

Table S2. The electron density (e/au^3), the values of H-bond energy (kJ mol^{-1}) evaluated using EML formula and the donor-acceptor interaction energies (kJ mol^{-1}) in the quaternary systems having guanine–thymine mismatch and adenine–thymine base pair. ^a

	ρ	$E_{\text{EML,HB}}$	$E_{\text{HB}}^{(2)}$
G [*] –T in	0.0364 (0.0386) <i>0.0195</i>	-43.84 (40.83) <i>-18.32</i>	87.78 (118.53) <i>30.25</i>
G [*] –T A–T			
A–T in	0.0212 (0.0418) <i>0.0054</i>	-20.55 (-46.61) <i>-4.20</i>	37.03 (121.21) <i>1.97</i>
G [*] –T A–T			
G [*] –T in	0.0346 (0.0367) <i>0.0218</i>	-40.54 (38.33) <i>-21.39</i>	83.26 (111.84) <i>36.23</i>
T–G [*] A–T			
A–T in	0.0284 (0.0320) <i>0.0025</i>	-31.16 (-31.95) <i>-1.84</i>	59.83 (87.19) <i>0.63</i>
T–G [*] A–T			
G–T [*] in	0.0700 (0.0394) <i>0.0198</i>	-101.68 (43.85) <i>-18.49</i>	257.94 (113.26) <i>33.97</i>
G–T [*] A–T			
A–T in	0.0218 (0.0415) <i>0.0051</i>	-21.44 (-46.06) <i>-3.95</i>	38.58 (126.23) <i>1.80</i>
G–T [*] A–T			
G–T [*] in	0.0562 (0.0390) <i>0.0240</i>	-76.82 (43.19) <i>-24.37</i>	189.37 (107.91) <i>44.98</i>
T [*] –G A–T			
A–T in	0.0277 (0.0318) <i>0.0026</i>	-30.25 (-31.61) <i>-1.84</i>	55.27 (84.68) <i>0.63</i>
T [*] –G A–T			

^a The normal data, data in the parentheses and italicized data correspond to HB1, HB2 and HB3, respectively.