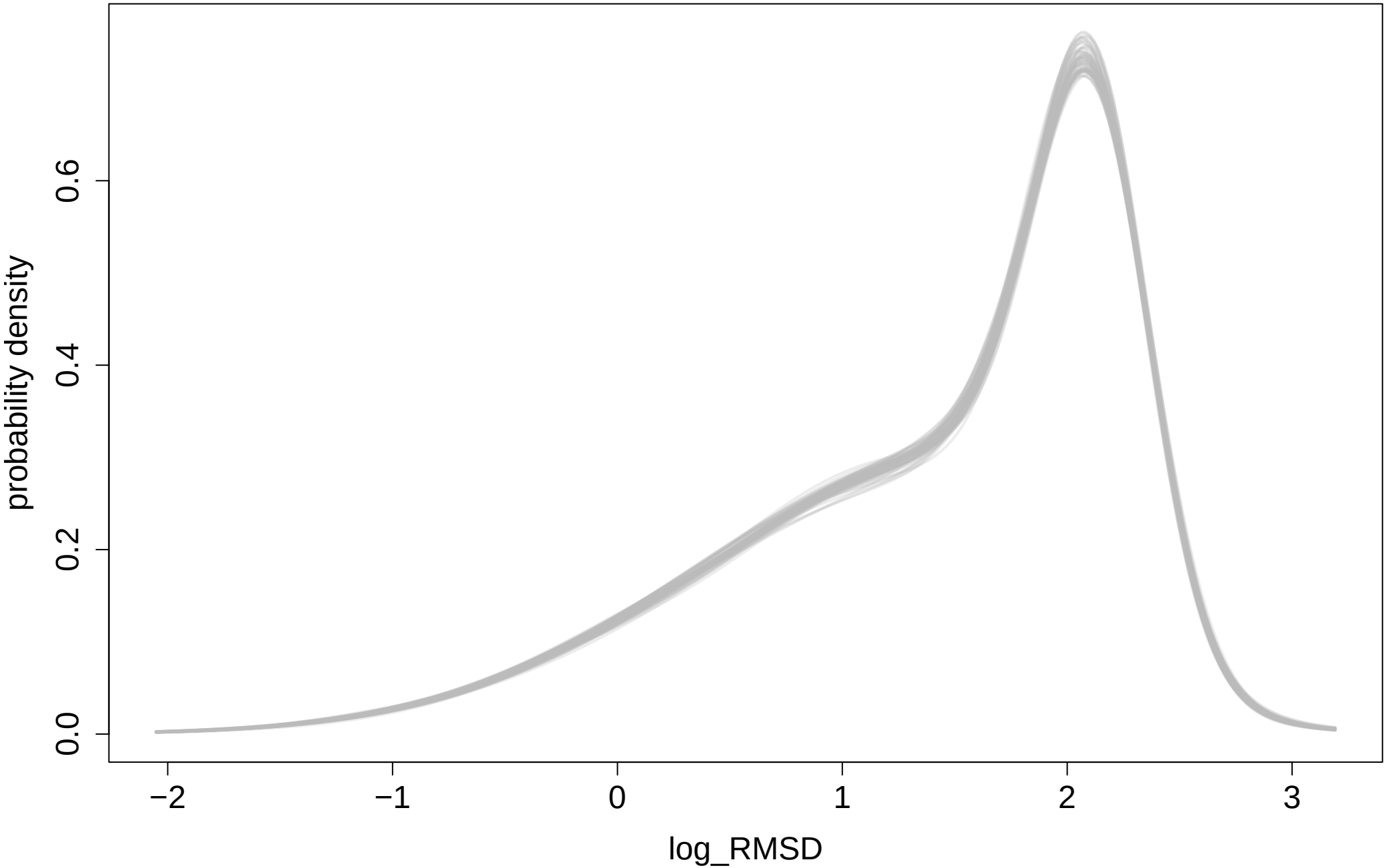
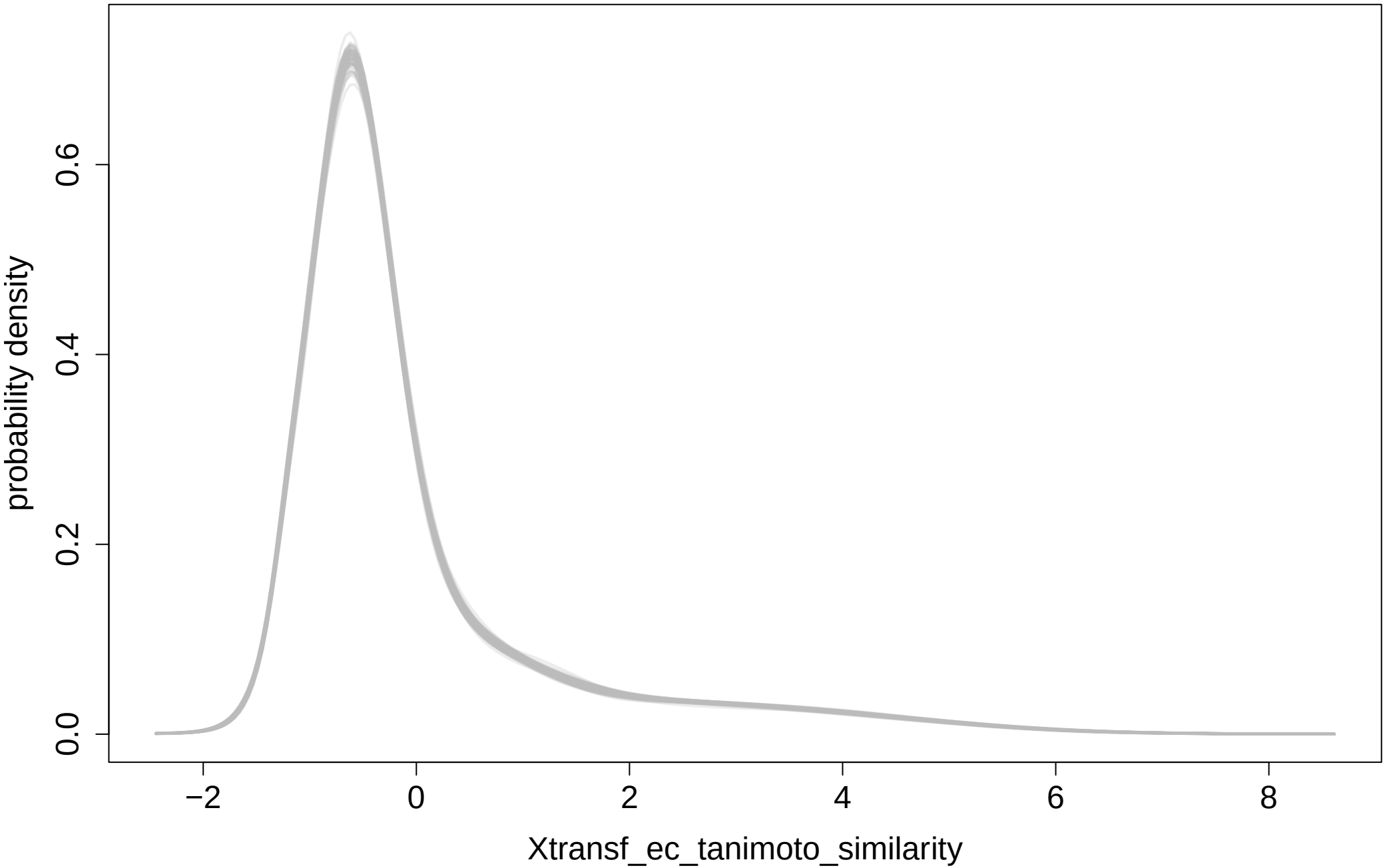
−− STATS maxD −−
min ESS = 3.10520549534621
max BMK = 0.716081098562101
max MCSE = 14.2504101981248
all stationary: FALSE
burn: 2040

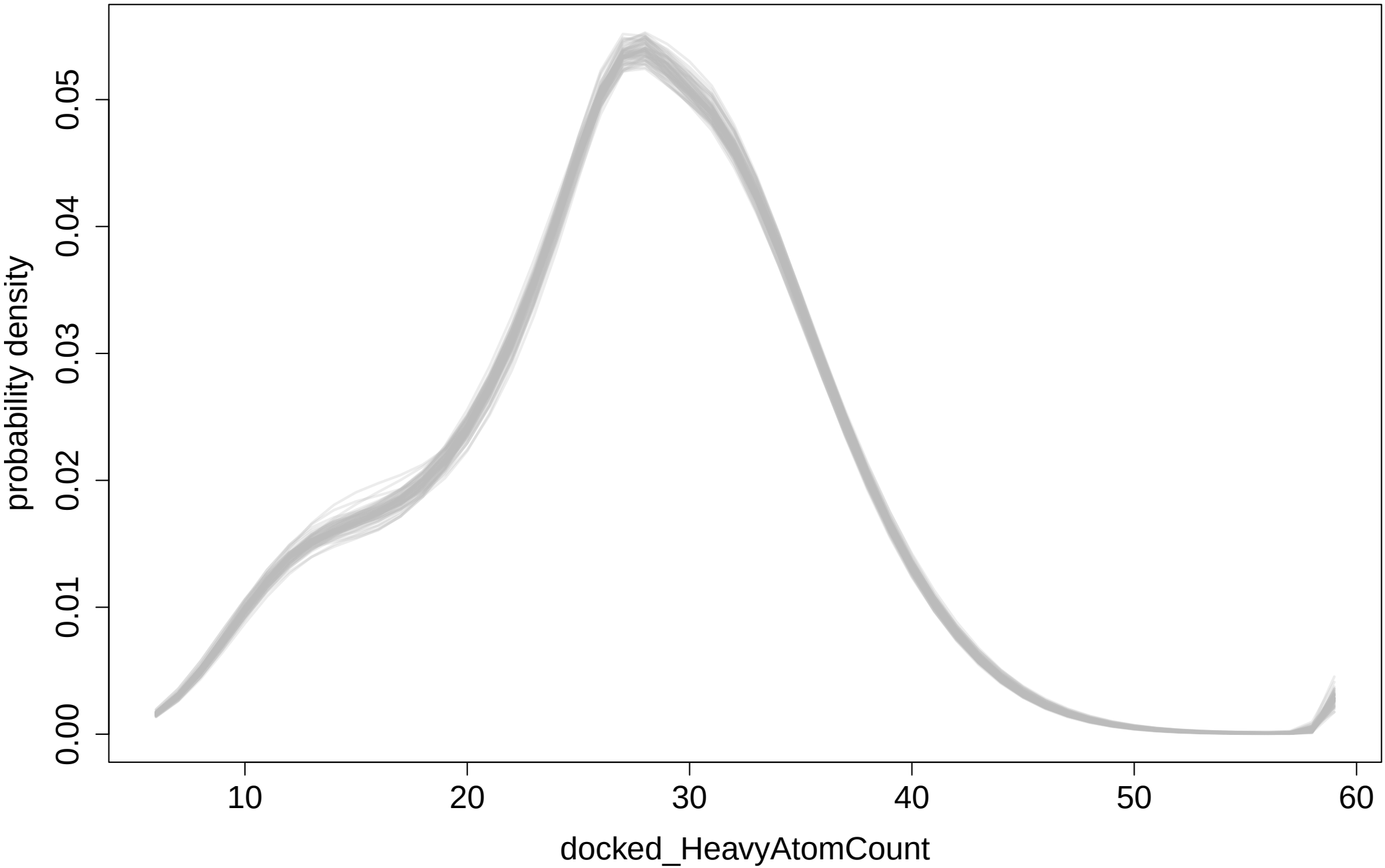
−− STATS 2D −−
min ESS = 896.57924939927
max BMK = 0.113819677933426
max MCSE = 3.67611518572781
all stationary: FALSE
burn: 0

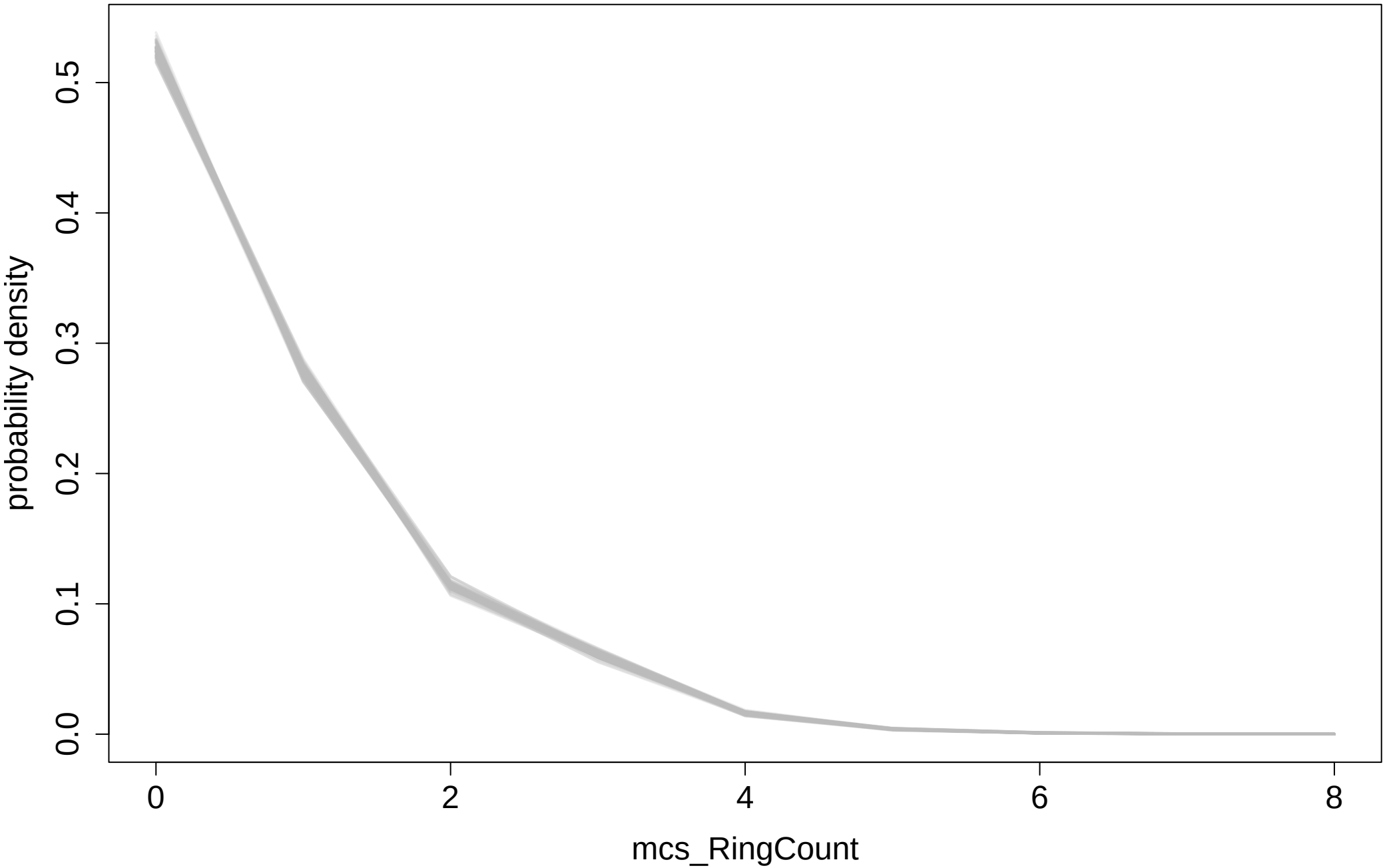
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 0.627852113064889
max MCSE = NaN
all stationary: FALSE
burn: 2040

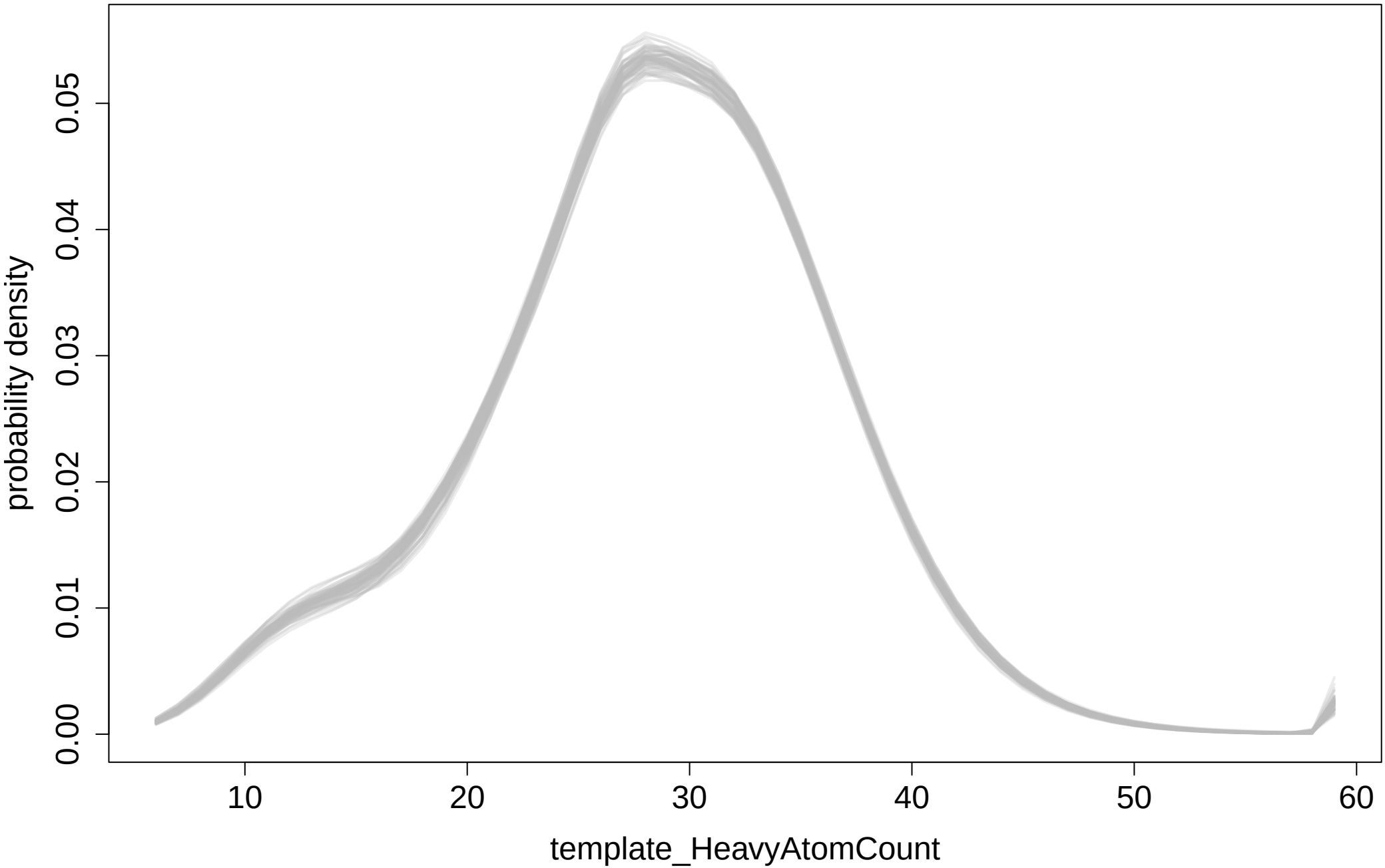
Occupied clusters: 61 of 91
LL: −110000 +− 102

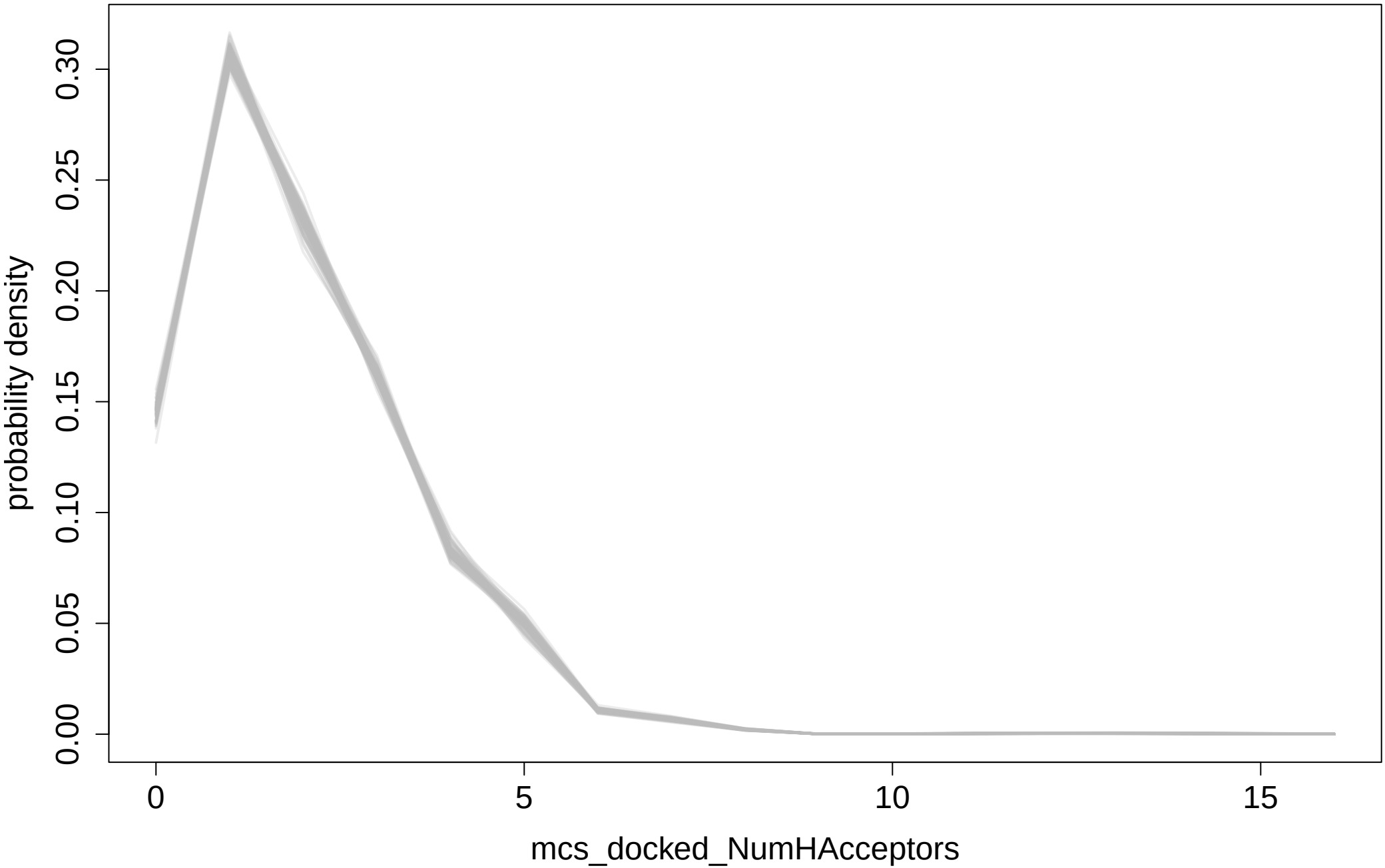

probability density
0.0
0.2
0.4
0.6
−2
−1
0
1
2
3
log_RMSD

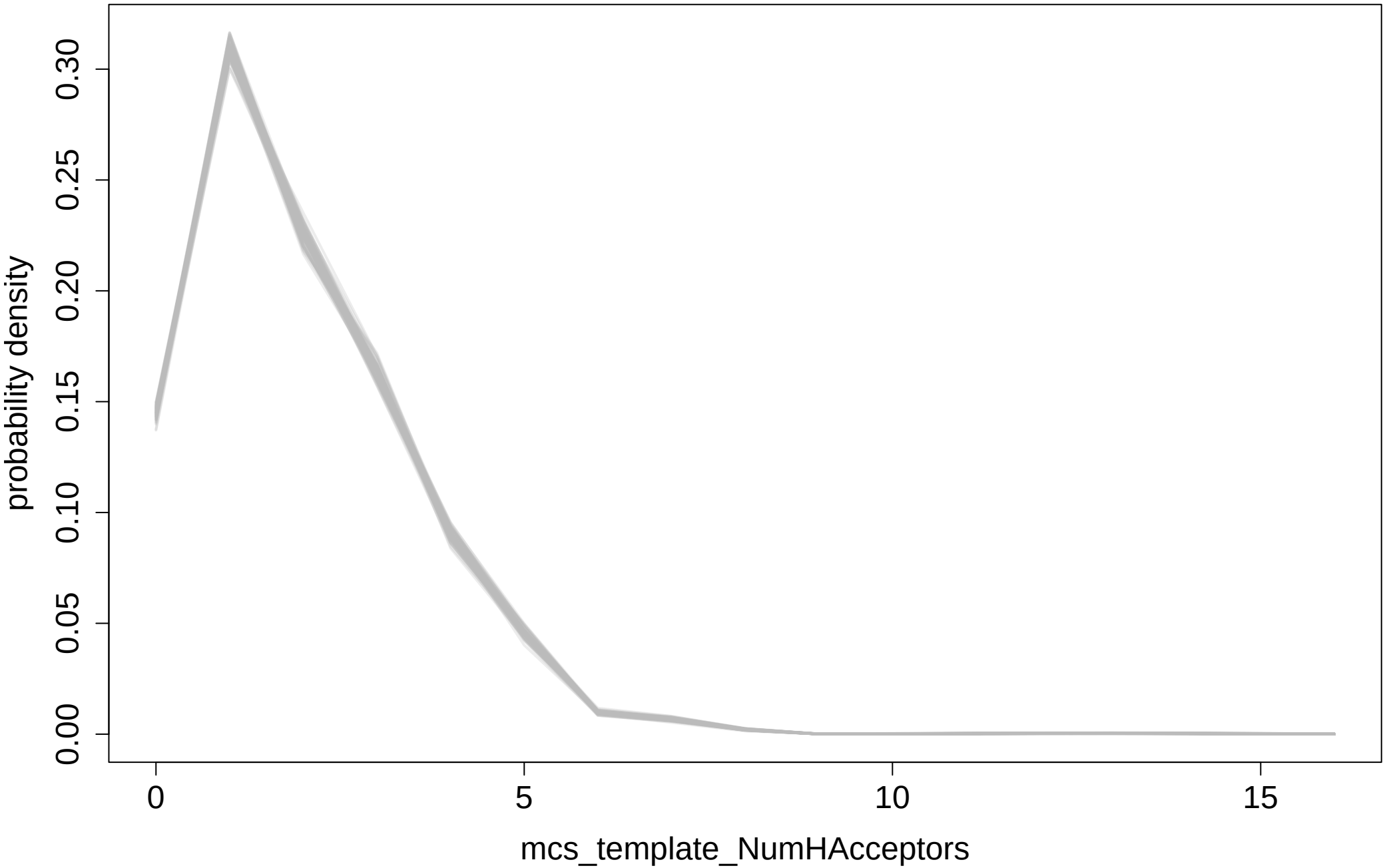

probability density
0.0
0.2
0.4
0.6
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity

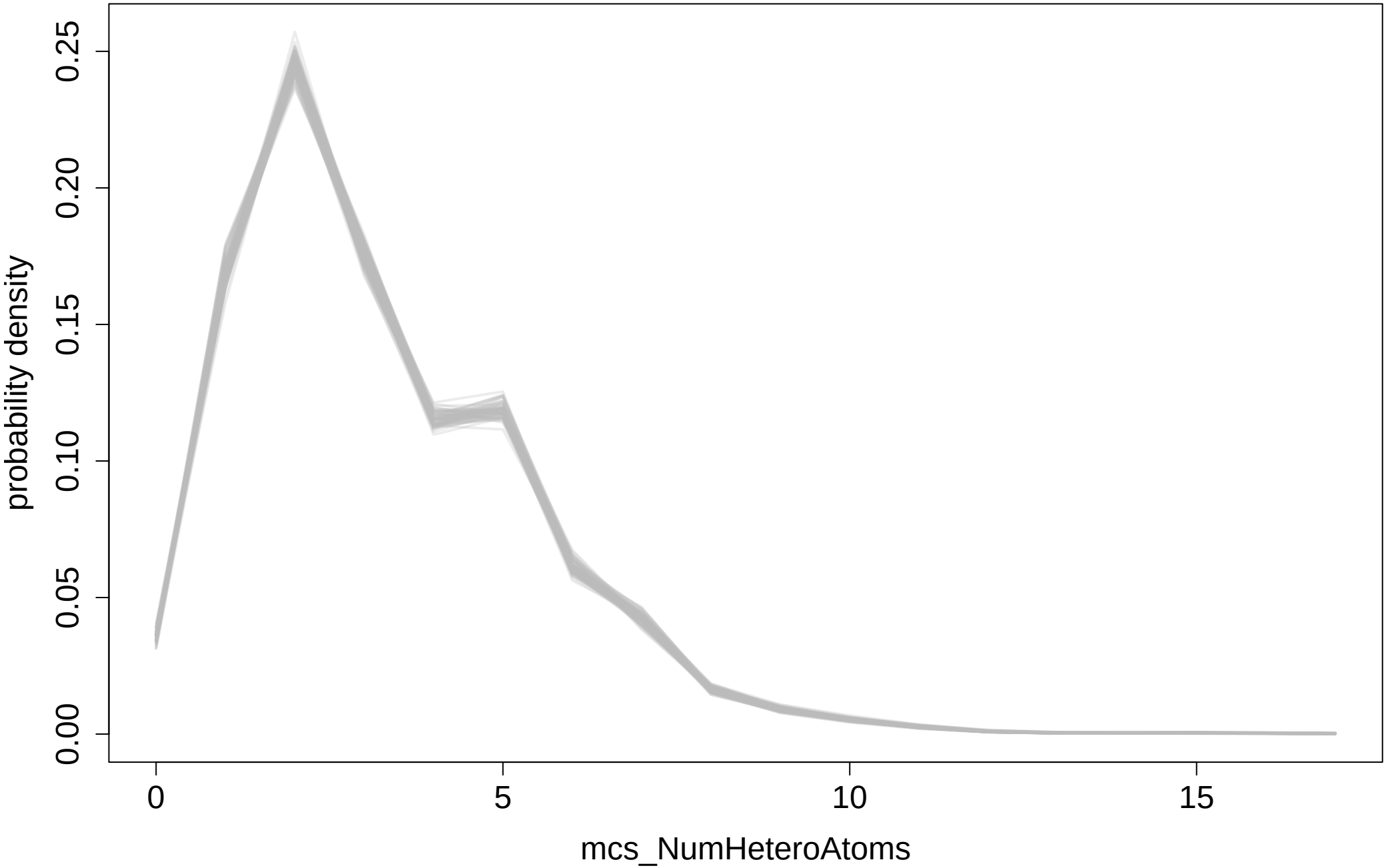

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
docked_HeavyAtomCount

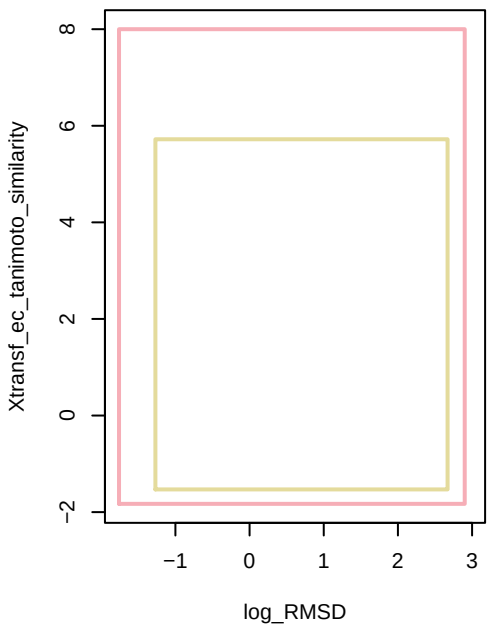

probability density
0.0
0.1
0.2
0.3
0.4
0.5
0
2
4
6
8
mcs_RingCount

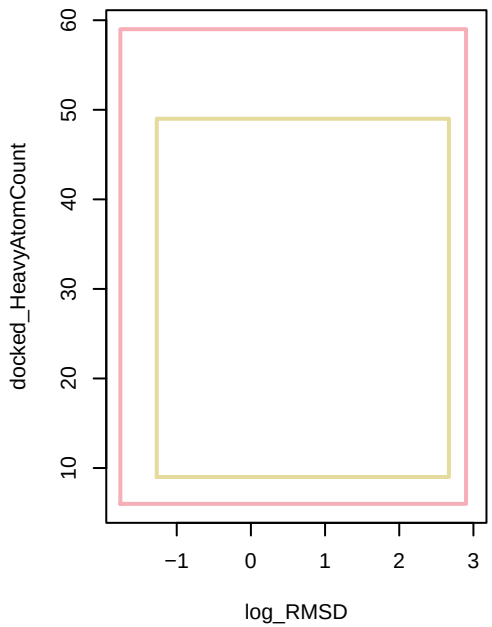

probability density
0.00
0.01
0.02
0.03
0.04
0.05
10
20
30
40
50
60
template_HeavyAtomCount

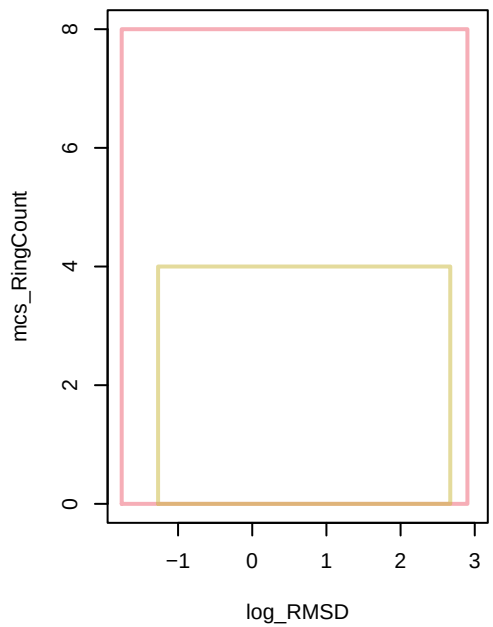

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_docked_NumHAcceptors

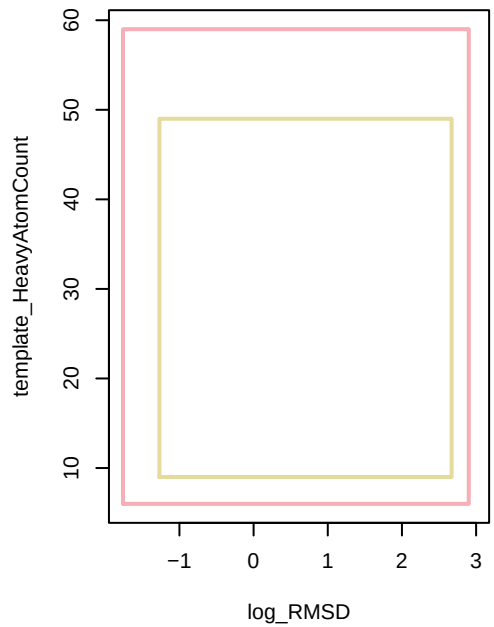

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0
5
10
15
mcs_template_NumHAcceptors

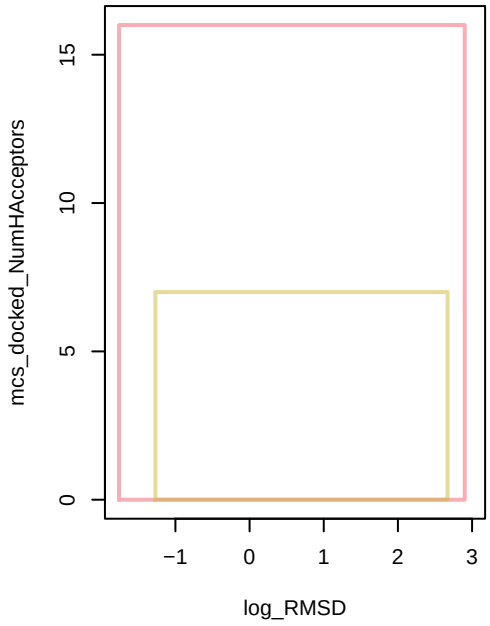

probability density
0.00
0.05
0.10
0.15
0.20
0.25
0
5
10
15
mcs_NumHeteroAtoms

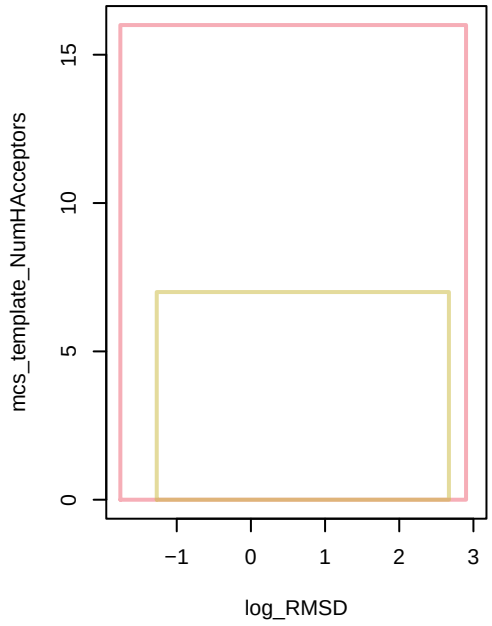

Xtransf_ec_tanimoto_similarity
log_RMSD

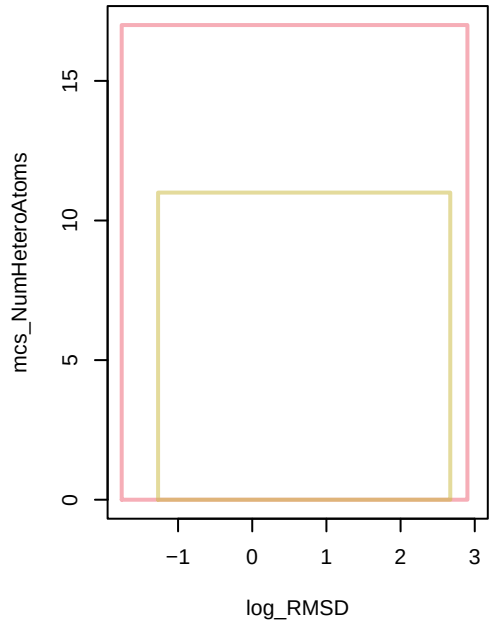

docked_HeavyAtomCount
log_RMSD

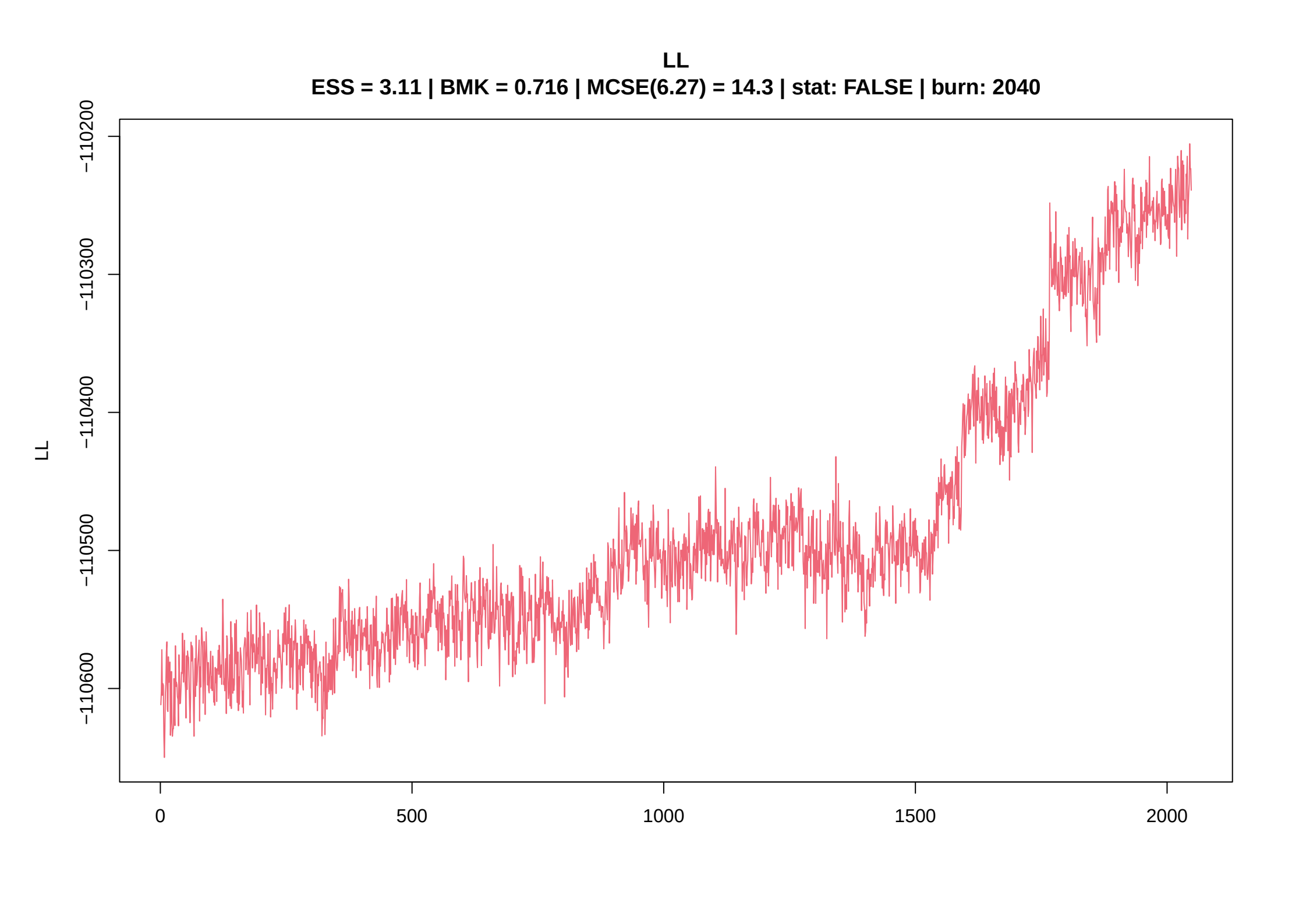

mcs_RingCount
log_RMSD

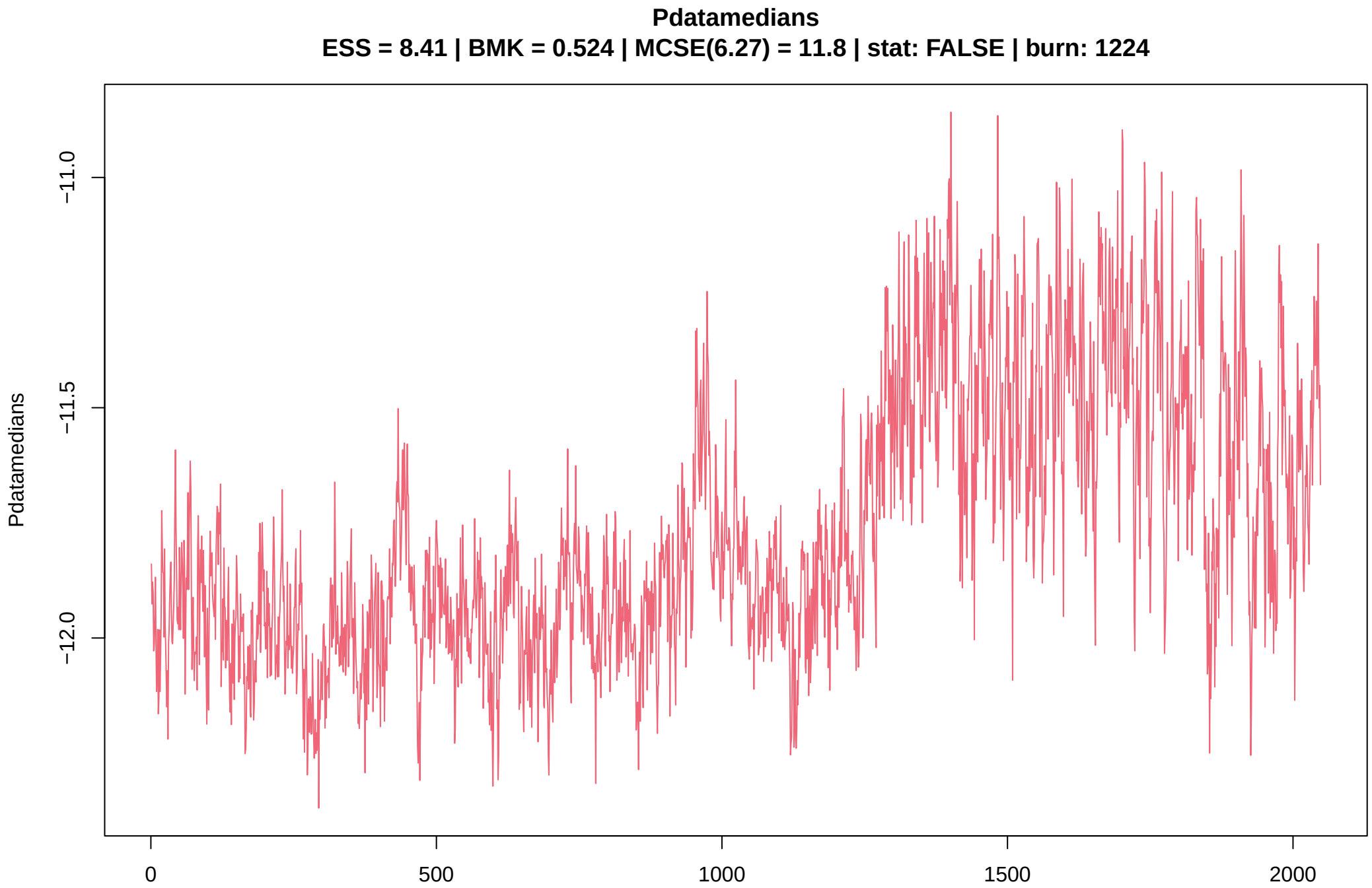

template_HeavyAtomCount
log_RMSD

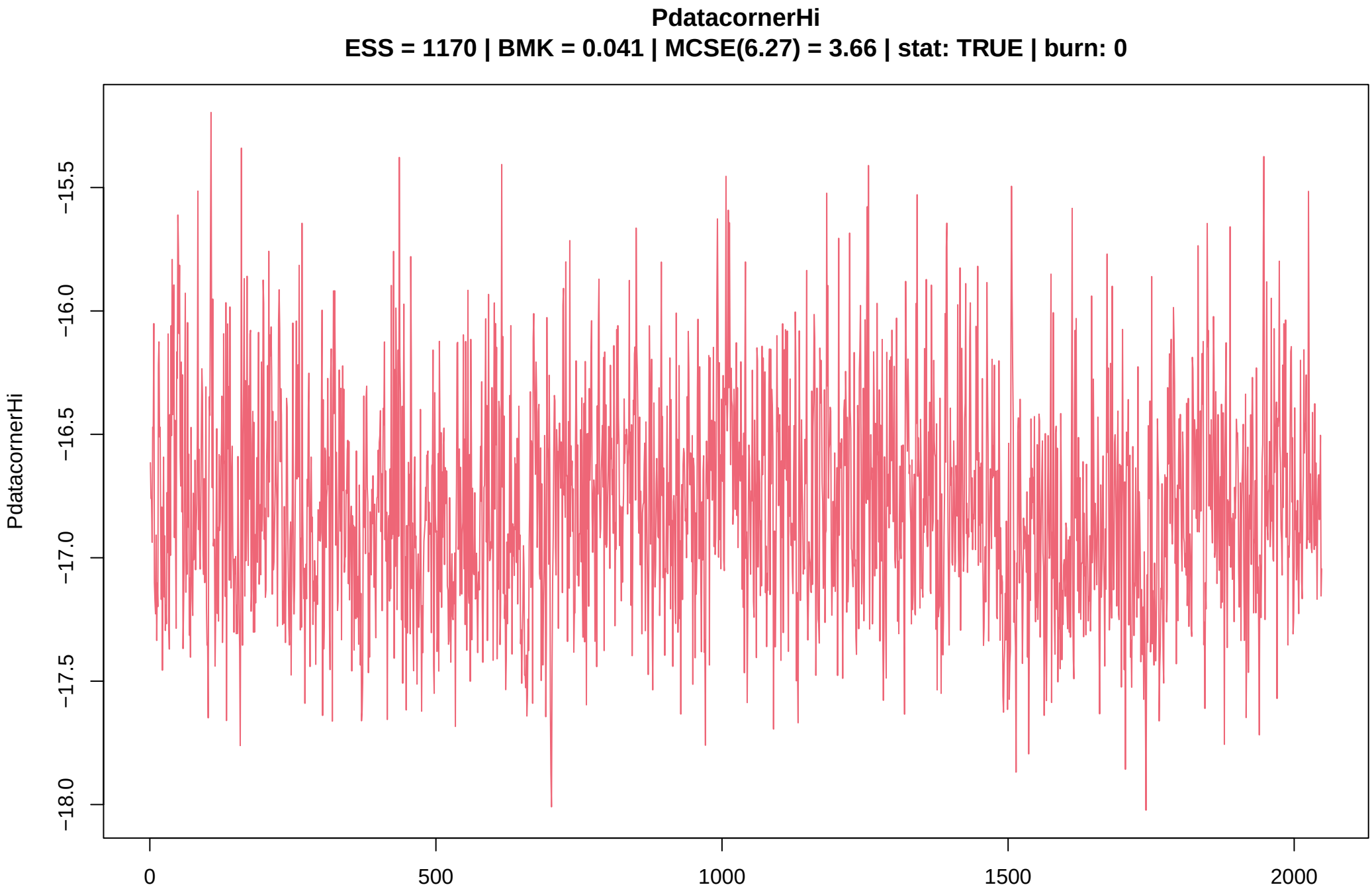

mcs_docked_NumHAcceptors
log_RMSD

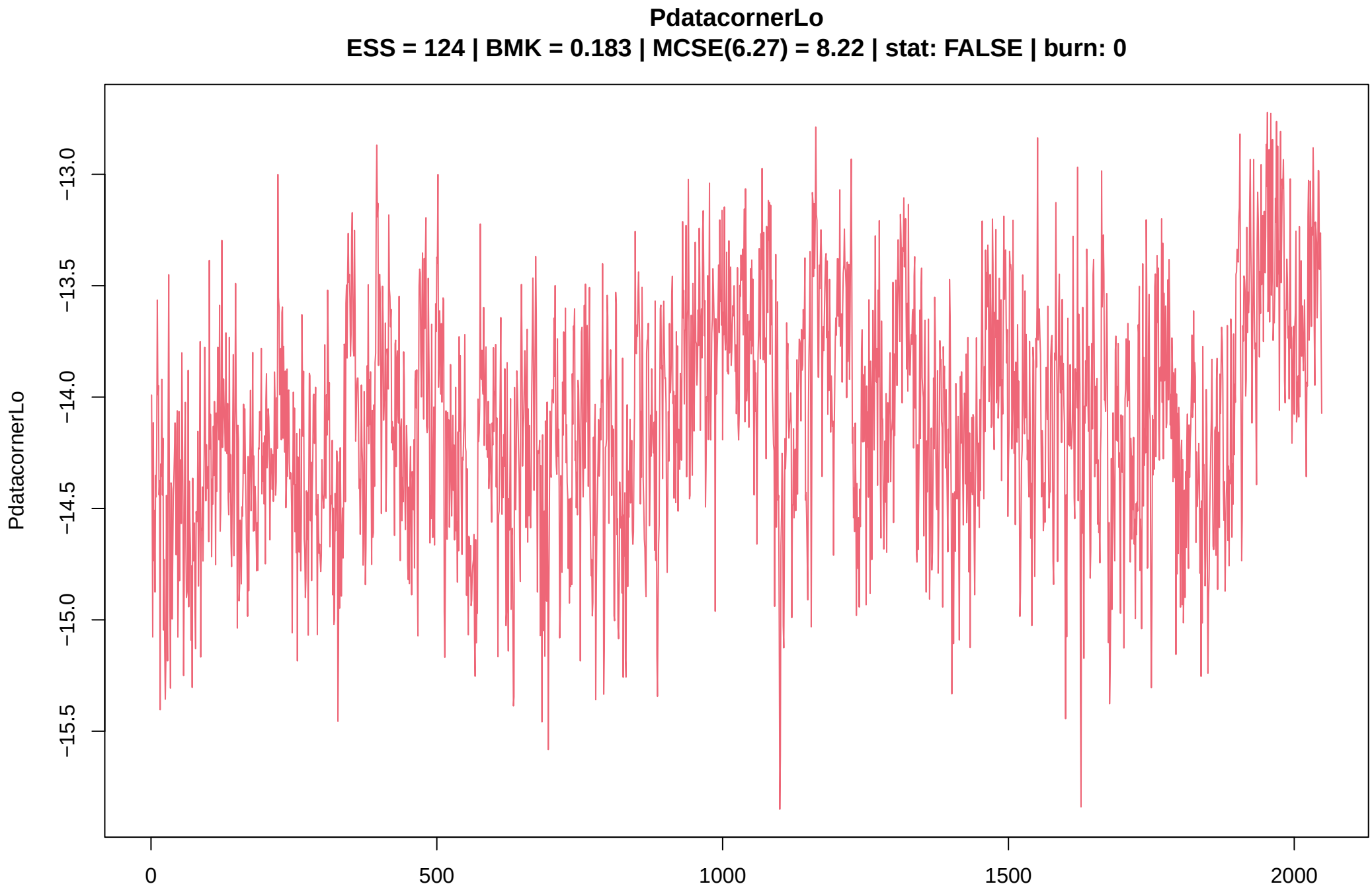

mcs_template_NumHAcceptors
log_RMSD

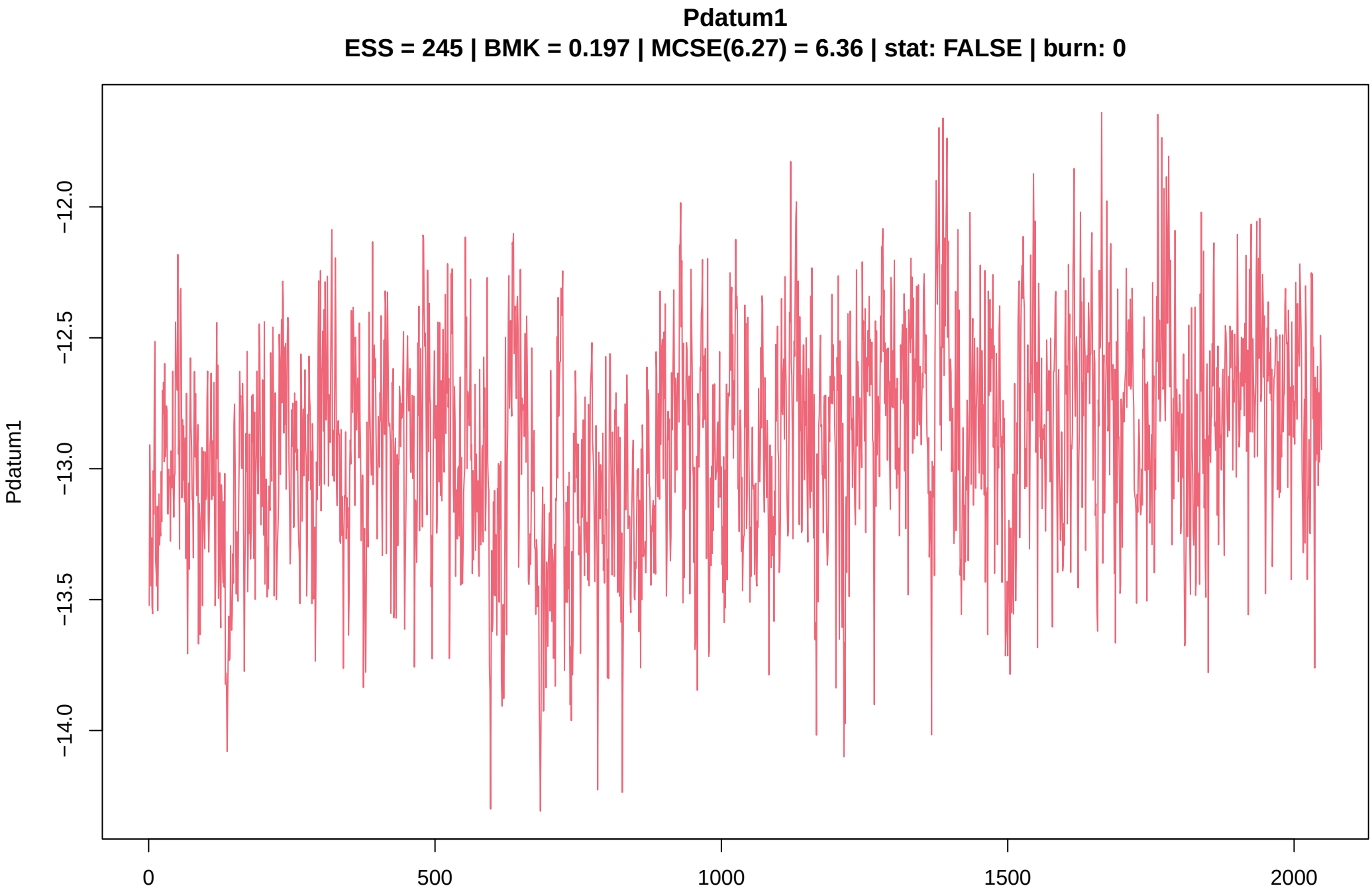

mcs_NumHeteroAtoms
log_RMSD

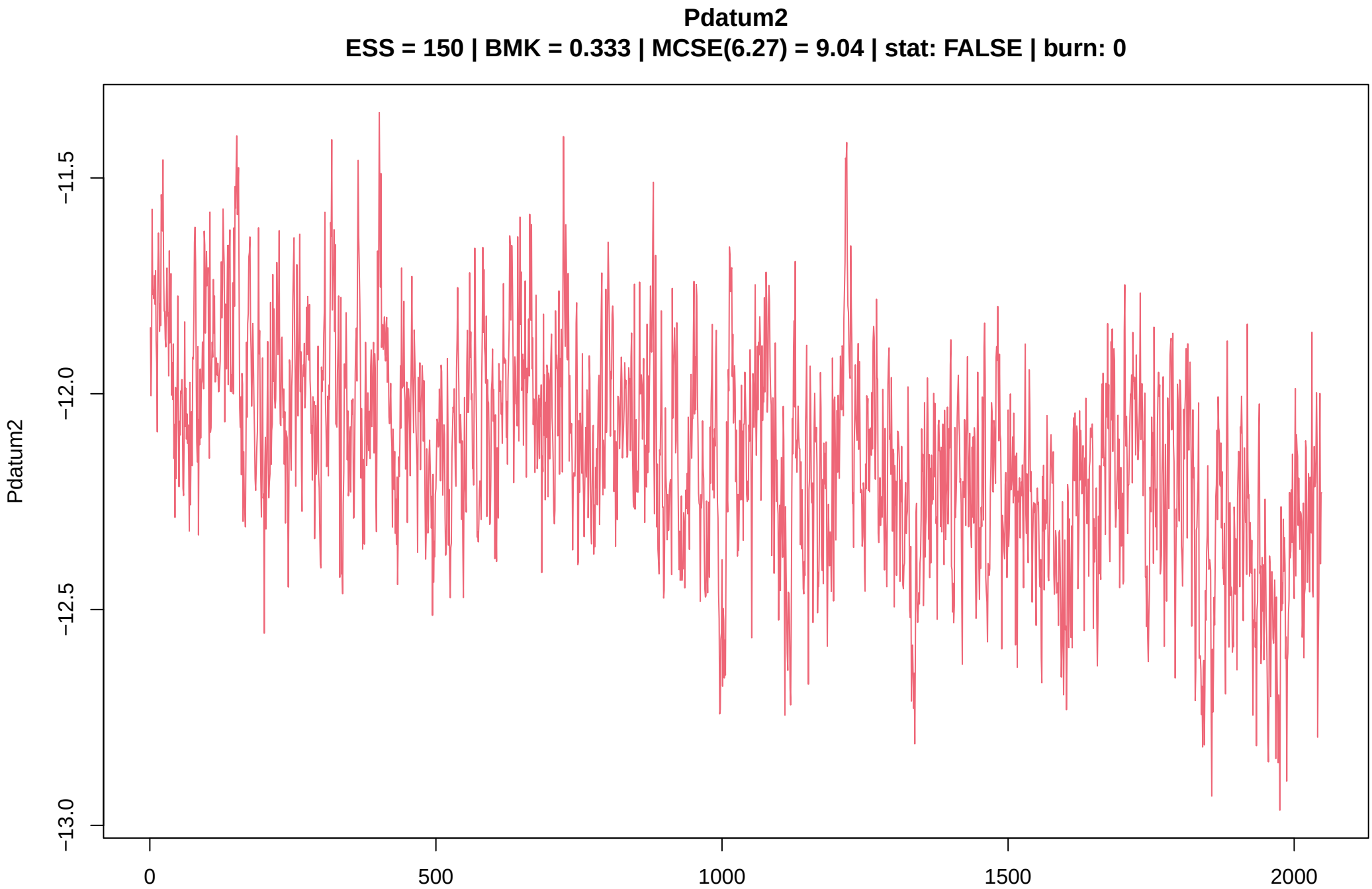

LL
ESS = 3.11 | BMK = 0.716 | MCSE(6.27) = 14.3 | stat: FALSE | burn: 2040
LL
−110200
−110300
−110400
−110500
−110600
0
500
1000
1500
2000

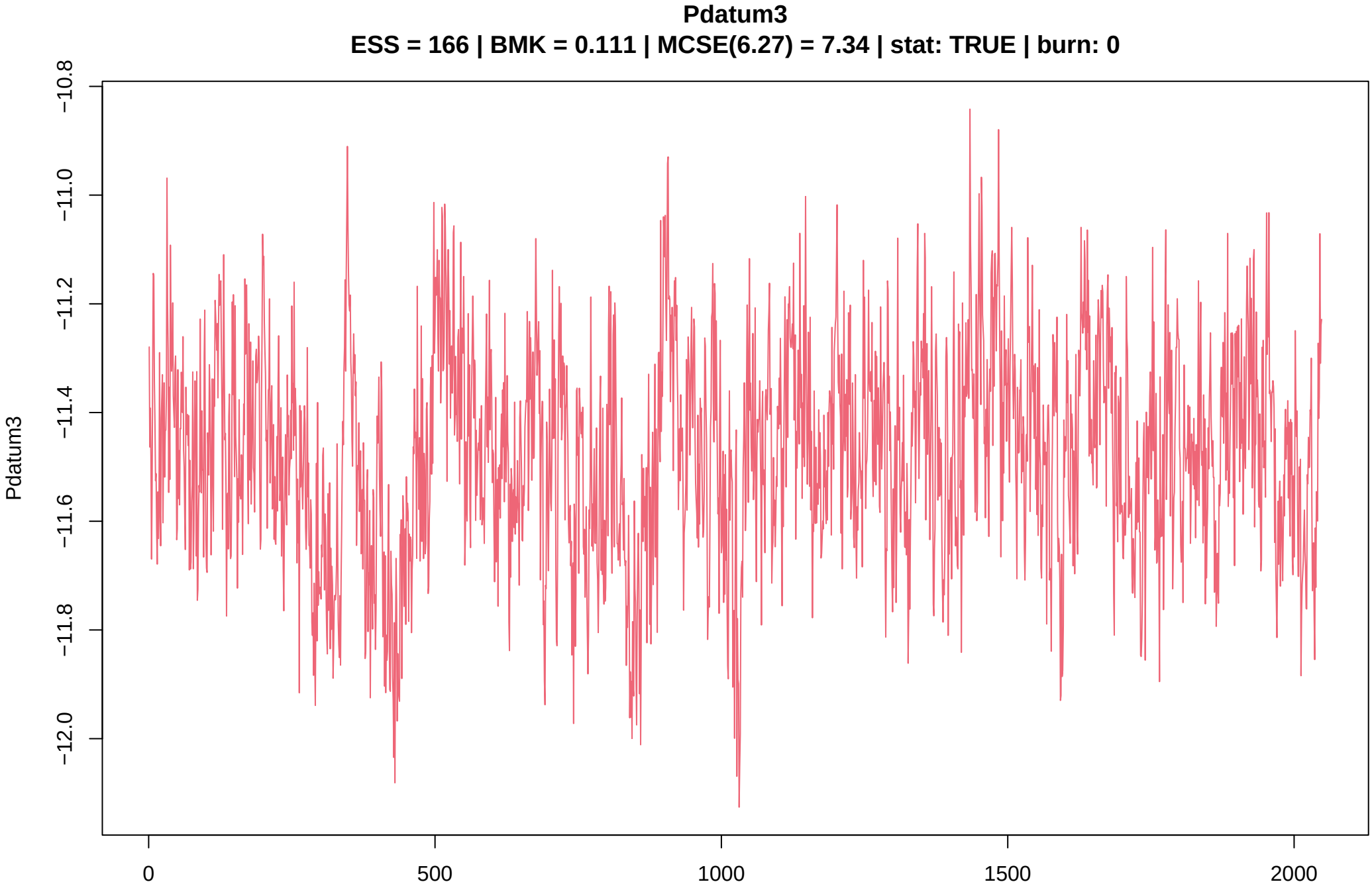

Pdatamedians
ESS = 8.41 | BMK = 0.524 | MCSE(6.27) = 11.8 | stat: FALSE | burn: 1224
Pdatamedians
−11.0
−11.5
−12.0
0
500
1000
1500
2000

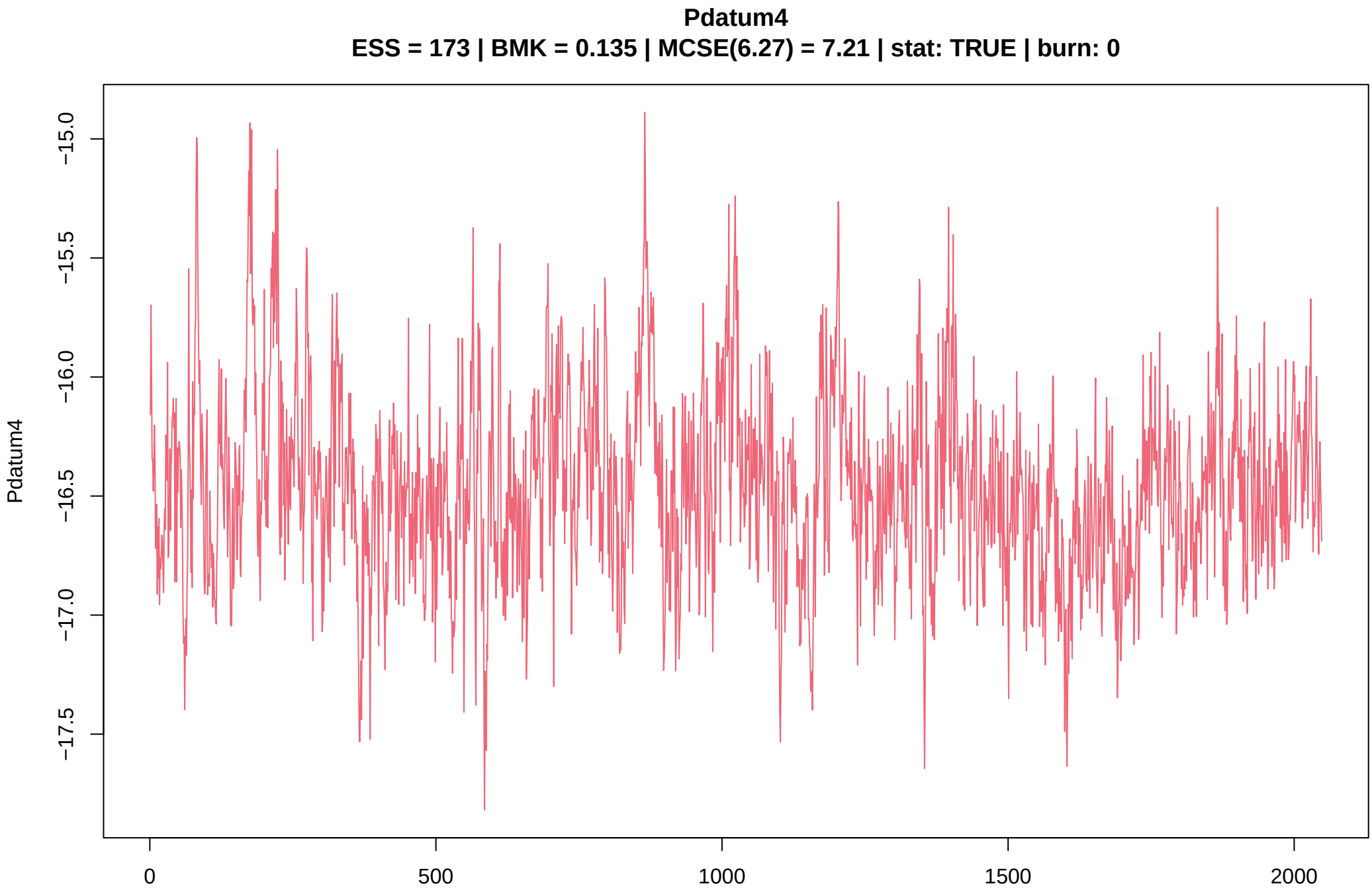

PdatacornerHi
ESS = 1170 | BMK = 0.041 | MCSE(6.27) = 3.66 | stat: TRUE | burn: 0
PdatacornerHi
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
0
500
1000
1500
2000

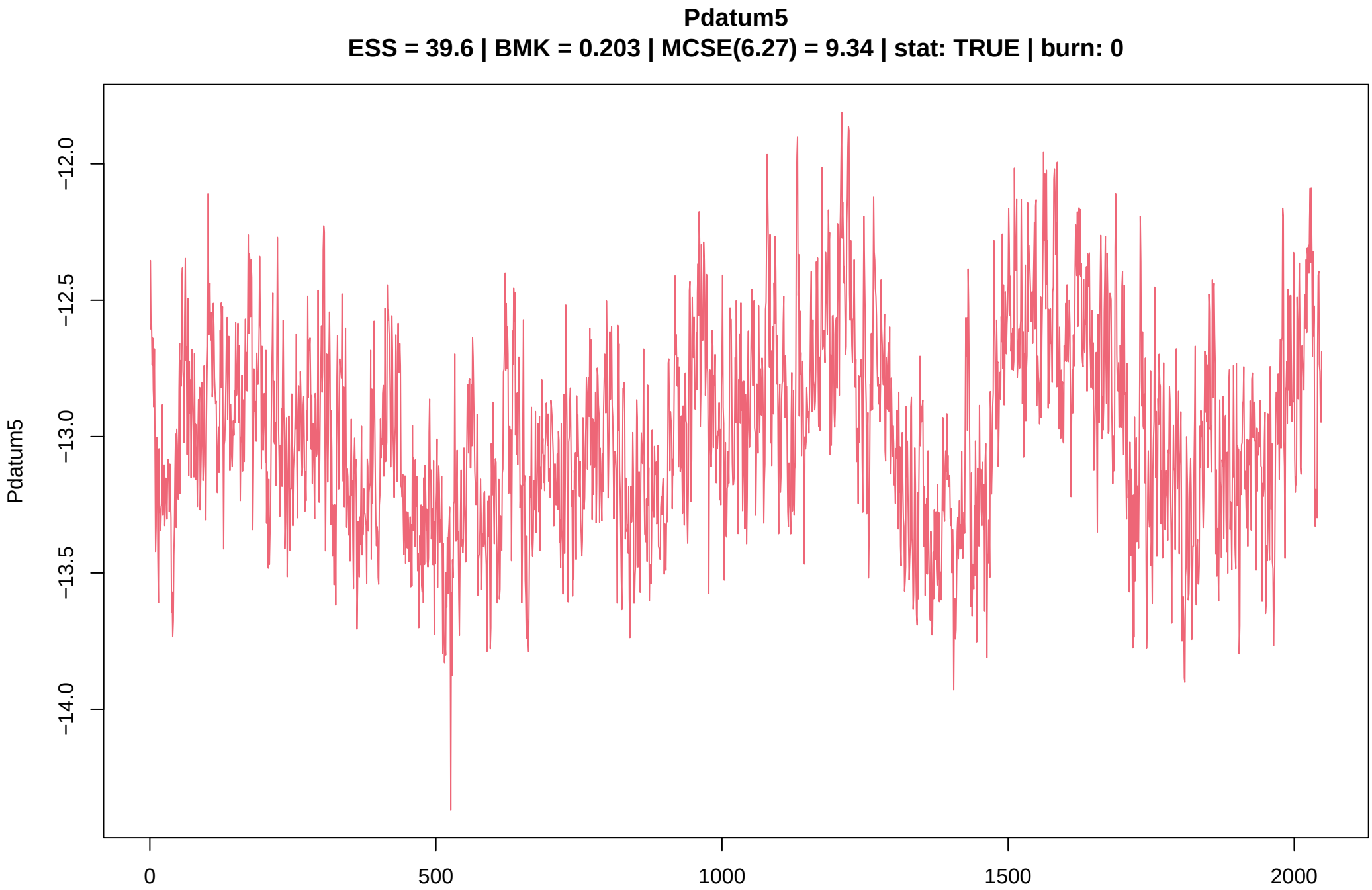

PdatacornerLo
ESS = 124 | BMK = 0.183 | MCSE(6.27) = 8.22 | stat: FALSE | burn: 0
PdatacornerLo
−13.0
−13.5
−14.0
−14.5
−15.0
−15.5
0
500
1000
1500
2000

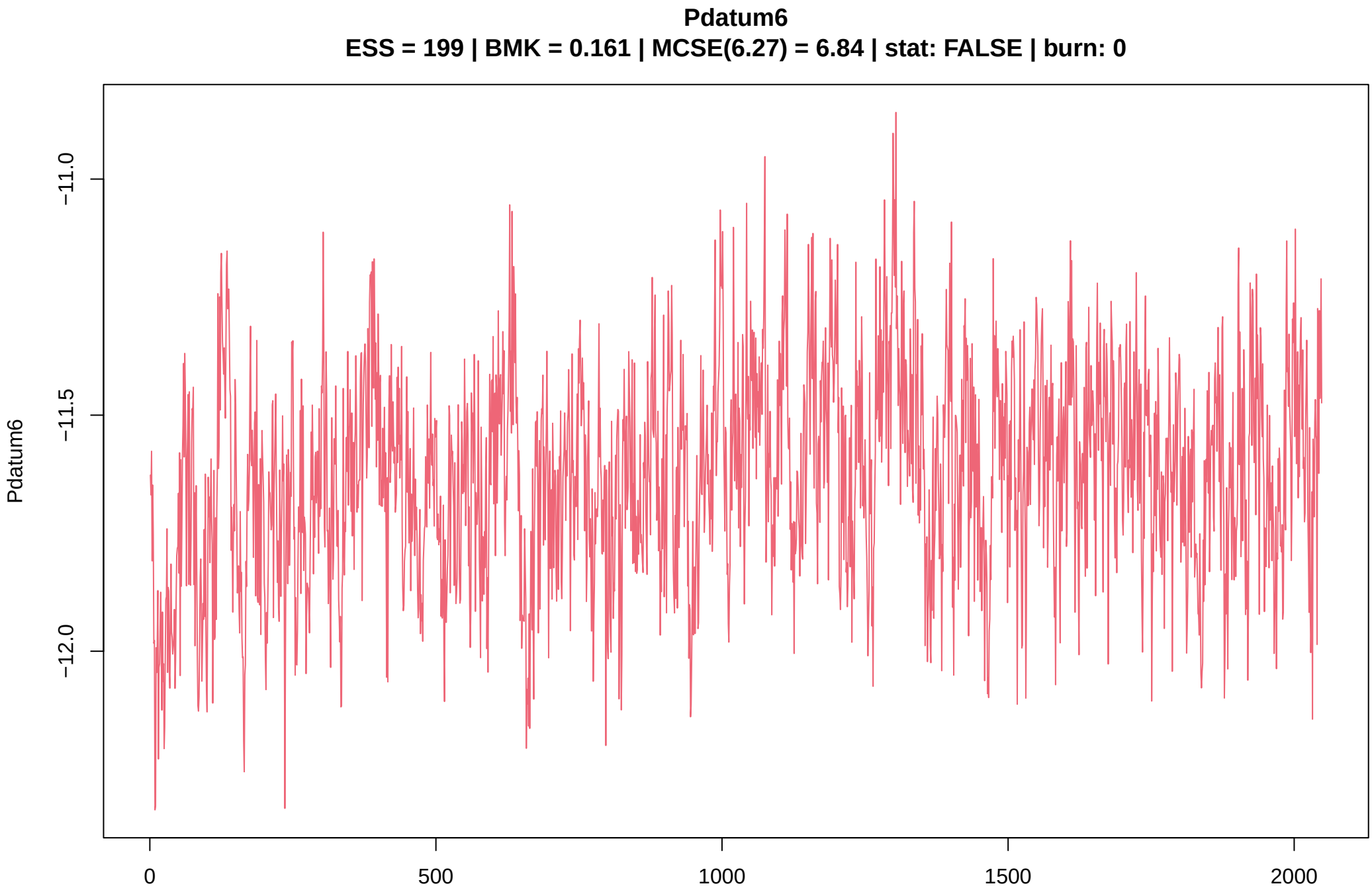

Pdatum1
ESS = 245 | BMK = 0.197 | MCSE(6.27) = 6.36 | stat: FALSE | burn: 0
Pdatum1
−12.0
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

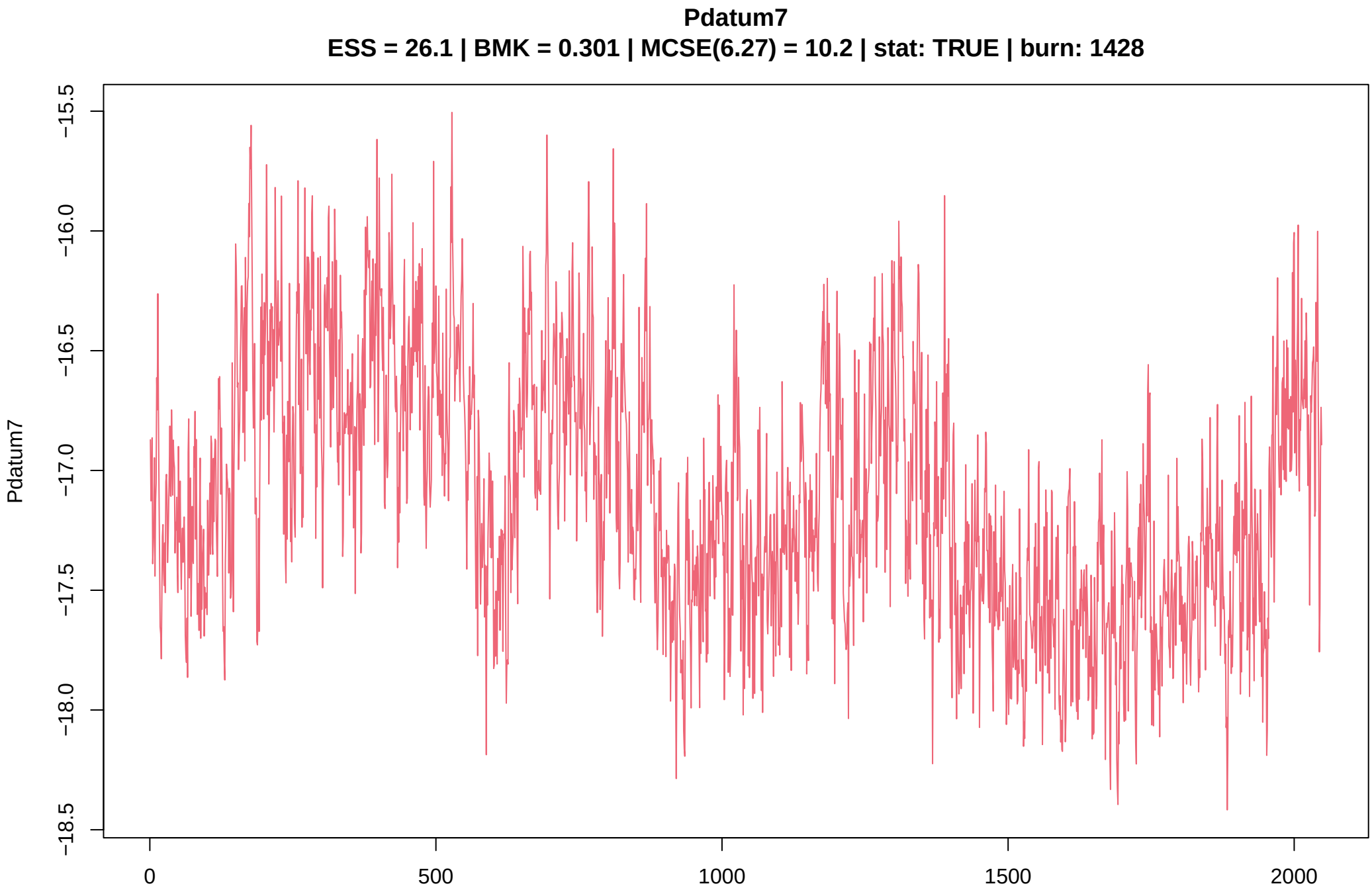

Pdatum2
ESS = 150 | BMK = 0.333 | MCSE(6.27) = 9.04 | stat: FALSE | burn: 0
Pdatum2
−11.5
−12.0
−12.5
−13.0
0
500
1000
1500
2000

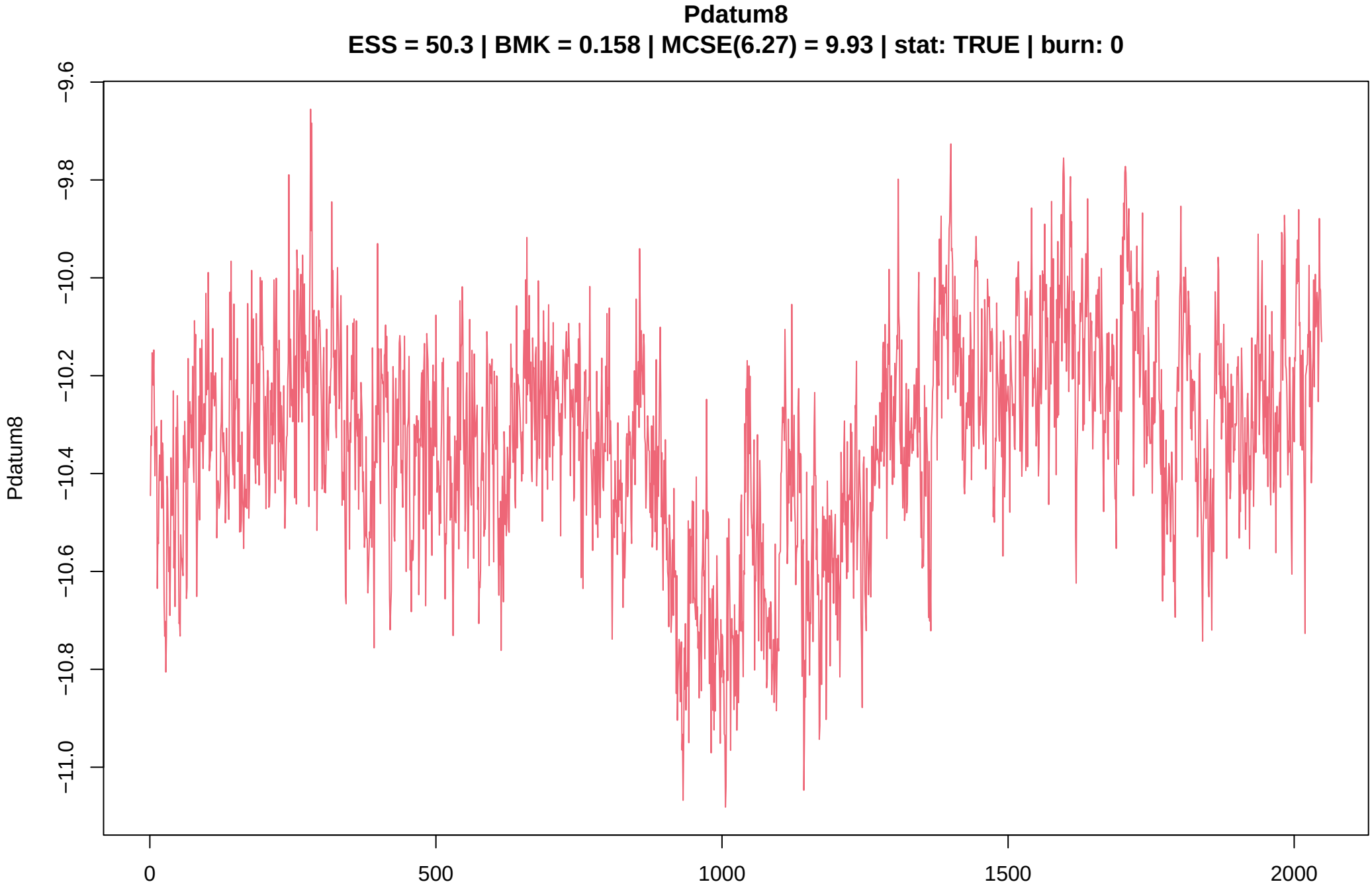

Pdatum3
ESS = 166 | BMK = 0.111 | MCSE(6.27) = 7.34 | stat: TRUE | burn: 0
Pdatum3
−10.8
−11.0
−11.2
−11.4
−11.6
−11.8
−12.0
0
500
1000
1500
2000

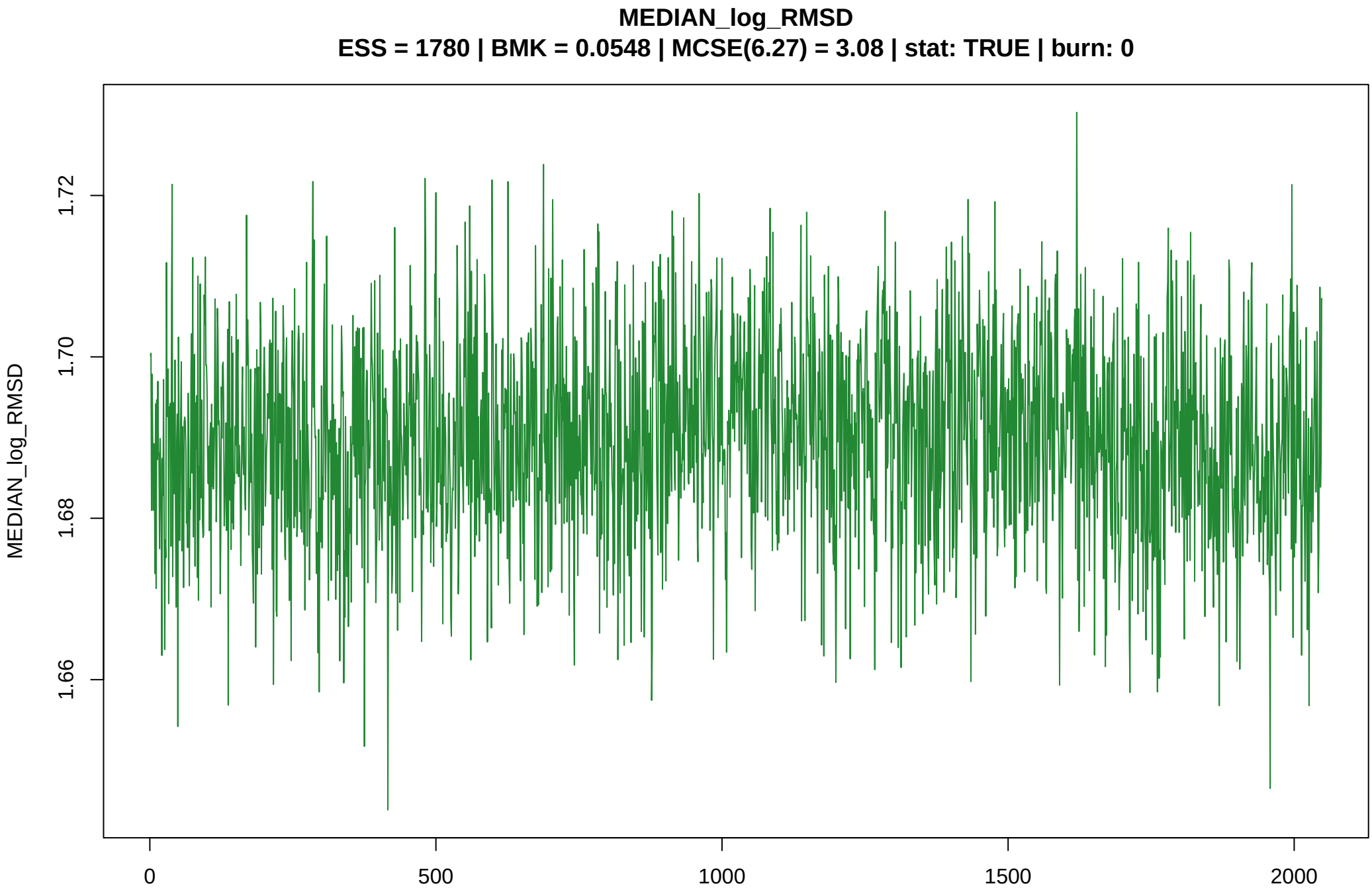

Pdatum4
ESS = 173 | BMK = 0.135 | MCSE(6.27) = 7.21 | stat: TRUE | burn: 0
Pdatum4
−15.0
−15.5
−16.0
−16.5
−17.0
−17.5
0
500
1000
1500
2000

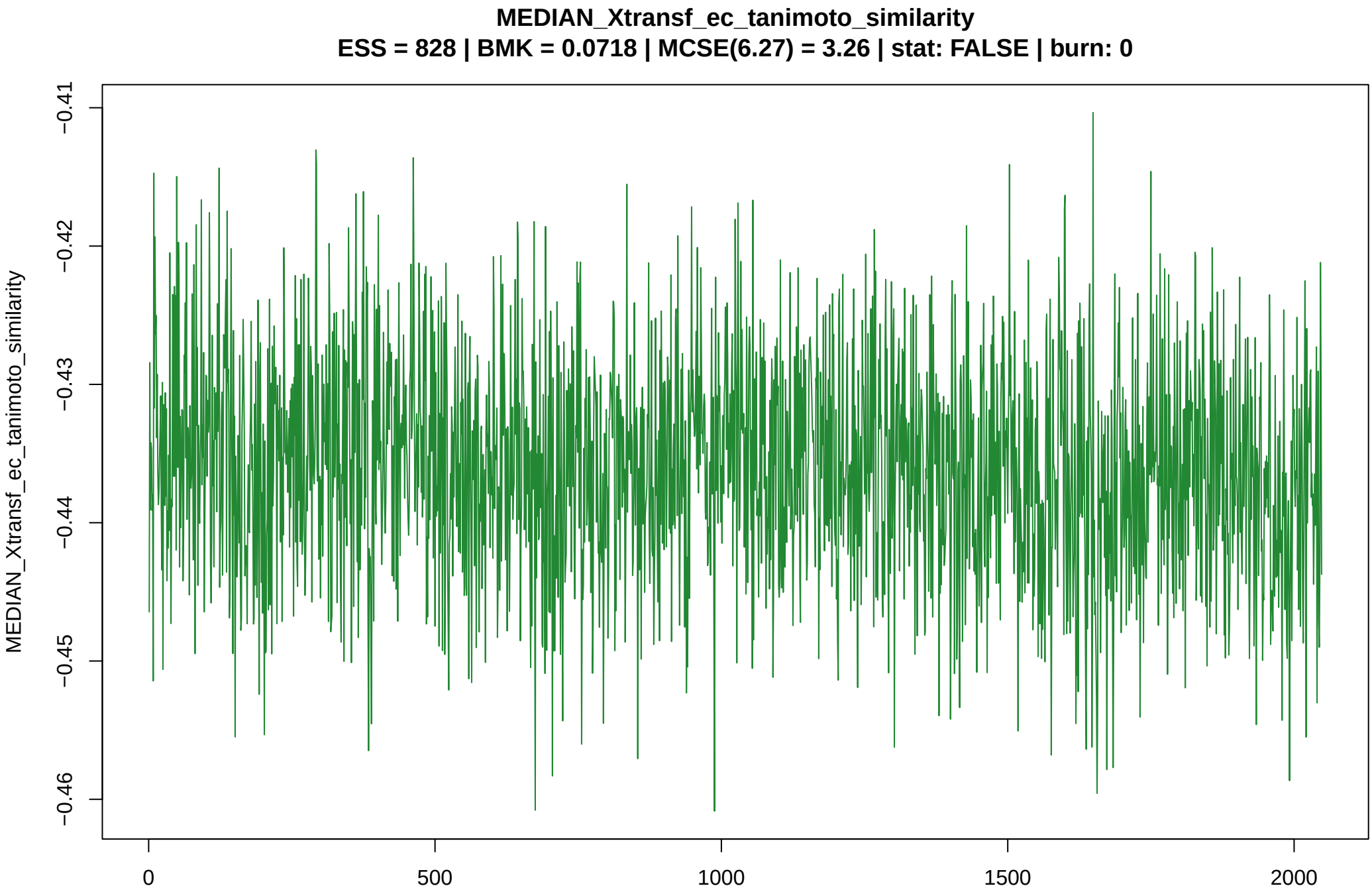

Pdatum5
ESS = 39.6 | BMK = 0.203 | MCSE(6.27) = 9.34 | stat: TRUE | burn: 0
Pdatum5
−12.0
−12.5
−13.0
−13.5
−14.0
0
500
1000
1500
2000

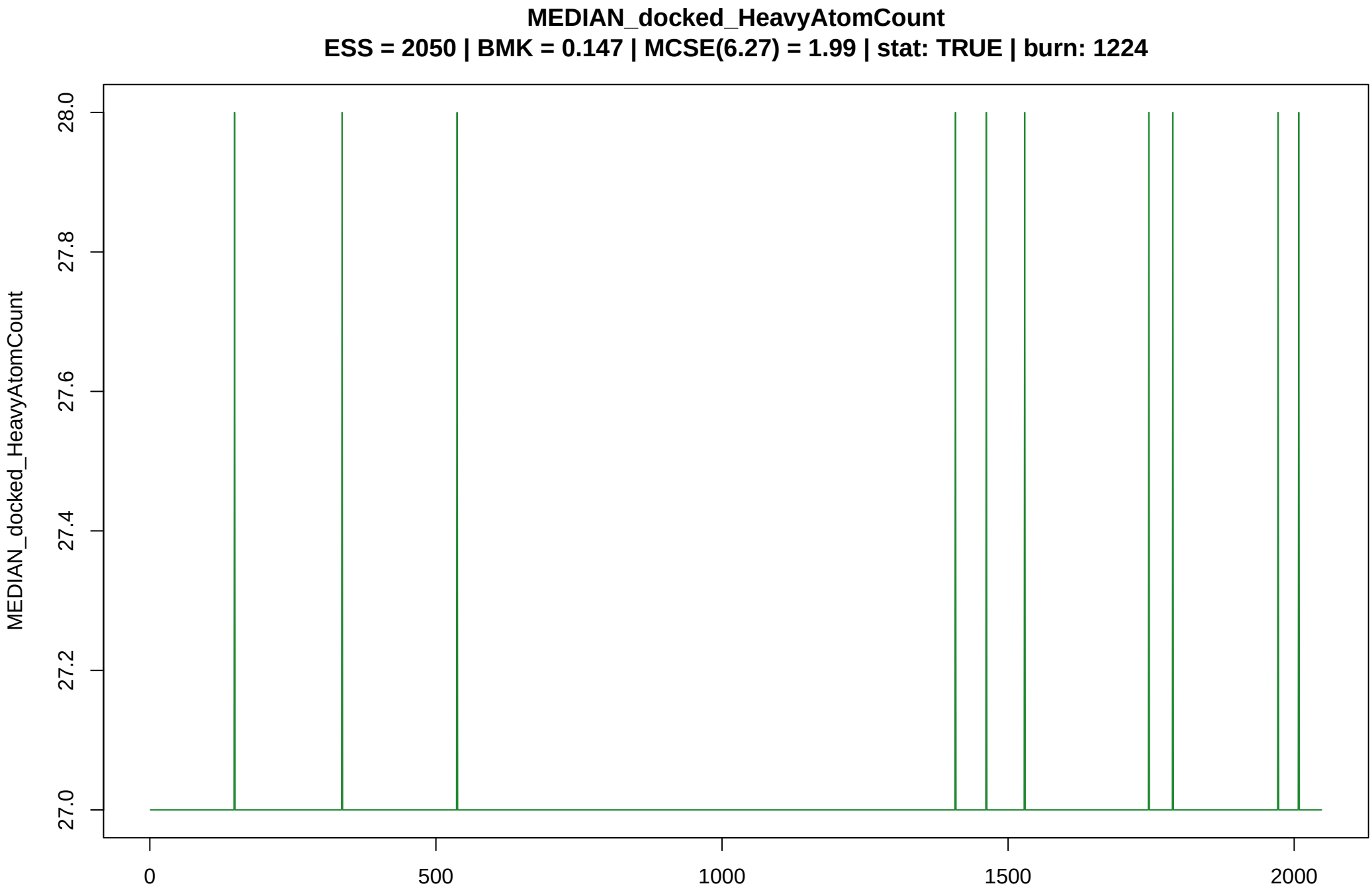

Pdatum6
ESS = 199 | BMK = 0.161 | MCSE(6.27) = 6.84 | stat: FALSE | burn: 0
Pdatum6
−11.0
−11.5
−12.0
0
500
1000
1500
2000

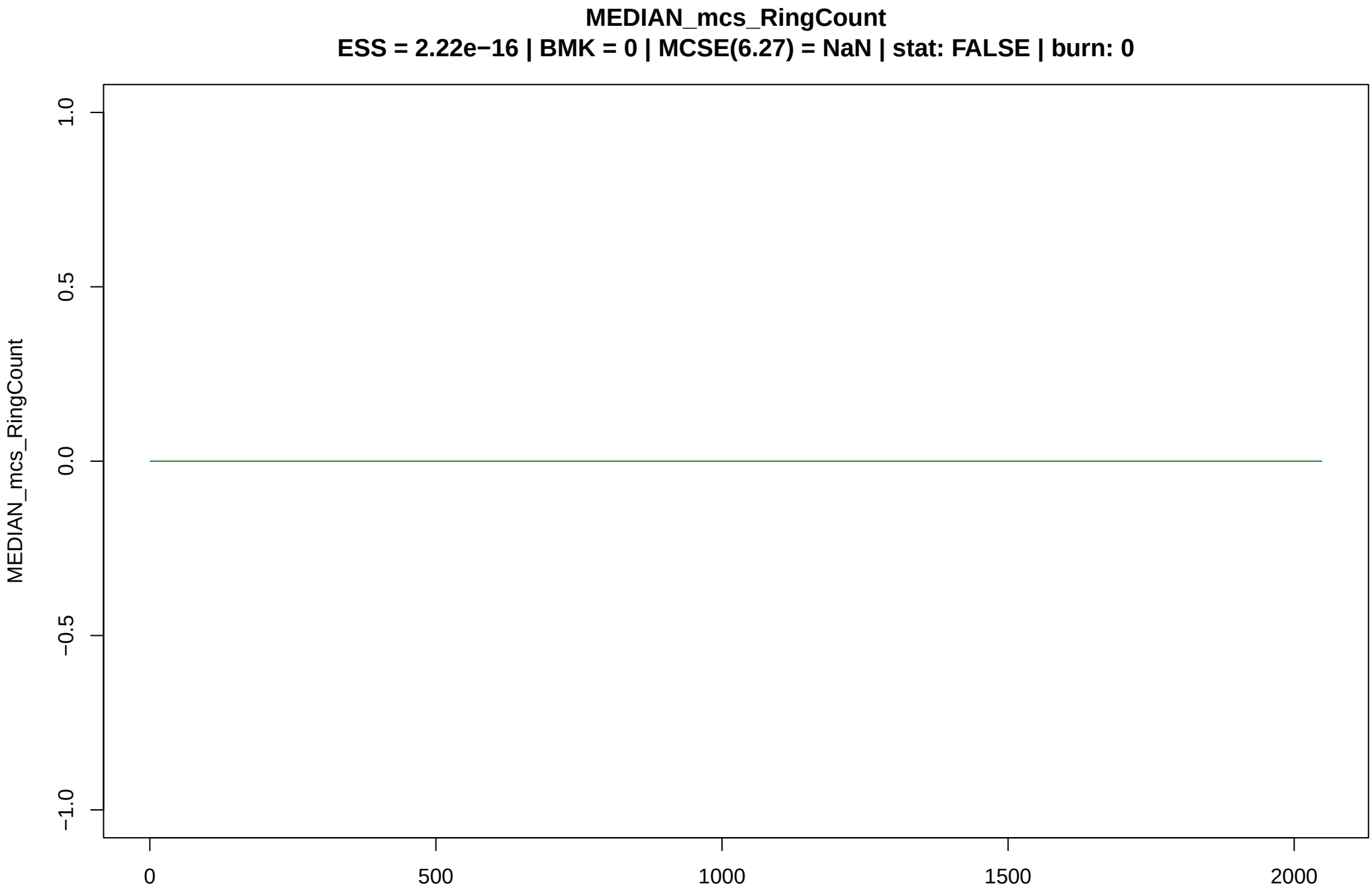

Pdatum7
ESS = 26.1 | BMK = 0.301 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 1428
Pdatum7
−15.5
−16.0
−16.5
−17.0
−17.5
−18.0
−18.5
0
500
1000
1500
2000

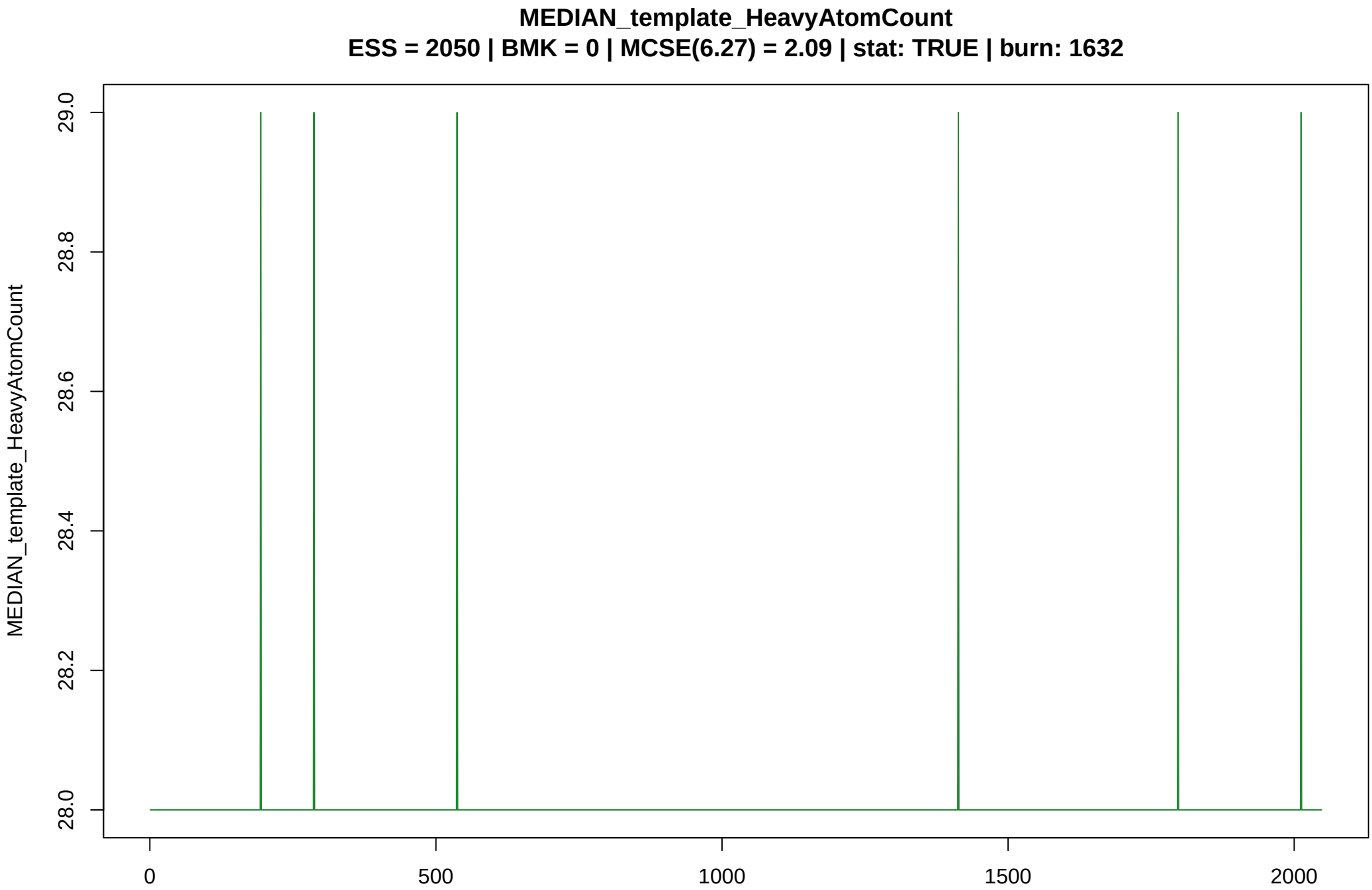

Pdatum8
ESS = 50.3 | BMK = 0.158 | MCSE(6.27) = 9.93 | stat: TRUE | burn: 0
Pdatum8
−9.6
−9.8
−10.0
−10.2
−10.4
−10.6
−10.8
−11.0
0
500
1000
1500
2000

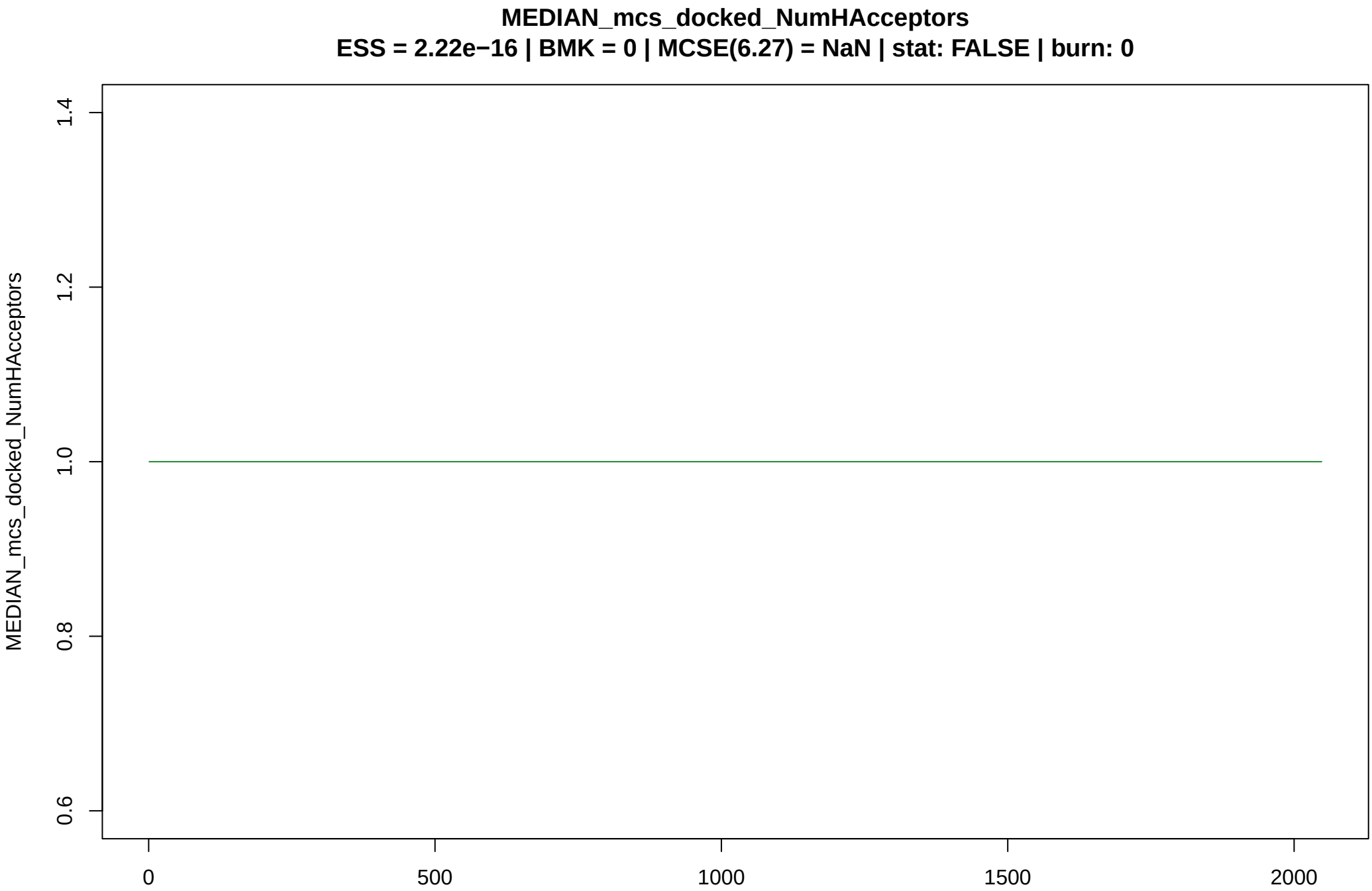

MEDIAN_log_RMSD
ESS = 1780 | BMK = 0.0548 | MCSE(6.27) = 3.08 | stat: TRUE | burn: 0
MEDIAN_log_RMSD
1.66
1.68
1.70
1.72
0
500
1000
1500
2000

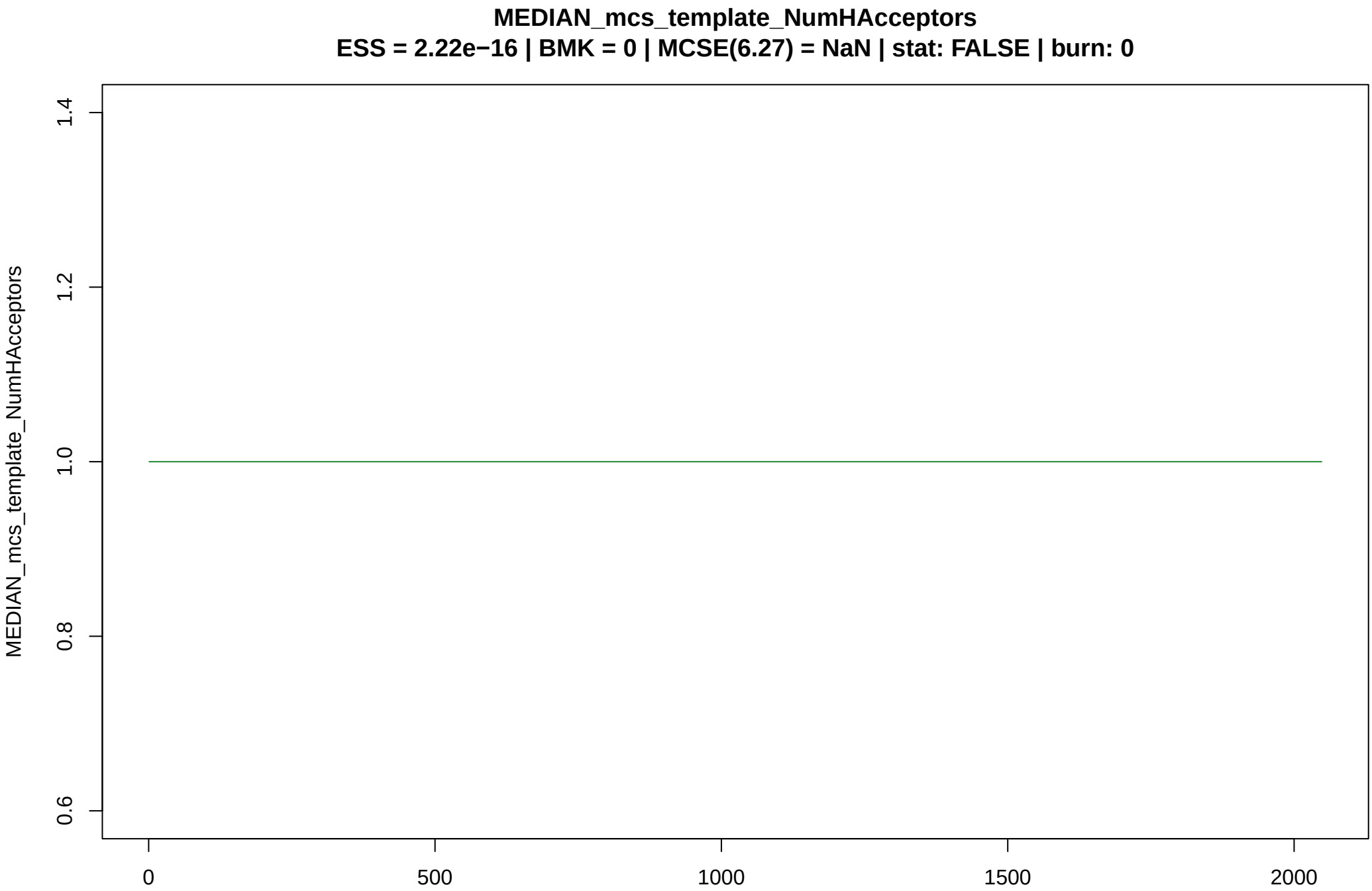

MEDIAN_Xtransf_ec_tanimoto_similarity
ESS = 828 | BMK = 0.0718 | MCSE(6.27) = 3.26 | stat: FALSE | burn: 0
MEDIAN_Xtransf_ec_tanimoto_similarity
−0.41
−0.42
−0.43
−0.44
−0.45
−0.46
0
500
1000
1500
2000

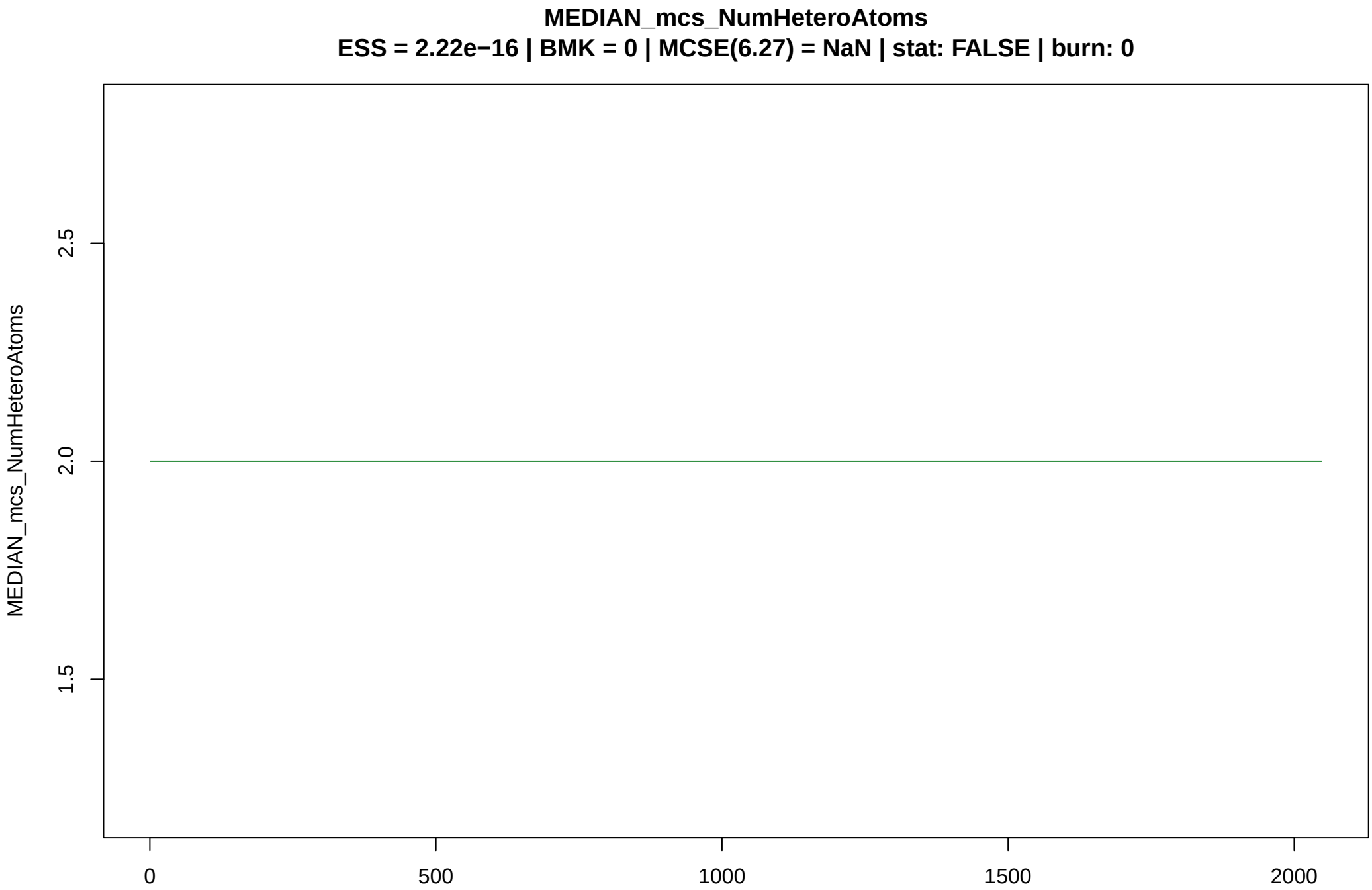

MEDIAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.147 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 1224
MEDIAN_docked_HeavyAtomCount
28.0
27.8
27.6
27.4
27.2
27.0
0
500
1000
1500
2000

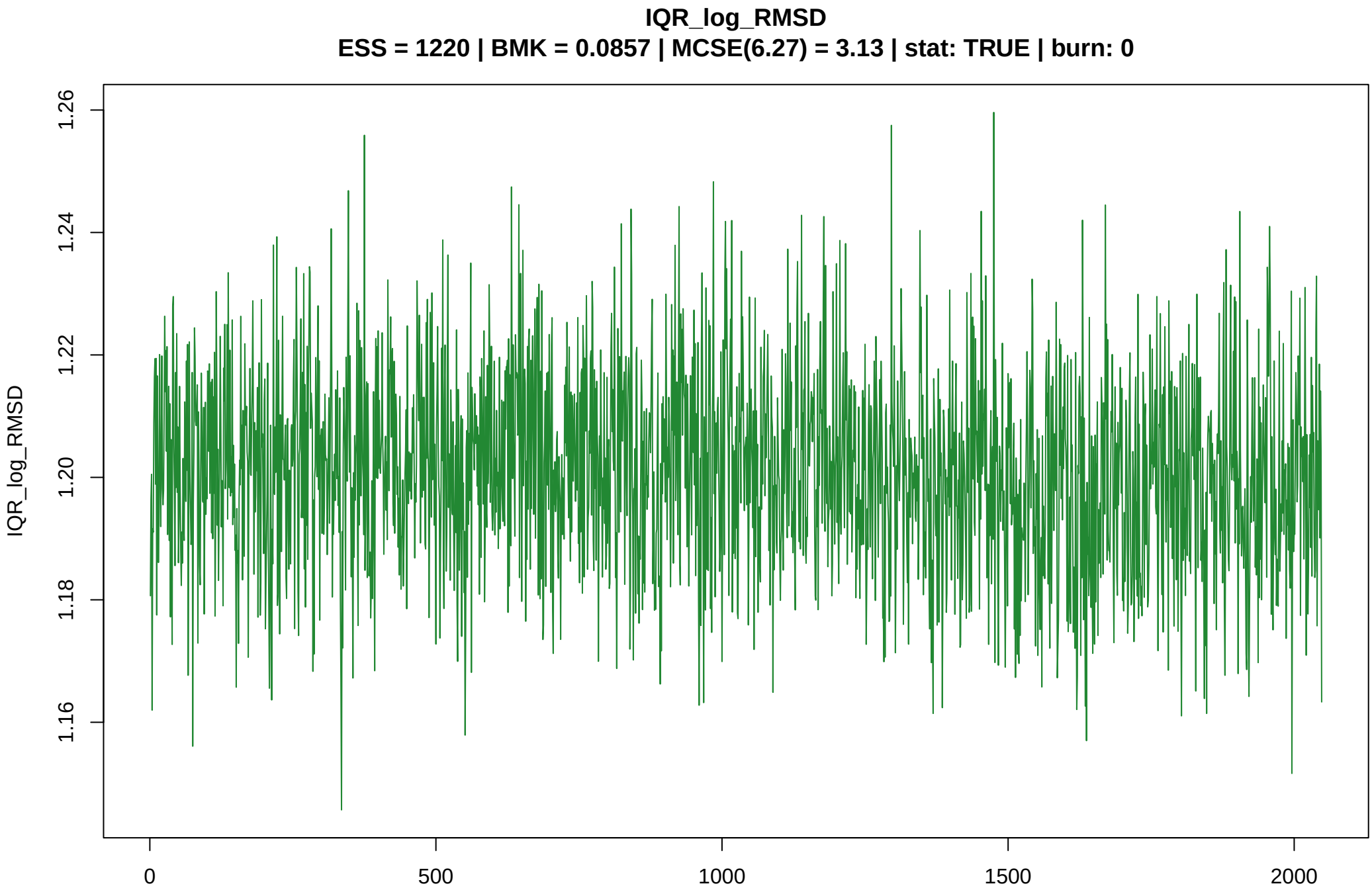

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

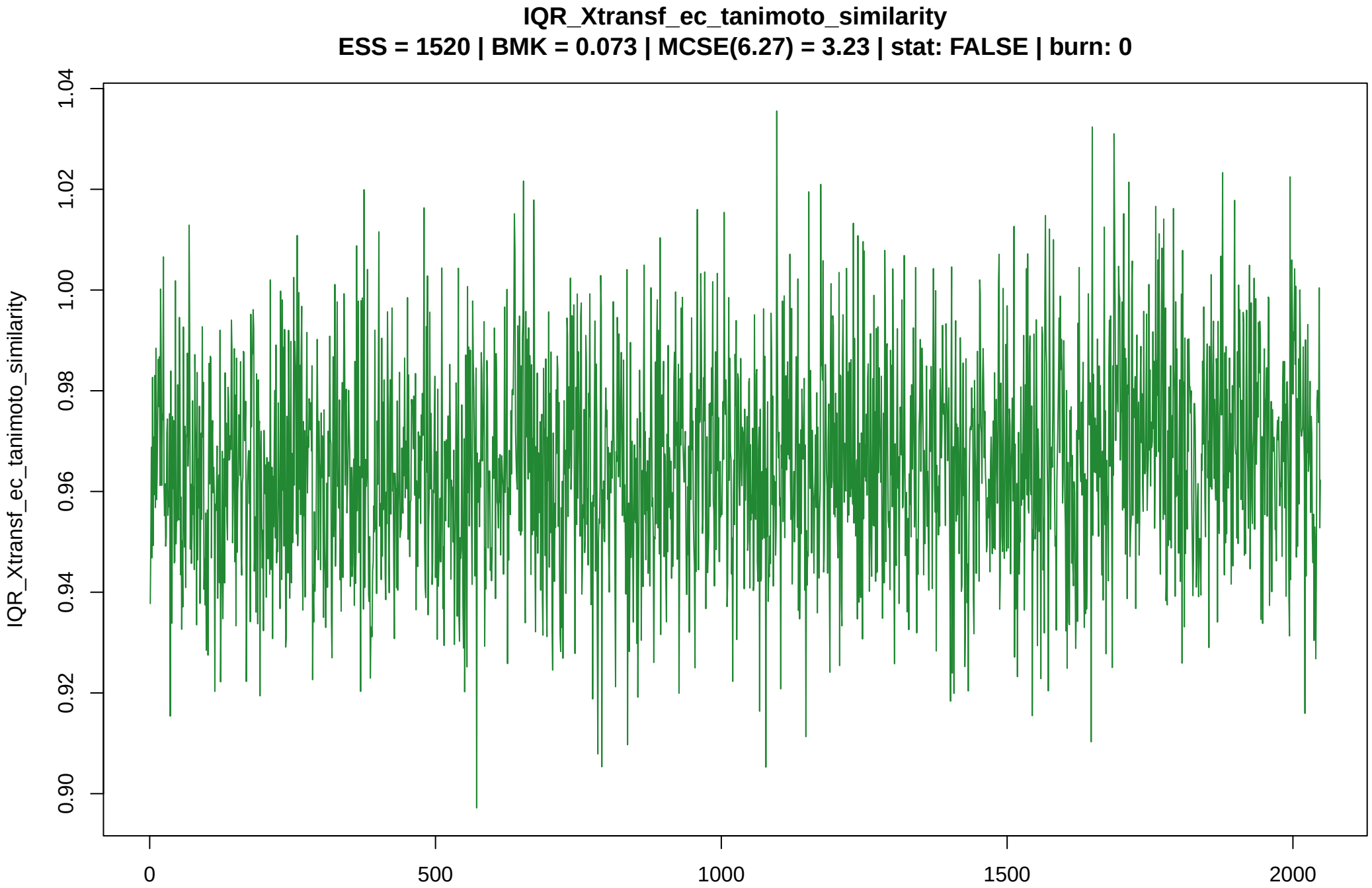

MEDIAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0 | MCSE(6.27) = 2.09 | stat: TRUE | burn: 1632
MEDIAN_template_HeavyAtomCount
29.0
28.8
28.6
28.4
28.2
28.0
0
500
1000
1500
2000

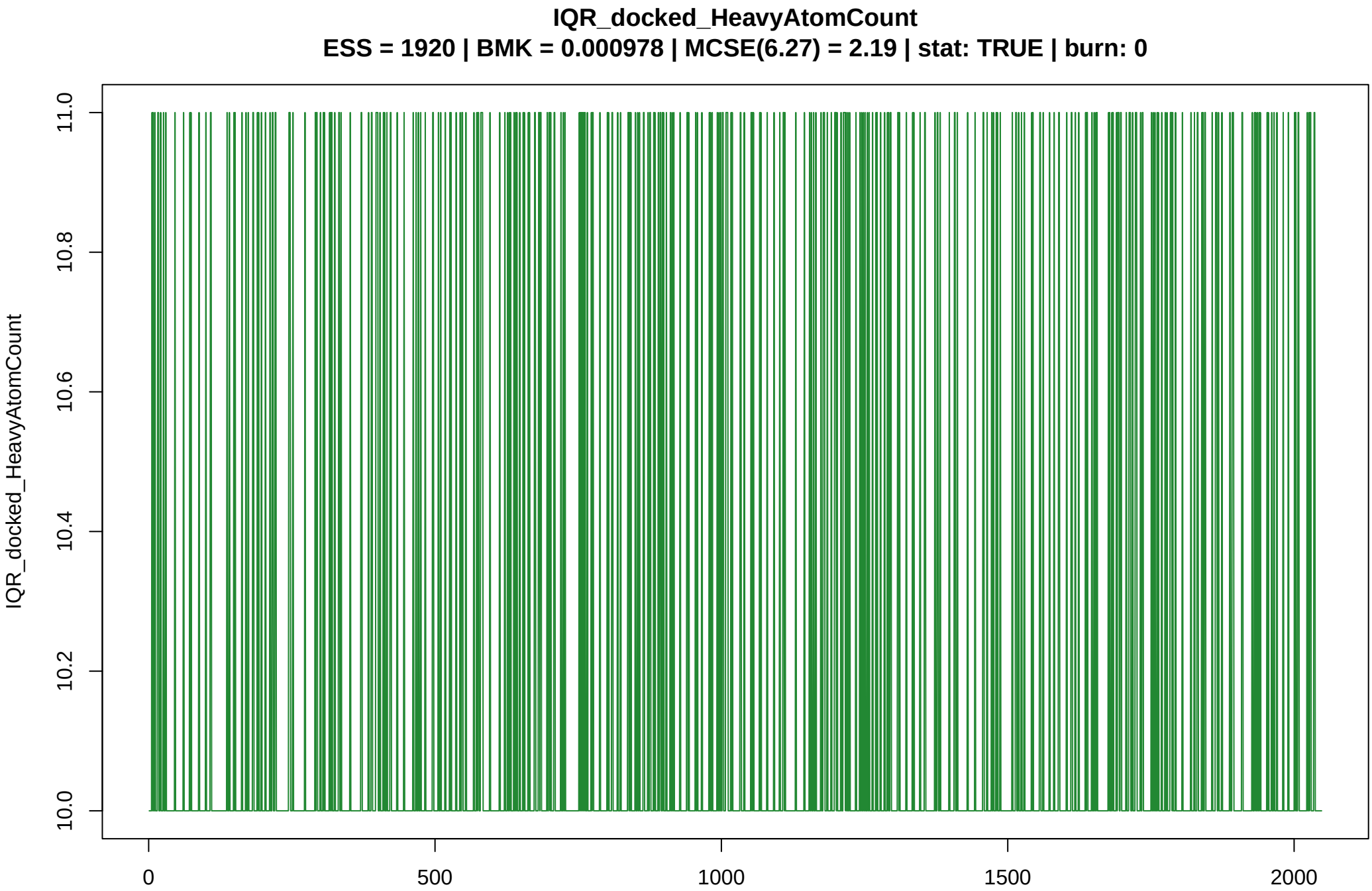

MEDIAN_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

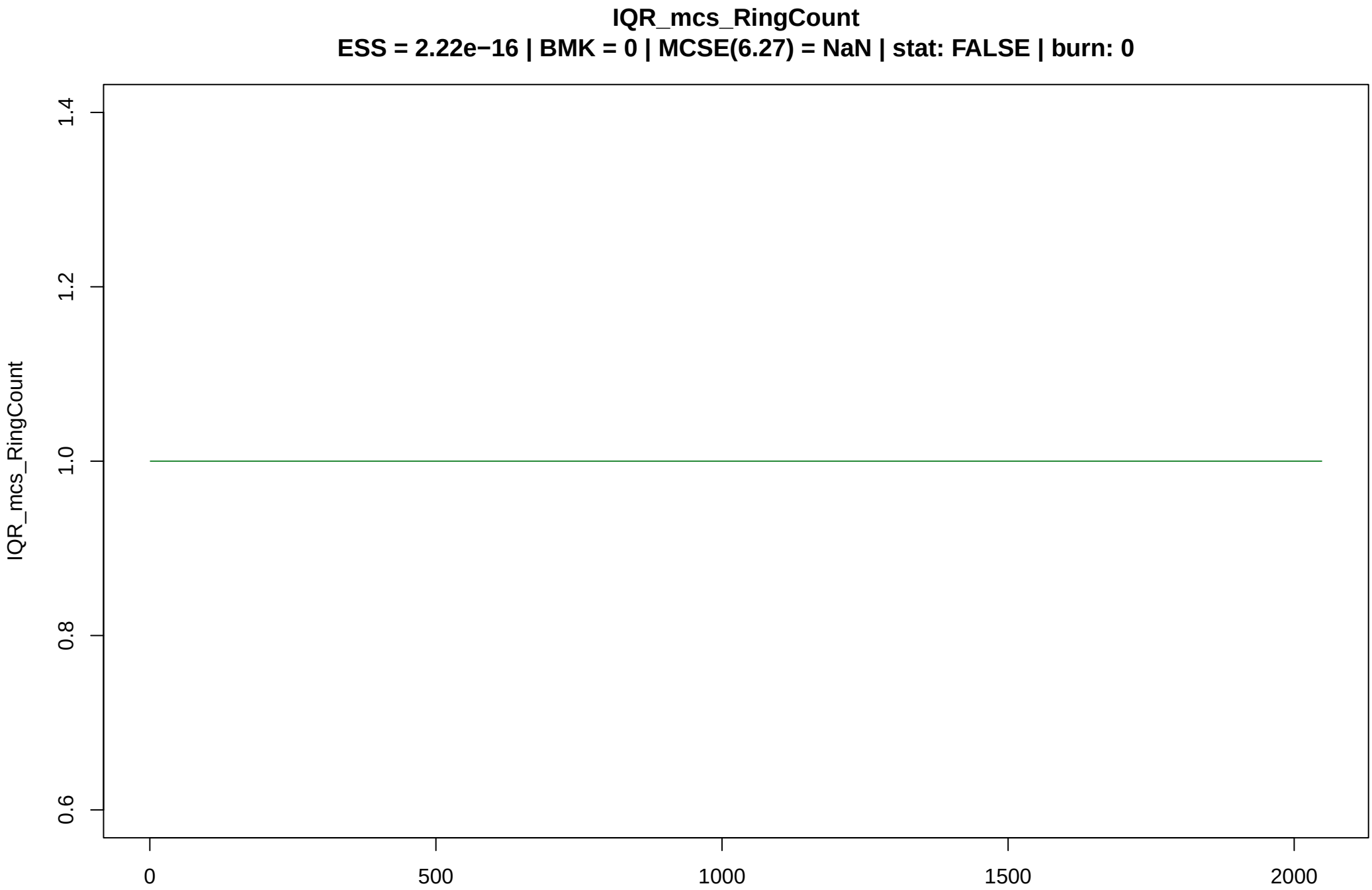

MEDIAN_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_template_NumHAcceptors
1.4
1.2
1.0
0.8
0.6
0
500
1000
1500
2000

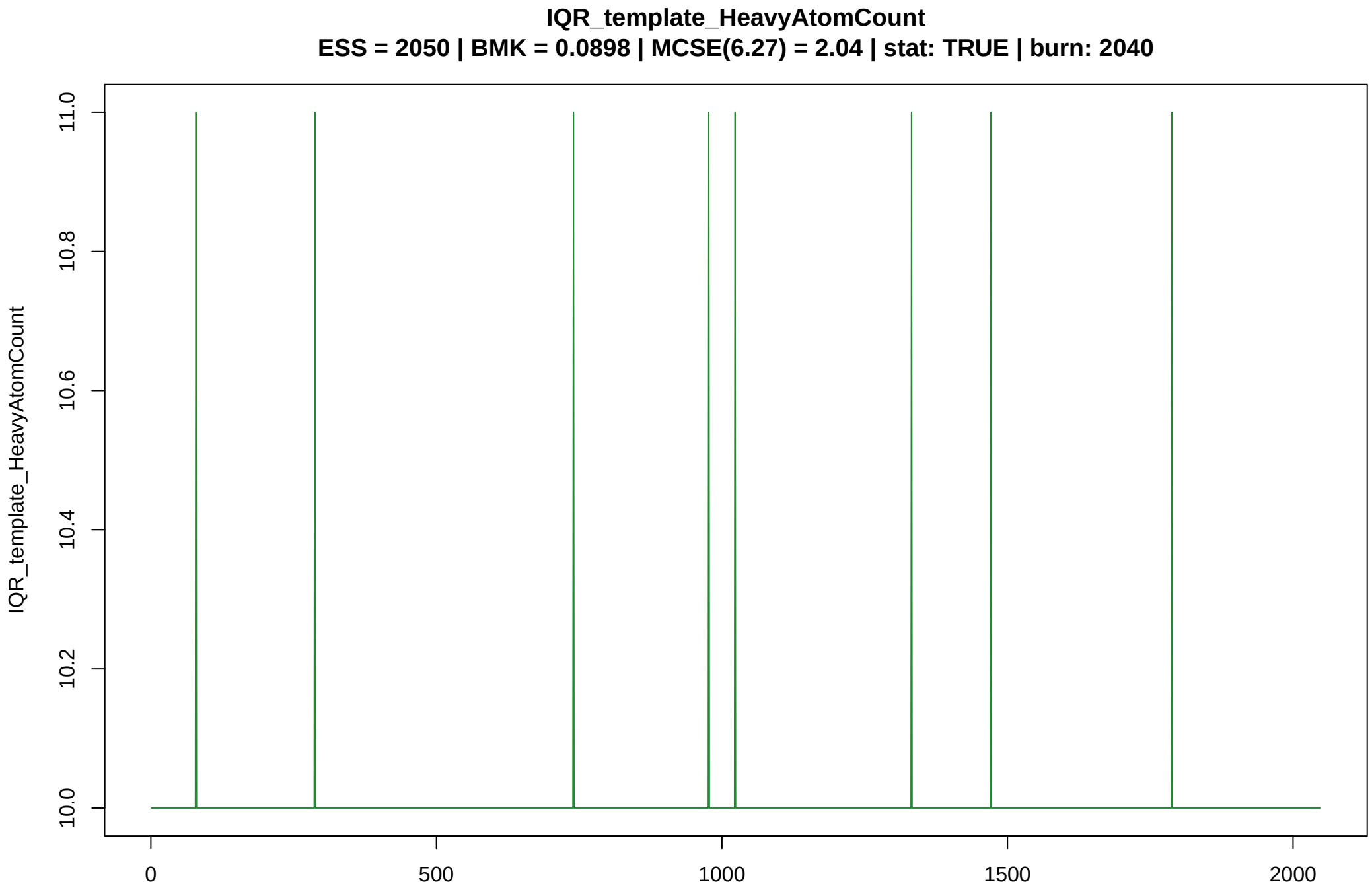

MEDIAN_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
0
500
1000
1500
2000

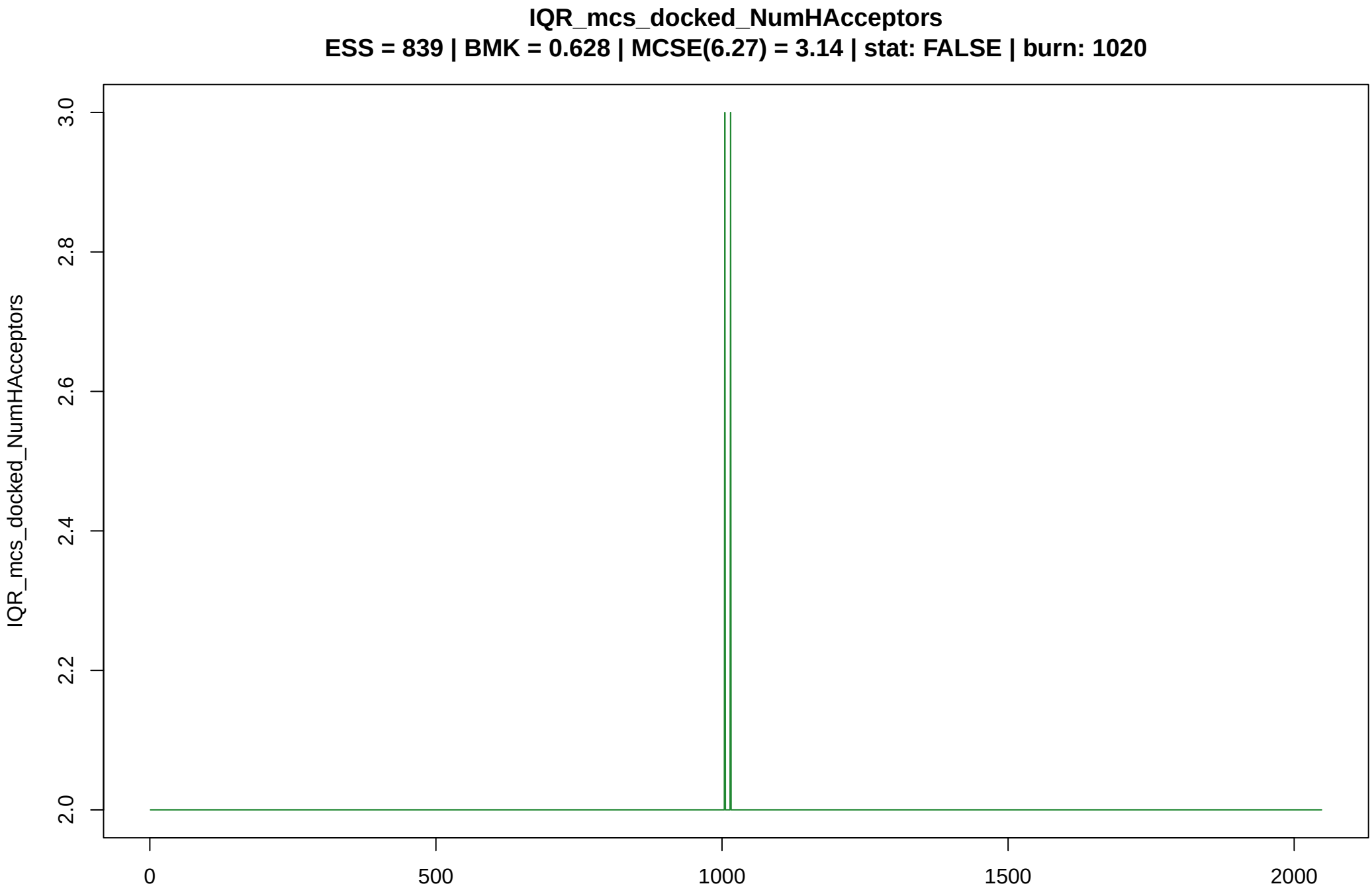

IQR_log_RMSD
ESS = 1220 | BMK = 0.0857 | MCSE(6.27) = 3.13 | stat: TRUE | burn: 0
IQR_log_RMSD
1.16
1.18
1.20
1.22
1.24
1.26
0
500
1000
1500
2000

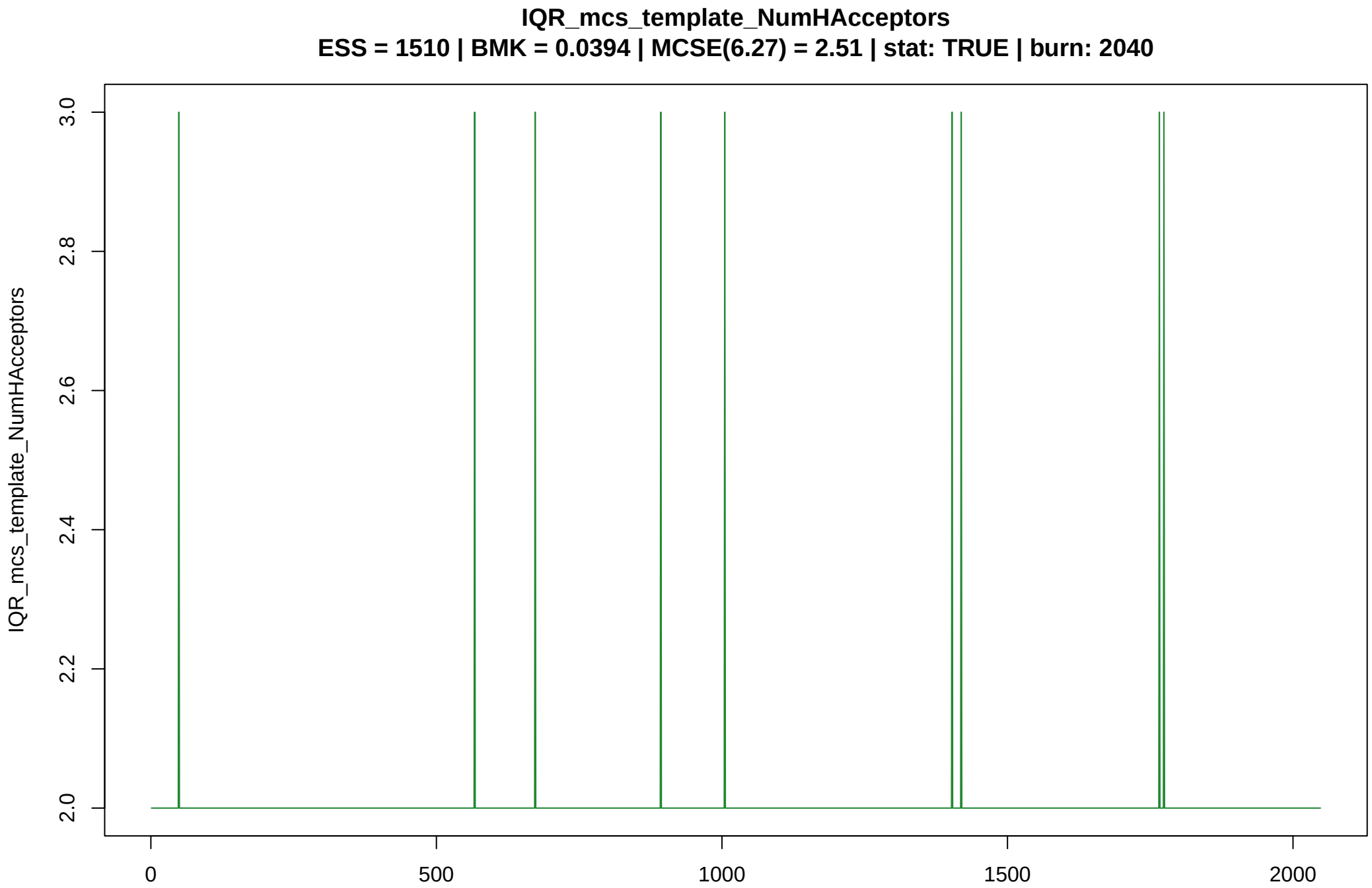

IQR_Xtransf_ec_tanimoto_similarity
ESS = 1520 | BMK = 0.073 | MCSE(6.27) = 3.23 | stat: FALSE | burn: 0
IQR_Xtransf_ec_tanimoto_similarity
0.90
0.92
0.94
0.96
0.98
1.00
1.02
1.04
0
500
1000
1500
2000

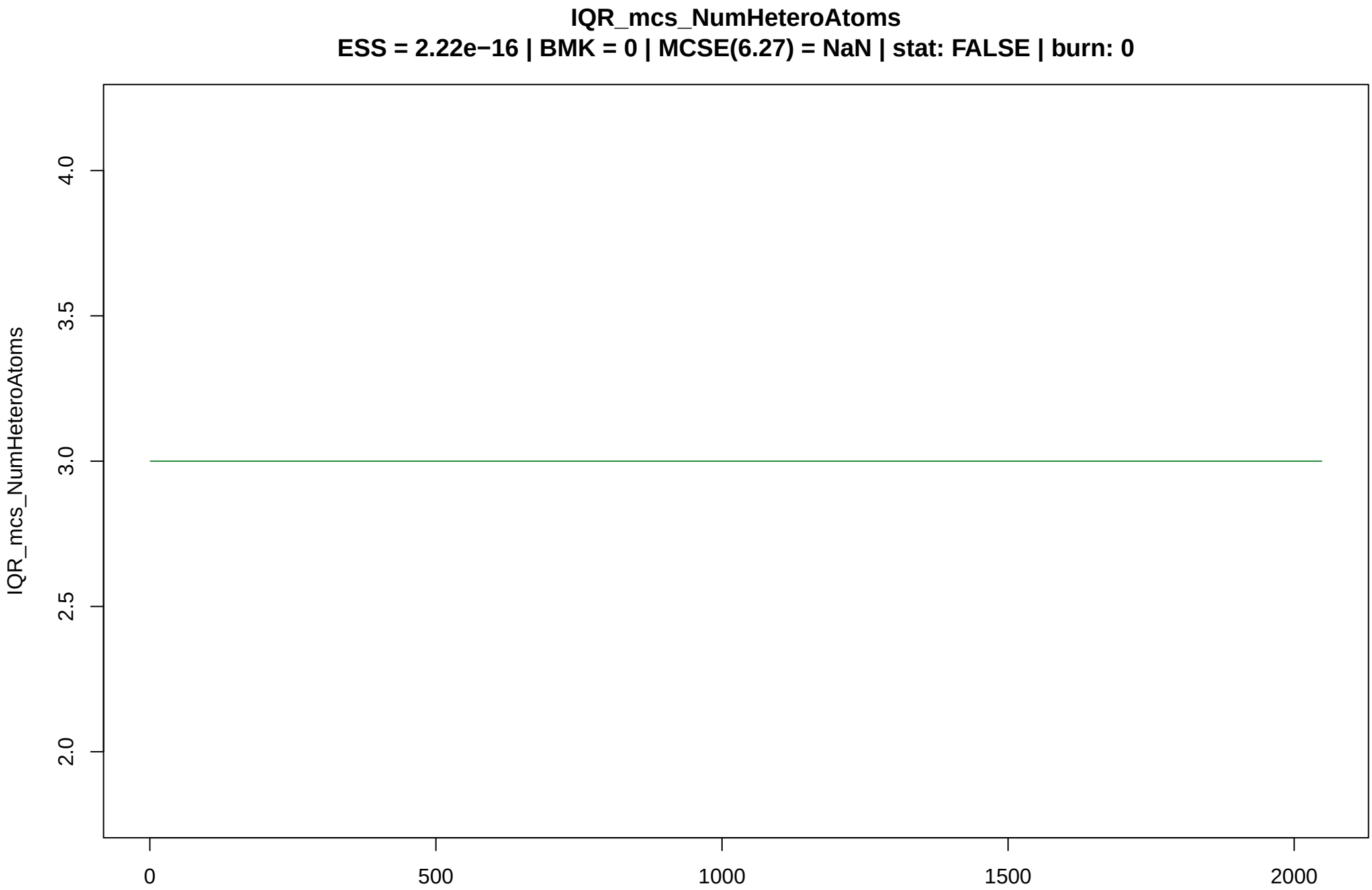

IQR_docked_HeavyAtomCount
ESS = 1920 | BMK = 0.000978 | MCSE(6.27) = 2.19 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
10.0
10.2
10.4
10.6
10.8
11.0
0
500
1000
1500
2000

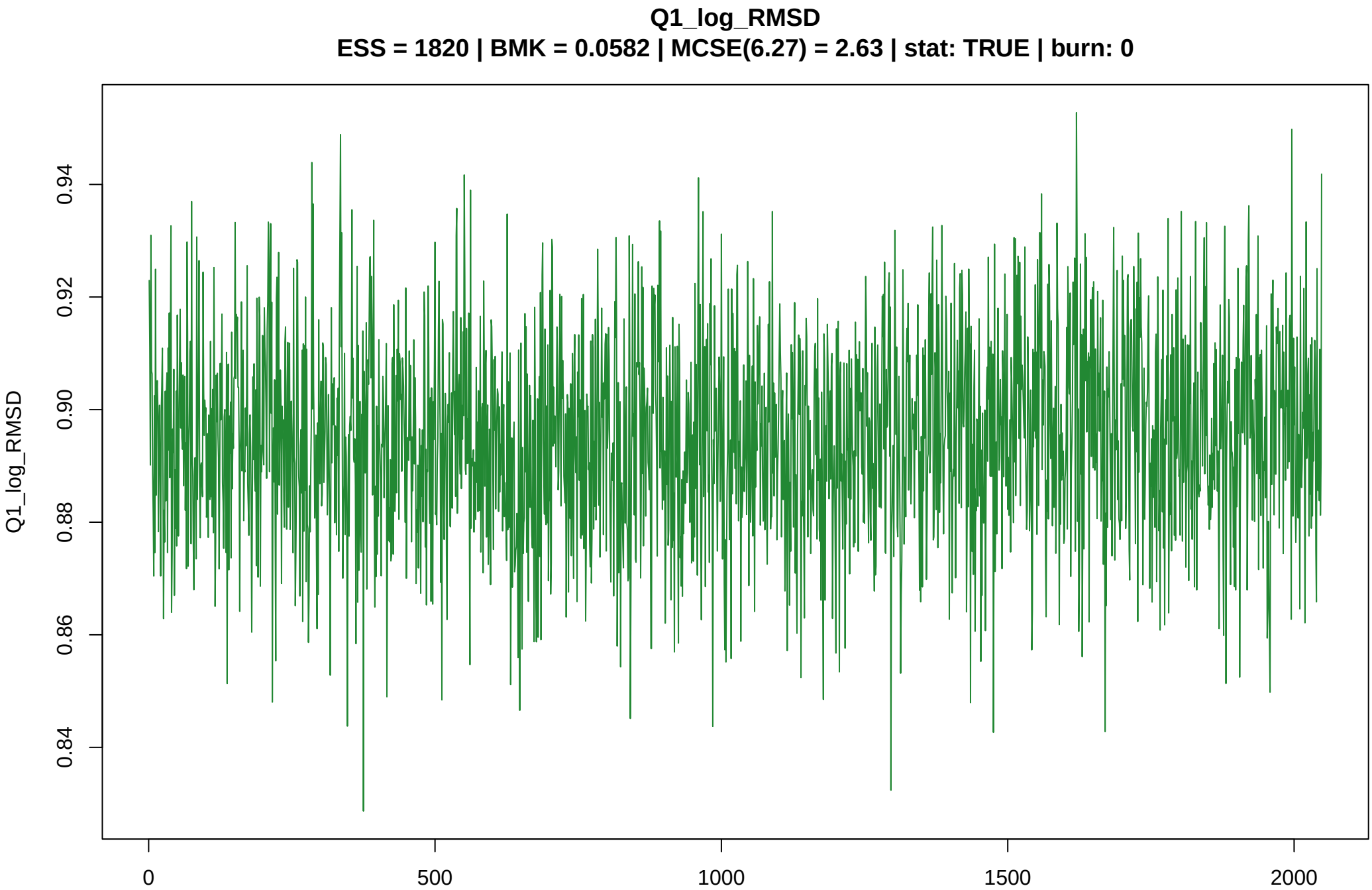

IQR_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

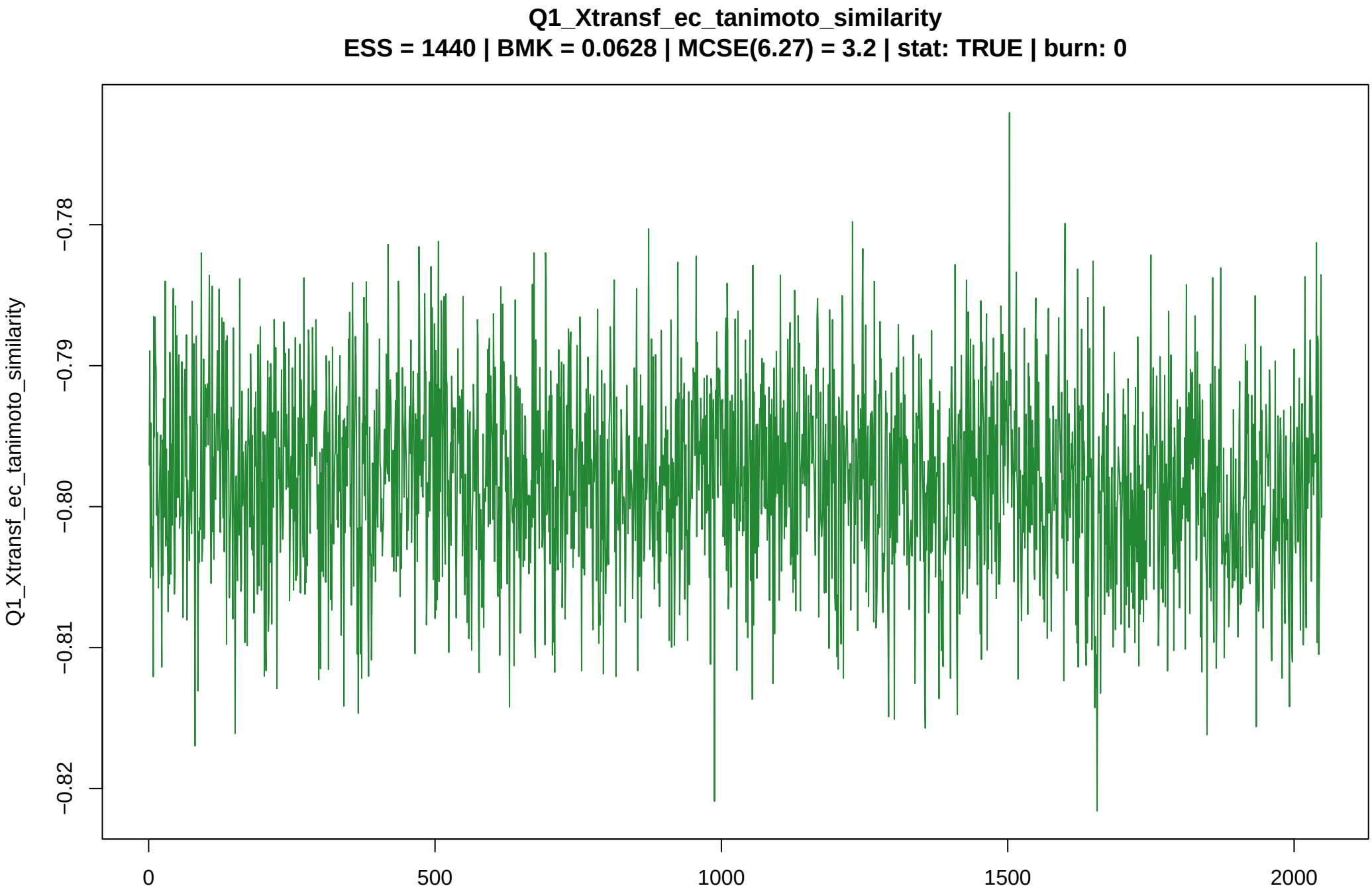

IQR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0898 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 2040
IQR_template_HeavyAtomCount
10.0
10.2
10.4
10.6
10.8
11.0
0
500
1000
1500
2000

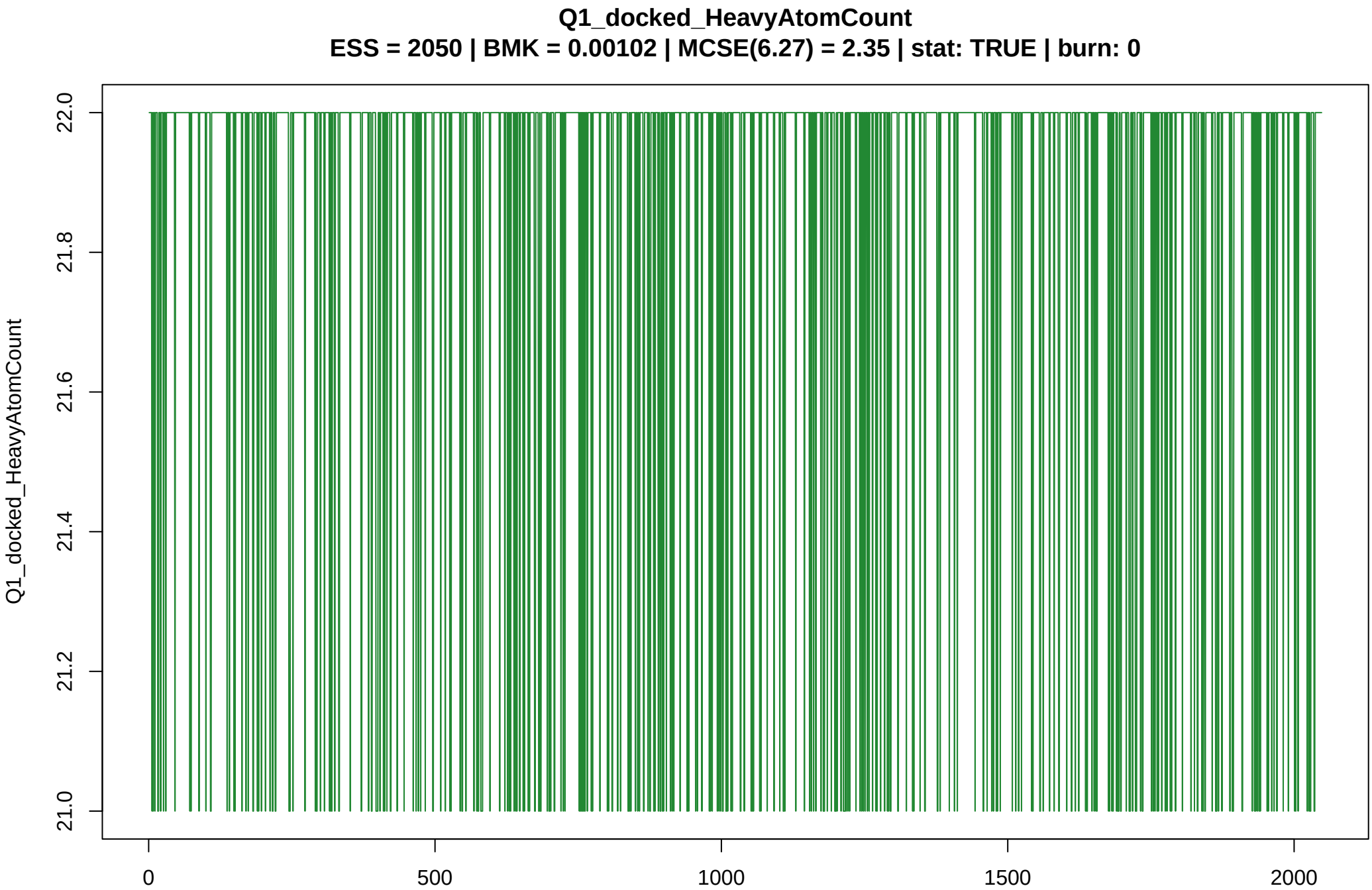

IQR_mcs_docked_NumHAcceptors
ESS = 839 | BMK = 0.628 | MCSE(6.27) = 3.14 | stat: FALSE | burn: 1020
IQR_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

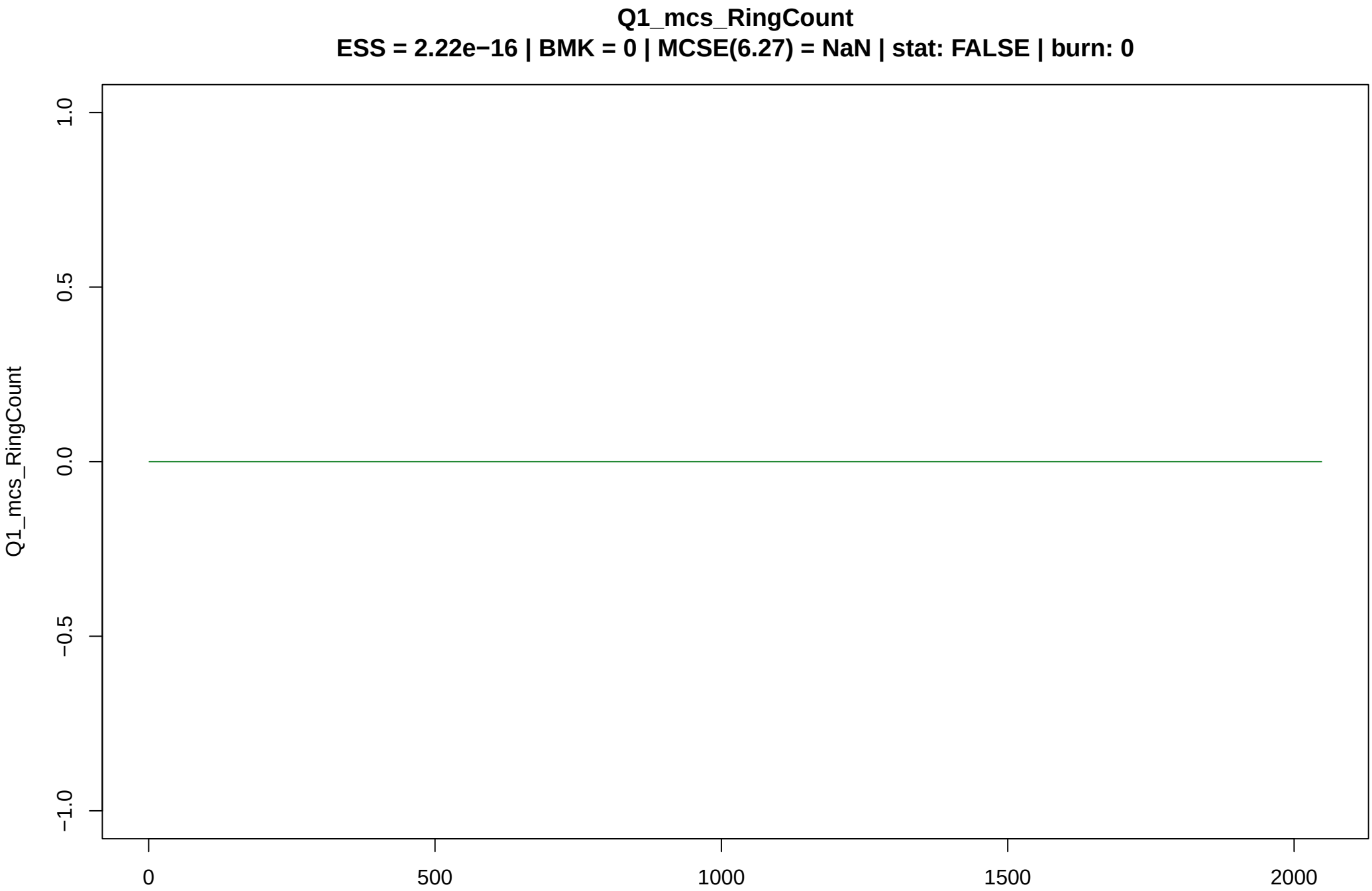

IQR_mcs_template_NumHAcceptors
ESS = 1510 | BMK = 0.0394 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 2040
IQR_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

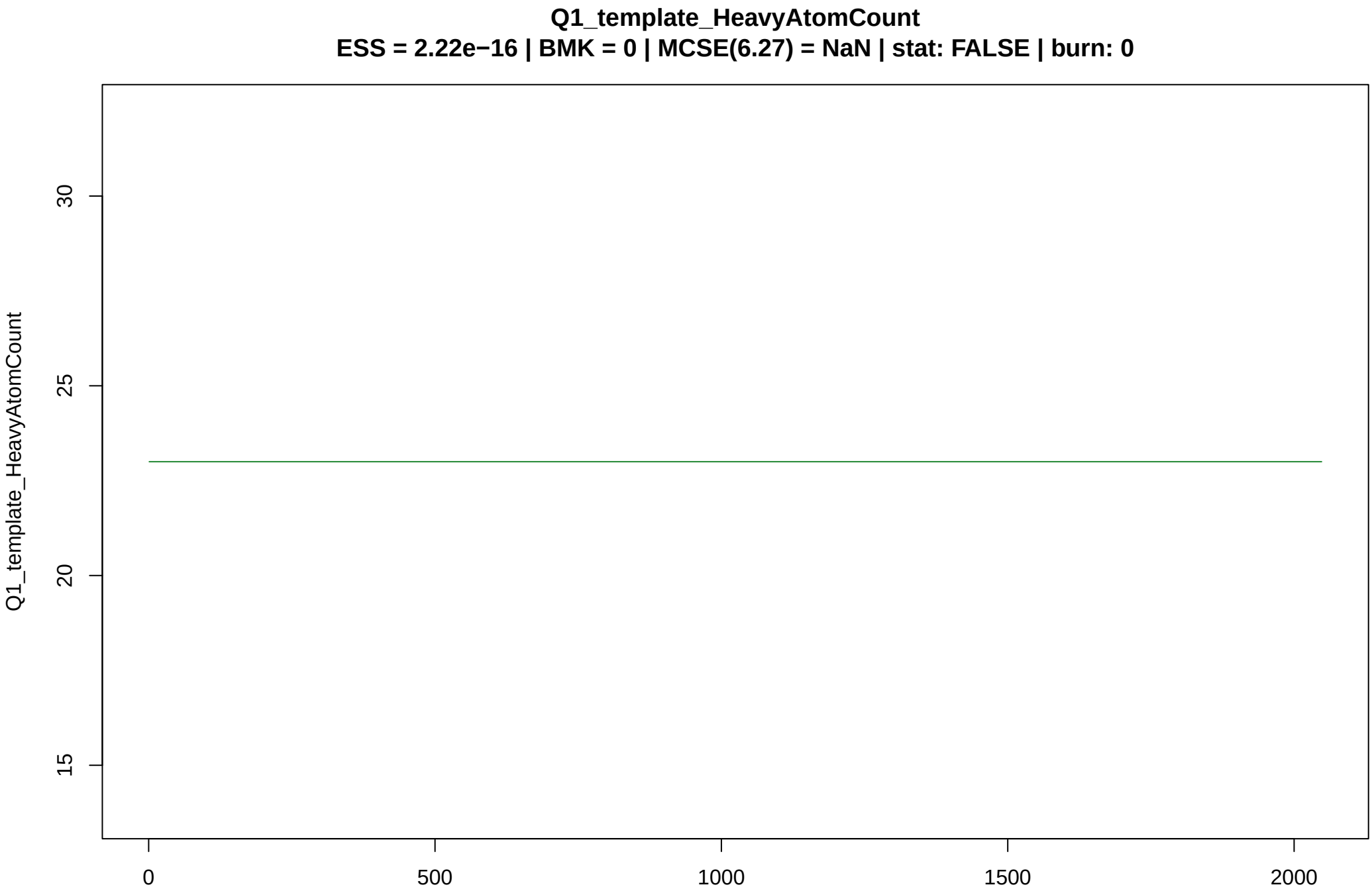

IQR_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
IQR_mcs_NumHeteroAtoms
2.0
2.5
3.0
3.5
4.0
0
500
1000
1500
2000

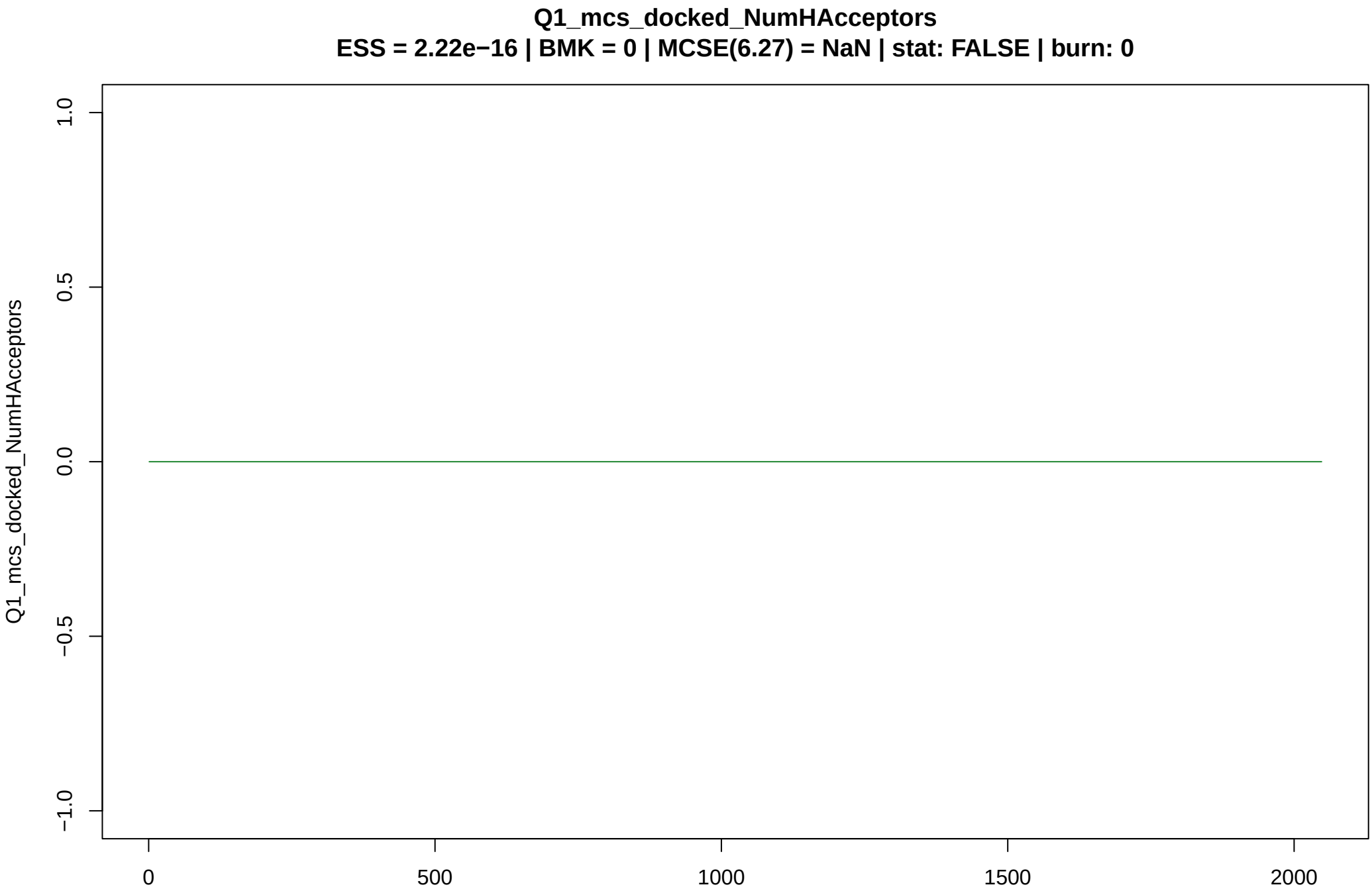

Q1_log_RMSD
ESS = 1820 | BMK = 0.0582 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0
Q1_log_RMSD
0.84
0.86
0.88
0.90
0.92
0.94
0
500
1000
1500
2000

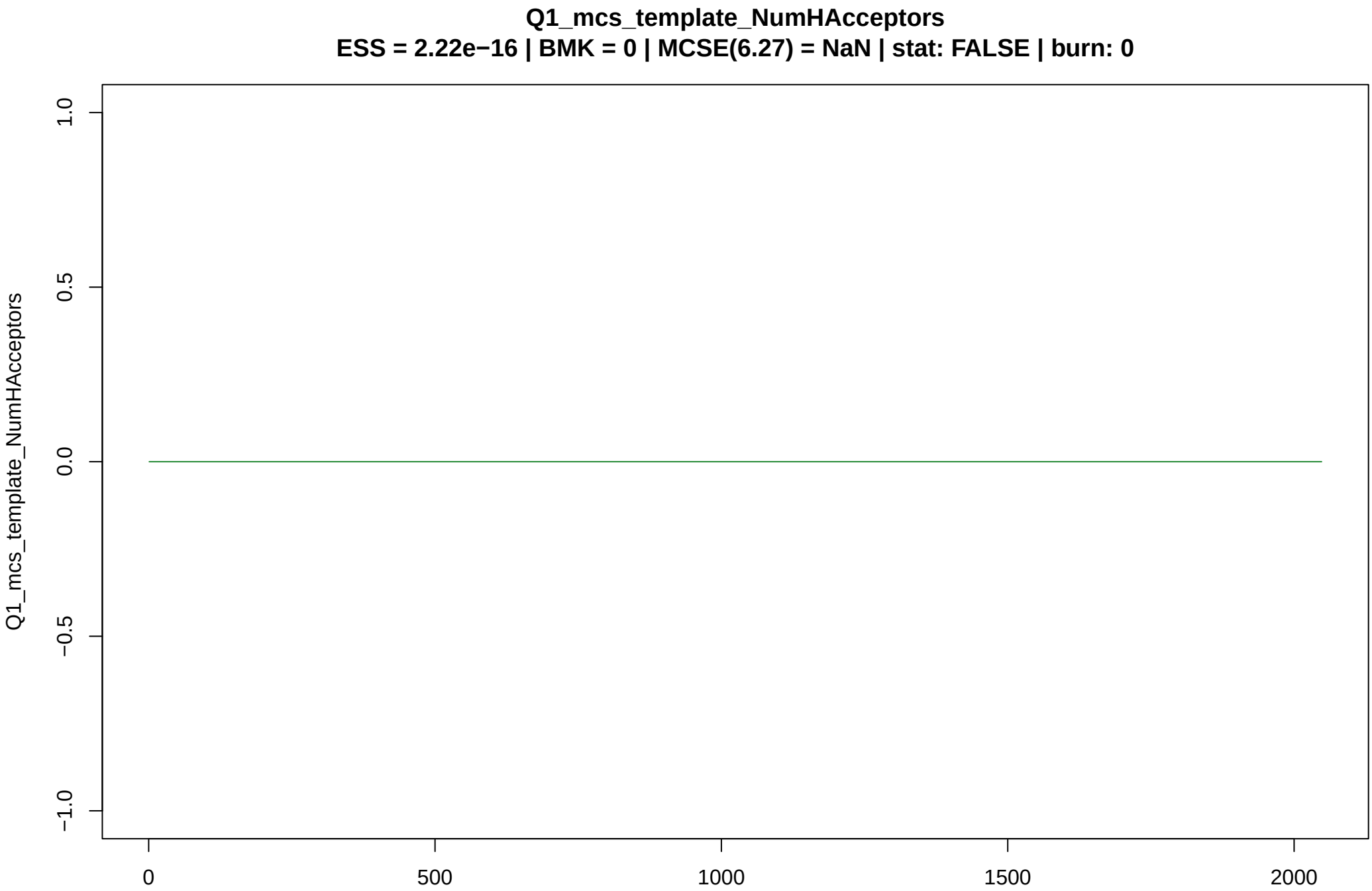

Q1_Xtransf_ec_tanimoto_similarity
ESS = 1440 | BMK = 0.0628 | MCSE(6.27) = 3.2 | stat: TRUE | burn: 0
Q1_Xtransf_ec_tanimoto_similarity
−0.78
−0.79
−0.80
−0.81
−0.82
0
500
1000
1500
2000

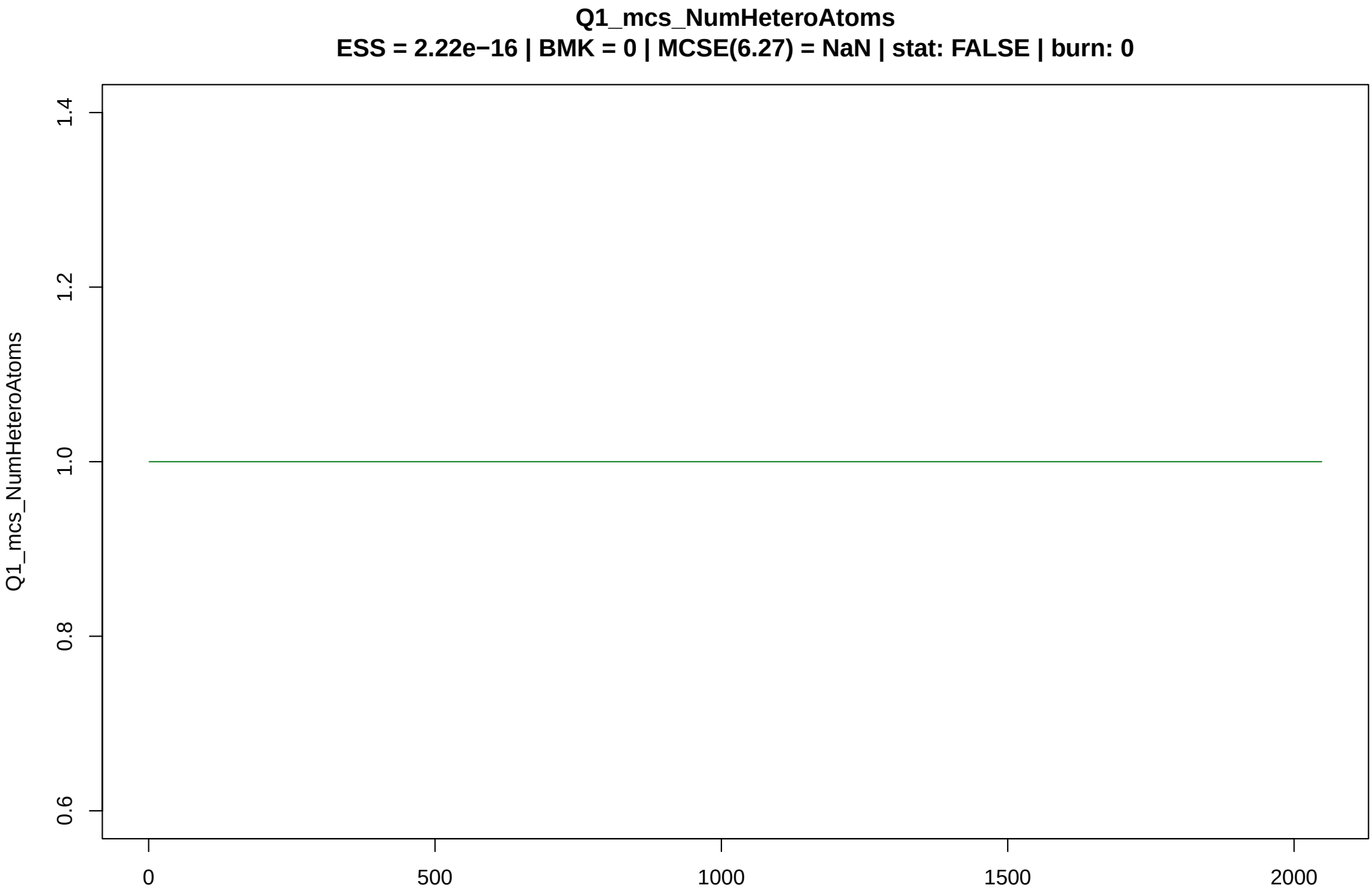

Q1_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.00102 | MCSE(6.27) = 2.35 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
22.0
21.8
21.6
21.4
21.2
21.0
0
500
1000
1500
2000

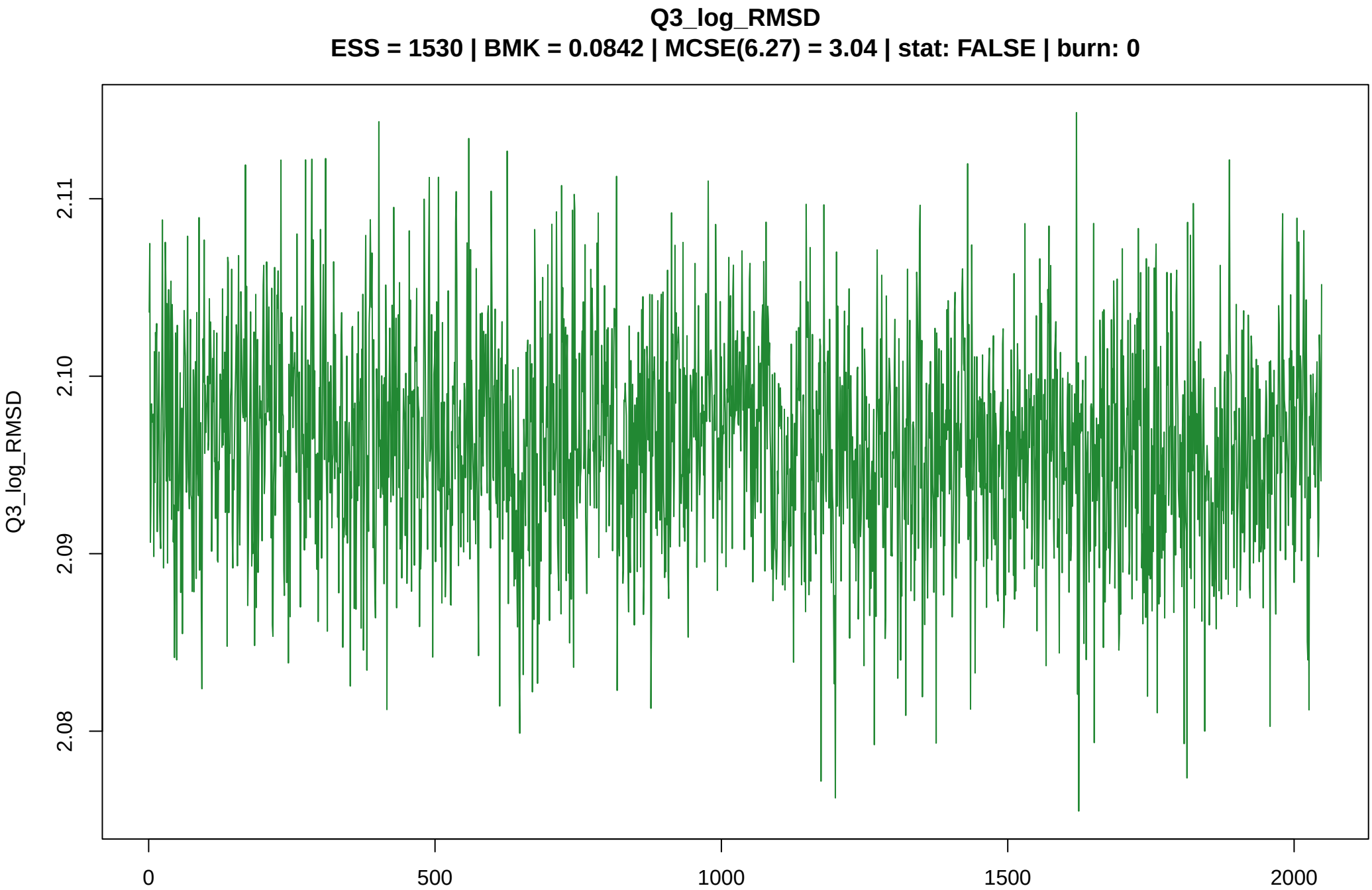

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

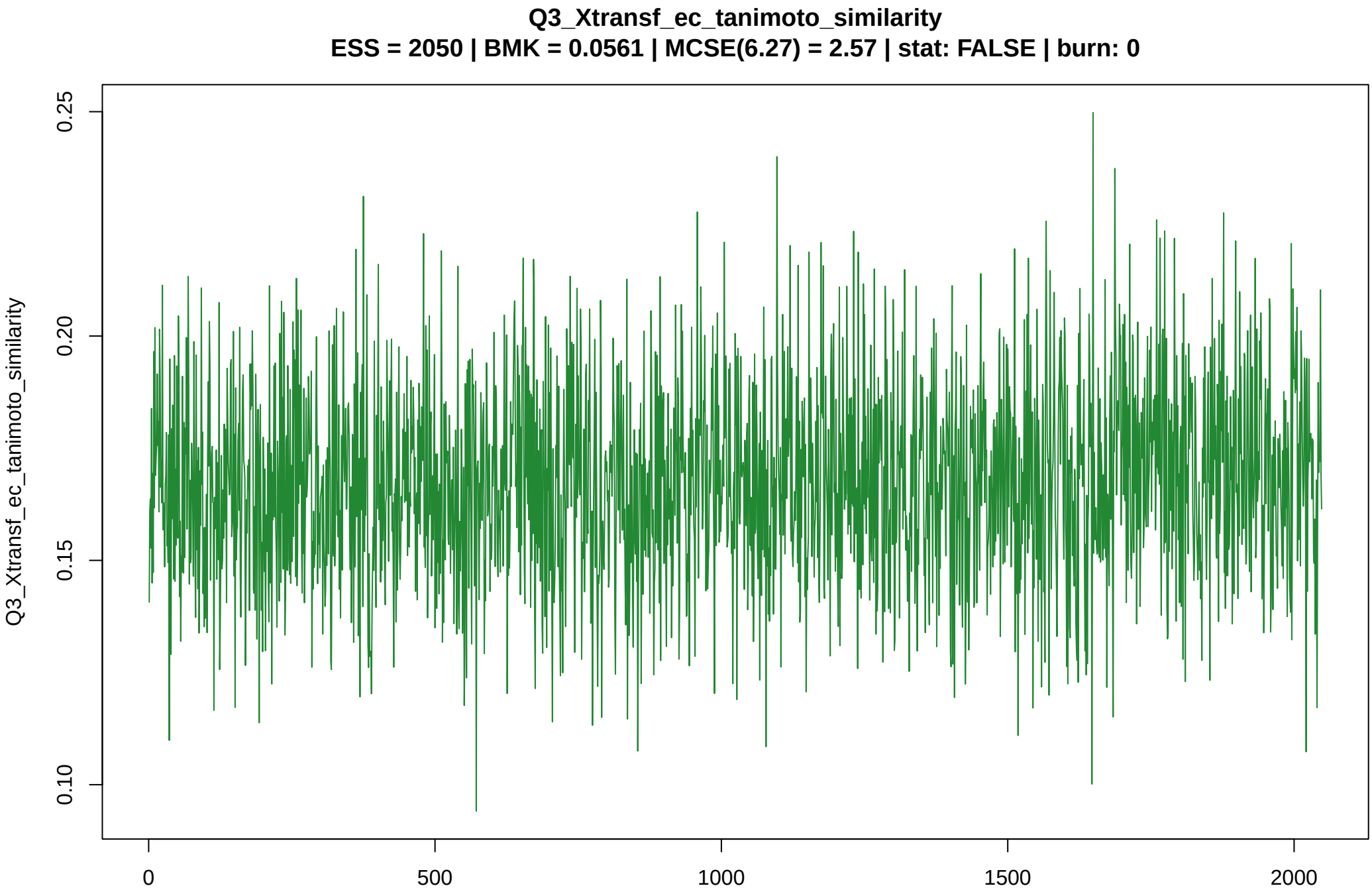

Q1_template_HeavyAtomCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_template_HeavyAtomCount
15
20
25
30
0
500
1000
1500
2000

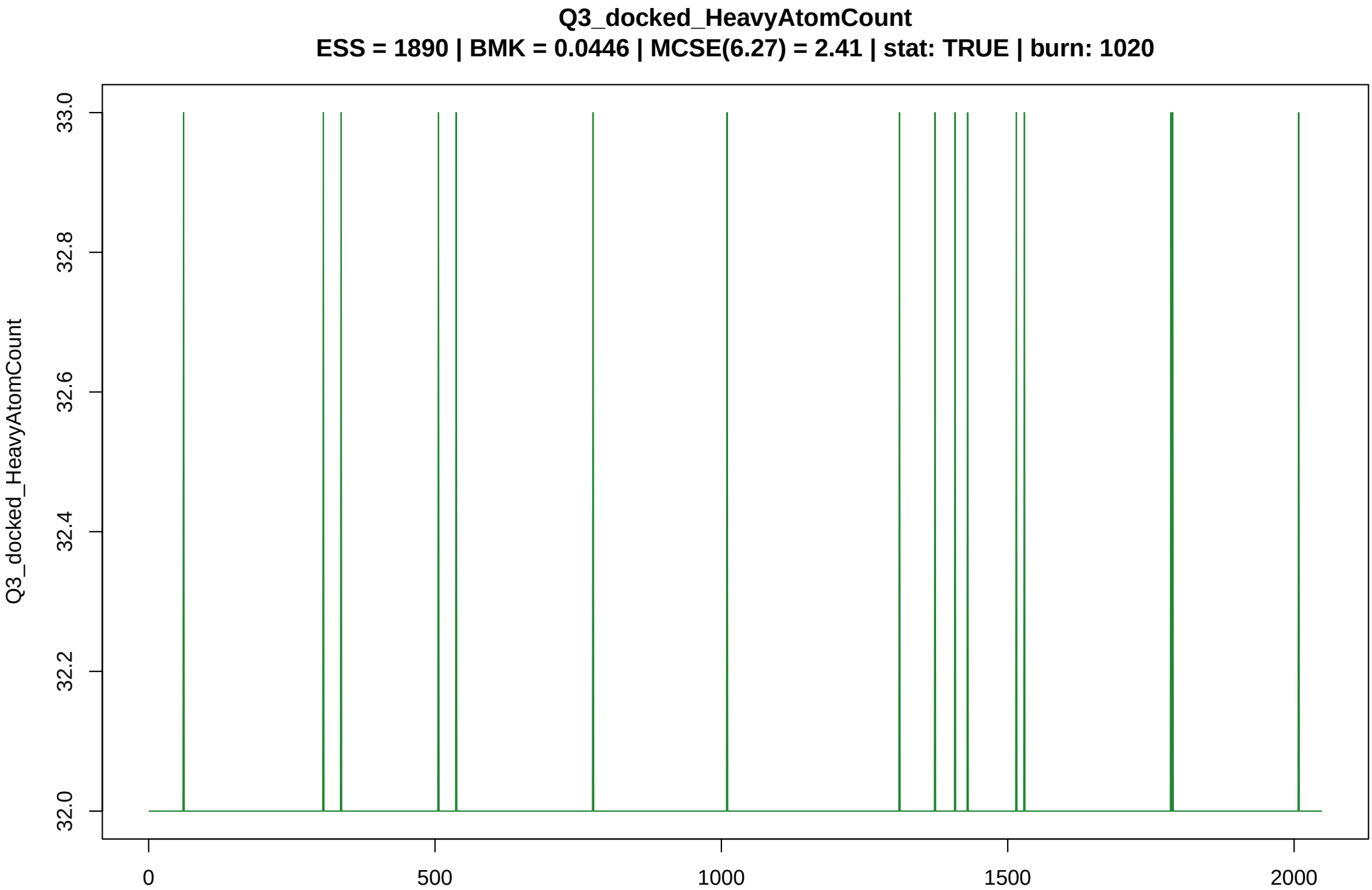

Q1_mcs_docked_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_docked_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

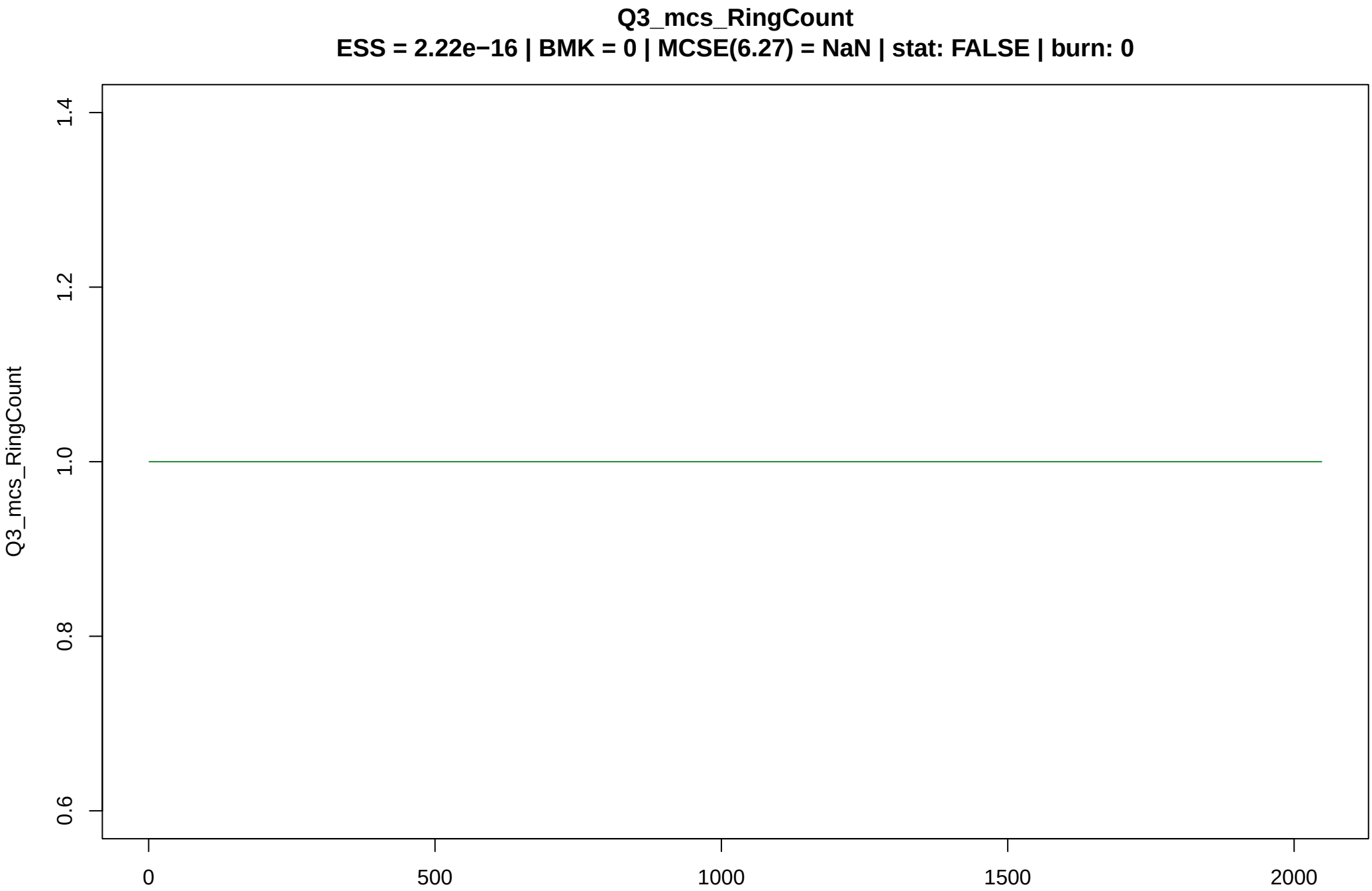

Q1_mcs_template_NumHAcceptors
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_template_NumHAcceptors
1.0
0.5
0.0
−0.5
−1.0
0
500
1000
1500
2000

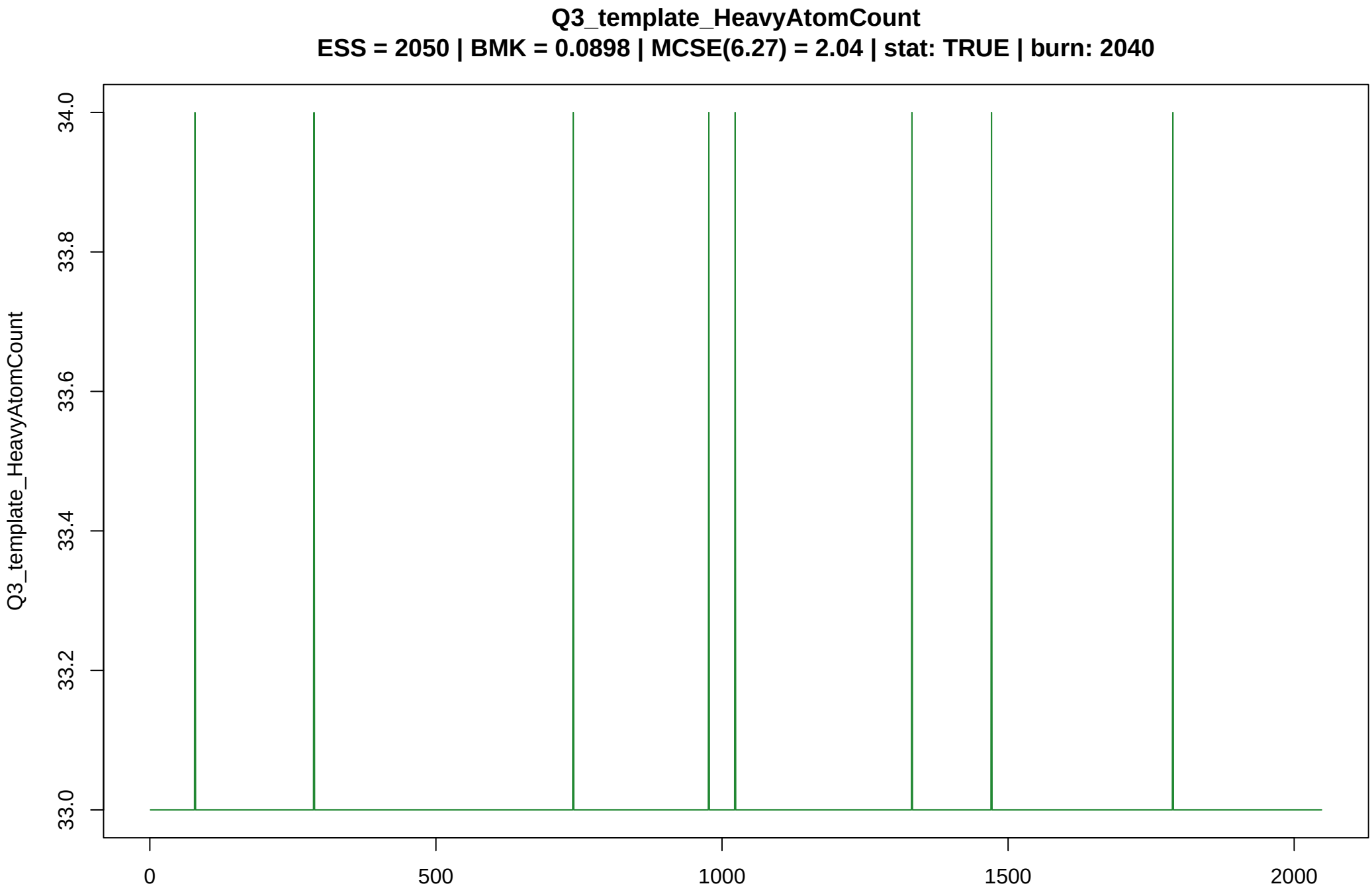

Q1_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_NumHeteroAtoms
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

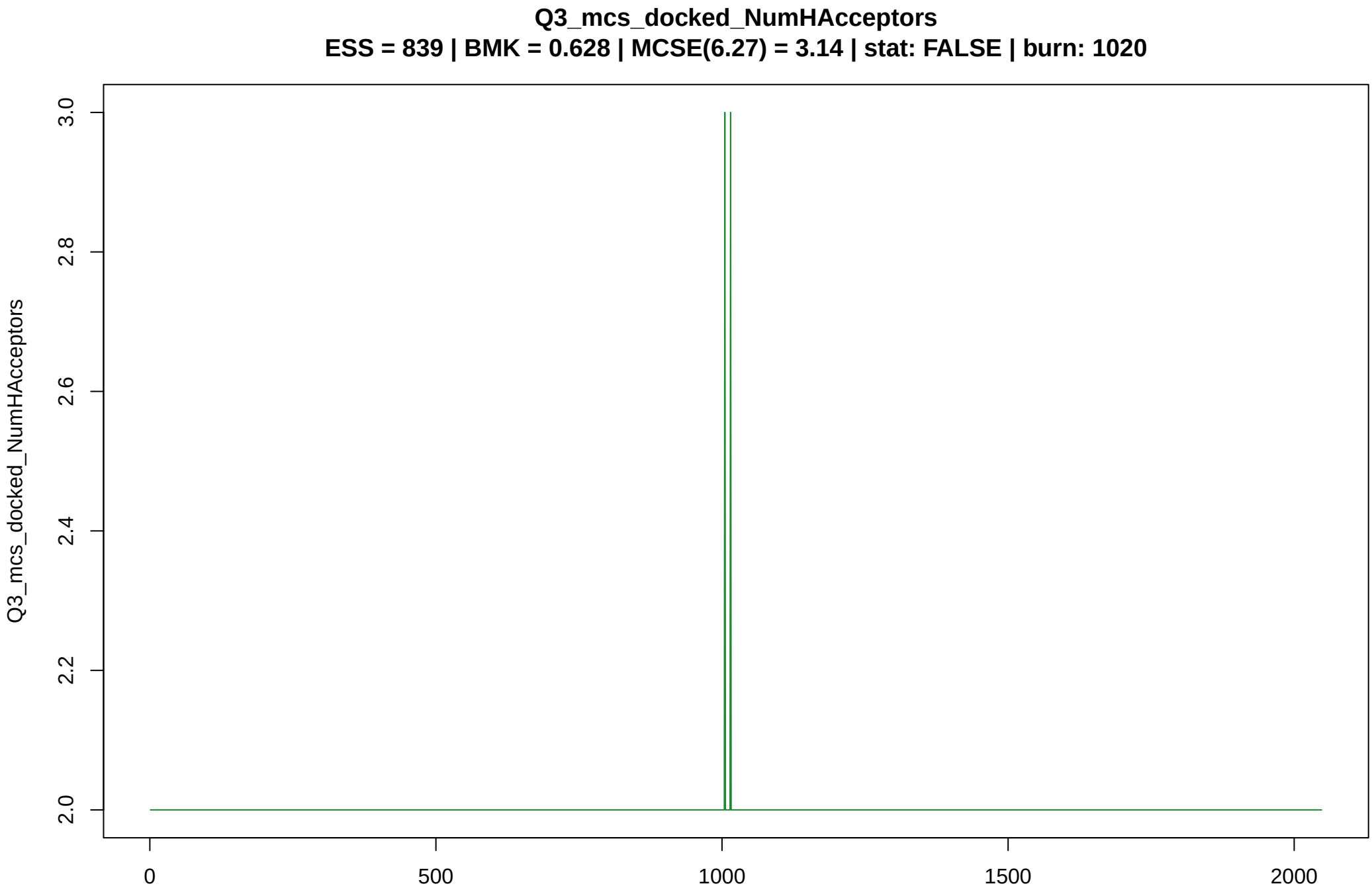

Q3_log_RMSD
ESS = 1530 | BMK = 0.0842 | MCSE(6.27) = 3.04 | stat: FALSE | burn: 0
Q3_log_RMSD
2.08
2.09
2.10
2.11
0
500
1000
1500
2000

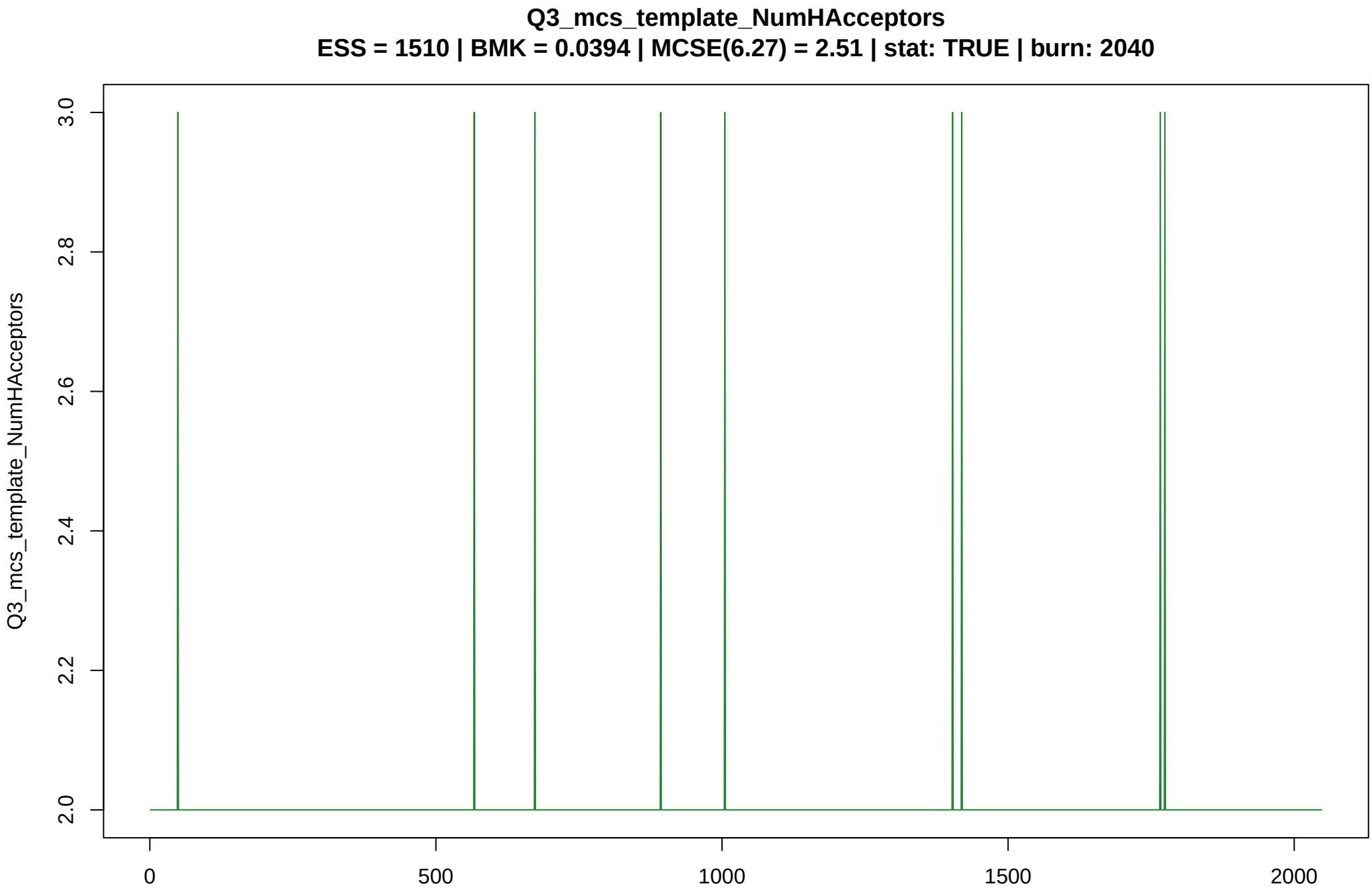

Q3_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0561 | MCSE(6.27) = 2.57 | stat: FALSE | burn: 0
Q3_Xtransf_ec_tanimoto_similarity
0.10
0.15
0.20
0.25
0
500
1000
1500
2000

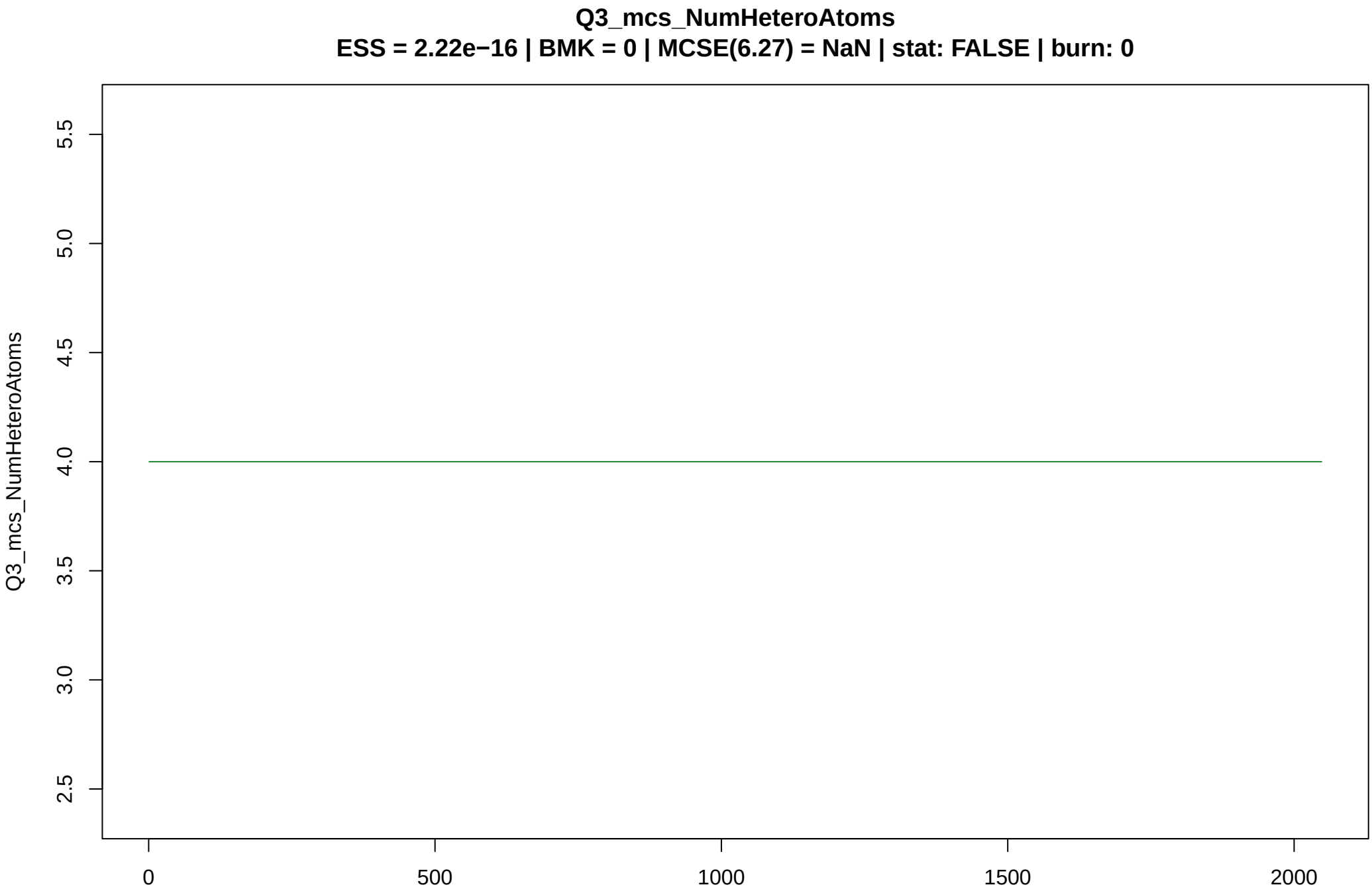

Q3_docked_HeavyAtomCount
ESS = 1890 | BMK = 0.0446 | MCSE(6.27) = 2.41 | stat: TRUE | burn: 1020
Q3_docked_HeavyAtomCount
33.0
32.8
32.6
32.4
32.2
32.0
0
500
1000
1500
2000

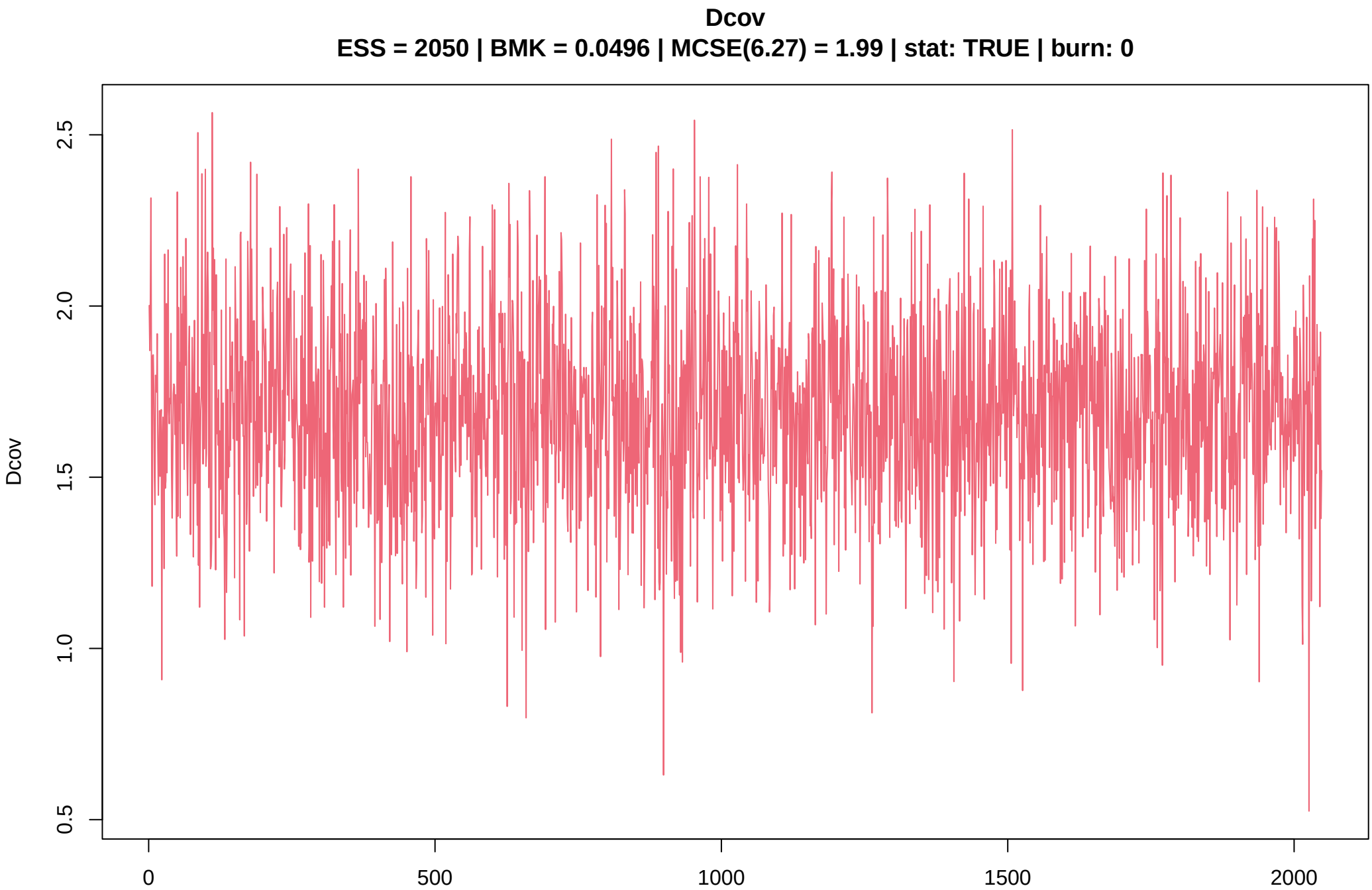

Q3_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_RingCount
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

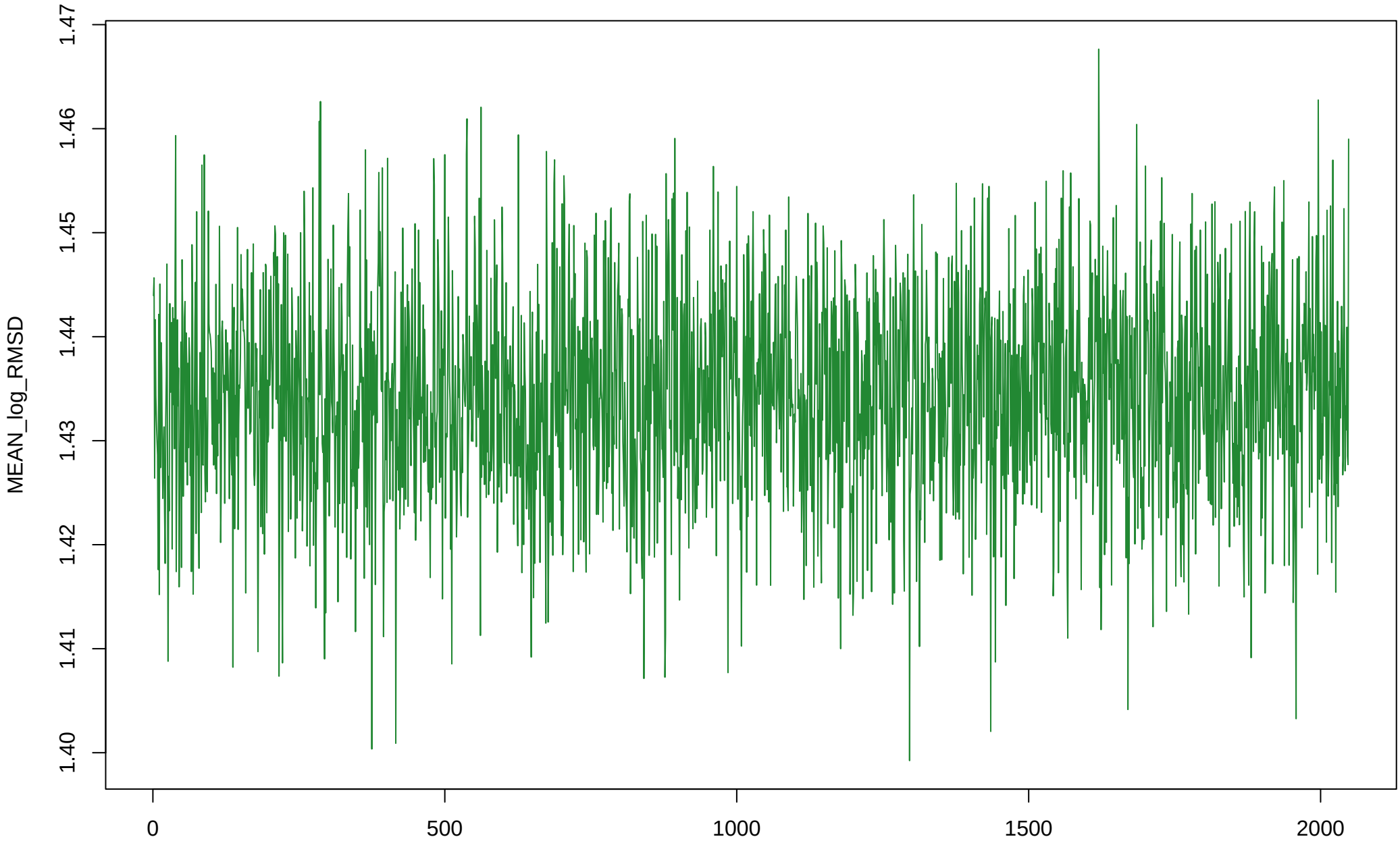

Q3_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0898 | MCSE(6.27) = 2.04 | stat: TRUE | burn: 2040
Q3_template_HeavyAtomCount
34.0
33.8
33.6
33.4
33.2
33.0
0
500
1000
1500
2000

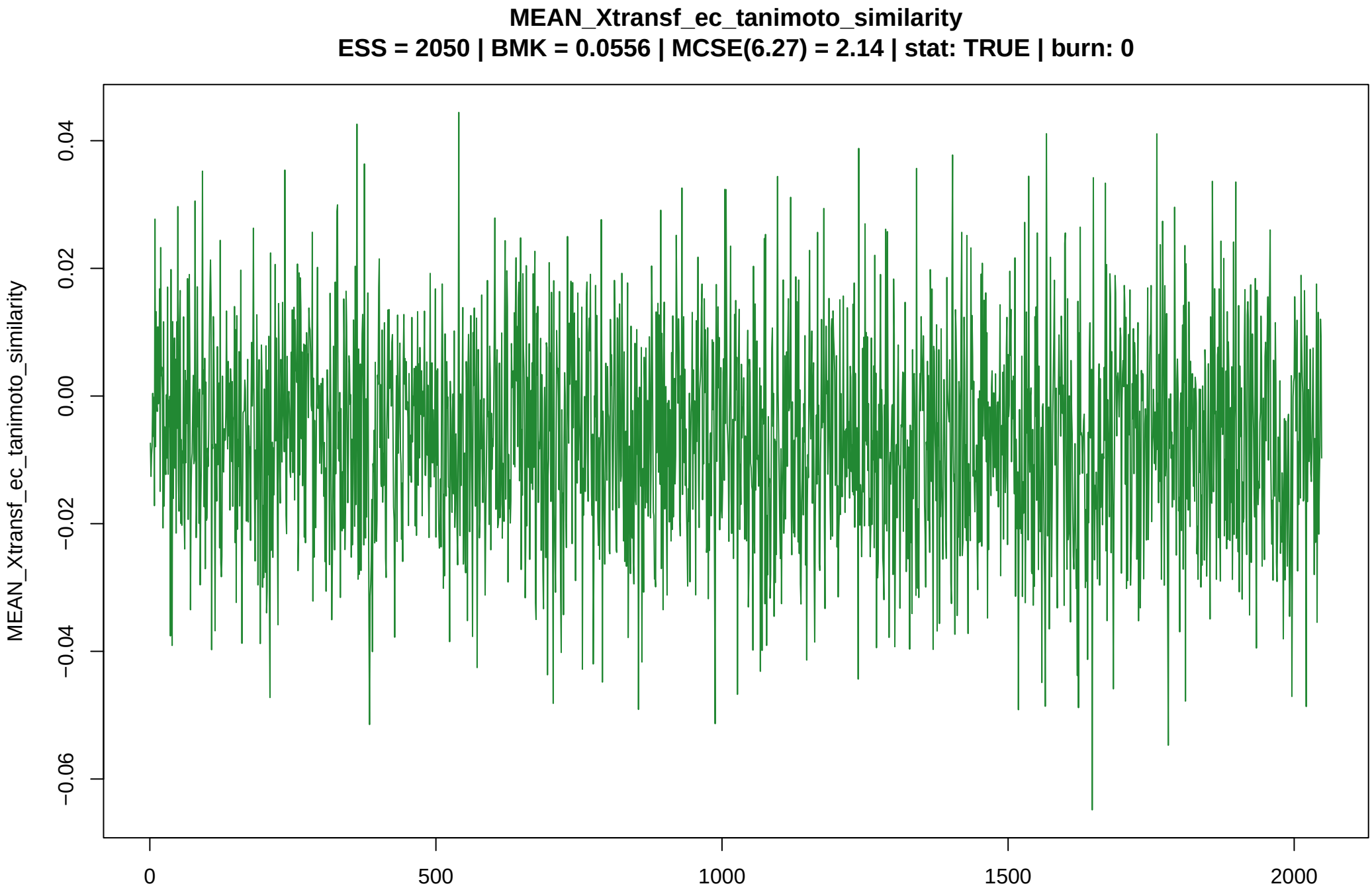

Q3_mcs_docked_NumHAcceptors
ESS = 839 | BMK = 0.628 | MCSE(6.27) = 3.14 | stat: FALSE | burn: 1020
Q3_mcs_docked_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

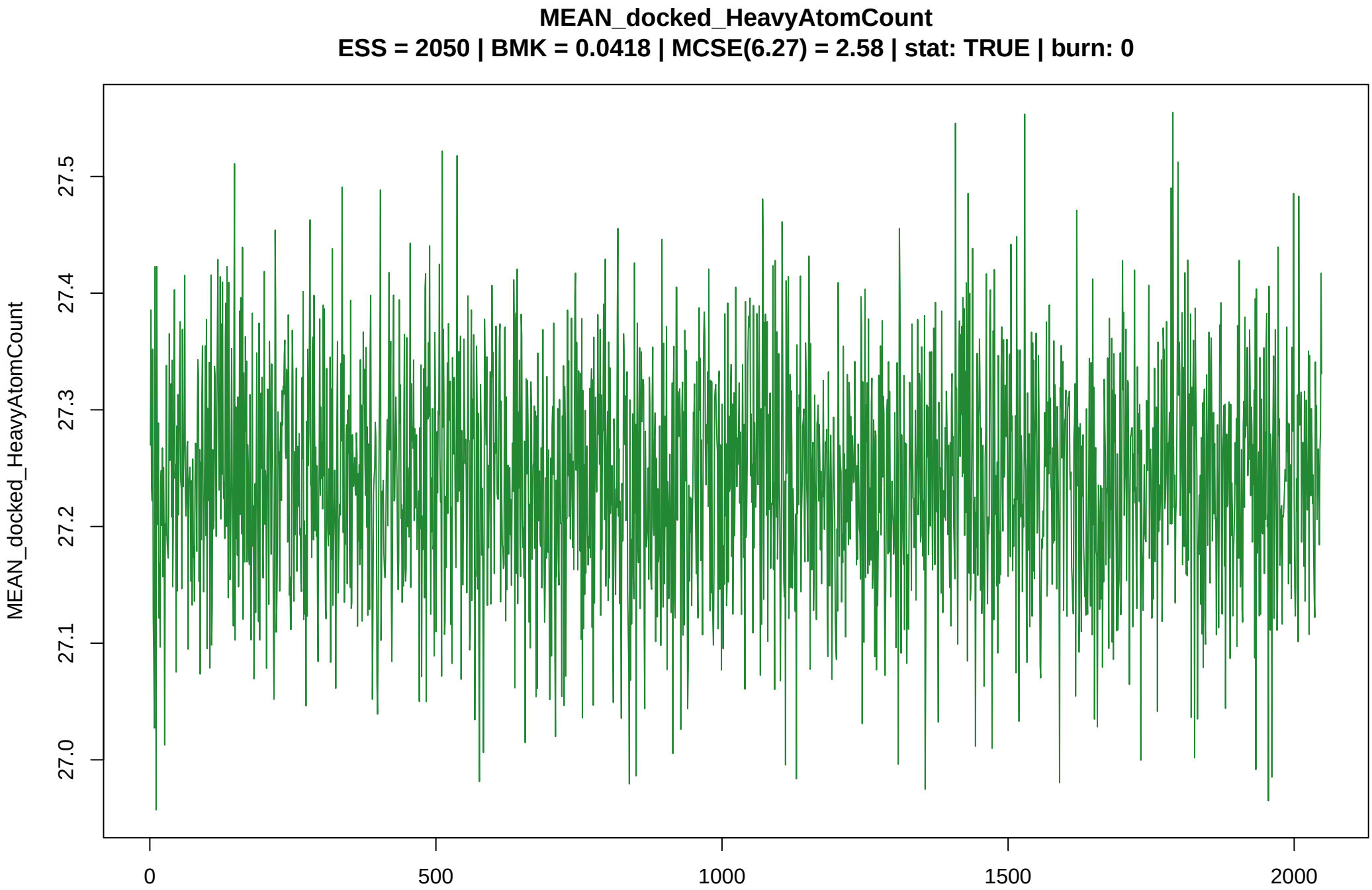

Q3_mcs_template_NumHAcceptors
ESS = 1510 | BMK = 0.0394 | MCSE(6.27) = 2.51 | stat: TRUE | burn: 2040
Q3_mcs_template_NumHAcceptors
3.0
2.8
2.6
2.4
2.2
2.0
0
500
1000
1500
2000

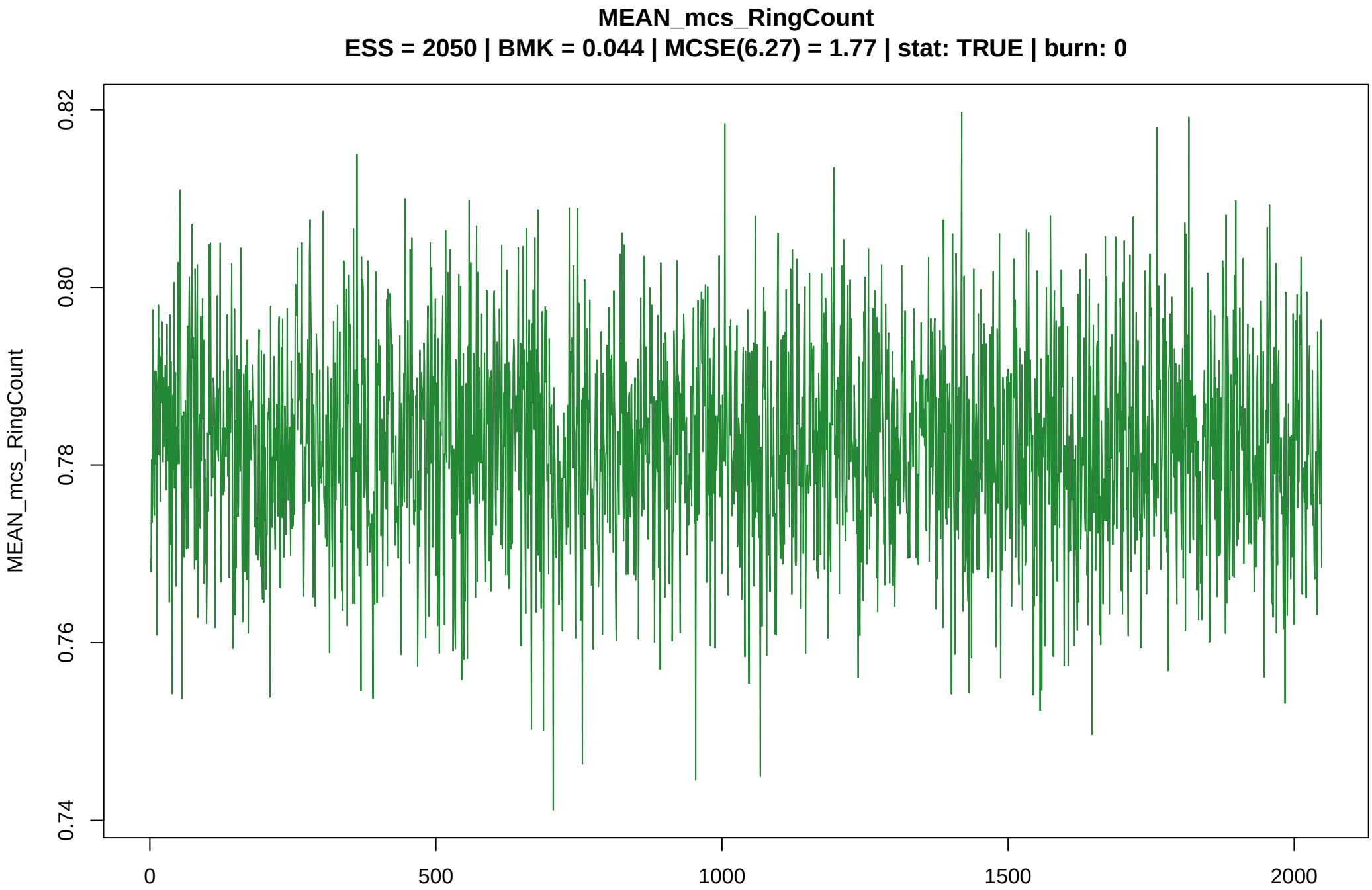

Q3_mcs_NumHeteroAtoms
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q3_mcs_NumHeteroAtoms
2.5
3.0
3.5
4.0
4.5
5.0
5.5
0
500
1000
1500
2000

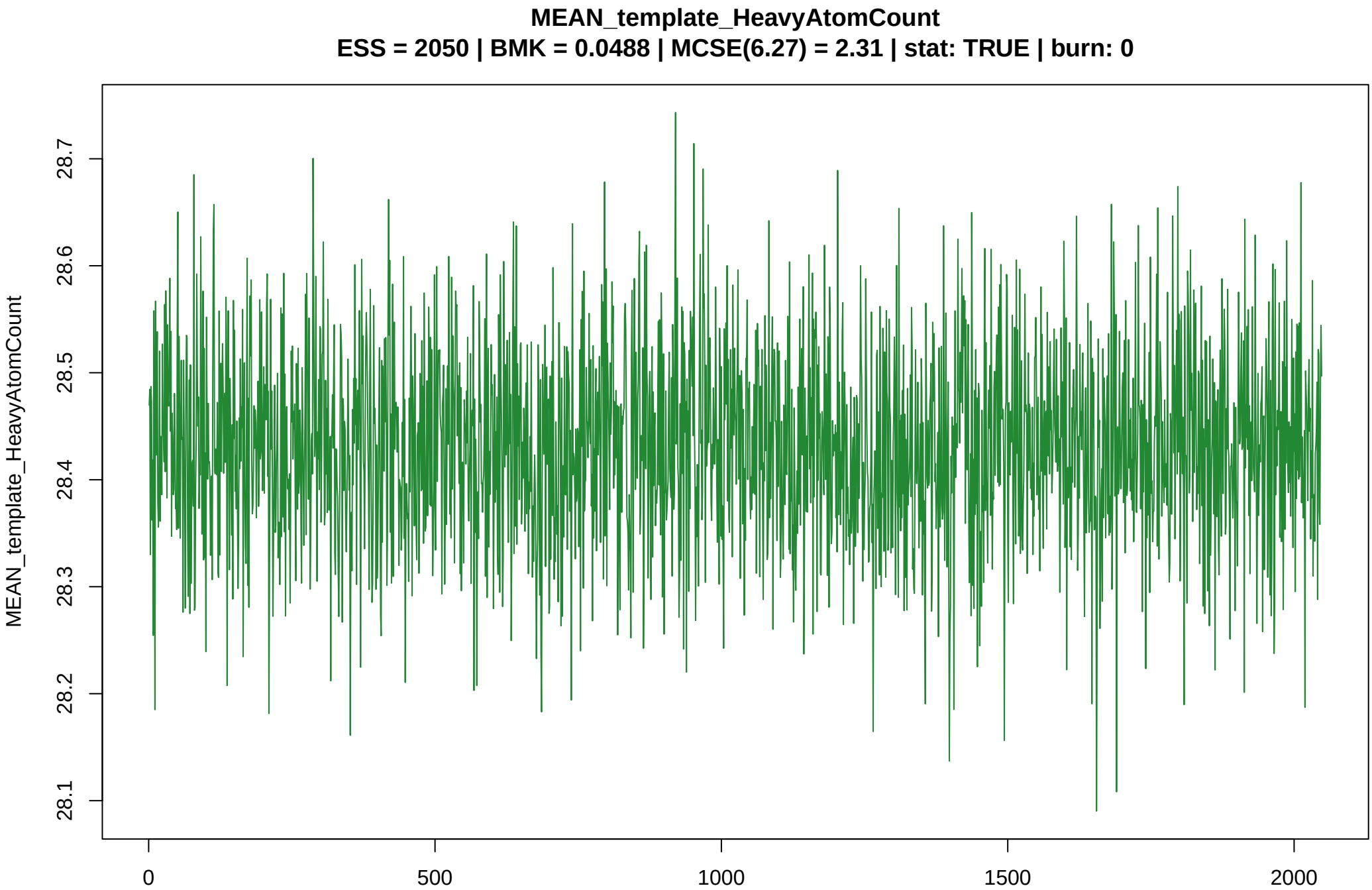

Dcov
ESS = 2050 | BMK = 0.0496 | MCSE(6.27) = 1.99 | stat: TRUE | burn: 0
Dcov
0.5
1.0
1.5
2.0
2.5
0
500
1000
1500
2000

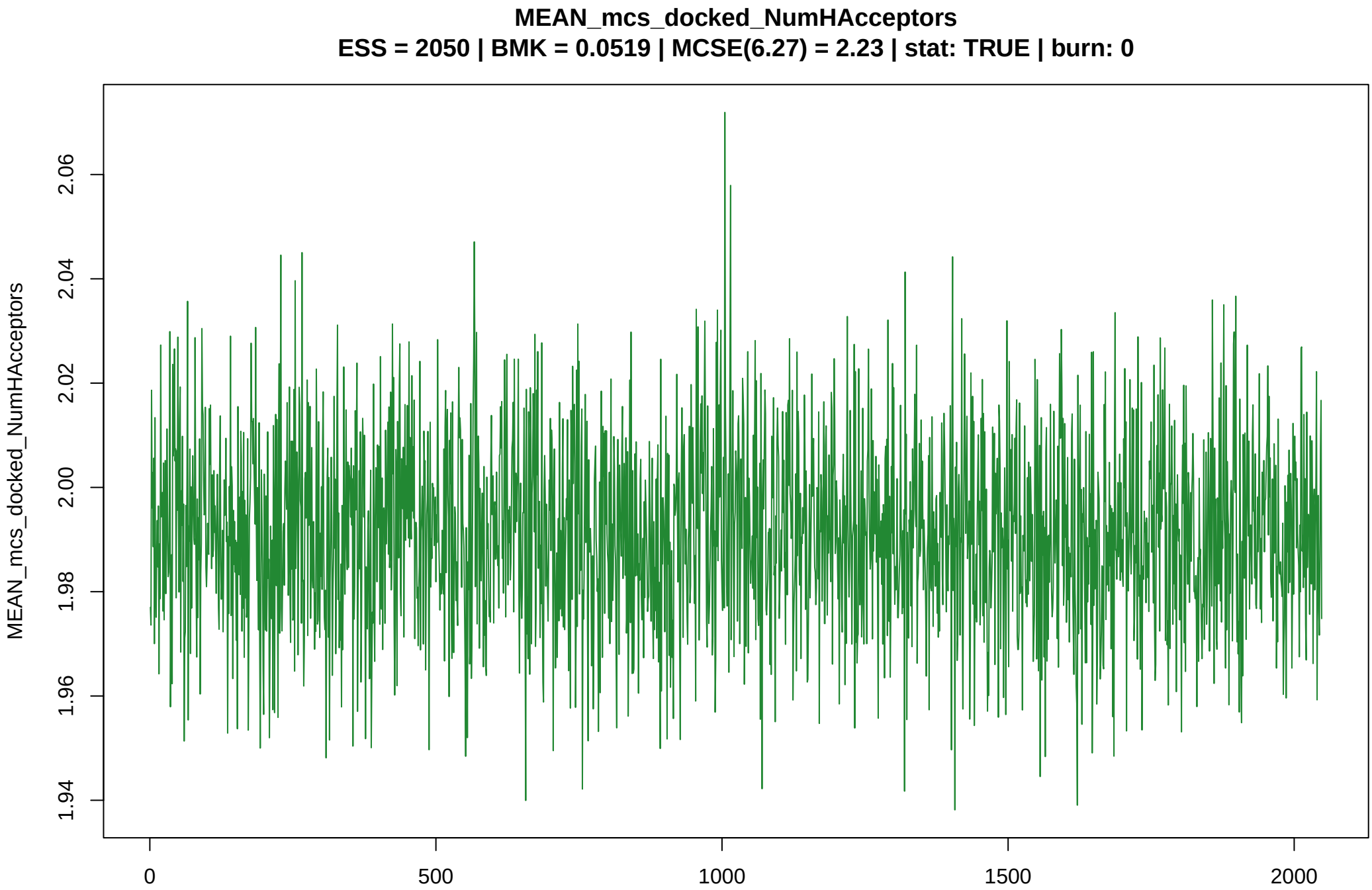

MEAN_log_RMSD
ESS = 2050 | BMK = 0.0679 | MCSE(6.27) = 1.86 | stat: TRUE | burn: 0
MEAN_log_RMSD
1.40
1.41
1.42
1.43
1.44
1.45
1.46
1.47
0
500
1000
1500
2000

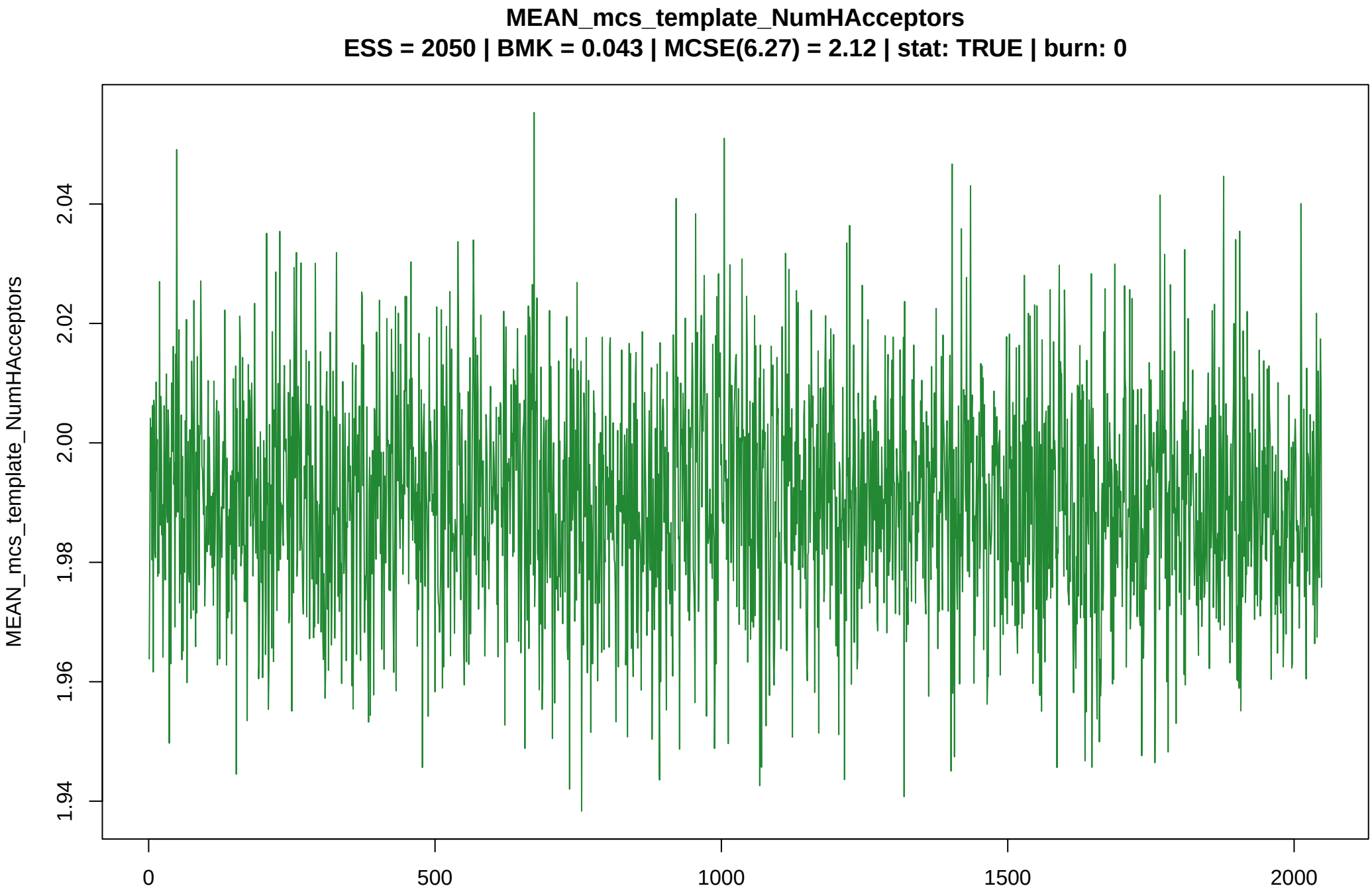

MEAN_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.0556 | MCSE(6.27) = 2.14 | stat: TRUE | burn: 0
MEAN_Xtransf_ec_tanimoto_similarity
0.04
0.02
0.00
−0.02
−0.04
−0.06
0
500
1000
1500
2000

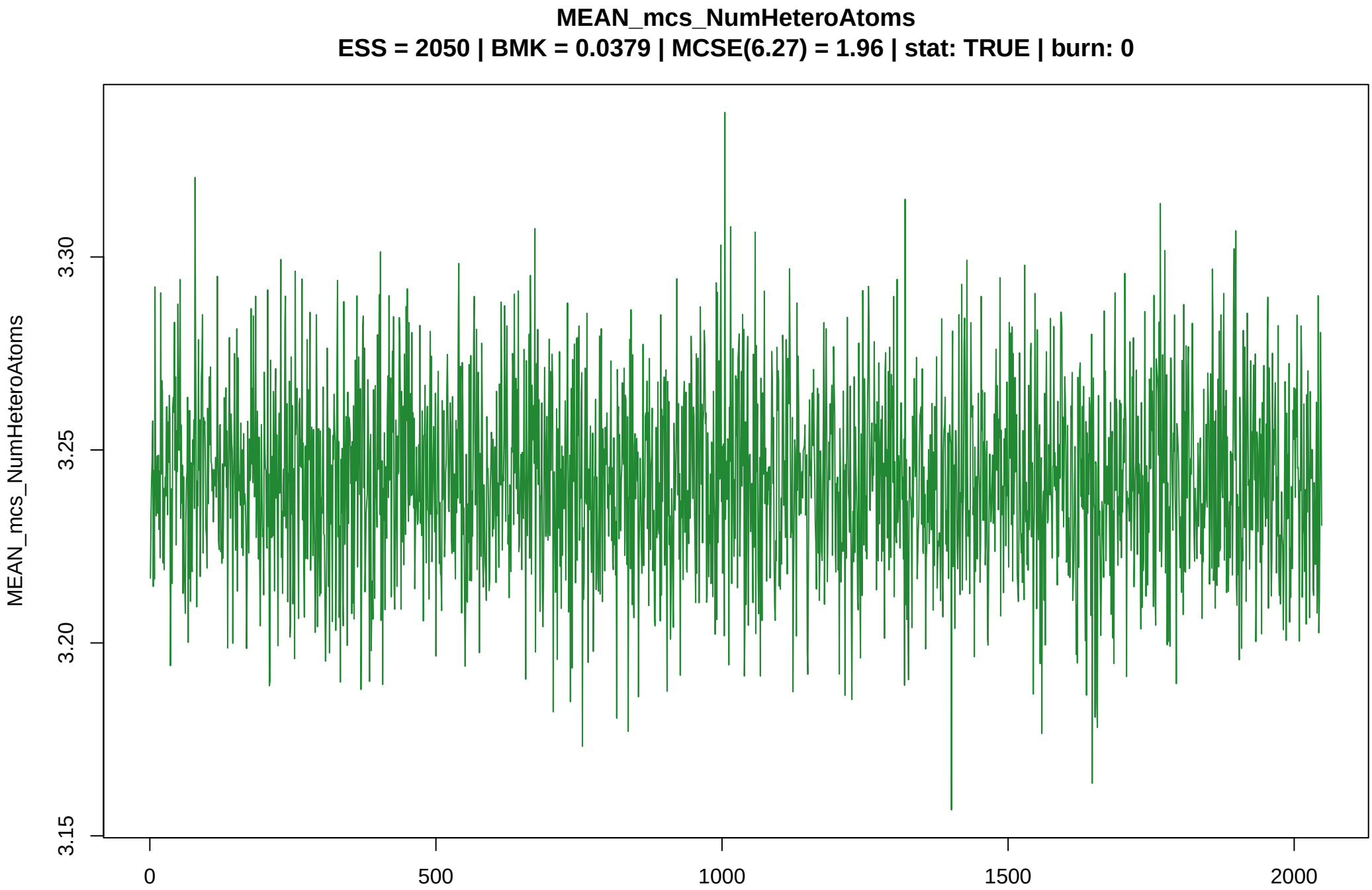

MEAN_docked_HeavyAtomCount
ESS = 2050 | BMK = 0.0418 | MCSE(6.27) = 2.58 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
27.0
27.1
27.2
27.3
27.4
27.5
0
500
1000
1500
2000

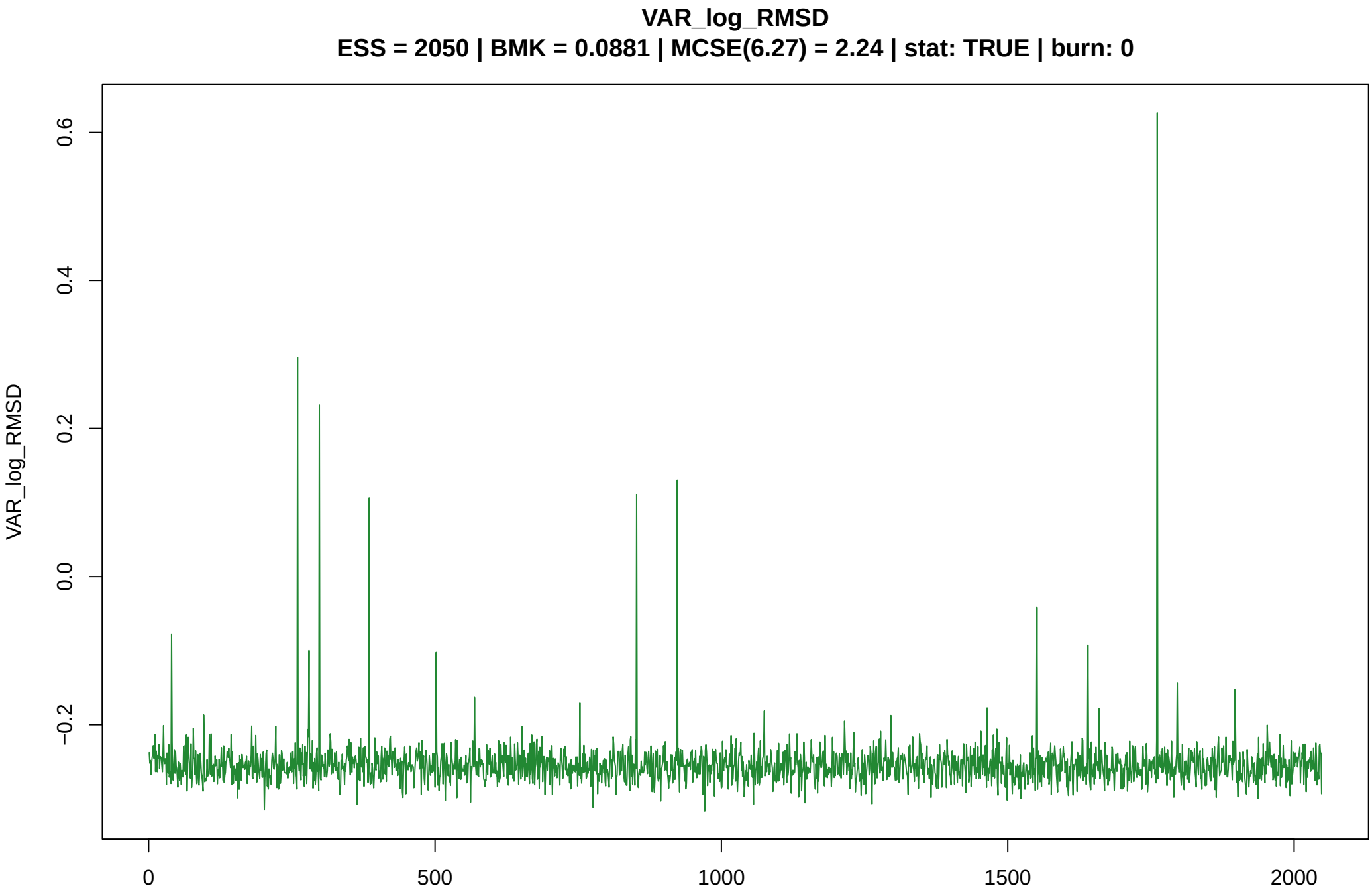

MEAN_mcs_RingCount
ESS = 2050 | BMK = 0.044 | MCSE(6.27) = 1.77 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.74
0.76
0.78
0.80
0.82
0
500
1000
1500
2000

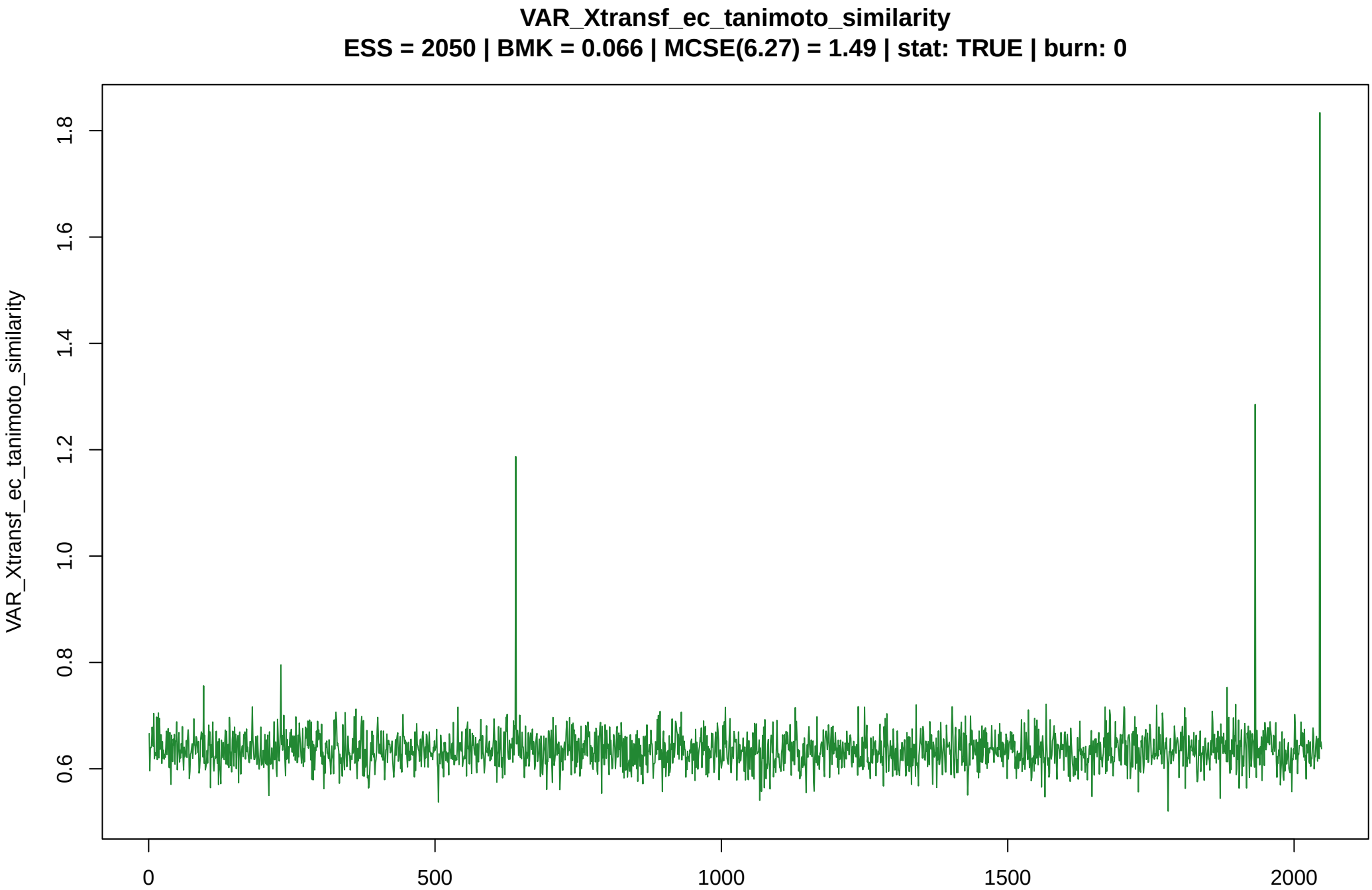

MEAN_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0488 | MCSE(6.27) = 2.31 | stat: TRUE | burn: 0
MEAN_template_HeavyAtomCount
28.1
28.2
28.3
28.4
28.5
28.6
28.7
0
500
1000
1500
2000

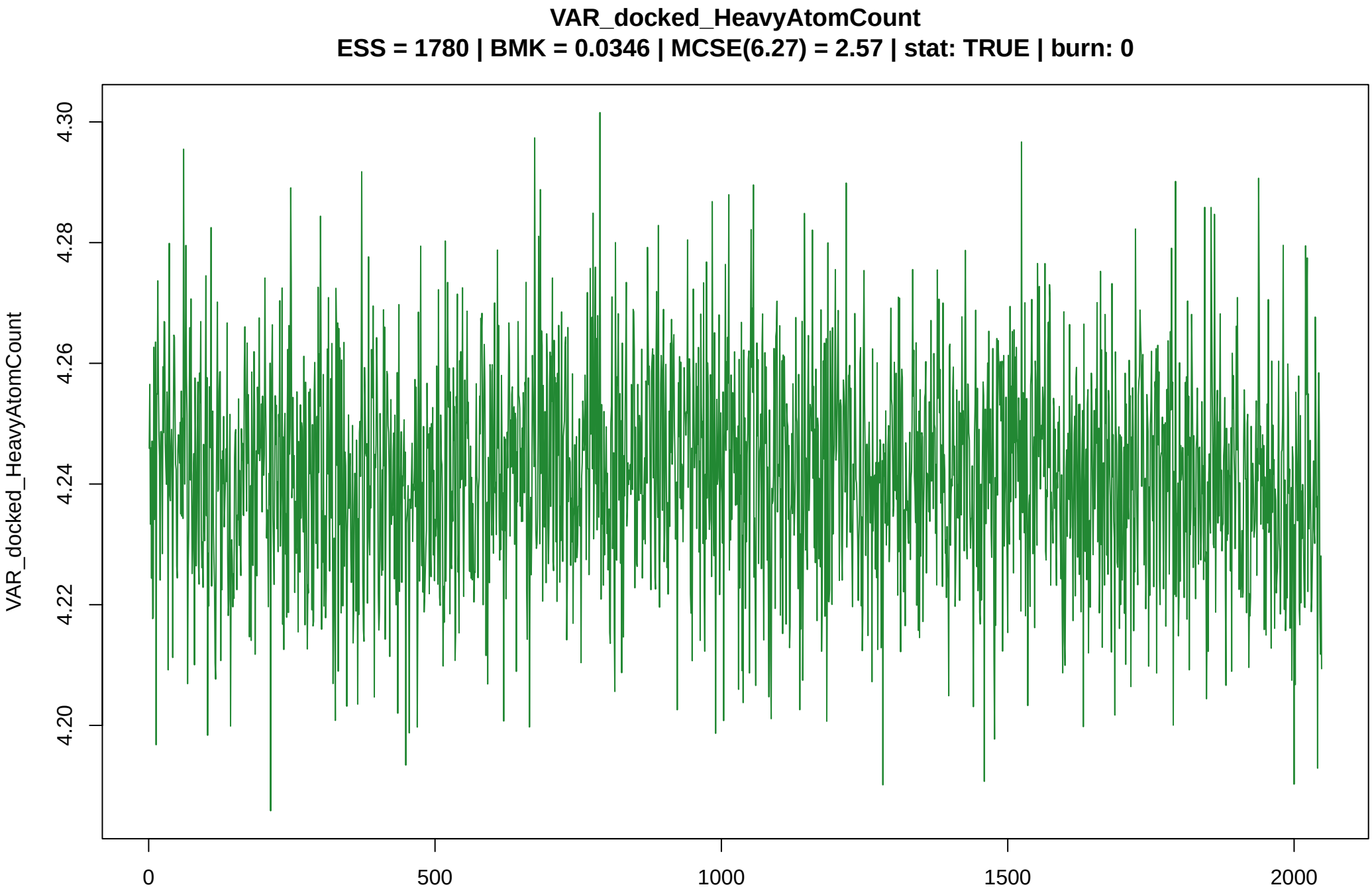

MEAN_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0519 | MCSE(6.27) = 2.23 | stat: TRUE | burn: 0
MEAN_mcs_docked_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
2.06
0
500
1000
1500
2000

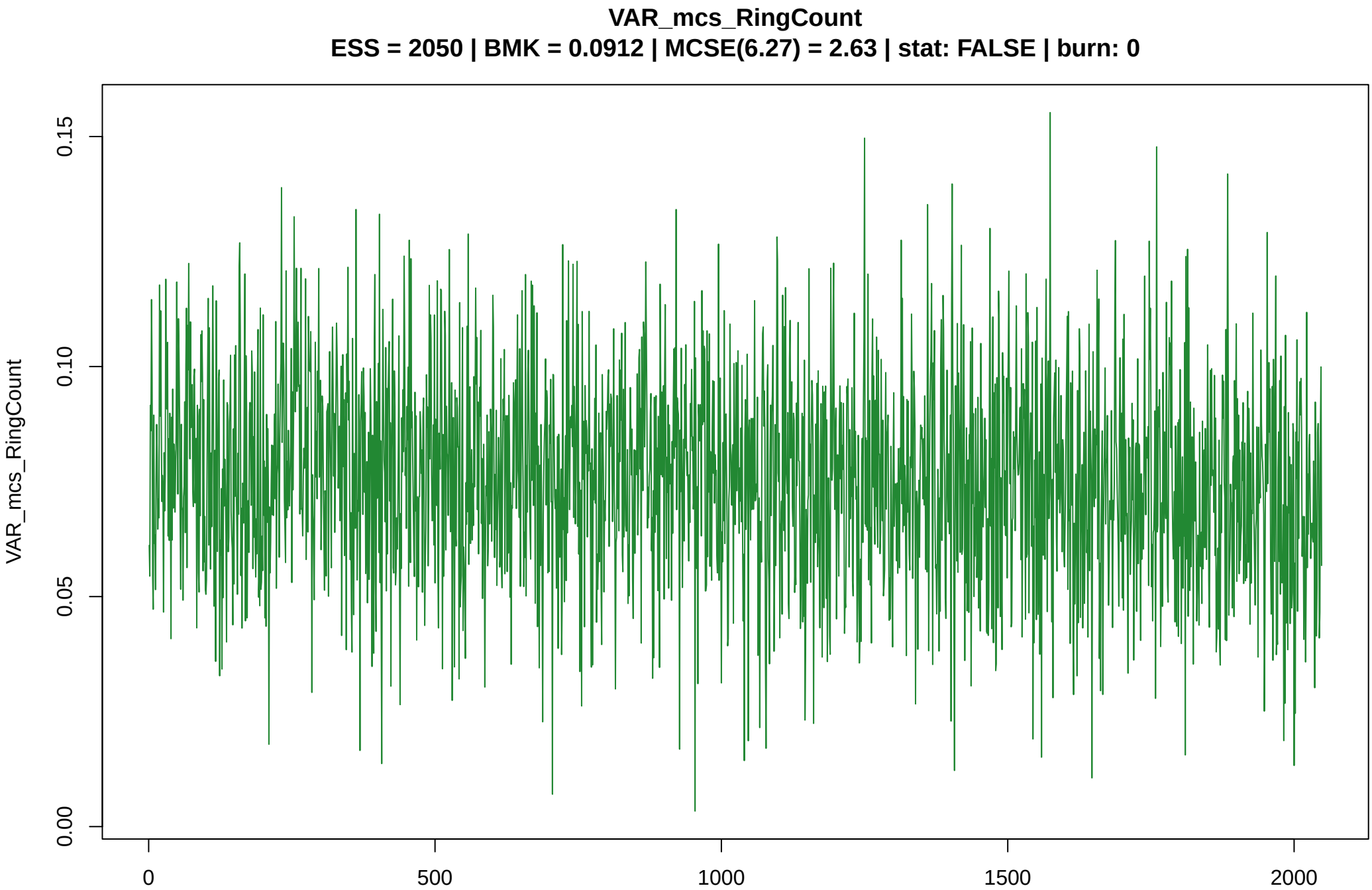

MEAN_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.043 | MCSE(6.27) = 2.12 | stat: TRUE | burn: 0
MEAN_mcs_template_NumHAcceptors
1.94
1.96
1.98
2.00
2.02
2.04
0
500
1000
1500
2000

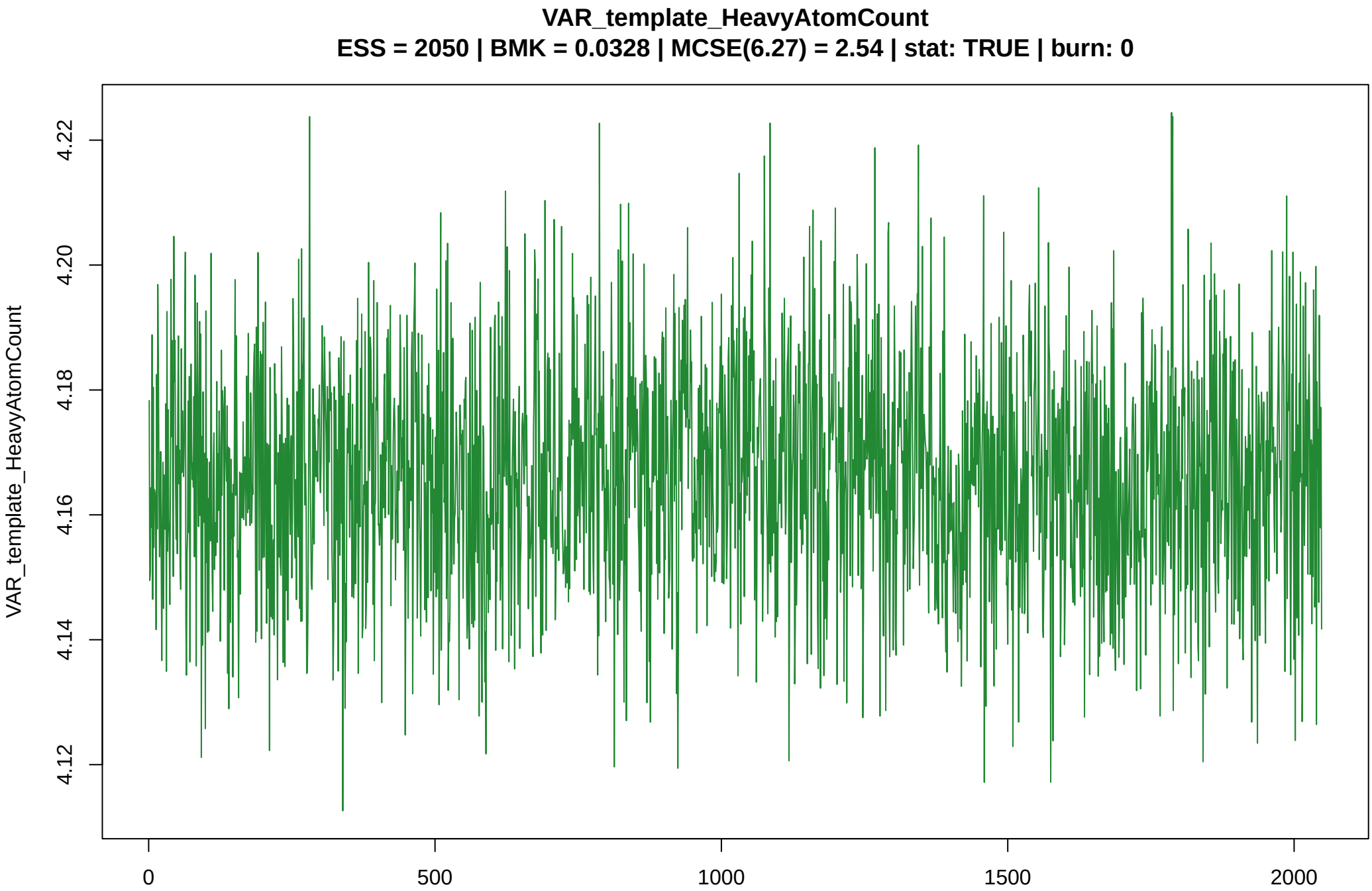

MEAN_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0379 | MCSE(6.27) = 1.96 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
3.15
3.20
3.25
3.30
0
500
1000
1500
2000

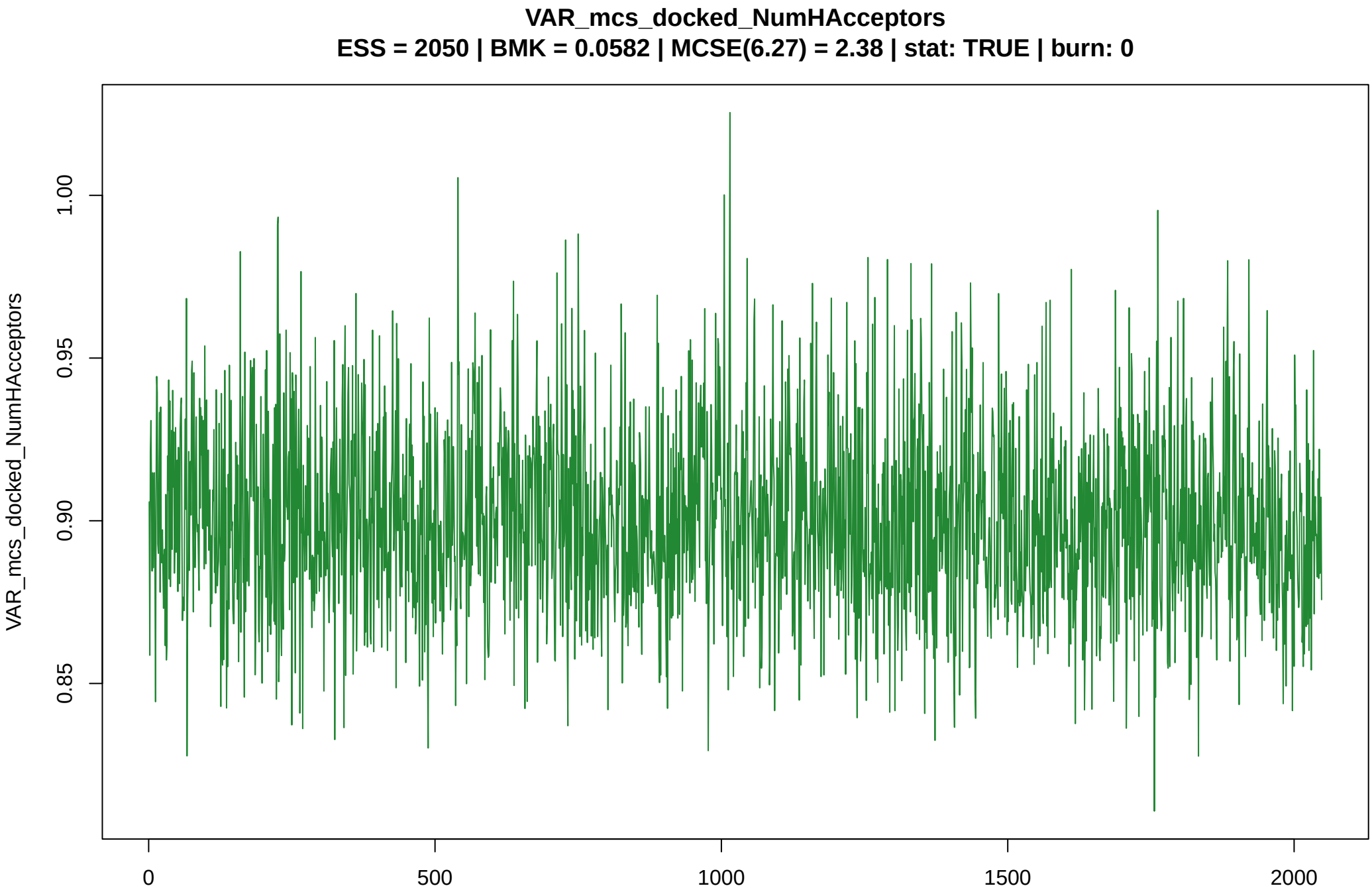

VAR_log_RMSD
ESS = 2050 | BMK = 0.0881 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0
VAR_log_RMSD
0.6
0.4
0.2
0.0
−0.2
0
500
1000
1500
2000

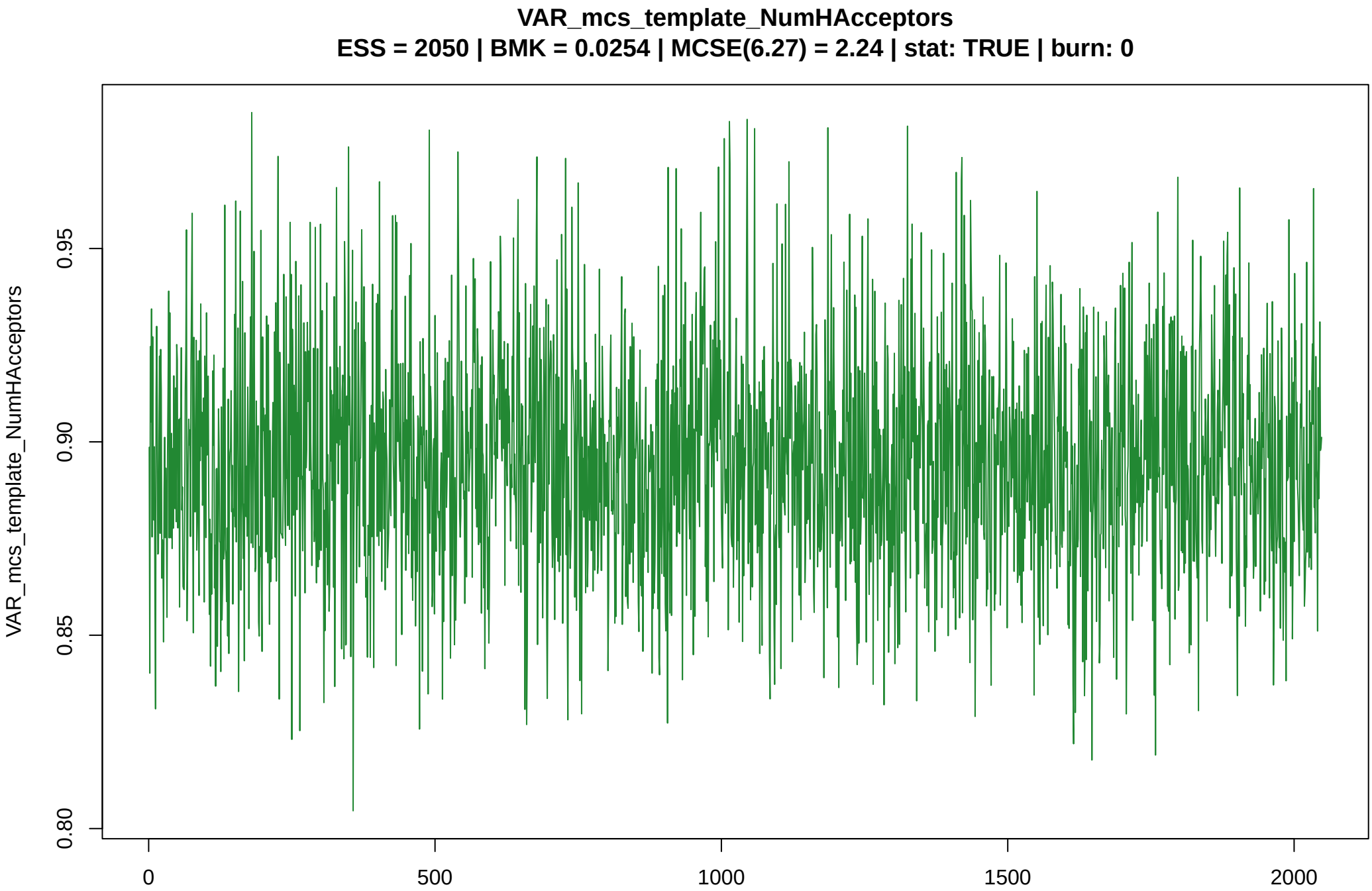

VAR_Xtransf_ec_tanimoto_similarity
ESS = 2050 | BMK = 0.066 | MCSE(6.27) = 1.49 | stat: TRUE | burn: 0
VAR_Xtransf_ec_tanimoto_similarity
0.6
0.8
1.0
1.2
1.4
1.6
1.8
0
500
1000
1500
2000

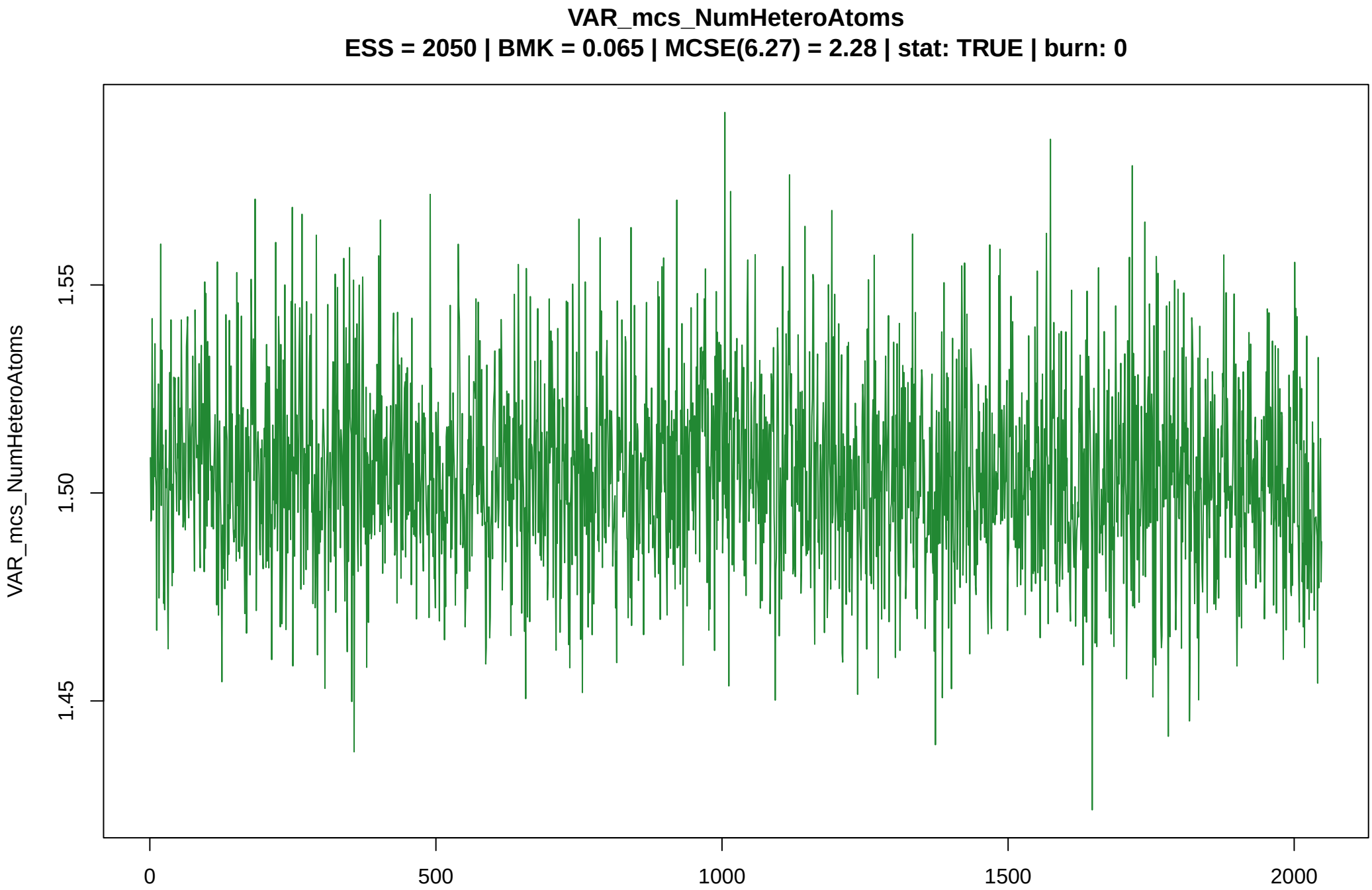

VAR_docked_HeavyAtomCount
ESS = 1780 | BMK = 0.0346 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0
VAR_docked_HeavyAtomCount
4.20
4.22
4.24
4.26
4.28
4.30
0
500
1000
1500
2000

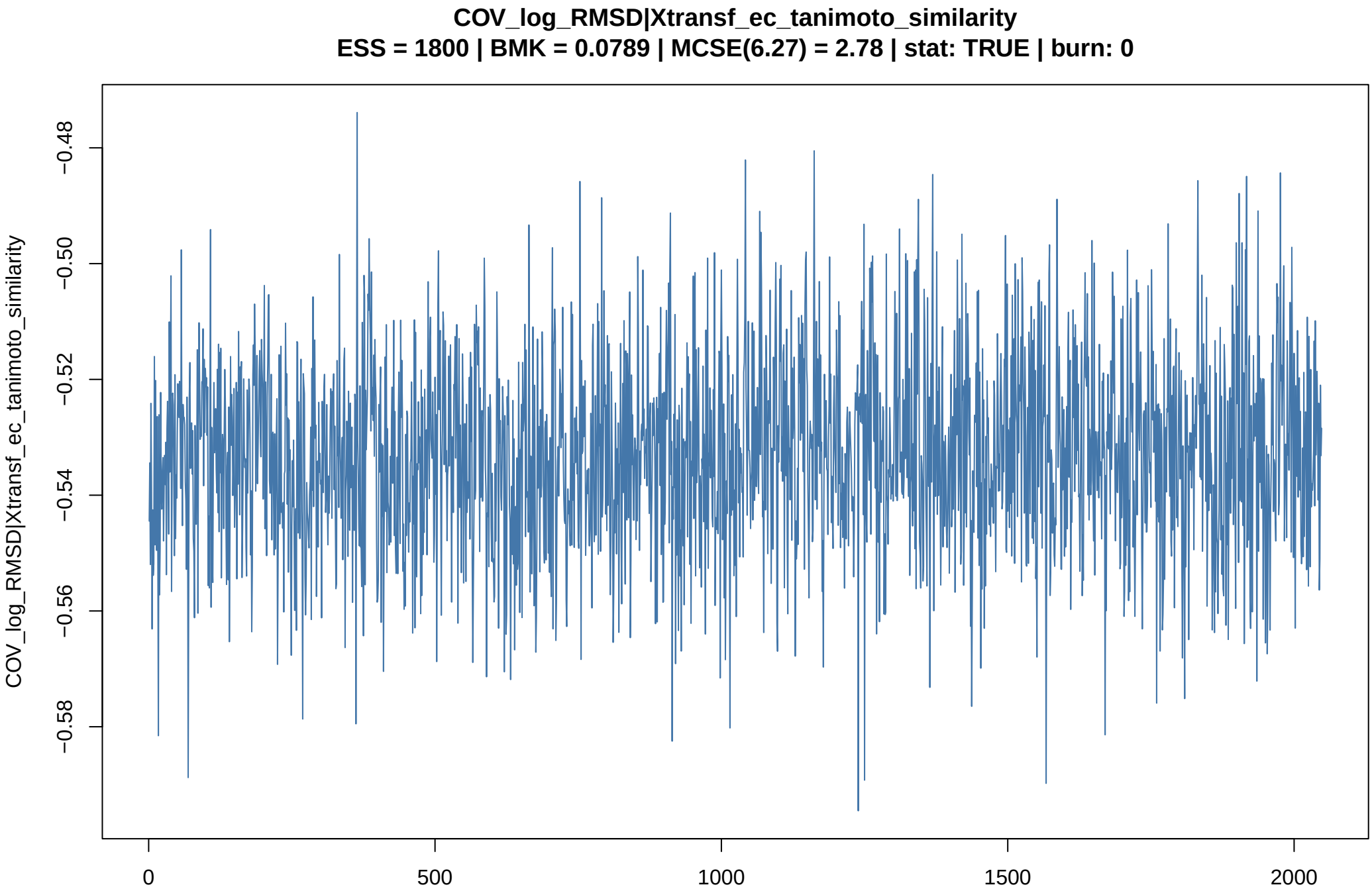

VAR_mcs_RingCount
ESS = 2050 | BMK = 0.0912 | MCSE(6.27) = 2.63 | stat: FALSE | burn: 0
VAR_mcs_RingCount
0.00
0.05
0.10
0.15
0
500
1000
1500
2000

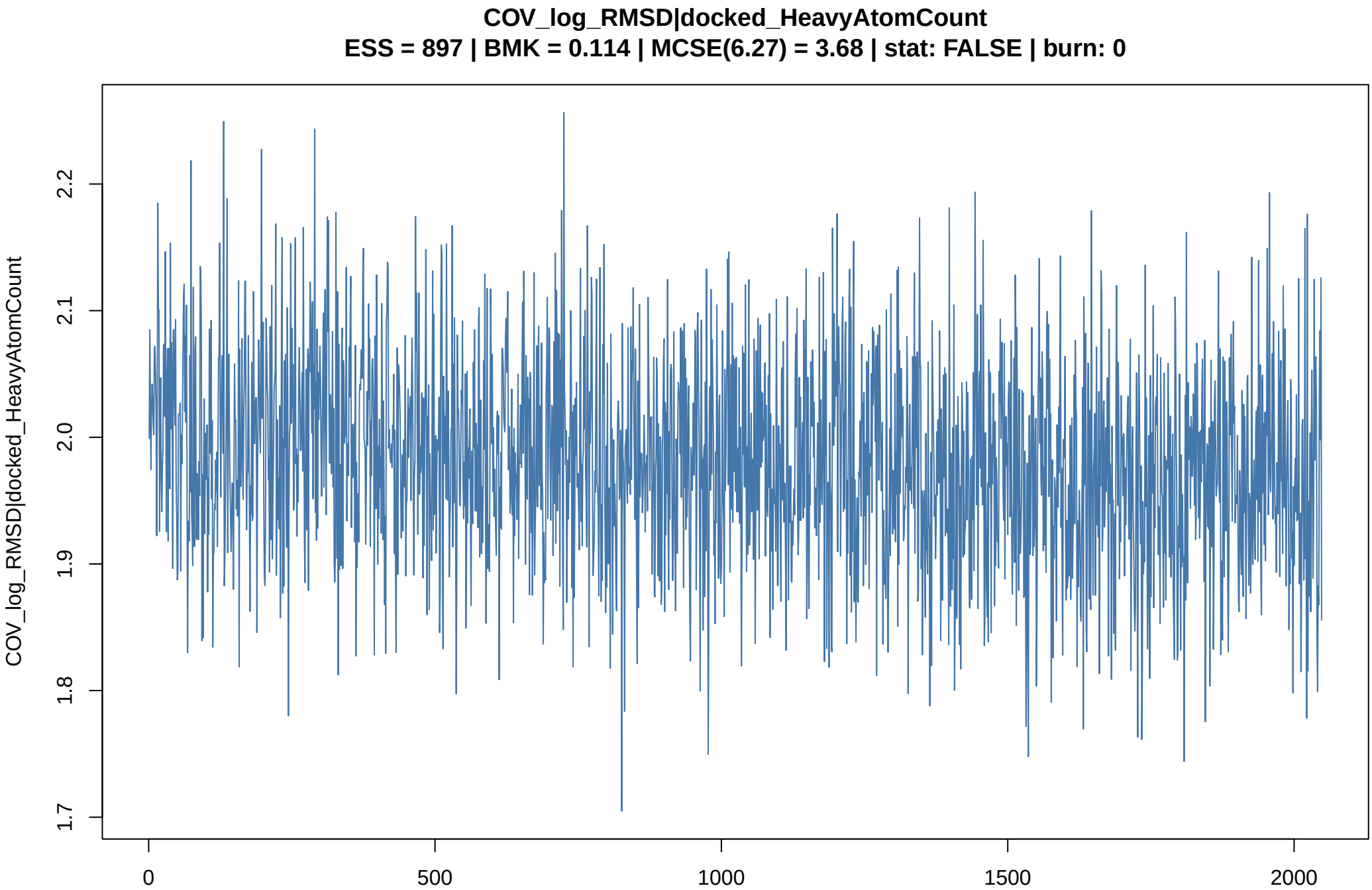

VAR_template_HeavyAtomCount
ESS = 2050 | BMK = 0.0328 | MCSE(6.27) = 2.54 | stat: TRUE | burn: 0
VAR_template_HeavyAtomCount
4.12
4.14
4.16
4.18
4.20
4.22
0
500
1000
1500
2000

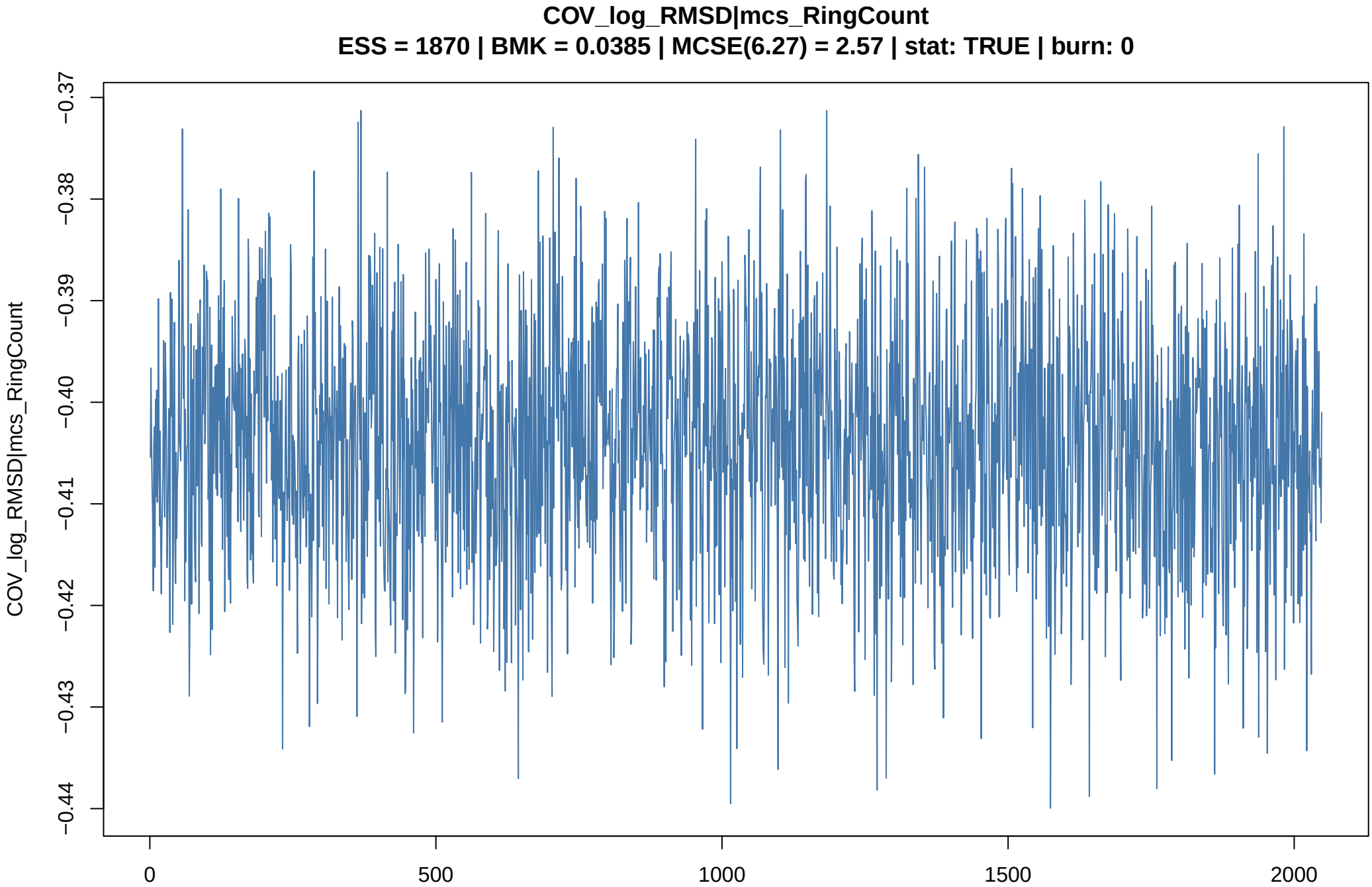

VAR_mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0582 | MCSE(6.27) = 2.38 | stat: TRUE | burn: 0
VAR_mcs_docked_NumHAcceptors
0.85
0.90
0.95
1.00
0
500
1000
1500
2000

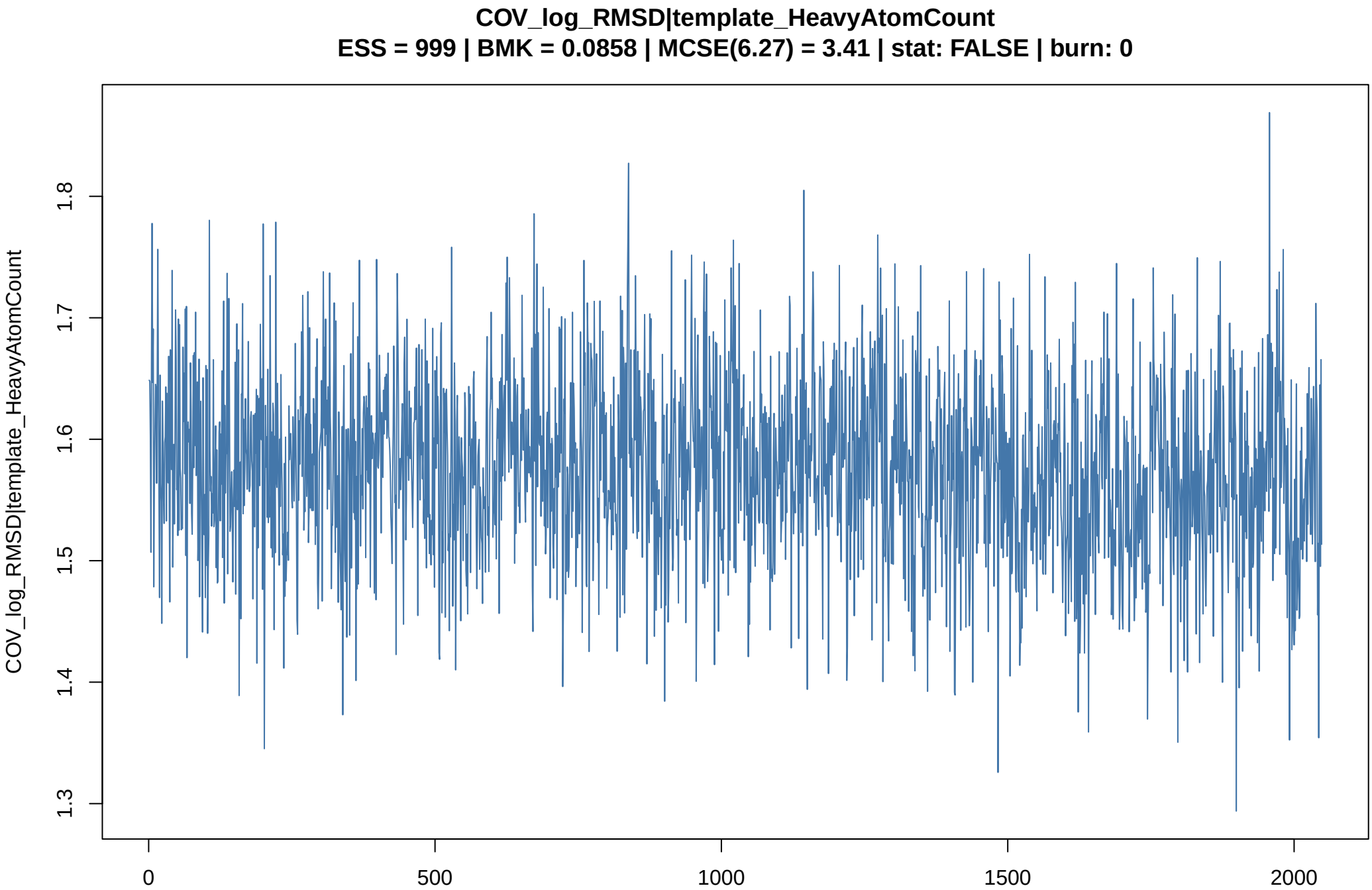

VAR_mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0254 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0
VAR_mcs_template_NumHAcceptors
0.80
0.85
0.90
0.95
0
500
1000
1500
2000

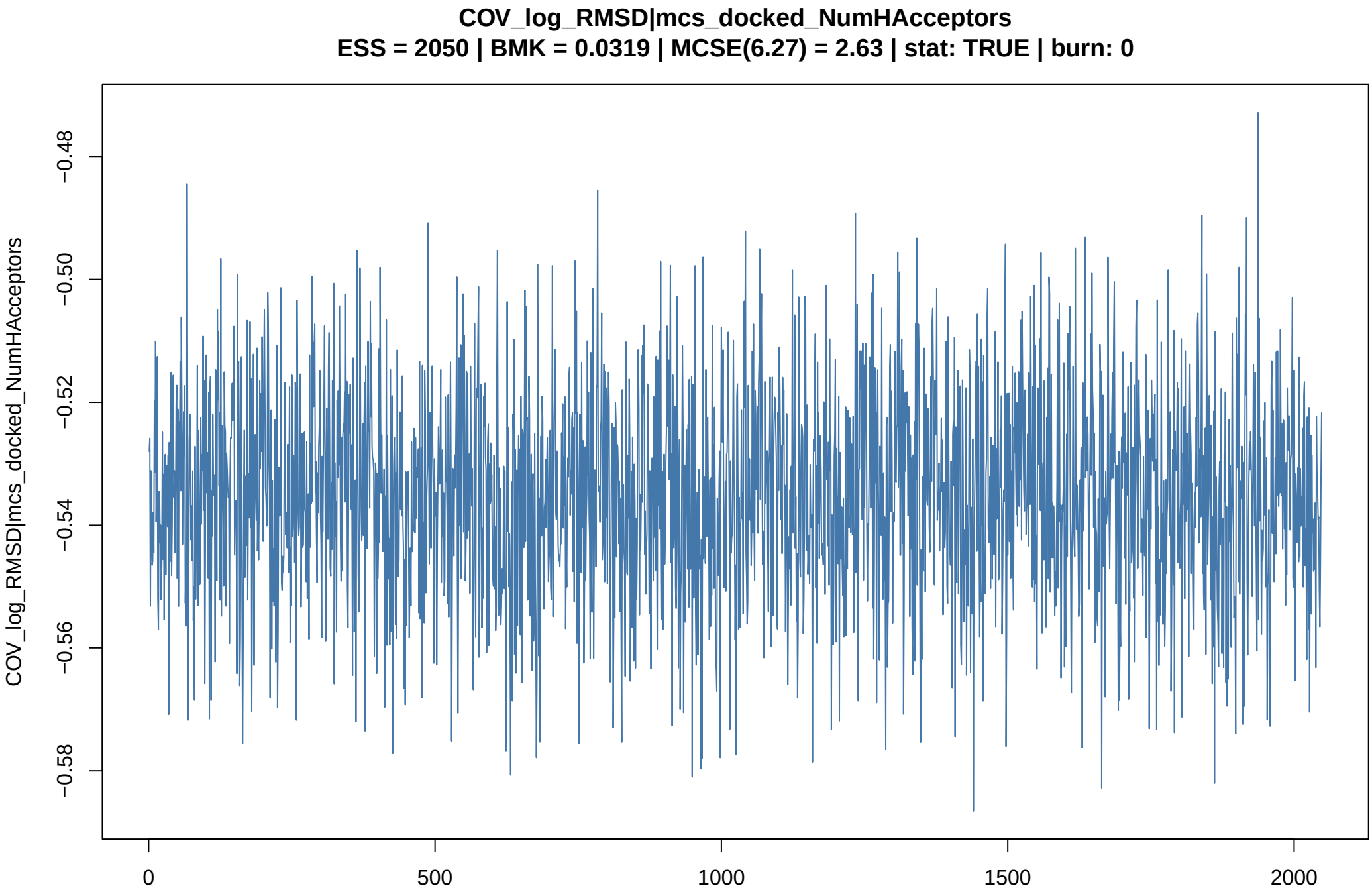

VAR_mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.065 | MCSE(6.27) = 2.28 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
1.45
1.50
1.55
0
500
1000
1500
2000

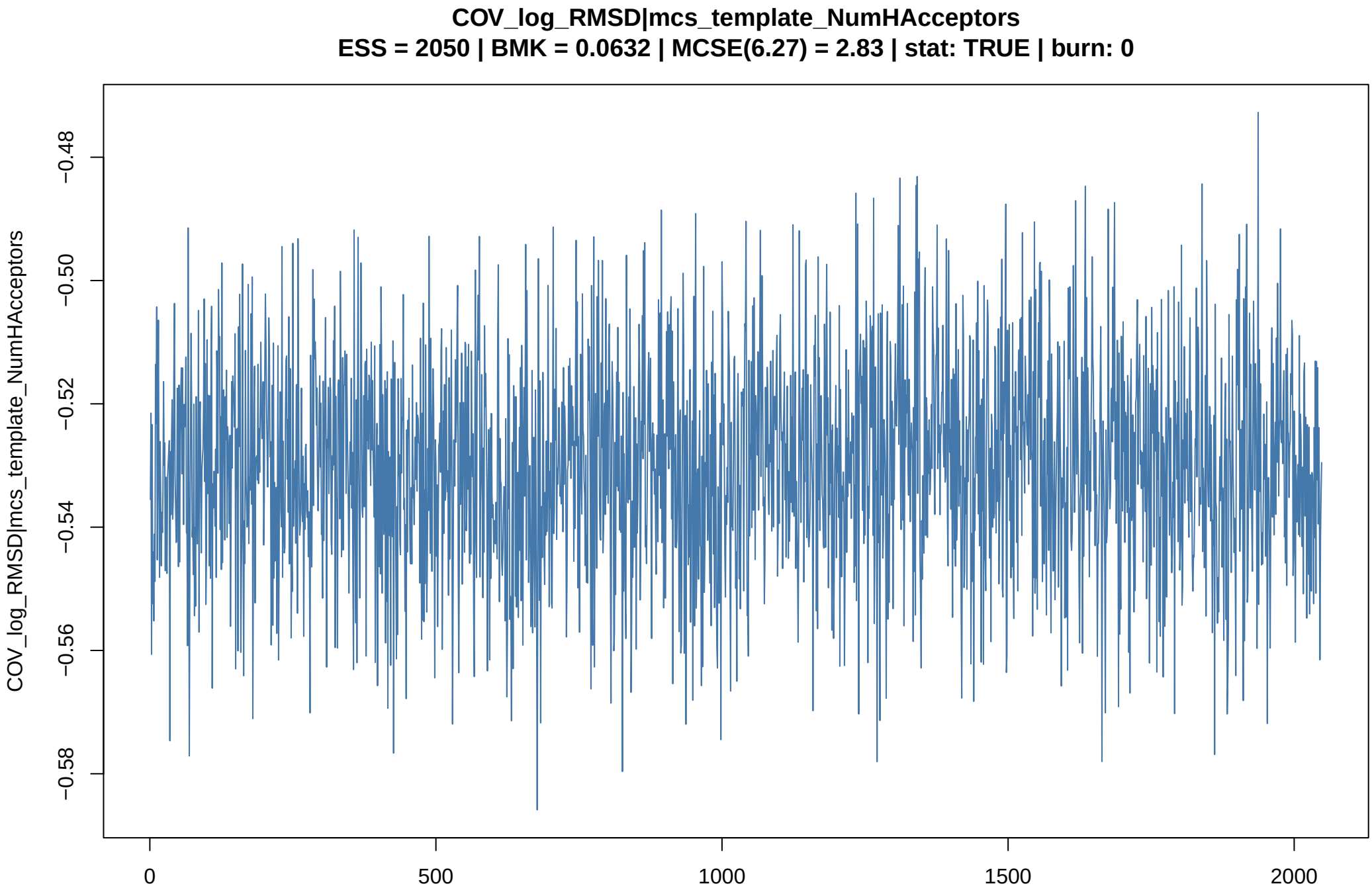

COV_log_RMSD|Xtransf_ec_tanimoto_similarity
ESS = 1800 | BMK = 0.0789 | MCSE(6.27) = 2.78 | stat: TRUE | burn: 0
COV_log_RMSD|Xtransf_ec_tanimoto_similarity
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

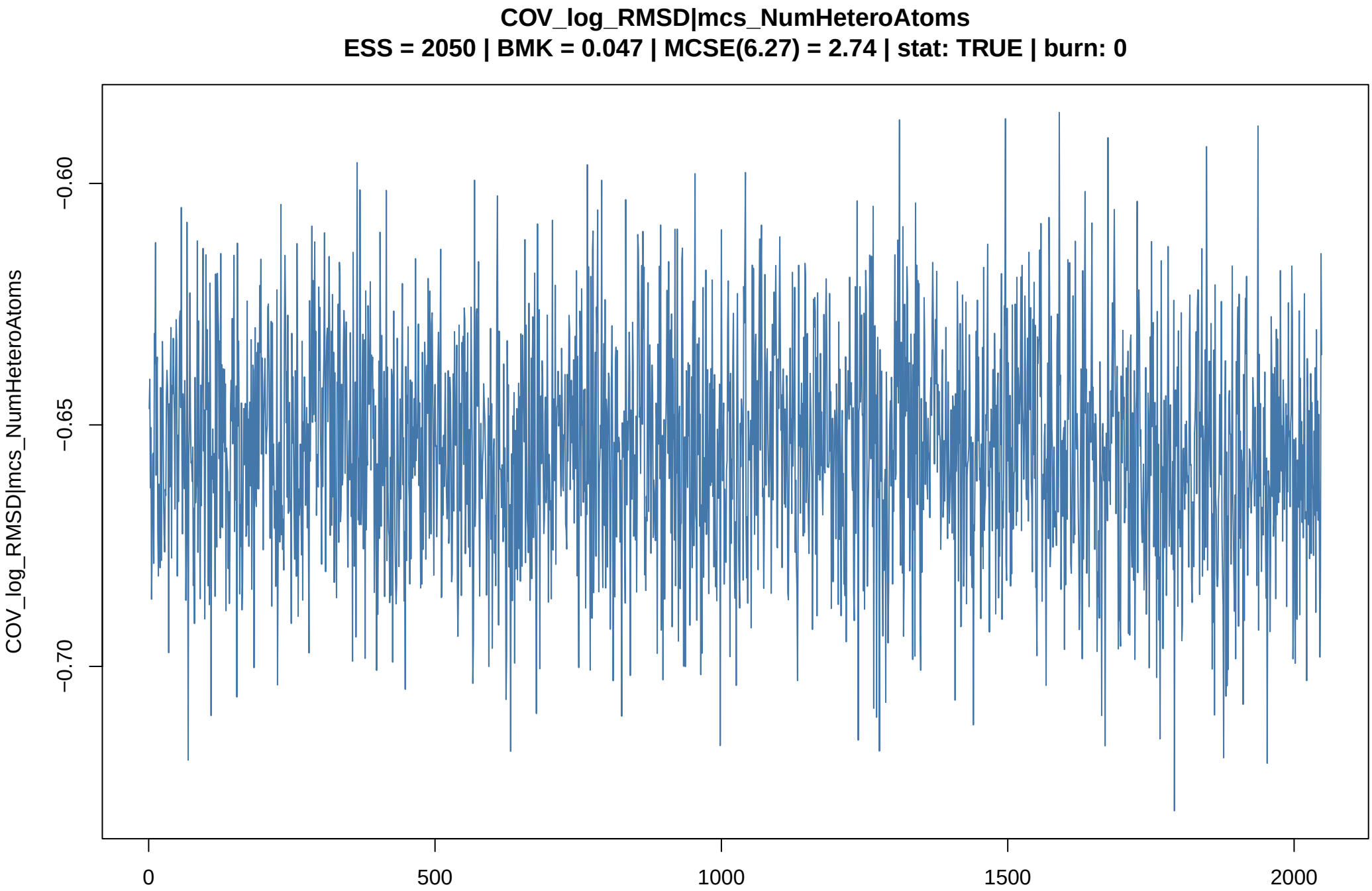

COV_log_RMSD|docked_HeavyAtomCount
ESS = 897 | BMK = 0.114 | MCSE(6.27) = 3.68 | stat: FALSE | burn: 0
COV_log_RMSD|docked_HeavyAtomCount
1.7
1.8
1.9
2.0
2.1
2.2
0
500
1000
1500
2000

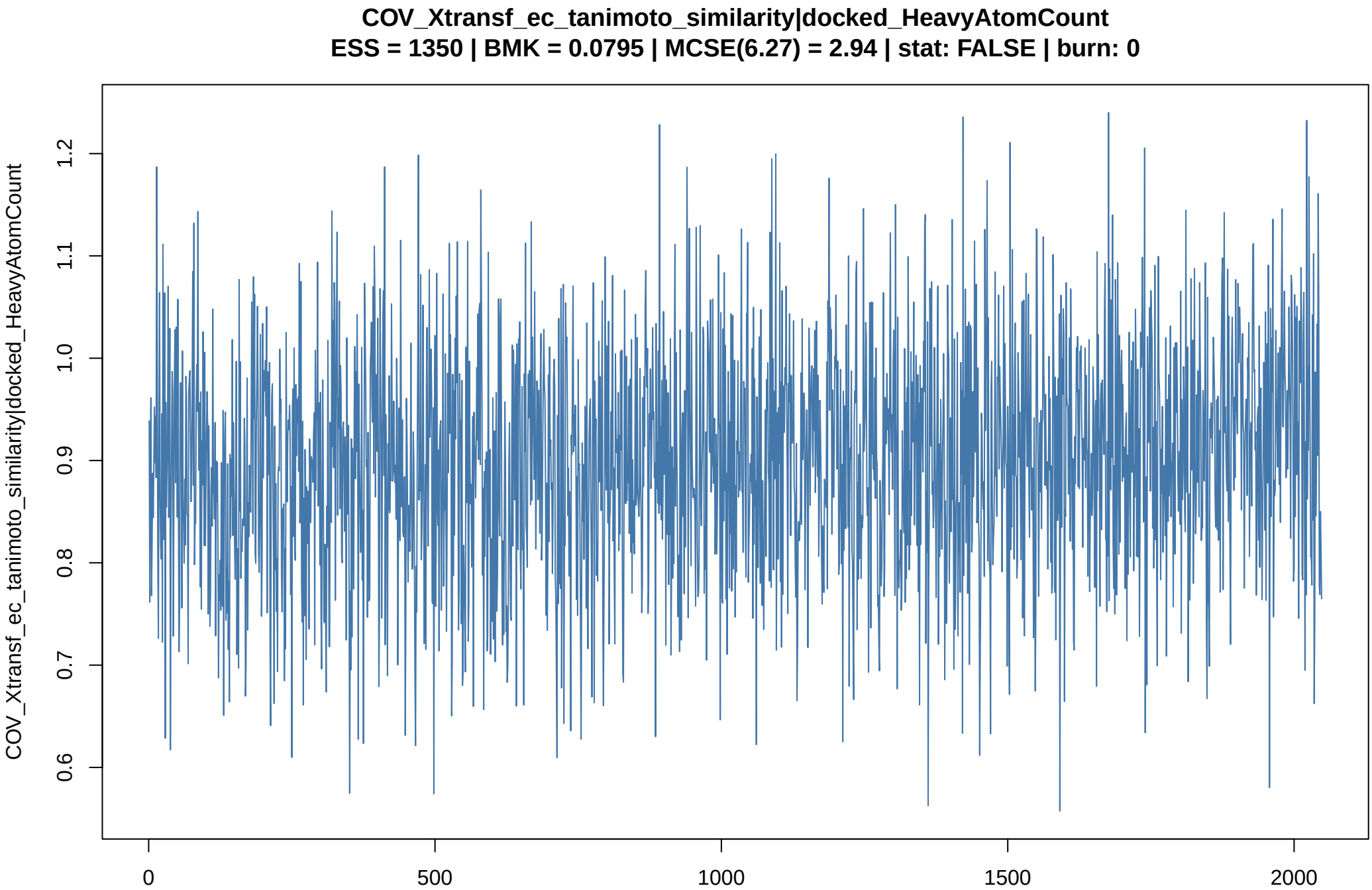

COV_log_RMSD|mcs_RingCount
ESS = 1870 | BMK = 0.0385 | MCSE(6.27) = 2.57 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_RingCount
−0.37
−0.38
−0.39
−0.40
−0.41
−0.42
−0.43
−0.44
0
500
1000
1500
2000

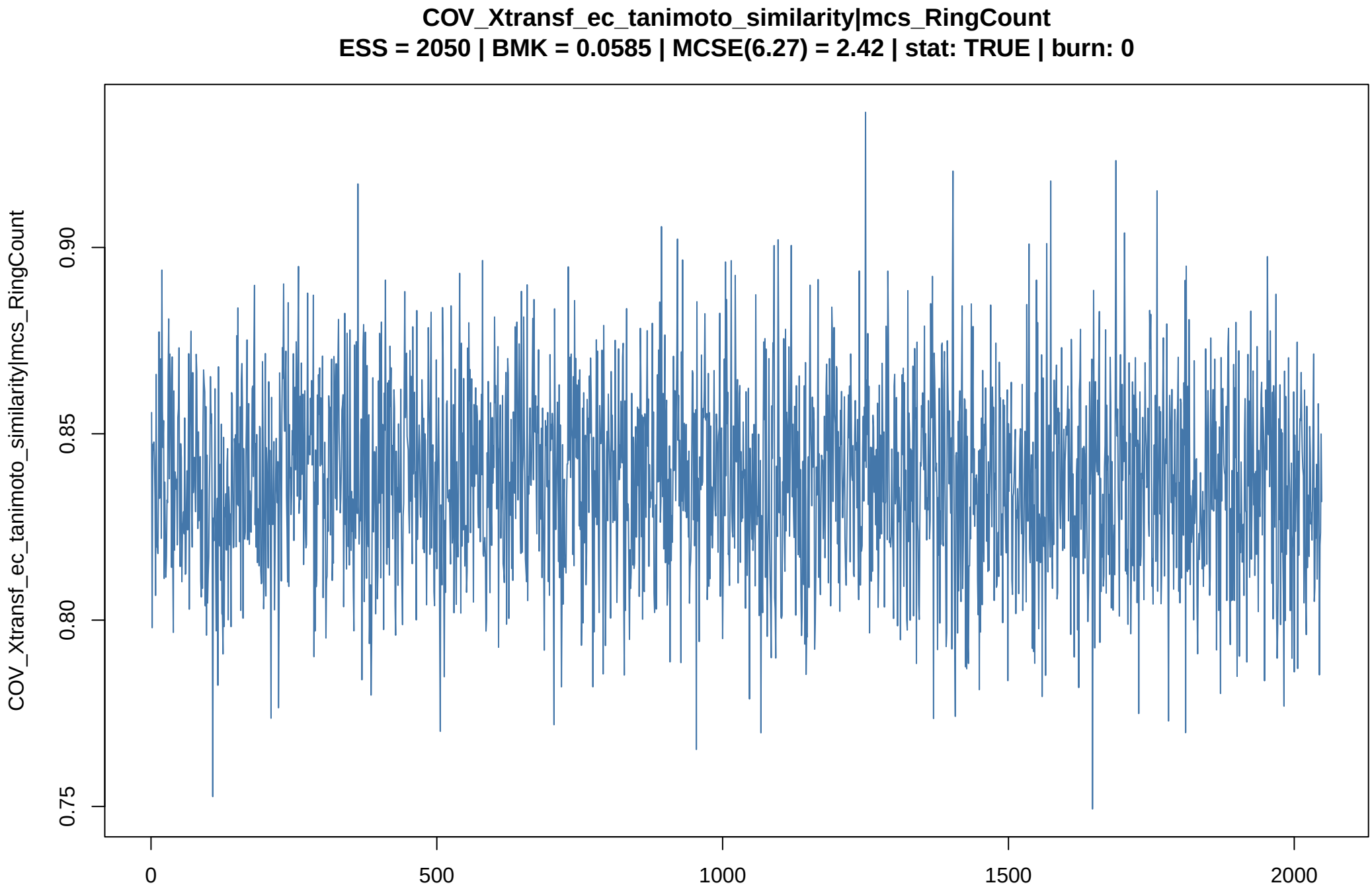

COV_log_RMSD|template_HeavyAtomCount
ESS = 999 | BMK = 0.0858 | MCSE(6.27) = 3.41 | stat: FALSE | burn: 0
COV_log_RMSD|template_HeavyAtomCount
1.3
1.4
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

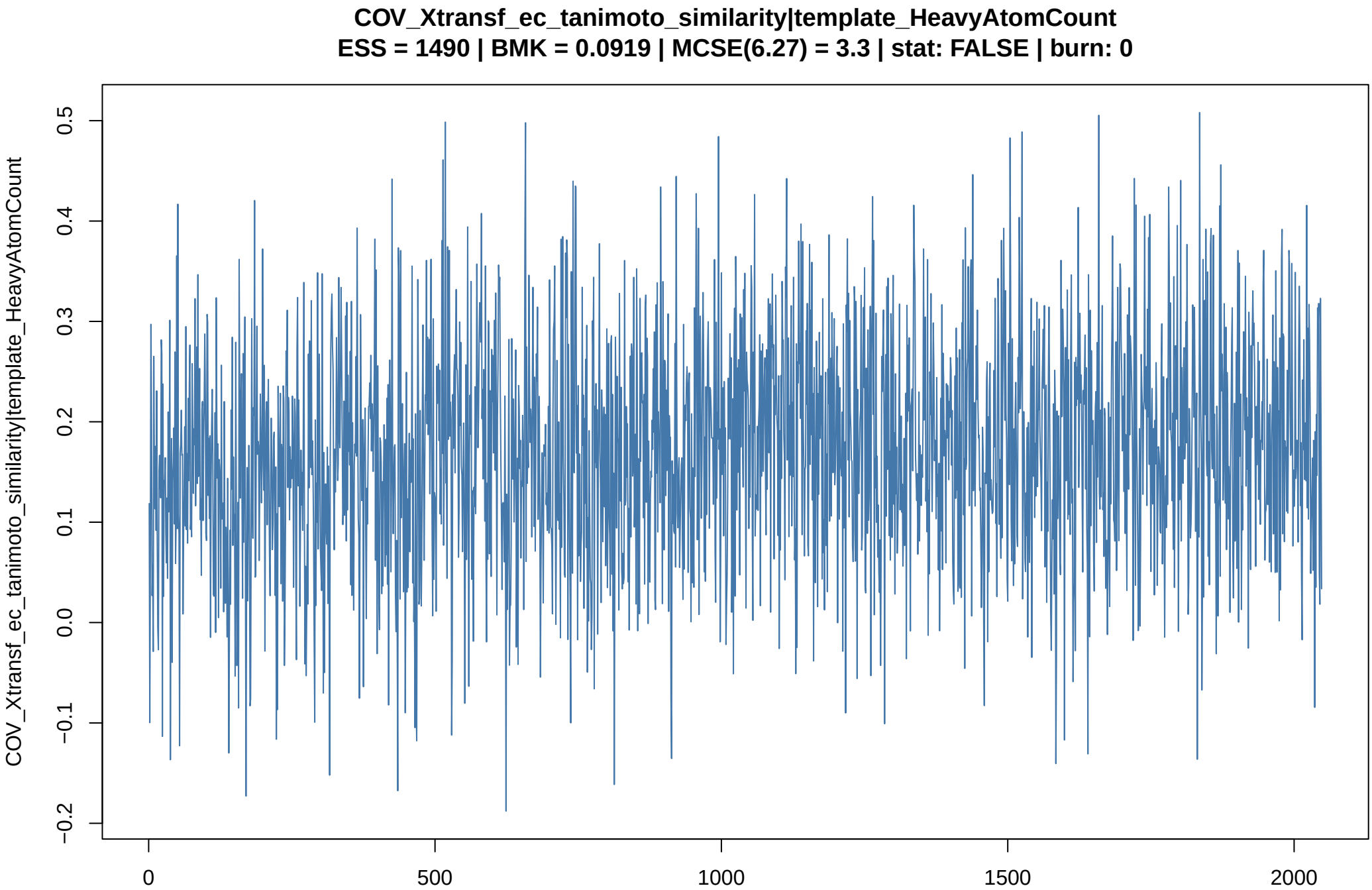

COV_log_RMSD|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0319 | MCSE(6.27) = 2.63 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_docked_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

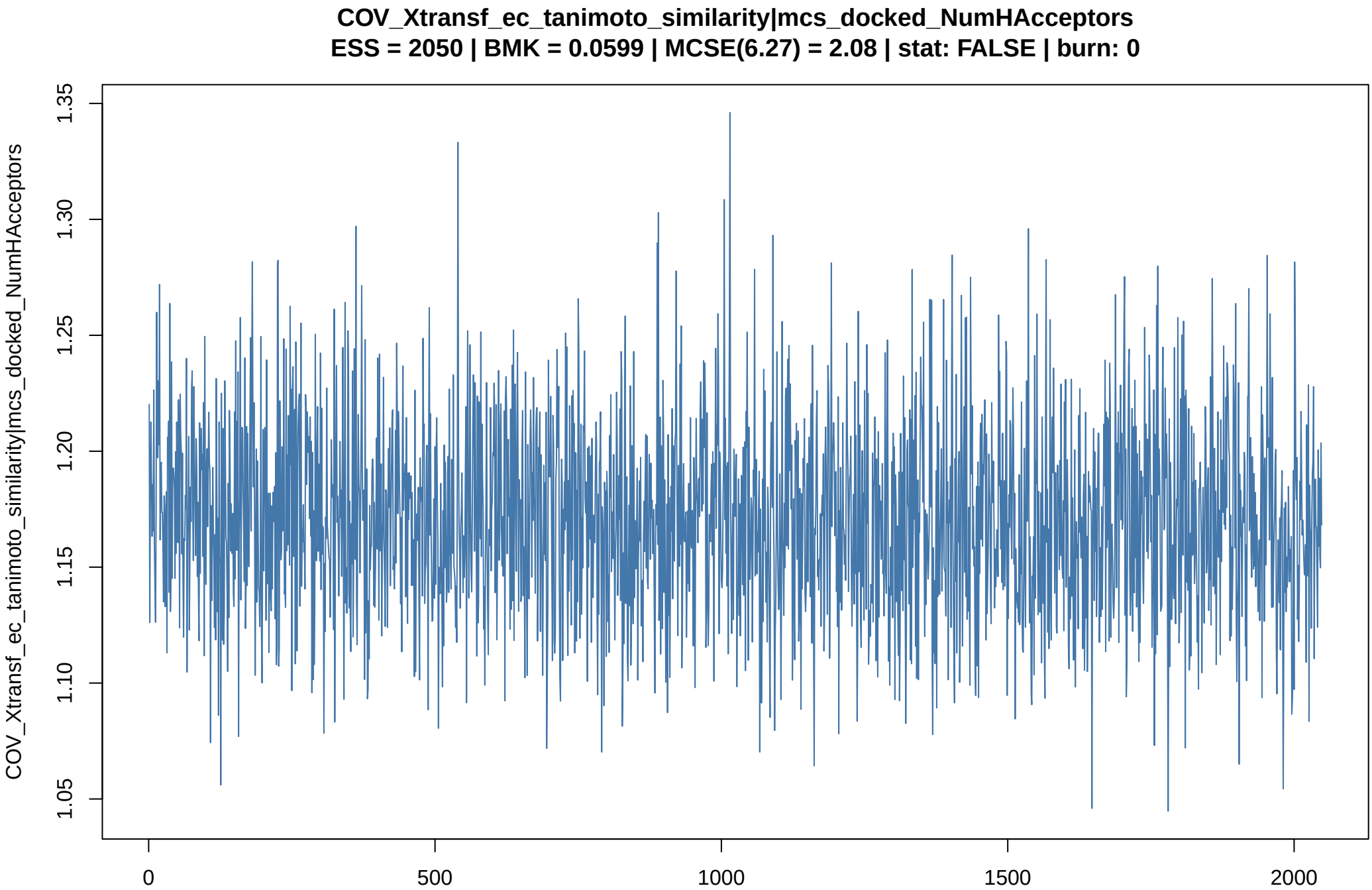

COV_log_RMSD|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0632 | MCSE(6.27) = 2.83 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_template_NumHAcceptors
−0.48
−0.50
−0.52
−0.54
−0.56
−0.58
0
500
1000
1500
2000

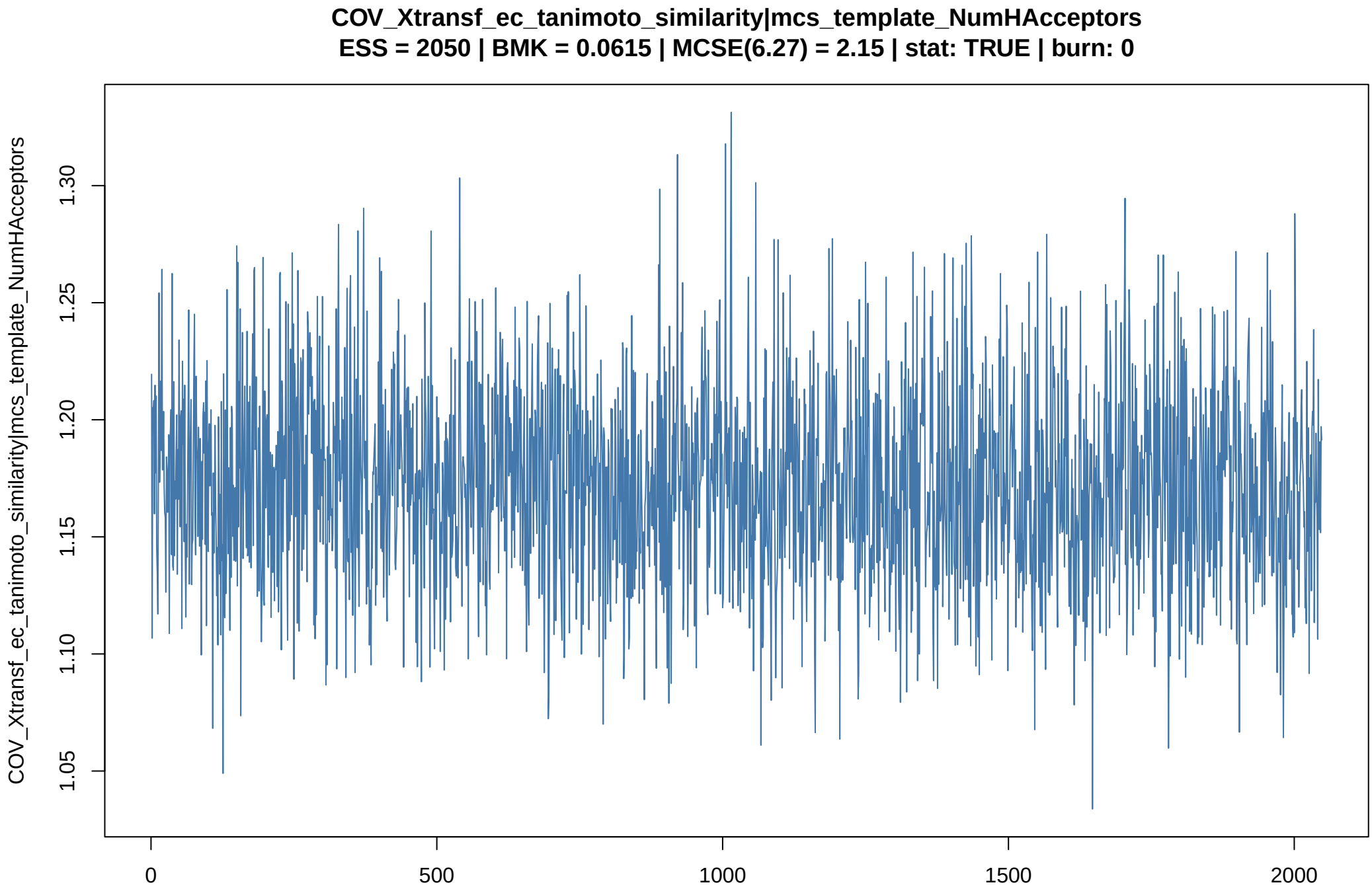

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.047 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0
COV_log_RMSD|mcs_NumHeteroAtoms
−0.60
−0.65
−0.70
0
500
1000
1500
2000

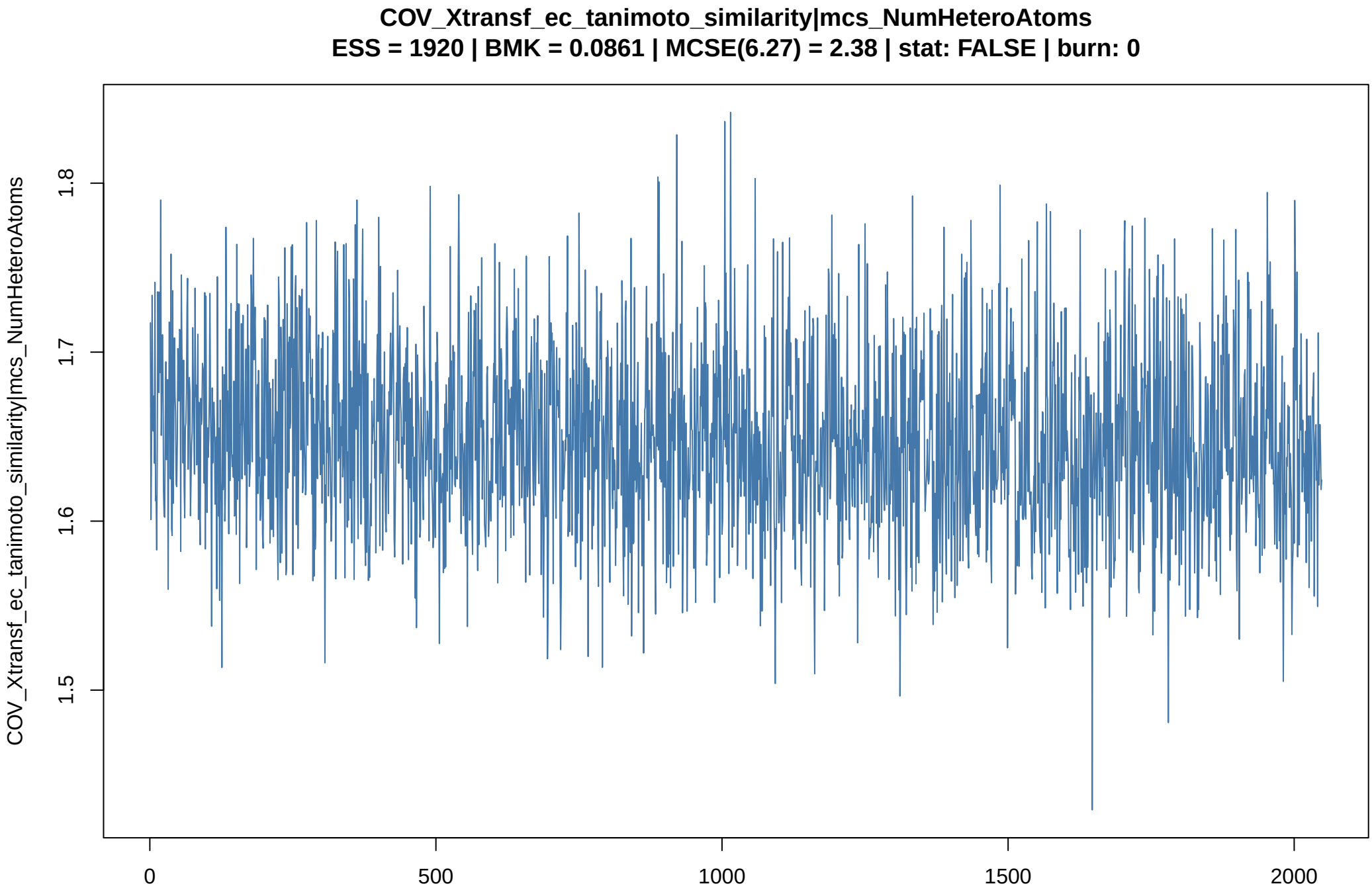

COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 1350 | BMK = 0.0795 | MCSE(6.27) = 2.94 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|docked_HeavyAtomCount
0.6
0.7
0.8
0.9
1.0
1.1
1.2
0
500
1000
1500
2000

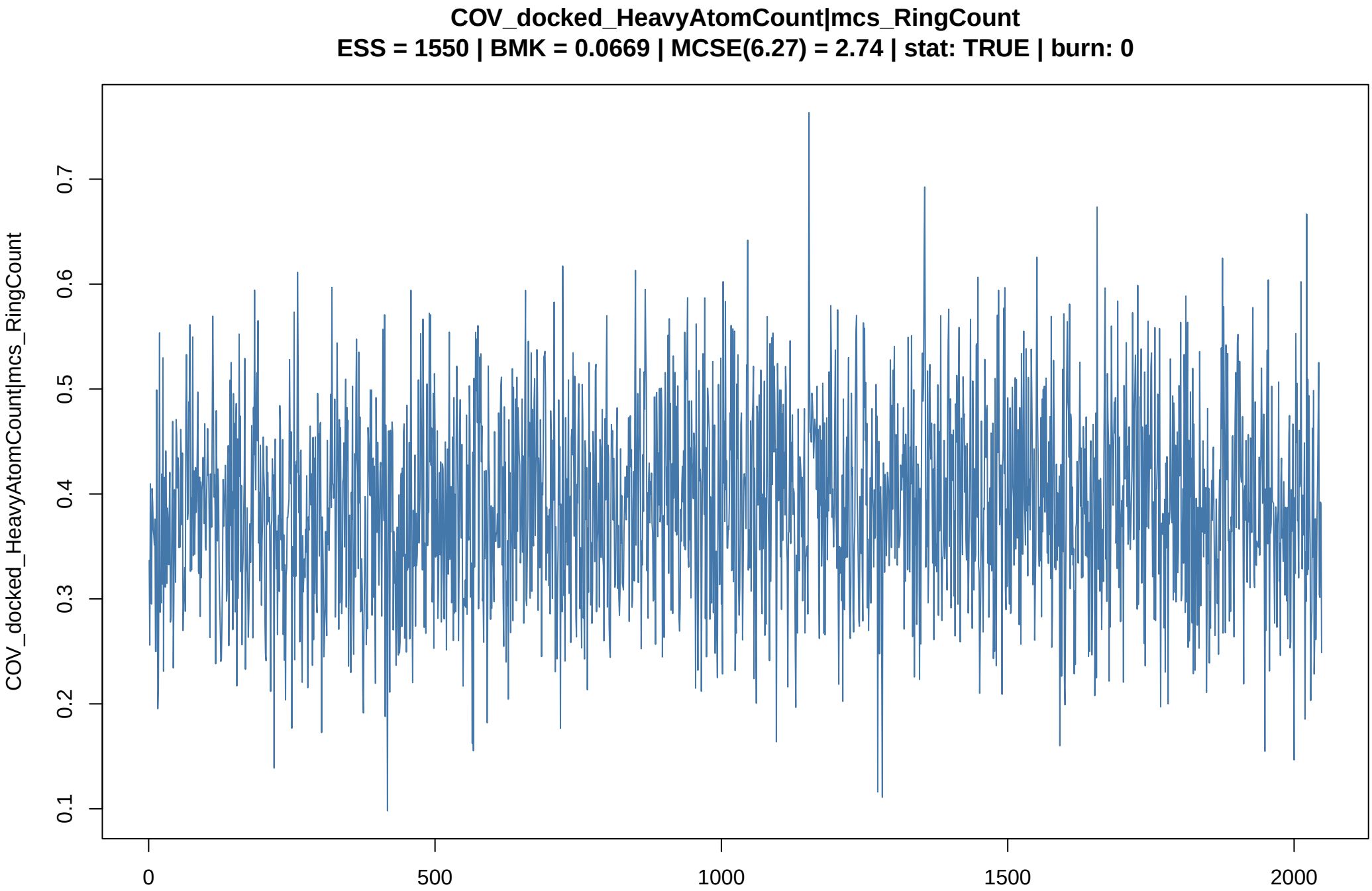

COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
ESS = 2050 | BMK = 0.0585 | MCSE(6.27) = 2.42 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_RingCount
0.75
0.80
0.85
0.90
0
500
1000
1500
2000

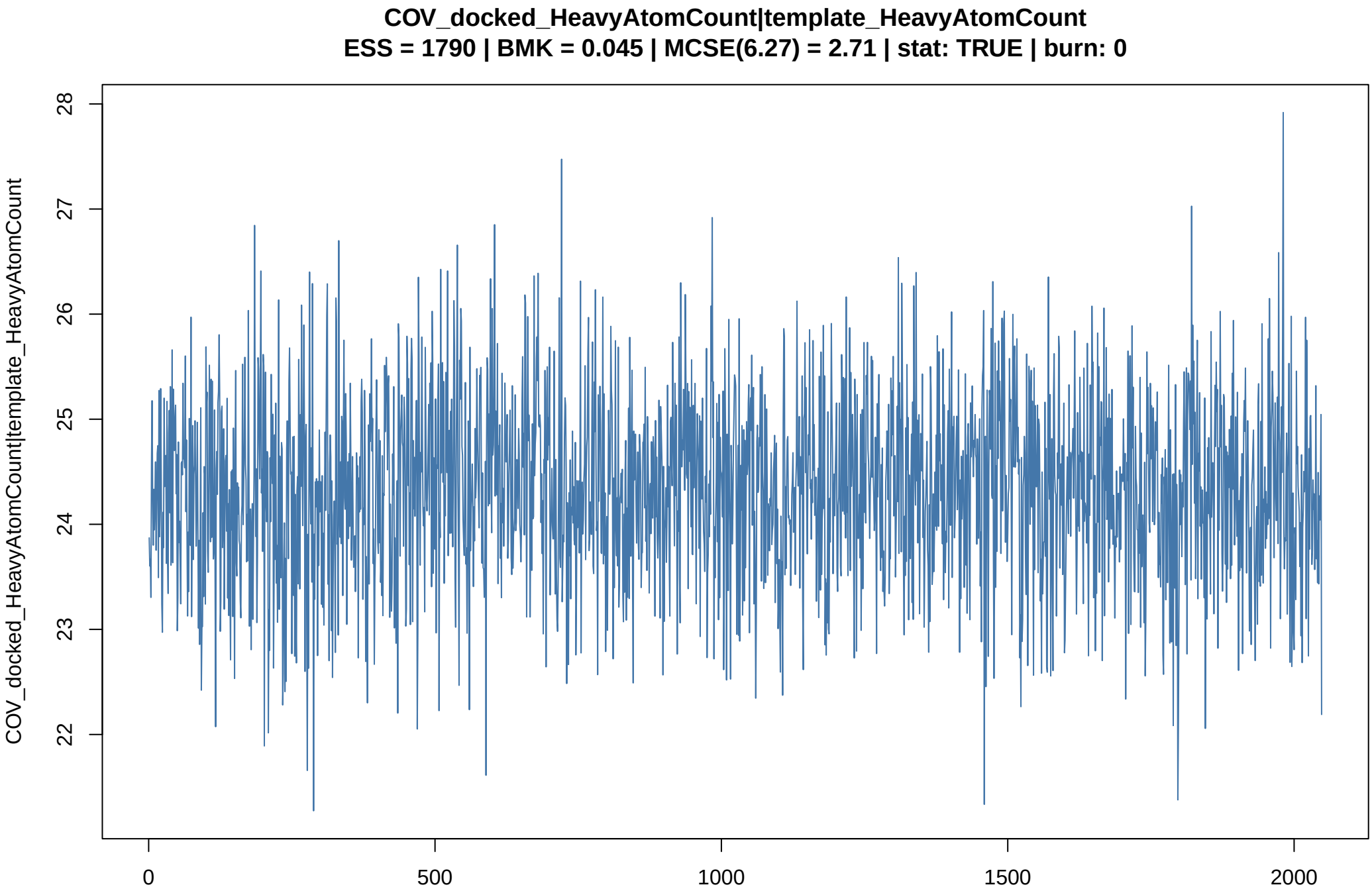

COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
ESS = 1490 | BMK = 0.0919 | MCSE(6.27) = 3.3 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|template_HeavyAtomCount
0.5
0.4
0.3
0.2
0.1
0.0
−0.1
−0.2
0
500
1000
1500
2000

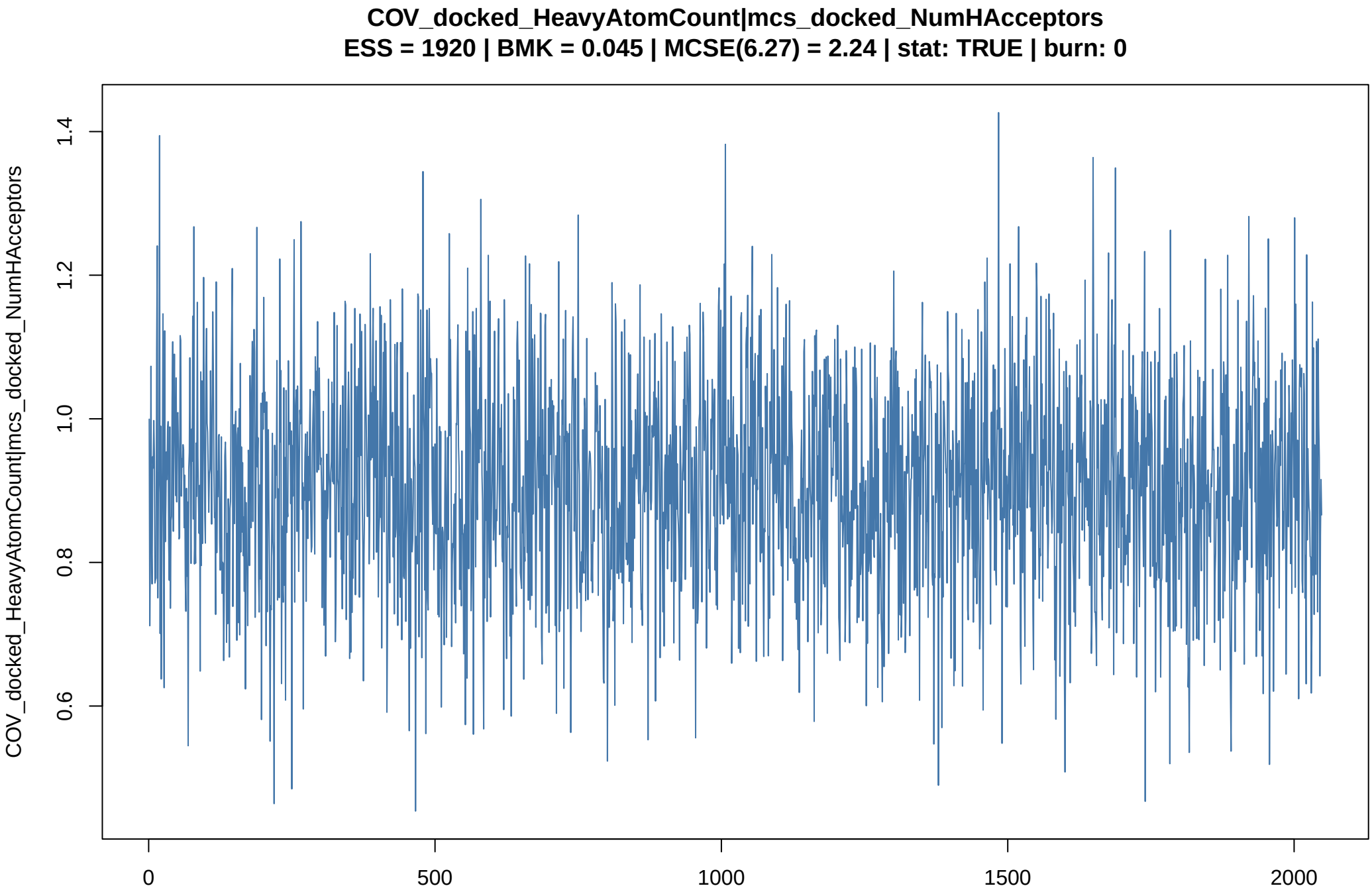

COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0599 | MCSE(6.27) = 2.08 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_docked_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
1.35
0
500
1000
1500
2000

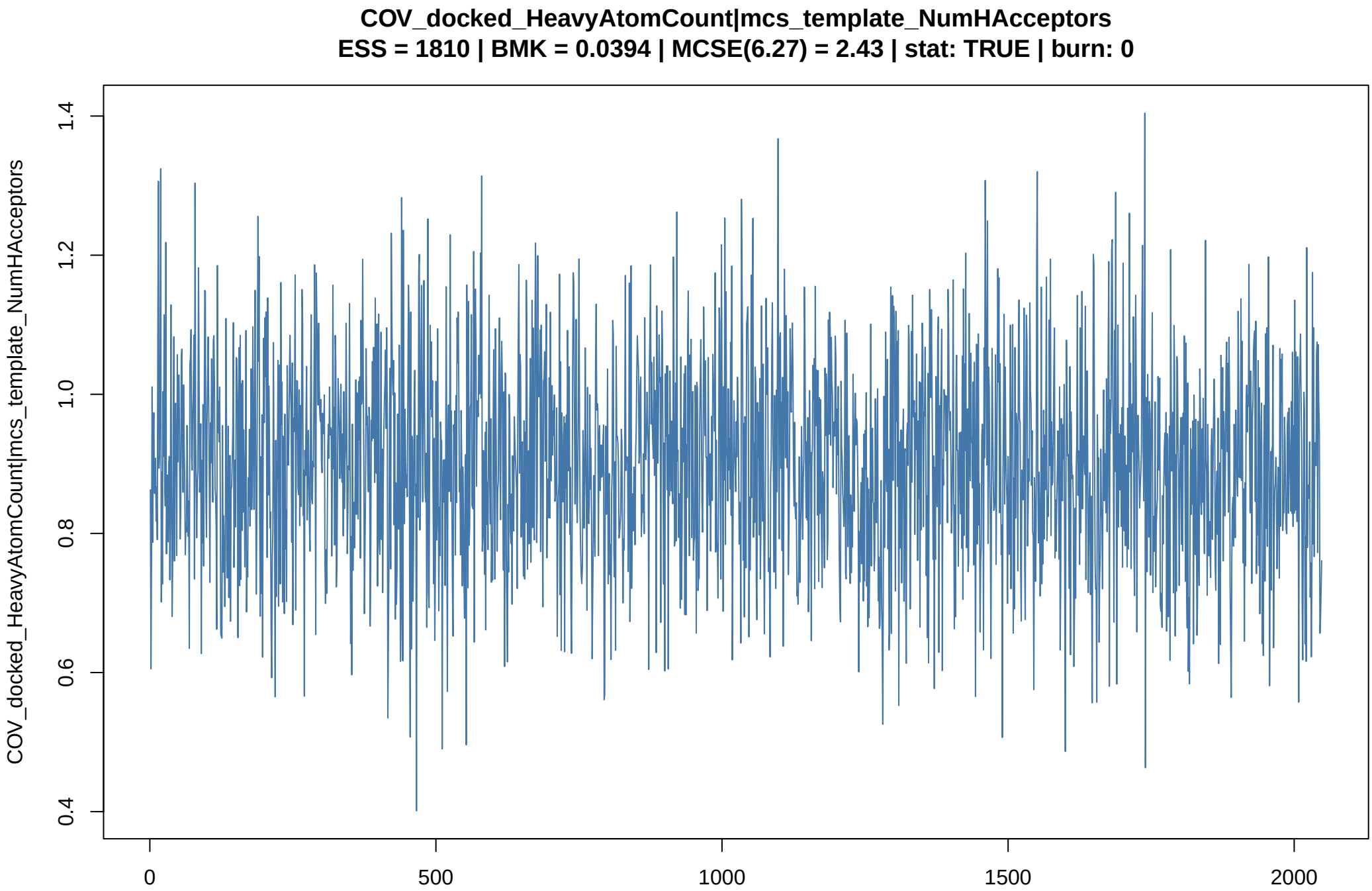

COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0615 | MCSE(6.27) = 2.15 | stat: TRUE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_template_NumHAcceptors
1.05
1.10
1.15
1.20
1.25
1.30
0
500
1000
1500
2000

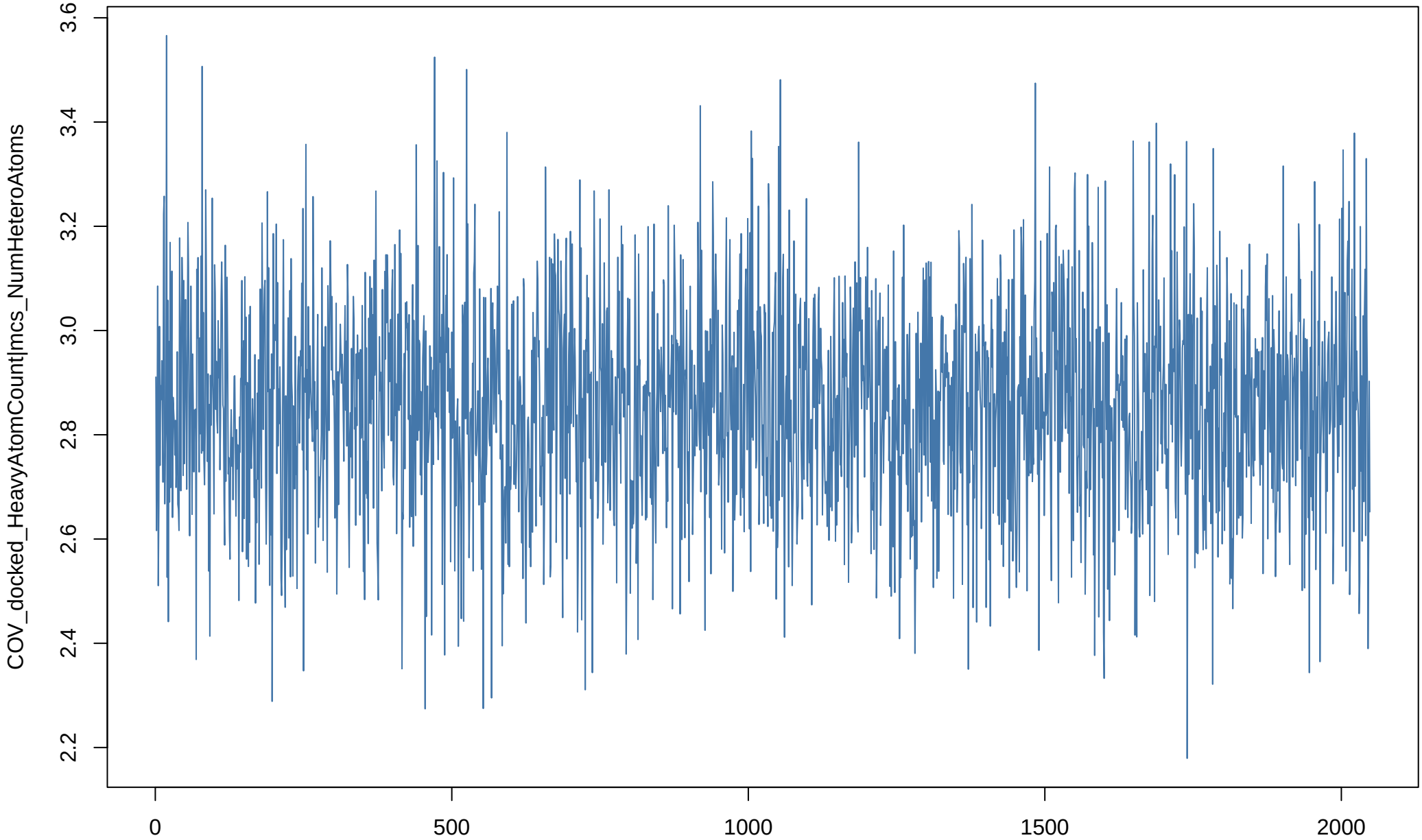

COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 1920 | BMK = 0.0861 | MCSE(6.27) = 2.38 | stat: FALSE | burn: 0
COV_Xtransf_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.5
1.6
1.7
1.8
0
500
1000
1500
2000

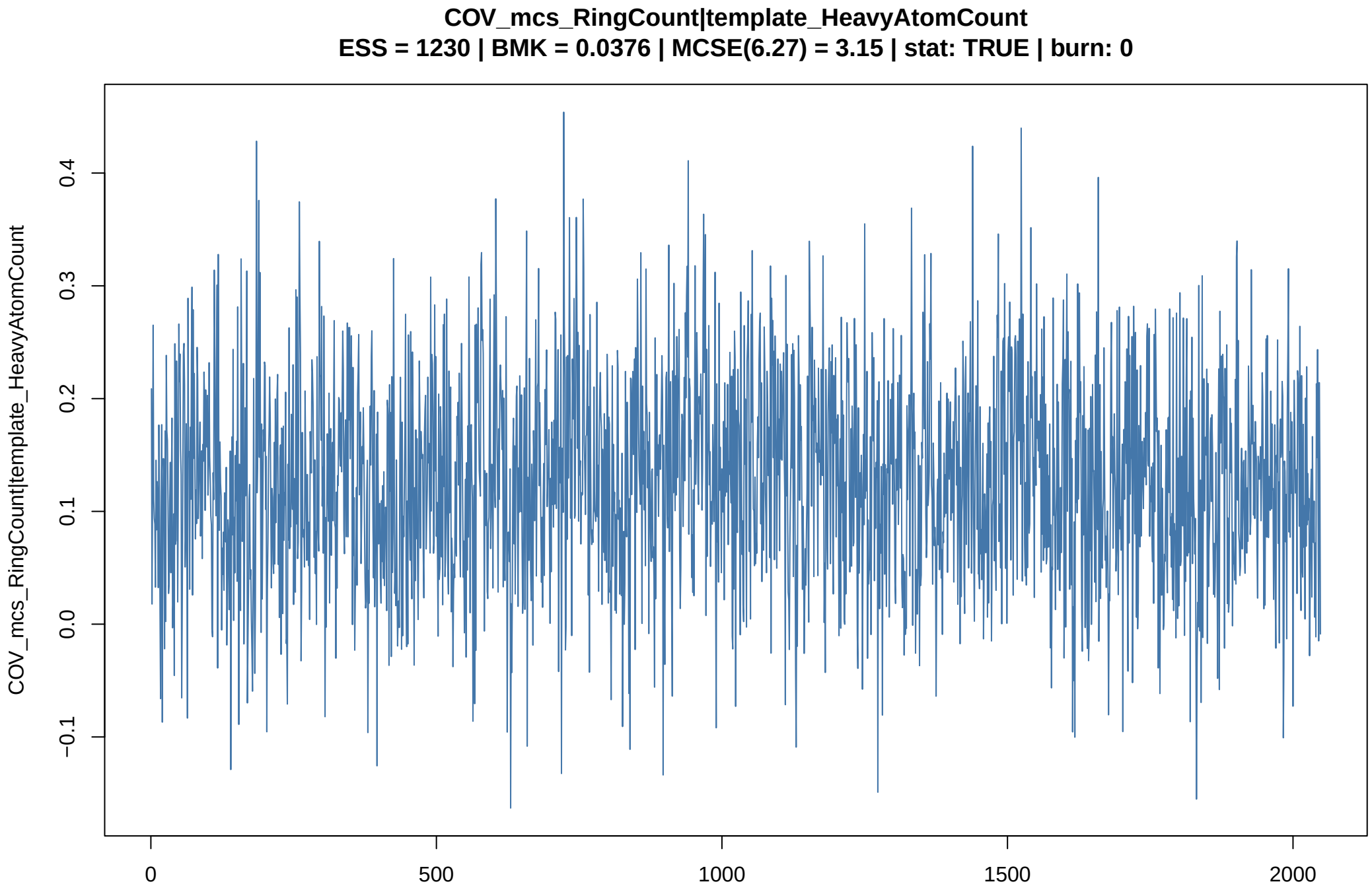

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 1550 | BMK = 0.0669 | MCSE(6.27) = 2.74 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0
500
1000
1500
2000

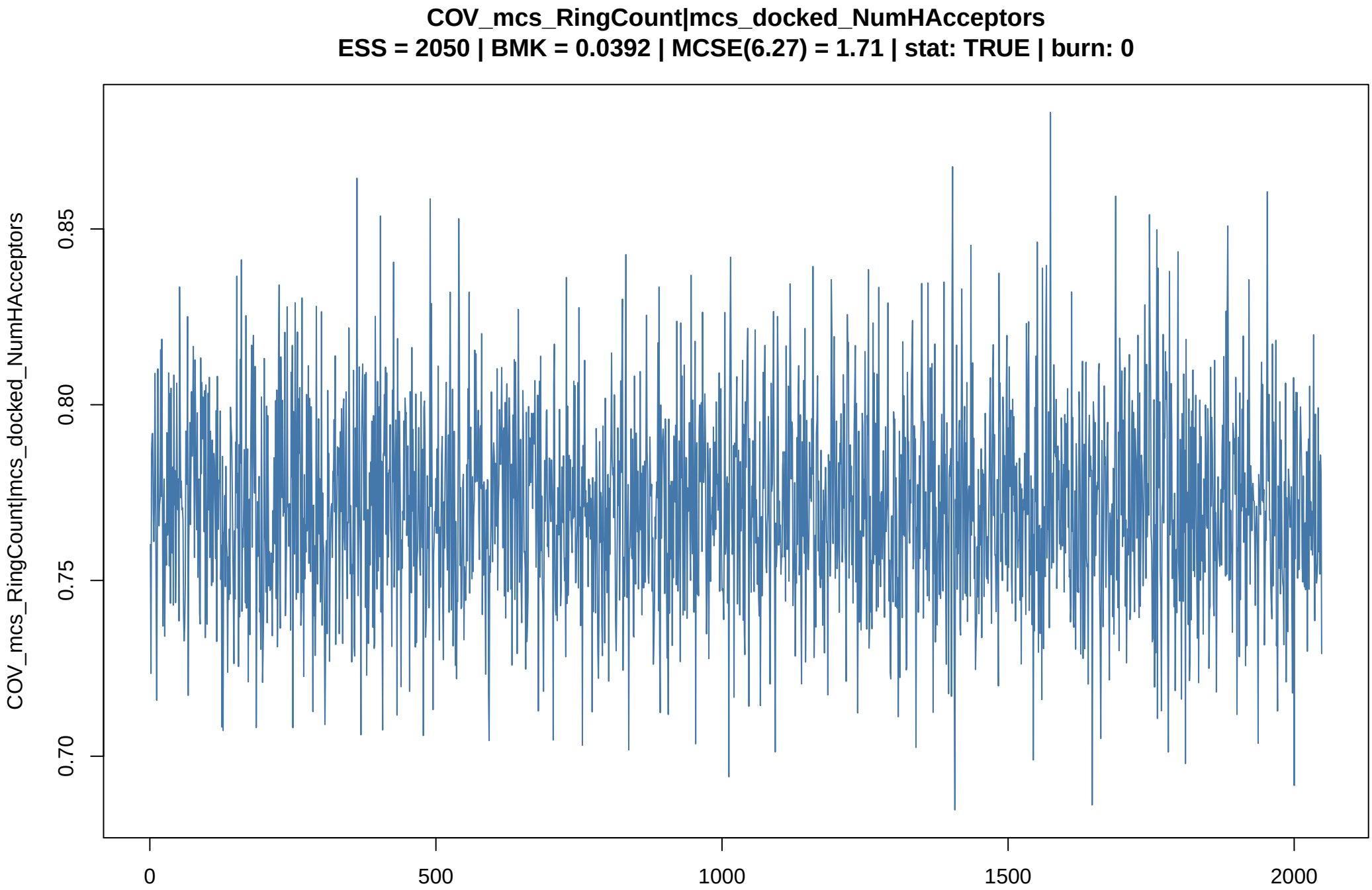

COV_docked_HeavyAtomCount|template_HeavyAtomCount
ESS = 1790 | BMK = 0.045 | MCSE(6.27) = 2.71 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|template_HeavyAtomCount
22
23
24
25
26
27
28
0
500
1000
1500
2000

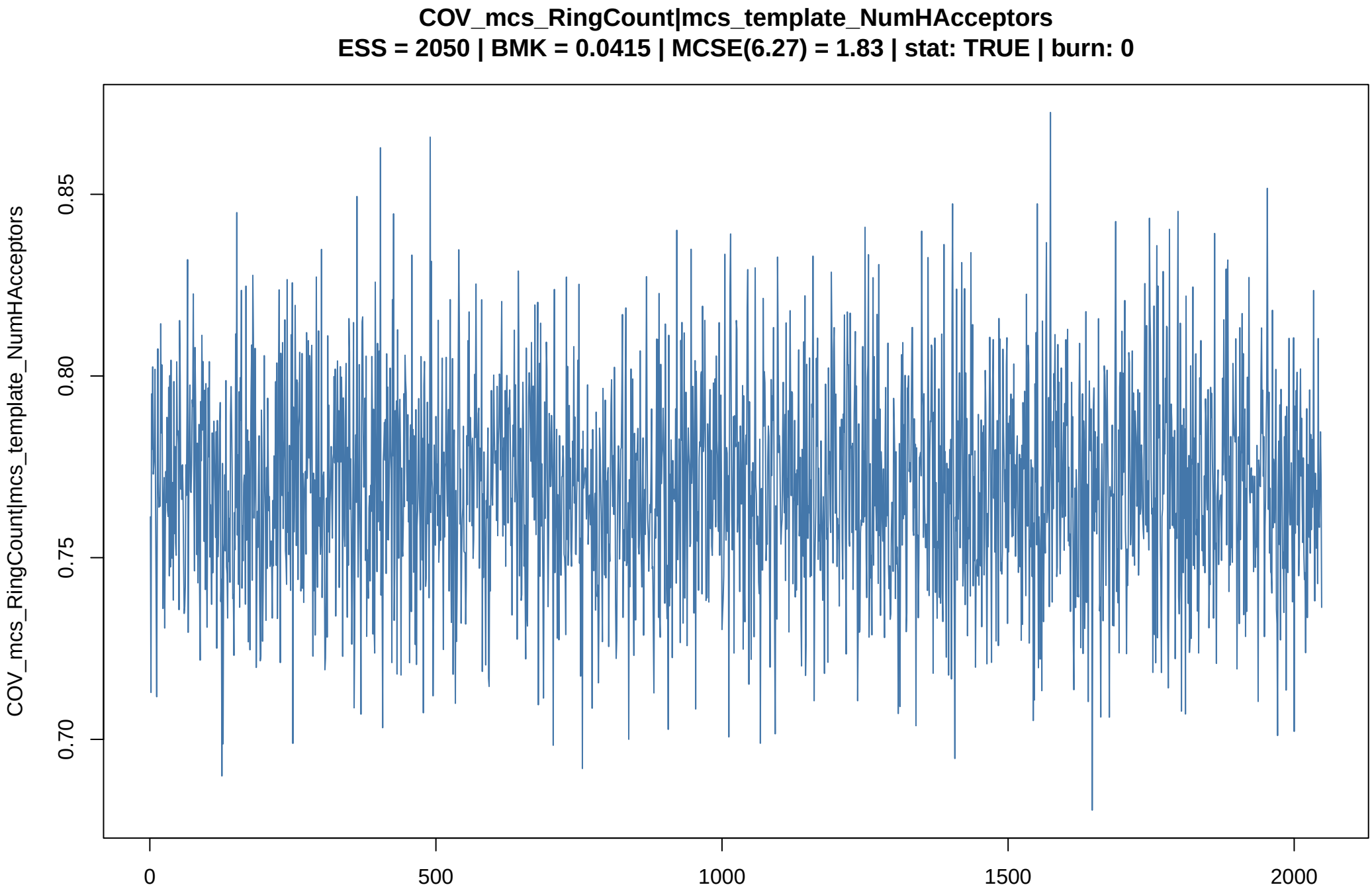

COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1920 | BMK = 0.045 | MCSE(6.27) = 2.24 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_docked_NumHAcceptors
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

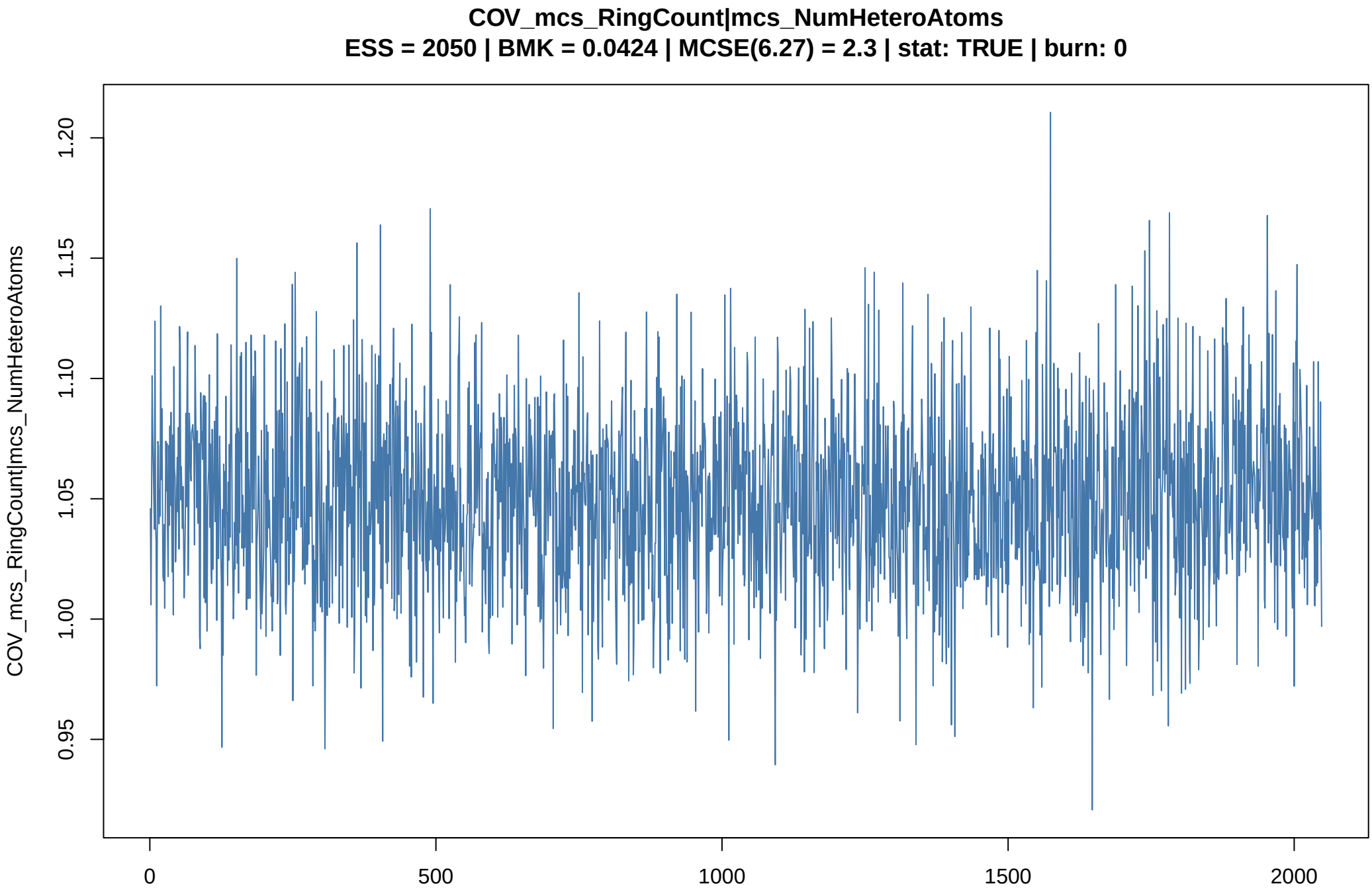

COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1810 | BMK = 0.0394 | MCSE(6.27) = 2.43 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_template_NumHAcceptors
0.4
0.6
0.8
1.0
1.2
1.4
0
500
1000
1500
2000

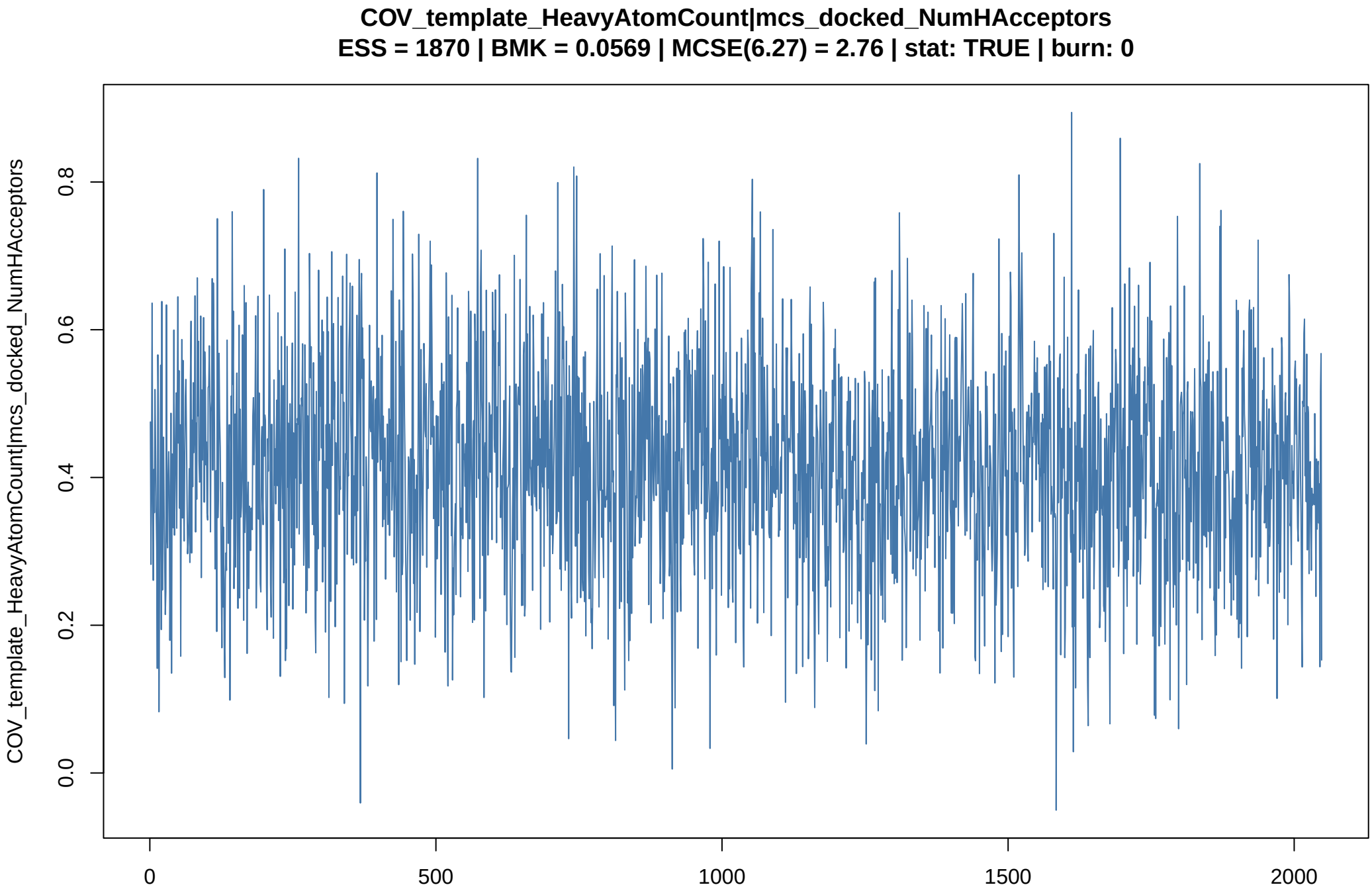

COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0424 | MCSE(6.27) = 2.47 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NumHeteroAtoms
2.2
2.4
2.6
2.8
3.0
3.2
3.4
3.6
0
500
1000
1500
2000

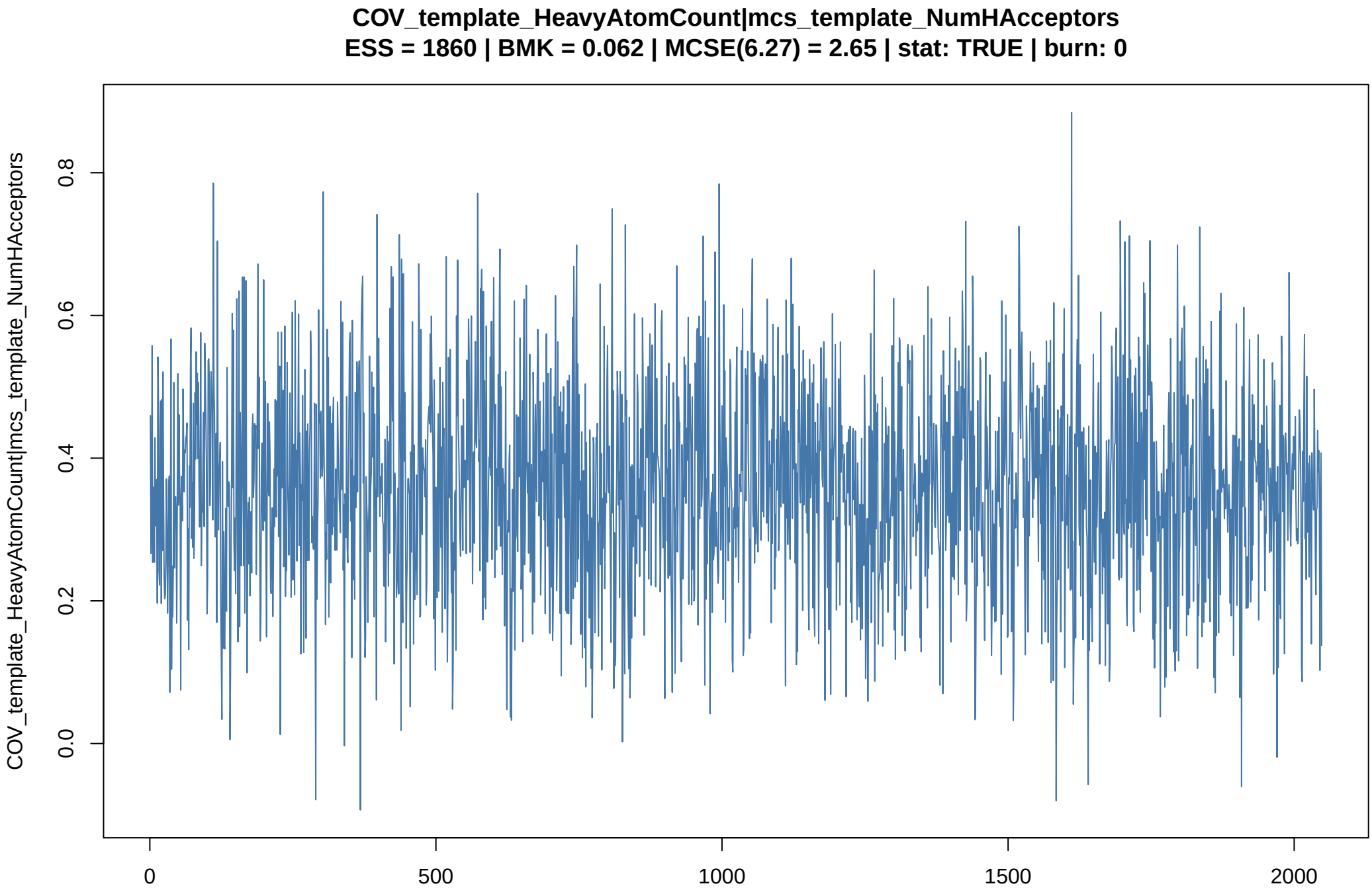

COV_mcs_RingCount|template_HeavyAtomCount
ESS = 1230 | BMK = 0.0376 | MCSE(6.27) = 3.15 | stat: TRUE | burn: 0
COV_mcs_RingCount|template_HeavyAtomCount
−0.1
0.0
0.1
0.2
0.3
0.4
0
500
1000
1500
2000

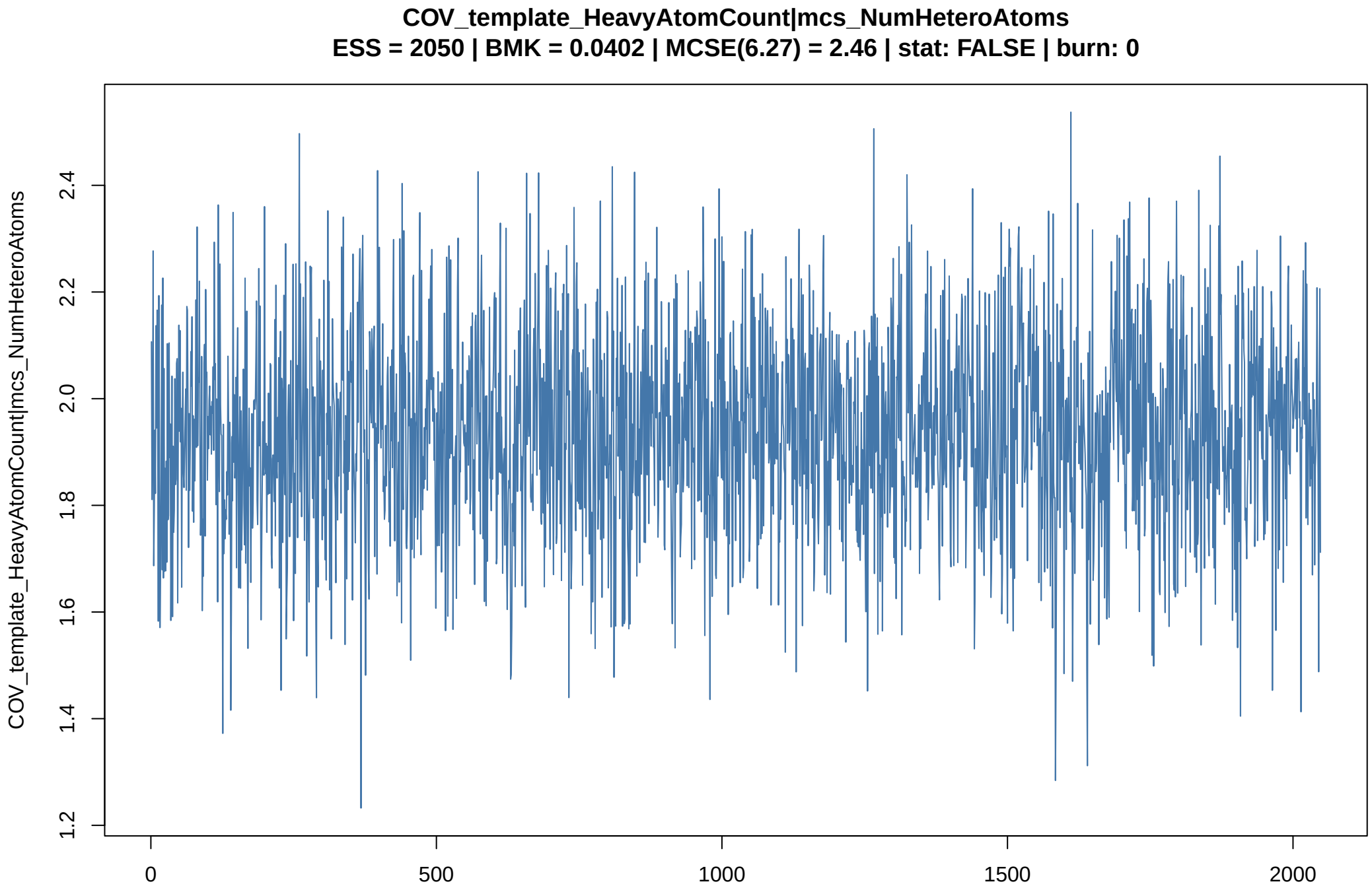

COV_mcs_RingCount|mcs_docked_NumHAcceptors
ESS = 2050 | BMK = 0.0392 | MCSE(6.27) = 1.71 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_docked_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

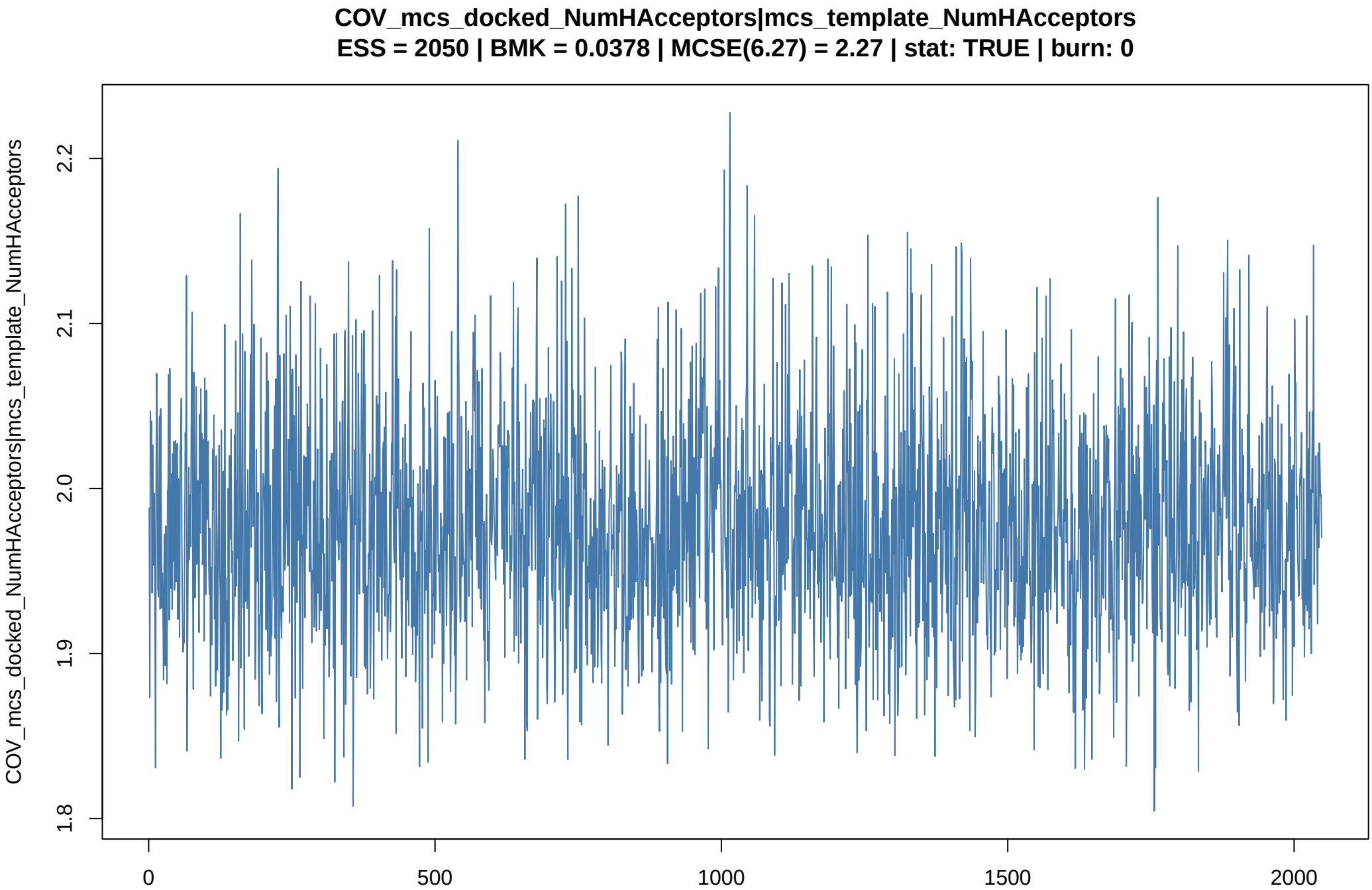

COV_mcs_RingCount|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0415 | MCSE(6.27) = 1.83 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_template_NumHAcceptors
0.70
0.75
0.80
0.85
0
500
1000
1500
2000

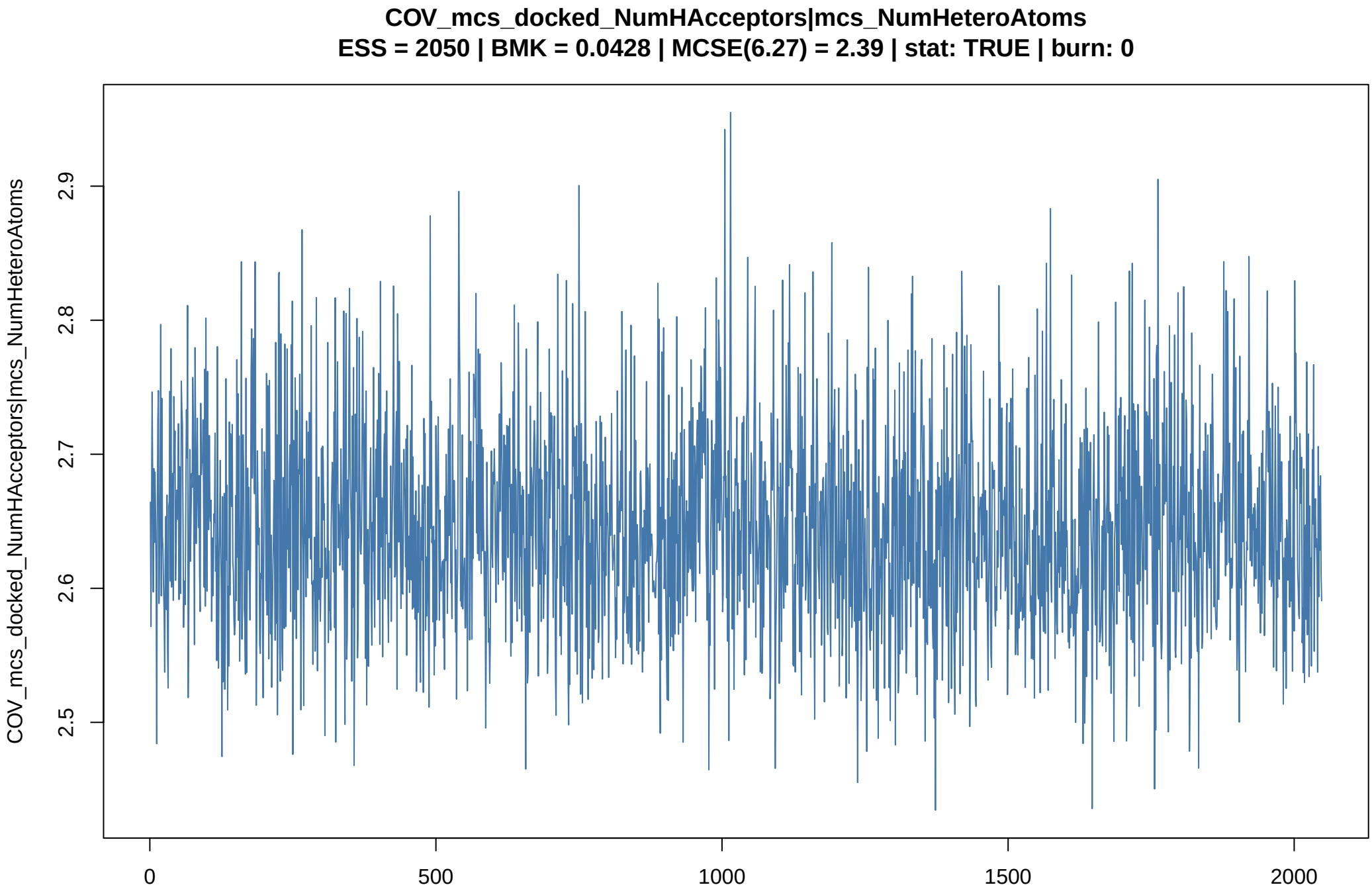

COV_mcs_RingCount|mcs_NumHeteroAtoms
ESS = 2050 | BMK = 0.0424 | MCSE(6.27) = 2.3 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NumHeteroAtoms
0.95
1.00
1.05
1.10
1.15
1.20
0
500
1000
1500
2000

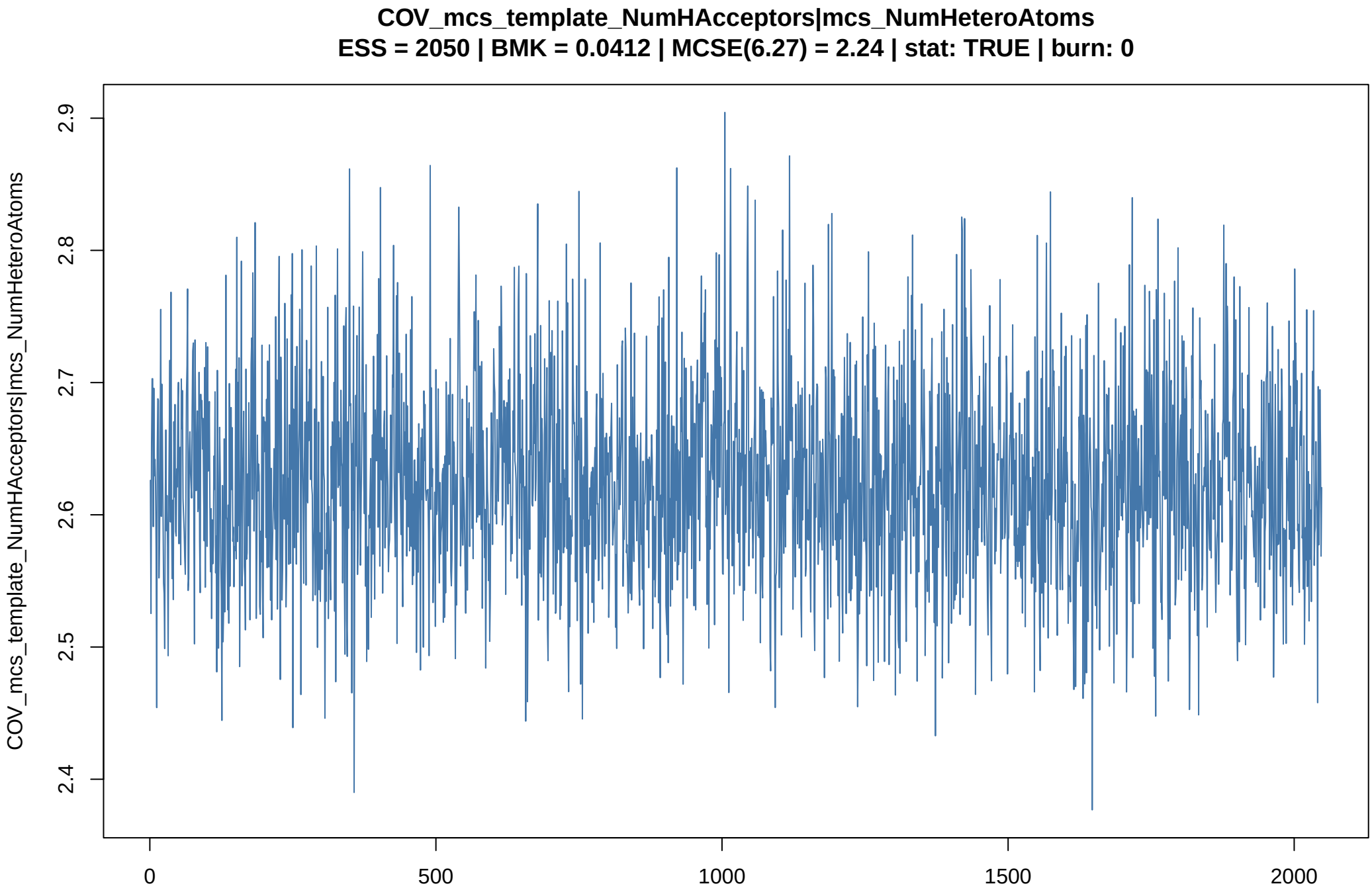

COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
ESS = 1870 | BMK = 0.0569 | MCSE(6.27) = 2.76 | stat: TRUE | burn: 0
COV_template_HeavyAtomCount|mcs_docked_NumHAcceptors
0.0
0.2
0.4
0.6
0.8
0
500
1000
1500
2000


COV_template_HeavyAtomCount|mcs_template_NumHAcceptors
ESS = 1860 | BMK = 0.062 | MCSE(6.27) = 2.65 | 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 = 0.0402 | MCSE(6.27) = 2.46 | stat: FALSE | burn: 0
COV_template_HeavyAtomCount|mcs_NumHeteroAtoms
1.2
1.4
1.6
1.8
2.0
2.2
2.4
0
500
1000
1500
2000


COV_mcs_docked_NumHAcceptors|mcs_template_NumHAcceptors
ESS = 2050 | BMK = 0.0378 | MCSE(6.27) = 2.27 | 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 = 0.0428 | MCSE(6.27) = 2.39 | 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 = 0.0412 | MCSE(6.27) = 2.24 | 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