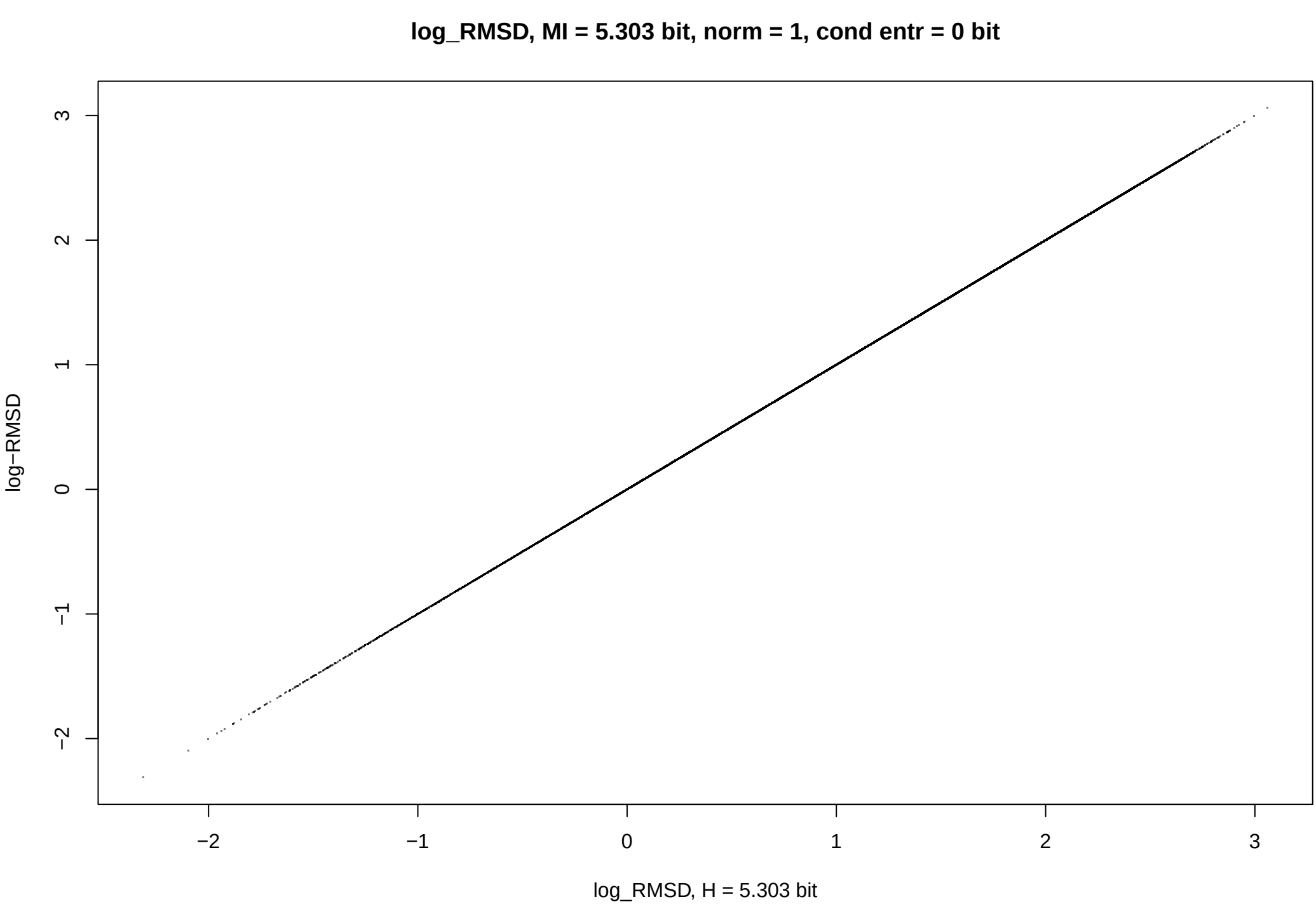
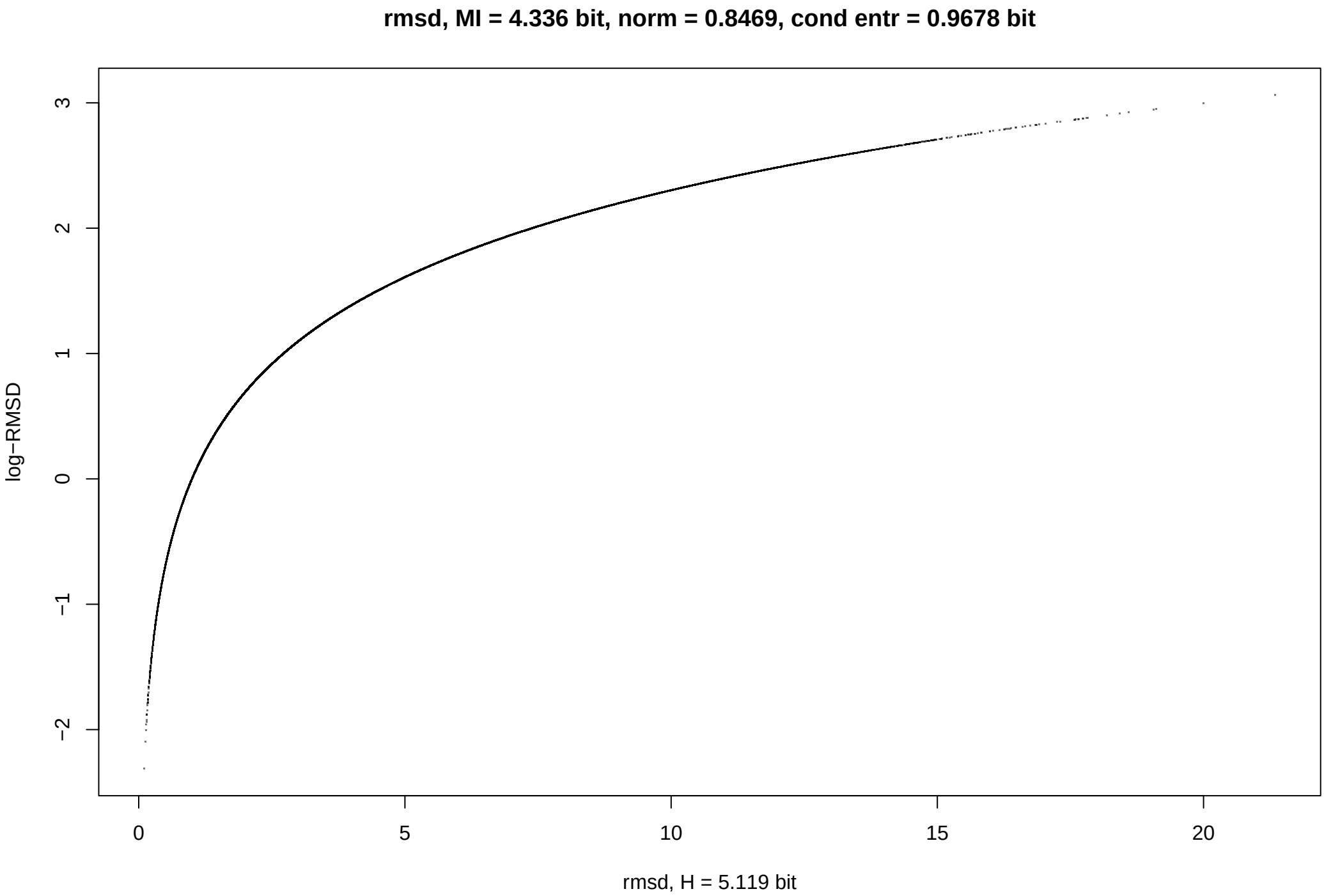
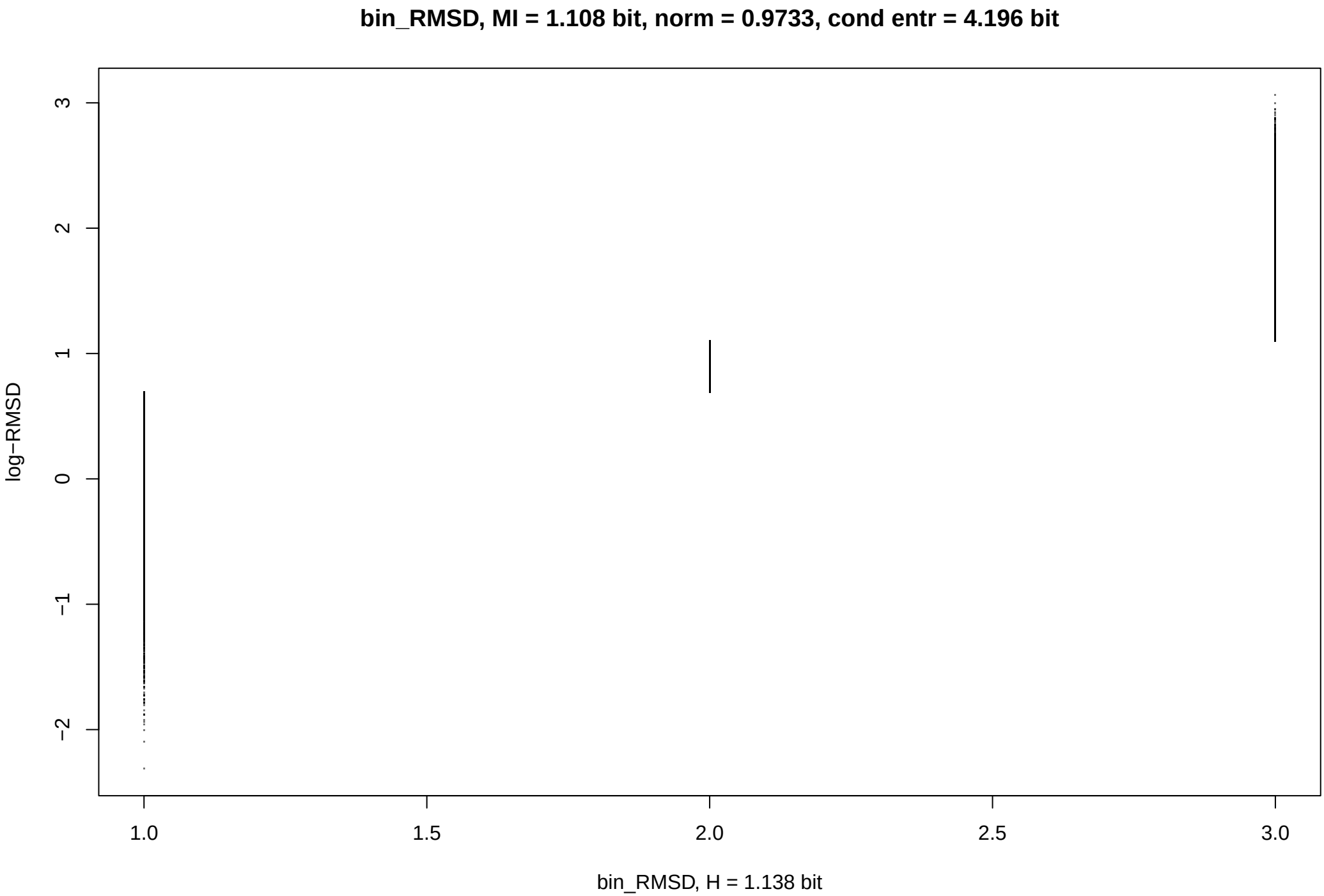
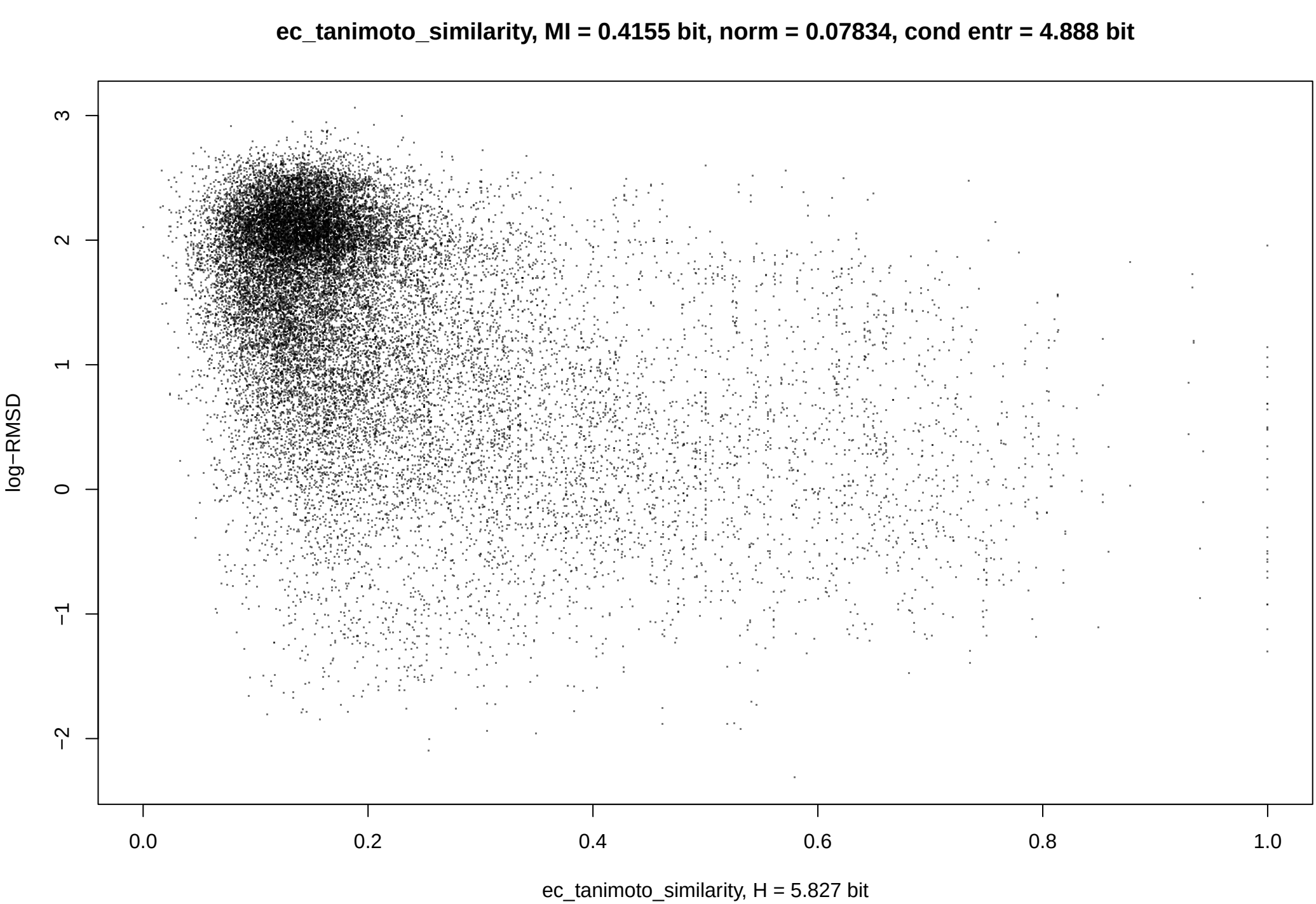
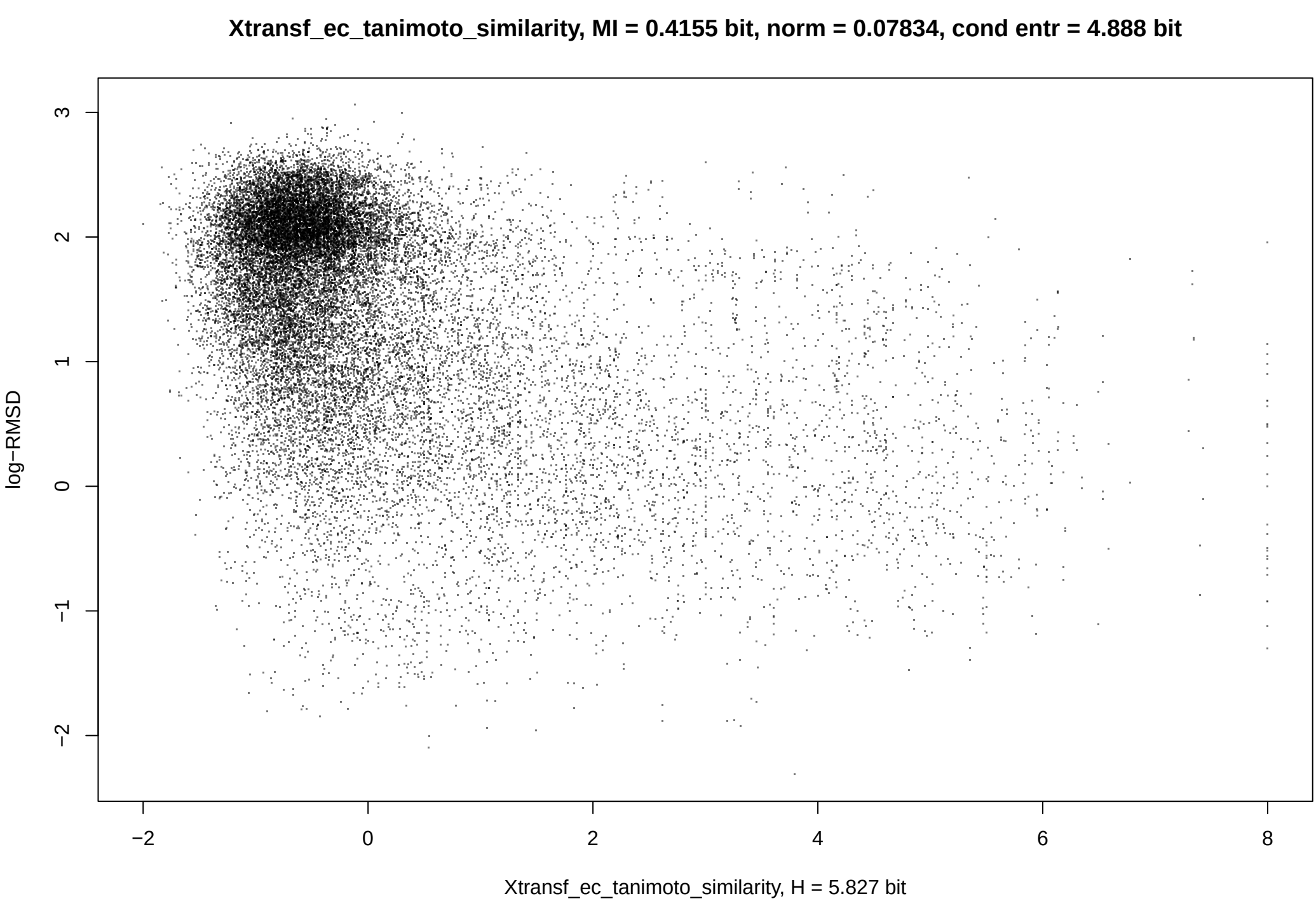
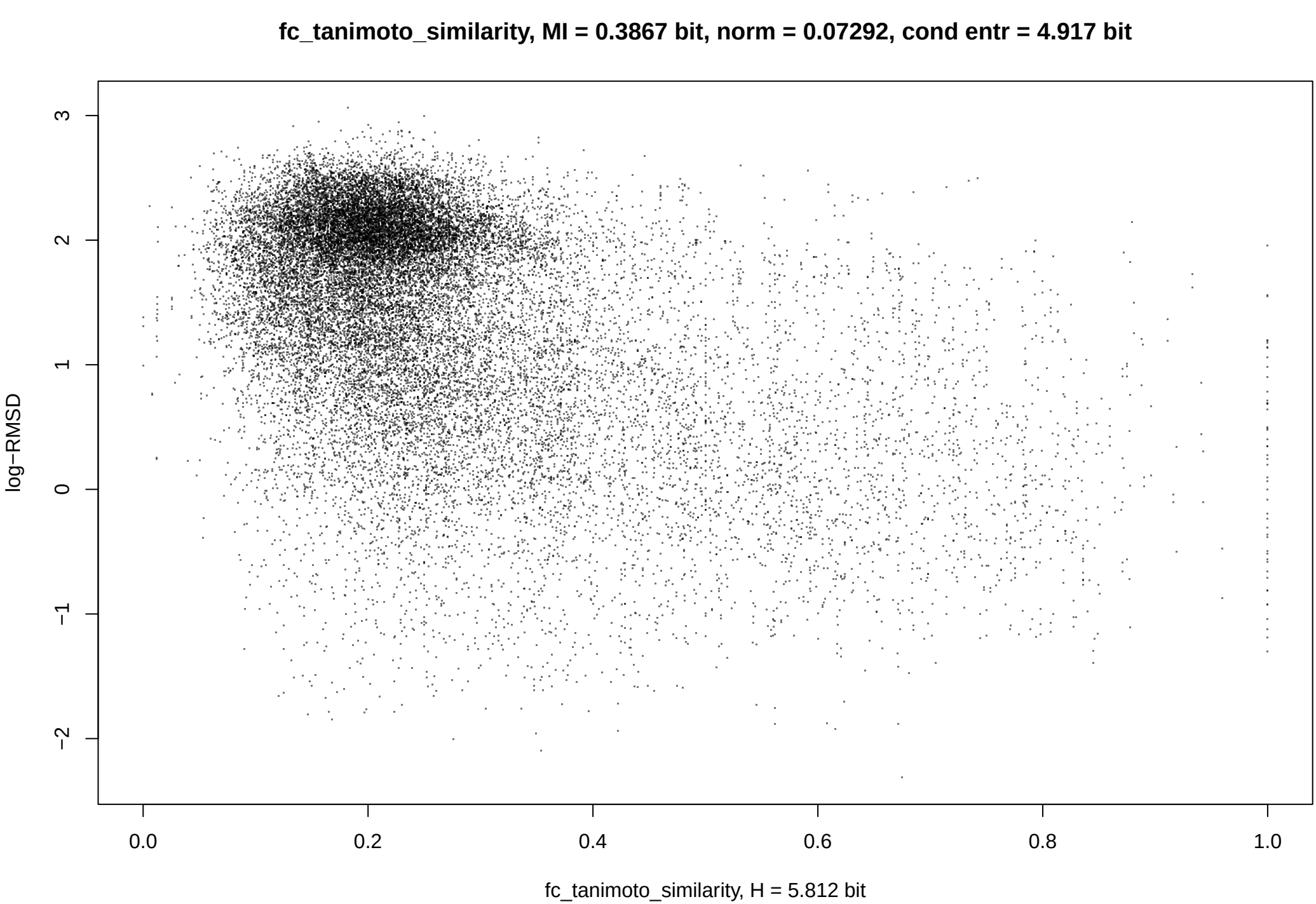

log_RMSD, MI = 5.303 bit, norm = 1, cond entr = 0 bit
log−RMSD
3
2
1
0
−1
−2
−2
−1
0
1
2
3
log_RMSD, H = 5.303 bit

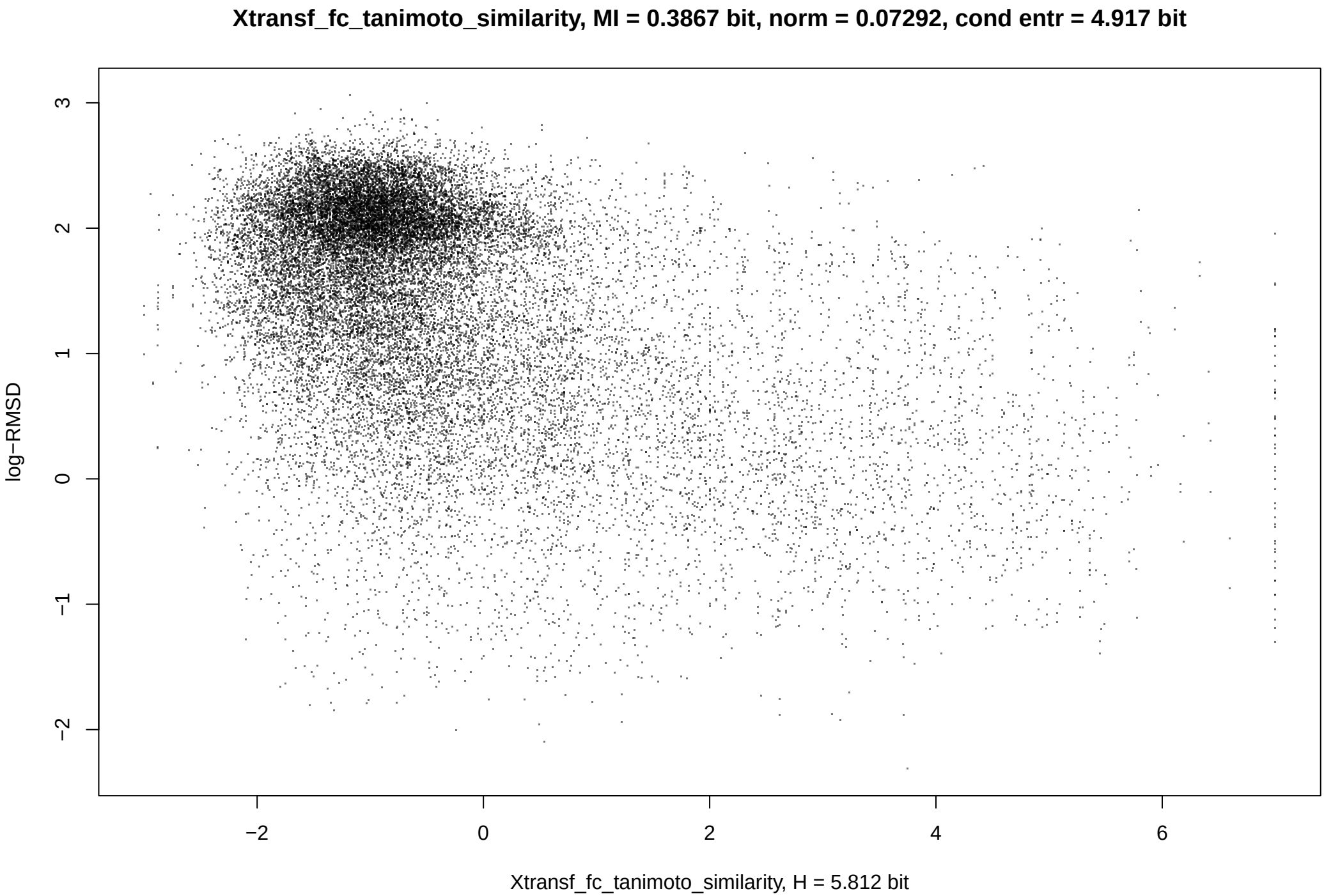

rmsd, MI = 4.336 bit, norm = 0.8469, cond entr = 0.9678 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
20
rmsd, H = 5.119 bit

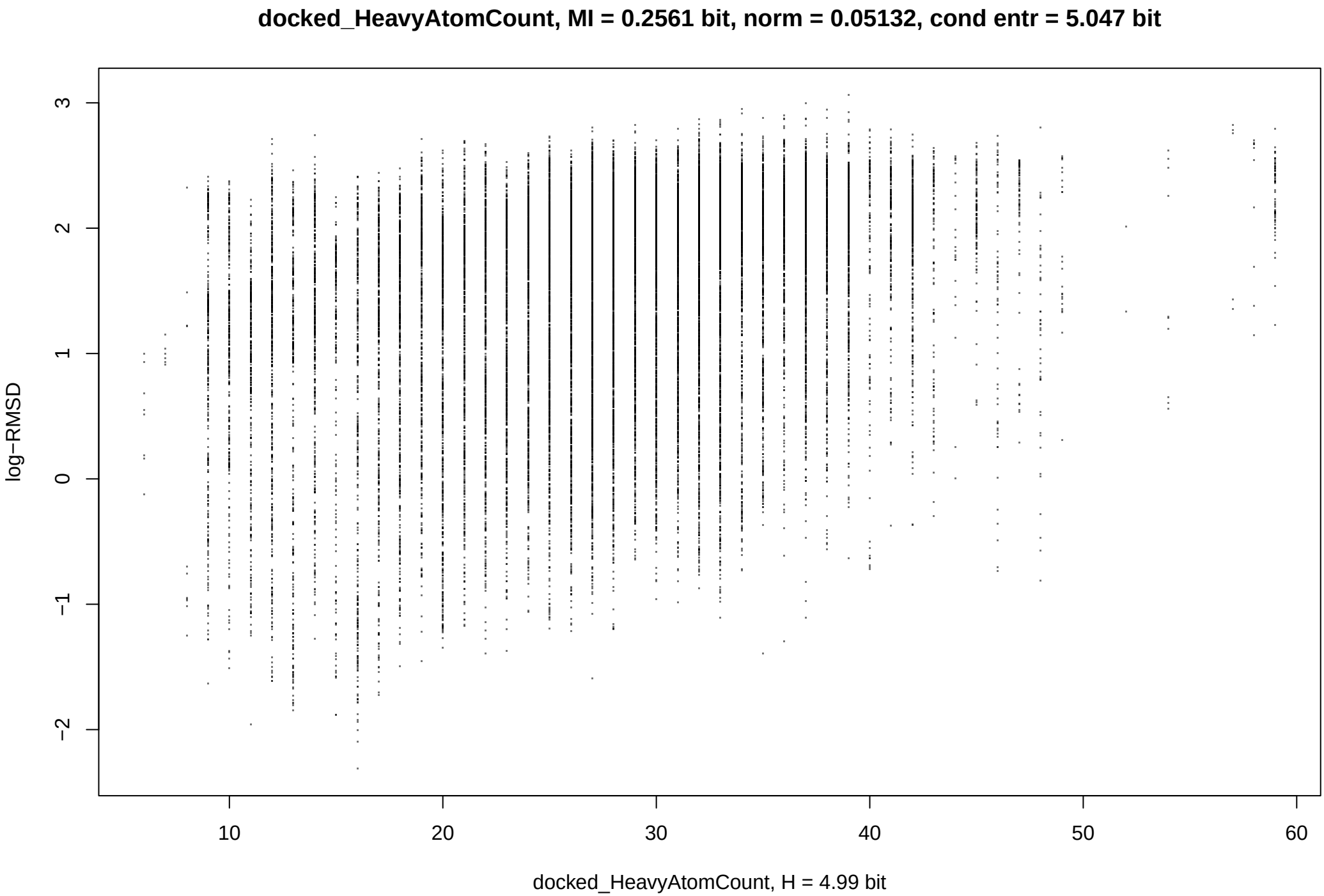

bin_RMSD, MI = 1.108 bit, norm = 0.9733, cond entr = 4.196 bit
log−RMSD
3
2
1
0
−1
−2
1.0
1.5
2.0
2.5
3.0
bin_RMSD, H = 1.138 bit

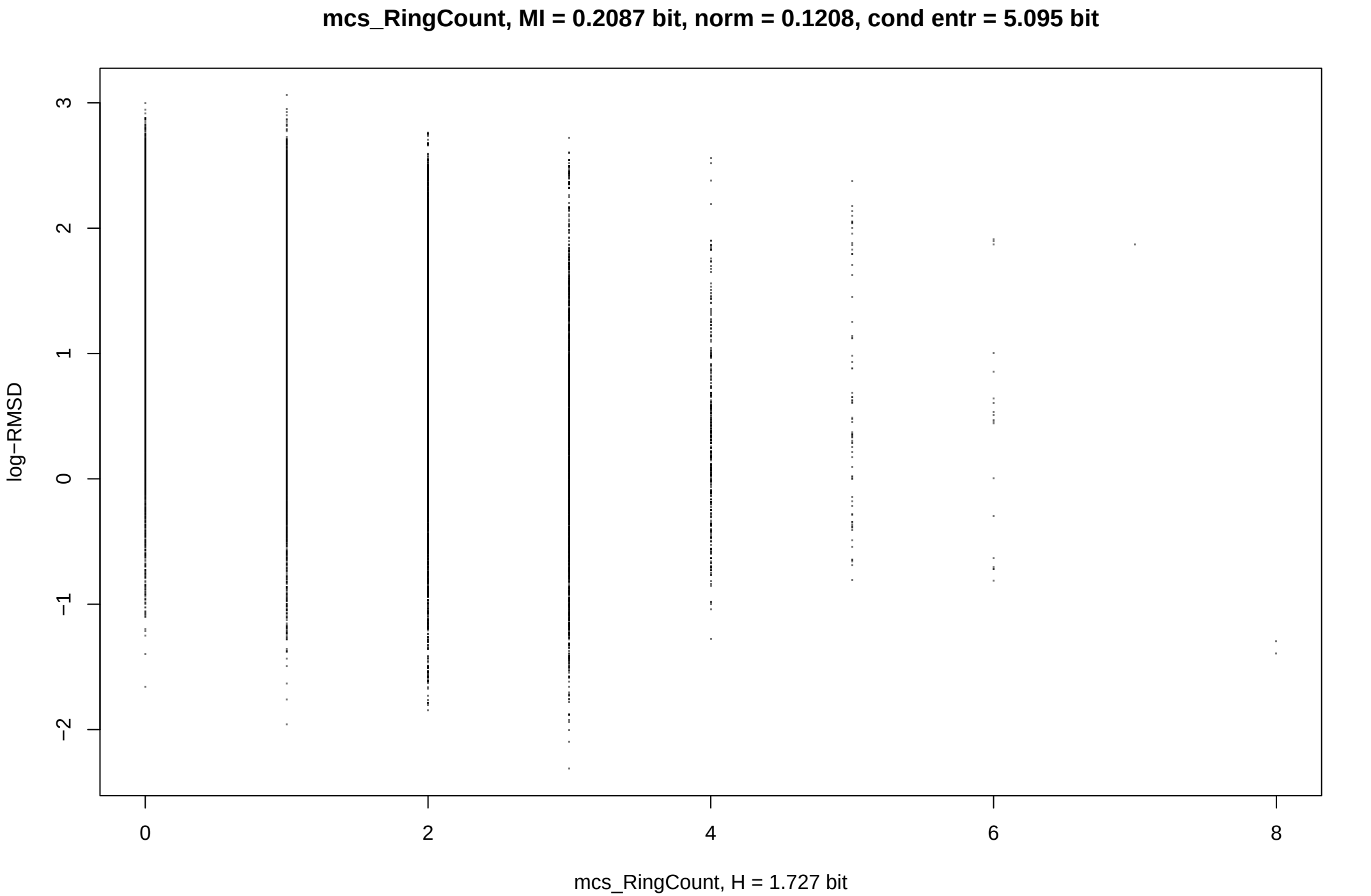

ec_tanimoto_similarity, MI = 0.4155 bit, norm = 0.07834, cond entr = 4.888 bit
log−RMSD
3
2
1
0
−1
−2
0.0
0.2
0.4
0.6
0.8
1.0
ec_tanimoto_similarity, H = 5.827 bit

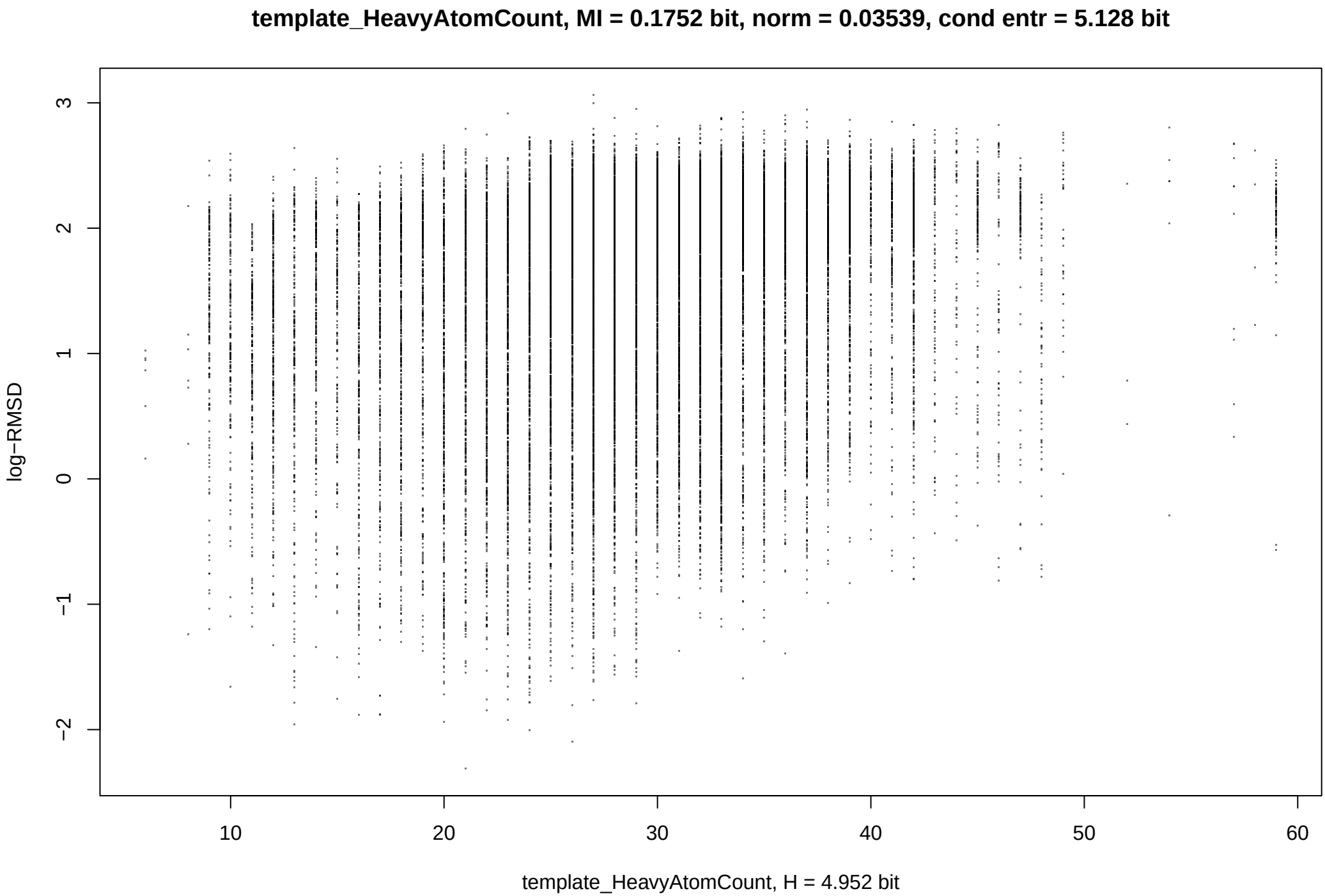

Xtransf_ec_tanimoto_similarity, MI = 0.4155 bit, norm = 0.07834, cond entr = 4.888 bit
log−RMSD
3
2
1
0
−1
−2
−2
0
2
4
6
8
Xtransf_ec_tanimoto_similarity, H = 5.827 bit

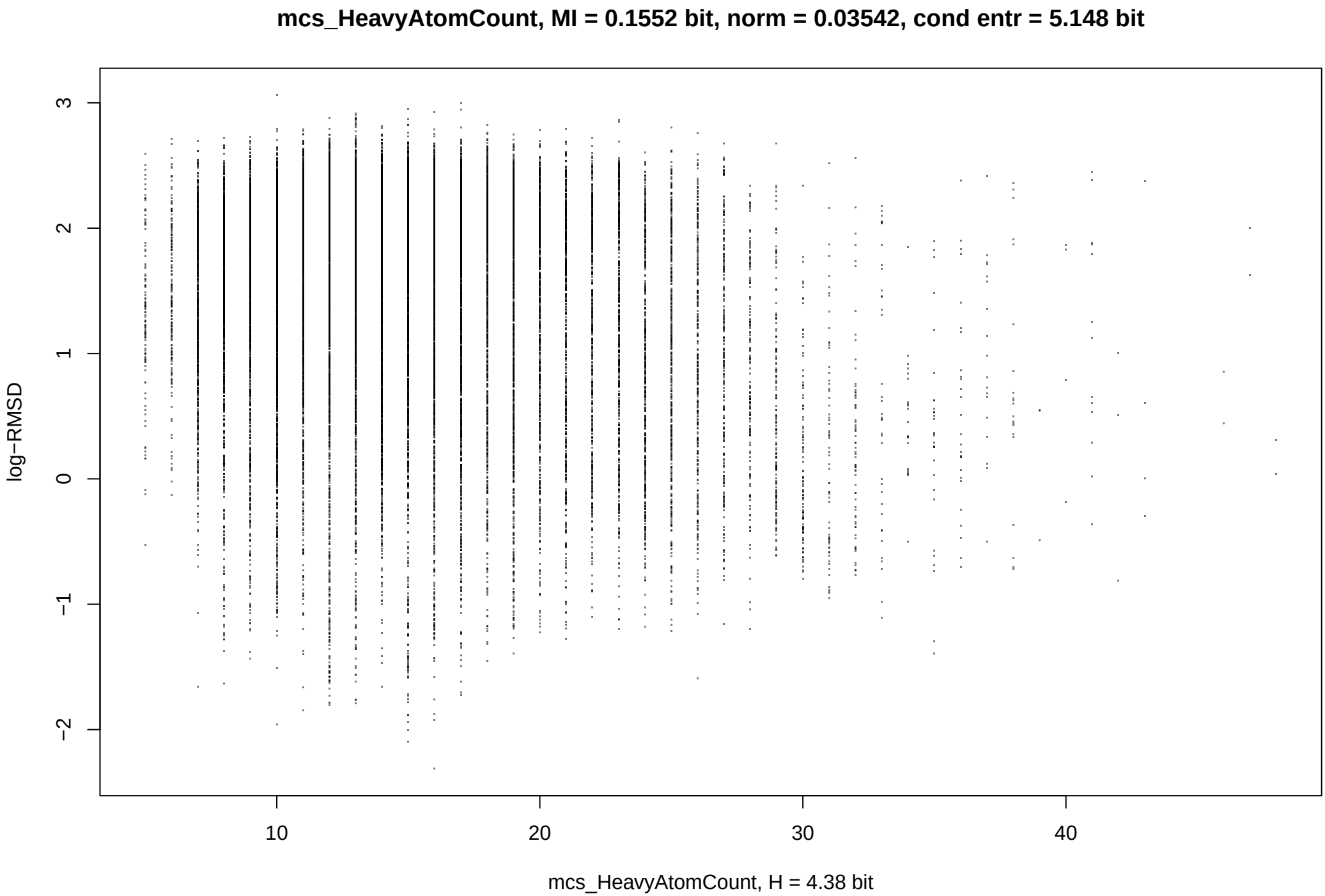

fc_tanimoto_similarity, MI = 0.3867 bit, norm = 0.07292, cond entr = 4.917 bit
log−RMSD
3
2
1
0
−1
−2
0.0
0.2
0.4
0.6
0.8
1.0
fc_tanimoto_similarity, H = 5.812 bit

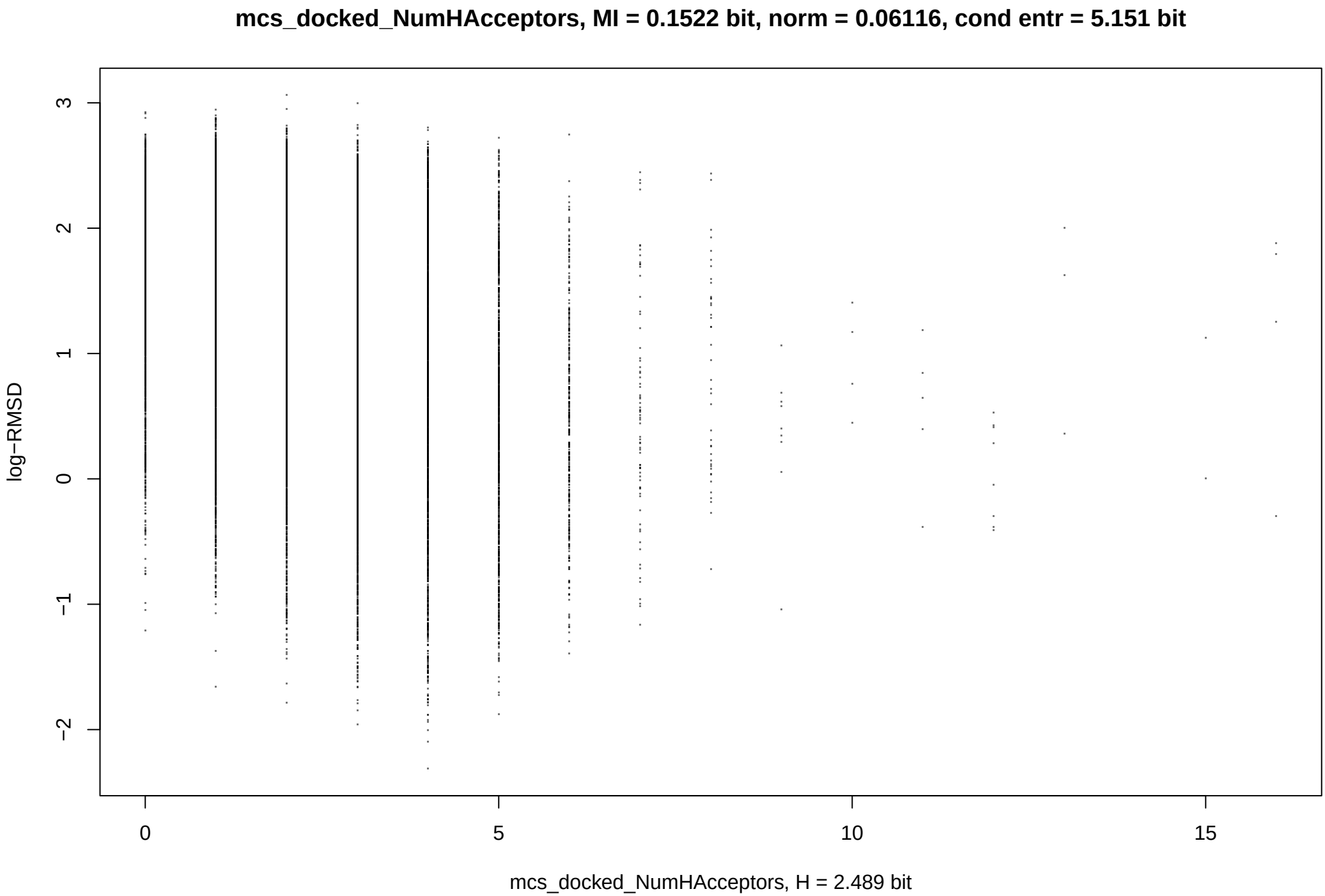

Xtransf_fc_tanimoto_similarity, MI = 0.3867 bit, norm = 0.07292, cond entr = 4.917 bit
log−RMSD
3
2
1
0
−1
−2
−2
0
2
4
6
Xtransf_fc_tanimoto_similarity, H = 5.812 bit

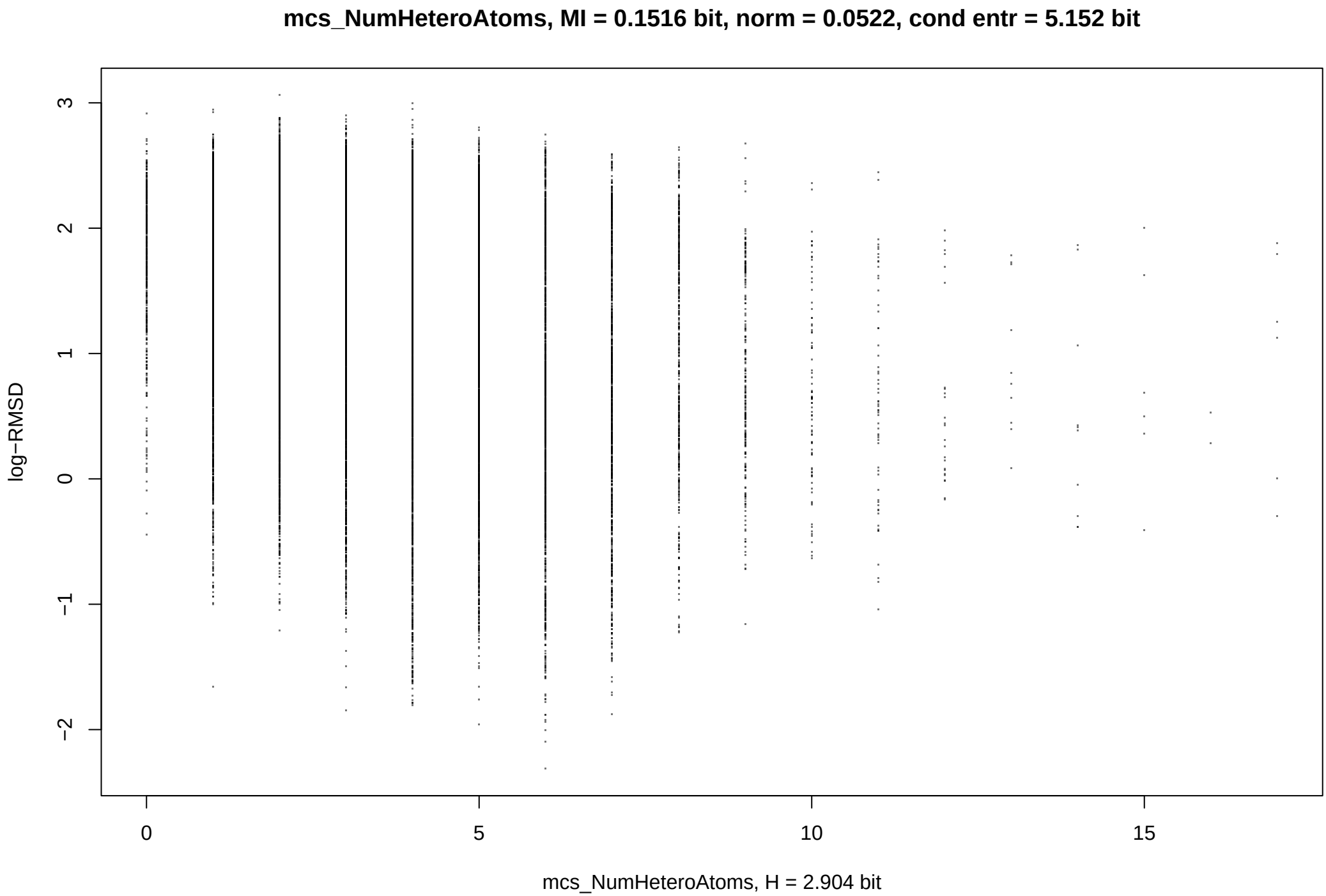

docked_HeavyAtomCount, MI = 0.2561 bit, norm = 0.05132, cond entr = 5.047 bit
log−RMSD
3
2
1
0
−1
−2
10
20
30
40
50
60
docked_HeavyAtomCount, H = 4.99 bit

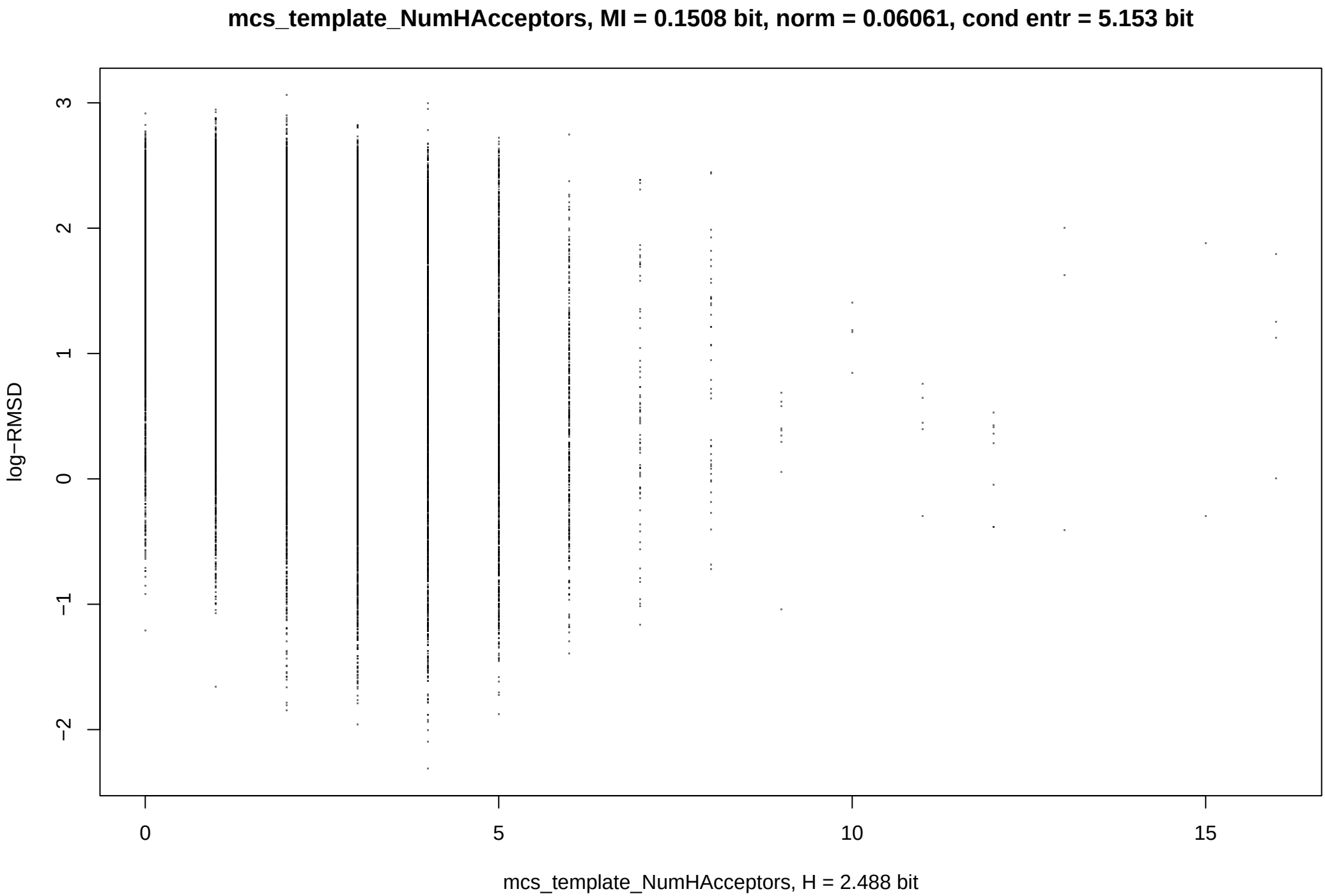

mcs_RingCount, MI = 0.2087 bit, norm = 0.1208, cond entr = 5.095 bit
log−RMSD
3
2
1
0
−1
−2
0
2
4
6
8
mcs_RingCount, H = 1.727 bit

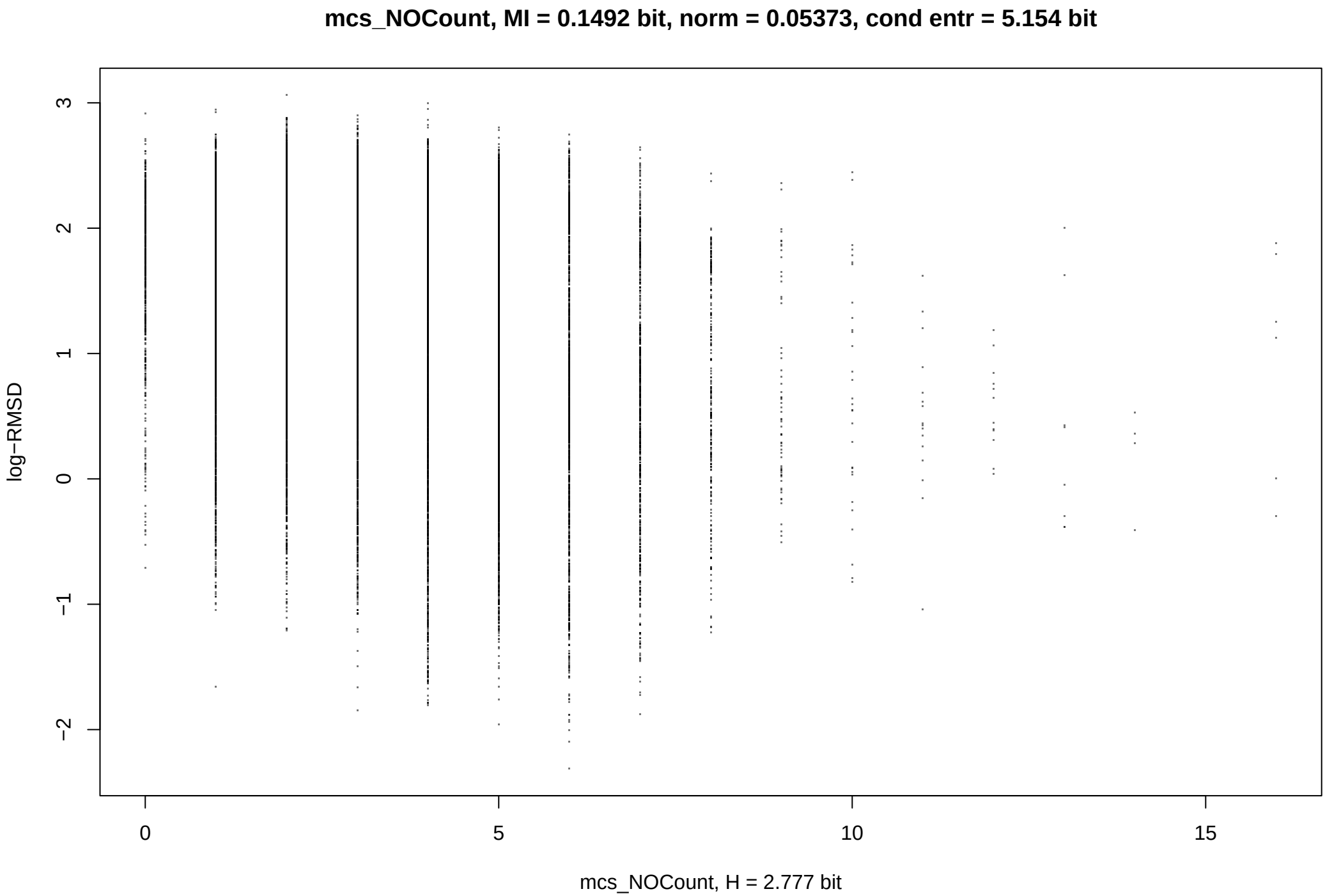

template_HeavyAtomCount, MI = 0.1752 bit, norm = 0.03539, cond entr = 5.128 bit
log−RMSD
3
2
1
0
−1
−2
10
20
30
40
50
60
template_HeavyAtomCount, H = 4.952 bit

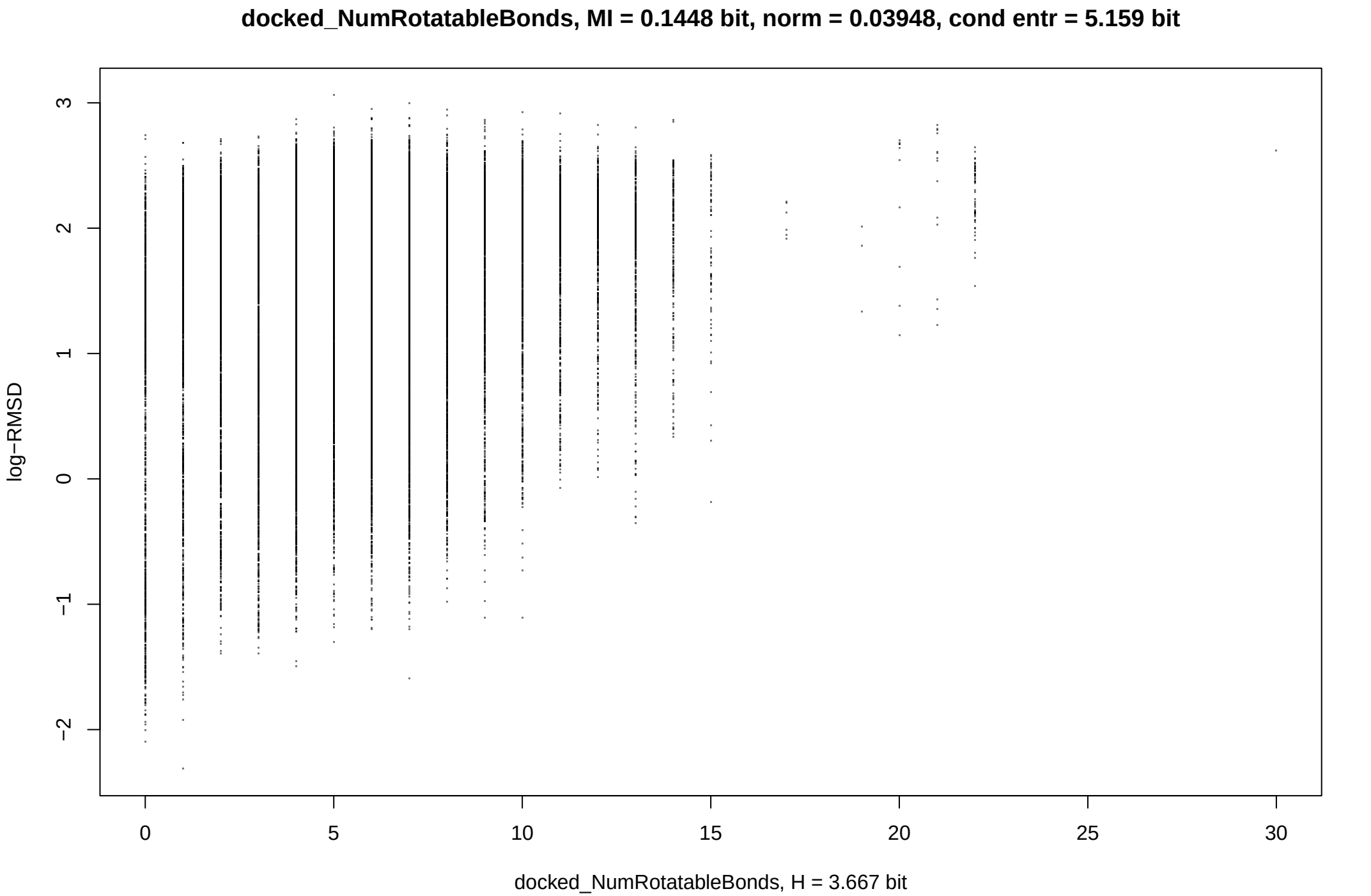

mcs_HeavyAtomCount, MI = 0.1552 bit, norm = 0.03542, cond entr = 5.148 bit
log−RMSD
3
2
1
0
−1
−2
10
20
30
40
mcs_HeavyAtomCount, H = 4.38 bit

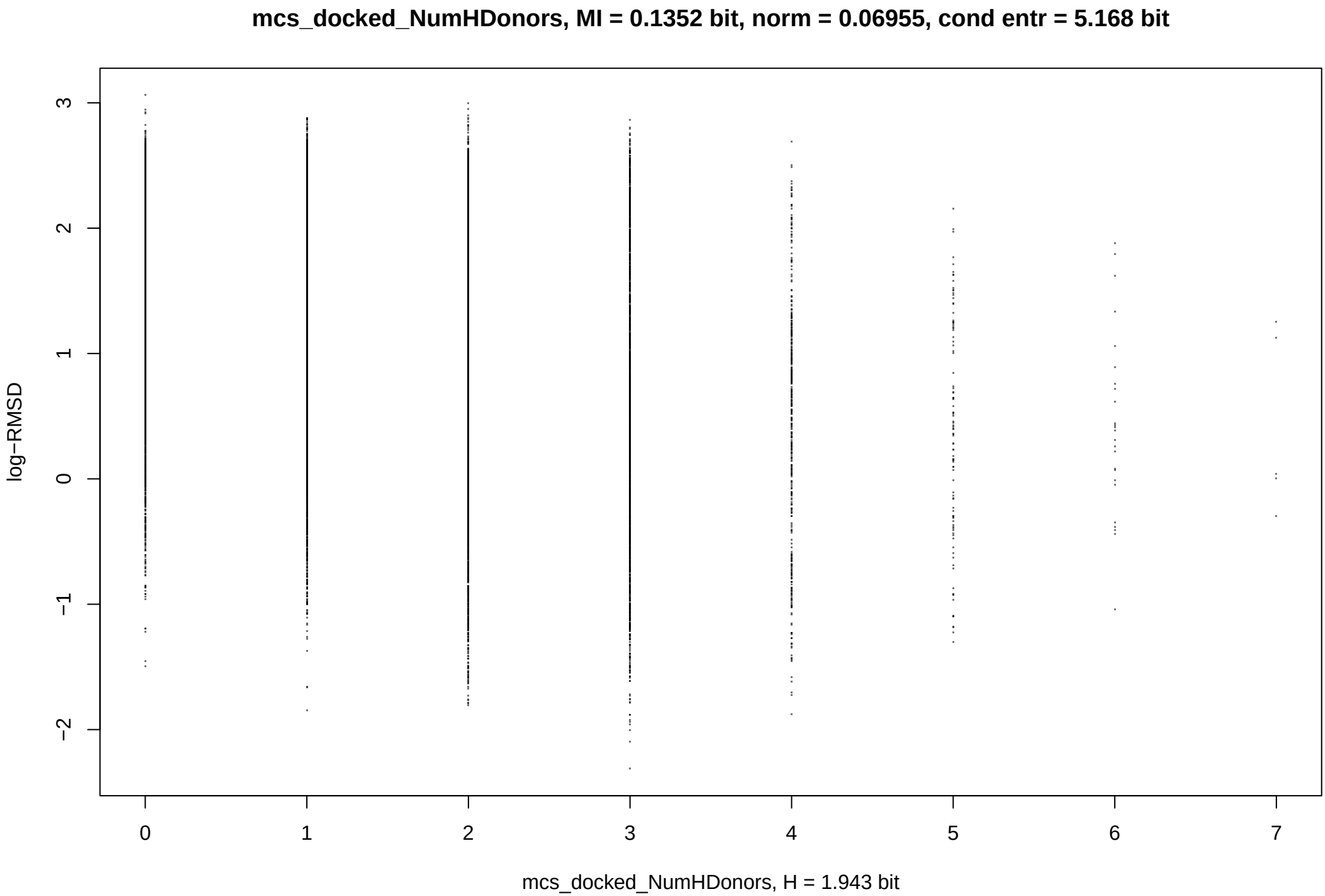

mcs_docked_NumHAcceptors, MI = 0.1522 bit, norm = 0.06116, cond entr = 5.151 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
mcs_docked_NumHAcceptors, H = 2.489 bit

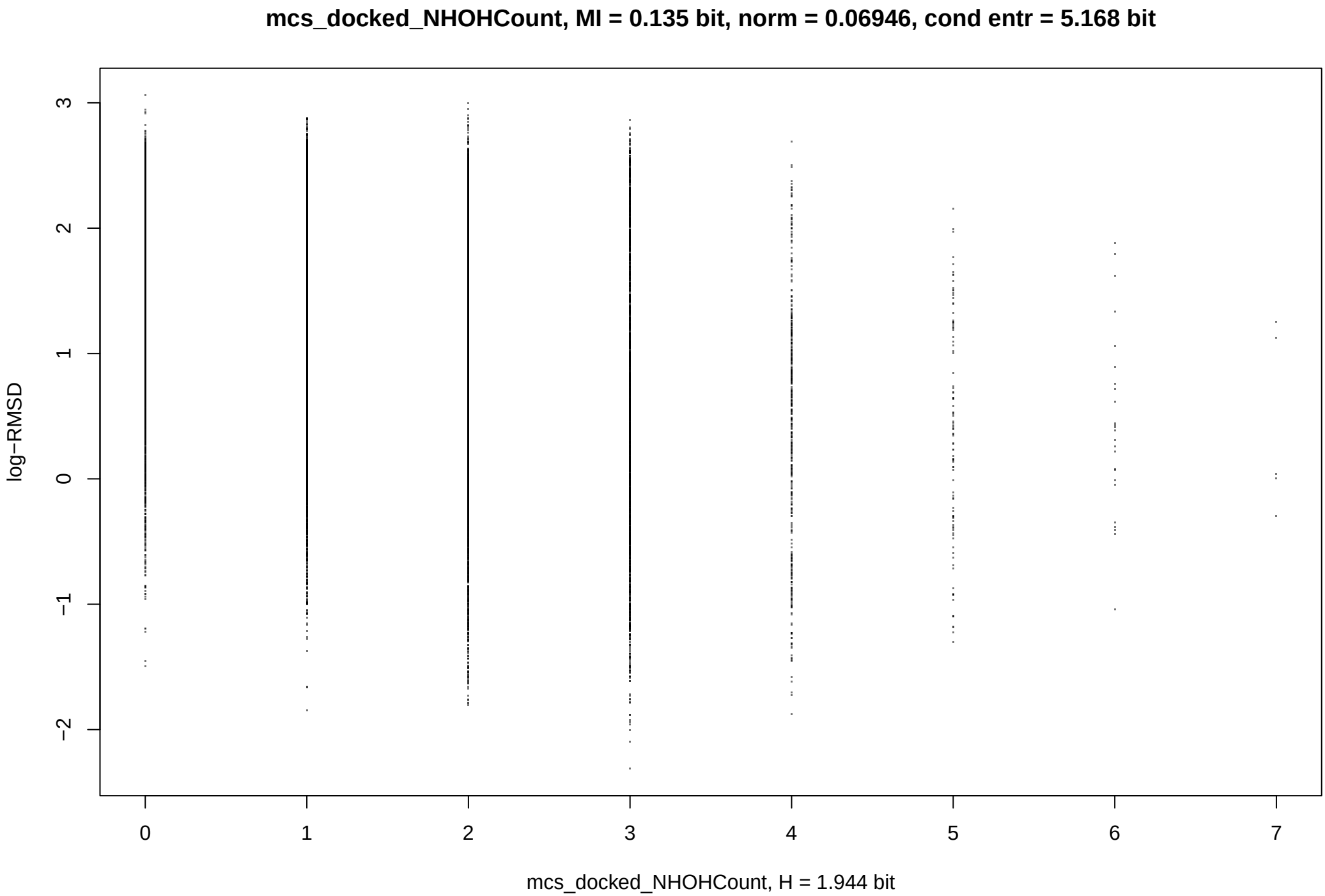

mcs_NumHeteroAtoms, MI = 0.1516 bit, norm = 0.0522, cond entr = 5.152 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
mcs_NumHeteroAtoms, H = 2.904 bit

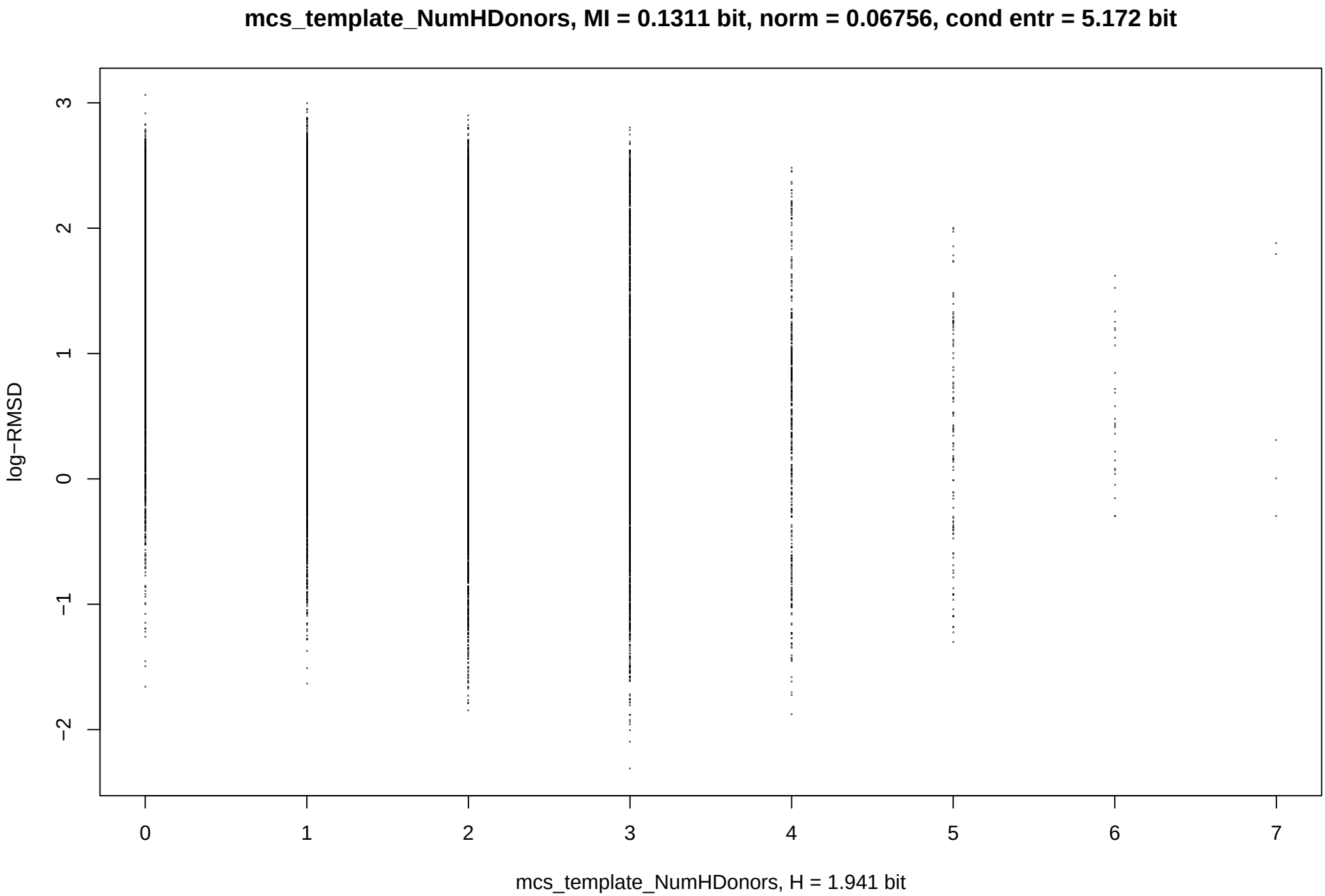

mcs_template_NumHAcceptors, MI = 0.1508 bit, norm = 0.06061, cond entr = 5.153 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
mcs_template_NumHAcceptors, H = 2.488 bit

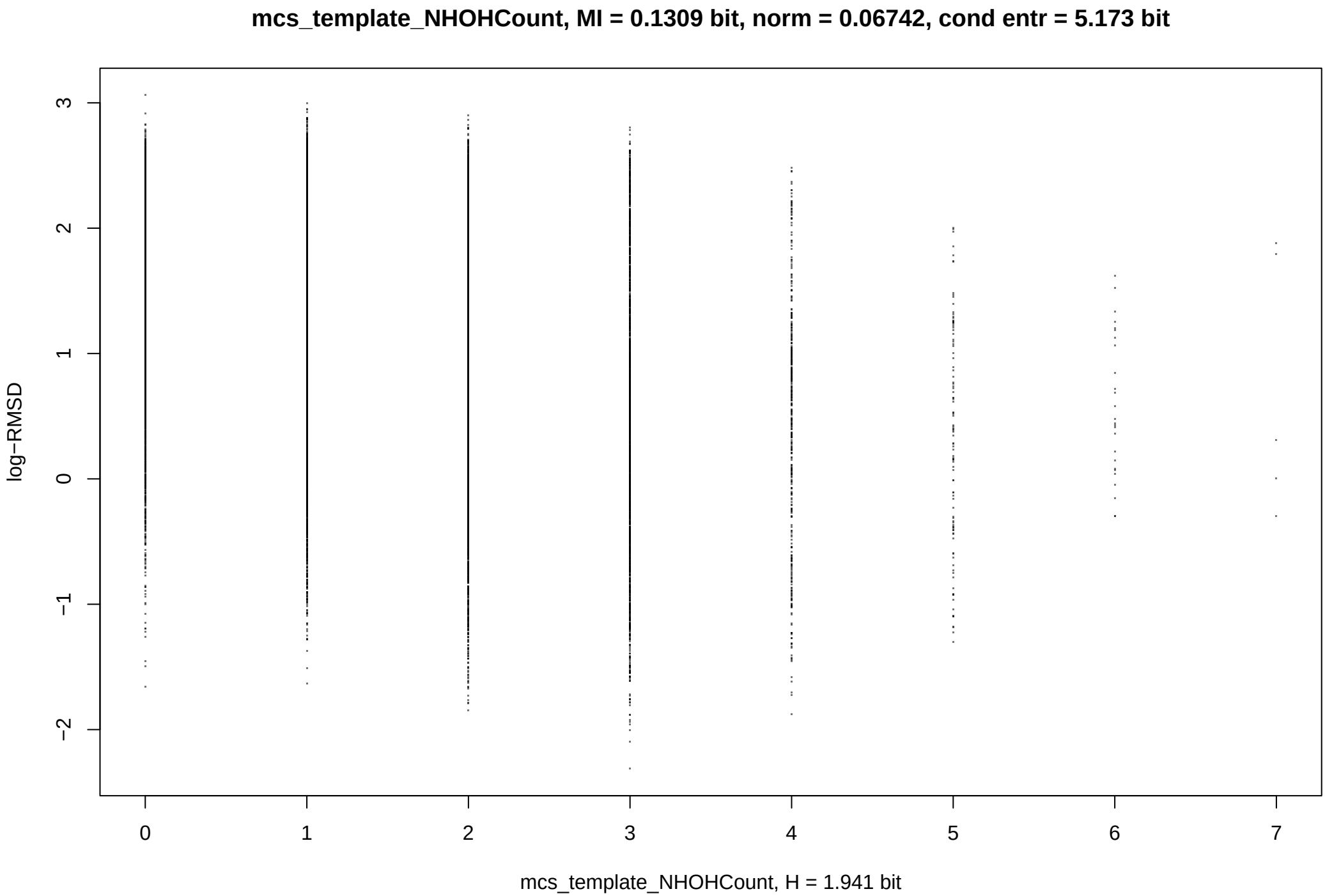

mcs_NOCount, MI = 0.1492 bit, norm = 0.05373, cond entr = 5.154 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
mcs_NOCount, H = 2.777 bit

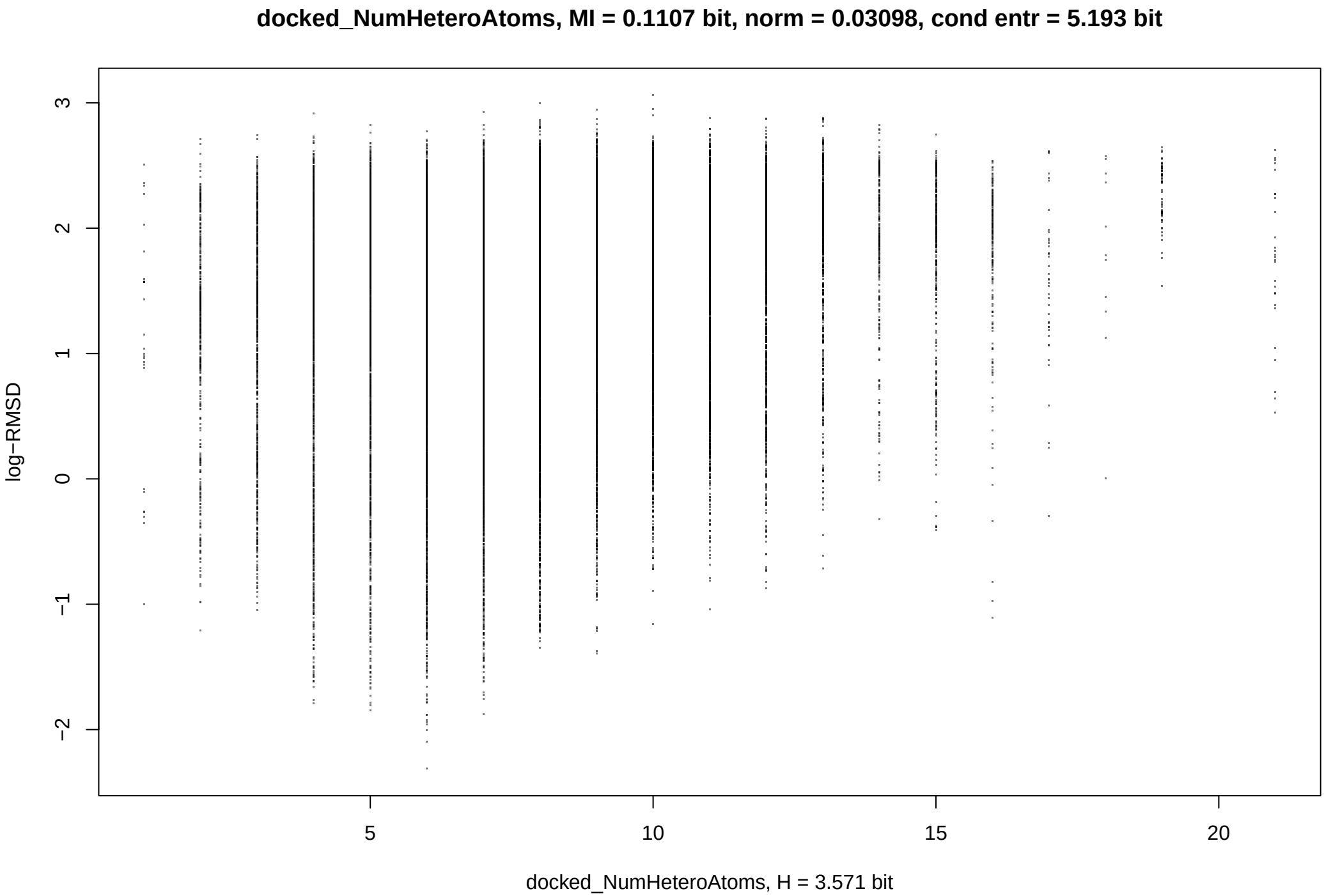

docked_NumRotatableBonds, MI = 0.1448 bit, norm = 0.03948, cond entr = 5.159 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
20
25
30
docked_NumRotatableBonds, H = 3.667 bit

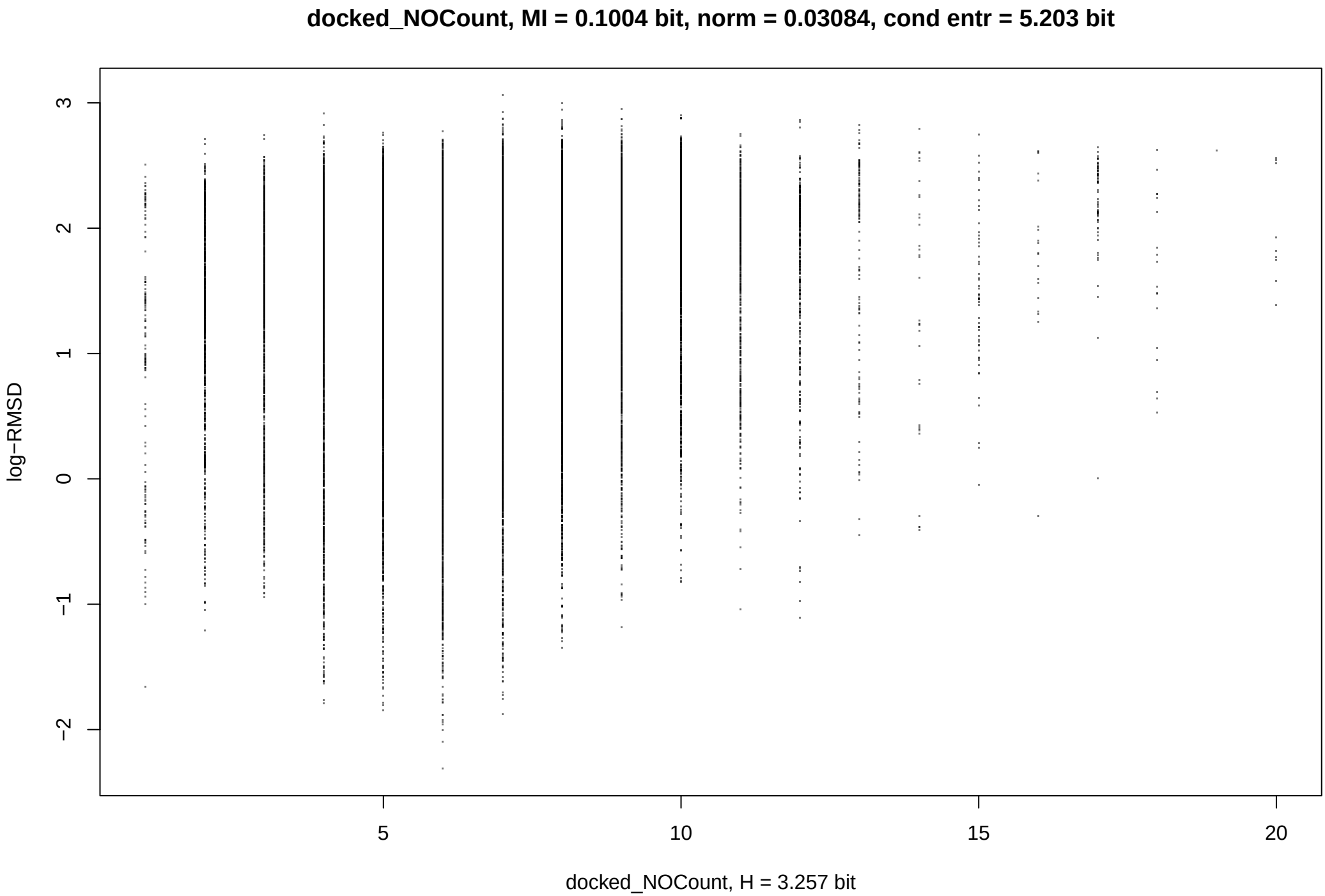

mcs_docked_NumHDonors, MI = 0.1352 bit, norm = 0.06955, cond entr = 5.168 bit
log−RMSD
3
2
1
0
−1
−2
0
1
2
3
4
5
6
7
mcs_docked_NumHDonors, H = 1.943 bit

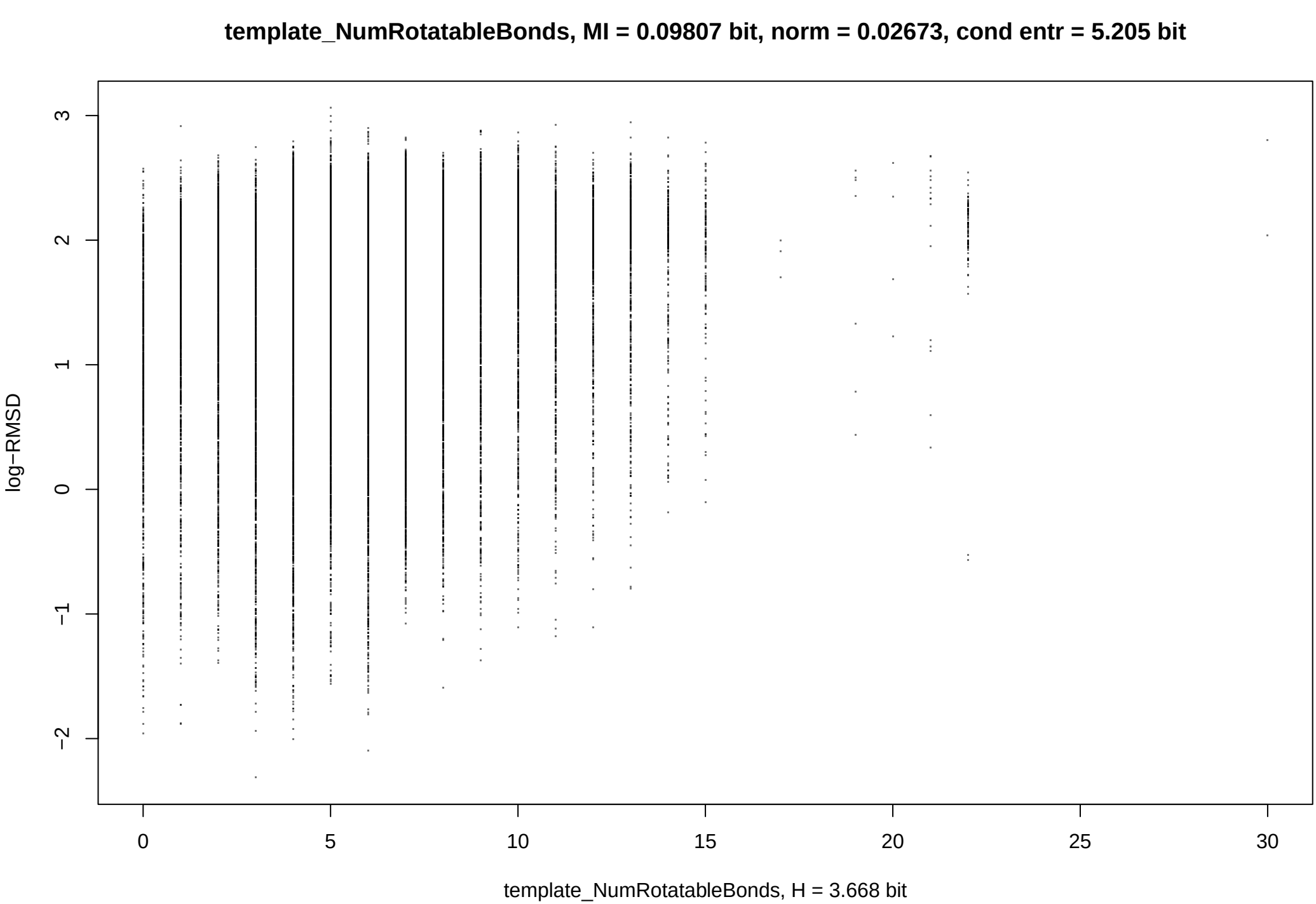

mcs_docked_NHOHCount, MI = 0.135 bit, norm = 0.06946, cond entr = 5.168 bit
log−RMSD
3
2
1
0
−1
−2
0
1
2
3
4
5
6
7
mcs_docked_NHOHCount, H = 1.944 bit

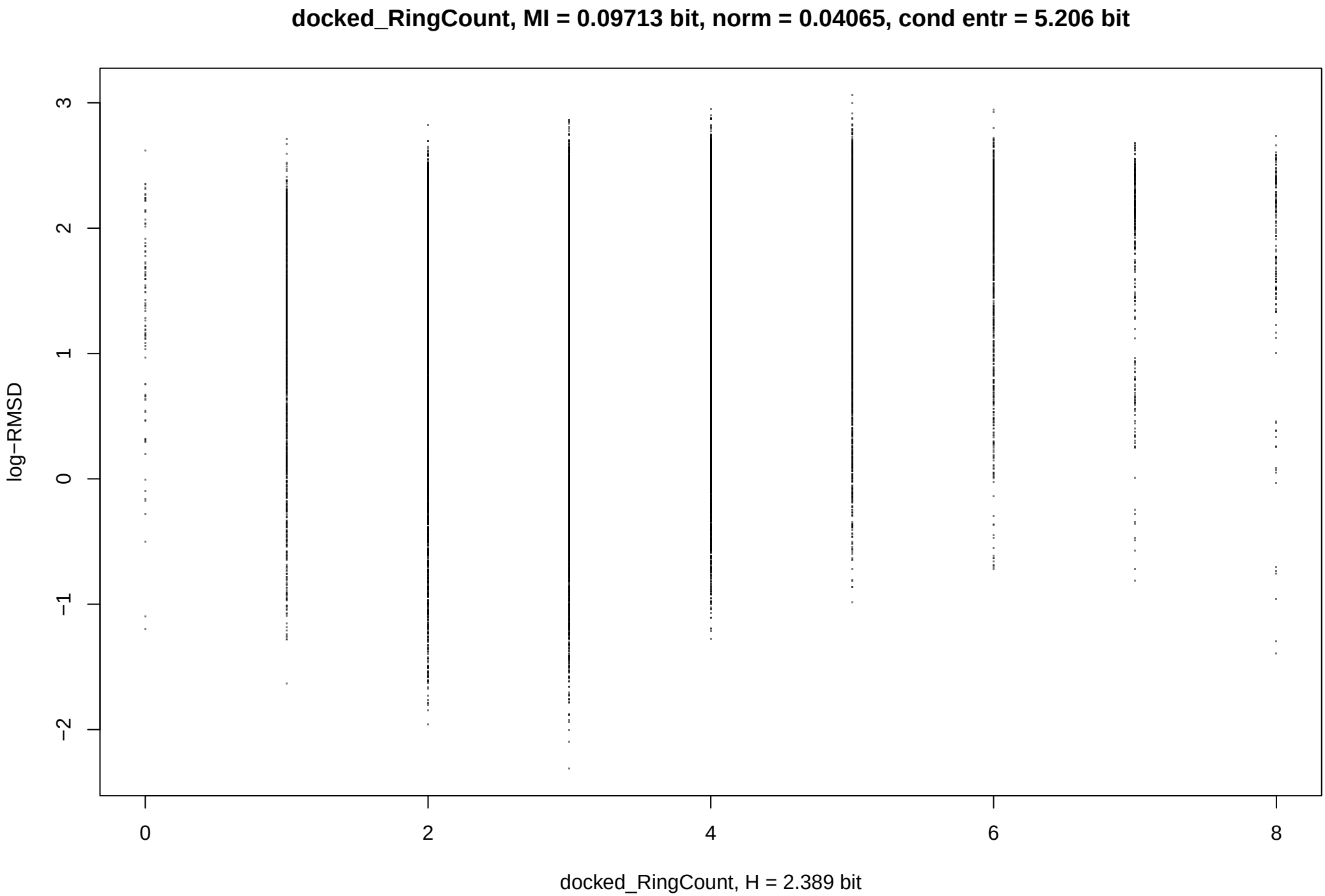

mcs_template_NumHDonors, MI = 0.1311 bit, norm = 0.06756, cond entr = 5.172 bit
log−RMSD
3
2
1
0
−1
−2
0
1
2
3
4
5
6
7
mcs_template_NumHDonors, H = 1.941 bit

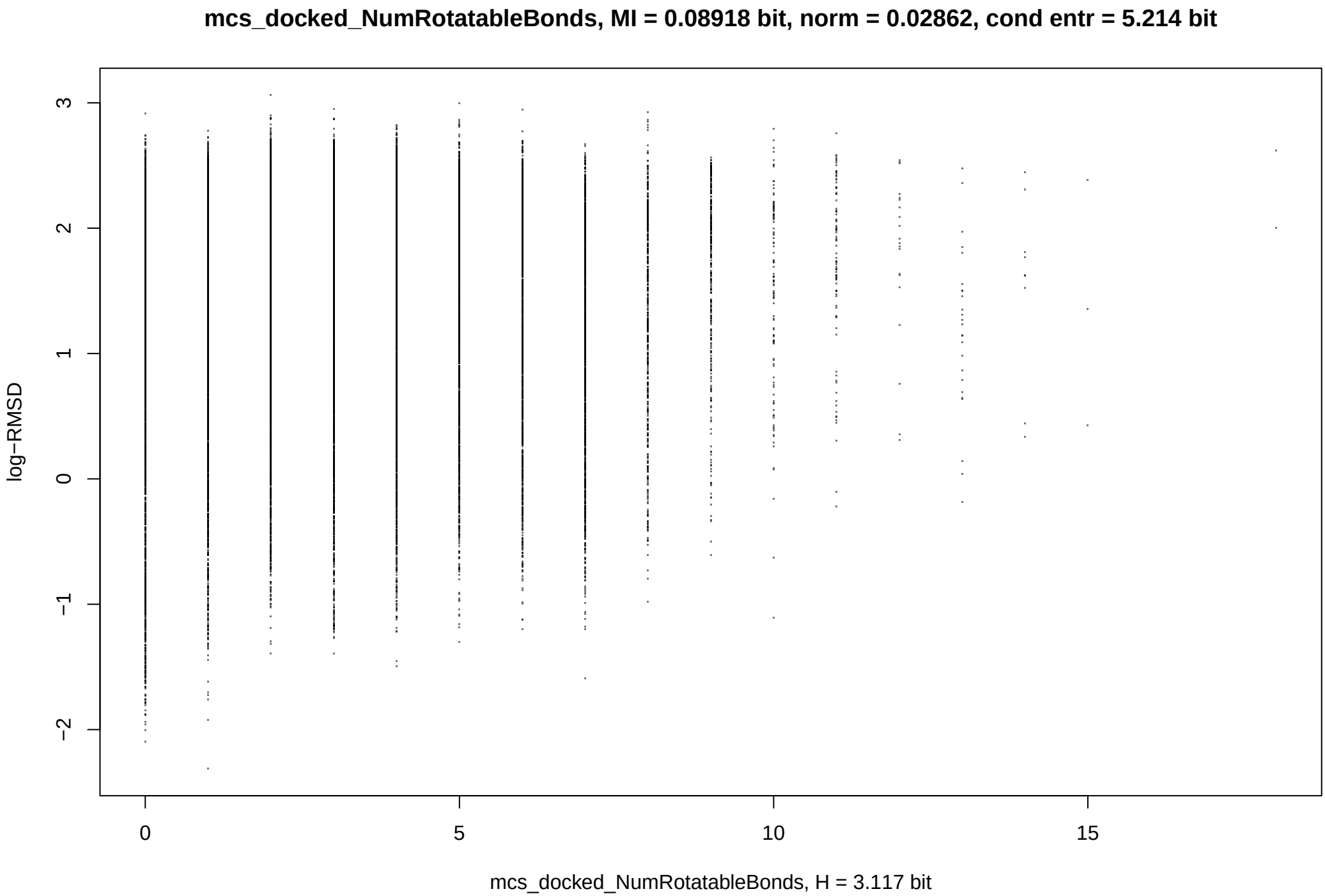

mcs_template_NHOHCount, MI = 0.1309 bit, norm = 0.06742, cond entr = 5.173 bit
log−RMSD
3
2
1
0
−1
−2
0
1
2
3
4
5
6
7
mcs_template_NHOHCount, H = 1.941 bit

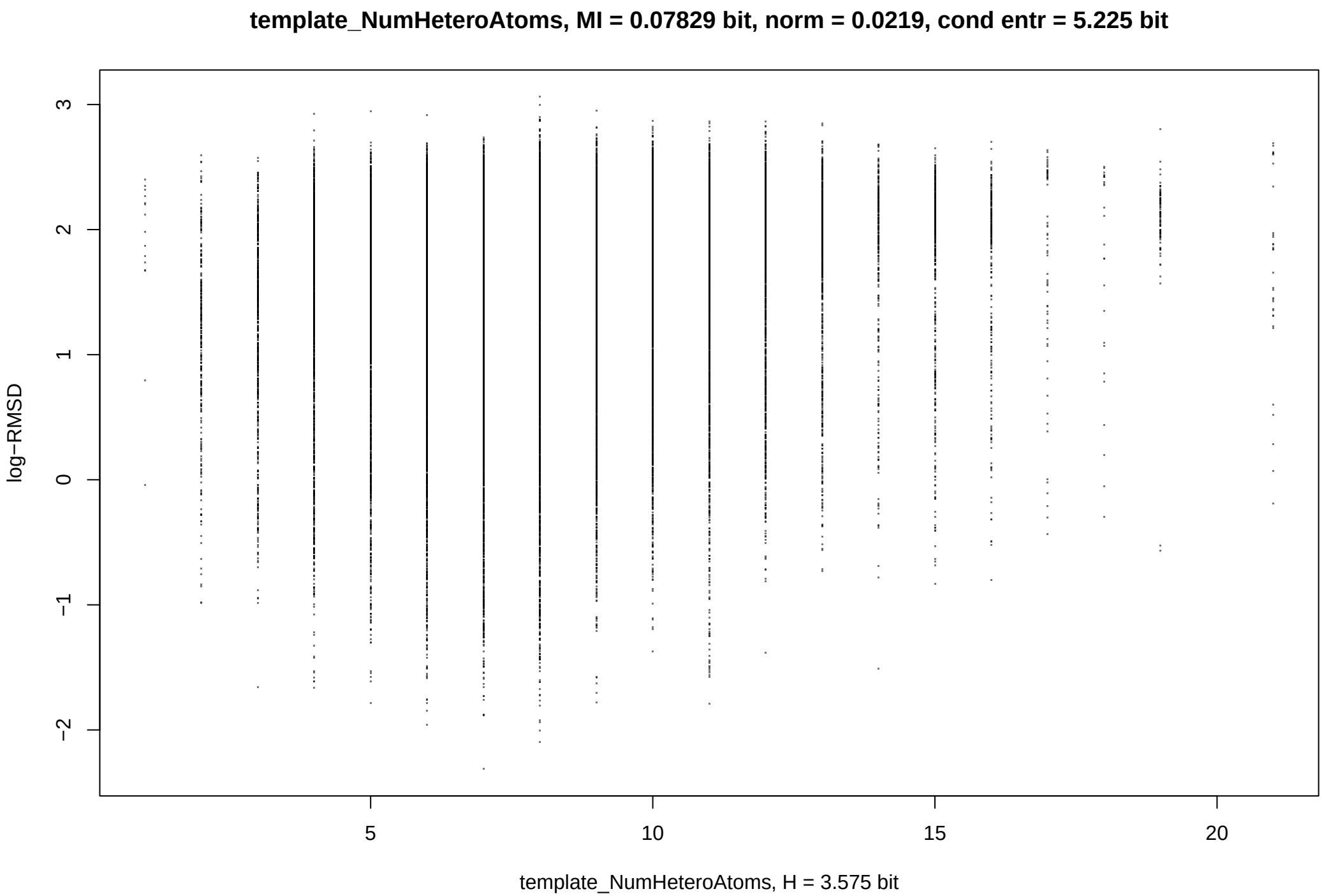

docked_NumHeteroAtoms, MI = 0.1107 bit, norm = 0.03098, cond entr = 5.193 bit
log−RMSD
3
2
1
0
−1
−2
5
10
15
20
docked_NumHeteroAtoms, H = 3.571 bit

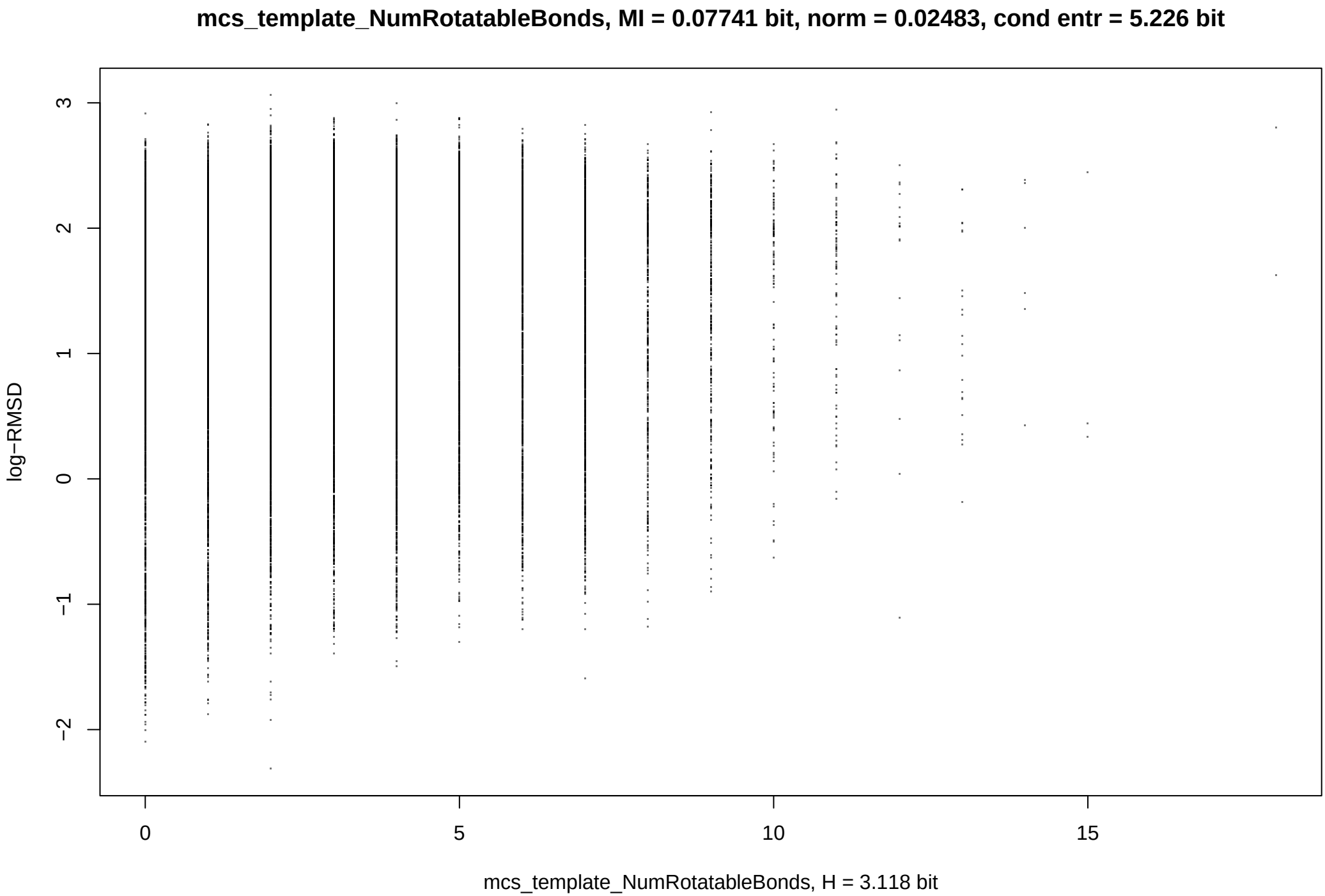

docked_NOCount, MI = 0.1004 bit, norm = 0.03084, cond entr = 5.203 bit
log−RMSD
3
2
1
0
−1
−2
5
10
15
20
docked_NOCount, H = 3.257 bit

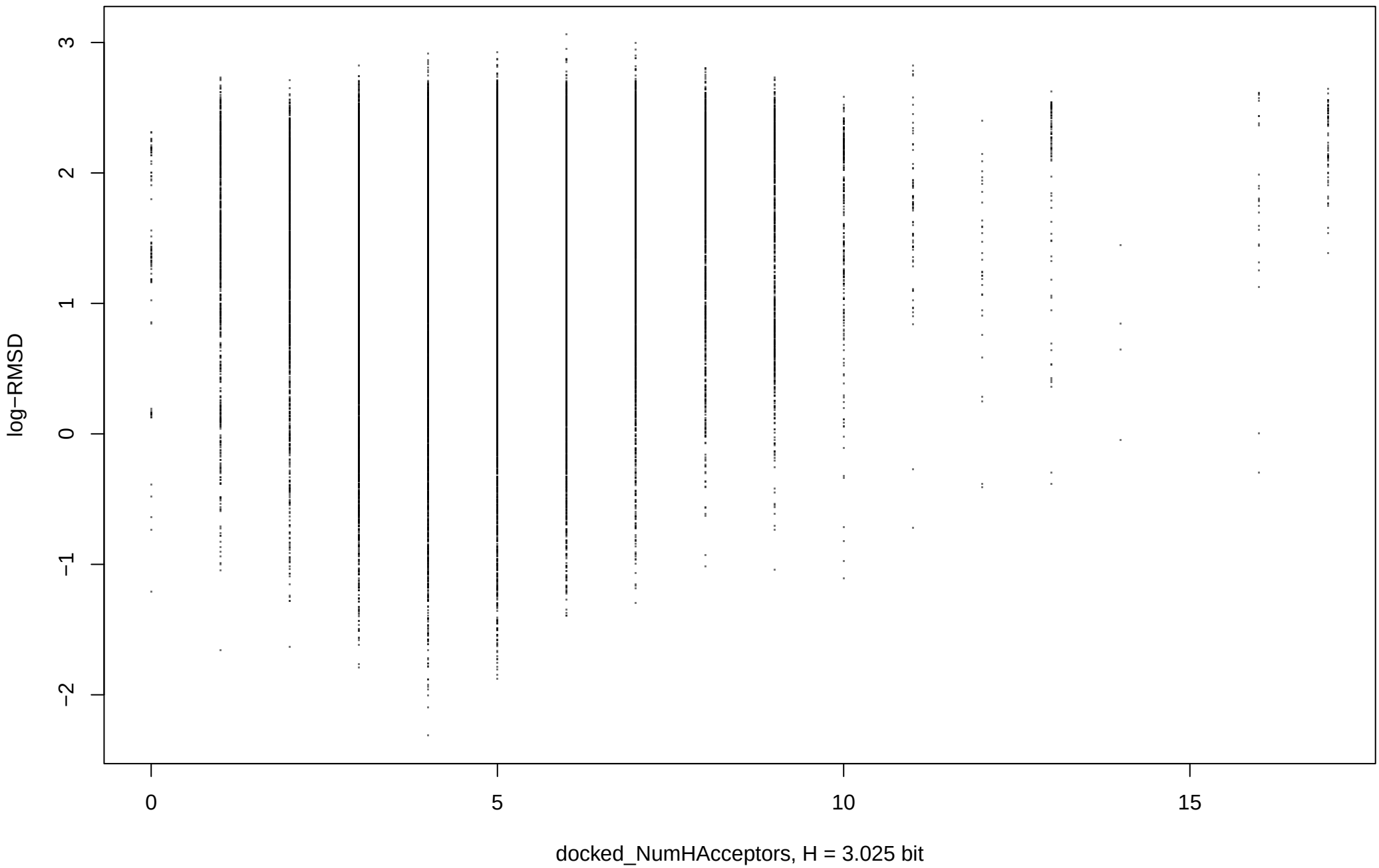

template_NumRotatableBonds, MI = 0.09807 bit, norm = 0.02673, cond entr = 5.205 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
20
25
30
template_NumRotatableBonds, H = 3.668 bit

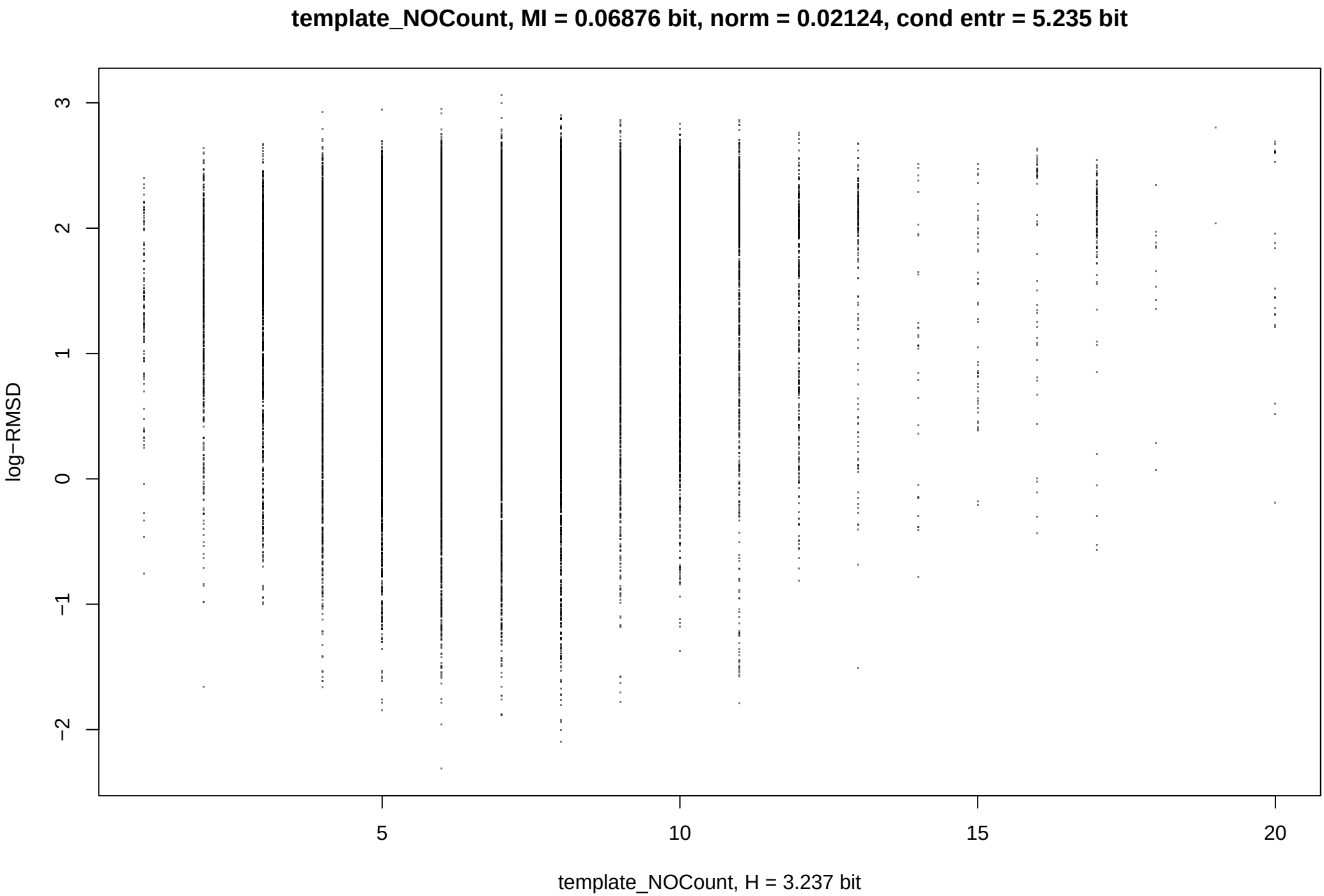

docked_RingCount, MI = 0.09713 bit, norm = 0.04065, cond entr = 5.206 bit
log−RMSD
3
2
1
0
−1
−2
0
2
4
6
8
docked_RingCount, H = 2.389 bit

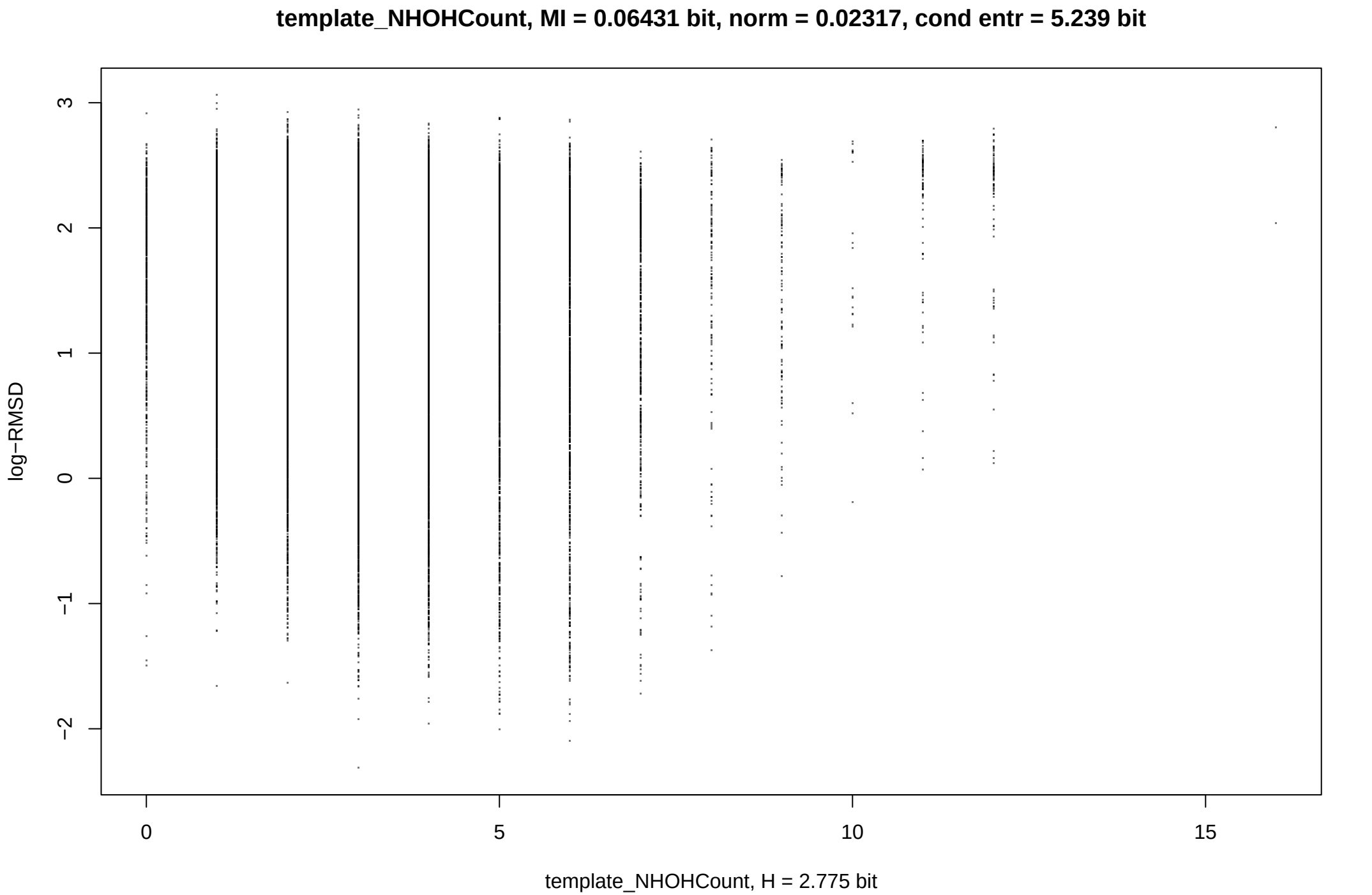

mcs_docked_NumRotatableBonds, MI = 0.08918 bit, norm = 0.02862, cond entr = 5.214 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
mcs_docked_NumRotatableBonds, H = 3.117 bit

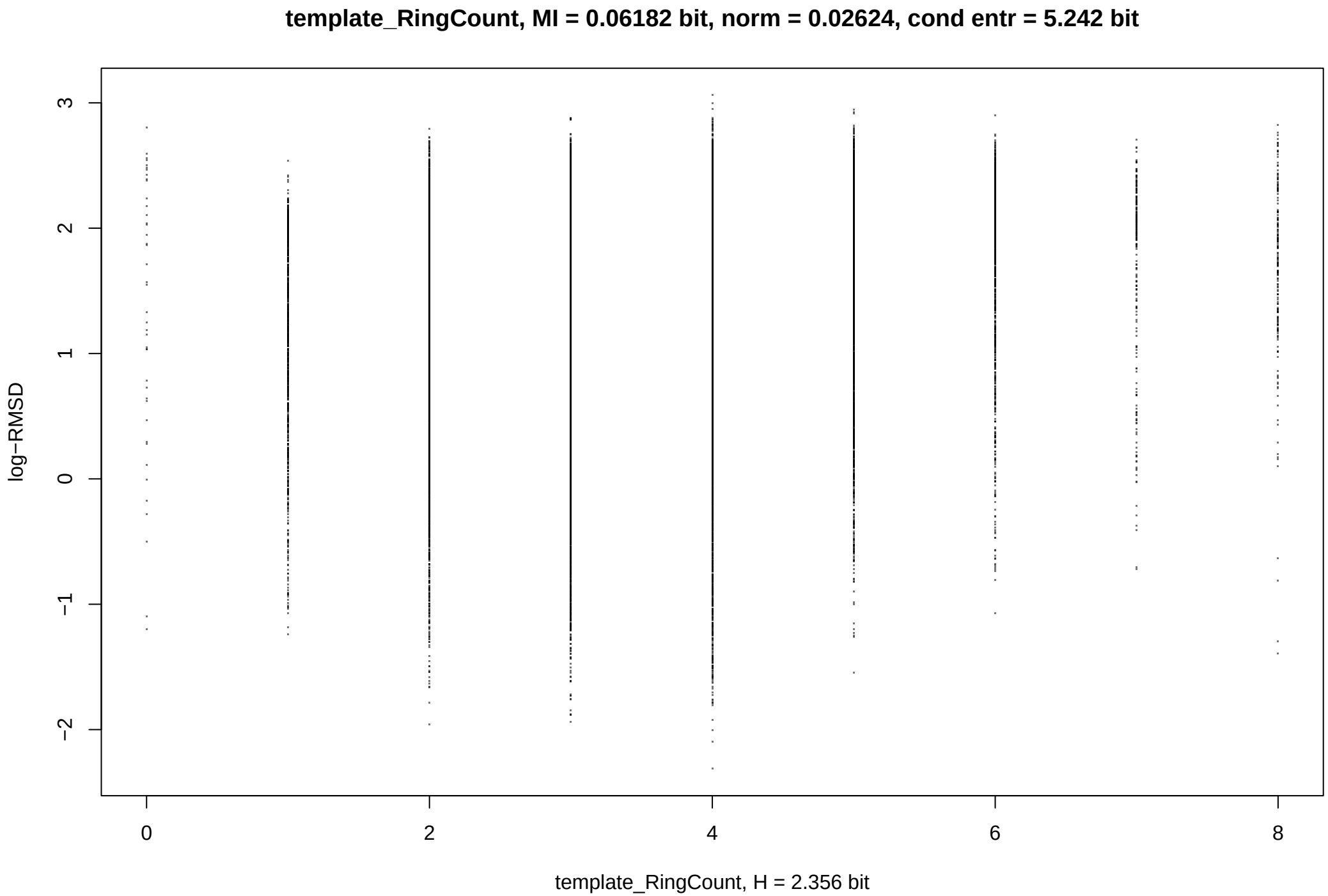

template_NumHeteroAtoms, MI = 0.07829 bit, norm = 0.0219, cond entr = 5.225 bit
log−RMSD
3
2
1
0
−1
−2
5
10
15
20
template_NumHeteroAtoms, H = 3.575 bit

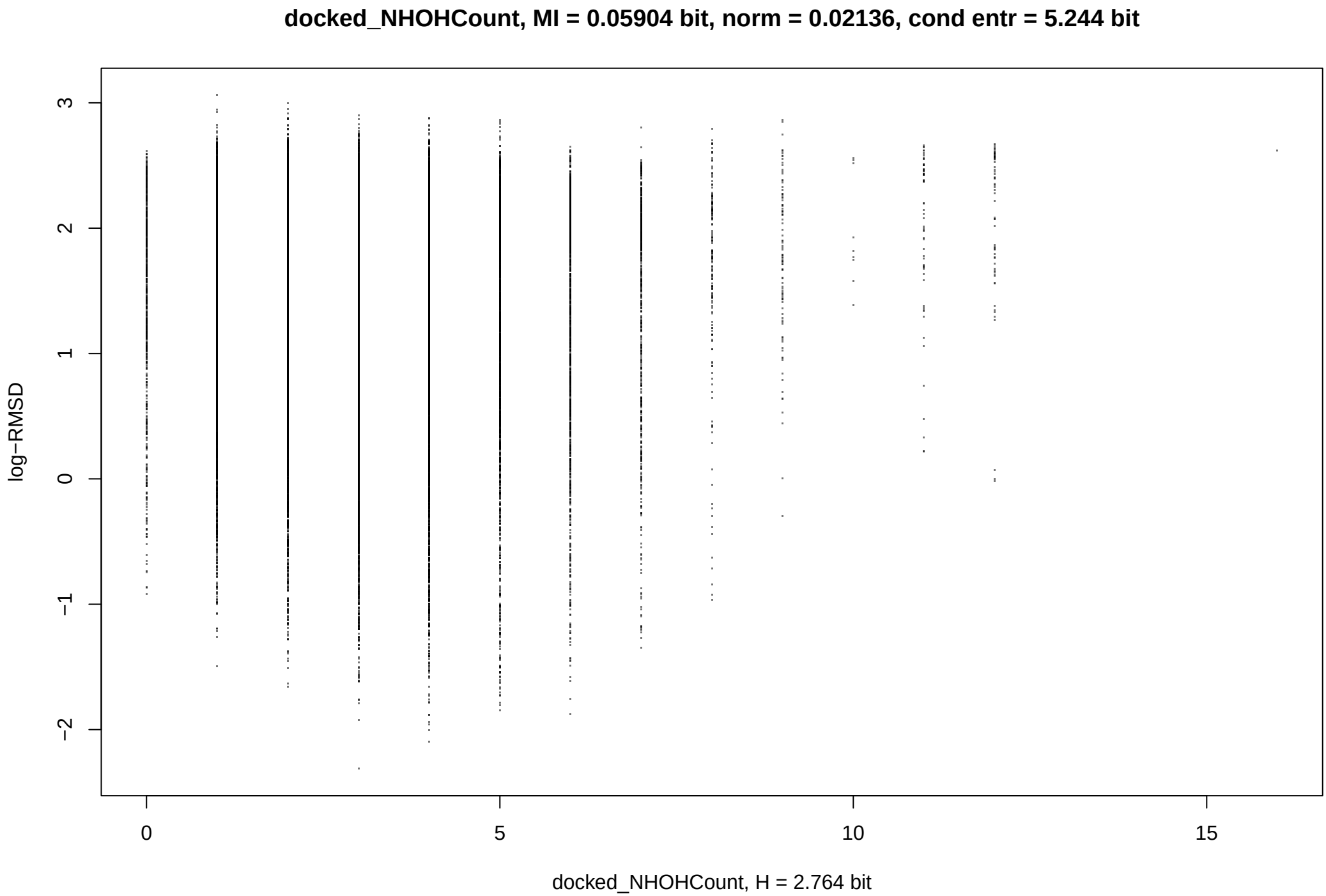

mcs_template_NumRotatableBonds, MI = 0.07741 bit, norm = 0.02483, cond entr = 5.226 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
mcs_template_NumRotatableBonds, H = 3.118 bit

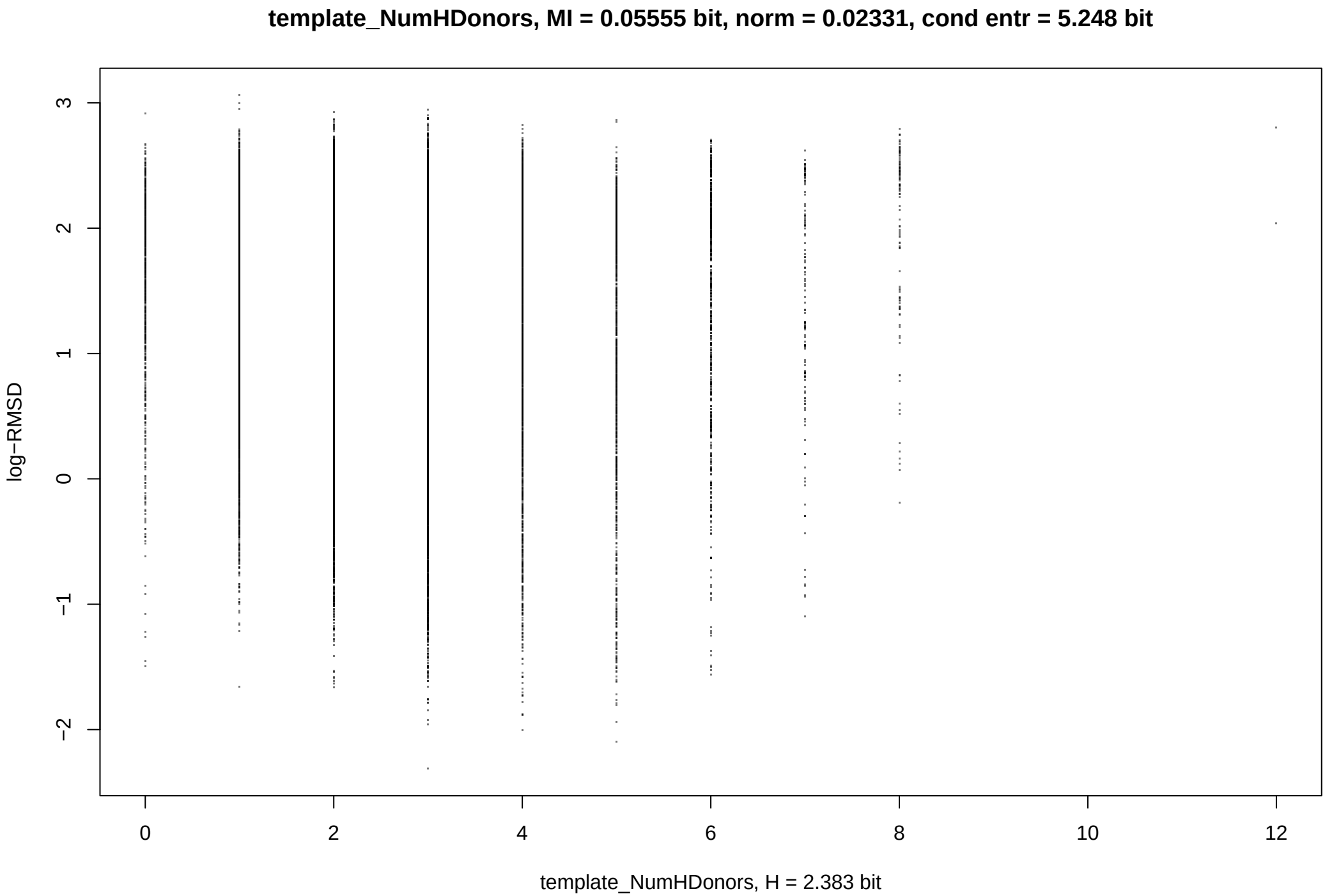

docked_NumHAcceptors, MI = 0.07647 bit, norm = 0.02528, cond entr = 5.227 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
docked_NumHAcceptors, H = 3.025 bit

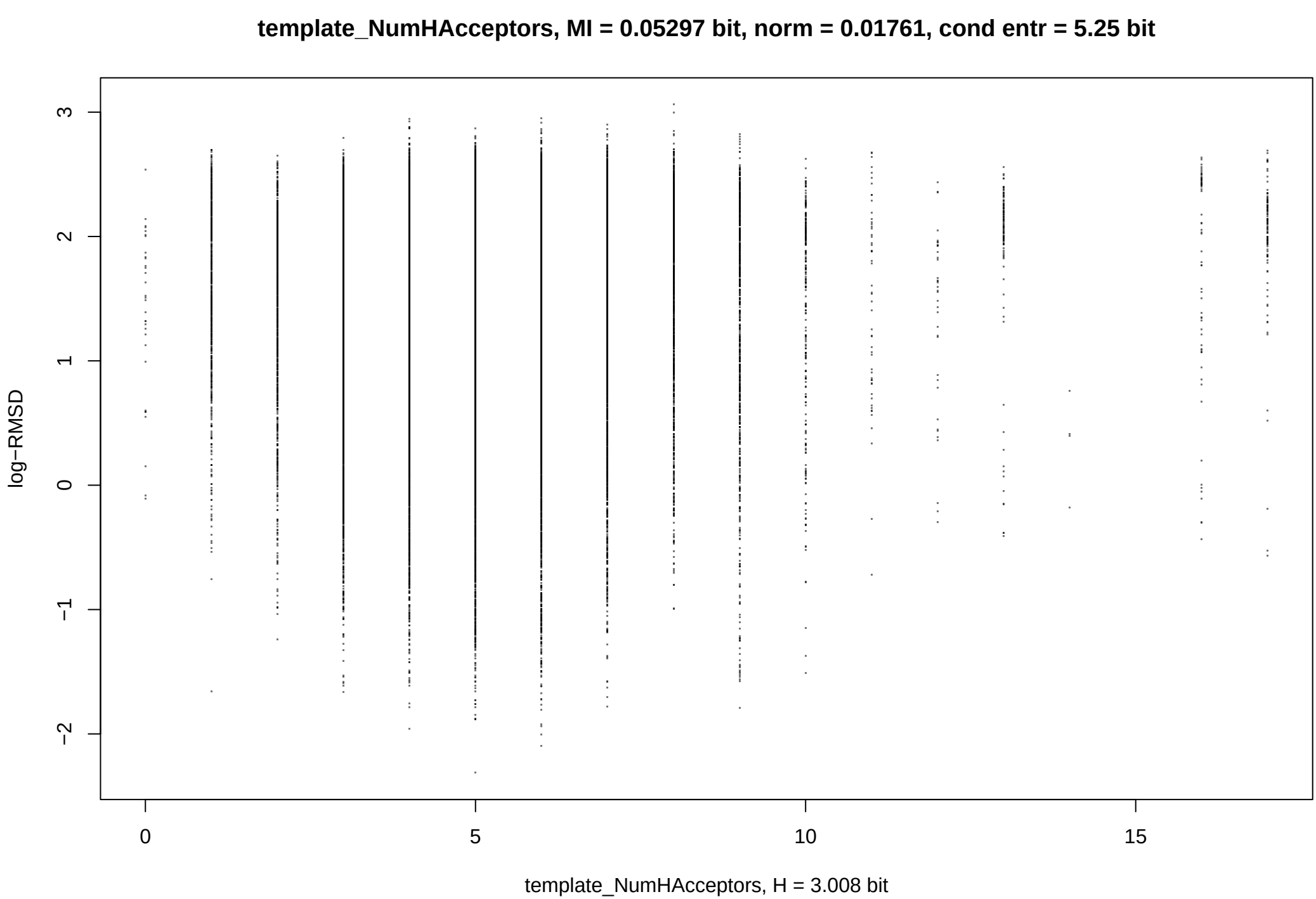

template_NOCount, MI = 0.06876 bit, norm = 0.02124, cond entr = 5.235 bit
log−RMSD
3
2
1
0
−1
−2
5
10
15
20
template_NOCount, H = 3.237 bit

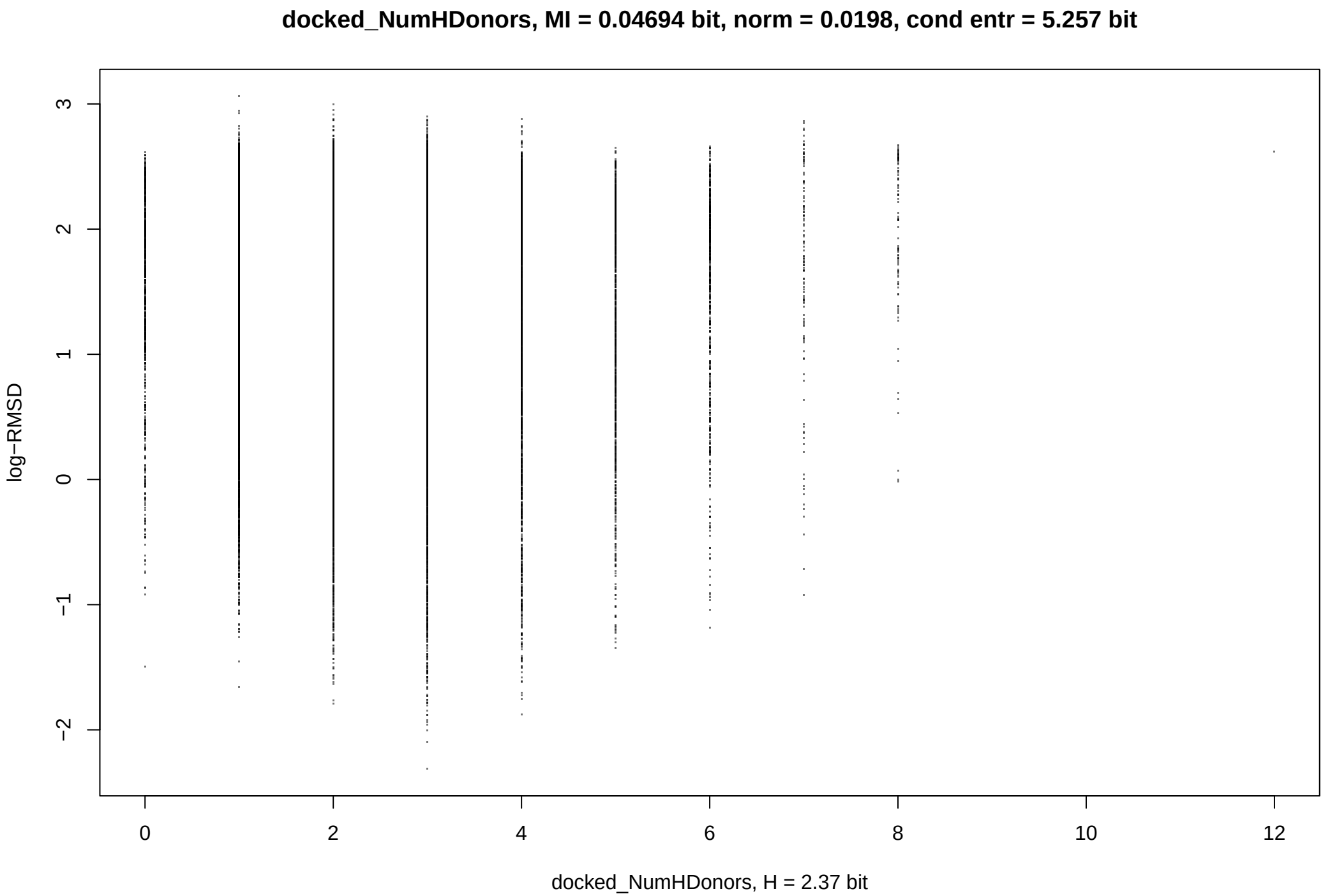

template_NHOHCount, MI = 0.06431 bit, norm = 0.02317, cond entr = 5.239 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
template_NHOHCount, H = 2.775 bit


template_RingCount, MI = 0.06182 bit, norm = 0.02624, cond entr = 5.242 bit
log−RMSD
3
2
1
0
−1
−2
0
2
4
6
8
template_RingCount, H = 2.356 bit


docked_NHOHCount, MI = 0.05904 bit, norm = 0.02136, cond entr = 5.244 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
docked_NHOHCount, H = 2.764 bit


template_NumHDonors, MI = 0.05555 bit, norm = 0.02331, cond entr = 5.248 bit
log−RMSD
3
2
1
0
−1
−2
0
2
4
6
8
10
12
template_NumHDonors, H = 2.383 bit


template_NumHAcceptors, MI = 0.05297 bit, norm = 0.01761, cond entr = 5.25 bit
log−RMSD
3
2
1
0
−1
−2
0
5
10
15
template_NumHAcceptors, H = 3.008 bit


docked_NumHDonors, MI = 0.04694 bit, norm = 0.0198, cond entr = 5.257 bit
log−RMSD
3
2
1
0
−1
−2
0
2
4
6
8
10
12
docked_NumHDonors, H = 2.37 bit