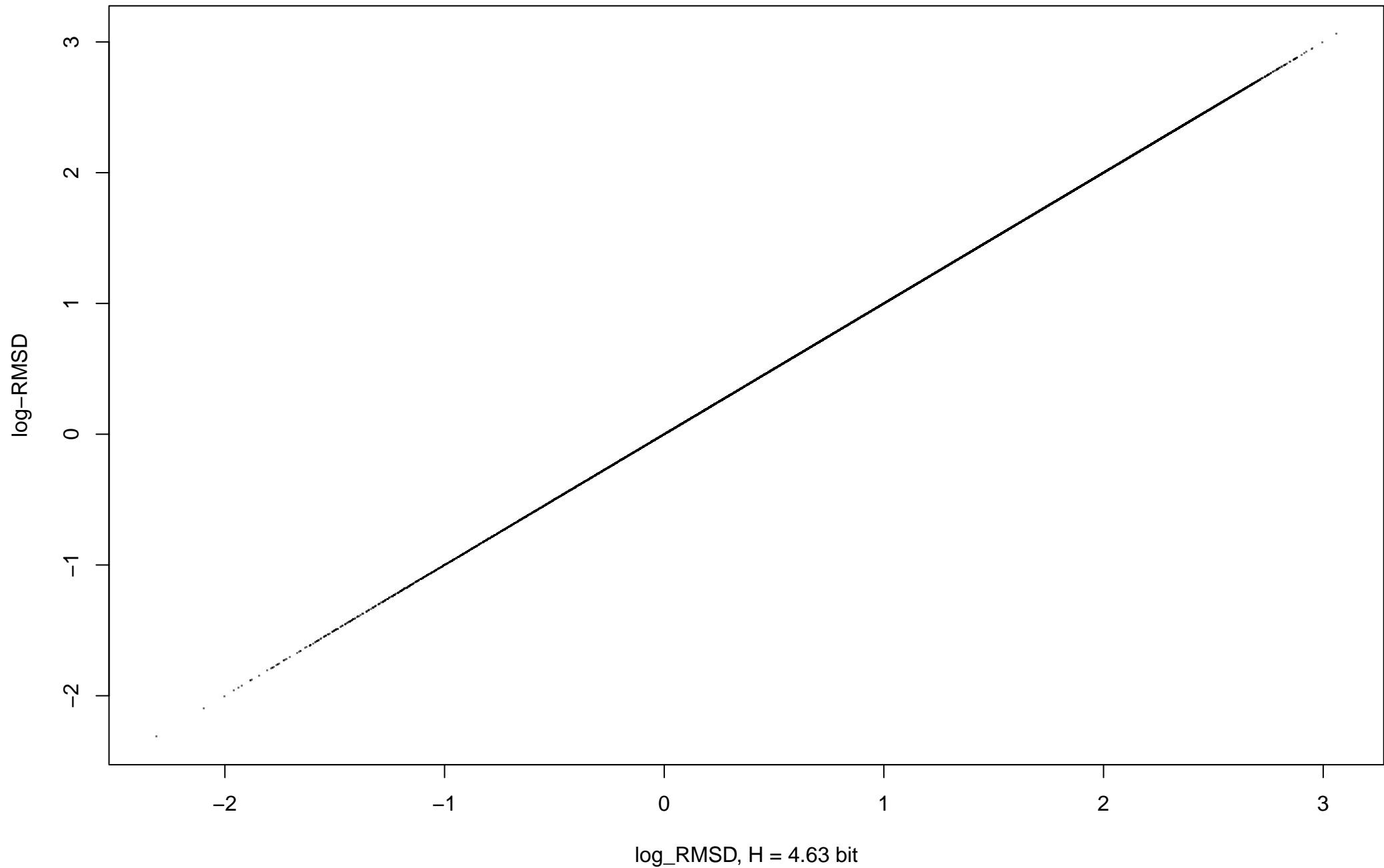
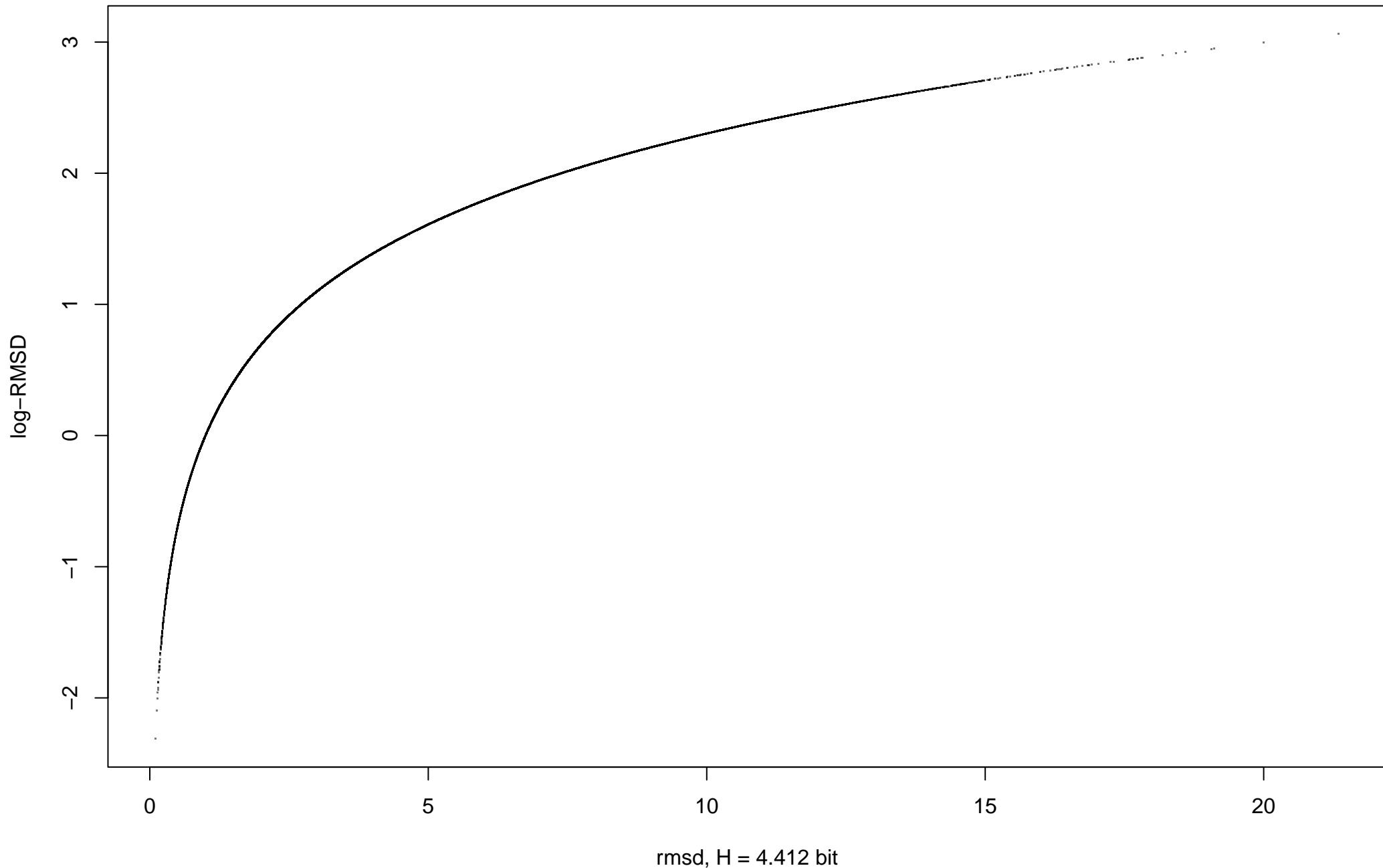


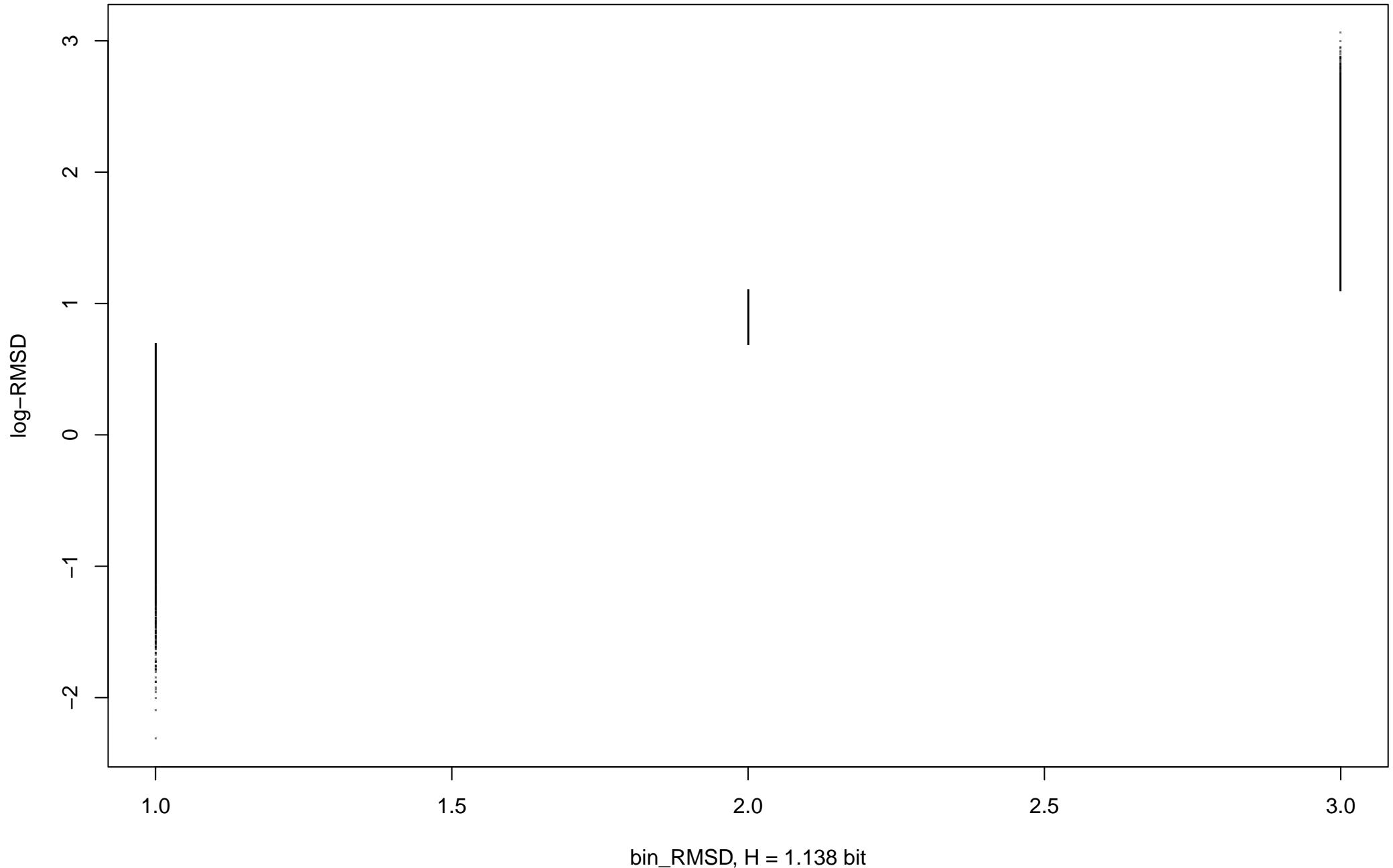
log_RMSD, MI = 4.63 bit, norm = 1, cond entr = 0 bit



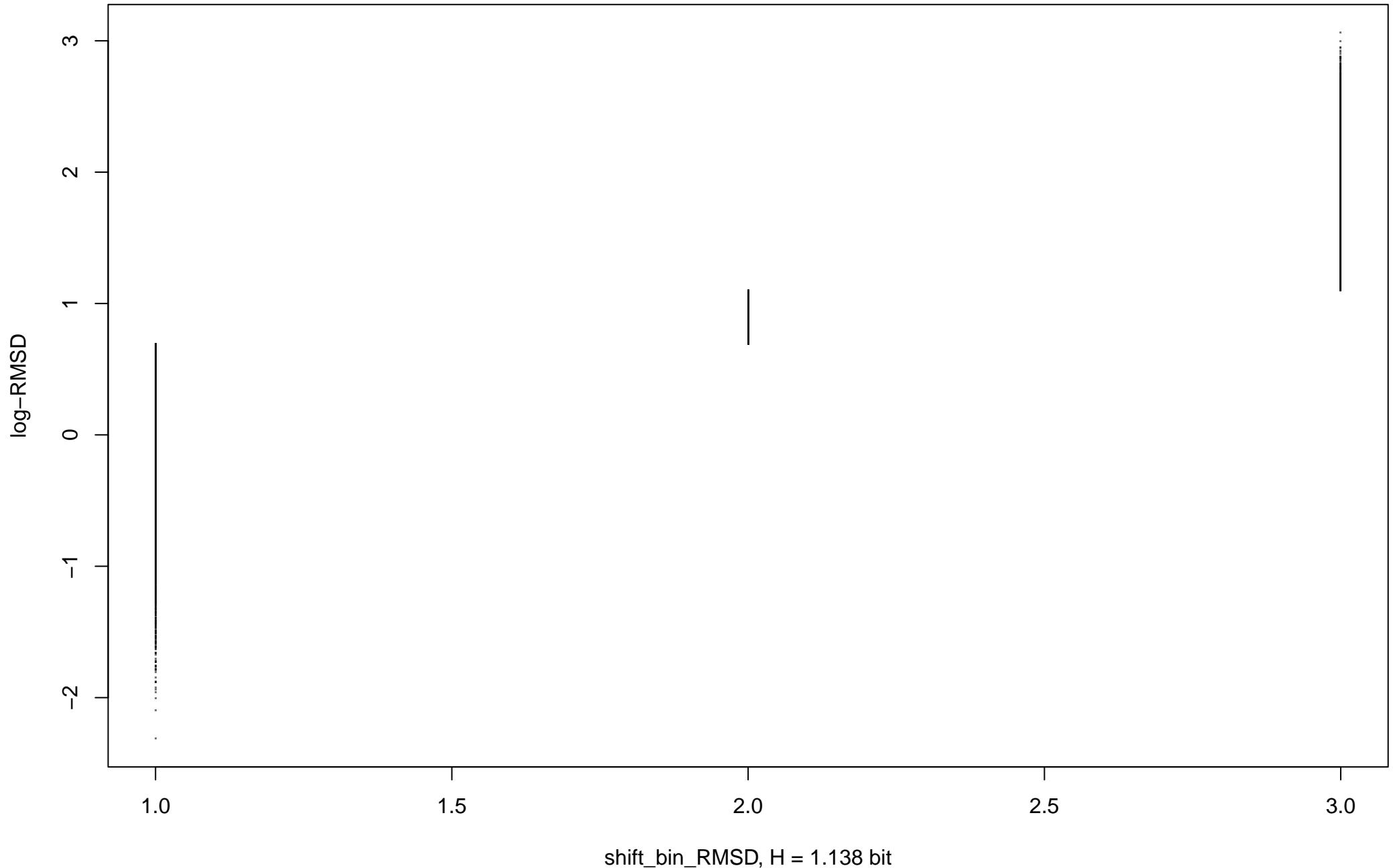
rmsd, MI = 3.556 bit, norm = 0.8059, cond entr = 1.074 bit



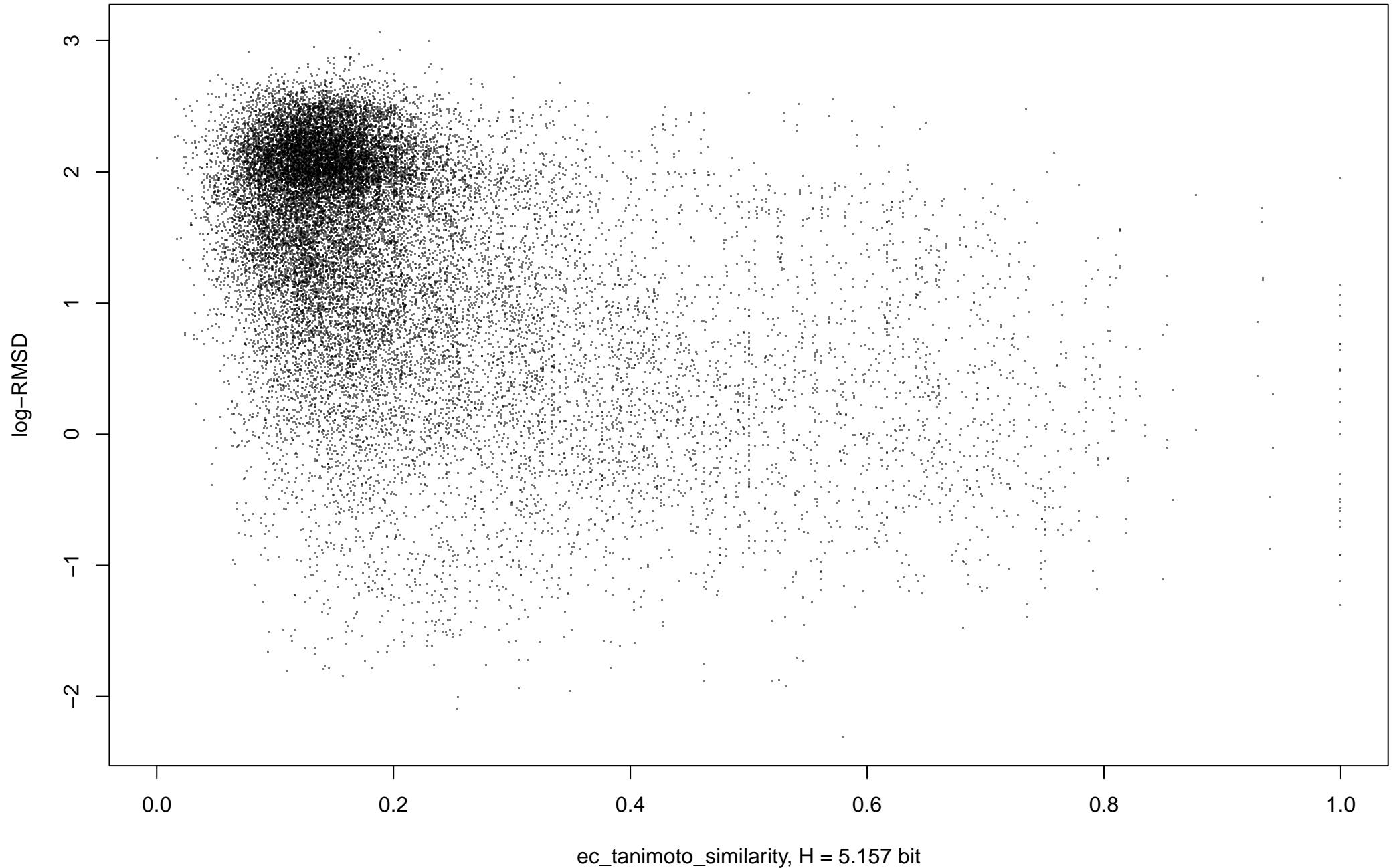
bin_RMSD, MI = 1.089 bit, norm = 0.9567, cond entr = 3.542 bit



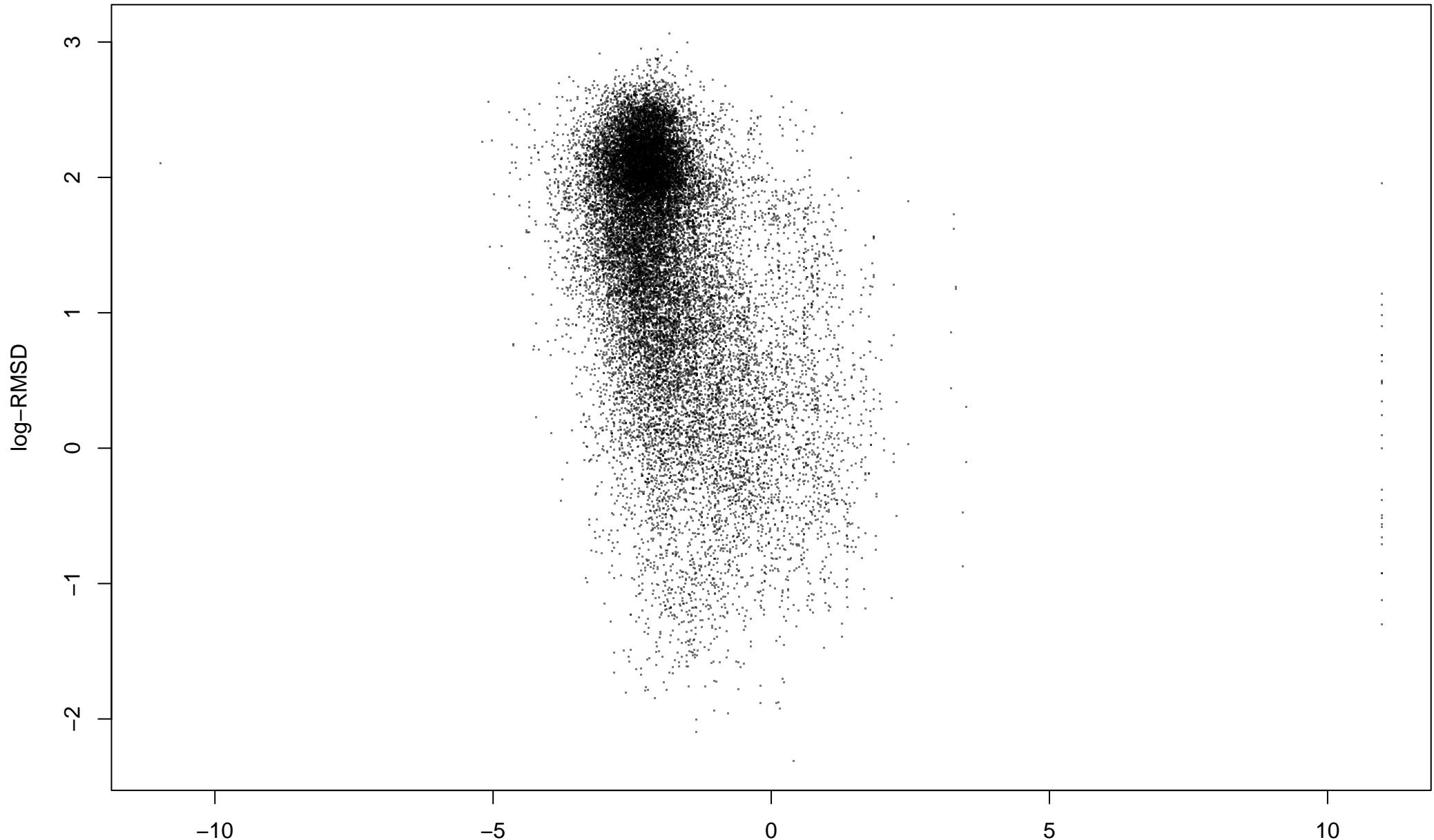
shift_bin_RMSD, MI = 1.089 bit, norm = 0.9567, cond entr = 3.542 bit



ec_tanimoto_similarity, MI = 0.2975 bit, norm = 0.06426, cond entr = 4.333 bit

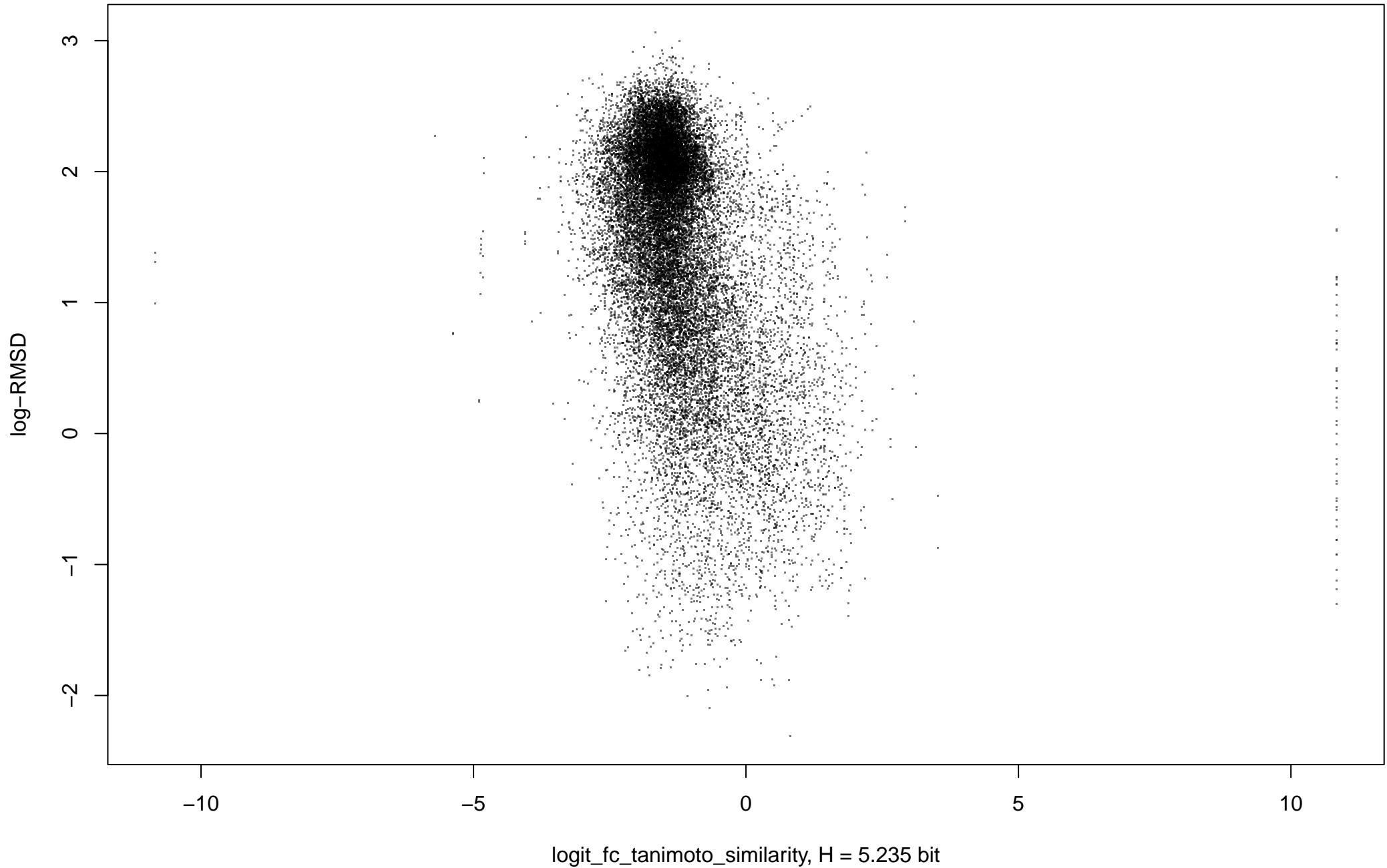


logit_ec_tanimoto_similarity, MI = 0.2857 bit, norm = 0.06171, cond entr = 4.344 bit

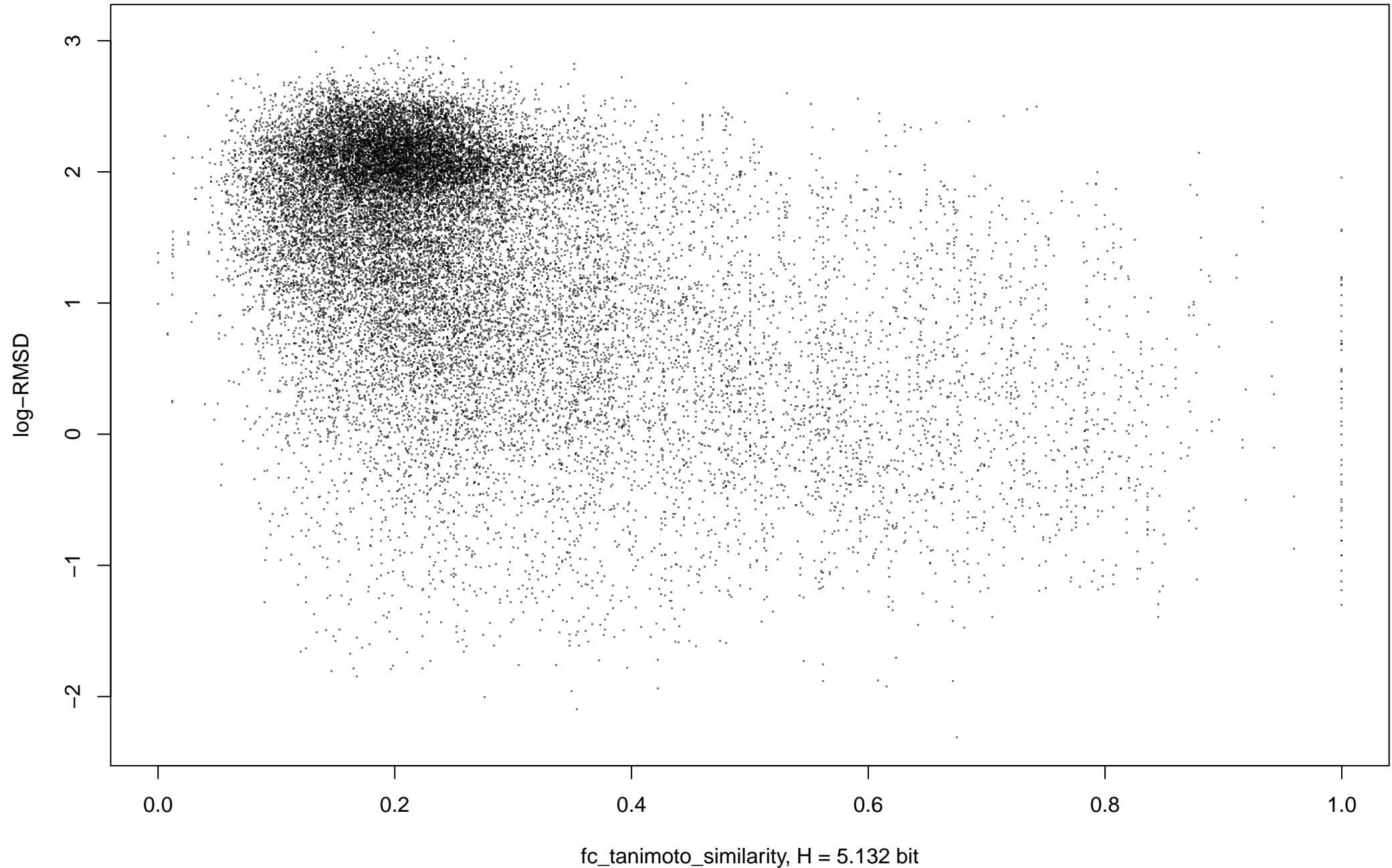


logit_ec_tanimoto_similarity, H = 5.207 bit

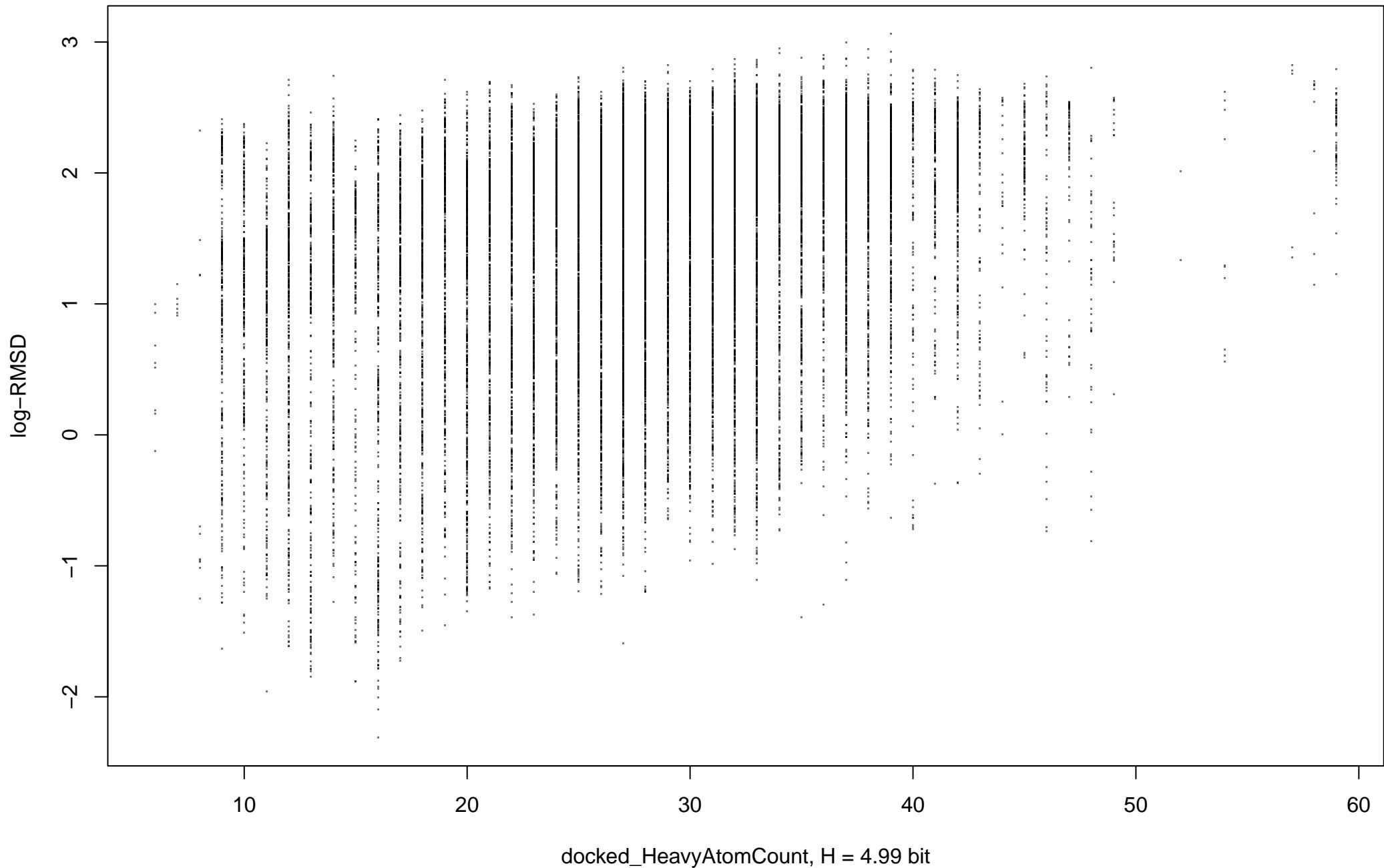
logit_fc_tanimoto_similarity, MI = 0.2834 bit, norm = 0.06121, cond entr = 4.347 bit



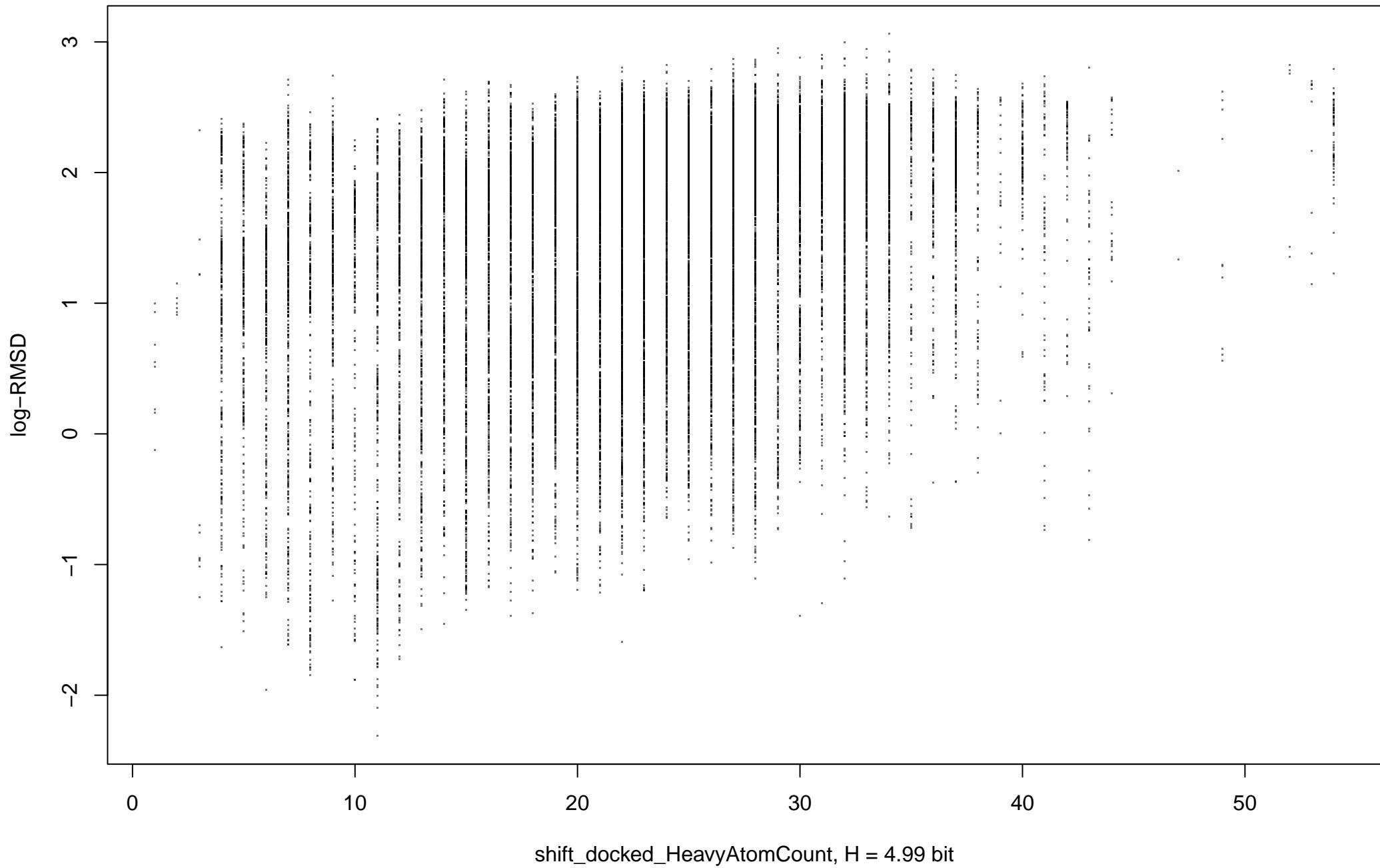
fc_tanimoto_similarity, MI = 0.2788 bit, norm = 0.06021, cond entr = 4.351 bit



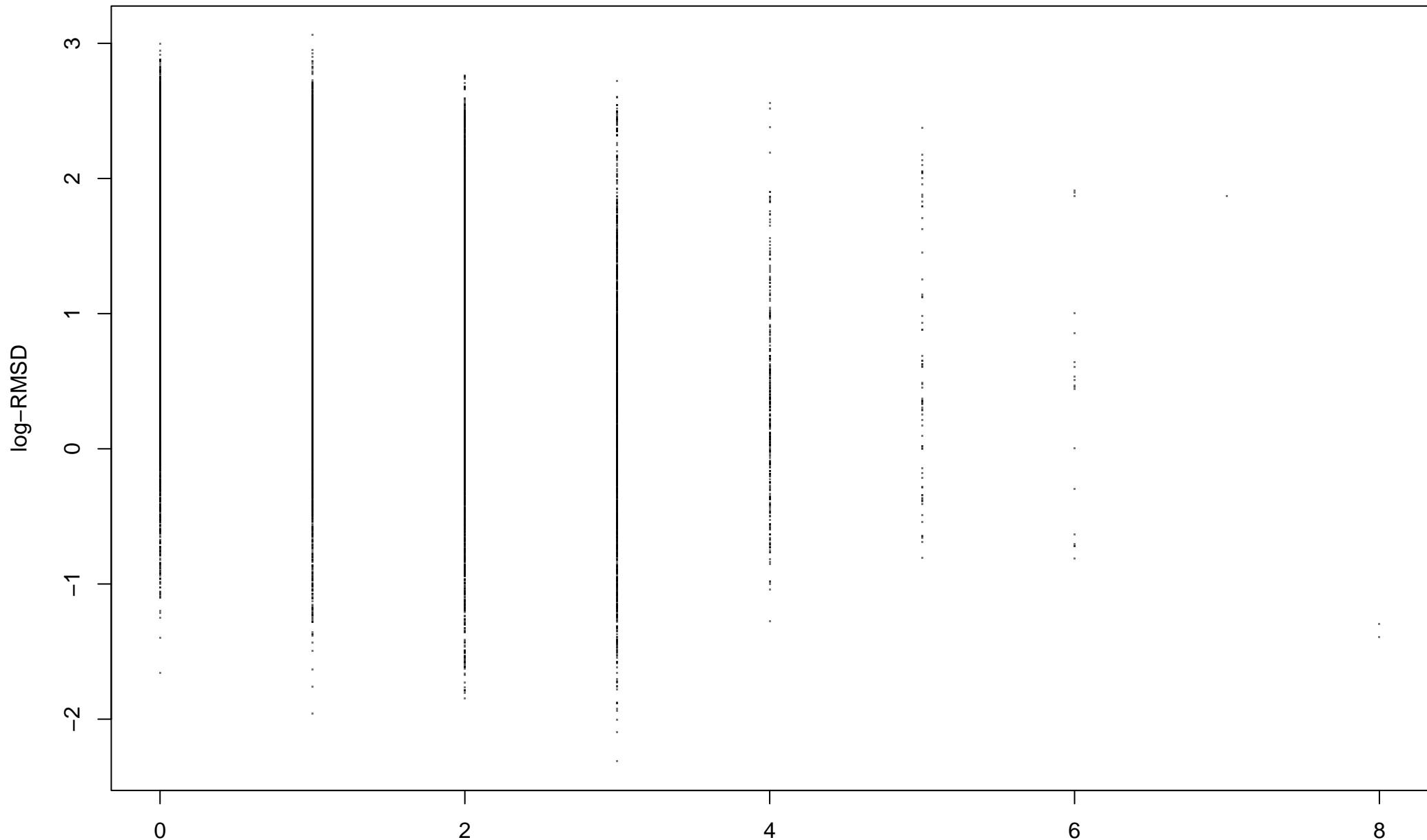
docked_HeavyAtomCount, MI = 0.2246 bit, norm = 0.04851, cond entr = 4.406 bit



shift_docked_HeavyAtomCount, MI = 0.2246 bit, norm = 0.04851, cond entr = 4.406 bit

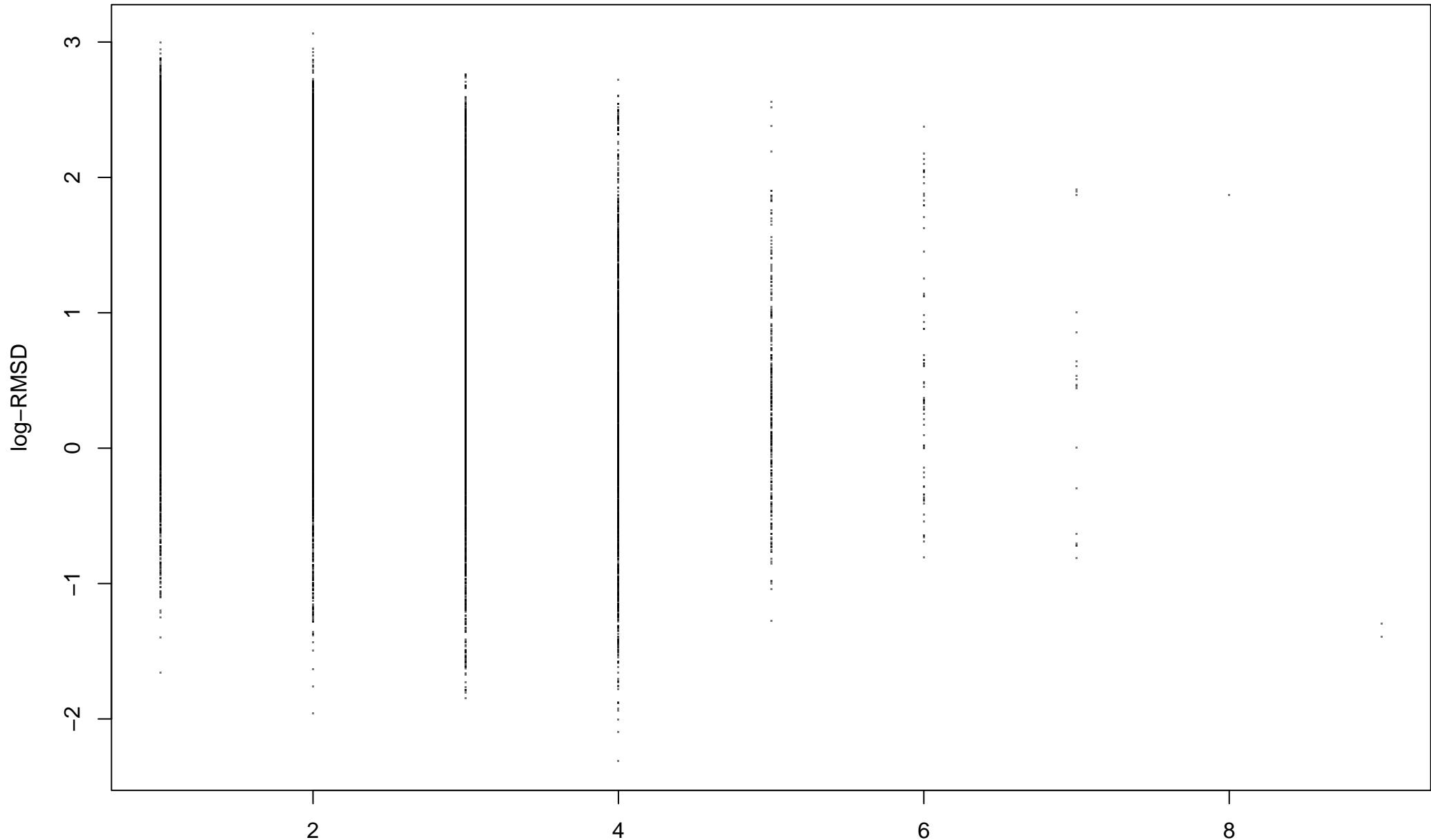


mcs_RingCount, MI = 0.2044 bit, norm = 0.1183, cond entr = 4.426 bit



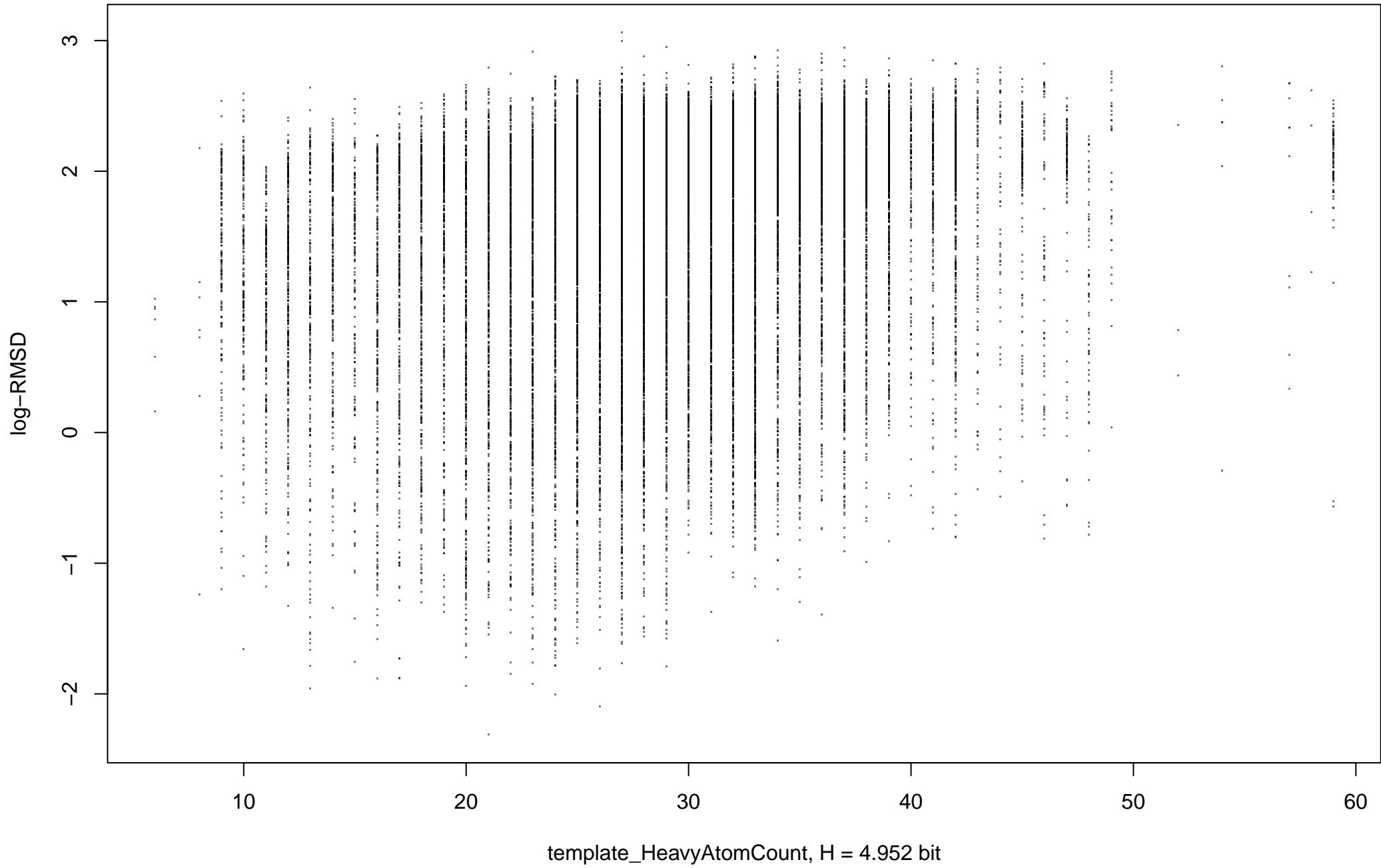
`mcs_RingCount, H = 1.727 bit`

shift_mcs_RingCount, MI = 0.2044 bit, norm = 0.1183, cond entr = 4.426 bit

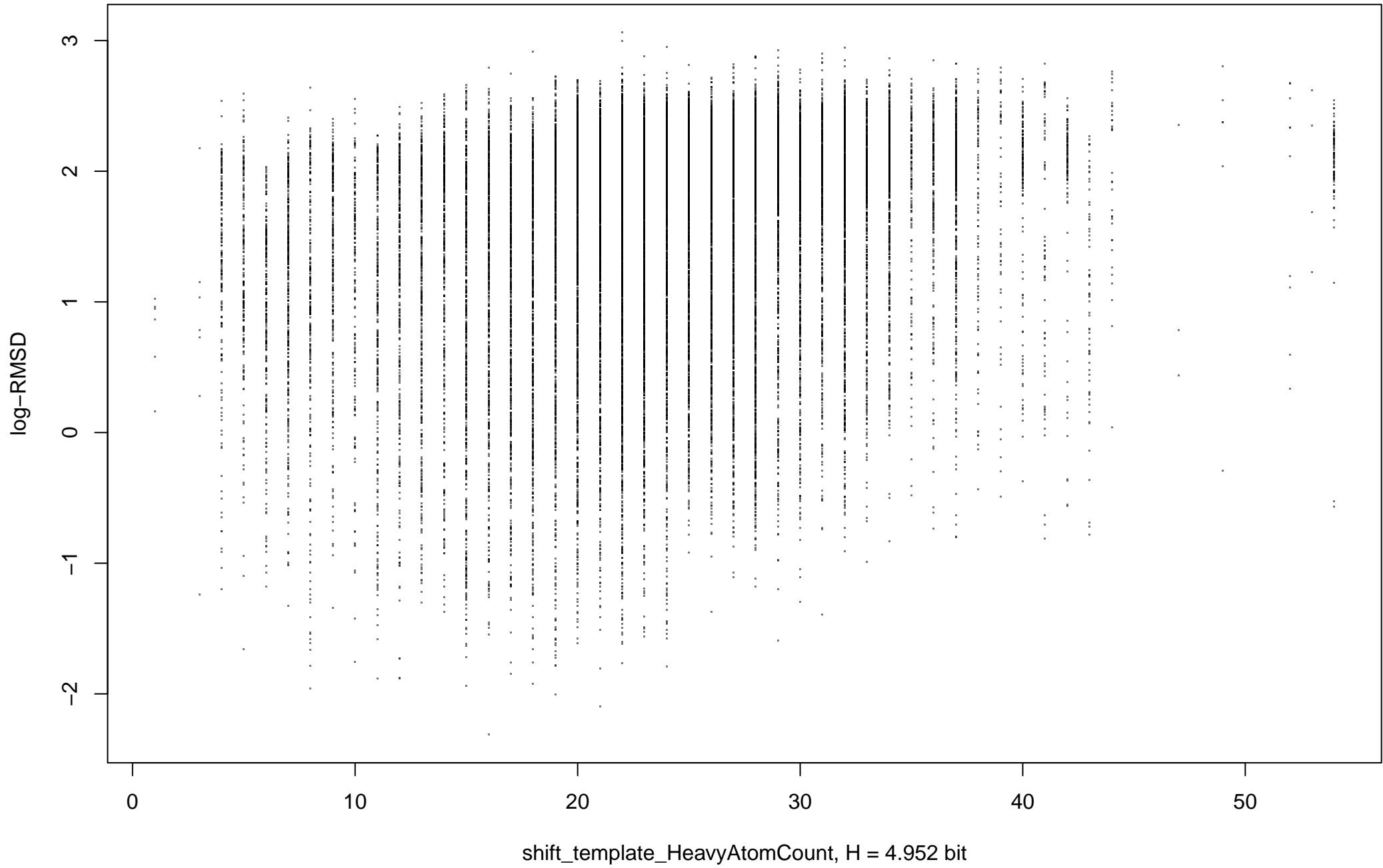


shift_mcs_RingCount, H = 1.727 bit

template_HeavyAtomCount, MI = 0.1477 bit, norm = 0.0319, cond entr = 4.483 bit

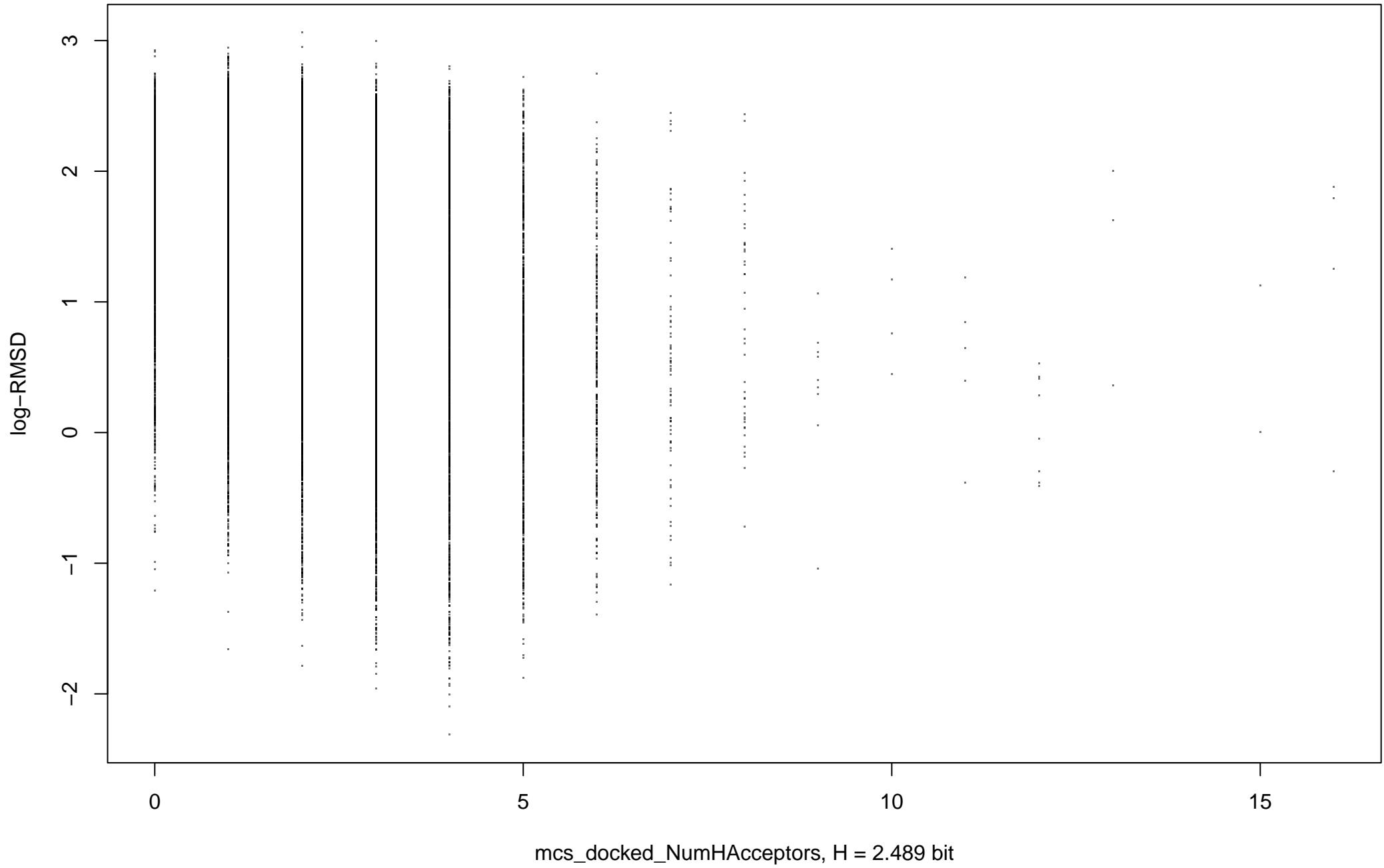


shift_template_HeavyAtomCount, MI = 0.1477 bit, norm = 0.0319, cond entr = 4.483 bit

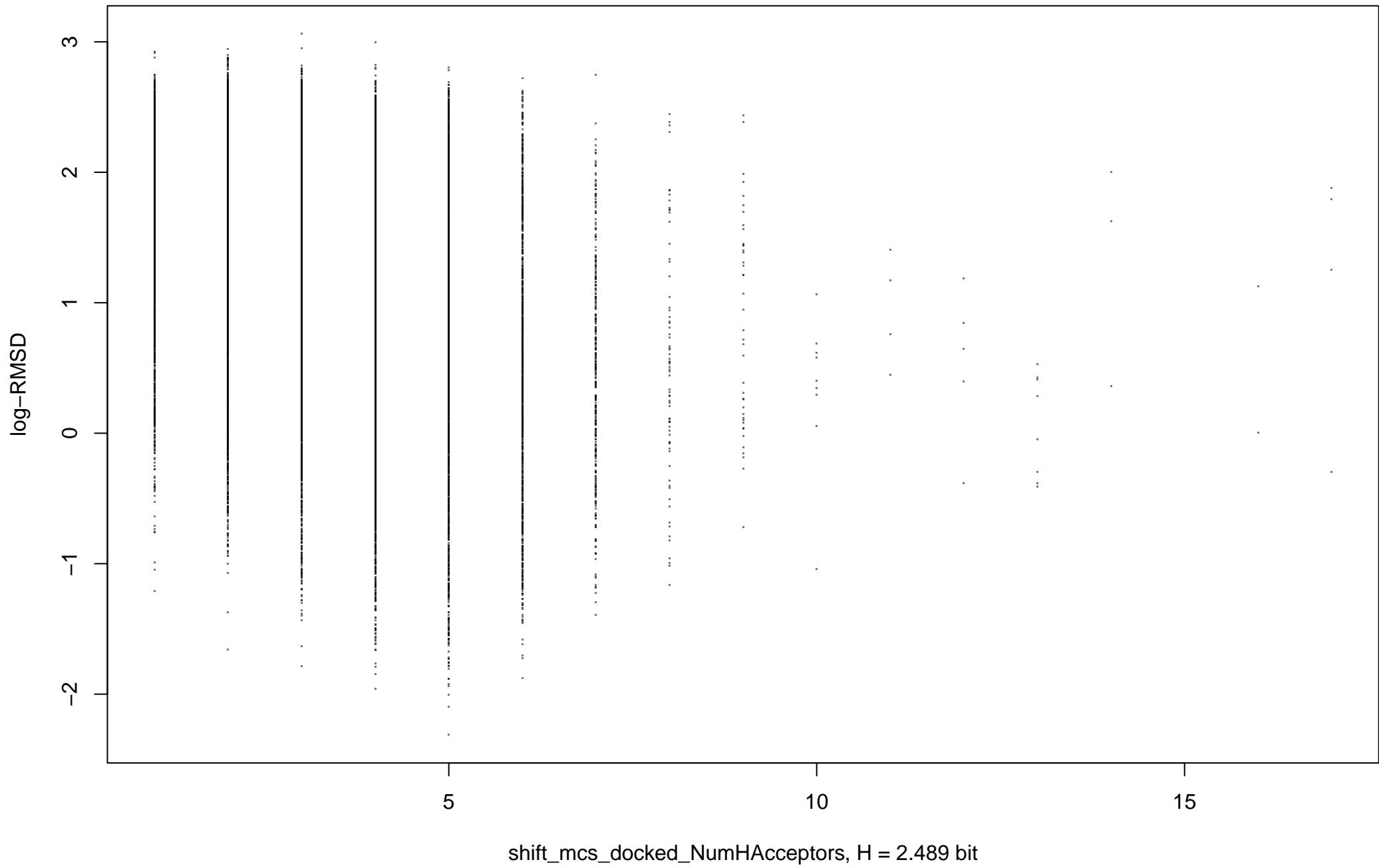


shift_template_HeavyAtomCount, H = 4.952 bit

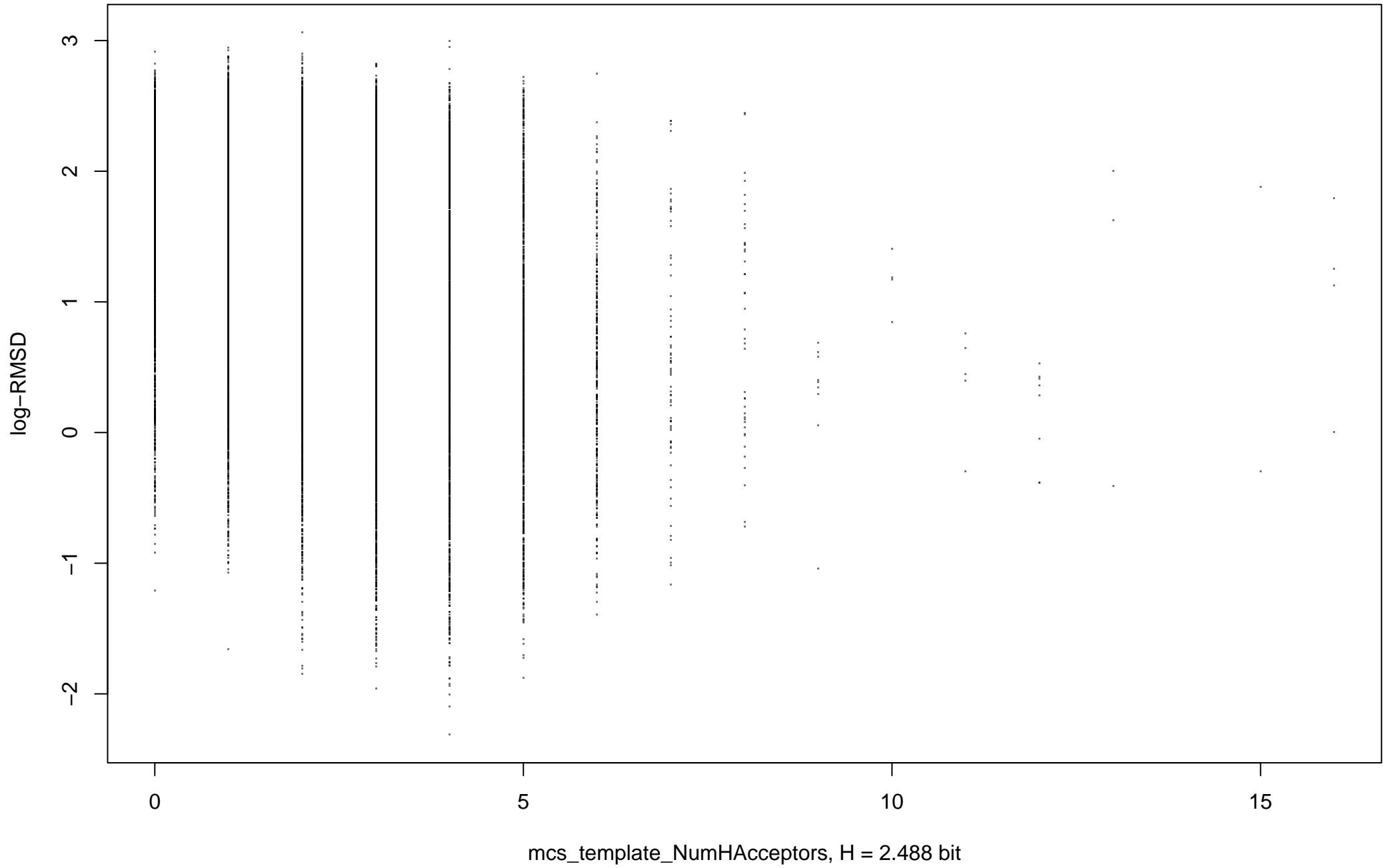
mcs_docked_NumHAcceptors, MI = 0.1462 bit, norm = 0.05874, cond entr = 4.484 bit



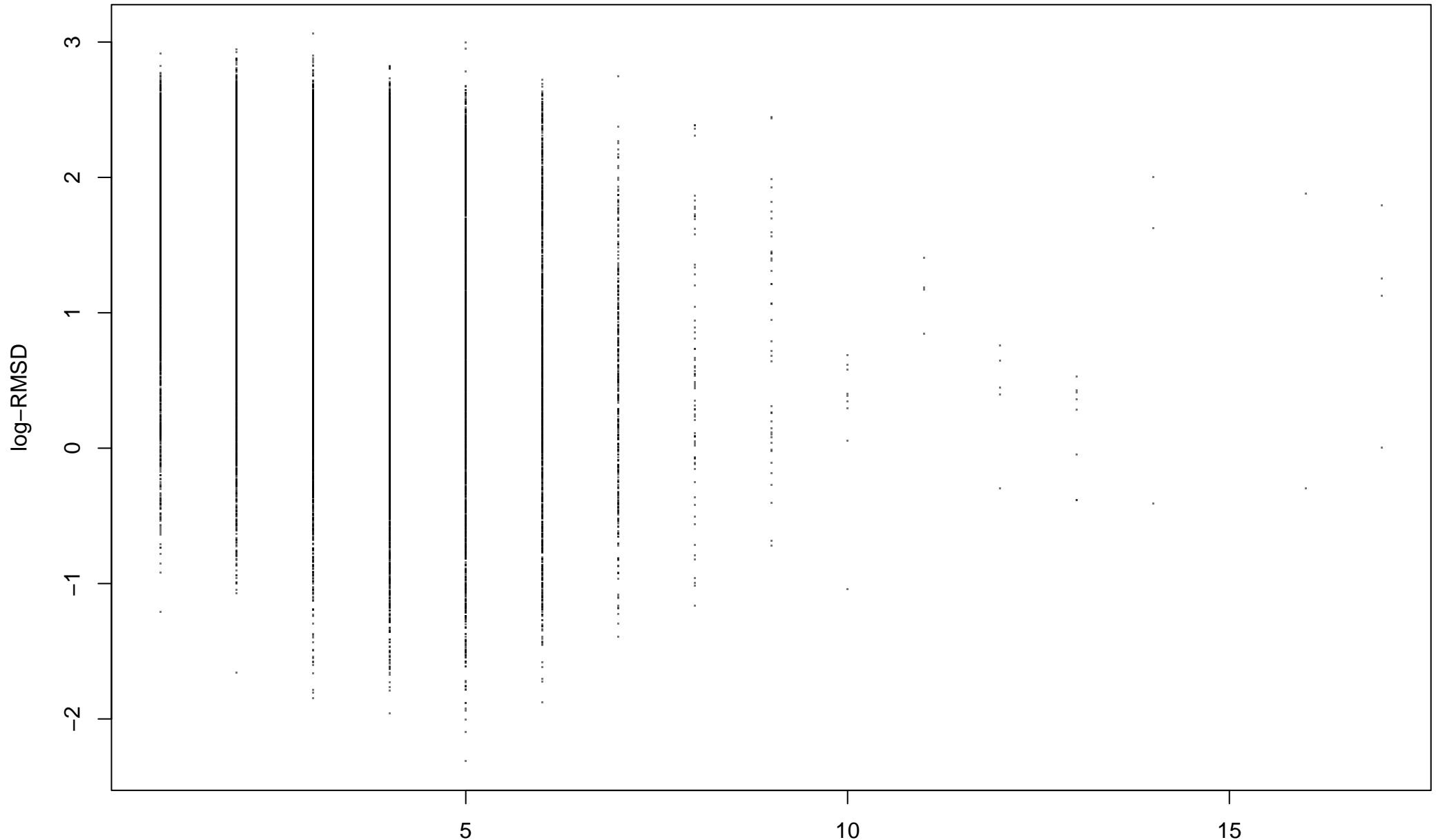
shift_mcs_docked_NumHAcceptors, MI = 0.1462 bit, norm = 0.05874, cond entr = 4.484 bit



mcs_template_NumHAcceptors, MI = 0.1452 bit, norm = 0.05837, cond entr = 4.485 bit

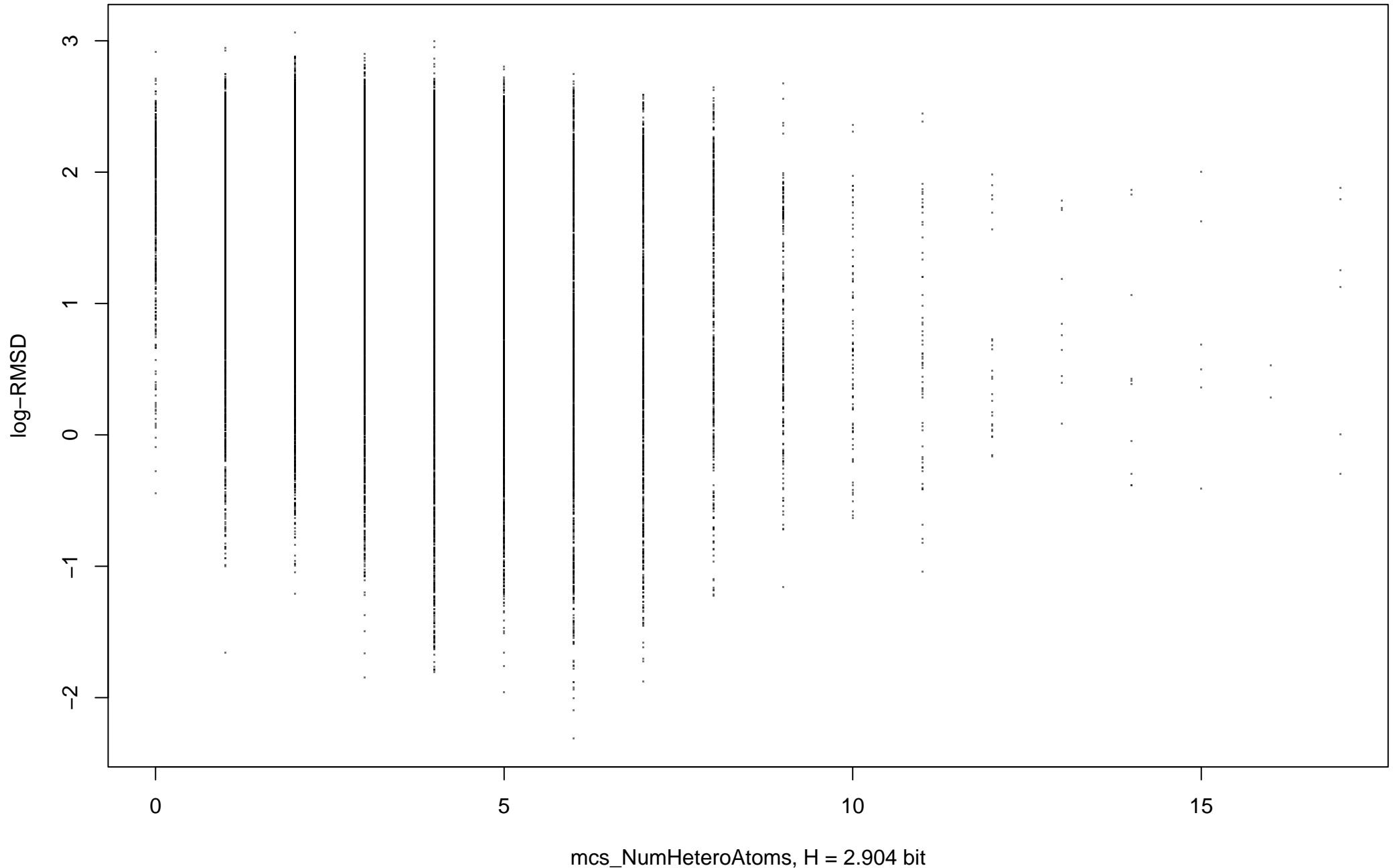


shift_mcs_template_NumHAcceptors, MI = 0.1452 bit, norm = 0.05837, cond entr = 4.485 bit

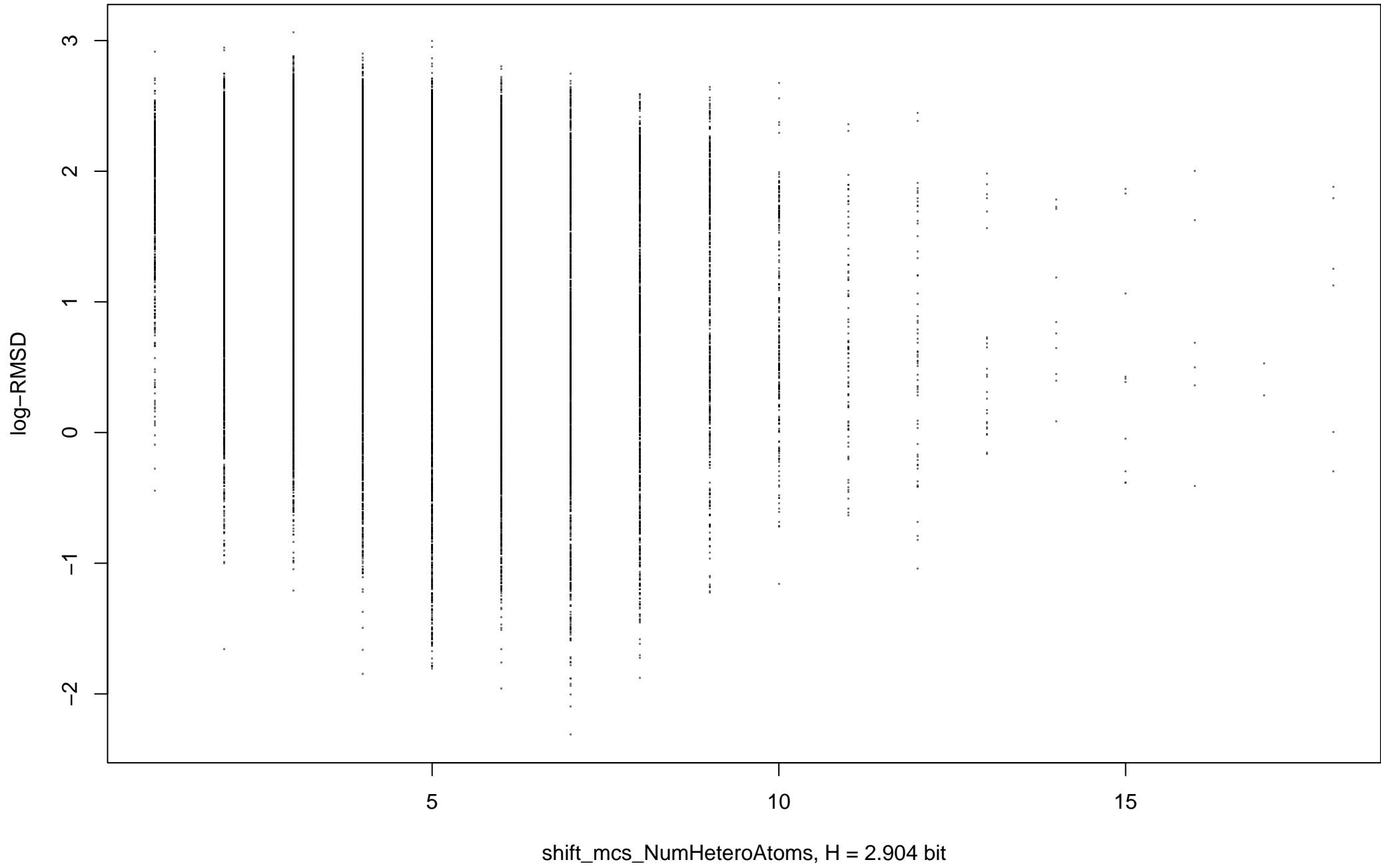


shift_mcs_template_NumHAcceptors, H = 2.488 bit

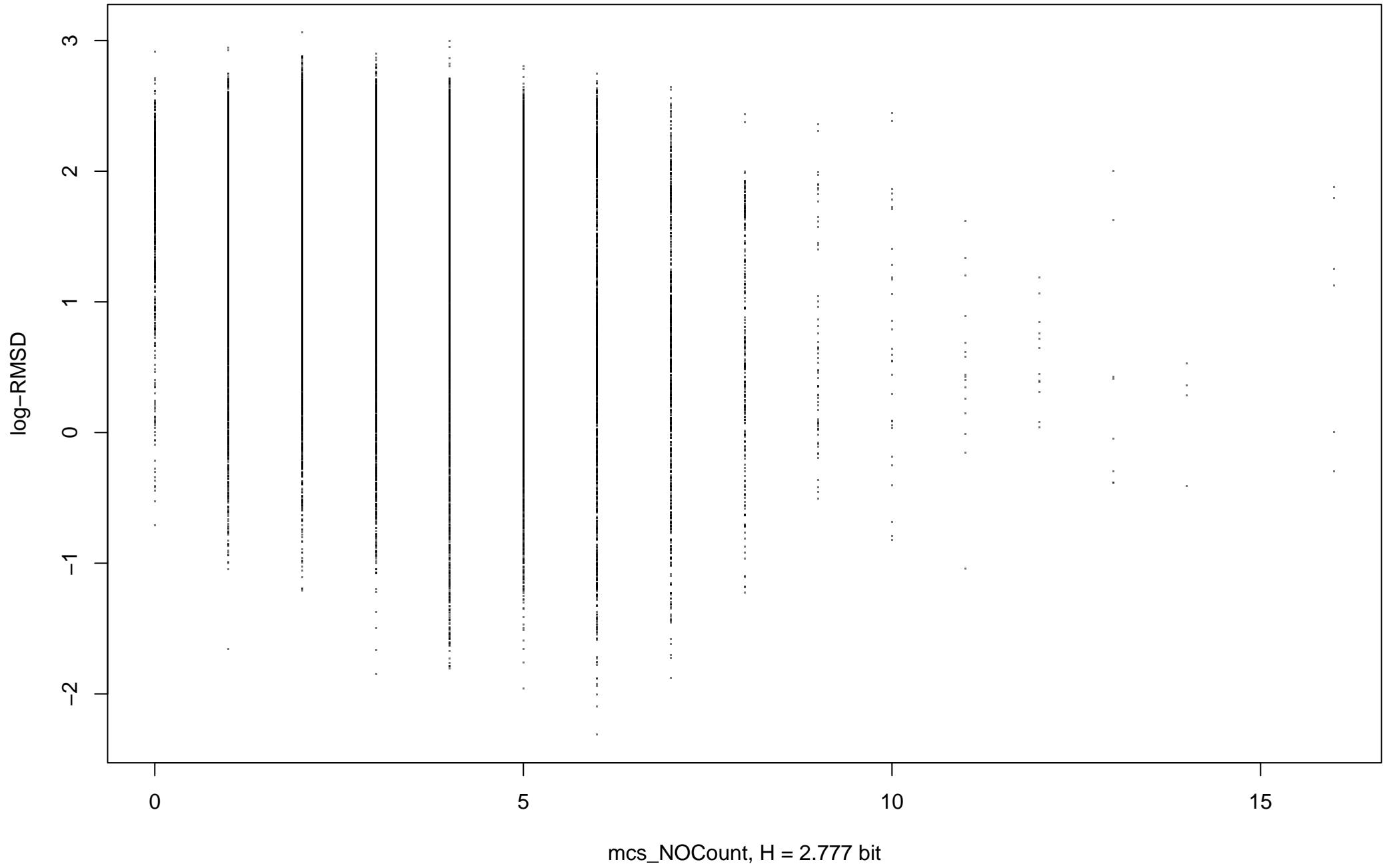
mcs_NumHeteroAtoms, MI = 0.1429 bit, norm = 0.04921, cond entr = 4.487 bit



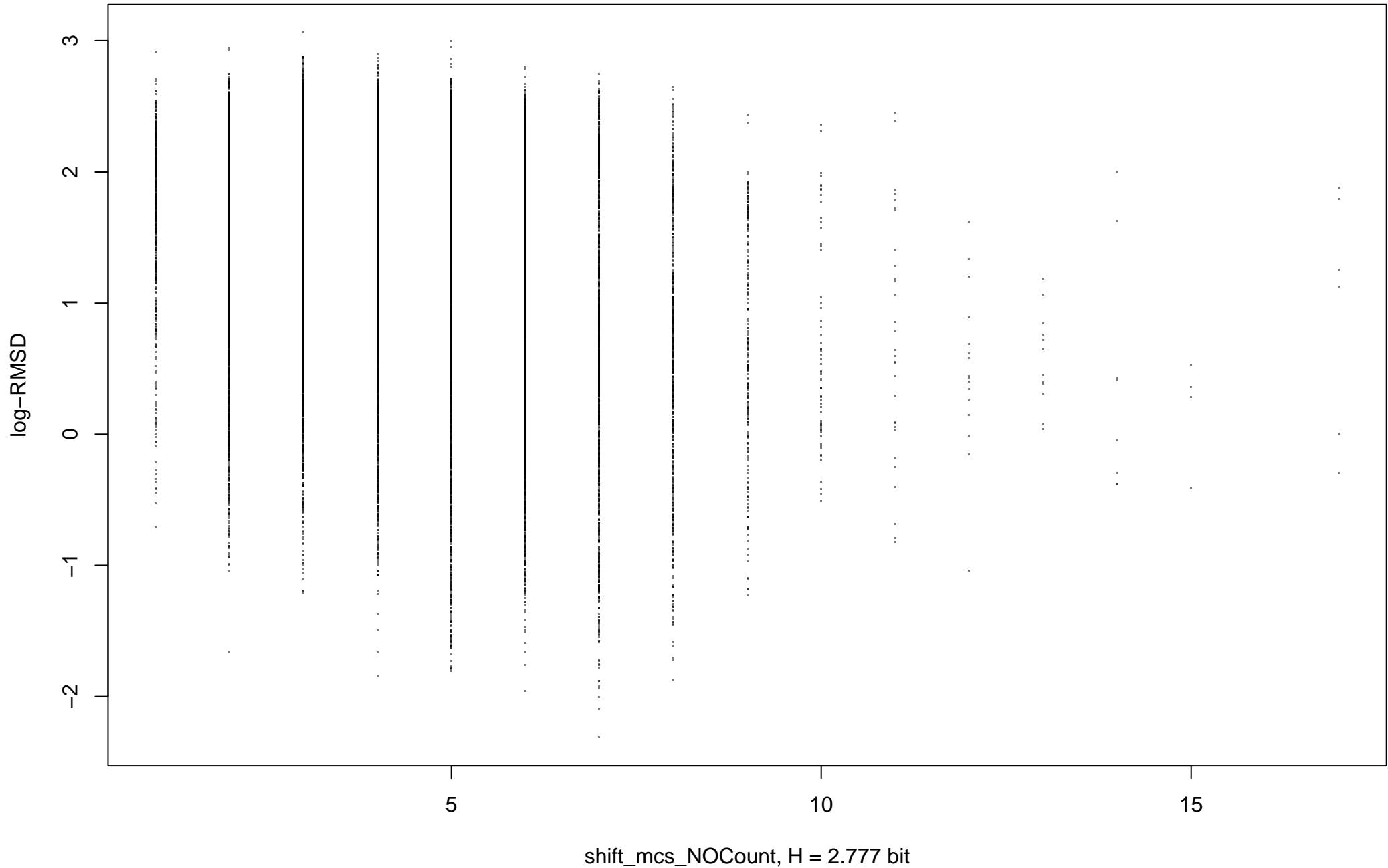
shift_mcs_NumHeteroAtoms, MI = 0.1429 bit, norm = 0.04921, cond entr = 4.487 bit



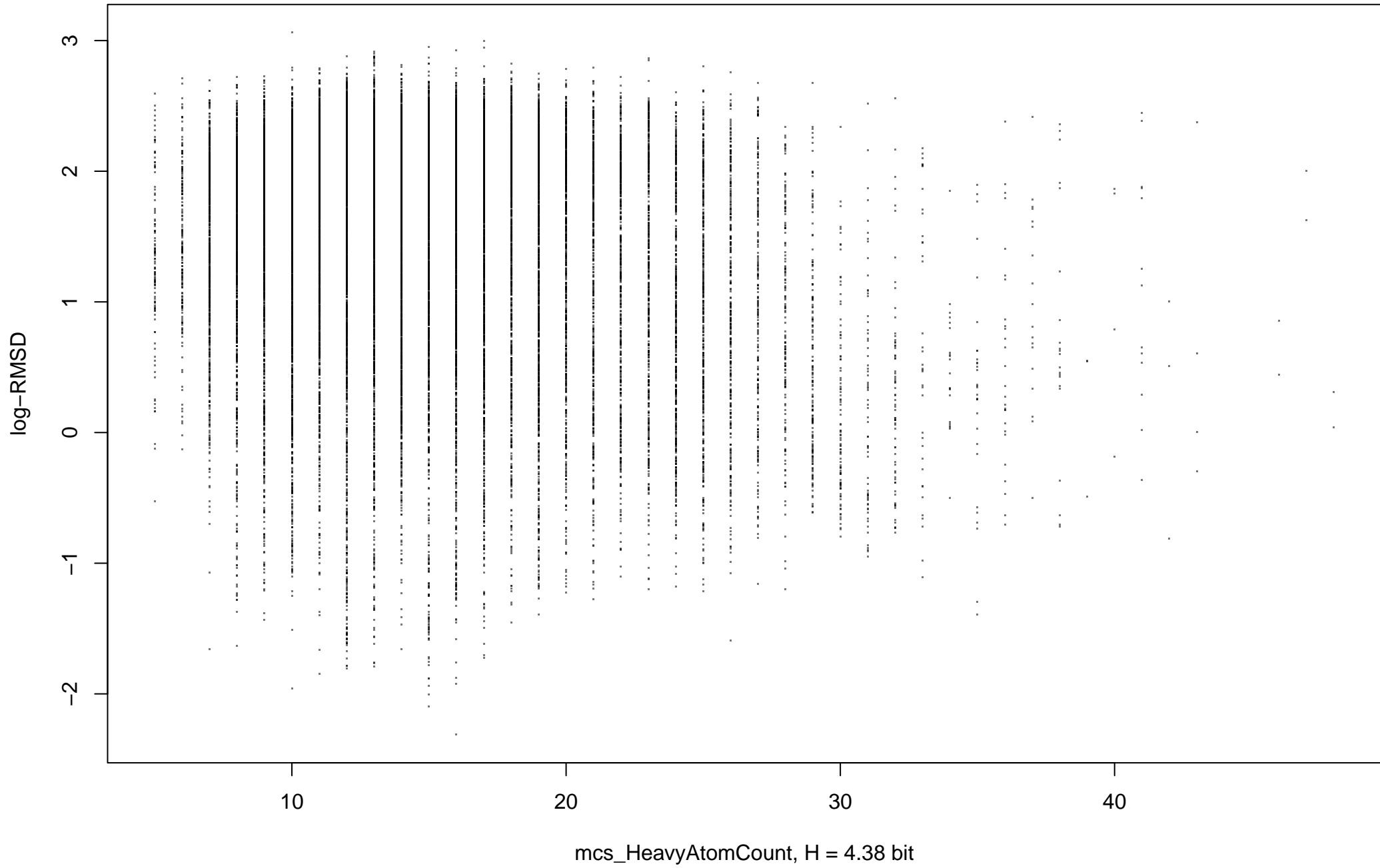
mcs_NOCount, MI = 0.1402 bit, norm = 0.0505, cond entr = 4.49 bit



shift_mcs_NOCount, MI = 0.1402 bit, norm = 0.0505, cond entr = 4.49 bit

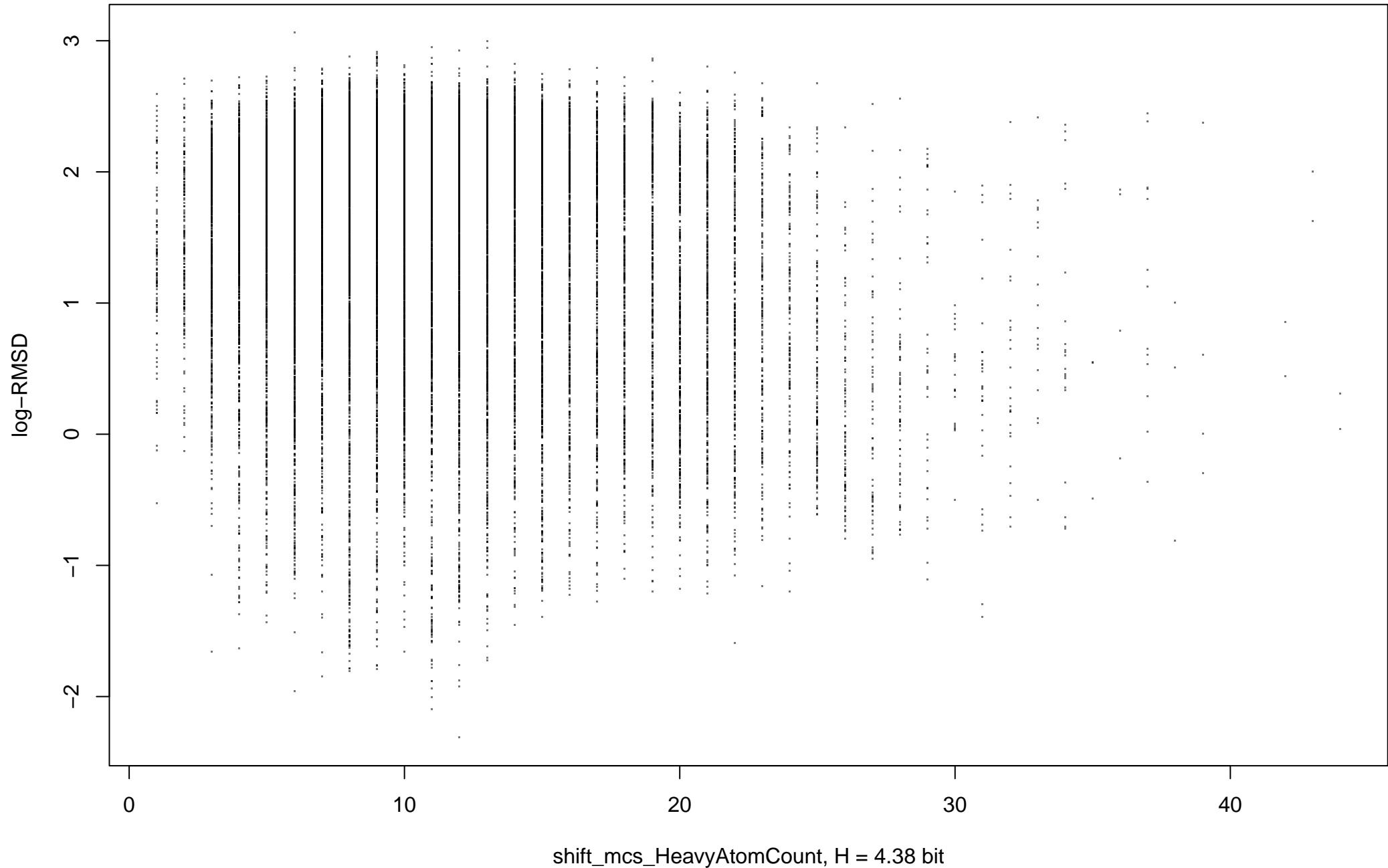


mcs_HeavyAtomCount, MI = 0.135 bit, norm = 0.03082, cond entr = 4.495 bit

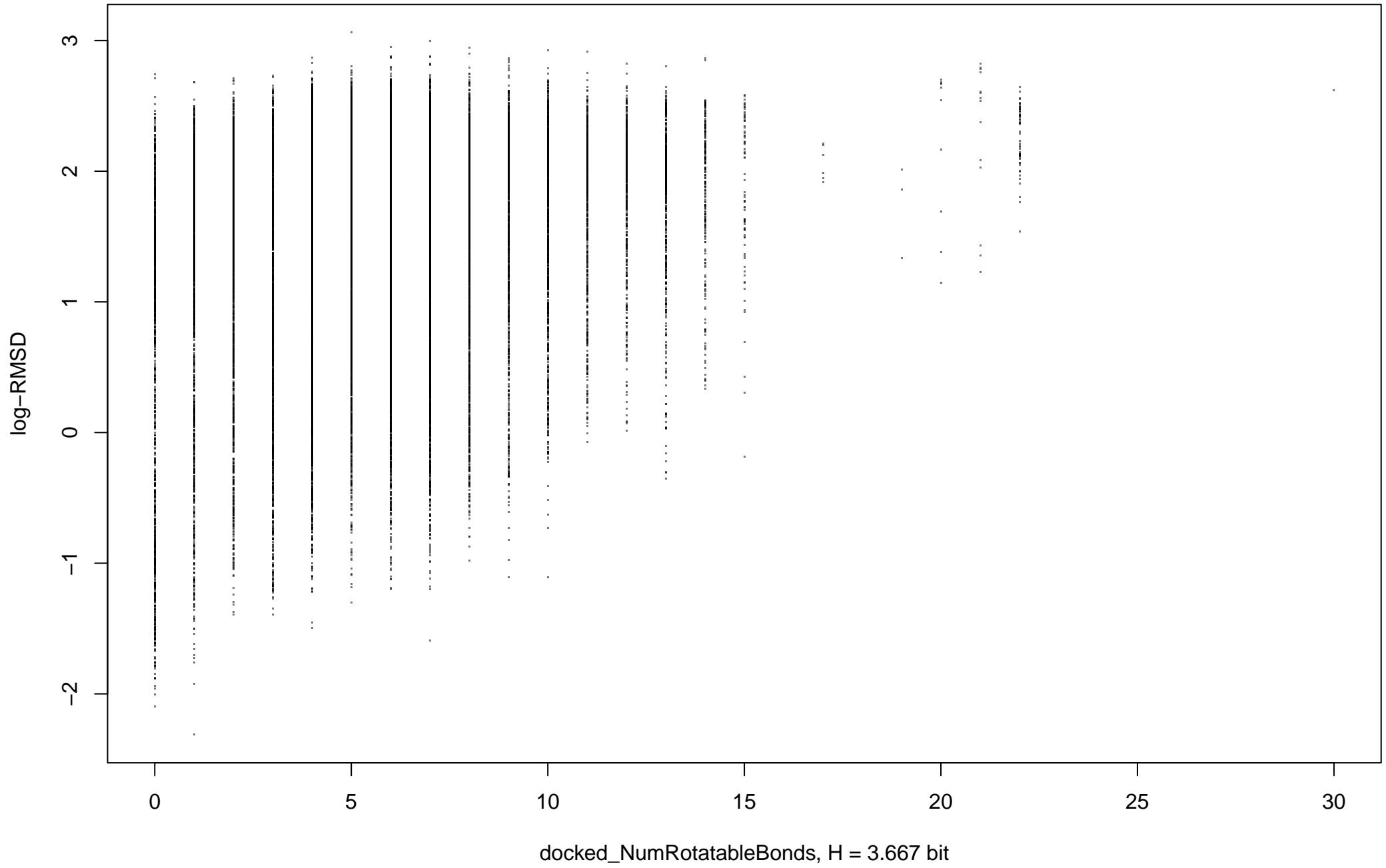


mcs_HeavyAtomCount, H = 4.38 bit

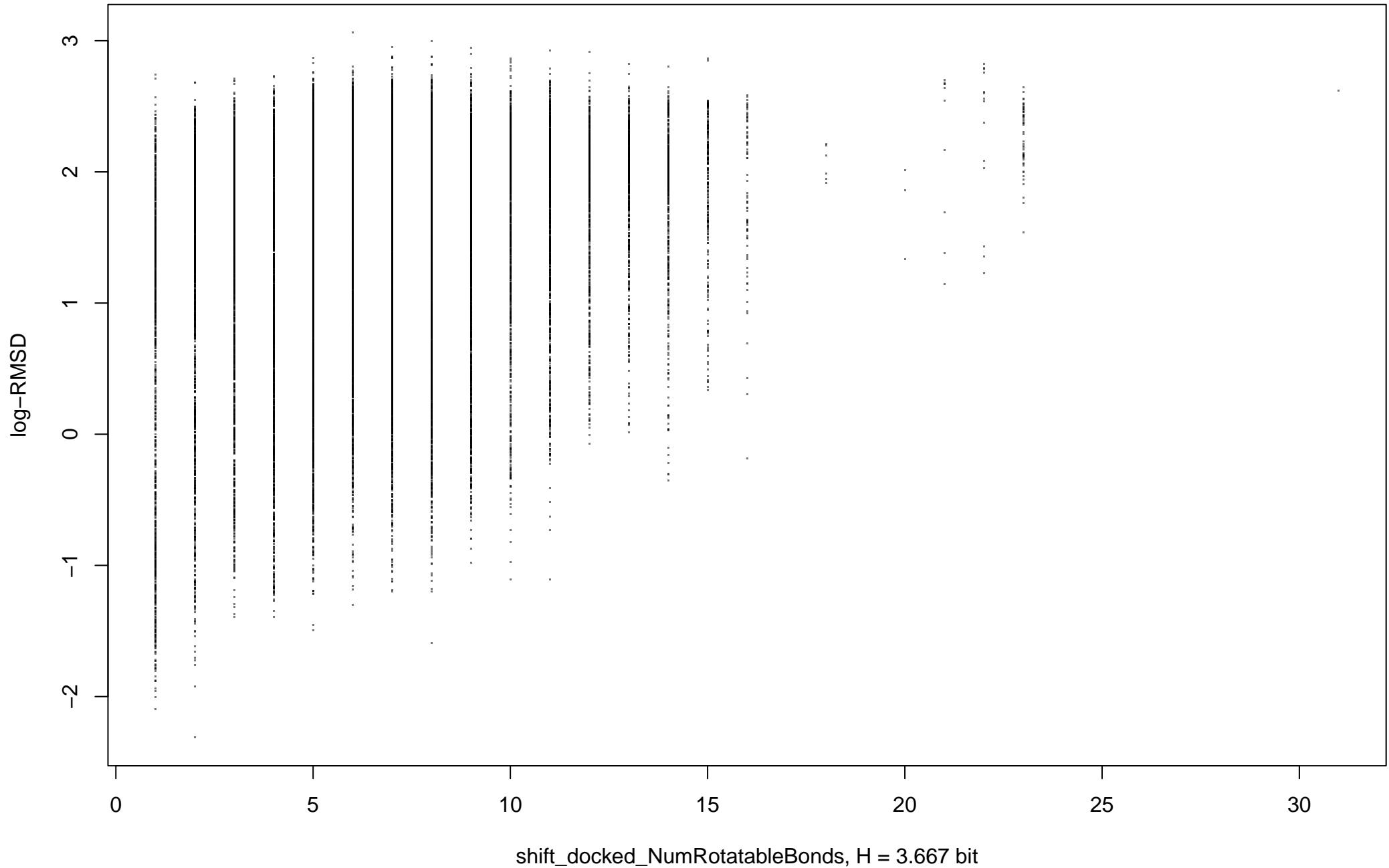
shift_mcs_HeavyAtomCount, MI = 0.135 bit, norm = 0.03082, cond entr = 4.495 bit



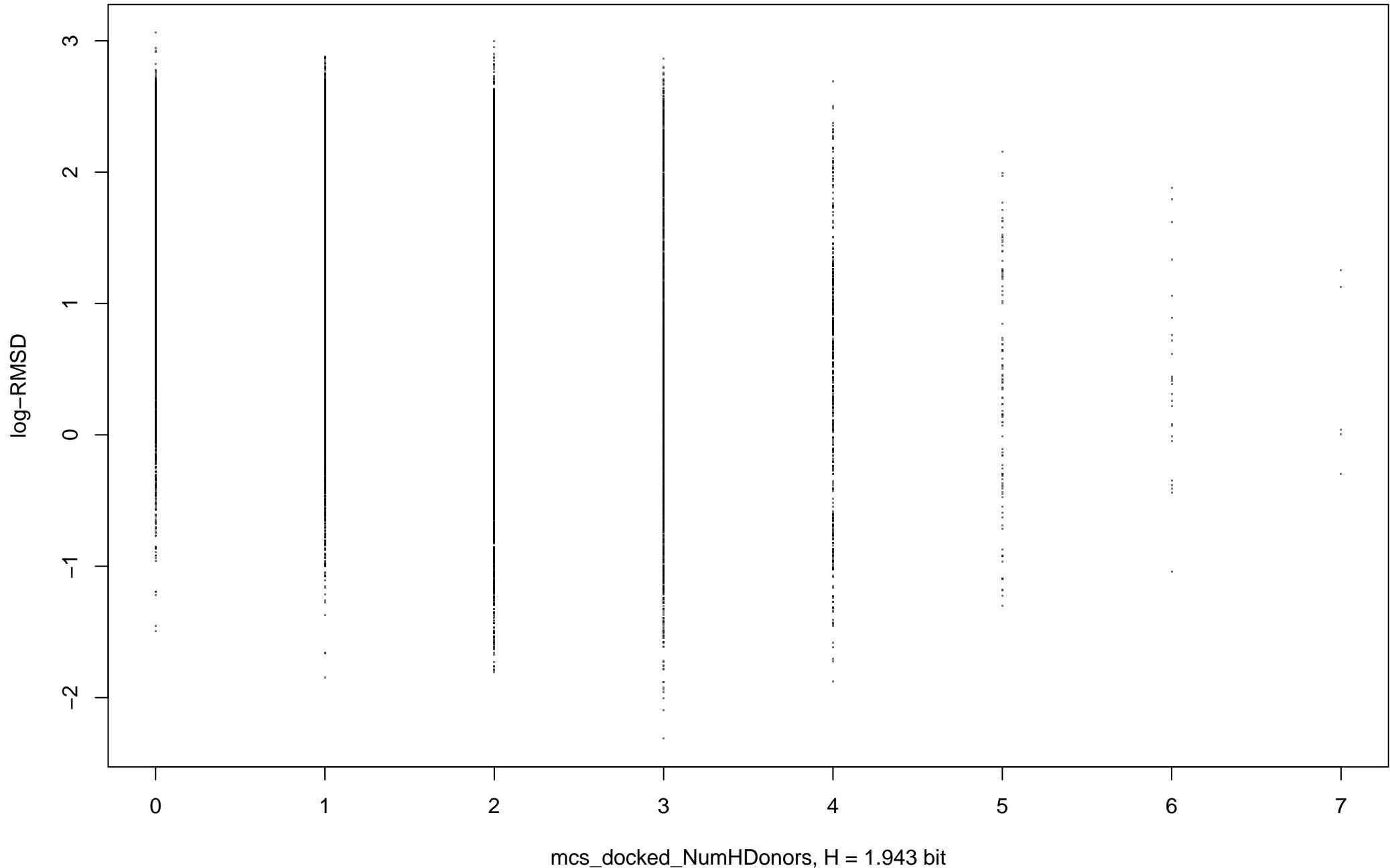
docked_NumRotatableBonds, MI = 0.1309 bit, norm = 0.0357, cond entr = 4.499 bit



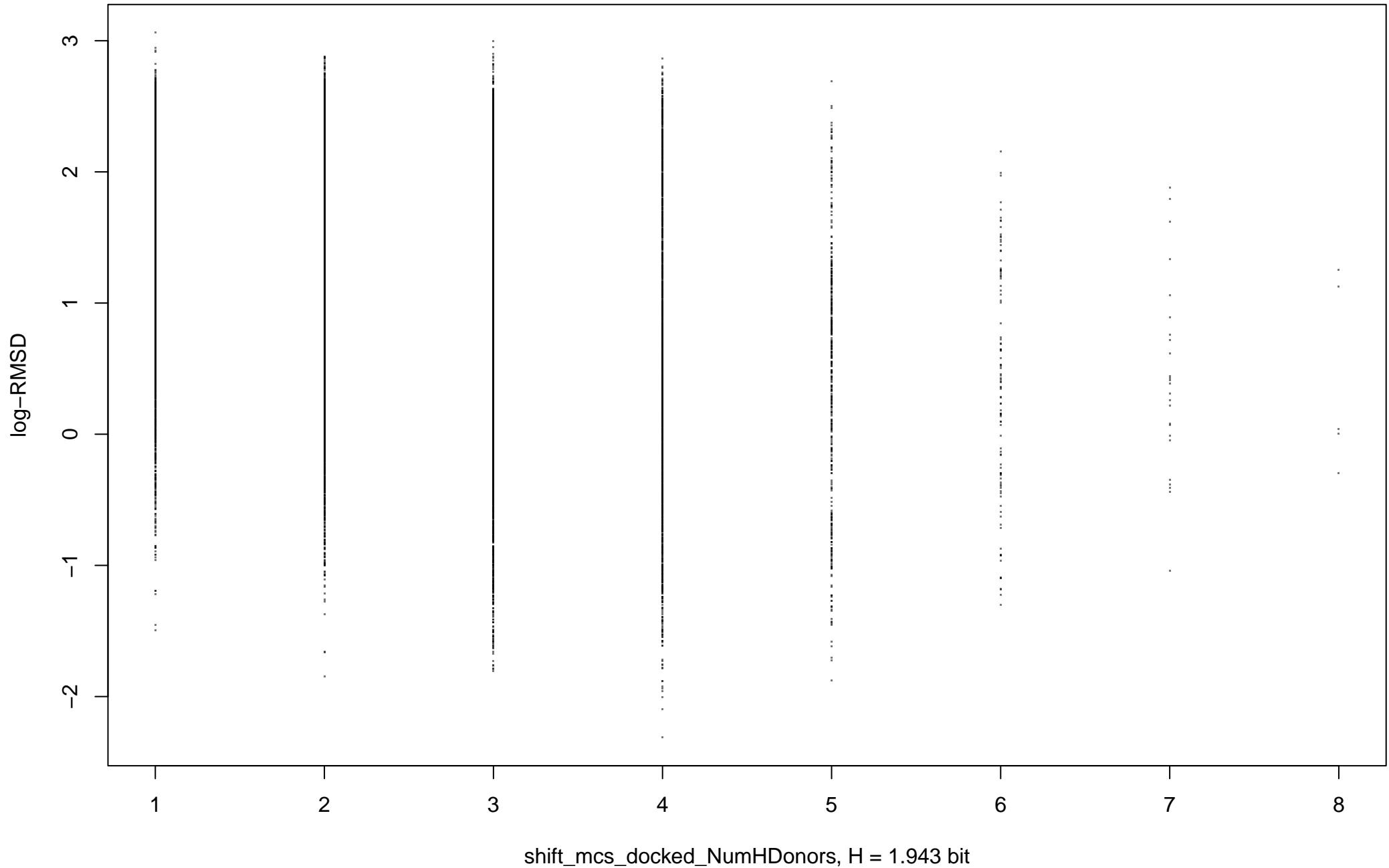
shift_docked_NumRotatableBonds, MI = 0.1309 bit, norm = 0.0357, cond entr = 4.499 bit



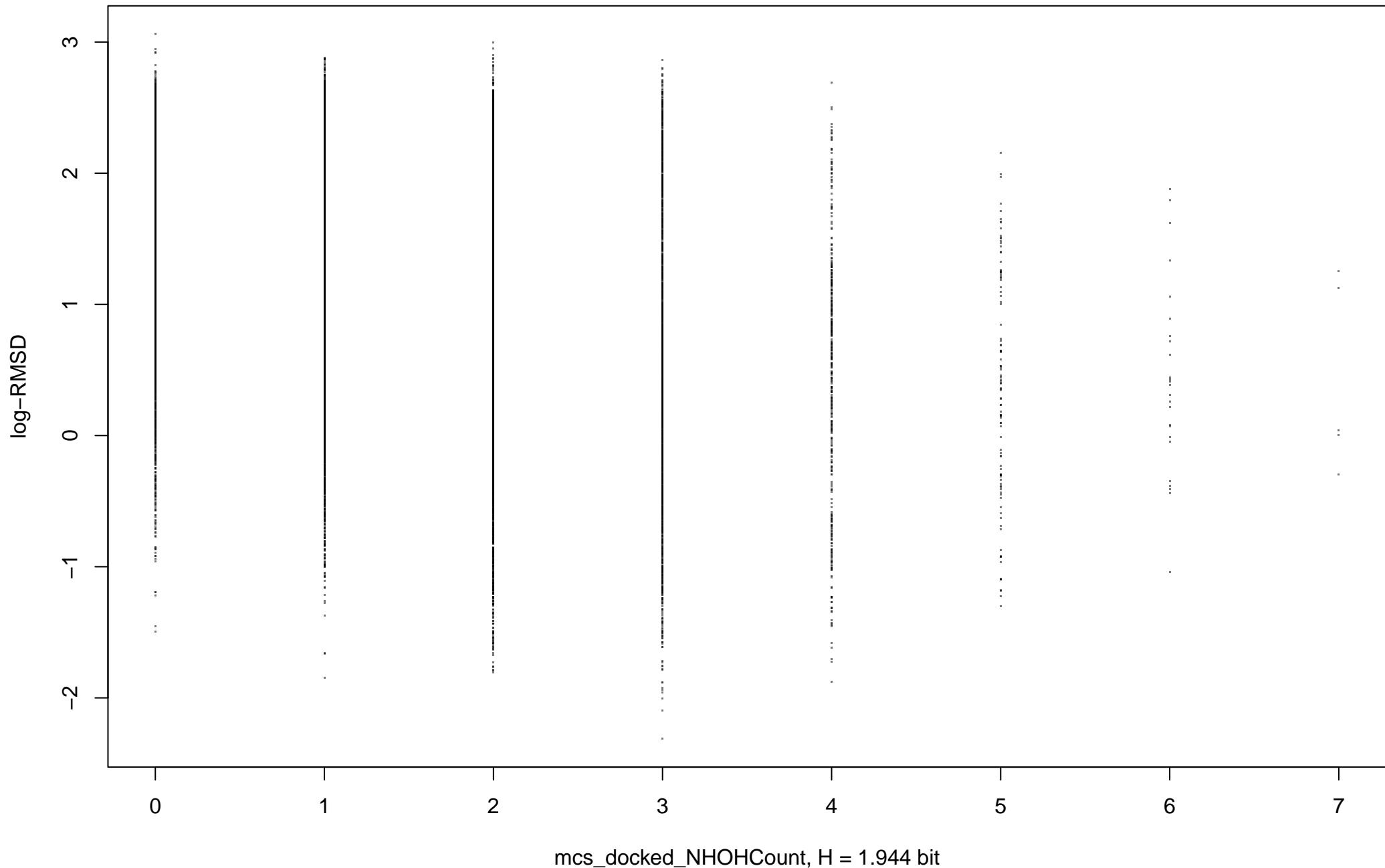
mcs_docked_NumHDonors, MI = 0.1293 bit, norm = 0.06654, cond entr = 4.501 bit



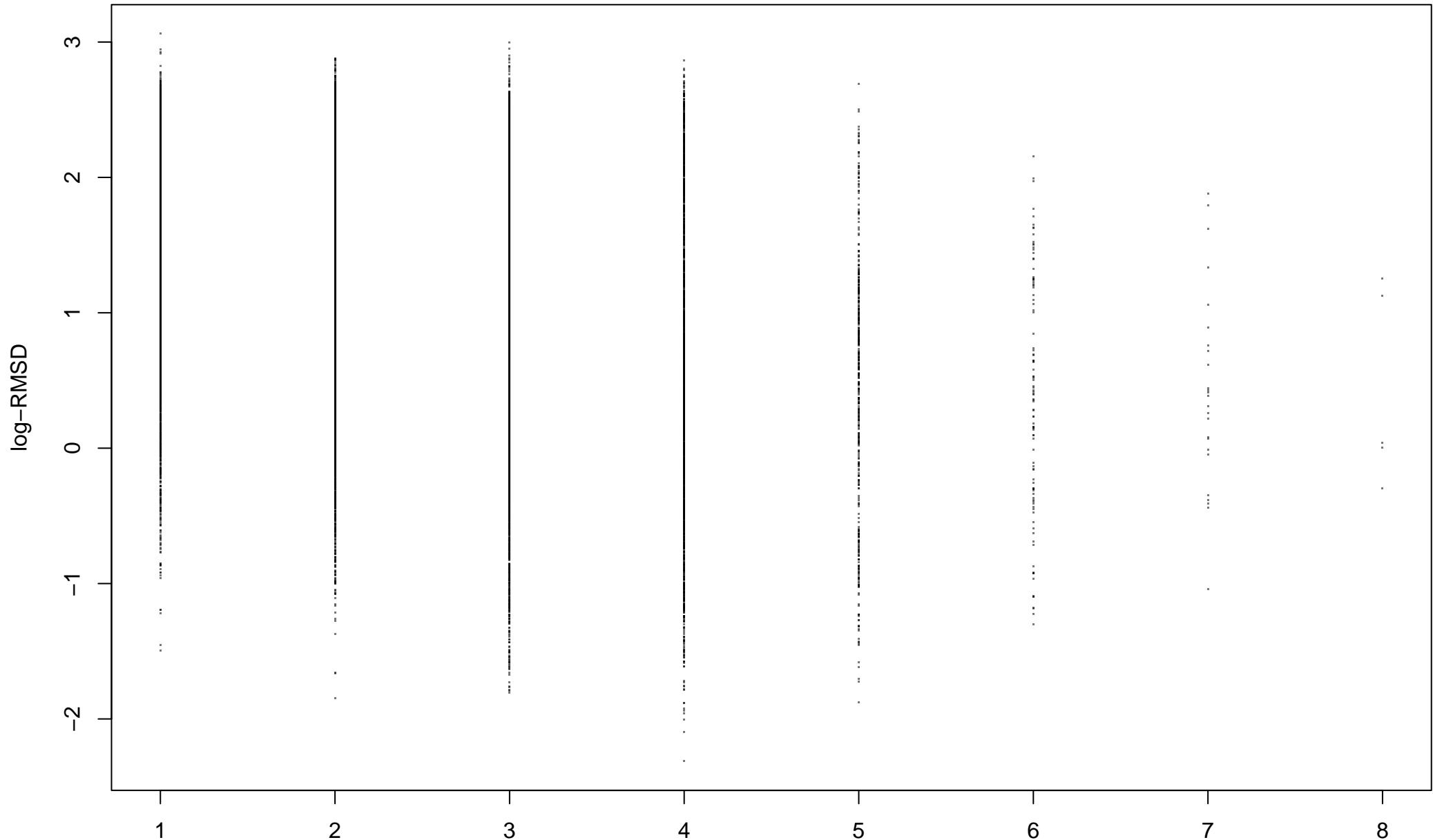
shift_mcs_docked_NumHDonors, MI = 0.1293 bit, norm = 0.06654, cond entr = 4.501 bit



mcs_docked_NHOHCount, MI = 0.1292 bit, norm = 0.06648, cond entr = 4.501 bit

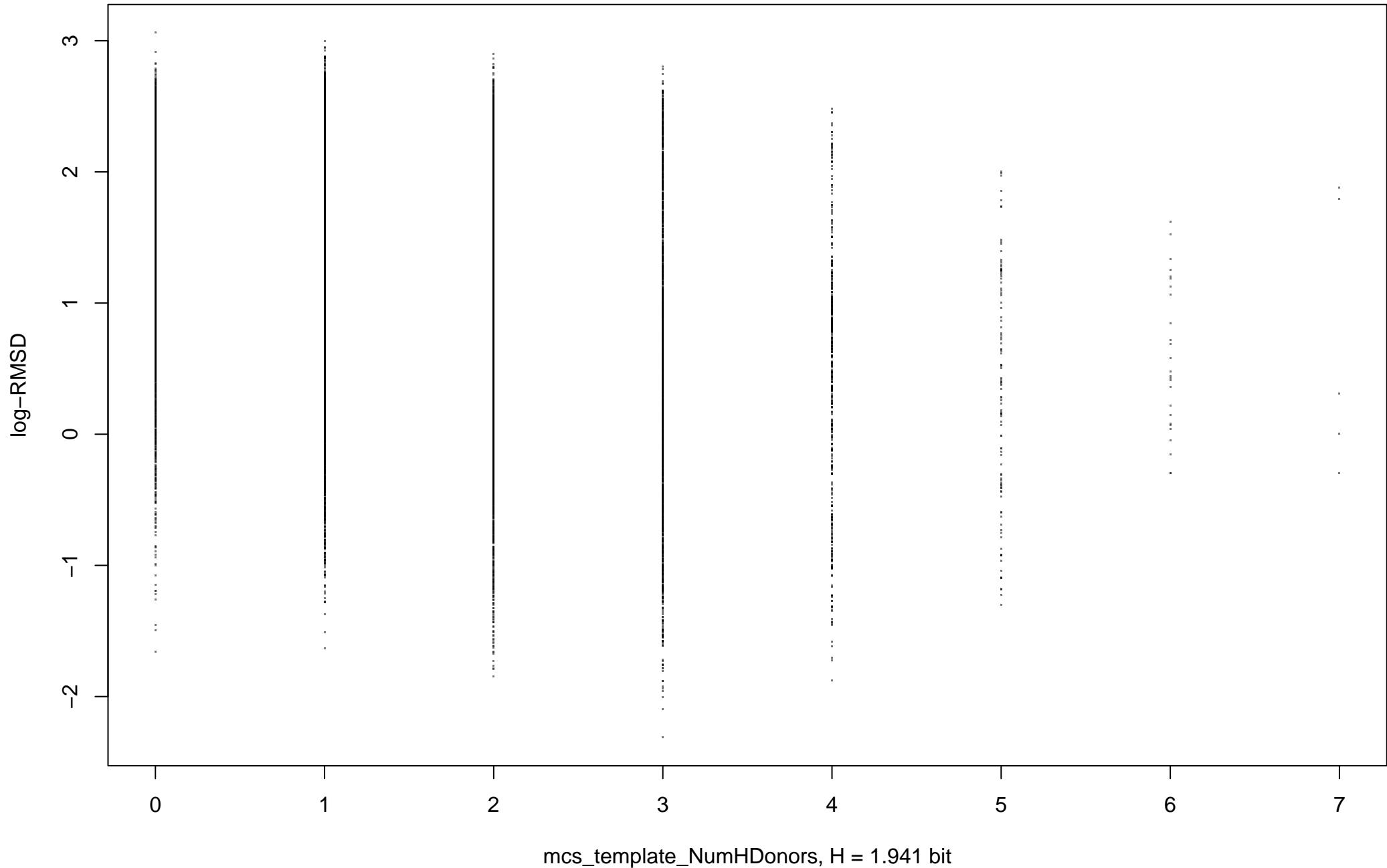


shift_mcs_docked_NHOHCount, MI = 0.1292 bit, norm = 0.06648, cond entr = 4.501 bit

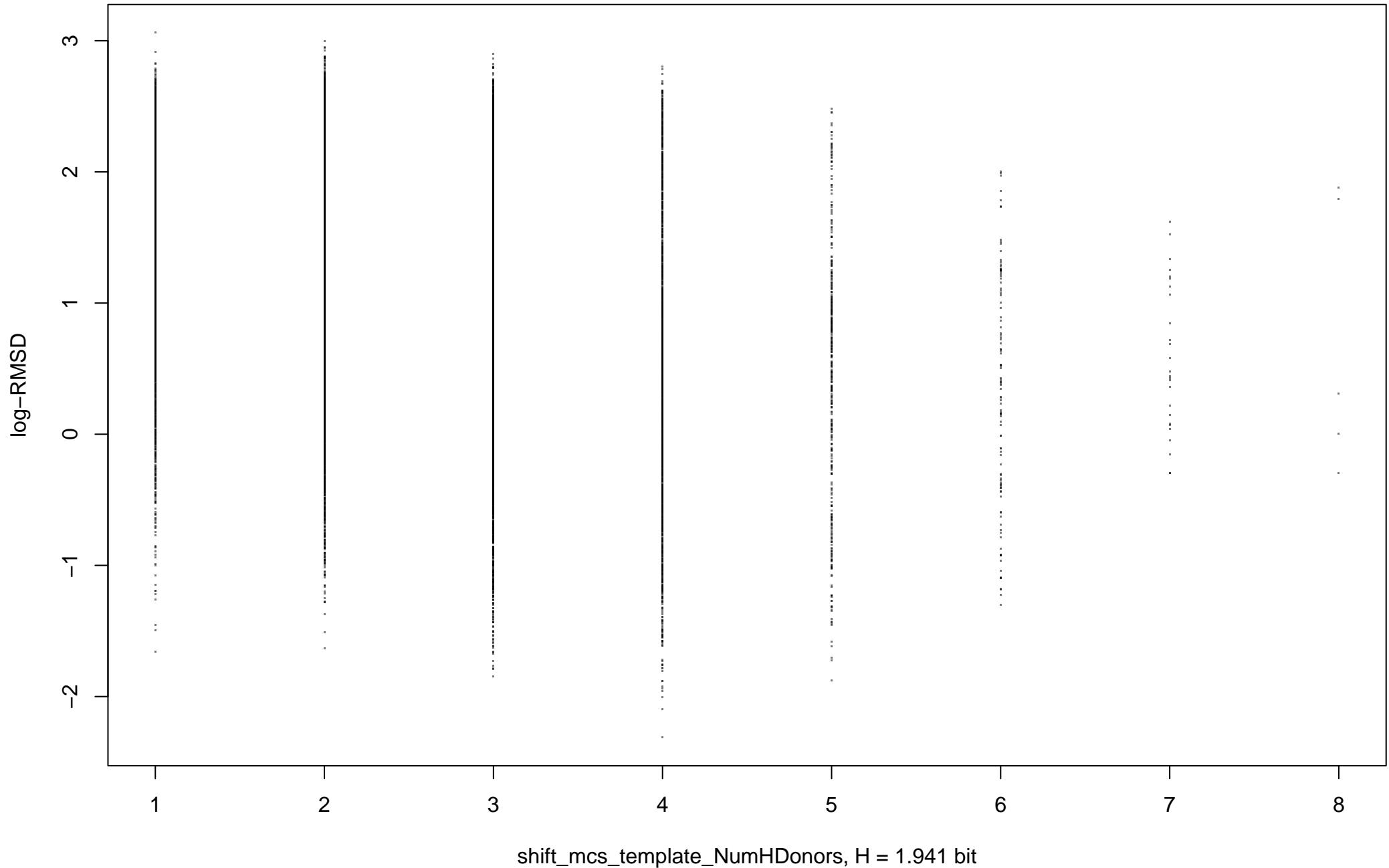


shift_mcs_docked_NHOHCount, H = 1.944 bit

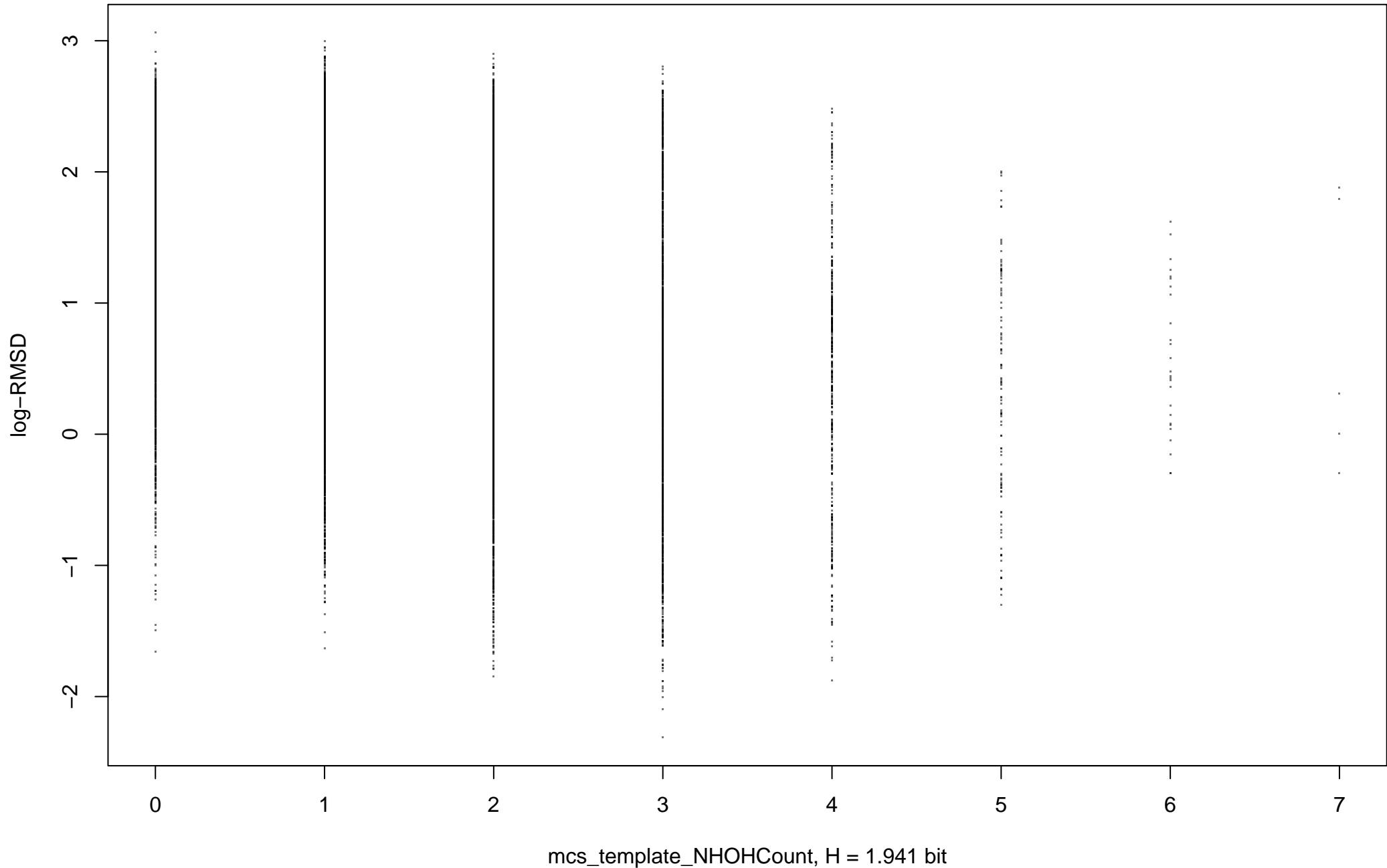
mcs_template_NumHDonors, MI = 0.126 bit, norm = 0.06492, cond entr = 4.504 bit



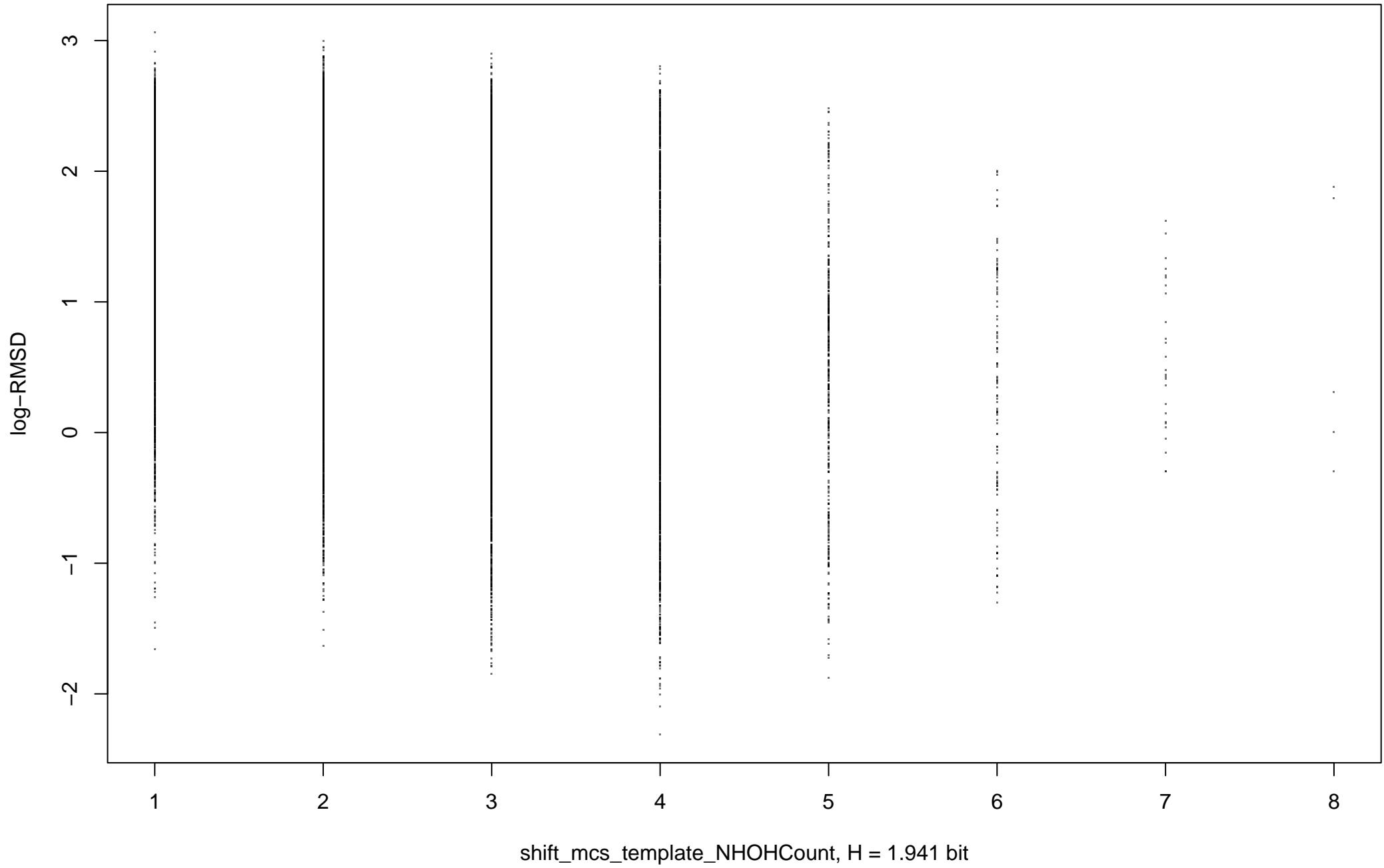
shift_mcs_template_NumHDonors, MI = 0.126 bit, norm = 0.06492, cond entr = 4.504 bit



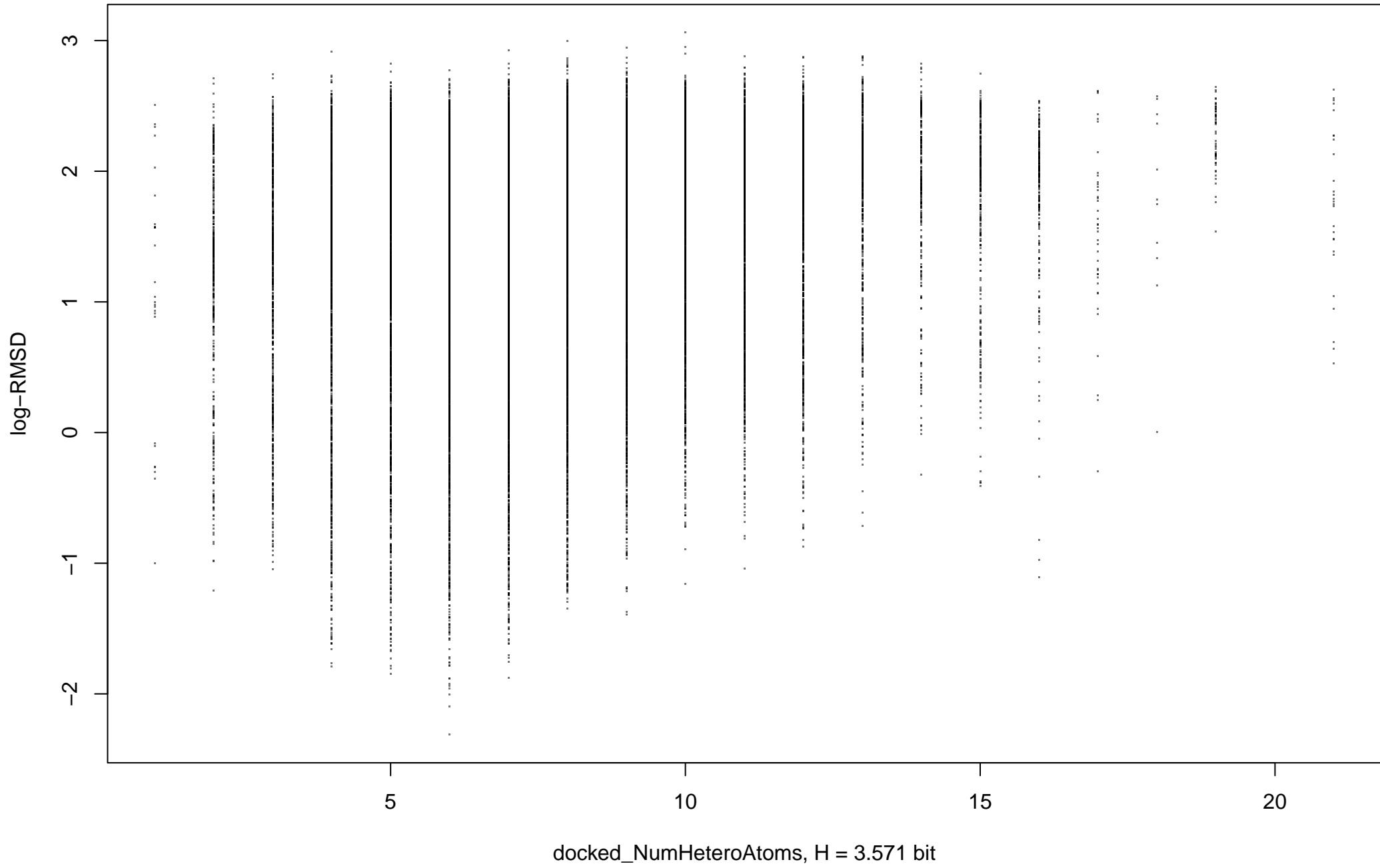
mcs_template_NHOHCount, MI = 0.1258 bit, norm = 0.06478, cond entr = 4.504 bit



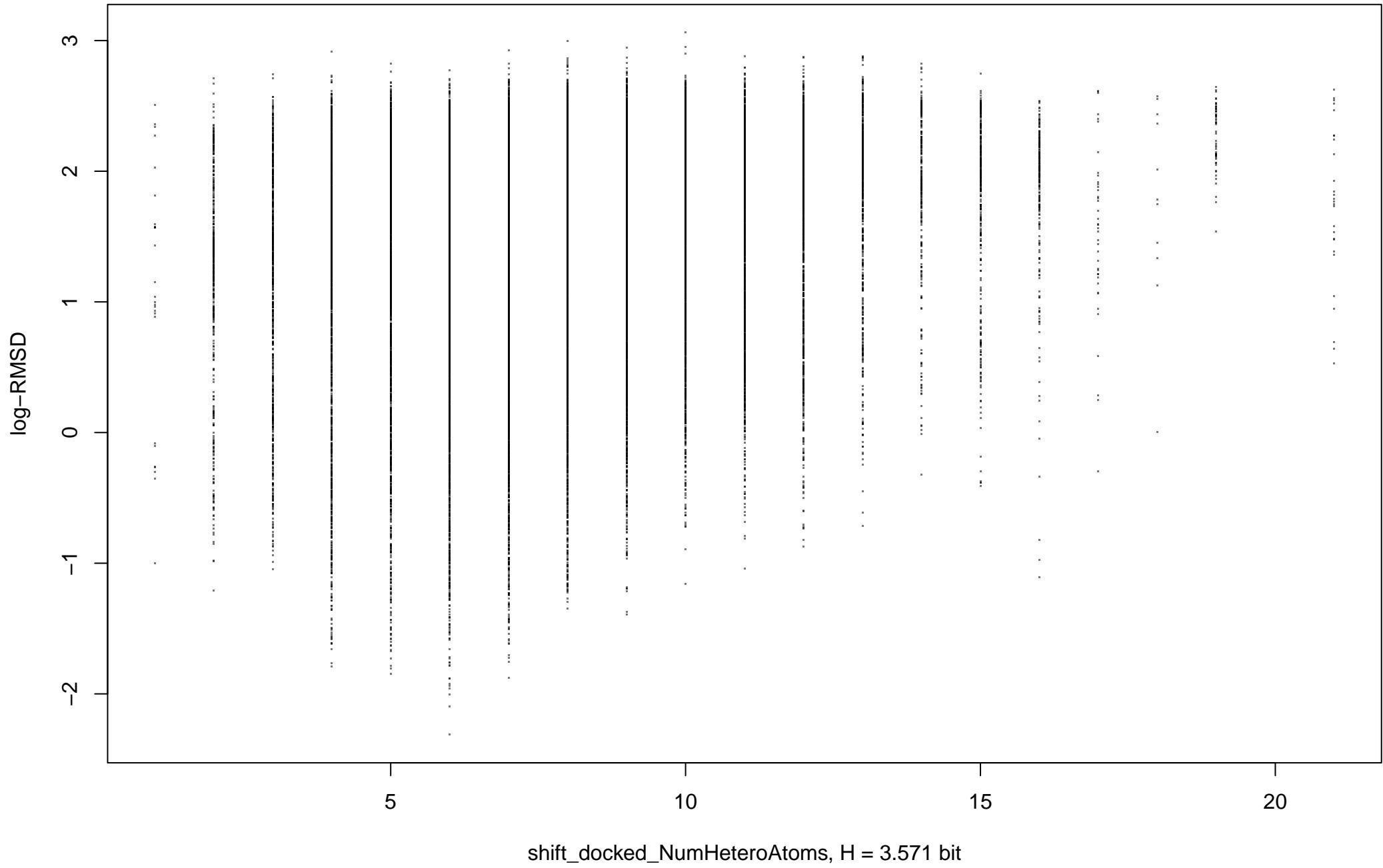
shift_mcs_template_NHOHCount, MI = 0.1258 bit, norm = 0.06478, cond entr = 4.504 bit



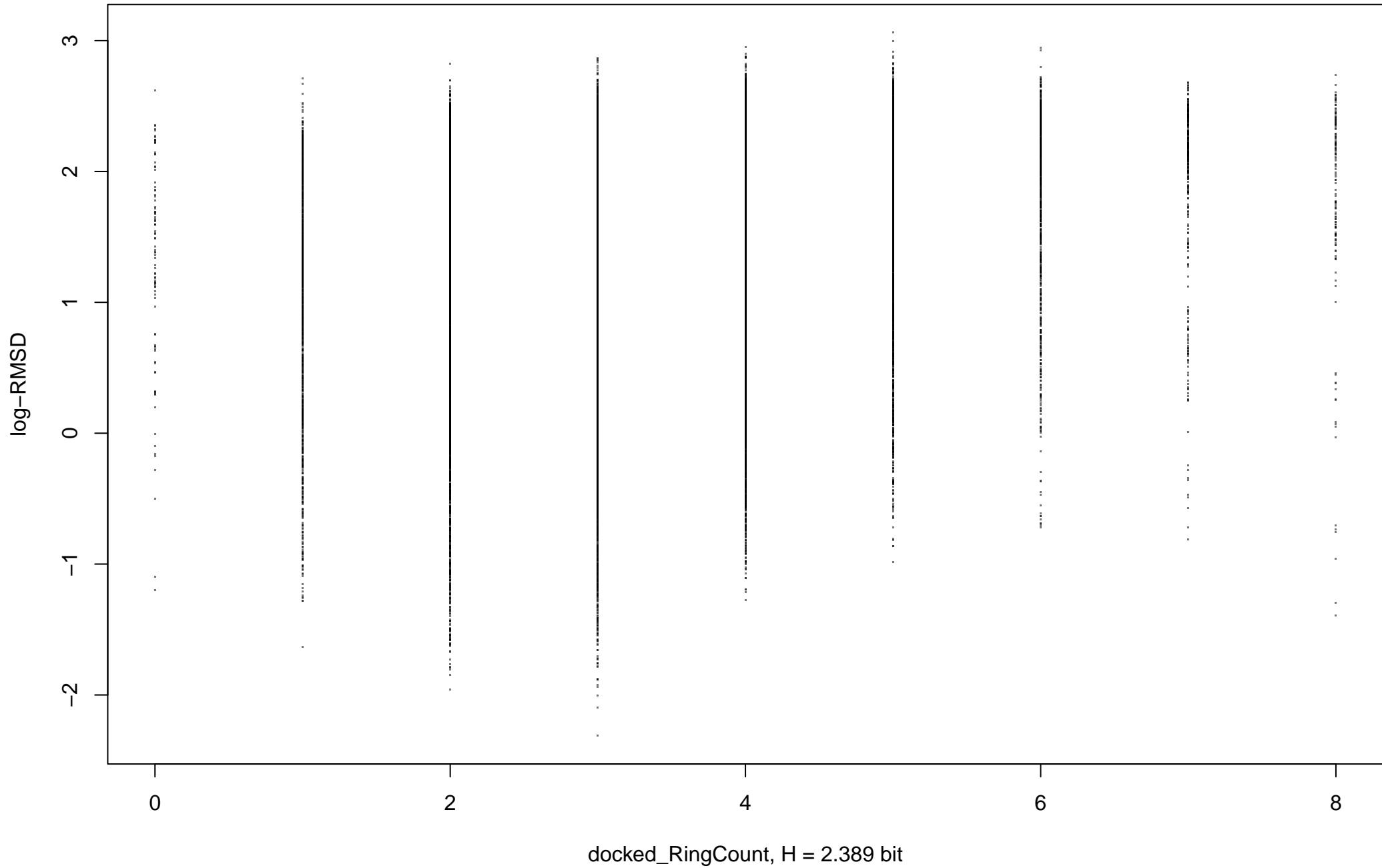
docked_NumHeteroAtoms, MI = 0.09698 bit, norm = 0.02716, cond entr = 4.533 bit



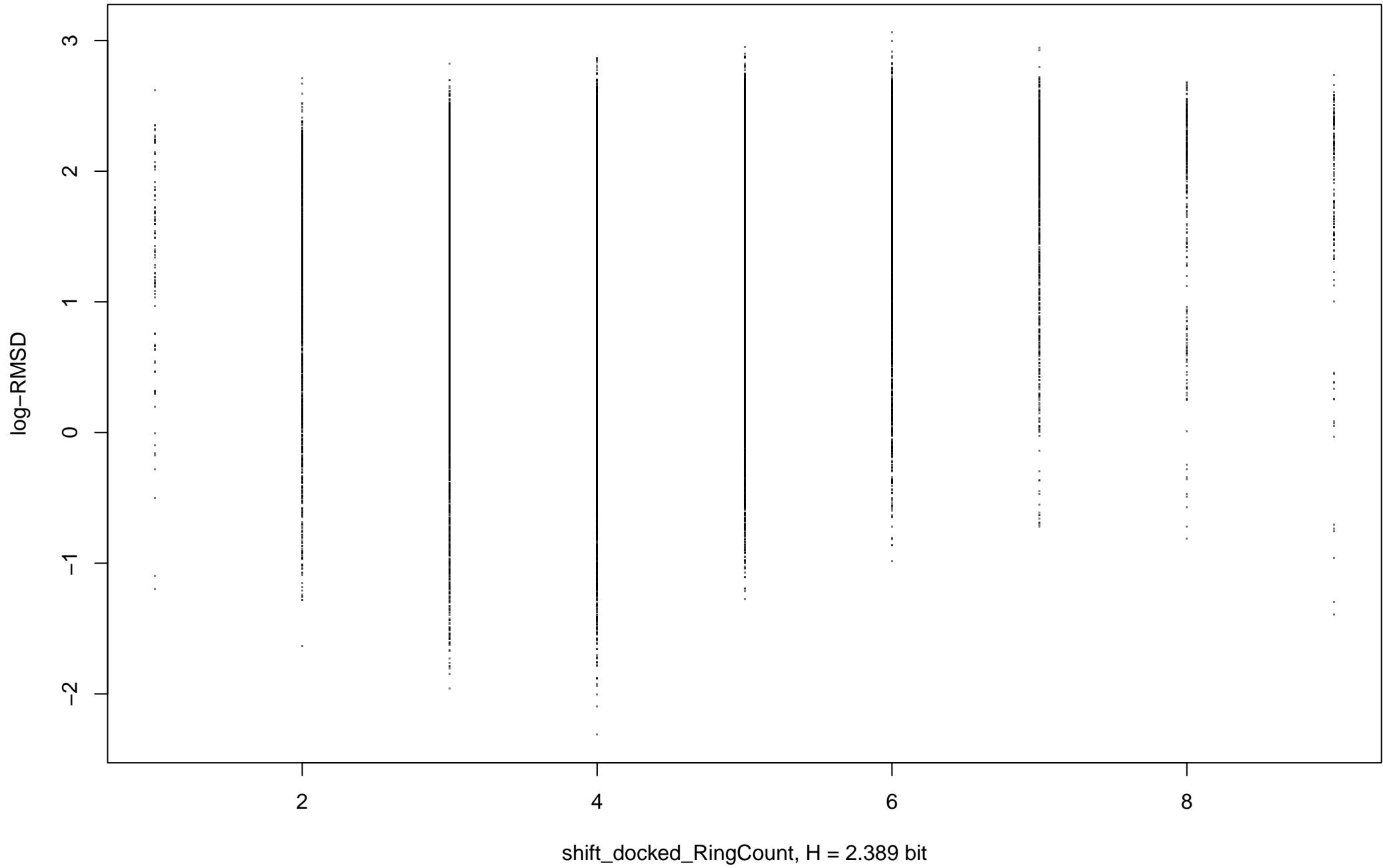
shift_docked_NumHeteroAtoms, MI = 0.09698 bit, norm = 0.02716, cond entr = 4.533 bit



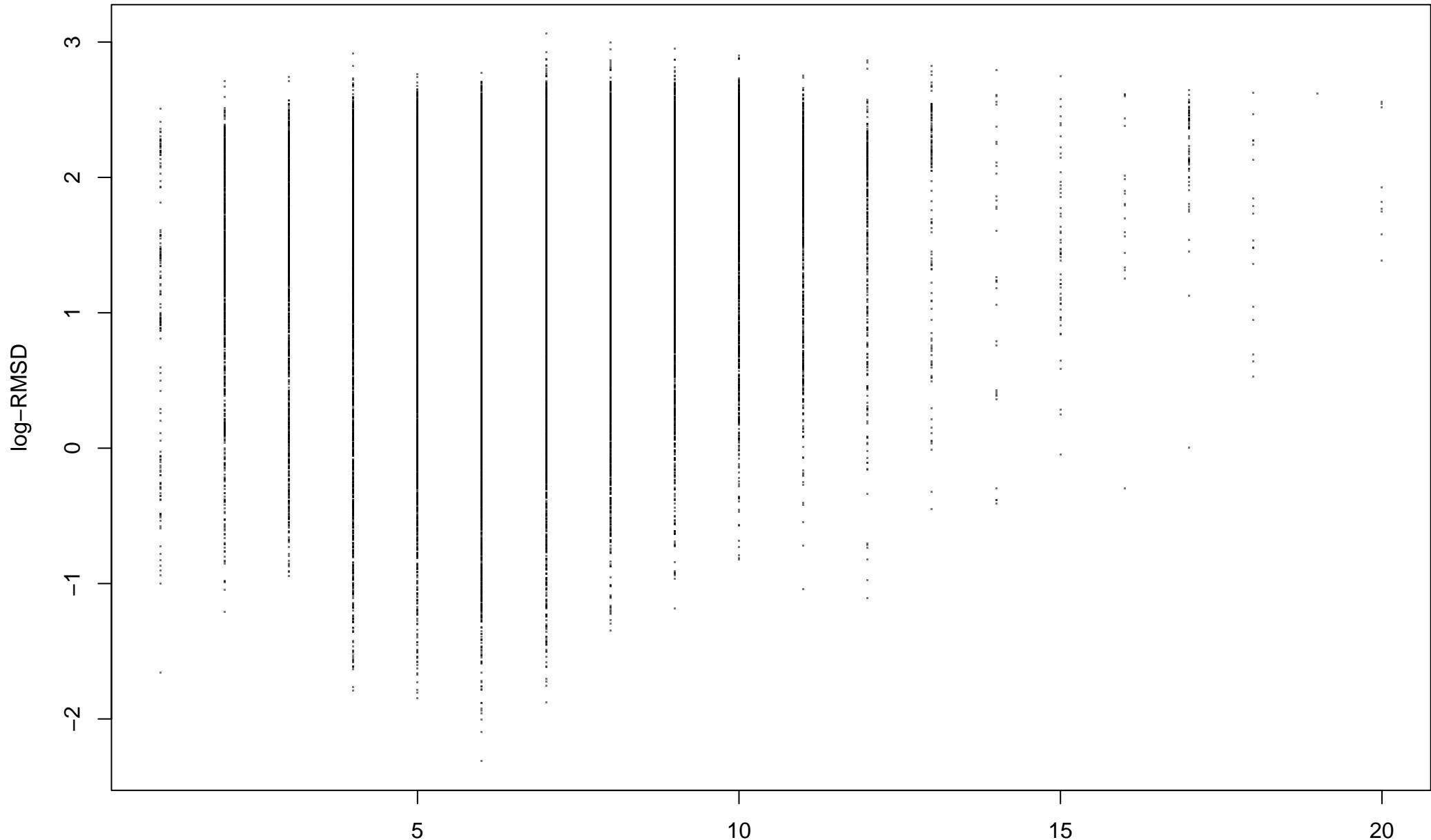
docked_RingCount, MI = 0.09028 bit, norm = 0.03779, cond entr = 4.54 bit



shift_docked_RingCount, MI = 0.09028 bit, norm = 0.03779, cond entr = 4.54 bit

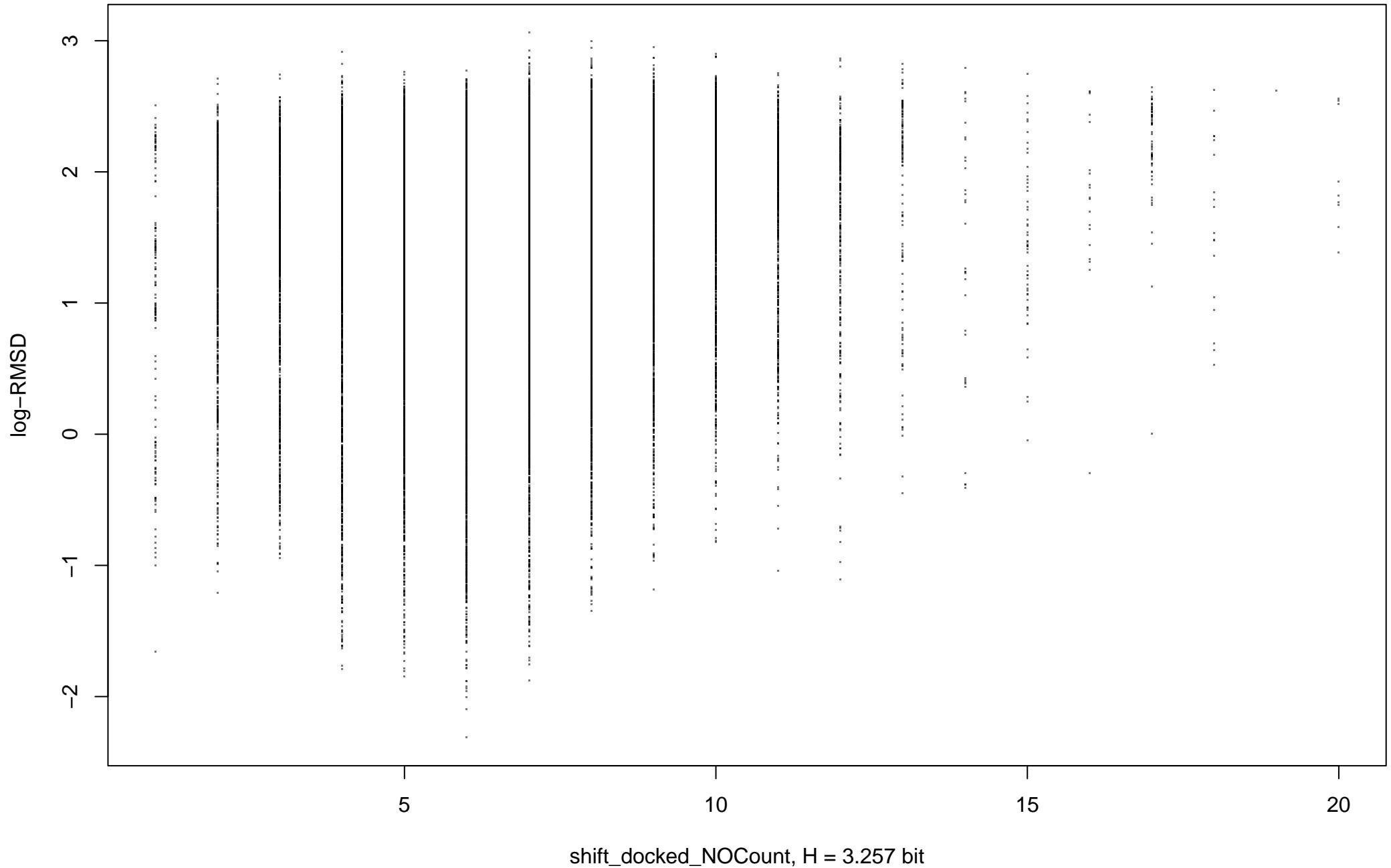


docked_NOCount, MI = 0.08995 bit, norm = 0.02762, cond entr = 4.54 bit

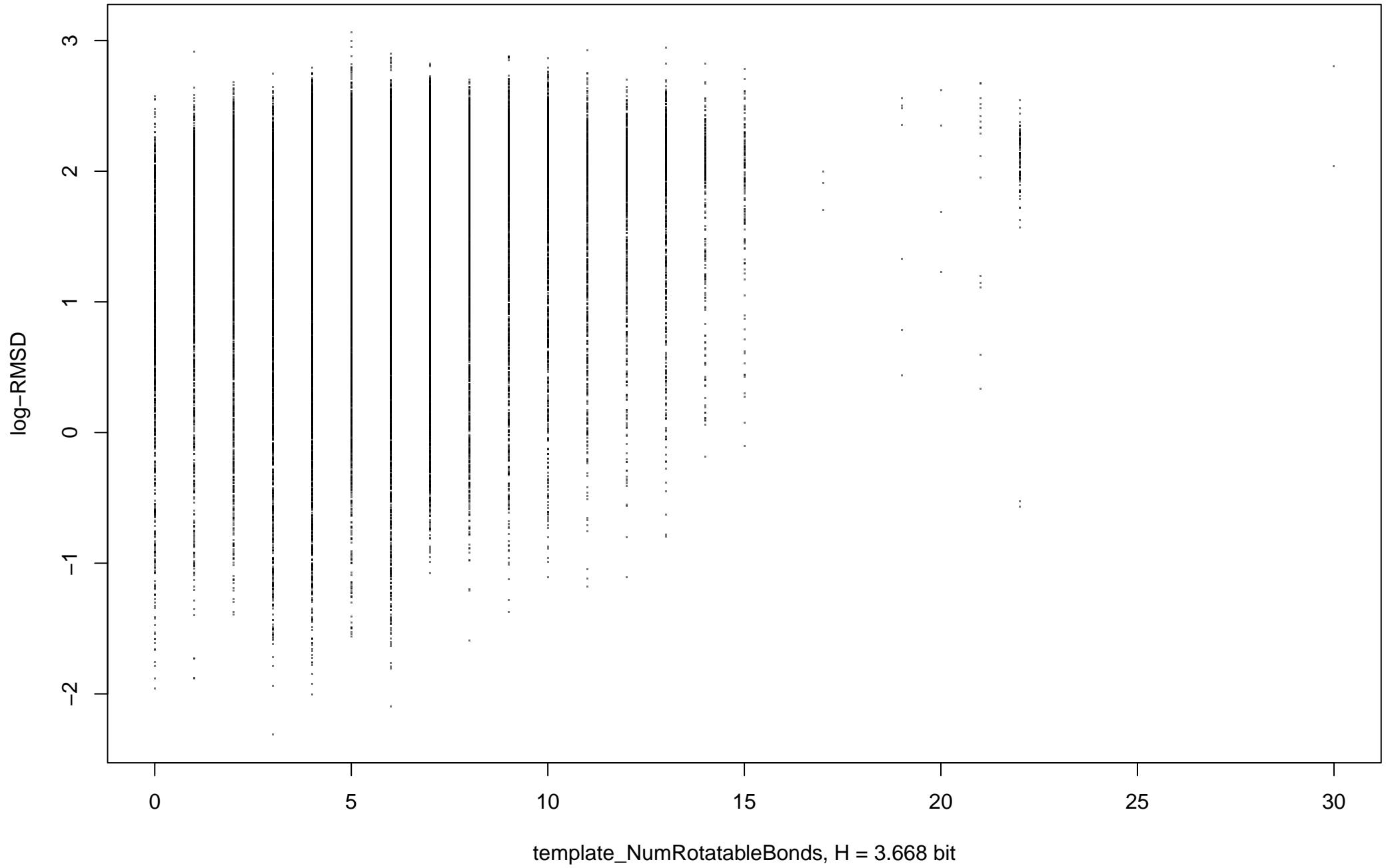


docked_NOCount, H = 3.257 bit

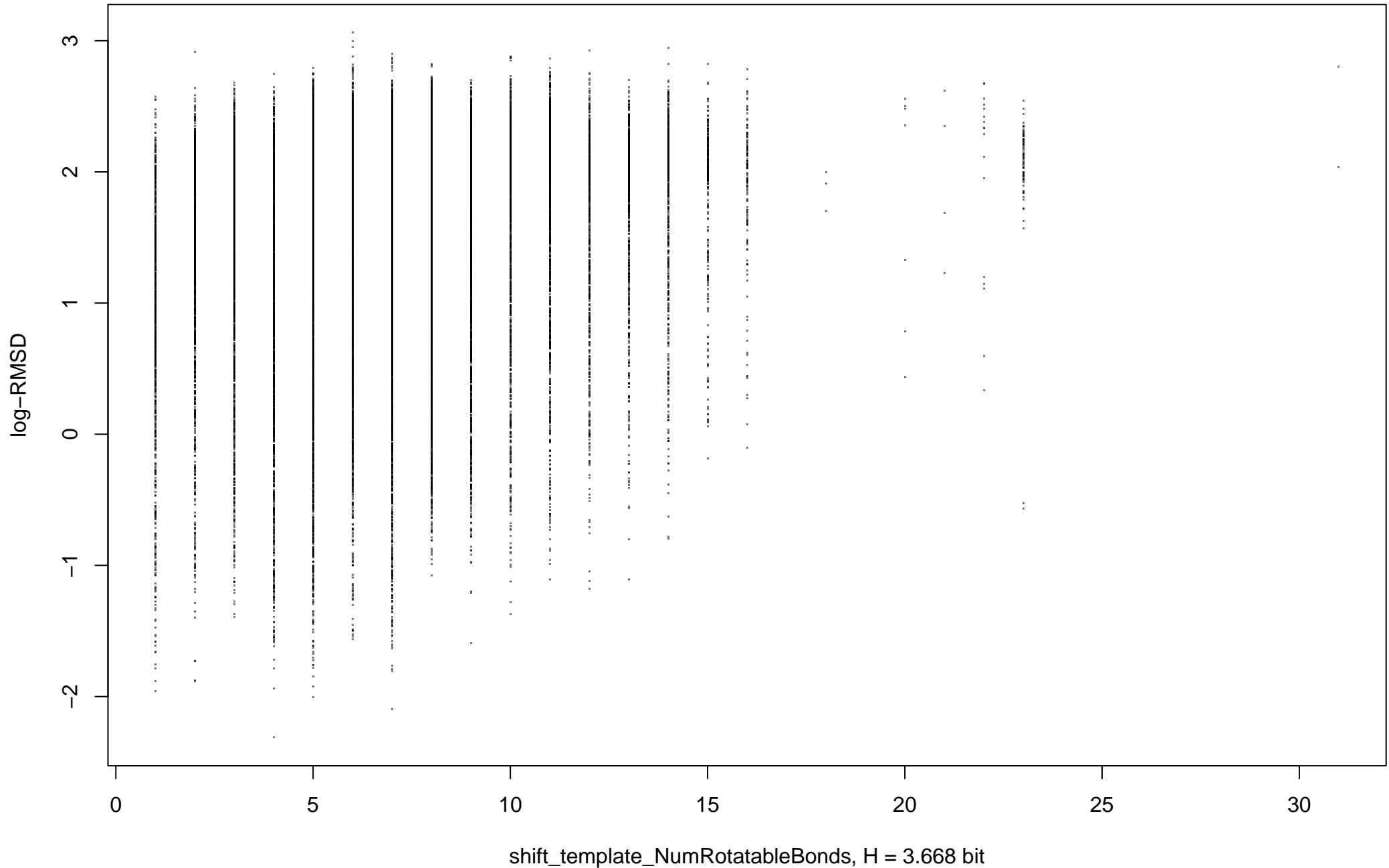
shift_docked_NOCount, MI = 0.08995 bit, norm = 0.02762, cond entr = 4.54 bit



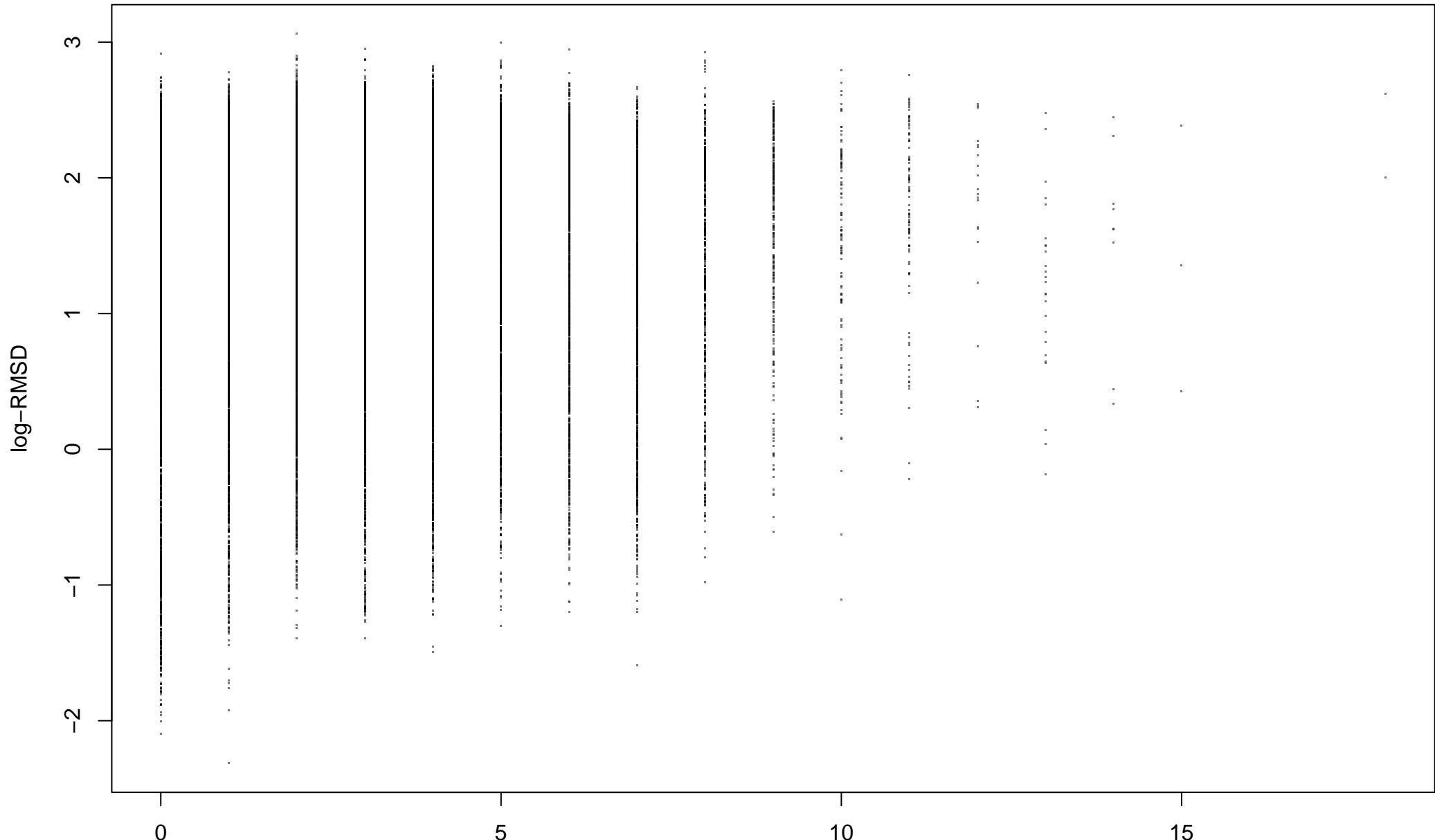
template_NumRotatableBonds, MI = 0.0868 bit, norm = 0.02366, cond entr = 4.543 bit



shift_template_NumRotatableBonds, MI = 0.0868 bit, norm = 0.02366, cond entr = 4.543 bit

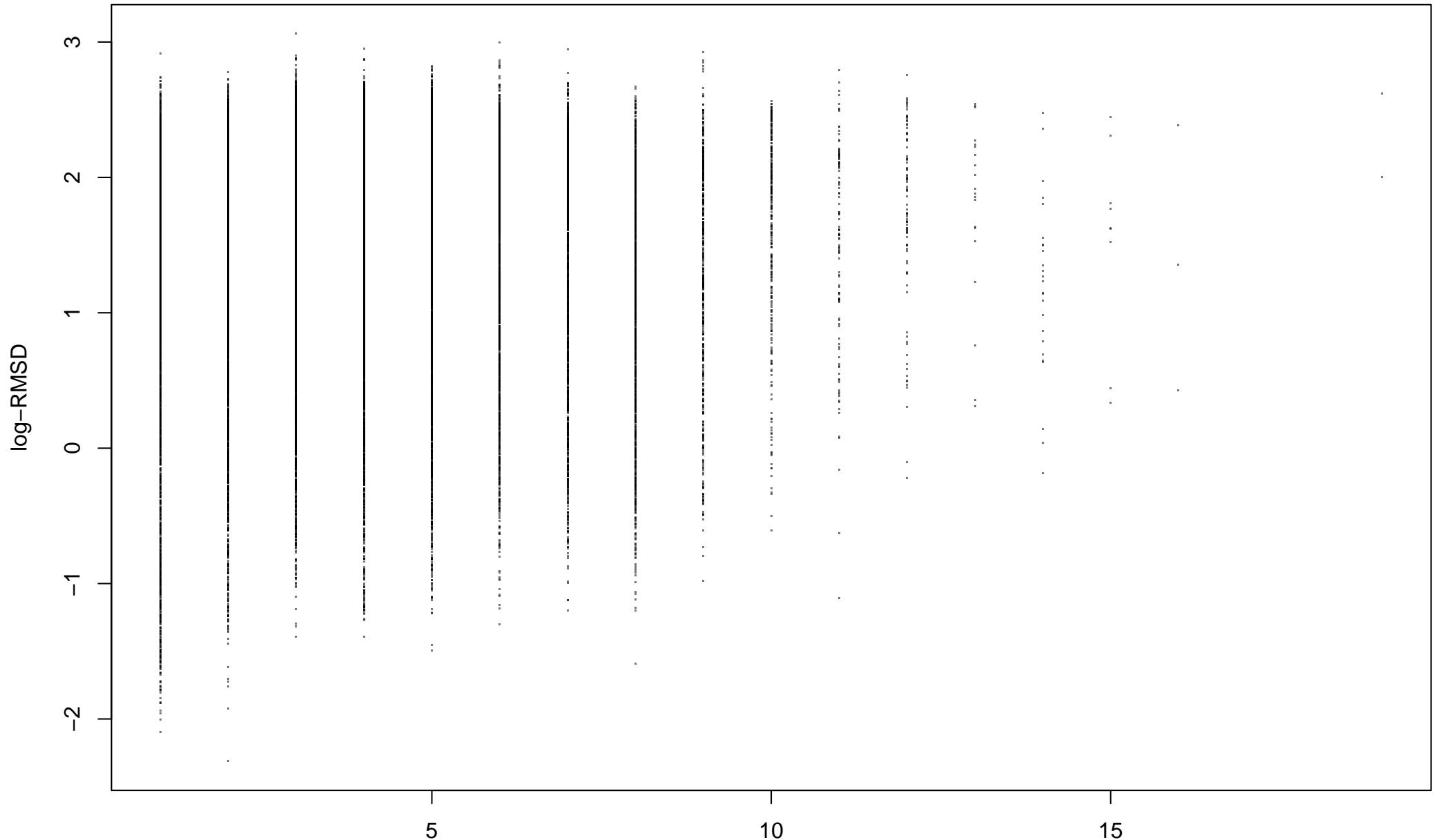


mcs_docked_NumRotatableBonds, MI = 0.07894 bit, norm = 0.02533, cond entr = 4.551 bit



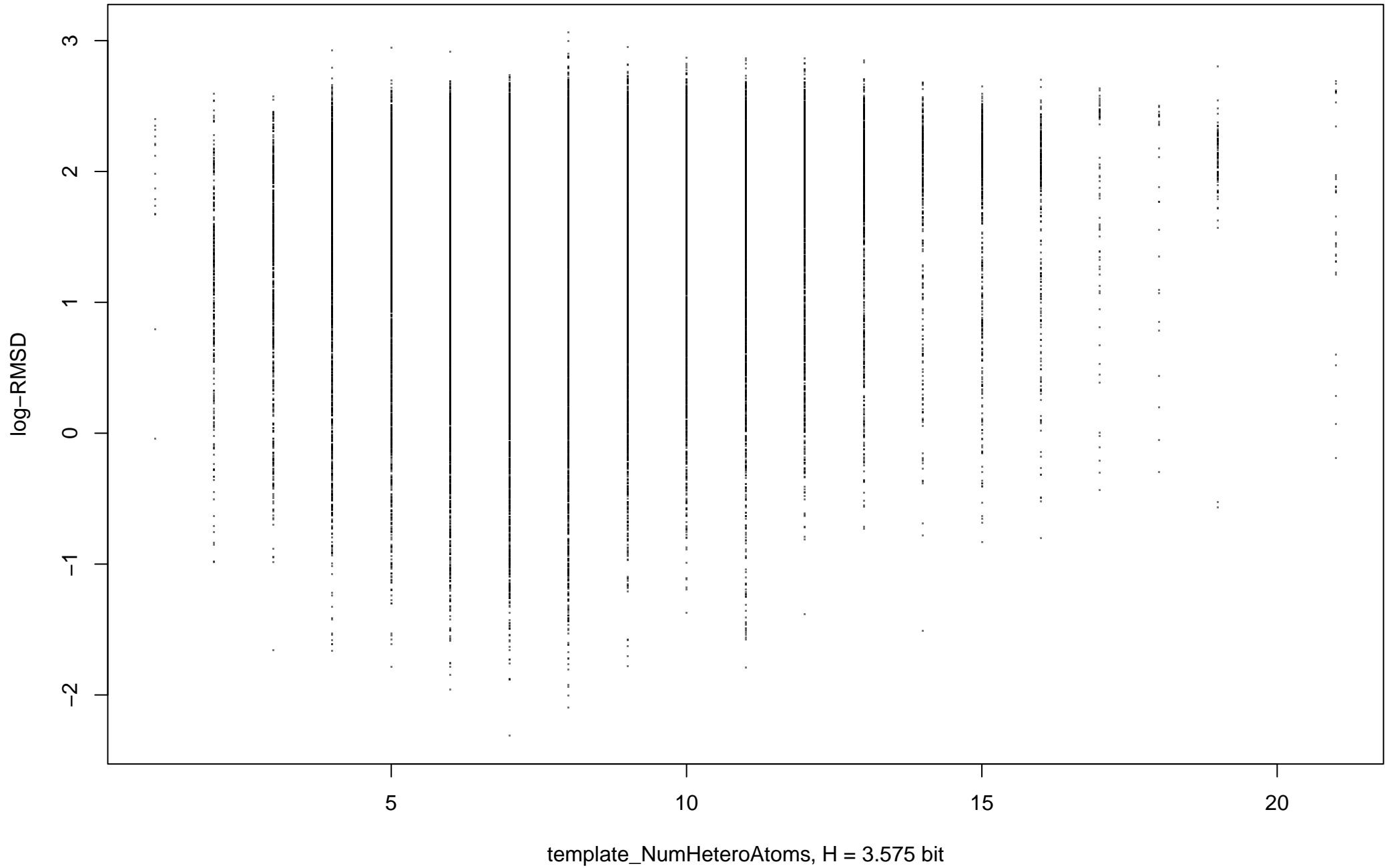
mcs_docked_NumRotatableBonds, H = 3.117 bit

shift_mcs_docked_NumRotatableBonds, MI = 0.07894 bit, norm = 0.02533, cond entr = 4.551 bit

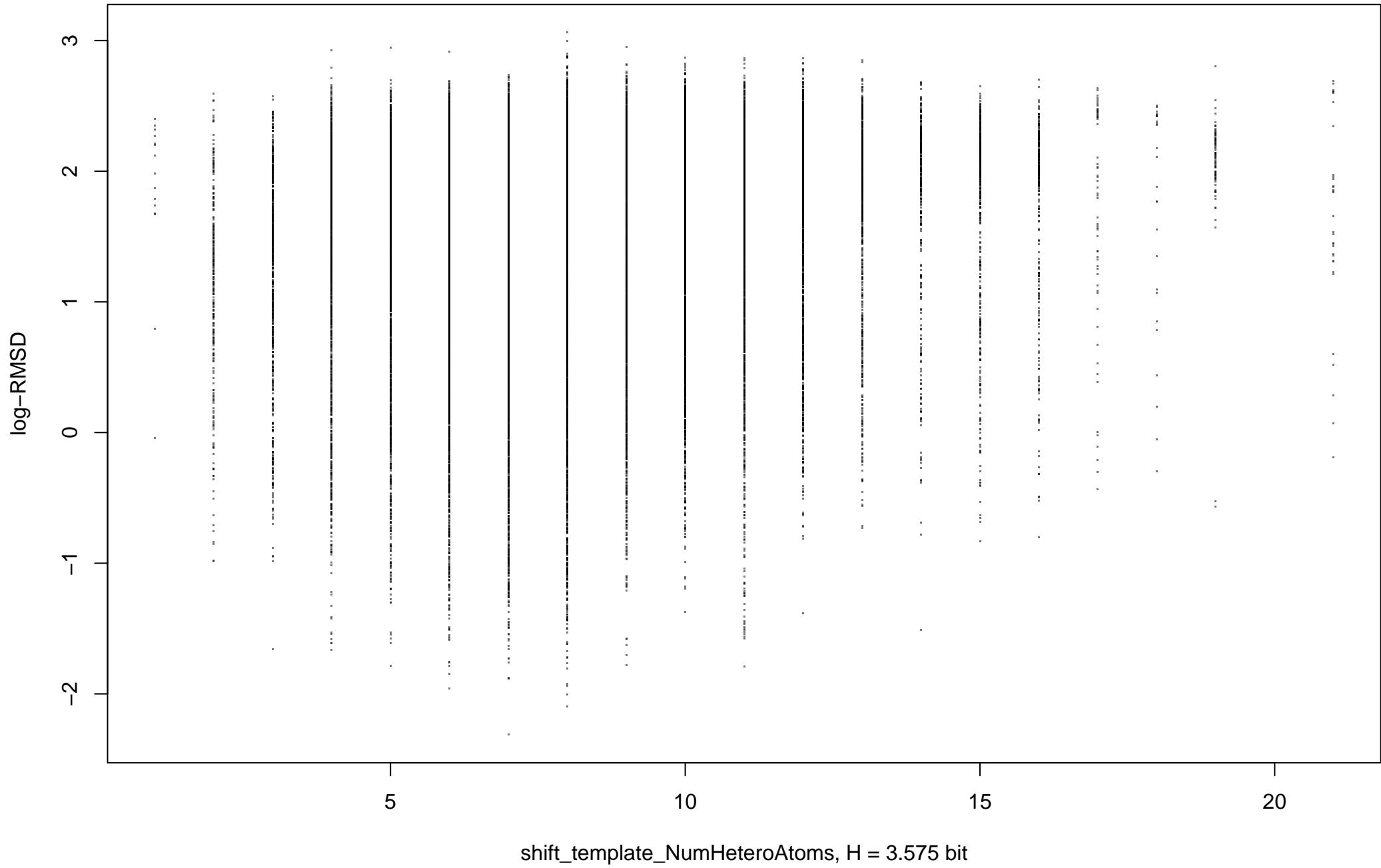


shift_mcs_docked_NumRotatableBonds, H = 3.117 bit

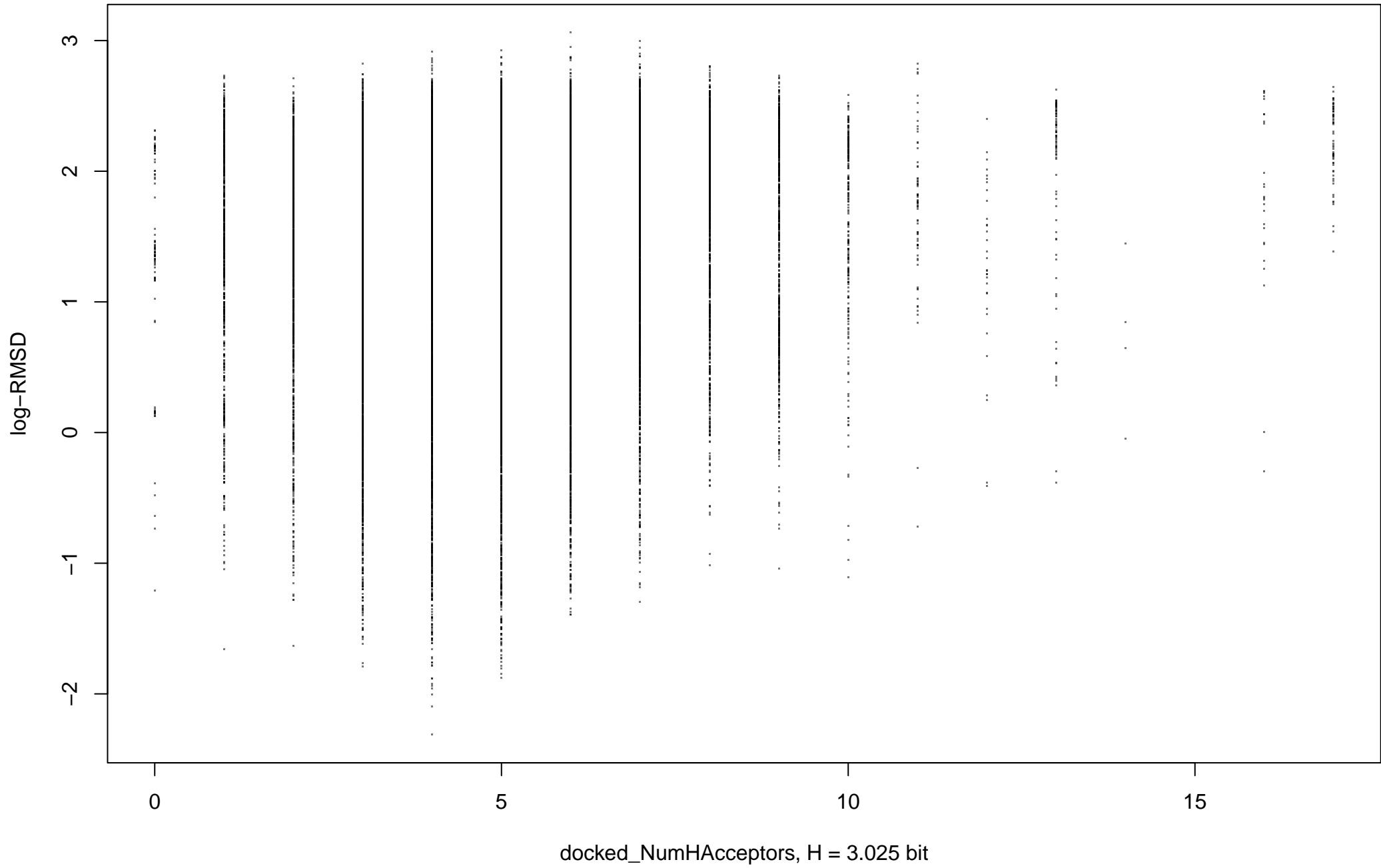
template_NumHeteroAtoms, MI = 0.06742 bit, norm = 0.01886, cond entr = 4.563 bit



shift_template_NumHeteroAtoms, MI = 0.06742 bit, norm = 0.01886, cond entr = 4.563 bit

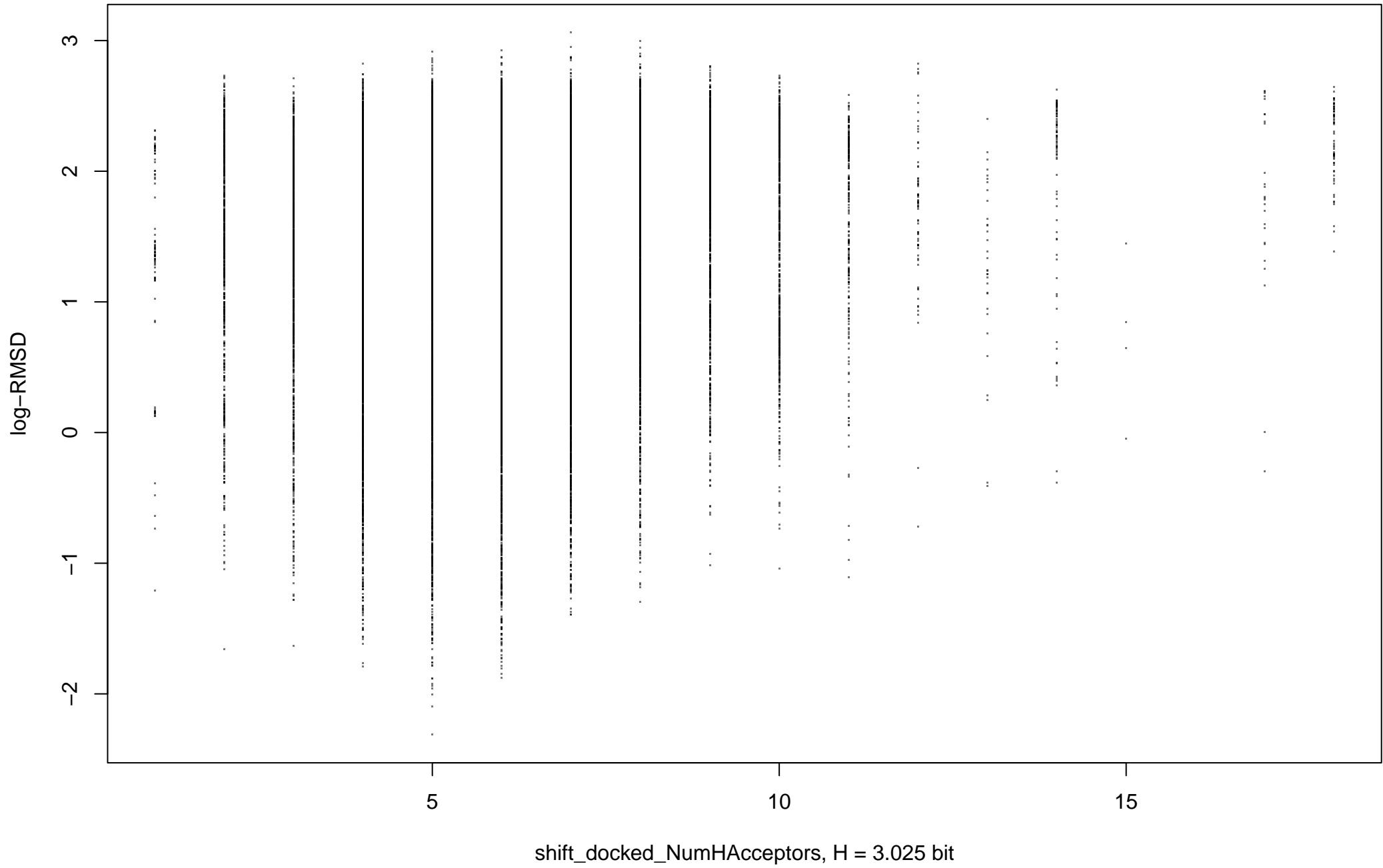


docked_NumHAcceptors, MI = 0.0672 bit, norm = 0.02221, cond entr = 4.563 bit

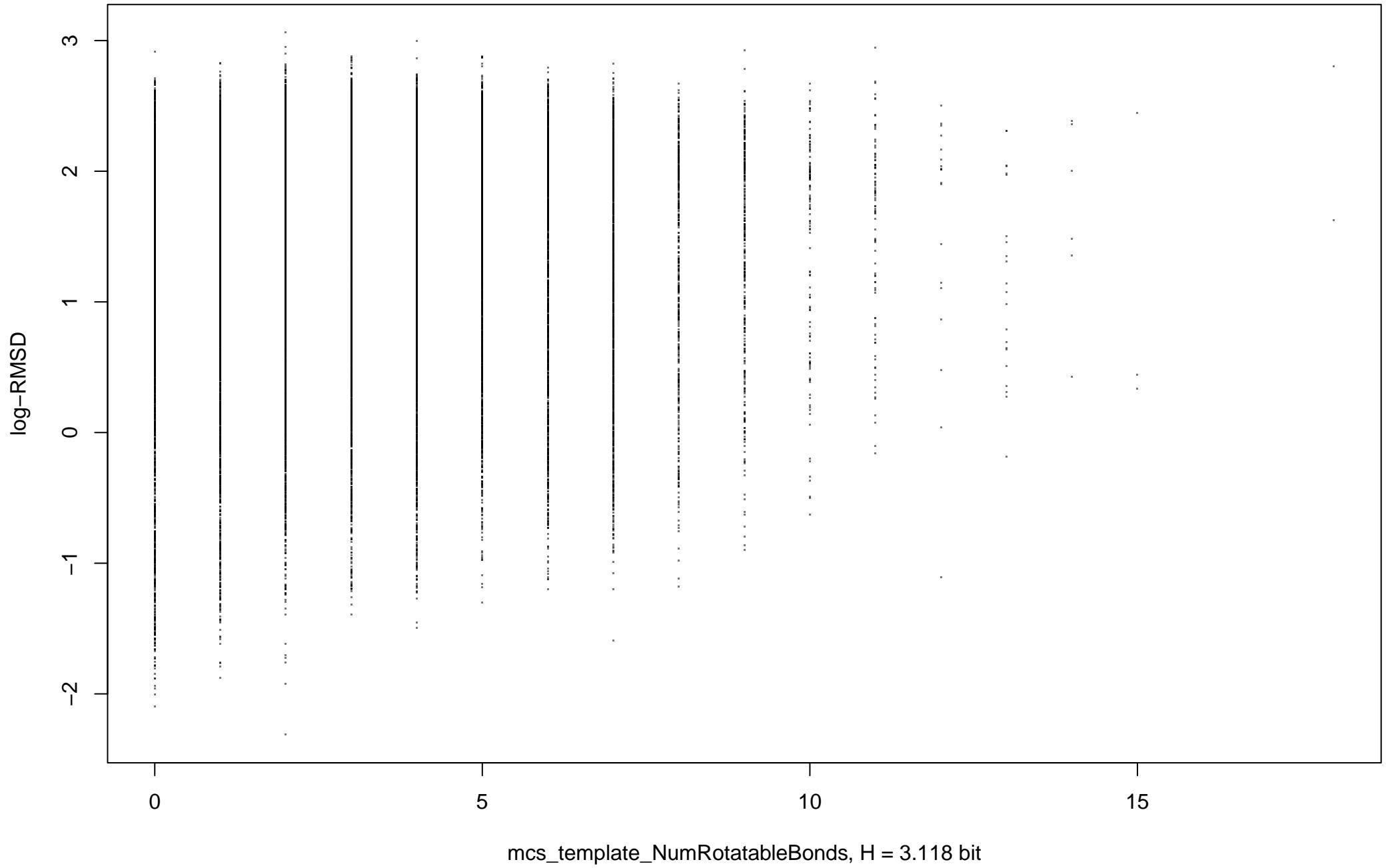


docked_NumHAcceptors, H = 3.025 bit

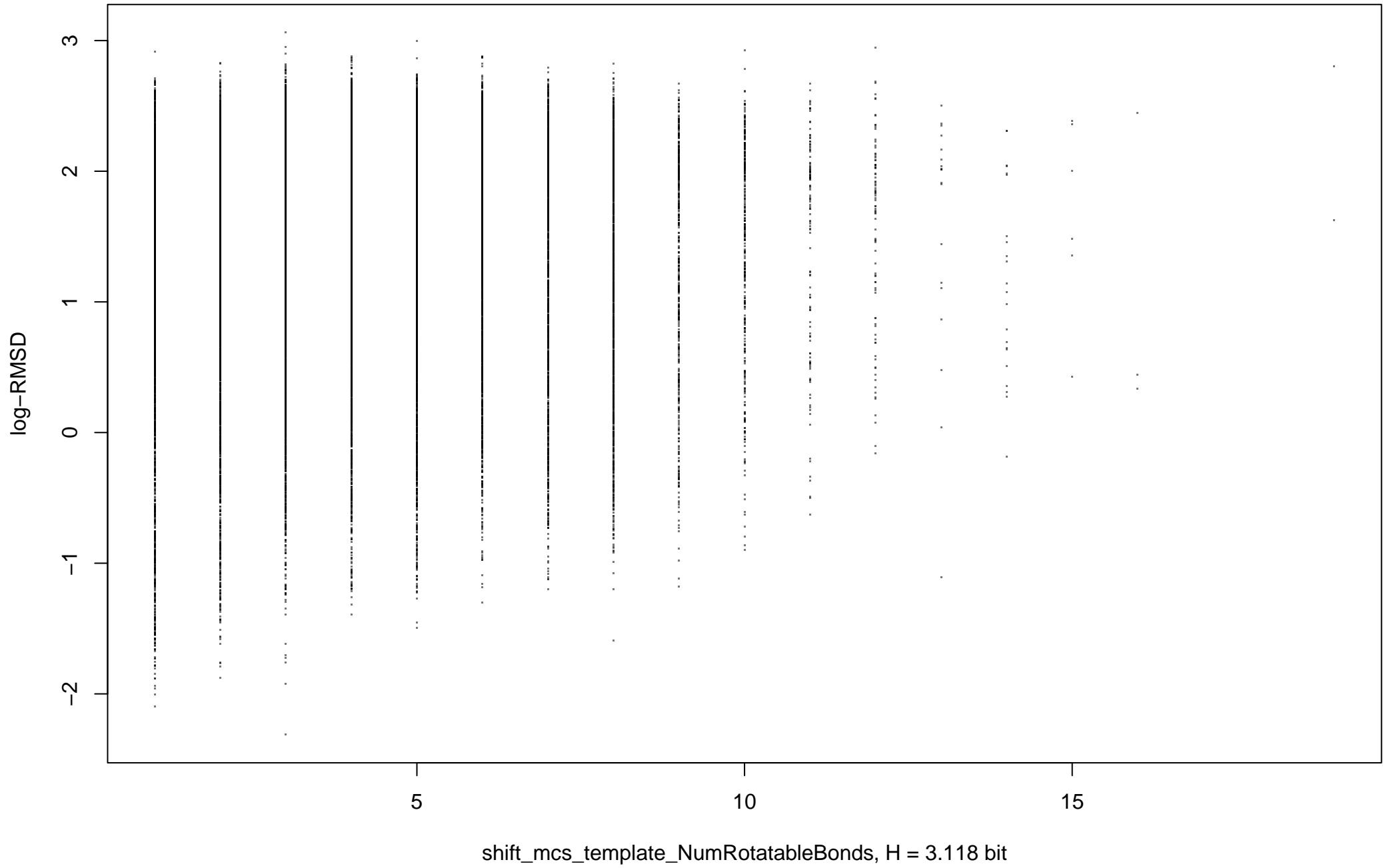
shift_docked_NumHAcceptors, MI = 0.0672 bit, norm = 0.02221, cond entr = 4.563 bit



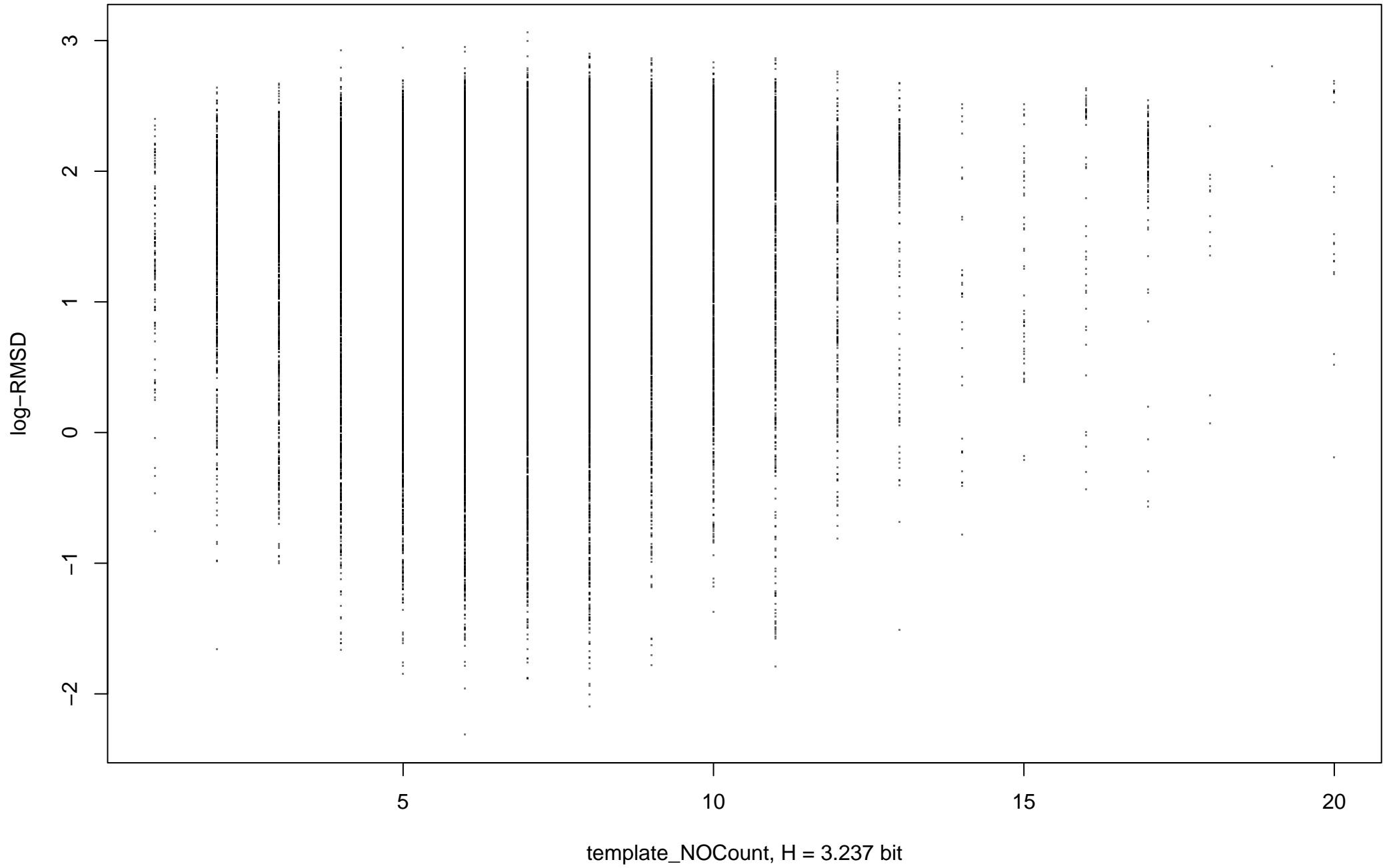
mcs_template_NumRotatableBonds, MI = 0.06717 bit, norm = 0.02154, cond entr = 4.563 bit



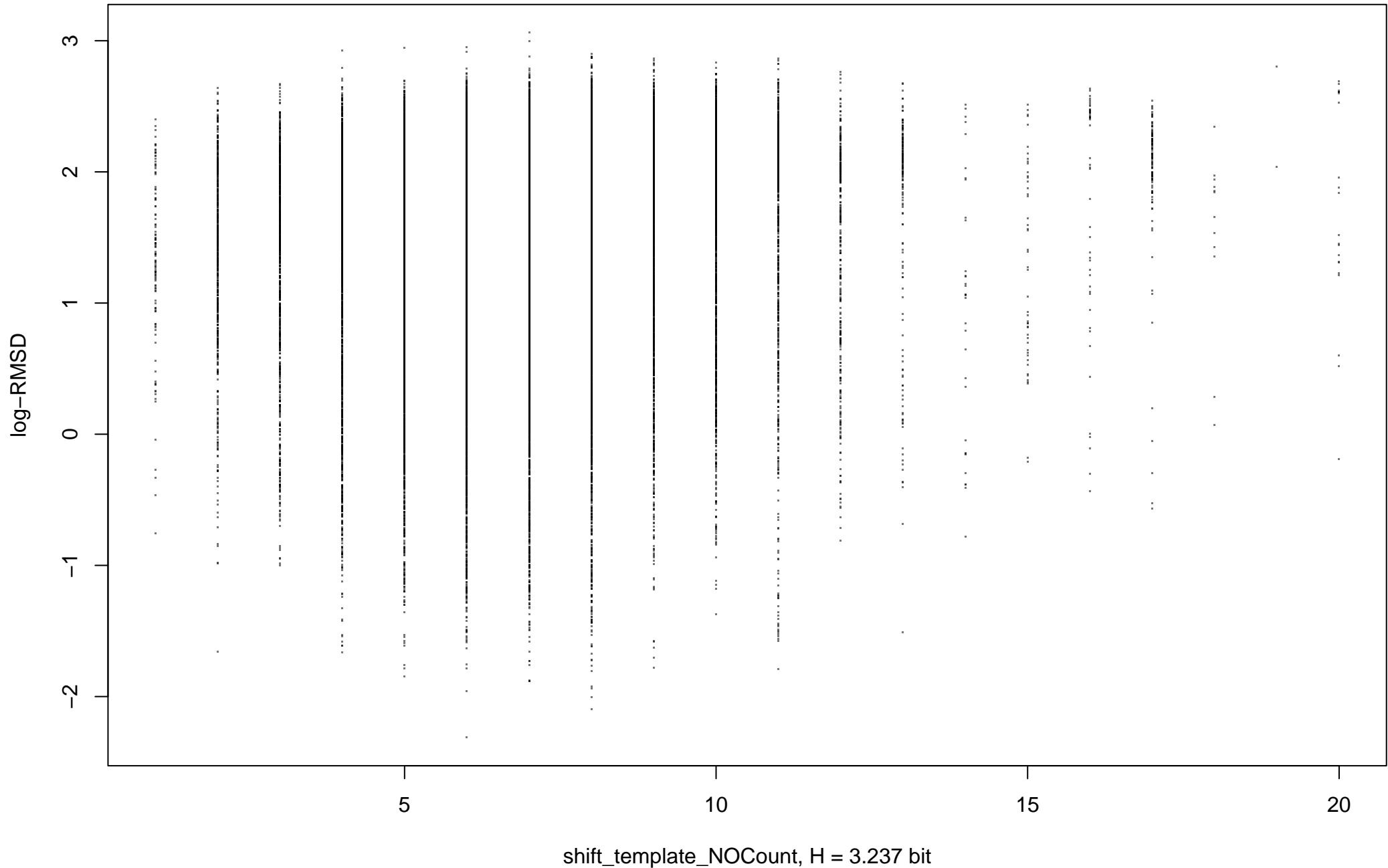
shift_mcs_template_NumRotatableBonds, MI = 0.06717 bit, norm = 0.02154, cond entr = 4.563 bit



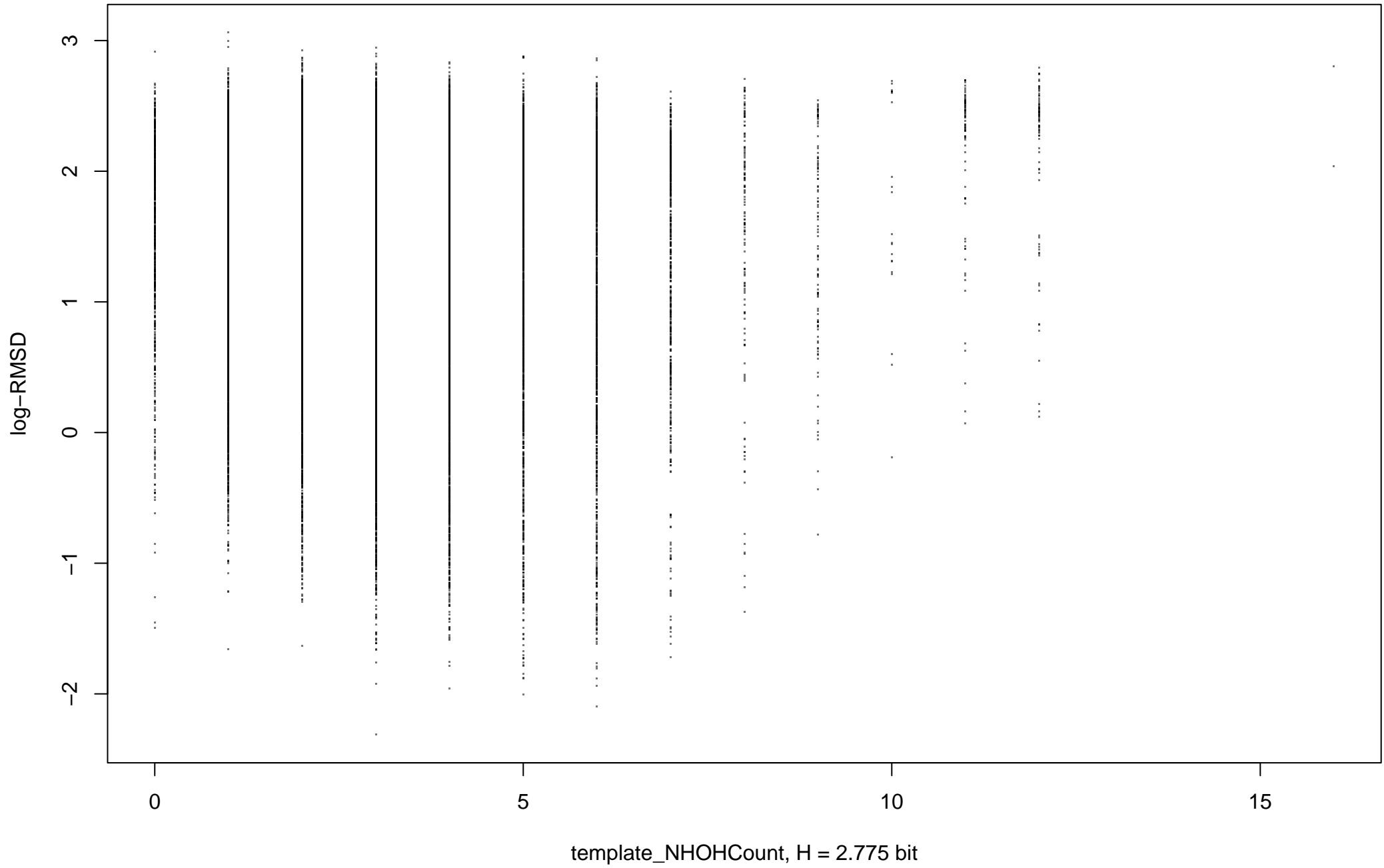
template_NOCount, MI = 0.0588 bit, norm = 0.01817, cond entr = 4.571 bit



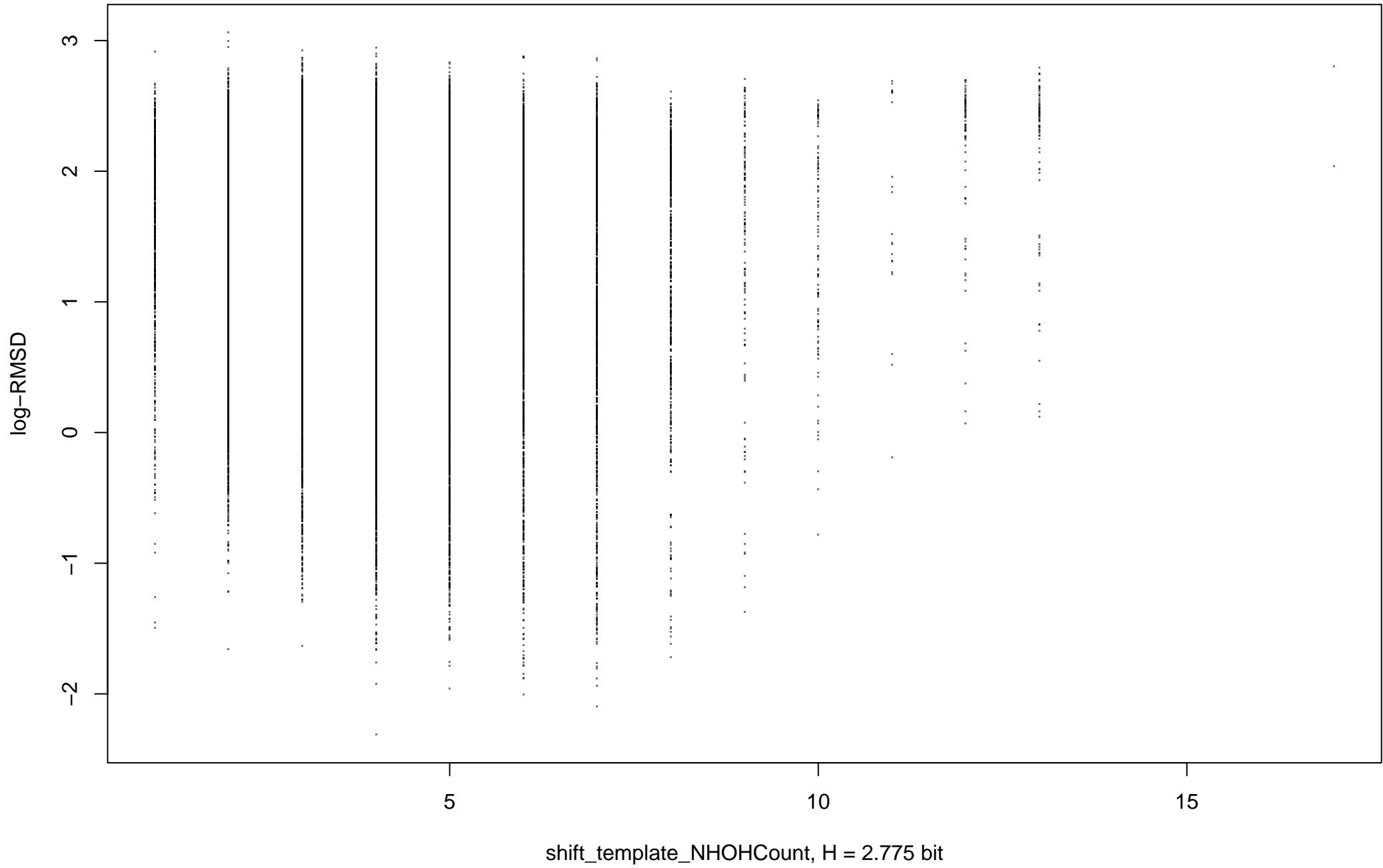
shift_template_NOCount, MI = 0.0588 bit, norm = 0.01817, cond entr = 4.571 bit



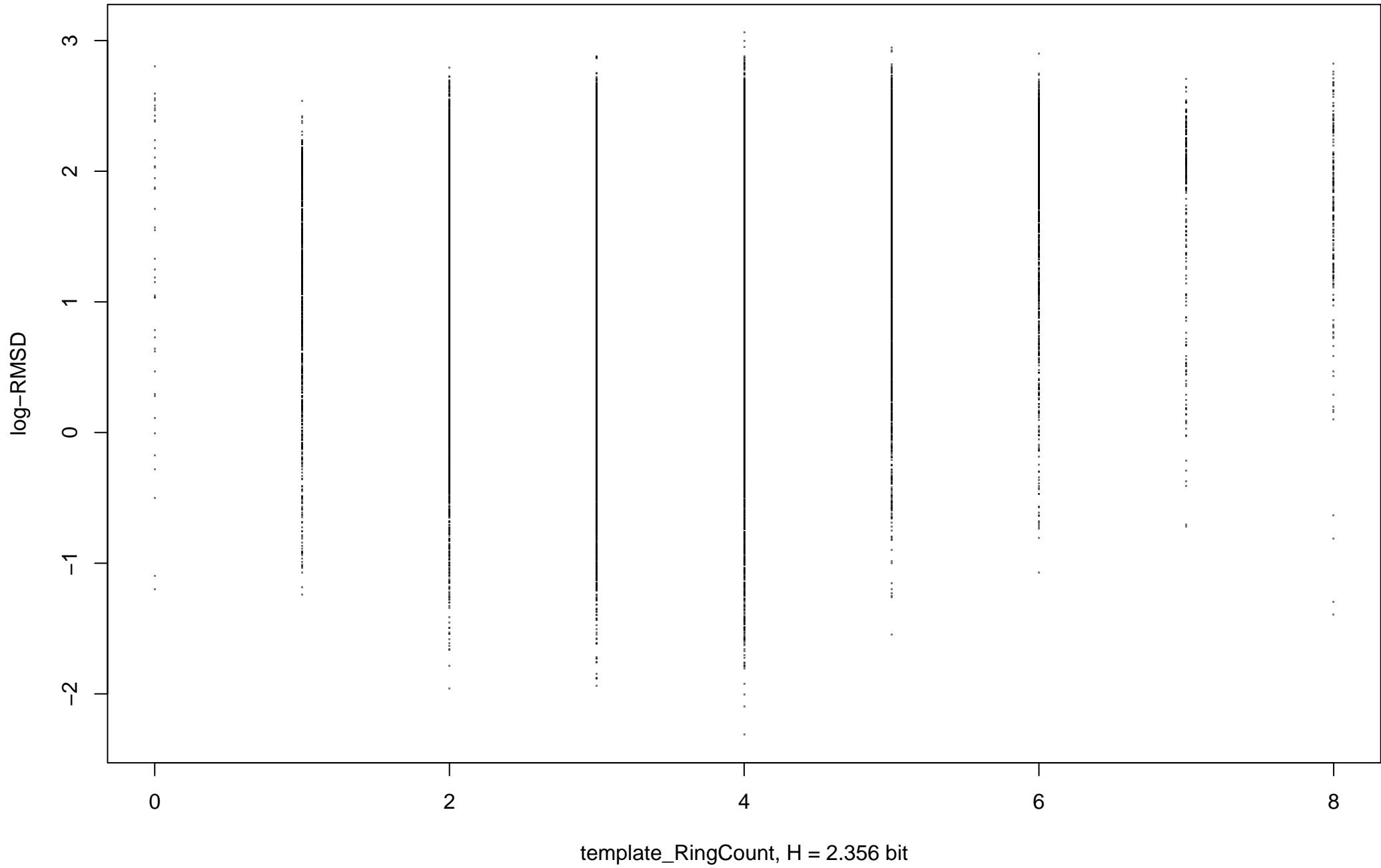
template_NHOHCount, MI = 0.05667 bit, norm = 0.02042, cond entr = 4.574 bit



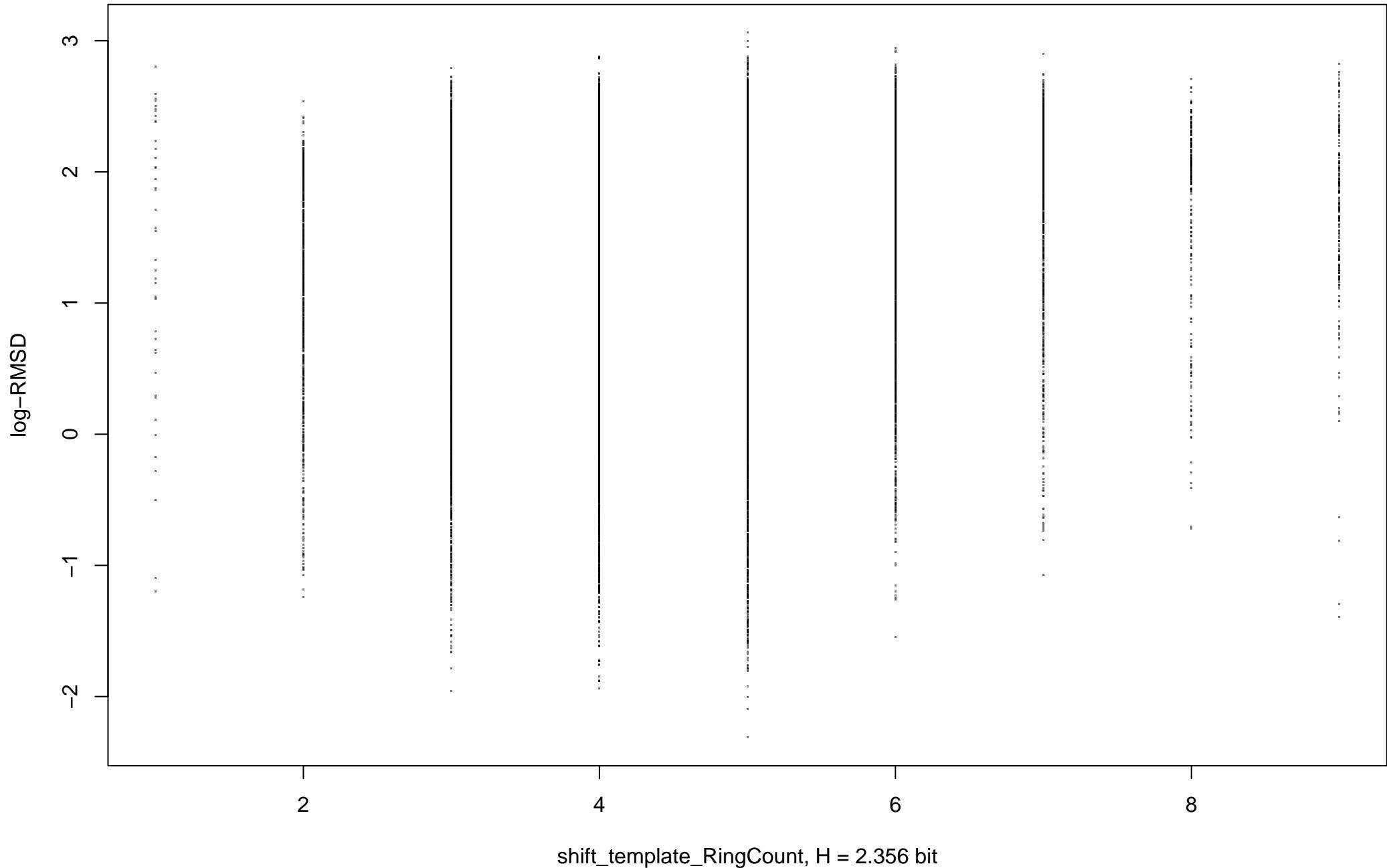
shift_template_NHOHCount, MI = 0.05667 bit, norm = 0.02042, cond entr = 4.574 bit



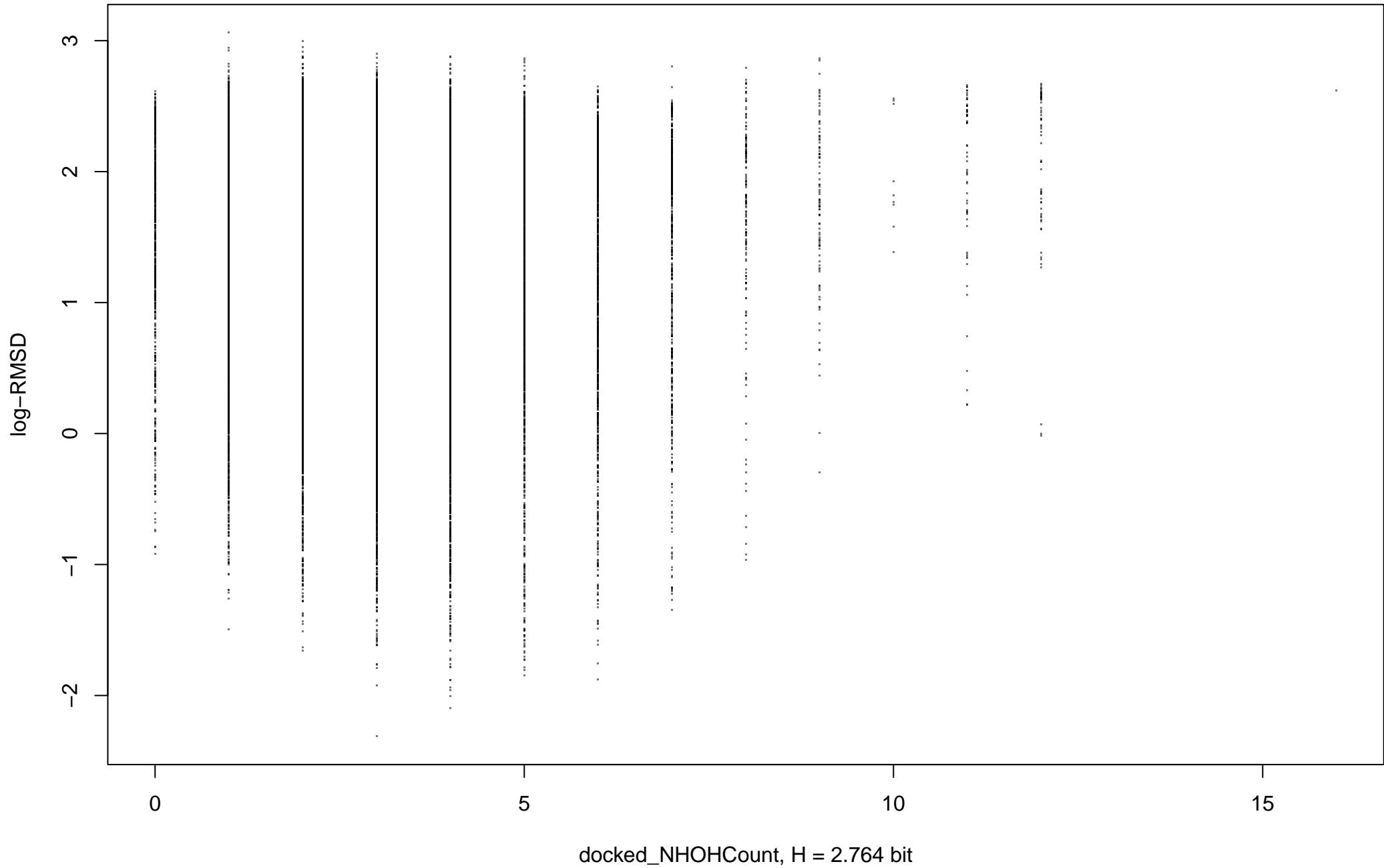
template_RingCount, MI = 0.05557 bit, norm = 0.02359, cond entr = 4.575 bit



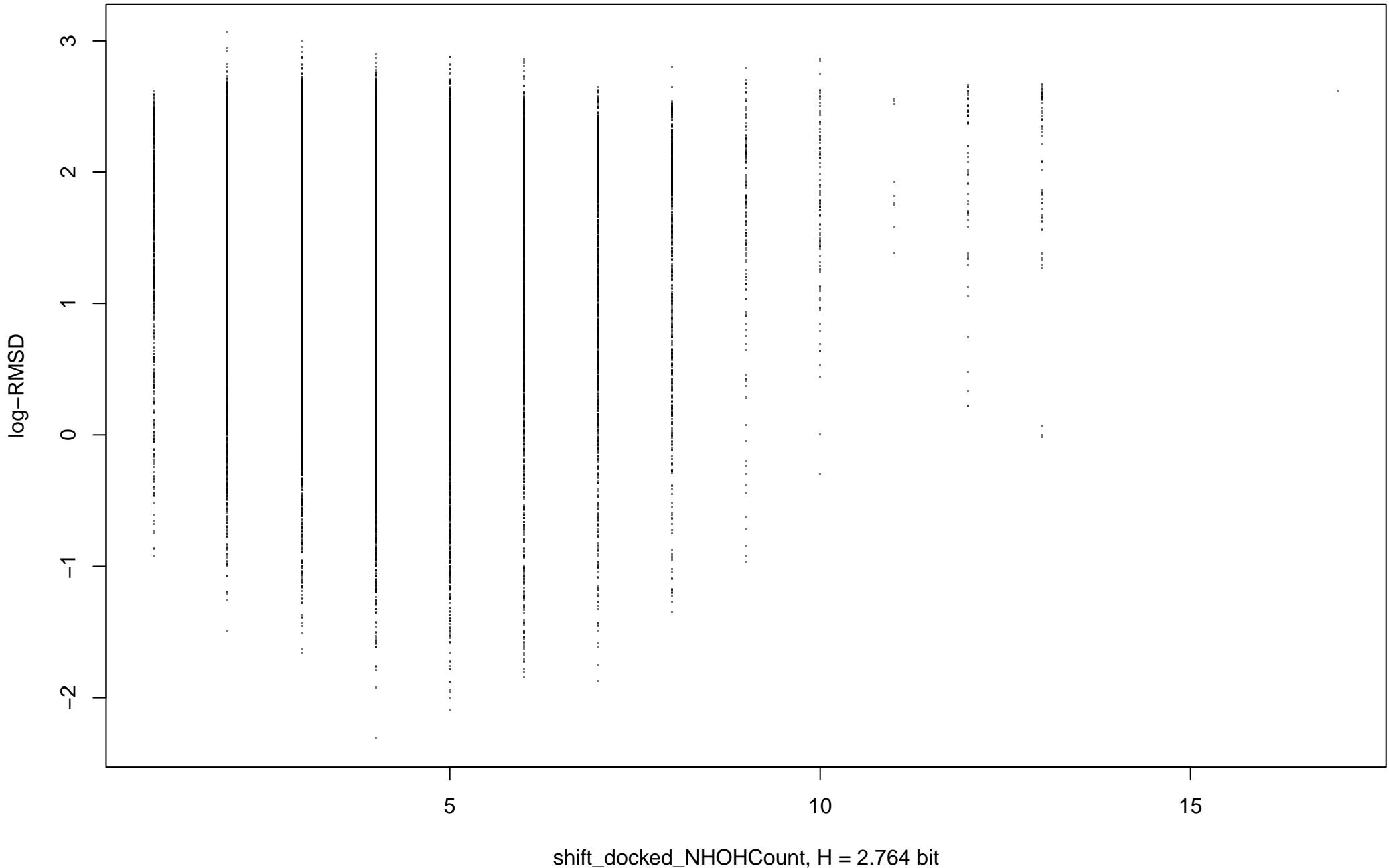
shift_template_RingCount, MI = 0.05557 bit, norm = 0.02359, cond entr = 4.575 bit



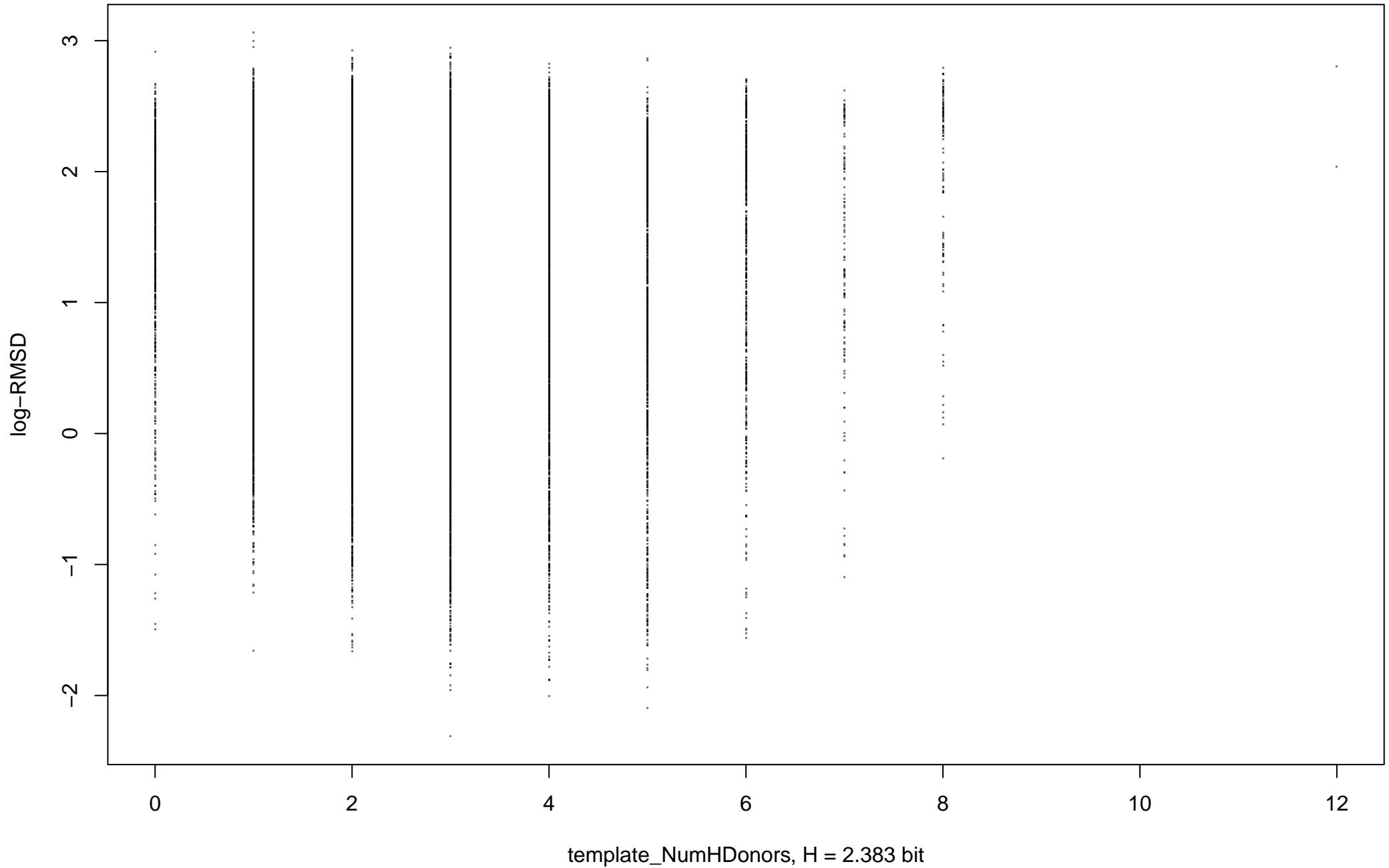
docked_NHOHCount, MI = 0.04974 bit, norm = 0.01799, cond entr = 4.58 bit



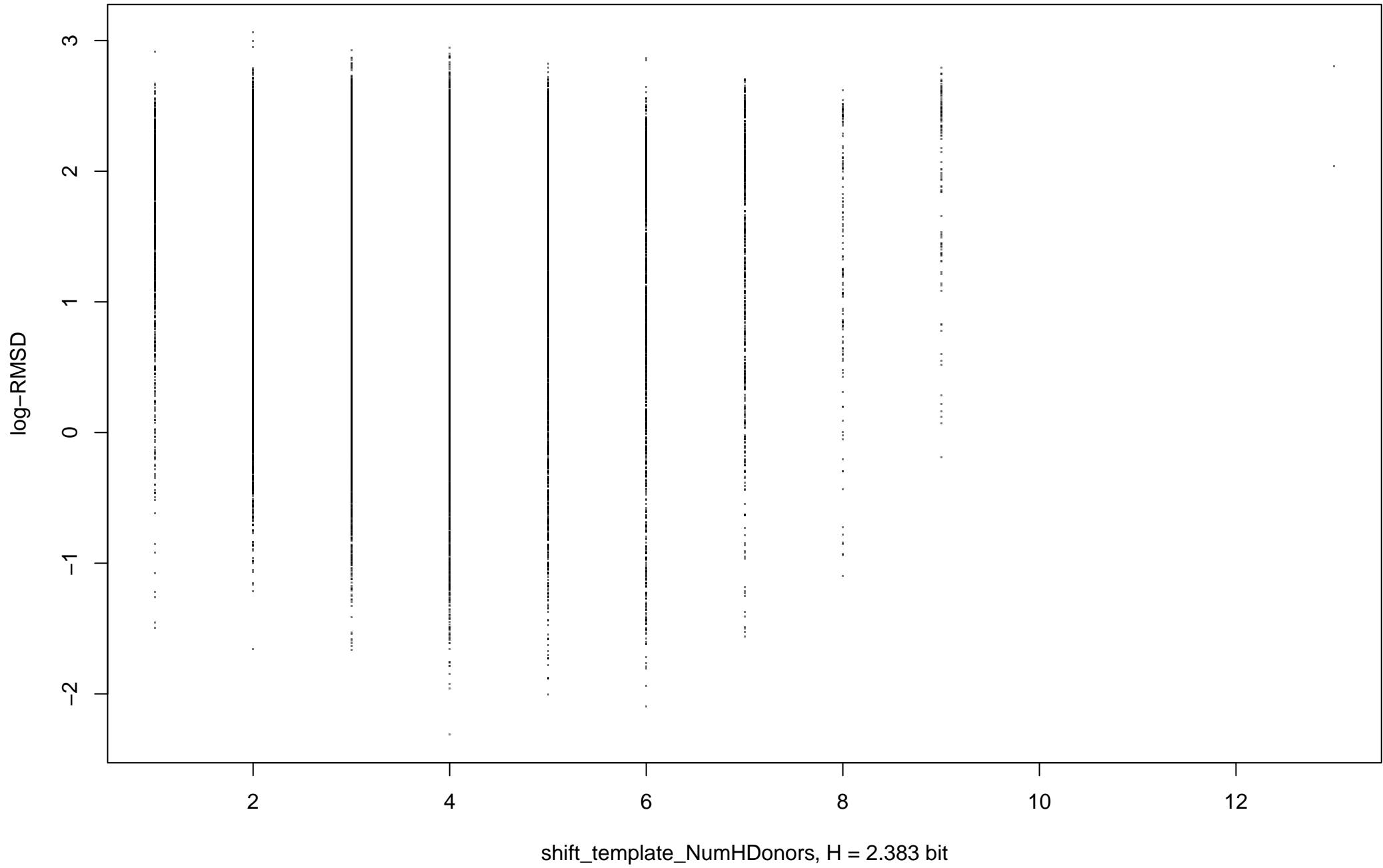
shift_docked_NHOHCount, MI = 0.04974 bit, norm = 0.01799, cond entr = 4.58 bit



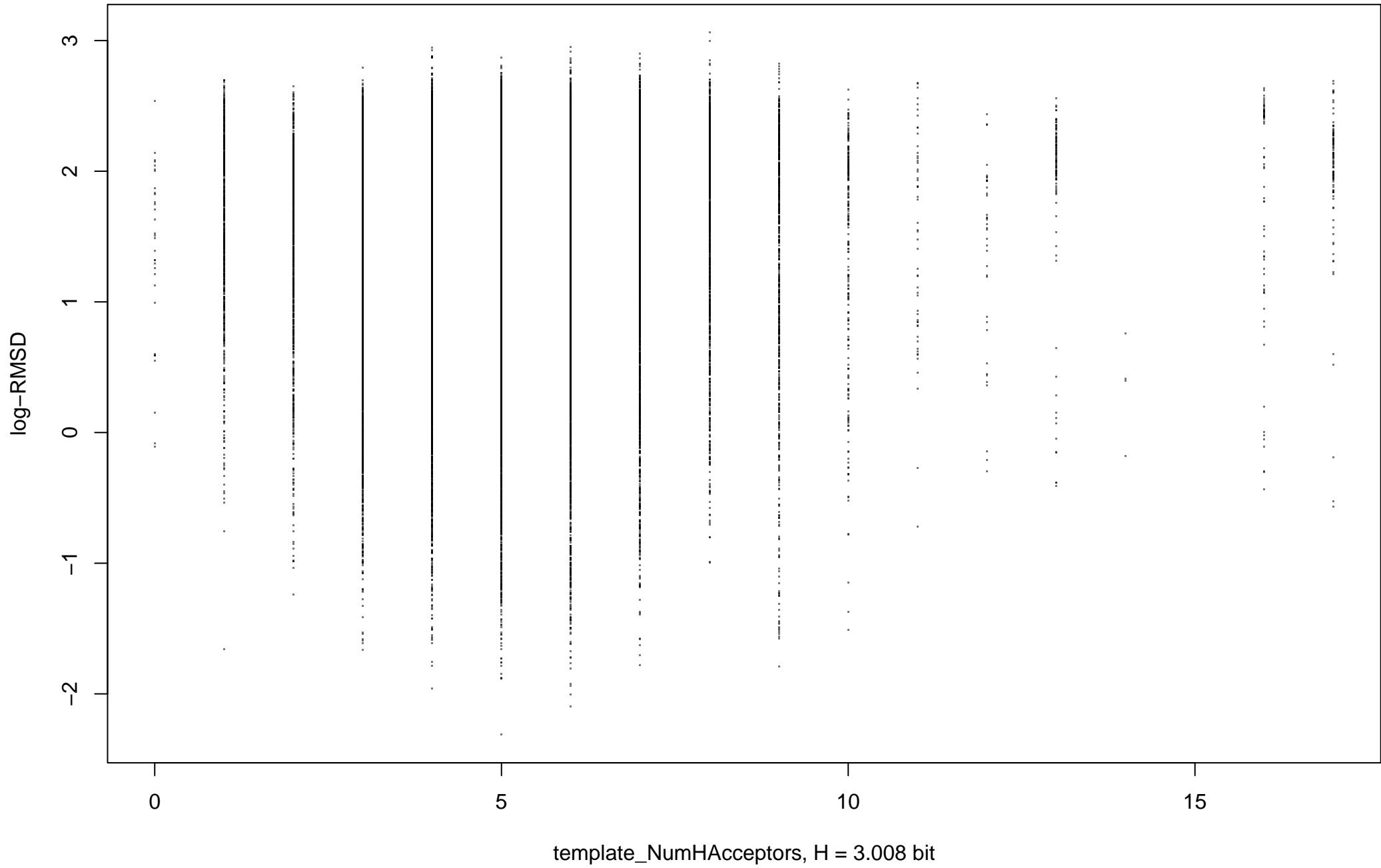
template_NumHDonors, MI = 0.04885 bit, norm = 0.0205, cond entr = 4.581 bit



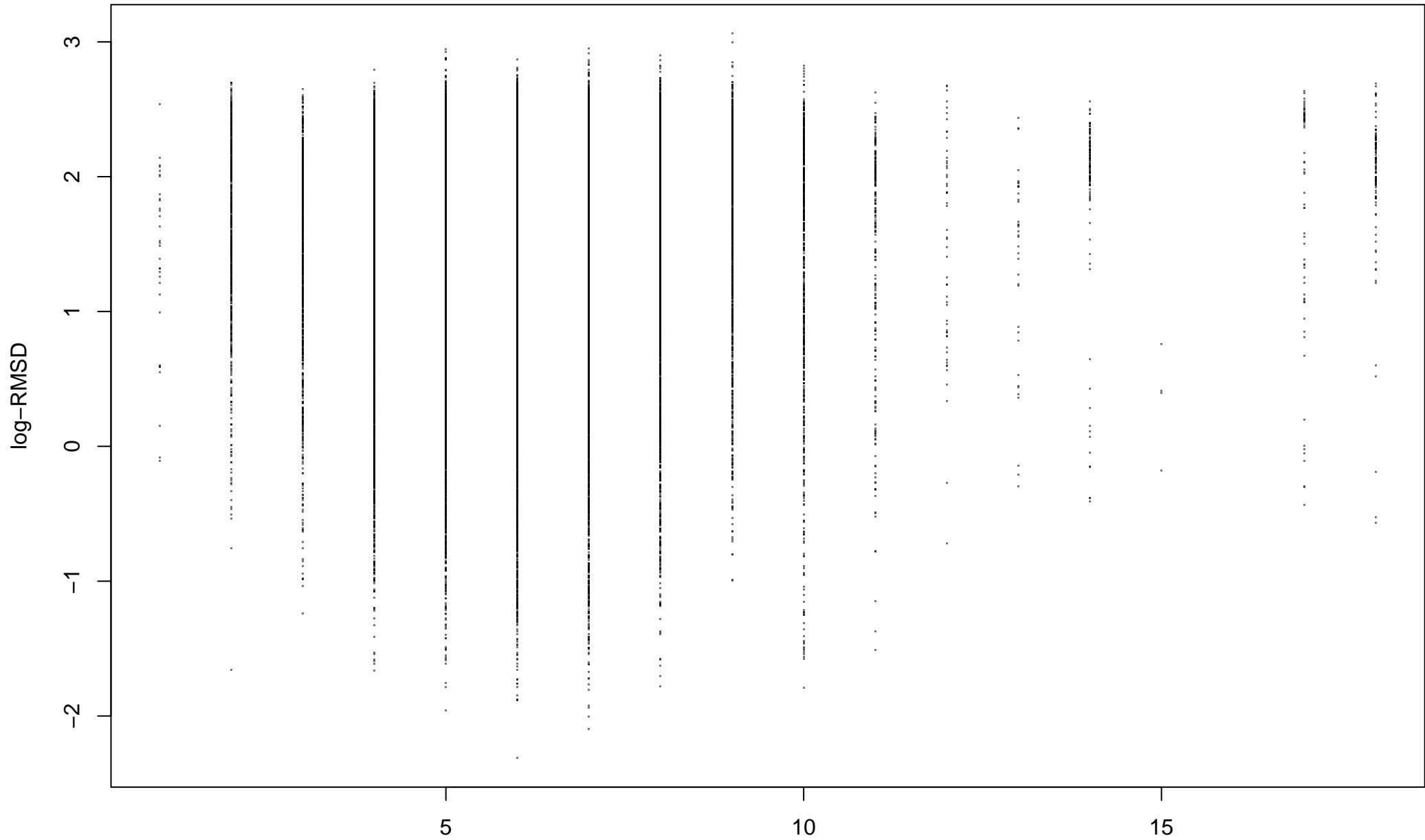
shift_template_NumHDonors, MI = 0.04885 bit, norm = 0.0205, cond entr = 4.581 bit



template_NumHAcceptors, MI = 0.04507 bit, norm = 0.01499, cond entr = 4.585 bit

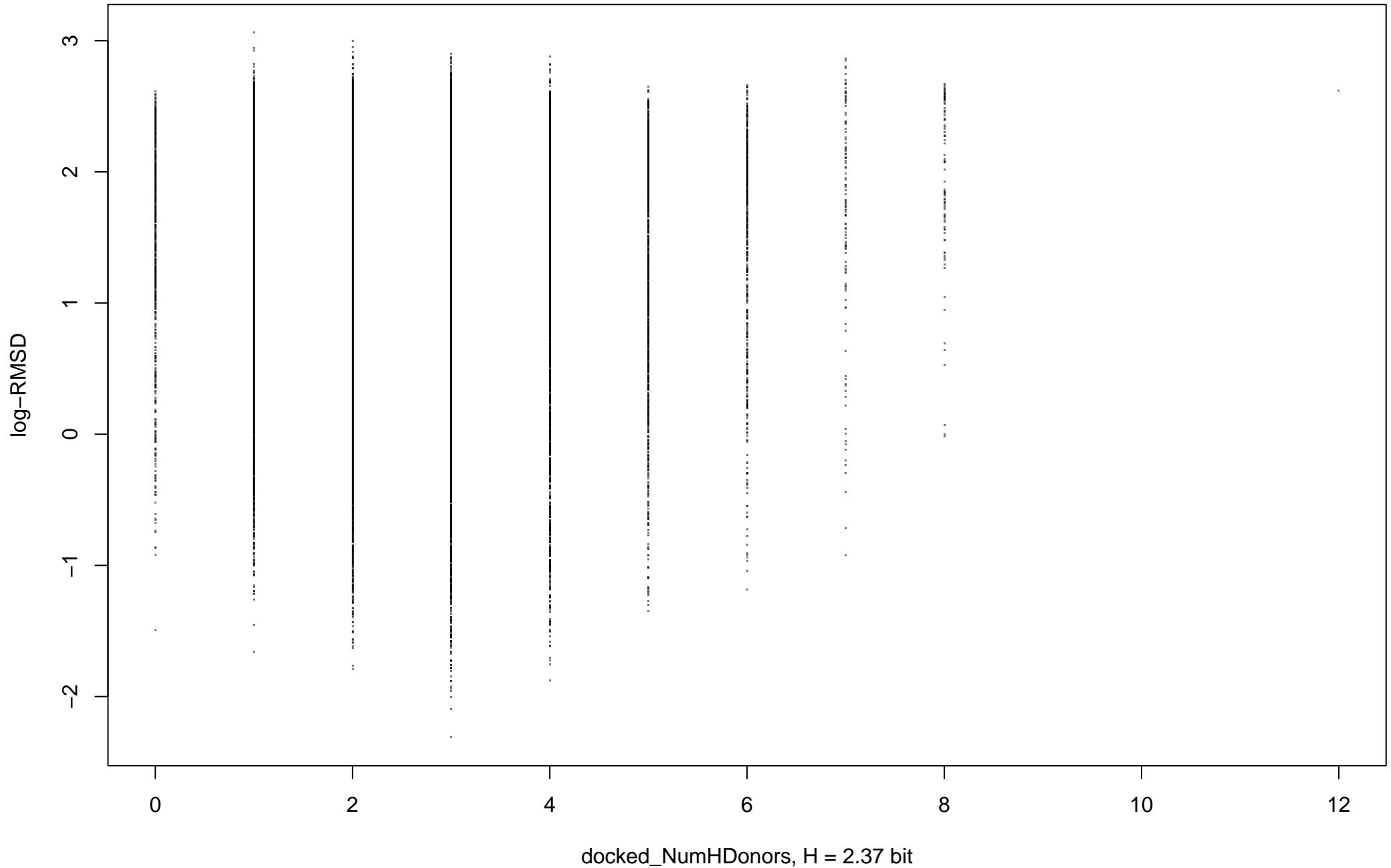


shift_template_NumHAcceptors, MI = 0.04507 bit, norm = 0.01499, cond entr = 4.585 bit



shift_template_NumHAcceptors, H = 3.008 bit

docked_NumHDonors, MI = 0.04122 bit, norm = 0.01739, cond entr = 4.589 bit



shift_docked_NumHDonors, MI = 0.04122 bit, norm = 0.01739, cond entr = 4.589 bit

