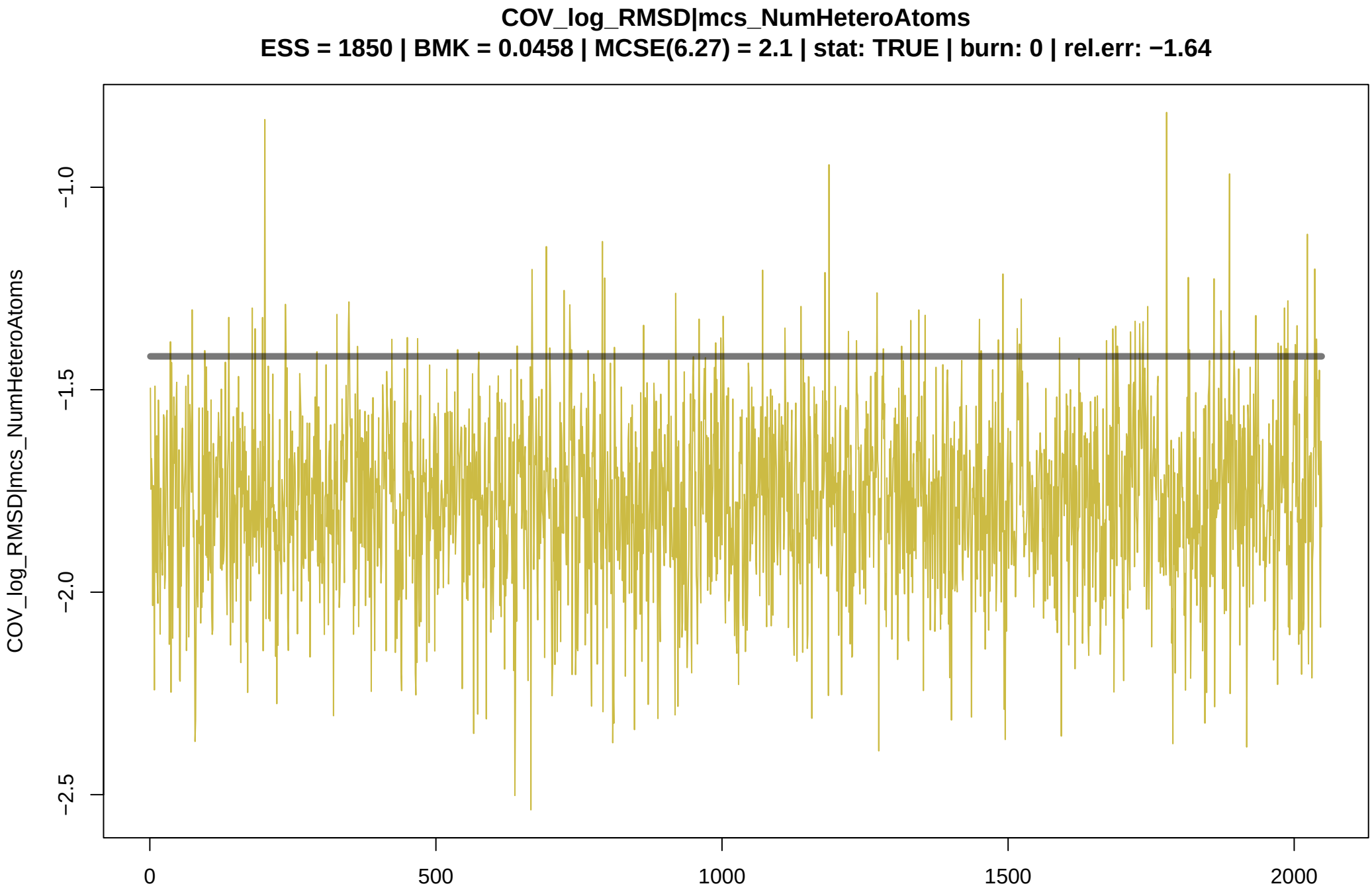

VAR_log_RMSD
ESS = 2050 | BMK = 0.0417 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0 | rel.err: 2.3
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

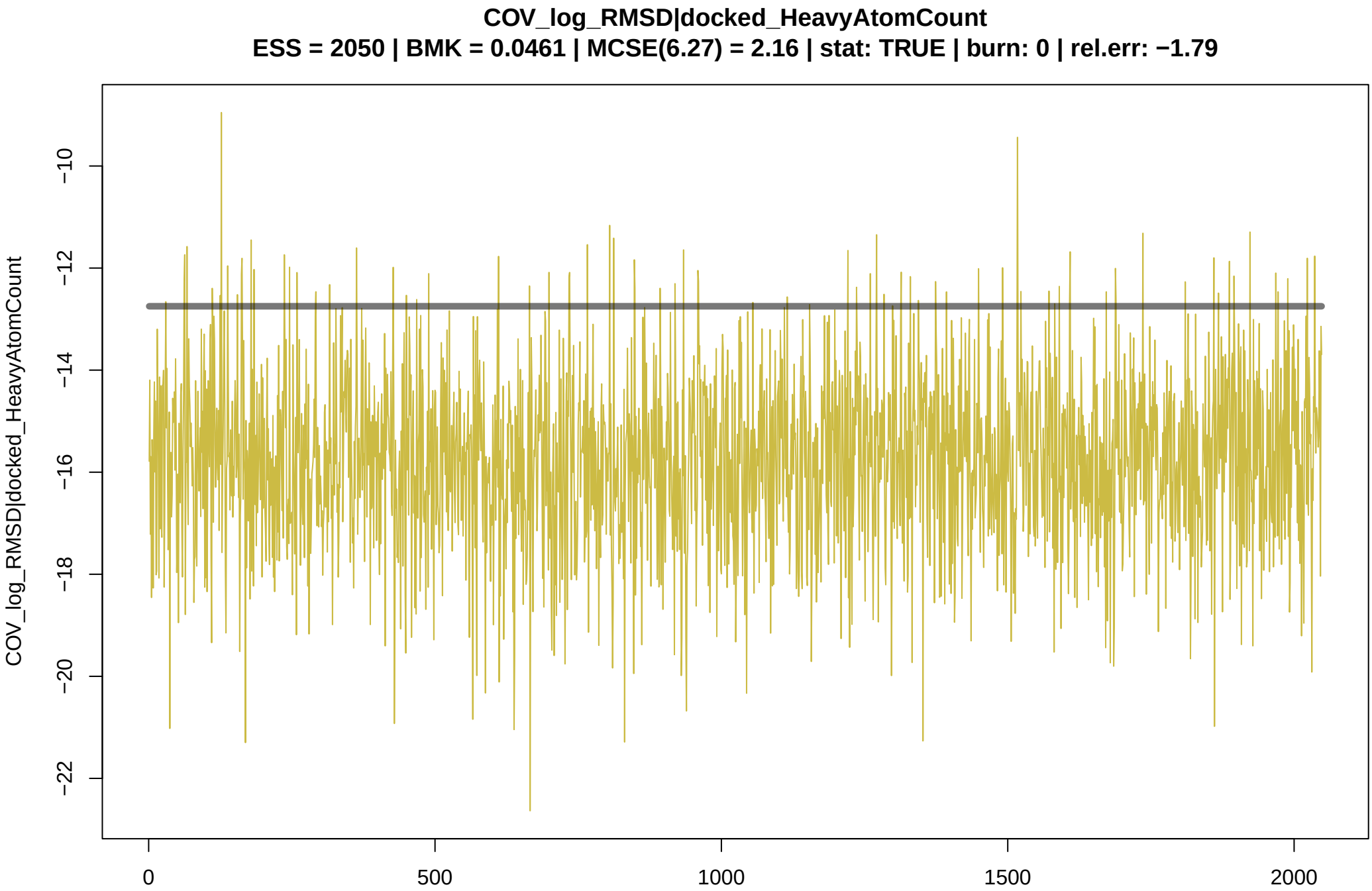

VAR_log_mcs_unbonded_polar_sasa
ESS = 1910 | BMK = 0.043 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0 | rel.err: 1.34
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

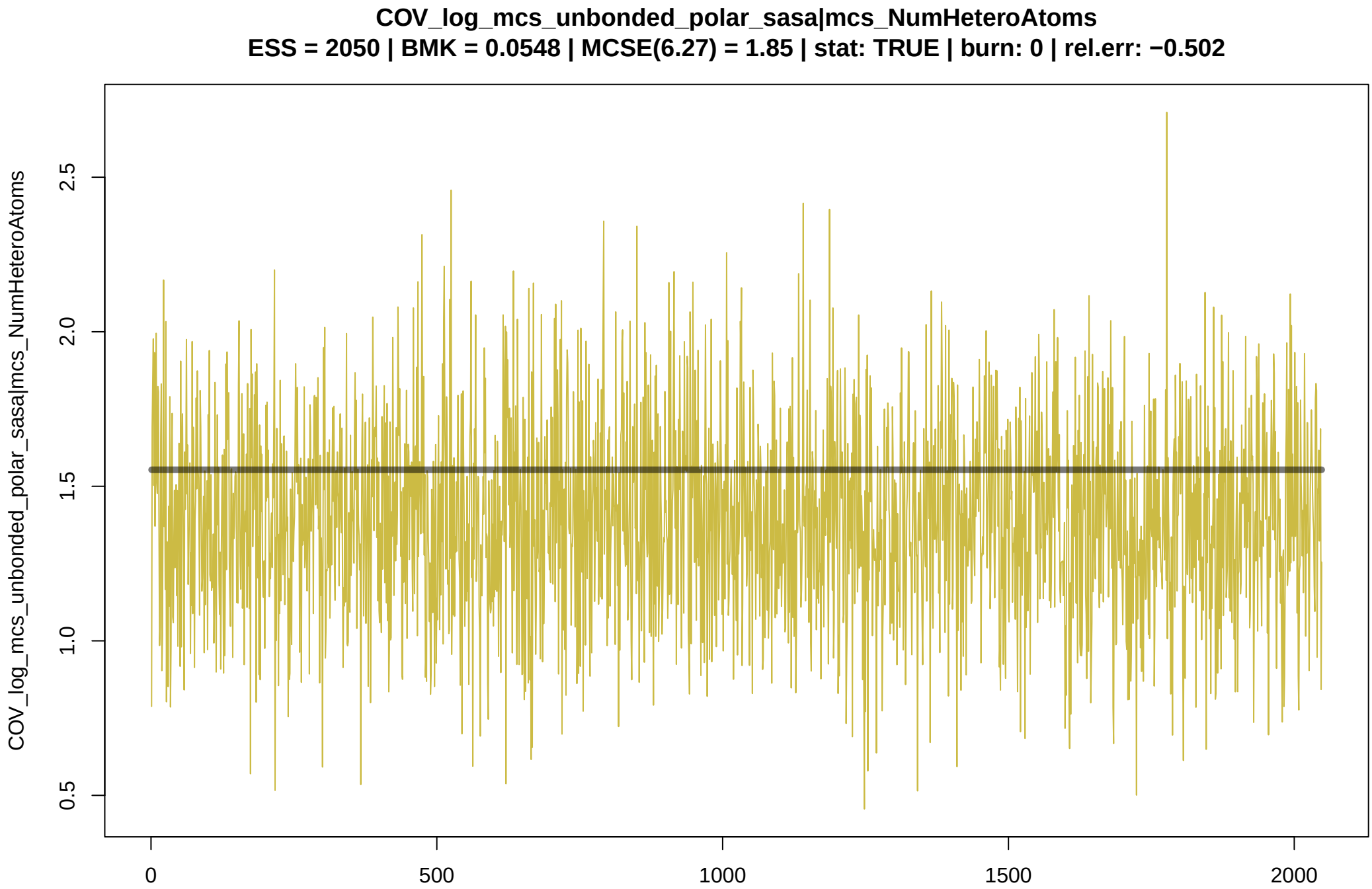

VAR_mcs_NumHeteroAtoms
ESS = 1470 | BMK = 0.0579 | MCSE(6.27) = 2.95 | stat: TRUE | burn: 0 | rel.err: 0.49
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

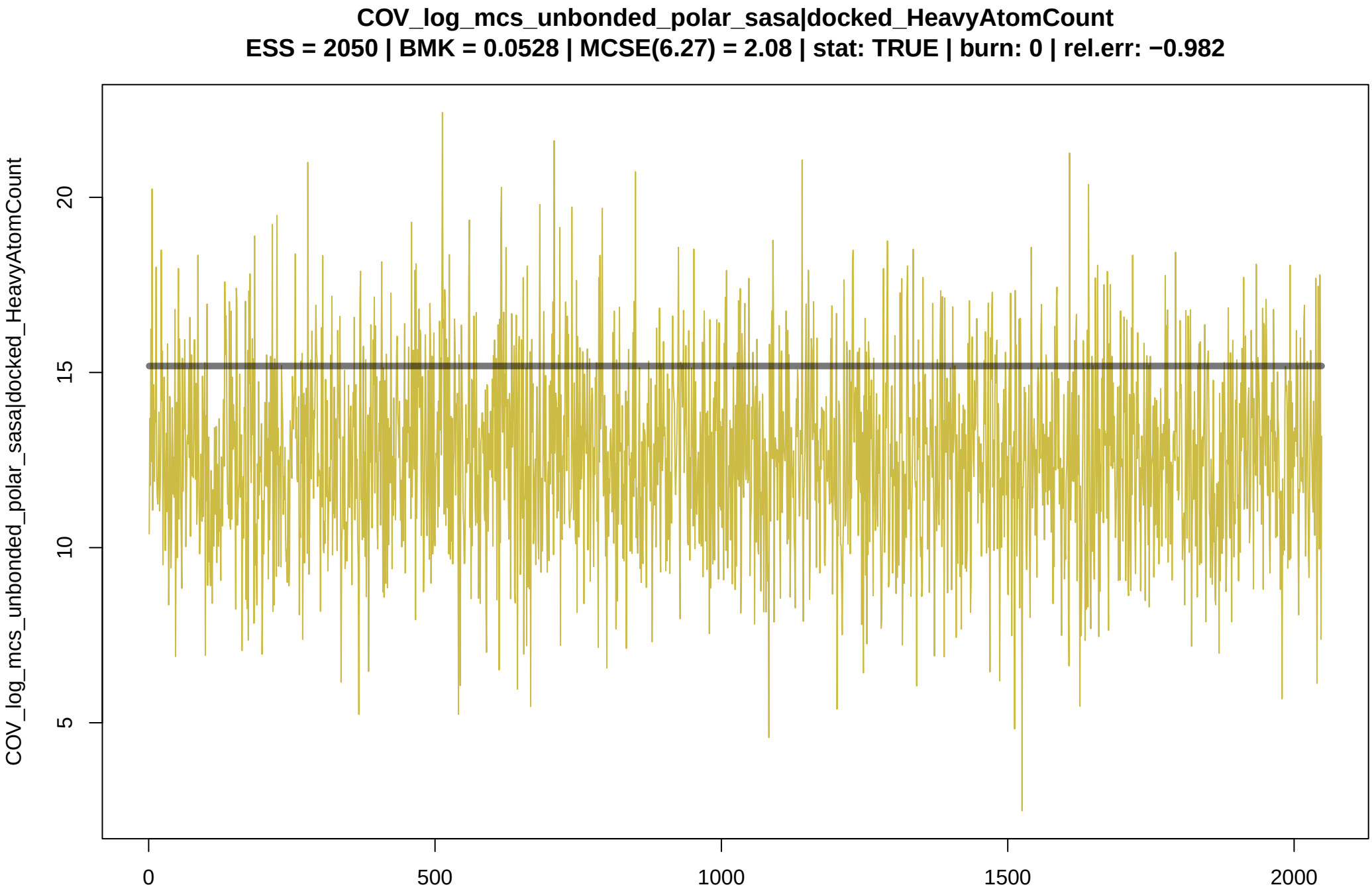

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.073 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0 | rel.err: 0.101
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

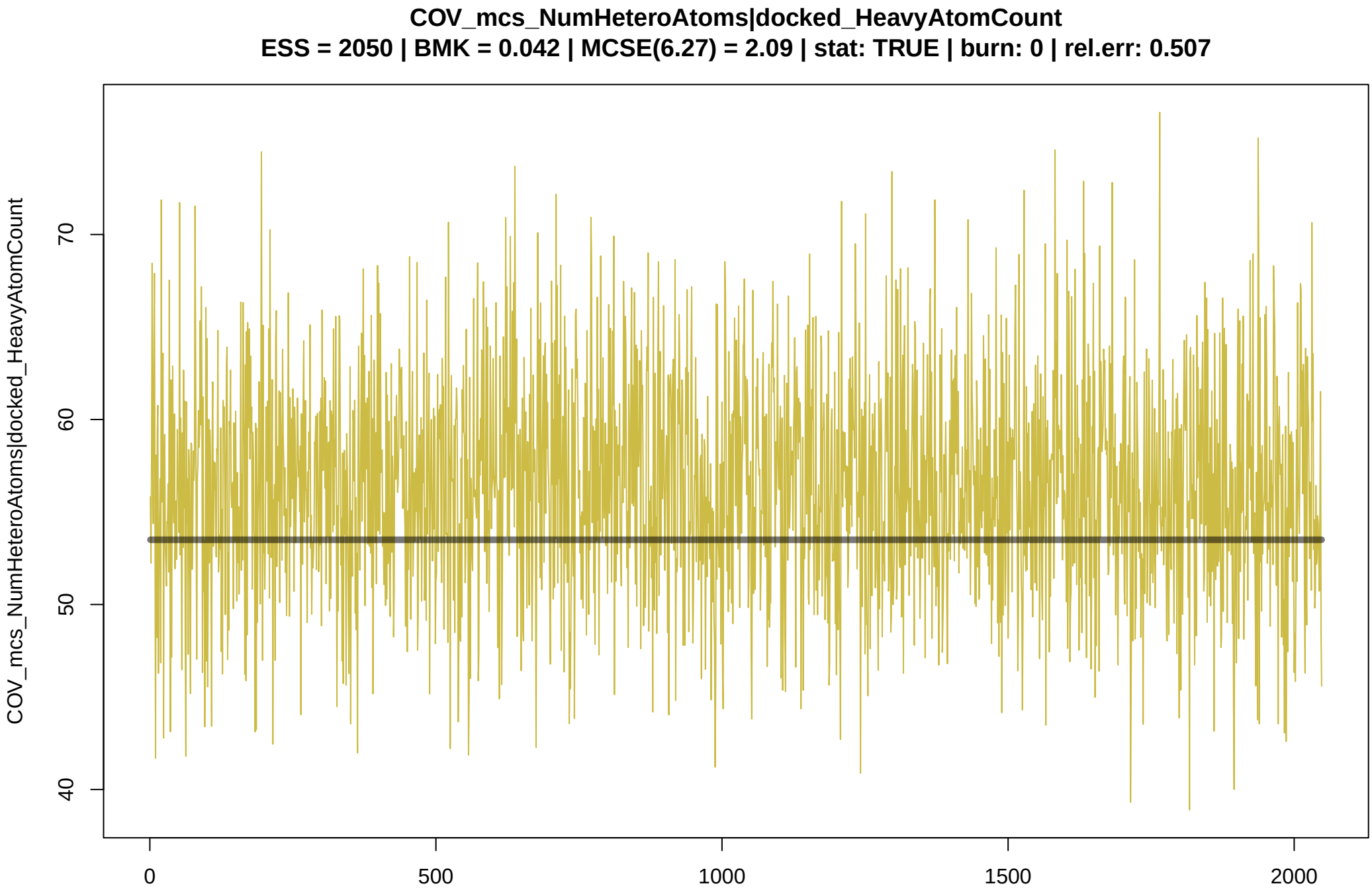

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1870 | BMK = 0.0597 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0 | rel.err: 0.532
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1850 | BMK = 0.0458 | MCSE(6.27) = 2.1 | 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 = 0.0461 | MCSE(6.27) = 2.16 | stat: TRUE | 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 = 2050 | BMK = 0.0548 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0 | rel.err: −0.502
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 = 0.0528 | MCSE(6.27) = 2.08 | stat: TRUE | burn: 0 | rel.err: −0.982
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 = 0.042 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.507
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
500
1000
1500
2000