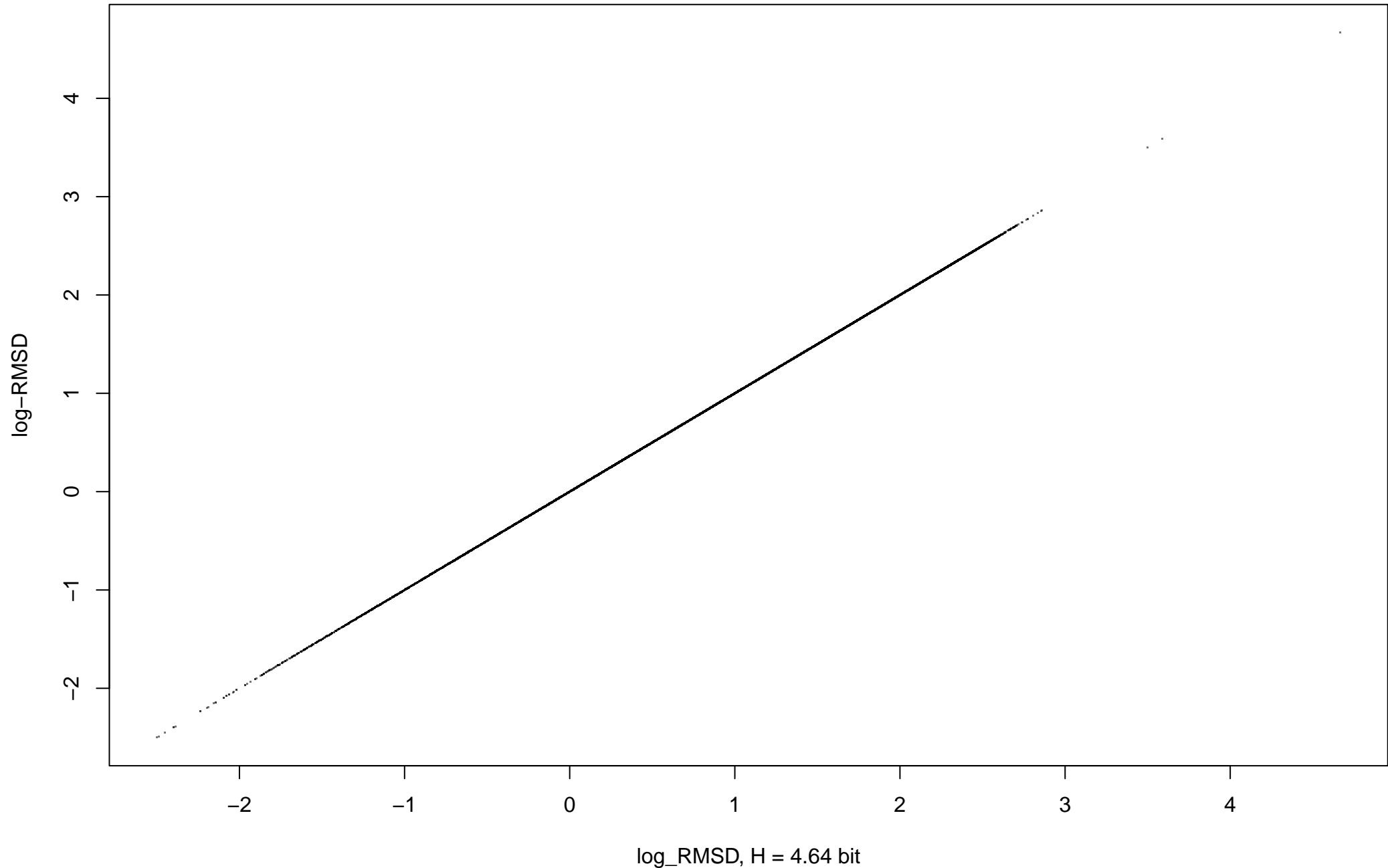
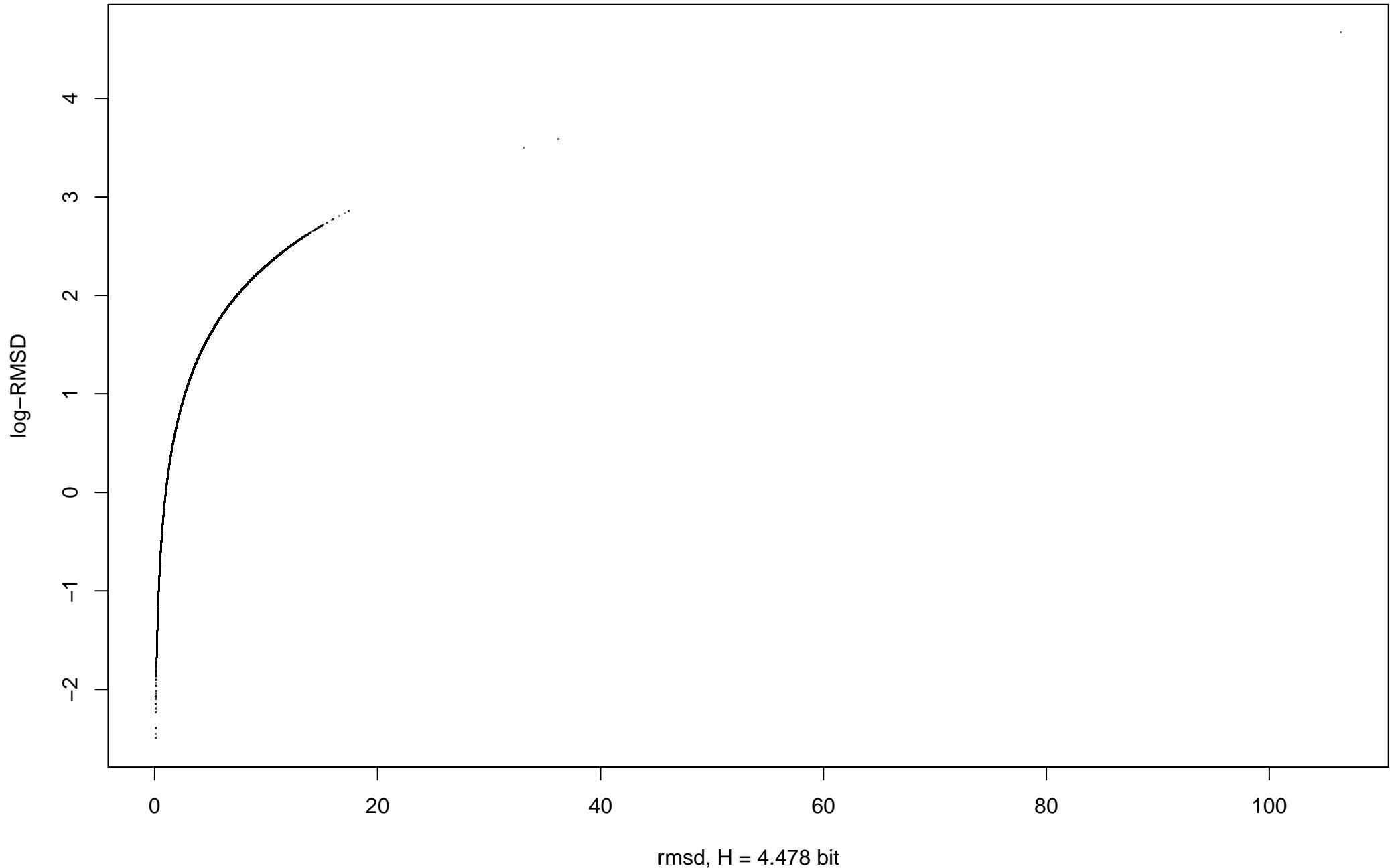


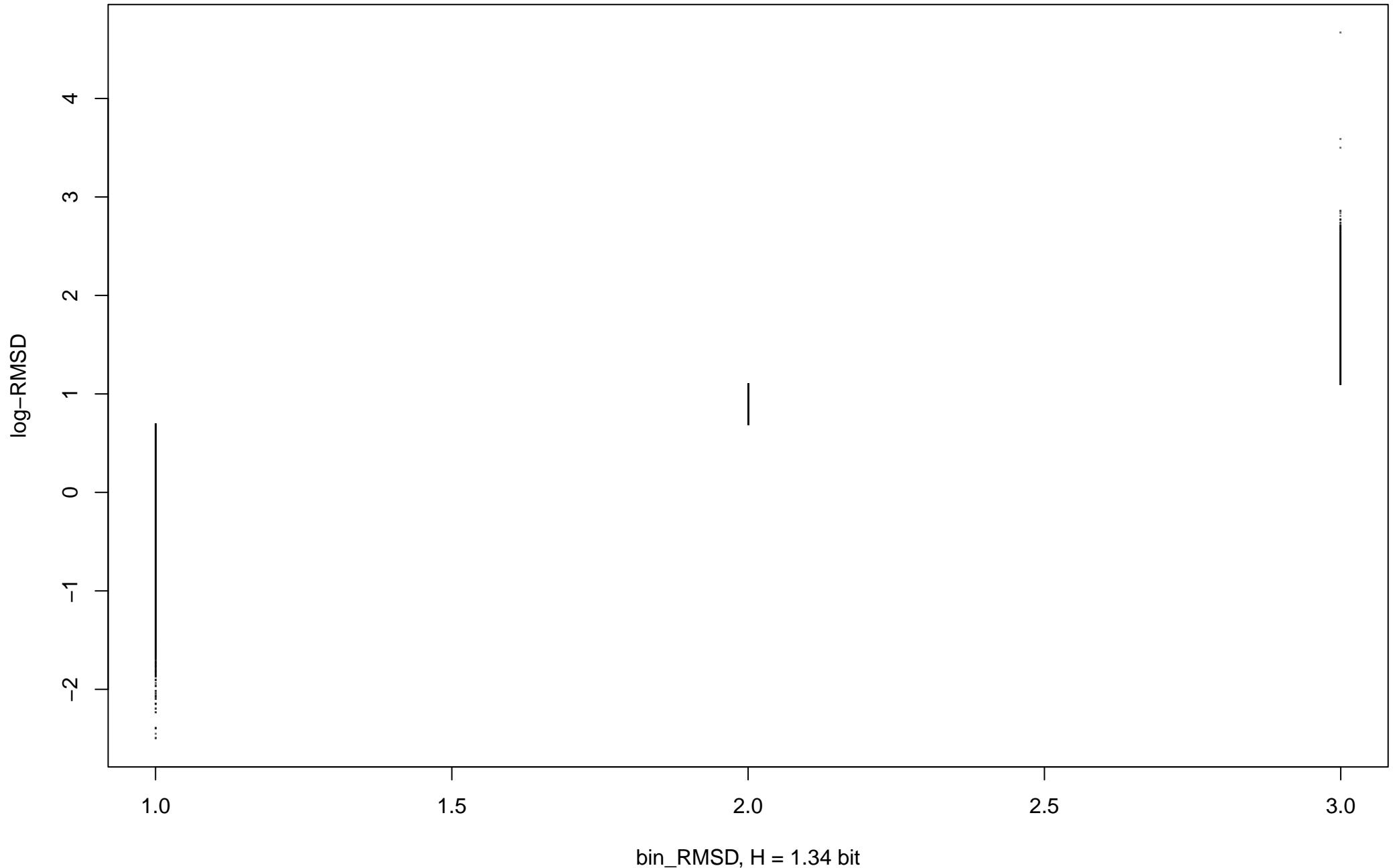
log_RMSD, MI = 4.64 bit, norm = 1, cond entr = 0 bit



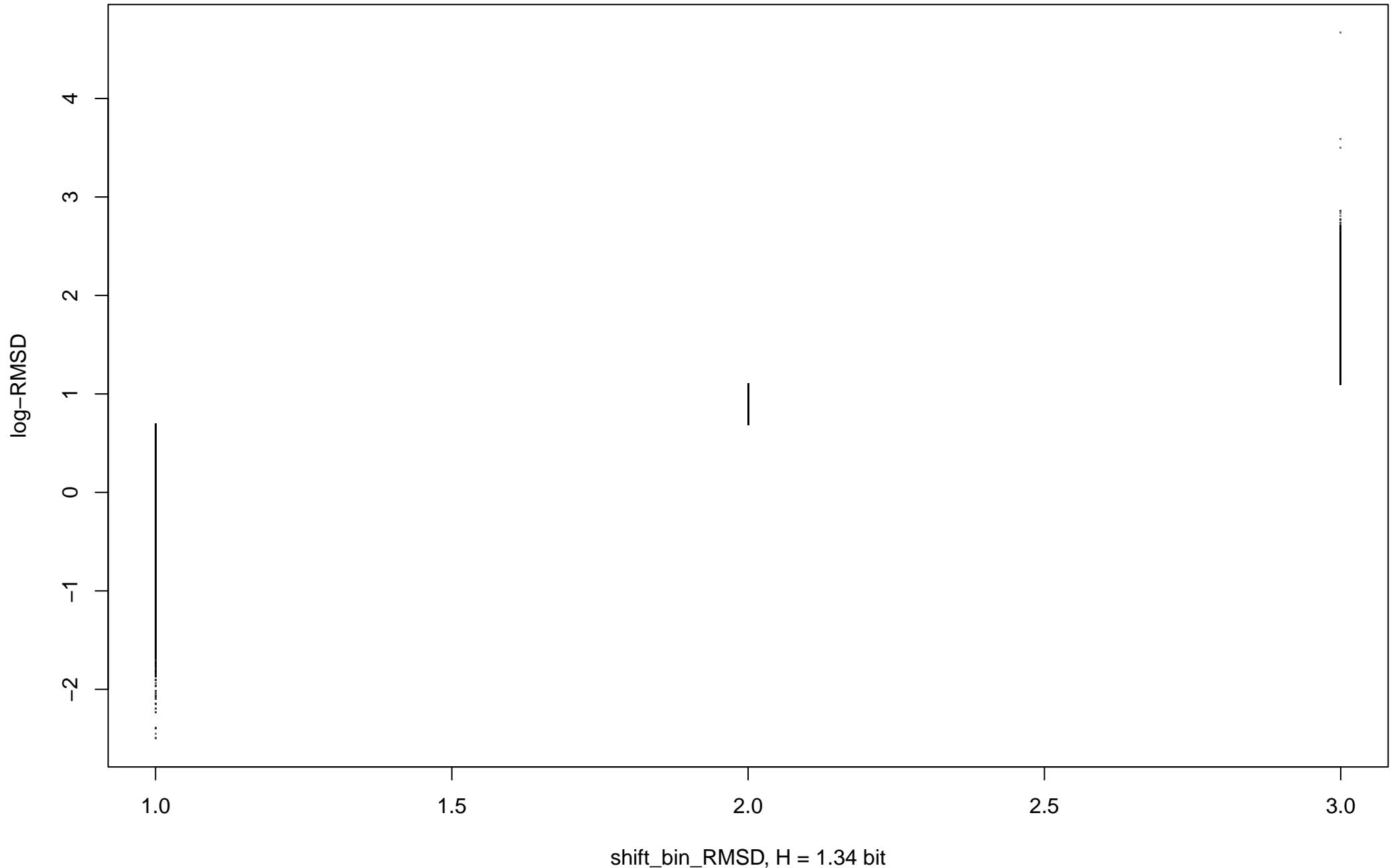
rmsd, MI = 3.743 bit, norm = 0.8358, cond entr = 0.8968 bit



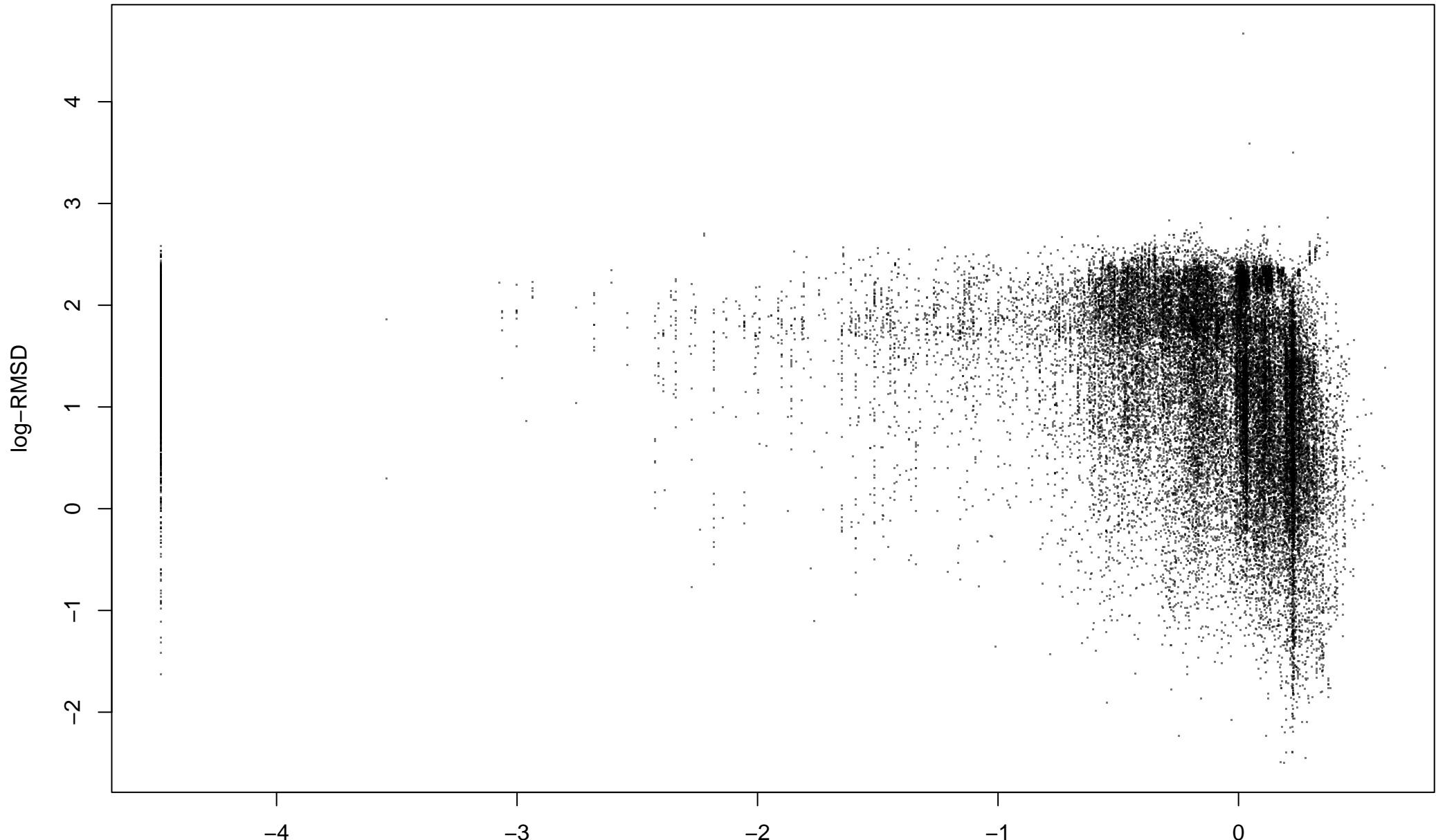
bin_RMSD, MI = 1.308 bit, norm = 0.9757, cond entr = 3.332 bit



shift_bin_RMSD, MI = 1.308 bit, norm = 0.9757, cond entr = 3.332 bit

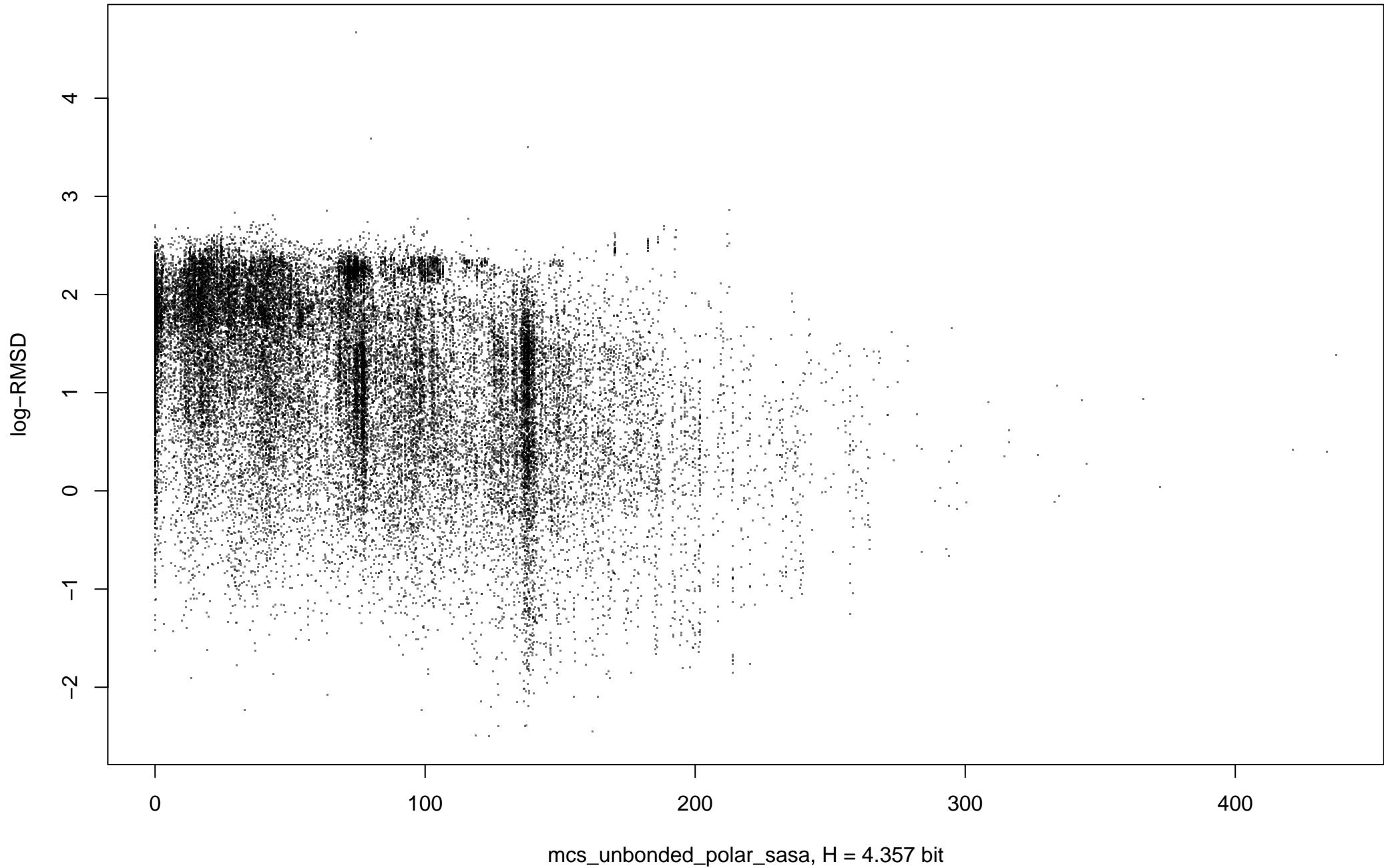


log_mcs_unbonded_polar_sasa, MI = 0.2213 bit, norm = 0.04769, cond entr = 4.418 bit

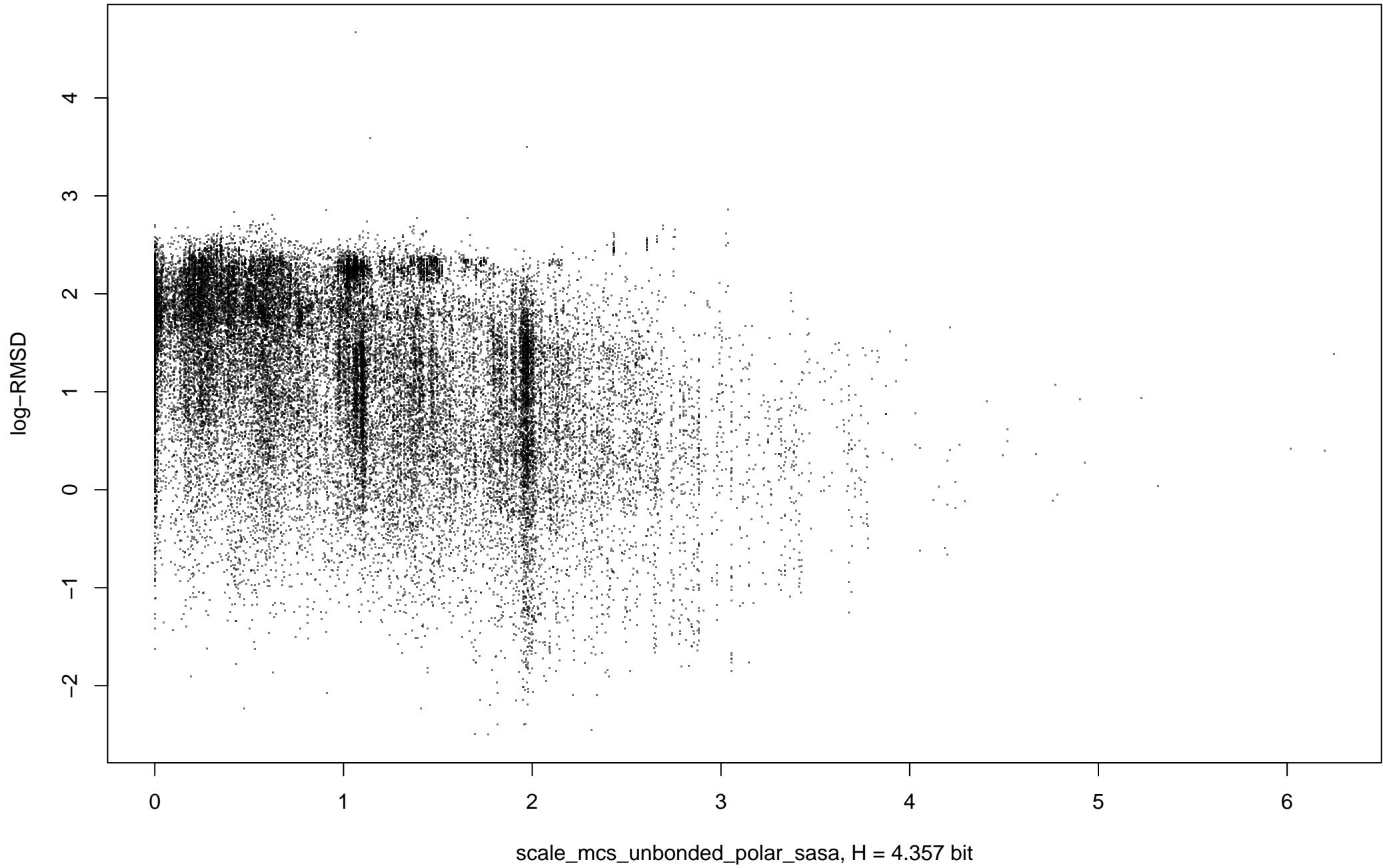


log_mcs_unbonded_polar_sasa, H = 4.644 bit

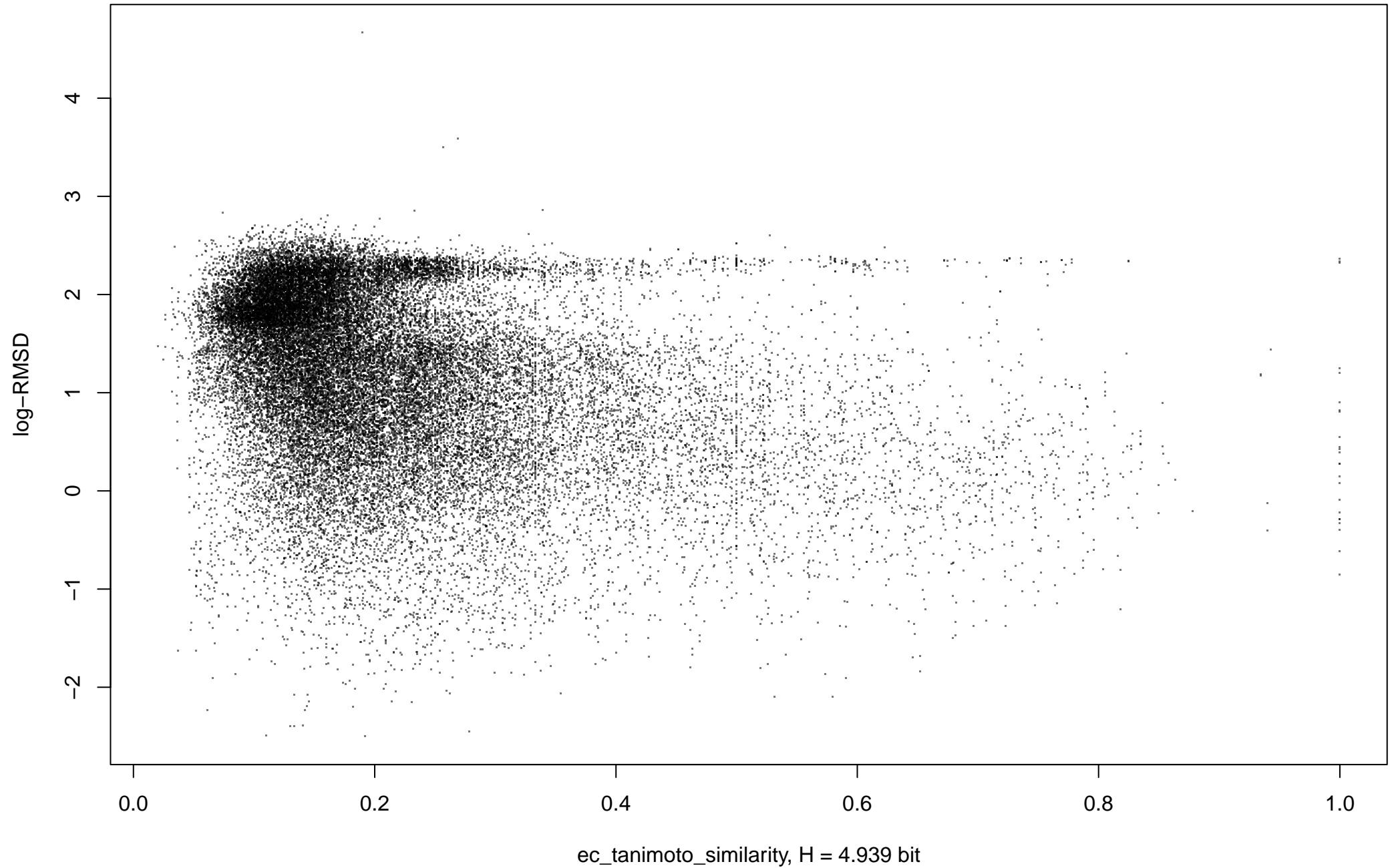
mcs_unbonded_polar_sasa, MI = 0.2024 bit, norm = 0.04646, cond entr = 4.437 bit



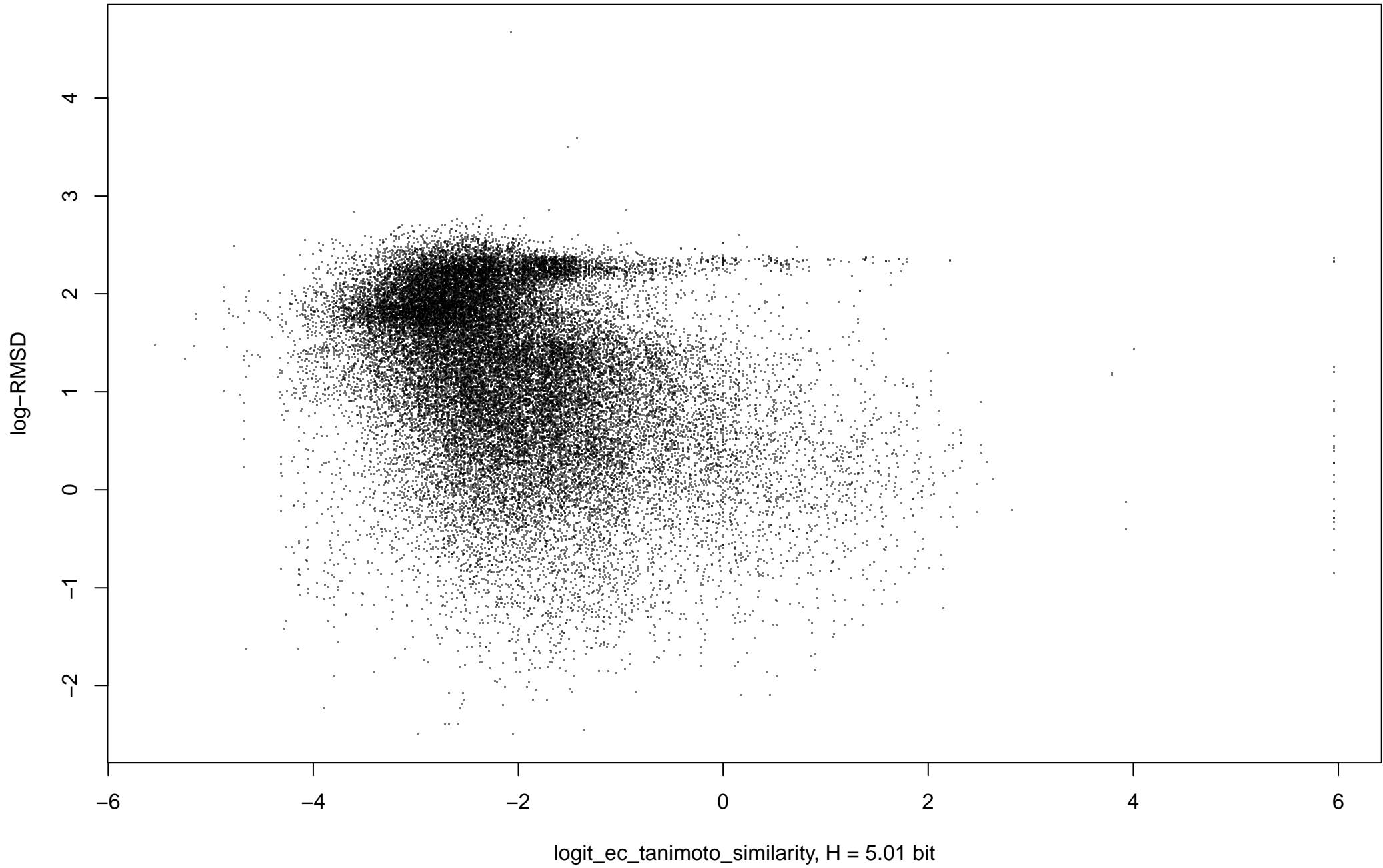
scale_mcs_unbonded_polar_sasa, MI = 0.2024 bit, norm = 0.04646, cond entr = 4.437 bit



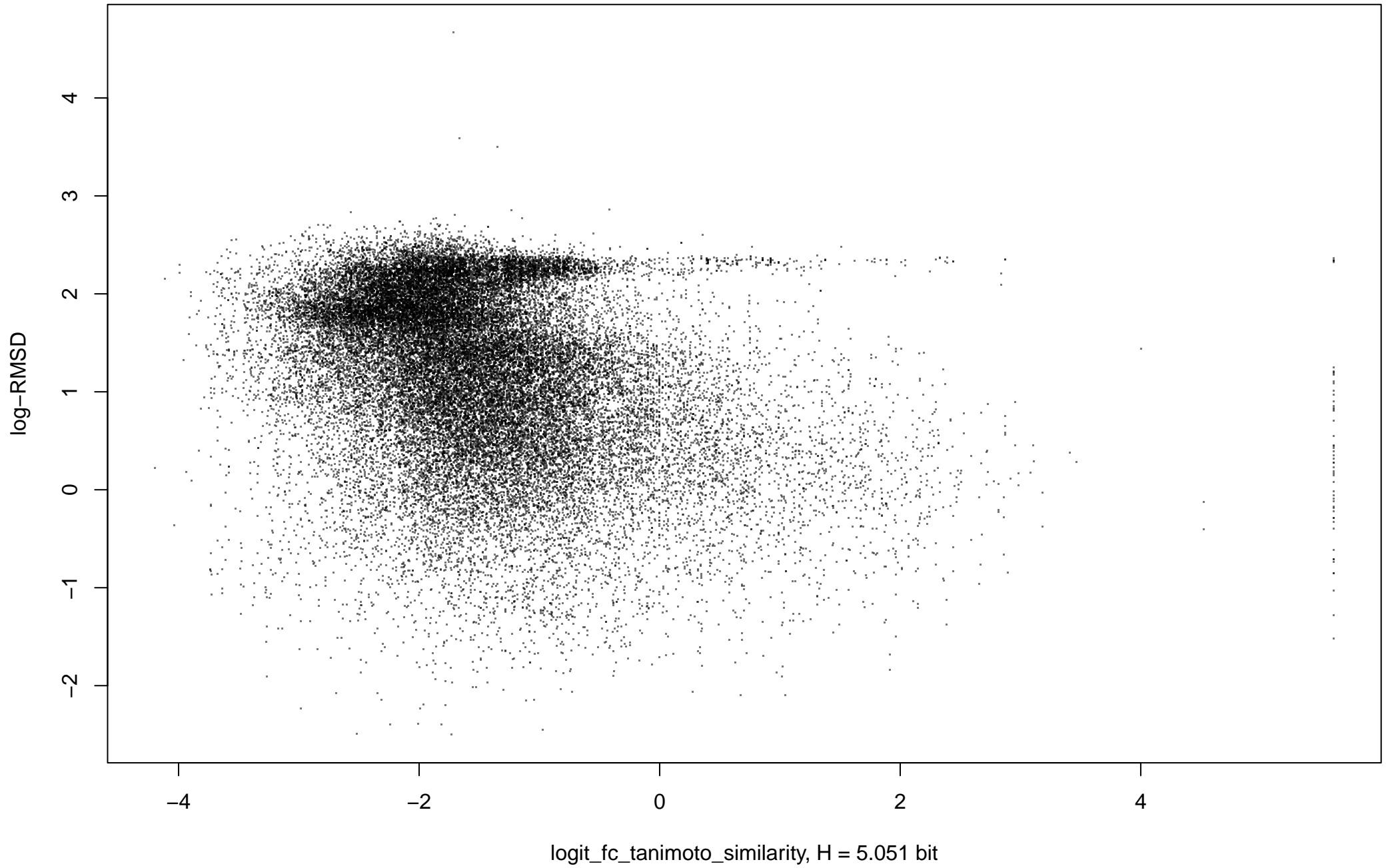
ec_tanimoto_similarity, MI = 0.2004 bit, norm = 0.04319, cond entr = 4.439 bit



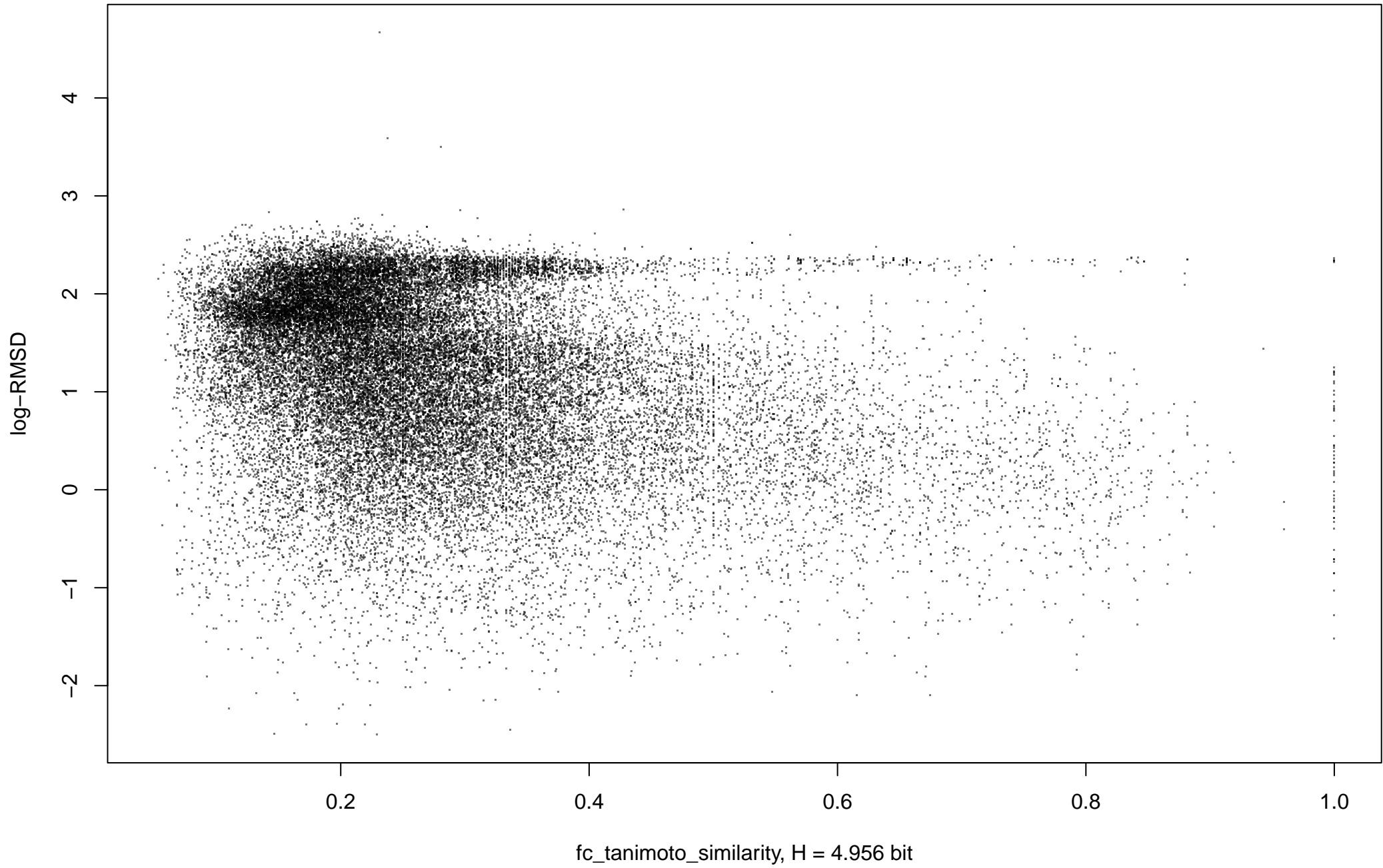
logit_ec_tanimoto_similarity, MI = 0.1958 bit, norm = 0.0422, cond entr = 4.444 bit



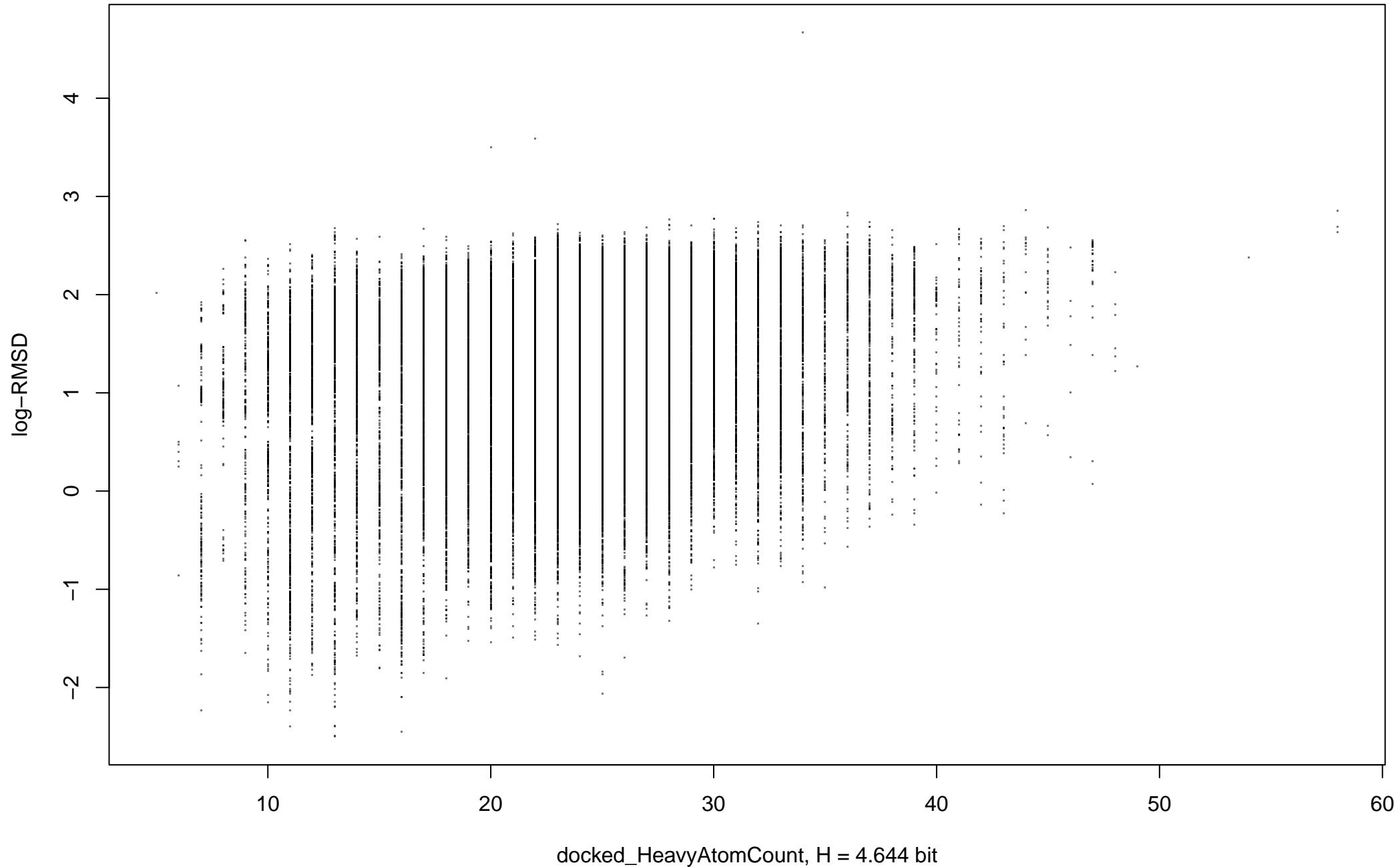
logit_fc_tanimoto_similarity, MI = 0.1863 bit, norm = 0.04015, cond entr = 4.453 bit



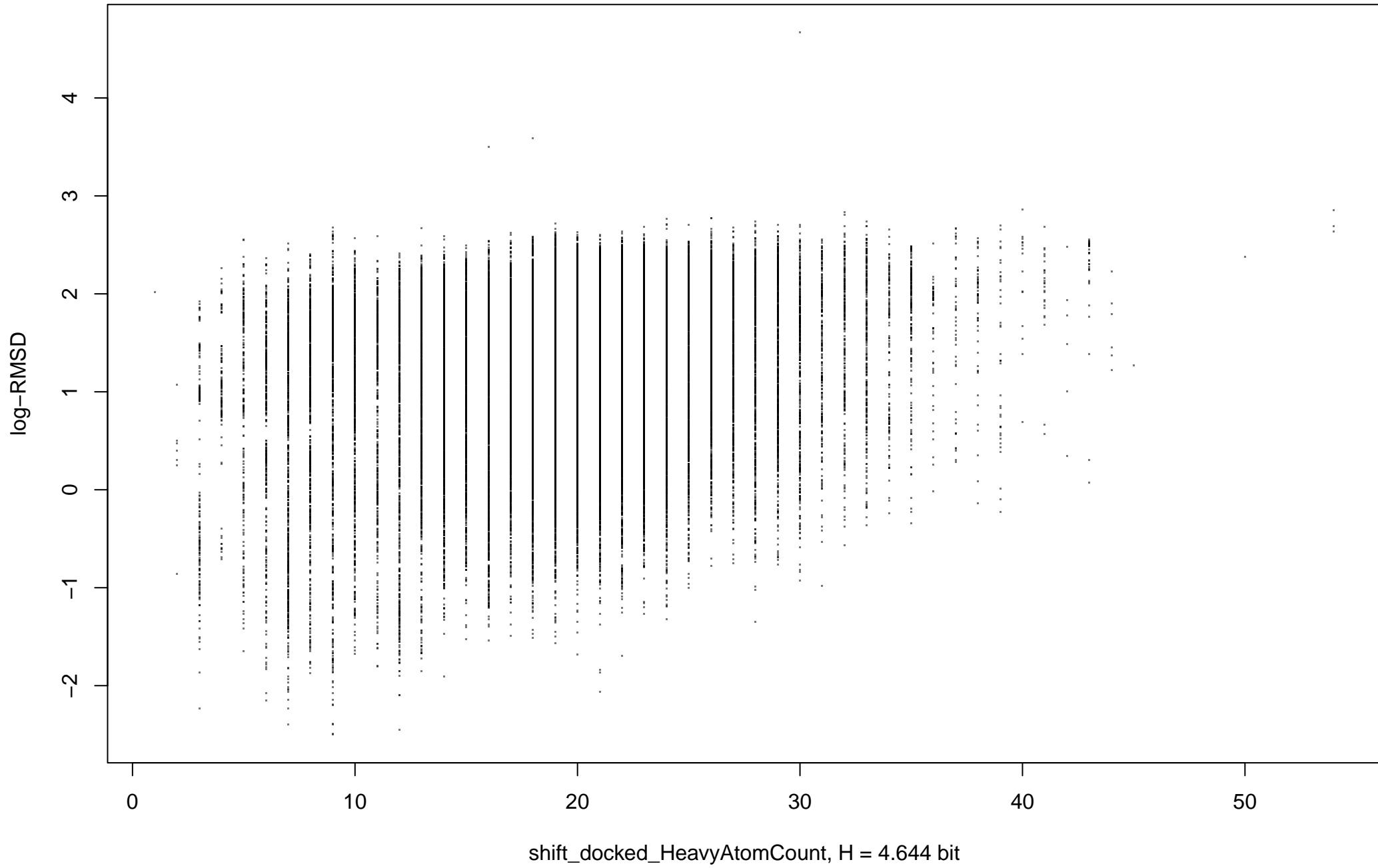
fc_tanimoto_similarity, MI = 0.1836 bit, norm = 0.03958, cond entr = 4.456 bit



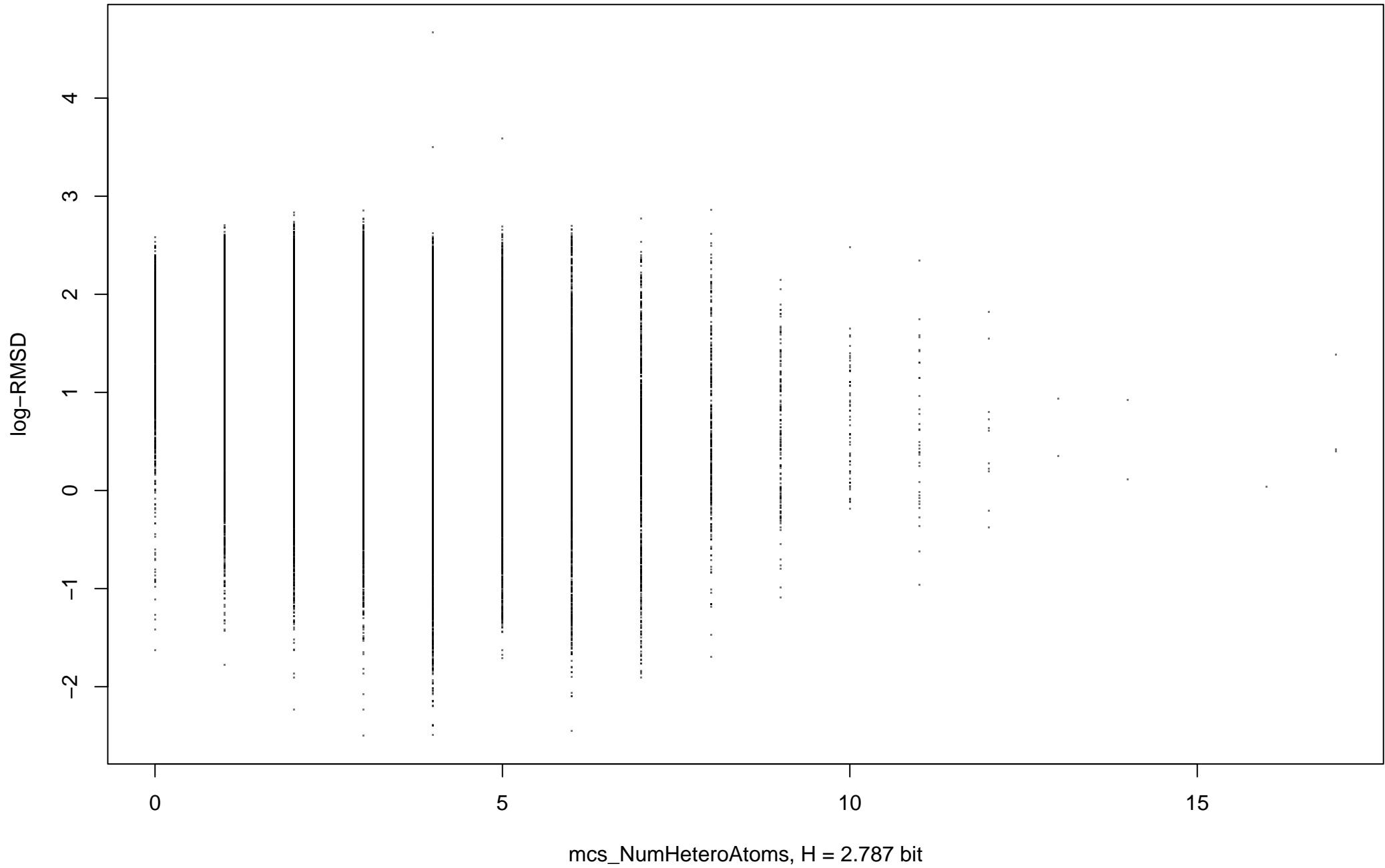
docked_HeavyAtomCount, MI = 0.16 bit, norm = 0.03449, cond entr = 4.48 bit



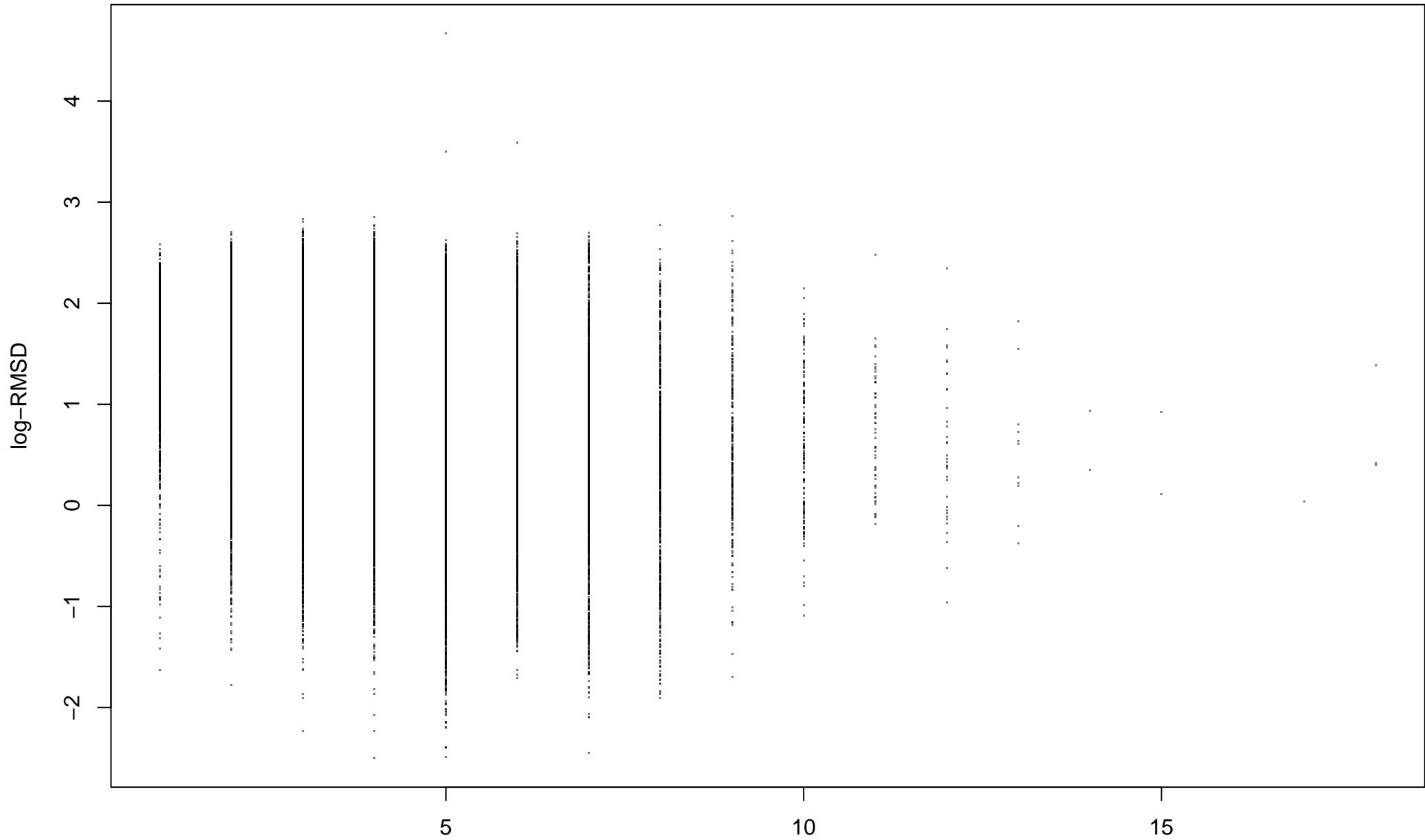
shift_docked_HeavyAtomCount, MI = 0.16 bit, norm = 0.03449, cond entr = 4.48 bit



mcs_NumHeteroAtoms, MI = 0.1592 bit, norm = 0.05712, cond entr = 4.48 bit

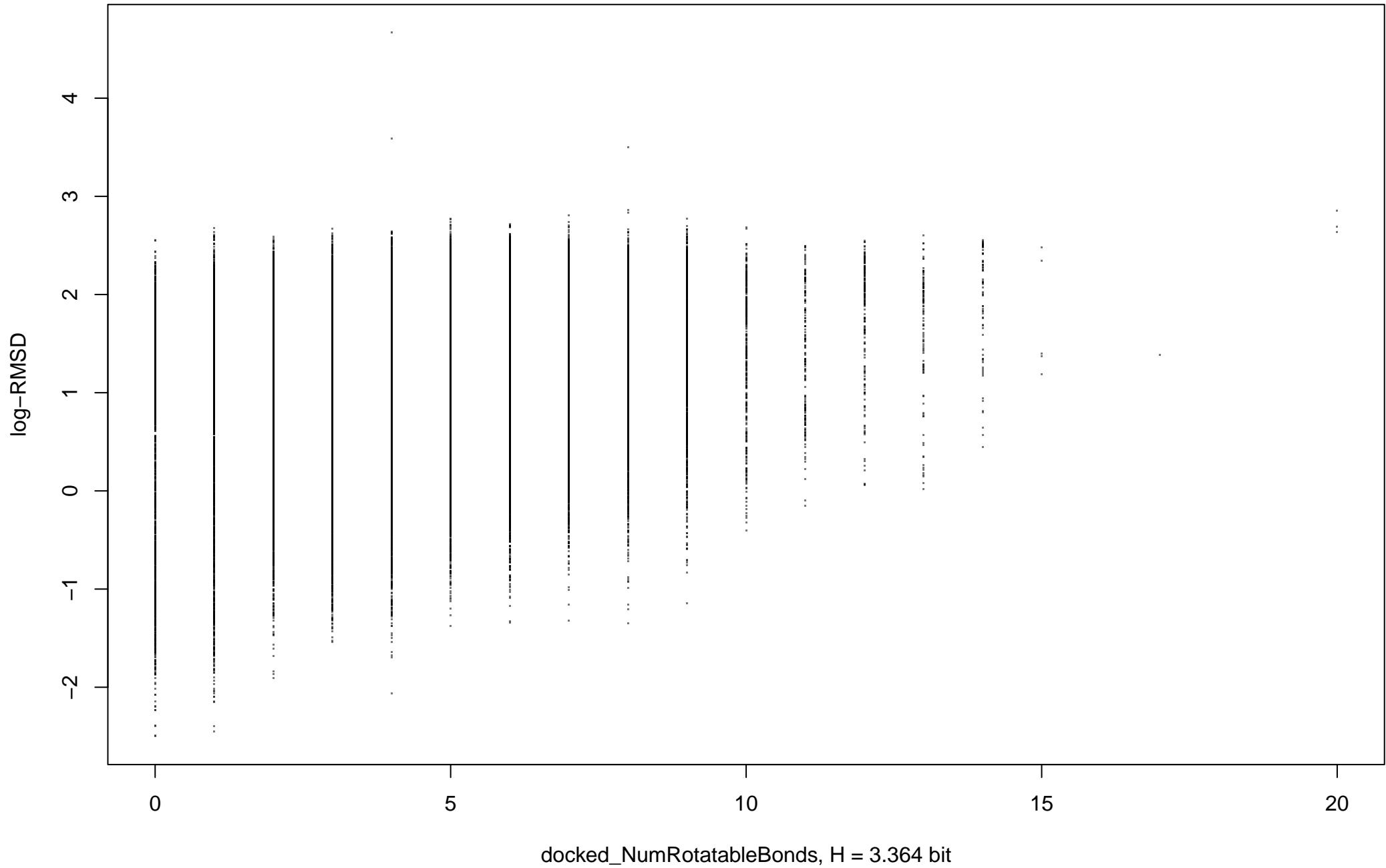


shift_mcs_NumHeteroAtoms, MI = 0.1592 bit, norm = 0.05712, cond entr = 4.48 bit

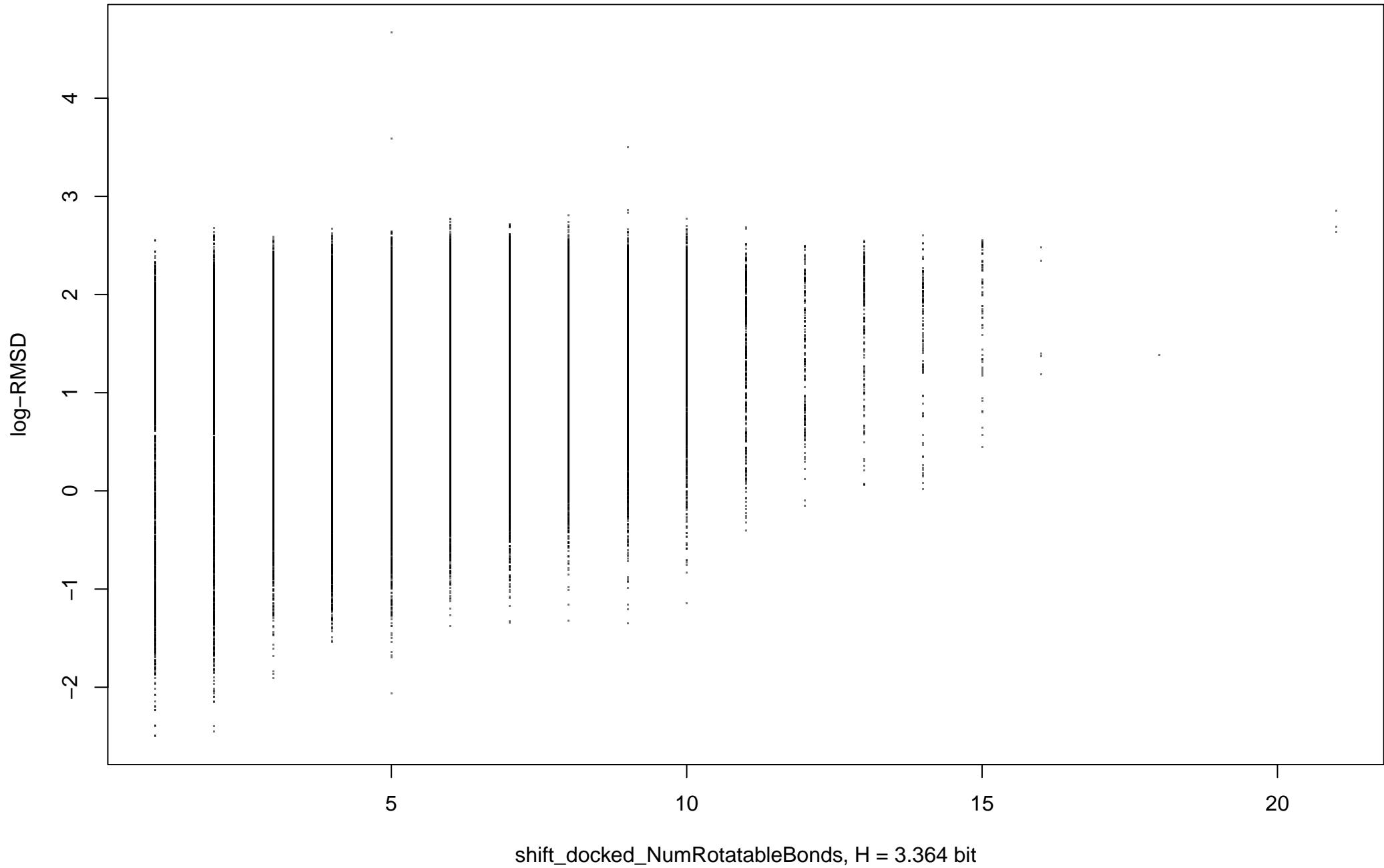


shift_mcs_NumHeteroAtoms, H = 2.787 bit

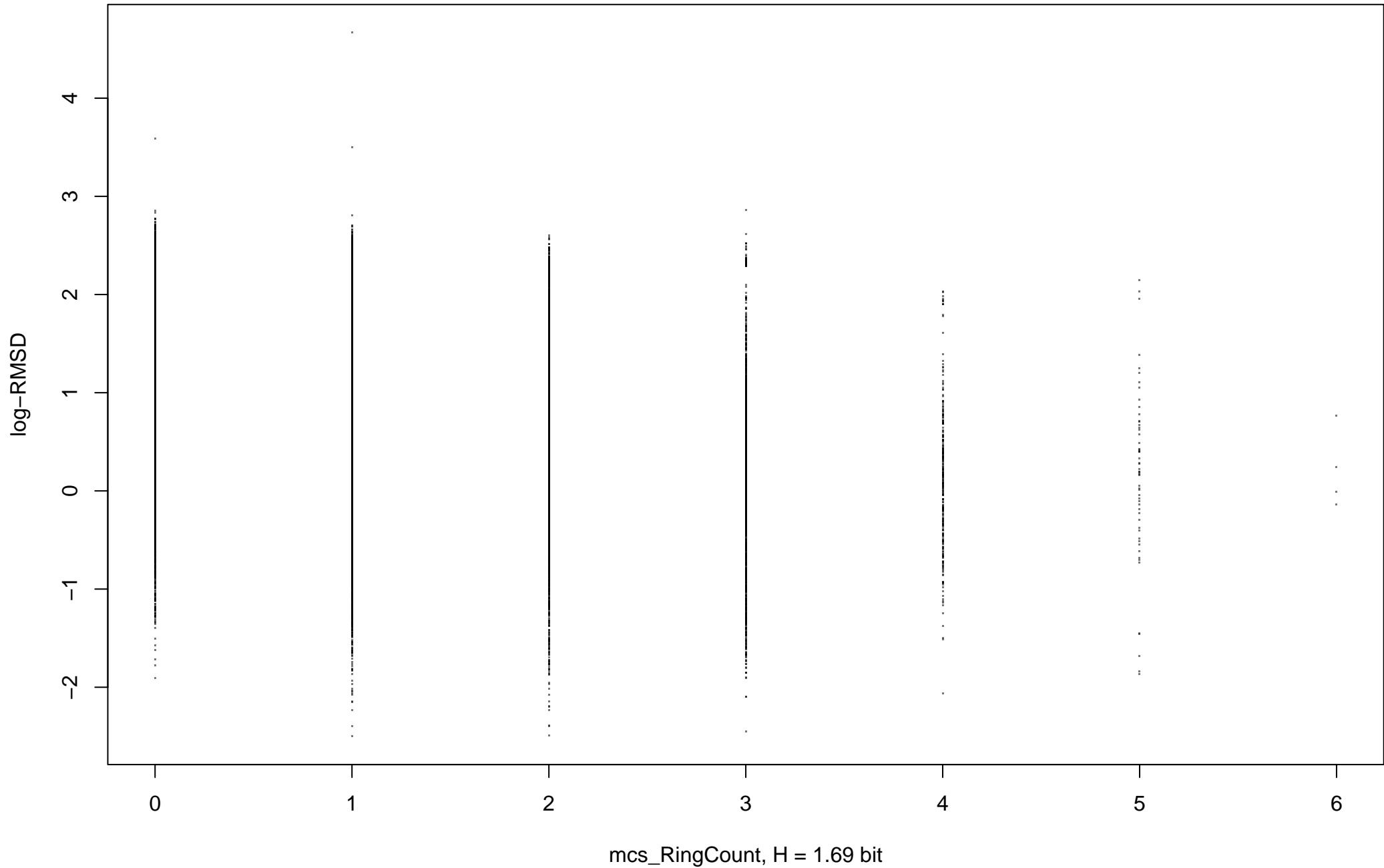
docked_NumRotatableBonds, MI = 0.1472 bit, norm = 0.04375, cond entr = 4.492 bit



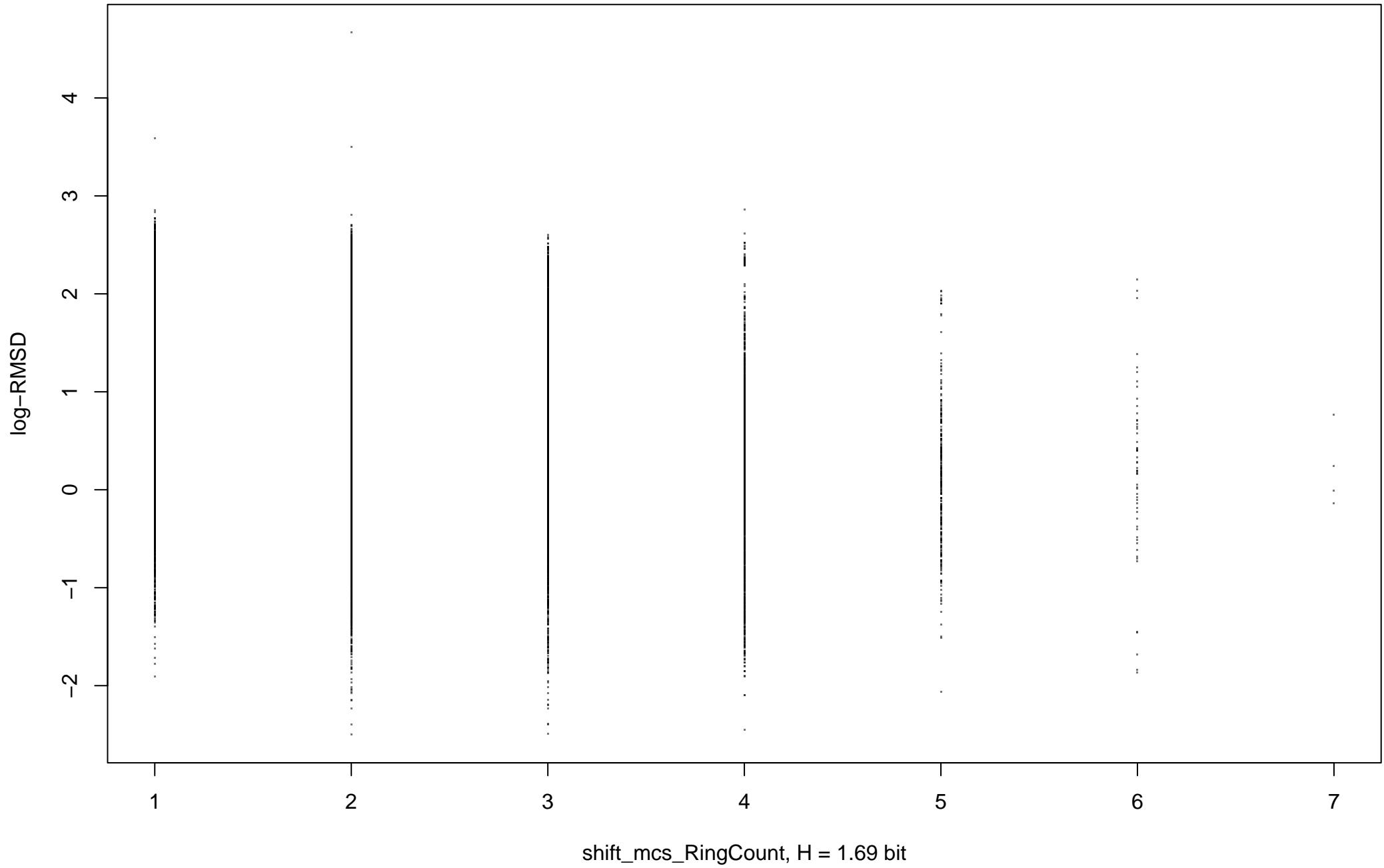
shift_docked_NumRotatableBonds, MI = 0.1472 bit, norm = 0.04375, cond entr = 4.492 bit



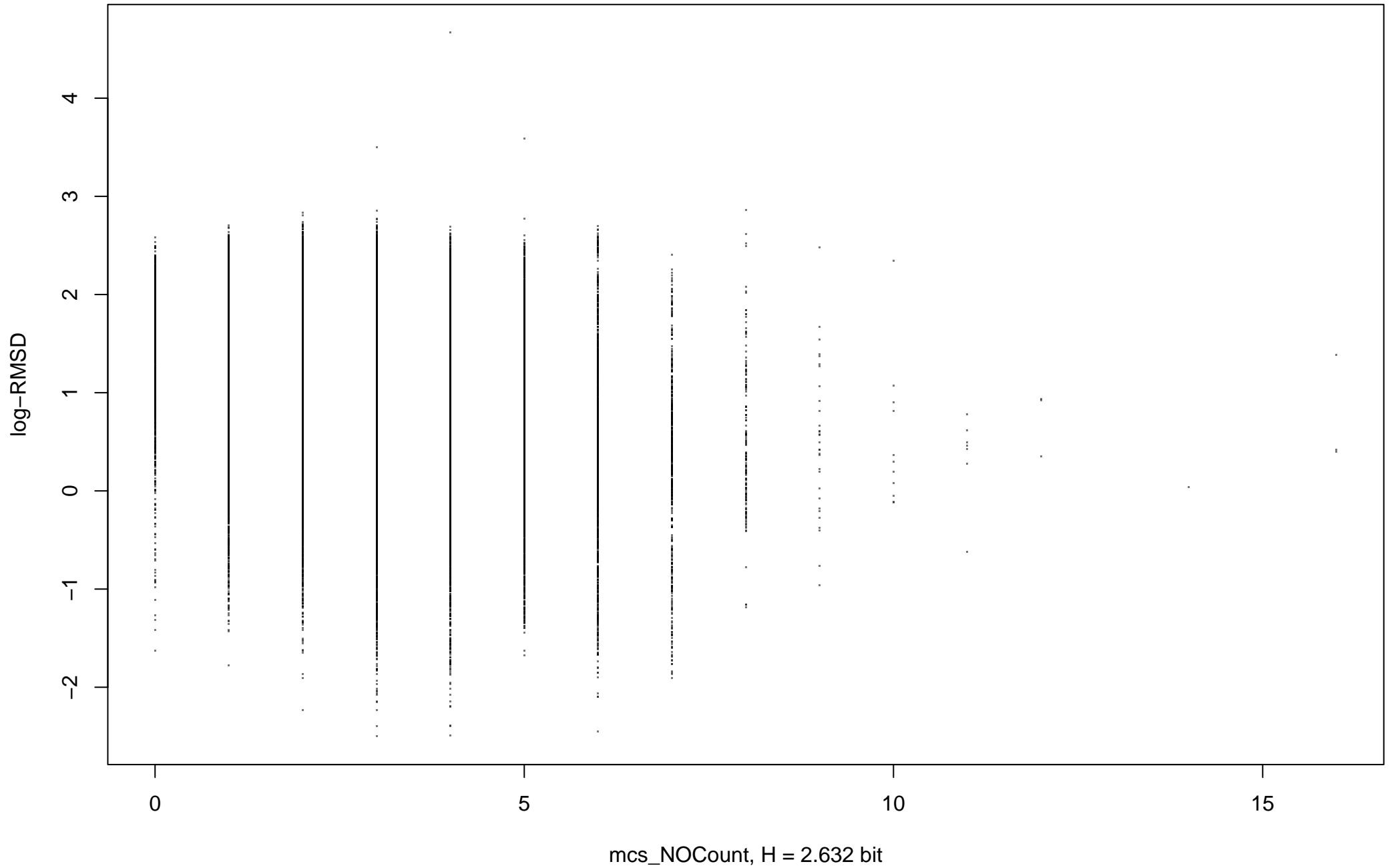
mcs_RingCount, MI = 0.1442 bit, norm = 0.0853, cond entr = 4.495 bit



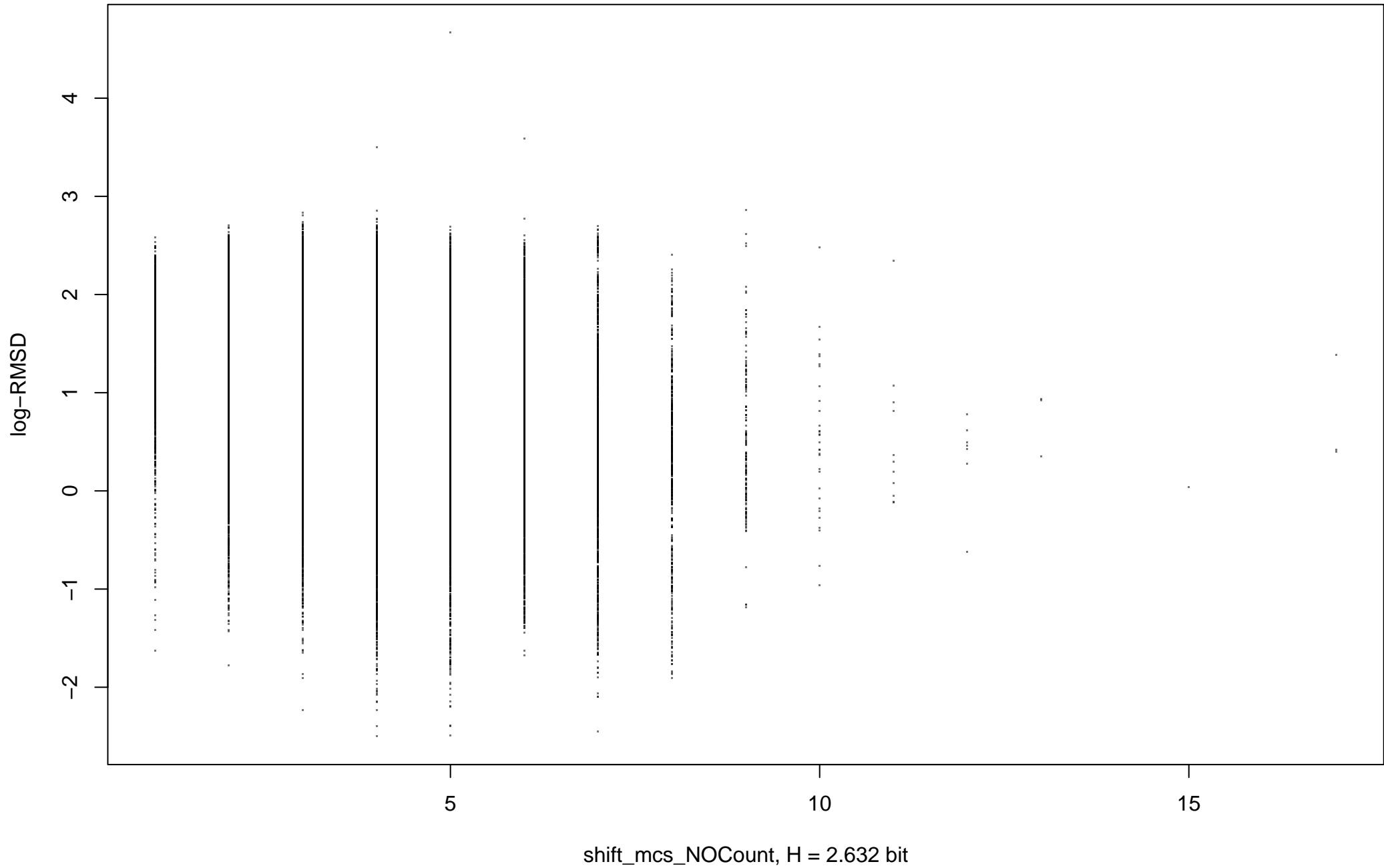
shift_mcs_RingCount, MI = 0.1442 bit, norm = 0.0853, cond entr = 4.495 bit



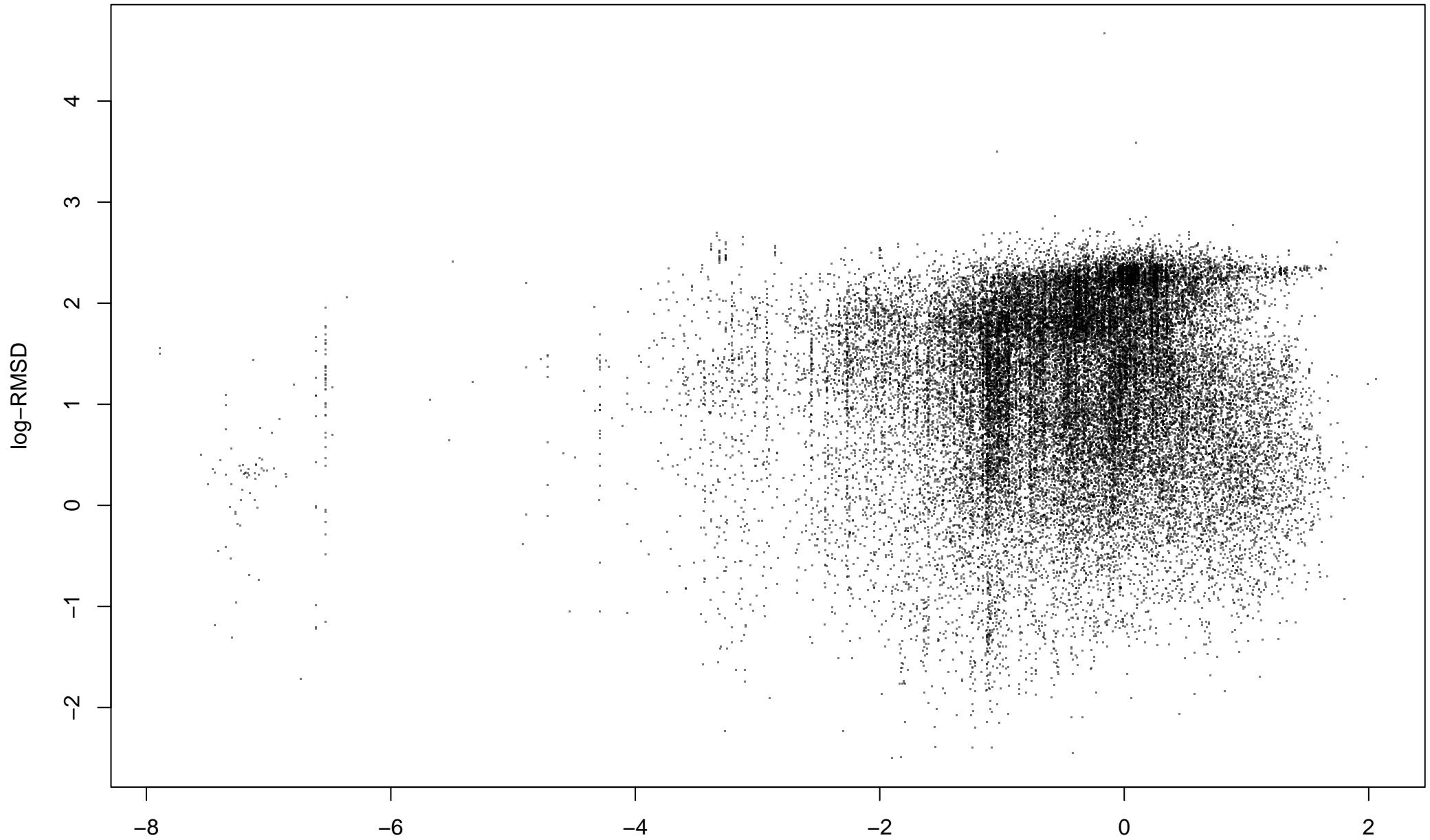
mcs_NOCount, MI = 0.1404 bit, norm = 0.05334, cond entr = 4.499 bit



shift_mcs_NOCount, MI = 0.1404 bit, norm = 0.05334, cond entr = 4.499 bit

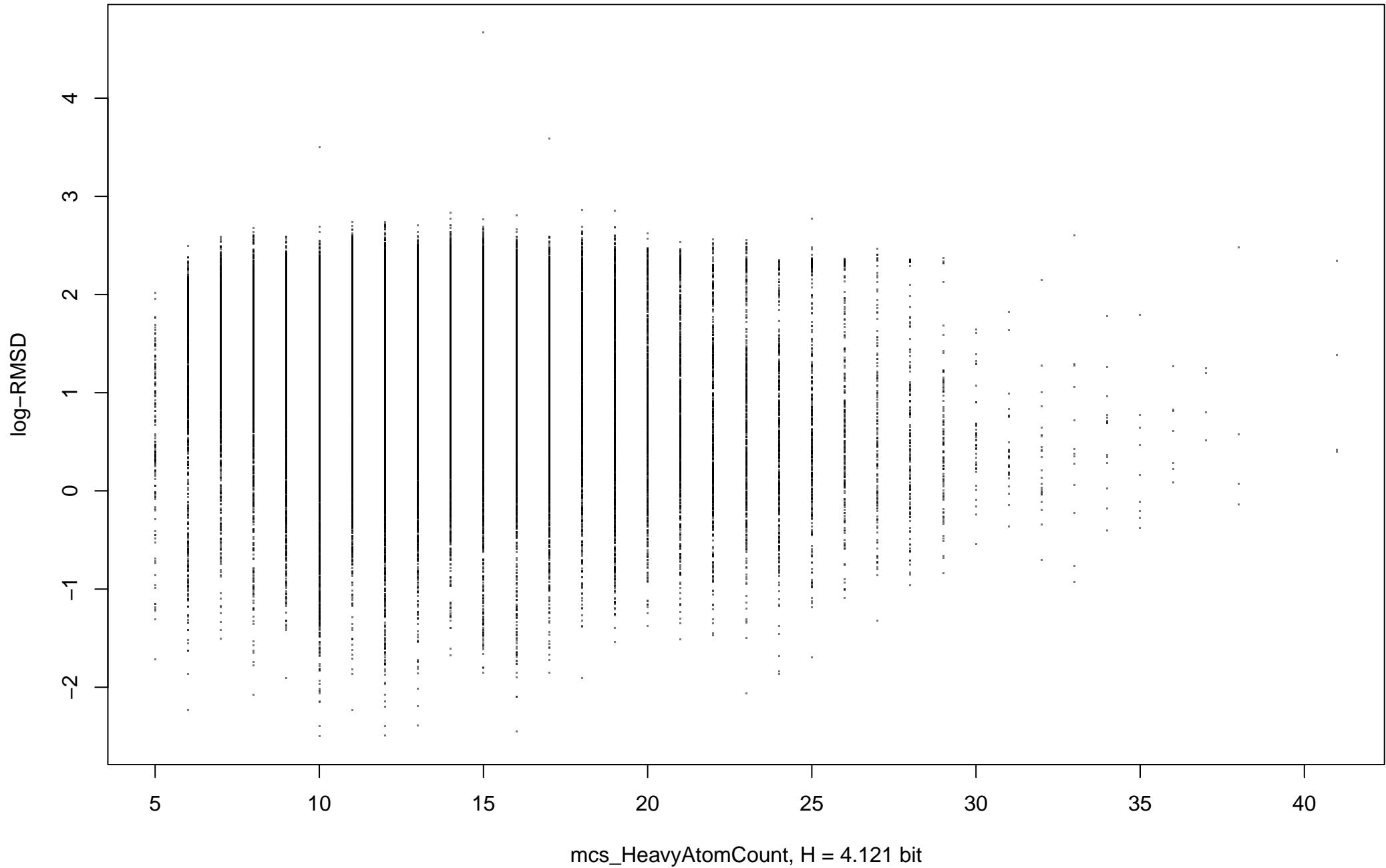


log_mcs_unbonded_apolar_sasa, MI = 0.1315 bit, norm = 0.02835, cond entr = 4.508 bit

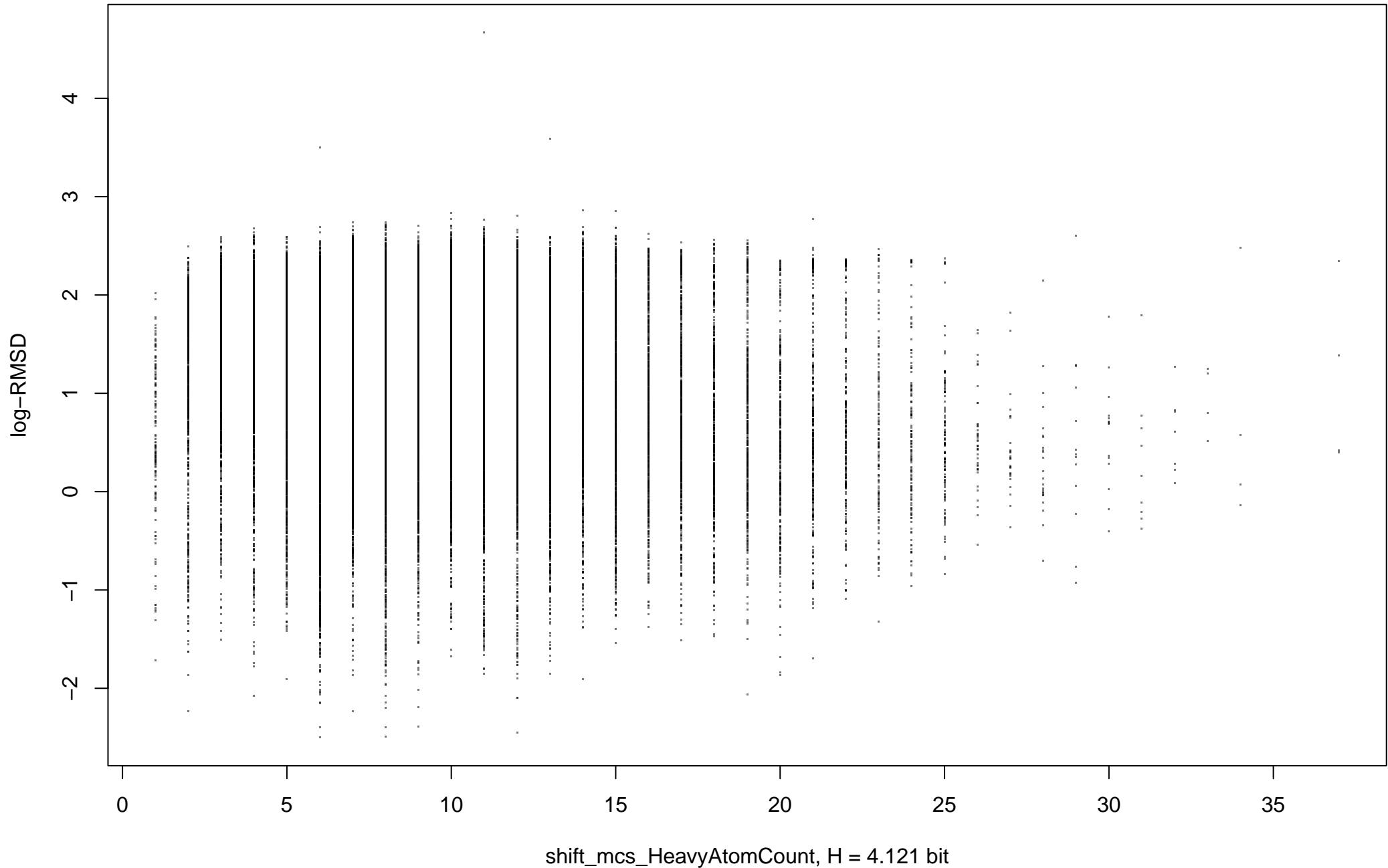


log_mcs_unbonded_apolar_sasa, H = 4.924 bit

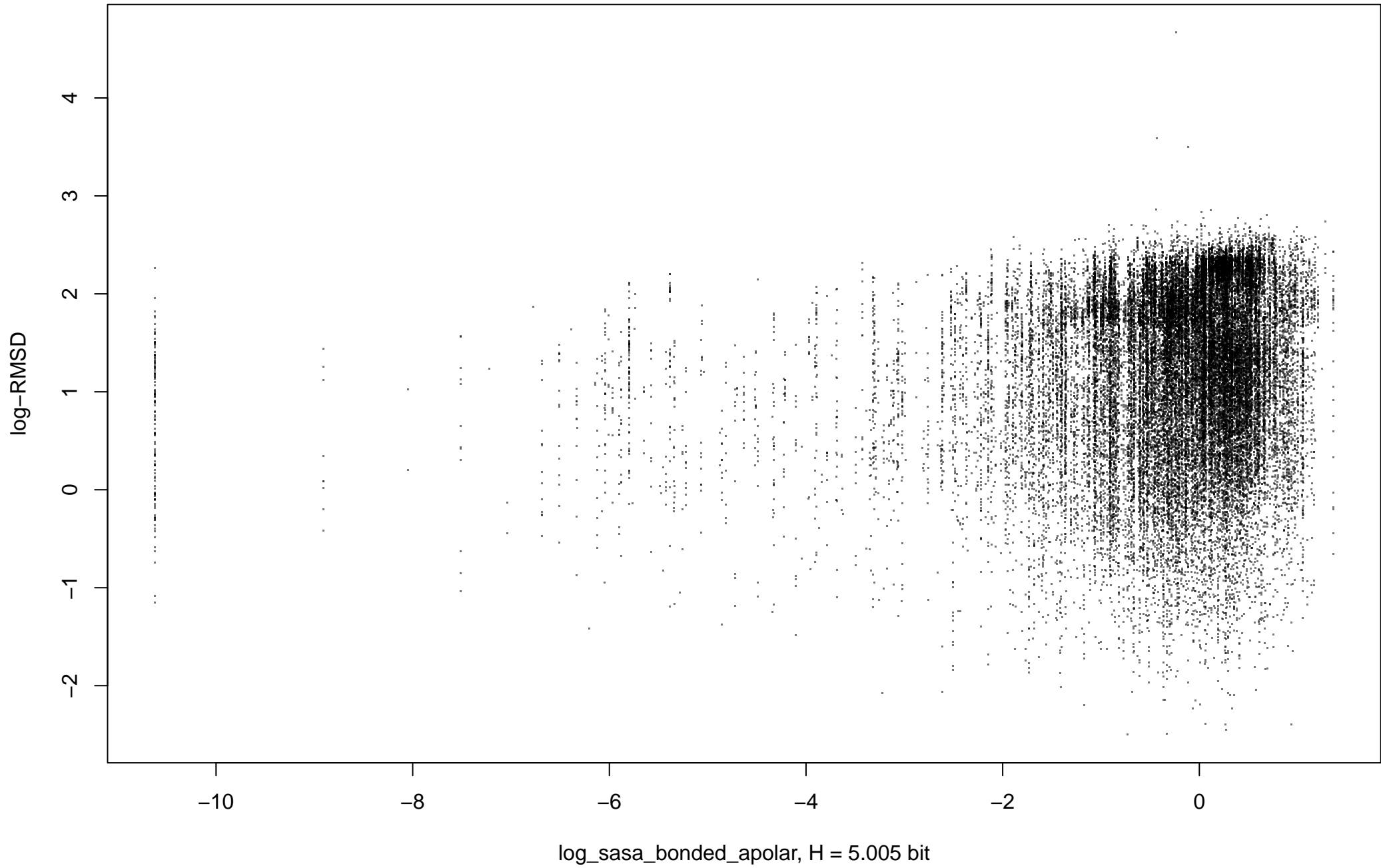
mcs_HeavyAtomCount, MI = 0.1268 bit, norm = 0.03078, cond entr = 4.513 bit



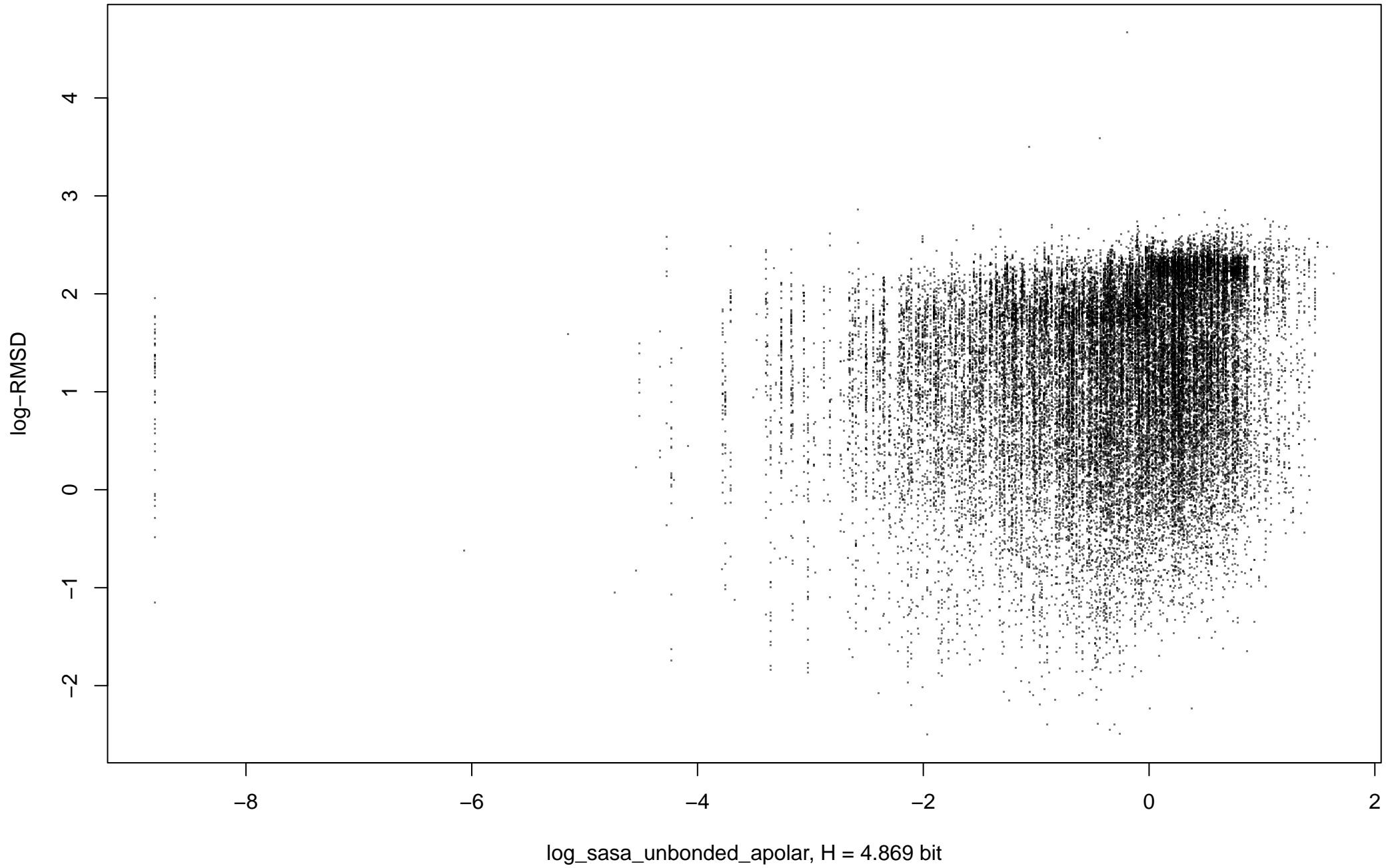
shift_mcs_HeavyAtomCount, MI = 0.1268 bit, norm = 0.03078, cond entr = 4.513 bit



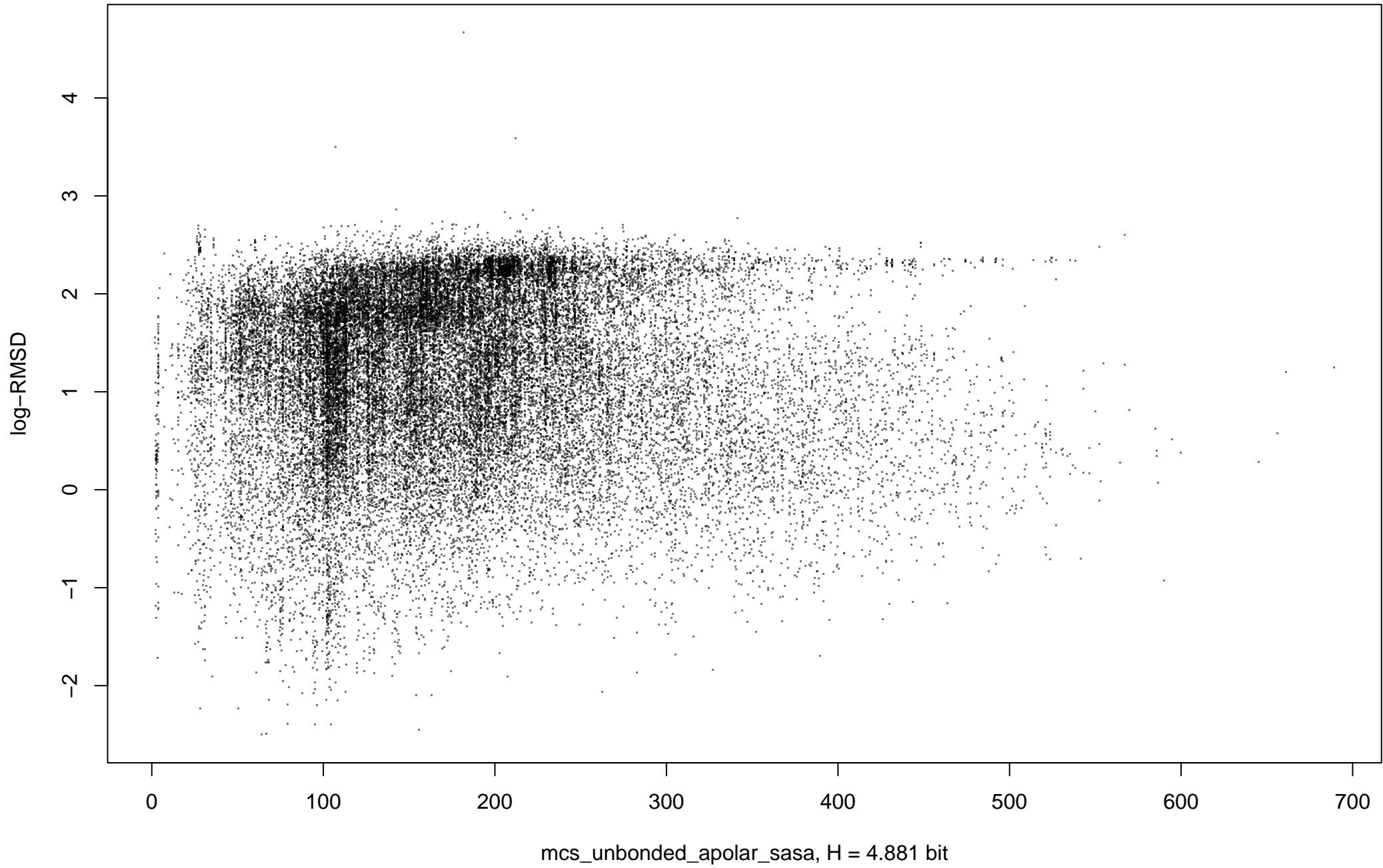
log_sasa_bonded_apolar, MI = 0.1266 bit, norm = 0.02729, cond entr = 4.513 bit



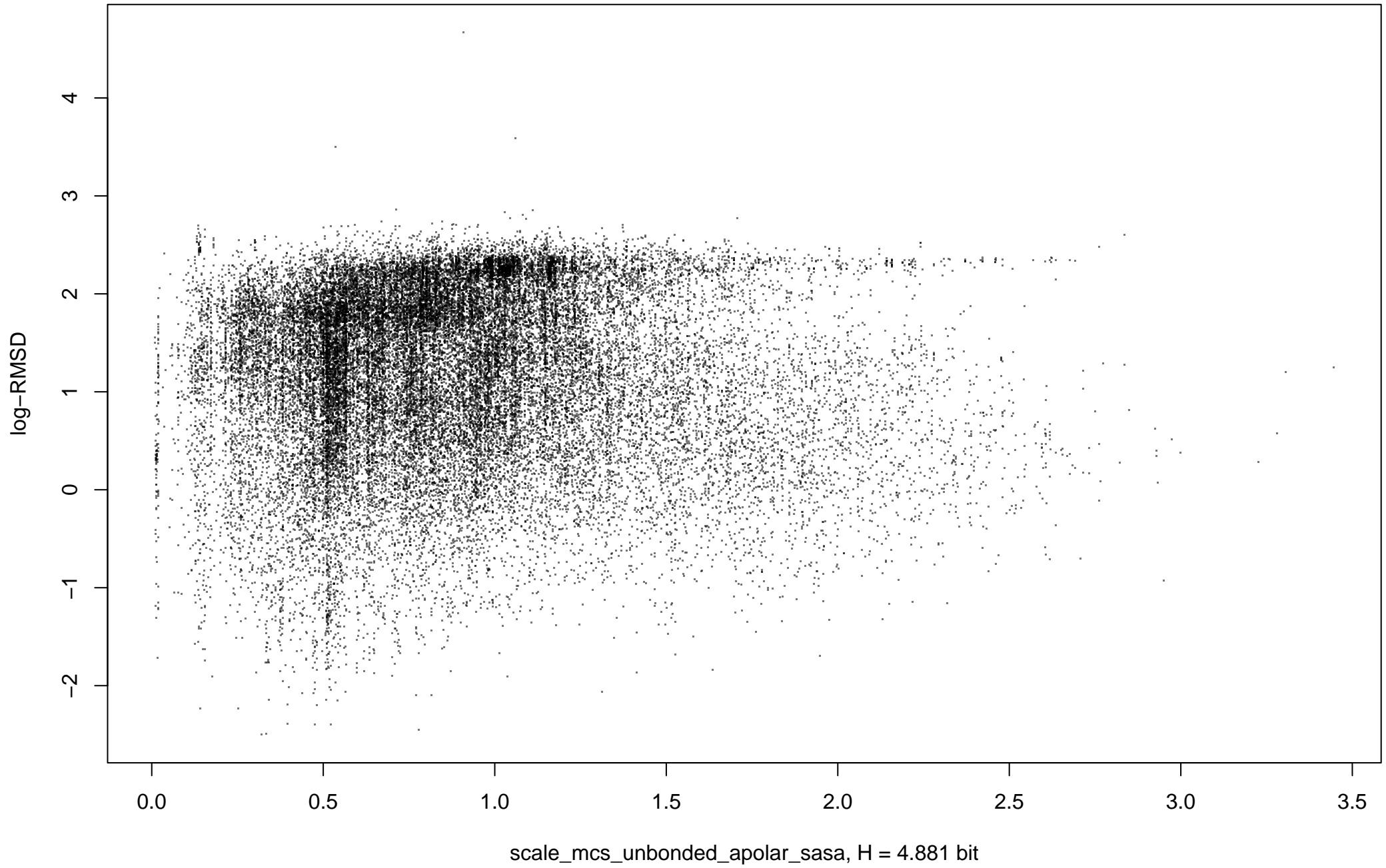
log_sasa_unbonded_apolar, MI = 0.126 bit, norm = 0.02715, cond entr = 4.514 bit



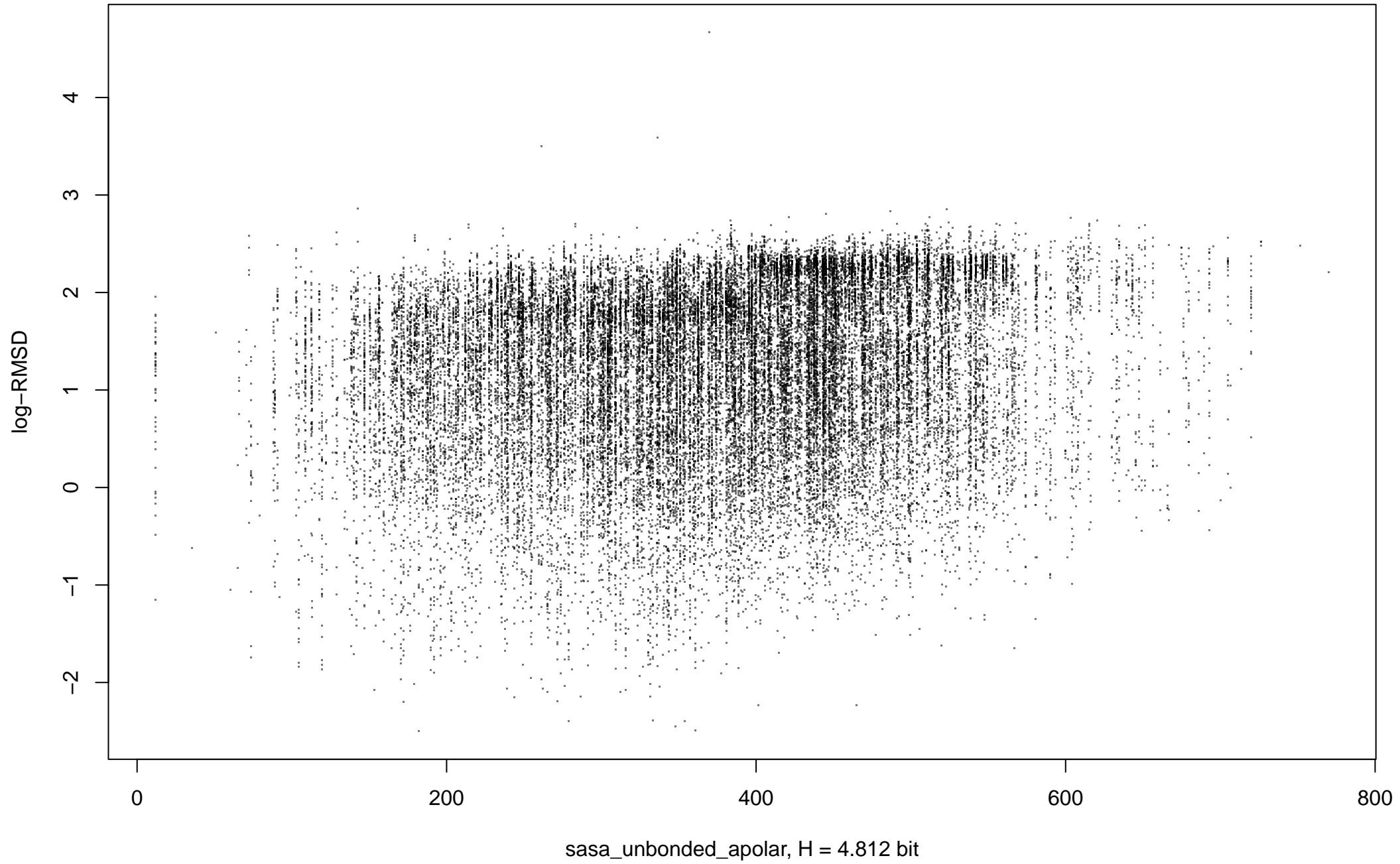
mcs_unbonded_apolar_sasa, MI = 0.1221 bit, norm = 0.02633, cond entr = 4.517 bit



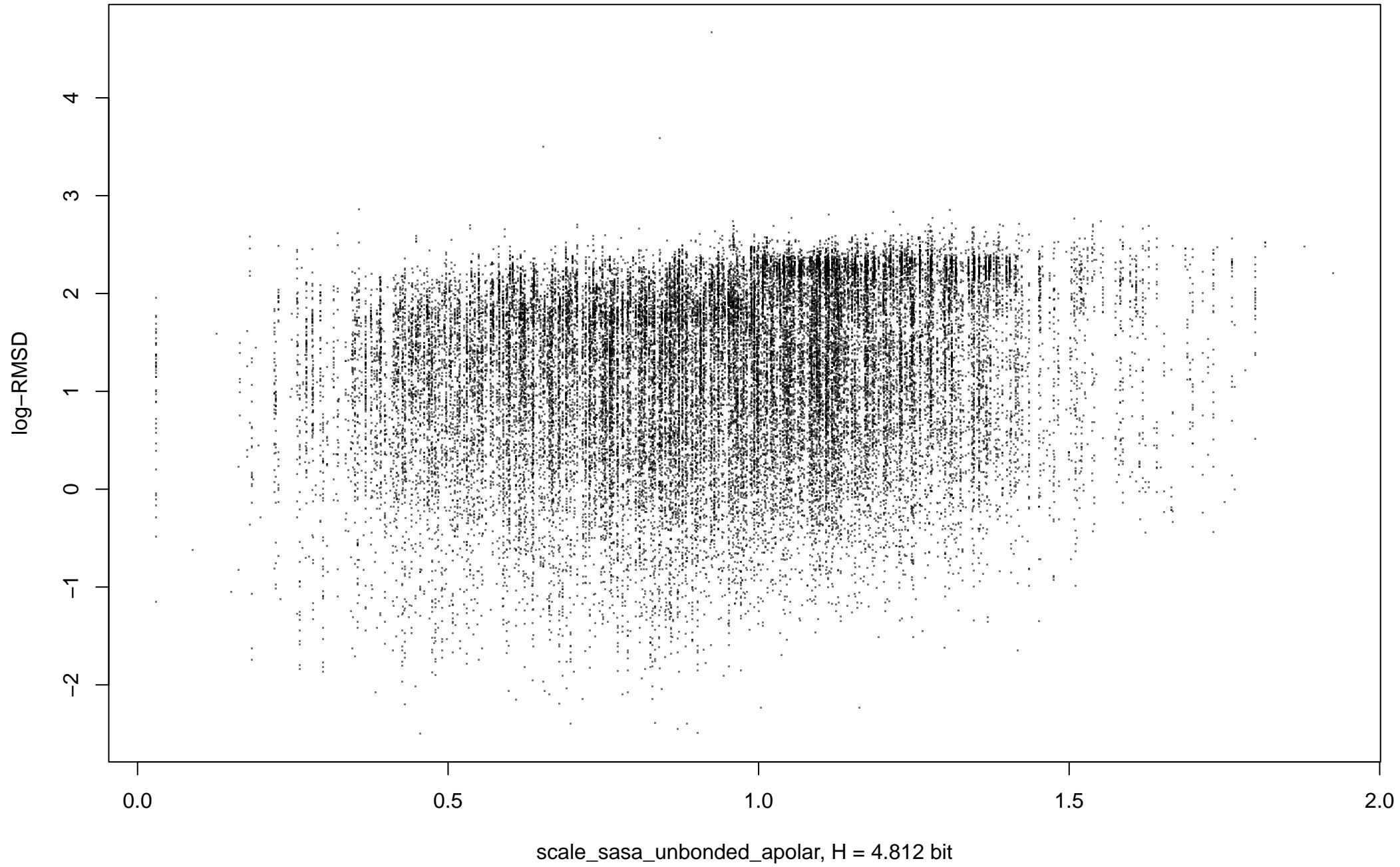
scale_mcs_unbonded_apolar_sasa, MI = 0.1221 bit, norm = 0.02633, cond entr = 4.517 bit



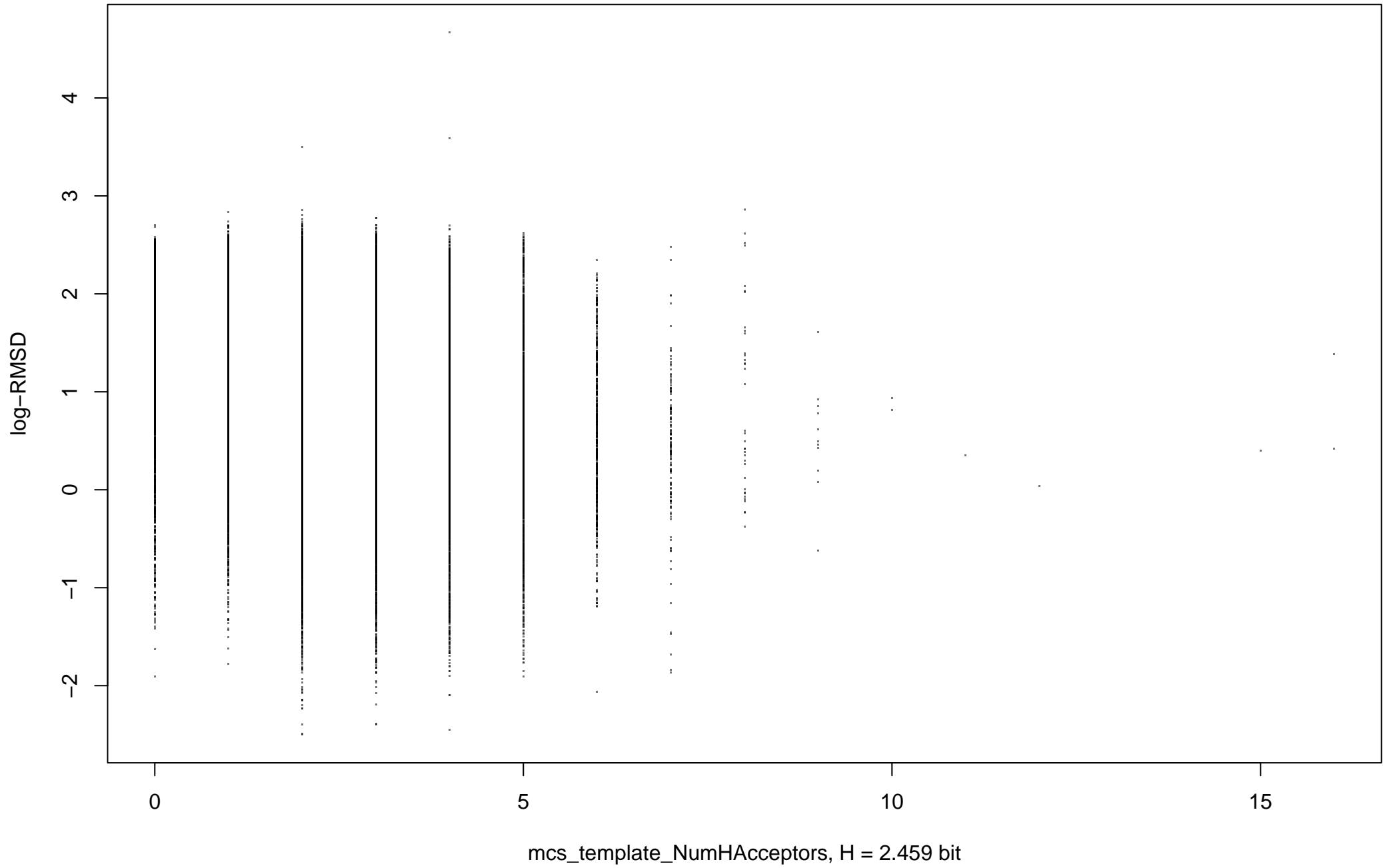
sasa_unbonded_apolar, MI = 0.1172 bit, norm = 0.02527, cond entr = 4.522 bit



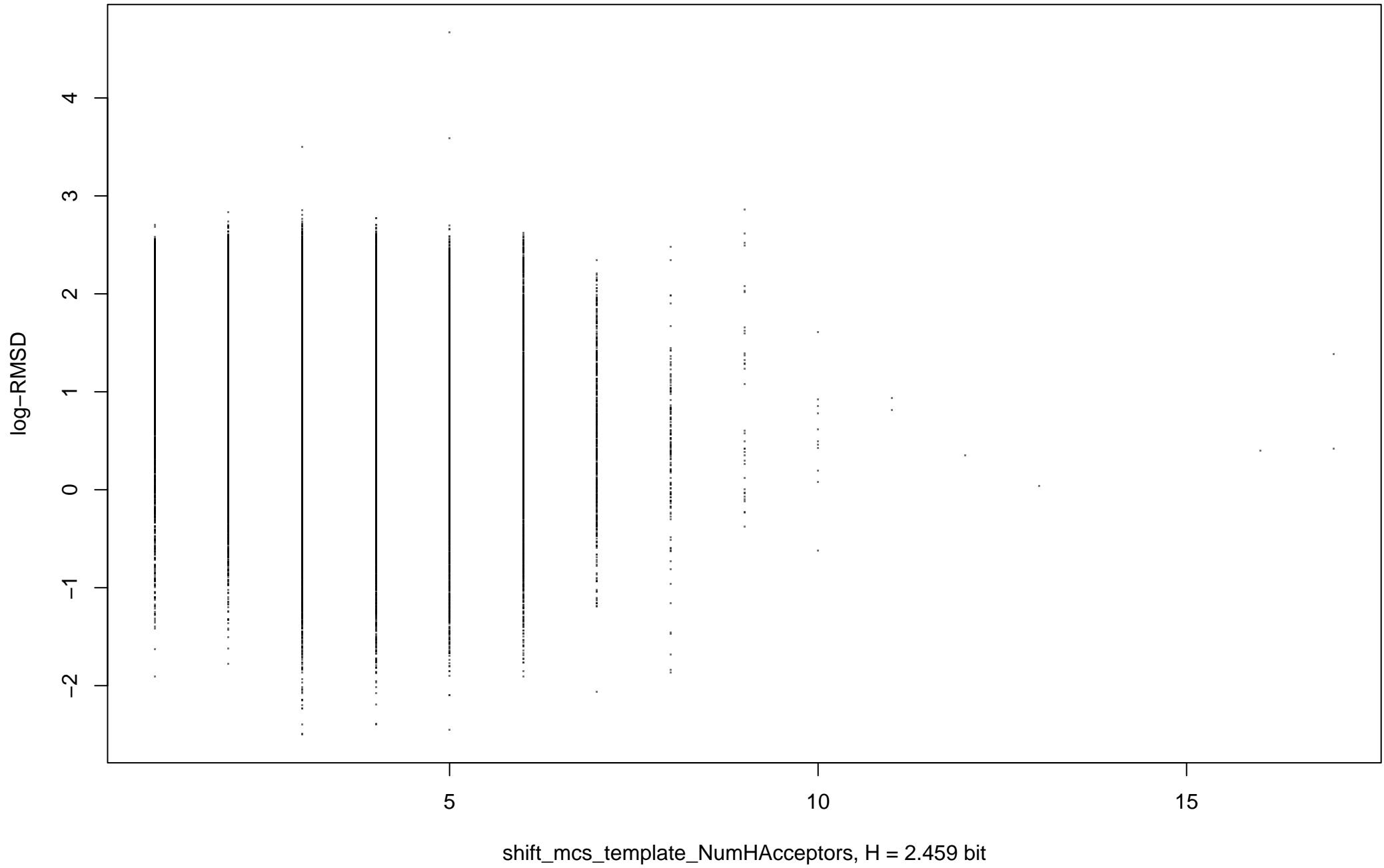
scale_sasa_unbonded_apolar, MI = 0.1172 bit, norm = 0.02527, cond entr = 4.522 bit



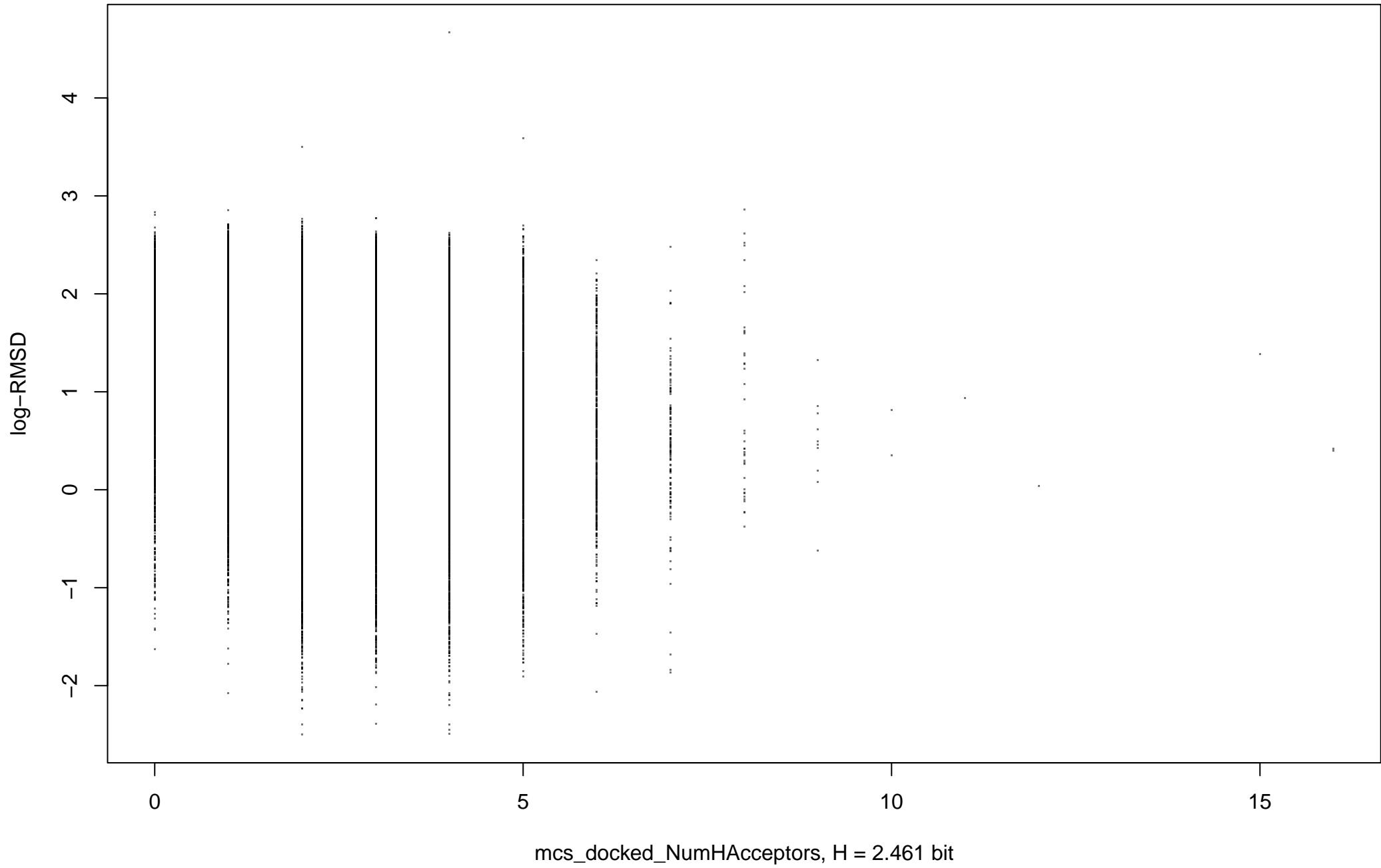
mcs_template_NumHAcceptors, MI = 0.1147 bit, norm = 0.04665, cond entr = 4.525 bit



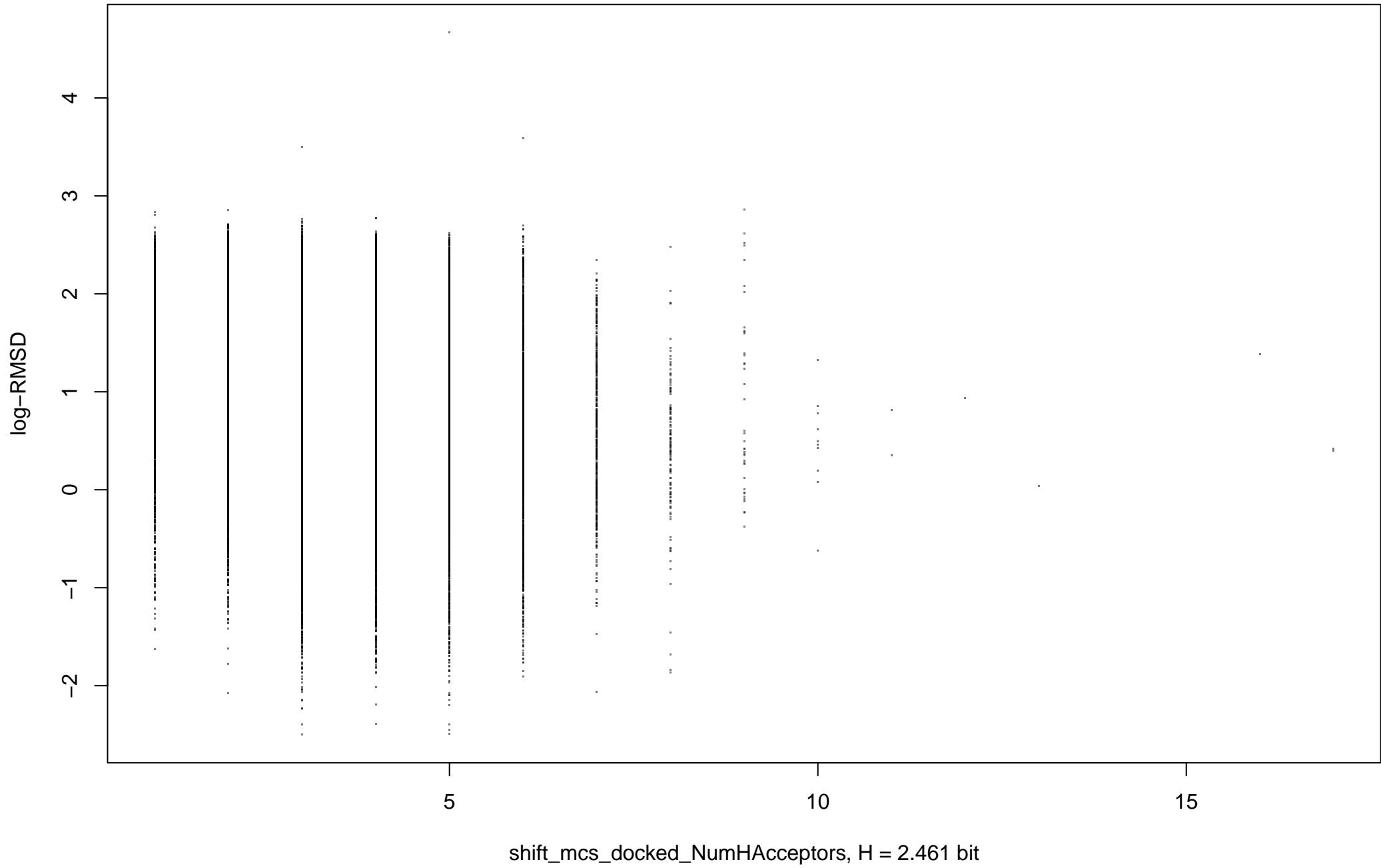
shift_mcs_template_NumHAcceptors, MI = 0.1147 bit, norm = 0.04665, cond entr = 4.525 bit



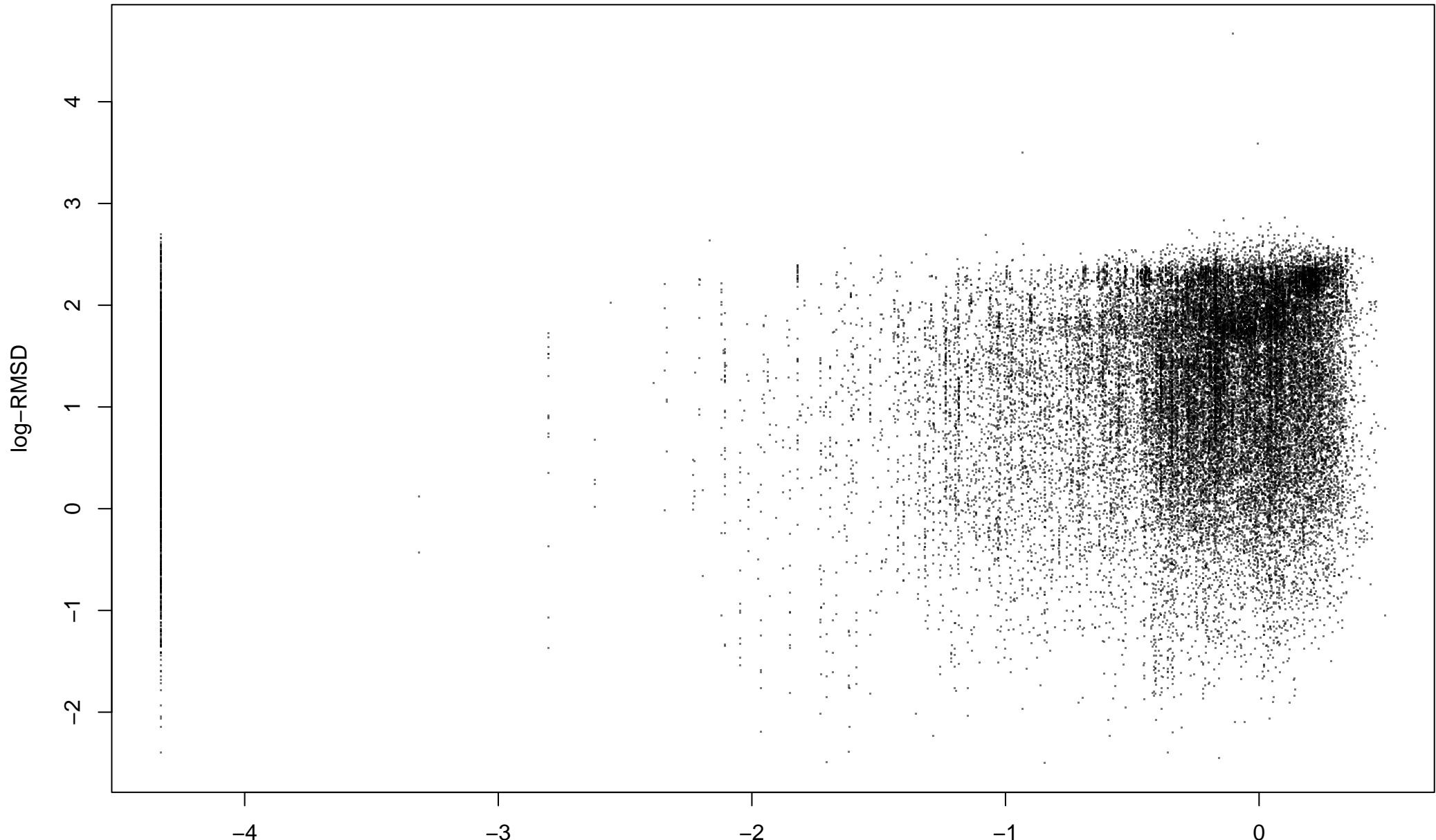
mcs_docked_NumHAcceptors, MI = 0.1145 bit, norm = 0.04651, cond entr = 4.525 bit



shift_mcs_docked_NumHAcceptors, MI = 0.1145 bit, norm = 0.04651, cond entr = 4.525 bit

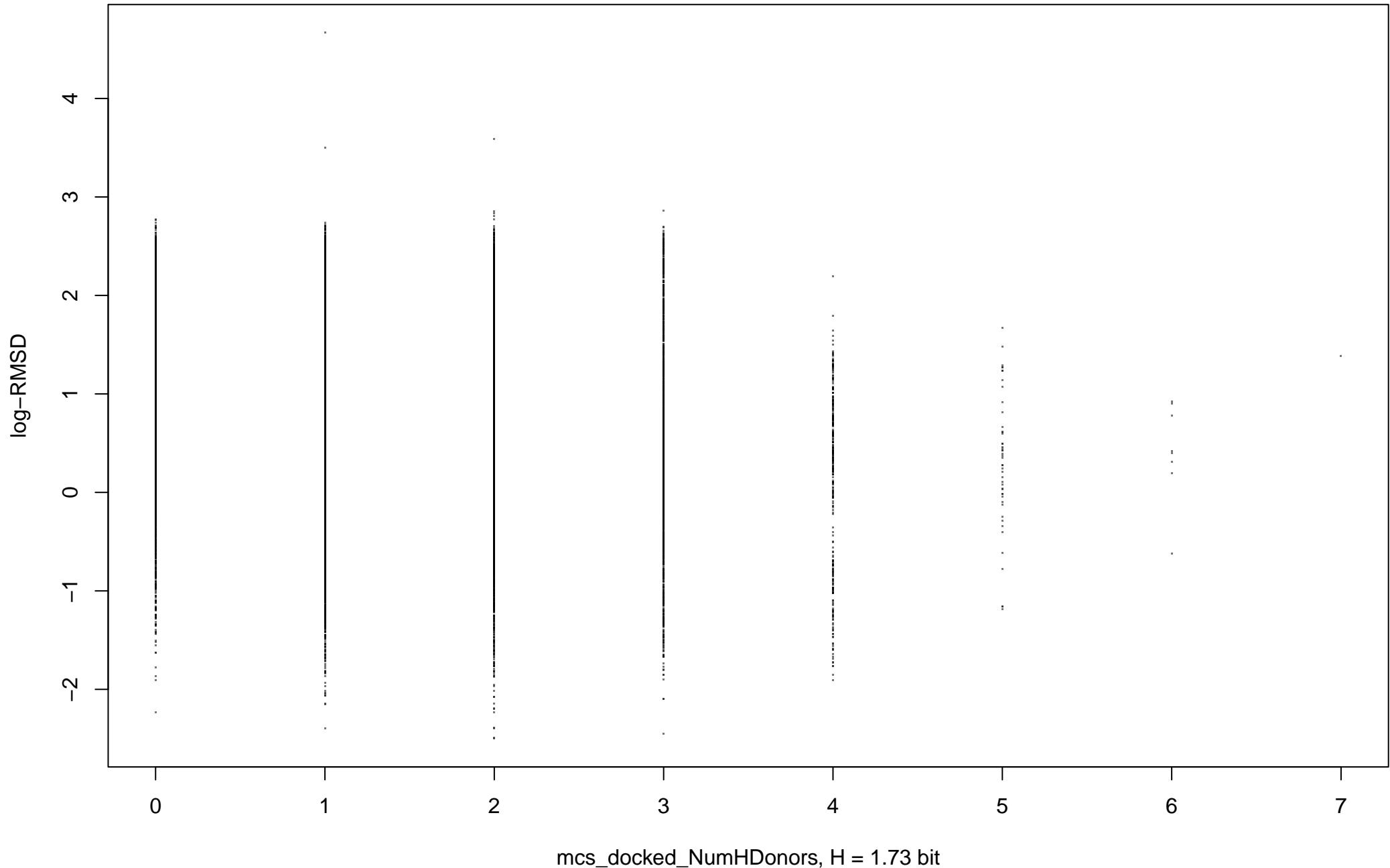


log_mcs_bonded_apolar_sasa, MI = 0.1046 bit, norm = 0.02254, cond entr = 4.535 bit

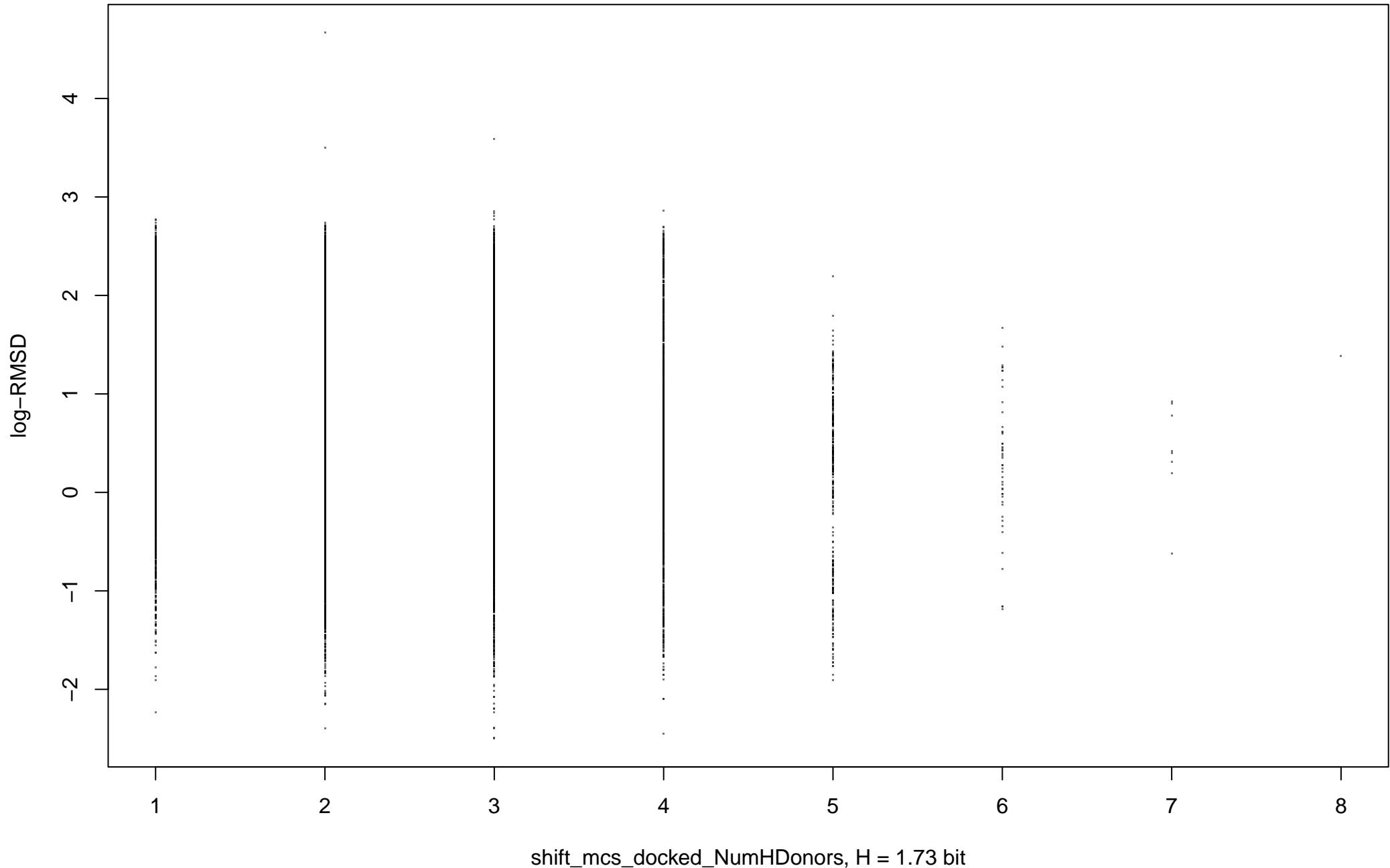


log_mcs_bonded_apolar_sasa, H = 4.886 bit

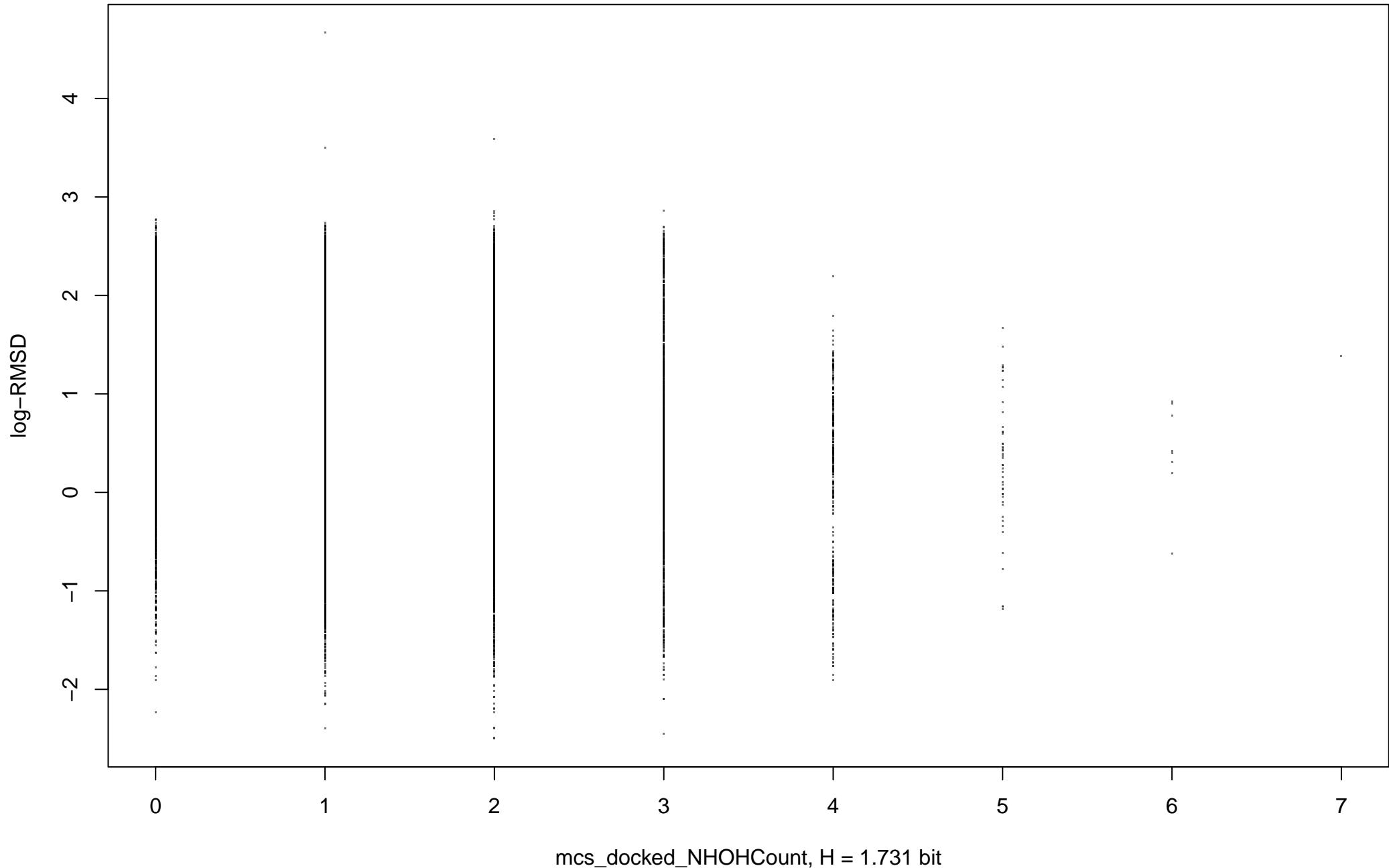
mcs_docked_NumHDonors, MI = 0.1033 bit, norm = 0.05968, cond entr = 4.536 bit



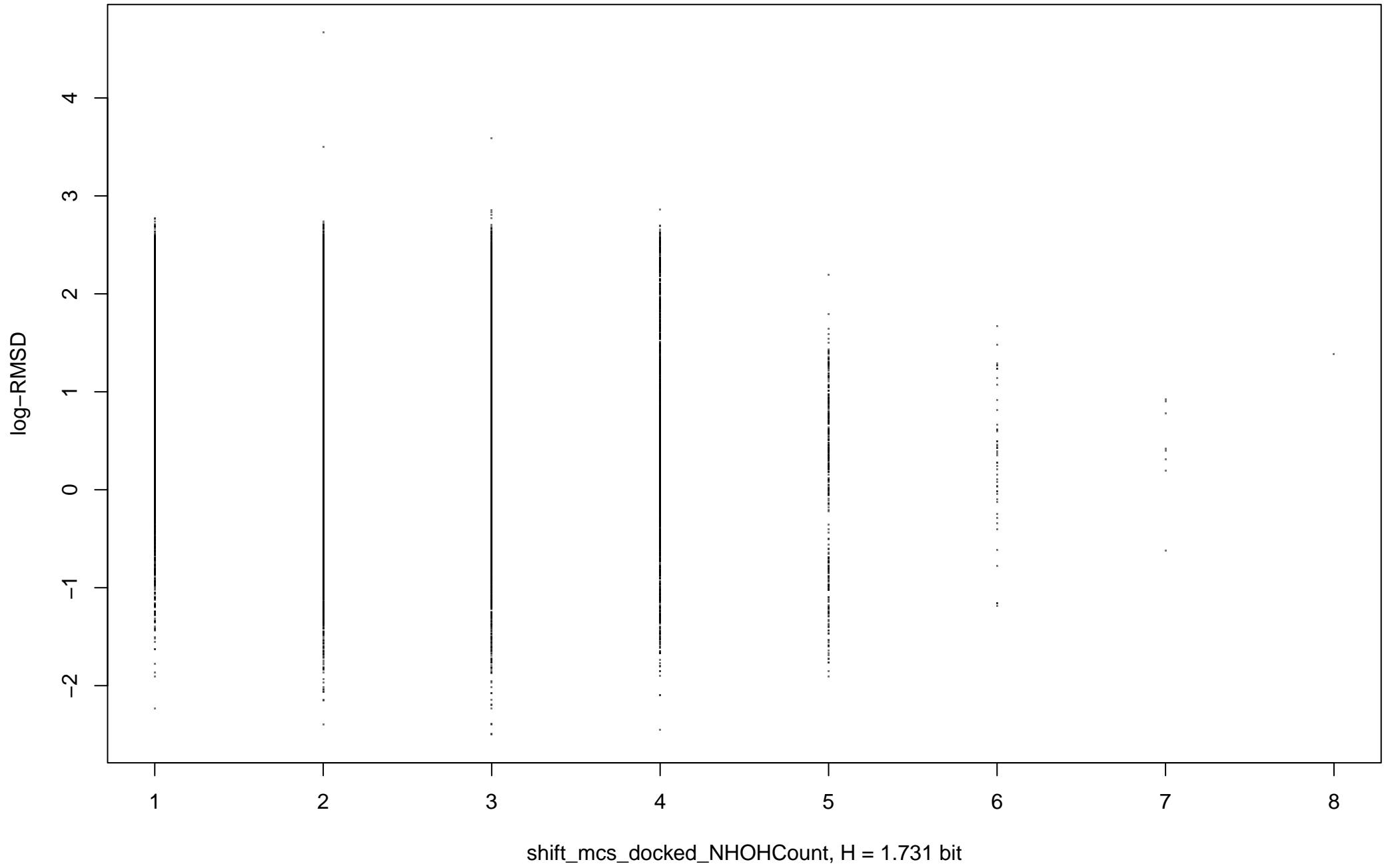
shift_mcs_docked_NumHDonors, MI = 0.1033 bit, norm = 0.05968, cond entr = 4.536 bit



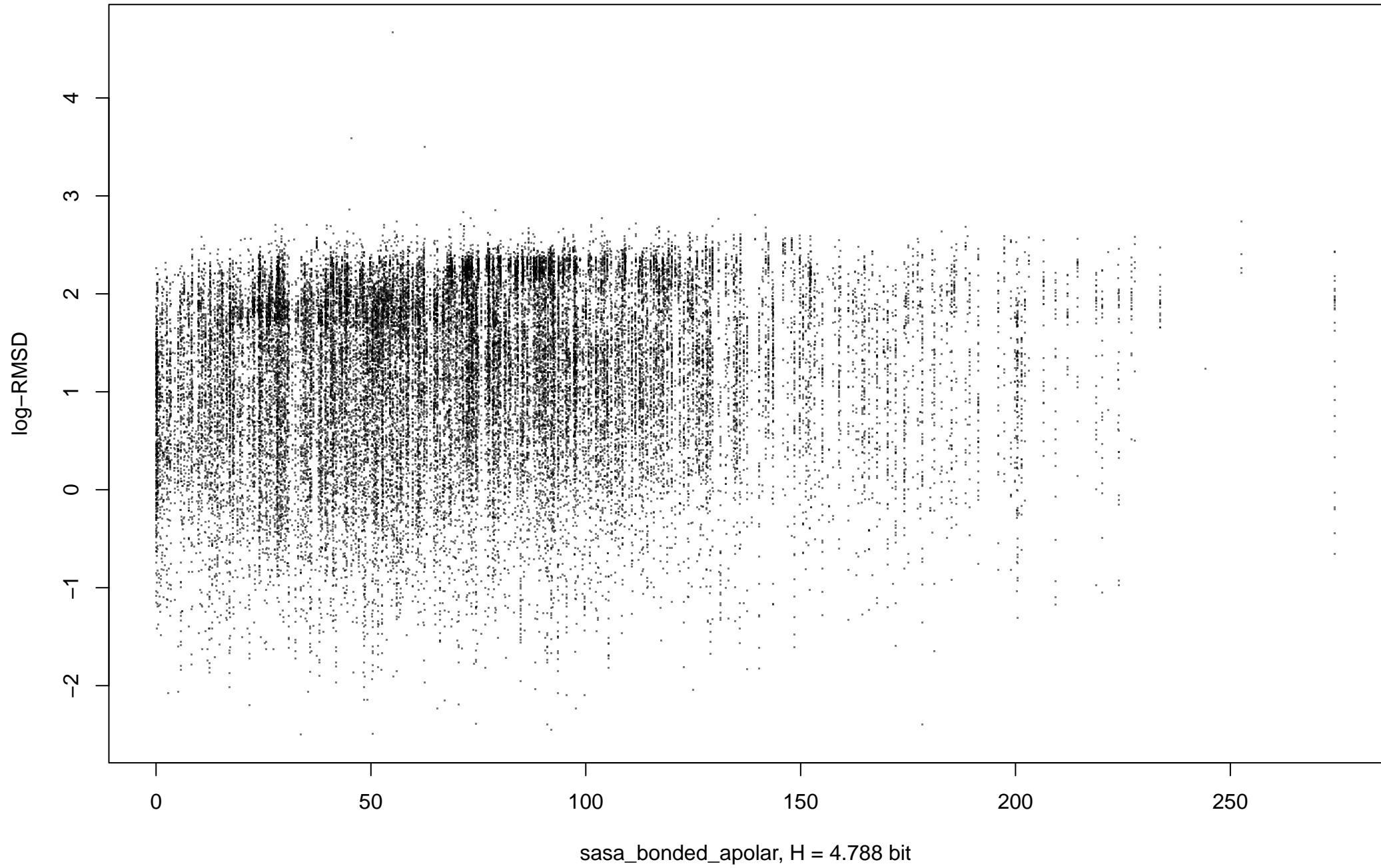
mcs_docked_NHOHCount, MI = 0.1032 bit, norm = 0.05965, cond entr = 4.536 bit



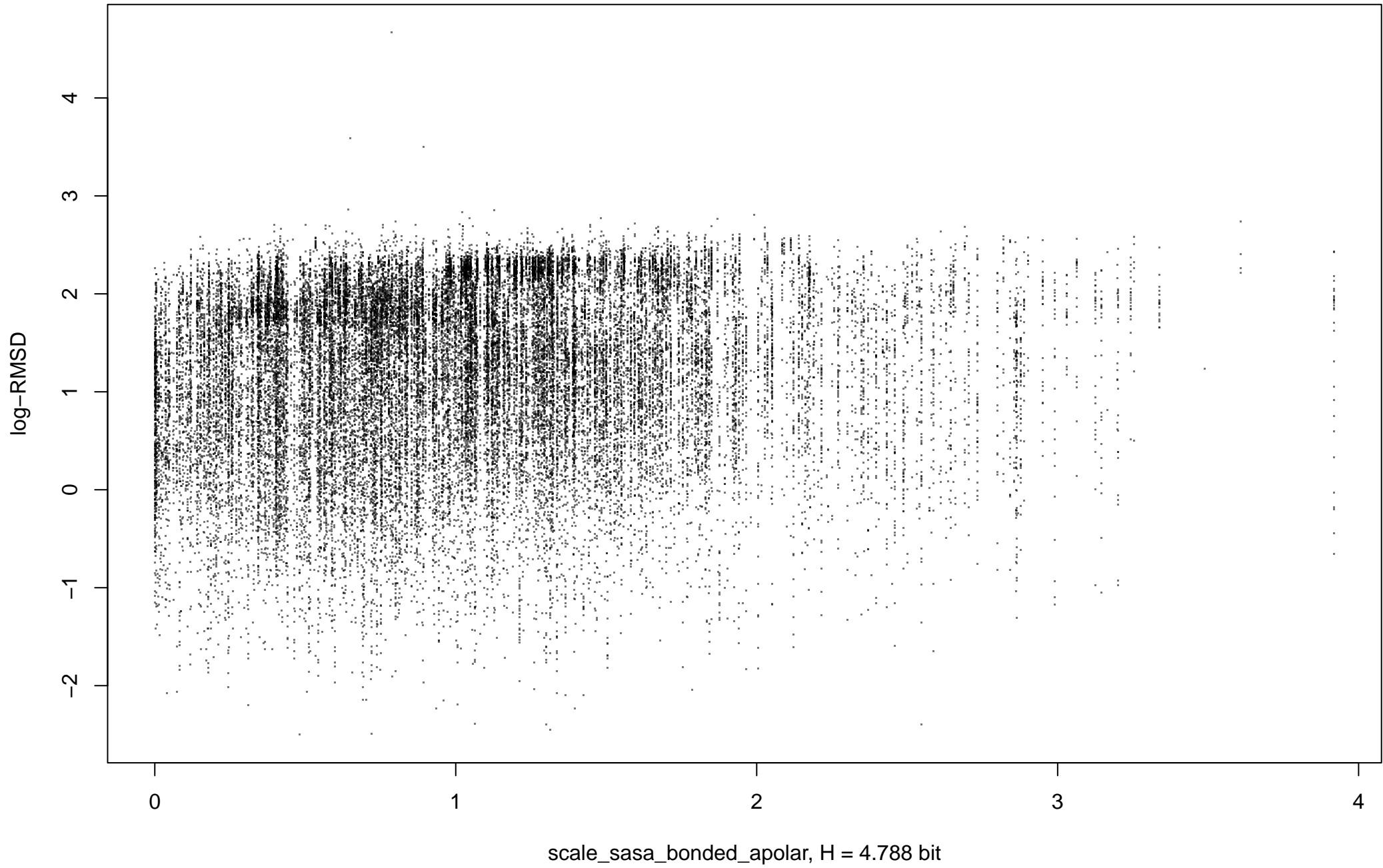
shift_mcs_docked_NHOHCount, MI = 0.1032 bit, norm = 0.05965, cond entr = 4.536 bit



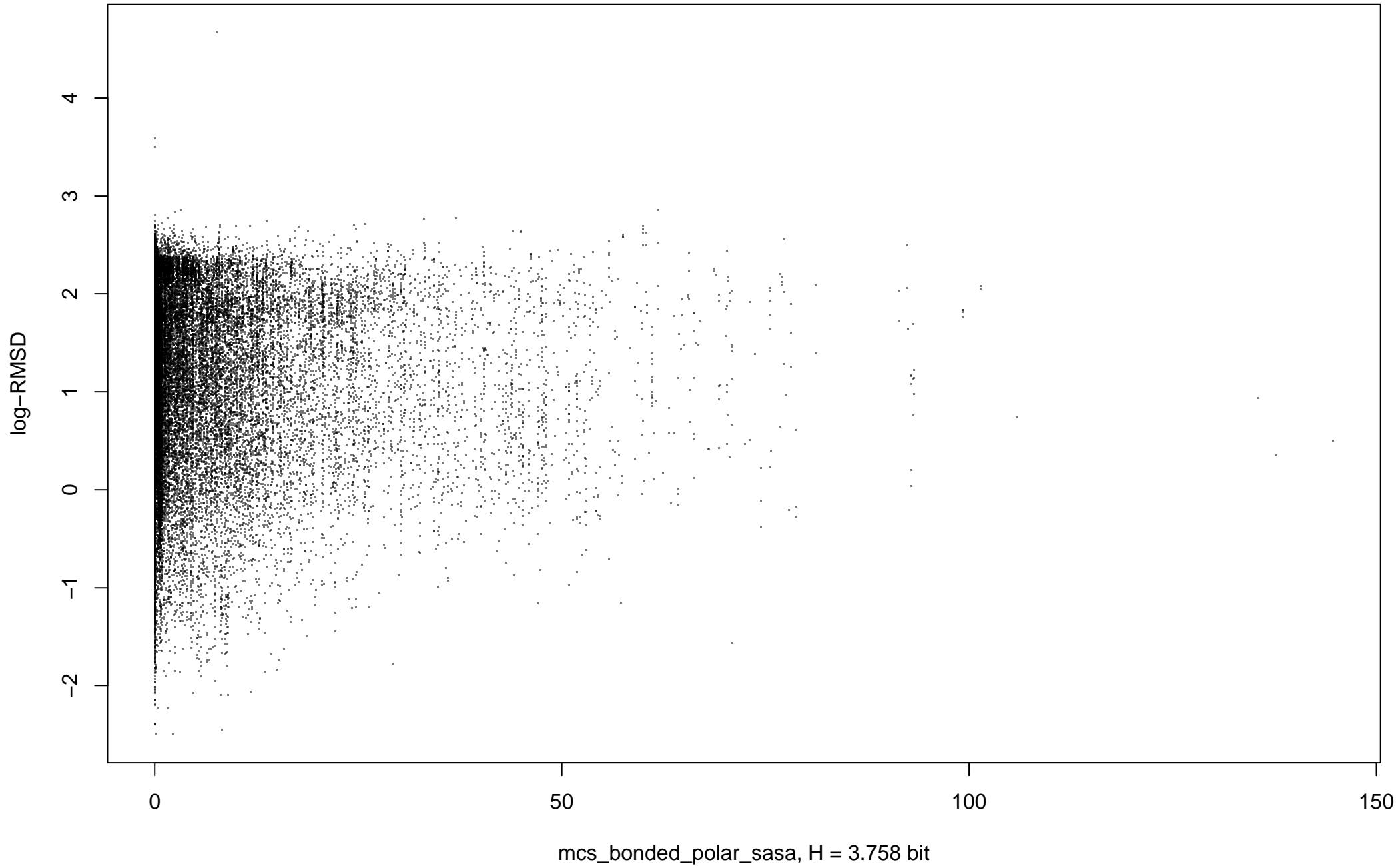
sasa_bonded_apolar, MI = 0.09878 bit, norm = 0.02129, cond entr = 4.541 bit



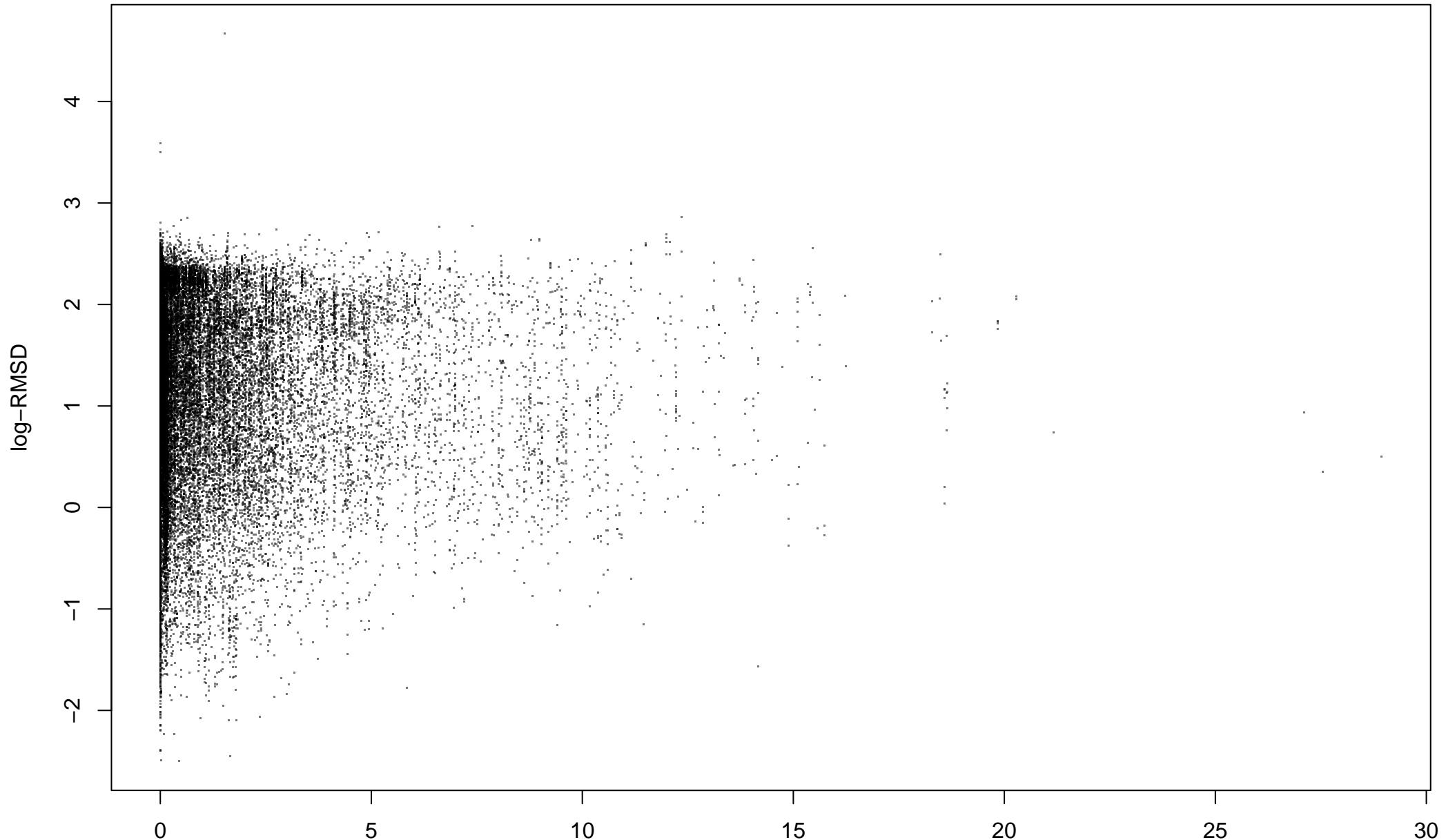
scale_sasa_bonded_apolar, MI = 0.09878 bit, norm = 0.02129, cond entr = 4.541 bit



mcs_bonded_polar_sasa, MI = 0.09754 bit, norm = 0.02595, cond entr = 4.542 bit

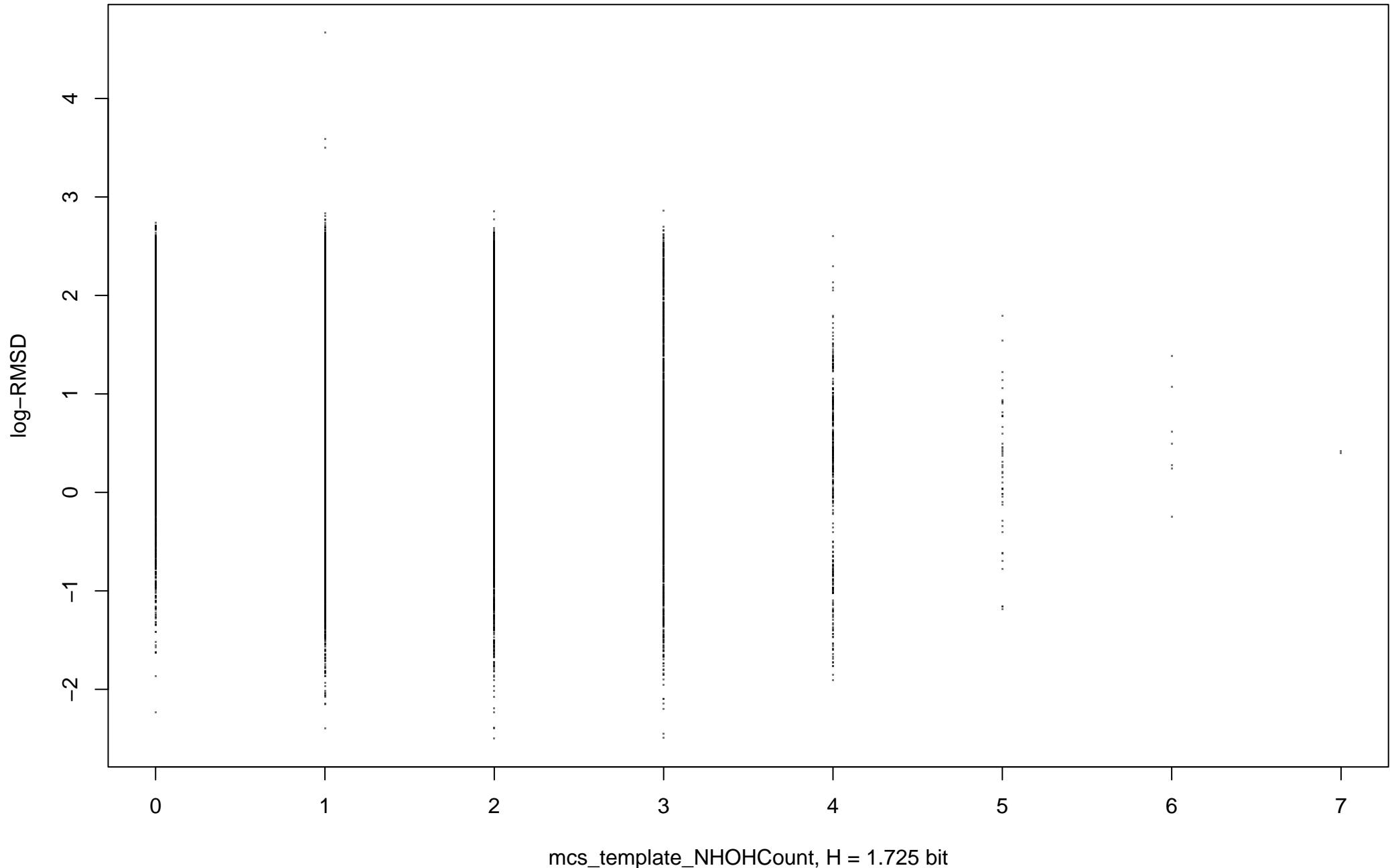


scale_mcs_bonded_polar_sasa, MI = 0.09754 bit, norm = 0.02595, cond entr = 4.542 bit

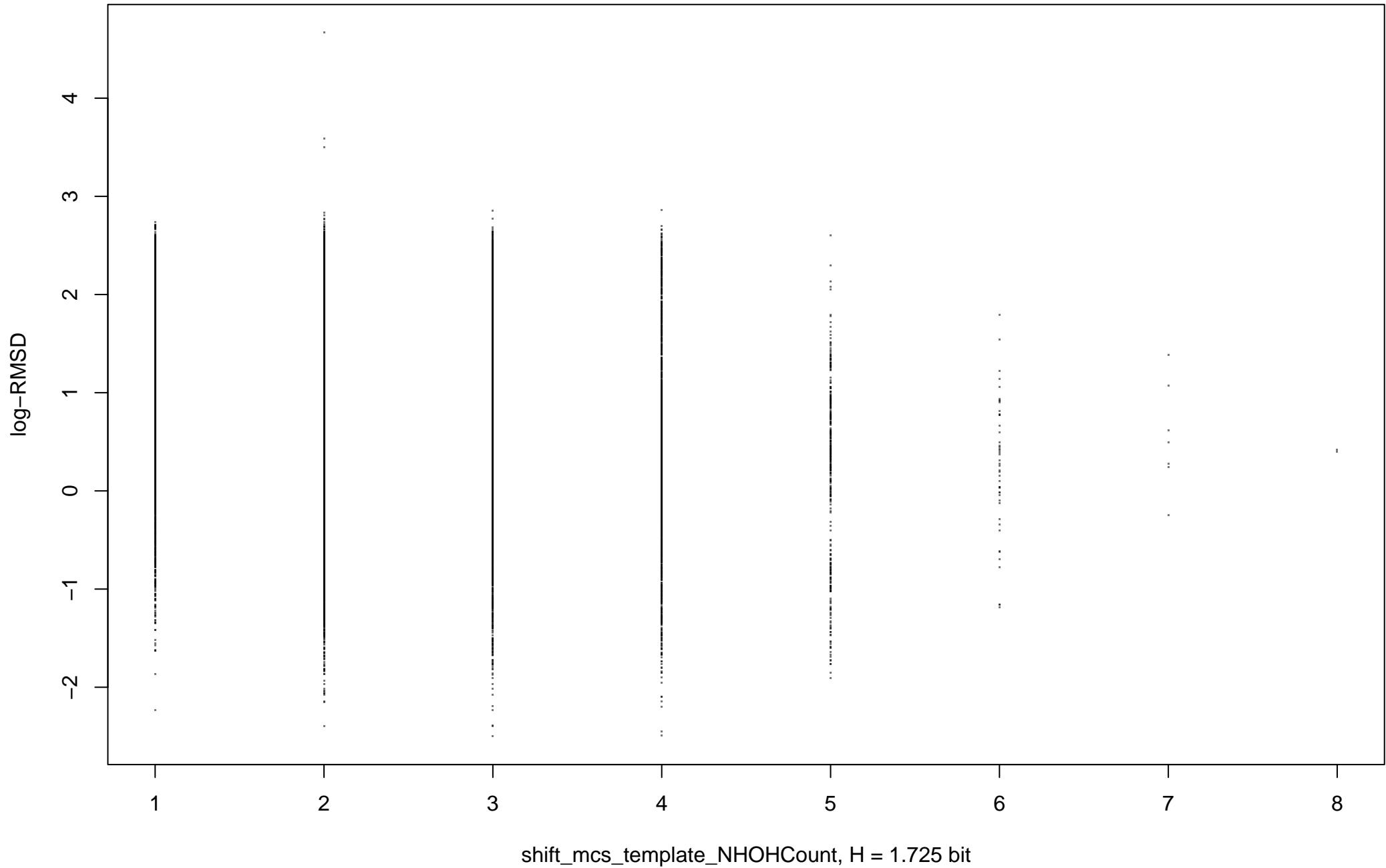


scale_mcs_bonded_polar_sasa, H = 3.758 bit

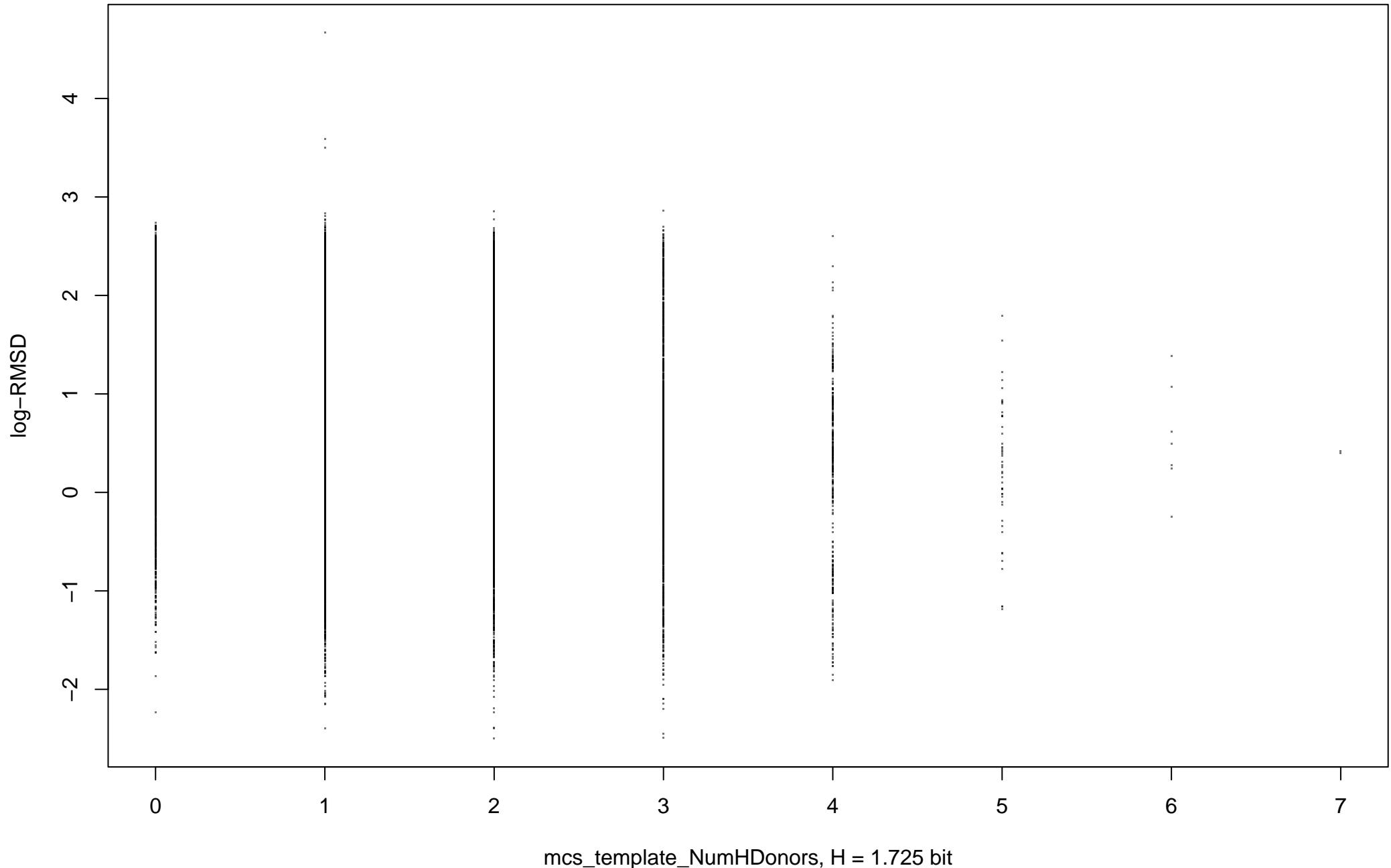
mcs_template_NHOHCount, MI = 0.09586 bit, norm = 0.05556, cond entr = 4.544 bit



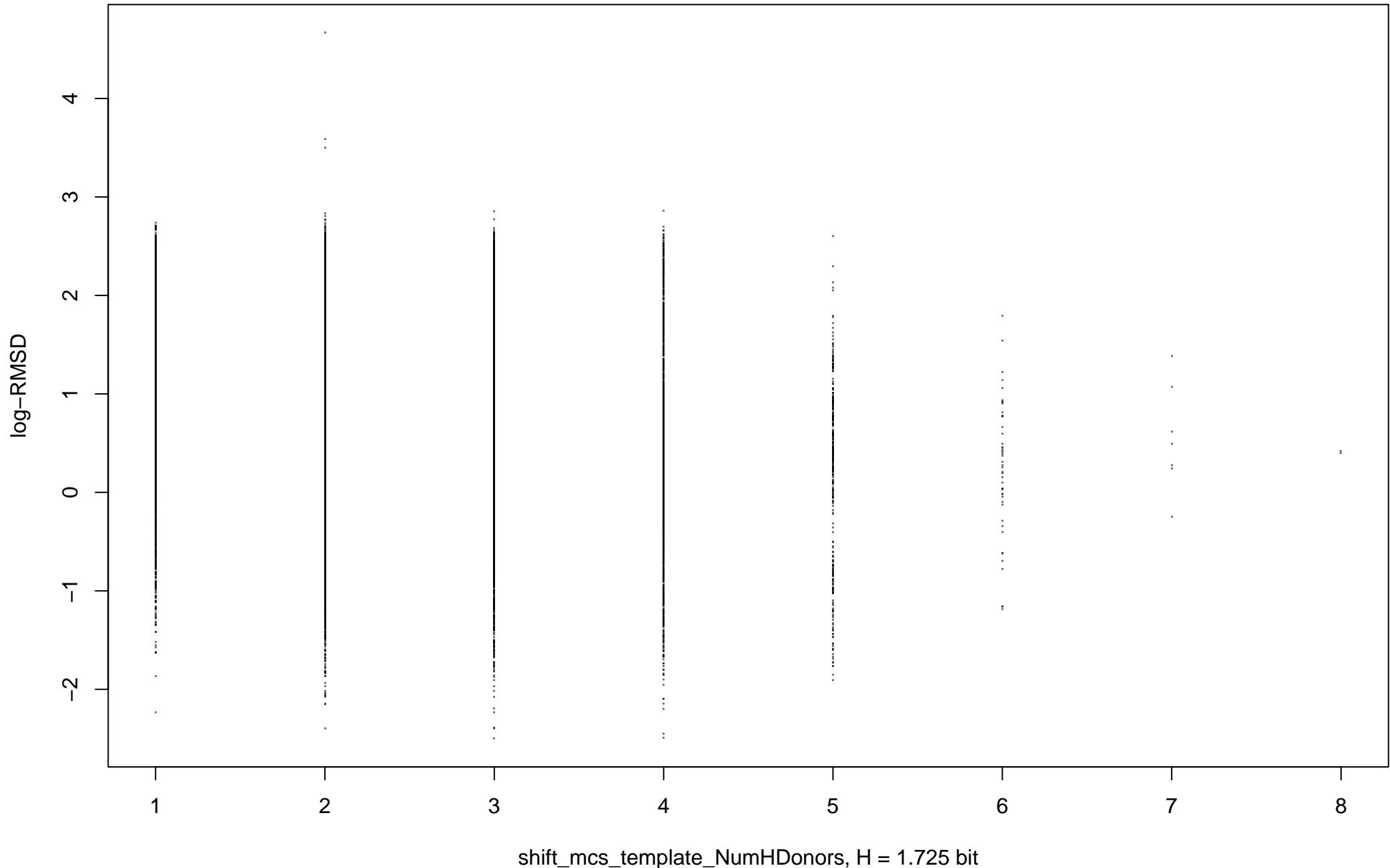
shift_mcs_template_NHOHCount, MI = 0.09586 bit, norm = 0.05556, cond entr = 4.544 bit



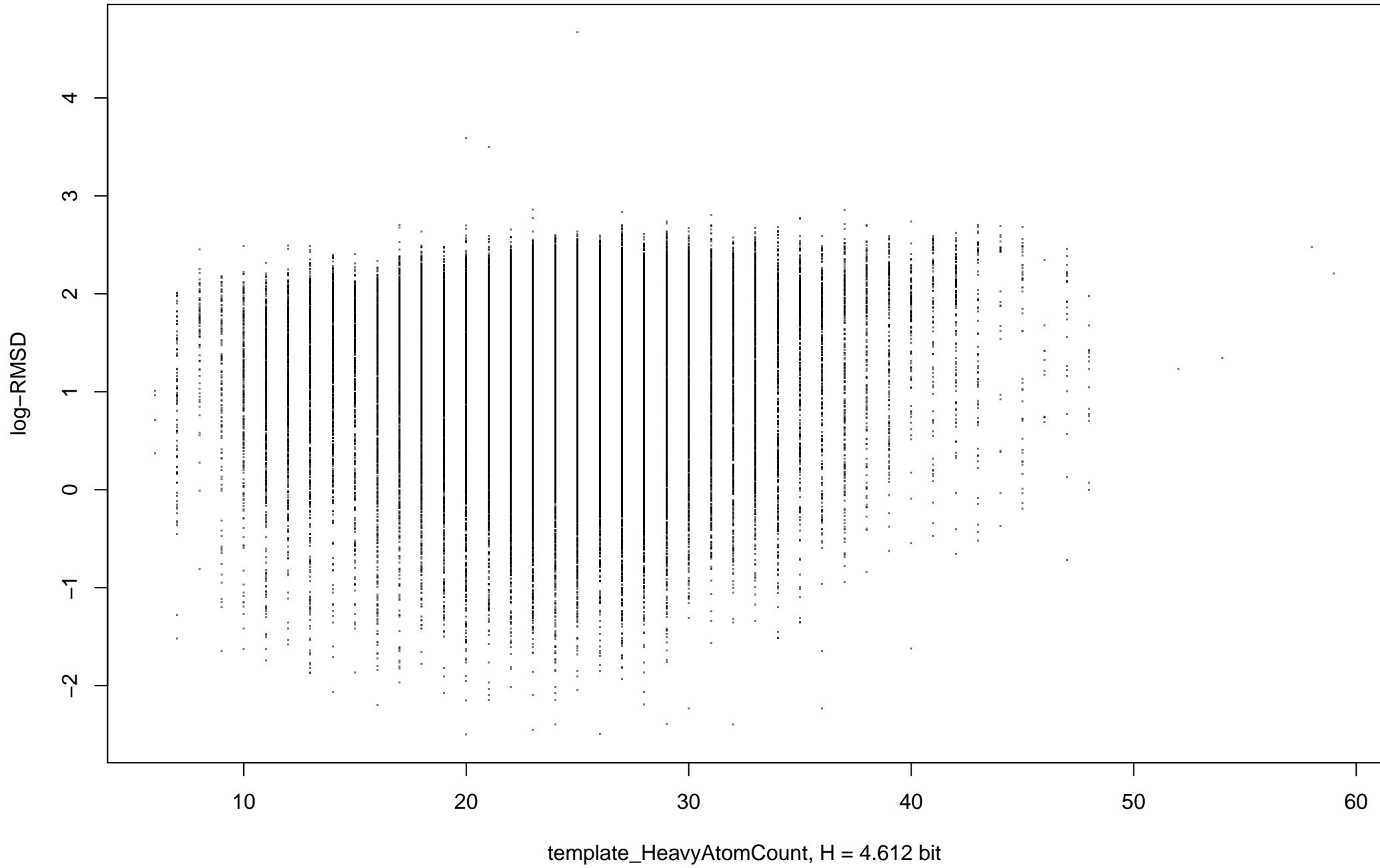
mcs_template_NumHDonors, MI = 0.09572 bit, norm = 0.0555, cond entr = 4.544 bit



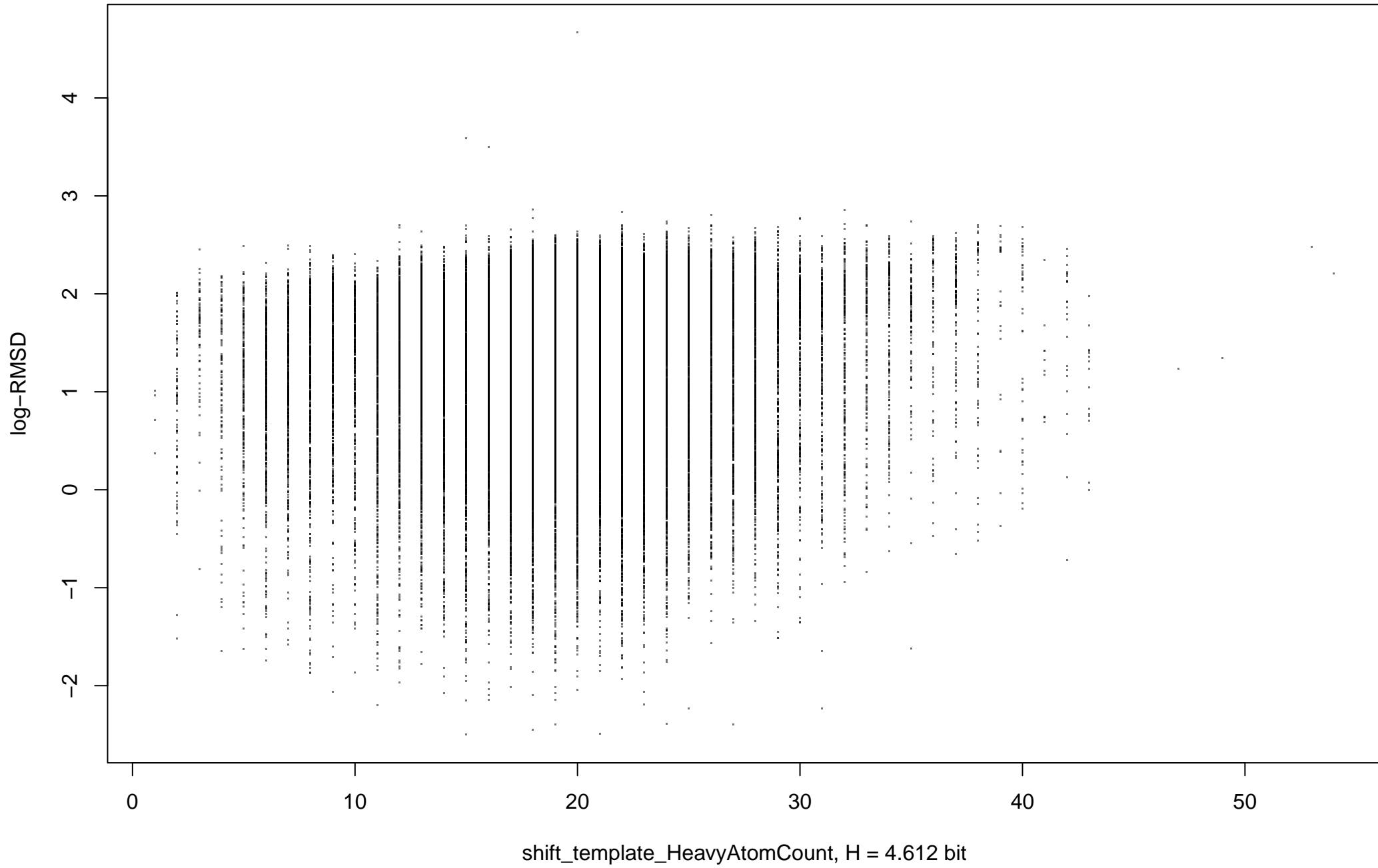
shift_mcs_template_NumHDonors, MI = 0.09572 bit, norm = 0.0555, cond entr = 4.544 bit



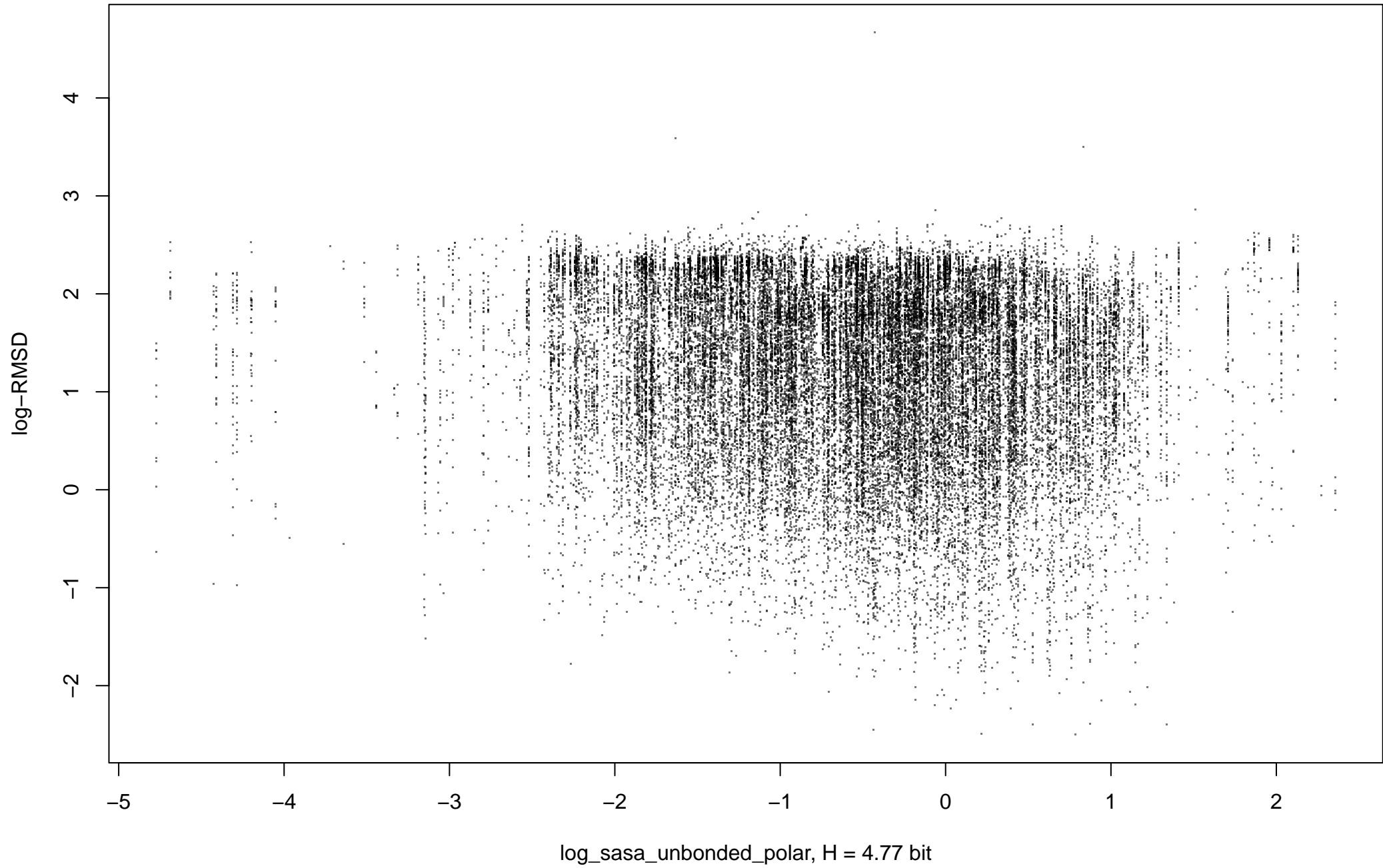
template_HeavyAtomCount, MI = 0.08976 bit, norm = 0.01946, cond entr = 4.55 bit



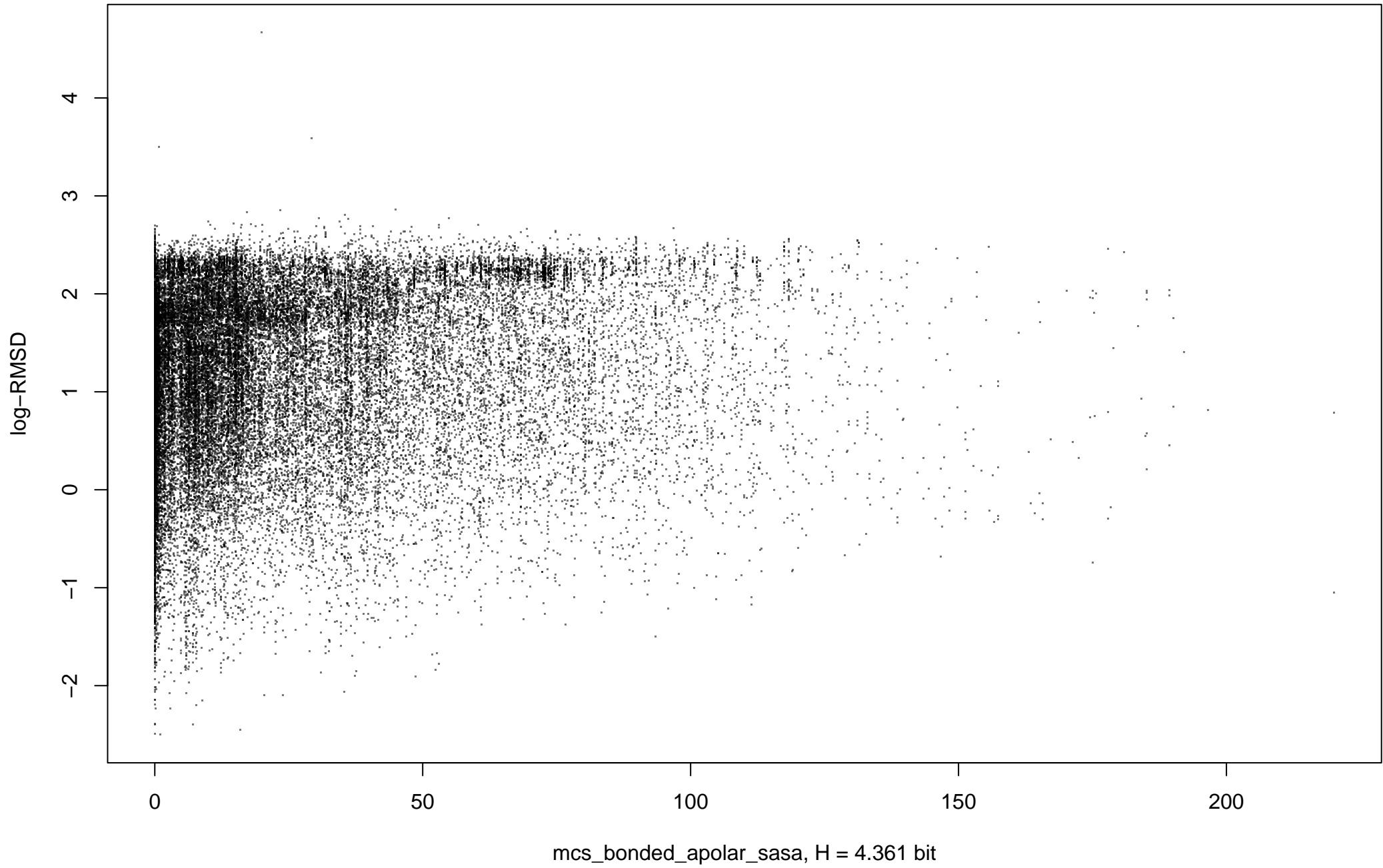
shift_template_HeavyAtomCount, MI = 0.08976 bit, norm = 0.01946, cond entr = 4.55 bit



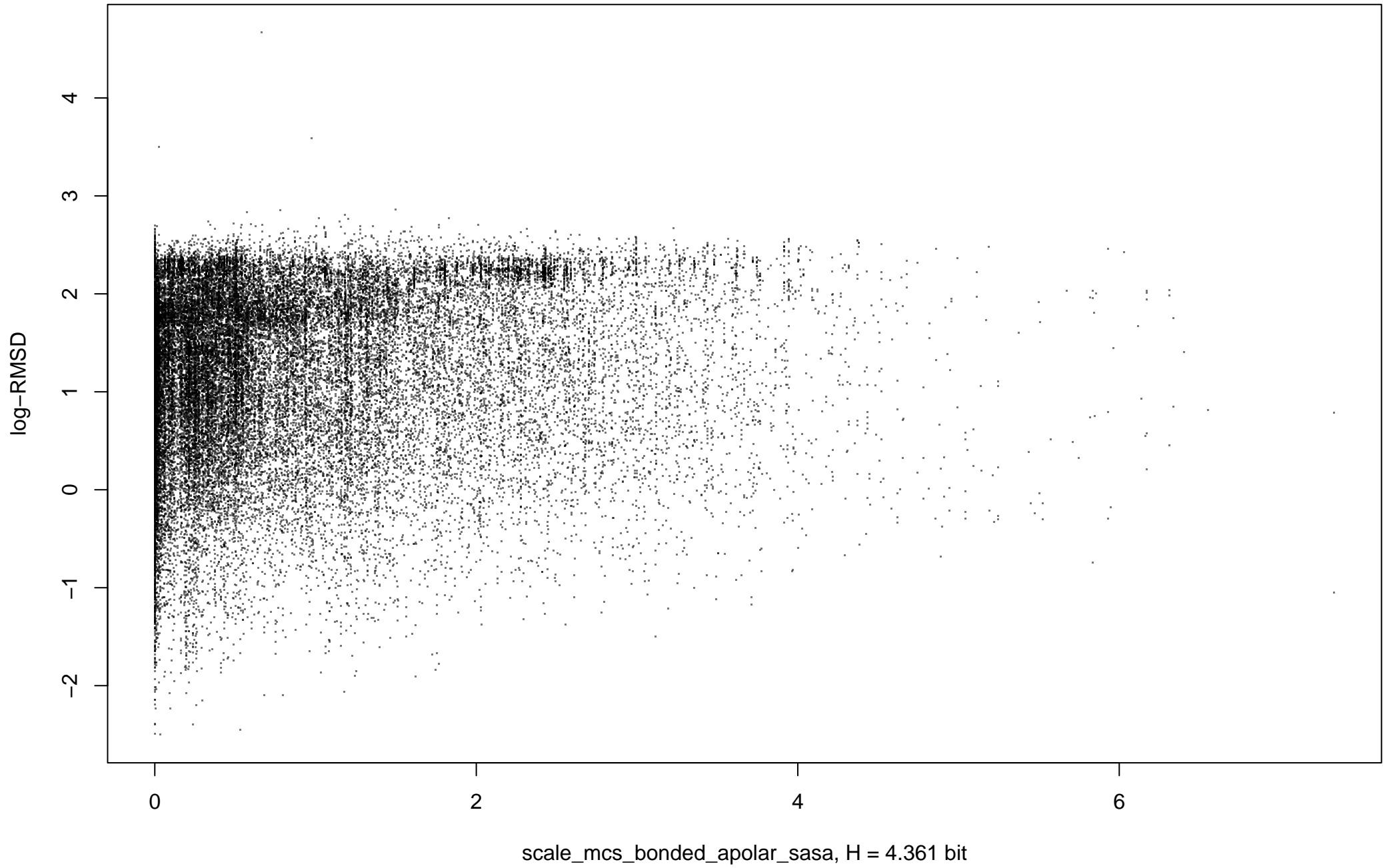
log_sasa_unbonded_polar, MI = 0.08541 bit, norm = 0.01841, cond entr = 4.554 bit



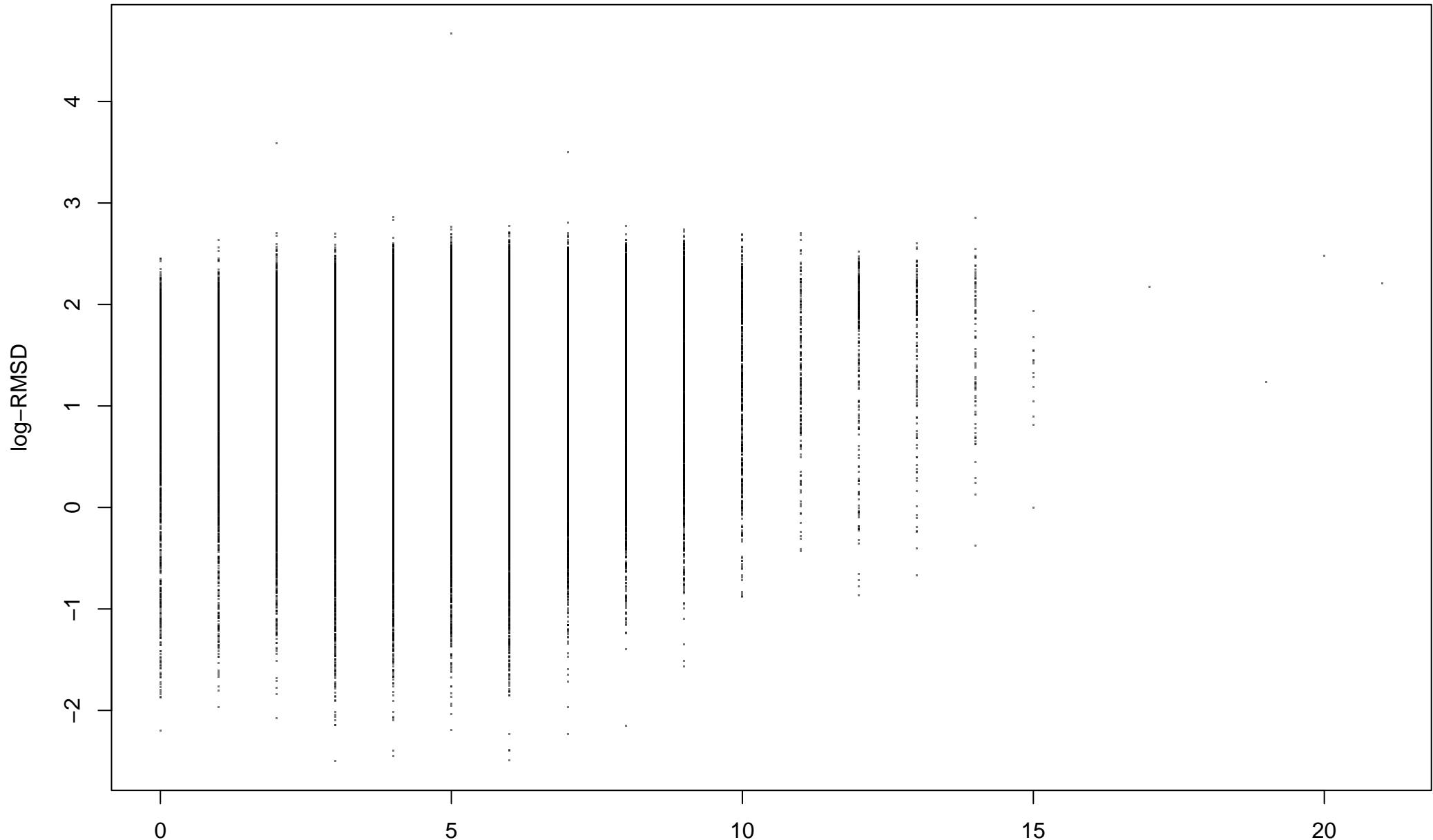
mcs_bonded_apolar_sasa, MI = 0.08474 bit, norm = 0.01943, cond entr = 4.555 bit



scale_mcs_bonded_apolar_sasa, MI = 0.08474 bit, norm = 0.01943, cond entr = 4.555 bit

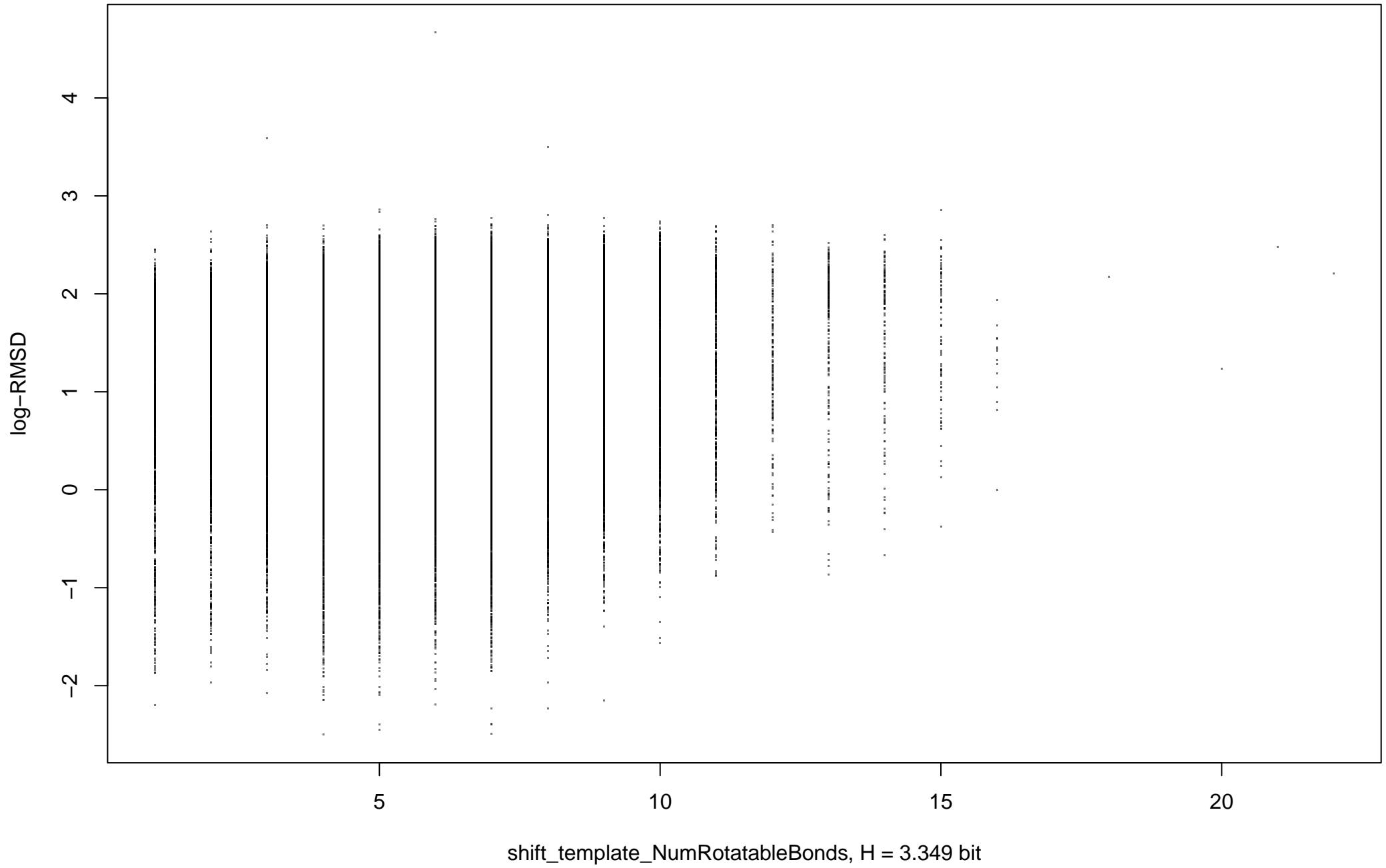


template_NumRotatableBonds, MI = 0.08426 bit, norm = 0.02516, cond entr = 4.555 bit

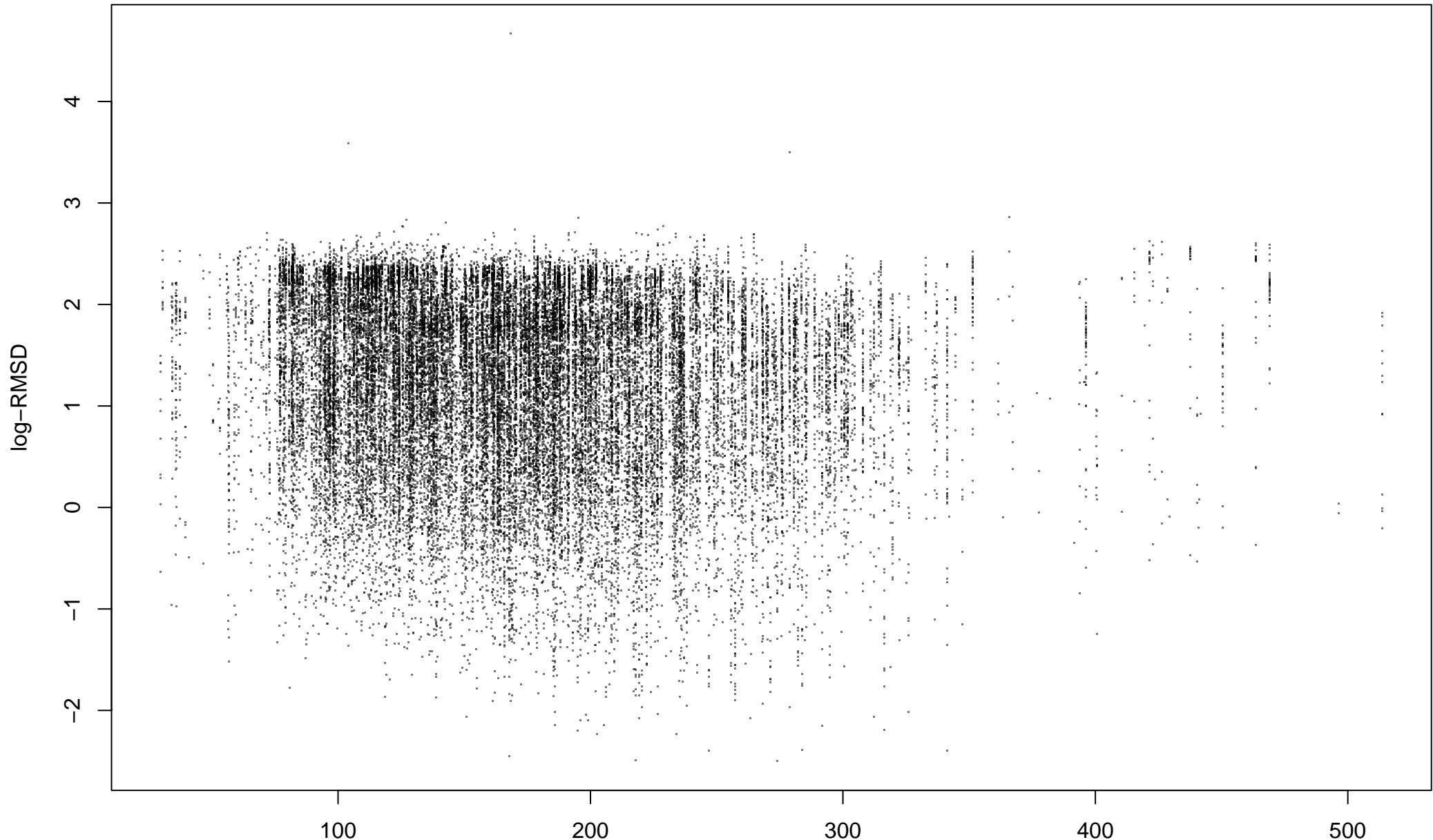


template_NumRotatableBonds, H = 3.349 bit

shift_template_NumRotatableBonds, MI = 0.08426 bit, norm = 0.02516, cond entr = 4.555 bit

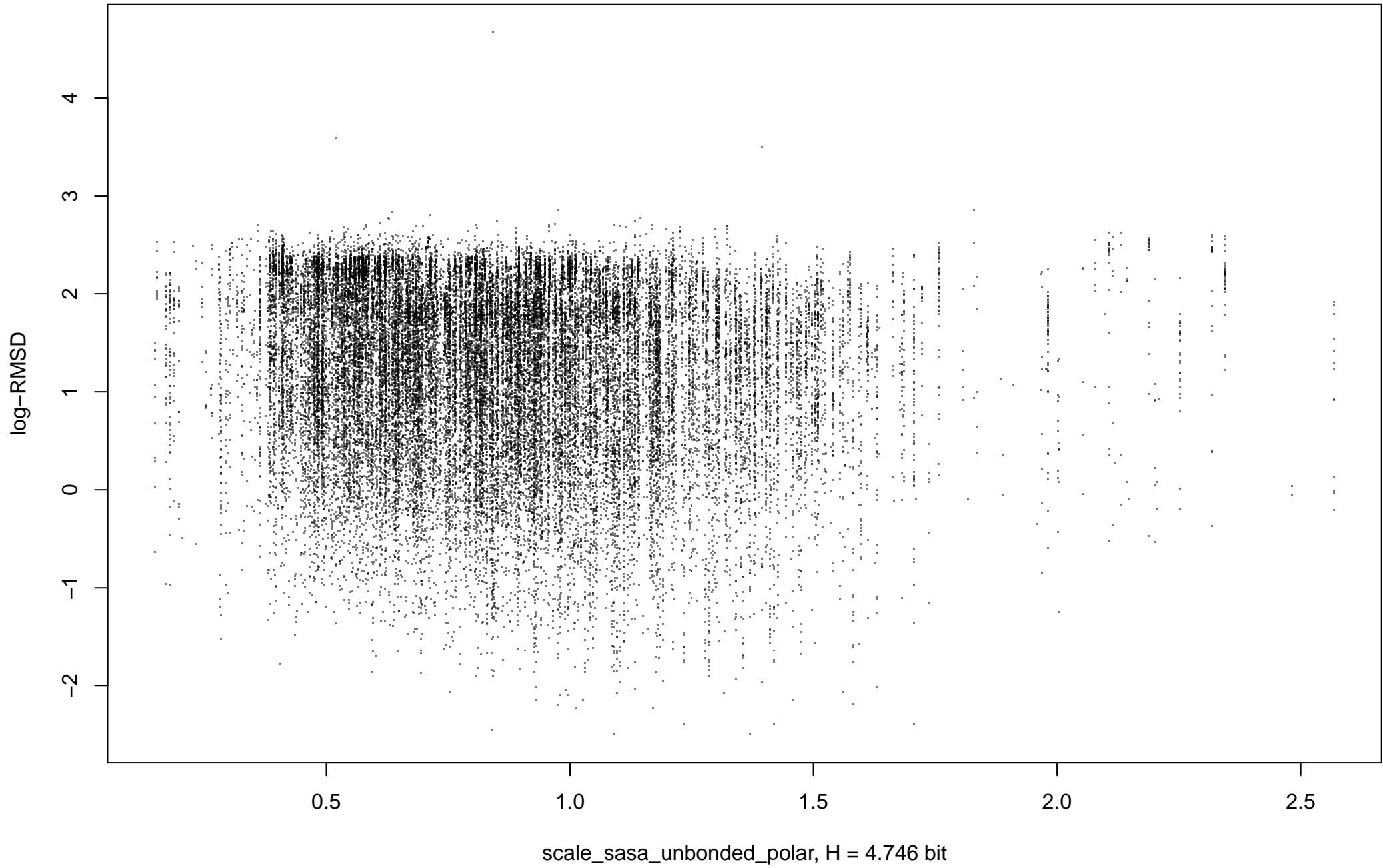


sasa_unbonded_polar, MI = 0.08421 bit, norm = 0.01815, cond entr = 4.555 bit

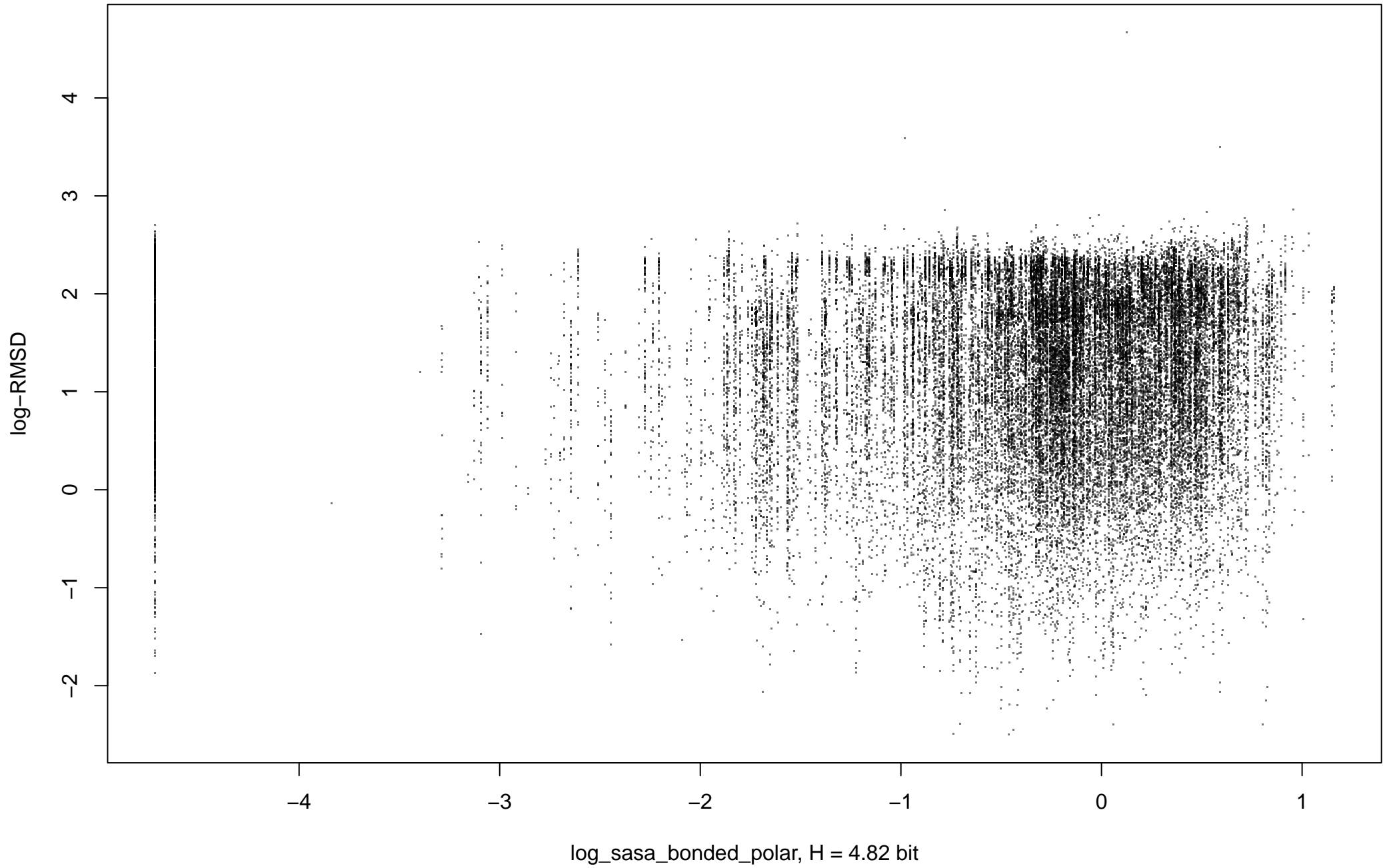


sasa_unbonded_polar, H = 4.746 bit

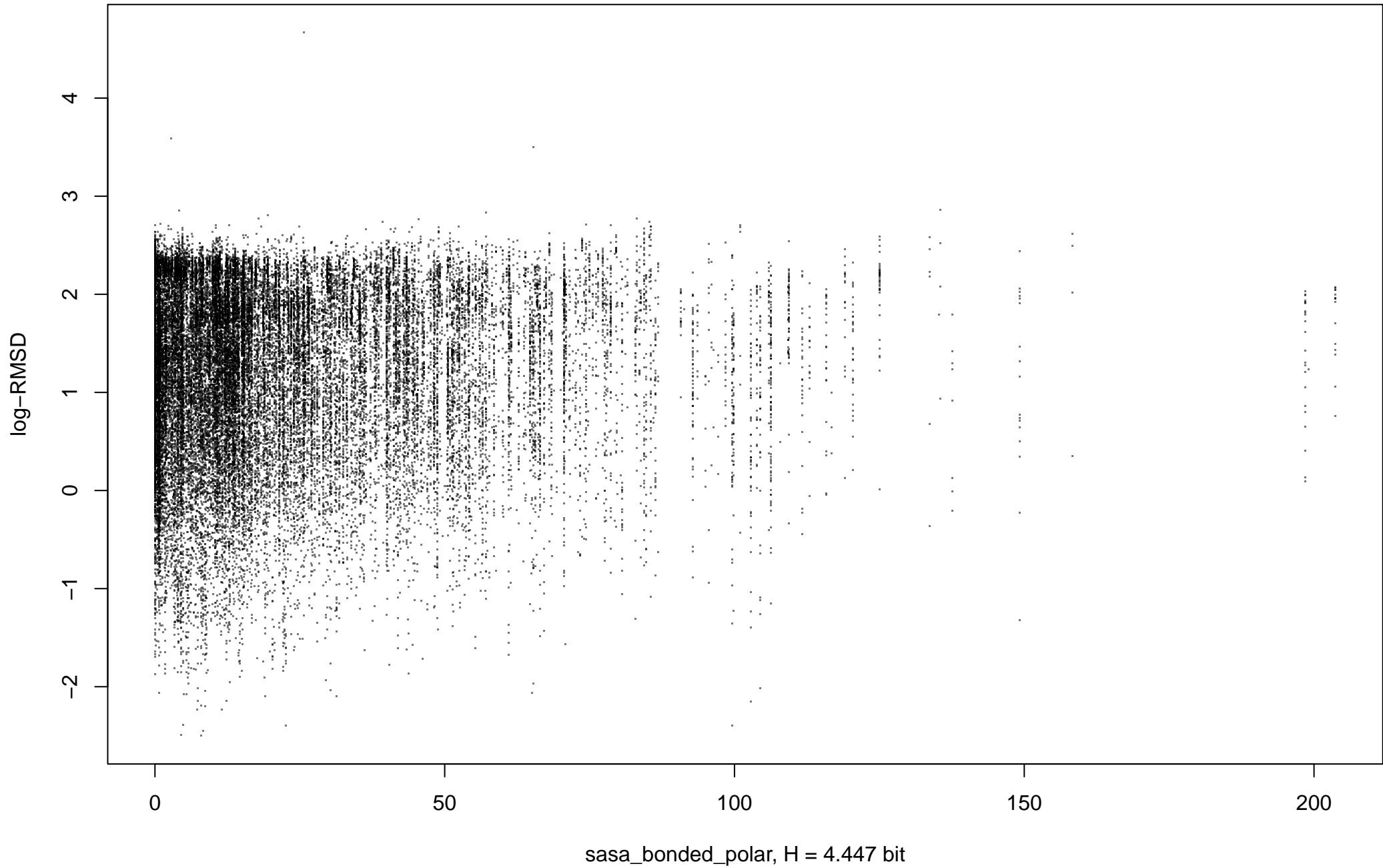
scale_sasa_unbonded_polar, MI = 0.08421 bit, norm = 0.01815, cond entr = 4.555 bit



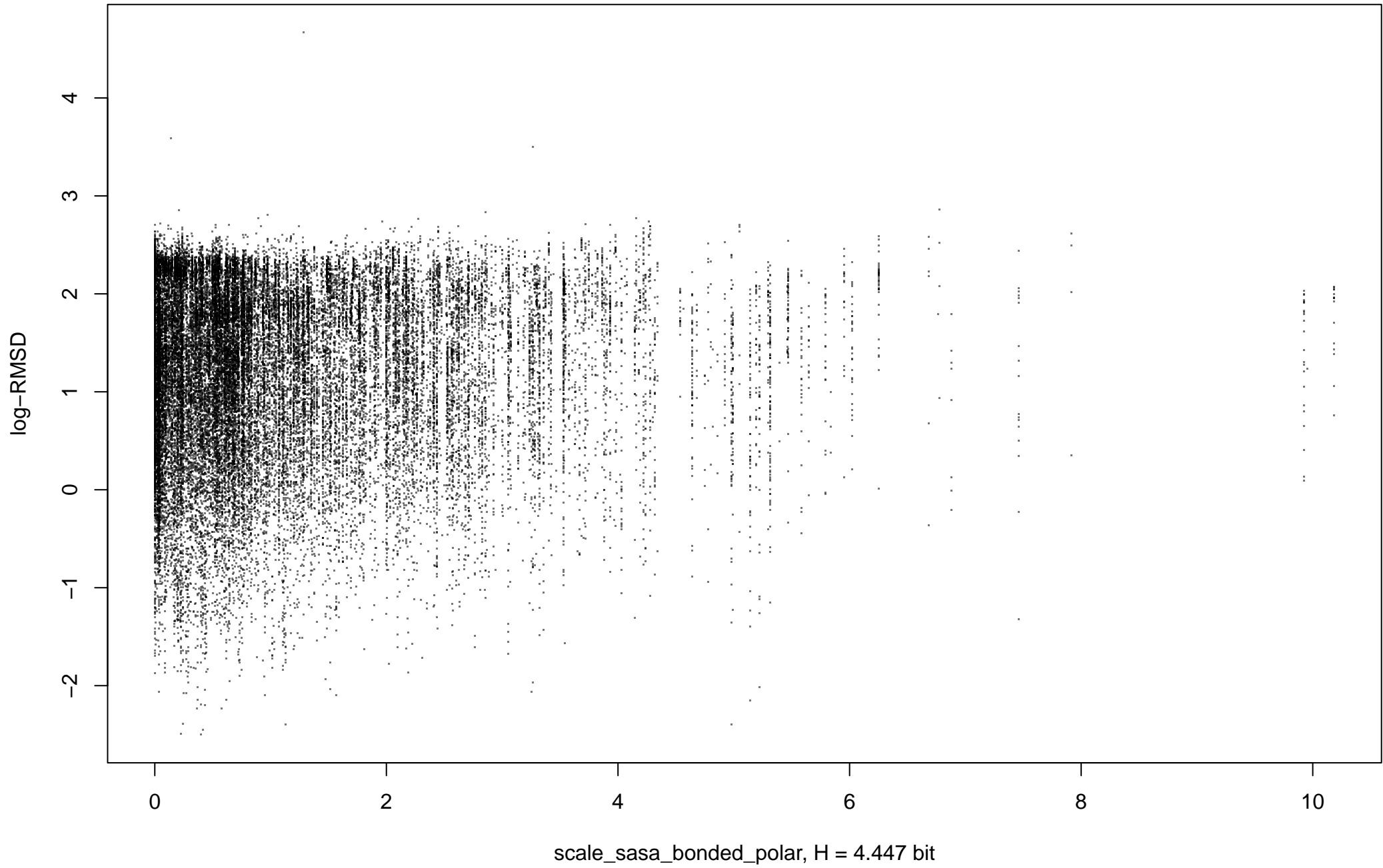
log_sasa_bonded_polar, MI = 0.07997 bit, norm = 0.01724, cond entr = 4.56 bit



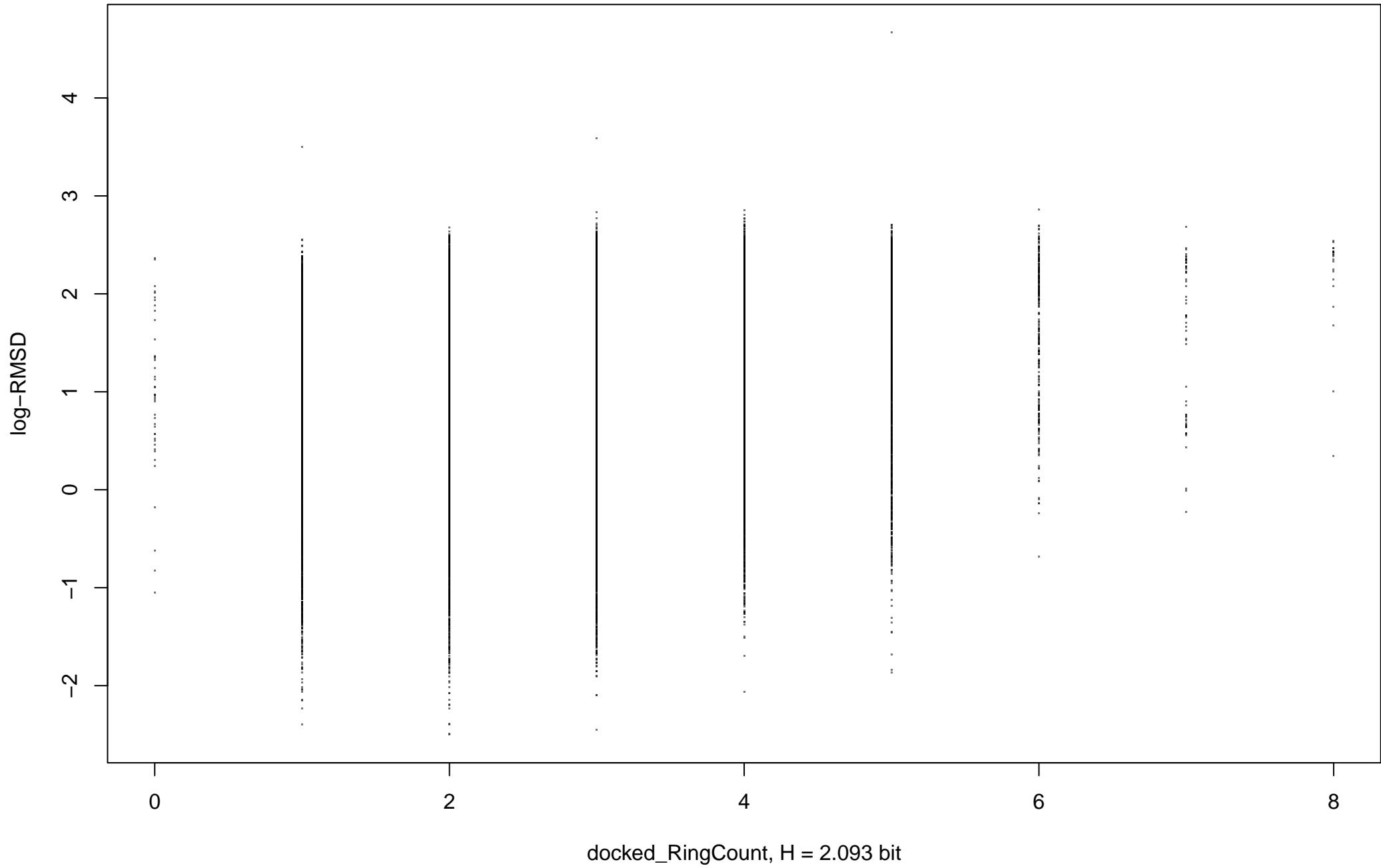
sasa_bonded_polar, MI = 0.07087 bit, norm = 0.01594, cond entr = 4.569 bit



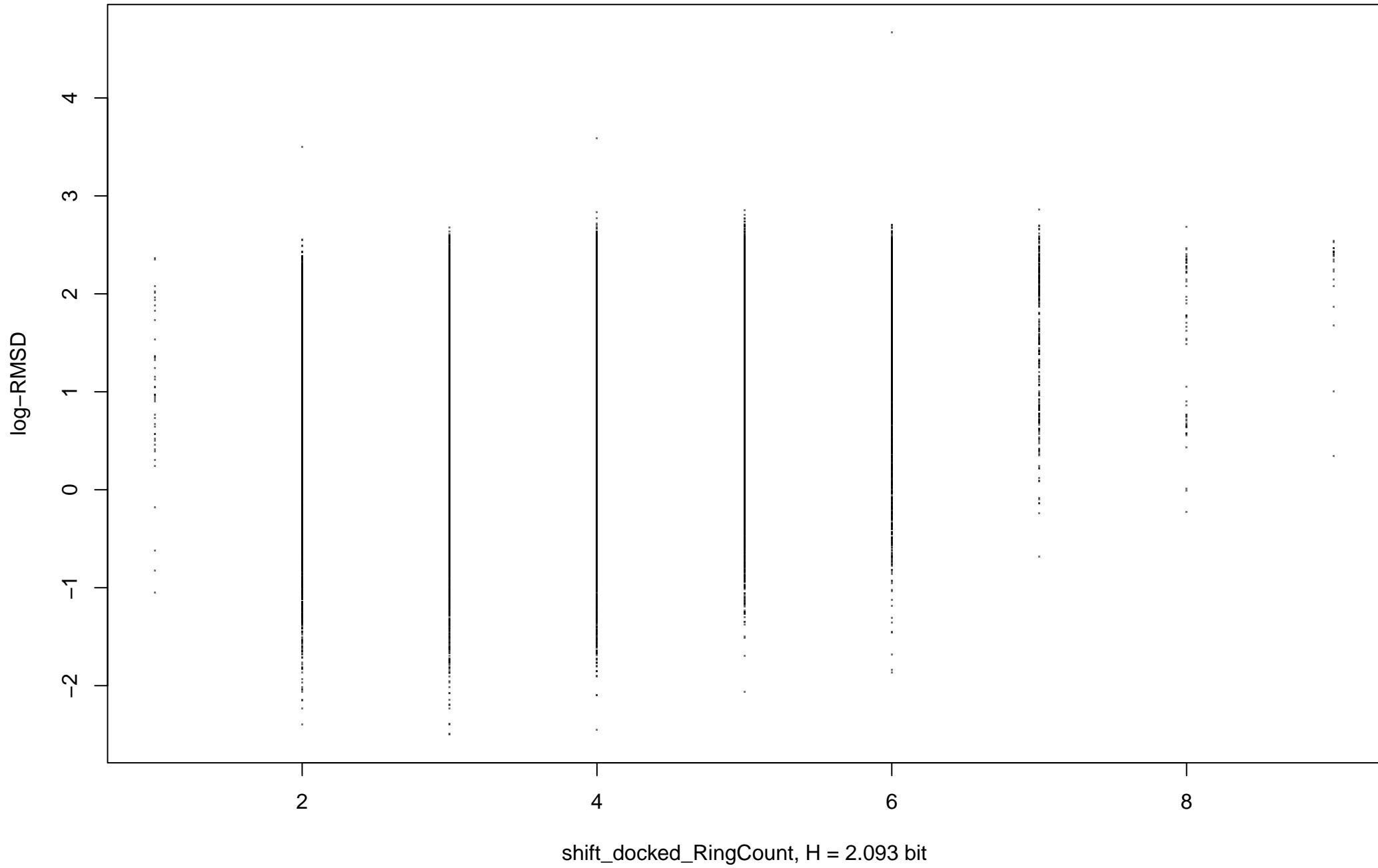
scale_sasa_bonded_polar, MI = 0.07087 bit, norm = 0.01594, cond entr = 4.569 bit



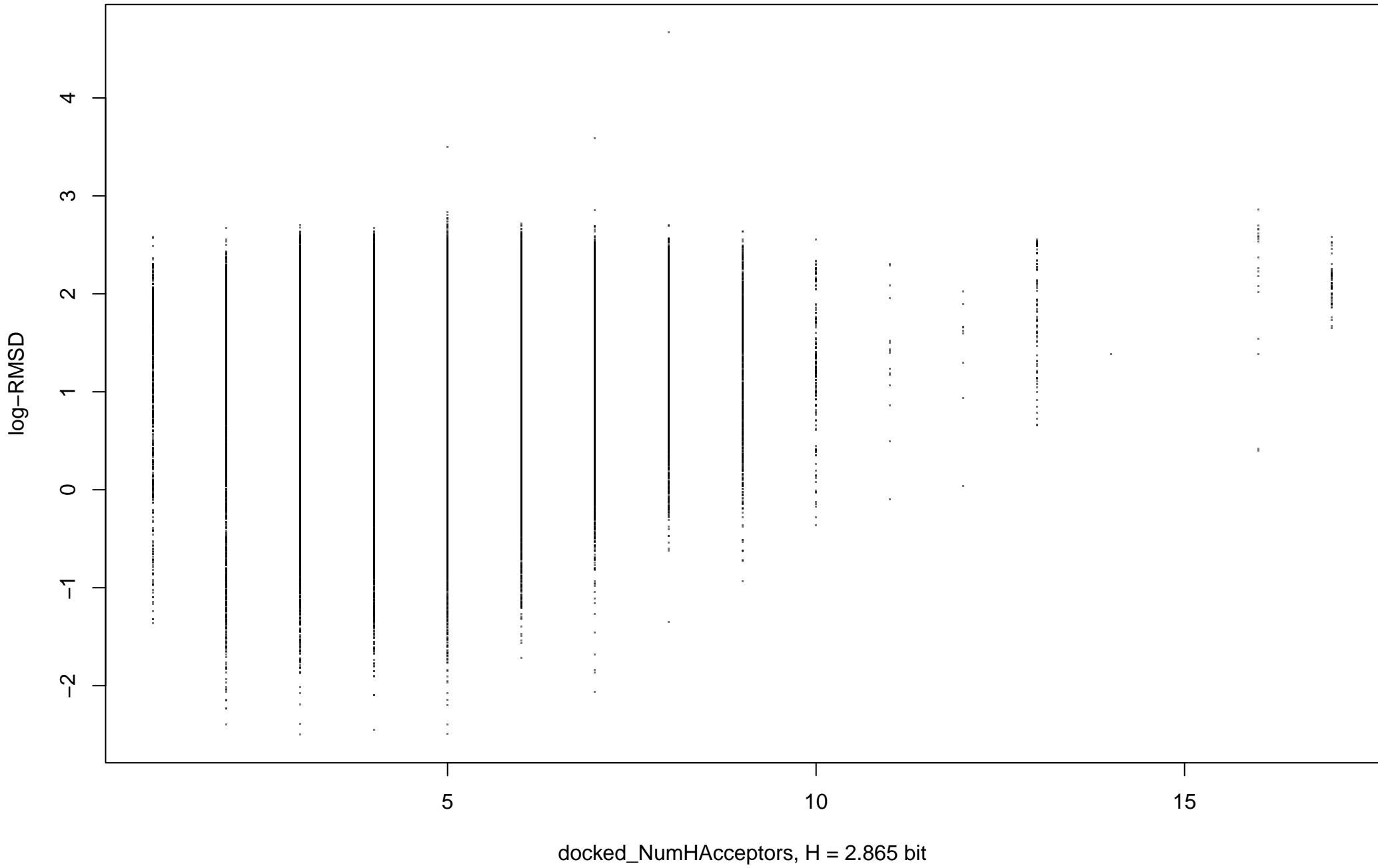
docked_RingCount, MI = 0.06292 bit, norm = 0.03006, cond entr = 4.577 bit



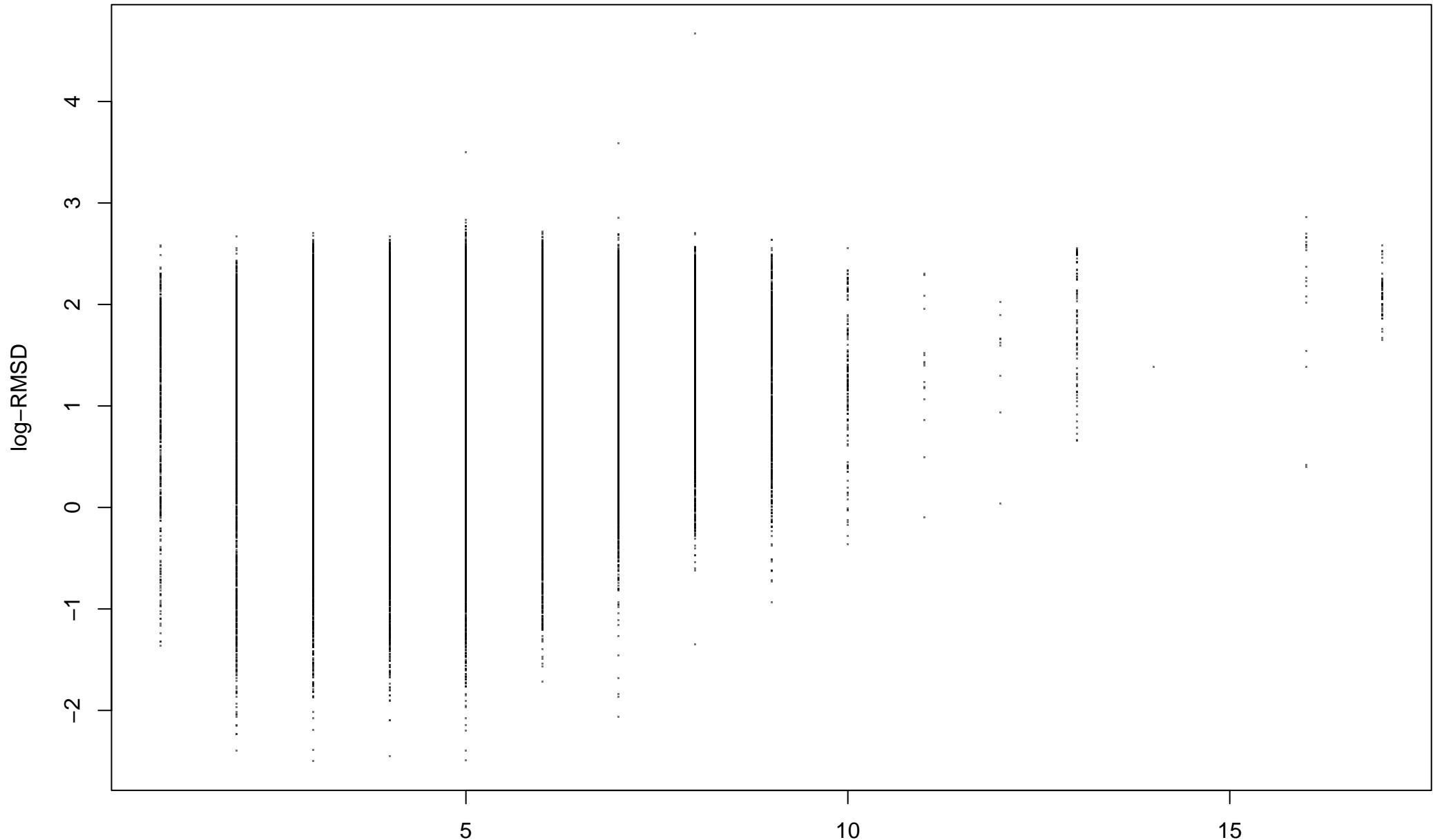
shift_docked_RingCount, MI = 0.06292 bit, norm = 0.03006, cond entr = 4.577 bit



docked_NumHAcceptors, MI = 0.05858 bit, norm = 0.02044, cond entr = 4.581 bit

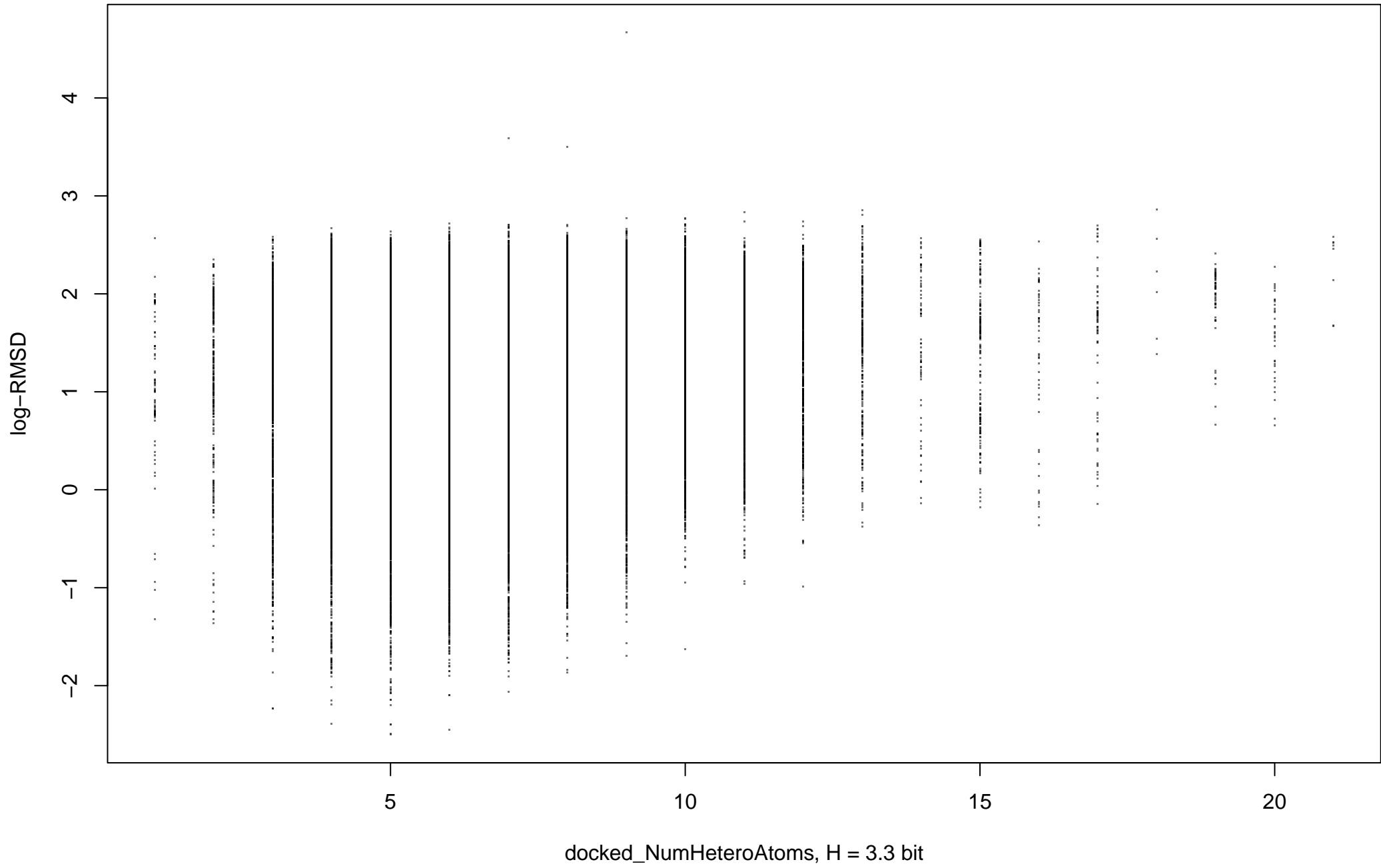


shift_docked_NumHAcceptors, MI = 0.05858 bit, norm = 0.02044, cond entr = 4.581 bit

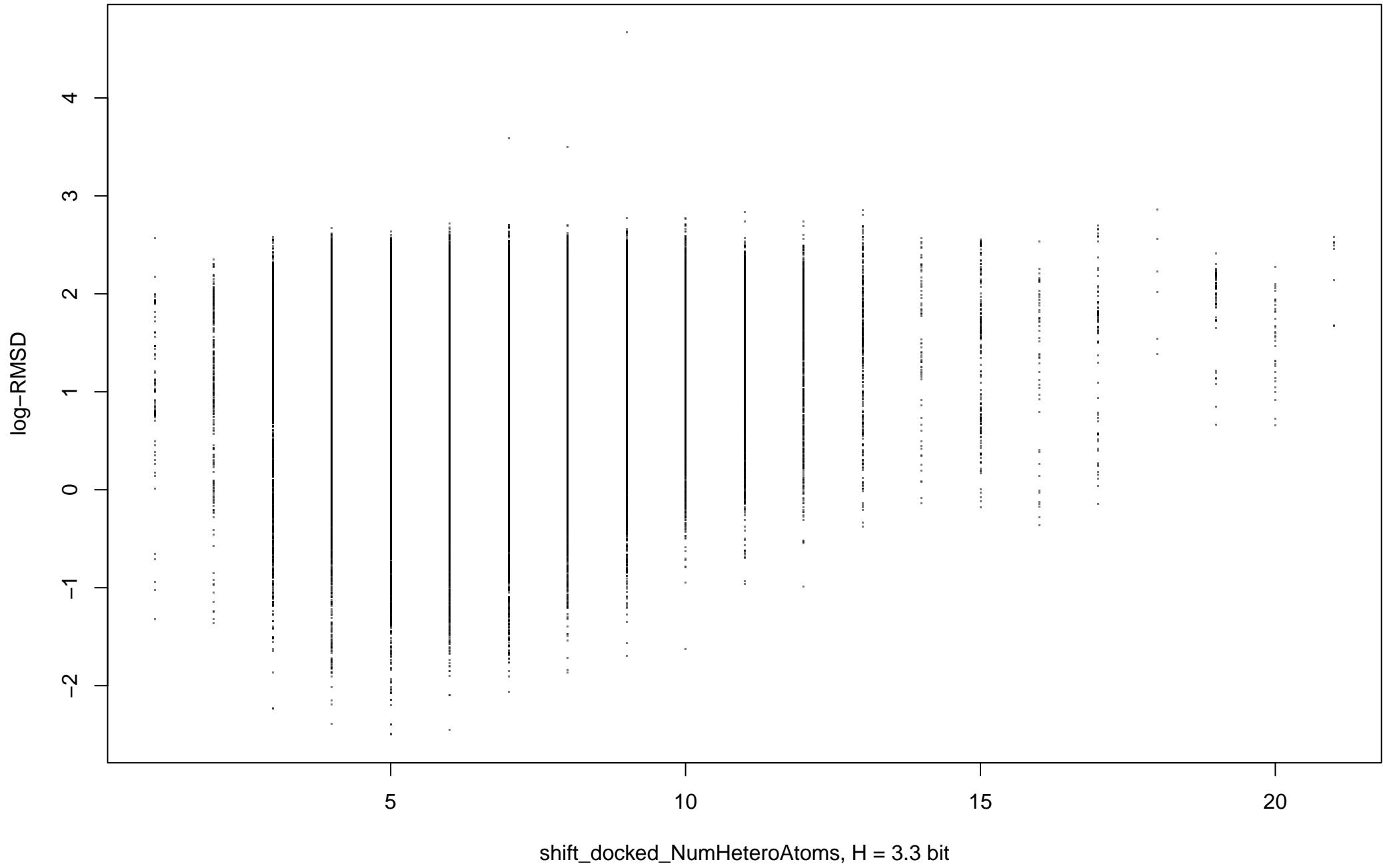


shift_docked_NumHAcceptors, H = 2.865 bit

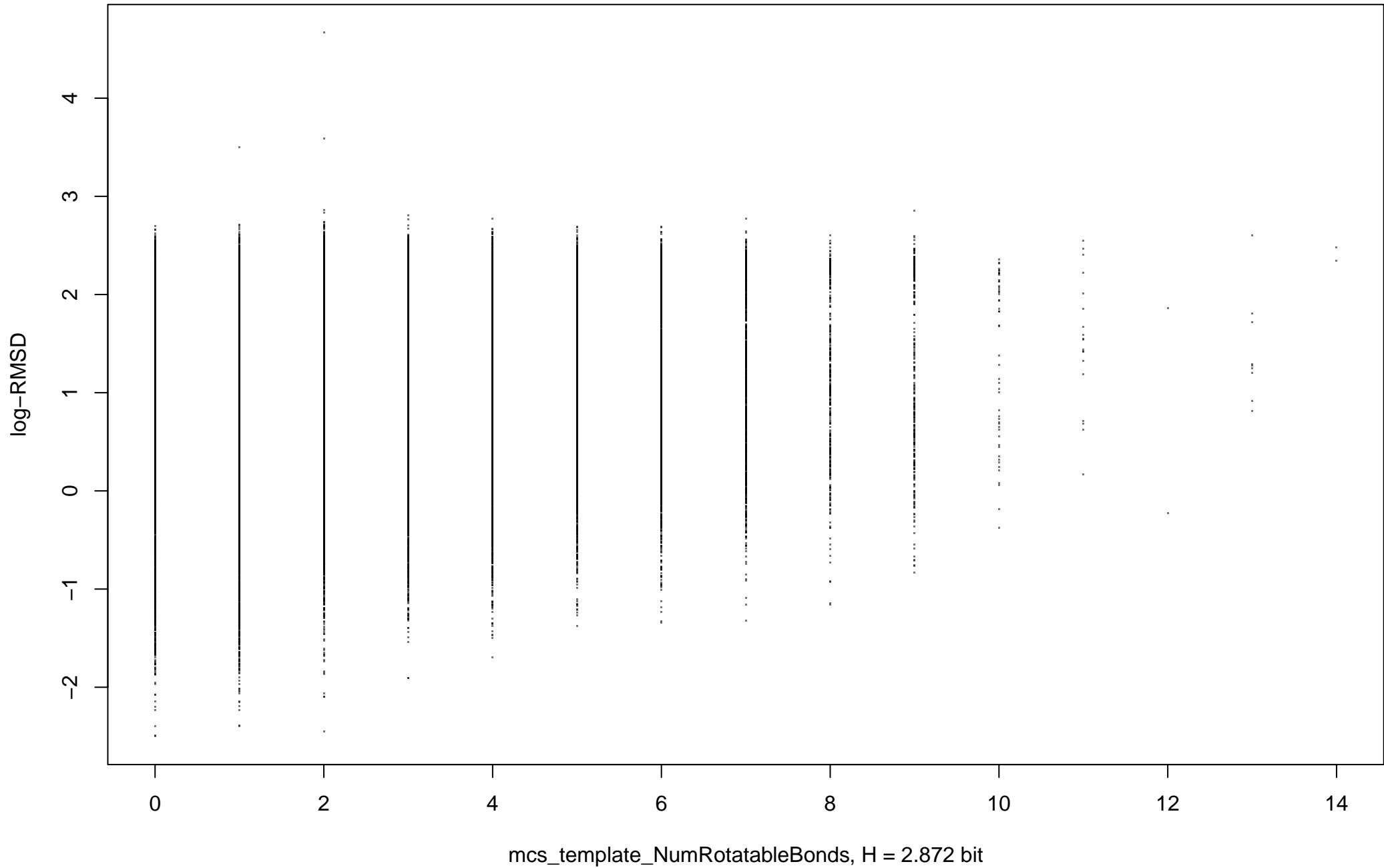
docked_NumHeteroAtoms, MI = 0.05832 bit, norm = 0.01767, cond entr = 4.581 bit



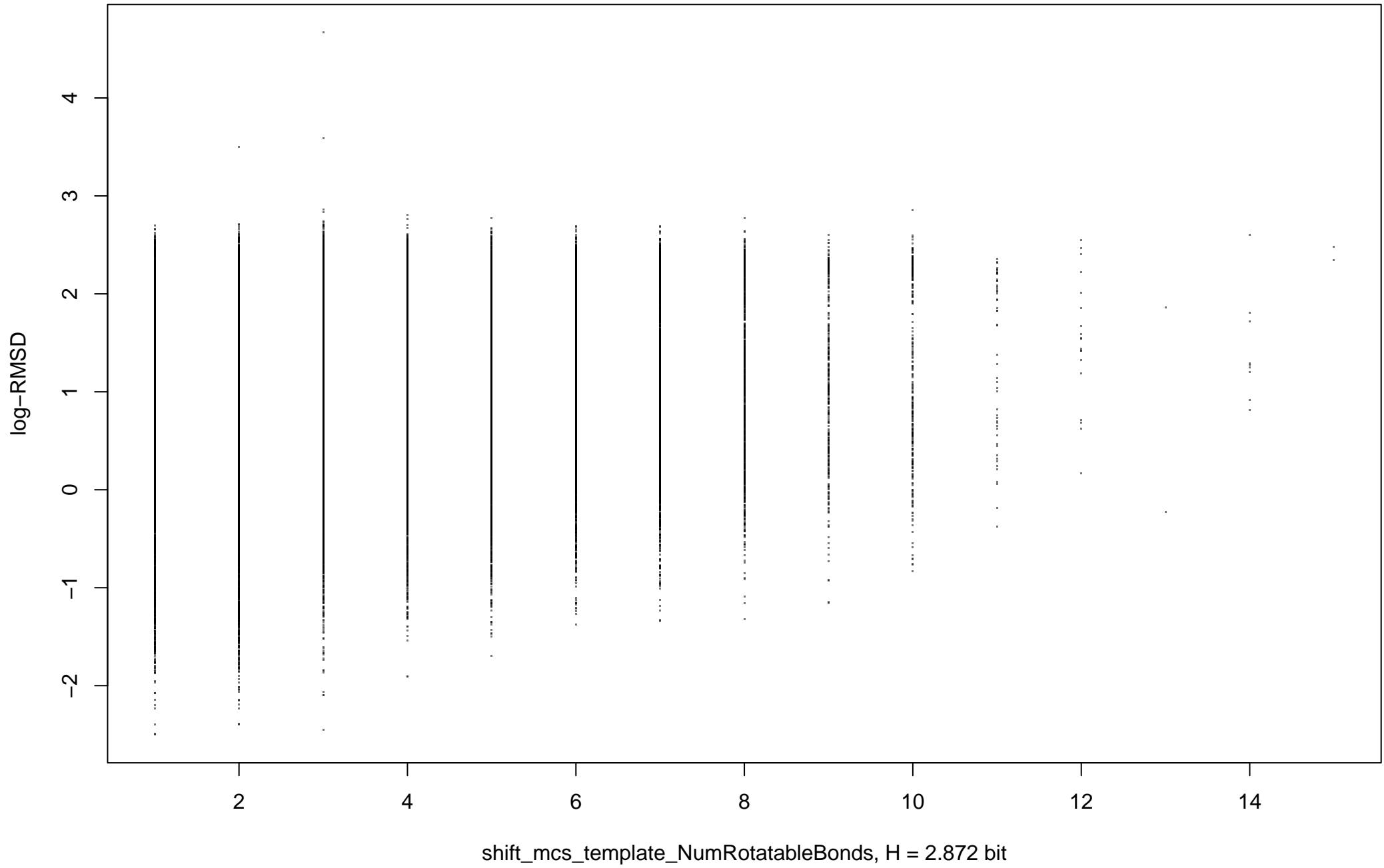
shift_docked_NumHeteroAtoms, MI = 0.05832 bit, norm = 0.01767, cond entr = 4.581 bit



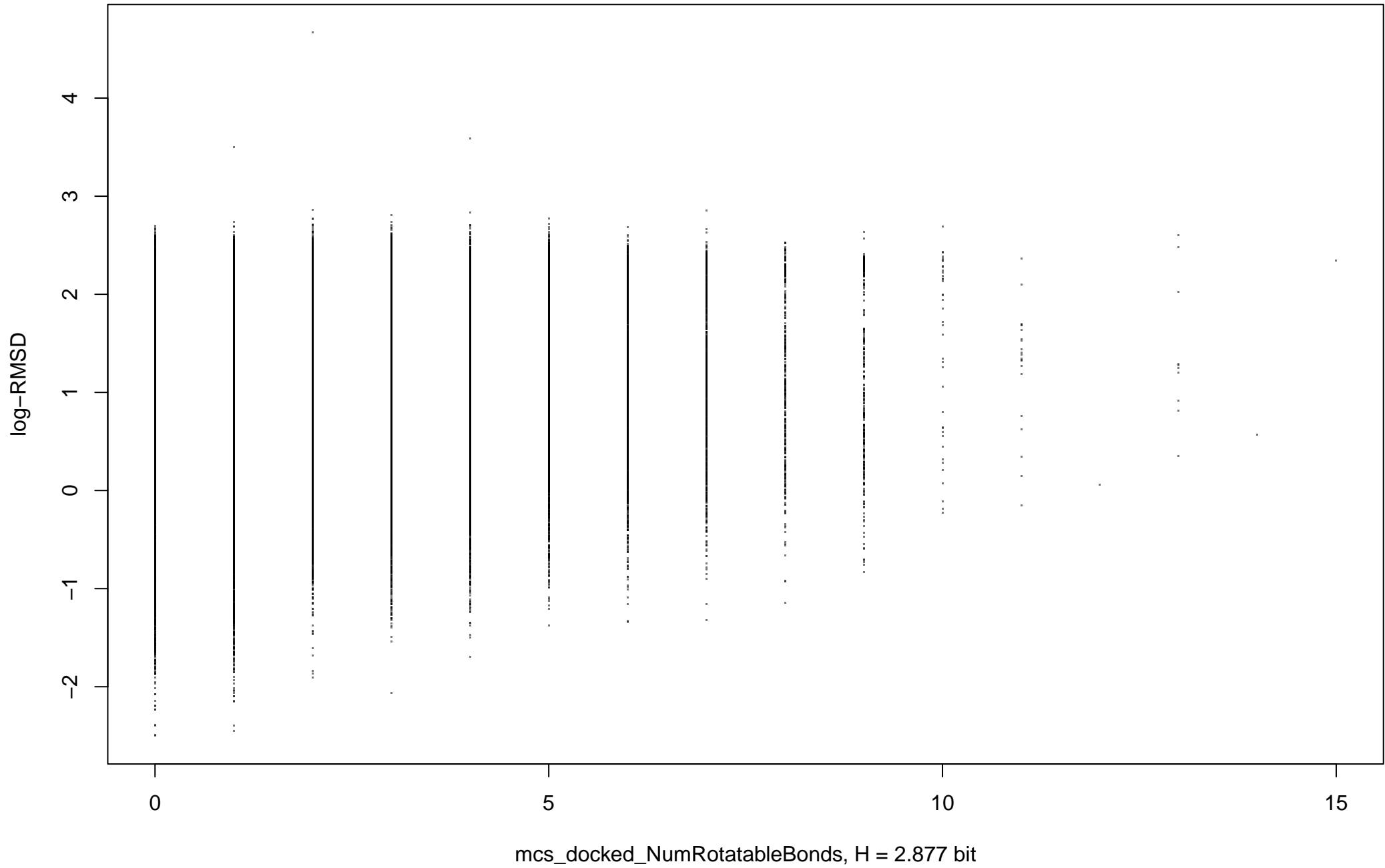
mcs_template_NumRotatableBonds, MI = 0.05825 bit, norm = 0.02028, cond entr = 4.581 bit



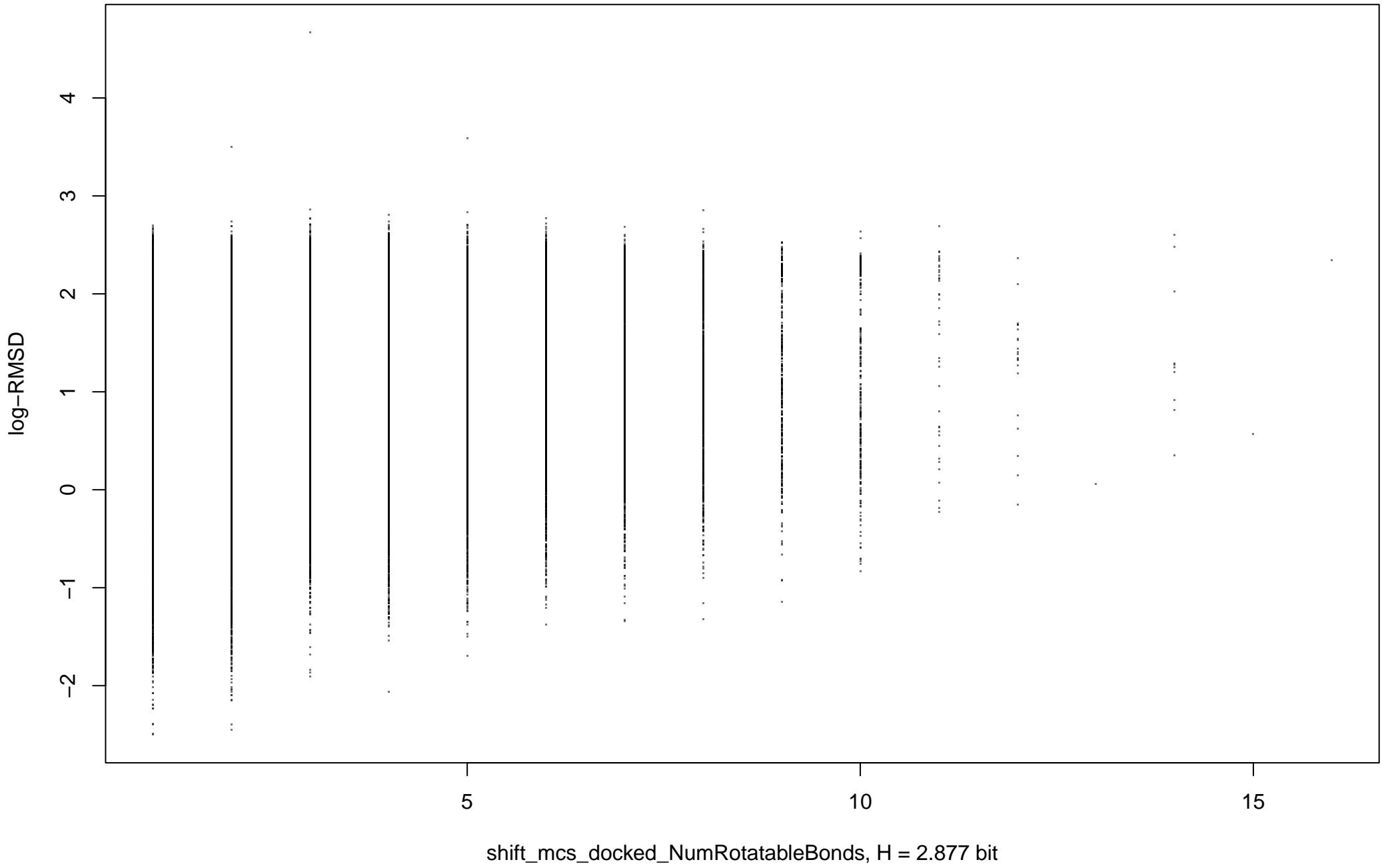
shift_mcs_template_NumRotatableBonds, MI = 0.05825 bit, norm = 0.02028, cond entr = 4.581 bit



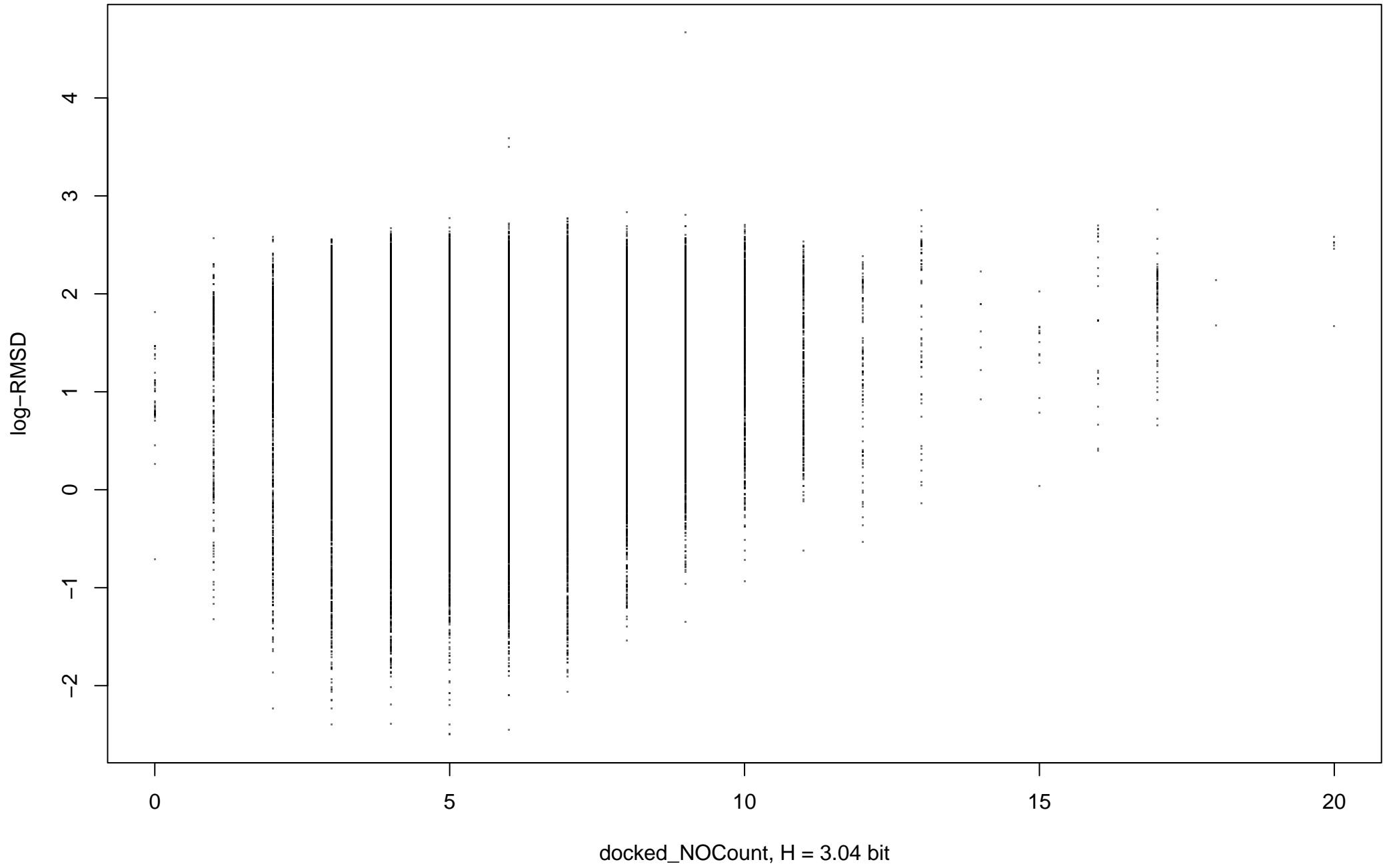
mcs_docked_NumRotatableBonds, MI = 0.05574 bit, norm = 0.01937, cond entr = 4.584 bit



shift_mcs_docked_NumRotatableBonds, MI = 0.05574 bit, norm = 0.01937, cond entr = 4.584 bit

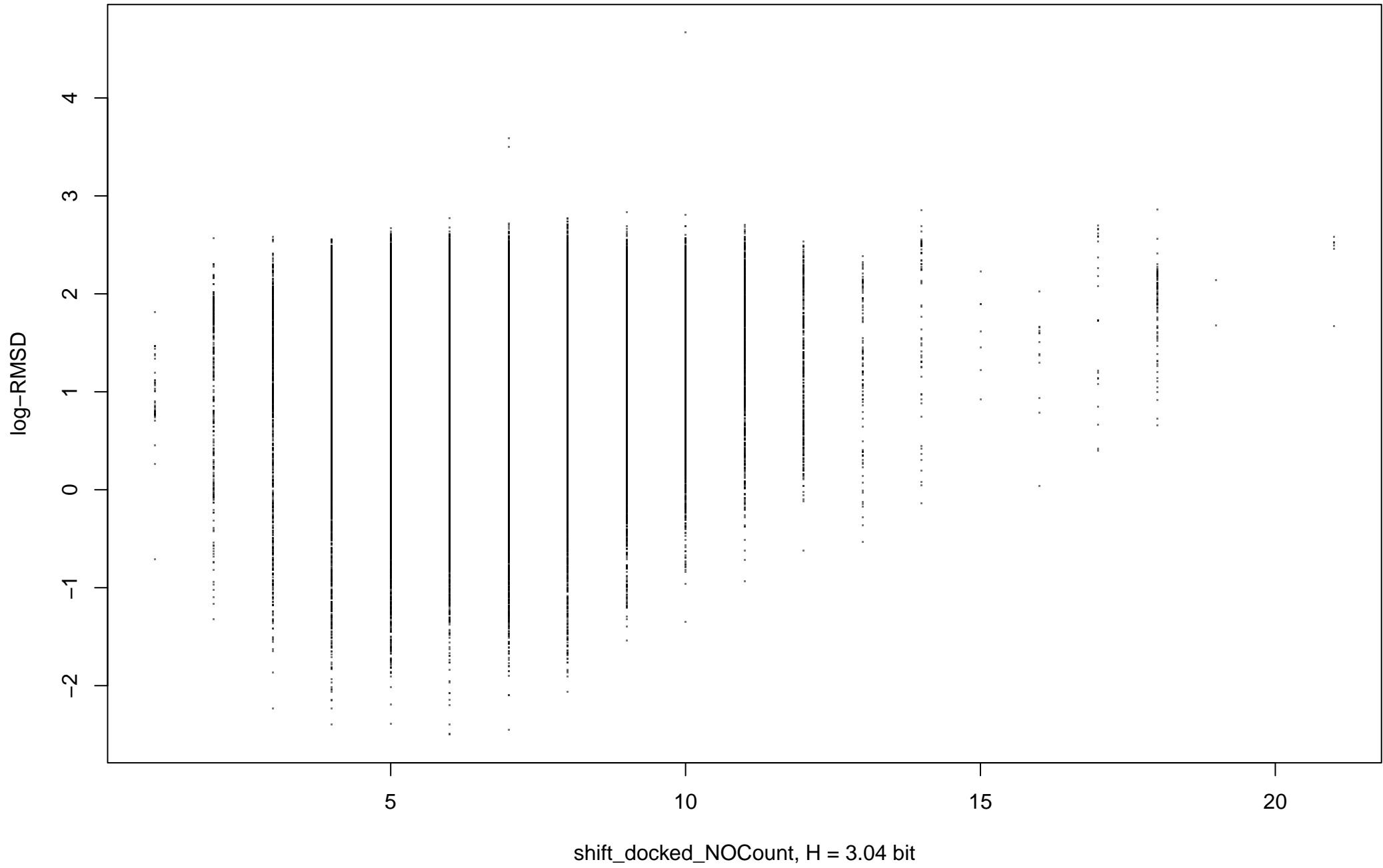


docked_NOCount, MI = 0.055 bit, norm = 0.01809, cond entr = 4.585 bit

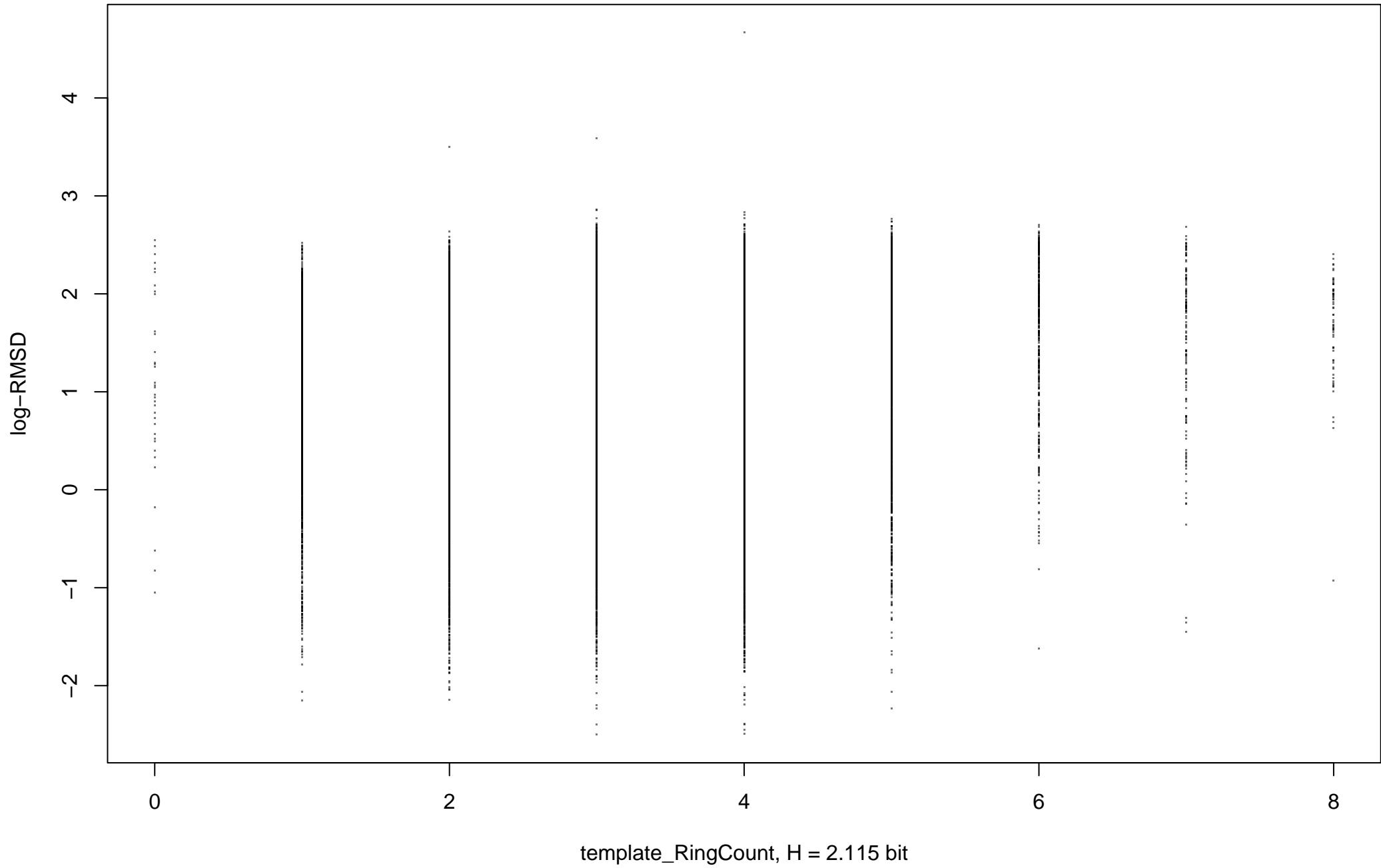


docked_NOCount, H = 3.04 bit

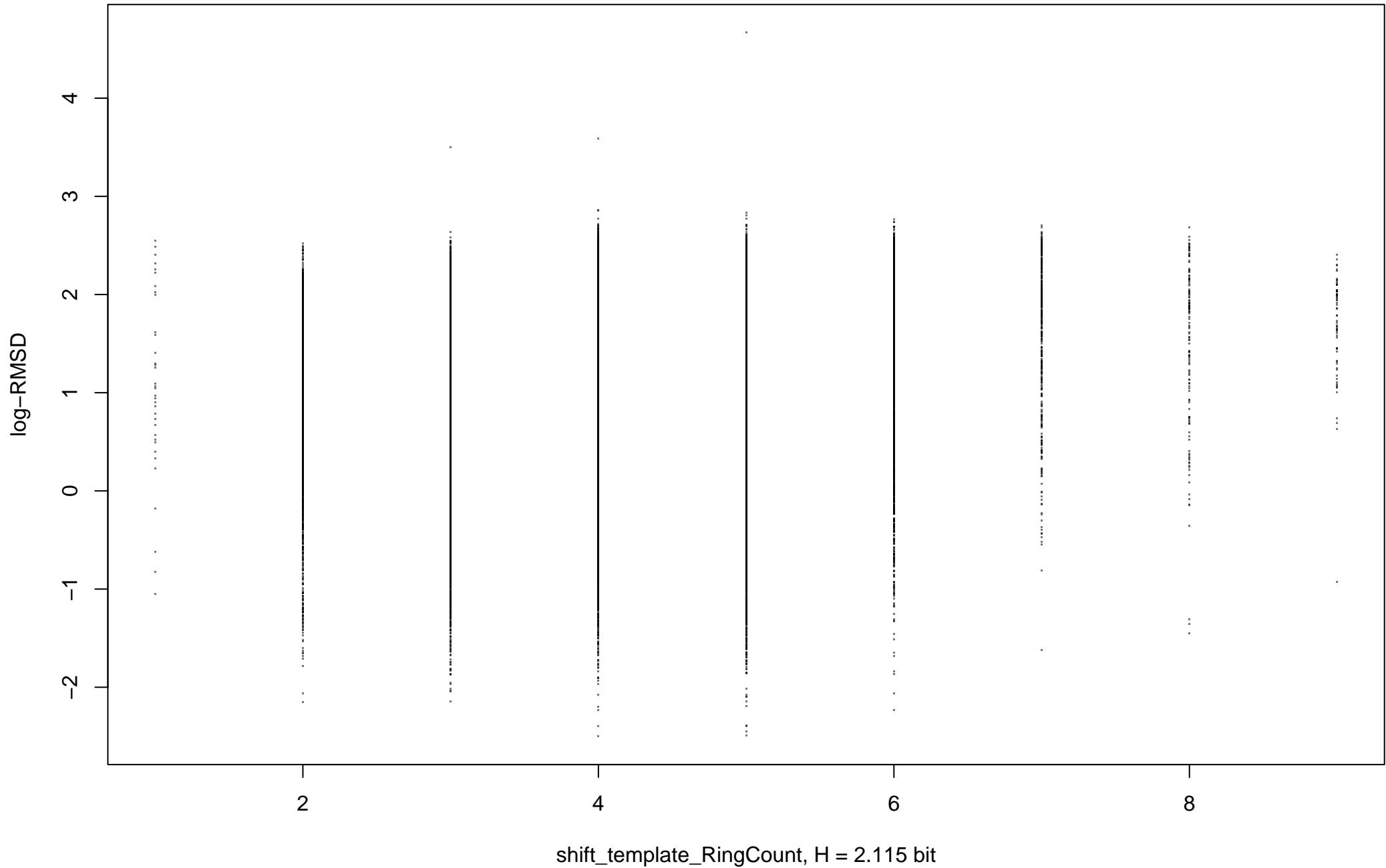
shift_docked_NOCount, MI = 0.055 bit, norm = 0.01809, cond entr = 4.585 bit



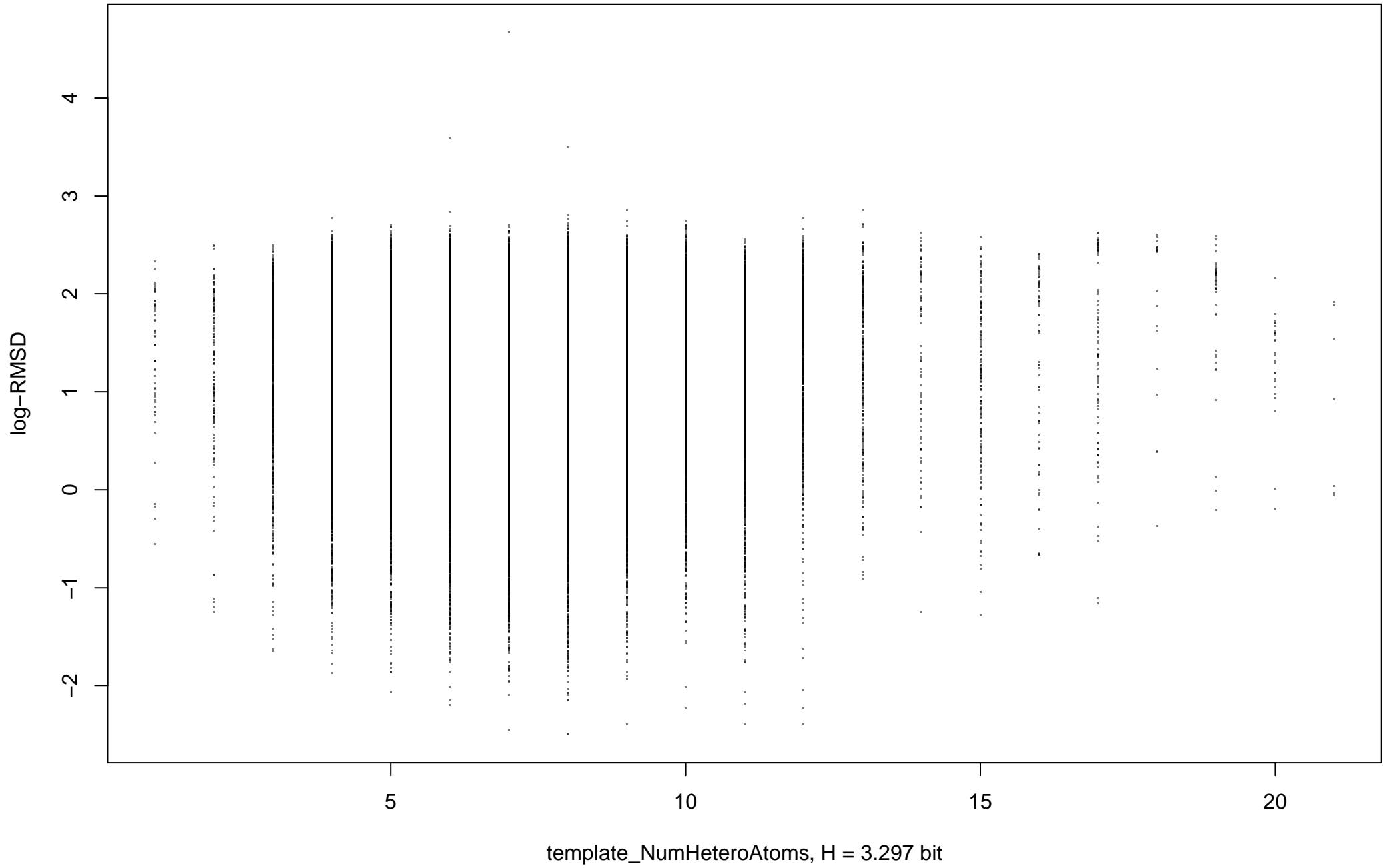
template_RingCount, MI = 0.04614 bit, norm = 0.02181, cond entr = 4.593 bit



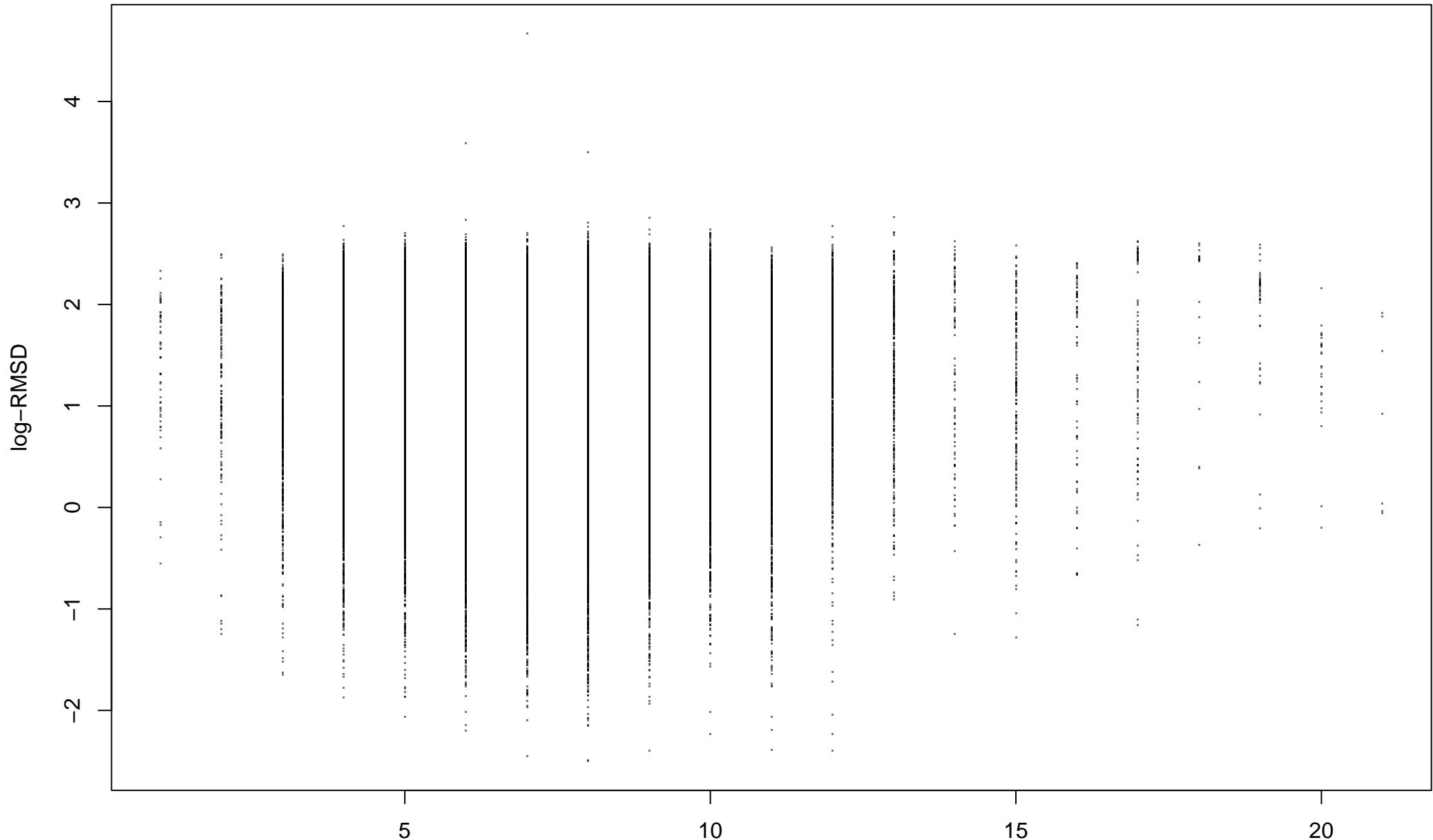
shift_template_RingCount, MI = 0.04614 bit, norm = 0.02181, cond entr = 4.593 bit



template_NumHeteroAtoms, MI = 0.04609 bit, norm = 0.01398, cond entr = 4.593 bit

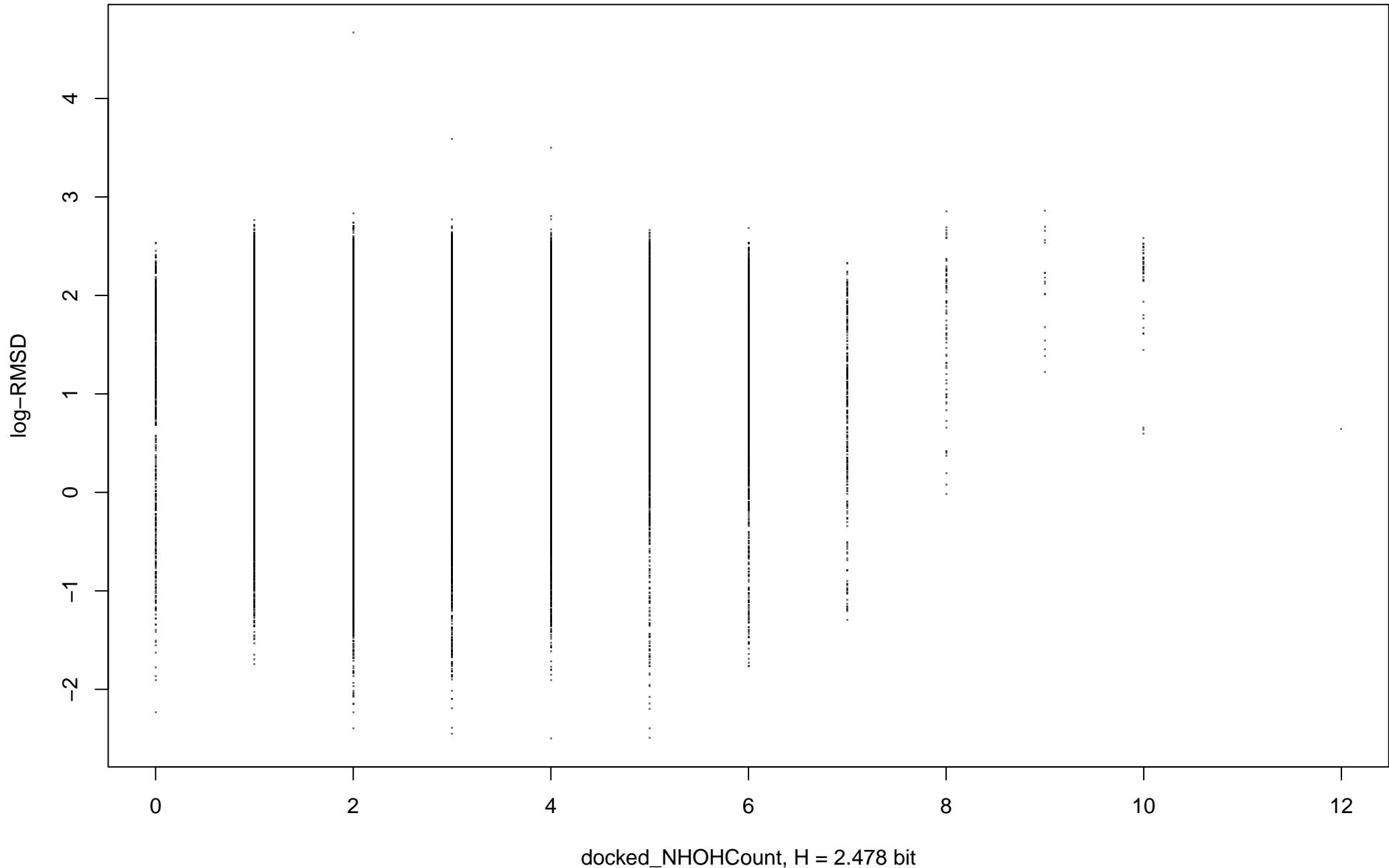


shift_template_NumHeteroAtoms, MI = 0.04609 bit, norm = 0.01398, cond entr = 4.593 bit

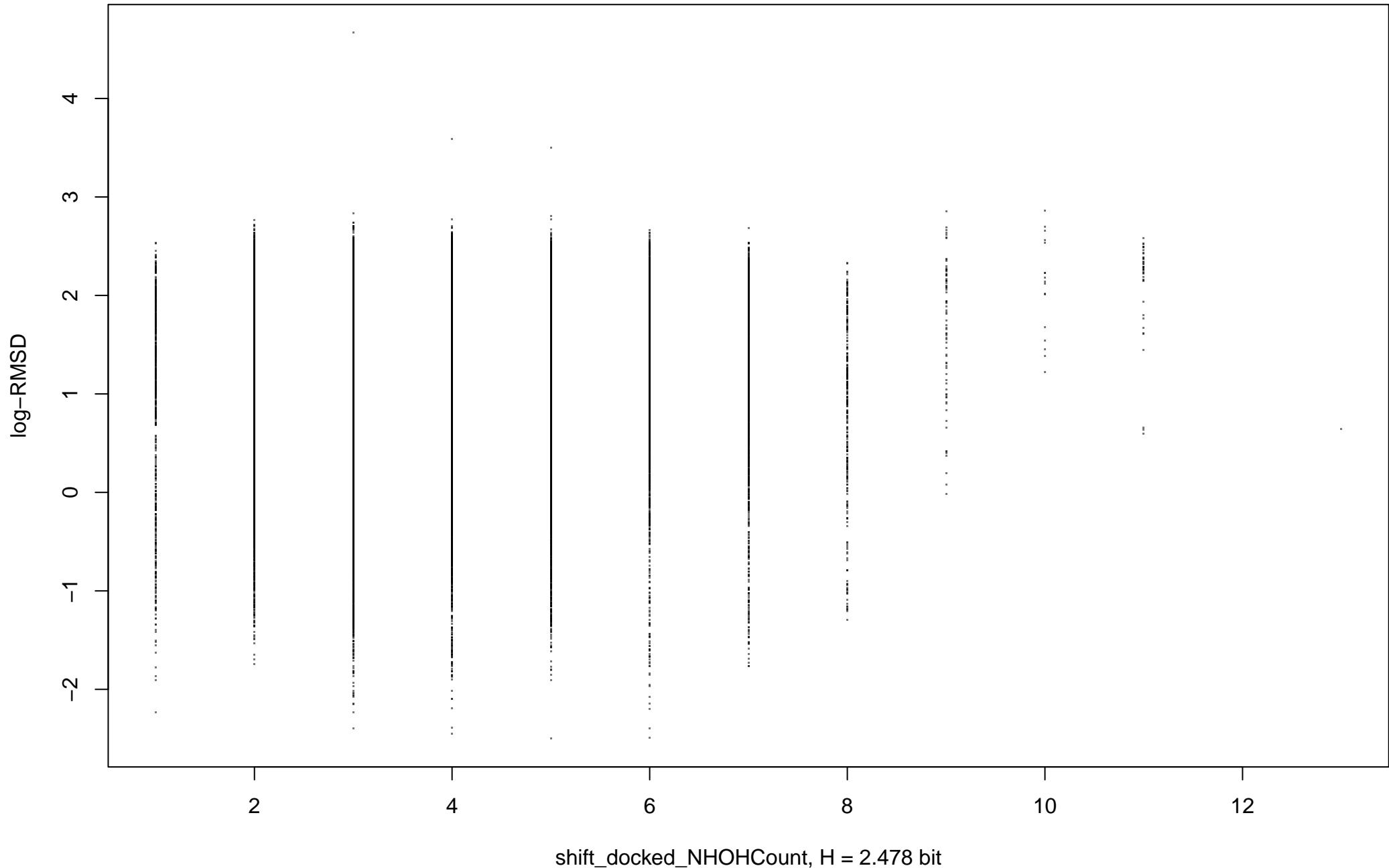


shift_template_NumHeteroAtoms, H = 3.297 bit

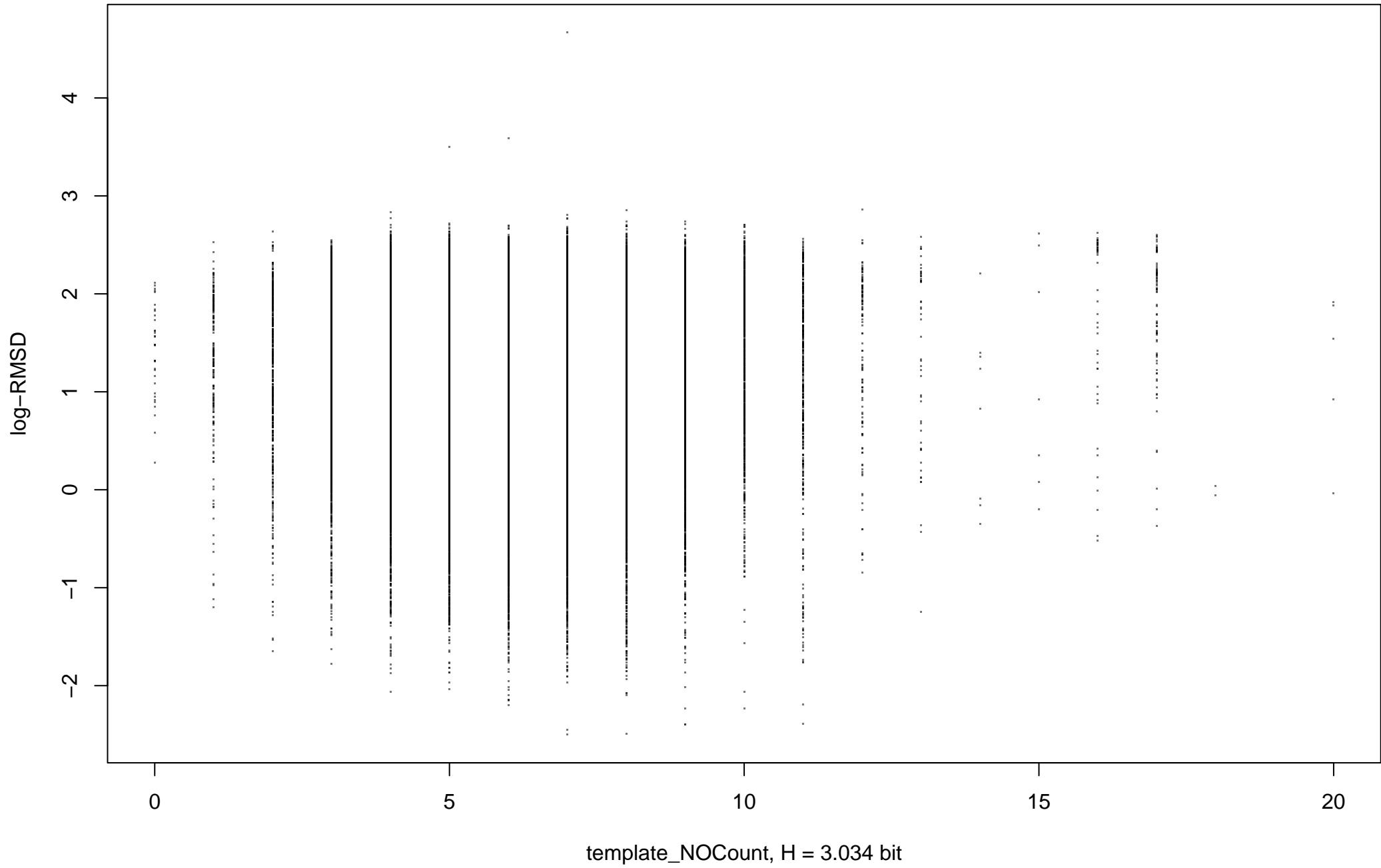
docked_NHOHCount, MI = 0.04592 bit, norm = 0.01853, cond entr = 4.594 bit



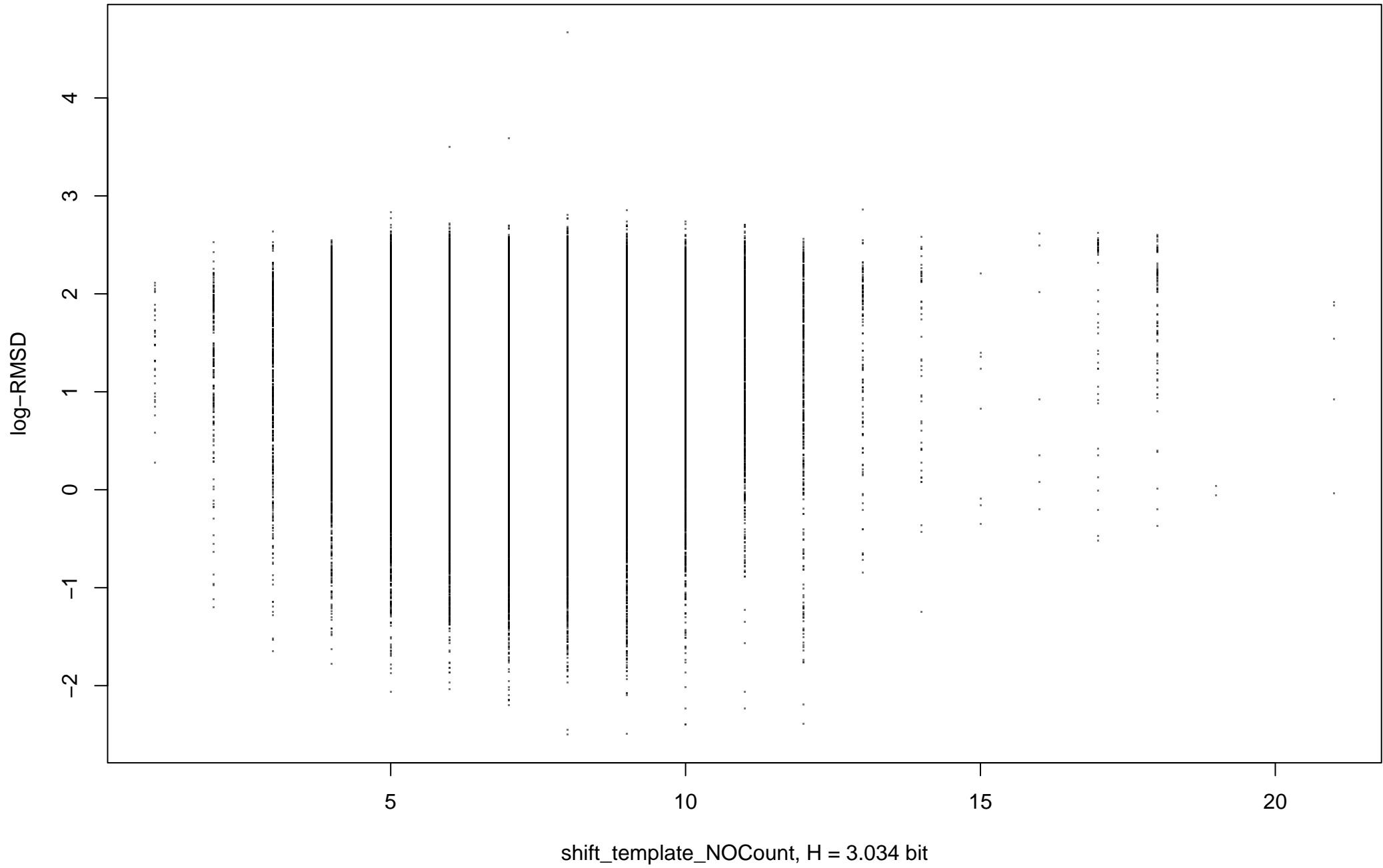
shift_docked_NHOHCount, MI = 0.04592 bit, norm = 0.01853, cond entr = 4.594 bit



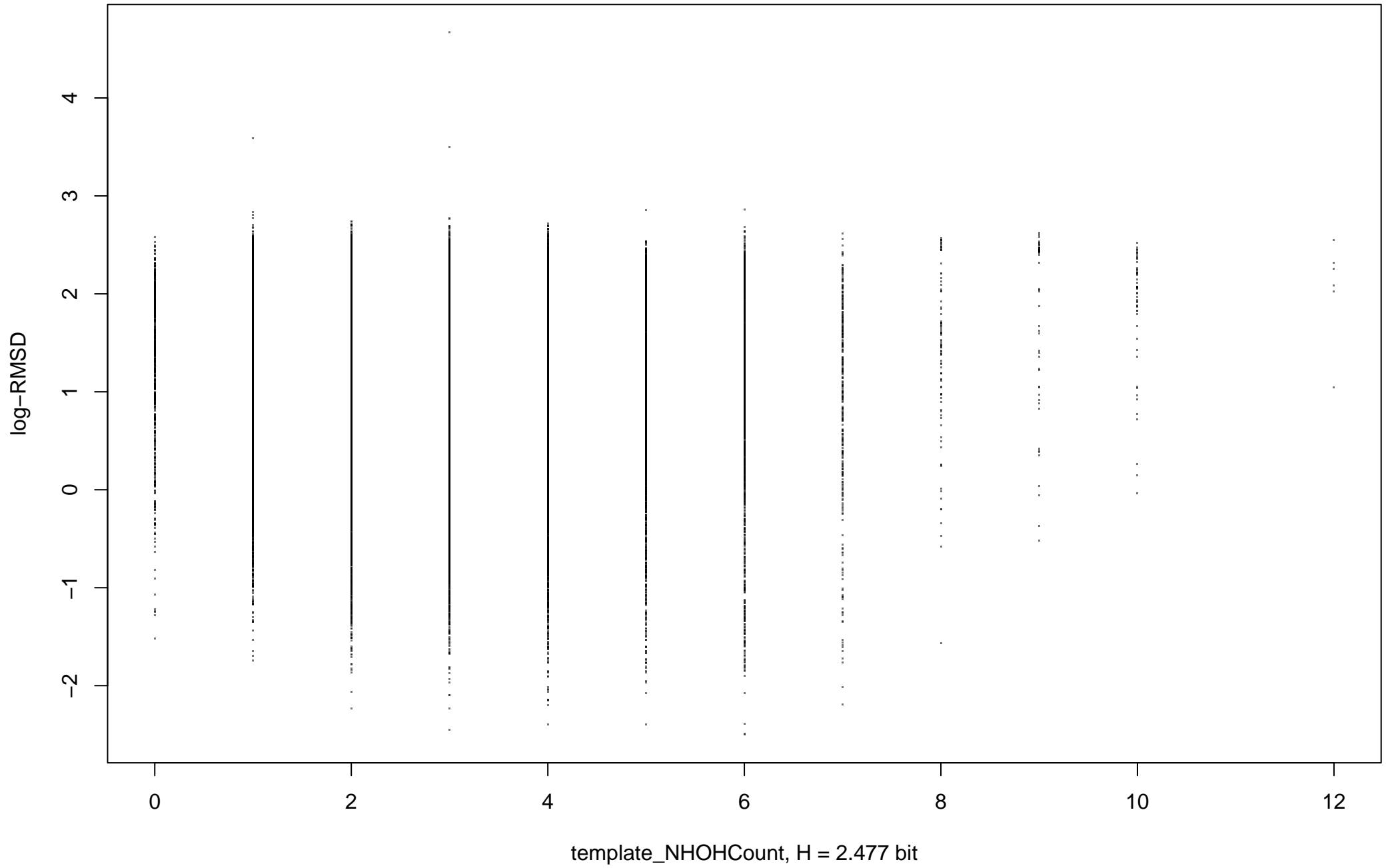
template_NOCount, MI = 0.04518 bit, norm = 0.01489, cond entr = 4.594 bit



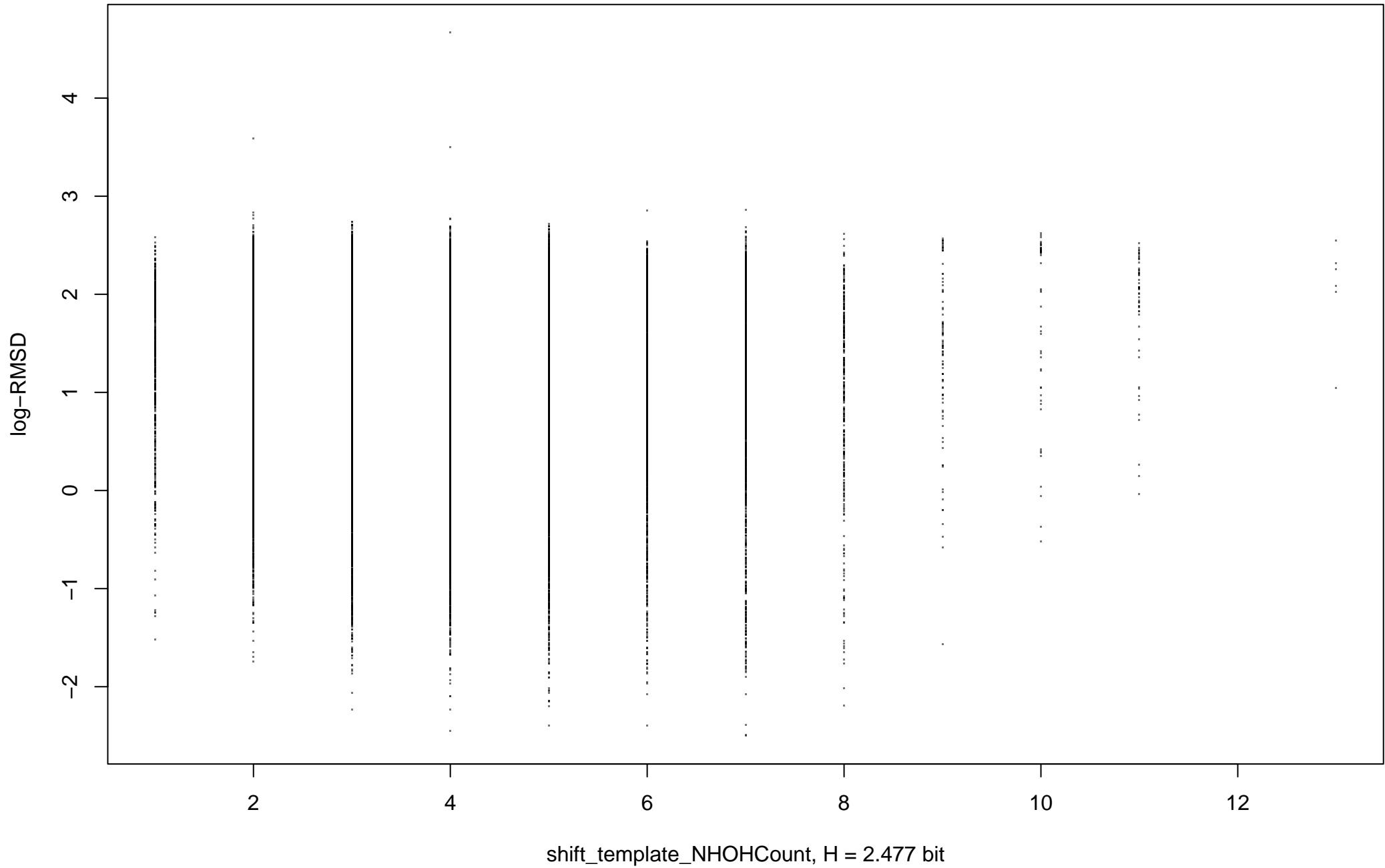
shift_template_NOCount, MI = 0.04518 bit, norm = 0.01489, cond entr = 4.594 bit



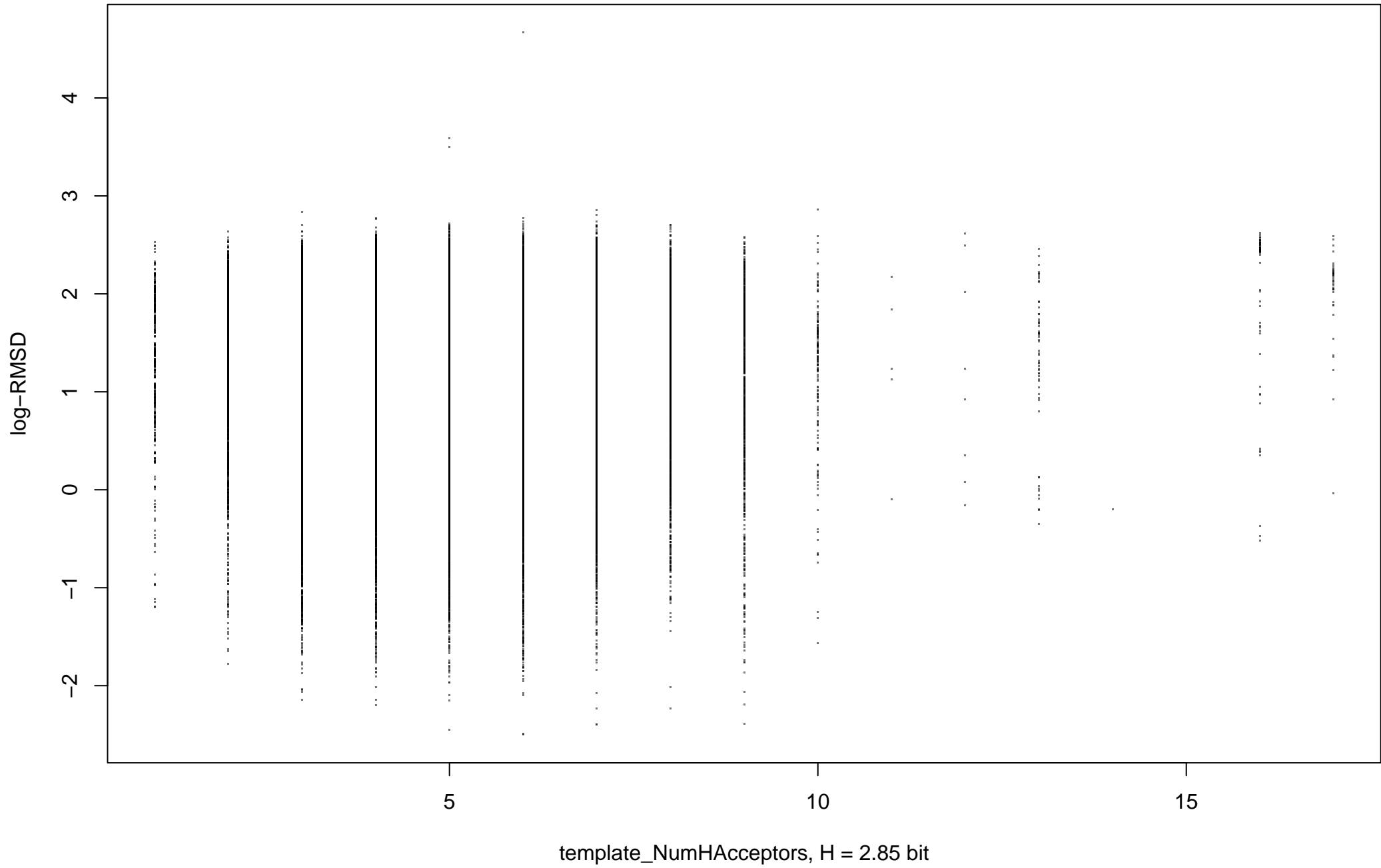
template_NHOHCount, MI = 0.04185 bit, norm = 0.0169, cond entr = 4.598 bit



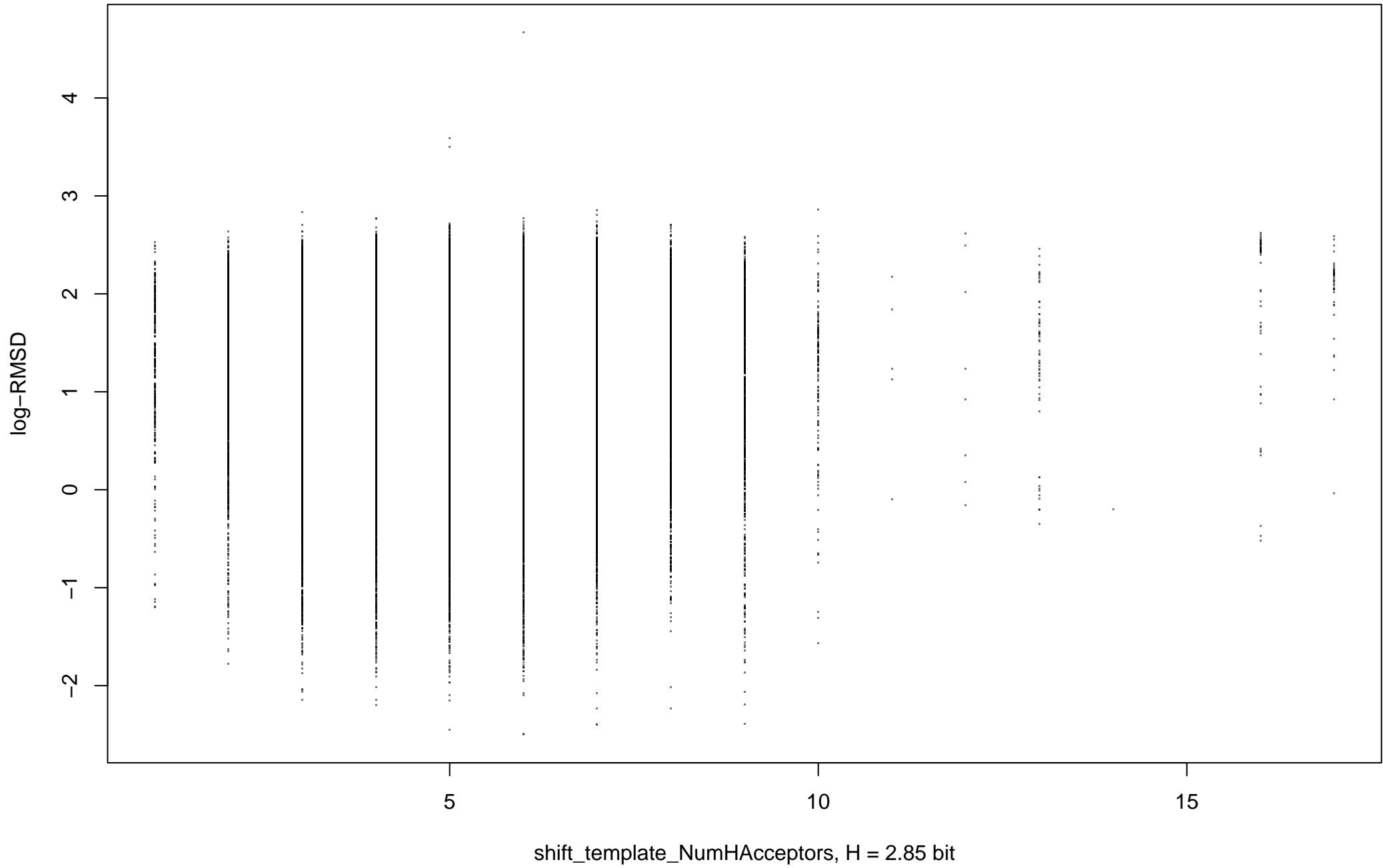
shift_template_NHOHCount, MI = 0.04185 bit, norm = 0.0169, cond entr = 4.598 bit



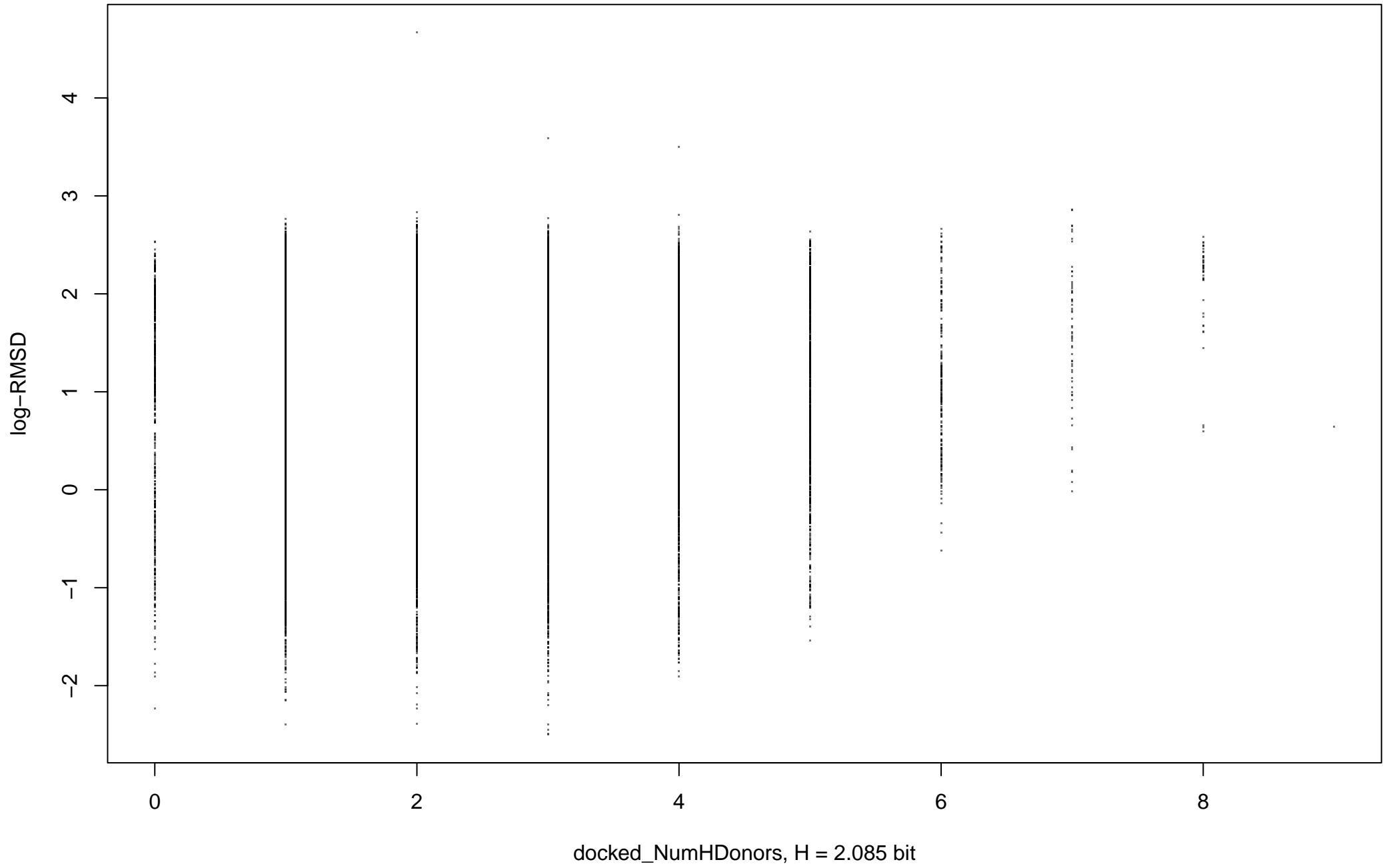
template_NumHAcceptors, MI = 0.0363 bit, norm = 0.01274, cond entr = 4.603 bit



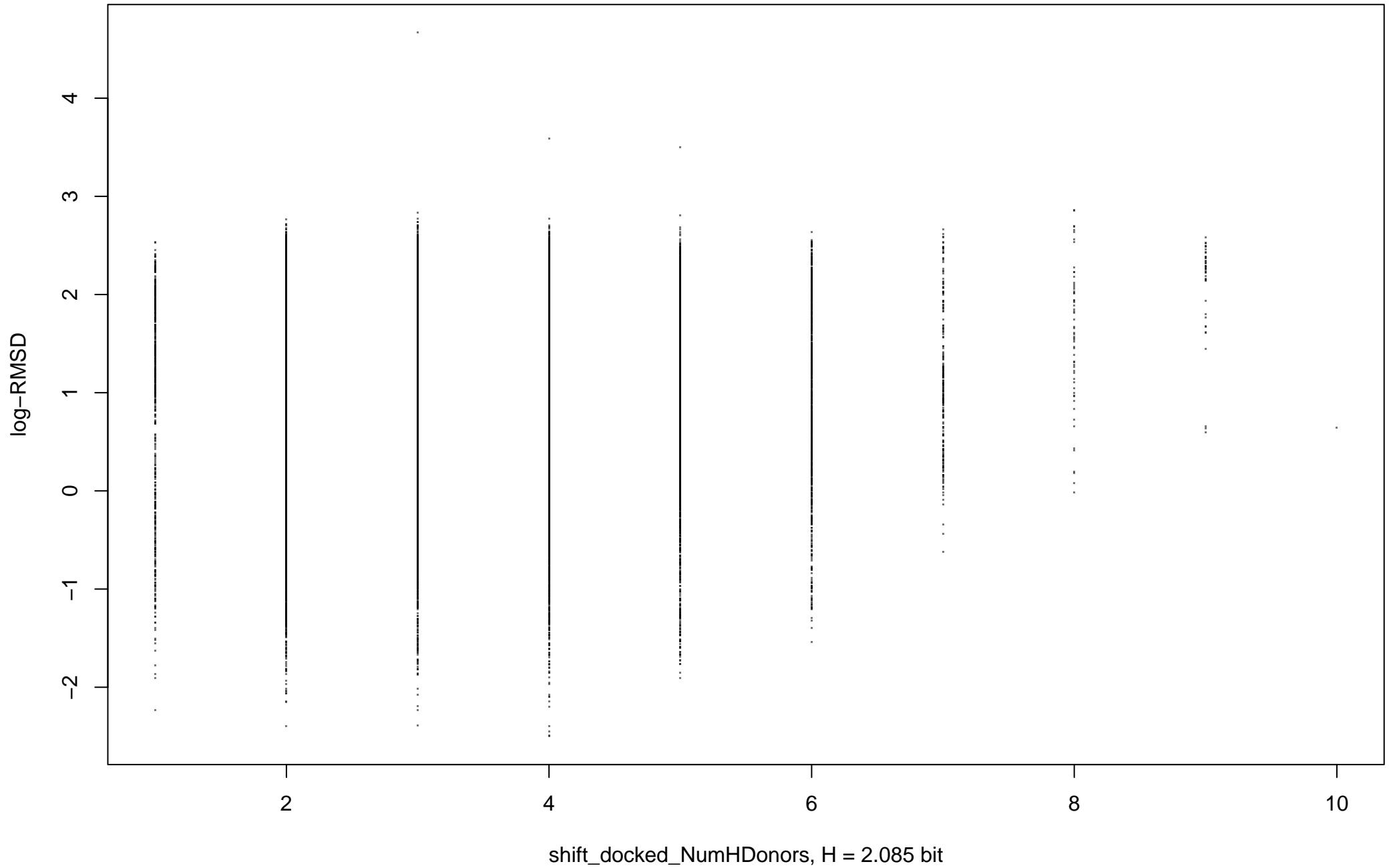
shift_template_NumHAcceptors, MI = 0.0363 bit, norm = 0.01274, cond entr = 4.603 bit



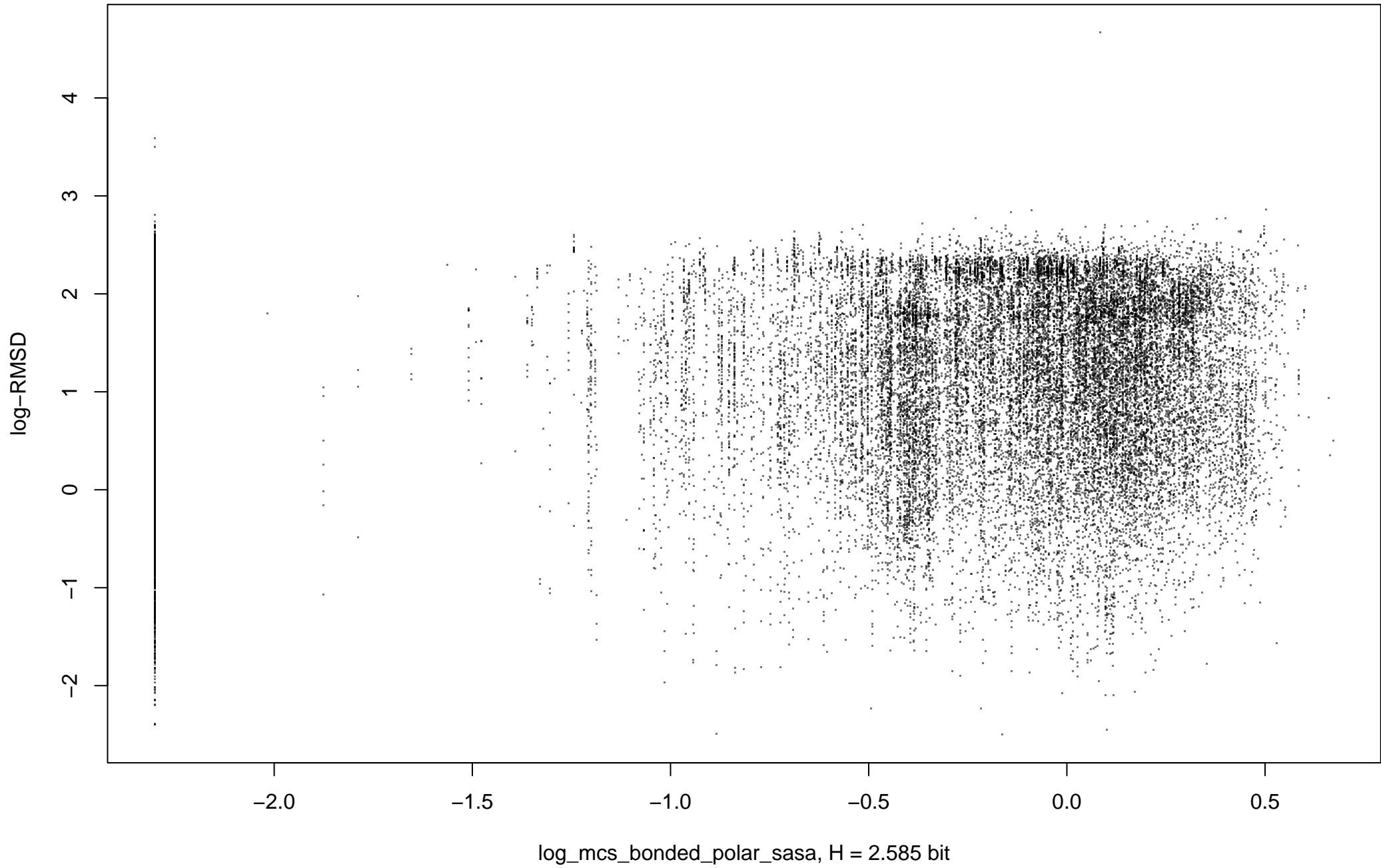
docked_NumHDonors, MI = 0.03314 bit, norm = 0.0159, cond entr = 4.606 bit



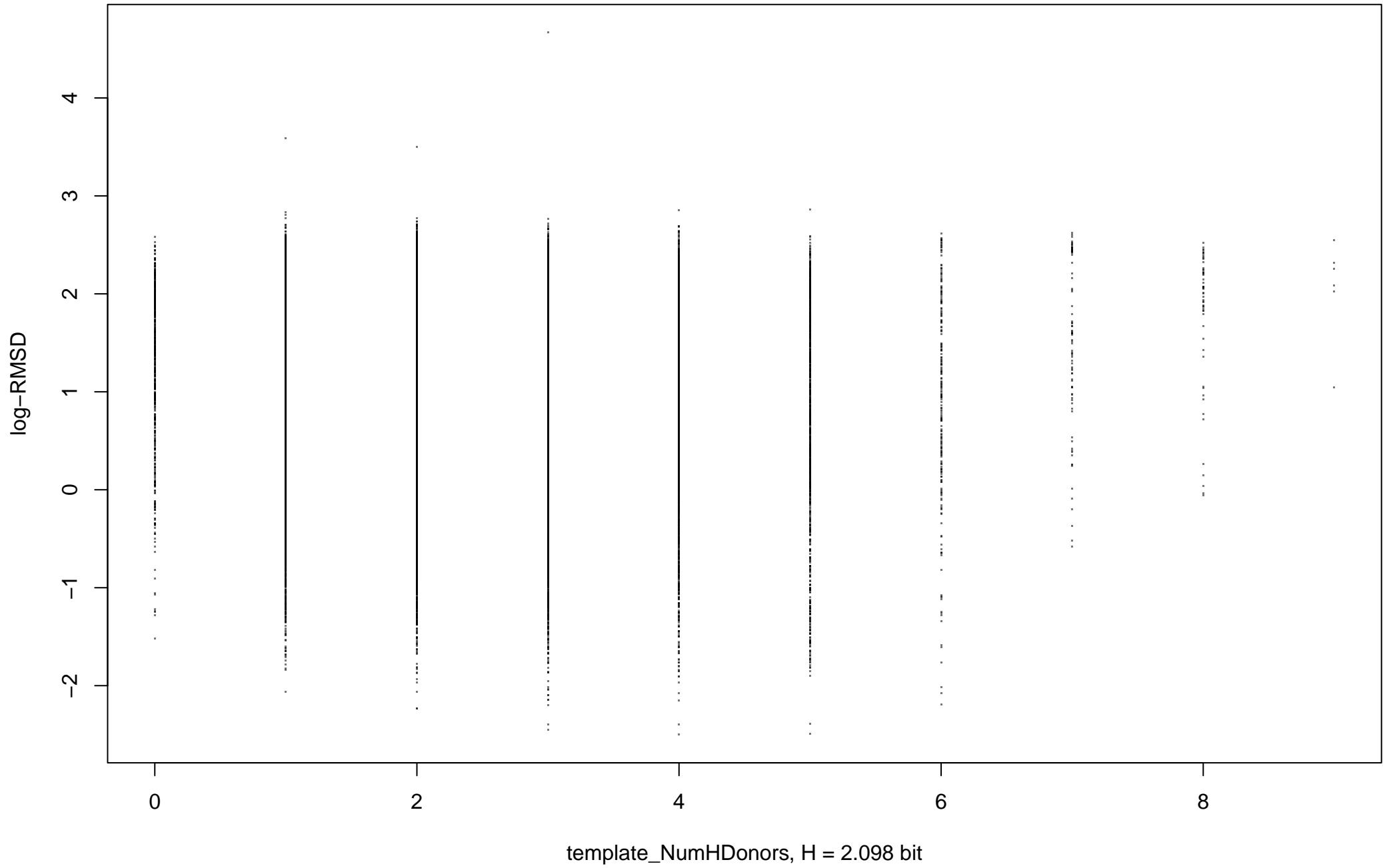
shift_docked_NuHDonors, MI = 0.03314 bit, norm = 0.0159, cond entr = 4.606 bit



log_mcs_bonded_polar_sasa, MI = 0.03126 bit, norm = 0.01209, cond entr = 4.608 bit



template_NumHDonors, MI = 0.03022 bit, norm = 0.01441, cond entr = 4.609 bit



shift_template_NumHDonors, MI = 0.03022 bit, norm = 0.01441, cond entr = 4.609 bit

