Effects of Extending the Computational Model on DNA–Protein T-shaped Interactions: The Case of Adenine–Histidine Dimers

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Supporting Information

Table SI-1. Strongest MP2/6-31G*(0.25) Interaction Energies (ΔE, kJ mol^{-1}) of (Neutral) Histidine (edge)–Adenine (face) Dimers as Determined by Varying R_1 (Å), α (°), and R_2 ((X-displacement, Y-displacement), Å)[a]

Model	θ	R_1	ΔE	α	ΔE	R_2	ΔE
Protein Backbone[b]							
HIS_δ'	2	4.7	–11.8	300	–14.5	—	
	3	4.3	–7.7	240	–10.7	—	
	B	4.4	–21.4	240	–26.6	(0, –0.5)	–27.6
	C	4.3	–12.8	300	–17.1	—	
	D	4.4	–12.8	120	–14.7	—	
HIS_ε'	1	4.5	–18.7	60	–21.0	—	
	2	4.7	–13.5	330	–14.5	—	
	A	4.5	–17.9	60	–25.3	(0, –0.5)	–26.2
	B	4.4	–19.8	240	–23.9	(0, –0.5)	–24.5
	C	4.3	–20.1	300	–25.2	(1, 1)	–27.6

[a] See Figure 1 for structures of histidine and adenine, Figure 4 for definitions of R_1, α, and R_2, and Figure 5 for definitions of edges (θ) considered in the present study. [b] Dimers between truncated adenine (A) and extended histidine (see Computational Details for definition of HIS_δ' and HIS_ε').

Table SI-2. Strongest MP2/6-31G*(0.25) Interaction Energies (ΔE, kJ mol^{-1}) of (Cationic) Protonated Histidine (edge)–Adenine (face) Dimers as Determined by Varying R_1 (Å), α (°), and R_2 ((X-displacement, Y-displacement), Å)[a]

Model	θ	R_1	ΔE	α	ΔE	R_2	ΔE
Protein Backbone[b]							
$HIS_{\delta\varepsilon}^{+\prime}$	1	4.3	–44.0	240	–47.7	(2, 1.5)	–57.8
	2	4.5	–32.2	240	–37.6	—	
	A	4.2	–44.8	300	–51.9	(2,0)	–53.4
	B	4.2	–43.9	240	–54.9	(0, –0.5)	–55.6
	B′	4.2	–43.3	240	–55.0	(0, 0)	–55.0

[a] See Figure 1 for structures of protonated histidine and adenine, Figure 4 for definitions of R_1, α, and R_2, and Figure 5 for definitions of edges (θ) considered in the present study. [b] Dimers between truncated adenine (A) and extended (protonated) histidine (see Computational Details for definition of $HIS_{\delta\varepsilon}^{+\prime}$).

Table SI-3. Strongest MP2/6-31G*(0.25) Interaction Energies (ΔE, kJ mol^{-1}) of (Neutral) Adenine (edge)–Histidine (face) Dimers as Determined by Varying R_1 (Å), α (°), and R_2 ((X-displacement, Y-displacement), Å)[a]

Model	θ	R_1	ΔE	α	ΔE	R_2	ΔE
Protein Backbone[b]							
HIS_δ'	1	3.2	–11.1	330	–14.0	—	
	2	2.5	–8.7	90	–9.5	—	
	3	3.2	–6.8	150	–13.5	—	
	4	2.3	–16.1	120	–29.8	(0.5, 1)	–34.0
	5	2.5	–9.5	150	–17.5	—	
	6	3.2	–9.5	150	–10.6	—	
	7	3.5	–13.3	330	–15.9	—	
	8	2.4	–20.7	300	–25.2	(0, 0)	–25.2
	A	3.8	–5.9	150	–9.7	—	
	B	3.6	–9.1	330	–10.4	—	
	C	3.4	–1.9	150	–18.6	—	
	D	2.6	–17.0	150	–21.8	(0.5, 0.5)	–24.3
	E	3.7	–5.4	150	–15.7	—	
	F	3.4	–10.0	330	–11.7	—	
	G	2.7	–14.5	330	–14.8	(0.5, 0.5)	–17.0
	H	3.5	–9.7	330	–12.8	—	
HIS_ε'	1	3.2	–10.5	330	–13.5	—	
	2	2.5	–9.0	90	–11.1	—	
	3	3.2	–5.6	150	–13.0	—	
	4	2.3	–17.2	120	–28.3	(0.5, 1)	–32.3
	5	2.4	–9.7	120	–16.4	—	
	6	3.2	–8.6	150	–10.0	—	
	7	3.2	–8.7	300	–13.7	—	
	8	2.4	–17.5	300	–22.5	(0.5, 1)	–22.8
	A	3.8	–6.5	150	–8.8	—	
	B	3.7	–8.2	330	–9.0	—	
	C	3.3	–3.7	120	–16.3	—	
	D	2.6	–17.4	150	–20.7	(0.5, 0.5)	–23.3
	E	3.7	–5.9	120	–13.6.	—	
	F	3.3	–7.3	330	–8.4	—	
	G	2.7	–14.7	330	–14.9	(0.5, 0.5)	–16.9
	H	3.3	–9.2	330	–11.7	—	
Deoxyribose[c]							
HIS′	1	3.2	–8.4	330	–8.9	—	
	2	2.6	–5.9	210	–7.5	—	
	6	3.3	–2.4	150	–10.5	—	
	7	3.3	–6.0	270	–13.0	—	
	8	2.4	–19.0	330	–21.2	(0, 0)	–21.2
	A	3.8	–3.5	150	–6.6	—	
	F	3.4	–2.6	300	–5.4	—	
	G	2.8	–8.9	180	–15.0	(0, 0.5)	–15.9
	H	3.4	–7.0	330	–8.7	—	

[a] See Figure 1 for structures of histidine and adenine, Figure 4 for definitions of R_1, α, and R_2, and Figure 5 for definitions of edges (θ) considered in the present study. [b] Dimers between truncated adenine (A) and extended histidine (see Computational Details for definition of HIS_δ' and HIS_ε'). [c] Dimers between truncated histidine (HIS) and extended adenine (A_{dR}).

Table SI-4. Strongest MP2/6-31G*(0.25) Interaction Energies (ΔE, kJ mol^{-1}) of (Cationic) Adenine (edge)–Protonated Histidine (face) Dimers as Determined by Varying R_1 (Å), α (°), and R_2 ((X-displacement, Y-displacement), Å)[a]

Model	θ	R_1	ΔE	α	ΔE	R_2	ΔE
Protein Backbone[b]							
$HIS_{\delta\varepsilon}^{+\prime}$	1	3.1	–33.5	240	–40.3	(–0.5, 0)	–41.1
	2	2.4	–29.9	150	–30.4	—	
	3	3.0	–34.5	60	–39.4	(0, 0)	–39.4
	4	2.4	–1.2	60	–2.6	—	
	5	2.6	3.3	60	1.6	—	
	6	3.1	–20.4	60	–24.4	—	
	7	3.6	–14.9	240	–17.8	—	
	8	2.5	–18.7	240	–22.6	—	
	A	3.5	–32.7	30	–32.8	(–0.5, 1)	–34.7
	B	3.5	–30.9	180	–32.2	(0, 1)	–34.4
	C	3.0	–30.0	60	–35.2	(1, –0.5)	–39.9
	D	2.9	11.0	30	9.9	—	
	E	3.5	–14.2	60	–16.7	—	
	F	3.4	–14.8	240	–20.4	—	
	G	2.9	–2.4	240	–3.4	—	
	H	3.4	–26.0	240	–34.6	(0.5, –0.5)	–36.4

[a] See Figure 1 for structures of protonated histidine and adenine, Figure 4 for definitions of R_1, α, and R_2, and Figure 5 for definitions of edges (θ) considered in the present study. [b] Dimers between truncated adenine (A) and extended (protonated) histidine (see Computational Details for definition of $HIS_{\delta\varepsilon}^{+\prime}$).