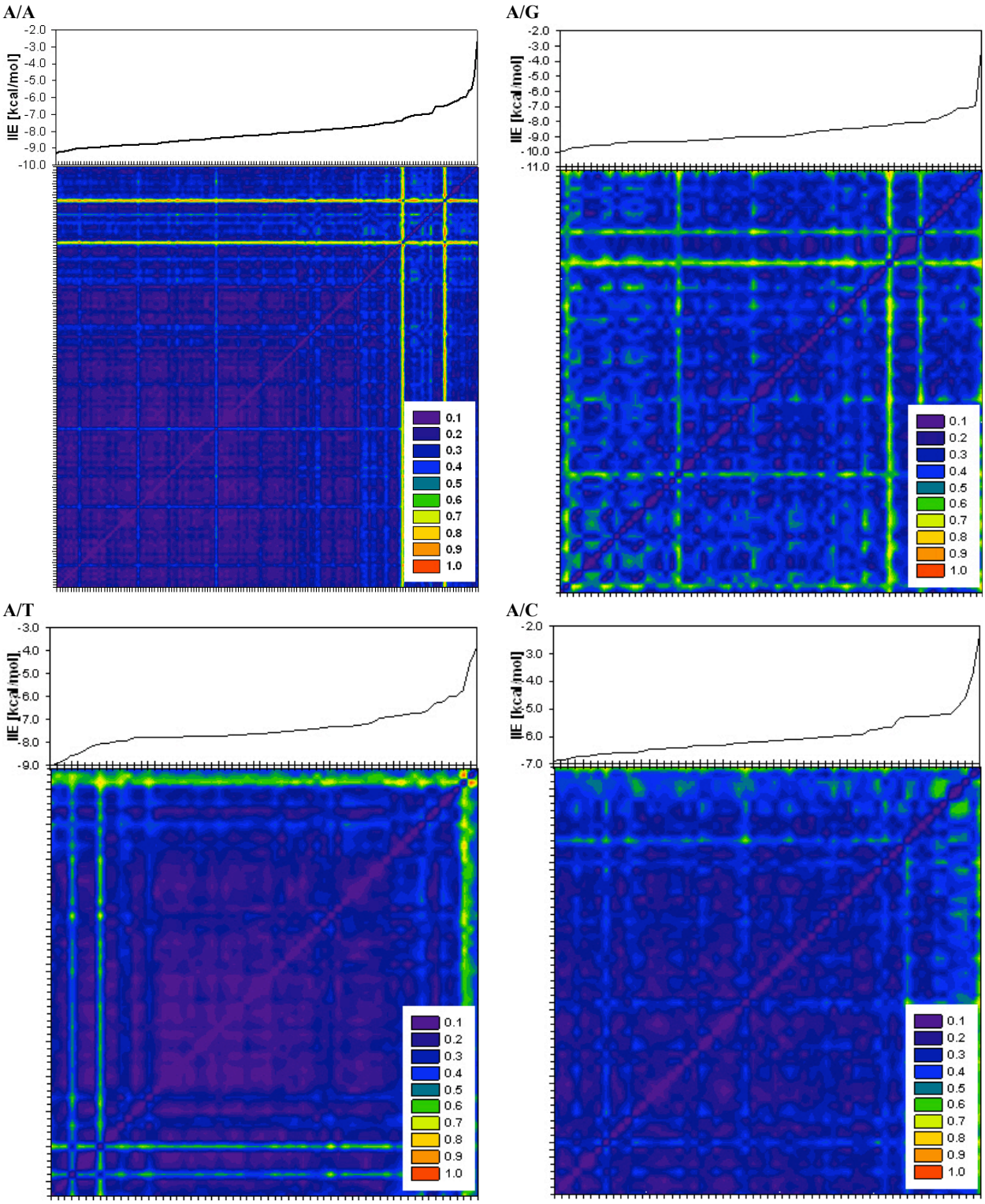

Fig. S1. The distributions of NRMSD (RMSD of normalized values of base step parameters: *shift*, *slide*, *rise*, *roll*, *tilt*, *twist*) characterizing structural diversity of 5'-adenine stacked with four nucleobases. The stacked pairs are denoted by tick mark on edges of the plot were ordered with increasing values of stacking energy (IIE in kcal/mol). The color scale is the same for all distributions and represent actual values of NRMSD resulting from comparison of all possible twosome stacked dimers.

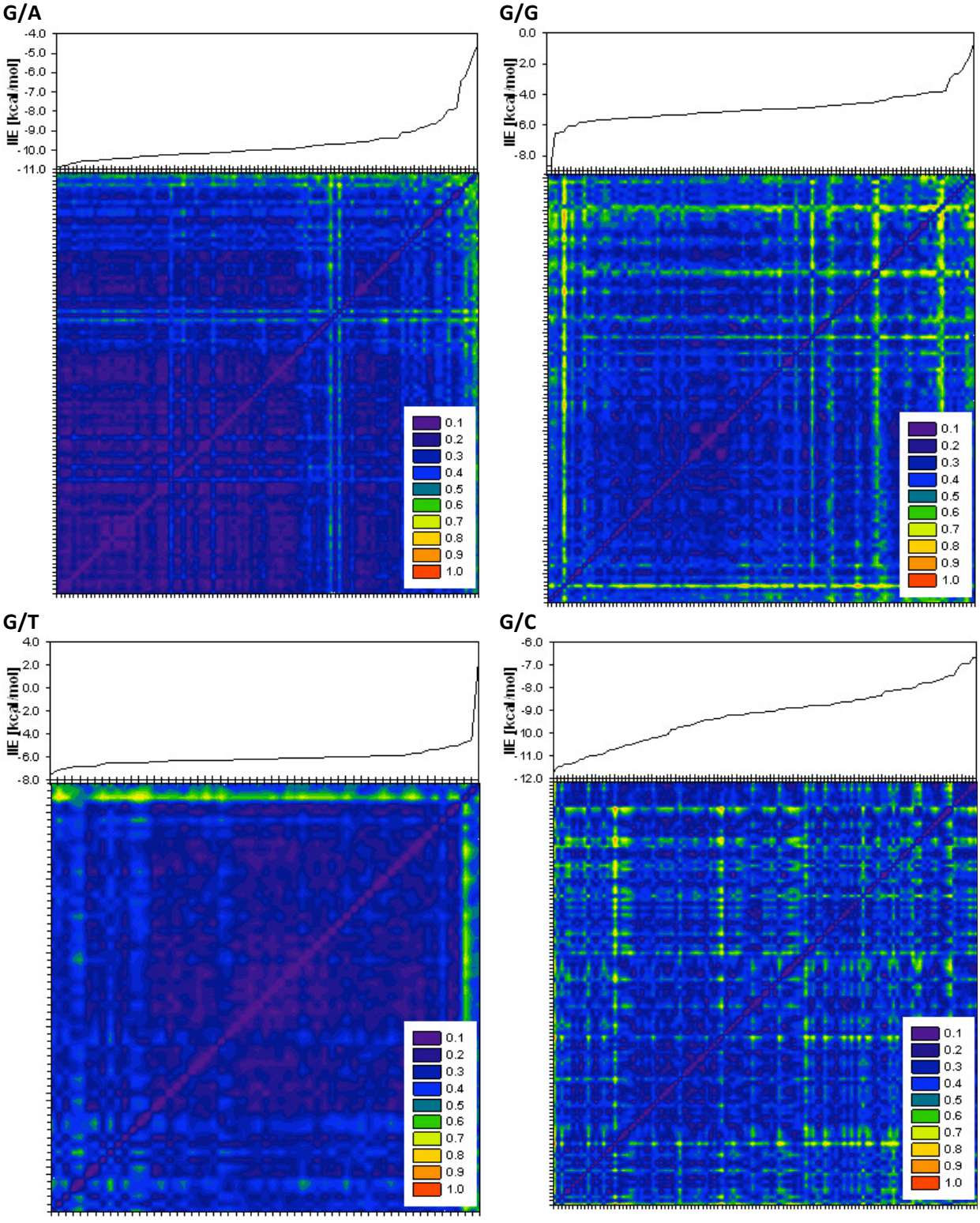

Fig. S2. The distributions of NRMSD characterizing structural diversity of 5'-guanine stacked with four nucleobases. Notation is the same as in Fig.S1

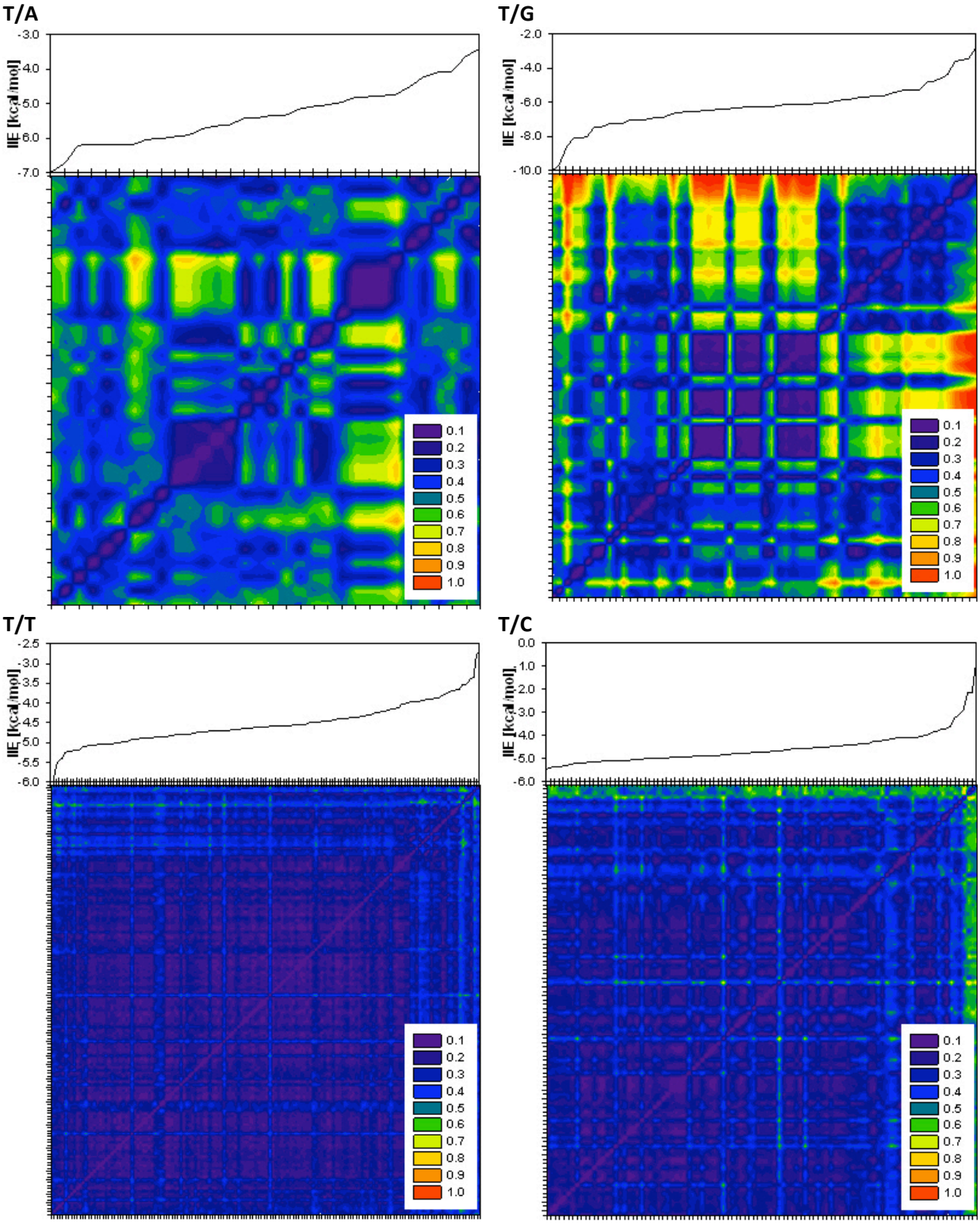

Fig. S3. The distributions of NRMSD characterizing structural diversity of 5'-thymine stacked with four nucleobases. Notating is the same as in Fig.S1

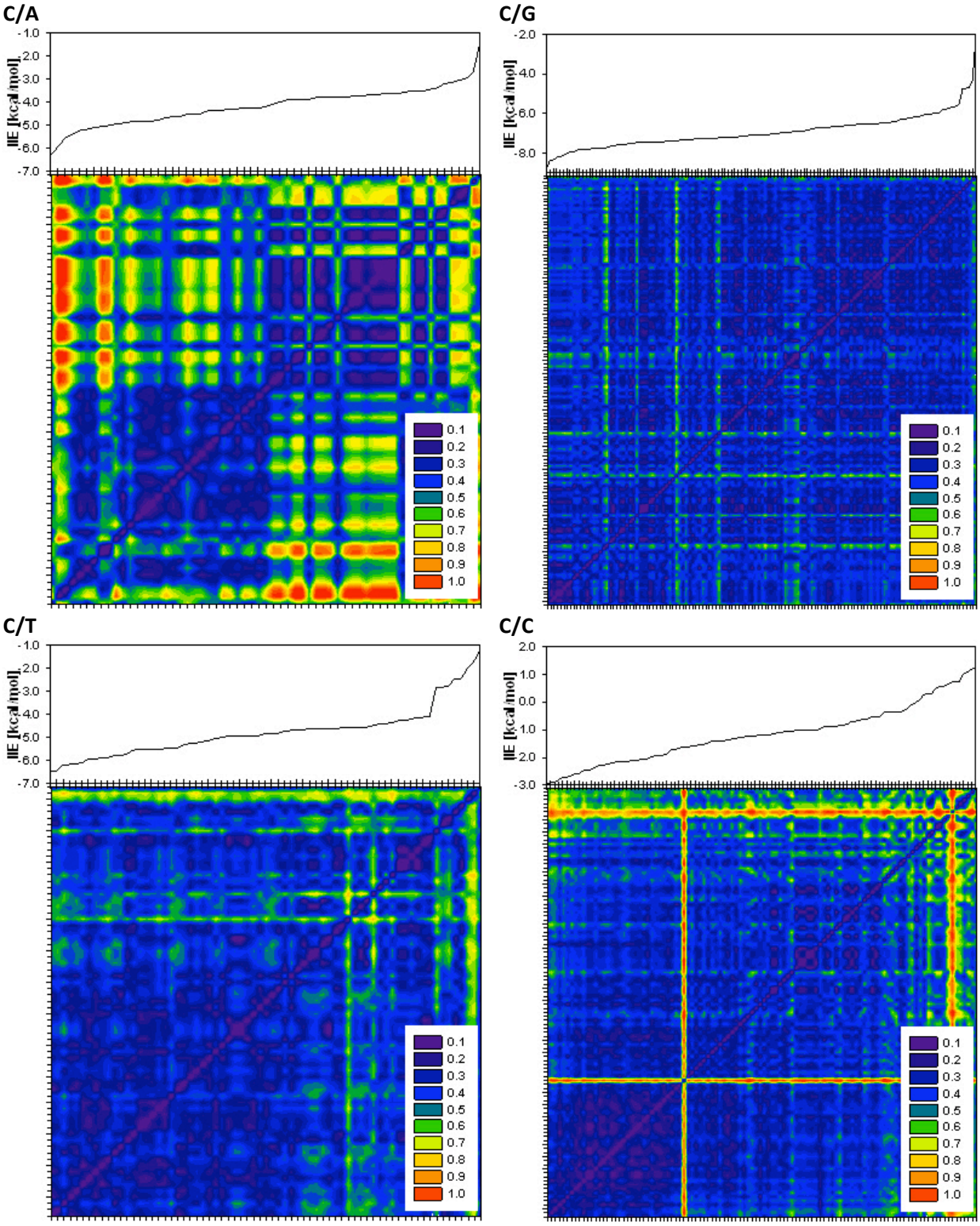

Fig. S4. The distributions of NRMSD characterizing structural diversity of 5'-cytosine stacked with four nucleobases. Notating is the same as in Fig.S1

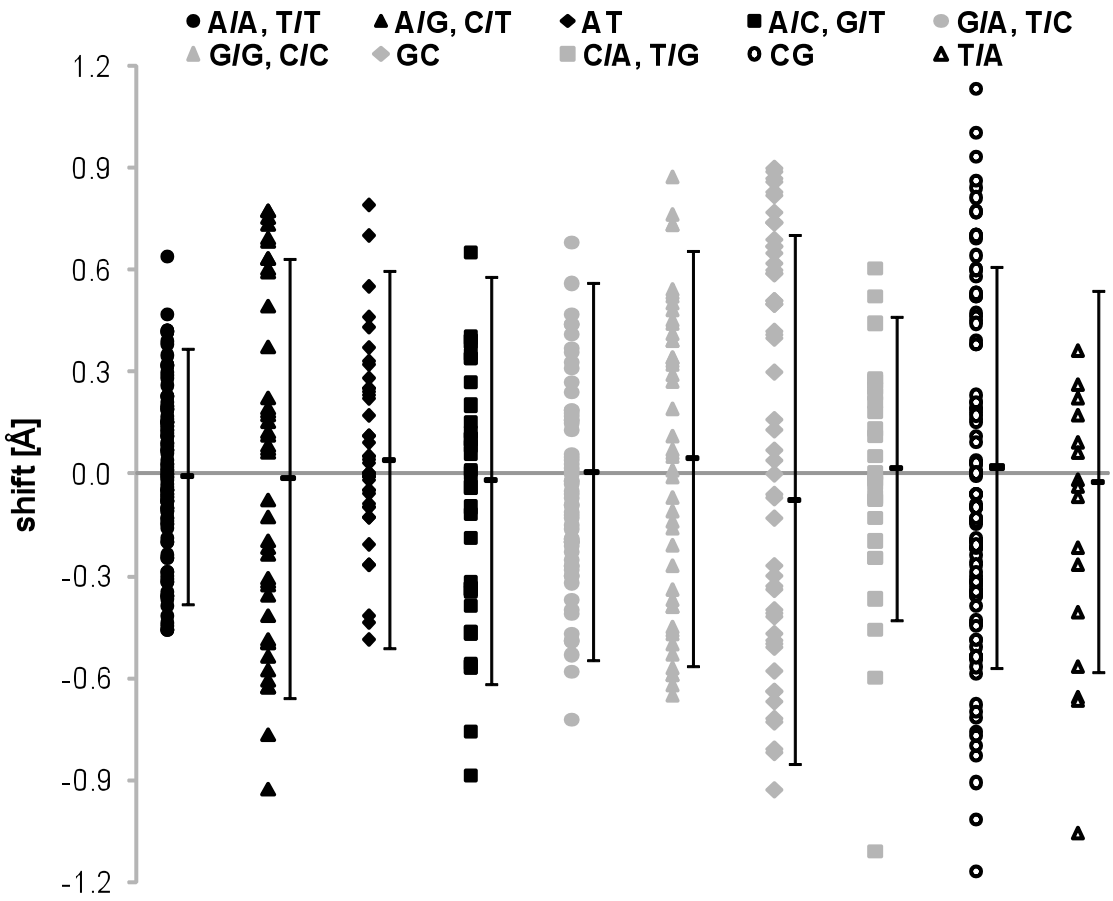

Fig. S5. The distributions of *shift* values characterizing all unique stacked pairs of nucleobases. Points correspond to the most representative structures only. They are characterized by smallest values of mean NRMSD (i.e. not higher than minimal value augmented by amount of the standard deviation). The mean value estimated for all stacked pairs along with corresponding standard deviation bars are also supplied next to each distribution.

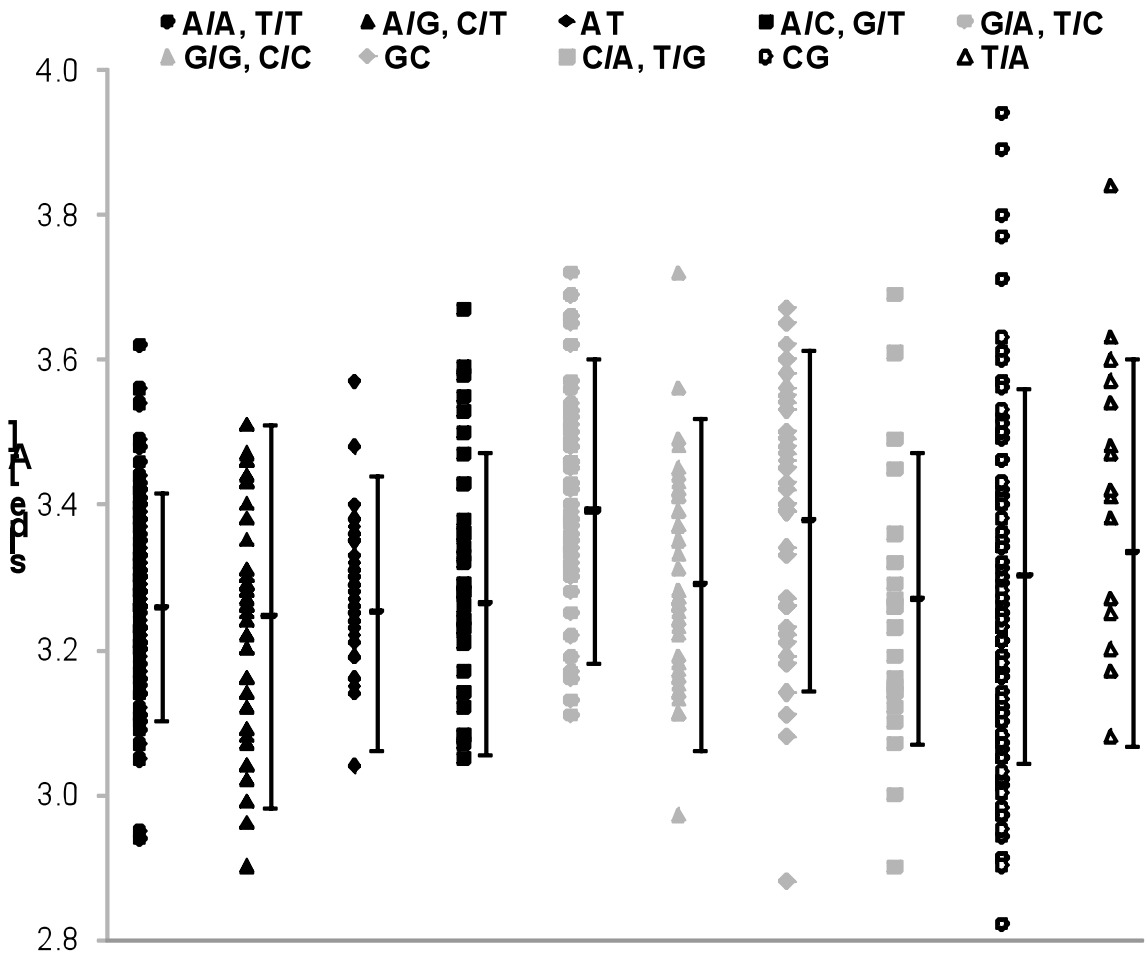

Fig. S6. The distributions of *rise* values characterizing all unique stacked pairs of nucleobases. For notation see Fig.S5

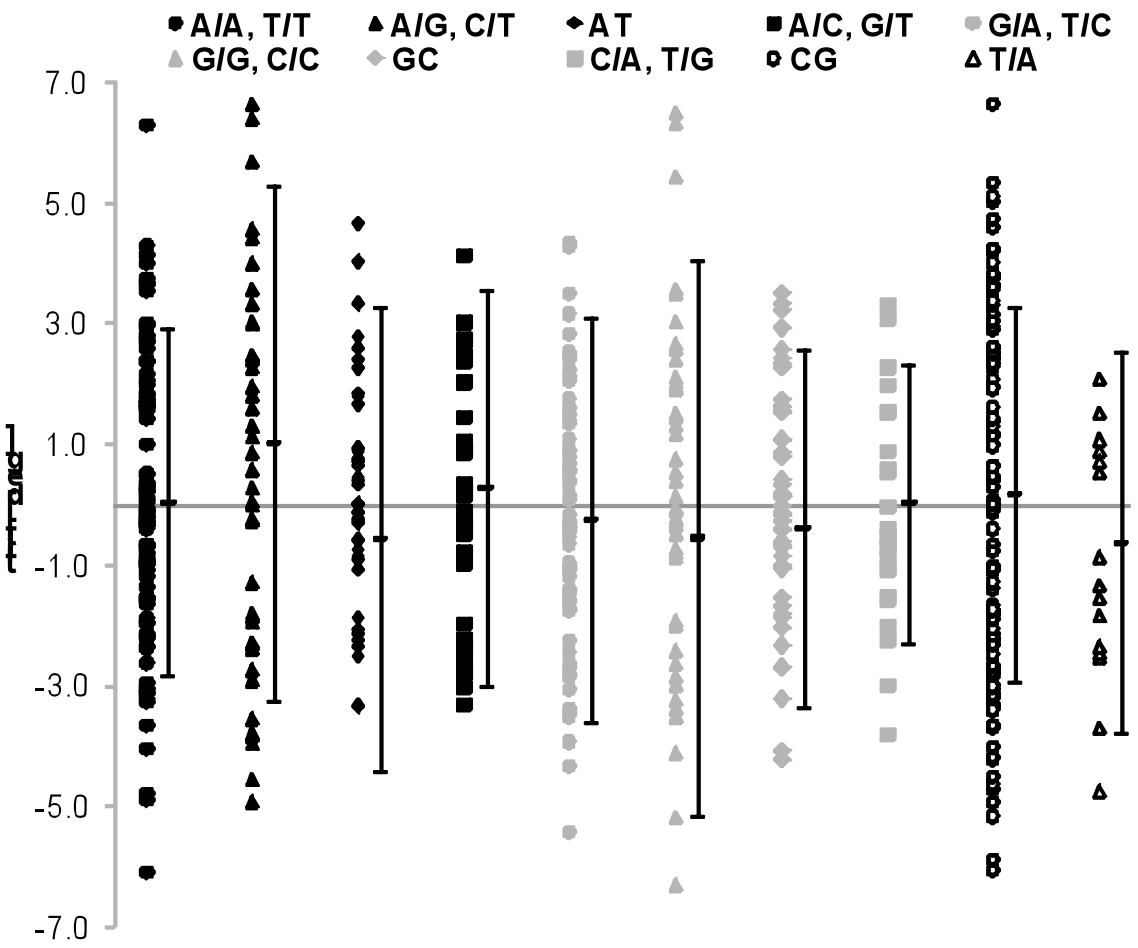

Fig. S7. The distributions of *titl* values characterizing all unique stacked pairs of nucleobases. For notation see Fig.S5

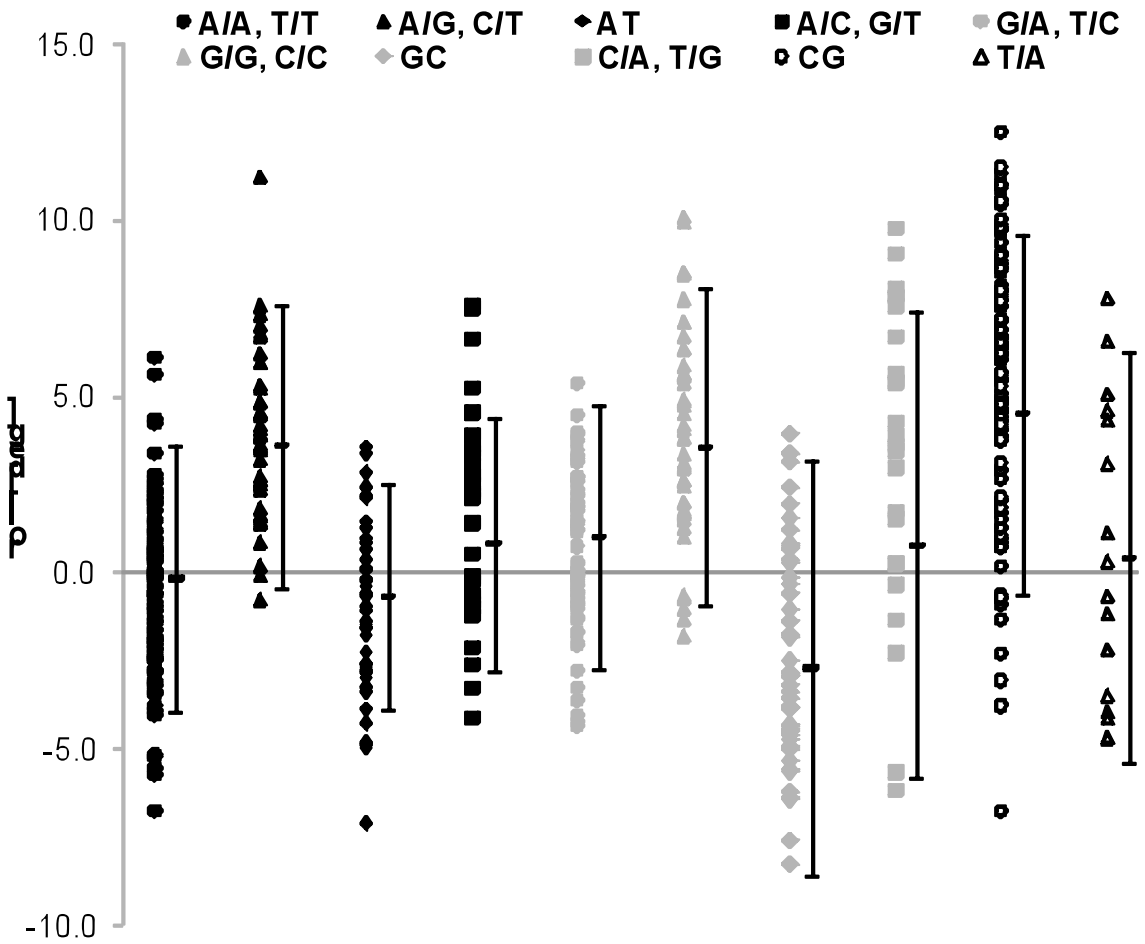

Fig. S8. The distributions of *roll* values characterizing all unique stacked pairs of nucleobases. For notation see Fig.S5

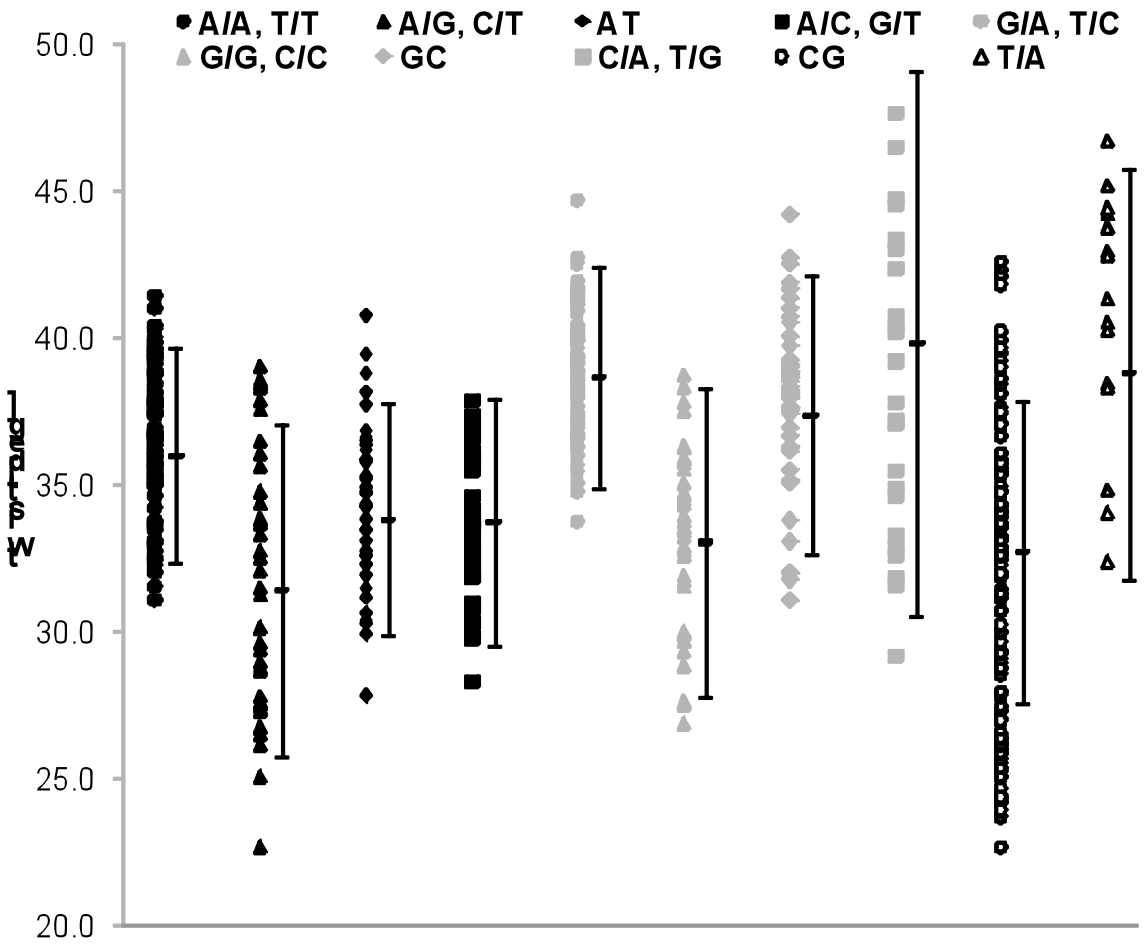

Fig. S9. The distributions of *twist* values characterizing all unique stacked pairs of nucleobases. For notation see Fig.S5

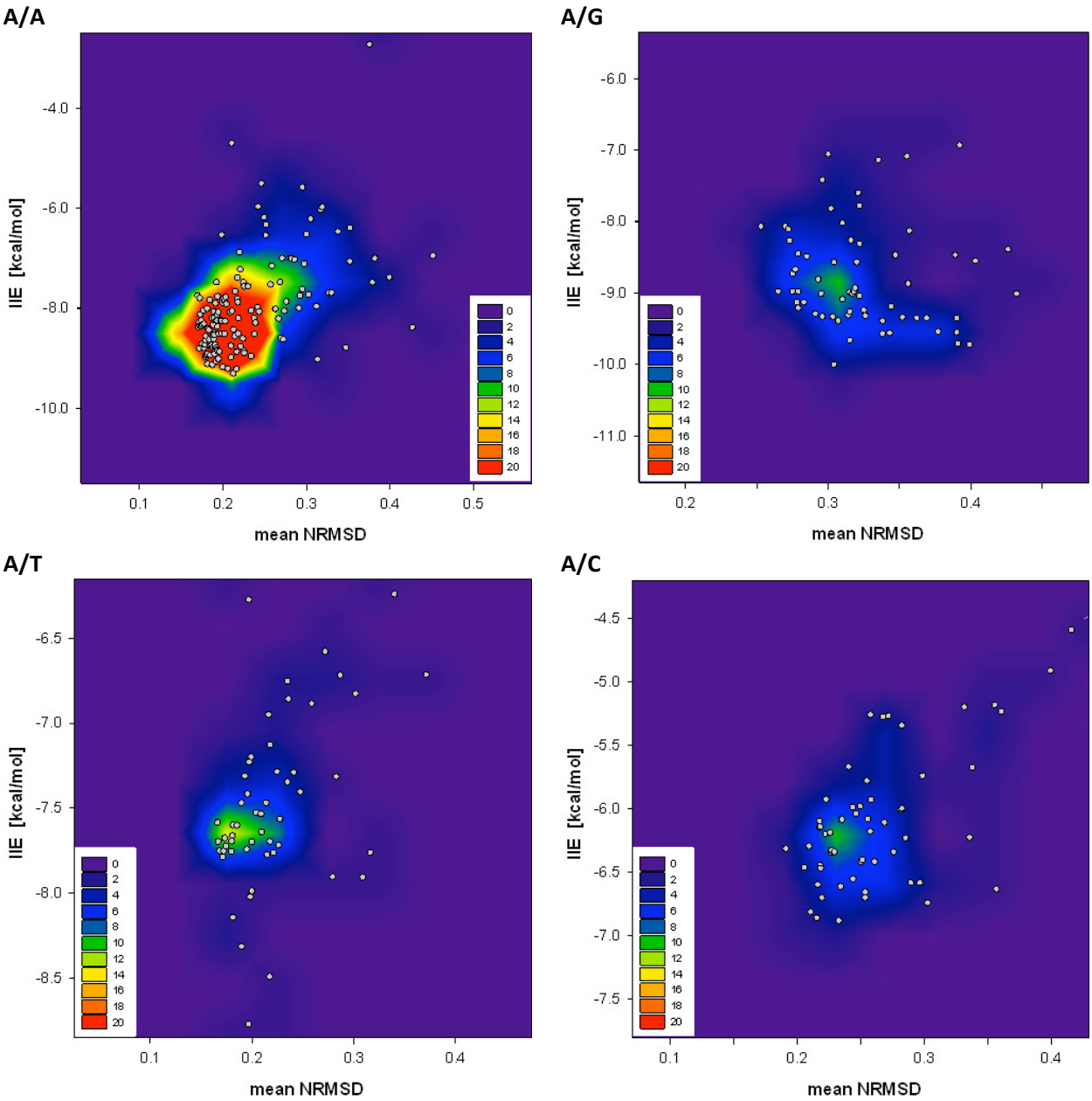

Fig. S10. The correlation between mean values of NRMSD and IIE of 5'-adenine stacked with four nucleobases. The mean NRMSD were estimated as average NMRSD values of given structure with respect of all stacked pairs of the same type. The color spectrum represent population percentages.

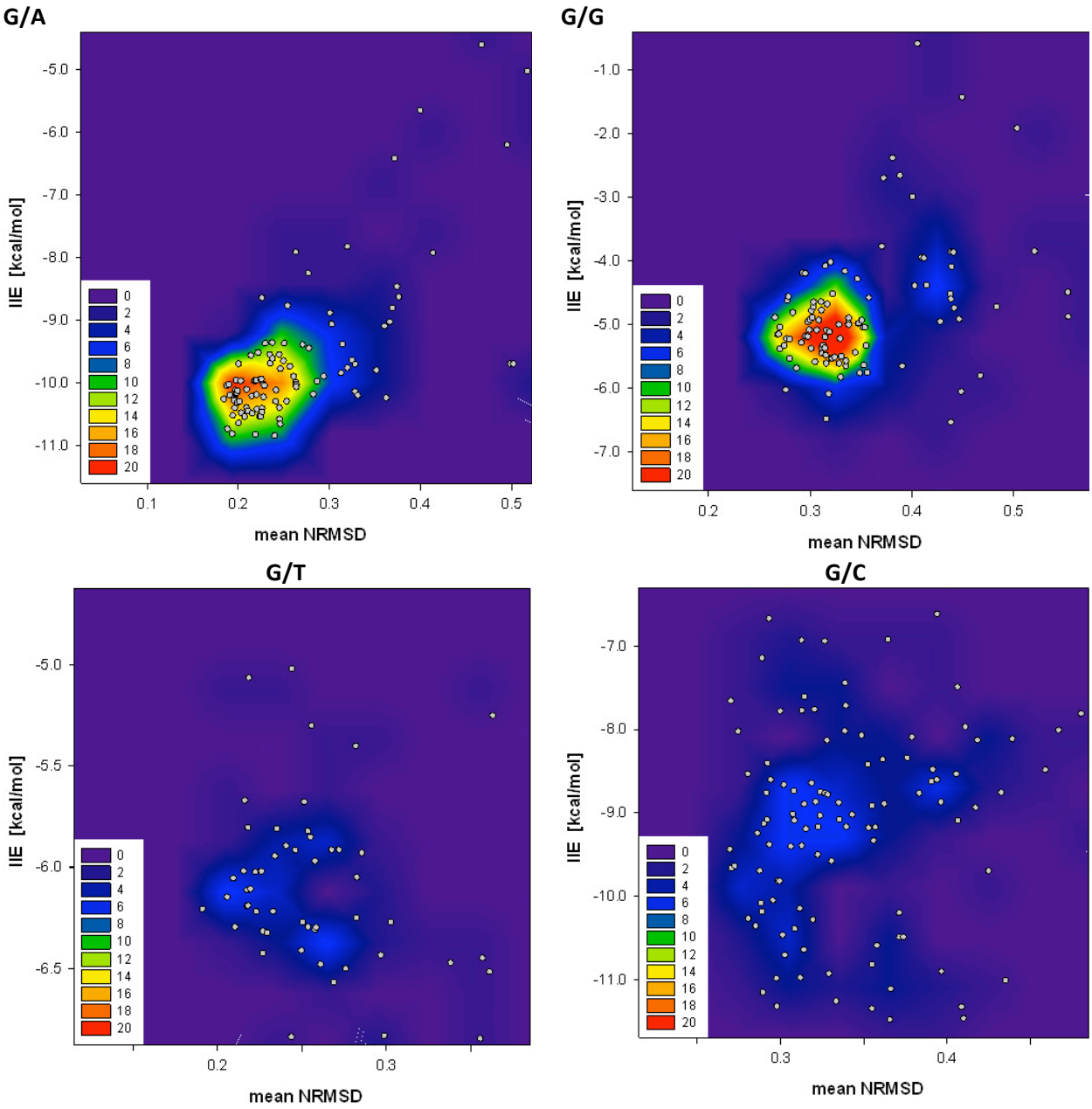

Fig. S11. The correlation between mean values of NRMSD and IIE of 5'-guanine stacked with four nucleobases. Notation is the same as in Fig.S10.

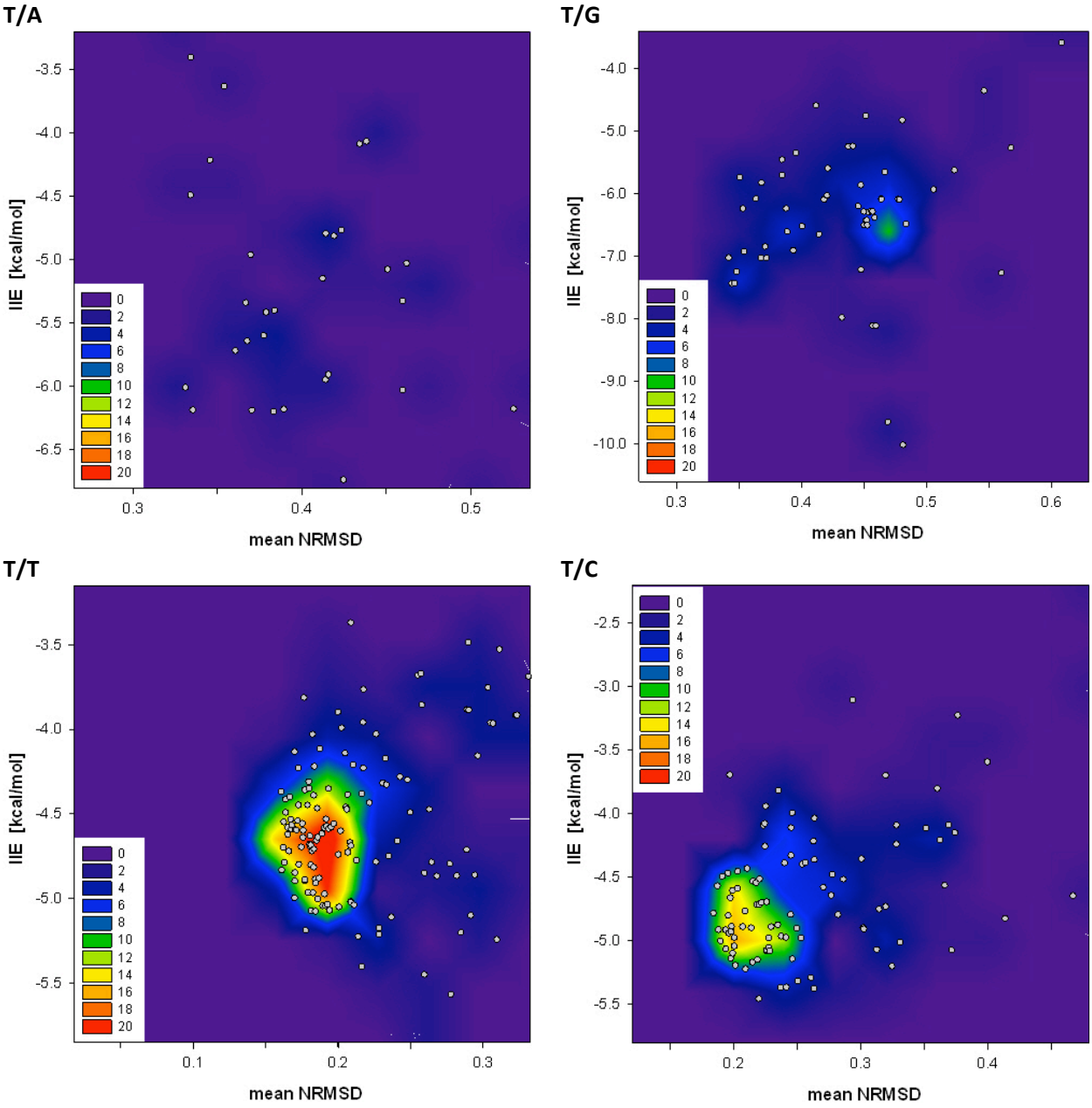

Fig. S12. The correlation between mean values of NRMSD and IIE of 5'-thymine stacked with four nucleobases. Notation is the same as in Fig.S10.

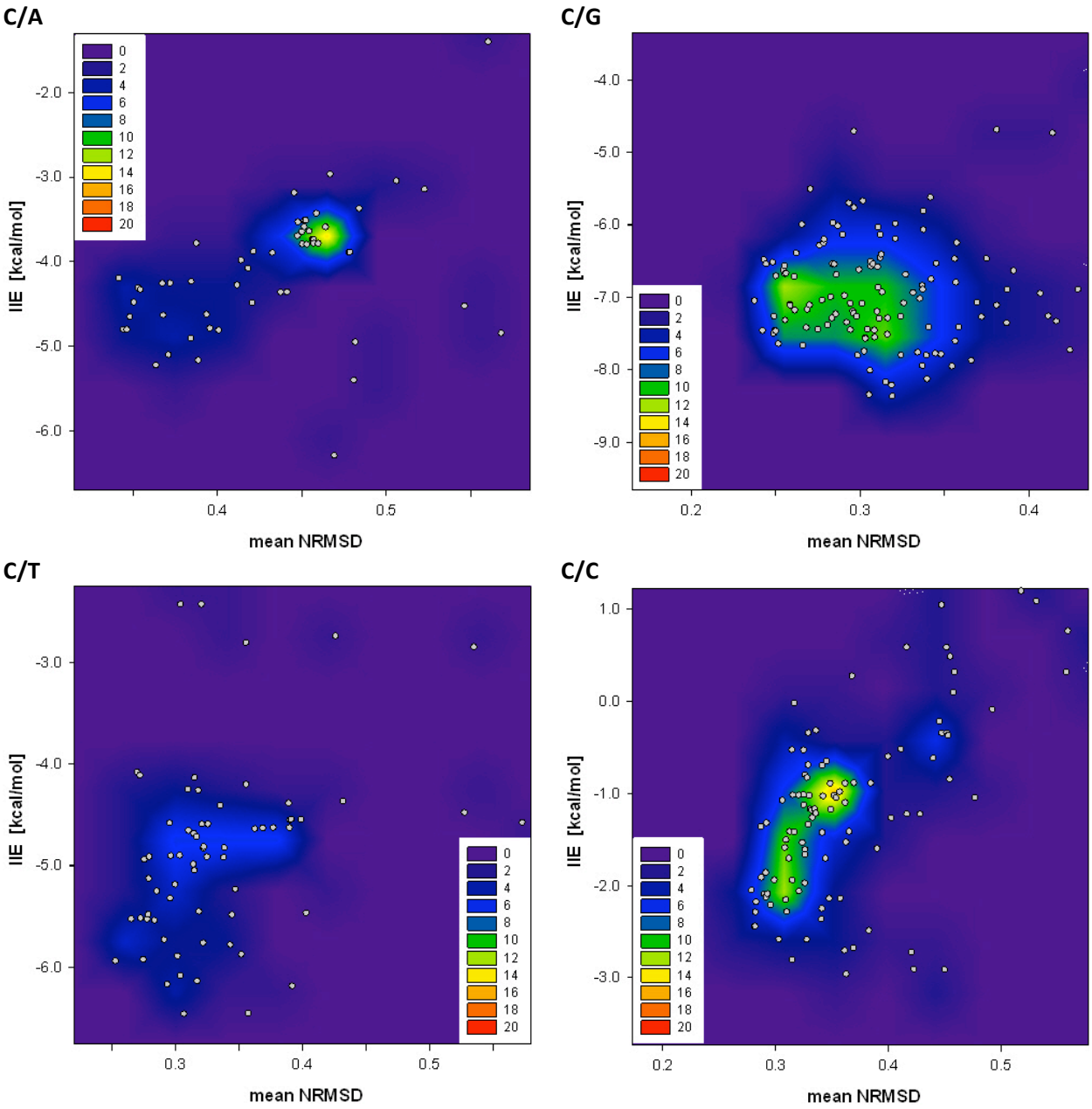

Fig. S13. The correlation between mean values of NRMSD and IIE of 5'-cytosine stacked with four nucleobases. Notation is the same as in Fig.S10.

Table S1. The experimental values of gas phase basicities (Gibbs free energy expressed in kcal/mol of protonation reaction in the gas phase) and pK_a (in water solution) of training set of heterocyclic compounds. Data taken from NIST chemistry web book (http://webbook.nist.gov/chemistry). The values of Gibbs free energy of proton solvation is assumed to be equal to -262.65 kcal/mol.

compound	**GPB**	**pK_a**
adenine	218.1	4.17
	328.0	9.75
guanine	222.0	3.30
cytosine	219.0	4.58
uracil	201.2	9.46
purine	212.3	2.52
pyridine	214.7	5.17
2-CH_3-pyridine	219.2	5.96
2-C_2H_5-pyridine	220.0	5.89
2-NH_2-pyridine	218.8	6.71
2-Cl-pyridine	208.0	0.49
3-CH3-pyridine	217.9	5.68
3-Cl-pyridine	208.3	2.84
3-Br-pyridine	209.9	2.85
3-NH_2-pyridine	220.5	6.03
4-CH_3-pyridine	218.8	6.00
2,3-diCH_3-pyridine	221.6	6.60
2,4-diCH_3-pyridine	222.5	6.72
3,5-diCH_3-pyridine	220.7	6.14
2,5-diCH_3-pyridine	221.5	6.47
2,6-diCH_3-pyridine	222.5	6.77
3,4-diCH_3-pyridine	221.2	6.52
4-Br-pyridine	211.8	3.71
imidazole	217.3	6.95
2-CH_3-imidazole	222.2	7.75
pyrazine	202.4	0.60
pyrimidine	204.5	1.30
pyridazine	209.6	2.33