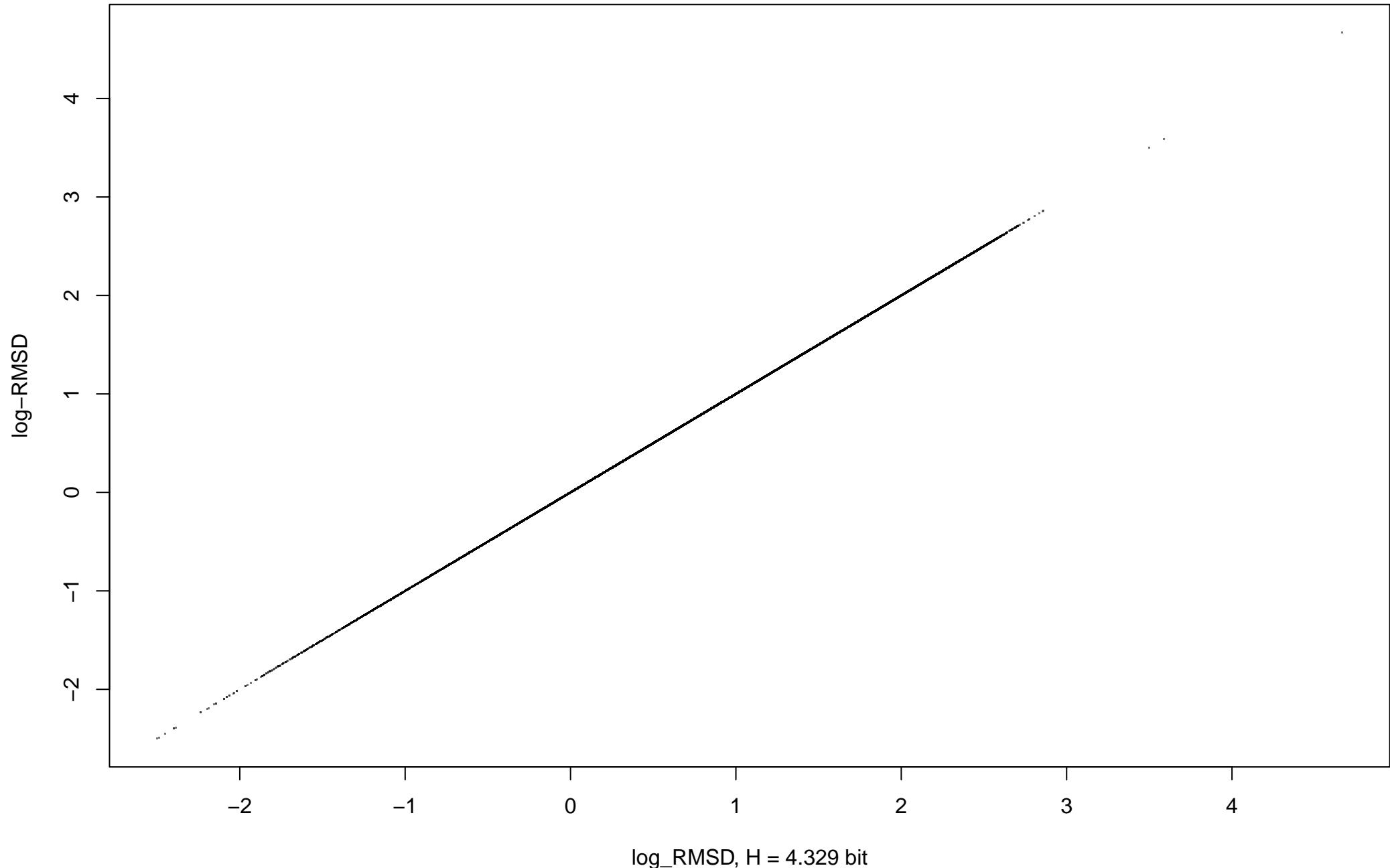
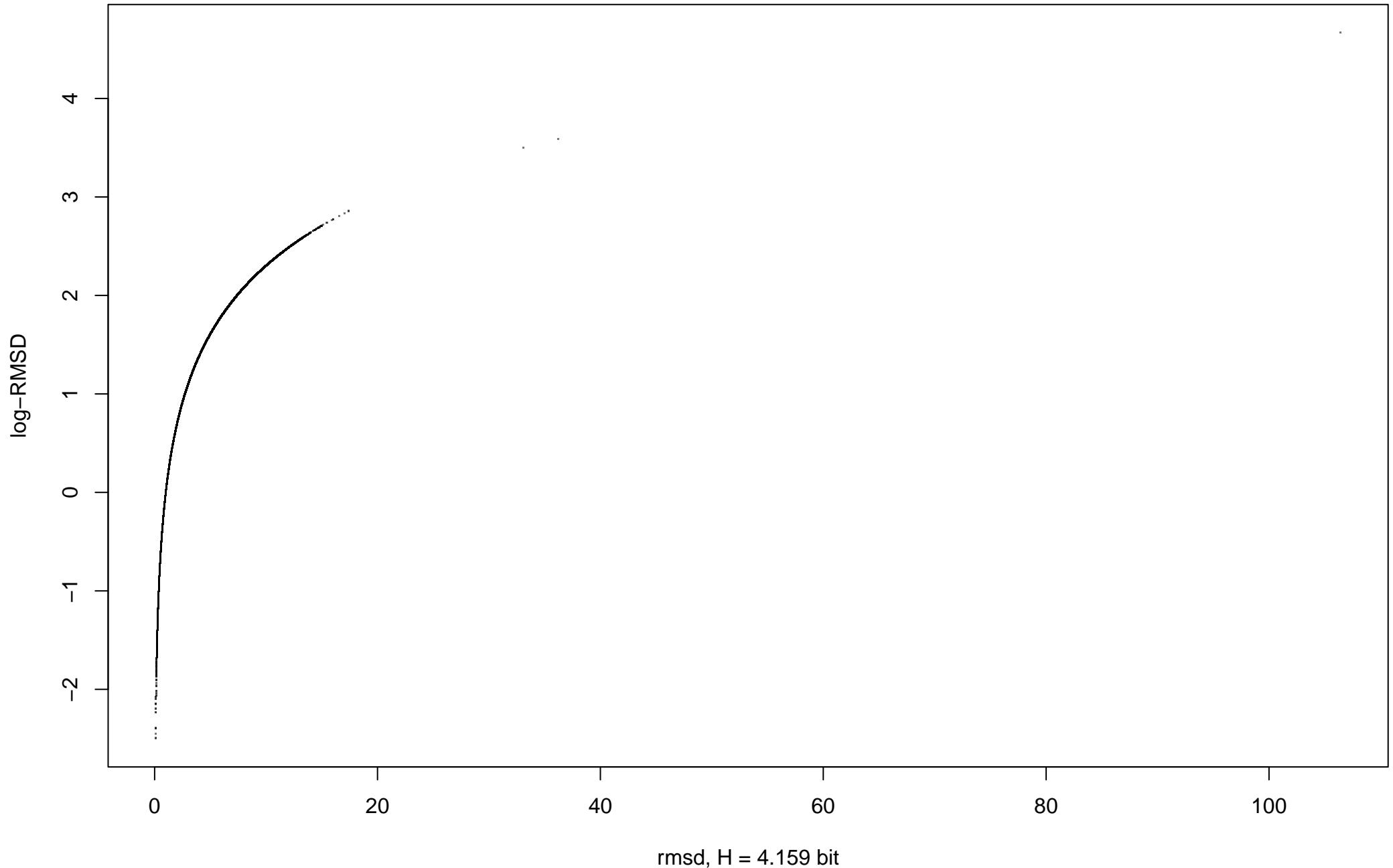


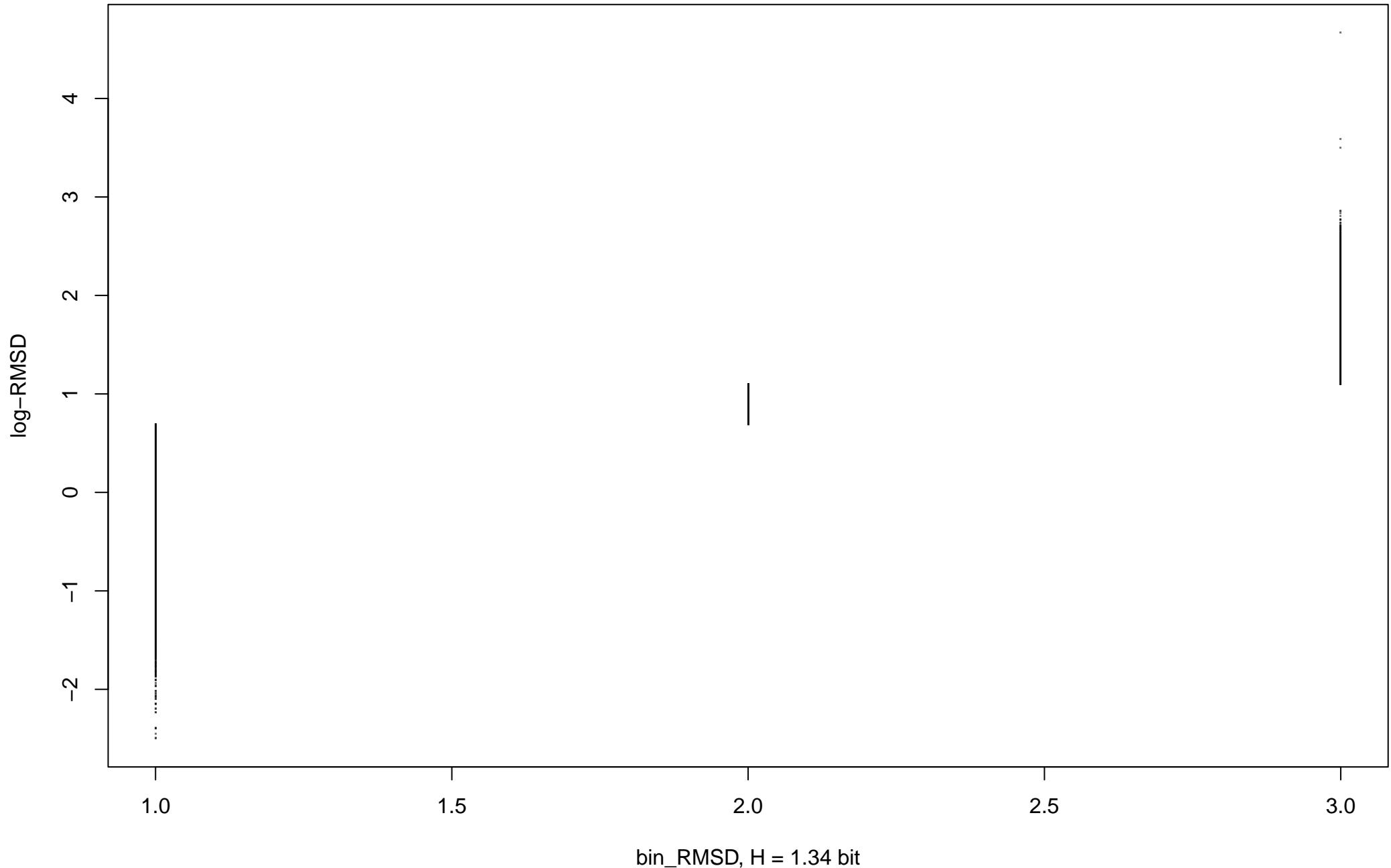
log_RMSD, MI = 4.329 bit, norm = 1, cond entr = 0 bit



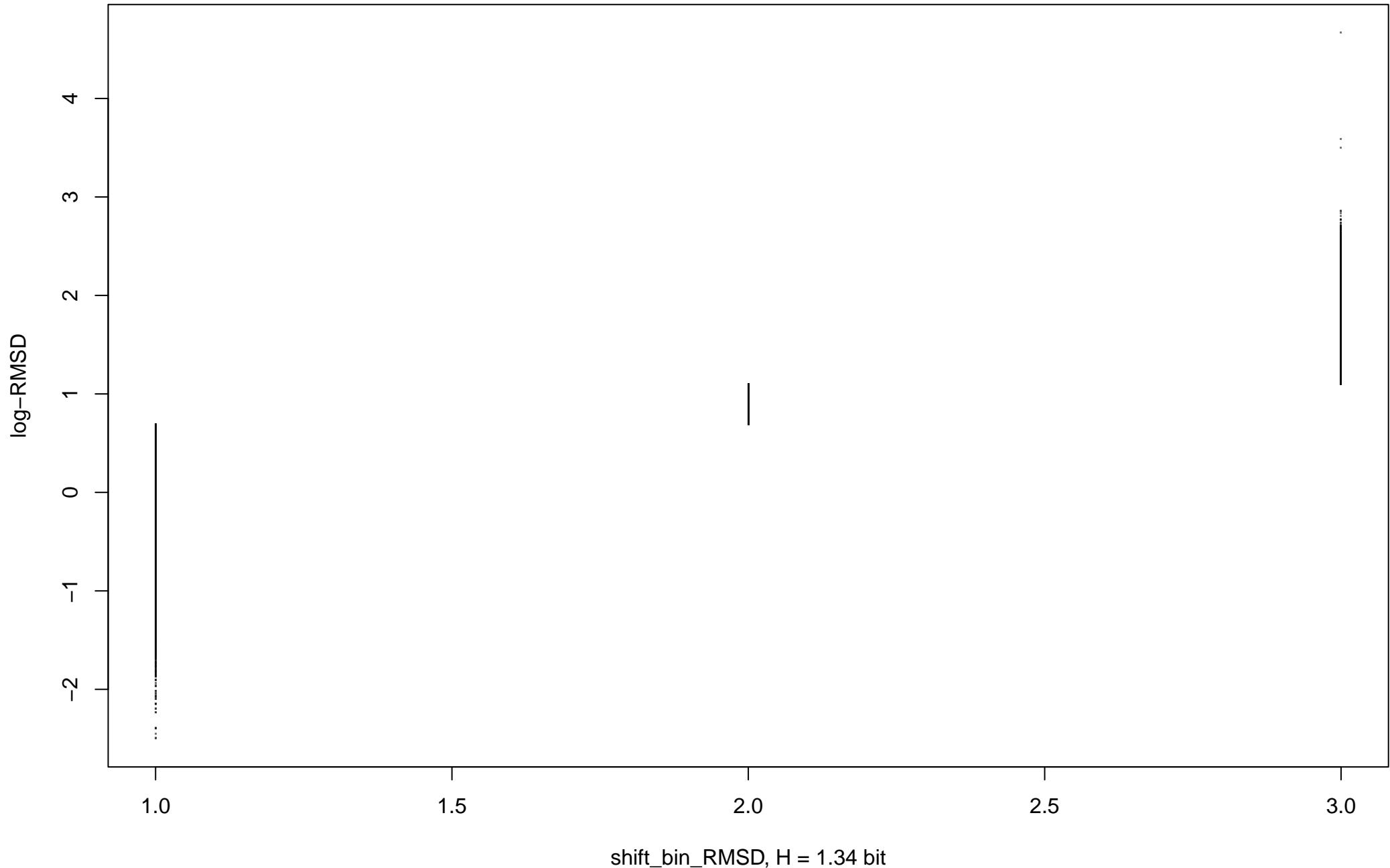
rmsd, MI = 3.338 bit, norm = 0.8026, cond entr = 0.9912 bit



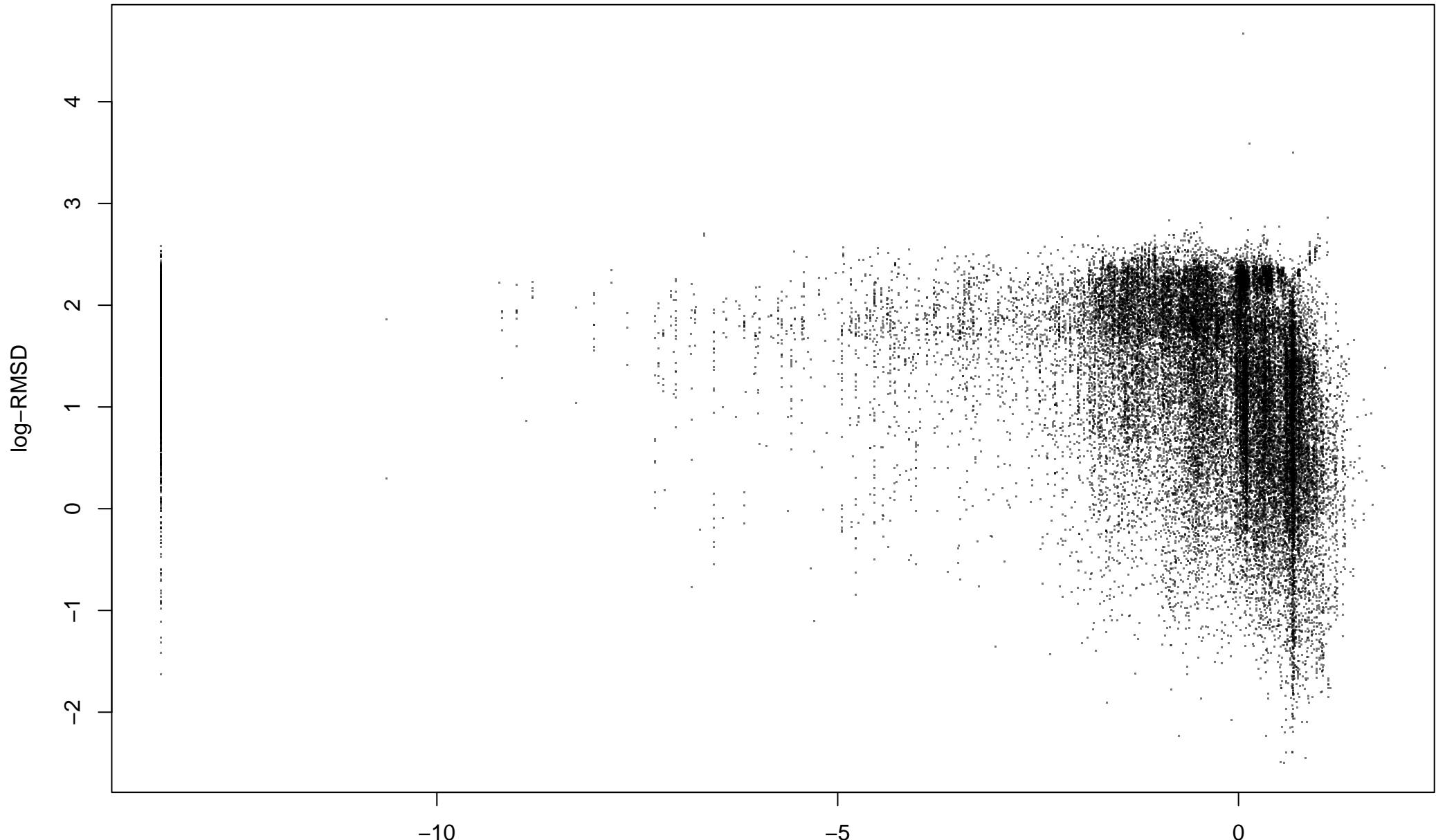
bin_RMSD, MI = 1.269 bit, norm = 0.9467, cond entr = 3.061 bit



shift_bin_RMSD, MI = 1.269 bit, norm = 0.9467, cond entr = 3.061 bit

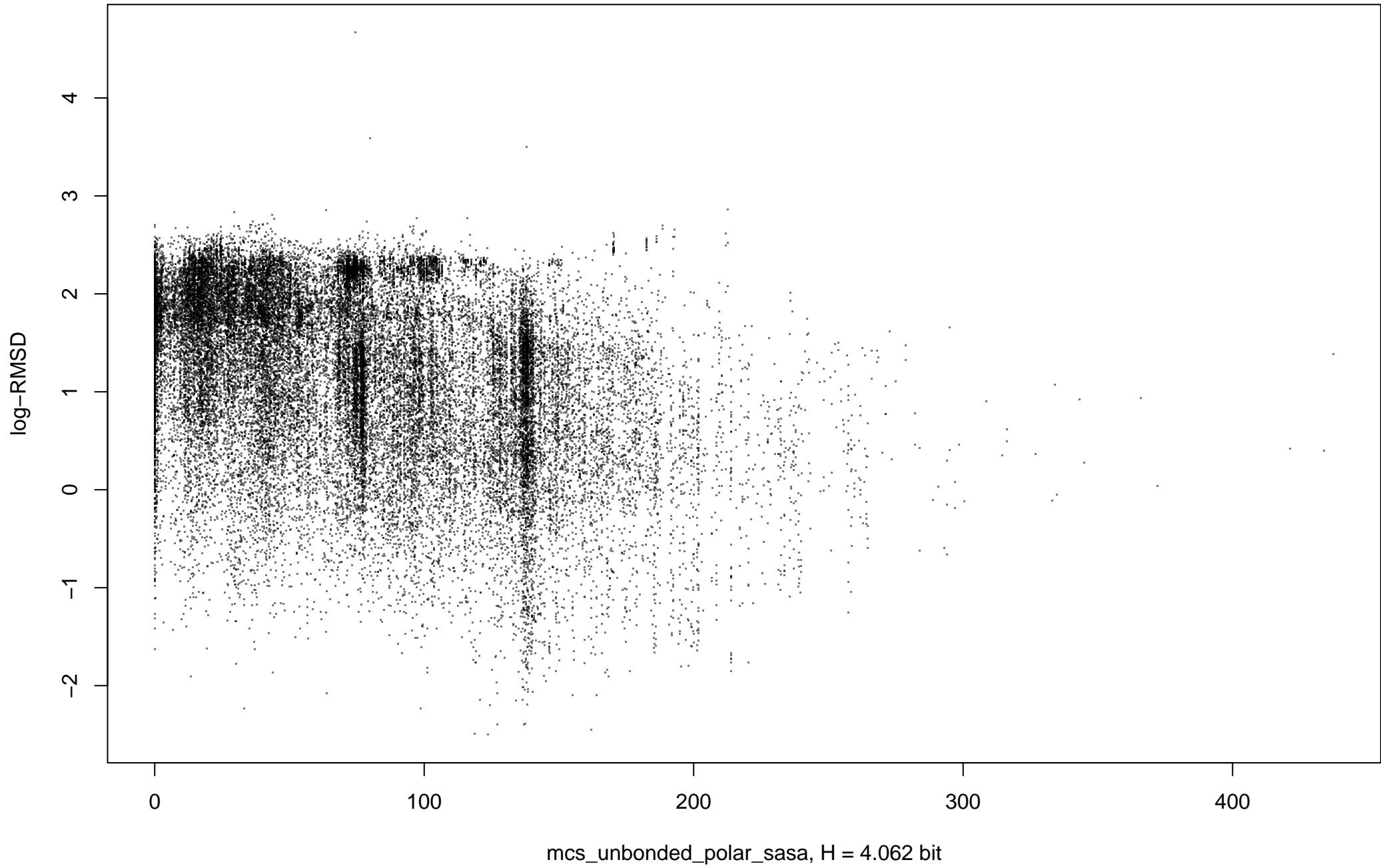


log_mcs_unbonded_polar_sasa, MI = 0.2064 bit, norm = 0.04766, cond entr = 4.123 bit

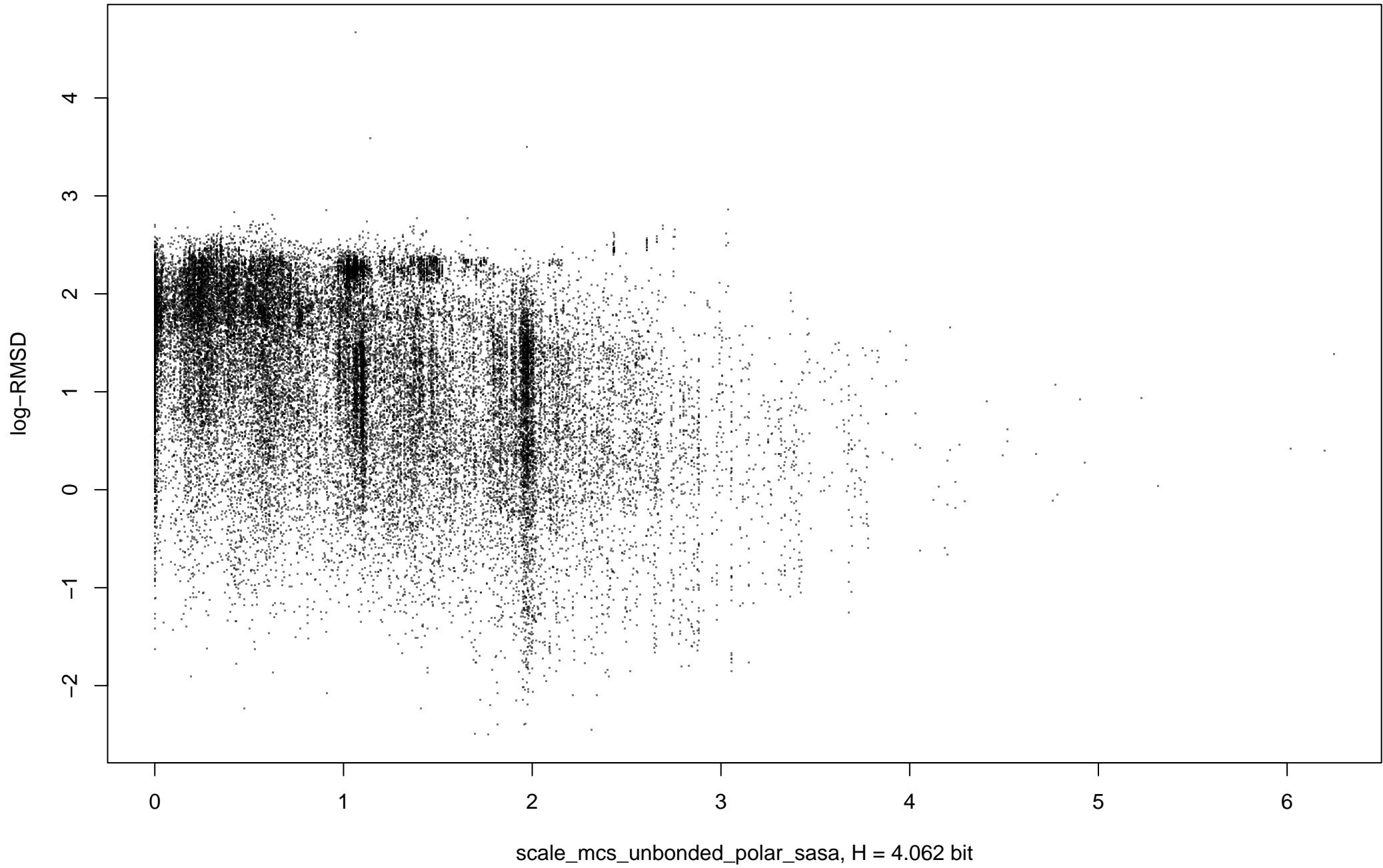


log_mcs_unbonded_polar_sasa, H = 4.367 bit

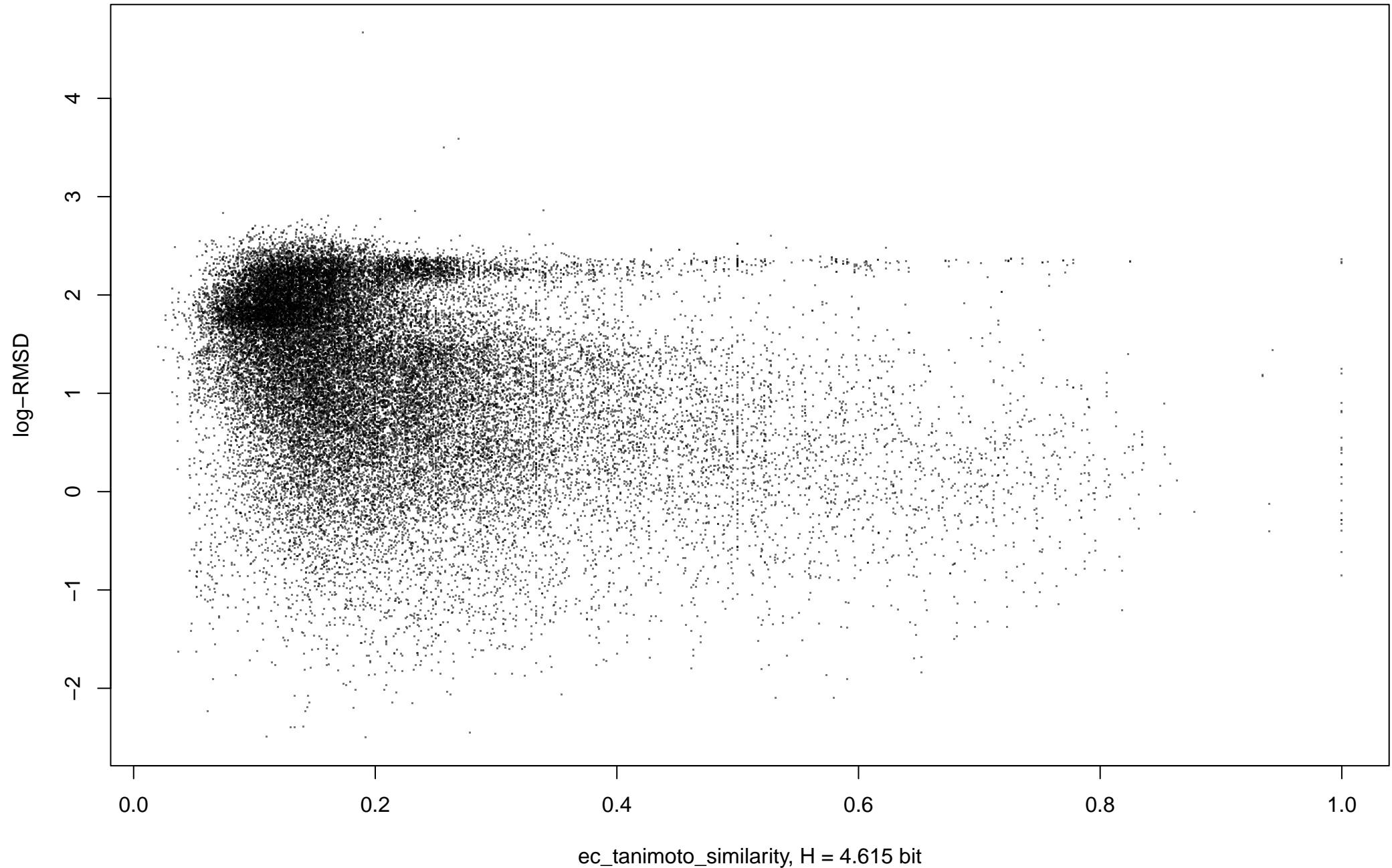
mcs_unbonded_polar_sasa, MI = 0.194 bit, norm = 0.04777, cond entr = 4.135 bit



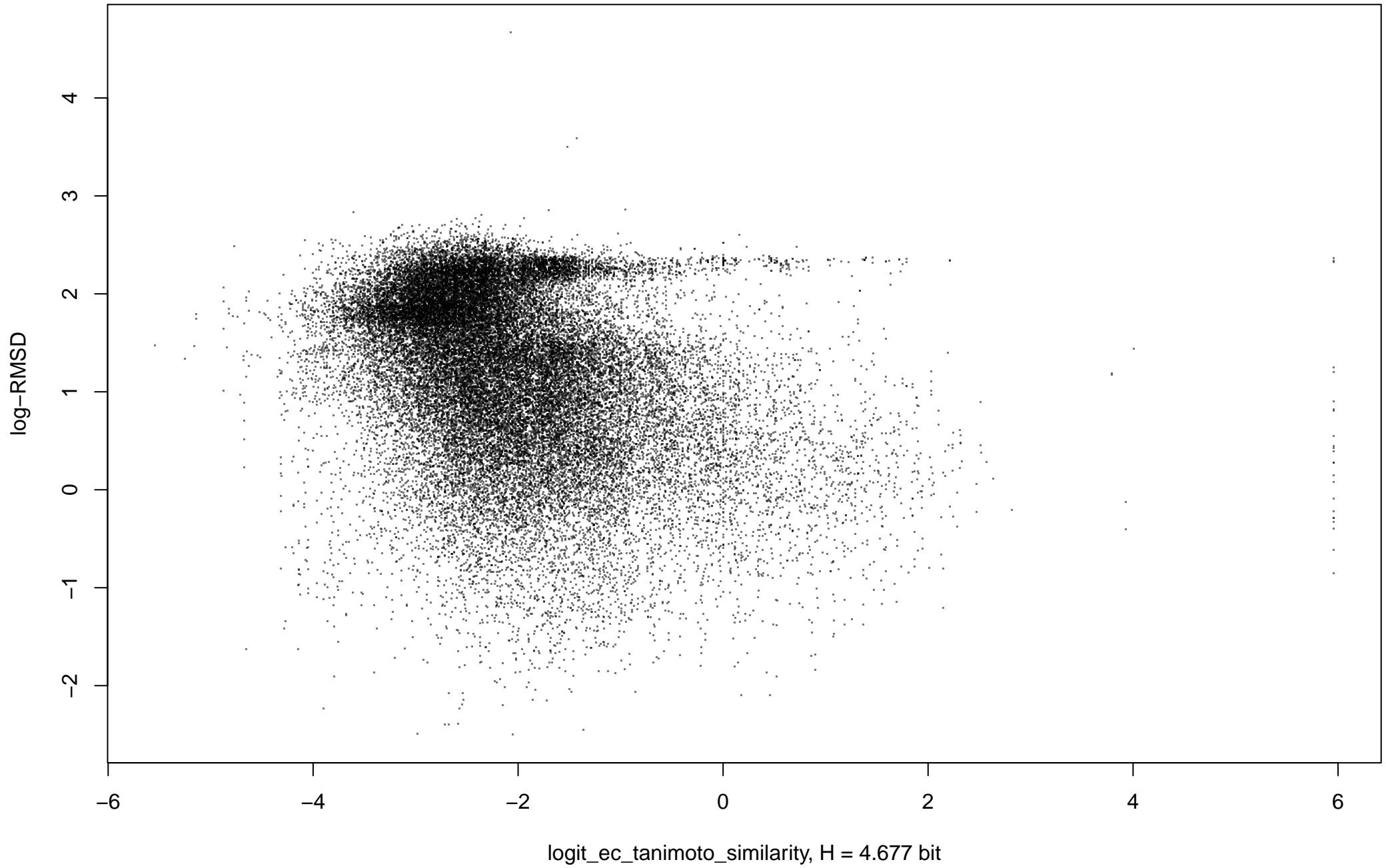
scale_mcs_unbonded_polar_sasa, MI = 0.194 bit, norm = 0.04777, cond entr = 4.135 bit



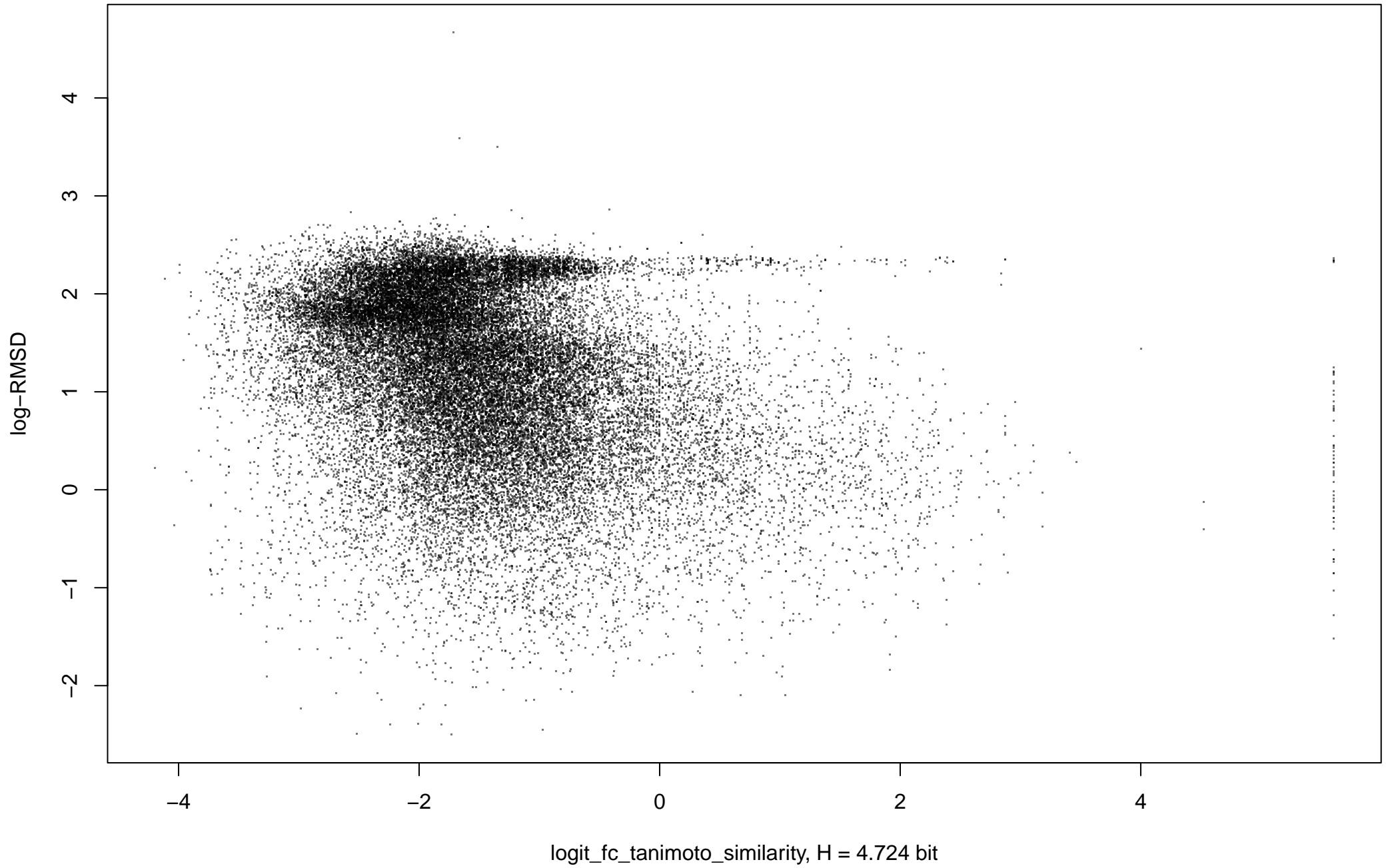
ec_tanimoto_similarity, MI = 0.1852 bit, norm = 0.04278, cond entr = 4.144 bit



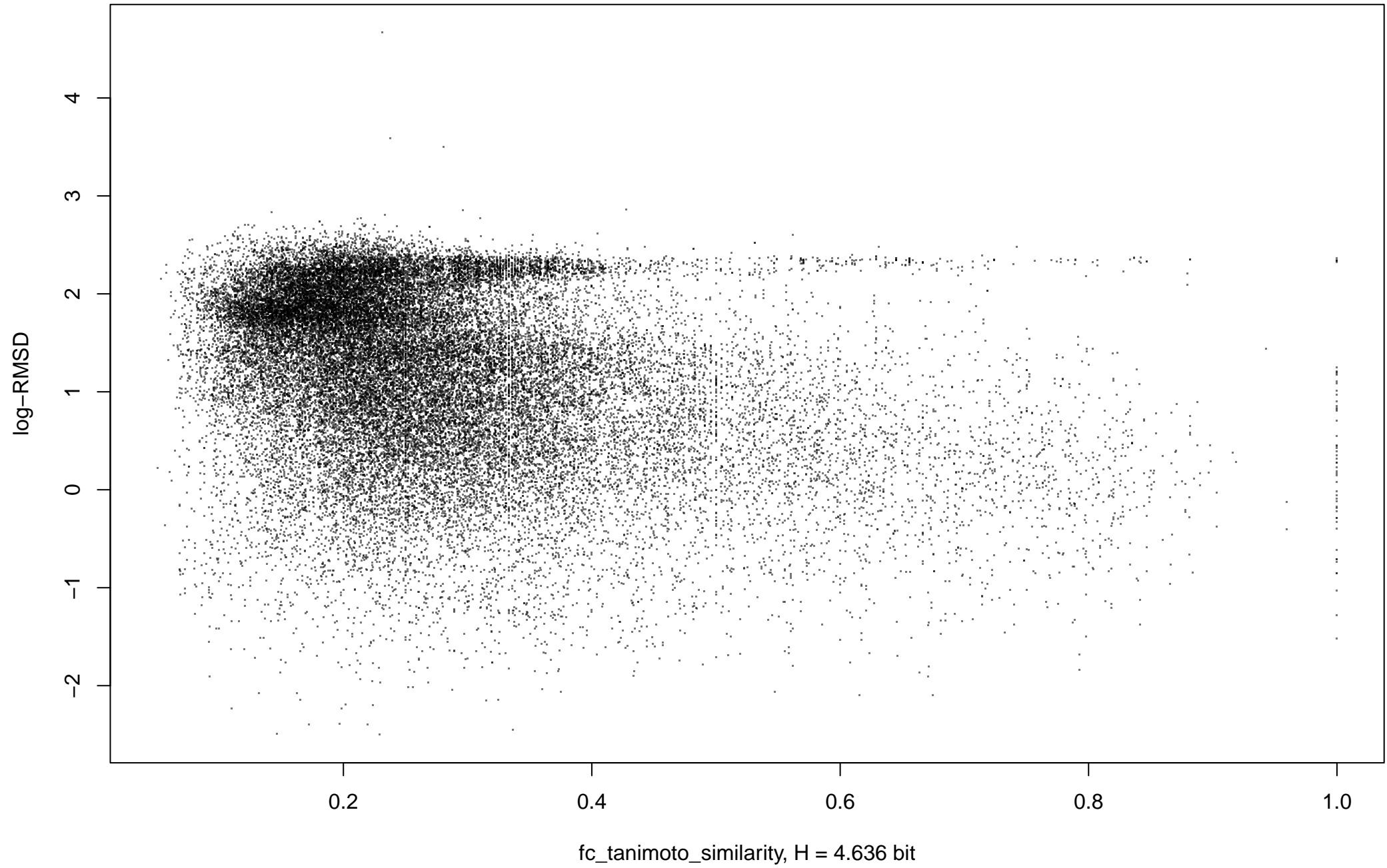
logit_ec_tanimoto_similarity, MI = 0.1817 bit, norm = 0.04197, cond entr = 4.148 bit



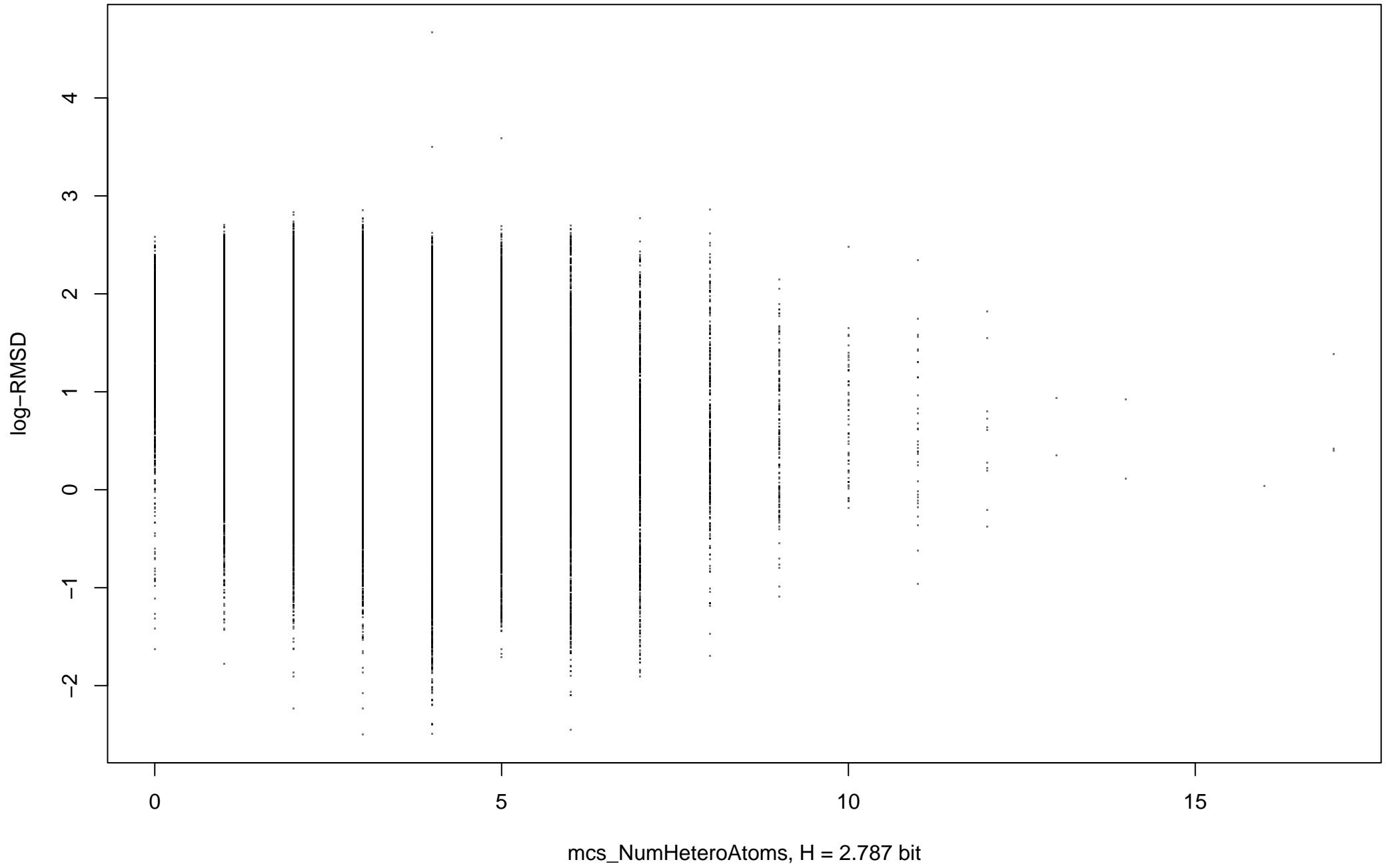
logit_fc_tanimoto_similarity, MI = 0.1707 bit, norm = 0.03943, cond entr = 4.159 bit



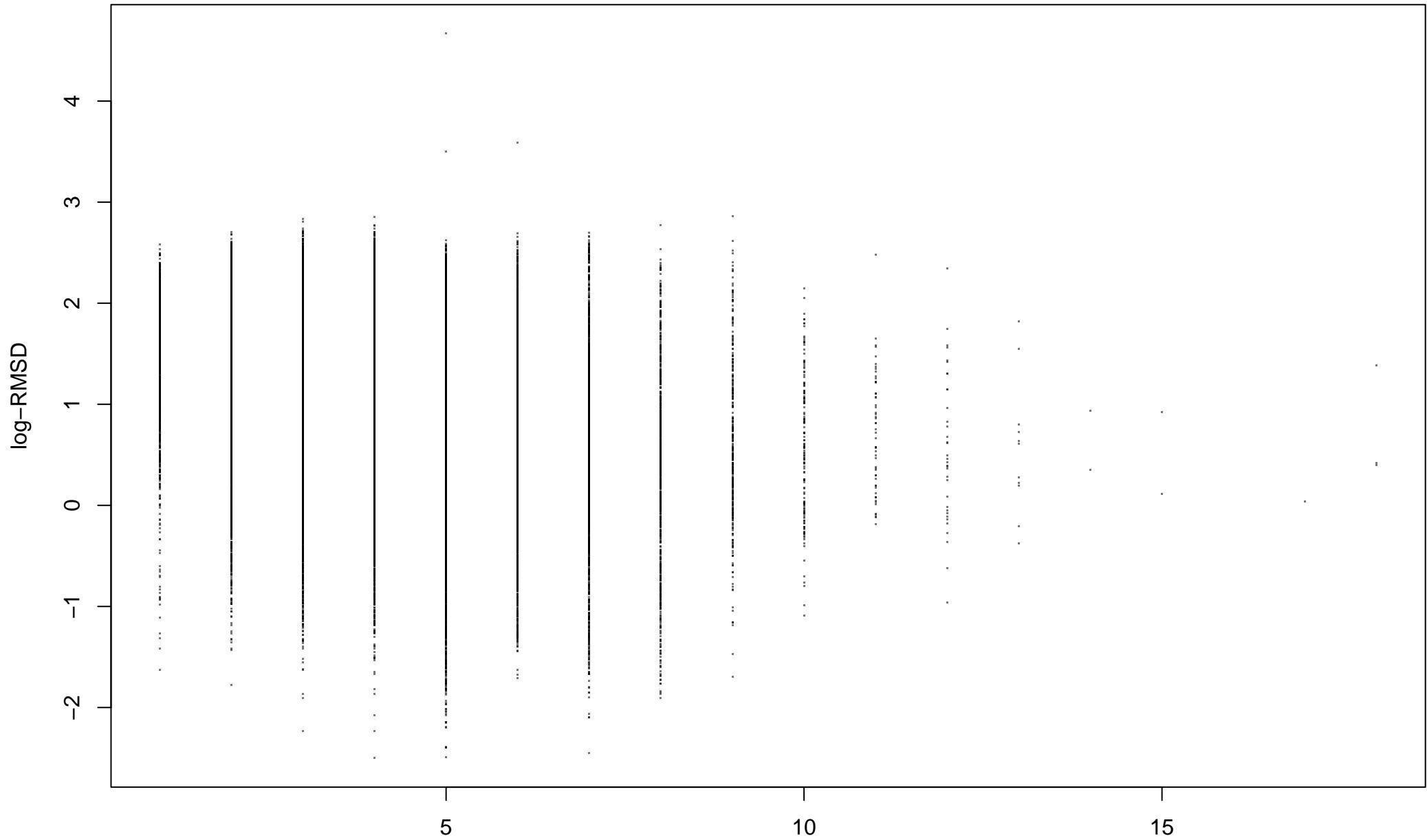
fc_tanimoto_similarity, MI = 0.1688 bit, norm = 0.03899, cond entr = 4.16 bit



mcs_NumHeteroAtoms, MI = 0.1567 bit, norm = 0.05623, cond entr = 4.173 bit

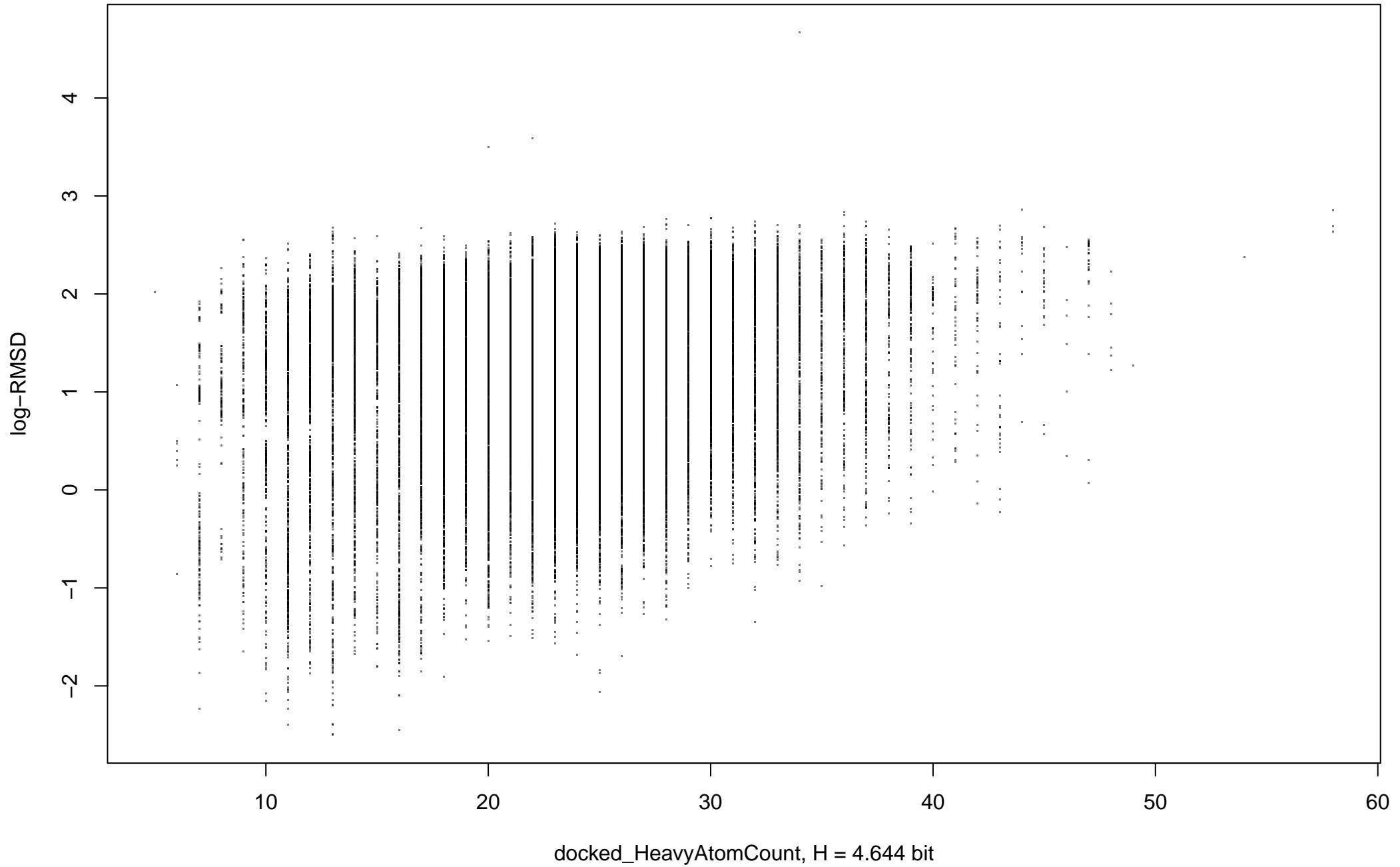


shift_mcs_NumHeteroAtoms, MI = 0.1567 bit, norm = 0.05623, cond entr = 4.173 bit

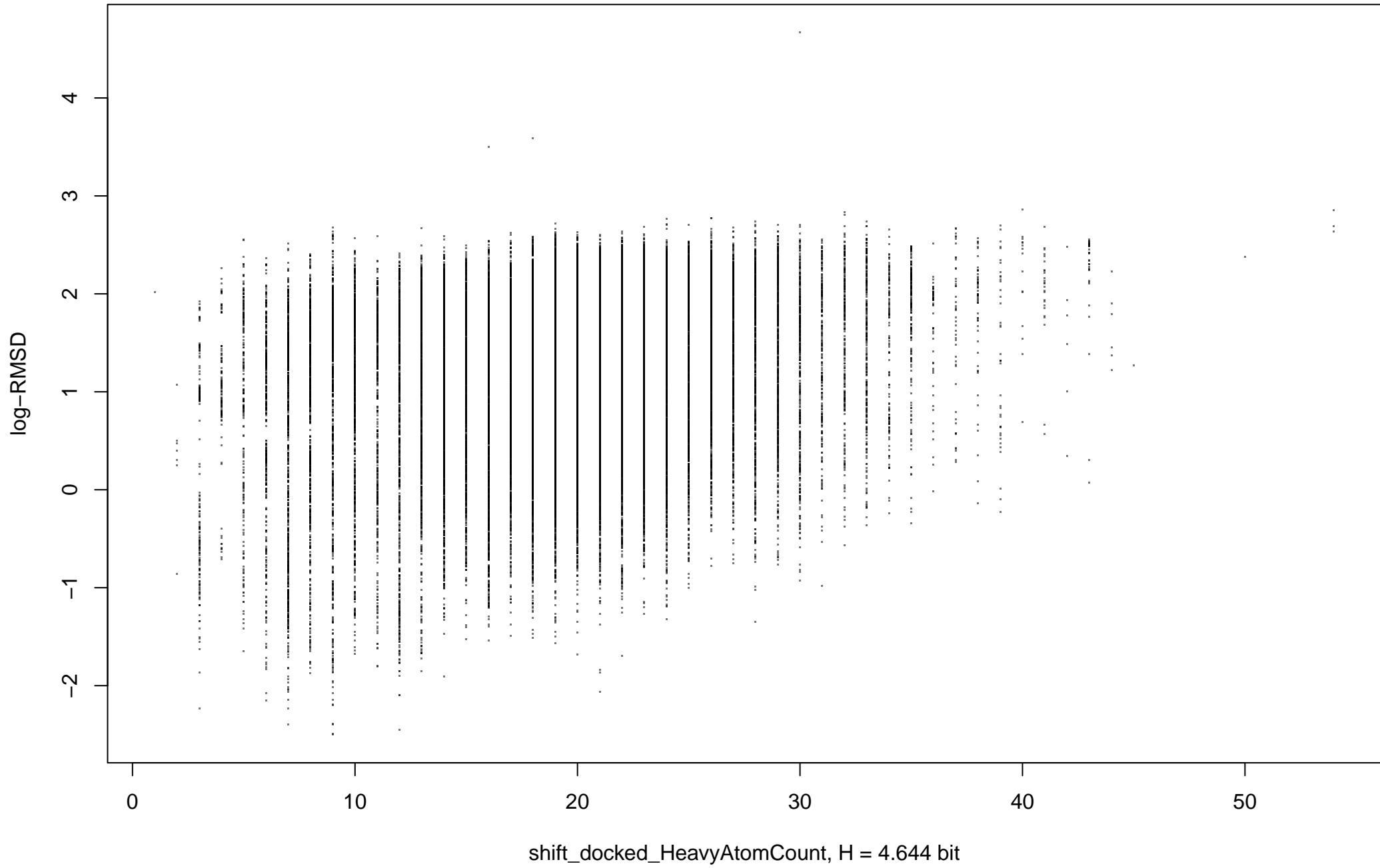


shift_mcs_NumHeteroAtoms, H = 2.787 bit

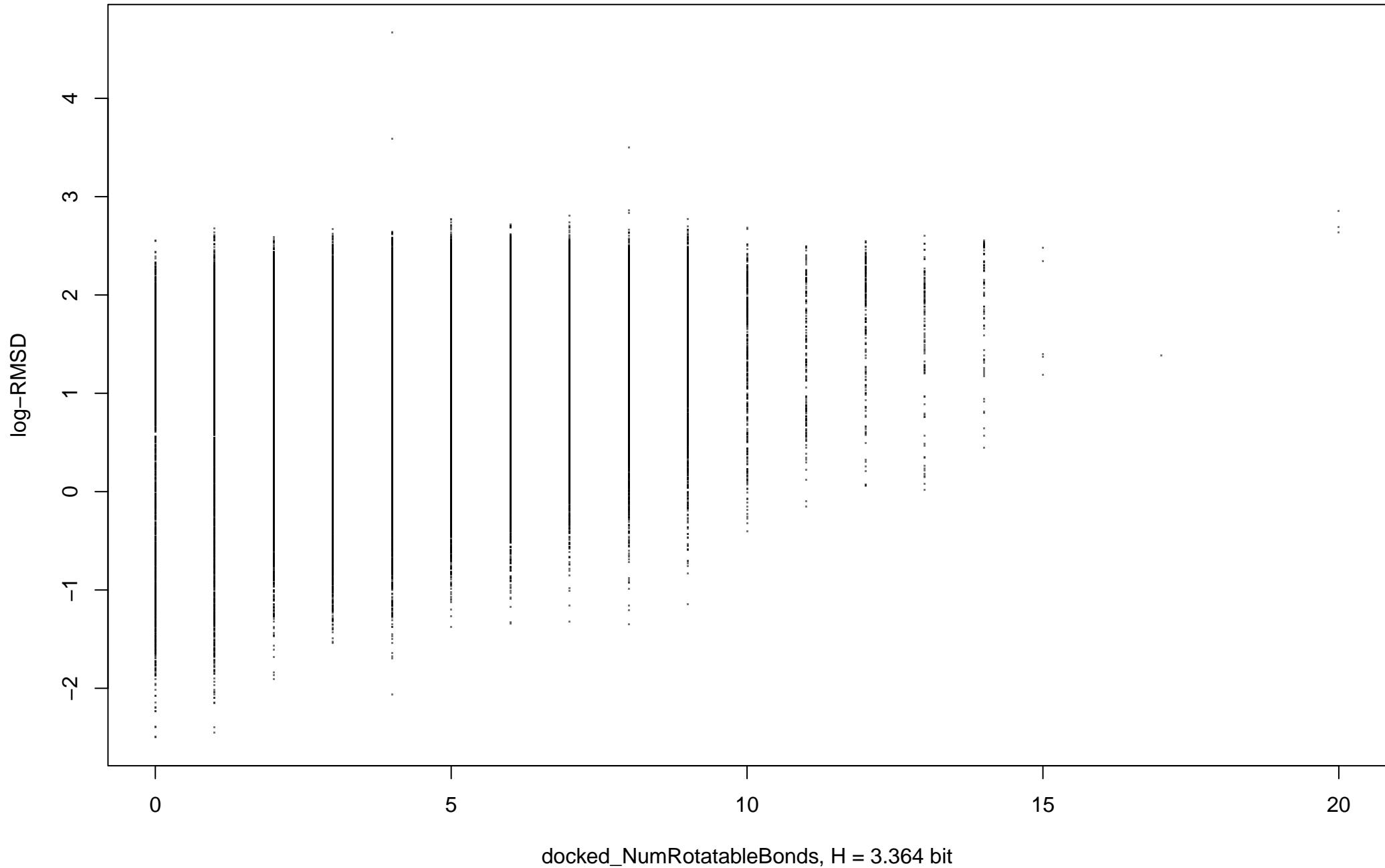
docked_HeavyAtomCount, MI = 0.1548 bit, norm = 0.03577, cond entr = 4.174 bit



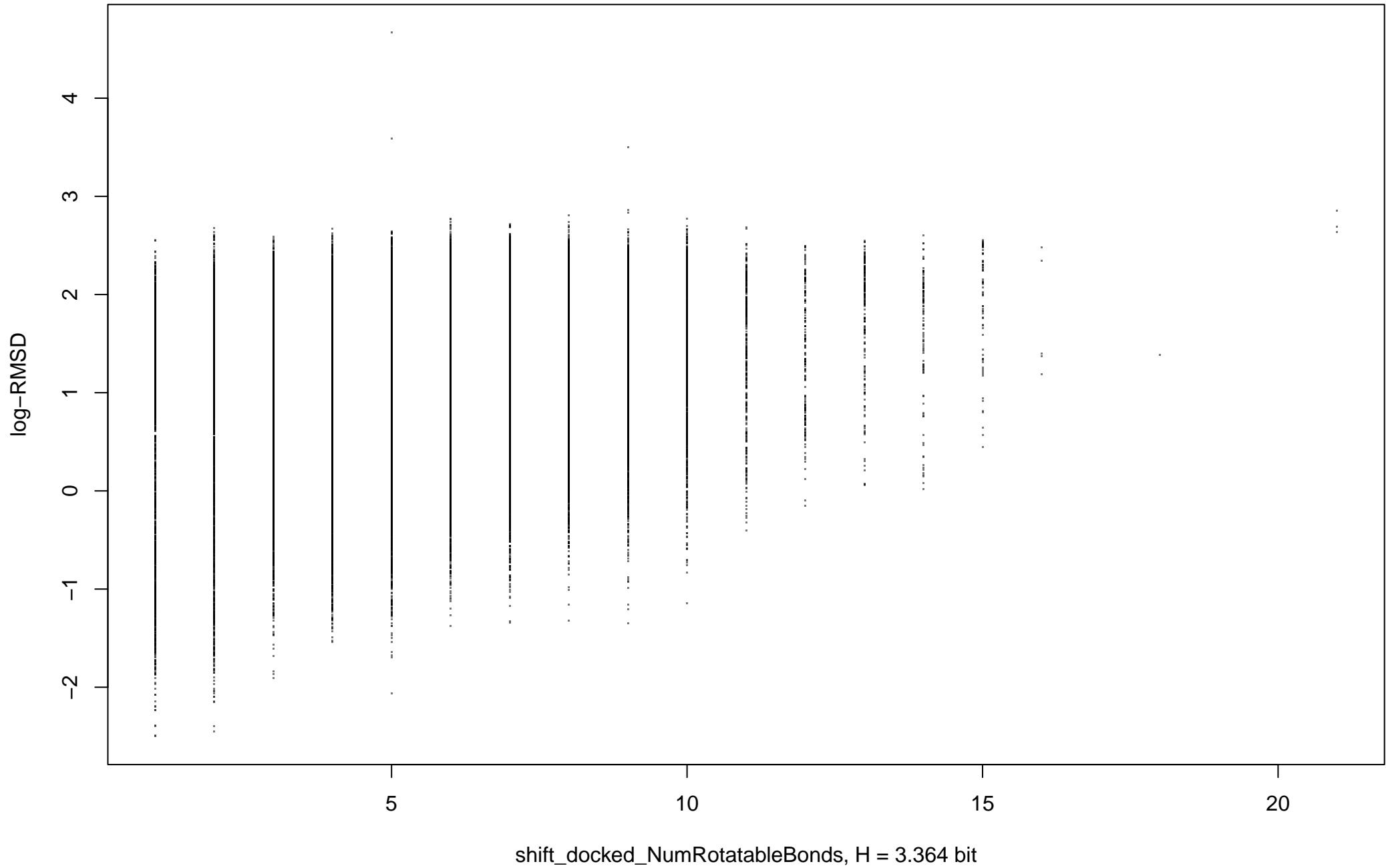
shift_docked_HeavyAtomCount, MI = 0.1548 bit, norm = 0.03577, cond entr = 4.174 bit



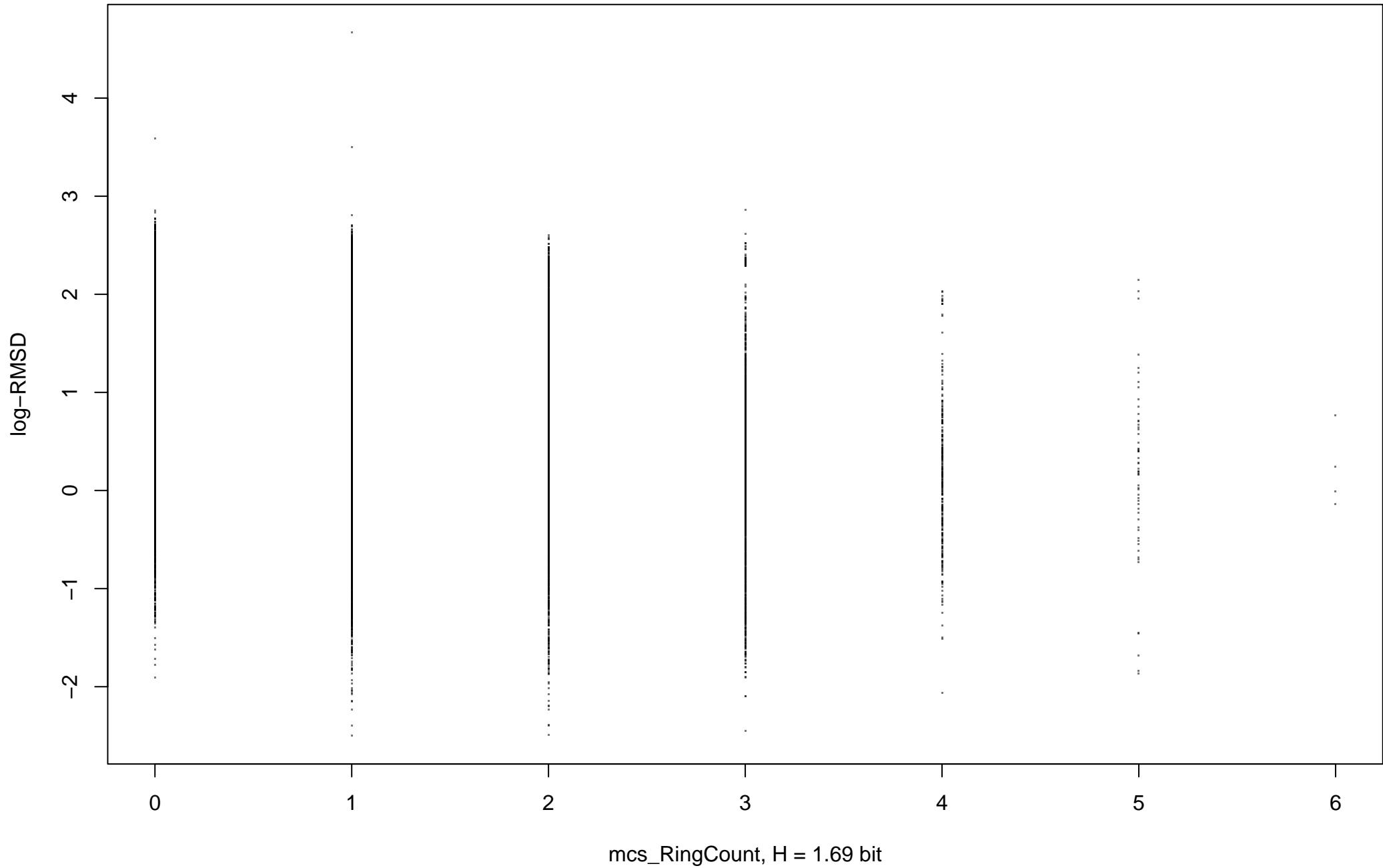
docked_NumRotatableBonds, MI = 0.145 bit, norm = 0.04309, cond entr = 4.184 bit



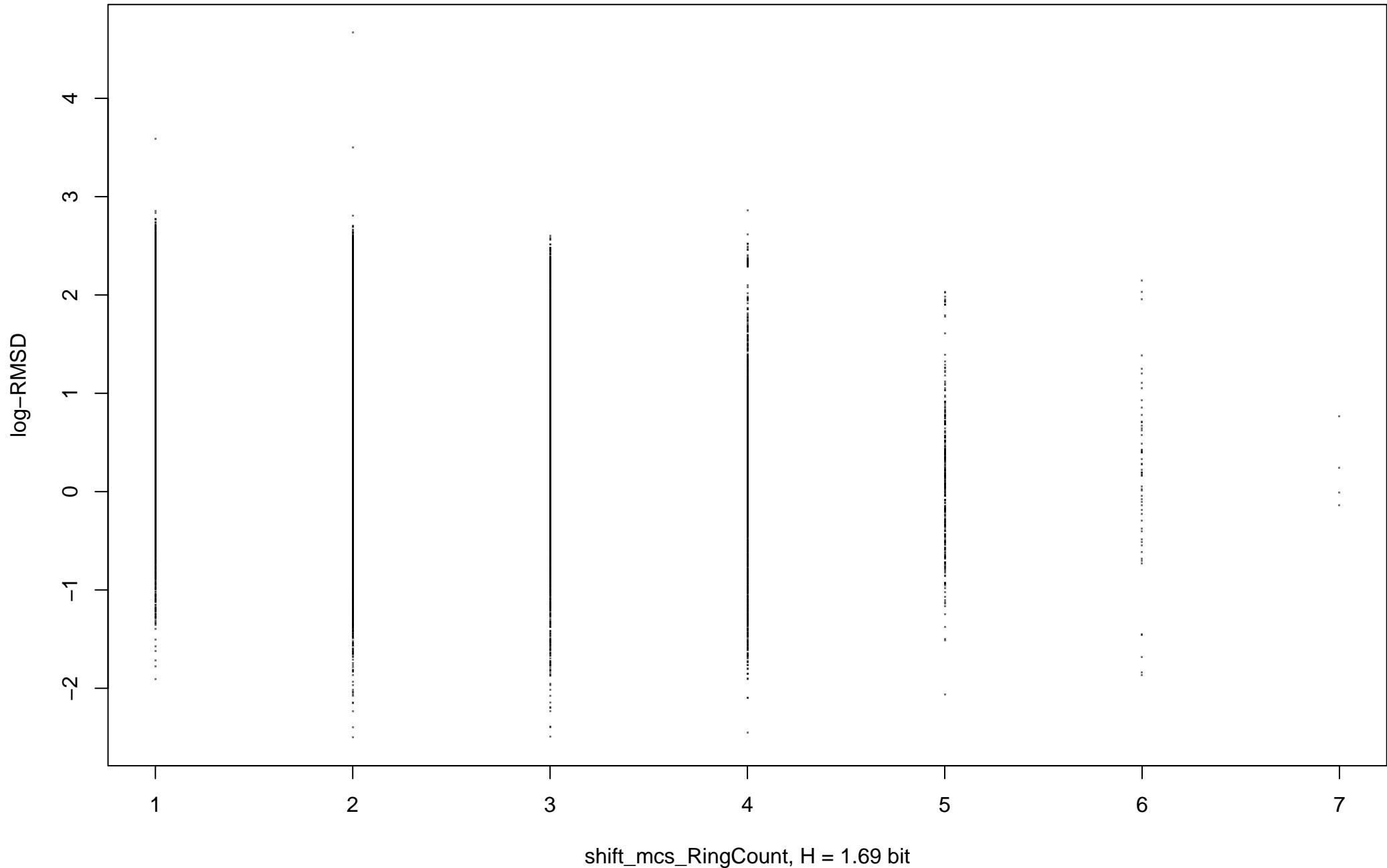
shift_docked_NumRotatableBonds, MI = 0.145 bit, norm = 0.04309, cond entr = 4.184 bit



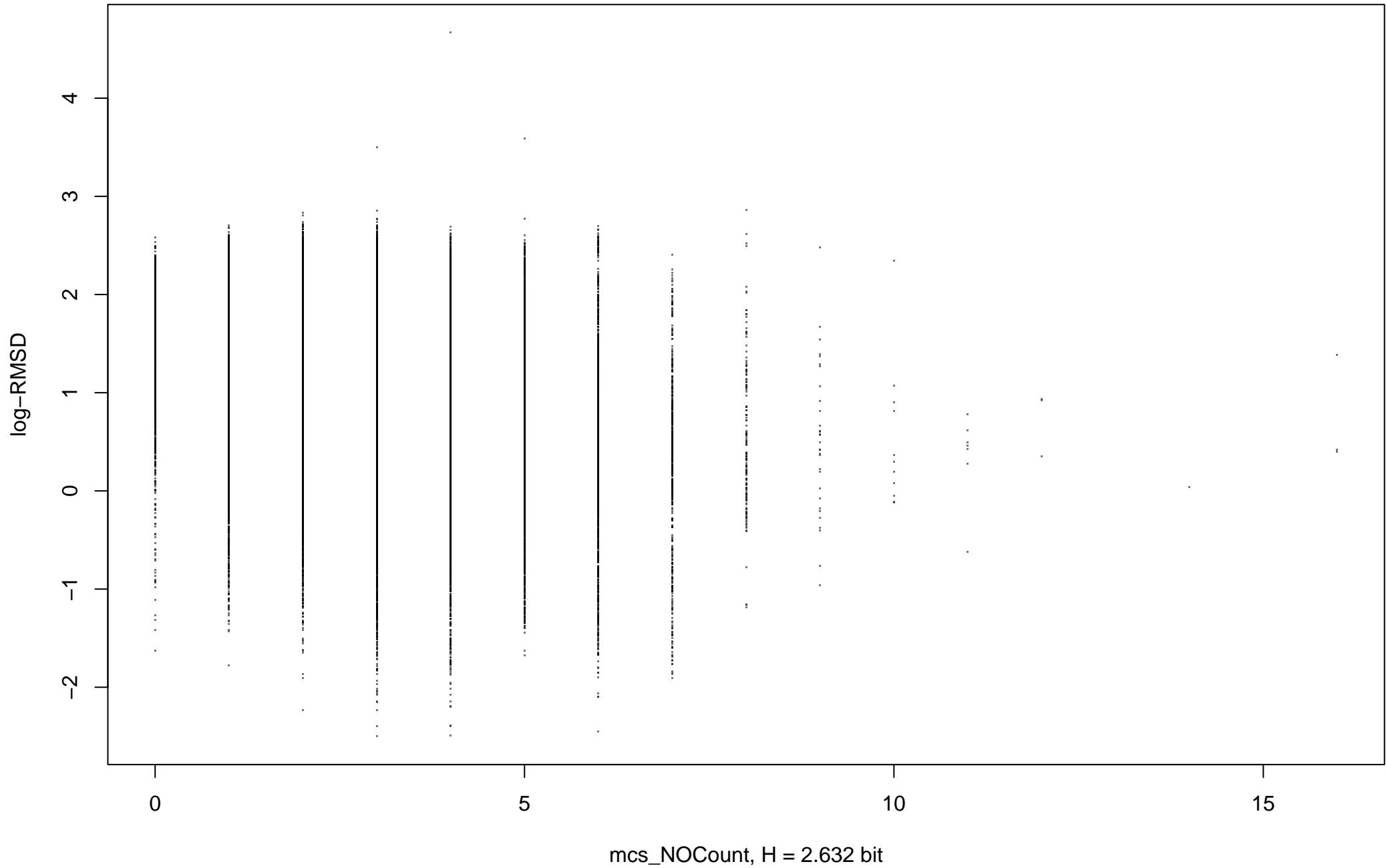
mcs_RingCount, MI = 0.1435 bit, norm = 0.08488, cond entr = 4.186 bit



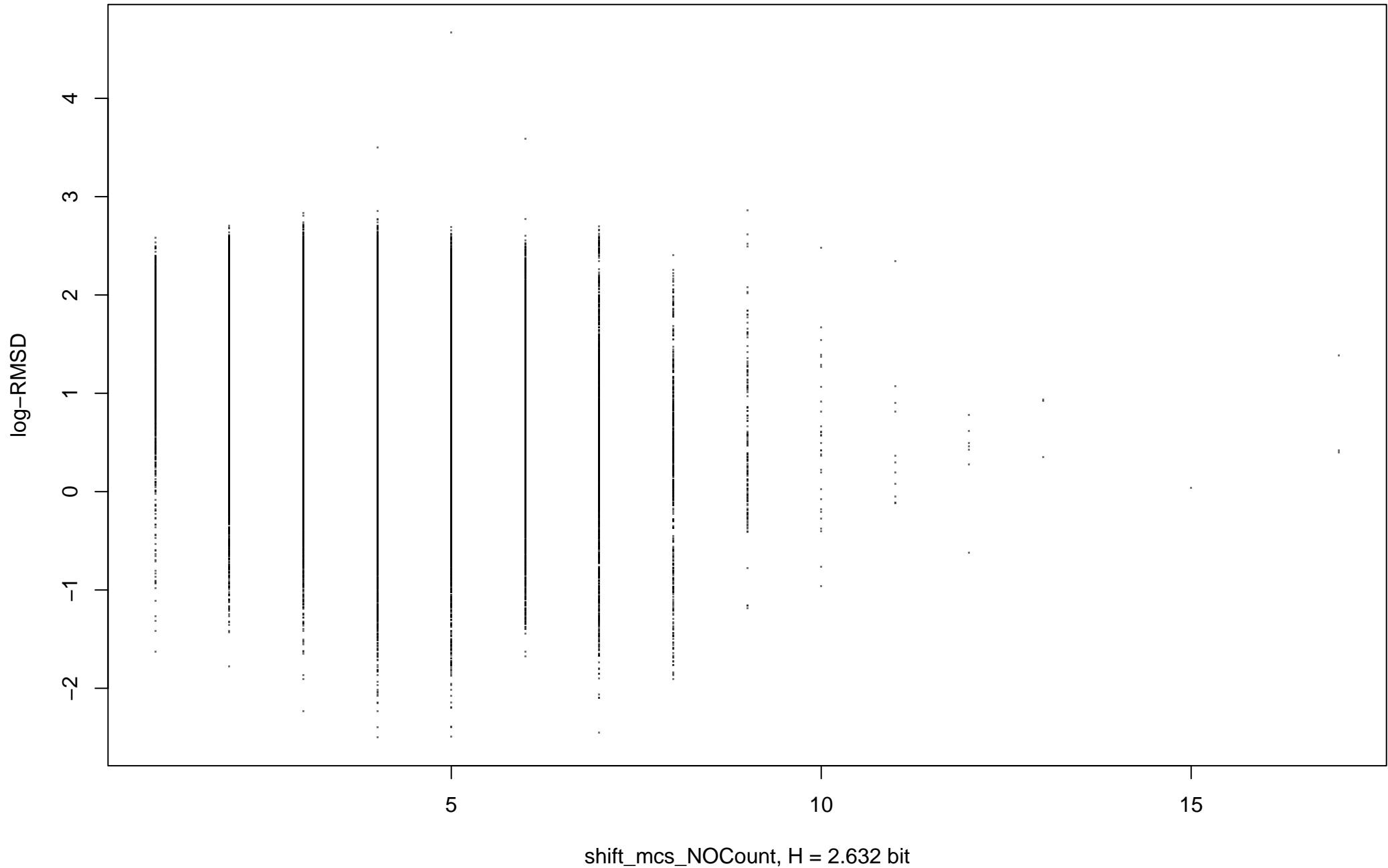
shift_mcs_RingCount, MI = 0.1435 bit, norm = 0.08488, cond entr = 4.186 bit



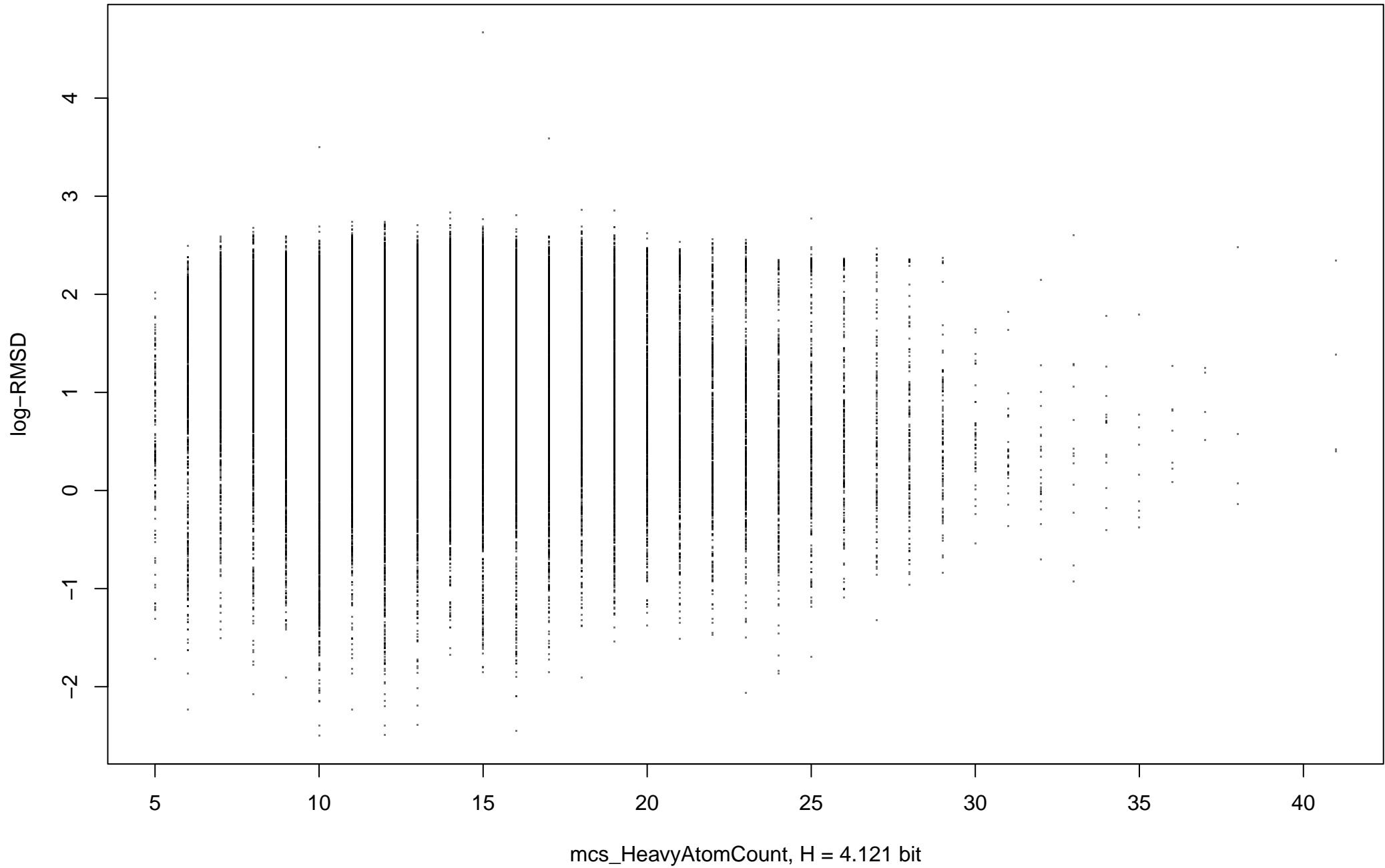
mcs_NOCount, MI = 0.1379 bit, norm = 0.0524, cond entr = 4.191 bit



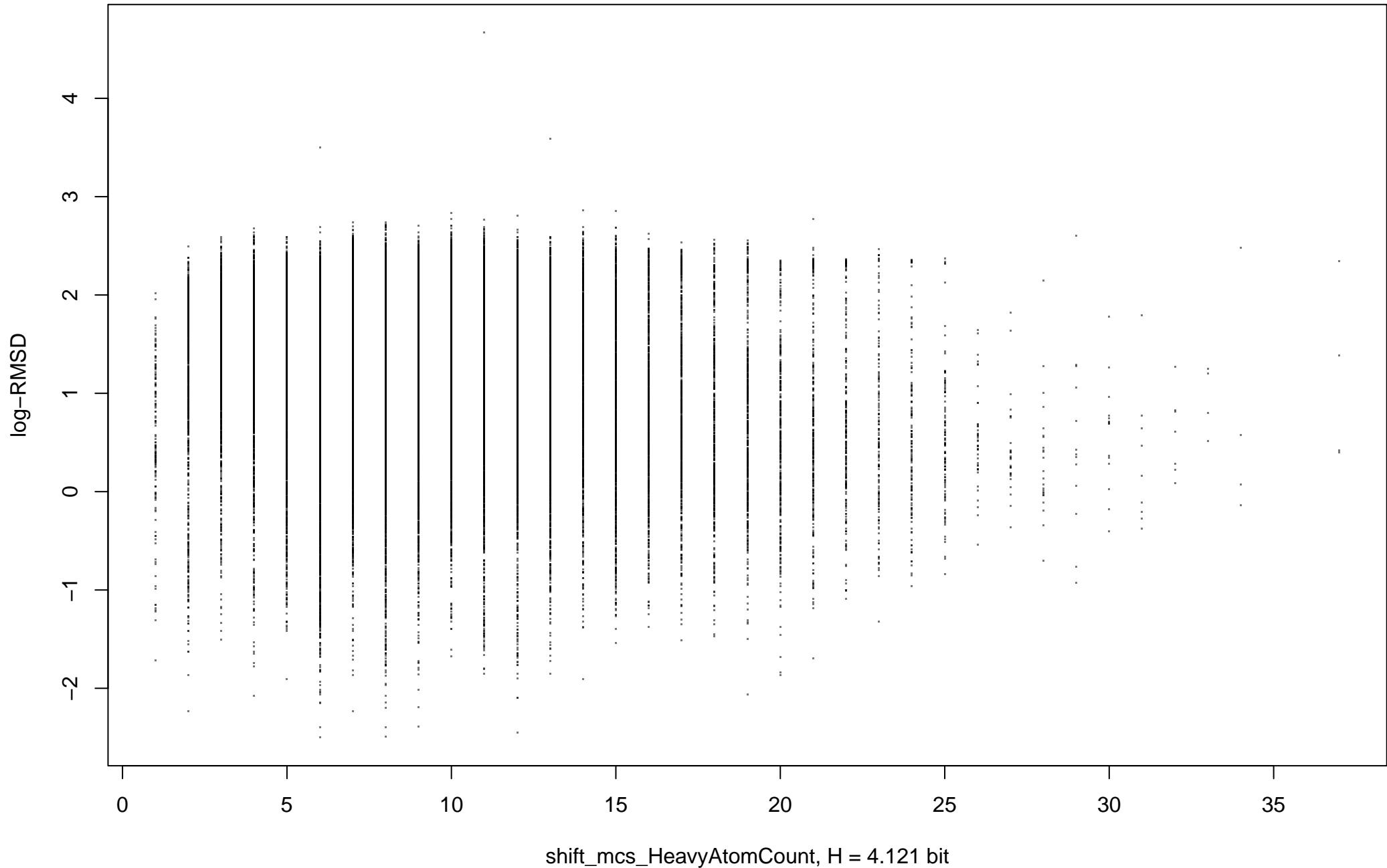
shift_mcs_NOCount, MI = 0.1379 bit, norm = 0.0524, cond entr = 4.191 bit



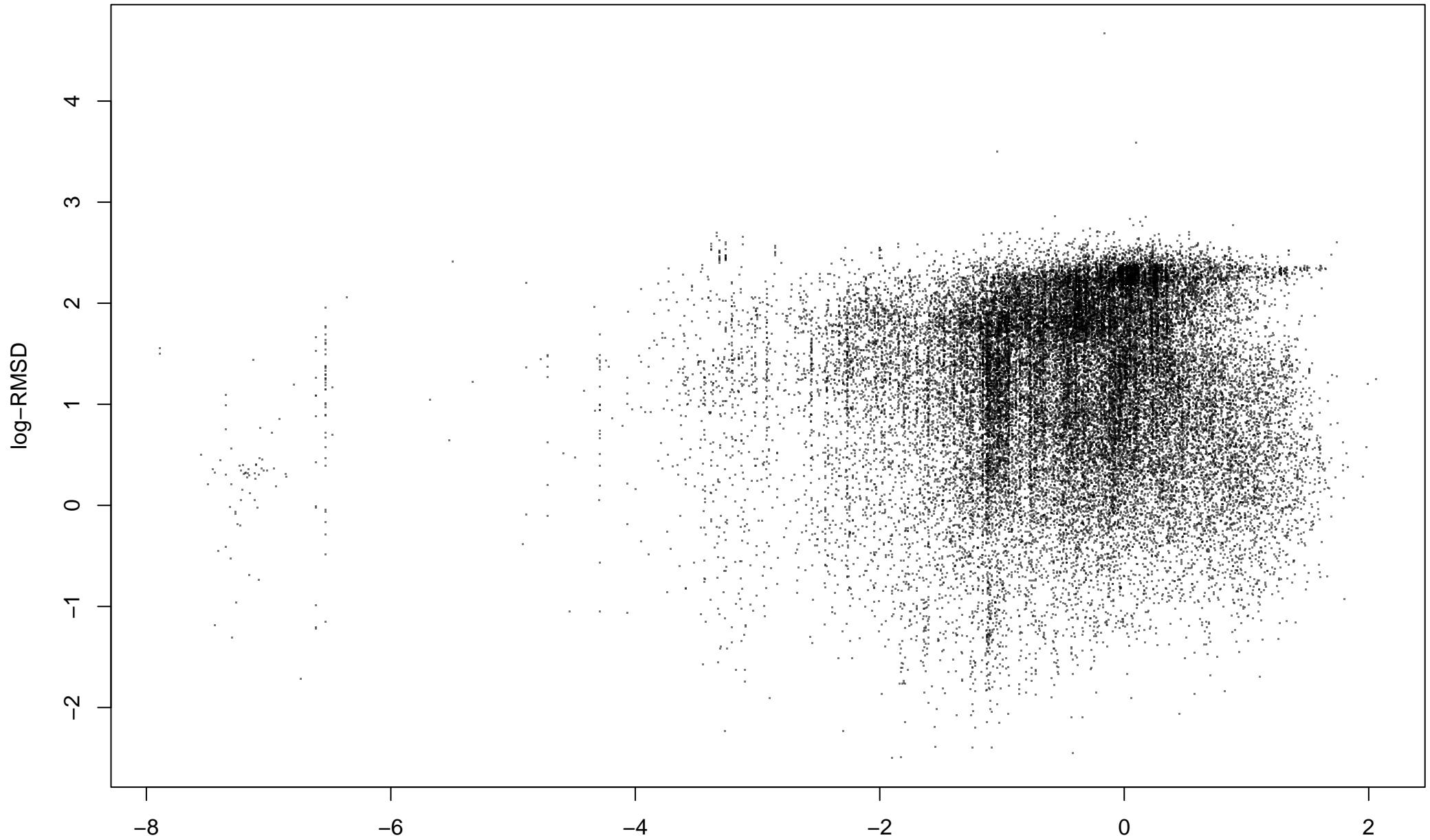
mcs_HeavyAtomCount, MI = 0.1235 bit, norm = 0.02997, cond entr = 4.206 bit



shift_mcs_HeavyAtomCount, MI = 0.1235 bit, norm = 0.02997, cond entr = 4.206 bit

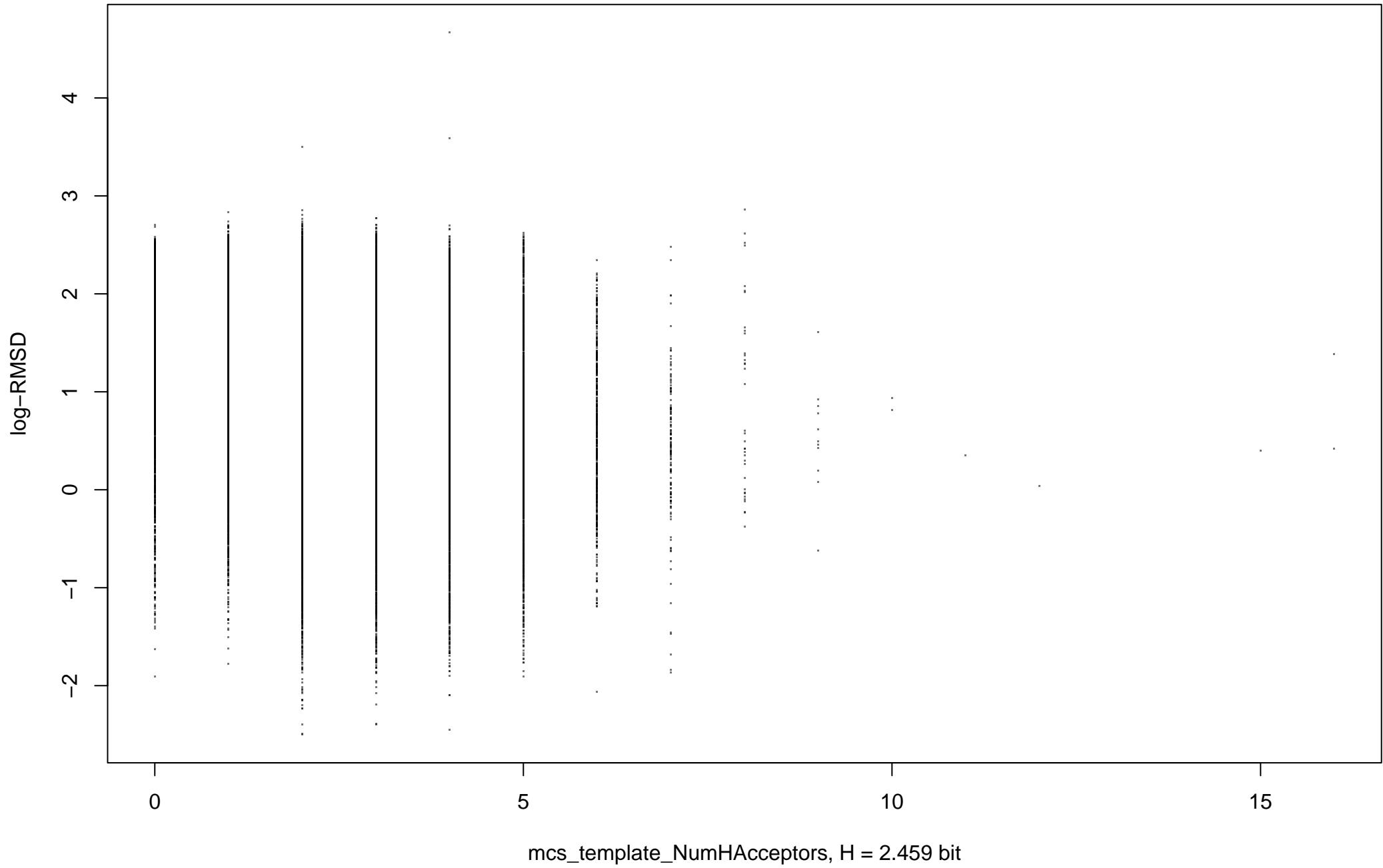


log_mcs_unbonded_apolar_sasa, MI = 0.1145 bit, norm = 0.02645, cond entr = 4.215 bit

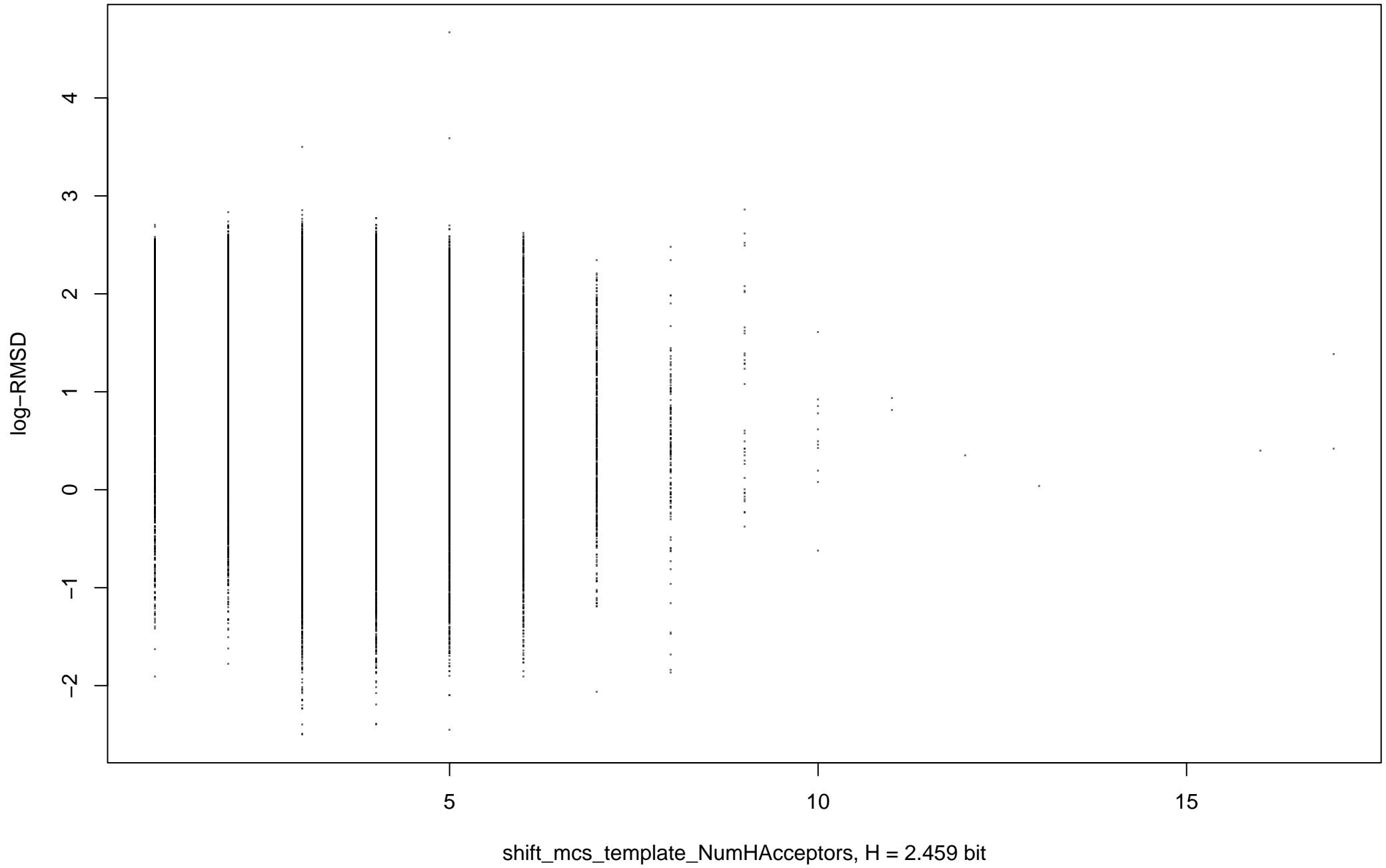


log_mcs_unbonded_apolar_sasa, H = 4.604 bit

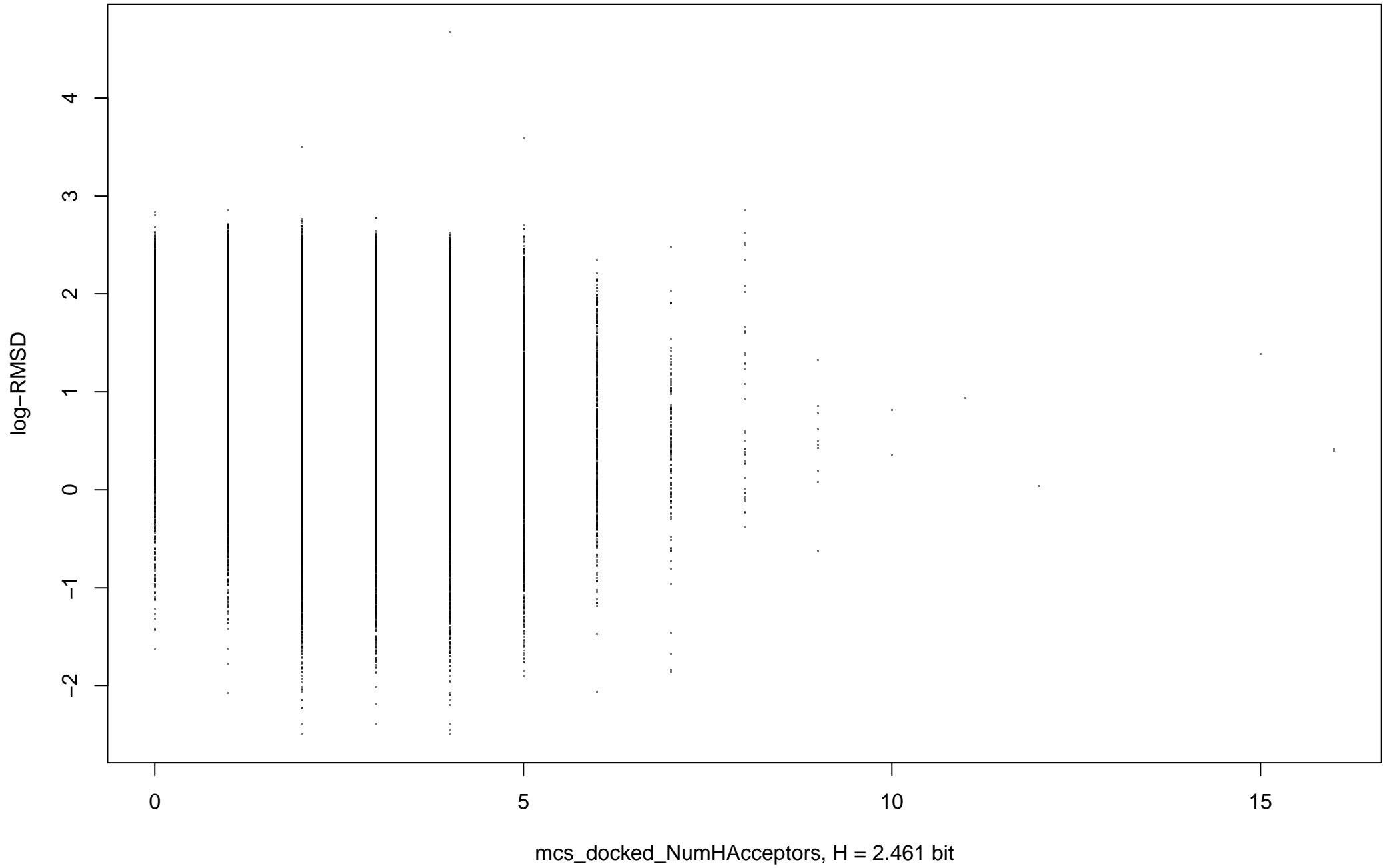
mcs_template_NumHAcceptors, MI = 0.1131 bit, norm = 0.04598, cond entr = 4.216 bit



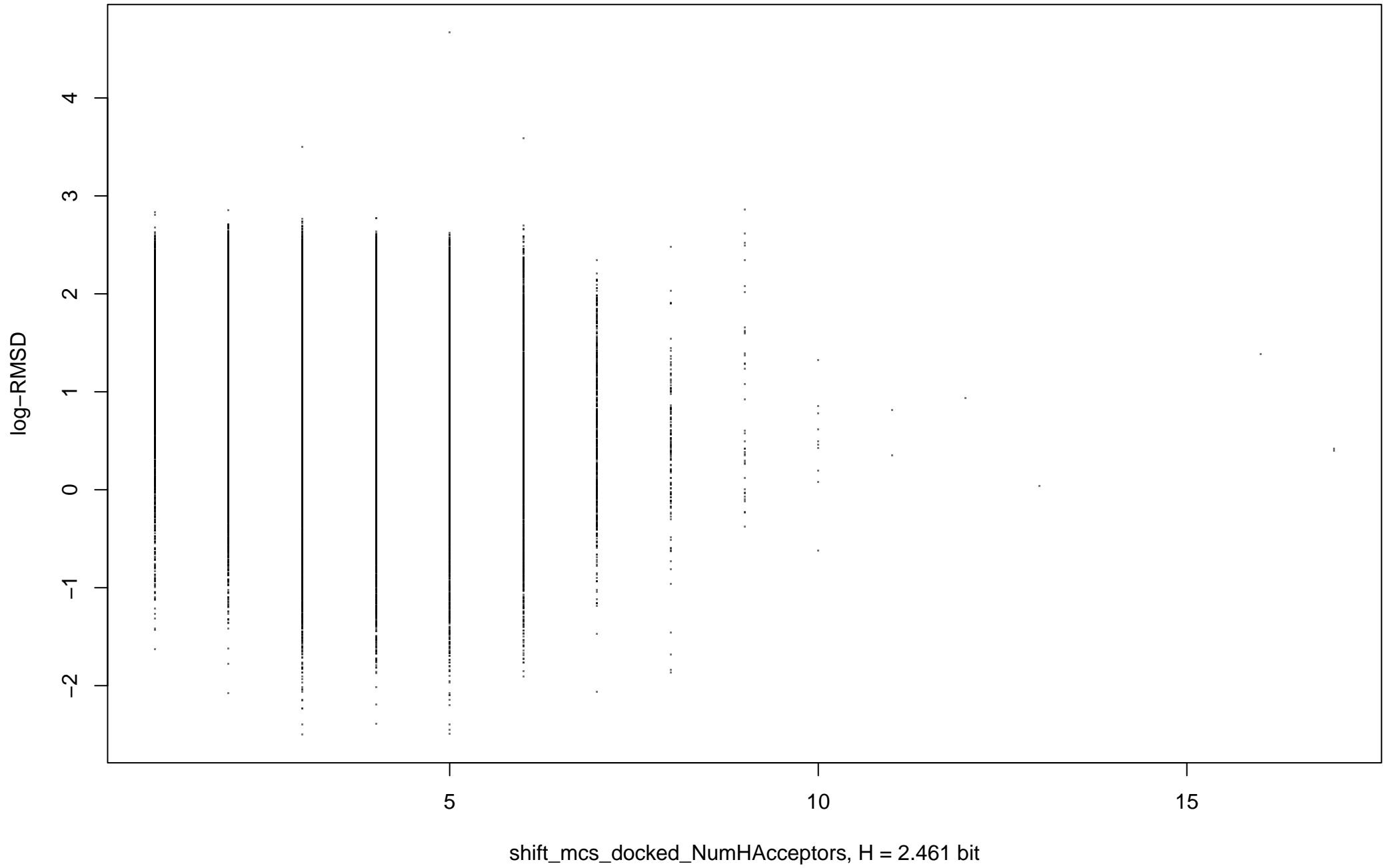
shift_mcs_template_NumHAcceptors, MI = 0.1131 bit, norm = 0.04598, cond entr = 4.216 bit



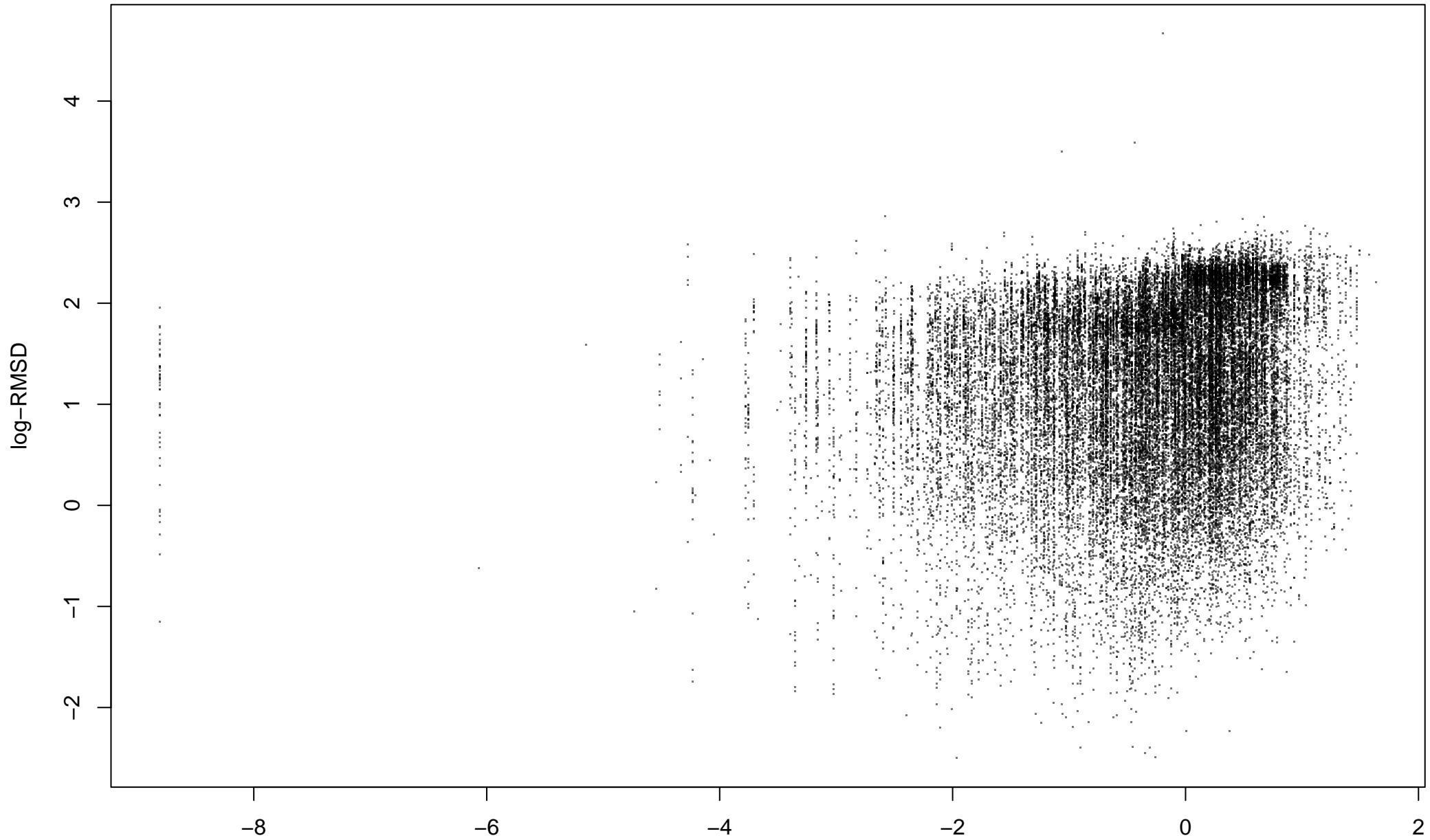
mcs_docked_NumHAcceptors, MI = 0.1129 bit, norm = 0.04589, cond entr = 4.216 bit



shift_mcs_docked_NumHAcceptors, MI = 0.1129 bit, norm = 0.04589, cond entr = 4.216 bit

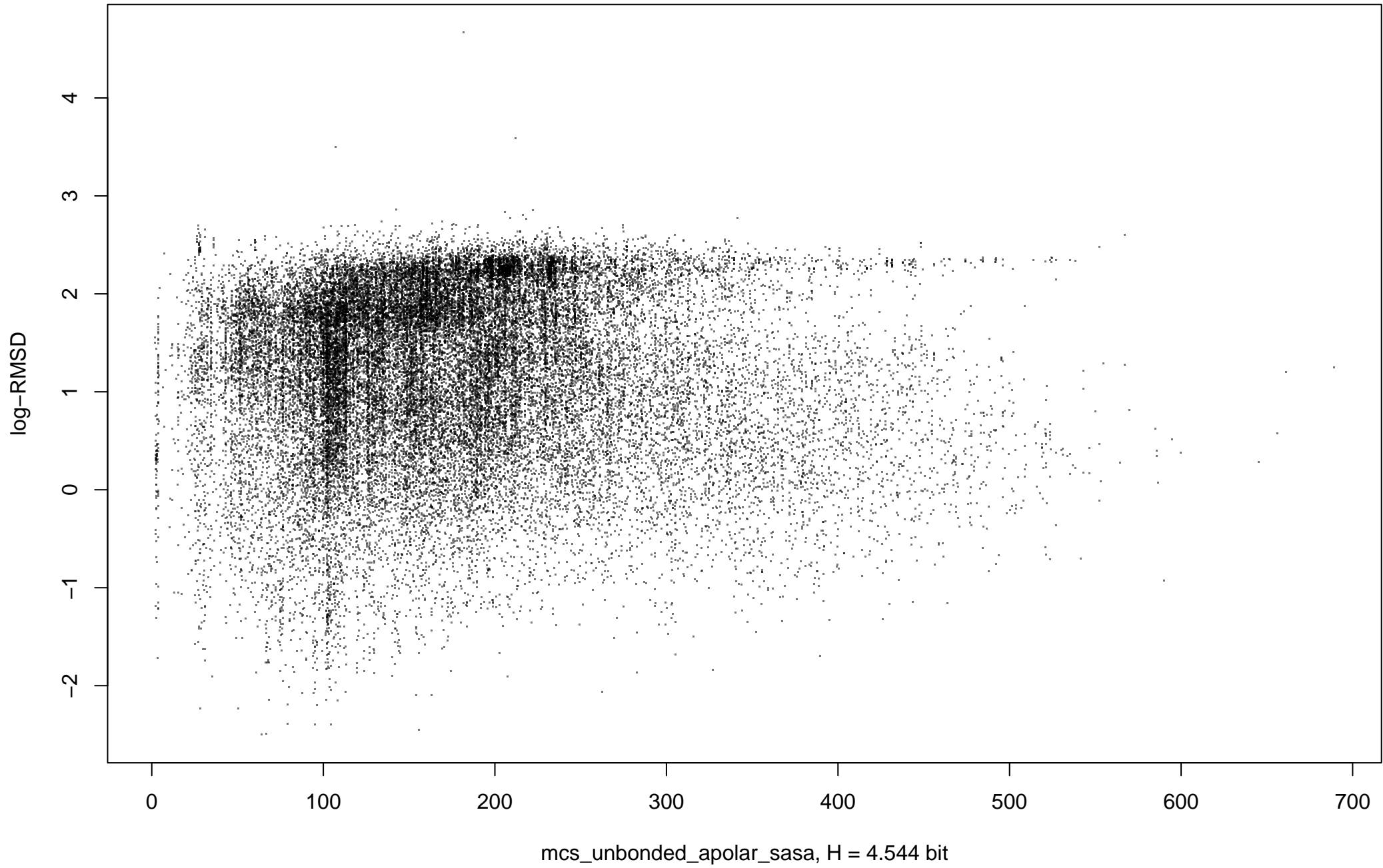


log_sasa_unbonded_apolar, MI = 0.1097 bit, norm = 0.02534, cond entr = 4.22 bit



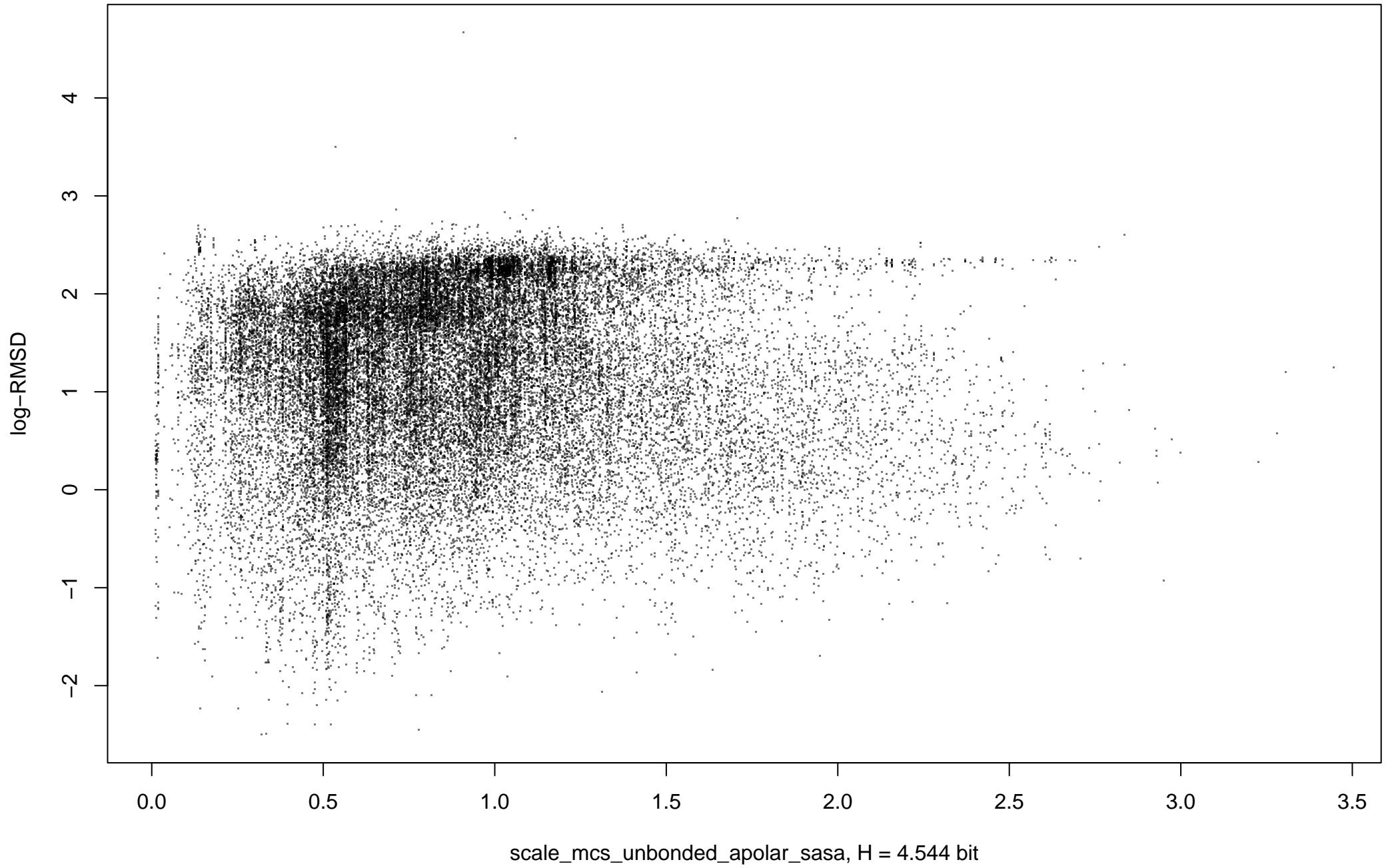
log_sasa_unbonded_apolar, H = 4.553 bit

mcs_unbonded_apolar_sasa, MI = 0.1084 bit, norm = 0.02505, cond entr = 4.221 bit

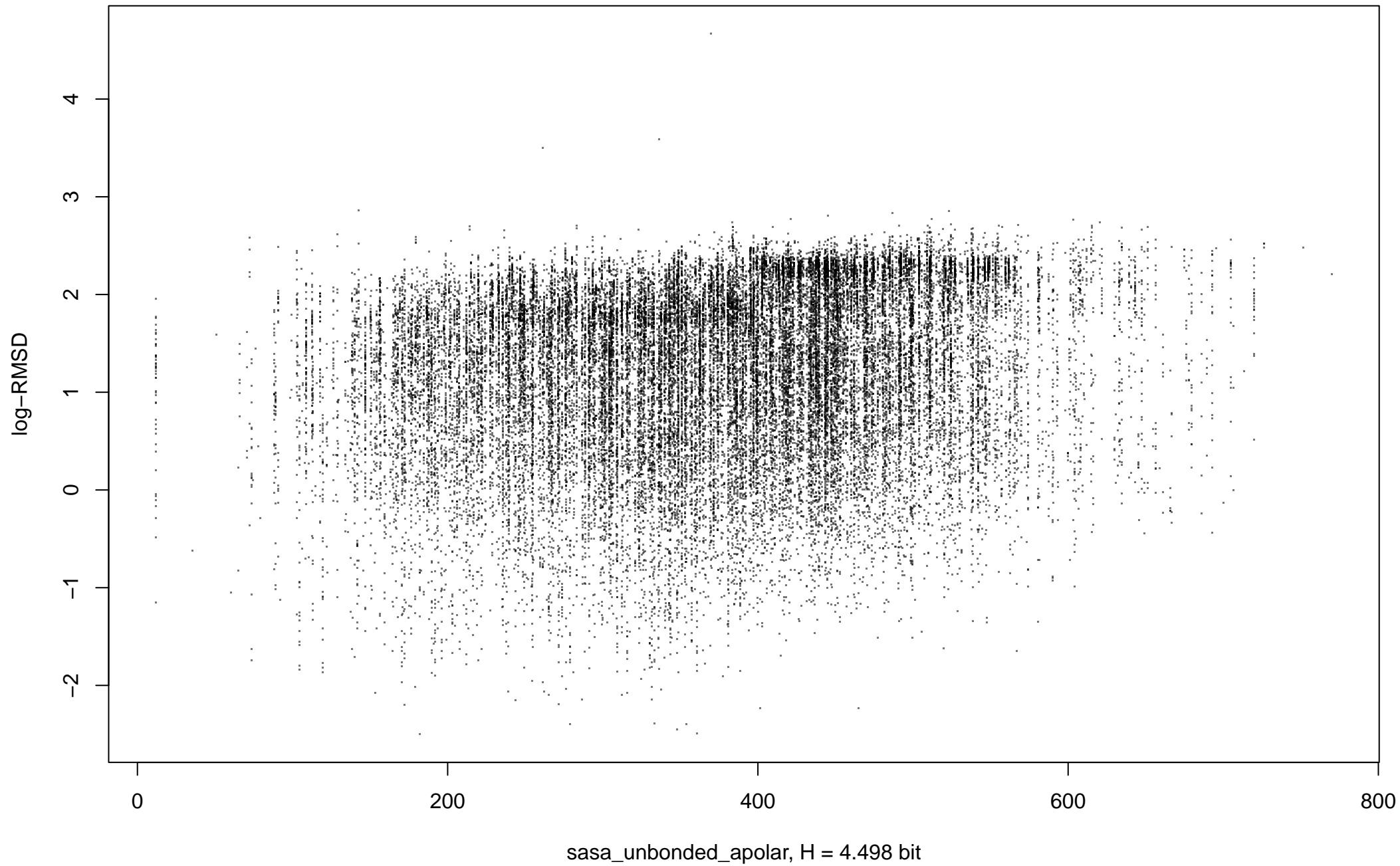


mcs_unbonded_apolar_sasa, H = 4.544 bit

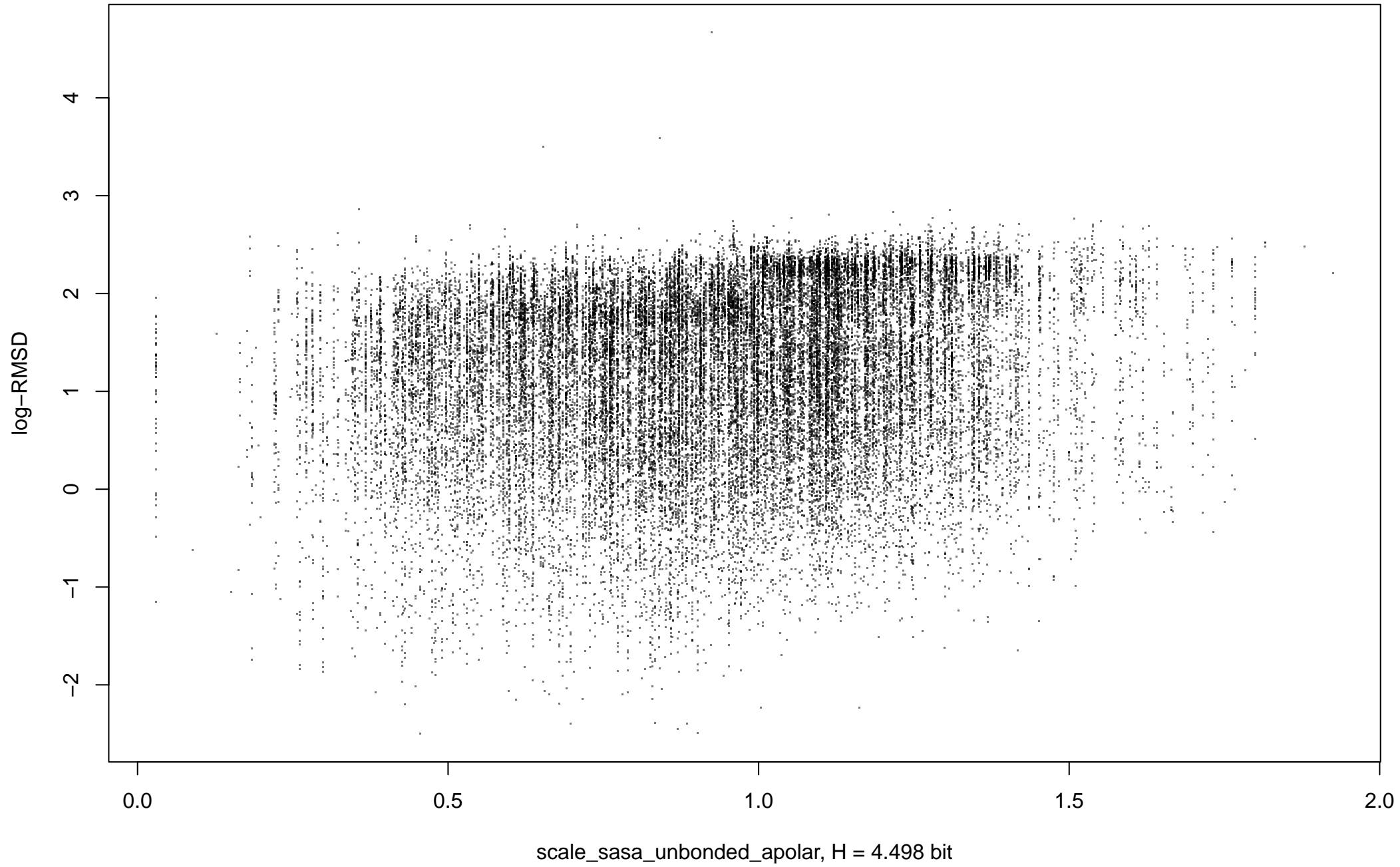
scale_mcs_unbonded_apolar_sasa, MI = 0.1084 bit, norm = 0.02505, cond entr = 4.221 bit



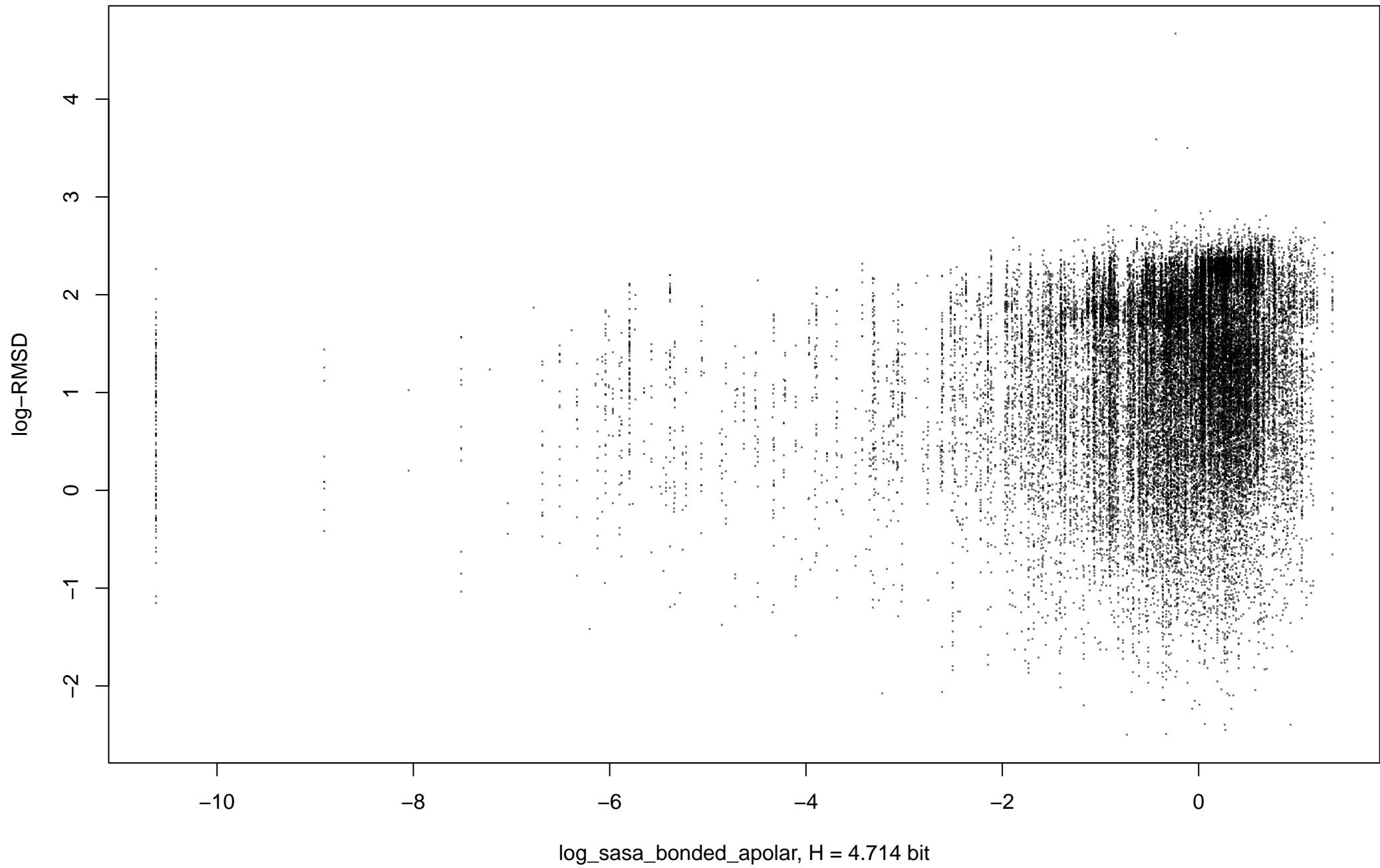
sasa_unbonded_apolar, MI = 0.1078 bit, norm = 0.02489, cond entr = 4.221 bit



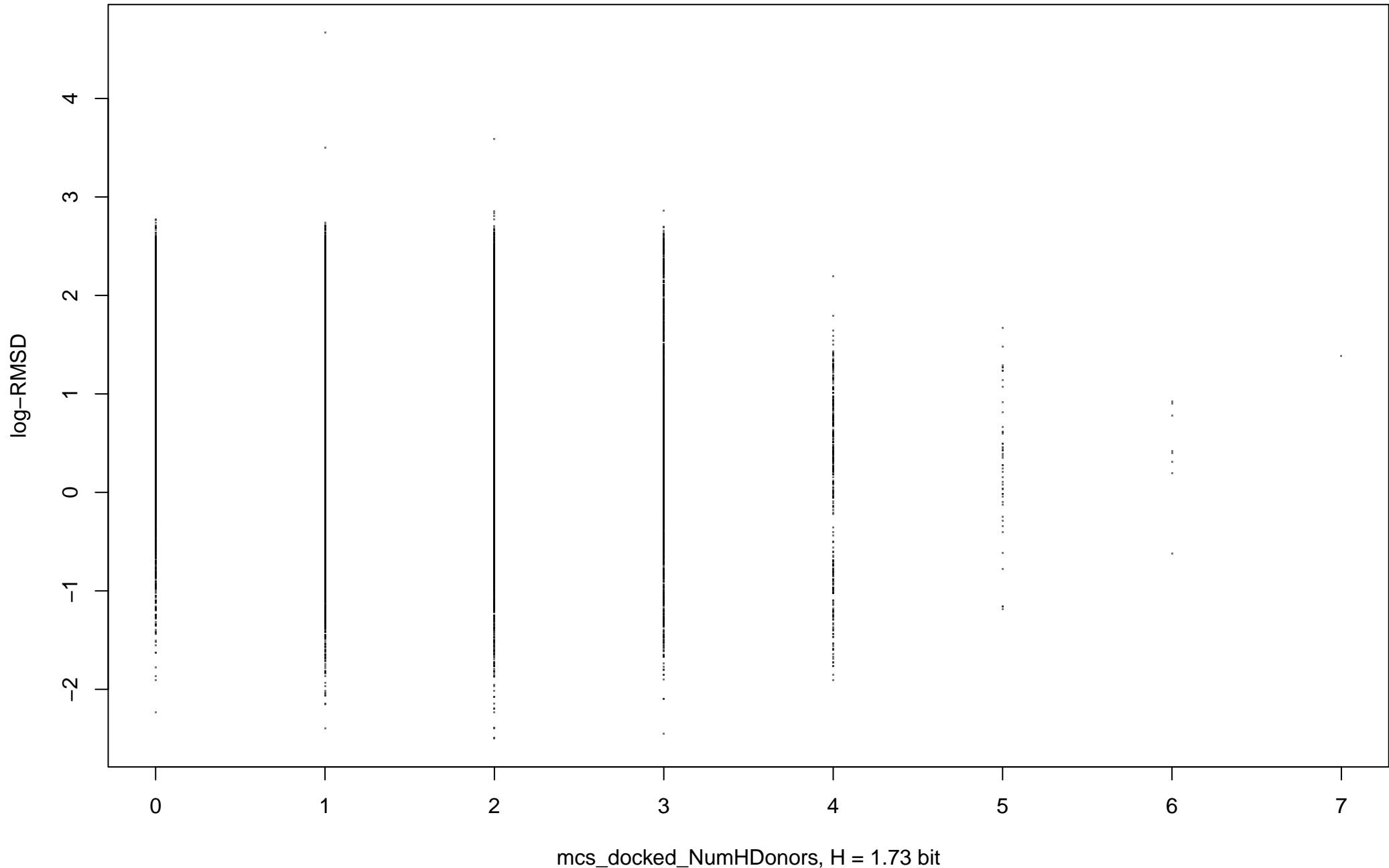
scale_sasa_unbonded_apolar, MI = 0.1078 bit, norm = 0.02489, cond entr = 4.221 bit



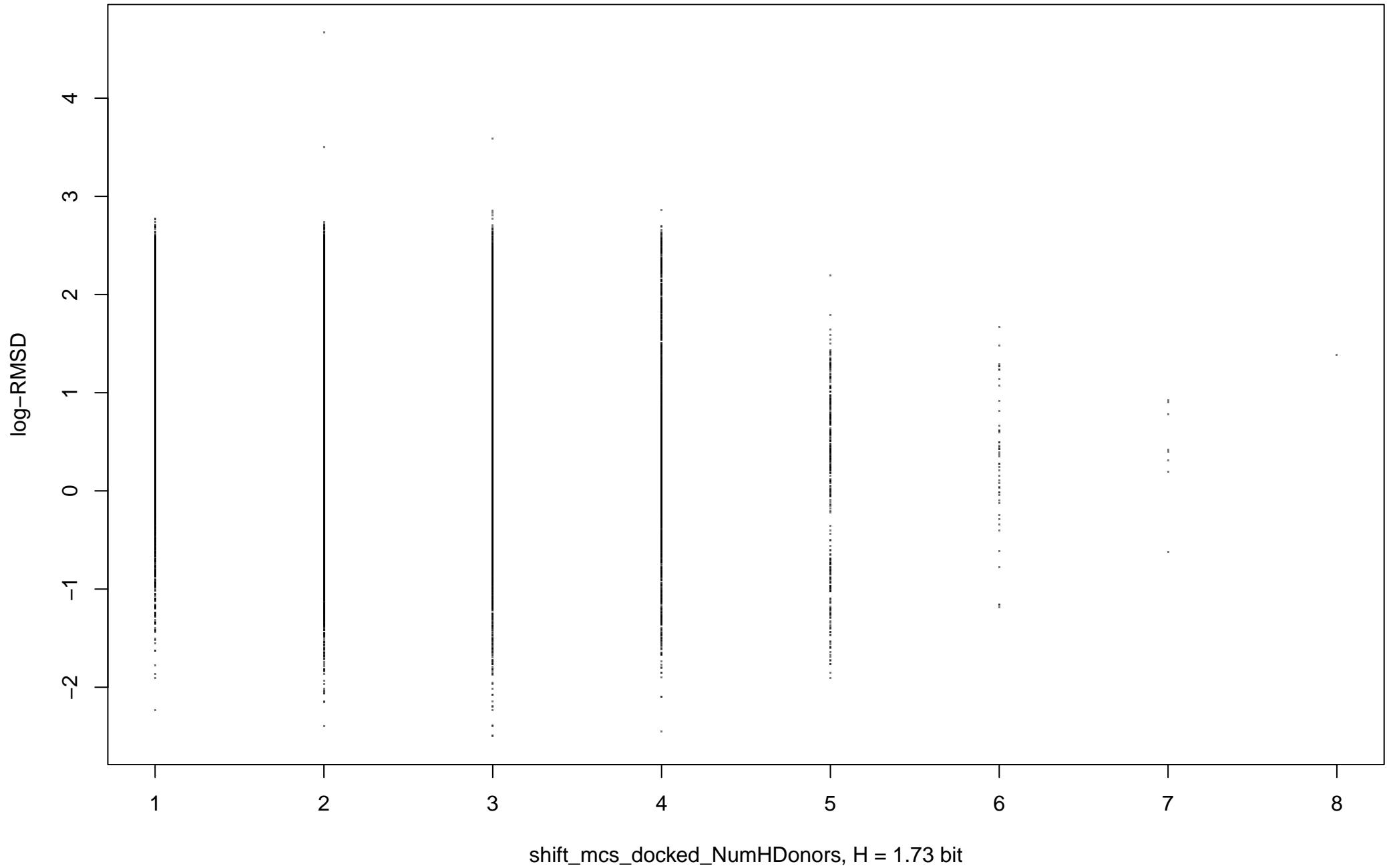
log_sasa_bonded_apolar, MI = 0.1063 bit, norm = 0.02455, cond entr = 4.223 bit



mcs_docked_NumHDonors, MI = 0.1026 bit, norm = 0.05929, cond entr = 4.227 bit

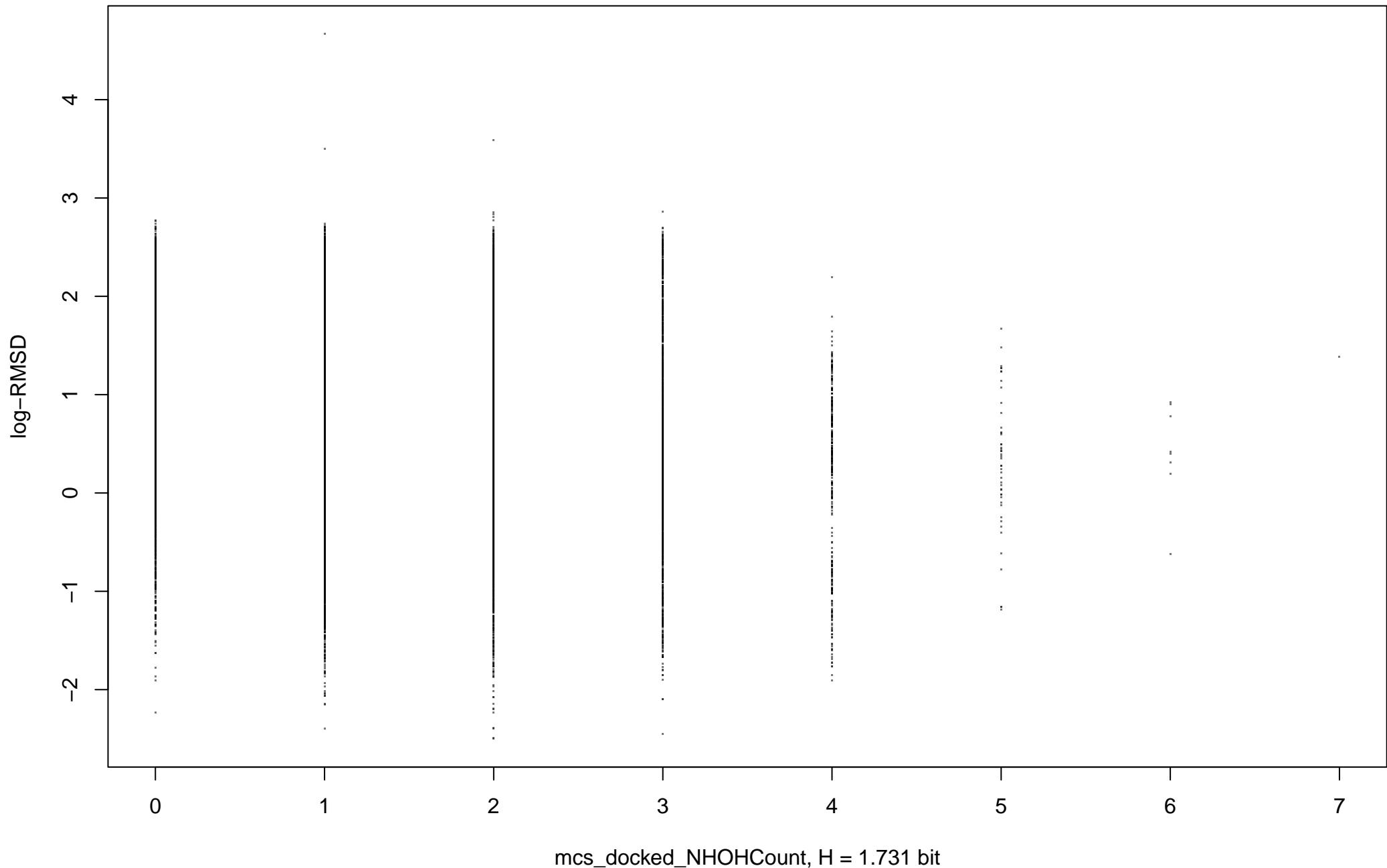


shift_mcs_docked_NumHDonors, MI = 0.1026 bit, norm = 0.05929, cond entr = 4.227 bit

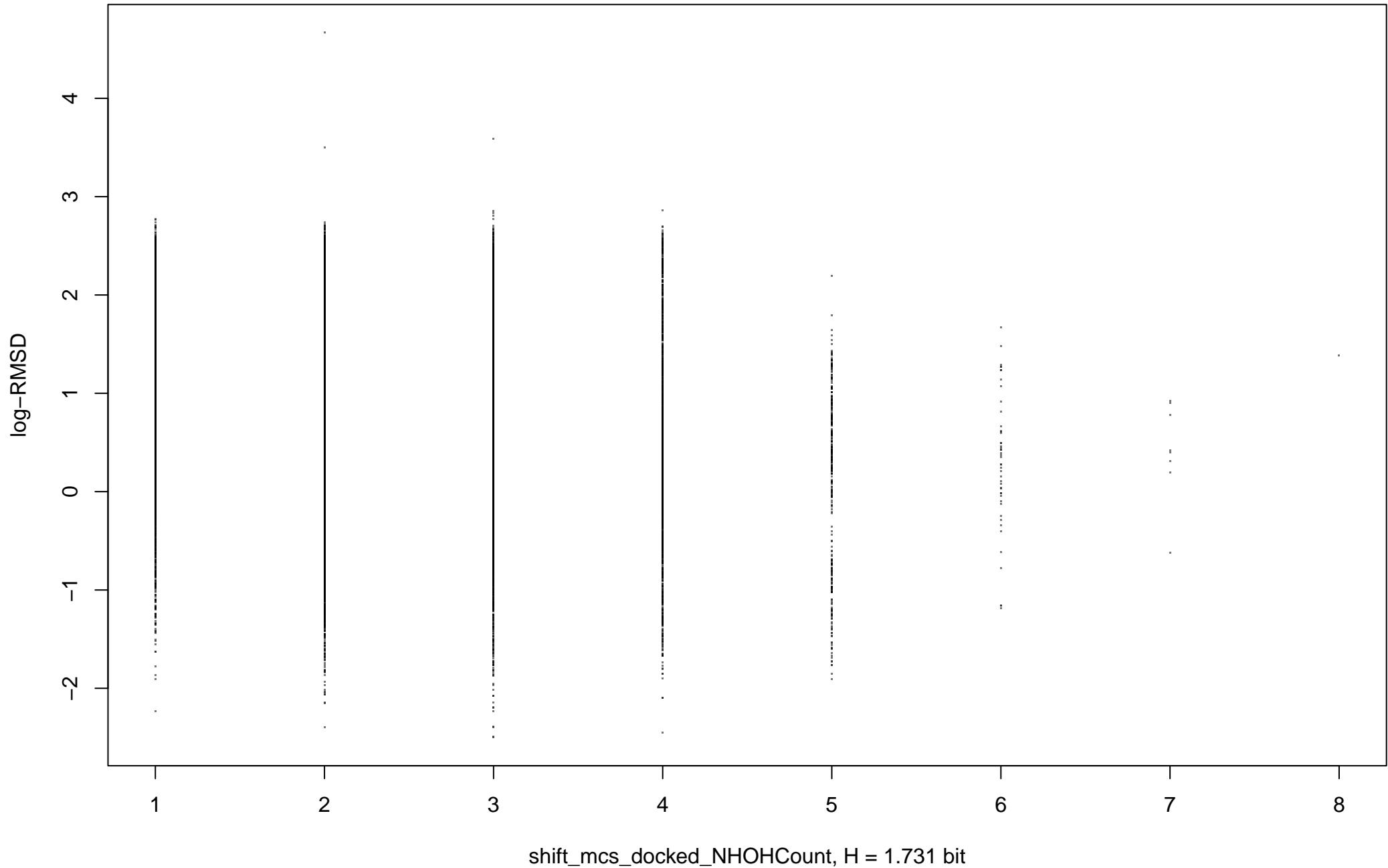


shift_mcs_docked_NumHDonors, H = 1.73 bit

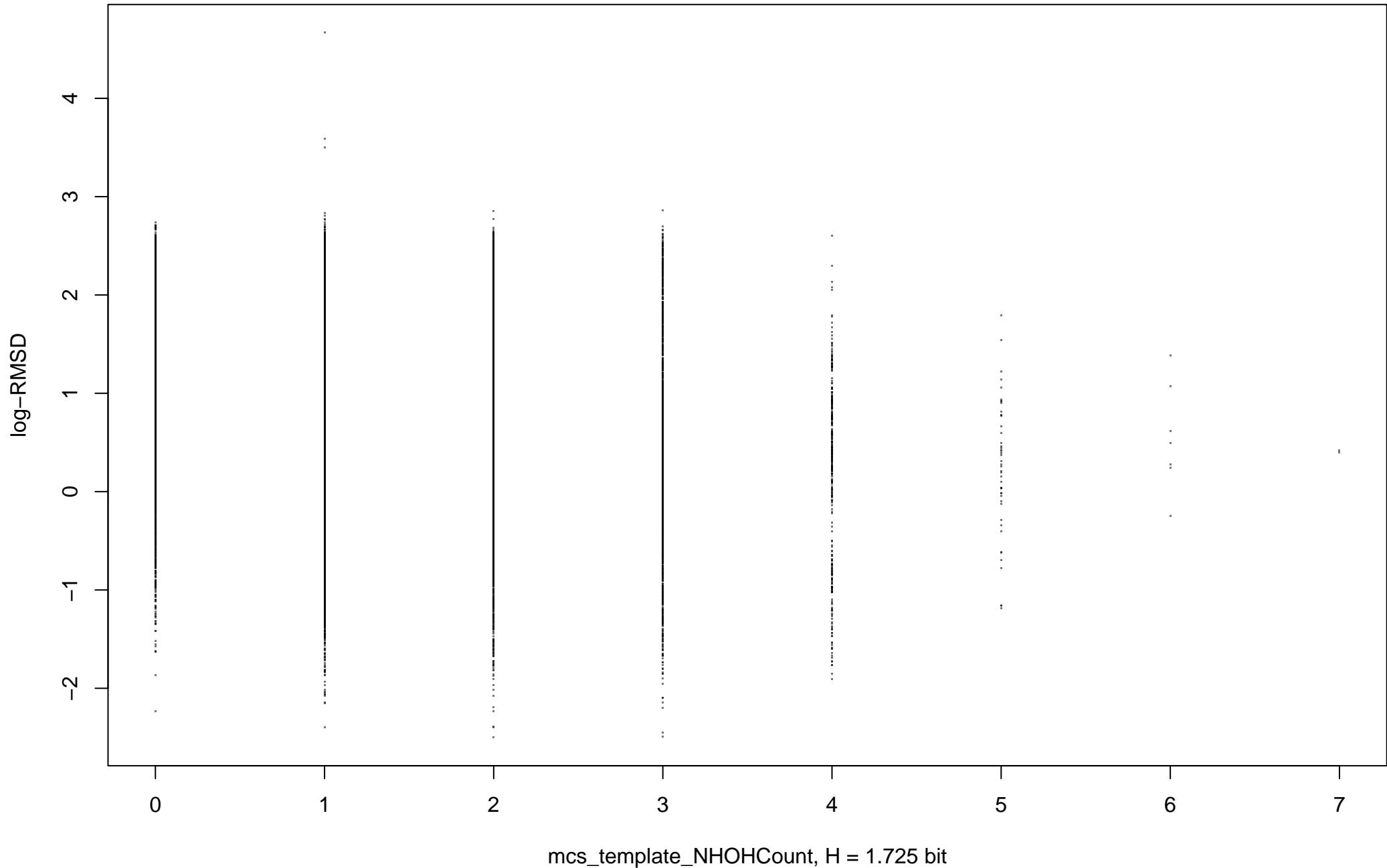
mcs_docked_NHOHCount, MI = 0.1025 bit, norm = 0.05925, cond entr = 4.227 bit



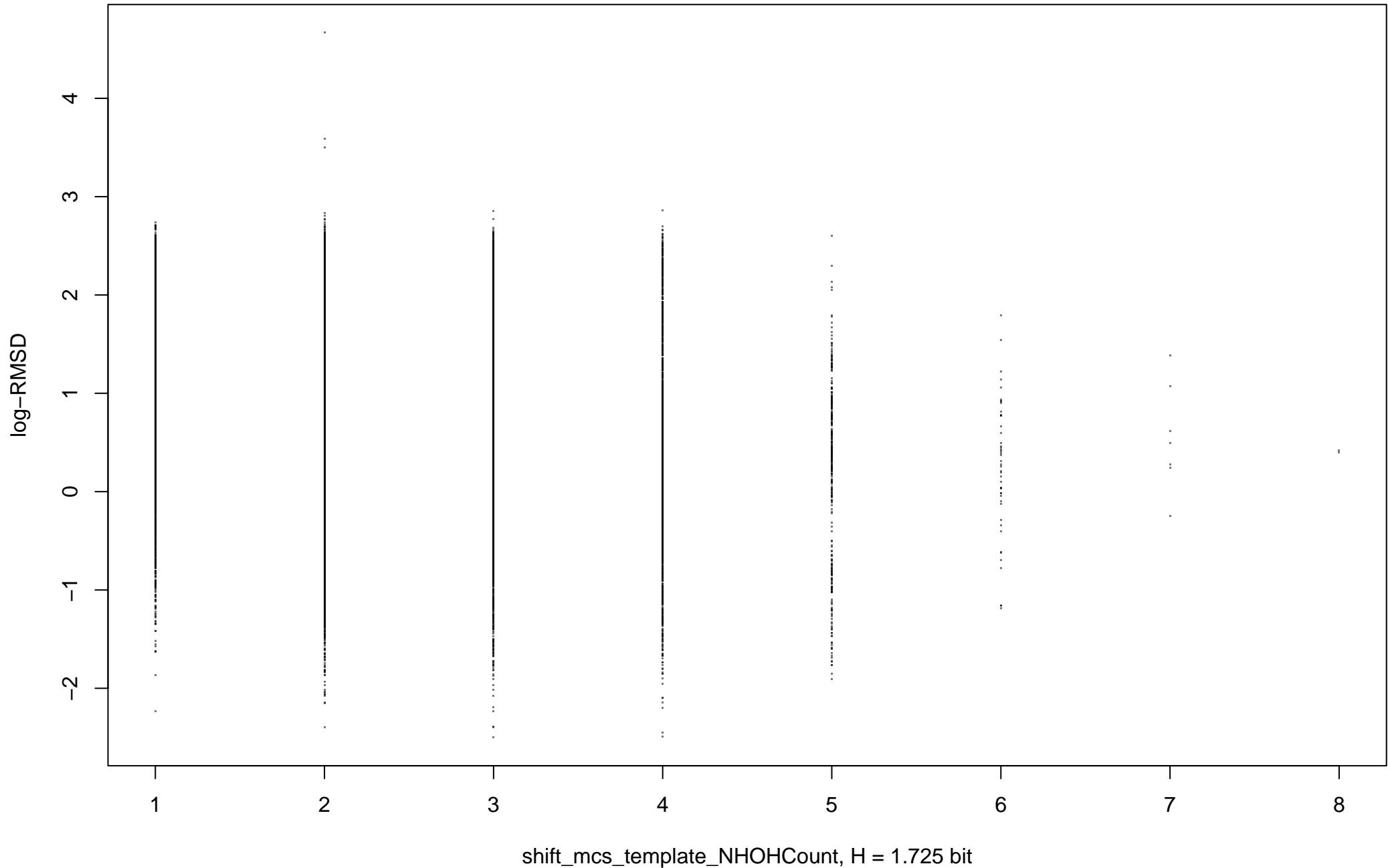
shift_mcs_docked_NHOHCount, MI = 0.1025 bit, norm = 0.05925, cond entr = 4.227 bit



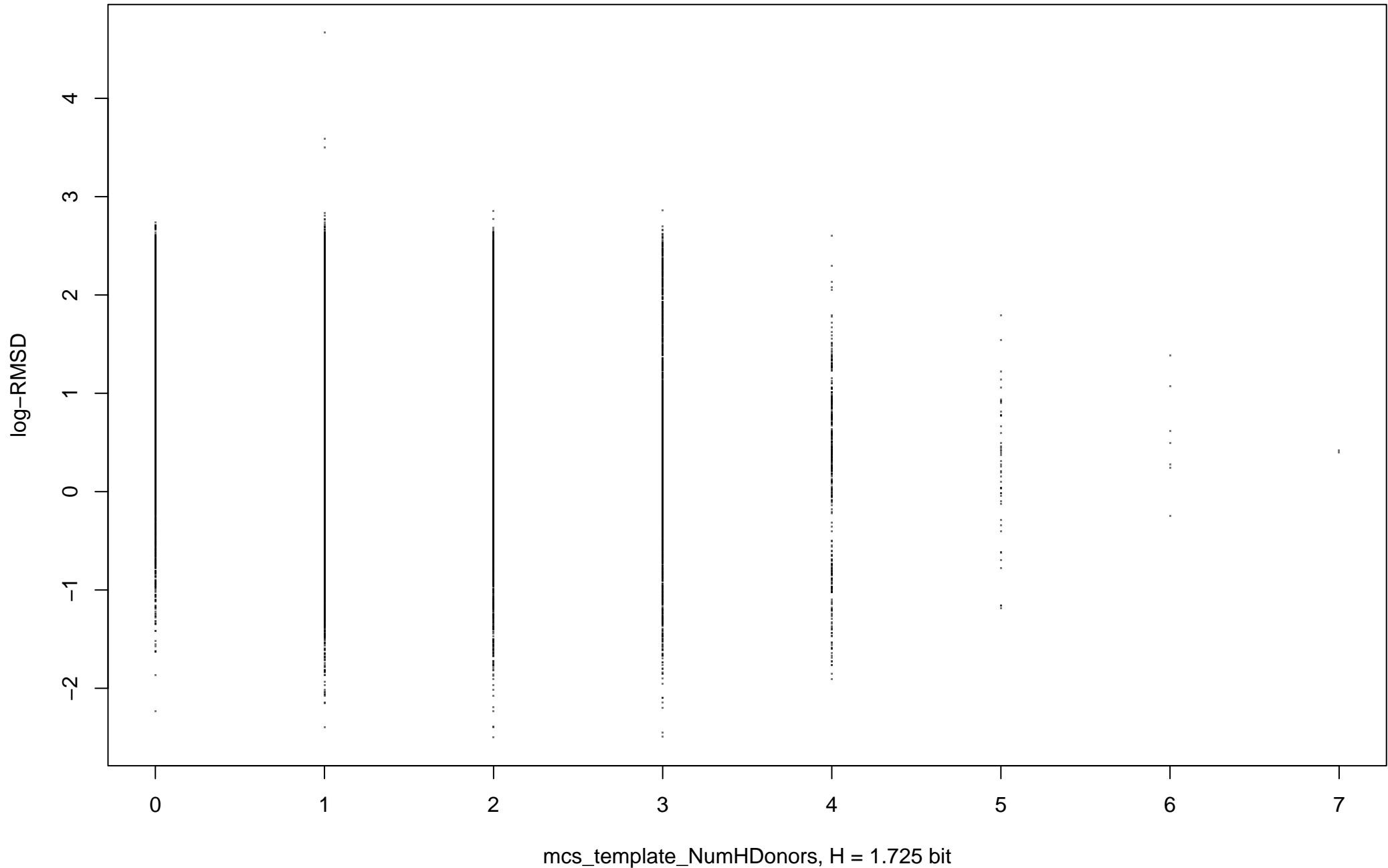
mcs_template_NHOHCount, MI = 0.0949 bit, norm = 0.05501, cond entr = 4.234 bit



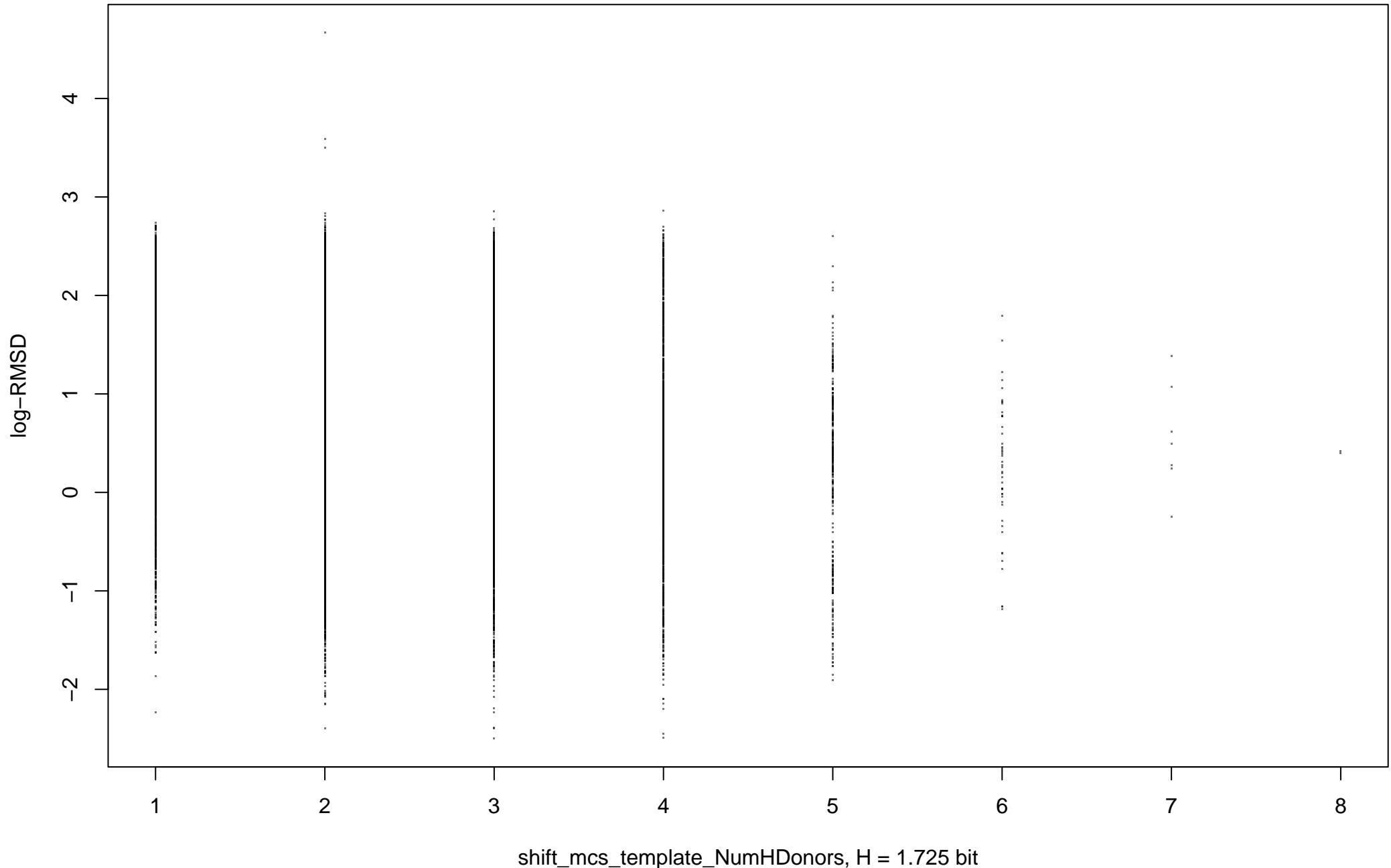
shift_mcs_template_NHOHCount, MI = 0.0949 bit, norm = 0.05501, cond entr = 4.234 bit



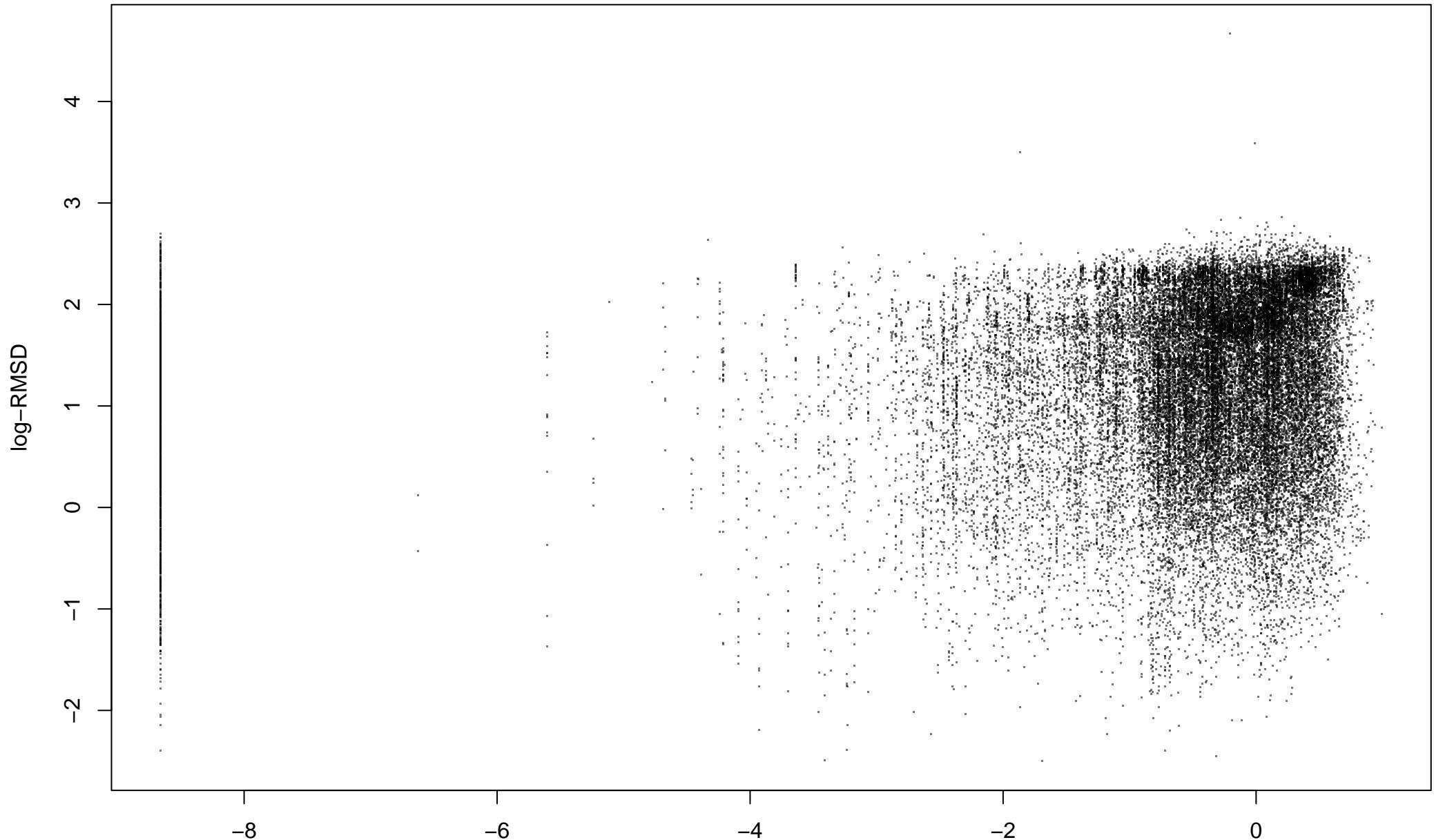
mcs_template_NumHDonors, MI = 0.09479 bit, norm = 0.05496, cond entr = 4.234 bit



shift_mcs_template_NumHDonors, MI = 0.09479 bit, norm = 0.05496, cond entr = 4.234 bit

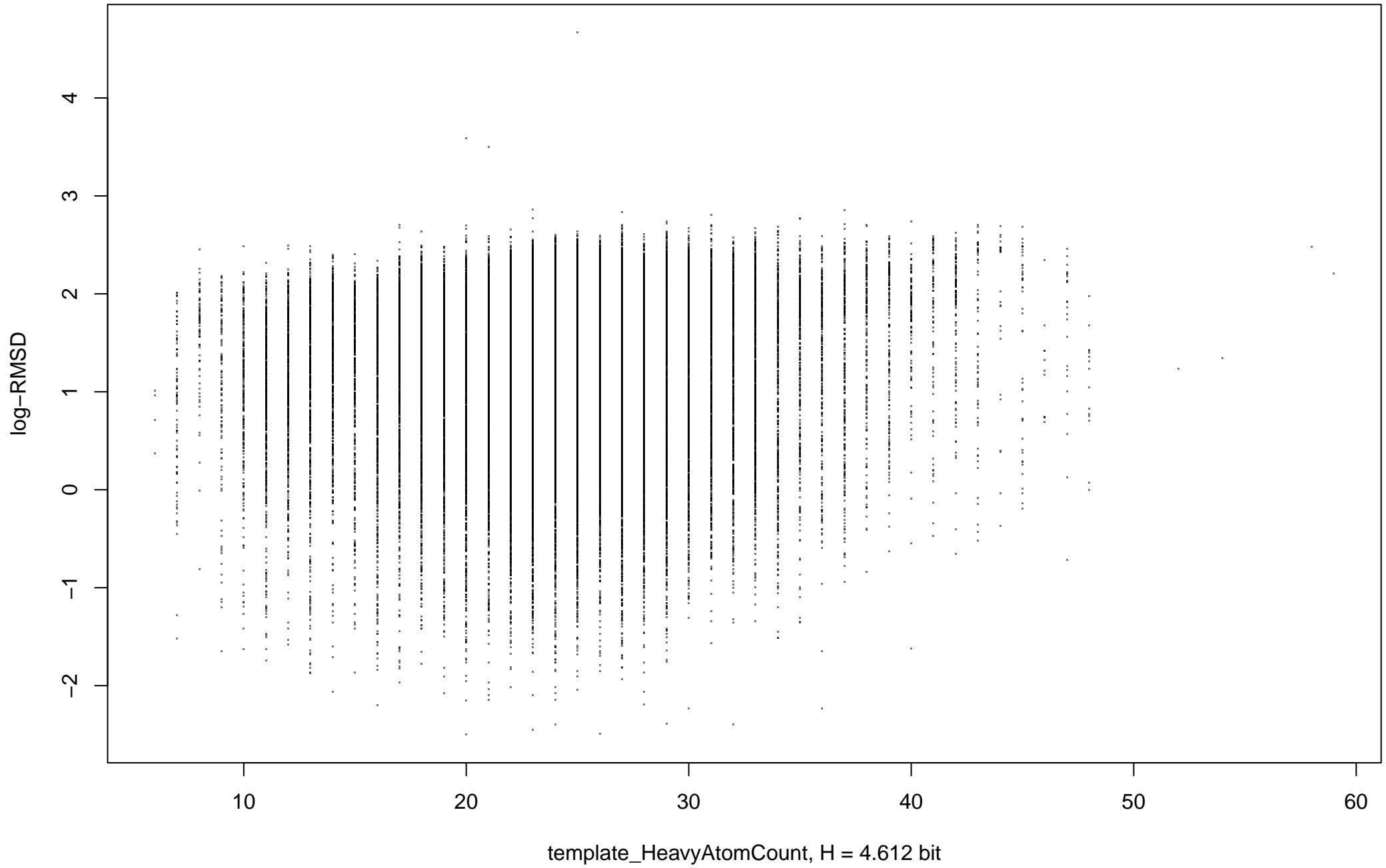


log_mcs_bonded_apolar_sasa, MI = 0.08883 bit, norm = 0.02052, cond entr = 4.24 bit

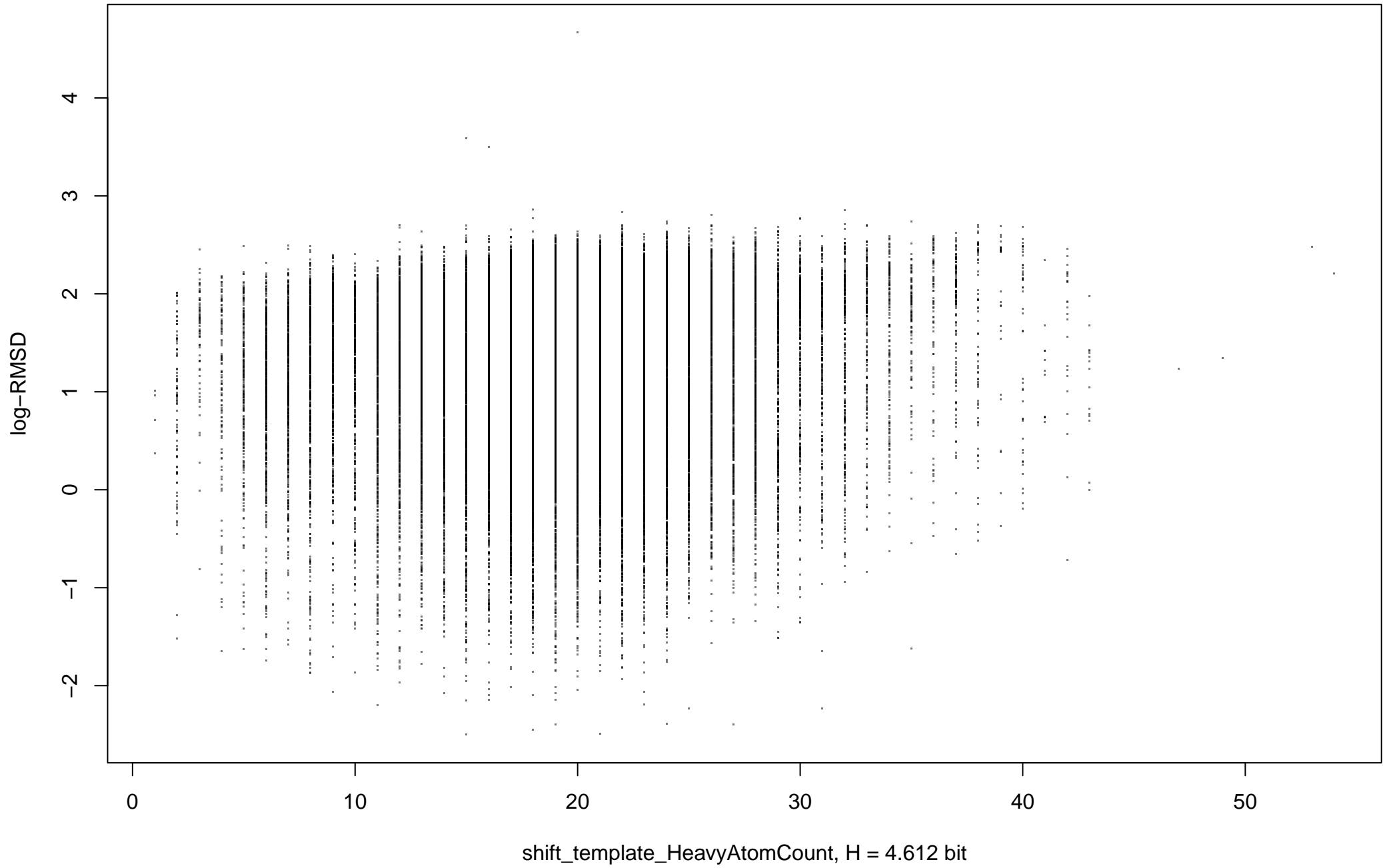


log_mcs_bonded_apolar_sasa, H = 4.586 bit

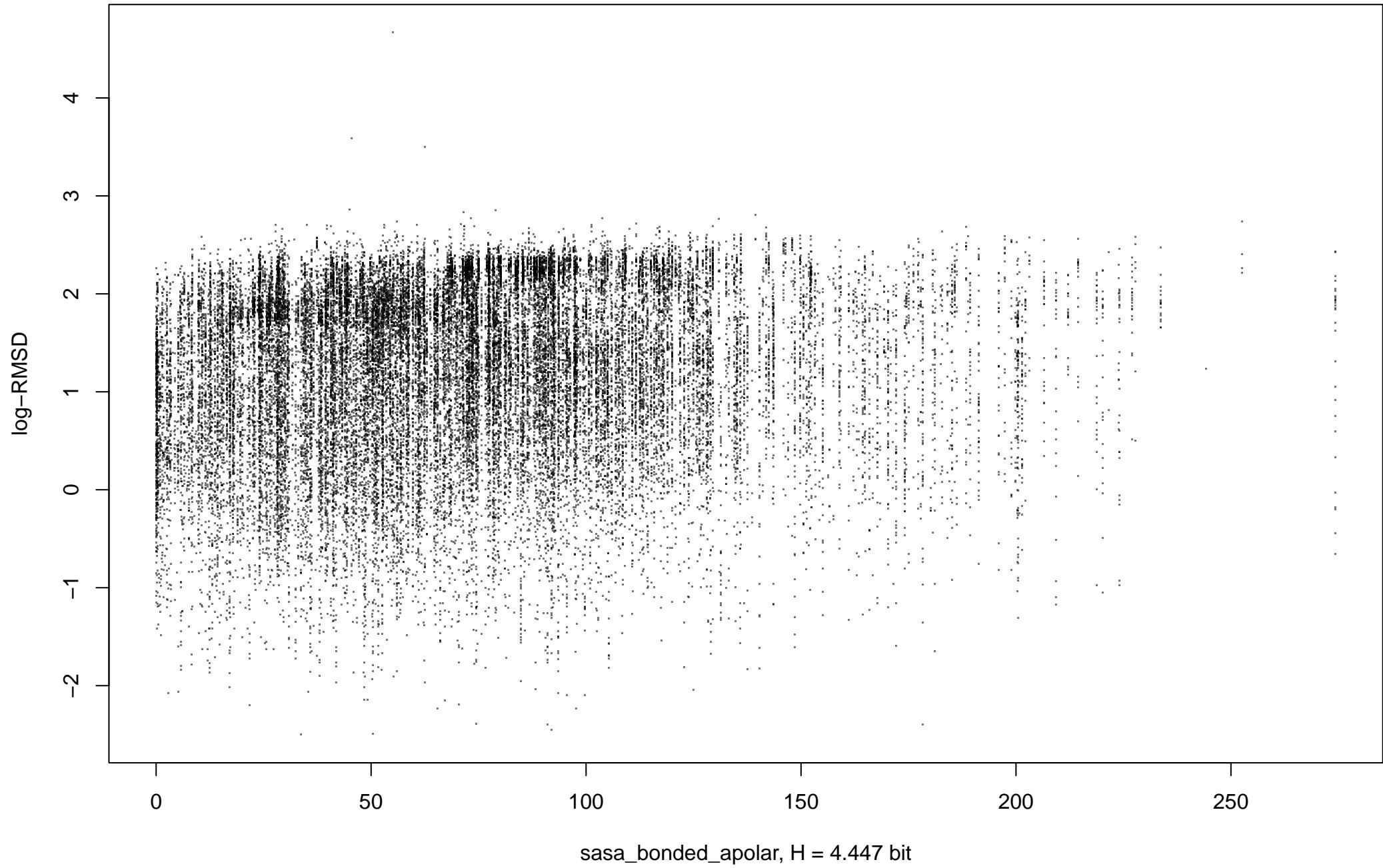
template_HeavyAtomCount, MI = 0.08498 bit, norm = 0.01963, cond entr = 4.244 bit



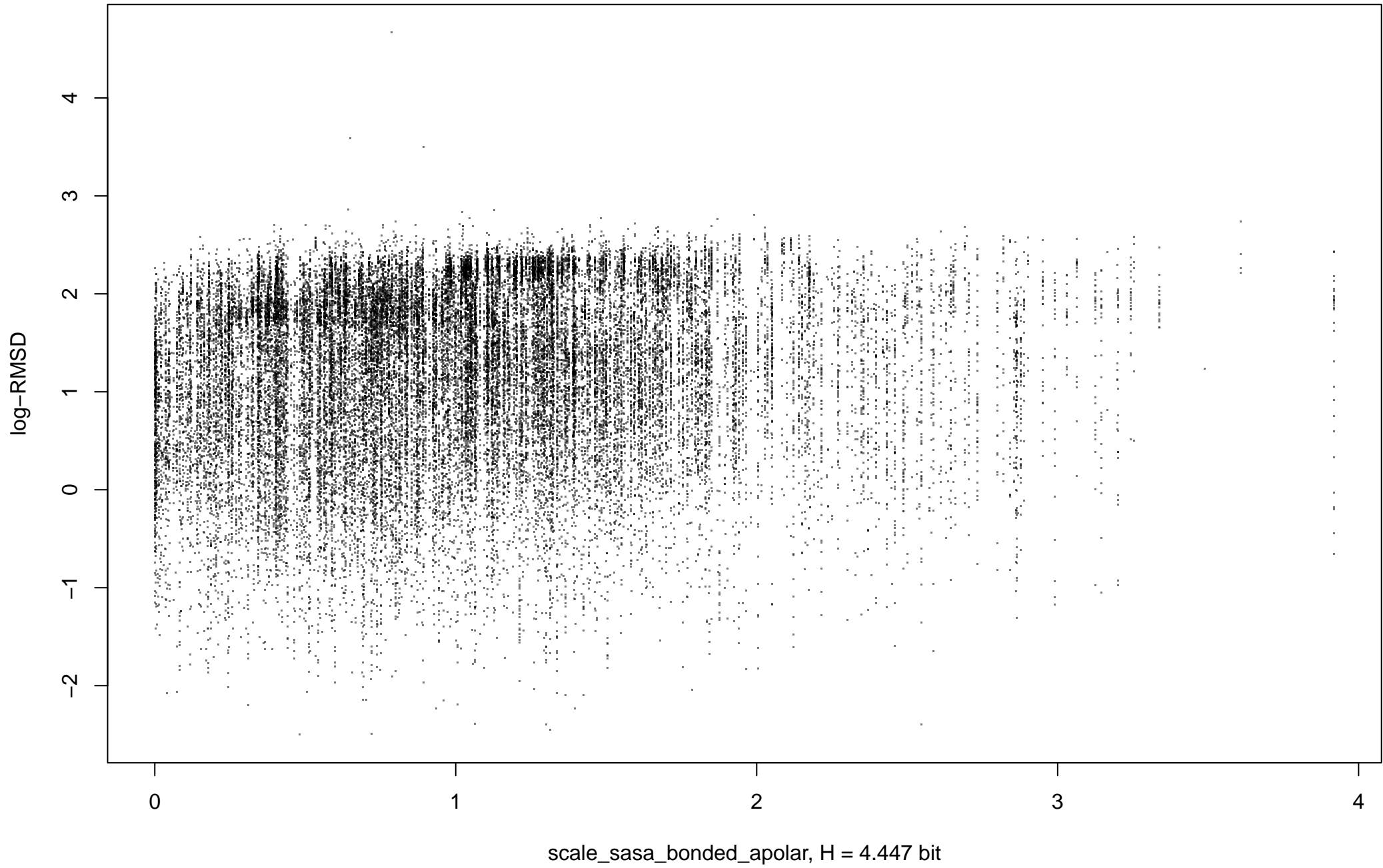
shift_template_HeavyAtomCount, MI = 0.08498 bit, norm = 0.01963, cond entr = 4.244 bit



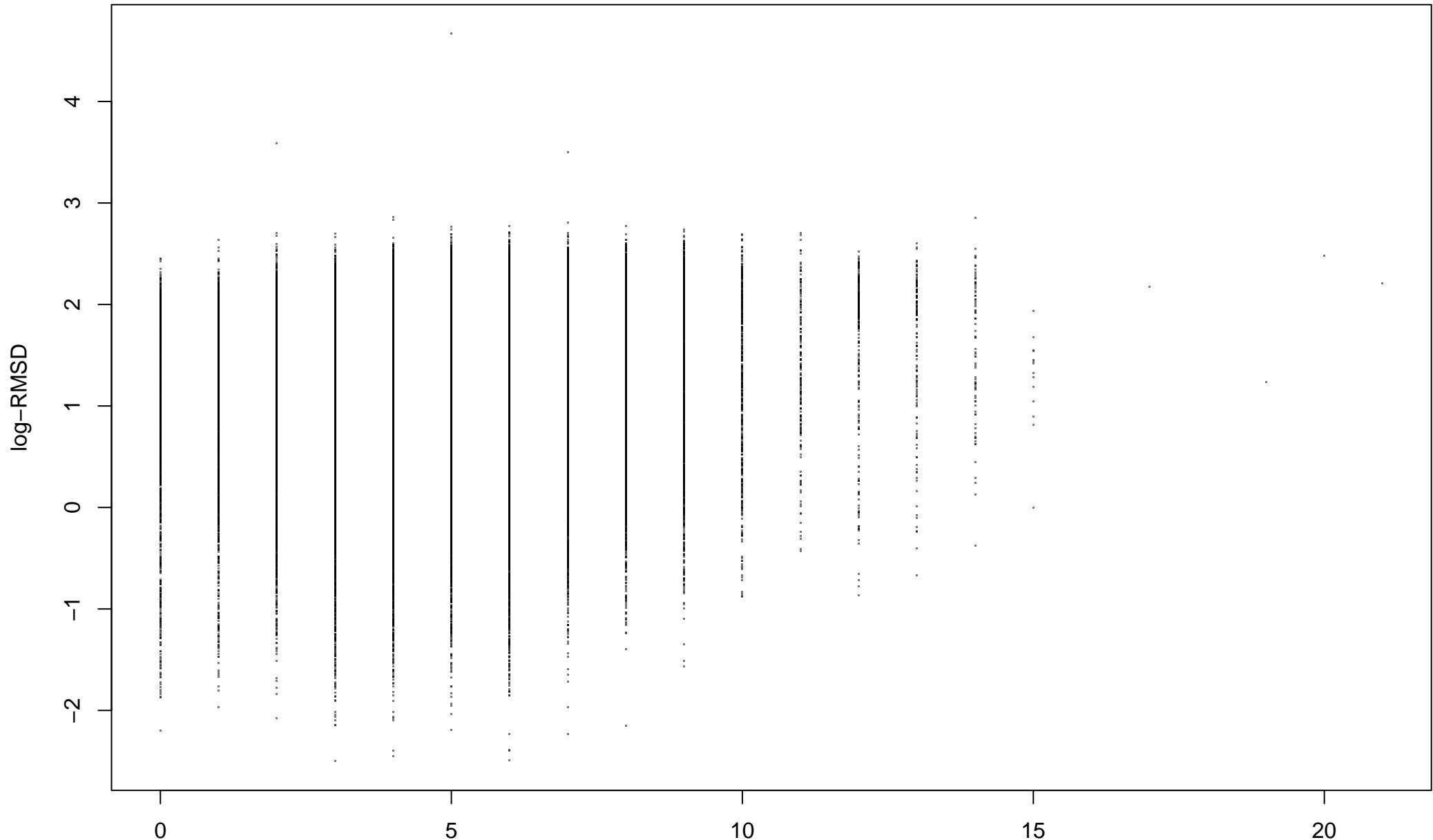
sasa_bonded_apolar, MI = 0.08496 bit, norm = 0.01963, cond entr = 4.244 bit



scale_sasa_bonded_apolar, MI = 0.08496 bit, norm = 0.01963, cond entr = 4.244 bit

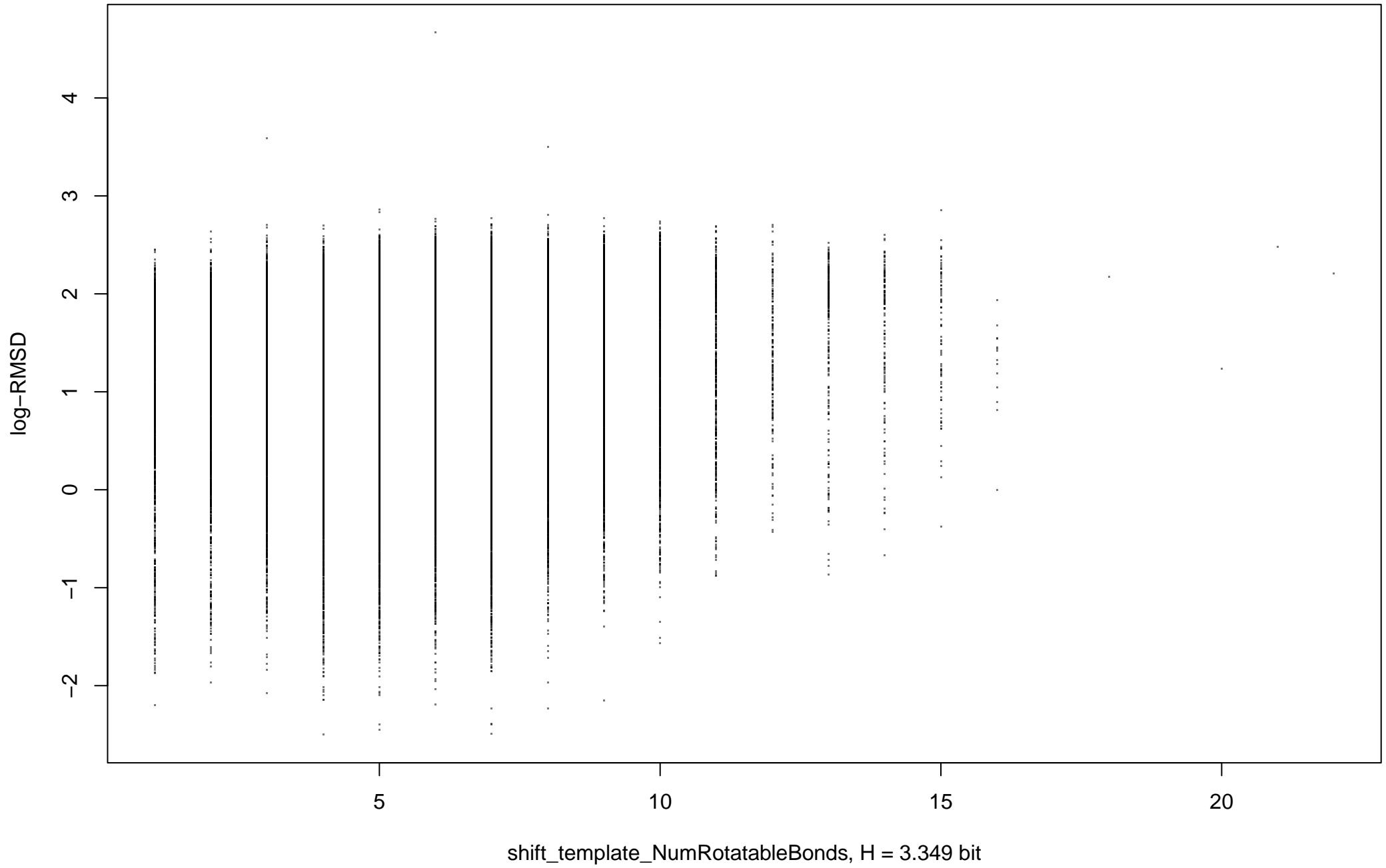


template_NumRotatableBonds, MI = 0.08131 bit, norm = 0.02428, cond entr = 4.248 bit

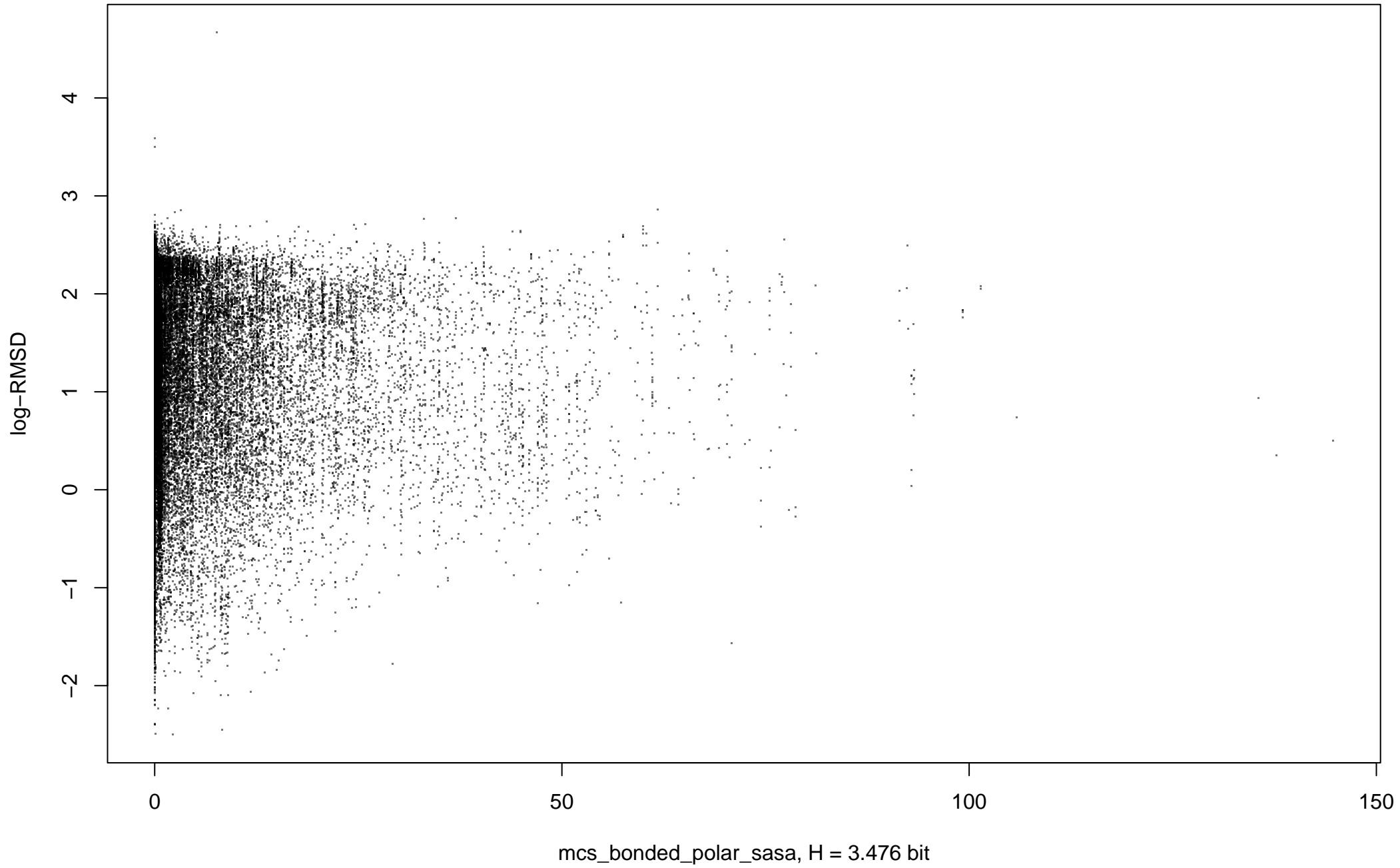


template_NumRotatableBonds, H = 3.349 bit

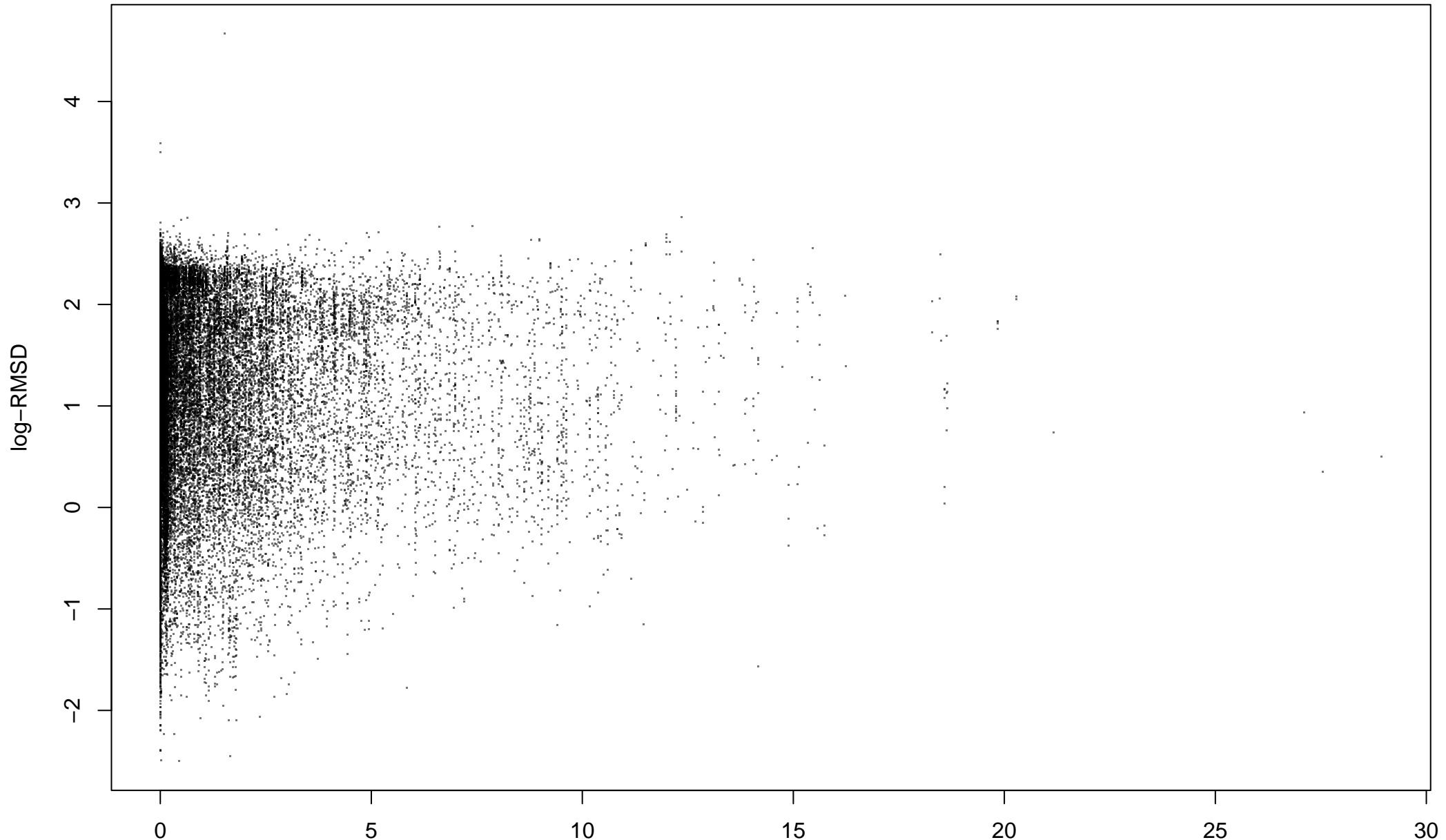
shift_template_NumRotatableBonds, MI = 0.08131 bit, norm = 0.02428, cond entr = 4.248 bit



mcs_bonded_polar_sasa, MI = 0.07245 bit, norm = 0.02084, cond entr = 4.257 bit

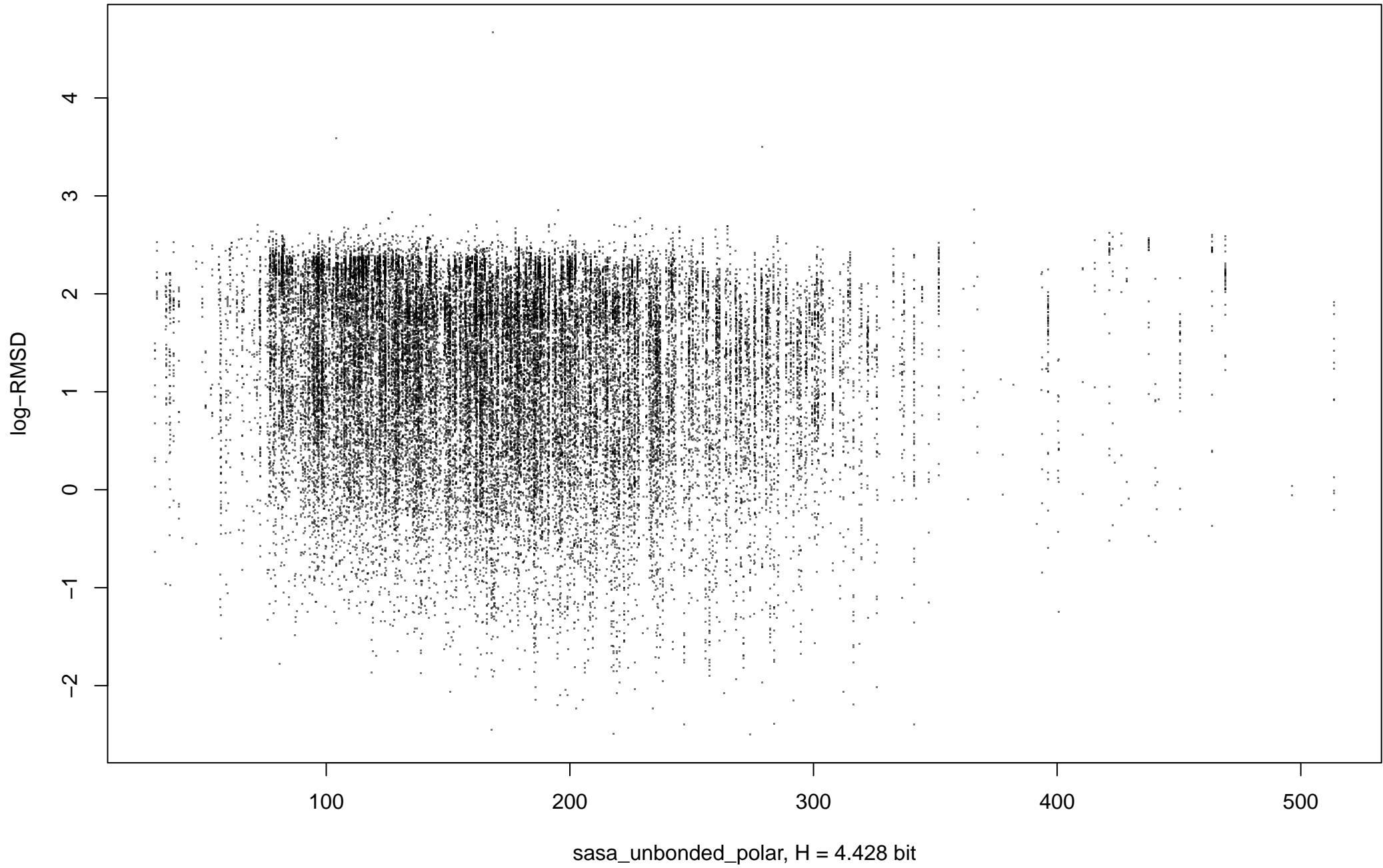


scale_mcs_bonded_polar_sasa, MI = 0.07245 bit, norm = 0.02084, cond entr = 4.257 bit

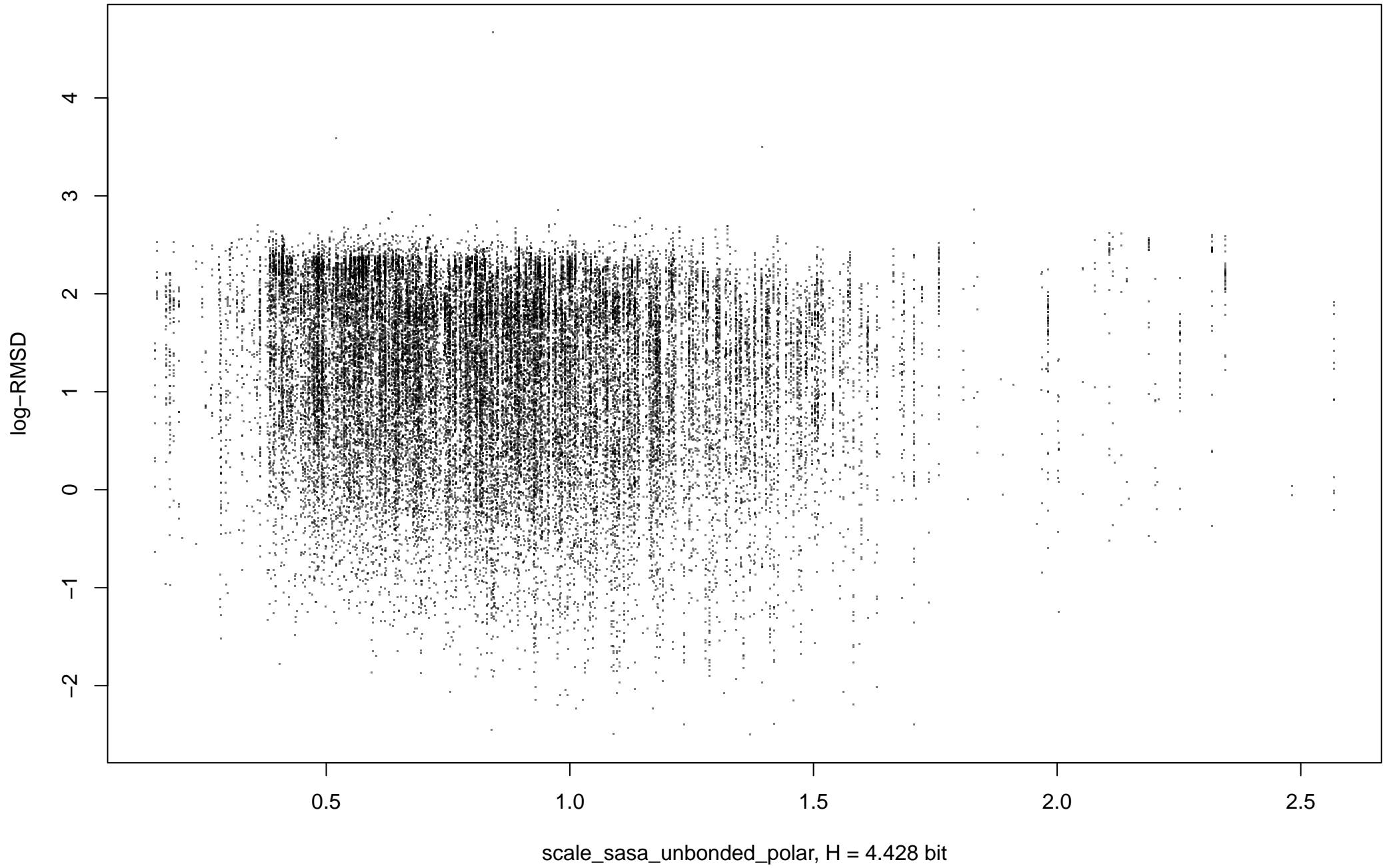


scale_mcs_bonded_polar_sasa, H = 3.476 bit

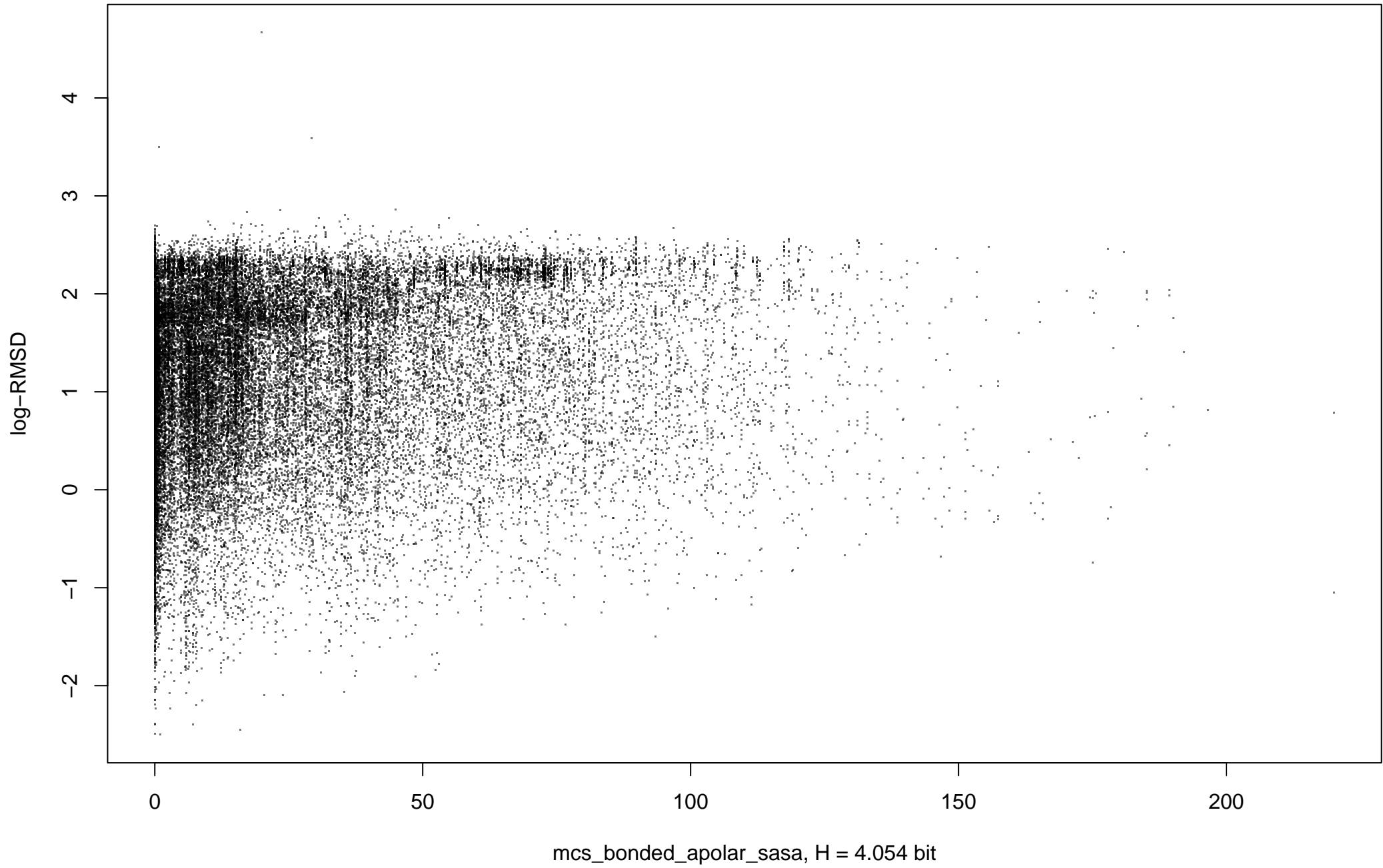
sasa_unbonded_polar, MI = 0.07114 bit, norm = 0.01643, cond entr = 4.258 bit



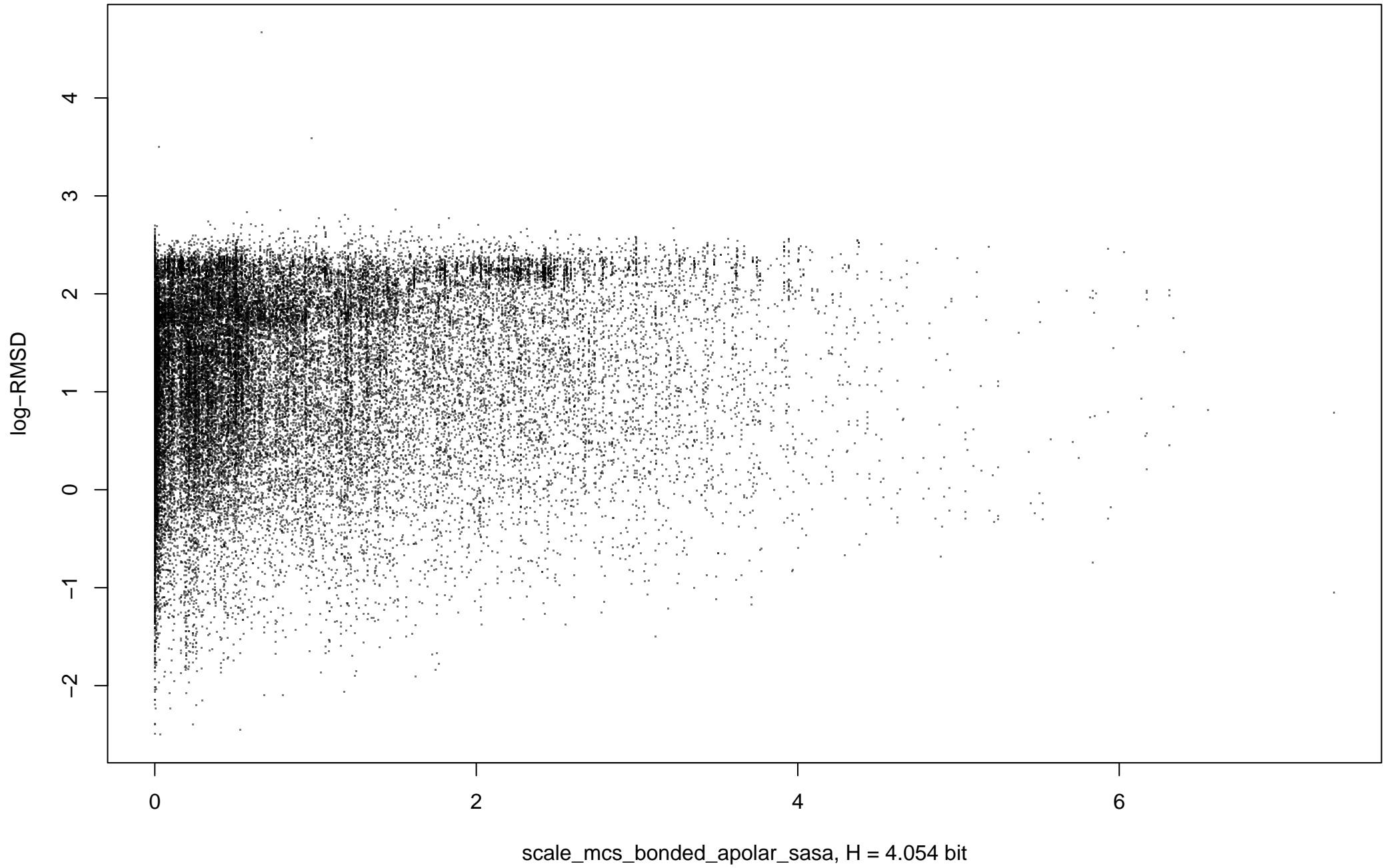
scale_sasa_unbonded_polar, MI = 0.07114 bit, norm = 0.01643, cond entr = 4.258 bit



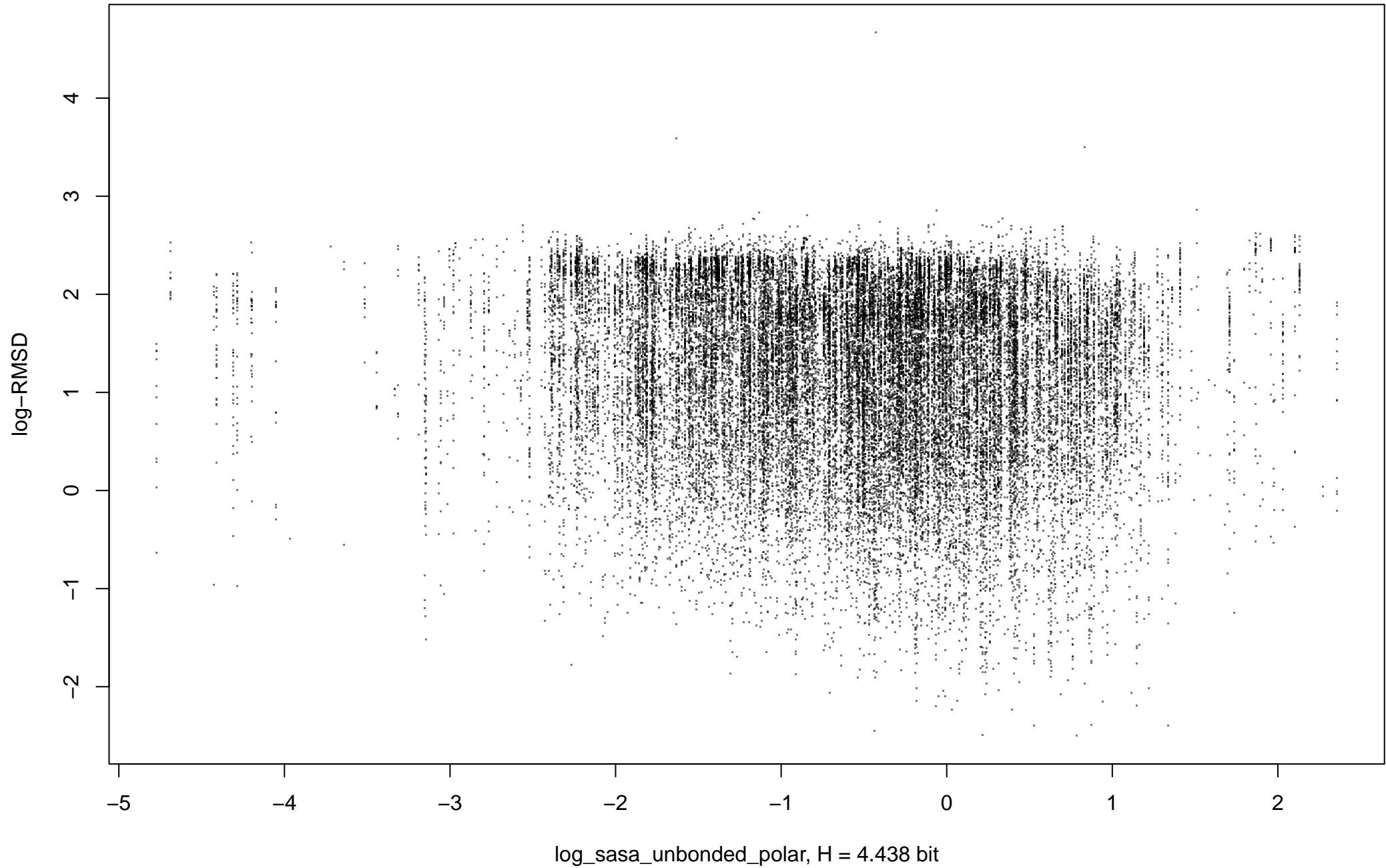
mcs_bonded_apolar_sasa, MI = 0.07072 bit, norm = 0.01745, cond entr = 4.259 bit



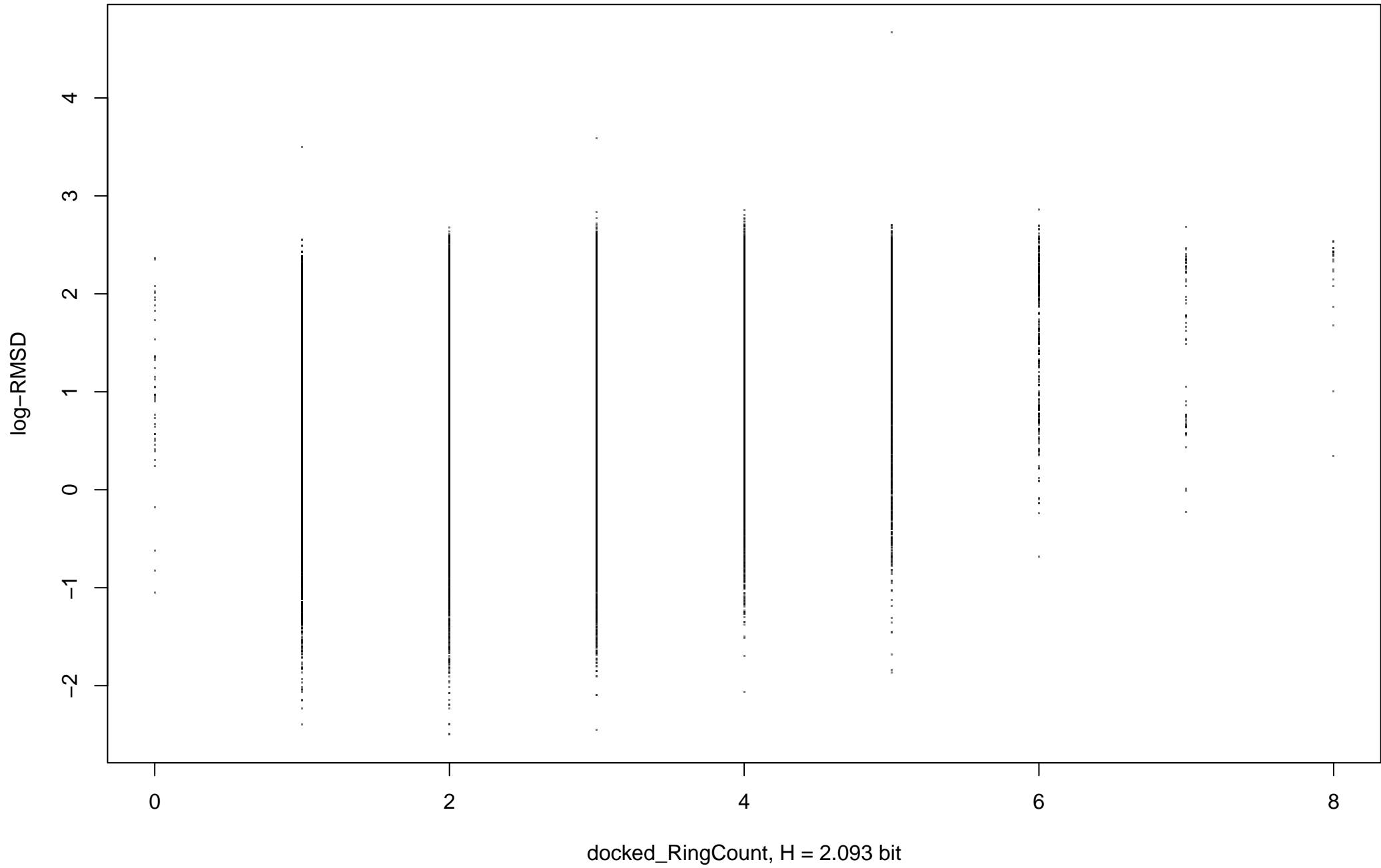
scale_mcs_bonded_apolar_sasa, MI = 0.07072 bit, norm = 0.01745, cond entr = 4.259 bit



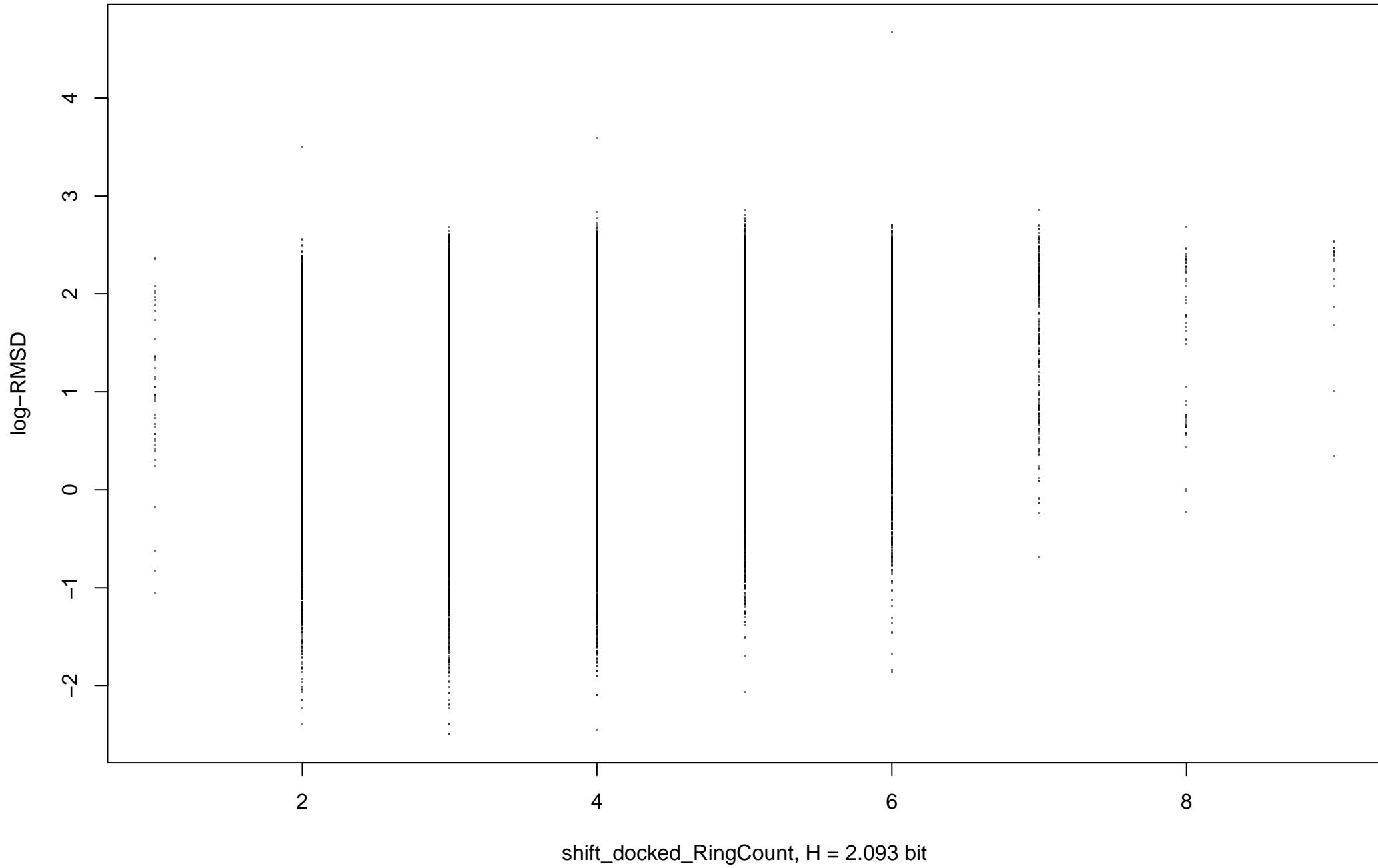
log_sasa_unbonded_polar, MI = 0.06765 bit, norm = 0.01563, cond entr = 4.262 bit



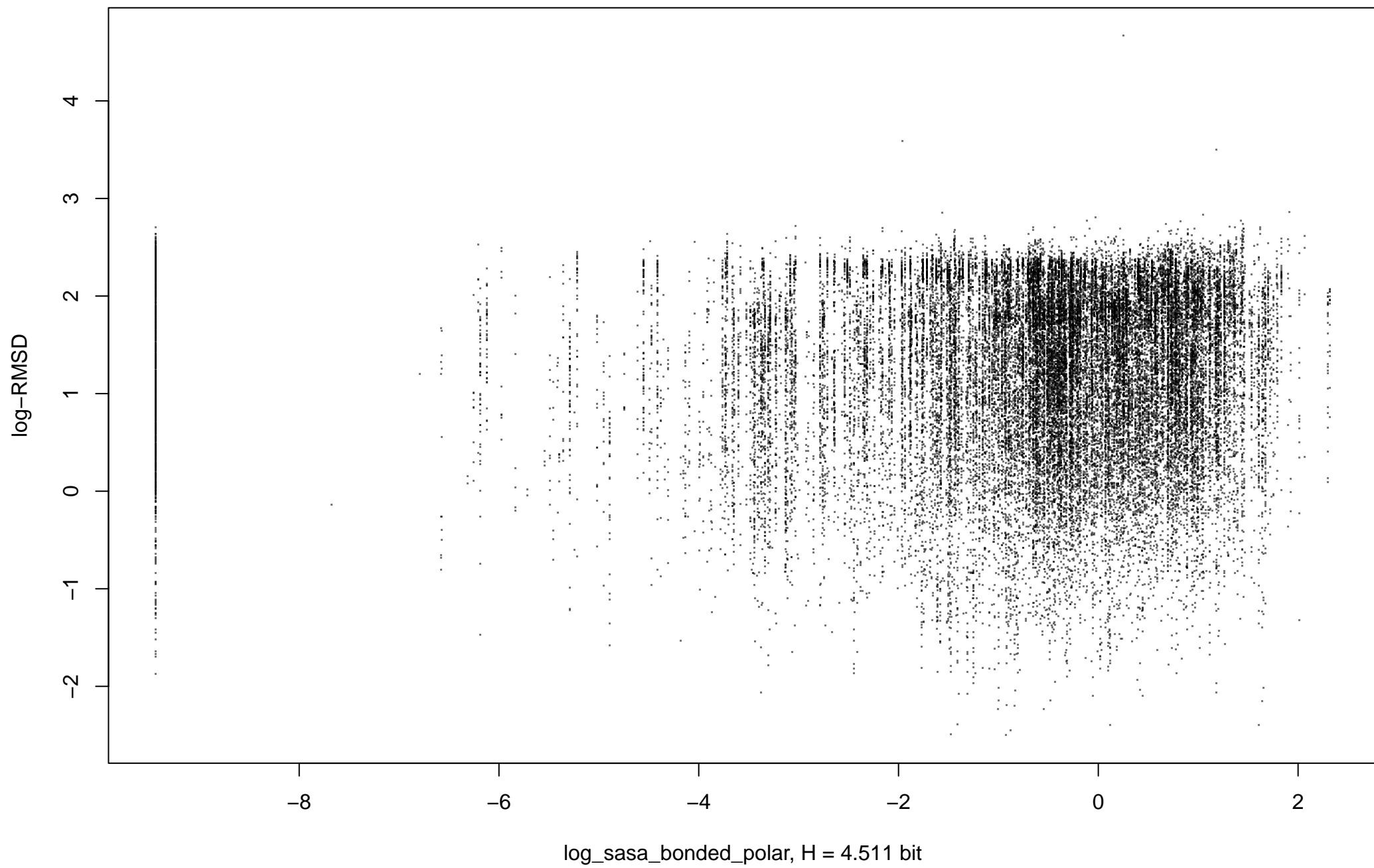
docked_RingCount, MI = 0.06232 bit, norm = 0.02977, cond entr = 4.267 bit



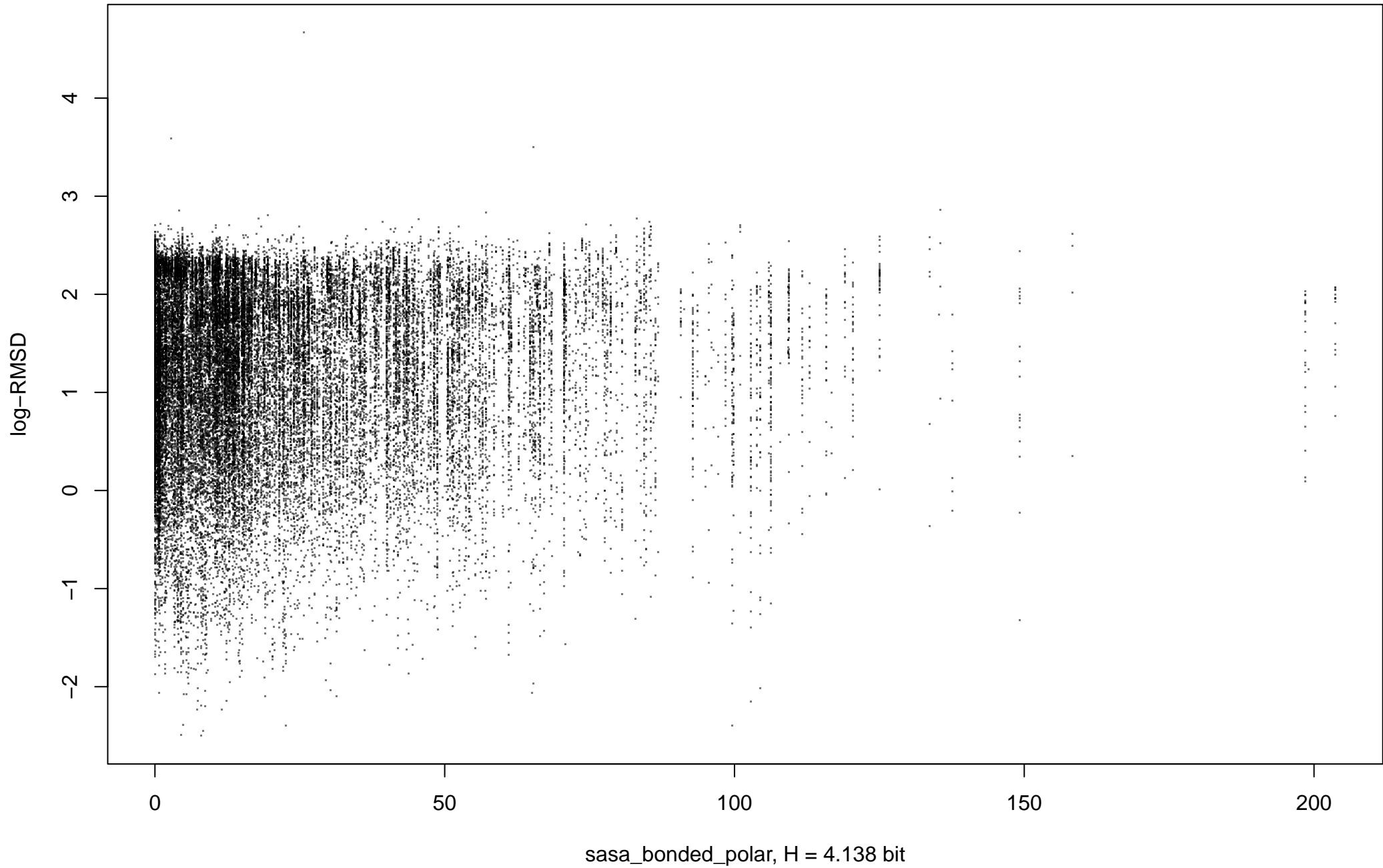
shift_docked_RingCount, MI = 0.06232 bit, norm = 0.02977, cond entr = 4.267 bit



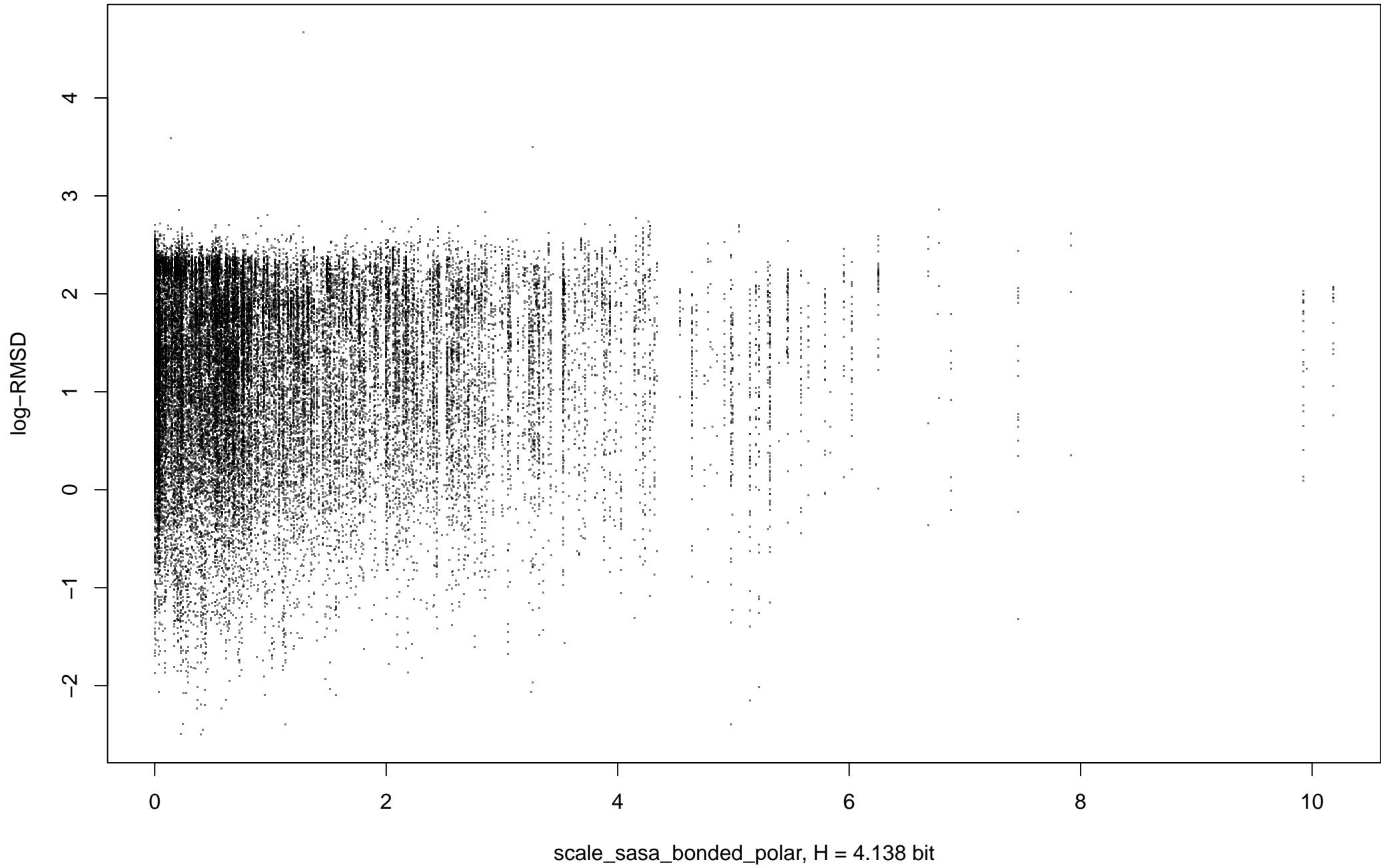
log_sasa_bonded_polar, MI = 0.05854 bit, norm = 0.01352, cond entr = 4.271 bit



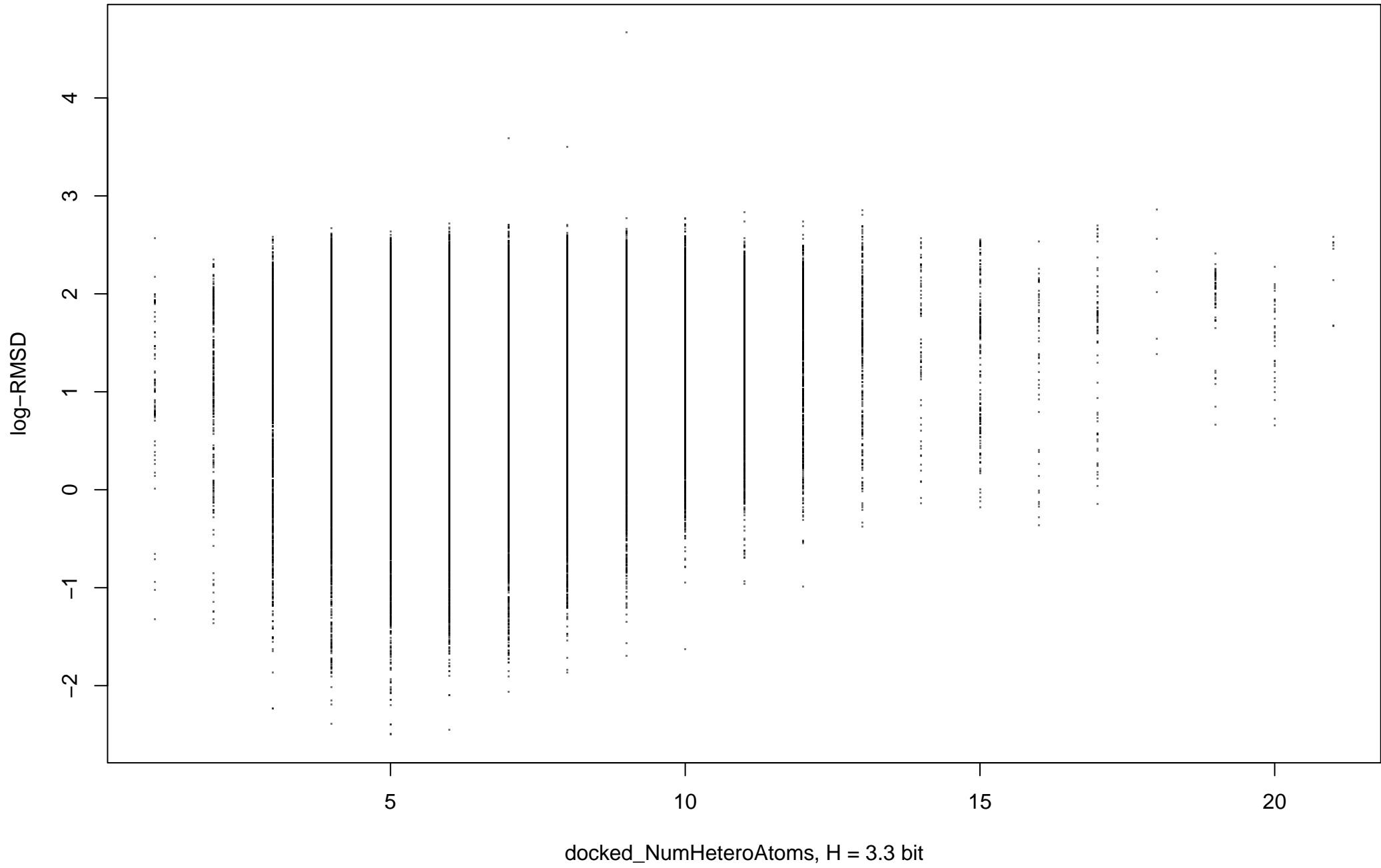
sasa_bonded_polar, MI = 0.05811 bit, norm = 0.01405, cond entr = 4.271 bit



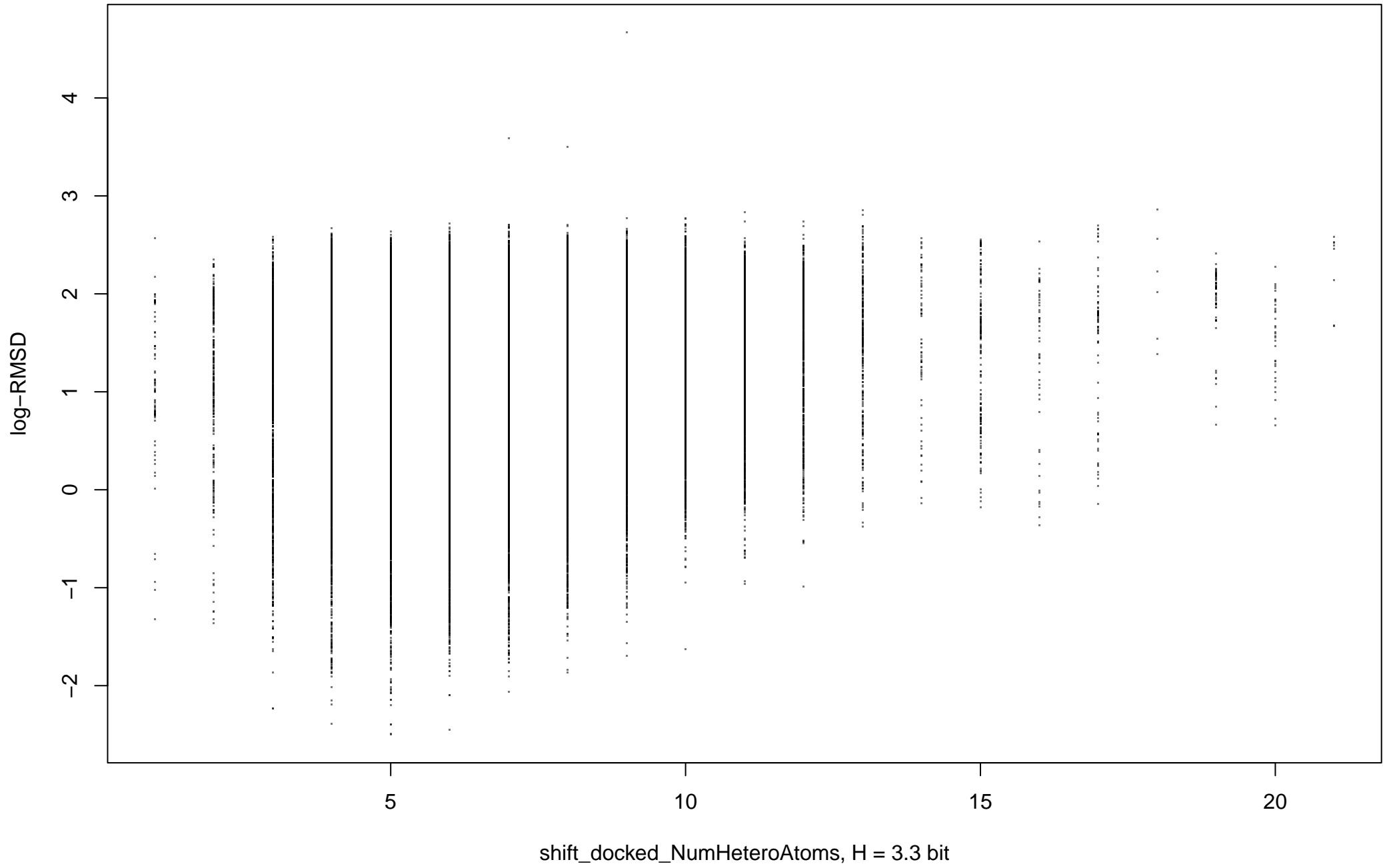
scale_sasa_bonded_polar, MI = 0.05811 bit, norm = 0.01405, cond entr = 4.271 bit



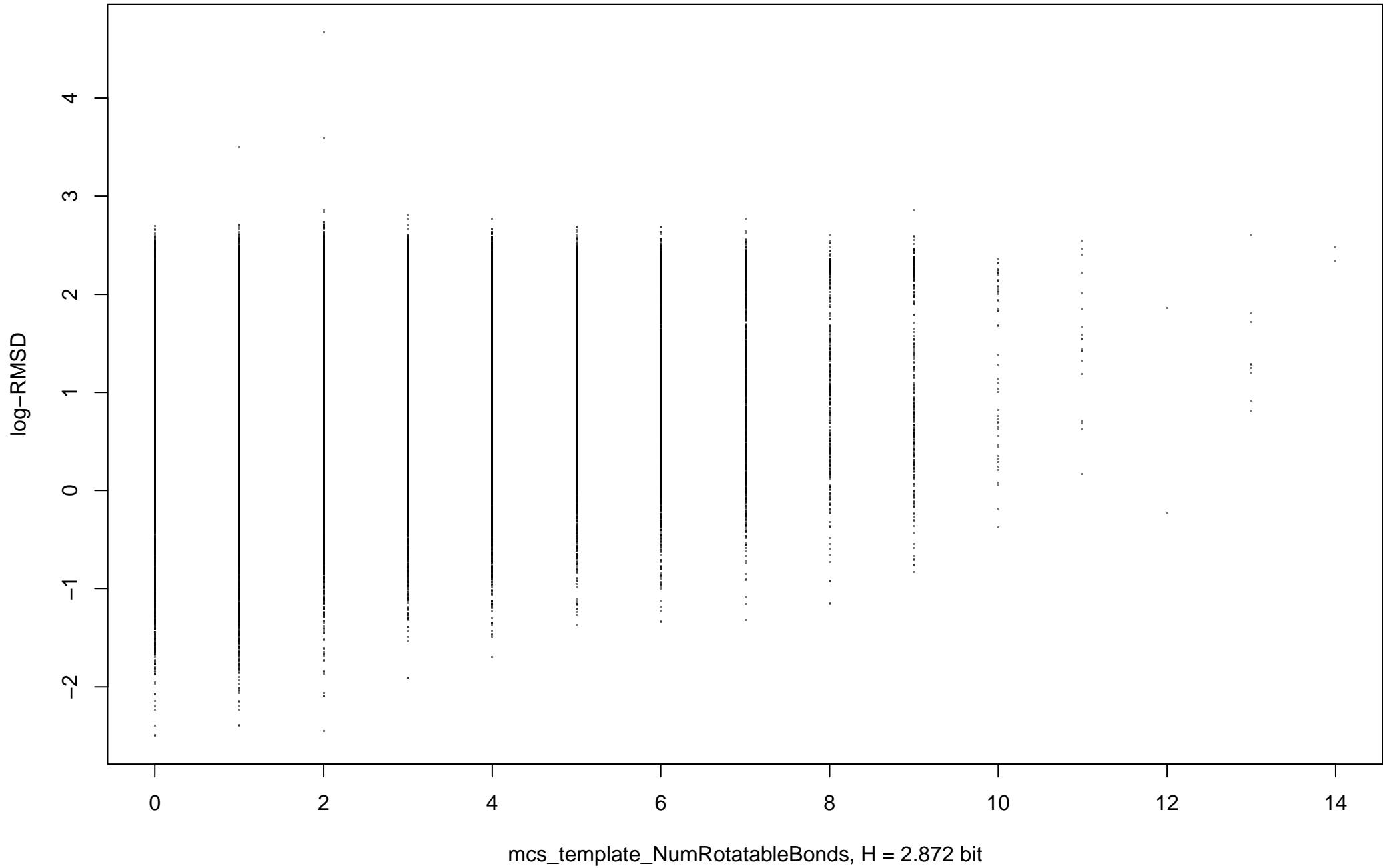
docked_NumHeteroAtoms, MI = 0.05716 bit, norm = 0.01732, cond entr = 4.272 bit



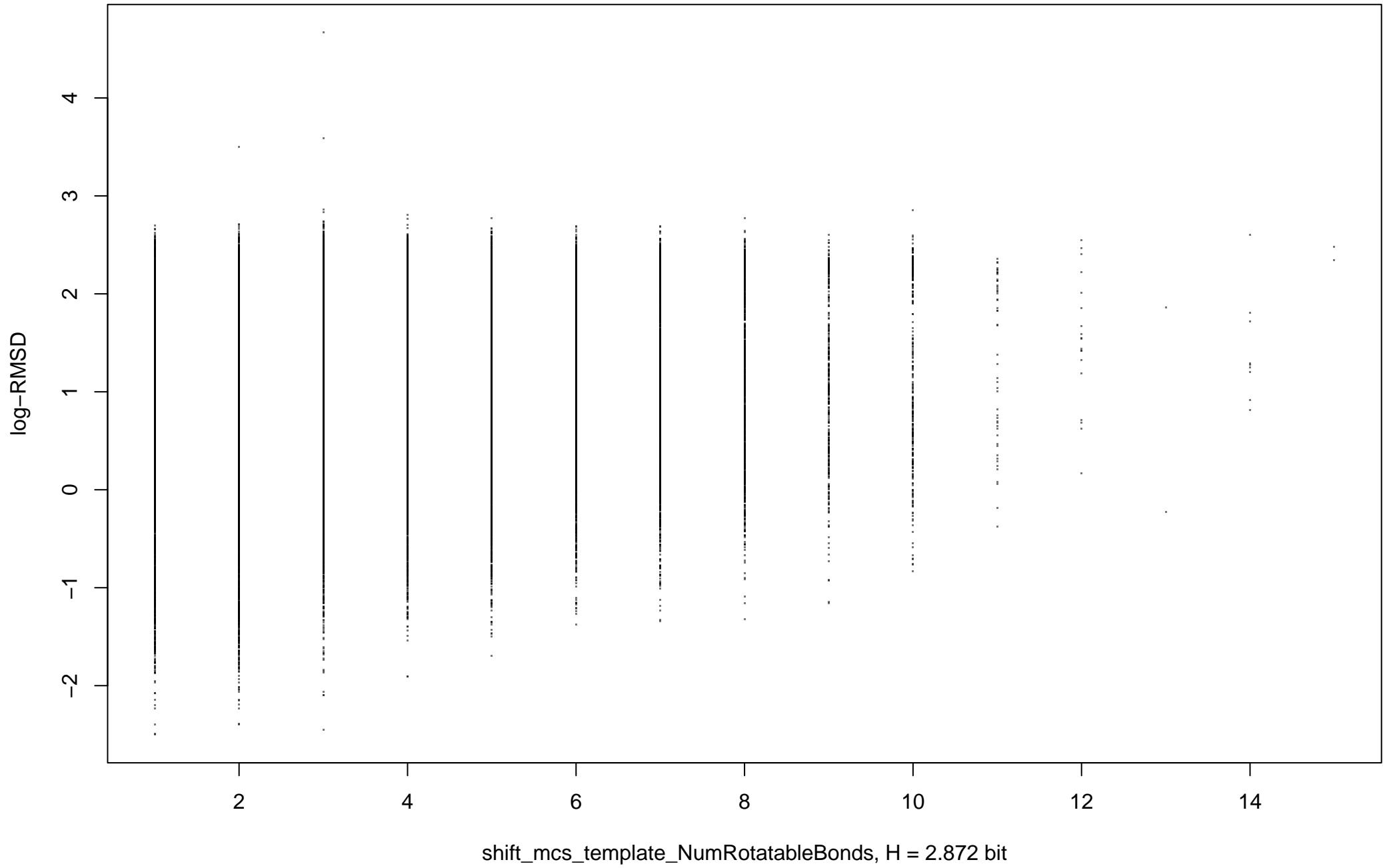
shift_docked_NumHeteroAtoms, MI = 0.05716 bit, norm = 0.01732, cond entr = 4.272 bit



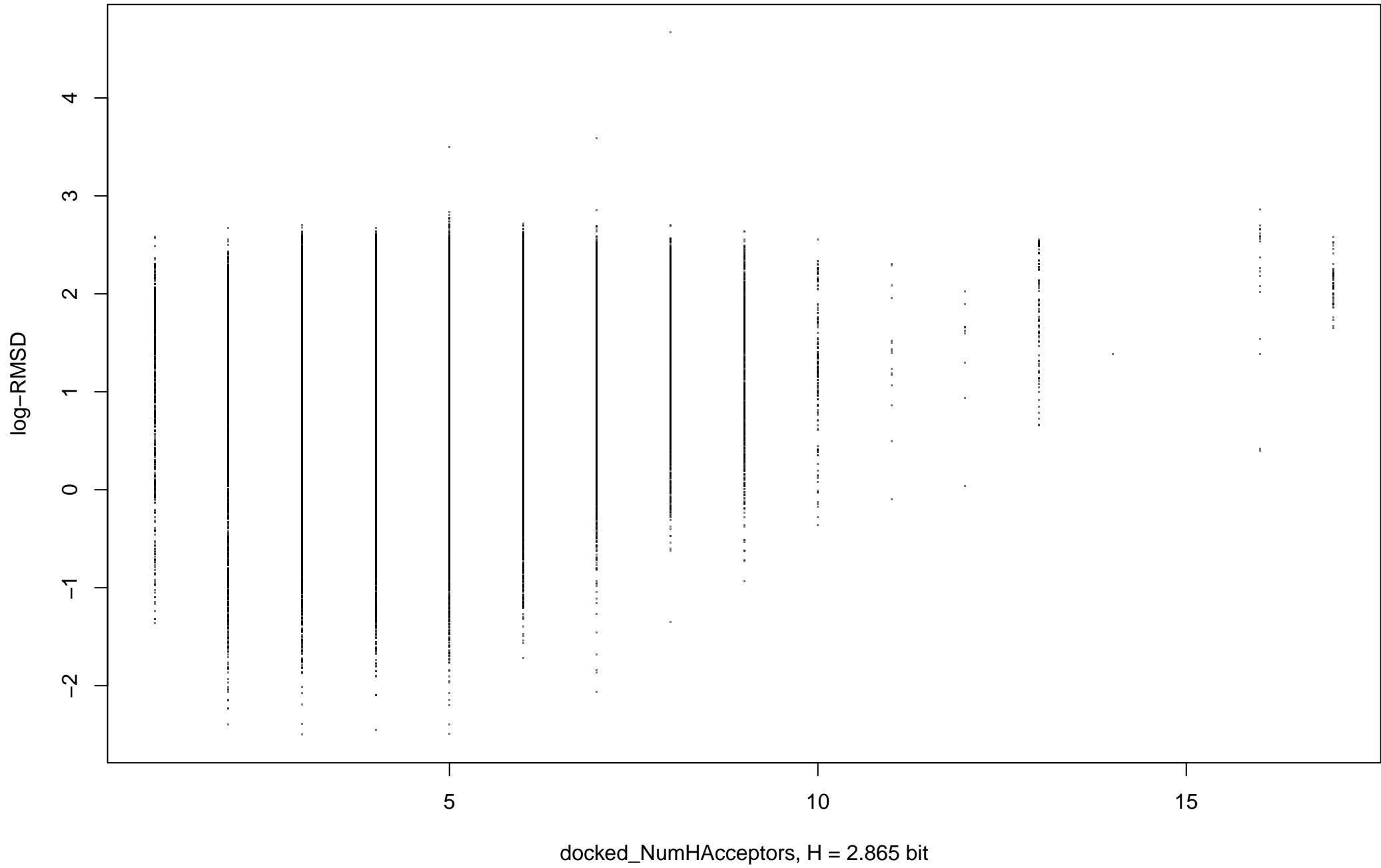
mcs_template_NumRotatableBonds, MI = 0.05709 bit, norm = 0.01988, cond entr = 4.272 bit



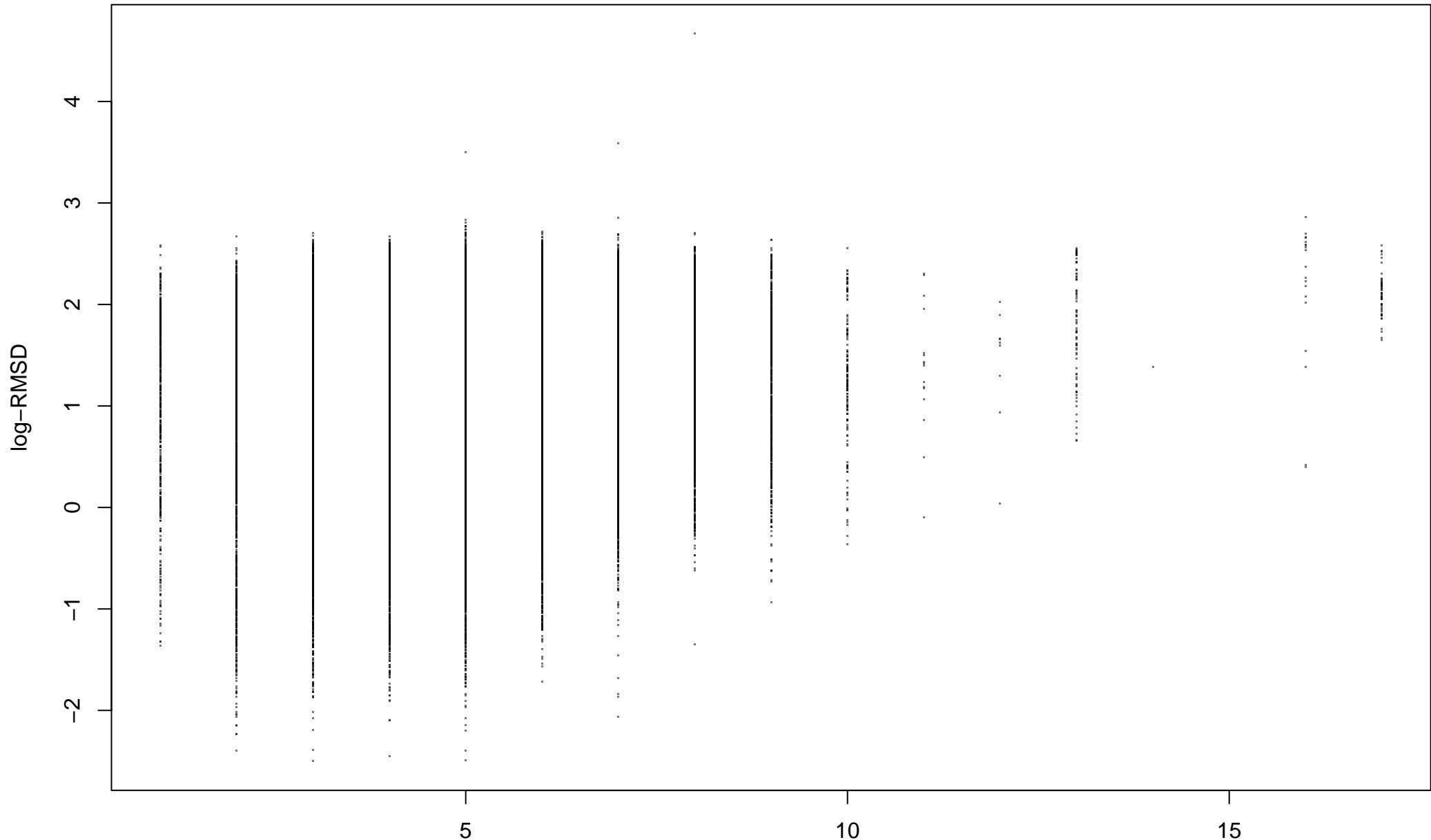
shift_mcs_template_NumRotatableBonds, MI = 0.05709 bit, norm = 0.01988, cond entr = 4.272 bit



docked_NumHAcceptors, MI = 0.056 bit, norm = 0.01954, cond entr = 4.273 bit

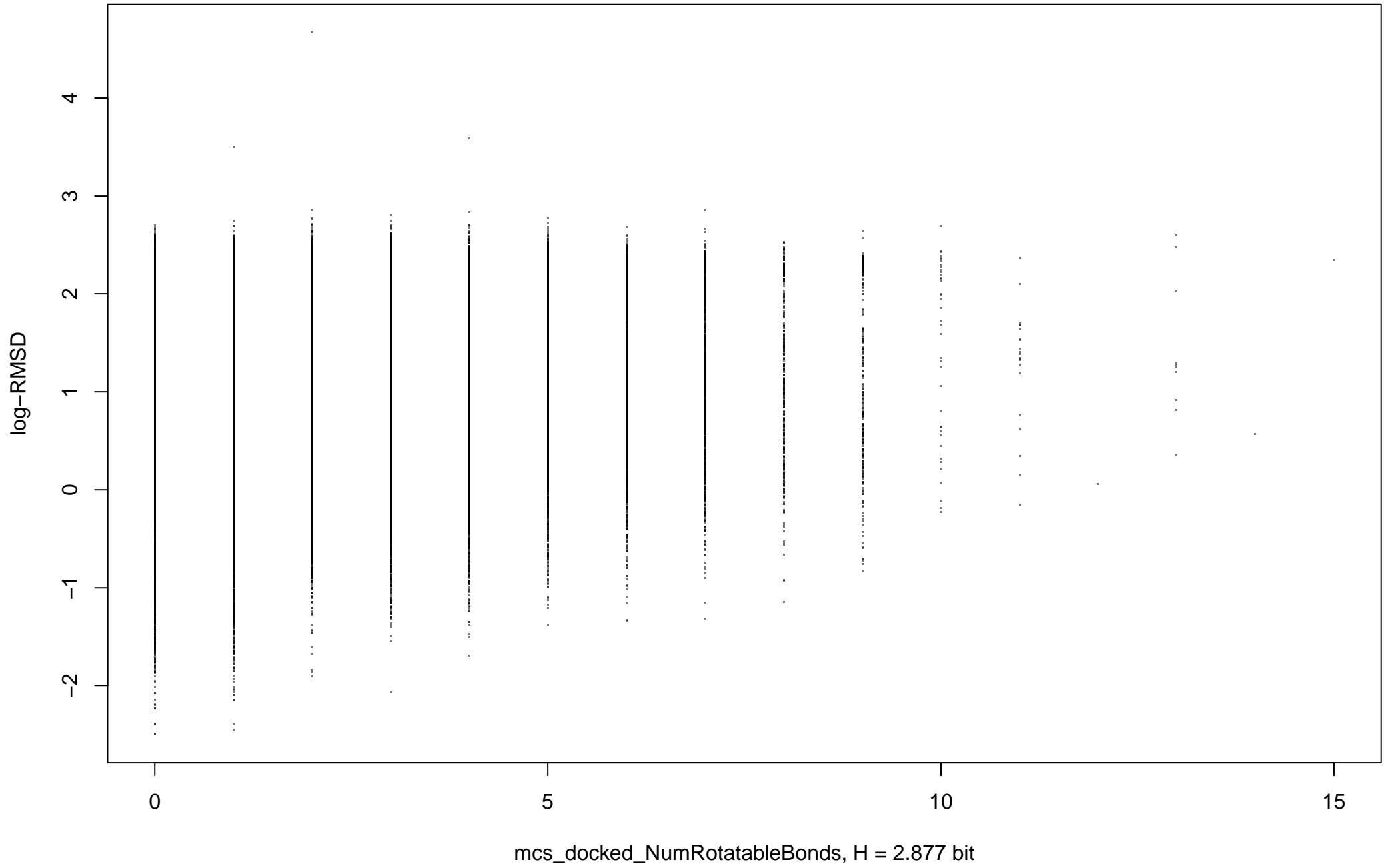


shift_docked_NumHAcceptors, MI = 0.056 bit, norm = 0.01954, cond entr = 4.273 bit

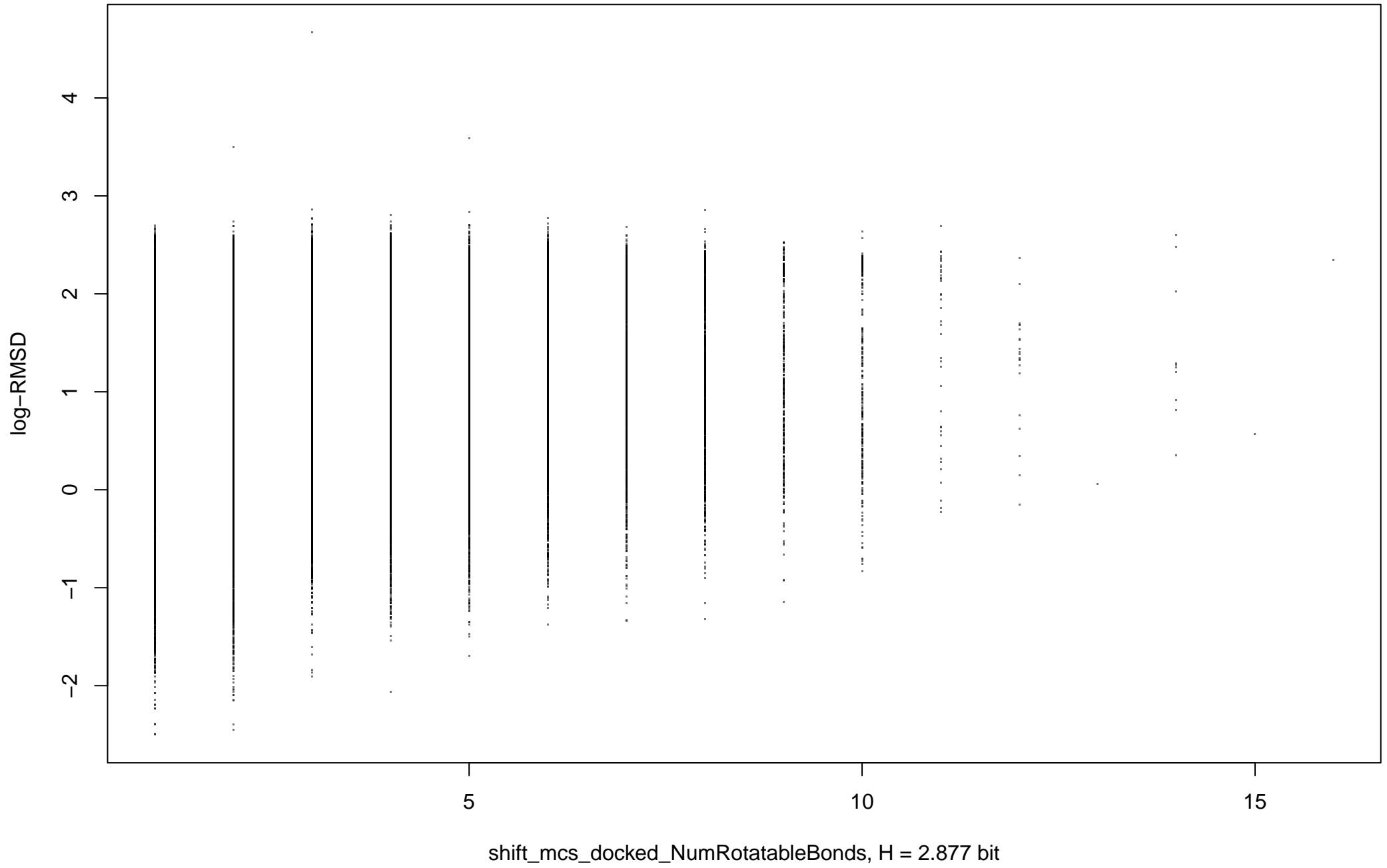


shift_docked_NumHAcceptors, H = 2.865 bit

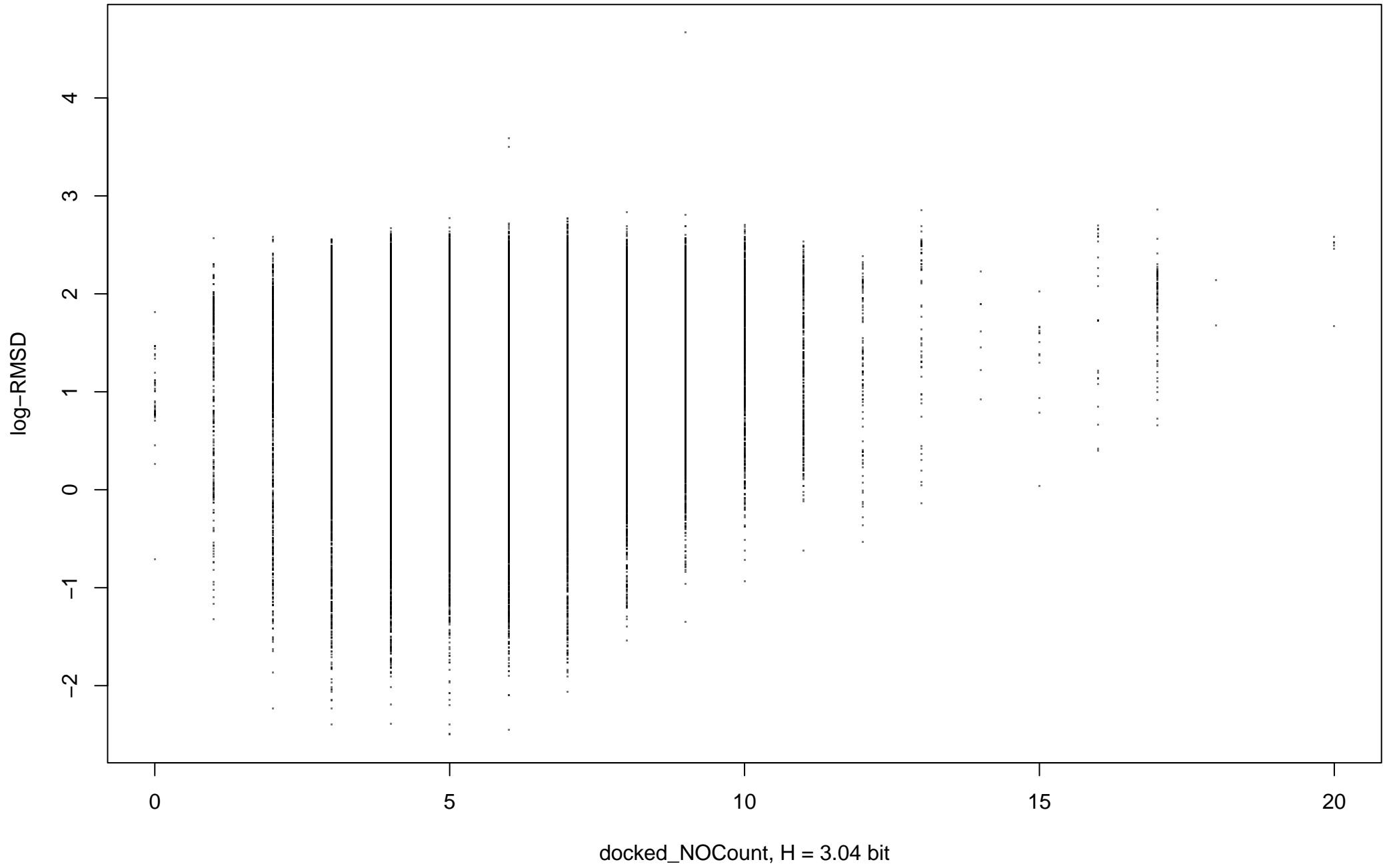
mcs_docked_NumRotatableBonds, MI = 0.05592 bit, norm = 0.01944, cond entr = 4.273 bit



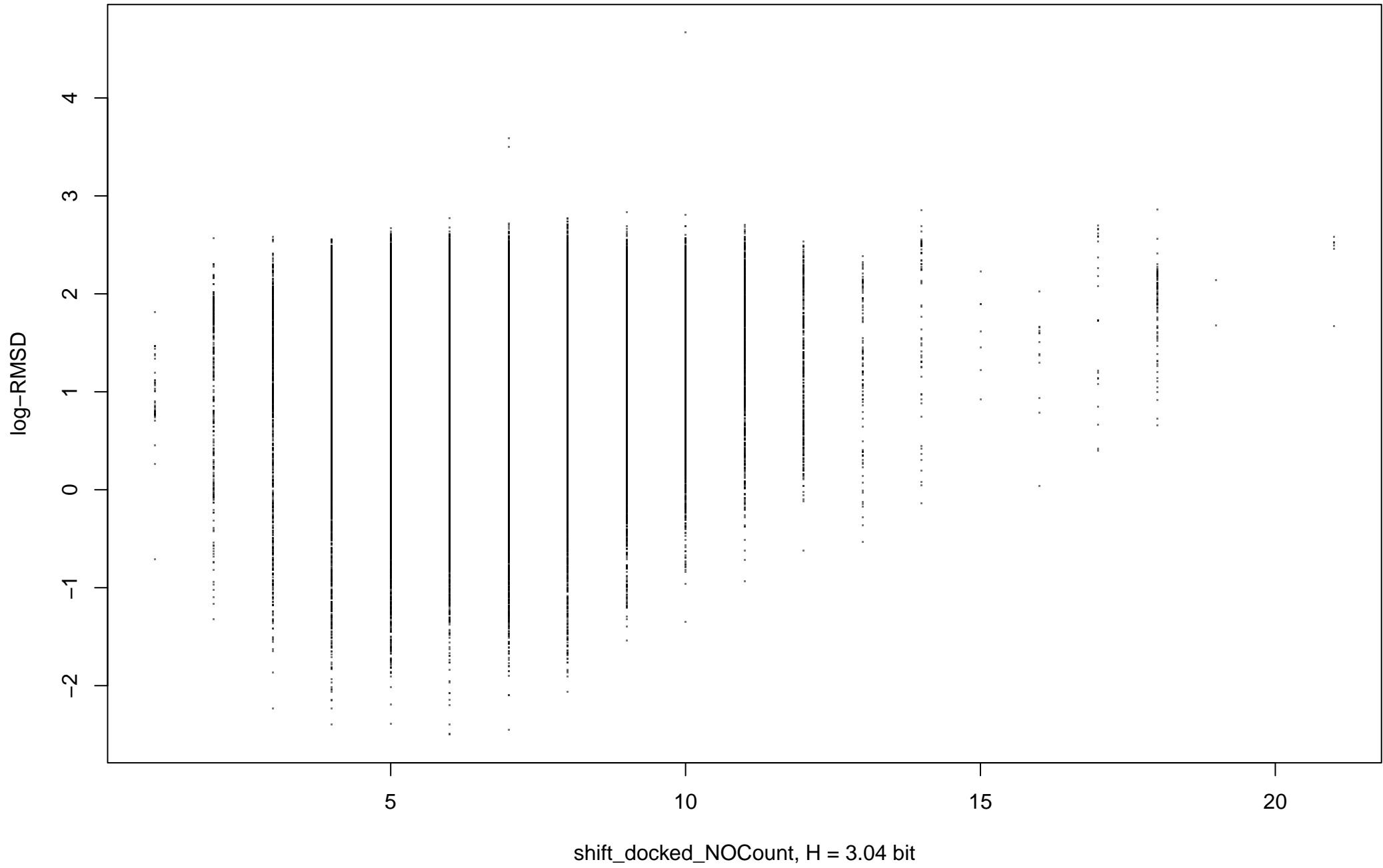
shift_mcs_docked_NumRotatableBonds, MI = 0.05592 bit, norm = 0.01944, cond entr = 4.273 bit



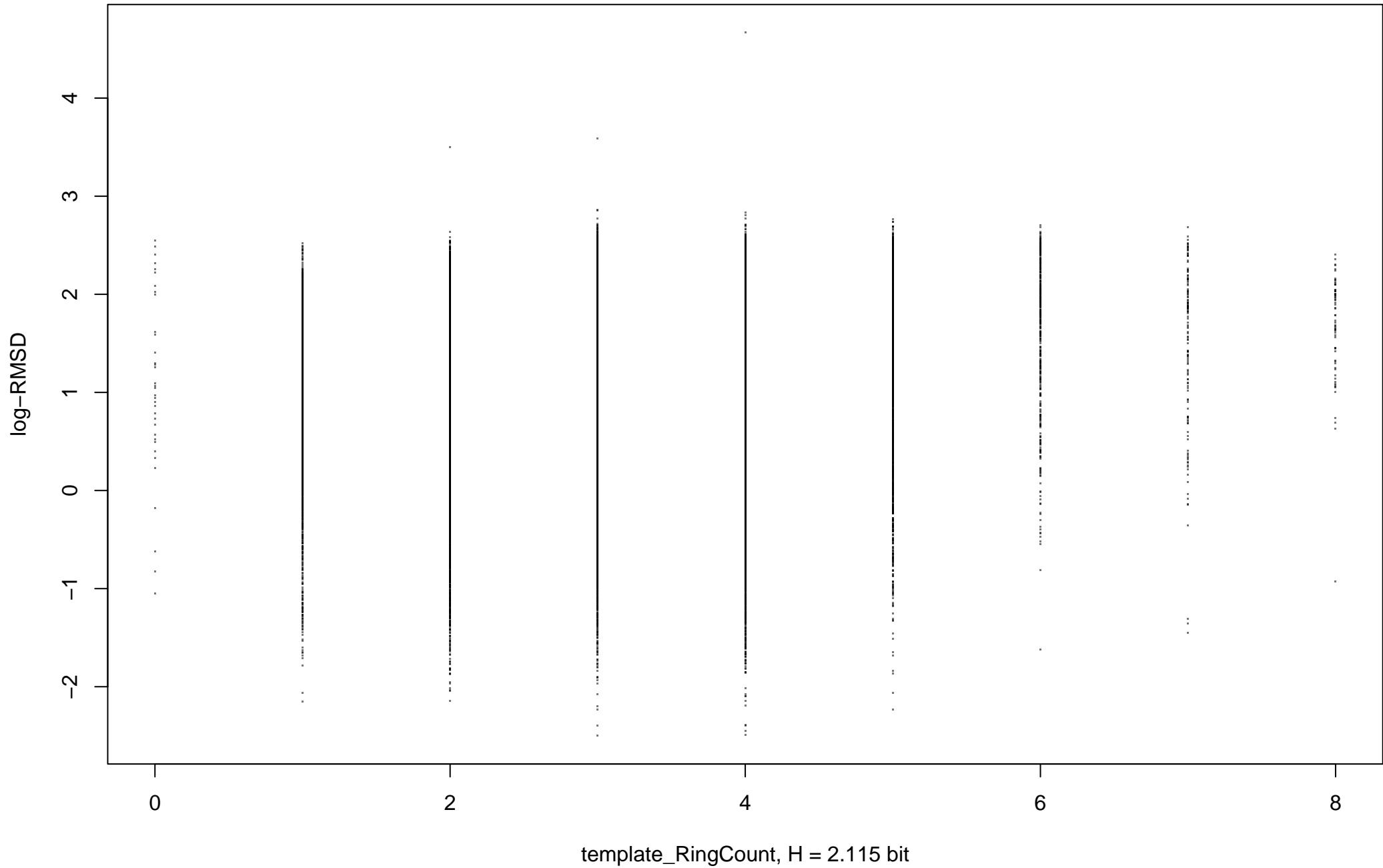
docked_NOCount, MI = 0.05359 bit, norm = 0.01763, cond entr = 4.276 bit



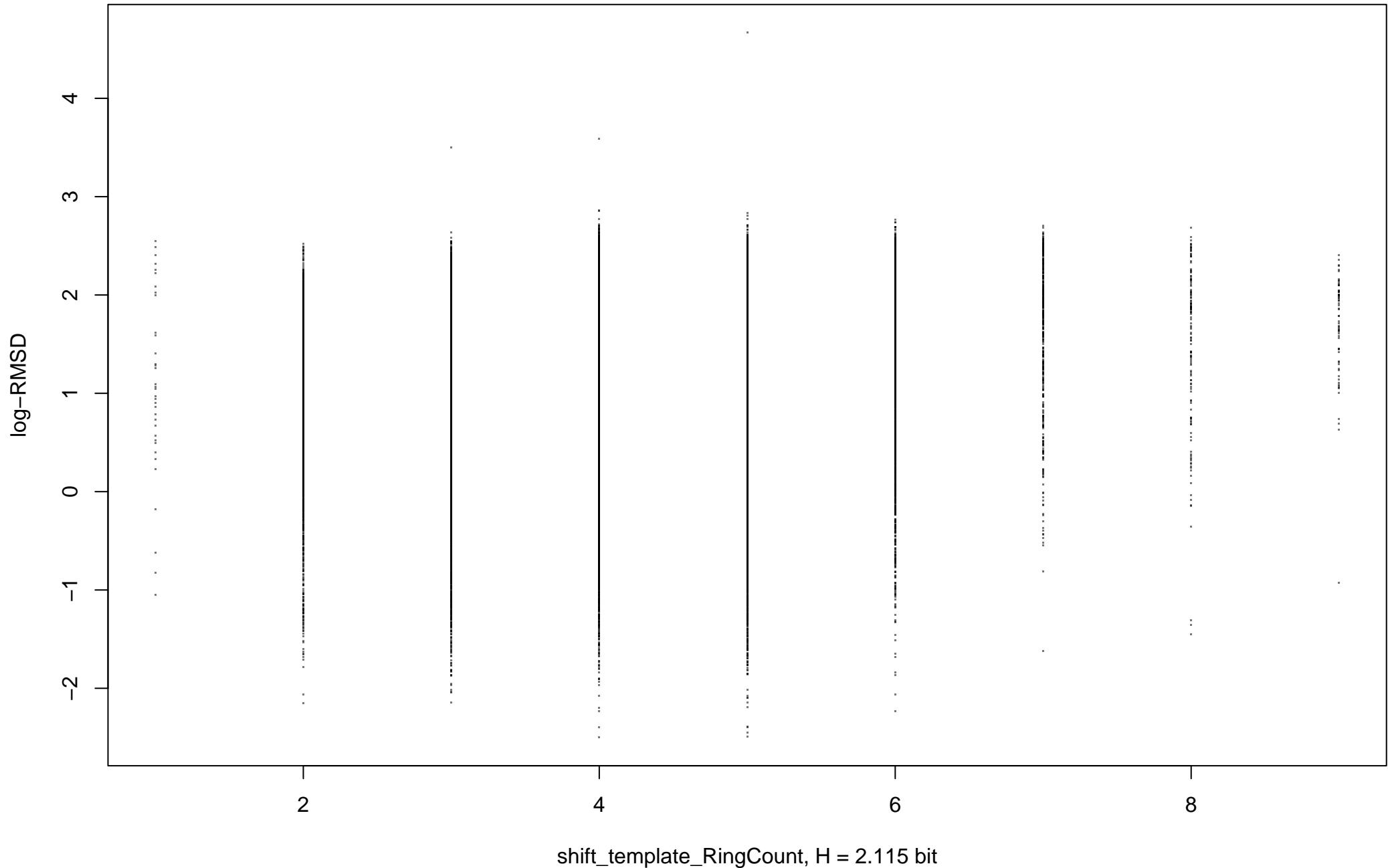
shift_docked_NOCount, MI = 0.05359 bit, norm = 0.01763, cond entr = 4.276 bit



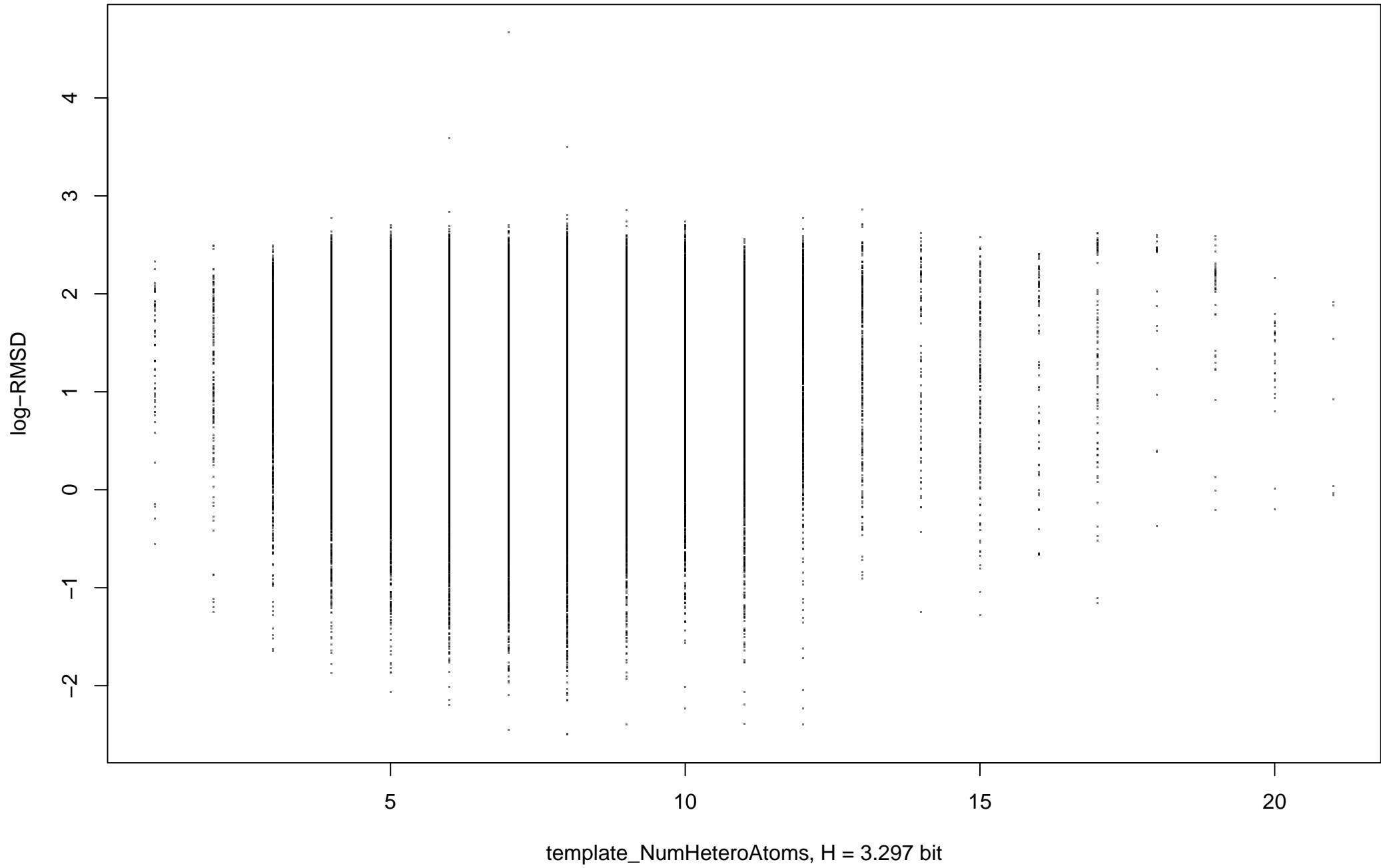
template_RingCount, MI = 0.04507 bit, norm = 0.02131, cond entr = 4.284 bit



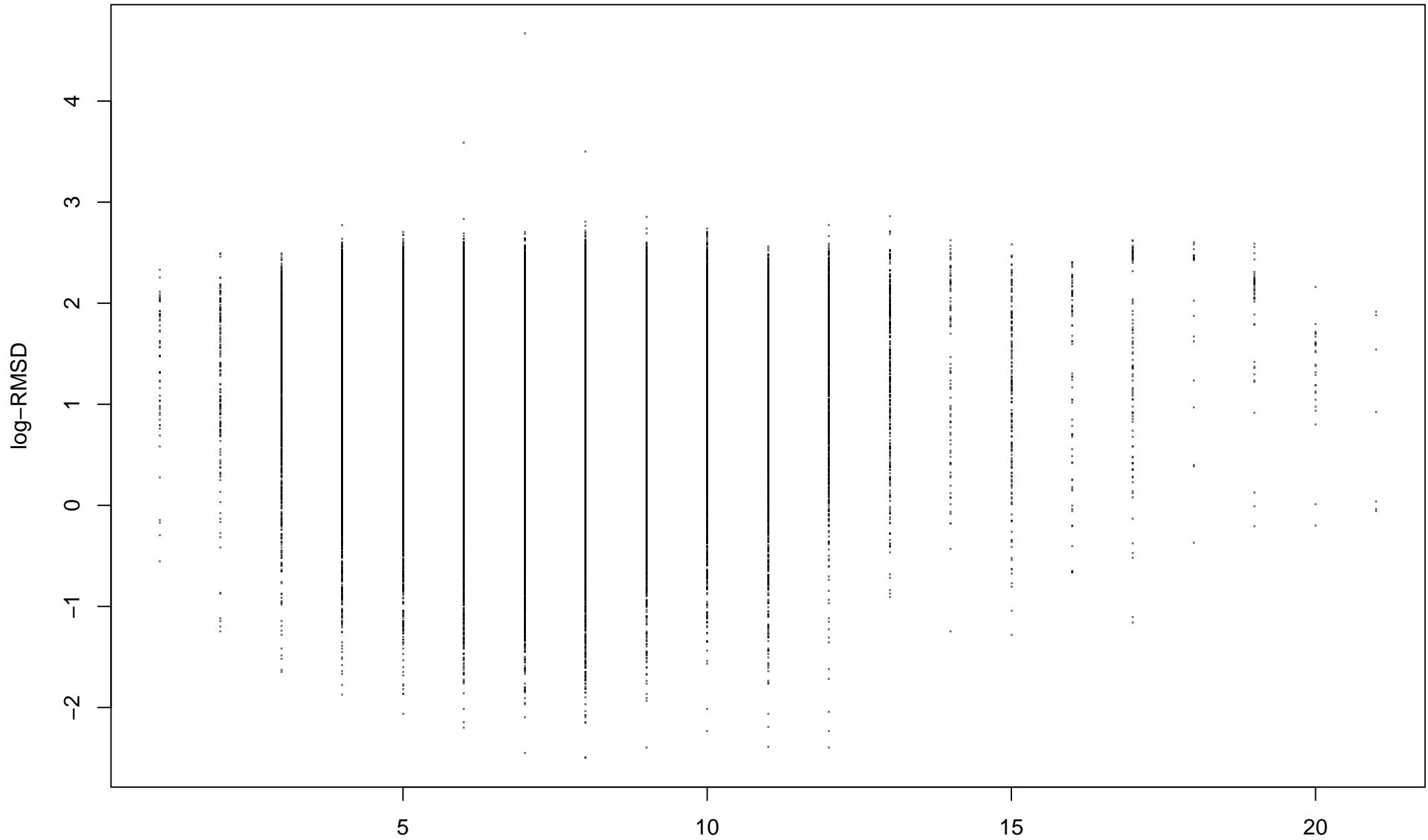
shift_template_RingCount, MI = 0.04507 bit, norm = 0.02131, cond entr = 4.284 bit



template_NumHeteroAtoms, MI = 0.0441 bit, norm = 0.01337, cond entr = 4.285 bit

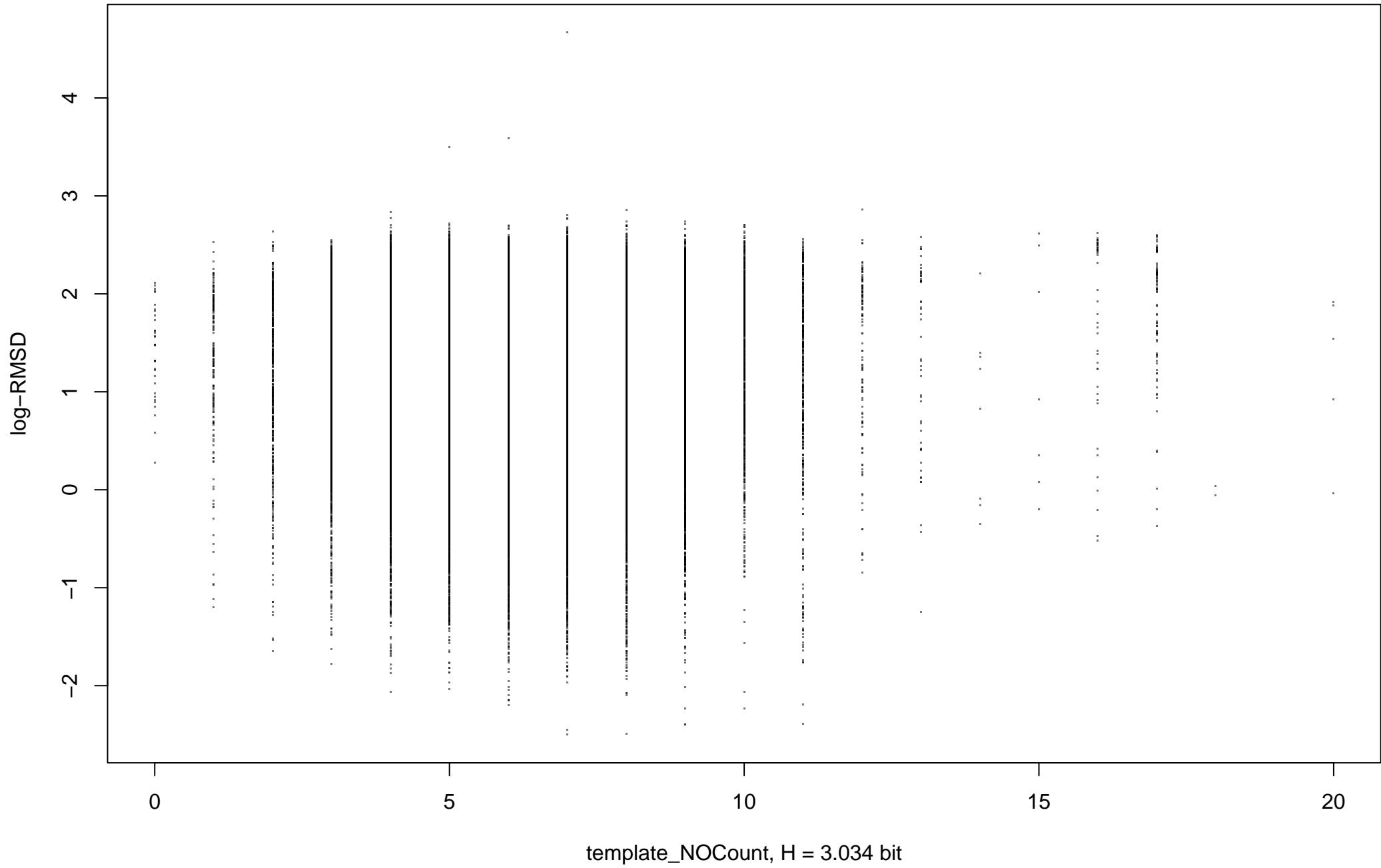


shift_template_NumHeteroAtoms, MI = 0.0441 bit, norm = 0.01337, cond entr = 4.285 bit

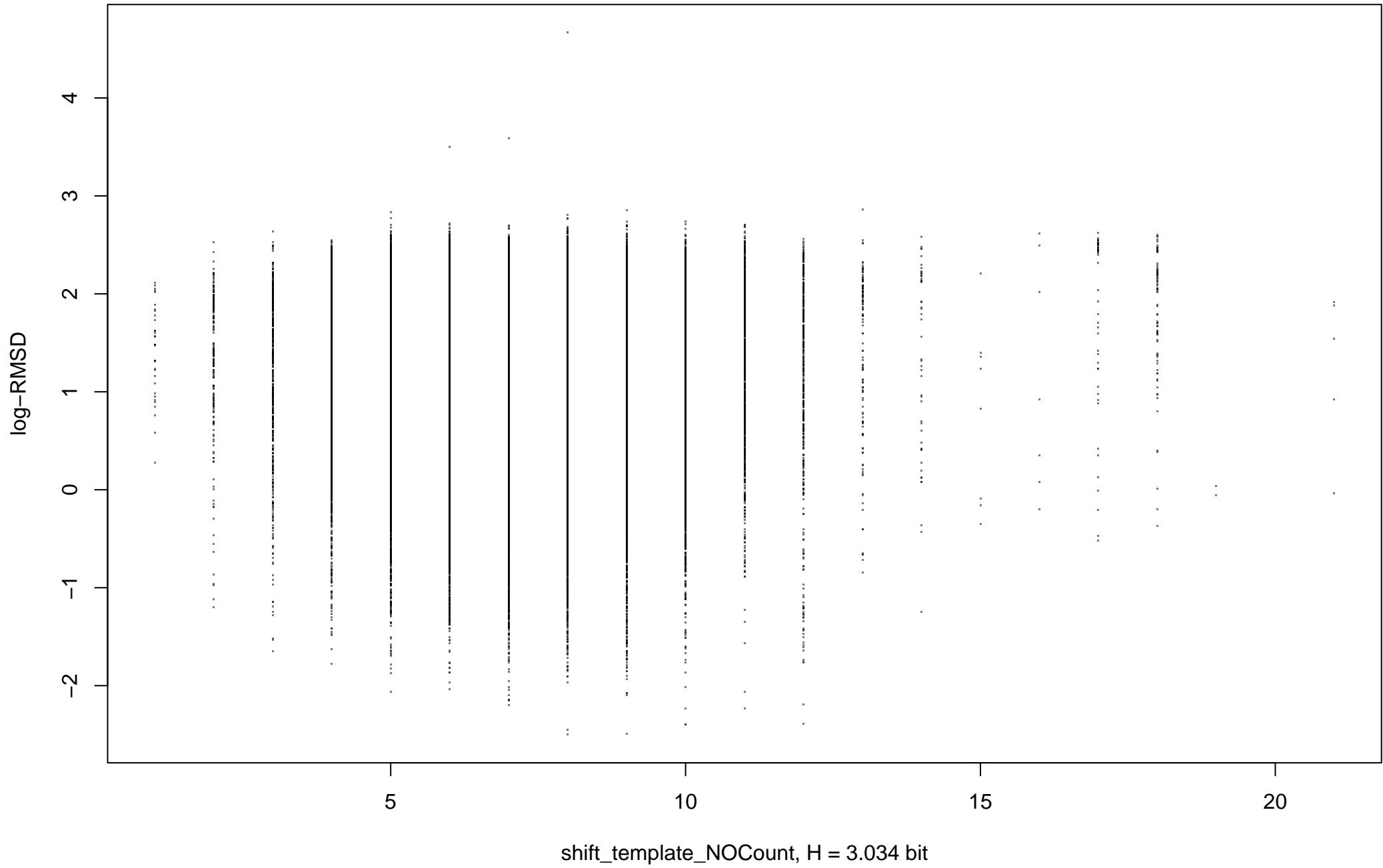


shift_template_NumHeteroAtoms, H = 3.297 bit

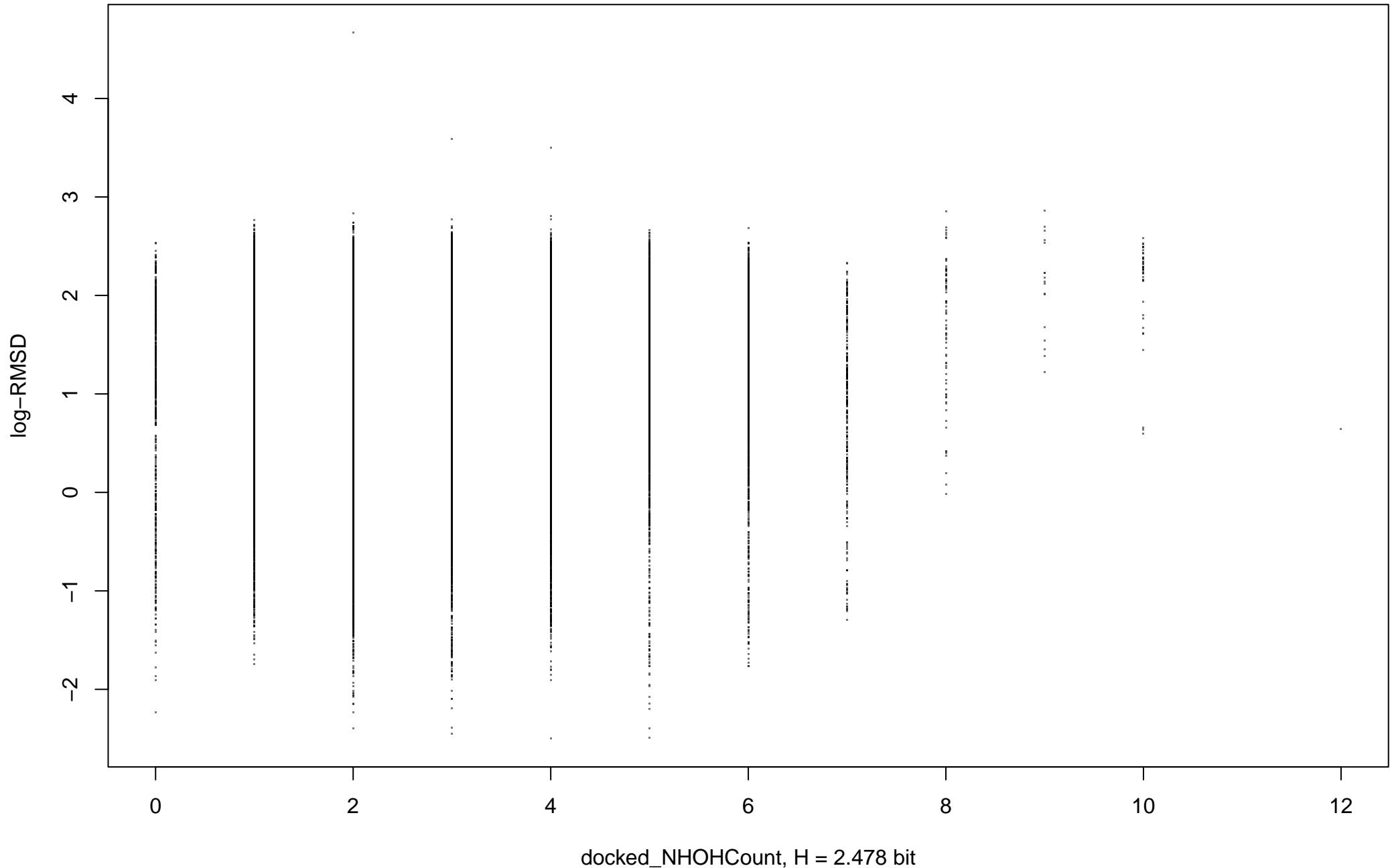
template_NOCount, MI = 0.04249 bit, norm = 0.01401, cond entr = 4.287 bit



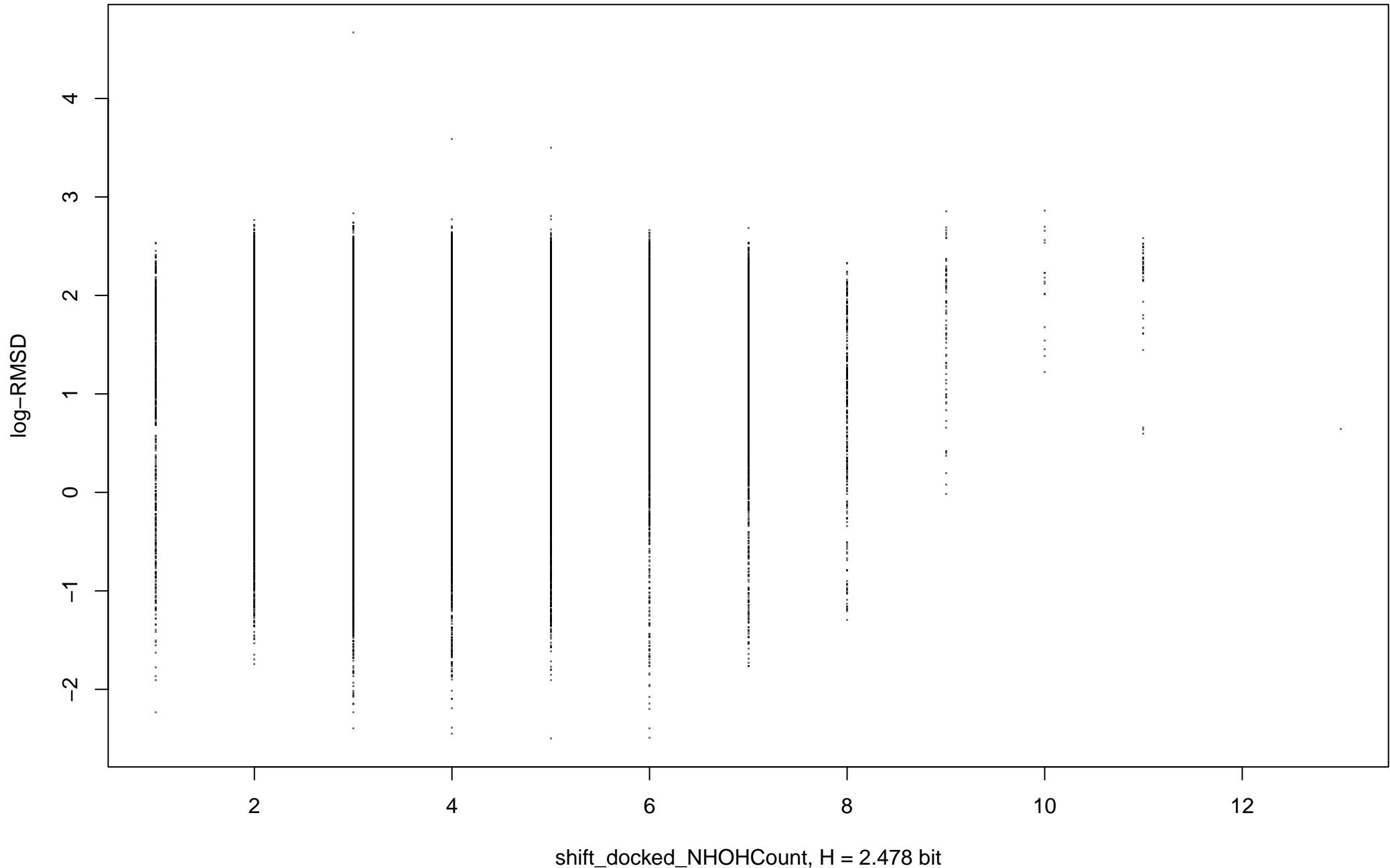
shift_template_NOCount, MI = 0.04249 bit, norm = 0.01401, cond entr = 4.287 bit



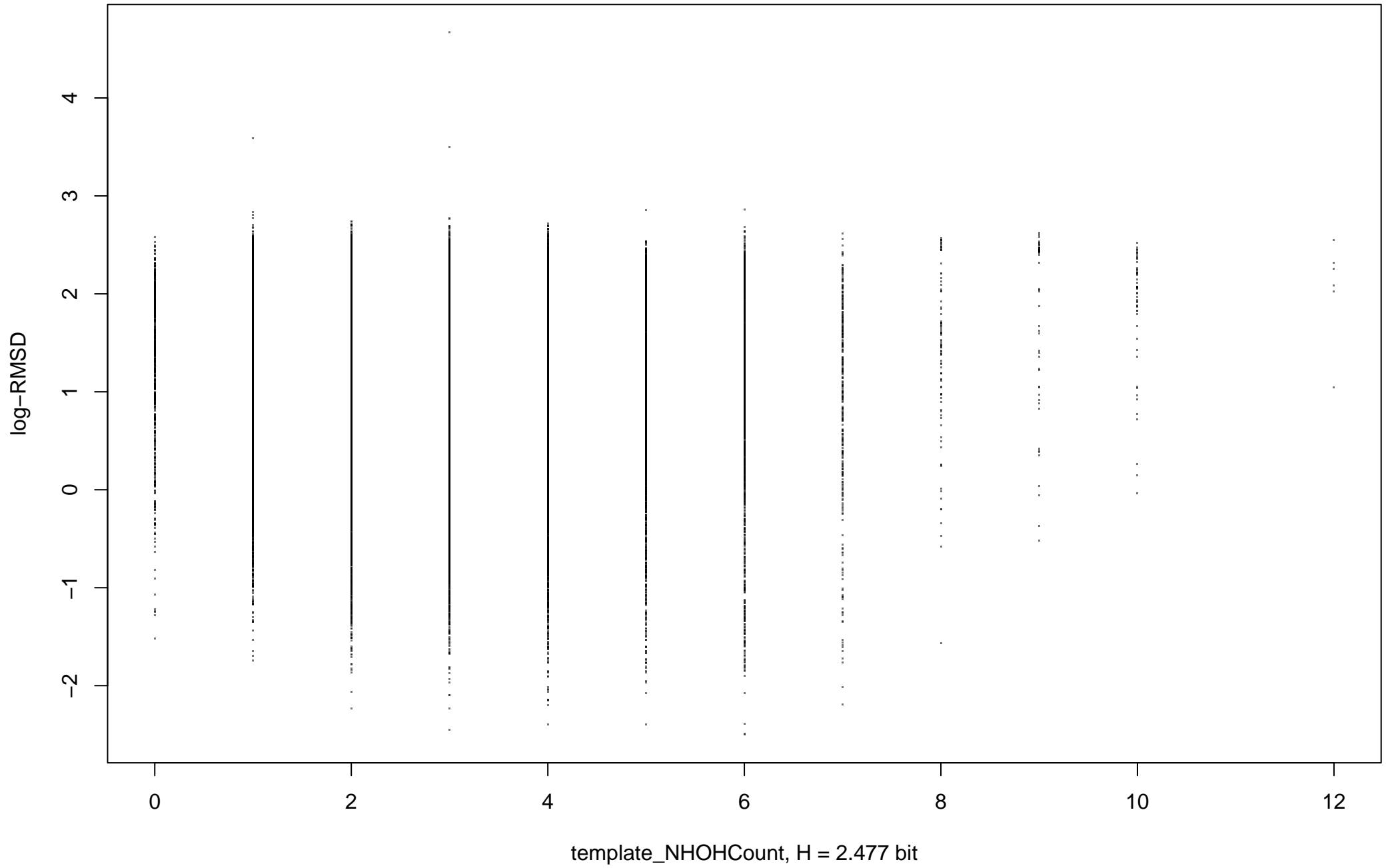
docked_NHOHCount, MI = 0.04175 bit, norm = 0.01685, cond entr = 4.288 bit



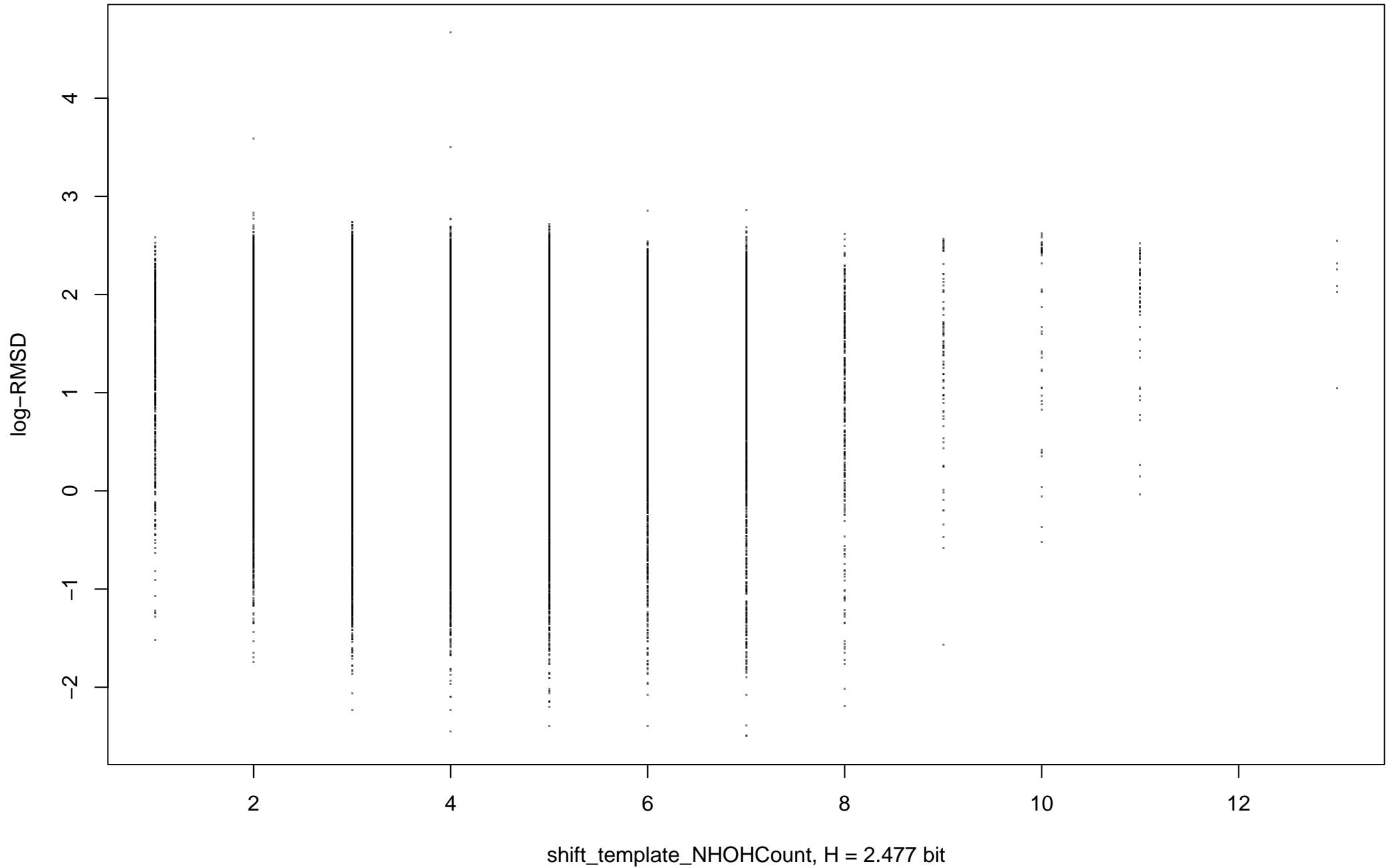
shift_docked_NHOHCount, MI = 0.04175 bit, norm = 0.01685, cond entr = 4.288 bit



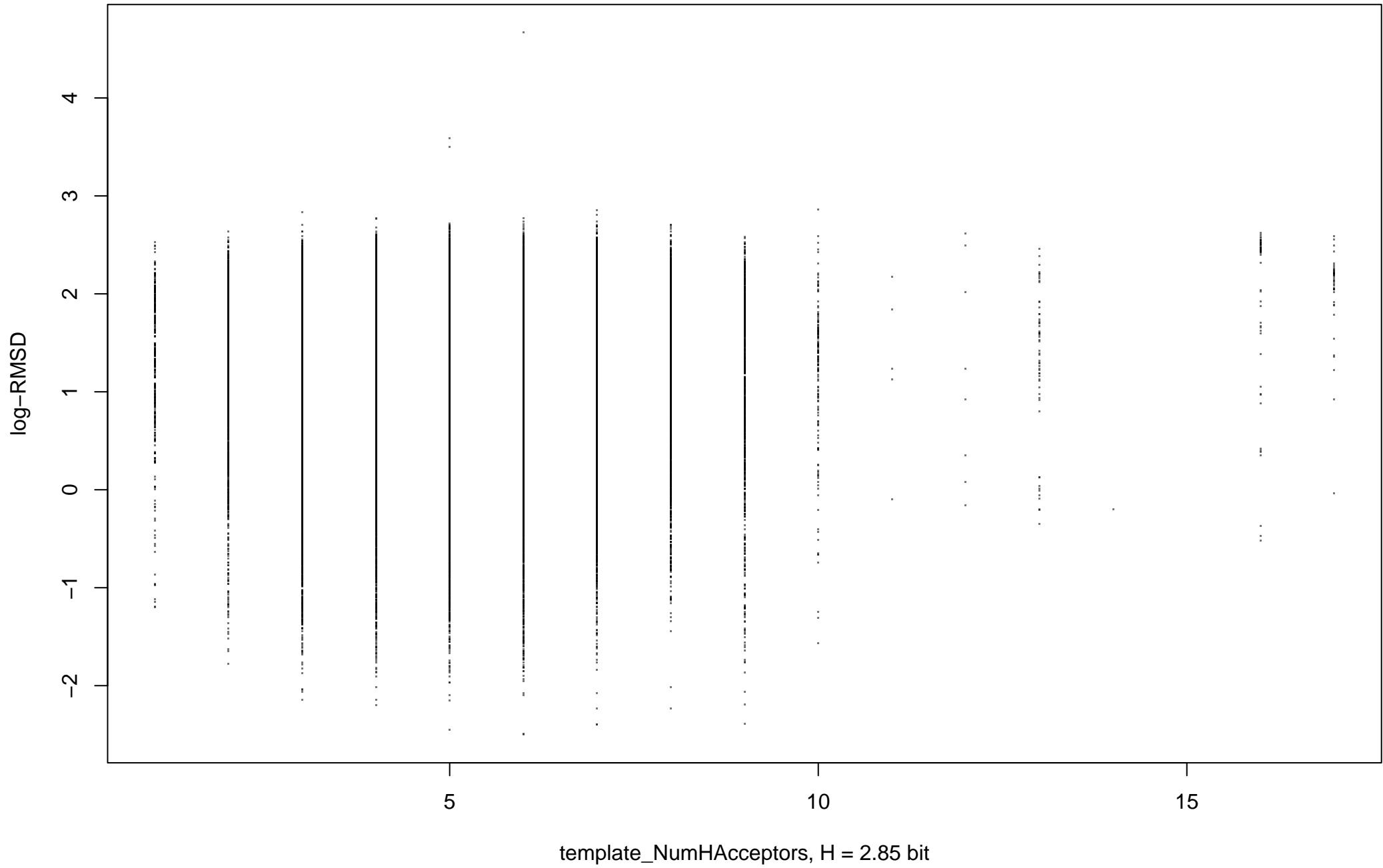
template_NHOHCount, MI = 0.04099 bit, norm = 0.01655, cond entr = 4.288 bit



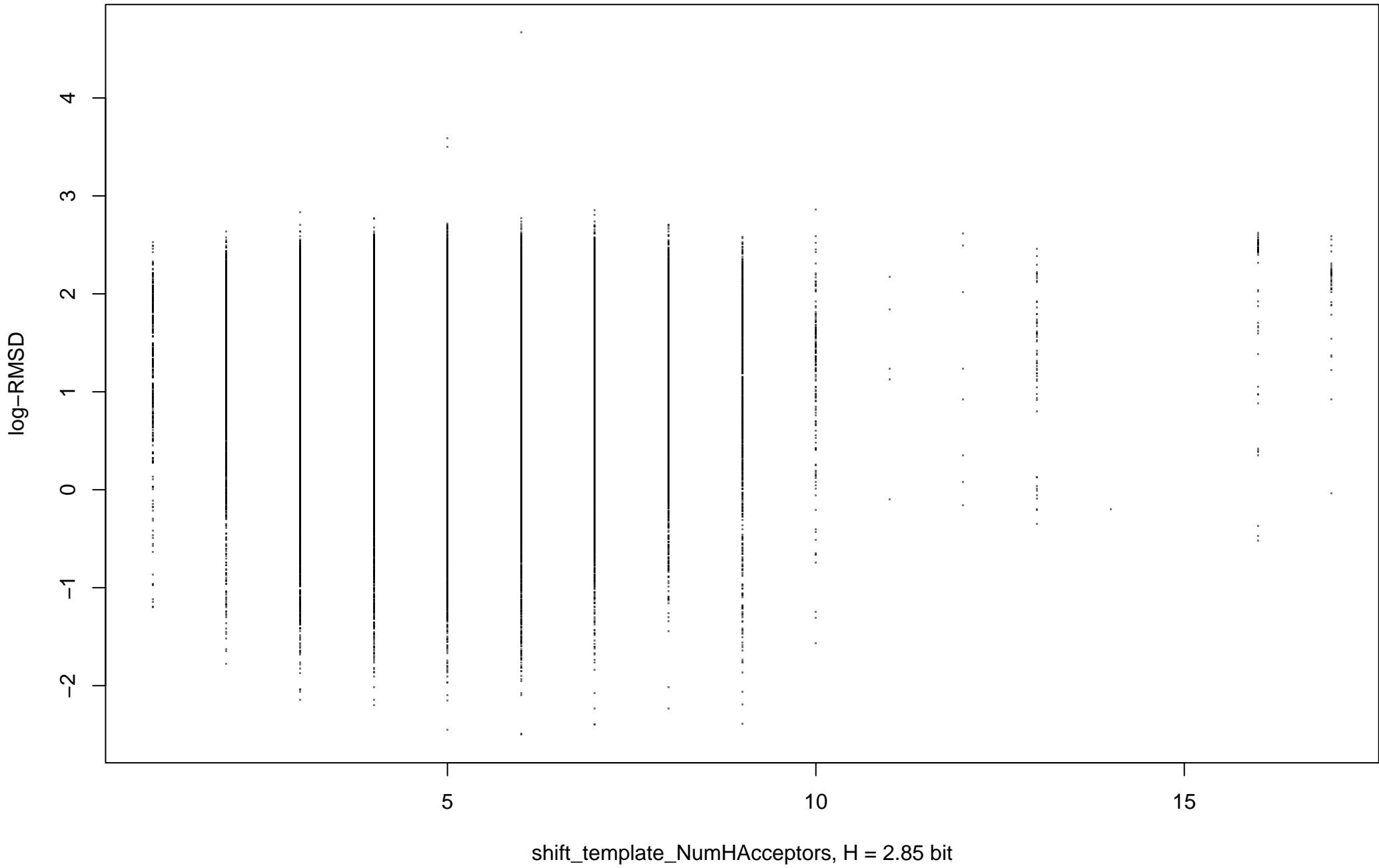
shift_template_NHOHCount, MI = 0.04099 bit, norm = 0.01655, cond entr = 4.288 bit



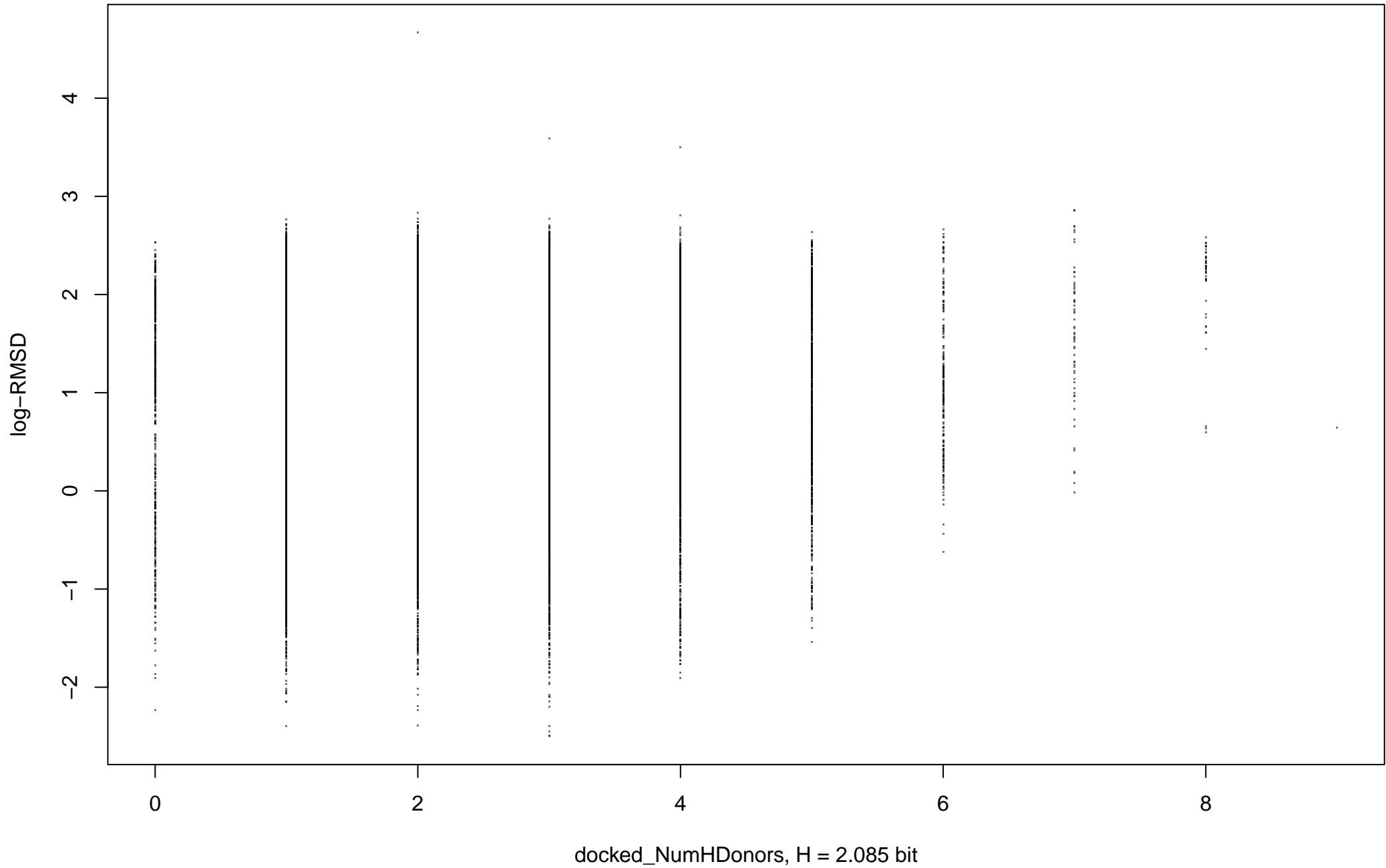
template_NumHAcceptors, MI = 0.03333 bit, norm = 0.01169, cond entr = 4.296 bit



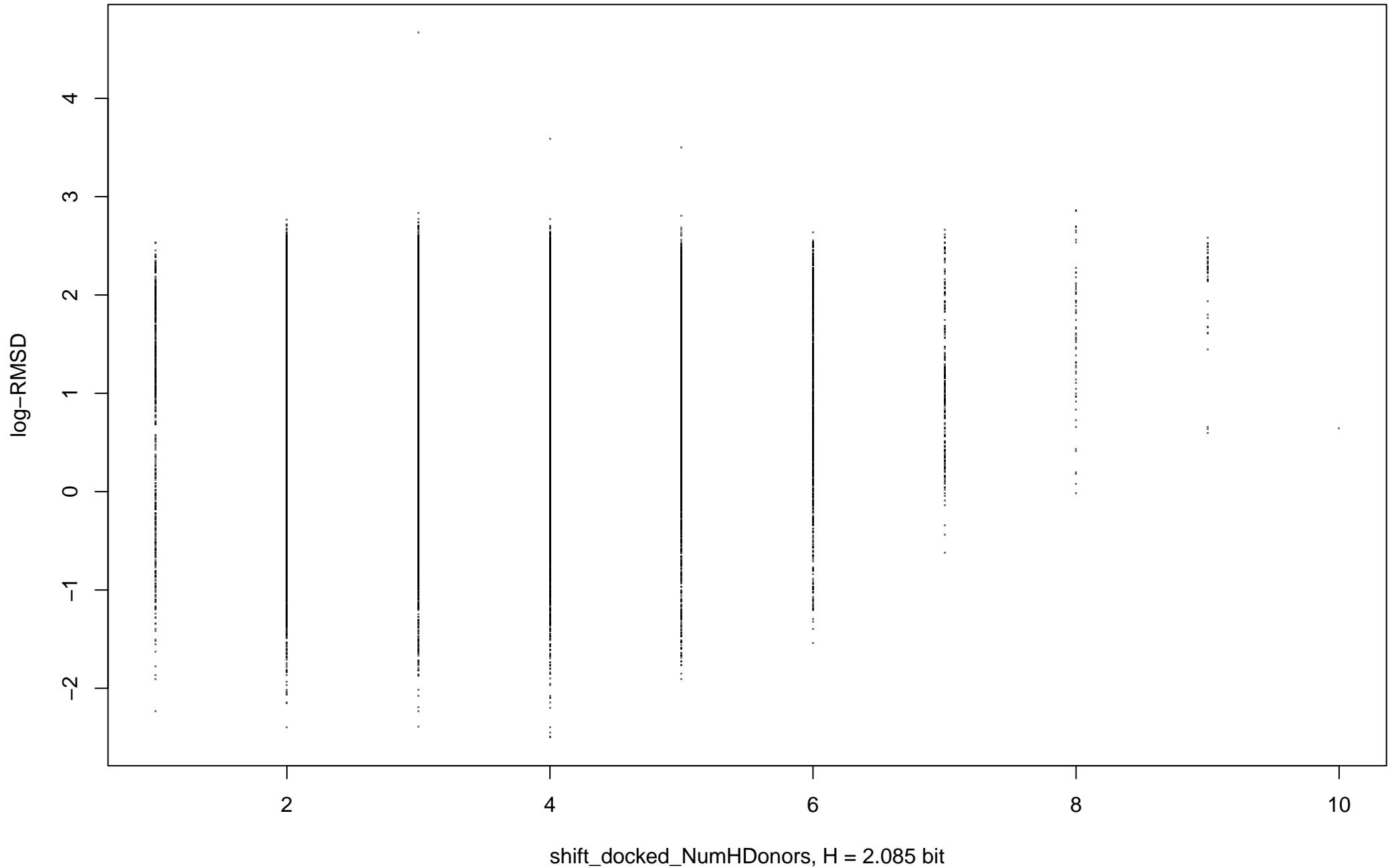
shift_template_NumHAcceptors, MI = 0.03333 bit, norm = 0.01169, cond entr = 4.296 bit



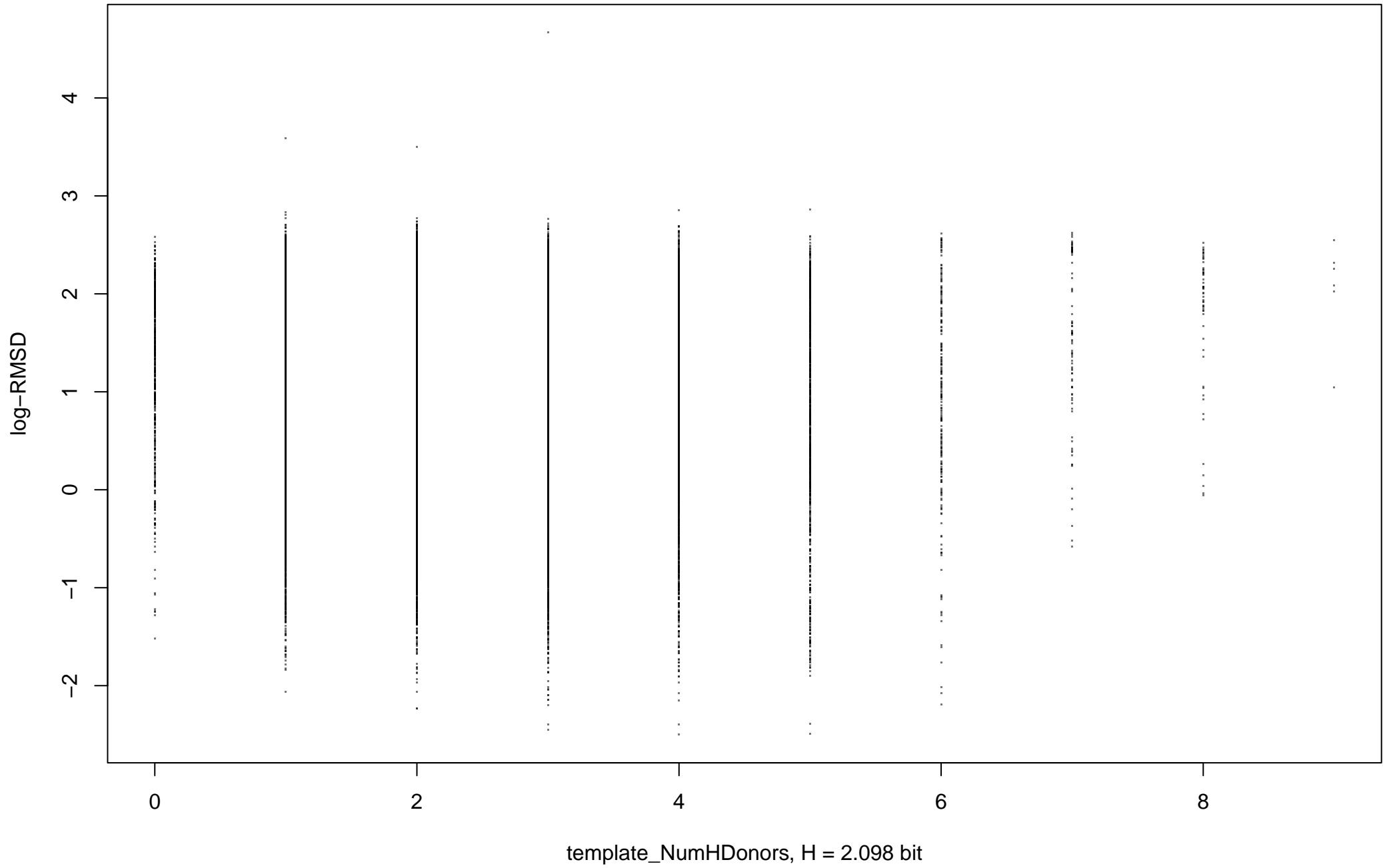
docked_NumHDonors, MI = 0.03068 bit, norm = 0.01472, cond entr = 4.299 bit



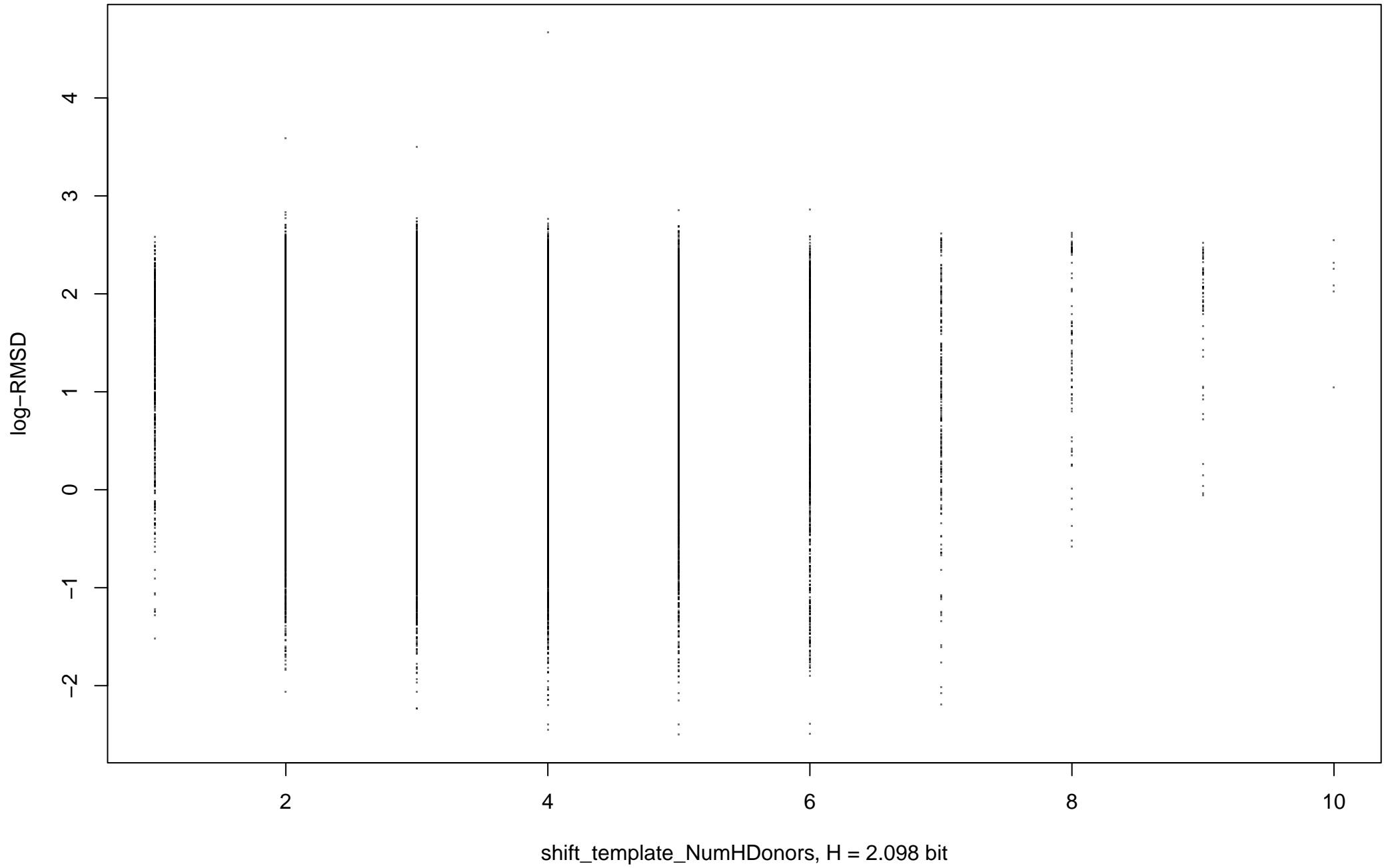
shift_docked_NumHDonors, MI = 0.03068 bit, norm = 0.01472, cond entr = 4.299 bit



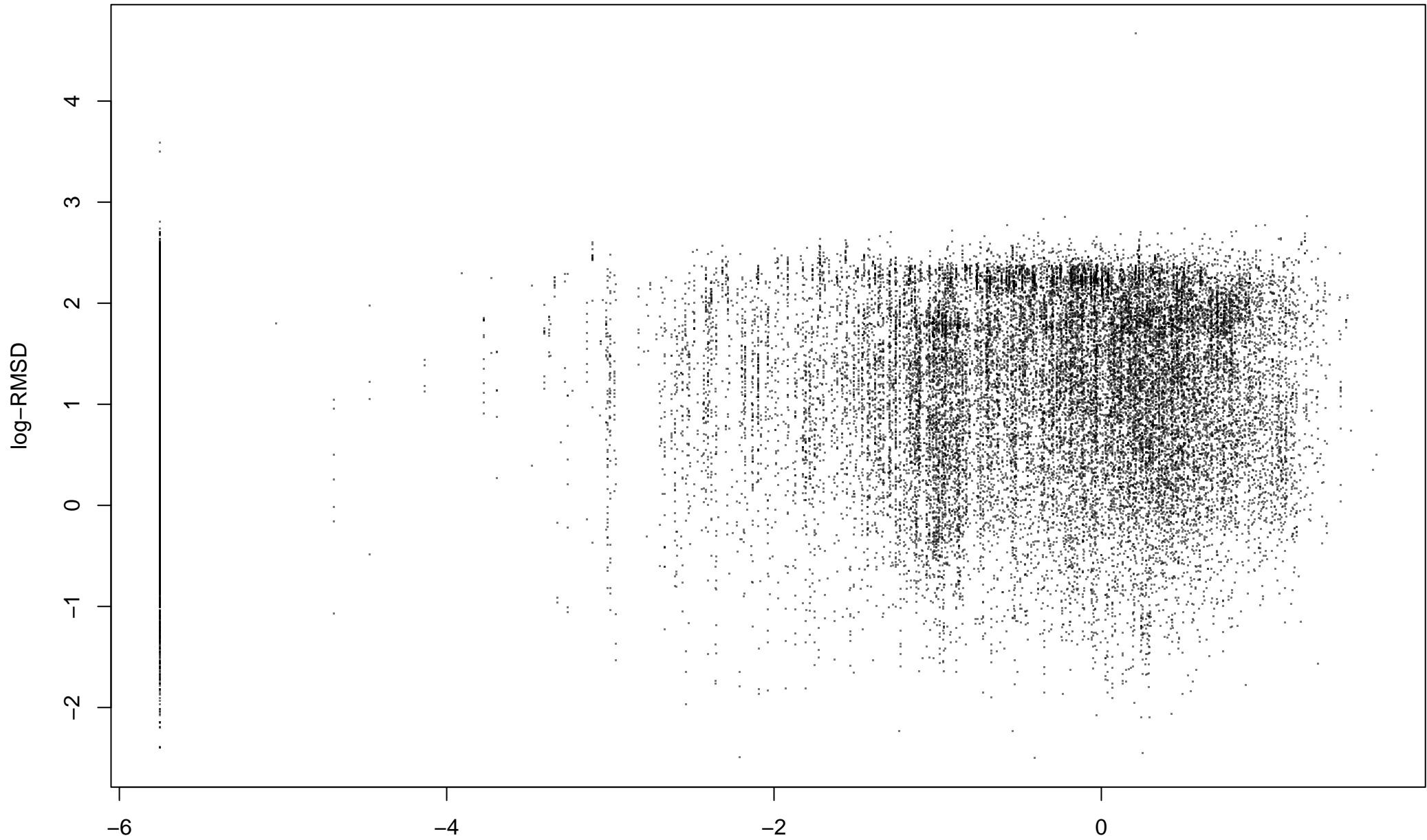
template_NumHDonors, MI = 0.0292 bit, norm = 0.01392, cond entr = 4.3 bit



shift_template_NumHDonors, MI = 0.0292 bit, norm = 0.01392, cond entr = 4.3 bit



log_mcs_bonded_polar_sasa, MI = 0.0276 bit, norm = 0.01184, cond entr = 4.302 bit



log_mcs_bonded_polar_sasa, H = 2.332 bit