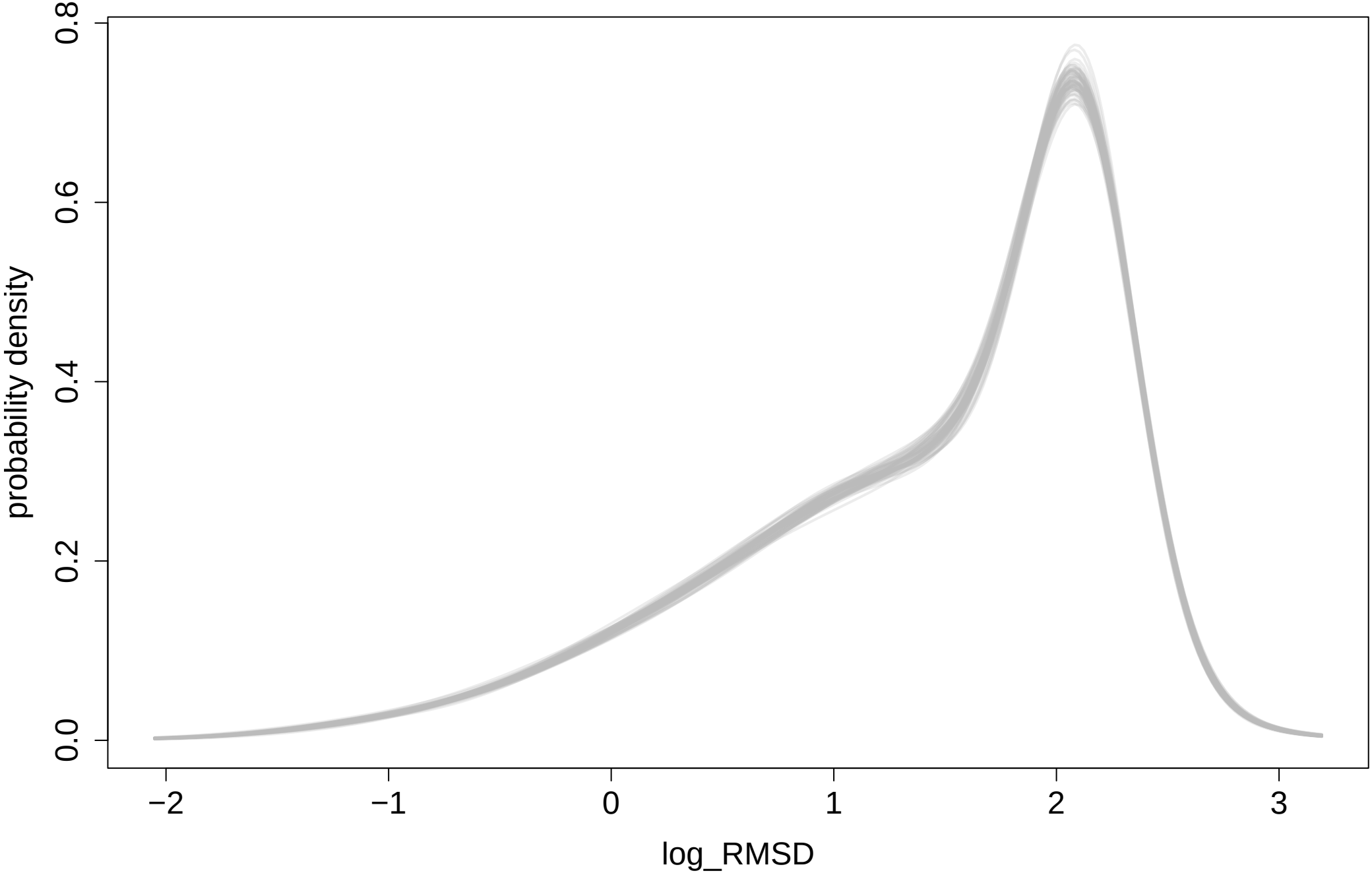
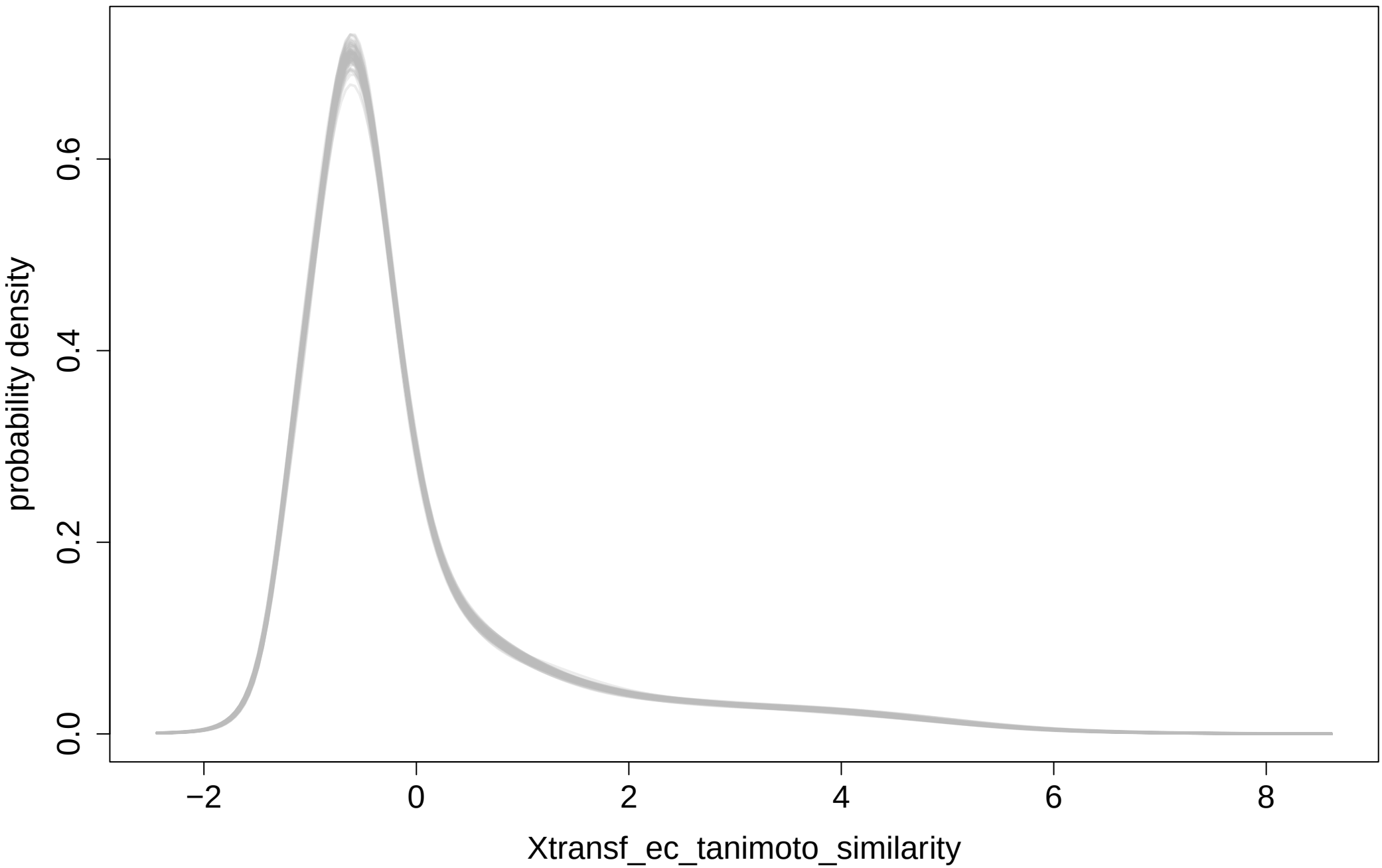
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.368082398398951
max MCSE = 10.4836915345577
all stationary: FALSE
burn: 0

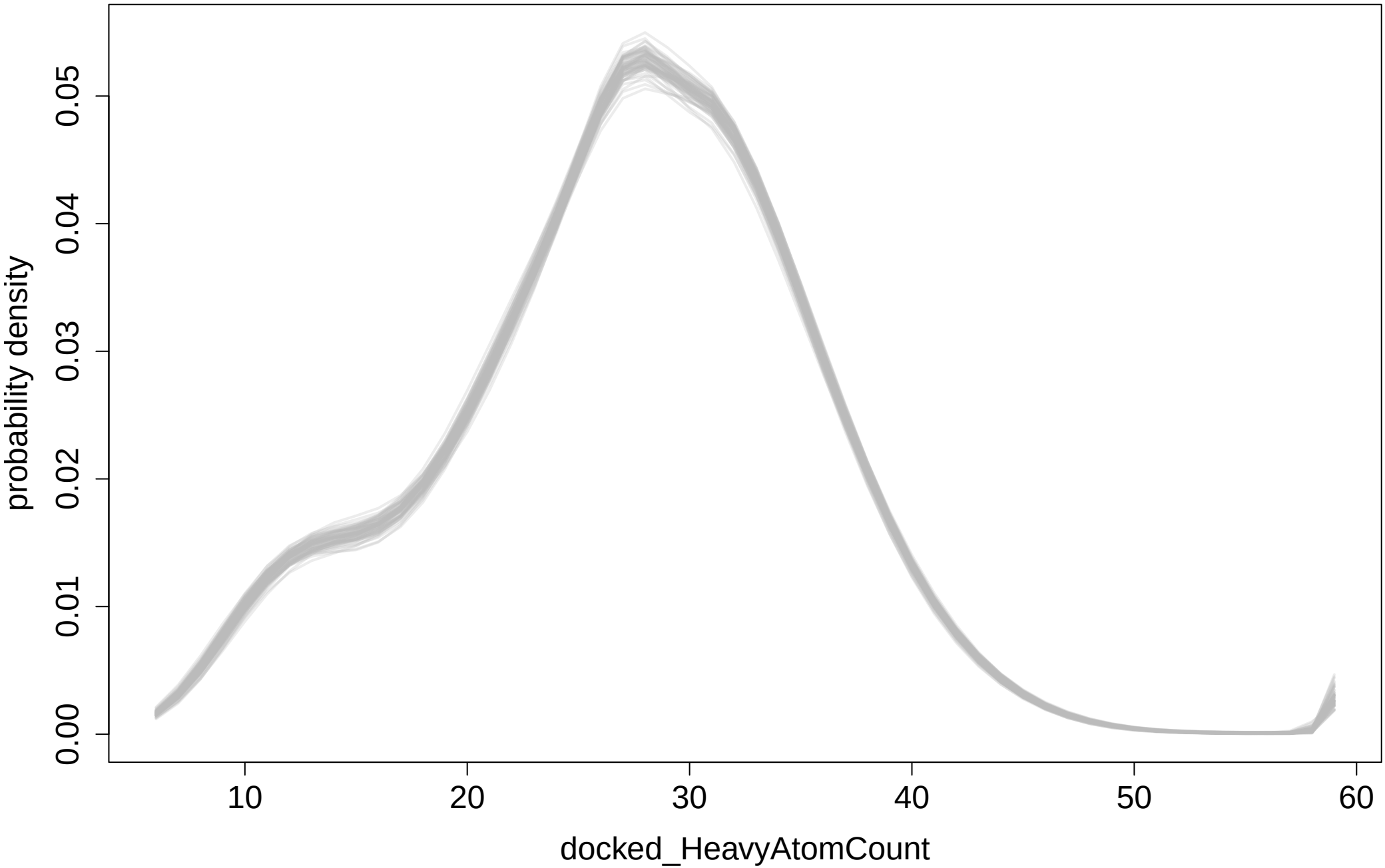
−− STATS 2D −−
min ESS = 1041.95695339855
max BMK = 0.103949175633807
max MCSE = 3.41568779846761
all stationary: FALSE
burn: 0

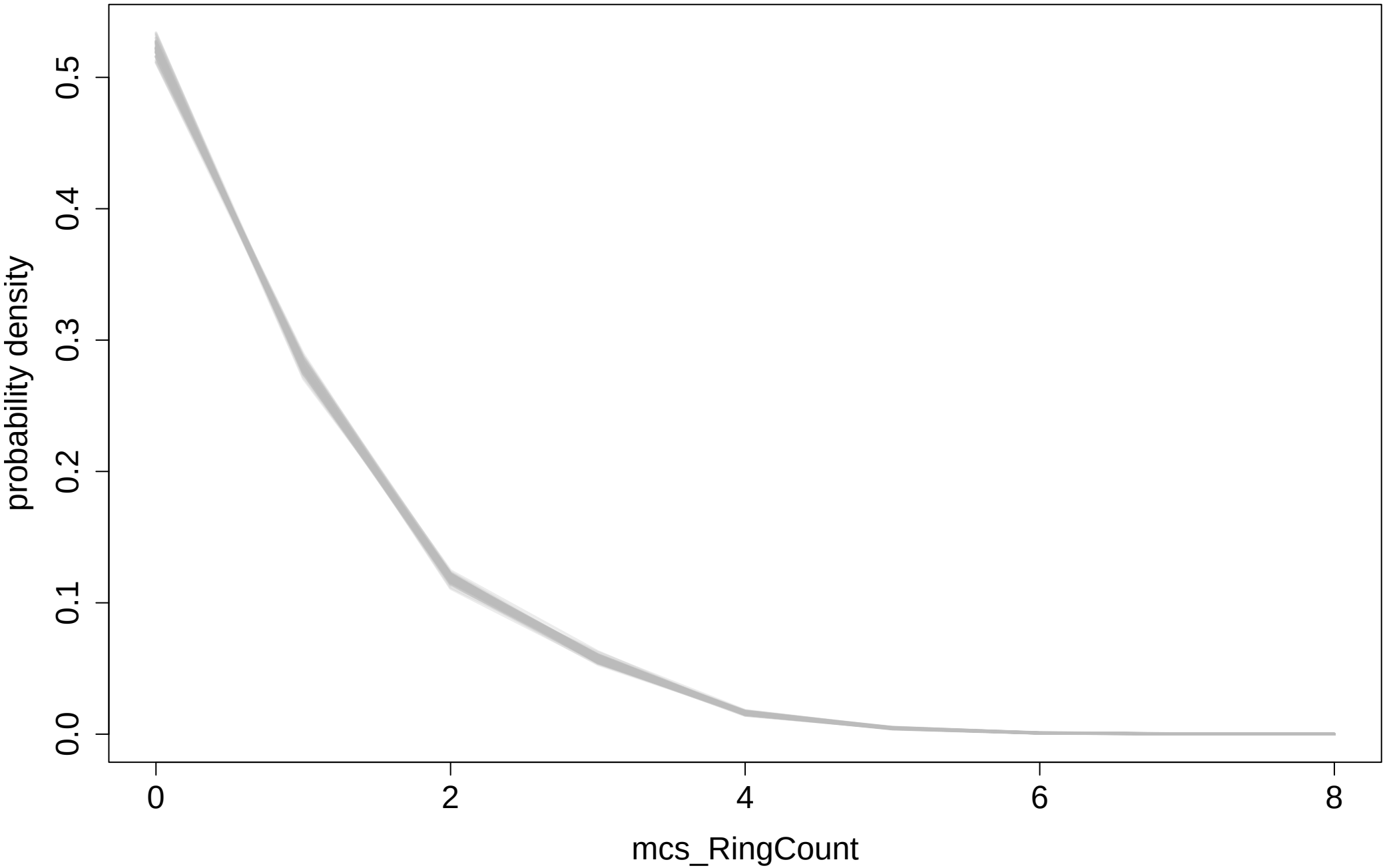
−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.627852113064889
max MCSE = NaN
all stationary: FALSE
burn: 2040

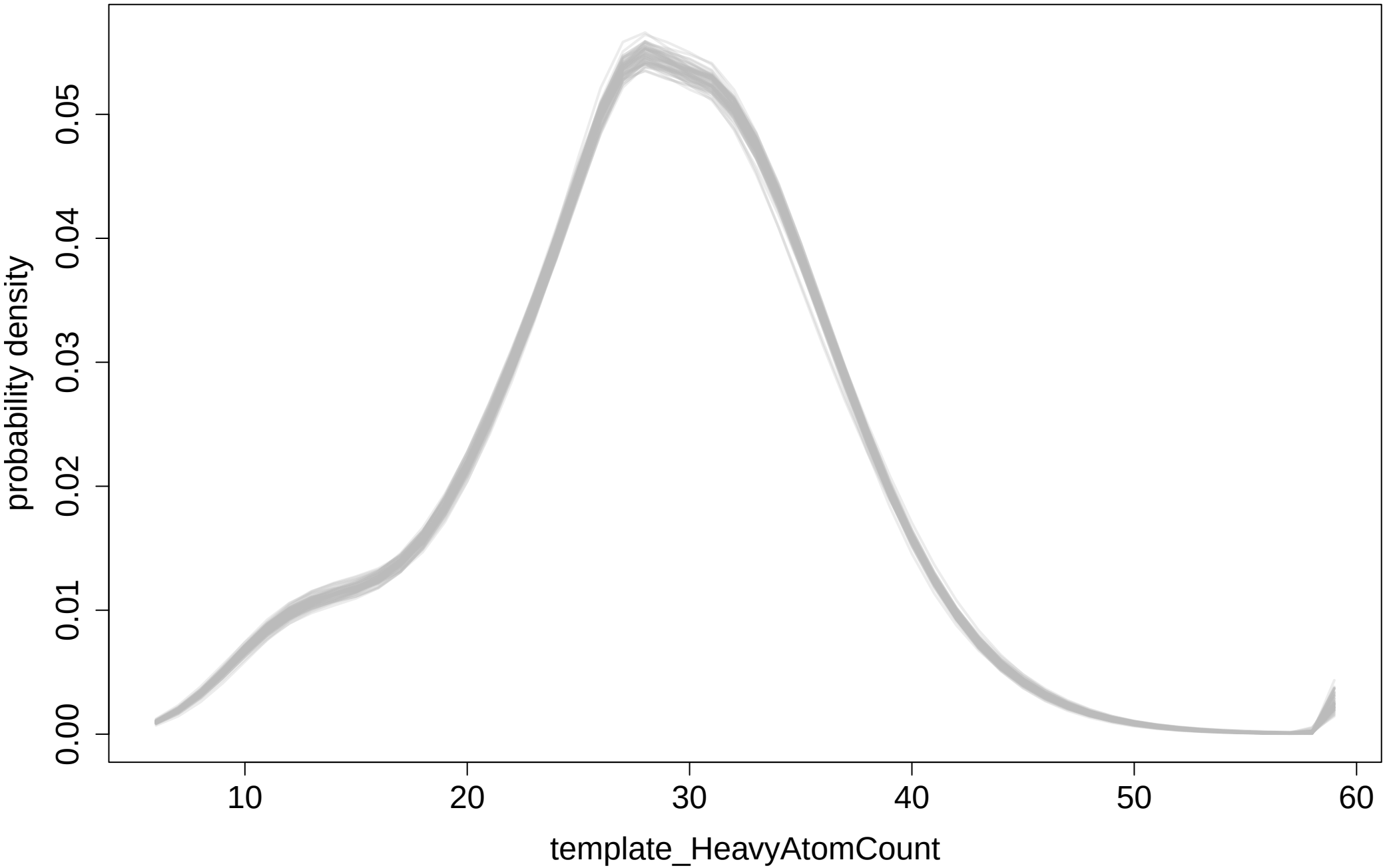
Occupied clusters: 62 of 64
LL: −110000 +− 28.6

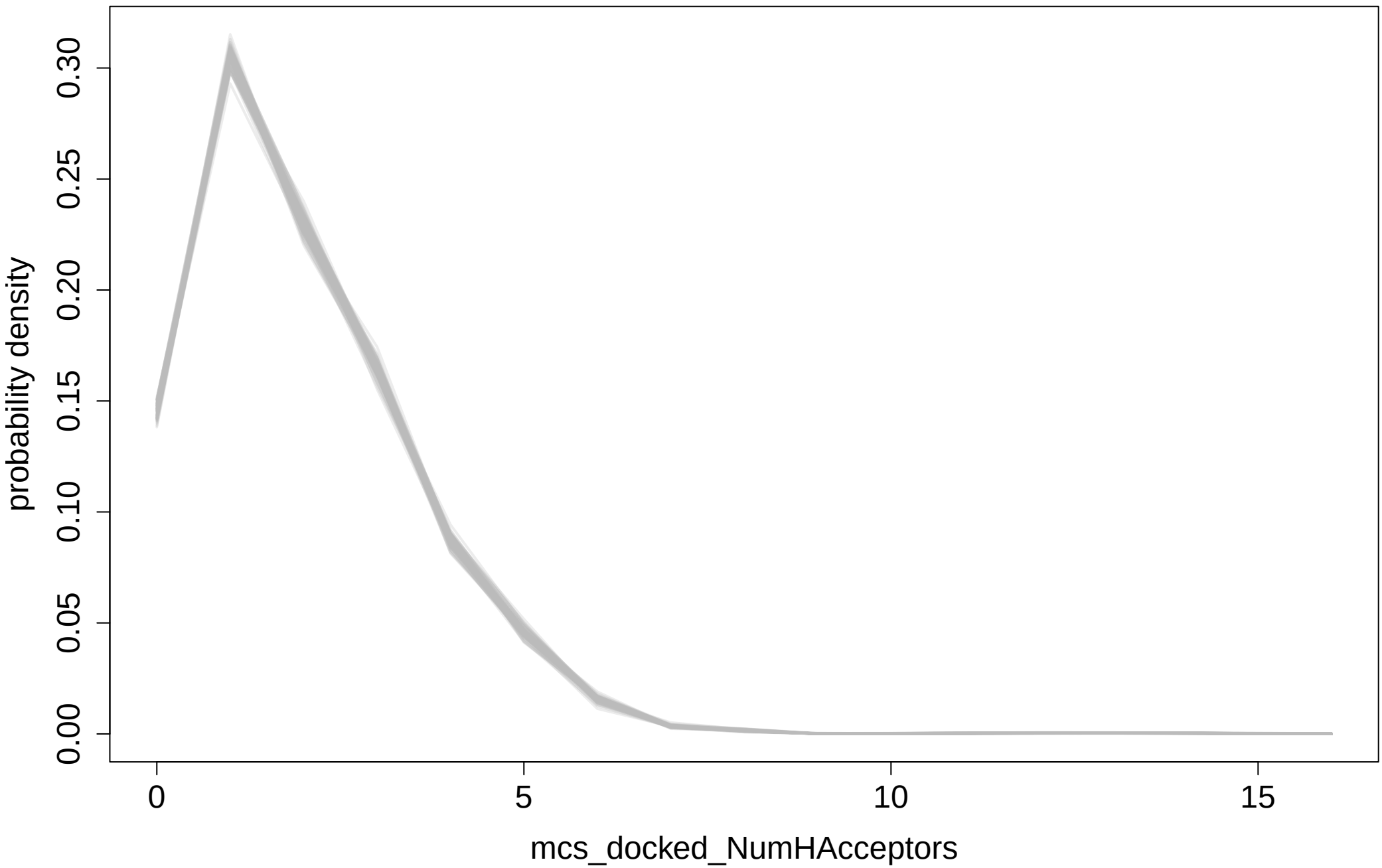

probability density
0.0
0.2
0.4
0.6
0.8
−2
−1
0
1
2
3
log_RMSD

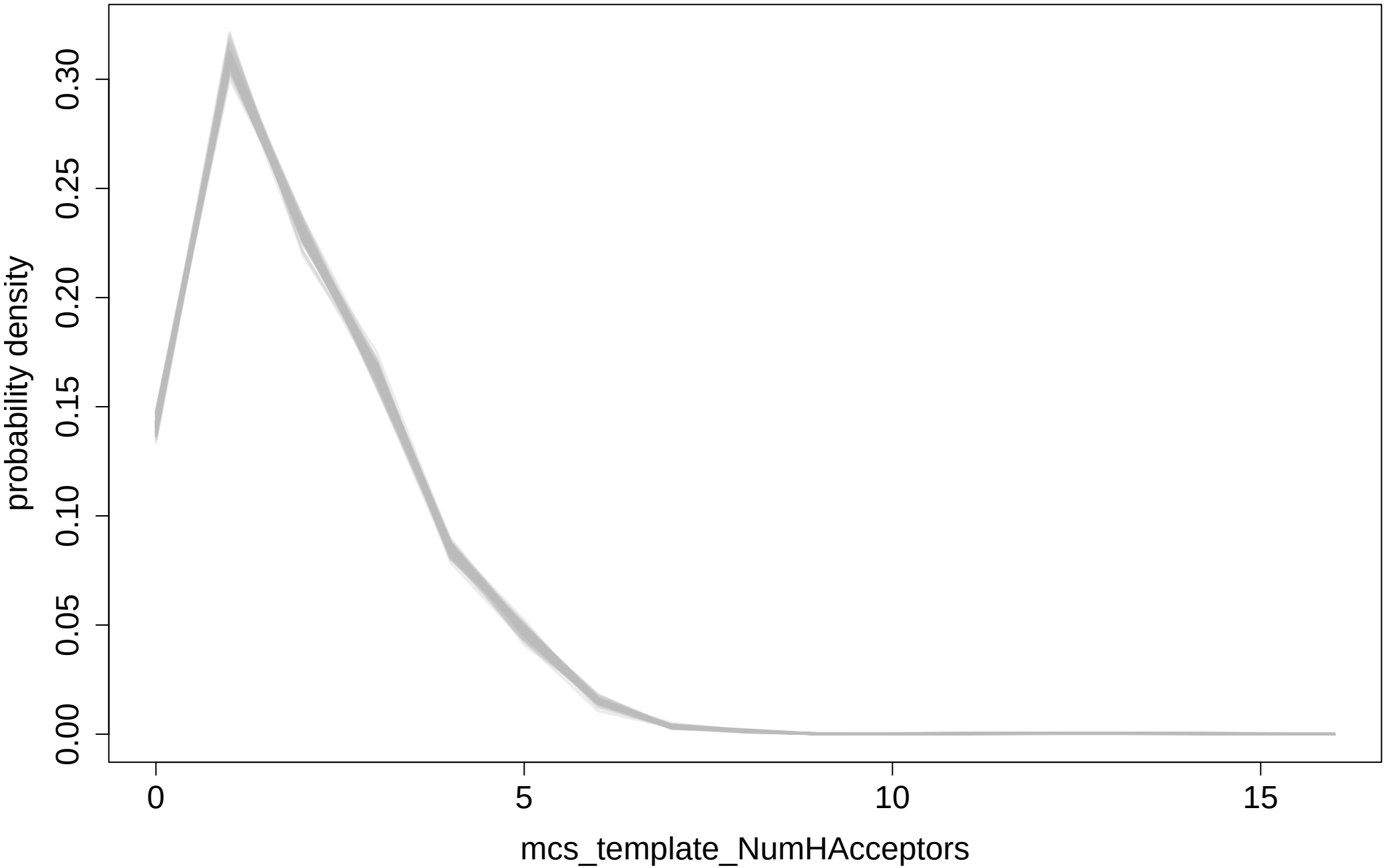

probability density
0.0
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

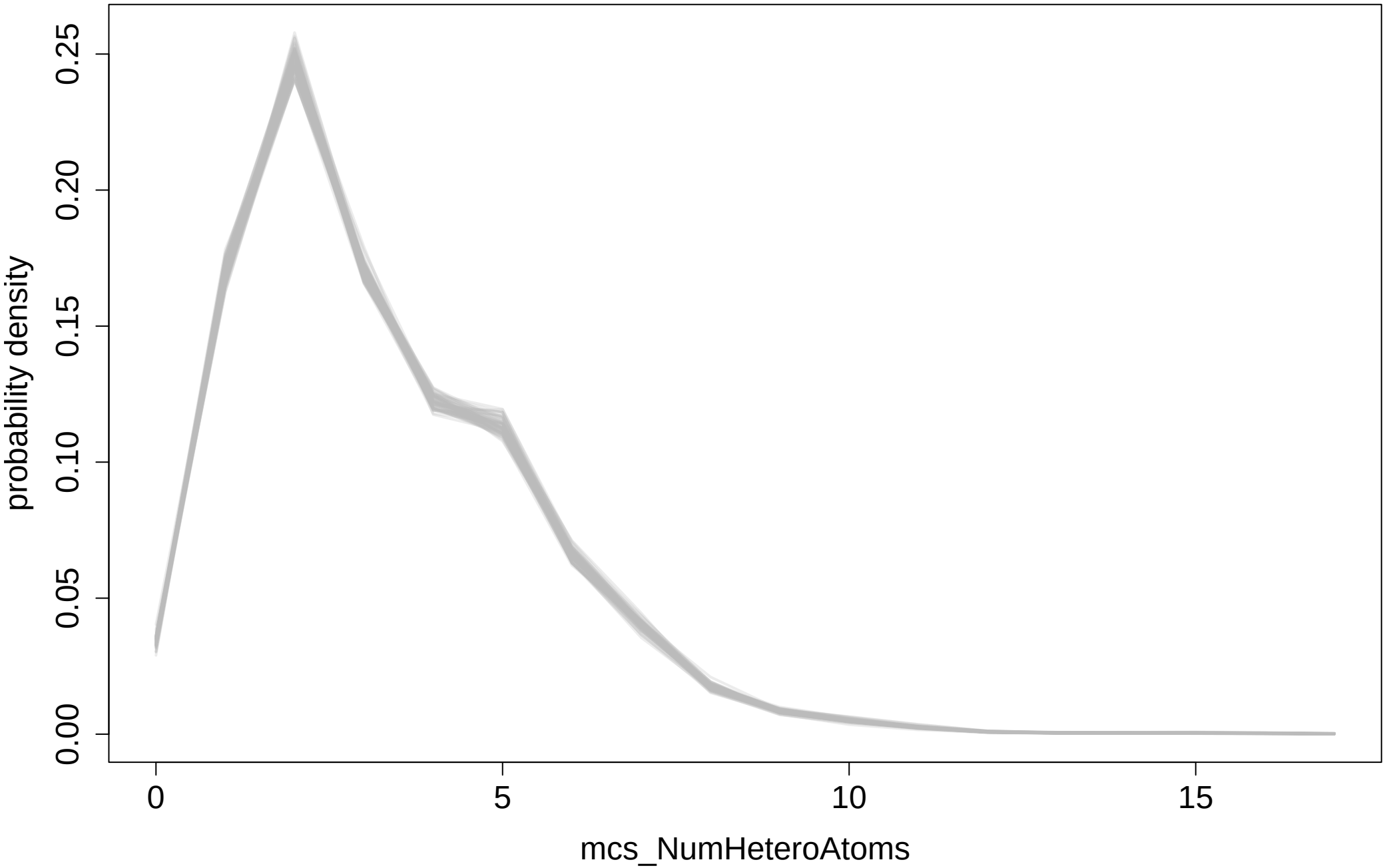

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

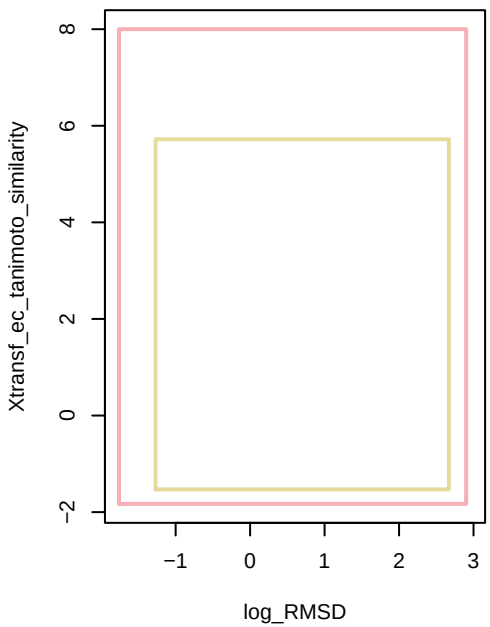

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

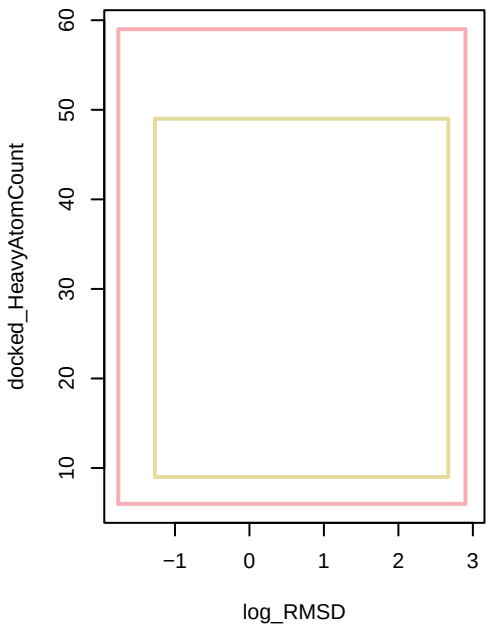

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

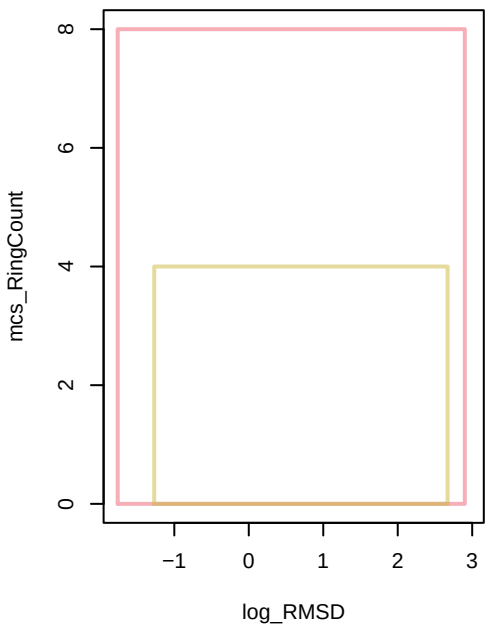

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_docked_NumHAcceptors

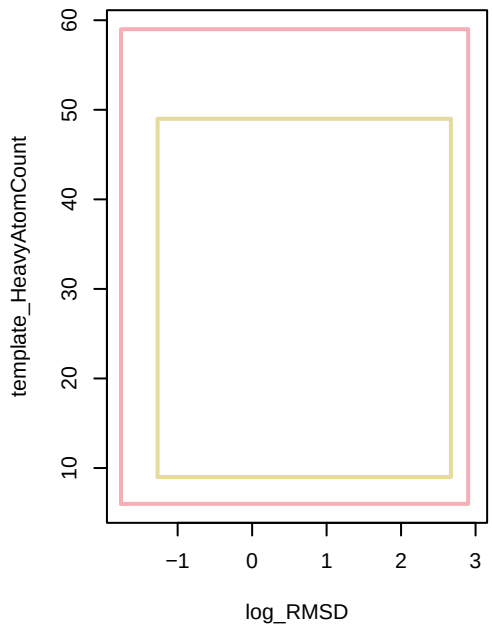

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_template_NumHAcceptors

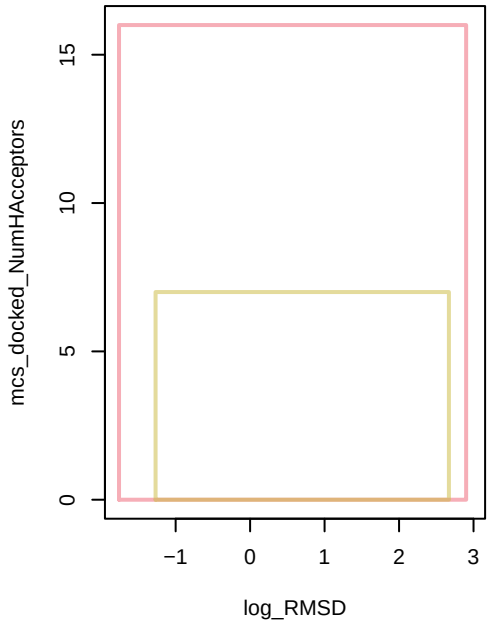

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

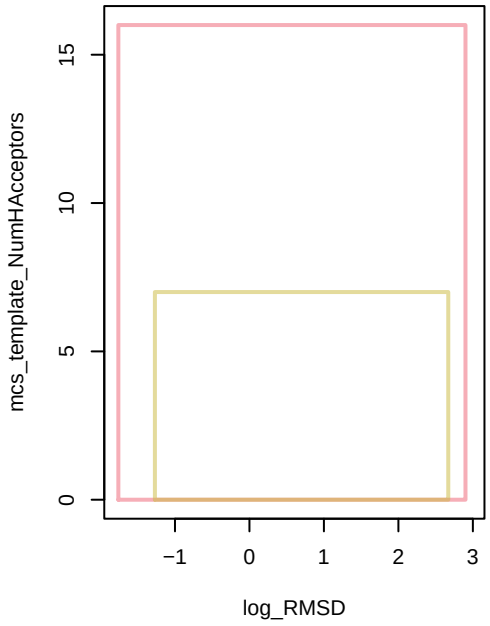

Xtransf_ec_tanimoto_similarity
log_RMSD

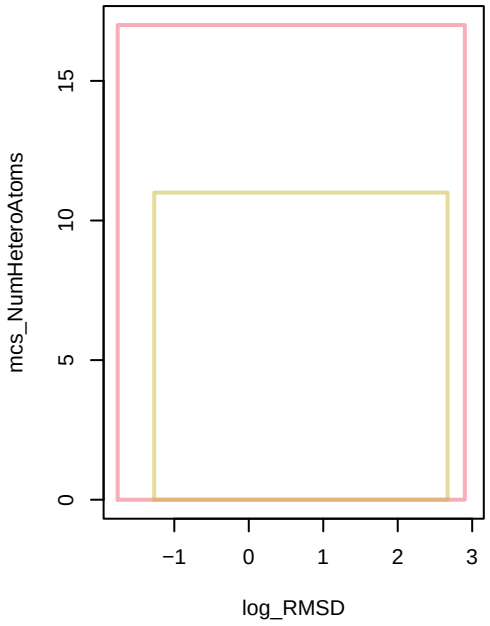

docked_HeavyAtomCount
log_RMSD

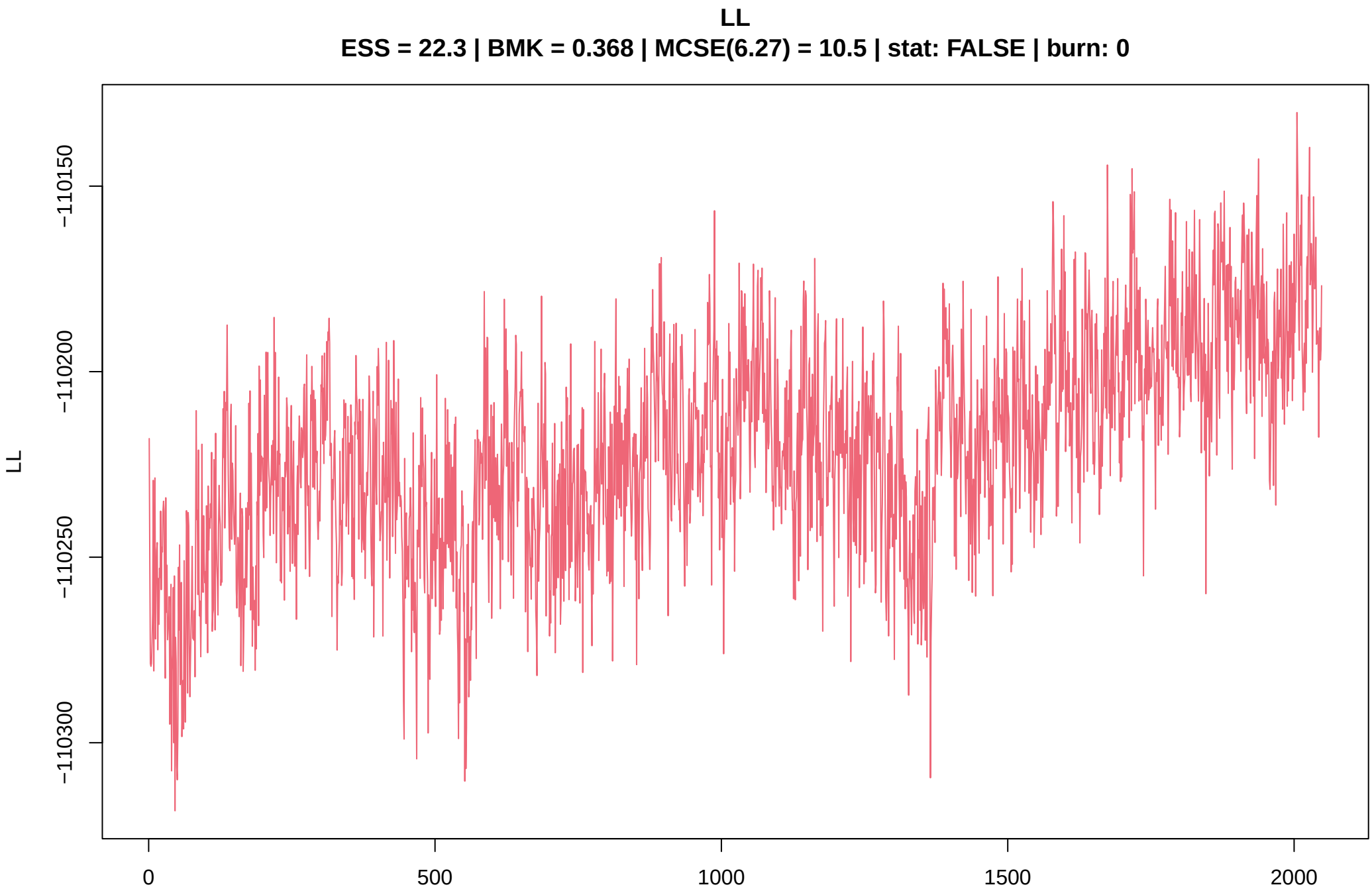

mcs_RingCount
log_RMSD

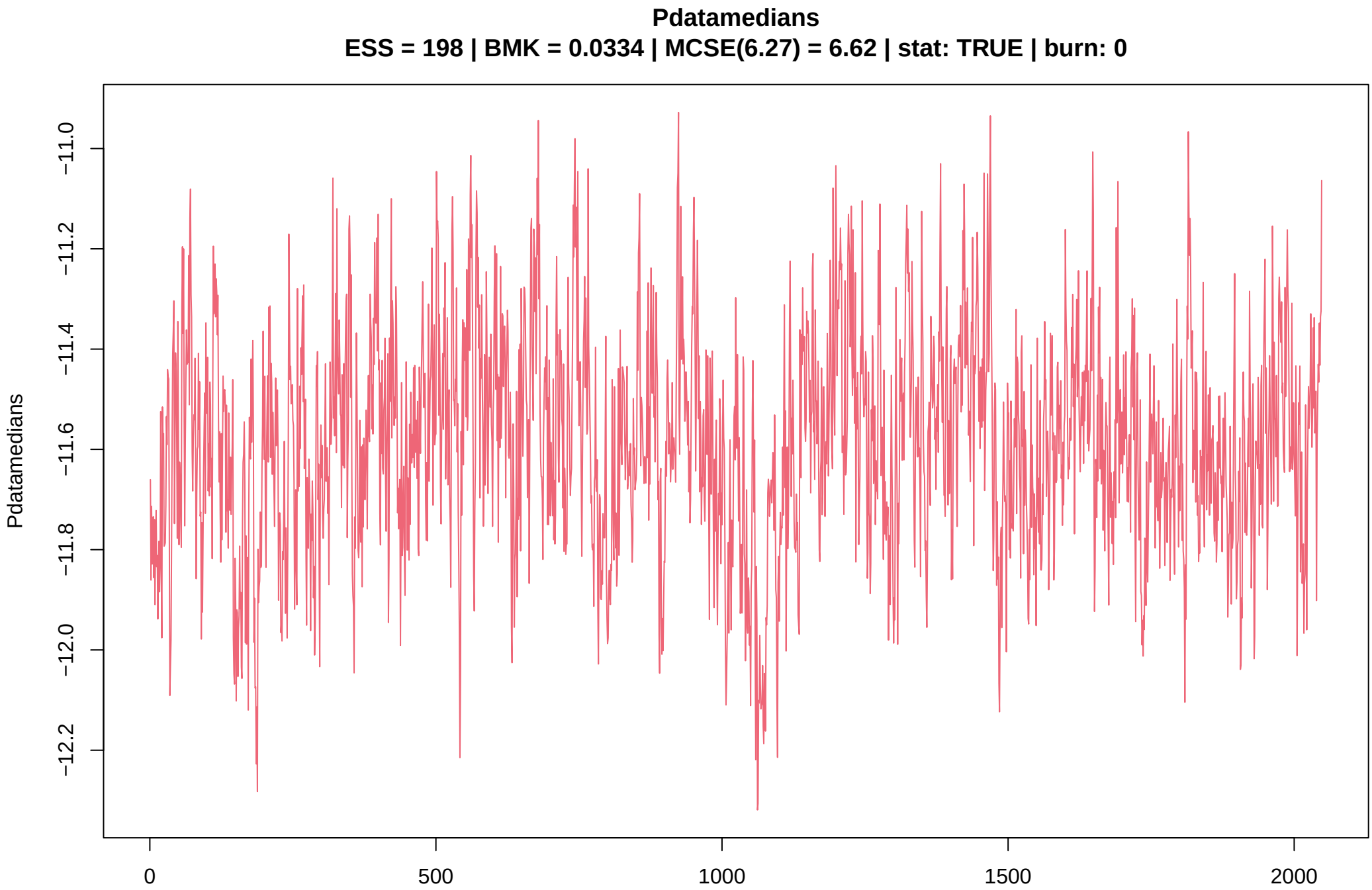

template_HeavyAtomCount
log_RMSD

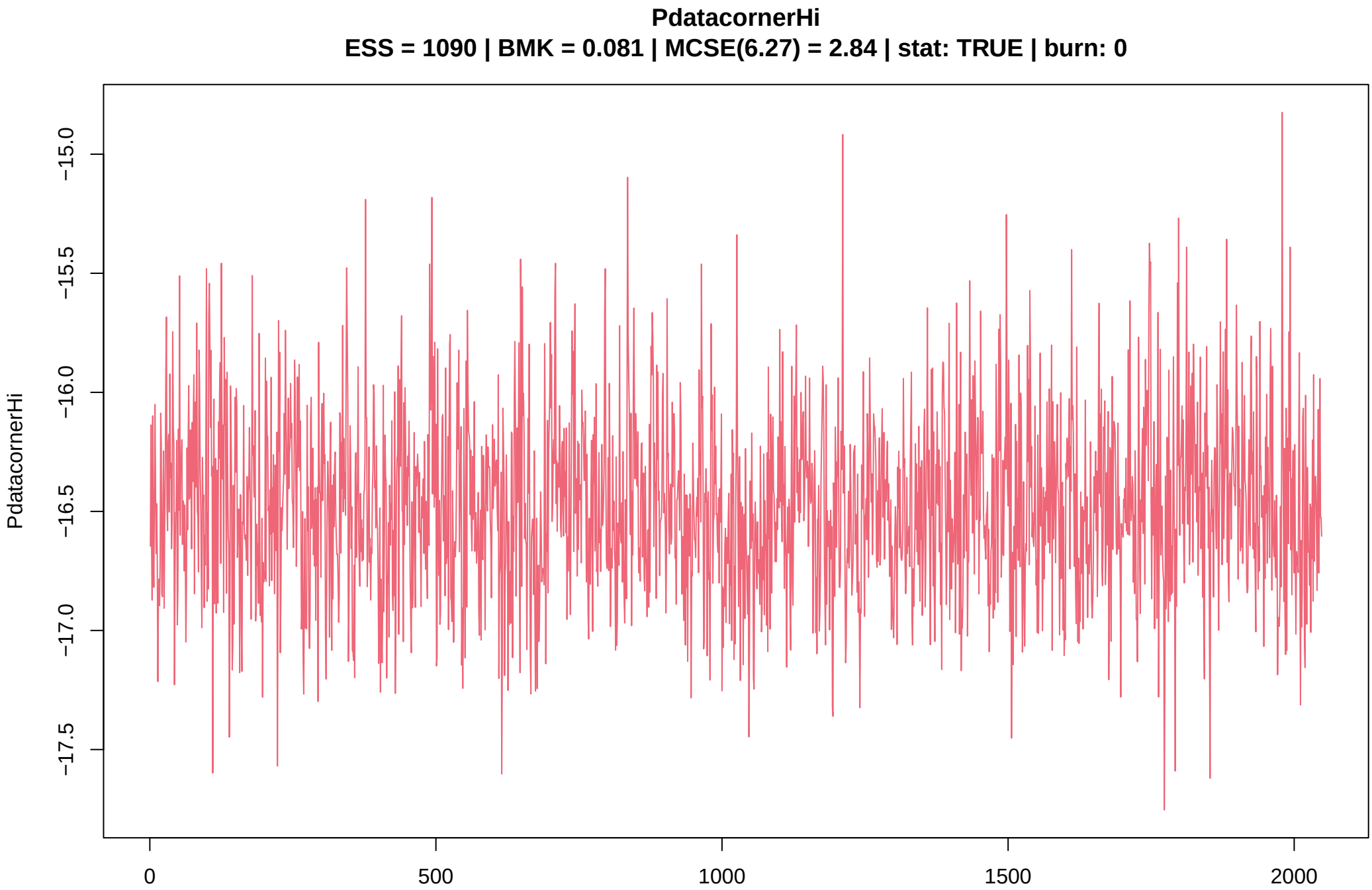

mcs_docked_NumHAcceptors
log_RMSD

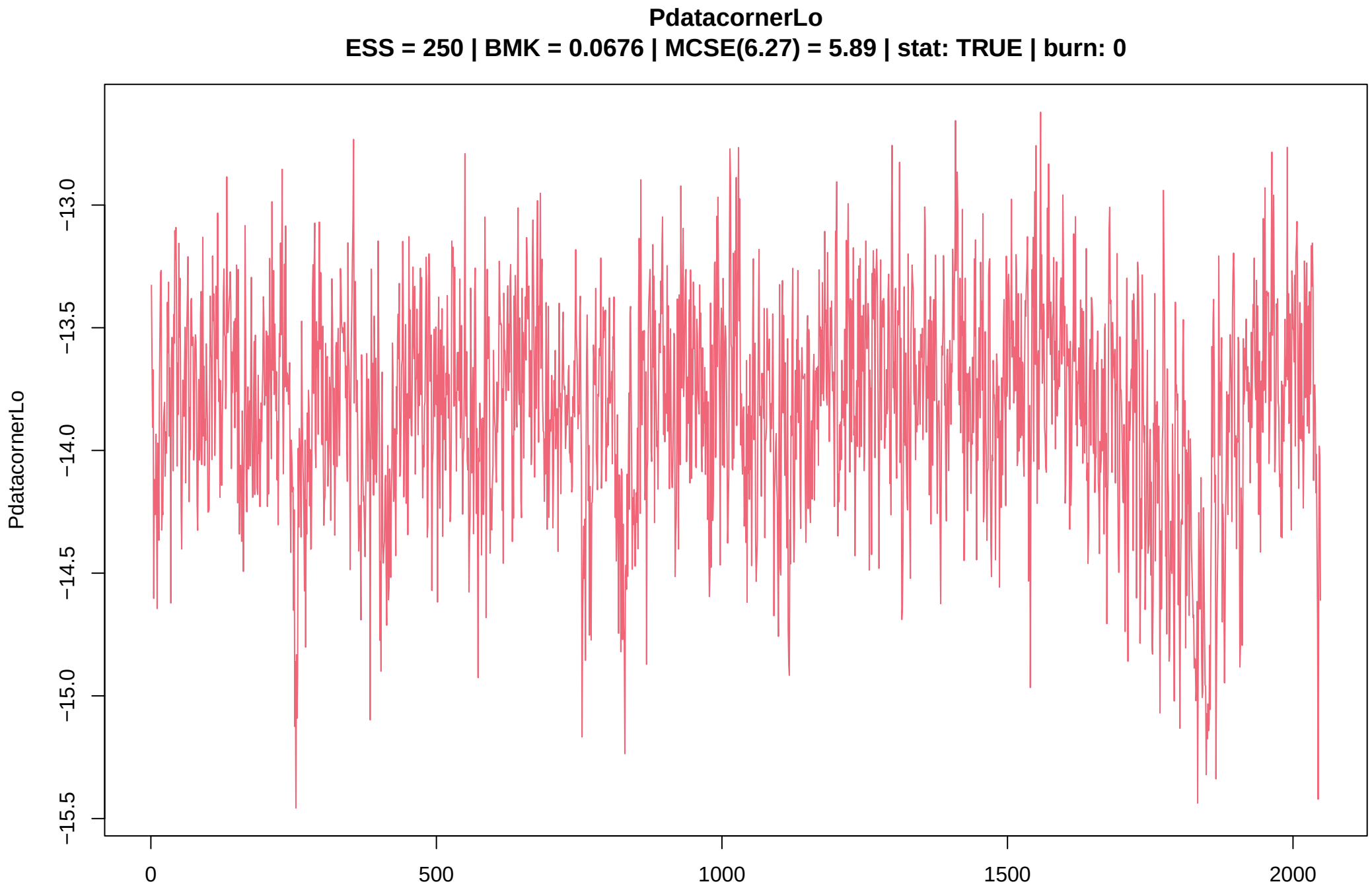

mcs_template_NumHAcceptors
log_RMSD

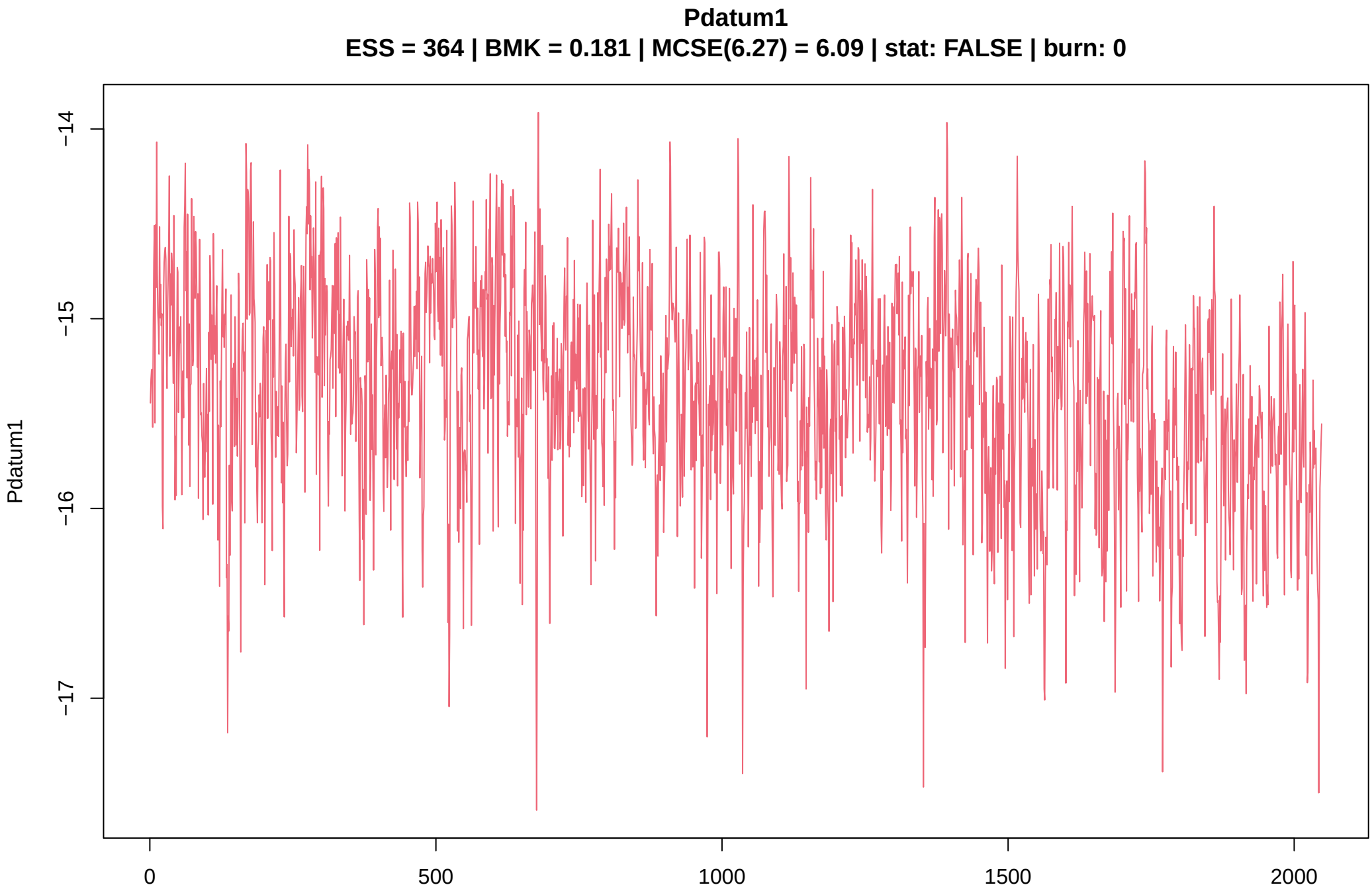

mcs_NumHeteroAtoms
log_RMSD

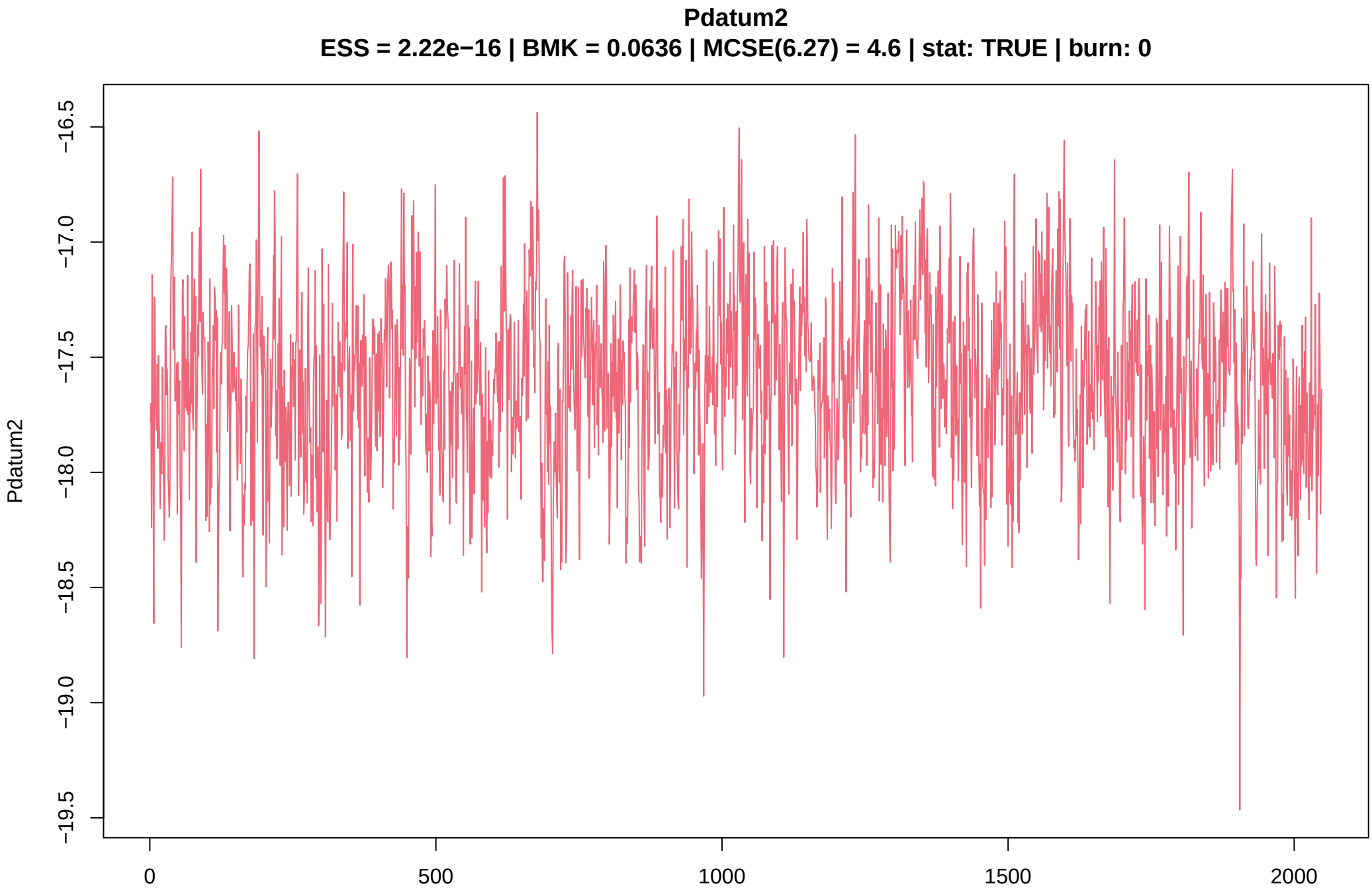

LL
ESS = 22.3 | BMK = 0.368 | MCSE(6.27) = 10.5 | stat: FALSE | burn: 0
LL
−110150
−110200
−110250
−110300
0
500
1000
1500
2000

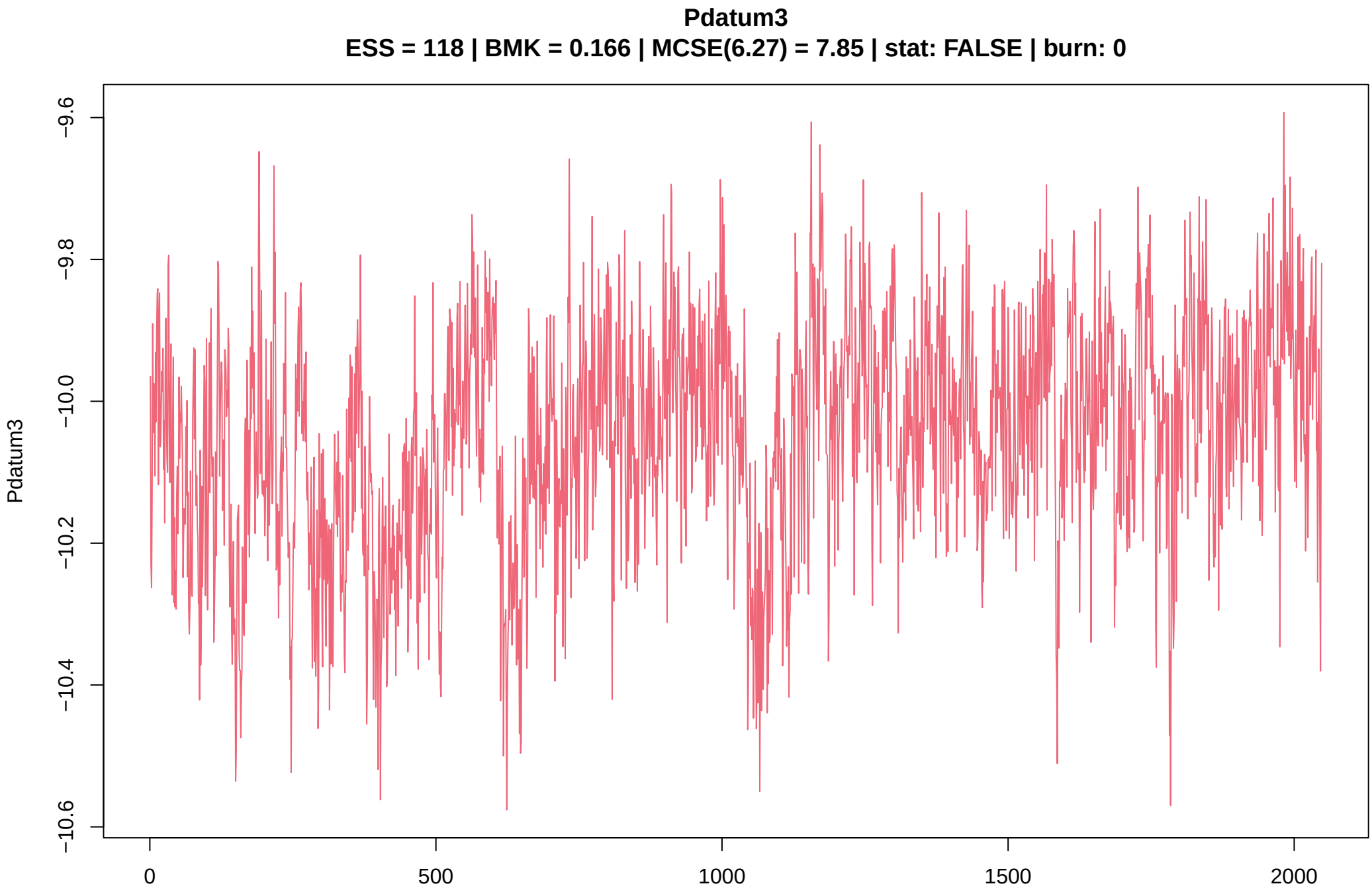

Pdatamedians
ESS = 198 | BMK = 0.0334 | MCSE(6.27) = 6.62 | stat: TRUE | burn: 0
Pdatamedians
−11.0
−11.2
−11.4
−11.6
−11.8
−12.0
−12.2
0
500
1000
1500
2000

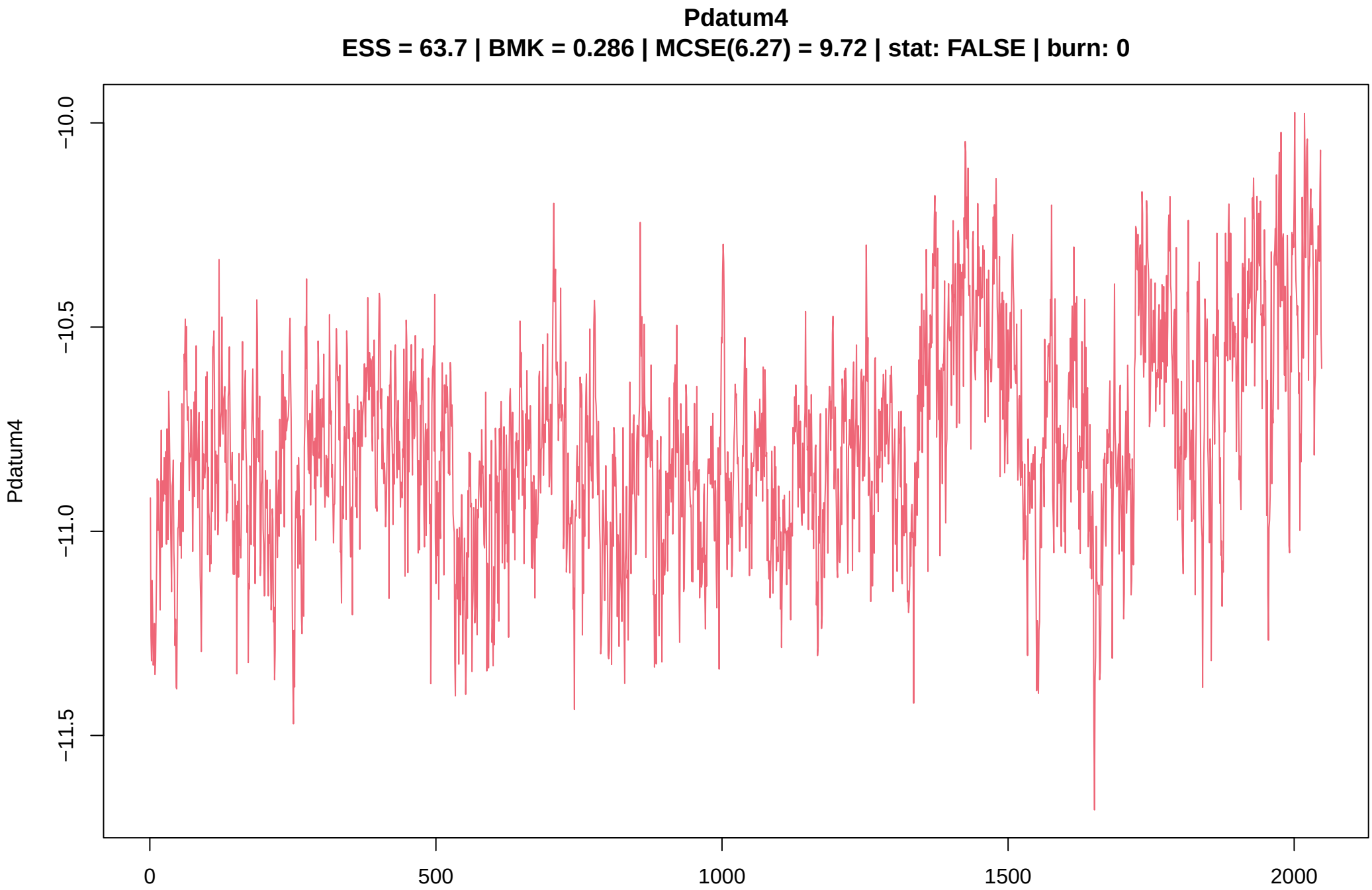

PdatacornerHi
ESS = 1090 | BMK = 0.081 | MCSE(6.27) = 2.84 | stat: TRUE | burn: 0
PdatacornerHi
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000

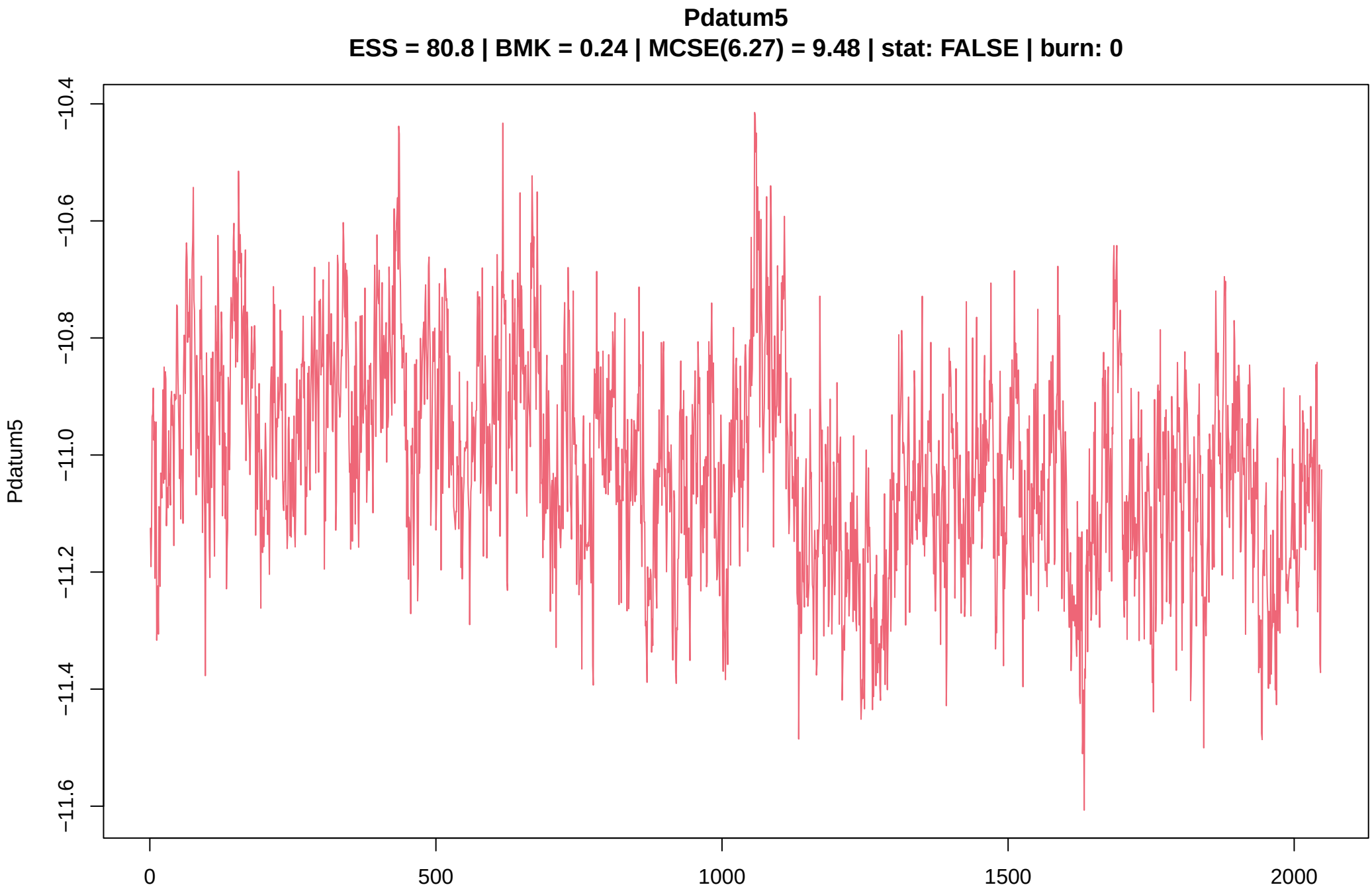

PdatacornerLo
ESS = 250 | BMK = 0.0676 | MCSE(6.27) = 5.89 | stat: TRUE | burn: 0
PdatacornerLo
−13.0
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

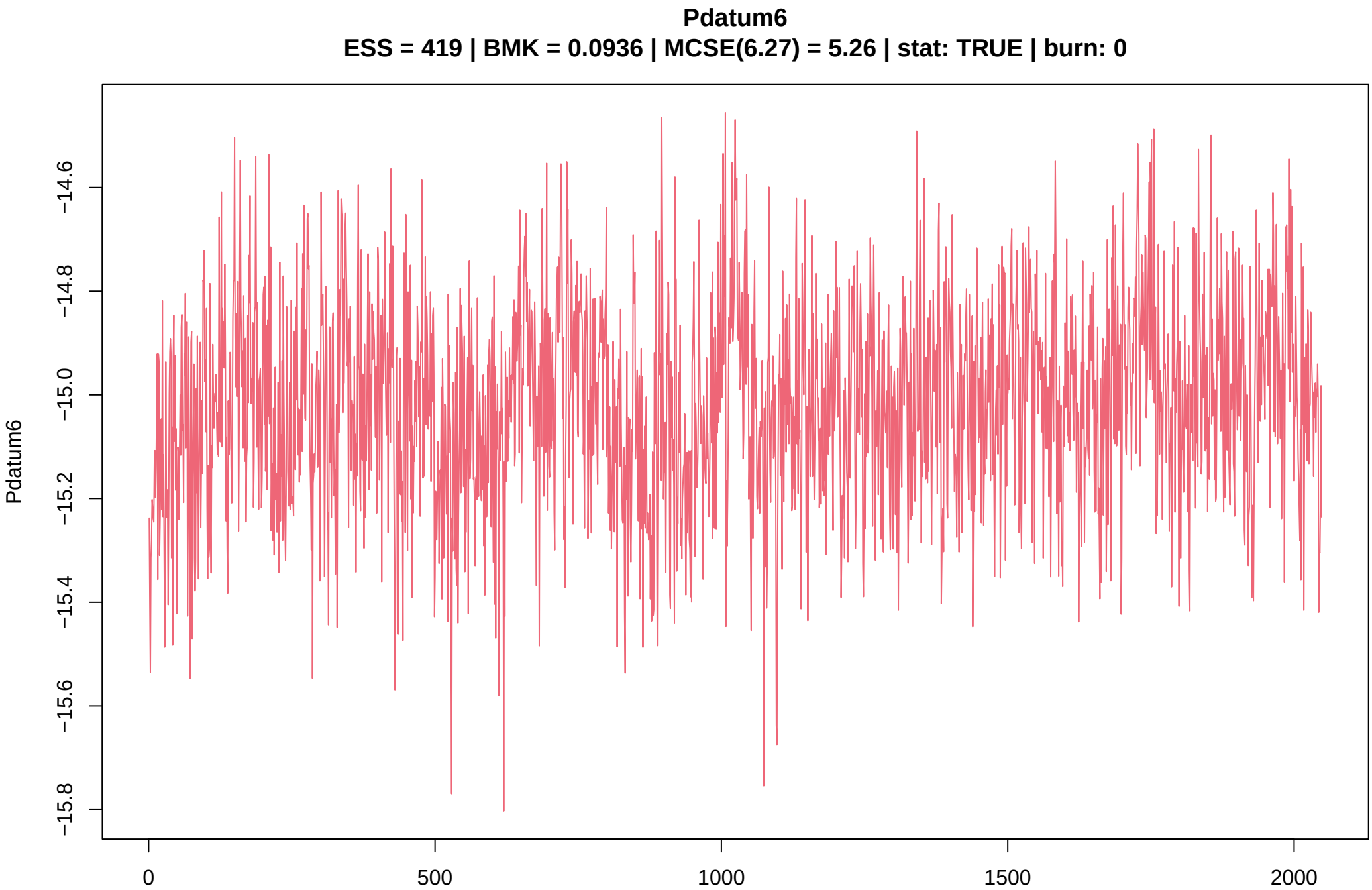

Pdatum1
ESS = 364 | BMK = 0.181 | MCSE(6.27) = 6.09 | stat: FALSE | burn: 0
Pdatum1
−14
−15
−16
−17
0
500
1000
1500
2000

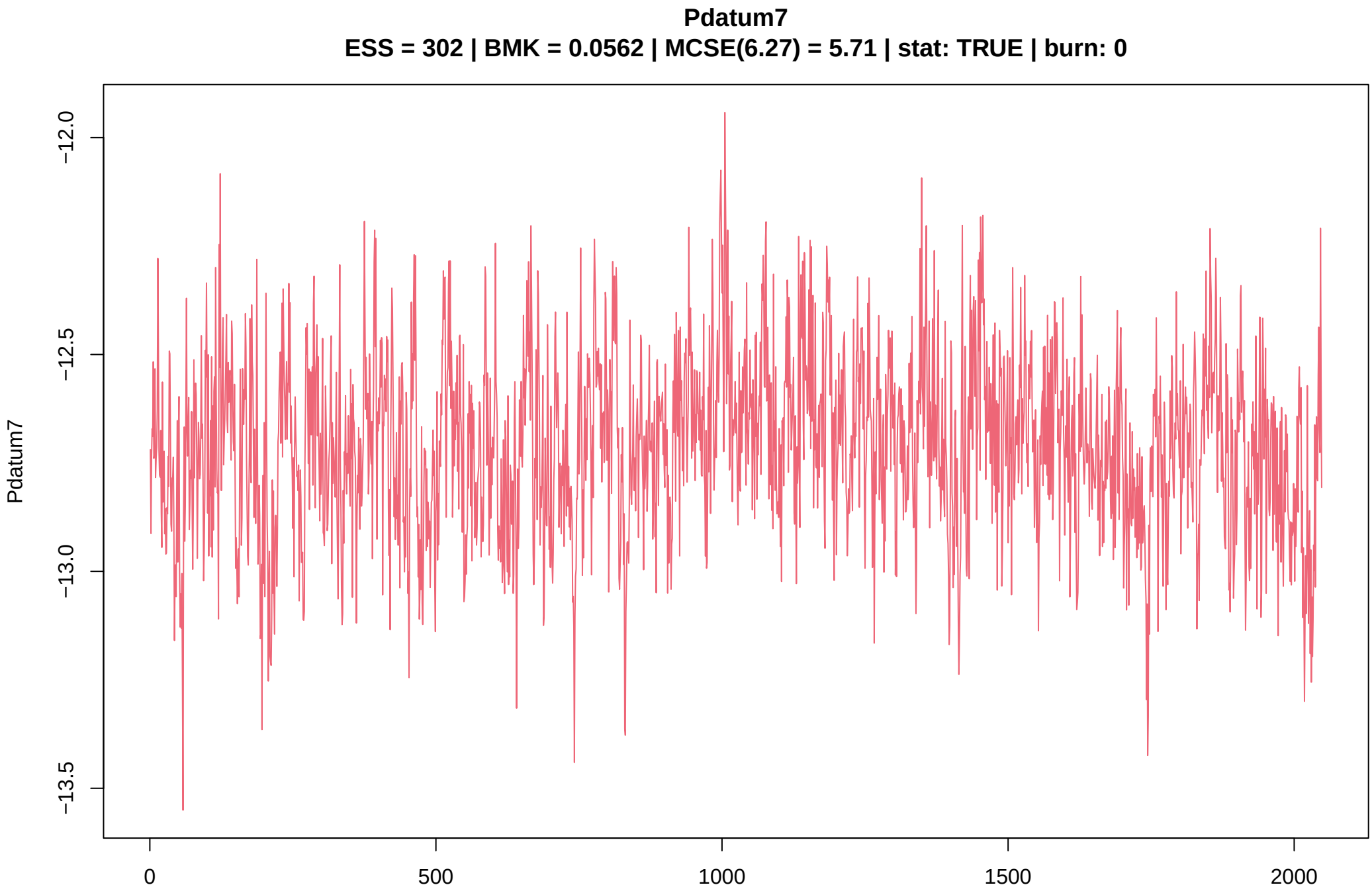

Pdatum2
ESS = 2.22e−16 | BMK = 0.0636 | MCSE(6.27) = 4.6 | stat: TRUE | burn: 0
Pdatum2
−16.5
−17.0
−17.5
−18.0
−18.5
−19.0
−19.5
0
500
1000
1500
2000

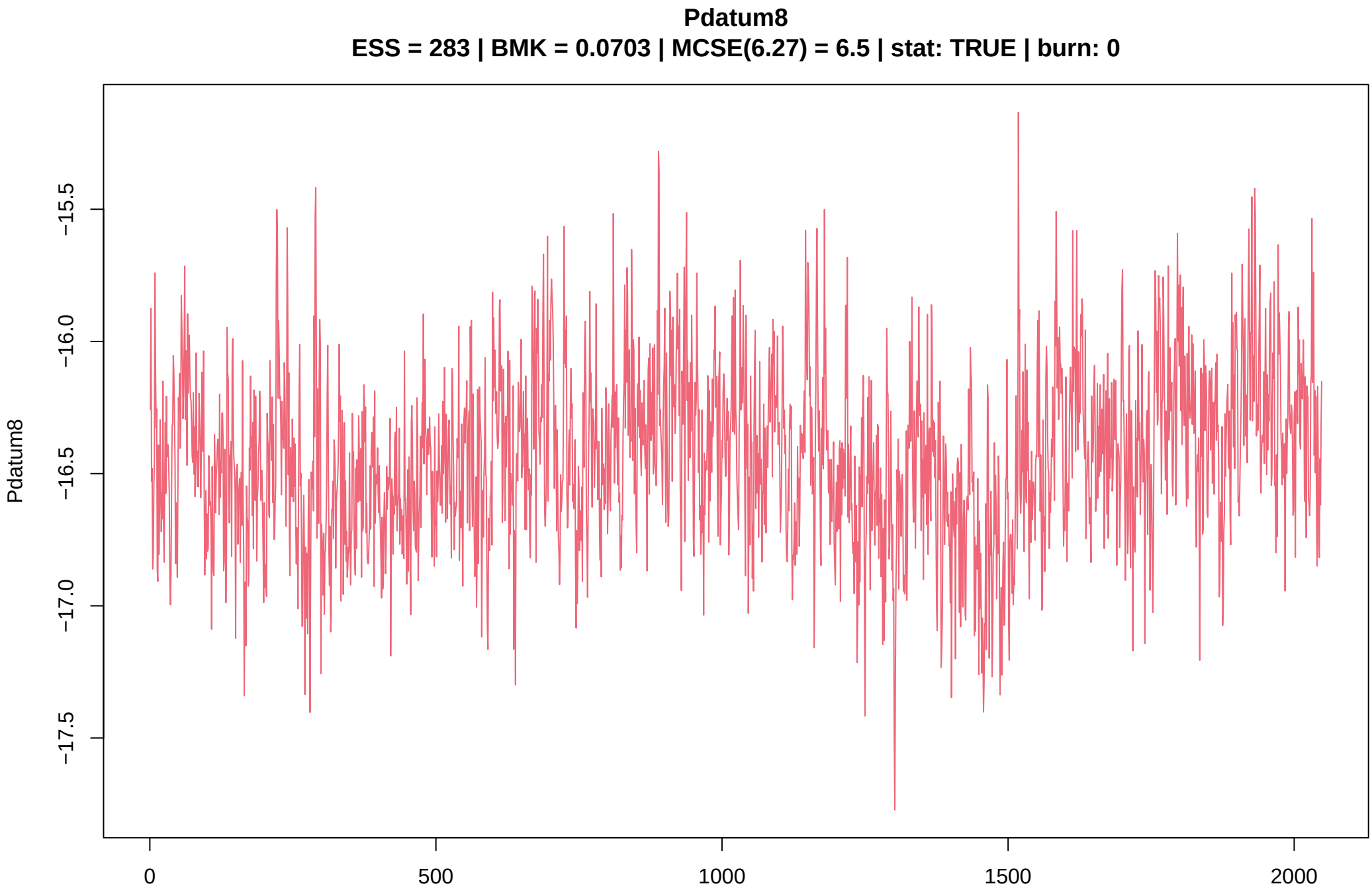

Pdatum3
ESS = 118 | BMK = 0.166 | MCSE(6.27) = 7.85 | stat: FALSE | burn: 0
Pdatum3
−9.6
−9.8
−10.0
−10.2
−10.4
−10.6
0
500
1000
1500
2000

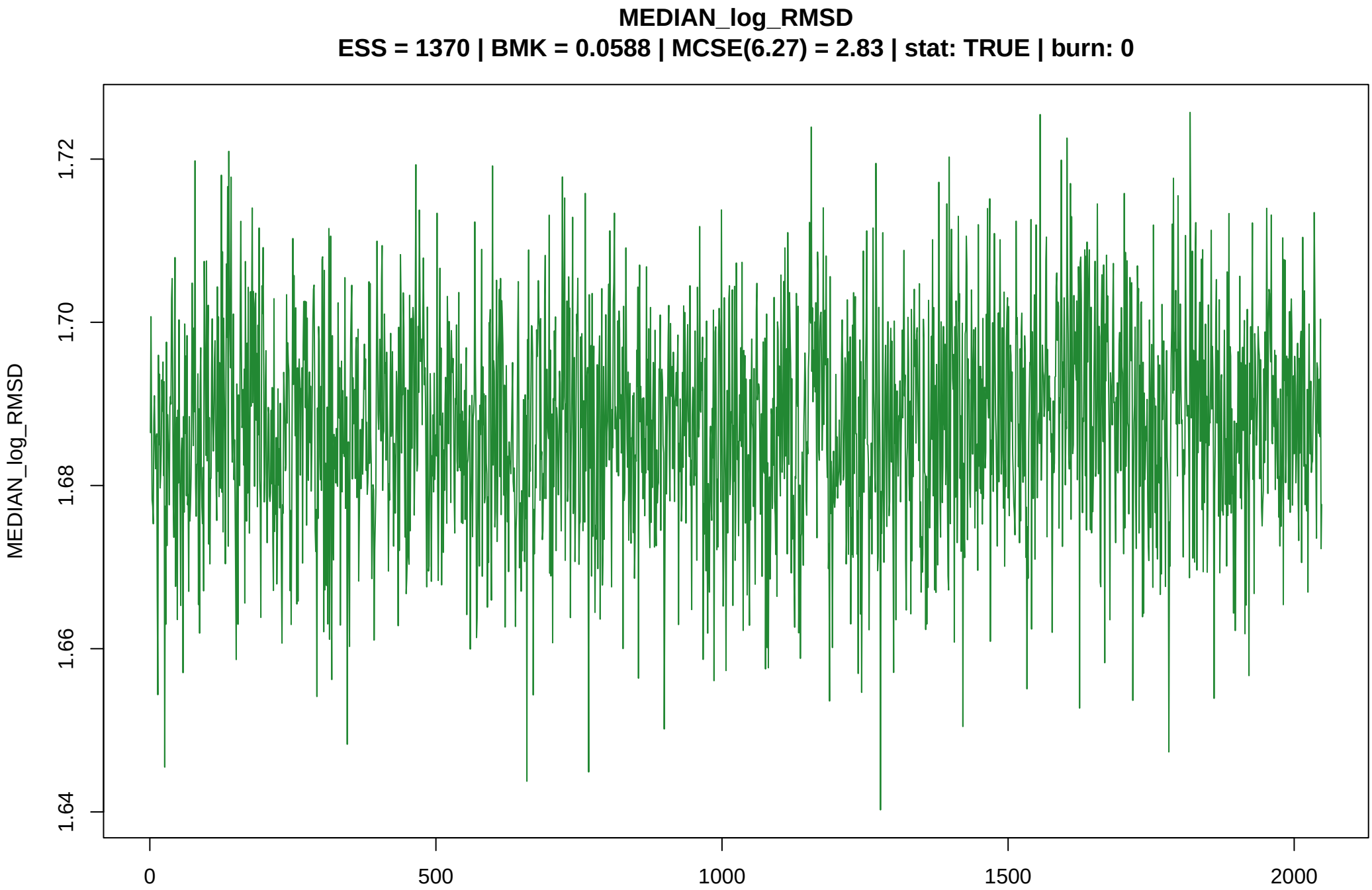

Pdatum4
ESS = 63.7 | BMK = 0.286 | MCSE(6.27) = 9.72 | stat: FALSE | burn: 0
Pdatum4
−10.0
−10.5
−11.0
−11.5
0
500
1000
1500
2000

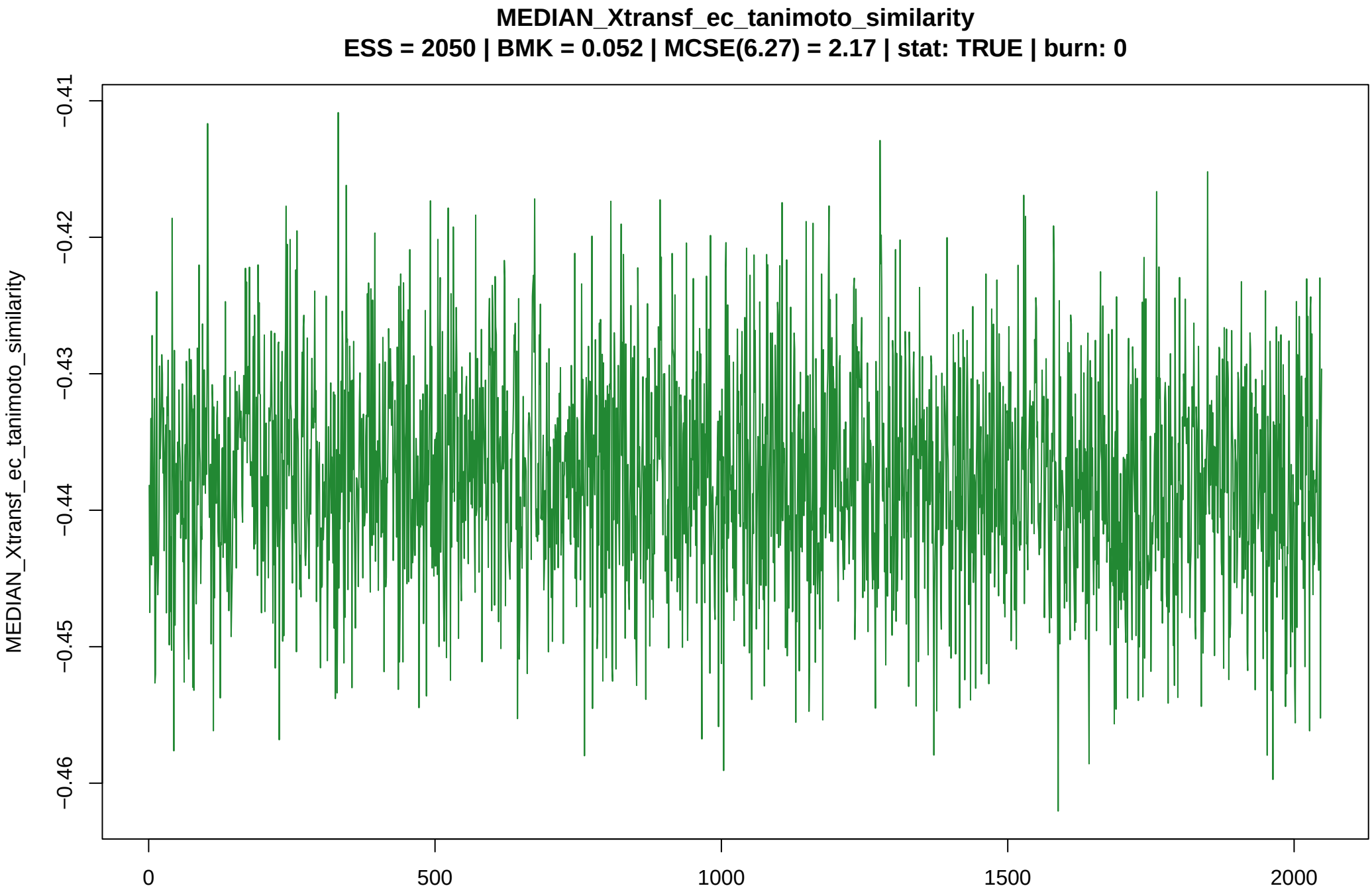

Pdatum5
ESS = 80.8 | BMK = 0.24 | MCSE(6.27) = 9.48 | stat: FALSE | burn: 0
Pdatum5
−10.4
−10.6
−10.8
−11.0
−11.2
−11.4
−11.6
0
500
1000
1500
2000

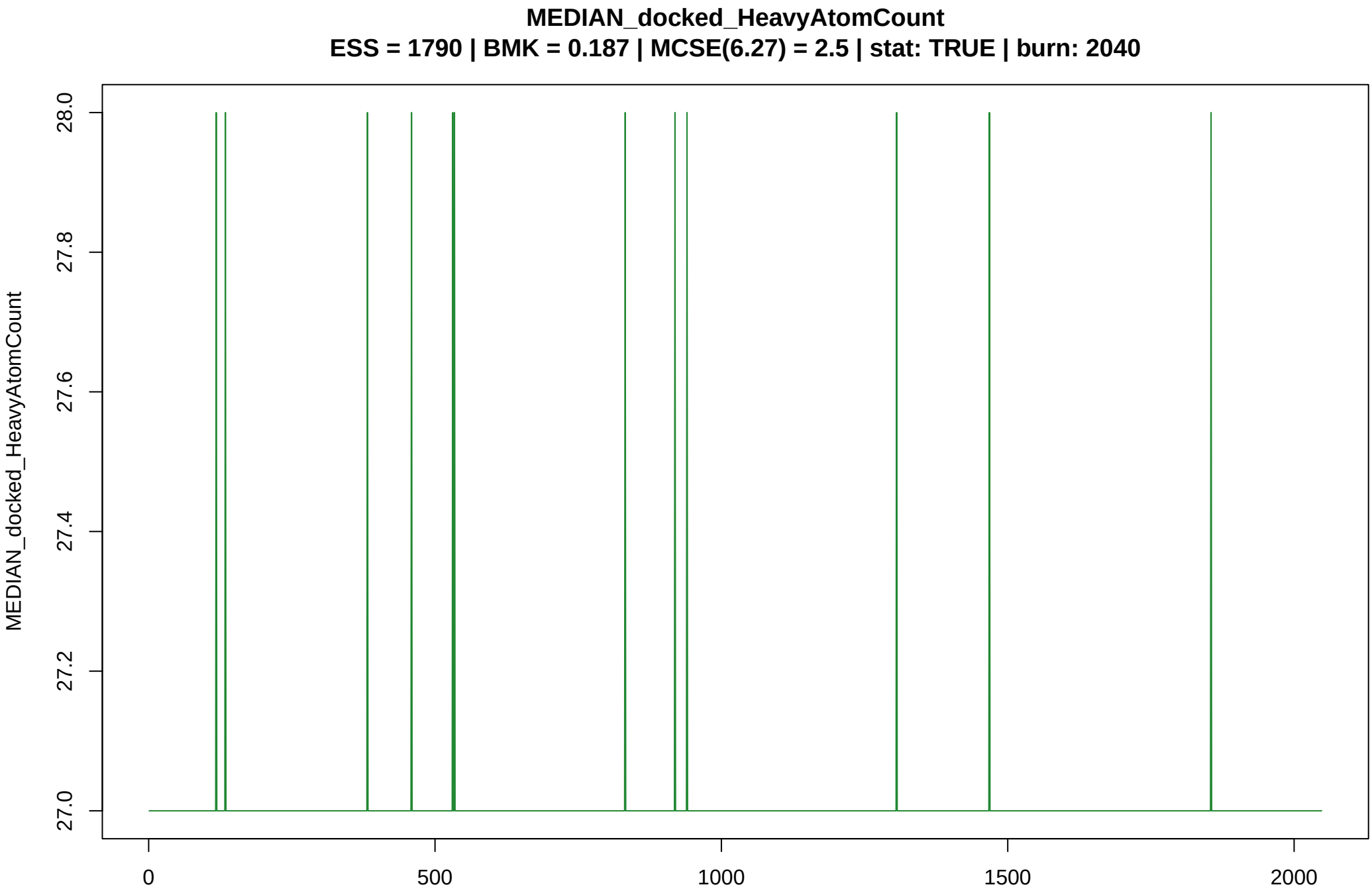

Pdatum6
ESS = 419 | BMK = 0.0936 | MCSE(6.27) = 5.26 | stat: TRUE | burn: 0
Pdatum6
−14.6
−14.8
−15.0
−15.2
−15.4
−15.6
−15.8
0
500
1000
1500
2000

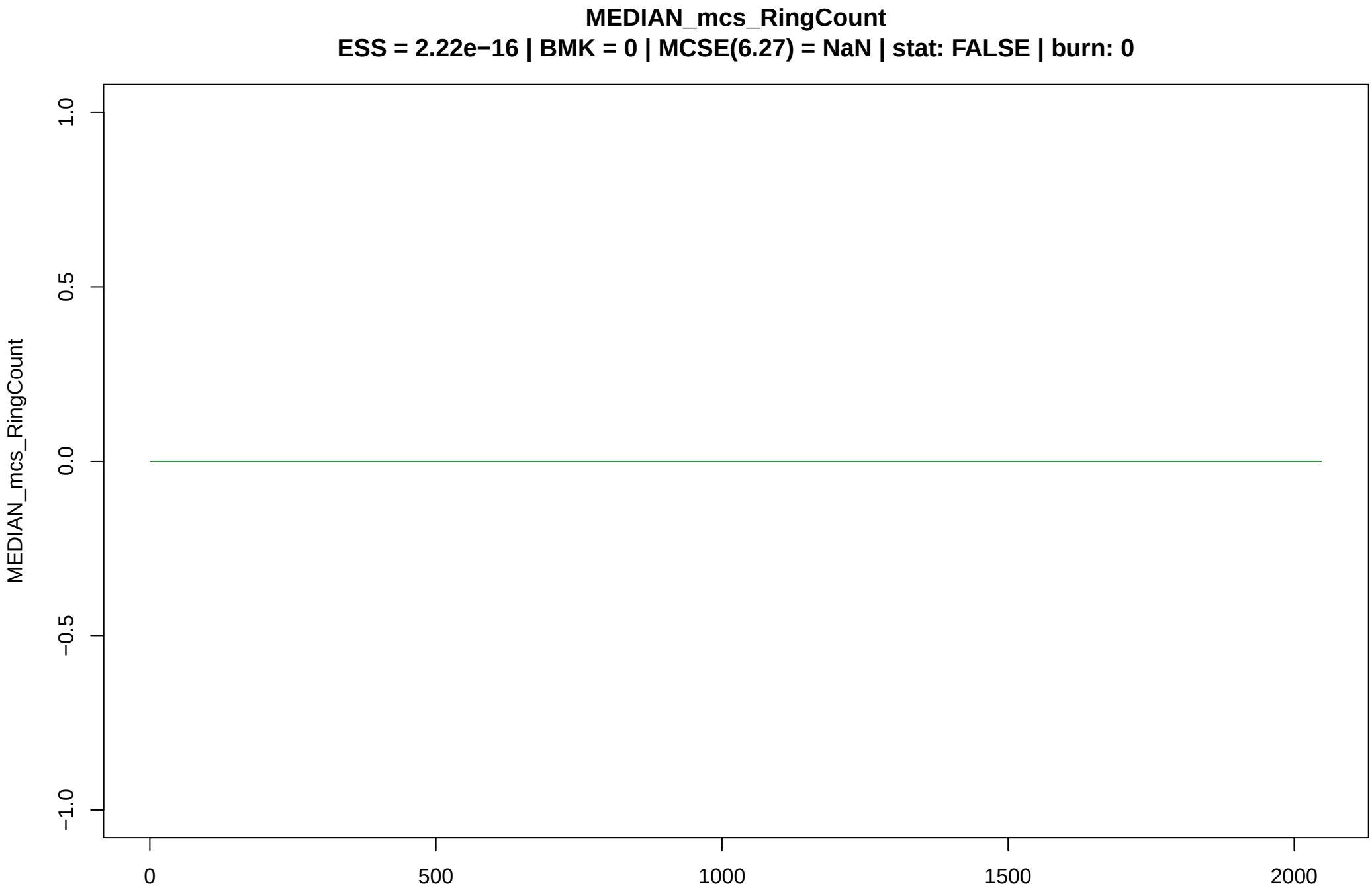

Pdatum7
ESS = 302 | BMK = 0.0562 | MCSE(6.27) = 5.71 | stat: TRUE | burn: 0
Pdatum7
−12.0
−12.5
−13.0
−13.5
0
500
1000
1500
2000

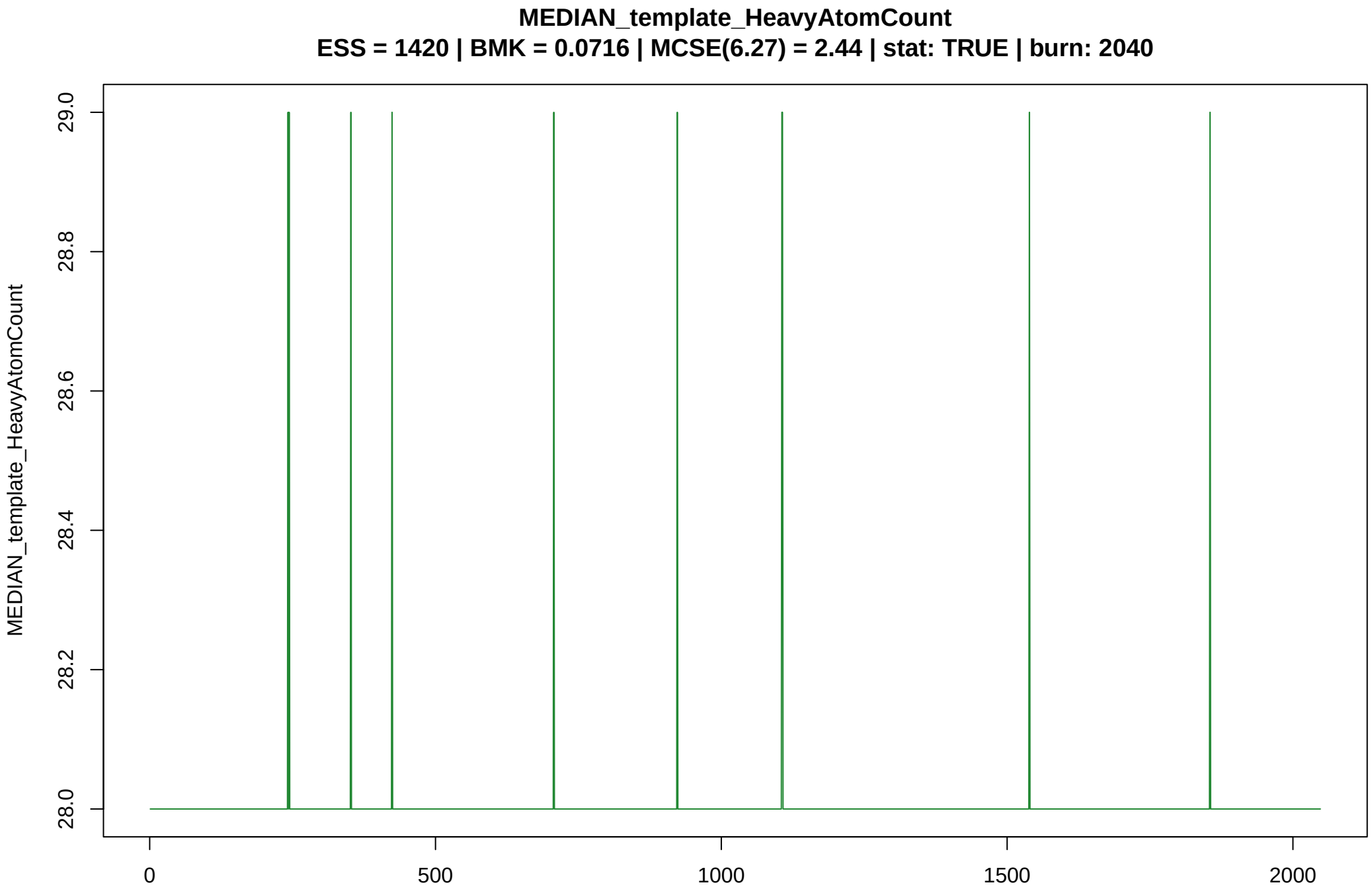

Pdatum8
ESS = 283 | BMK = 0.0703 | MCSE(6.27) = 6.5 | stat: TRUE | burn: 0
Pdatum8
−15.5
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000

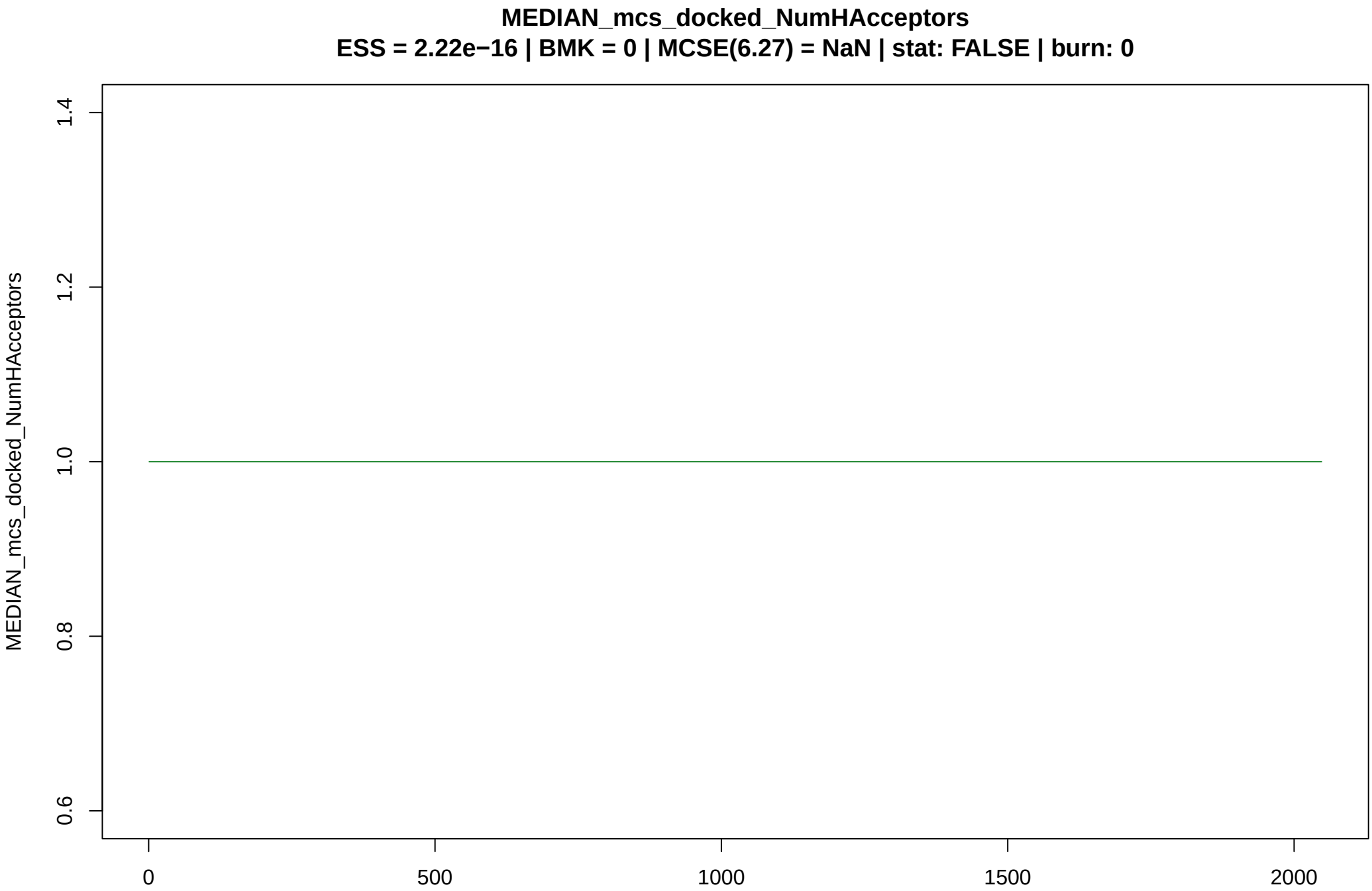

MEDIAN_log_RMSD
ESS = 1370 | BMK = 0.0588 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
1.64
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

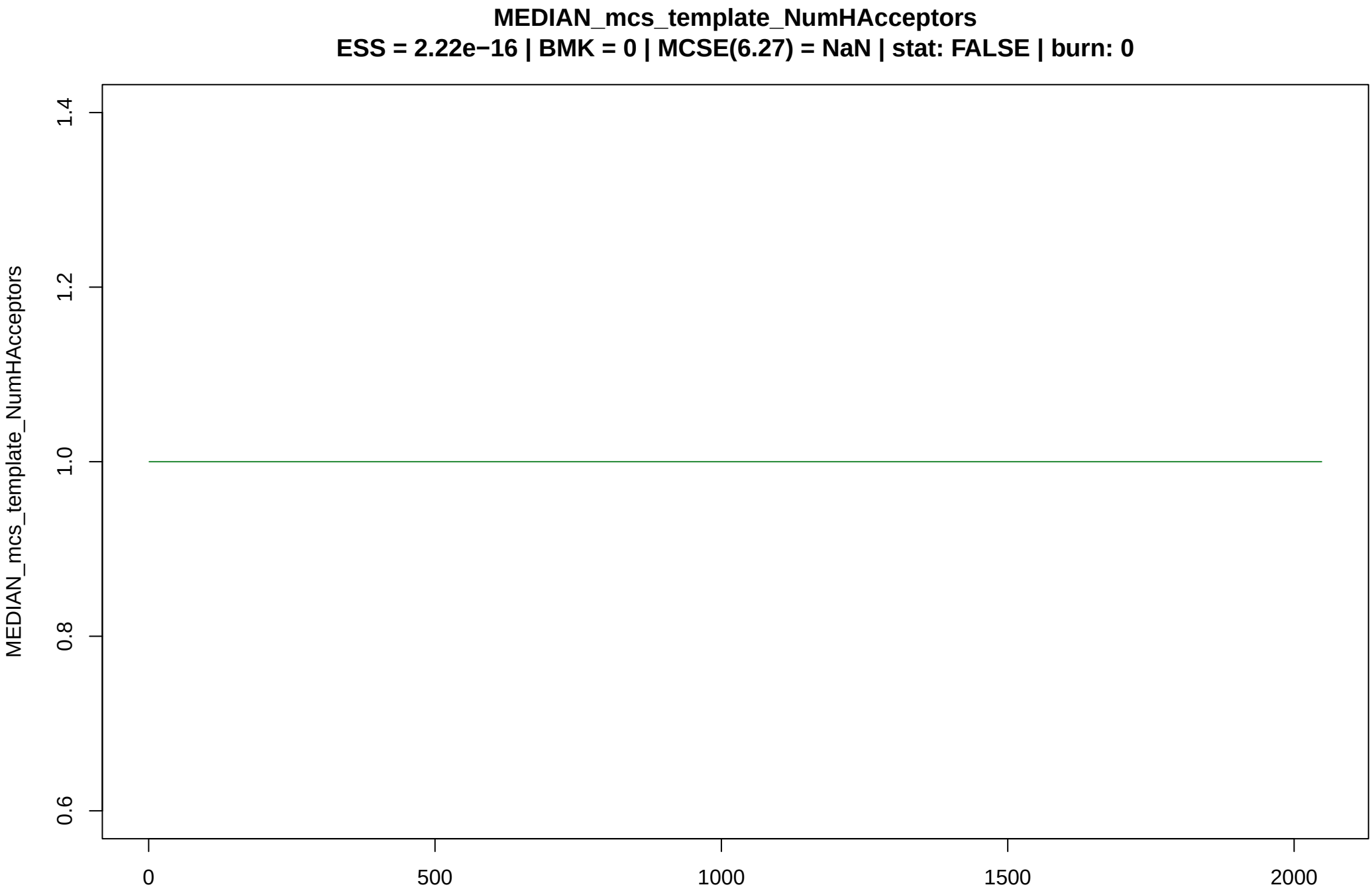

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.052 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.41
−0.42
−0.43
−0.44
−0.45
−0.46
0
500
1000
1500
2000

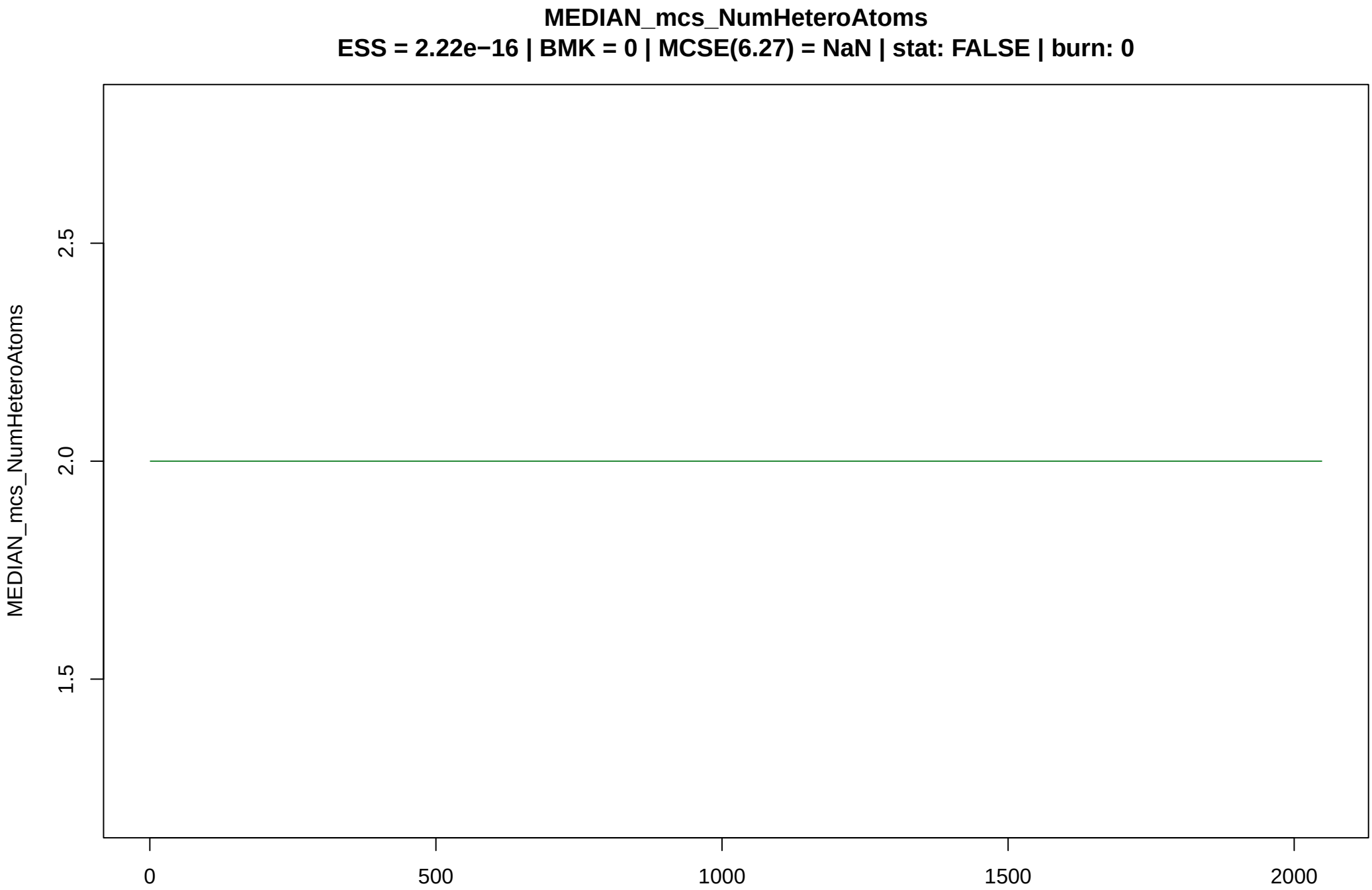

MEDIAN_docked_HeavyAtomCount
ESS = 1790 | BMK = 0.187 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 2040
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

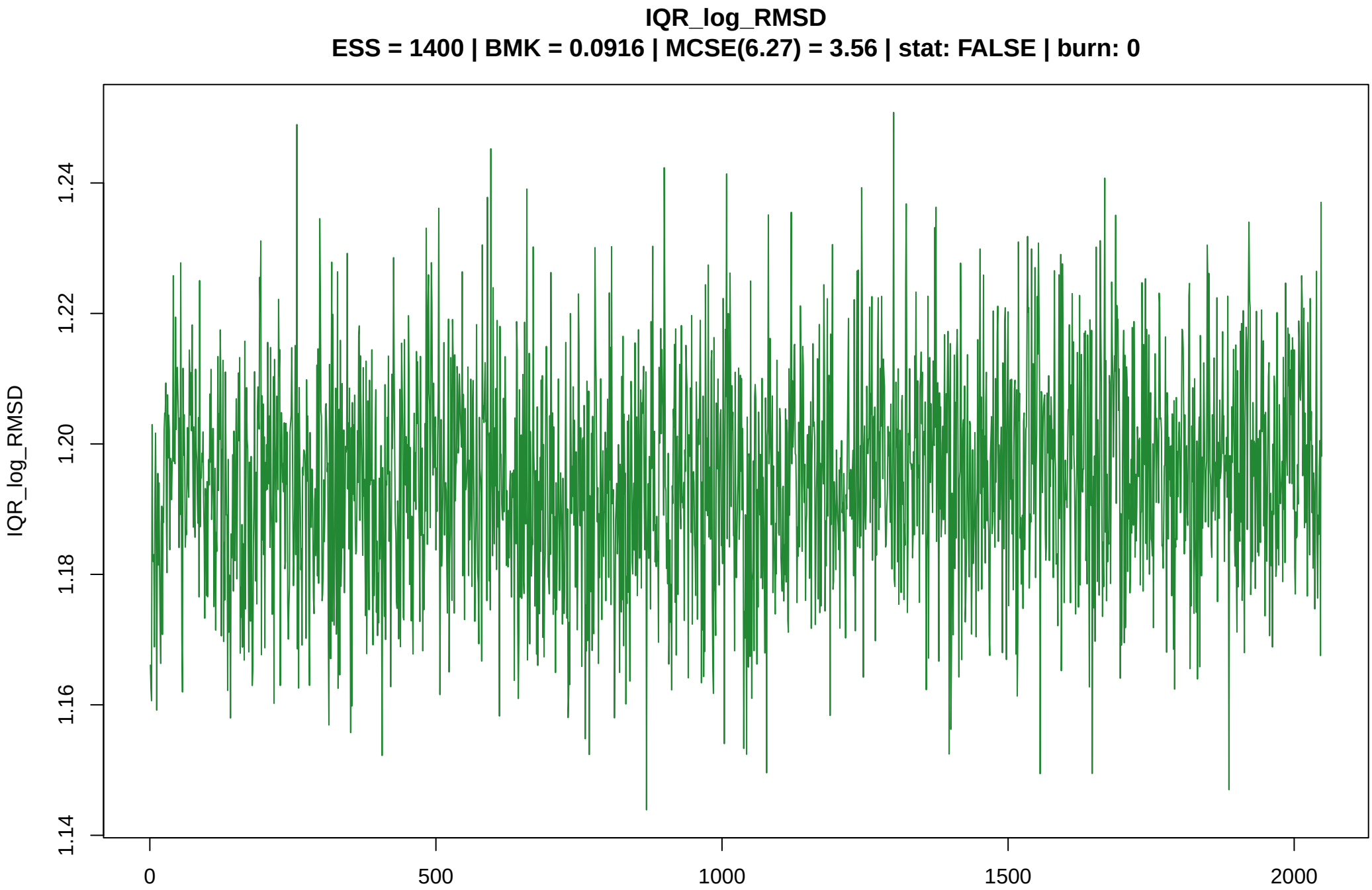

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

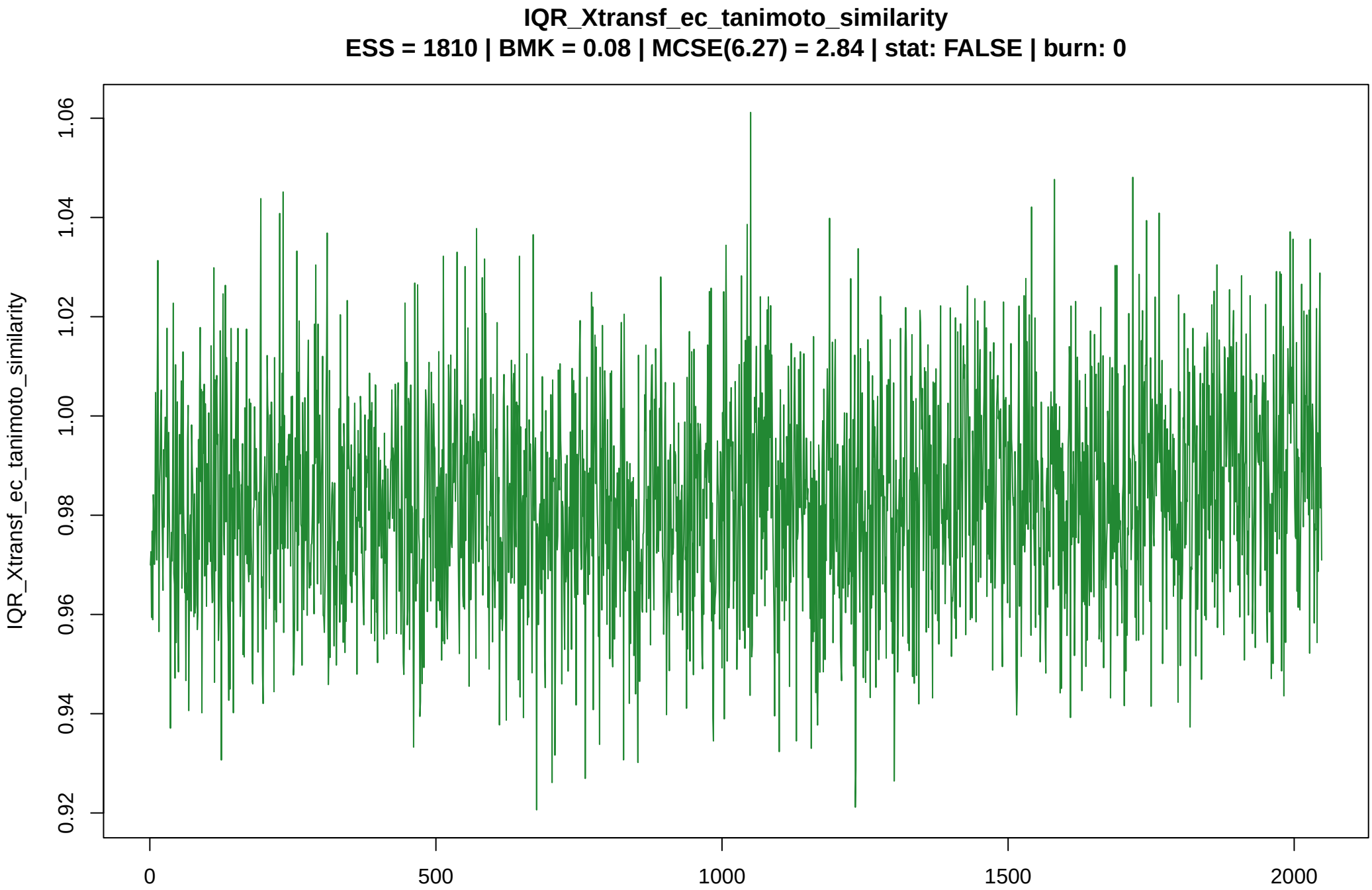

MEDIAN_template_HeavyAtomCount
ESS = 1420 | BMK = 0.0716 | MCSE(6.27) = 2.44 | stat: TRUE | burn: 2040
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

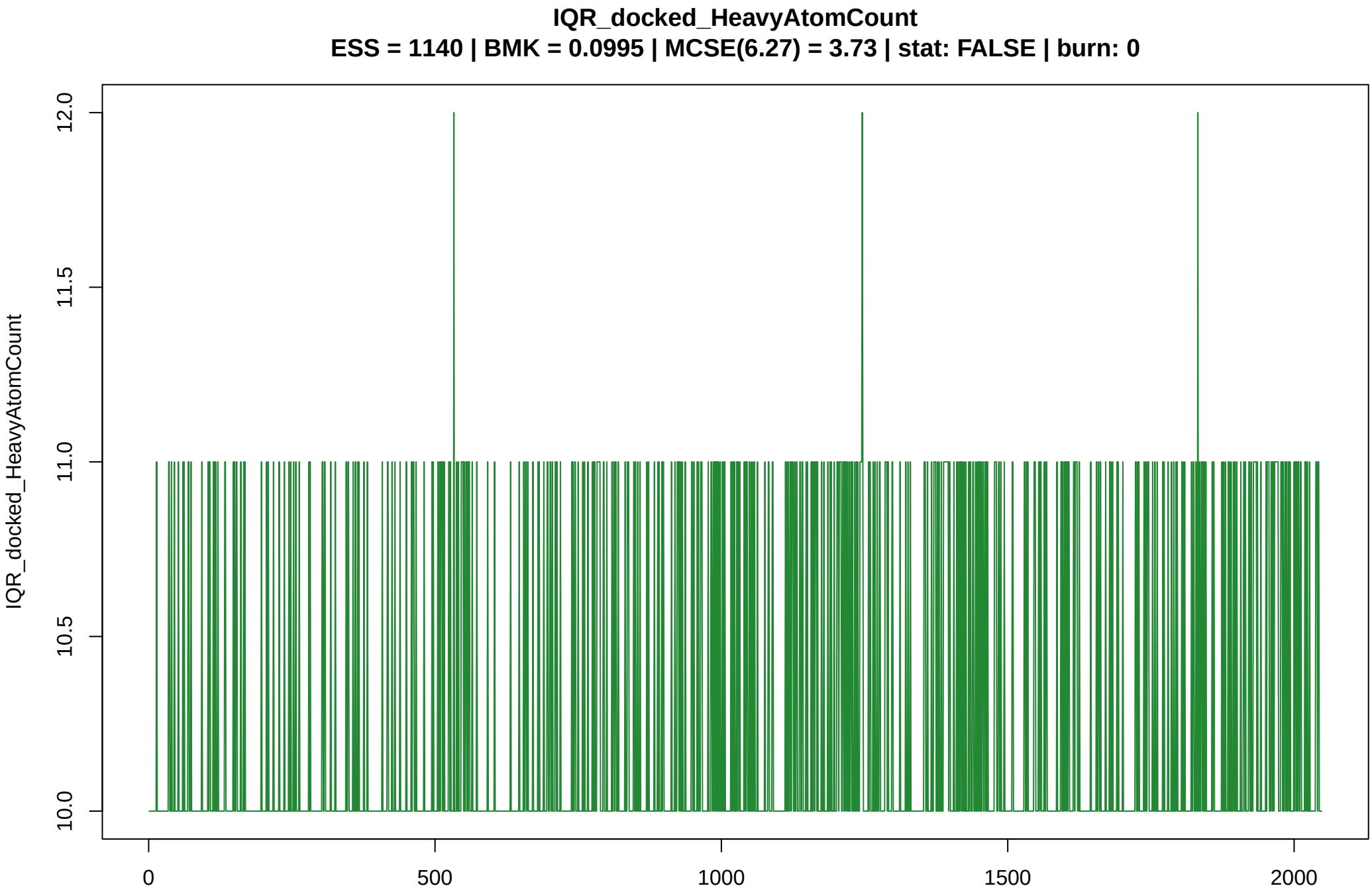

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

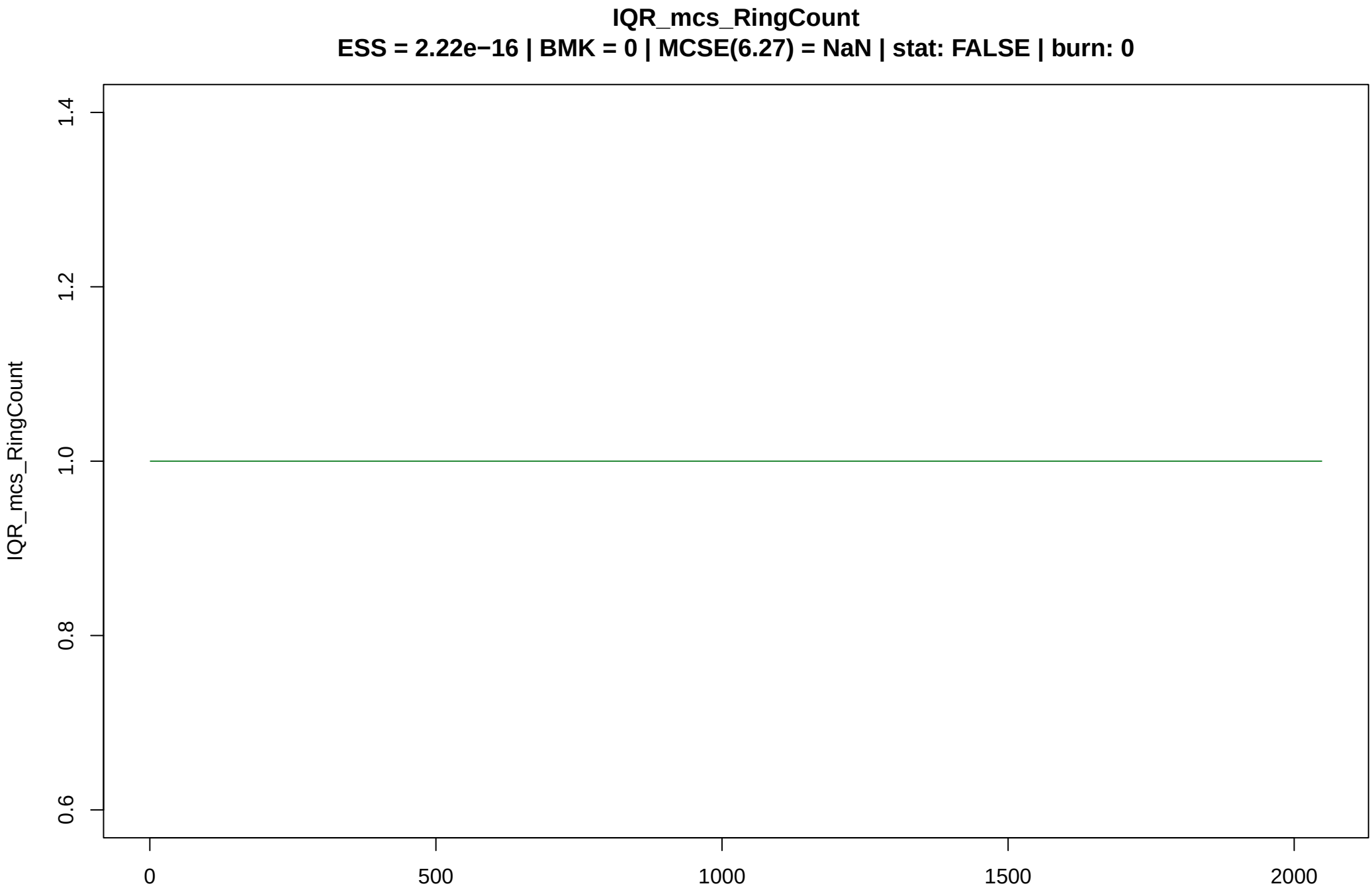

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

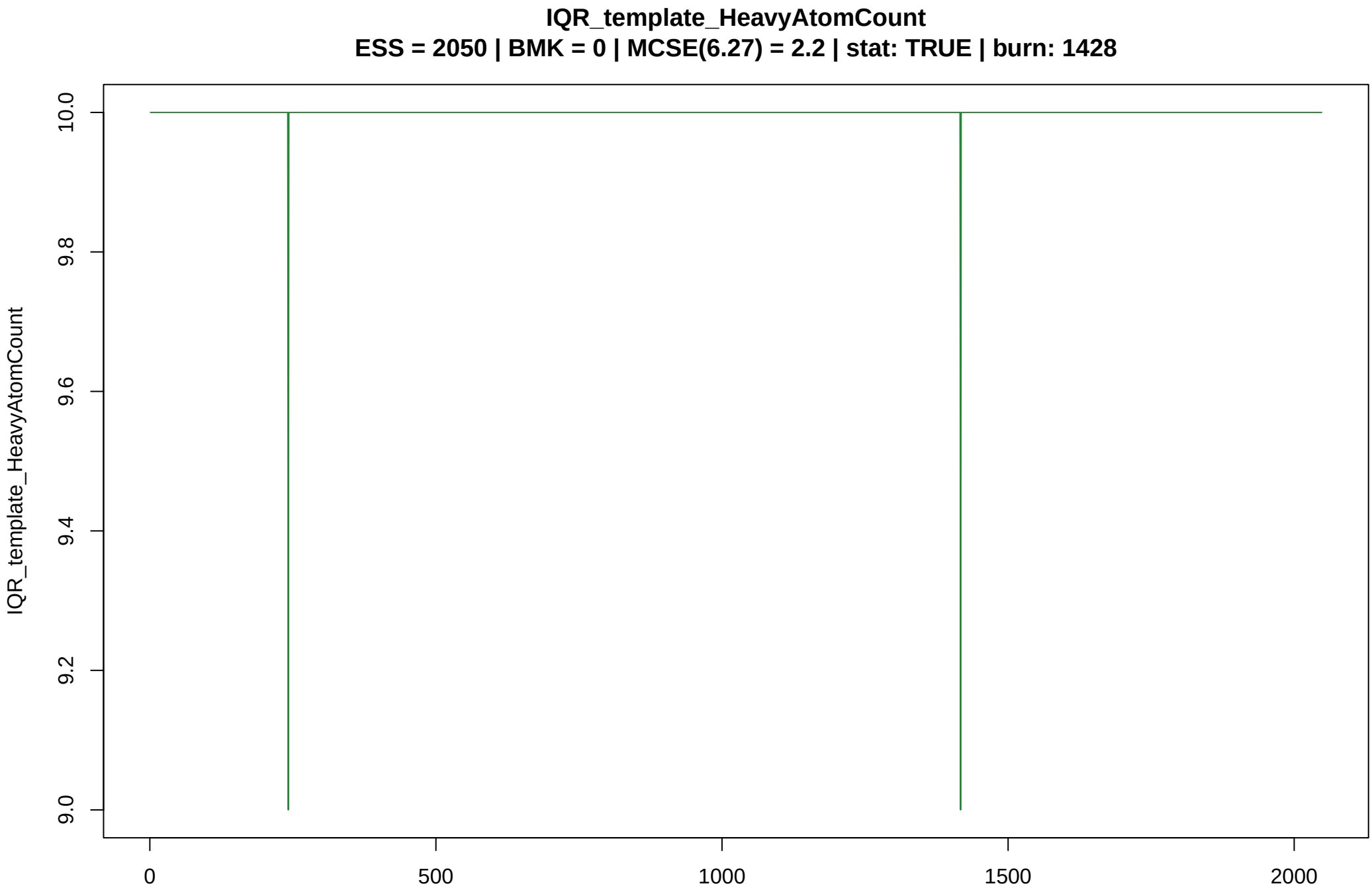

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

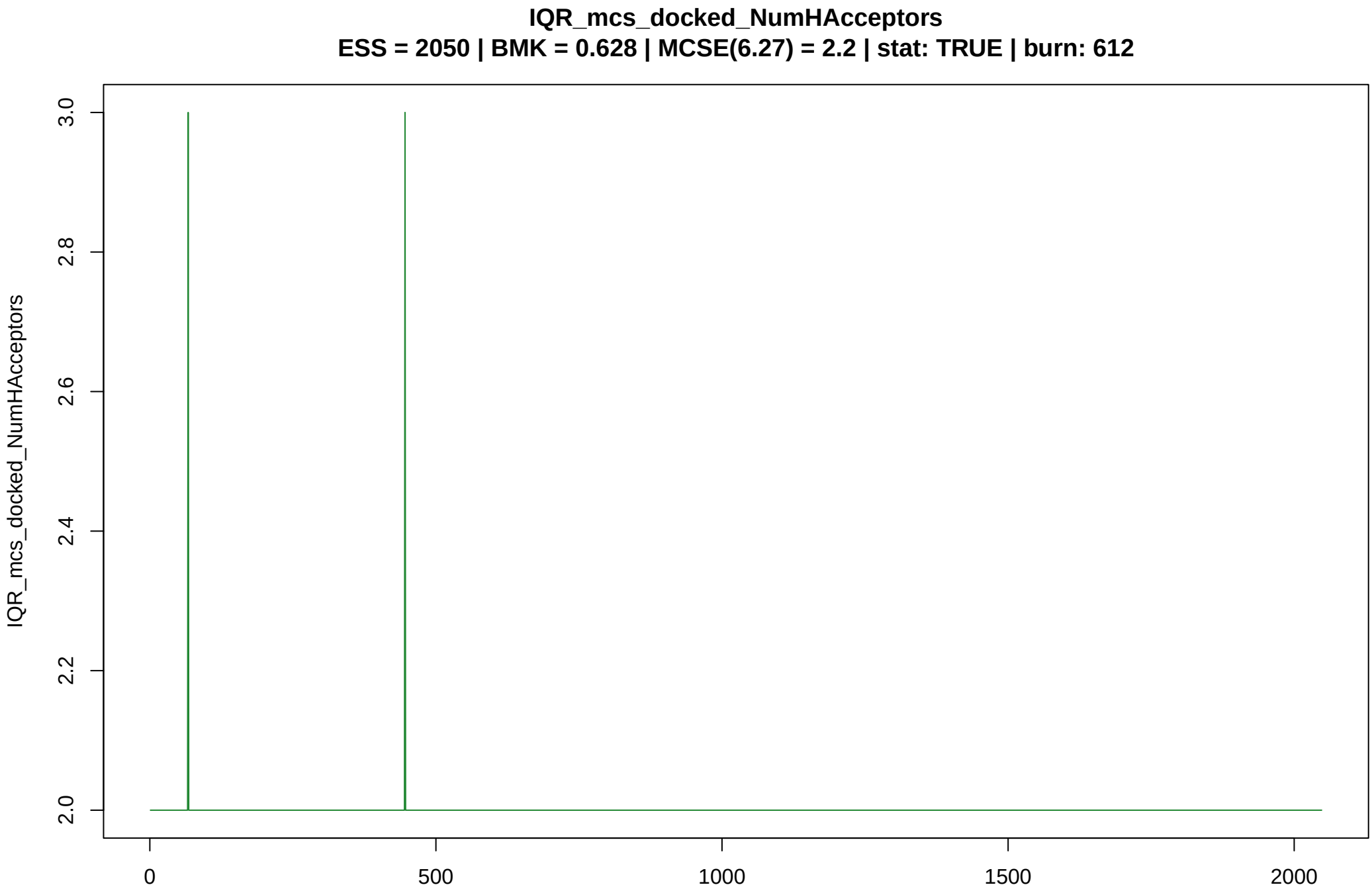

IQR_log_RMSD
ESS = 1400 | BMK = 0.0916 | MCSE(6.27) = 3.56 | stat: FALSE | burn: 0
IQR_log_RMSD
1.14
1.16
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

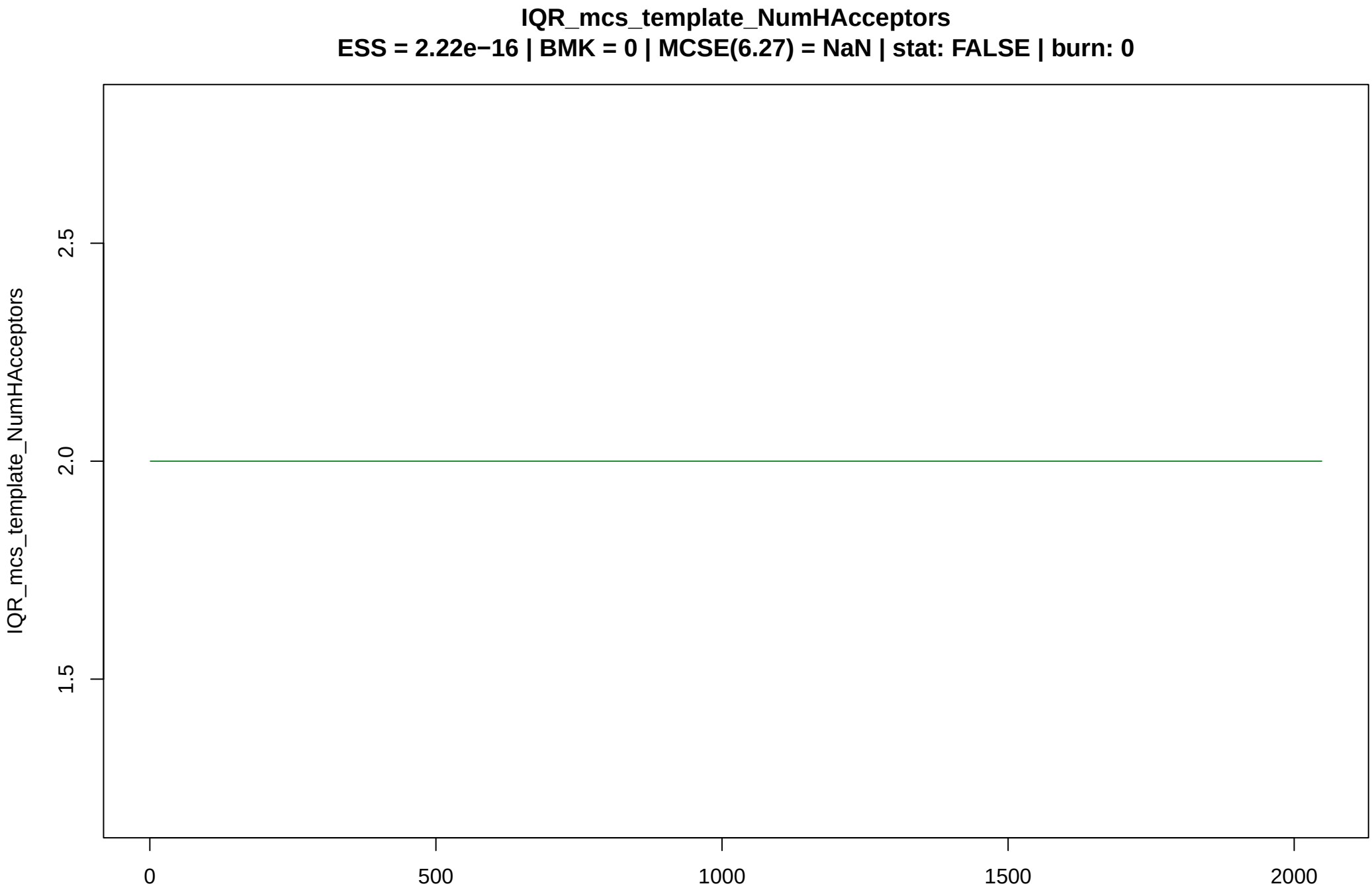

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1810 | BMK = 0.08 | MCSE(6.27) = 2.84 | stat: FALSE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.92
0.94
0.96
0.98
1.00
1.02
1.04
1.06
0
500
1000
1500
2000

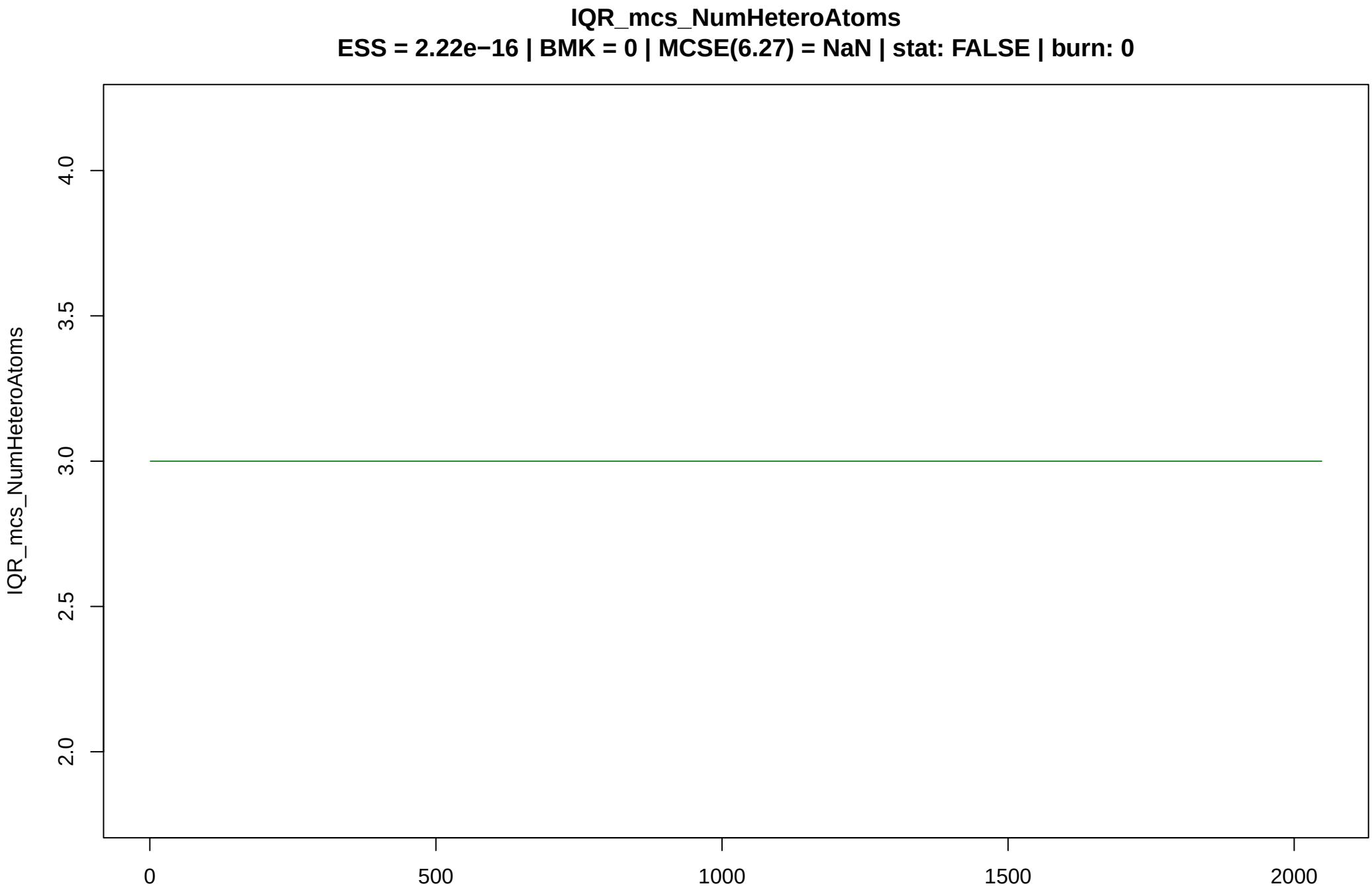

IQR_docked_HeavyAtomCount
ESS = 1140 | BMK = 0.0995 | MCSE(6.27) = 3.73 | stat: FALSE | burn: 0
IQR_docked_HeavyAtomCount
12.0
11.5
11.0
10.5
10.0
0
500
1000
1500
2000

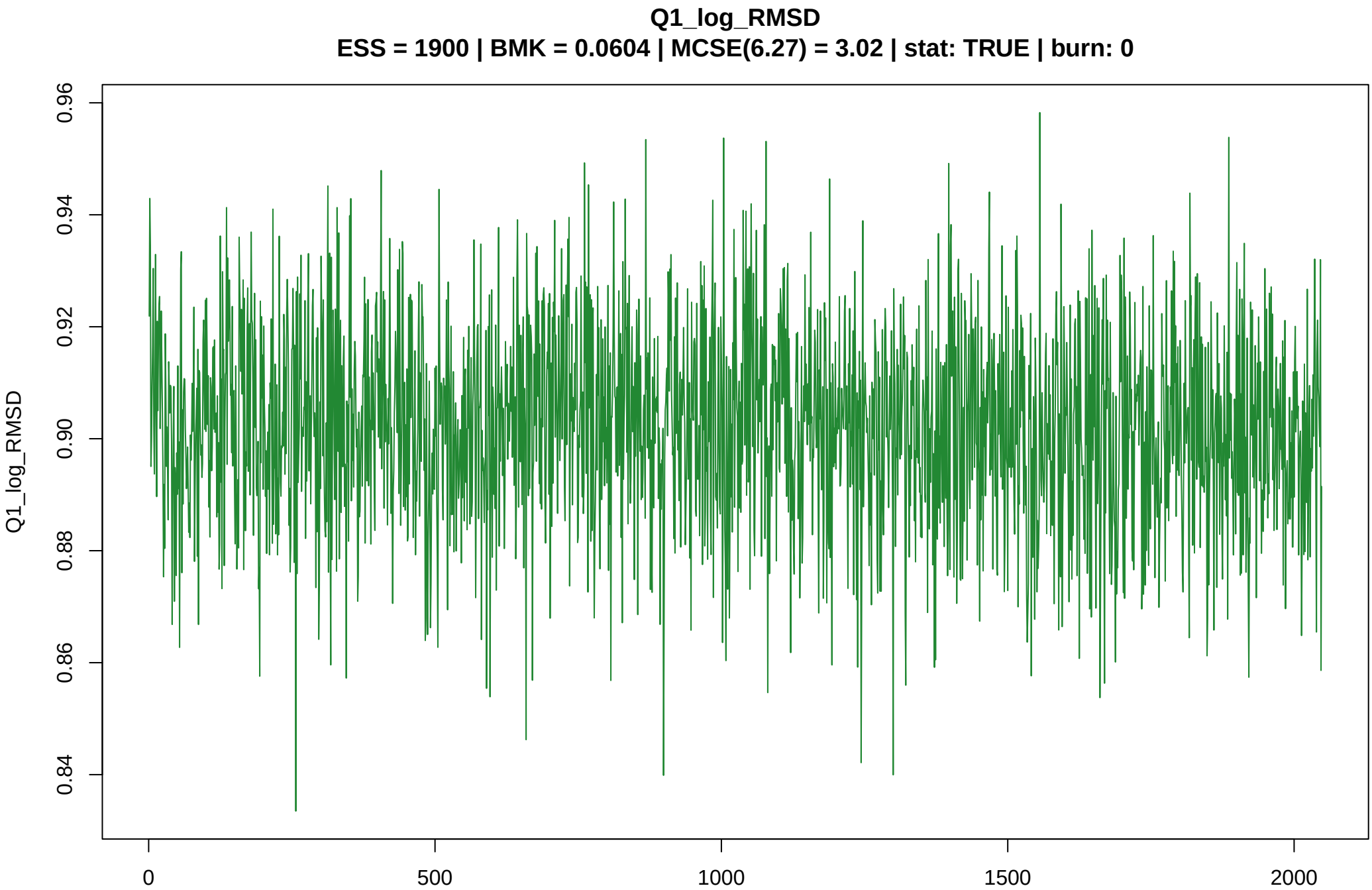

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

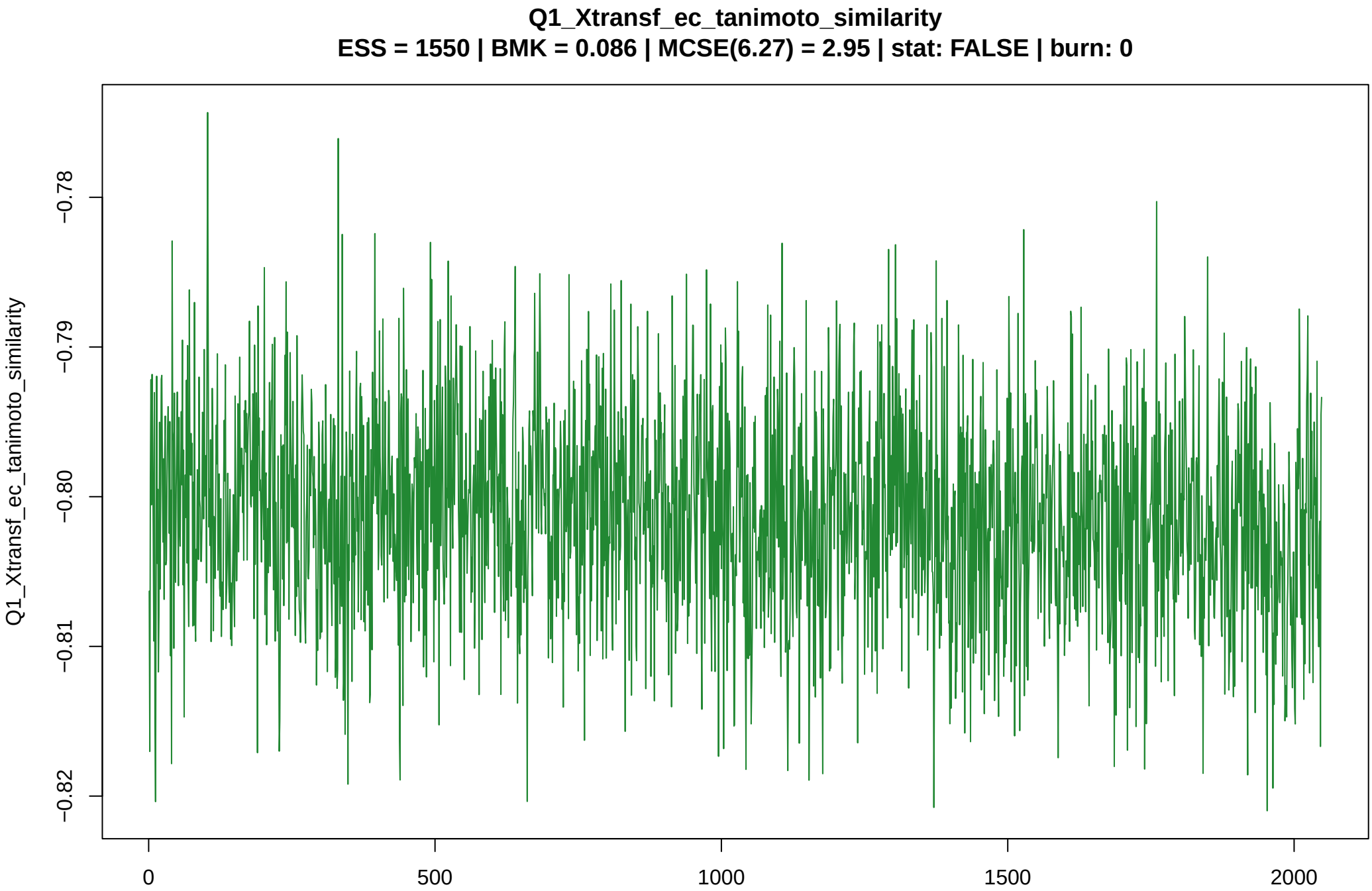

IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1428
IQR_template_HeavyAtomCount
10.0
9.8
9.6
9.4
9.2
9.0
0
500
1000
1500
2000

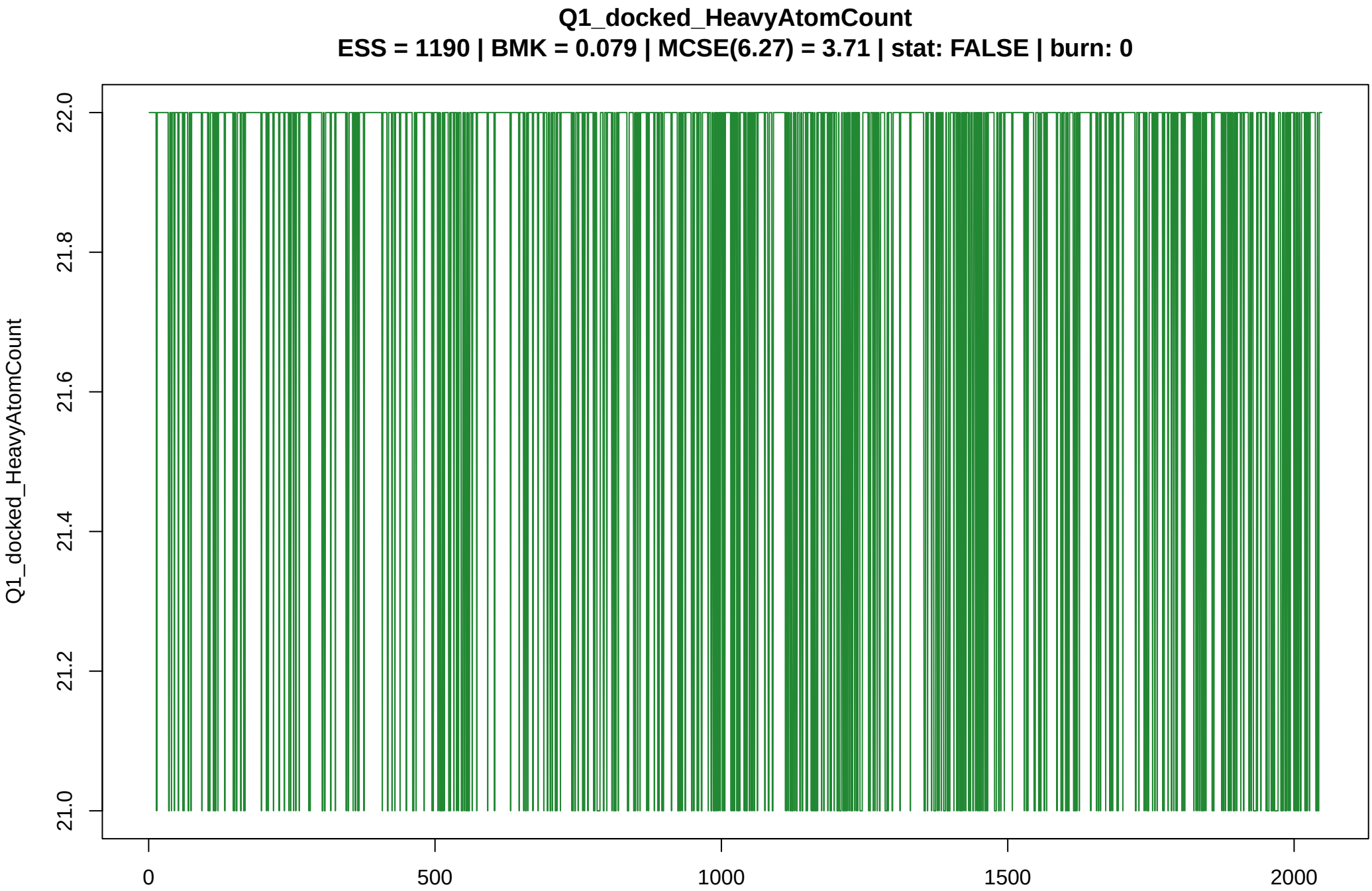

IQR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 612
IQR_mcs_docked_NumHAcceptors
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

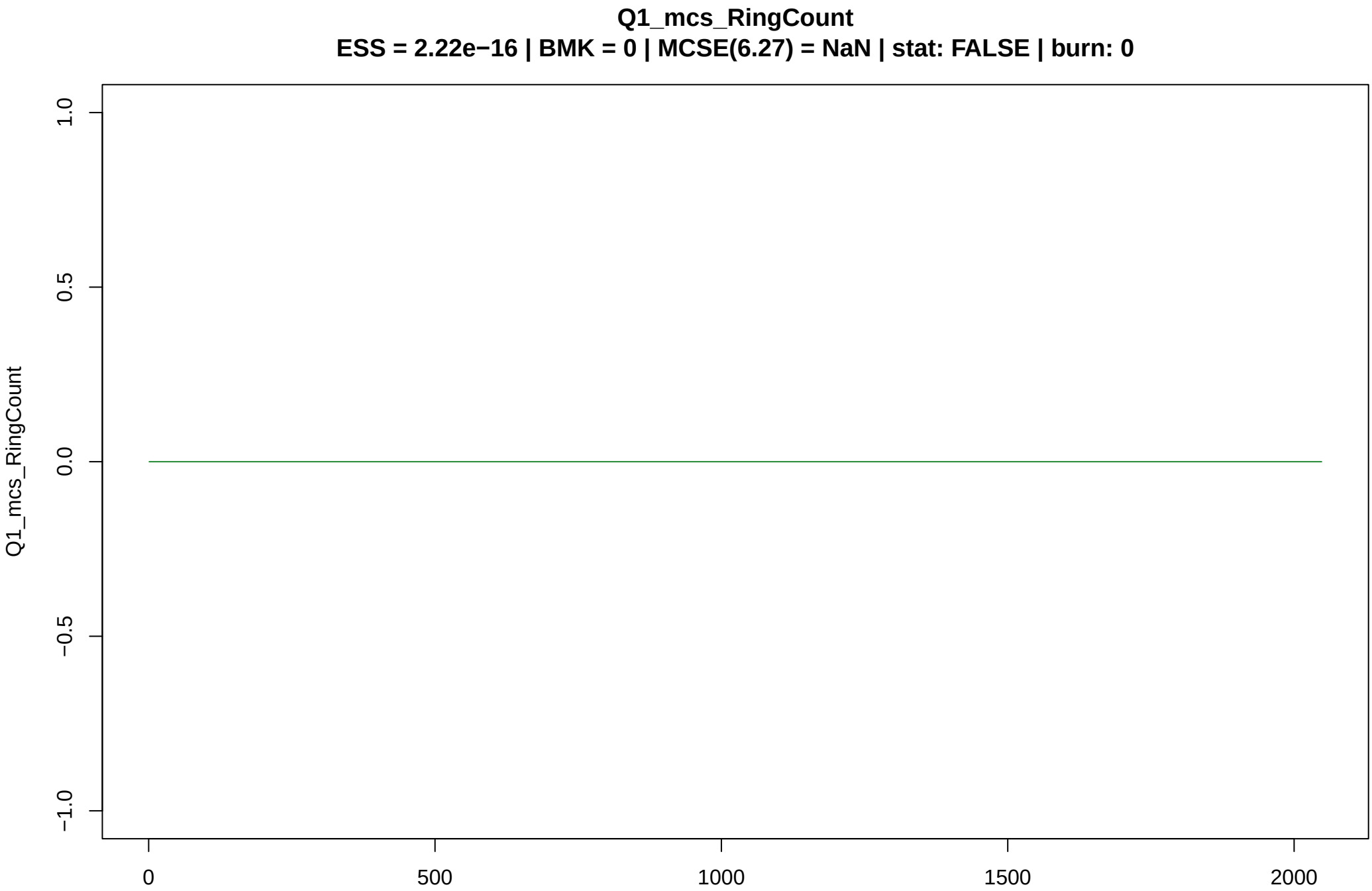

IQR_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_template_NumHAcceptors
2.5
2.0
1.5
0
500
1000
1500
2000

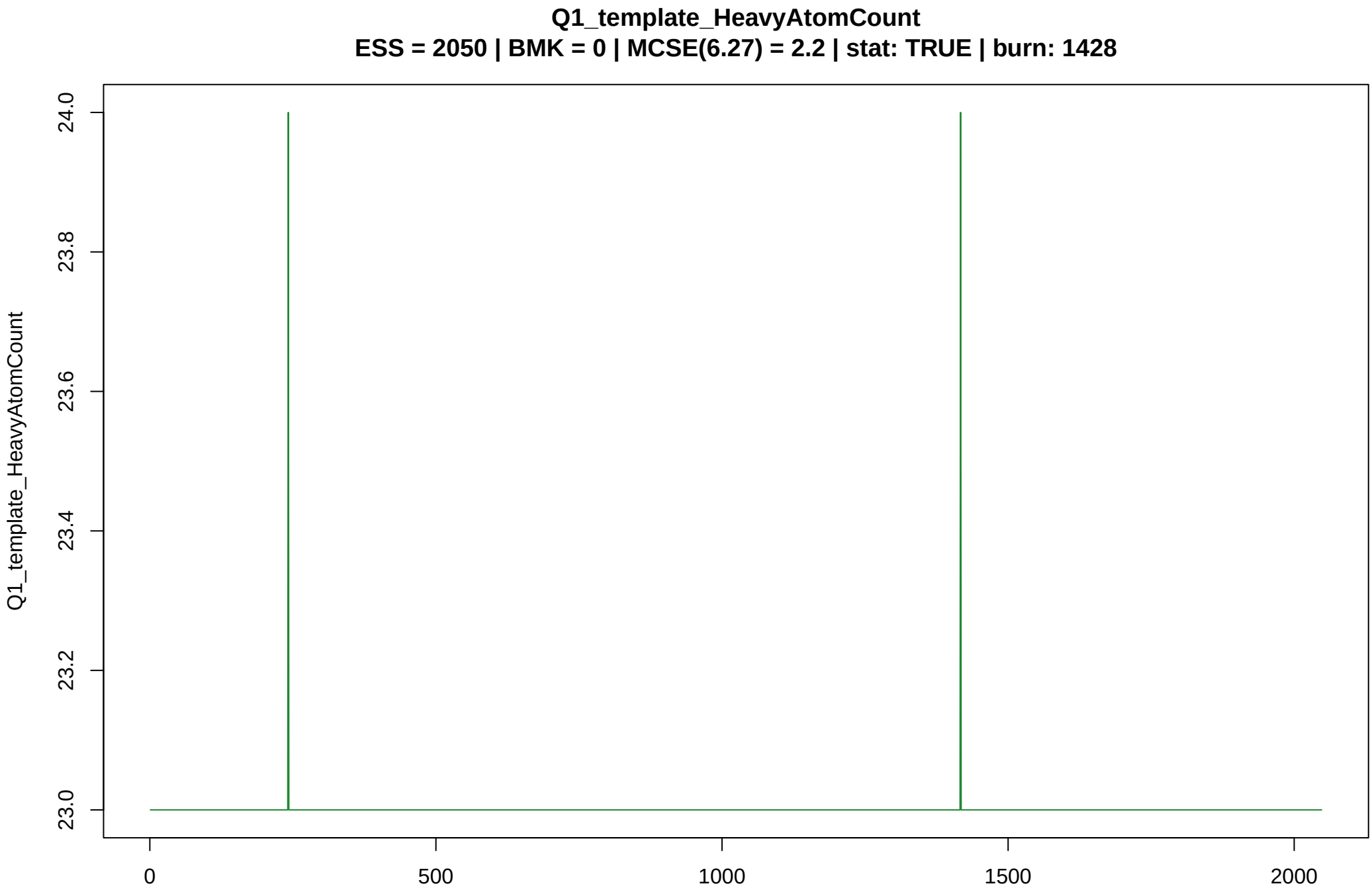

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

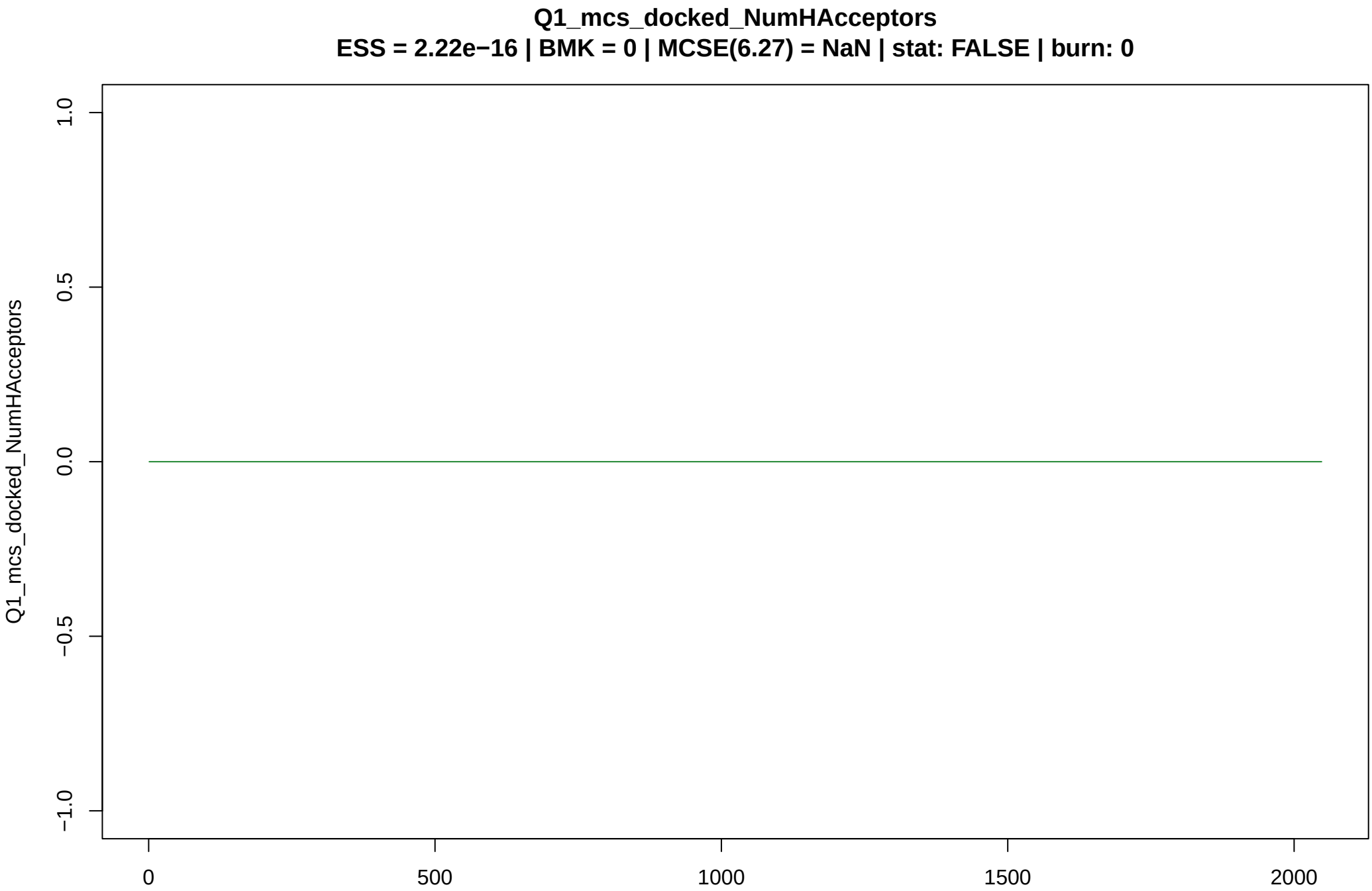

Q1_log_RMSD
ESS = 1900 | BMK = 0.0604 | MCSE(6.27) = 3.02 | stat: TRUE | burn: 0
Q1_log_RMSD
0.84
0.86
0.88
0.90
0.92
0.94
0.96
0
500
1000
1500
2000

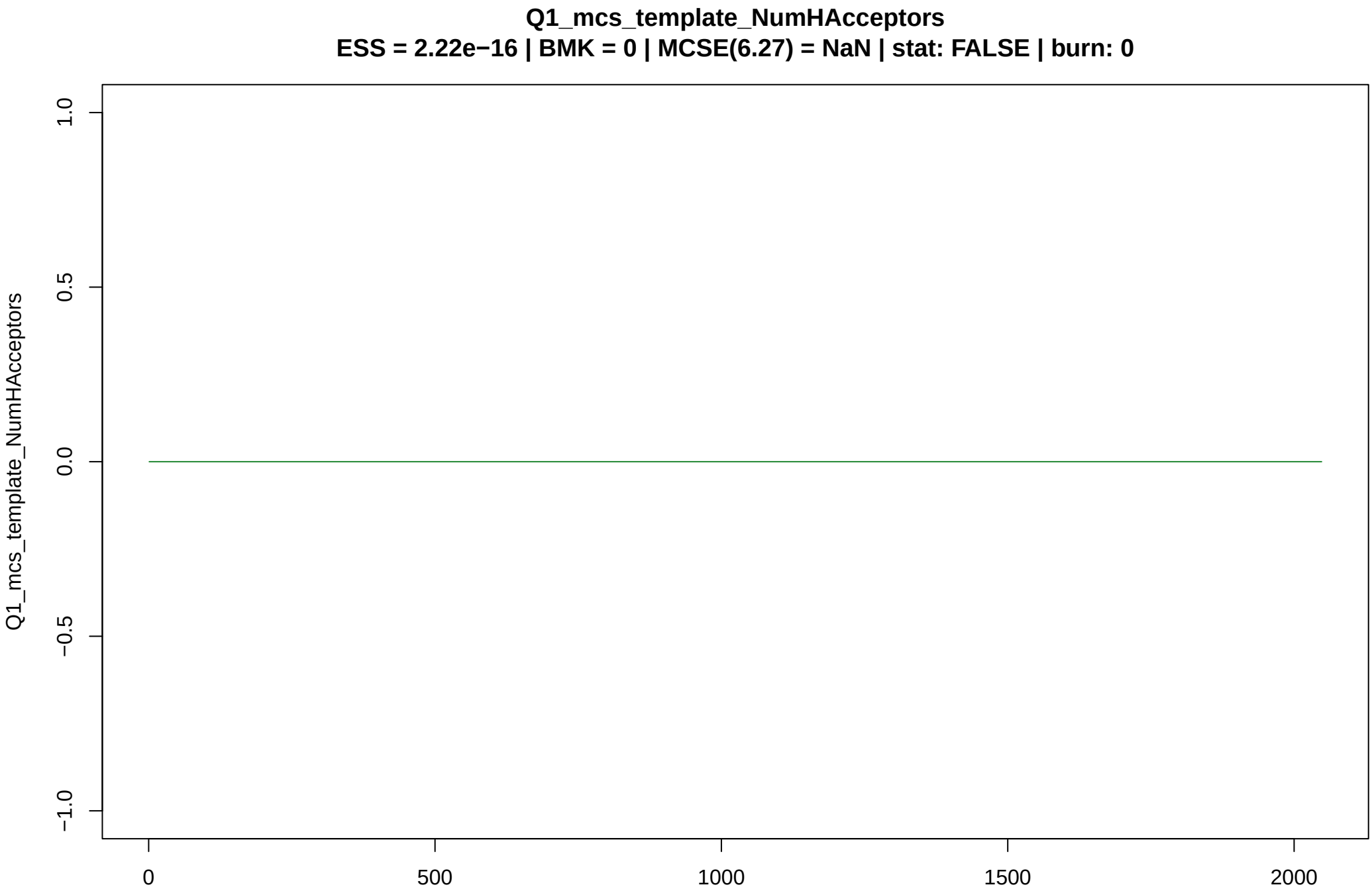

Q1_Xtransf_ec_tanimoto_similarity
ESS = 1550 | BMK = 0.086 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

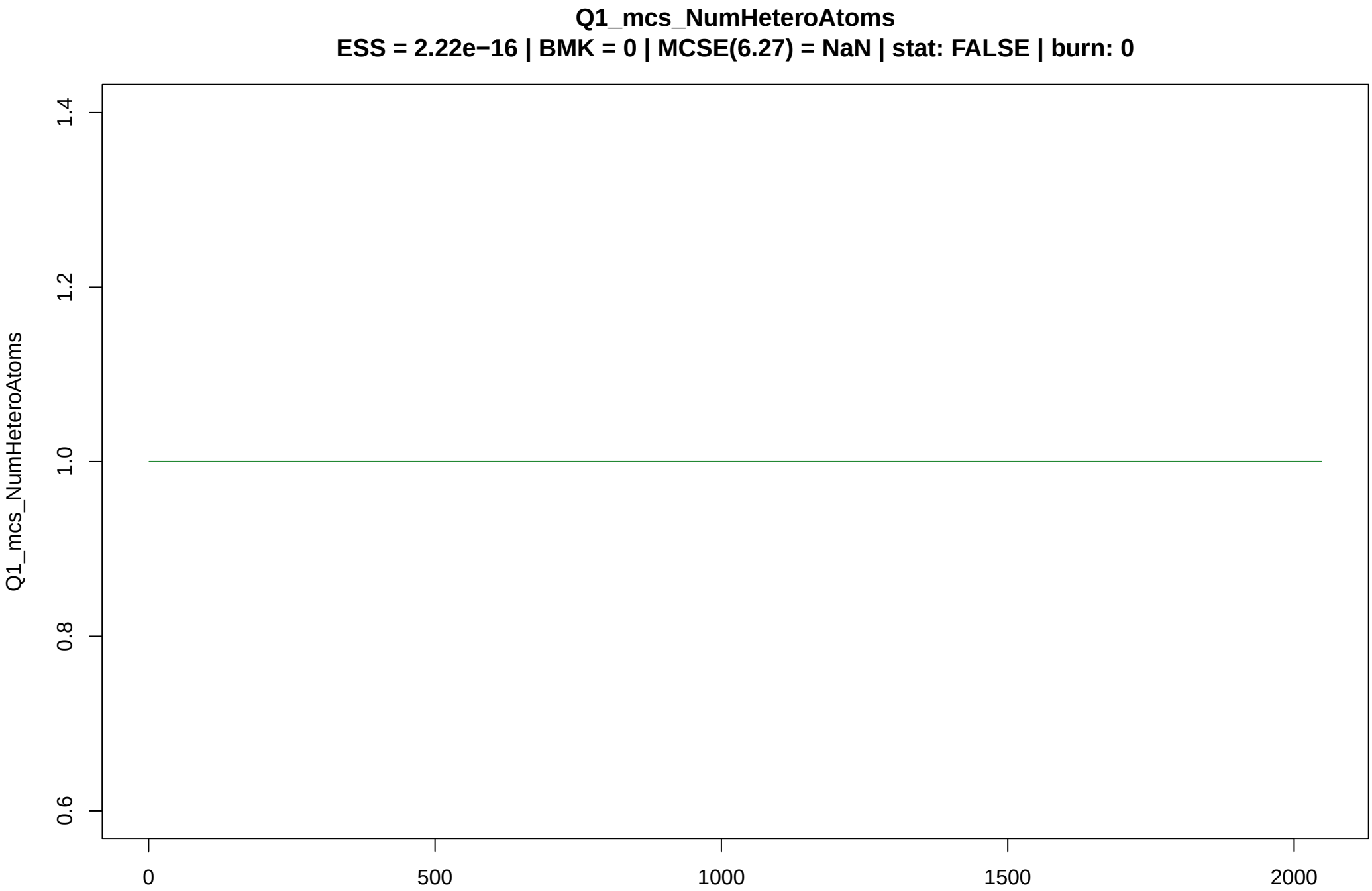

Q1_docked_HeavyAtomCount
ESS = 1190 | BMK = 0.079 | MCSE(6.27) = 3.71 | stat: FALSE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

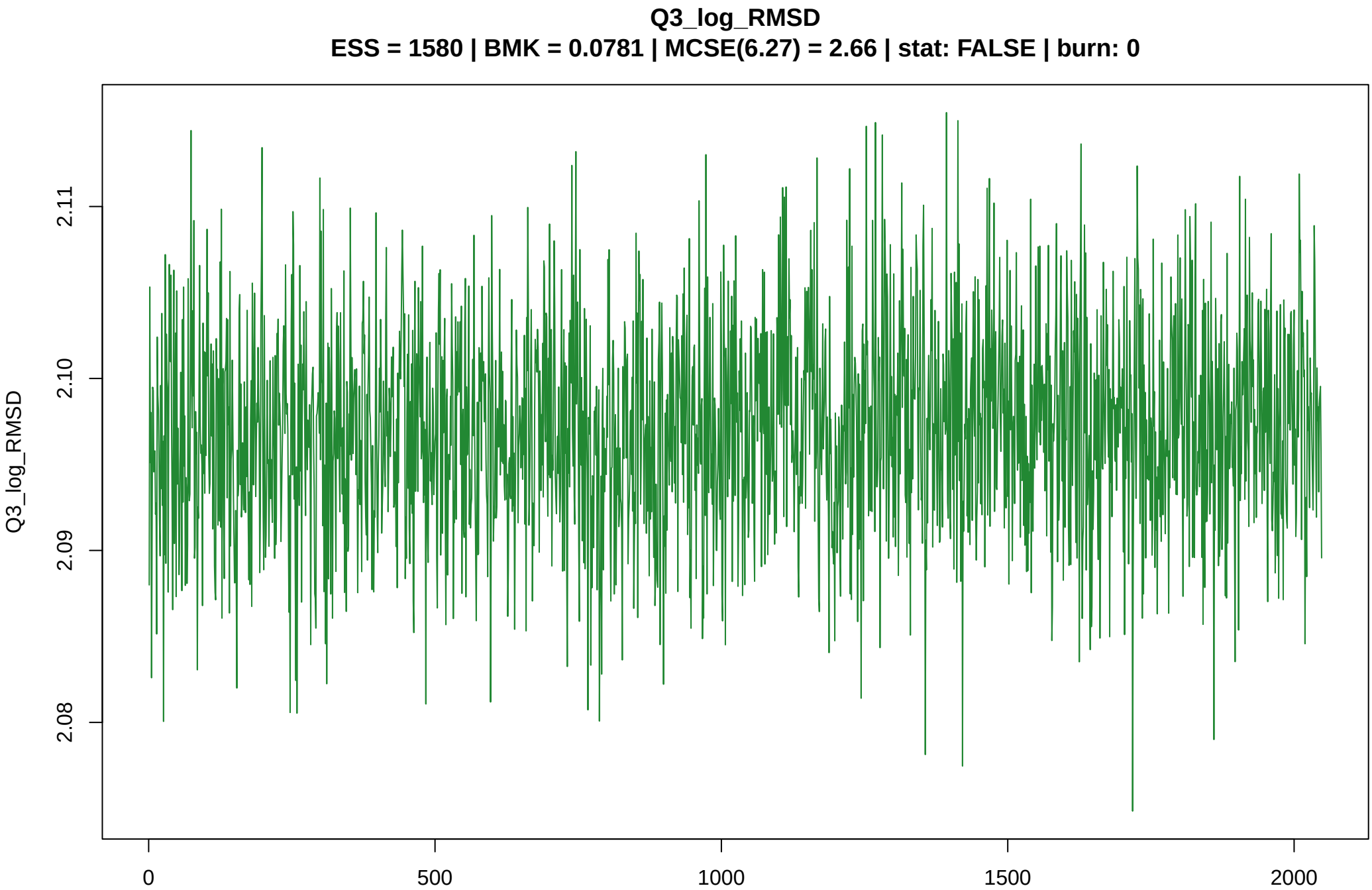

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

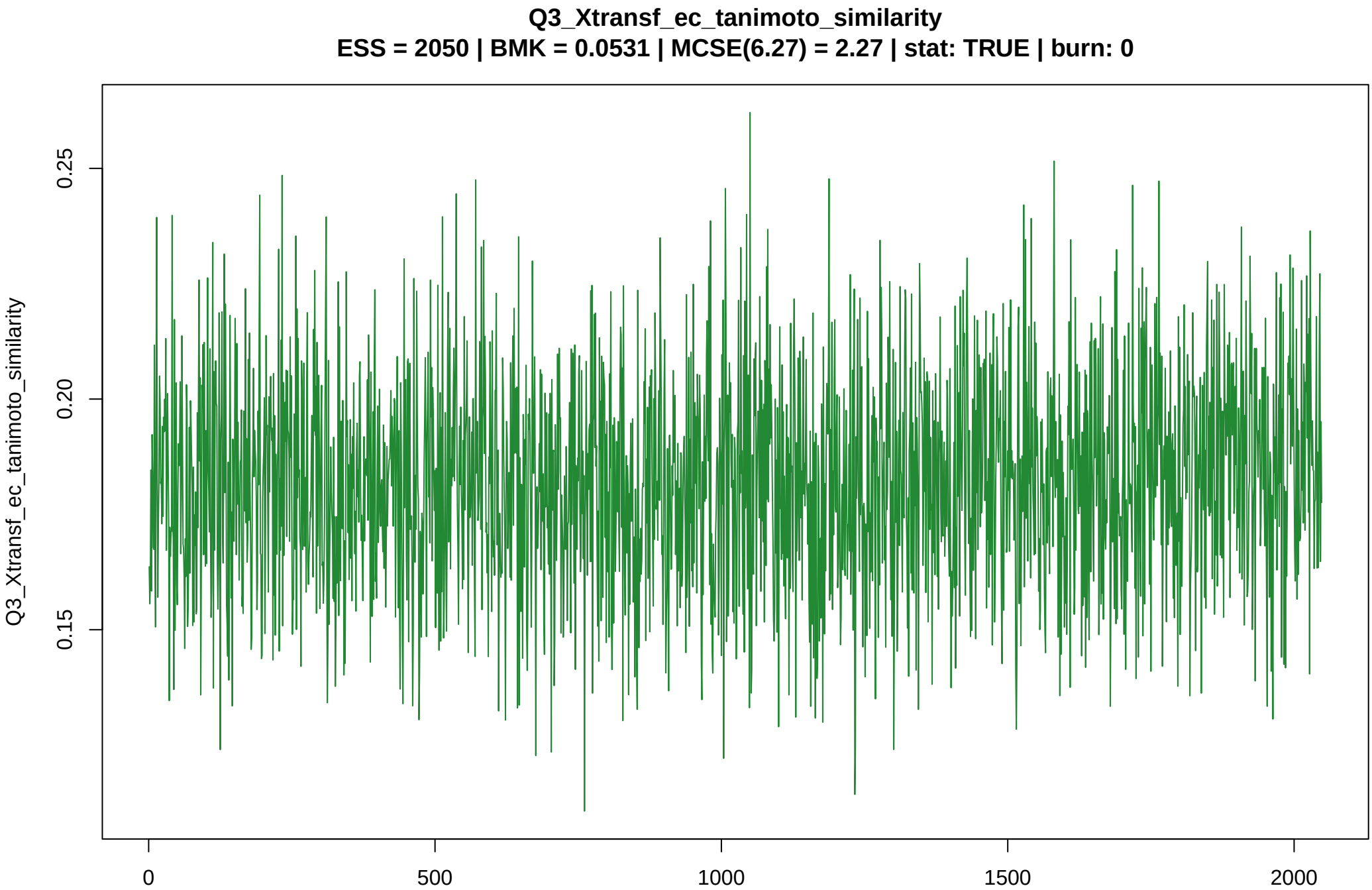

Q1_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 1428
Q1_template_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

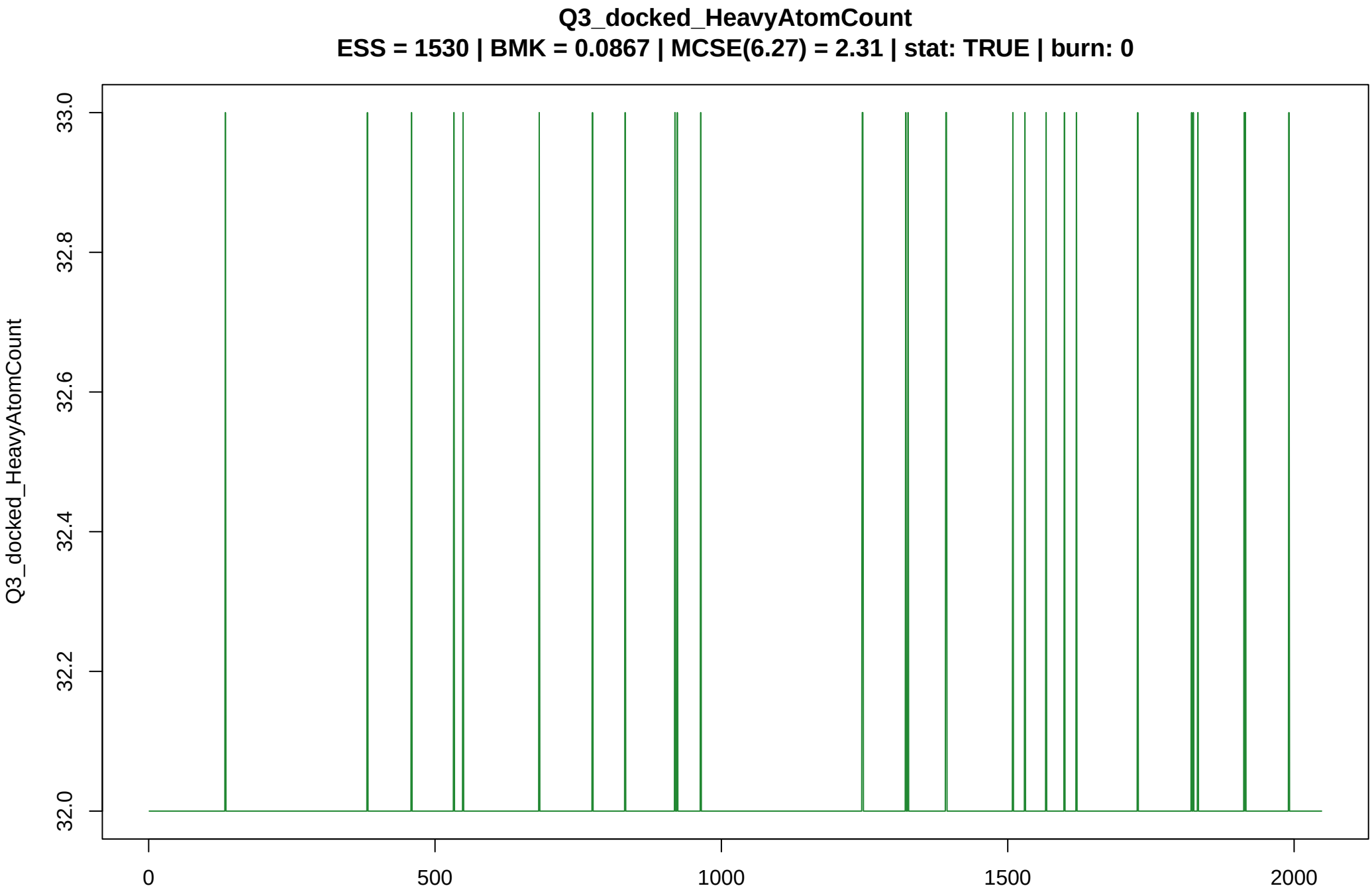

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

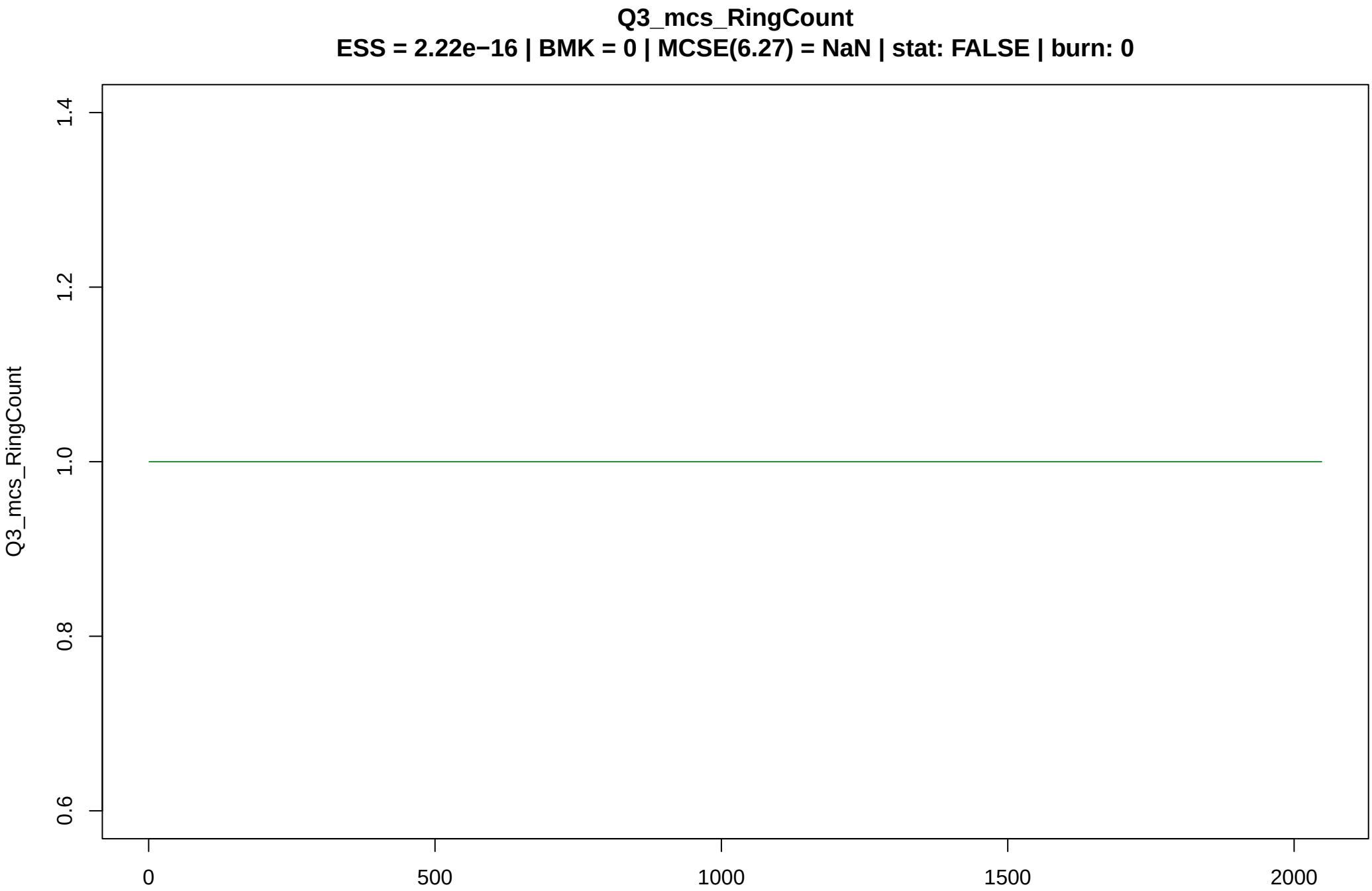

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

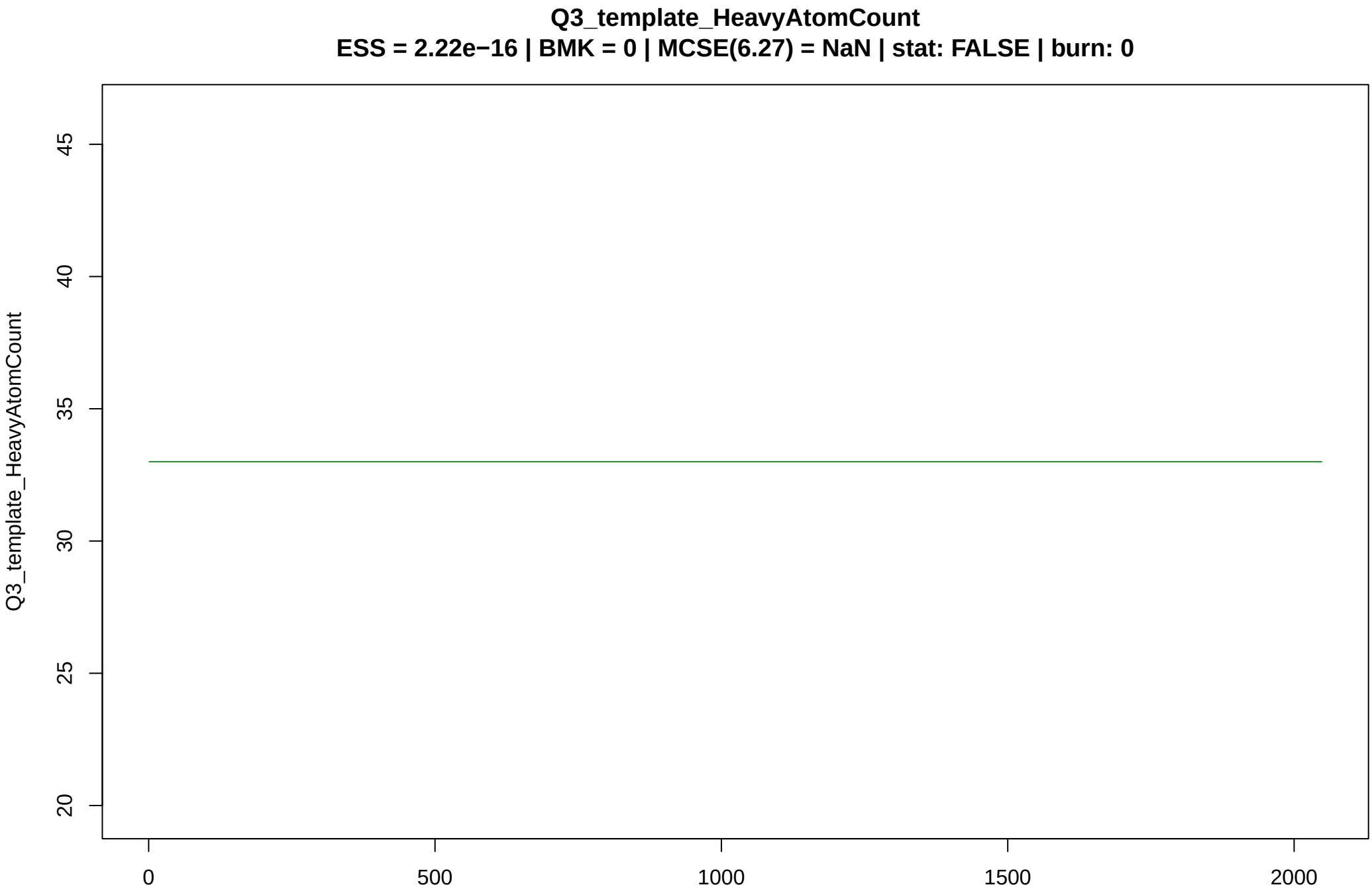

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

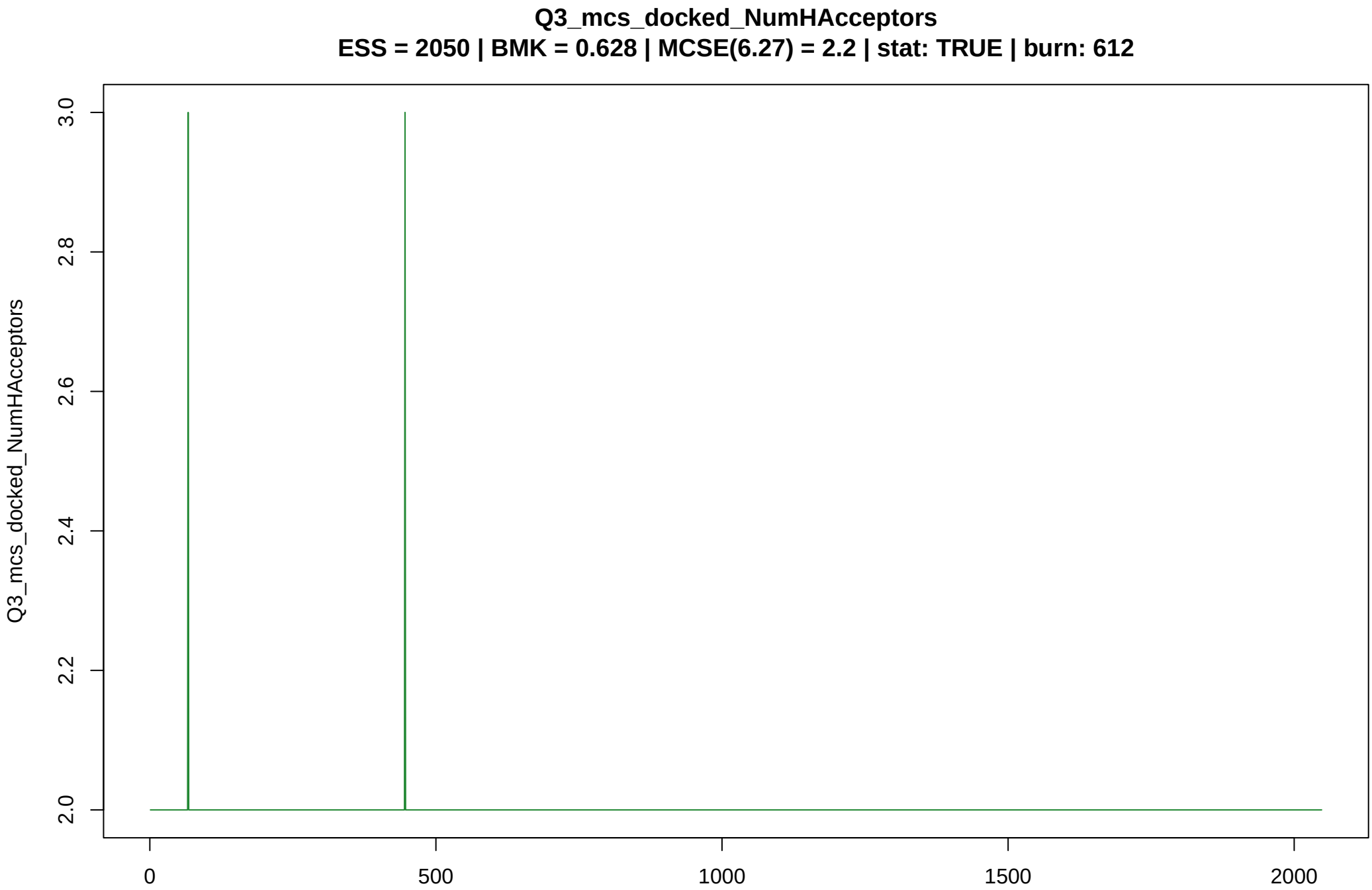

Q3_log_RMSD
ESS = 1580 | BMK = 0.0781 | MCSE(6.27) = 2.66 | stat: FALSE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
0
500
1000
1500
2000

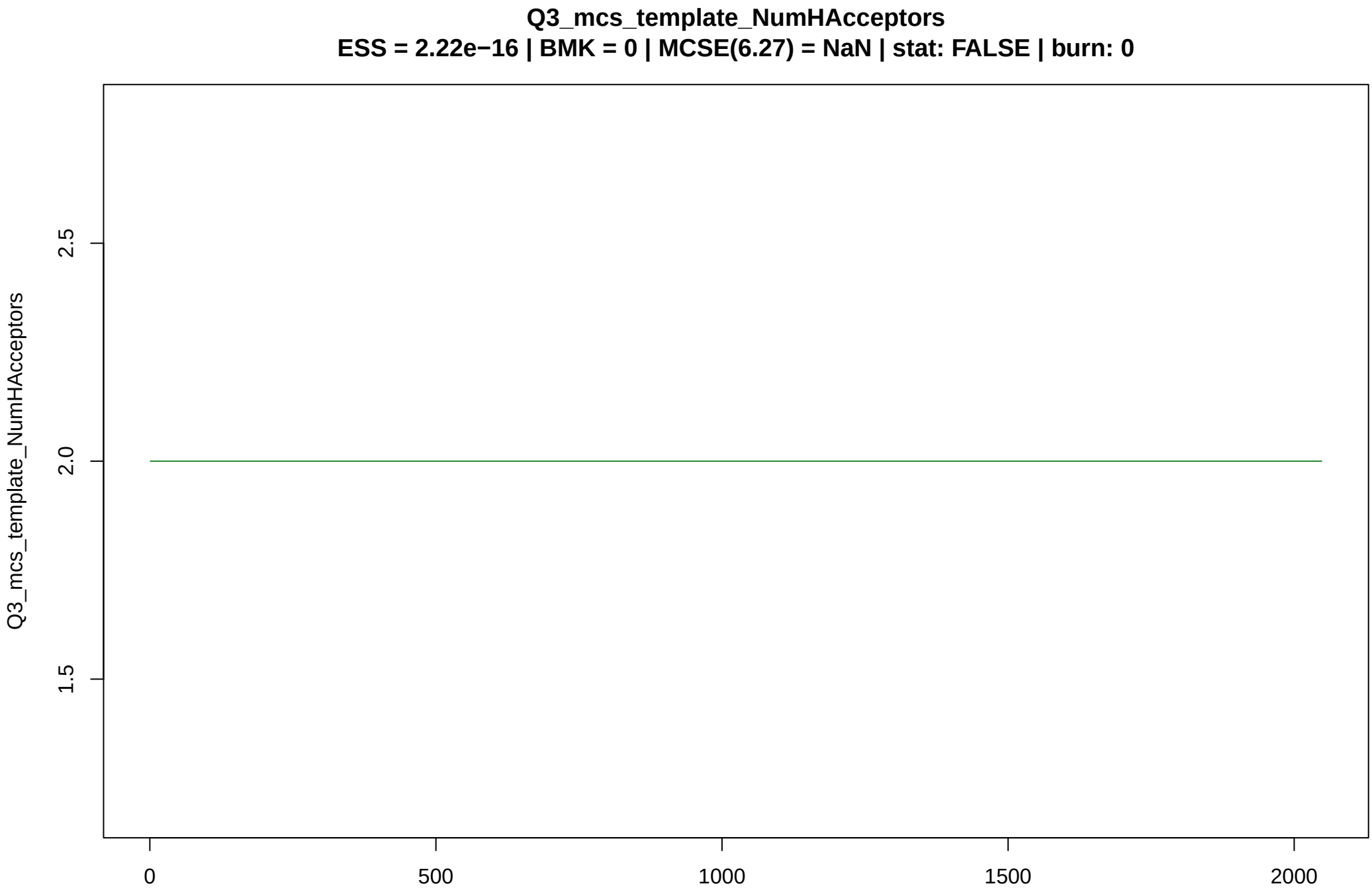

Q3_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0531 | MCSE(6.27) = 2.27 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.15
0.20
0.25
0
500
1000
1500
2000

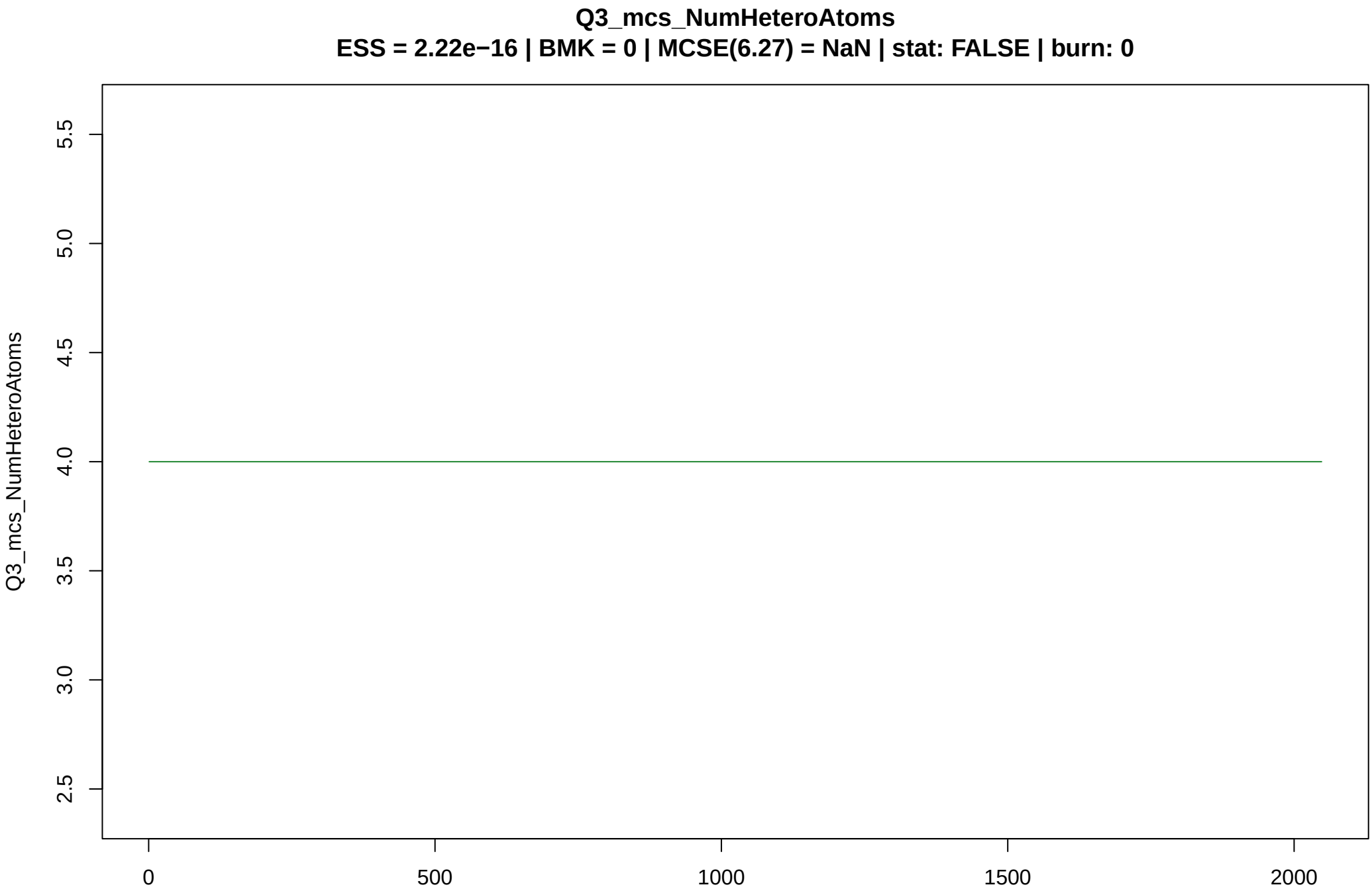

Q3_docked_HeavyAtomCount
ESS = 1530 | BMK = 0.0867 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

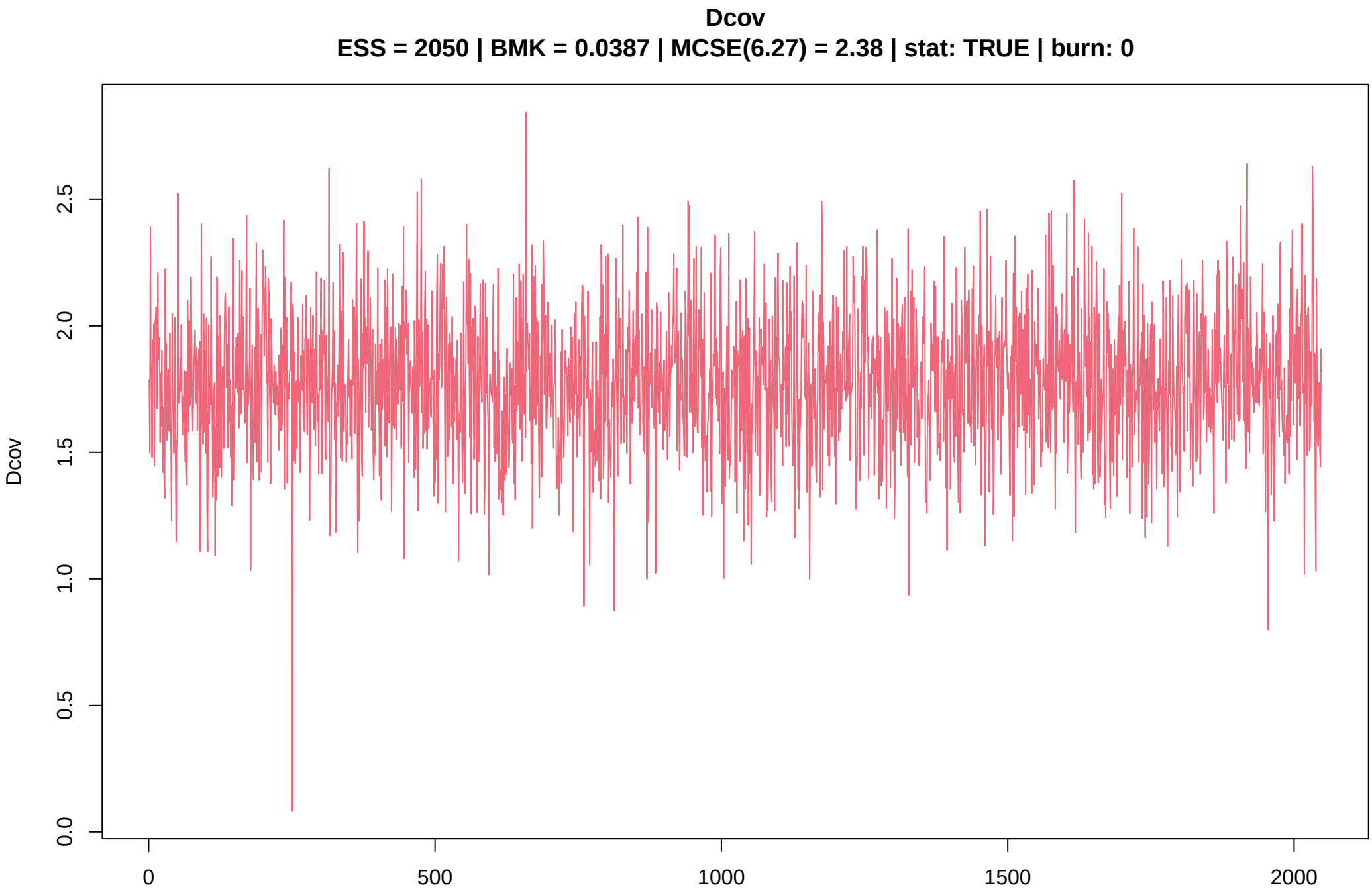

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

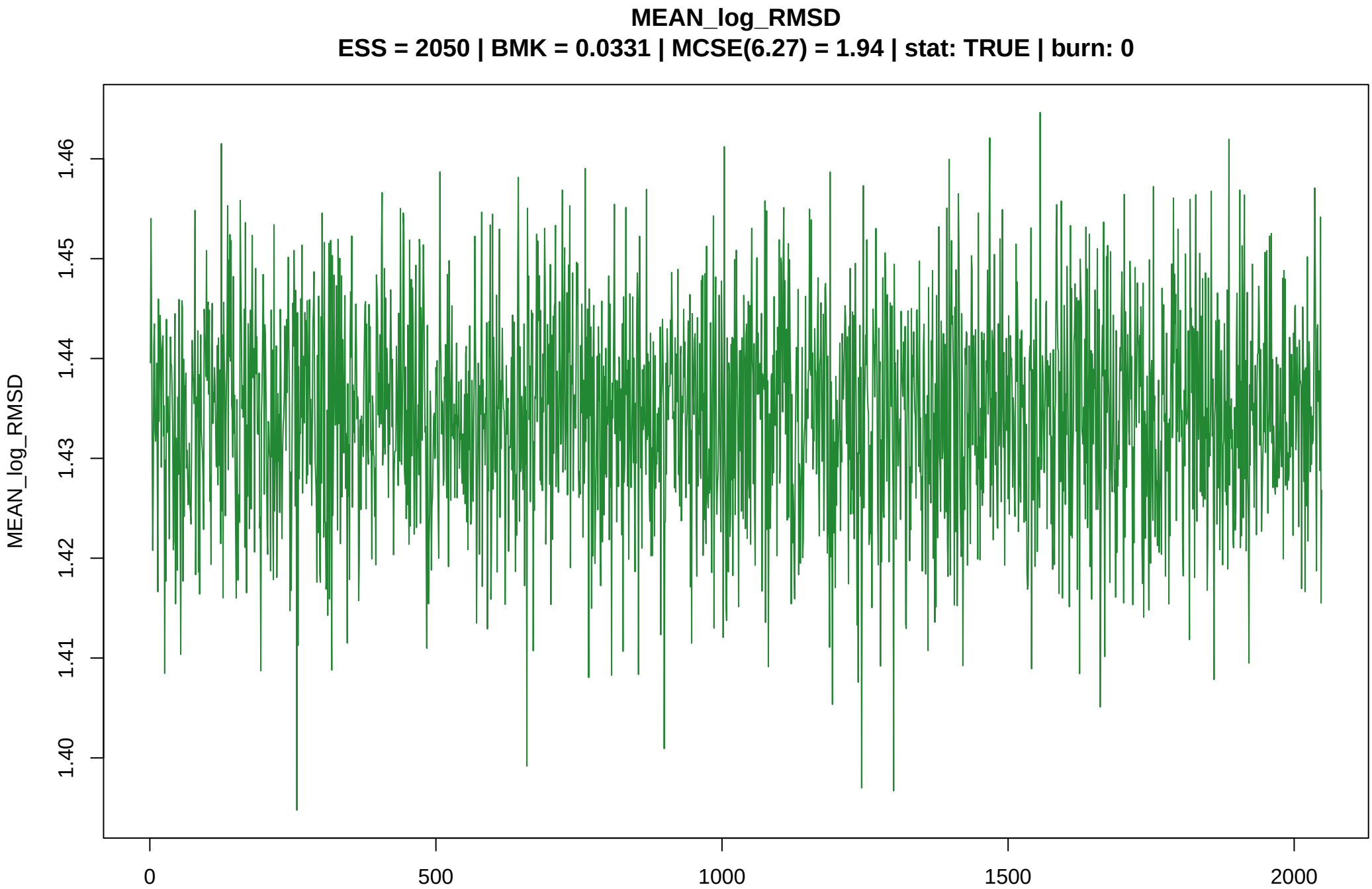

Q3_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_template_HeavyAtomCount
20
25
30
35
40
45
0
500
1000
1500
2000

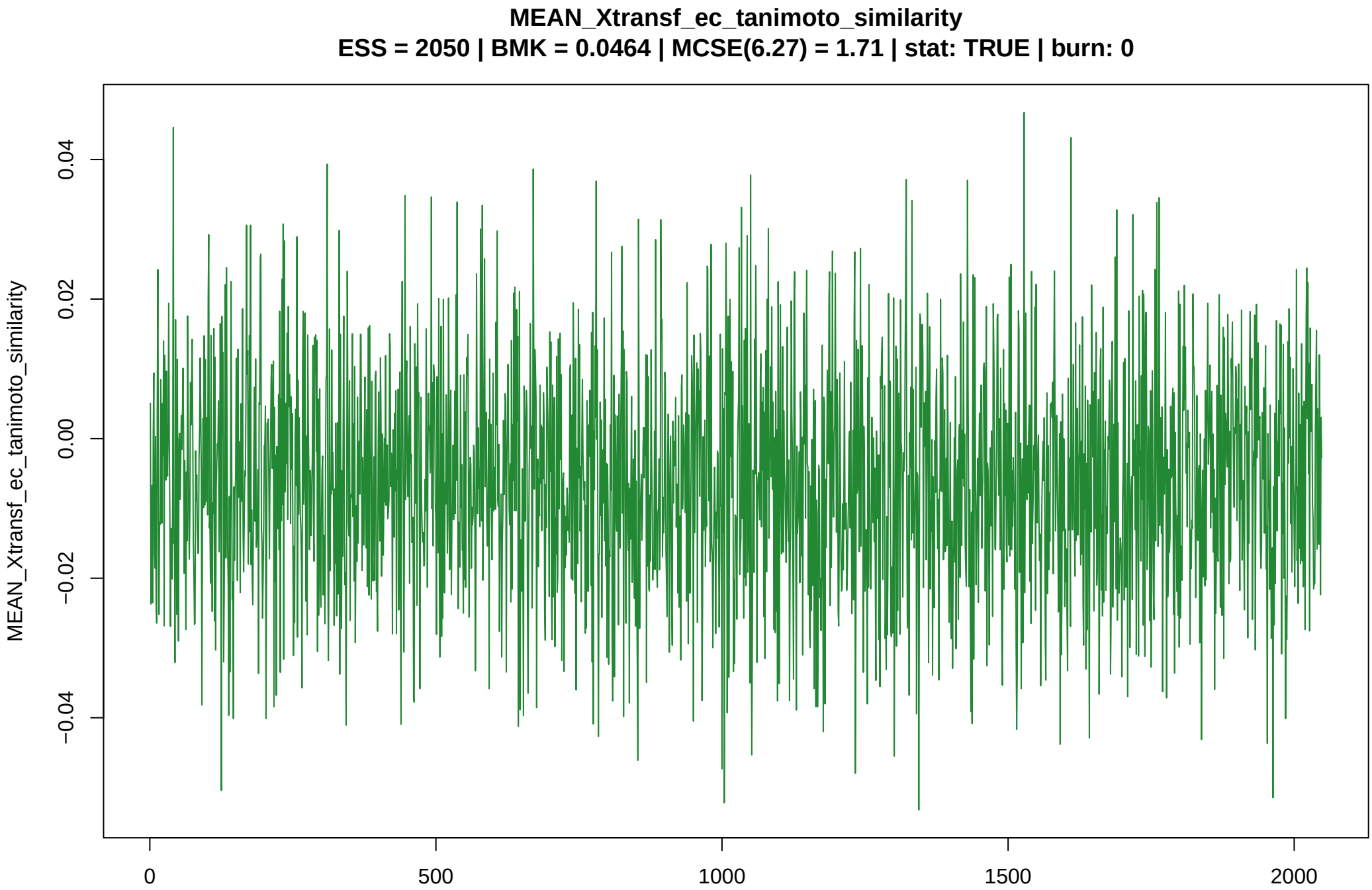

Q3_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.628 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 612
Q3_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

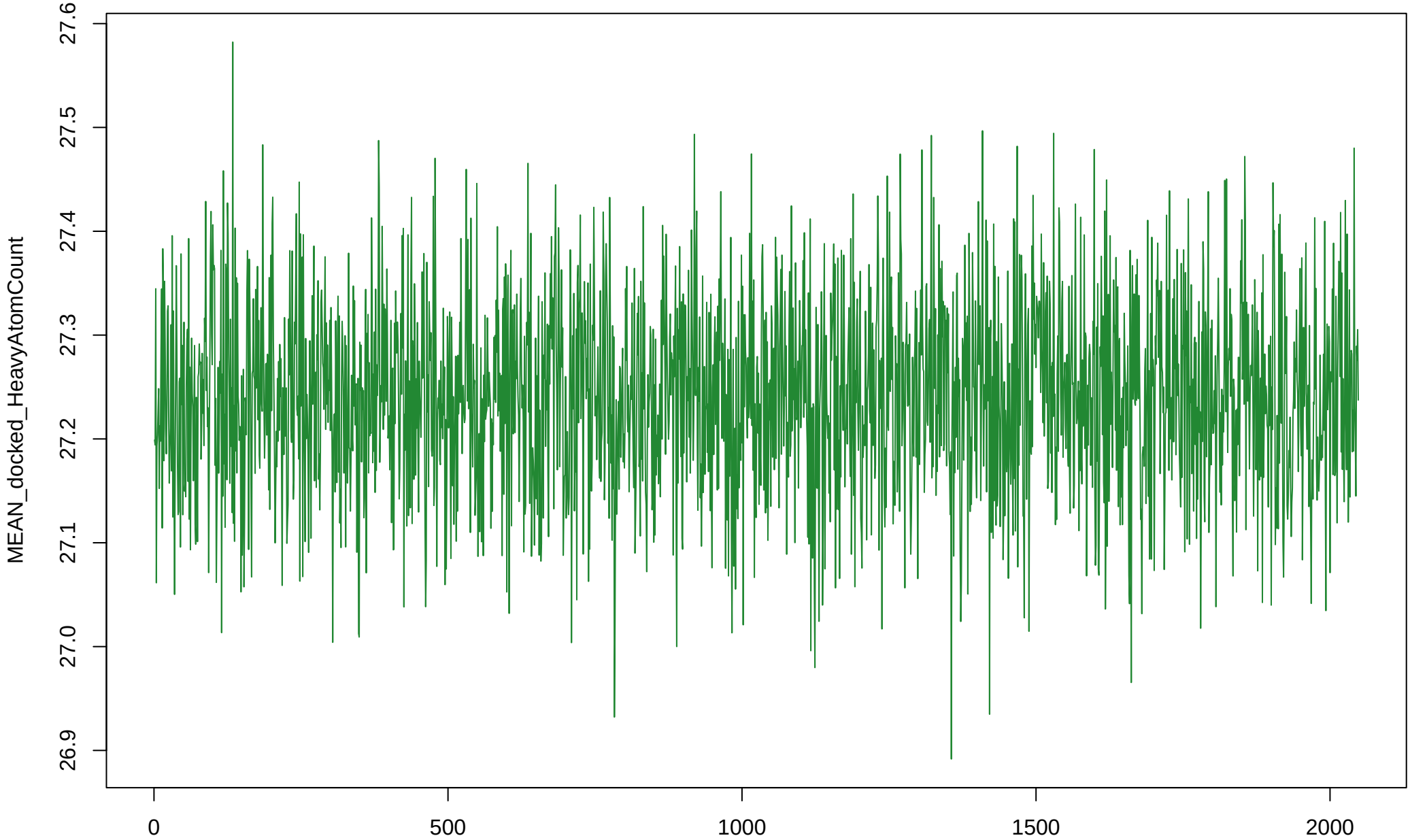

Q3_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_template_NumHAcceptors
2.5
2.0
1.5
0
500
1000
1500
2000

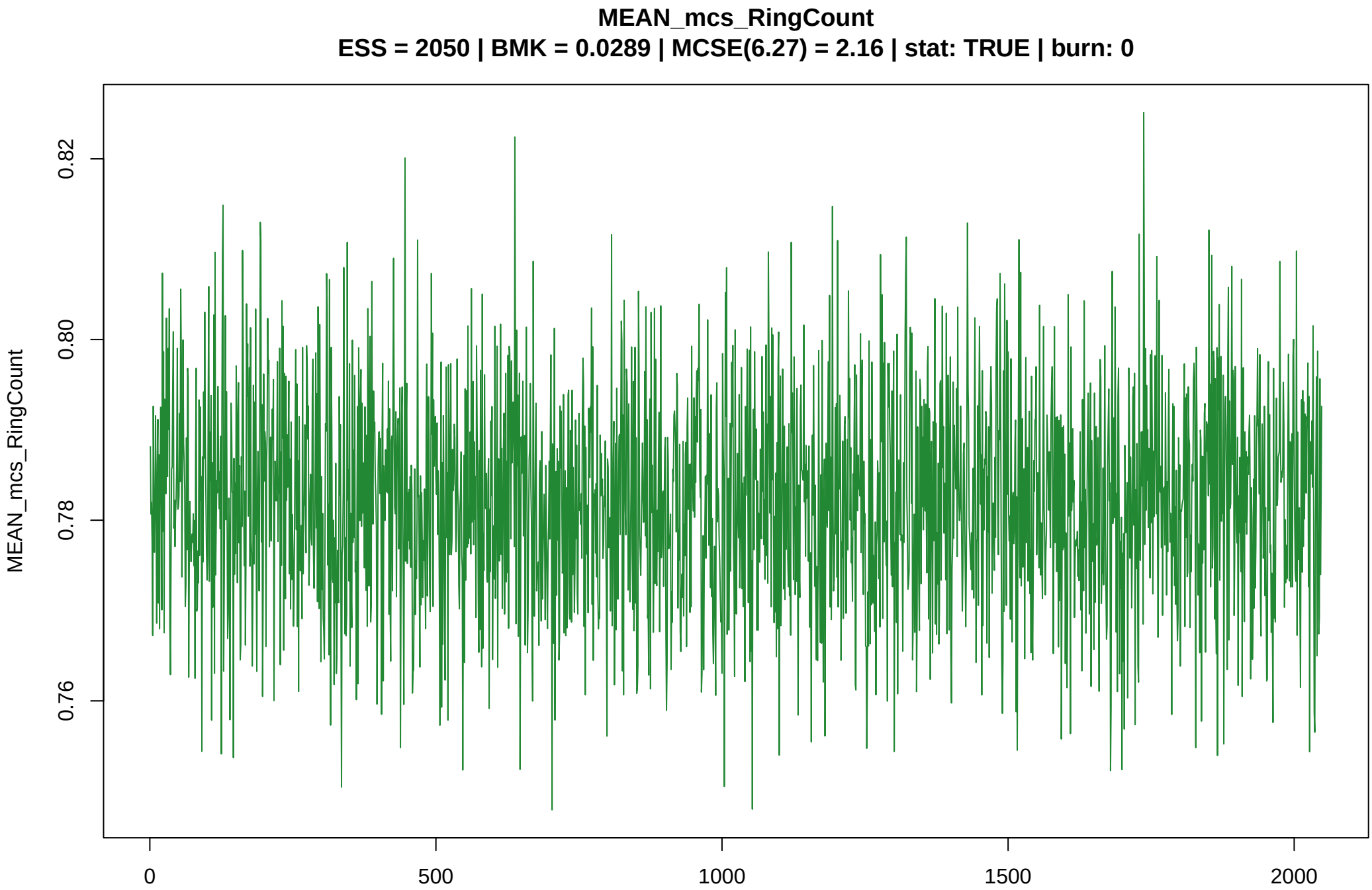

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

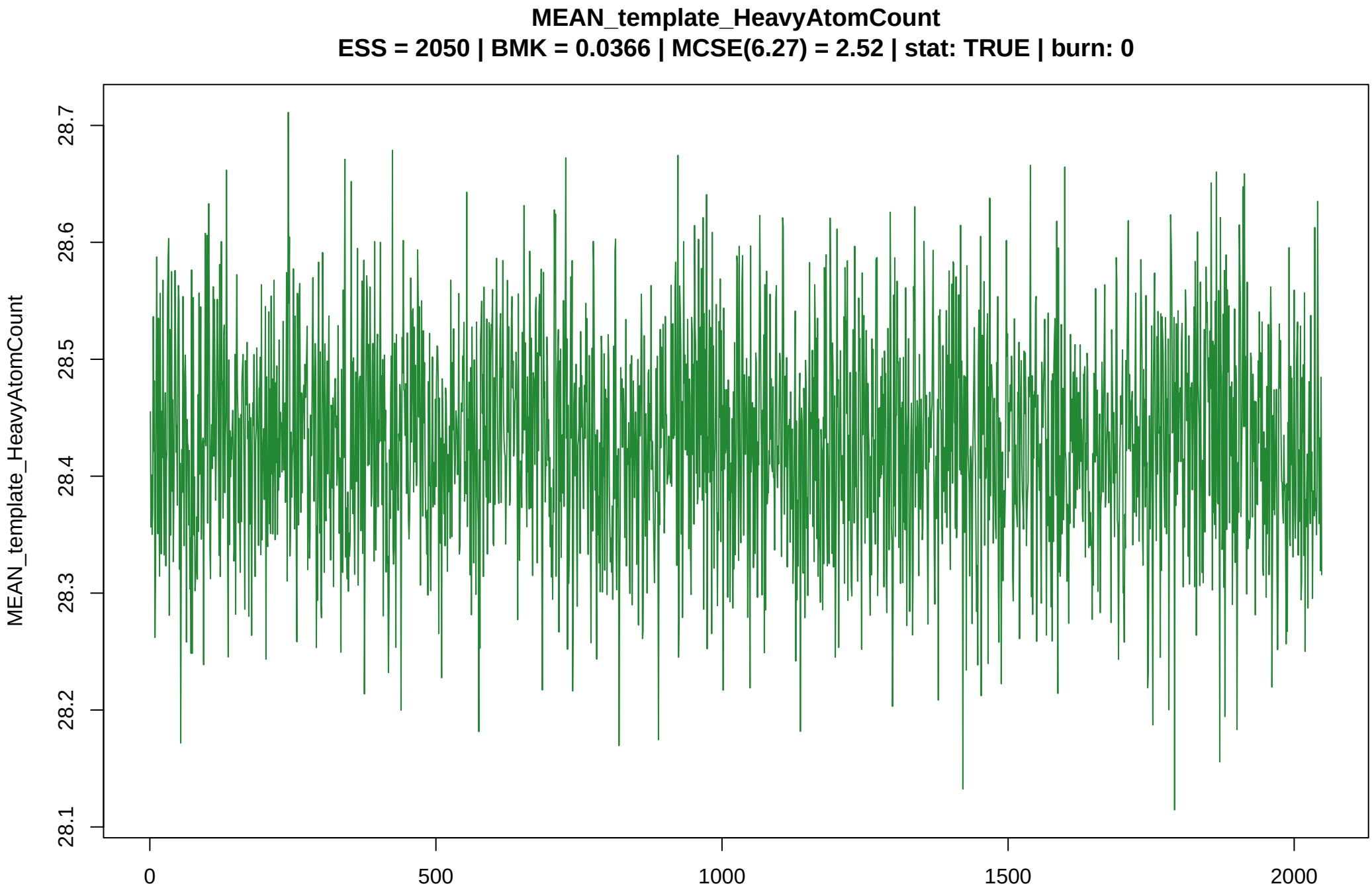

Dcov
ESS = 2050 | BMK = 0.0387 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
Dcov
0.0
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000

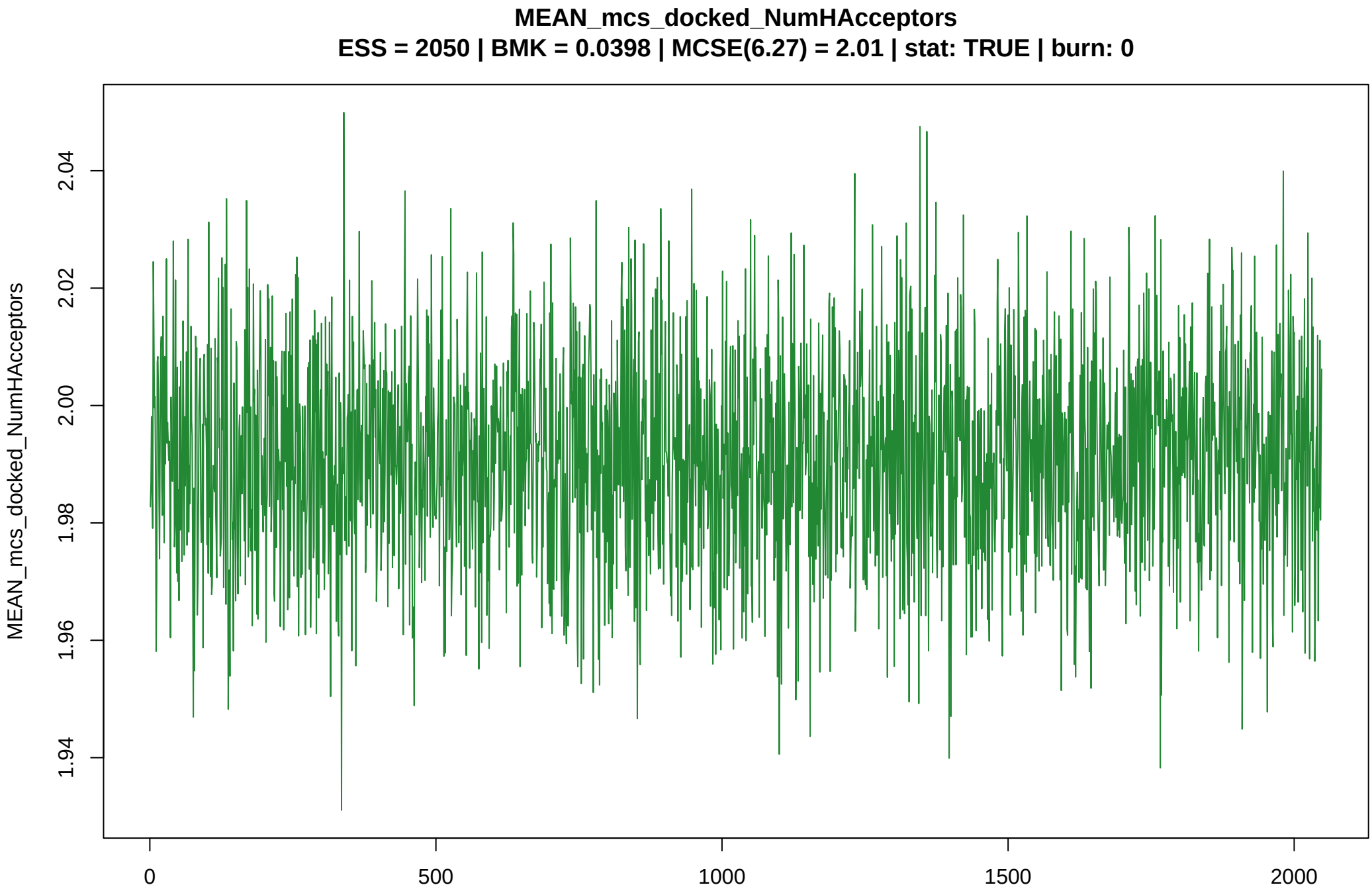

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0331 | MCSE(6.27) = 1.94 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.40
1.41
1.42
1.43
1.44
1.45
1.46
0
500
1000
1500
2000

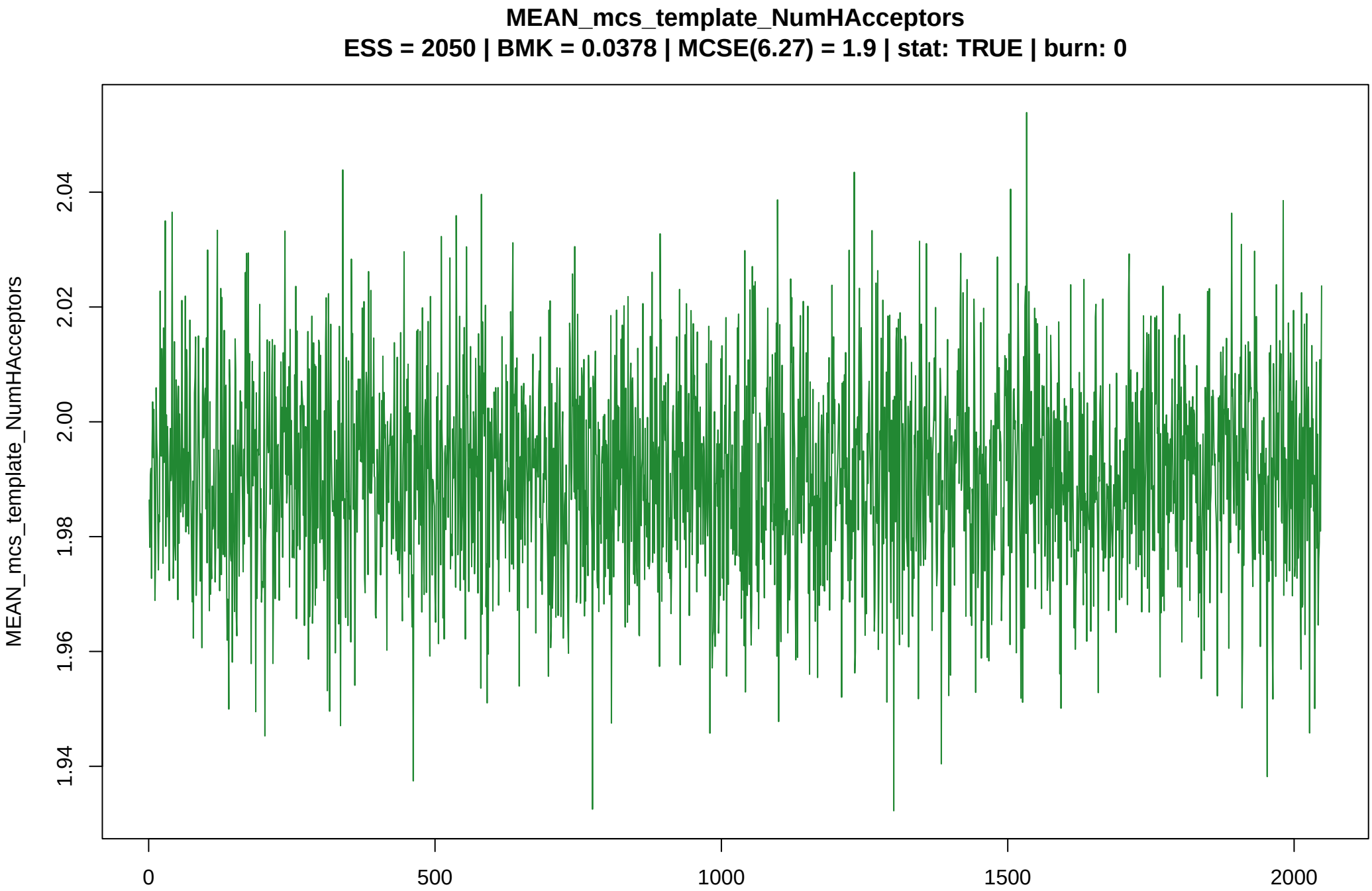

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0464 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
0
500
1000
1500
2000

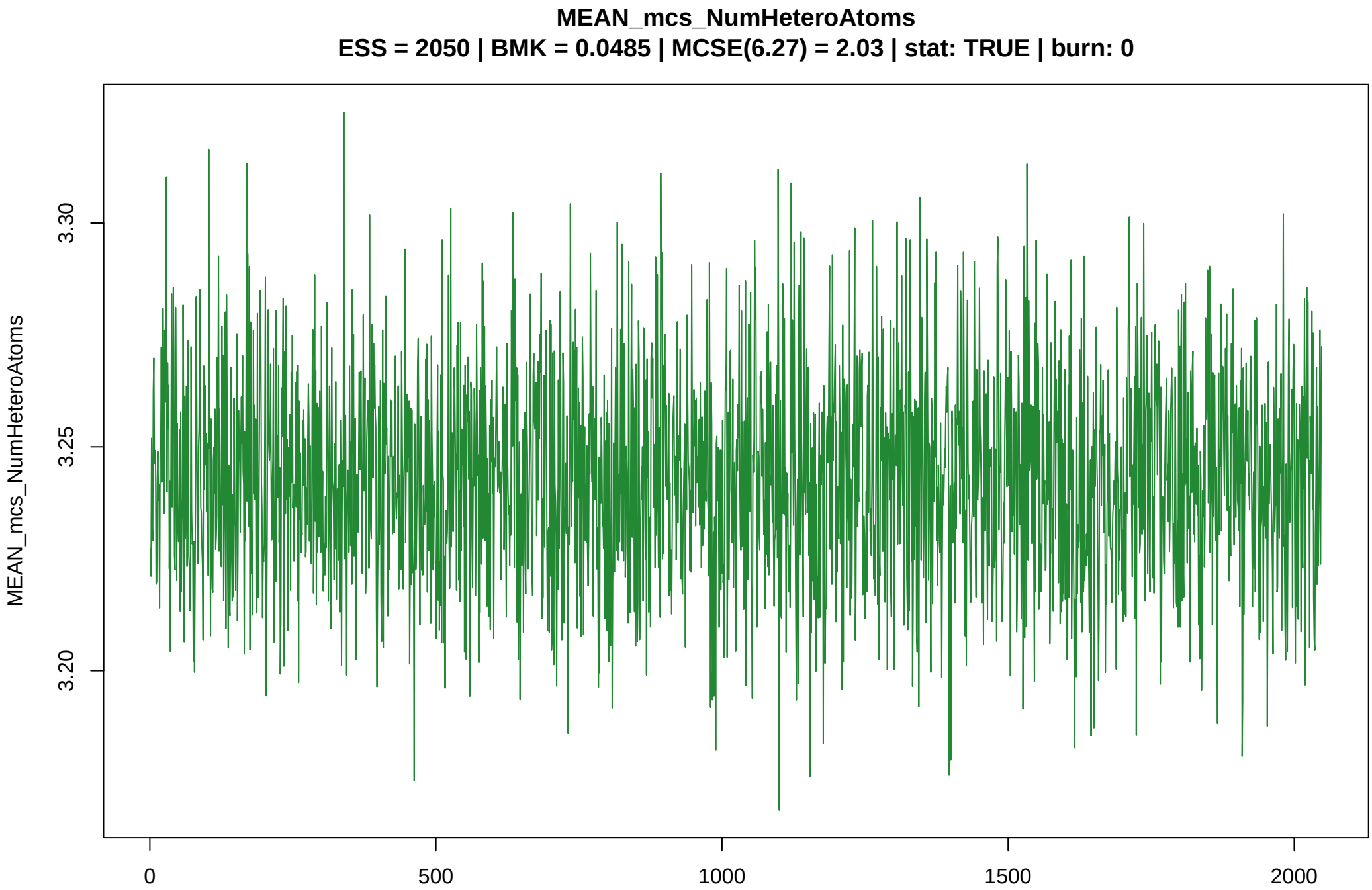

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0345 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
26.9
27.0
27.1
27.2
27.3
27.4
27.5
27.6
0
500
1000
1500
2000

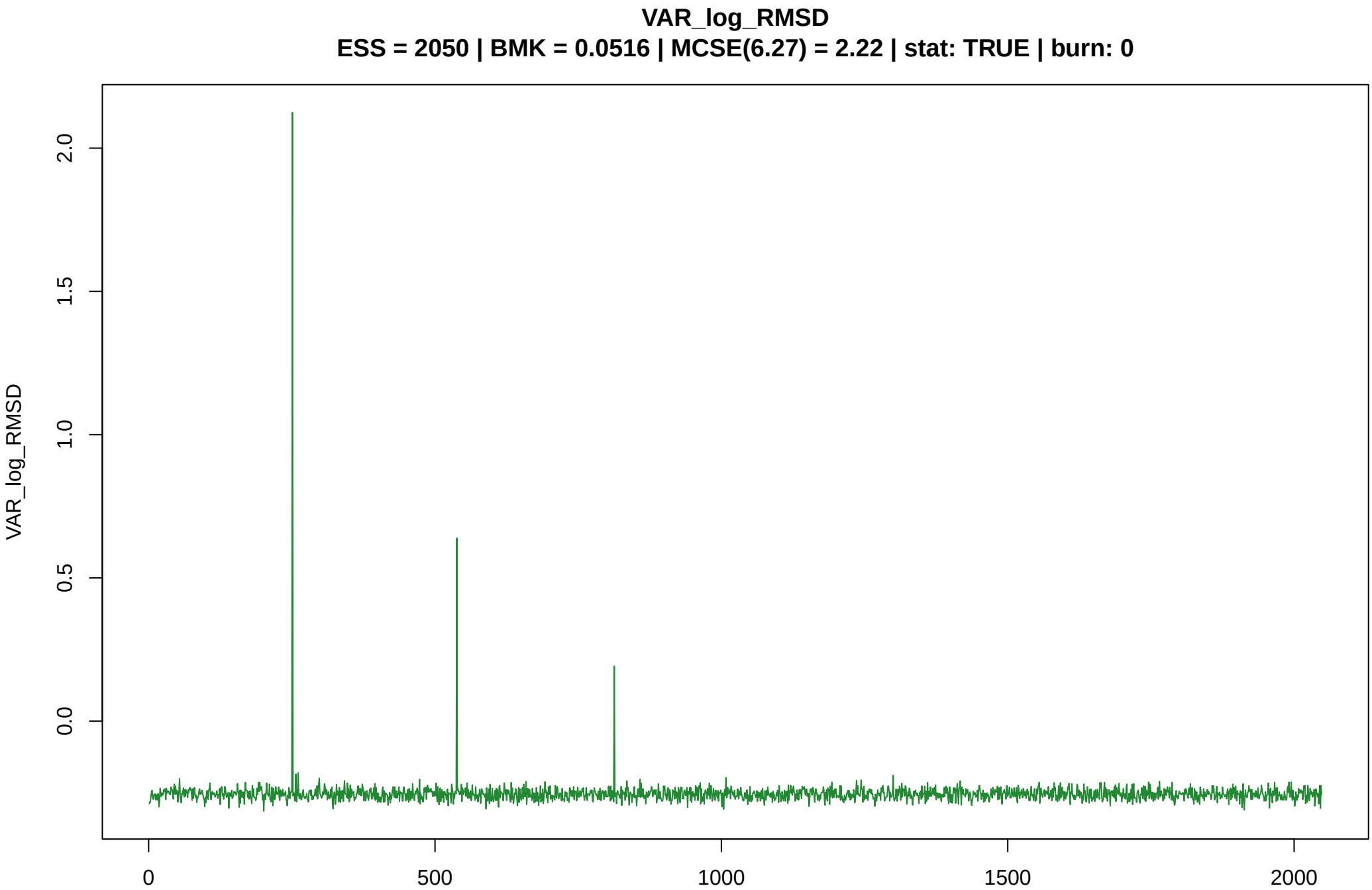

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0289 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

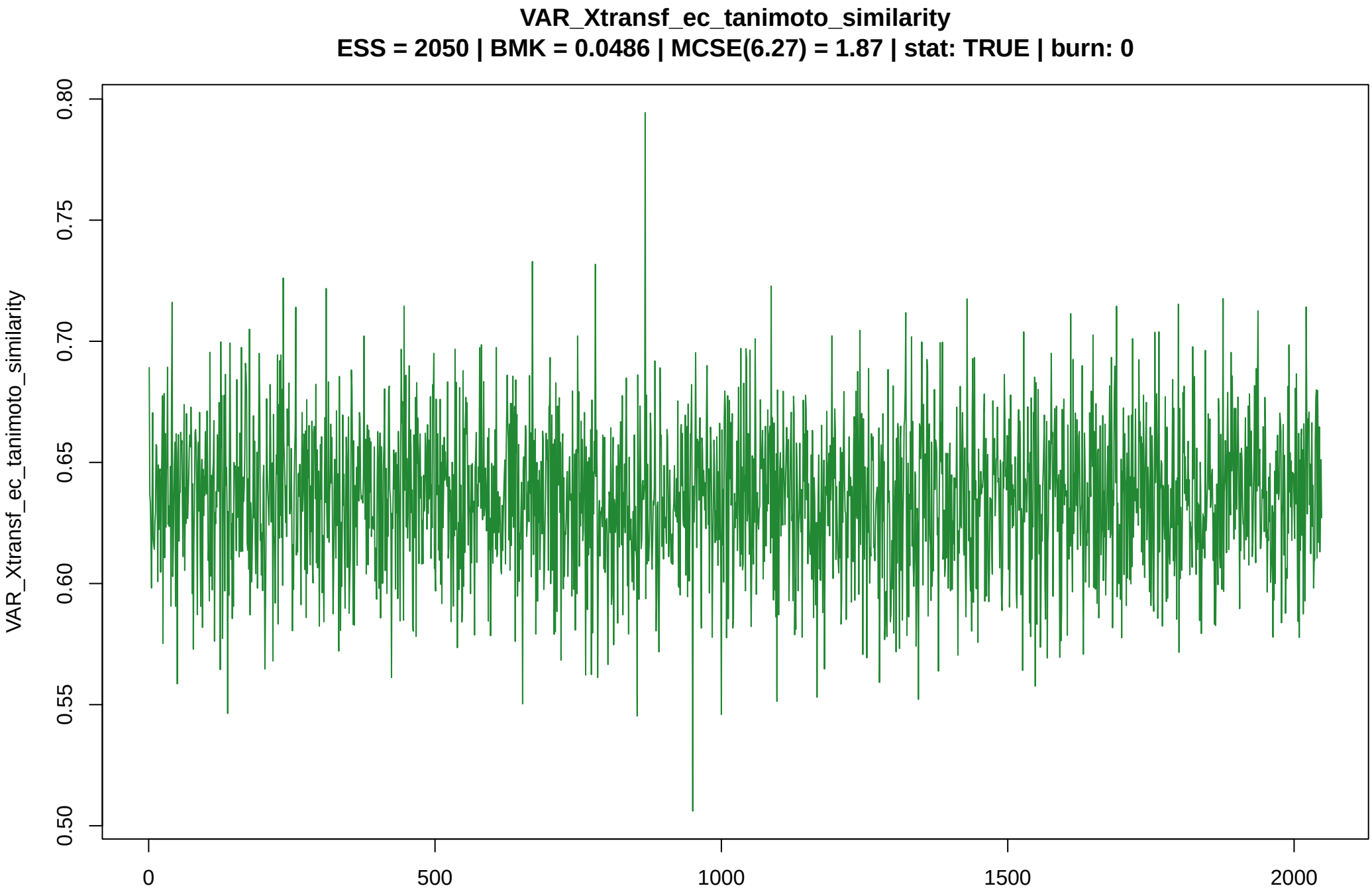

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0366 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
28.1
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

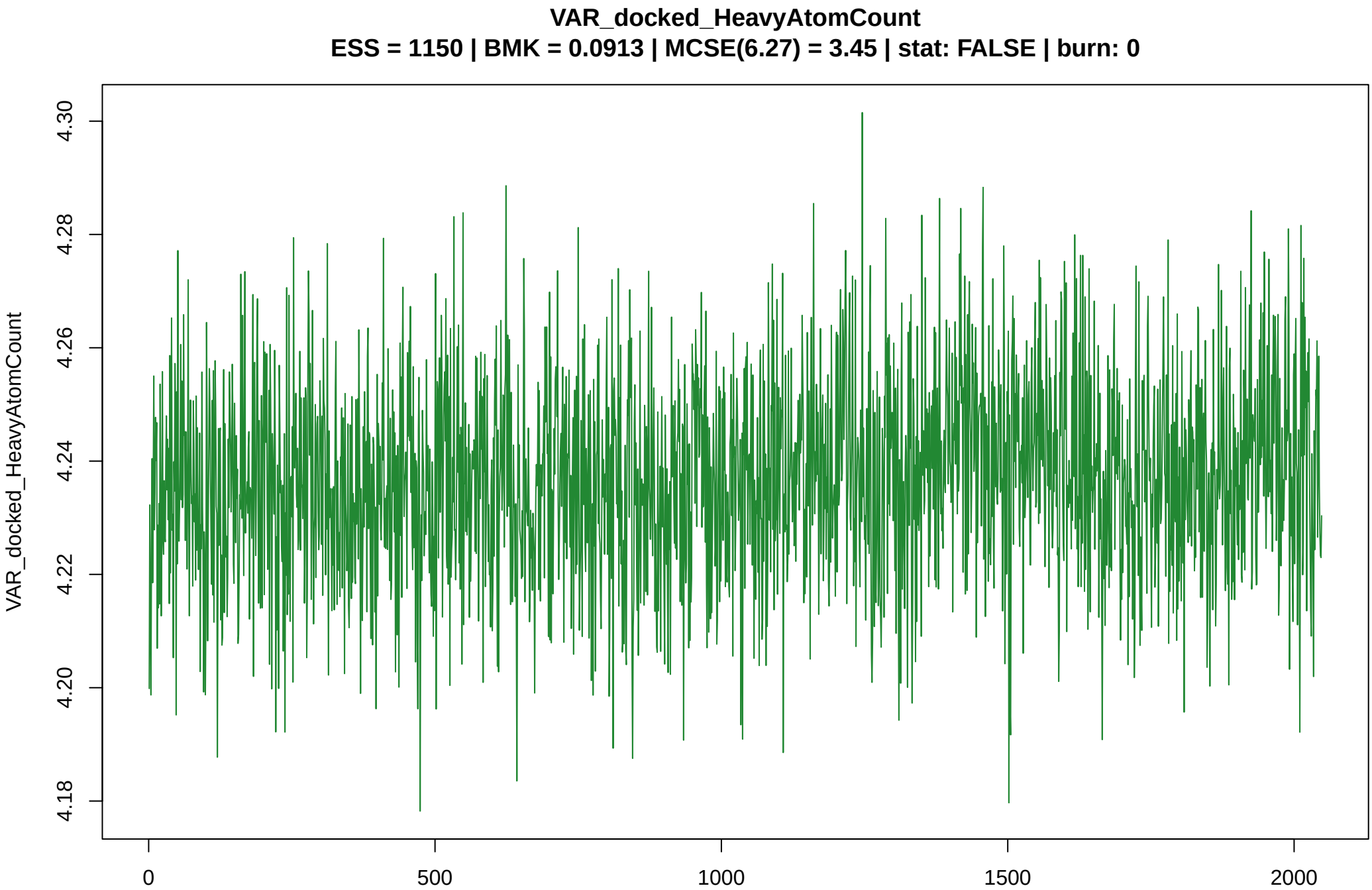

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0398 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

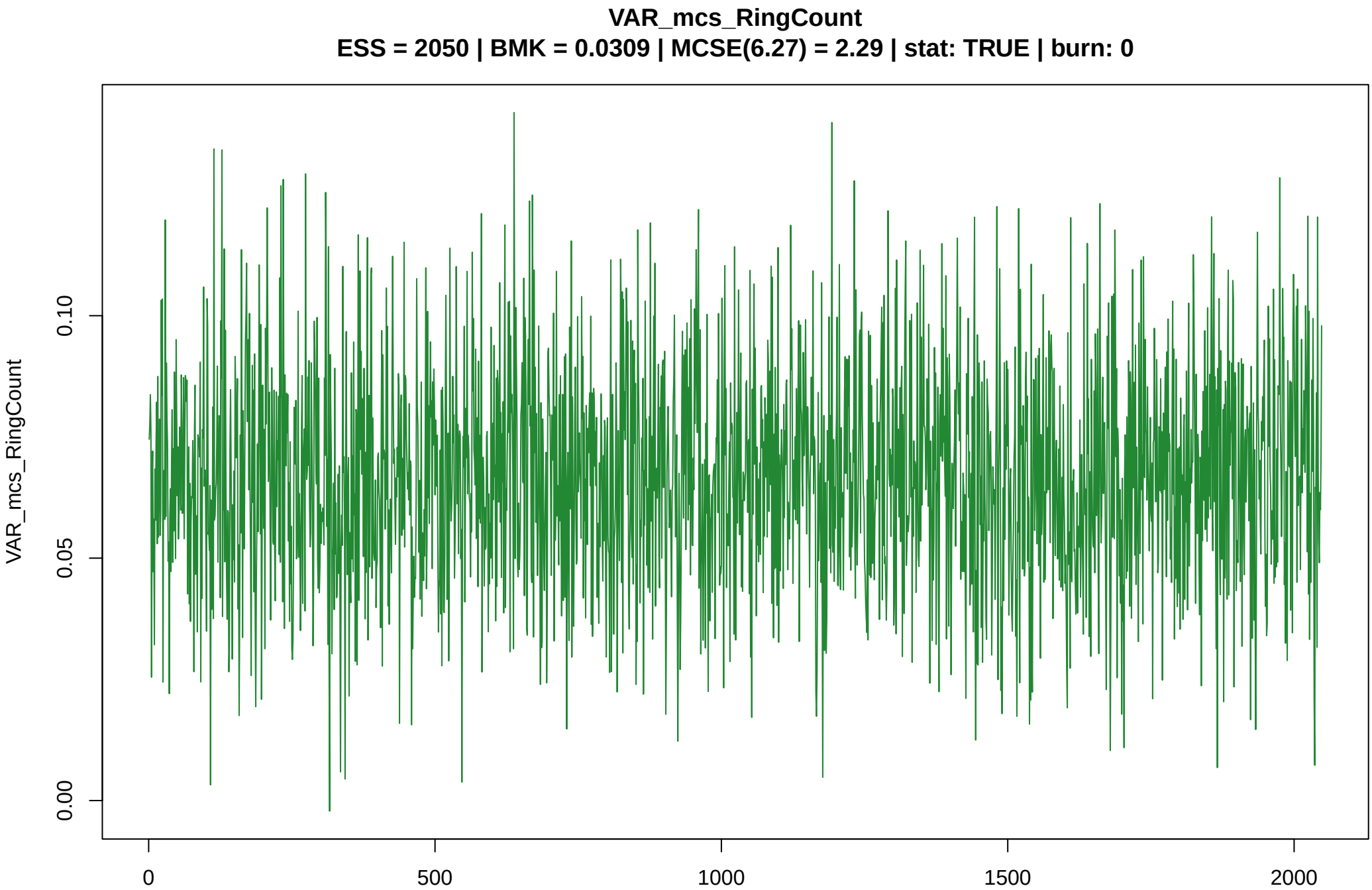

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0378 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

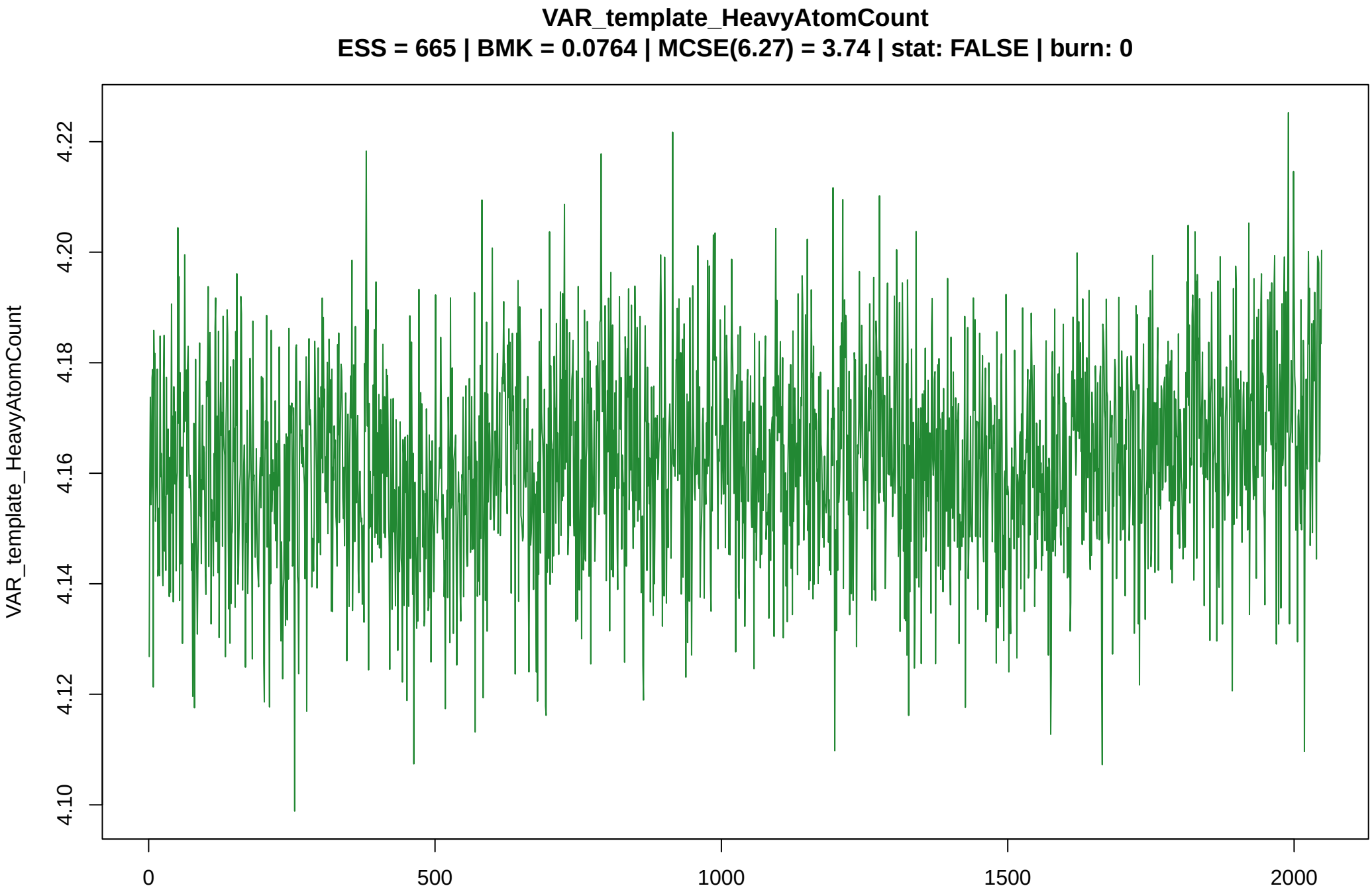

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0485 | MCSE(6.27) = 2.03 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.20
3.25
3.30
0
500
1000
1500
2000

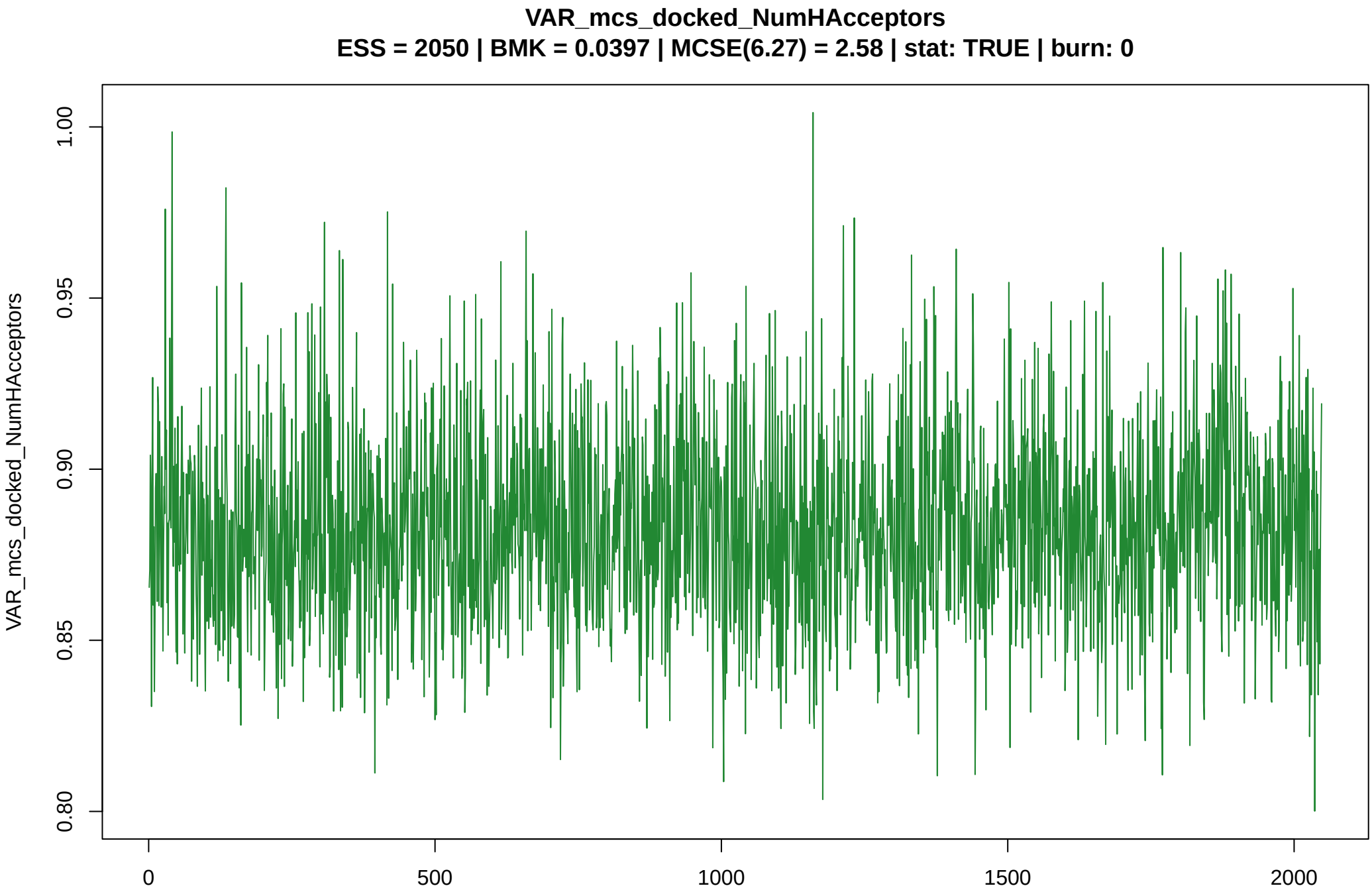

VAR_log_RMSD
ESS = 2050 | BMK = 0.0516 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
VAR_log_RMSD
0.0
0.5
1.0
1.5
2.0
0
500
1000
1500
2000

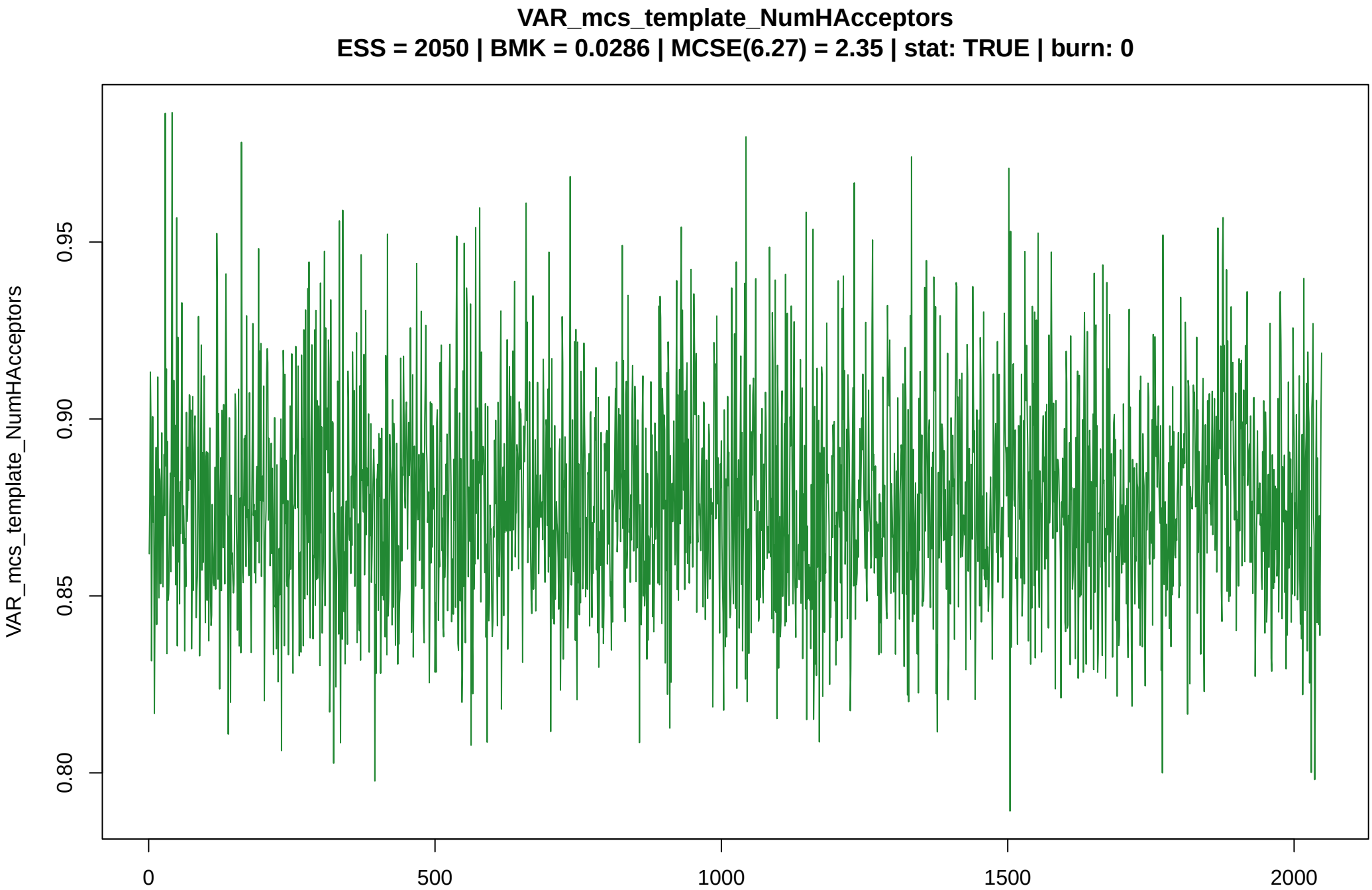

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0486 | MCSE(6.27) = 1.87 | stat: TRUE | burn: 0
VAR_Xtransf_ec_tanimoto_similarity
0.50
0.55
0.60
0.65
0.70
0.75
0.80
0
500
1000
1500
2000

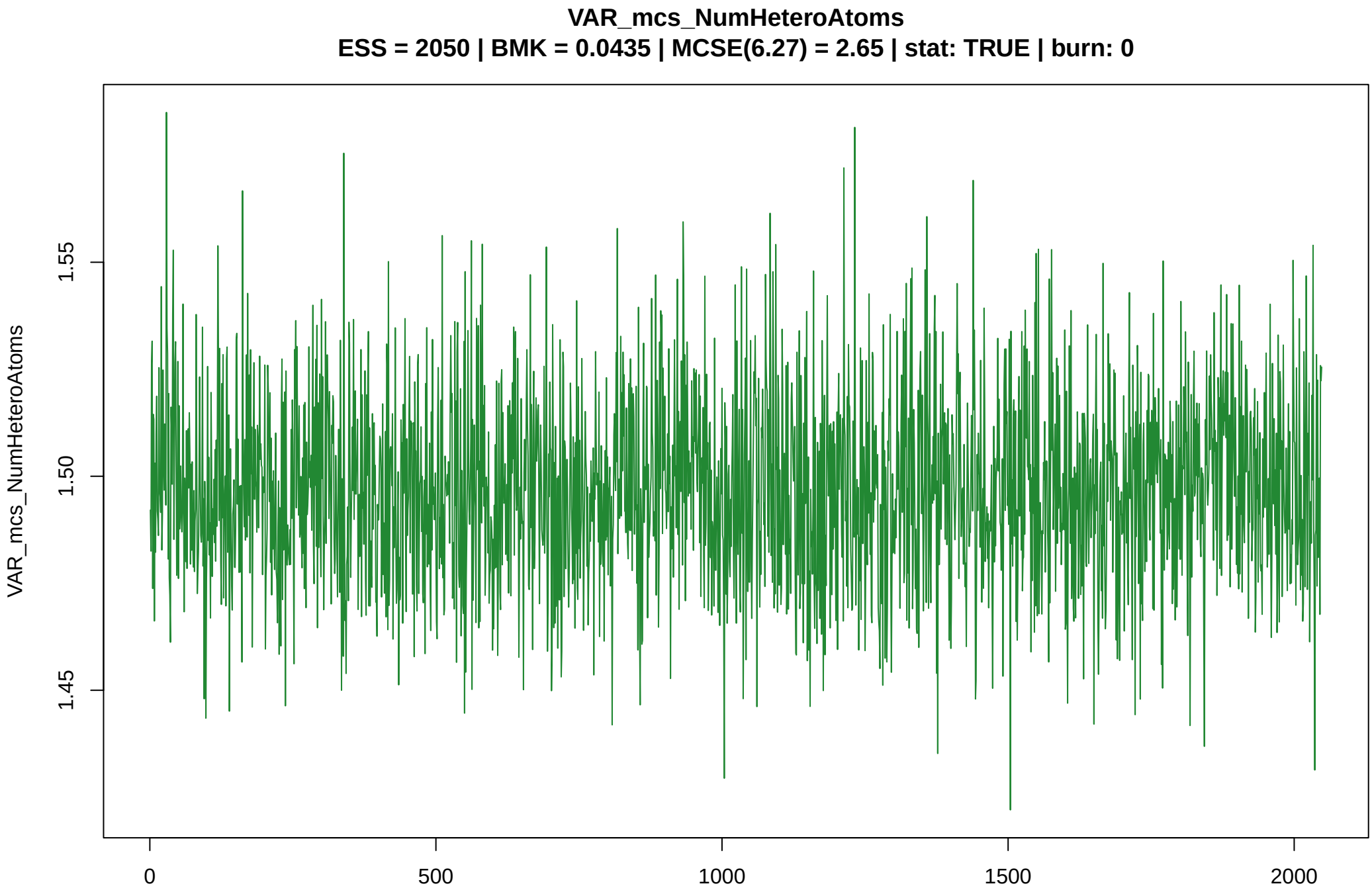

VAR_docked_HeavyAtomCount
ESS = 1150 | BMK = 0.0913 | MCSE(6.27) = 3.45 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
4.18
4.20
4.22
4.24
4.26
4.28
4.30
0
500
1000
1500
2000

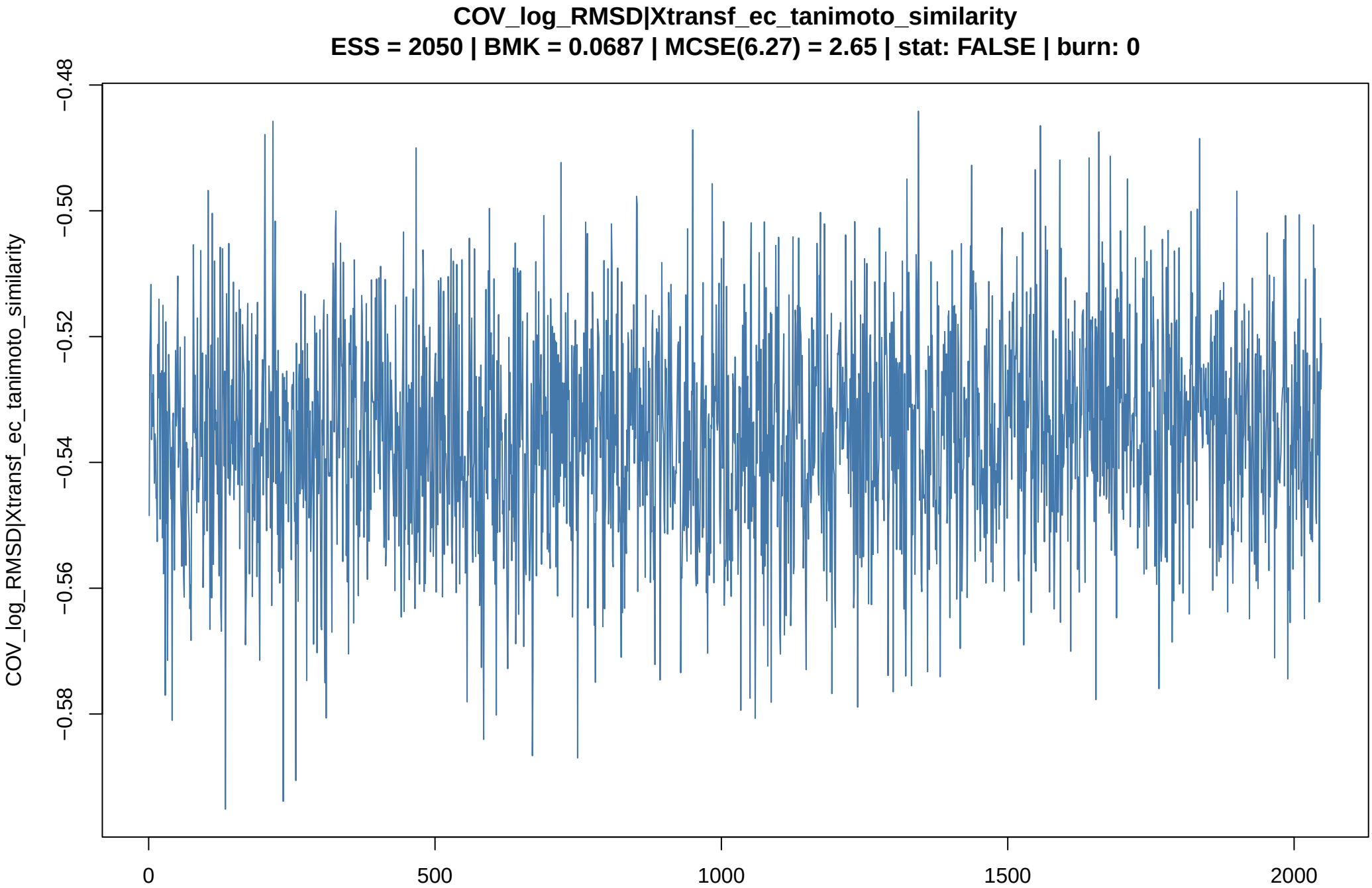

VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0309 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0
VAR_mcs_RingCount
0.00
0.05
0.10
0
500
1000
1500
2000

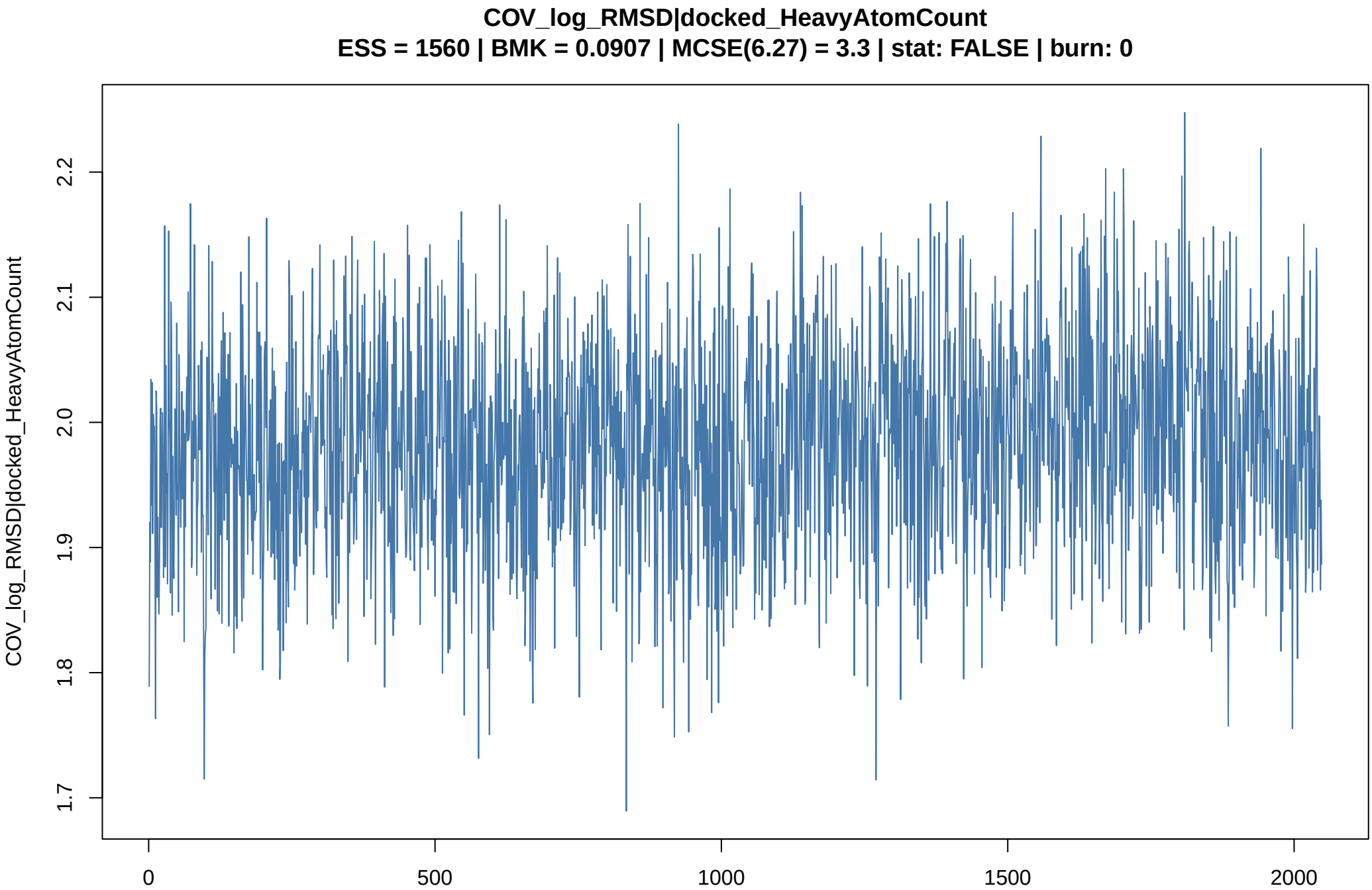

VAR_template_HeavyAtomCount
ESS = 665 | BMK = 0.0764 | MCSE(6.27) = 3.74 | stat: FALSE | burn: 0
VAR_template_HeavyAtomCount
4.10
4.12
4.14
4.16
4.18
4.20
4.22
0
500
1000
1500
2000

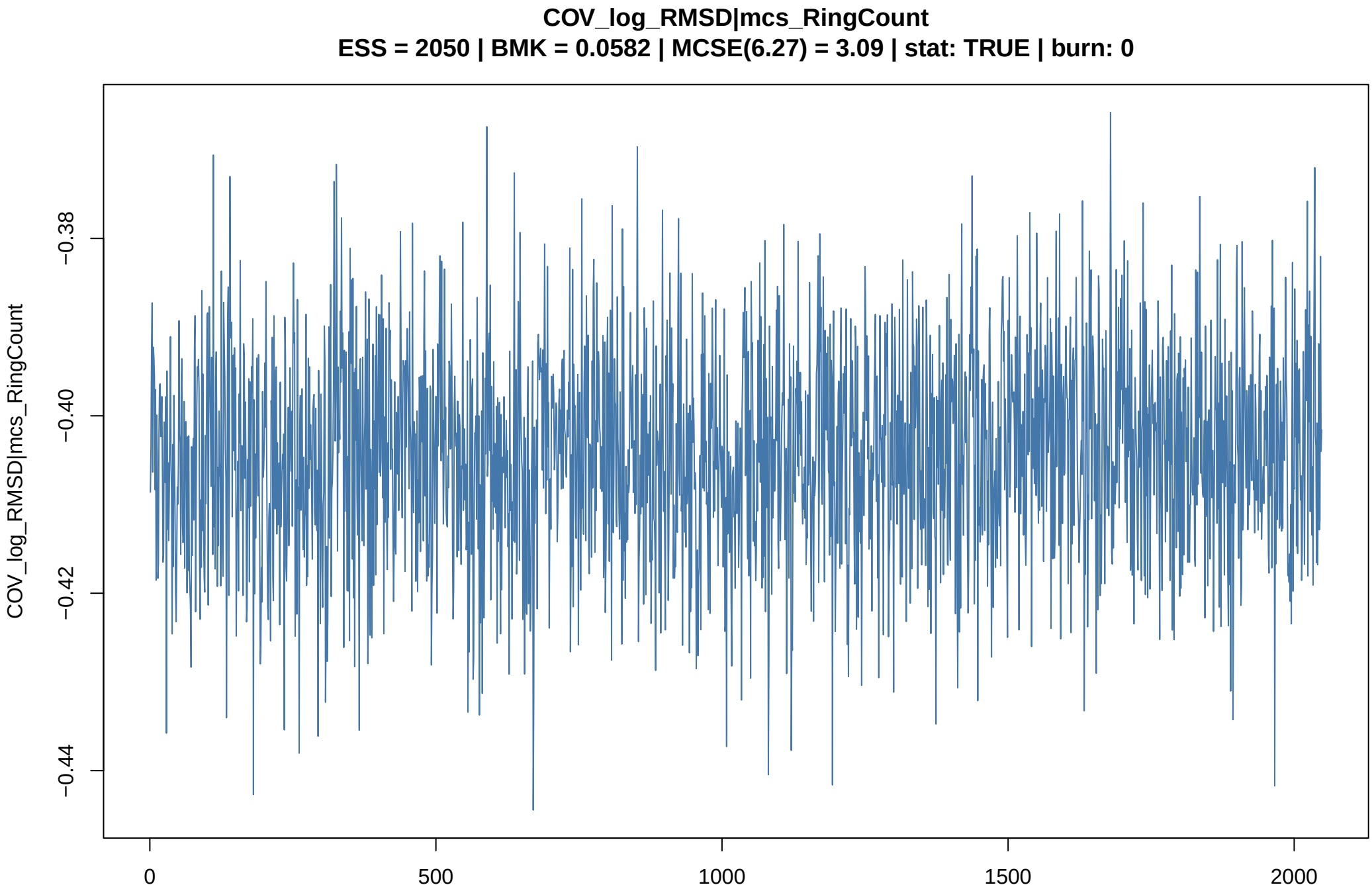

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0397 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
1.00
0.95
0.90
0.85
0.80
0
500
1000
1500
2000

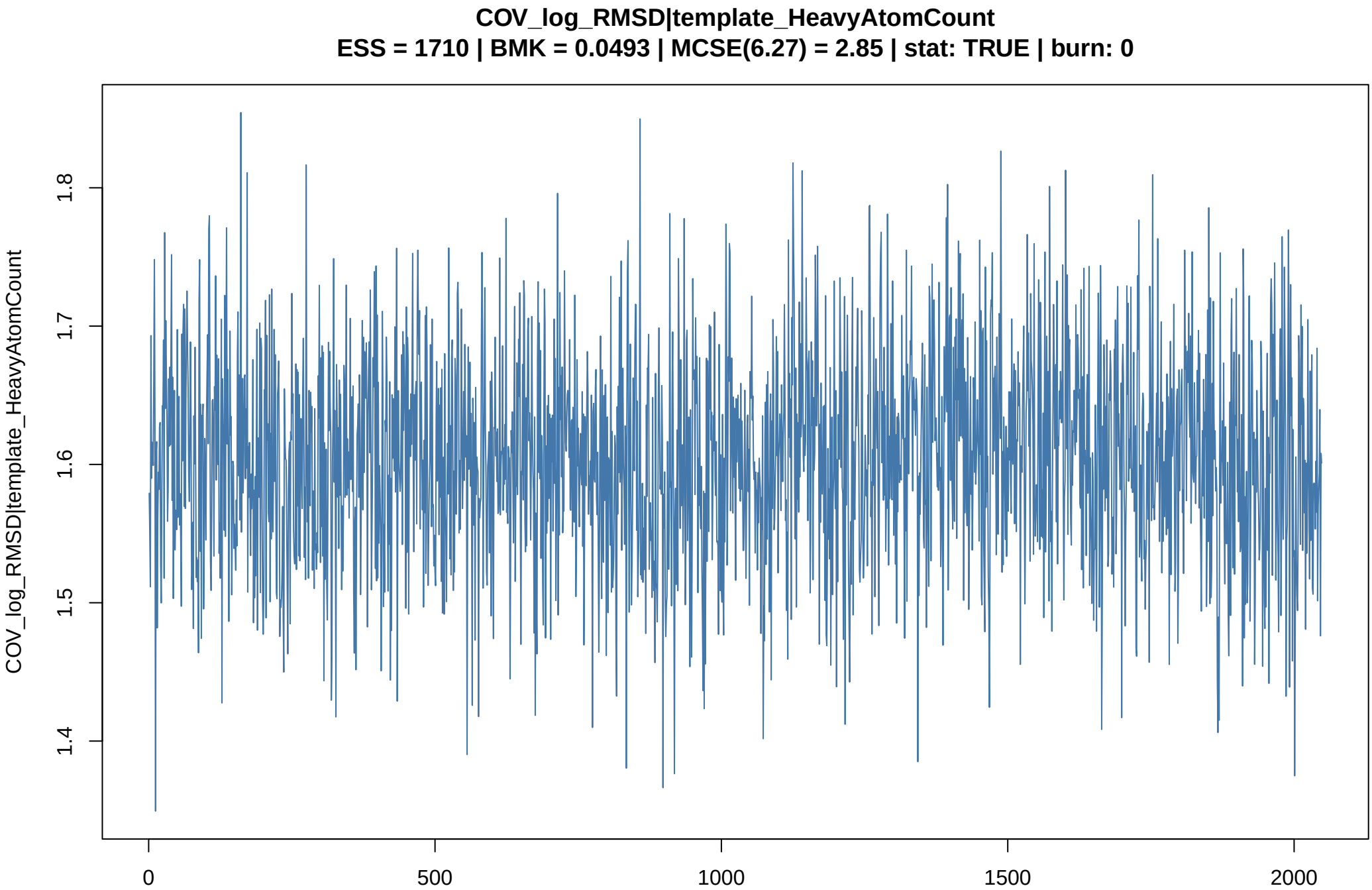

VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0286 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

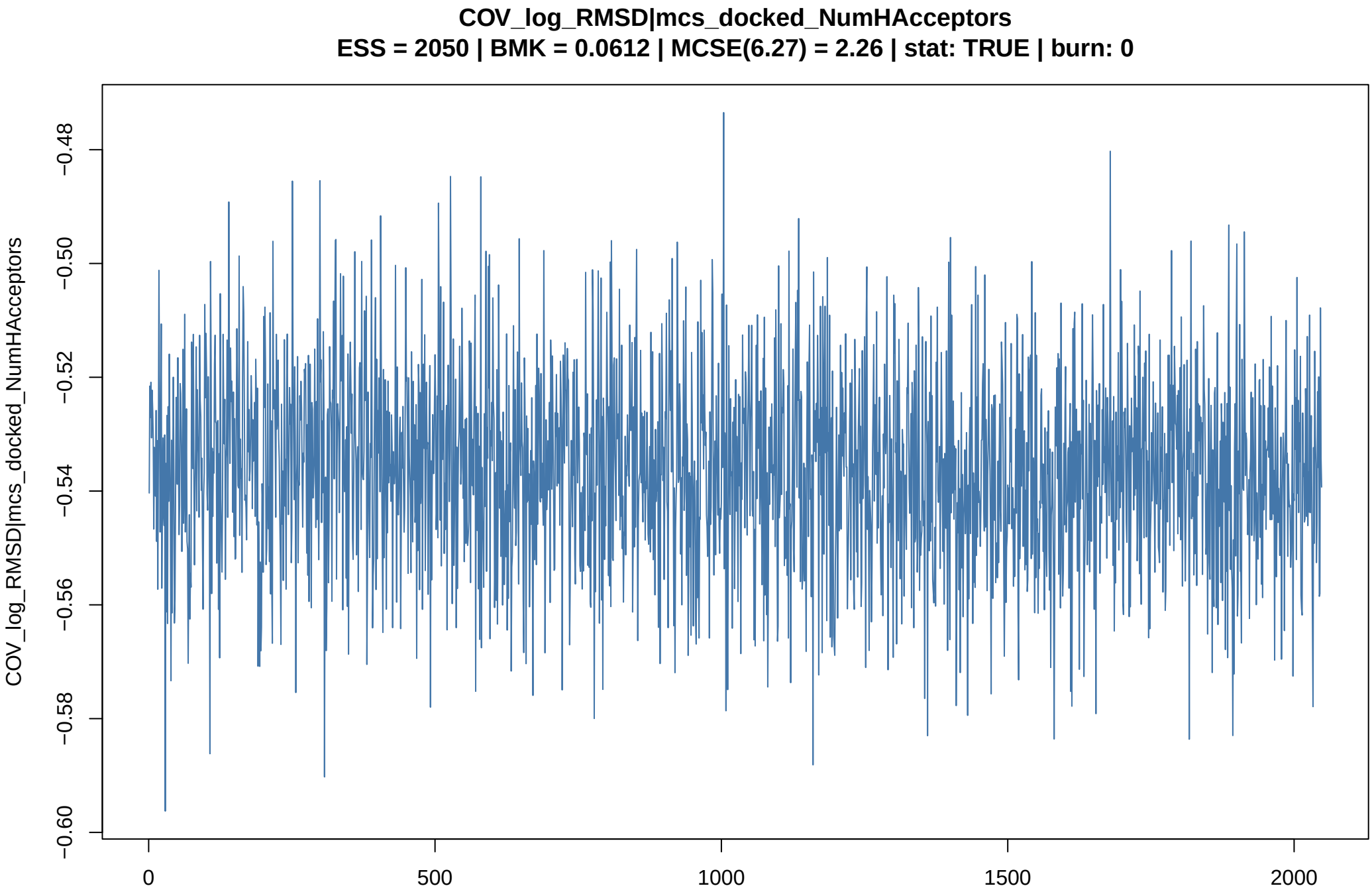

VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0435 | MCSE(6.27) = 2.65 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
1.45
1.50
1.55
0
500
1000
1500
2000

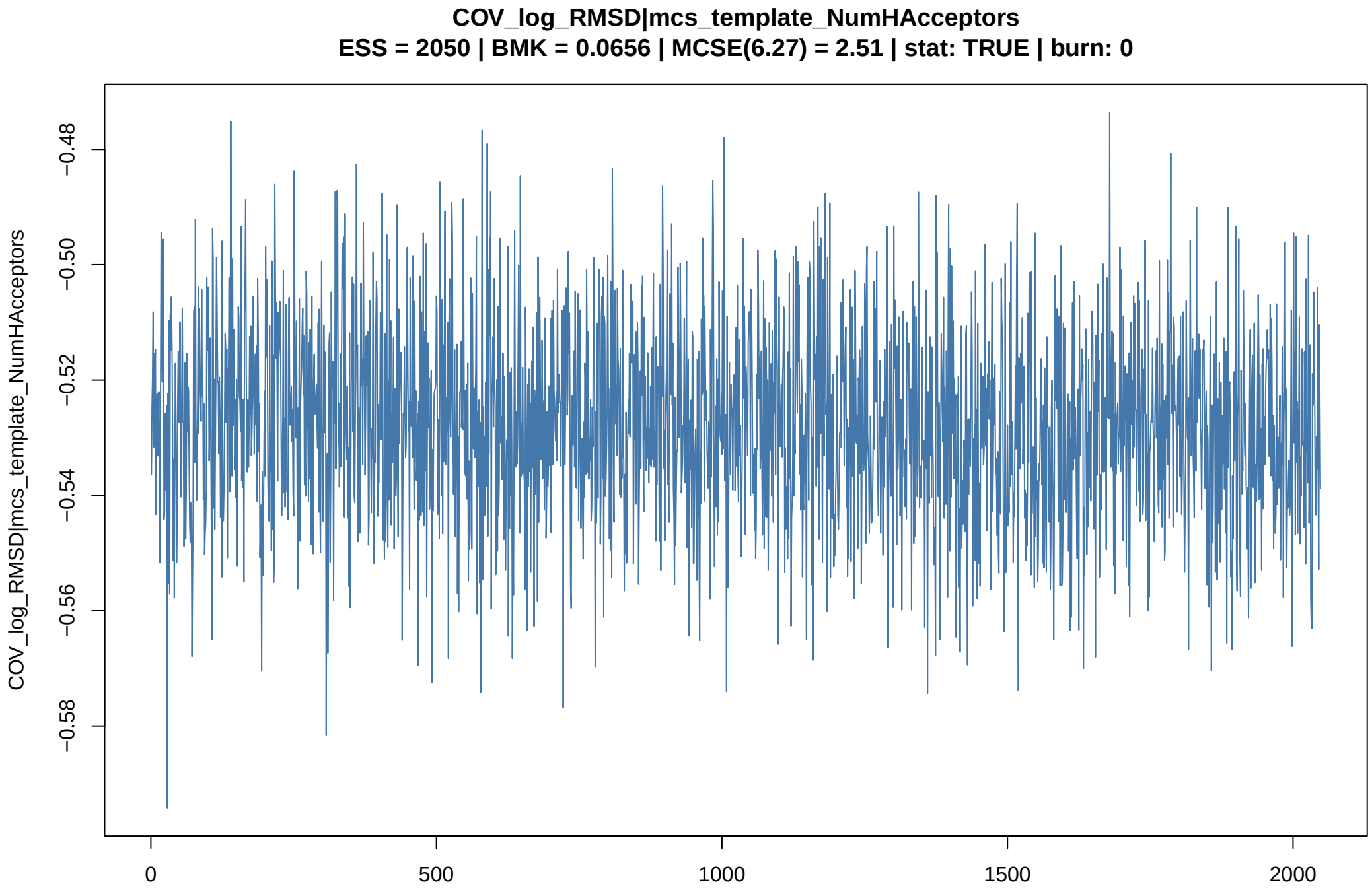

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0687 | MCSE(6.27) = 2.65 | stat: FALSE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

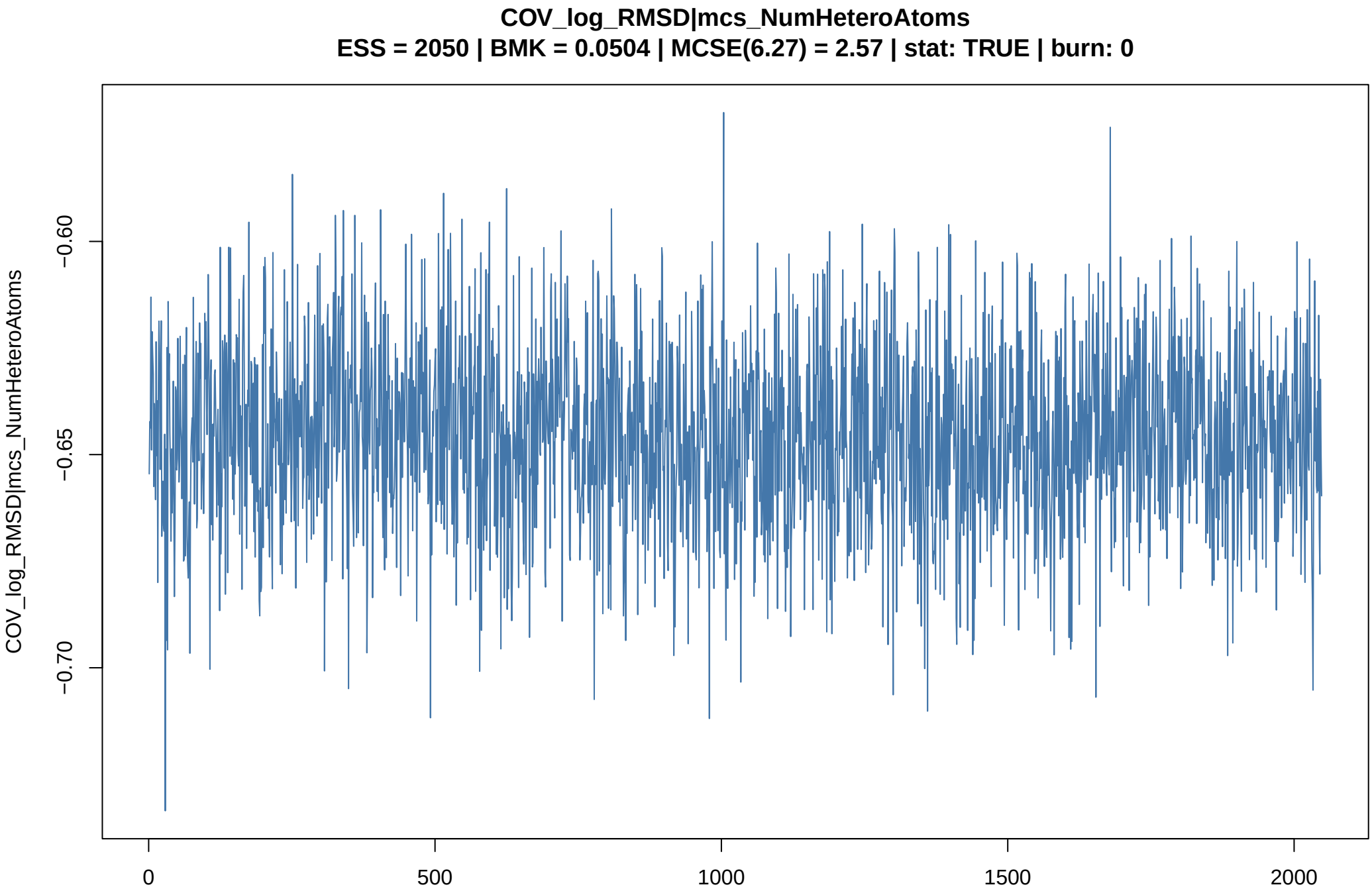

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1560 | BMK = 0.0907 | MCSE(6.27) = 3.3 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.7
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

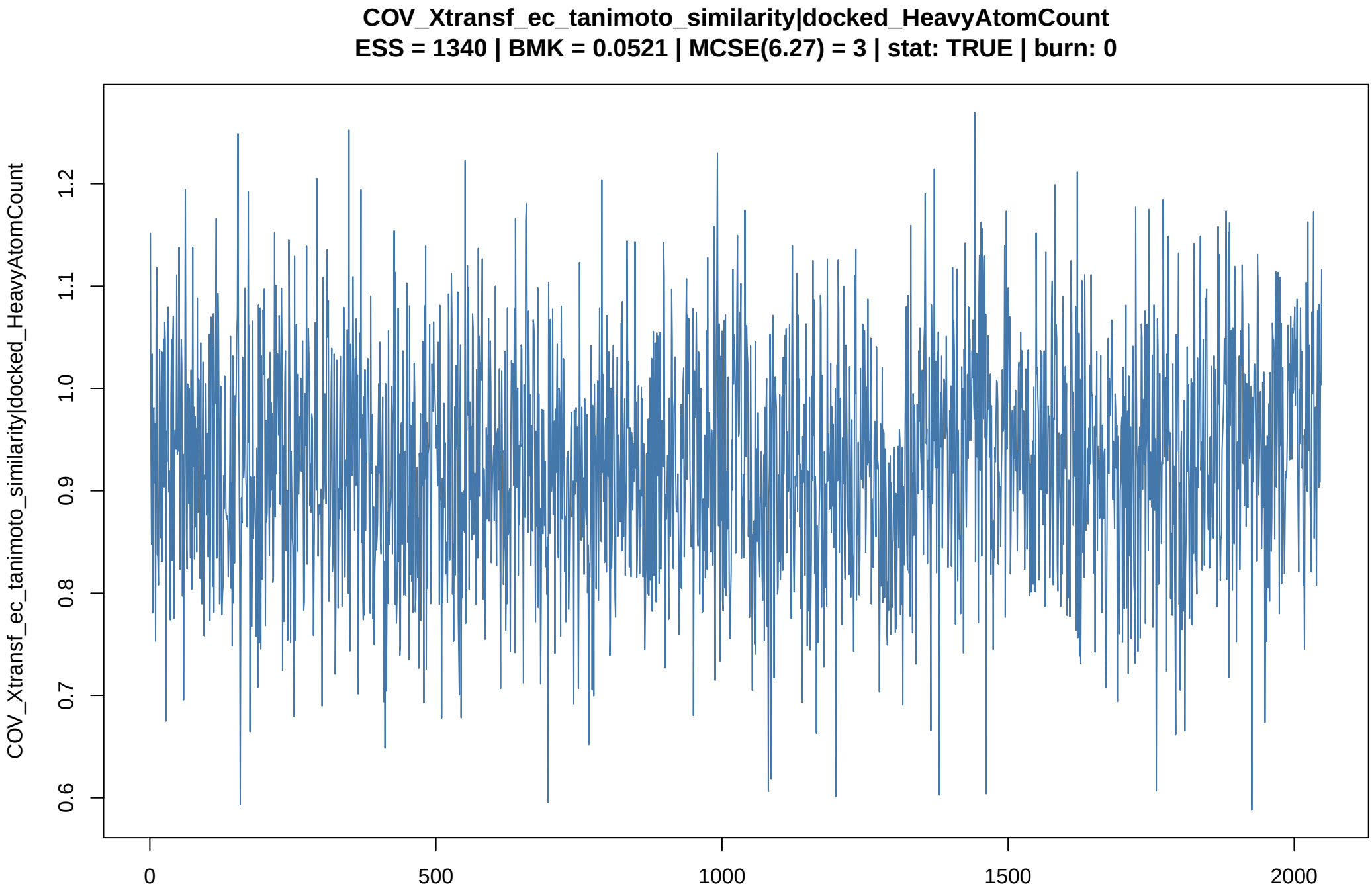

COV_log_RMSD|mcs_RingCount
ESS = 2050 | BMK = 0.0582 | MCSE(6.27) = 3.09 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.38
−0.40
−0.42
−0.44
0
500
1000
1500
2000

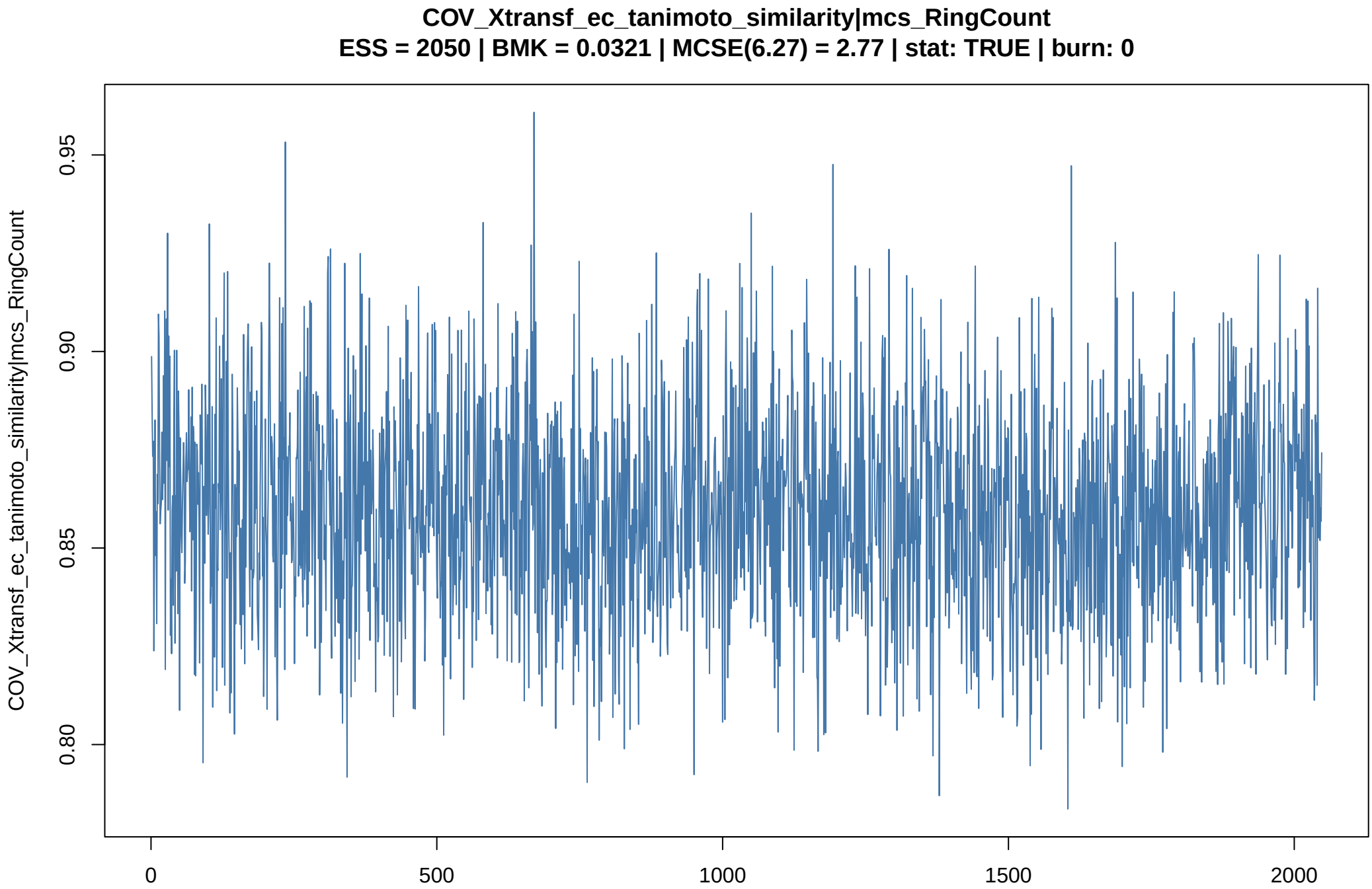

COV_log_RMSD|template_HeavyAtomCount
ESS = 1710 | BMK = 0.0493 | MCSE(6.27) = 2.85 | stat: TRUE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

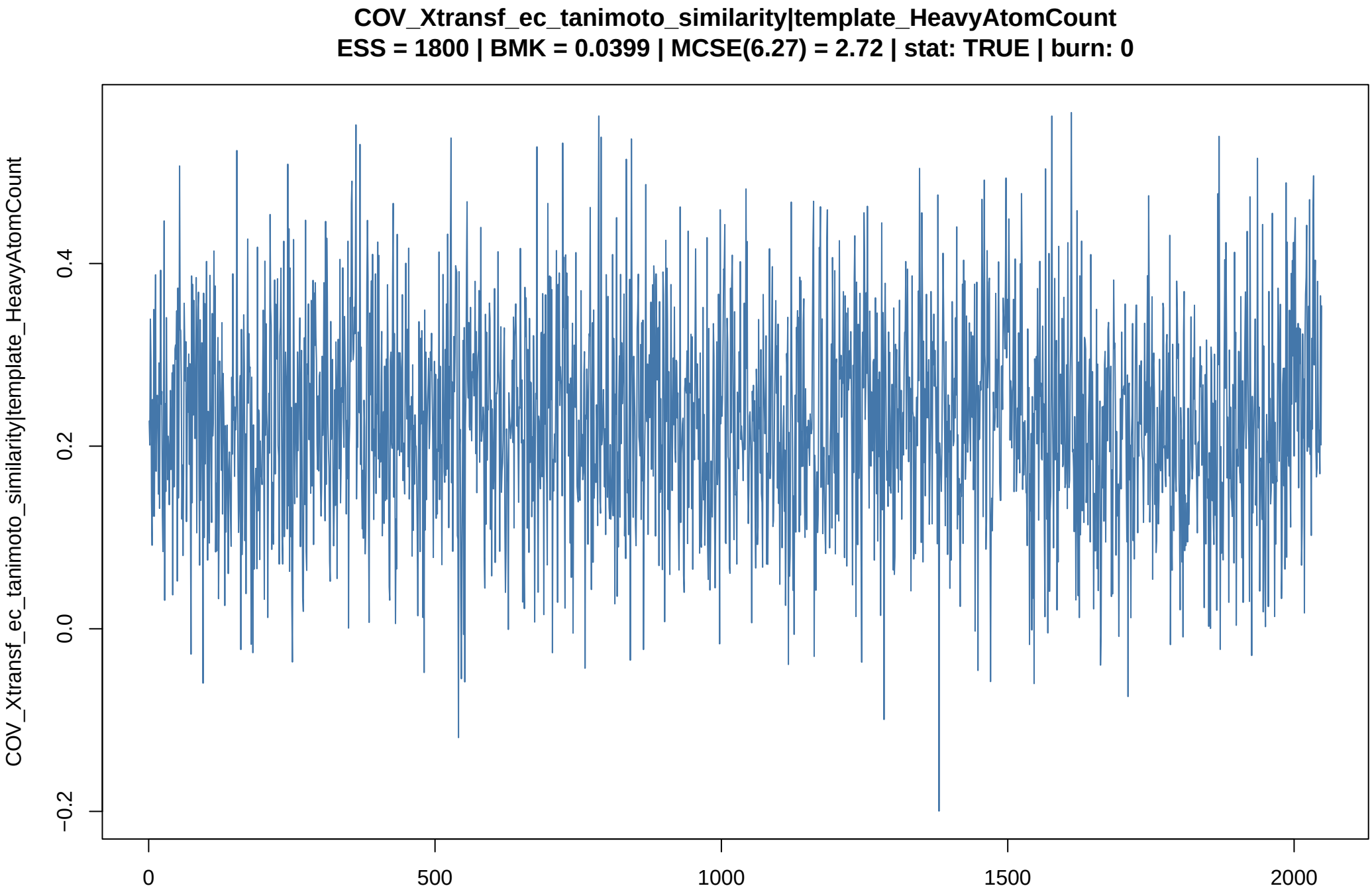

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0612 | MCSE(6.27) = 2.26 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
−0.60
0
500
1000
1500
2000

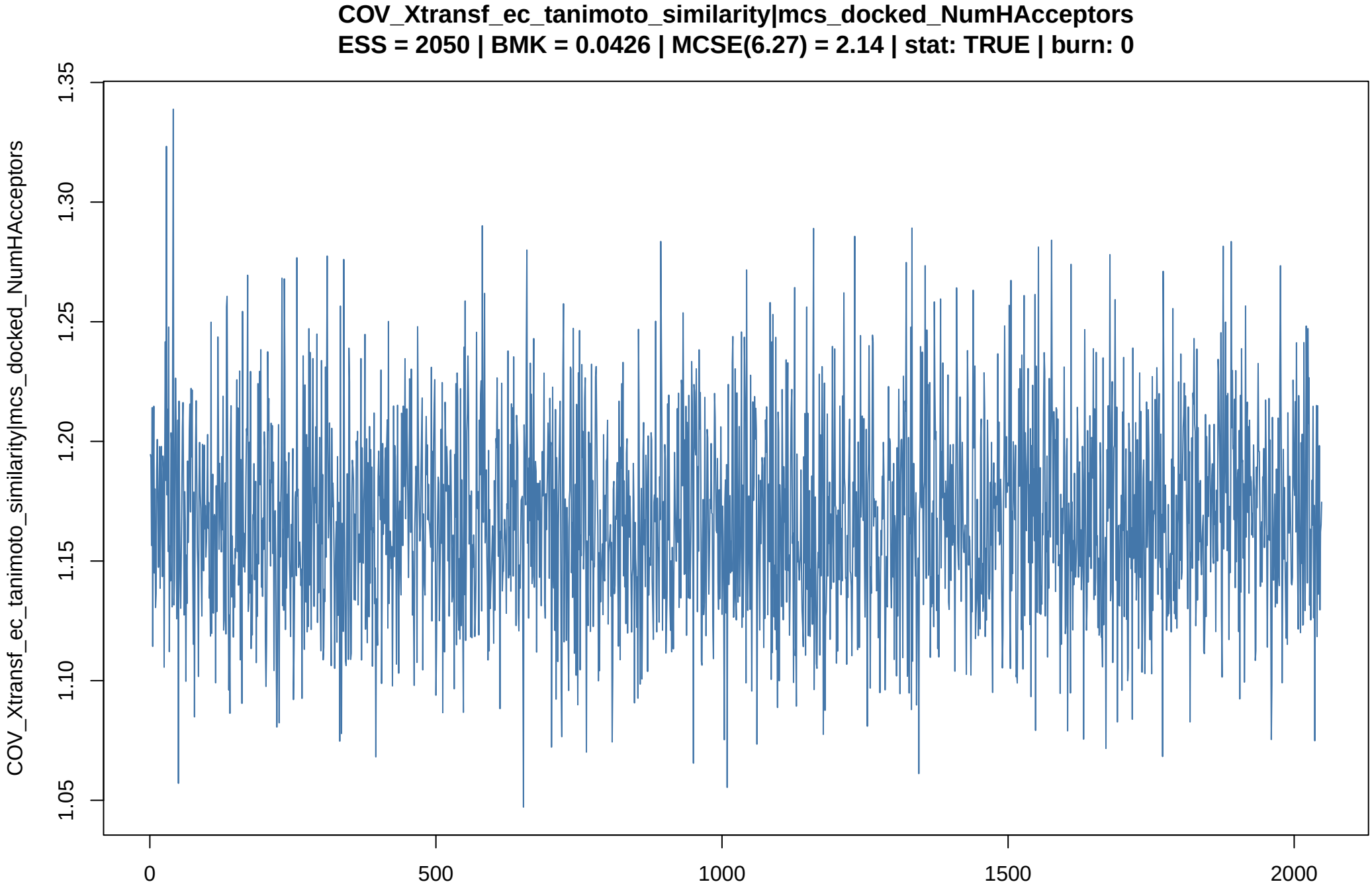

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0656 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

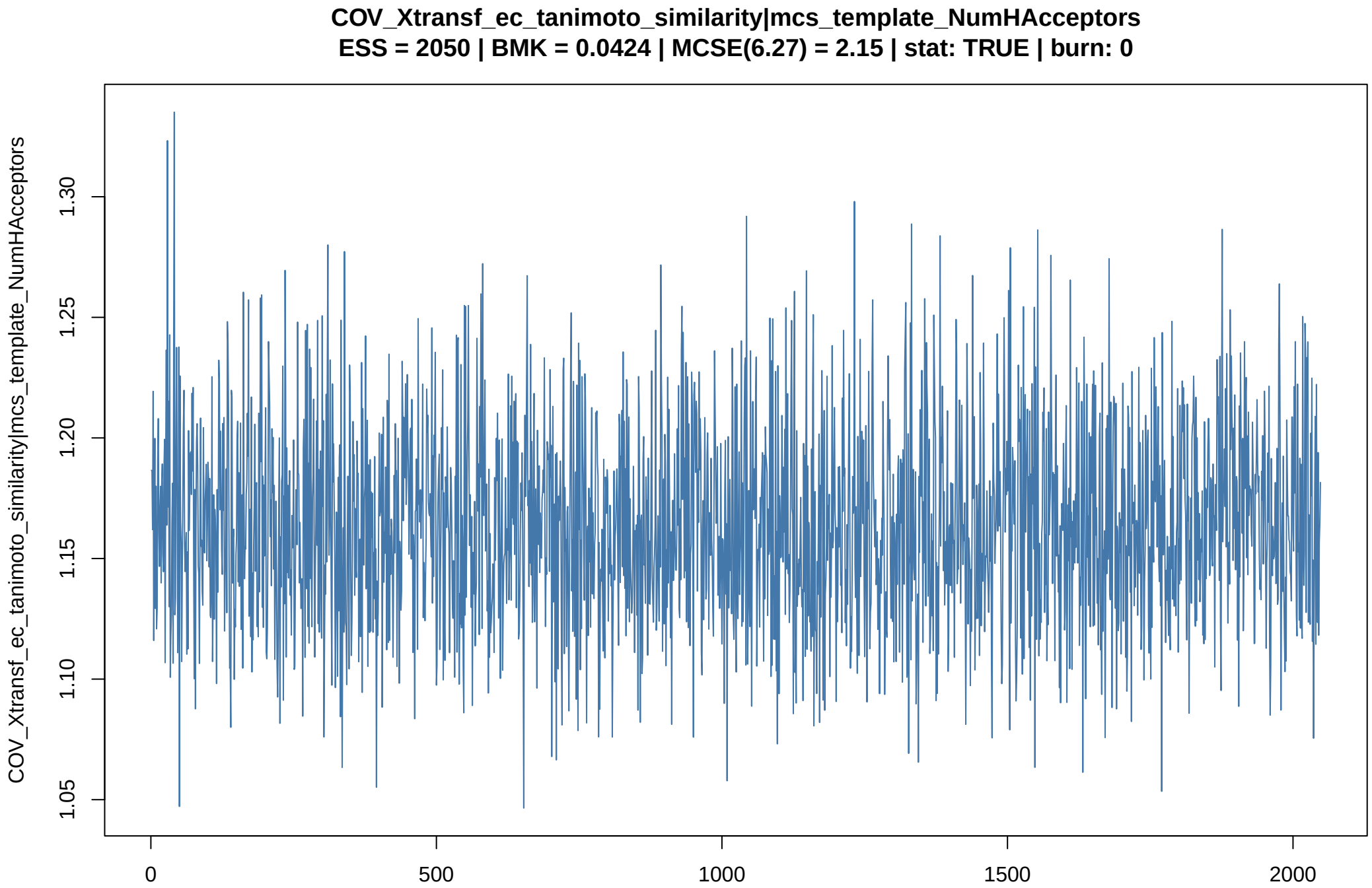

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0504 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.60
−0.65
−0.70
0
500
1000
1500
2000

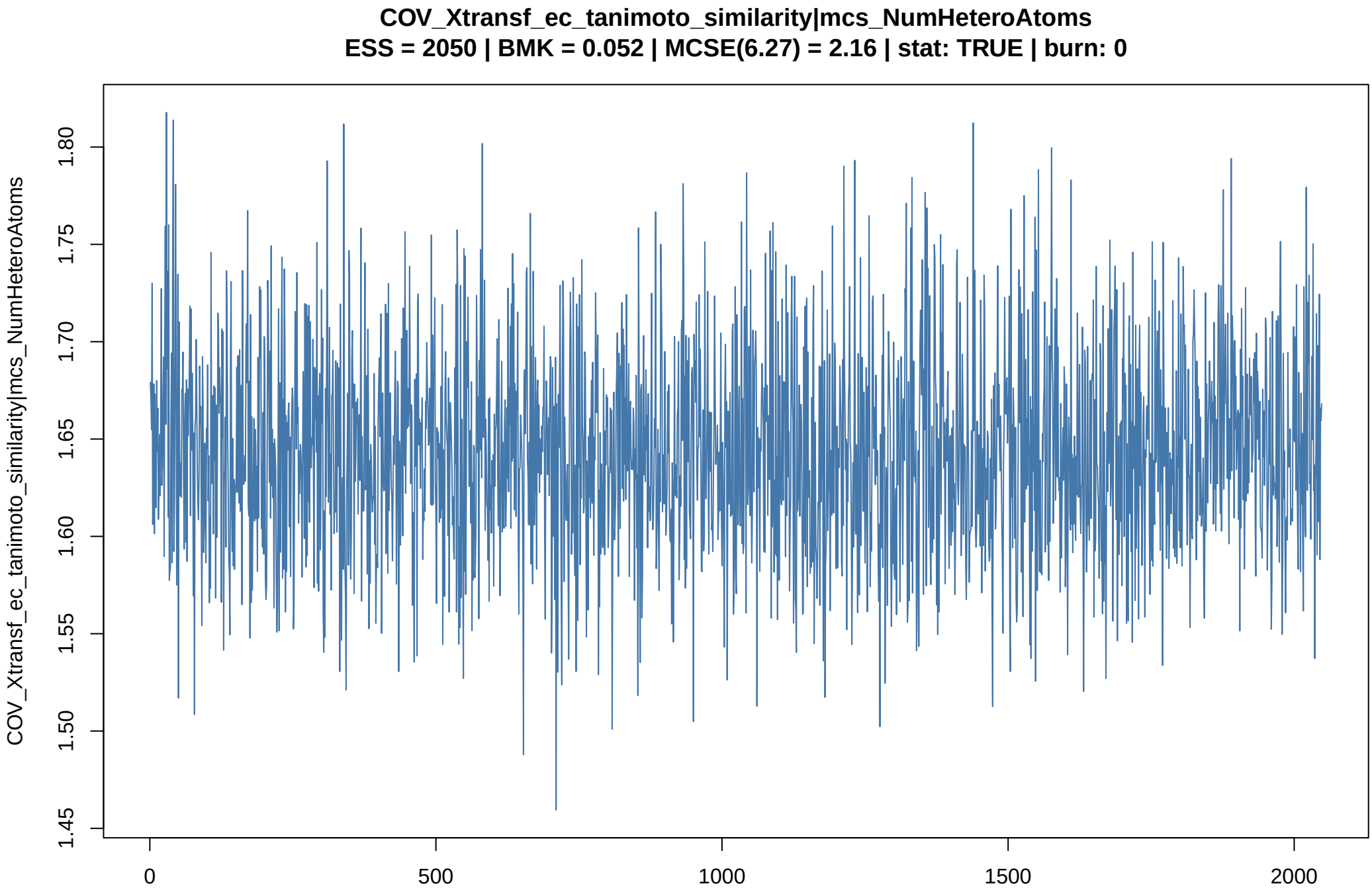

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1340 | BMK = 0.0521 | MCSE(6.27) = 3 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.7
0.8
0.9
1.0
1.1
1.2
0
500
1000
1500
2000

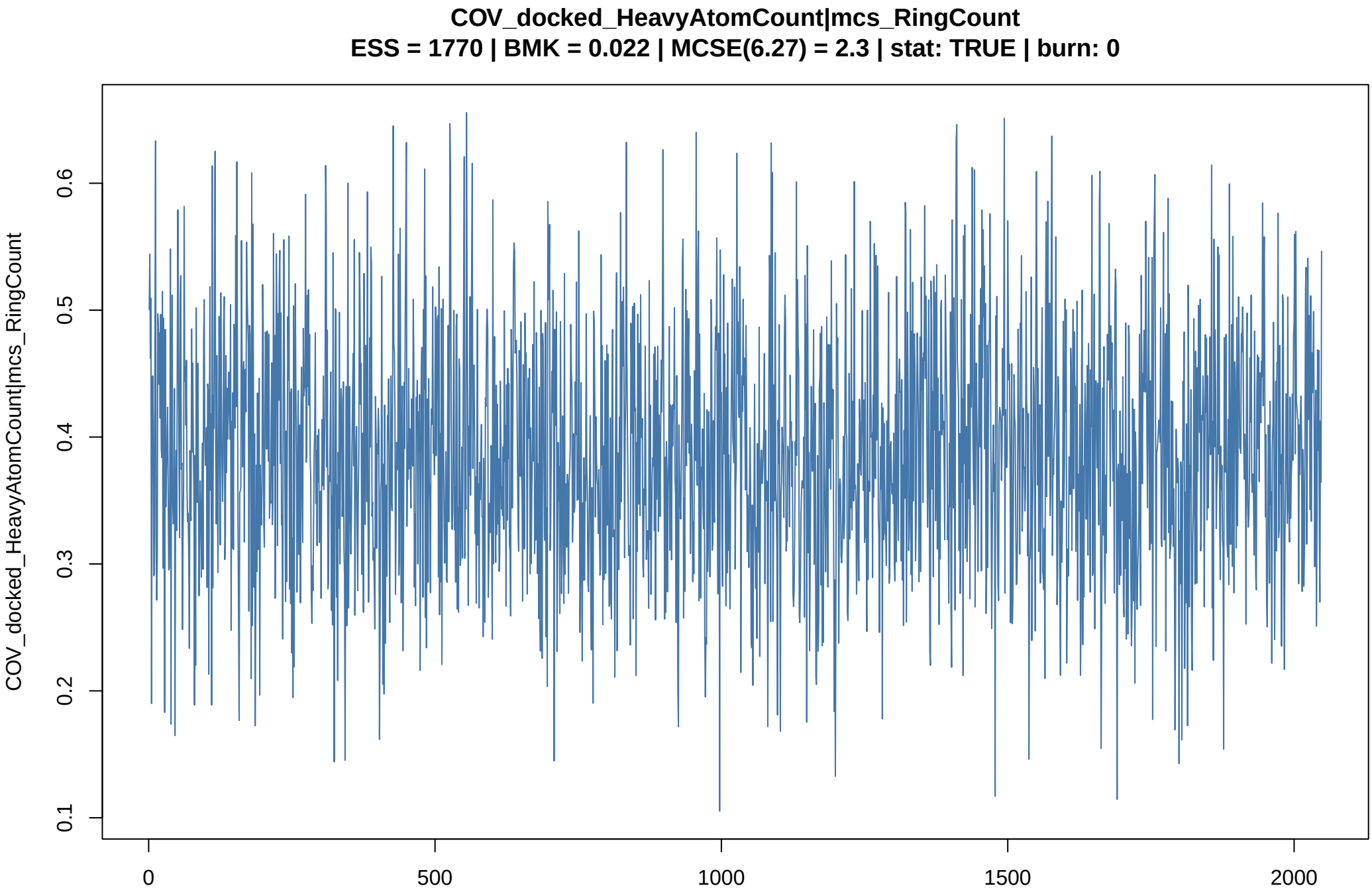

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 2050 | BMK = 0.0321 | MCSE(6.27) = 2.77 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

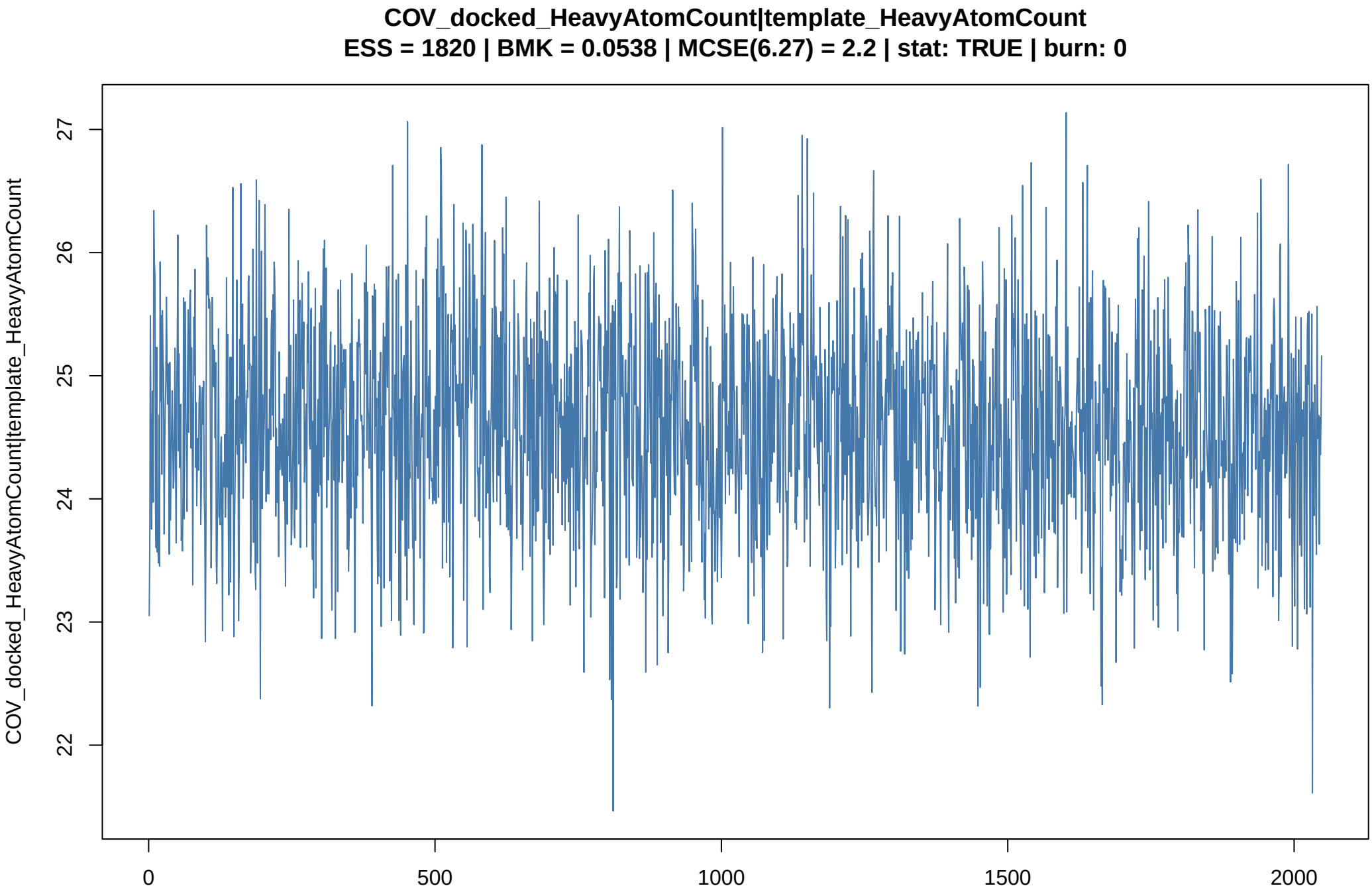

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1800 | BMK = 0.0399 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
−0.2
0.0
0.2
0.4
0
500
1000
1500
2000

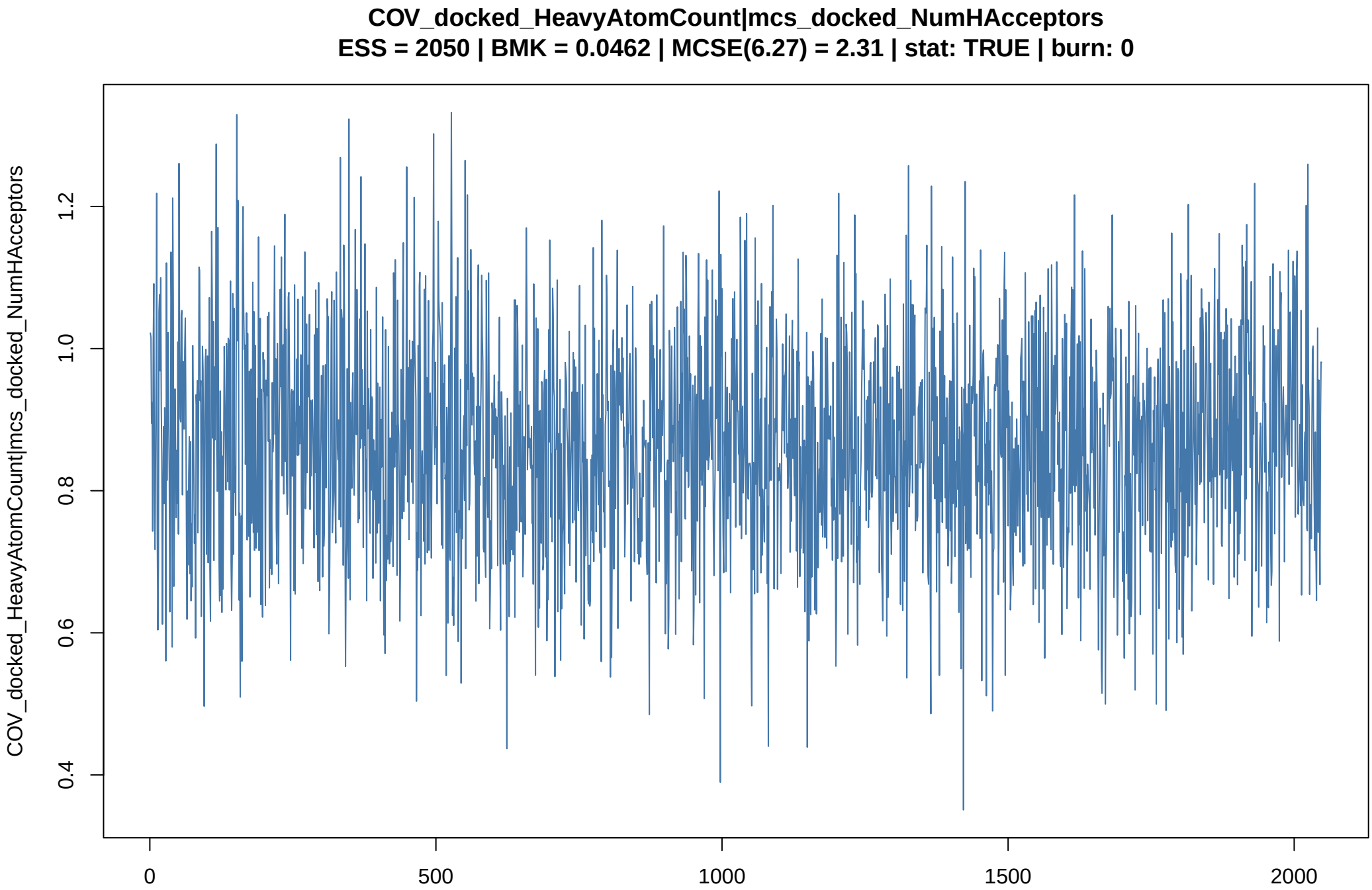

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0426 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
1.35
0
500
1000
1500
2000

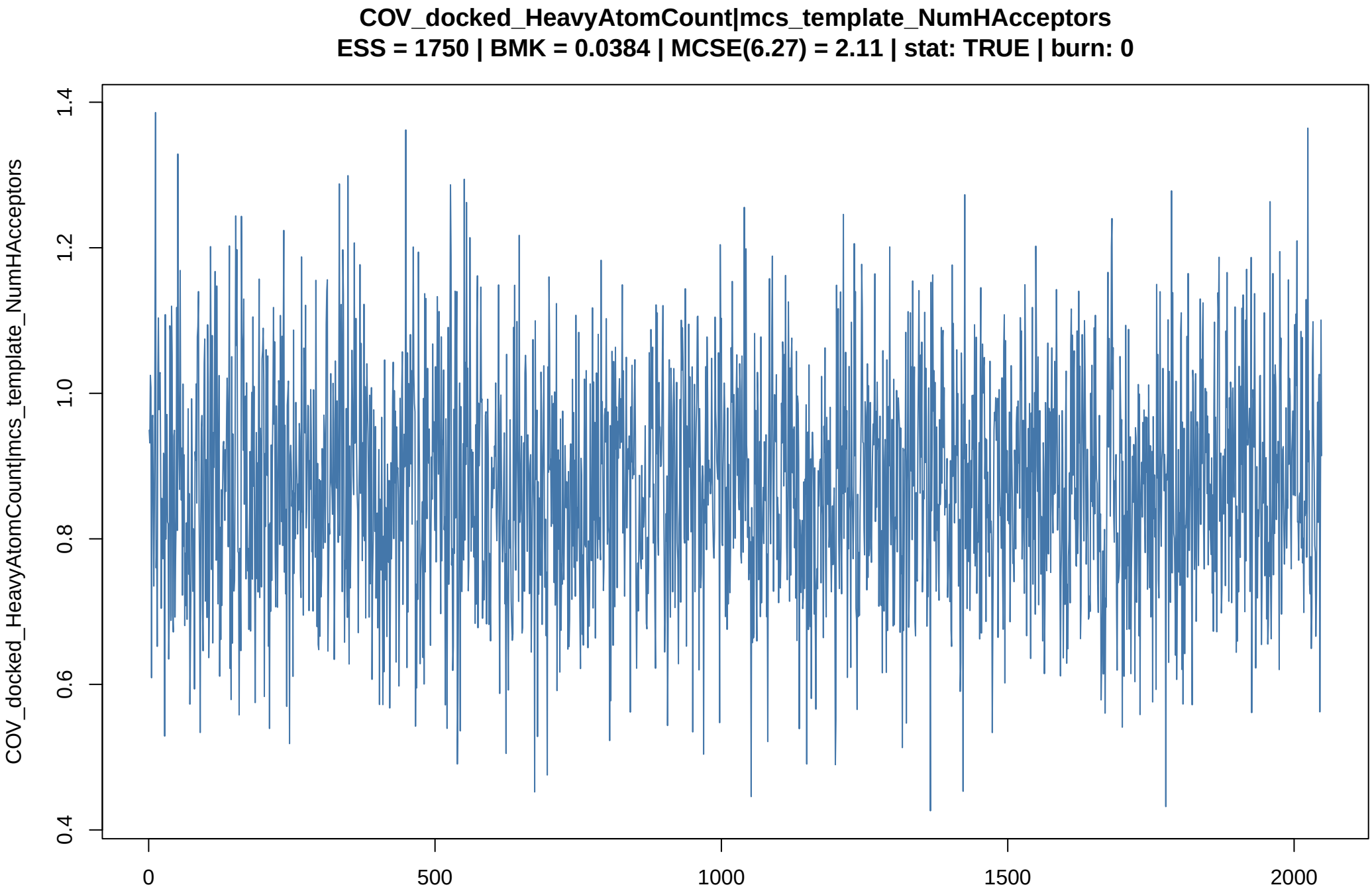

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0424 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

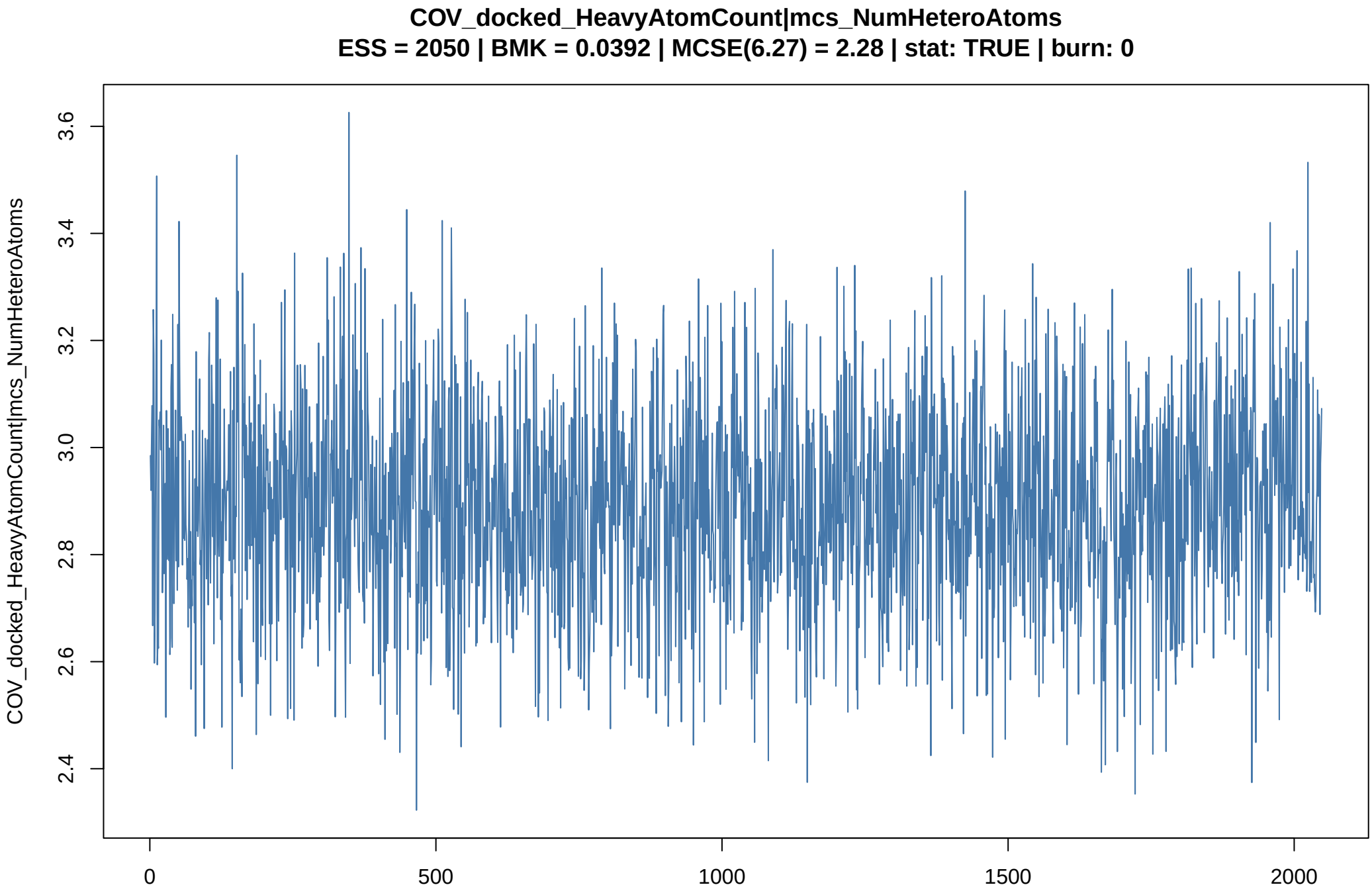

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.052 | MCSE(6.27) = 2.16 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.45
1.50
1.55
1.60
1.65
1.70
1.75
1.80
0
500
1000
1500
2000

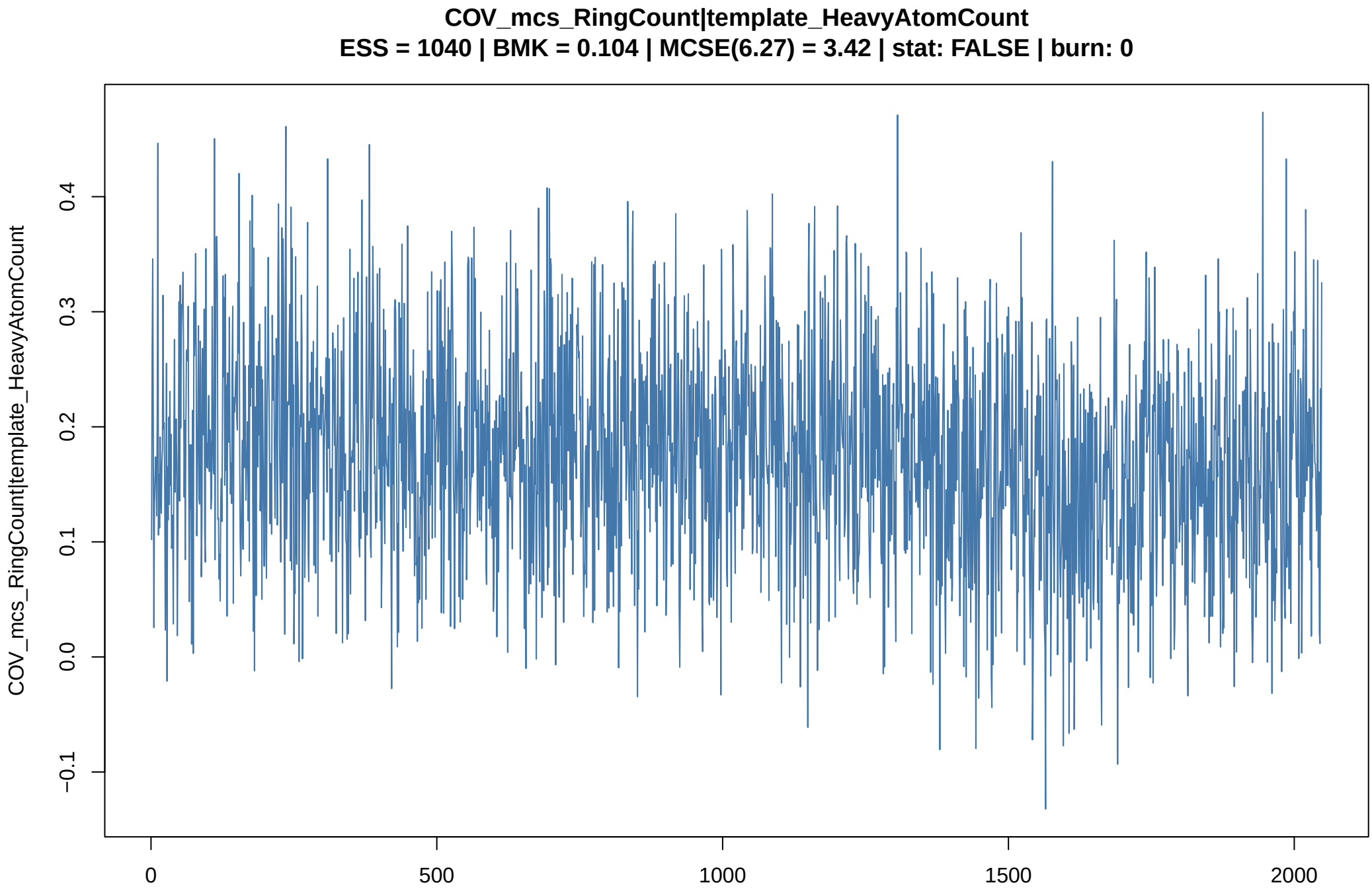

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1770 | BMK = 0.022 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0
500
1000
1500
2000

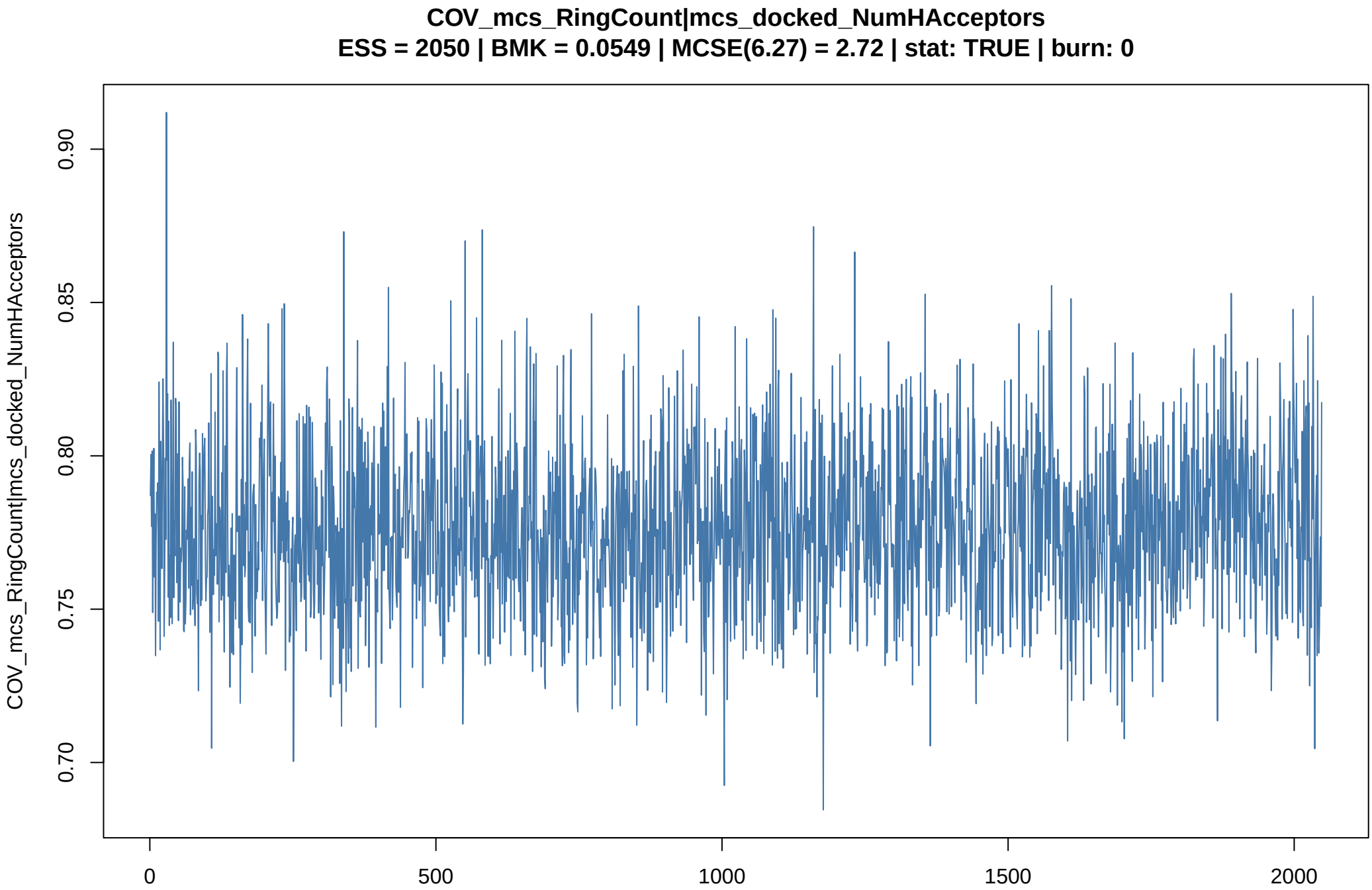

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1820 | BMK = 0.0538 | MCSE(6.27) = 2.2 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
22
23
24
25
26
27
0
500
1000
1500
2000

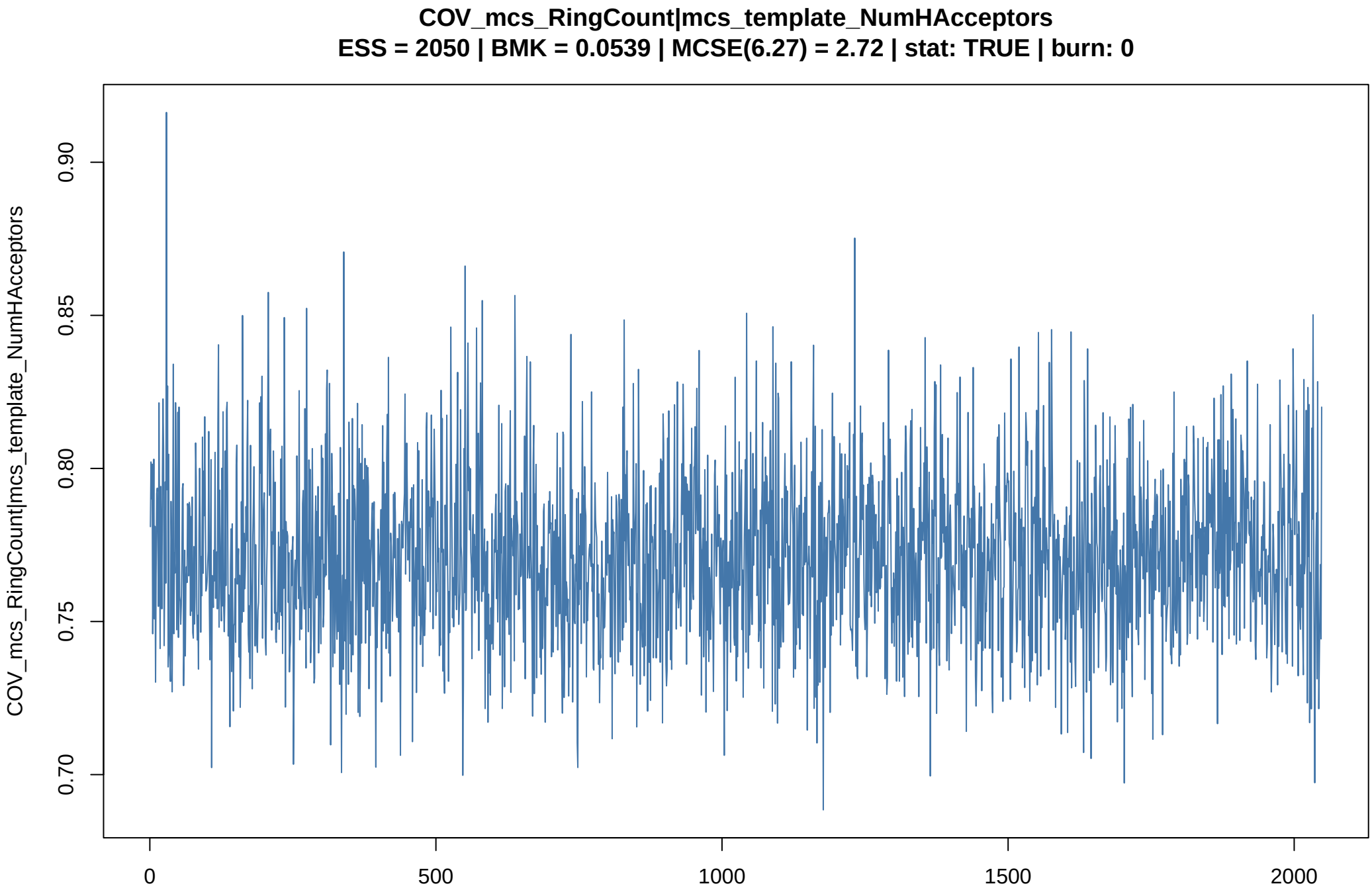

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0462 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

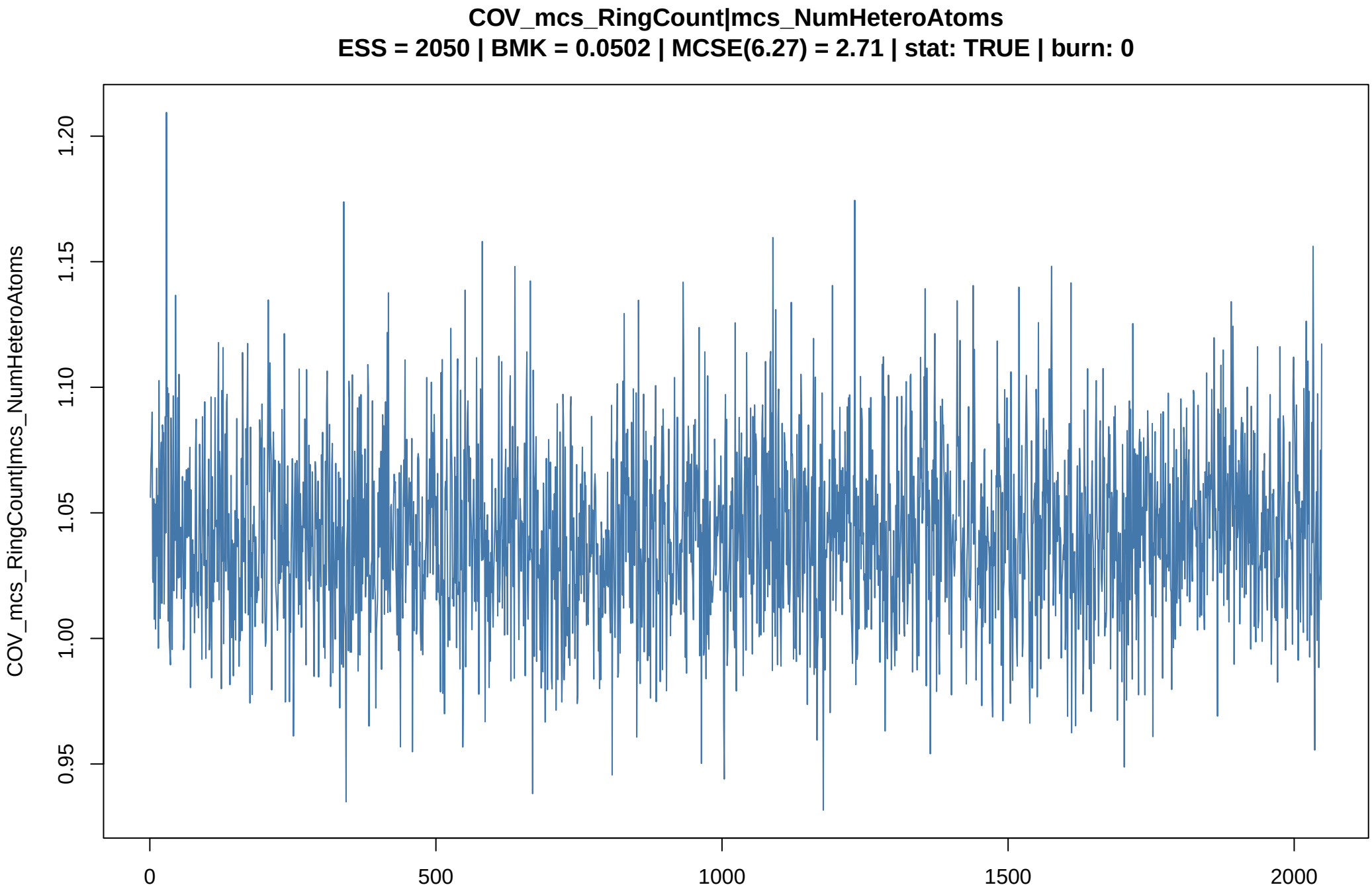

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1750 | BMK = 0.0384 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

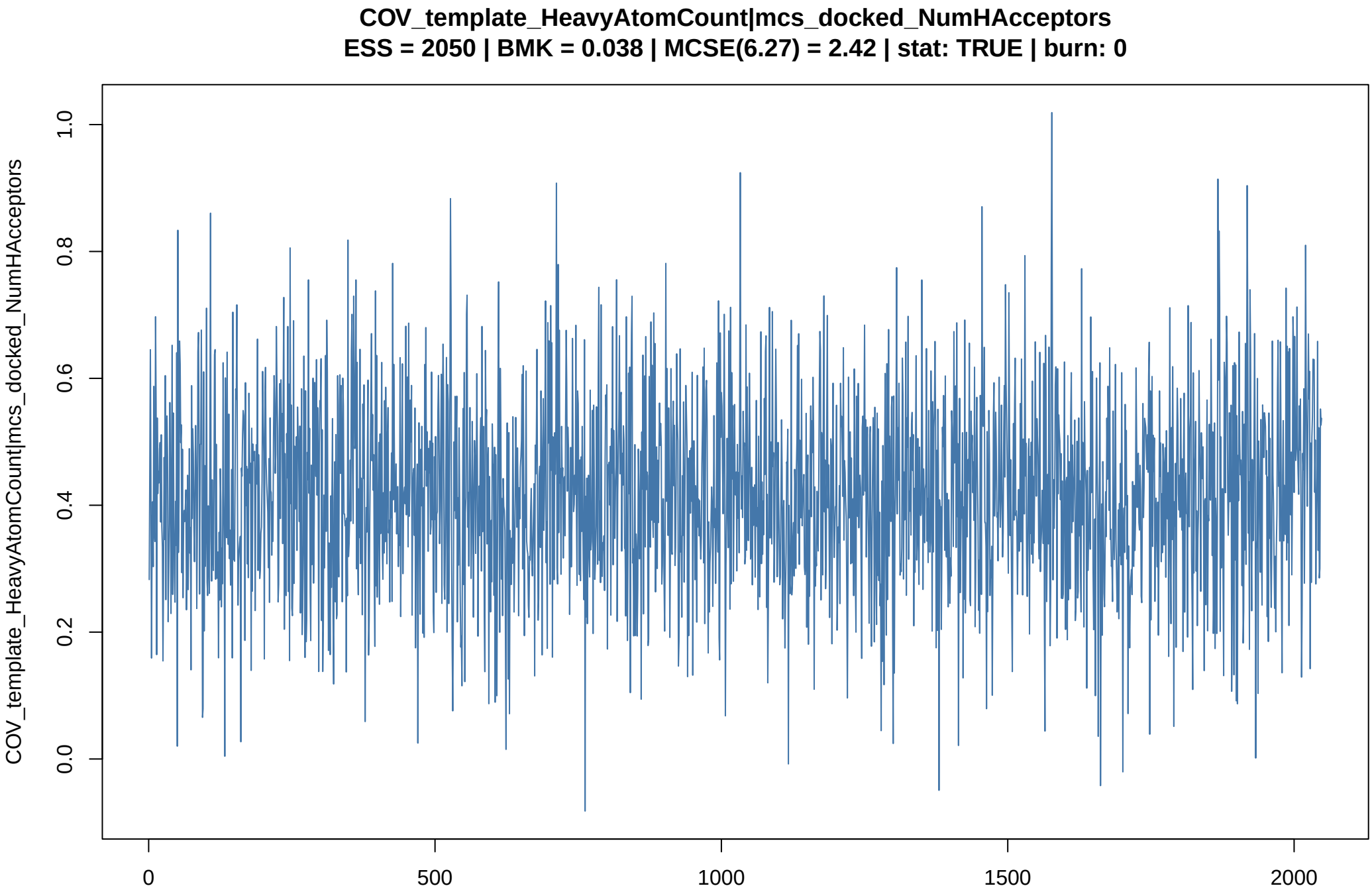

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0392 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.4
2.6
2.8
3.0
3.2
3.4
3.6
0
500
1000
1500
2000

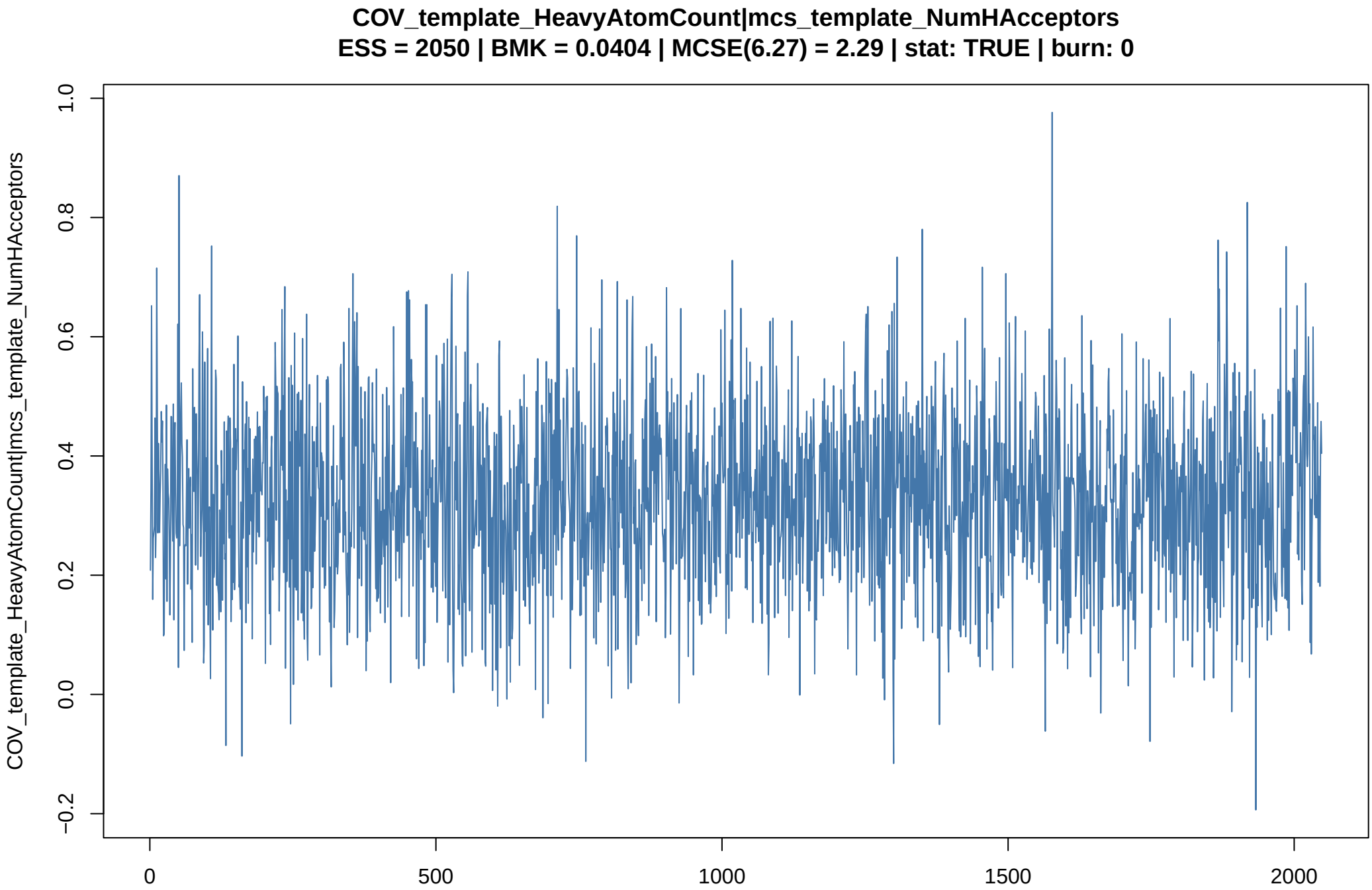

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1040 | BMK = 0.104 | MCSE(6.27) = 3.42 | stat: FALSE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
0.4
0.3
0.2
0.1
0.0
−0.1
0
500
1000
1500
2000

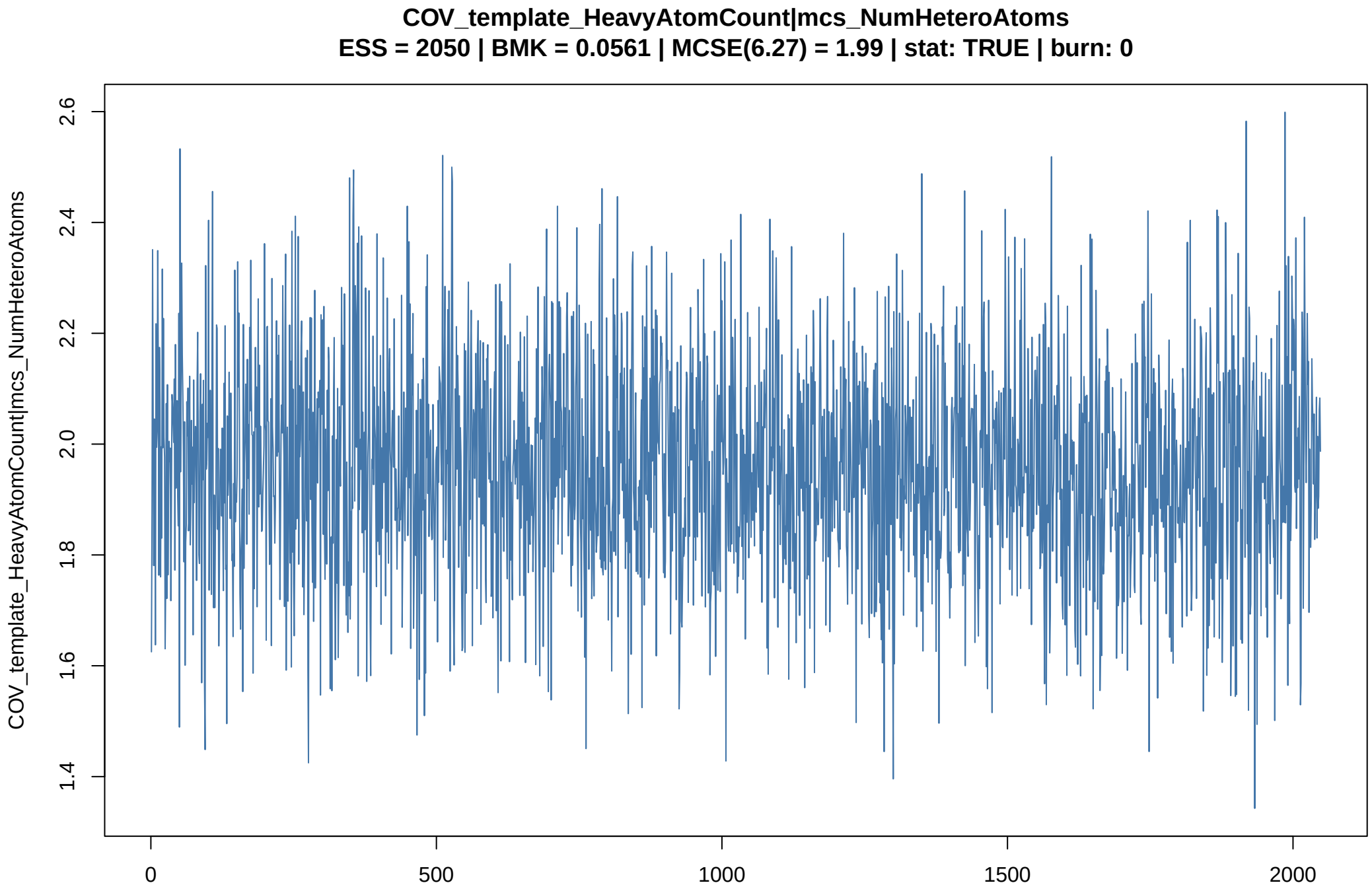

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0549 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0.90
0
500
1000
1500
2000

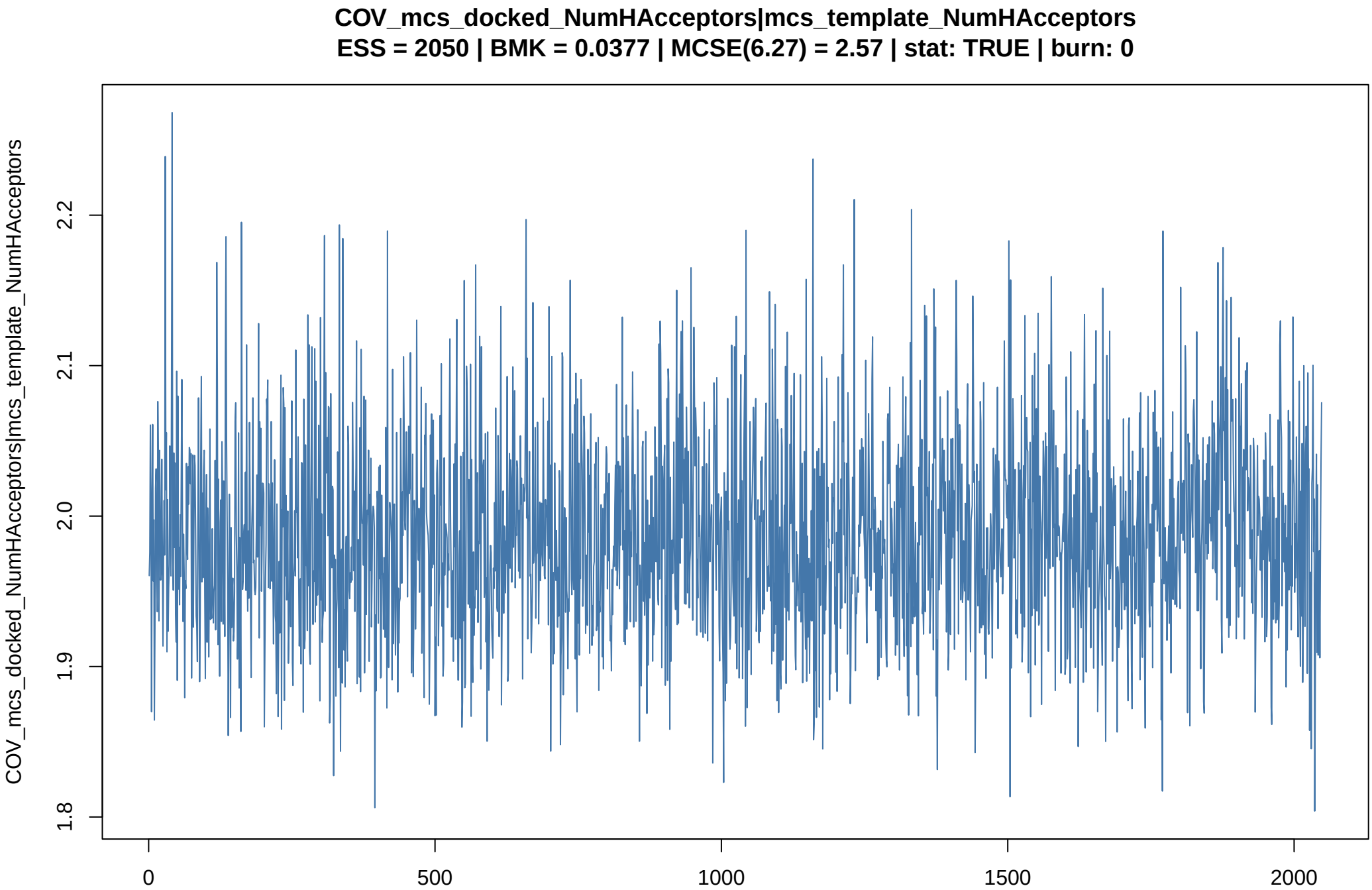

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0539 | MCSE(6.27) = 2.72 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0.90
0
500
1000
1500
2000

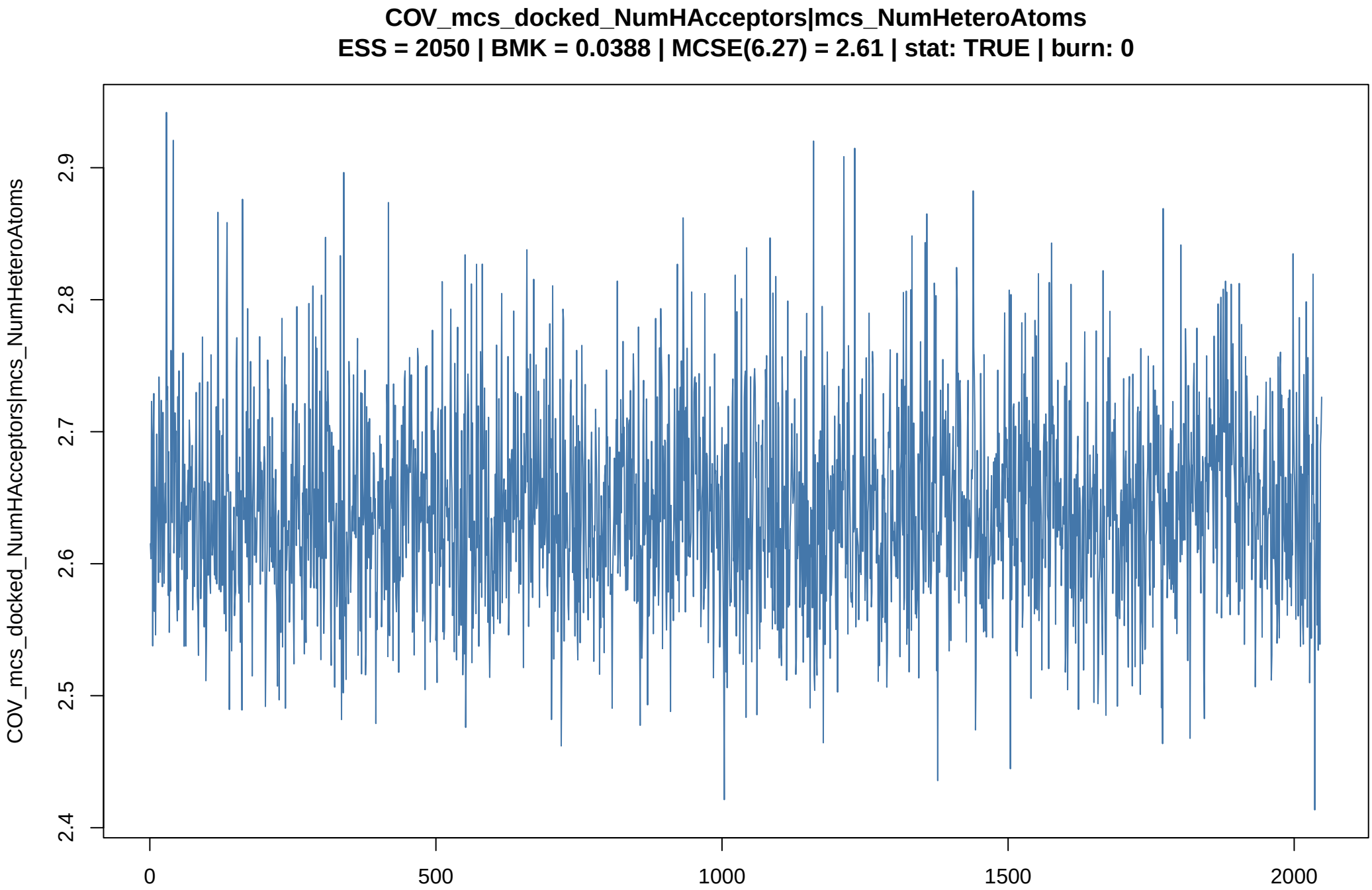

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
1.20
0
500
1000
1500
2000

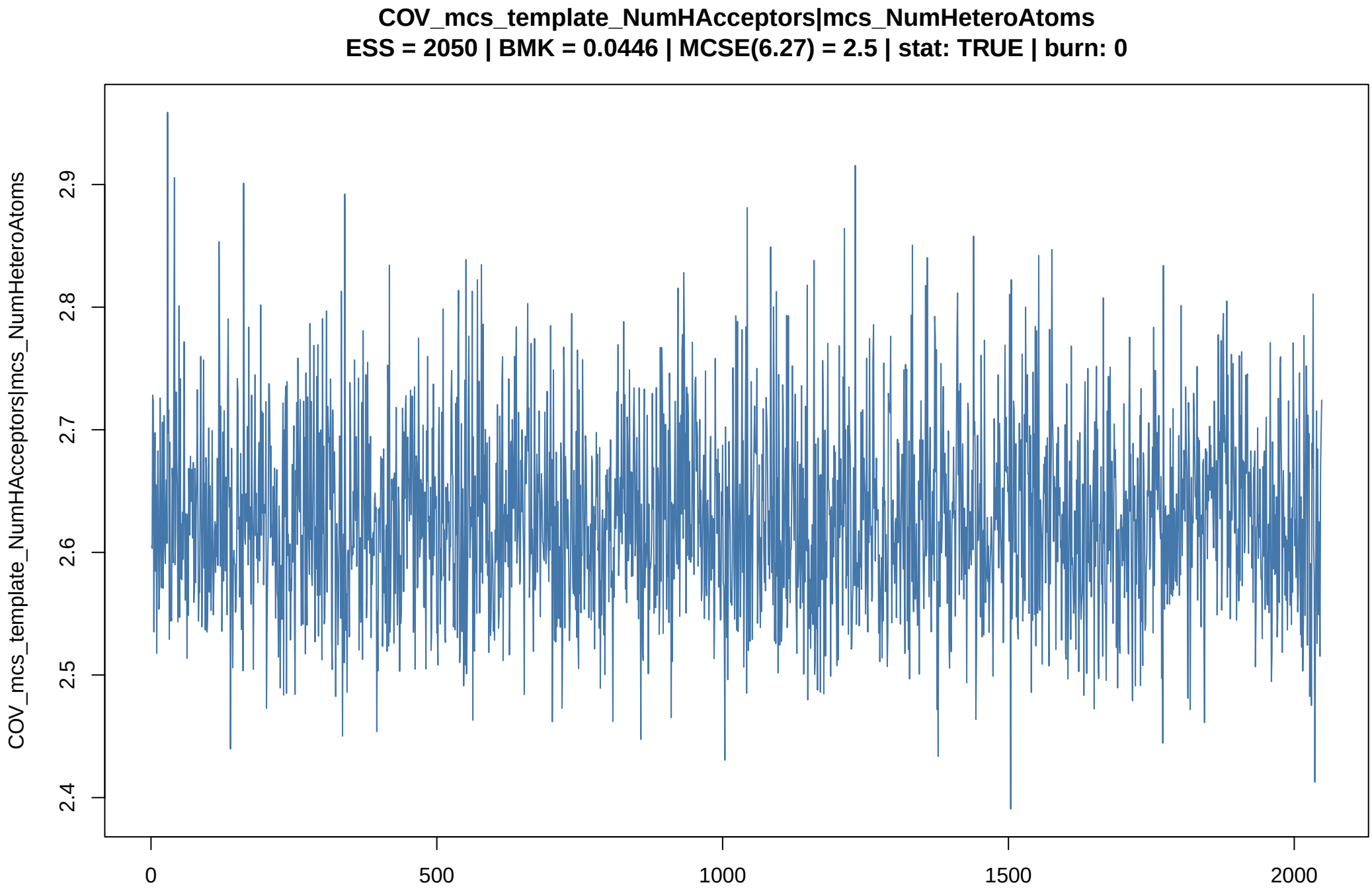

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.038 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0404 | MCSE(6.27) = 2.29 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
1.0
0.8
0.6
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0561 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
1.4
1.6
1.8
2.0
2.2
2.4
2.6
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0377 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0388 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
2.4
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0446 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0
COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
2.4
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000