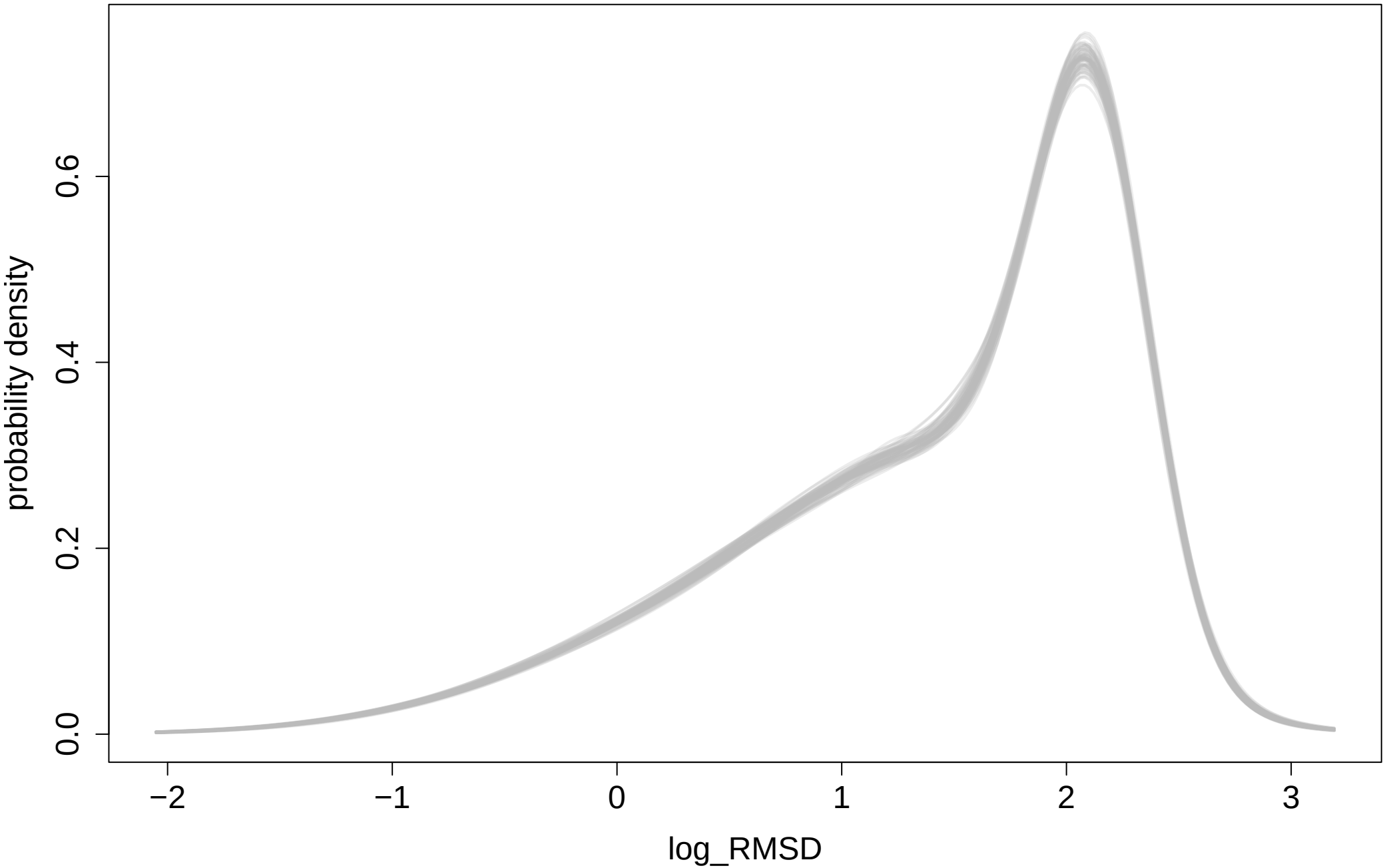
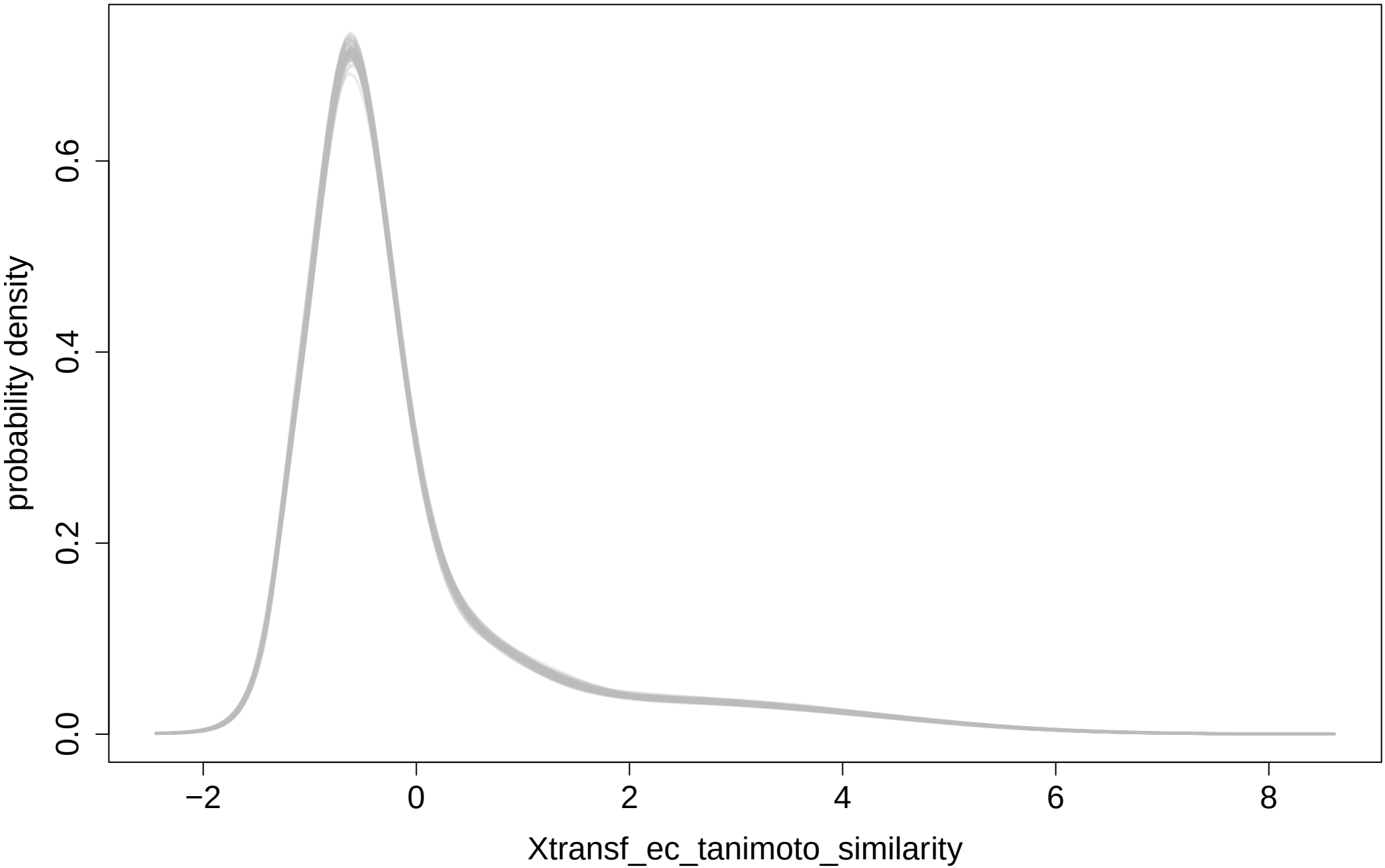
−− STATS maxD −−
min ESS = 2.2044604925031e−16
max BMK = 0.803249900715993
max MCSE = 14.6421102407174
all stationary: FALSE
burn: 1020

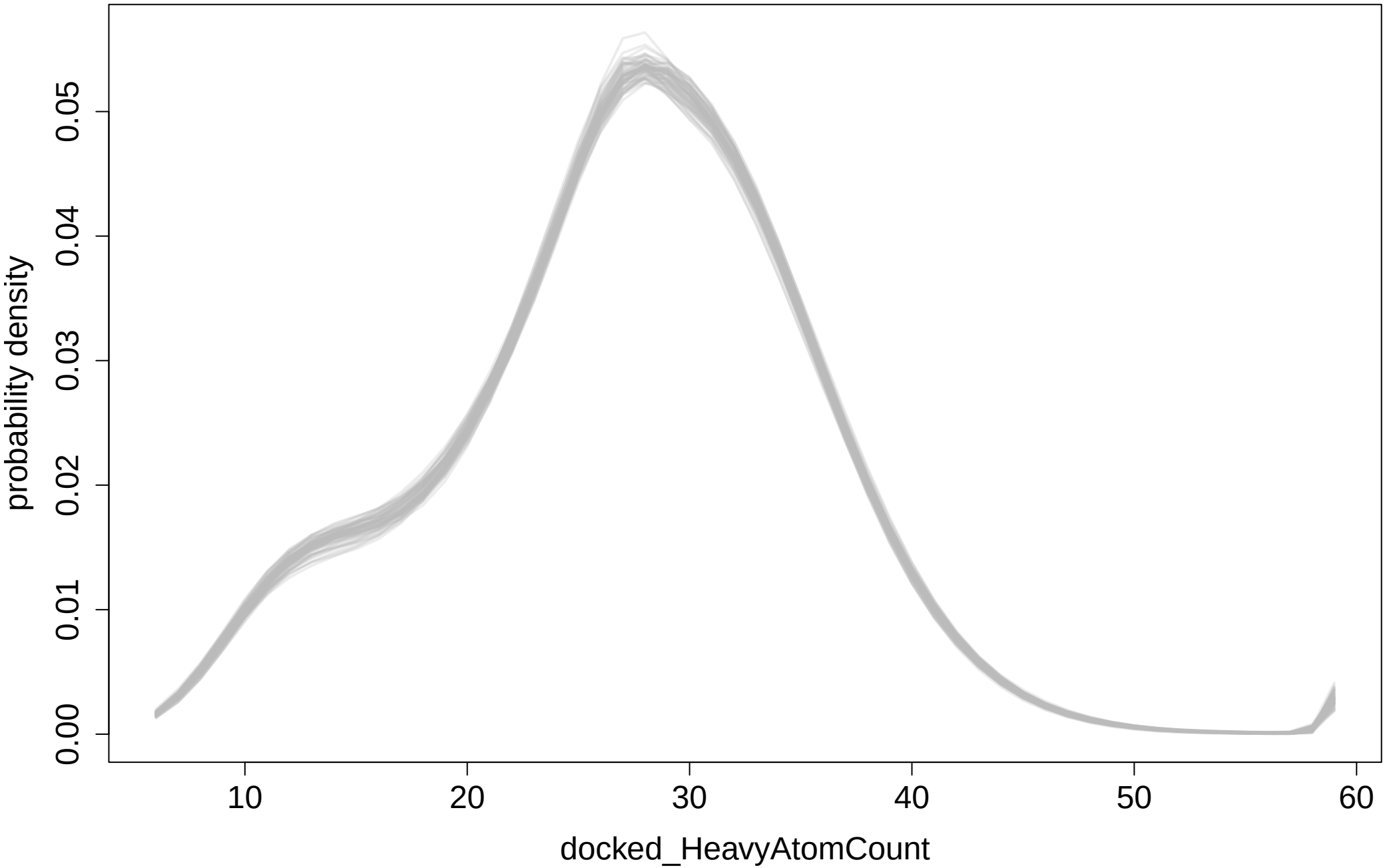
−− STATS 2D −−
min ESS = 1565.59462957779
max BMK = 0.0615459776356086
max MCSE = 3.04383113251057
all stationary: FALSE
burn: 0

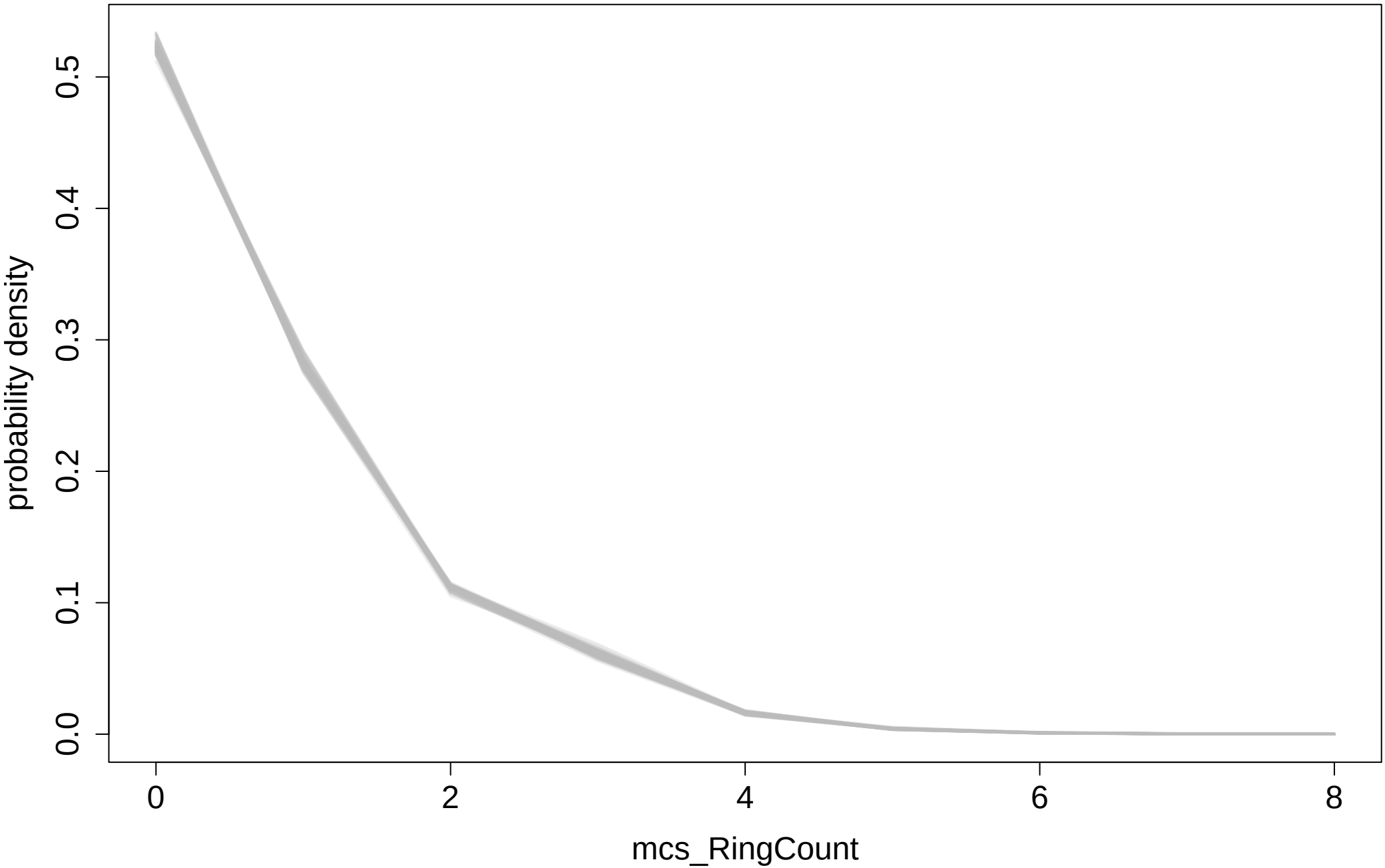
−− STATS 1D −−
min ESS = 2.2044604925031e−16
max BMK = 0.203634255156498
max MCSE = NaN
all stationary: FALSE
burn: 2040

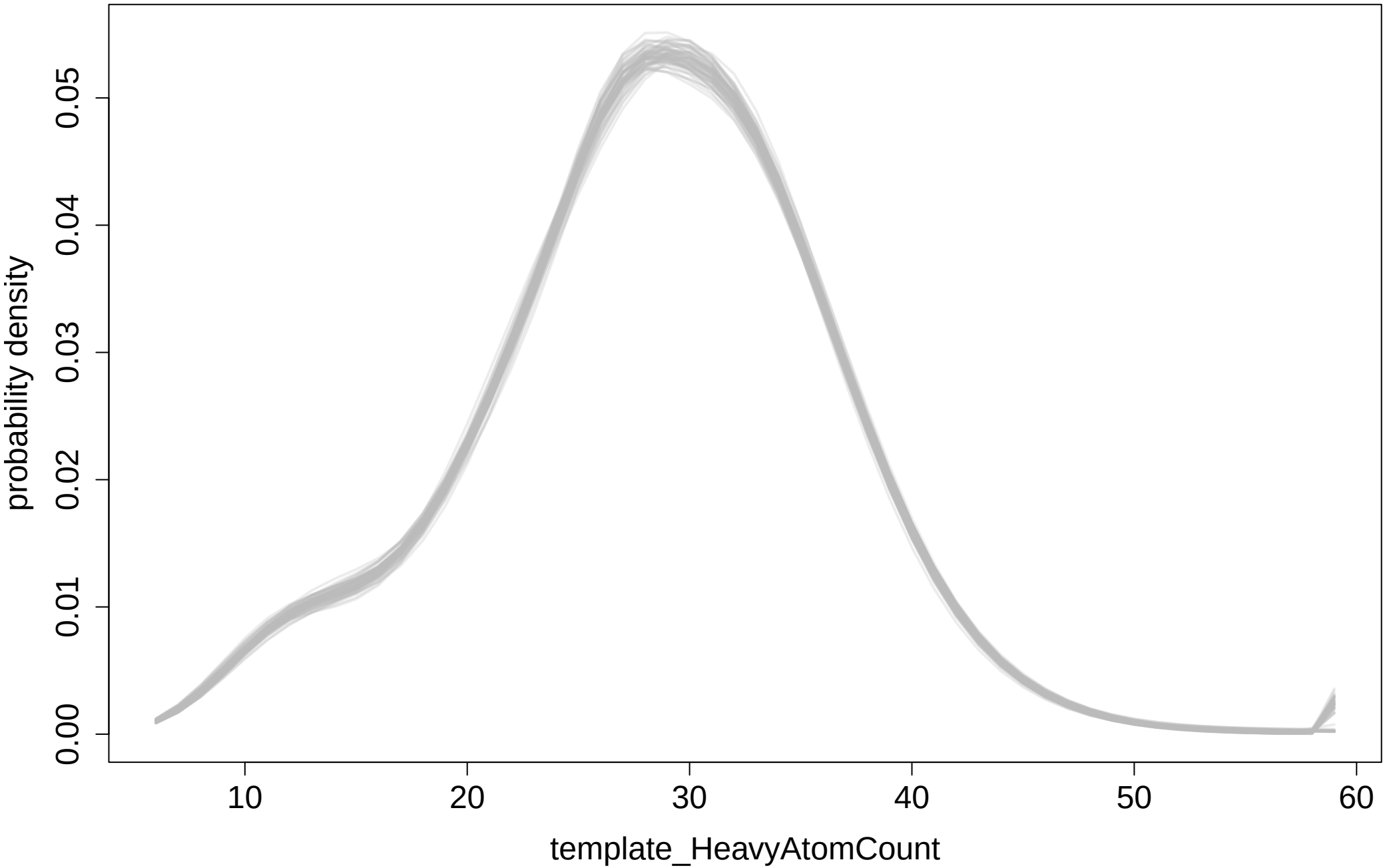
Occupied clusters: 57 of 91
LL: −111000 +− 88.3

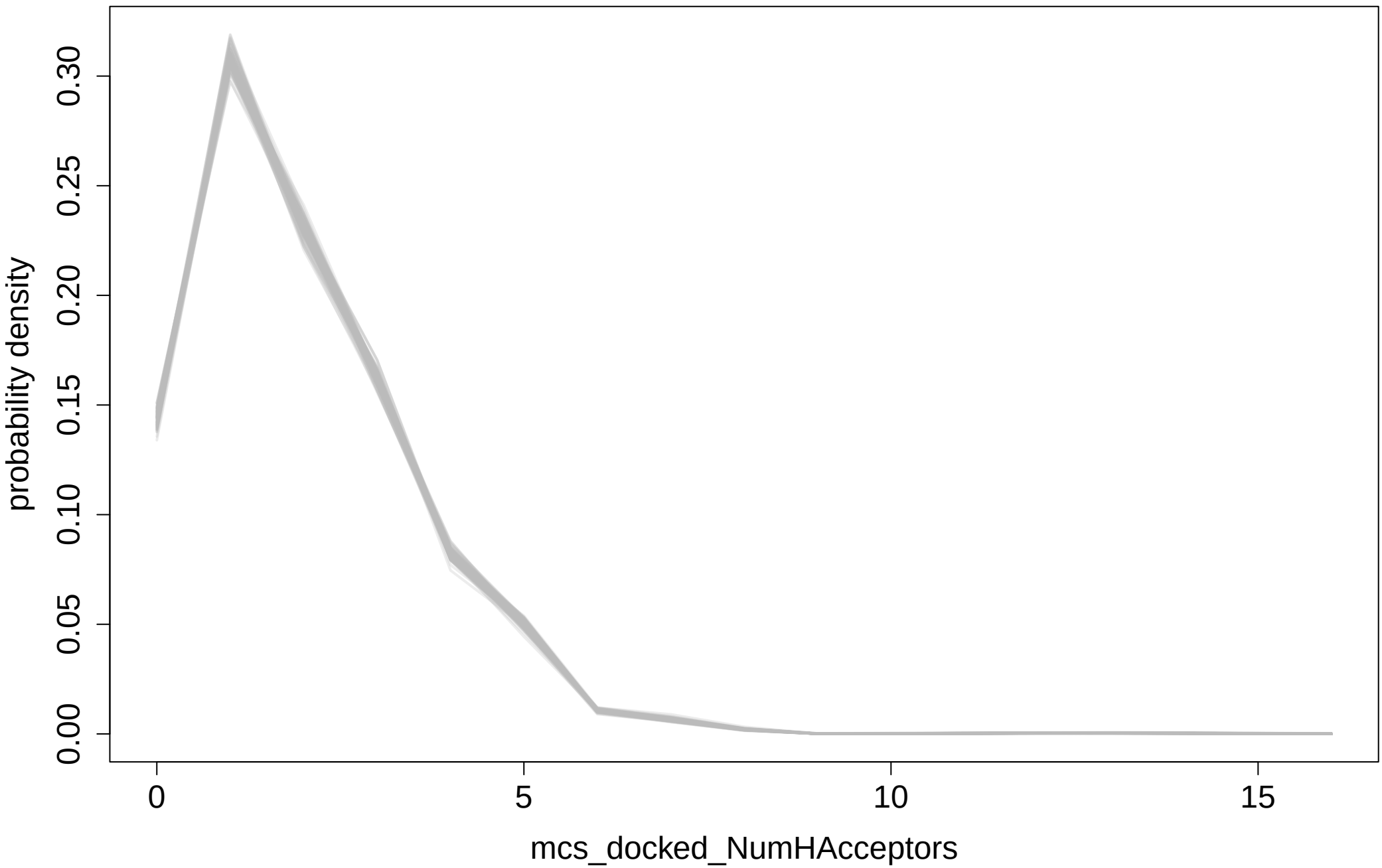

probability density
0.0
0.2
0.4
0.6
−2
−1
0
1
2
3
log_RMSD

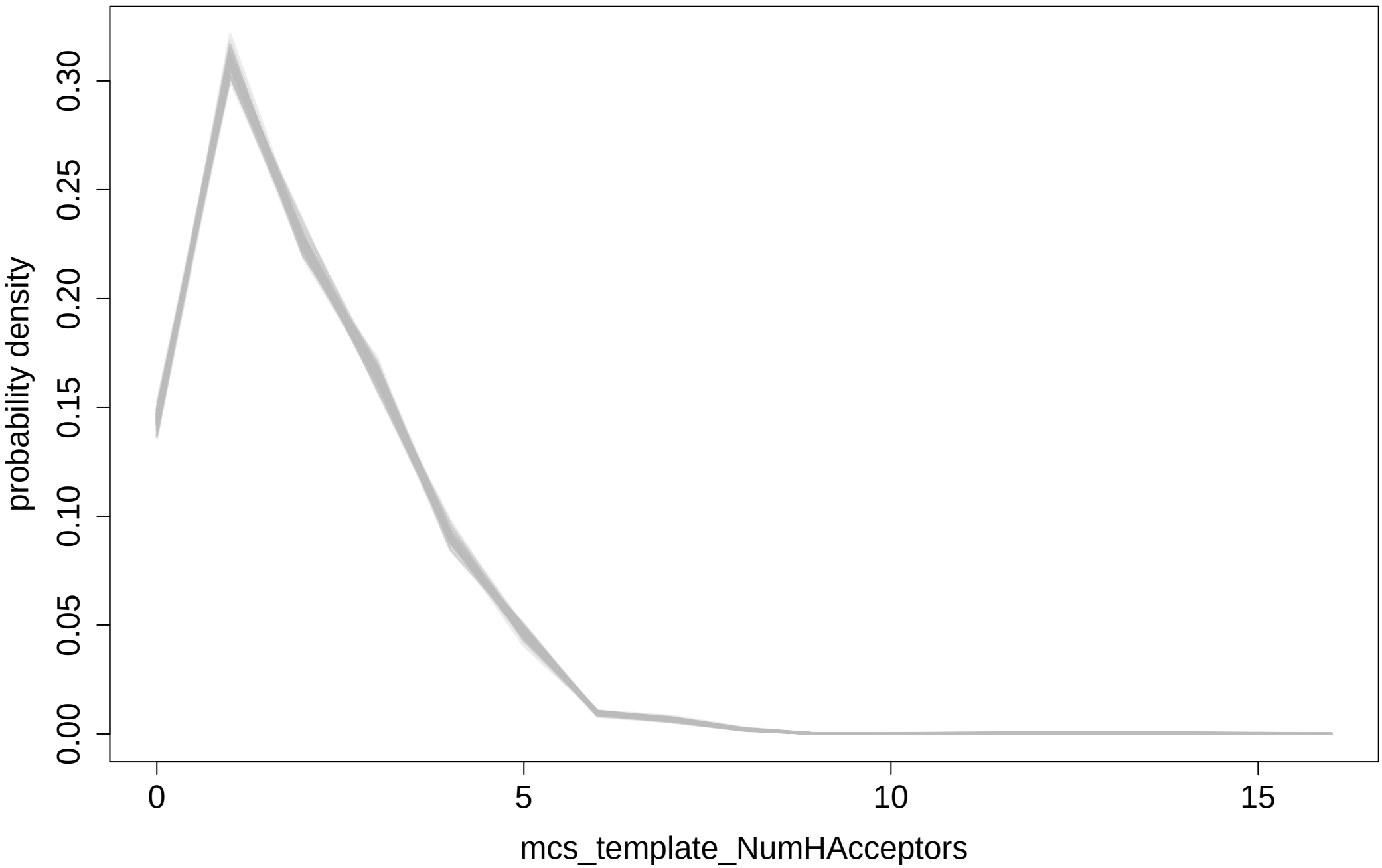

probability density
0.0
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

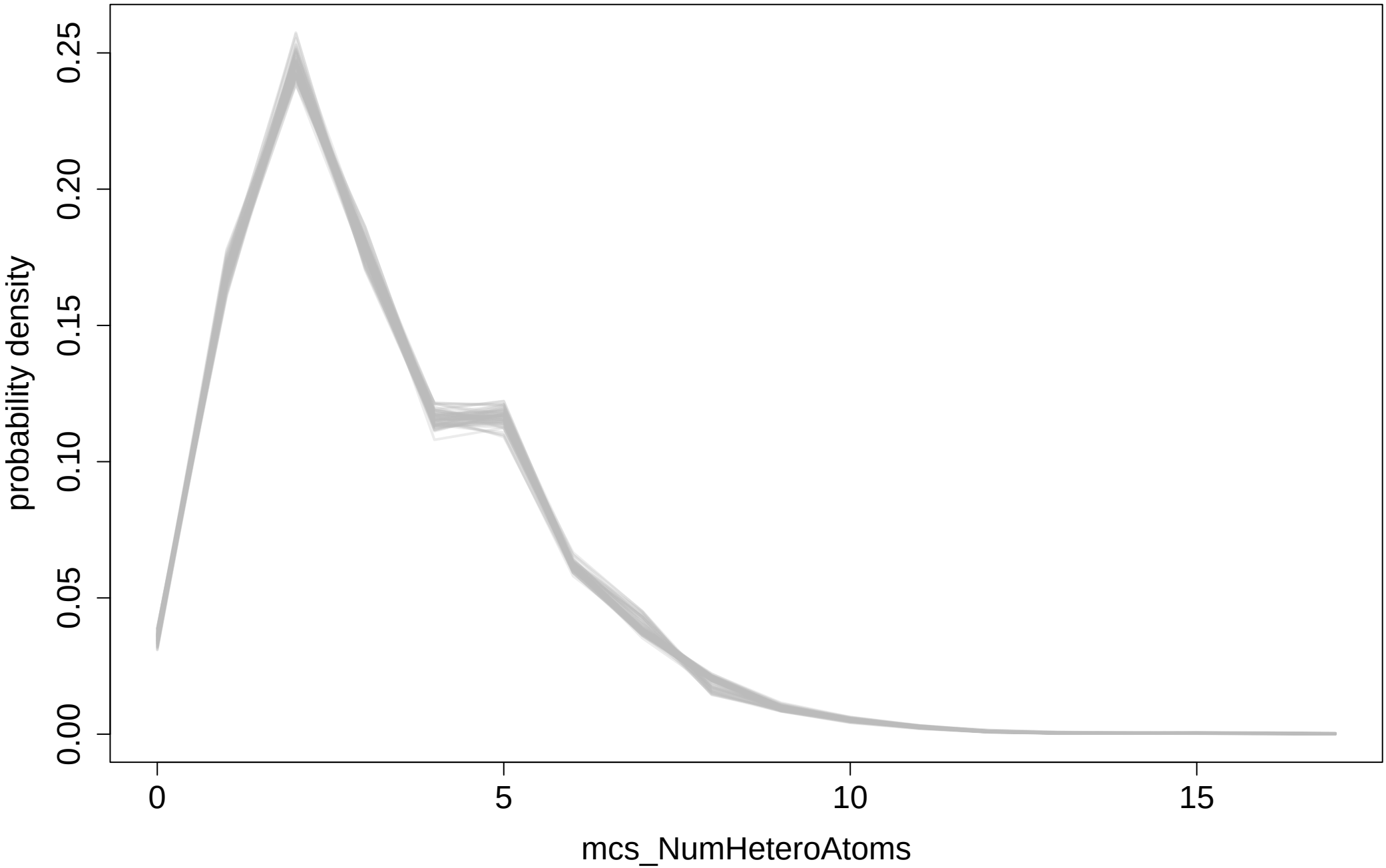

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

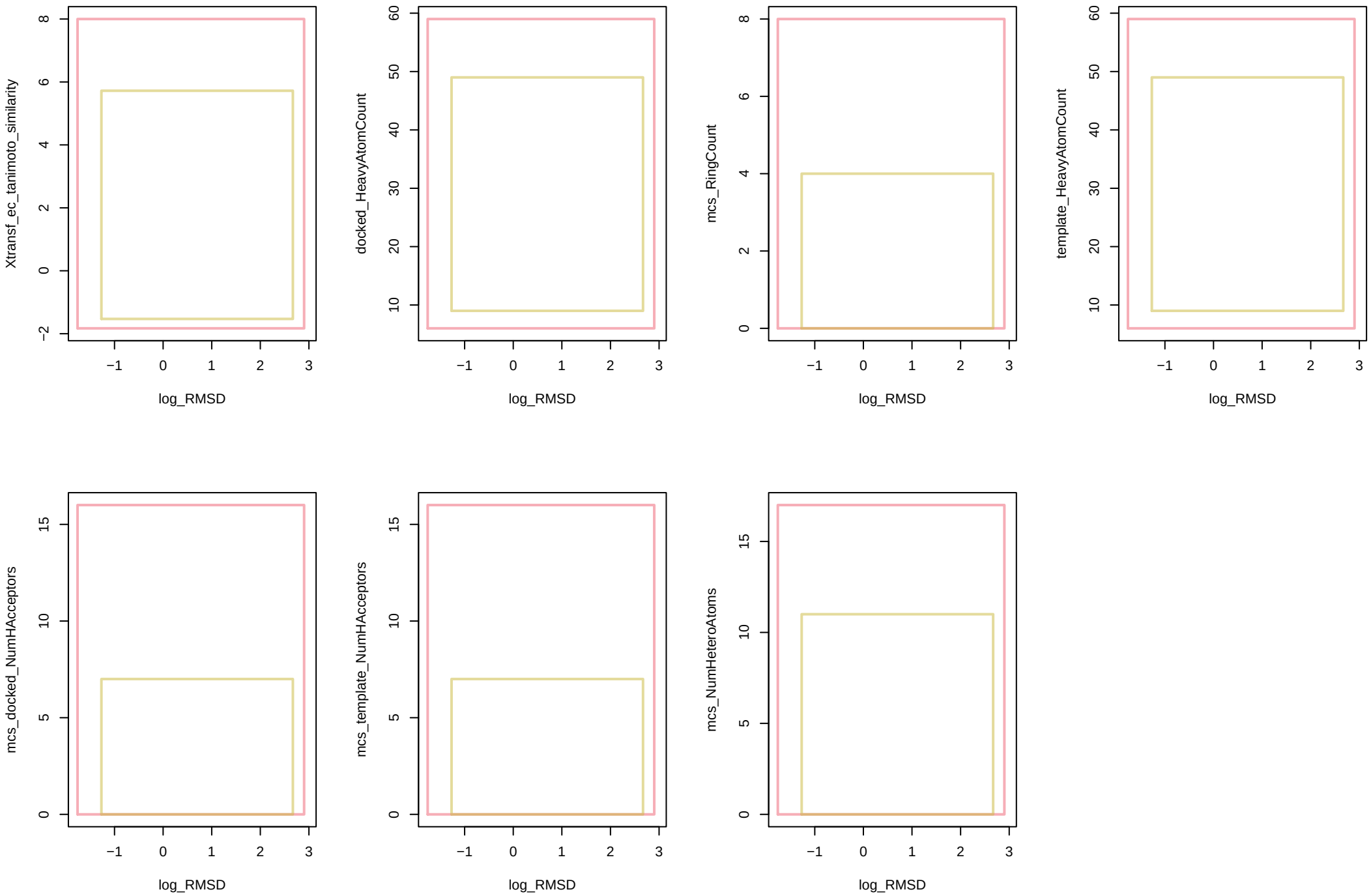

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

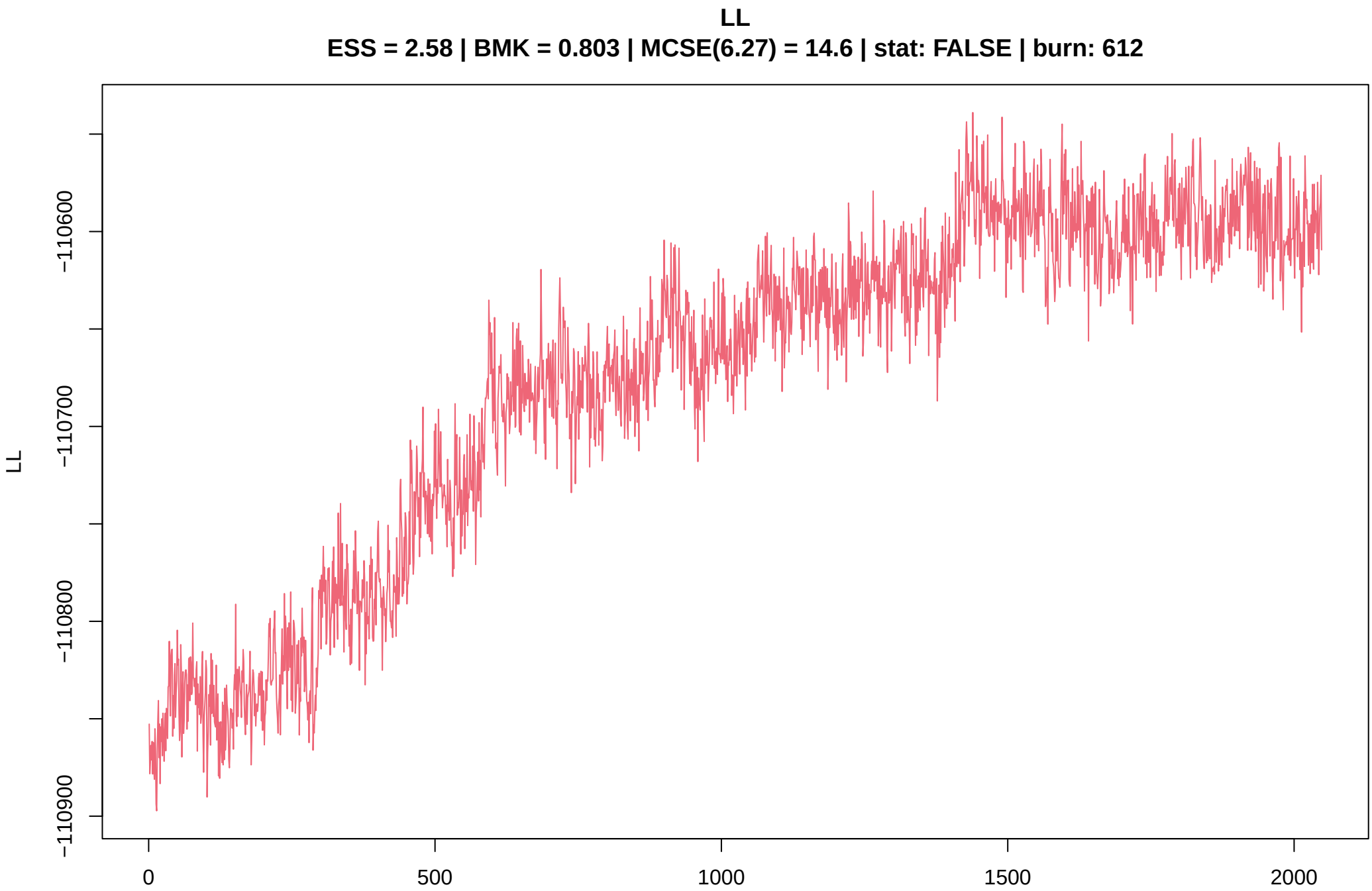

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

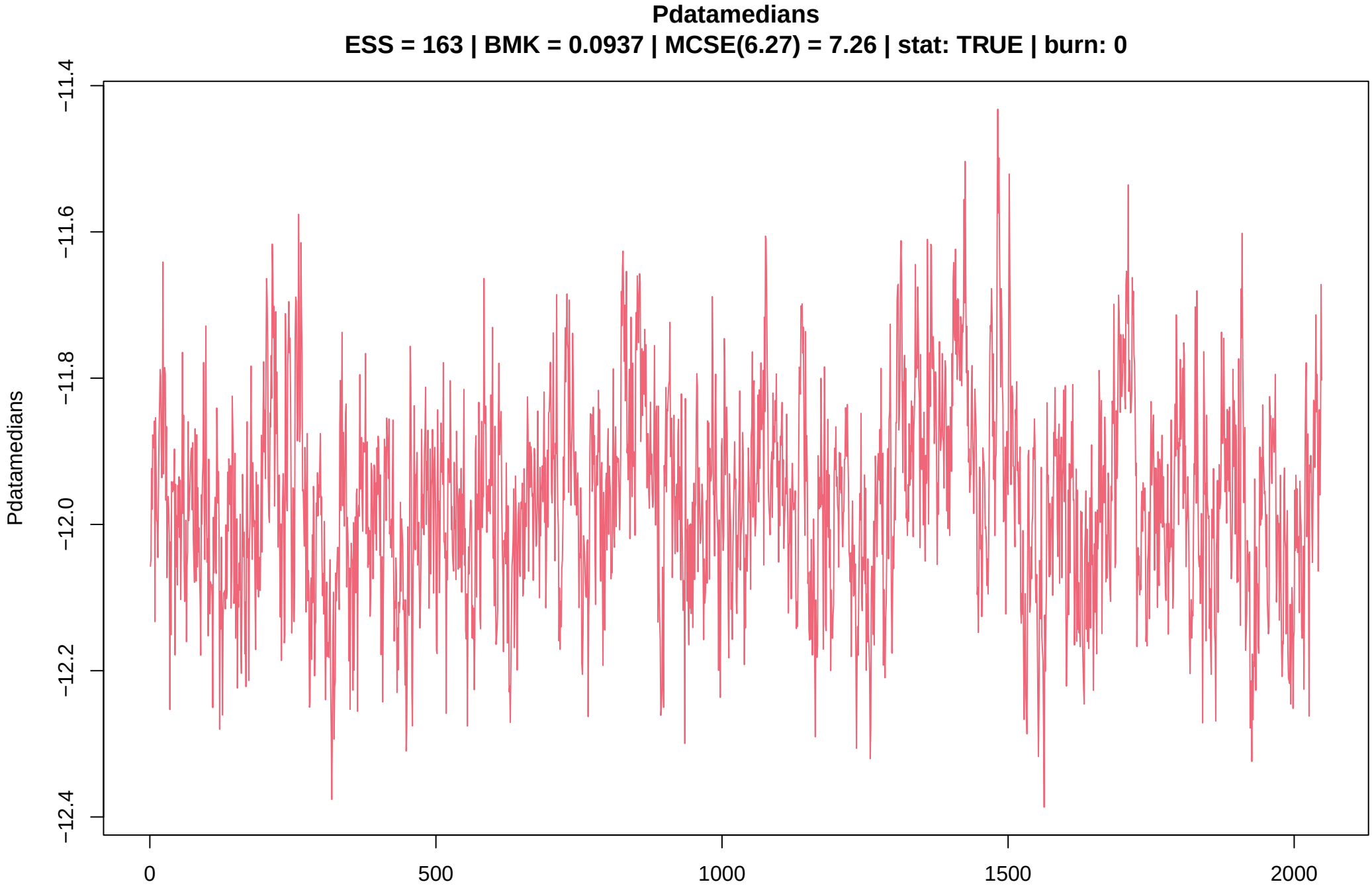

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_docked_NumHAcceptors

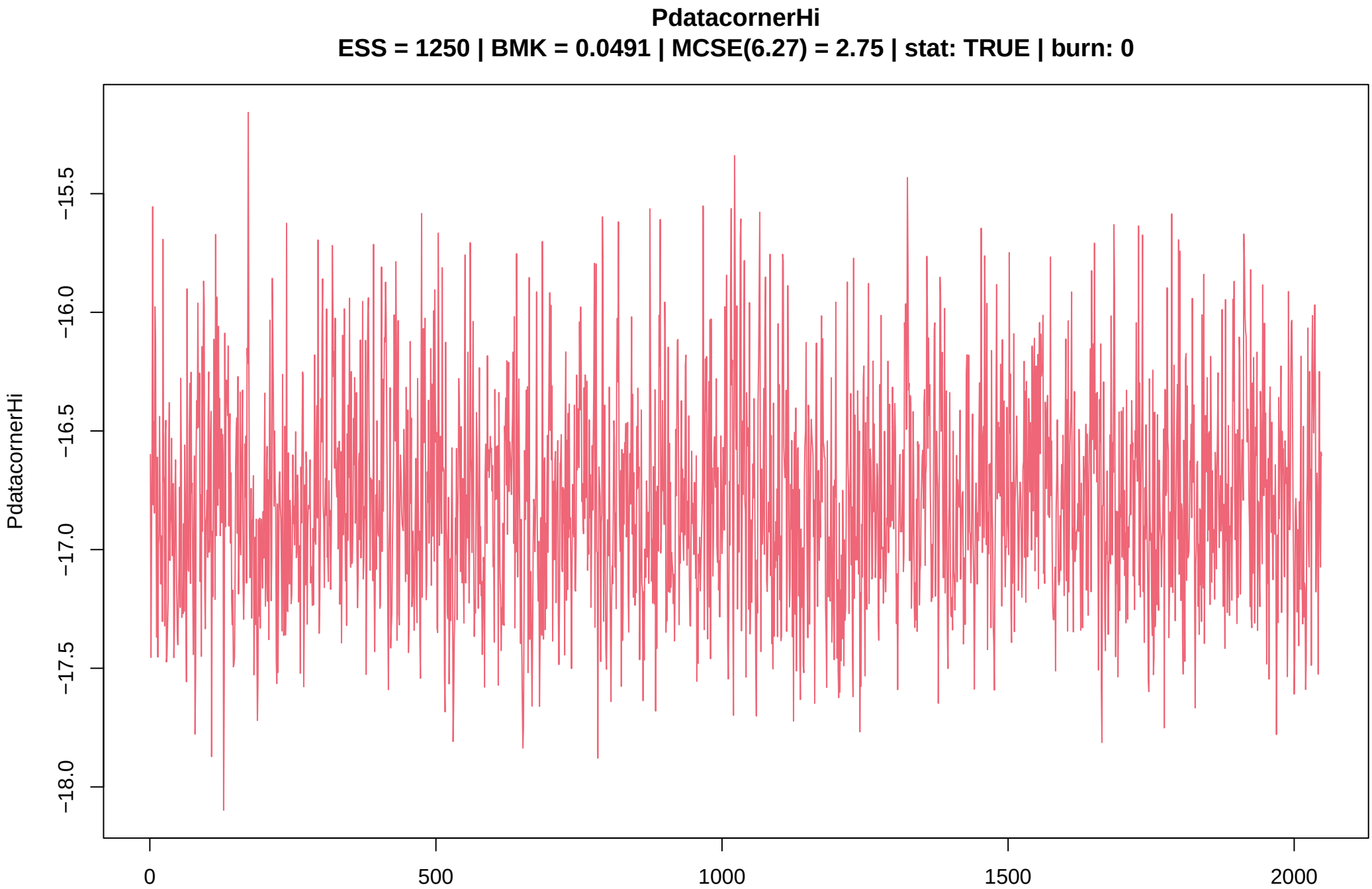

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_template_NumHAcceptors

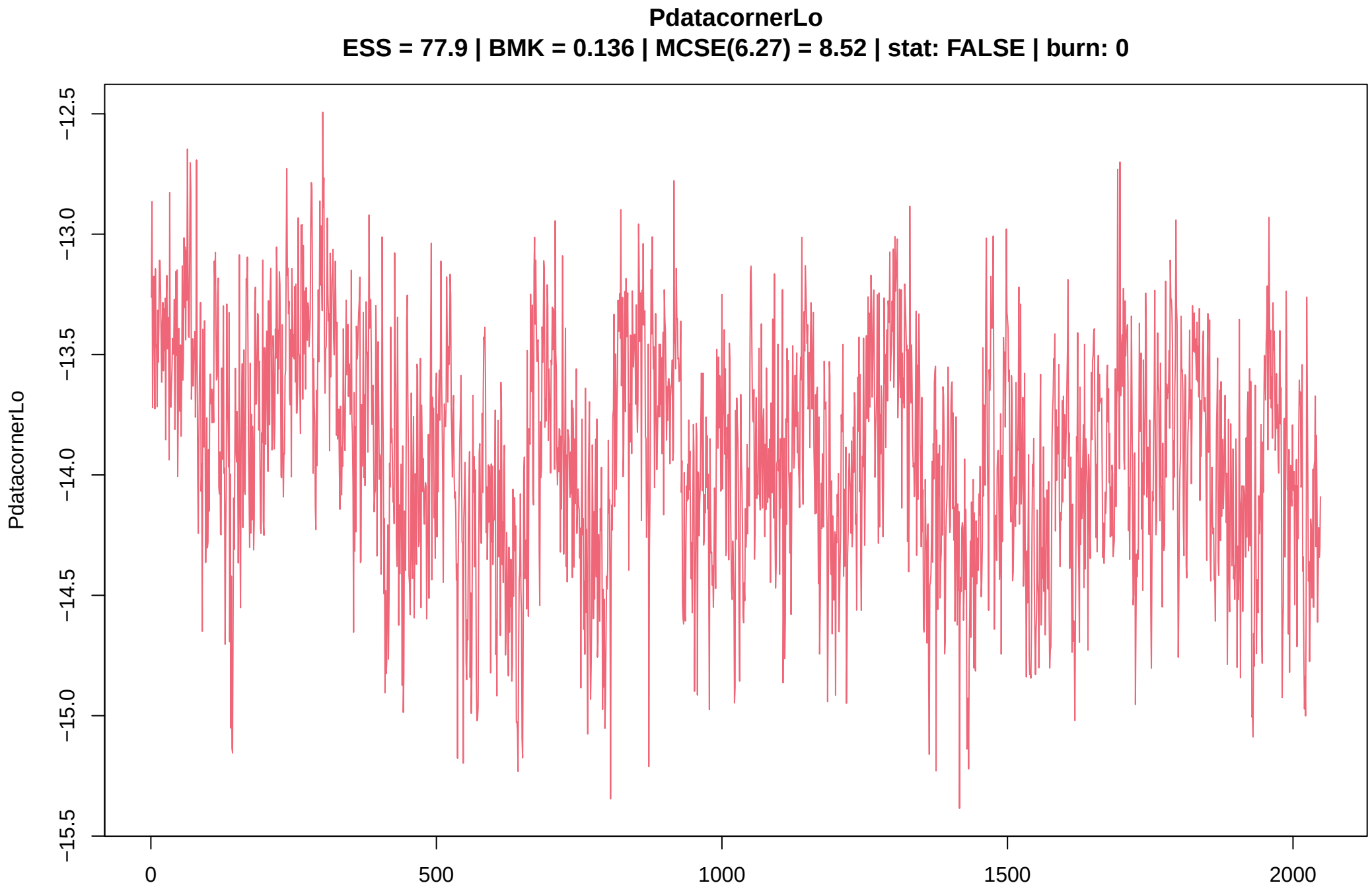

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

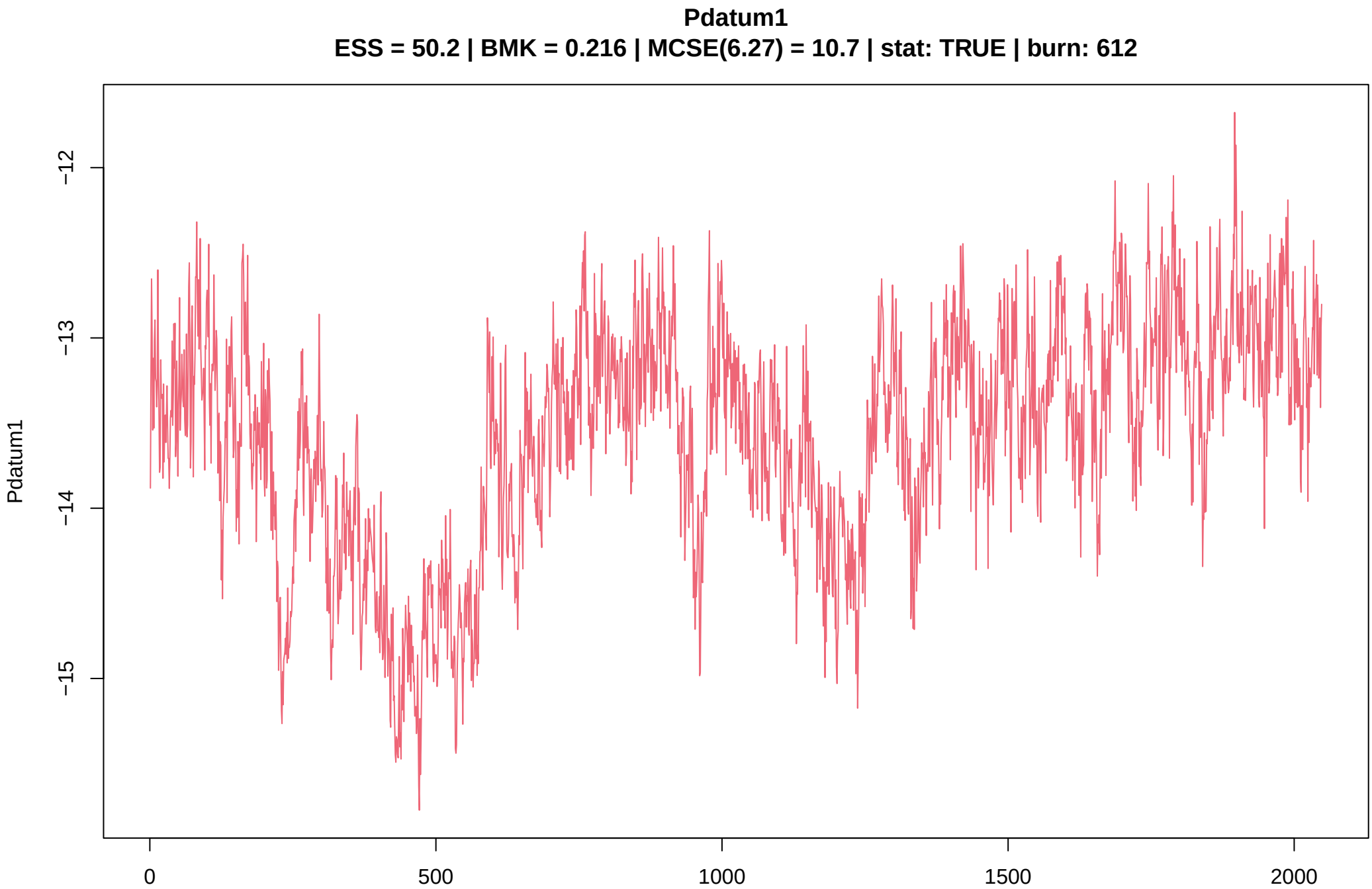

Xtransf_ec_tanimoto_similarity
docked_HeavyAtomCount
mcs_RingCount
template_HeavyAtomCount
mcs_docked_NumHAcceptors
mcs_template_NumHAcceptors
mcs_NumHeteroAtoms
log_RMSD

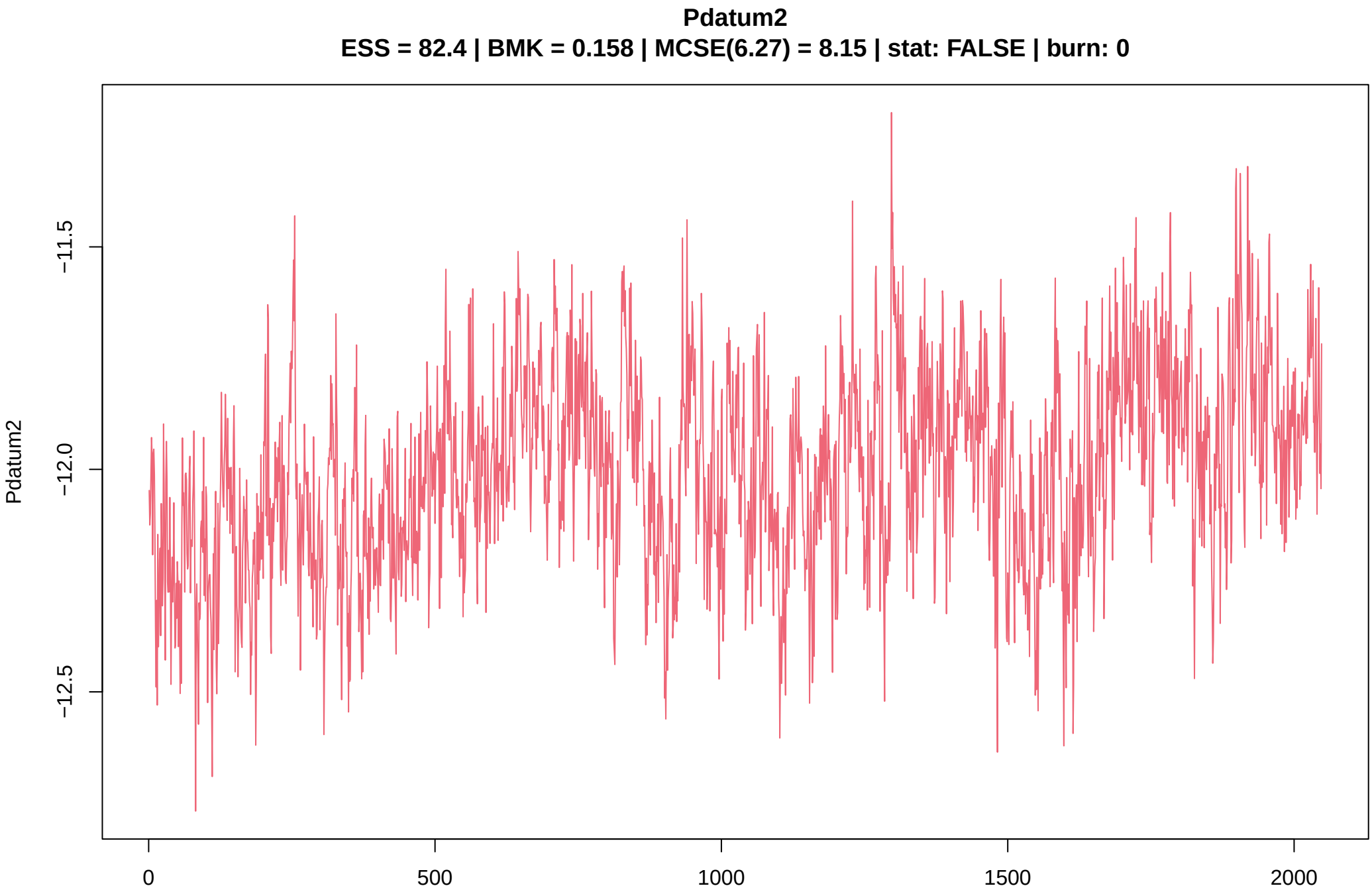

LL
ESS = 2.58 | BMK = 0.803 | MCSE(6.27) = 14.6 | stat: FALSE | burn: 612
LL
−110600
−110700
−110800
−110900
0
500
1000
1500
2000

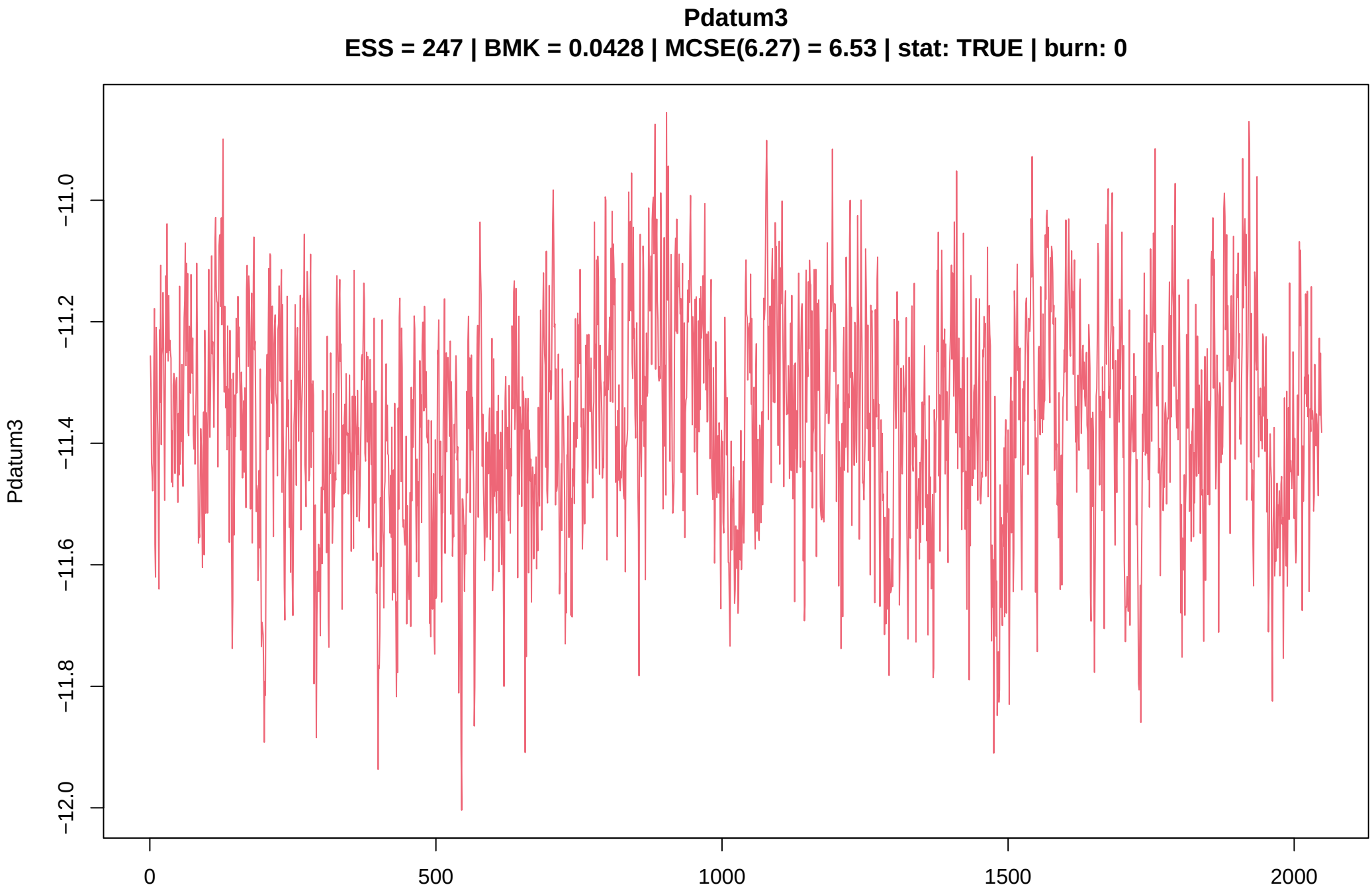

Pdatamedians
ESS = 163 | BMK = 0.0937 | MCSE(6.27) = 7.26 | stat: TRUE | burn: 0
Pdatamedians
−11.4
−11.6
−11.8
−12.0
−12.2
−12.4
0
500
1000
1500
2000

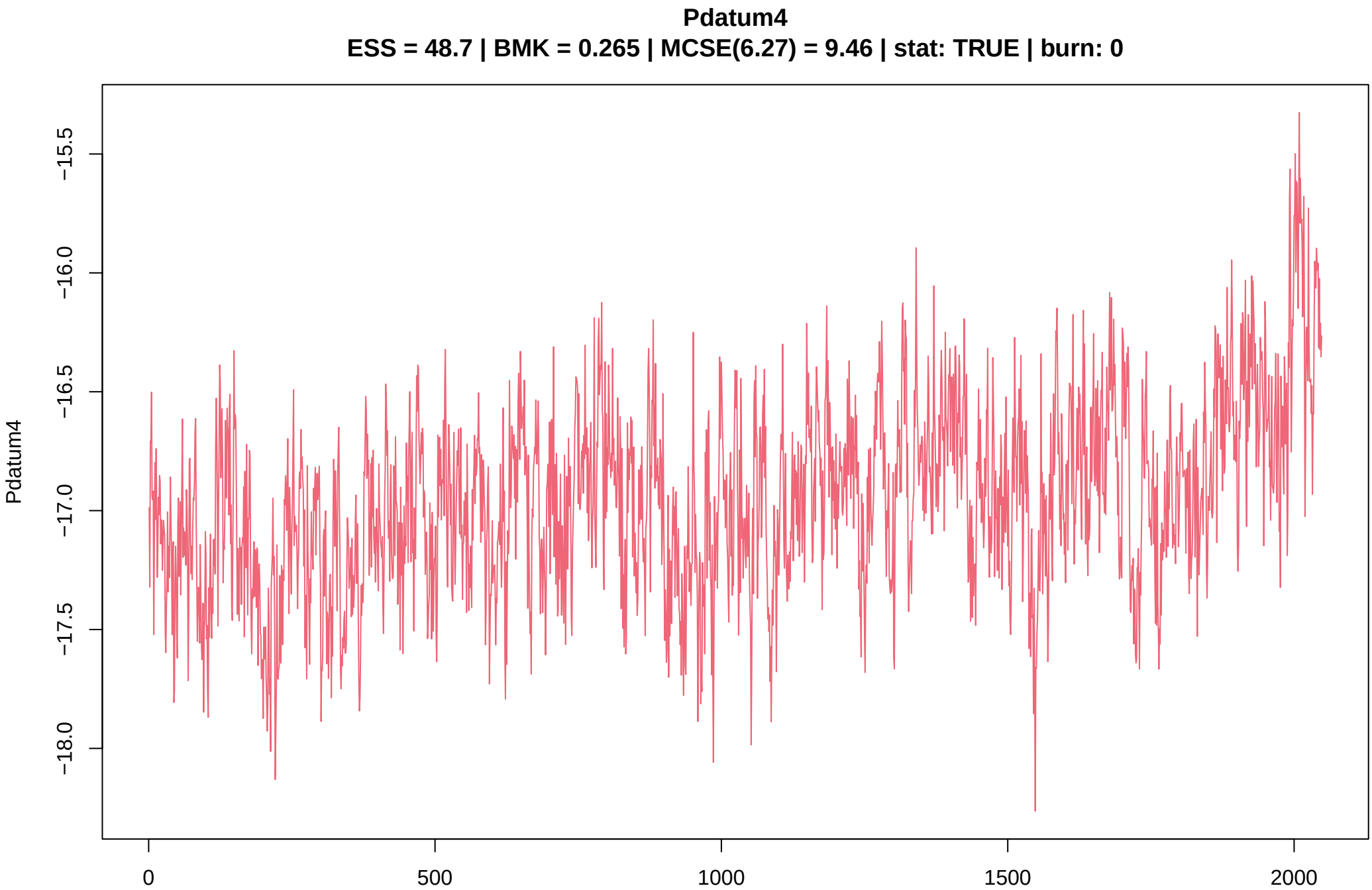

PdatacornerHi
ESS = 1250 | BMK = 0.0491 | MCSE(6.27) = 2.75 | stat: TRUE | burn: 0
PdatacornerHi
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

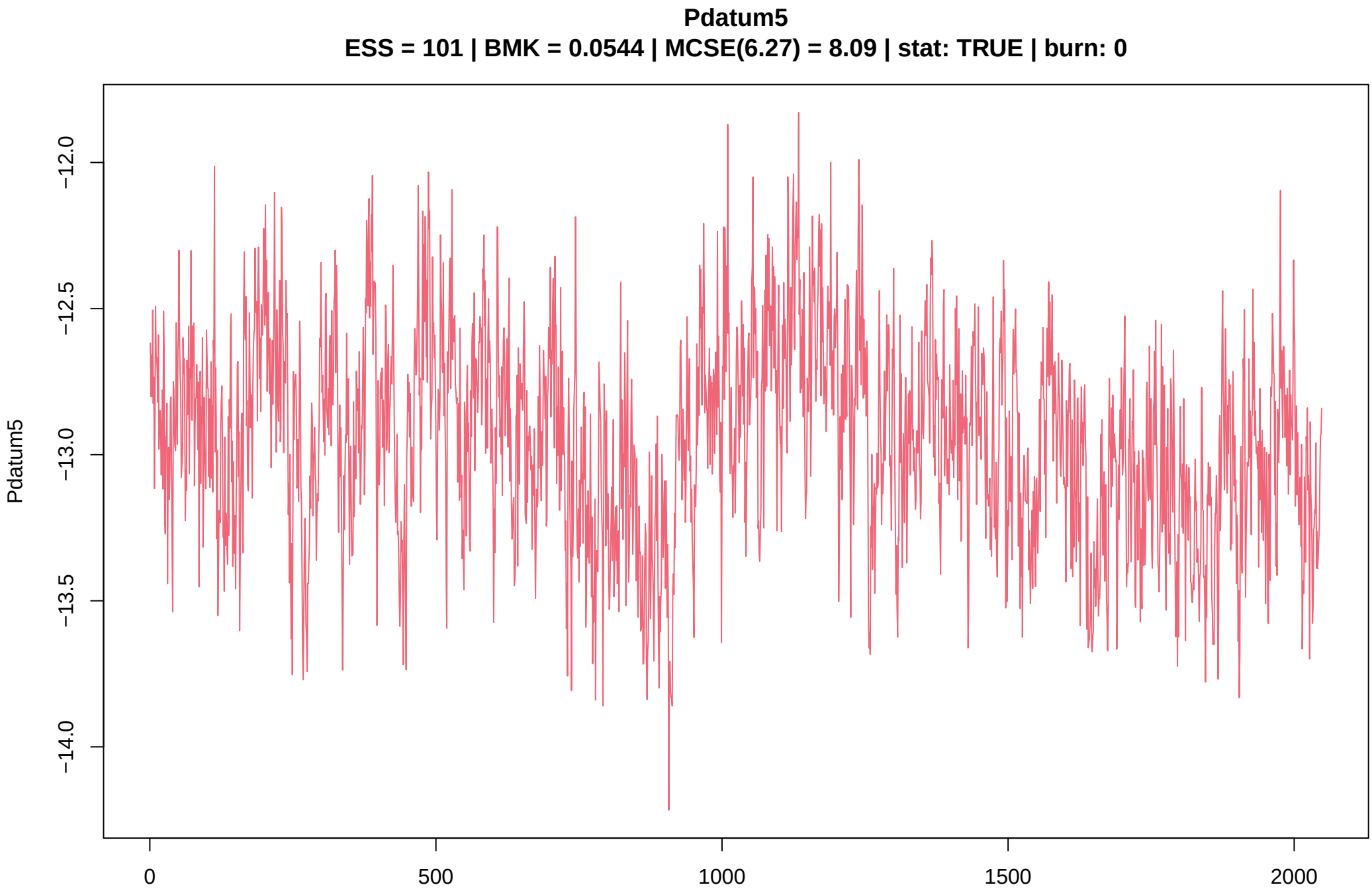

PdatacornerLo
ESS = 77.9 | BMK = 0.136 | MCSE(6.27) = 8.52 | stat: FALSE | burn: 0
PdatacornerLo
−12.5
−13.0
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

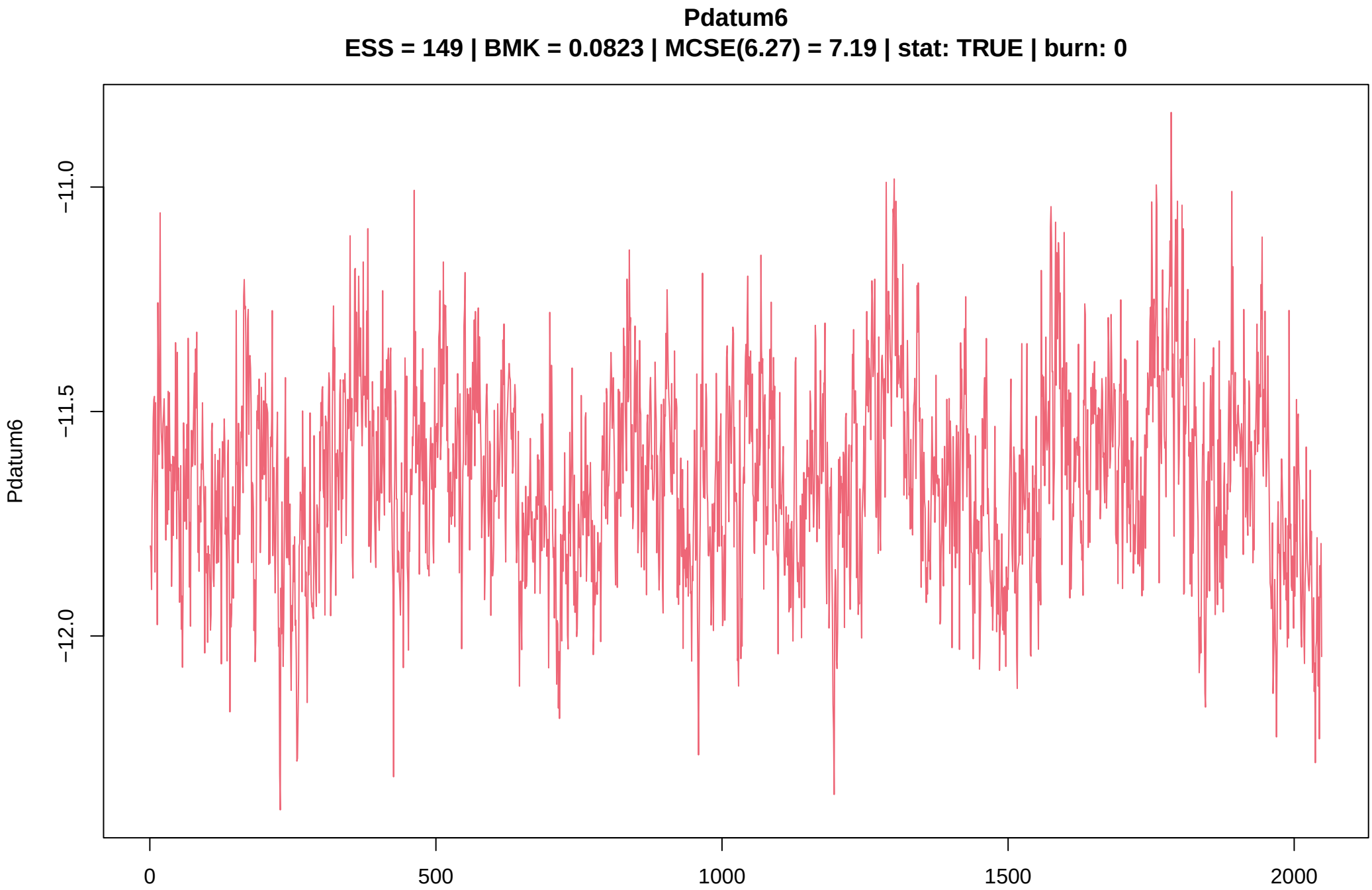

Pdatum1
ESS = 50.2 | BMK = 0.216 | MCSE(6.27) = 10.7 | stat: TRUE | burn: 612
Pdatum1
−12
−13
−14
−15
0
500
1000
1500
2000

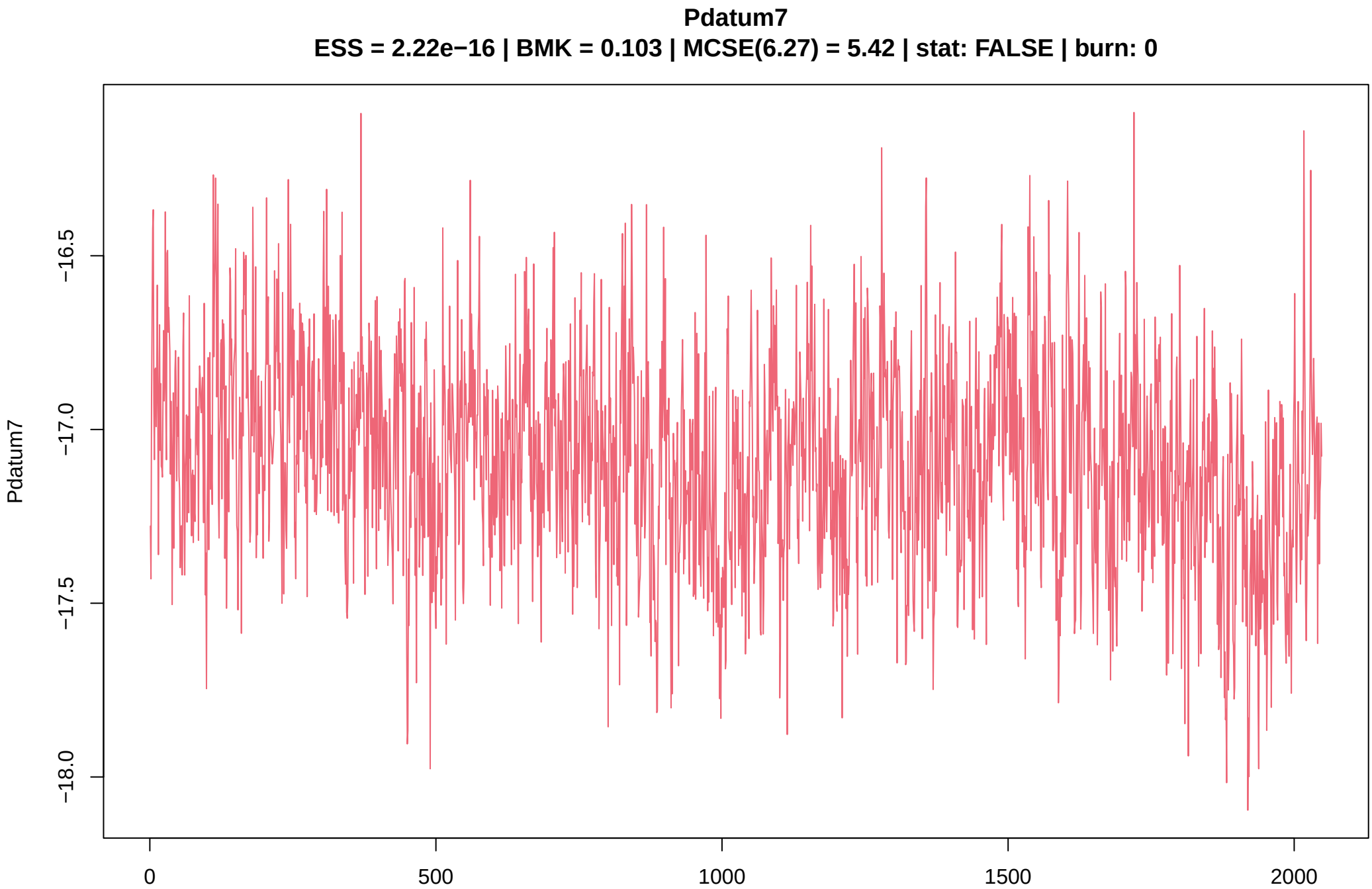

Pdatum2
ESS = 82.4 | BMK = 0.158 | MCSE(6.27) = 8.15 | stat: FALSE | burn: 0
Pdatum2
−11.5
−12.0
−12.5
0
500
1000
1500
2000

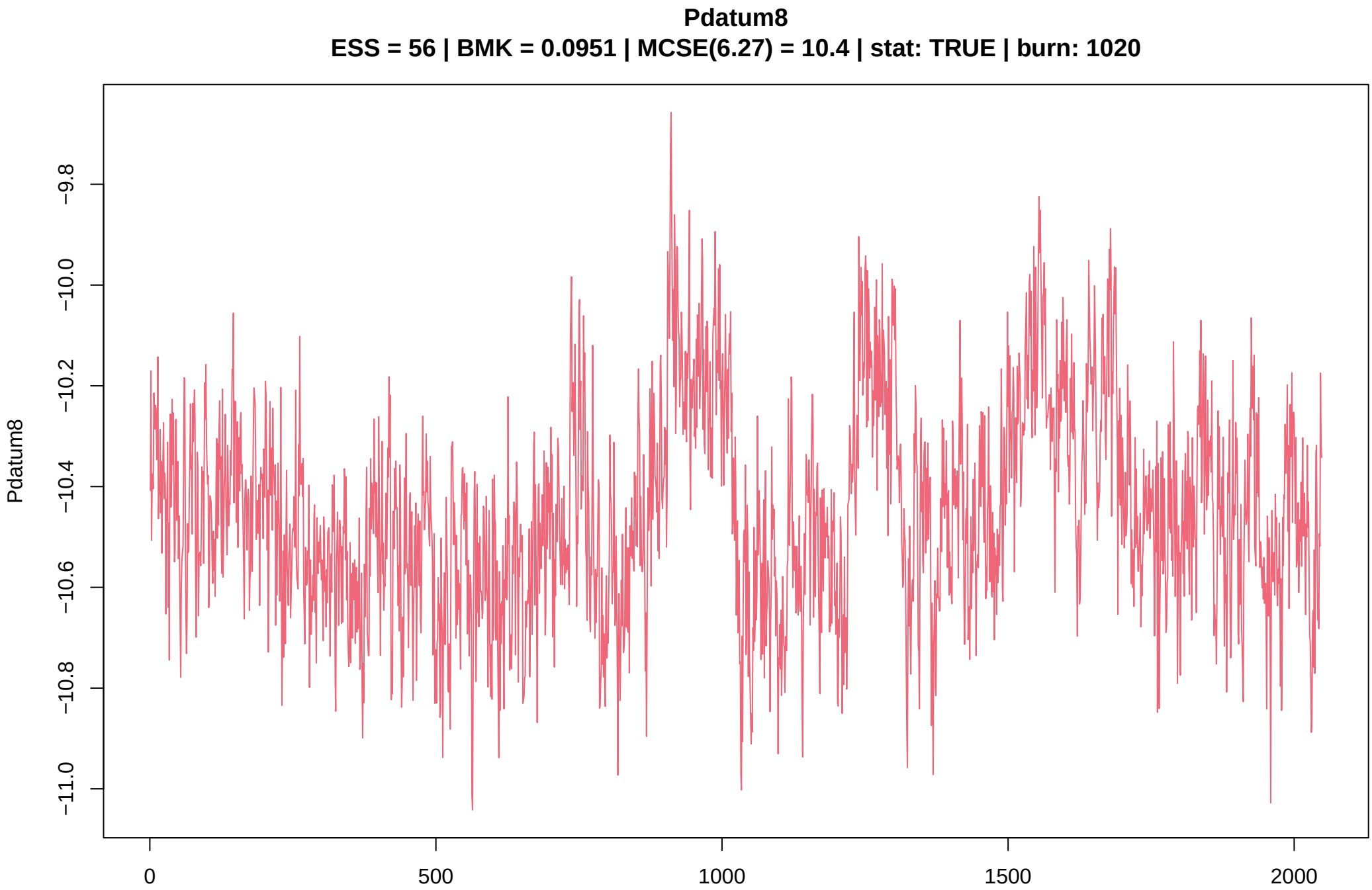

Pdatum3
ESS = 247 | BMK = 0.0428 | MCSE(6.27) = 6.53 | stat: TRUE | burn: 0
Pdatum3
−11.0
−11.2
−11.4
−11.6
−11.8
−12.0
0
500
1000
1500
2000

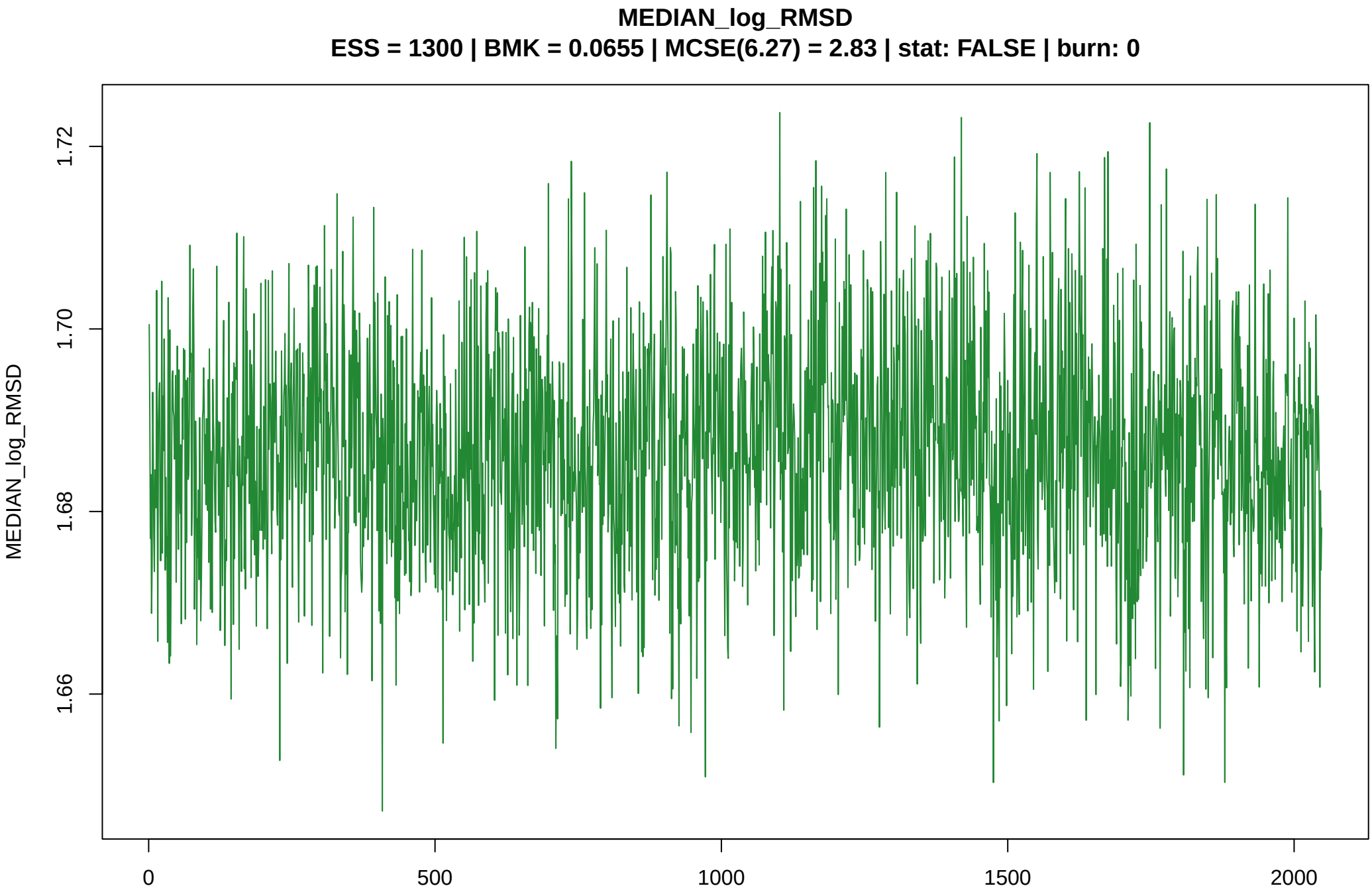

Pdatum4
ESS = 48.7 | BMK = 0.265 | MCSE(6.27) = 9.46 | stat: TRUE | burn: 0
Pdatum4
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

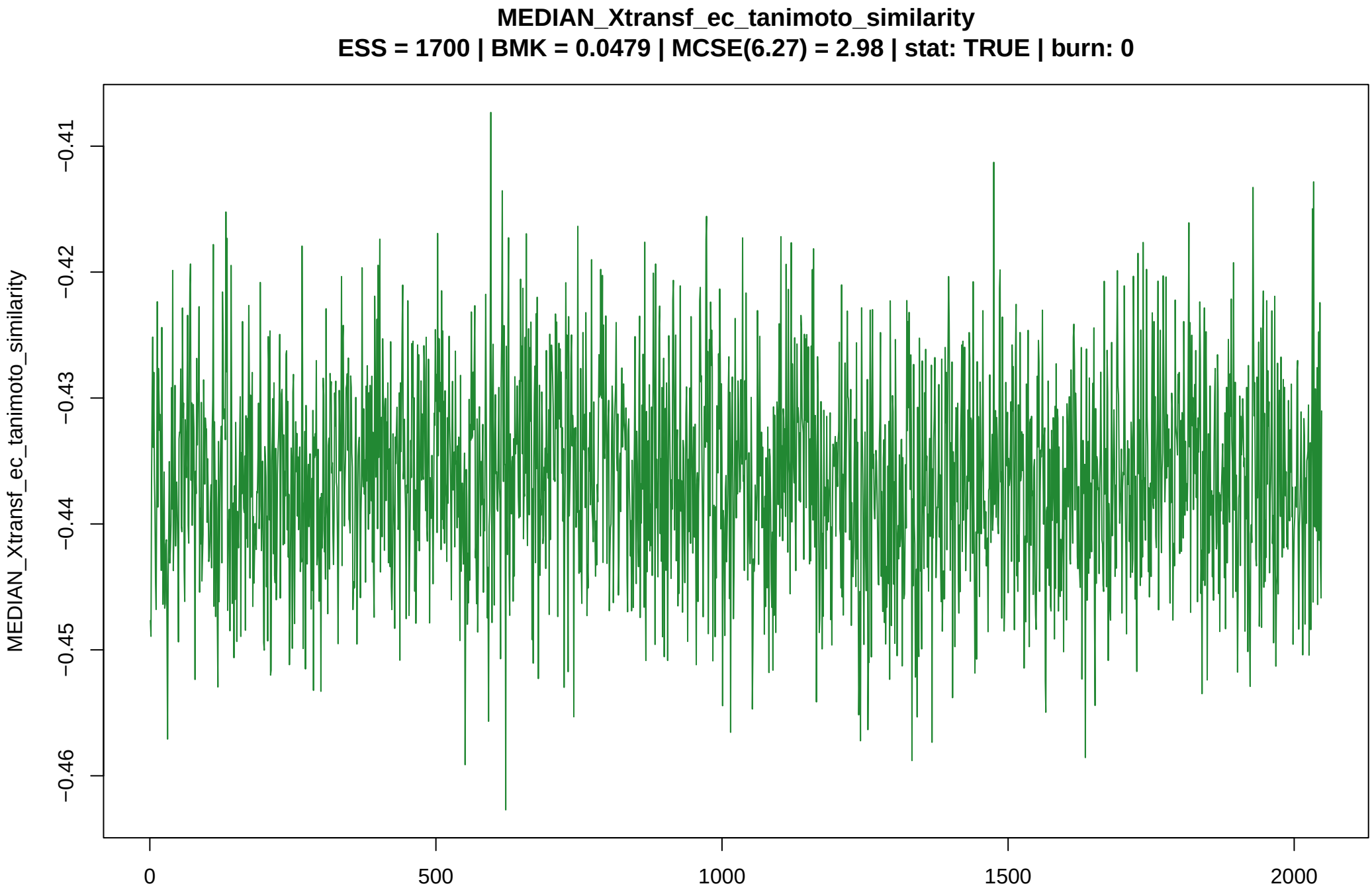

Pdatum5
ESS = 101 | BMK = 0.0544 | MCSE(6.27) = 8.09 | stat: TRUE | burn: 0
Pdatum5
−12.0
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

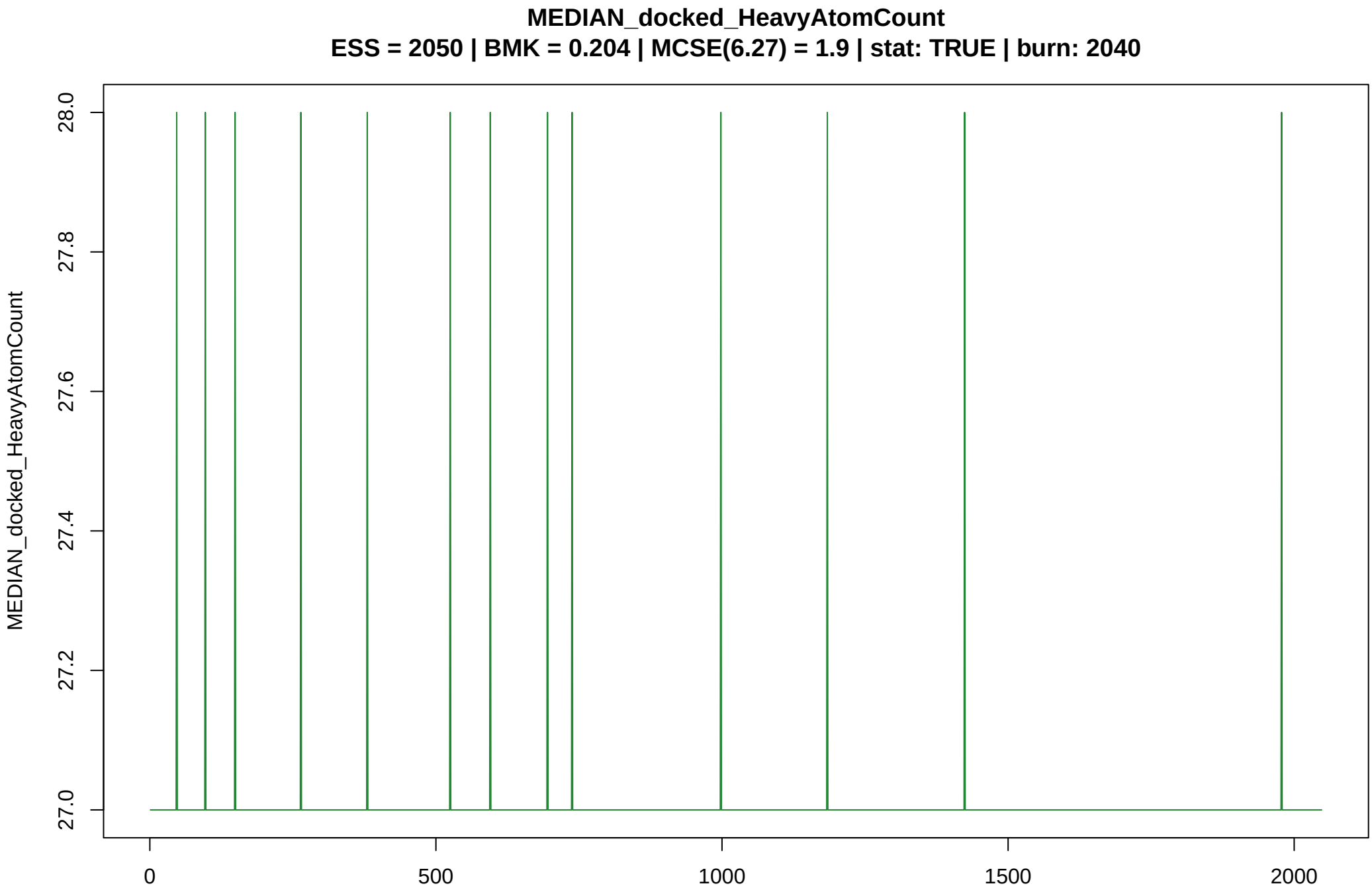

Pdatum6
ESS = 149 | BMK = 0.0823 | MCSE(6.27) = 7.19 | stat: TRUE | burn: 0
Pdatum6
−11.0
−11.5
−12.0
0
500
1000
1500
2000

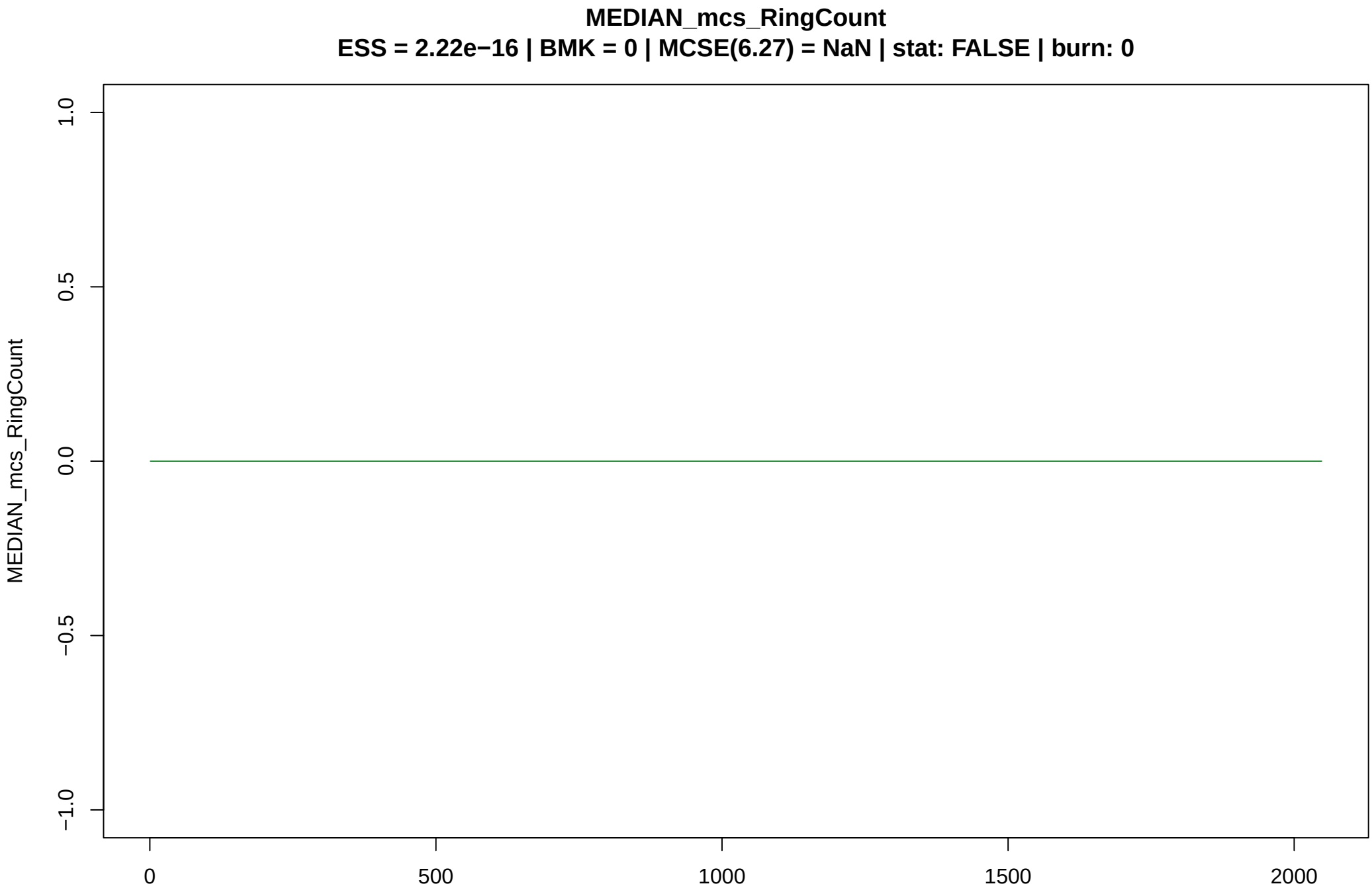

Pdatum7
ESS = 2.22e−16 | BMK = 0.103 | MCSE(6.27) = 5.42 | stat: FALSE | burn: 0
Pdatum7
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

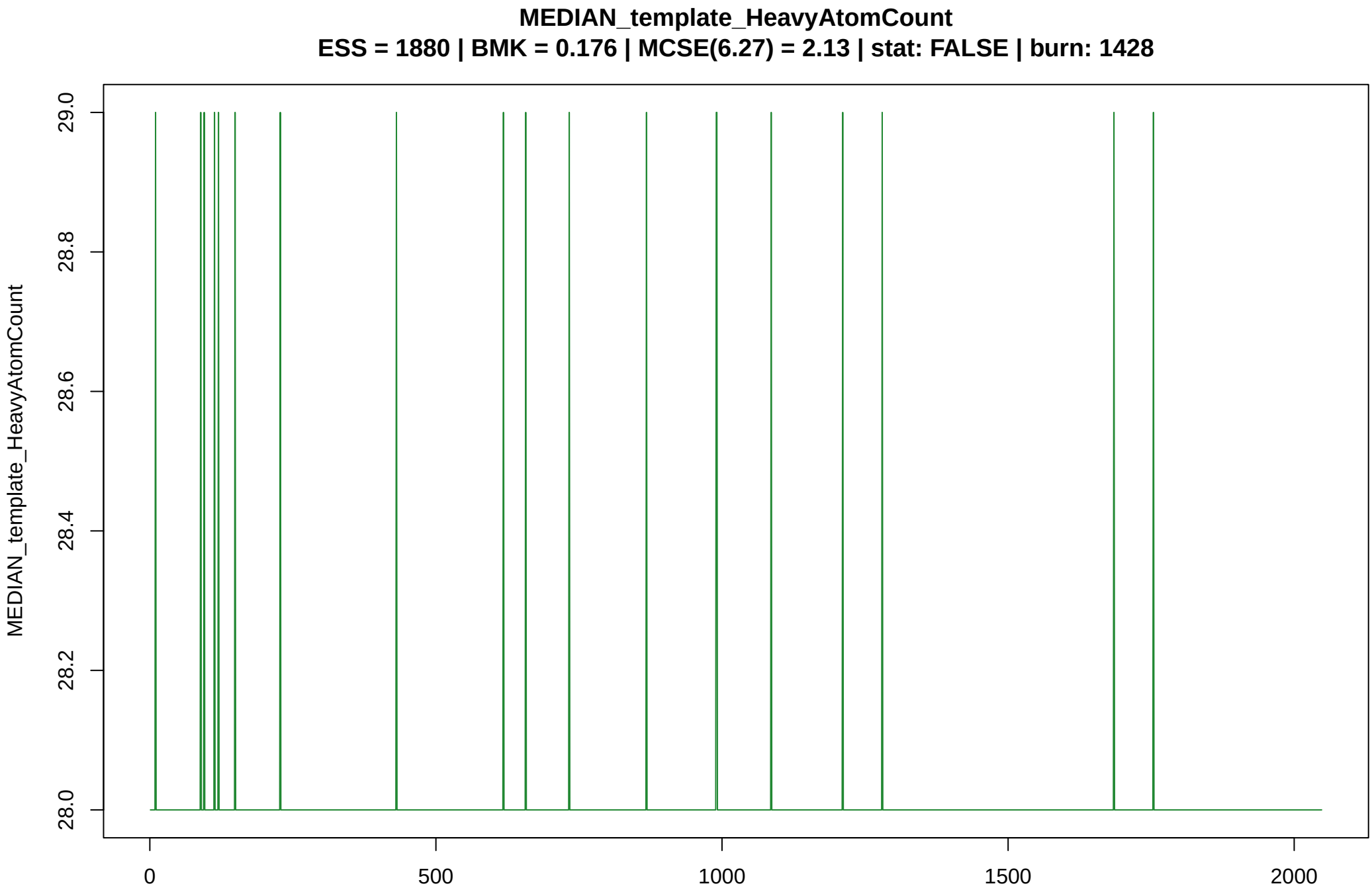

Pdatum8
ESS = 56 | BMK = 0.0951 | MCSE(6.27) = 10.4 | stat: TRUE | burn: 1020
Pdatum8
−9.8
−10.0
−10.2
−10.4
−10.6
−10.8
−11.0
0
500
1000
1500
2000

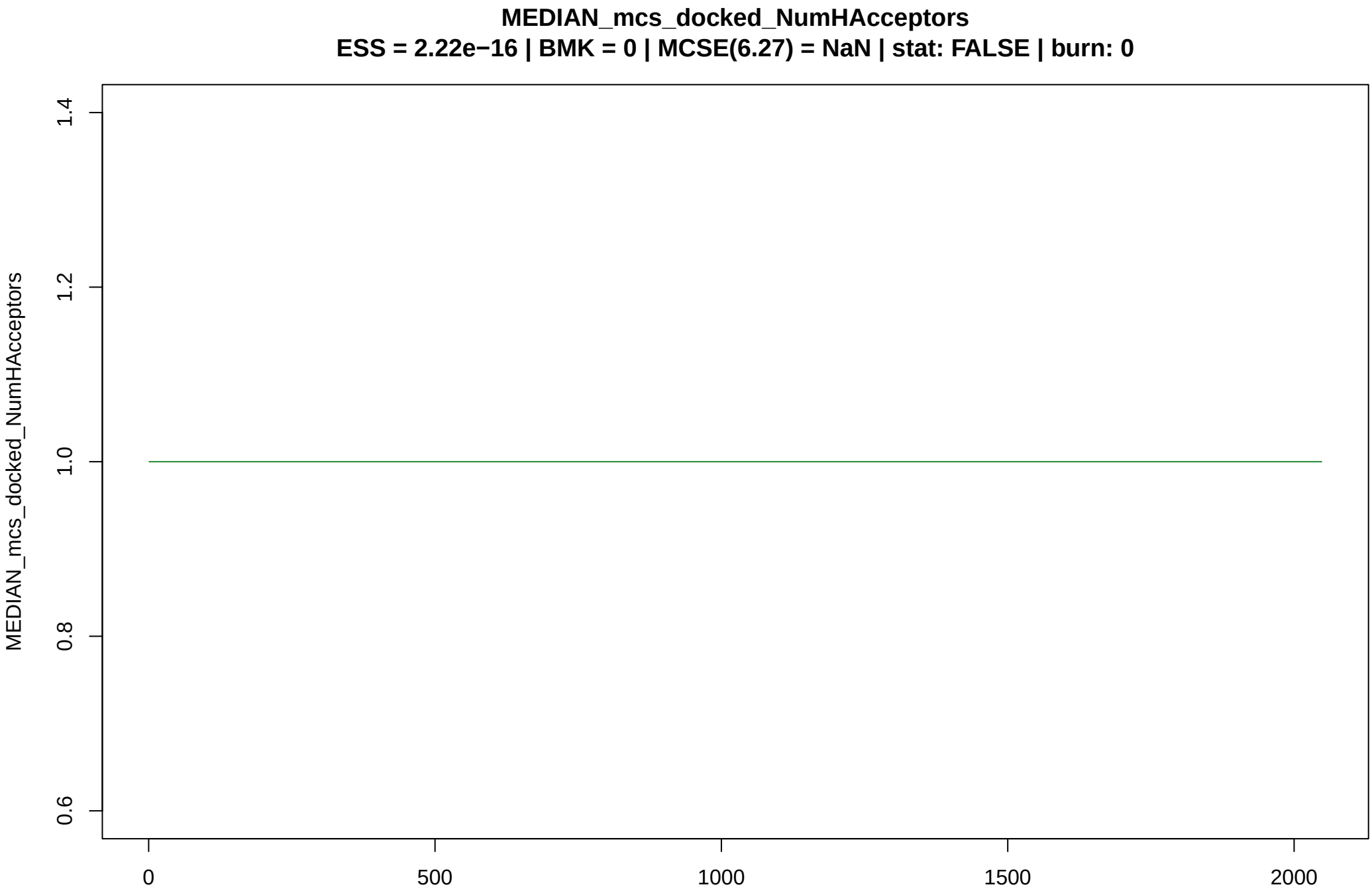

MEDIAN_log_RMSD
ESS = 1300 | BMK = 0.0655 | MCSE(6.27) = 2.83 | stat: FALSE | burn: 0
MEDIAN_log_RMSD
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

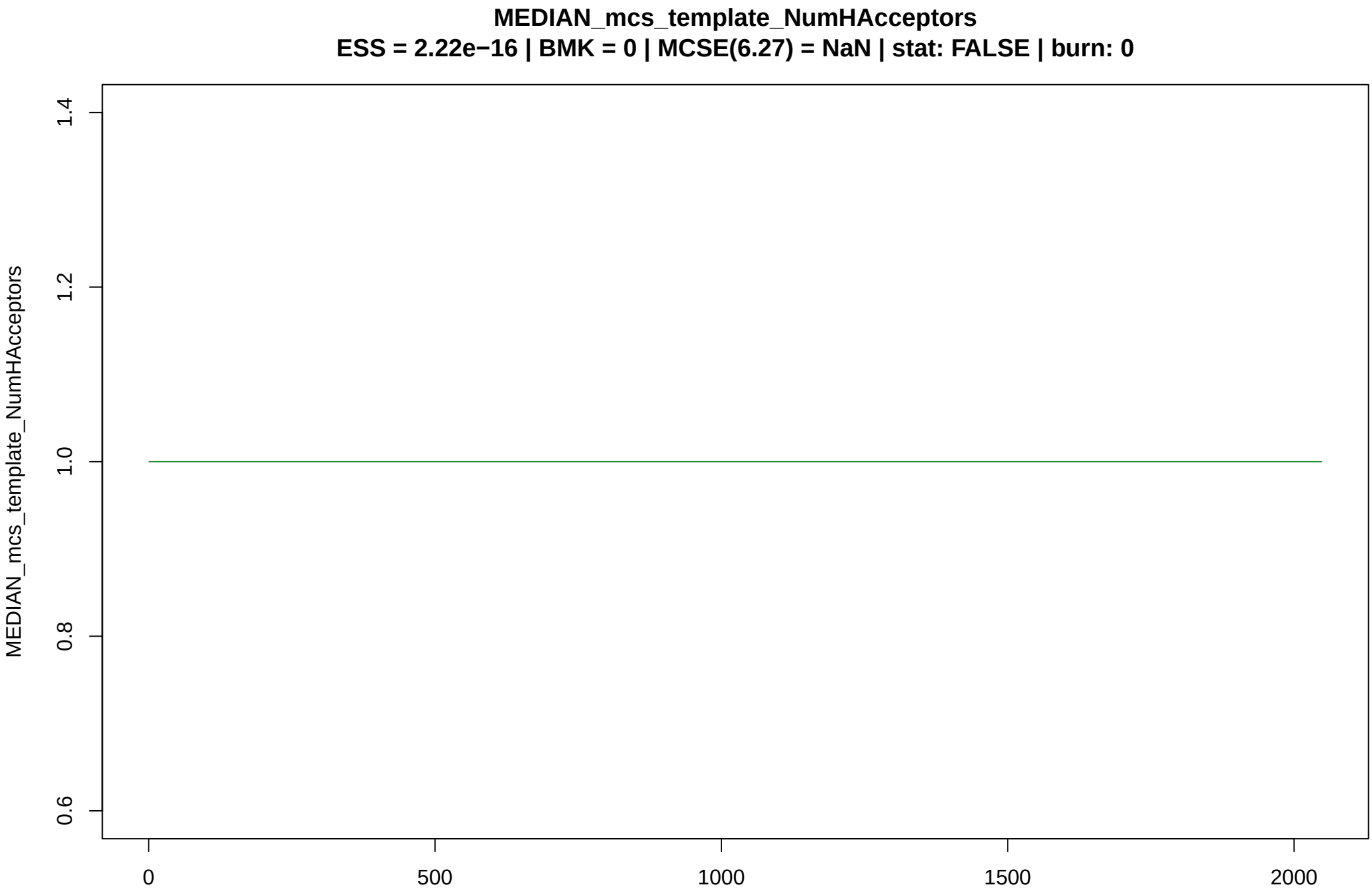

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 1700 | BMK = 0.0479 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.41
−0.42
−0.43
−0.44
−0.45
−0.46
0
500
1000
1500
2000

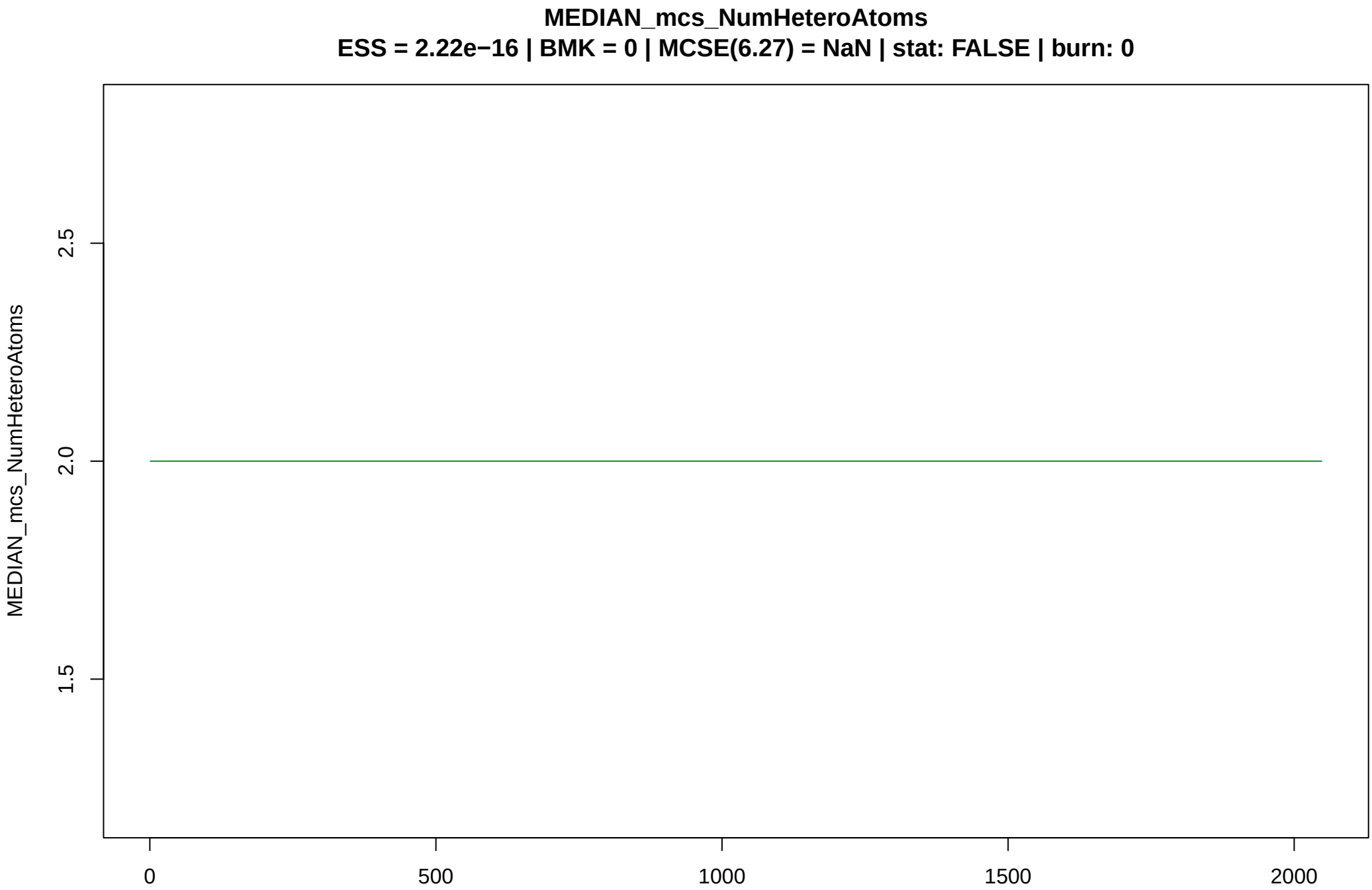

MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.204 | MCSE(6.27) = 1.9 | stat: TRUE | burn: 2040
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

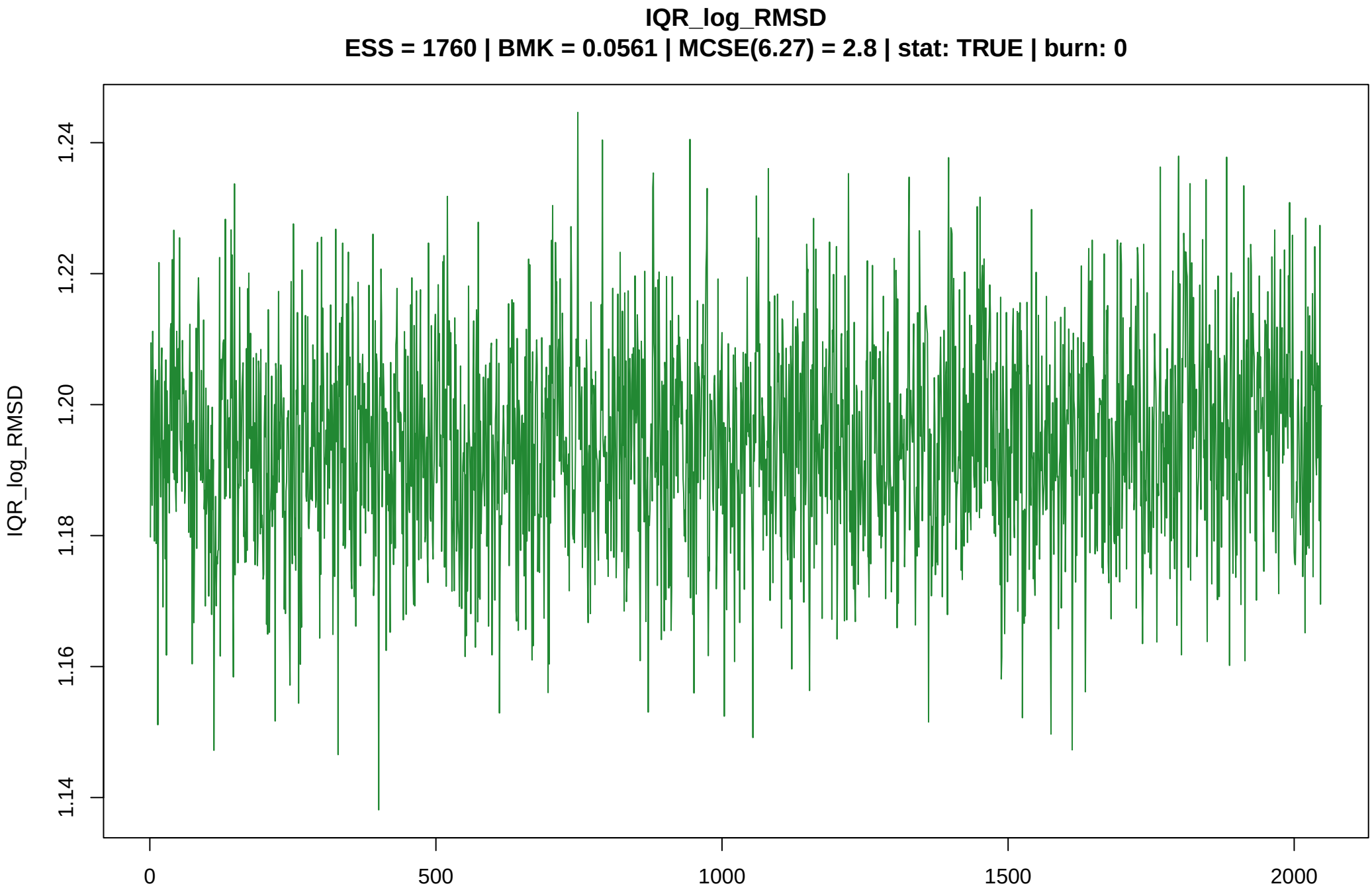

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

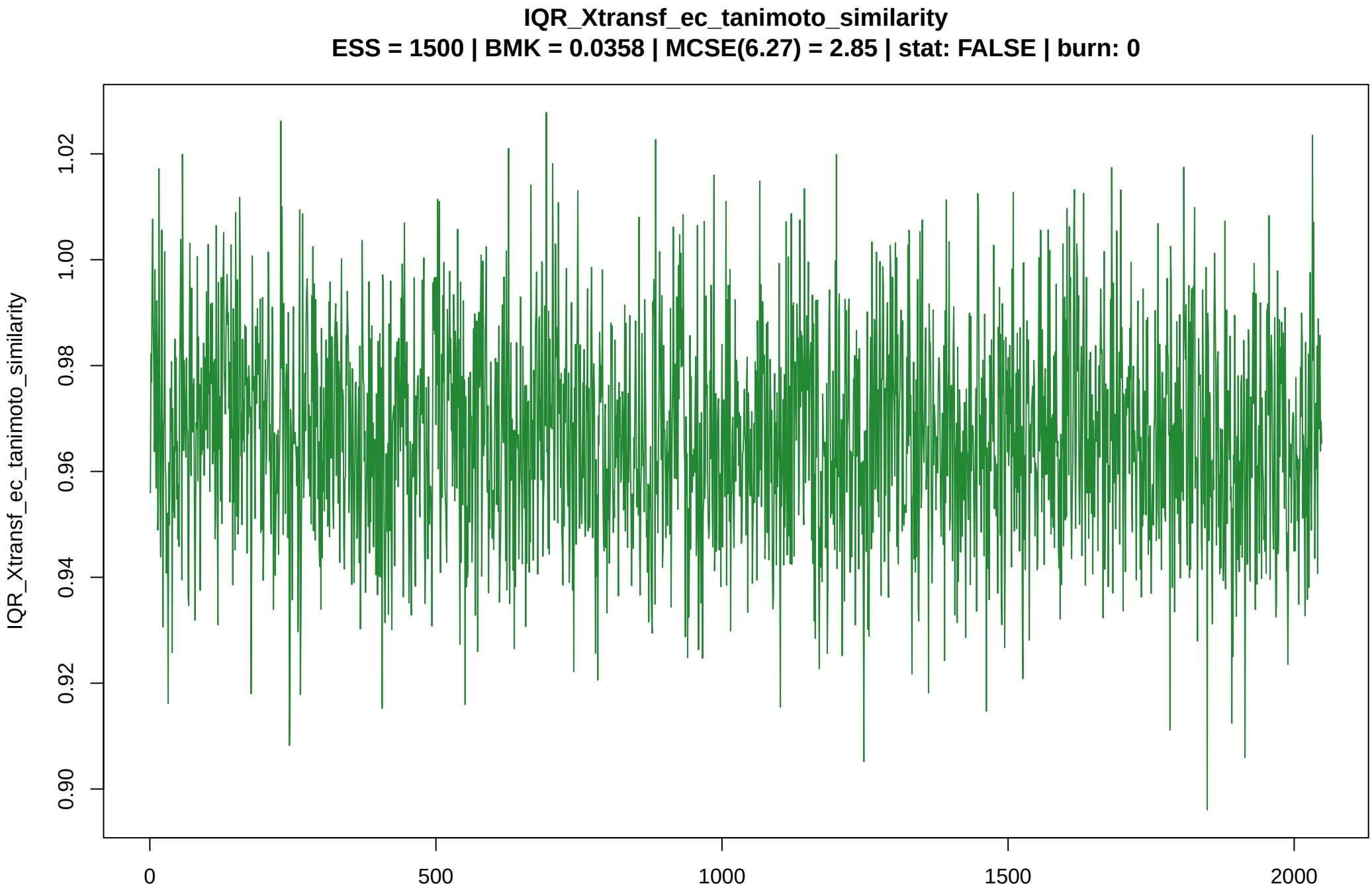

MEDIAN_template_HeavyAtomCount
ESS = 1880 | BMK = 0.176 | MCSE(6.27) = 2.13 | stat: FALSE | burn: 1428
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

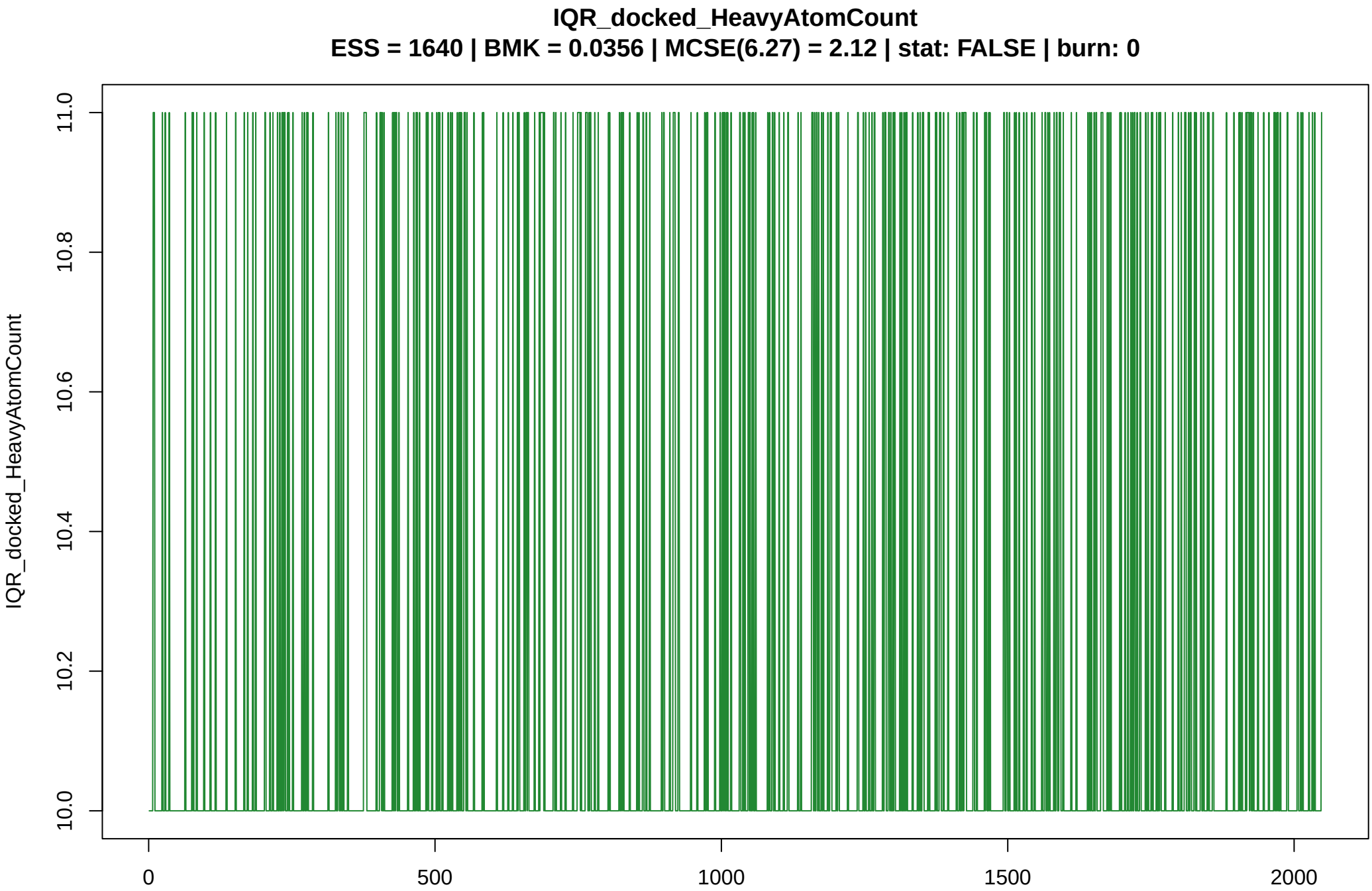

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

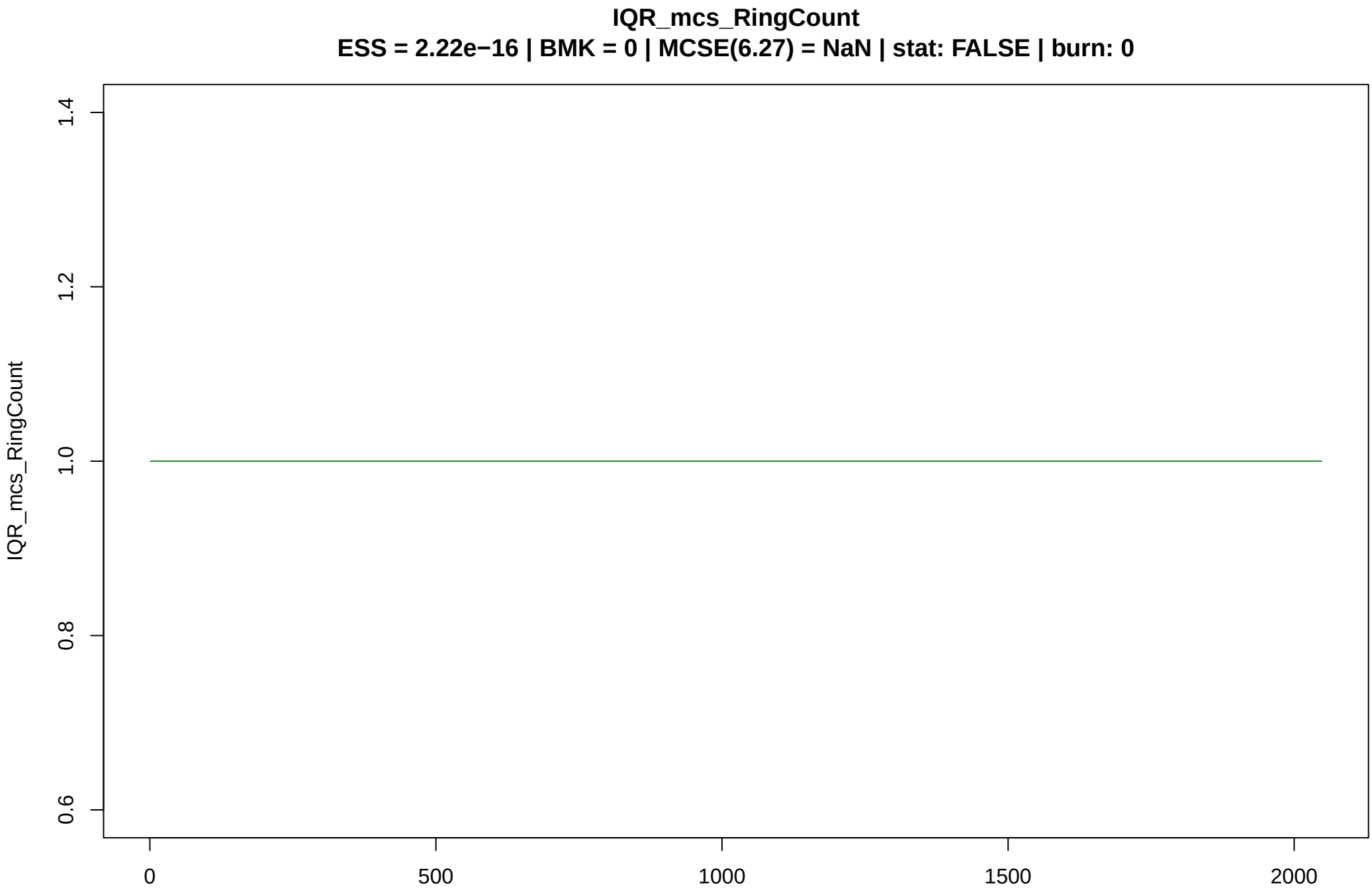

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

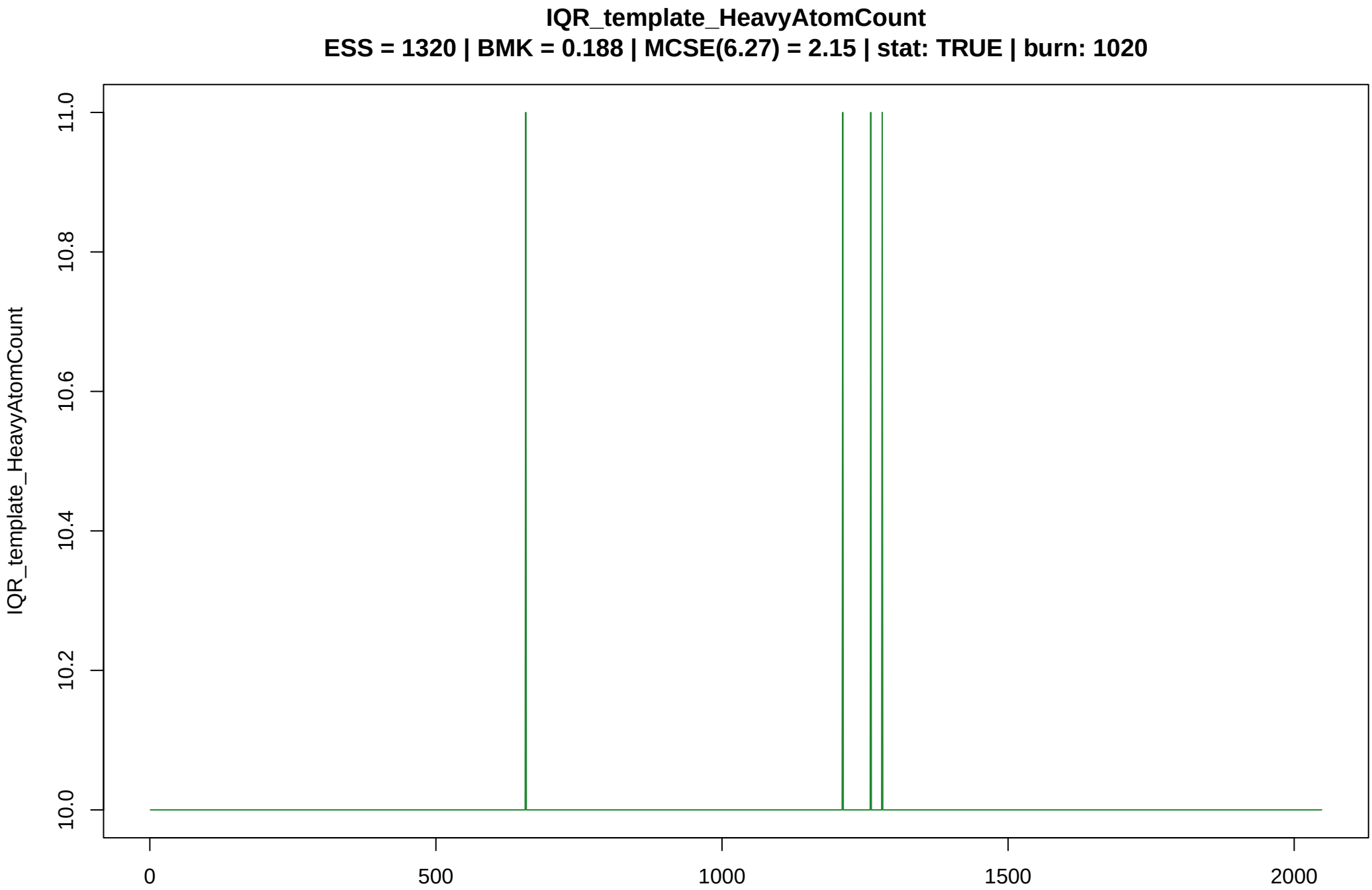

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

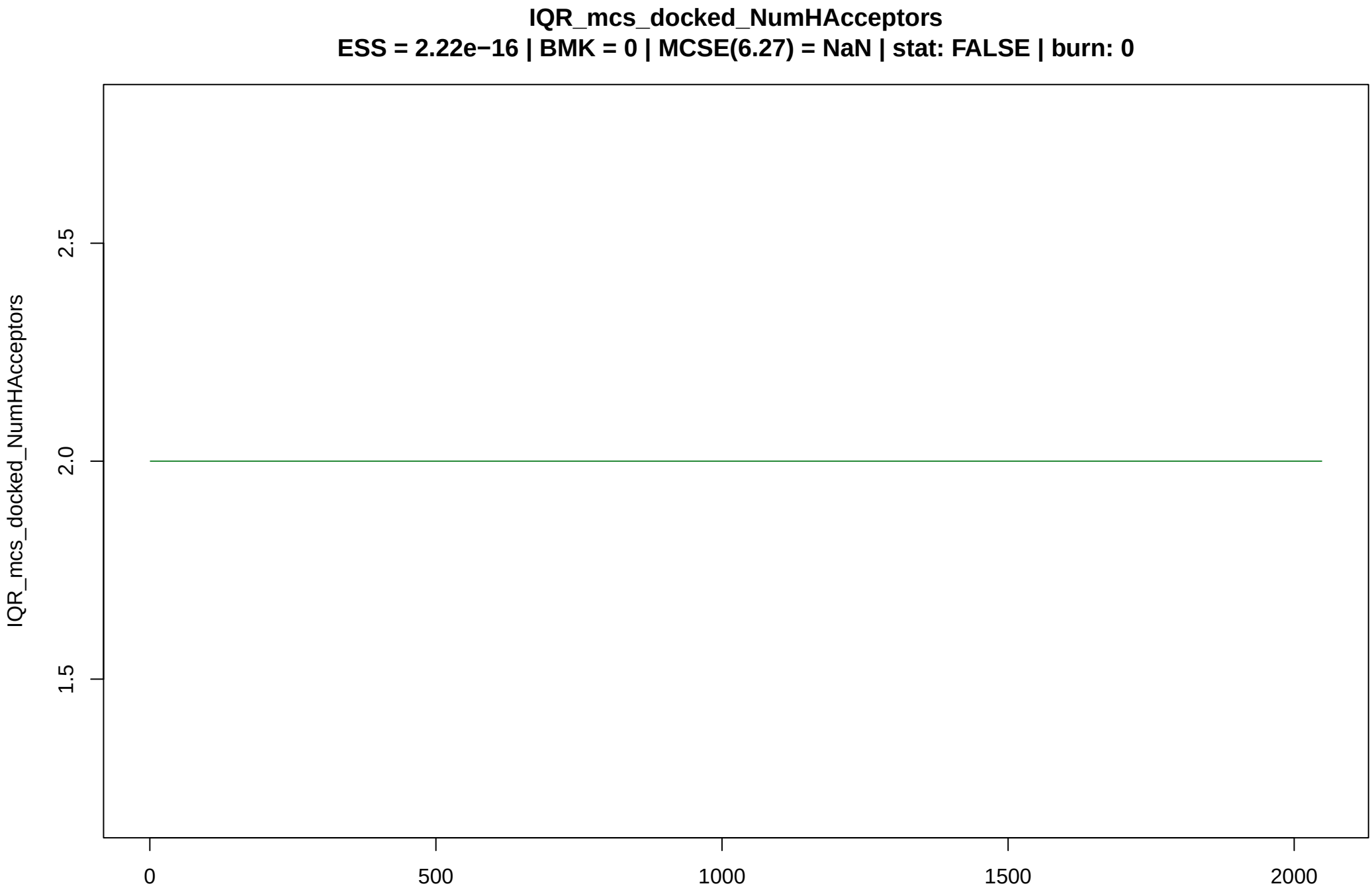

IQR_log_RMSD
ESS = 1760 | BMK = 0.0561 | MCSE(6.27) = 2.8 | stat: TRUE | burn: 0
IQR_log_RMSD
1.14
1.16
1.18
1.20
1.22
1.24
0
500
1000
1500
2000

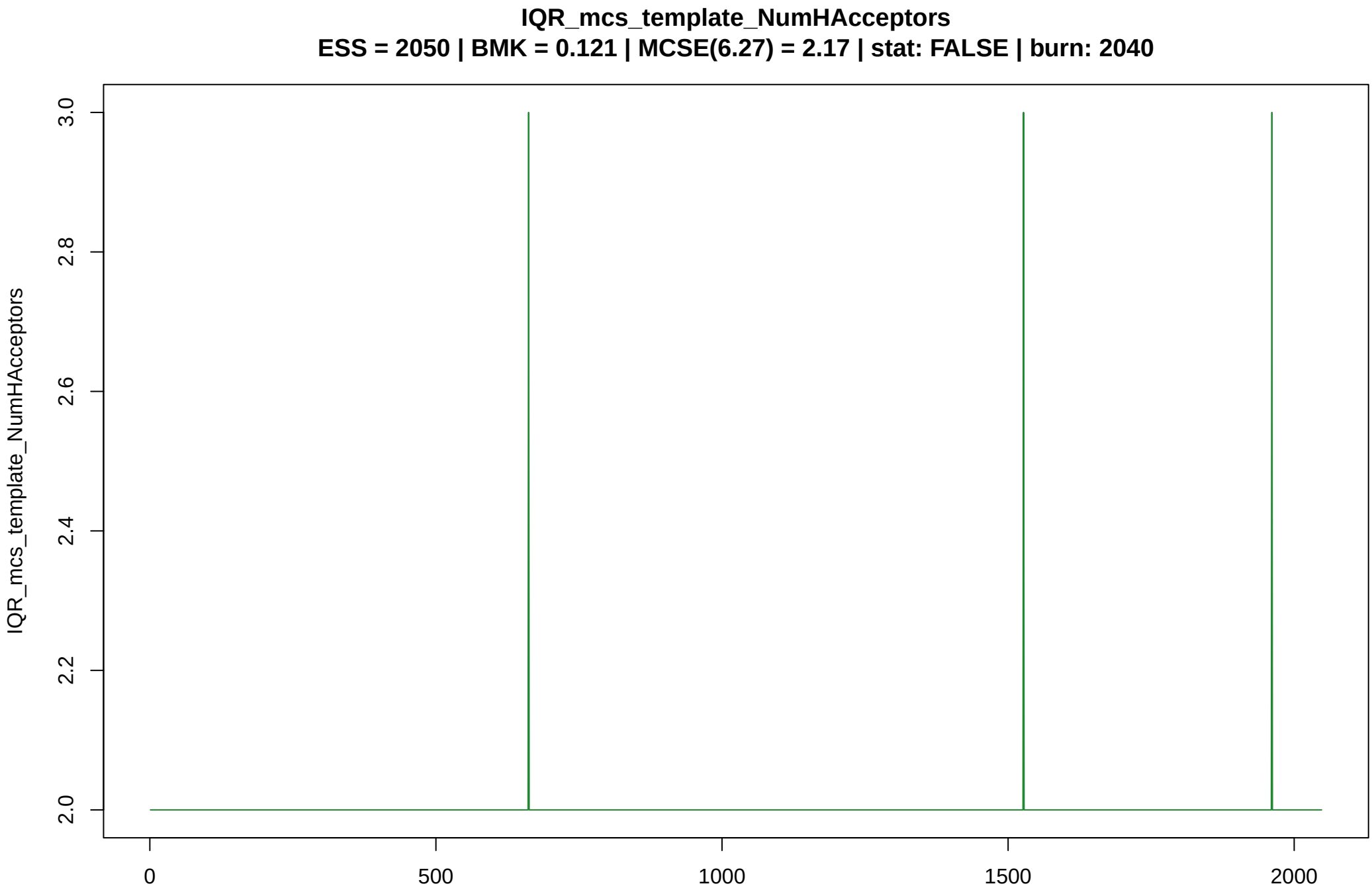

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1500 | BMK = 0.0358 | MCSE(6.27) = 2.85 | stat: FALSE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.90
0.92
0.94
0.96
0.98
1.00
1.02
0
500
1000
1500
2000

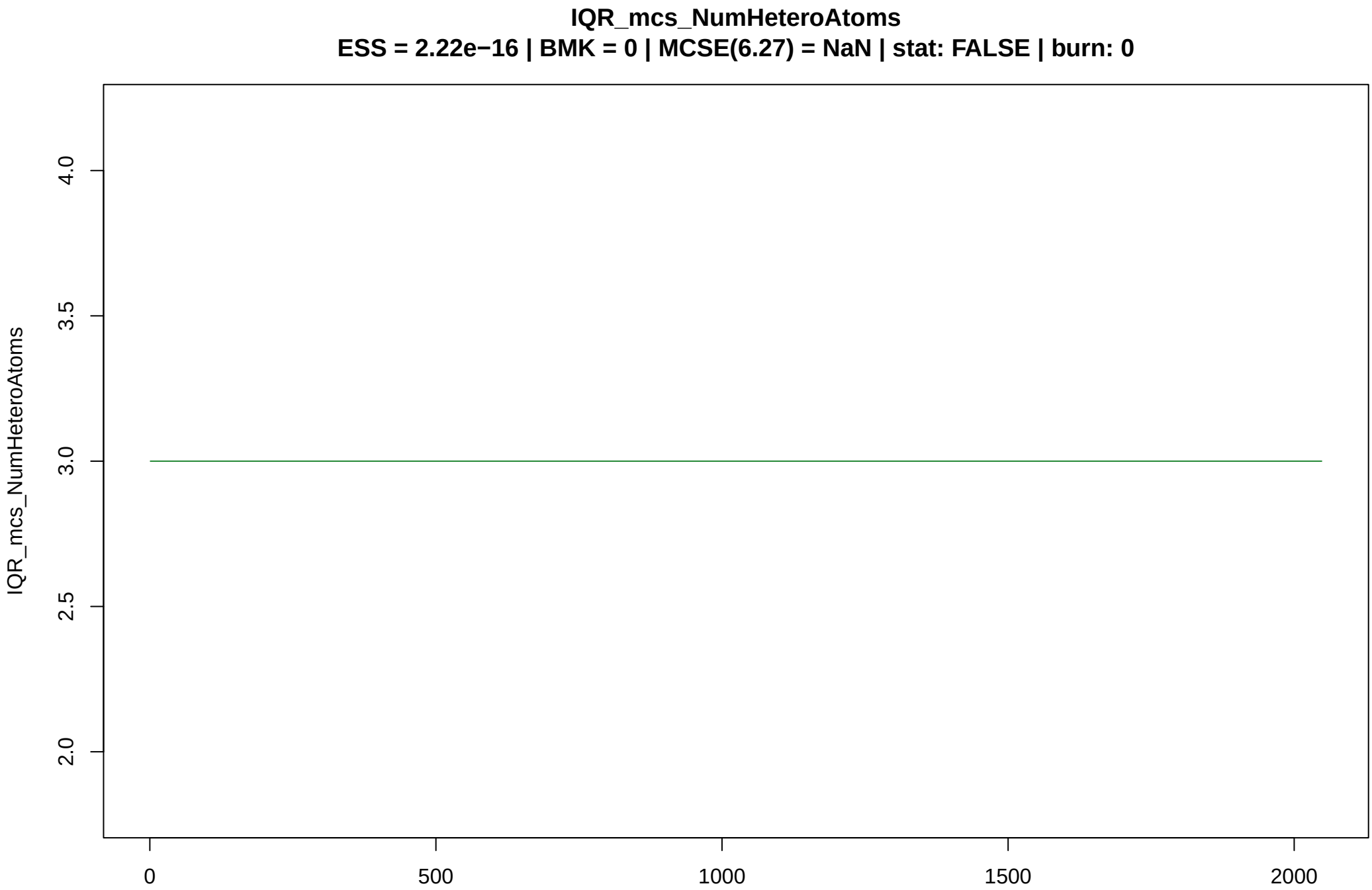

IQR_docked_HeavyAtomCount
ESS = 1640 | BMK = 0.0356 | MCSE(6.27) = 2.12 | stat: FALSE | burn: 0
IQR_docked_HeavyAtomCount
10.0
10.2
10.4
10.6
10.8
11.0
0
500
1000
1500
2000

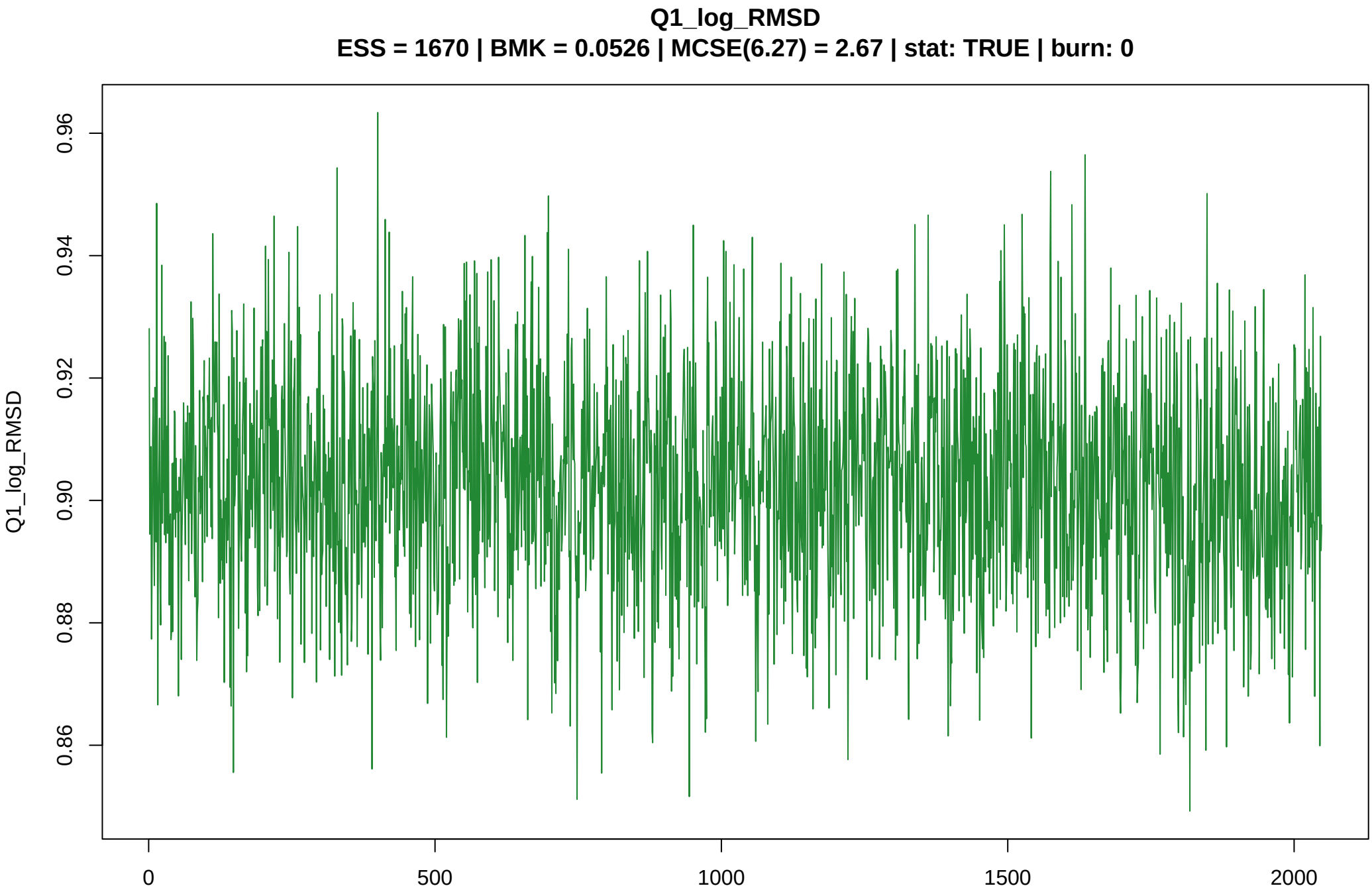

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

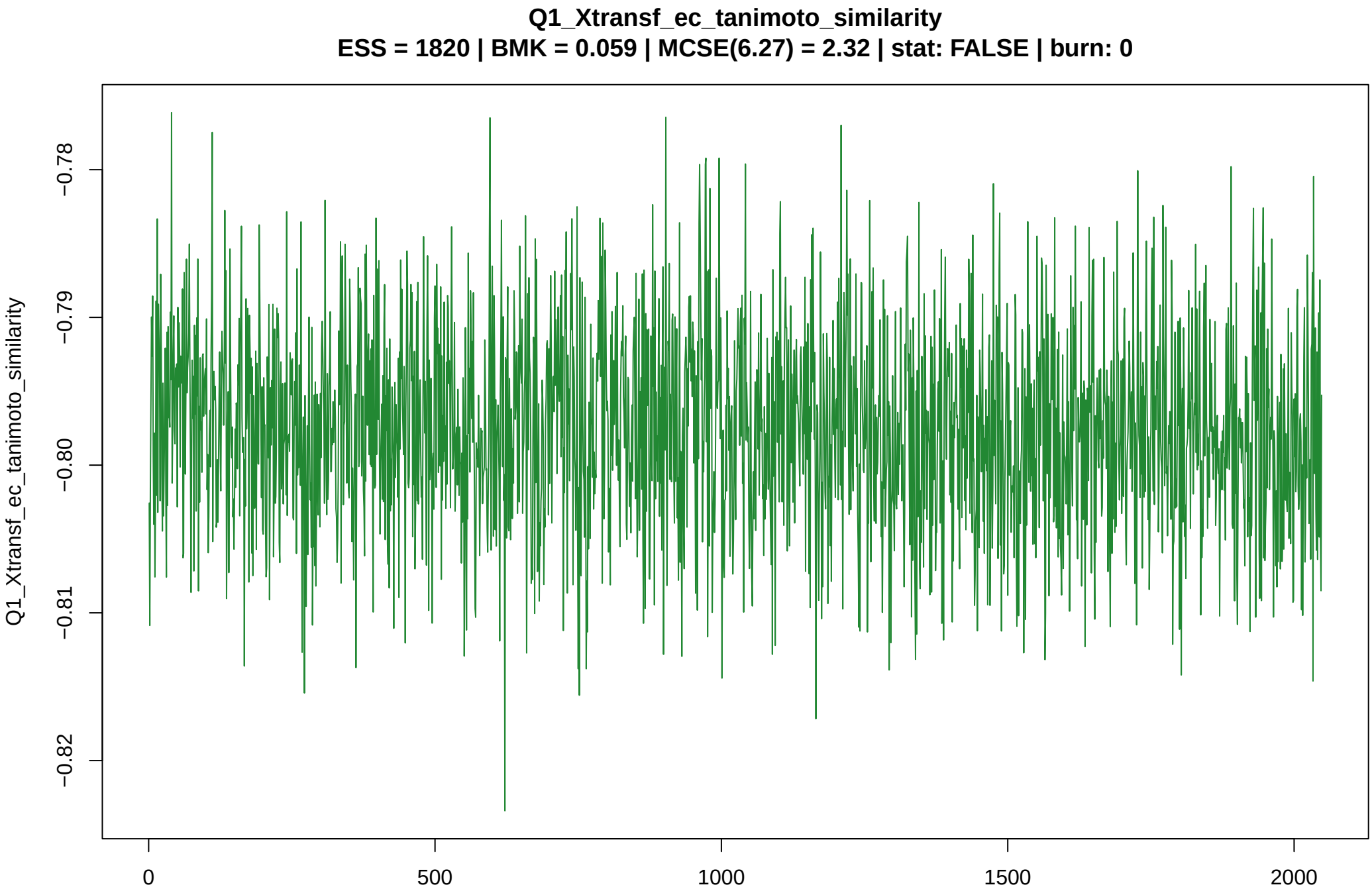

IQR_template_HeavyAtomCount
ESS = 1320 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1020
IQR_template_HeavyAtomCount
11.0
10.8
10.6
10.4
10.2
10.0
0
500
1000
1500
2000

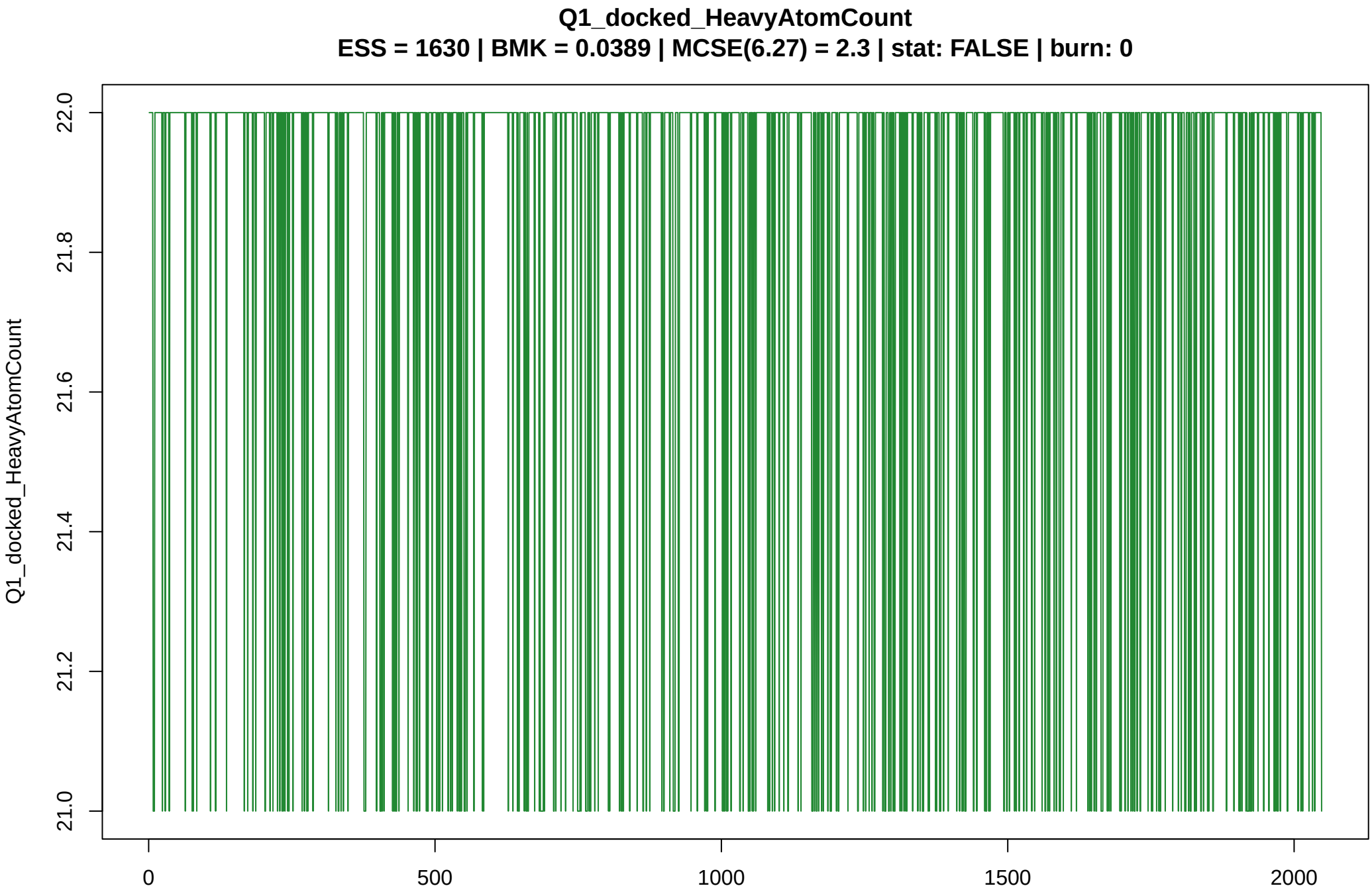

IQR_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_docked_NumHAcceptors
2.5
2.0
1.5
0
500
1000
1500
2000

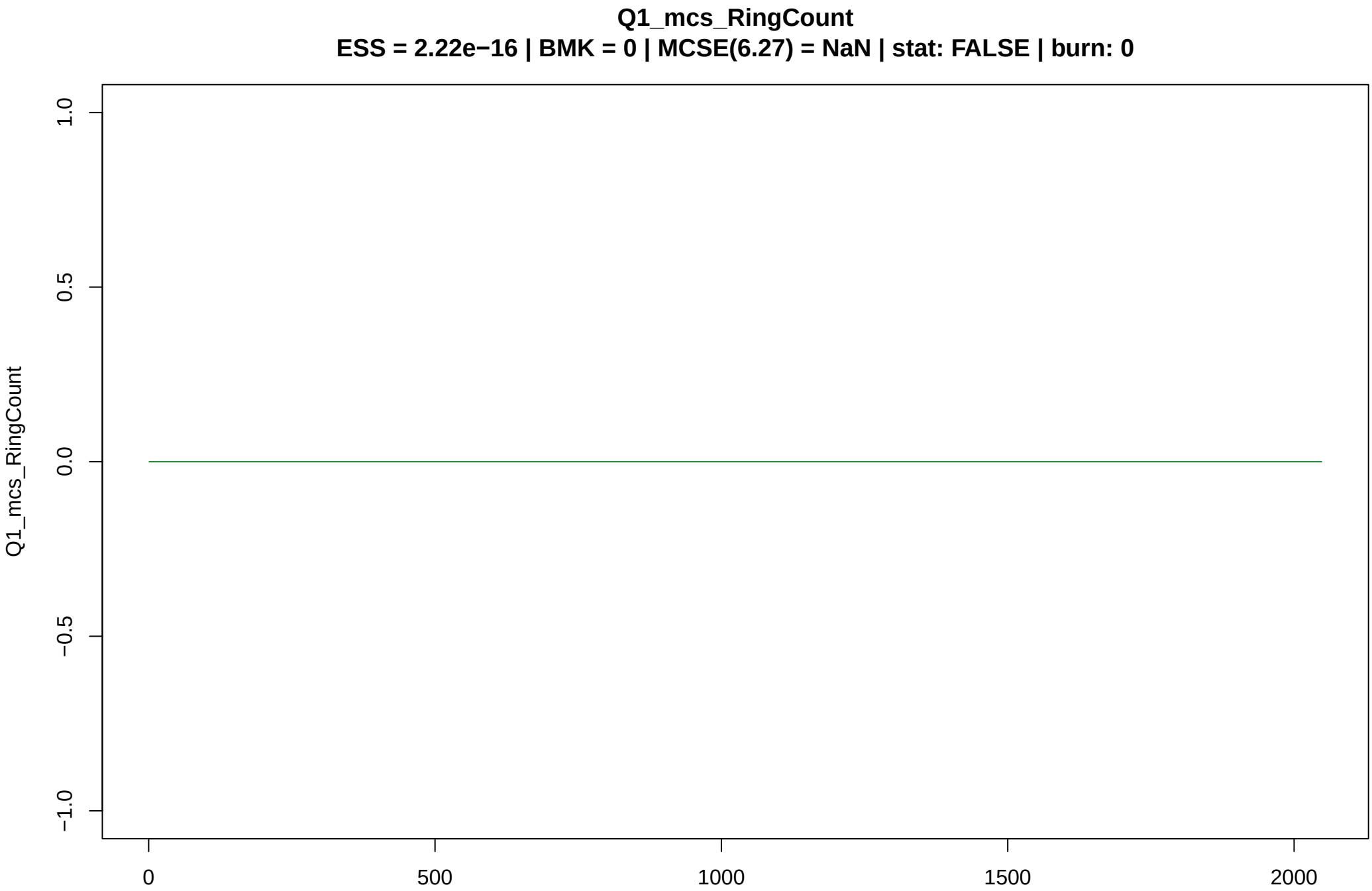

IQR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 2040
IQR_mcs_template_NumHAcceptors
2.0
2.2
2.4
2.6
2.8
3.0
0
500
1000
1500
2000

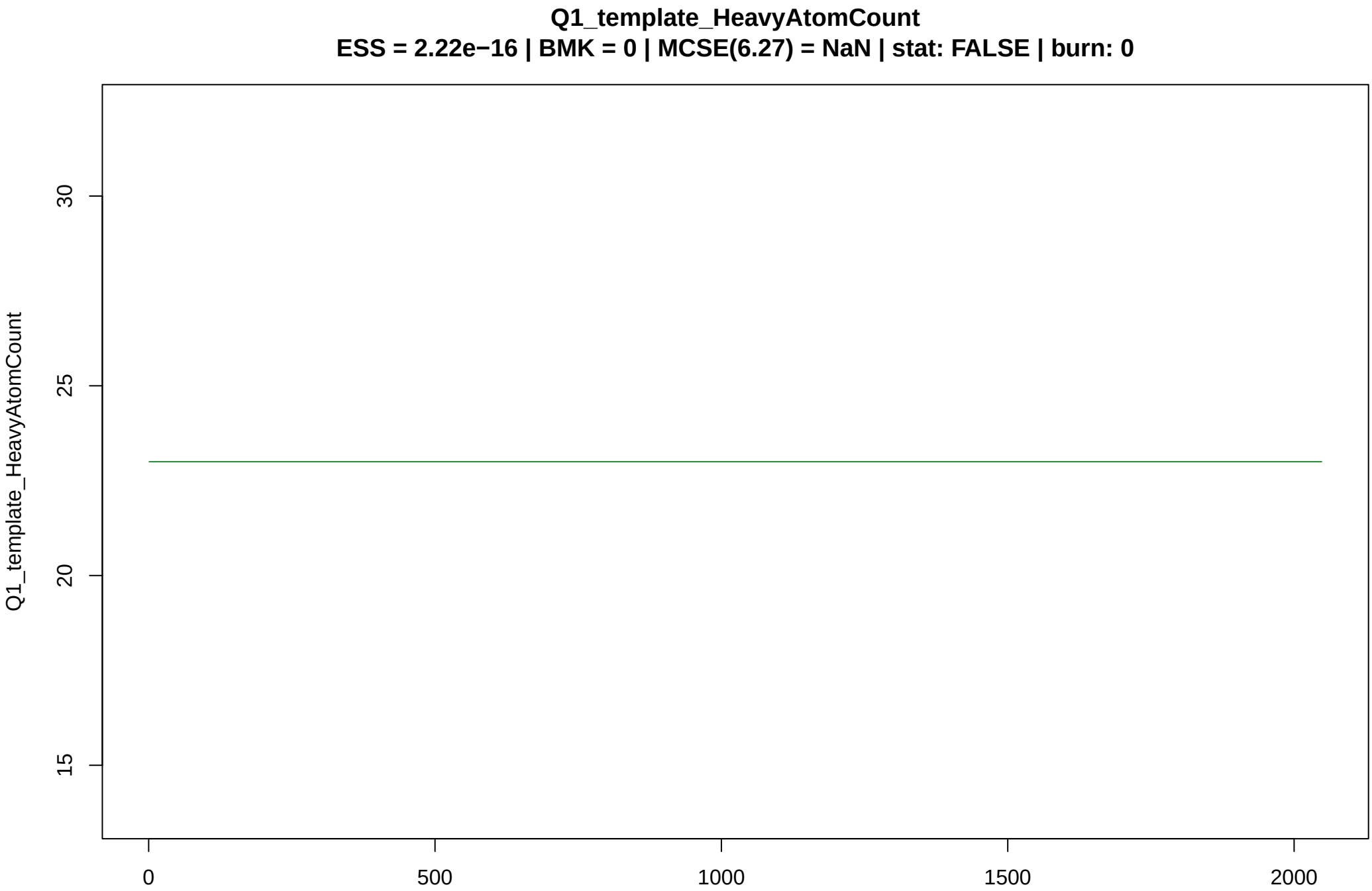

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

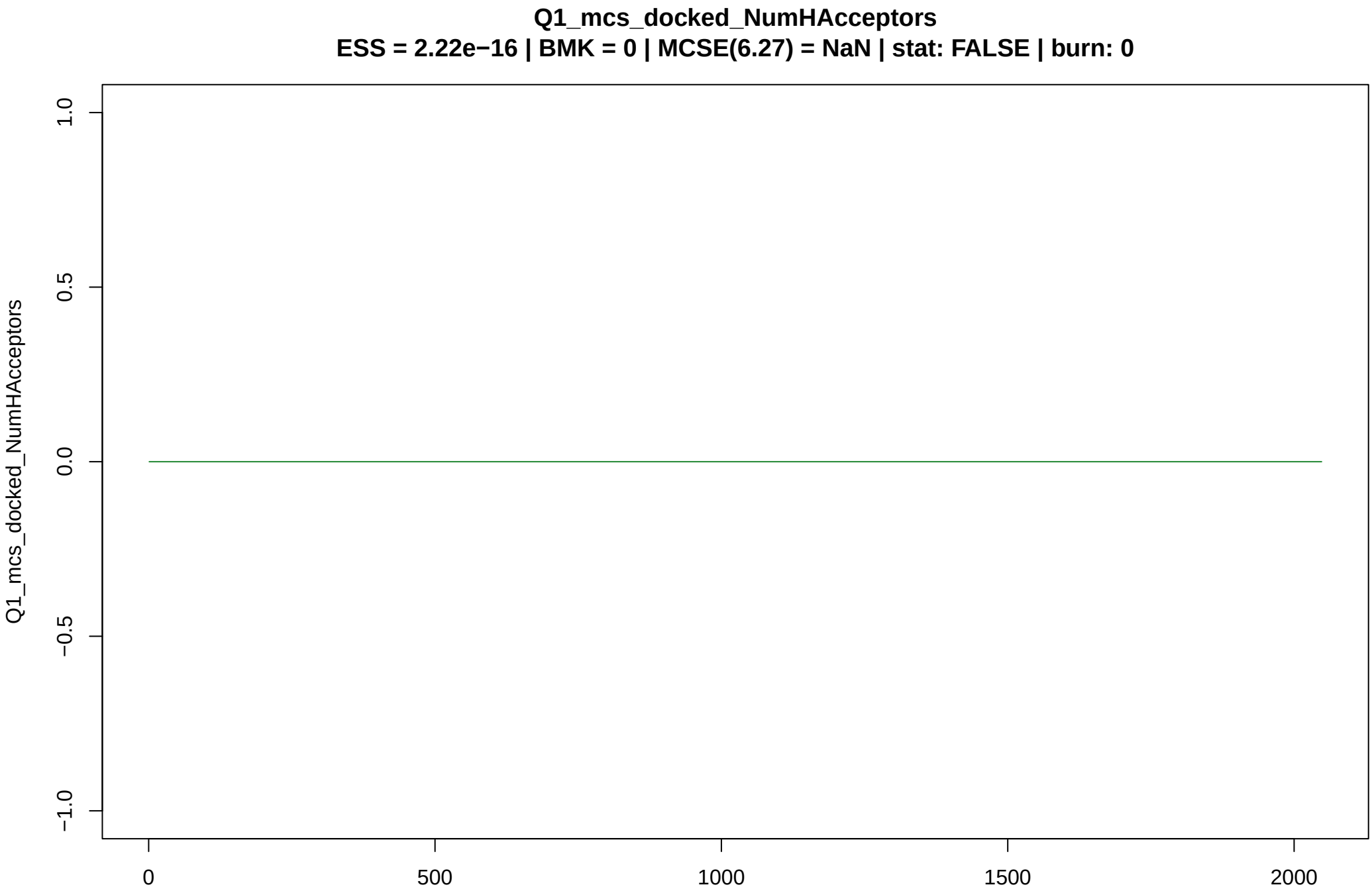

Q1_log_RMSD
ESS = 1670 | BMK = 0.0526 | MCSE(6.27) = 2.67 | stat: TRUE | burn: 0
Q1_log_RMSD
0.86
0.88
0.90
0.92
0.94
0.96
0
500
1000
1500
2000

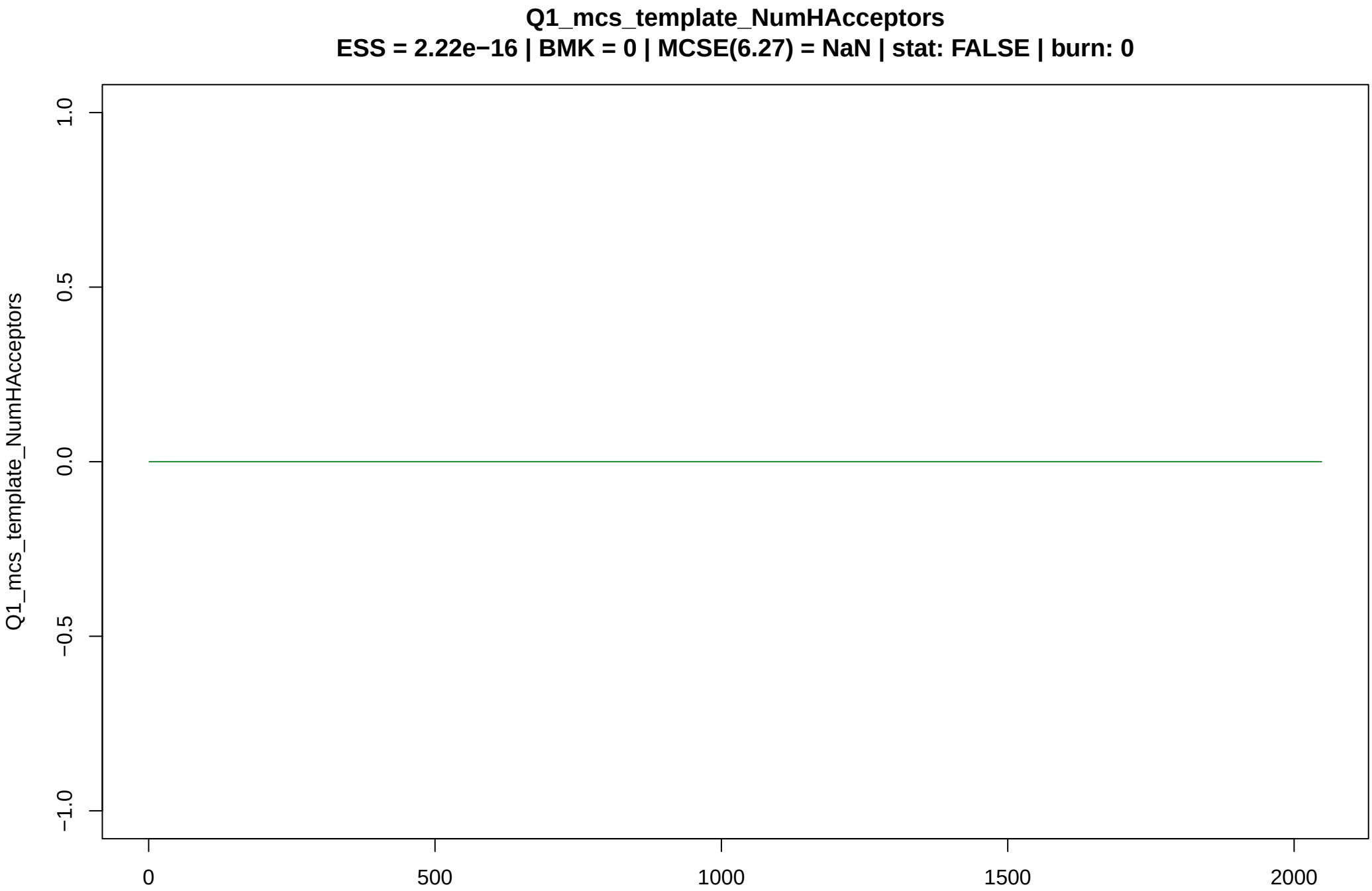

Q1_Xtransf_ec_tanimoto_similarity
ESS = 1820 | BMK = 0.059 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

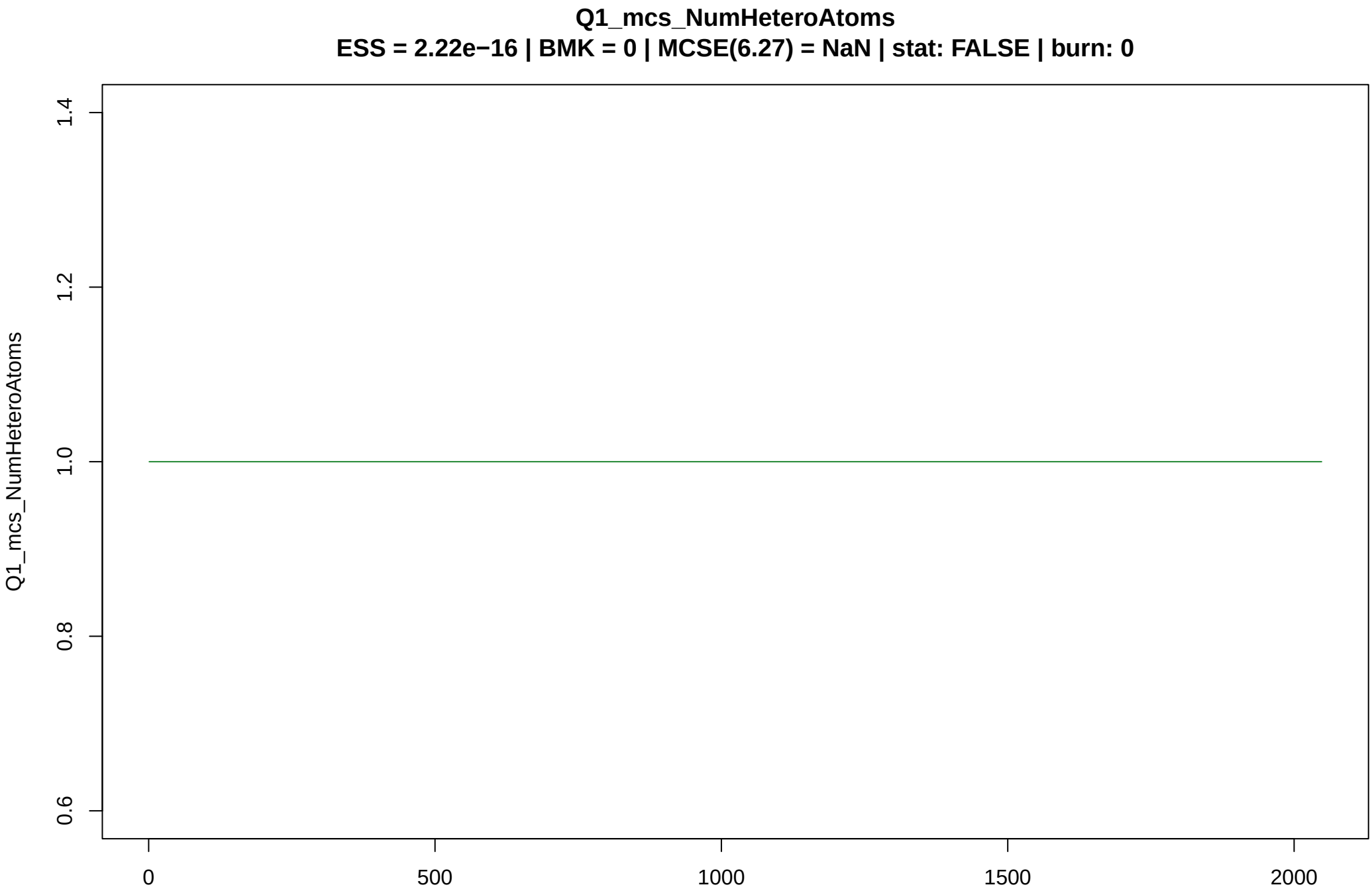

Q1_docked_HeavyAtomCount
ESS = 1630 | BMK = 0.0389 | MCSE(6.27) = 2.3 | stat: FALSE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

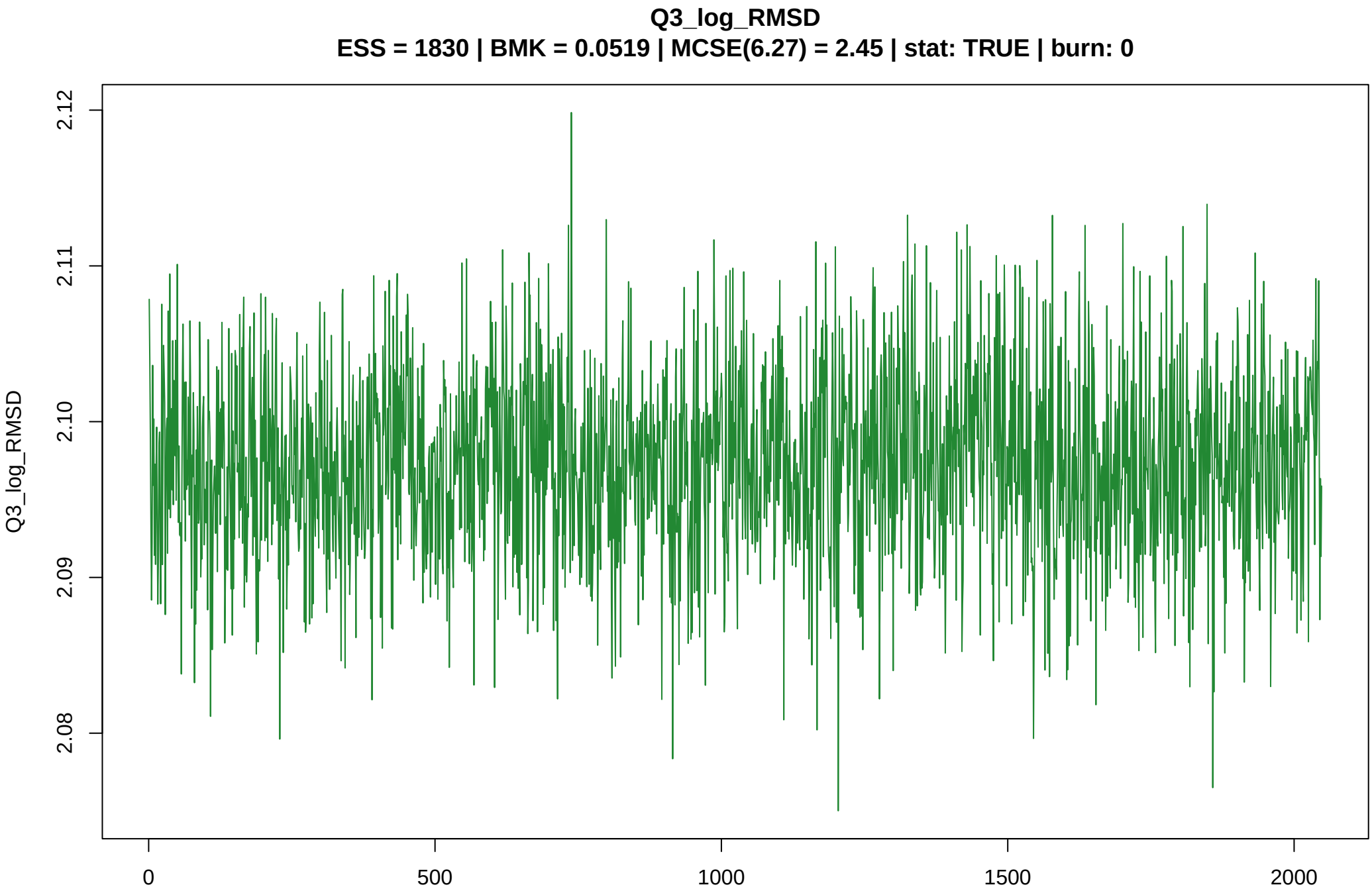

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

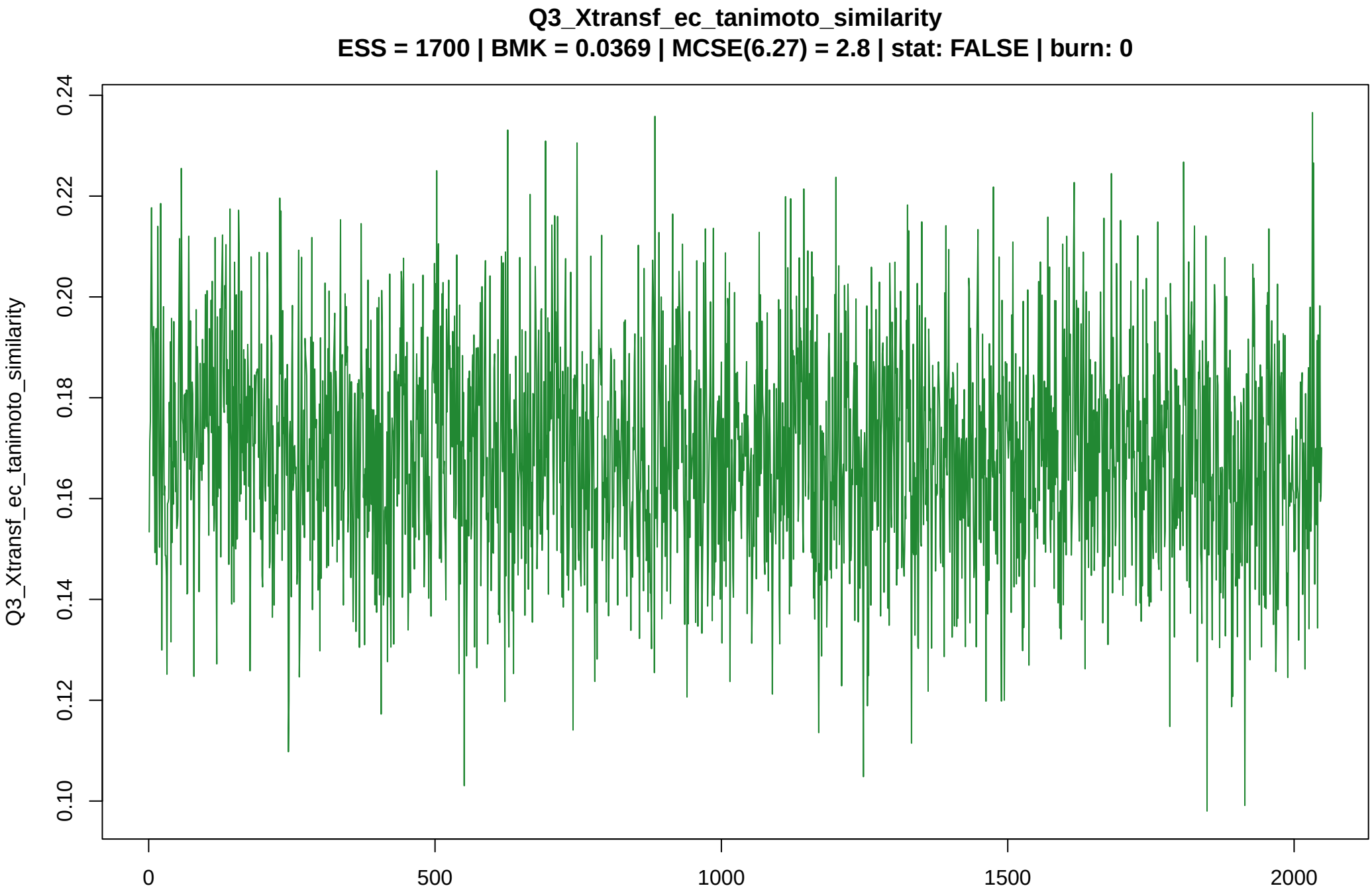

Q1_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_template_HeavyAtomCount
15
20
25
30
0
500
1000
1500
2000

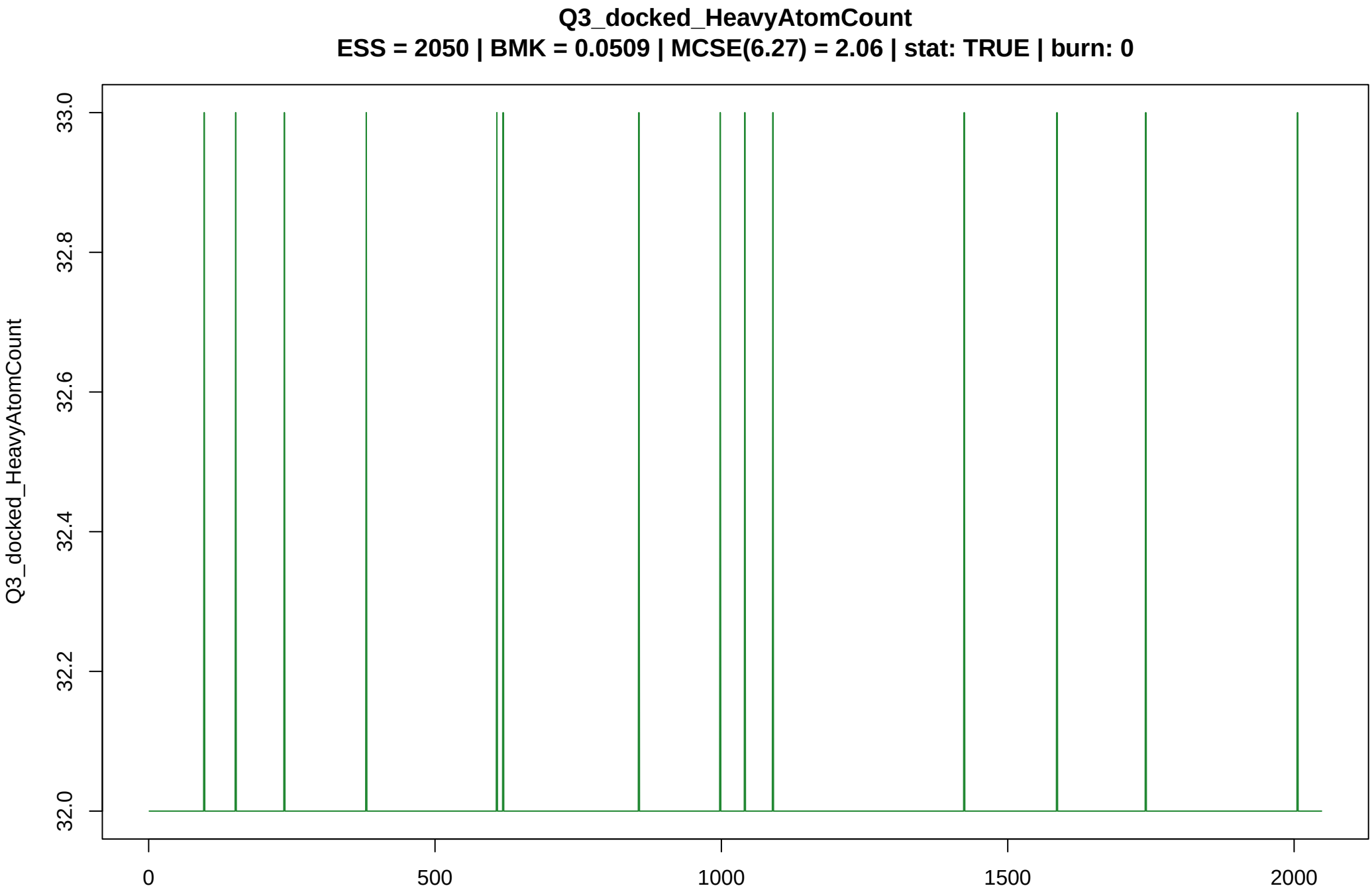

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

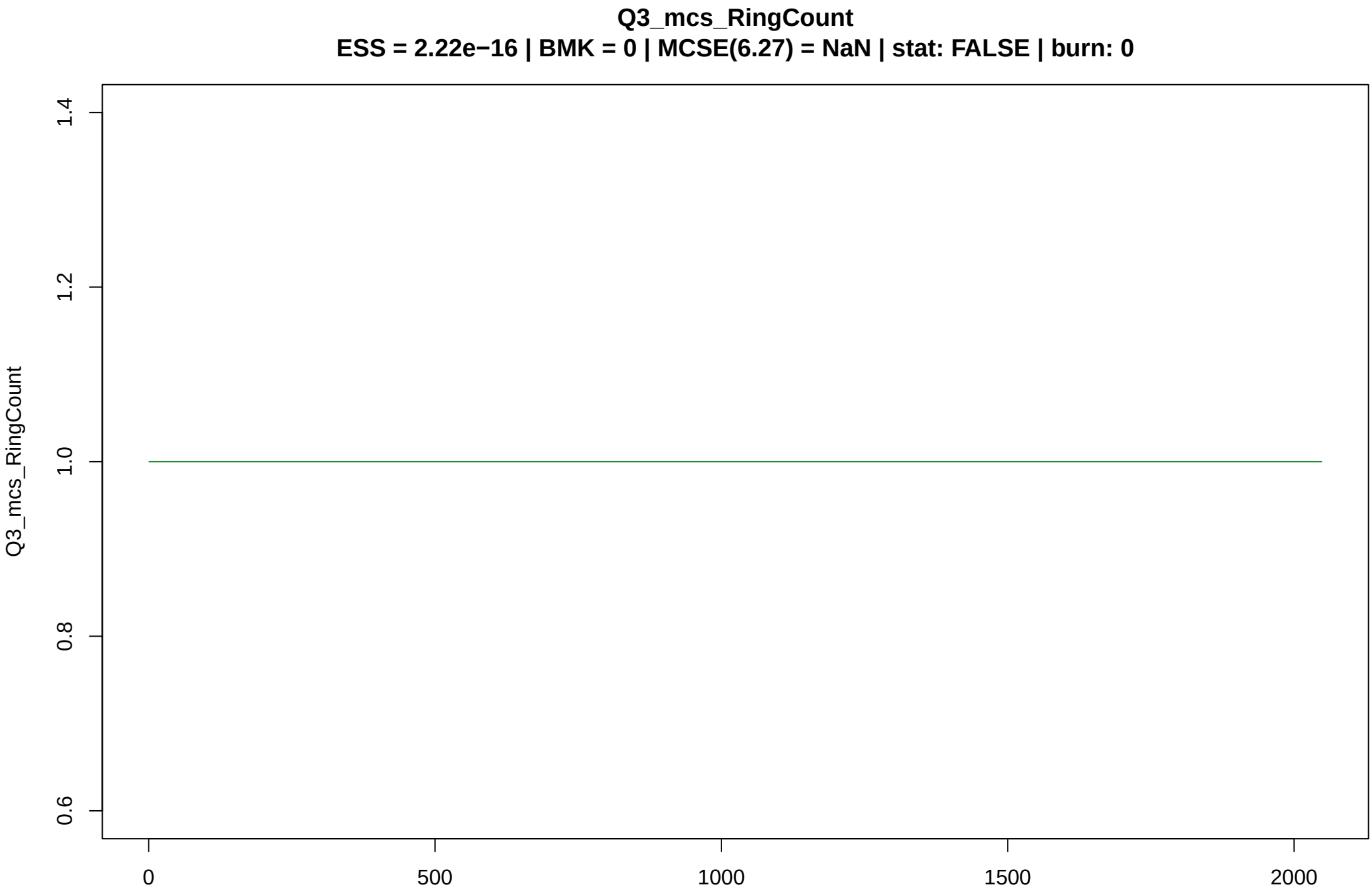

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

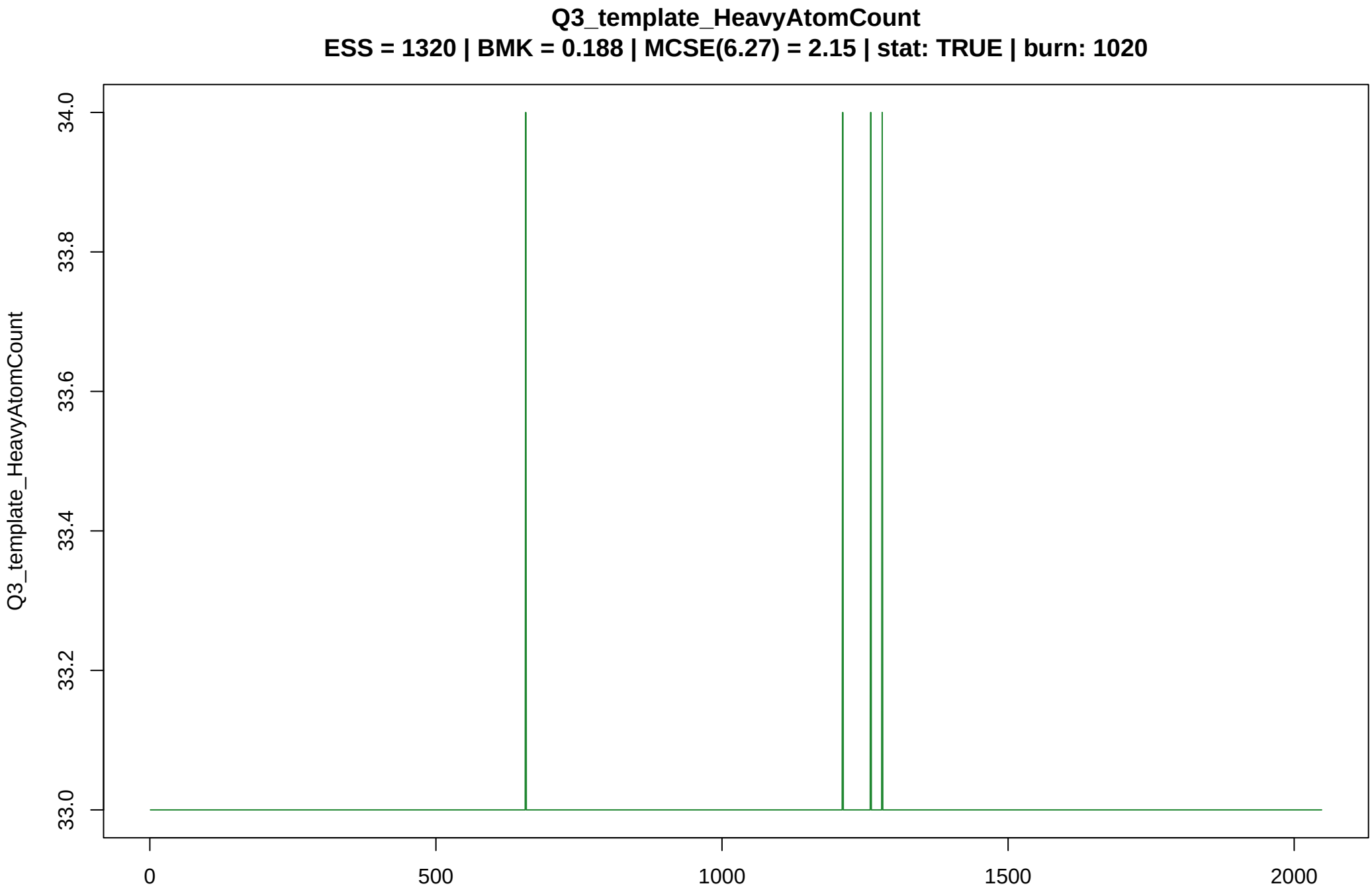

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

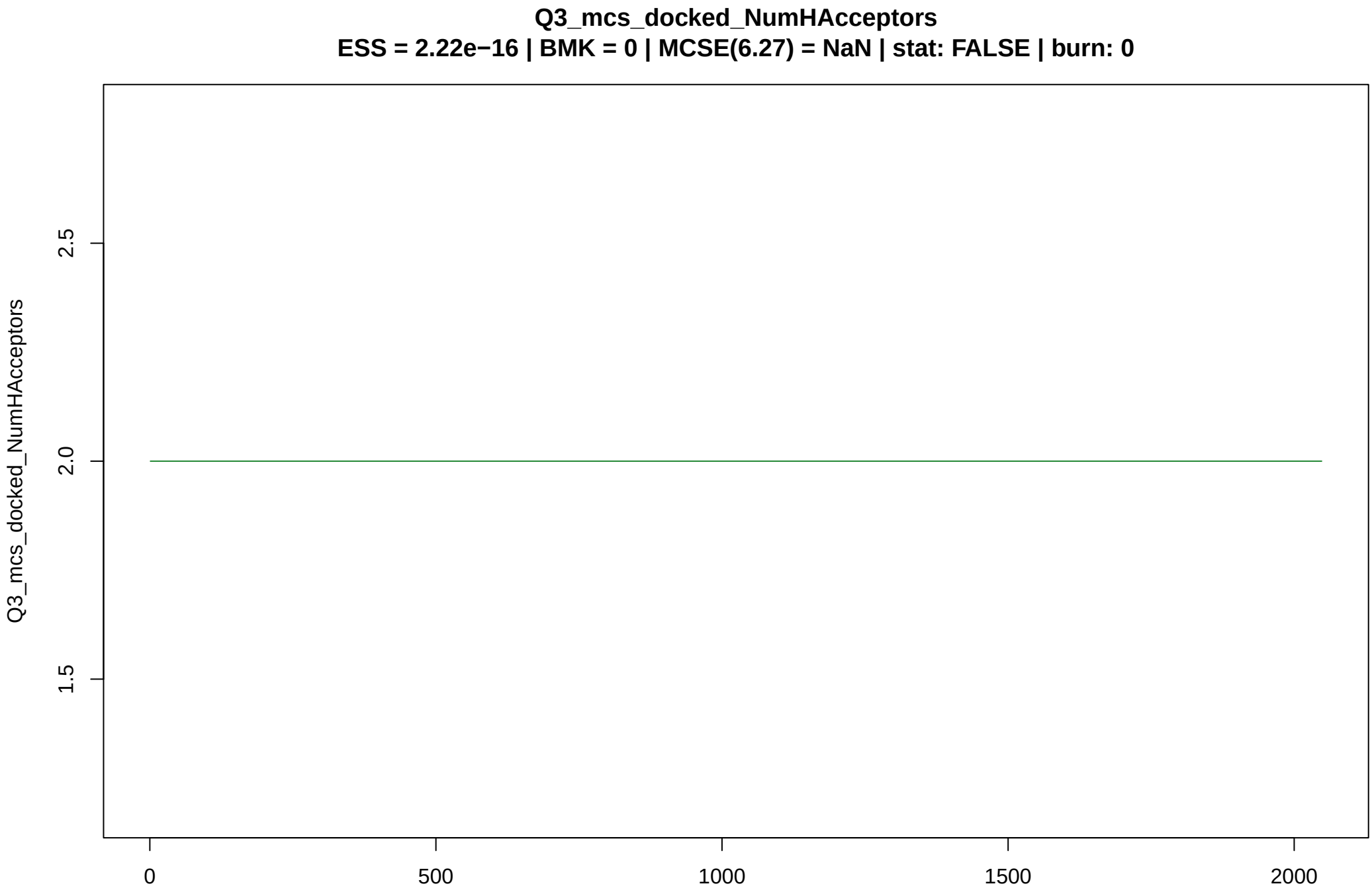

Q3_log_RMSD
ESS = 1830 | BMK = 0.0519 | MCSE(6.27) = 2.45 | stat: TRUE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
2.12
0
500
1000
1500
2000

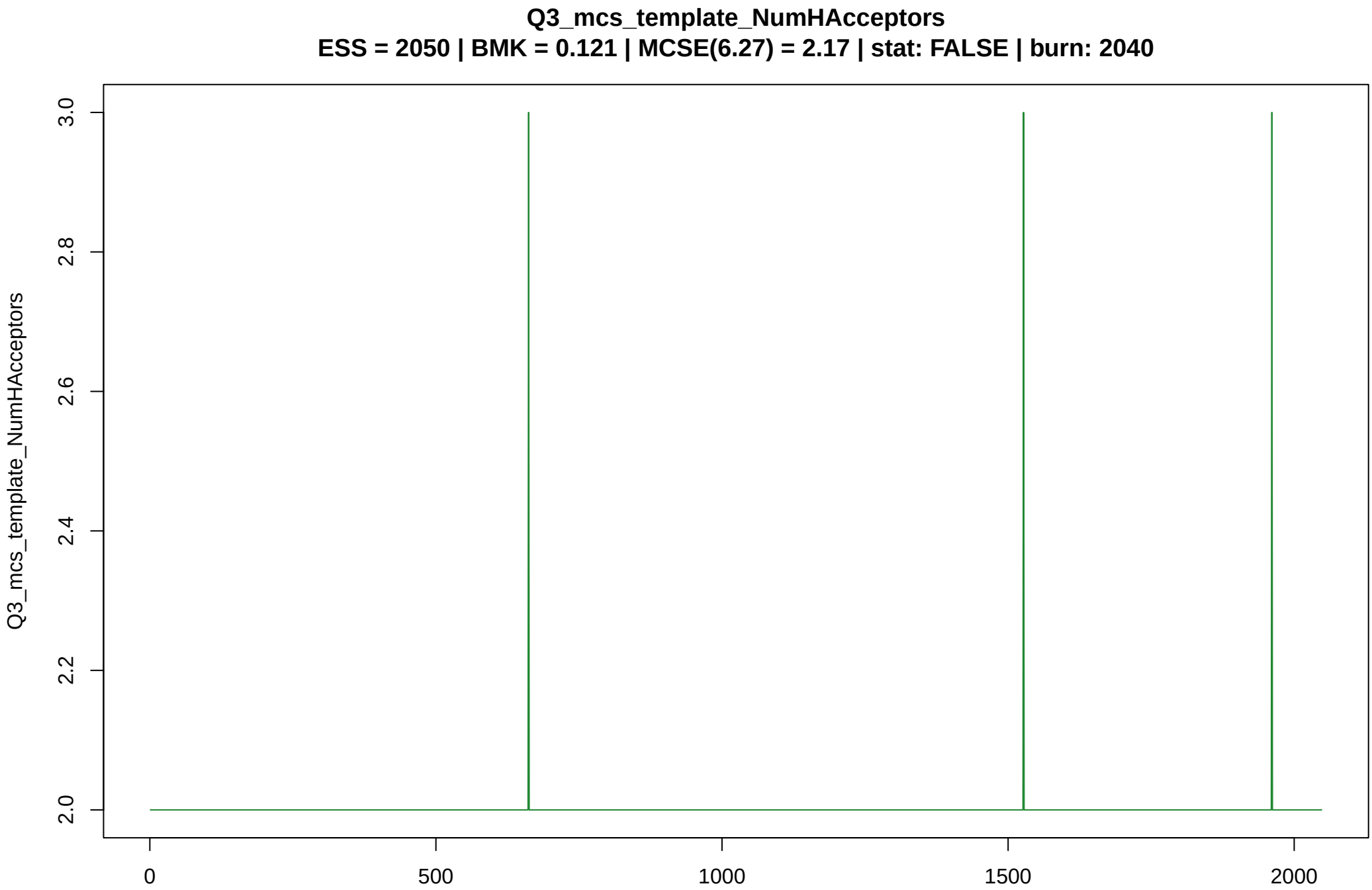

Q3_Xtransf_ec_tanimoto_similarity
ESS = 1700 | BMK = 0.0369 | MCSE(6.27) = 2.8 | stat: FALSE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.10
0.12
0.14
0.16
0.18
0.20
0.22
0.24
0
500
1000
1500
2000

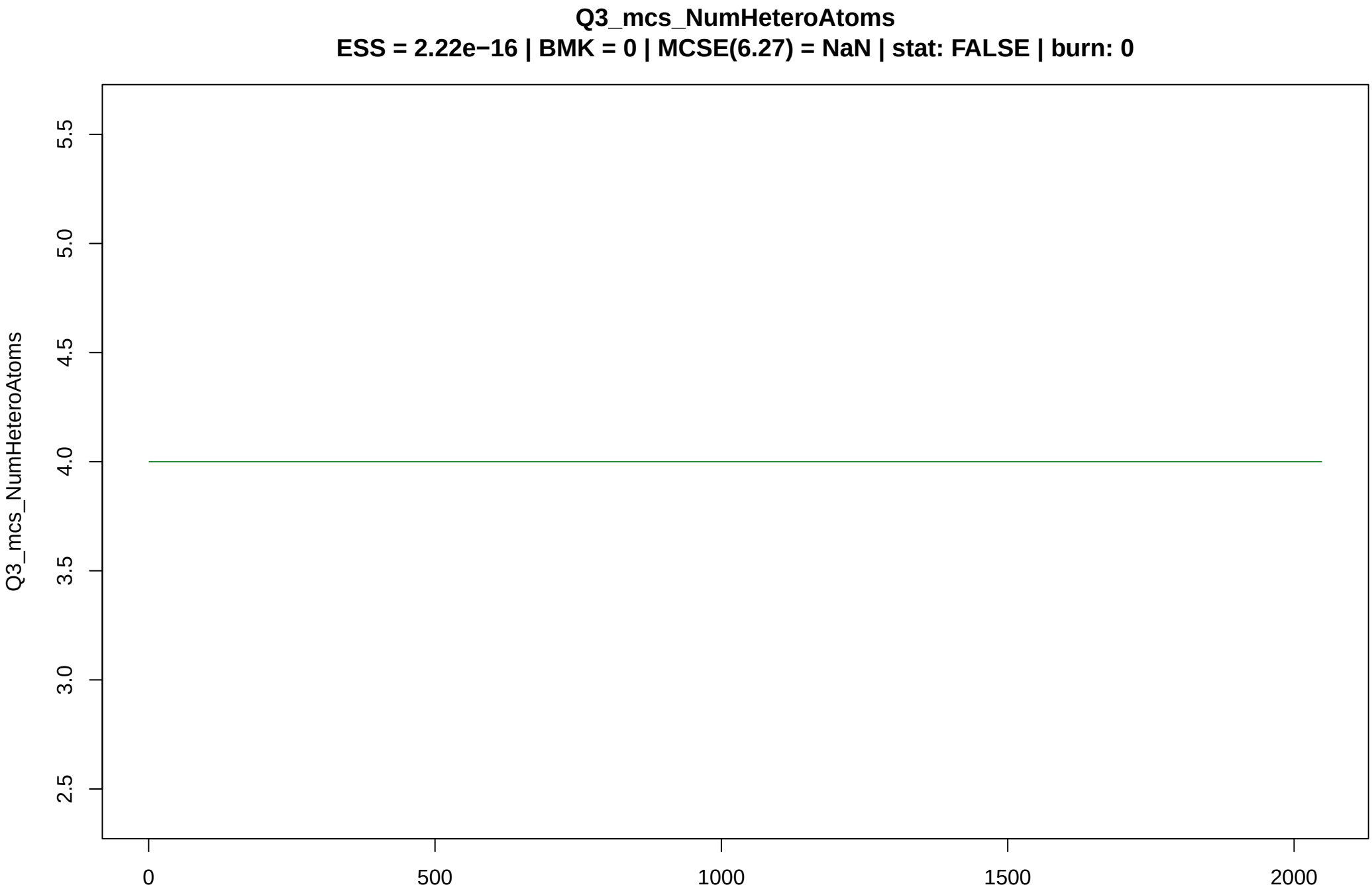

Q3_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0509 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

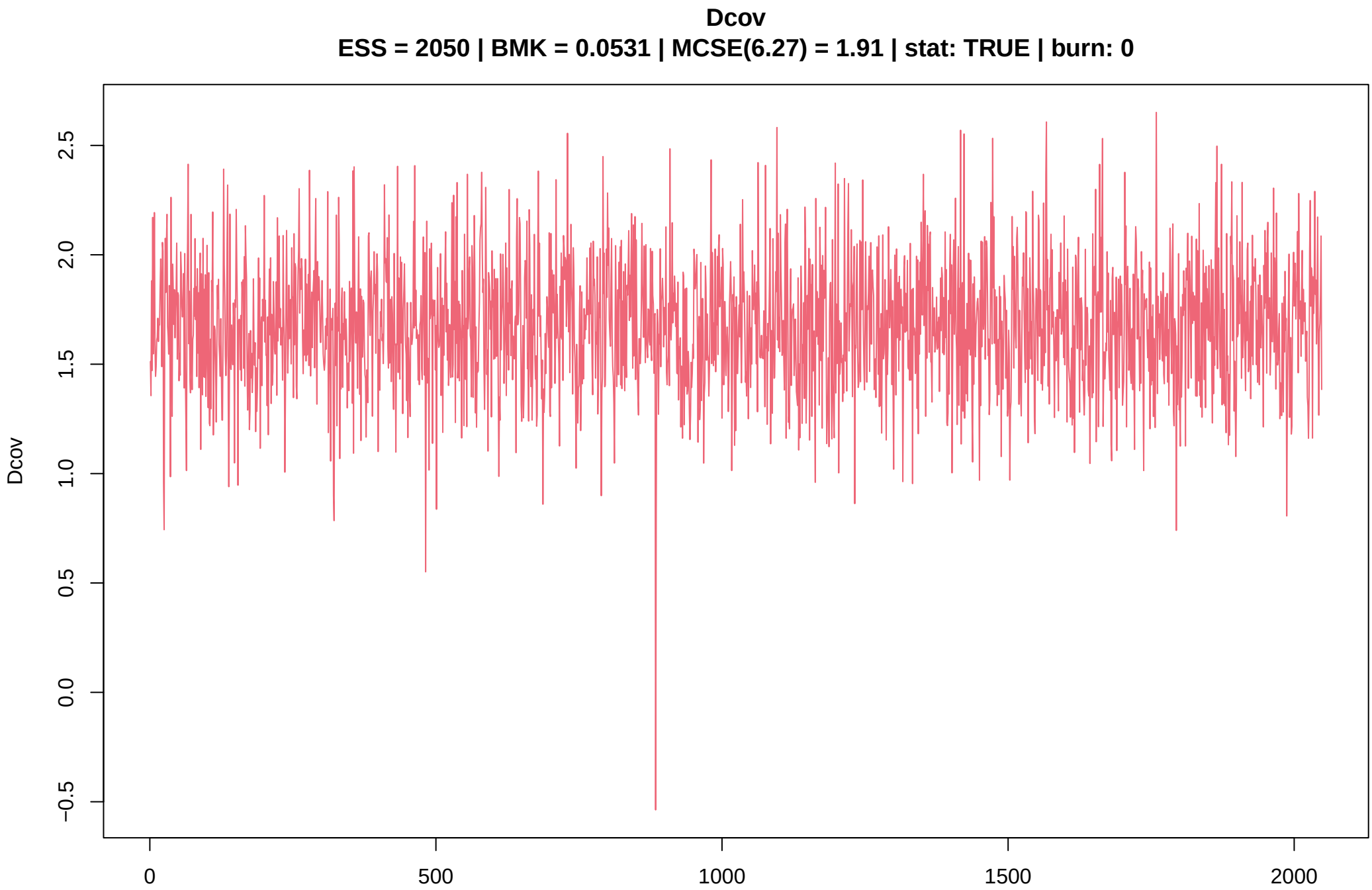

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

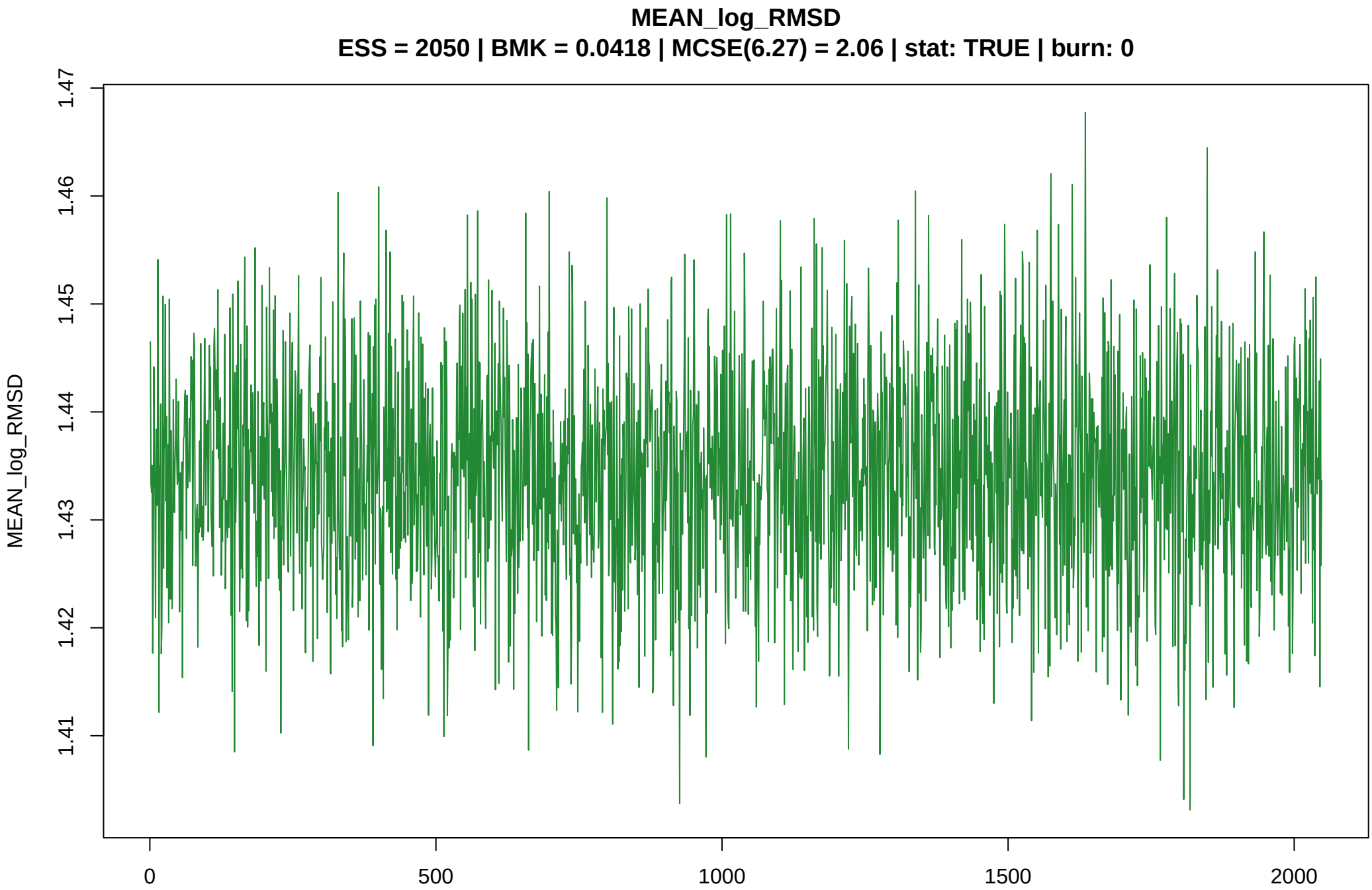

Q3_template_HeavyAtomCount
ESS = 1320 | BMK = 0.188 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 1020
Q3_template_HeavyAtomCount
34.0
33.8
33.6
33.4
33.2
33.0
0
500
1000
1500
2000

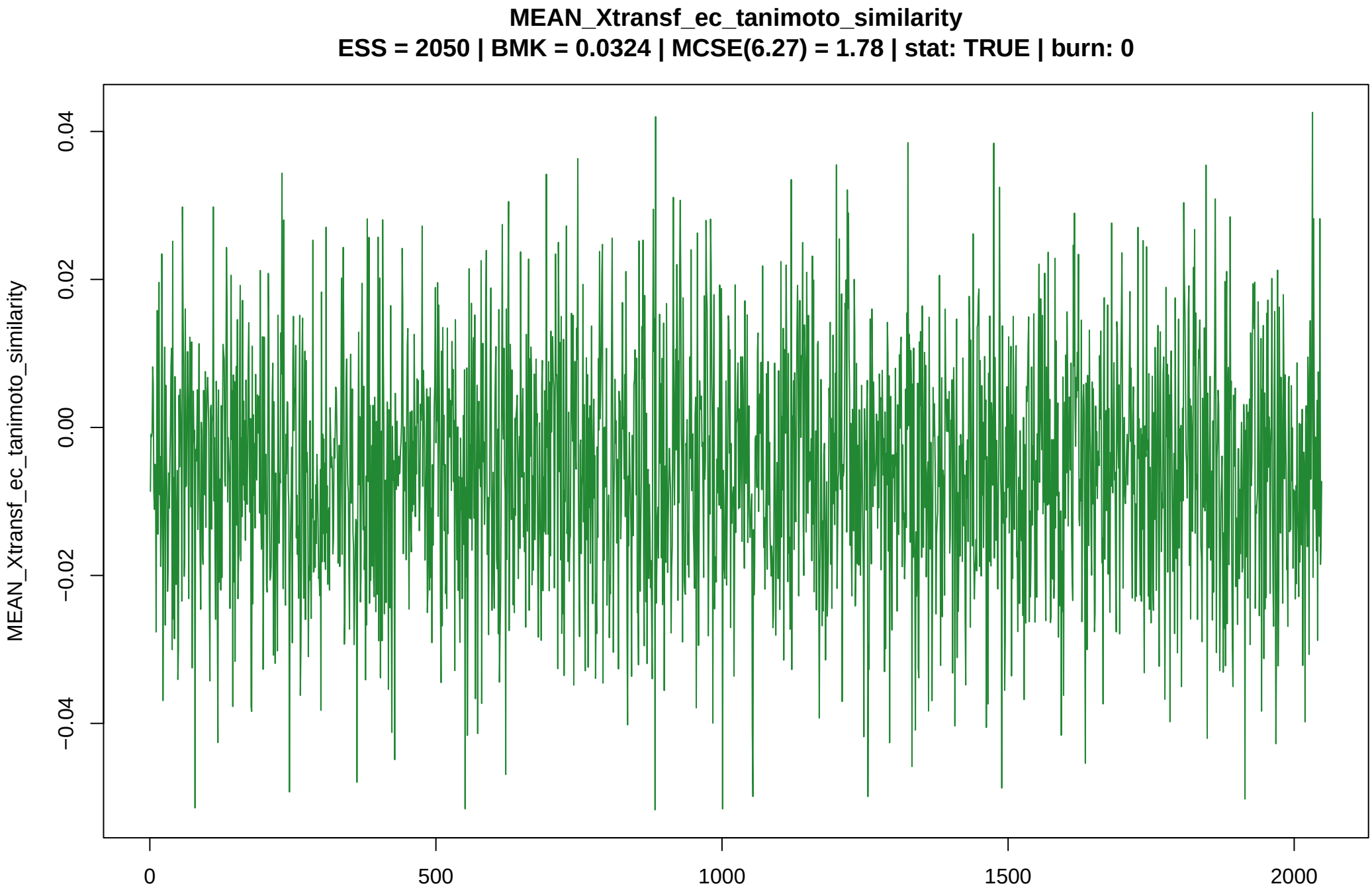

Q3_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_docked_NumHAcceptors
1.5
2.0
2.5
0
500
1000
1500
2000

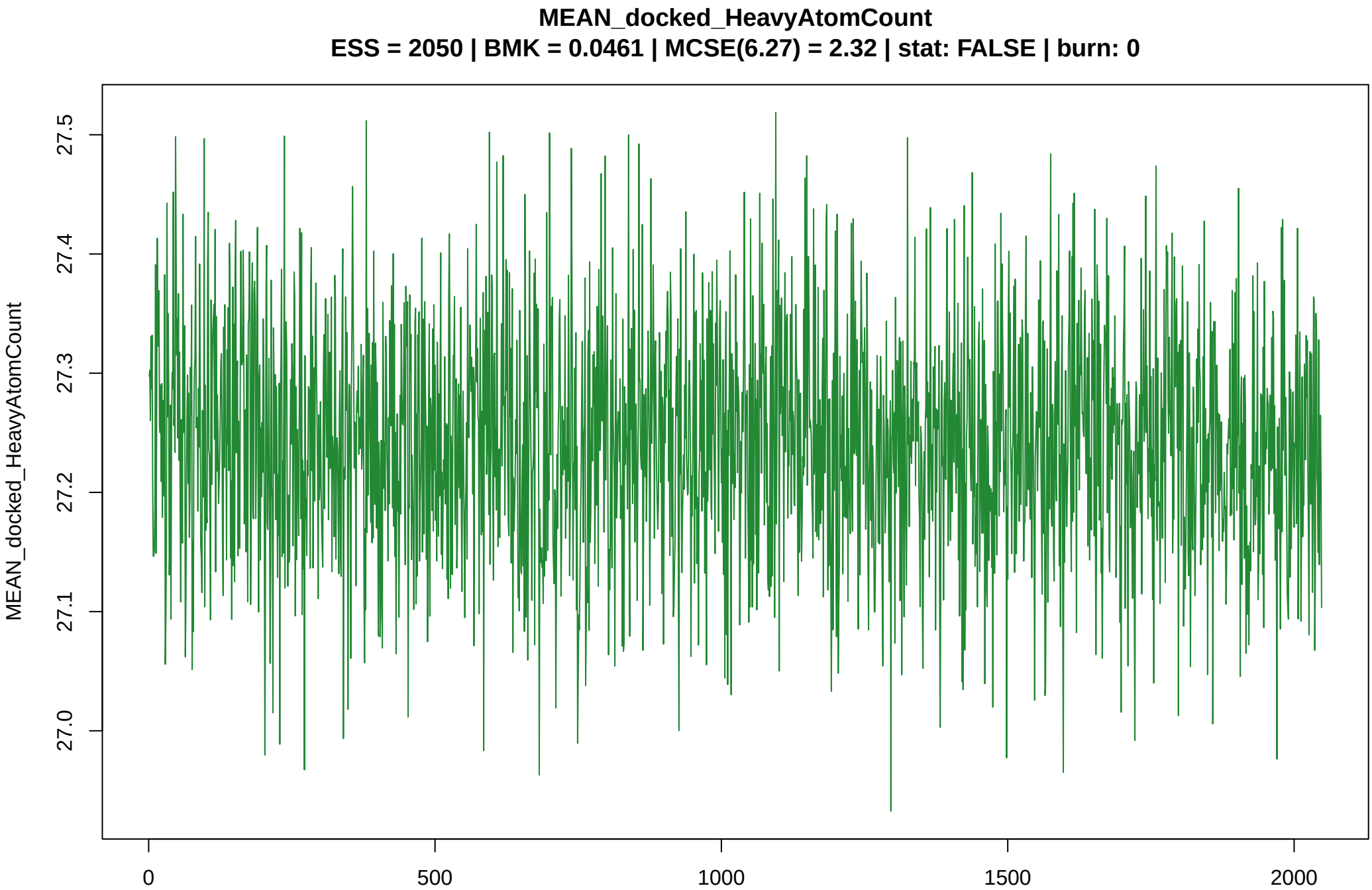

Q3_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.121 | MCSE(6.27) = 2.17 | stat: FALSE | burn: 2040
Q3_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

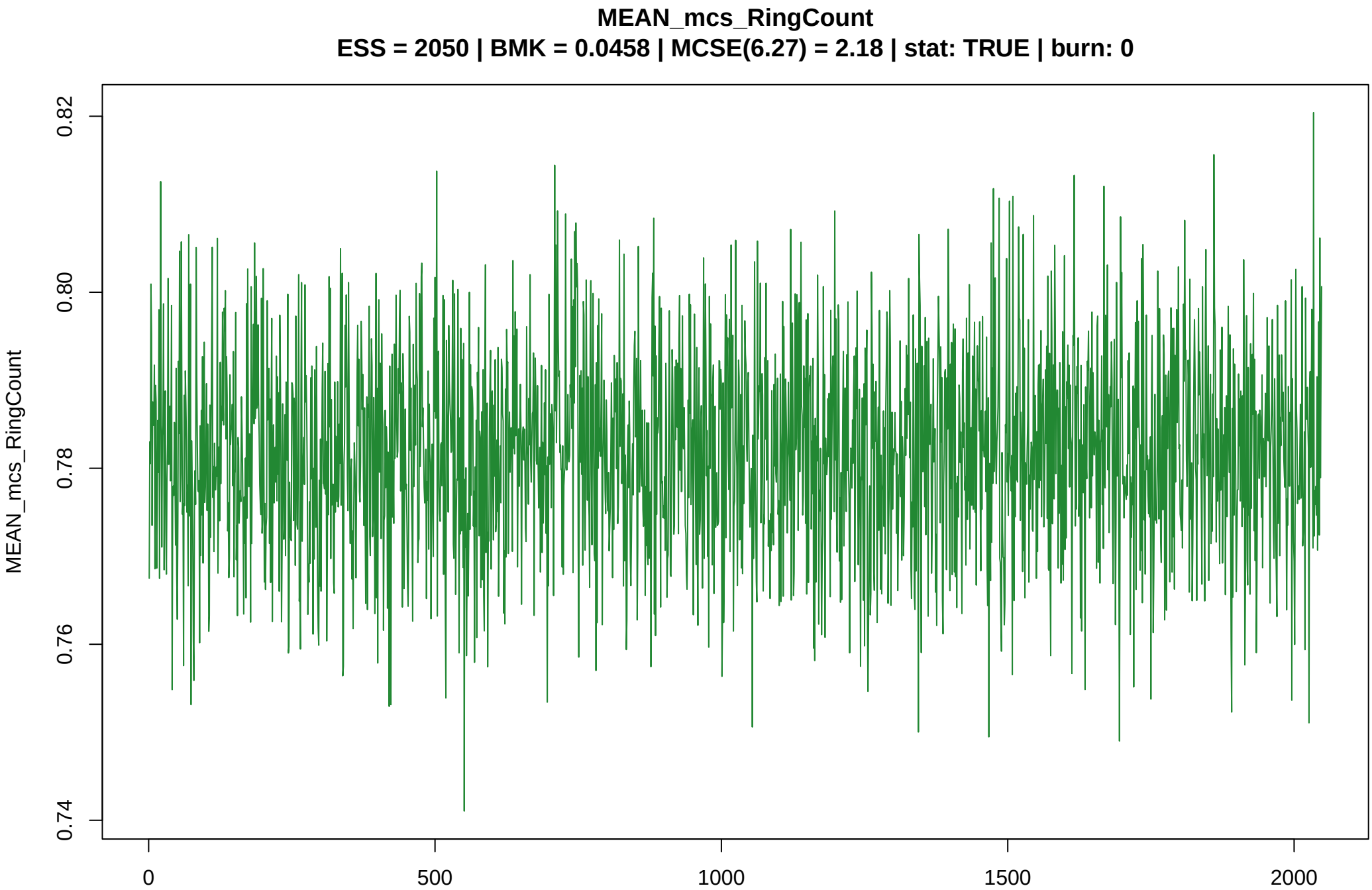

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

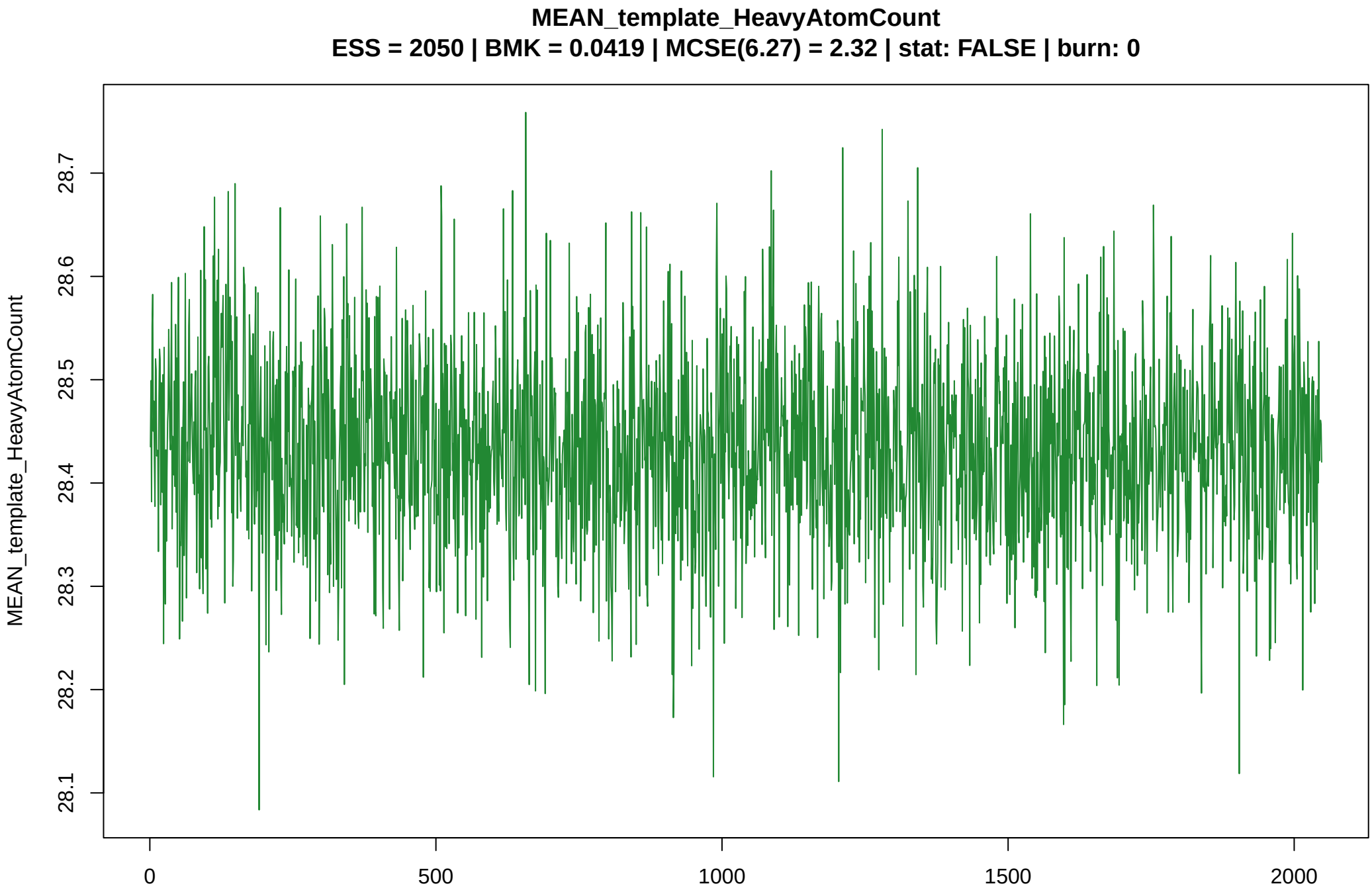

Dcov
ESS = 2050 | BMK = 0.0531 | MCSE(6.27) = 1.91 | stat: TRUE | burn: 0
Dcov
−0.5
0.0
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000

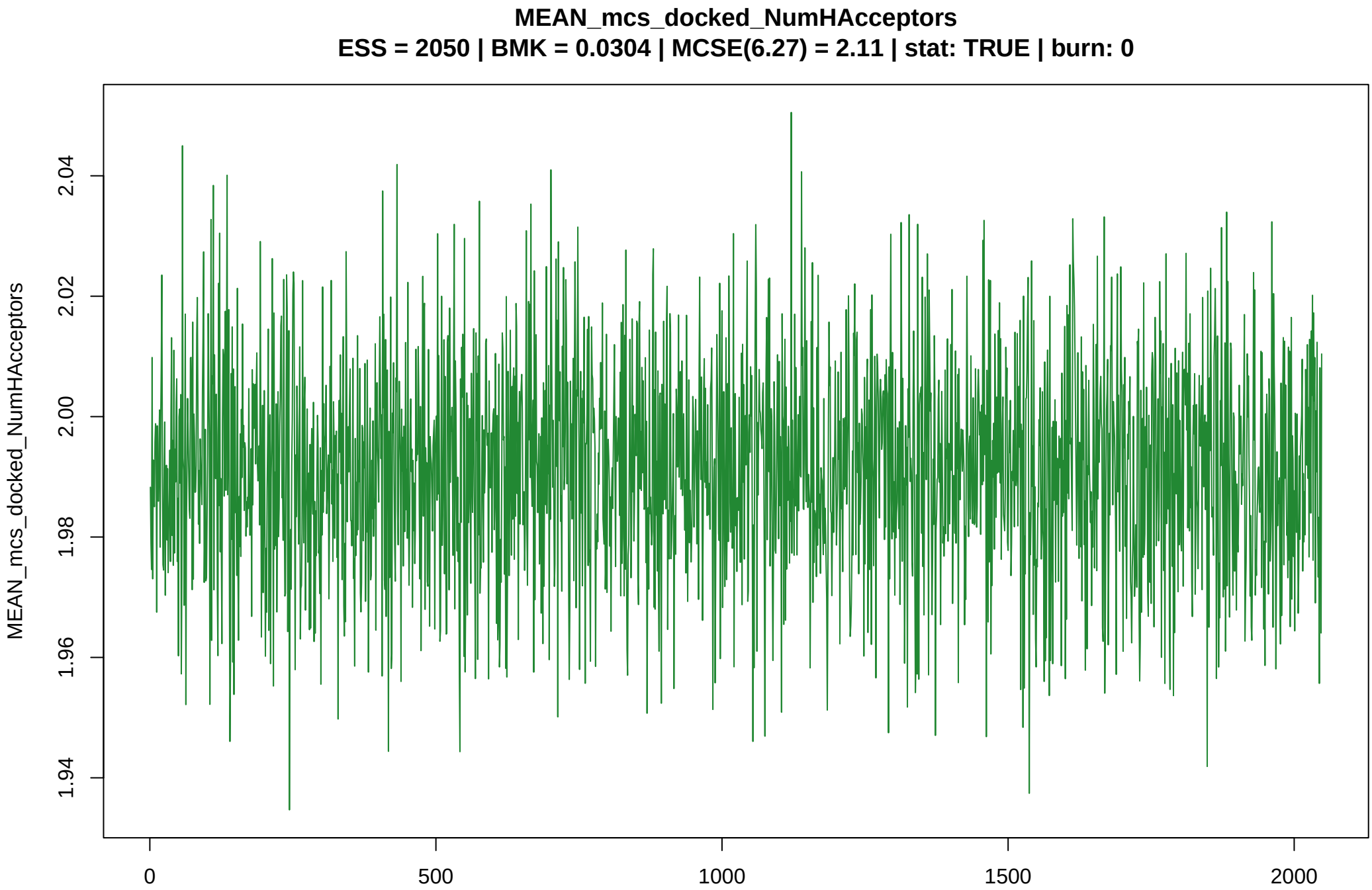

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.06 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.41
1.42
1.43
1.44
1.45
1.46
1.47
0
500
1000
1500
2000

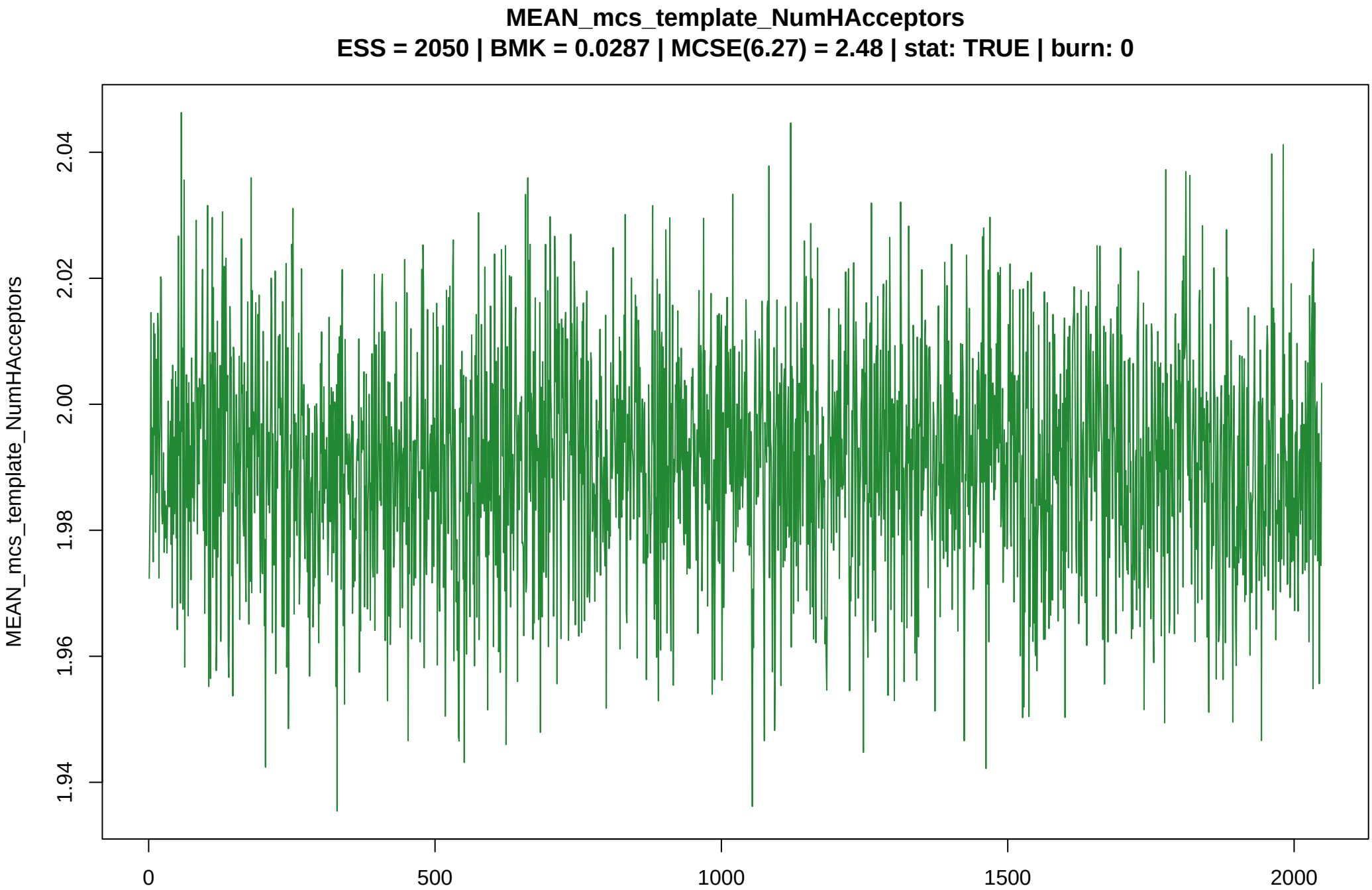

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0324 | MCSE(6.27) = 1.78 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
0
500
1000
1500
2000

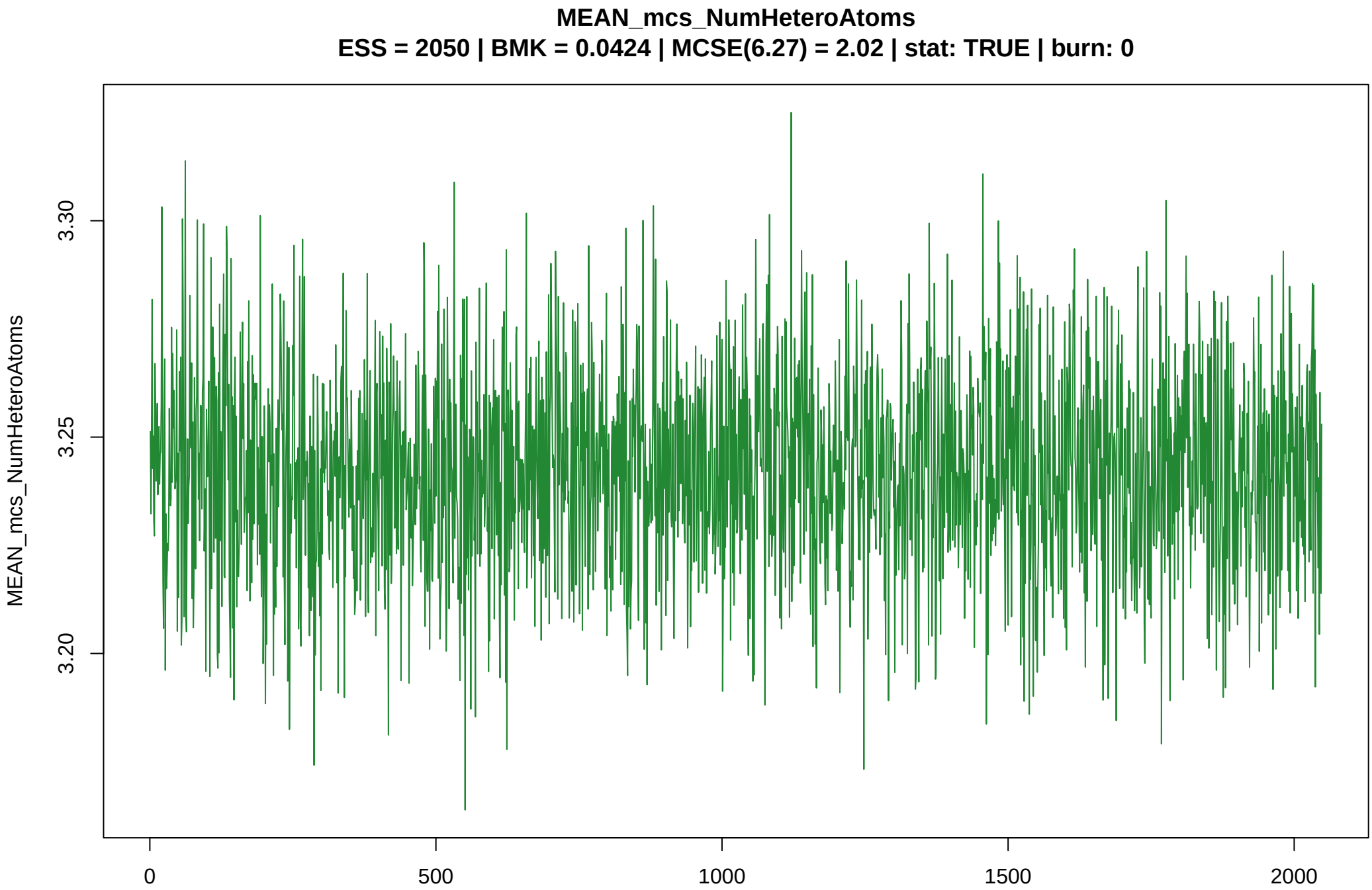

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0461 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0
MEAN_docked_HeavyAtomCount
27.0
27.1
27.2
27.3
27.4
27.5
0
500
1000
1500
2000

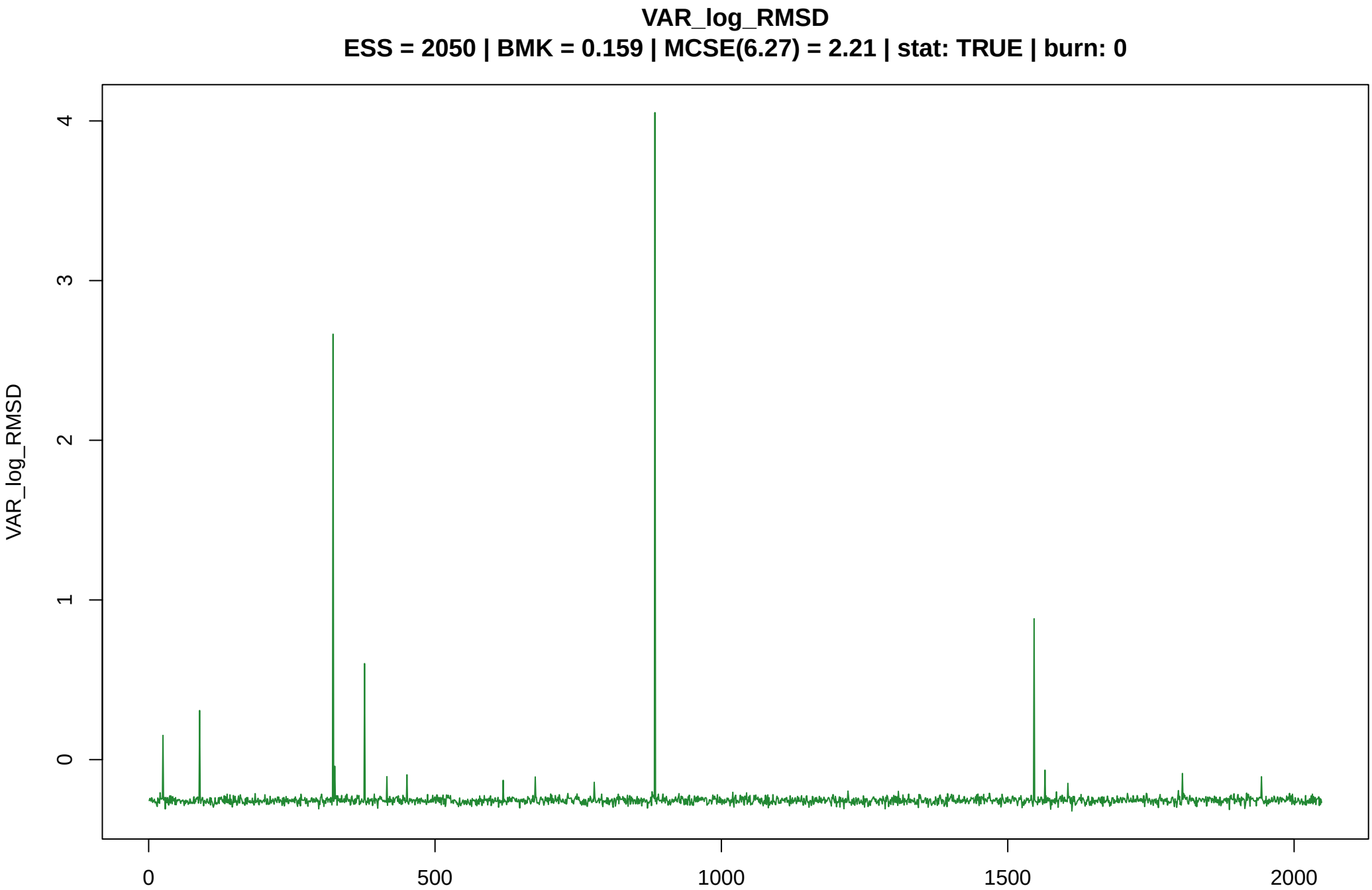

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.0458 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

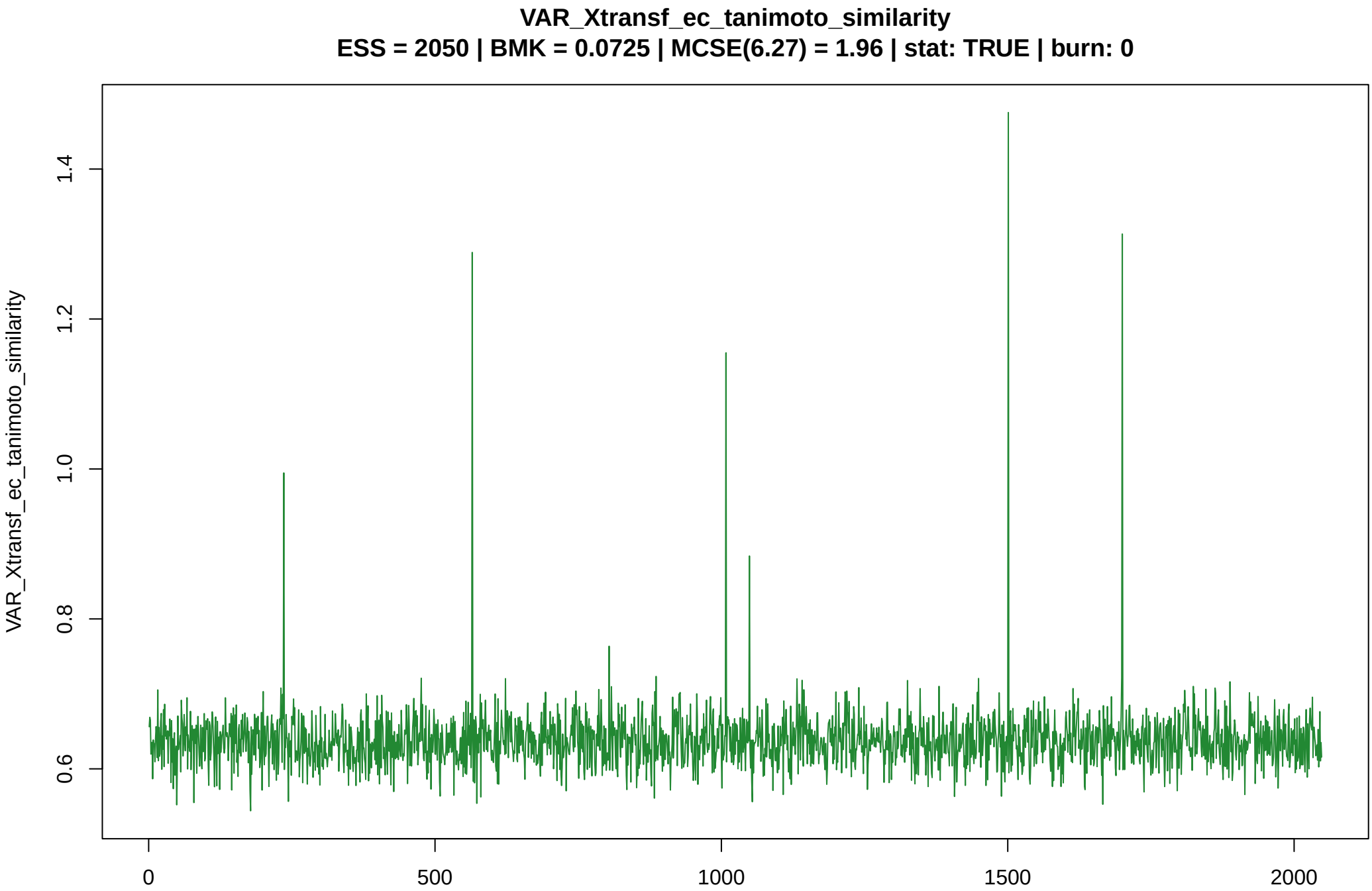

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0419 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0
MEAN_template_HeavyAtomCount
28.1
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

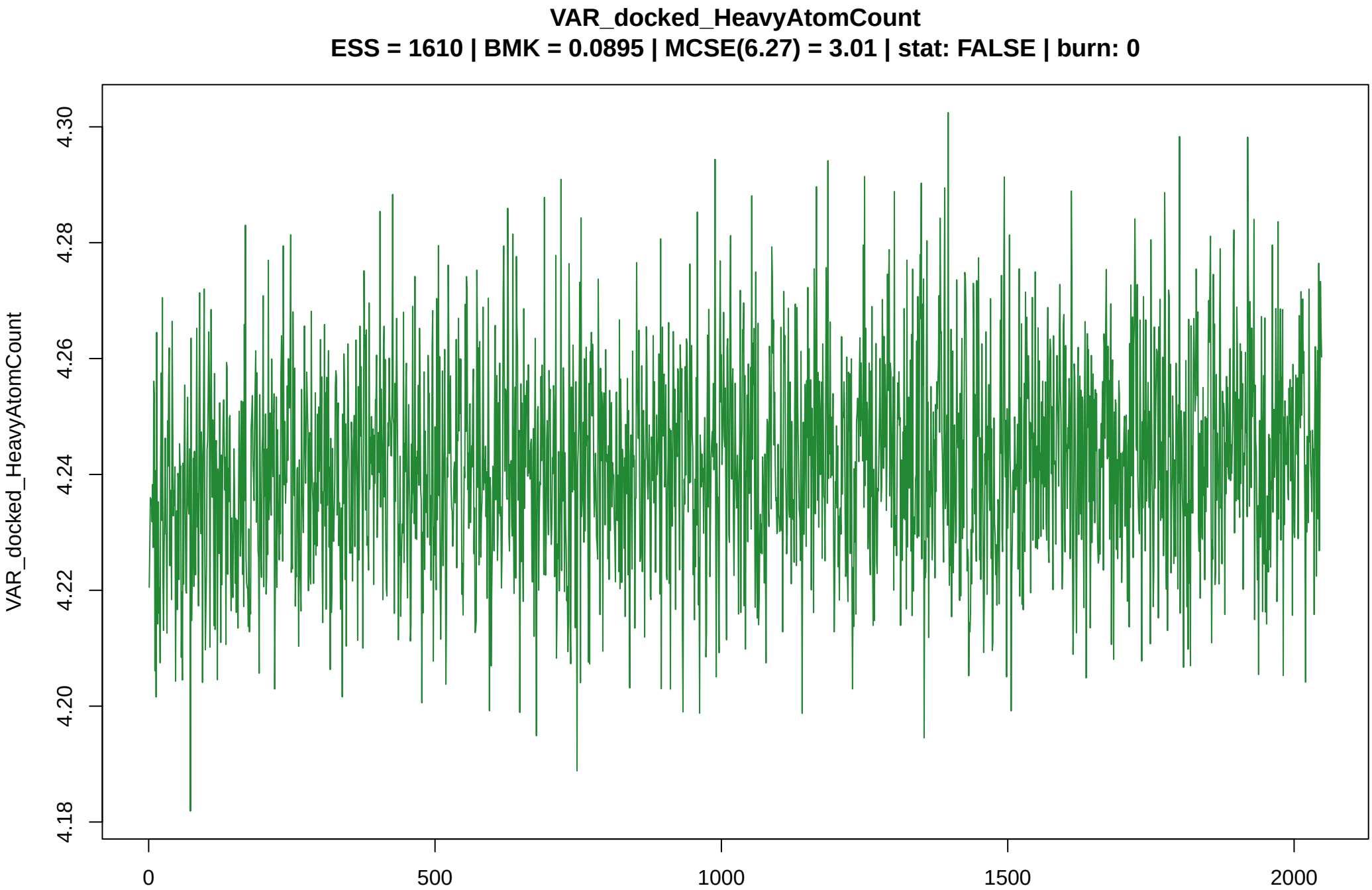

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0304 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

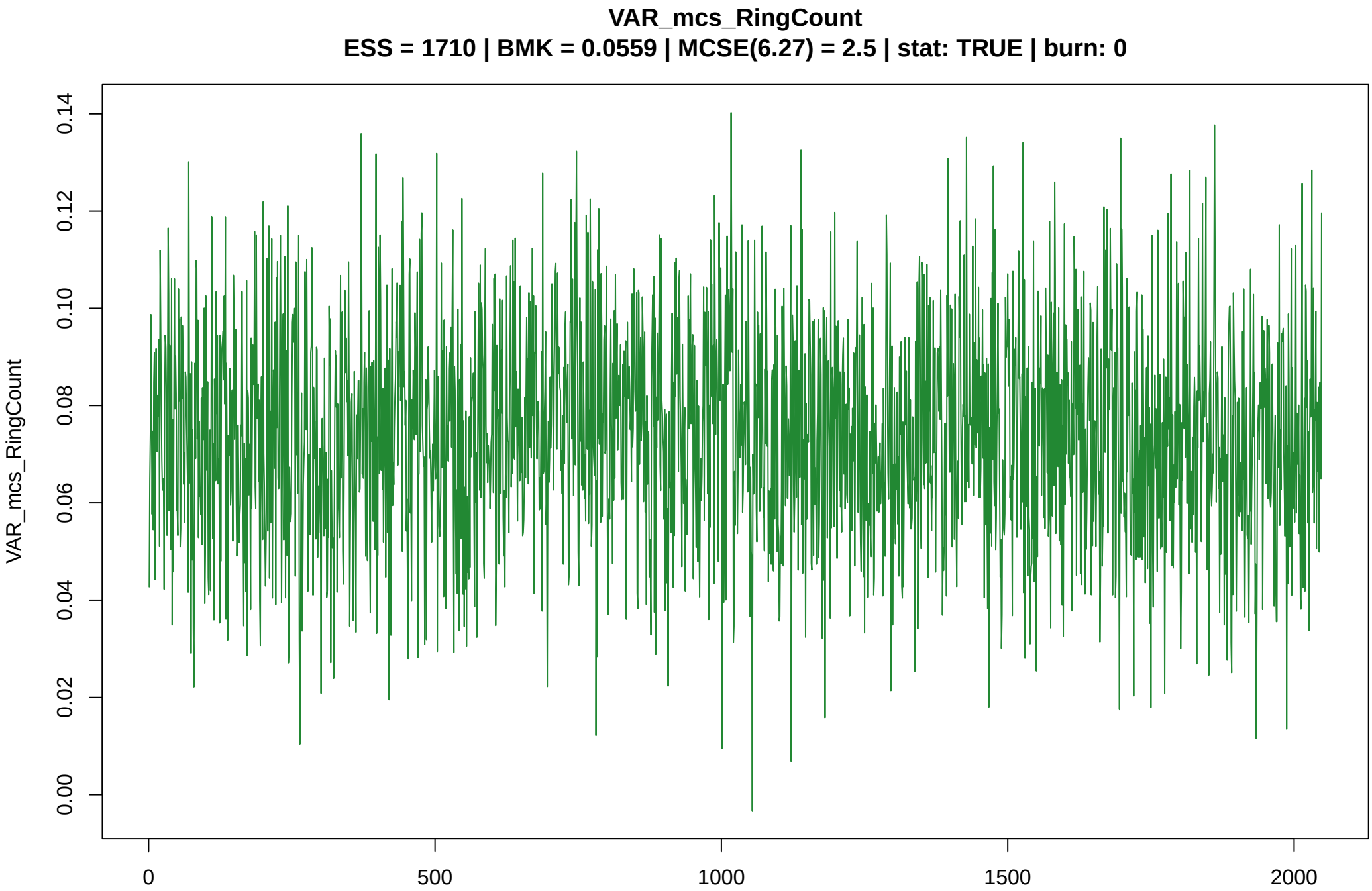

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0287 | MCSE(6.27) = 2.48 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

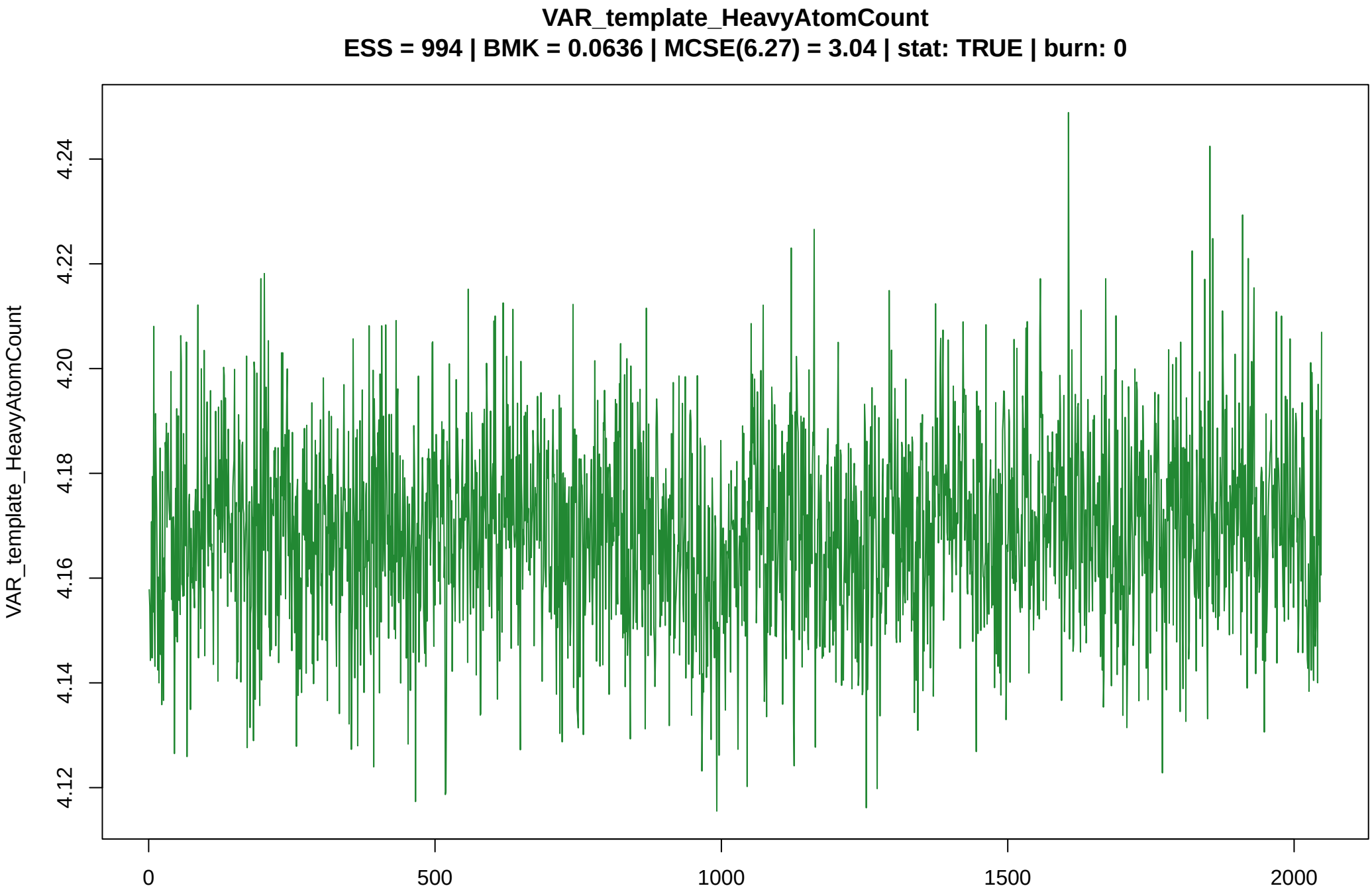

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0424 | MCSE(6.27) = 2.02 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.20
3.25
3.30
0
500
1000
1500
2000

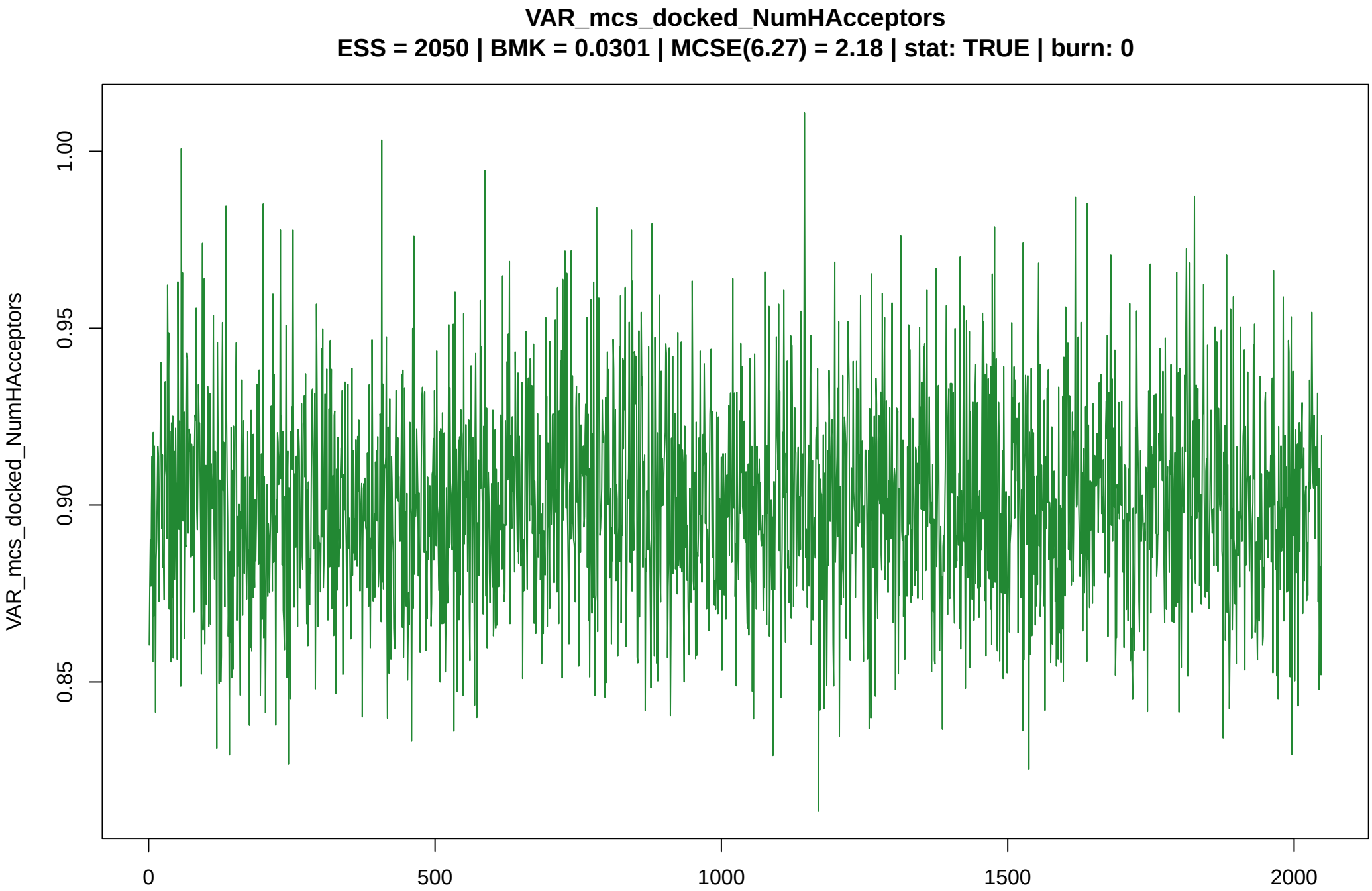

VAR_log_RMSD
ESS = 2050 | BMK = 0.159 | MCSE(6.27) = 2.21 | stat: TRUE | burn: 0
VAR_log_RMSD
0
1
2
3
4
0
500
1000
1500
2000

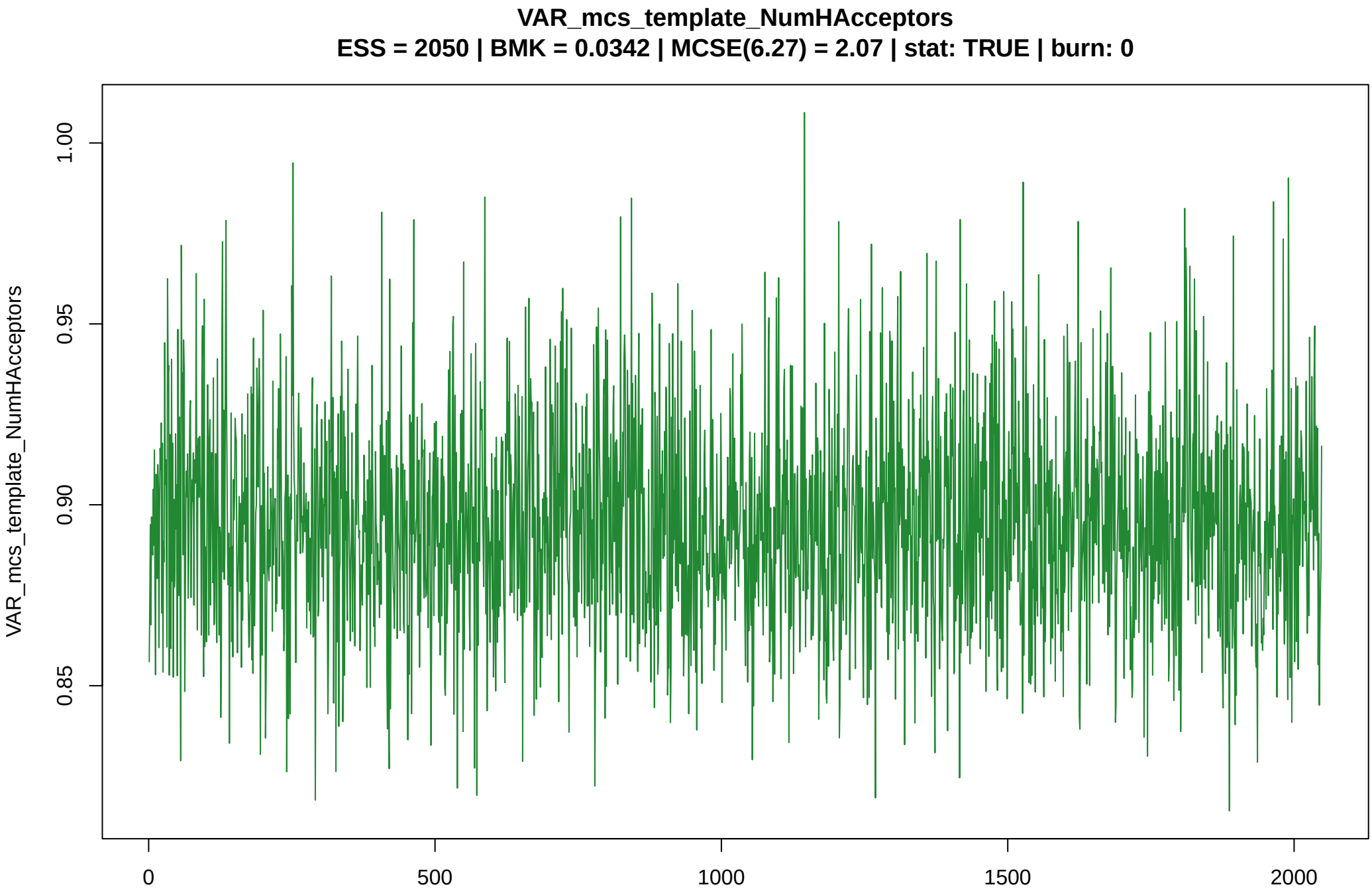

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0725 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0
VAR_Xtransf_ec_tanimoto_similarity
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

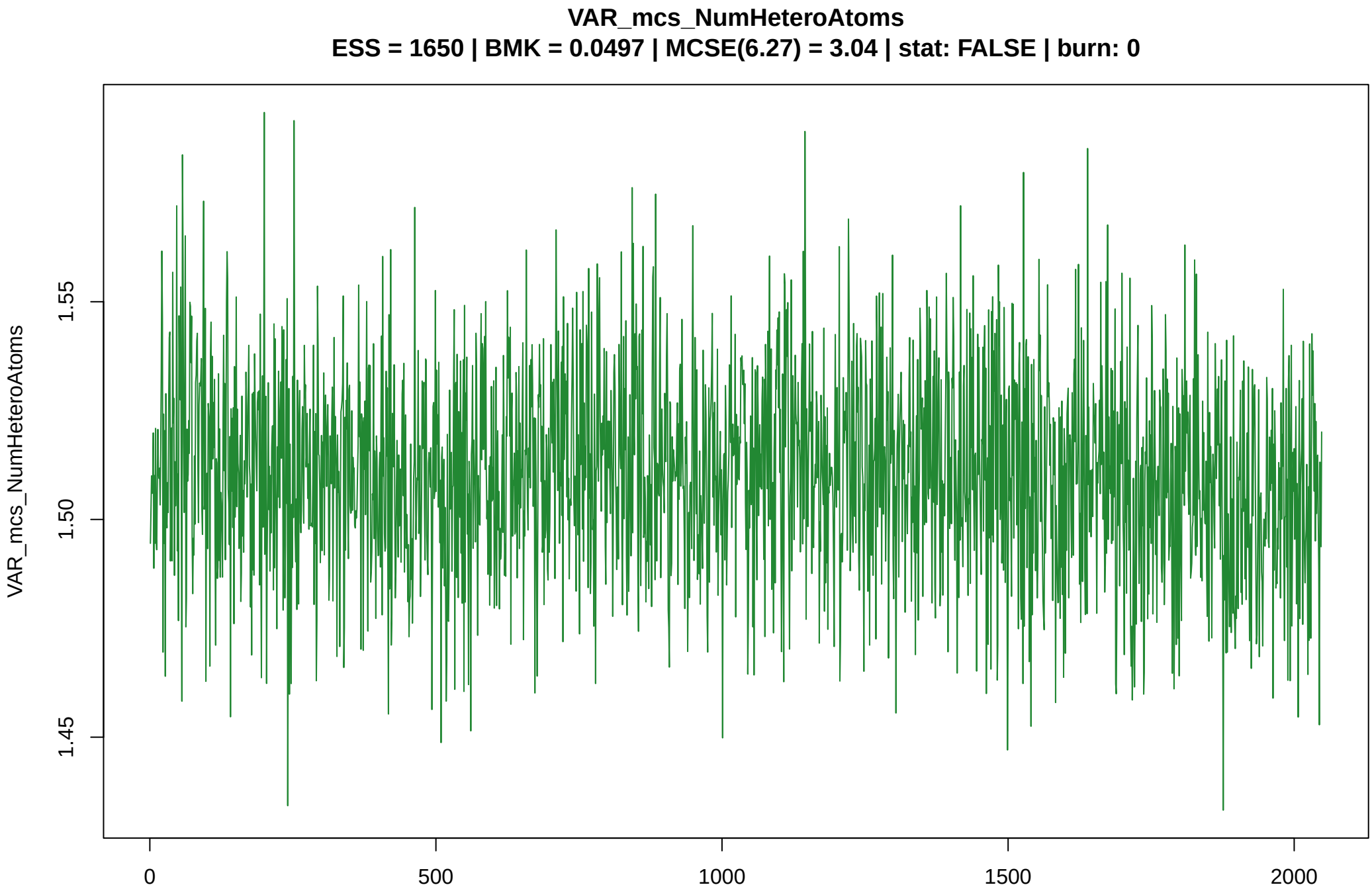

VAR_docked_HeavyAtomCount
ESS = 1610 | BMK = 0.0895 | MCSE(6.27) = 3.01 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
4.18
4.20
4.22
4.24
4.26
4.28
4.30
0
500
1000
1500
2000

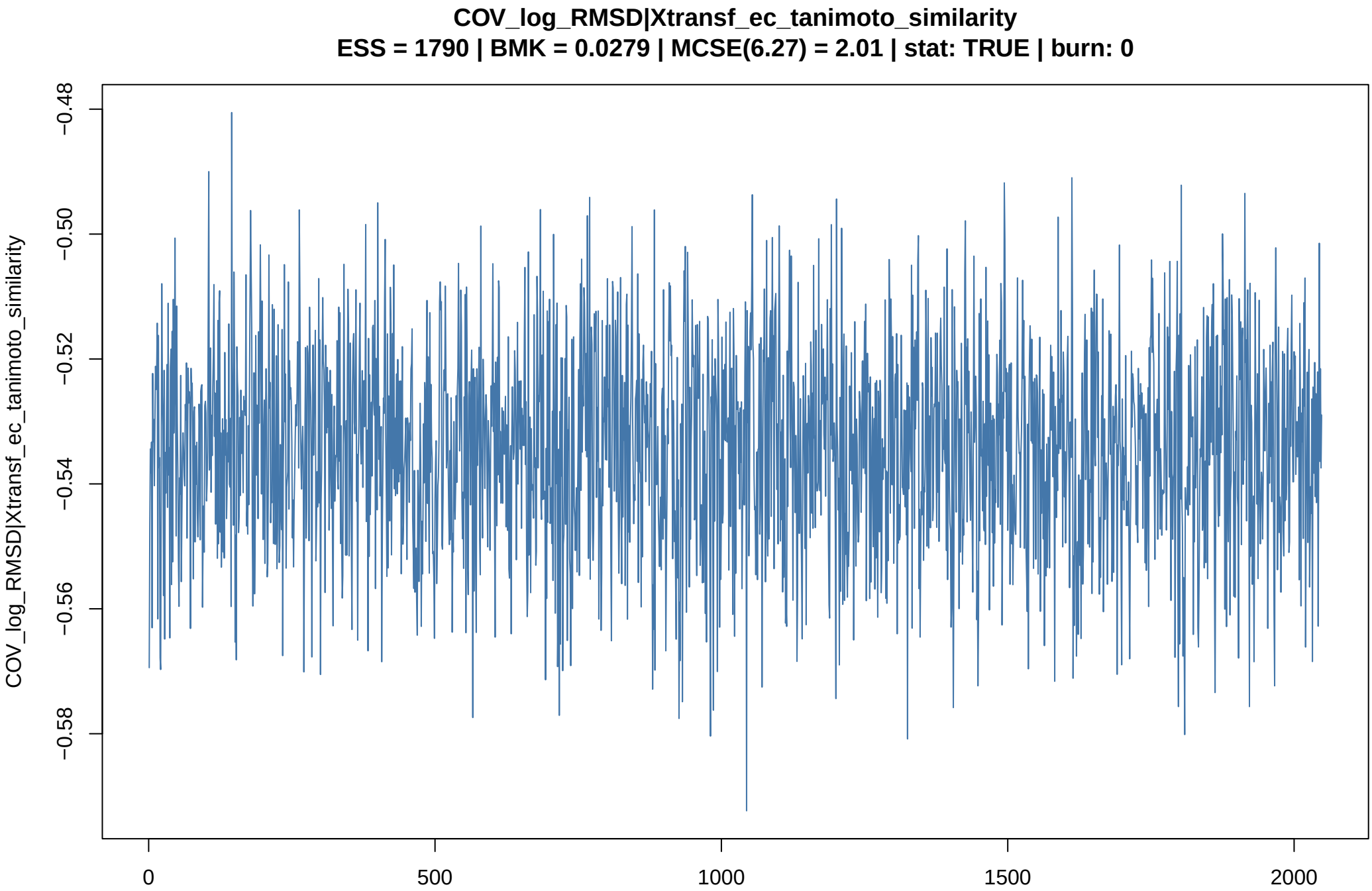

VAR_mcs_RingCount
ESS = 1710 | BMK = 0.0559 | MCSE(6.27) = 2.5 | stat: TRUE | burn: 0
VAR_mcs_RingCount
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0
500
1000
1500
2000

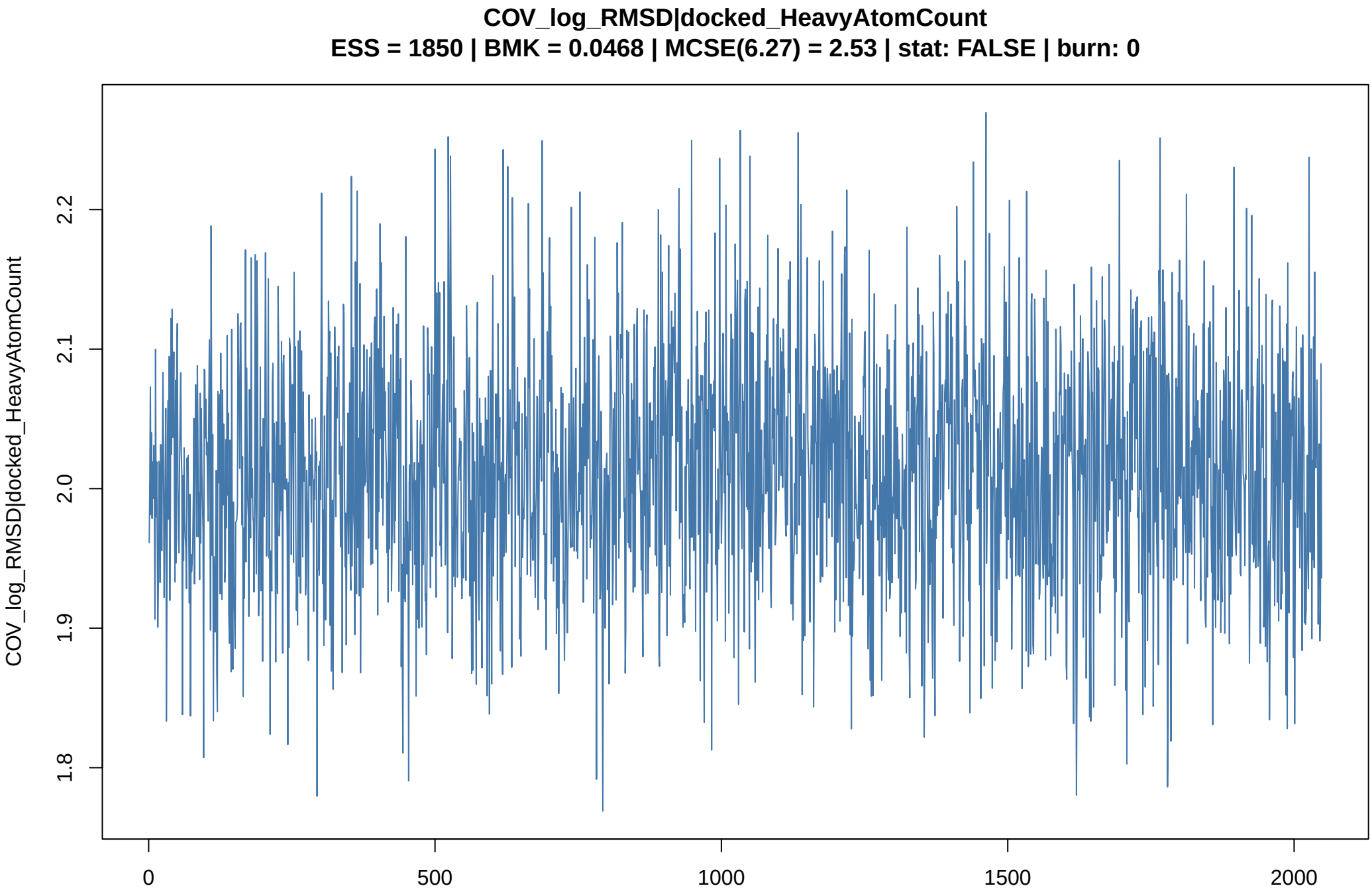

VAR_template_HeavyAtomCount
ESS = 994 | BMK = 0.0636 | MCSE(6.27) = 3.04 | stat: TRUE | burn: 0
VAR_template_HeavyAtomCount
4.12
4.14
4.16
4.18
4.20
4.22
4.24
0
500
1000
1500
2000

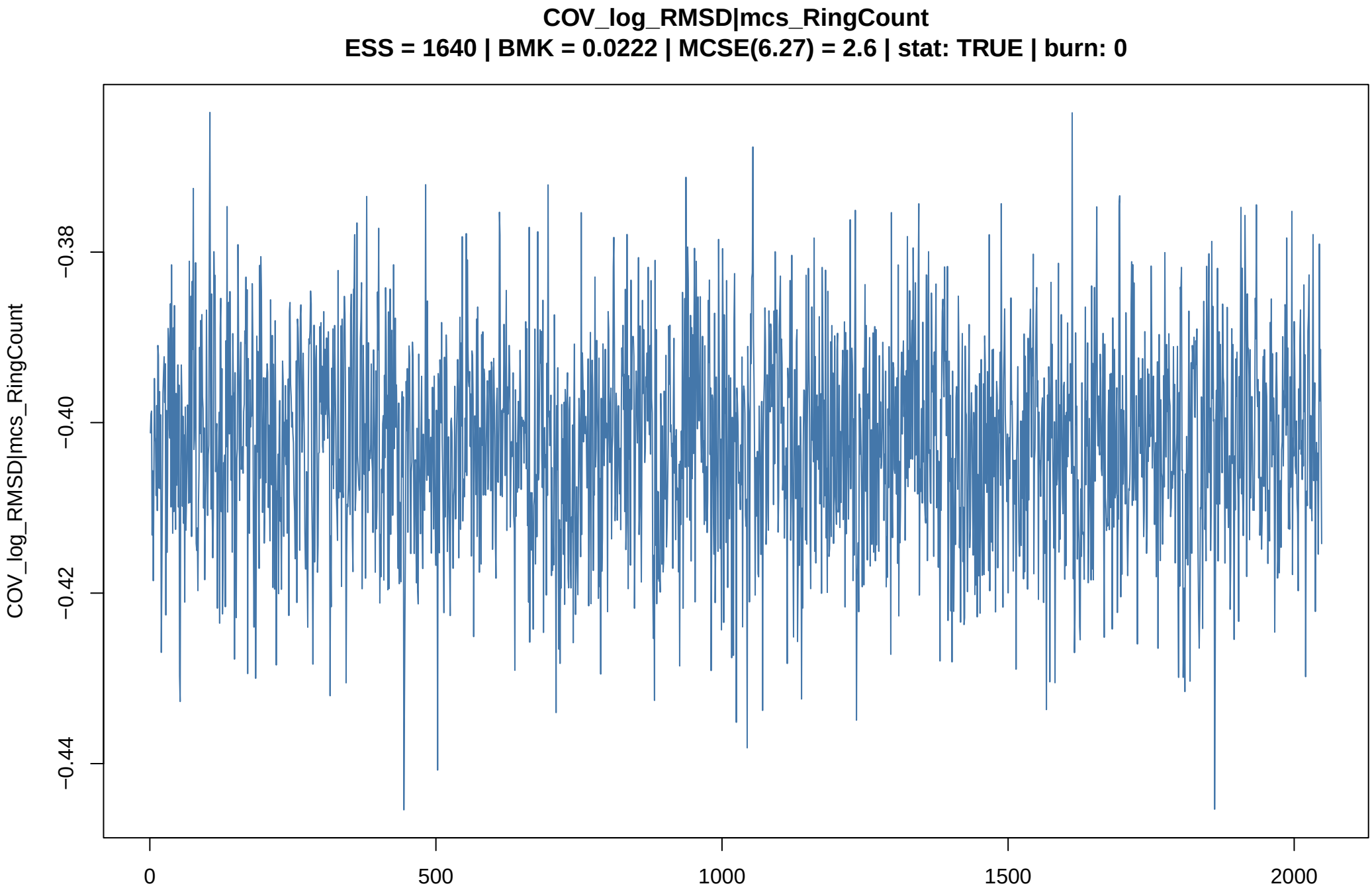

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0301 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
1.00
0.95
0.90
0.85
0
500
1000
1500
2000

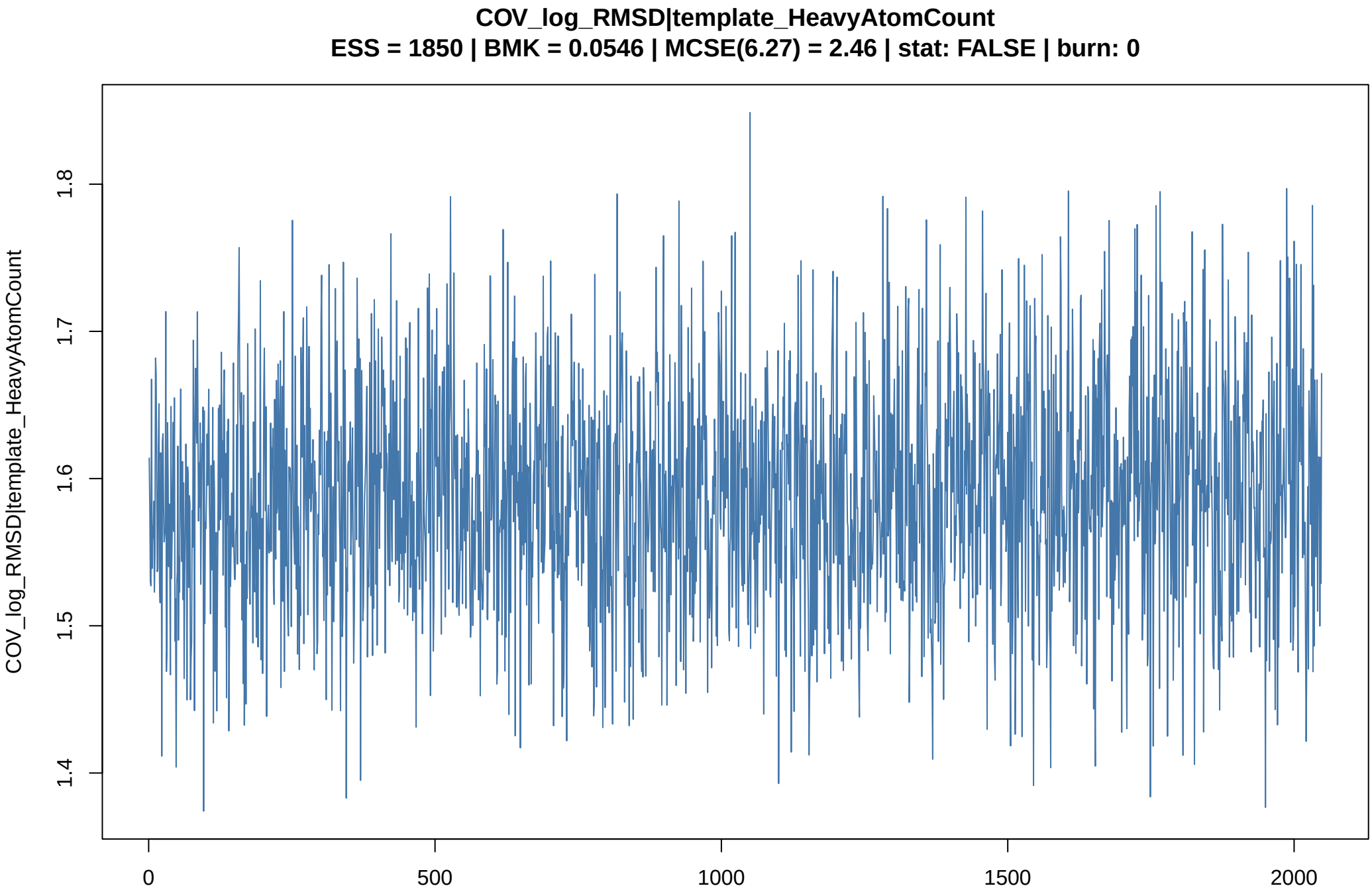

VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0342 | MCSE(6.27) = 2.07 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
1.00
0.95
0.90
0.85
0
500
1000
1500
2000

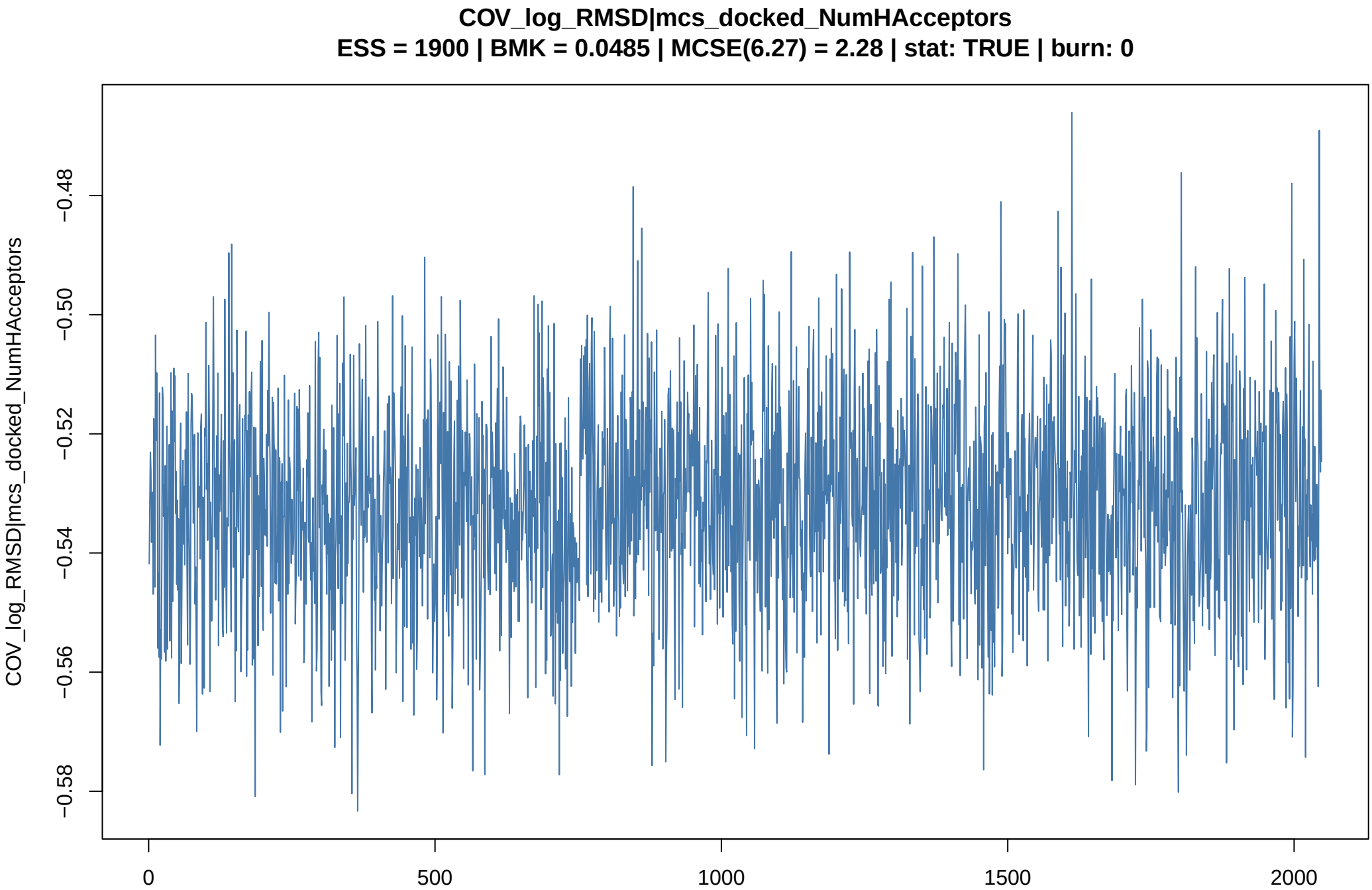

VAR_mcs_NumHeteroAtoms
ESS = 1650 | BMK = 0.0497 | MCSE(6.27) = 3.04 | stat: FALSE | burn: 0
VAR_mcs_NumHeteroAtoms
1.45
1.50
1.55
0
500
1000
1500
2000

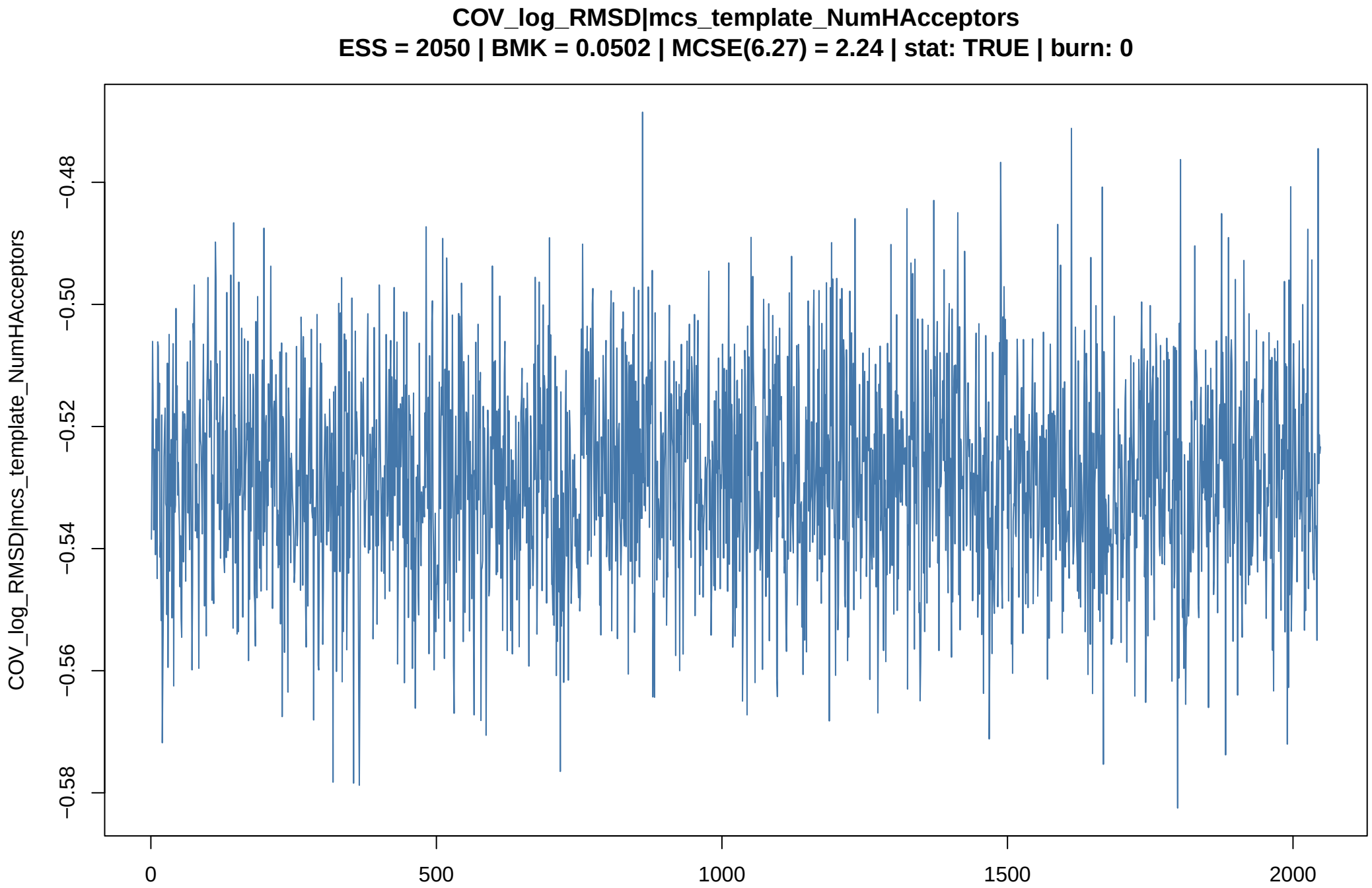

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1790 | BMK = 0.0279 | MCSE(6.27) = 2.01 | stat: TRUE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

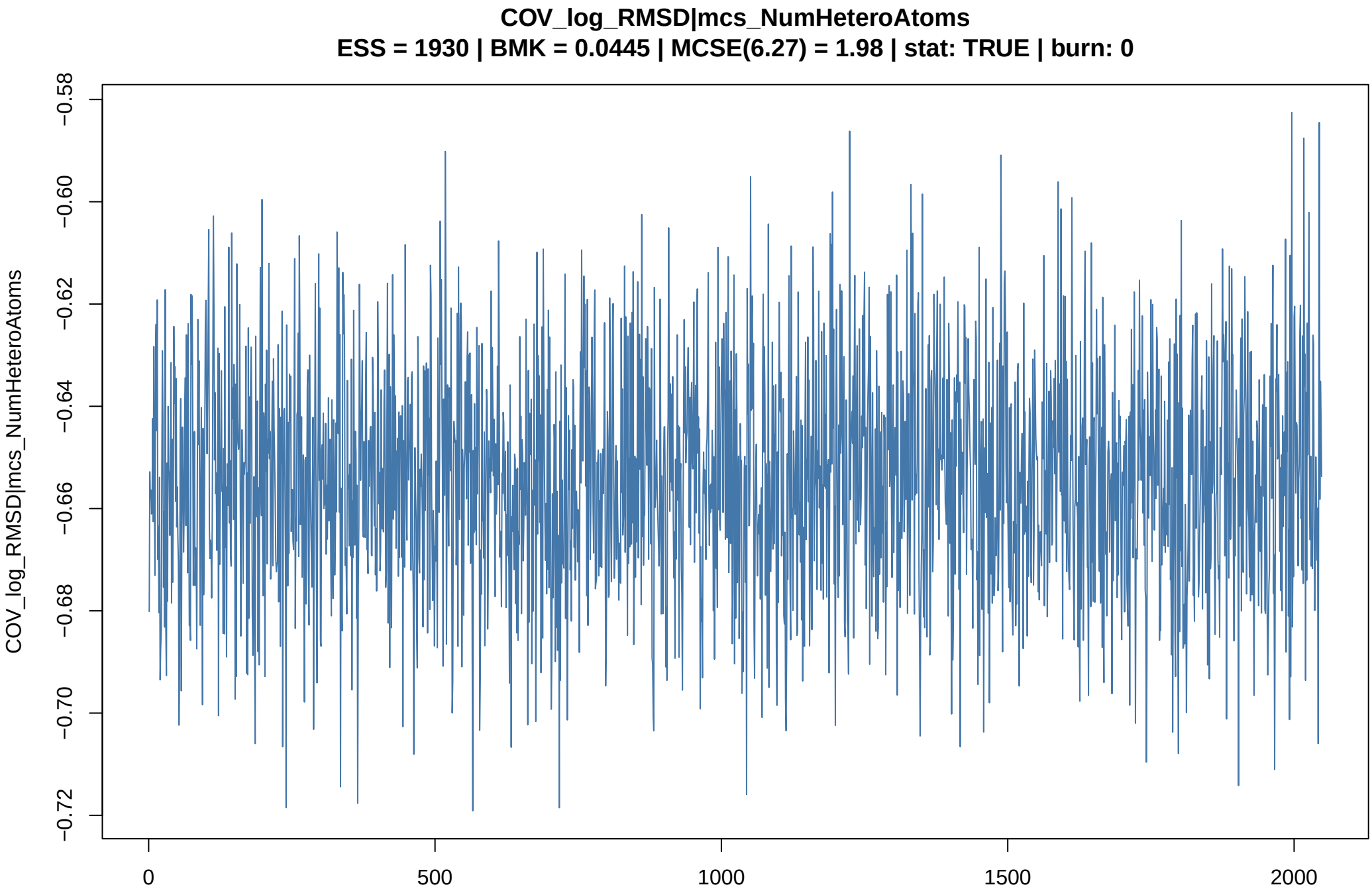

COV_log_RMSD|docked_HeavyAtomCount
ESS = 1850 | BMK = 0.0468 | MCSE(6.27) = 2.53 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

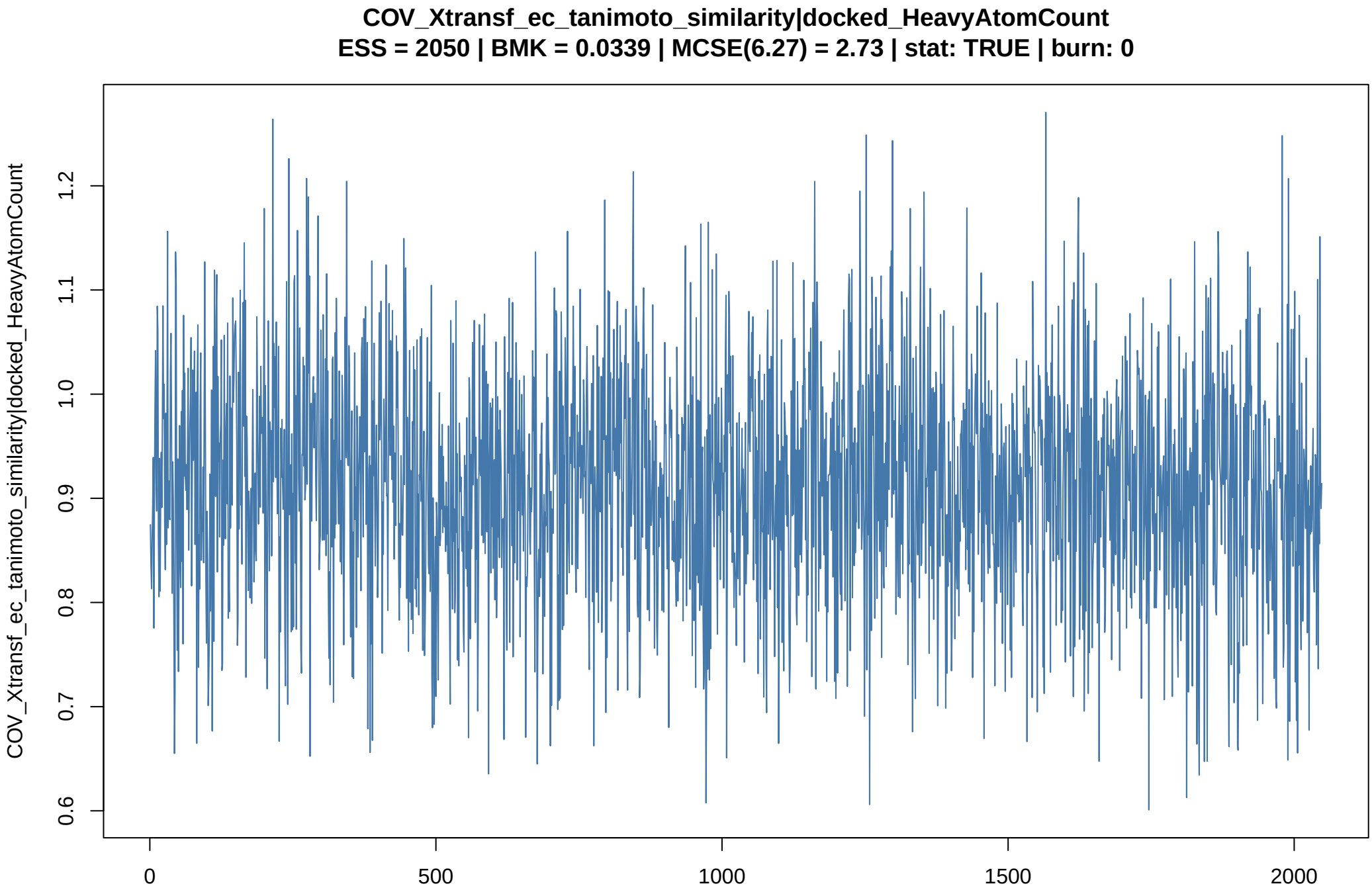

COV_log_RMSD|mcs_RingCount
ESS = 1640 | BMK = 0.0222 | MCSE(6.27) = 2.6 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.38
−0.40
−0.42
−0.44
0
500
1000
1500
2000

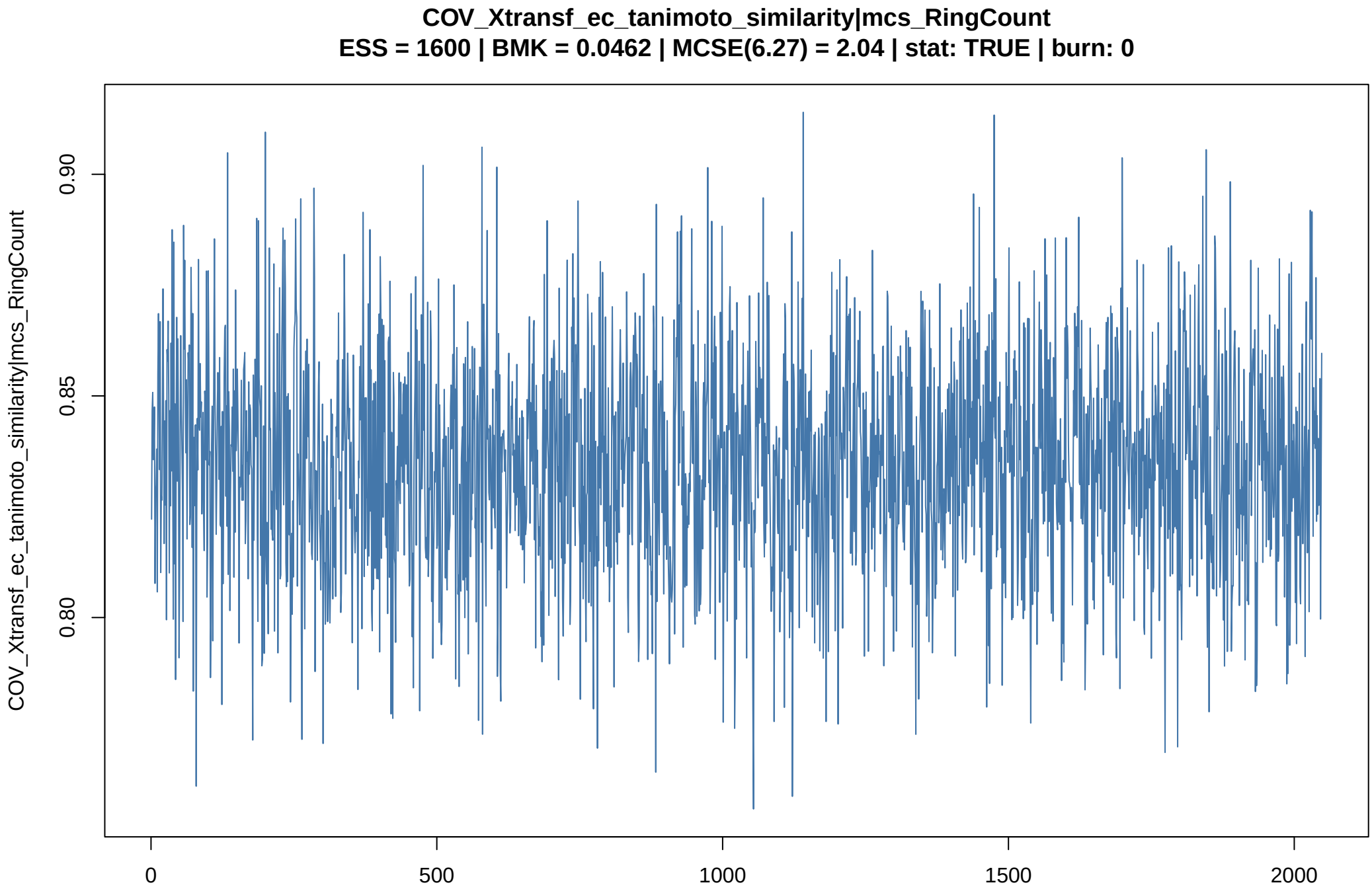

COV_log_RMSD|template_HeavyAtomCount
ESS = 1850 | BMK = 0.0546 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

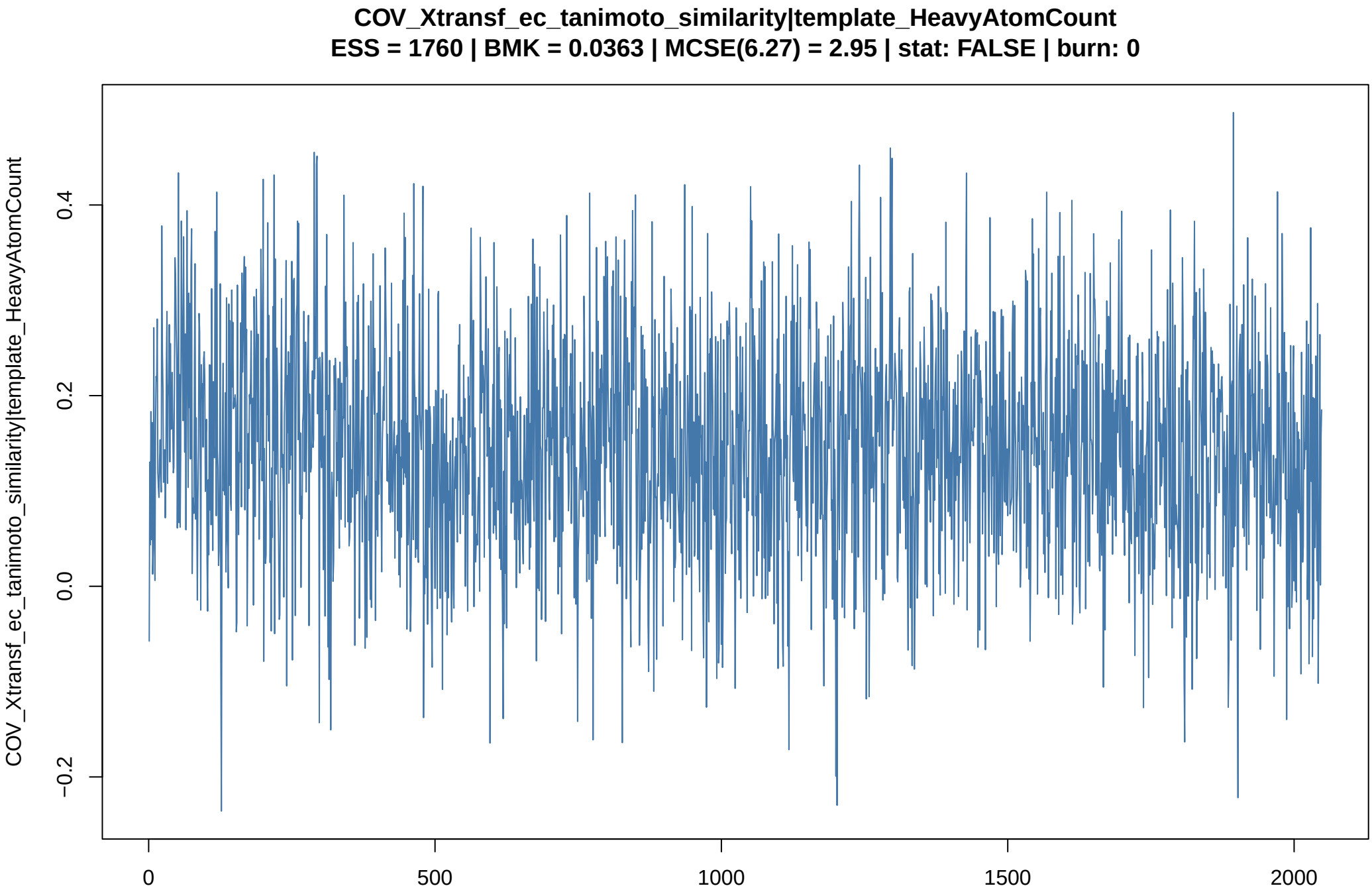

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 1900 | BMK = 0.0485 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

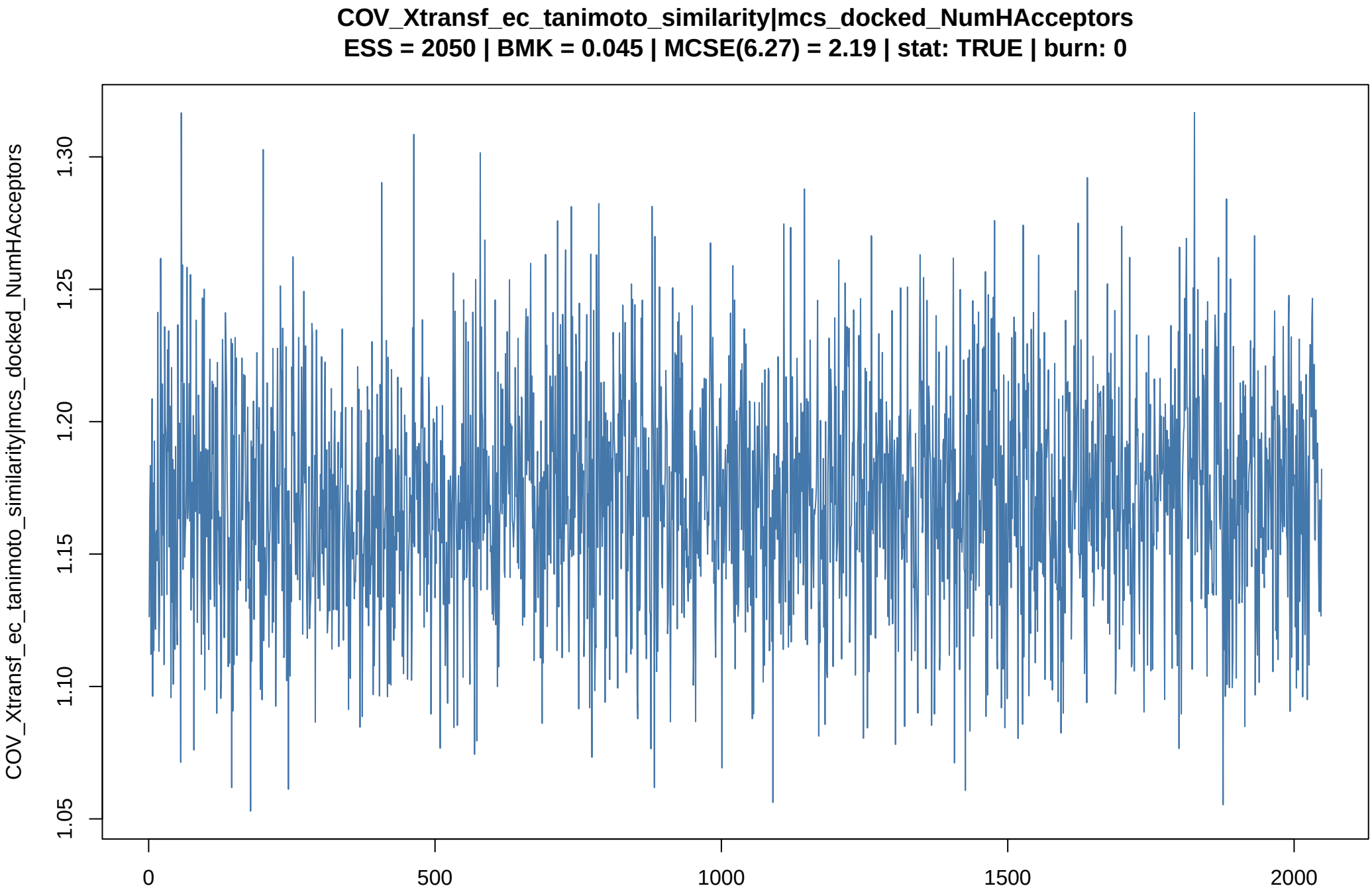

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0502 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

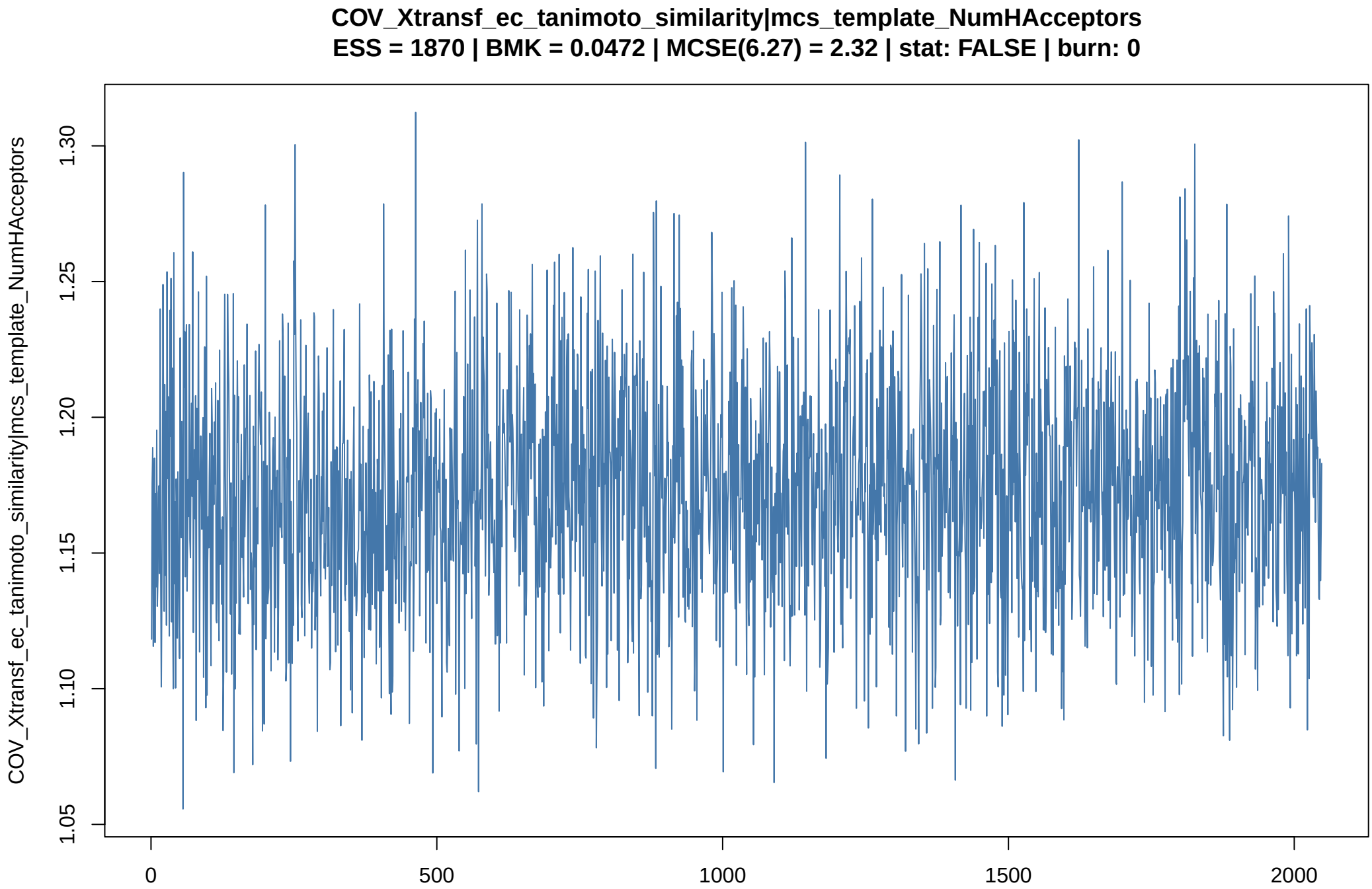

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 1930 | BMK = 0.0445 | MCSE(6.27) = 1.98 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.58
−0.60
−0.62
−0.64
−0.66
−0.68
−0.70
−0.72
0
500
1000
1500
2000

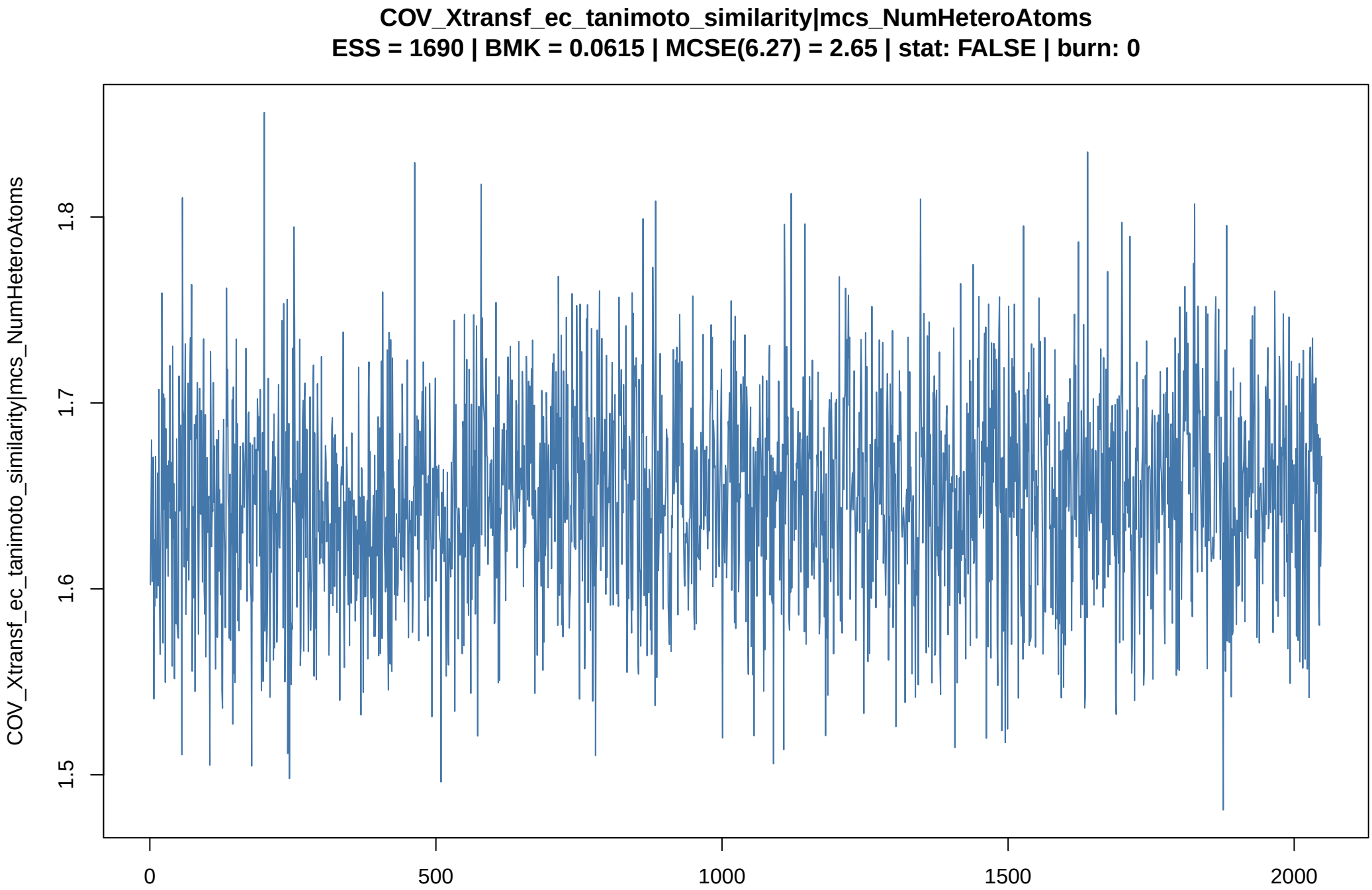

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0339 | MCSE(6.27) = 2.73 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.7
0.8
0.9
1.0
1.1
1.2
0
500
1000
1500
2000

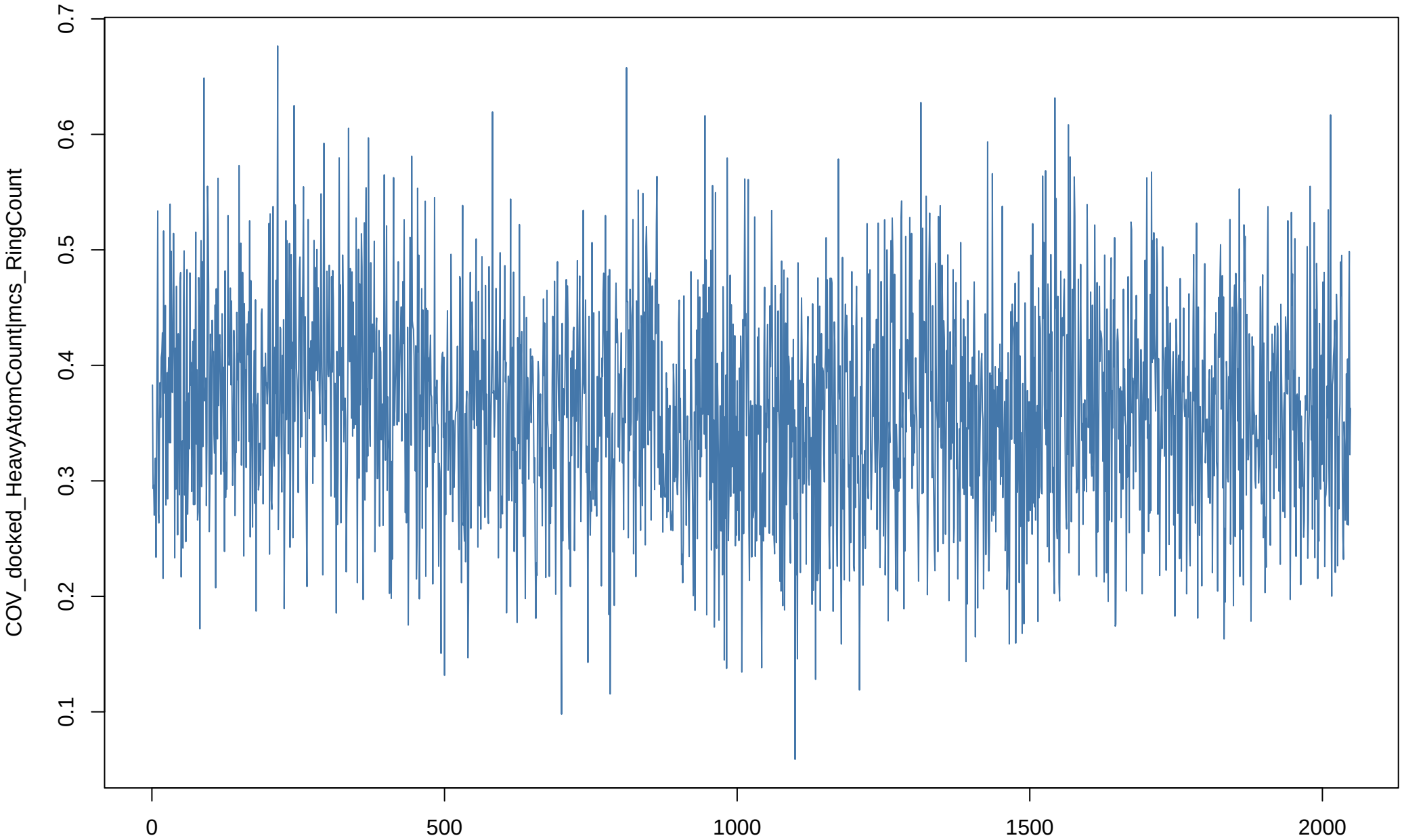

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 1600 | BMK = 0.0462 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.80
0.85
0.90
0
500
1000
1500
2000

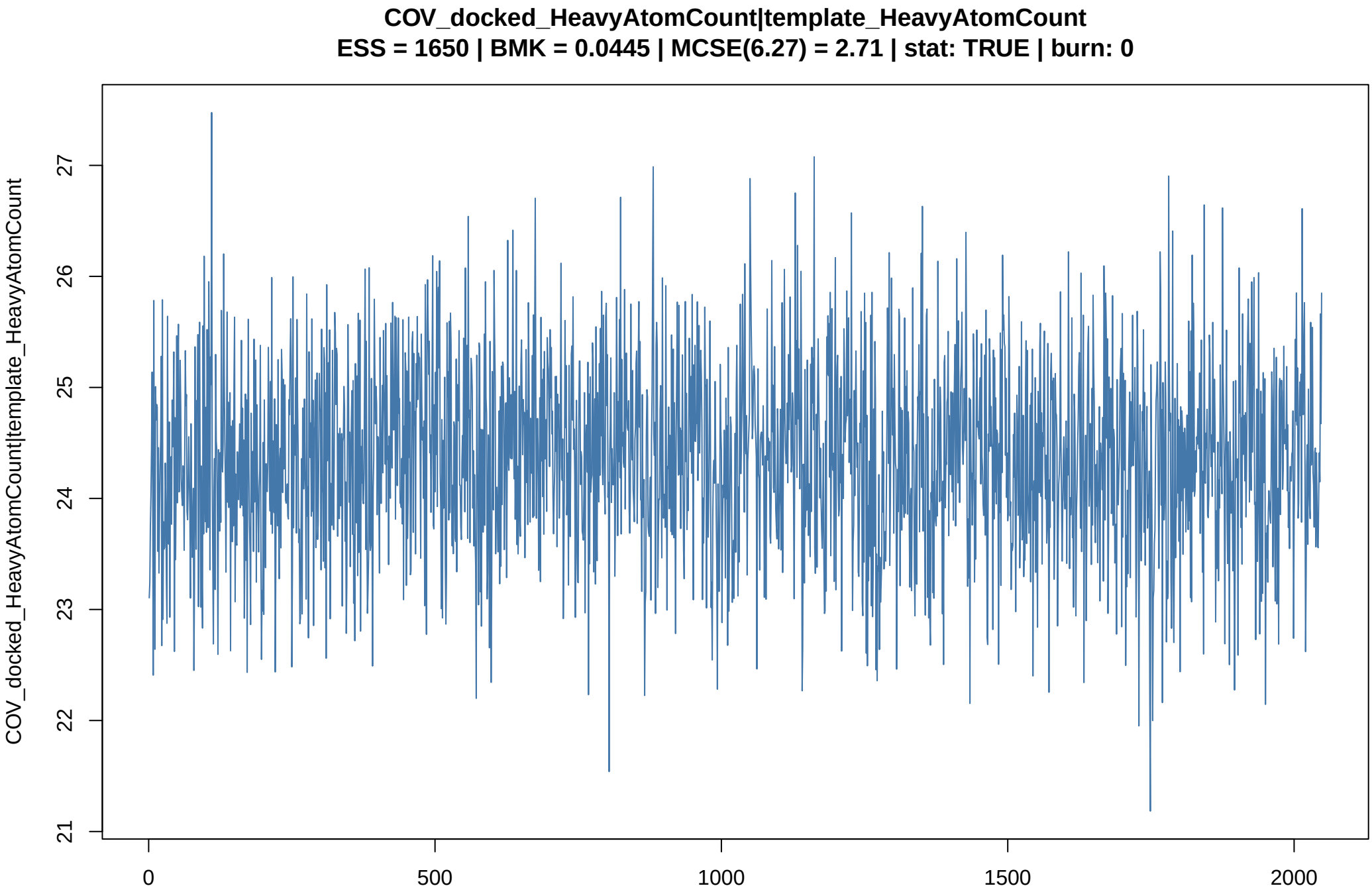

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1760 | BMK = 0.0363 | MCSE(6.27) = 2.95 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

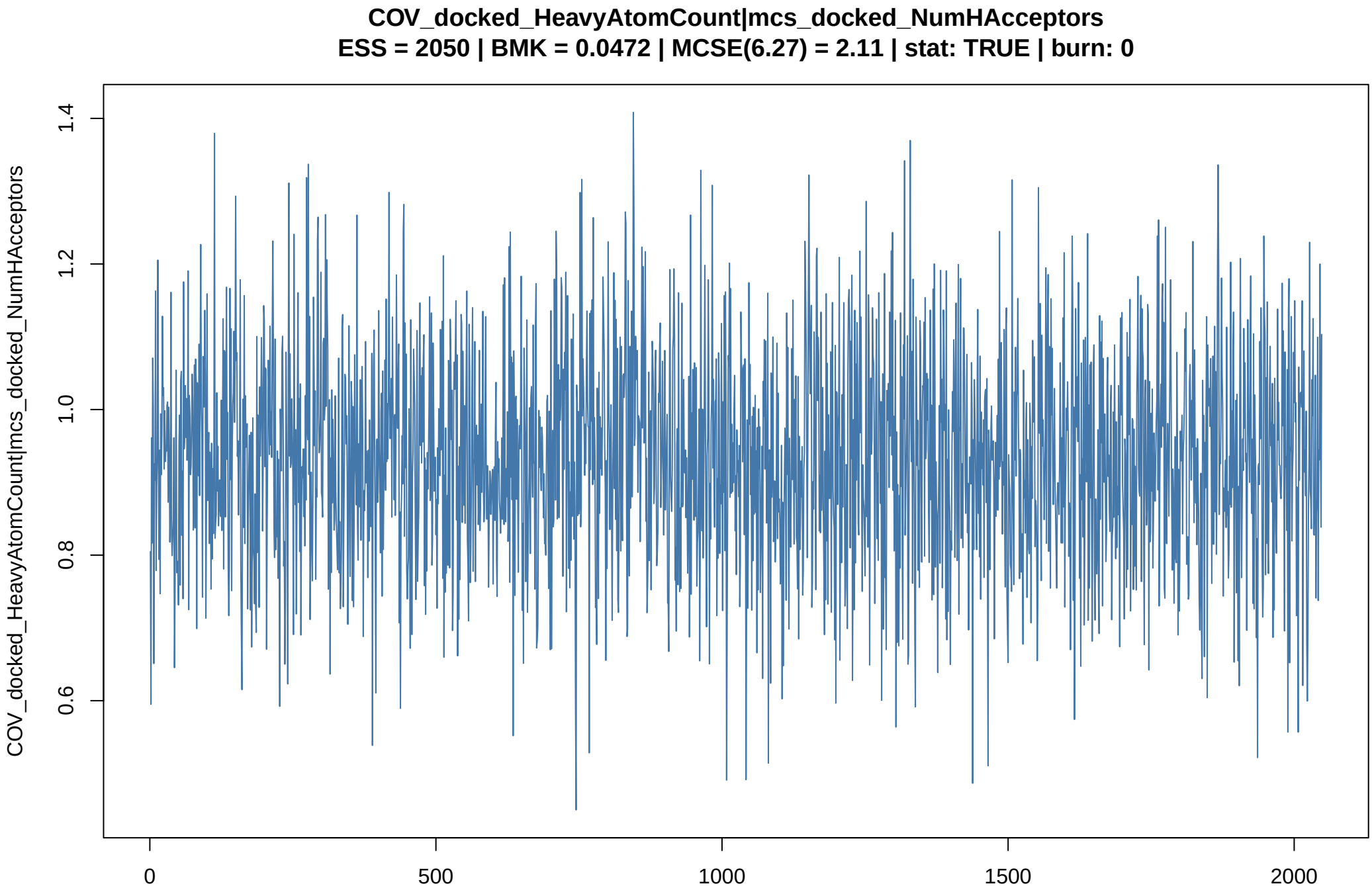

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.045 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

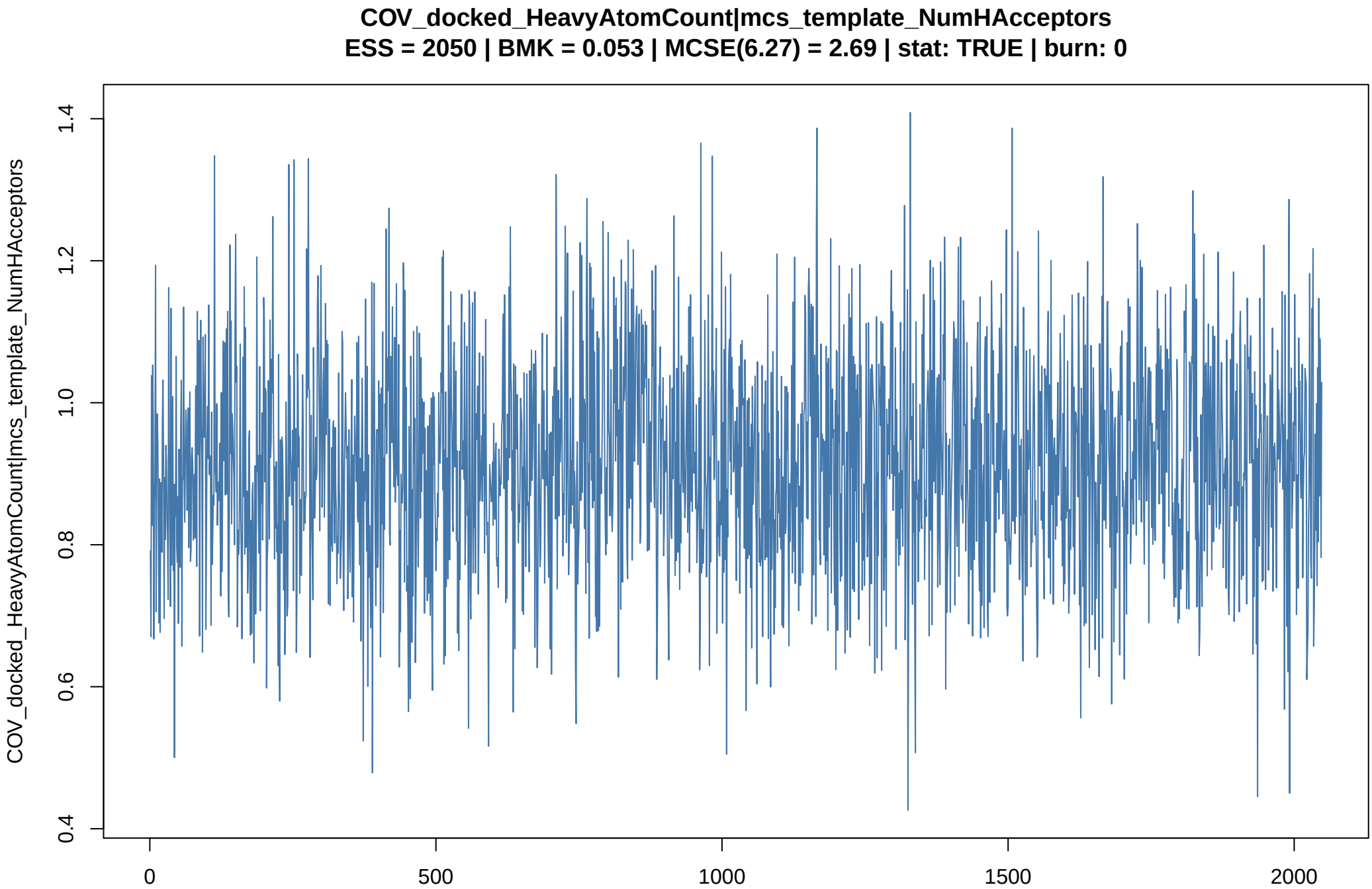

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 1870 | BMK = 0.0472 | MCSE(6.27) = 2.32 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

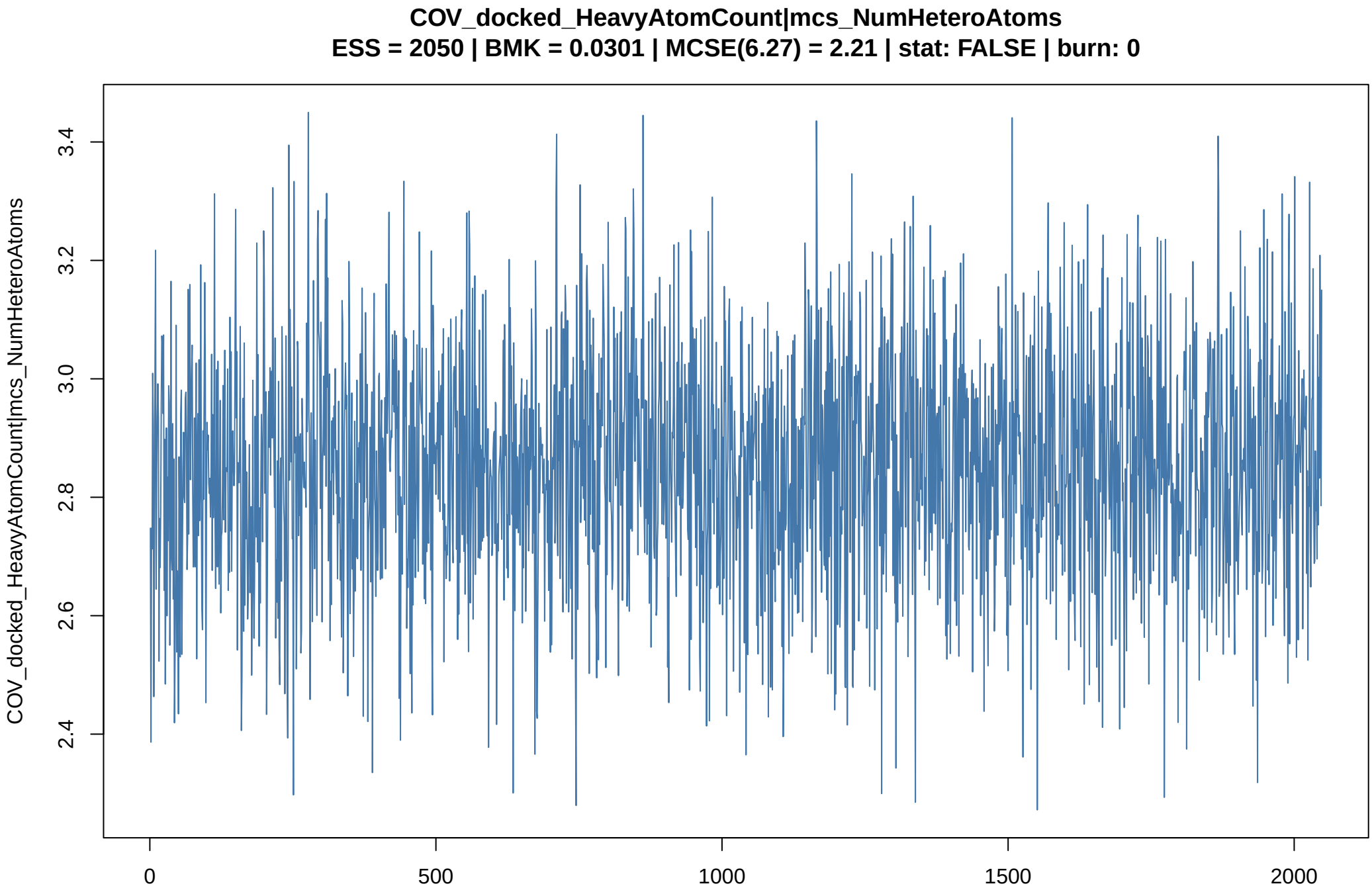

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1690 | BMK = 0.0615 | MCSE(6.27) = 2.65 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

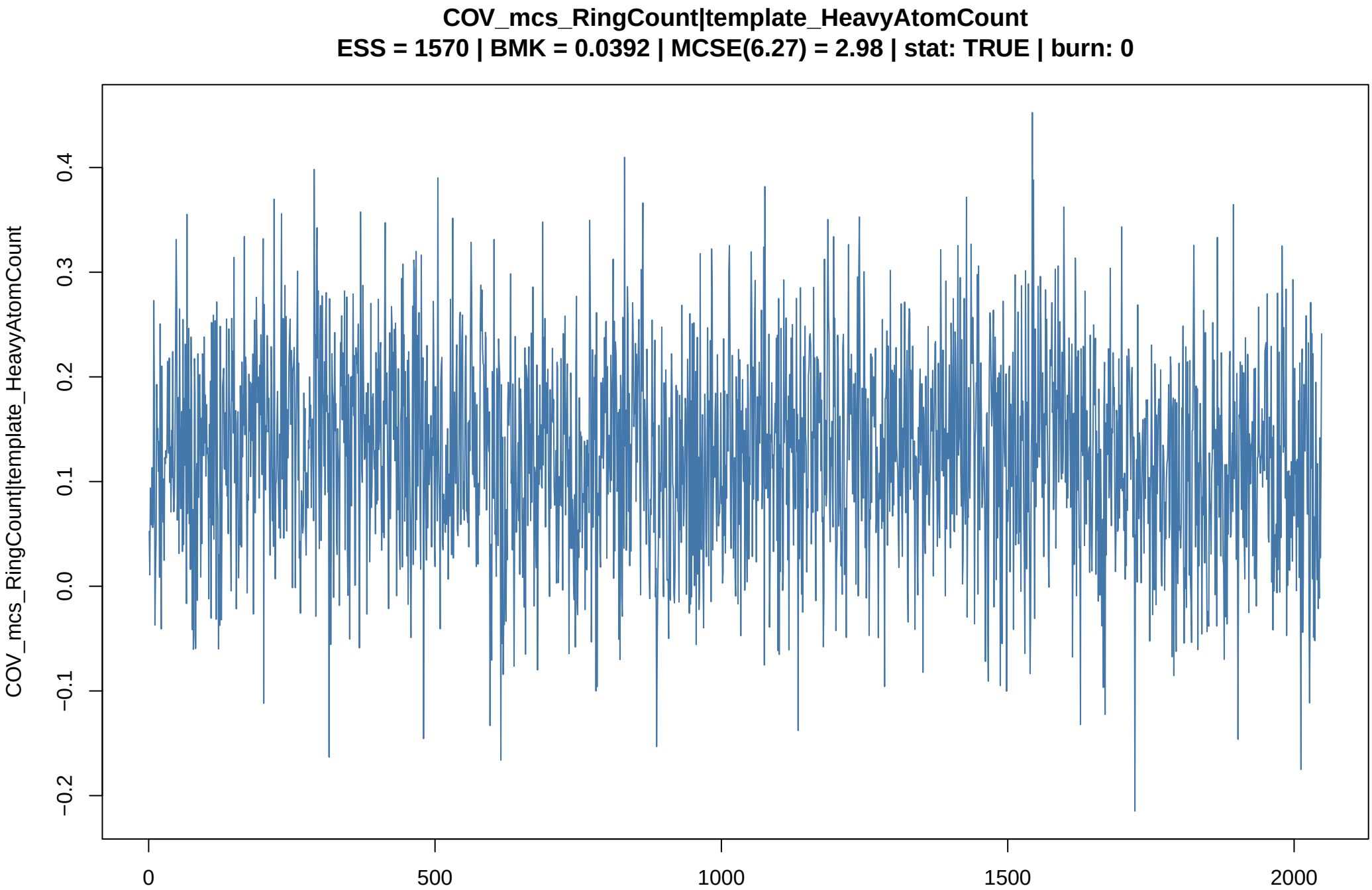

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1910 | BMK = 0.0558 | MCSE(6.27) = 3.04 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000

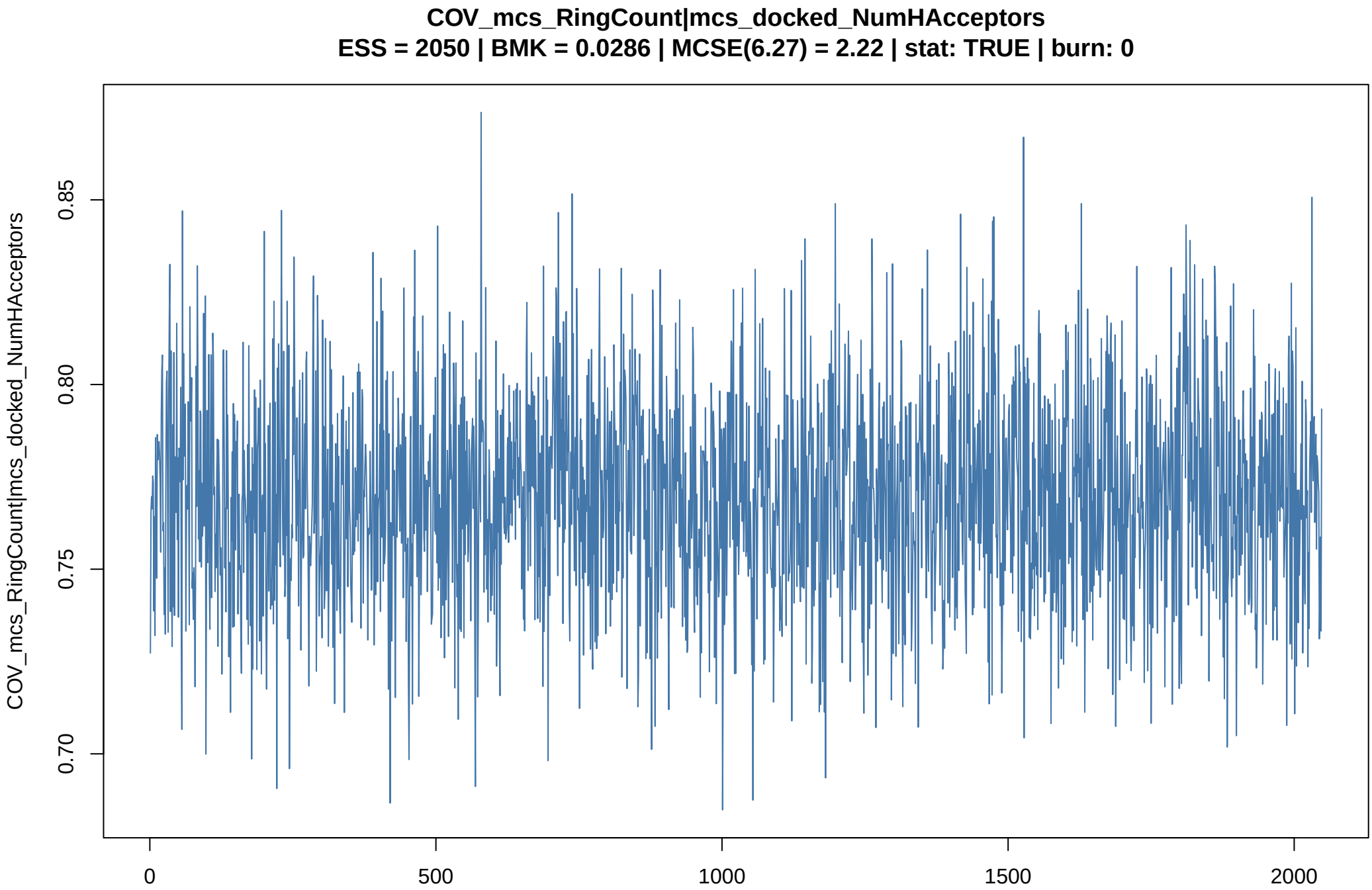

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1650 | BMK = 0.0445 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
21
22
23
24
25
26
27
0
500
1000
1500
2000

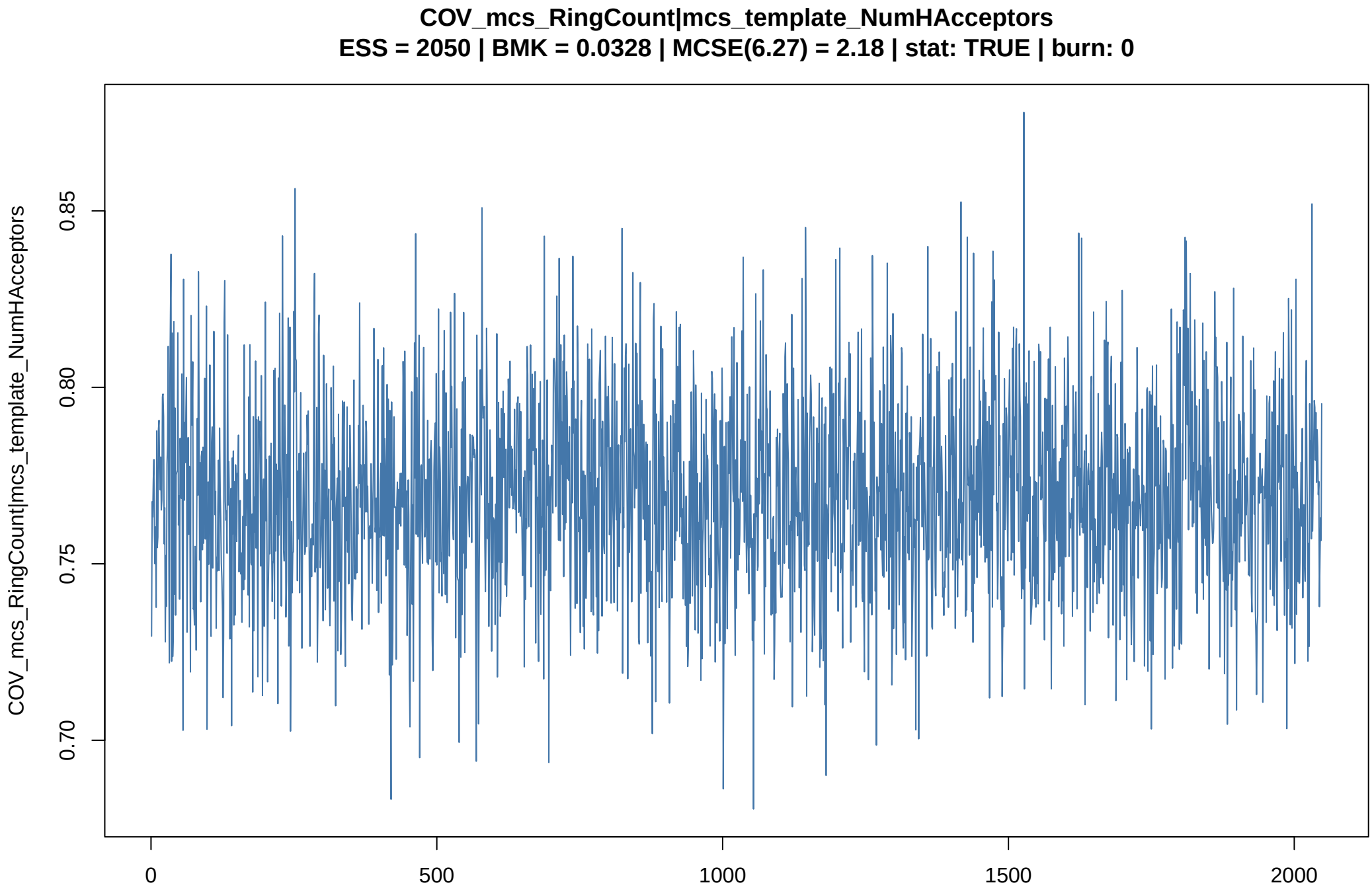

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0472 | MCSE(6.27) = 2.11 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

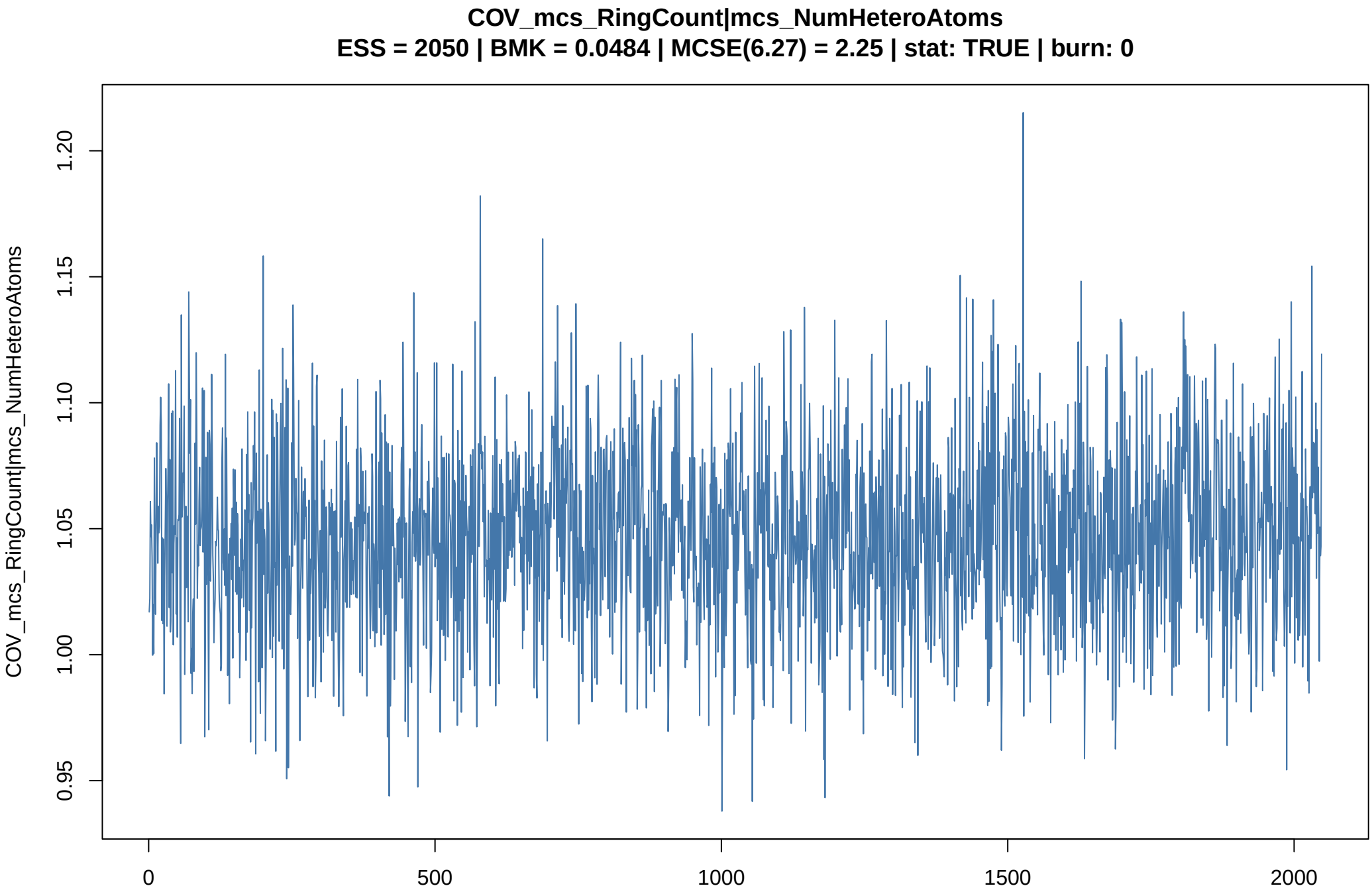

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.053 | MCSE(6.27) = 2.69 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

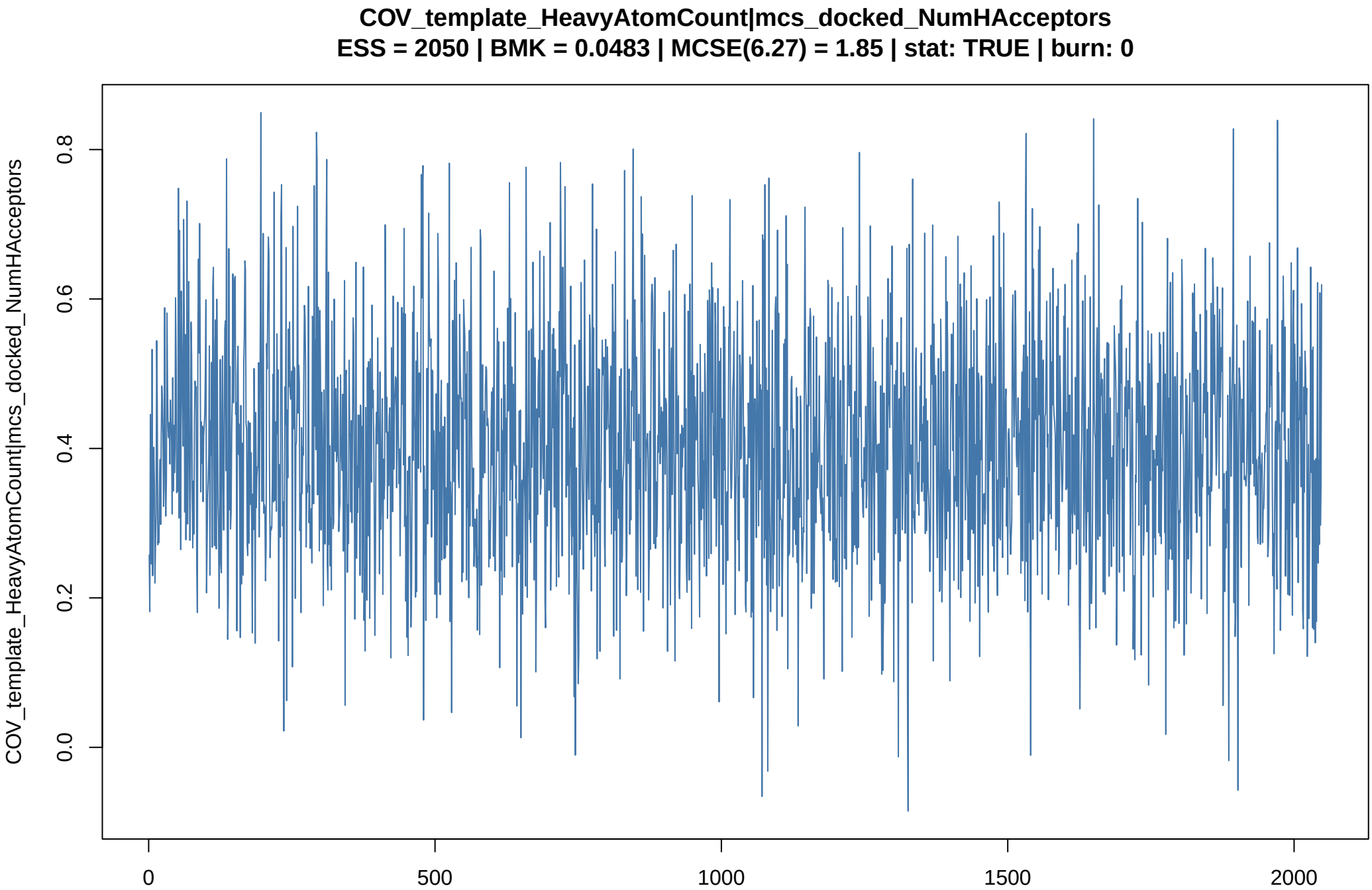

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0301 | MCSE(6.27) = 2.21 | stat: FALSE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.4
2.6
2.8
3.0
3.2
3.4
0
500
1000
1500
2000

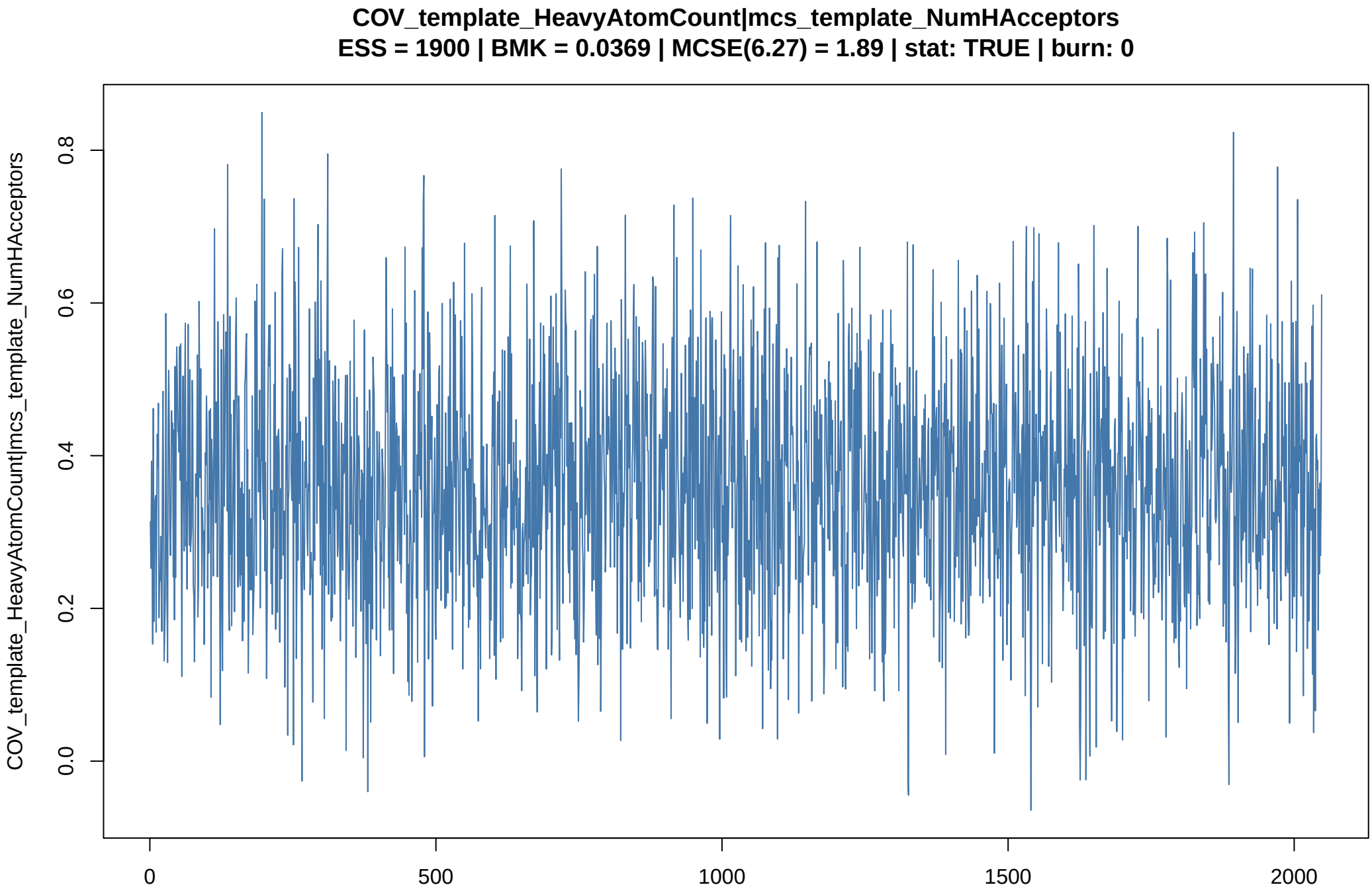

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1570 | BMK = 0.0392 | MCSE(6.27) = 2.98 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
−0.2
−0.1
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

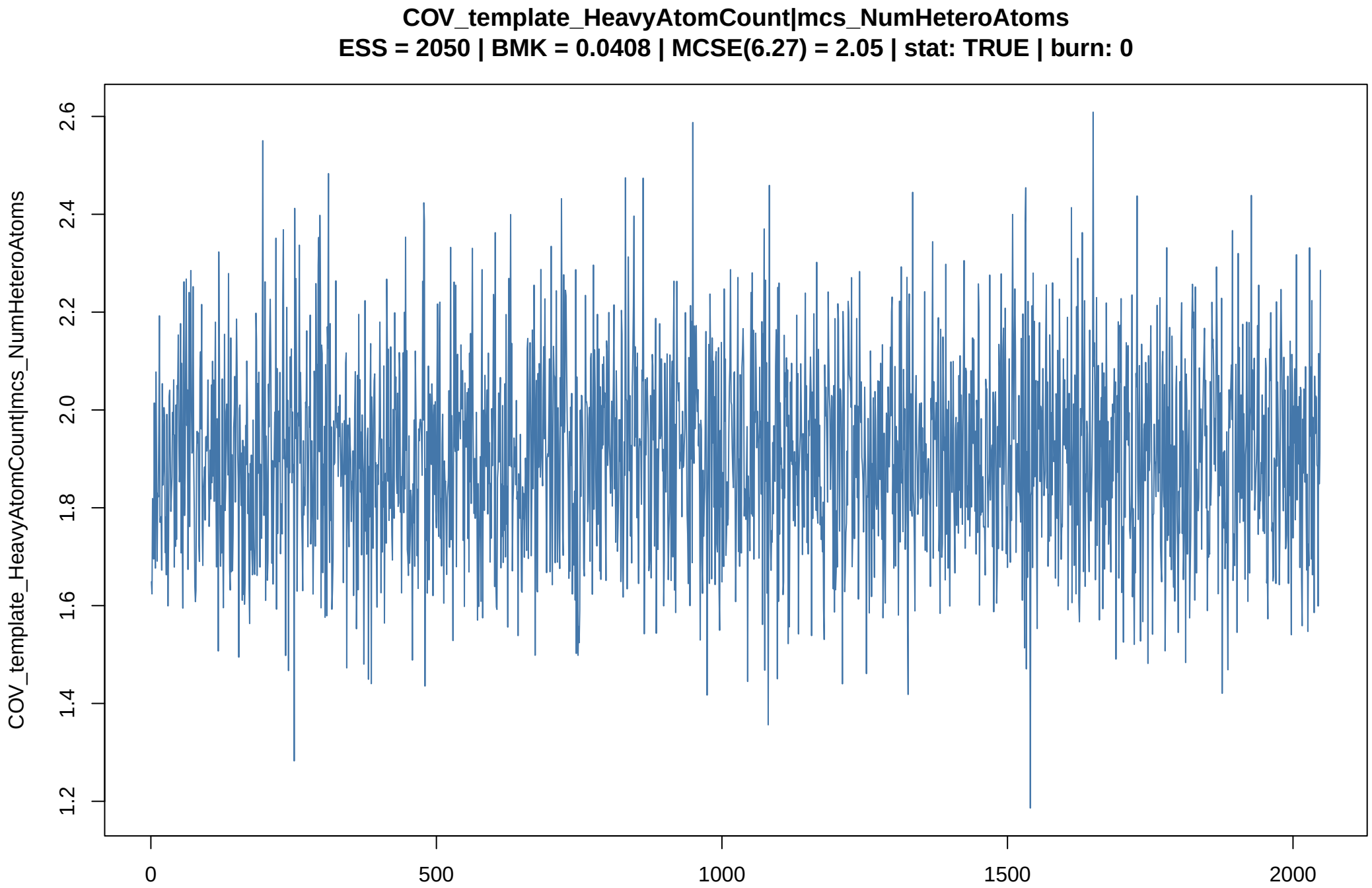

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0286 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

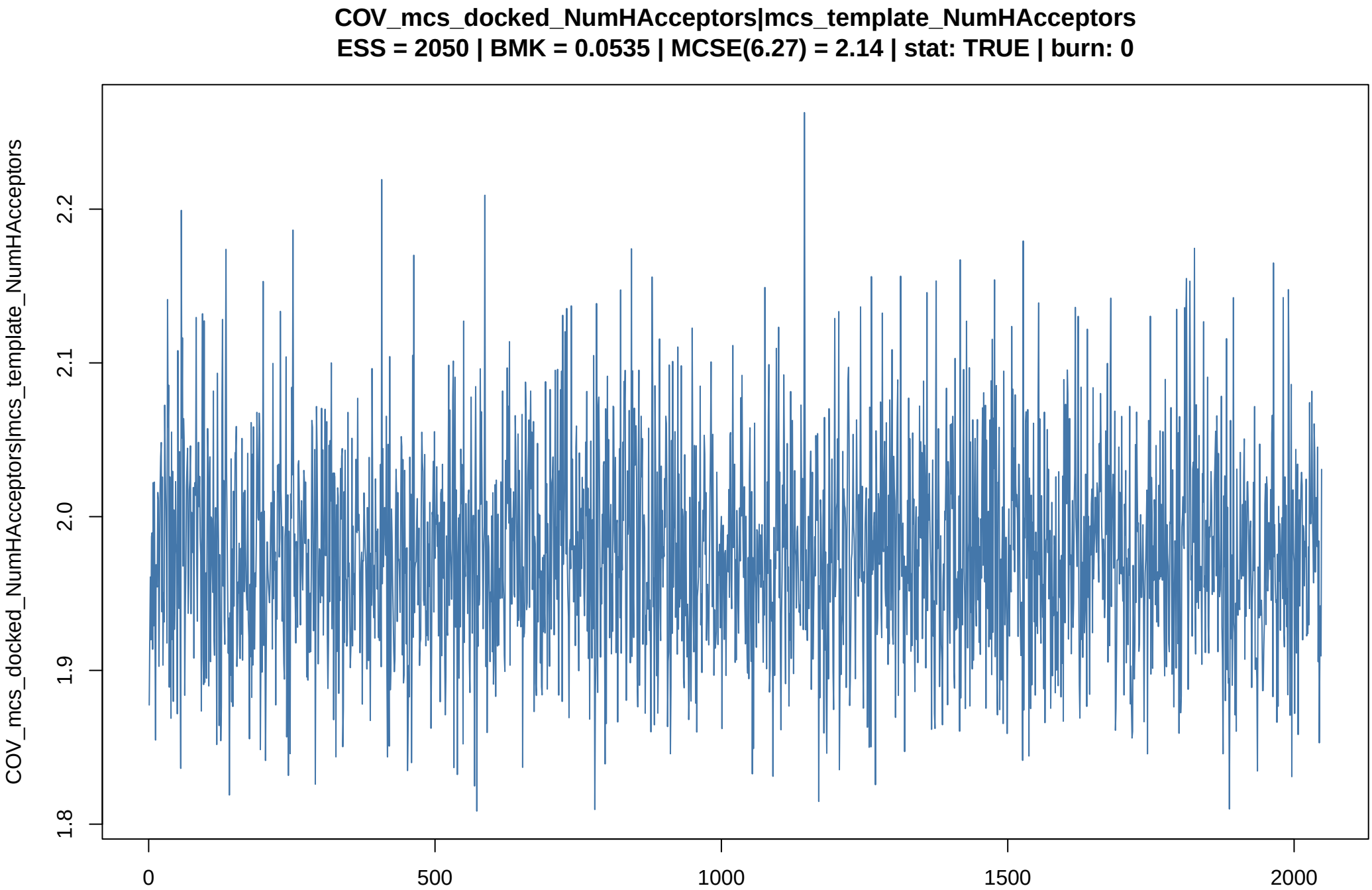

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0328 | MCSE(6.27) = 2.18 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

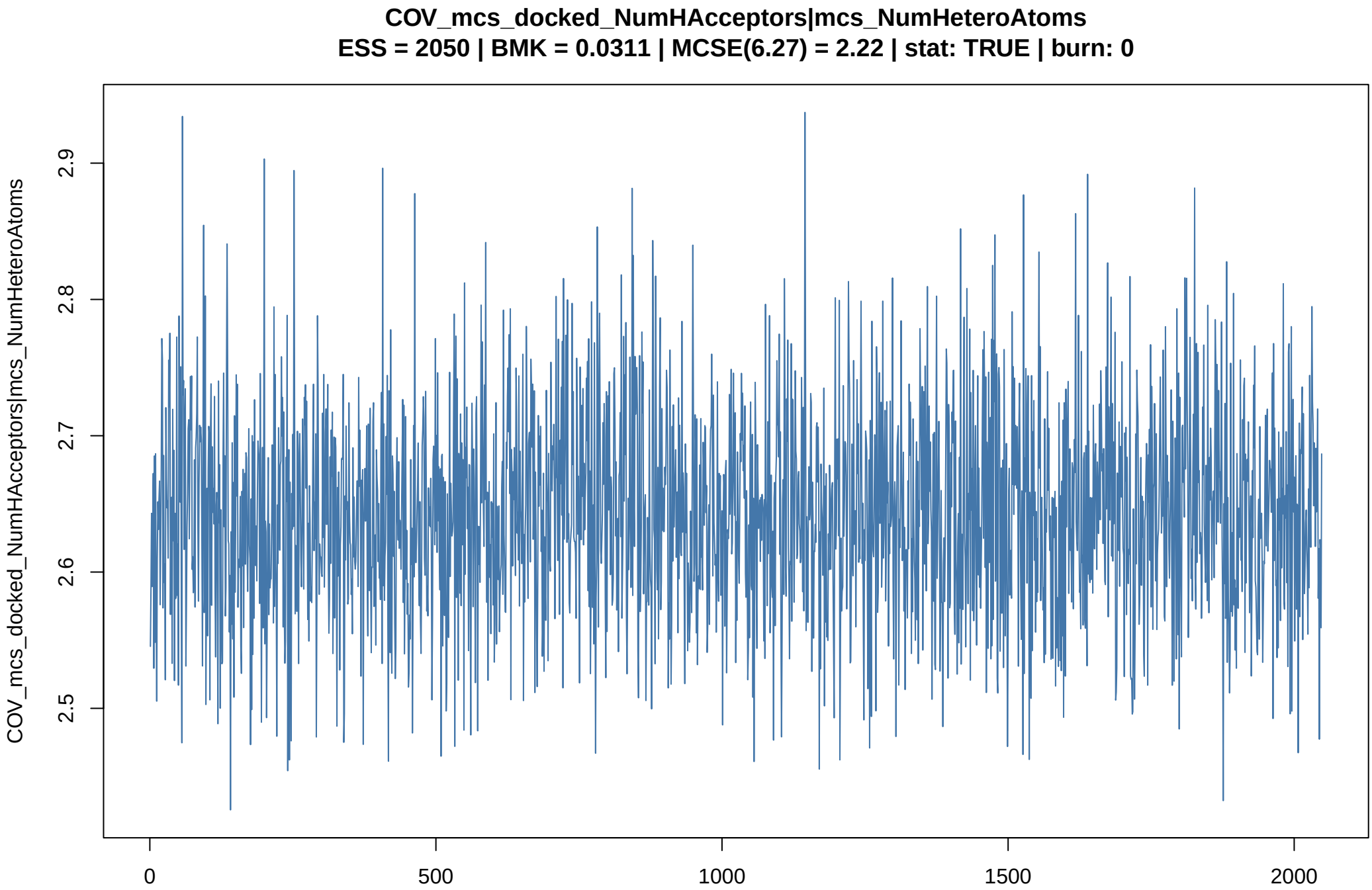

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0484 | MCSE(6.27) = 2.25 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
1.20
0
500
1000
1500
2000

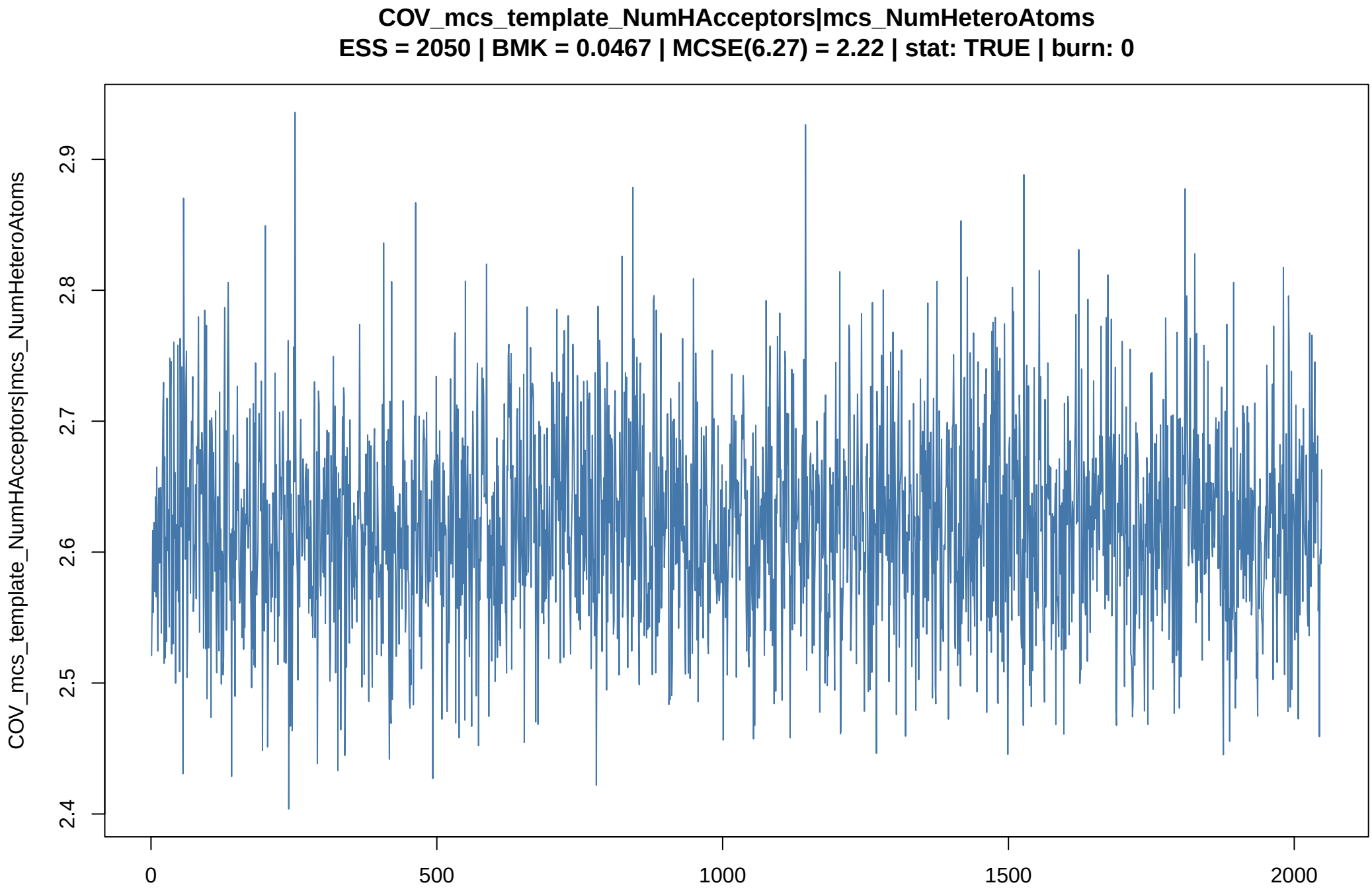

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0483 | MCSE(6.27) = 1.85 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1900 | BMK = 0.0369 | MCSE(6.27) = 1.89 | 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 = 0.0408 | MCSE(6.27) = 2.05 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
1.2
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 = 0.0535 | MCSE(6.27) = 2.14 | 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 = 0.0311 | MCSE(6.27) = 2.22 | stat: TRUE | burn: 0
COV_mcs_docked_NumHAcceptors|mcs_NumHeteroAtoms
2.5
2.6
2.7
2.8
2.9
0
500
1000
1500
2000


COV_mcs_template_NumHAcceptors|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0467 | MCSE(6.27) = 2.22 | 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