

Table S1. List of CSV and Python^a files available in the Supplemental Material that contain dual-donor-to-acceptor-pair instances corresponding to Figure 5, Figure 8C, and Supplemental Figure S2. For each row, a .csv and a .py file is available.

	File Name	Description
1	Supplemental_Data_S1	A(N6) dual-donation to G(N3)/N(O2') within sheared GA base pairs (n = 1,518) corresponding to Figure 5A.
2	Supplemental_Data_S2	A(N6) dual-donation to G(N3)/N(O2') within sheared GA base pairs where the N2 of the G is also a dual-donating amine (n = 186). This is a subset of row 1, and focus is on the G in the file (e.g., the don_resi column represents the G).
3	Supplemental_Data_S3	A(N6) dual-donation to G(N3)/N(O2') within a WC/H A-minor motif (n = 40).
4	Supplemental_Data_S4	A(N6) dual-donation to G(N3)/N(O2') within a WC/H A-minor motif where the N2 of the G is also a dual-donating amine (n = 38). This is a subset of row 3 that corresponds to Figure 5B. Focus is on the G in the file (e.g., the don_resi column represents the G).
5	Supplemental_Data_S5	A(N6) dual-donation to G(N3)/N(O2') within a WC/H A-minor motif where the dual-donating G(N2) donates an H-bond to the N1 of the A bearing the dual-donating A(N6) (n = 31). This is a subset of row 4.
6	Supplemental_Data_S6	A(N6) dual-donation to G(N3)/N(O2') within a WC/H A-minor motif where the dual-donating G(N2) donates an H-bond to the N7 of the A bearing the dual-donating A(N6) (n = 3). This is a subset of row 4.
7	Supplemental_Data_S7	A(N6) dual-donation to A(N7)/N(NPO) within a trans AA base pair (n = 458) corresponding to Figure 5C.
8	Supplemental_Data_S8	A(N6) dual-donation to A(N7)/N(NPO) within a trans AA base pair where the N6 of the partner A is also a dual-donating amine (n = 75). This is a subset of row 7, and focus is on the pairing A in the file (e.g., the don_resi column represents the second A).
9	Supplemental_Data_S9	C(N4) dual-donation to G(O6)/N(NPO) where the C and G form a canonical base pair (n = 1,398) corresponding to Figure 5D.
10	Supplemental_Data_S10	G(N2) dual-donation to A(N3)/C(O2) within a type I A-minor motif (n = 2,178) corresponding to Figure 5E.
11	Supplemental_Data_S11	G(N2) dual-donation to A(N3)/C(O2) within a type I A-minor motif where the N6 of the A is also a dual-donating amine (n = 179). This is a subset of row 10, and focus is on the A in the file (e.g., the don_resi column represents the A).
12	Supplemental_Data_S12	G(N2) dual-donation to A(N7)/N(NPO) where the N7 and NPO belong to the same A (n = 790) corresponding to Figure 5F, not all of which are involved in tetraloops.

13	Supplemental_Data_S13	G(N2) dual-donation to A(N7)/N(NPO) where the N7 and NPO belong to the same A that also has a dual-donating amine (n = 23). This is a subset of row 12, and focus is on the A in the file (e.g., the don_resi column represents the A).
14	Supplemental_Data_S14	C(N4) dual-donation to AA(O)/G(O6) (n = 243) corresponding to Supplemental Figure S2A.
15	Supplemental_Data_S15	G(N2) dual-donation to AA(O)/C(O2) (n = 965) corresponding to Supplemental Figure S2B.
16	Supplemental_Data_S16	All residues that are within Location 1 (n = 285) corresponding to Figure 8C.
17	Supplemental_Data_S17	All residues that are within Location 2 (n = 272) corresponding to Figure 8C.
18	Supplemental_Data_S18	Residues in Location 1 of Figure 8C that are connected to the 5'-end of a residue in Location 2 of the same plot (n = 83).

^aThe Python files are intended to be run using PyMOL (see Methods).