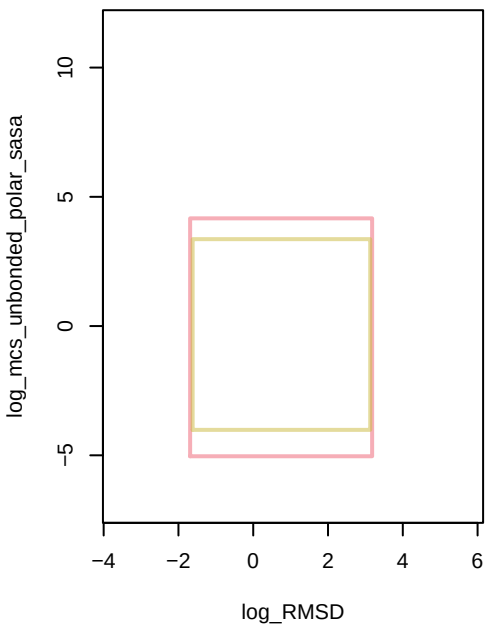
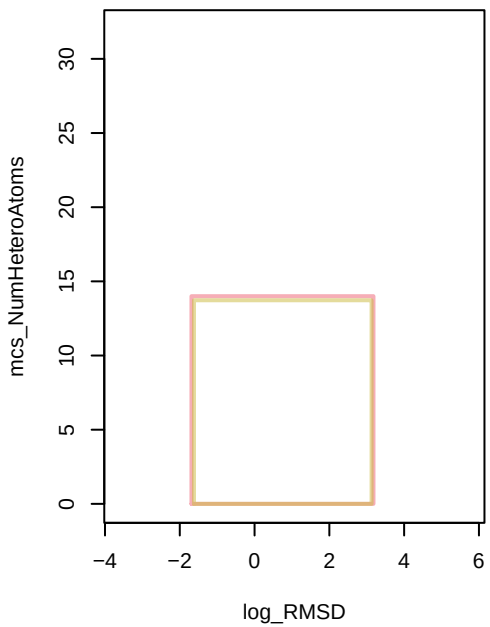
−− STATS maxD −−
min ESS = 62.105170171398
max BMK = 0.209192702022583
max MCSE = 8.77288384594454
all stationary: FALSE
burn: 0
max rel.err.: 2.14337939791671

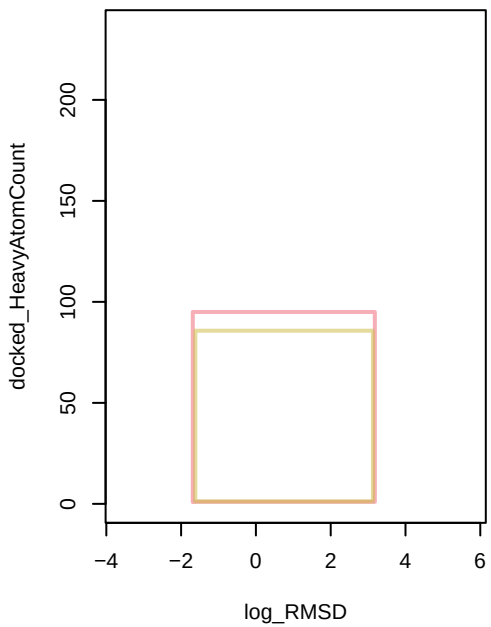
−− STATS 2D −−
min ESS = 1480.96869317278
max BMK = 0.0647086146895888
max MCSE = 2.61625635034241
all stationary: TRUE
burn: 0
max rel.err.: 1.76702544317149

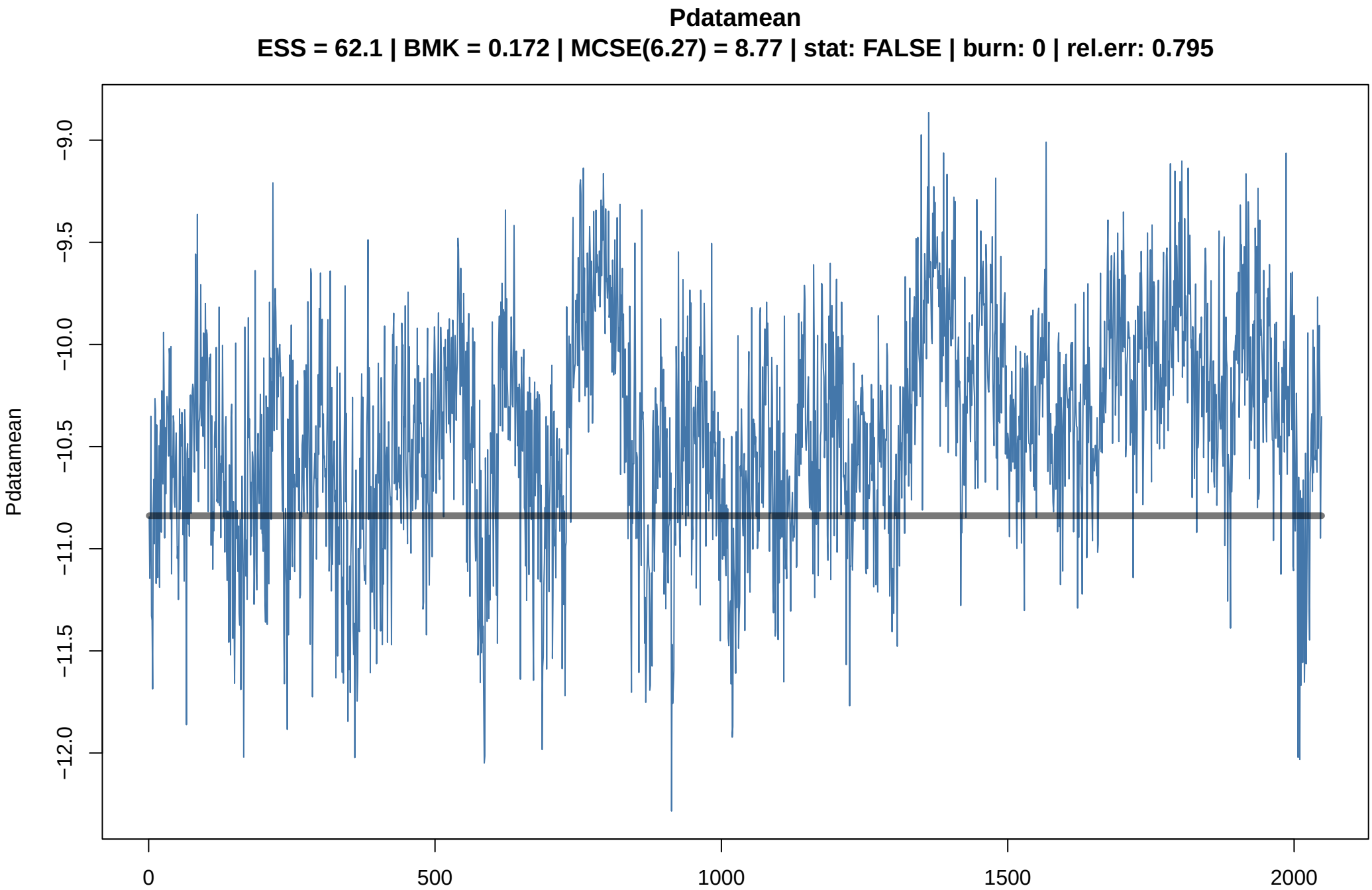
−− STATS 1D −−
min ESS = 1071.62537306162
max BMK = 0.084306434294174 1
max MCSE = 3.23586322677185
all stationary: FALSE
burn: 0
max rel.err.: 2.23667360811149

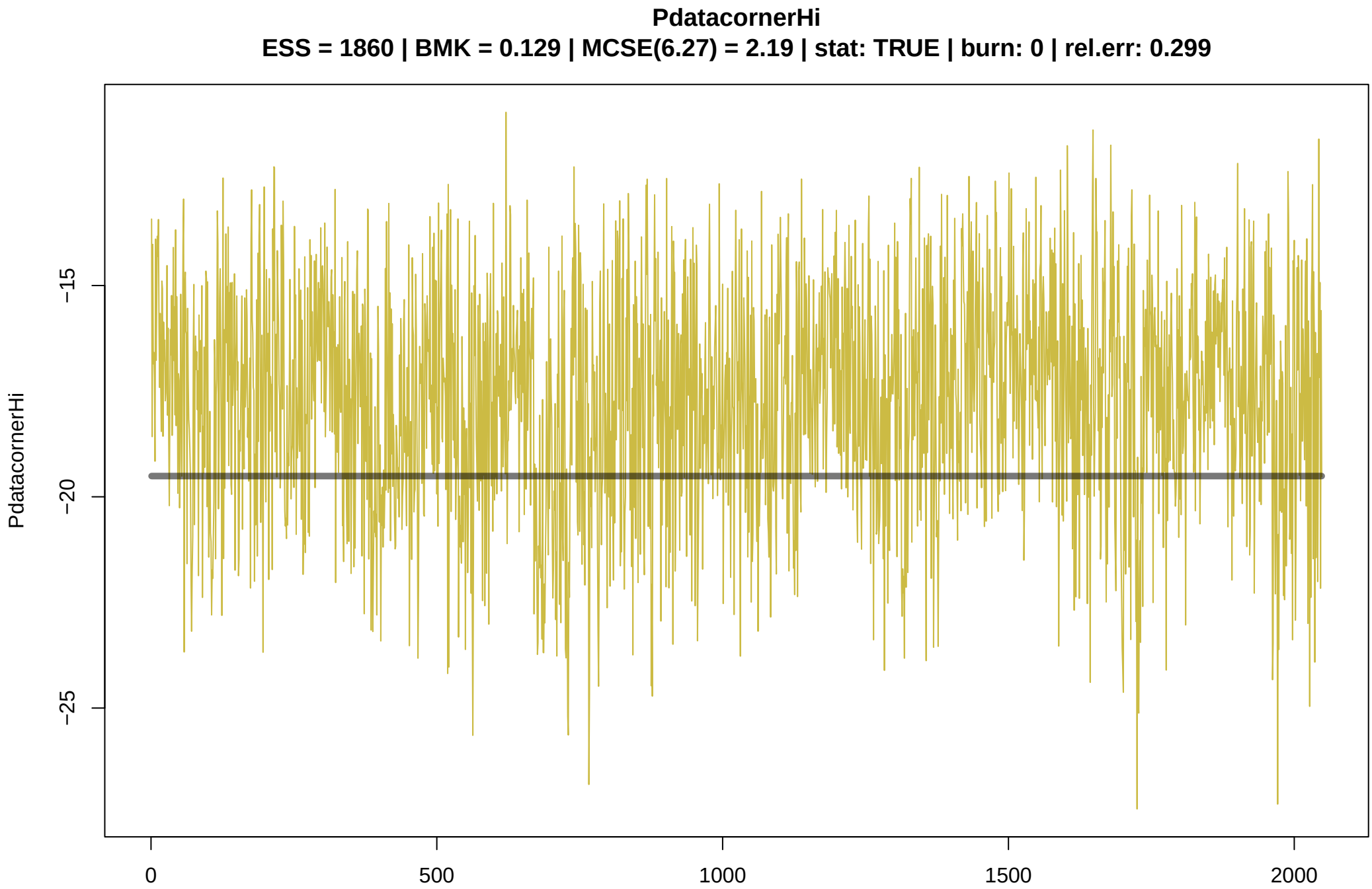
Occupied clusters: 10 of 16

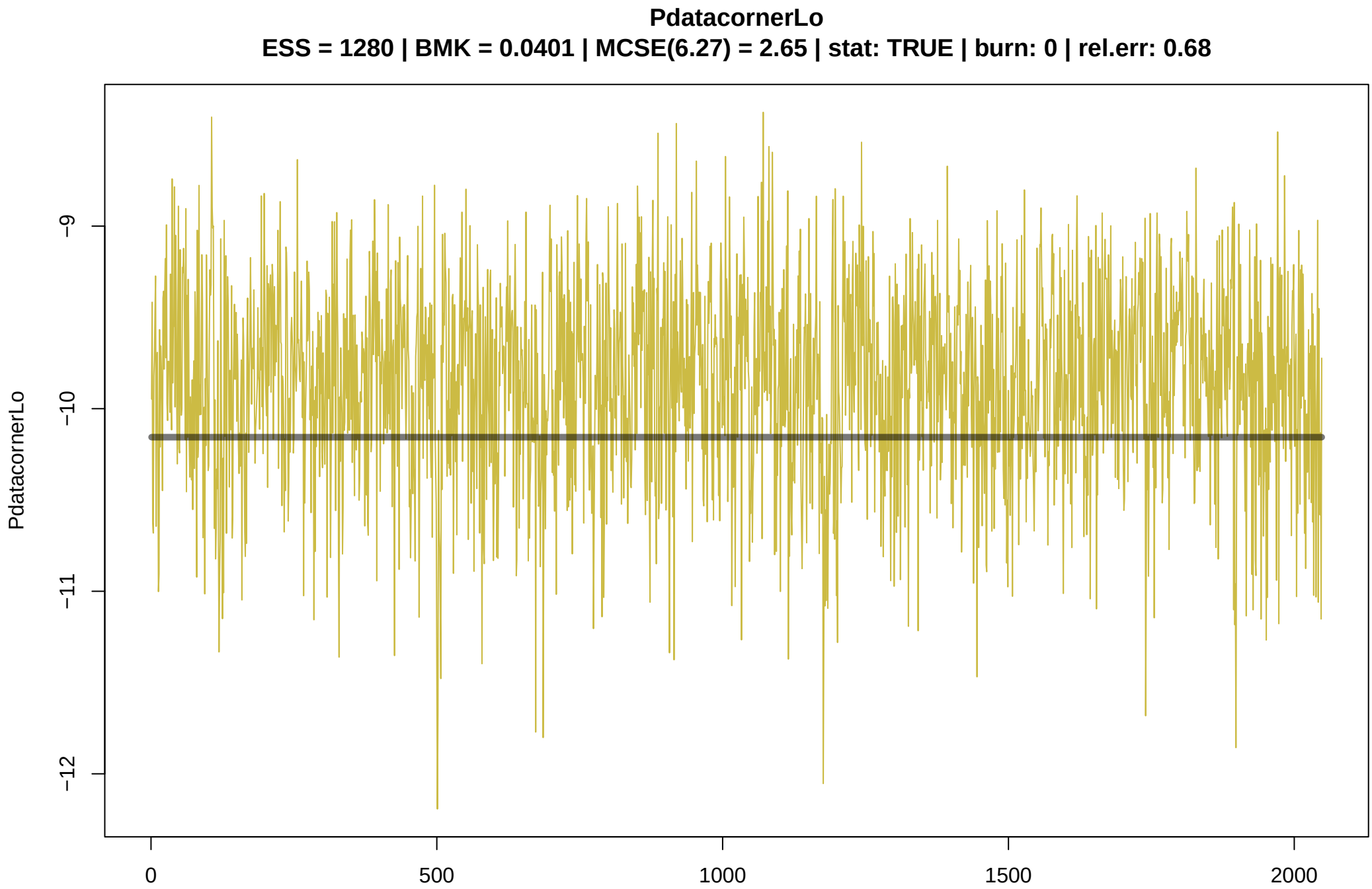

log_mcs_unbonded_polar_sasa
10
5
0
−5
−4
−2
0
2
4
6
log_RMSD

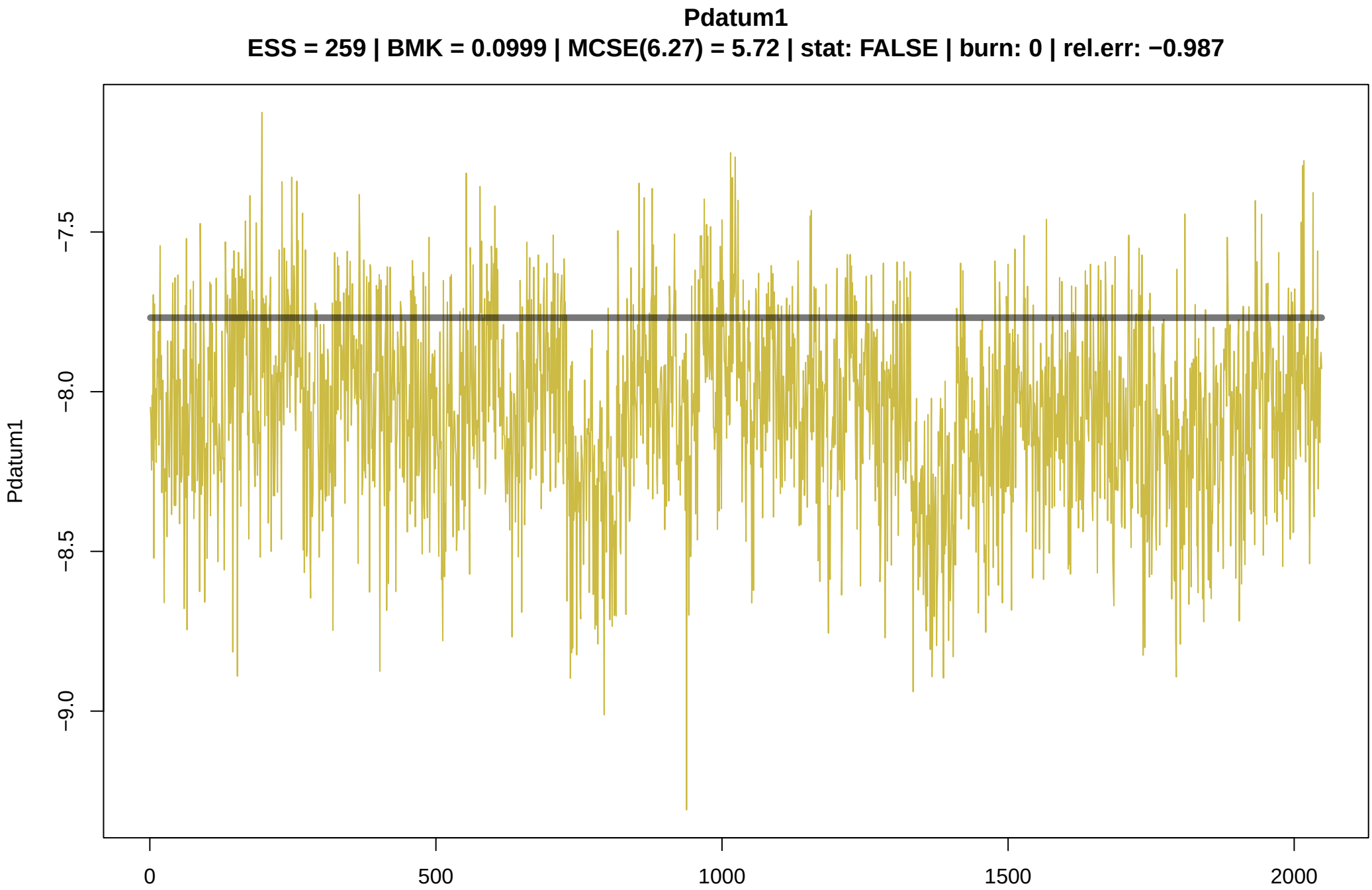

mcs_NumHeteroAtoms
30
25
20
15
10
5
0
−4
−2
0
2
4
6
log_RMSD

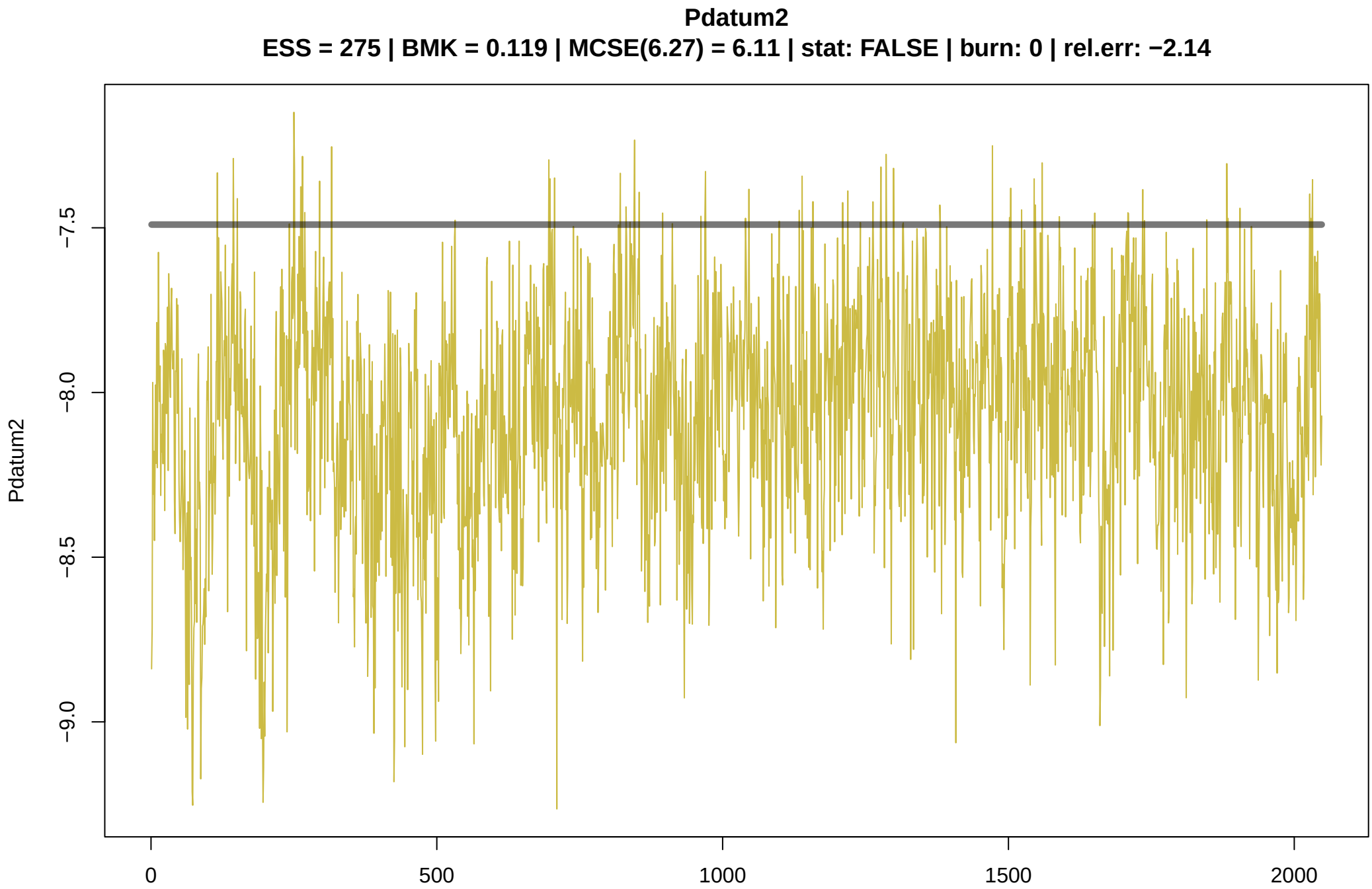

docked_HeavyAtomCount
200
150
100
50
0
−4
−2
0
2
4
6
log_RMSD

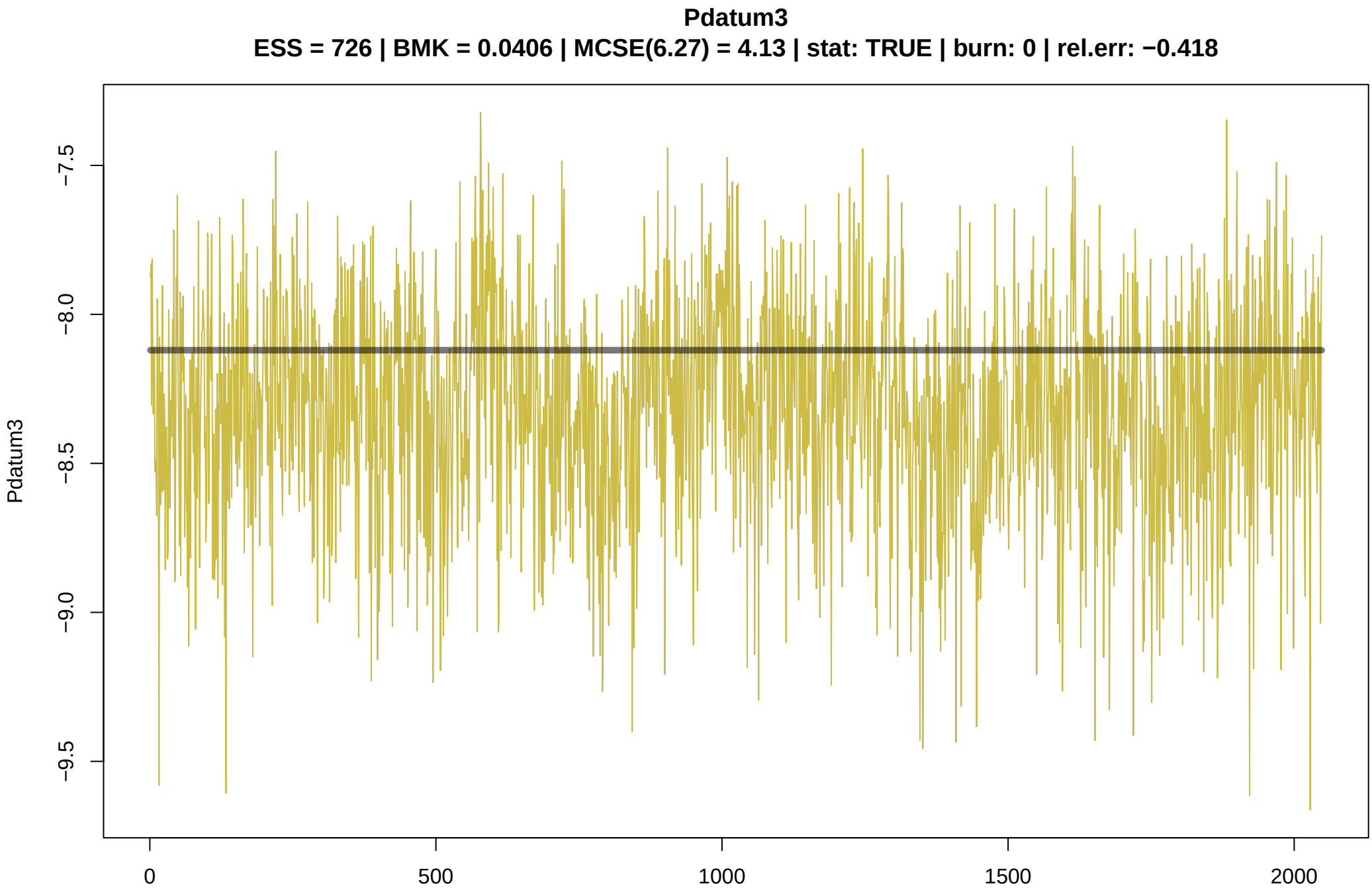

Pdatamean
ESS = 62.1 | BMK = 0.172 | MCSE(6.27) = 8.77 | stat: FALSE | burn: 0 | rel.err: 0.795
Pdatamean
−9.0
−9.5
−10.0
−10.5
−11.0
−11.5
−12.0
0
500
1000
1500
2000

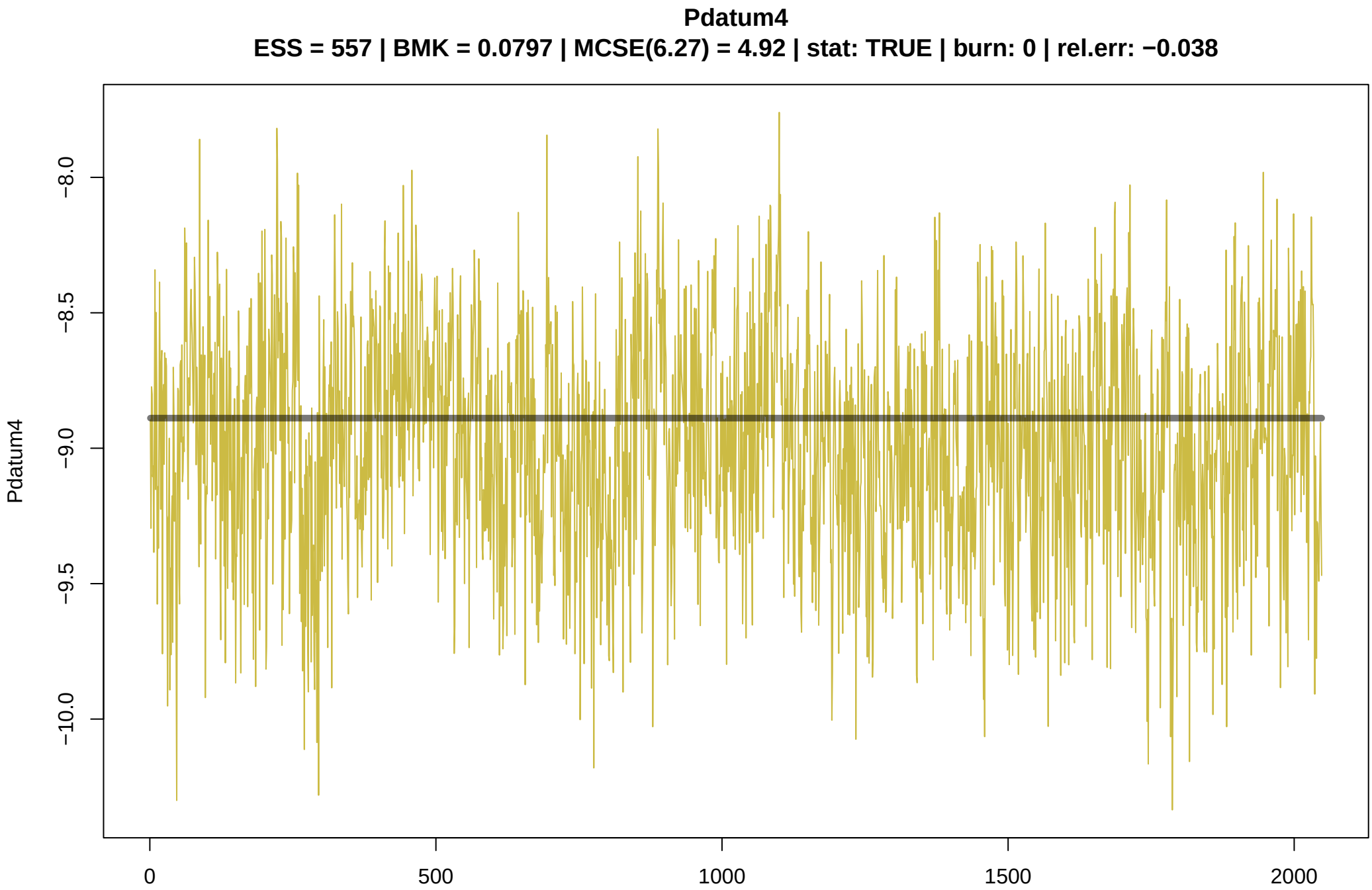

PdatacornerHi
ESS = 1860 | BMK = 0.129 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: 0.299
PdatacornerHi
−15
−20
−25
0
500
1000
1500
2000

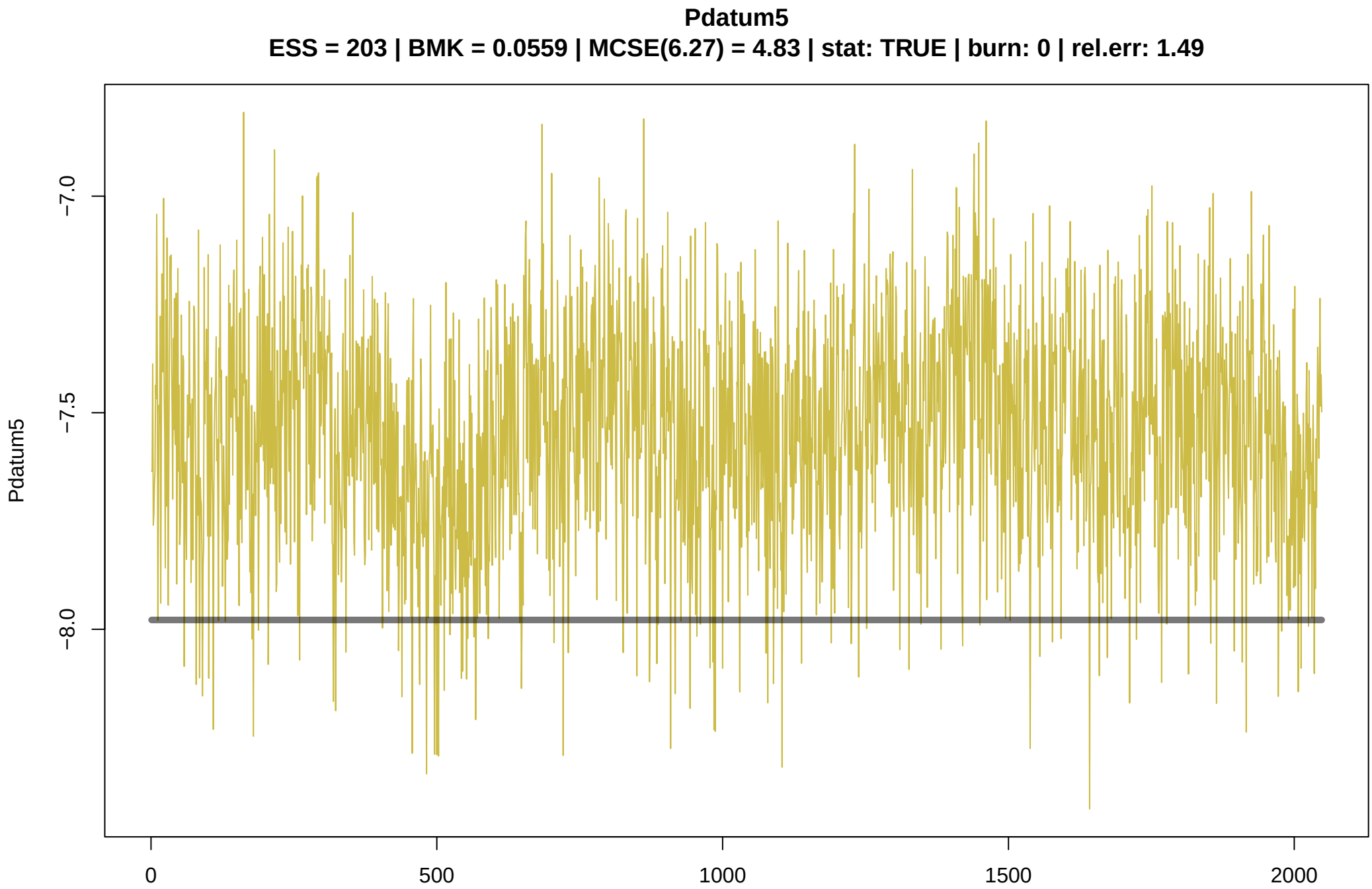

PdatacornerLo
ESS = 1280 | BMK = 0.0401 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0 | rel.err: 0.68
PdatacornerLo
−9
−10
−11
−12
0
500
1000
1500
2000

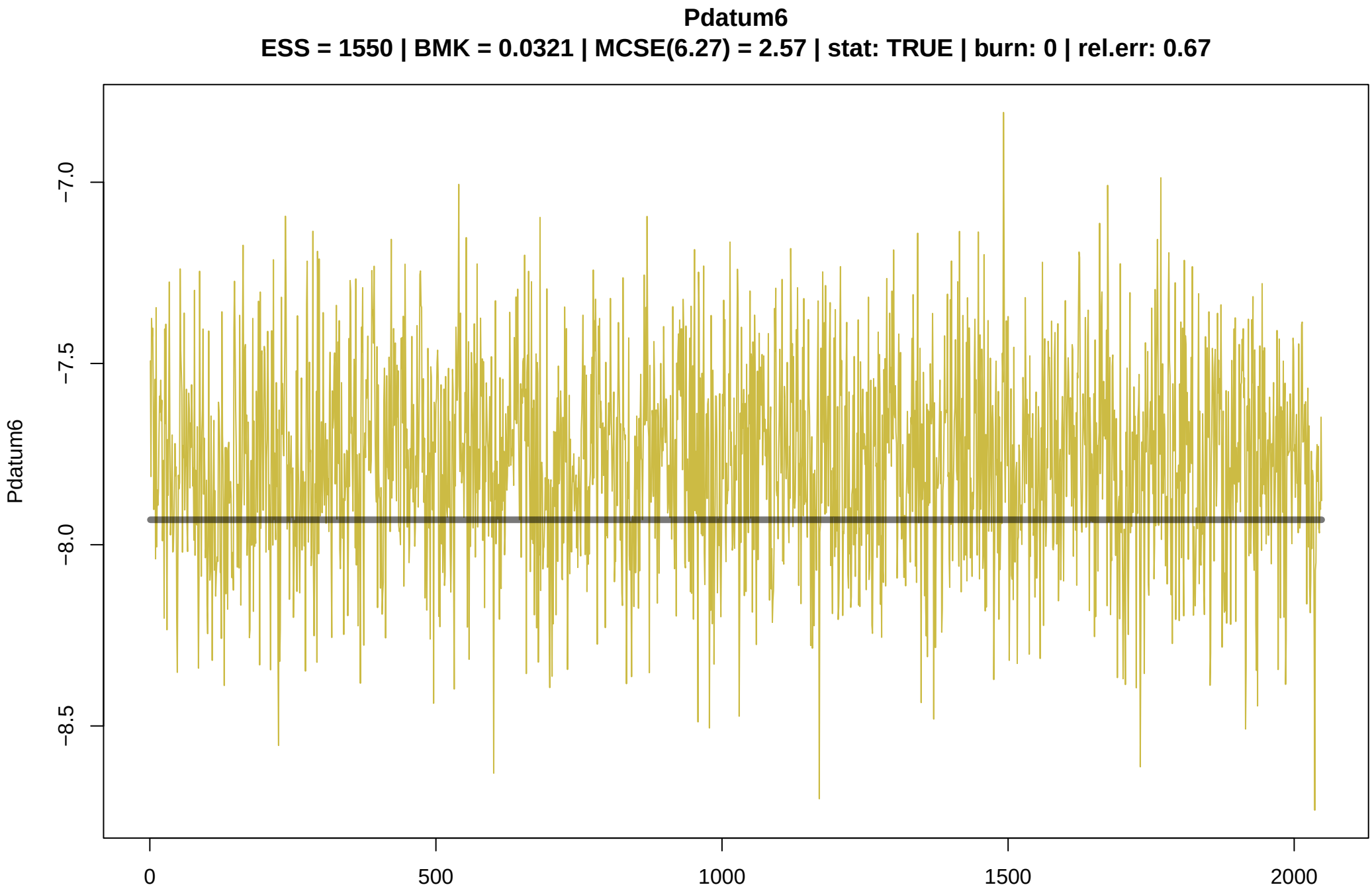

Pdatum1
ESS = 259 | BMK = 0.0999 | MCSE(6.27) = 5.72 | stat: FALSE | burn: 0 | rel.err: −0.987
Pdatum1
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

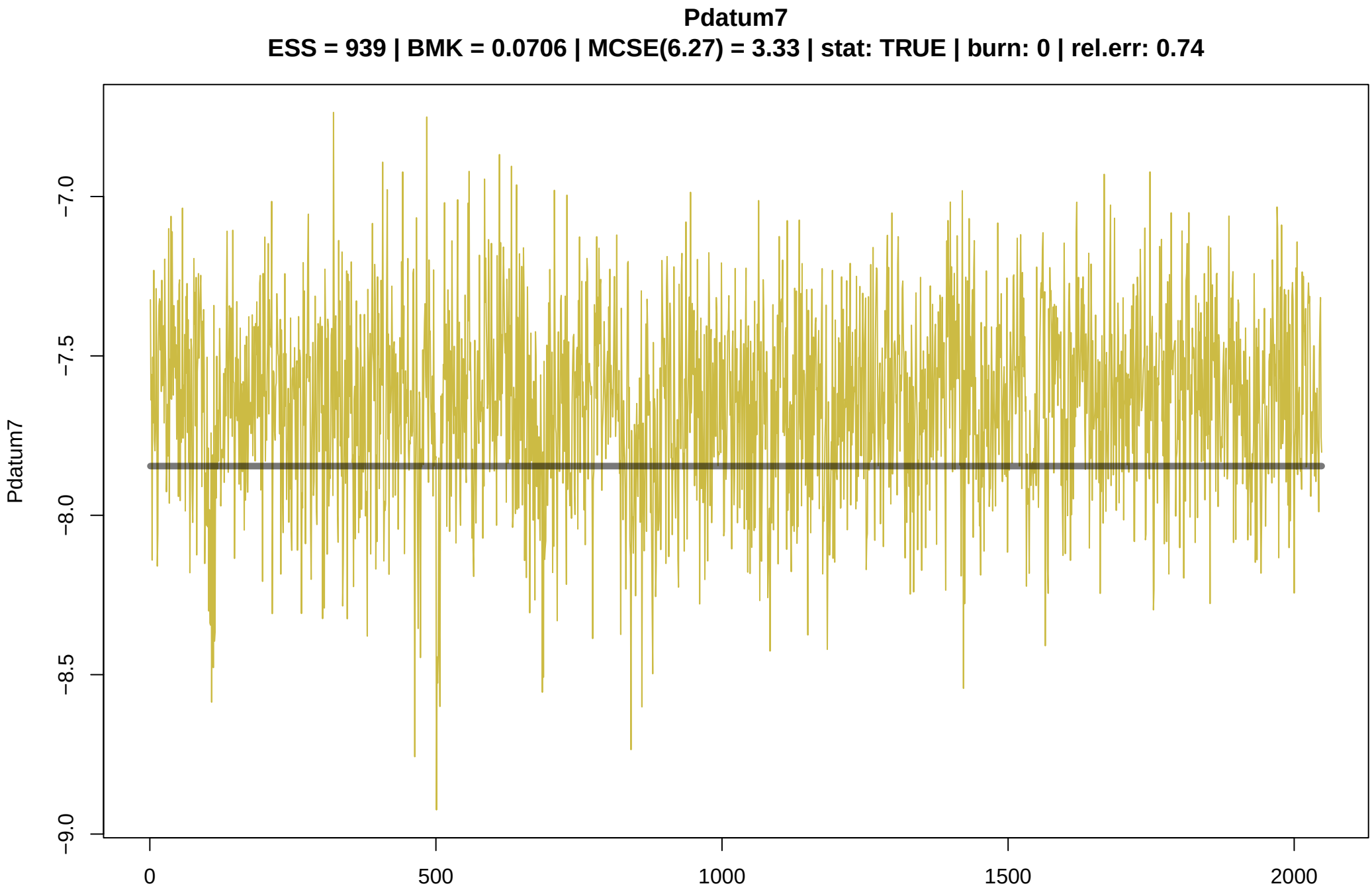

Pdatum2
ESS = 275 | BMK = 0.119 | MCSE(6.27) = 6.11 | stat: FALSE | burn: 0 | rel.err: −2.14
Pdatum2
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

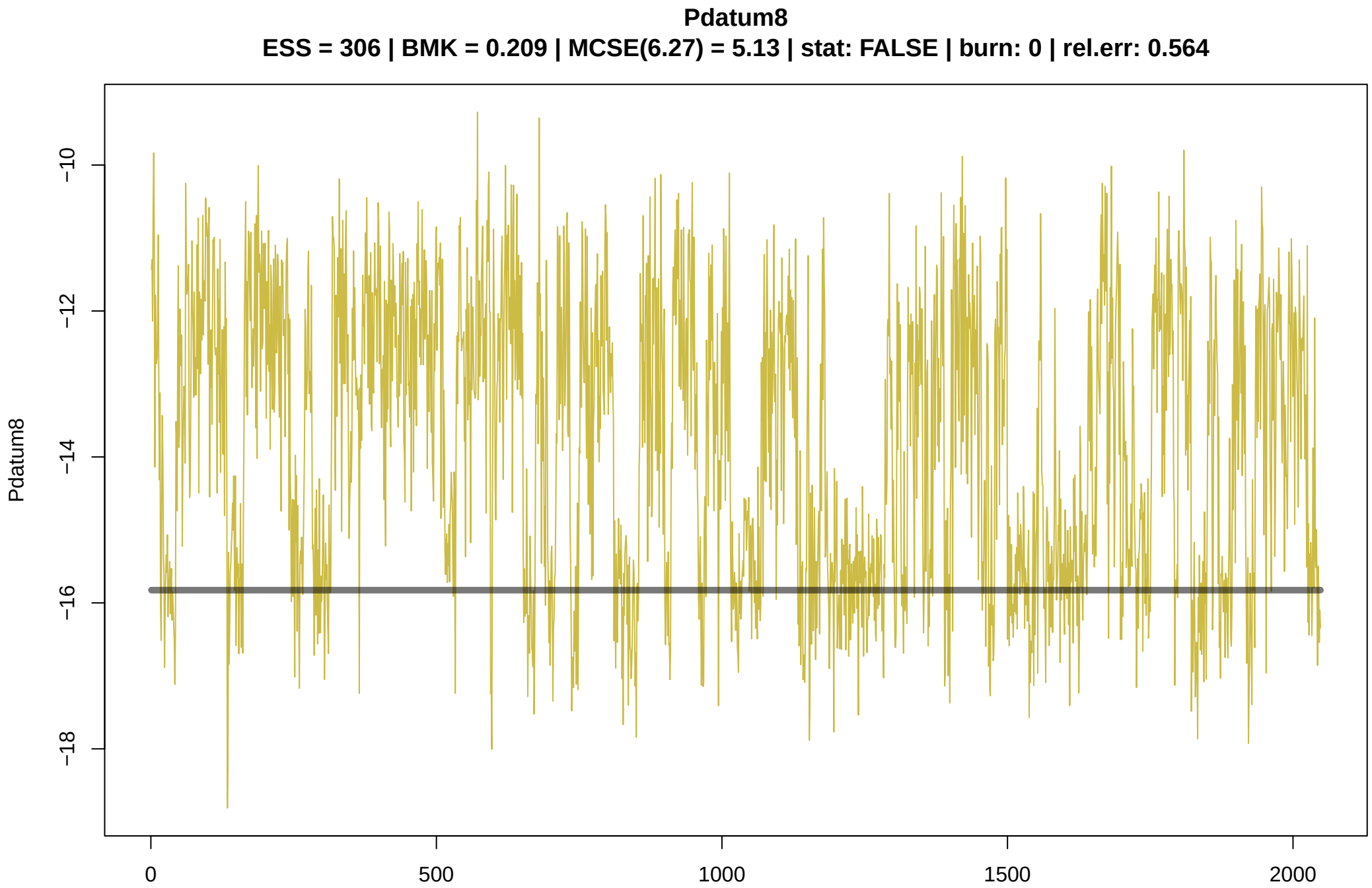

Pdatum3
ESS = 726 | BMK = 0.0406 | MCSE(6.27) = 4.13 | stat: TRUE | burn: 0 | rel.err: −0.418
Pdatum3
−7.5
−8.0
−8.5
−9.0
−9.5
0
500
1000
1500
2000

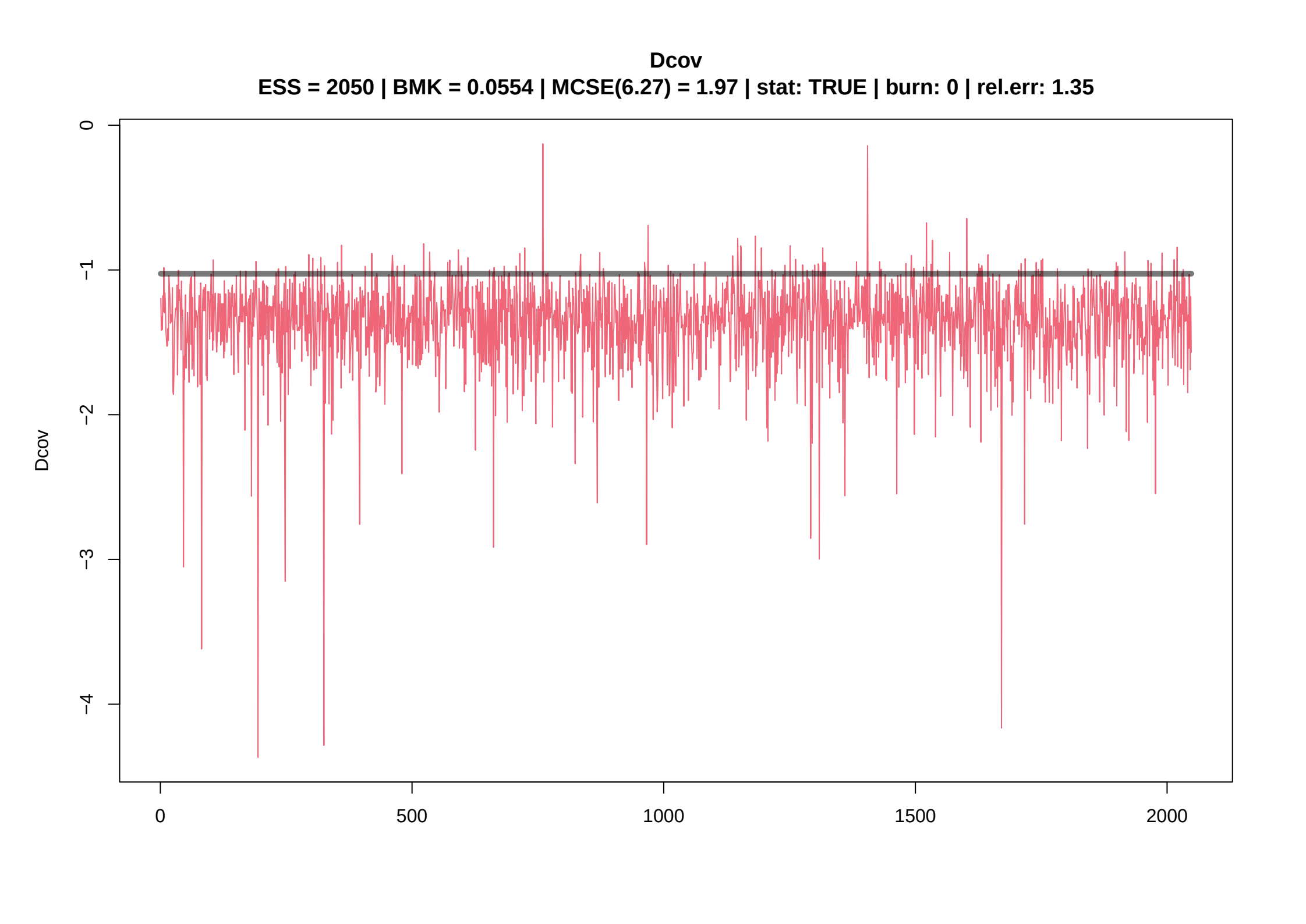

Pdatum4
ESS = 557 | BMK = 0.0797 | MCSE(6.27) = 4.92 | stat: TRUE | burn: 0 | rel.err: −0.038
Pdatum4
−8.0
−8.5
−9.0
−9.5
−10.0
0
500
1000
1500
2000

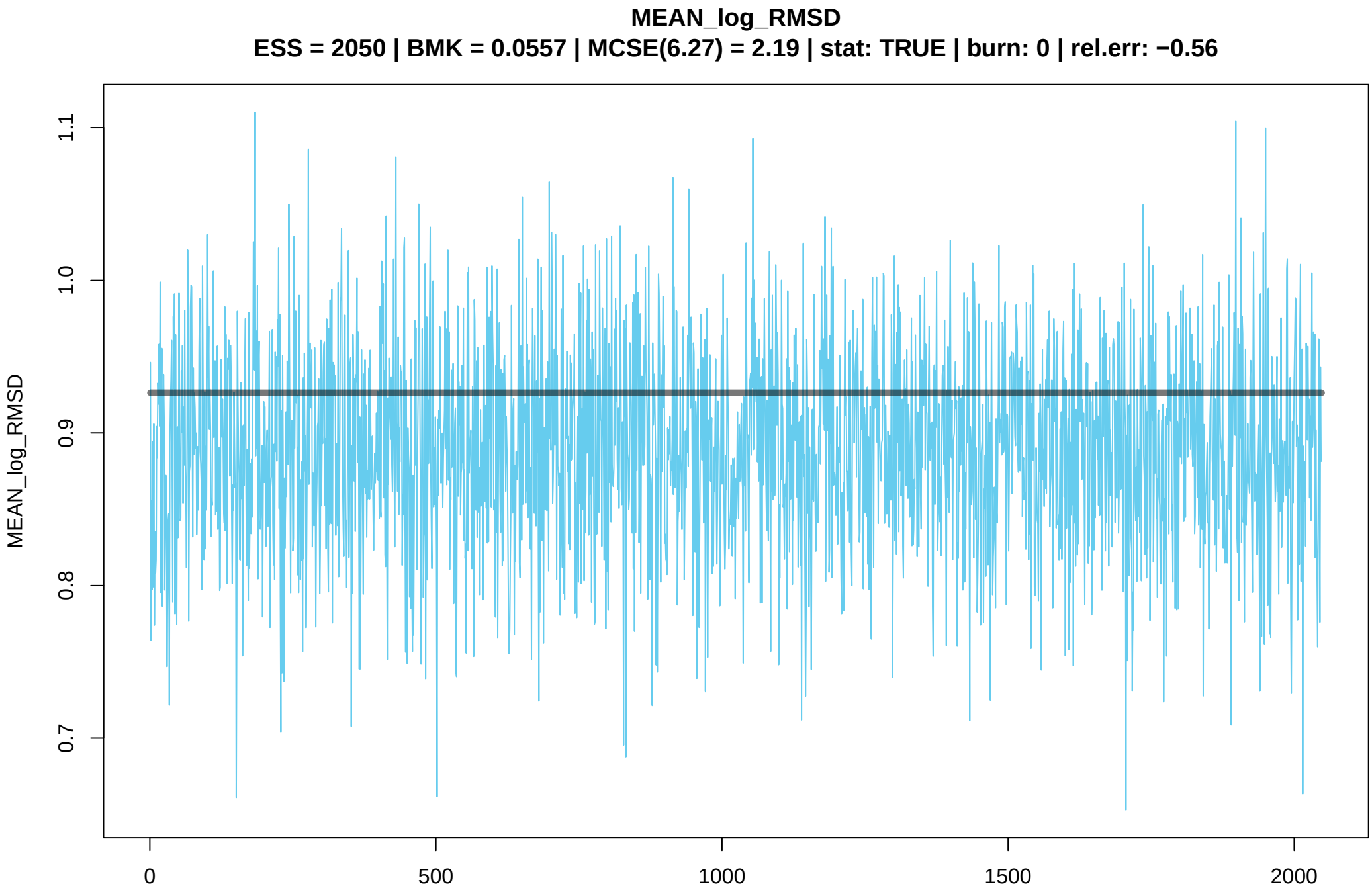

Pdatum5
ESS = 203 | BMK = 0.0559 | MCSE(6.27) = 4.83 | stat: TRUE | burn: 0 | rel.err: 1.49
Pdatum5
−7.0
−7.5
−8.0
0
500
1000
1500
2000

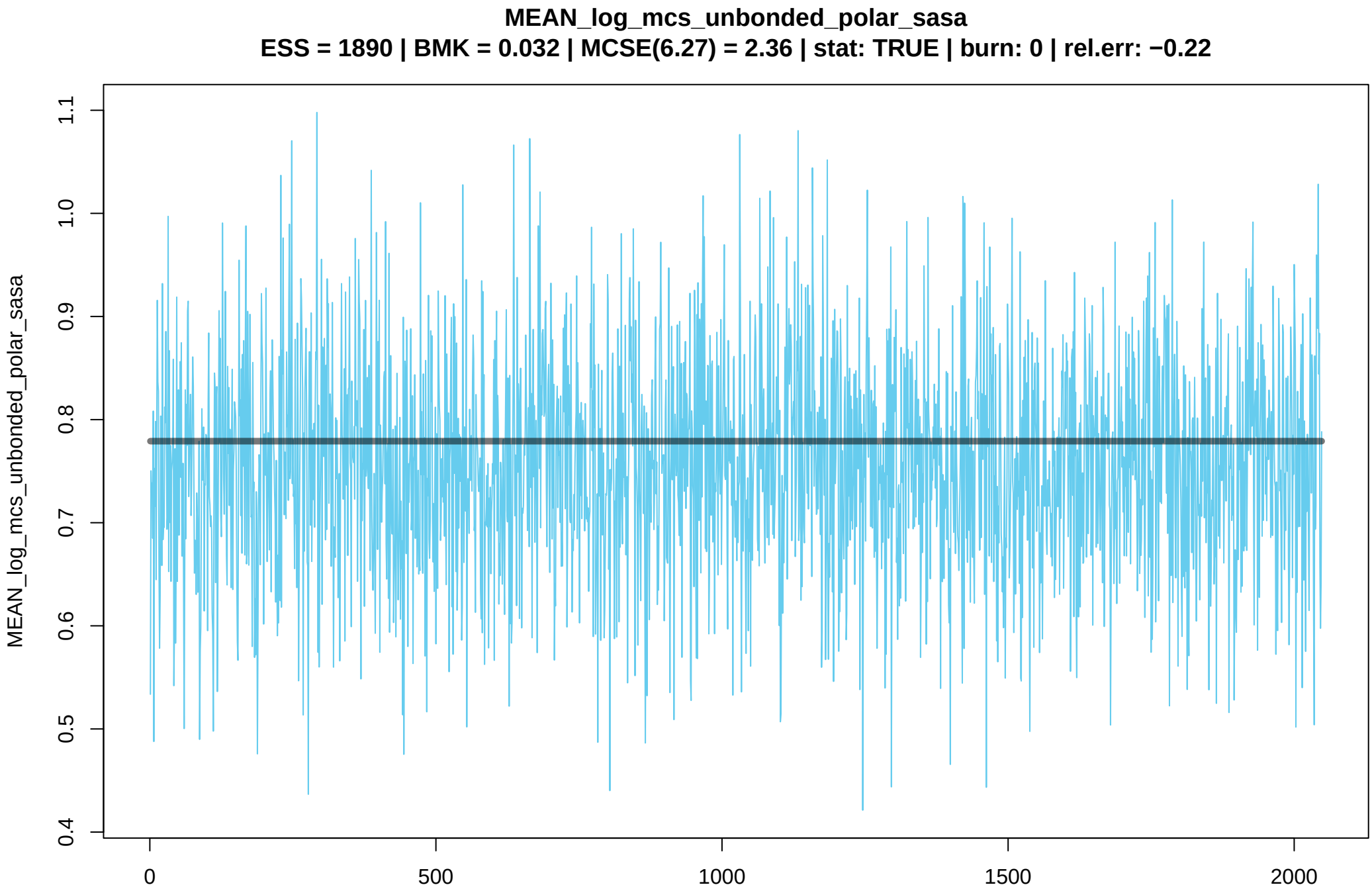

Pdatum6
ESS = 1550 | BMK = 0.0321 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0 | rel.err: 0.67
Pdatum6
−7.0
−7.5
−8.0
−8.5
0
500
1000
1500
2000

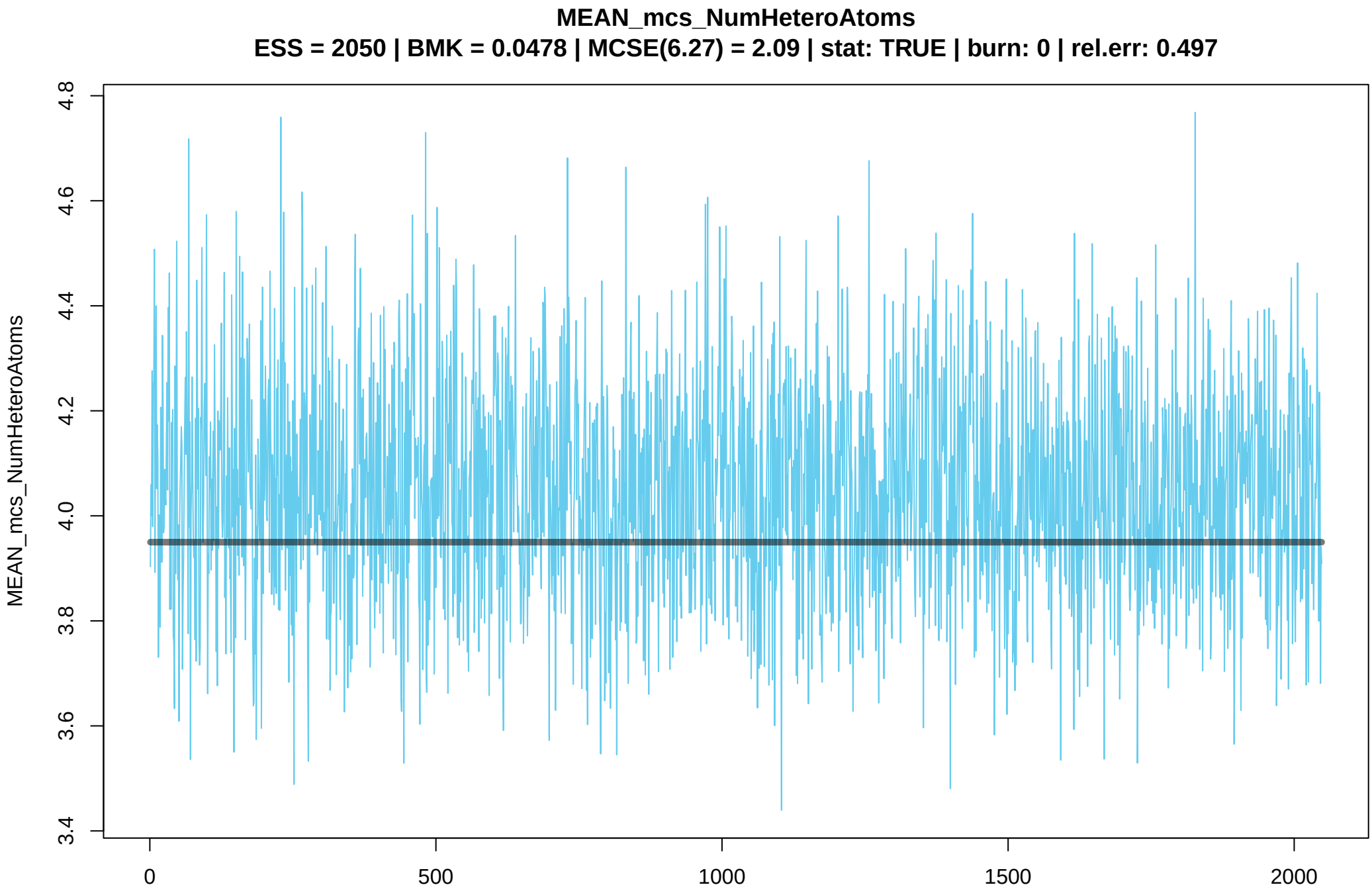

Pdatum7
ESS = 939 | BMK = 0.0706 | MCSE(6.27) = 3.33 | stat: TRUE | burn: 0 | rel.err: 0.74
Pdatum7
−7.0
−7.5
−8.0
−8.5
−9.0
0
500
1000
1500
2000

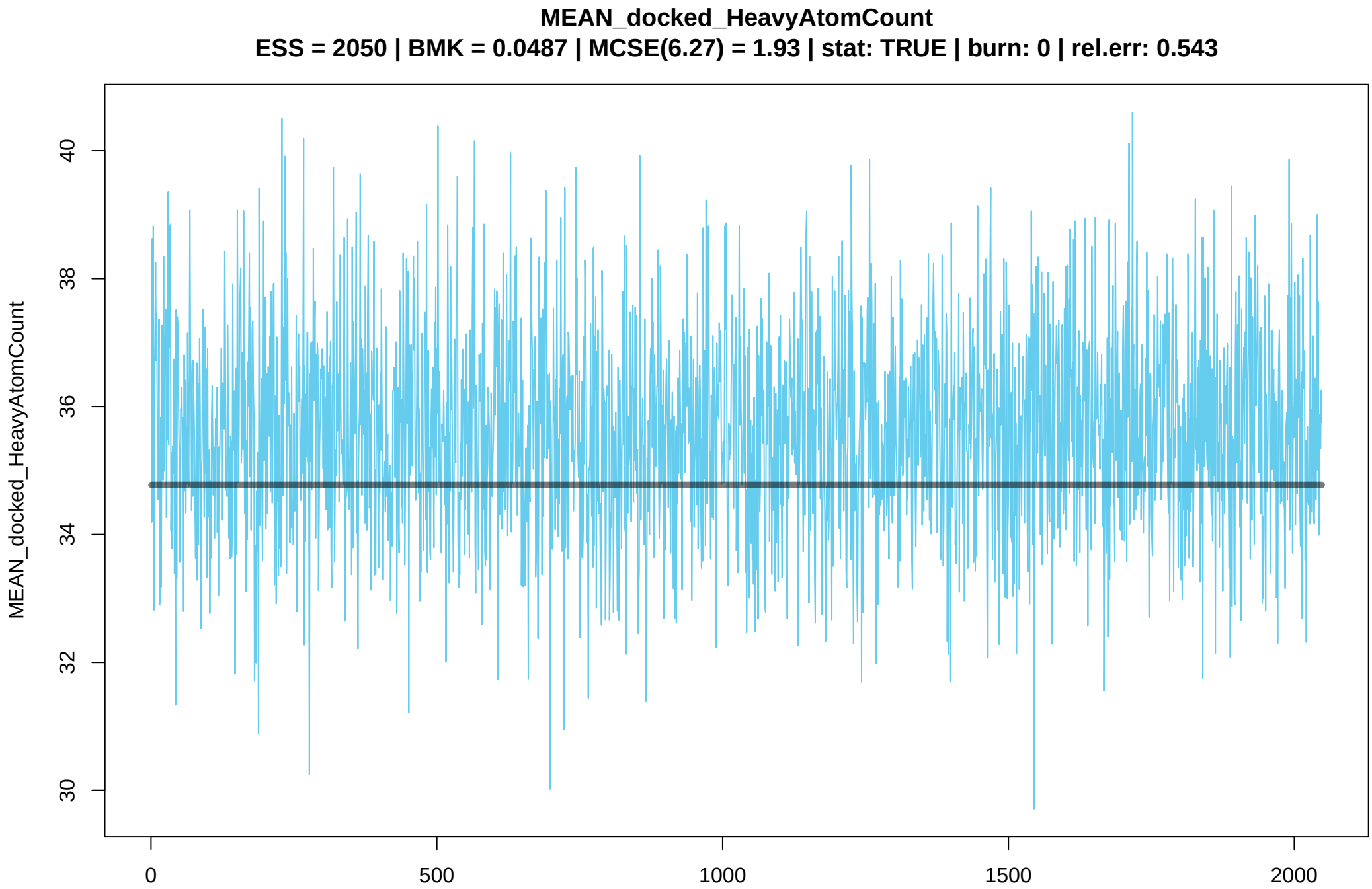

Pdatum8
ESS = 306 | BMK = 0.209 | MCSE(6.27) = 5.13 | stat: FALSE | burn: 0 | rel.err: 0.564
Pdatum8
−10
−12
−14
−16
−18
0
500
1000
1500
2000

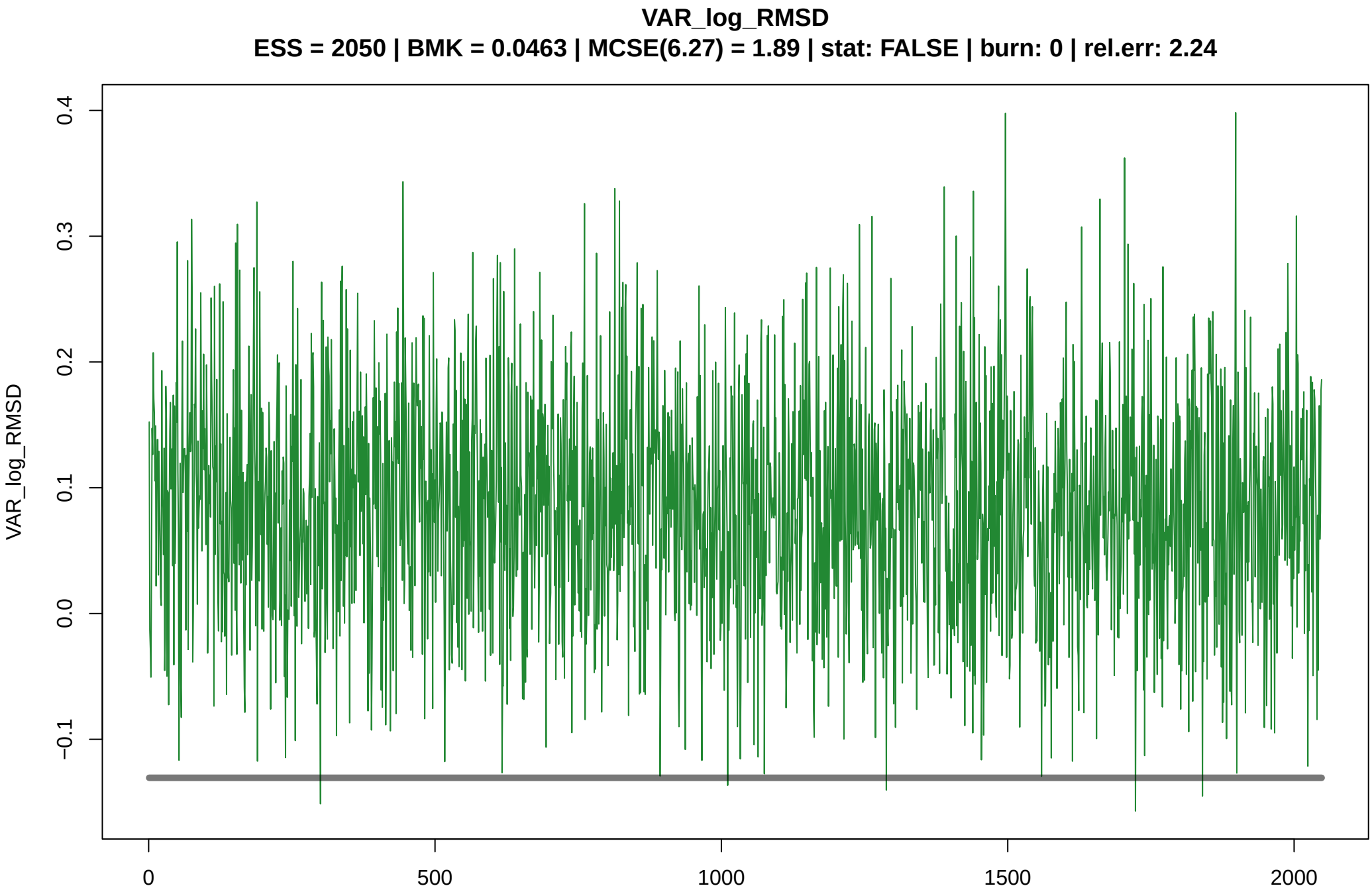

Dcov
ESS = 2050 | BMK = 0.0554 | MCSE(6.27) = 1.97 | stat: TRUE | burn: 0 | rel.err: 1.35
Dcov
0
−1
−2
−3
−4
0
500
1000
1500
2000

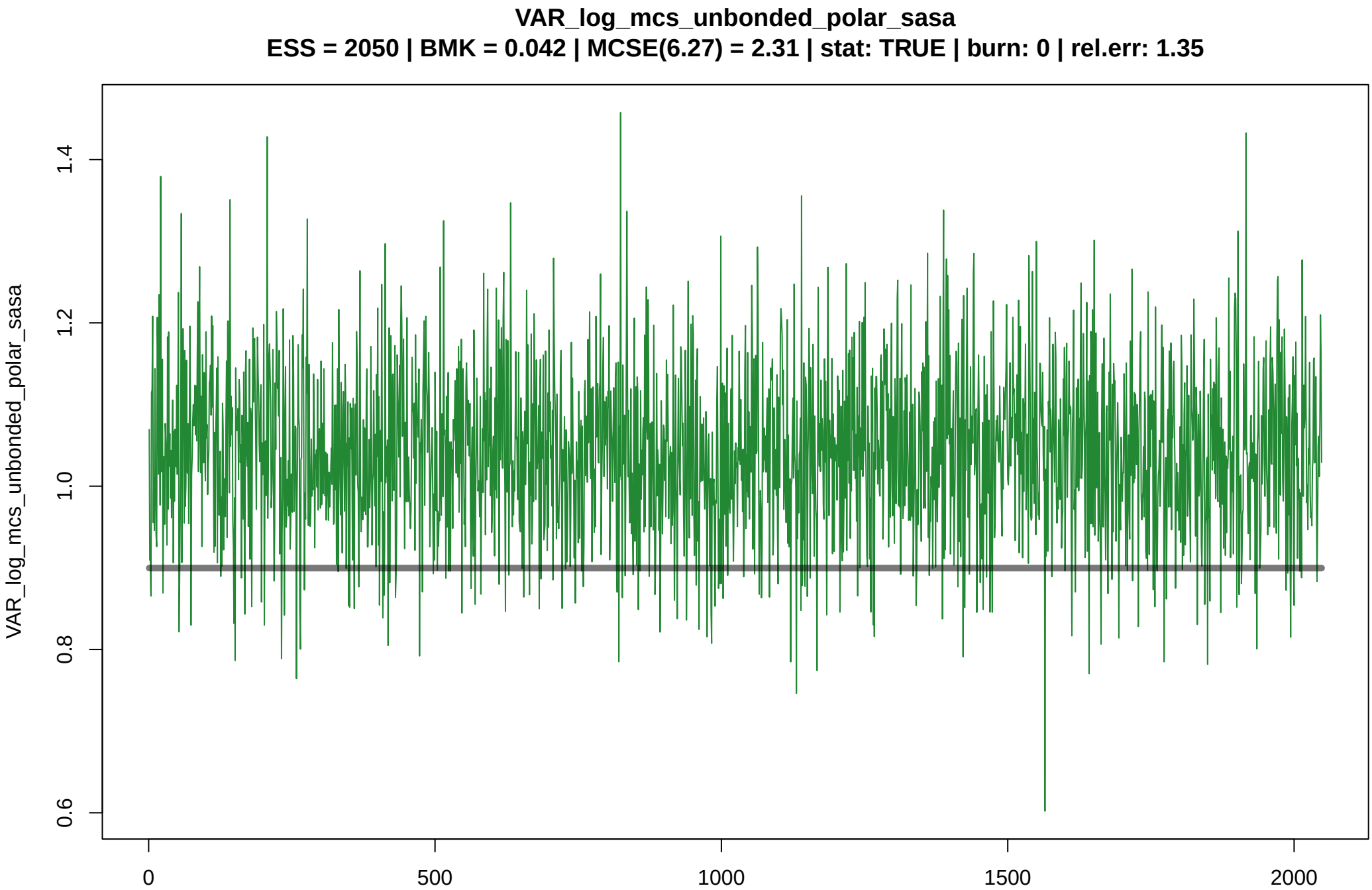

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0557 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0 | rel.err: −0.56
MEAN_log_RMSD
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

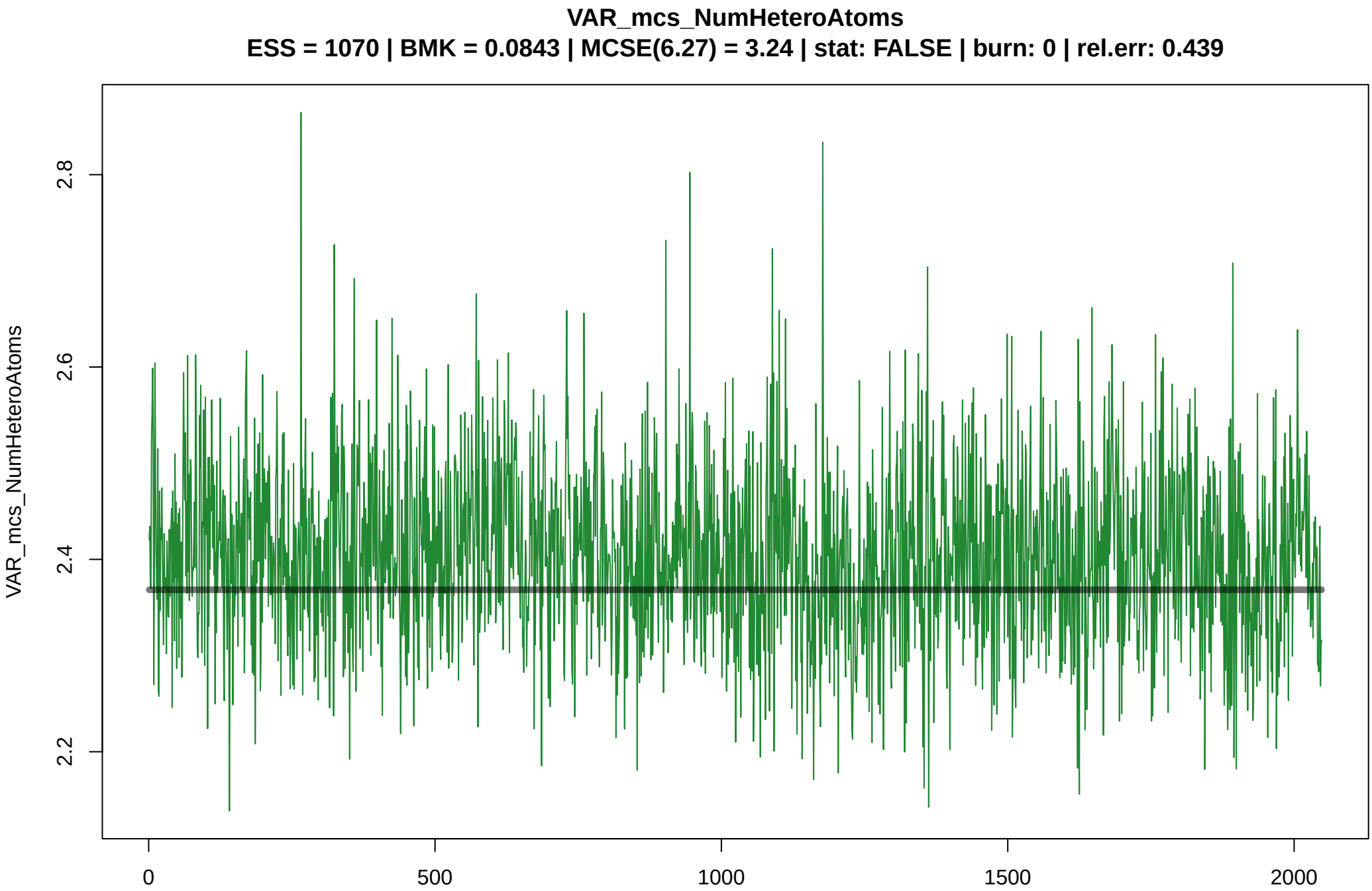

MEAN_log_mcs_unbonded_polar_sasa
ESS = 1890 | BMK = 0.032 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0 | rel.err: −0.22
MEAN_log_mcs_unbonded_polar_sasa
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
0
500
1000
1500
2000

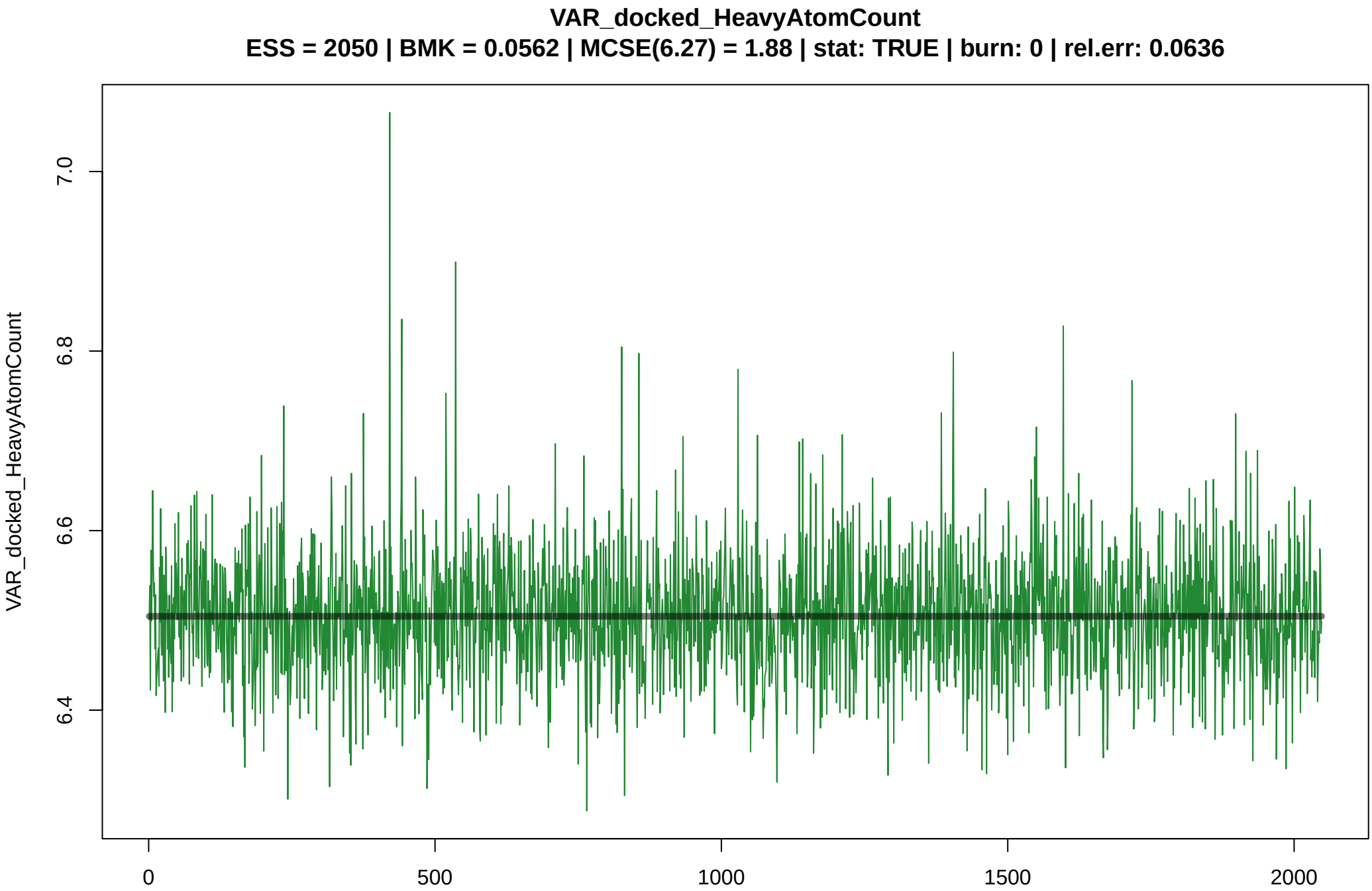

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0478 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0 | rel.err: 0.497
MEAN_mcs_NumHeteroAtoms
3.4
3.6
3.8
4.0
4.2
4.4
4.6
4.8
0
500
1000
1500
2000

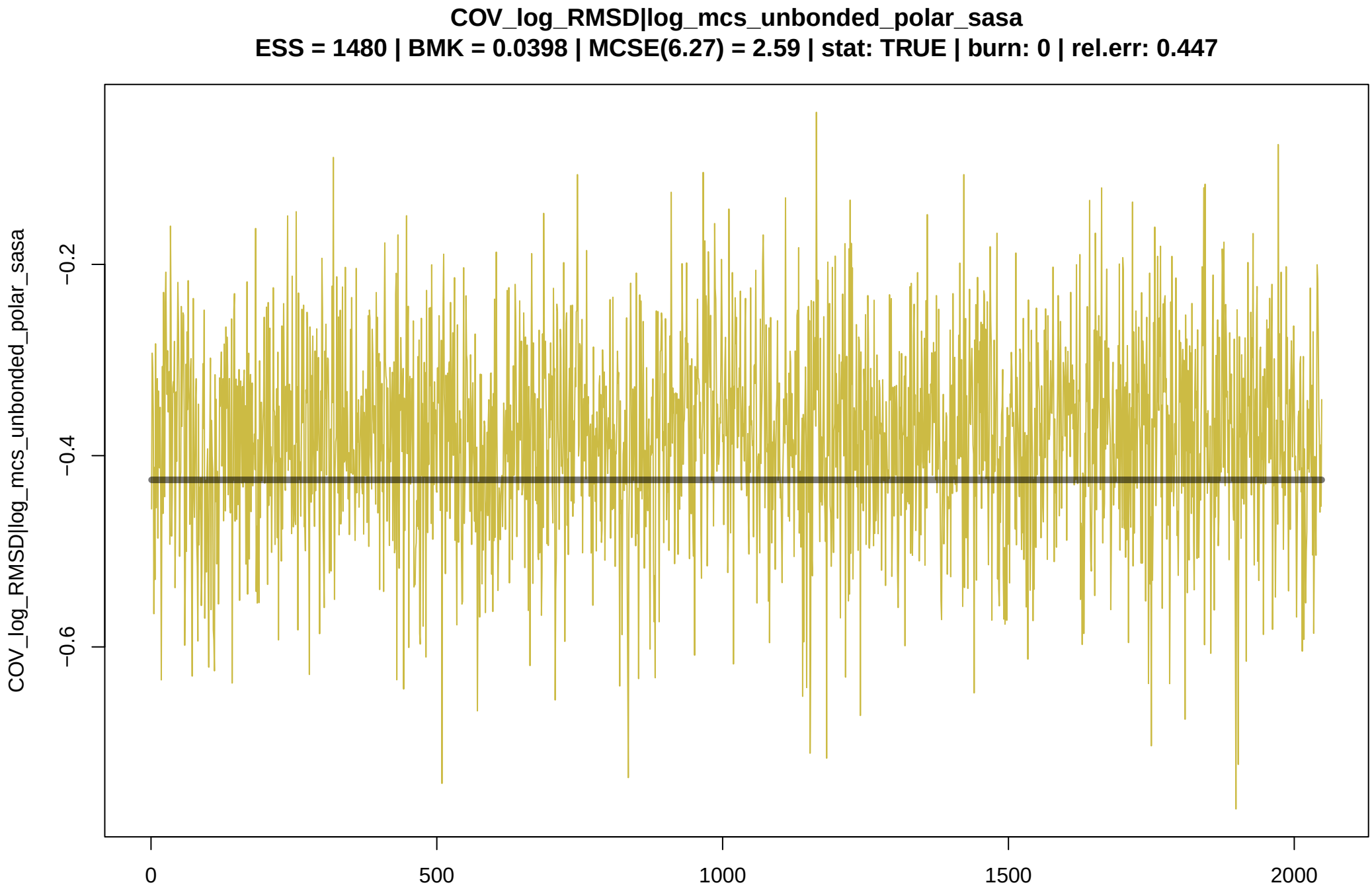

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0487 | MCSE(6.27) = 1.93 | stat: TRUE | burn: 0 | rel.err: 0.543
MEAN_docked_HeavyAtomCount
30
32
34
36
38
40
0
500
1000
1500
2000

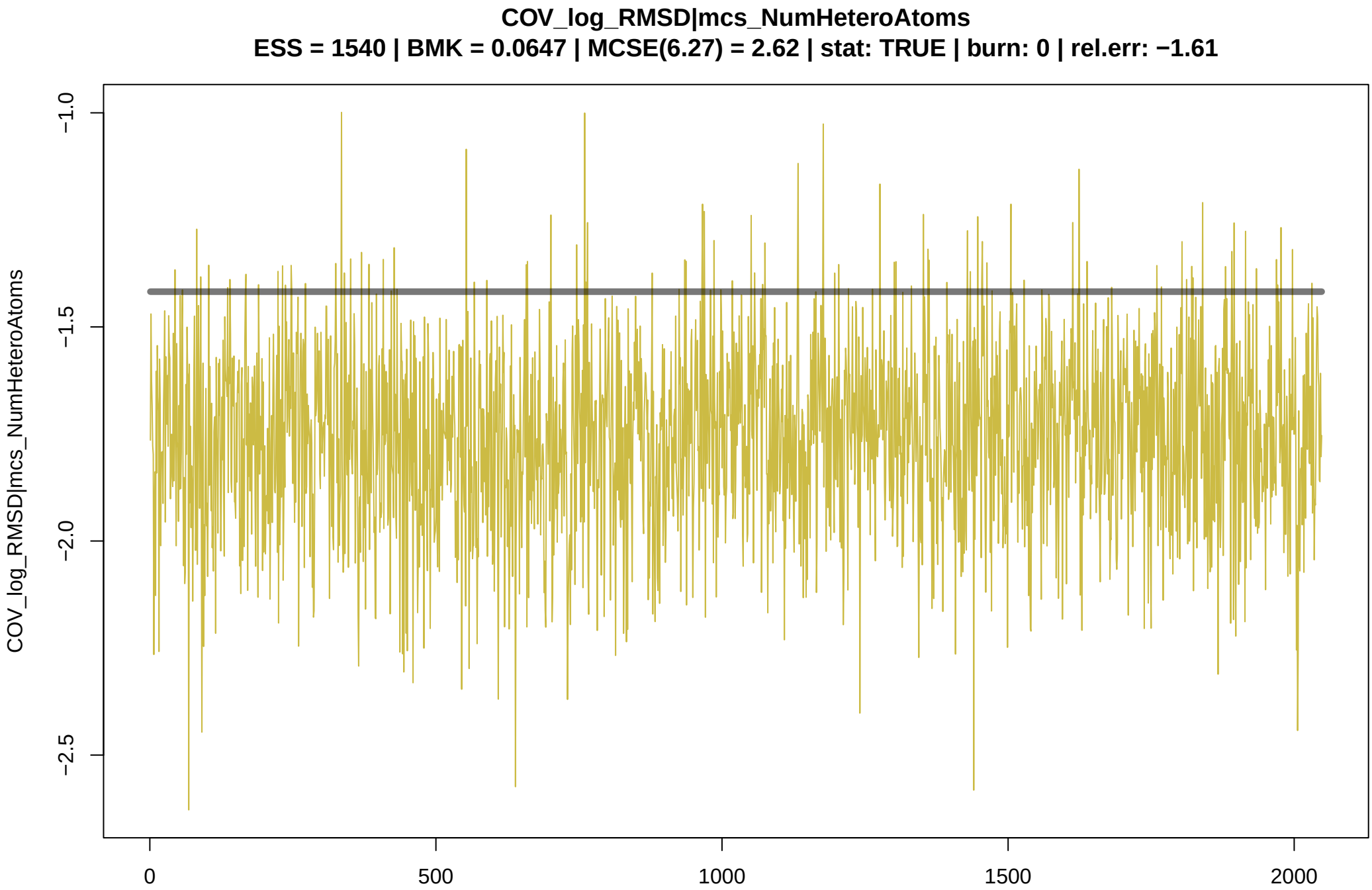

VAR_log_RMSD
ESS = 2050 | BMK = 0.0463 | MCSE(6.27) = 1.89 | stat: FALSE | burn: 0 | rel.err: 2.24
VAR_log_RMSD
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000

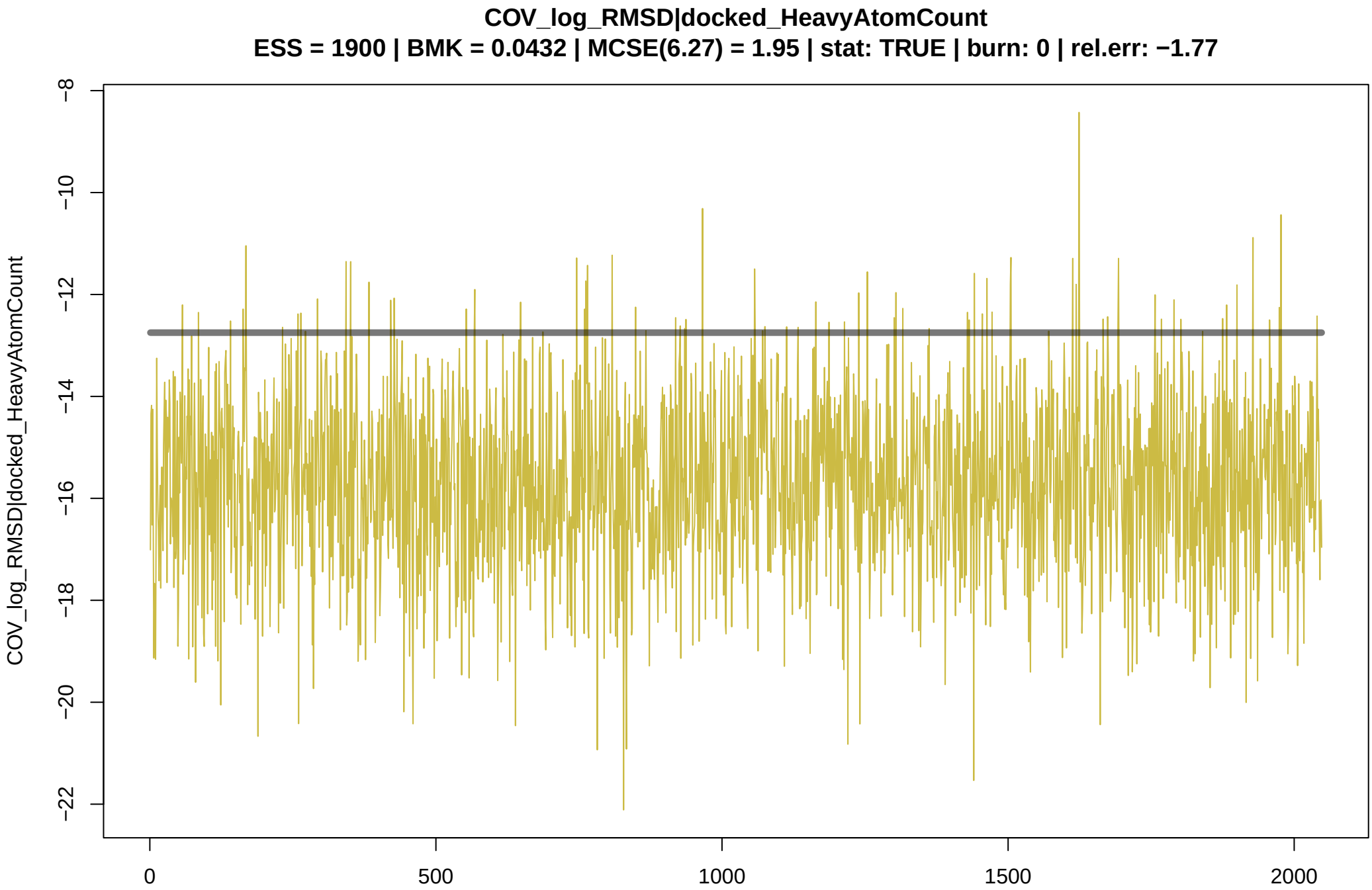

VAR_log_mcs_unbonded_polar_sasa
ESS = 2050 | BMK = 0.042 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0 | rel.err: 1.35
VAR_log_mcs_unbonded_polar_sasa
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

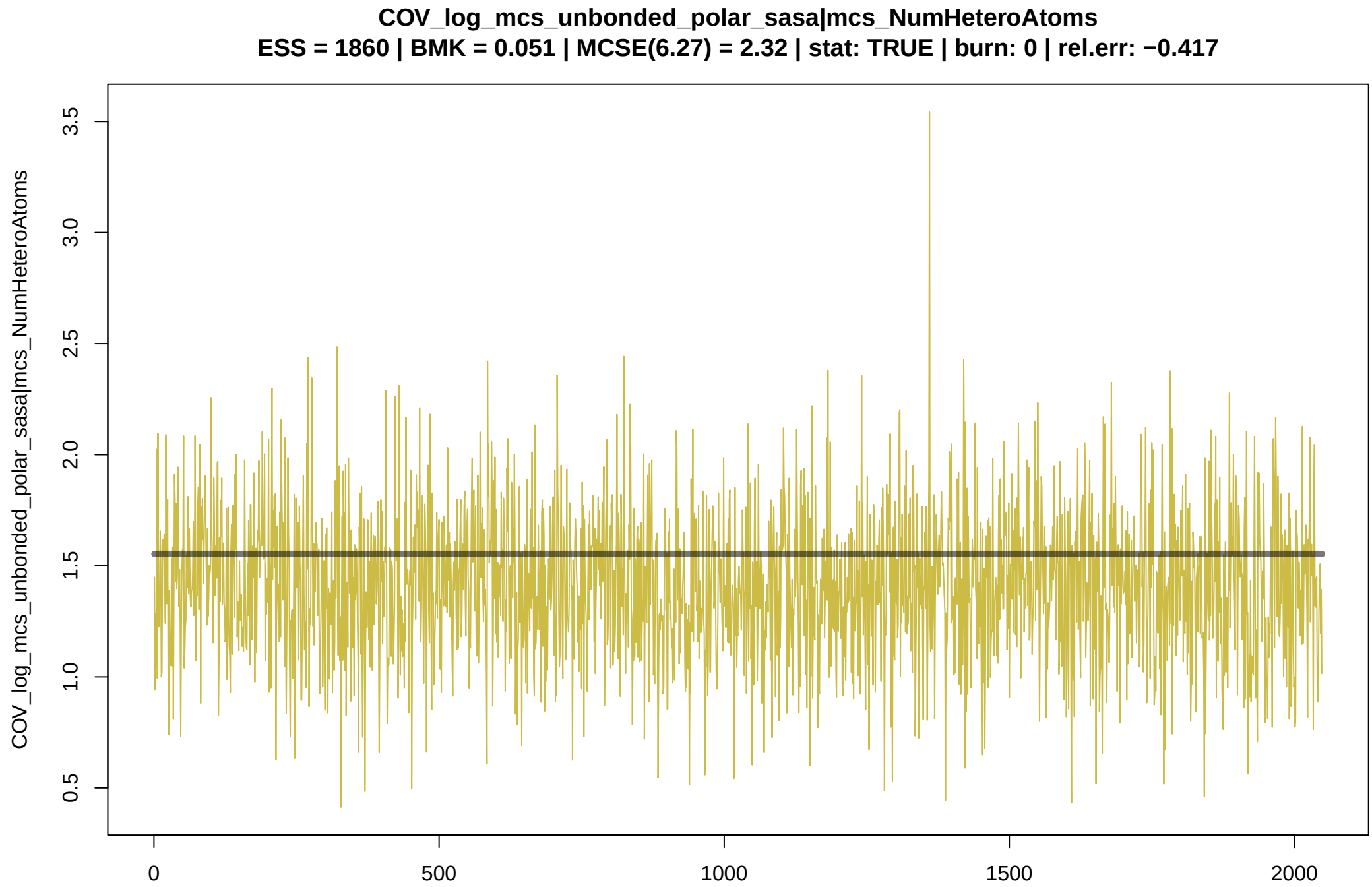

VAR_mcs_NumHeteroAtoms
ESS = 1070 | BMK = 0.0843 | MCSE(6.27) = 3.24 | stat: FALSE | burn: 0 | rel.err: 0.439
VAR_mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
0
500
1000
1500
2000

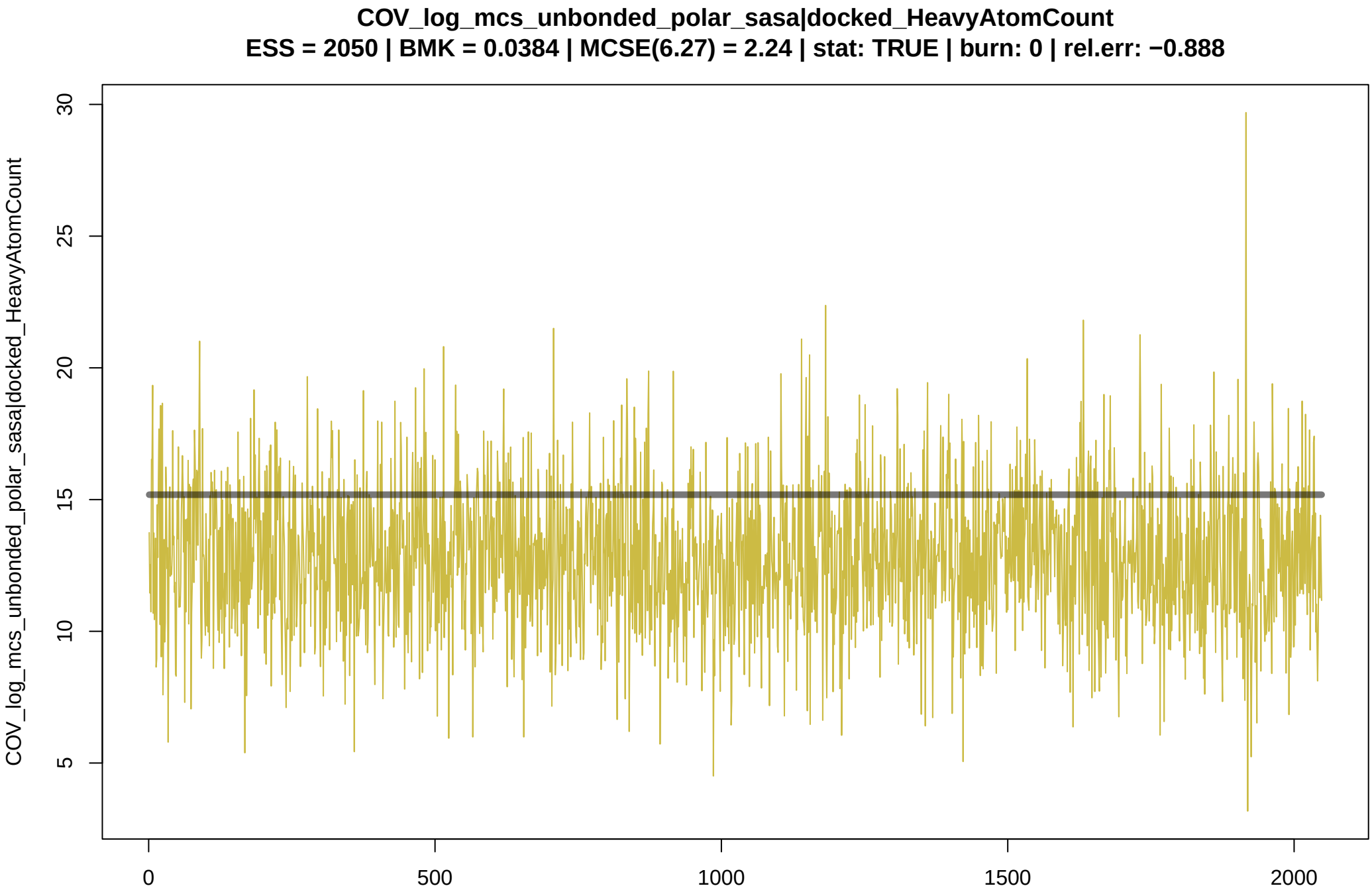

VAR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0562 | MCSE(6.27) = 1.88 | stat: TRUE | burn: 0 | rel.err: 0.0636
VAR_docked_HeavyAtomCount
7.0
6.8
6.6
6.4
0
500
1000
1500
2000

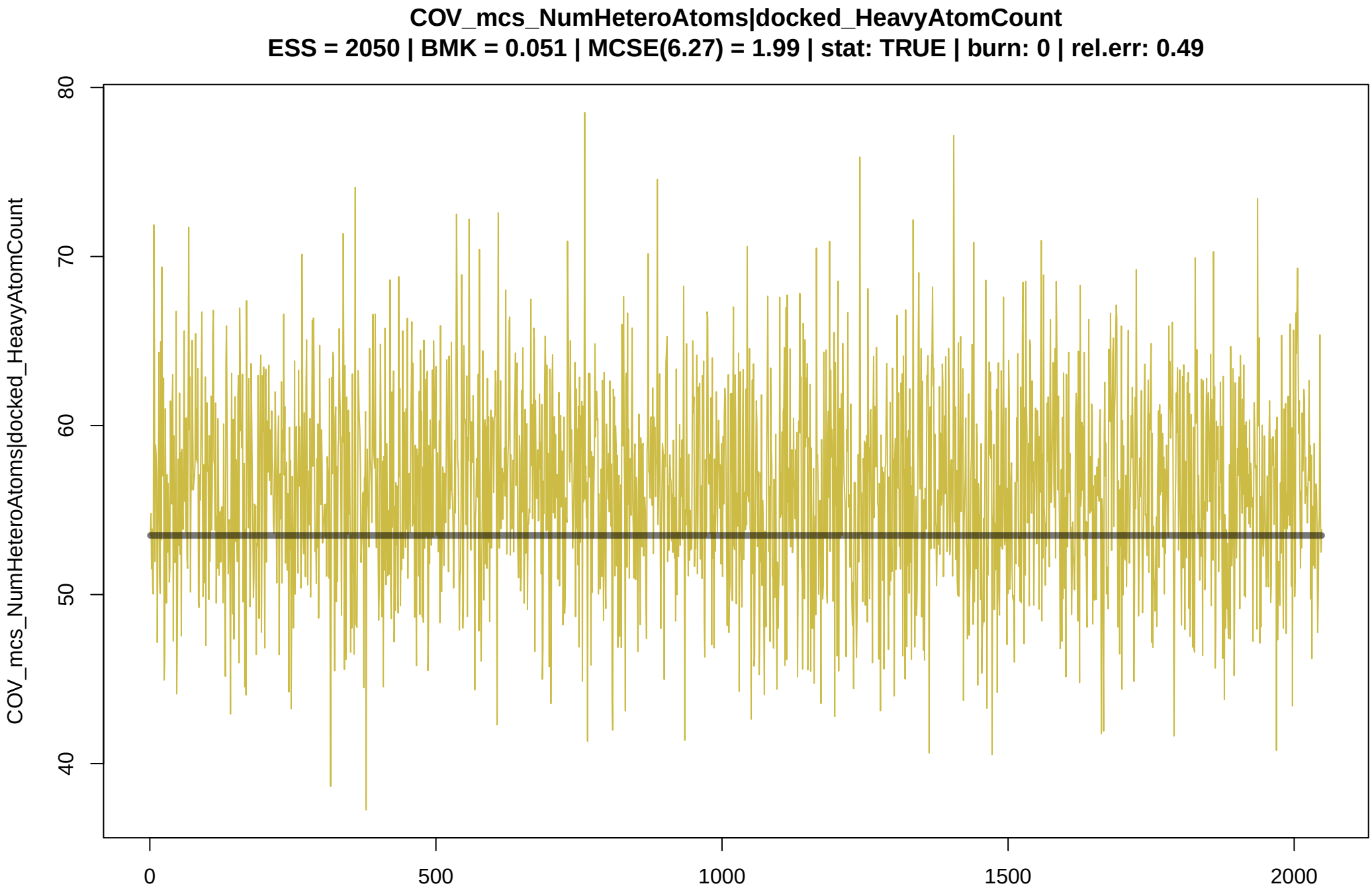

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 1480 | BMK = 0.0398 | MCSE(6.27) = 2.59 | stat: TRUE | burn: 0 | rel.err: 0.447
COV_log_RMSD|log_mcs_unbonded_polar_sasa
−0.2
−0.4
−0.6
0
500
1000
1500
2000


COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1540 | BMK = 0.0647 | MCSE(6.27) = 2.62 | 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 = 1900 | BMK = 0.0432 | MCSE(6.27) = 1.95 | stat: TRUE | burn: 0 | rel.err: −1.77
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 = 1860 | BMK = 0.051 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0 | rel.err: −0.417
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.5
1.0
1.5
2.0
2.5
3.0
3.5
0
500
1000
1500
2000


COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0384 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0 | rel.err: −0.888
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
5
10
15
20
25
30
0
500
1000
1500
2000


COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.051 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0 | rel.err: 0.49
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
80
70
60
50
40
0
500
1000
1500
2000