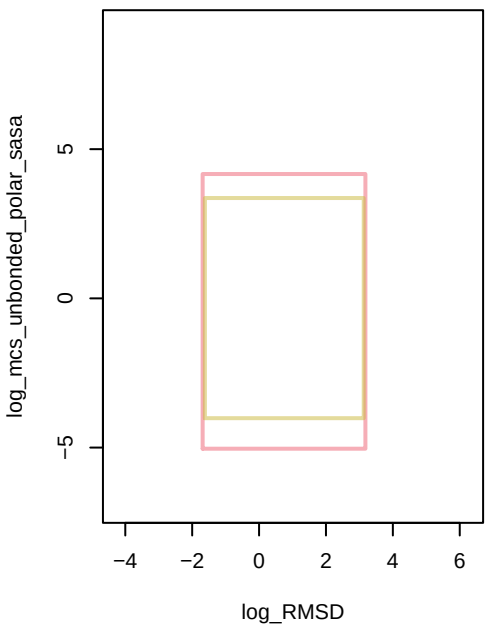
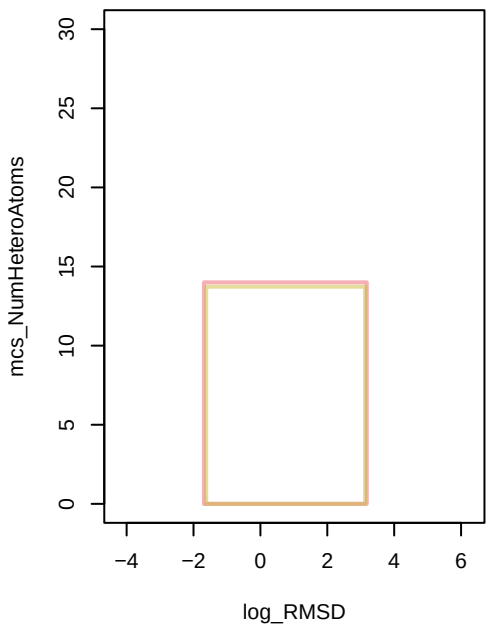
−− STATS maxD −−
min ESS = 131.525732984592
max BMK = 0.168607999608427
max MCSE = 7.2136827628264
all stationary: FALSE
burn: 0
max rel.err.: 1.90878407299402

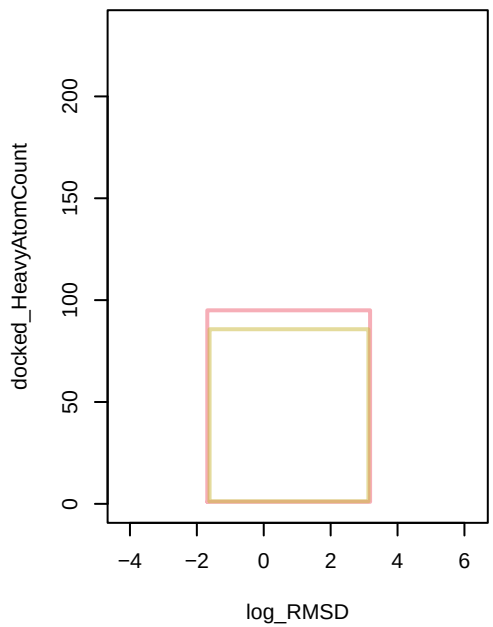
−− STATS 2D −−
min ESS = 1614.44257168966
max BMK = 0.067634953344977
max MCSE = 2.5282119029574
all stationary: TRUE
burn: 0
max rel.err.: 1.74053544499318

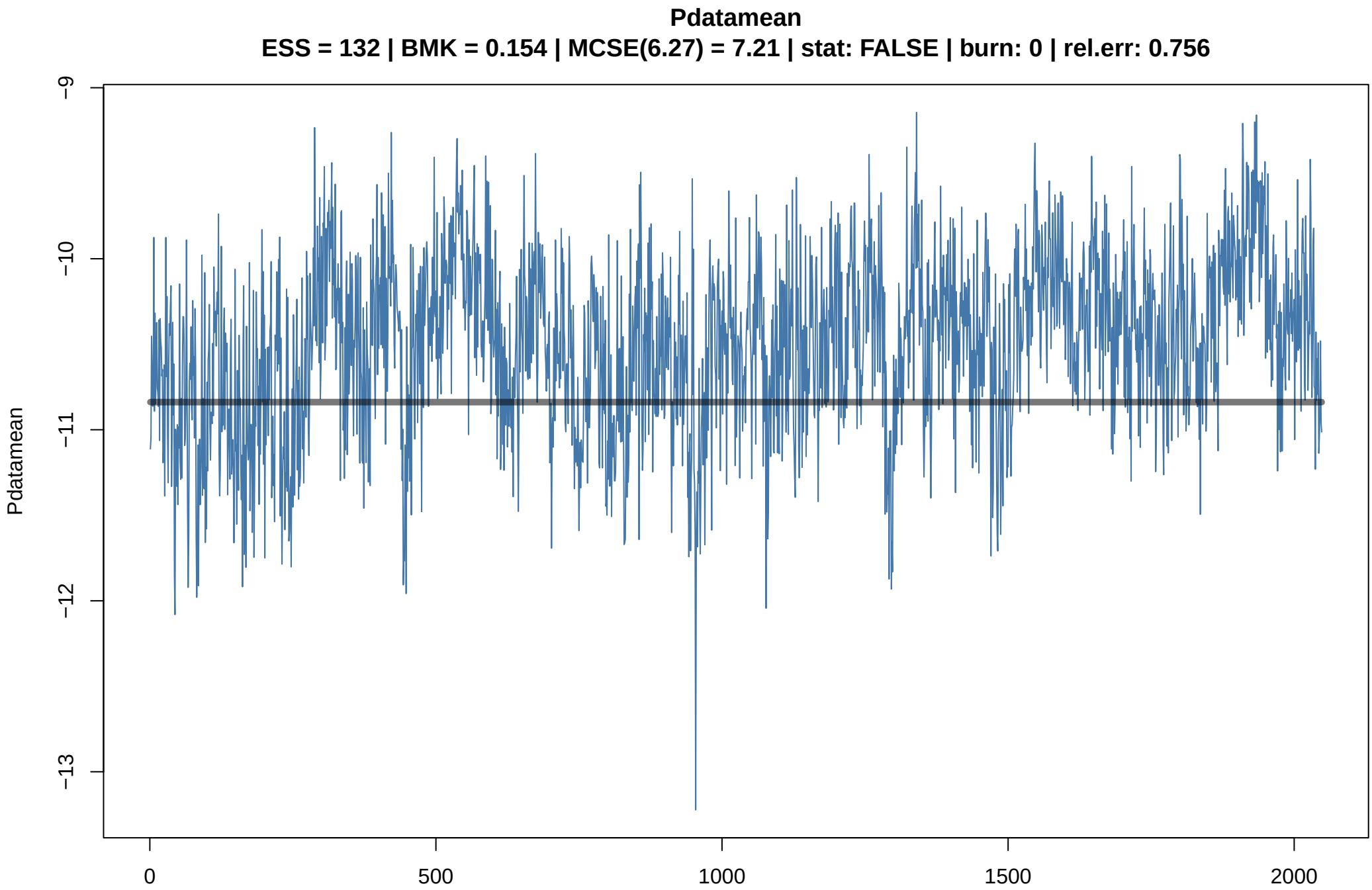
−− STATS 1D −−
min ESS = 1692.05406500034
max BMK = 0.074837512465284
max MCSE = 2.90099073427199
all stationary: TRUE
burn: 0
max rel.err.: 2.28514093787467

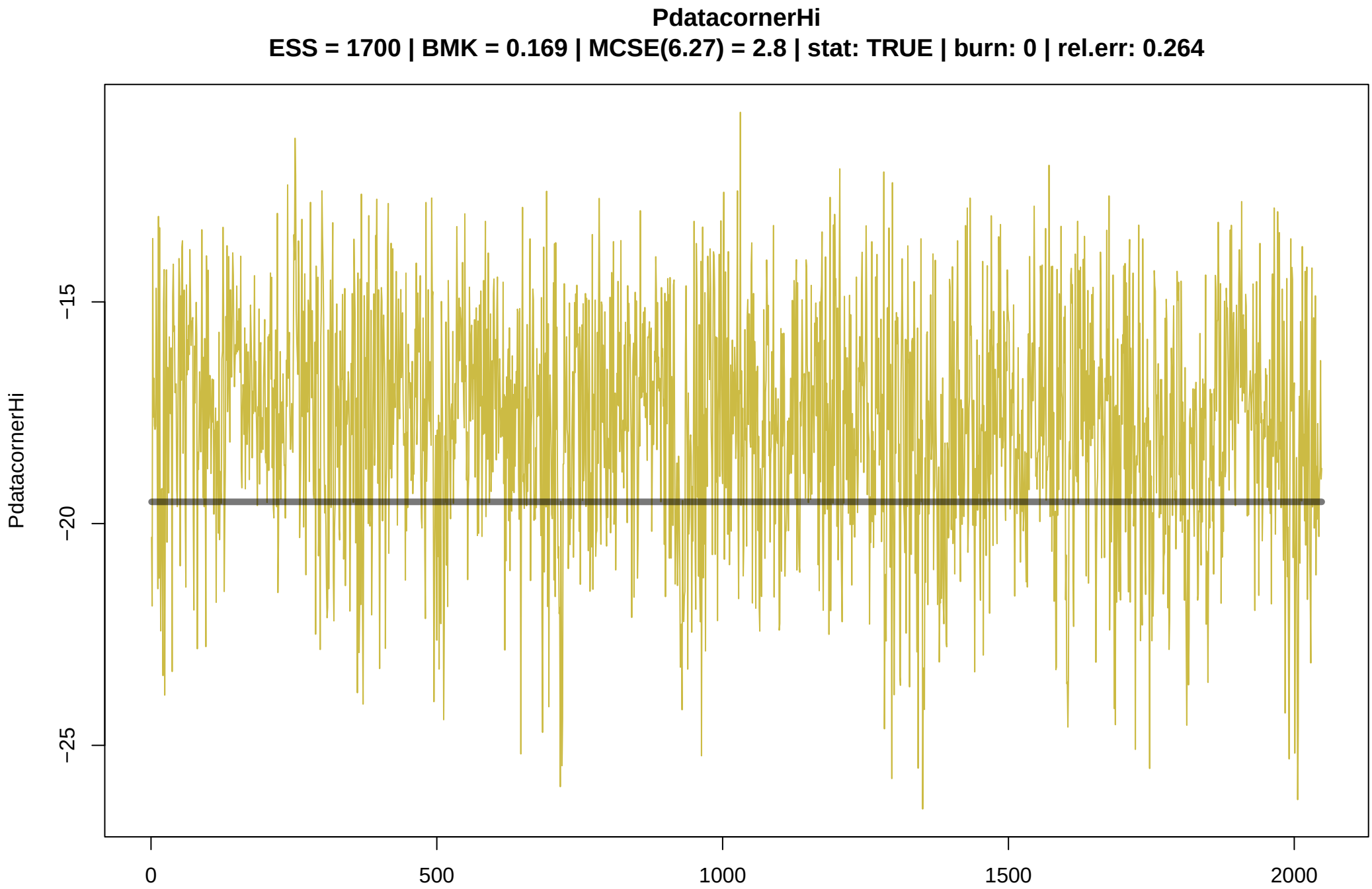
Occupied clusters: 10 of 16

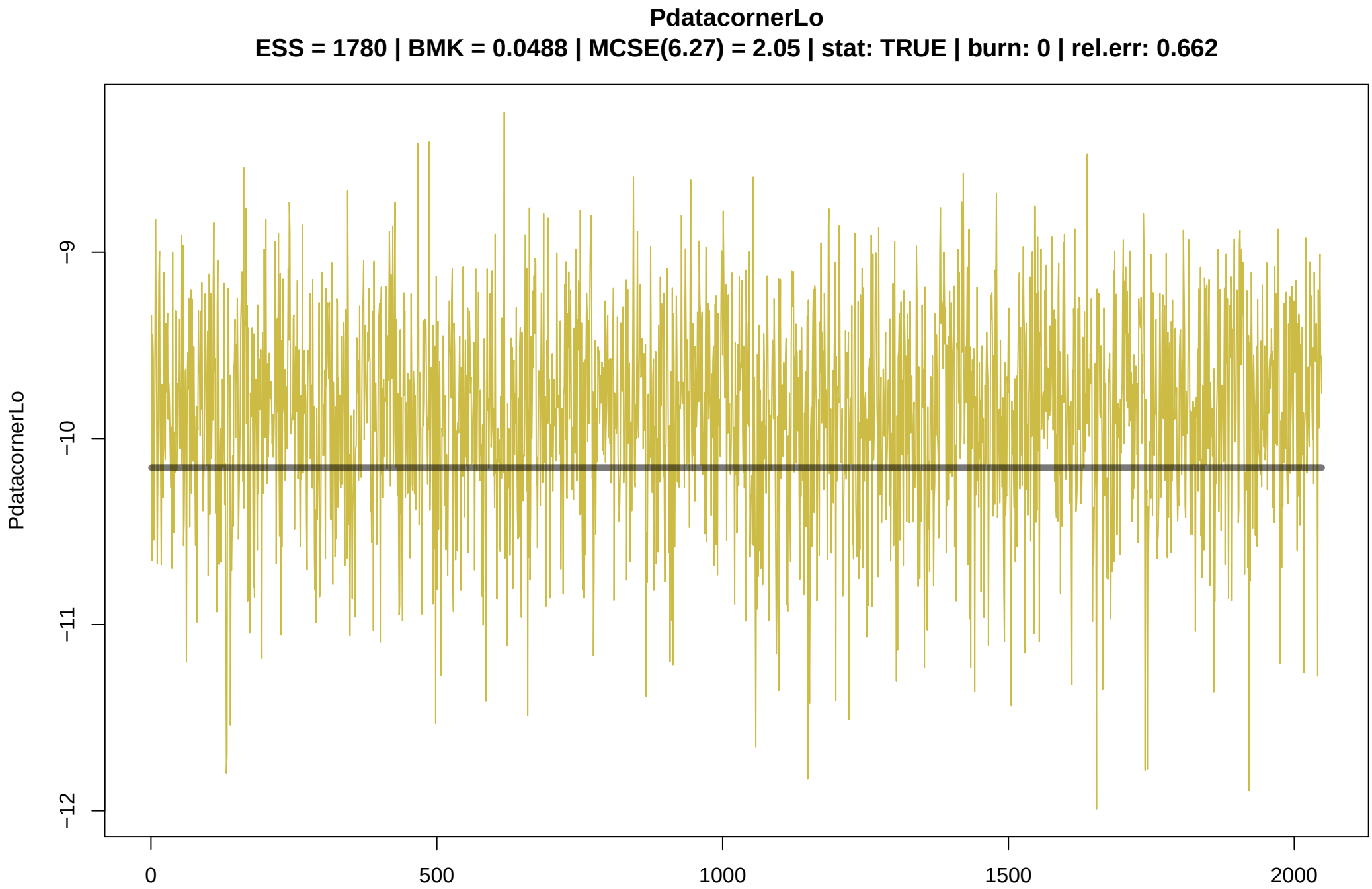

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
6
log_RMSD

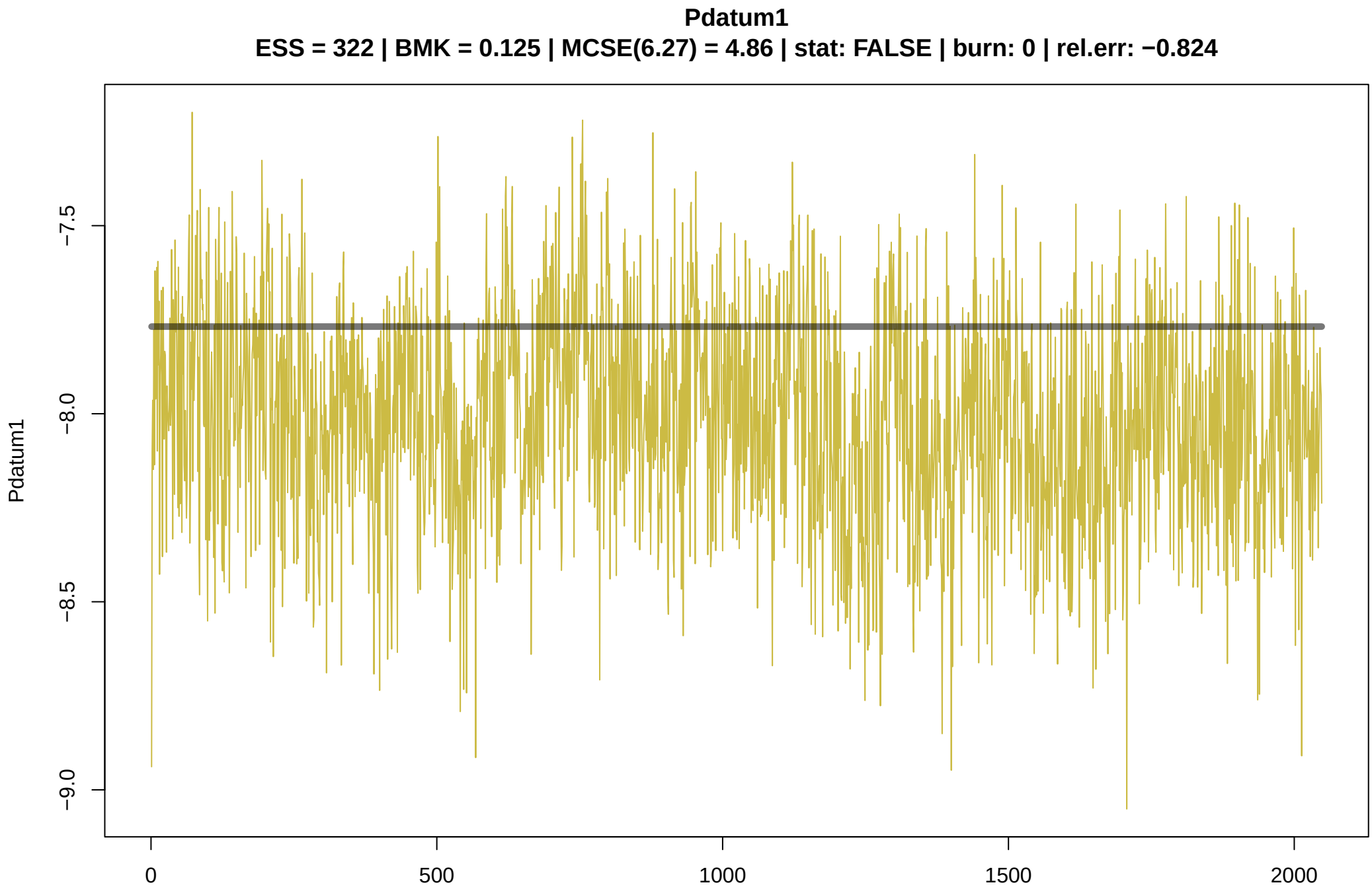

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

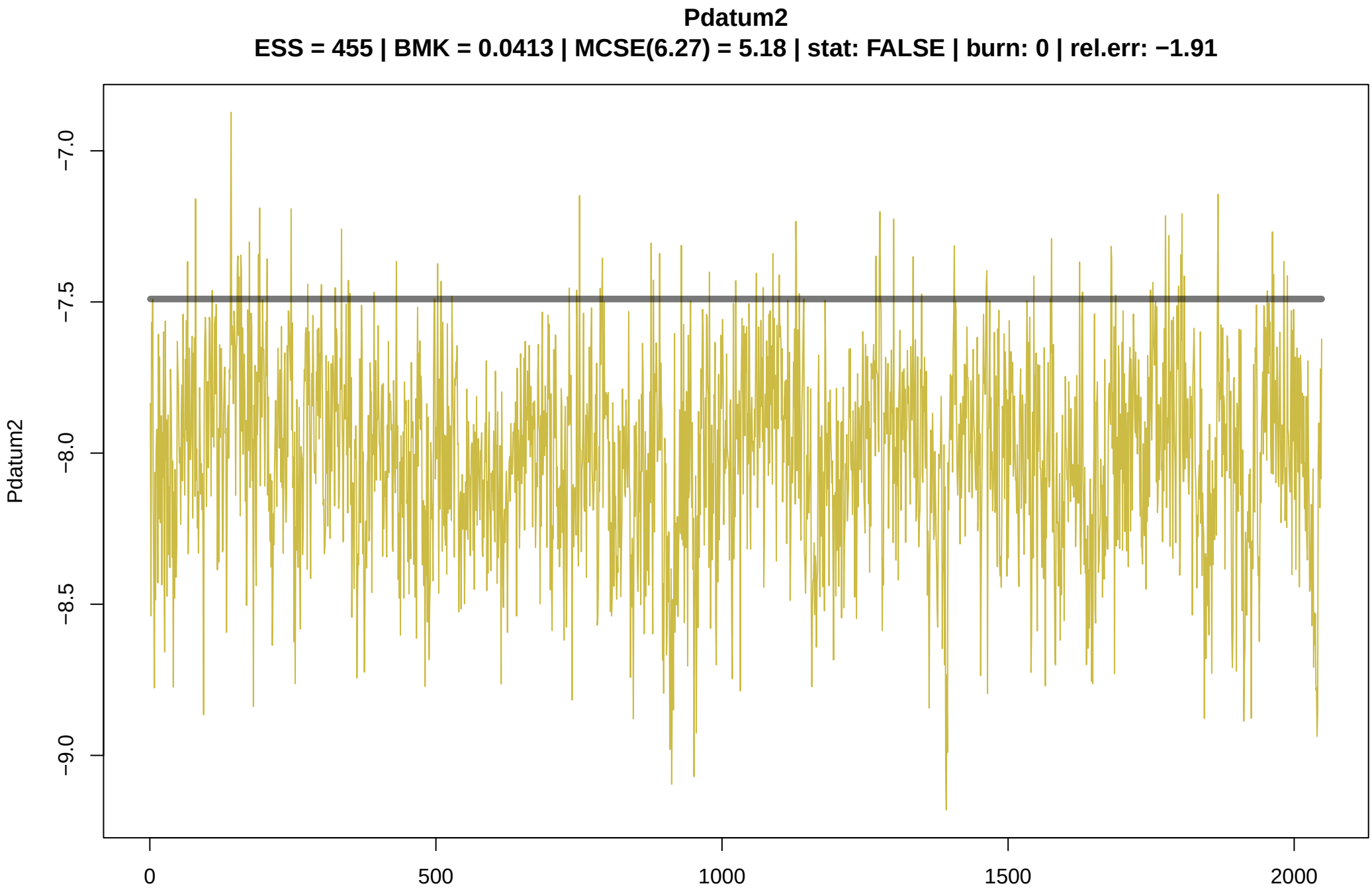

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

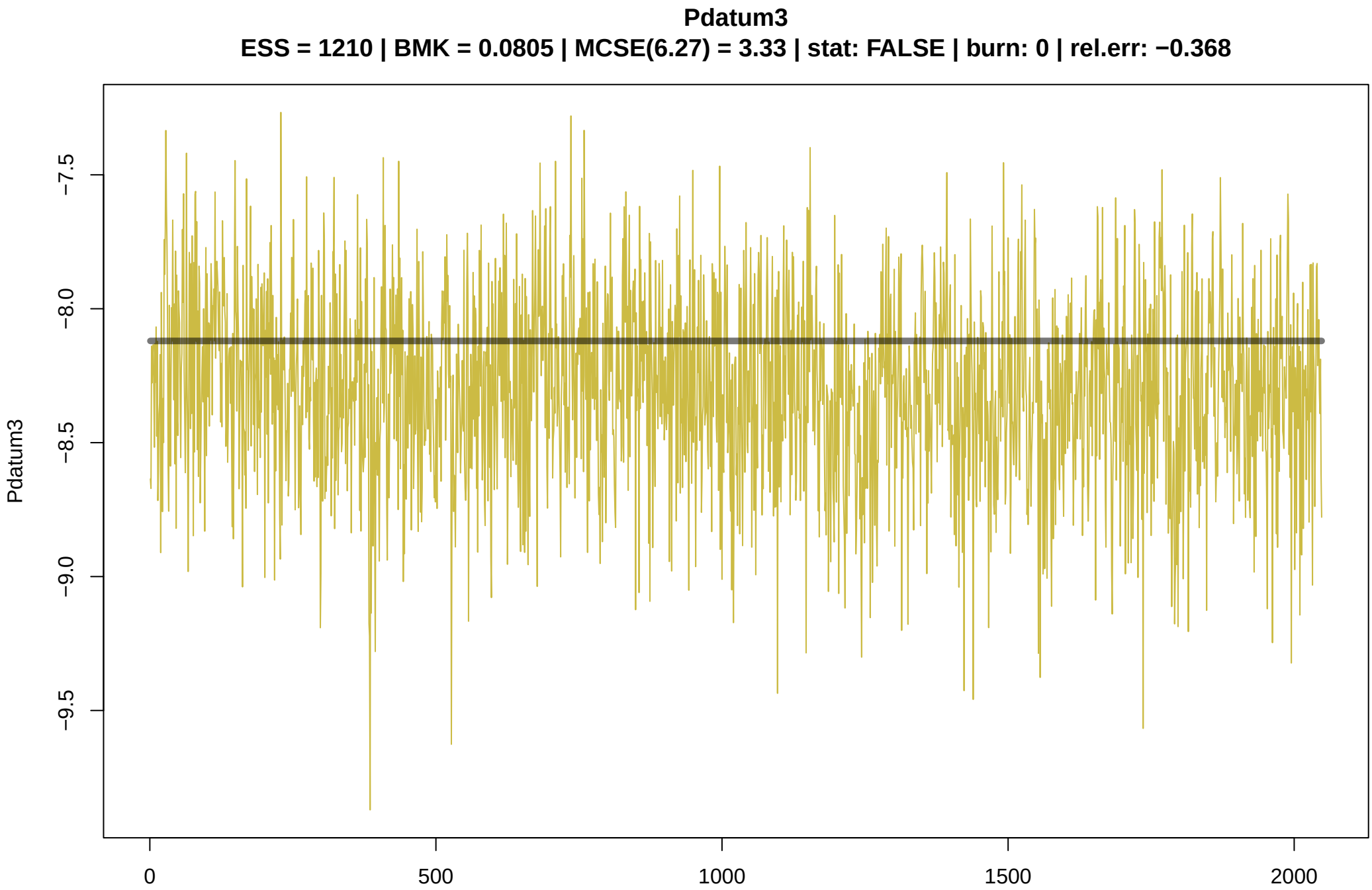

Pdatamean
ESS = 132 | BMK = 0.154 | MCSE(6.27) = 7.21 | stat: FALSE | burn: 0 | rel.err: 0.756
Pdatamean
−9
−10
−11
−12
−13
0
500
1000
1500
2000

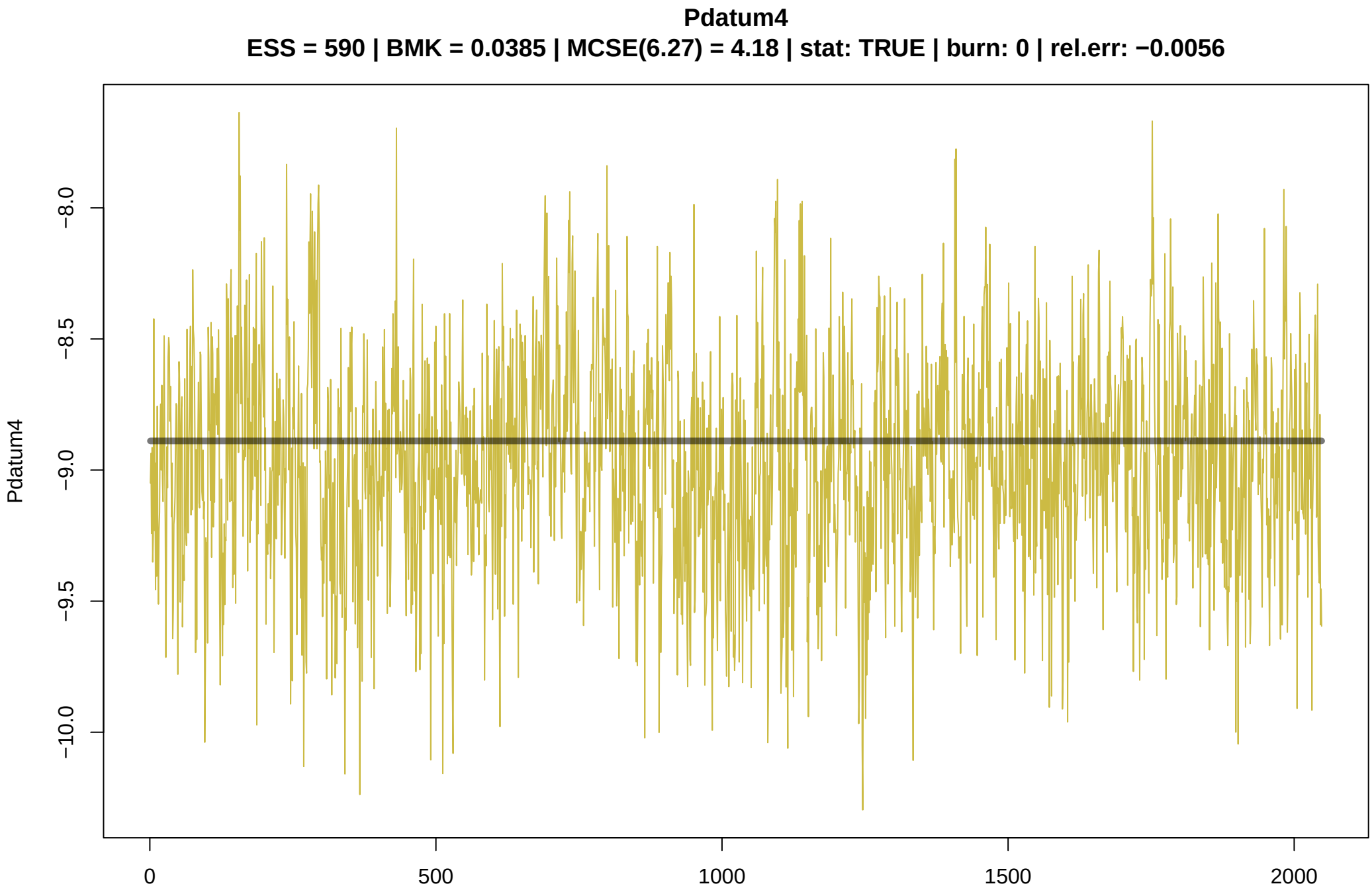

PdatacornerHi
ESS = 1700 | BMK = 0.169 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0 | rel.err: 0.264
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

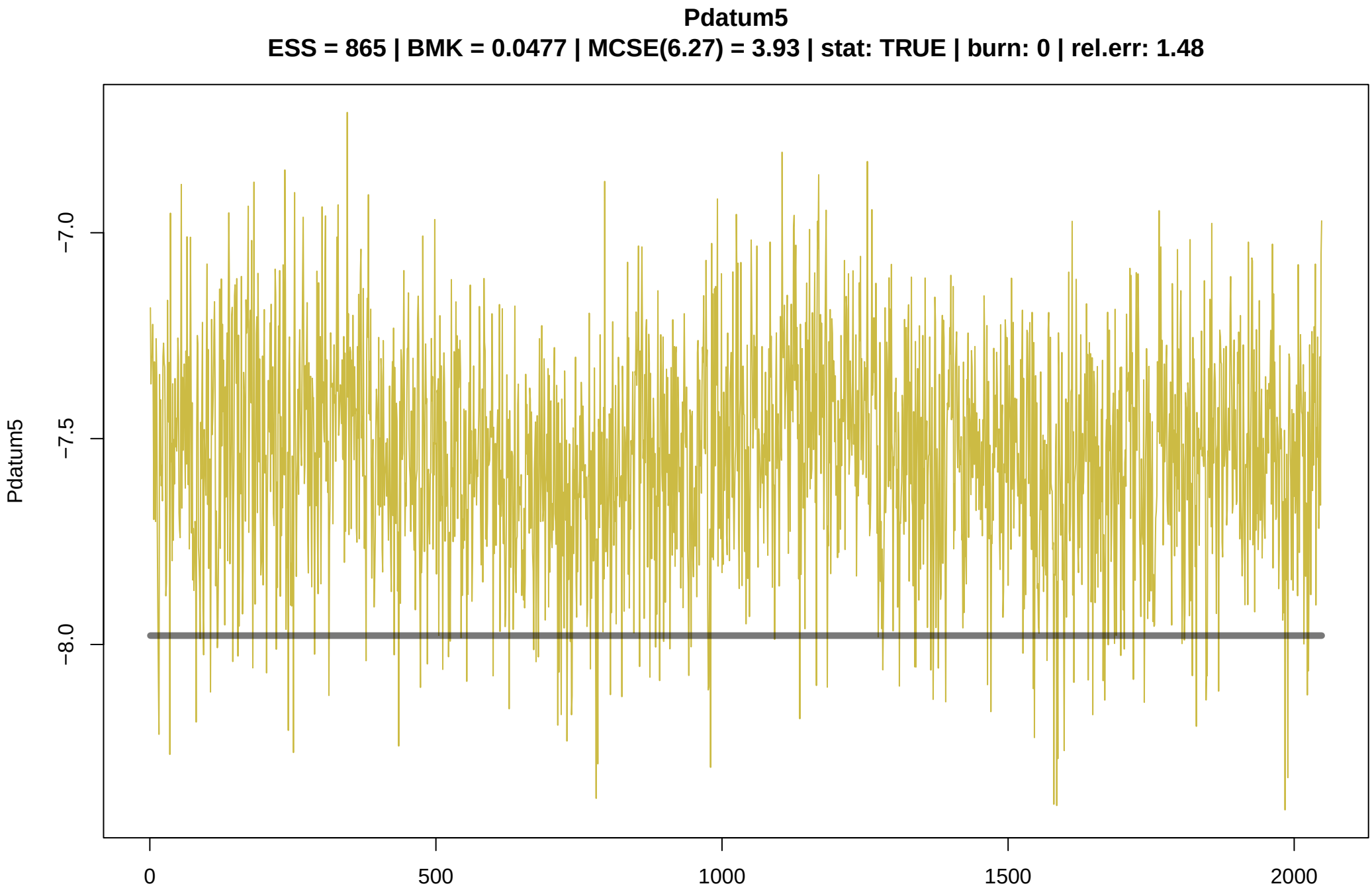

PdatacornerLo
ESS = 1780 | BMK = 0.0488 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0 | rel.err: 0.662
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

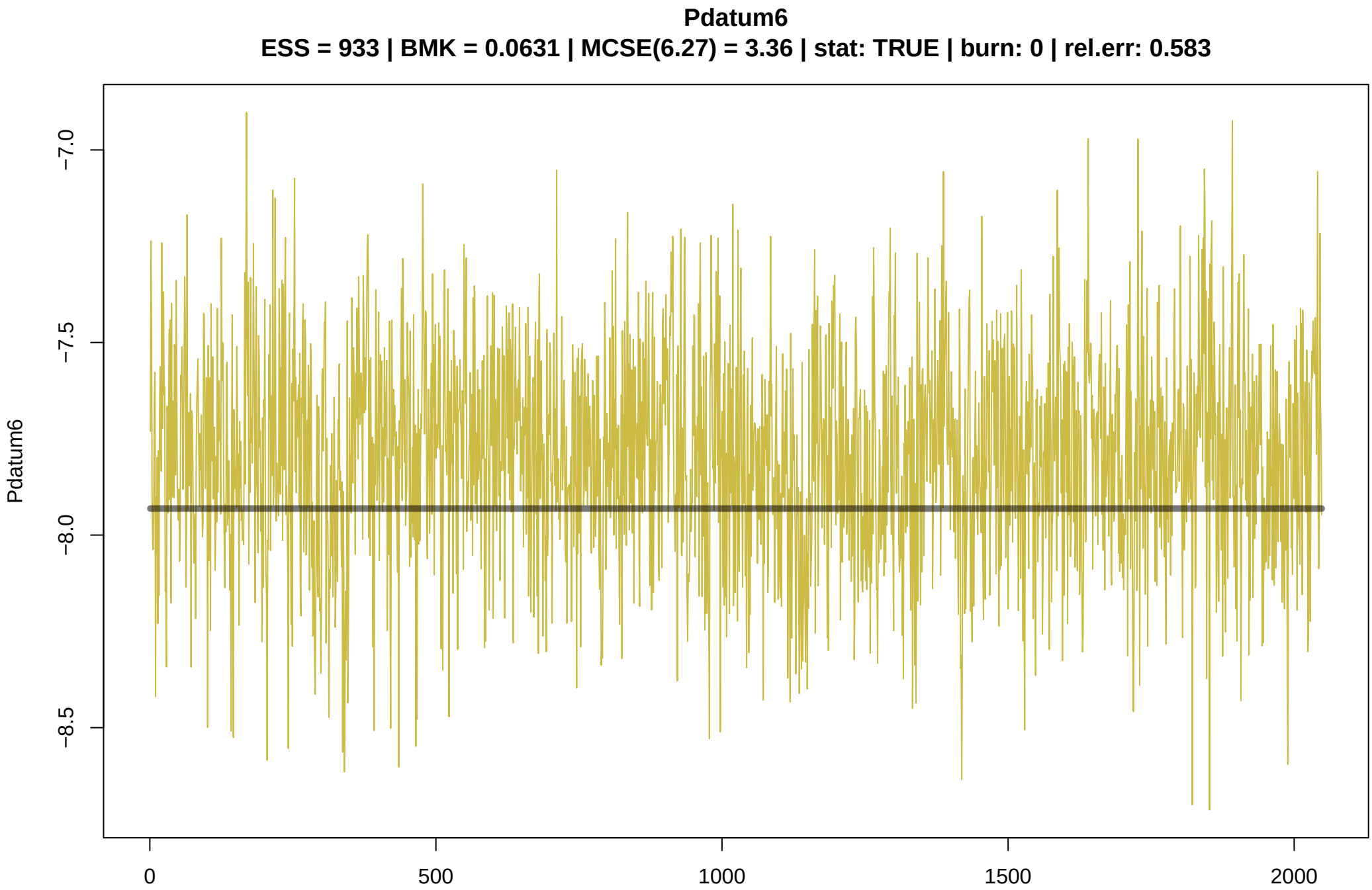

Pdatum1
ESS = 322 | BMK = 0.125 | MCSE(6.27) = 4.86 | stat: FALSE | burn: 0 | rel.err: −0.824
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

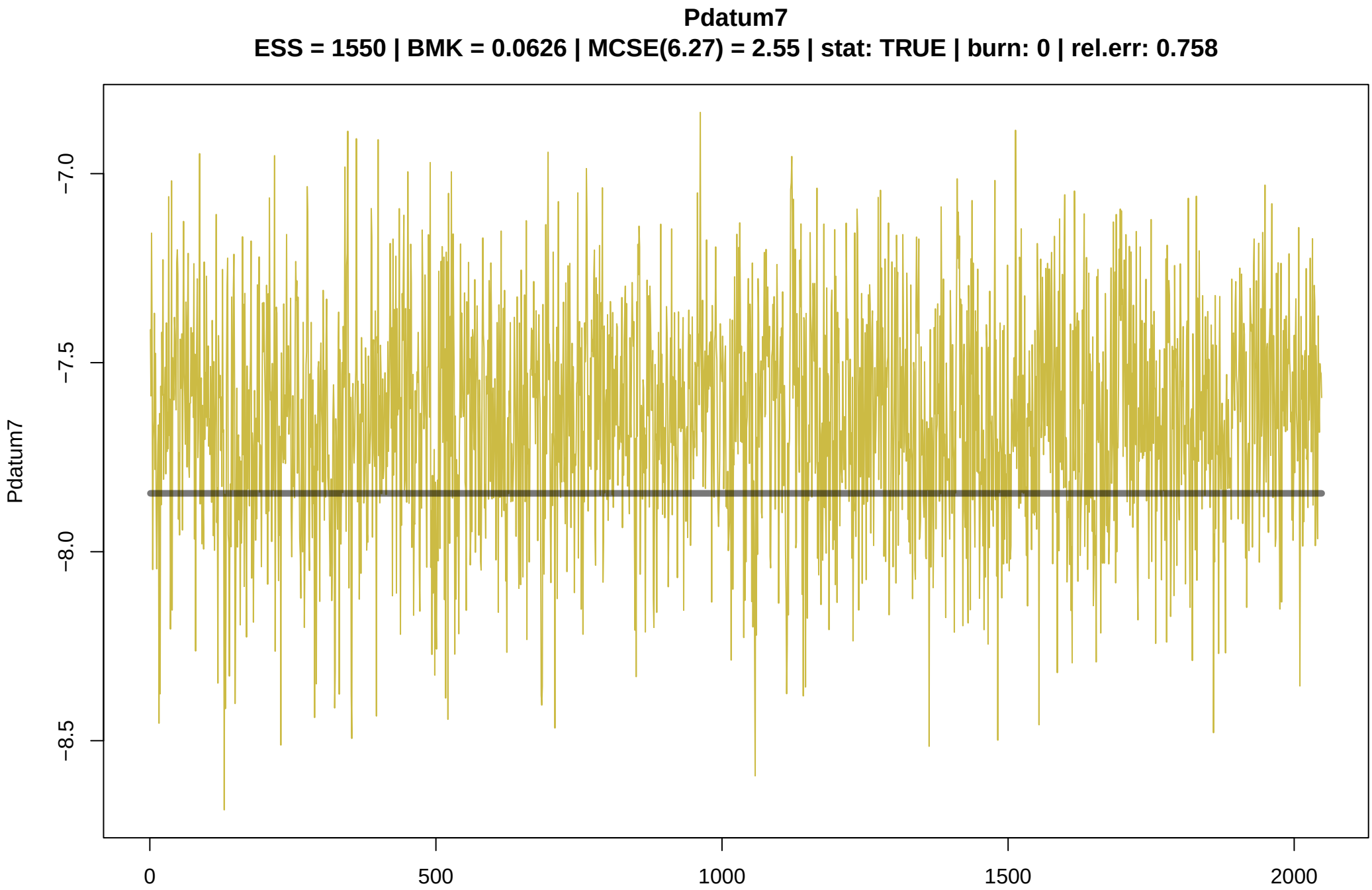

Pdatum2
ESS = 455 | BMK = 0.0413 | MCSE(6.27) = 5.18 | stat: FALSE | burn: 0 | rel.err: −1.91
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

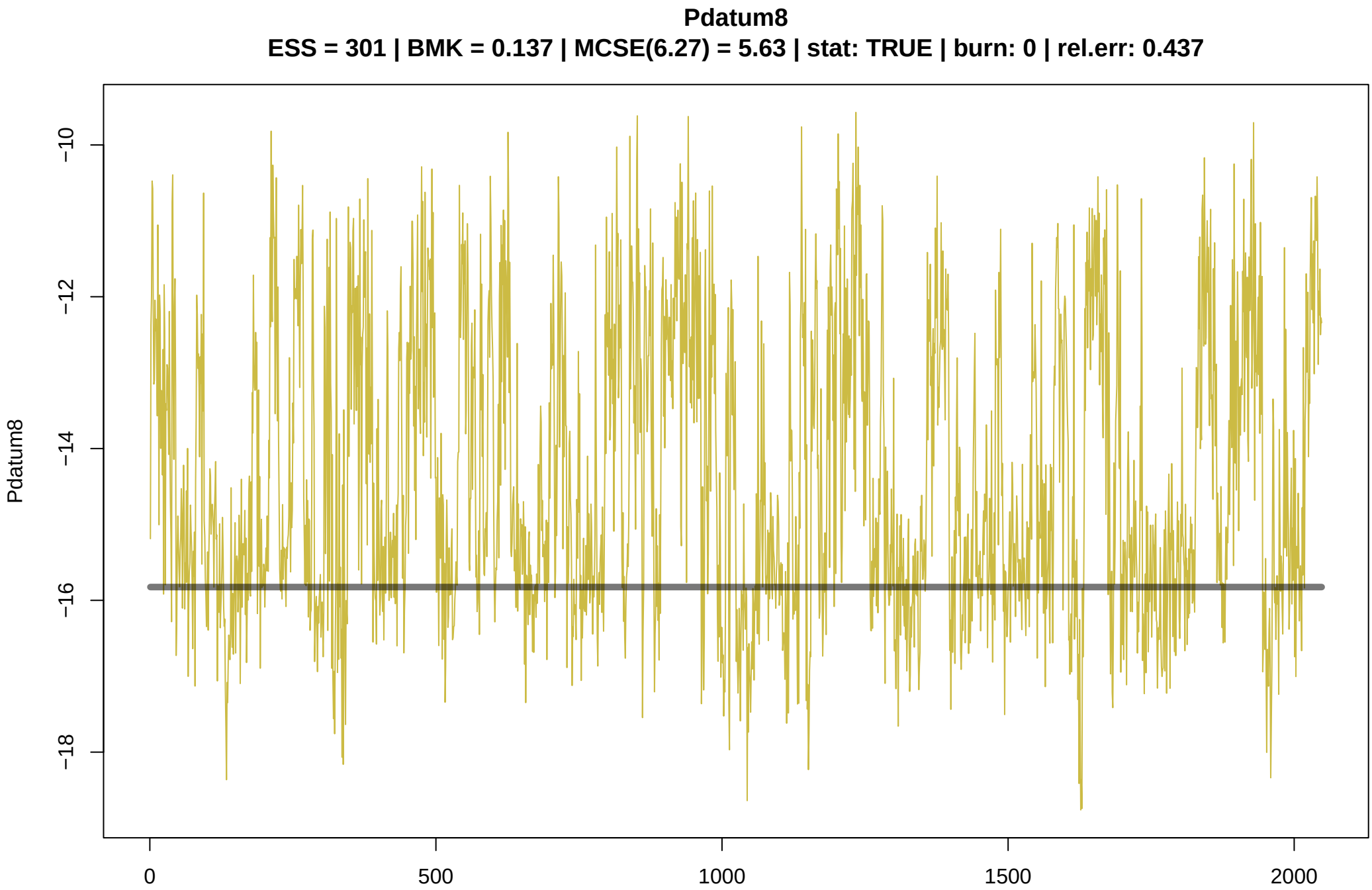

Pdatum3
ESS = 1210 | BMK = 0.0805 | MCSE(6.27) = 3.33 | stat: FALSE | burn: 0 | rel.err: −0.368
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

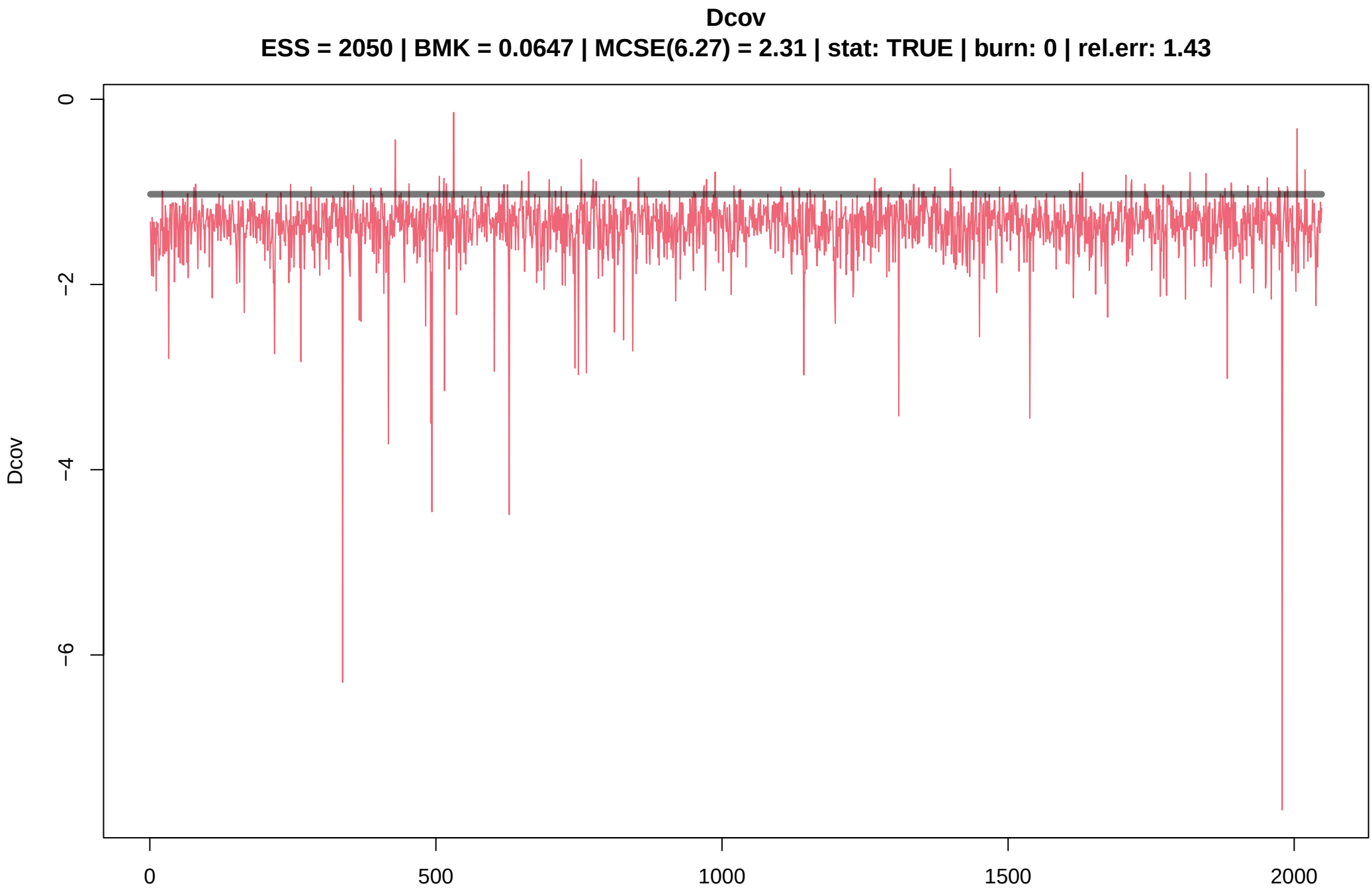

Pdatum4
ESS = 590 | BMK = 0.0385 | MCSE(6.27) = 4.18 | stat: TRUE | burn: 0 | rel.err: −0.0056
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

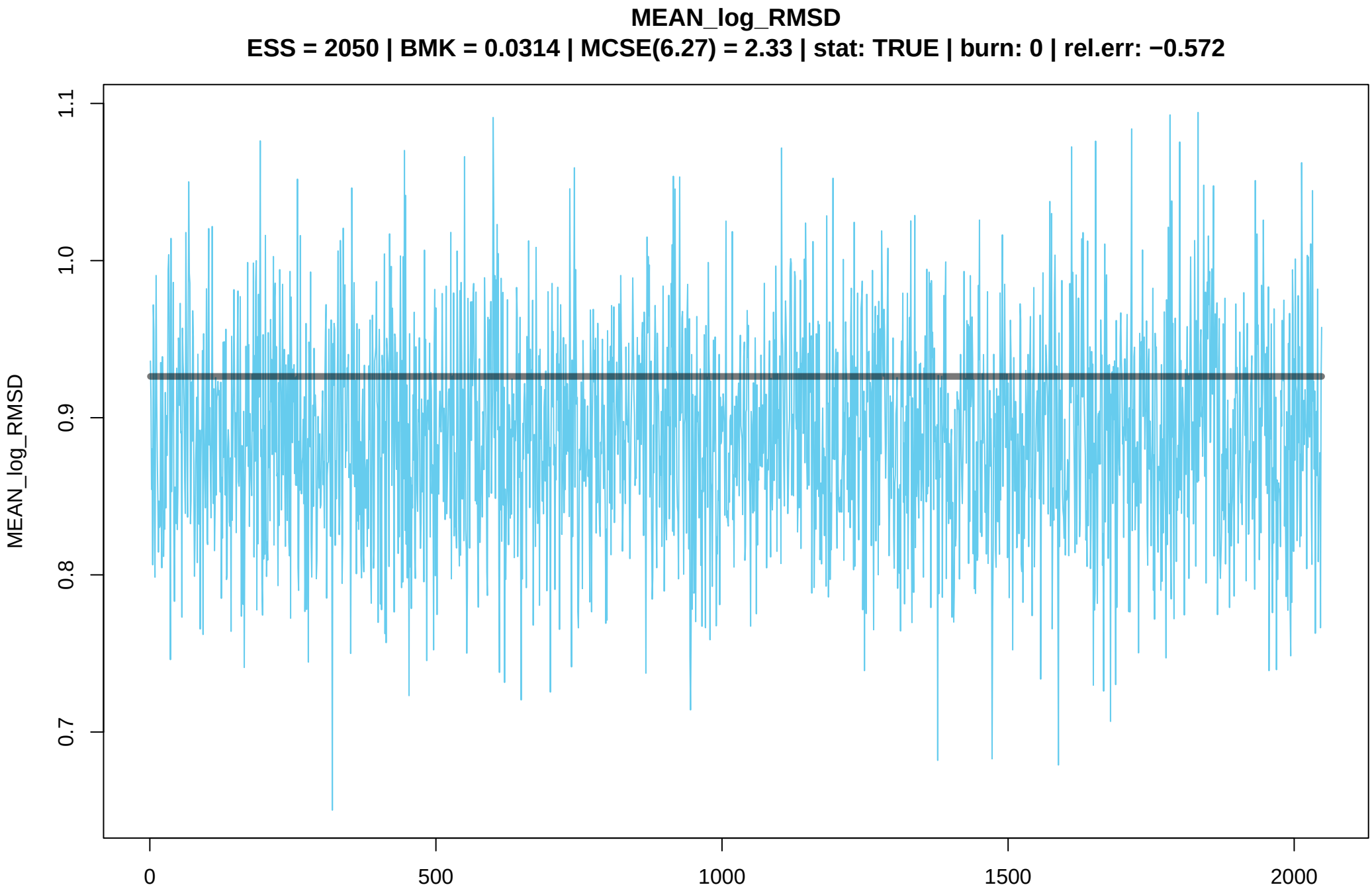

Pdatum5
ESS = 865 | BMK = 0.0477 | MCSE(6.27) = 3.93 | stat: TRUE | burn: 0 | rel.err: 1.48
Pdatum5
−7.0
−7.5
−8.0
0
500
1000
1500
2000

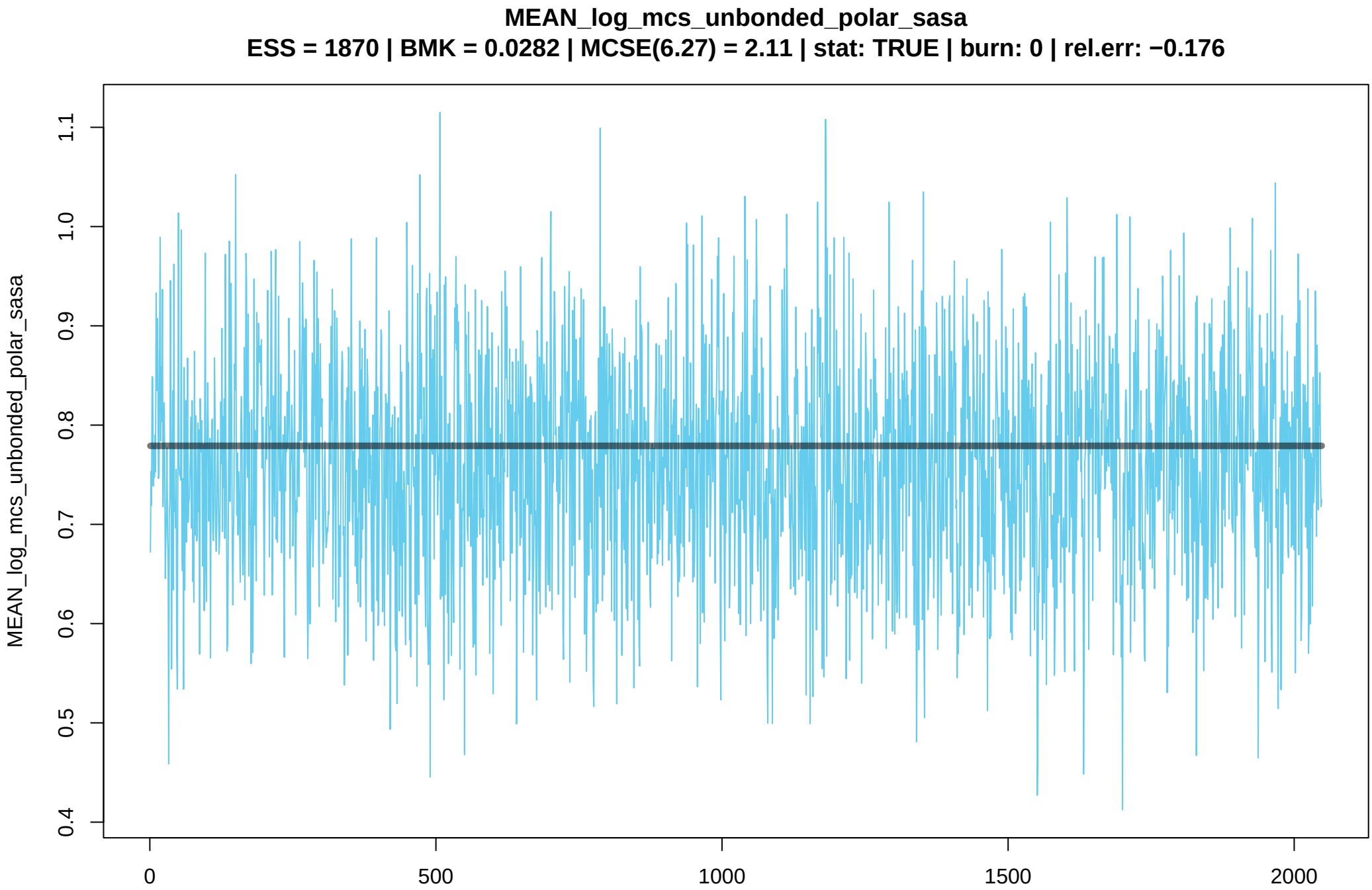

Pdatum6
ESS = 933 | BMK = 0.0631 | MCSE(6.27) = 3.36 | stat: TRUE | burn: 0 | rel.err: 0.583
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

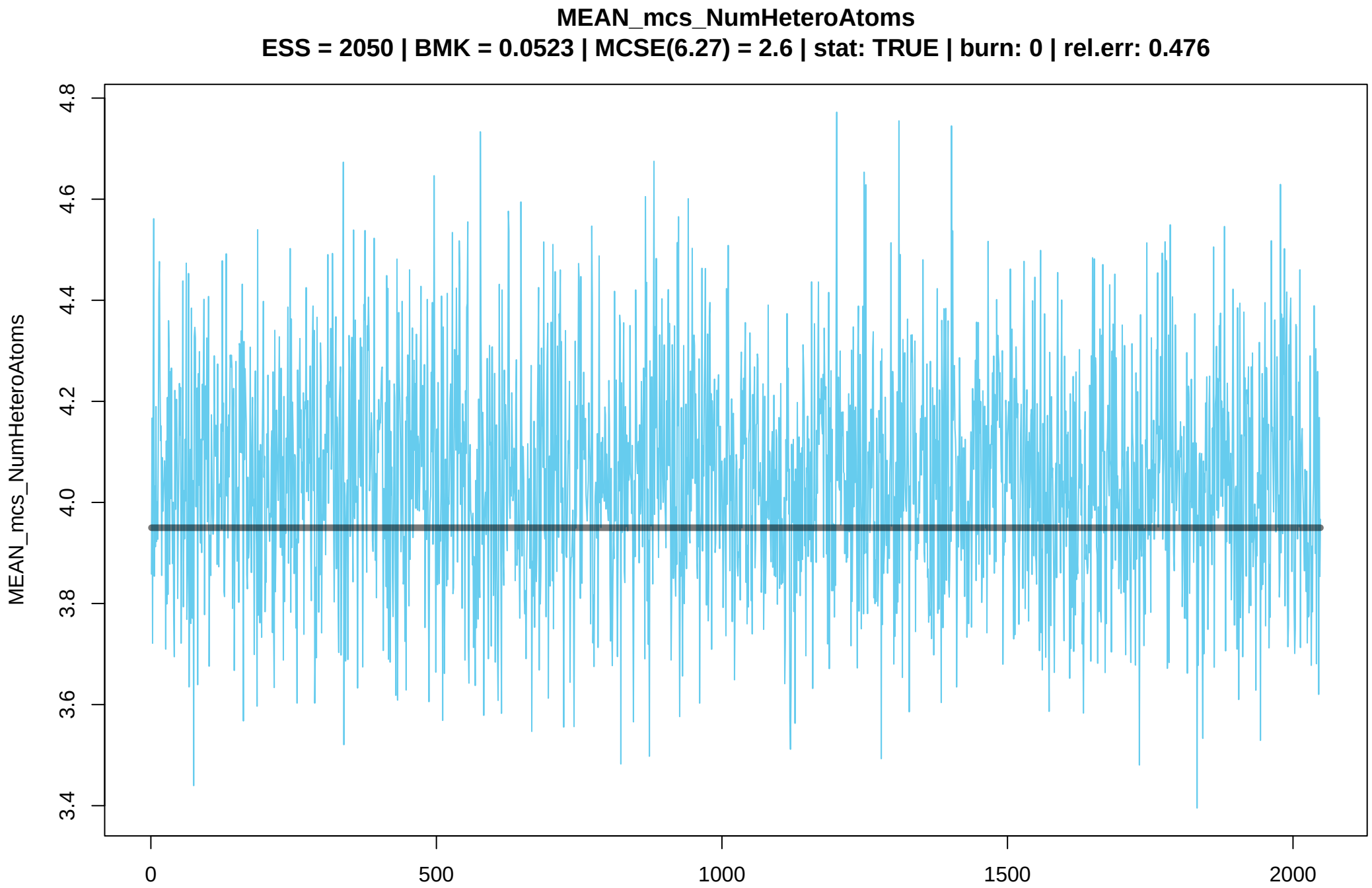

Pdatum7
ESS = 1550 | BMK = 0.0626 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 0.758
Pdatum7
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

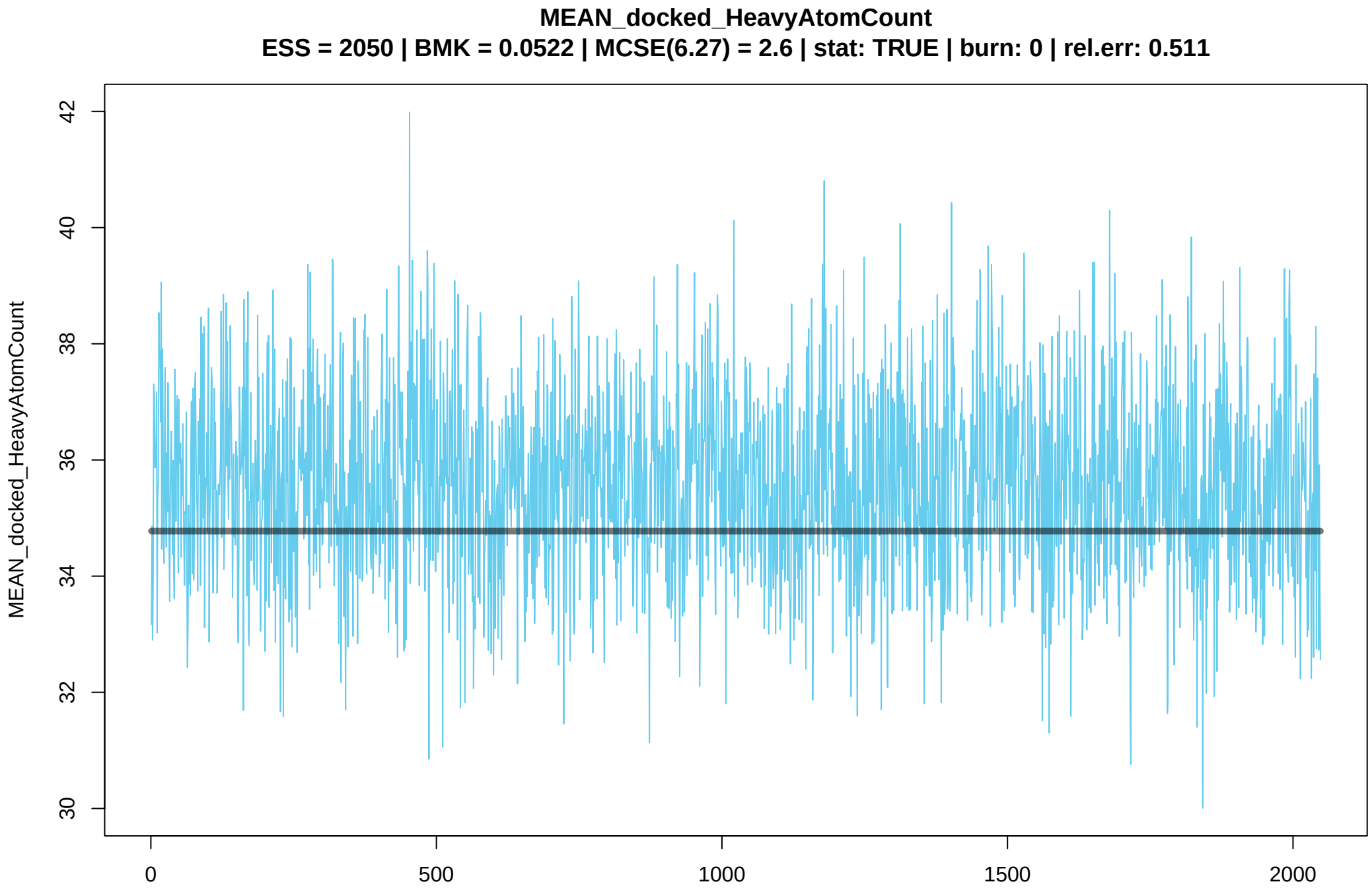

Pdatum8
ESS = 301 | BMK = 0.137 | MCSE(6.27) = 5.63 | stat: TRUE | burn: 0 | rel.err: 0.437
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

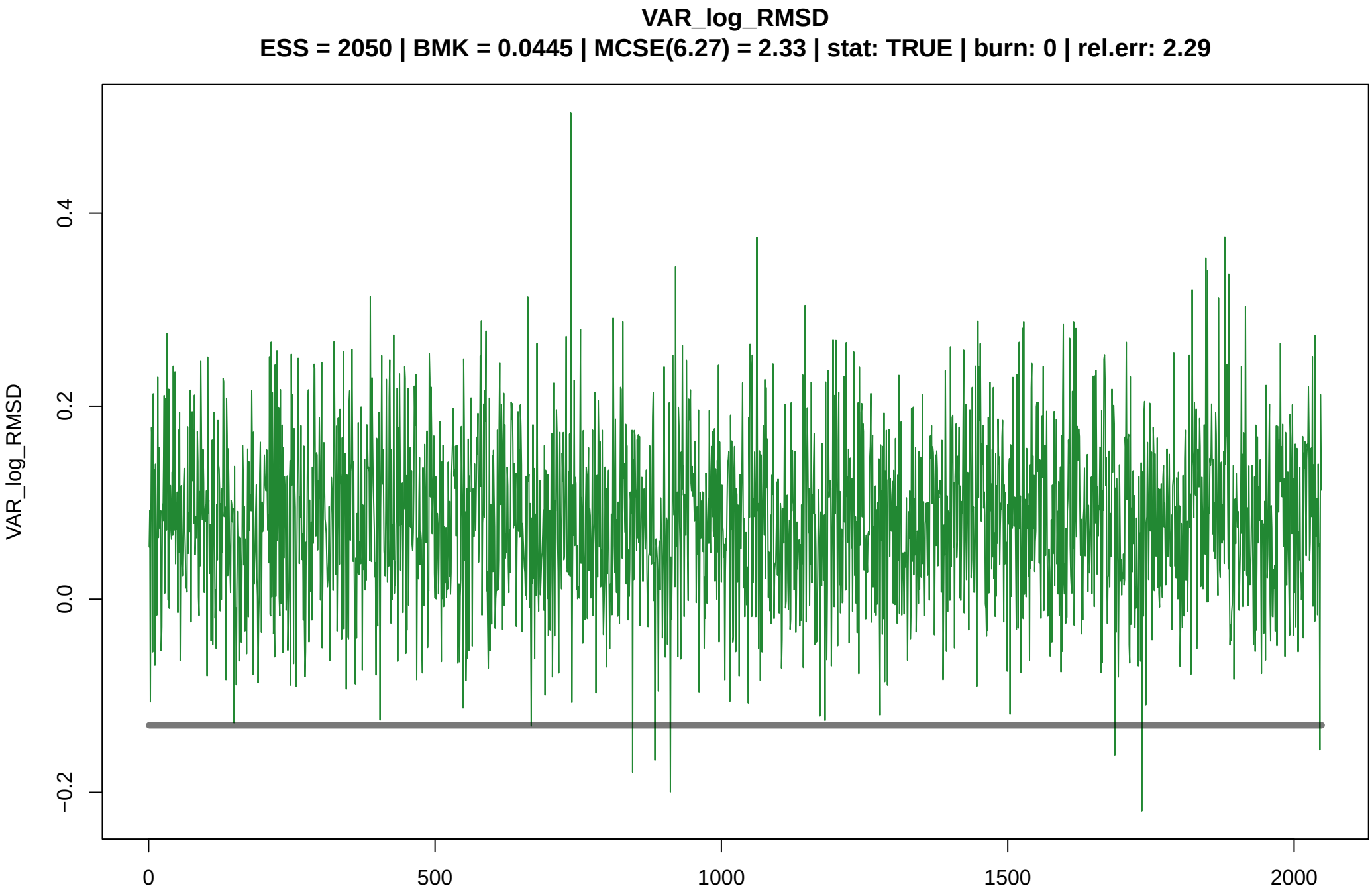

Dcov
ESS = 2050 | BMK = 0.0647 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: 1.43
Dcov
0
−2
−4
−6
0
500
1000
1500
2000

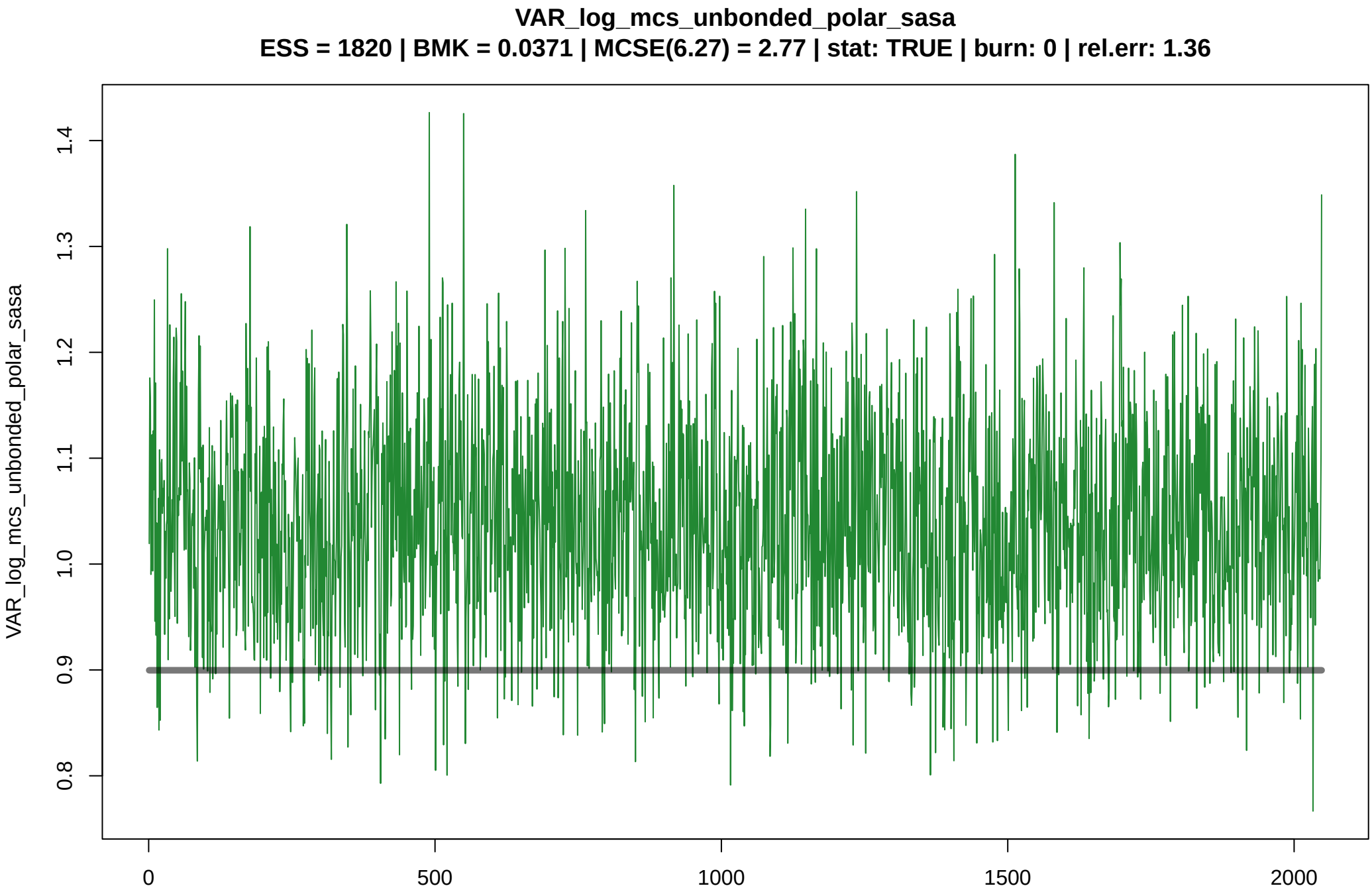

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0314 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: −0.572
MEAN_log_RMSD
1.1
1.0
0.9
0.8
0.7
0
500
1000
1500
2000

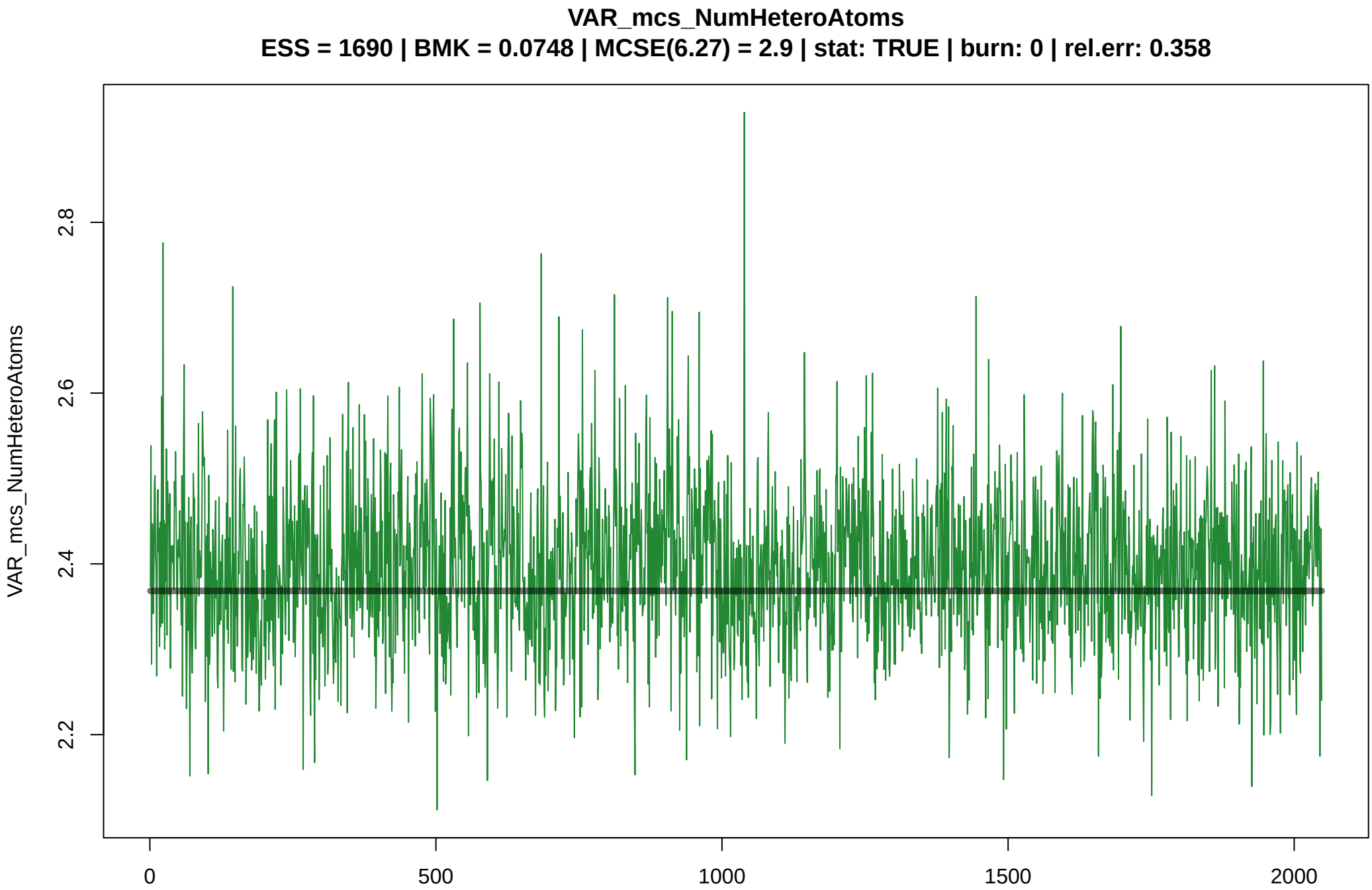

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1870 | BMK = 0.0282 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: −0.176
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

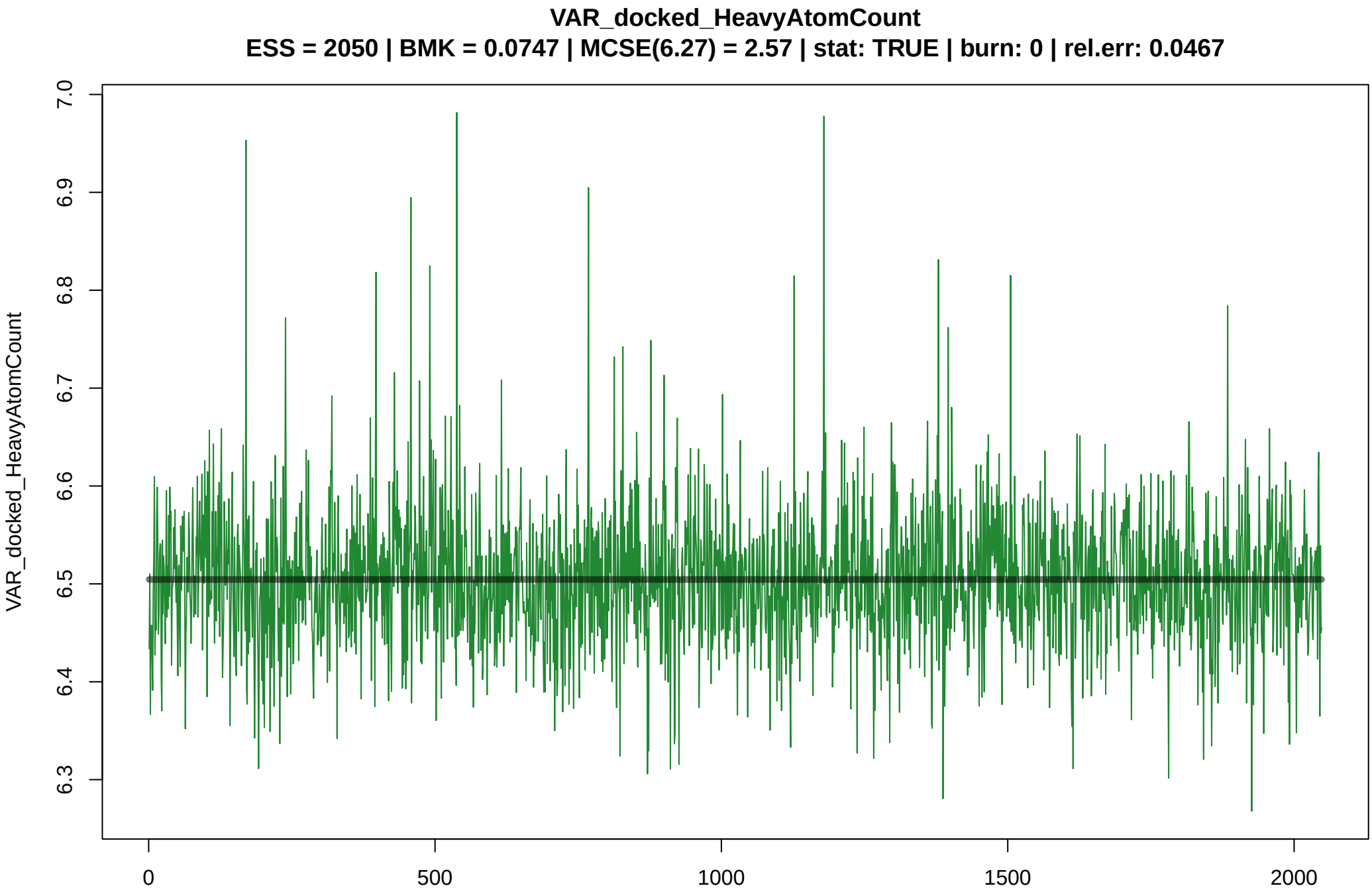

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0523 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 0.476
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

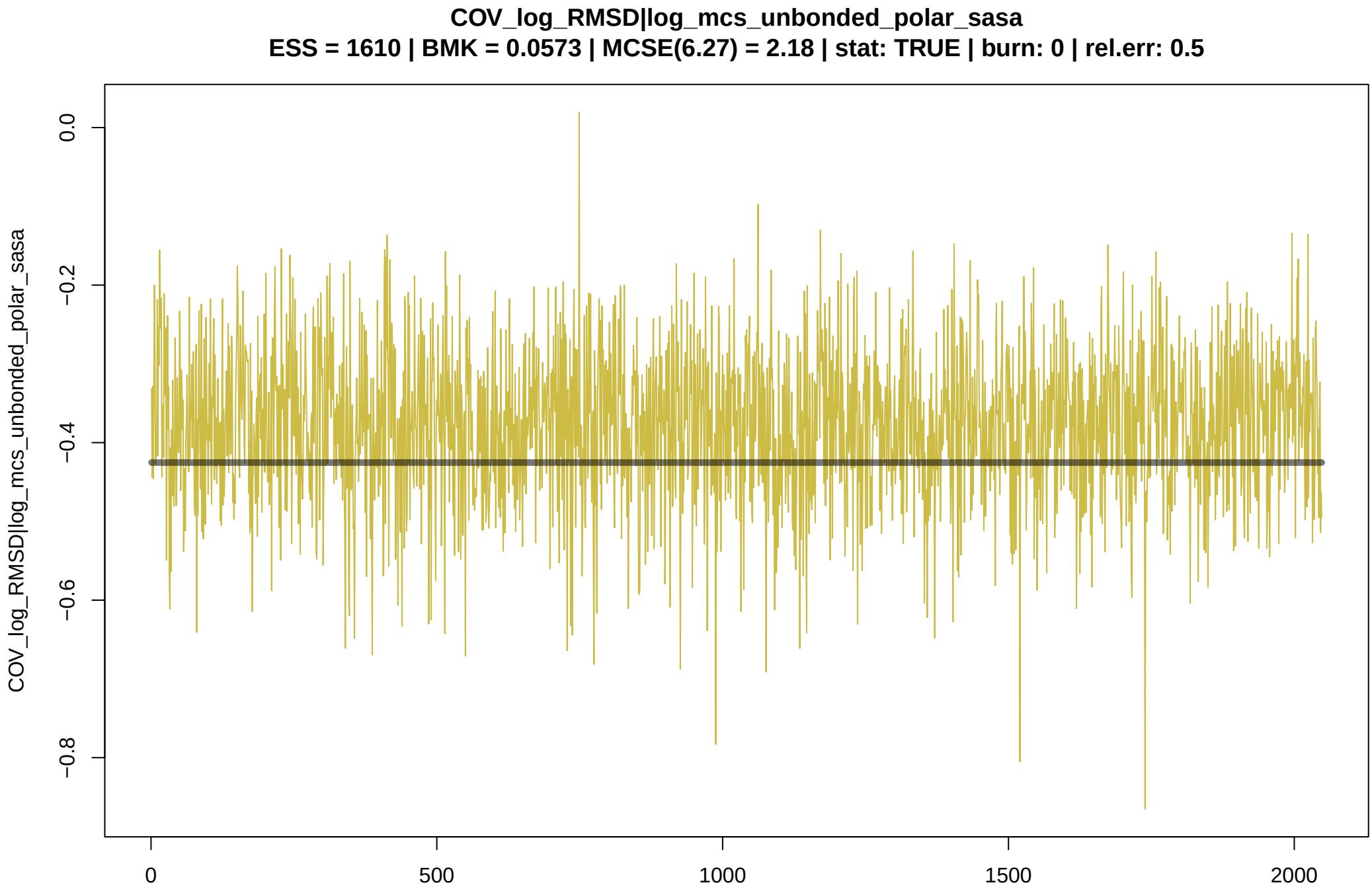

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0522 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0 | rel.err: 0.511
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
42
0
500
1000
1500
2000

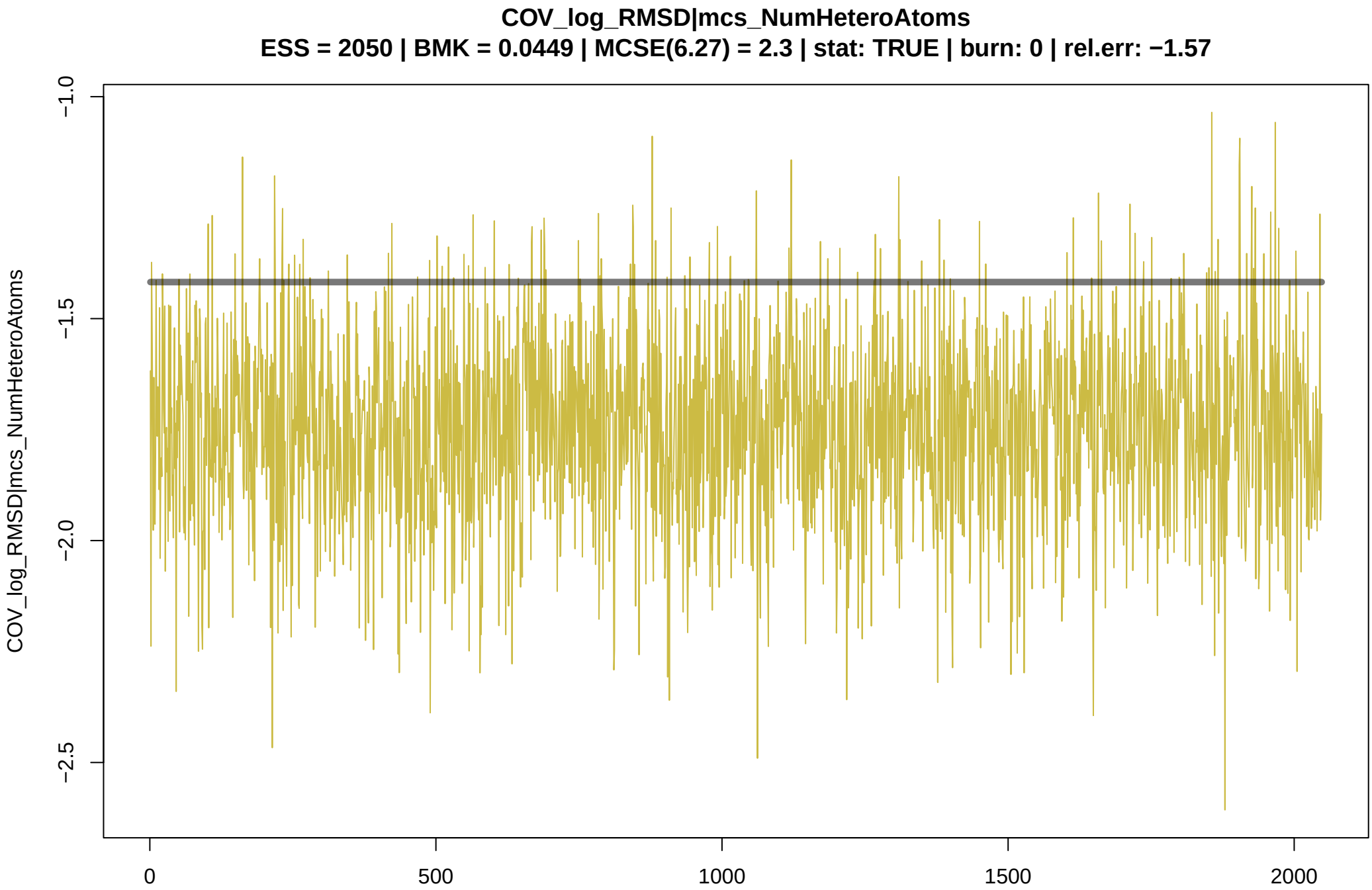

VAR_log_RMSD
ESS = 2050 | BMK = 0.0445 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0 | rel.err: 2.29
VAR_log_RMSD
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

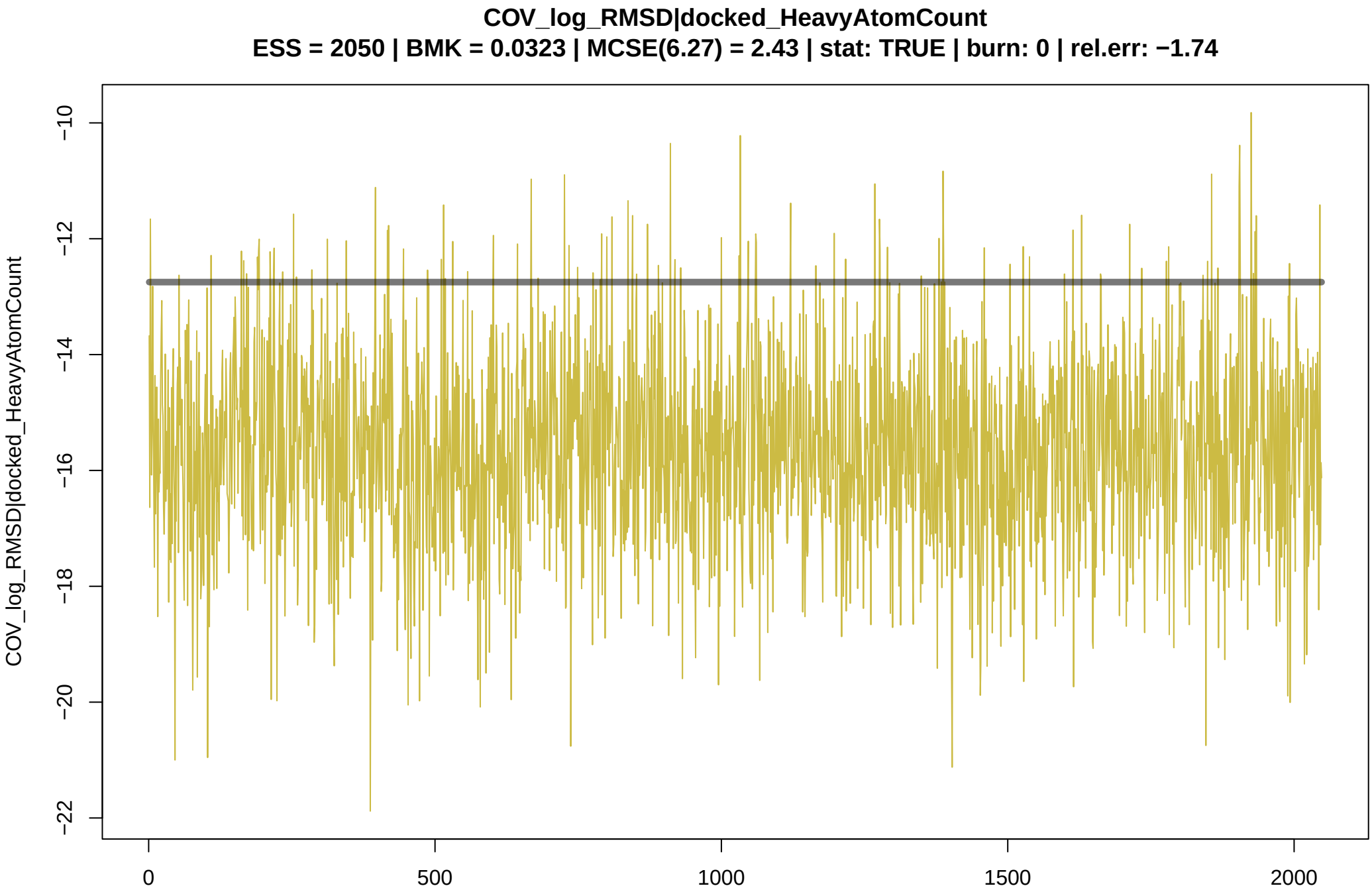

VAR_log_mcs_unbonded_polar_sasa
ESS = 1820 | BMK = 0.0371 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0 | rel.err: 1.36
VAR_log_mcs_unbonded_polar_sasa
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

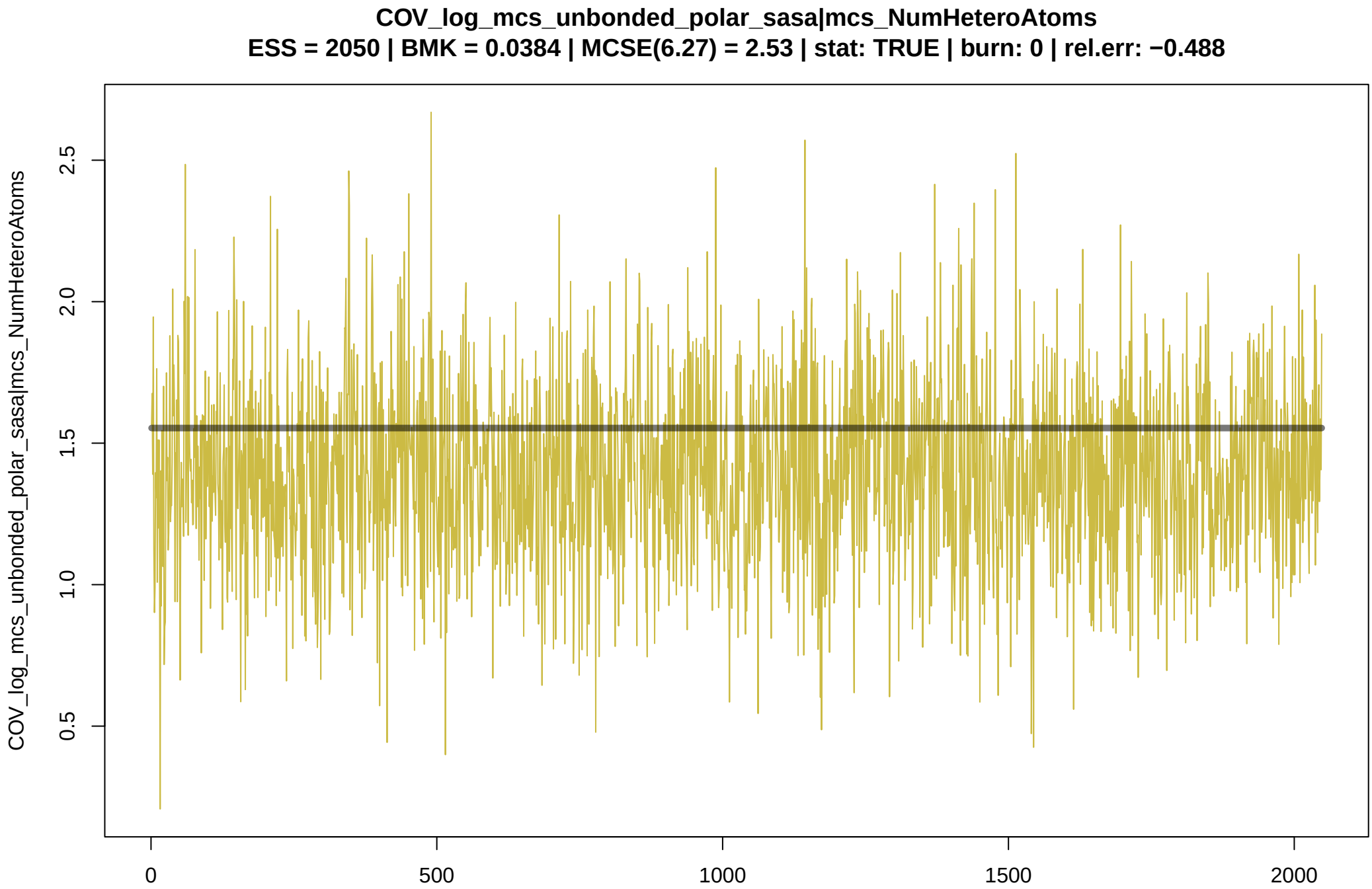

VAR_mcs_NumHeteroAtoms
ESS = 1690 | BMK = 0.0748 | MCSE(6.27) = 2.9 | stat: TRUE | burn: 0 | rel.err: 0.358
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

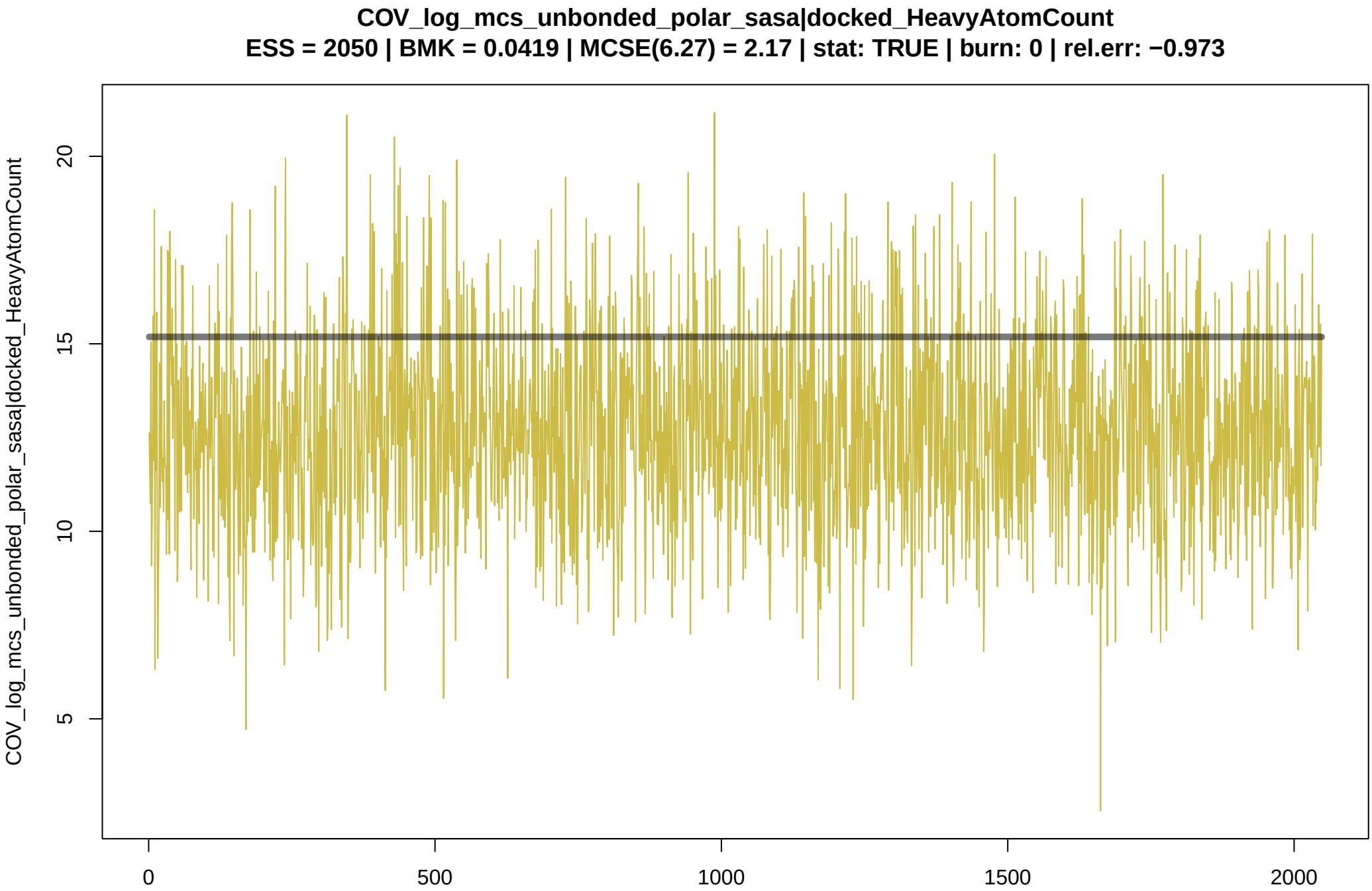

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0747 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: 0.0467
VAR_docked_HeavyAtomCount
7.0
6.9
6.8
6.7
6.6
6.5
6.4
6.3
0
500
1000
1500
2000

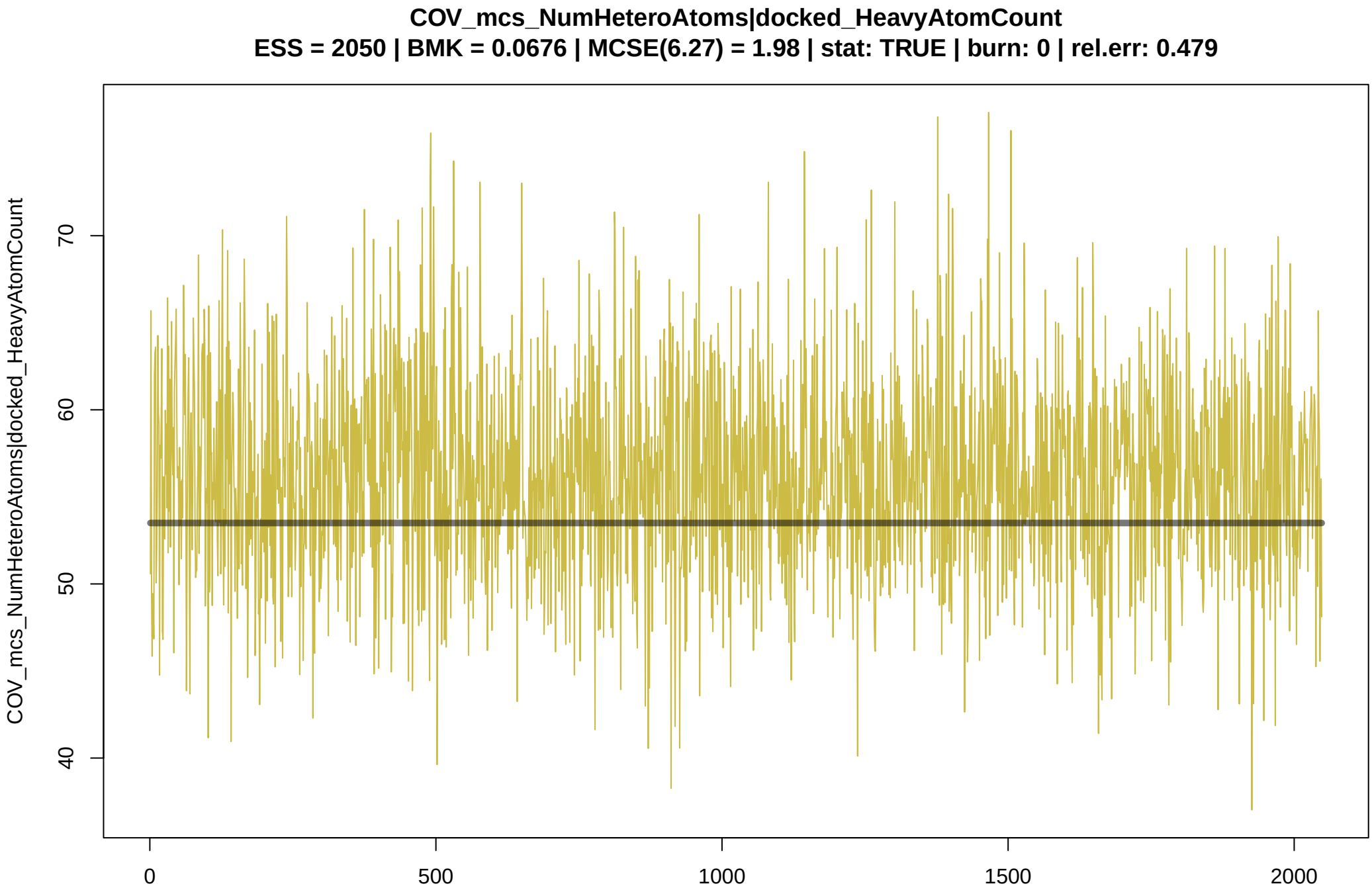

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1610 | BMK = 0.0573 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0 | rel.err: 0.5
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.0
−0.2
−0.4
−0.6
−0.8
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0449 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0 | rel.err: −1.57
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 = 0.0323 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0 | rel.err: −1.74
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 = 0.0384 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: −0.488
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 = 0.0419 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0 | rel.err: −0.973
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 = 0.0676 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0 | rel.err: 0.479
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
500
1000
1500
2000