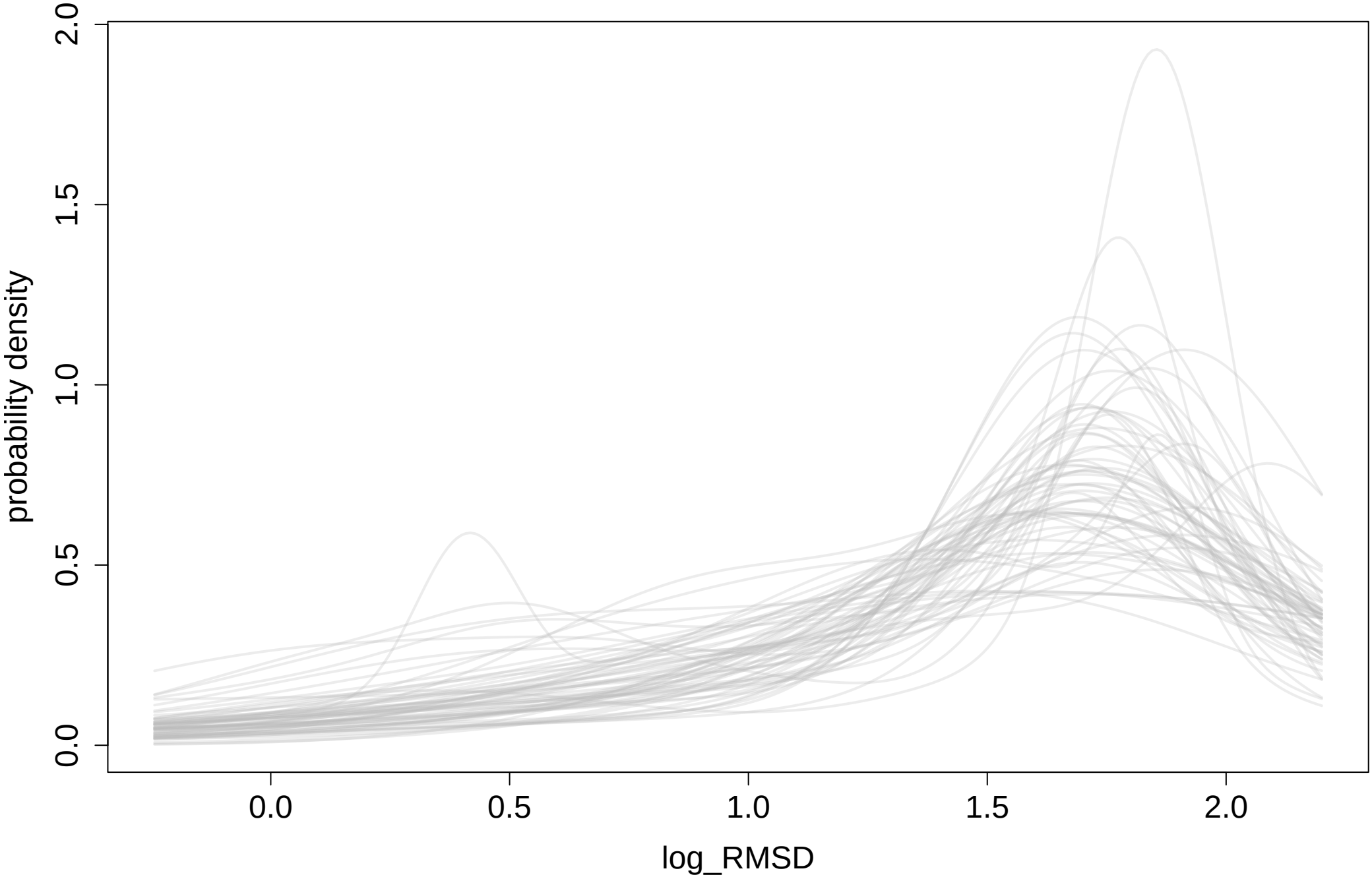
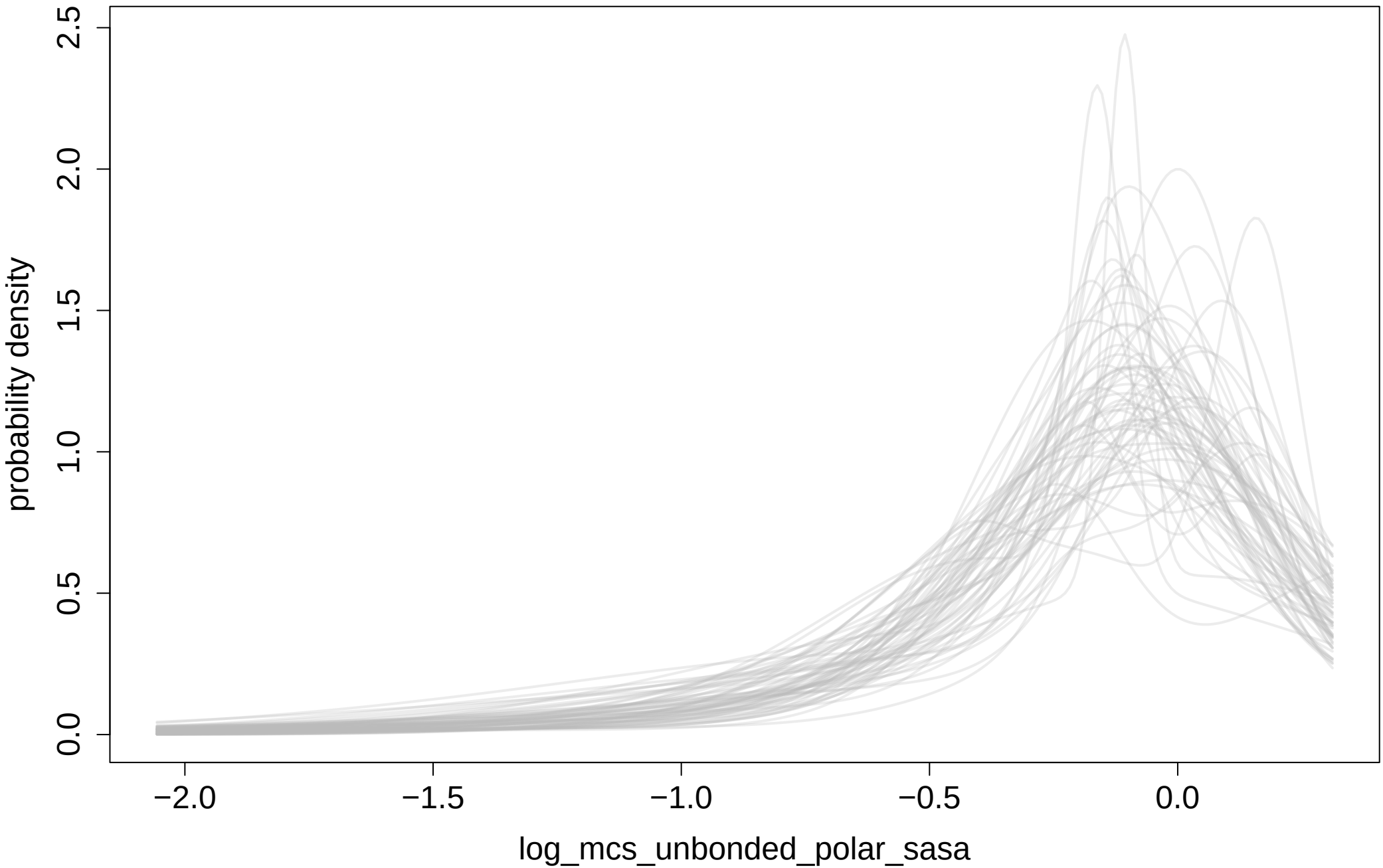
−− STATS maxD −−
min ESS = 27.2260526137046
max BMK = 0.363177149379179
max MCSE = 13.0501082813377
all stationary: FALSE
burn: 200

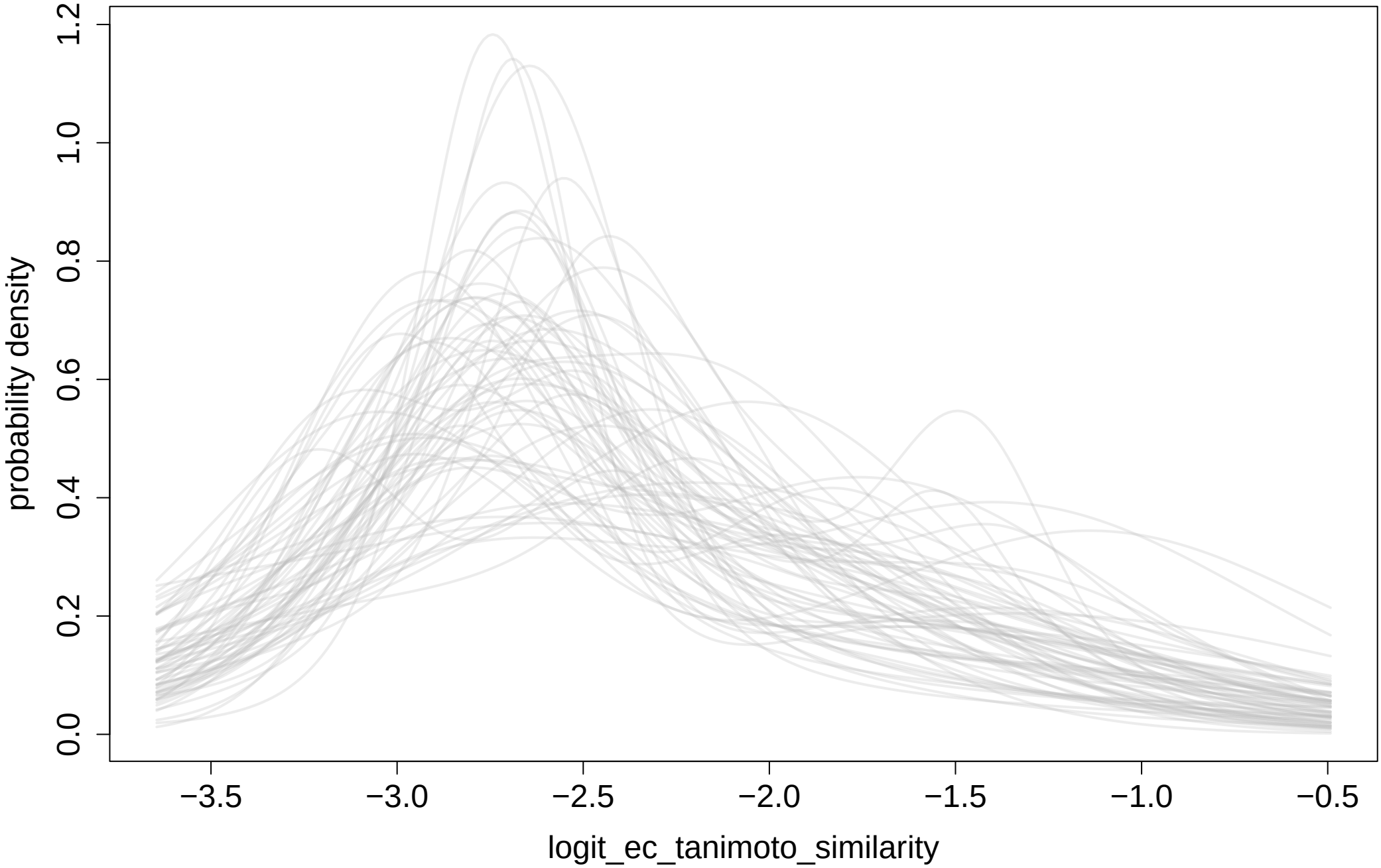
−− STATS 2D −−
min ESS = 13.4291850117879
max BMK = 0.305785952764289
max MCSE = 22.7371921300517
all stationary: FALSE
burn: 160

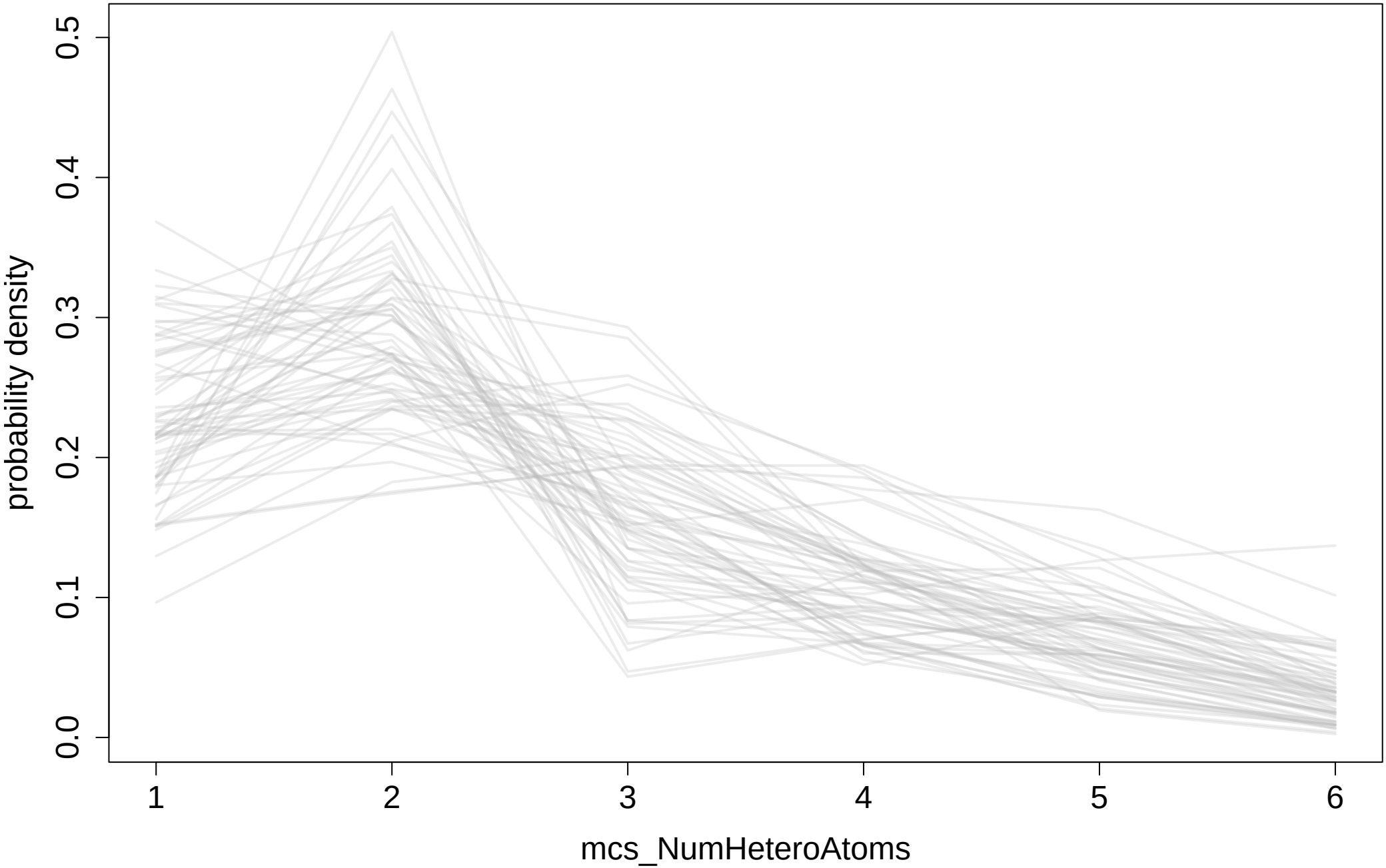
−− STATS 1D −−
min ESS = 2.2204604925031e−16
max BMK = 0.246592158469434
max MCSE = NaN
all stationary: FALSE
burn: 200

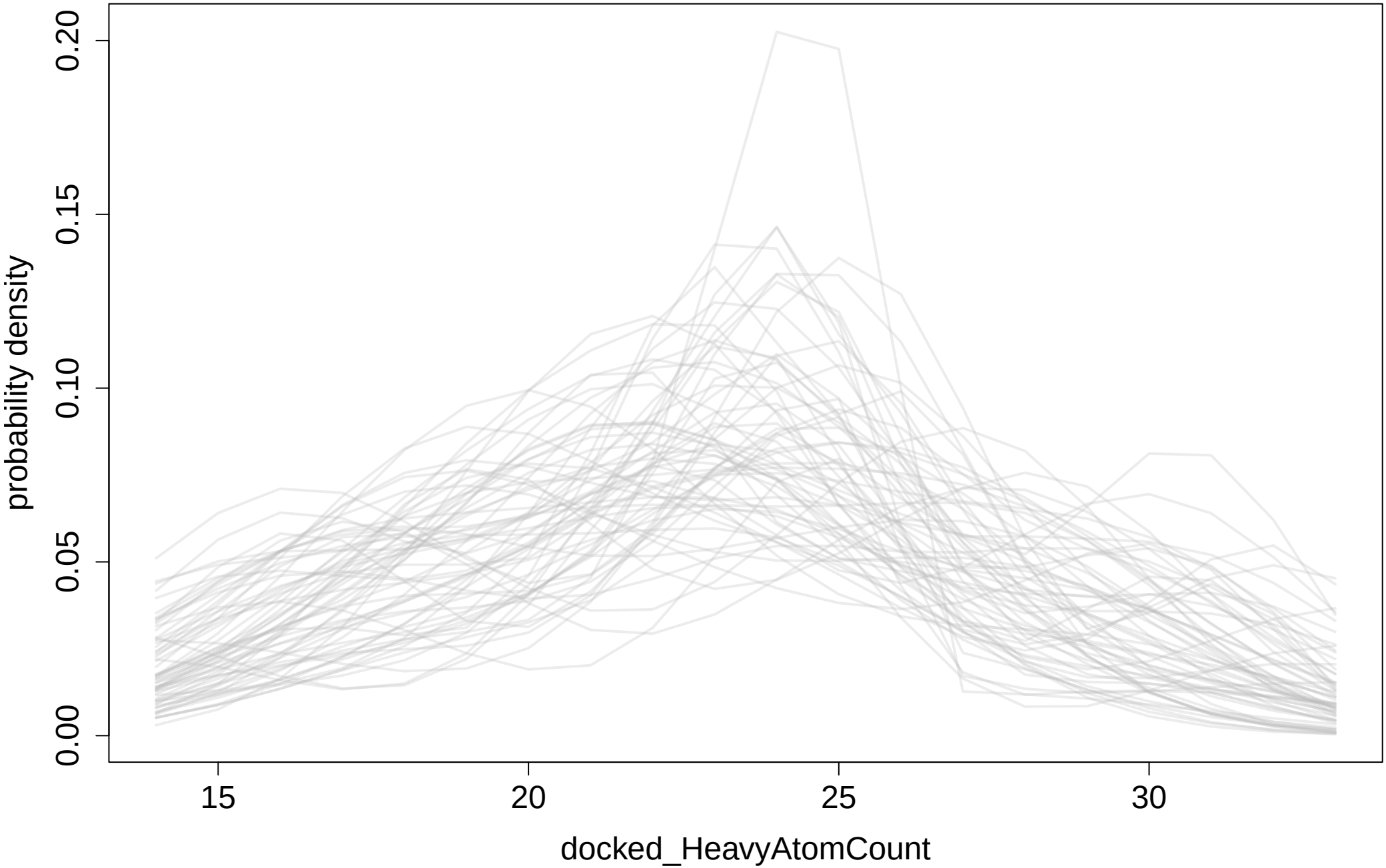
Occupied clusters: 4 of 4
LL: −186 +− 5.42

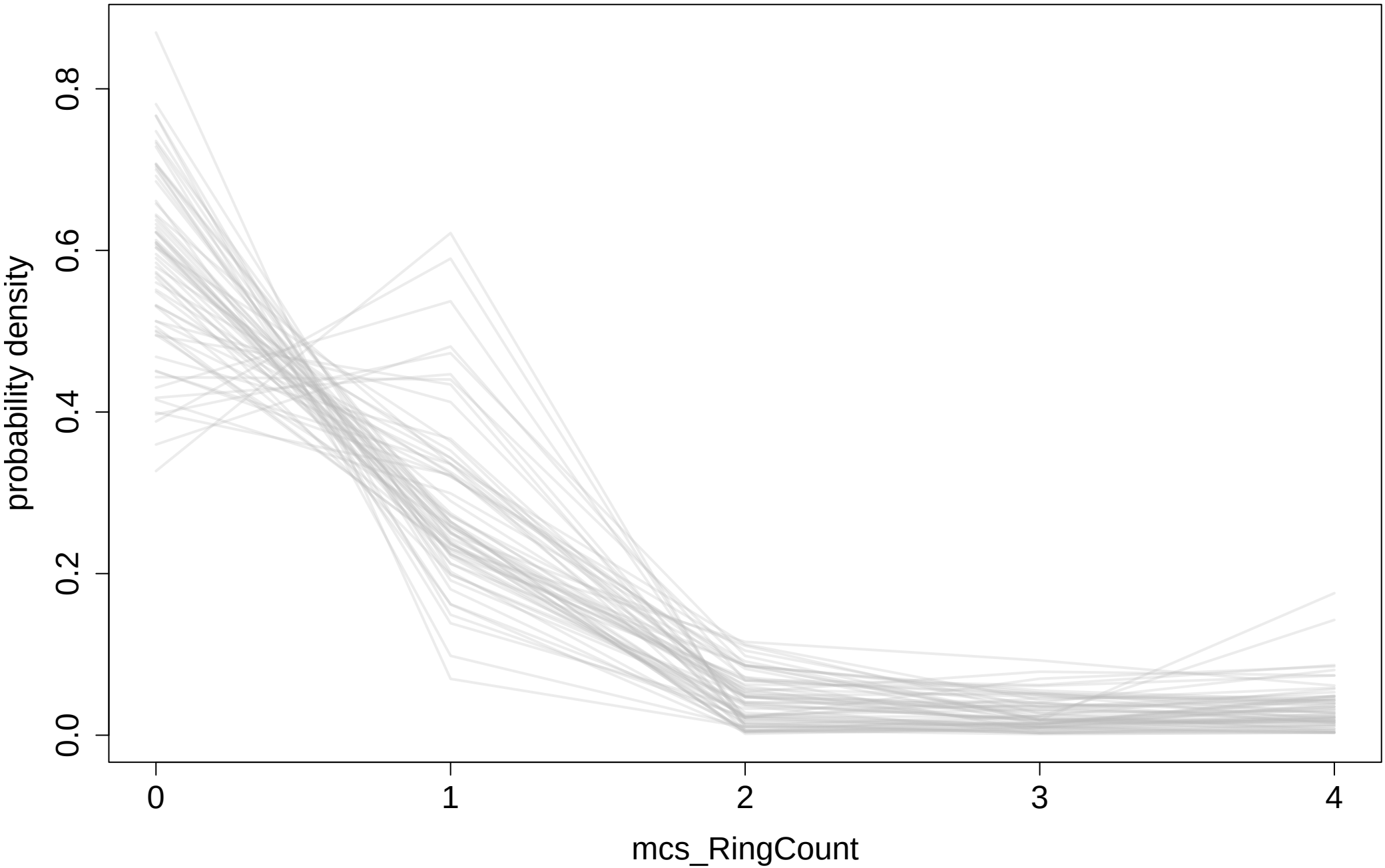

probability density
0.0
0.5
1.0
1.5
2.0
0.0
0.5
1.0
1.5
2.0
log_RMSD

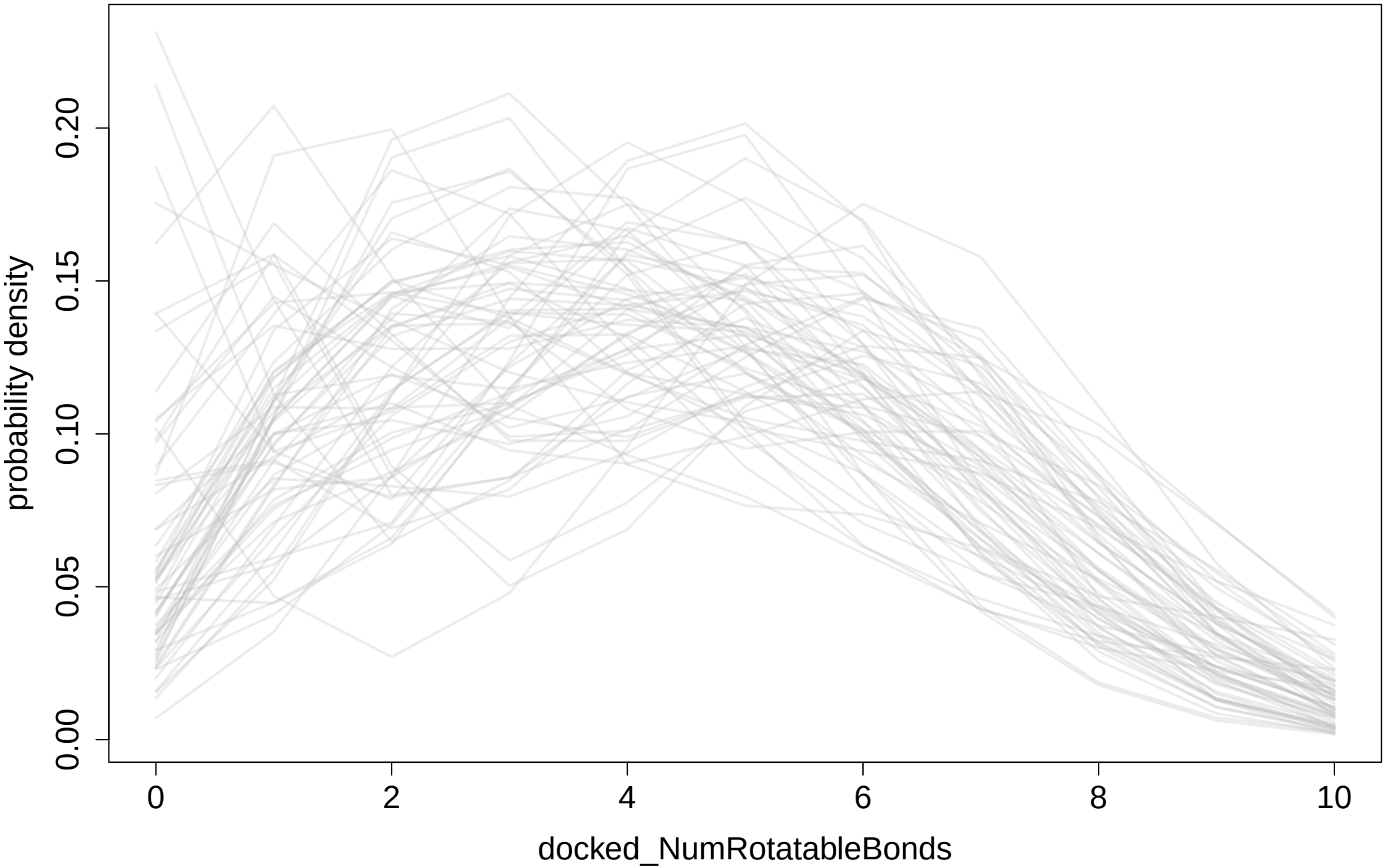

probability density
0.0
0.5
1.0
1.5
2.0
2.5
−2.0
−1.5
−1.0
−0.5
0.0
log_mcs_unbonded_polar_sasa

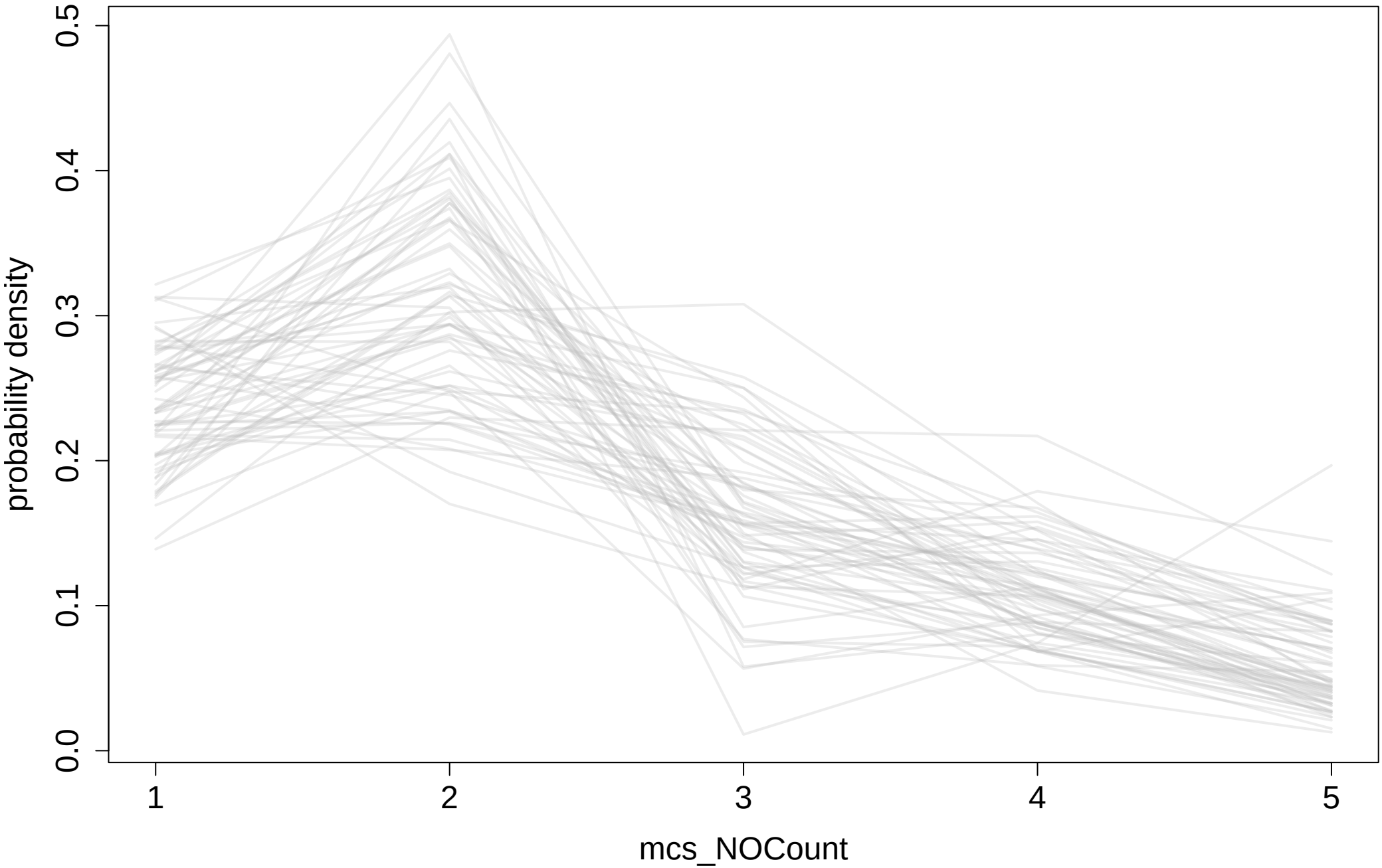

probability density
0.0
0.2
0.4
0.6
0.8
1.0
1.2
−3.5
−3.0
−2.5
−2.0
−1.5
−1.0
−0.5
logit_ec_tanimoto_similarity

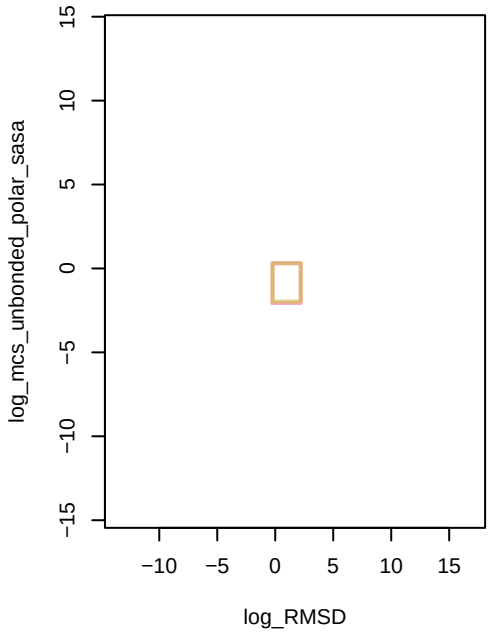

probability density
0.0
0.1
0.2
0.3
0.4
0.5
1
2
3
4
5
6
mcs_NumHeteroAtoms

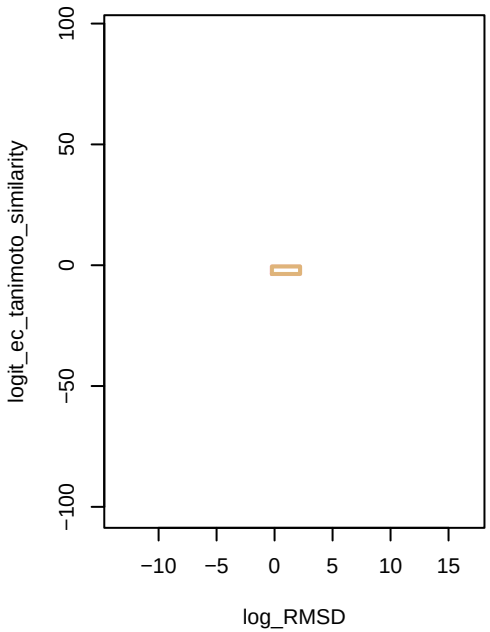

probability density
0.00
0.05
0.10
0.15
0.20
15
20
25
30
docked_HeavyAtomCount

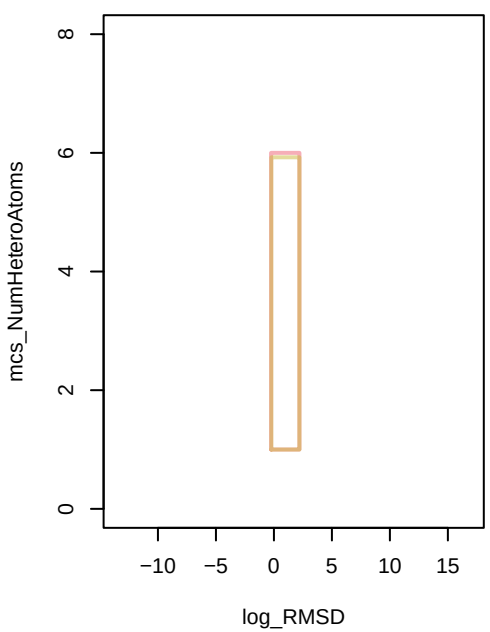

probability density
0.0
0.2
0.4
0.6
0.8
0
1
2
3
4
mcs_RingCount

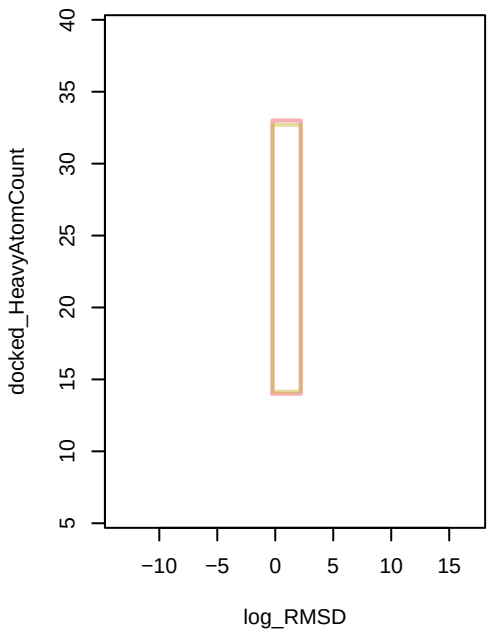

probability density
0.00
0.05
0.10
0.15
0.20
0
2
4
6
8
10
docked_NumRotatableBonds

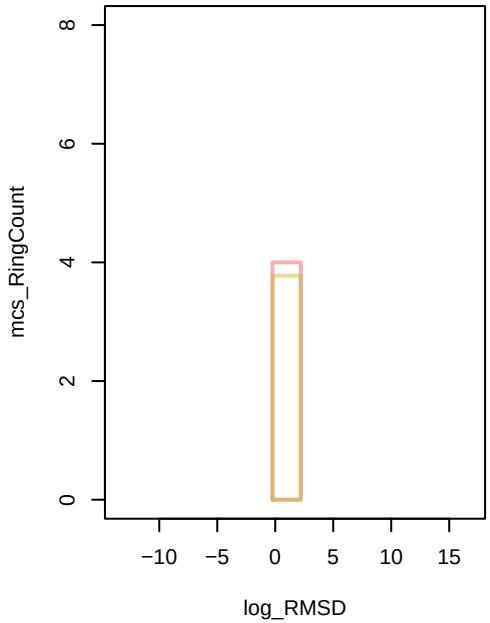

probability density
0.0
0.1
0.2
0.3
0.4
0.5
1
2
3
4
5
mcs_NOCount

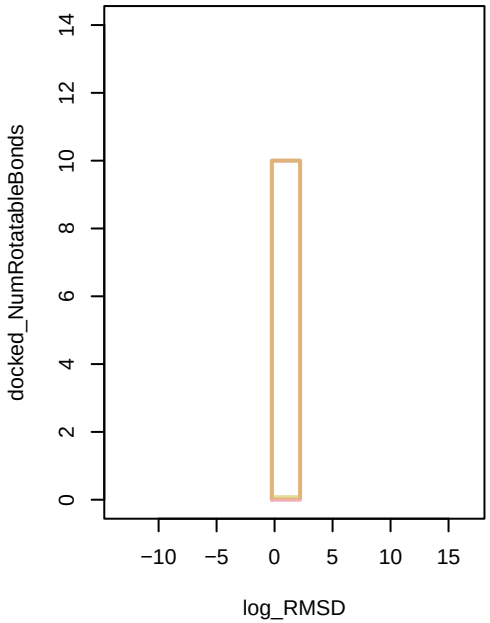

log_mcs_unbonded_polar_sasa
15
10
5
0
−5
−10
−15
−10
−5
0
5
10
15
log_RMSD

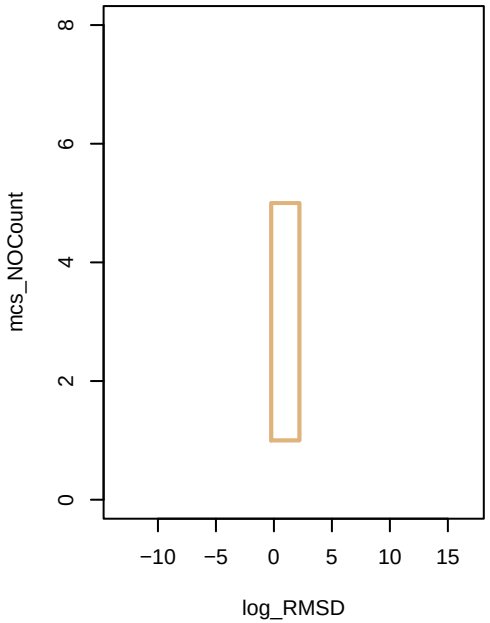

logit_ec_tanimoto_similarity
100
50
0
−50
−100
−10
−5
0
5
10
15
log_RMSD

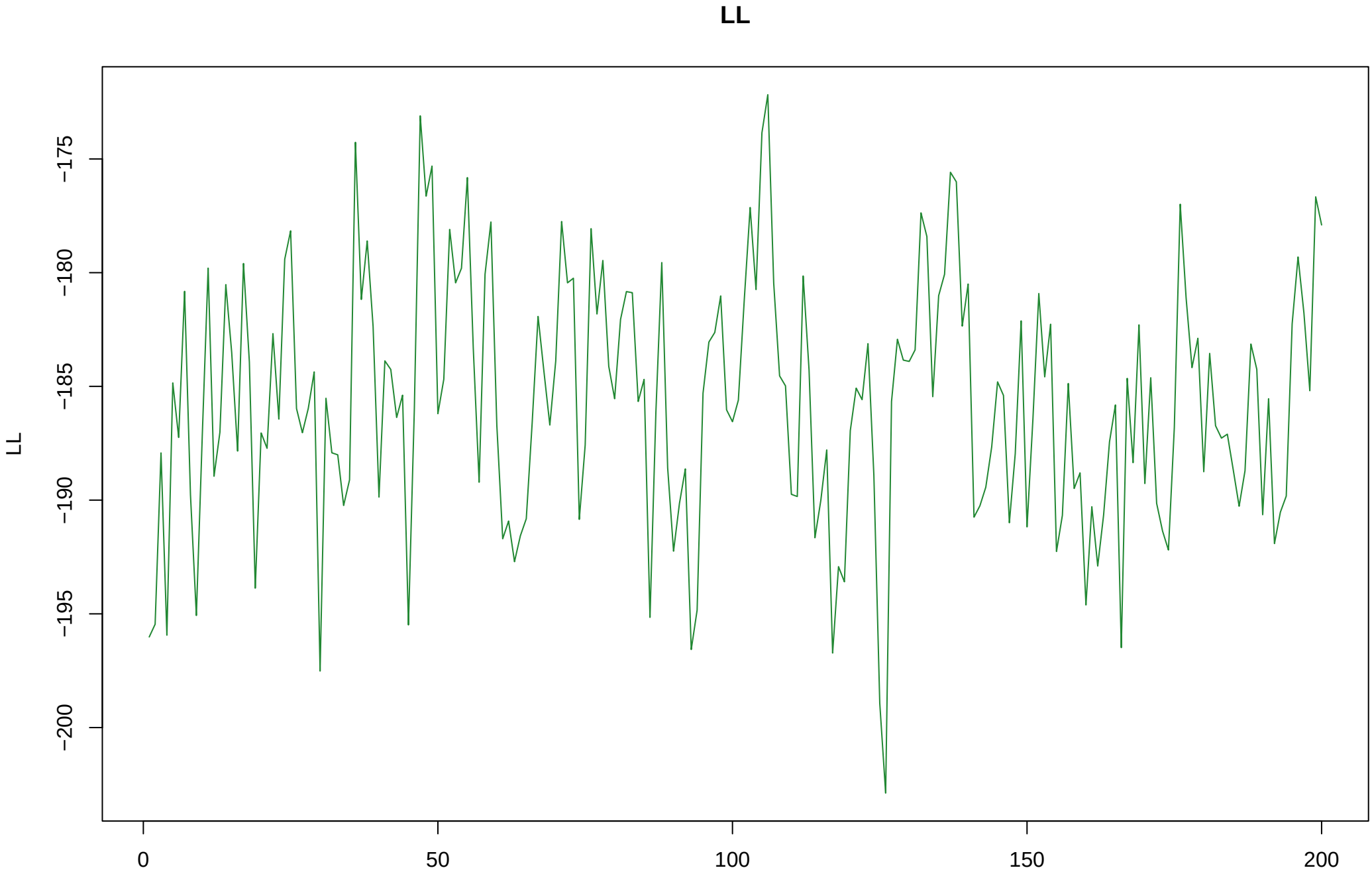

mcs_NumHeteroAtoms
8
6
4
2
0
−10
−5
0
5
10
15
log_RMSD

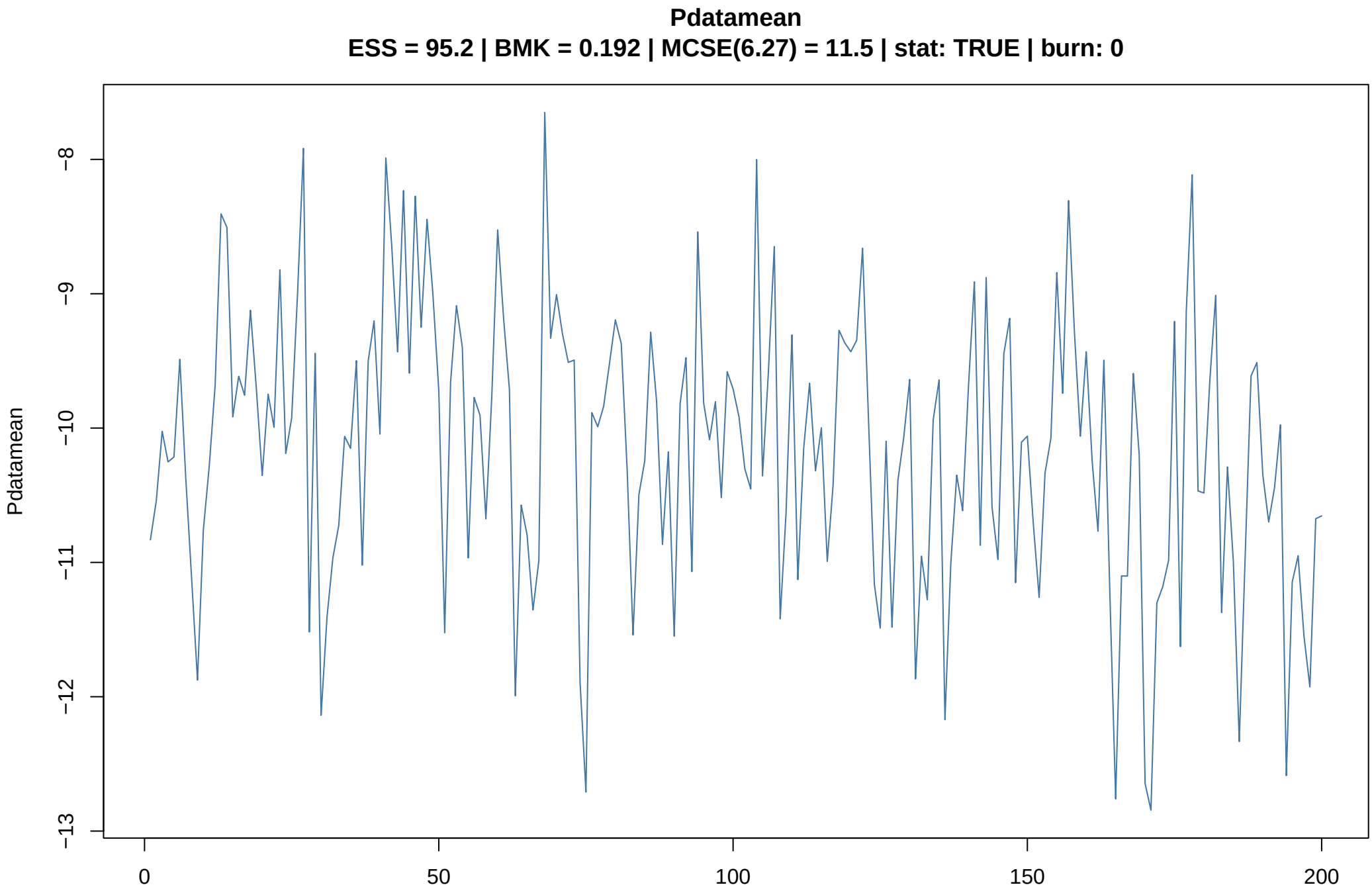

docked_HeavyAtomCount
40
35
30
25
20
15
10
5
−10
−5
0
5
10
15
log_RMSD

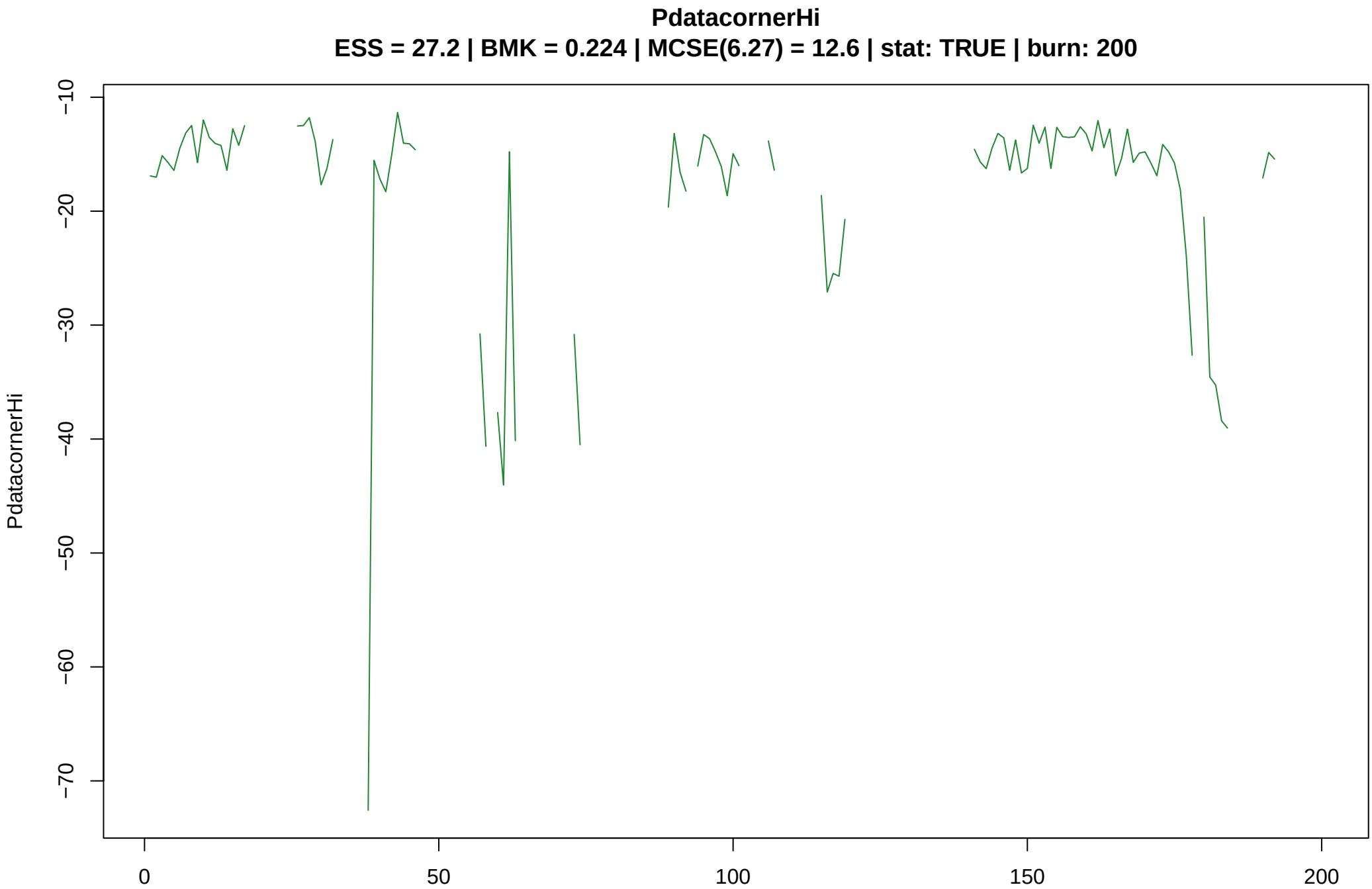

mcs_RingCount
8
6
4
2
0
−10
−5
0
5
10
15
log_RMSD

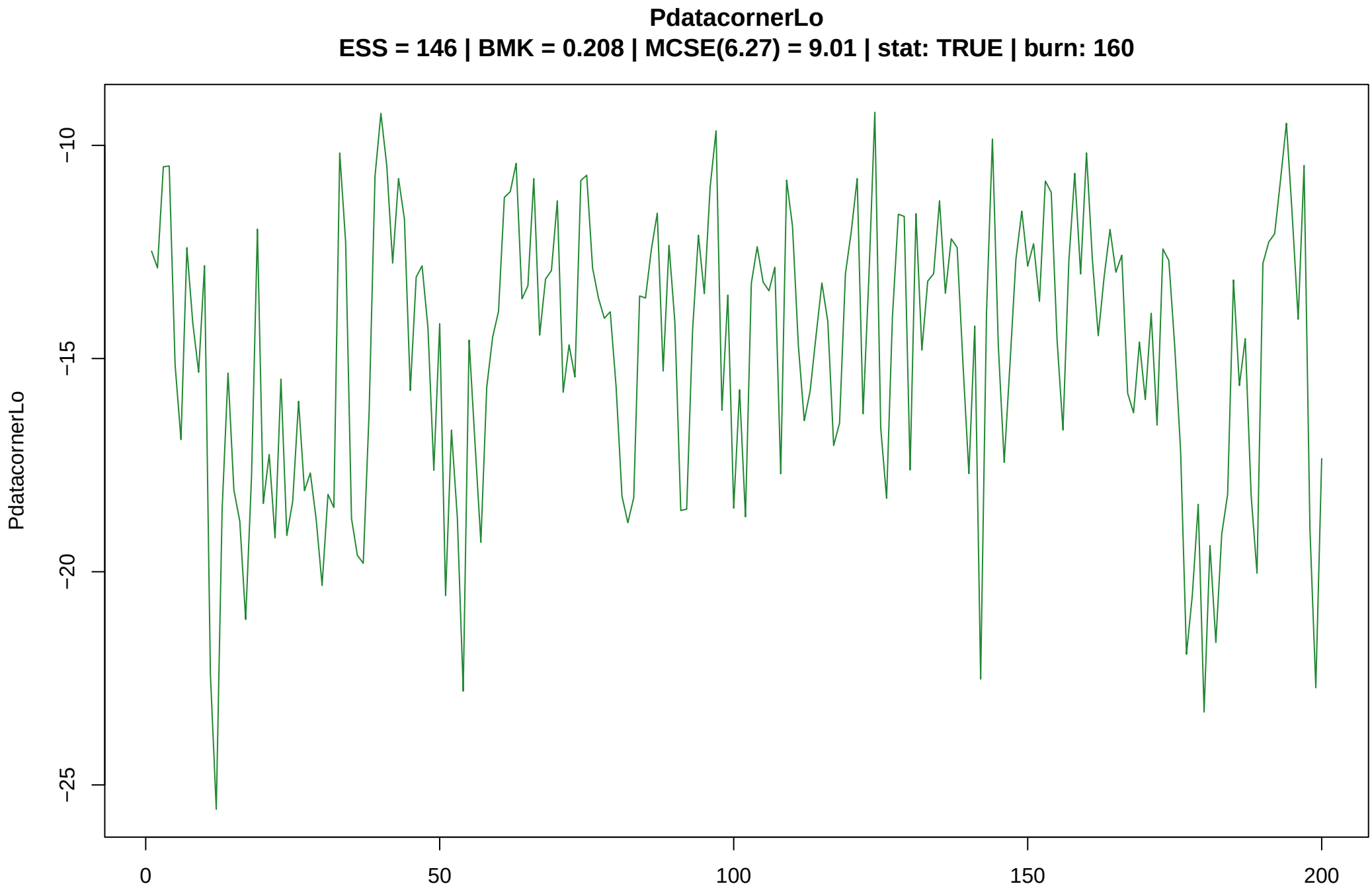

docked_NumRotatableBonds
14
12
10
8
6
4
2
0
−10
−5
0
5
10
15
log_RMSD

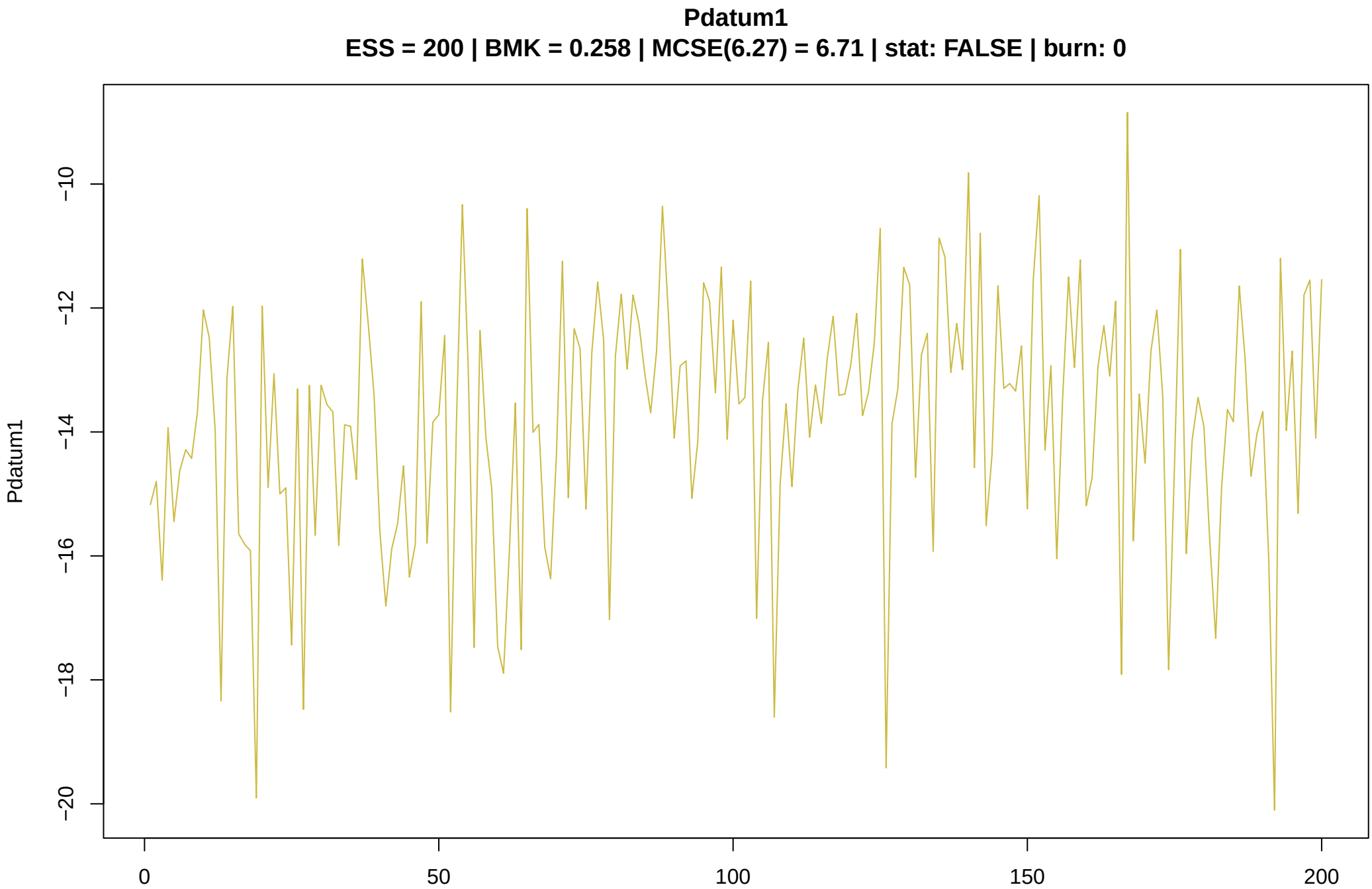

mcs_NOCount
8
6
4
2
0
−10
−5
0
5
10
15
log_RMSD

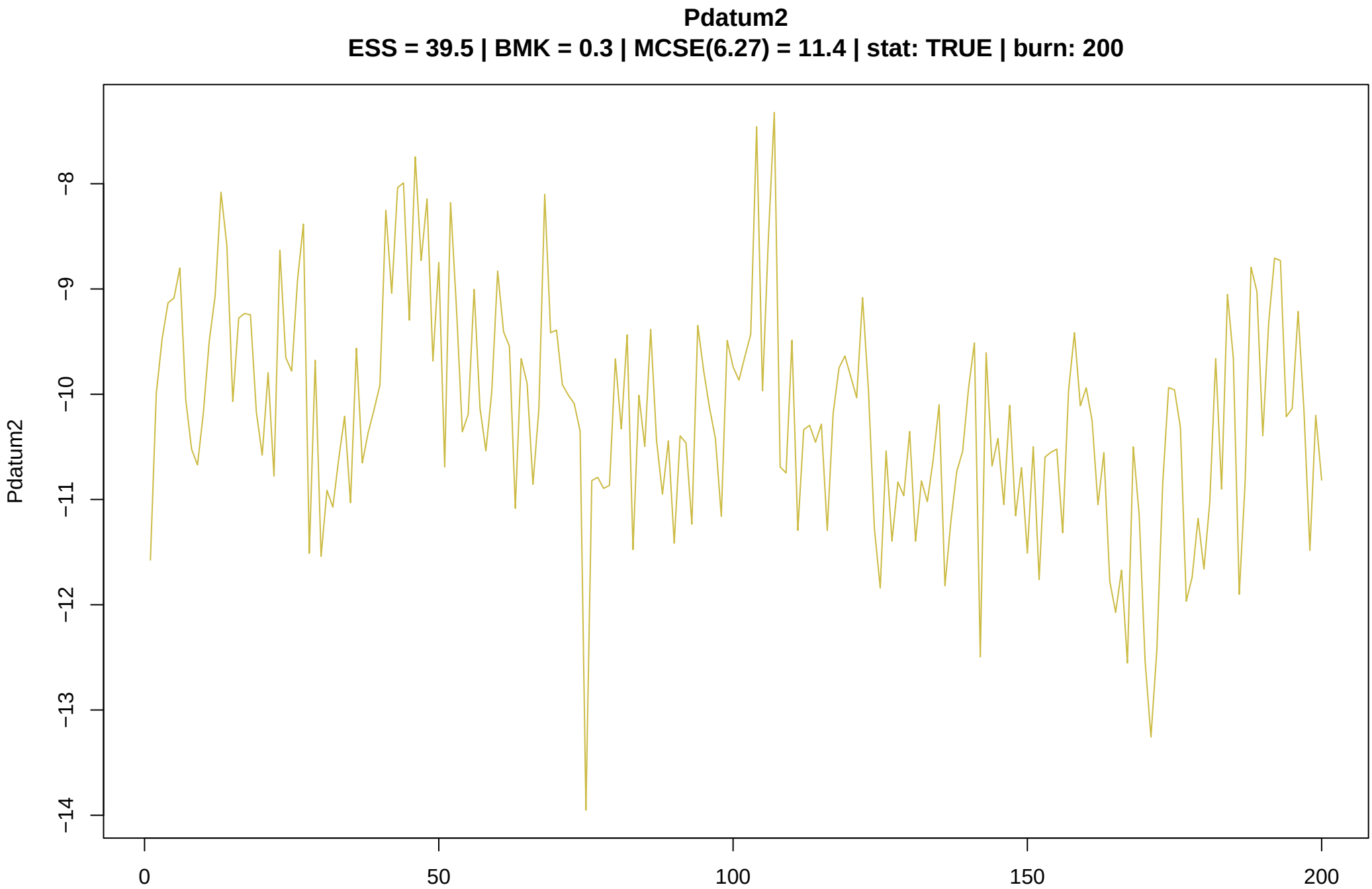

LL
LL
−175
−180
−185
−190
−195
−200
0
50
100
150
200

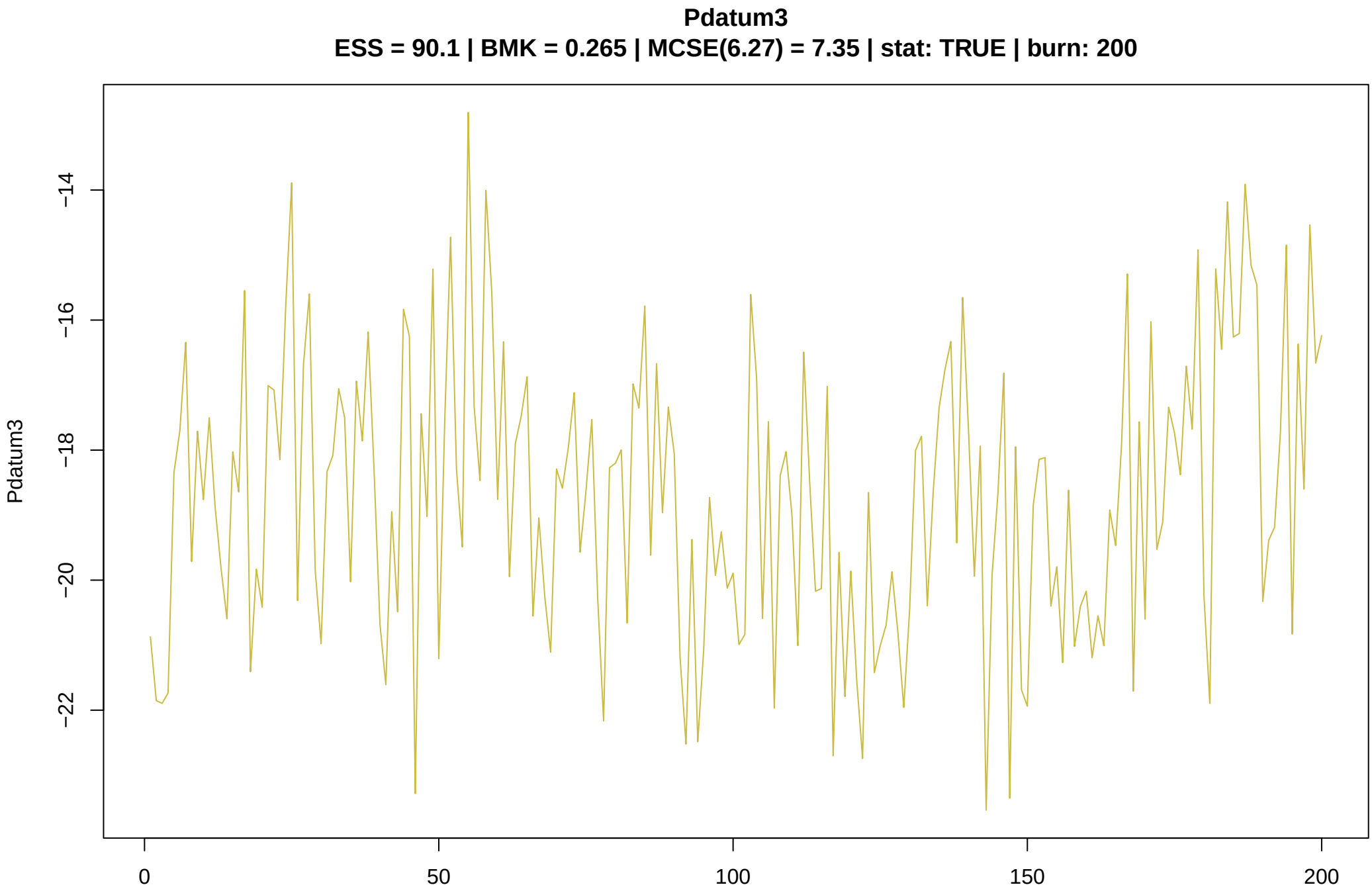

Pdatamean
ESS = 95.2 | BMK = 0.192 | MCSE(6.27) = 11.5 | stat: TRUE | burn: 0
Pdatamean
−8
−9
−10
−11
−12
−13
0
50
100
150
200

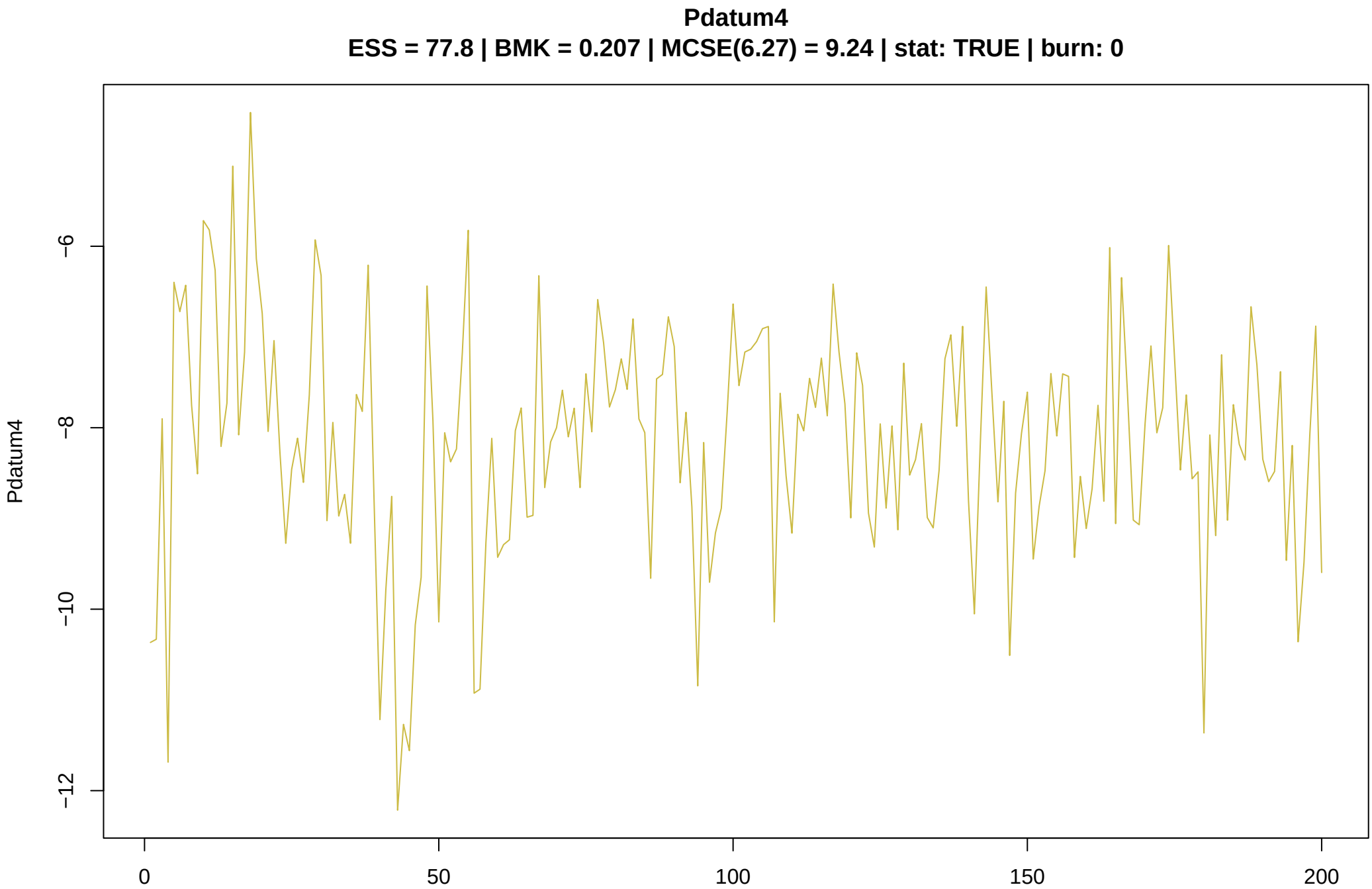

PdatacornerHi
ESS = 27.2 | BMK = 0.224 | MCSE(6.27) = 12.6 | stat: TRUE | burn: 200
PdatacornerHi
−10
−20
−30
−40
−50
−60
−70
0
50
100
150
200

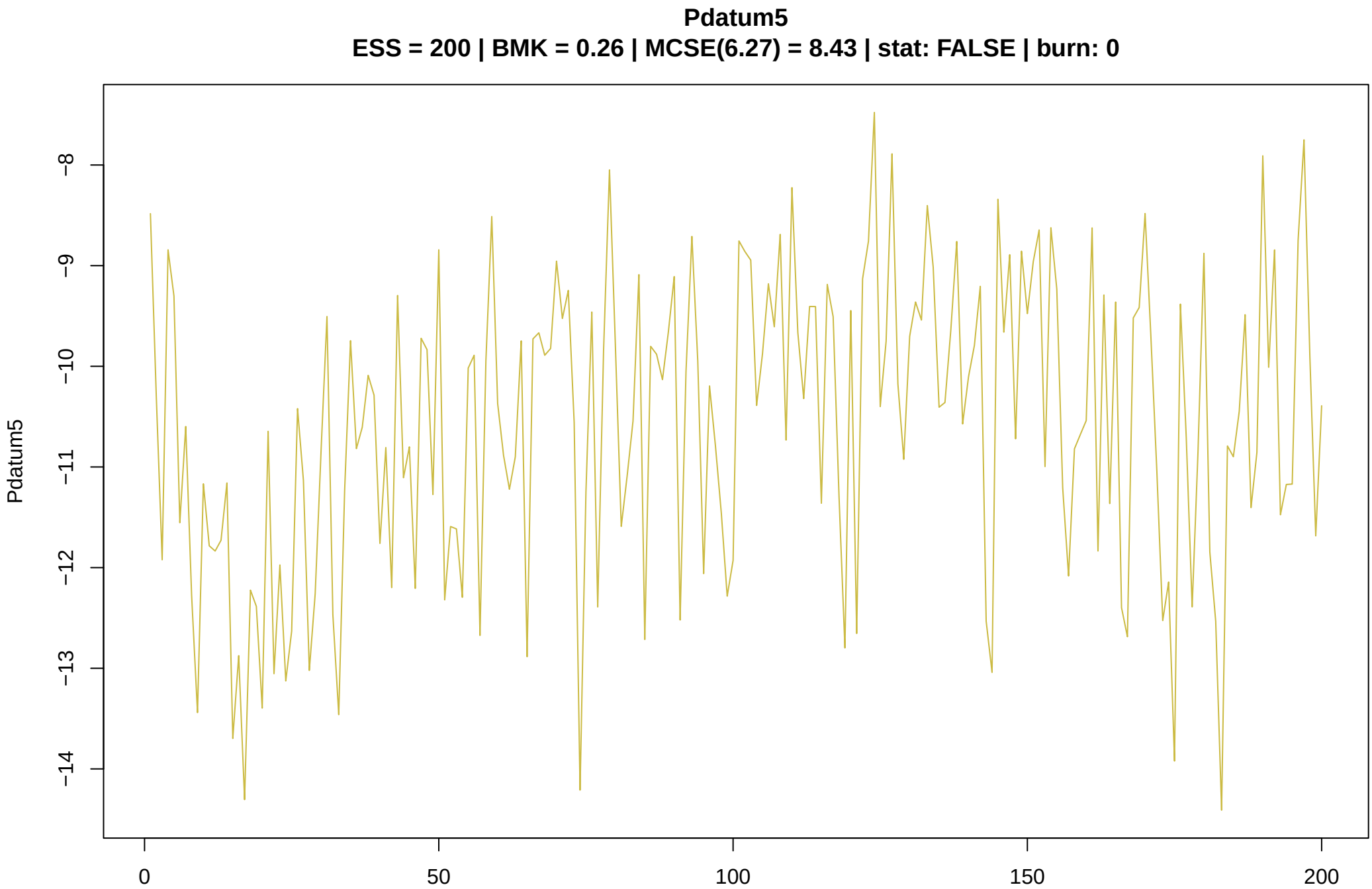

PdatacornerLo
ESS = 146 | BMK = 0.208 | MCSE(6.27) = 9.01 | stat: TRUE | burn: 160
PdatacornerLo
−10
−15
−20
−25
0
50
100
150
200

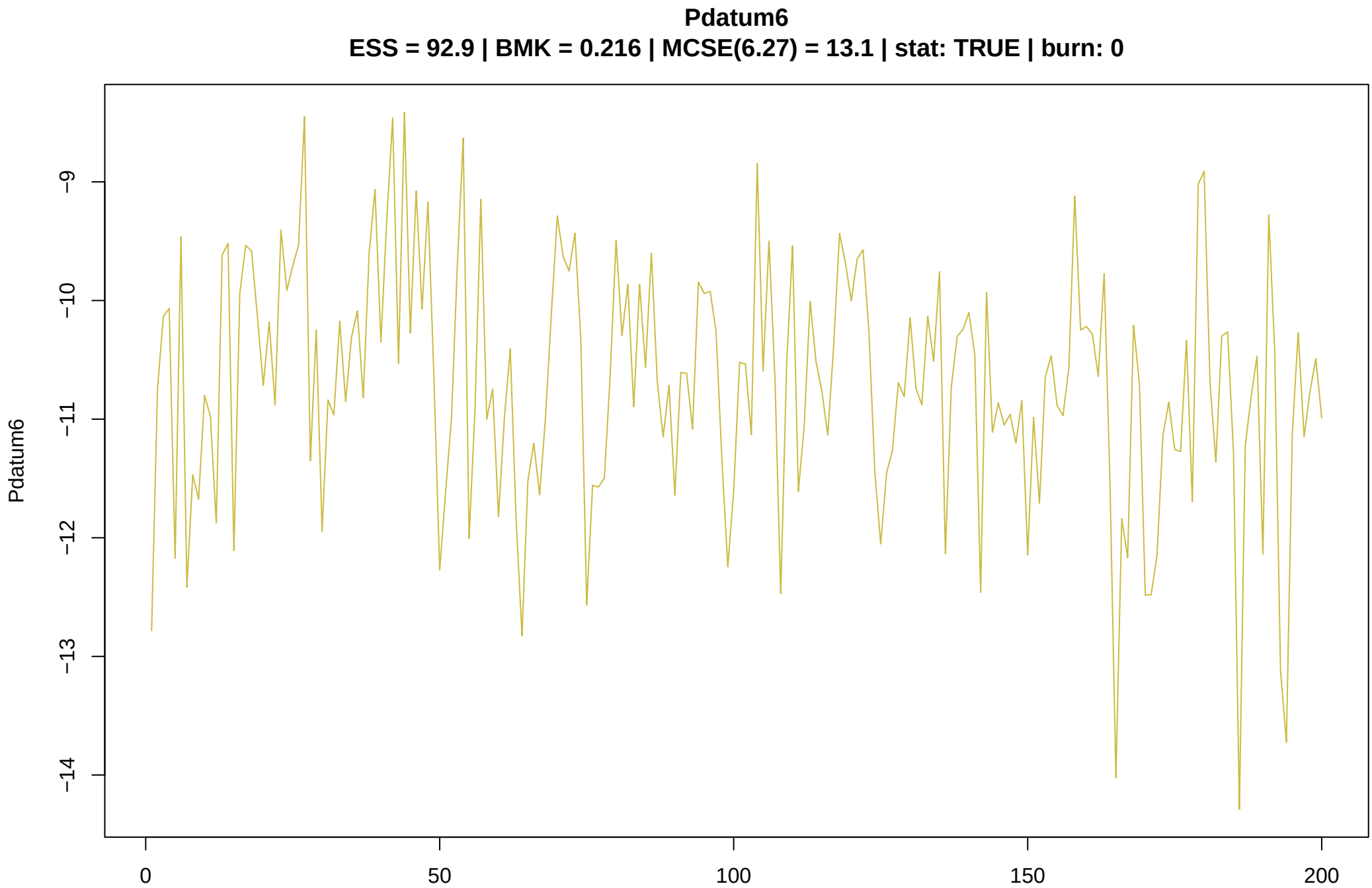

Pdatum1
ESS = 200 | BMK = 0.258 | MCSE(6.27) = 6.71 | stat: FALSE | burn: 0
Pdatum1
−10
−12
−14
−16
−18
−20
0
50
100
150
200

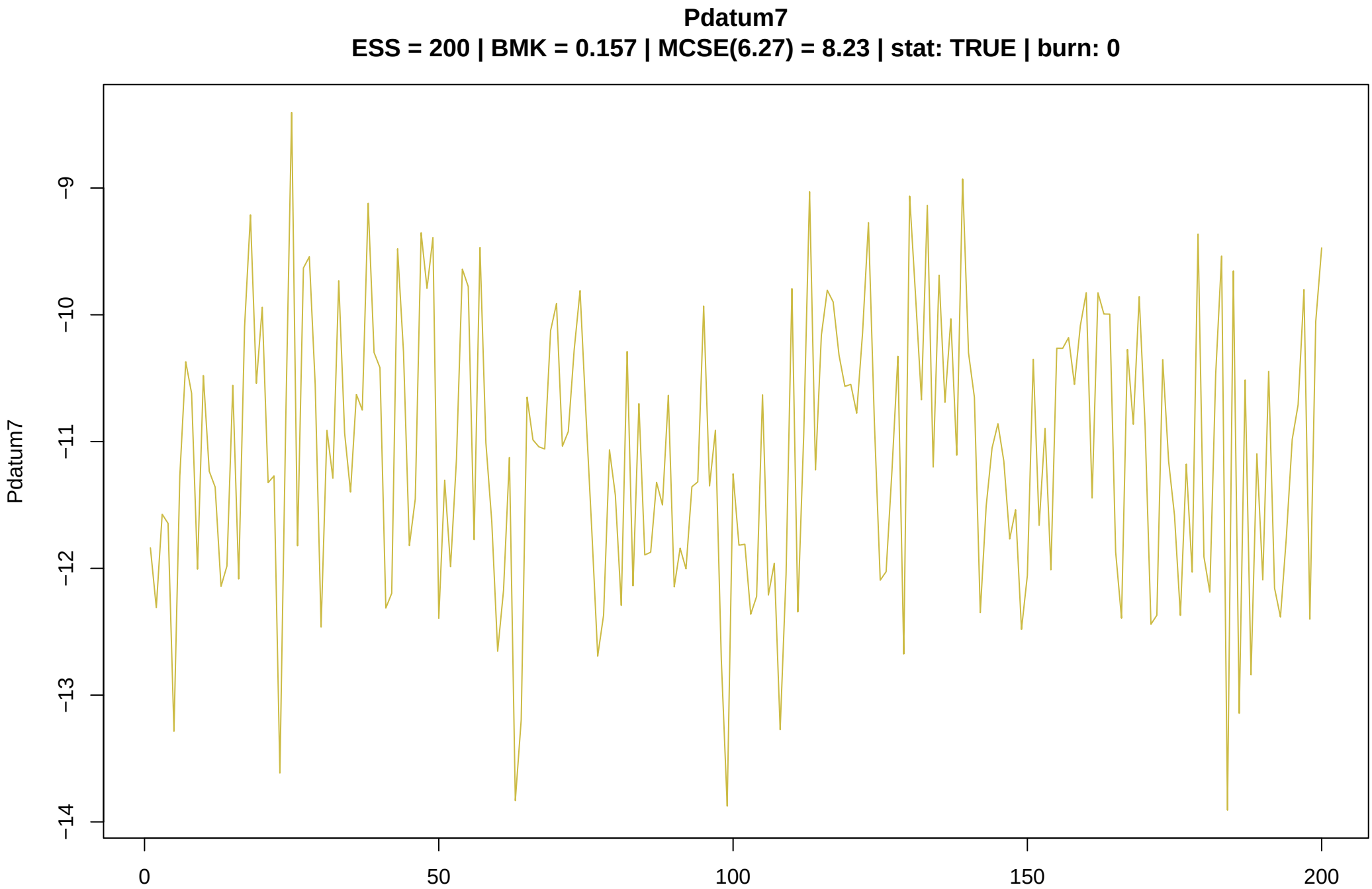

Pdatum2
ESS = 39.5 | BMK = 0.3 | MCSE(6.27) = 11.4 | stat: TRUE | burn: 200
Pdatum2
−8
−9
−10
−11
−12
−13
−14
0
50
100
150
200

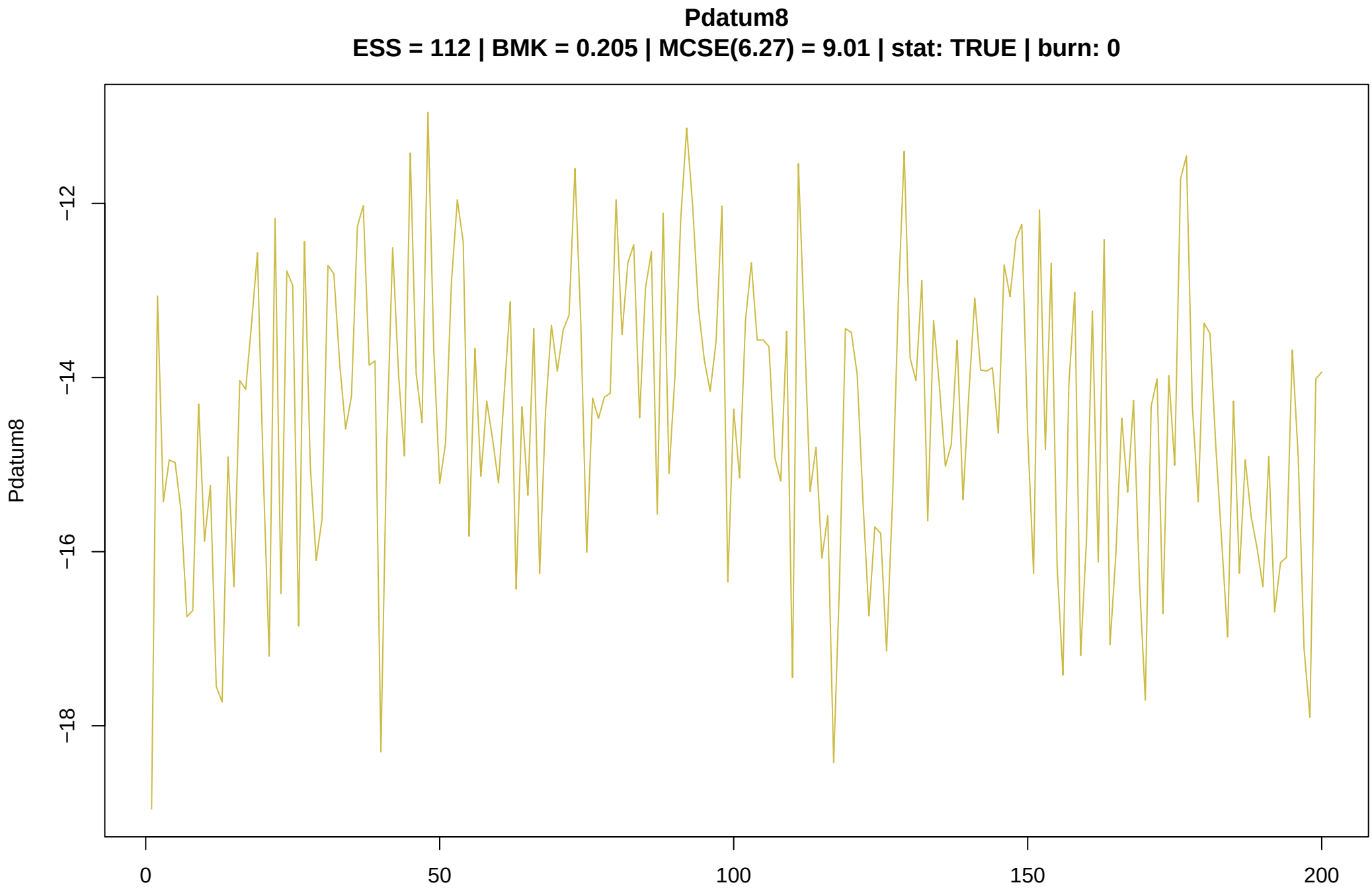

Pdatum3
ESS = 90.1 | BMK = 0.265 | MCSE(6.27) = 7.35 | stat: TRUE | burn: 200
Pdatum3
−14
−16
−18
−20
−22
0
50
100
150
200

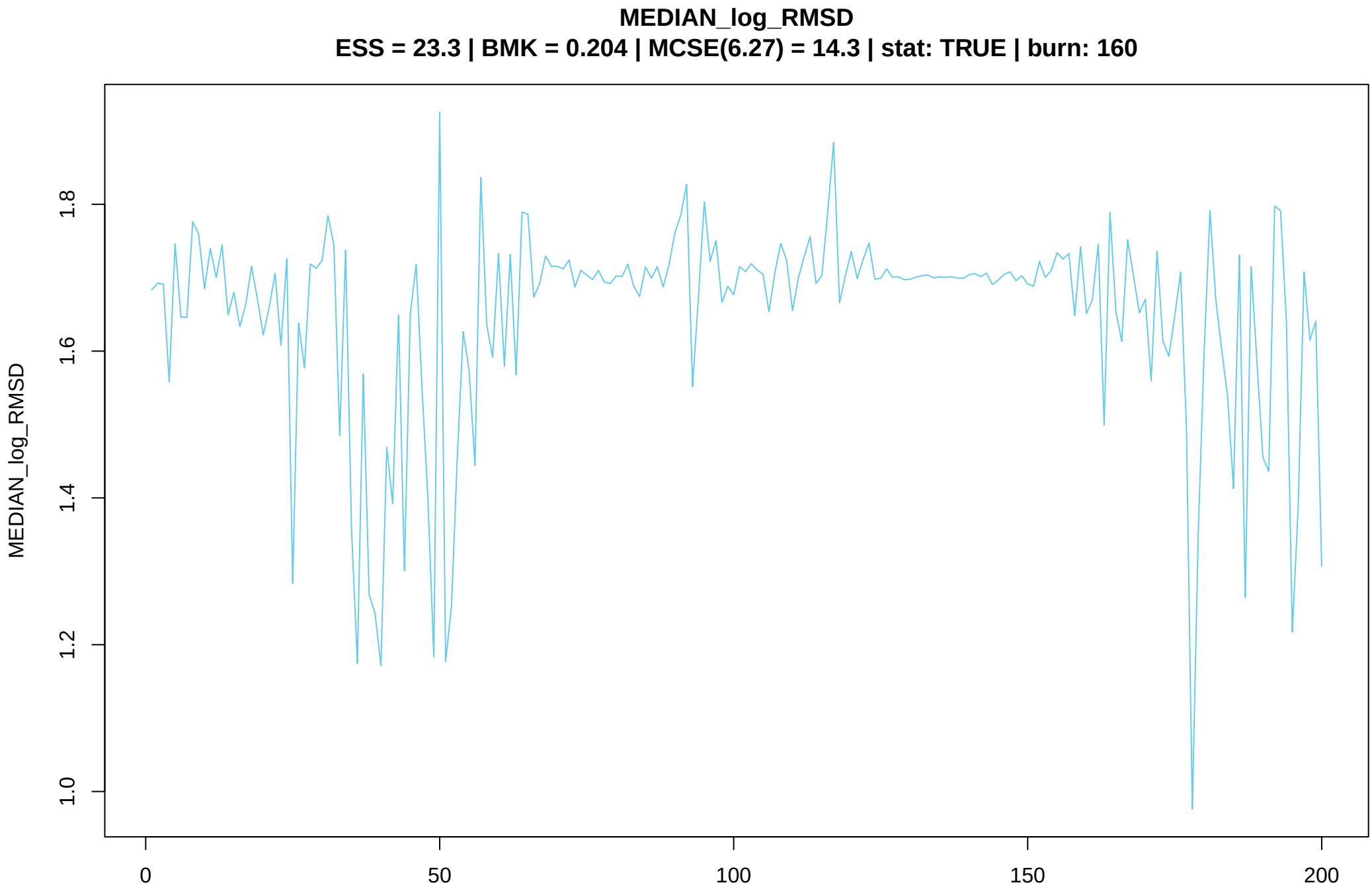

Pdatum4
ESS = 77.8 | BMK = 0.207 | MCSE(6.27) = 9.24 | stat: TRUE | burn: 0
Pdatum4
−6
−8
−10
−12
0
50
100
150
200

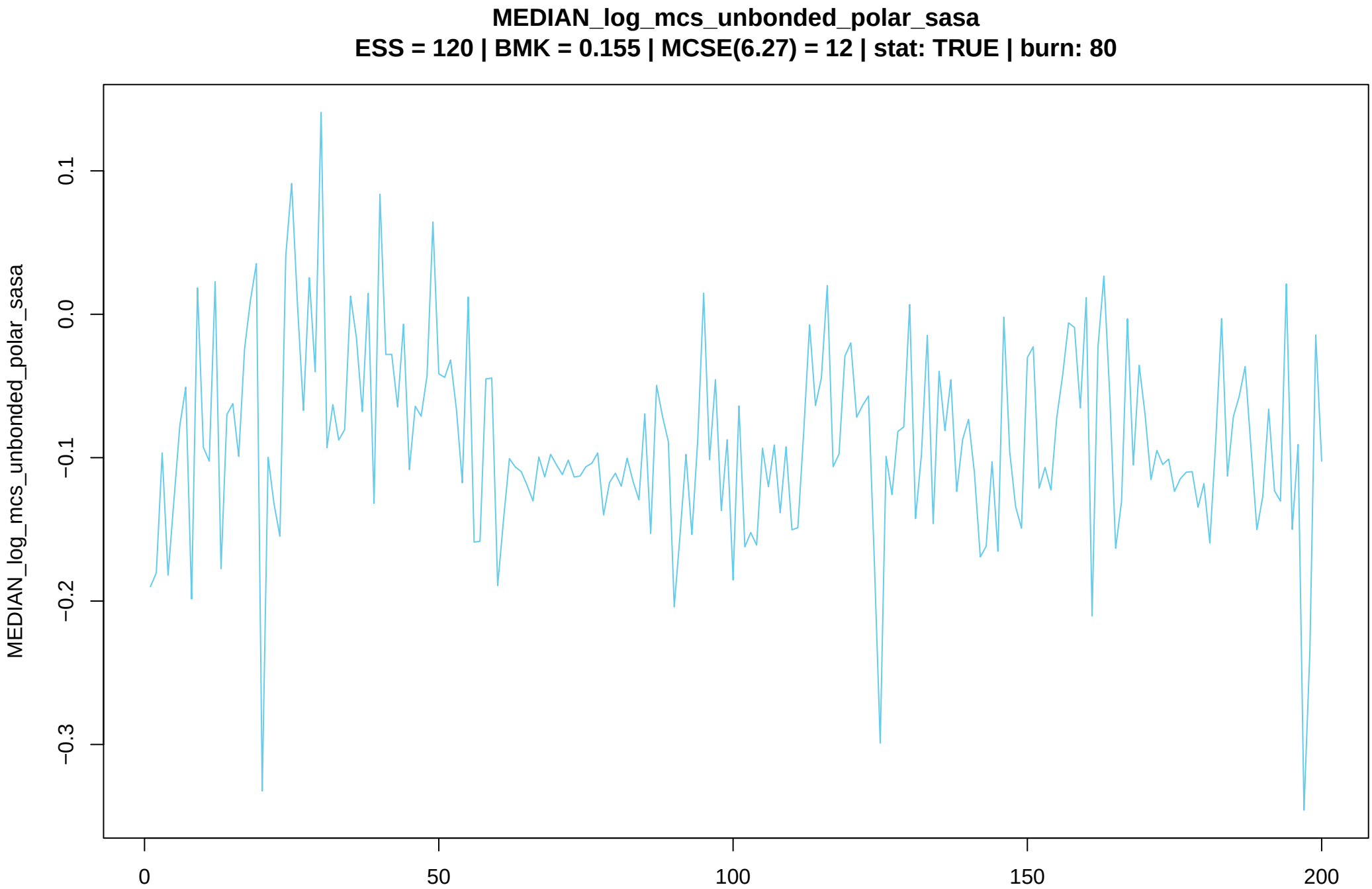

Pdatum5
ESS = 200 | BMK = 0.26 | MCSE(6.27) = 8.43 | stat: FALSE | burn: 0
Pdatum5
−8
−9
−10
−11
−12
−13
−14
0
50
100
150
200

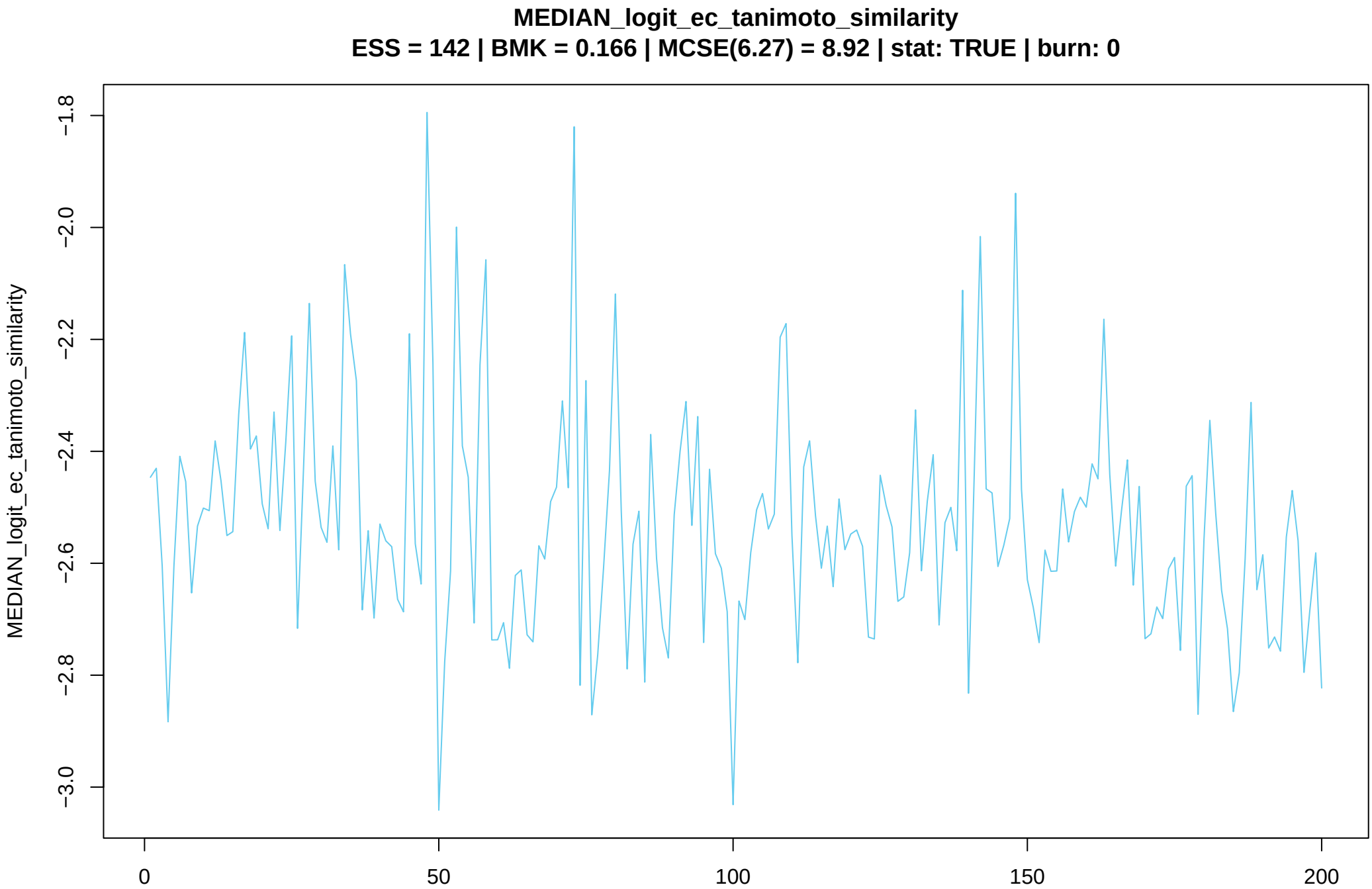

Pdatum6
ESS = 92.9 | BMK = 0.216 | MCSE(6.27) = 13.1 | stat: TRUE | burn: 0
Pdatum6
−9
−10
−11
−12
−13
−14
0
50
100
150
200

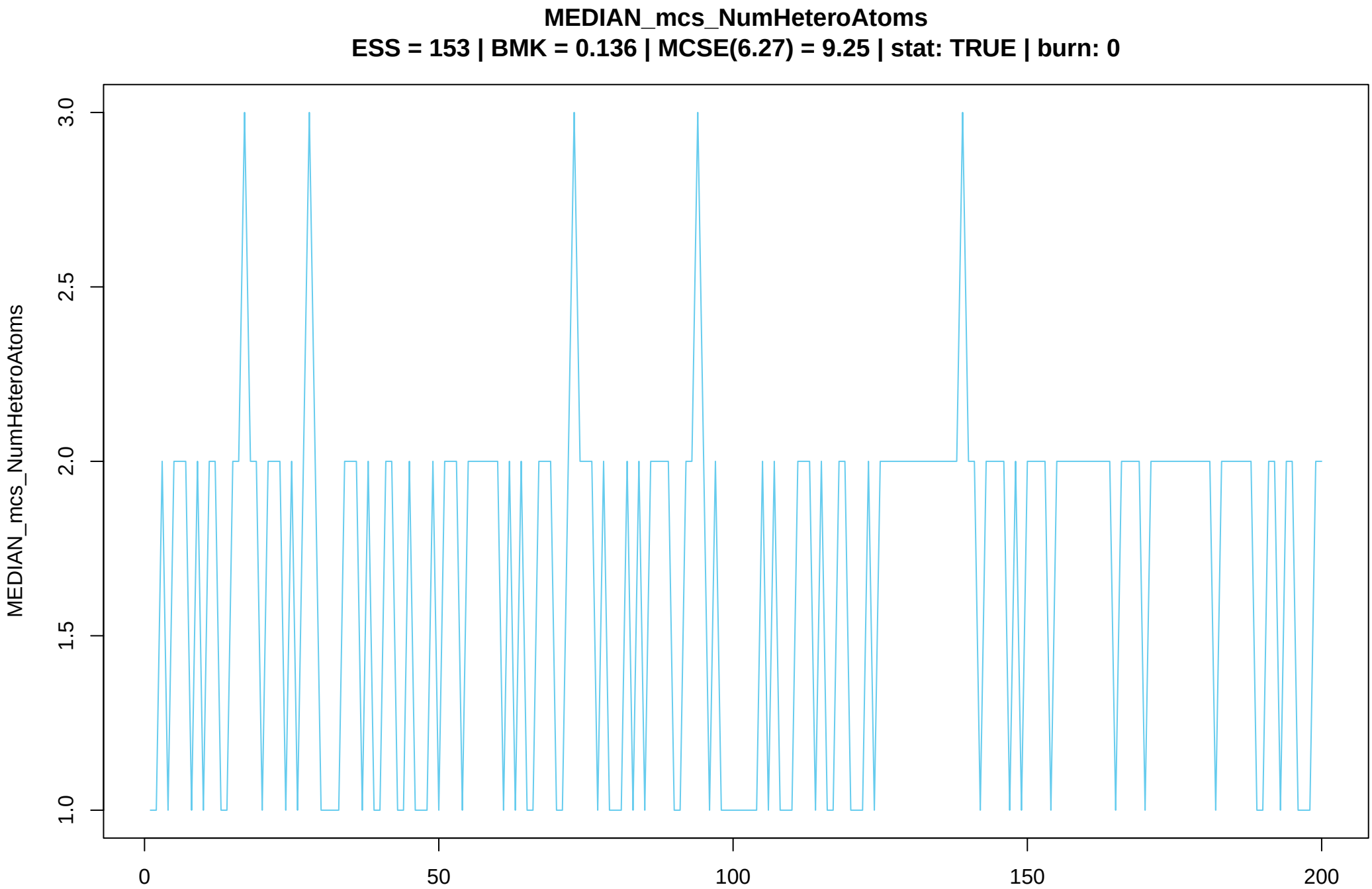

Pdatum7
ESS = 200 | BMK = 0.157 | MCSE(6.27) = 8.23 | stat: TRUE | burn: 0
Pdatum7
−9
−10
−11
−12
−13
−14
0
50
100
150
200

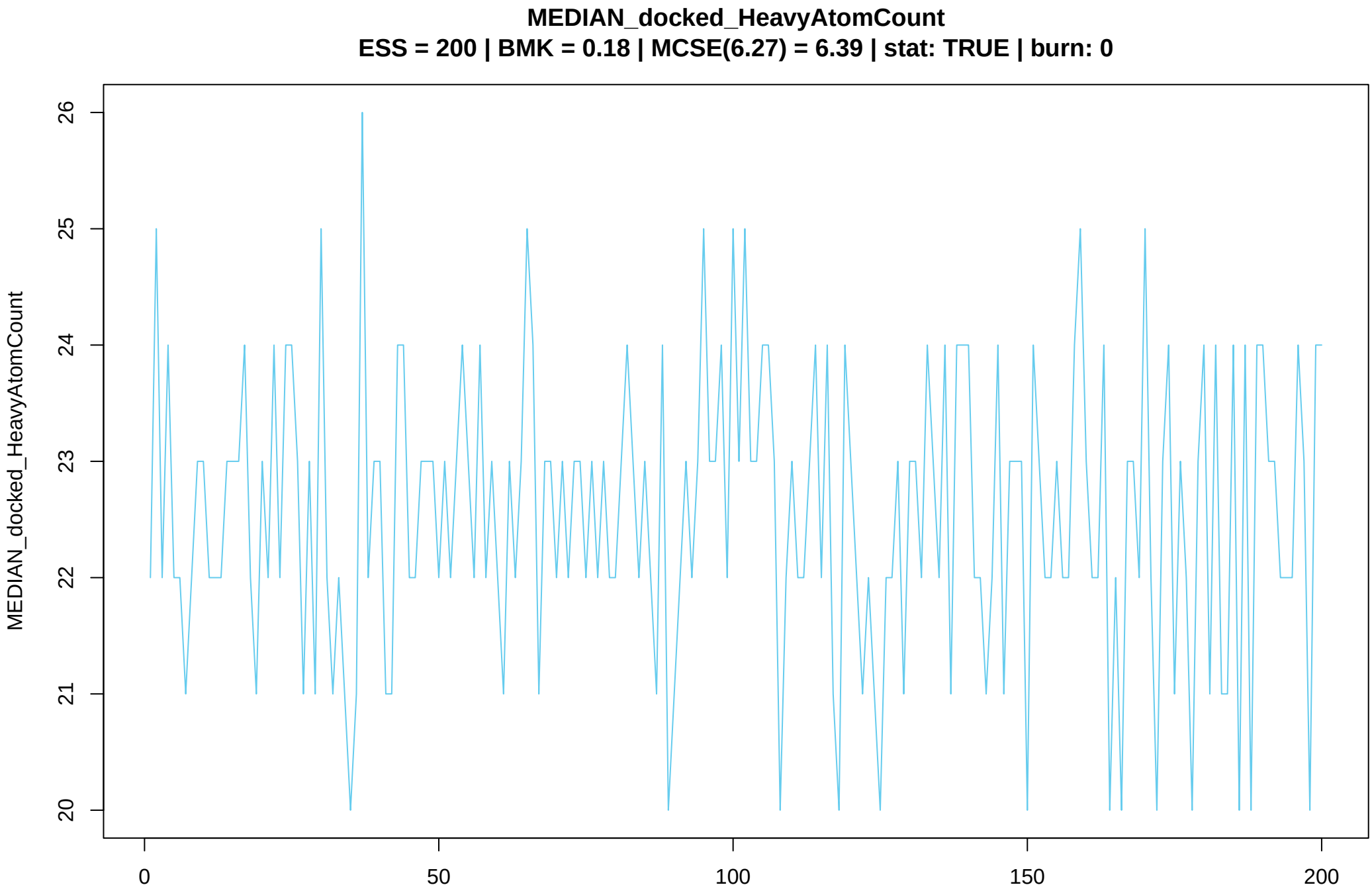

Pdatum8
ESS = 112 | BMK = 0.205 | MCSE(6.27) = 9.01 | stat: TRUE | burn: 0
Pdatum8
−12
−14
−16
−18
0
50
100
150
200

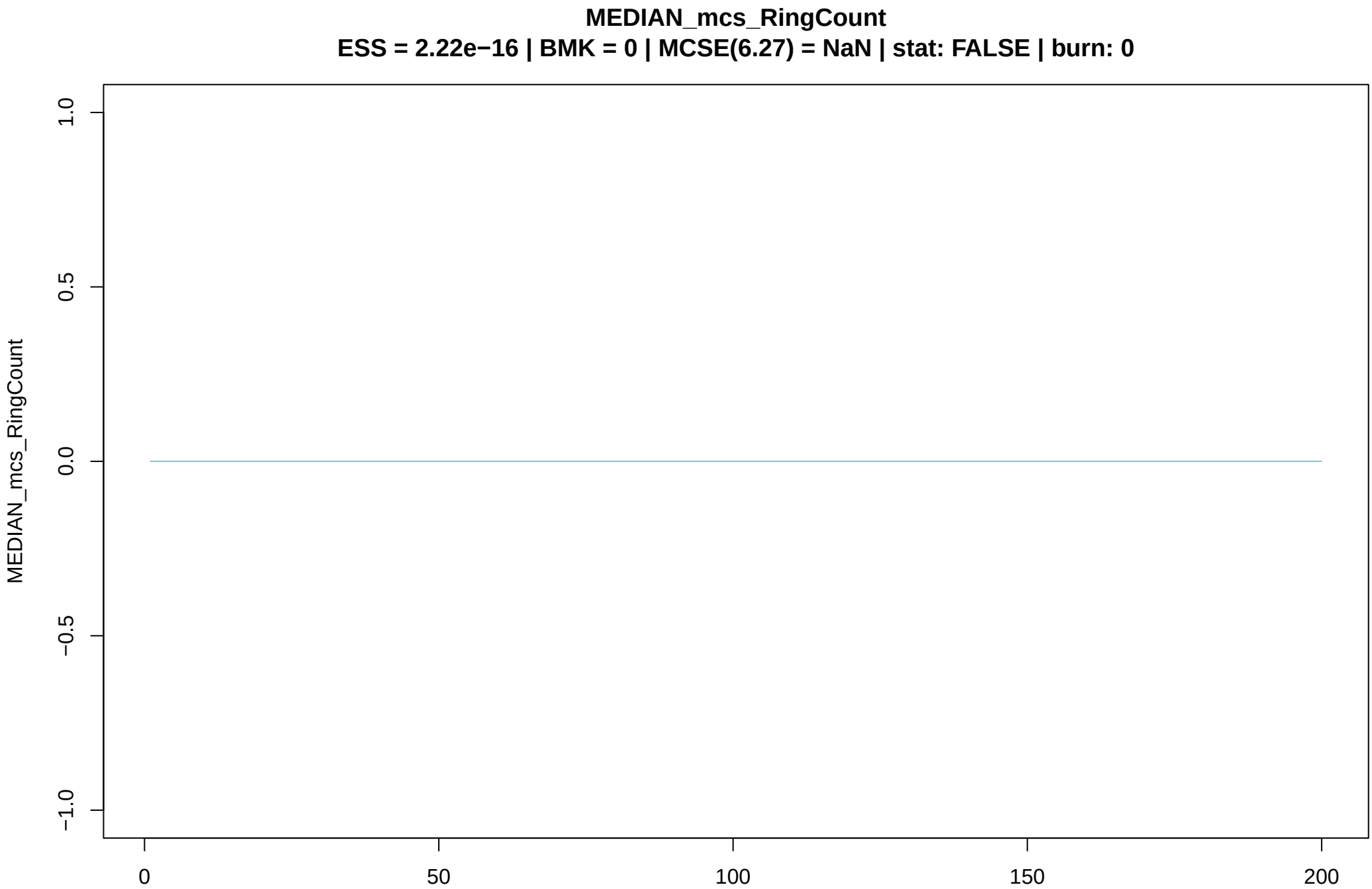

MEDIAN_log_RMSD
ESS = 23.3 | BMK = 0.204 | MCSE(6.27) = 14.3 | stat: TRUE | burn: 160
MEDIAN_log_RMSD
1.0
1.2
1.4
1.6
1.8
0
50
100
150
200

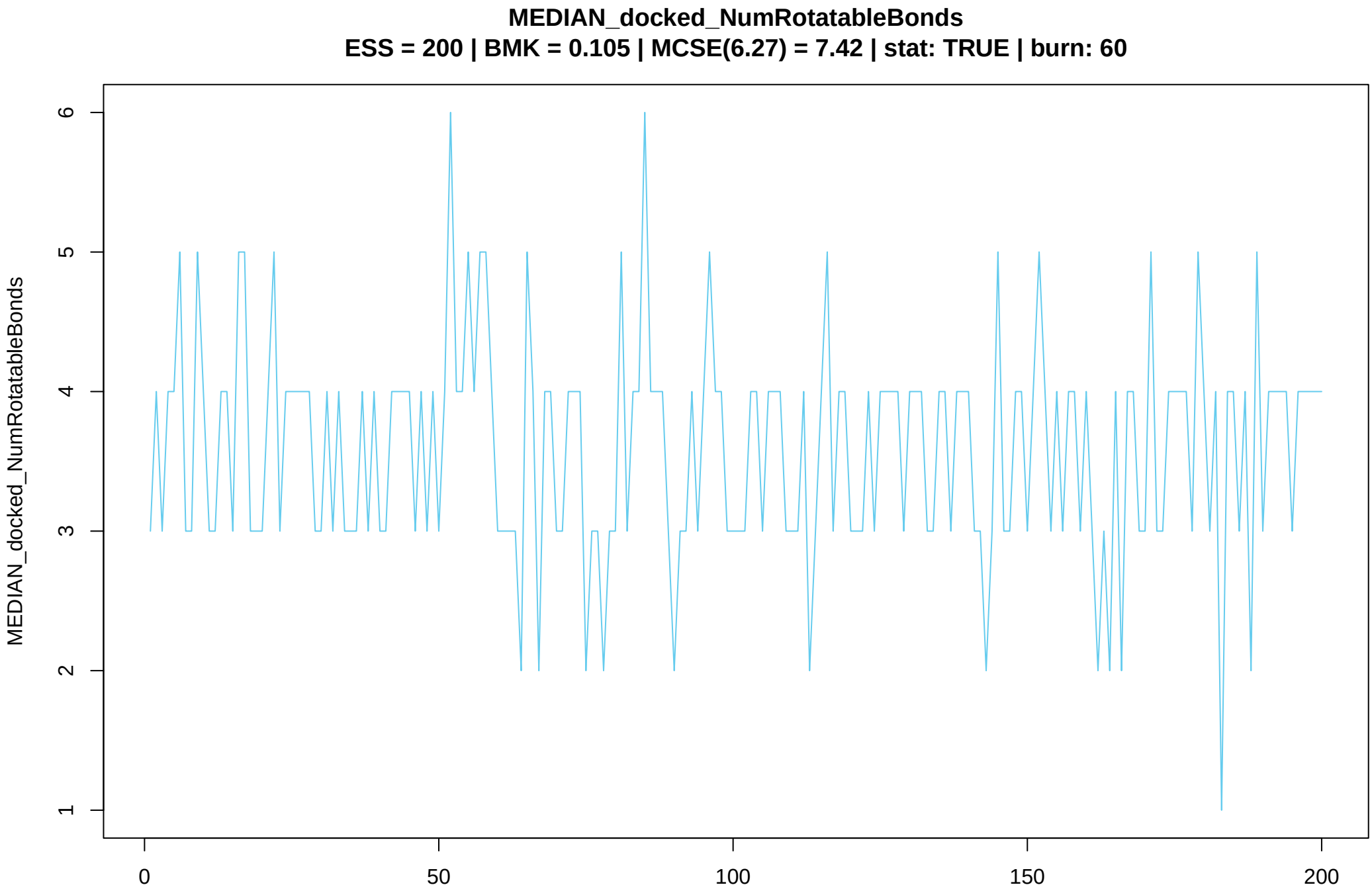

MEDIAN_log_mcs_unbonded_polar_sasa
ESS = 120 | BMK = 0.155 | MCSE(6.27) = 12 | stat: TRUE | burn: 80
MEDIAN_log_mcs_unbonded_polar_sasa
0.1
0.0
−0.1
−0.2
−0.3
0
50
100
150
200

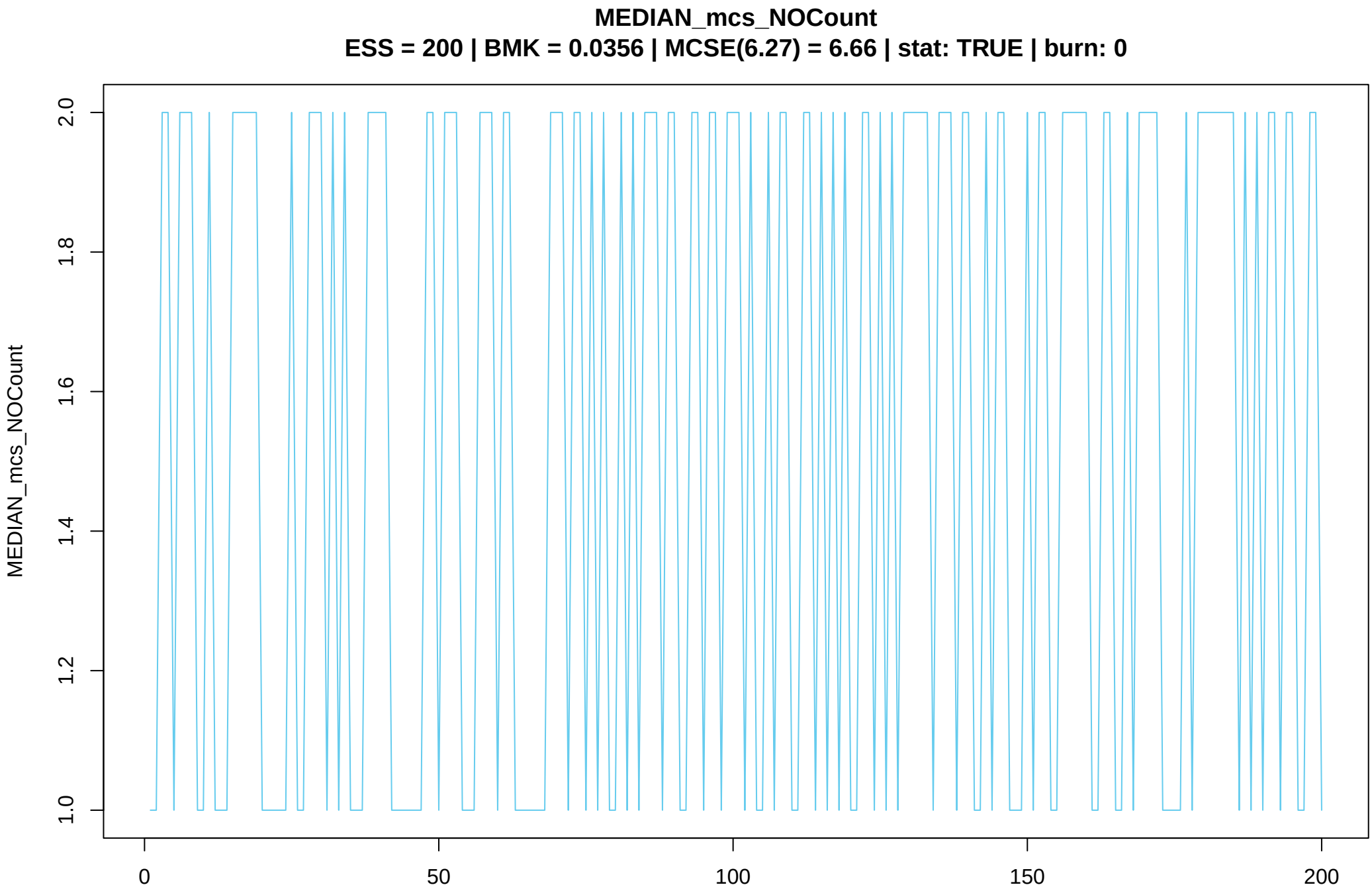

MEDIAN_logit_ec_tanimoto_similarity
ESS = 142 | BMK = 0.166 | MCSE(6.27) = 8.92 | stat: TRUE | burn: 0
MEDIAN_logit_ec_tanimoto_similarity
−1.8
−2.0
−2.2
−2.4
−2.6
−2.8
−3.0
0
50
100
150
200

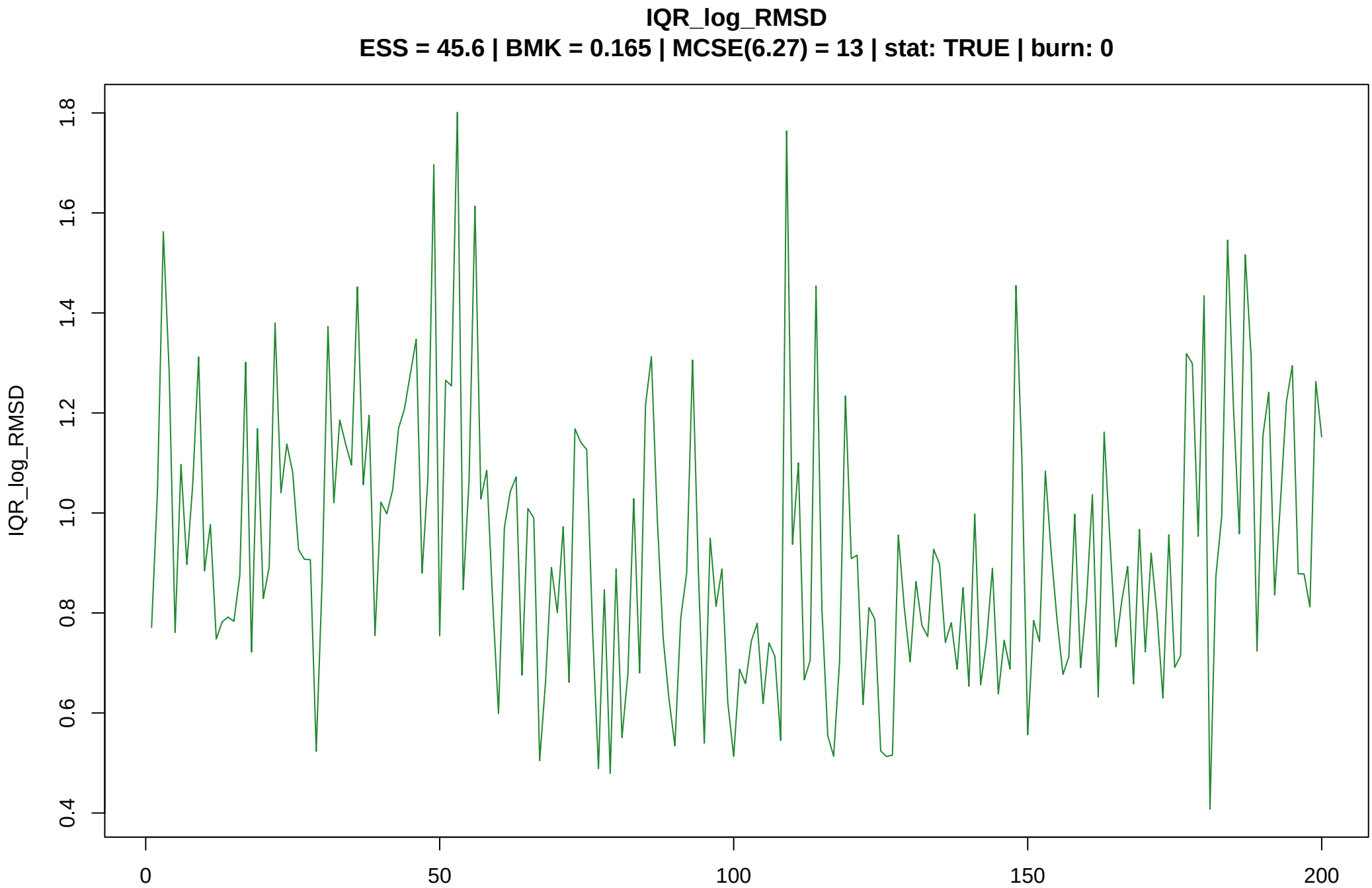

MEDIAN_mcs_NumHeteroAtoms
ESS = 153 | BMK = 0.136 | MCSE(6.27) = 9.25 | stat: TRUE | burn: 0
MEDIAN_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
0
50
100
150
200

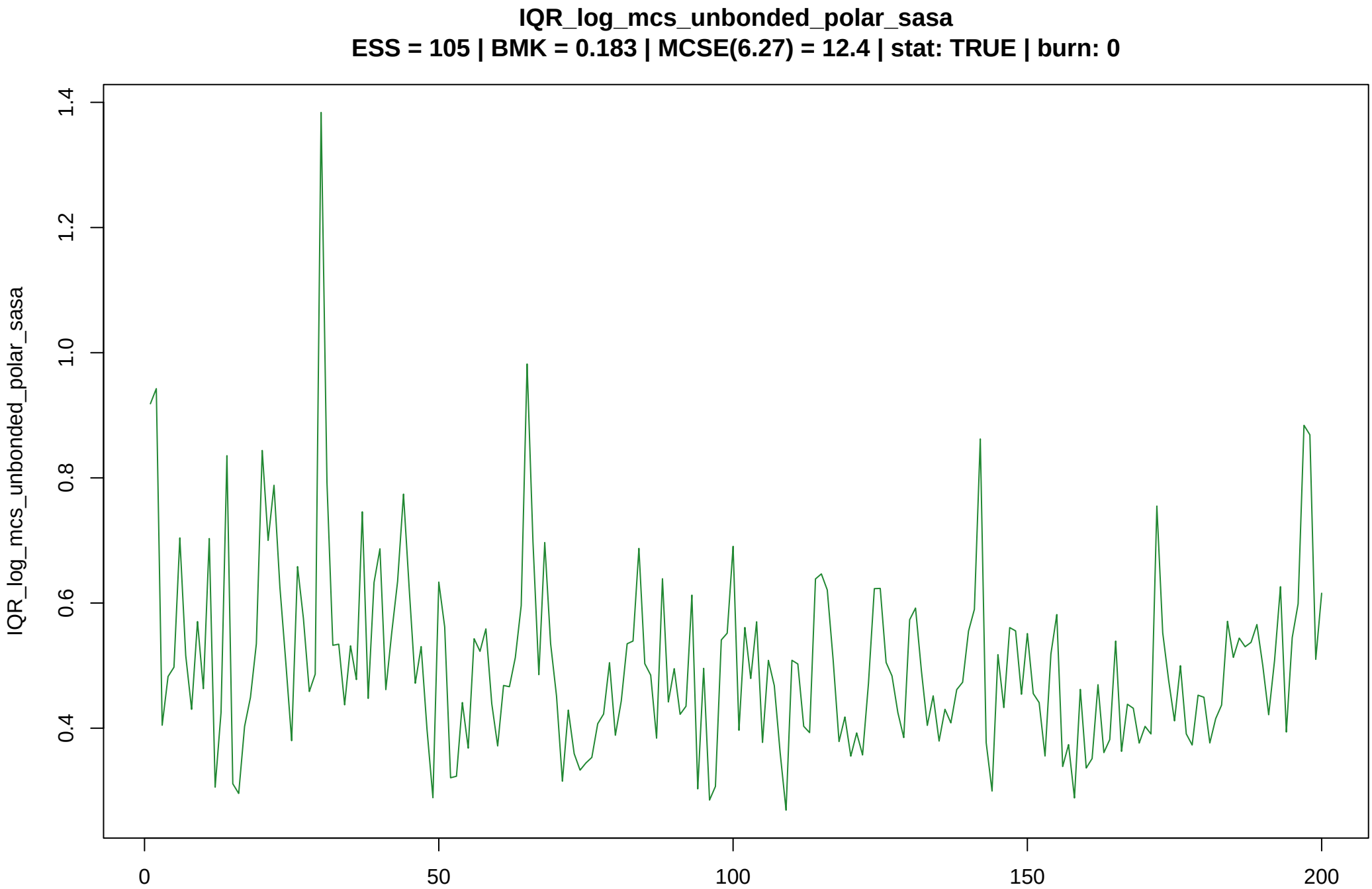

MEDIAN_docked_HeavyAtomCount
ESS = 200 | BMK = 0.18 | MCSE(6.27) = 6.39 | stat: TRUE | burn: 0
MEDIAN_docked_HeavyAtomCount
20
21
22
23
24
25
26
0
50
100
150
200

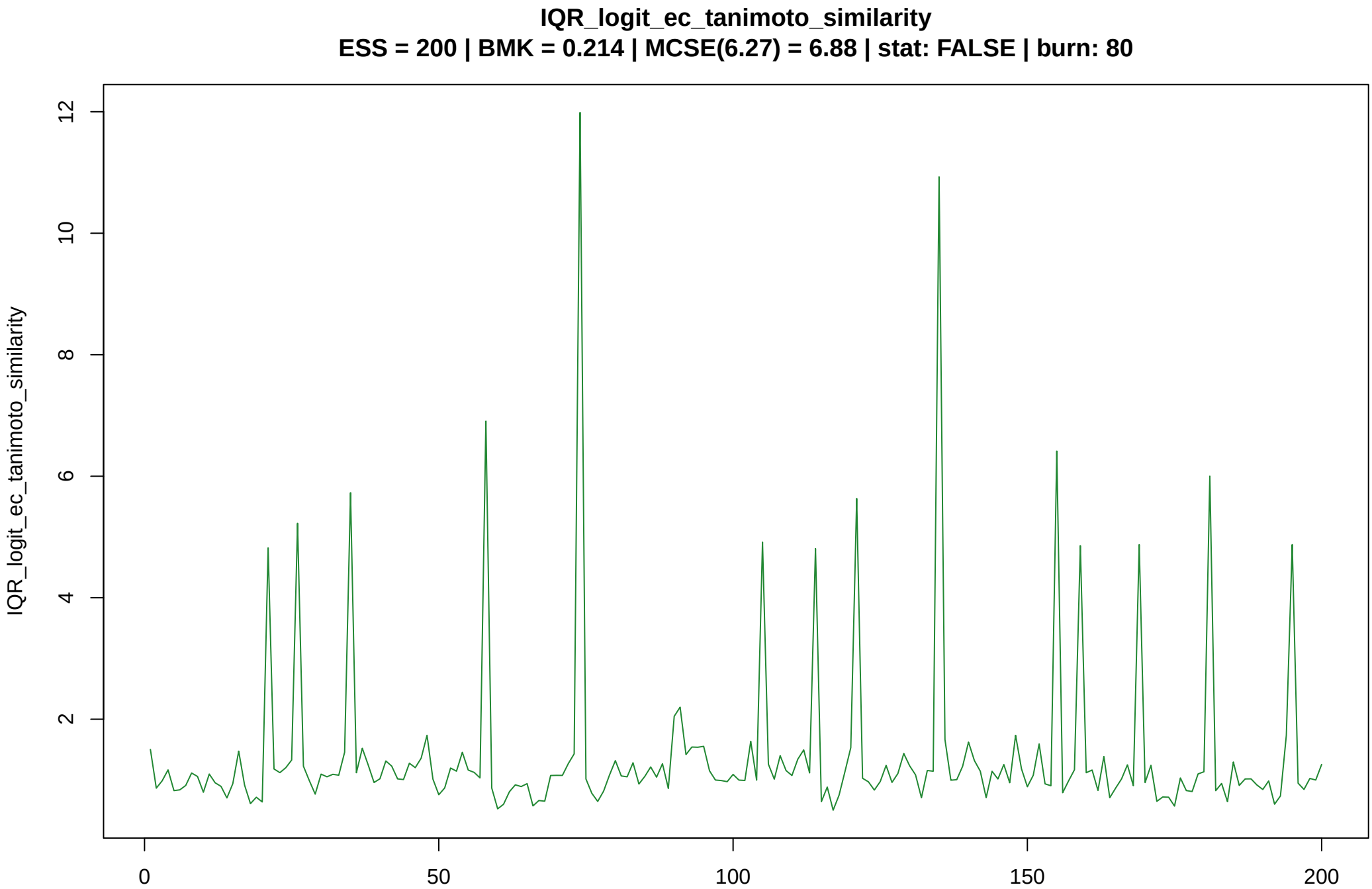

MEDIAN_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
MEDIAN_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
50
100
150
200

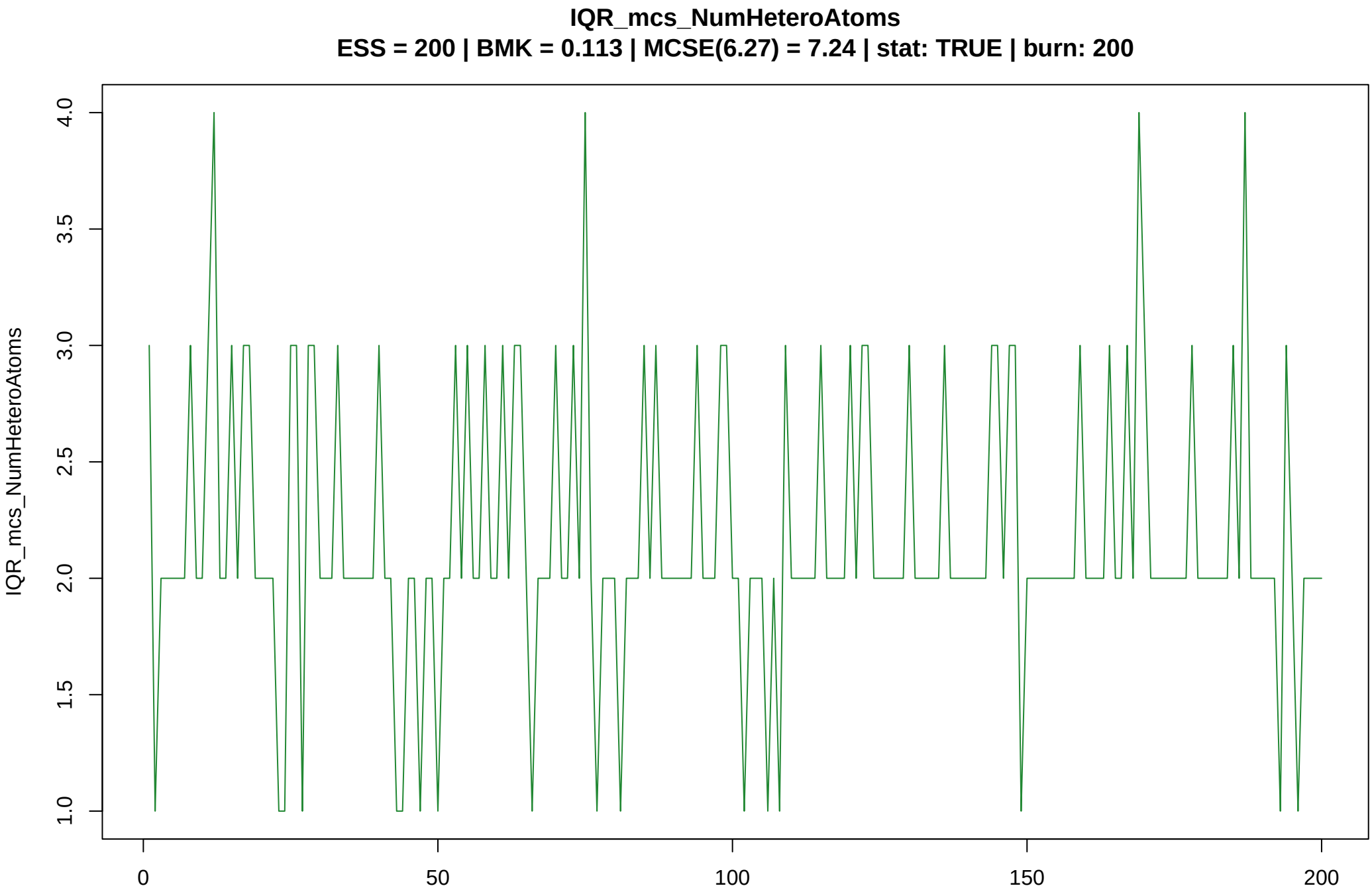

MEDIAN_docked_NumRotatableBonds
ESS = 200 | BMK = 0.105 | MCSE(6.27) = 7.42 | stat: TRUE | burn: 60
MEDIAN_docked_NumRotatableBonds
1
2
3
4
5
6
0
50
100
150
200

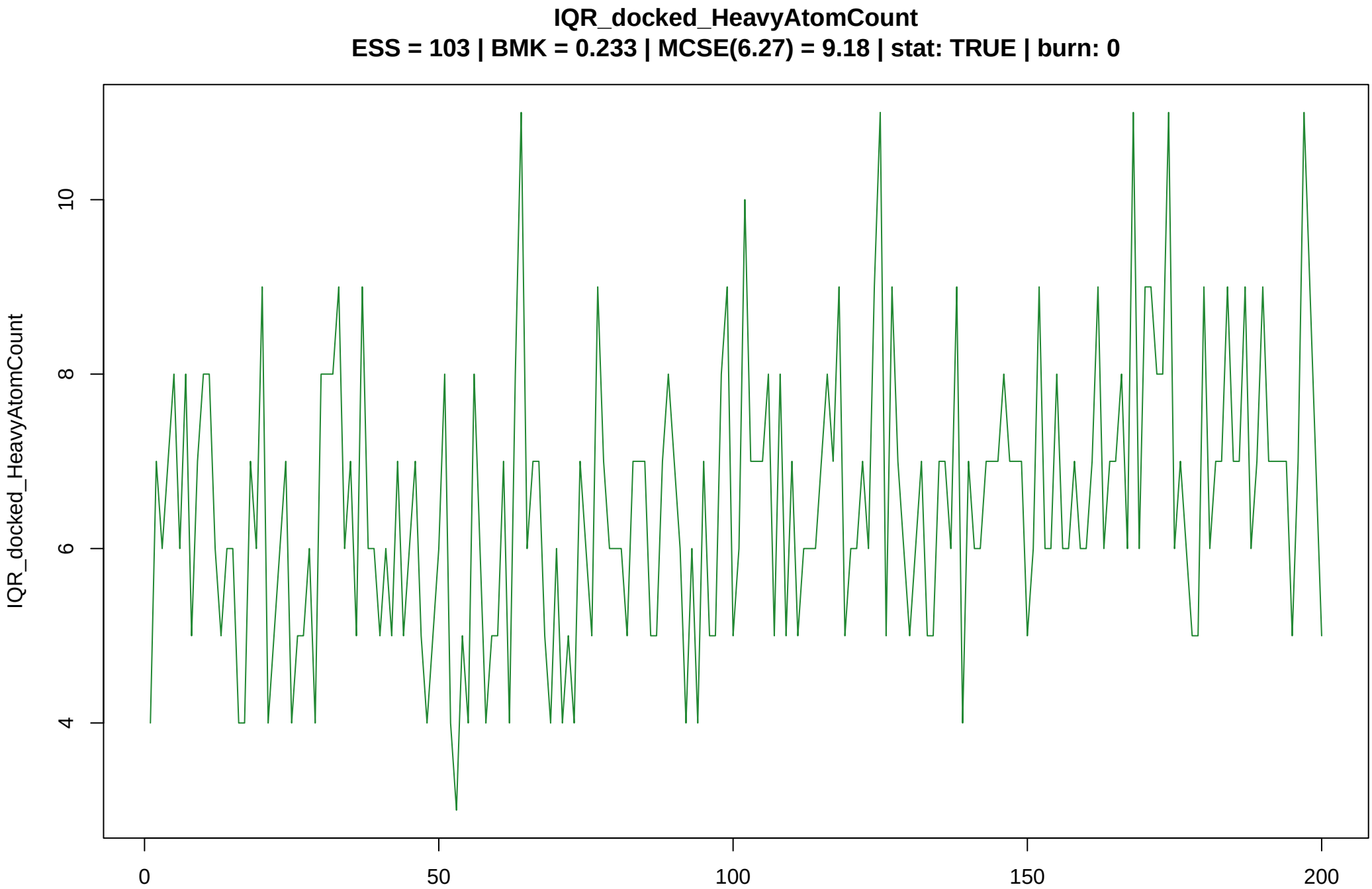

MEDIAN_mcs_NOCount
ESS = 200 | BMK = 0.0356 | MCSE(6.27) = 6.66 | stat: TRUE | burn: 0
MEDIAN_mcs_NOCount
1.0
1.2
1.4
1.6
1.8
2.0
0
50
100
150
200

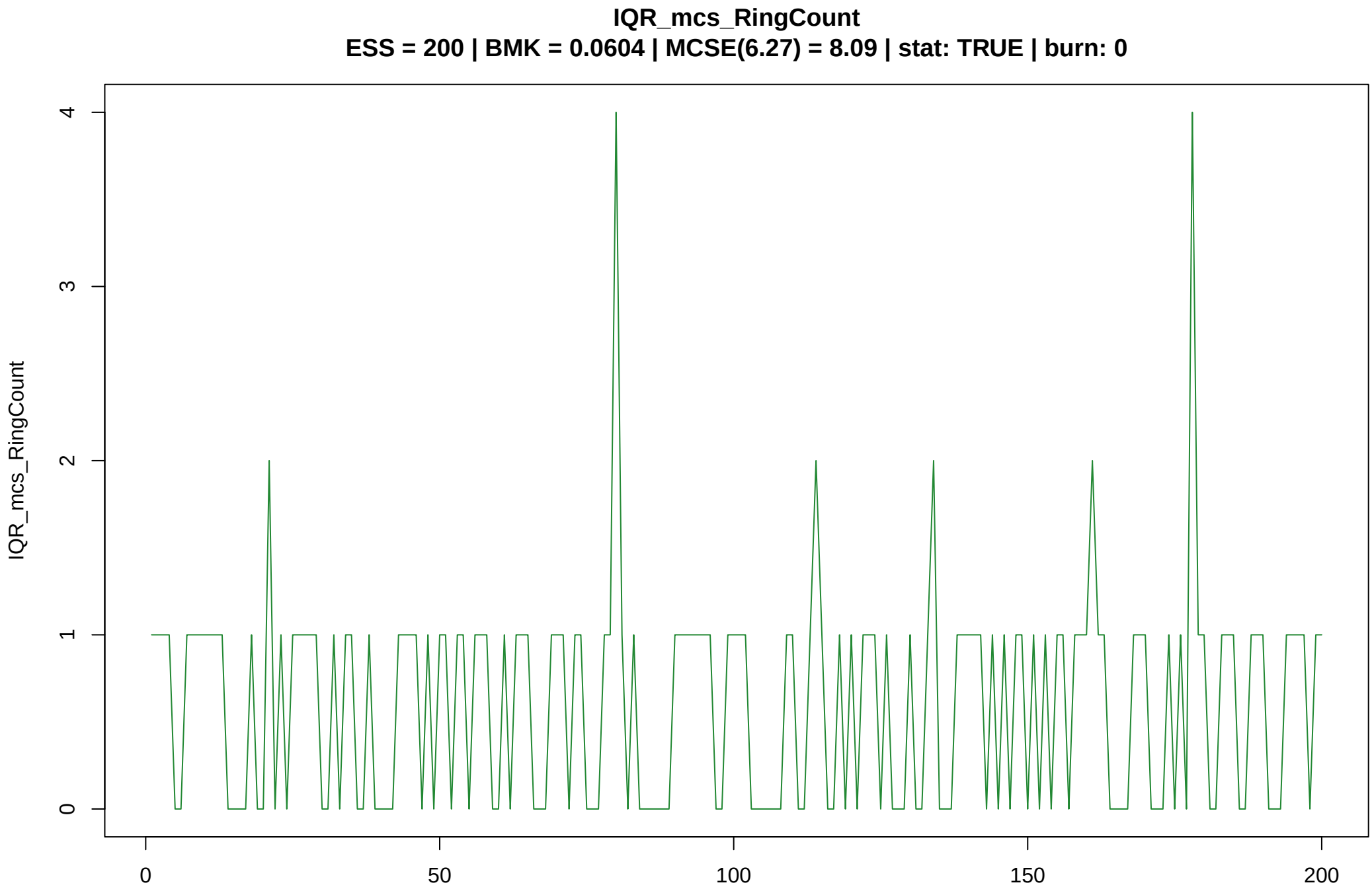

IQR_log_RMSD
ESS = 45.6 | BMK = 0.165 | MCSE(6.27) = 13 | stat: TRUE | burn: 0
IQR_log_RMSD
0.4
0.6
0.8
1.0
1.2
1.4
1.6
1.8
0
50
100
150
200

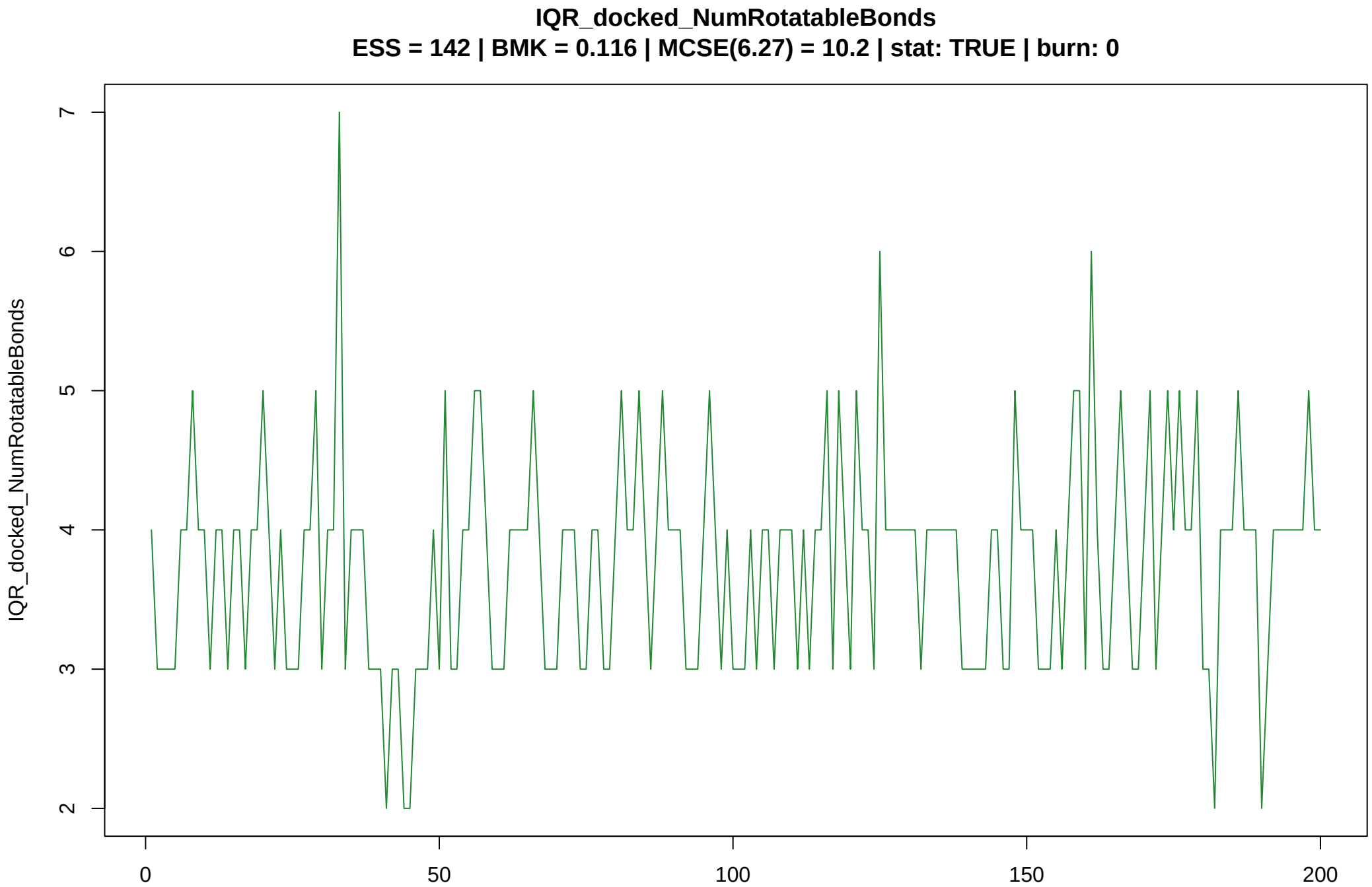

IQR_log_mcs_unbonded_polar_sasa
ESS = 105 | BMK = 0.183 | MCSE(6.27) = 12.4 | stat: TRUE | burn: 0
IQR_log_mcs_unbonded_polar_sasa
0.4
0.6
0.8
1.0
1.2
1.4
0
50
100
150
200

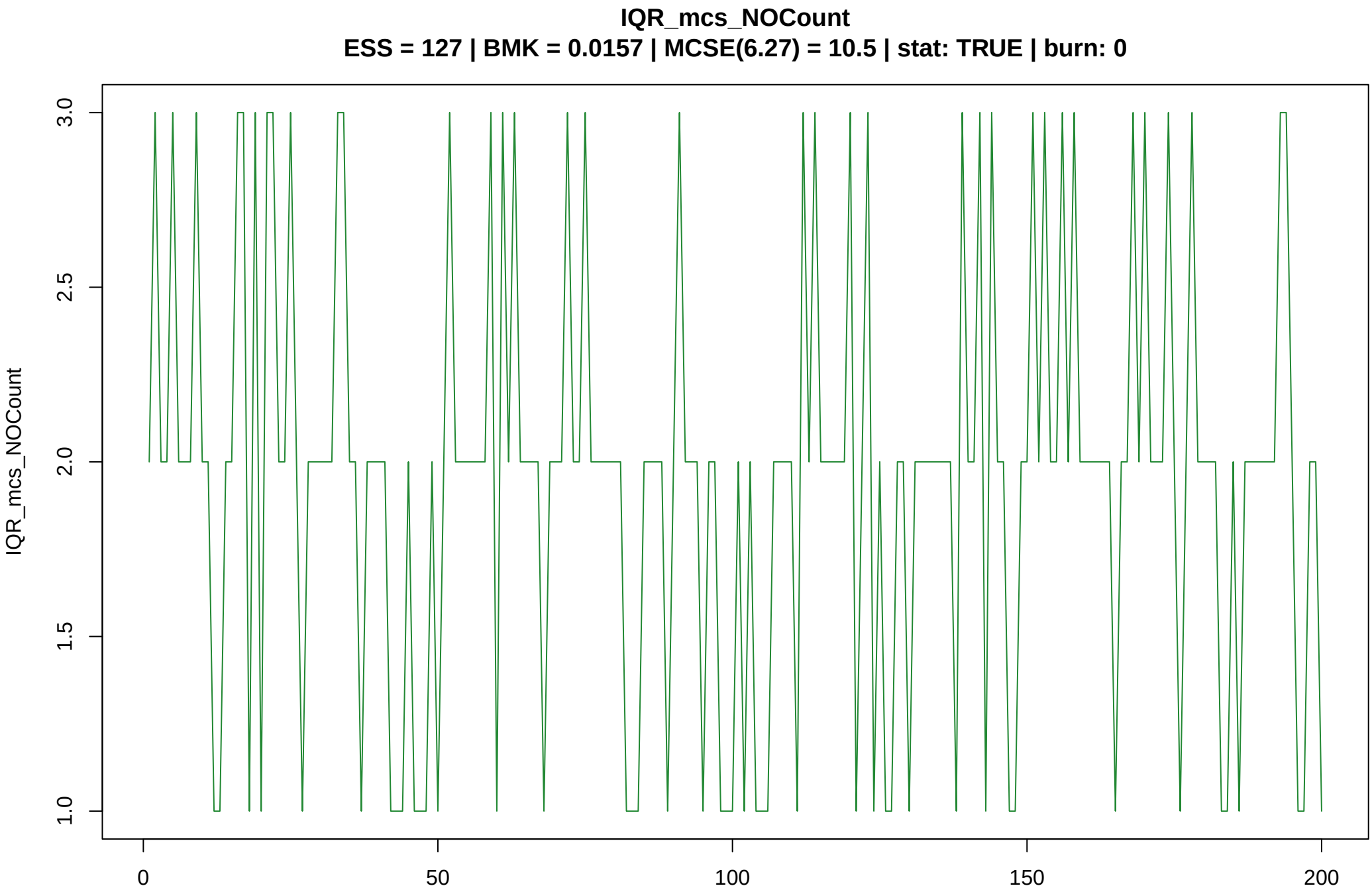

IQR_logit_ec_tanimoto_similarity
ESS = 200 | BMK = 0.214 | MCSE(6.27) = 6.88 | stat: FALSE | burn: 80
IQR_logit_ec_tanimoto_similarity
2
4
6
8
10
12
0
50
100
150
200

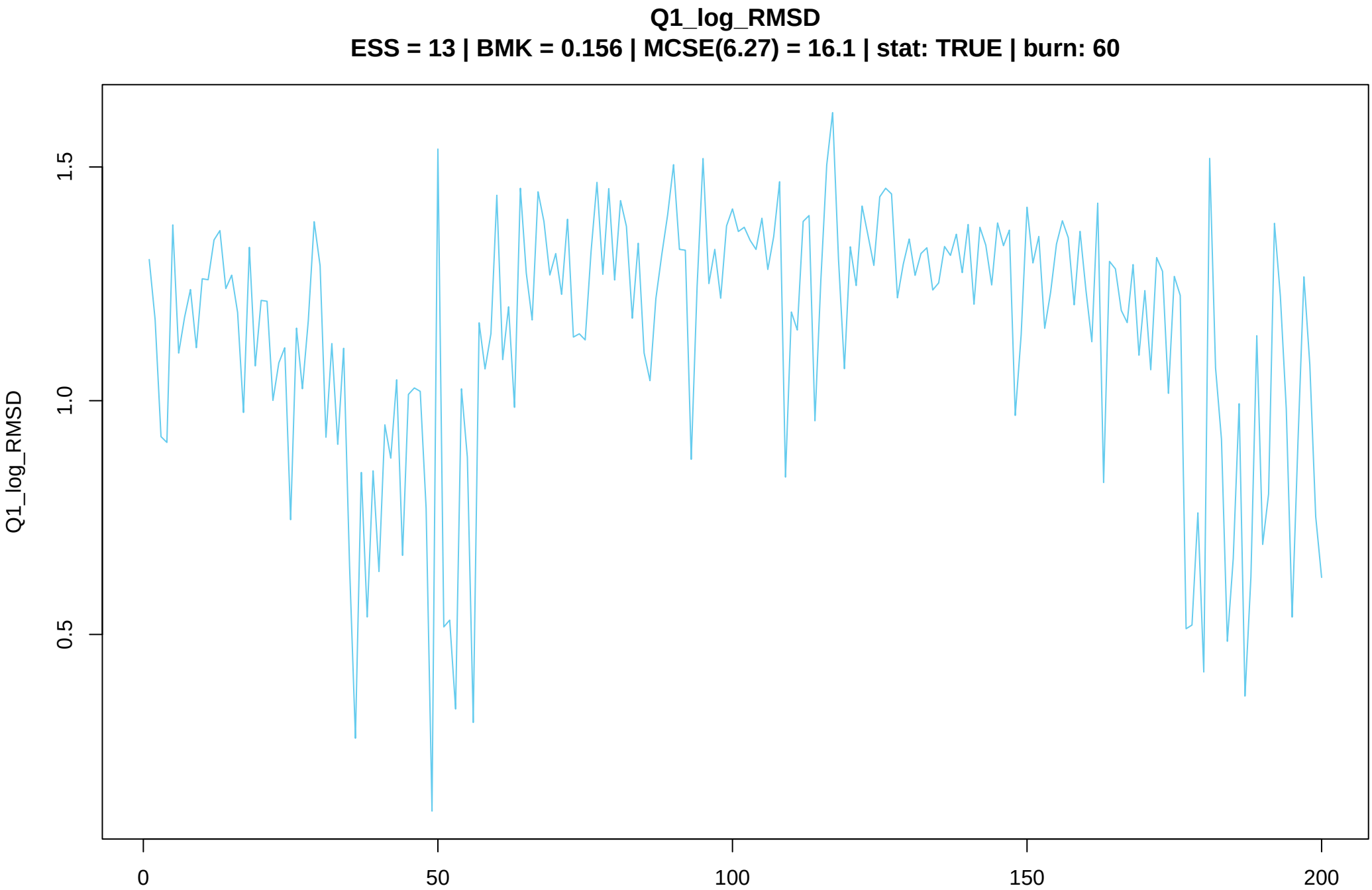

IQR_mcs_NumHeteroAtoms
ESS = 200 | BMK = 0.113 | MCSE(6.27) = 7.24 | stat: TRUE | burn: 200
IQR_mcs_NumHeteroAtoms
1.0
1.5
2.0
2.5
3.0
3.5
4.0
0
50
100
150
200

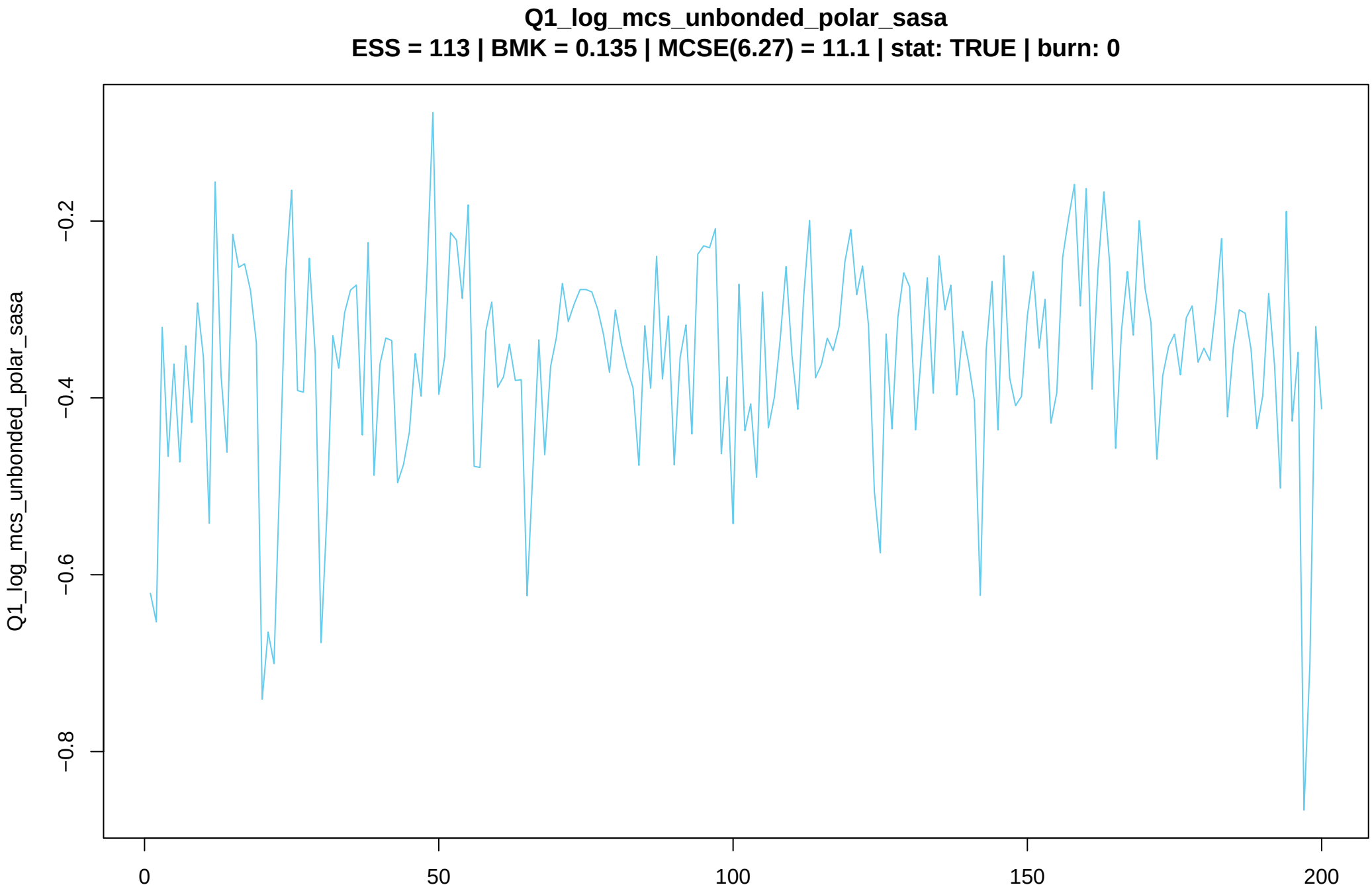

IQR_docked_HeavyAtomCount
ESS = 103 | BMK = 0.233 | MCSE(6.27) = 9.18 | stat: TRUE | burn: 0
IQR_docked_HeavyAtomCount
4
6
8
10
0
50
100
150
200

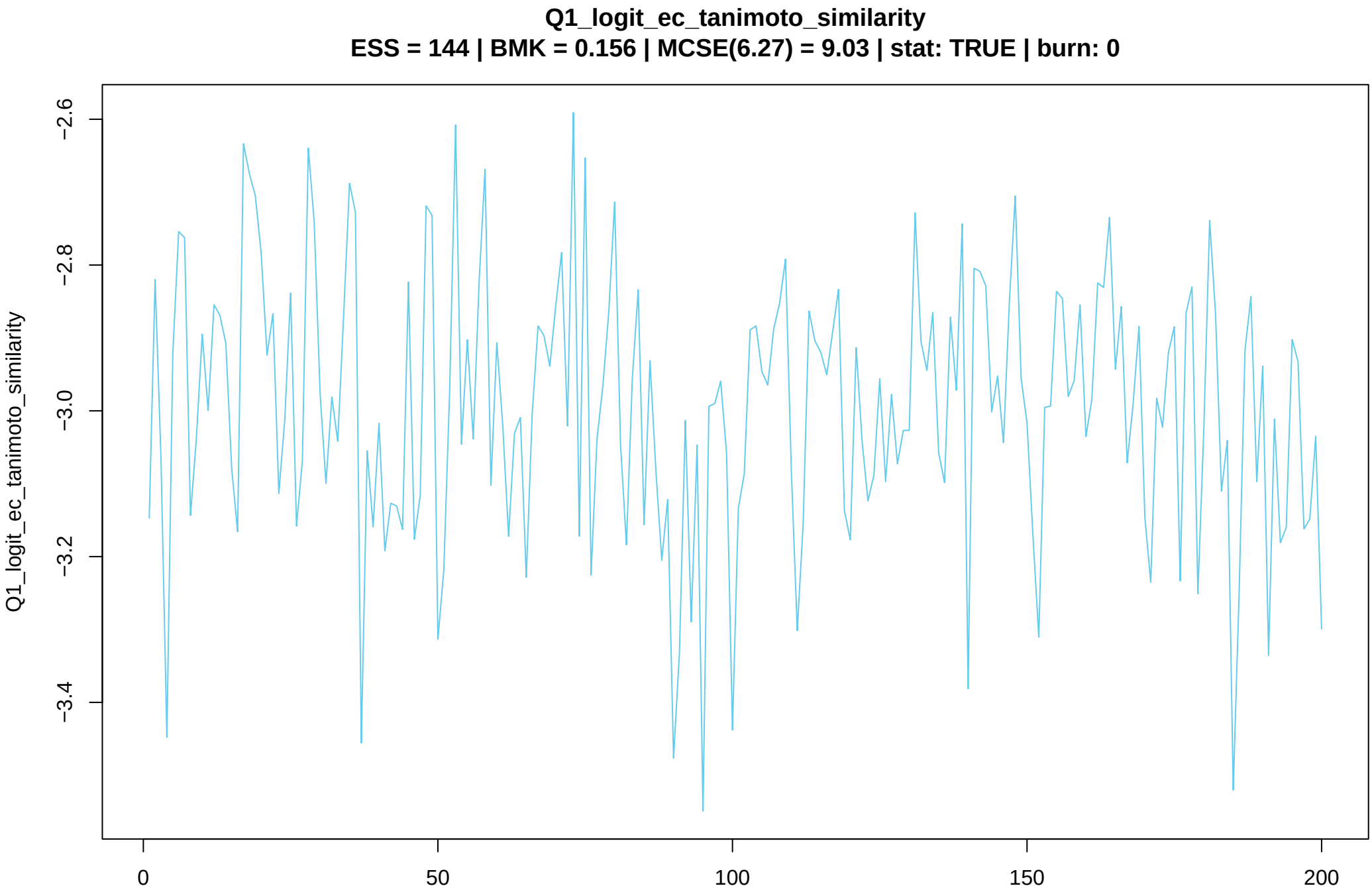

IQR_mcs_RingCount
ESS = 200 | BMK = 0.0604 | MCSE(6.27) = 8.09 | stat: TRUE | burn: 0
IQR_mcs_RingCount
0
1
2
3
4
0
50
100
150
200

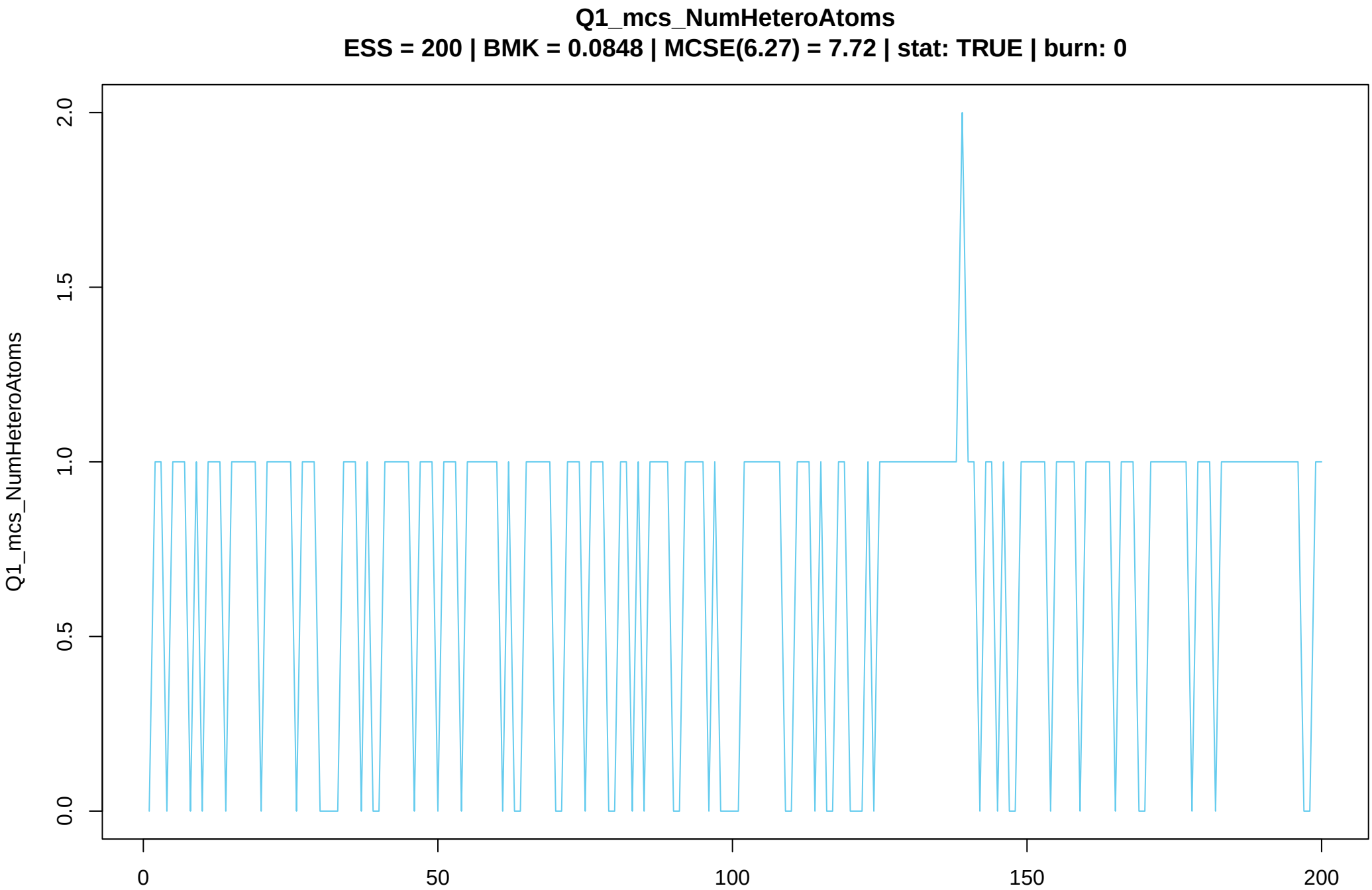

IQR_docked_NumRotatableBonds
ESS = 142 | BMK = 0.116 | MCSE(6.27) = 10.2 | stat: TRUE | burn: 0
IQR_docked_NumRotatableBonds
2
3
4
5
6
7
0
50
100
150
200

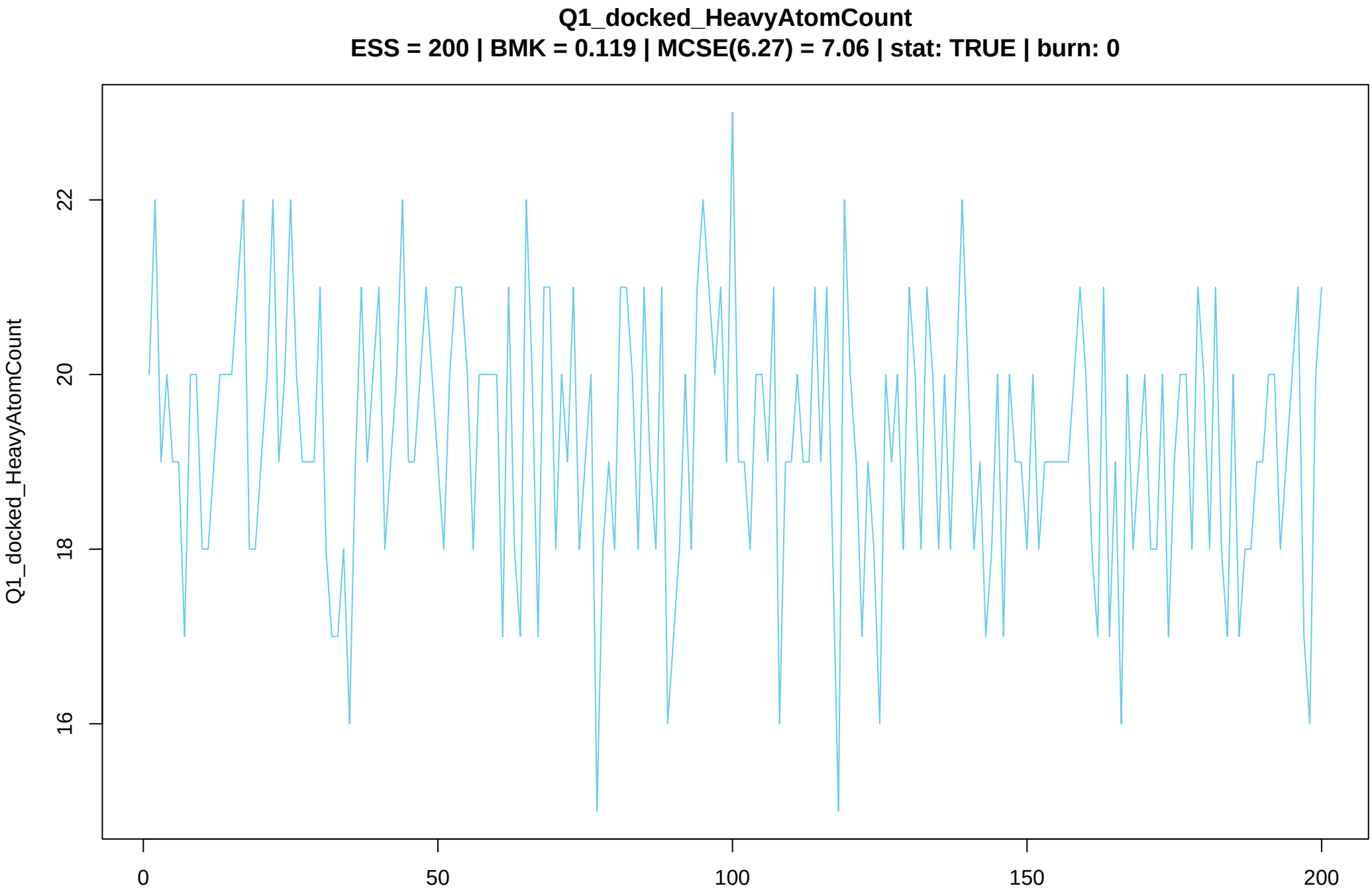

IQR_mcs_NOCount
ESS = 127 | BMK = 0.0157 | MCSE(6.27) = 10.5 | stat: TRUE | burn: 0
IQR_mcs_NOCount
1.0
1.5
2.0
2.5
3.0
0
50
100
150
200

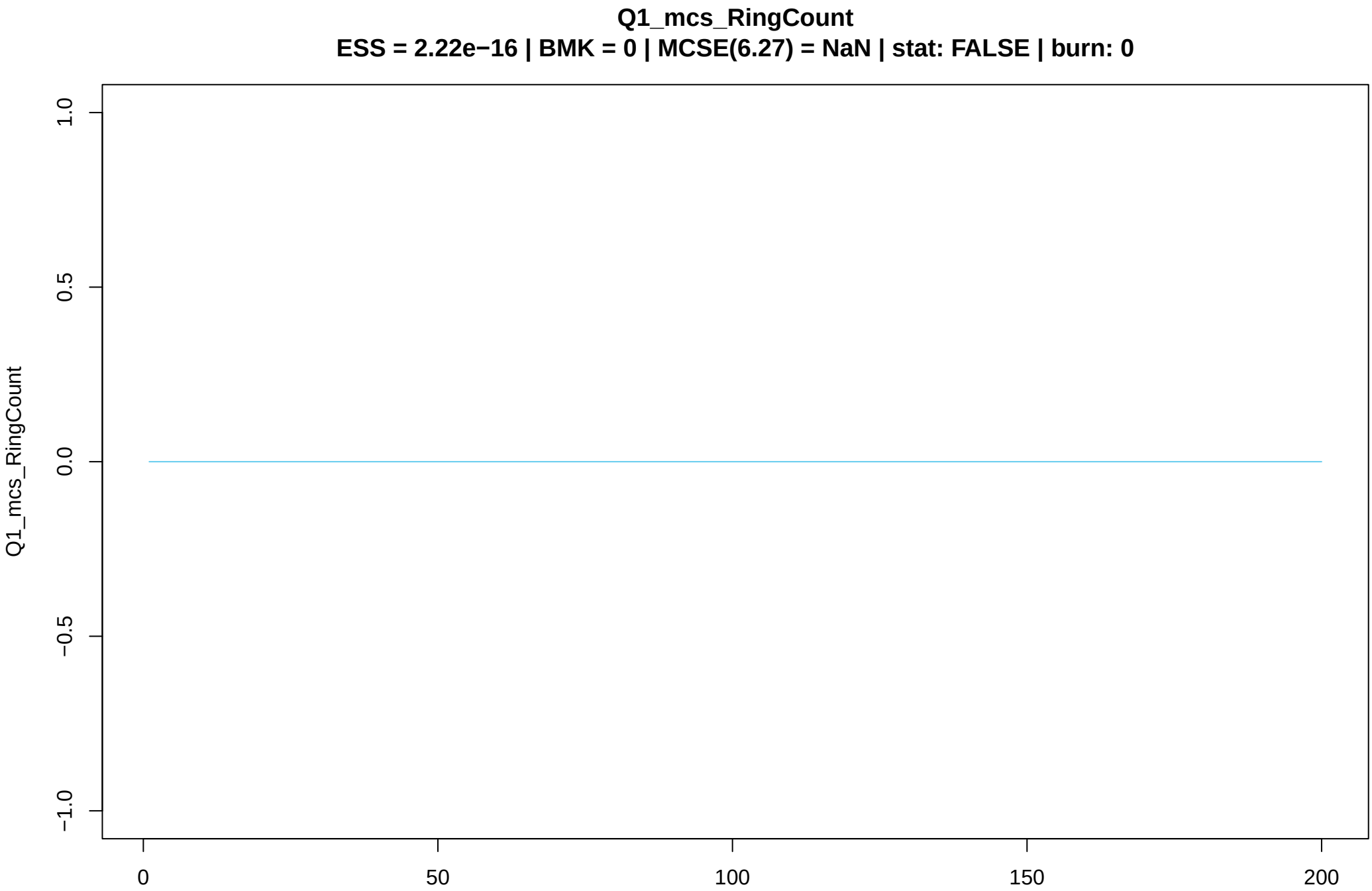

Q1_log_RMSD
ESS = 13 | BMK = 0.156 | MCSE(6.27) = 16.1 | stat: TRUE | burn: 60
Q1_log_RMSD
0.5
1.0
1.5
0
50
100
150
200

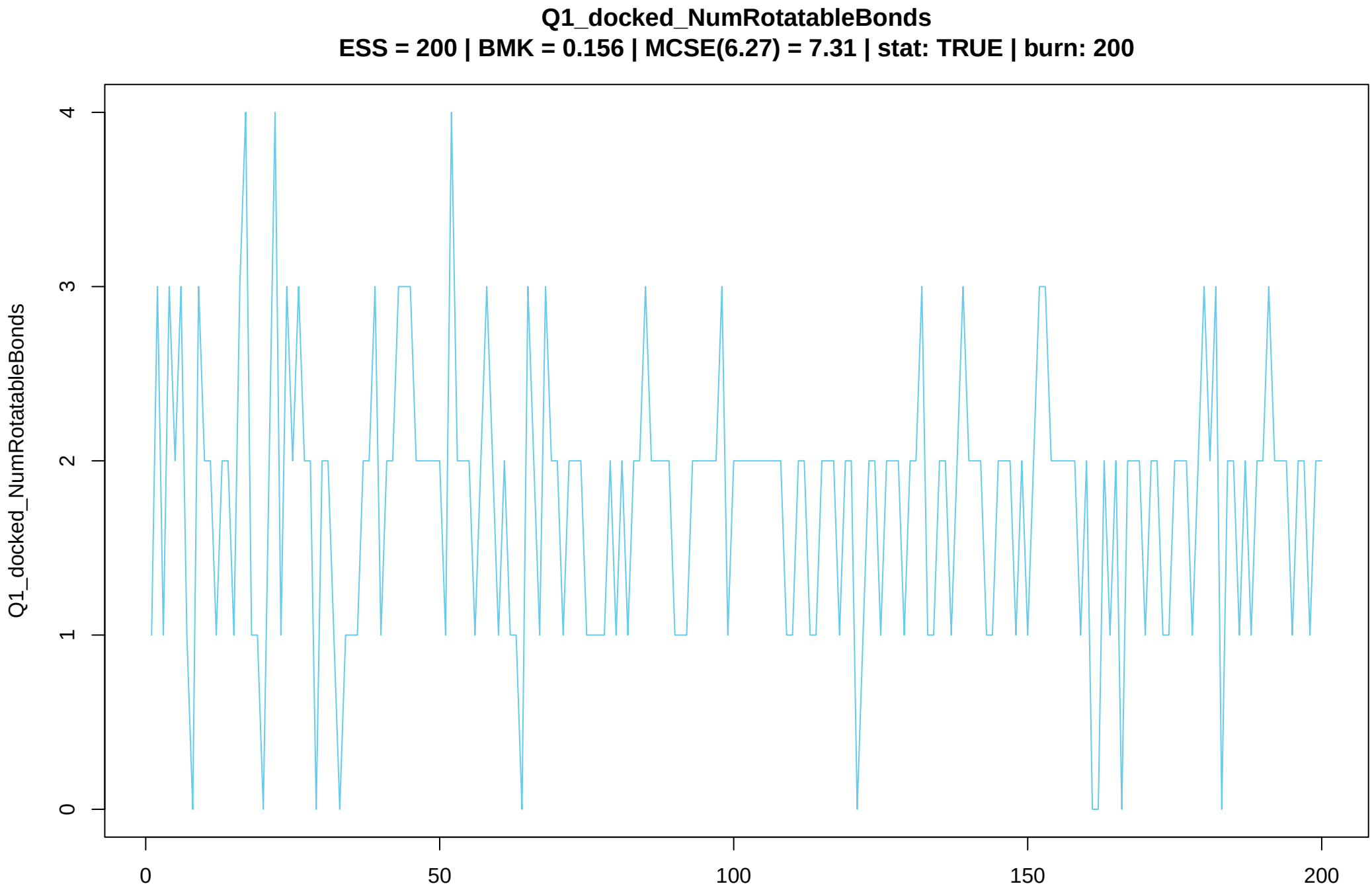

Q1_log_mcs_unbonded_polar_sasa
ESS = 113 | BMK = 0.135 | MCSE(6.27) = 11.1 | stat: TRUE | burn: 0
Q1_log_mcs_unbonded_polar_sasa
−0.2
−0.4
−0.6
−0.8
0
50
100
150
200

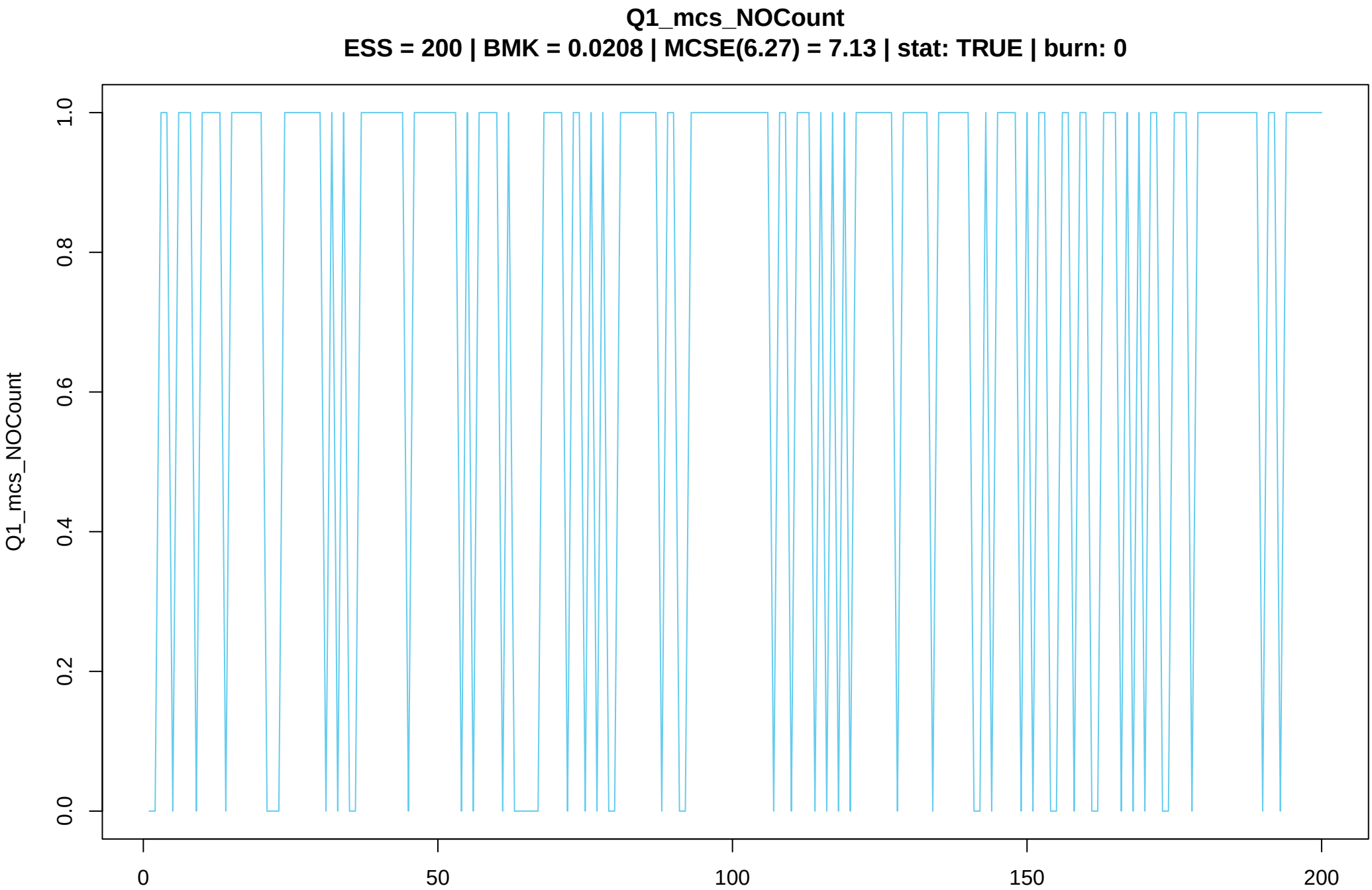

Q1_logit_ec_tanimoto_similarity
ESS = 144 | BMK = 0.156 | MCSE(6.27) = 9.03 | stat: TRUE | burn: 0
Q1_logit_ec_tanimoto_similarity
−2.6
−2.8
−3.0
−3.2
−3.4
0
50
100
150
200

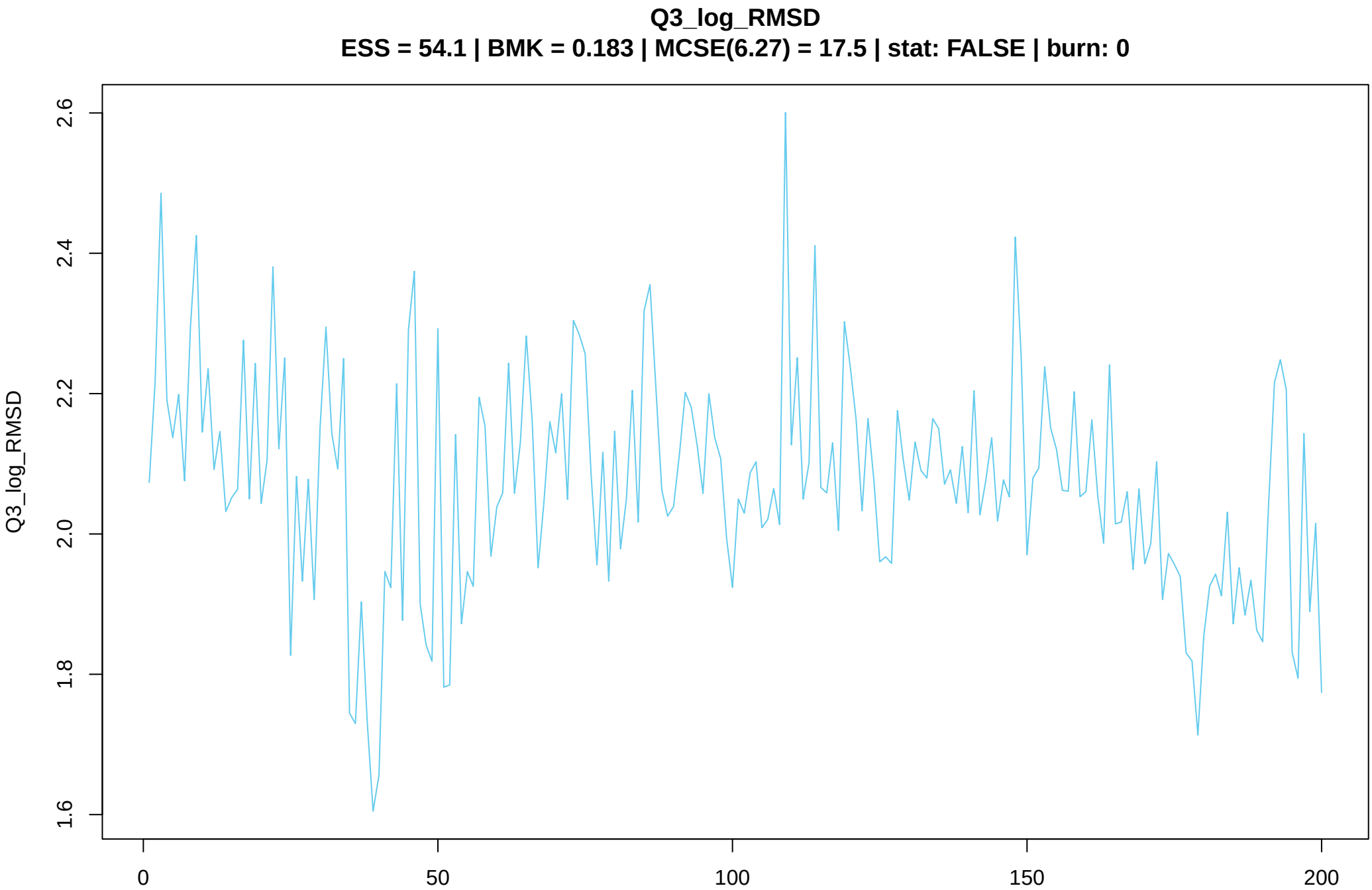

Q1_mcs_NumHeteroAtoms
ESS = 200 | BMK = 0.0848 | MCSE(6.27) = 7.72 | stat: TRUE | burn: 0
Q1_mcs_NumHeteroAtoms
0.0
0.5
1.0
1.5
2.0
0
50
100
150
200

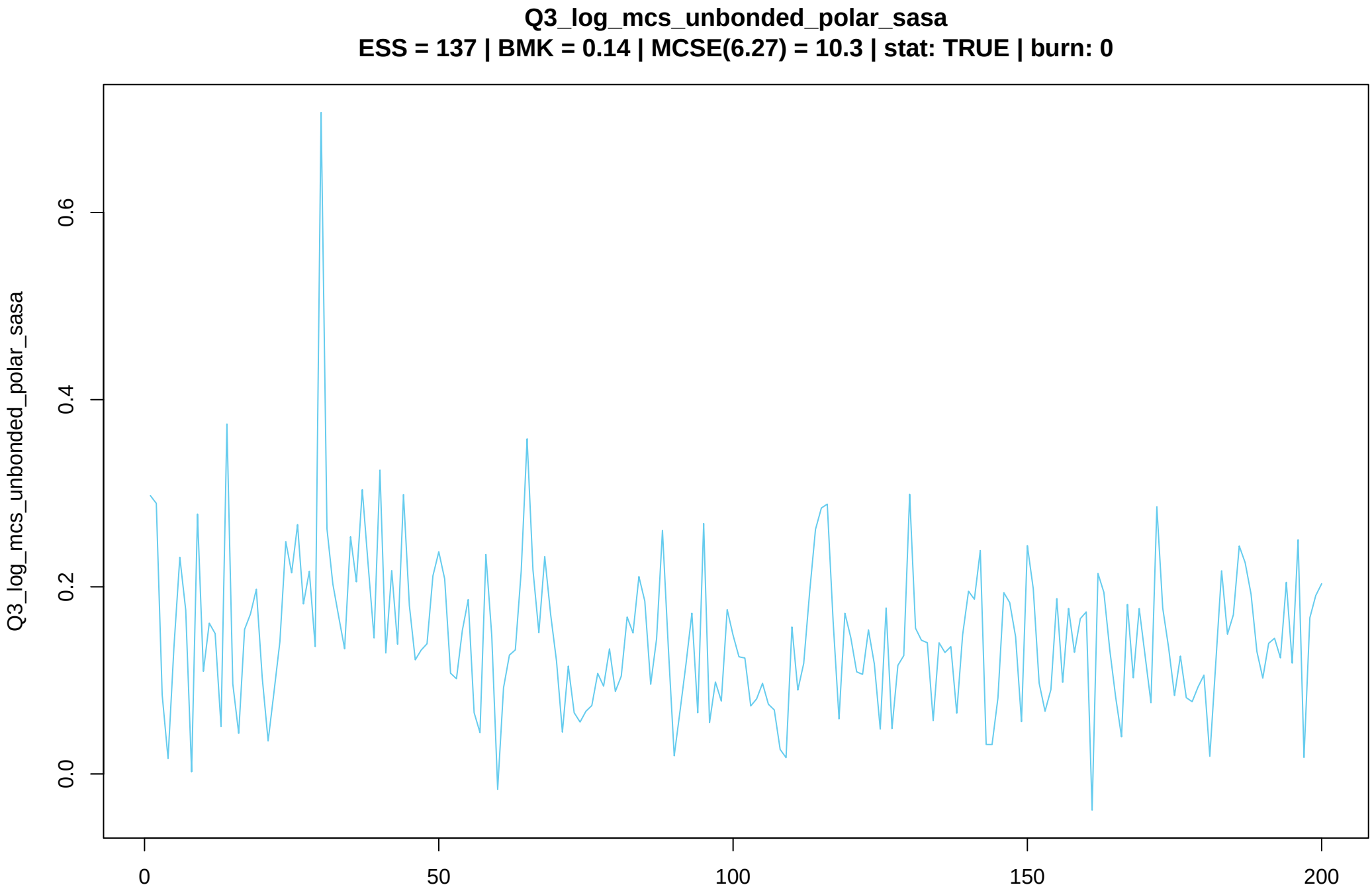

Q1_docked_HeavyAtomCount
ESS = 200 | BMK = 0.119 | MCSE(6.27) = 7.06 | stat: TRUE | burn: 0
Q1_docked_HeavyAtomCount
16
18
20
22
0
50
100
150
200

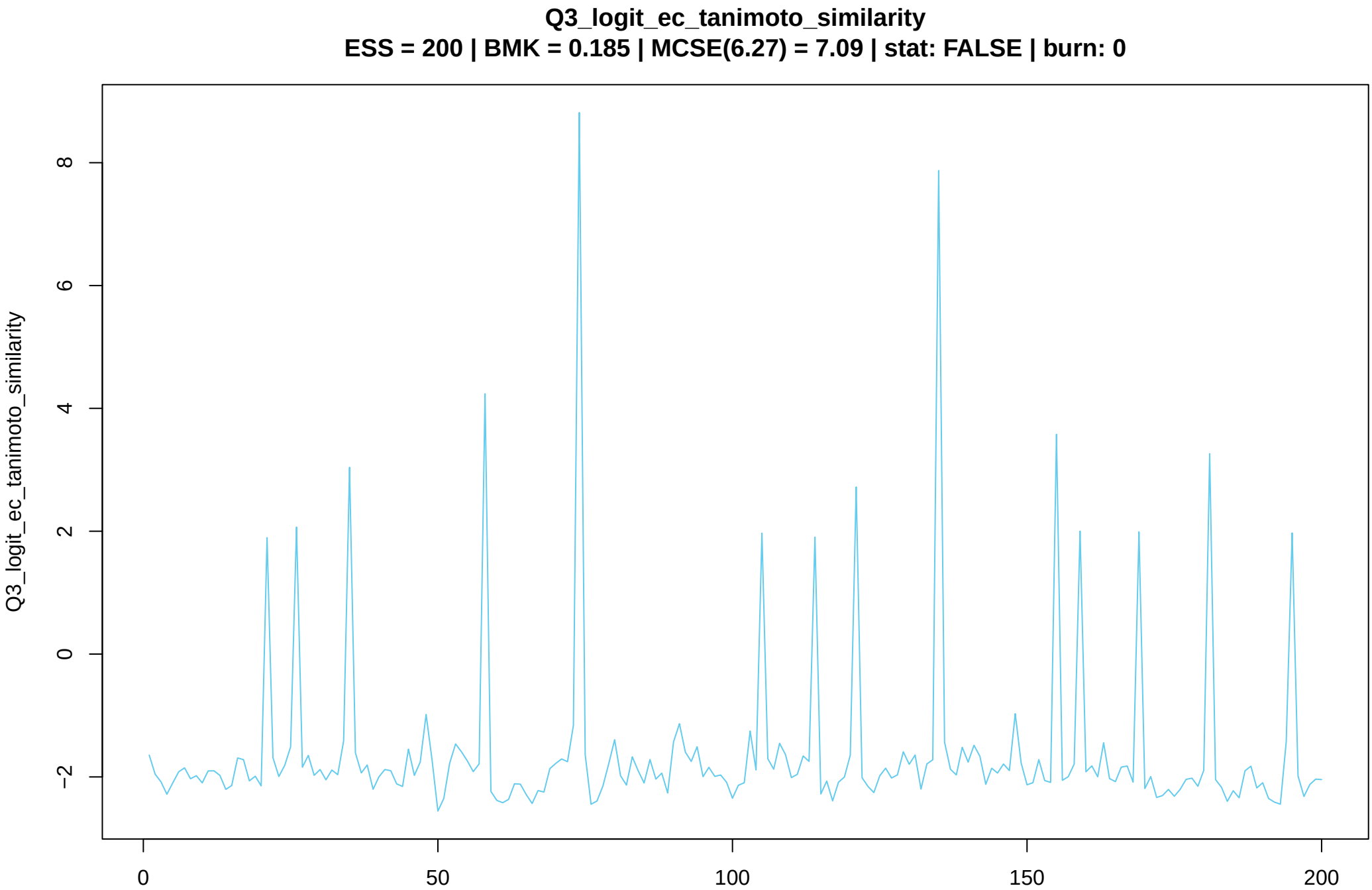

Q1_mcs_RingCount
ESS = 2.22e−16 | BMK = 0 | MCSE(6.27) = NaN | stat: FALSE | burn: 0
Q1_mcs_RingCount
1.0
0.5
0.0
−0.5
−1.0
0
50
100
150
200

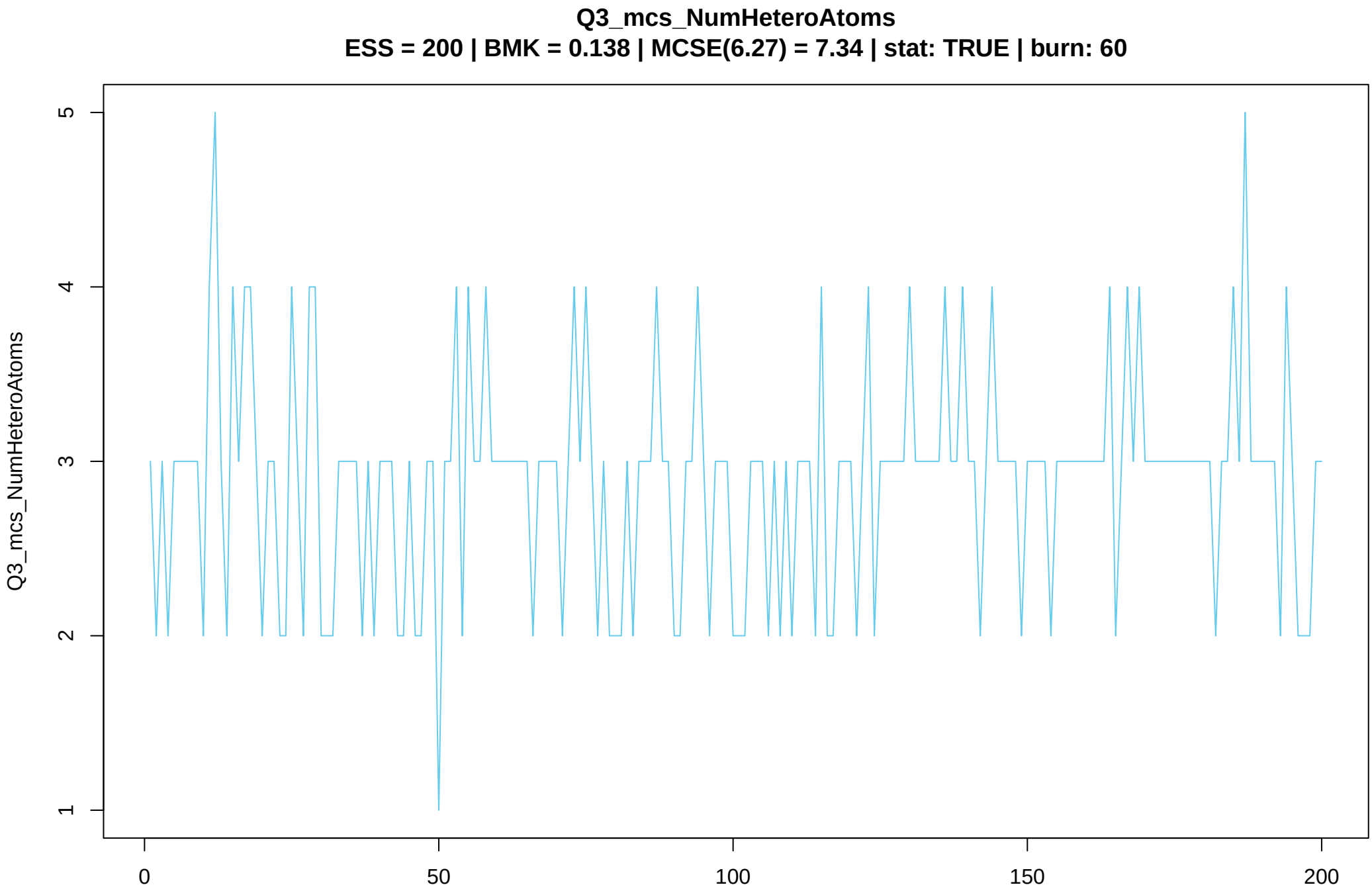

Q1_docked_NumRotatableBonds
ESS = 200 | BMK = 0.156 | MCSE(6.27) = 7.31 | stat: TRUE | burn: 200
Q1_docked_NumRotatableBonds
0
1
2
3
4
0
50
100
150
200

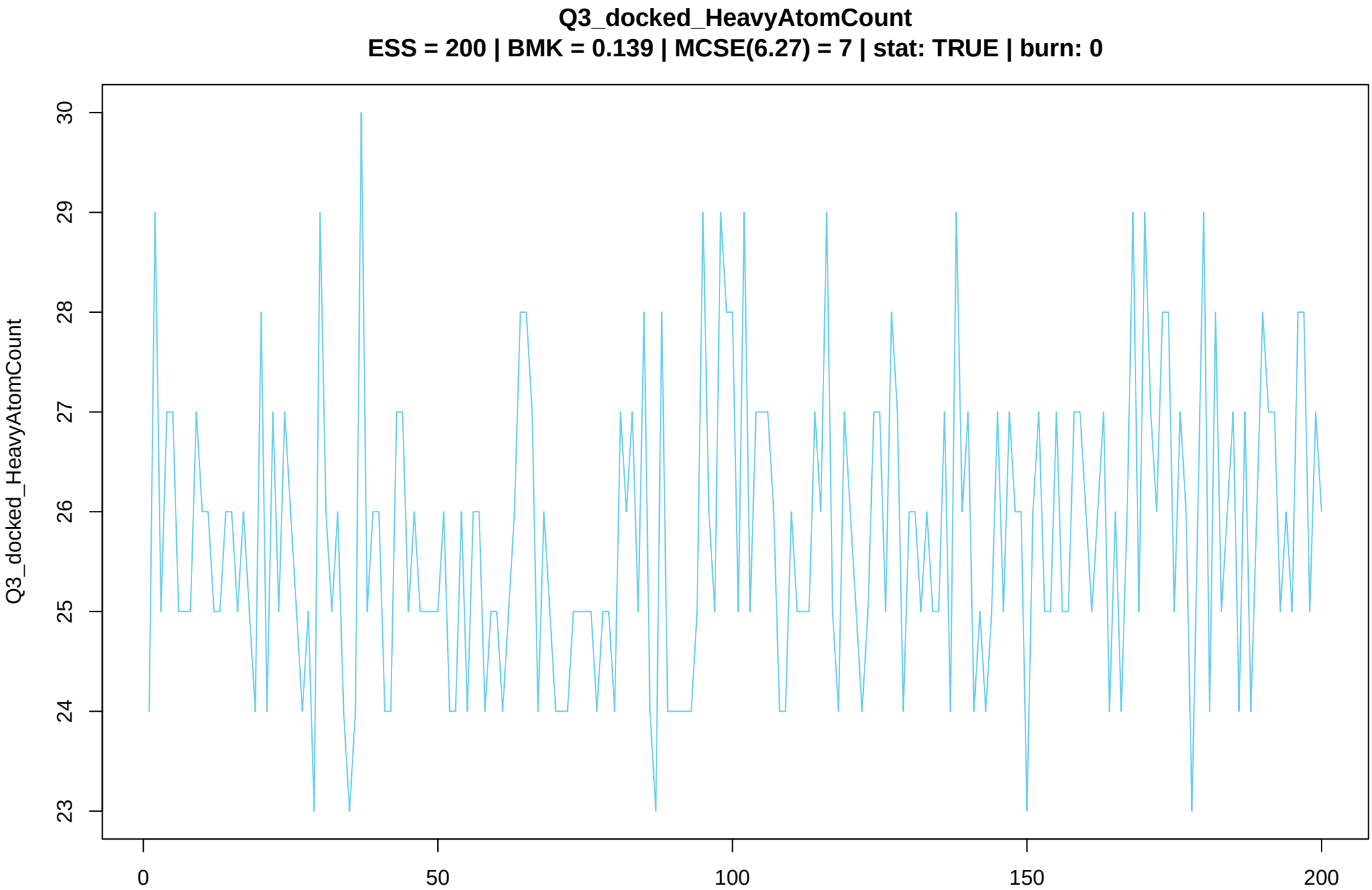

Q1_mcs_NOCount
ESS = 200 | BMK = 0.0208 | MCSE(6.27) = 7.13 | stat: TRUE | burn: 0
Q1_mcs_NOCount
0.0
0.2
0.4
0.6
0.8
1.0
0
50
100
150
200

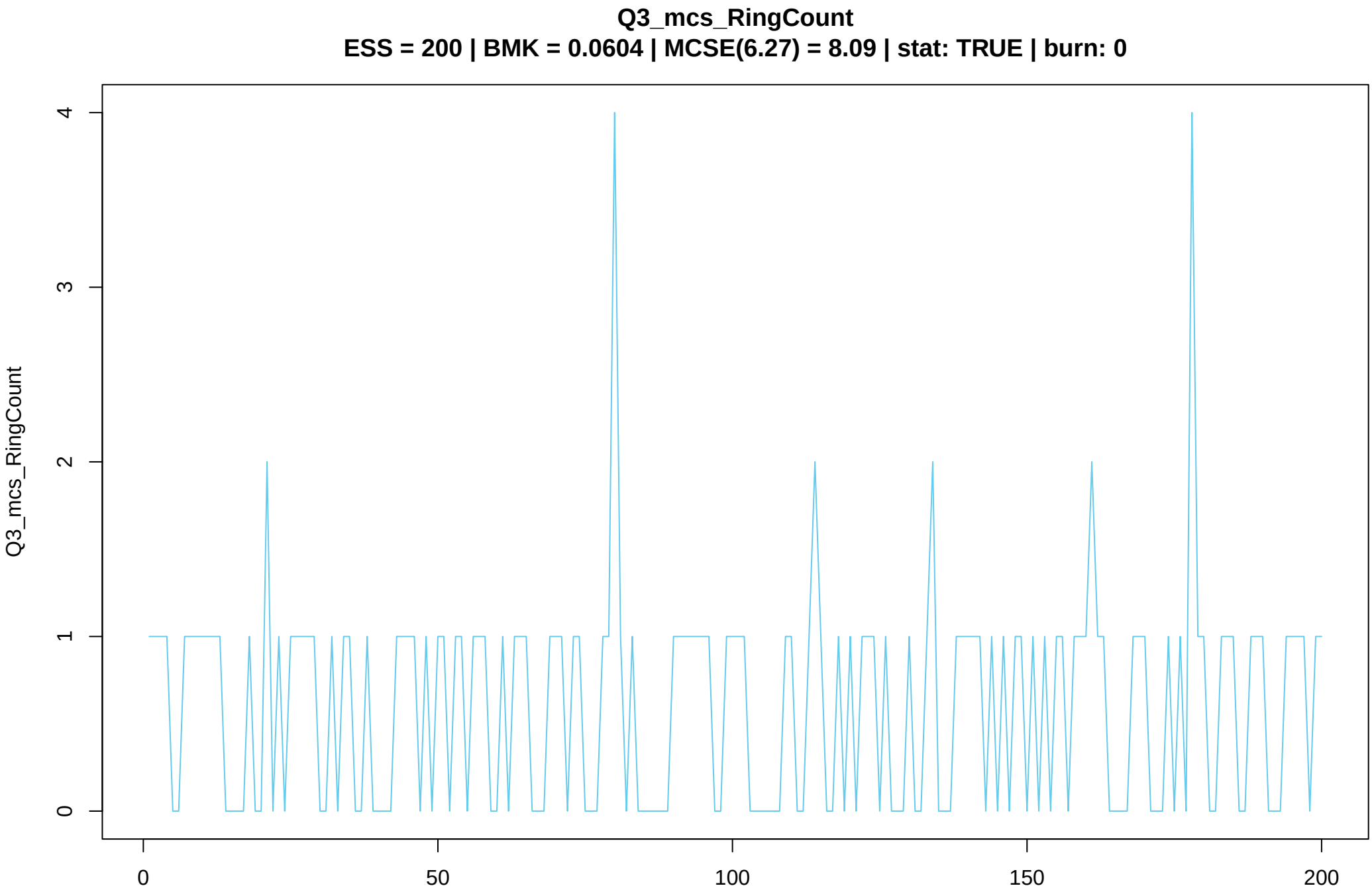

Q3_log_RMSD
ESS = 54.1 | BMK = 0.183 | MCSE(6.27) = 17.5 | stat: FALSE | burn: 0
Q3_log_RMSD
1.6
1.8
2.0
2.2
2.4
2.6
0
50
100
150
200

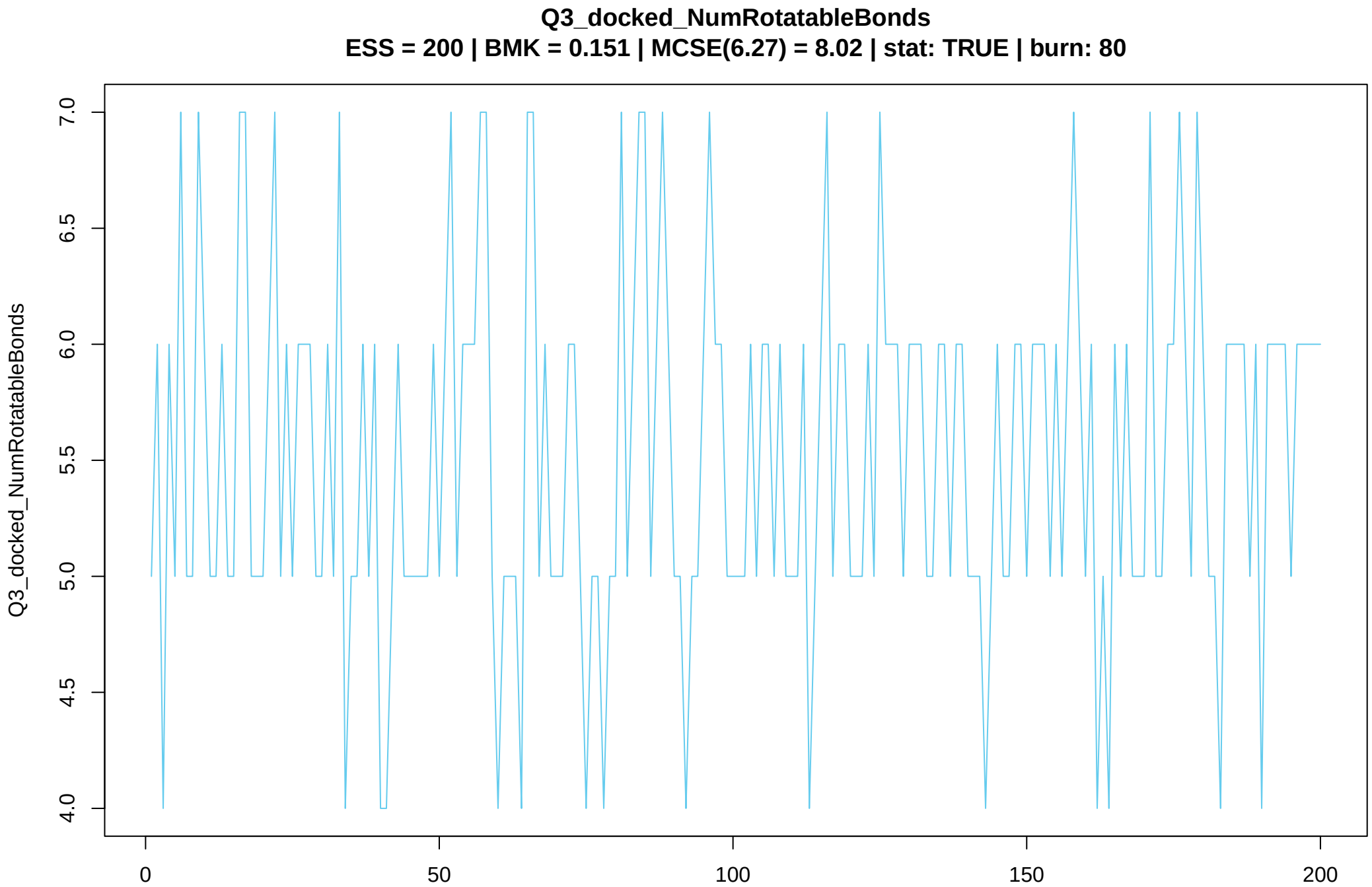

Q3_log_mcs_unbonded_polar_sasa
ESS = 137 | BMK = 0.14 | MCSE(6.27) = 10.3 | stat: TRUE | burn: 0
Q3_log_mcs_unbonded_polar_sasa
0.0
0.2
0.4
0.6
0
50
100
150
200

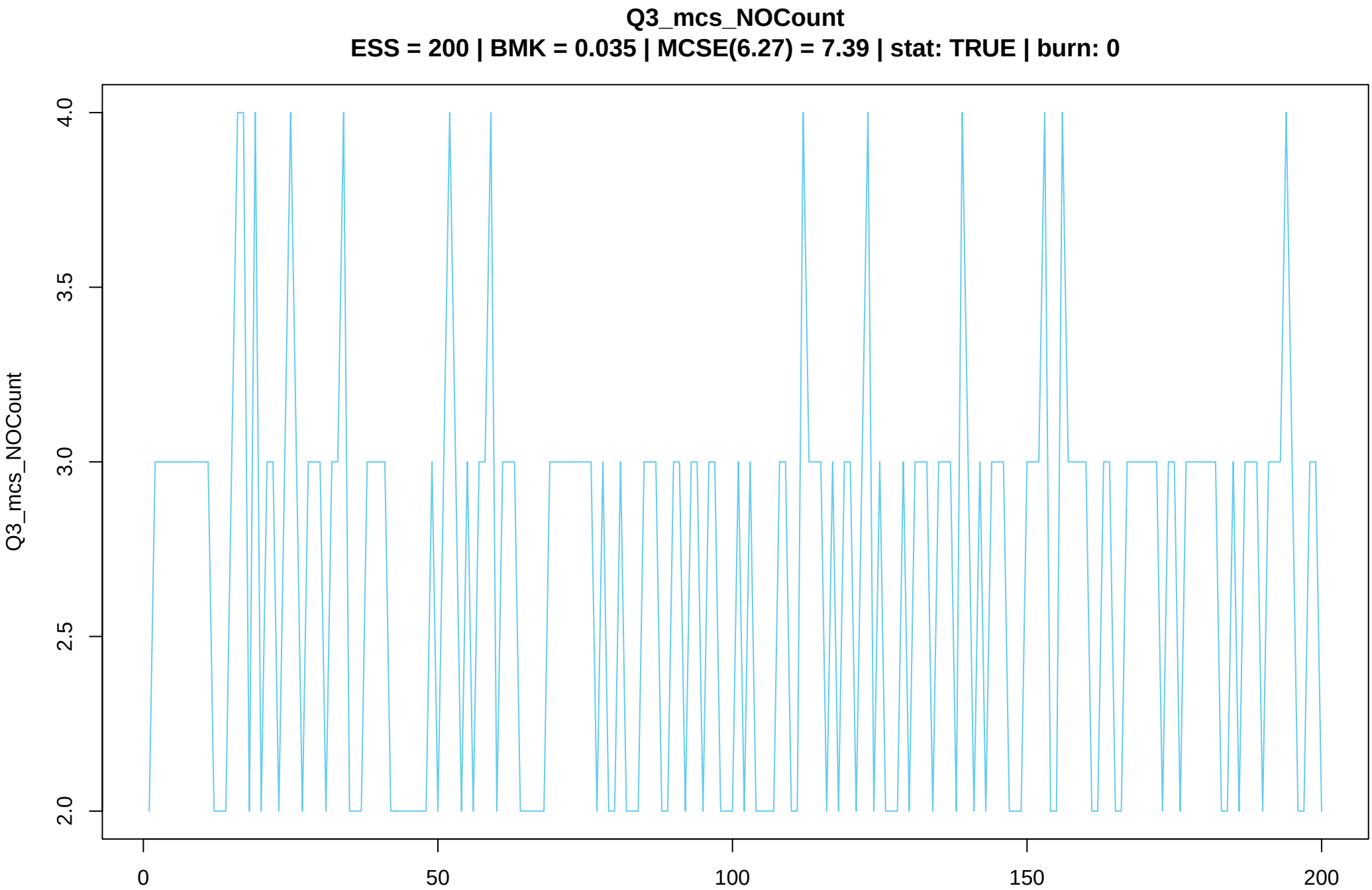

Q3_logit_ec_tanimoto_similarity
ESS = 200 | BMK = 0.185 | MCSE(6.27) = 7.09 | stat: FALSE | burn: 0
Q3_logit_ec_tanimoto_similarity
8
6
4
2
0
−2
0
50
100
150
200

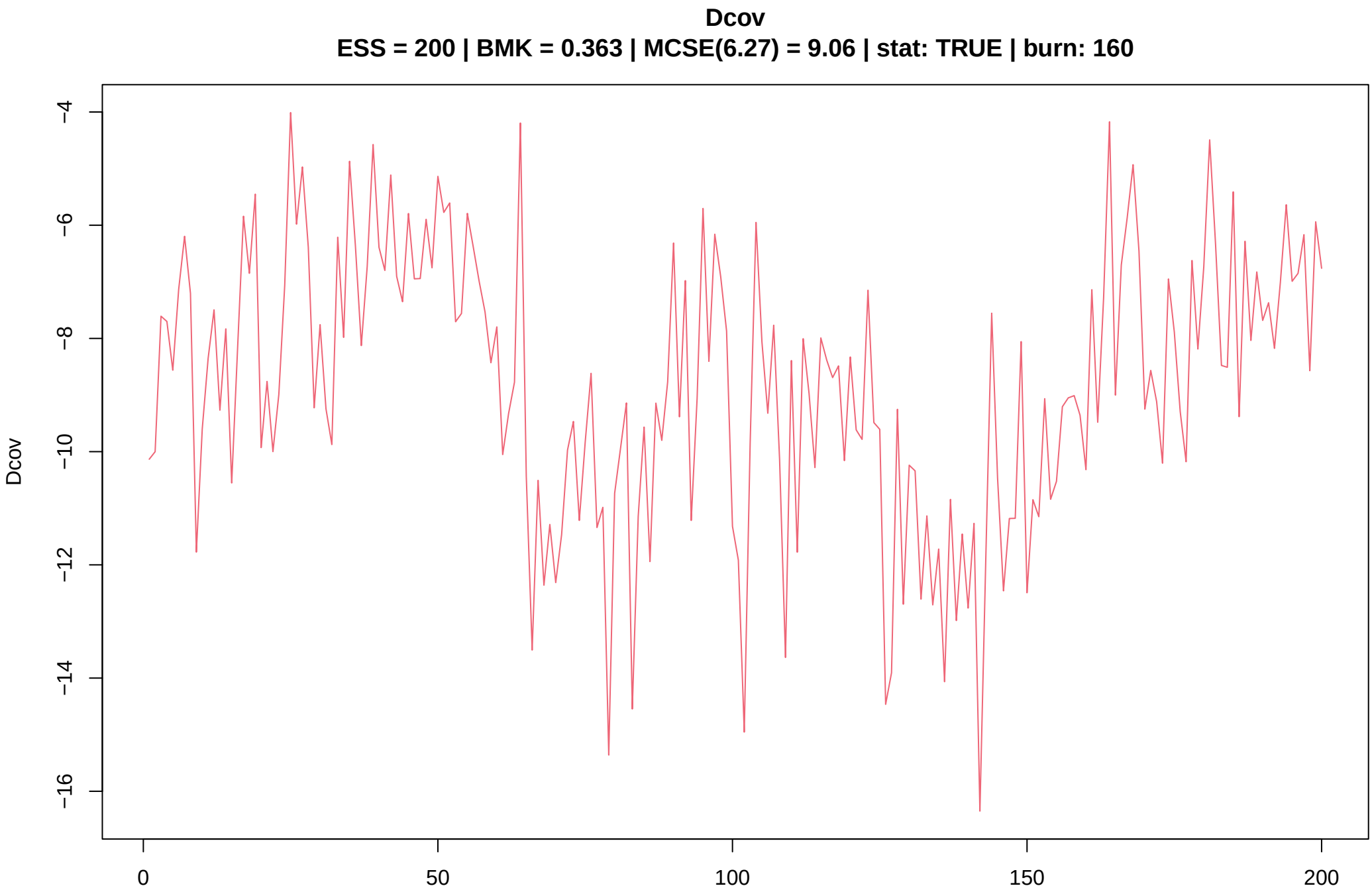

Q3_mcs_NumHeteroAtoms
ESS = 200 | BMK = 0.138 | MCSE(6.27) = 7.34 | stat: TRUE | burn: 60
Q3_mcs_NumHeteroAtoms
1
2
3
4
5
0
50
100
150
200

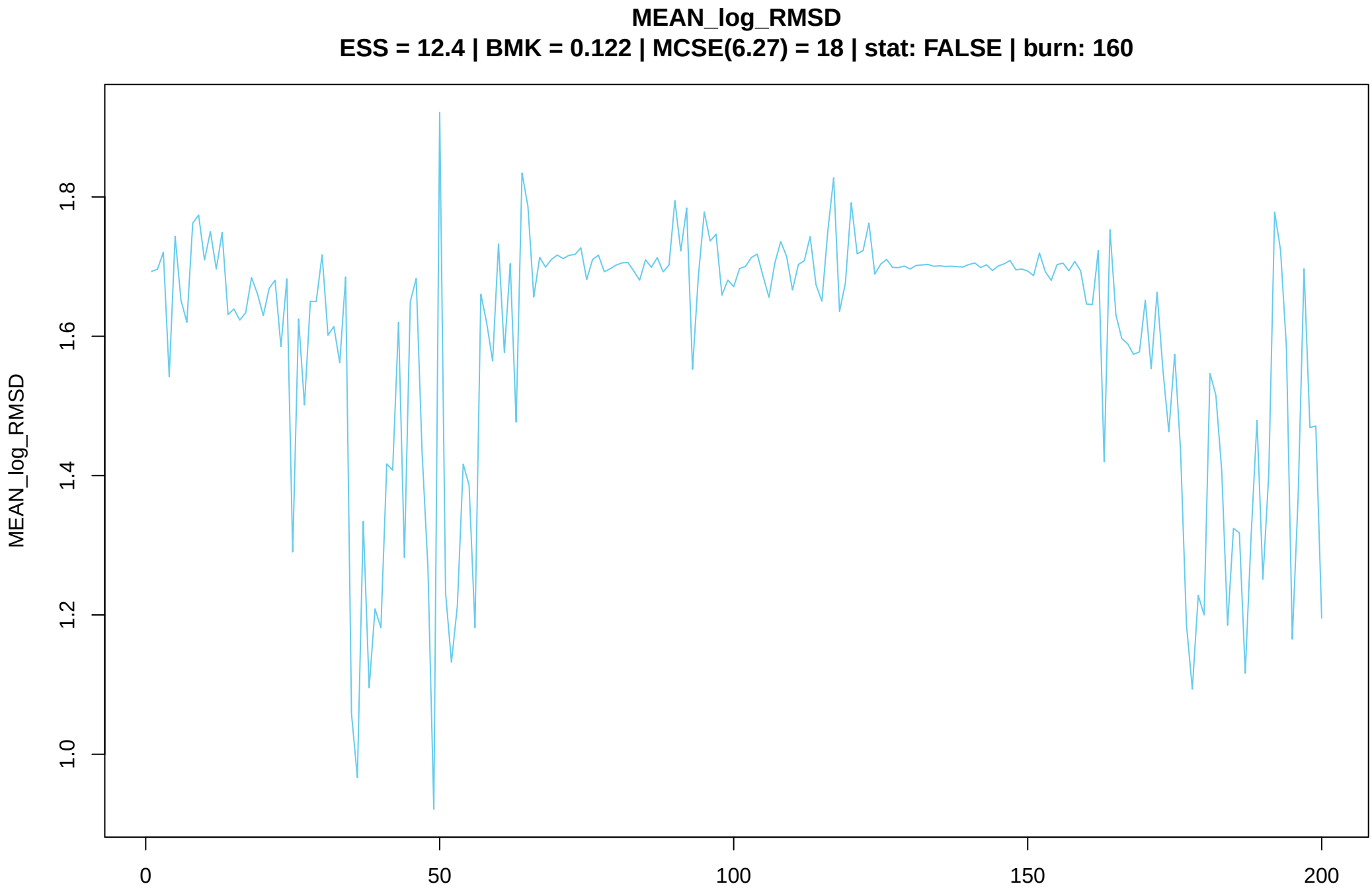

Q3_docked_HeavyAtomCount
ESS = 200 | BMK = 0.139 | MCSE(6.27) = 7 | stat: TRUE | burn: 0
Q3_docked_HeavyAtomCount
23
24
25
26
27
28
29
30
0
50
100
150
200

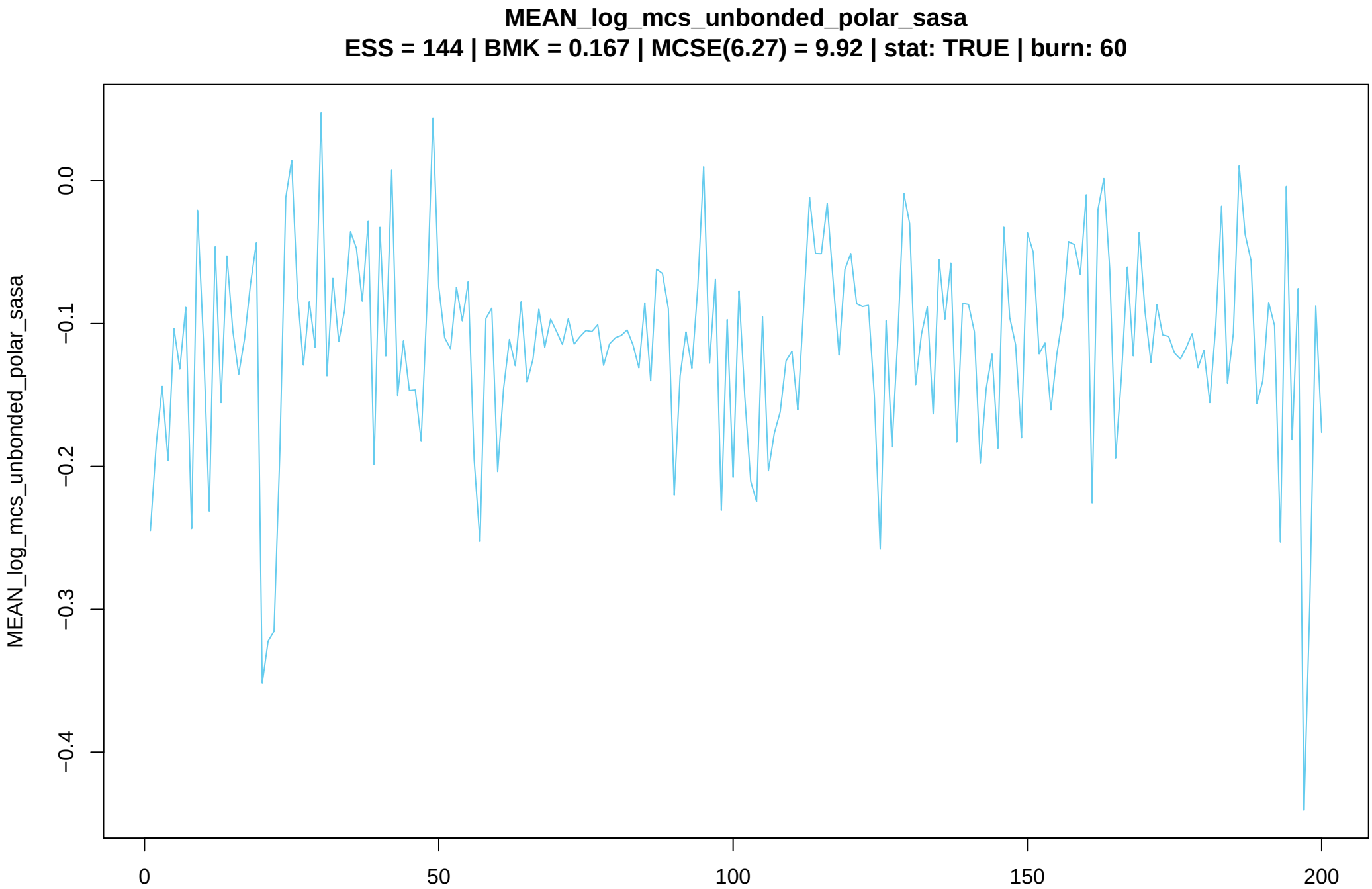

Q3_mcs_RingCount
ESS = 200 | BMK = 0.0604 | MCSE(6.27) = 8.09 | stat: TRUE | burn: 0
Q3_mcs_RingCount
0
1
2
3
4
0
50
100
150
200

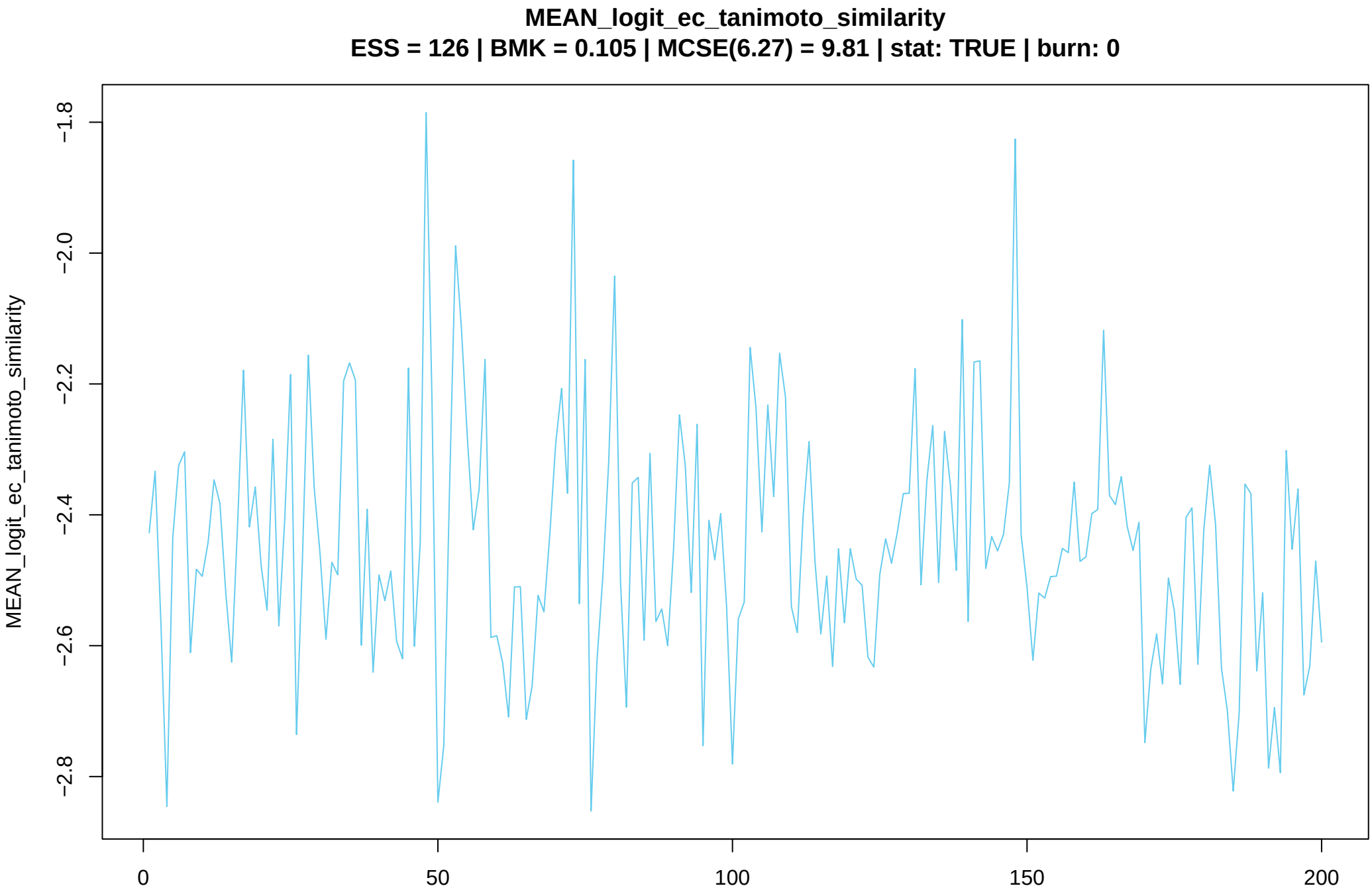

Q3_docked_NumRotatableBonds
ESS = 200 | BMK = 0.151 | MCSE(6.27) = 8.02 | stat: TRUE | burn: 80
Q3_docked_NumRotatableBonds
4.0
4.5
5.0
5.5
6.0
6.5
7.0
0
50
100
150
200

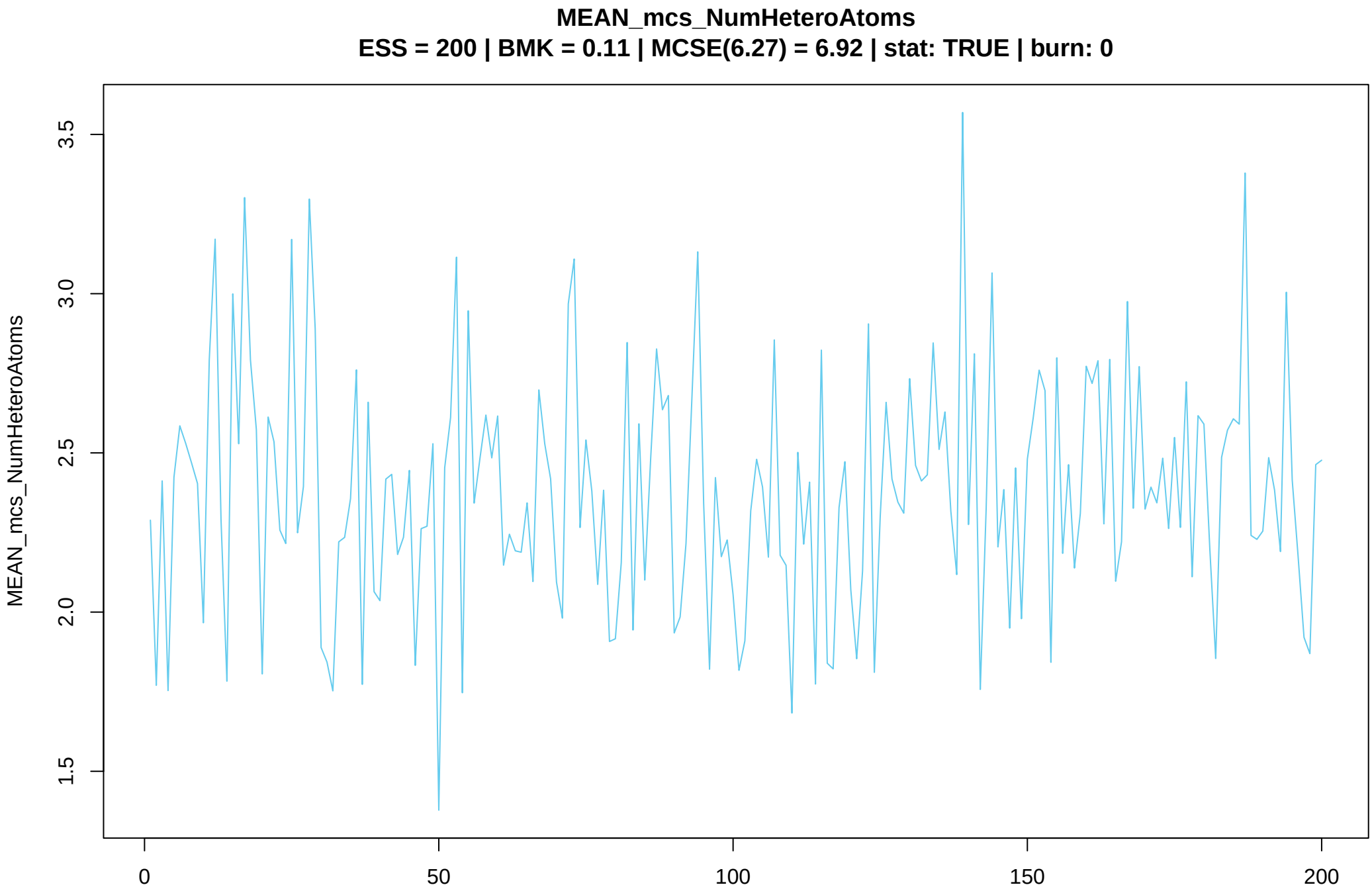

Q3_mcs_NOCount
ESS = 200 | BMK = 0.035 | MCSE(6.27) = 7.39 | stat: TRUE | burn: 0
Q3_mcs_NOCount
2.0
2.5
3.0
3.5
4.0
0
50
100
150
200

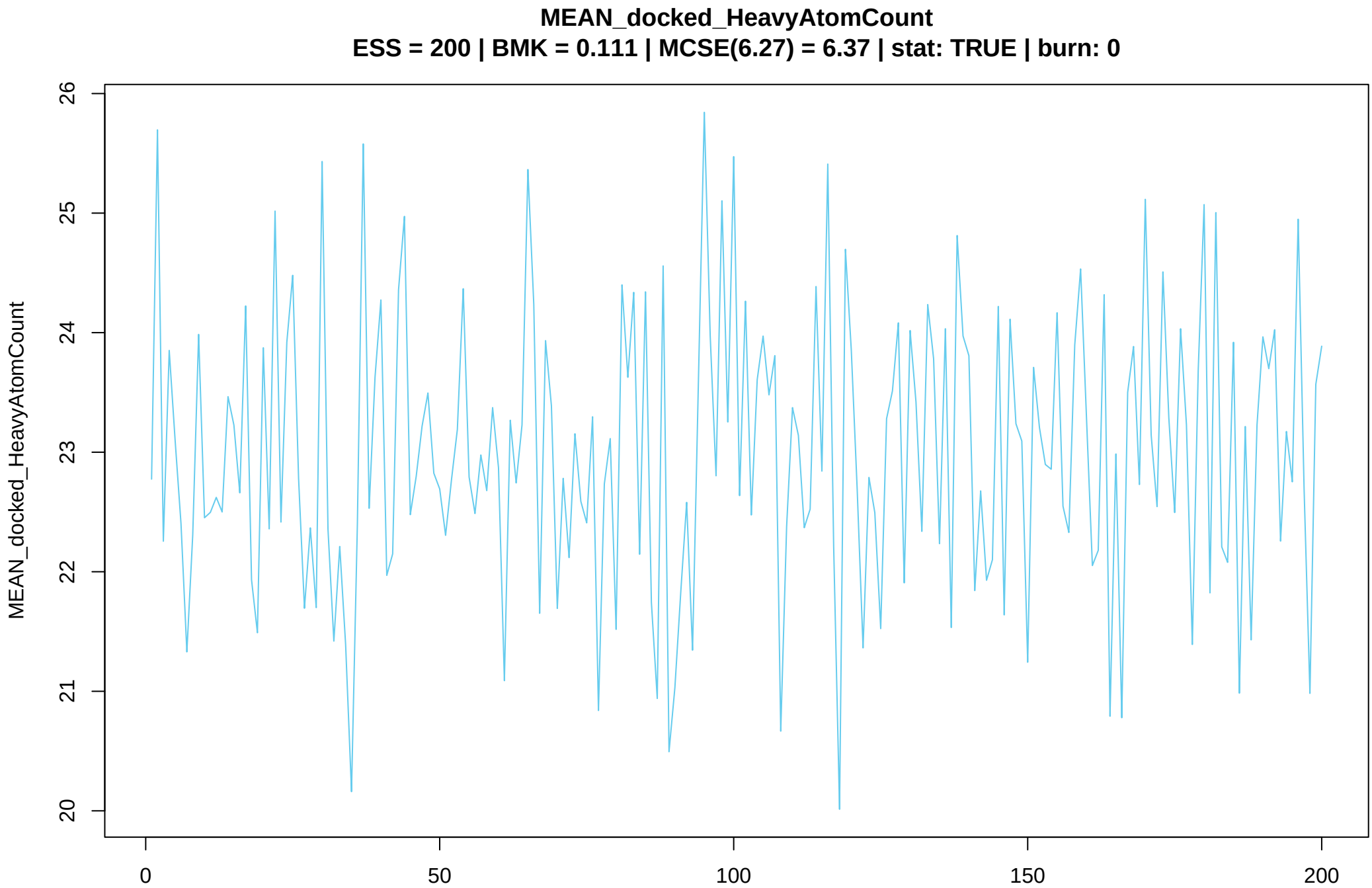

Dcov
ESS = 200 | BMK = 0.363 | MCSE(6.27) = 9.06 | stat: TRUE | burn: 160
Dcov
−4
−6
−8
−10
−12
−14
−16
0
50
100
150
200

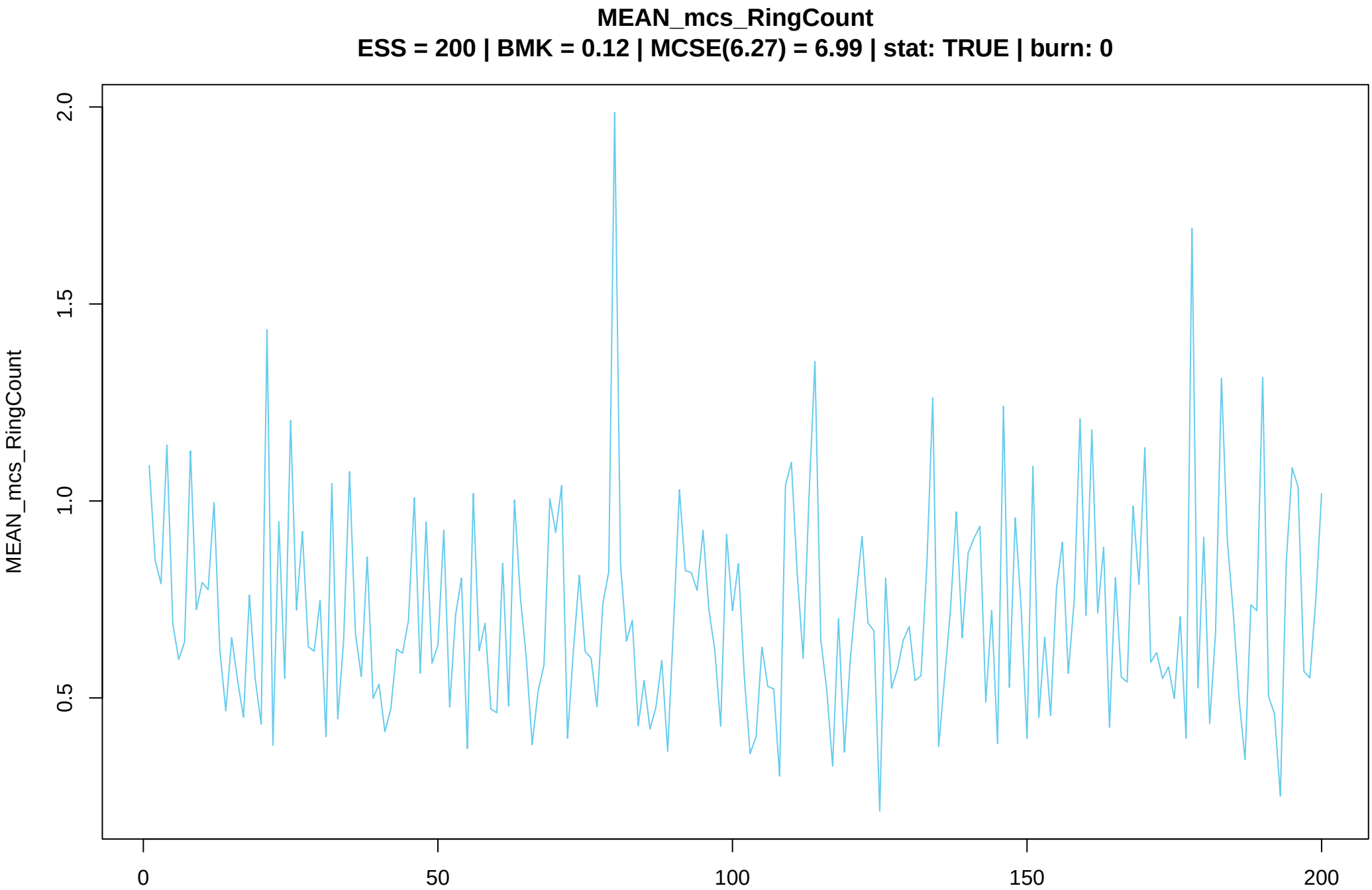

MEAN_log_RMSD
ESS = 12.4 | BMK = 0.122 | MCSE(6.27) = 18 | stat: FALSE | burn: 160
MEAN_log_RMSD
1.0
1.2
1.4
1.6
1.8
0
50
100
150
200

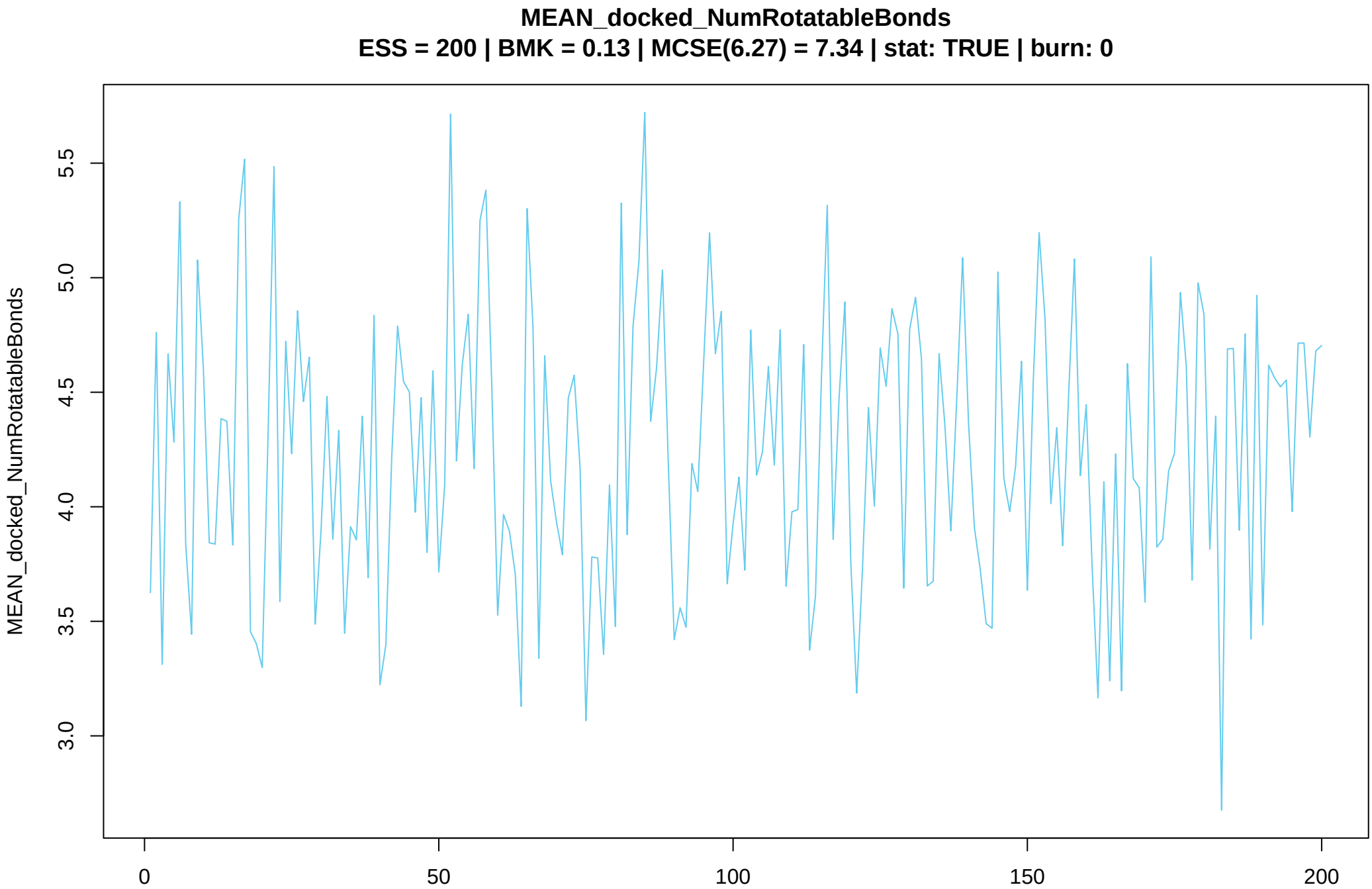

MEAN_log_mcs_unbonded_polar_sasa
ESS = 144 | BMK = 0.167 | MCSE(6.27) = 9.92 | stat: TRUE | burn: 60
MEAN_log_mcs_unbonded_polar_sasa
0.0
−0.1
−0.2
−0.3
−0.4
0
50
100
150
200

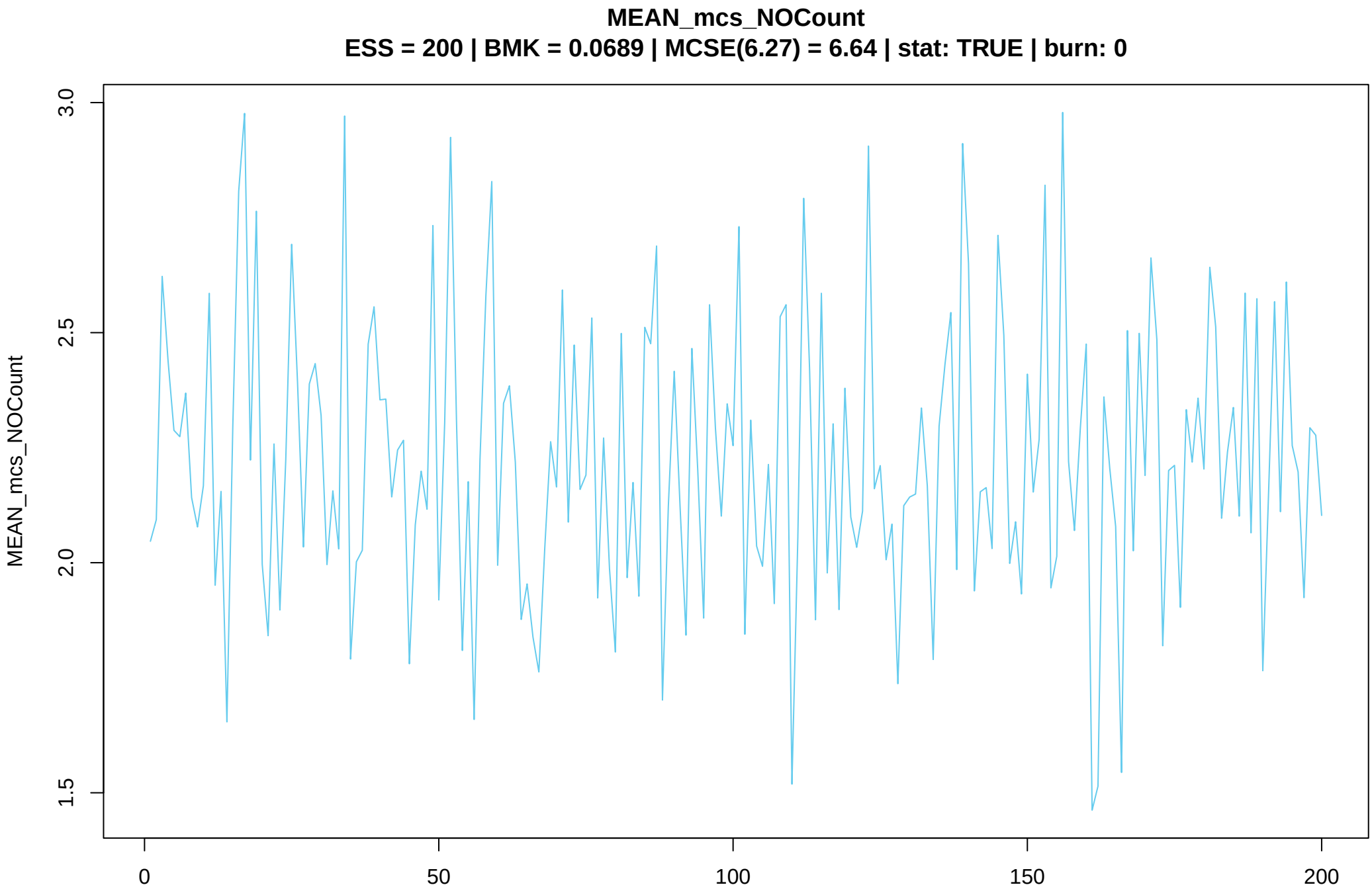

MEAN_logit_ec_tanimoto_similarity
ESS = 126 | BMK = 0.105 | MCSE(6.27) = 9.81 | stat: TRUE | burn: 0
MEAN_logit_ec_tanimoto_similarity
−1.8
−2.0
−2.2
−2.4
−2.6
−2.8
0
50
100
150
200

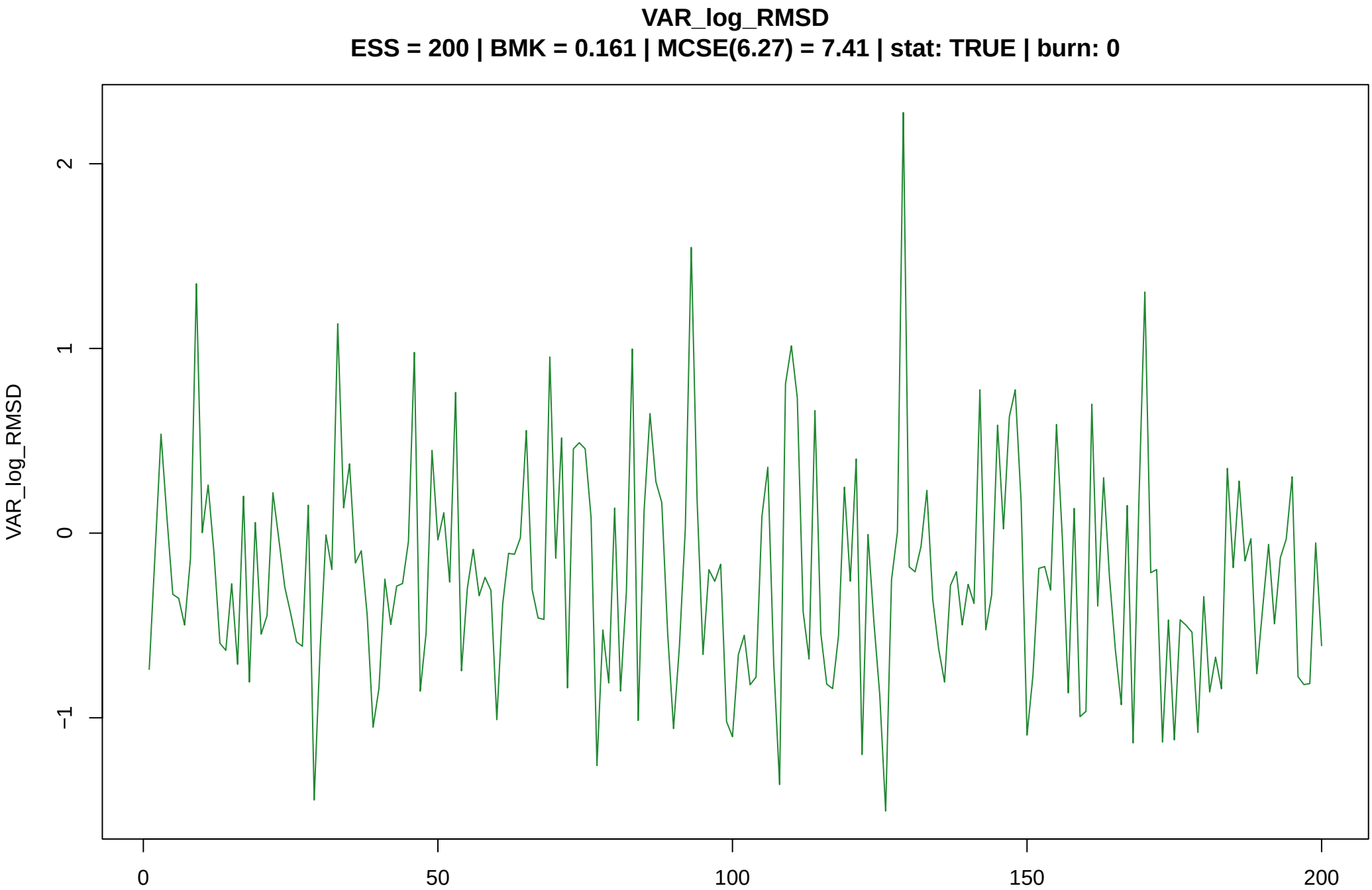

MEAN_mcs_NumHeteroAtoms
ESS = 200 | BMK = 0.11 | MCSE(6.27) = 6.92 | stat: TRUE | burn: 0
MEAN_mcs_NumHeteroAtoms
1.5
2.0
2.5
3.0
3.5
0
50
100
150
200

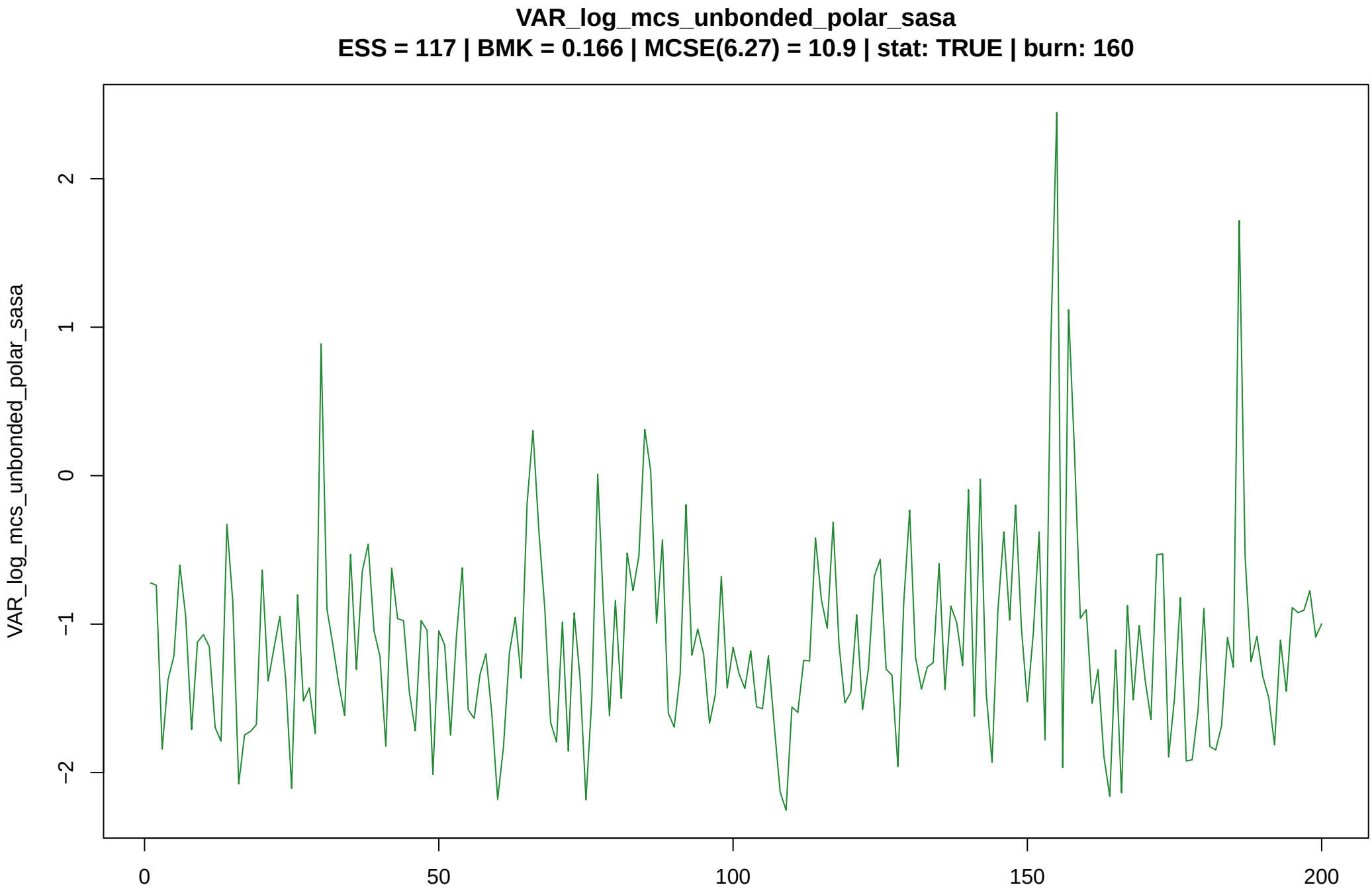

MEAN_docked_HeavyAtomCount
ESS = 200 | BMK = 0.111 | MCSE(6.27) = 6.37 | stat: TRUE | burn: 0
MEAN_docked_HeavyAtomCount
20
21
22
23
24
25
26
0
50
100
150
200

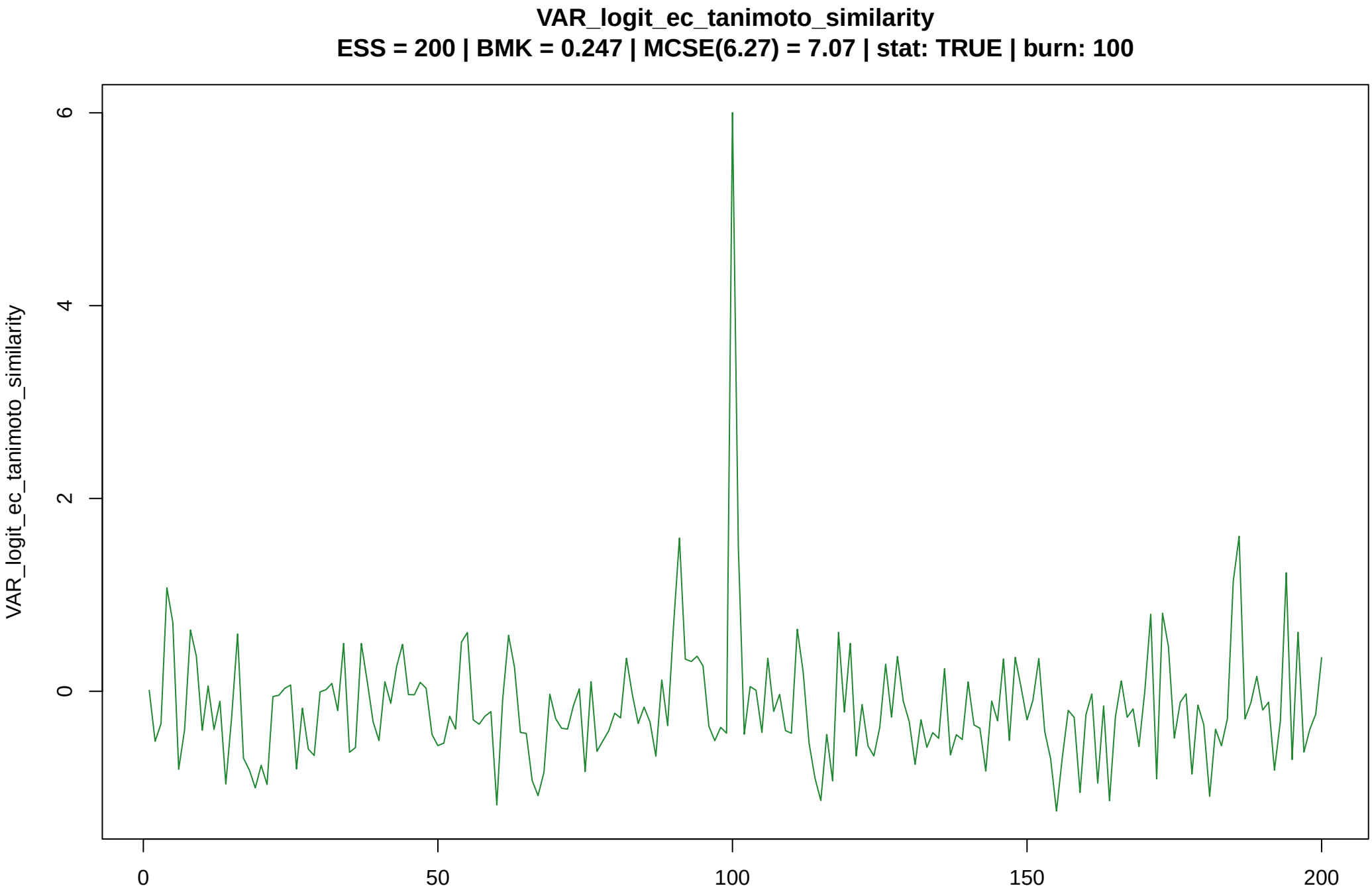

MEAN_mcs_RingCount
ESS = 200 | BMK = 0.12 | MCSE(6.27) = 6.99 | stat: TRUE | burn: 0
MEAN_mcs_RingCount
0.5
1.0
1.5
2.0
0
50
100
150
200

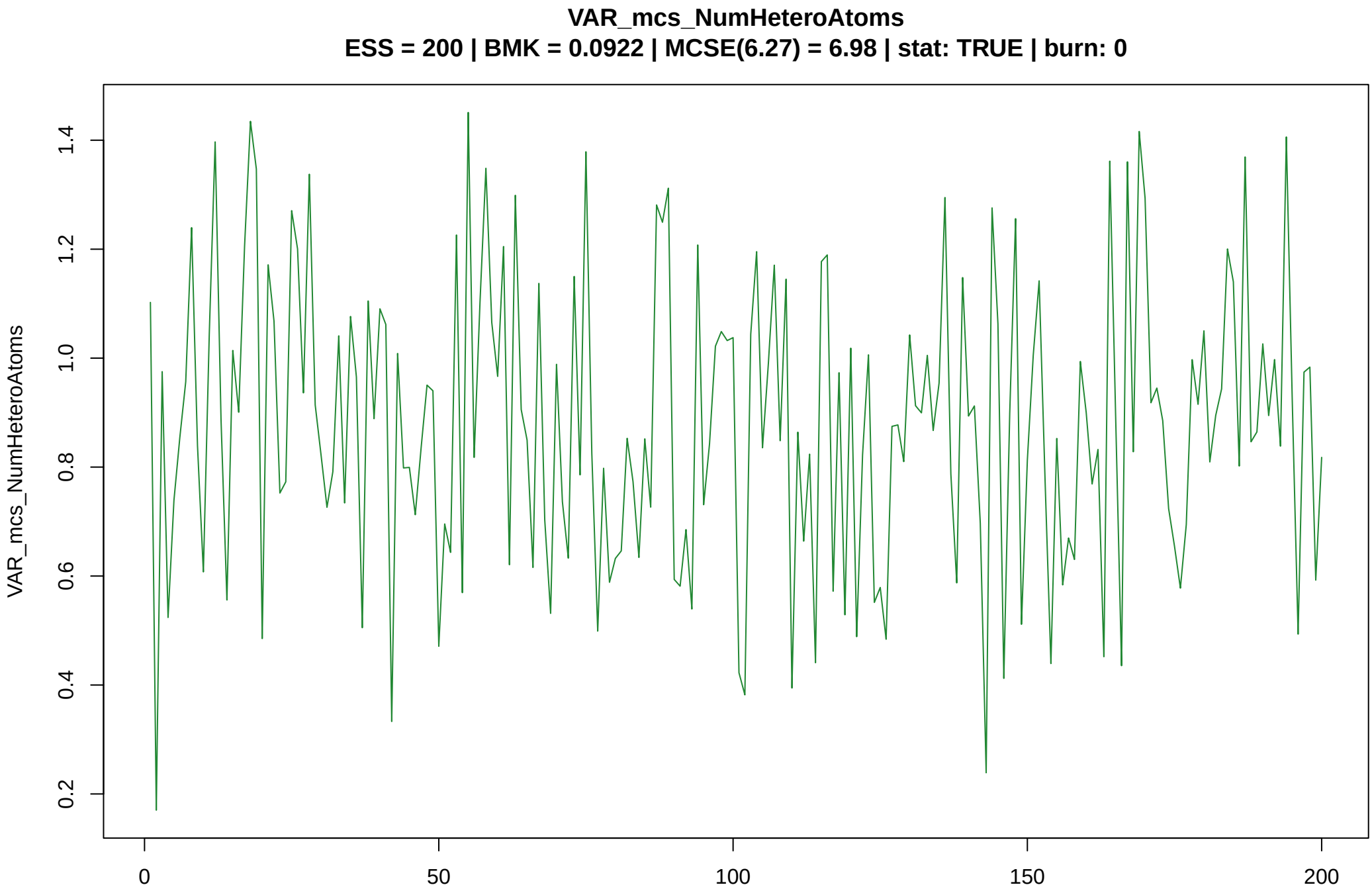

MEAN_docked_NumRotatableBonds
ESS = 200 | BMK = 0.13 | MCSE(6.27) = 7.34 | stat: TRUE | burn: 0
MEAN_docked_NumRotatableBonds
3.0
3.5
4.0
4.5
5.0
5.5
0
50
100
150
200

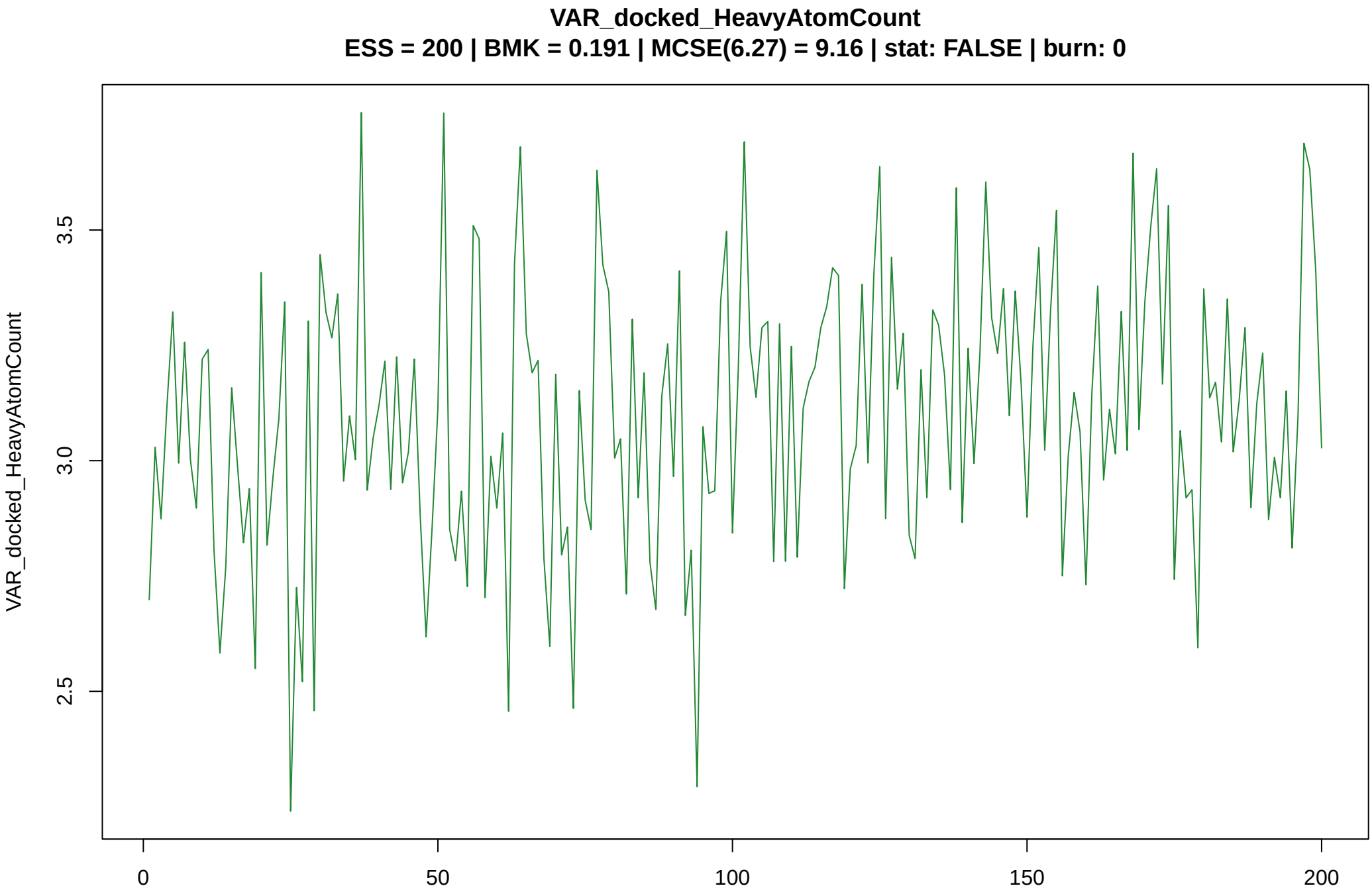

MEAN_mcs_NOCount
ESS = 200 | BMK = 0.0689 | MCSE(6.27) = 6.64 | stat: TRUE | burn: 0
MEAN_mcs_NOCount
3.0
2.5
2.0
1.5
0
50
100
150
200

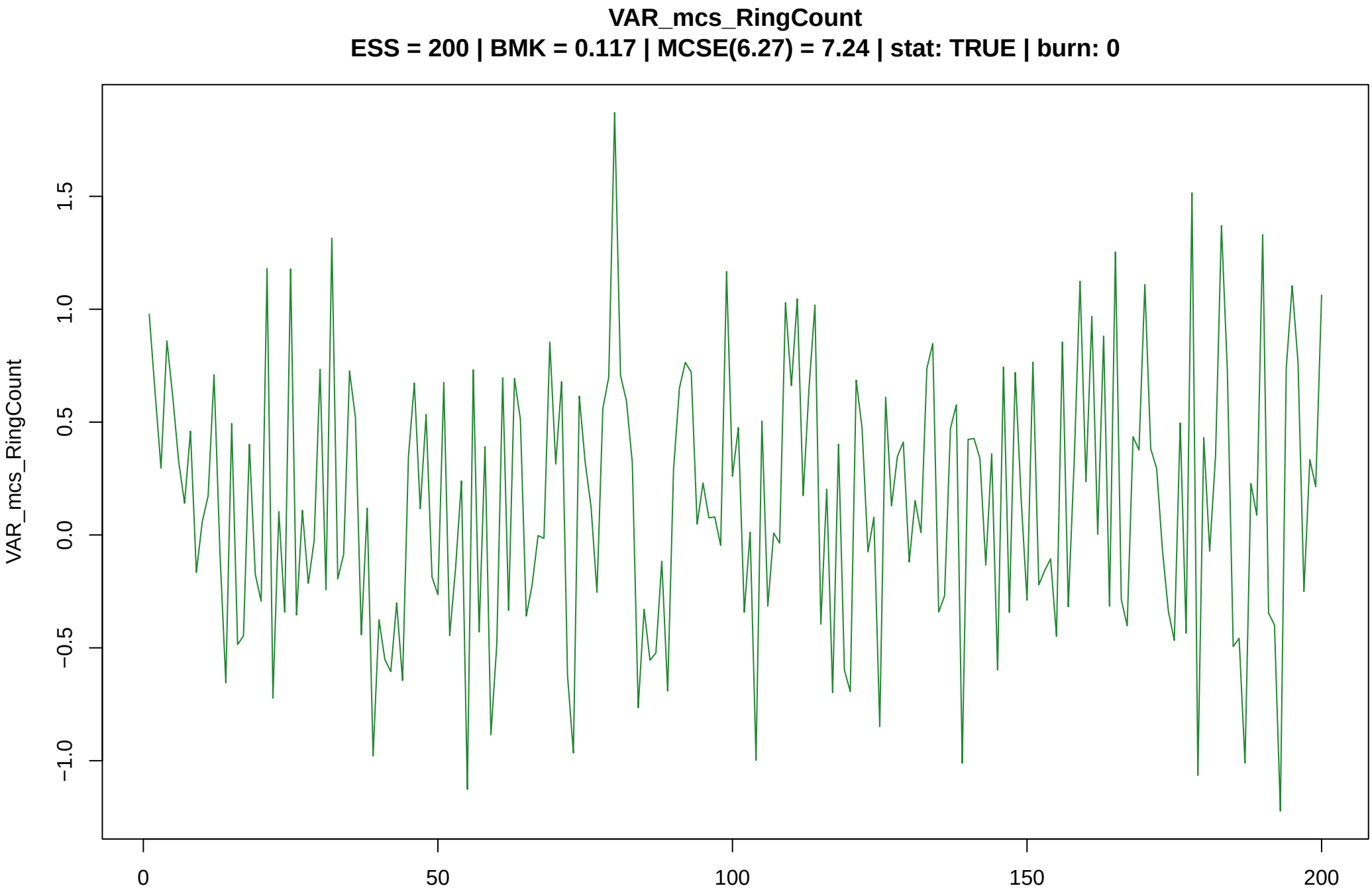

VAR_log_RMSD
ESS = 200 | BMK = 0.161 | MCSE(6.27) = 7.41 | stat: TRUE | burn: 0
VAR_log_RMSD
2
1
0
−1
0
50
100
150
200

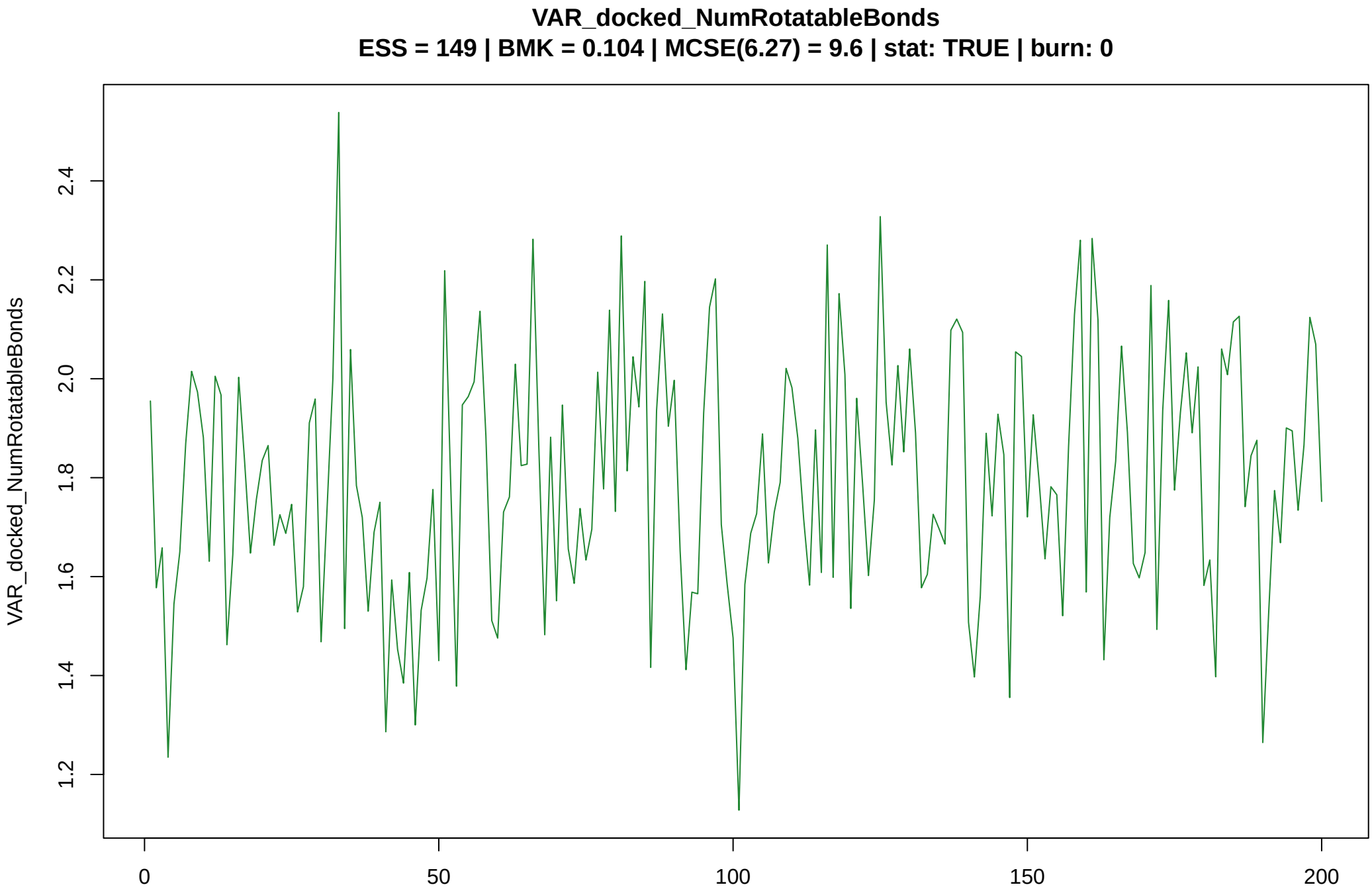

VAR_log_mcs_unbonded_polar_sasa
ESS = 117 | BMK = 0.166 | MCSE(6.27) = 10.9 | stat: TRUE | burn: 160
VAR_log_mcs_unbonded_polar_sasa
2
1
0
−1
−2
0
50
100
150
200

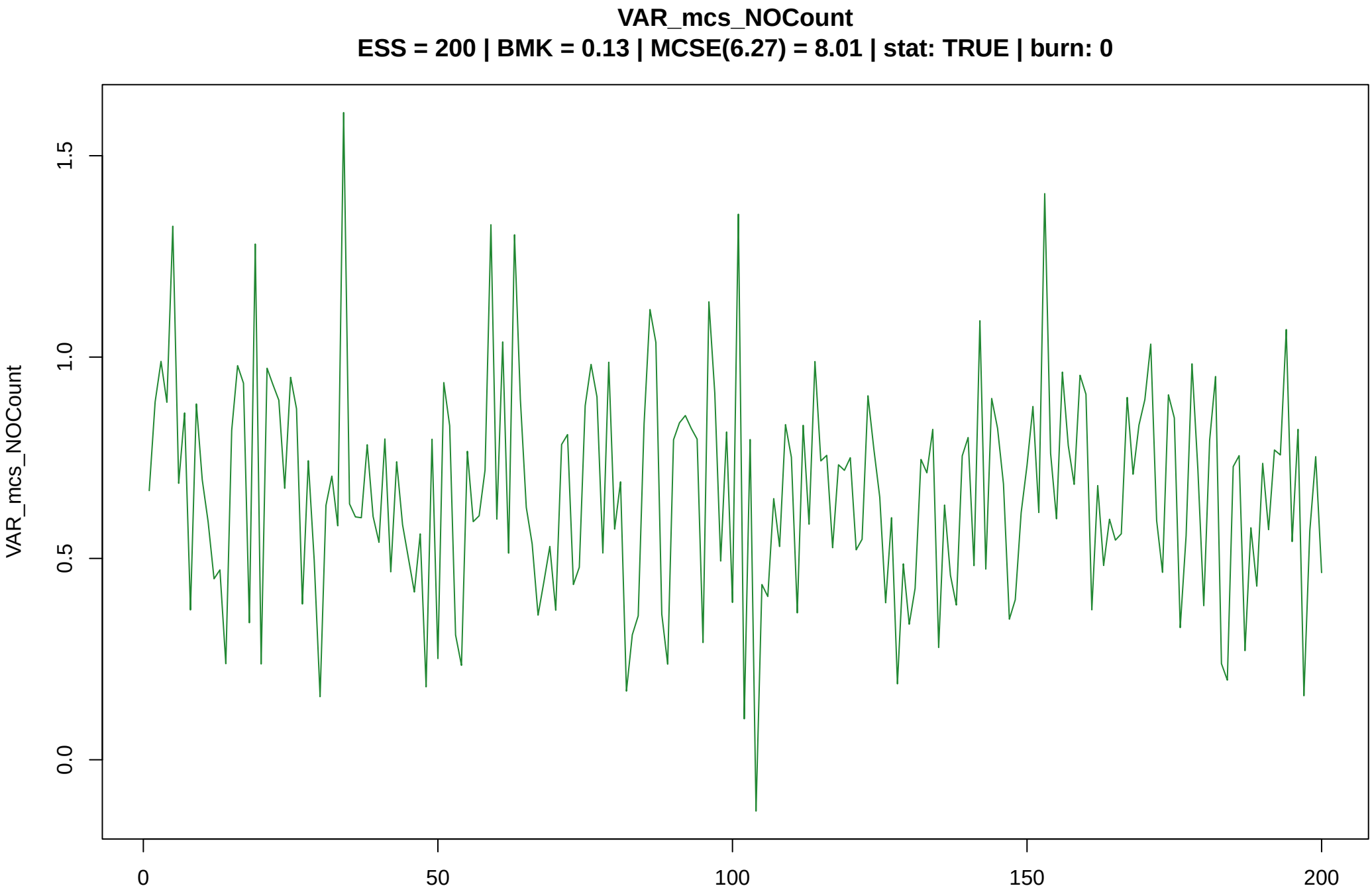

VAR_logit_ec_tanimoto_similarity
ESS = 200 | BMK = 0.247 | MCSE(6.27) = 7.07 | stat: TRUE | burn: 100
VAR_logit_ec_tanimoto_similarity
0
2
4
6
0
50
100
150
200

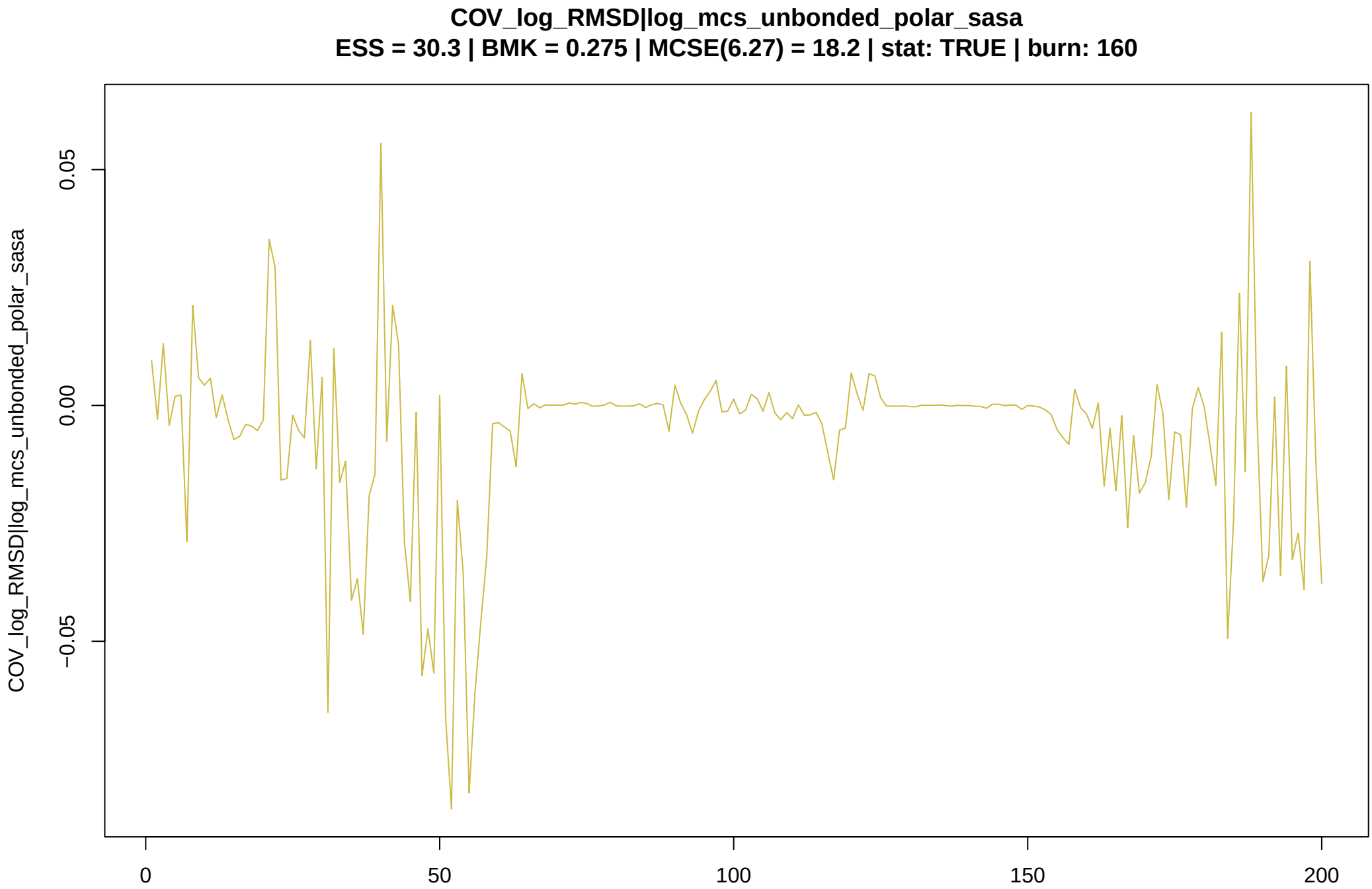

VAR_mcs_NumHeteroAtoms
ESS = 200 | BMK = 0.0922 | MCSE(6.27) = 6.98 | stat: TRUE | burn: 0
VAR_mcs_NumHeteroAtoms
0.2
0.4
0.6
0.8
1.0
1.2
1.4
0
50
100
150
200

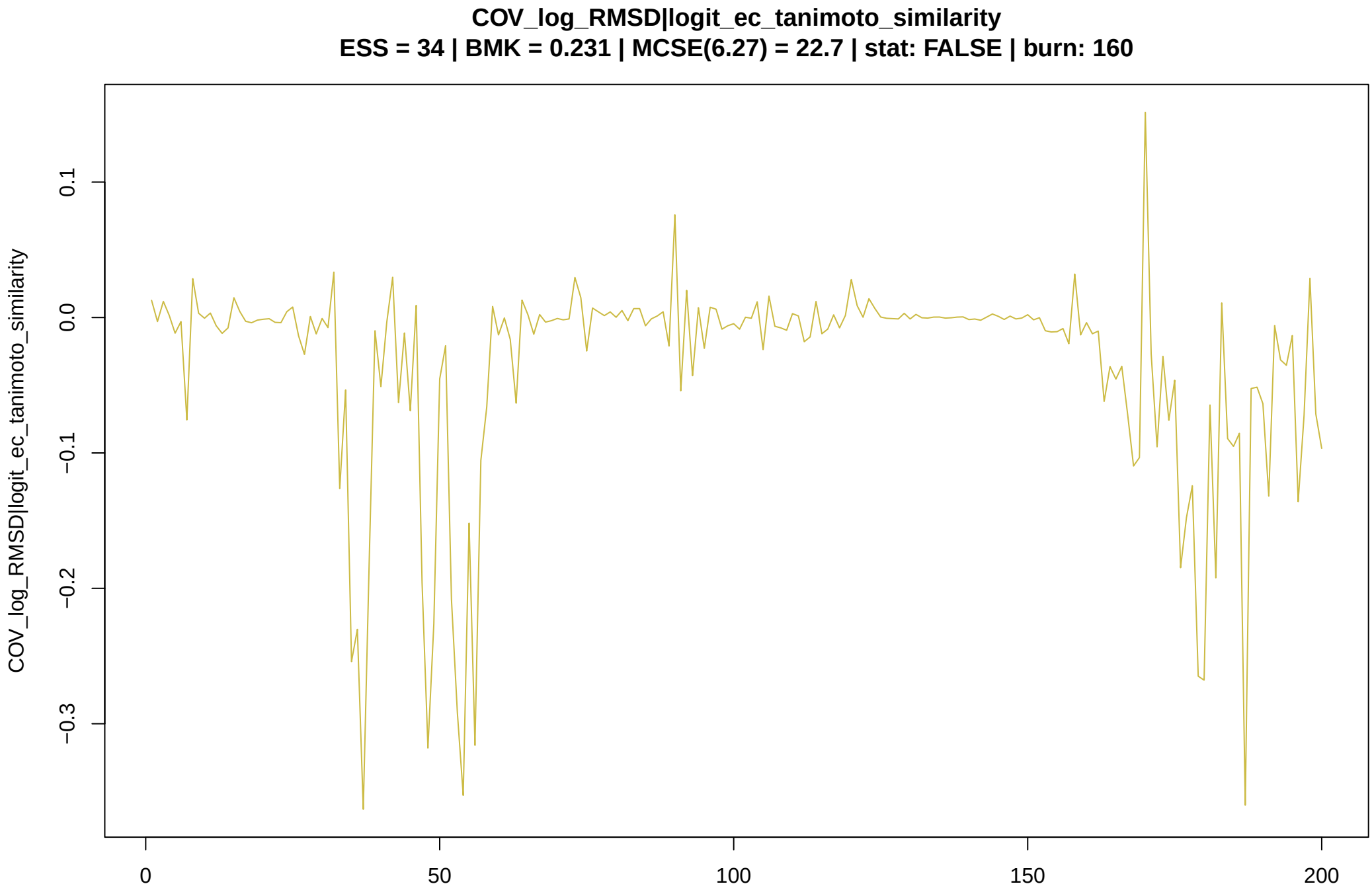

VAR_docked_HeavyAtomCount
ESS = 200 | BMK = 0.191 | MCSE(6.27) = 9.16 | stat: FALSE | burn: 0
VAR_docked_HeavyAtomCount
2.5
3.0
3.5
0
50
100
150
200

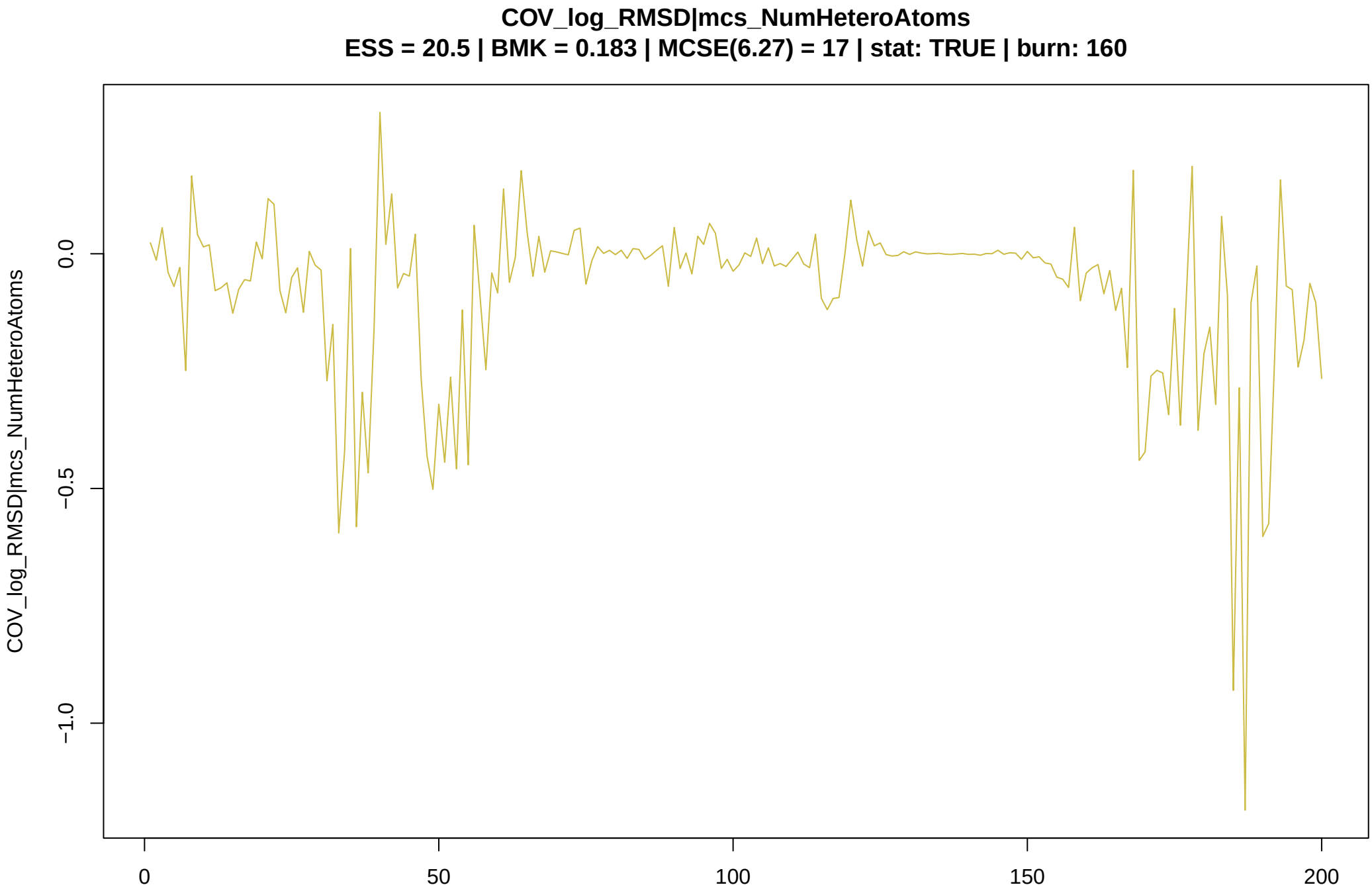

VAR_mcs_RingCount
ESS = 200 | BMK = 0.117 | MCSE(6.27) = 7.24 | stat: TRUE | burn: 0
VAR_mcs_RingCount
−1.0
−0.5
0.0
0.5
1.0
1.5
0
50
100
150
200

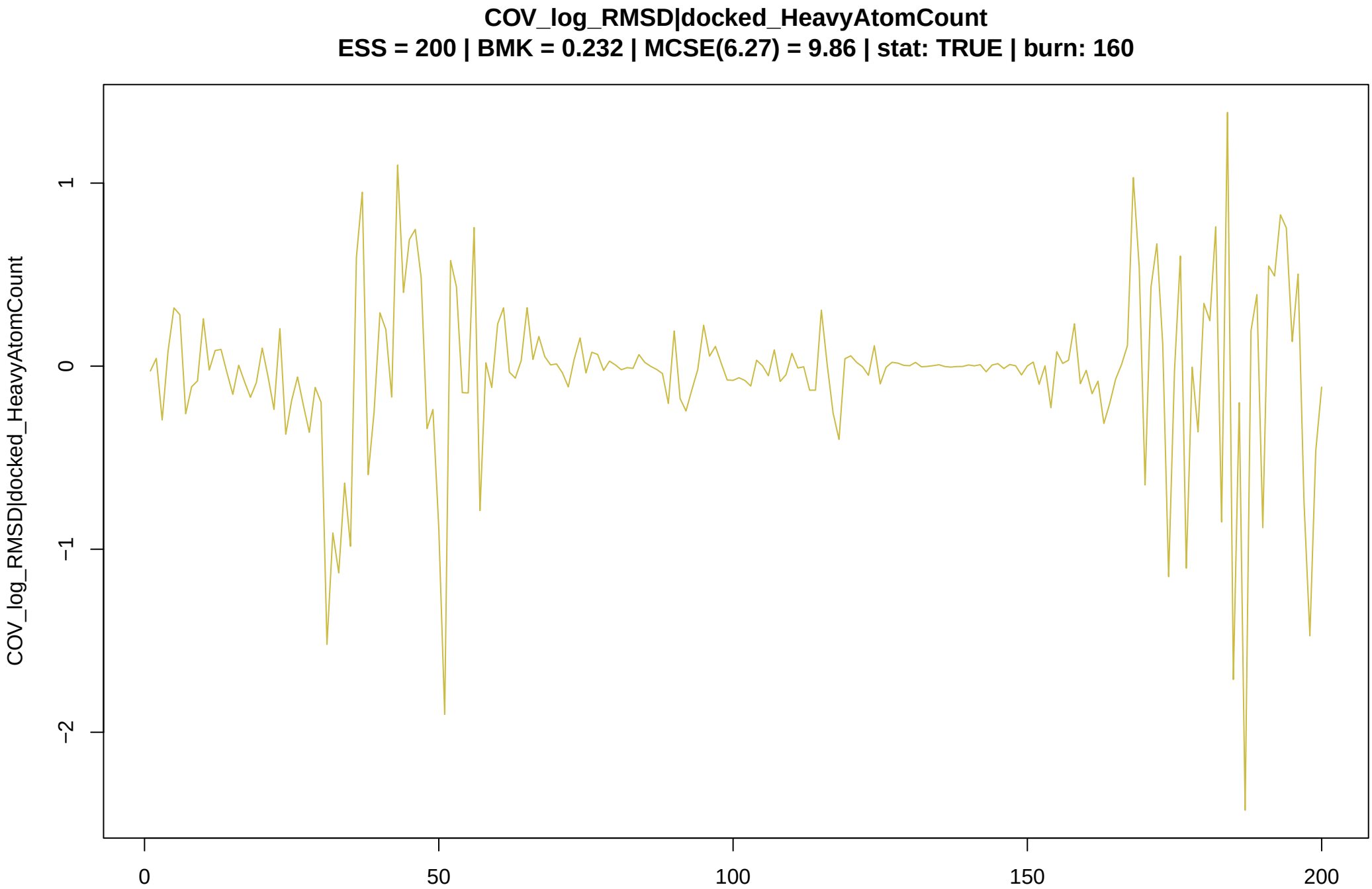

VAR_docked_NumRotatableBonds
ESS = 149 | BMK = 0.104 | MCSE(6.27) = 9.6 | stat: TRUE | burn: 0
VAR_docked_NumRotatableBonds
1.2
1.4
1.6
1.8
2.0
2.2
2.4
0
50
100
150
200

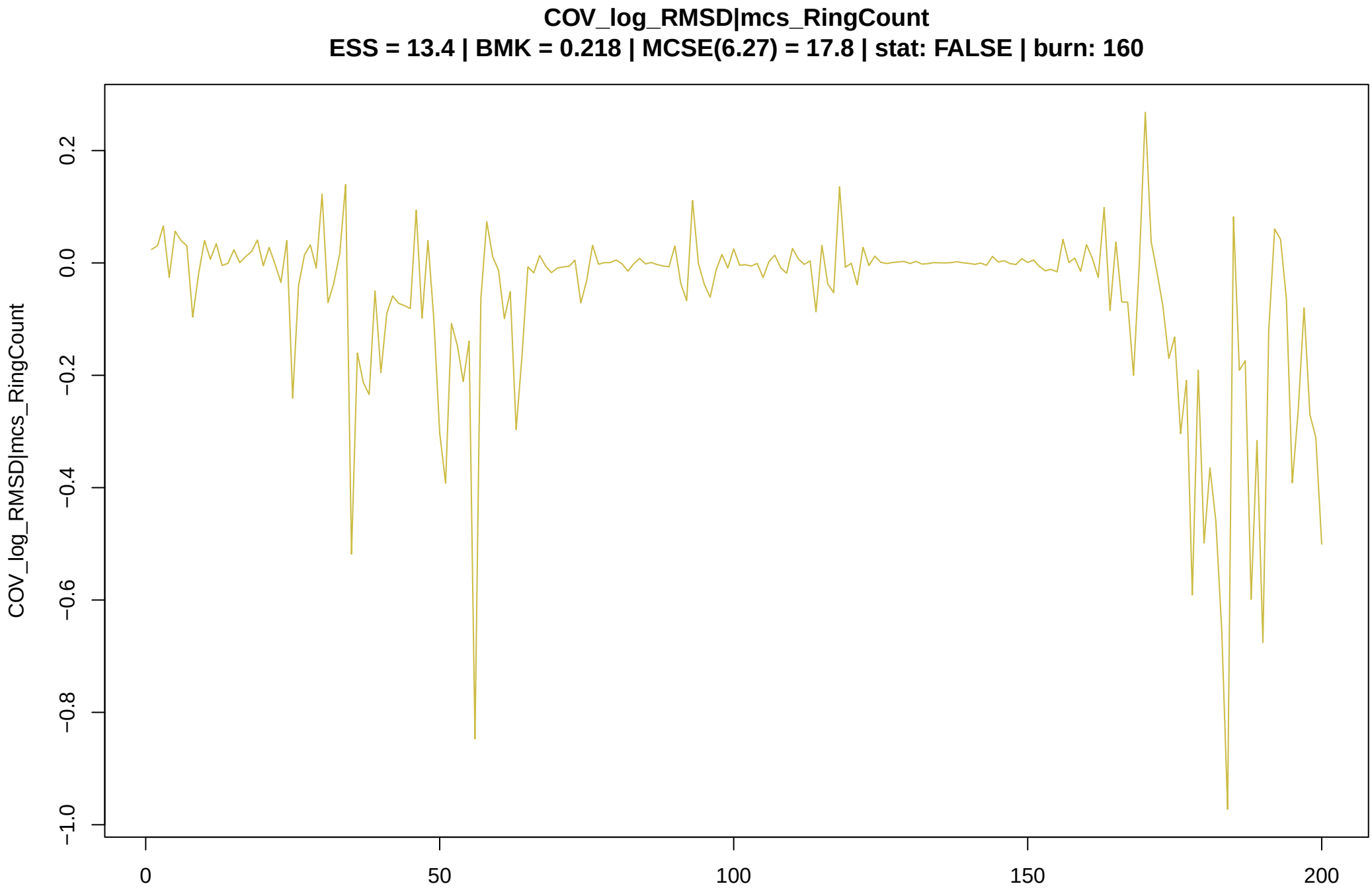

VAR_mcs_NOCount
ESS = 200 | BMK = 0.13 | MCSE(6.27) = 8.01 | stat: TRUE | burn: 0
VAR_mcs_NOCount
0.0
0.5
1.0
1.5
0
50
100
150
200

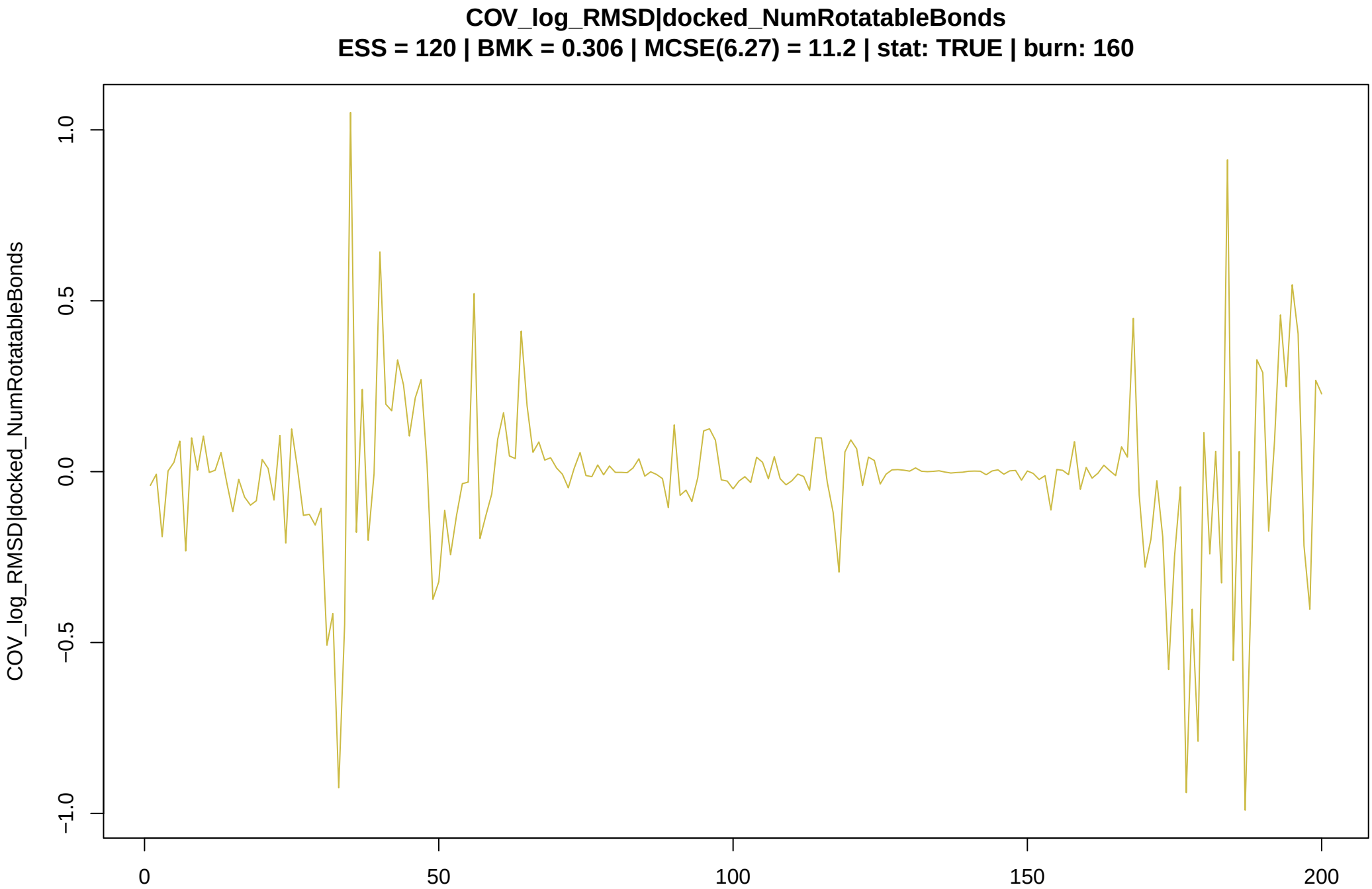

COV_log_RMSD|log_mcs_unbonded_polar_sasa
ESS = 30.3 | BMK = 0.275 | MCSE(6.27) = 18.2 | stat: TRUE | burn: 160
COV_log_RMSD|log_mcs_unbonded_polar_sasa
0.05
0.00
−0.05
0
50
100
150
200

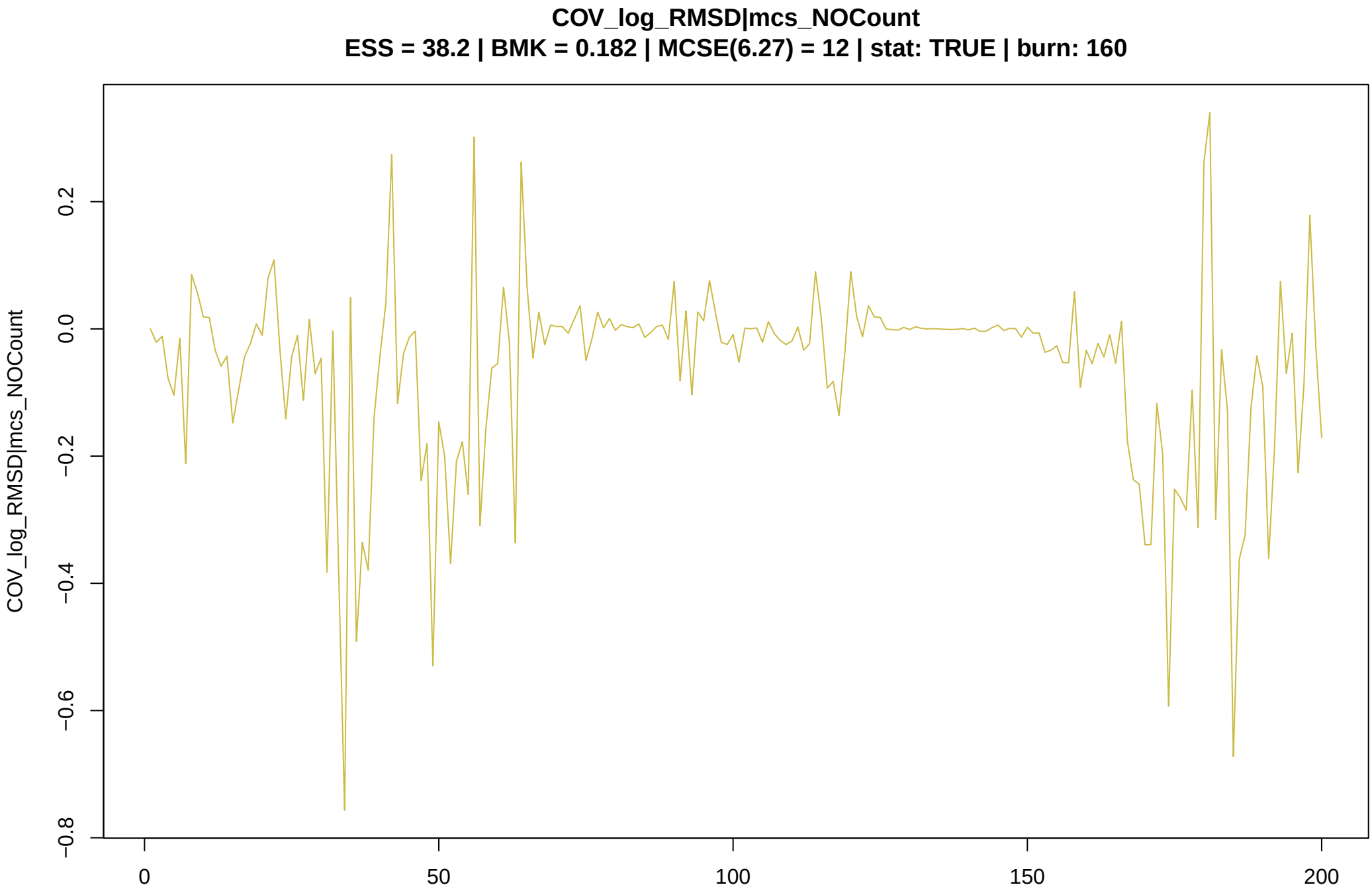

COV_log_RMSD|logit_ec_tanimoto_similarity
ESS = 34 | BMK = 0.231 | MCSE(6.27) = 22.7 | stat: FALSE | burn: 160
COV_log_RMSD|logit_ec_tanimoto_similarity
0.1
0.0
−0.1
−0.2
−0.3
0
50
100
150
200

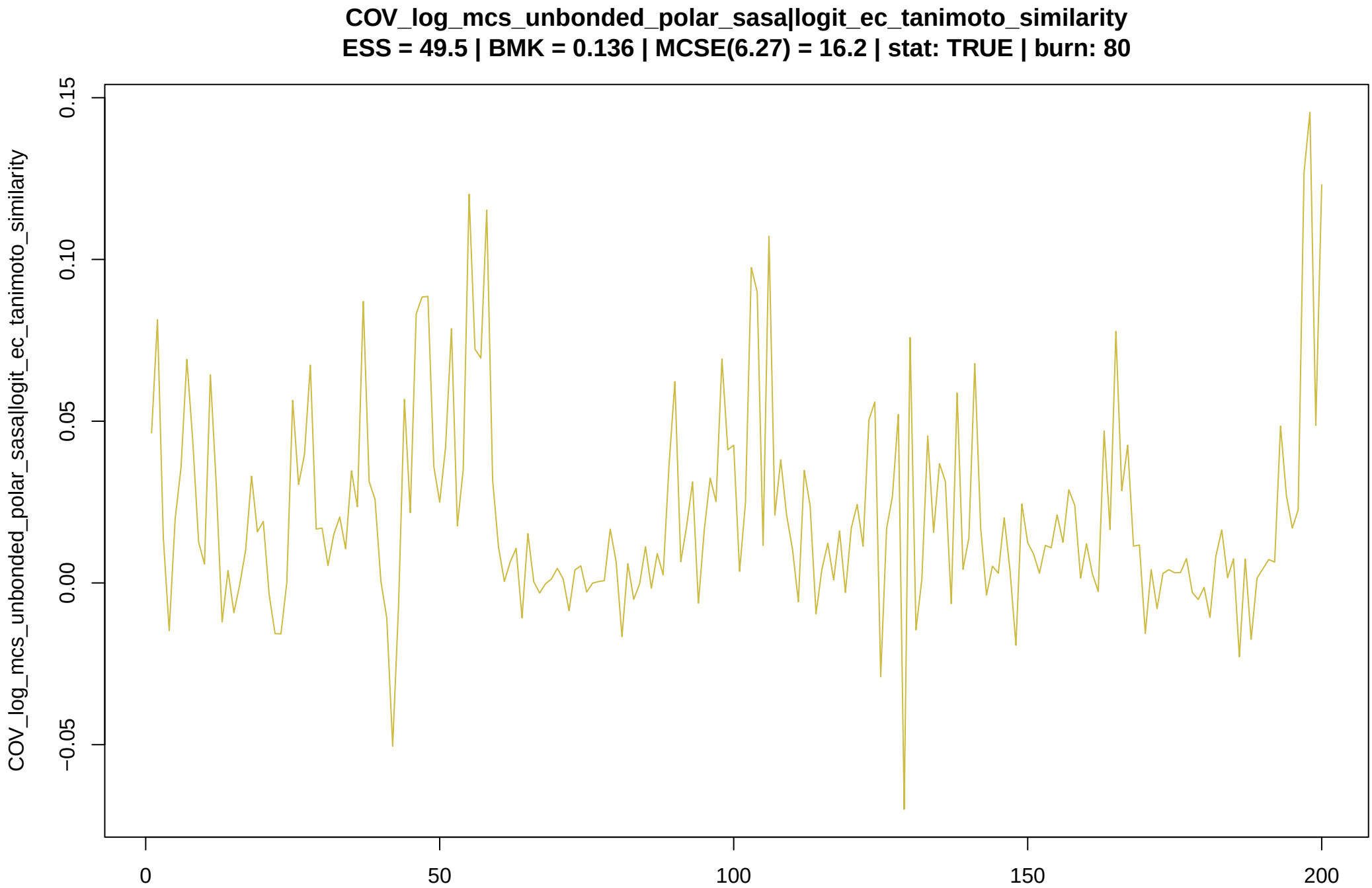

COV_log_RMSD|mcs_NumHeteroAtoms
ESS = 20.5 | BMK = 0.183 | MCSE(6.27) = 17 | stat: TRUE | burn: 160
COV_log_RMSD|mcs_NumHeteroAtoms
0.0
−0.5
−1.0
0
50
100
150
200

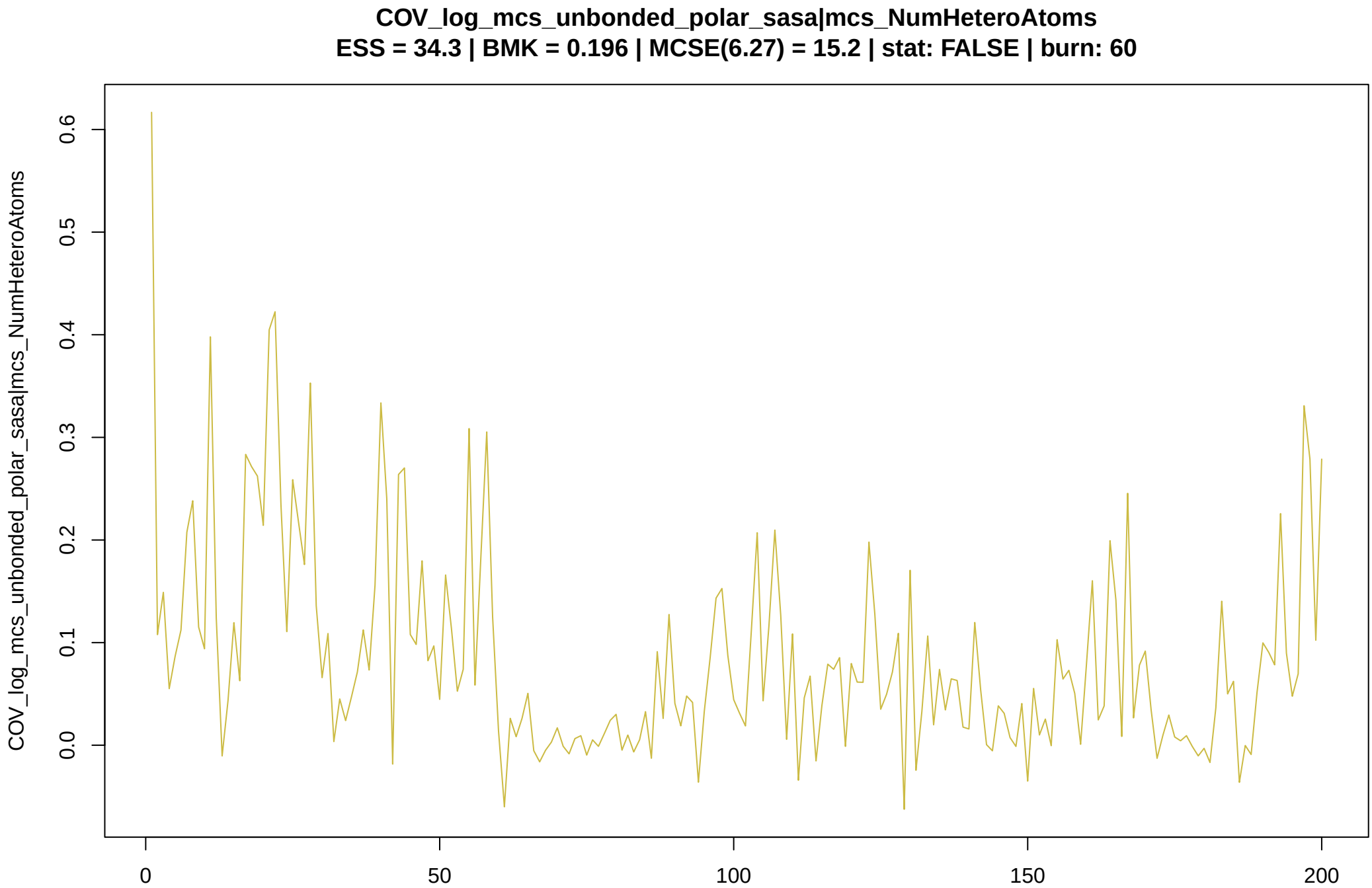

COV_log_RMSD|docked_HeavyAtomCount
ESS = 200 | BMK = 0.232 | MCSE(6.27) = 9.86 | stat: TRUE | burn: 160
COV_log_RMSD|docked_HeavyAtomCount
1
0
−1
−2
0
50
100
150
200

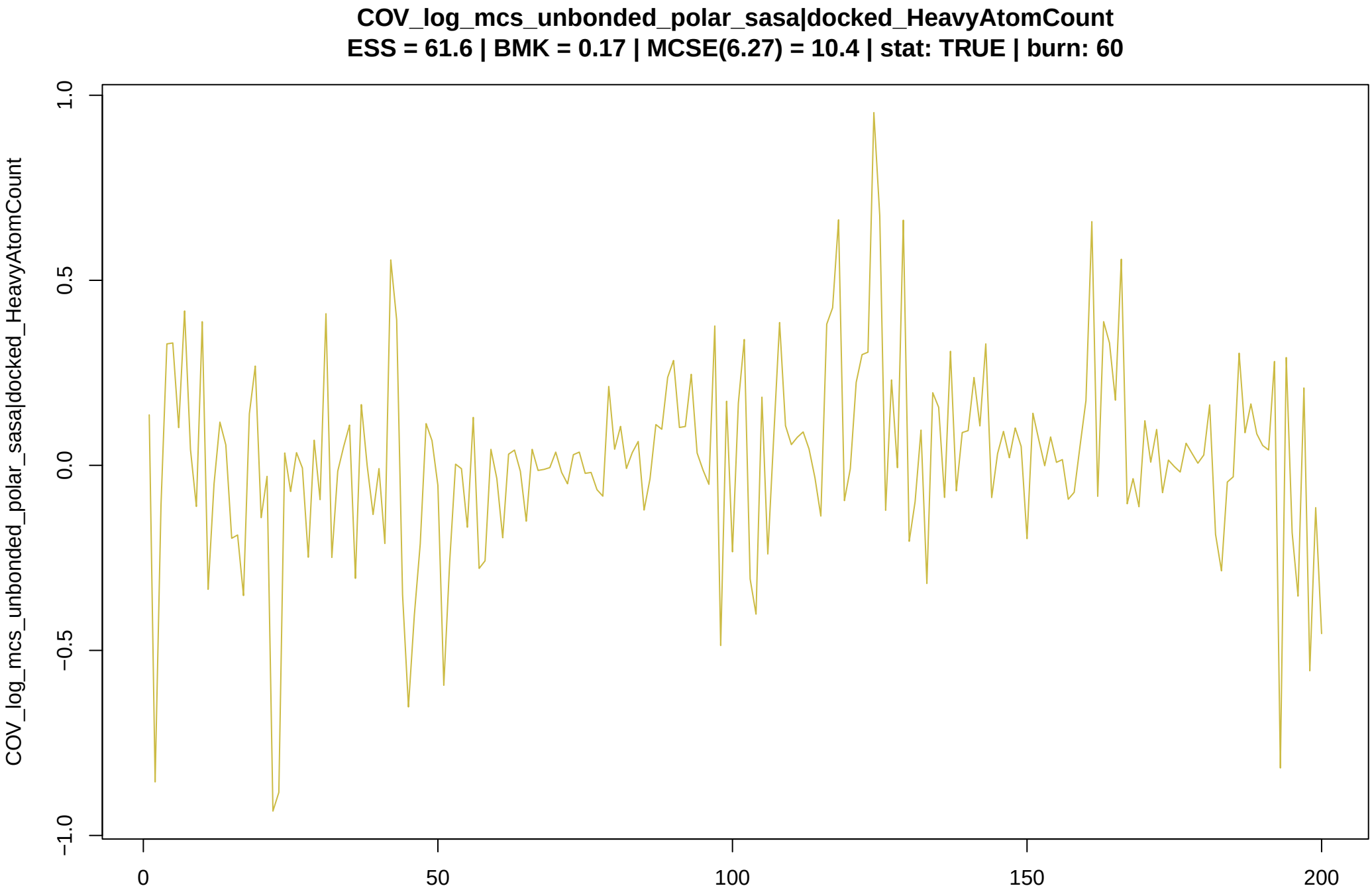

COV_log_RMSD|mcs_RingCount
ESS = 13.4 | BMK = 0.218 | MCSE(6.27) = 17.8 | stat: FALSE | burn: 160
COV_log_RMSD|mcs_RingCount
0.2
0.0
−0.2
−0.4
−0.6
−0.8
−1.0
0
50
100
150
200

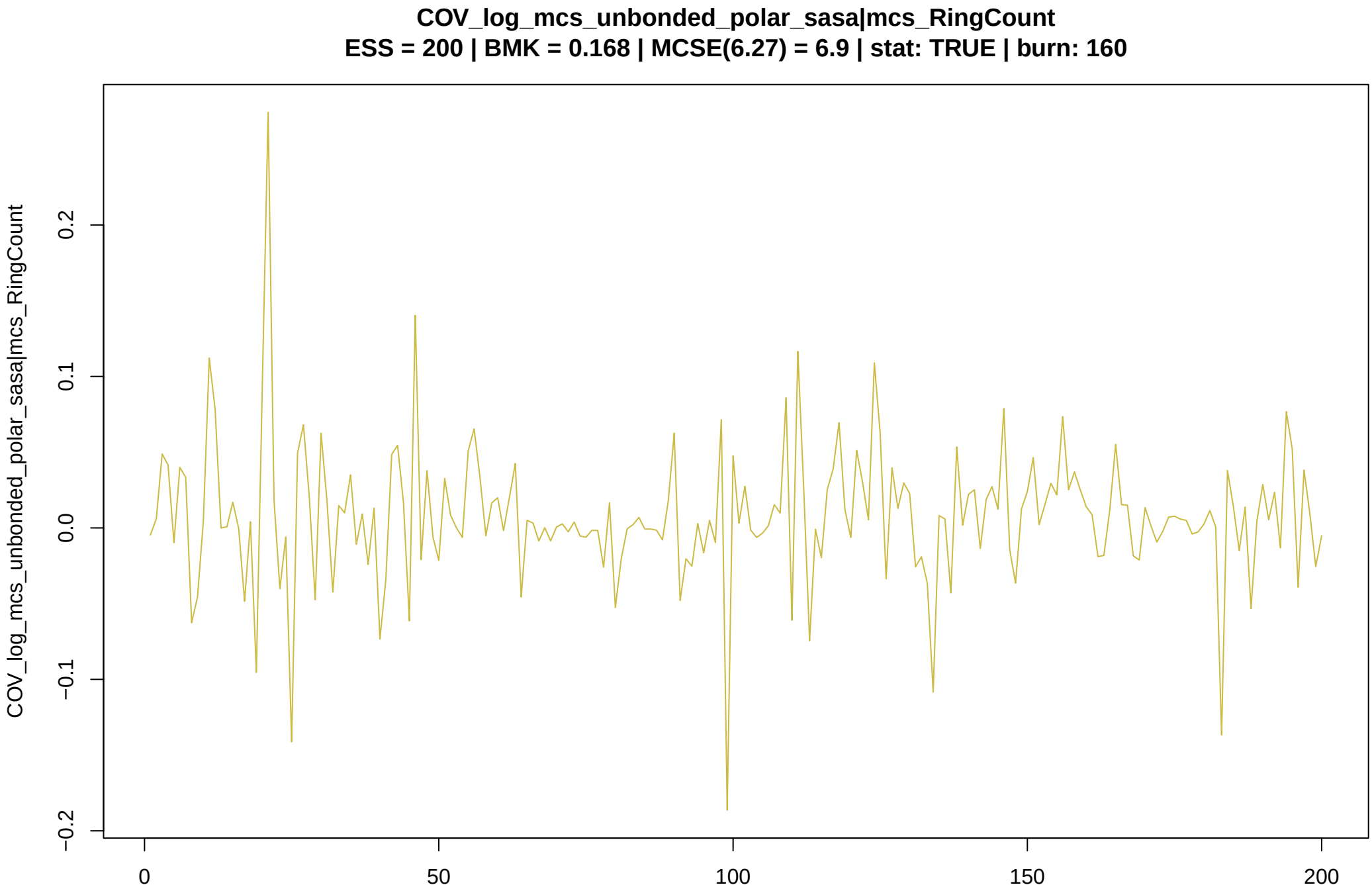

COV_log_RMSD|docked_NumRotatableBonds
ESS = 120 | BMK = 0.306 | MCSE(6.27) = 11.2 | stat: TRUE | burn: 160
COV_log_RMSD|docked_NumRotatableBonds
1.0
0.5
0.0
−0.5
−1.0
0
50
100
150
200

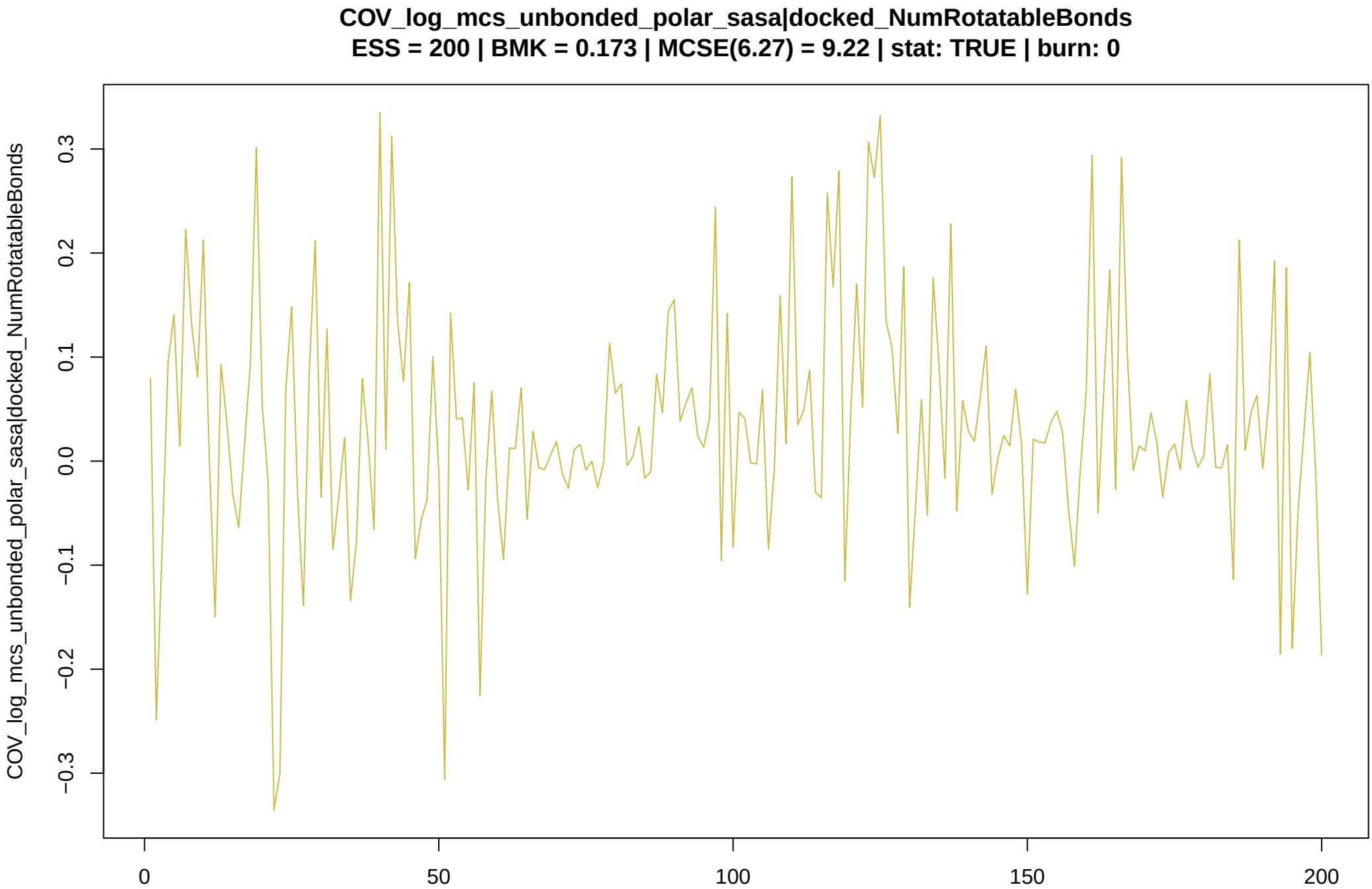

COV_log_RMSD|mcs_NOCount
ESS = 38.2 | BMK = 0.182 | MCSE(6.27) = 12 | stat: TRUE | burn: 160
COV_log_RMSD|mcs_NOCount
0.2
0.0
−0.2
−0.4
−0.6
−0.8
0
50
100
150
200

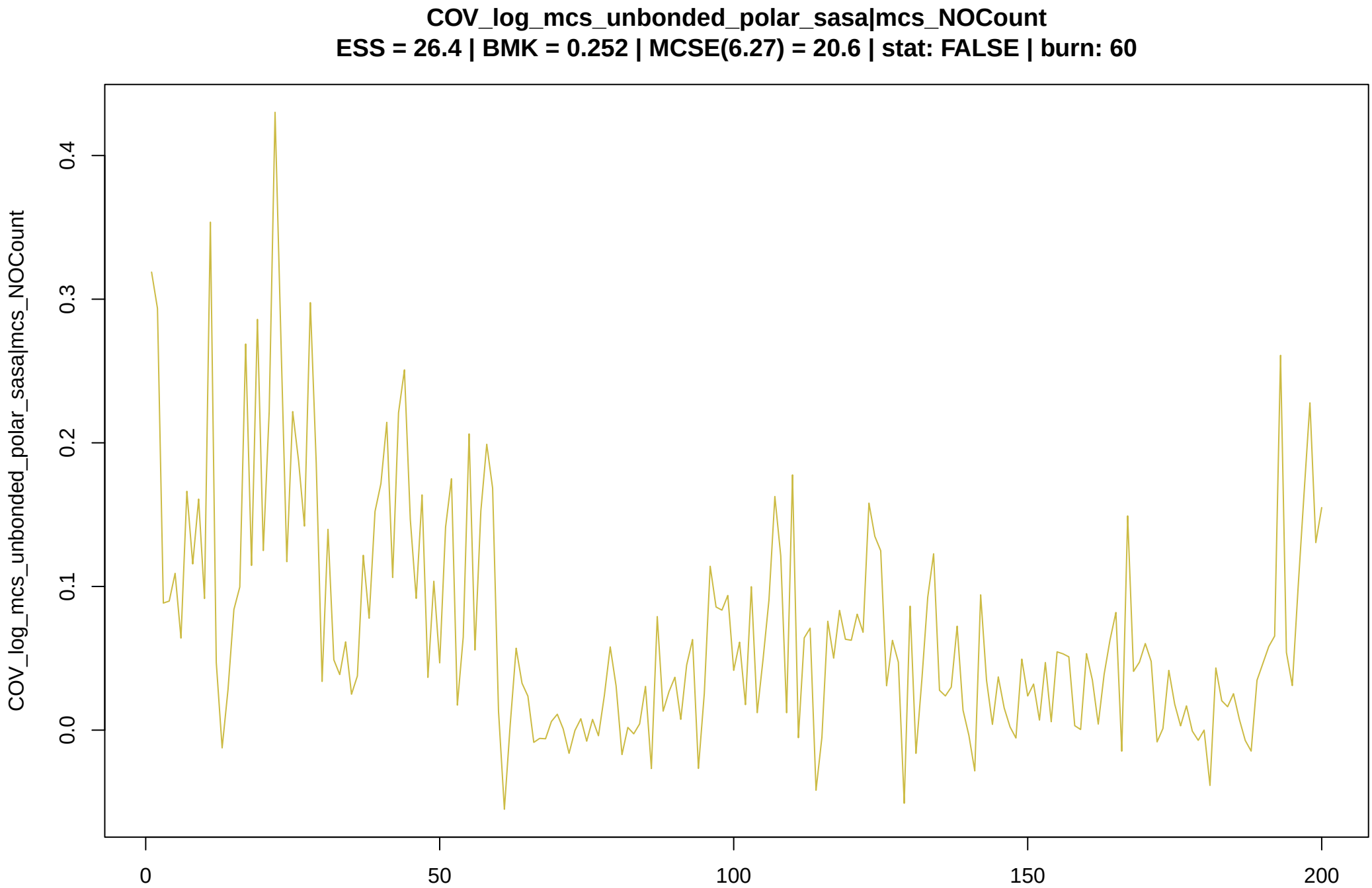

COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
ESS = 49.5 | BMK = 0.136 | MCSE(6.27) = 16.2 | stat: TRUE | burn: 80
COV_log_mcs_unbonded_polar_sasa|logit_ec_tanimoto_similarity
0.15
0.10
0.05
0.00
−0.05
0
50
100
150
200

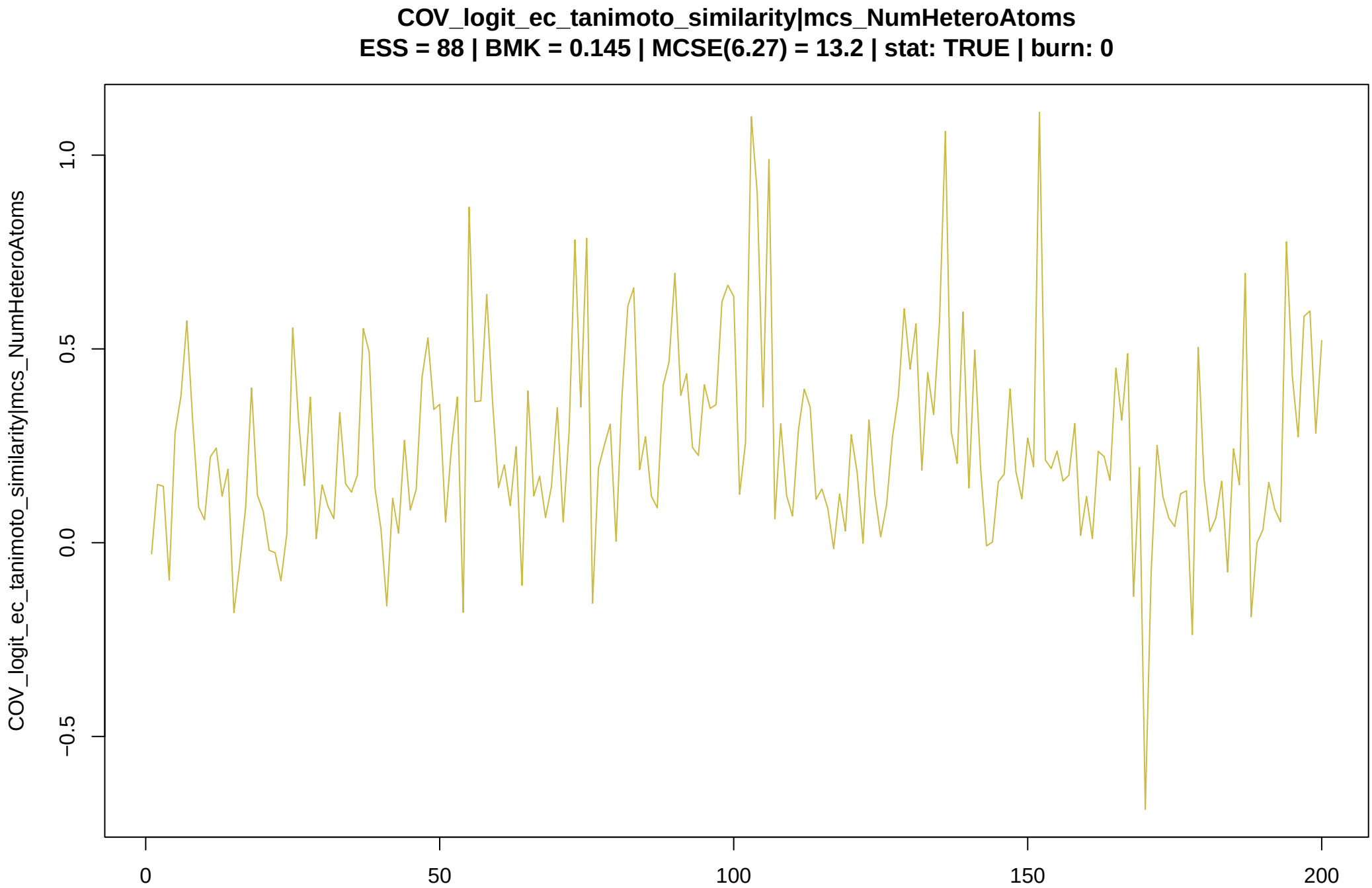

COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
ESS = 34.3 | BMK = 0.196 | MCSE(6.27) = 15.2 | stat: FALSE | burn: 60
COV_log_mcs_unbonded_polar_sasa|mcs_NumHeteroAtoms
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0
50
100
150
200

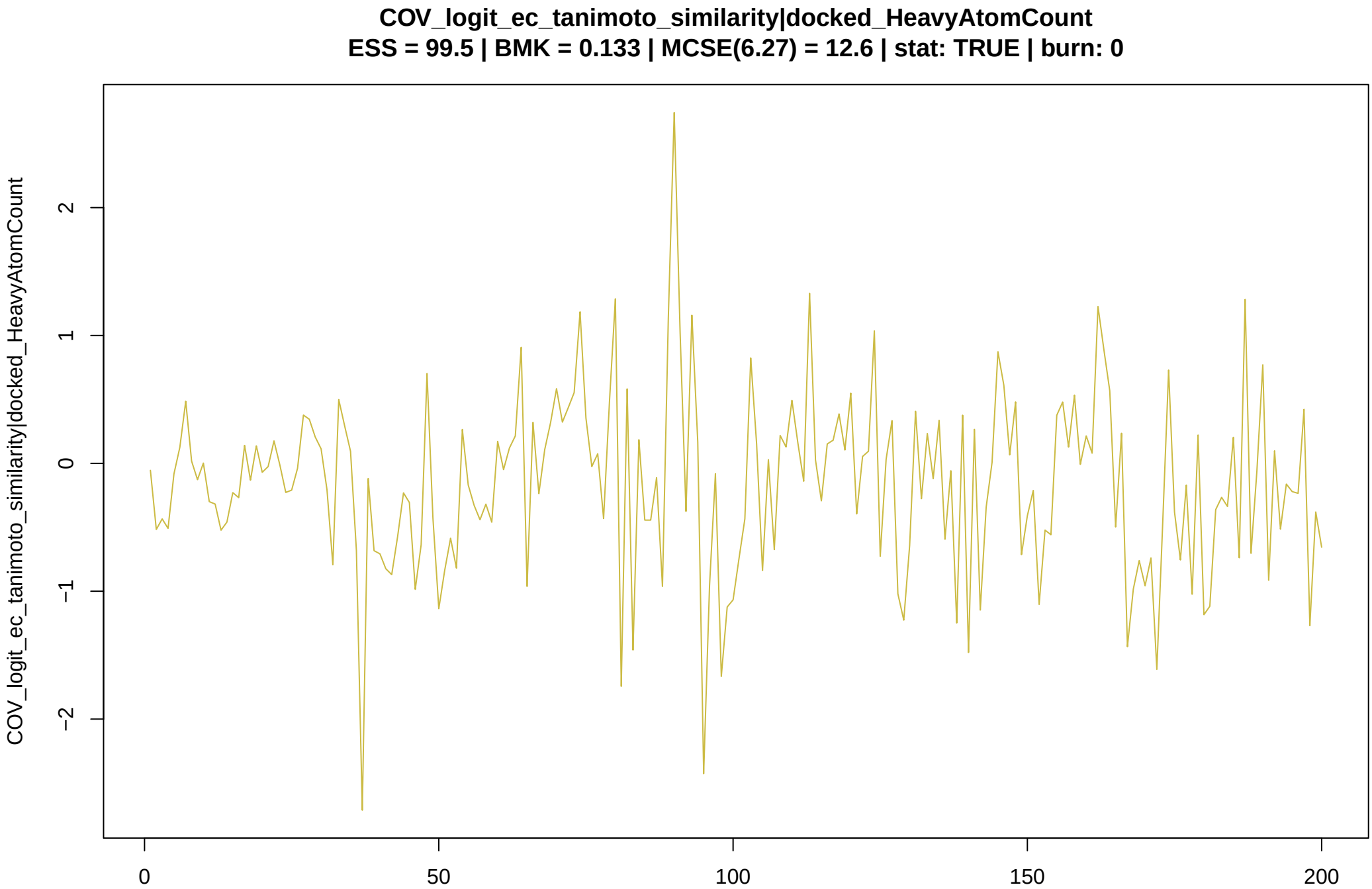

COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
ESS = 61.6 | BMK = 0.17 | MCSE(6.27) = 10.4 | stat: TRUE | burn: 60
COV_log_mcs_unbonded_polar_sasa|docked_HeavyAtomCount
1.0
0.5
0.0
−0.5
−1.0
0
50
100
150
200

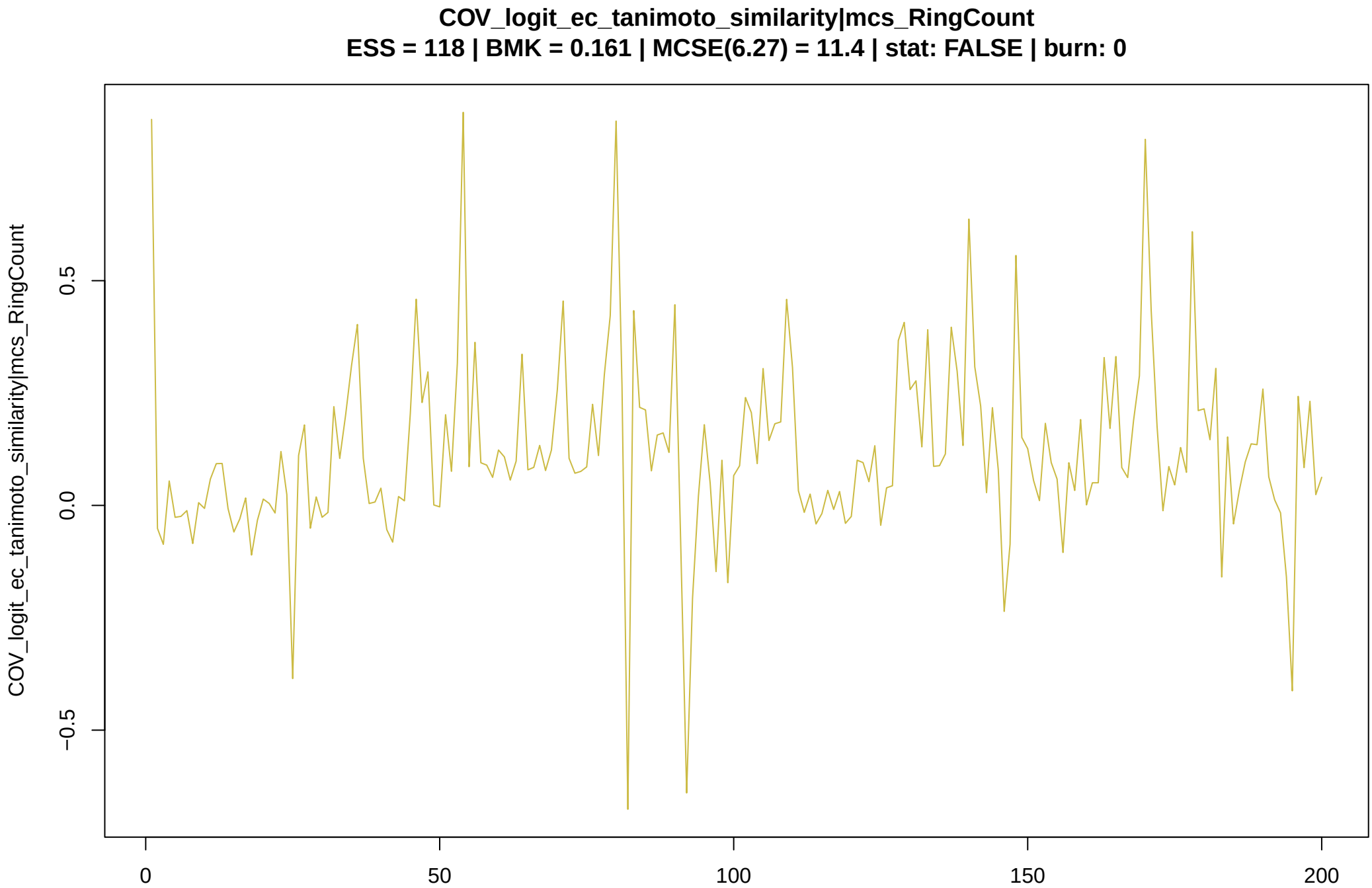

COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
ESS = 200 | BMK = 0.168 | MCSE(6.27) = 6.9 | stat: TRUE | burn: 160
COV_log_mcs_unbonded_polar_sasa|mcs_RingCount
0.2
0.1
0.0
−0.1
−0.2
0
50
100
150
200

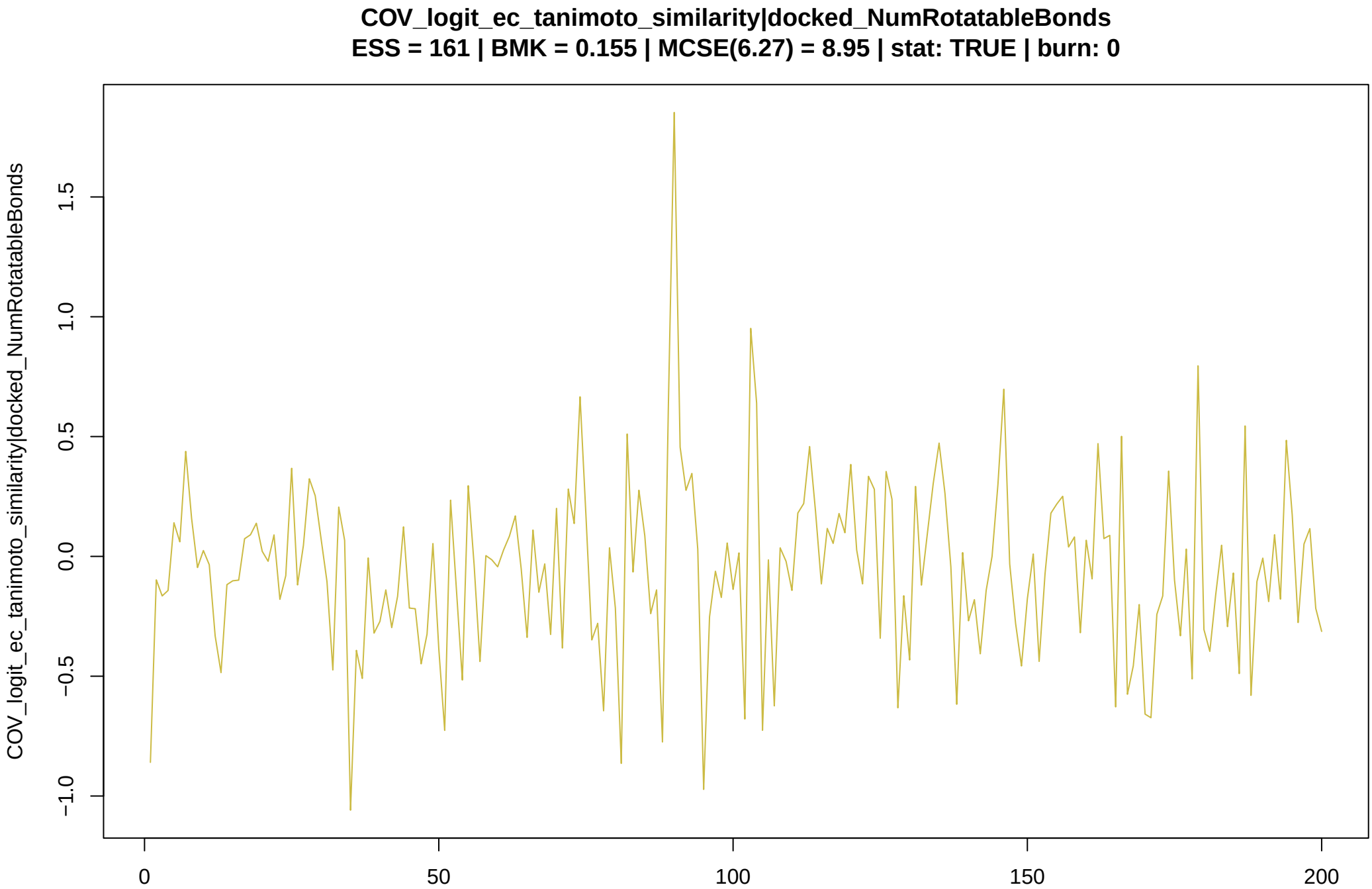

COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
ESS = 200 | BMK = 0.173 | MCSE(6.27) = 9.22 | stat: TRUE | burn: 0
COV_log_mcs_unbonded_polar_sasa|docked_NumRotatableBonds
0.3
0.2
0.1
0.0
−0.1
−0.2
−0.3
0
50
100
150
200

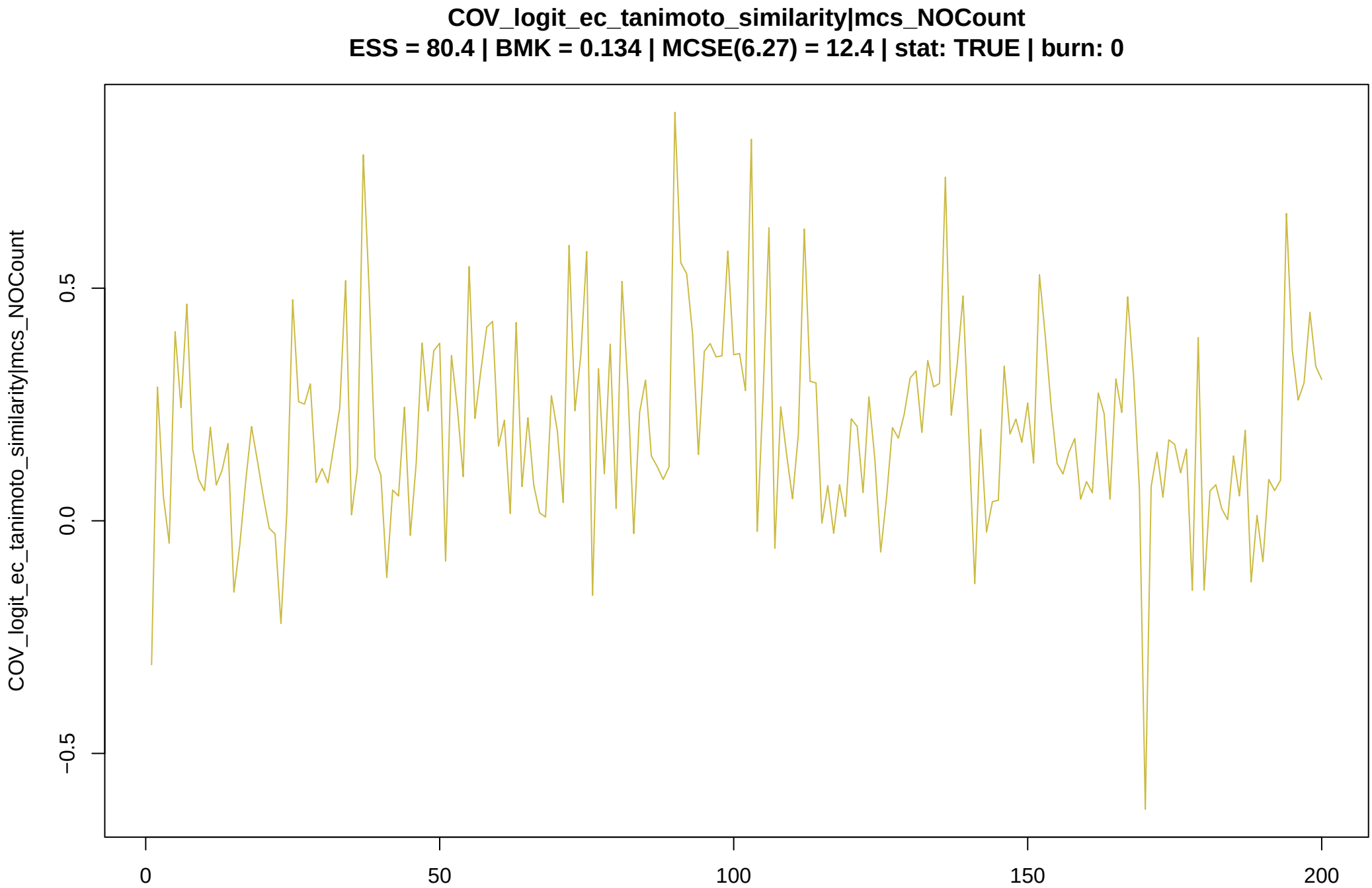

COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
ESS = 26.4 | BMK = 0.252 | MCSE(6.27) = 20.6 | stat: FALSE | burn: 60
COV_log_mcs_unbonded_polar_sasa|mcs_NOCount
0.0
0.1
0.2
0.3
0.4
0
50
100
150
200

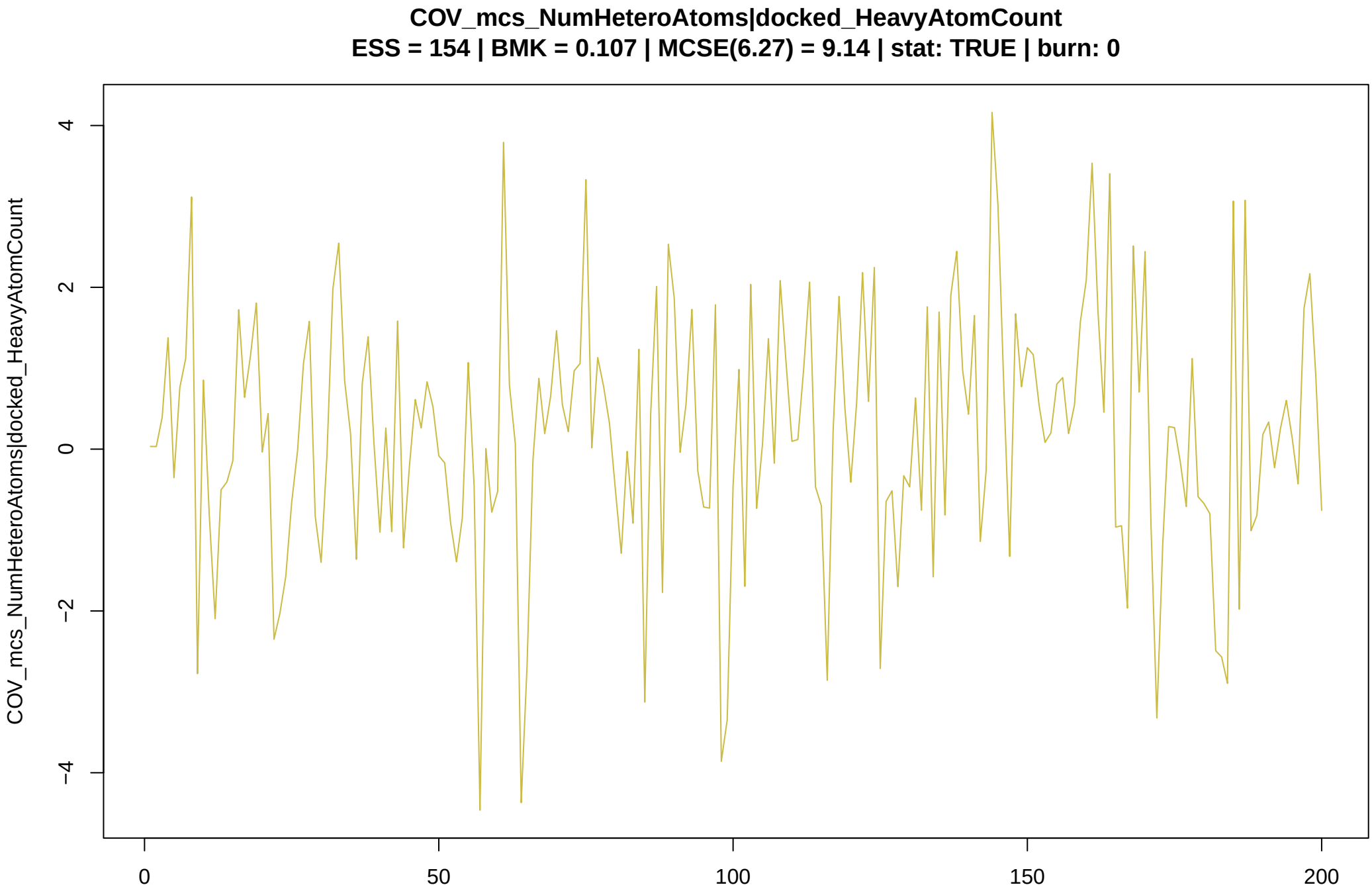

COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
ESS = 88 | BMK = 0.145 | MCSE(6.27) = 13.2 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NumHeteroAtoms
1.0
0.5
0.0
−0.5
0
50
100
150
200

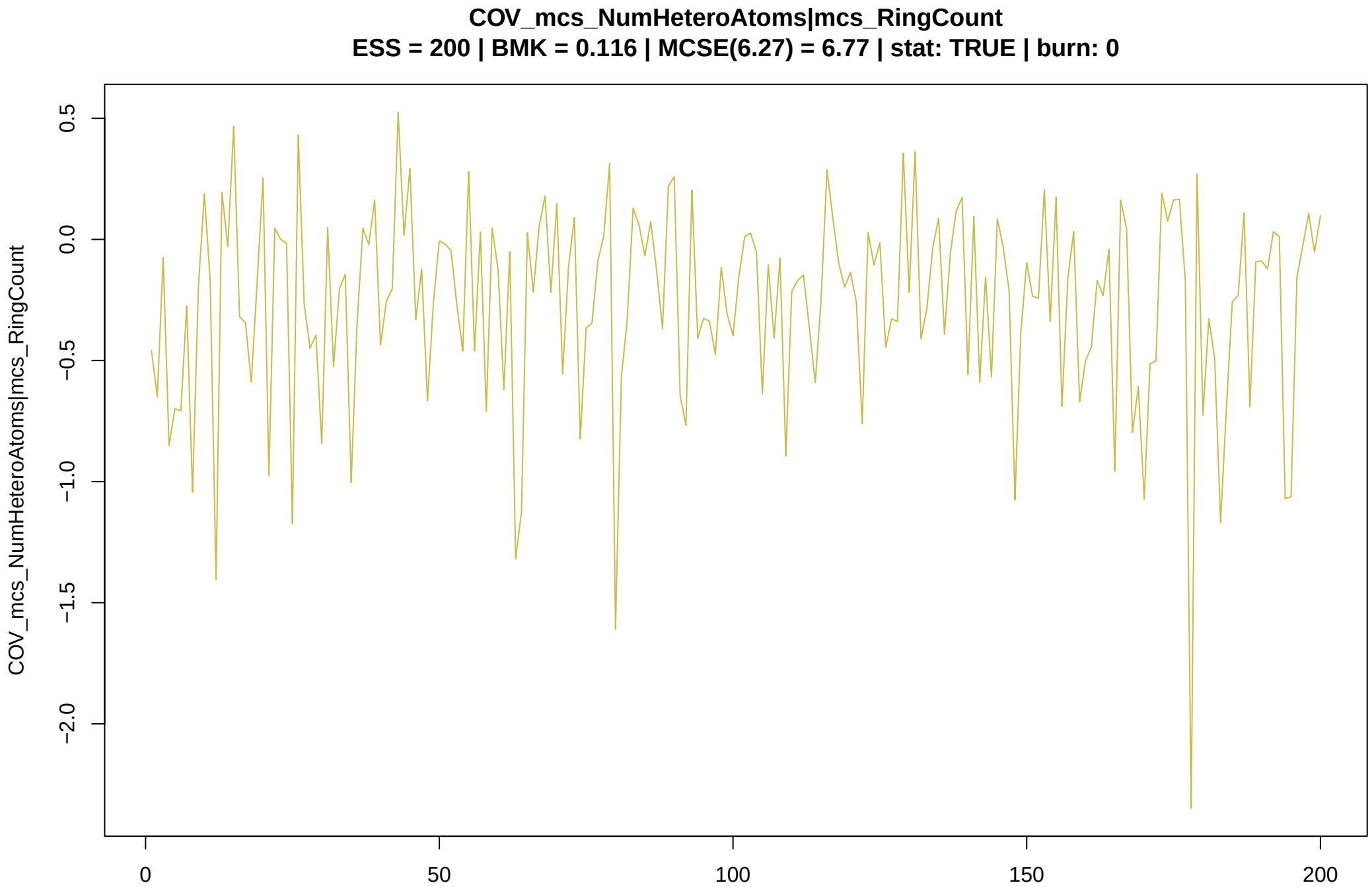

COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
ESS = 99.5 | BMK = 0.133 | MCSE(6.27) = 12.6 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_HeavyAtomCount
2
1
0
−1
−2
0
50
100
150
200

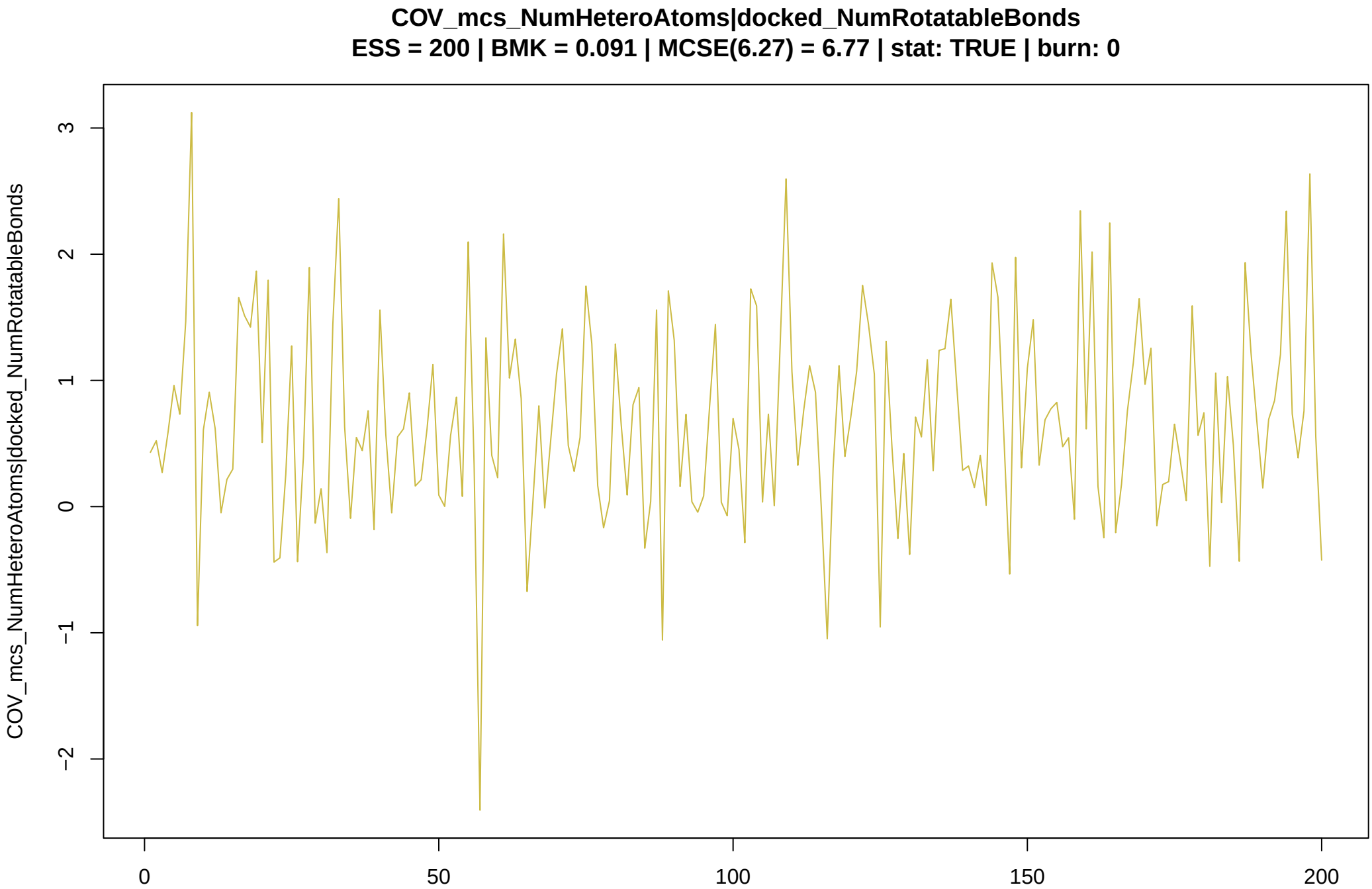

COV_logit_ec_tanimoto_similarity|mcs_RingCount
ESS = 118 | BMK = 0.161 | MCSE(6.27) = 11.4 | stat: FALSE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_RingCount
0.5
0.0
−0.5
0
50
100
150
200

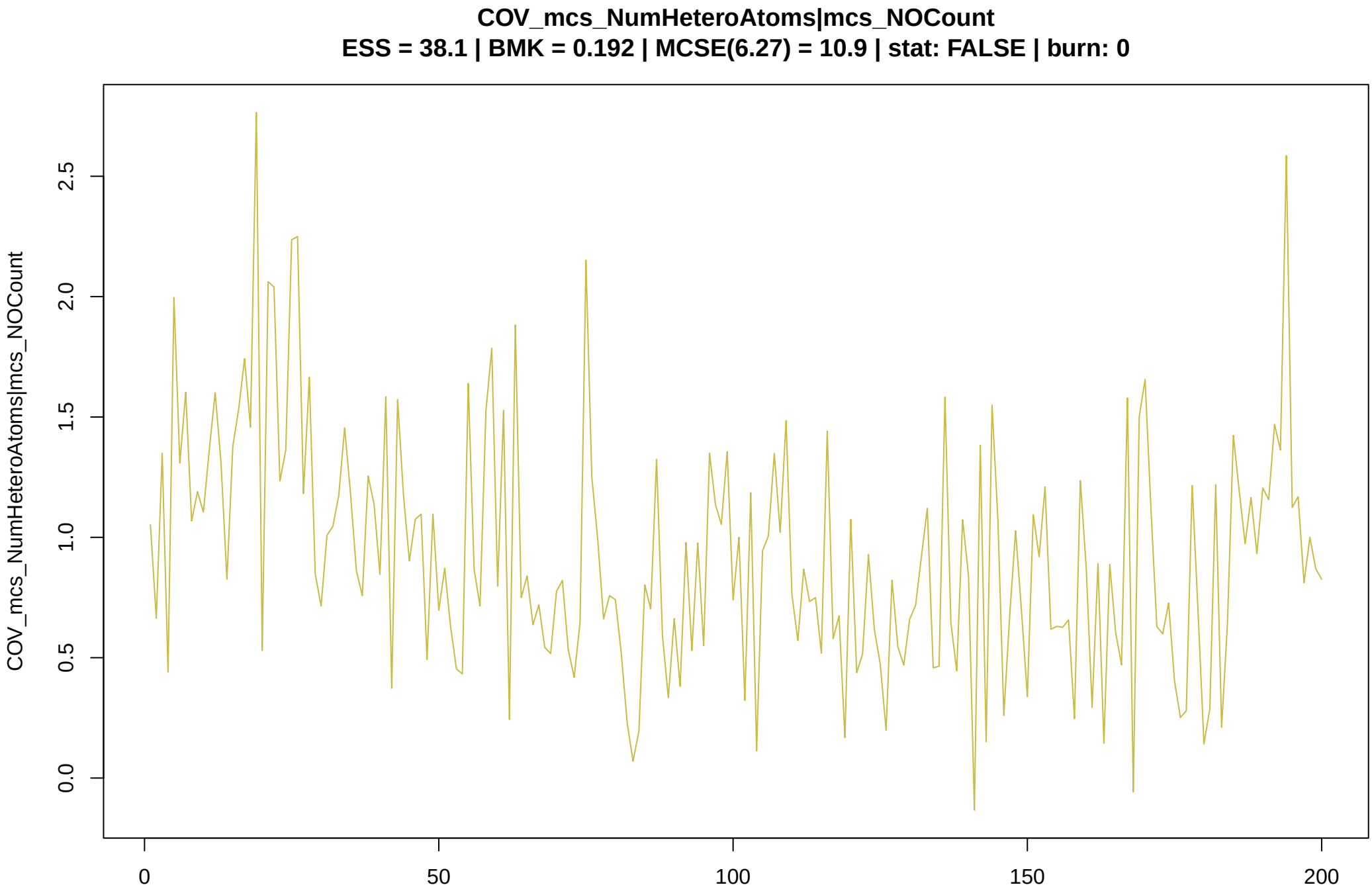

COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
ESS = 161 | BMK = 0.155 | MCSE(6.27) = 8.95 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|docked_NumRotatableBonds
−1.0
−0.5
0.0
0.5
1.0
1.5
0
50
100
150
200

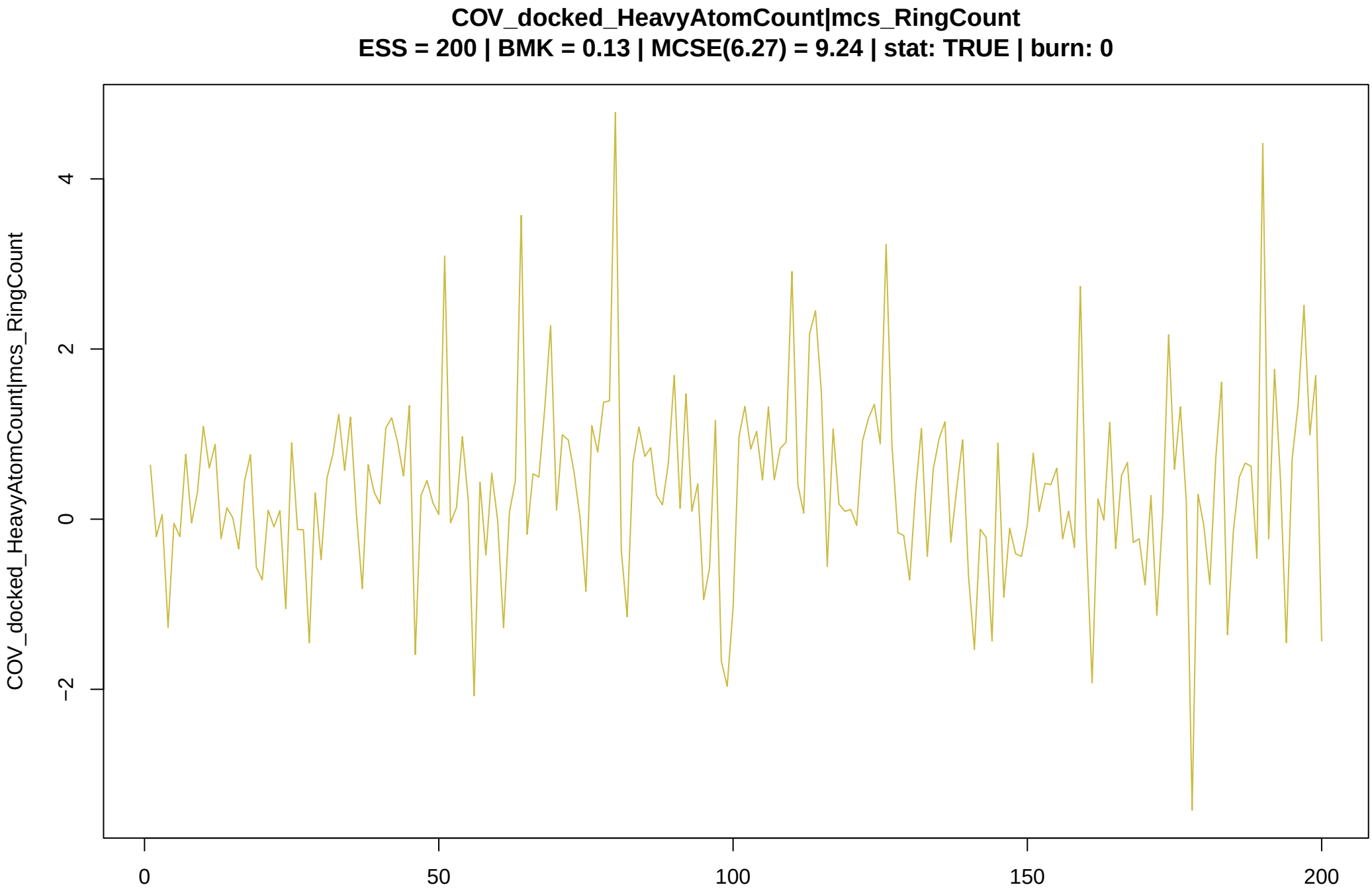

COV_logit_ec_tanimoto_similarity|mcs_NOCount
ESS = 80.4 | BMK = 0.134 | MCSE(6.27) = 12.4 | stat: TRUE | burn: 0
COV_logit_ec_tanimoto_similarity|mcs_NOCount
0.5
0.0
−0.5
0
50
100
150
200

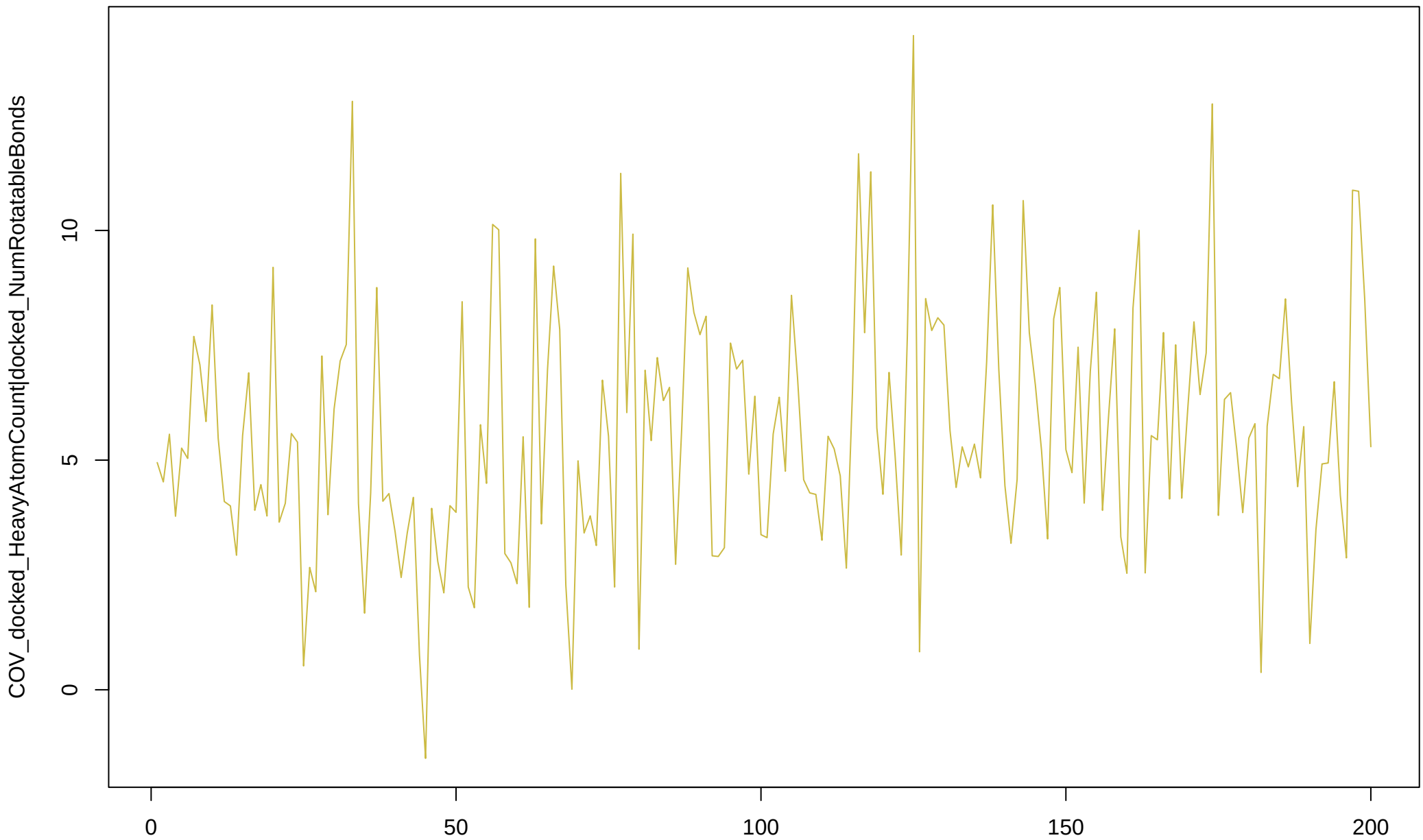

COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
ESS = 154 | BMK = 0.107 | MCSE(6.27) = 9.14 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_HeavyAtomCount
4
2
0
−2
−4
0
50
100
150
200

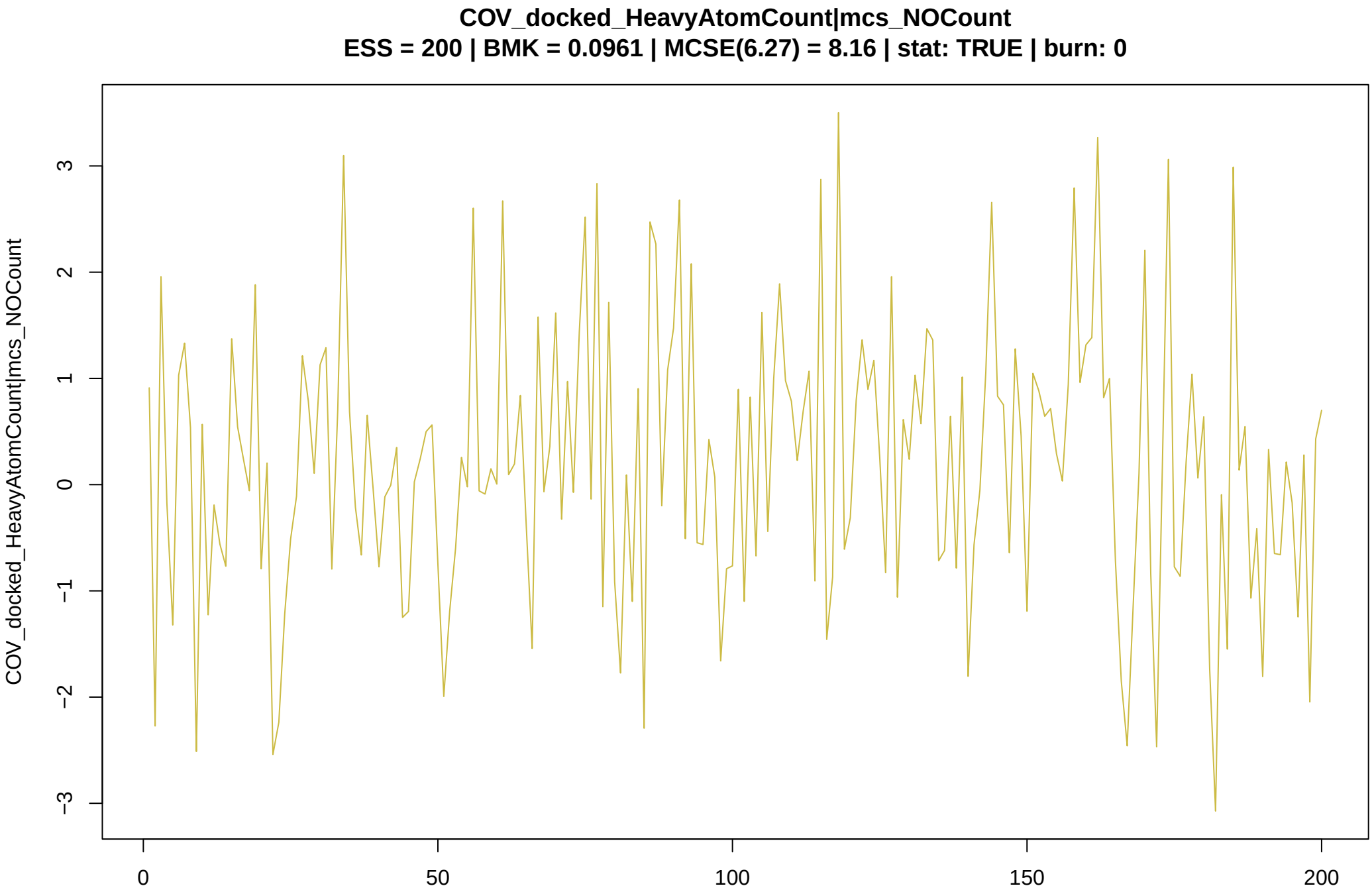

COV_mcs_NumHeteroAtoms|mcs_RingCount
ESS = 200 | BMK = 0.116 | MCSE(6.27) = 6.77 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_RingCount
0.5
0.0
−0.5
−1.0
−1.5
−2.0
0
50
100
150
200

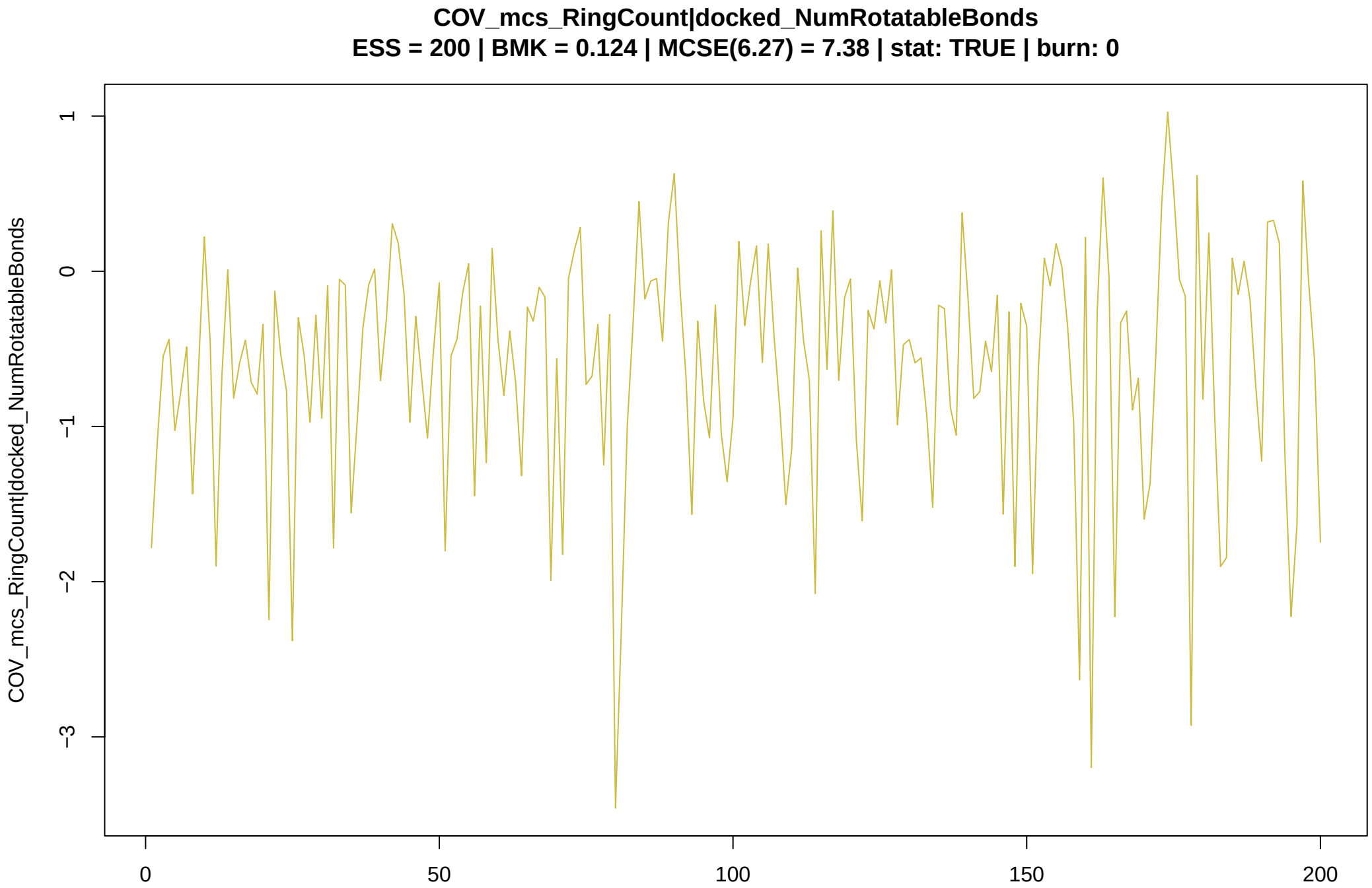

COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
ESS = 200 | BMK = 0.091 | MCSE(6.27) = 6.77 | stat: TRUE | burn: 0
COV_mcs_NumHeteroAtoms|docked_NumRotatableBonds
3
2
1
0
−1
−2
0
50
100
150
200

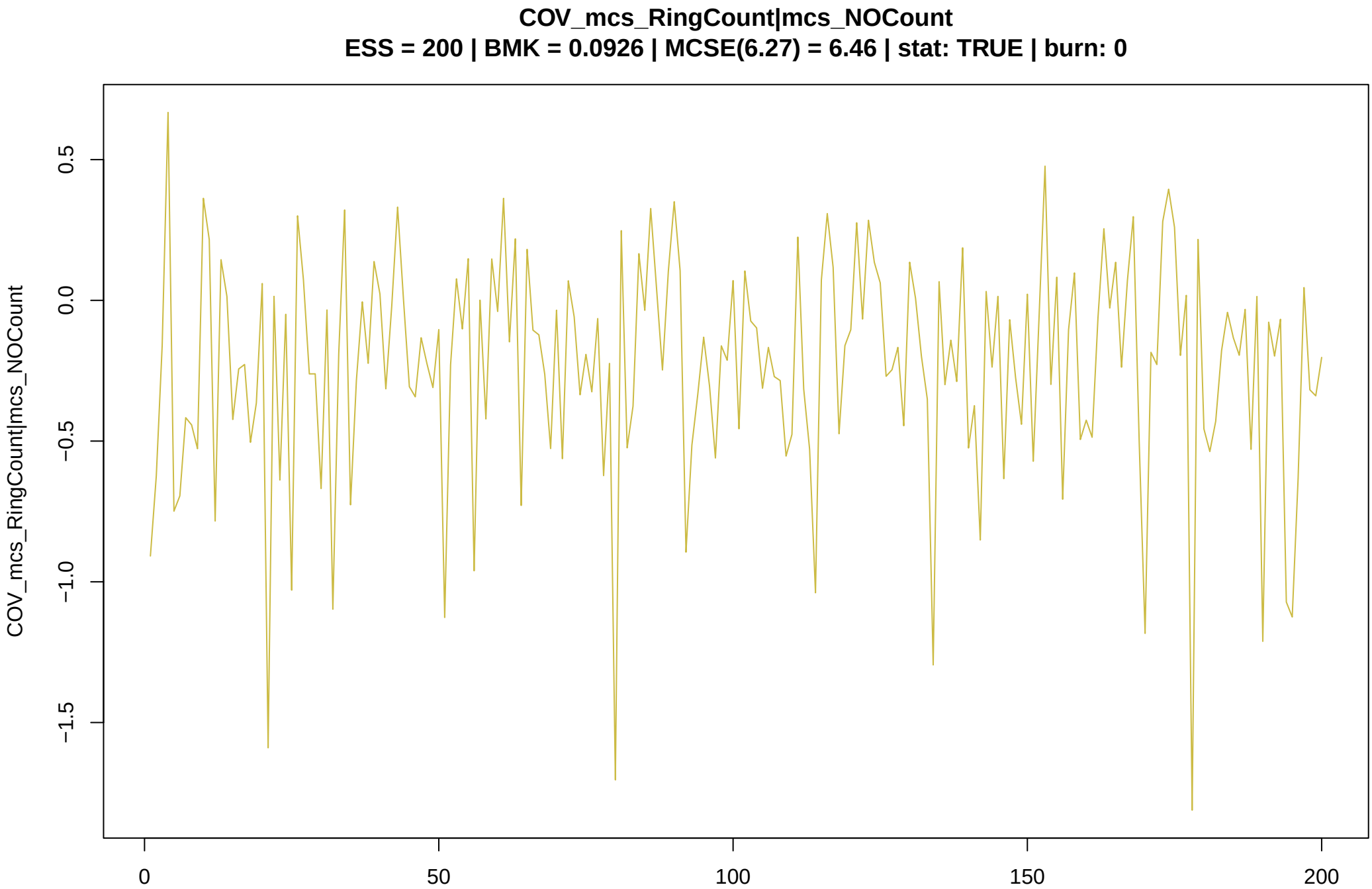

COV_mcs_NumHeteroAtoms|mcs_NOCount
ESS = 38.1 | BMK = 0.192 | MCSE(6.27) = 10.9 | stat: FALSE | burn: 0
COV_mcs_NumHeteroAtoms|mcs_NOCount
0.0
0.5
1.0
1.5
2.0
2.5
0
50
100
150
200

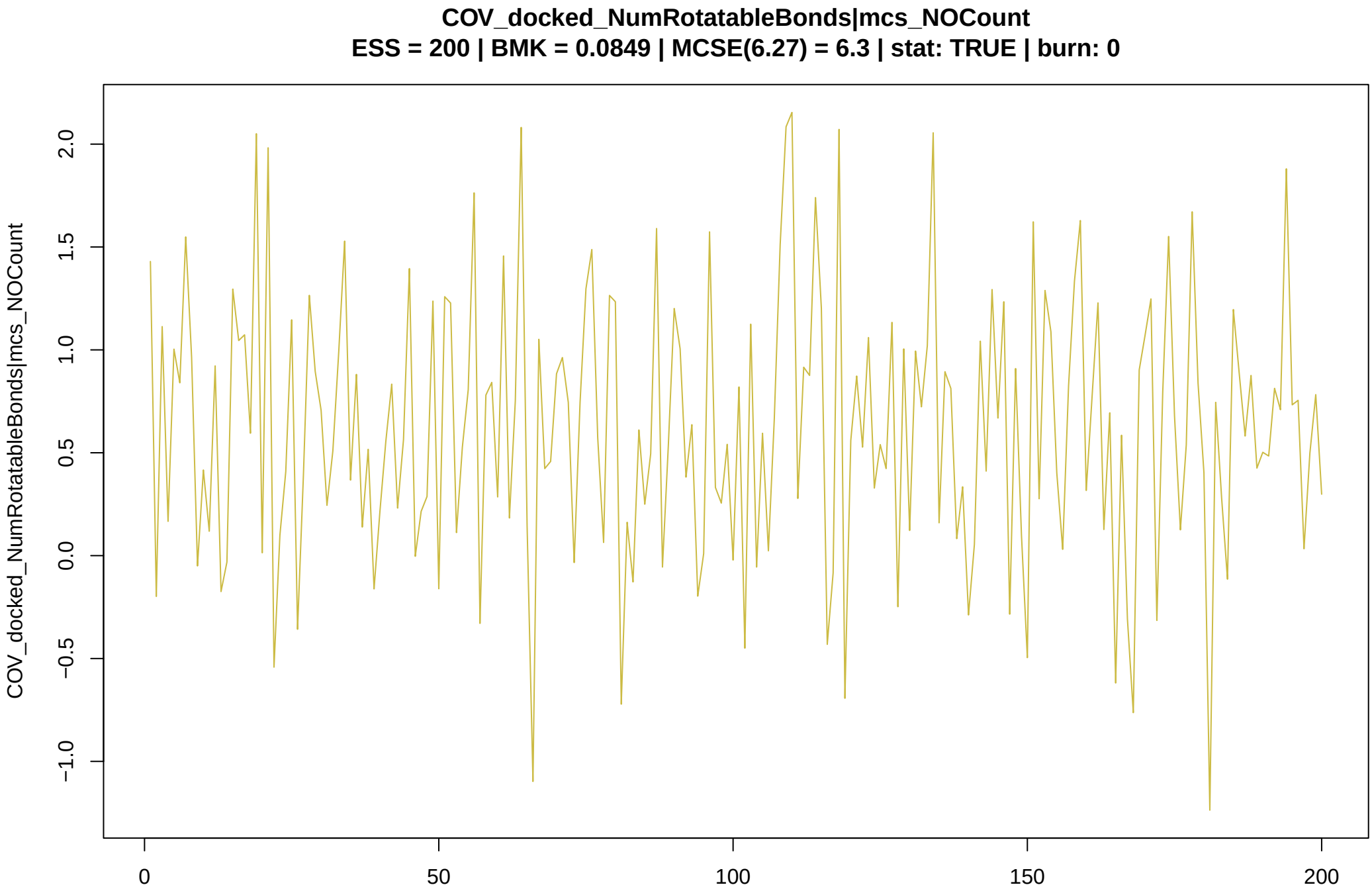

COV_docked_HeavyAtomCount|mcs_RingCount
ESS = 200 | BMK = 0.13 | MCSE(6.27) = 9.24 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_RingCount
4
2
0
−2
0
50
100
150
200


COV_docked_HeavyAtomCount|docked_NumRotatableBonds
ESS = 148 | BMK = 0.152 | MCSE(6.27) = 8.92 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|docked_NumRotatableBonds
0
5
10
0
50
100
150
200


COV_docked_HeavyAtomCount|mcs_NOCount
ESS = 200 | BMK = 0.0961 | MCSE(6.27) = 8.16 | stat: TRUE | burn: 0
COV_docked_HeavyAtomCount|mcs_NOCount
3
2
1
0
−1
−2
−3
0
50
100
150
200


COV_mcs_RingCount|docked_NumRotatableBonds
ESS = 200 | BMK = 0.124 | MCSE(6.27) = 7.38 | stat: TRUE | burn: 0
COV_mcs_RingCount|docked_NumRotatableBonds
1
0
−1
−2
−3
0
50
100
150
200


COV_mcs_RingCount|mcs_NOCount
ESS = 200 | BMK = 0.0926 | MCSE(6.27) = 6.46 | stat: TRUE | burn: 0
COV_mcs_RingCount|mcs_NOCount
0.5
0.0
−0.5
−1.0
−1.5
0
50
100
150
200


COV_docked_NumRotatableBonds|mcs_NOCount
ESS = 200 | BMK = 0.0849 | MCSE(6.27) = 6.3 | stat: TRUE | burn: 0
COV_docked_NumRotatableBonds|mcs_NOCount
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
0
50
100
150
200