Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supporting information for: Role of N7 protonation of guanine in determining structure, stability and function of RNA base pairs

Antarip Halder[1], Sohini Bhattacharya[1], Ayan Datta[2], Dhananjay Bhattacharyya[3], and Abhijit Mitra[1,*]

[1]Center for Computational Natural Sciences and Bioinformatics (CCNSB), International Institute of Information Technology (IIIT-H), Gachibowli, Hyderabad 500032, India
[2]Department of Spectroscopy, Indian Association for the Cultivation of Science, 2A&2B Raja S. C. Mullick Road, Jadavpur, Kolkata-700032, India
[3]Computational Science Division, Saha Institute of Nuclear Physics(SINP), 1/AF, Bidhannagar, Kolkata 700064, India

Short Title: Role of N7 protonation of guanine

Key Words: Structural bioinformatics, N7 protonated guanine, Class II protonated nucleobases, DFT, pH dependence of base pair geometry, Levitt base pair, molecular switch

S1 Computational details

S1.1 RMSD calculation

We have saved all the crystal and optimized geometries in .mol2 format and used the following .tcl script to calculate the RMSD between the crystal geometry (`s01_crystal.mol2` in the following example) and different optimized geometries using VMD package. It is to be noted that we have considered only the heavy atoms for the purpose.

```
set inp [lindex $argv 0]
set trj .
set trj1 .
mol load mol2 $trj1/s01_crystal.mol2
mol new $trj/s01_${inp}.mol2
set out [open ${inp}.rms w]
set sel1 [atomselect 0 "not hydrogen"]
set sel2 [atomselect 1 "not hydrogen"]
set tmat [measure fit $sel1 $sel2]
$sel2 move $tmat
set rmsd [measure rmsd $sel1 $sel2]
puts $out "final rmsd:  $rmsd"
close $out
```

S1.2 Interaction energy calculation

The gas phase intrinsic interaction energy of a base pairing interaction AB, involving two bases A and B is calculated via the following protocol.

- The base pair AB is optimized to its ground state, in gas phase, at M05-2X/6-311G+(2d,2p) level of theory.
- Single point energy of the optimized geometry of the base pair AB and the individual bases A and B are calculated at MP2/aug-cc-pVDZ level of theory. In each case, the MP2 level single point energy has two components – the HF term (E^{HF}) and the correlation term (E^{Corr}).
- We calculate the HF component and Correlation component of the MP2 level interaction energy (ΔE^{MP2}_{gas}) as,

$$\begin{aligned} \Delta E^{HF}_{gas} &= E^{HF}_{gas}(AB) - E^{HF}_{gas}(A) - E^{HF}_{gas}(B) \\ \Delta E^{Corr}_{gas} &= E^{Corr}_{gas}(AB) - E^{Corr}_{gas}(A) - E^{Corr}_{gas}(B) \\ \Delta E^{MP2}_{gas} &= \Delta E^{HF}_{gas} + \Delta E^{Corr}_{gas} \end{aligned} \tag{1}$$

- This MP2 level interaction energy (ΔE^{MP2}_{gas}) is further corrected for Basis Set Superposition Error (BSSE) and we obtain the final gas phase interaction energy as,

$$\Delta E^{gas}_{int} = \Delta E^{MP2}_{gas} + E^{BSSE} \tag{2}$$

where, E^{BSSE} is the BSSE correction term at MP2/aug-cc-pVDZ level.

- To account for the effect of polar solvent environment on the gas phase interaction energy of the base pairs, we have calculated the single point energy of the gas phase optimized geometry of the based pairs and individual bases with dielectric constant of pure water 78.4 in CPCM model, at the same MP2/aug-cc-pVDZ level. Similarly we obtain the HF and correlation component and BSSE corrected interaction energy with solvent effects as,

$$\begin{aligned} \Delta E_{sol}^{HF} &= E_{sol}^{HF}(AB) - E_{sol}^{HF}(A) - E_{sol}^{HF}(B) \\ \Delta E_{sol}^{Corr} &= E_{sol}^{Corr}(AB) - E_{sol}^{Corr}(A) - E_{sol}^{Corr}(B) \\ \Delta E_{sol}^{MP2} &= \Delta E_{sol}^{HF} + \Delta E_{sol}^{Corr} \\ \Delta E_{int}^{sol} &= \Delta E_{sol}^{MP2} + E^{BSSE} \end{aligned} \tag{3}$$

It is to be noted that E^{BSSE} is the same as that for ΔE_{int}^{gas} calculation.

- We also have calculated the solvent phase optimized geometry of the base pairs at M05-2X/6-311G+(2d,2p) level of theory by including the solvent effect (ε=78.4) within the optimization subroutine. Interaction energy of the solvent phase optimized geometry has also been calculated at MP2/aug-cc-pVDZ level with BSSE correction. In this case the BSSE correction energy has been calculated at gas phase using the solvent phase optimized geometry. Therefore we have,

$$\Delta E_{int}(Sol) = (E_{AB}^{MP2}(Sol) - E_{A}^{MP2}(Sol) - E_{B}^{MP2}(Sol)) + E_{gas}^{BSSE} \tag{4}$$

S2 Natural Bond Orbital analysis

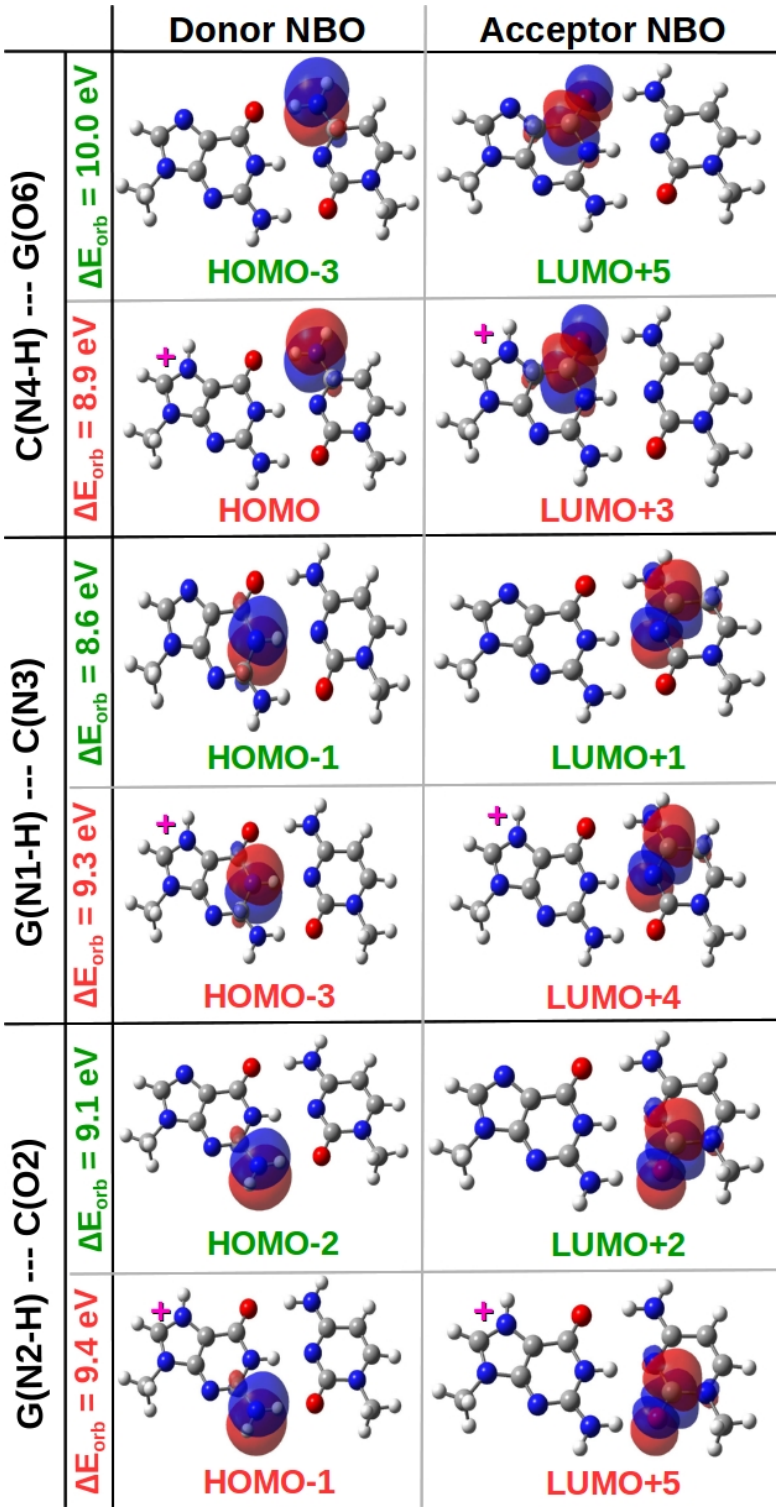

Figure S1 Distribution of donor and acceptor NBOs and their energies (in eV) corresponding to the three noncanonical interactions detected in canonical G:C base pair in its neutral and N7 protonated state. Energy difference (ΔE_{orb}) between the donor and acceptor NBO are also reported.

S3 Context analysis of Gr:C W:W Cis

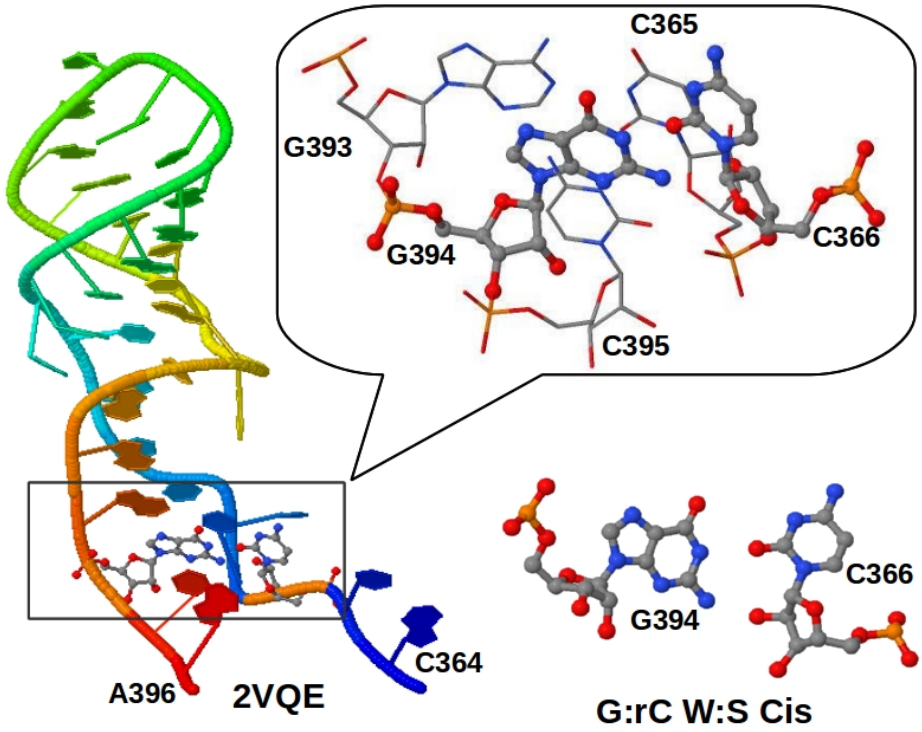

Figure S2 Context of occurrence of G:rC W:W Cis base pair.

S4 Optimized geometry

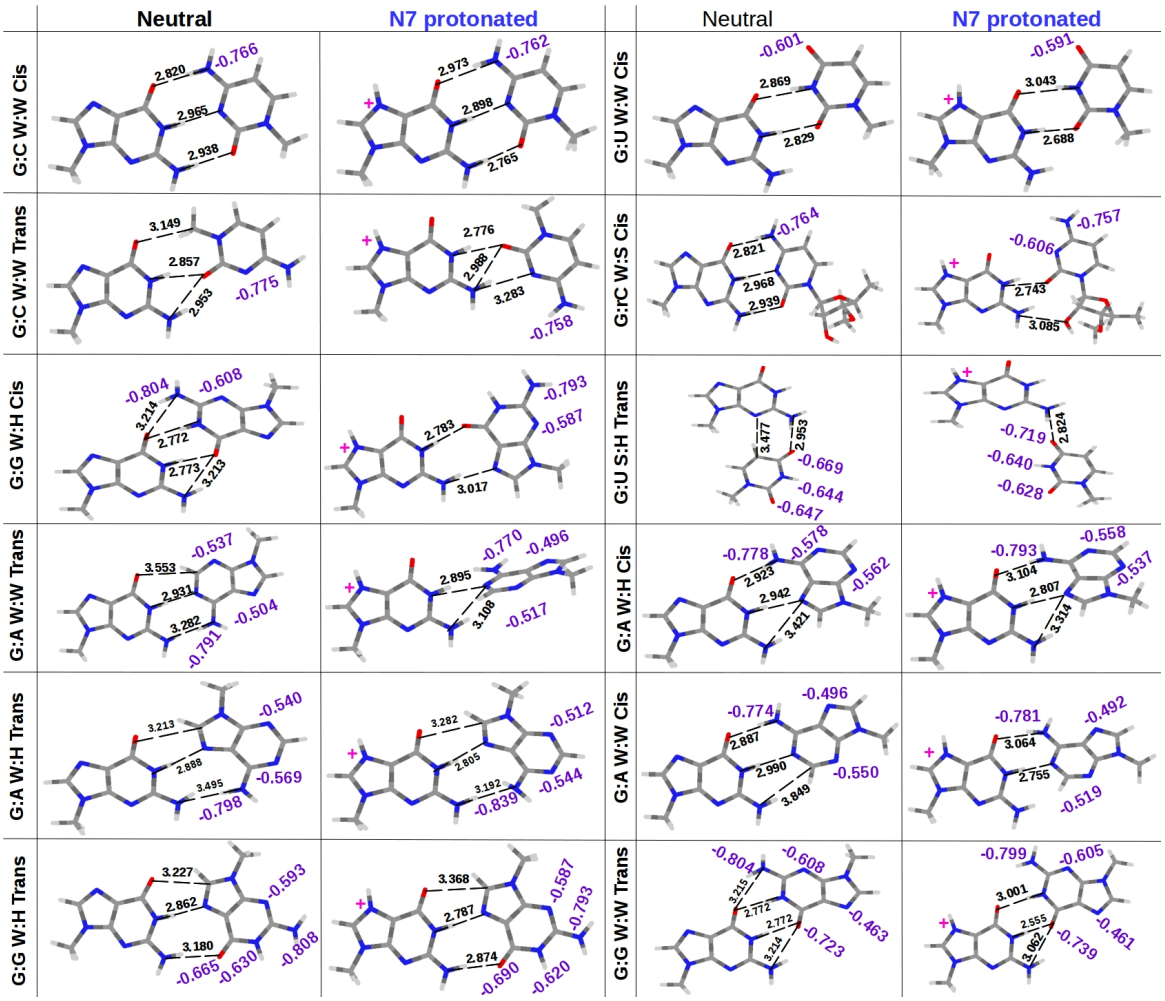

Figure S3 M05-2X/6-311G+(2d,2p) level gas phase optimized geometries of the studied base pairs involving WatsonCrick edge of guanine. Distance between heavy atoms are given in $\AA$ unit. NBO charges of the free polar sites of the second base are given in atomic unit.

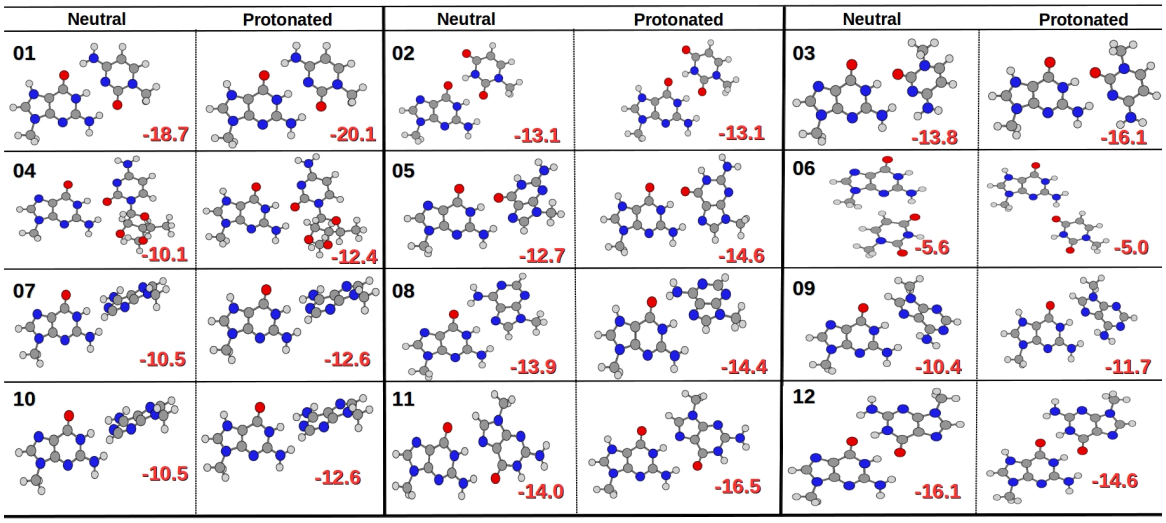

Figure S4 Solvent phase optimized geometry (at M05-2X/6-311G+(2d,2p) level) and their interaction energy in kcal/mol unit (at MP2/aug-CC-pVDZ level) . Base pairs involving sugar edge of guanine is shown in tube model.

S5 Interaction energy

Table S1 Different components of the interaction energy in gas phase and solvent phase at MP2/aug-ccpVDZ level of theory.

		Gas phase energies							Solvent phase energies						
System		ΔE_{HF}	ΔE_{corr}	ΔE_{MP2}	%HF	%corr	E^{BSSE}	ΔE_{total}	ΔE_{HF}	ΔE_{corr}	ΔE_{MP2}	%HF	%corr	E^{BSSE}	ΔE_{total}
1	Neutral	-25.6	-7.2	-32.8	78.0	22.0	4.5	-28.3	-9.3	-10.0	-19.4	48.2	51.8	4.5	-14.9
G:C W:W Cis	Protonated	-35.6	-8.0	-43.6	81.7	18.3	4.6	-38.9	-10.8	-10.5	-21.4	50.7	49.3	4.6	-16.7
2	Neutral	-13.7	-6.0	-19.7	69.4	30.6	3.5	-16.1	-6.4	-7.3	-13.7	46.7	53.3	3.5	-10.2
G:U W:W Cis	Protonated	-19.8	-6.5	-26.3	75.3	24.7	3.8	-22.5	-6.6	-7.8	-14.4	45.8	54.2	3.8	-10.6
3	Neutral	-15.9	-5.2	-21.1	75.2	24.8	3.3	-17.8	-4.4	-7.5	-11.9	36.6	63.4	3.3	-8.6
G:C W:W Trans	Protonated	-29.4	-5.2	-34.6	85.1	14.9	3.2	-31.4	-7.3	-7.0	-14.2	51.0	49.0	3.2	-11.1
4	Neutral	-25.6	-7.5	-33.1	77.4	22.6	4.6	-28.5	-9.2	-10.2	-19.4	47.2	52.8	4.6	-14.8
G:rC W:S Cis	Protonated	-33.9	-6.7	-40.6	83.4	16.6	4.0	-36.6	-8.3	-8.5	-16.8	49.1	50.9	4.0	-12.8
5	Neutral	-26.8	-6.3	-33.1	81.1	18.9	4.4	-28.7	-7.5	-9.7	-17.2	43.6	56.4	4.4	-12.8
G:G H:W Cis	Protonated	-29.5	-6.5	-36.0	81.9	18.1	3.6	-32.5	-7.3	-7.8	-15.1	48.5	51.5	3.6	-11.5
6	Neutral	-6.0	-5.9	-11.9	50.7	49.3	3.1	-8.8	-1.8	-6.7	-8.5	20.9	79.1	3.1	-5.3
G:U S:H Trans	Protonated	-13.3	-2.5	-15.8	84.3	15.7	1.7	-14.1	-2.7	-3.3	-6.0	44.8	55.2	1.7	-4.3
7	Neutral	-7.7	-7.7	-15.4	49.9	50.1	3.5	-11.9	-2.5	-8.6	-11.1	22.6	77.4	3.5	-7.6
G:A W:W Trans	Protonated	-15.7	-8.5	-24.3	64.8	35.2	3.6	-20.7	-4.3	-8.5	-12.8	33.9	66.1	3.6	-9.3
8	Neutral	-12.7	-8.6	-21.3	59.5	40.5	4.0	-17.2	-5.3	-9.5	-14.8	36.0	64.0	4.0	-10.7
G:A W:H Cis	Protonated	-16.5	-10.0	-26.6	62.2	37.8	4.4	-22.2	-5.5	-10.5	-16.0	34.2	65.8	4.4	-11.6
9	Neutral	-10.5	-7.7	-18.1	57.8	42.2	3.8	-14.3	-2.6	-8.8	-11.4	22.7	77.3	3.8	-7.6
G:A W:H Trans	Protonated	-18.0	-9.7	-27.7	65.0	35.0	4.3	-23.5	-4.1	-10.4	-14.5	28.1	71.9	4.3	-10.2
10	Neutral	-12.3	-8.5	-20.8	59.2	40.8	3.8	-16.9	-4.1	-9.3	-13.4	30.4	69.6	3.8	-9.5
G:A W:W Cis	Protonated	-18.2	-10.4	-28.6	63.6	36.4	4.3	-24.3	-4.7	-10.8	-15.6	30.5	69.5	4.3	-11.2
11	Neutral	-17.1	-6.6	-23.7	72.0	28.0	3.8	-19.8	-5.4	-8.8	-14.2	37.7	62.3	3.8	-10.4
G:G H:W Trans	Protonated	-32.3	-8.2	-40.5	79.7	20.3	4.3	-36.2	-7.7	-10.1	-17.9	43.3	56.7	4.3	-13.6
12	Neutral	-26.8	-6.2	-33.1	81.1	18.9	4.4	-28.7	-7.5	-9.7	-17.2	43.6	56.4	4.4	-12.8
G:G W:W Trans	Protonated	-31.9	-6.3	-38.2	83.4	16.6	4.4	-33.7	-8.0	-9.4	-17.3	46.1	53.9	4.4	-12.9
13	Neutral	-7.7	-8.3	-16.0	47.9	52.1	3.6	-12.4	-3.2	-8.7	-11.9	27.2	72.8	3.6	-8.3
rG:A S:W Trans	Protonated	-11.0	-8.9	-19.9	55.5	44.5	3.6	-16.3	-3.3	-8.8	-12.2	27.4	72.6	3.6	-8.5
14	Neutral	-7.0	-8.8	-15.8	44.4	55.6	3.8	-12.0	-3.2	-9.2	-12.4	26.1	73.9	3.8	-8.6
rG:A S:H Trans	Protonated	-8.7	-13.4	-22.1	39.3	60.7	5.1	-17.0	1.1	-13.8	-12.7	-8.3	108.3	3.8	-9.0

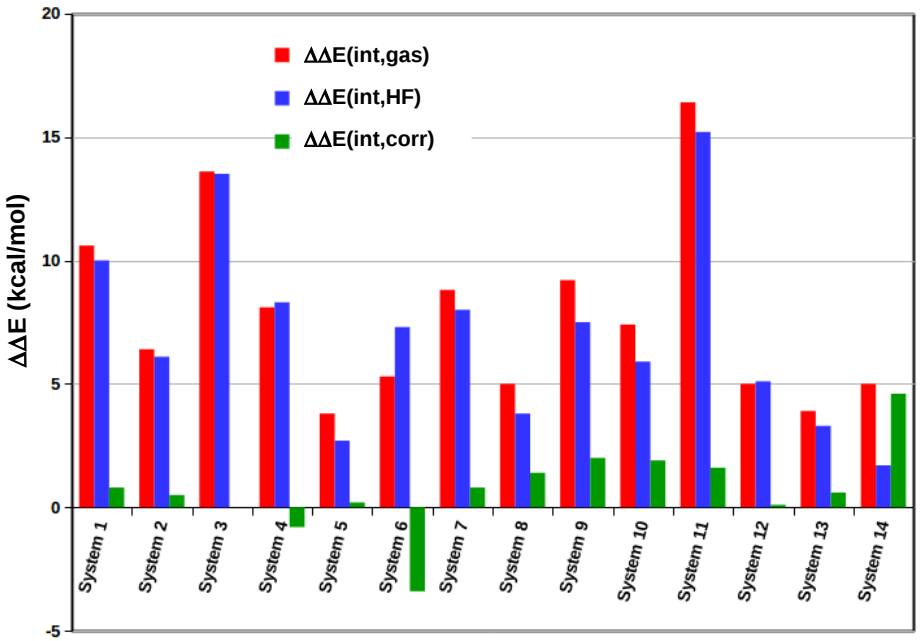

Figure S5 Difference between the BSSE corrected gas phase interaction energy (ΔΔE(int,gas)), its HF component (ΔΔE(int,HF)) and correlation component (ΔΔE(int,corr)) of base pairs optimized as (i)neutral and (ii)guanine N7 protonated species. Therefore, $\Delta\Delta E(\mathrm{int,X}) = \Delta\mathrm{E(int,X)}$ of neutral species $- \Delta\mathrm{E(int,X)}$ of protonated species.

S6 Inter Base Pair parameters from NUPARM

Table S2 Base pair orientation parameters calculated by NUPARM (Mukherjee, Bansal, Bhattacharyya (2006) *J. Comp. Aided Mol. Des.*), RMSD values and C1′-C1′ distance (in Å) for the crystal geometry and gas and solvent phase optimized ground state geometries (with and without proton at N7 of guanine) of the base pairing systems are reported.

				Rotational Parameters			Translational Parameters				
Sl No	Base Pair			Buckle	Open	Propel	Stagger	Shear	Stretch	RMSD	C1′-C1′
1	G:C W:W Cis	Crystal		3.8	3.43	-16.55	-0.05	-0.35	2.7		10.248
		Neutral	gas	2.32	-3.63	-2.68	-0.08	-0.18	2.96	0.26	10.698
			sol	2.7	-1.24	-8.75	-0.11	0.16	2.96	0.23	10.686
		Protonated	gas	0.20	1.94	0.24	0.00	0.28	2.88	0.27	10.523
			sol	5.47	0.44	-6.69	-0.01	0.19	2.93	0.27	10.617
2	G:U W:W Cis	Crystal		-11.8	6.91	-14.42	-0.47	-2.25	2.76		10.271
		Neutral	gas	-0.21	0.98	-3.33	-0.10	-2.43	2.85	0.2	10.393
			sol	-8.65	-0.47	-8.1	0.03	-2.31	2.89	0.19	10.438
		Protonated	gas	-0.13	7.60	-0.10	0.00	-2.31	2.89	0.21	10.226
			sol	-8.74	2.57	-7.66	0.01	-2.3	2.89	0.17	10.359
3	G:C W:W Trans	Crystal		-4.21	6.46	-4.26	-0.11	-2.57	2.81		10.443
		Neutral	gas	10.20	76.56	6.13	-0.32	-4.10	3.08	3.24	8.549
			sol	6.98	10.58	32.14	-0.15	-2.33	2.96	3.27	10.474
		Protonated	gas	-1.04	18.62	-1.24	-0.01	-3.41	2.83	0.51	10.141
			sol	0.03	11.61	-0.1	0	-2.54	2.94	0.16	10.434
4	G:rC W:S Cis	Crystal		15.07	-33.19	-19.13	-0.06	3.68	3.17		9.062
		Neutral	gas	2.14	-3.66	-0.80	-0.06	-0.20	2.96	1.94	10.705
			sol	2.48	48.21	-21.23	0.06	-2.42	3.66	0.45	4.600
		Protonated	gas	7.54	38.96	-8.76	0.21	-2.14	3.44	0.64	9.526
			sol	-21.98	38.38	-23.17	0.02	-2.14	3.4	0.84	4.394
5	G:G W:H Cis	Crystal		8.47	-1.33	-0.5	0.16	-2.92	3.05		11.63
		Neutral	gas	-19.48	0.03	8.02	0.00	2.00	2.76	1.85	13.09
			sol	-11.71	-6.03	-37.66	-0.2	-2.54	2.93	0.62	11.455
		Protonated	gas	0.50	-4.58	0.14	0.00	-3.10	2.91	0.21	11.733
			sol	3.09	-4.57	-6.18	-0.05	2.77	2.96	0.22	11.632
6	G:U S:H Trans	Crystal		-2.17	18.04	9.13	0.35	4.04	3.84		11.019
		Neutral	gas	-158.88	11.16	68.49	-0.74	-3.23	0.15	2.17	6.196
			sol	-148.12	21.01	82.09	0.3	-3.3	0.26	2.19	6.370
		Protonated	gas	-29.27	15.86	21.73	-0.15	-5.99	0.2	0.71	10.095
			sol	0.74	42.83	18.08	-0.04	-5.58	0.47	0.29	10.569

Continued to next page.

Continued from previous page.

Base pair orientation parameters calculated by NUPARM (Mukherjee, Bansal, Bhattacharyya (2006) *J. Comp. Aided Mol. Des.*), RMSD values and C1′-C1′ distance (in *Å*) for the crystal geometry and gas and solvent phase optimized ground state geometries (with and without proton at N7 of guanine) of the base pairing systems are reported.

				Rotational Parameters			Translational Parameters				
Sl No	Base Pair			Buckle	Open	Propel	Stagger	Shear	Stretch	RMSD	C1′-C1′
7	G:A W:W Trans	Crystal		23.53	15.48	34.68	-0.05	0.22	2		12.734
		Neutral	gas	11.95	10.91	24.44	-0.09	-0.31	2.91	0.36	12.869
			sol	-17.17	12.54	79.1	0.47	-0.75	0.91	0.91	12.691
		Protonated	gas	28.92	11.6	-90.12	-0.41	-1.02	2.68	1.46	12.413
			sol	-15.44	16.34	86.5	0.64	-0.86	1.27	1.27	12.633
8	G:A W:H Cis	Crystal		6.05	-2.51	13.7	0.28	-0.06	2.88		10.919
		Neutral	gas	7.52	-3.88	29.72	0.27	0.35	2.91	0.28	10.965
			sol	12.81	-4.78	35.78	0.39	0.27	2.9	0.35	11.018
		Protonated	gas	18.02	-1.38	46.7	0.37	0.5	2.74	0.47	10.916
			sol	13.98	-3.62	41.33	0.43	0.27	2.83	0.45	10.973
9	G:A W:H Trans	Crystal		4.56	3.29	-18.12	1.8	1.09	2.75		11.554
		Neutral	gas	-4.16	14.32	-13.78	0.25	-0.11	2.87	0.69	10.867
			sol	37.81	2.79	-28.72	0.72	0.06	2.86	0.84	10.586
		Protonated	gas	33.99	4.8	-13.76	0.63	0.14	2.73	0.77	10.706
			sol	33.56	6.7	-21.37	0.56	0.04	2.84	0.84	10.649
10	G:A W:W Cis	Crystal		21.04	2.14	-36.06	-0.74	-0.58	2.68		12.592
		Neutral	gas	12.81	-3.62	28.53	0.41	0.16	2.96	0.33	12.863
			sol	13.6	-3.66	37.24	0.43	0.08	2.94	0.41	12.907
		Protonated	gas	7.89	4.39	37.04	0.37	0.08	2.73	0.43	12.666
			sol	8.82	-0.37	35.09	0.36	0.03	2.87	0.41	12.839
11	G:G W:H Trans	Crystal		11.52	-0.62	0.09	0.03	-0.25	2.67		10.966
		Neutral	gas	-11.17	10.99	-2.9	0.04	0.18	2.86	0.4	11.011
			sol	5.34	-4.14	-9.47	-0.06	0.18	2.89	0.28	11.198
		Protonated	gas	1.71	3.76	0.37	0.01	0.27	2.78	0.26	11.143
			sol	7.95	-3.88	-5.2	-0.01	0.21	2.83	0.23	11.155
12	G:G W:W Trans	Crystal		23.11	-1.03	-10.75	0.05	2.54	3.01		13.516
		Neutral	gas	18.9	0	-7.9	0	2.01	2.76	0.28	13.099
			sol	12.6	0	-7.91	0	2.13	2.8	0.25	13.291
		Protonated	gas	0.04	-11.19	-1.08	-0.05	2.18	2.78	0.45	13.316
			sol	6.27	-3.68	-6.25	-0.04	2.2	2.81	0.32	13.373

S7 Context analysis of G:G W:H Cis base pair over a nonredundant set of 167 RNA crystal structures.

Table S3 G:G W:H Cis base pair (not the part of any triples and quartets)

Sl No.	Structure	1st Nucleotide	2nd Nucleotide	Geometry(1:2)
1	3TVF.pdb	566 G (A)	299 G (A)	H:WC
2	3TVF.pdb	12 G (B)	9 G (B)	H:WC
3	1VQO.pdb	607 G (0)	604 G (0)	H:WC
4	2XG0.pdb	2345 G (A)	2371 G (A)	H:WC
5	4GAQ.pdb	177 G (A)	145 G (A)	H:WC
6	4GAQ.pdb	566 G (A)	299 G (A)	H:WC
7	2VQE.pdb	566 G (A)	299 G (A)	H:WC
8	2XQD.pdb	566 G (A)	299 G (A)	H:WC
9	3KNH.pdb	566 G (A)	299 G (A)	H:WC
10	3KNH.pdb	1160 G (A)	1182 G (A)	H:WC
11	3V2D.pdb	2345 G (A)	2371 G (A)	H:WC
12	2Y10.pdb	566 G (A)	299 G (A)	H:WC
13	2Y10.pdb	1142 G (A)	1139 G (A)	H:WC
14	2ZJR.pdb	2324 G (X)	2350 G (X)	H:WC
15	3PYN.pdb	566 G (A)	299 G (A)	H:WC
16	3U5B.pdb	163 G (2)	151 G (2)	H:WC
17	3U5B.pdb	571 G (2)	553 G (2)	H:WC
18	3U5B.pdb	613 G (2)	371 G (2)	H:WC
19	3U5B.pdb	1277 G (2)	1273 G (2)	H:WC
20	3KIQ.pdb	566 G (a)	299 G (a)	H:WC
21	3KNL.pdb	566 G (A)	299 G (A)	H:WC
22	3KNN.pdb	566 G (A)	299 G (A)	H:WC
23	3R8N.pdb	177 G (A)	145 G (A)	H:WC
24	3R8N.pdb	566 G (A)	299 G (A)	H:WC
25	3KIT.pdb	2345 G (A)	2371 G (A)	H:WC
26	4DH9.pdb	68 G (A)	64 G (A)	H:WC
27	4DH9.pdb	566 G (A)	299 G (A)	H:WC
28	3PYU.pdb	566 G (A)	299 G (A)	H:WC
29	3UZ6.pdb	566 G (A)	299 G (A)	H:WC
30	3R8S.pdb	2345 G (A)	2371 G (A)	H:WC
31	3KIR.pdb	2345 G (A)	2371 G (A)	H:WC
32	3UZ8.pdb	2345 G (A)	2371 G (A)	H:WC
33	3D2V.pdb	66 G (A)	48 G (A)	H:WC
34	3D2V.pdb	66 G (B)	48 G (B)	H:WC
35	3UYE.pdb	2345 G (A)	2371 G (A)	H:WC

Table S4 Quartets involving a G:G W:H Cis base pair

Sl. No.	Structure	1st Nucleotide	2nd Nucleotide	Geometry (1:2)	3rd Nucleotide	Geometry (1:3)	4th Nucleotide	Geometry (1:4)
1	3UYE.pdb	2349 G (A)	2382 G (A)	H:WC	2368 C (A)	W:WC	644 A (A)	S:WT
2	2VQE.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC	152 A (A)	s:sT
3	2XQD.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC	152 A (A)	s:sT
4	2Y10.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC	152 A (A)	s:sT
5	3PYN.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC	152 A (A)	s:sT
6	3KIQ.pdb	68 G (a)	101 A (a)	W:WC	64 G (a)	H:WC	152 A (a)	s:sT
7	3KNL.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC	152 A (A)	s:sT
8	3R8N.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC	152 A (A)	s:sT
9	1VQO.pdb	184 G (0)	153 C (0)	W:WC	186 A (0)	S:SC	150 G (0)	H:WC
10	2XG0.pdb	2349 G (A)	2368 C (A)	W:WC	644 A (A)	S:WT	2382 G (A)	H:WC
11	3V2D.pdb	2349 G (A)	2368 C (A)	W:WC	644 A (A)	S:WT	2382 G (A)	H:WC
12	3KIT.pdb	2349 G (A)	2368 C (A)	W:WC	644 A (A)	S:WT	2382 G (A)	H:WC
13	3R8S.pdb	2349 G (A)	2368 C (A)	W:WC	644 A (A)	S:WT	2382 G (A)	H:WC
14	3KIR.pdb	2349 G (A)	2368 C (A)	W:WC	644 A (A)	S:WT	2382 G (A)	H:WC
15	3UZ8.pdb	2349 G (A)	2368 C (A)	W:WC	644 A (A)	S:WT	2382 G (A)	H:WC

Table S5 Triplets involving a G:G W:H Cis base pair

Sl No.	Structure	1st Nucleotide	2nd Nucleotide	Geometry(1:2)	3rd Nucleotide	Geometry(1:3)
1	4GAQ.pdb	97 G (A)	94 G (A)	H:WC	73 C (A)	W:WC
2	4GAQ.pdb	1142 G (A)	1139 G (A)	H:WC	1132 C (A)	W:WC
3	1DDY.pdb	228 G (C)	210 G (C)	H:WC	218 C (C)	W:WC
4	1DDY.pdb	428 G (E)	410 G (E)	H:WC	418 C (E)	W:WC
5	1U9S.pdb	176 G (A)	218 G (A)	H:WC	194 C (A)	W:WC
6	3R8N.pdb	1160 G (A)	1182 G (A)	H:WC	1176 A (A)	W:WC
7	3UZ8.pdb	1091 G (A)	1071 G (A)	H:WC	1100 C (A)	W:WC
8	3UYE.pdb	1091 G (A)	1071 G (A)	H:WC	1100 C (A)	W:WC
9	3TVF.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC
10	4GAQ.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC
11	2XQD.pdb	1160 G (A)	1176 A (A)	W:WC	1182 G (A)	H:WC
12	2Y10.pdb	1160 G (A)	1176 A (A)	W:WC	1182 G (A)	H:WC
13	3PYN.pdb	1160 G (A)	1176 A (A)	W:WC	1182 G (A)	H:WC
14	3PYU.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC
15	3UZ6.pdb	68 G (A)	101 A (A)	W:WC	64 G (A)	H:WC
16	3TVF.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
17	3TVF.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
18	1VQO.pdb	84 G (0)	62 C (0)	W:WC	56 G (0)	H:WC
19	1VQO.pdb	702 G (0)	726 C (0)	W:WC	744 G (0)	H:WC
20	4ARC.pdb	12 G (B)	23 C (B)	W:WC	9 G (B)	H:WC
21	2XG0.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC
22	4GAQ.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
23	4GAQ.pdb	10 G (V)	25 C (V)	W:WC	44 G (V)	H:WC
24	2VQE.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
25	2VQE.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
26	2VQE.pdb	1142 G (A)	1132 C (A)	W:WC	1139 G (A)	H:WC
27	4AS1.pdb	12 G (B)	23 C (B)	W:WC	9 G (B)	H:WC
28	2XQD.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
29	2XQD.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
30	2XQD.pdb	10 G (Y)	25 C (Y)	W:WC	44 G (Y)	H:WC
31	1U6B.pdb	130 G (B)	177 C (B)	W:WC	206 G (C)	H:WC
32	3KNH.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
33	3KNH.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
34	3V2D.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC
35	1DDY.pdb	28 G (A)	18 C (A)	W:WC	10 G (A)	H:WC
36	1DDY.pdb	628 G (G)	618 C (G)	W:WC	610 G (G)	H:WC
37	1U9S.pdb	177 G (A)	193 C (A)	W:WC	188 G (A)	H:WC
38	2Y10.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
39	2Y10.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
40	2Y10.pdb	10 G (Y)	25 C (Y)	W:WC	44 G (Y)	H:WC
41	3U5D.pdb	1266 G (1)	1275 C (1)	W:WC	1246 G (1)	H:WC
42	2ZJR.pdb	87 G (X)	65 C (X)	W:WC	59 G (X)	H:WC
43	2ZJR.pdb	1102 G (X)	1111 C (X)	W:WC	1082 G (X)	H:WC
44	2ZJR.pdb	2328 G (X)	2347 C (X)	W:WC	2361 G (X)	H:WC
45	3PYN.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
46	3PYN.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
47	3U5B.pdb	325 G (2)	343 C (2)	W:WC	322 G (2)	H:WC
48	3U5B.pdb	326 G (2)	342 C (2)	W:WC	337 G (2)	H:WC
49	3KIQ.pdb	254 G (a)	272 C (a)	W:WC	251 G (a)	H:WC
50	3KNL.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
51	3KNL.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
52	3KNN.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
53	3KNN.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
54	3R8N.pdb	97 G (A)	73 C (A)	W:WC	94 G (A)	H:WC
55	3R8N.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
56	3R8N.pdb	255 G (A)	271 C (A)	W:WC	266 G (A)	H:WC
57	3R8N.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
58	3KIT.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC
59	4DH9.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
60	4DH9.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
61	4DH9.pdb	1142 G (A)	1132 C (A)	W:WC	1139 G (A)	H:WC
62	2BTE.pdb	12 G (B)	23 C (B)	W:WC	9 G (B)	H:WC
63	2BTE.pdb	12 G (E)	23 C (E)	W:WC	9 G (E)	H:WC
64	3PYU.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
65	3PYU.pdb	1142 G (A)	1132 C (A)	W:WC	1139 G (A)	H:WC
66	3UZ6.pdb	254 G (A)	272 C (A)	W:WC	251 G (A)	H:WC
67	3UZ6.pdb	1057 G (A)	1203 C (A)	W:WC	1053 G (A)	H:WC
68	1MMS.pdb	1091 G (C)	1100 C (C)	W:WC	1071 G (C)	H:WC
69	1MMS.pdb	1091 G (D)	1100 C (D)	W:WC	1071 G (D)	H:WC
70	3R8S.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC
71	3KIR.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC
72	3UZ8.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC
73	3UYE.pdb	88 G (A)	66 C (A)	W:WC	60 G (A)	H:WC

S8 Full reference of Gaussian 09 package

Gaussian 09, Revision C.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, .; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.