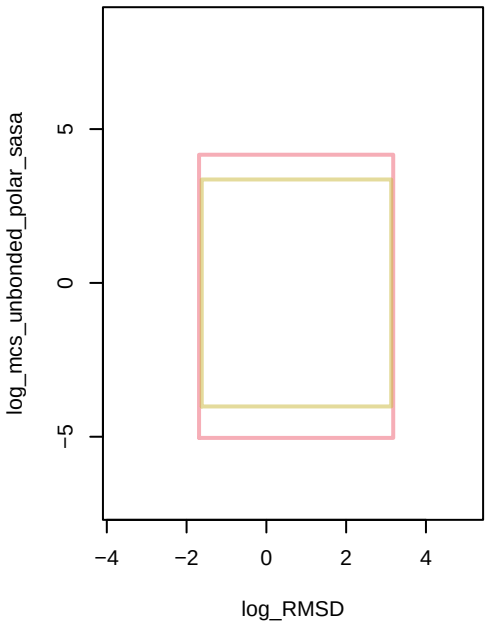
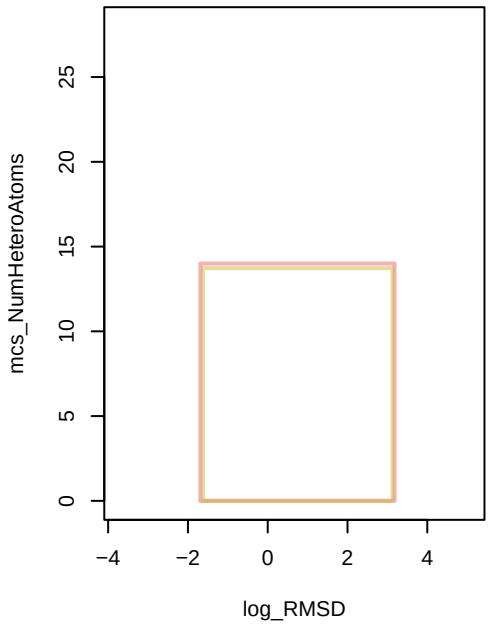
−− STATS maxD −−
min ESS = 63.1807761168363
max BMK = 0.168799048693644
max MCSE = 9.16071071742675
all stationary: FALSE
burn: 0
max rel.err.: 2.23428194820732

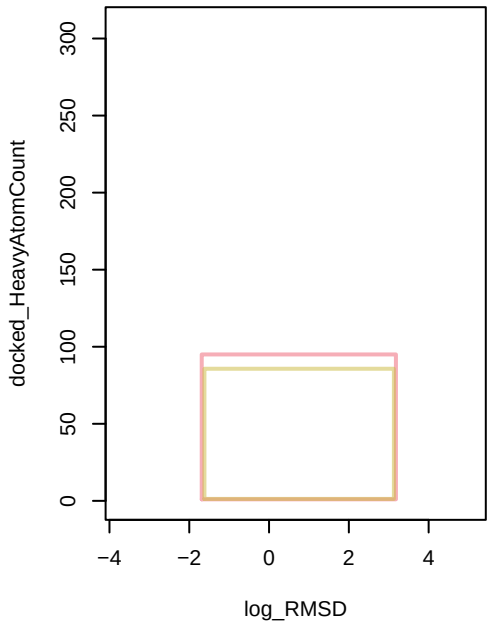
−− STATS 2D −−
min ESS = 1730.85886482235
max BMK = 0.0440427988316472
max MCSE = 2.82625388020113
all stationary: TRUE
burn: 0
max rel.err.: 1.81861546250648

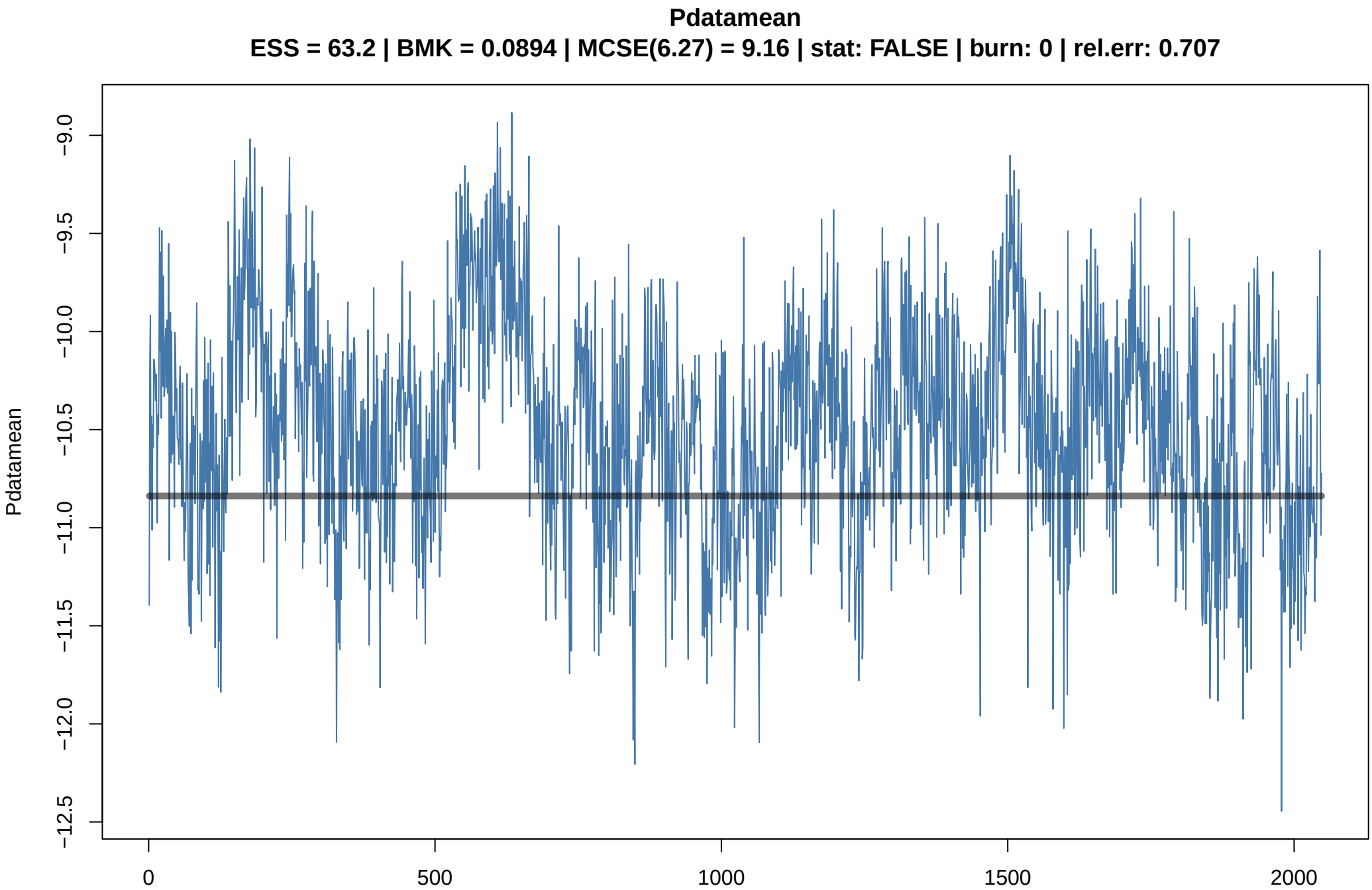
−− STATS 1D −−
min ESS = 1647.48804466916
max BMK = 0.0576383125559659
max MCSE = 3.10843426600398
all stationary: TRUE
burn: 0
max rel.err.: 2.33593942314373

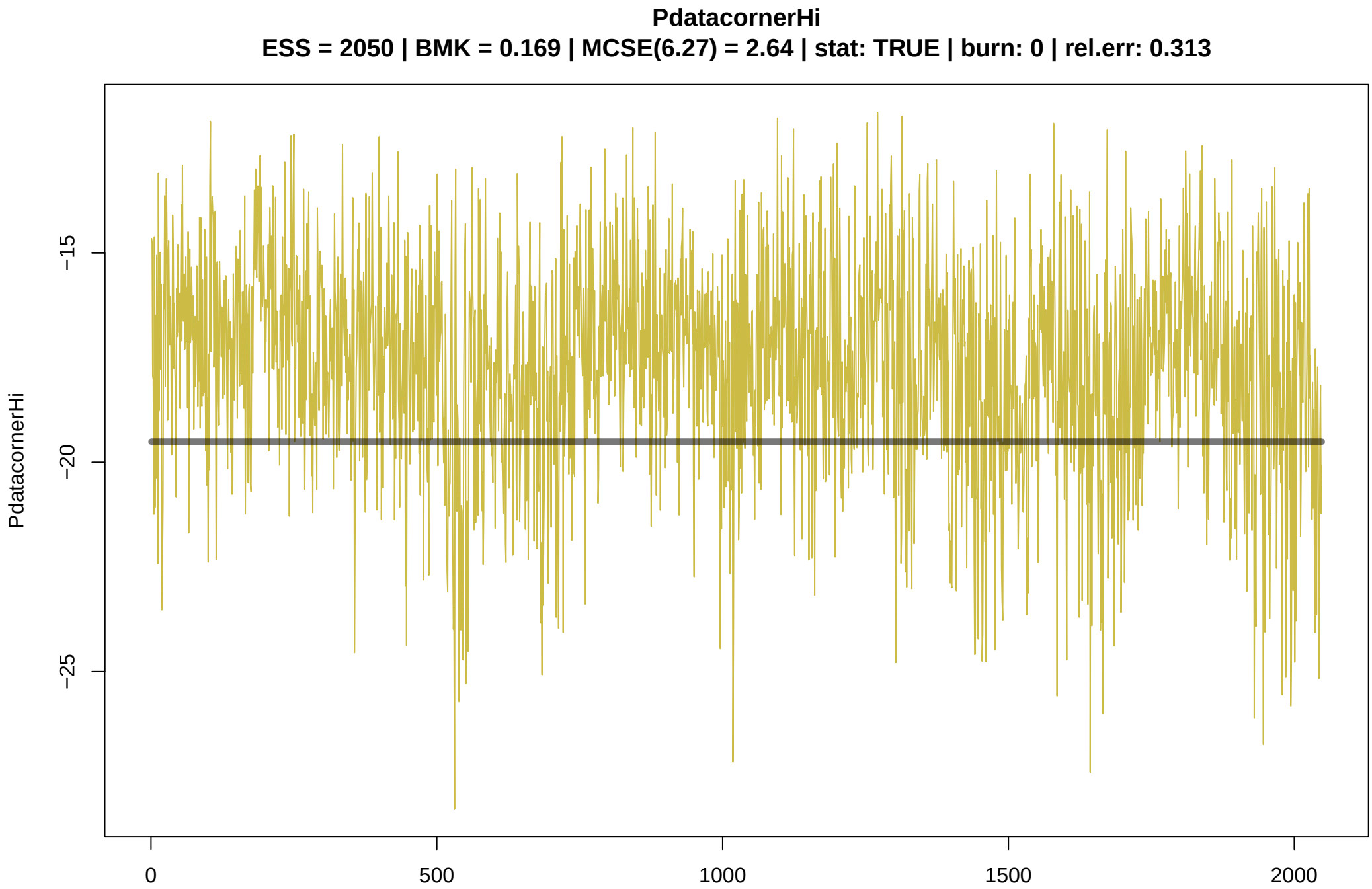
Occupied clusters: 10 of 16

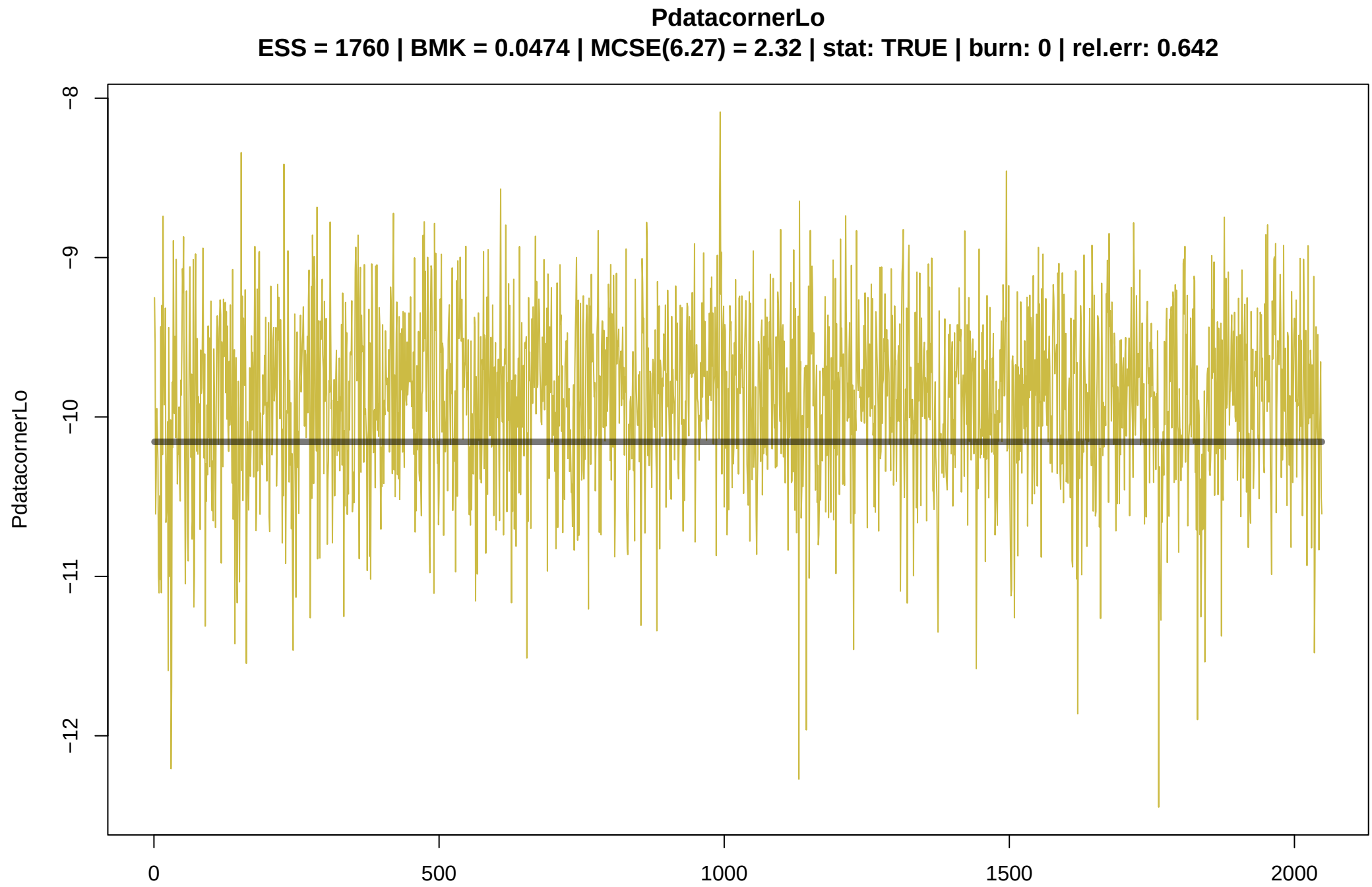

log_mcs_unbonded_polar_sasa
5
0
−5
−4
−2
0
2
4
log_RMSD

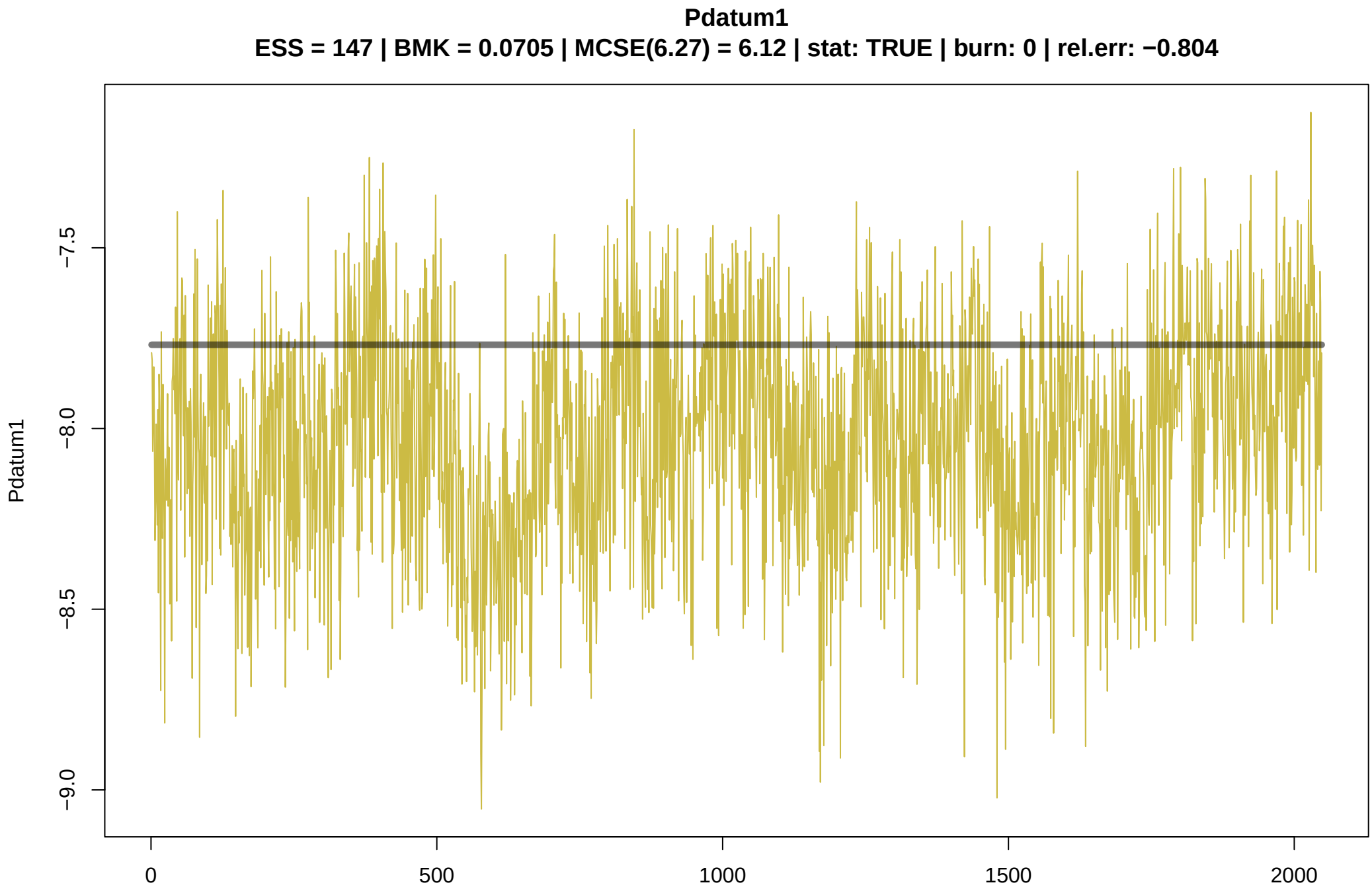

mcs_NumHeteroAtoms
25
20
15
10
5
0
−4
−2
0
2
4
log_RMSD

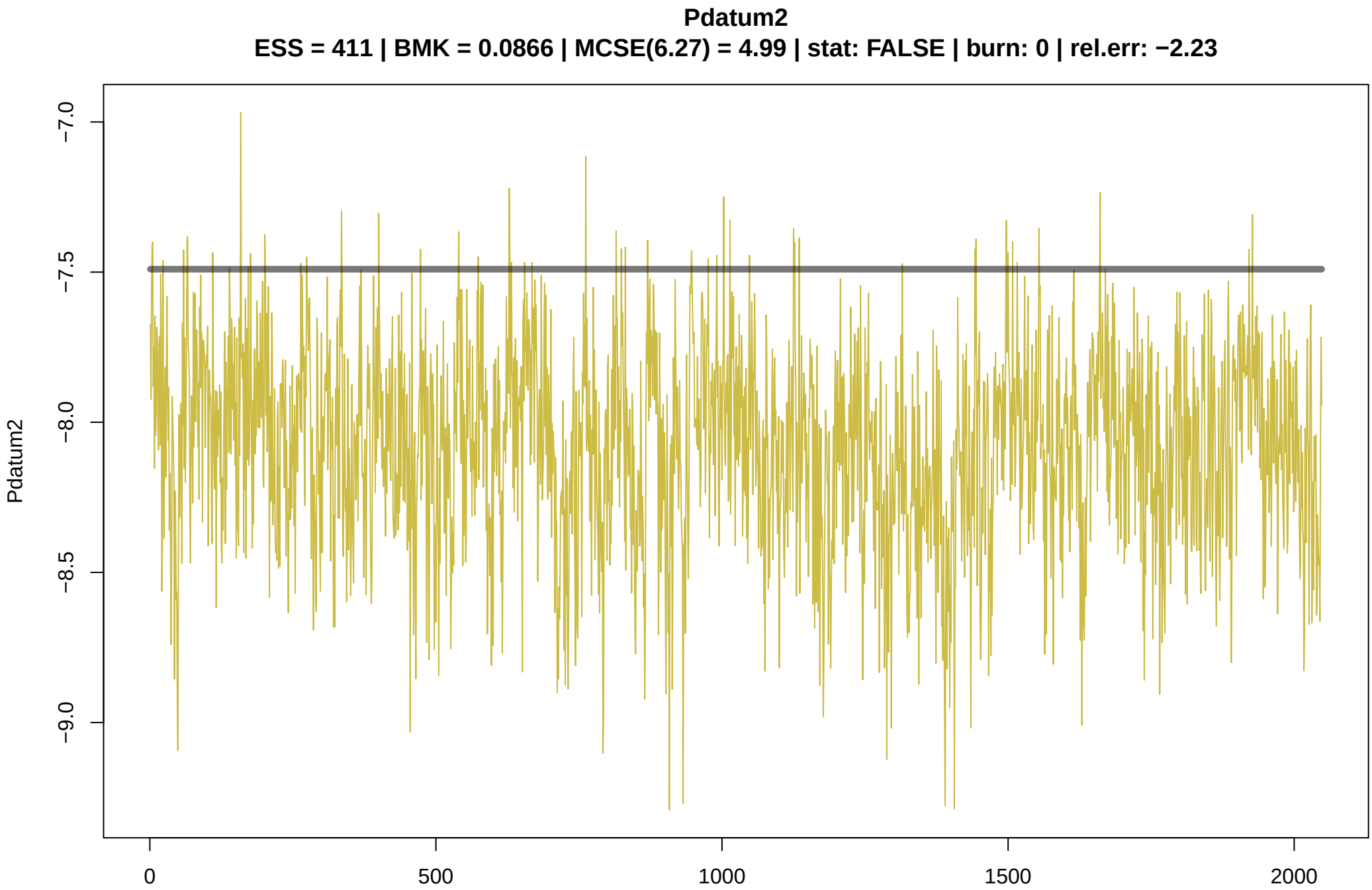

docked_HeavyAtomCount
300
250
200
150
100
50
0
−4
−2
0
2
4
log_RMSD

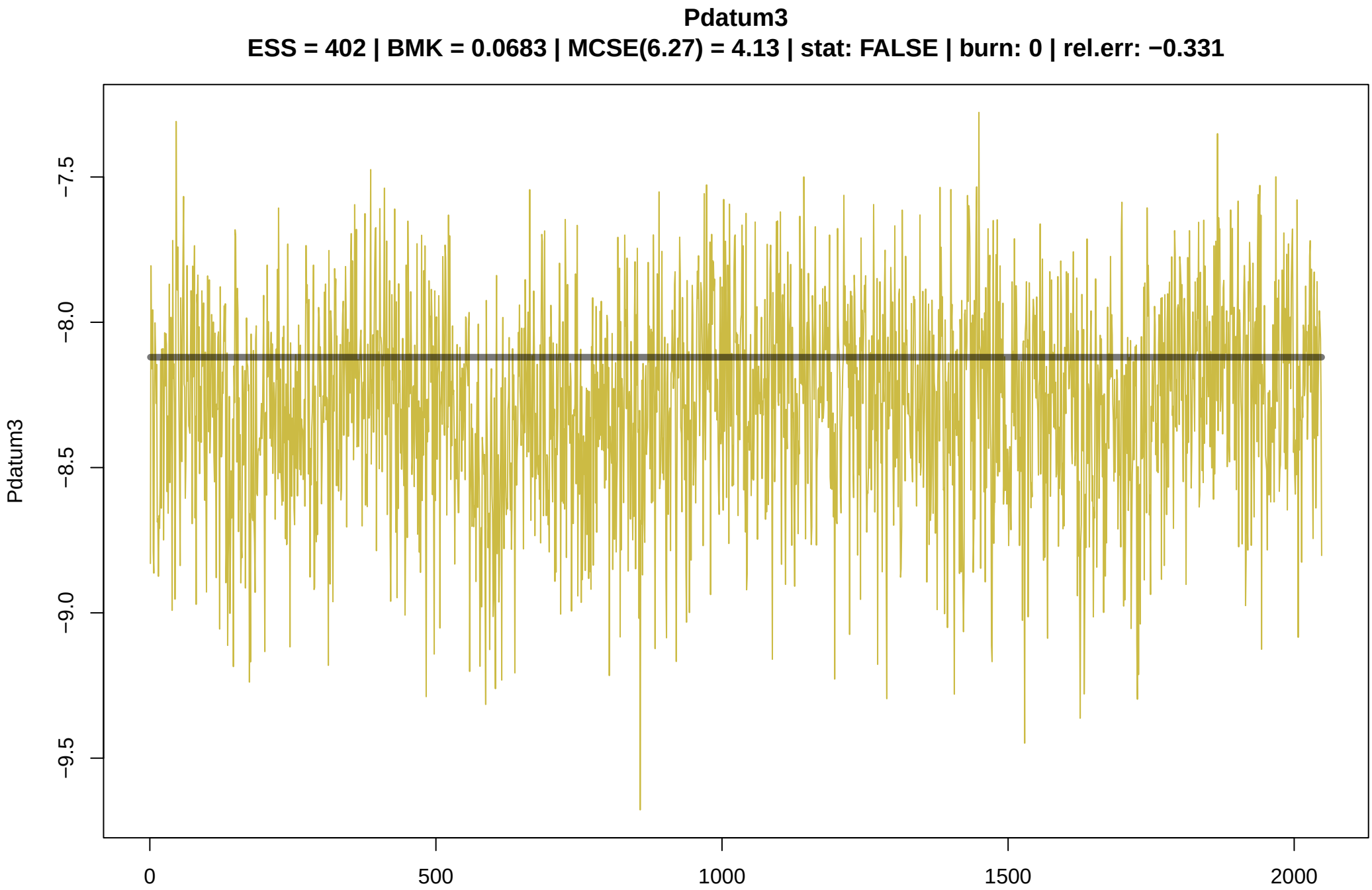

Pdatamean
ESS = 63.2 | BMK = 0.0894 | MCSE(6.27) = 9.16 | stat: FALSE | burn: 0 | rel.err: 0.707
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
−12.5
0
500
1000
1500
2000

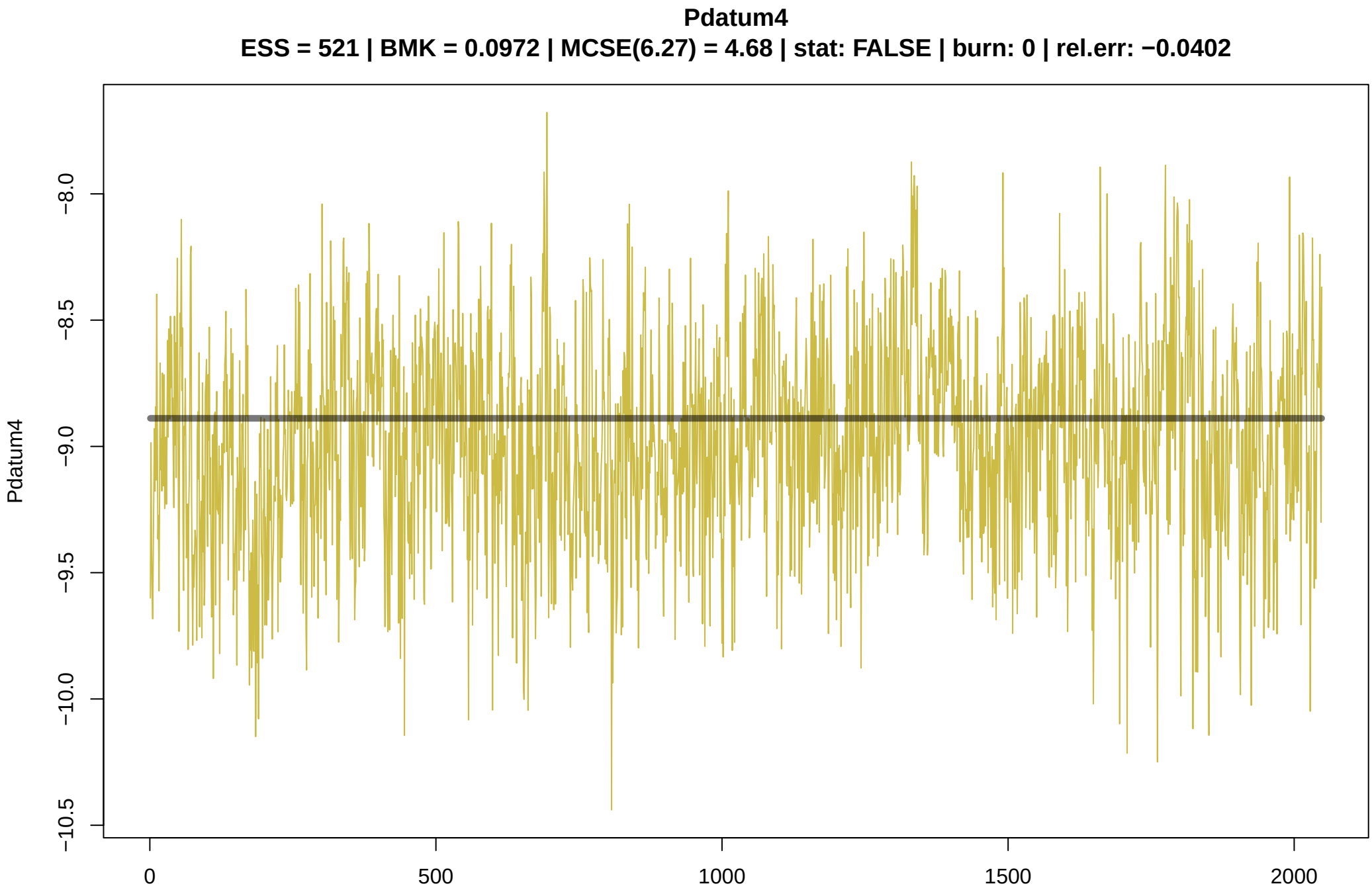

PdatacornerHi
ESS = 2050 | BMK = 0.169 | MCSE(6.27) = 2.64 | stat: TRUE | burn: 0 | rel.err: 0.313
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

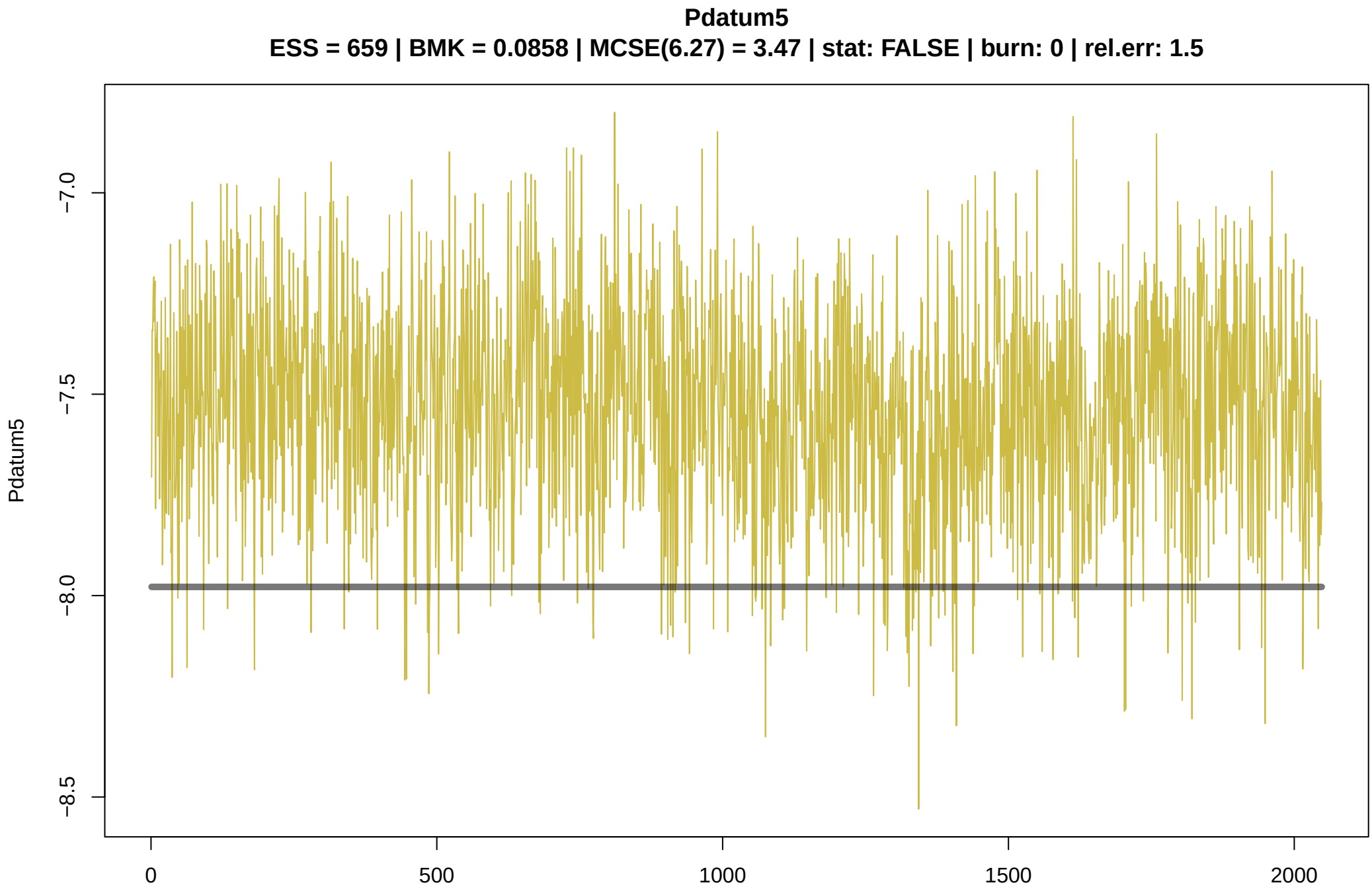

PdatacornerLo
ESS = 1760 | BMK = 0.0474 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: 0.642
PdatacornerLo
−8
−9
−10
−11
−12
0
500
1000
1500
2000

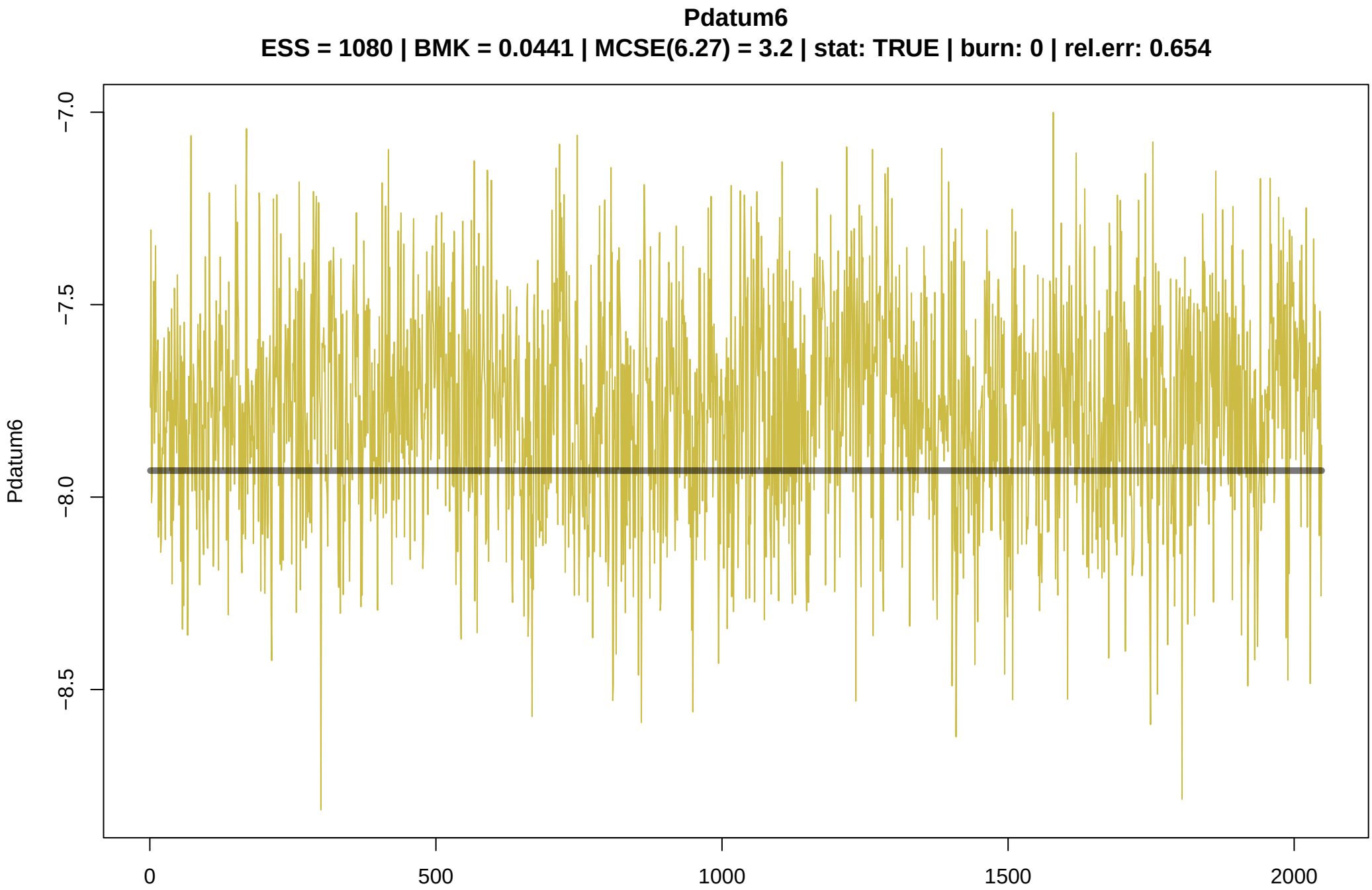

Pdatum1
ESS = 147 | BMK = 0.0705 | MCSE(6.27) = 6.12 | stat: TRUE | burn: 0 | rel.err: −0.804
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

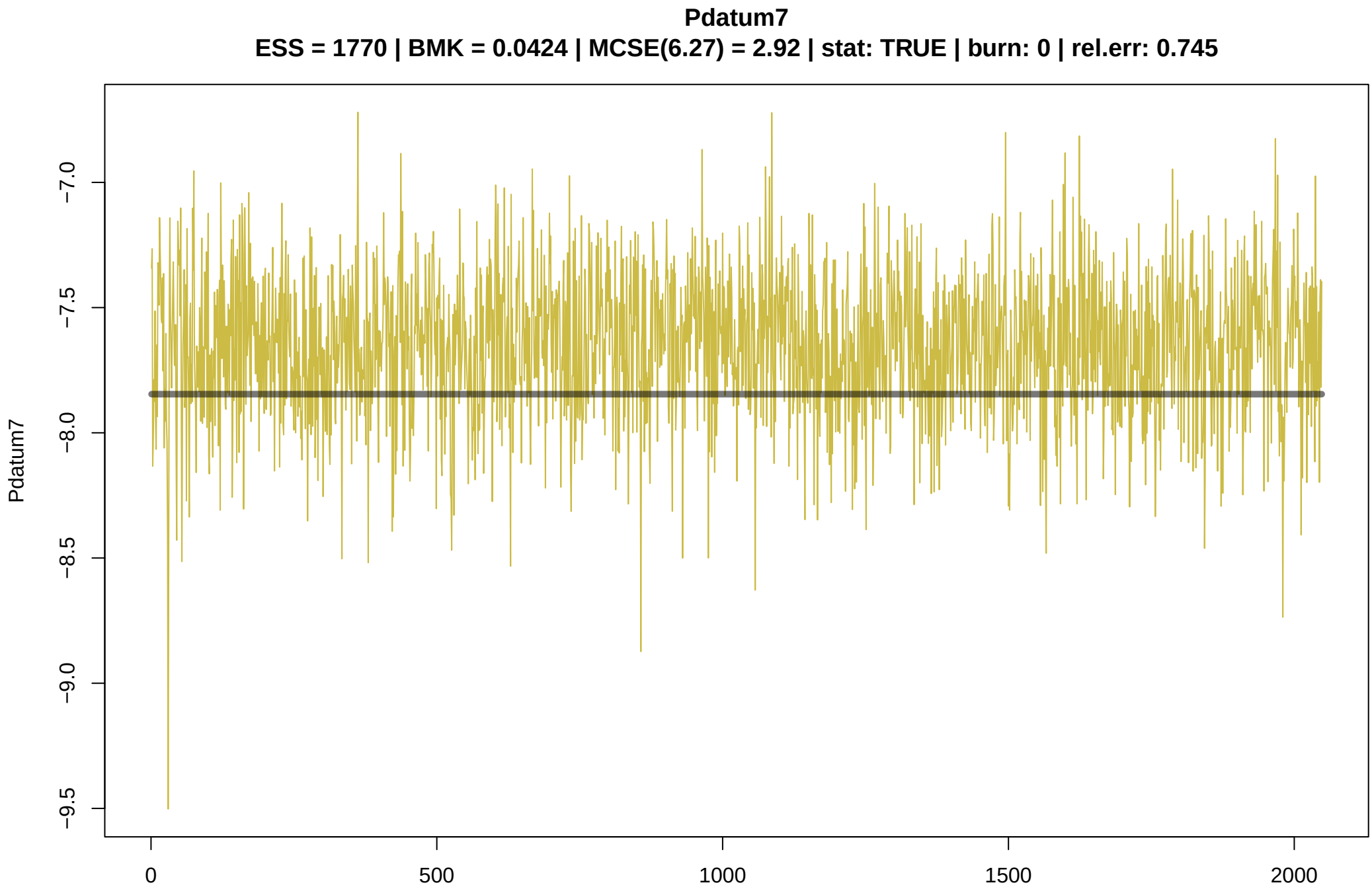

Pdatum2
ESS = 411 | BMK = 0.0866 | MCSE(6.27) = 4.99 | stat: FALSE | burn: 0 | rel.err: −2.23
Pdatum2
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

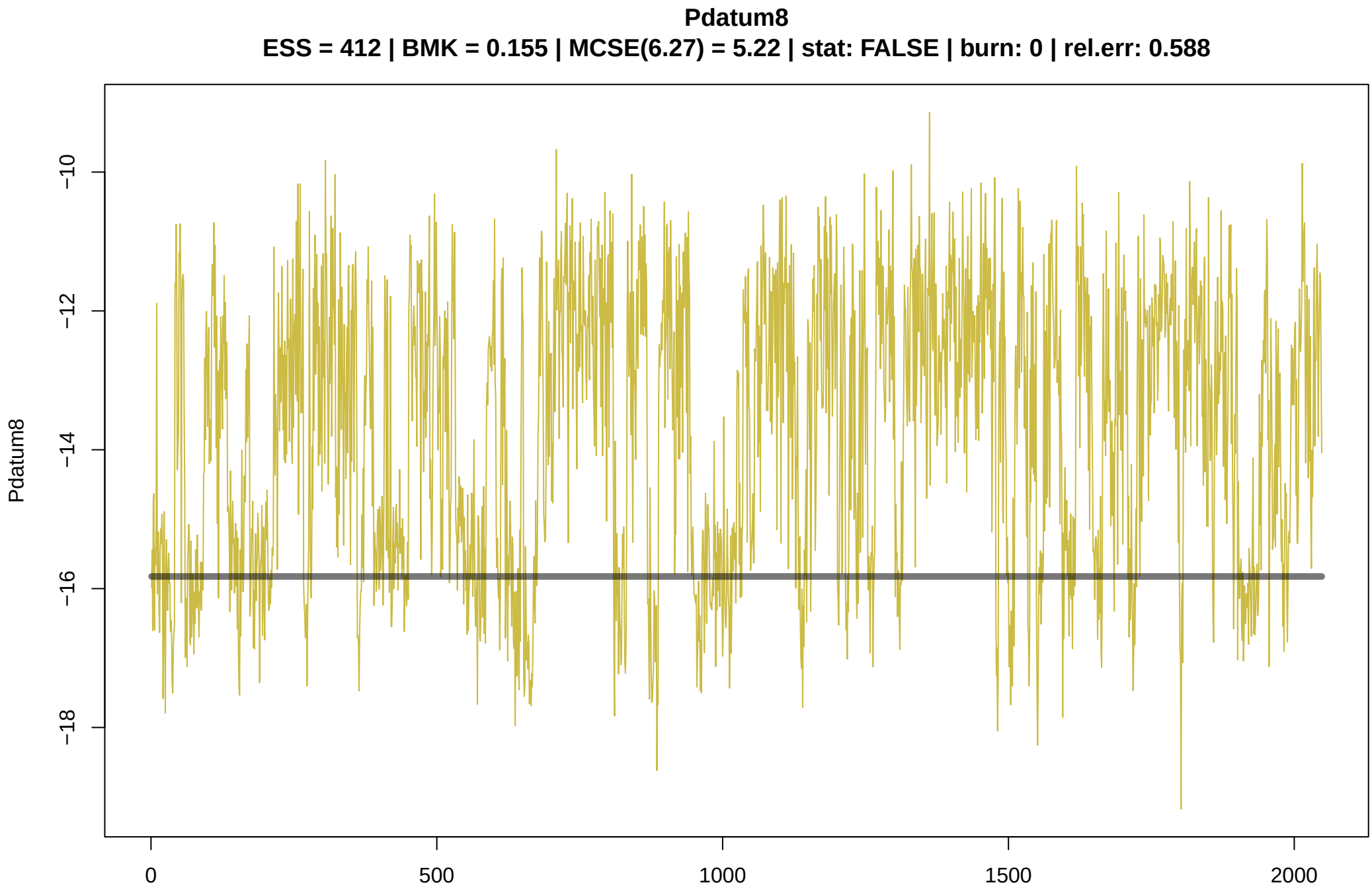

Pdatum3
ESS = 402 | BMK = 0.0683 | MCSE(6.27) = 4.13 | stat: FALSE | burn: 0 | rel.err: −0.331
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

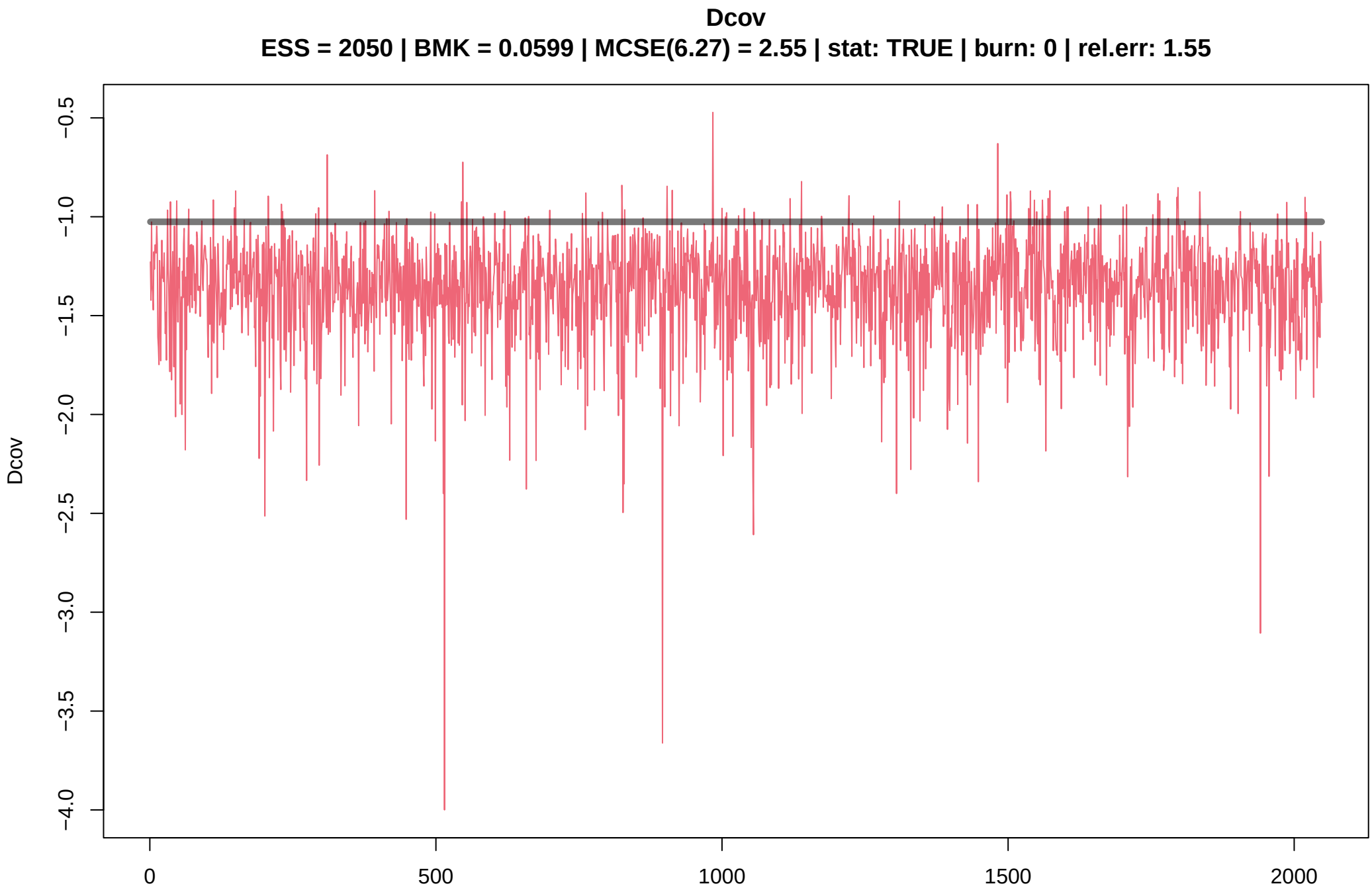

Pdatum4
ESS = 521 | BMK = 0.0972 | MCSE(6.27) = 4.68 | stat: FALSE | burn: 0 | rel.err: −0.0402
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
−10.5
0
500
1000
1500
2000

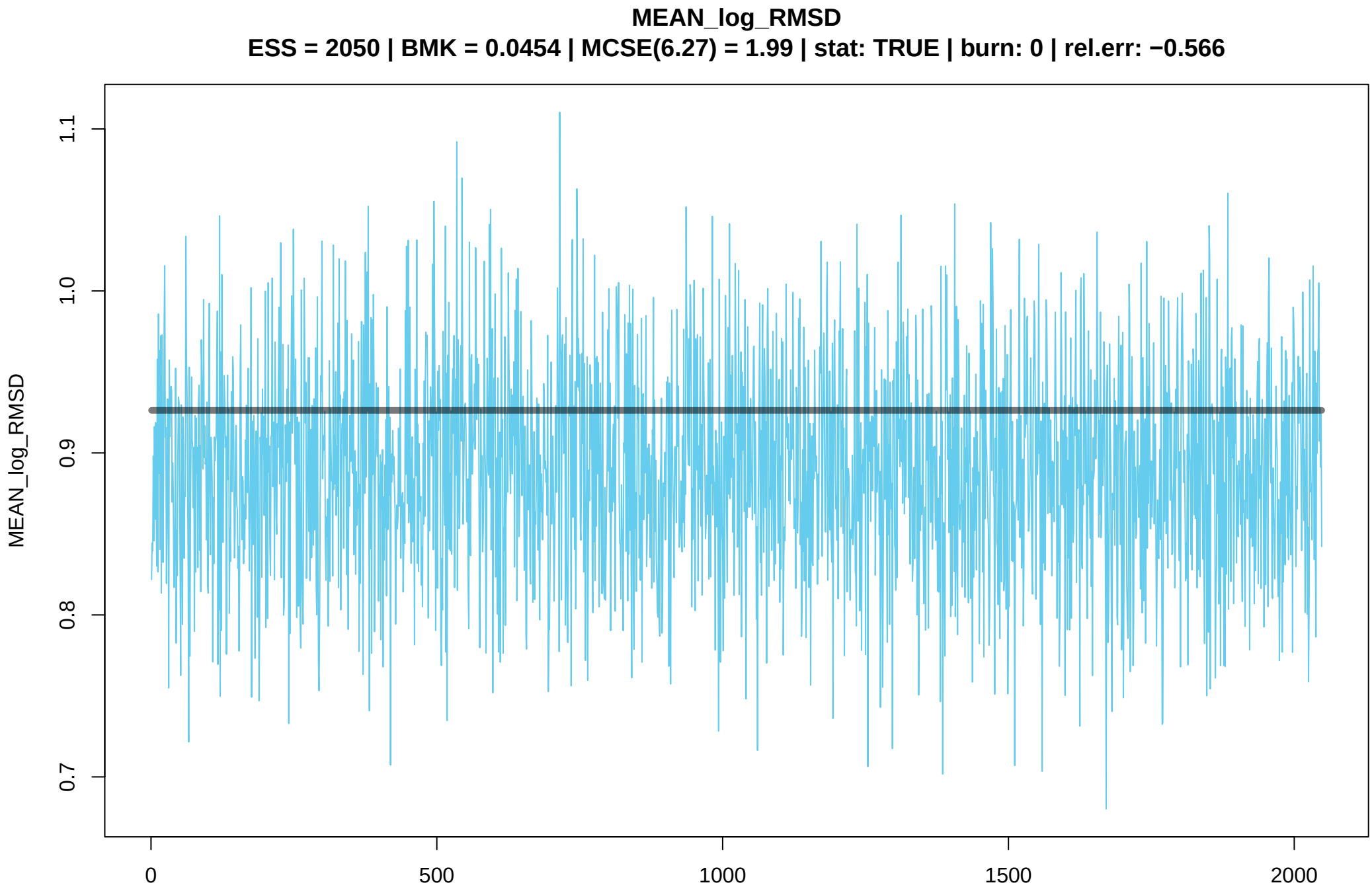

Pdatum5
ESS = 659 | BMK = 0.0858 | MCSE(6.27) = 3.47 | stat: FALSE | burn: 0 | rel.err: 1.5
Pdatum5
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

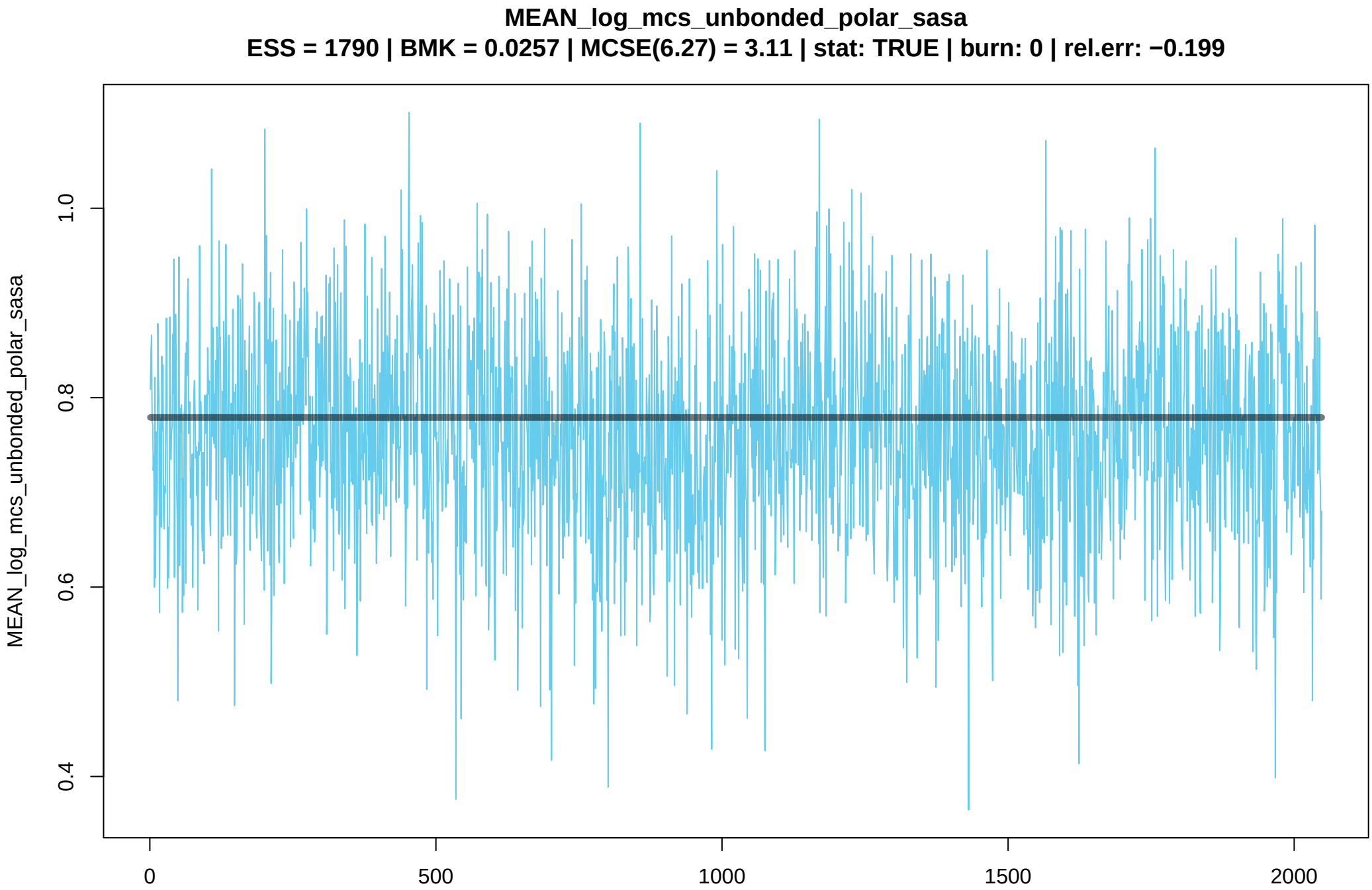

Pdatum6
ESS = 1080 | BMK = 0.0441 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0 | rel.err: 0.654
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

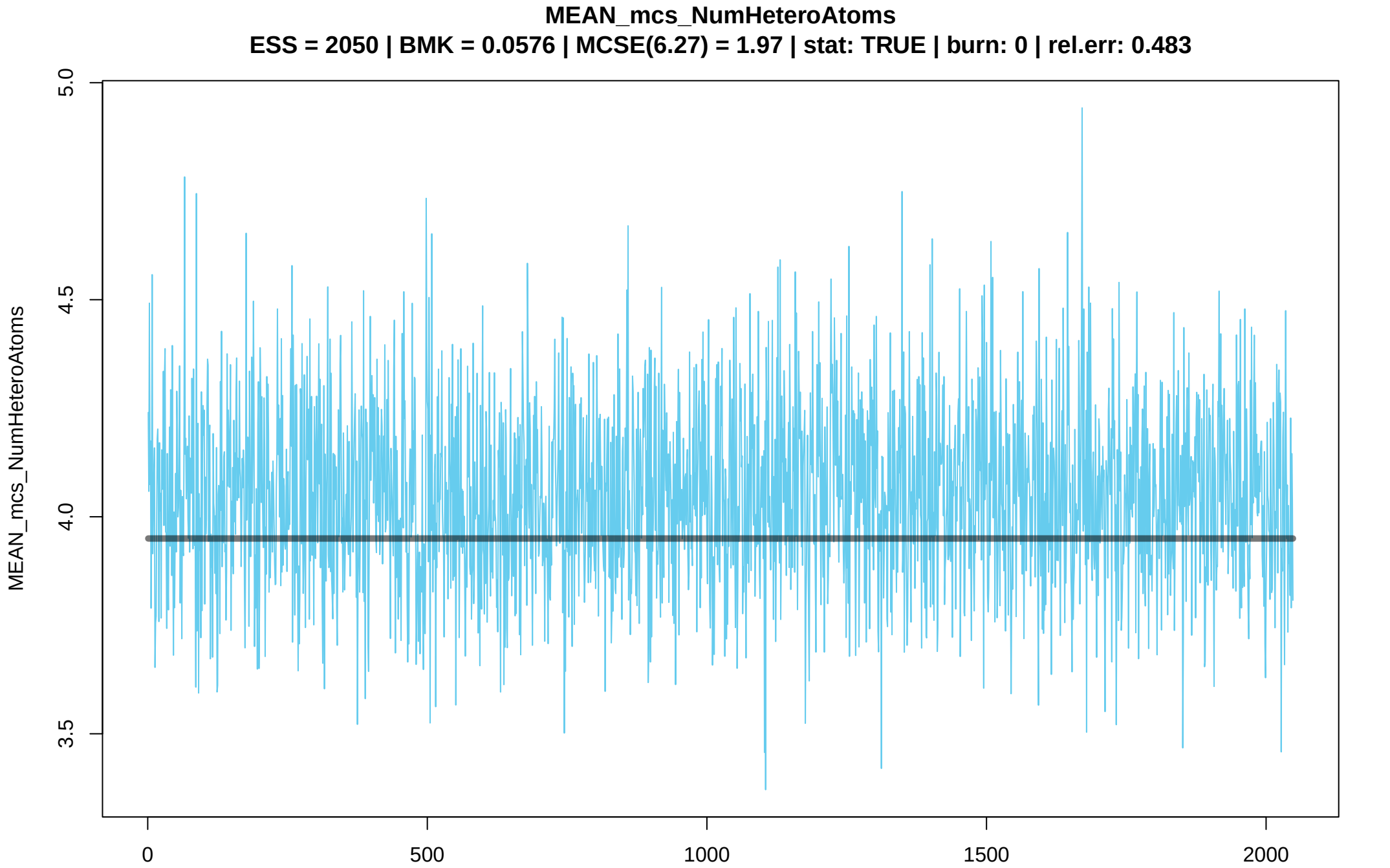

Pdatum7
ESS = 1770 | BMK = 0.0424 | MCSE(6.27) = 2.92 | stat: TRUE | burn: 0 | rel.err: 0.745
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

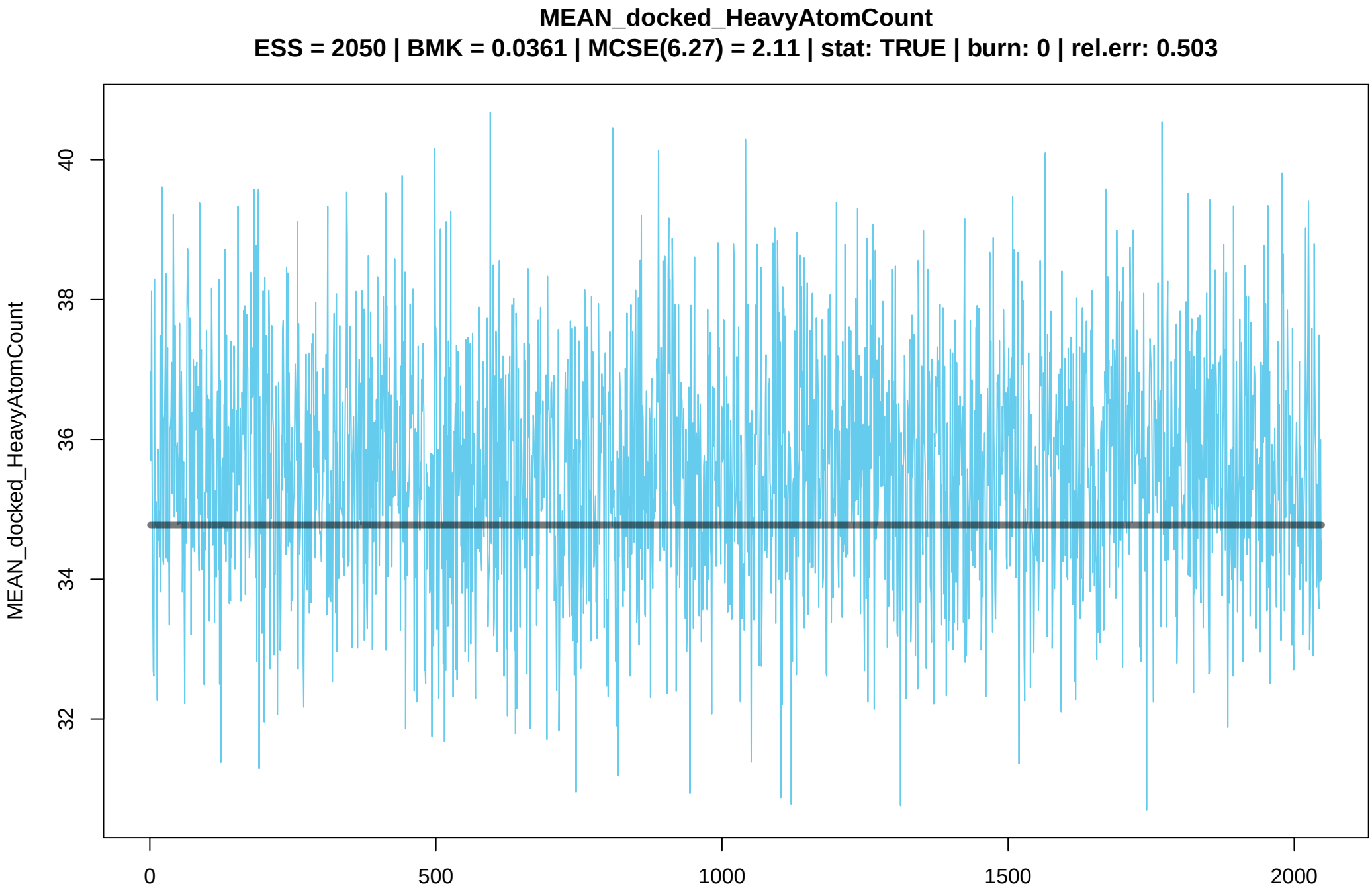

Pdatum8
ESS = 412 | BMK = 0.155 | MCSE(6.27) = 5.22 | stat: FALSE | burn: 0 | rel.err: 0.588
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

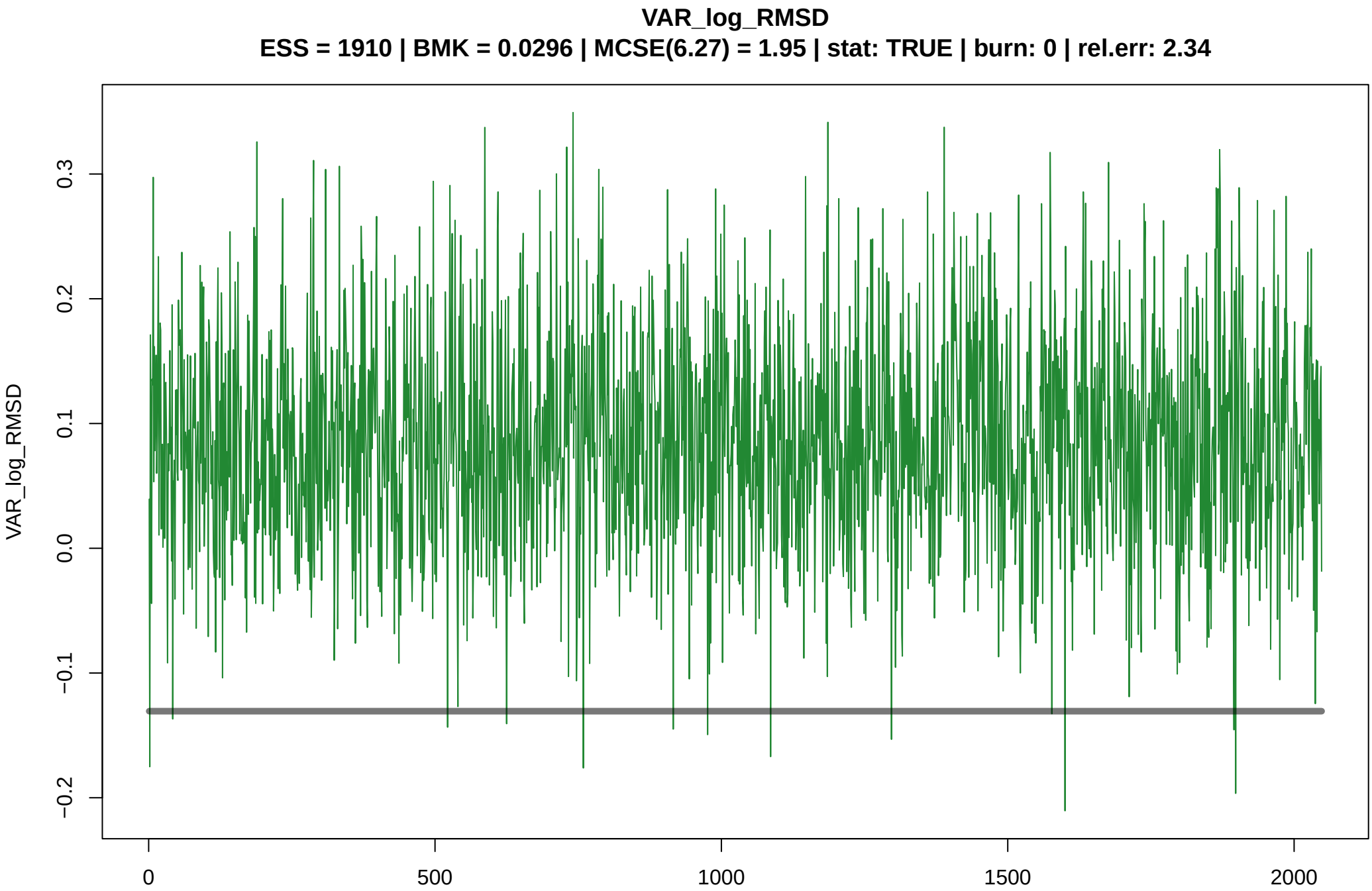

Dcov
ESS = 2050 | BMK = 0.0599 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0 | rel.err: 1.55
Dcov
−0.5
−1.0
−1.5
−2.0
−2.5
−3.0
−3.5
−4.0
0
500
1000
1500
2000

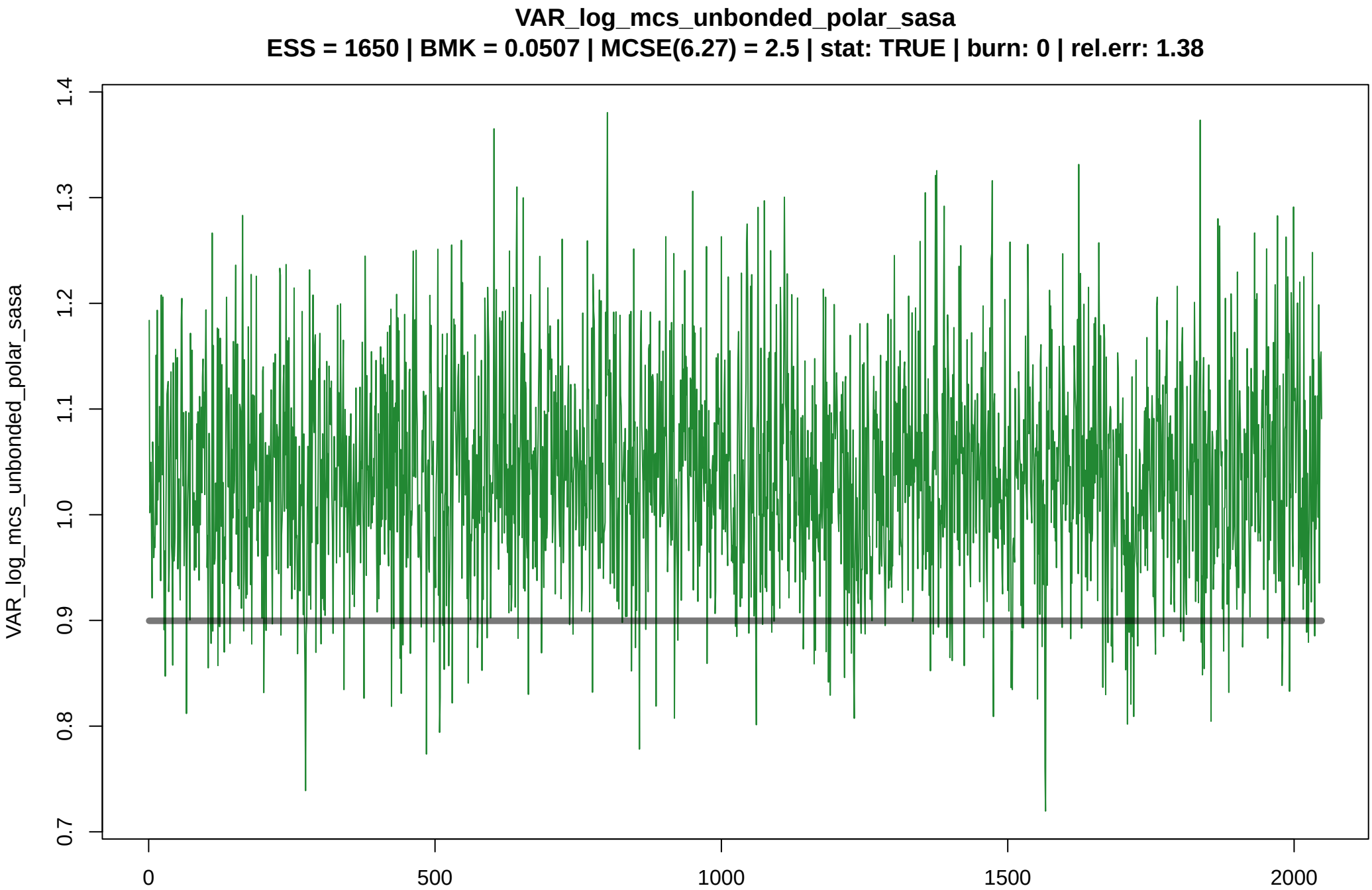

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0454 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: −0.566
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

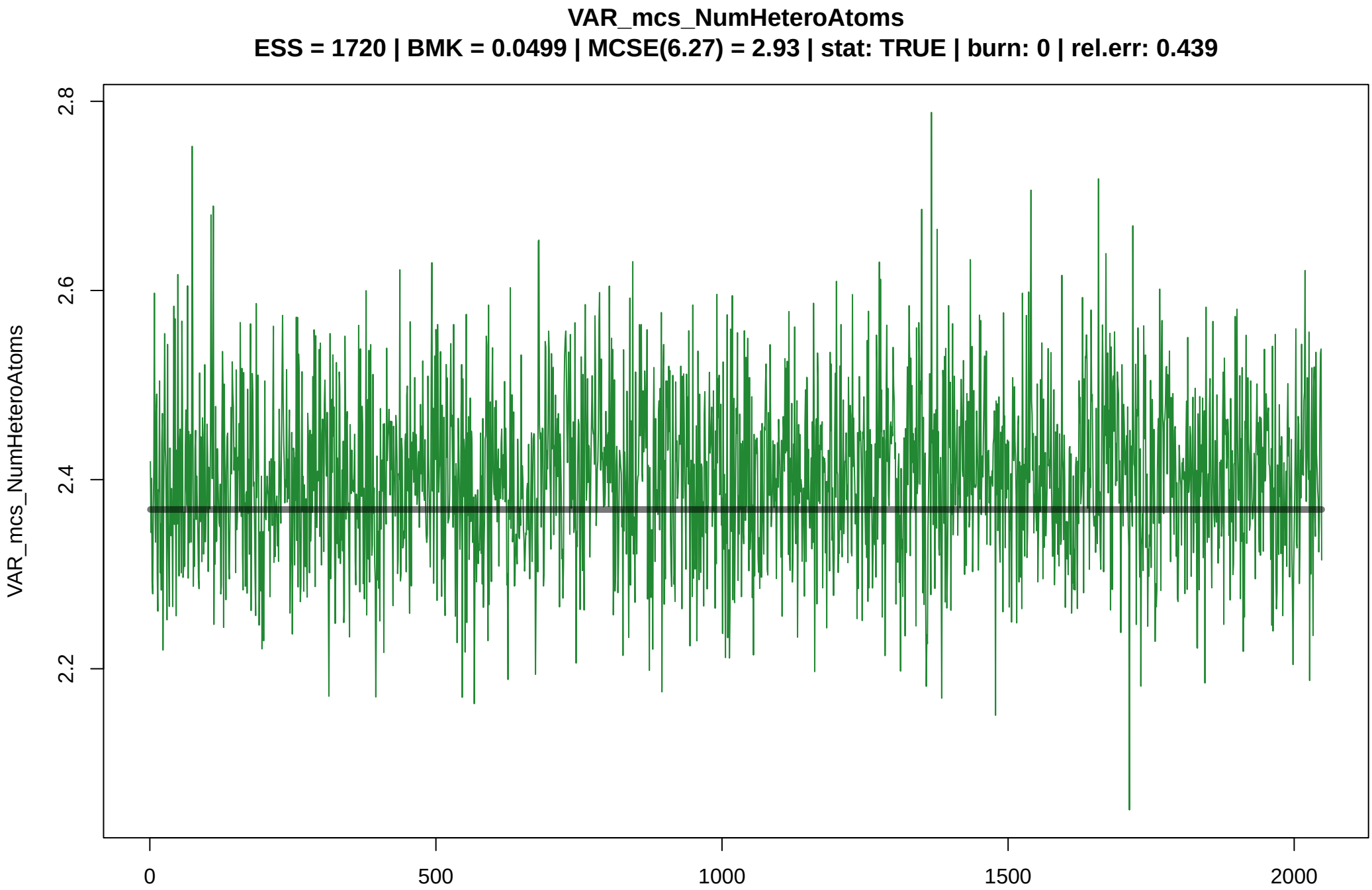

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1790 | BMK = 0.0257 | MCSE(6.27) = 3.11 | stat: TRUE | burn: 0 | rel.err: −0.199
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
0
500
1000
1500
2000

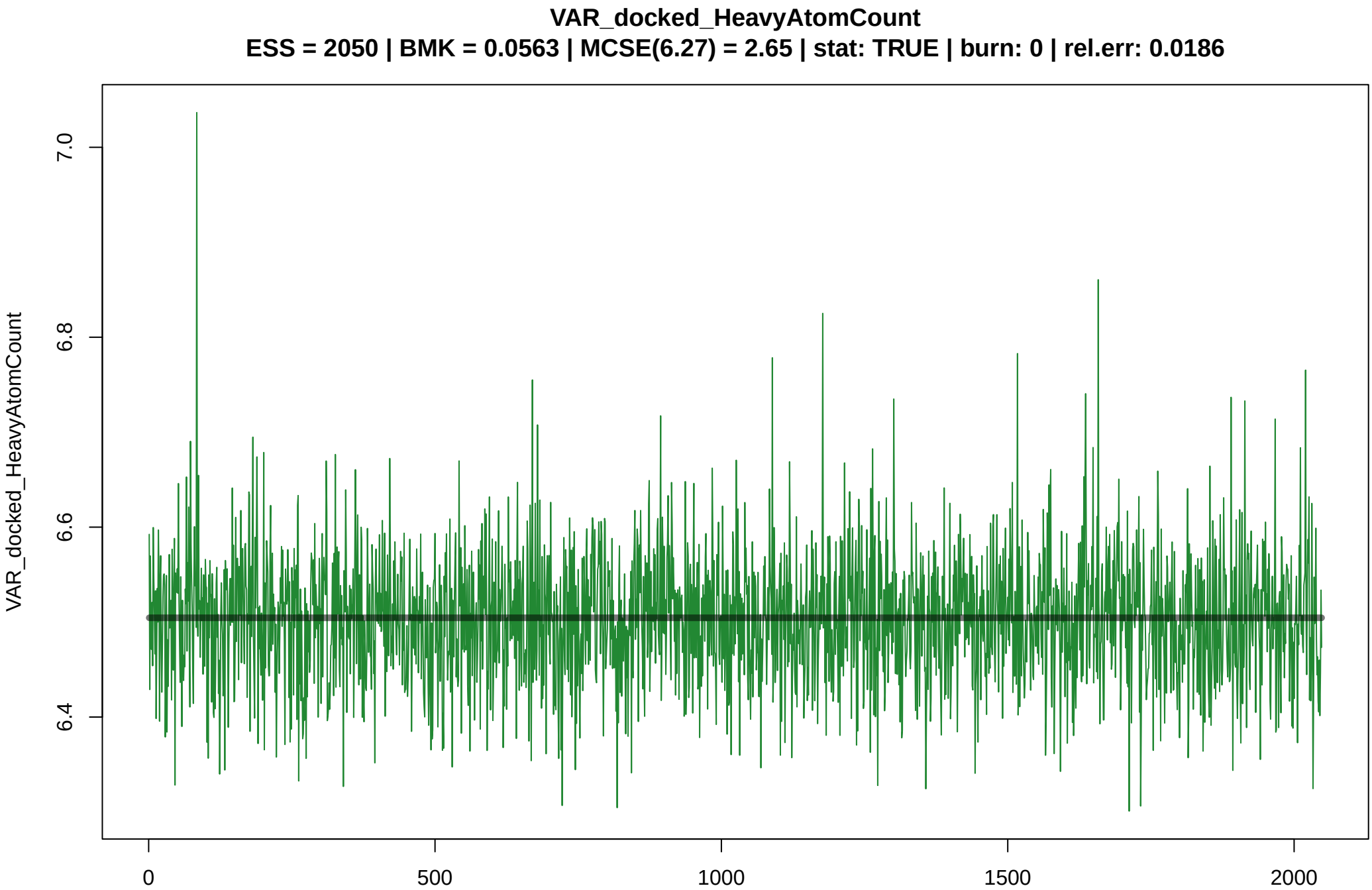

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0576 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0 | rel.err: 0.483
MEAN_mcs_NumHeteroAtoms
5.0
4.5
4.0
3.5
0
500
1000
1500
2000

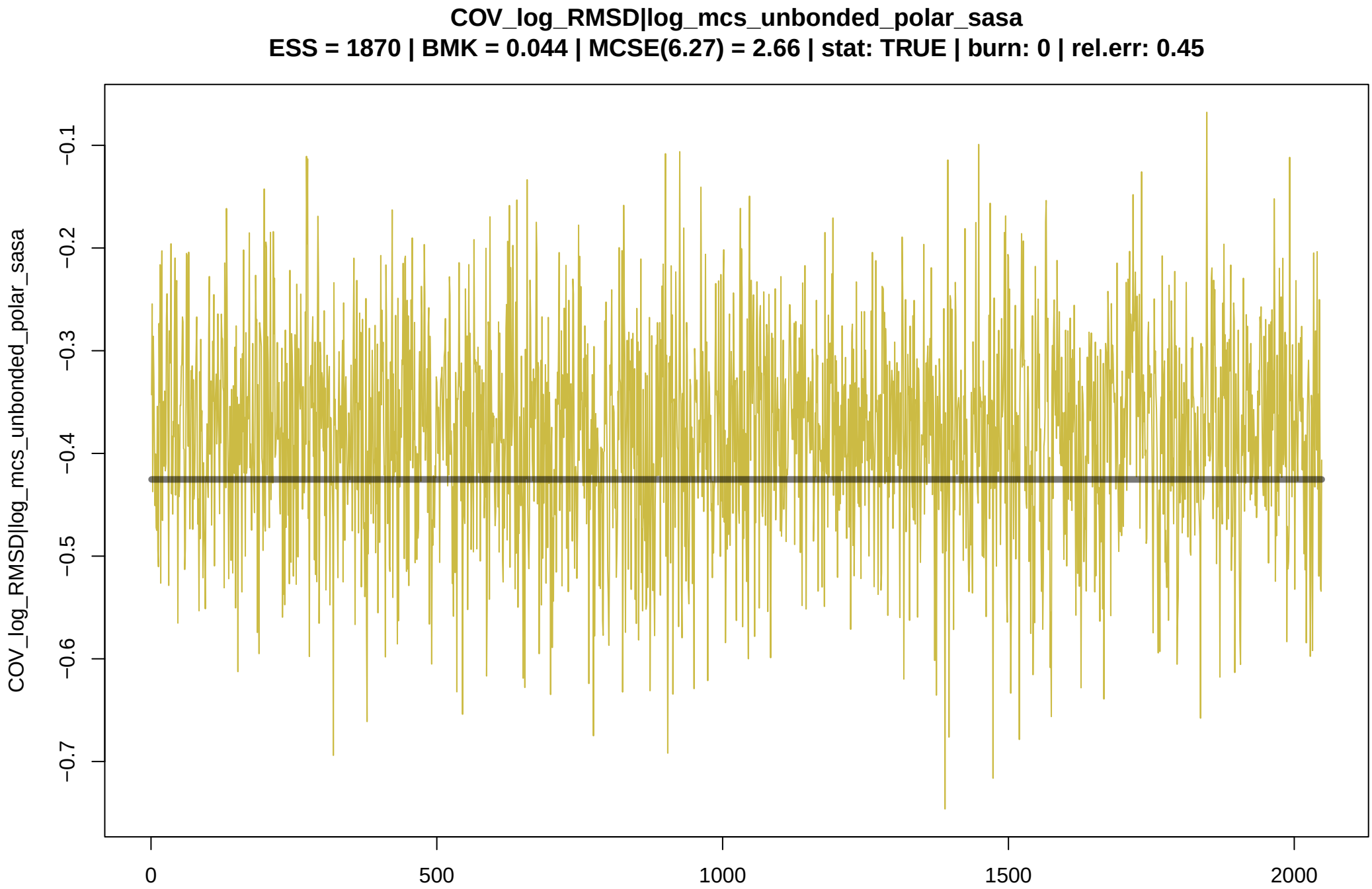

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0361 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0 | rel.err: 0.503
MEAN_docked_HeavyAtomCount
32
34
36
38
40
0
500
1000
1500
2000

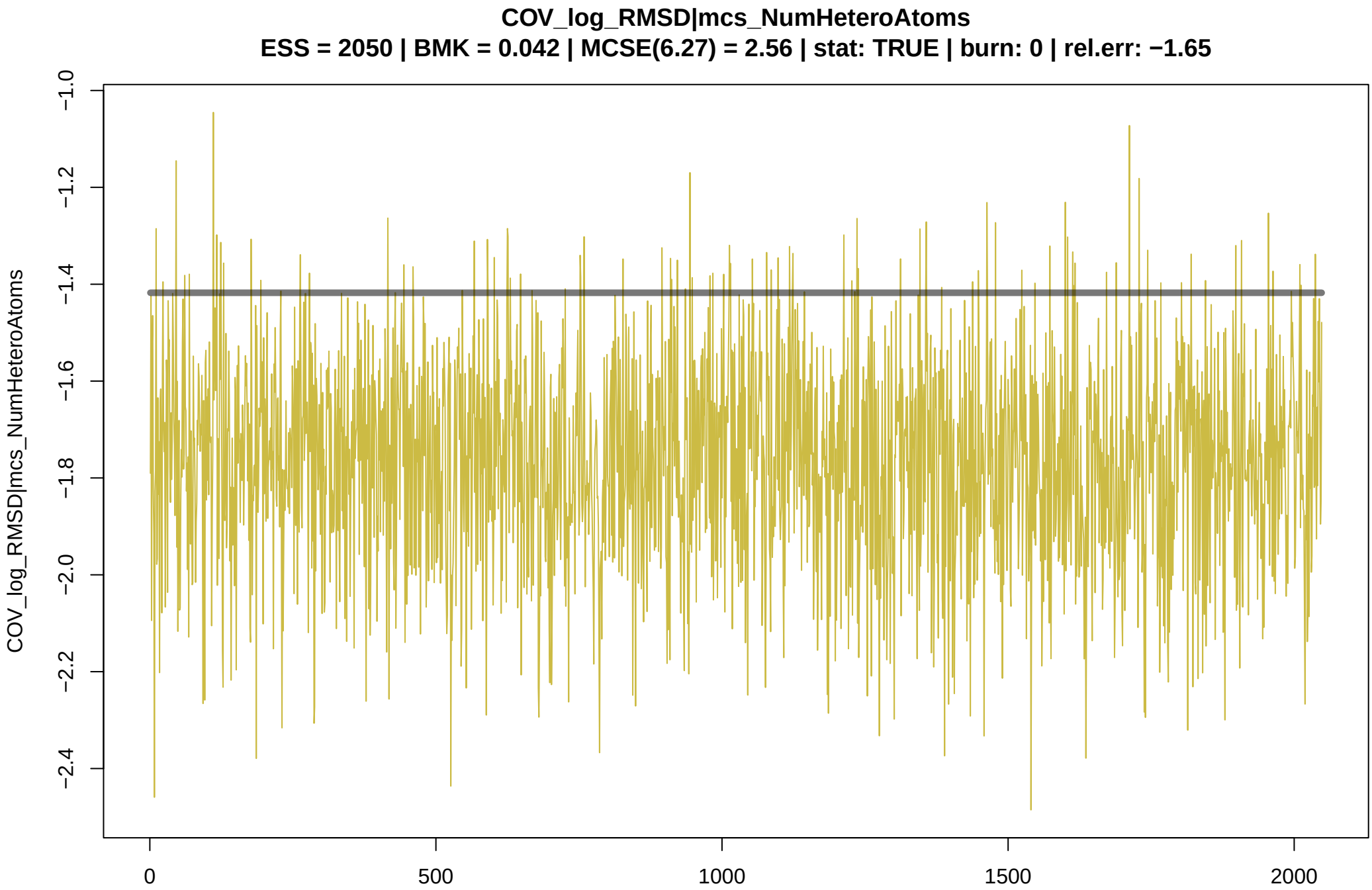

VAR_log_RMSD
ESS = 1910 | BMK = 0.0296 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: 2.34
VAR_log_RMSD
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

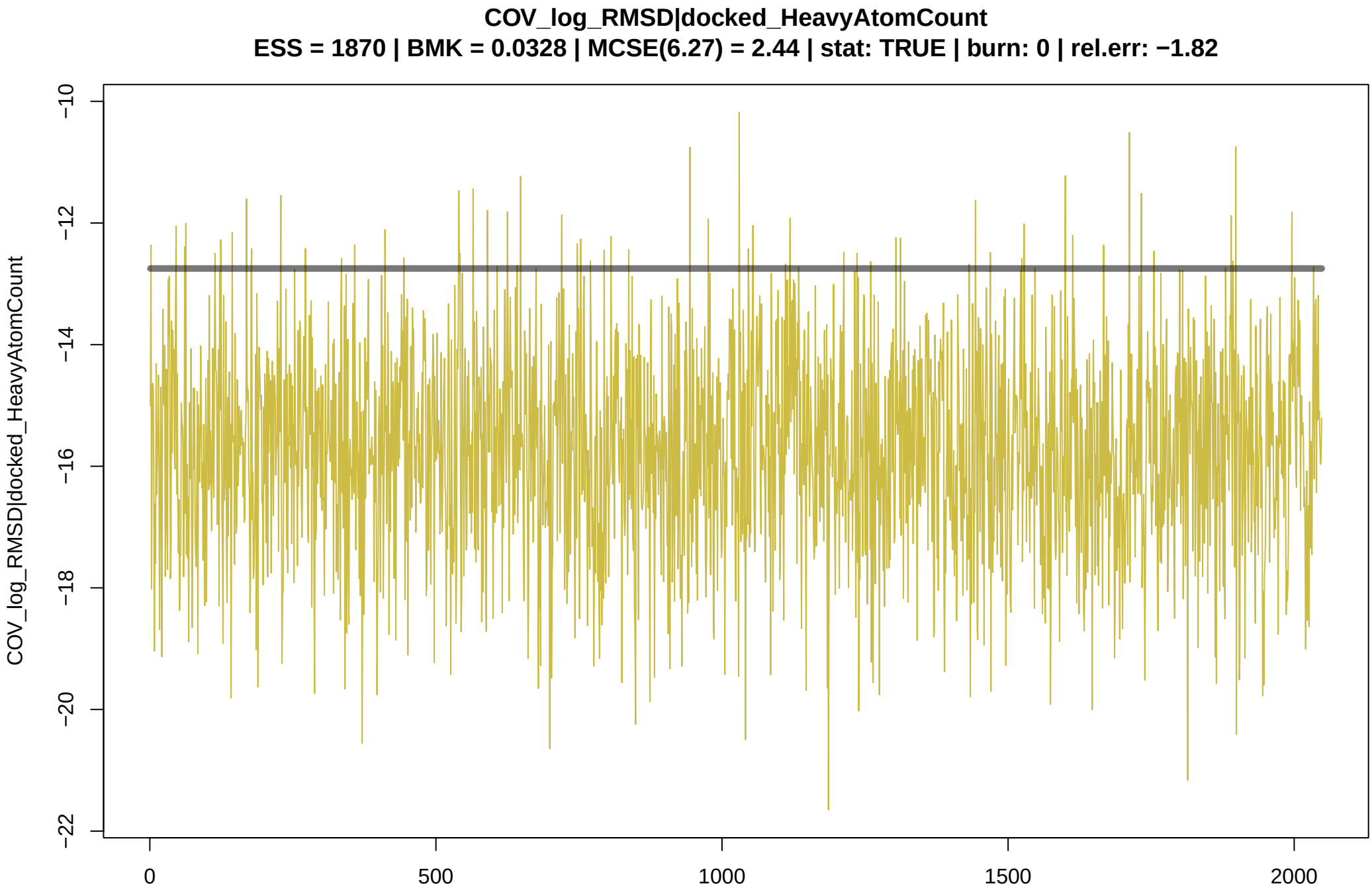

VAR_log_mcs_unbonded_polar_sasa
ESS = 1650 | BMK = 0.0507 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0 | rel.err: 1.38
VAR_log_mcs_unbonded_polar_sasa
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4
0
500
1000
1500
2000

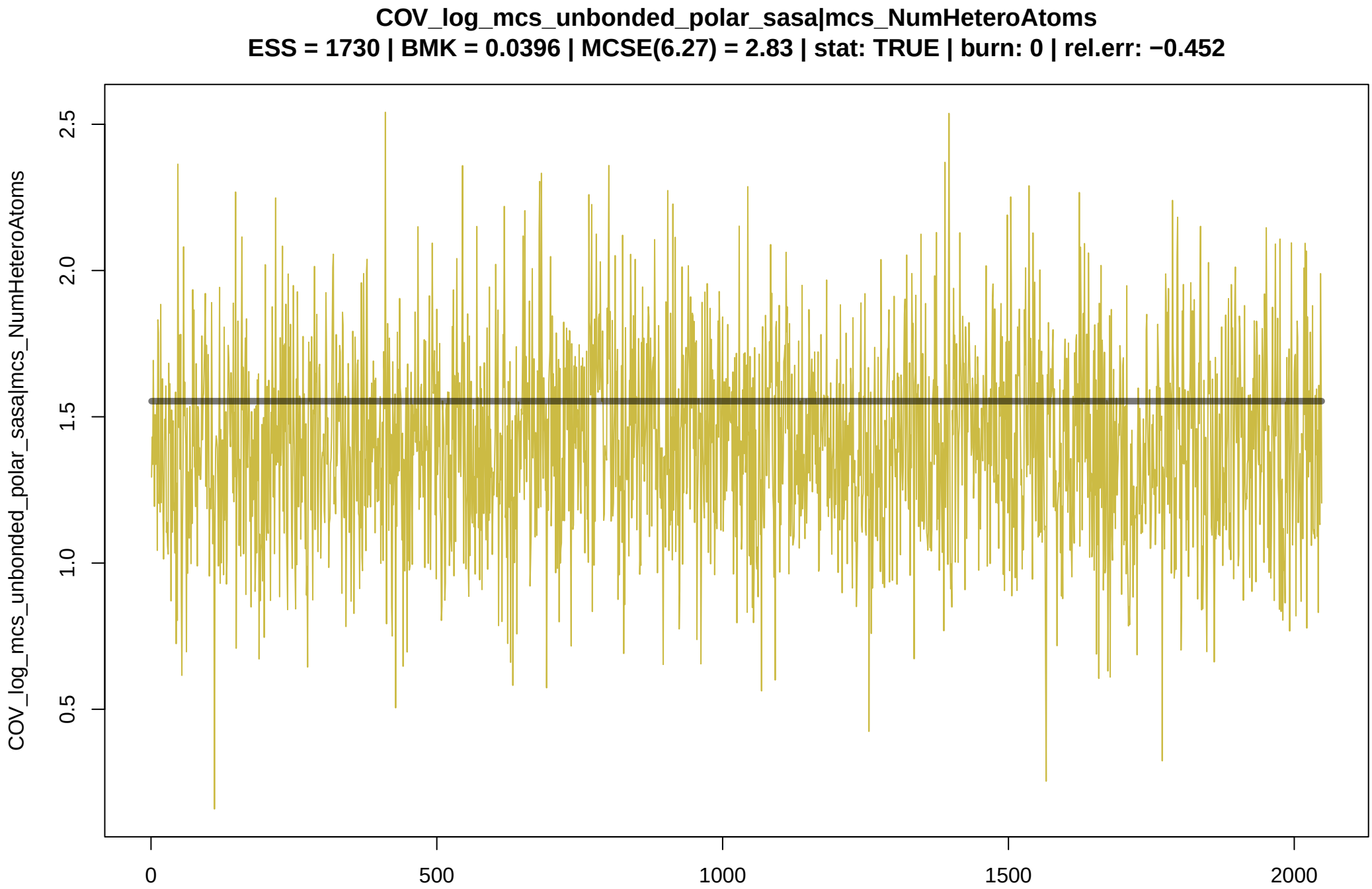

VAR_mcs_NumHeteroAtoms
ESS = 1720 | BMK = 0.0499 | MCSE(6.27) = 2.93 | stat: TRUE | burn: 0 | rel.err: 0.439
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

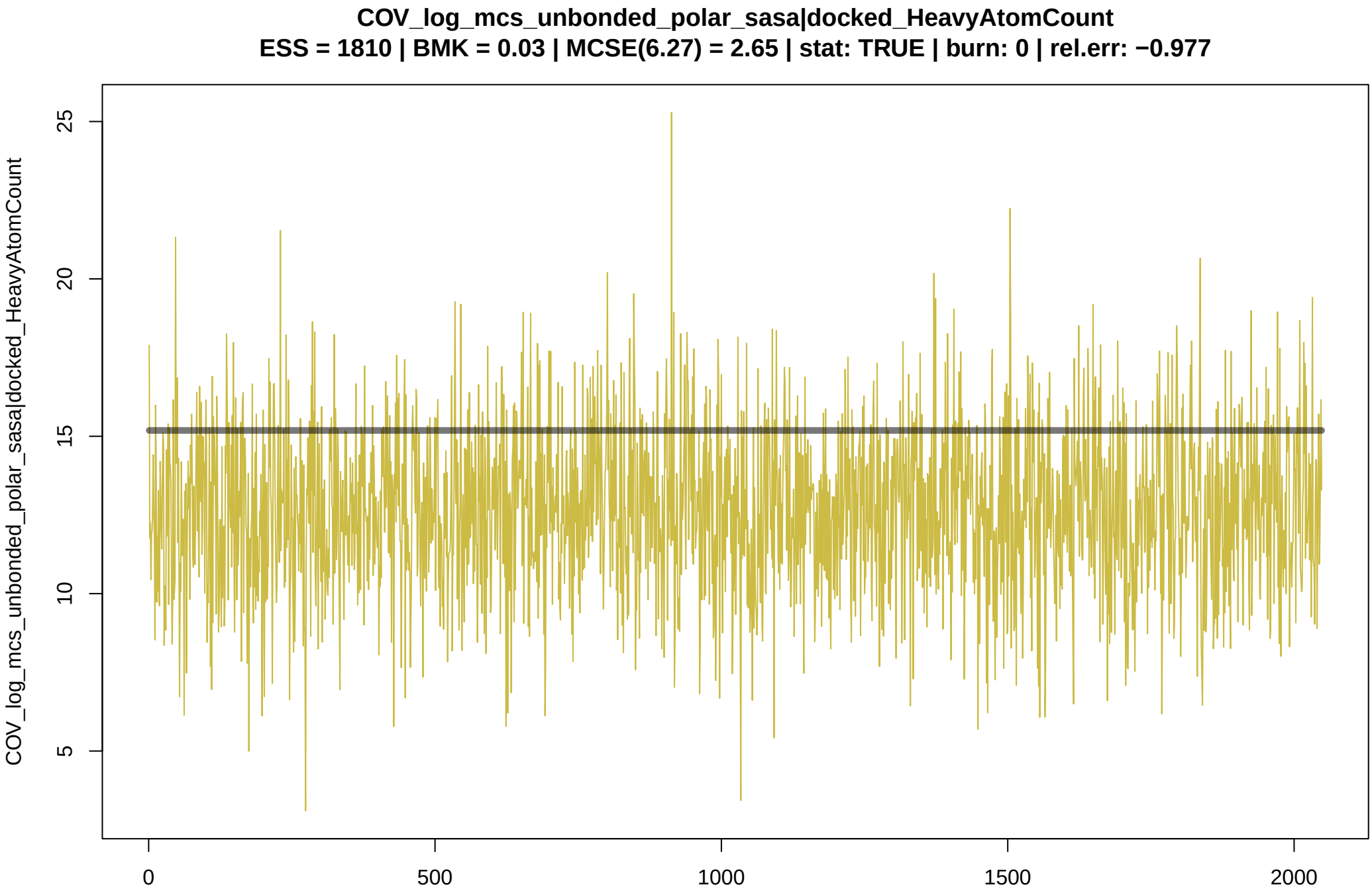

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0563 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: 0.0186
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

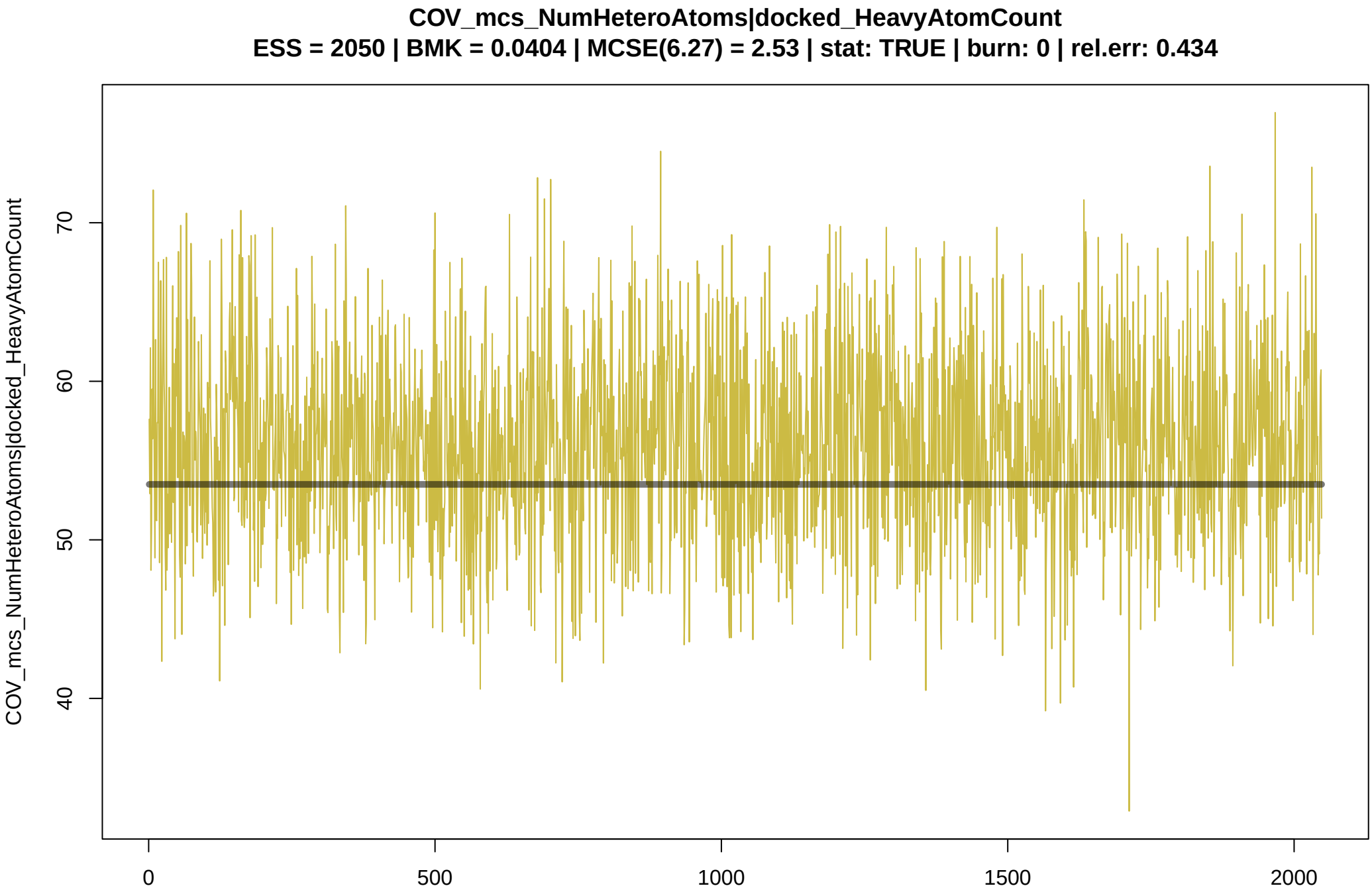

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1870 | BMK = 0.044 | MCSE(6.27) = 2.66 | stat: TRUE | burn: 0 | rel.err: 0.45
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.1
−0.2
−0.3
−0.4
−0.5
−0.6
−0.7
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 2.56 | stat: TRUE | burn: 0 | rel.err: −1.65
COV_log_RMSD|mcs_NumHeteroAtoms
−1.0
−1.2
−1.4
−1.6
−1.8
−2.0
−2.2
−2.4
0
500
1000
1500
2000


COV_log_RMSD|docked_HeavyAtomCount
ESS = 1870 | BMK = 0.0328 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 0 | rel.err: −1.82
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 = 1730 | BMK = 0.0396 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0 | rel.err: −0.452
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 = 1810 | BMK = 0.03 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: −0.977
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
25
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0404 | MCSE(6.27) = 2.53 | stat: TRUE | burn: 0 | rel.err: 0.434
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
40
50
60
70
0
500
1000
1500
2000