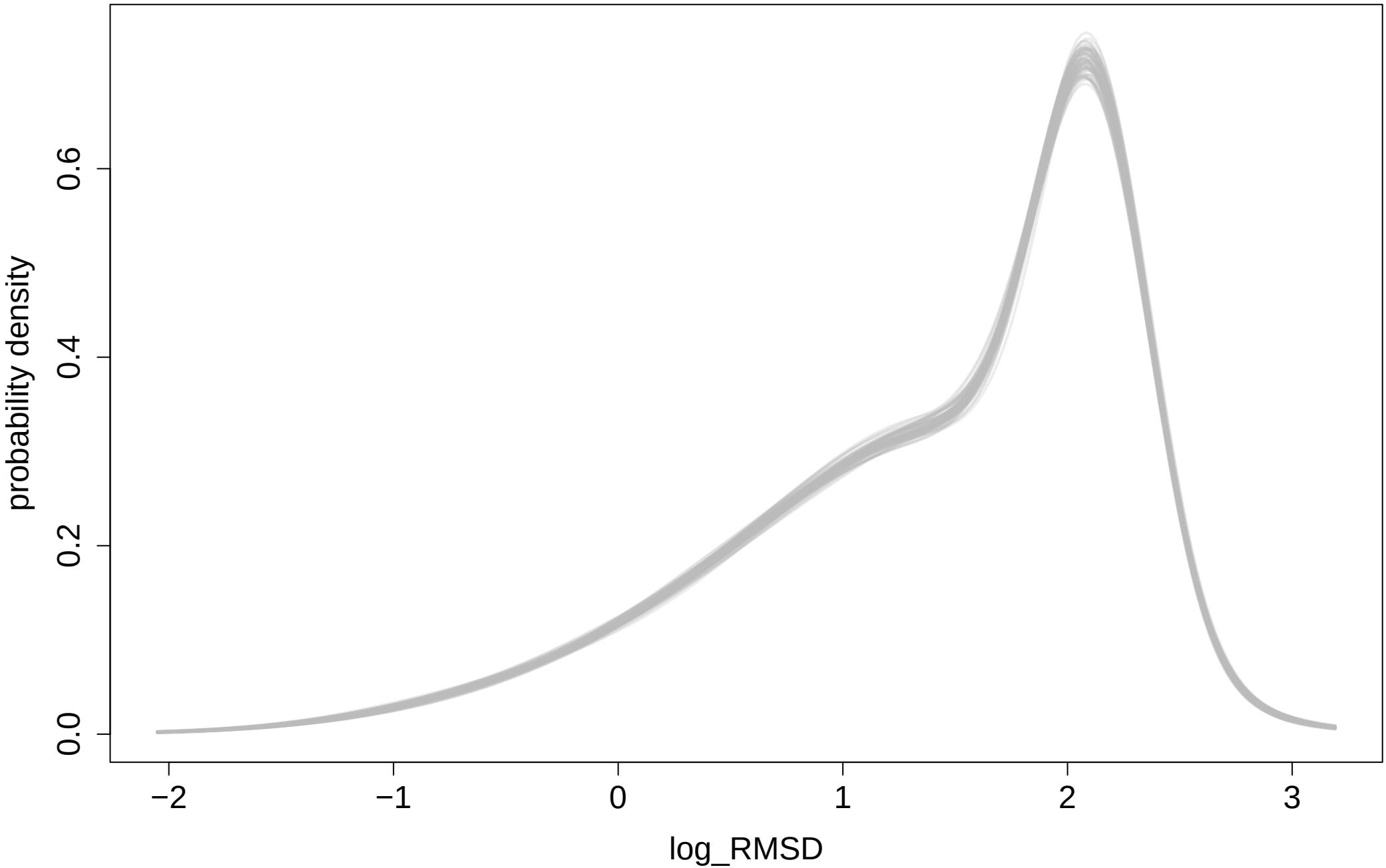
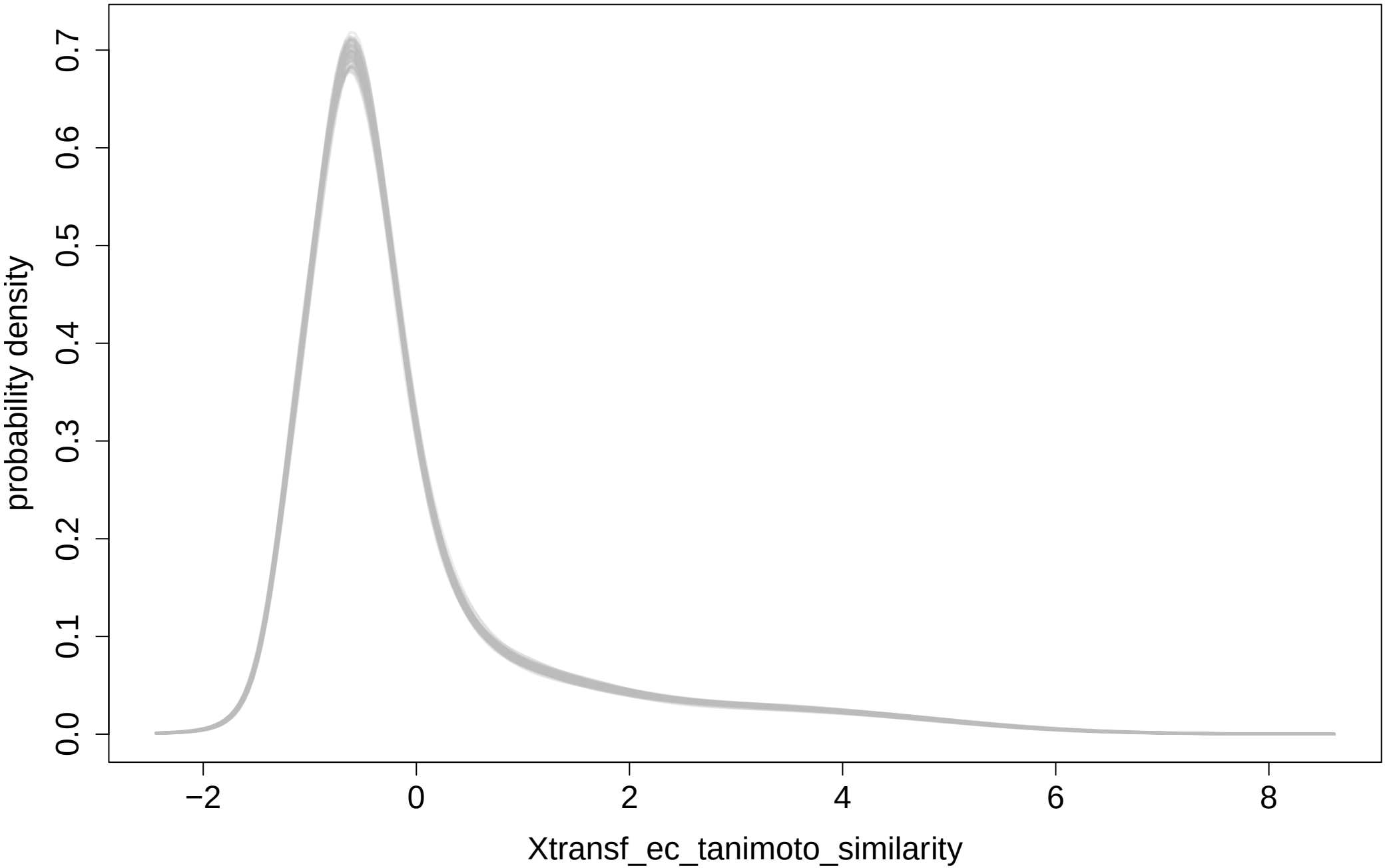
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.322658373783011
max MCSE = 12.0611033103647
all stationary: FALSE
burn: 2040

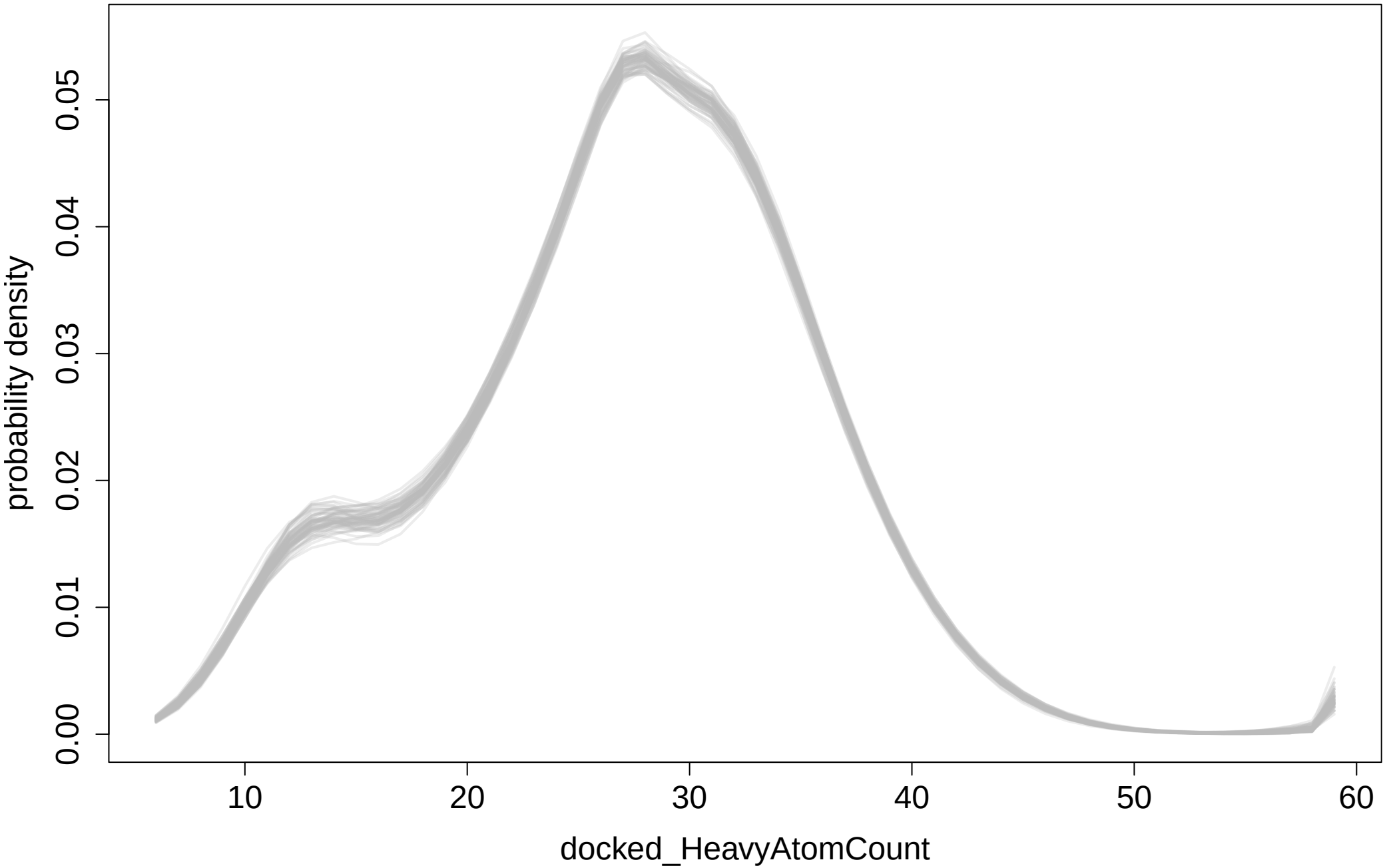
−− STATS 2D −−
min ESS = 1383.5482983437
max BMK = 0.0540073635065904
max MCSE = 3.01167497791719
all stationary: TRUE
burn: 0

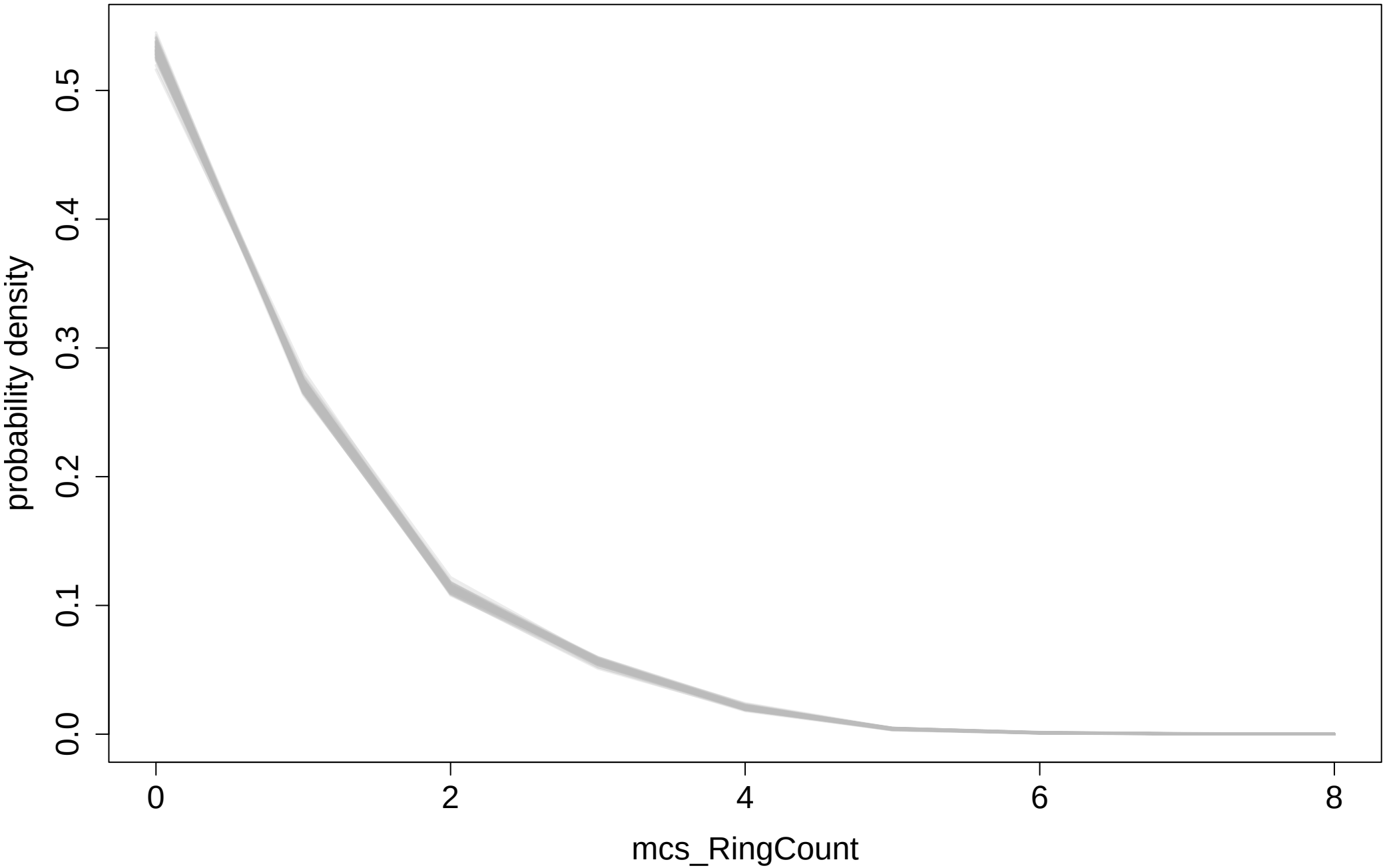
−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.871696503711511
max MCSE = NaN
all stationary: FALSE
burn: 2040

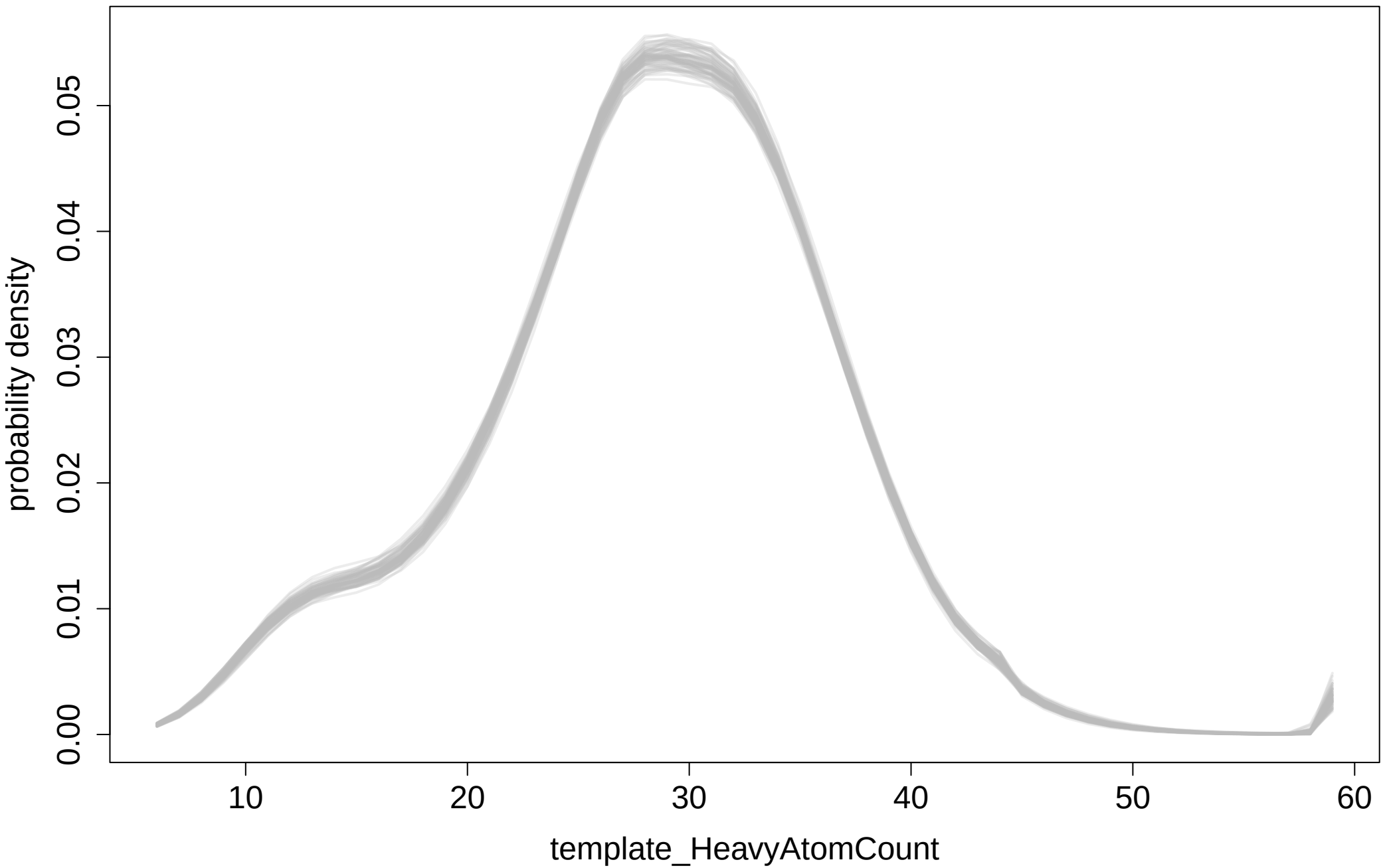
Occupied clusters: 49 of 91
LL: −112000 +− 32.8

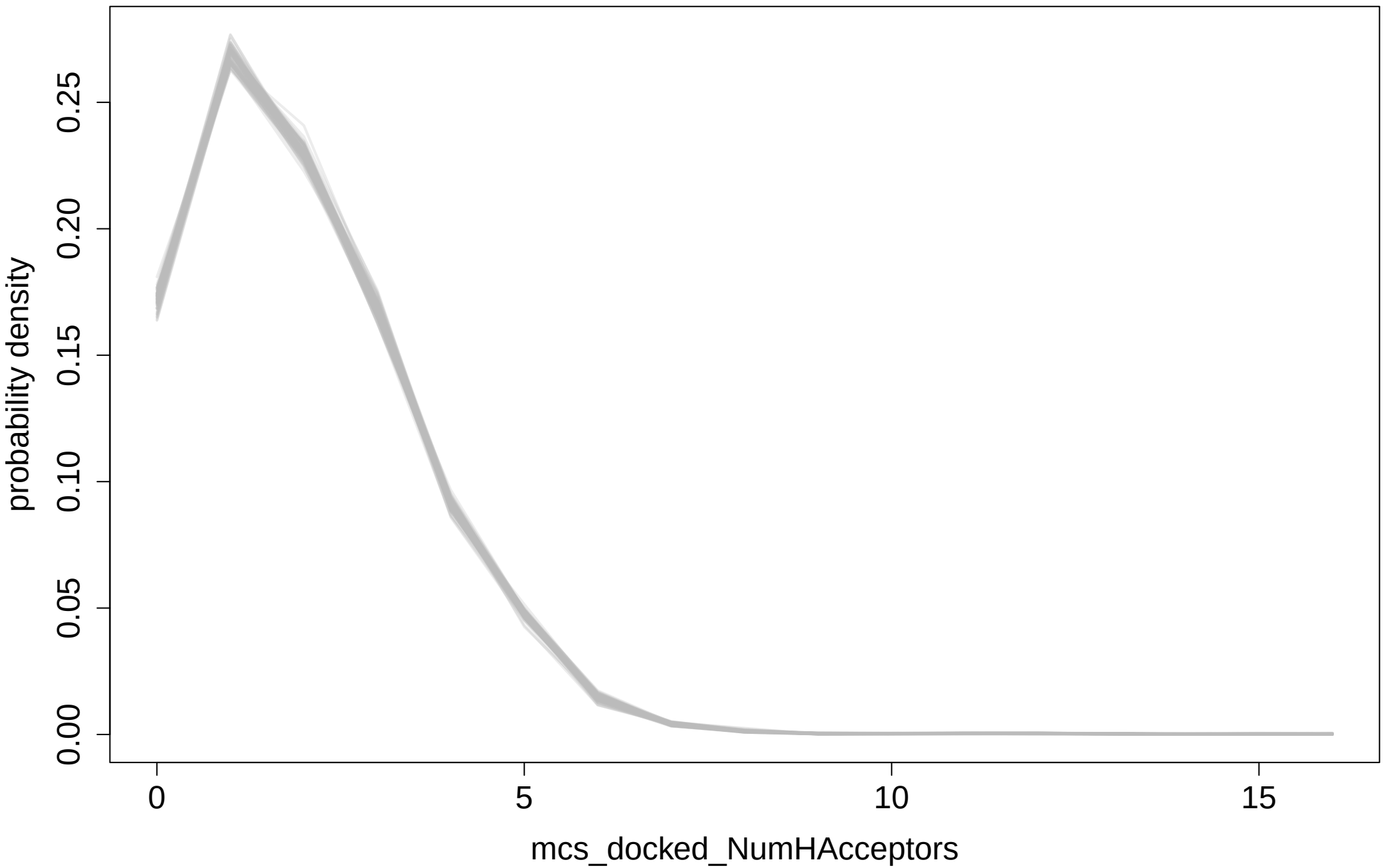

probability density
0.0
0.2
0.4
0.6
−2
−1
0
1
2
3
log_RMSD

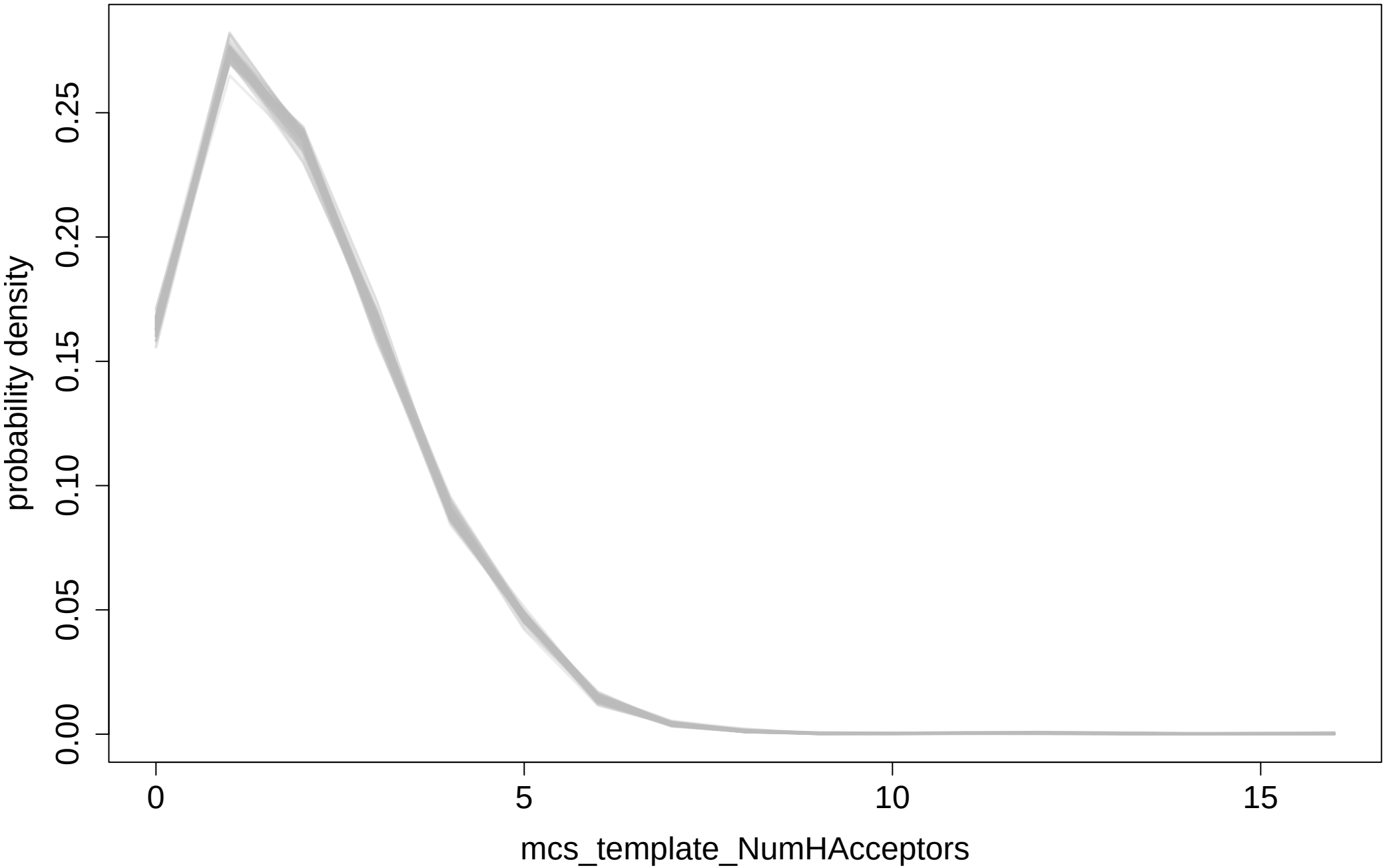

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

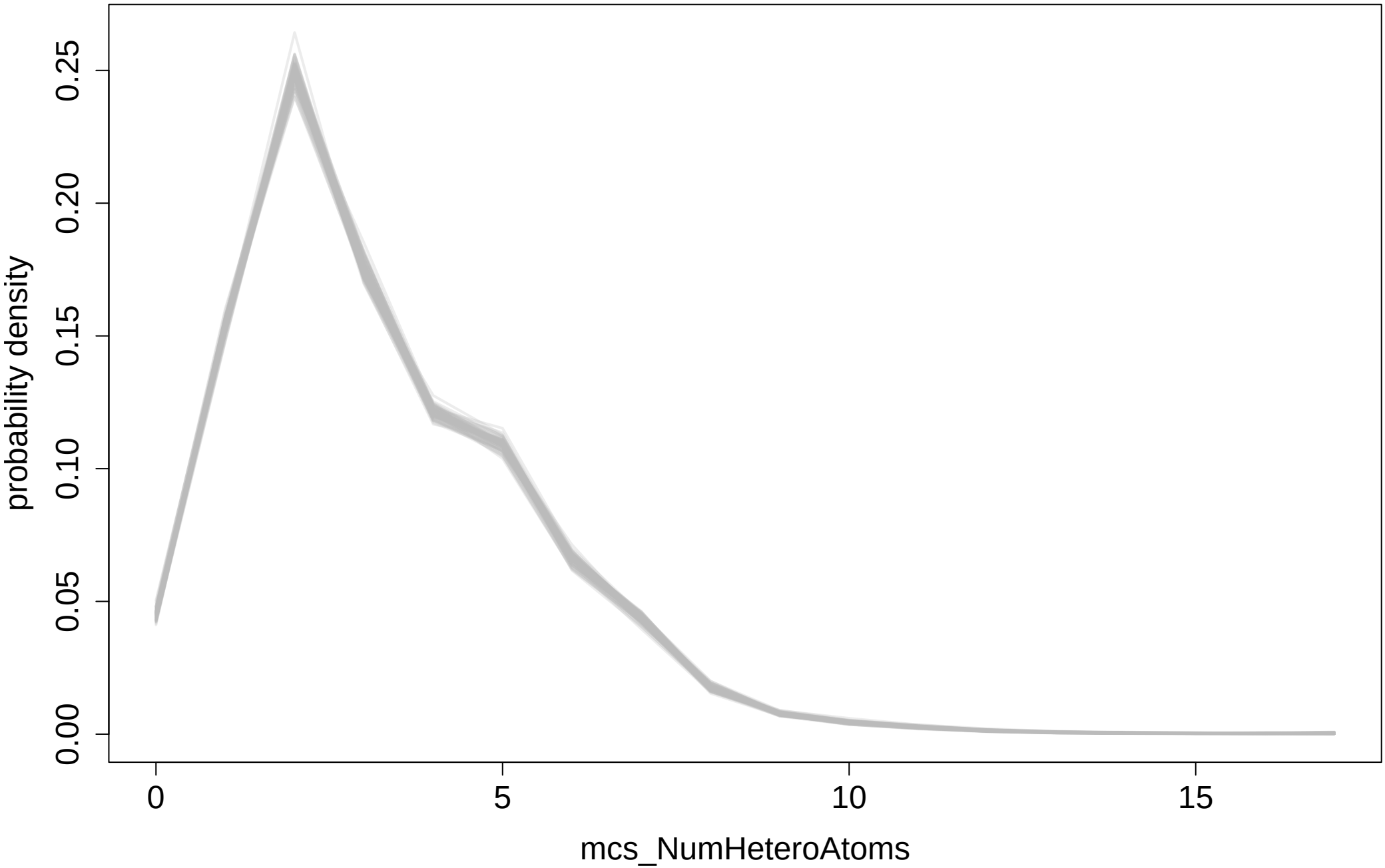

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

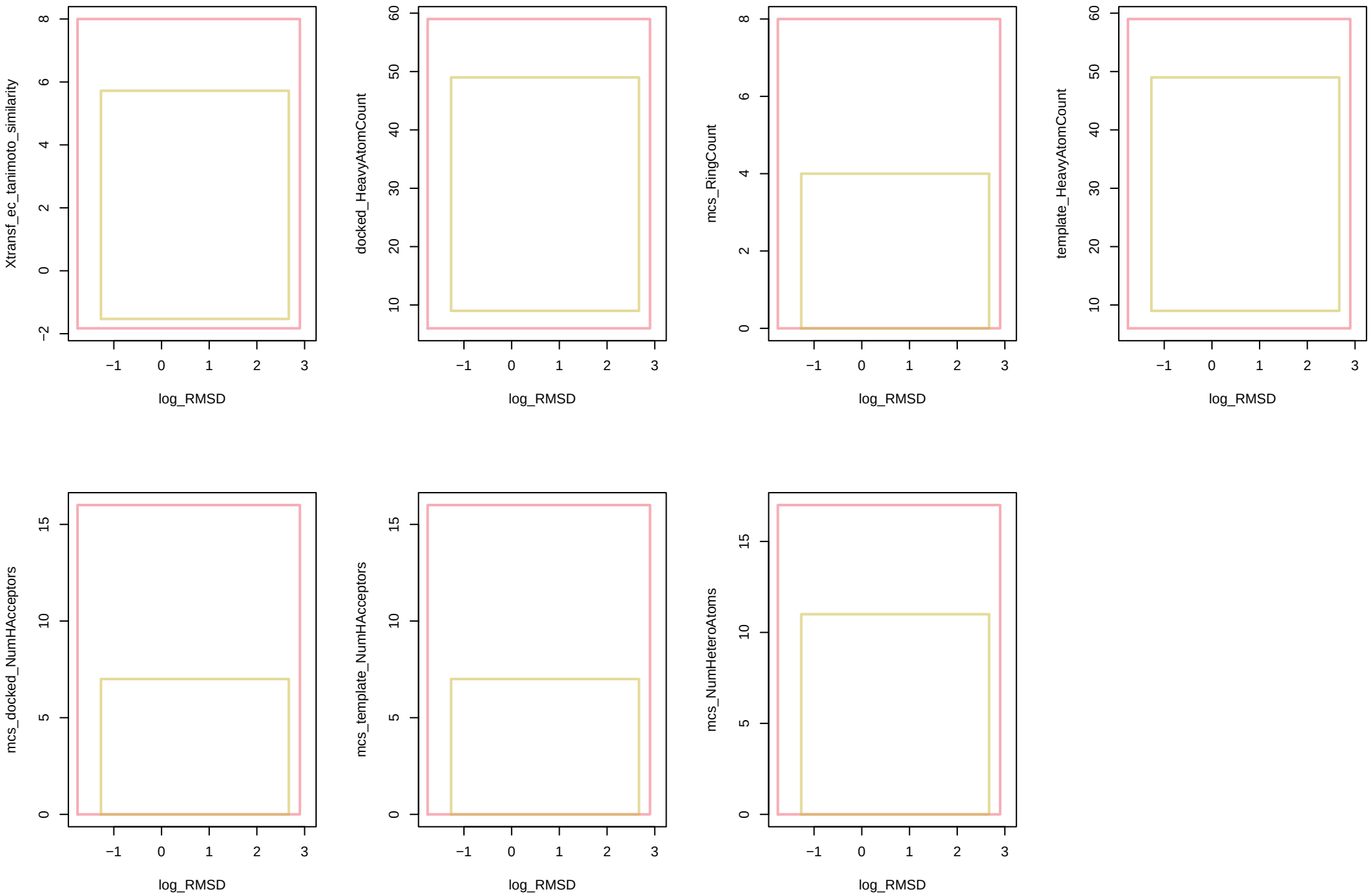

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

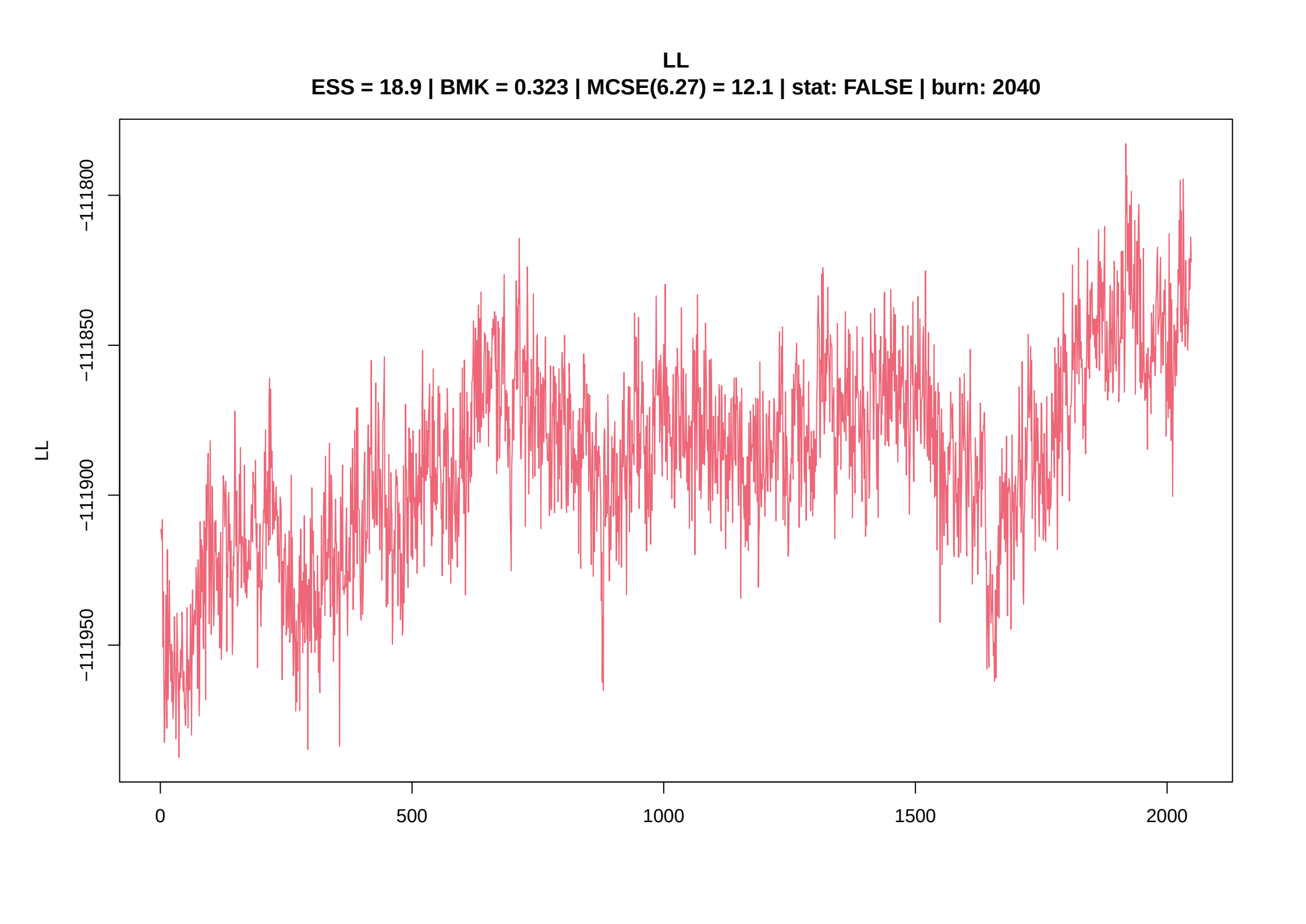

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

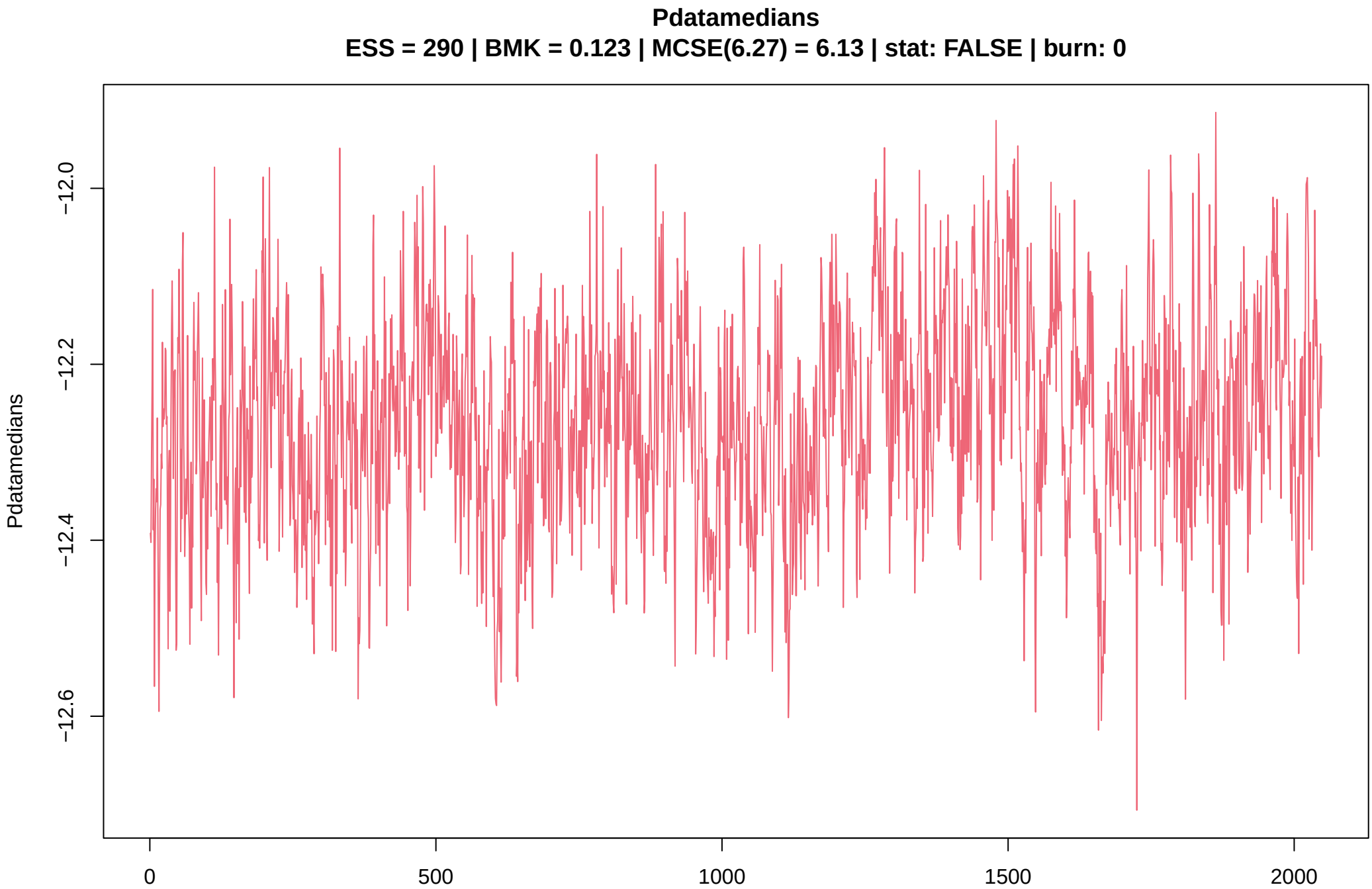

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_docked_NumHAcceptors

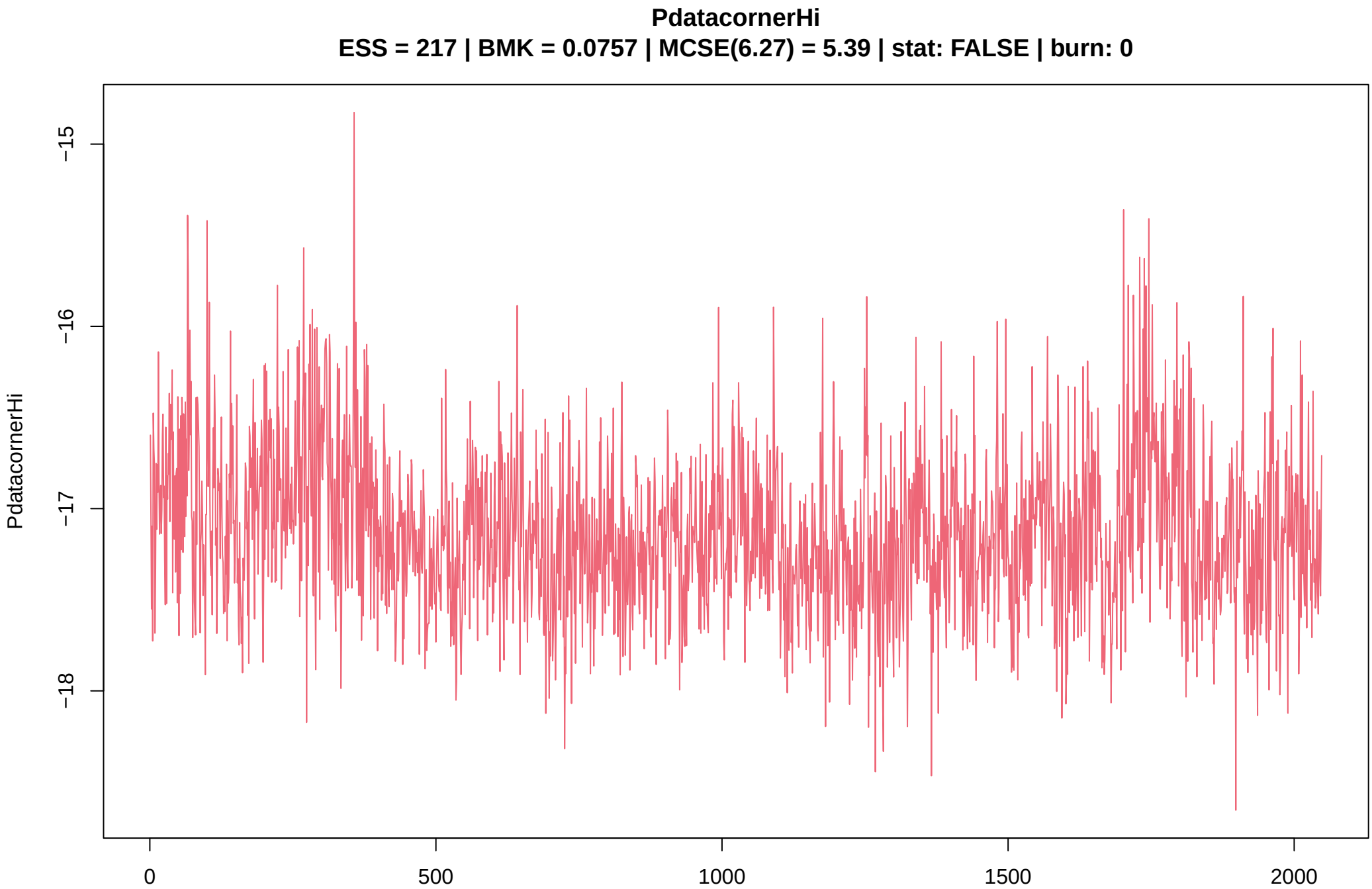

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_template_NumHAcceptors

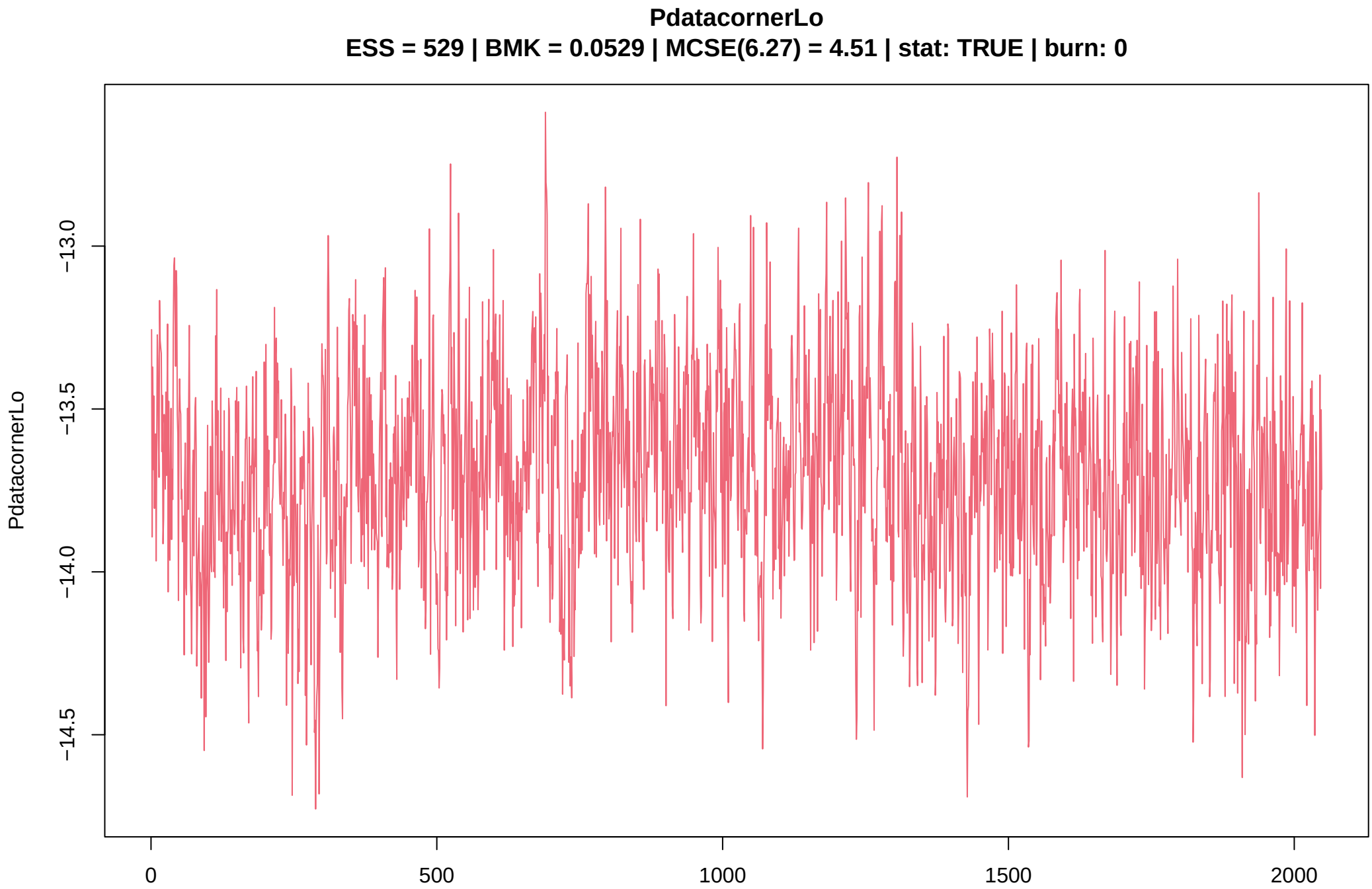

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

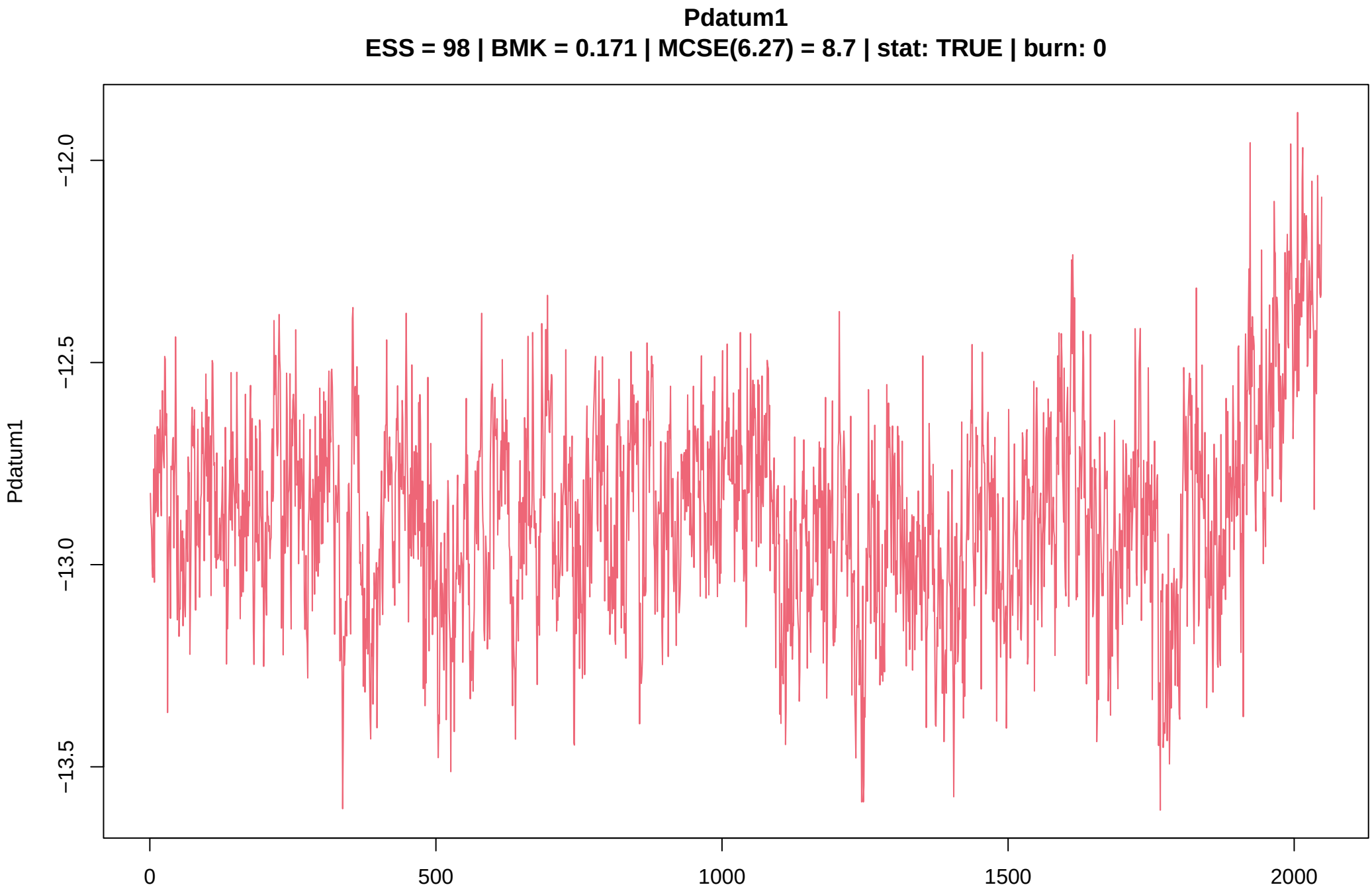

Xtransf_ec_tanimoto_similarity
docked_HeavyAtomCount
mcs_RingCount
template_HeavyAtomCount
mcs_docked_NumHAcceptors
mcs_template_NumHAcceptors
mcs_NumHeteroAtoms
log_RMSD

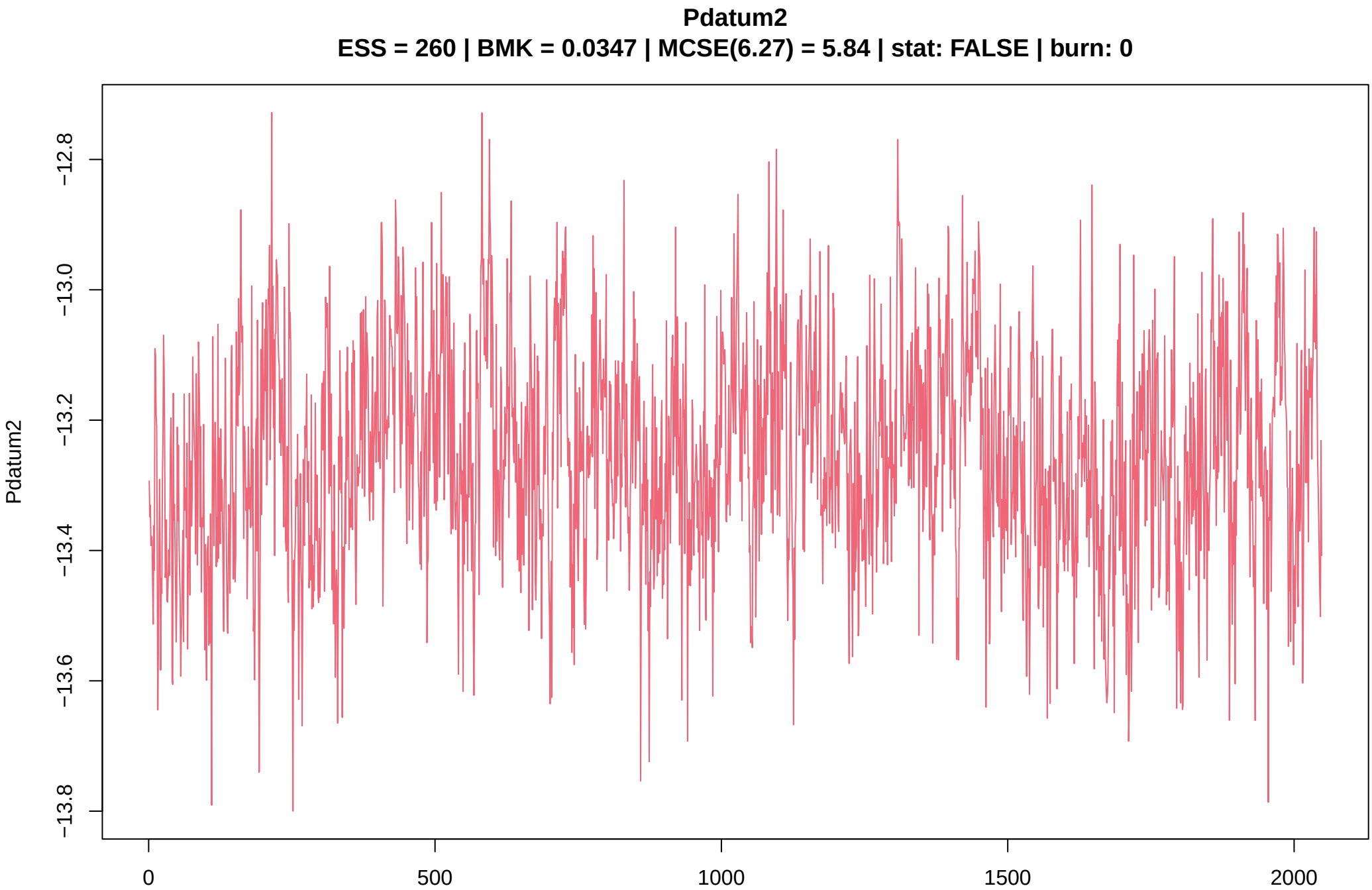

LL
ESS = 18.9 | BMK = 0.323 | MCSE(6.27) = 12.1 | stat: FALSE | burn: 2040
LL
−111800
−111850
−111900
−111950
0
500
1000
1500
2000

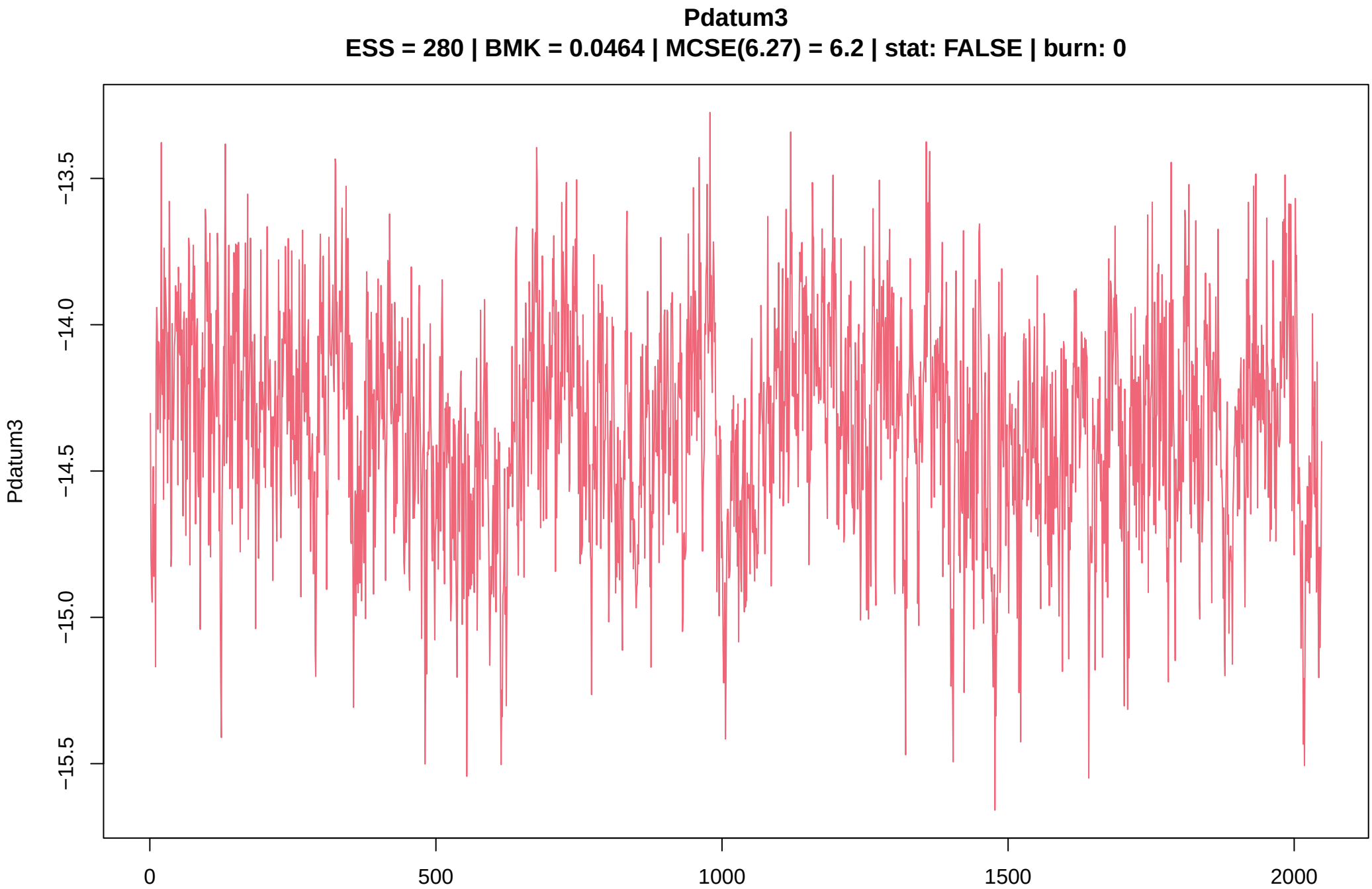

Pdatamedians
ESS = 290 | BMK = 0.123 | MCSE(6.27) = 6.13 | stat: FALSE | burn: 0
Pdatamedians
−12.0
−12.2
−12.4
−12.6
0
500
1000
1500
2000

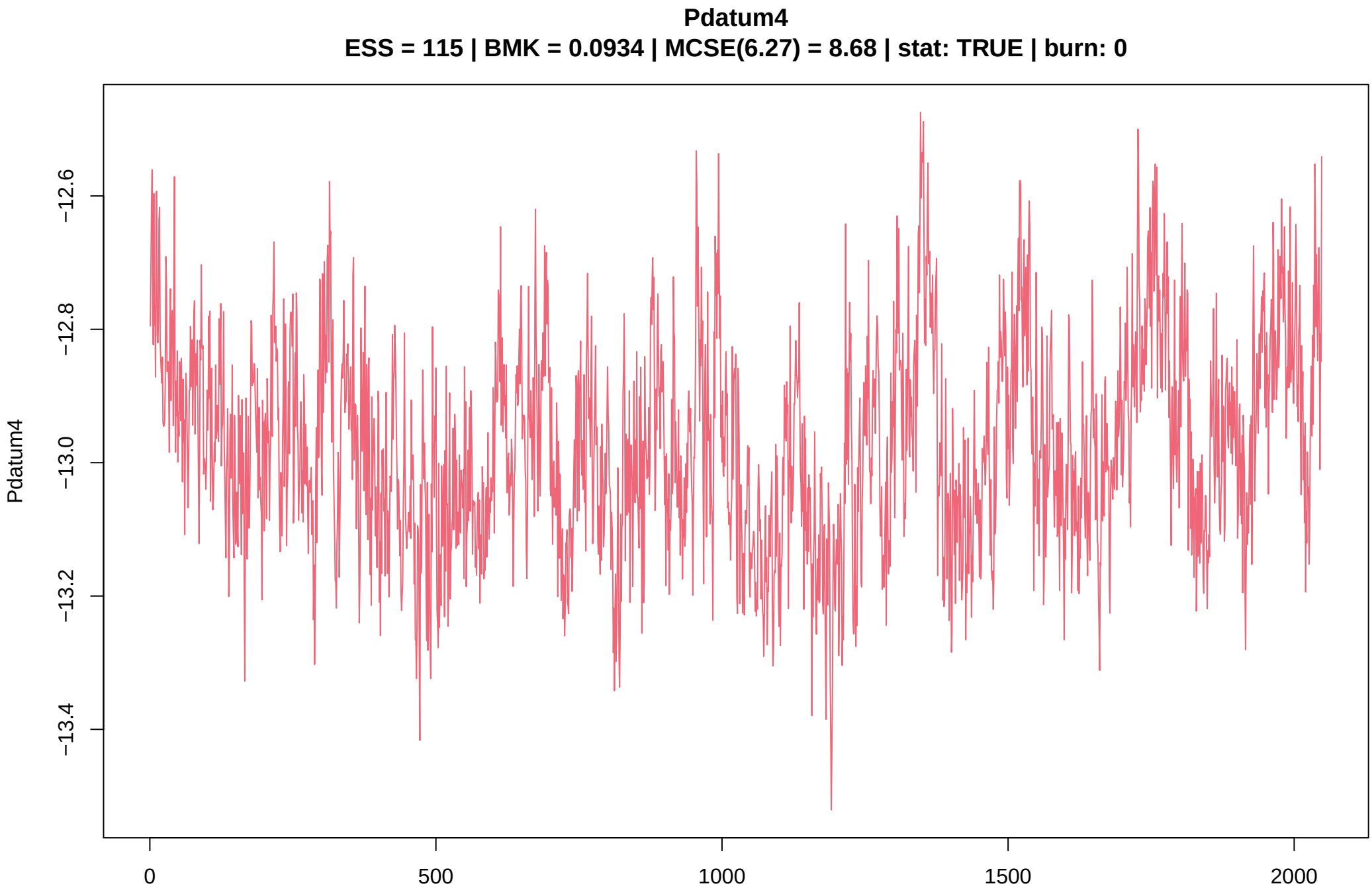

PdatacornerHi
ESS = 217 | BMK = 0.0757 | MCSE(6.27) = 5.39 | stat: FALSE | burn: 0
PdatacornerHi
−15
−16
−17
−18
0
500
1000
1500
2000

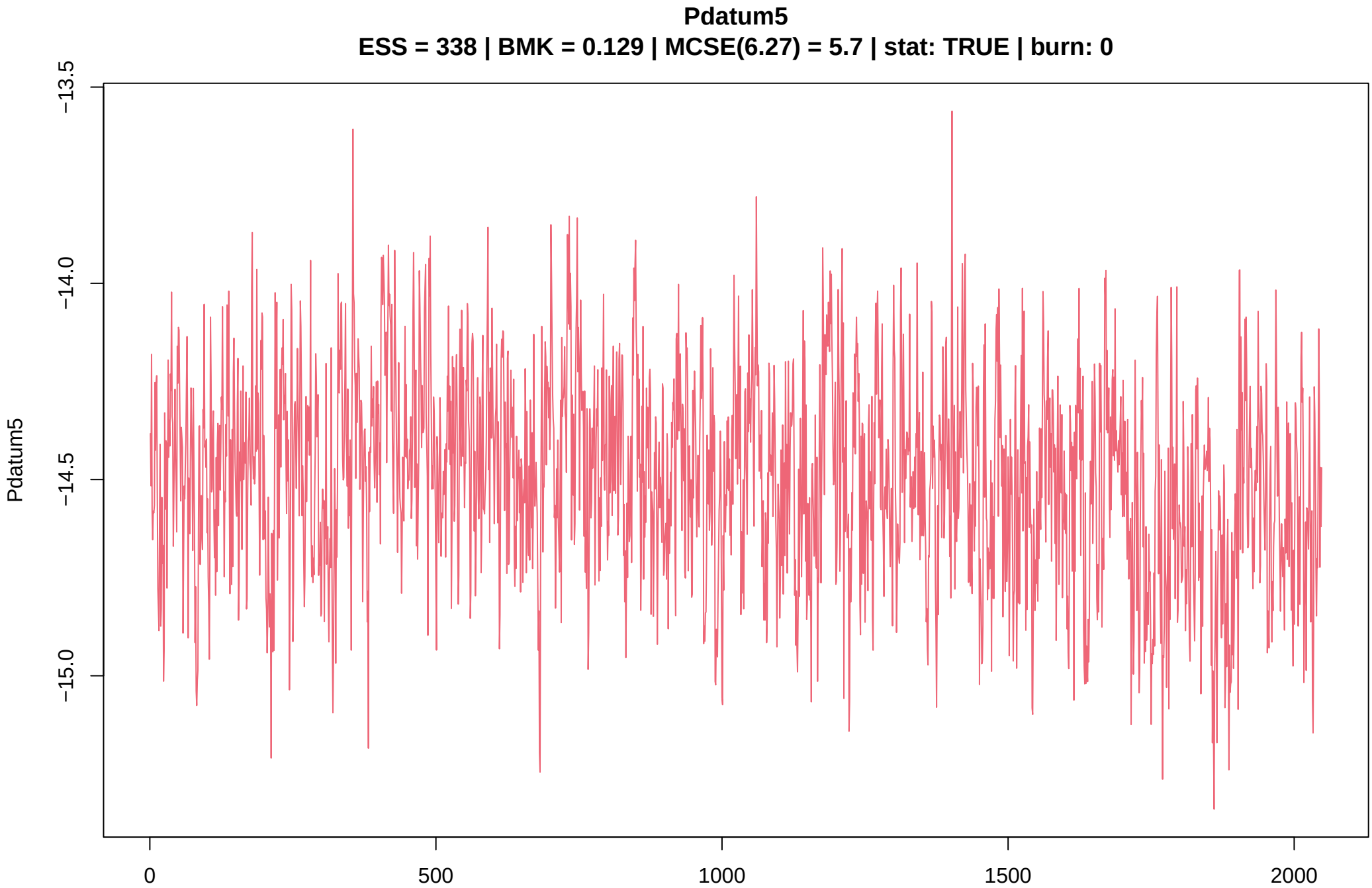

PdatacornerLo
ESS = 529 | BMK = 0.0529 | MCSE(6.27) = 4.51 | stat: TRUE | burn: 0
PdatacornerLo
−13.0
−13.5
−14.0
−14.5
0
500
1000
1500
2000

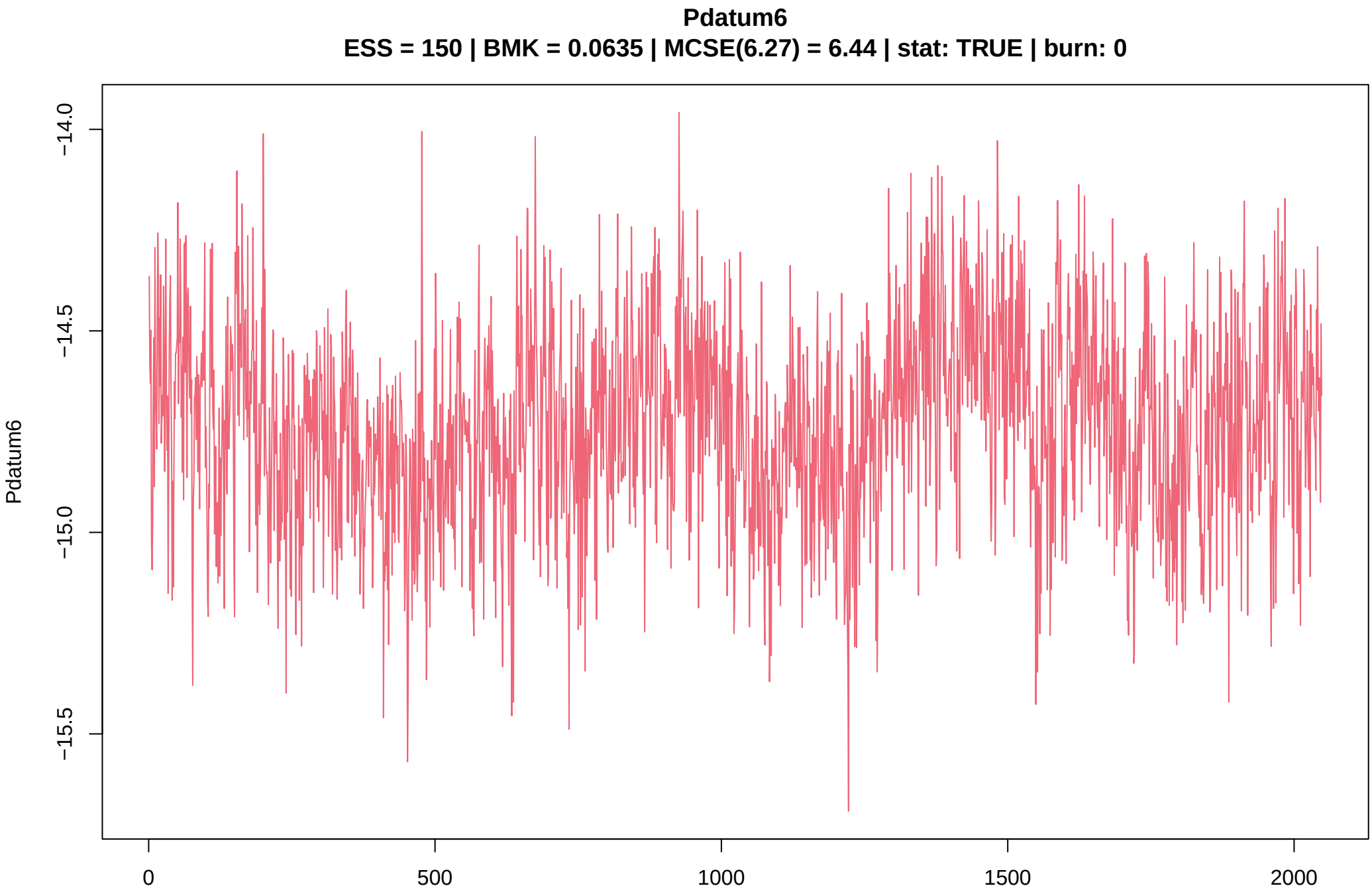

Pdatum1
ESS = 98 | BMK = 0.171 | MCSE(6.27) = 8.7 | stat: TRUE | burn: 0
Pdatum1
−12.0
−12.5
−13.0
−13.5
0
500
1000
1500
2000

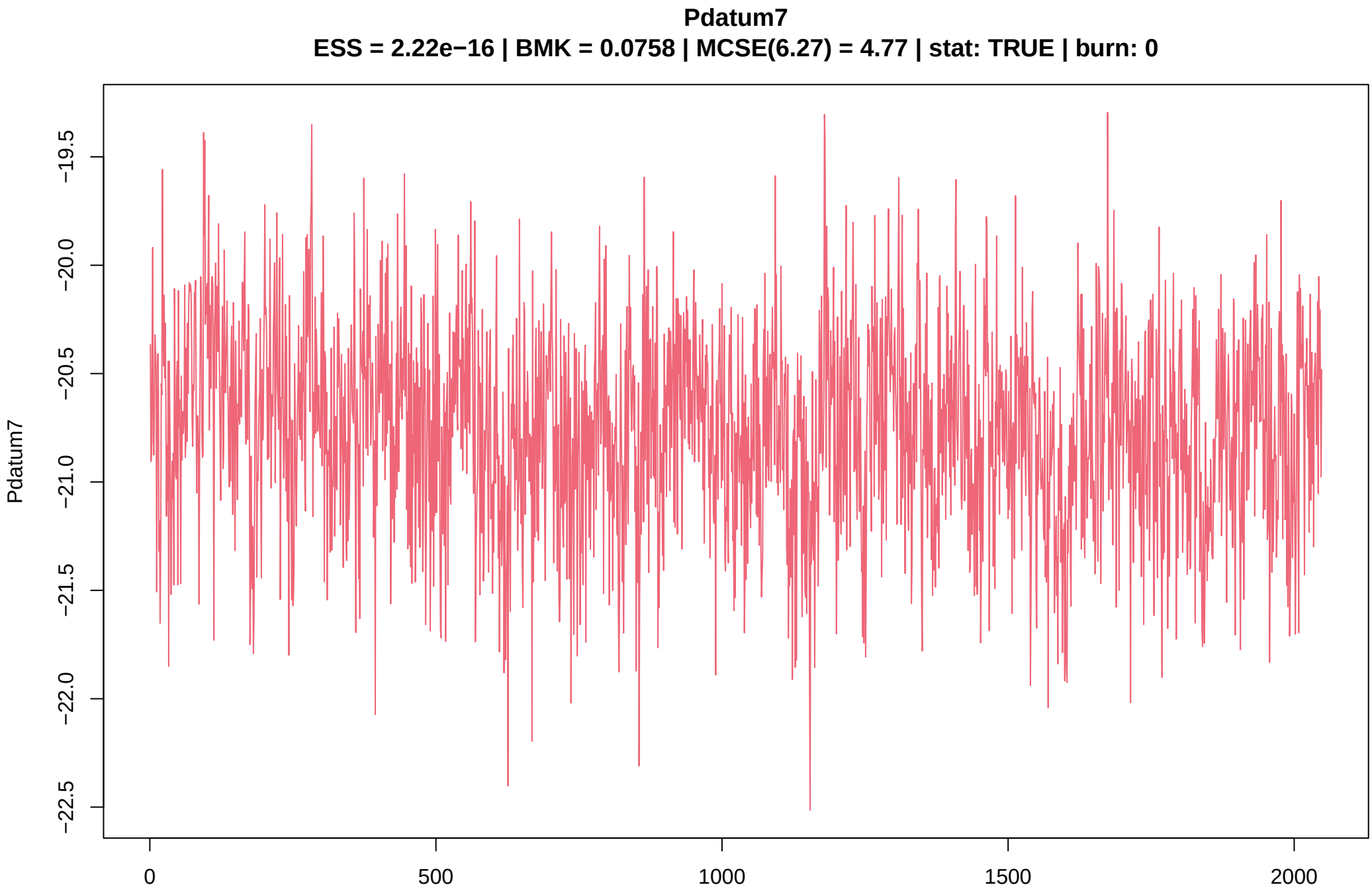

Pdatum2
ESS = 260 | BMK = 0.0347 | MCSE(6.27) = 5.84 | stat: FALSE | burn: 0
Pdatum2
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
0
500
1000
1500
2000

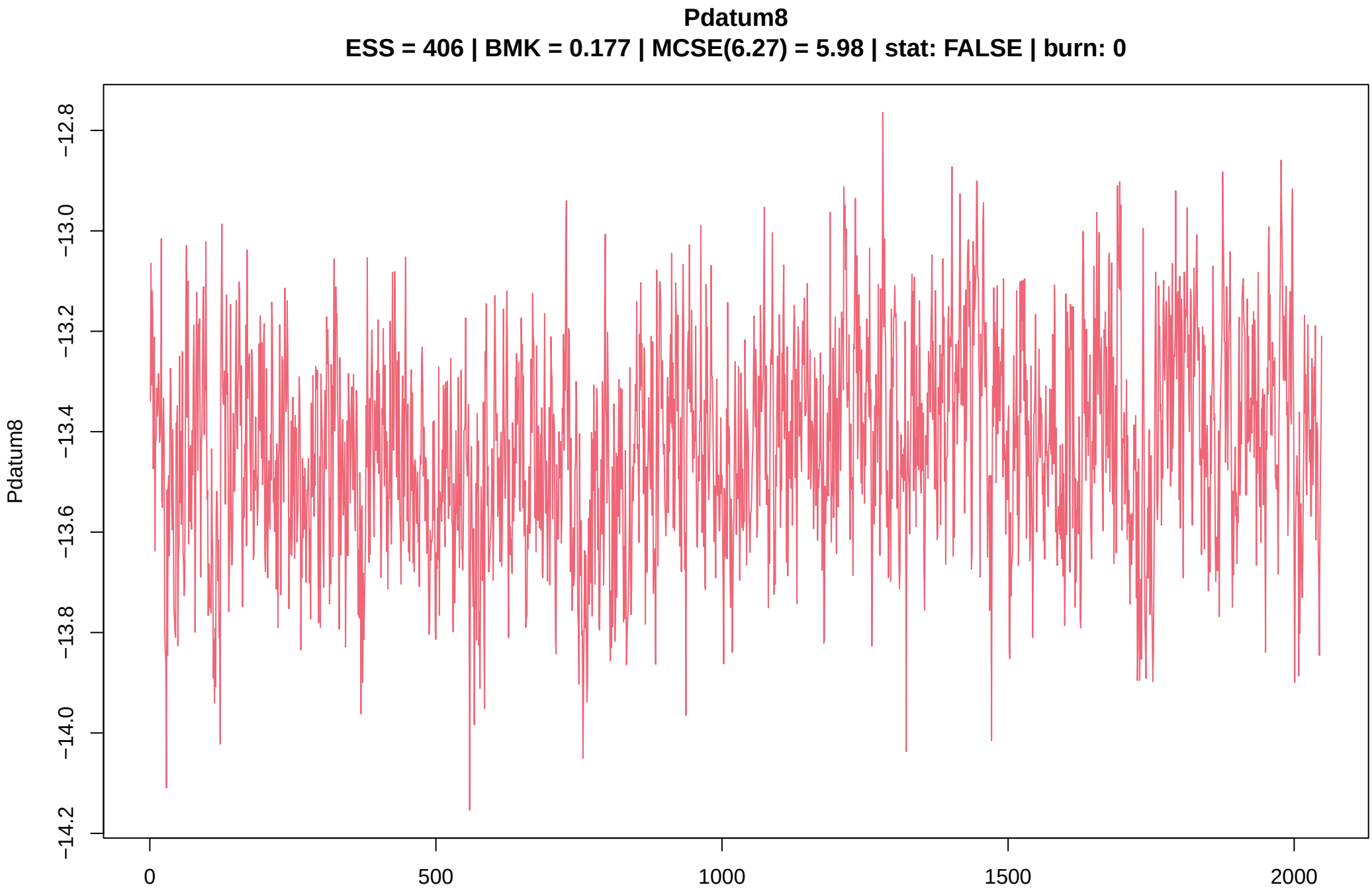

Pdatum3
ESS = 280 | BMK = 0.0464 | MCSE(6.27) = 6.2 | stat: FALSE | burn: 0
Pdatum3
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

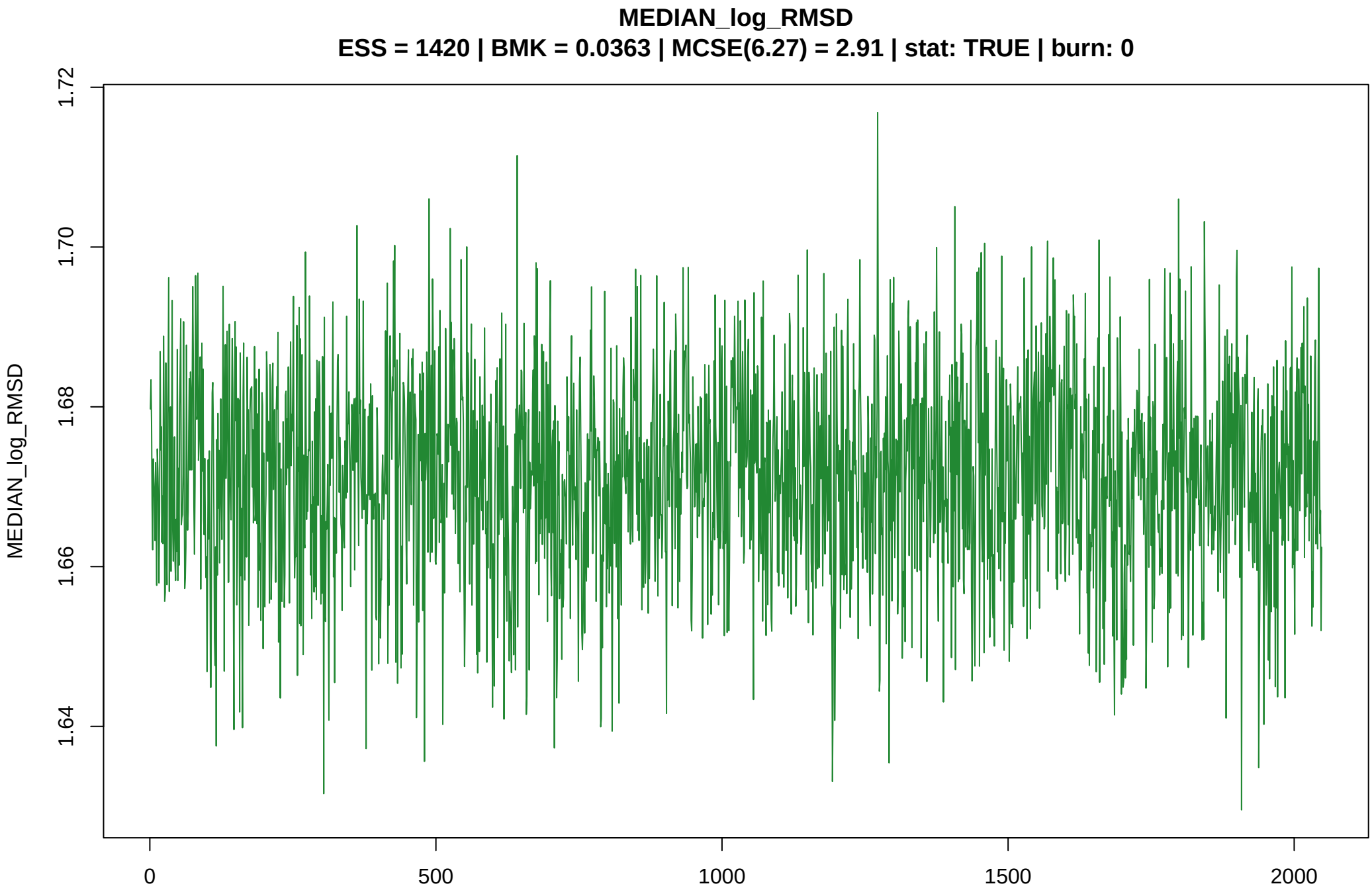

Pdatum4
ESS = 115 | BMK = 0.0934 | MCSE(6.27) = 8.68 | stat: TRUE | burn: 0
Pdatum4
−12.6
−12.8
−13.0
−13.2
−13.4
0
500
1000
1500
2000

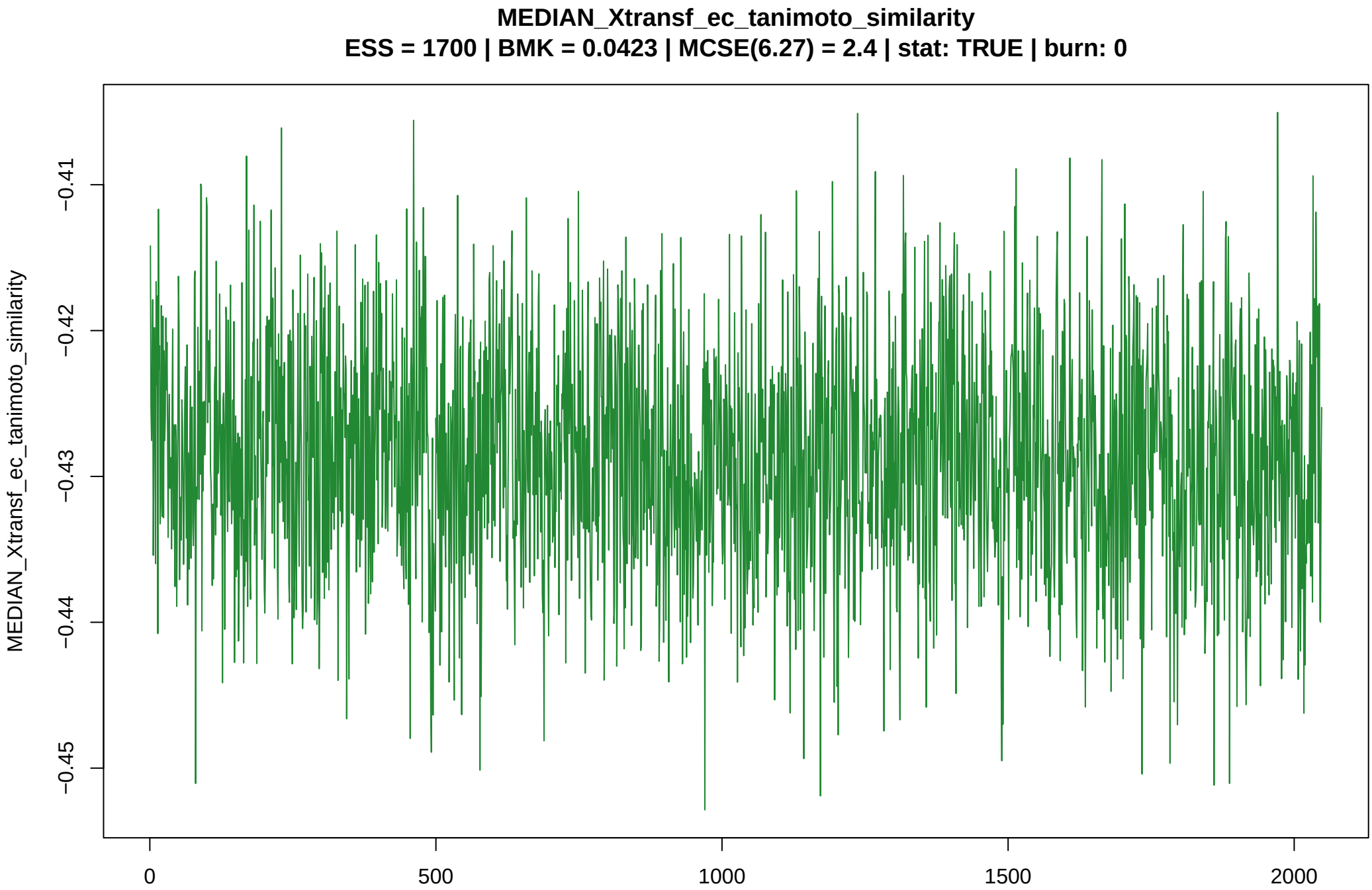

Pdatum5
ESS = 338 | BMK = 0.129 | MCSE(6.27) = 5.7 | stat: TRUE | burn: 0
Pdatum5
−13.5
−14.0
−14.5
−15.0
0
500
1000
1500
2000

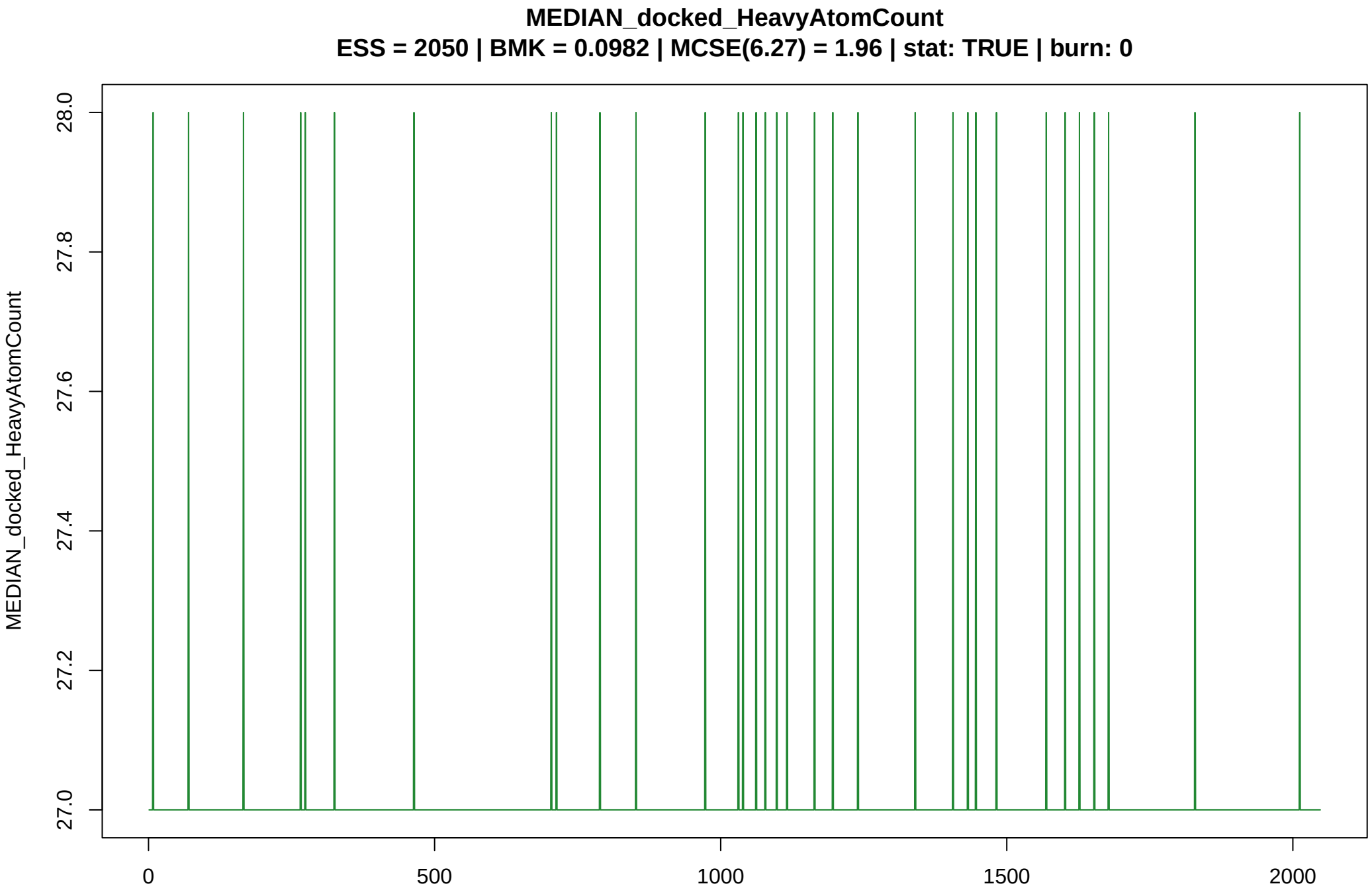

Pdatum6
ESS = 150 | BMK = 0.0635 | MCSE(6.27) = 6.44 | stat: TRUE | burn: 0
Pdatum6
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

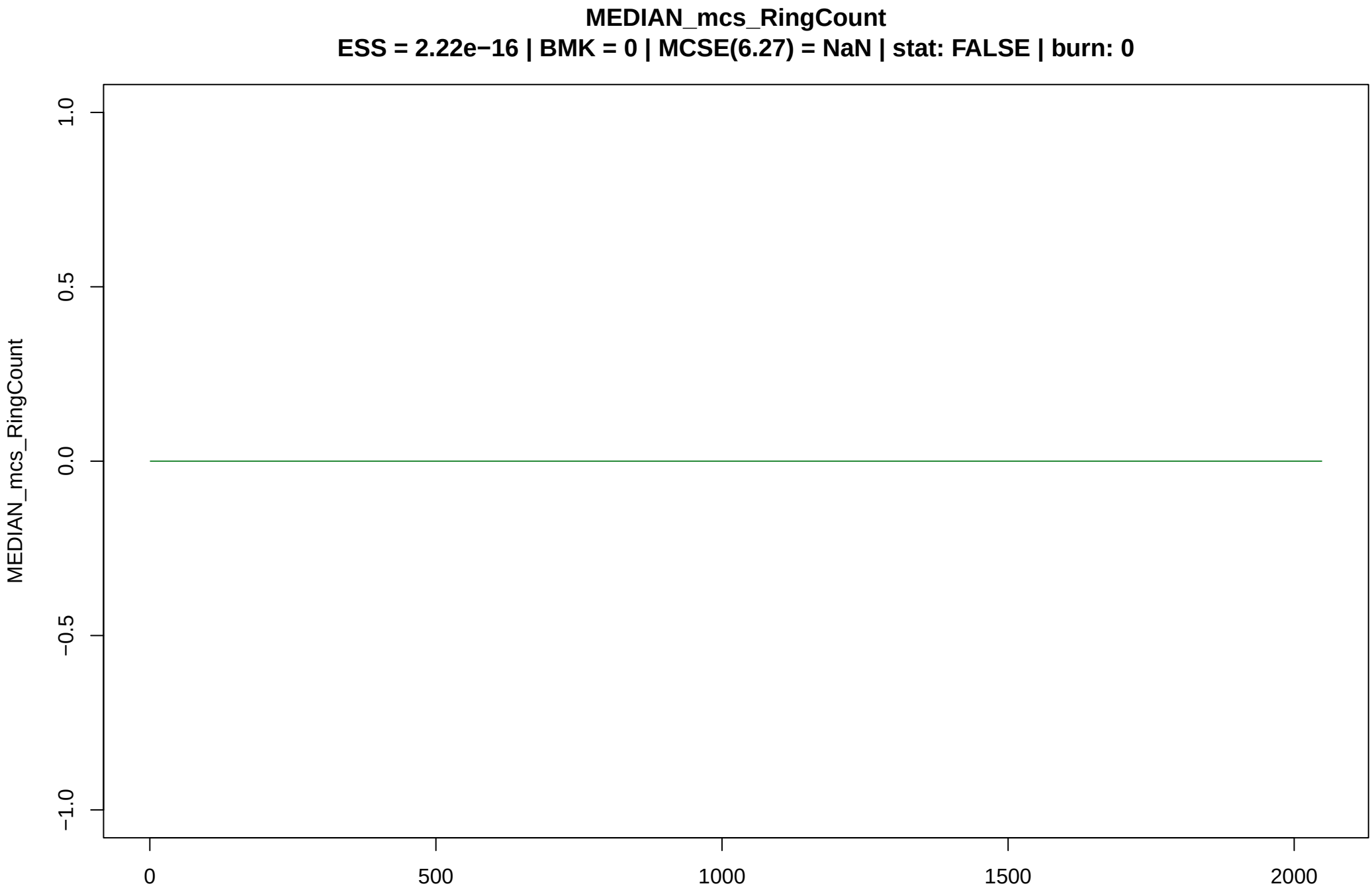

Pdatum7
ESS = 2.22e−16 | BMK = 0.0758 | MCSE(6.27) = 4.77 | stat: TRUE | burn: 0
Pdatum7
−19.5
−20.0
−20.5
−21.0
−21.5
−22.0
−22.5
0
500
1000
1500
2000

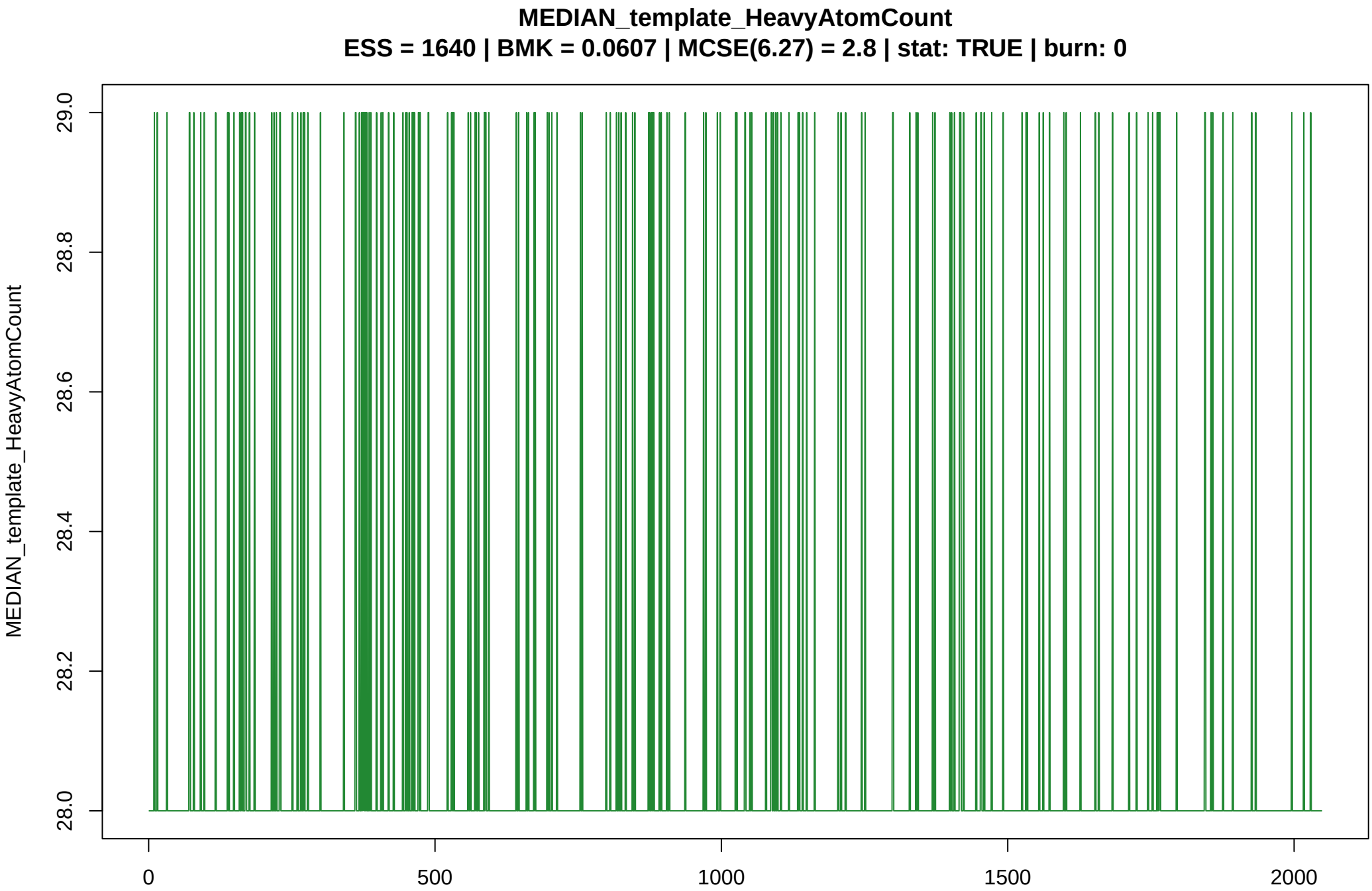

Pdatum8
ESS = 406 | BMK = 0.177 | MCSE(6.27) = 5.98 | stat: FALSE | burn: 0
Pdatum8
−12.8
−13.0
−13.2
−13.4
−13.6
−13.8
−14.0
−14.2
0
500
1000
1500
2000

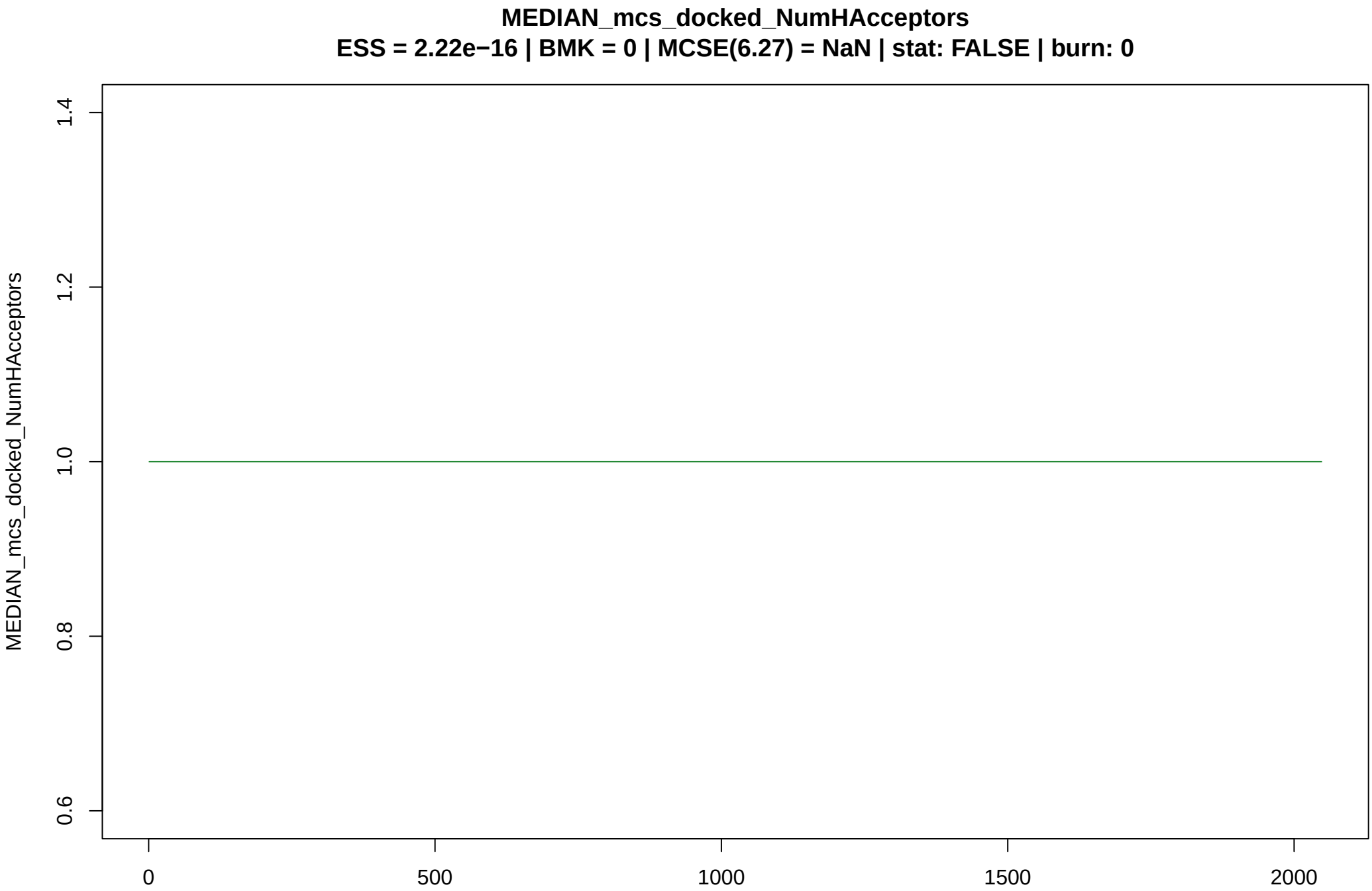

MEDIAN_log_RMSD
ESS = 1420 | BMK = 0.0363 | MCSE(6.27) = 2.91 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
1.72
1.70
1.68
1.66
1.64
0
500
1000
1500
2000

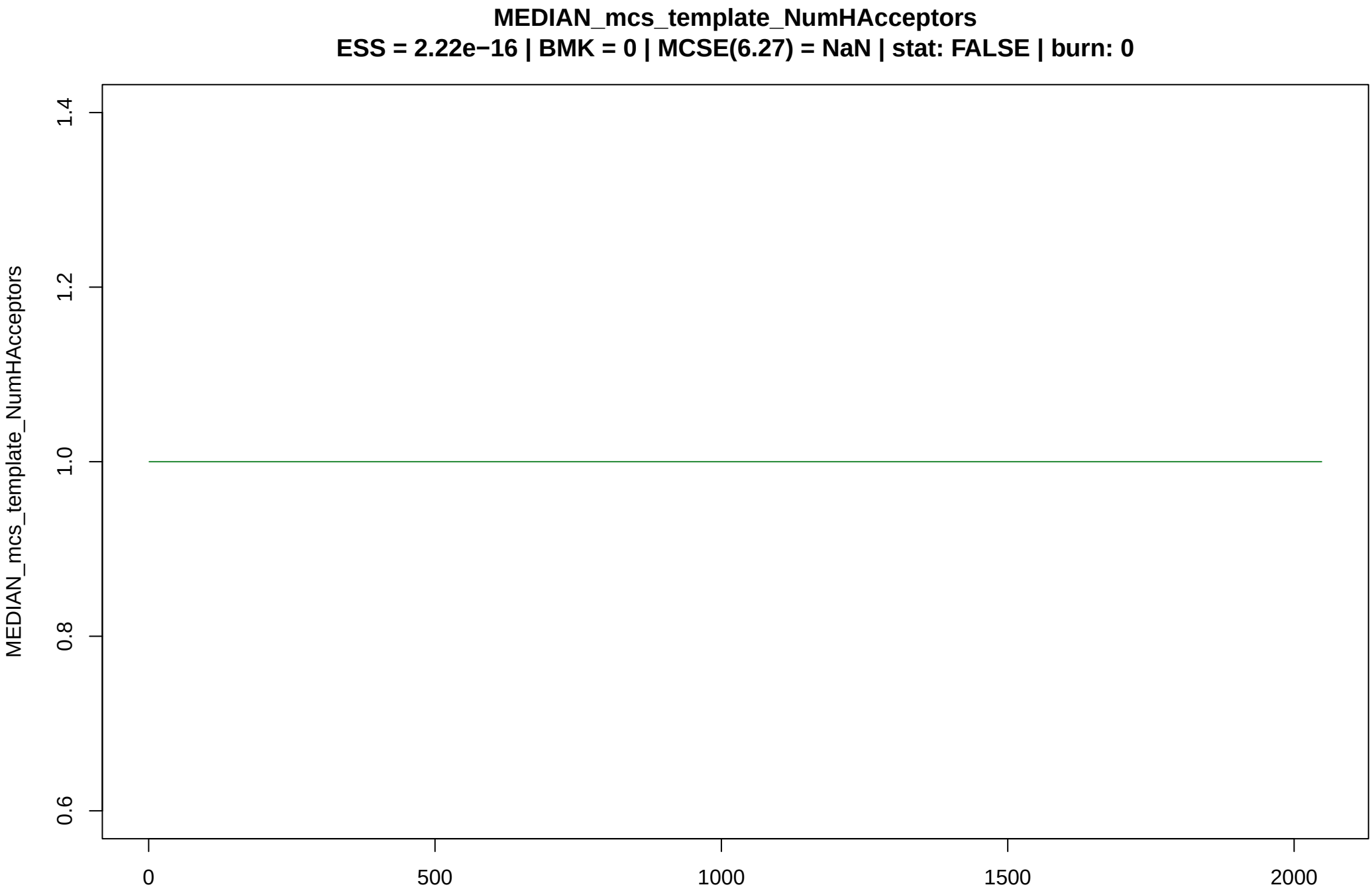

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1700 | BMK = 0.0423 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.41
−0.42
−0.43
−0.44
−0.45
0
500
1000
1500
2000

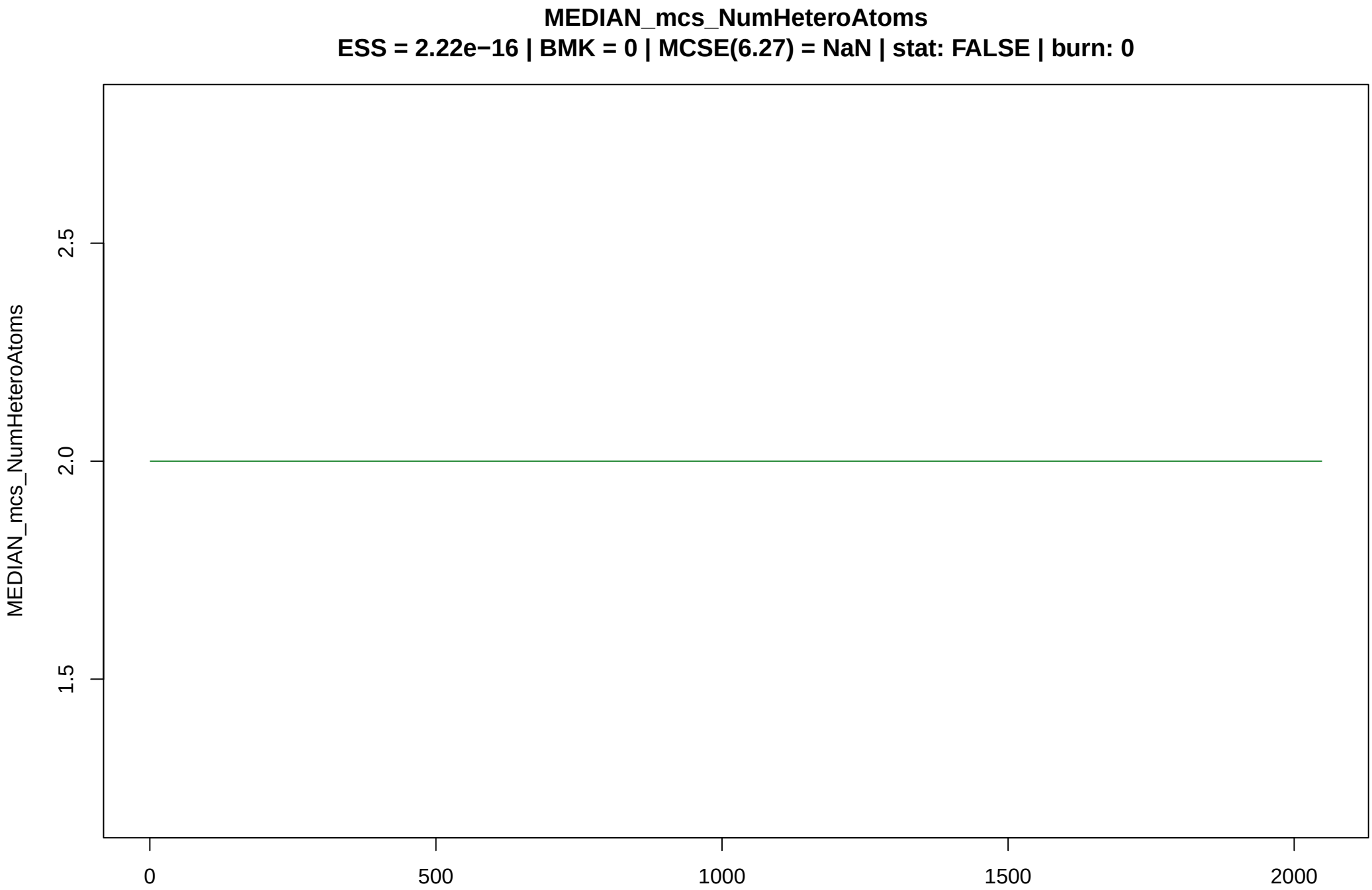

MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0982 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

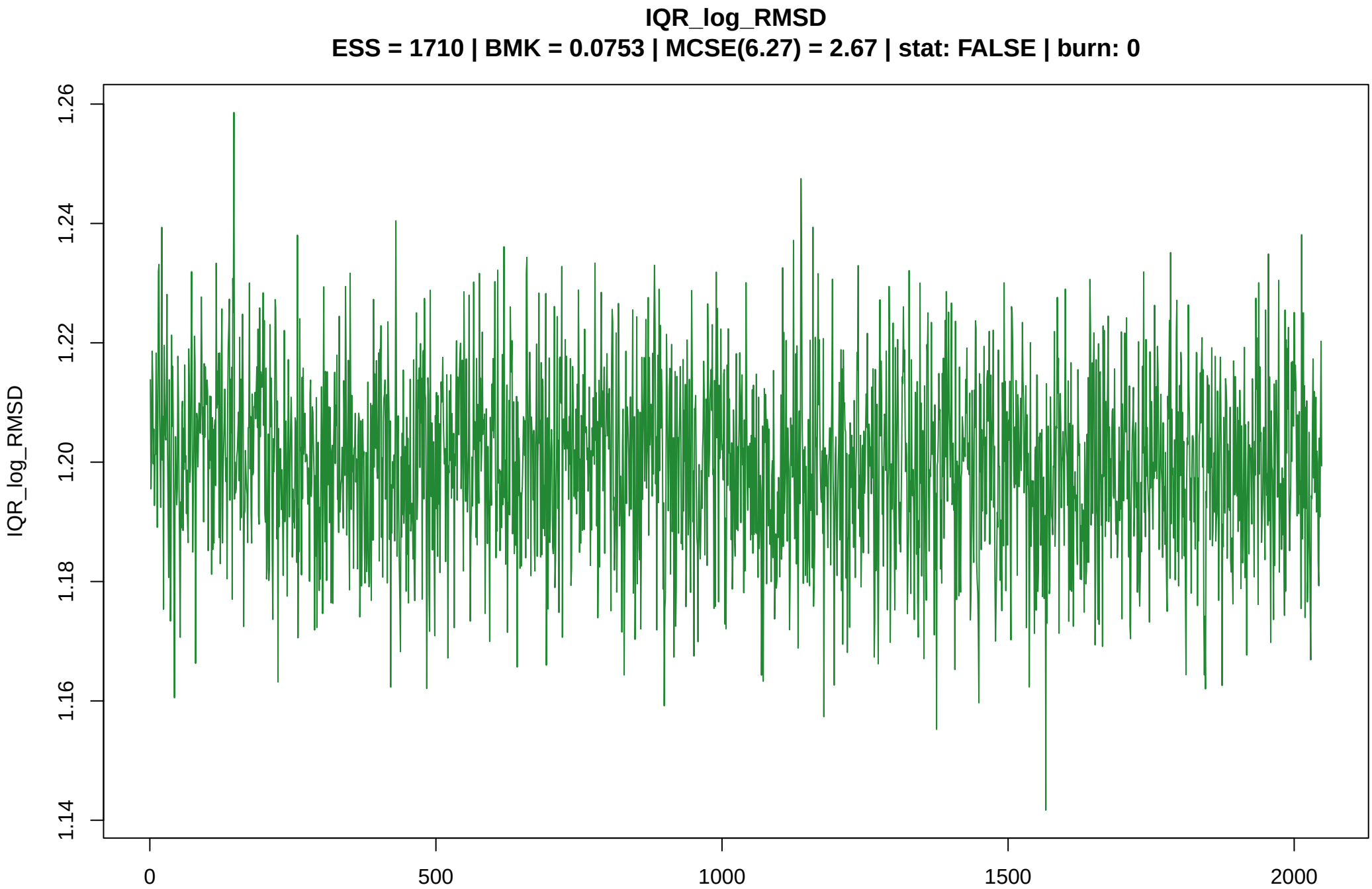

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

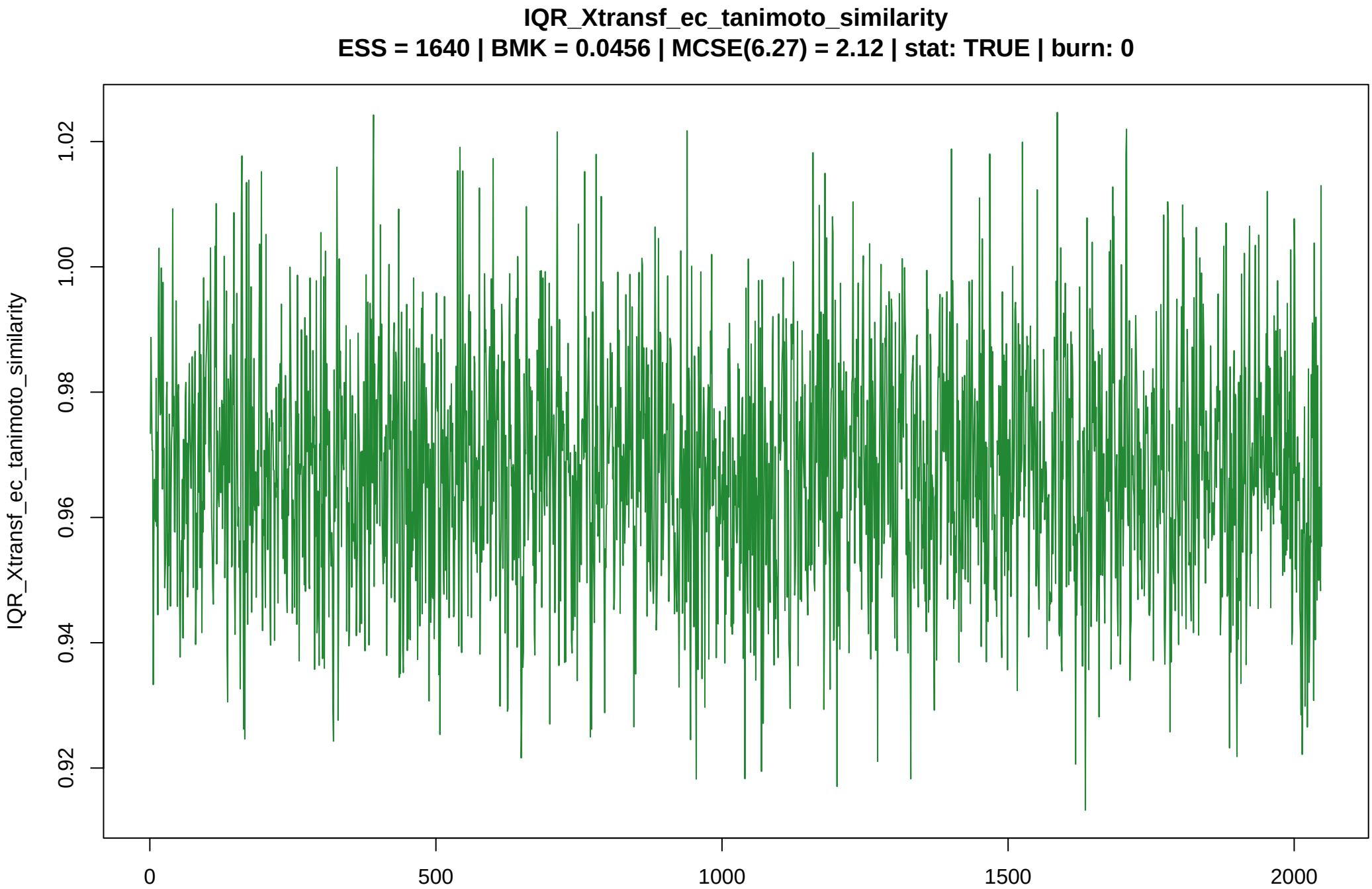

MEDIAN_template_HeavyAtomCount
ESS = 1640 | BMK = 0.0607 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

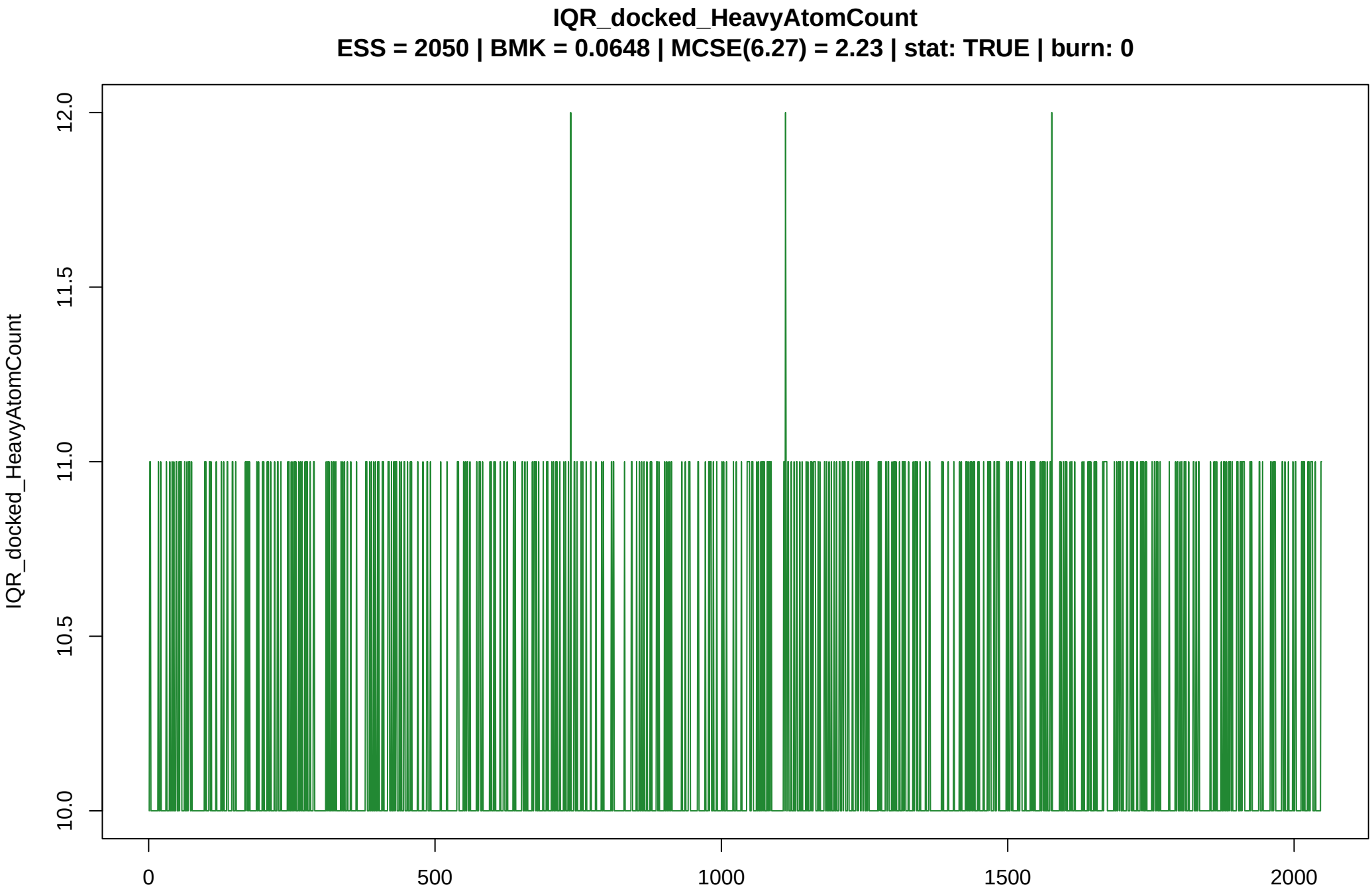

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

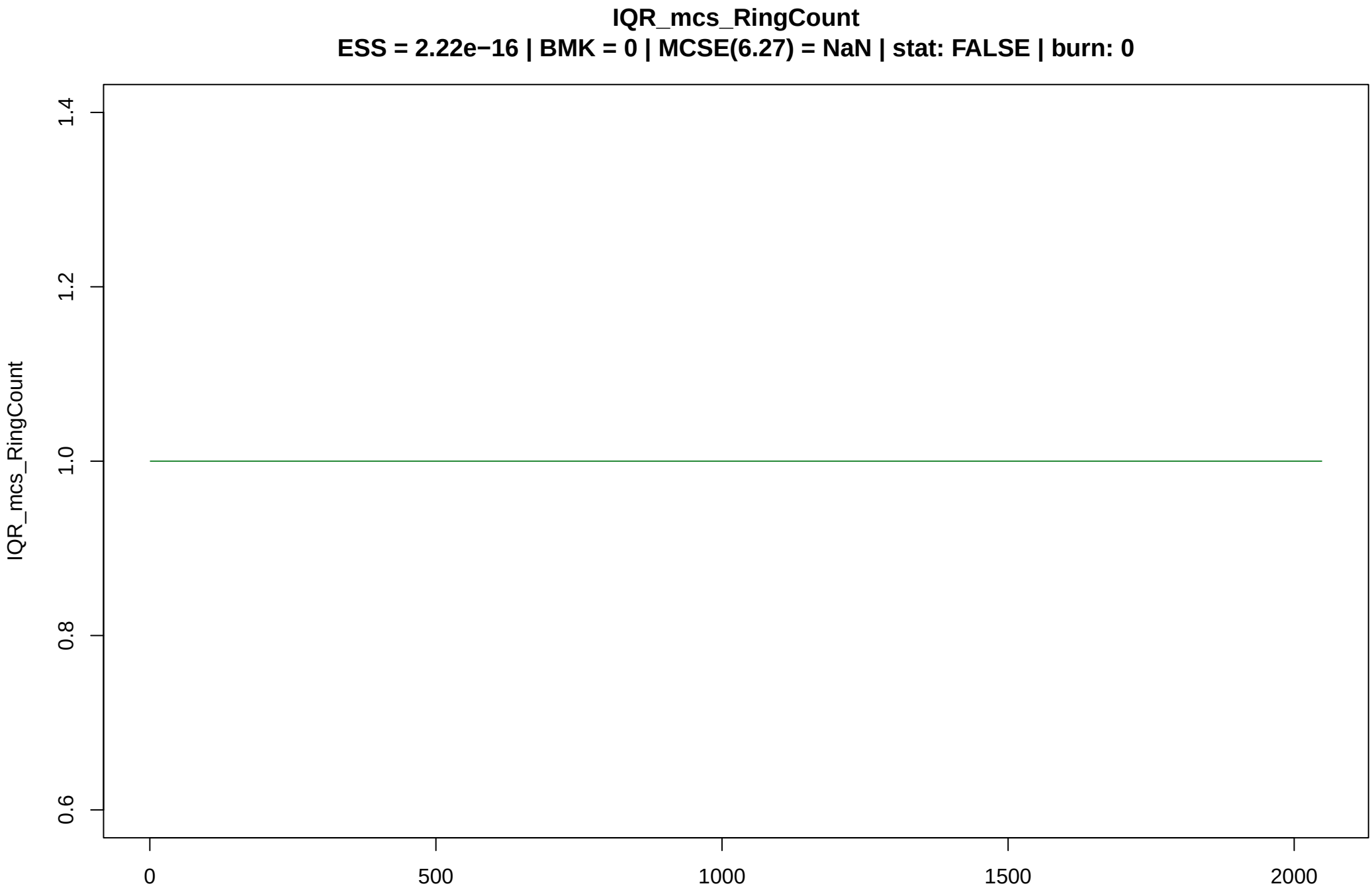

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

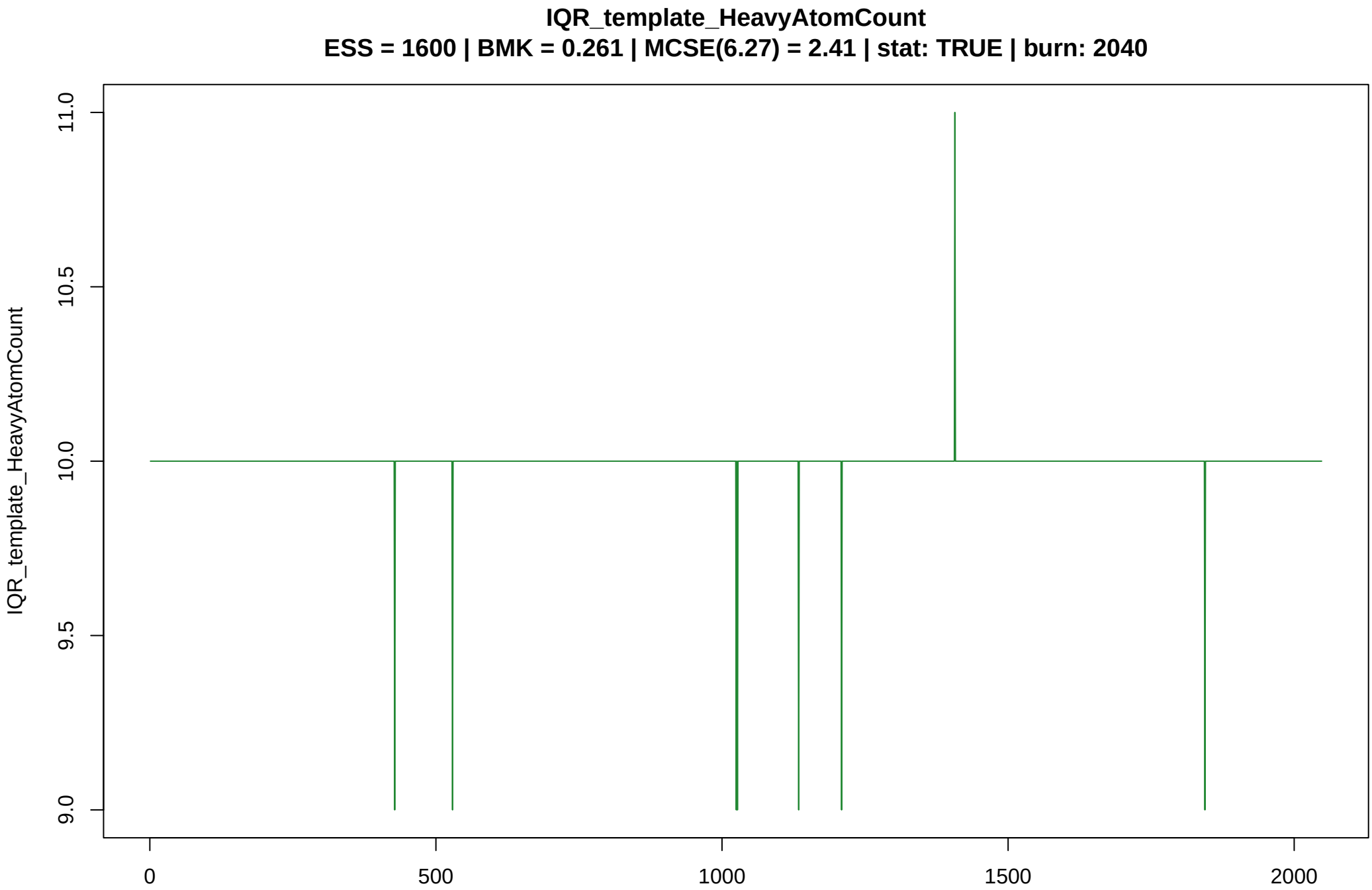

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

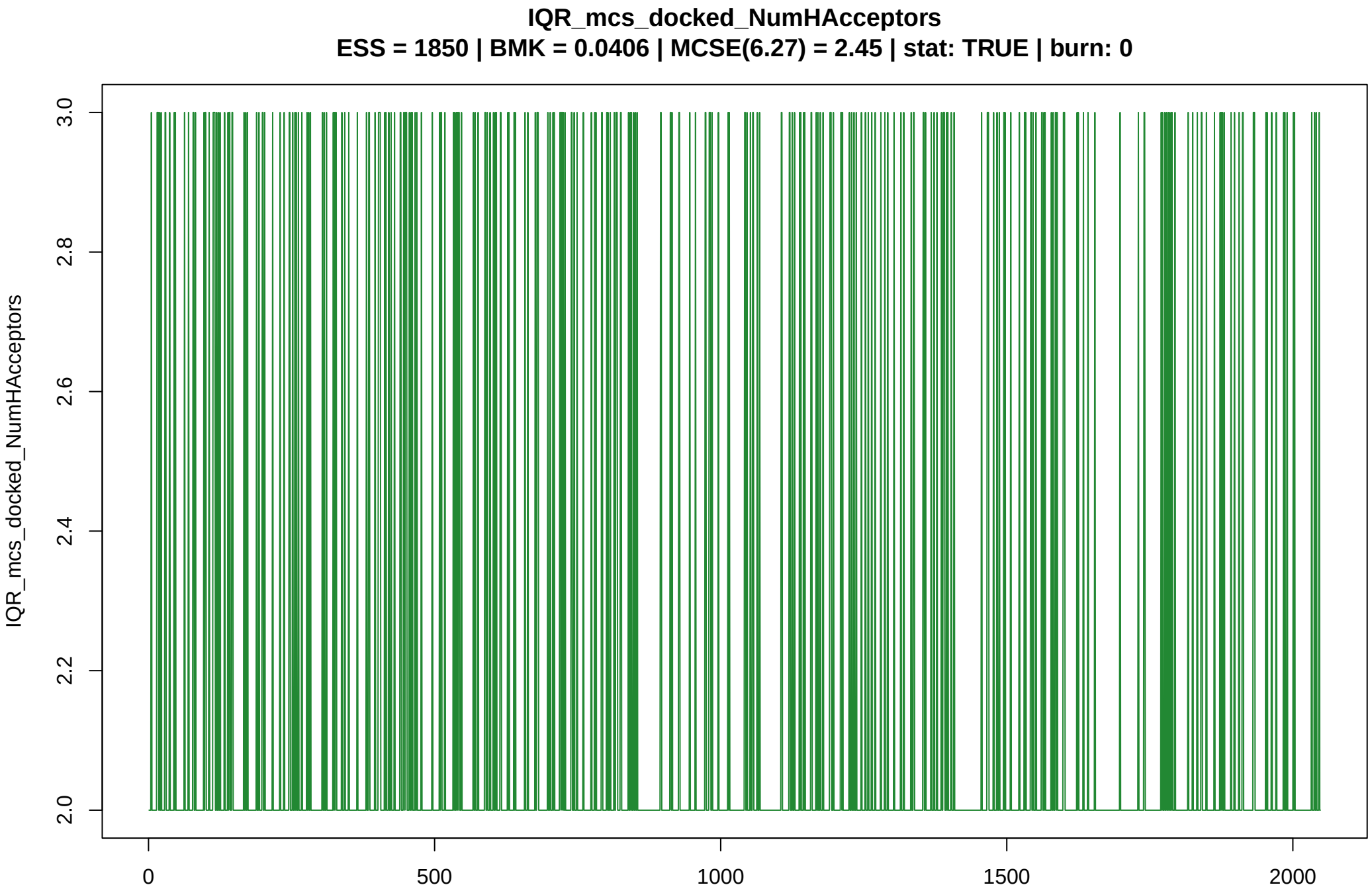

IQR_log_RMSD
ESS = 1710 | BMK = 0.0753 | MCSE(6.27) = 2.67 | stat: FALSE | burn: 0
IQR_log_RMSD
1.14
1.16
1.18
1.20
1.22
1.24
1.26
0
500
1000
1500
2000

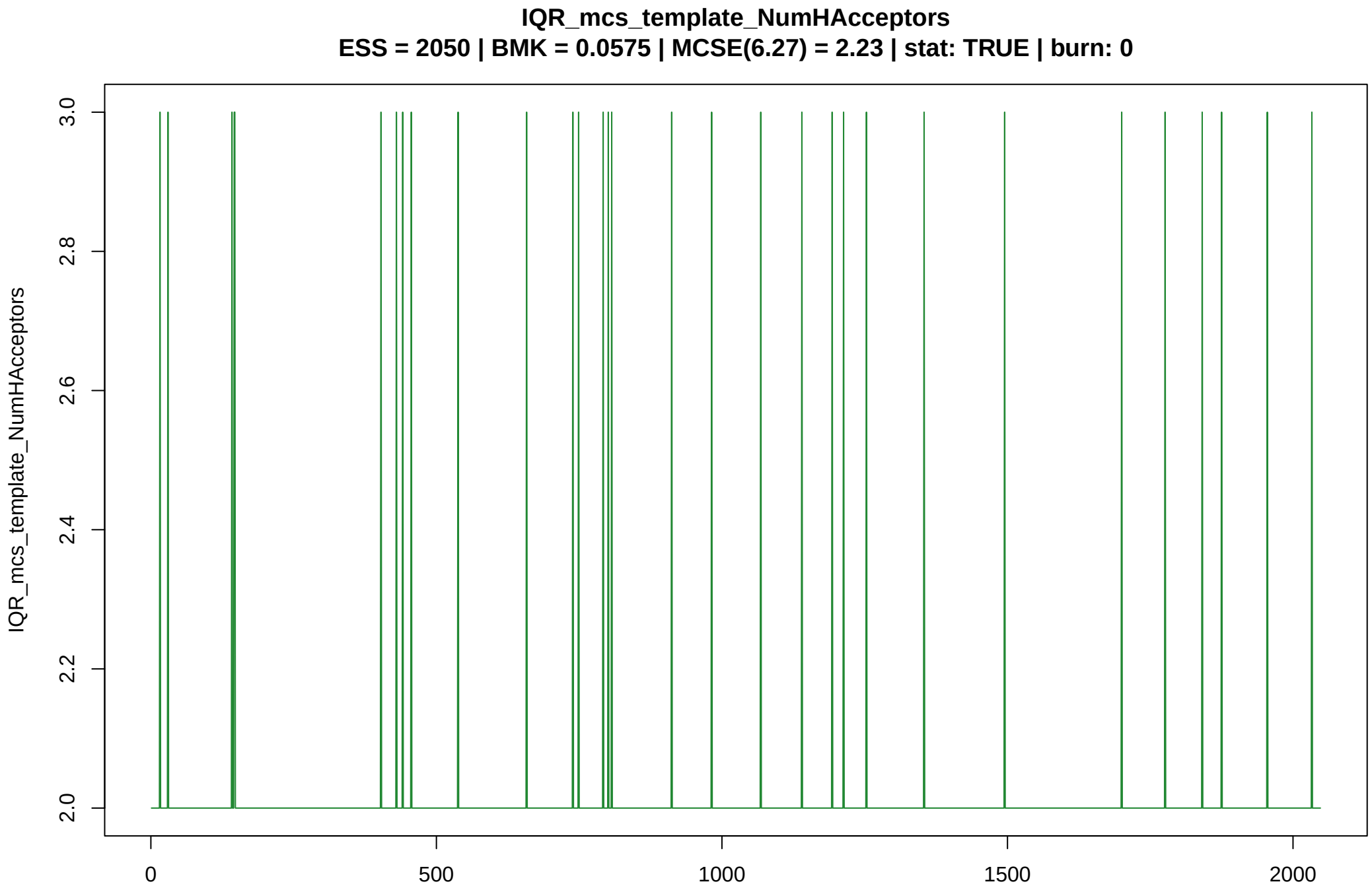

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1640 | BMK = 0.0456 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.92
0.94
0.96
0.98
1.00
1.02
0
500
1000
1500
2000

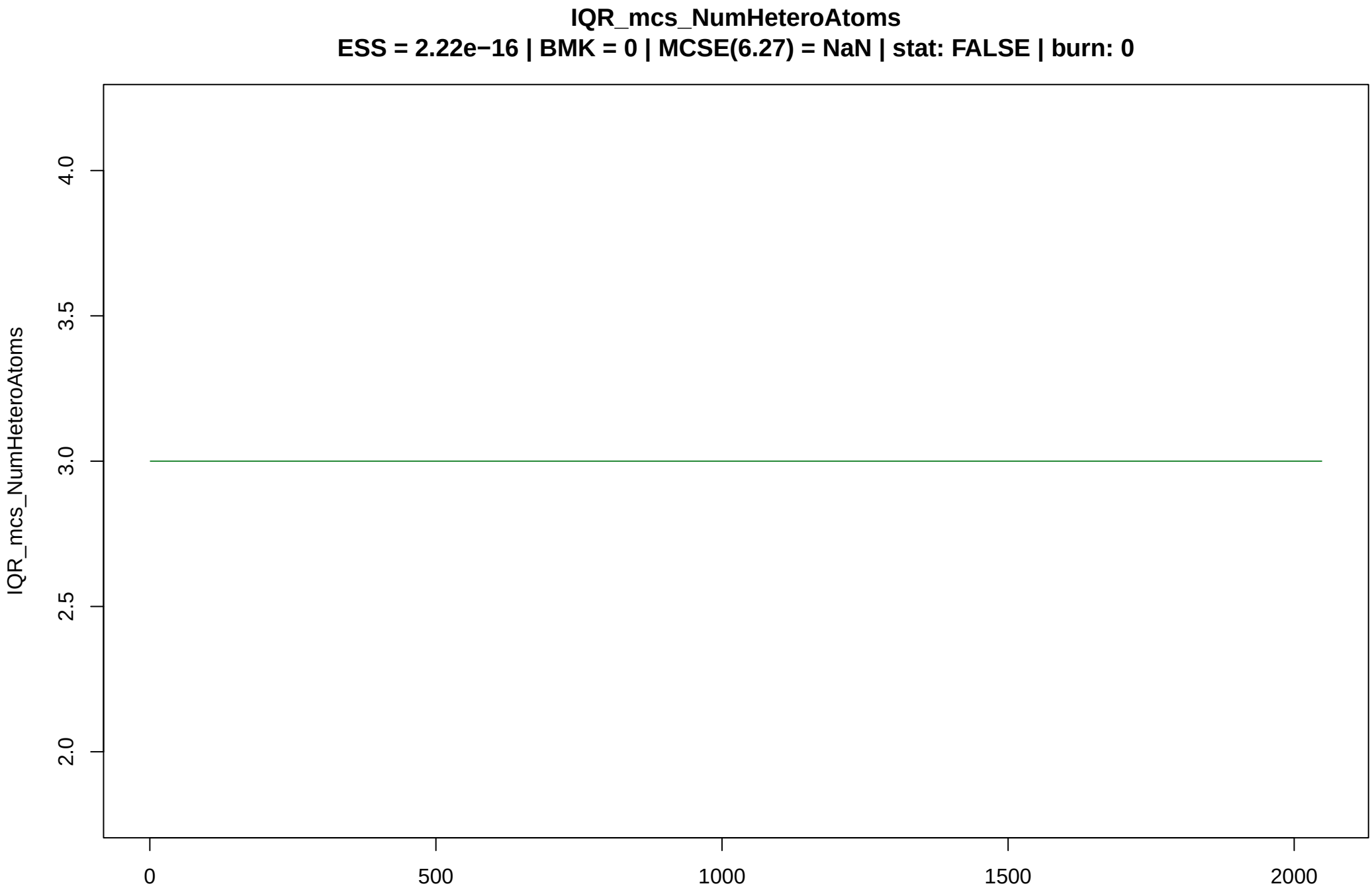

IQR_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0648 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
12.0
11.5
11.0
10.5
10.0
0
500
1000
1500
2000

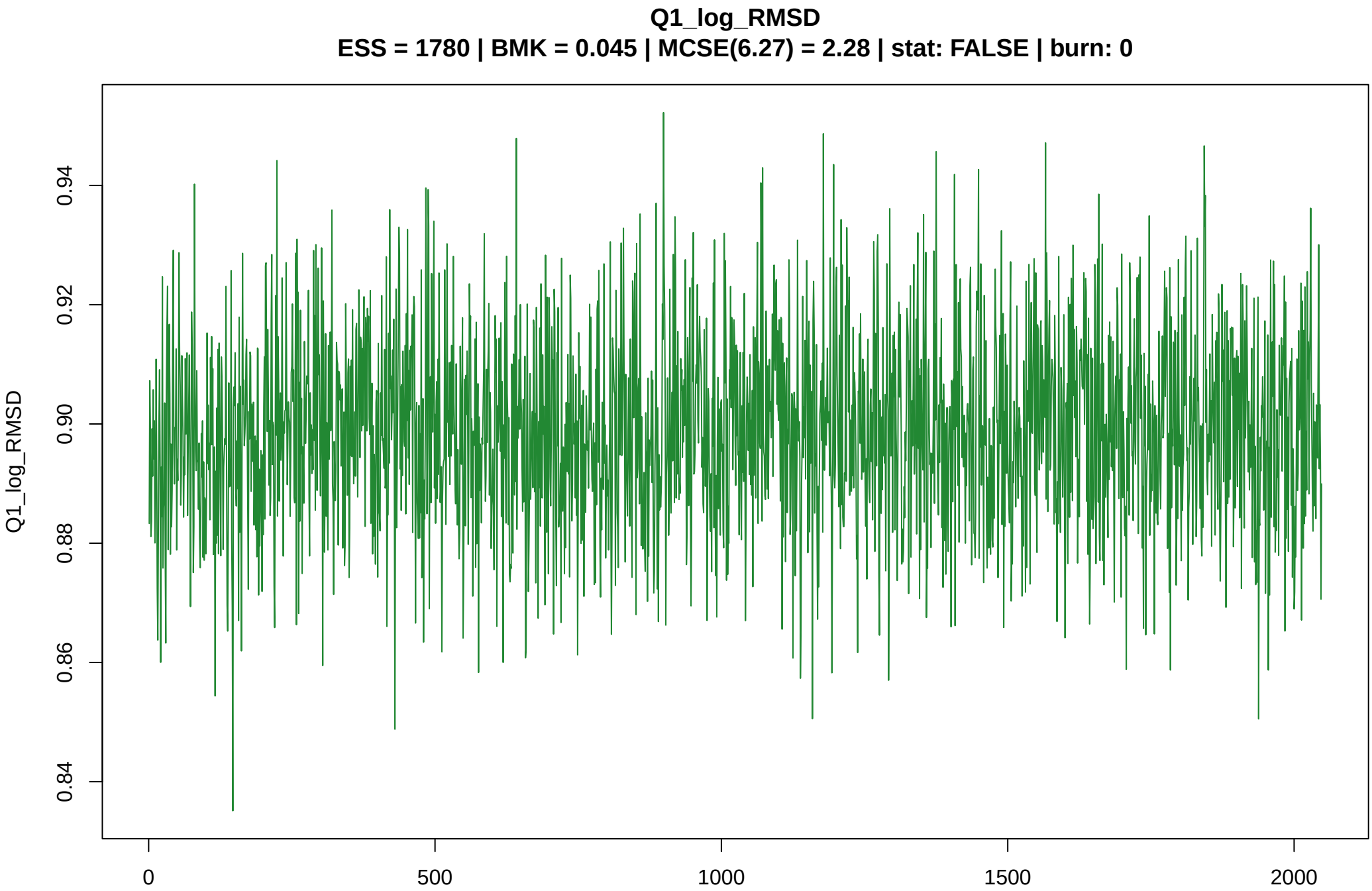

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

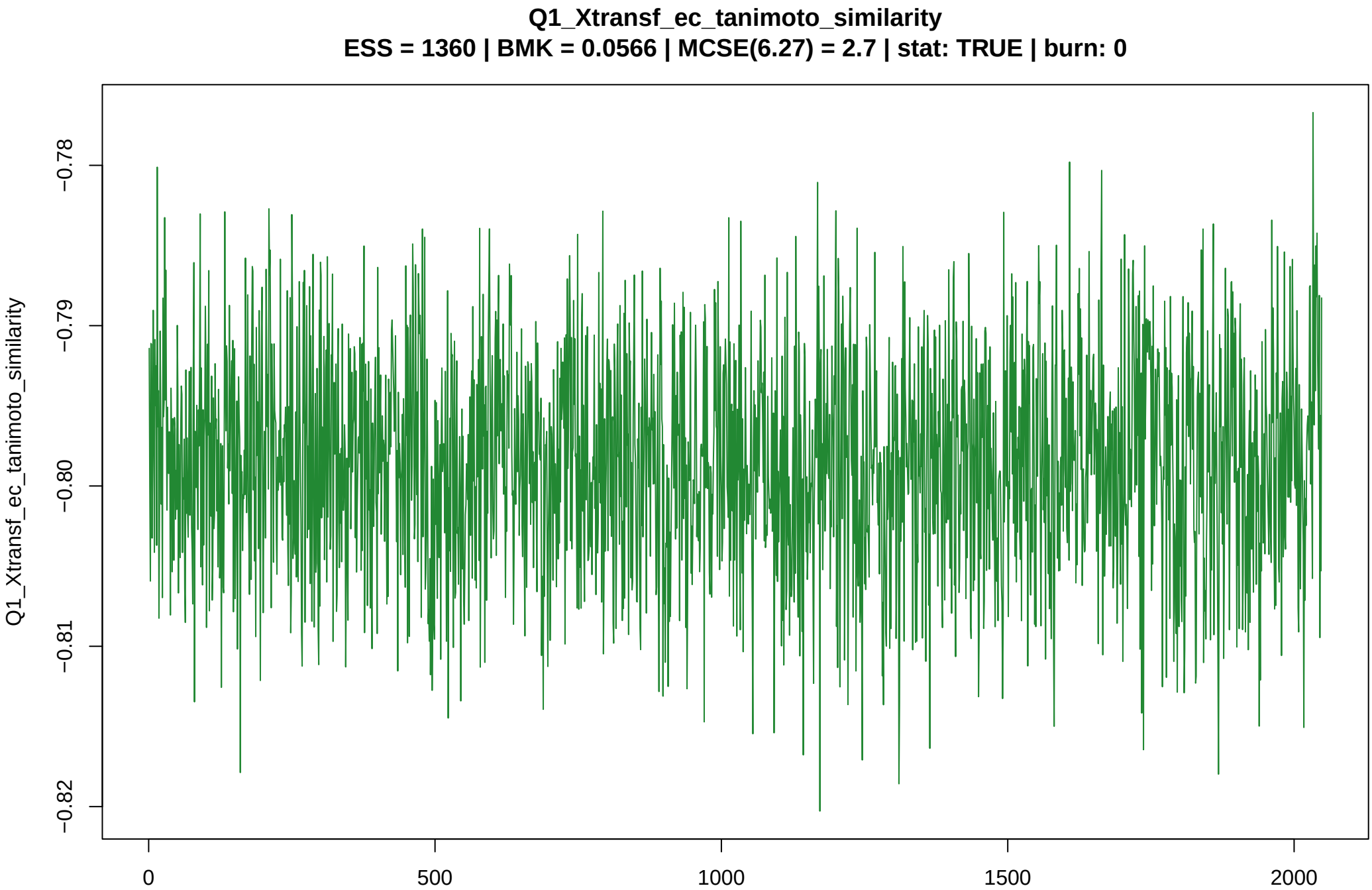

IQR_template_HeavyAtomCount
ESS = 1600 | BMK = 0.261 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 2040
IQR_template_HeavyAtomCount
11.0
10.5
10.0
9.5
9.0
0
500
1000
1500
2000

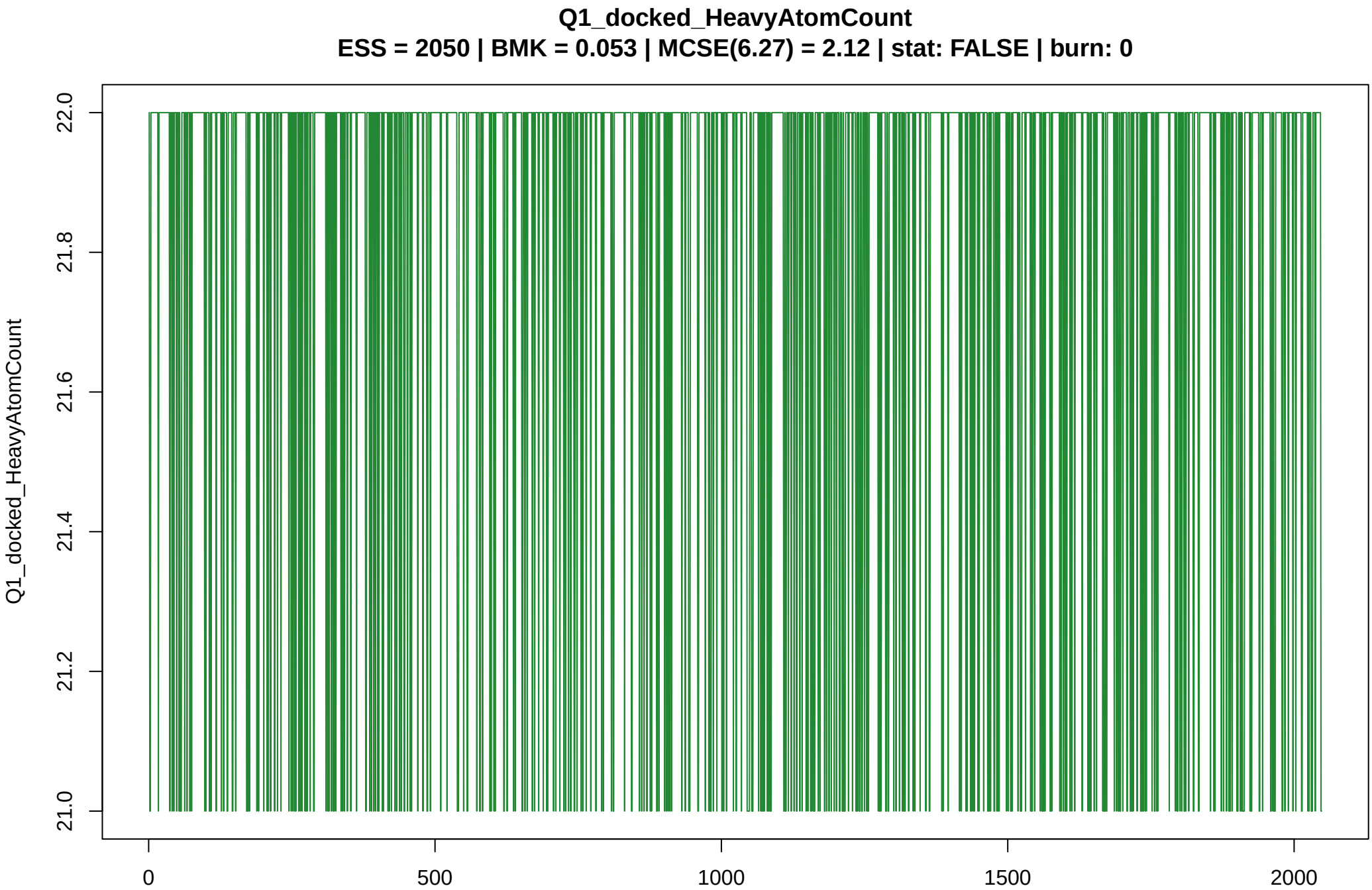

IQR_mcs_docked_NumHAcceptors
ESS = 1850 | BMK = 0.0406 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
IQR_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

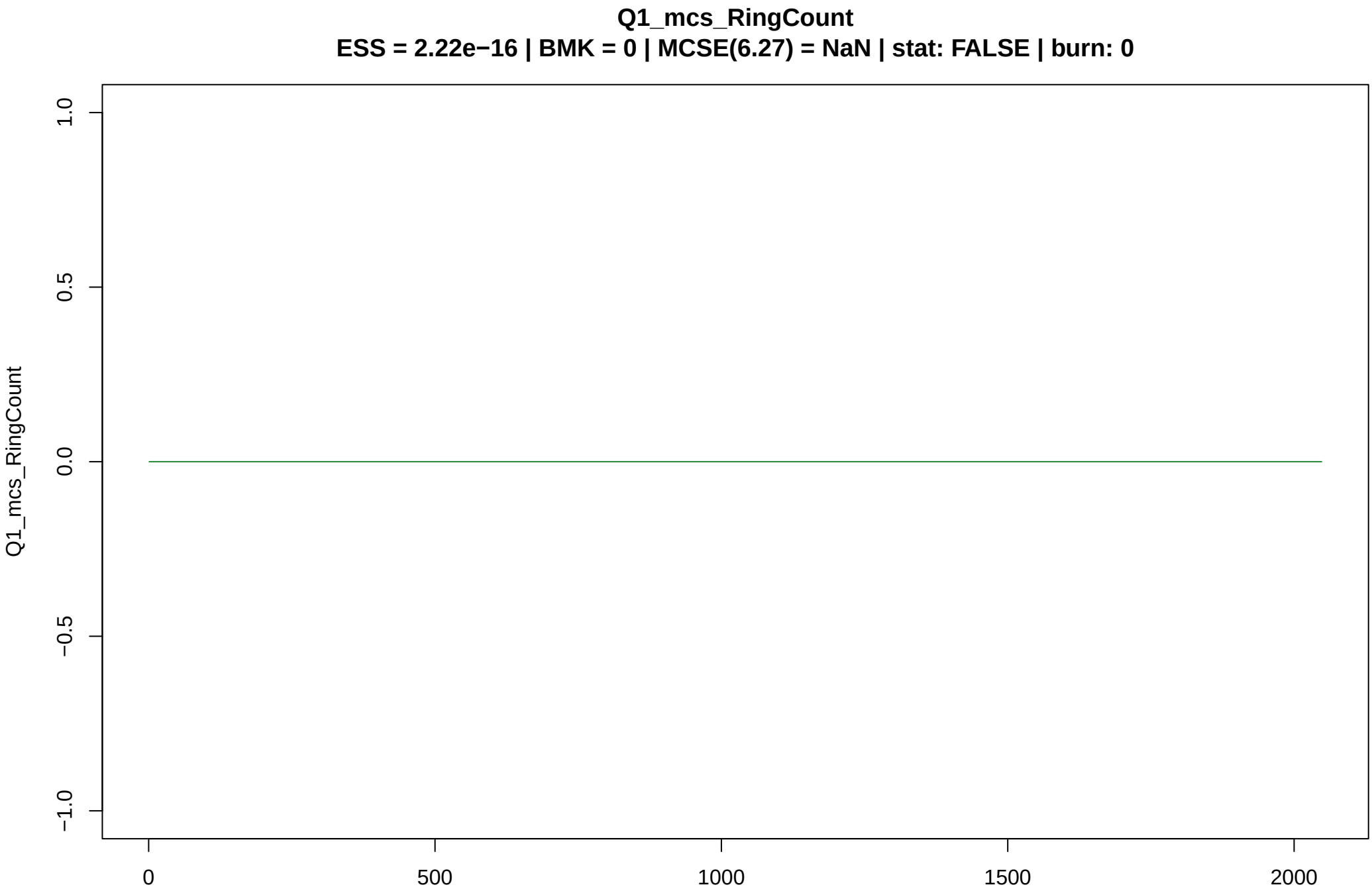

IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0575 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0
IQR_mcs_template_NumHAcceptors
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

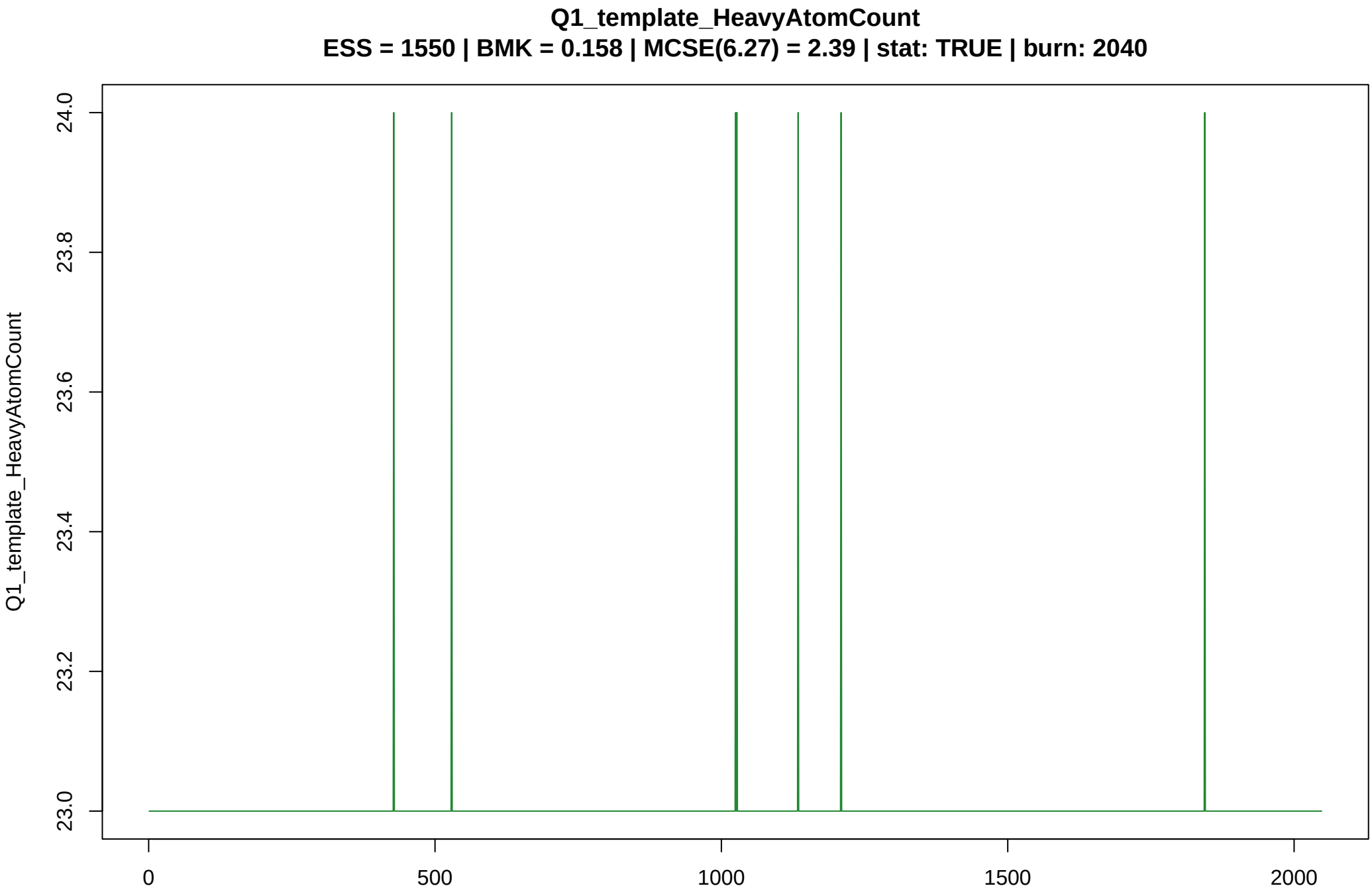

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

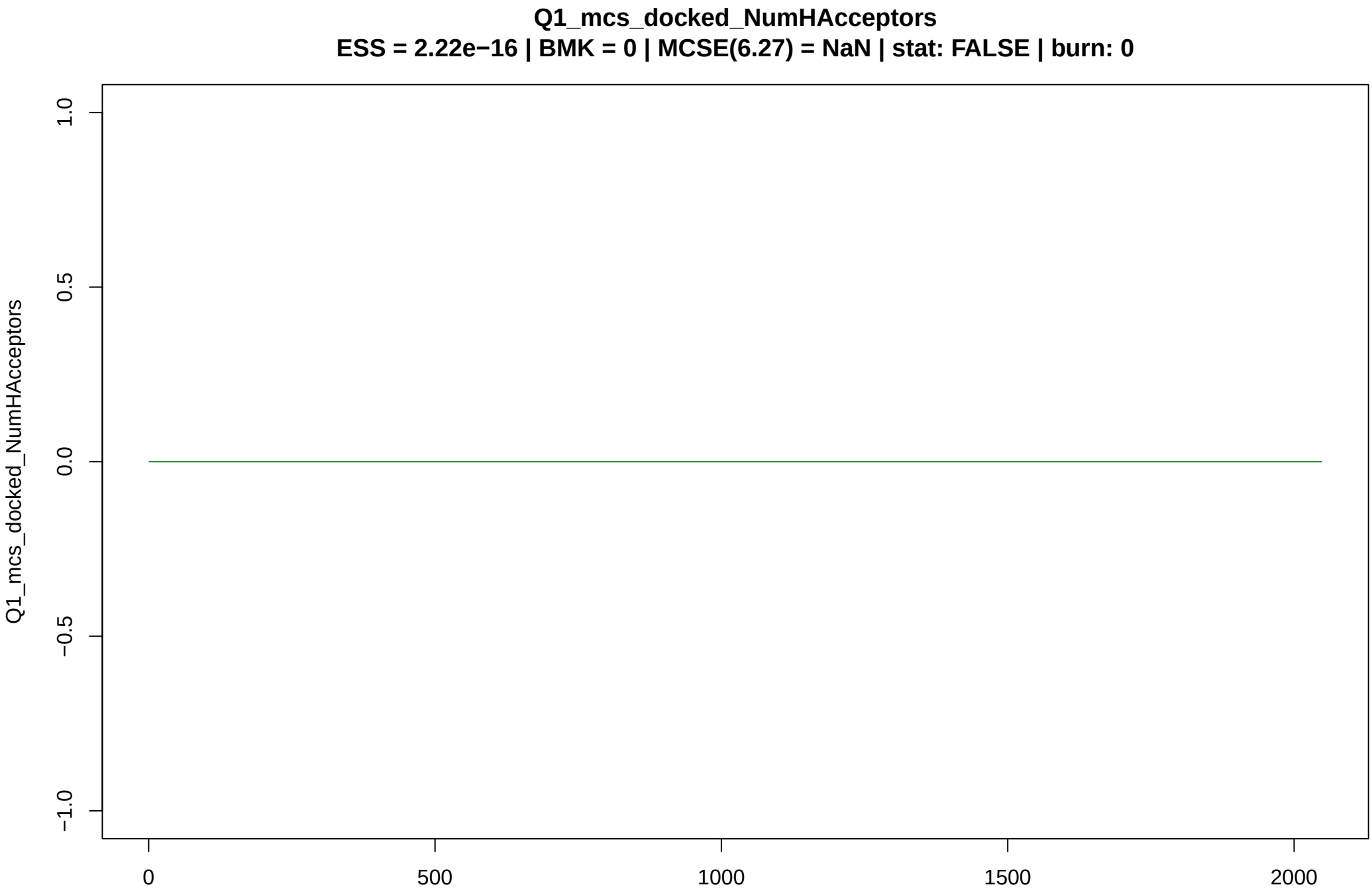

Q1_log_RMSD
ESS = 1780 | BMK = 0.045 | MCSE(6.27) = 2.28 | stat: FALSE | burn: 0
Q1_log_RMSD
0.84
0.86
0.88
0.90
0.92
0.94
0
500
1000
1500
2000

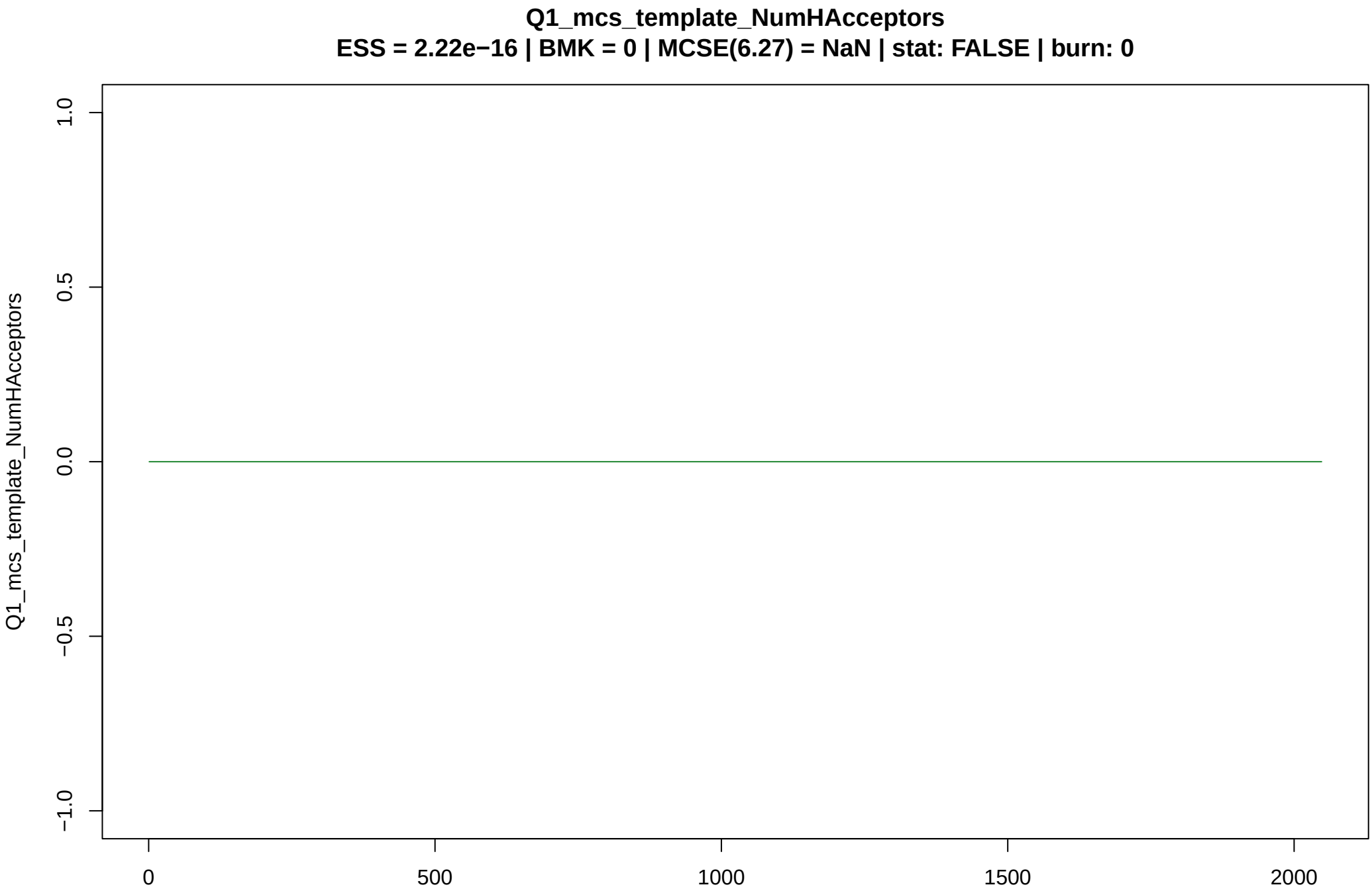

Q1_Xtransf_ec_tanimoto_similarity
ESS = 1360 | BMK = 0.0566 | MCSE(6.27) = 2.7 | stat: TRUE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

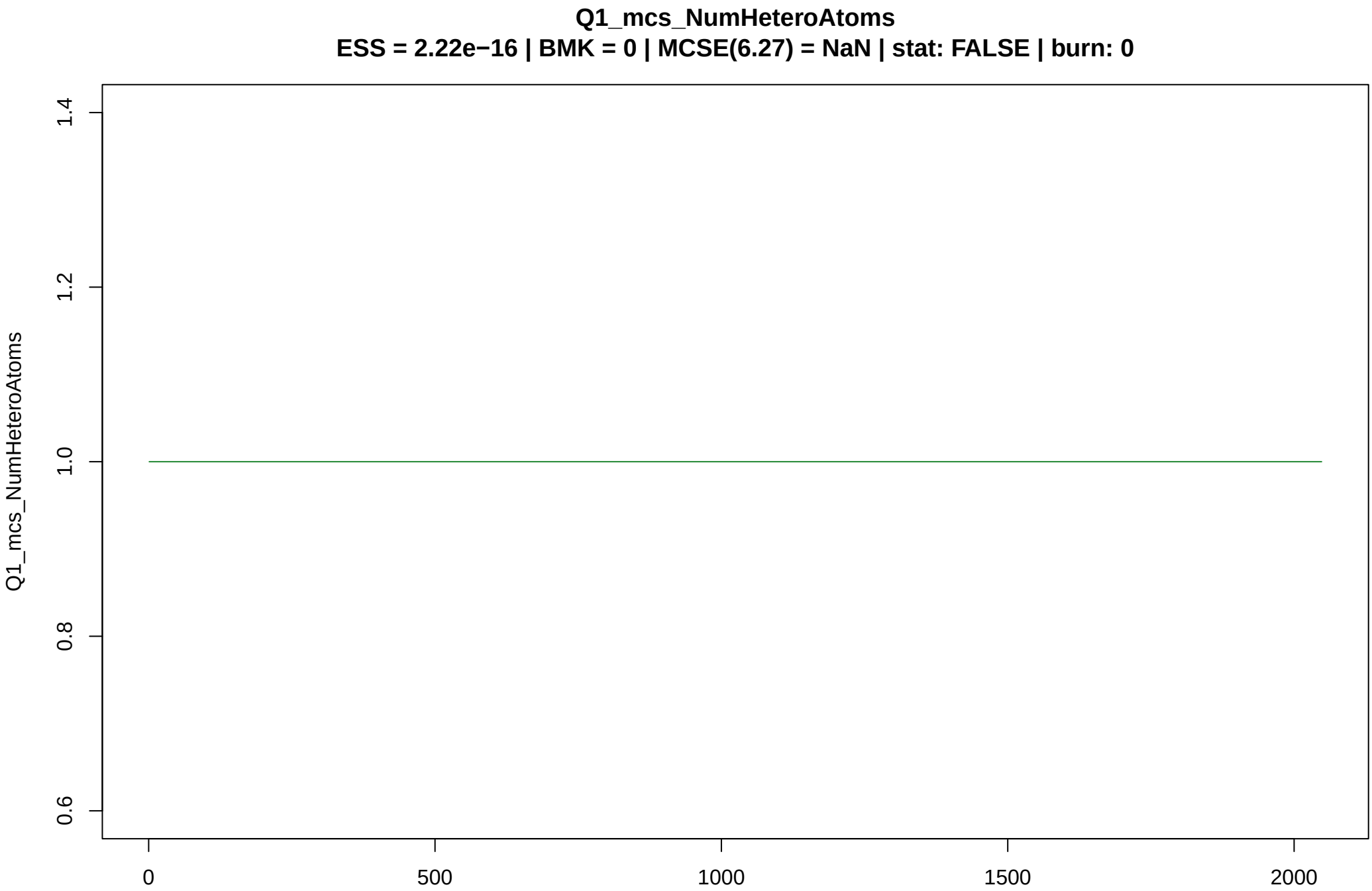

Q1_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.053 | MCSE(6.27) = 2.12 | stat: FALSE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

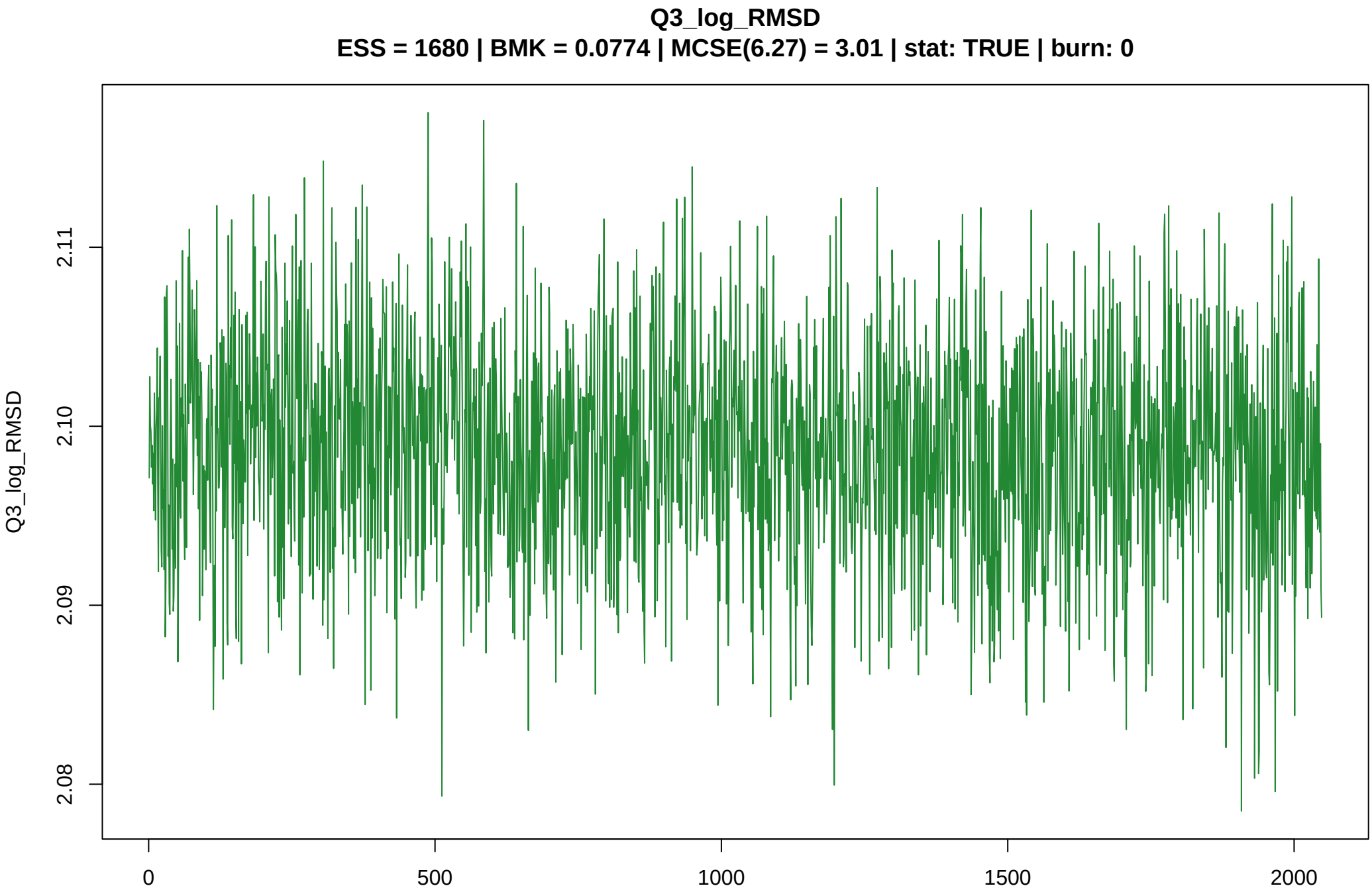

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

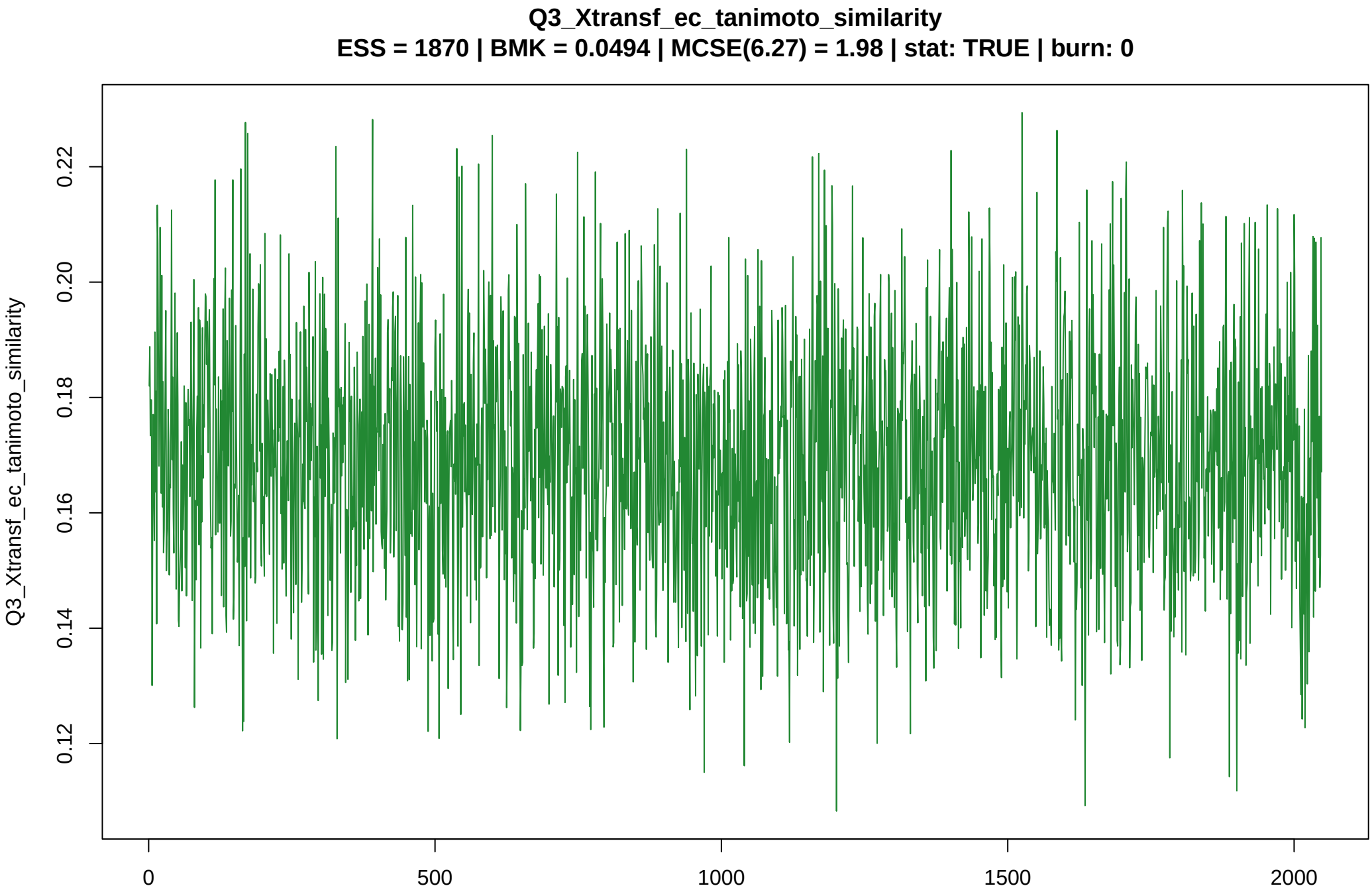

Q1_template_HeavyAtomCount
ESS = 1550 | BMK = 0.158 | MCSE(6.27) = 2.39 | stat: TRUE | burn: 2040
Q1_template_HeavyAtomCount
24.0
23.8
23.6
23.4
23.2
23.0
0
500
1000
1500
2000

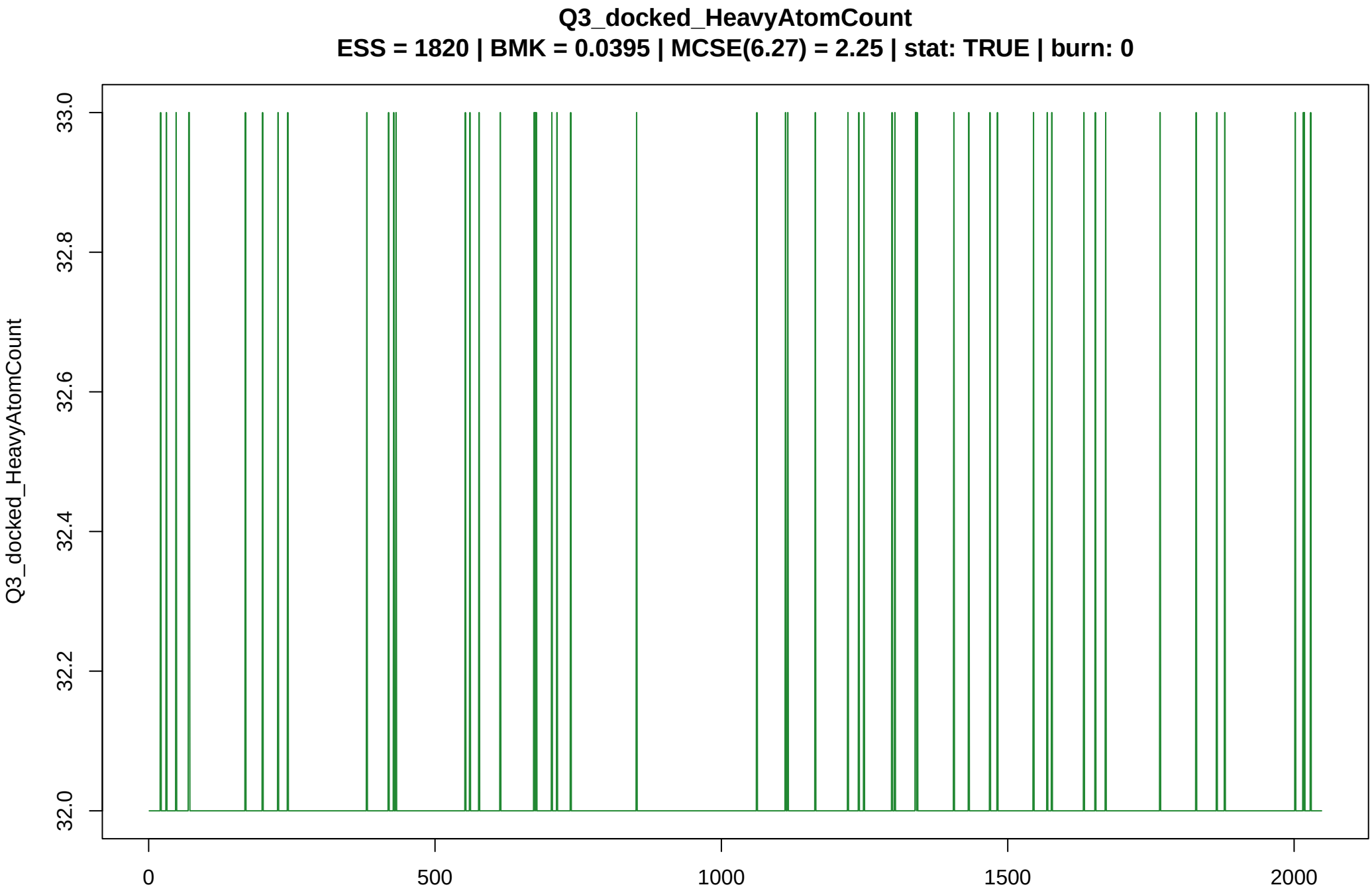

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

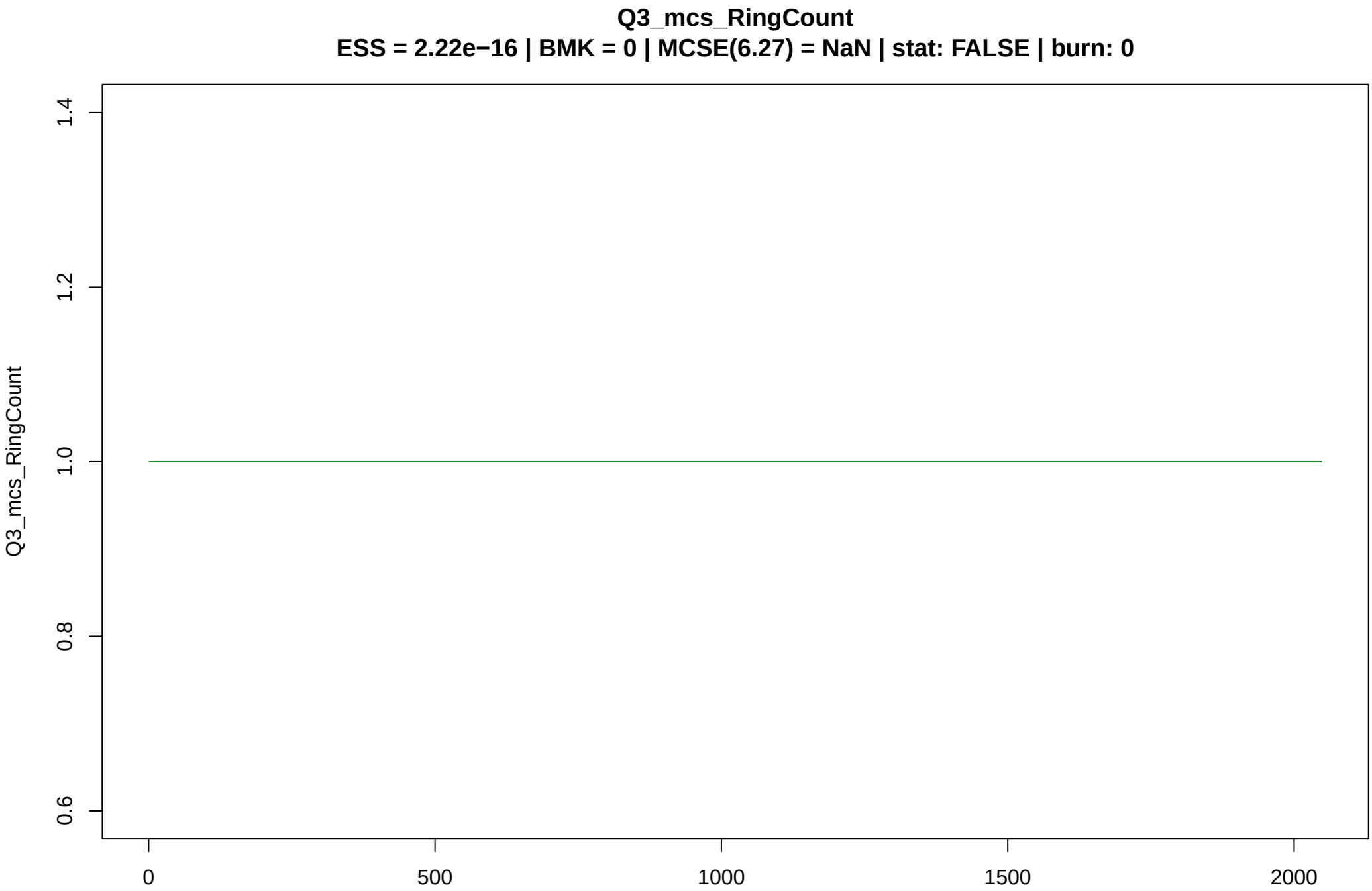

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

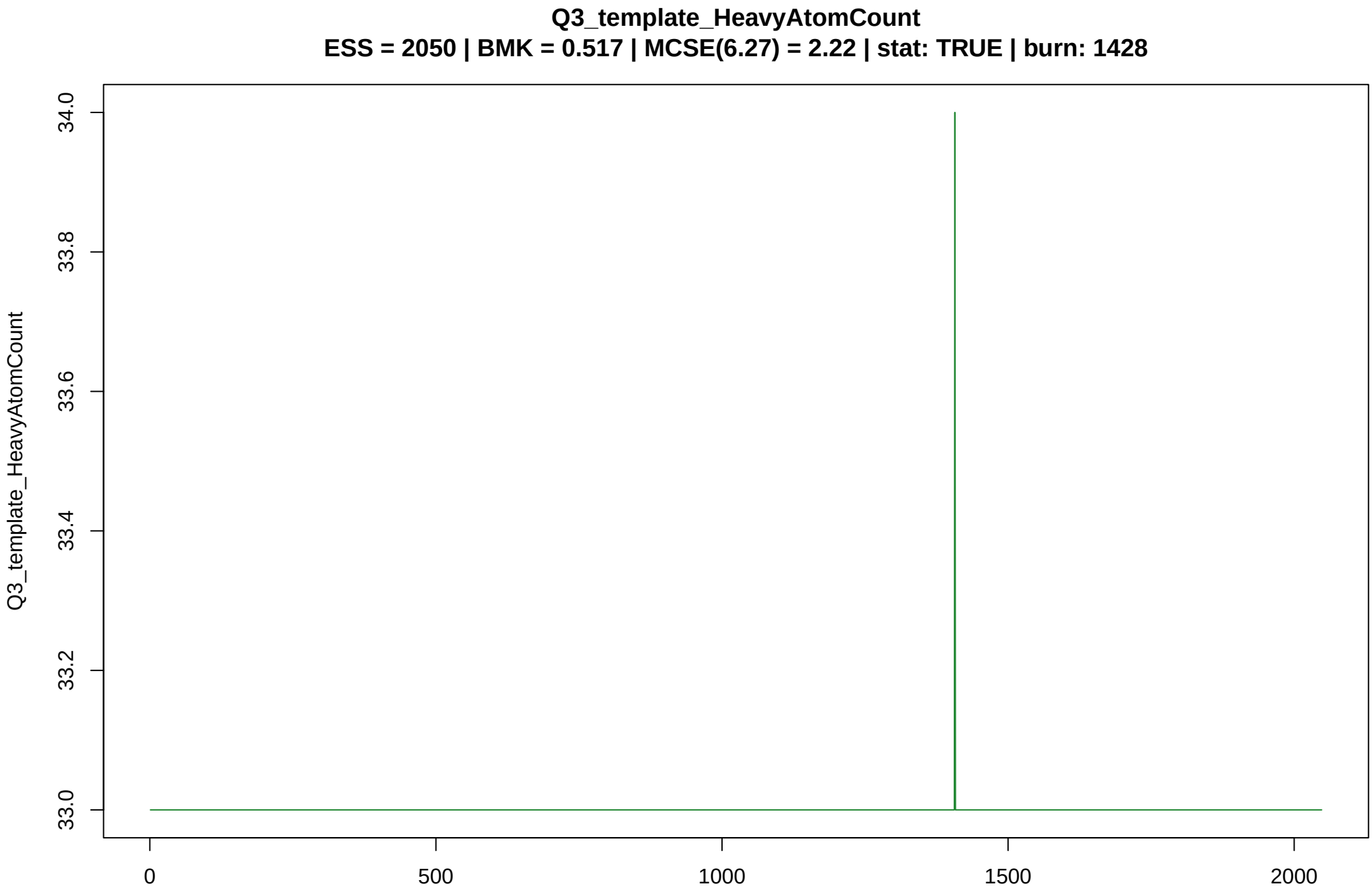

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

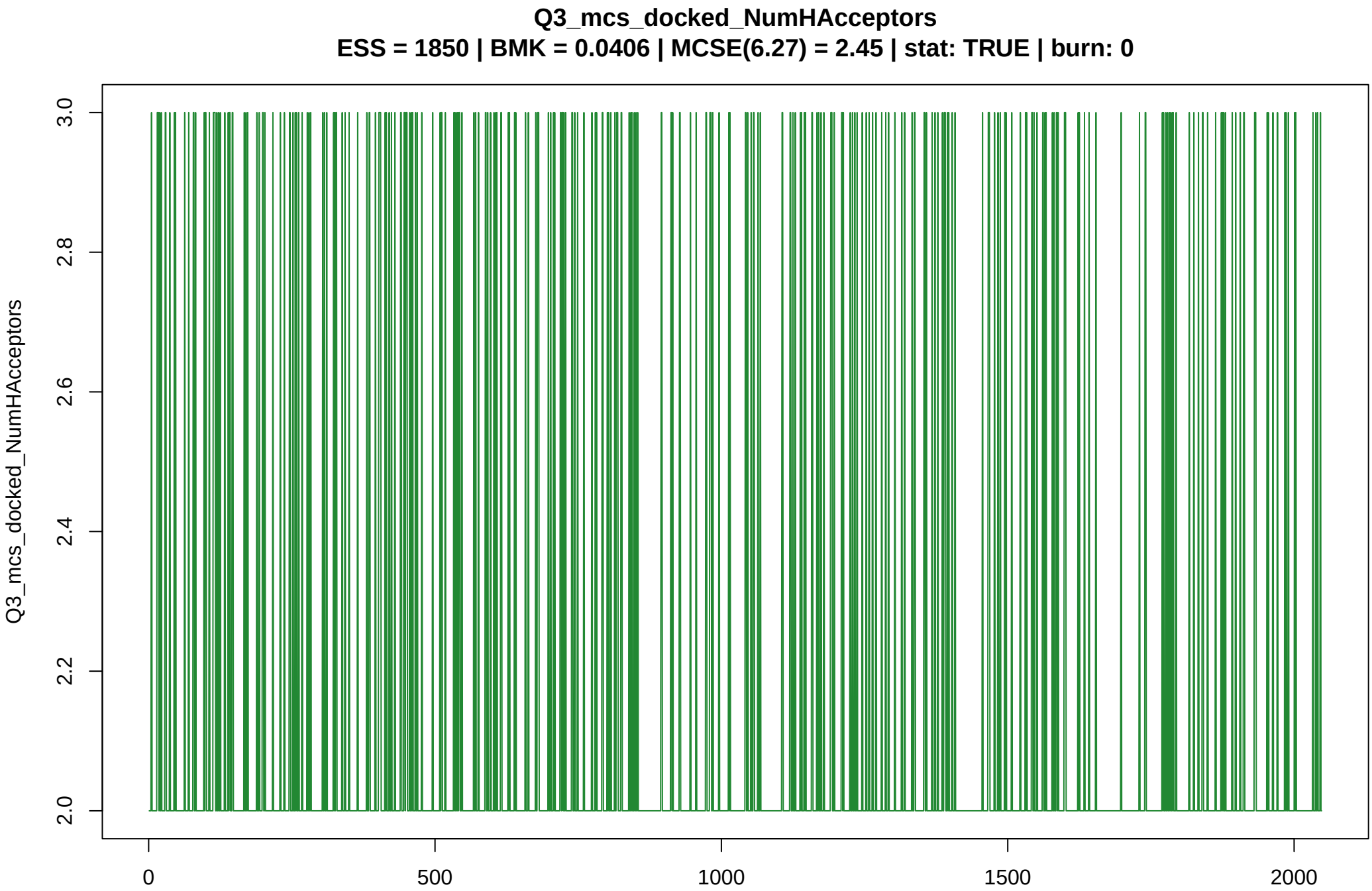

Q3_log_RMSD
ESS = 1680 | BMK = 0.0774 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
0
500
1000
1500
2000

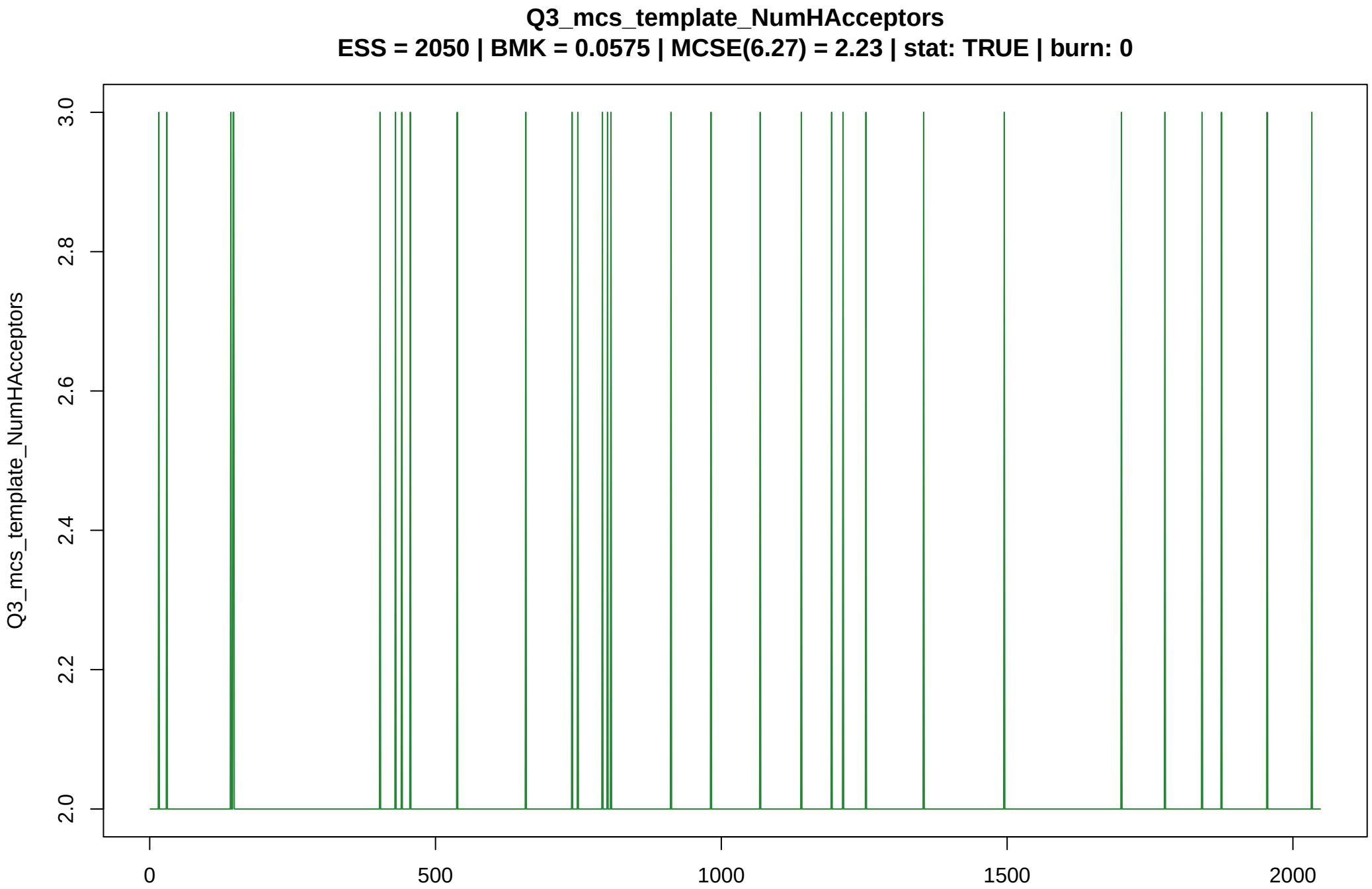

Q3_Xtransf_ec_tanimoto_similarity
ESS = 1870 | BMK = 0.0494 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.12
0.14
0.16
0.18
0.20
0.22
0
500
1000
1500
2000

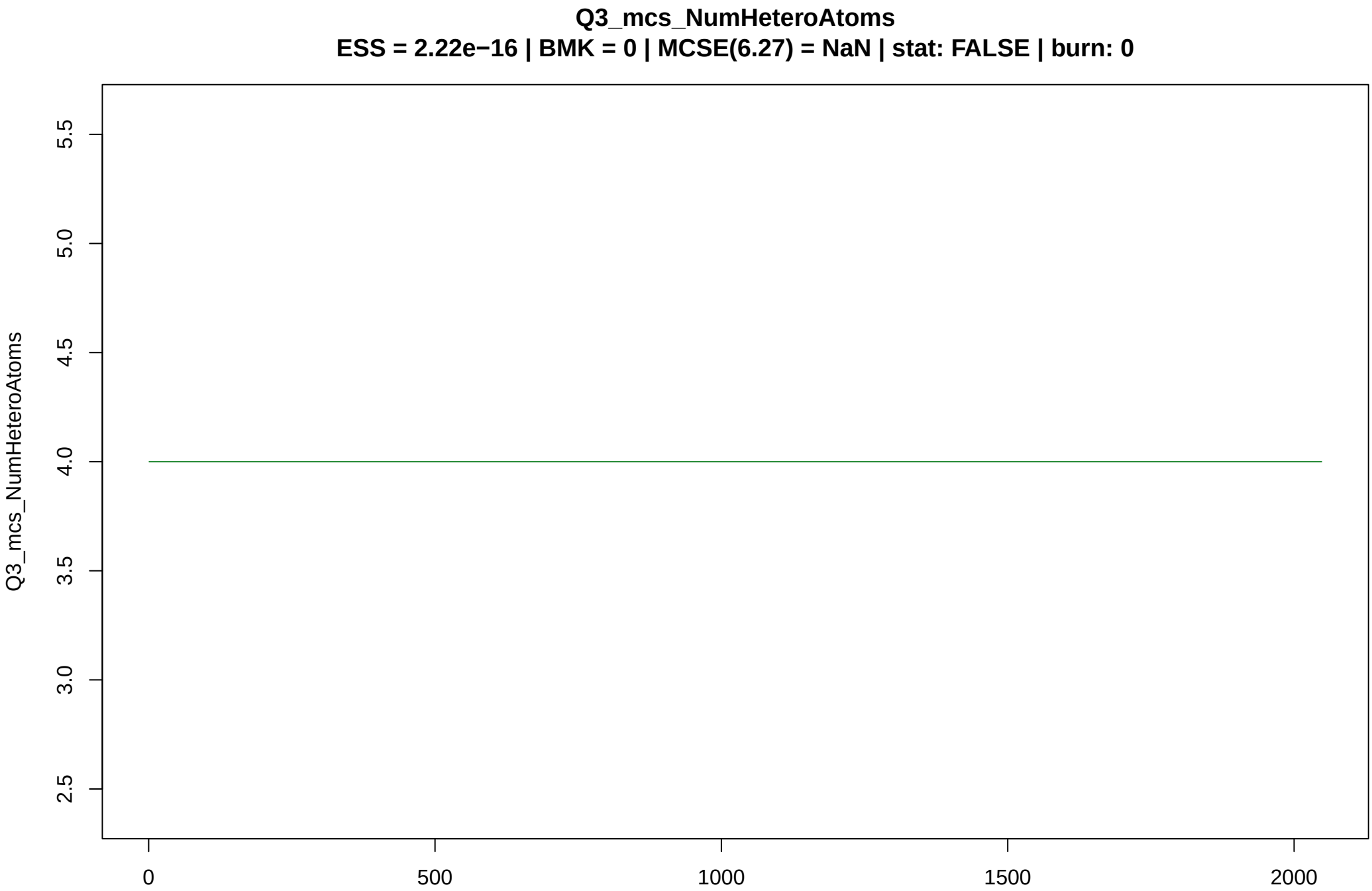

Q3_docked_HeavyAtomCount
ESS = 1820 | BMK = 0.0395 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
32.0
32.2
32.4
32.6
32.8
33.0
0
500
1000
1500
2000

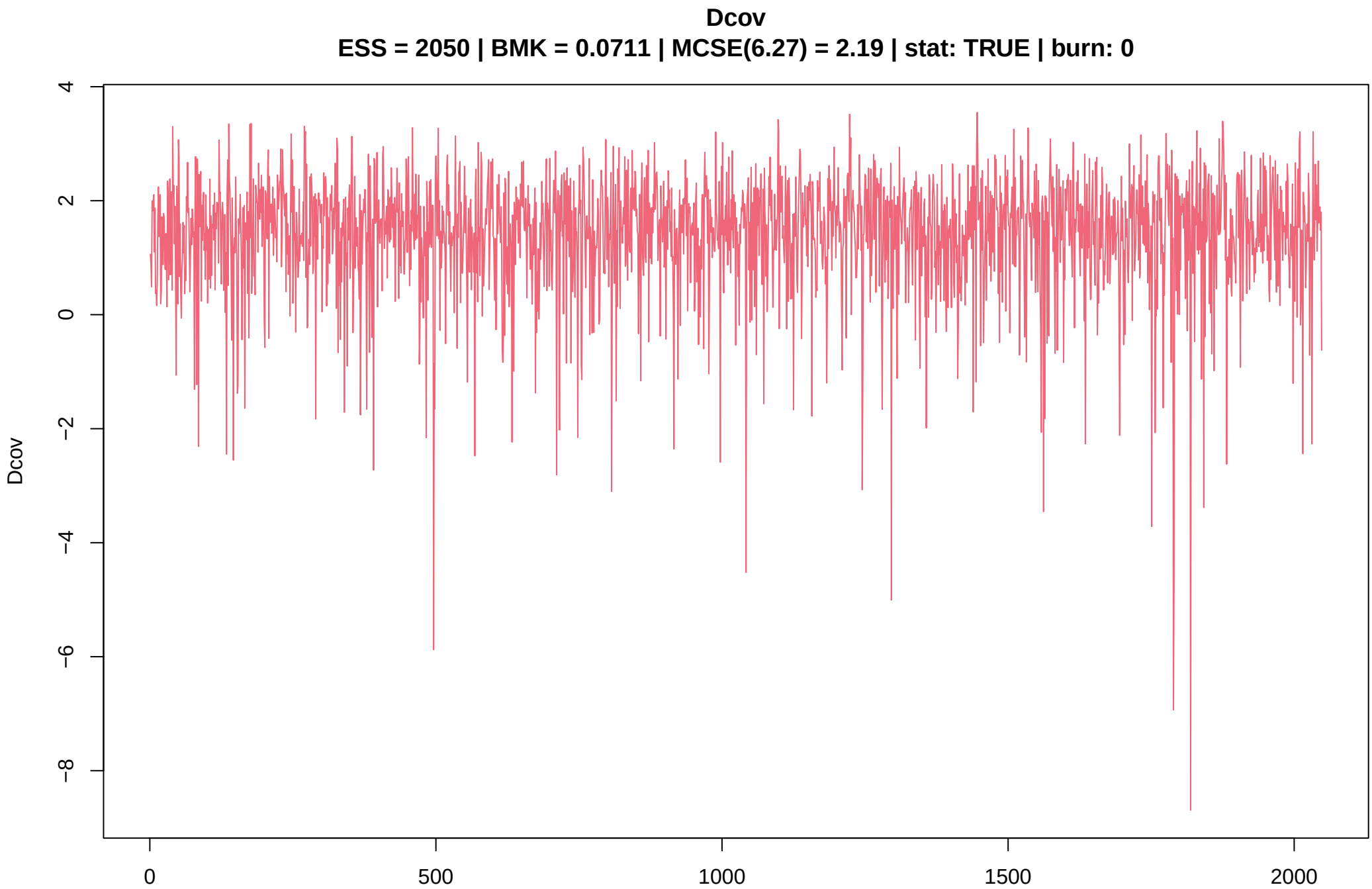

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

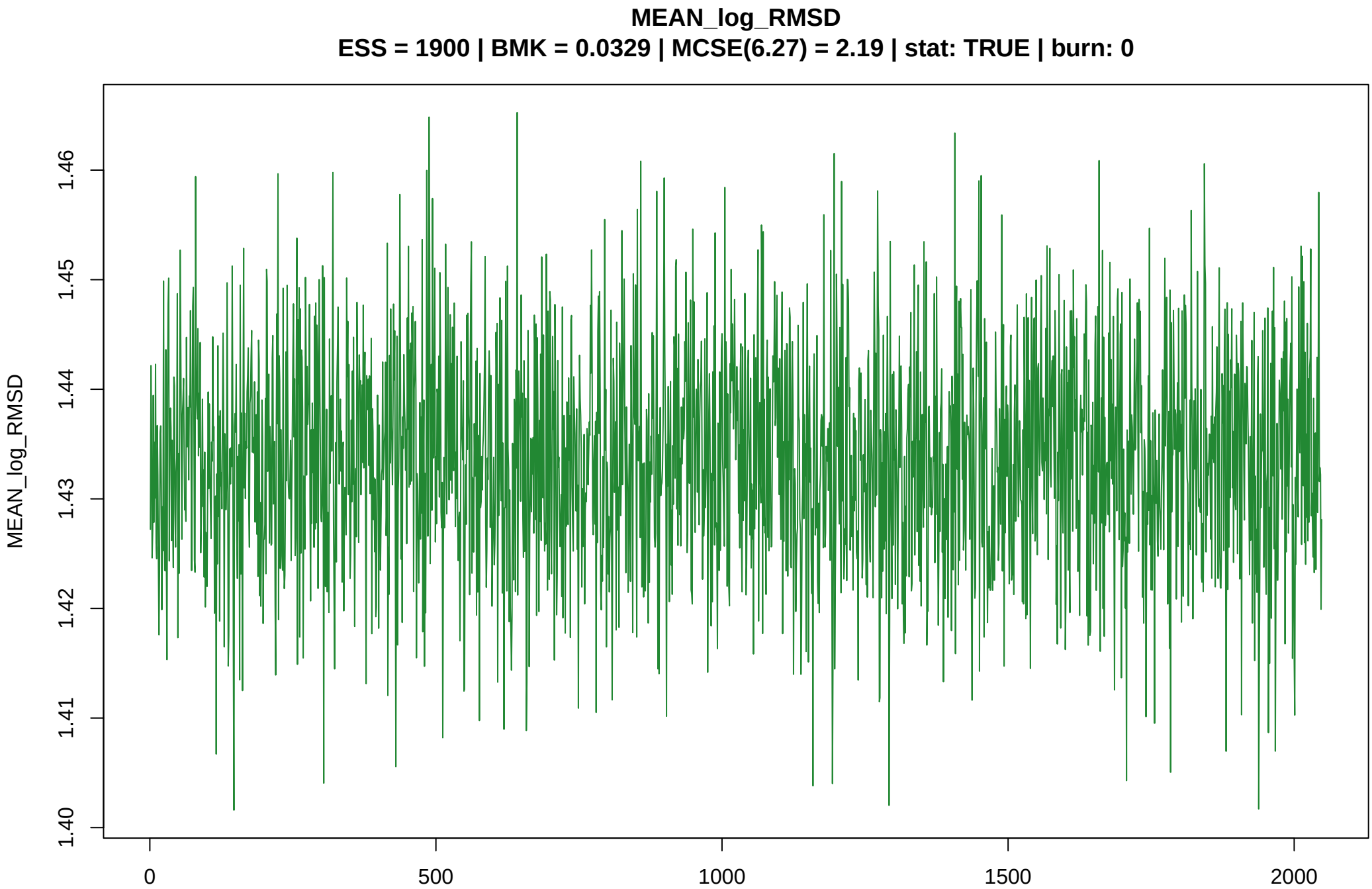

Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.517 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 1428
Q3_template_HeavyAtomCount
34.0
33.8
33.6
33.4
33.2
33.0
0
500
1000
1500
2000

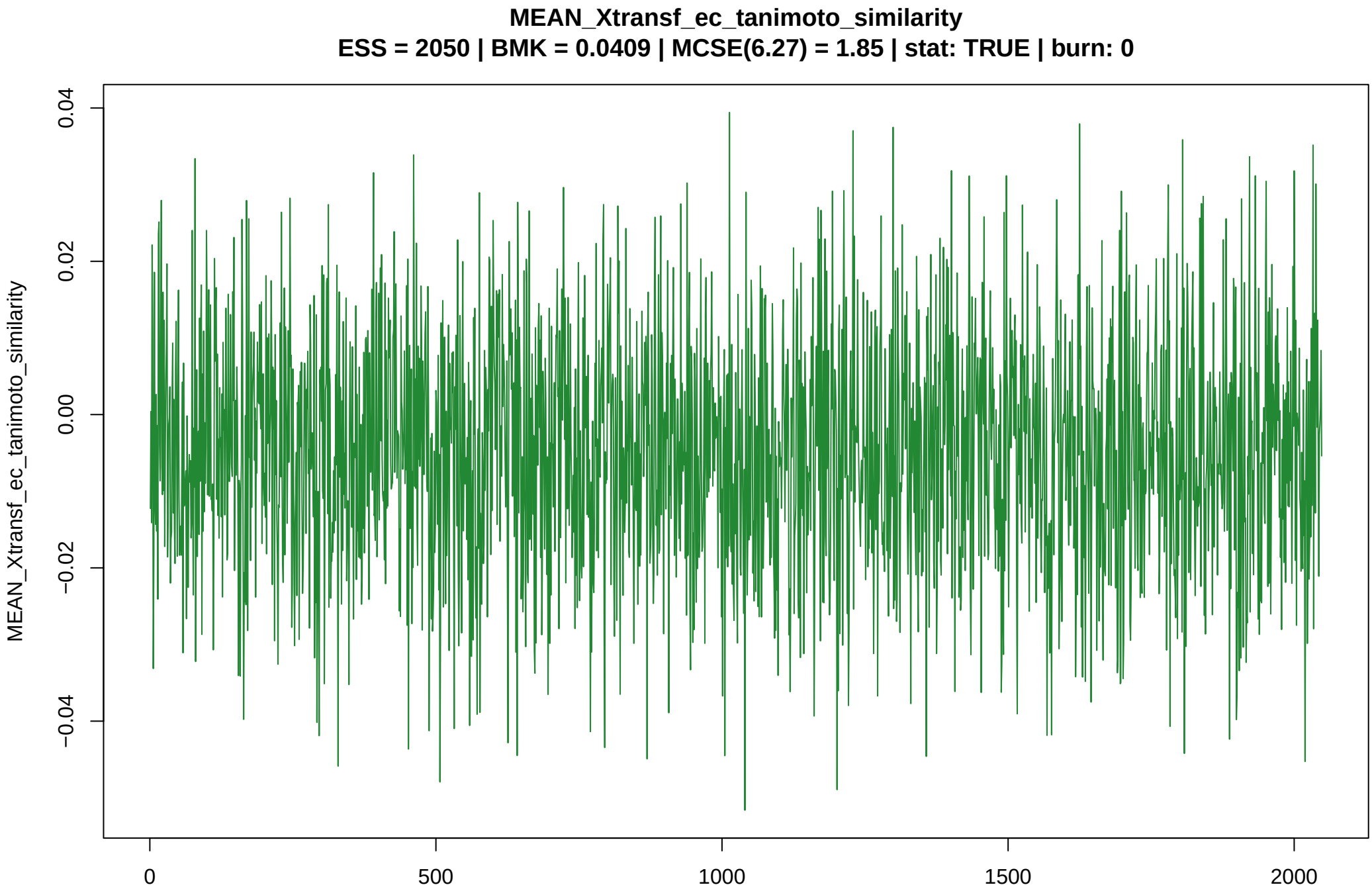

Q3_mcs_docked_NumHAcceptors
ESS = 1850 | BMK = 0.0406 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
Q3_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

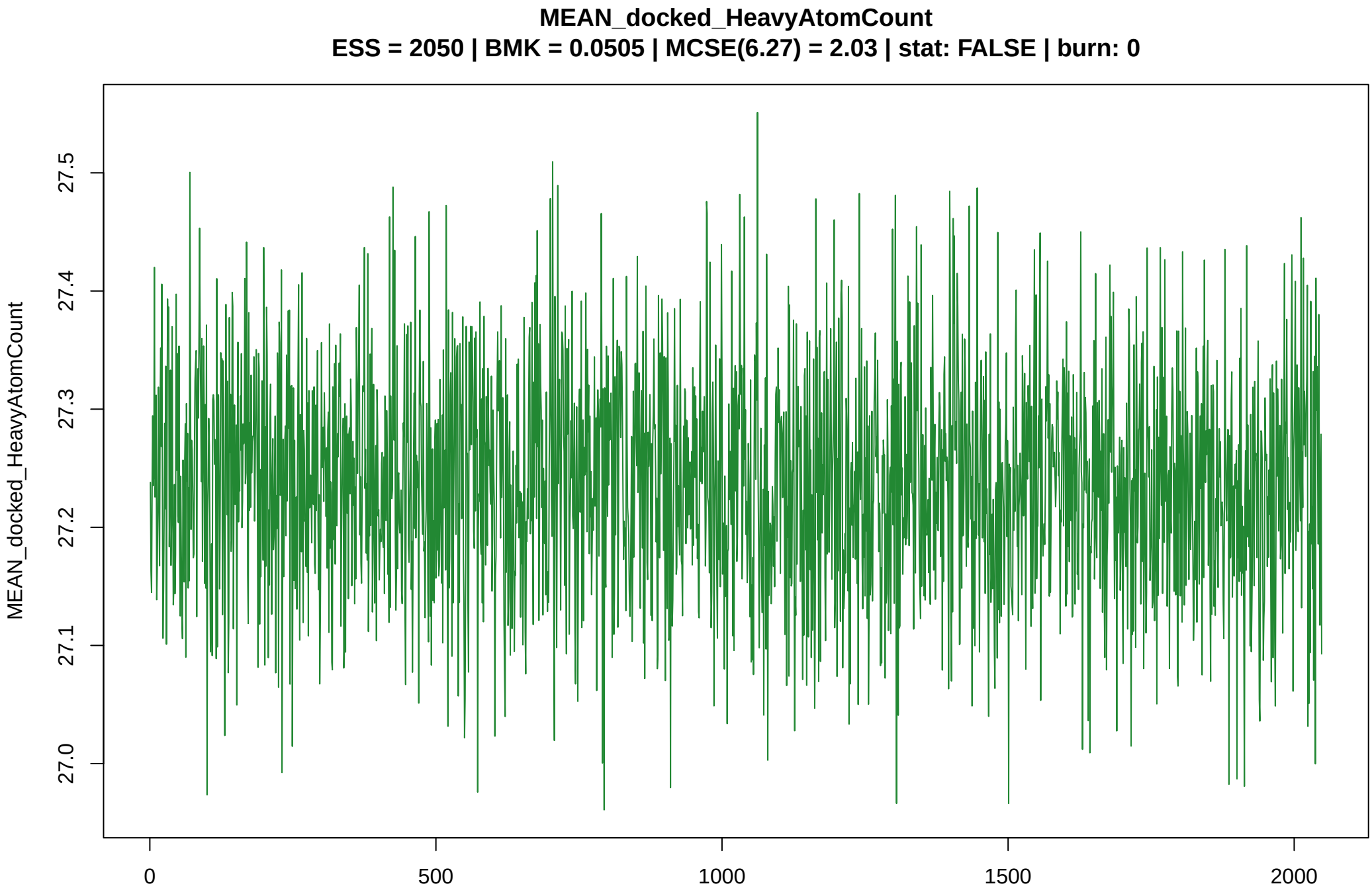

Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0575 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0
Q3_mcs_template_NumHAcceptors
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

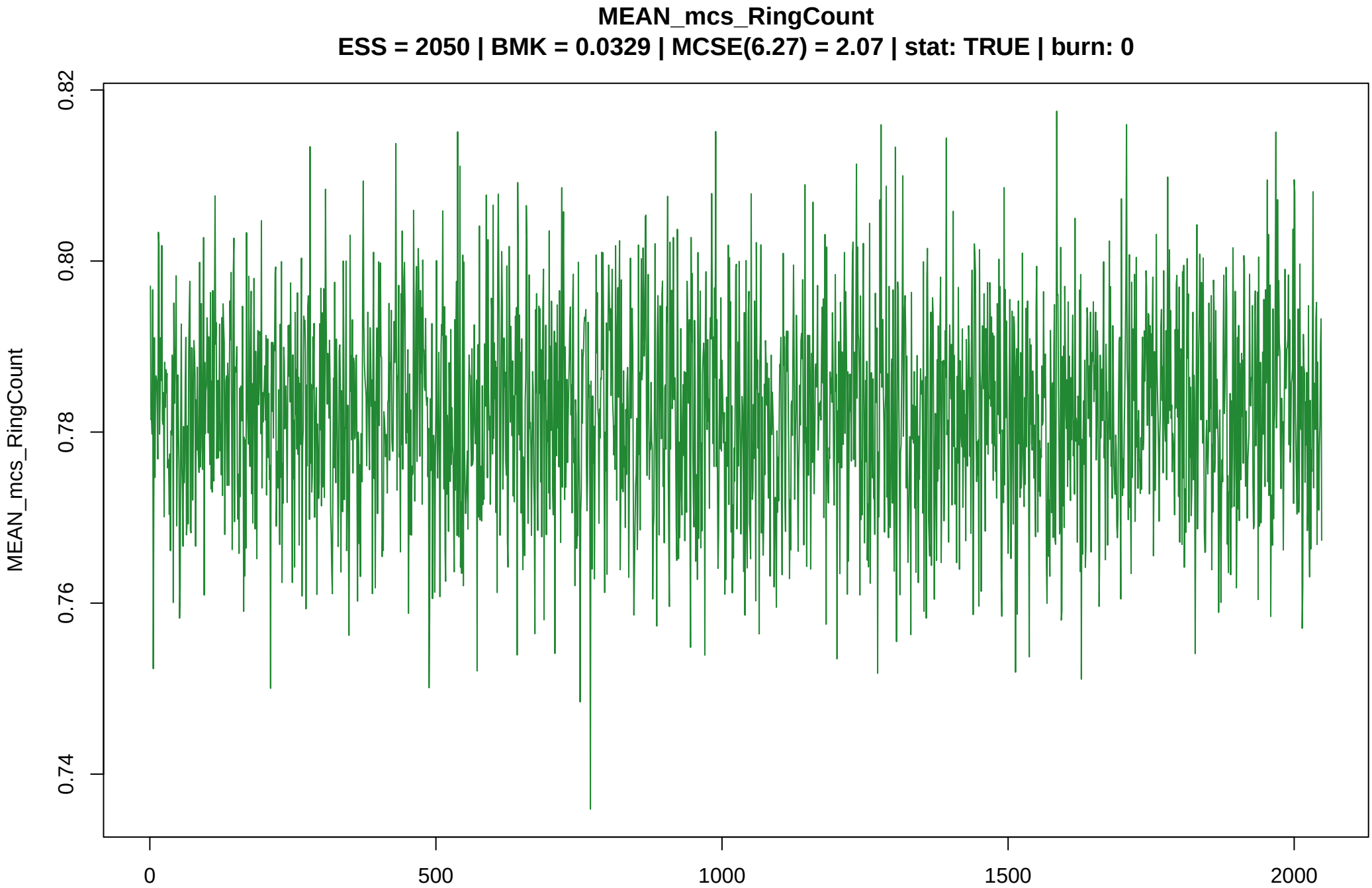

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

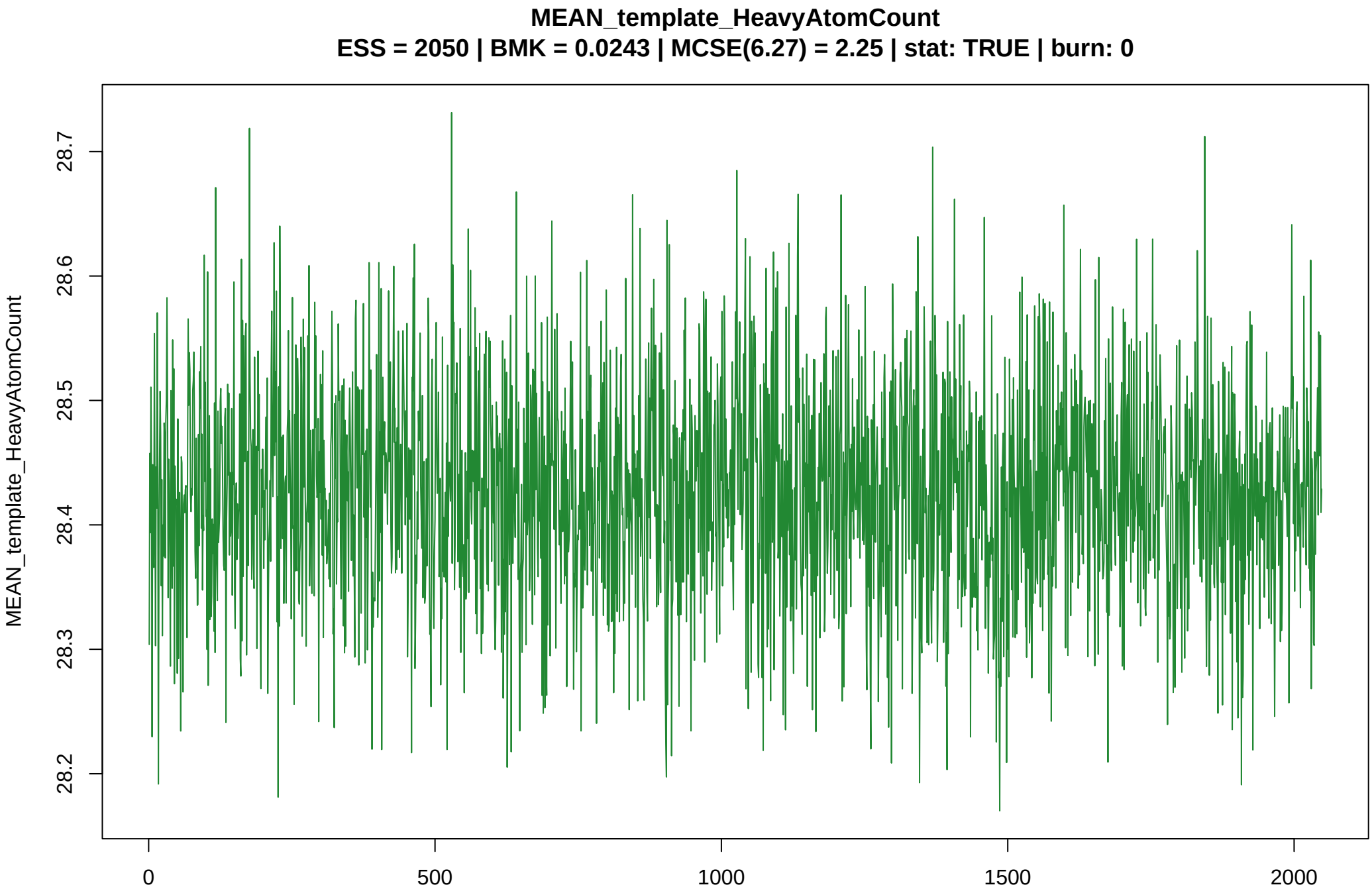

Dcov
ESS = 2050 | BMK = 0.0711 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
Dcov
4
2
0
−2
−4
−6
−8
0
500
1000
1500
2000

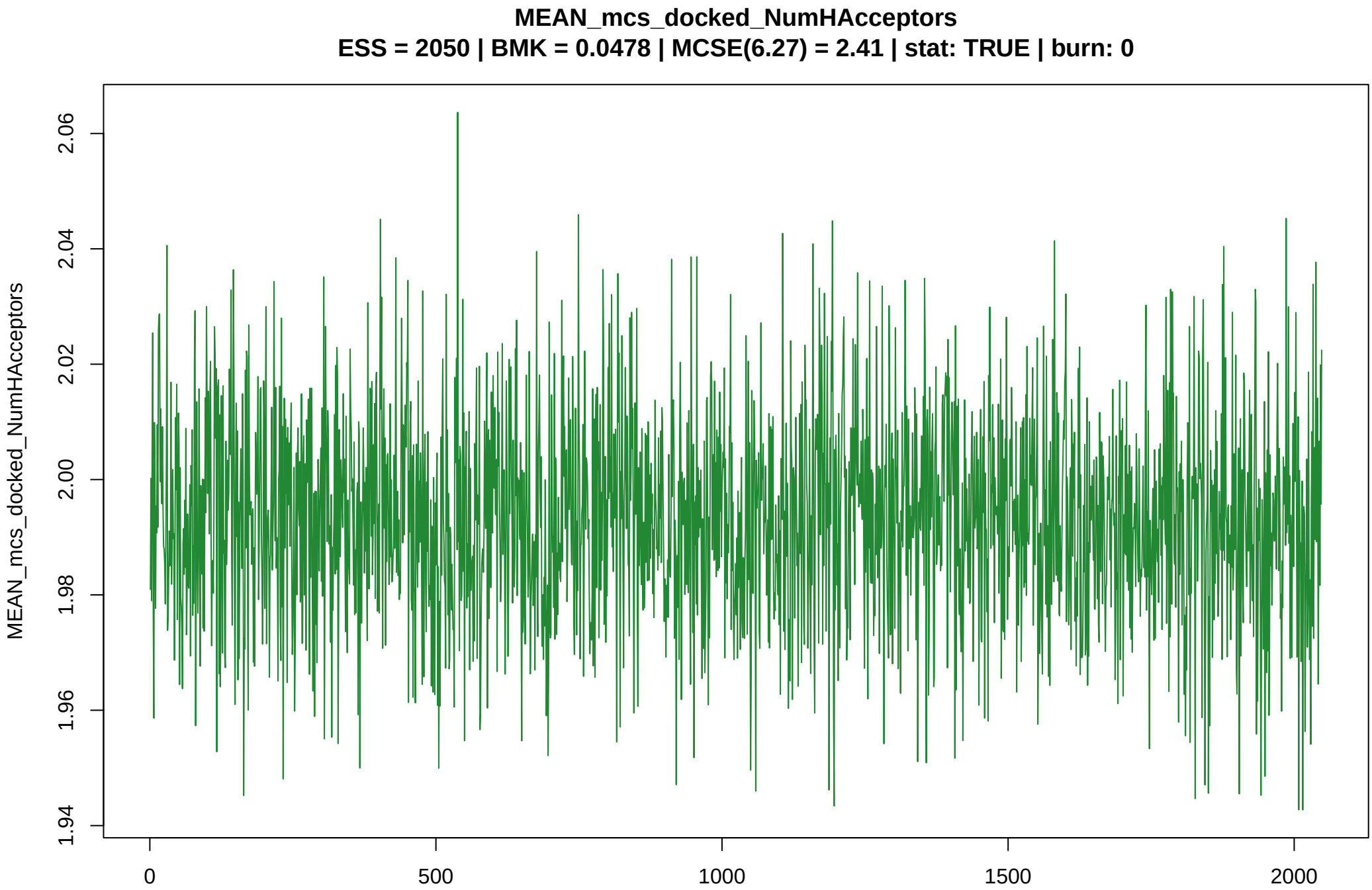

MEAN_log_RMSD
ESS = 1900 | BMK = 0.0329 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.40
1.41
1.42
1.43
1.44
1.45
1.46
0
500
1000
1500
2000

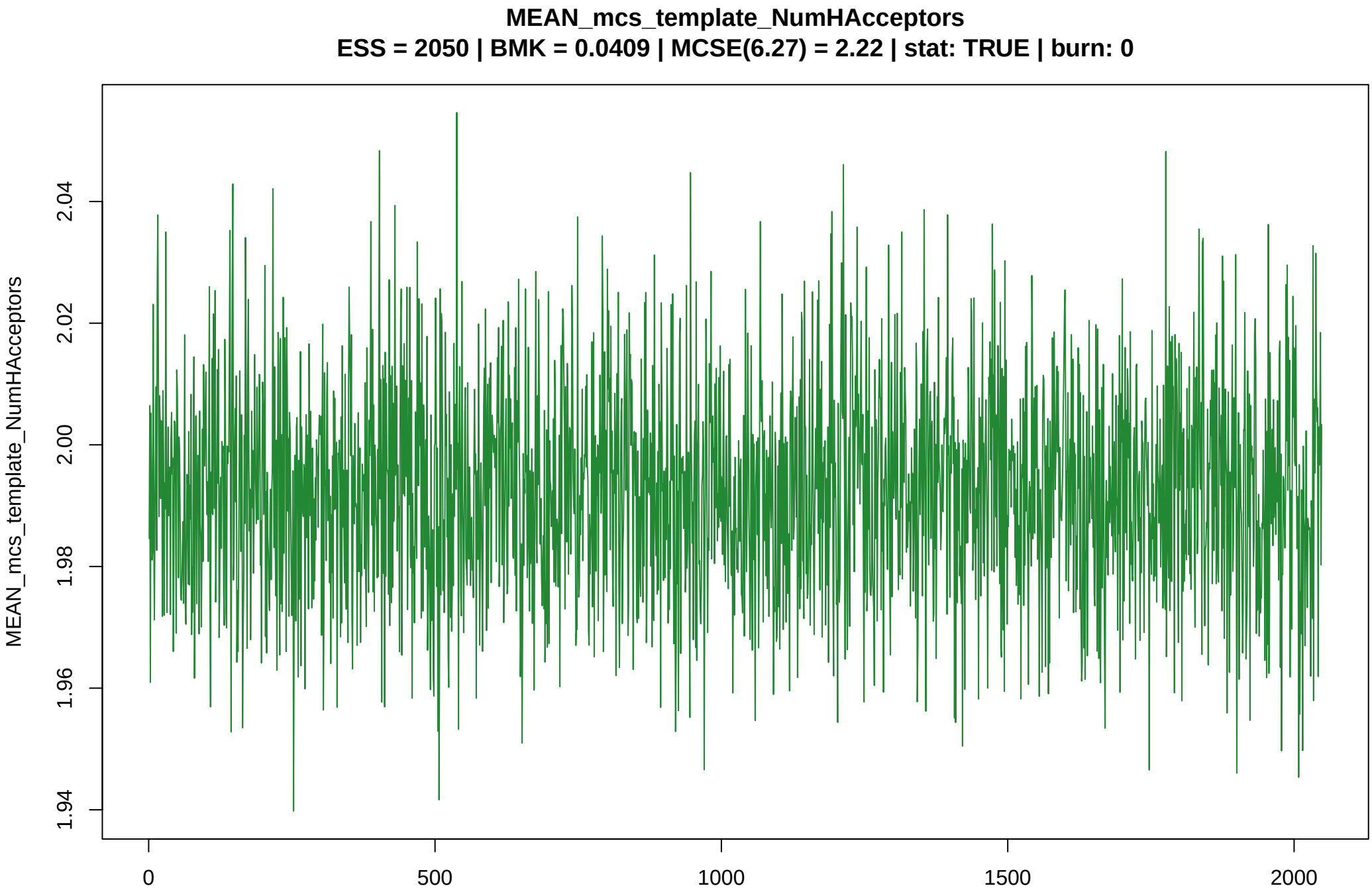

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0409 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
0
500
1000
1500
2000

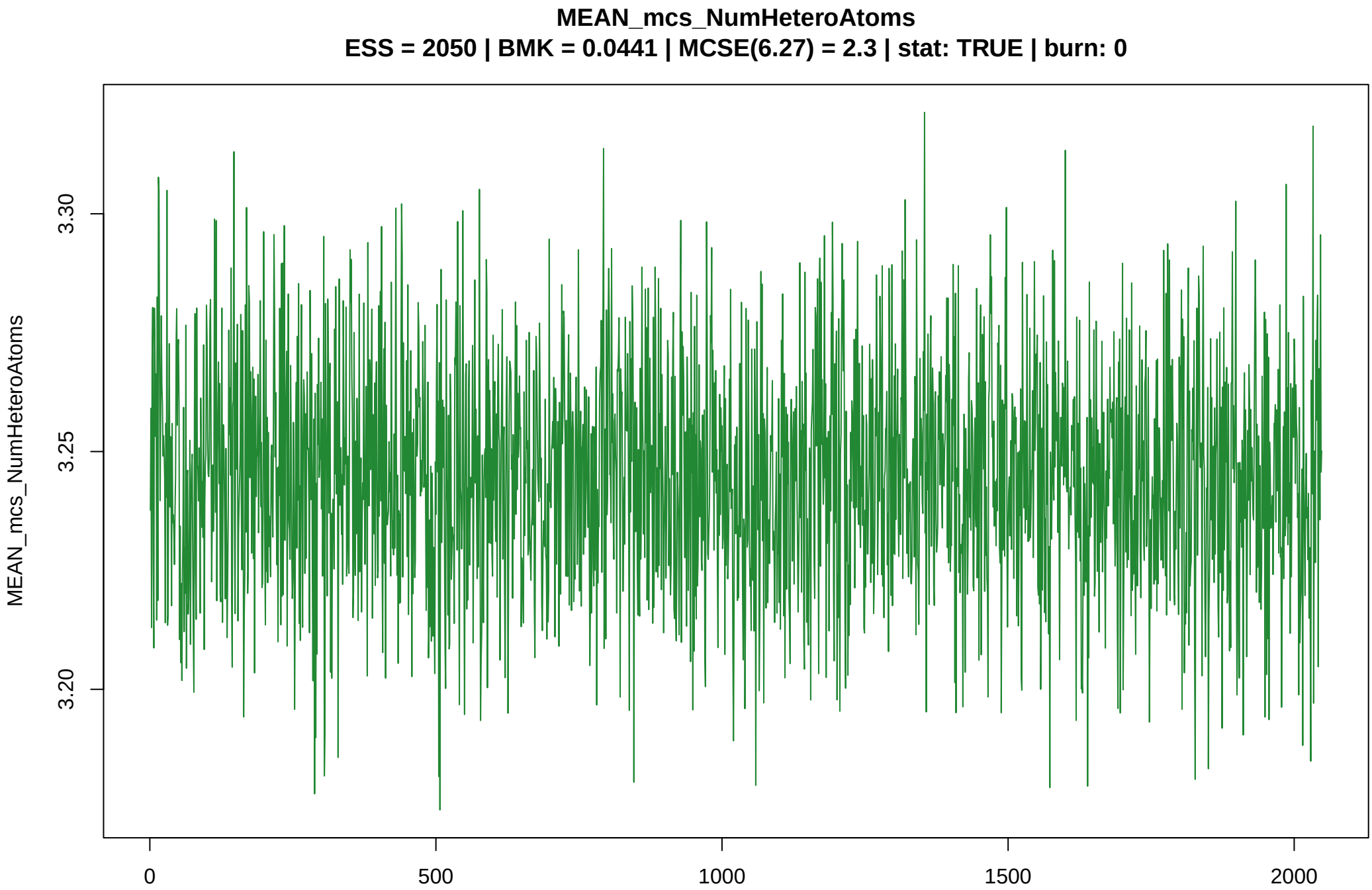

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0505 | MCSE(6.27) = 2.03 | stat: FALSE | burn: 0
MEAN_docked_HeavyAtomCount
27.0
27.1
27.2
27.3
27.4
27.5
0
500
1000
1500
2000

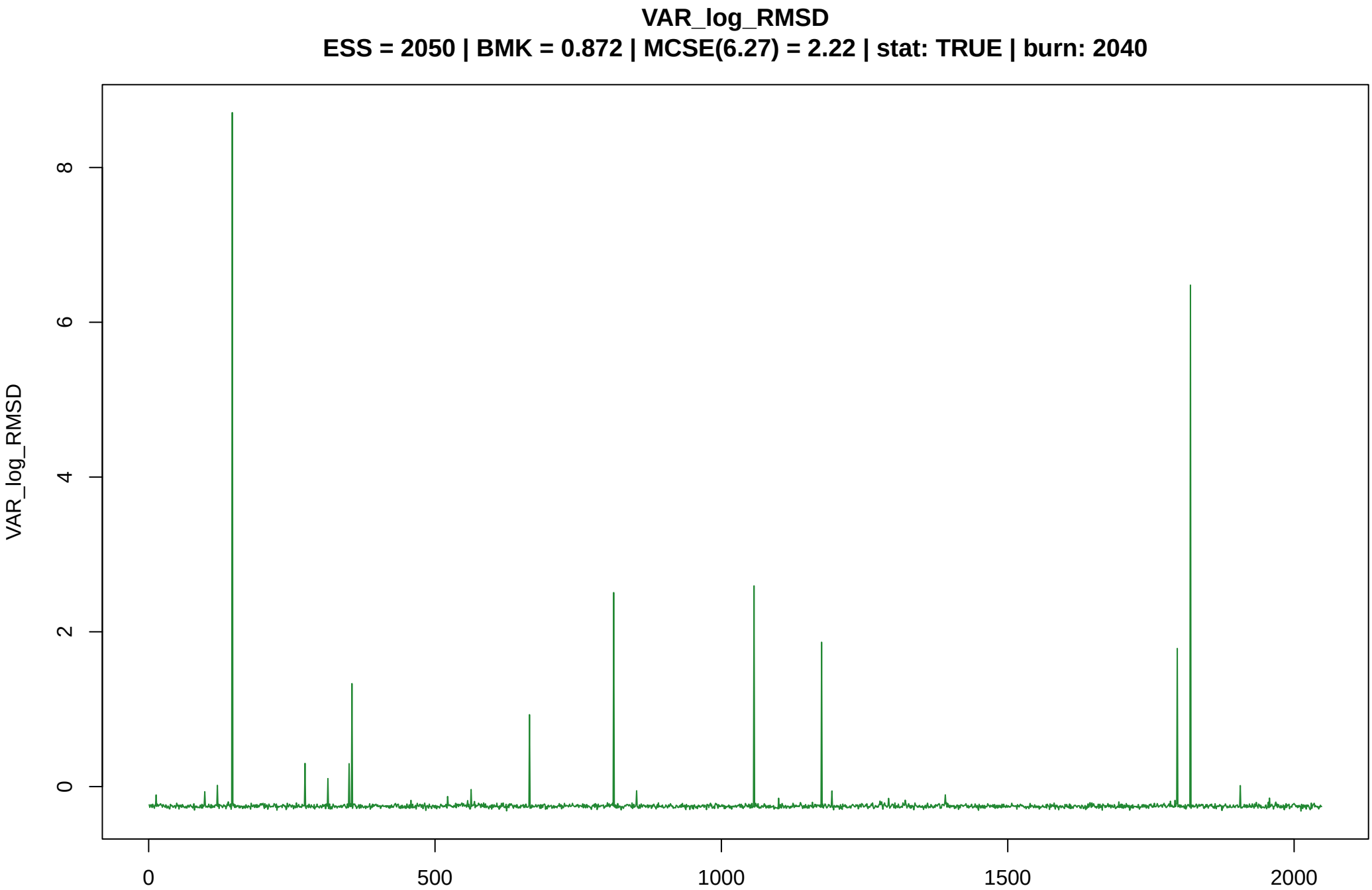

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0329 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

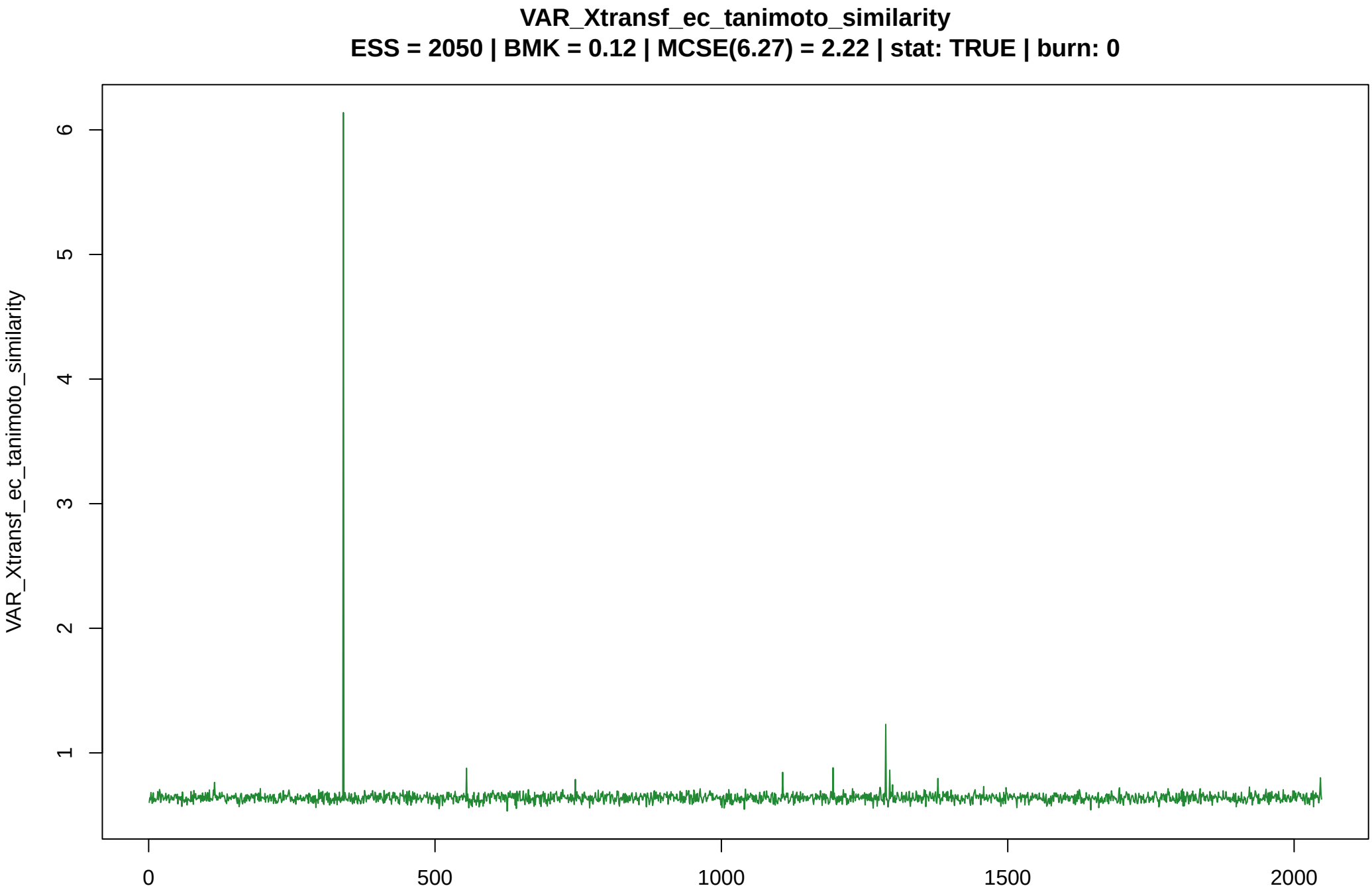

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0243 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

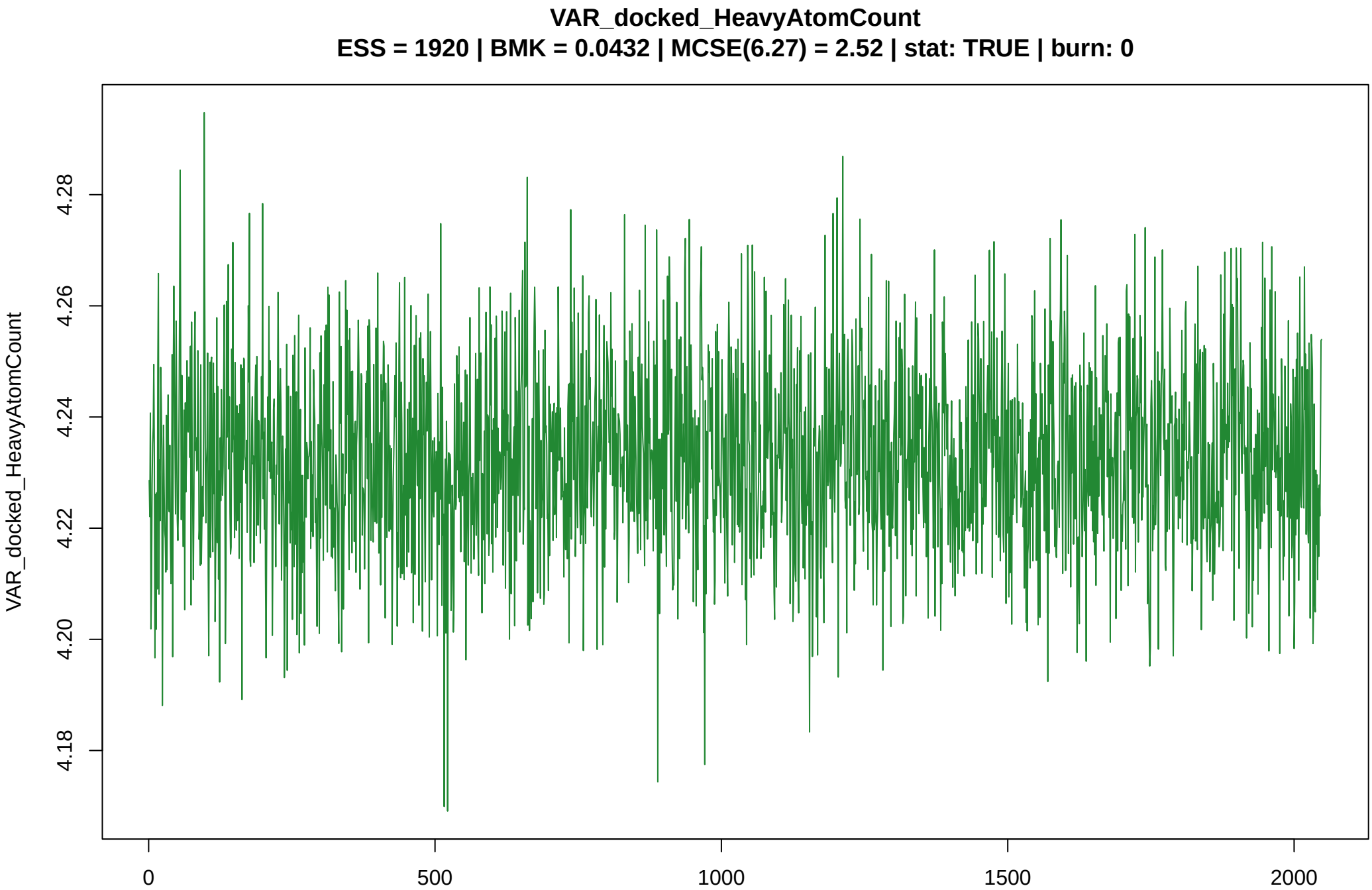

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0478 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
2.06
0
500
1000
1500
2000

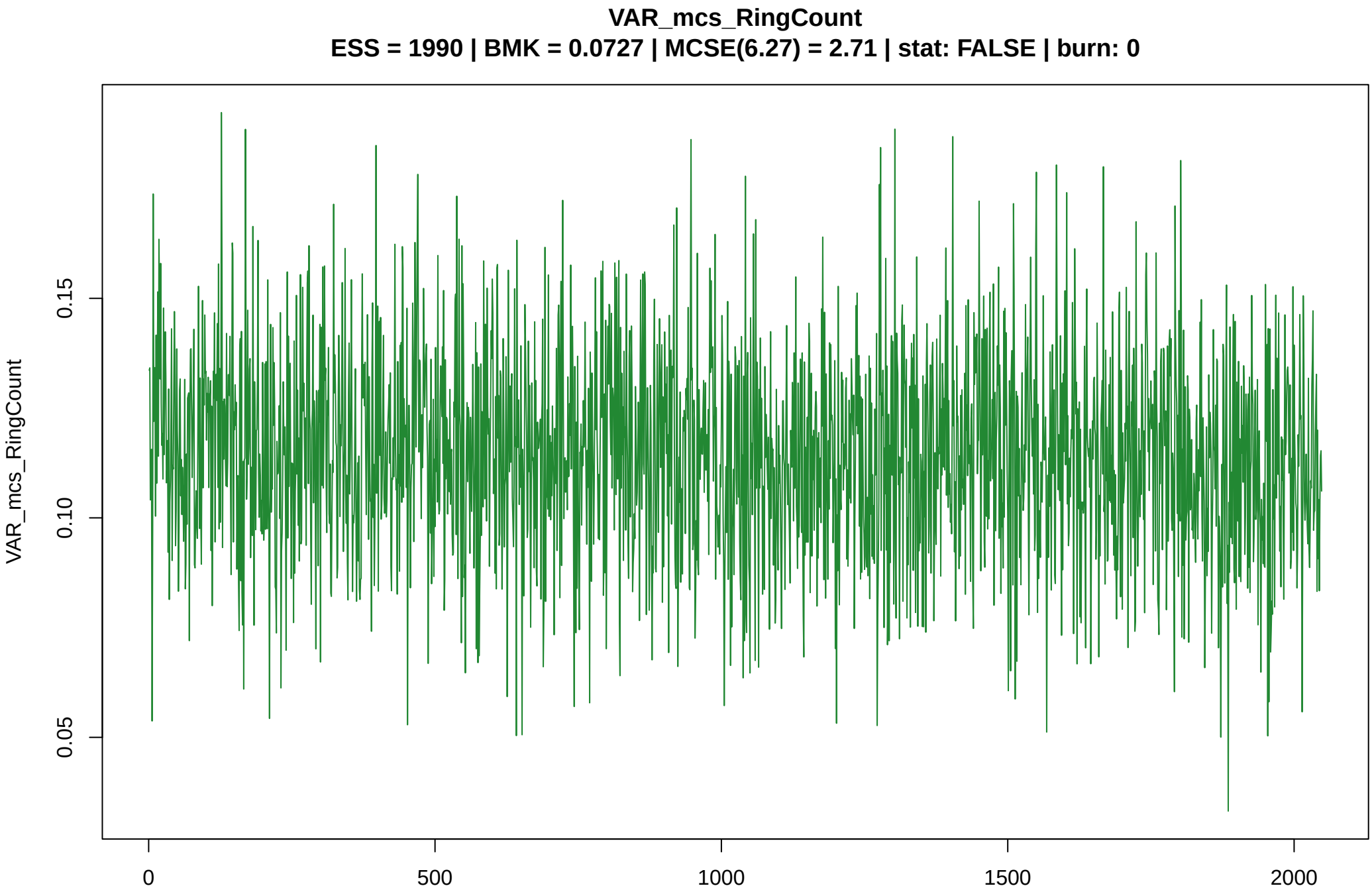

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0409 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

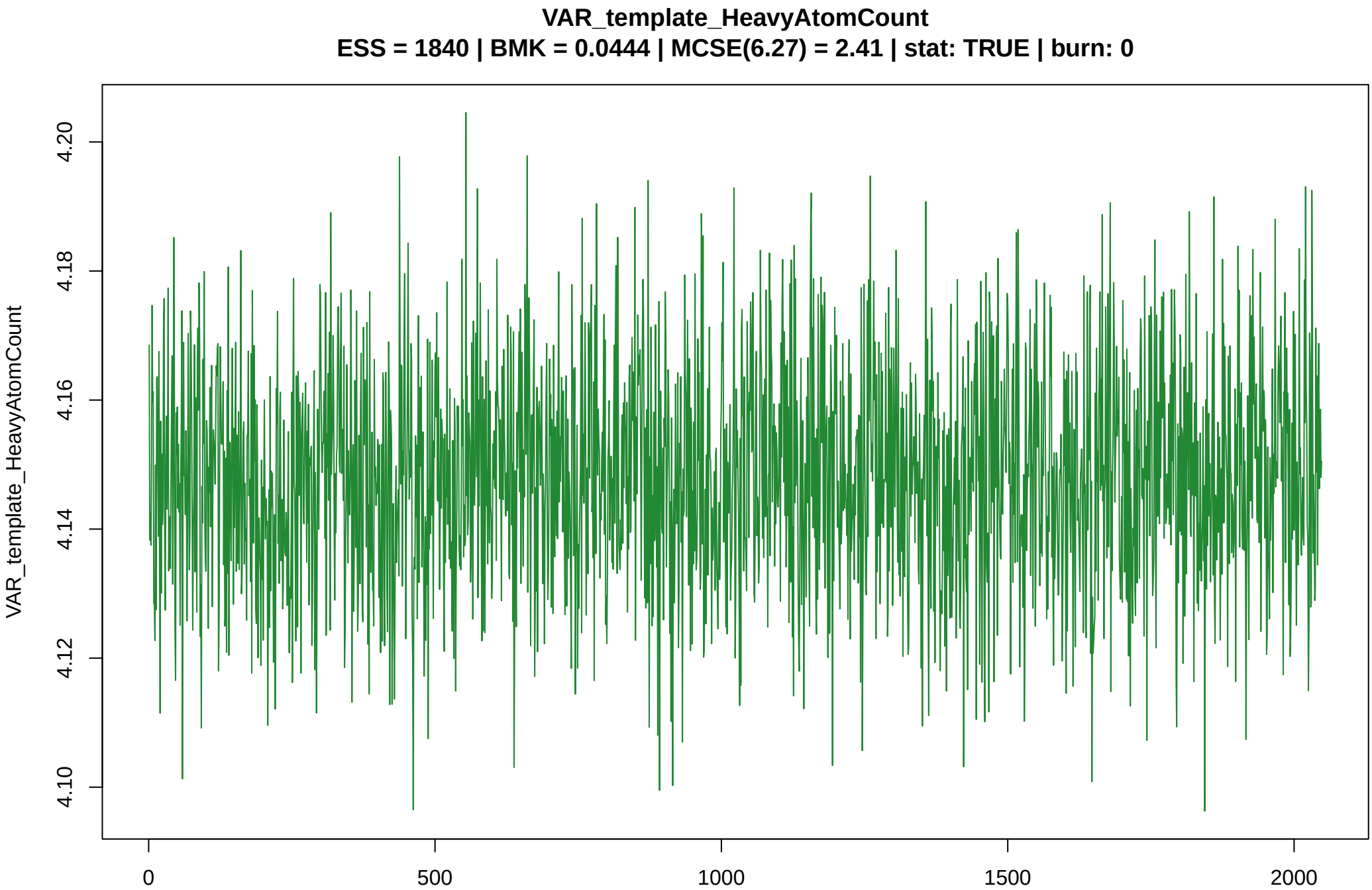

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0441 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.20
3.25
3.30
0
500
1000
1500
2000

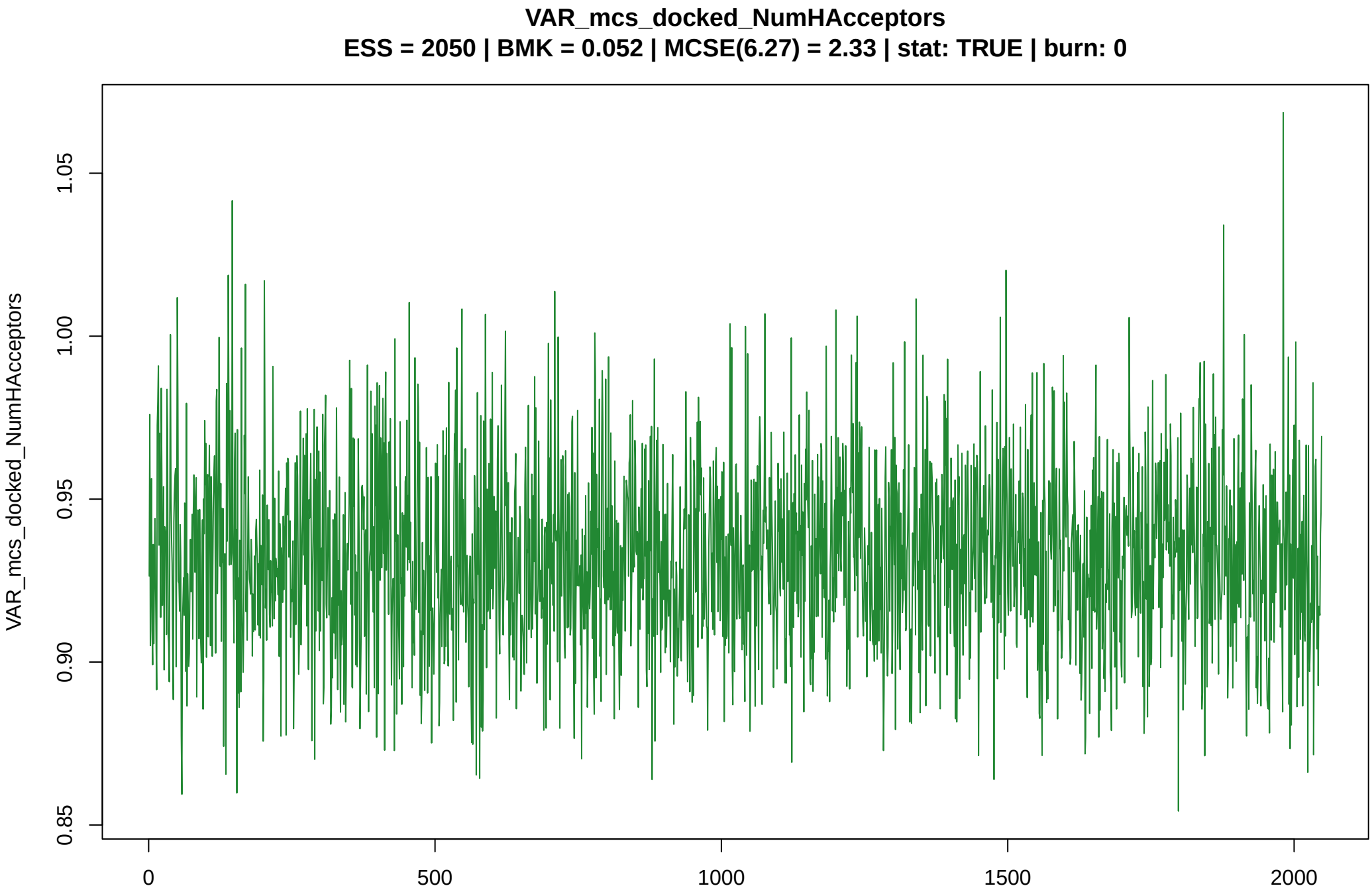

VAR_log_RMSD
ESS = 2050 | BMK = 0.872 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 2040
VAR_log_RMSD
0
2
4
6
8
0
500
1000
1500
2000

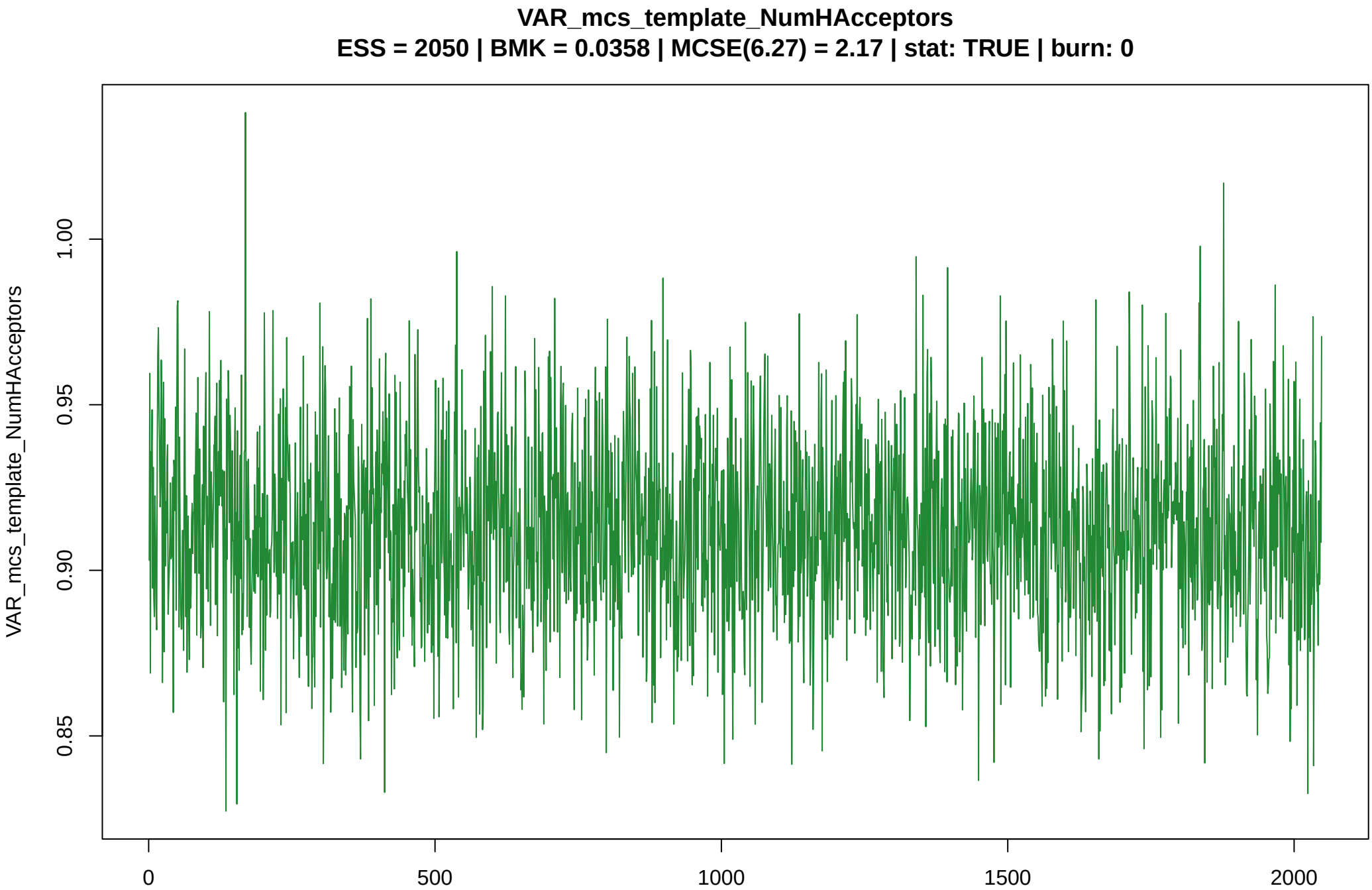

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.12 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
VAR_Xtransf_ec_tanimoto_similarity
1
2
3
4
5
6
0
500
1000
1500
2000

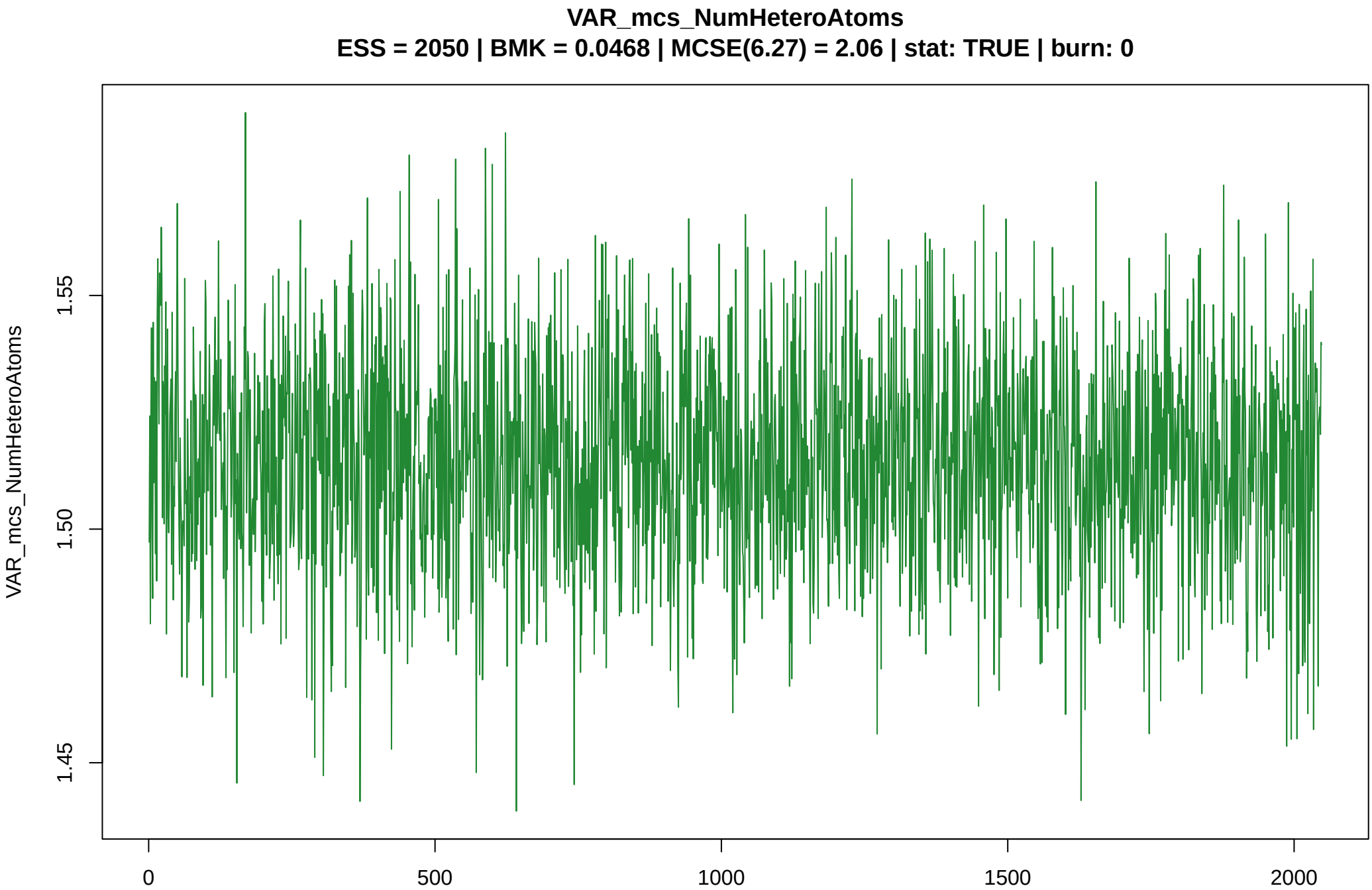

VAR_docked_HeavyAtomCount
ESS = 1920 | BMK = 0.0432 | MCSE(6.27) = 2.52 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
4.18
4.20
4.22
4.24
4.26
4.28
0
500
1000
1500
2000

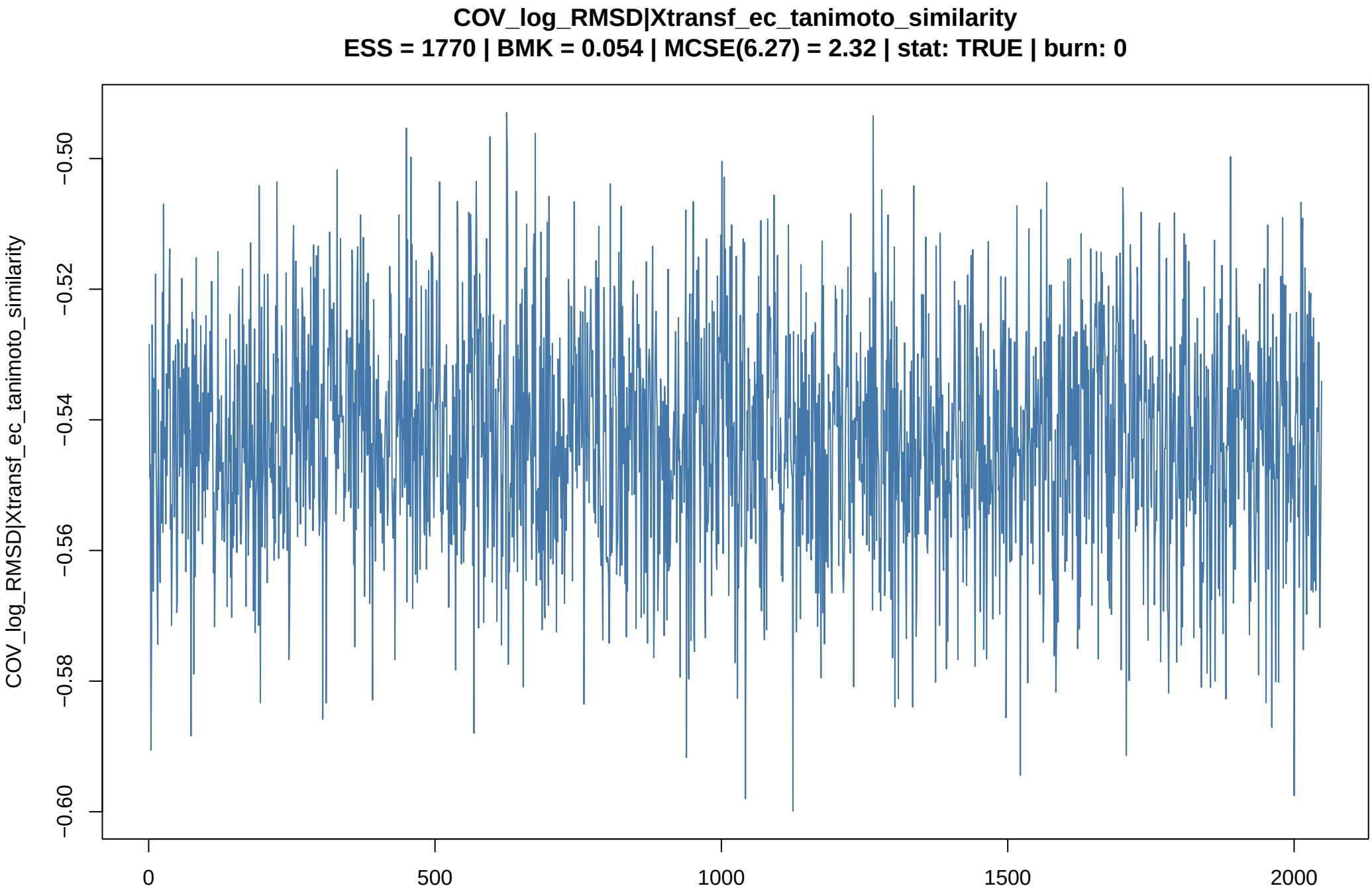

VAR_mcs_RingCount
ESS = 1990 | BMK = 0.0727 | MCSE(6.27) = 2.71 | stat: FALSE | burn: 0
VAR_mcs_RingCount
0.05
0.10
0.15
0
500
1000
1500
2000

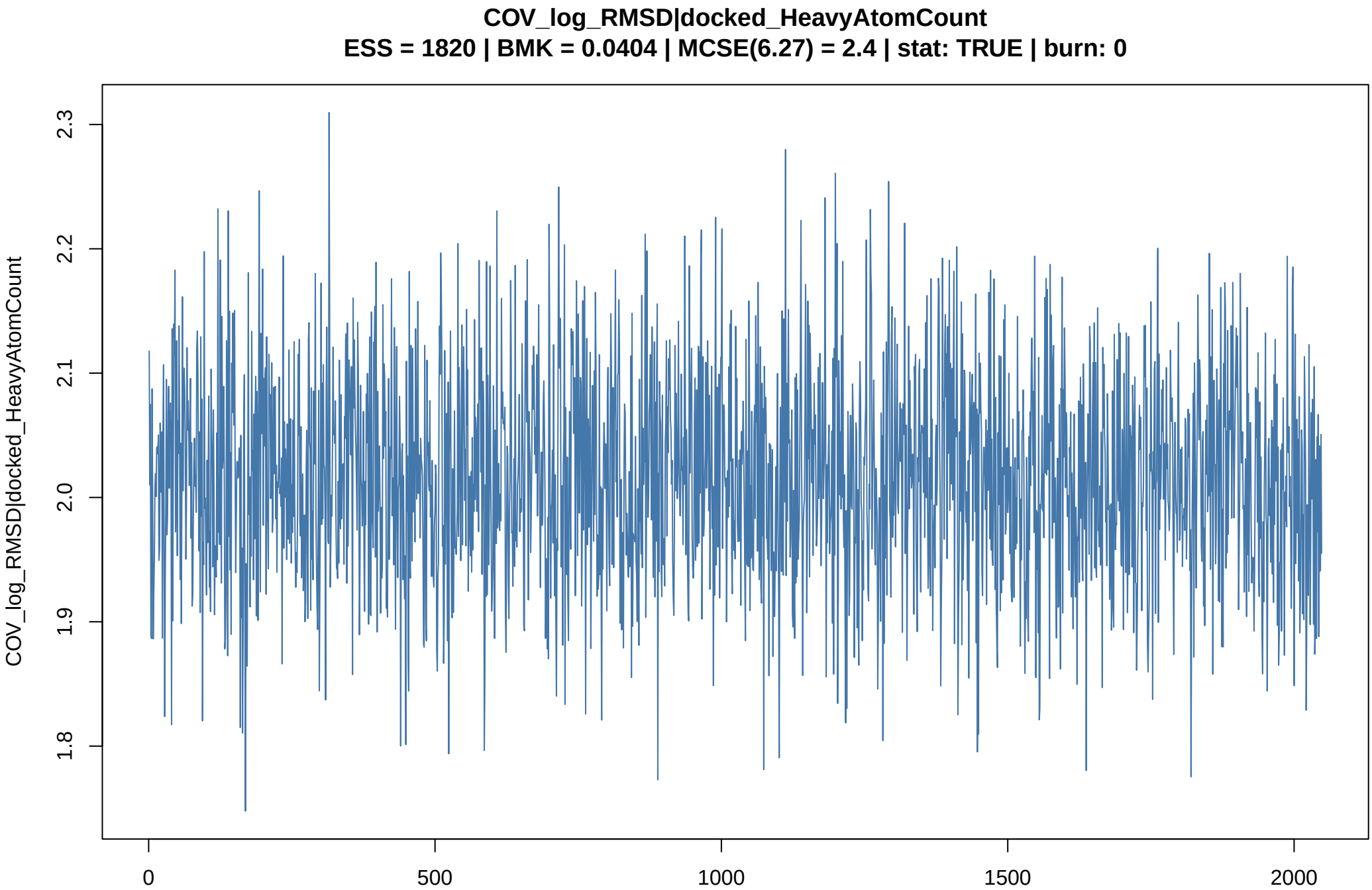

VAR_template_HeavyAtomCount
ESS = 1840 | BMK = 0.0444 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 0
VAR_template_HeavyAtomCount
4.10
4.12
4.14
4.16
4.18
4.20
0
500
1000
1500
2000

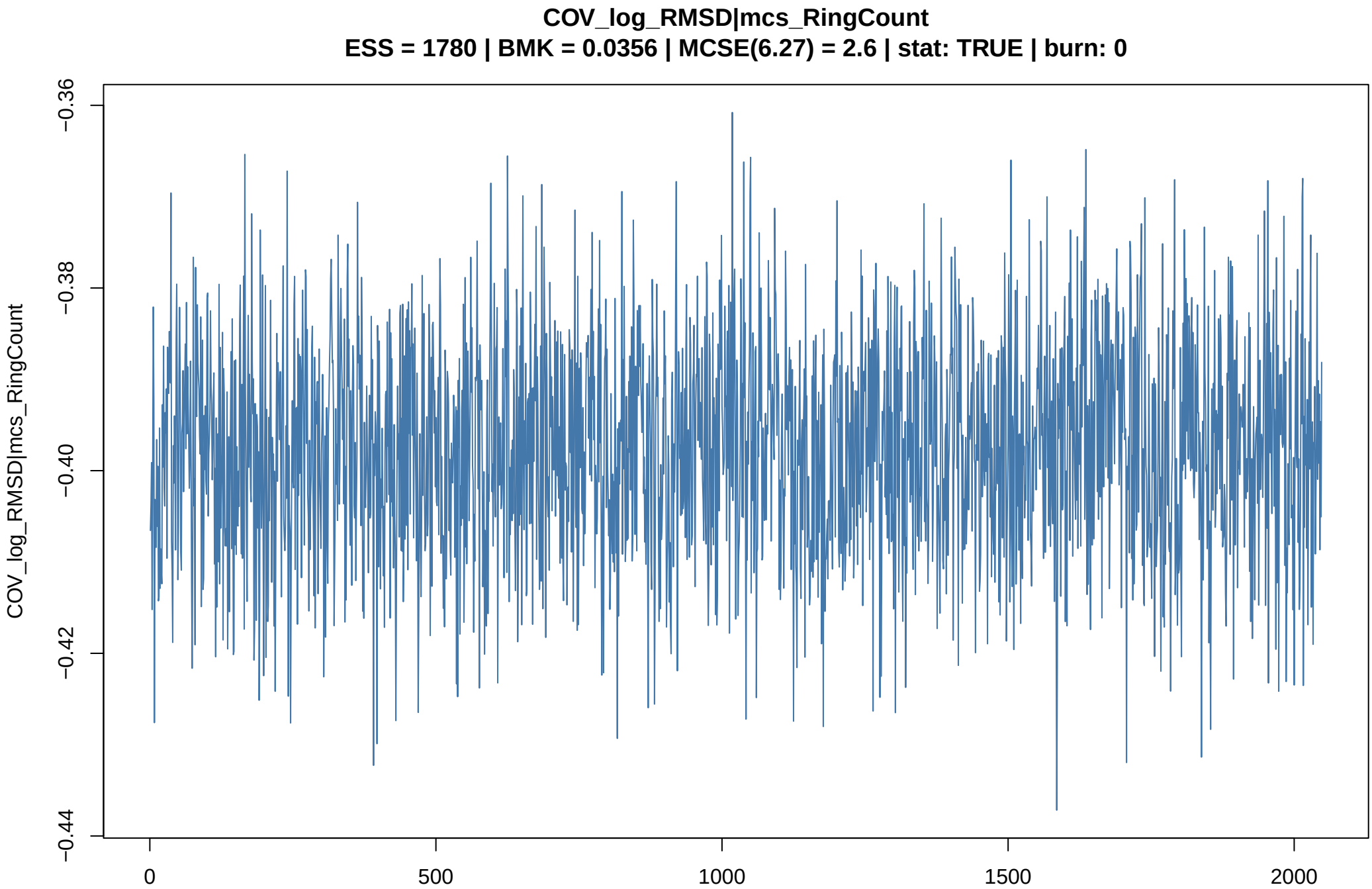

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.052 | MCSE(6.27) = 2.33 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
0.85
0.90
0.95
1.00
1.05
0
500
1000
1500
2000

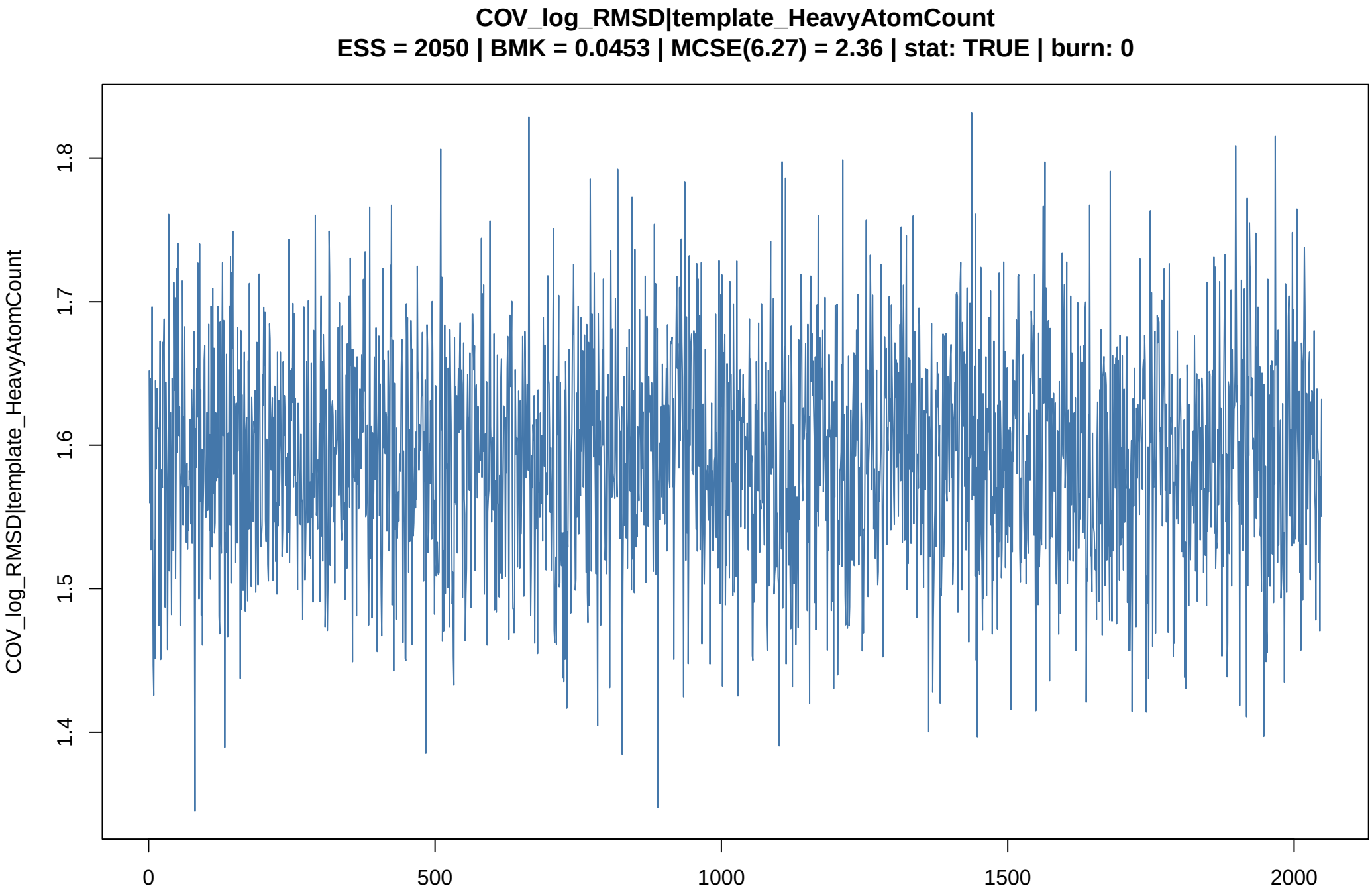

VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0358 | MCSE(6.27) = 2.17 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
0.85
0.90
0.95
1.00
0
500
1000
1500
2000

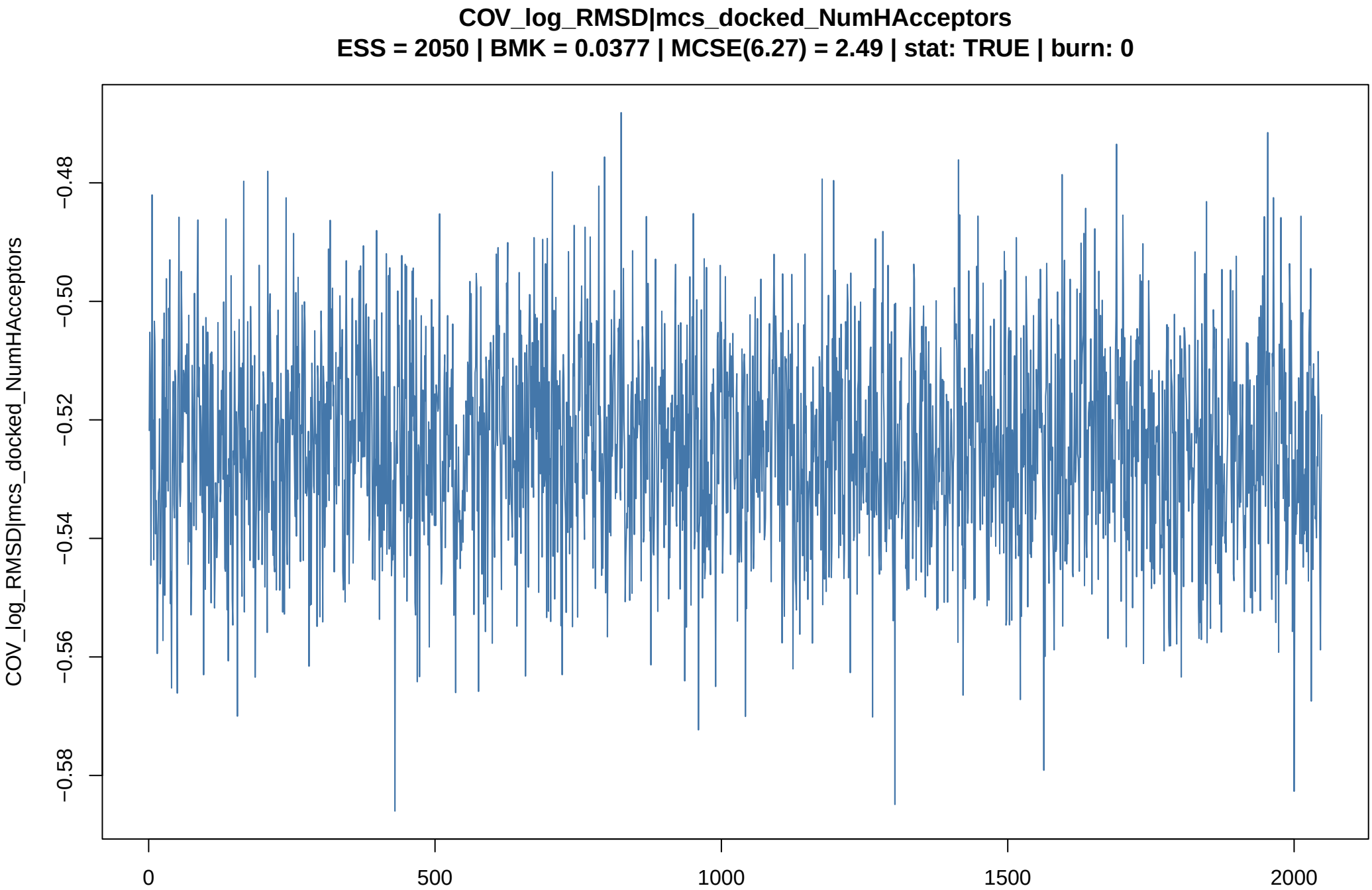

VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0468 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
1.45
1.50
1.55
0
500
1000
1500
2000

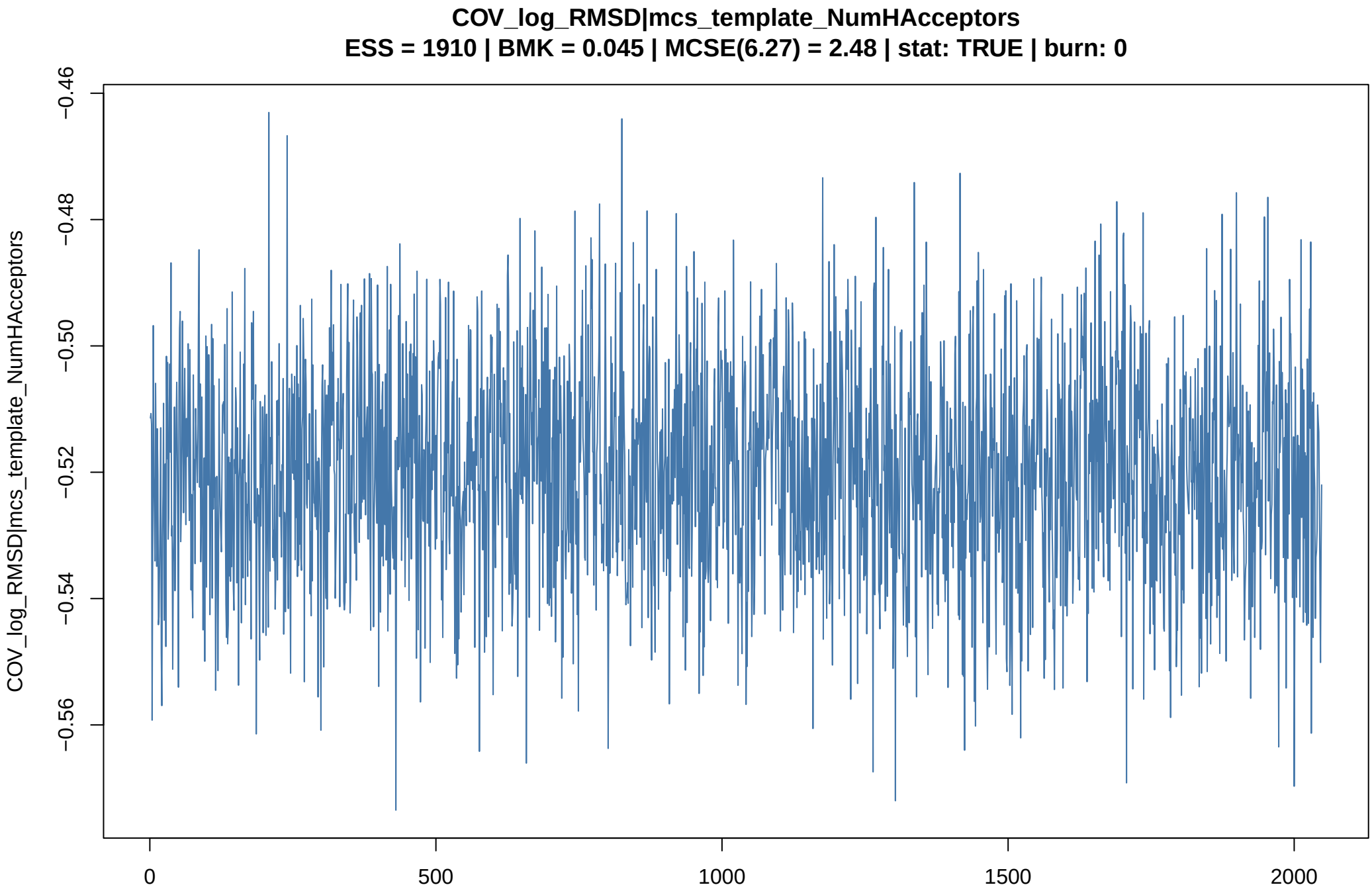

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1770 | BMK = 0.054 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.50
−0.52
−0.54
−0.56
−0.58
−0.60
0
500
1000
1500
2000

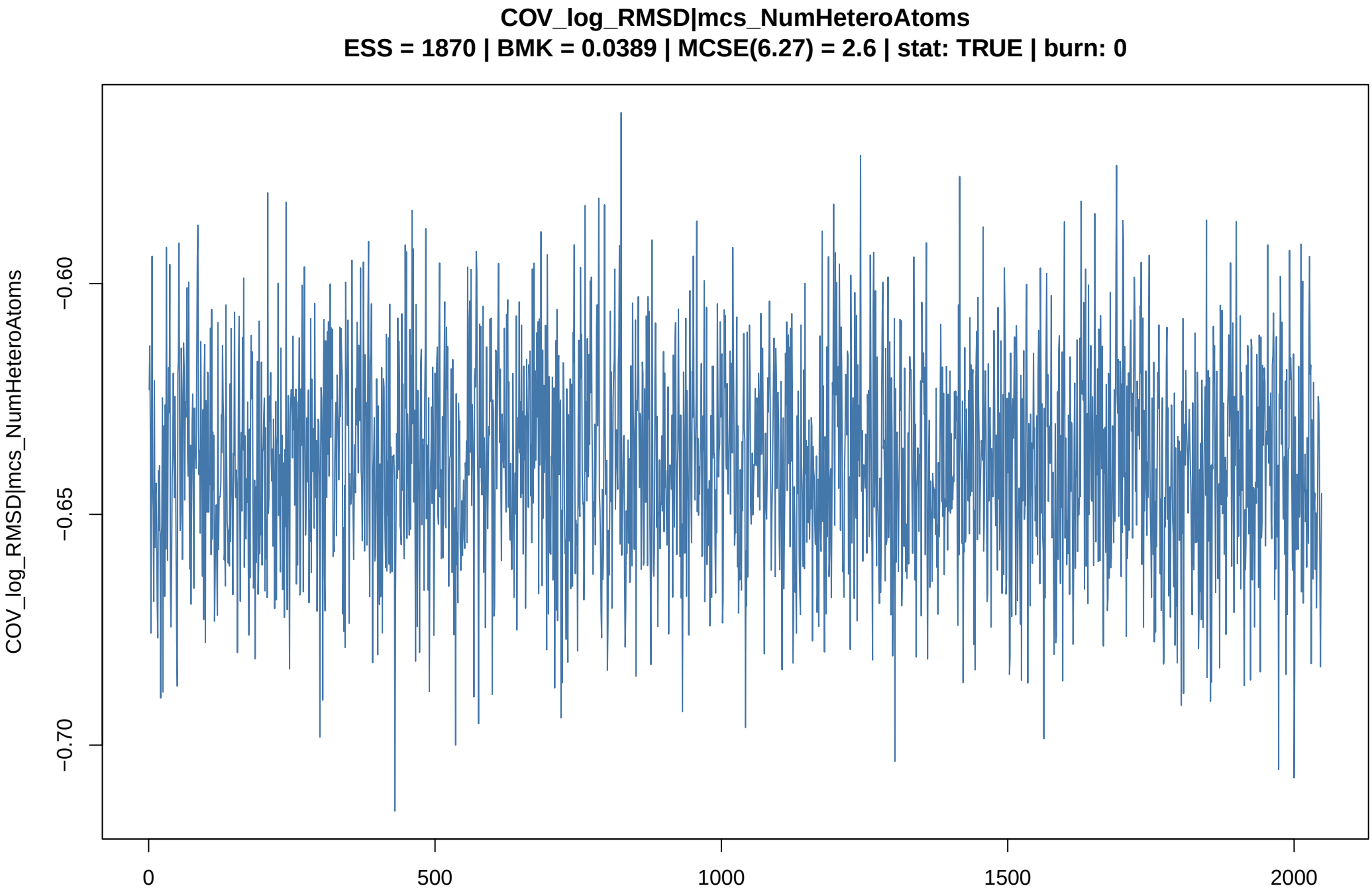

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1820 | BMK = 0.0404 | MCSE(6.27) = 2.4 | stat: TRUE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.8
1.9
2.0
2.1
2.2
2.3
0
500
1000
1500
2000

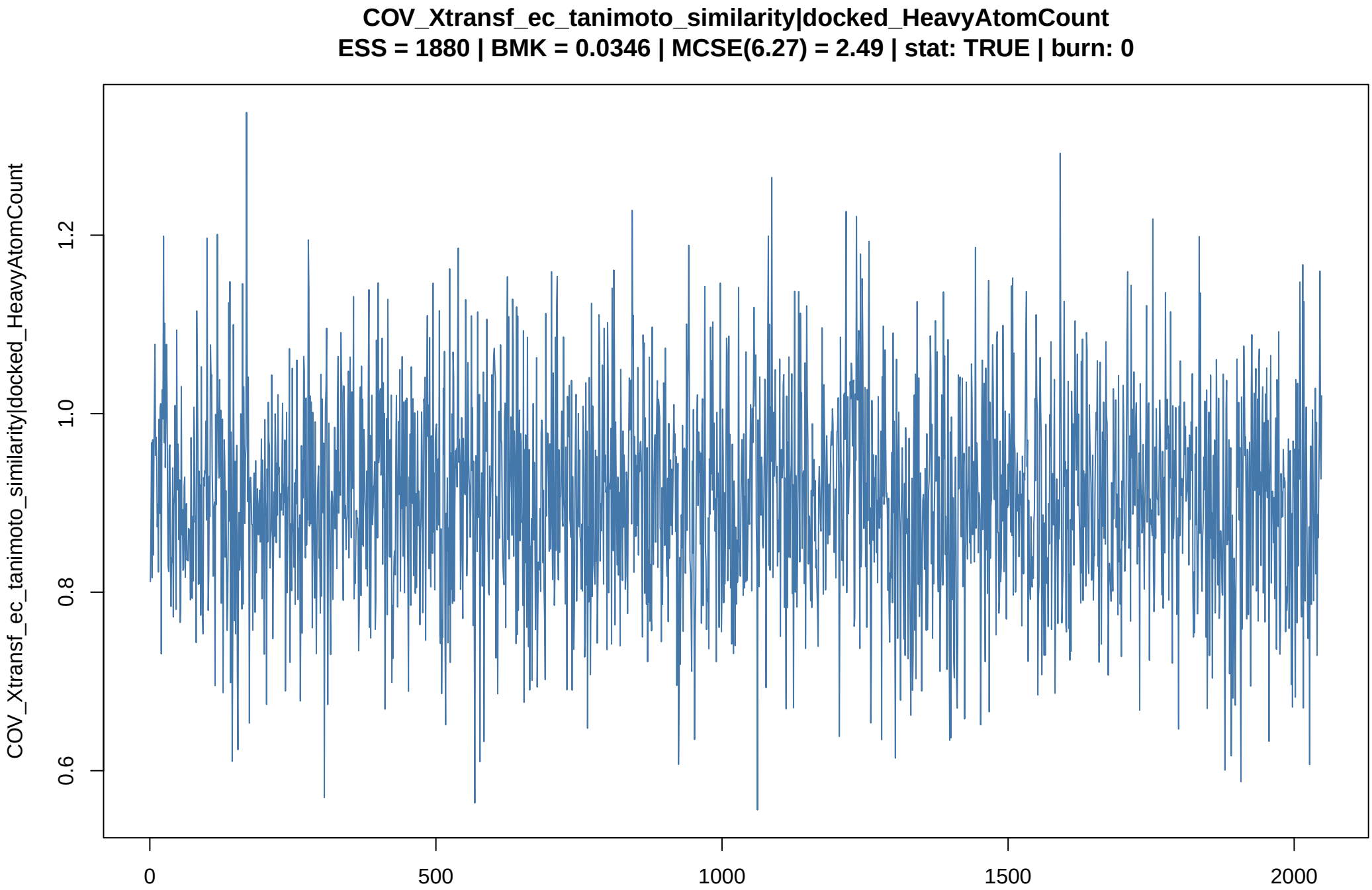

COV_log_RMSD|mcs_RingCount
ESS = 1780 | BMK = 0.0356 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.36
−0.38
−0.40
−0.42
−0.44
0
500
1000
1500
2000

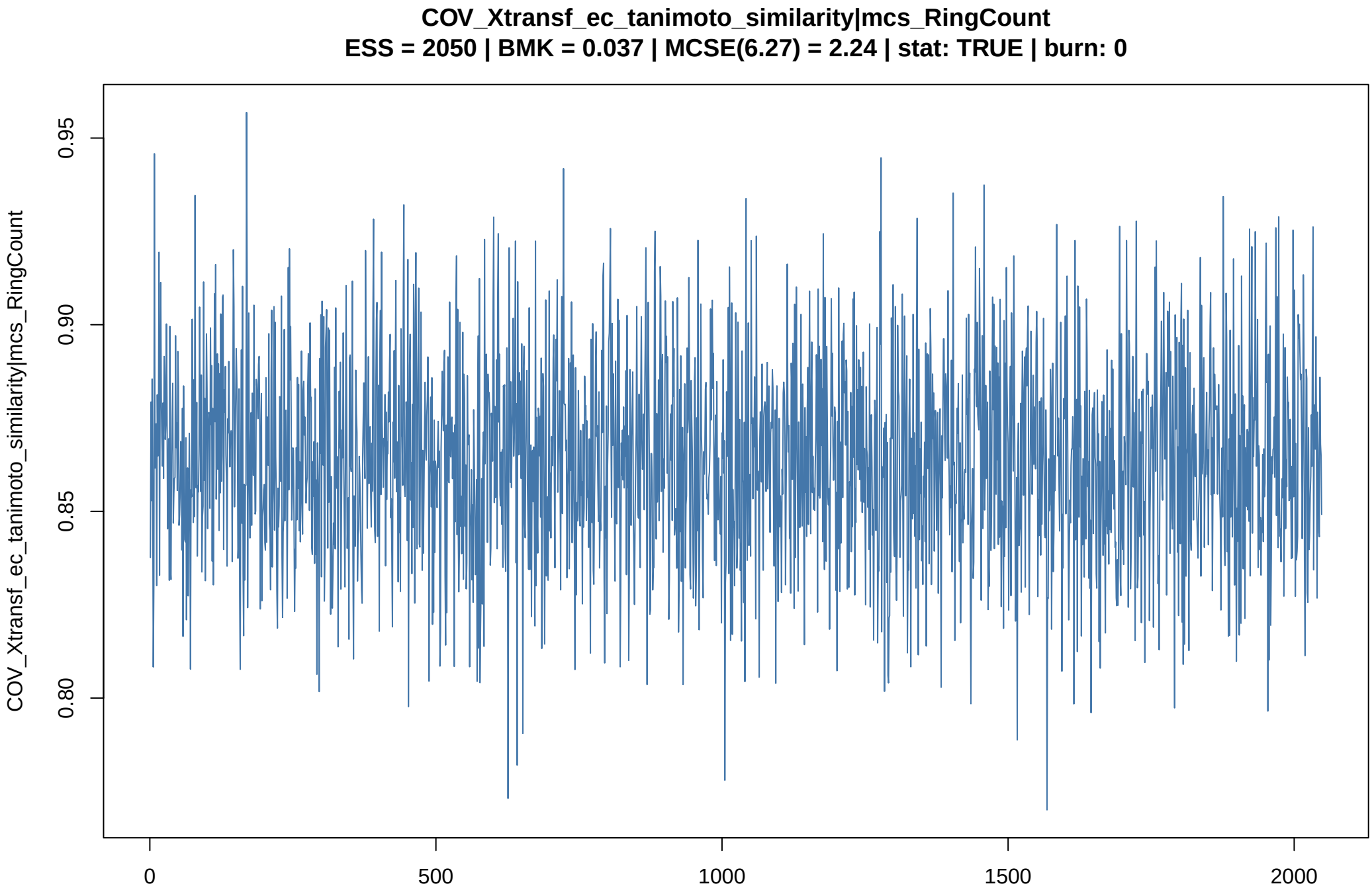

COV_log_RMSD|template_HeavyAtomCount
ESS = 2050 | BMK = 0.0453 | MCSE(6.27) = 2.36 | stat: TRUE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

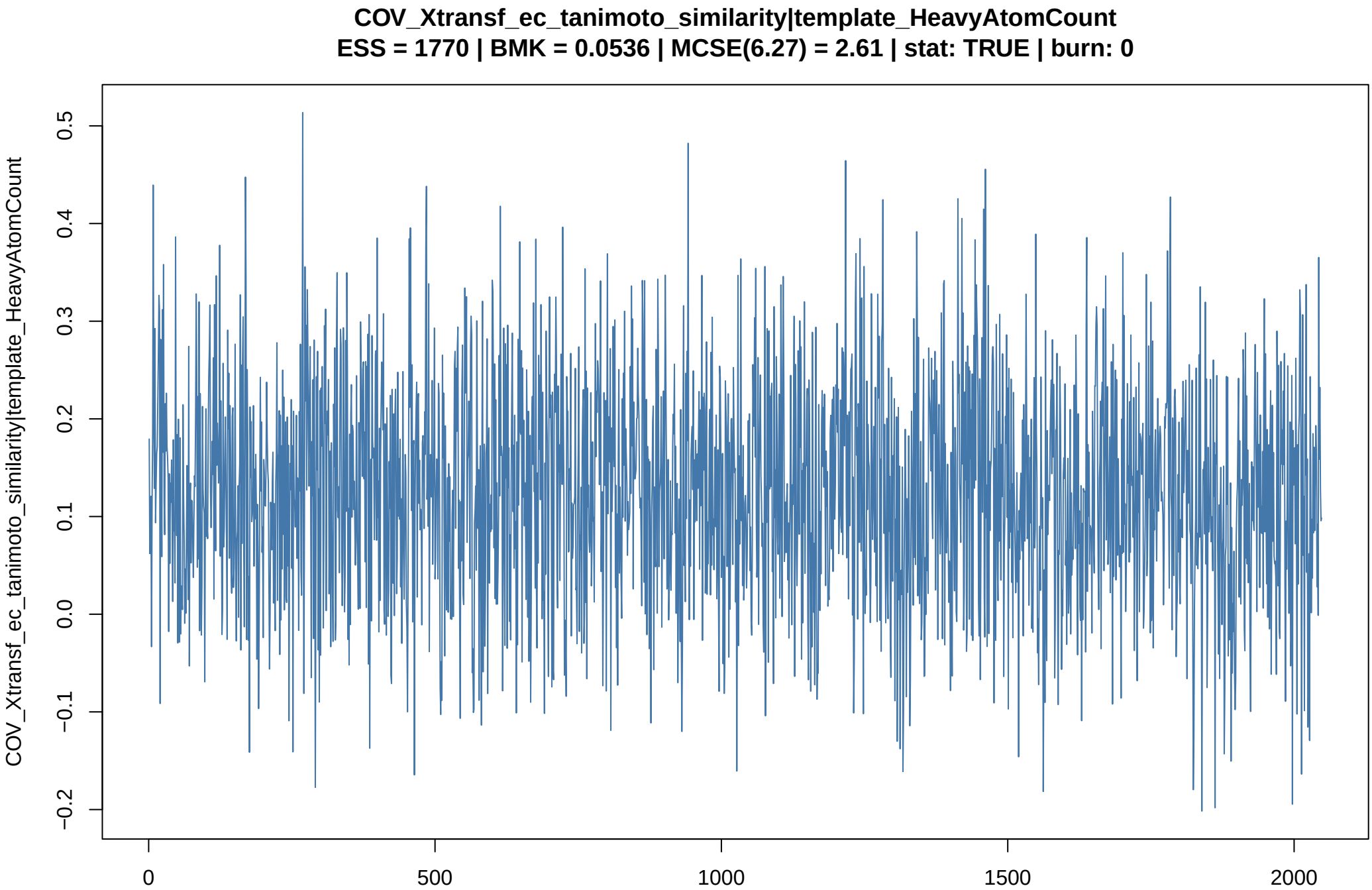

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0377 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

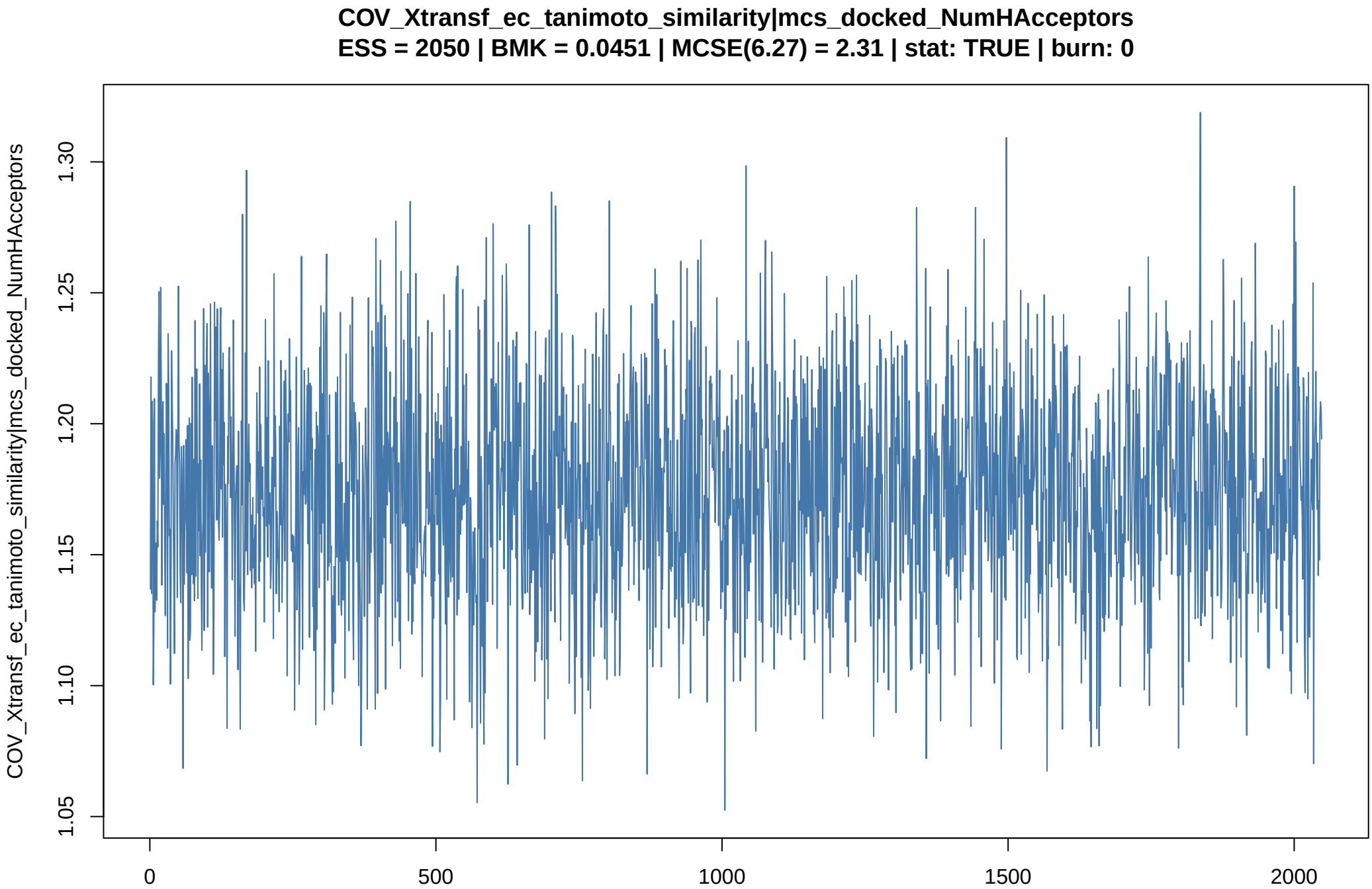

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 1910 | BMK = 0.045 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.46
−0.48
−0.50
−0.52
−0.54
−0.56
0
500
1000
1500
2000

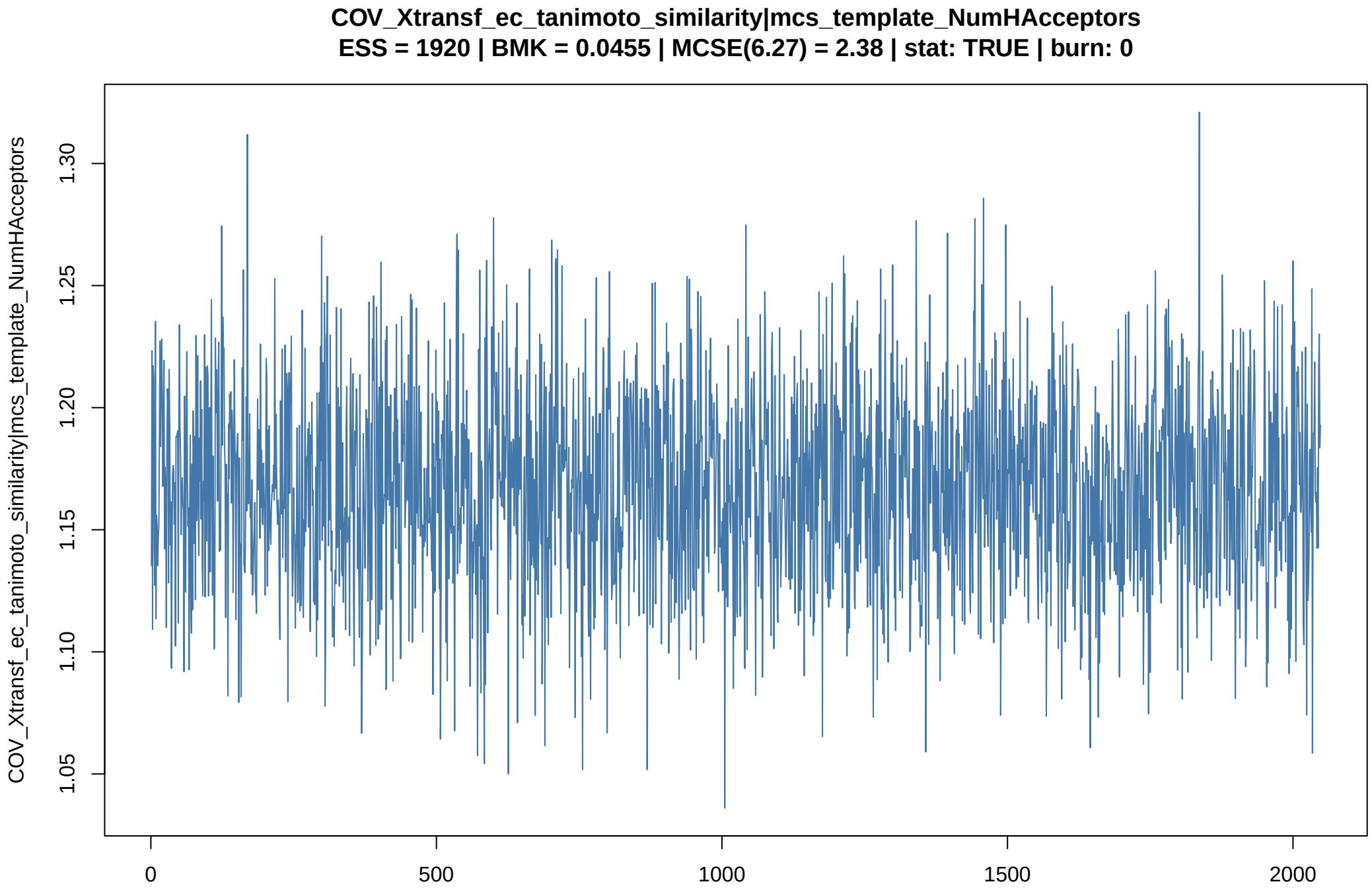

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1870 | BMK = 0.0389 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.60
−0.65
−0.70
0
500
1000
1500
2000

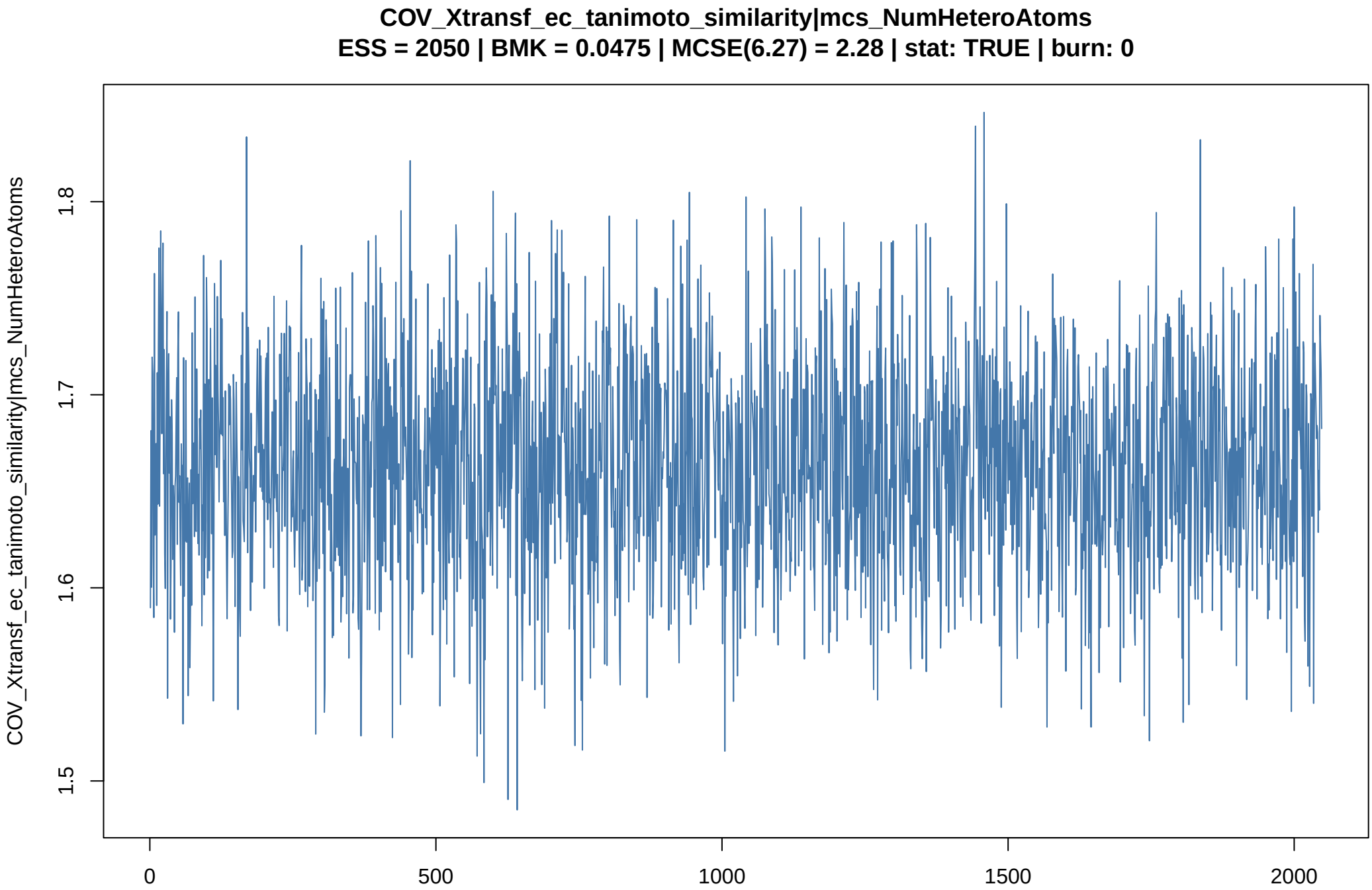

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1880 | BMK = 0.0346 | MCSE(6.27) = 2.49 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.8
1.0
1.2
0
500
1000
1500
2000

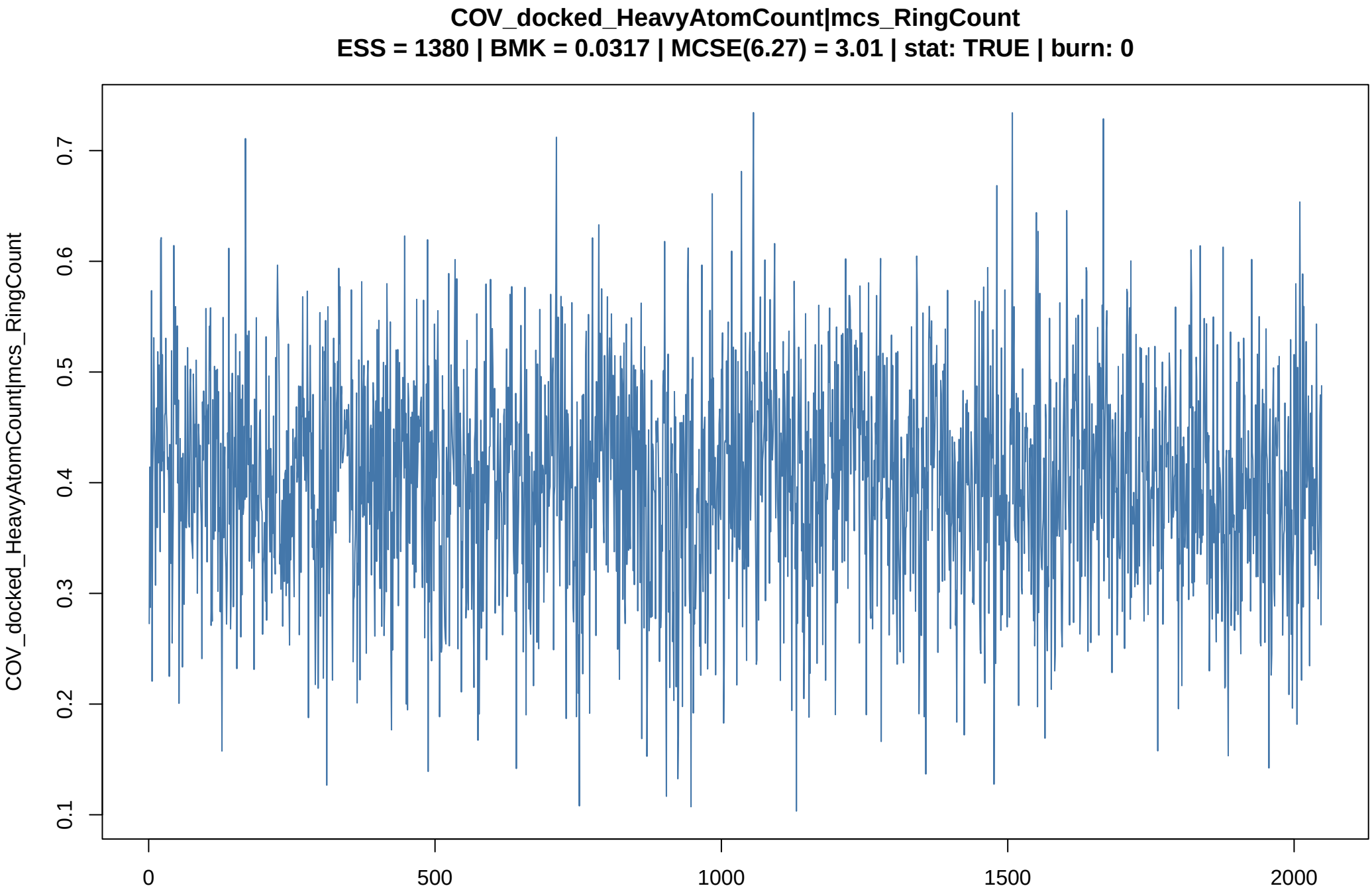

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 2050 | BMK = 0.037 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

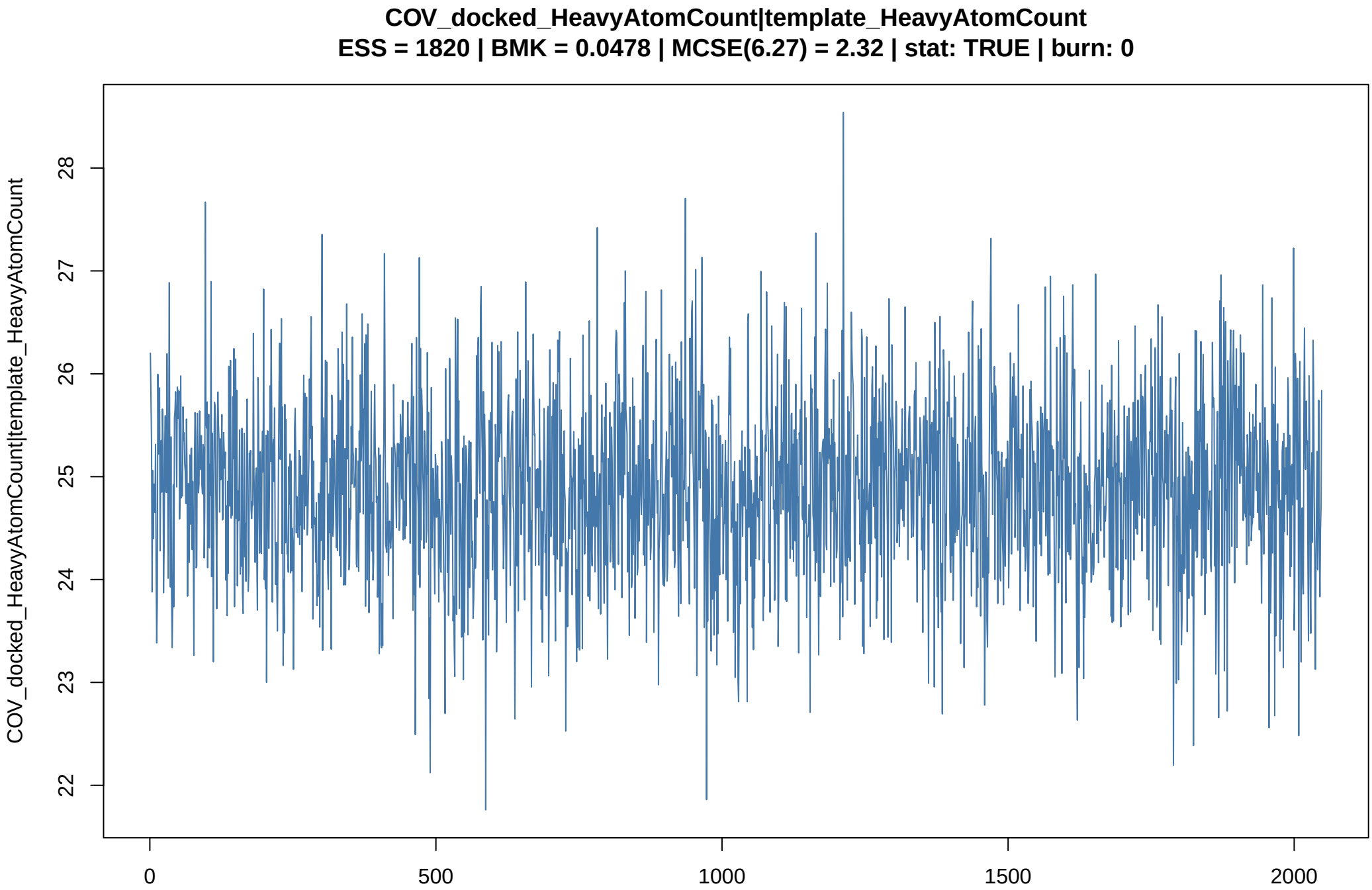

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1770 | BMK = 0.0536 | MCSE(6.27) = 2.61 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

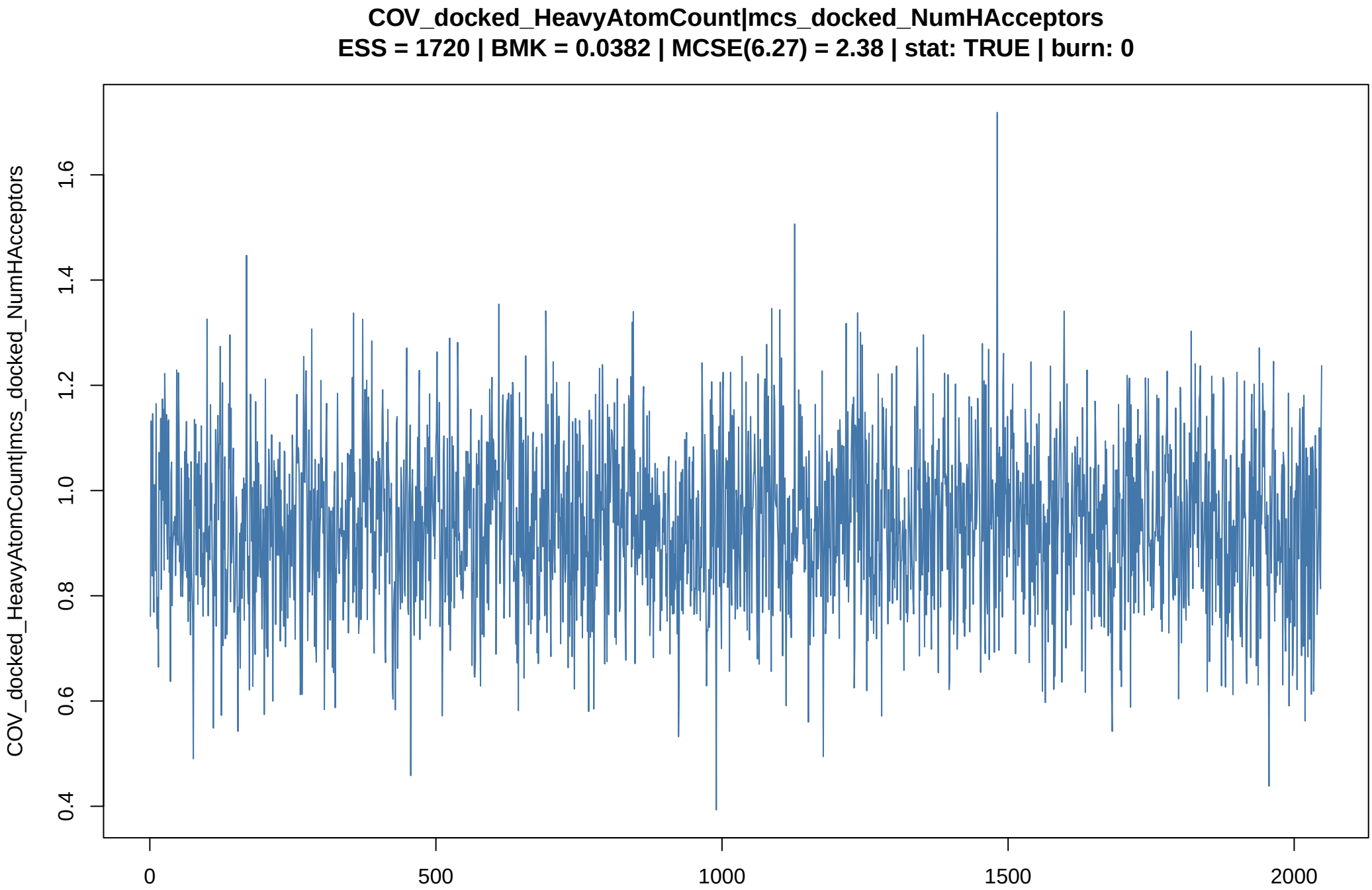

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0451 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

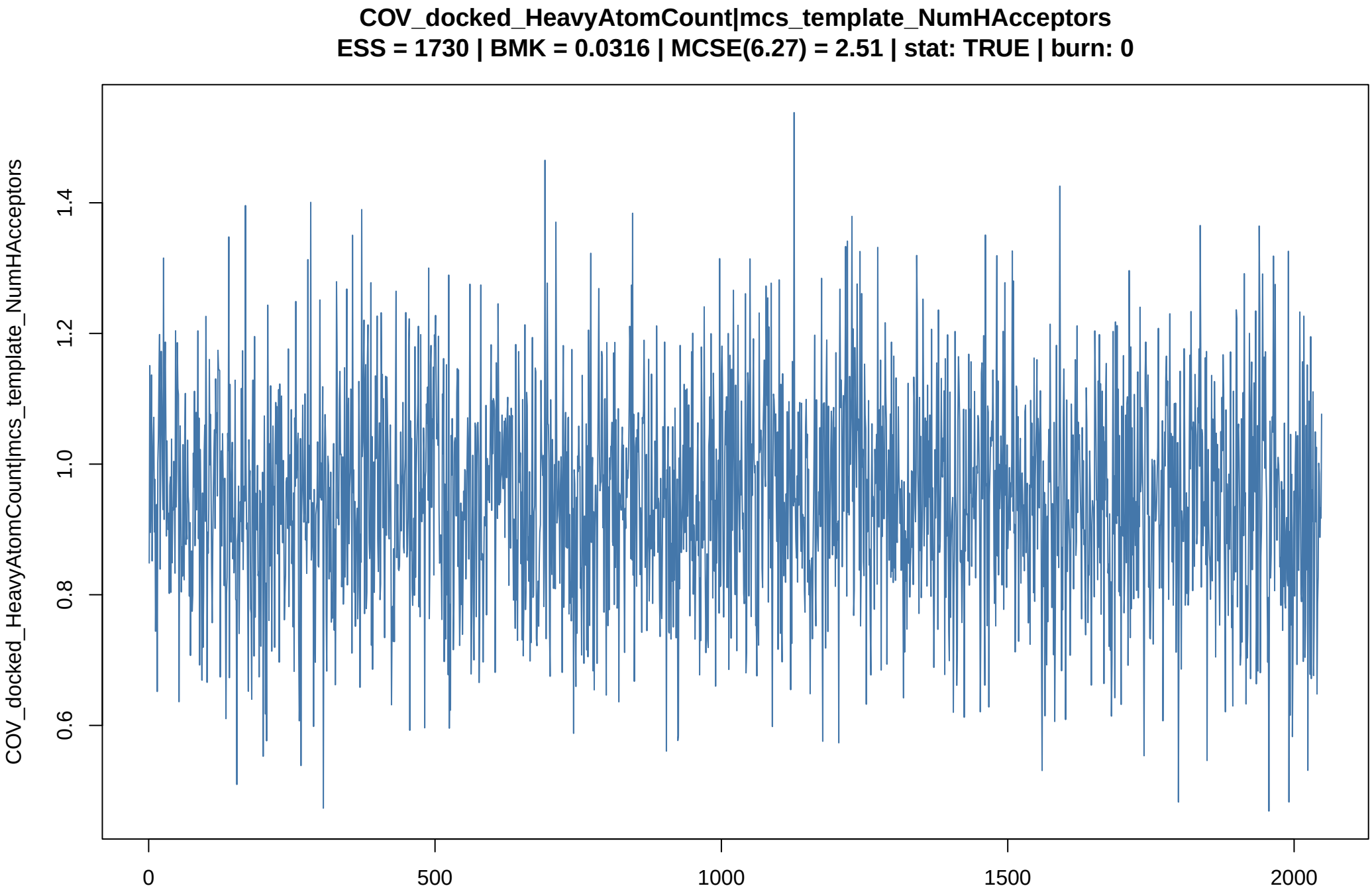

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 1920 | BMK = 0.0455 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

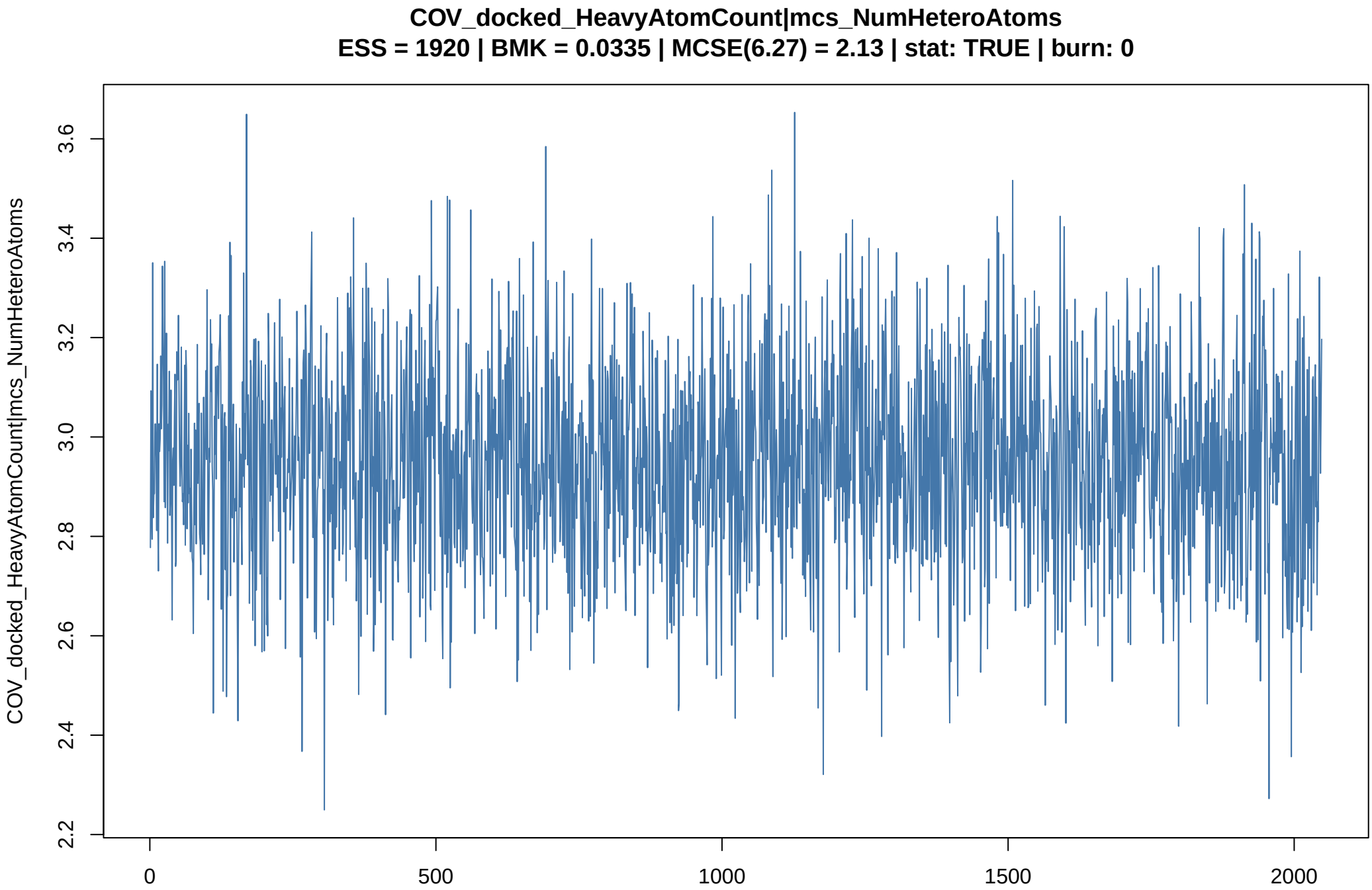

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0475 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

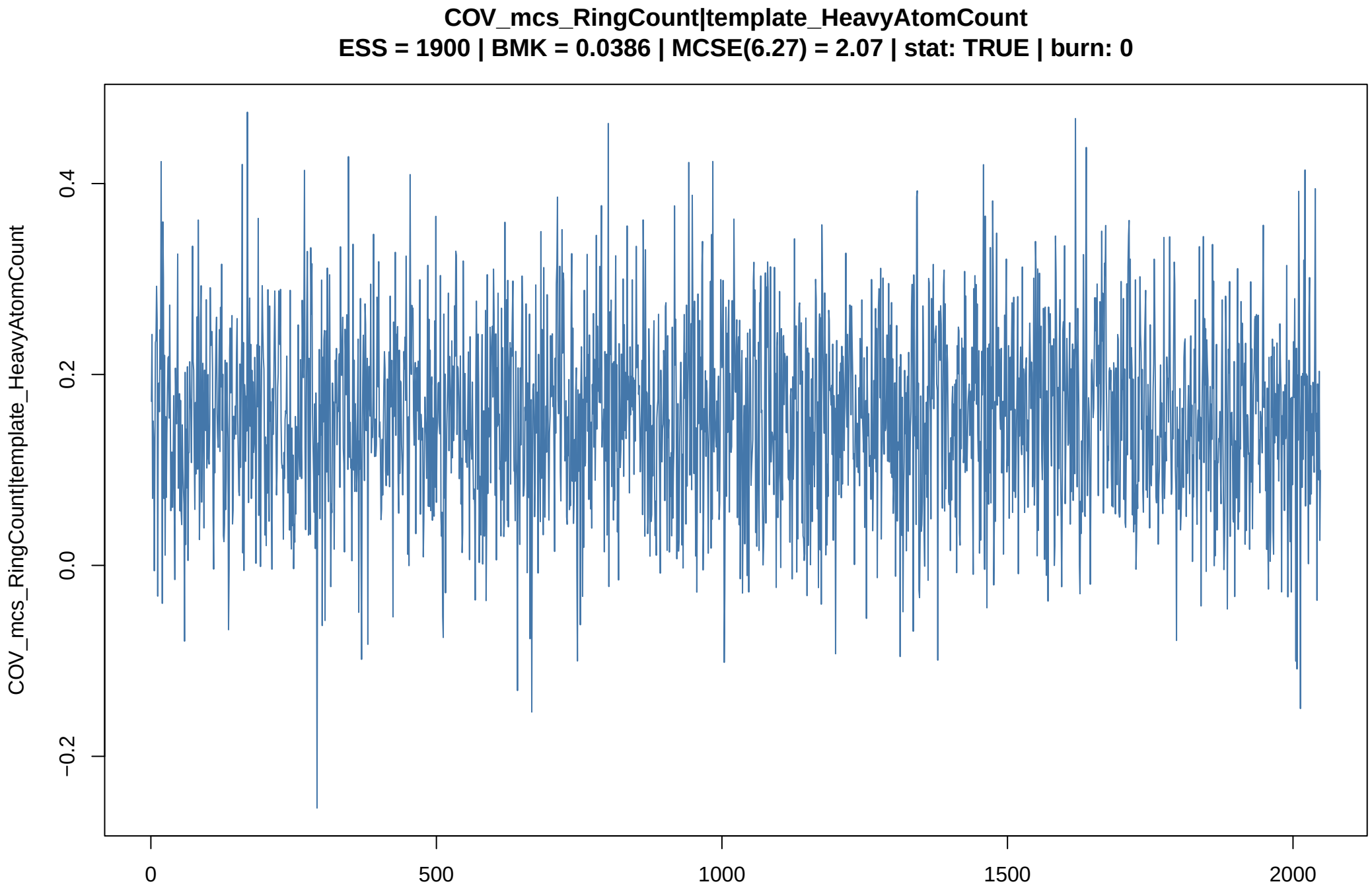

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1380 | BMK = 0.0317 | MCSE(6.27) = 3.01 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000

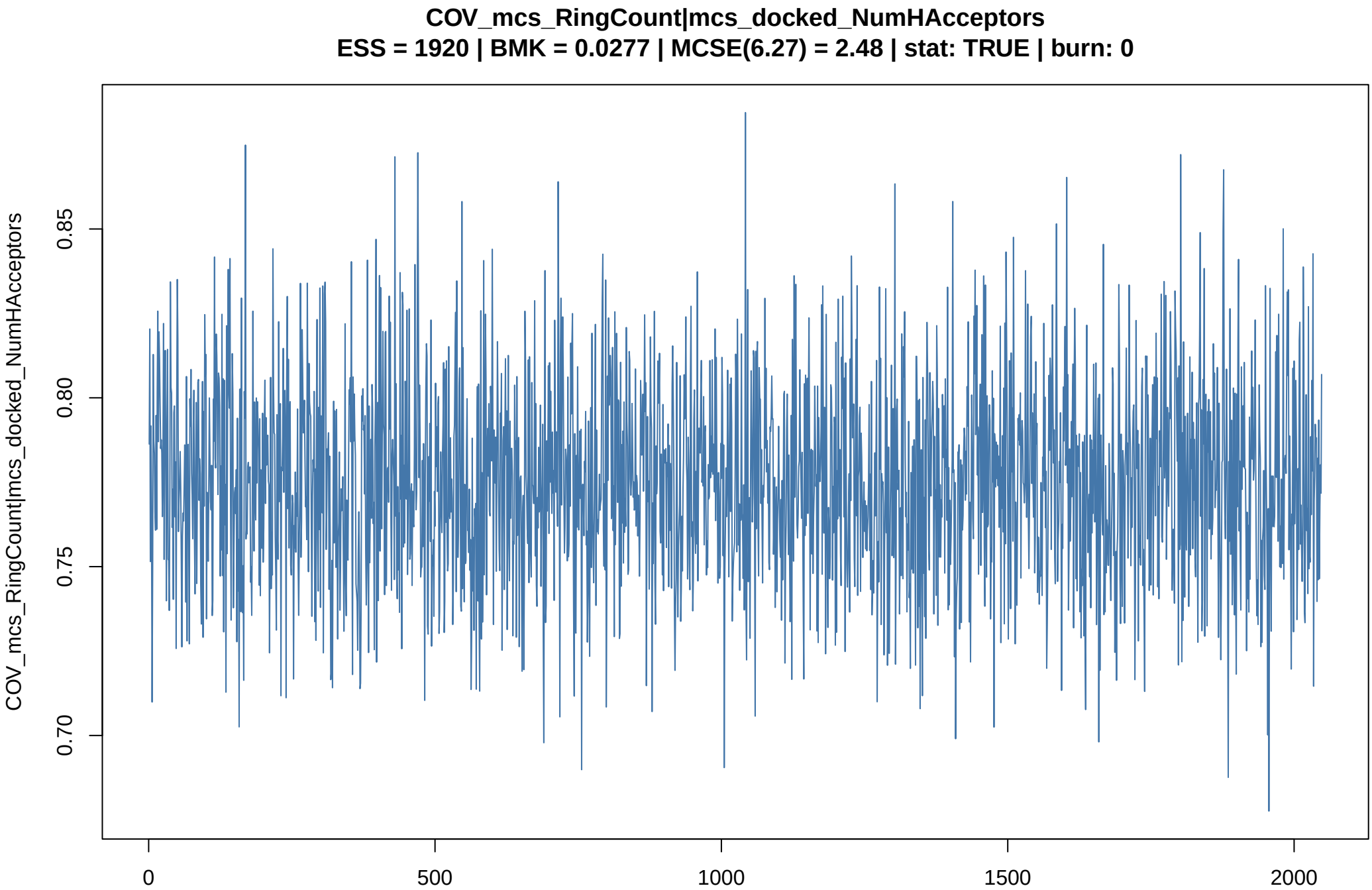

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1820 | BMK = 0.0478 | MCSE(6.27) = 2.32 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
22
23
24
25
26
27
28
0
500
1000
1500
2000

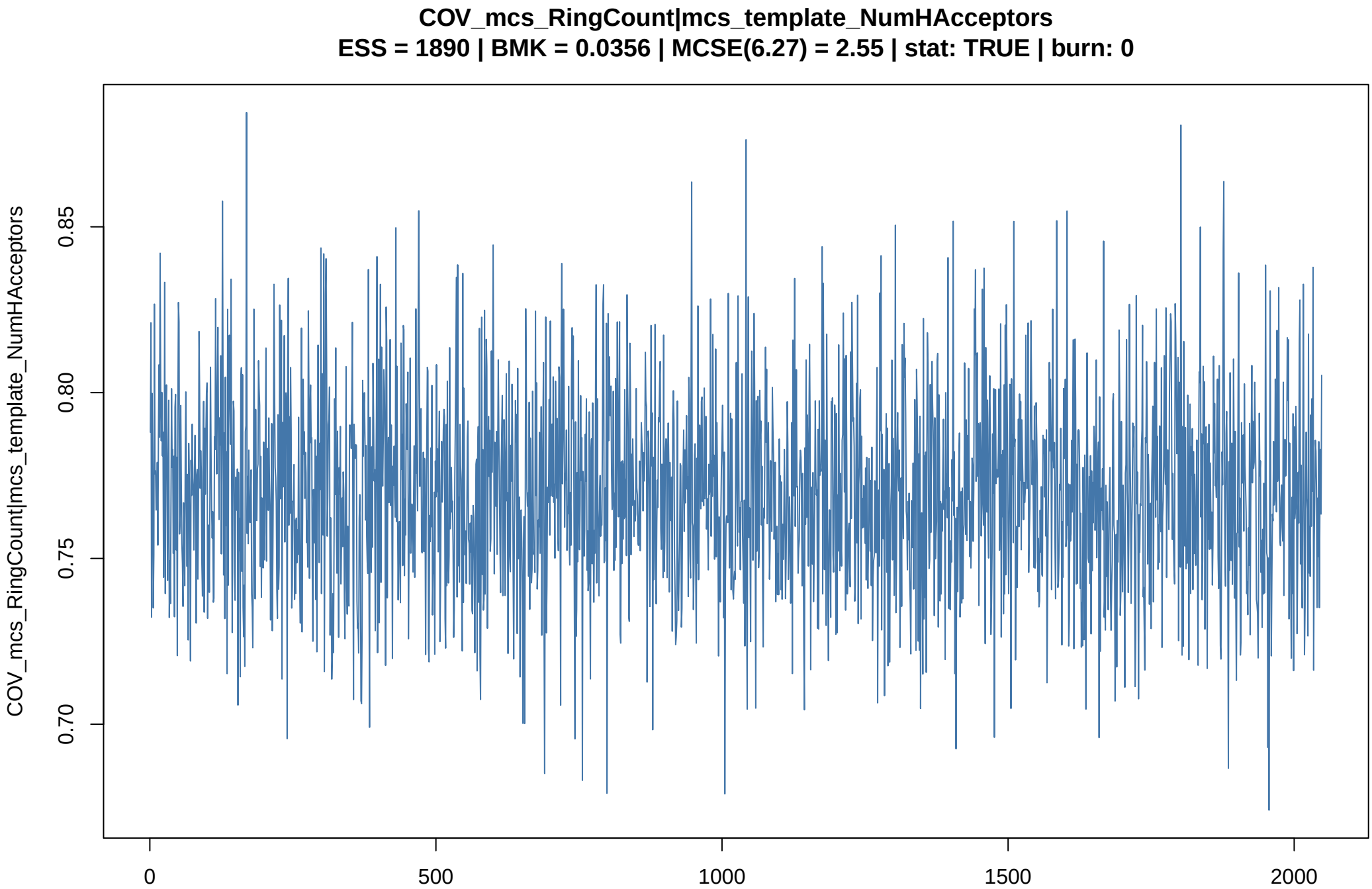

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1720 | BMK = 0.0382 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
1.6
0
500
1000
1500
2000

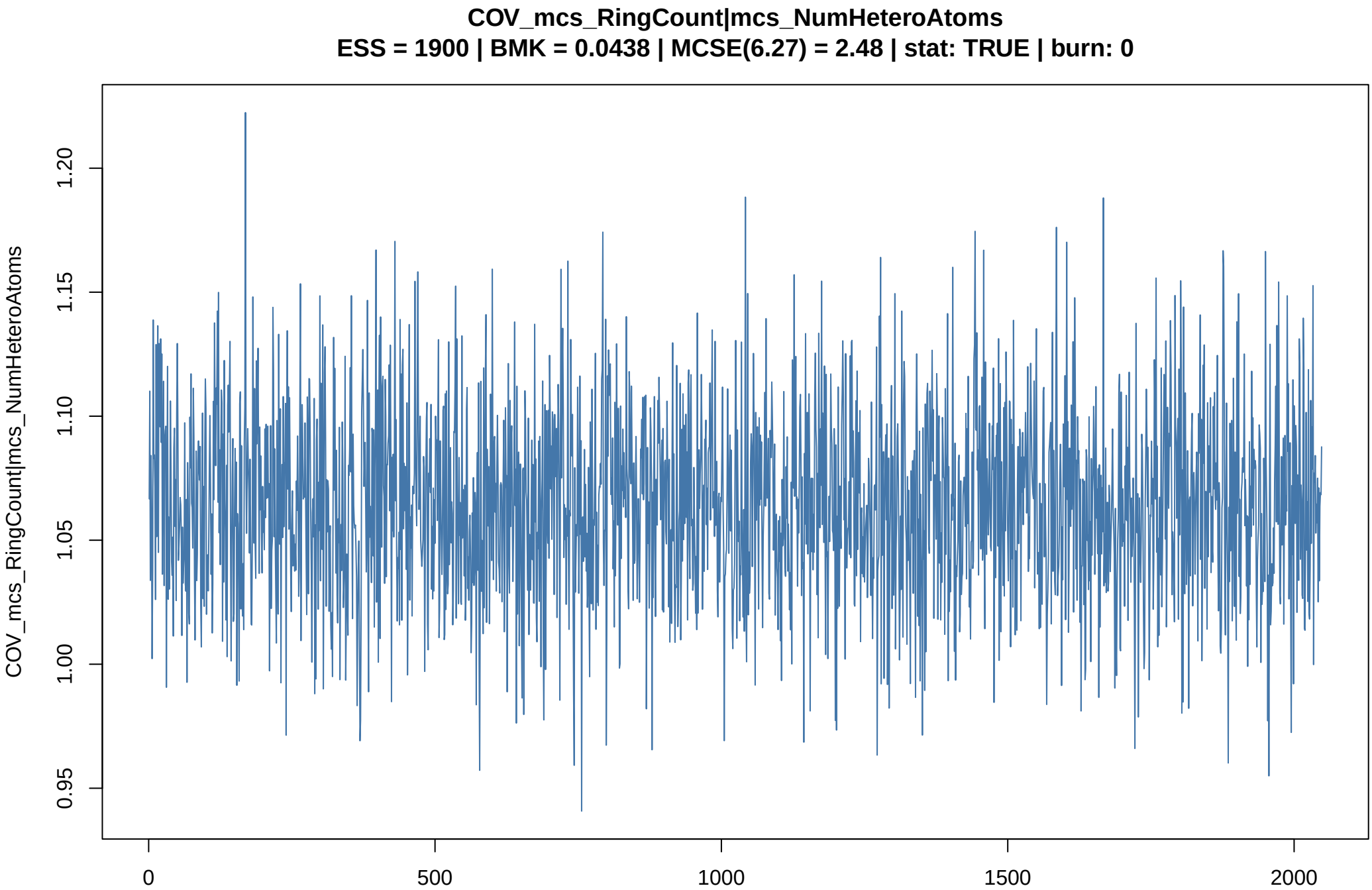

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1730 | BMK = 0.0316 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

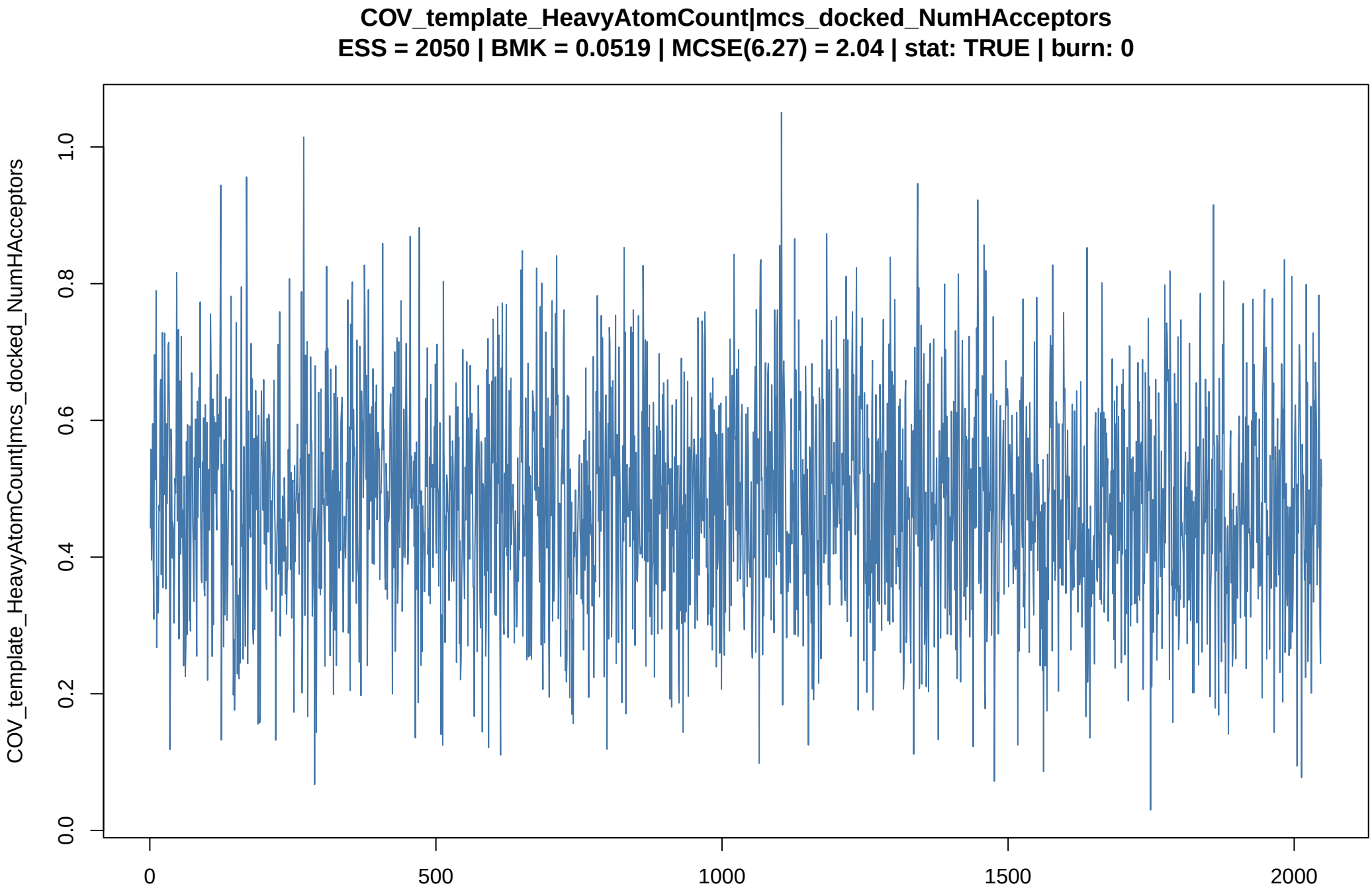

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0335 | MCSE(6.27) = 2.13 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
0
500
1000
1500
2000

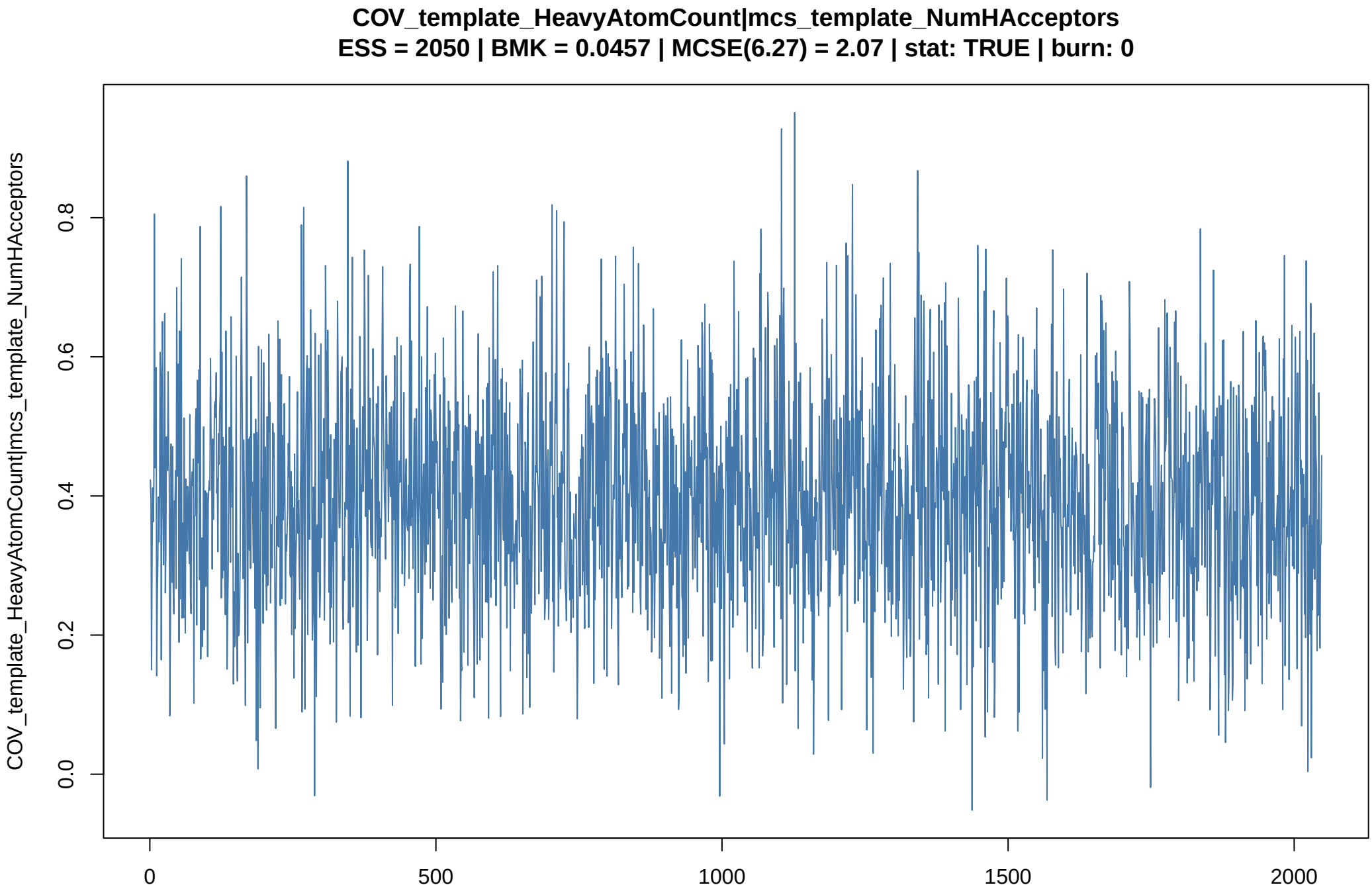

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1900 | BMK = 0.0386 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

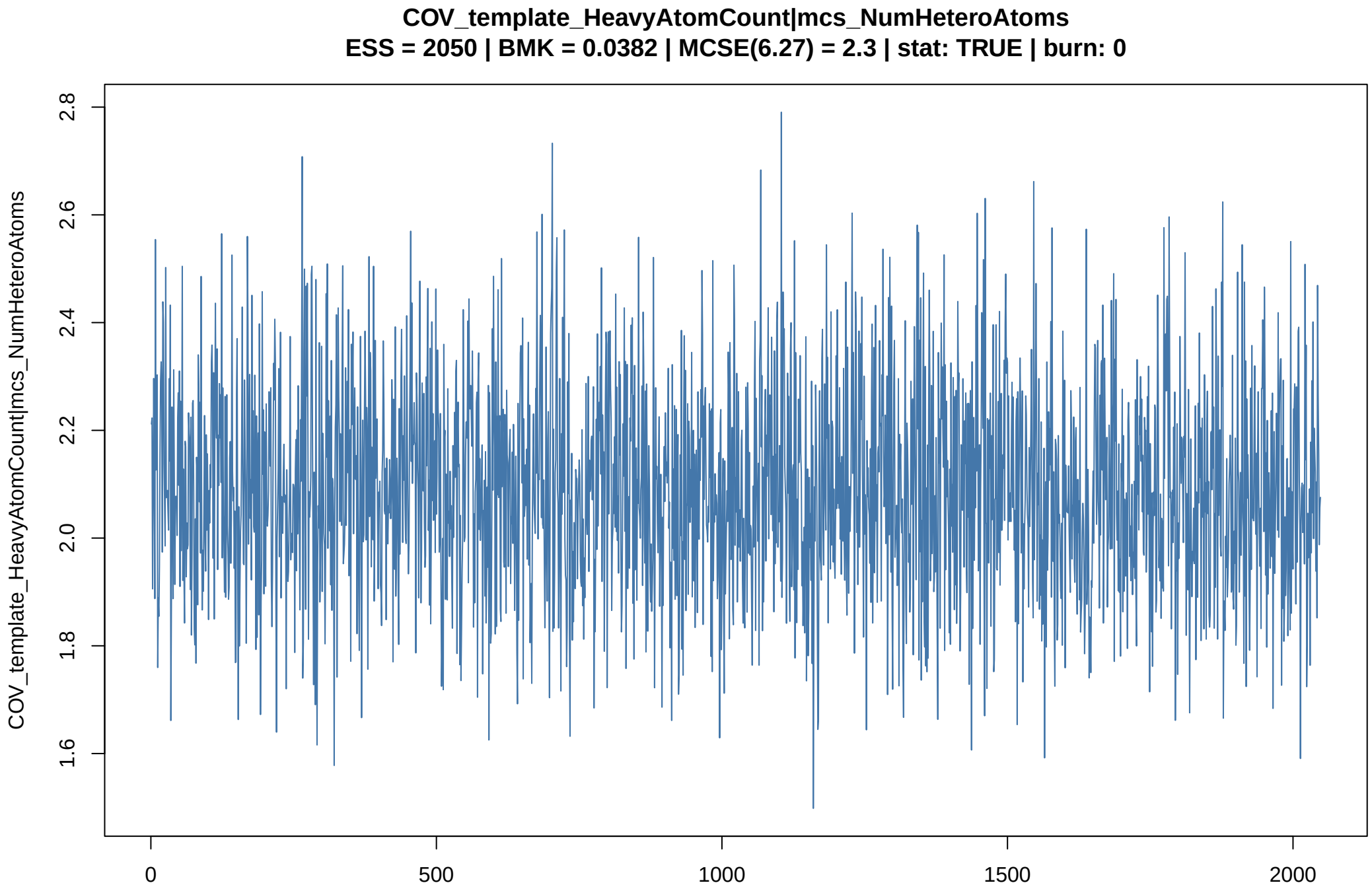

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 1920 | BMK = 0.0277 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

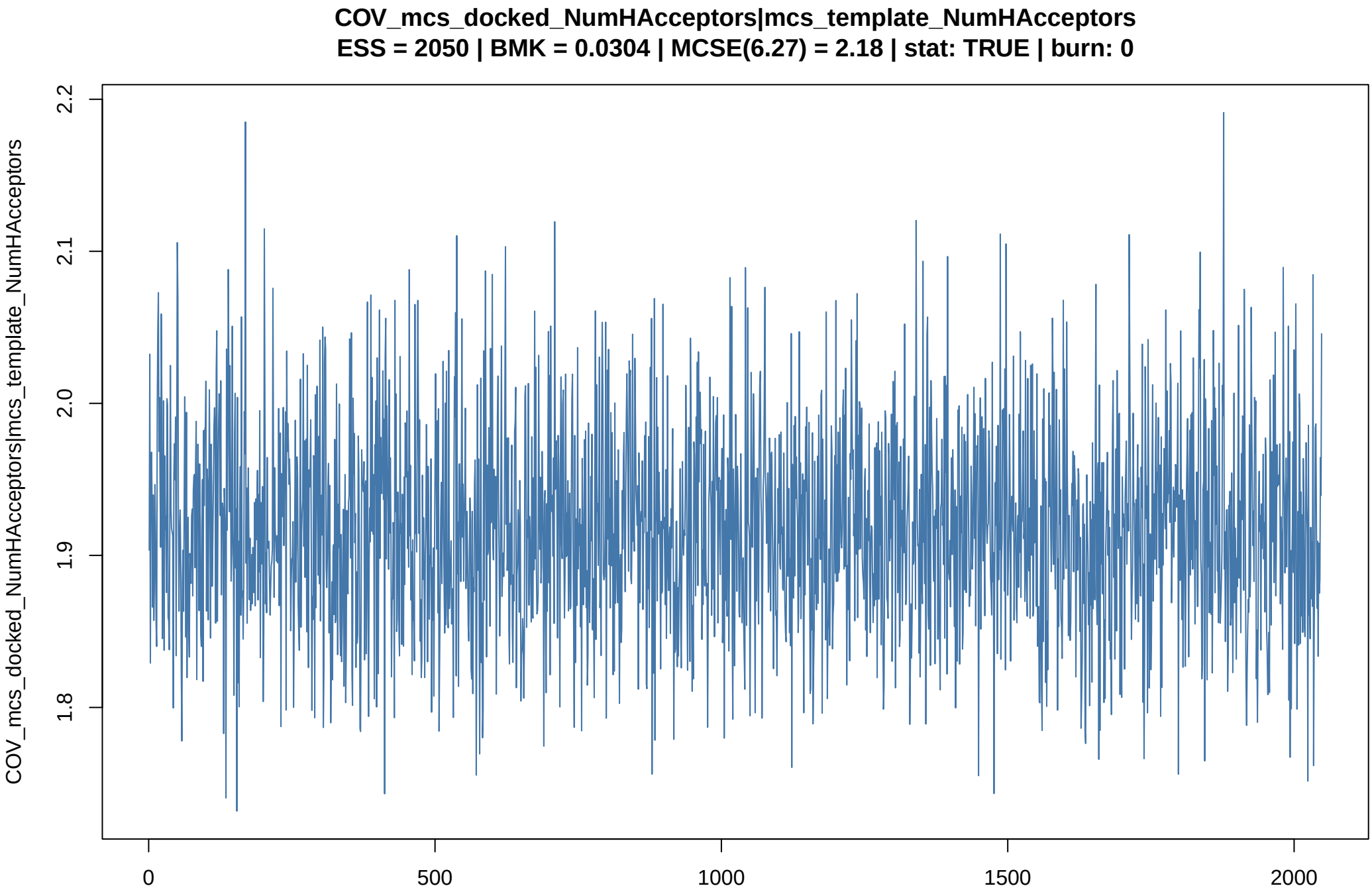

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 1890 | BMK = 0.0356 | MCSE(6.27) = 2.55 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

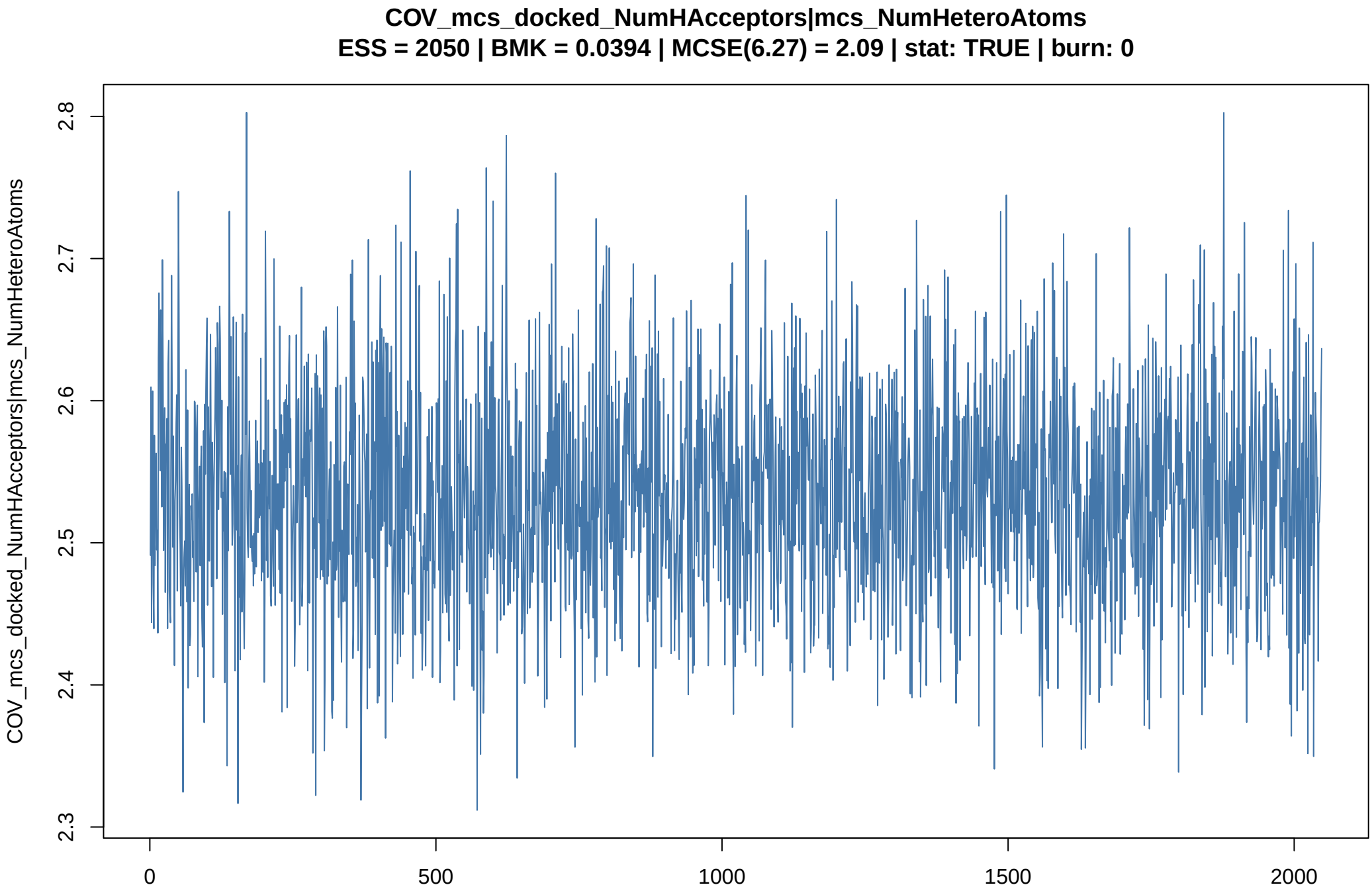

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 1900 | BMK = 0.0438 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
1.20
0
500
1000
1500
2000

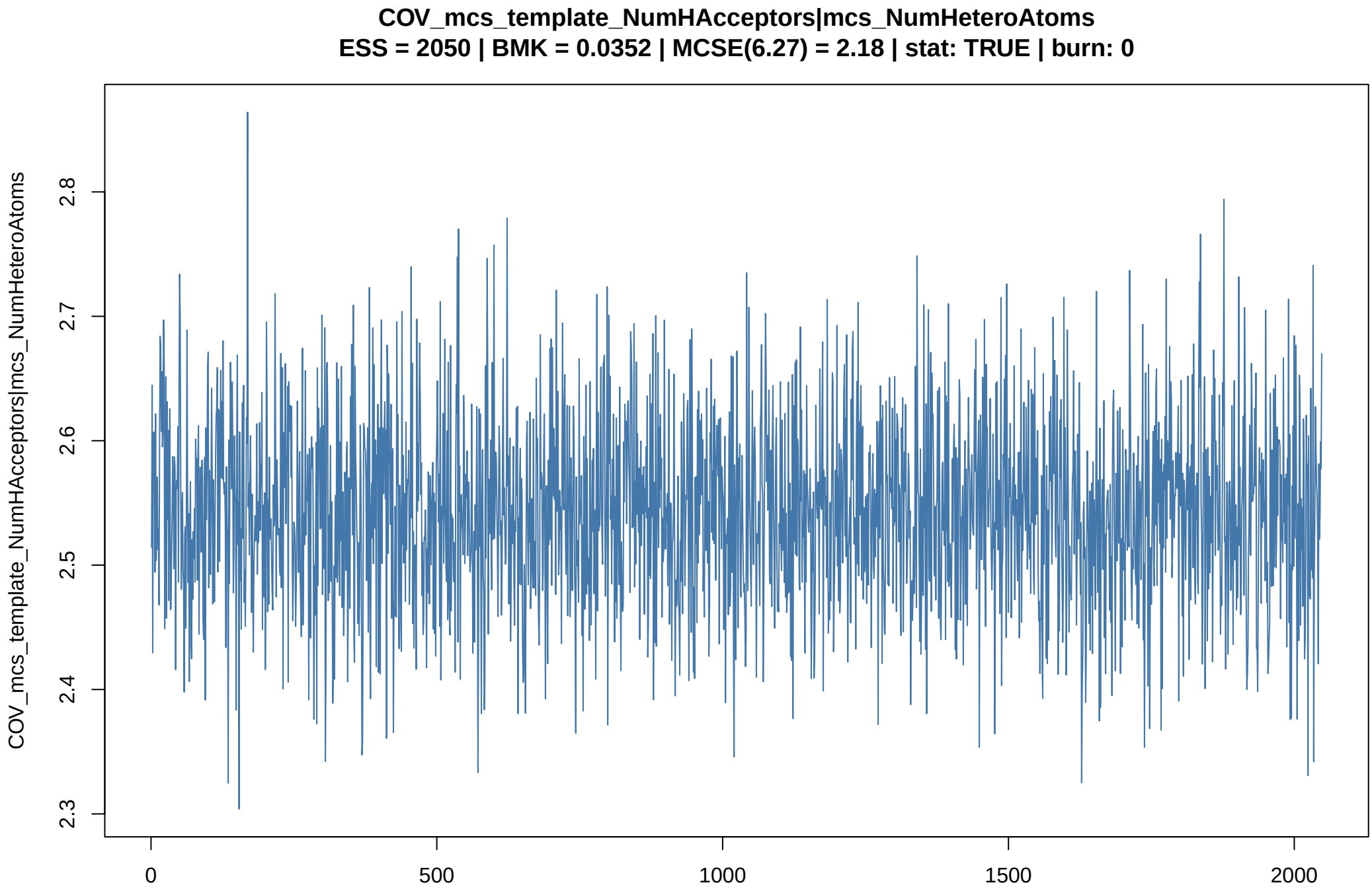

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0519 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
1.0
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0457 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0382 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
1.6
1.8
2.0
2.2
2.4
2.6
2.8
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0304 | MCSE(6.27) = 2.18 | 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 = 0.0394 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0352 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
2.3
2.4
2.5
2.6
2.7
2.8
0
500
1000
1500
2000