Electronic Supplementary Information (ESI)

New palladium(II) and platinum(II) 5,5-diethylbarbiturate complexes with 2-phenylpyridine, 2,2'-bipyridine and 2,2'-dipyridylamine: synthesis, structures, DNA/protein binding, molecular docking, antioxidant activity and cytotoxicity

Ceyda Icsel, Veysel T. Yilmaz,* Hale Samli, Yunus Kaya, William T. A. Harrison, Orhan Buyukgungor

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Fig. S1 Stability of complexes **1**, **2** and **5** in MeOH and a saline solution (0.9% NaCl). Stability values are expressed as the percentage of the complexes remaining in the solution after 24 h.

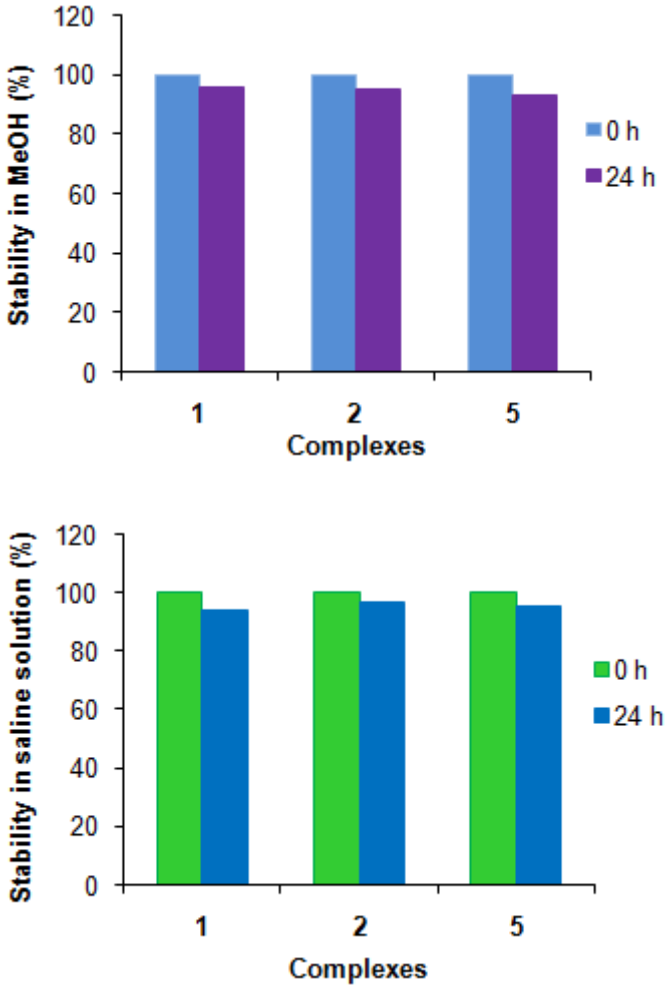


Fig. S2 Electronic absorption spectra of complexes **1**–**6** (25 μM each) upon the titration of FS-DNA (0–50 μM) in Tris-HCl buffer. The arrow shows the increases in absorbance with respect to an increase in the FS-DNA concentration. The inset shows the linear fit of [DNA]/($\varepsilon_a - \varepsilon_f$) vs. [DNA].

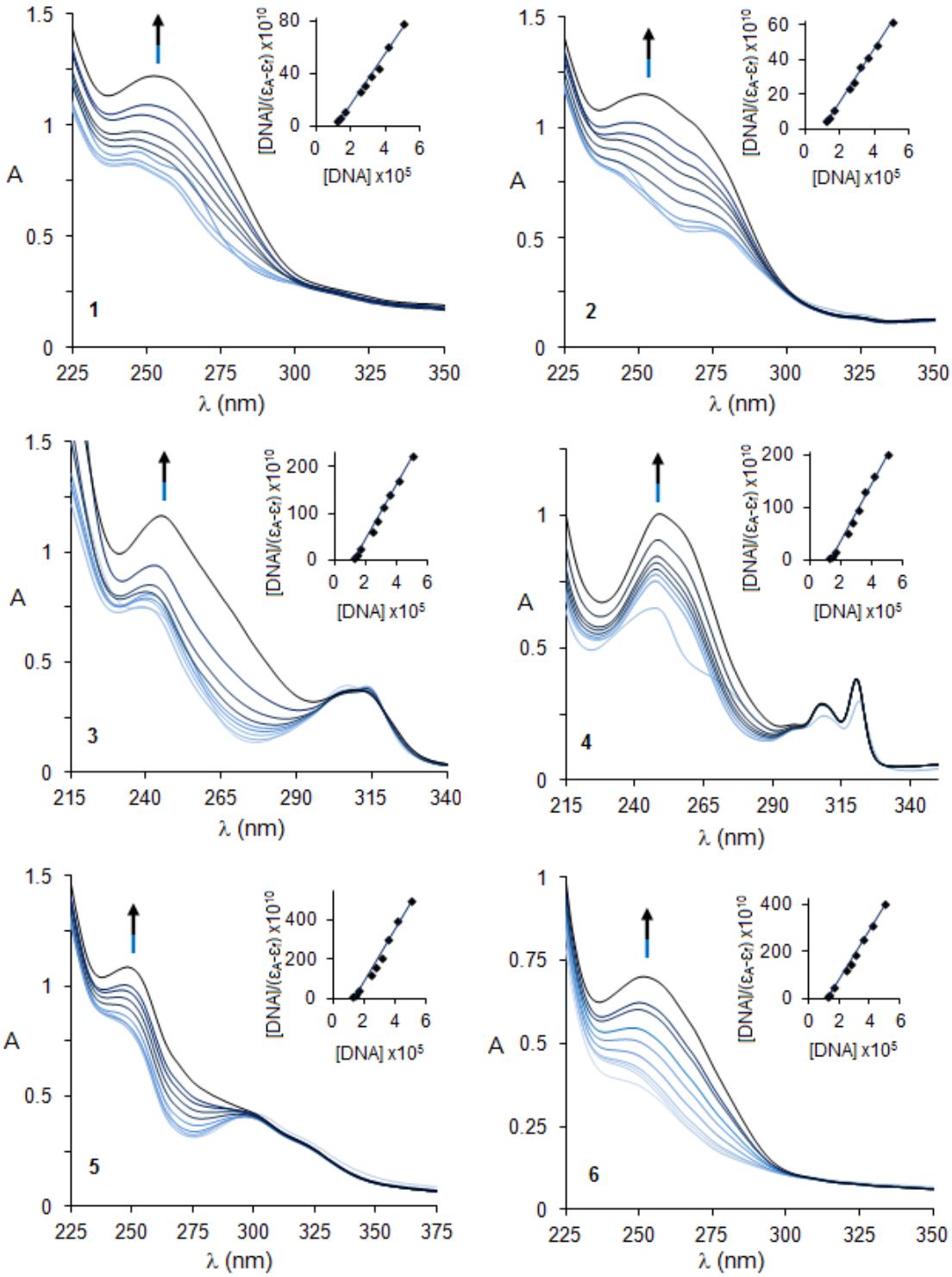


Fig. S3 Emission spectra of EB bound to DNA in the absence and presence of increasing concentrations of complexes **1**–**6** (12.5–100 μM) in Tris-HCl buffer. [EB] = 5.0 μM, [DNA] 50.0 μM. The arrows show the changes in intensity upon increasing amounts of the complexs. Insets: Stern-Volmer plot of the fluorescence data.

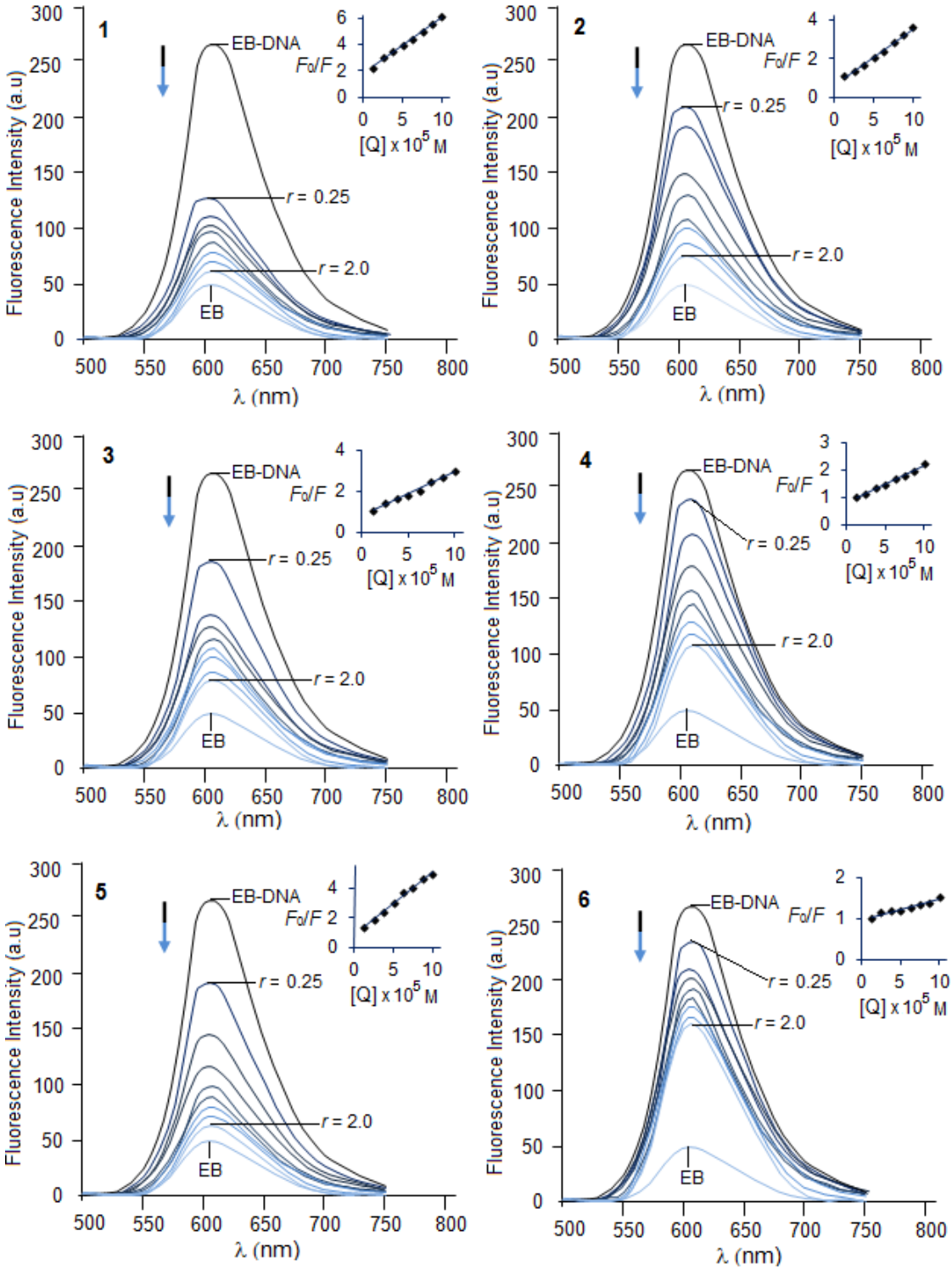
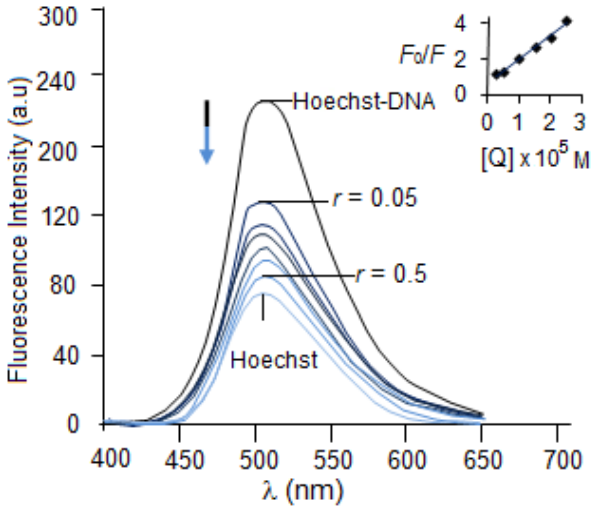
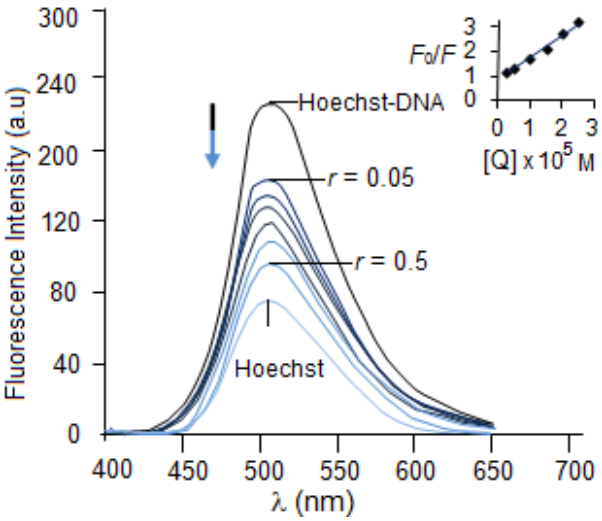


Fig. S4 Emission spectra of Hoechst 33258-bound DNA solutions in the absence and presence of increasing concentrations of complexes **1** and **3** (2.5–25 μM) in Tris-HCl buffer. [Hoechst 33258] = 5.0 μM, [DNA] 50.0 μM. The arrows show the changes in intensity upon increasing amounts of the complexes. Insets: Stern-Volmer plot of the fluorescence data.



(1)



(3)

Fig. S5 The relative viscosity of FS-DNA upon addition of increasing amounts of complexes **1**−**6** in Tris-HCl buffer. η is the viscosity of DNA in the presence of complex, and η_0 is the viscosity of DNA alone. r = 0.25−2.0.

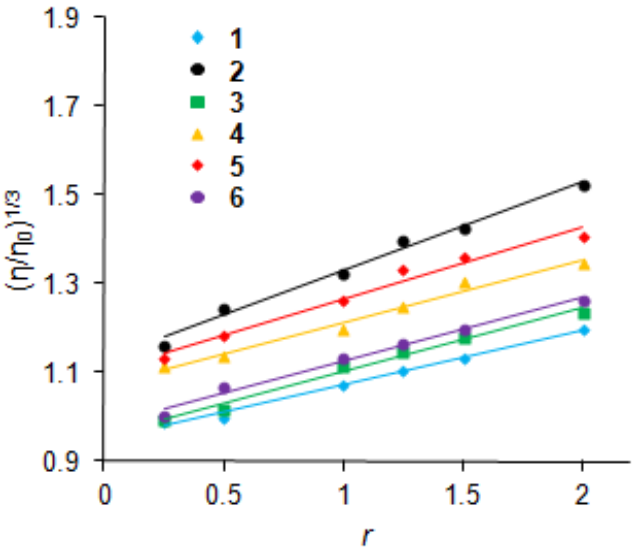


Fig. S6 Thermal denaturation profiles of FS-DNA in the absence and in the presence of complexes **1**−**6** in Tris-HCl buffer at r = 0.5.

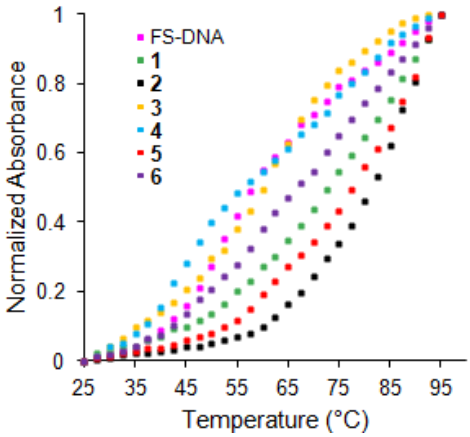


Fig. S7 Computational docking models (using the Autodock/Vina software) illustrating the interactions between DNA and complexes **1**–**6**.

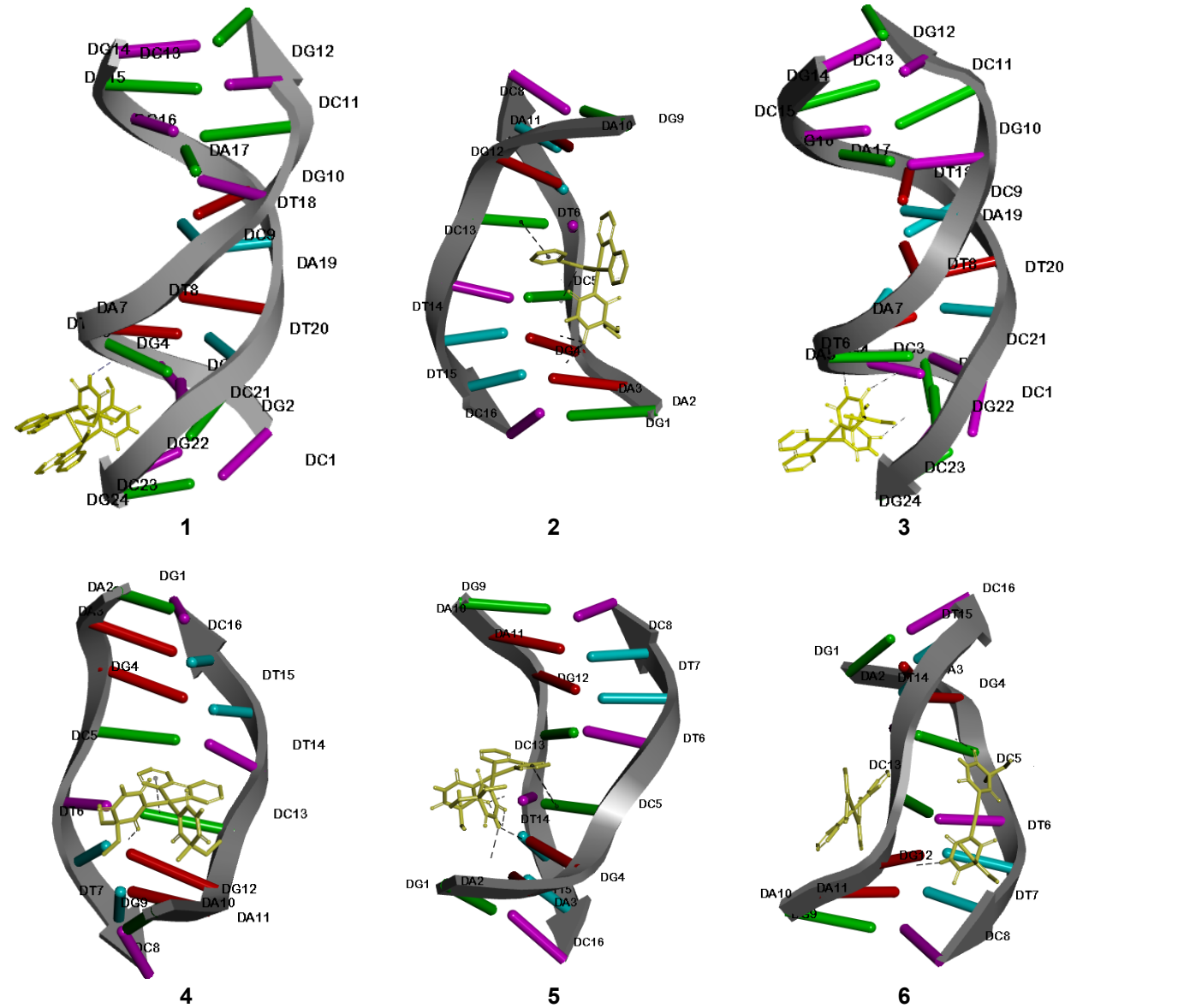


Table S1 Hydrogen bonding interactions and the binding free energy of the most stable docking conformations for complexes **1**−**6** docked into DNA

Complexes	Donor (D–H)	Acceptor (H···A)	H···A (Å)	ΔG (kJ mol^{-1})
1	N6–H6 (barb)	O (DG4)	2.28	−32.22
2	N–H (DA3)	O1 (barb)	2.31	−29.71
	N–H (DA2)	O1 (barb)	2.48	
3	N–H (DG2)	O6 (barb)	2.54	−29.71
	N–H (DG4)	O3 (barb)	2.10	
	N4–H4 (barb)	O (DG4)	2.37	
4	N–H (DA11)	O1 (barb)	2.08	−28.03
5	N–H (DA3)	O6 (barb)	2.28	−30.96
	N–H (DC13)	O1 (barb)	2.31	
	N–H (DA3)	O1 (barb)	2.54	
	N7–H7 (barb)	N7 (DA3)	2.59	
	N7–H7 (barb)	N7 (DA2)	2.79	
6	N–H (DC5)	O2 (barb)	2.18	−27.61
	N4–H4 (barb)	N (DA11)	2.89	