Occurrence and Stability of Lone Pair-π and OH-π Interactions between Water and Nucleobases in Functional RNAs

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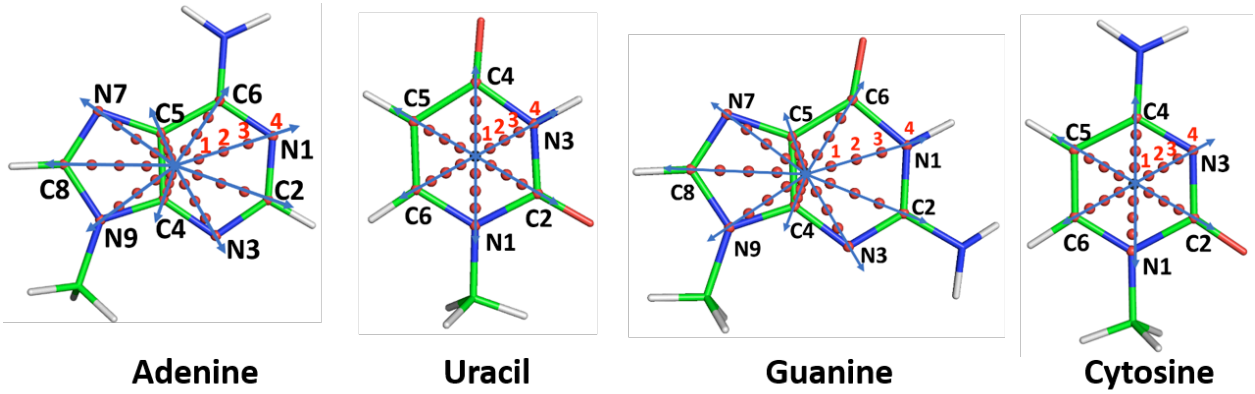


Figure S1. Grid positions for the calculation of the interaction energy for different projections of O^W on the nucleobase plane. Four steps along each of the lines connecting the nucleobase centroid to the ring atoms were considered. Atoms along each line were labeled as 1 to 4 (from the centroid towards the ring) preceded by the atom name. For instance, N1-1 represents the geometry with the O^W atom positioned above the first point connecting the ring centroid to the N1 atom. The distance between O^W and the nucleobase plane was set to the ideal values of 3.0 and 3.5 Å for the lp-π and OH-π geometries, respectively.

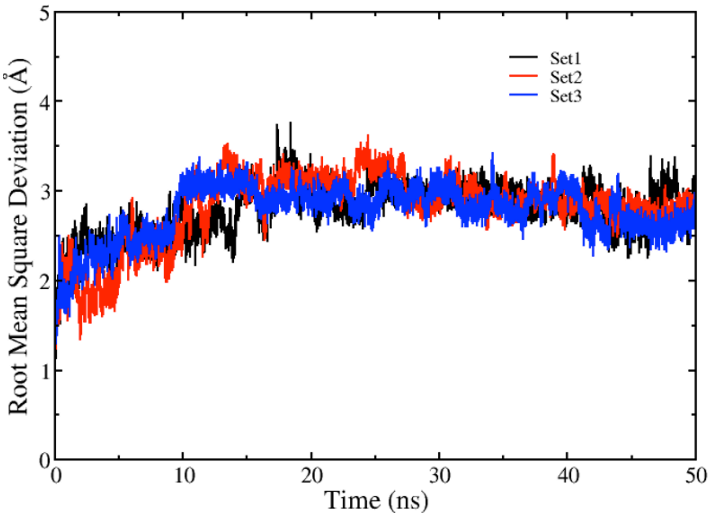


Figure S2. RMSD profile of the three sets of independent simulations we ran. In the main text, results corresponding to the Set 1 are reported.

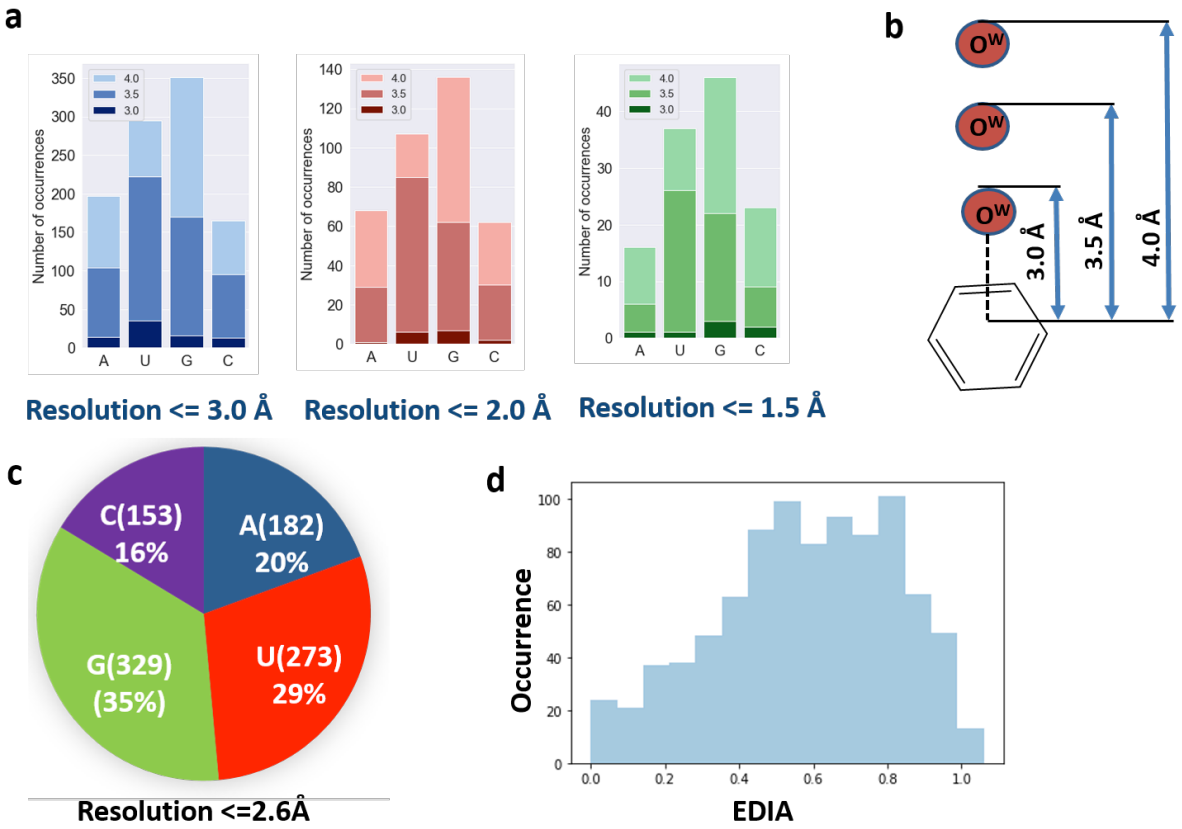


Figure S3. a) Distances distribution (within 3.0, 3.5 and 4.0 Å) of O^W from the nucleobase plane for the observed water-nucleobase stacking contacts in RNA structures at different resolution cutoffs. **b**) Scheme of the geometrical description of the distance cutoffs used in **a**). **c**) Distribution of nucleobases involved in water-nucleobase stacking contacts with a resolution cutoff of <=2.6 Å; **d**) Distribution of EDIA values for the O^W atoms of water molecules involved in water-nucleobase stacking contacts (see the Methods section in the text).

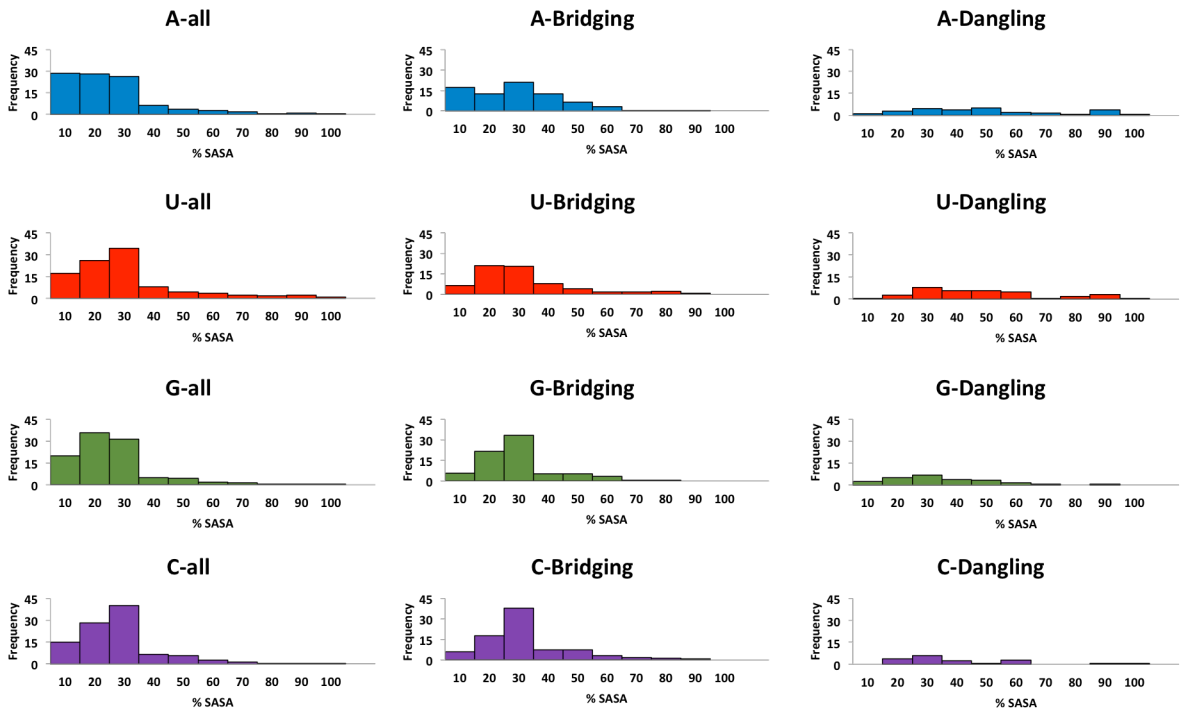


Figure S4. Frequencies of nucleobases at different solvent accessible surface area (SASA) percentage ranges: all the nucleobases in the dataset of 293 PDBs (left), nucleobases found stacked to bridging waters (middle), and nucleobases found stacked to dangling waters (right). The SASA values were calculated with FreeSASA (Simon Mitternacht, 2016, FreeSASA: An open source C library for solvent accessible surface area calculation. F1000Research 5:189; doi: 10.12688/f1000research.7931.1), by setting a standard probe radius of 1.4 Å. For each of the four nucleobases, a maximum SASA value was set at the value obtained for the most exposed nucleobase of that type in the analysed dataset. These maximum values were: 247.3 $Å^2$ for A, from A8 in 1NLC_A; 214.7 $Å^2$ for U, from U19 in 2OIU_P; 273.2 $Å^2$ for G, from G1 in 1B7F_P; and 218.4 $Å^2$ for C, from C122 in 1S72_9. Visual check confirmed that the above bases are fully exposed to the solvent in the corresponding RNA structures. The percentage SASA for each nucleobase was then obtained by dividing the measured SASA by the maximum value possible for that nucleobase and multiplying by 100.

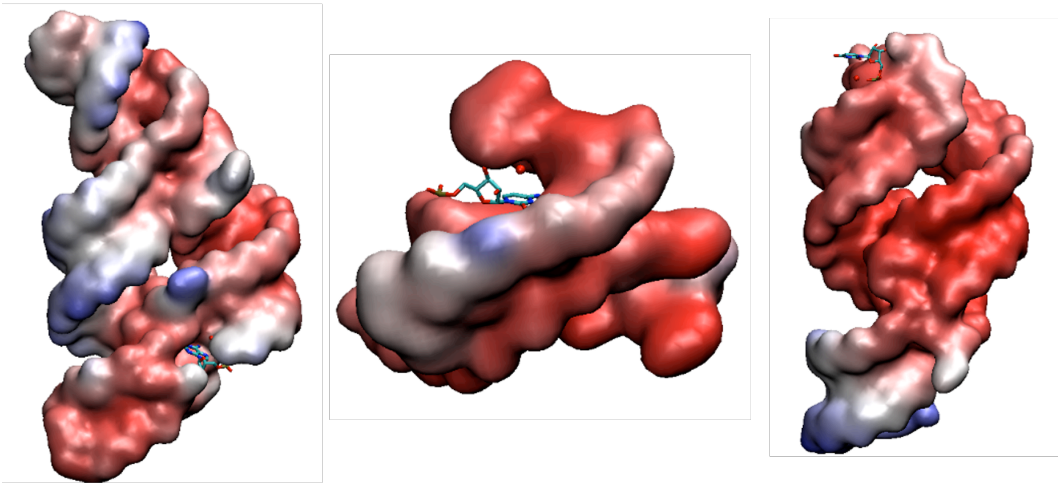


Figure S5. Examples of bridging water-nucleobase stacking interactions at representative values of % SASA: 6, 15 and 74 %. A surface representation of the RNA structure is given, while the stacked nucleobase is shown in stick and the stacked water as a little red sphere centered on its oxygen atom.

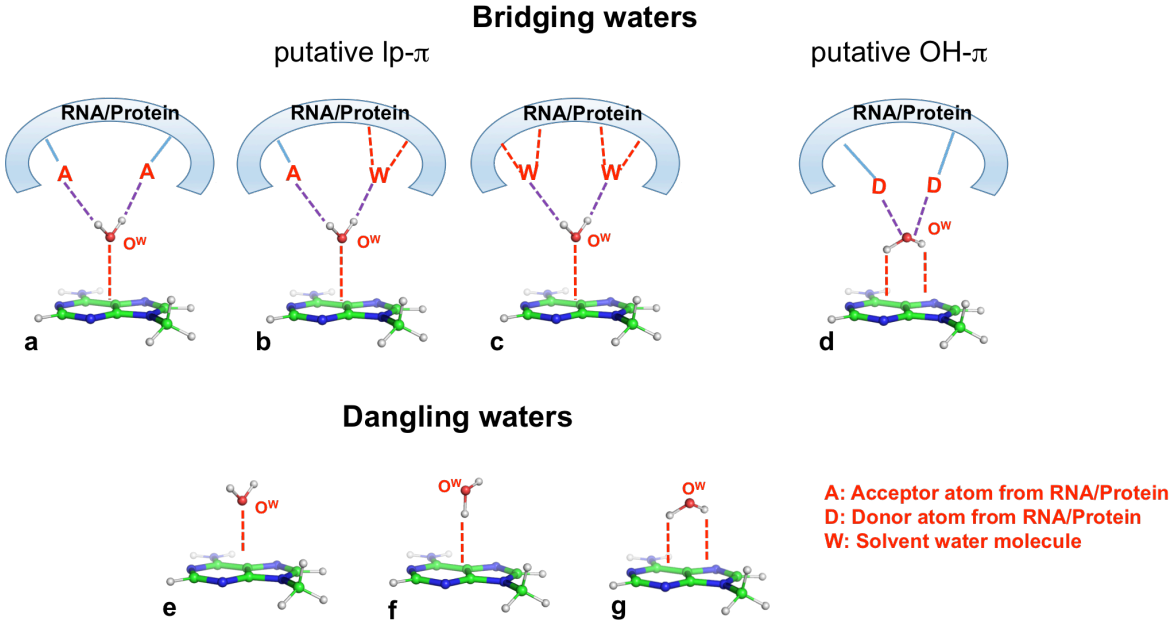


Figure S6. Schematic representation of bridging stacking waters (top panel, **a-d**) and dangling stacking waters (bottom panel, **e-g**). In the top panel, a schematic representation of the structural context is provided, when leading to a possible assignment of the interactions as lp-π (**a-c**) or OH-π (**d**). In the putative lp-π interactions, both the hydrogen atoms on O^W appear to be engaged in H-bonds with acceptor atoms from surrounding residues, while in the OH-π interactions both the lone pairs on O^W appear to be engaged in H-bonds with donor atoms from surrounding residues. Ambiguous cases, where only one hydrogen/lone pair on O^W is at H-bonding distance from an acceptor/donor atom from surrounding residues, are not shown. "A" stands for an acceptor atom from the RNA/Protein and "W" for a crystal water. The blue curve, representing the RNA/protein surrounding at H-bonding distance from the stacked water is clearly absent in case of the dangling waters.

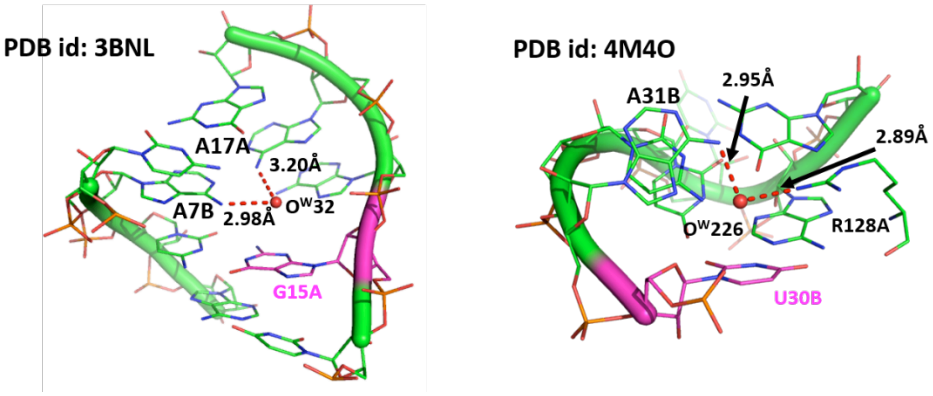


Figure S7. Examples of water-nucleobase stacking contacts where the O^W (represented as a small red sphere) was found at H-bond distance from two heavy donor atoms, thus representing putative OH-π stacking contacts. The nucleobases involved in the stacking contacts are in magenta. Red dashed lines represent the distances between the donors and O^W atom.

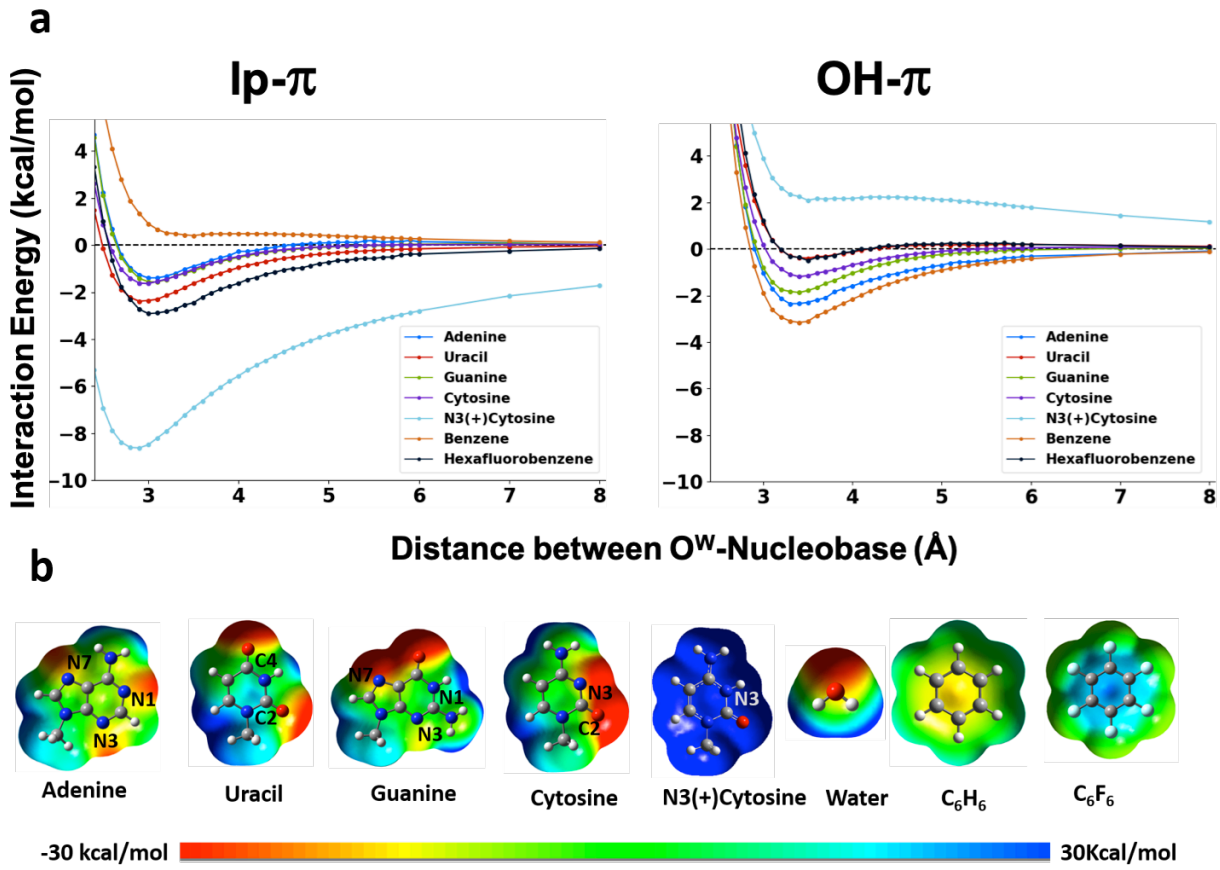
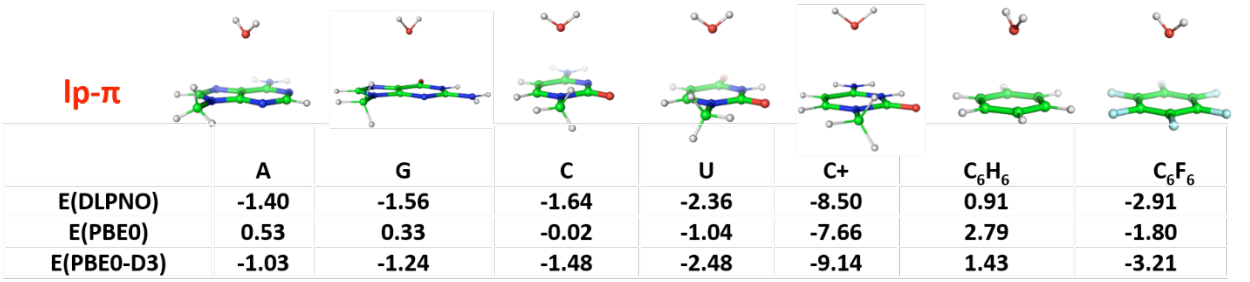
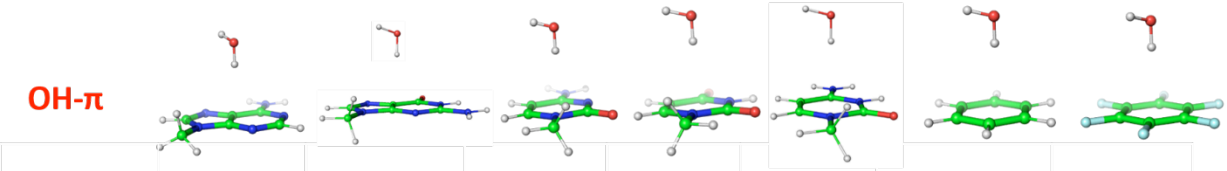


Figure S8. **a**) Potential Energy Curves for all the nucleobases (A, U, G, C, and C^+), benzene and hexafluorobenzene, with water oriented to give rise to pure lp-π (left) and OH-π (right) interactions. Interaction energies in kcal/mol (y-axis) are reported *versus* the O^W-ring distances, varying between 2.4 Å and 8.0 Å (x-axis); **b**) electrostatic potentials of nucleobases, water, benzene and hexafluorobenzene. Electrostatic potentials were mapped on electron density isosurfaces corresponding to a value of 0.0004 atomic units, and are scaled between –30 and 30 kcal/mol.



	A	G	C	U	C+	C_6H_6	C_6F_6
E(DLPNO)	-1.40	-1.56	-1.64	-2.36	-8.50	0.91	-2.91
E(PBE0)	0.53	0.33	-0.02	-1.04	-7.66	2.79	-1.80
E(PBE0-D3)	-1.03	-1.24	-1.48	-2.48	-9.14	1.43	-3.21



	A	G	C	U	C+	C_6H_6	C_6F_6
E(DLPNO)	-2.30	-1.79	-1.15	-0.40	2.09	-3.11	-0.49
E(PBE0)	-1.03	-0.36	0.30	0.94	3.79	-2.07	1.01
E(PBE0-D3)	-2.64	-1.98	-1.27	-0.61	2.20	-3.52	-0.49

Figure S9. Geometries and energies of model geometries corresponding to lp-π and OH-π interactions between water and the aromatic ring of the four nucleobases, of benzene and of hexafluorobenzene. Energies were calculated at reference DLPNO/CBS; and PBE0/TZVP that corresponds to electrostatic energy contribution and PBE0-D3/TZVP that includes the explicit dispersion contribution for interaction energy calculation.

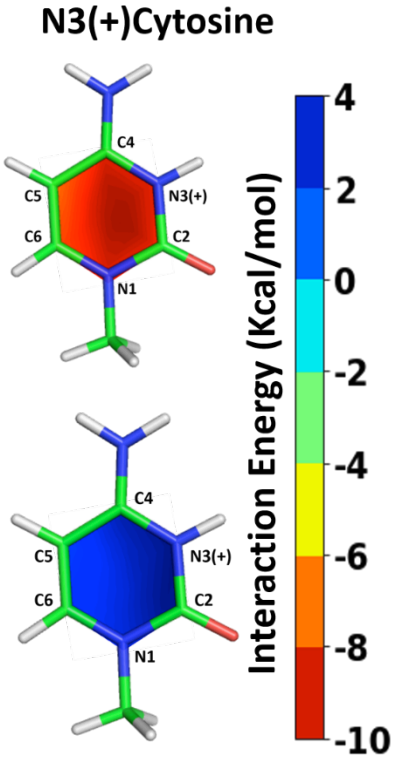


Figure S10. Contour diagrams showing the interaction energies for the lp-π and OH-π interactions between water and the N3-protonated cytosine (C^+) base. Energy values are color coded, from red (-10 kcal/mol) to blue (+4 kcal/mol). Singe point energies were calculated for both the types of interaction on a grid made of 4 points for each line connecting the nucleobase centroid to each atom of the ring. Water-nucleobase distances were frozen at 3.0 Å and 3.5 Å for the lp-π and the OH-π interaction, respectively.

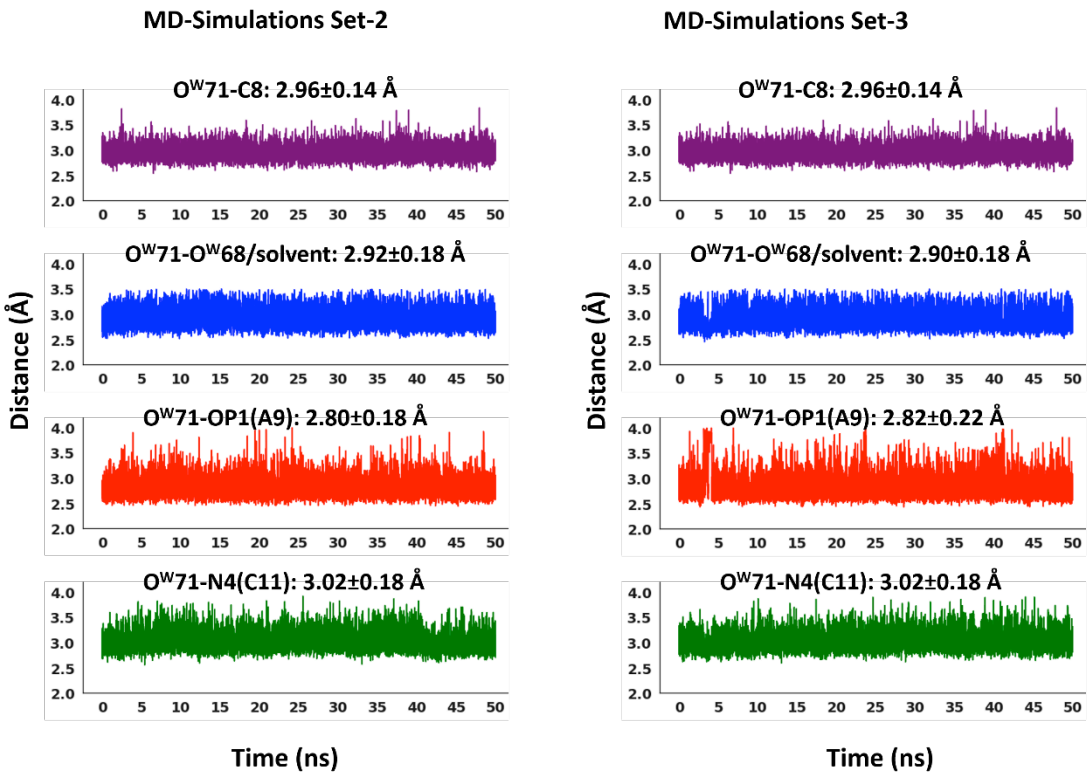


Figure S11. Time evolution of all the relevant distances for the O^W71-C8 stacking contact from the other two sets of independent MD trajectories. The color code of the plots is the same used in Figure 7. Average distance and standard deviation values are also given in the relative plots.

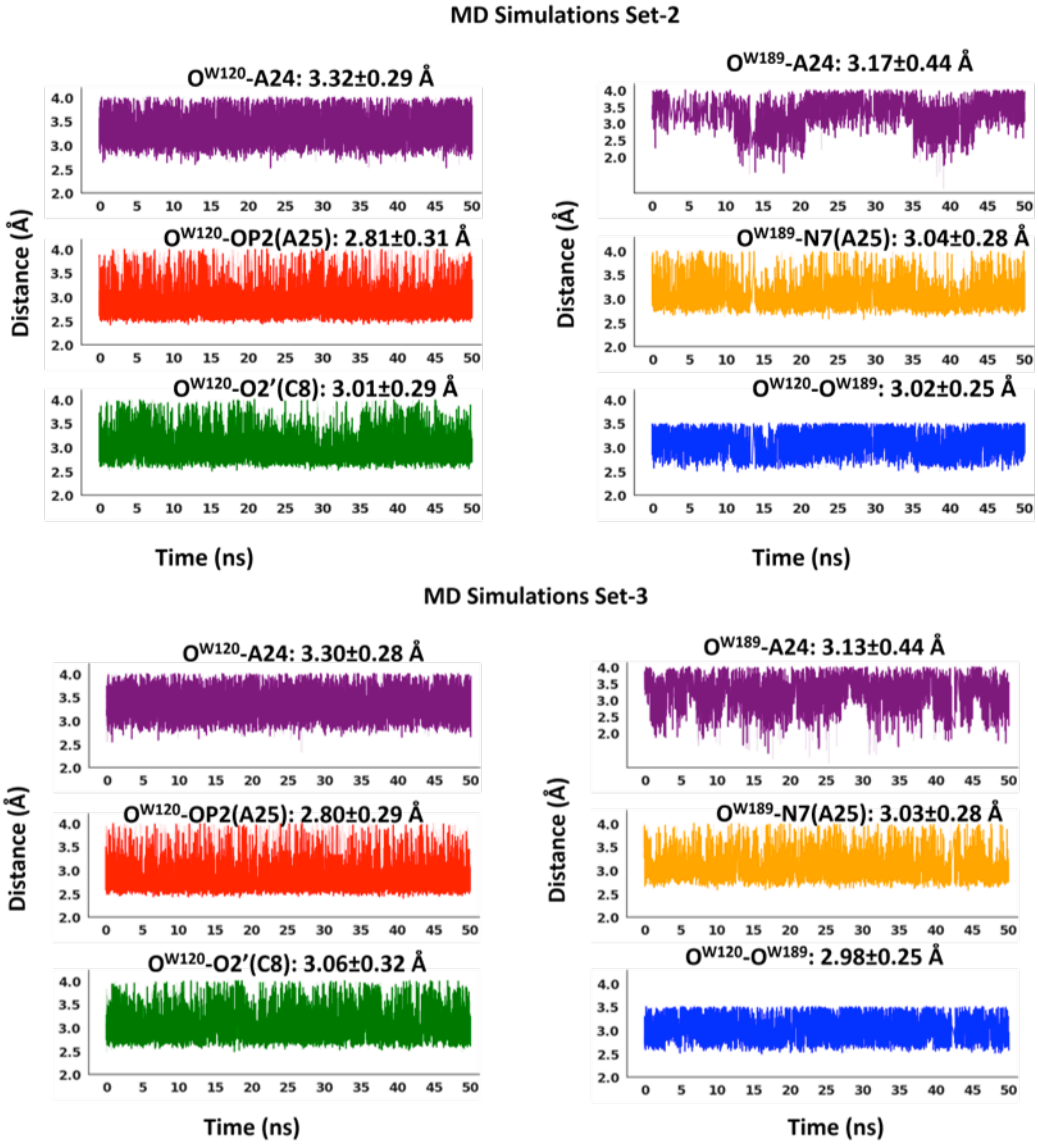


Figure S12. Time evolution of the relevant distances for the A24-O^{W}120/ O^{W} 189 stacking contact from the other two sets of independent MD trajectories. The color code of the plots is the same used in Figure 8. Average distance and standard deviation values are also given in the relative plots.

Molecular dynamics simulations results for the two water-nucleobase stacking contacts involving dangling waters: O^W175-A9 and O^W73-A20

Regarding the O^W175-A9 contact, analysis of our three independent MD trajectories evidenced that a water molecule remains stacked on the A9 base (although O^W175 gets replaced by bulk solvent waters) under dynamic conditions (in ~92% of the frames), maintaining an OH-π interaction. In the figure below, the average distance between O^W175 and the A9 base plane is reported for the three simulations.

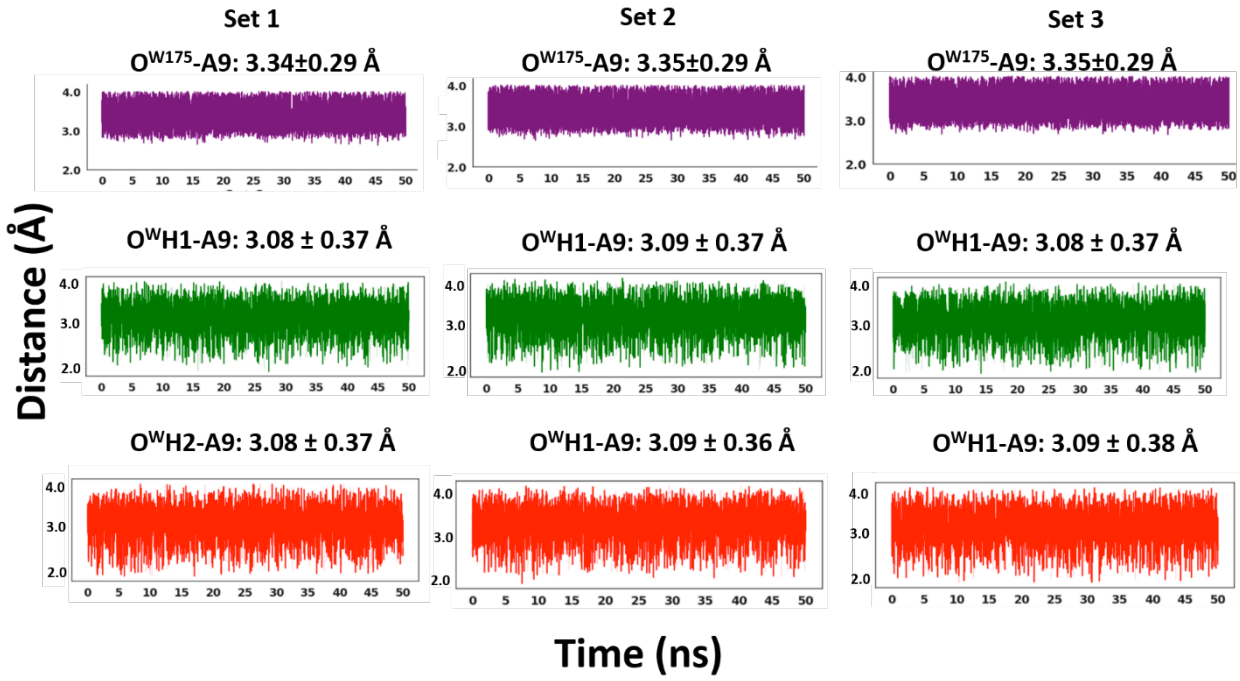


Figure S13. Time evolution of the distances between the oxygen and the hydrogen atoms of water-175 and the plane of nucleobase A9 for the three performed simulations. Average distance and standard deviation values are also given in the relative plots. Only frames matching both a NP-O^W distance < 4.0 Å and one between the NP-O-H angles < 90° are considered in the analysis.

As for the O^W73-A20 contact, it is clearly unstable under dynamic conditions. During the simulation time, indeed, O^W73 does not remain at stacking distance from the A20 nucleobase, apart from a fraction of frames, ranging between 20% and 39% for the three simulations (see the Figure below, reporting the distance along the simulation time between O^W73 and the A20 plane).

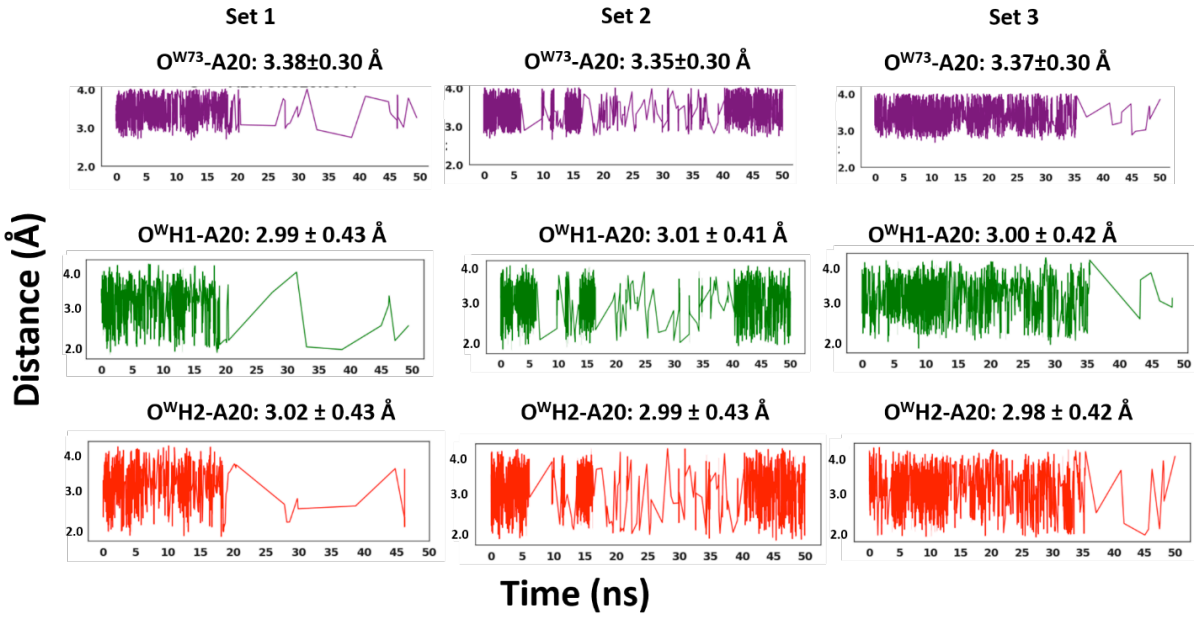


Figure S14. The time evolution of the distances between the oxygen and the hydrogen atoms of water-73 and the plane of nucleobase A20 is reported for the three performed simulations. Average distance and standard deviation values, calculated only on the frames where the contact is maintained (20%, 35% and 39%, respectively), are also given in the relative plots. Only frames matching both a NP-O^W distance < 4.0 Å and one between the NP-O-H angles < 90° are considered in the analysis.

Table S1. Instances of nucleobase-water stacking contacts with specification of involved nucleobase and water, PDB ID, and water oxygen EDIA (Electron Density for Individual Atoms) value (it is "NA" for water molecules for which the EDIA value could not be obtained, as the electron density map is not available for the corresponding X-ray structure). Putative protonated A and C nucleobases are indicated by adding a + sign to the nucleobase in the first column.

Nucleobase	Water	PDB ID	EDIA
Adenine-Water Stacking Contacts			
A_0_1117	HOH_0_6023	1s72	0.65
A_0_1123	HOH_0_5521	1s72	0.24
A_0_1132	HOH_0_3419	1s72	0.15
A_0_1150	HOH_G_4499	1s72	0.82
A_0_120	HOH_2_3012	1s72	0.83
A_0_1200	HOH_0_5253	1s72	0.17
A_0_1232	HOH_0_8805	1s72	0.42
A_0_1487	HOH_0_7109	1s72	0.15
A_0_1502	HOH_0_9437	1s72	0.48
A_0_1572	HOH_0_5162	1s72	0.10
A_0_1653	HOH_0_3547	1s72	0.18
A_0_1653	HOH_0_9279	1s72	0.66
A_0_1712	HOH_0_5765	1s72	0.25
A_0_1733	HOH_0_9660	1s72	0.43
A_0_1836	HOH_0_4875	1s72	0.58
A_0_1839	HOH_0_5023	1s72	0.28
A_0_1840	HOH_0_8621	1s72	0.54
A_0_189	HOH_0_8616	1s72	0.31
A_0_2038	HOH_B_8622	1s72	0.35
A_0_2062	HOH_0_4160	1s72	0.47
A_0_2101	HOH_0_8836	1s72	0.53
A_0_2238	HOH_0_6164	1s72	0.17
A_0_2455	HOH_0_3599	1s72	0.29
A_0_2460	HOH_0_4312	1s72	0.84
A_0_2483	HOH_0_3803	1s72	0.91
A_0_2485-(+)	HOH_0_9765	1s72	0.23
A_0_2488	HOH_0_4290	1s72	0.43
A_0_2509	HOH_0_6222	1s72	0.41
A_0_2509	HOH_0_8756	1s72	0.47
A_0_2697	HOH_0_4105	1s72	0.82
A_0_2743	HOH_0_5576	1s72	0.24
A_0_2840	HOH_0_7140	1s72	0.16
A_0_2896	HOH_X_4132	1s72	0.19
A_0_331	HOH_0_6338	1s72	0.01

A_0_37	HOH_0_4186	1s72	0.40
A_0_395	HOH_0_9812	1s72	0.41
A_0_442	HOH_0_9794	1s72	0.38
A_0_459	HOH_0_4174	1s72	0.64
A_0_462	HOH_0_4383	1s72	0.21
A_0_513	HOH_2_7177	1s72	0.40
A_0_513	HOH_2_7692	1s72	0.56
A_0_565	HOH_0_4500	1s72	0.02
A_0_67	HOH_S_8339	1s72	0.47
A_0_674	HOH_0_4441	1s72	0.44
A_0_721	HOH_0_9863	1s72	0.62
A_0_766	HOH_0_4679	1s72	0.41
A_0_867	HOH_0_8845	1s72	0.57
A_0_907	HOH_0_5051	1s72	0.56
A_0_922	HOH_0_8846	1s72	0.77
A_0_923	HOH_0_3803	1s72	0.91
A_0_923	HOH_0_5533	1s72	0.61
A_0_939	HOH_0_3152	1s72	0.51
A_9_3	HOH_9_8477	1s72	0.12
A_9_52	HOH_9_8392	1s72	0.04
A_A_1	HOH_A_2003	4un3	0.77
A_A_1311	HOH_A_5103	4qcn	NA
A_A_14	HOH_A_1099	2qwy	0.24
A_A_17	HOH_A_158	3td0	0.83
A_A_18	HOH_A_164	3td0	0.72
A_A_1817	HOH_A_4013	4qcn	NA
A_A_1992	HOH_A_4016	4qcn	NA
A_A_1993	HOH_A_4825	4qcn	NA
A_A_2	HOH_A_134	4u34	0.94
A_A_2	HOH_A_137	4u35	0.53
A_A_20	HOH_A_73	1l2x	0.76
A_A_2082	HOH_A_5134	4qcn	NA
A_A_21	HOH_A_661	2a43	0.53
A_A_22	HOH_A_2040	4bw0	0.55
A_A_24	HOH_A_120	1l2x	0.73
A_A_24	HOH_A_189	1l2x	0.45
A_A_24	HOH_A_544	2a43	0.92
A_A_24	HOH_A_551	2a43	0.73
A_A_2497	HOH__A3682	4kj9	NA
A_A_2614	HOH_A_4045	4qcn	NA
A_A_29	HOH_A_2140	3zp8	0.81
A_A_335	HOH_A_4019	4qcn	NA
A_A_4	HOH_A_79	3nj6	0.99
A_A_43	HOH_A_123	3d2v	0.70
A_A_50	HOH_A_173	3d2v	0.59
A_A_53	HOH_B_59	3tzr	0.39

A_A_55	HOH_A_399	4lvz	0.95
A_A_6	HOH_A_17	283d	NA
A_A_62	HOH_A_453	4lvz	0.75
A_A_7	HOH_A_16	3nj6	0.93
A_A_7	HOH_A_21	3nj7	0.94
A_A_7	HOH_A_46	3nj7	0.49
A_A_7	HOH_A_68	3nj6	0.94
A_A_72	HOH_A_231	4jf2	0.96
A_A_9	HOH_A_71	2r22	0.97
A_A_9	HOH_A_80	2r20	0.77
A_A_9	HOH_A_95	1u0b	0.39
A_B_1492	HOH_A_156	2oe5	0.81
A_B_15	HOH_B_191	1d4r	0.35
A_B_20	HOH_B_104	3cgp	0.74
A_B_20	HOH_B_117	3cgp	0.74
A_B_20	HOH_B_52	3ibk	0.35
A_B_20	HOH_B_86	3cgr	0.65
A_B_22	HOH_B_106	2r20	0.66
A_B_23	HOH_B_194	3d2v	0.20
A_B_27	HOH_B_222	2hw8	0.53
A_B_304	HOH_B_1278	1et4	0.55
A_B_31	HOH_B_2008	4aq7	0.86
A_B_38	HOH_B_2059	2vpl	0.16
A_B_38	HOH_B_2064	2vpl	0.08
A_B_38(+)	HOH_B_82	3rg5	0.35
A_B_39	HOH_B_302	2fqn	0.82
A_B_40	HOH_B_165	3td0	0.77
A_B_404	HOH_B_623	1k8w	0.49
A_B_413	HOH_A_523	1k8w	0.99
A_B_44	HOH_A_666	4n0t	0.91
A_B_45	HOH_B_215	4n0t	0.86
A_B_5	HOH_A_158	3q0q	0.59
A_B_50	HOH_B_310	3d2v	0.67
A_B_56	HOH_B_386	3egz	0.58
A_B_56	HOH_B_395	4n0t	0.75
A_B_56	HOH_B_434	3egz	0.56
A_B_57	HOH_B_332	3d2v	0.52
A_B_57	HOH_B_506	3nkb	0.59
A_B_58	HOH_B_144	3ivn	0.55
A_B_6	HOH_A_47	3q0s	0.78
A_B_68	HOH_B_159	1csl	0.67
A_B_7	HOH_A_139	3k62	0.90
A_B_7	HOH_A_149	3k5z	0.64
A_B_7	HOH_A_262	1g2e	0.48
A_B_7	HOH_A_576	3k5y	0.48
A_B_7	HOH_B_17	3nj7	0.92

A_B_7	HOH_B_2047	2atw	0.85
A_B_7	HOH_B_34	3nj7	0.76
A_B_8	HOH_B_1009	3dd2	0.84
A_B_93	HOH_B_264	4n0t	0.68
A_C_11	HOH_C_218	1t0e	0.74
A_C_11	HOH_C_50	1m8y	0.81
A_C_12	HOH_C_102	4ig8	0.12
A_C_1284	HOH_C_1350	1n35	0.24
A_C_15	HOH_A_2051	4c8z	0.65
A_C_15	HOH_A_362	1q96	0.79
A_C_15	HOH_C_376	1q96	0.68
A_C_16	HOH_A_119	1m8w	0.72
A_C_16	HOH_C_227	3ova	0.85
A_C_17	HOH_C_227	3ova	0.85
A_C_3	HOH_A_408	3t5n	0.48
A_C_35	HOH_A_340	2zm5	0.79
A_C_4	HOH_A_113	3q0p	0.36
A_C_4	HOH_B_370	4mdx	0.81
A_C_416	HOH_C_1605	1et4	0.48
A_C_57	HOH_C_1025	2pn4	0.79
A_C_7	HOH_C_18	3nj7	0.92
A_C_7	HOH_C_26	3nj7	0.84
A_C_76	HOH_C_520	2fmt	NA
A_D_109	HOH_D_16	3p59	0.87
A_D_11	HOH_D_218	1m8y	0.46
A_D_15	HOH_D_176	1yz9	0.51
A_D_16	HOH_B_256	1m8w	0.55
A_D_1953	HOH_D_2027	2bh2	NA
A_D_2	HOH_D_210	4m30	0.13
A_D_30	HOH_D_2034	2vpl	0.21
A_D_37	HOH_D_550	2fmt	NA
A_D_4	HOH_D_112	3nj7	0.8
A_D_5	HOH_D_117	4ht9	0.49
A_D_58	HOH_D_203	4nku	0.5
A_D_7	HOH_D_15	3nj7	0.97
A_D_7	HOH_D_44	3nj7	0.66
A_D_76	HOH_D_523	2fmt	NA
A_E_1	HOH_B_448	1ytu	0.67
A_E_116	HOH_E_1284	1et4	0.48
A_E_29	HOH_A_447	3eph	0.28
A_E_54	HOH_E_112	3p59	0.72
A_E_7	HOH_E_24	3nj7	0.86
A_E_7	HOH_E_38	3nj7	0.73
A_F_2	HOH_F_174	3gpq	0.37
A_F_22	HOH_F_2024	2y9h	0.48
A_F_37	HOH_F_45	1q2r	0.24

A_F_39	HOH_F_99	3rw6	0.49
A_F_44	HOH_F_75	3rw6	0.69
A_F_58	HOH_F_88	3eph	0.82
A_F_7	HOH_F_20	3nj7	0.83
A_F_7	HOH_F_48	3nj7	0.66
A_H_3	HOH_B_2059	4b3g	0.56
A_H_4	HOH_H_2003	4b3g	0.26
A_H_40	HOH_H_64	3rw6	0.92
A_P_7	HOH_P_181	3ok4	0.81
A_R_12	HOH_A_2041	2bu1	0.45
A_R_3	HOH_R_66	2tmv	NA
A_R_38	HOH_R_275	4kzd	0.43
A_R_65	HOH_R_992	1b23	0.03
A_R_68	HOH_R_10	3iab	0.50
A_S_2	HOH_Q_101	4g7o	0.42
A_V_4	HOH_N_150	3ok4	0.77
A_X_105	HOH_X_371	2qbz	0.24
A_X_15 (+)	HOH_X_120	3wbm	0.87
A_X_41	HOH_X_404	2gdi	0.45
A_X_44	HOH_X_451	2gdi	0.79
A_X_503	HOH_X_704	4peh	0.69
A_X_61	HOH_X_431	2qbz	0.36
A_X_75	HOH_X_373	2gdi	0.63
A_Y_44	HOH_Y_343	2gdi	0.39
A_Y_41	HOH_Y_303	2gdi	0.26
			Uracil-Water Stacking Contacts
U_0_1009	HOH_0_3800	1s72	0.83
U_0_1017	HOH_0_9564	1s72	0.27
U_0_1047	HOH_0_4097	1s72	0.62
U_0_1062	HOH_0_9365	1s72	0.55
U_0_1109	HOH_J_247	1s72	0.78
U_0_1136	HOH_0_4468	1s72	0.40
U_0_1220	HOH_0_5489	1s72	0.21
U_0_1264	HOH_0_3068	1s72	0.62
U_0_1310	HOH_0_5322	1s72	0.21
U_0_1359	HOH_0_4211	1s72	0.36
U_0_1446	HOH_S_8344	1s72	0.54
U_0_1447	HOH_0_6288	1s72	0.42
U_0_1454	HOH_0_4793	1s72	0.53
U_0_1473	HOH_0_9258	1s72	0.23
U_0_1488	HOH_0_8837	1s72	0.22
U_0_1503	HOH_0_9132	1s72	0.47
U_0_1696	HOH_0_6912	1s72	0.81
U_0_170	HOH_0_8545	1s72	0.52
U_0_170	HOH_0_8675	1s72	0.57
U_0_1724	HOH_0_4194	1s72	0.32

U_0_1771	HOH_0_4322	1s72	0.31
U_0_1813	HOH_0_6210	1s72	0.20
U_0_1835	HOH_0_9532	1s72	0.39
U_0_1838	HOH_0_5023	1s72	0.28
U_0_1850	HOH_0_5230	1s72	0.63
U_0_1890	HOH_0_4580	1s72	0.38
U_0_1980	HOH_0_8778	1s72	0.59
U_0_2059	HOH_0_9467	1s72	0.57
U_0_2117	HOH_0_4348	1s72	0.48
U_0_2278	HOH_0_6216	1s72	0.62
U_0_2330	HOH_0_3494	1s72	0.47
U_0_2419	HOH_0_8632	1s72	0.83
U_0_2424	HOH_0_8614	1s72	0.51
U_0_2473	HOH_0_6717	1s72	0.55
U_0_2484	HOH_0_9127	1s72	0.41
U_0_2512	HOH_0_4846	1s72	0.56
U_0_2541	HOH_0_6922	1s72	0.79
U_0_2645	HOH_0_5553	1s72	0.56
U_0_2837	HOH_B_8579	1s72	0.15
U_0_325	HOH_0_5053	1s72	0.13
U_0_374	HOH_0_8538	1s72	0.84
U_0_454	HOH_0_3591	1s72	0.08
U_0_454	HOH_0_8546	1s72	0.22
U_0_488	HOH_0_3563	1s72	0.76
U_0_55	HOH_0_4853	1s72	0.38
U_0_651	HOH_0_9519	1s72	0.57
U_0_675	HOH_0_4494	1s72	0.47
U_0_713	HOH_0_3450	1s72	0.15
U_0_713	HOH_0_9645	1s72	0.25
U_0_714	HOH_0_5515	1s72	0.63
U_0_753	HOH_0_5024	1s72	0.37
U_0_777	HOH_0_7071	1s72	0.36
U_0_779	HOH_0_5003	1s72	0.42
U_0_831	HOH_0_8880	1s72	0.72
U_0_840	HOH_0_6533	1s72	0.35
U_0_845	HOH_0_5153	1s72	0.67
U_0_866	HOH_0_8845	1s72	0.57
U_9_82	HOH_9_8400	1s72	0.44
U_A_1006	HOH_A_9120	4rkv	0.49
U_A_106	HOH_A_206	3d0u	0.81
U_A_11	HOH_A_95	2zy6	0.30
U_A_1286	HOH_A_4935	4qcn	NA
U_A_13	HOH_A_128	4e5c	0.86
U_A_13	HOH_A_169	2zy6	0.90
U_A_17	HOH_A_559	2a43	0.80
U_A_17	HOH_A_691	2a43	0.92

U_A_18	HOH_A_260	3d2v	0.29
U_A_2	HOH_A_221	4jah	0.54
U_A_2069	HOH_A_5226	4qcn	NA
U_A_209	HOH_A_1208	1et4	0.34
U_A_209	HOH_A_1713	1et4	0.47
U_A_223	HOH_A_1366	1et4	0.68
U_A_227	HOH_A_1153	1et4	0.98
U_A_2420	HOH_A_4331	4qcn	NA
U_A_2443	HOH_A_4334	4qcn	NA
U_A_25	HOH_A_111	397d	0.99
U_A_3	HOH_A_116	2g91	NA
U_A_3	HOH_A_36	165d	NA
U_A_31	HOH_A_1026	2qwy	0.50
U_A_34	HOH_A_337	3fo4	0.74
U_A_34	HOH_A_422	3la5	0.78
U_A_36	HOH_A_353	3la5	0.58
U_A_36	HOH_A_360	3fo4	0.74
U_A_369	HOH__A3555	4KJ9	NA
U_A_39	HOH_A_254	4p5j	0.92
U_A_39	HOH_A_328	3d2v	0.48
U_A_4	HOH_A_108	4mce	0.85
U_A_4	HOH_A_227	2awe	0.32
U_A_40	HOH_A_259	3la5	1.03
U_A_42	HOH_A_258	4lvz	0.93
U_A_458	HOH_A_4514	4qcn	NA
U_A_47	HOH_A_113	1i9v	NA
U_A_49	HOH_A_298	3la5	0.88
U_A_49	HOH_A_327	3fo4	0.84
U_A_49	HOH_A_711	4lx6	0.37
U_A_5	HOH_A_161	3gx5	0.23
U_A_5	HOH_A_2016	2vuq	0.54
U_A_5	HOH_A_2034	2v7r	0.47
U_A_5	HOH_A_29	255d	NA
U_A_5	HOH_A_40	1fuf	1.02
U_A_51	HOH_A_215	4enb	0.35
U_A_6	HOH_A_166	280d	0.50
U_A_6	HOH_A_20	413d	NA
U_A_6	HOH_B_46	1fuf	0.98
U_A_62	HOH_A_451	3la5	0.83
U_A_64	HOH_B_2105	4un3	0.80
U_A_69	HOH_A_497	4lvz	0.50
U_A_7	HOH_A_27	422d	0.31
U_A_7	HOH_A_5016	1qbp	NA
U_A_7	HOH_A_87	1f27	NA
U_A_80	HOH_A_13	439d	0.80
U_A_80	HOH_A_335	354d	NA

U_A_814	HOH_A_4660	4qcn	NA
U_B_1	HOH_A_13	3k62	0.98
U_B_1	HOH_A_131	3k5z	0.67
U_B_1	HOH_A_19	3k64	0.95
U_B_1	HOH_A_19	3qgc	0.89
U_B_1	HOH_A_21	3k5y	0.62
U_B_1	HOH_A_31	3k5q	0.78
U_B_1	HOH_A_65	3k61	0.65
U_B_1	HOH_A_8	3k5q	0.74
U_B_113	HOH_B_136	2g3s	0.60
U_B_12	HOH_B_103	4ngd	0.76
U_B_12	HOH_B_104	2g91	NA
U_B_12	HOH_B_112	4ngd	0.55
U_B_12	HOH_B_340	1j6s	0.47
U_B_12	HOH_B_352	1jzv	0.56
U_B_12	HOH_B_42	165d	NA
U_B_13	HOH_B_114	4e5c	0.51
U_B_16	HOH_B_128	4e5c	0.89
U_B_162	HOH_B_339	1jid	0.91
U_B_17	HOH_B_70	3sj2	0.70
U_B_19	HOH_B_33	1fuf	0.96
U_B_19	HOH_B_33	422d	0.43
U_B_19	HOH_B_59	3cgp	0.74
U_B_2	HOH_A_652	4j7l	0.32
U_B_2	HOH_B_12	3nmr	0.81
U_B_2	HOH_B_12	3nna	0.82
U_B_2	HOH_B_8	3nnc	0.90
U_B_20	HOH_A_79	1fuf	0.82
U_B_20	HOH_B_108	4kxt	0.81
U_B_2006	HOH_B_2225	4rkv	0.47
U_B_201	HOH_B_347	4o41	0.49
U_B_22	HOH_B_5000	1qbp	NA
U_B_24	HOH_B_593	3nkb	0.68
U_B_28	HOH_B_446	3egz	0.26
U_B_30	HOH_A_258	4m4o	0.79
U_B_30	HOH_B_226	4m4o	0.53
U_B_309	HOH_B_1148	1et4	0.62
U_B_327	HOH_B_1192	1et4	0.85
U_B_33	HOH_B_278	4m4o	0.37
U_B_33	HOH_B_87	3rg5	0.50
U_B_34	HOH_B_141	3rg5	0.57
U_B_34	HOH_B_616	2zzm	0.49
U_B_35	HOH_B_322	3d2v	0.21
U_B_38	HOH_B_271	4n0t	0.69
U_B_4	HOH_B_2006	2xs7	0.98
U_B_4	HOH_B_2008	2xs7	0.94

U_B_4	HOH_B_2029	2xs2	0.92
U_B_41	HOH_B_176	3d2v	0.03
U_B_5	HOH_A_1444	3pey	0.76
U_B_5	HOH_A_306	1g2e	0.86
U_B_5	HOH_B_1088	2atw	0.39
U_B_5	HOH_B_26	1fxl	0.70
U_B_502	HOH_B_703	4jk0	0.69
U_B_6	HOH_B_218	4mce	0.65
U_B_6210	HOH_A_6205	3b31	0.11
U_B_6210	HOH_B_6242	3b31	0.26
U_B_6212	HOH_B_6227	3b31	0.05
U_B_7	HOH_A_1022	3i5y	0.43
U_B_7	HOH_A_637	3qgc	0.72
U_B_7	HOH_B_2024	2xs2	0.82
U_B_72	HOH_A_2055	4aq7	0.52
U_B_8	HOH_B_133	1qf6	0.07
U_B_8	HOH_B_202	4kyy	0.37
U_B_80	HOH_B_30	1feu	0.43
U_B_80	HOH_B_3126	4qcn	NA
U_B_9	HOH_B_1050	2asb	0.78
U_B_9	HOH_B_1120	2atw	0.58
U_B_9	HOH_B_155	3rg5	0.78
U_B_9	HOH_B_157	3rg5	0.59
U_C_1	HOH_C_203	4rge	0.90
U_C_11	HOH_D_137	4qik	0.73
U_C_12	HOH_C_1096	2qwy	0.01
U_C_12	HOH_C_31	2qux	0.65
U_C_14	HOH_E_157	2qux	0.41
U_C_2	HOH_C_214	4jah	0.8
U_C_2	HOH_C_243	4mdx	0.85
U_C_2	HOH_C_70	3bsb	0.32
U_C_205	HOH_C_1610	2g3s	0.49
U_C_3	HOH_C_2010	2xs5	0.93
U_C_3	HOH_C_85	3mdi	0.86
U_C_30	HOH_C_176	280d	0.39
U_C_37	HOH_C_3004	1qbp	NA
U_C_4	HOH_C_105	3mdg	0.64
U_C_409	HOH_A_407	1r3e	0.86
U_C_409	HOH_C_1289	1et4	0.61
U_C_427	HOH_C_1264	1et4	0.82
U_C_5	HOH_A_53	3fht	0.61
U_C_5	HOH_C_36	3q0p	0.75
U_C_5	HOH_C_37	3oin	0.75
U_C_9	HOH_B_537	1zh5	0.89
U_D_1	HOH_A_2293	4d25	0.53
U_D_1	HOH_D_121	3boy	0.50

U_D_10	HOH_D_108	4jah	0.79
U_D_108	HOH_D_1113	2q1o	0.70
U_D_15	HOH_D_274	3boy	0.16
U_D_1522	HOH_D_625	3ftf	0.13
U_D_17	HOH_D_241	4oog	0.35
U_D_2	HOH_D_121	3boy	0.50
U_D_21	HOH_D_217	4oog	0.17
U_D_3	HOH_D_119	4qm6	0.67
U_D_3	HOH_D_2007	2xs5	0.89
U_D_32	HOH_D_318	1jzv	0.74
U_D_4	HOH_D_121	2awe	0.67
U_D_4	HOH_D_171	2awe	0.36
U_D_42	HOH_D_81	280d	0.62
U_D_5	HOH_B_519	3fht	0.67
U_D_5	HOH_D_1030	3snp	0.14
U_D_509	HOH_D_1198	1et4	0.47
U_D_52	HOH_D_3005	1qbp	NA
U_D_527	HOH_D_1193	1et4	0.81
U_D_6	HOH_D_323	2grb	0.68
U_D_8	HOH_D_230	3boy	0.21
U_D_9	HOH_B_130	3bsx	0.11
U_D_9	HOH_D_205	4e48	0.60
U_E_109	HOH_E_1587	1et4	0.60
U_E_1209	HOH_A_2019	2i82	0.84
U_E_127	HOH_E_1200	1et4	0.99
U_E_2	HOH_E_117	4jah	0.49
U_E_210	HOH_E_940	1sds	0.65
U_E_25	HOH_E_104	4j1g	0.84
U_E_2596	HOH_E_2778	4lgt	0.57
U_E_27	HOH_E_2048	4c7o	0.20
U_E_32	HOH_E_533	3hax	0.73
U_E_4	HOH_E_119	4jah	0.61
U_E_4	HOH_E_75	2awe	0.60
U_E_409	HOH_E_60	1r3e	NA
U_E_47	HOH_E_130	3eph	0.41
U_E_6	HOH_E_684	2db3	0.70
U_E_8	HOH_E_28	3nnh	0.58
U_E_80	HOH_E_337	1feu	0.64
U_F_10	HOH_F_115	4jah	0.61
U_F_12	HOH_F_26	2qux	0.59
U_F_210	HOH_F_928	1sds	0.76
U_F_37	HOH_F_106	4m6d	0.47
U_F_4	HOH_G_41	2awe	0.62
U_F_46	HOH_F_88	3rw6	0.45
U_F_5	HOH_F_1296	2db3	0.50
U_F_51	HOH_F_83	3eph	0.84

U_F_6	HOH_A_501	3hax	0.88
U_F_6	HOH_B_2912	2db3	0.81
U_G_405	HOH_G_66	2g3s	0.98
U_G_5	HOH_G_1003	2db3	0.56
U_G_6	HOH_C_2961	2db3	0.71
U_H_38	HOH_H_101	3rw6	0.36
U_H_4	HOH_H_145	2awe	0.27
U_H_413	HOH_H_438	2g3s	0.73
U_H_5	HOH_H_928	2db3	0.79
U_I_505	HOH_I_556	2g3s	0.52
U_I_8	HOH_B_2285	1h38	NA
U_J_1	HOH_J_9	3t5q	0.96
U_J_37	HOH_J_105	4m6d	0.38
U_J_513	HOH_J_522	2g3s	0.85
U_K_3	HOH_K_362	3rer	0.65
U_N_80	HOH_N_511	1dfu	0.78
U_O_8	HOH_O_2006	1h38	NA
U_P_10	HOH_P_149	1b7f	NA
U_P_7	HOH_P_44	1urn	0.53
U_Q_15	HOH_Q_2019	2bgg	0.32
U_Q_16	HOH_Q_2018	2bgg	0.52
U_Q_38	HOH_Q_79	2oiu	0.71
U_Q_7	HOH_Q_121	1urn	0.63
U_Q_8	HOH_Q_141	1urn	0.47
U_R_1	HOH_H_422	1m8v	0.47
U_R_12	HOH_B_839	4wrt	0.52
U_R_17C	HOH_R_9050	2nz4	0.59
U_R_6	HOH_R_108	4krf	0.51
U_S_105	HOH_S_9032	2nz4	0.84
U_S_7	HOH_S_14	3r2d	0.68
U_T_20	HOH_T_1272	1qu2	0.95
U_T_20	HOH_T_1281	1qu2	0.73
U_U_12	HOH_U_218	3ts2	0.77
U_U_7	HOH_U_216	3ts2	0.49
U_W_149	HOH_W_2069	1gtf	0.34
U_X_23	HOH_X_313	2qbz	0.50
U_X_25	HOH_X_427	2gdi	0.78
U_X_28	HOH_X_352	2gdi	0.47
U_X_34	HOH_X_305	4tzx	0.07
U_X_49	HOH_X_243	4tzx	0.62
U_X_49	HOH_X_253	1y26	0.66
U_X_52	HOH_X_206	2gdi	0.46
U_Y_25	HOH_Y_259	2gdi	0.44
			Guanine-Water Stacking Contacts
G_0_1002	HOH_0_9141	1s72	0.44
G_0_1175	HOH_0_5242	1s72	0.03

G_0_1190	HOH_0_7173	1s72	0.28
G_0_1216	HOH_0_8786	1s72	0.59
G_0_1239	HOH_0_9920	1s72	0.27
G_0_1376	HOH_0_4008	1s72	0.56
G_0_1438	HOH_0_4204	1s72	0.55
G_0_1475	HOH_0_4666	1s72	0.46
G_0_1484	HOH_0_8618	1s72	0.31
G_0_150	HOH_0_5434	1s72	0.47
G_0_1614	HOH_0_4128	1s72	0.28
G_0_1703	HOH_0_5264	1s72	0.23
G_0_1723	HOH_0_6887	1s72	0.80
G_0_175	HOH_0_4038	1s72	0.43
G_0_175	HOH_0_9248	1s72	0.65
G_0_1752	HOH_0_5575	1s72	0.66
G_0_1752	HOH_0_7037	1s72	0.45
G_0_1837	HOH_0_5867	1s72	0.50
G_0_1868	HOH_0_4471	1s72	0.40
G_0_1873	HOH_0_4707	1s72	0.01
G_0_1979	HOH_0_8790	1s72	0.42
G_0_2013	HOH_0_4913	1s72	0.48
G_0_2046	HOH_0_9715	1s72	0.38
G_0_2072	HOH_0_9849	1s72	0.27
G_0_2075	HOH_0_9852	1s72	0.31
G_0_2136	HOH_0_9877	1s72	0.69
G_0_219	HOH_3_8566	1s72	0.81
G_0_2270	HOH_0_8789	1s72	0.62
G_0_2344	HOH_0_4419	1s72	0.92
G_0_2421	HOH_0_4095	1s72	0.60
G_0_2428	HOH_0_3288	1s72	0.29
G_0_2442	HOH_0_8703	1s72	0.85
G_0_2459	HOH_0_4312	1s72	0.84
G_0_2516	HOH_0_4936	1s72	0.07
G_0_2525	HOH_0_3548	1s72	0.44
G_0_2570	HOH_0_4335	1s72	0.04
G_0_2611	HOH_0_8757	1s72	0.68
G_0_2611	HOH_0_9265	1s72	0.62
G_0_2617	HOH_0_5201	1s72	0.35
G_0_264	HOH_0_6748	1s72	0.11
G_0_2643	HOH_0_5292	1s72	0.49
G_0_2643	HOH_0_6544	1s72	0.33
G_0_2882	HOH_0_6443	1s72	0.58
G_0_301	HOH_0_5339	1s72	0.48
G_0_304	HOH_0_9871	1s72	0.16
G_0_381	HOH_0_5186	1s72	0.18
G_0_553	HOH_0_3580	1s72	0.21
G_0_588	HOH_0_5317	1s72	0.02

G_0_702	HOH_0_9001	1s72	0.55
G_0_775	HOH_0_3941	1s72	0.55
G_0_869	HOH_0_3187	1s72	0.64
G_0_901	HOH_0_8636	1s72	0.69
G_A_1	HOH_A_390	1qcu	0.06
G_A_1	HOH_A_56	1fuf	0.62
G_A_10	HOH_A_378	1q96	0.73
G_A_108	HOH_C_799	3p4b	0.70
G_A_11	HOH_A_105	3sj2	0.76
G_A_1271	HOH__A3417	4KJ9	NA
G_A_13	HOH_A_131	3gx5	0.38
G_A_13	HOH_A_159	3td1	0.27
G_A_13	HOH_A_186	1f27	NA
G_A_13	HOH_A_201	1d4r	0.31
G_A_1312	HOH_W_4002	4qcn	NA
G_A_14	HOH_A_334	2fqn	0.69
G_A_1423	HOH_A_4018	4qcn	NA
G_A_15	HOH_B_32	3bnl	0.14
G_A_1502	HOH_A_4090	4qcn	NA
G_A_17	HOH_A_38	1t0e	0.65
G_A_1728	HOH_A_5250	4qcn	NA
G_A_19	HOH_A_107	3td0	0.79
G_A_2	HOH_A_114	1l2x	0.71
G_A_2	HOH_A_116	1p79	0.50
G_A_2	HOH_A_196	3cjz	0.65
G_A_2	HOH_A_408	1q96	0.38
G_A_2045	HOH_A_5198	4qcn	NA
G_A_21	HOH_A_141	397d	0.79
G_A_2262	HOH_A_5031	4qcn	NA
G_A_2269	HOH__A3510	4KJ9	NA
G_A_24	HOH_A_235	3d0u	0.33
G_A_24	HOH_A_427	1nuv	0.64
G_A_26	HOH_A_97	2zy6	0.56
G_A_28	HOH_A_272	3e5c	0.07
G_A_28	HOH_A_94	2zy6	0.33
G_A_2841	HOH_A_4688	4qcn	NA
G_A_29	HOH_A_113	3ivn	0.75
G_A_295	HOH__A3229	4KJ9	NA
G_A_3	HOH_A_107	3r1c	0.93
G_A_3	HOH_A_182	3td0	0.76
G_A_3	HOH_A_210	1j9h	NA
G_A_31	HOH_A_256	3e5c	0.15
G_A_31	HOH_A_259	3e5c	0.17
G_A_32	HOH_A_281	3la5	0.80
G_A_33	HOH_A_2066	4un3	0.86
G_A_36	HOH_A_2179	3zp8	0.49

G_A_36	HOH_A_2180	3zp8	0.91
G_A_37	HOH_A_297	4lvz	0.75
G_A_38	HOH_A_314	3la5	0.69
G_A_38	HOH_A_458	3fo4	0.44
G_A_4	HOH_A_102	3sj2	0.90
G_A_4	HOH_A_2026	2v6w	0.70
G_A_4	HOH_A_41	3gvn	0.90
G_A_4	HOH_A_498	4lvz	0.78
G_A_44	HOH_A_126	3la5	0.85
G_A_46	HOH_A_93	1csl	0.73
G_A_47	HOH_A_221	4oji	0.29
G_A_5	HOH_A_1153	2qwy	0.10
G_A_5	HOH_A_19	3cgp	0.98
G_A_51	HOH_A_9	3p59	0.83
G_A_54	HOH_A_321	4lvz	0.81
G_A_584	HOH_A_4759	4qcn	NA
G_A_6	HOH_A_486	3r1c	0.66
G_A_6	HOH_A_506	2a43	0.94
G_A_6	HOH_A_51	420d	NA
G_A_6	HOH_A_85	3r1d	0.67
G_A_60	HOH_A_145	3d2v	0.70
G_A_62	HOH_A_483	3fo4	0.64
G_A_7	HOH_A_221	1xpe	NA
G_A_7	HOH_A_241	1nlc	0.09
G_A_72	HOH_A_358	354d	NA
G_A_72	HOH_A_402	3fo4	0.78
G_A_72	HOH_A_701	4lx6	0.67
G_A_72	HOH_B_339	354d	NA
G_A_721	HOH_A_4044	4QCN	NA
G_A_75	HOH_A_329	354d	NA
G_A_76	HOH_A_339	4wfl	0.41
G_A_77	HOH_A_213	3d0u	0.24
G_A_786	HOH_A_5320	4qcn	NA
G_A_8	HOH_A_131	3sj2	0.61
G_A_8	HOH_A_26	255d	NA
G_A_855	HOH_A_4044	4qcn	NA
G_A_9	HOH_A_26	3r1d	0.78
G_A_9	HOH_A_301	4qlm	0.19
G_B_1	HOH_B_34	2dr8	0.53
G_B_10	HOH_B_2001	2bte	0.77
G_B_10	HOH_B_802	1qrs	0.58
G_B_102	HOH_B_313	2ho7	0.26
G_B_11	HOH_B_1207	2asb	0.40
G_B_11	HOH_B_233	2hw8	0.58
G_B_12	HOH_B_113	1d4r	0.91
G_B_12	HOH_B_118	1d4r	0.56

G_B_12	HOH_B_205	1j9h	NA
G_B_13	HOH_B_102	1dqh	0.45
G_B_135	HOH_B_425	1jid	0.24
G_B_138	HOH_B_376	1jid	0.60
G_B_14	HOH_B_175	3sj2	0.58
G_B_15	HOH_A_31	3bnl	0.24
G_B_1530	HOH_A_614	3r9w	0.20
G_B_16	HOH_B_50	479d	0.40
G_B_166	HOH_B_440	1lng	NA
G_B_167	HOH_B_424	1lng	NA
G_B_17	HOH_B_111	1dqh	0.76
G_B_17	HOH_B_42	3ibk	0.34
G_B_17	HOH_D_7327	1qbp	NA
G_B_177	HOH_B_2	1l9a	NA
G_B_2	HOH_A_70	3q0r	0.78
G_B_2	HOH_B_101	3qgc	0.79
G_B_2	HOH_B_133	3k5y	0.46
G_B_2	HOH_B_179	3k64	0.80
G_B_2	HOH_B_208	3k62	0.74
G_B_2	HOH_B_2104	2vpl	0.56
G_B_2	HOH_B_213	3k5z	0.35
G_B_2	HOH_B_274	3k5q	0.46
G_B_2	HOH_B_275	3k61	0.37
G_B_20	HOH_B_58	2r22	0.78
G_B_20	HOH_B_62	2r20	0.76
G_B_202	HOH_B_358	4o41	0.36
G_B_21	HOH_B_57	353d	NA
G_B_21	HOH_B_71	1mzp	0.31
G_B_2125	HOH_B_2314	3umy	0.64
G_B_24	HOH_B_2079	2y8w	0.67
G_B_24	HOH_B_260	3d2v	0.31
G_B_24	HOH_B_63	1t0d	0.51
G_B_27	HOH_A_217	4e48	0.56
G_B_28	HOH_A_317	4m4o	0.59
G_B_4	HOH_B_116	4kq0	0.28
G_B_412	HOH_A_575	1k8w	0.88
G_B_42	HOH_B_303	2fqn	0.90
G_B_5	HOH_A_158	3q0r	0.55
G_B_5	HOH_B_102	3v74	0.97
G_B_5	HOH_B_2013	2val	0.35
G_B_503	HOH_B_207	1j1u	0.77
G_B_513	HOH_B_719	4jk0	0.31
G_B_54	HOH_B_242	4m4o	0.57
G_B_55	HOH_A_1082	4n0t	0.74
G_B_55	HOH_B_220	4n0t	0.93
G_B_599	HOH_A_561	3ol8	0.65

G_B_6	HOH_B_164	3r1c	0.70
G_B_6	HOH_B_21	3r1d	0.99
G_B_60	HOH_B_109	3d2v	0.80
G_B_63	HOH_B_564	3nkb	0.80
G_B_67	HOH_B_3103	4qcn	NA
G_B_72	HOH_B_3117	4qcn	NA
G_B_72	HOH_C_351	1feu	0.78
G_B_75	HOH_B_196	1feu	0.68
G_B_8	HOH_B_39	3sj2	0.87
G_B_9	HOH_B_1047	466d	0.58
G_B_9	HOH_B_119	4u35	0.74
G_B_9	HOH_B_66	3r1d	0.54
G_B_901	HOH_B_1176	2zuf	0.81
G_B_96	HOH_B_391	4n0t	0.31
G_B_98	HOH_A_390	354d	NA
G_C_1	HOH_A_440	3ova	0.89
G_C_1	HOH_C_35	3nj7	0.67
G_C_10	HOH_A_188	1jbr	0.41
G_C_10	HOH_C_379	1q96	0.71
G_C_10	HOH_C_382	1q96	0.72
G_C_12	HOH_C_159	1d4r	0.43
G_C_12	HOH_C_49	2ez6	0.64
G_C_13	HOH_C_143	1d4r	0.55
G_C_14	HOH_C_243	1t0e	0.82
G_C_14	HOH_E_102	1m8w	0.52
G_C_16	HOH_C_117	3qrp	0.77
G_C_16	HOH_E_181	2qux	0.57
G_C_21	HOH_C_156	1j9h	NA
G_C_22	HOH_C_441	1ooa	NA
G_C_25	HOH_C_2007	4c8z	0.48
G_C_25	HOH_C_2015	4c8y	0.74
G_C_26	HOH_A_2093	4c8y	0.91
G_C_3	HOH_A_3179	1wpu	0.46
G_C_3	HOH_C_328	1wpu	0.58
G_C_412	HOH_A_395	1r3e	0.68
G_C_412	HOH_C_2	1r3e	0.96
G_C_426	HOH_C_1188	1et4	0.48
G_C_45	HOH_C_2046	1efw	0.42
G_C_5	HOH_A_3012	1wmq	0.79
G_C_5	HOH_C_2018	2xsl	0.89
G_C_693	HOH_C_786	3ol9	0.03
G_C_7	HOH_D_86	1t0d	0.73
G_C_9	HOH_C_94	3r1d	0.84
G_C_916	HOH_A_496	3kmq	0.68
G_C_98	HOH_B_10	1feu	0.72
G_D_1	HOH_D_204	4n48	0.60

G_D_1	HOH_D_43	3nj7	0.76
G_D_10	HOH_D_427	1jbs	0.82
G_D_110	HOH_D_120	2pn4	0.83
G_D_14	HOH_D_207	4oog	0.40
G_D_19	HOH_D_44	3boy	1.01
G_D_1934	HOH_B_2299	1il2	0.66
G_D_2	HOH_D_111	3q0o	0.24
G_D_2	HOH_D_2003	4afy	0.75
G_D_2	HOH_D_317	2grb	0.73
G_D_20	HOH_D_113	4qik	0.37
G_D_201	HOH_D_409	1yls	0.09
G_D_208	HOH_A_916	1sds	0.86
G_D_22	HOH_D_231	4oog	0.29
G_D_24	HOH_D_50	1t0d	0.49
G_D_3	HOH_B_3145	1wpu	0.77
G_D_3	HOH_D_181	1wpu	0.07
G_D_3	HOH_D_203	3r1c	0.87
G_D_30	HOH_D_142	1j9h	NA
G_D_36	HOH_B_2055	2vpl	0.54
G_D_4	HOH_C_53	3glp	0.70
G_D_408	HOH_D_120	1r3e	0.46
G_D_47	HOH_B_4009	1qbp	NA
G_D_5	HOH_B_3005	1wpu	0.98
G_D_5	HOH_D_42	3boy	0.93
G_D_501	HOH_D_1472	1et4	0.47
G_D_8	HOH_D_1059	435d	0.78
G_D_9	HOH_D_126	3r1d	0.53
G_E_1	HOH_A_1463	4g0a	0.86
G_E_1	HOH_B_1717	1tfw	0.68
G_E_1	HOH_E_82	3nj7	0.52
G_E_1	HOH_E_83	2hvy	0.71
G_E_12	HOH_E_78	2hvy	0.51
G_E_19	HOH_E_164	1nuv	0.78
G_E_208	HOH_B_923	1sds	0.98
G_E_2588	HOH_E_2731	4lgt	1.04
G_E_3	HOH_E_445	3r1c	0.64
G_E_302	HOH_F_361	2g3s	0.54
G_E_4	HOH_E_102	1m8w	0.52
G_E_4	HOH_E_118	4kq0	0.33
G_E_72	HOH_F_341	1feu	0.86
G_E_9	HOH_A_338	3hjw	0.81
G_E_9	HOH_E_212	3r1d	0.57
G_F_14	HOH_F_63	3rw6	0.47
G_F_18	HOH_F_109	3rw6	0.57
G_F_208	HOH_C_883	1sds	0.91
G_F_211	HOH_C_866	1sds	0.90

G_F_24	HOH_F_40	1zx7	0.75
G_F_32	HOH_F_61	2ozb	0.41
G_F_35	HOH_F_123	3rw6	0.16
G_F_47	HOH_F_69	3rw6	0.35
G_F_599	HOH_E_524	3ol8	0.69
G_F_9	HOH_B_140	1m8w	0.51
G_G_2	HOH_A_529	1tfw	0.65
G_G_24	HOH_G_237	1nuv	0.60
G_G_4	HOH_G_2001	4bwm	0.80
G_G_6	HOH_G_450	3r1c	0.90
G_H_1	HOH_H_1847	2o5i	1.0
G_H_14	HOH_H_72	3rw6	0.33
G_H_1510	HOH_H_2071	2i82	0.75
G_H_18	HOH_H_68	3rw6	0.49
G_H_9	HOH_B_2015	1yvp	0.71
G_H_9	HOH_P_181	3ok4	0.81
G_I_3	HOH_I_453	3r1c	0.70
G_I_6	HOH_I_427	3r1c	0.89
G_J_3	HOH_J_154	3r1c	0.93
G_J_599	HOH_I_521	3ol8	0.81
G_J_6	HOH_J_113	3r1c	0.82
G_J_7	HOH_J_104	4gha	0.66
G_K_3	HOH_K_431	3r1c	0.93
G_K_6	HOH_K_433	3r1c	0.84
G_K_693	HOH_K_1234	3ol9	0.11
G_L_3	HOH_L_176	3r1c	0.83
G_L_6	HOH_L_155	3r1c	0.82
G_M_3	HOH_M_139	3r1c	0.92
G_M_6	HOH_M_390	3r1c	0.66
G_M_98	HOH_M_537	1dfu	0.55
G_M_98	HOH_N_508	1dfu	0.64
G_N_599	HOH_M_515	3ol8	0.77
G_N_72	HOH_M_507	1dfu	0.27
G_N_72	HOH_M_527	1dfu	0.73
G_N_75	HOH_P_100	1dfu	0.87
G_O_1	HOH_O_2002	1h38	NA
G_O_16	HOH_O_26	2qux	0.75
G_O_6	HOH_O_463	3r1c	0.52
G_O_693	HOH_O_816	3ol9	0.13
G_O_7	HOH_O_27	2qux	0.44
G_Q_1	HOH_Q_89	2oiu	0.41
G_Q_3	HOH_Q_9	3r1c	0.80
G_Q_6	HOH_Q_361	3r1c	0.69
G_R_2	HOH_R_14	3r2c	0.92
G_R_3	HOH_A_2324	1qln	0.51
G_R_6	HOH_R_468	3r1c	0.50

G_S_2	HOH_S_151	3r2c	0.93
G_T_6	HOH_T_335	3r1c	0.65
G_U_3	HOH_U_336	3r1c	0.66
G_U_6	HOH_U_69	3r1c	0.80
G_V_21	HOH_V_311	3ts2	0.21
G_V_58	HOH_V_158	3q3z	0.05
G_W_106	HOH_W_2005	1gtf	0.48
G_W_126	HOH_W_2037	1gtf	0.63
G_W_151	HOH_W_2072	1gtf	0.65
G_W_6	HOH_W_473	3r1c	0.81
G_X_11	HOH_X_522	3czw	0.12
G_X_164	HOH_X_382	2qbz	0.63
G_X_168	HOH_X_368	2qbz	0.19
G_X_29	HOH_X_223	2gdi	0.20
G_X_72	HOH_X_201	2gdi	0.47
G_X_72	HOH_X_365	2gdi	0.79
G_X_73	HOH_X_315	2qbz	0.62
G_X_78	HOH_X_384	2gdi	0.76
G_X_8	HOH_X_537	3czw	0.37
G_Y_29	HOH_Y_347	2gdi	0.28
G_b_6	HOH_b_367	3r1c	0.53
G_d_3	HOH_d_355	3r1c	0.75
G_e_3	HOH_e_411	3r1c	0.45
G_e_6	HOH_e_479	3r1c	0.69
G_g_3	HOH_g_412	3r1c	0.64
G_j_6	HOH_j_386	3r1c	0.60
Cytosine-Water Stacking Contacts			
C_0_1043	HOH_0_9699	1s72	0.44
C_0_1083	HOH_0_8565	1s72	0.88
C_0_1184	HOH_0_5744	1s72	0.39
C_0_1353	HOH_0_3118	1s72	0.51
C_0_1365	HOH_0_9967	1s72	0.51
C_0_1602	HOH_0_4496	1s72	0.52
C_0_1708	HOH_0_4214	1s72	0.55
C_0_1708	HOH_P_162	1s72	0.52
C_0_1753	HOH_0_3604	1s72	0.15
C_0_1772	HOH_0_4776	1s72	0.53
C_0_1864	HOH_0_4162	1s72	0.72
C_0_1872	HOH_0_6799	1s72	0.48
C_0_2360	HOH_0_6163	1s72	0.16
C_0_2427	HOH_0_8777	1s72	0.40
C_0_2450	HOH_0_4676	1s72	0.34
C_0_2508	HOH_0_6222	1s72	0.41
C_0_2526	HOH_0_6452	1s72	0.31
C_0_2526	HOH_0_7097	1s72	0.30
C_0_2737	HOH_0_5643	1s72	0.25

C_0_282	HOH_0_9864	1s72	0.75
C_0_2833	HOH_0_6615	1s72	0.15
C_0_2839	HOH_0_5231	1s72	0.53
C_0_284	HOH_0_9126	1s72	0.39
C_0_2895	HOH_0_9077	1s72	0.62
C_0_31	HOH_0_5634	1s72	0.52
C_0_31	HOH_T_5160	1s72	0.42
C_0_376	HOH_0_9815	1s72	0.14
C_0_438	HOH_0_9934	1s72	0.53
C_0_687	HOH_0_6695	1s72	0.59
C_0_770	HOH_0_3530	1s72	0.46
C_0_789	HOH_0_4509	1s72	0.58
C_0_899	HOH_0_4310	1s72	0.54
C_0_905	HOH_0_4683	1s72	0.57
C_9_122	HOH_9_8423	1s72	0.40
C_A_10	HOH_A_103	4e6b	0.76
C_A_101	HOH_A_508	402d	0.15
C_A_11	HOH_A_228	4e48	0.35
C_A_12	HOH_A_33	1t0d	0.69
C_A_12	HOH_A_53	1t0e	0.57
C_A_15	HOH_A_57	3bnt	0.30
C_A_15	HOH_B_54	3mei	0.61
C_A_1677	HOH_A_4923	4qcn	NA
C_A_1710	HOH_A_4489	4qcn	NA
C_A_2	HOH_A_132	3glp	0.66
C_A_2	HOH_A_44	3cgr	0.78
C_A_20	HOH_A_118	1nlc	0.88
C_A_20	HOH_A_242	4oji	0.52
C_A_21	HOH_A_190	3td1	0.45
C_A_23	HOH_D_223	3bnq	0.68
C_A_2443	HOH__A3497	4KJ9	NA
C_A_28	HOH_A_382	3fo4	0.80
C_A_34	HOH_A_119	3gx5	0.58
C_A_39	HOH_A_427	3fo4	0.41
C_A_4	HOH_A_53	1kd5	0.90
C_A_44	HOH_A_151	3ivn	0.78
C_A_46	HOH_A_346	4lvz	0.59
C_A_47	HOH_A_347	3la5	0.42
C_A_5	HOH_A_117	3glp	0.91
C_A_5	HOH_A_159	1j9h	NA
C_A_5	HOH_A_206	4e48	0.49
C_A_5	HOH_A_218	4oji	0.42
C_A_53	HOH_A_12	3la5	0.93
C_A_54	HOH_A_377	3la5	0.36
C_A_54	HOH_A_432	3la5	0.89
C_A_54	HOH_A_466	3fo4	0.57

C_A_54	HOH_A_712	4lx6	0.72
C_A_6	HOH_A_126	4e5c	0.93
C_A_67	HOH_A_2141	4un3	0.48
C_A_67	HOH_A_2213	4un5	0.65
C_A_7	HOH_A_317	3bnq	0.38
C_A_7(+)	HOH_A_530	2a43	1.0
C_A_7	HOH_A_59	2ao5	0.45
C_A_7	HOH_A_65	3syw	0.67
C_A_72	HOH_A_86	1u0b	0.74
C_A_74	HOH_A_292	4p5j	0.53
C_A_79	HOH_A_307	3dir	0.24
C_A_8(+)	HOH_A_71	1l2x	0.98
C_A_99	HOH_A_1871	4KJA	NA
C_B_11	HOH_A_1181	4w5o	0.82
C_B_11	HOH_B_2036	2y8w	0.57
C_B_112	HOH_B_516	402d	0.09
C_B_13	HOH_B_258	1nlc	0.55
C_B_14	HOH_B_162	1j9h	NA
C_B_15	HOH_B_47	2r22	0.73
C_B_15	HOH_B_49	2r20	0.91
C_B_16	HOH_B_104	1dqh	0.69
C_B_17	HOH_B_60	353d	NA
C_B_170	HOH_B_12	1l9a	NA
C_B_19	HOH_A_217	1lnt	0.90
C_B_201	HOH_A_396	4knq	0.41
C_B_212	HOH_B_416	4j5v	0.01
C_B_215	HOH_B_411	4j5v	0.03
C_B_218	HOH_B_403	1lng	NA
C_B_218	HOH_B_405	4j5v	0.54
C_B_22	HOH_B_64	3cgs	0.76
C_B_25	HOH_B_211	4e48	0.57
C_B_25	HOH_B_624	3nkb	0.72
C_B_37	HOH_B_203	4e48	0.58
C_B_4	HOH_B_207	3bnq	0.51
C_B_4	HOH_B_244	4k31	0.81
C_B_4	HOH_B_62	1kd5	0.63
C_B_41(+)	HOH_B_503	3nkb	0.86
C_B_415	HOH_A_577	1k8w	0.82
C_B_42	HOH_A_422	3egz	0.56
C_B_44	HOH_B_133	3ivn	0.64
C_B_45	HOH_B_319	1m5o	0.77
C_B_45	HOH_B_411	3egz	0.52
C_B_5	HOH_B_206	4msr	0.85
C_B_598	HOH_A_648	4k4y	0.30
C_B_67	HOH_A_1408	4oo8	0.45
C_B_69	HOH_B_44	3gvn	0.84

C_B_7	HOH_A_312	3bnq	0.70
C_B_7	HOH_B_59	3syw	0.64
C_B_8	HOH_R_299	3ok4	0.85
C_B_934	HOH_B_1175	2zuf	0.48
C_C_12	HOH_C_24	1zx7	0.52
C_C_17	HOH_C_39	1m8y	0.75
C_C_2	HOH_C_106	4qm6	0.95
C_C_23	HOH_B_227	3bnq	0.53
C_C_23	HOH_C_121	1j9h	NA
C_C_3	HOH_C_12	2ao5	NA
C_C_4	HOH_C_267	4k31	0.81
C_C_8	HOH_C_167	1yz9	0.73
C_C_9	HOH_C_262	1t0e	0.33
C_D_11	HOH_D_118	3og8	0.50
C_D_13	HOH_A_712	2i91	0.38
C_D_1535	HOH_D_96	3iev	0.82
C_D_2	HOH_B_535	4o8j	0.97
C_D_2	HOH_D_104	4qm6	1.03
C_D_2	HOH_D_14	3glp	0.97
C_D_20	HOH_D_98	3vjr	0.87
C_D_32	HOH_D_112	1j9h	NA
C_D_34	HOH_D_325	1jzv	0.55
C_D_4	HOH_D_2007	4d25	0.59
C_D_5	HOH_C_325	3bnq	0.60
C_D_5	HOH_D_12	3glp	1.06
C_D_5	HOH_D_13	3q0o	0.62
C_D_5	HOH_D_202	4e48	0.46
C_E_11	HOH_E_2013	4c7o	0.47
C_E_303	HOH_E_319	2g3s	0.72
C_E_55(+)	HOH_F_13	3p59	0.55
C_E_6	HOH_A_119	1m8w	0.72
C_F_10	HOH_F_333	1yvp	0.91
C_F_311	HOH_F_356	2g3s	0.59
C_F_35	HOH_F_91	3eph	0.05
C_F_6	HOH_B_256	1m8w	0.55
C_G_12	HOH_G_23	1zx7	0.58
C_G_408	HOH_J_542	2g3s	0.83
C_G_8	HOH_A_2008	1yvp	0.68
C_G_8	HOH_A_2130	1yvp	0.61
C_G_9	HOH_G_736	1tfw	0.34
C_H_427	HOH_G_636	1duq	NA
C_H_7	HOH_B_2140	1yvp	0.73
C_H_8	HOH_B_2021	1yvp	0.73
C_H_8	HOH_B_2054	1yvp	0.92
C_J_61	HOH_C_519	1tfw	0.86
C_R_1	HOH_F_413	4u8t	0.55

C_U_20	HOH_U_210	3ts2	0.20
C_X_12	HOH_X_104	3wbm	0.89
C_X_23	HOH_X_225	2gdi	0.46
C_X_24	HOH_X_479	2gdi	0.22
C_X_502	HOH_C_715	4pei	0.71
C_X_53	HOH_X_235	1y26	0.52
C_Y_23	HOH_Y_263	2gdi	0.53

Table S2. Screening of the environment near the O^W that is stacking to a nucleobase, in order to classify it as a possible lp-π contact (at least 2 acceptor atoms within H-bonding distance from O^W). **Instances corresponding to Figure S4a[288 instances]**

PDB ID:	Base	Water	Surrounding acceptor atoms near Water
4u34	A_A_2	HOH_A_134	OP2-G_A_3,N7-G_A_3
2r20	A_A_9	HOH_A_80	OP2-A_A_10,N7-A_A_10
4u35	A_A_2	HOH_A_137	OP2-G_A_3,N7-G_A_3
3dd2	A_B_8	HOH_B_1009	OP2-A_B_9,N7-A_B_9
2r22	A_A_9	HOH_A_71	OP2-A_A_10,N7-A_A_10
2r20	A_B_22	HOH_B_106	OP2-A_B_23,N7-A_B_23
3p59	A_D_109	HOH_D_16	N7-G_C_60,O6-G_C_60,O6-G_D_107,N3-C_D_108
2fmt	A_C_76	HOH_C_520	O2-C_C_75,N3-C_C_75
2gdi	A_X_75	HOH_X_373	OP2-G_X_76,N7-G_X_76
1l2x	A_A_24	HOH_A_189	O2'-C_A_8,N7-A_A_25
1b23	A_R_65	HOH_R_992	OP2-A_R_66,N7-A_R_66
3egz	A_B_56	HOH_B_386	O2'-A_B_55,N3-A_B_55
4ig8	A_C_12	HOH_C_102	OP2-A_C_13,N7-A_C_13
1t0e	A_C_11	HOH_C_218	OP2-G_C_12,N7-G_C_12
3rg5	A_B_38	HOH_B_82	O2-U_B_33,OP2-A_B_37,N7-A_B_37
4m30	A_D_2	HOH_D_210	OP2-A_D_3,N7-A_D_3
1g2e	A_B_7	HOH_A_262	OP2-U_B_8,O-LEU_A_80
3zp8	A_A_29	HOH_A_2140	O3'-A_A_27,OP1-A_A_28
2a43	A_A_24	HOH_A_551	O2'-C_A_7,N7-A_A_25
3td0	A_A_17	HOH_A_158	OP1-G_A_19,N7-G_A_19
4lvz	A_A_55	HOH_A_399	O6-G_A_24,O2'-G_A_54,N3-G_A_54
3td0	A_B_40	HOH_B_165	OP1-G_B_42,N7-G_B_42
2hw8	A_B_27	HOH_B_222	O3'-G_B_23,OP1-C_B_24
3eph	A_E_29	HOH_A_447	OP2-G_E_30,N7-G_E_30

2qbz	A_X_61	HOH_X_431	O2-C_X_78,N3-C_X_78,N7-A_X_79
3d2v	A_B_23	HOH_B_194	OP2-G_B_24,N7-G_B_24
1k8w	A_B_404	HOH_B_623	OP2-A_B_405,N7-A_B_405
3ok4	A_V_4	HOH_N_150	P-A_N_7,OP2-A_N_7,OP2-U_V_5,OP2-C_4_3
3ok4	A_P_7	HOH_P_181	OP2-G_H_10,N7-G_H_10,OP2-C_P_8,OP2-U_X_6
2vpl	A_B_38	HOH_B_2064	O3'-G_B_34,P-A_B_35,OP1-A_B_35
1q2r	A_F_37	HOH_F_45	O2-C_F_32,O2-C_F_39
1et4	A_C_416	HOH_C_1605	O2-U_C_415,OP2-A_C_417,N7-A_C_417
3eph	A_F_58	HOH_F_88	O5'-U_F_59,OP2-C_F_60
4n0t	A_B_45	HOH_B_215	OG1-THR_A_202,N7-A_B_47
4n0t	A_B_93	HOH_B_264	OP2-A_B_94,N7-A_B_94
1et4	A_E_116	HOH_E_1284	O2-U_E_115,OP2-A_E_117,N7-A_E_117
1s72	A_0_939	HOH_0_3152	O2'-U_0_1028,O2-U_0_1028
1s72	A_0_1132	HOH_0_3419	O2'-G_0_1131,N3-G_0_1131,O3'-G_0_2522,OP1-U_0_2523
1s72	A_0_2455	HOH_0_3599	N1-A_0_2437,O2-C_0_2454,N3-C_0_2454
1s72	A_0_2062	HOH_0_4160	O3'-C_0_2651,O2'-C_0_2651
1s72	A_0_37	HOH_0_4186	OP2-G_0_38,N7-G_0_38
1s72	A_0_2488	HOH_0_4290	N3-C_0_2487,O2-U_0_2535
1s72	A_0_565	HOH_0_4500	N1-A_0_593,N3-A_0_593,O4'-G_0_1265
1s72	A_0_907	HOH_0_5051	OP2-A_0_908,N7-A_0_908
1s72	A_0_1572	HOH_0_5162	O4'-G_0_1496,O2'-G_0_1496,N1-A_0_1626
1s72	A_0_1200	HOH_0_5253	O2-U_0_1198,O5'-C_0_1201,O4'-C_0_1201
1s72	A_0_1123	HOH_0_5521	OP2-U_0_1122,O4'-C_0_1238,O2'-C_0_1238
1s72	A_0_923	HOH_0_5533	O4'-G_0_2481,O4-U_0_2484
1s72	A_0_1712	HOH_0_5765	N1-A_0_1711,O2-C_0_1816
1s72	A_0_2238	HOH_0_6164	P-C_0_2239,OP2-C_0_2239,O5'-C_0_2239
1s72	A_0_331	HOH_0_6338	O3'-U_0_346,O2'-U_0_346
1s72	A_0_1487	HOH_0_7109	O2'-A_0_1413,N3-A_0_1413,O4'-A_0_1414
1s72	A_0_2840	HOH_0_7140	O2'-C_0_2839,OP2-A_0_2841,N7-A_0_2841,O6-G_0_2842
1s72	A_0_189	HOH_0_8616	N3-C_0_188,O4'-G_0_206,O2'-G_0_206
1s72	A_0_1840	HOH_0_8621	P-U_0_832,OP1-U_0_832,OP2-U_0_832
1s72	A_0_2101	HOH_0_8836	OP1-A_0_2479,OP2-G_0_2480,OG-SER_C_63
1s72	A_0_1502	HOH_0_9437	O3'-G_0_1445,O2'-G_0_1445
1s72	A_0_1733	HOH_0_9660	N1-A_0_1732,O3'-A_0_2089,O2'-A_0_2089
1s72	A_0_2485	HOH_0_9765	O2'-C_0_2105,O2-C_0_2105,O2-U_0_2484
1s72	A_0_395	HOH_0_9812	O2'-A_0_216,O4'-G_0_394
1s72	A_0_721	HOH_0_9863	N1-A_0_708,O-VAL_O_113
1s72	A_9_52	HOH_9_8392	O4'-C_9_31,O2'-C_9_31
1s72	A_9_3	HOH_9_8477	O4'-U_9_2,O3'-U_9_2
1s72	A_0_2038	HOH_B_8622	OP2-A_0_2039,N7-A_0_2039

1s72	A_0_2896	HOH_X_4132	O2'-A_0_2727,N3-A_0_2727
3b31	U_B_6210	HOH_A_6205	O2'-A_A_6184,N3-A_A_6184
1feu	U_B_80	HOH_B_30	OP2-G_B_81,N7-G_B_81
4jah	U_E_2	HOH_E_117	OP2-G_E_3,N7-G_E_3
4e48	U_D_9	HOH_D_205	OP2-G_D_10,N7-G_D_10
3fo4	U_A_49	HOH_A_327	N3-A_A_21,O2-U_A_47
4jah	U_F_10	HOH_F_115	OP2-G_F_11,N7-G_F_11
3ftf	U_D_1522	HOH_D_625	OP2-G_D_1523,N7-G_D_1523
1qf6	U_B_8	HOH_B_133	N7-G_B_15,O6-G_B_15
2q1o	U_D_108	HOH_D_1113	OP2-G_D_109,N7-G_D_109
3la5	U_A_49	HOH_A_298	N3-A_A_21,O2-C_A_47
2v7r	U_A_5	HOH_A_2034	OP2-G_A_6,N7-G_A_6
4lvz	U_A_42	HOH_A_258	O2'-G_A_41,N3-G_A_41
4lx6	U_A_49	HOH_A_711	N3-A_A_21,O2-C_A_47
2vuq	U_A_5	HOH_A_2016	OP2-G_A_6,N7-G_A_6
3hax	U_F_6	HOH_A_501	OG1-THR_A_83,OP2-G_F_8,O5'-G_F_8,OP1-A_F_9
2g91	U_B_12	HOH_B_104	OP2-G_B_13,N7-G_B_13
1r3e	U_E_409	HOH_E_60	O3'-C_E_411,O5'-G_E_412
3k5q	U_B_1	HOH_A_8	OH-TYR_A_501,OP2-G_B_2
2qbz	U_X_23	HOH_X_313	OP2-U_X_24,OP1-A_X_25,O4-U_X_161
4tzx	U_X_49	HOH_X_243	N3-A_X_21,O2-U_X_47
1r3e	U_C_409	HOH_A_407	OP2-C_C_411,OP1-G_C_412,OG1-THR_A_46
1et4	U_A_209	HOH_A_1208	O5'-G_A_210,O4'-G_A_210,N7-G_A_226
4e5c	U_B_16	HOH_B_128	OP2-G_B_17,N7-G_B_17
1i9v	U_A_47	HOH_A_113	O3'-C_A_49,O2'-C_A_49
4j1g	U_E_25	HOH_E_104	O2-U_E_24,O4-U_E_24
2g3s	U_B_113	HOH_B_136	OP2-G_B_114,N7-G_B_114
3d2v	U_B_41	HOH_B_176	O5'-G_B_1,OP2-G_B_2
2g3s	U_C_205	HOH_C_1610	OP2-G_C_206,N7-G_C_206
1et4	U_B_309	HOH_B_1148	O5'-G_B_310,O4'-G_B_310,N7-G_B_326
1dfu	U_N_80	HOH_N_511	OP2-G_N_81,N7-G_N_81
3boy	U_D_1	HOH_D_121	OP2-U_D_2,O4'-U_D_2
3boy	U_D_8	HOH_D_230	OP2-U_D_9,O5'-U_D_9,O4'-U_D_9
3boy	U_D_15	HOH_D_274	OP2-U_D_16,O4'-U_D_16
2g3s	U_G_405	HOH_G_66	OP2-G_G_406,N7-G_G_406
2g3s	U_H_413	HOH_H_438	OP2-G_H_414,N7-G_H_414
3eph	U_E_47	HOH_E_130	N7-A_E_21,N7-G_E_46
2g3s	U_J_513	HOH_J_522	OP2-G_J_514,N7-G_J_514
1et4	U_C_409	HOH_C_1289	O5'-G_C_410,O4'-G_C_410,N7-G_C_426
3eph	U_F_51	HOH_F_83	OP2-A_F_52,O5'-A_F_52,N7-A_F_52
1et4	U_D_509	HOH_D_1198	O5'-G_D_510,N7-G_D_526
2bgg	U_Q_15	HOH_Q_2019	OP1-U_Q_16,O3'-U_Q_16

4n0t	U_B_38	HOH_B_271	N7-G_B_39,O2'-A_B_40
1et4	U_E_109	HOH_E_1587	O5'-G_E_110,O4'-G_E_110,N7-G_E_126
4qik	U_C_11	HOH_D_137	N7-G_C_12,O6-G_D_12
4wrt	U_R_12	HOH_B_839	O-ASN_B_670,OD1-ASN_B_670
1s72	U_0_454	HOH_0_3591	O2'-U_0_1362,O4'-G_0_1363
1s72	U_0_1724	HOH_0_4194	OP1-C_0_1431,OP2-C_0_1725
1s72	U_0_1359	HOH_0_4211	O4'-A_0_2101,N3-G_0_2537
1s72	U_0_1771	HOH_0_4322	O2'-A_0_1886,N3-A_0_1886
1s72	U_0_675	HOH_0_4494	OP1-A_0_674,O5'-A_0_674
1s72	U_0_55	HOH_0_4853	N7-G_0_56,N1-A_0_70
1s72	U_0_779	HOH_0_5003	OP2-A_0_780,N7-A_0_780
1s72	U_0_1838	HOH_0_5023	P-A_0_1839,OP2-A_0_1839,O5'-A_0_1839,N1-A_0_2622
1s72	U_0_325	HOH_0_5053	OP2-G_0_326,N7-G_0_326
1s72	U_0_1220	HOH_0_5489	OP2-G_0_1221,N7-G_0_1221
1s72	U_0_1813	HOH_0_6210	OP2-A_0_1815,O4-U_0_1817
1s72	U_0_777	HOH_0_7071	O4'-U_0_470,O2-C_0_881
1s72	U_0_170	HOH_0_8545	O2'-A_0_169,N3-G_0_219
1s72	U_0_454	HOH_0_8546	O2'-G_0_640,N3-G_0_640,O4'-G_0_641
1s72	U_0_2424	HOH_0_8614	O2'-G_0_2295,O4'-A_0_2425
1s72	U_0_170	HOH_0_8675	O4'-G_0_219,N3-G_0_219
1s72	U_0_1980	HOH_0_8778	O3'-C_0_2626,O2'-C_0_2626
1s72	U_0_1488	HOH_0_8837	O2'-G_0_786,N3-G_0_786,O4'-G_0_787
1s72	U_0_866	HOH_0_8845	N7-A_0_776,O5'-A_0_867
1s72	U_0_2484	HOH_0_9127	O2'-G_0_2481,N3-G_0_2481
1s72	U_0_1835	HOH_0_9532	O4'-A_0_876,O2-C_0_1834
1s72	U_0_1017	HOH_0_9564	OP2-A_0_1018,N7-A_0_1018
1s72	U_0_2837	HOH_B_8579	O2'-G_0_2845,OE1-GLU_B_22,OE2-GLU_B_22
4oji	G_A_47	HOH_A_221	OP2-G_A_48,N7-G_A_48
3sj2	G_A_8	HOH_A_131	OP2-G_A_9,N7-G_A_9
4e48	G_B_27	HOH_A_217	O2-U_A_15,O2-U_B_26
3czw	G_X_11	HOH_X_522	OP2-A_X_12,N7-A_X_12
2val	G_B_5	HOH_B_2013	OP2-A_B_6,N7-A_B_6
1f27	G_A_13	HOH_A_186	OP2-A_A_14,N7-A_A_14
3hjw	G_E_9	HOH_A_338	OG1-THR_A_83,OP2-G_E_11,O5'-G_E_11,OP1-C_E_12
2gdi	G_X_29	HOH_X_223	O3'-U_X_28,O2-U_X_28,OP2-C_X_30
2ho7	G_B_102	HOH_B_313	P-G_B_128,OP2-G_B_128,N7-G_B_128
4qlm	G_A_9	HOH_A_301	O5'-A_A_10,O3'-A_A_10,P-A_A_11,OP2-A_A_11,O5'-A_A_11,N7-A_A_11
3czw	G_X_8	HOH_X_537	OP2-A_X_9,N7-A_X_9
4wfl	G_A_76	HOH_A_339	P-G_A_77,OP2-G_A_77
2oiu	G_Q_1	HOH_Q_89	O6-G_Q_2,O4-U_Q_49,O4-U_Q_50
1csl	G_A_46	HOH_A_93	OP2-G_A_47,N7-G_A_47

2gdi	G_X_72	HOH_X_365	O2'-G_X_21,N1-A_X_43
2zy6	G_A_26	HOH_A_97	O4-U_A_8,OP2-A_A_27
1qrs	G_B_10	HOH_B_802	O2'-A_B_26,N3-A_B_26
1feu	G_B_75	HOH_B_196	O4-U_B_74,O2-U_C_103,OD2-ASP_A_87
3sj2	G_B_8	HOH_B_39	OP2-G_B_9,N7-G_B_9
1nuv	G_A_24	HOH_A_427	N7-A_A_25,O6-G_A_26
3q3z	G_V_58	HOH_V_158	N1-A_V_18,O2'-A_V_57,N3-A_V_57,O4'-C2E_V_84
3la5	G_A_44	HOH_A_126	OP2-A_A_45,N7-A_A_45
1d4r	G_B_12	HOH_B_113	O6-G_A_16,N7-G_B_13,O6-G_B_13
4o41	G_B_202	HOH_B_358	OP2-A_B_203,N7-A_B_203
3sj2	G_B_14	HOH_B_175	OP2-G_B_15,N7-G_B_15
1nlc	G_A_7	HOH_A_241	OP2-A_A_8,N7-G_A_9,O6-G_A_9
4oog	G_D_22	HOH_D_231	N7-G_D_23,O6-G_D_23
3r1c	G_A_3	HOH_A_107	OP2-G_A_4,N7-G_A_4
1t0e	G_C_14	HOH_C_243	OP2-U_C_15,O4-SO4_C_201
1fuf	G_A_1	HOH_A_56	N7-G_A_2,O2'-U_B_20
1nuv	G_E_19	HOH_E_164	OP2-G_E_20,N7-G_E_20
1feu	G_E_72	HOH_F_341	O6-G_F_102,O4-U_F_103
4kq0	G_B_4	HOH_B_116	OP2-G_B_5,N7-G_B_5
1lng	G_B_166	HOH_B_440	O3'-G_B_167,O2'-G_B_167,O2'-G_B_214
2v6w	G_A_4	HOH_A_2026	OP2-A_A_5,N7-A_A_5
3td1	G_A_13	HOH_A_159	OP2-A_A_14,N7-A_A_14
2dr8	G_B_1	HOH_B_34	N1-A_B_32,OD1-ASN_A_292
2gdi	G_Y_29	HOH_Y_347	O4'-U_Y_28,O2-U_Y_28,OP2-C_Y_30
4lvz	G_A_54	HOH_A_321	O2'-A_A_22,N7-A_A_55
1qcu	G_A_1	HOH_A_390	OP2-G_A_2,N7-G_A_2,OP2-C_C_102
1r3e	G_D_408	HOH_D_120	OP1-G_D_412,N7-G_D_412
2ez6	G_C_12	HOH_C_49	P-A_C_14,OP2-A_C_14
4kq0	G_E_4	HOH_E_118	OP2-G_E_5,N7-G_E_5
3r1c	G_E_3	HOH_E_445	OP2-G_E_4,N7-G_E_4
1l9a	G_B_177	HOH_B_2	N1-A_B_176,N3-C_B_221,N3-G_B_222
4c8y	G_C_26	HOH_A_2093	OP2-G_C_27,N7-G_C_27
3gvn	G_A_4	HOH_A_41	OP2-A_A_5,N7-A_A_5
1efw	G_C_45	HOH_C_2046	O4'-A_C_9,N3-A_C_9,O4'-G7M_C_46
2qbz	G_X_73	HOH_X_315	O2-C_X_69,OP2-A_X_72,N7-A_X_72
4n48	G_D_1	HOH_D_204	OP2-A_D_2,N7-A_D_2,O2G-MGT_D_101,O2B-MGT_D_101
4lvz	G_A_4	HOH_A_498	OP2-A_A_5,N7-A_A_5,O6-G_A_6
2xsl	G_C_5	HOH_C_2018	OP2-A_C_6,N7-A_C_6
1dqh	G_B_13	HOH_B_102	OP2-G_B_14,N7-G_B_14
1dqh	G_B_17	HOH_B_111	OP2-G_B_18,N7-G_B_18
4c8z	G_C_25	HOH_C_2007	N3-G_C_21,O4'-A_C_23,N7-A_C_24

3r1c	G_J_6	HOH_J_113	OP2-G_J_7,N7-G_J_7
3ts2	G_V_21	HOH_V_311	O2'-C_V_20,O6-G_V_22
3d0u	G_A_77	HOH_A_213	O3'-G_A_111,O2'-G_A_111,O2'-G_A_152
1wpu	G_C_3	HOH_A_3179	O-GLY_A_101,O-LEU_A_102
3r1c	G_K_6	HOH_K_433	OP2-G_K_7,N7-G_K_7
4un3	G_A_33	HOH_A_2066	O3'-A_A_34,P-A_A_35,OP1-A_A_35,OP2-A_A_35
3rw6	G_H_18	HOH_H_68	N3-A_H_17,N1-A_H_45
3rw6	G_H_14	HOH_H_72	O2-C_H_10,O2'-G_H_52,N3-G_H_52
3ova	G_C_1	HOH_A_440	OD1-ASN_A_292,N1-A_C_32
3rw6	G_F_14	HOH_F_63	O2-C_F_10,O2'-G_F_52,N3-G_F_52
3d2v	G_B_24	HOH_B_260	OP2-G_B_25,N7-G_B_25
3r1c	G_M_3	HOH_M_139	OP2-G_M_4,N7-G_M_4
3ok4	G_H_9	HOH_P_181	OP2-G_H_10,N7-G_H_10,OP2-C_P_8,OP2-U_X_6
3r1c	G_M_6	HOH_M_390	OP2-G_M_7,N7-G_M_7
1dfu	G_N_75	HOH_P_100	O2-U_M_103,O4-U_N_74,OD1-ASP_P_90
3rw6	G_F_18	HOH_F_109	OP2-G_F_19,N7-G_F_19
3rw6	G_F_35	HOH_F_123	O2-C_F_25,N3-C_F_25,N3-G_F_26,O2-U_F_34
2g3s	G_E_302	HOH_F_361	O2-C_F_316,N3-C_F_316
3r2c	G_R_2	HOH_R_14	N3-G_R_1,OP2-C_R_3
3r2c	G_S_2	HOH_S_151	N3-G_S_1,OP2-C_S_3
3r1c	G_Q_3	HOH_Q_9	OP2-G_Q_4,N7-G_Q_4
2vpl	G_B_2	HOH_B_2104	O2-C_B_49,N3-C_B_49
3r1c	G_Q_6	HOH_Q_361	OP2-G_Q_7,N7-G_Q_7
1et4	G_C_426	HOH_C_1188	O2-U_C_409,O2-C_C_421,O2'-A_C_425
3r1c	G_U_3	HOH_U_336	OP2-G_U_4,N7-G_U_4
3r1c	G_W_6	HOH_W_473	OP2-G_W_7,N7-G_W_7
4c8y	G_C_25	HOH_C_2015	N3-G_C_21,N7-A_C_24
3r1c	G_e_6	HOH_e_479	OP2-G_e_7,N7-G_e_7
3r1c	G_g_3	HOH_g_412	OP2-G_g_4,N7-G_g_4
1et4	G_D_501	HOH_D_1472	OP2-G_D_502,N7-G_D_502
4n0t	G_B_96	HOH_B_391	N1-A_B_34,OP2-A_B_97
3ol9	G_C_693	HOH_C_786	OP2-A_C_694,N7-A_C_694
2qux	G_O_7	HOH_O_27	OP2-A_O_8,N7-A_O_8
1tfw	G_E_1	HOH_B_1717	N1-A_H_73,OD1-ASN_B_292
3ol9	G_K_693	HOH_K_1234	OP2-A_K_694,N7-A_K_694
3ol9	G_O_693	HOH_O_816	OP2-A_O_694,N7-A_O_694
1s72	G_0_2428	HOH_0_3288	O2-C_0_2427,O2'-C_0_2464,O2-C_0_2464
1s72	G_0_553	HOH_0_3580	OP2-G_0_554,N7-G_0_554
1s72	G_0_775	HOH_0_3941	OP2-A_0_776,N7-A_0_867
1s72	G_0_2570	HOH_0_4335	OP2-C_0_2565,N1-A_0_2569
1s72	G_0_1868	HOH_0_4471	OP2-A_0_1869,N7-A_0_1869
1s72	G_0_1475	HOH_0_4666	OP2-A_0_1476,N7-A_0_1476

1s72	G_0_2516	HOH_0_4936	N1-A_0_2503,OP2-A_0_2517
1s72	G_0_381	HOH_0_5186	N7-G_0_406,O6-G_0_406
1s72	G_0_2617	HOH_0_5201	OP1-C_0_1750,O2'-OMG_0_2588
1s72	G_0_1703	HOH_0_5264	OP2-G_0_1704,N7-G_0_1704
1s72	G_0_588	HOH_0_5317	OP2-U_0_567,N7-G_0_568,O6-G_0_568
1s72	G_0_301	HOH_0_5339	OP2-A_0_302,N7-A_0_302
1s72	G_0_1837	HOH_0_5867	OP1-U_0_883,OP2-U_0_883
1s72	G_0_264	HOH_0_6748	O6-G_0_246,OH-TYR_M_5
1s72	G_0_1190	HOH_0_7173	O2-U_0_1187,O4'-A_0_1189,N3-A_0_1189
1s72	G_0_1484	HOH_0_8618	O4-U_0_1457,N7-A_0_1458,N7-A_0_1485
1s72	G_0_901	HOH_0_8636	O2-C_0_764,N3-C_0_764,O2-U_0_900
1s72	G_0_1979	HOH_0_8790	O2'-C_0_2625,O2-C_0_2625,O4'-C_0_2626
1s72	G_0_2046	HOH_0_9715	N1-A_0_1729,N7-A_0_1732
1s72	G_0_2072	HOH_0_9849	O2'-C_0_2533,O2-C_0_2533,O4'-C_0_2534
1s72	G_0_2075	HOH_0_9852	N3-A_0_2062,OP1-U_0_2064
1s72	G_0_1239	HOH_0_9920	OP2-G_0_1240,N7-G_0_1240
1j9h	C_A_5	HOH_A_159	OP2-G_A_6,N7-G_A_6
3egz	C_B_42	HOH_A_422	OD1-ASP_A_287,OD2-ASP_A_287
4k31	C_B_4	HOH_B_244	OP2-G_B_5,N7-G_B_5
1j9h	C_B_14	HOH_B_162	OP2-G_B_15,N7-G_B_15
1j9h	C_C_23	HOH_C_121	OP2-G_C_24,N7-G_C_24
1j9h	C_D_32	HOH_D_112	OP2-G_D_33,N7-G_D_33
3fo4	C_A_28	HOH_A_382	OP2-G_A_29,N7-G_A_29
4k31	C_C_4	HOH_C_267	OP2-G_C_5,N7-G_C_5
3fo4	C_A_54	HOH_A_466	OP2-G_A_55,N7-G_A_55
3mei	C_A_15	HOH_B_54	OP1-U_A_16,O6-G_B_8
1lng	C_B_218	HOH_B_403	O6-G_B_204,O2'-G_B_217,N3-G_B_217
4j5v	C_B_212	HOH_B_416	OP2-G_B_213,N7-G_B_213
2ao5	C_C_3	HOH_C_12	OP2-G_C_4,O5'-G_C_4,O4'-G_C_4,N7-G_C_4
1yz9	C_C_8	HOH_C_167	OP2-G_C_9,N7-G_C_9
3cgr	C_A_2	HOH_A_44	OP2-G_A_3,N7-G_A_3
4lx6	C_A_54	HOH_A_712	O2'-A_A_24,N3-A_A_24
3la5	C_A_54	HOH_A_377	OP2-A_A_55,N7-A_A_55
1duq	C_H_427	HOH_G_636	O2'-A_H_426,N3-A_H_426
3td1	C_A_21	HOH_A_190	OP2-G_A_22,N7-G_A_22
4lvz	C_A_46	HOH_A_346	OP2-A_A_47,N7-A_A_47
1lnt	C_B_19	HOH_A_217	O6-G_A_7,O2'-G_B_18,N3-G_B_18
3la5	C_A_54	HOH_A_432	O2'-A_A_24,N3-A_A_24,O4'-C_A_53
3gvn	C_B_69	HOH_B_44	OP2-A_B_70,N7-A_B_70
4p5j	C_A_74	HOH_A_292	N1-A_A_40,OP1-U_A_73
1k8w	C_B_415	HOH_A_577	N3-A_B_413,OD1-ASN_A_26
2g3s	C_E_303	HOH_E_319	OP2-G_E_304,N7-G_E_304

3ok4	C_B_8	HOH_R_299	N7-G_B_9,OP2-A_J_7,P-U_R_5,OP2-U_R_5,O5'-U_R_5
4oo8	C_B_67	HOH_A_1408	O-THR_A_1098,OP2-A_B_68
2g3s	C_F_311	HOH_F_356	OP2-G_F_312,N7-G_F_312
4w5o	C_B_11	HOH_A_1181	OE1-GLU_A_637,O-GLY_A_670
4qm6	C_C_2	HOH_C_106	OE1-GLN_A_83,OG-SER_A_85
4qm6	C_D_2	HOH_D_104	OE1-GLN_B_83,OG-SER_B_85
4un3	C_A_67	HOH_A_2141	OP2-A_A_68,O-THR_B_1098
4un5	C_A_67	HOH_A_2213	OP2-A_A_68,O-THR_B_1098
1s72	C_0_770	HOH_0_3530	OP2-G_0_771,N7-G_0_771
1s72	C_0_1753	HOH_0_3604	O2-U_0_1749,N7-G_0_1751
1s72	C_0_1708	HOH_0_4214	O3'-G_0_1760,OP1-U_0_1761,O-LYS_P_81
1s72	C_0_899	HOH_0_4310	O2'-A_0_897,N3-A_0_897
1s72	C_0_905	HOH_0_4683	OP2-C_0_906,O-ARG_L_8
1s72	C_0_2737	HOH_0_5643	OP1-G_0_2738,O5'-G_0_2738,OP2-A_0_2739
1s72	C_0_1184	HOH_0_5744	O2-C_0_1183,N3-C_0_1183
1s72	C_0_2526	HOH_0_6452	O2'-C_0_2496,O2-C_0_2496
Instances corresponding to Figure S4b[52 instances]			
2oe5	A_B_1492	HOH_A_156	O6-G_A_1408,O-HOH_A_199,O-HOH_B_193,O-HOH_B_202,O-HOH_B_202
3nj7	A_A_7	HOH_A_21	N7-G_A_8,O-HOH_A_46,O-HOH_A_64,O-HOH_A_65
3nj6	A_A_7	HOH_A_68	N7-G_A_8,O-HOH_A_16,O-HOH_A_22,O-HOH_A_33
3nj7	A_B_7	HOH_B_17	N7-G_B_8,O-HOH_B_34,O-HOH_B_110
3nj7	A_C_7	HOH_C_18	N7-G_C_8,O-HOH_C_26,O-HOH_C_50,O-HOH_C_168
3nj7	A_D_7	HOH_D_15	N7-G_D_8,O-HOH_D_44,O-HOH_D_102
3nj7	A_E_7	HOH_E_24	N7-G_E_8,O-HOH_E_38,O-HOH_E_107
3nj7	A_F_7	HOH_F_20	N7-G_F_8,O-HOH_E_159,O-HOH_F_48,O-HOH_F_175
2a43	A_A_24	HOH_A_544	O5'-A_A_25,O-HOH_A_551,O-HOH_A_602
3tzr	A_A_53	HOH_B_59	N7-G_B_107,O-HOH_A_26,O-HOH_B_22
1k8w	A_B_413	HOH_A_523	OP1-G_B_412,O-HOH_B_526,O-HOH_B_535
4kyy	U_B_8	HOH_B_202	OP2-U_B_9,O-HOH_B_207,O-HOH_B_236
1f27	U_A_7	HOH_A_87	O6-G_B_27,O-HOH_A_44,O-HOH_A_94,O-HOH_A_129
3k62	U_B_1	HOH_A_13	OG-SER_A_554,O-HOH_A_18,O-HOH_A_83
2gdi	U_X_28	HOH_X_352	O6-G_X_31,O-HOH_X_216,O-HOH_X_412
3k64	U_B_1	HOH_A_19	OG-SER_A_554,O-HOH_A_24,O-HOH_A_115
2zy6	U_A_13	HOH_A_169	OP2-C_A_15,O-HOH_A_179,O-HOH_A_182
3fo4	U_A_34	HOH_A_337	N7-A_A_64,O-HOH_A_446,O-HOH_A_457
2awe	U_A_4	HOH_A_227	OP2-G_A_5,O-HOH_A_222,O-HOH_D_49,O-HOH_D_64
2g91	U_A_3	HOH_A_116	N7-G_A_4,O-HOH_A_120,O-HOH_A_162,O-HOH_A_172,O-HOH_A_180,O-HOH_A_184
1jzv	U_B_12	HOH_B_352	OP2-C_B_14,O-HOH_B_312,O-HOH_B_351
1jzv	U_D_32	HOH_D_318	OP1-C_D_34,O-HOH_D_310,O-HOH_D_356
2i82	U_E_1209	HOH_A_2019	O4-U_E_1215,O-HOH_E_2074,O-HOH_E_2198

4e5c	U_A_13	HOH_A_128	N7-G_A_14,O-HOH_A_148,O-HOH_A_177
1zh5	U_C_9	HOH_B_537	O-LYS_B_54,O-HOH_C_11,O-HOH_C_36
4mdx	U_C_2	HOH_C_243	O5'-U_C_1,O-HOH_B_415,O-HOH_C_234
2g3s	U_I_505	HOH_I_556	N7-G_I_506,O-HOH_I_515,O-HOH_I_566
4u35	G_B_9	HOH_B_119	OP2-U_B_10,O-HOH_B_117,O-HOH_B_121
3nj7	G_C_1	HOH_C_35	N7-G_C_2,O-HOH_C_36,O-HOH_C_76,O-HOH_C_113
3nj7	G_D_1	HOH_D_43	N7-G_D_2,O-HOH_D_52,O-HOH_D_63,O-HOH_D_87
1feu	G_B_72	HOH_C_351	O4-U_C_103,O-HOH_C_347,O-HOH_C_353
1t0e	G_A_17	HOH_A_38	N7-G_A_18,O-HOH_A_66,O-HOH_A_72
3fo4	G_A_72	HOH_A_402	OP2-A_A_73,O-HOH_A_404,O-HOH_A_438,O-HOH_A_484
3la5	G_A_32	HOH_A_281	OP2-A_A_33,O-HOH_A_161,O-HOH_A_234,O-HOH_A_324
2a43	G_A_6	HOH_A_506	OP2-C_A_9,O-HOH_A_206,O-HOH_A_532,O-HOH_A_675
4lvz	G_A_37	HOH_A_297	N7-G_A_38,O-HOH_A_212,O-HOH_A_272
3r1c	G_G_6	HOH_G_450	N7-G_G_7,O-HOH_G_260,O-HOH_G_300,O-HOH_G_301
1yls	G_D_201	HOH_D_409	N7-G_D_202,O-HOH_D_405,O-HOH_D_406,O-HOH_D_407,O-HOH_D_408
3r1c	G_I_6	HOH_I_427	N7-G_I_7,O-HOH_I_118,O-HOH_I_428
3r1c	G_L_6	HOH_L_155	N7-G_L_7,O-HOH_L_315,O-HOH_L_522
1dfu	G_N_72	HOH_M_527	O4-U_M_103,O-HOH_M_507,O-HOH_N_563
1dfu	G_M_98	HOH_M_537	OP2-A_M_99,O-HOH_M_543,O-HOH_N_508,O-HOH_N_530
1dfu	G_M_98	HOH_N_508	O4-U_N_77,O-HOH_M_537,O-HOH_N_507,O-HOH_N_530,O-HOH_N_540
2r20	C_B_15	HOH_B_49	N7-G_B_16,O-HOH_B_48,O-HOH_B_66
2r22	C_B_15	HOH_B_47	N7-G_B_16,O-HOH_B_46,O-HOH_B_61
3bnt	C_A_15	HOH_A_57	OP2-A_A_16,O-HOH_A_69,O-HOH_A_71
3bnq	C_A_23	HOH_D_223	N1-A_D_15,O-HOH_C_316,O-HOH_D_238
1t0e	C_C_9	HOH_C_262	N7-G_C_10,O-HOH_C_210,O-HOH_C_241
2ao5	C_A_7	HOH_A_59	N7-G_A_8,O-HOH_A_85,O-HOH_A_131
1nlc	C_B_13	HOH_B_258	N7-A_B_14,O-HOH_A_168,O-HOH_B_155,O-HOH_B_321
3cgs	C_B_22	HOH_B_64	N7-G_B_23,O-HOH_B_43,O-HOH_B_49,O-HOH_B_71
3wbm	C_X_12	HOH_X_104	OP2-C_X_13,O-HOH_A_102,O-HOH_X_106
Instances corresponding to Figure S4c[9 instances]			
2tmv	A_R_3	HOH_R_66	O-HOH_R_35,O-HOH_R_65
4n0t	A_B_44	HOH_A_666	O-HOH_A_615,O-HOH_B_236,O-HOH_B_350
4rge	U_C_1	HOH_C_203	O-HOH_C_204,O-HOH_C_225
1et4	U_A_209	HOH_A_1713	O-HOH_A_1208,O-HOH_A_1371,O-HOH_A_1465
1et4	U_D_527	HOH_D_1193	O-HOH_D_1181,O-HOH_D_1324
1feu	G_C_98	HOH_B_10	O-HOH_B_12,O-HOH_B_13,O-HOH_B_251
1j9h	G_B_12	HOH_B_205	O-HOH_B_148,O-HOH_B_158,O-HOH_B_200,O-HOH_B_220

1j9h	G_C_21	HOH_C_156	O-HOH_C_116,O-HOH_C_136,O-HOH_C_140,O-HOH_C_143,O-HOH_C_208,O-HOH_D_133
3d2v	G_A_60	HOH_A_145	O-HOH_A_104,O-HOH_A_348,O-HOH_A_383
Instances corresponding to Figure S4d, where single acceptor/water is present near the O^W			
3ibk	A_B_20	HOH_B_52	O4-U_B_18
1l2x	A_A_20	HOH_A_73	O-HOH_A_37
2atw	A_B_7	HOH_B_2047	O-HOH_B_1083
1csl	A_B_68	HOH_B_159	O-HOH_B_123
2fmt	A_D_76	HOH_D_523	N3-C_D_75
3ivn	A_B_58	HOH_B_144	OP2-U_B_59
1m8y	A_C_11	HOH_C_50	O-HOH_C_30
1m8y	A_D_11	HOH_D_218	OP2-A_D_16
4ht9	A_D_5	HOH_D_117	O-HOH_D_111
3t5n	A_C_3	HOH_A_408	O2-U_C_4
3egz	A_B_56	HOH_B_434	O-HOH_B_386
2zm5	A_C_35	HOH_A_340	O-HOH_C_124
3k62	A_B_7	HOH_A_139	O-HOH_A_720
4un3	A_A_1	HOH_A_2003	O-HOH_A_2002
2a43	A_A_21	HOH_A_661	O-HOH_A_588
4lvz	A_A_62	HOH_A_453	O2'-G_A_63
3wbm	A_X_15	HOH_X_120	OP2-C_X_16
1n35	A_C_1284	HOH_C_1350	O2-U_C_1283
1et4	A_B_304	HOH_B_1278	OP2-C_B_305
3rw6	A_F_39	HOH_F_99	OP2-A_F_40
3ova	A_C_16	HOH_C_227	O2-U_C_14
3ova	A_C_17	HOH_C_227	O2-U_C_14
4aq7	A_B_31	HOH_B_2008	O5'-U_B_32
2vpl	A_D_30	HOH_D_2034	N7-G_D_31
1m8w	A_D_16	HOH_B_256	O-HOH_B_246
1s72	A_0_2697	HOH_0_4105	O-HOH_0_5563
1s72	A_0_2460	HOH_0_4312	O-HOH_0_9683
1s72	A_0_513	HOH_2_7692	O-HOH_2_7177
4mce	U_A_4	HOH_A_108	OP2-G_A_5
2gdi	U_X_52	HOH_X_206	OP2-G_X_86
3nnh	U_E_8	HOH_E_28	O-HOH_E_29
4mce	U_B_6	HOH_B_218	N7-G_B_7
1j6s	U_B_12	HOH_B_340	O-HOH_B_366
2xs2	U_B_7	HOH_B_2024	O-HOH_A_2047
2xs2	U_B_4	HOH_B_2029	O-HOH_B_2010
3i5y	U_B_7	HOH_A_1022	O-GLY_A_244
3nmr	U_B_2	HOH_B_12	O-HOH_A_200

2xs7	U_B_4	HOH_B_2006	O-HOH_B_2008
4o41	U_B_201	HOH_B_347	O-HOH_B_352
2gdi	U_X_25	HOH_X_427	O-HOH_X_479
2xs5	U_D_3	HOH_D_2007	O-HOH_D_2008
4oog	U_D_17	HOH_D_241	OP2-G_D_16
1fuf	U_A_5	HOH_A_40	O-HOH_A_48
4rkv	U_A_1006	HOH_A_9120	O-HOH_A_9123
3nna	U_B_2	HOH_B_12	O-HOH_A_200
3rg5	U_B_33	HOH_B_87	OP2-A_B_36
2awe	U_D_4	HOH_D_171	O-HOH_D_125
4j7l	U_B_2	HOH_A_652	OH-TYR_A_189
3bsx	U_D_9	HOH_B_130	OH-TYR_B_900
3la5	U_A_36	HOH_A_353	O-HOH_A_167
1g2e	U_B_5	HOH_A_306	O-HOH_A_239
3d2v	U_A_18	HOH_A_260	O4-U_A_19
1qu2	U_T_20	HOH_T_1272	O-HOH_T_1281
3rg5	U_B_9	HOH_B_155	O-HOH_B_157
3rg5	U_B_9	HOH_B_157	O-HOH_B_155
3oin	U_C_5	HOH_C_37	OP1-A_C_8
1qu2	U_T_20	HOH_T_1281	O-HOH_T_1272
4tzx	U_X_34	HOH_X_305	N1-A_X_64
3mdg	U_C_4	HOH_C_105	O-SER_A_58
3fht	U_D_5	HOH_B_519	OE1-GLN_B_256
1et4	U_A_223	HOH_A_1366	O-HOH_A_1455
3d0u	U_A_106	HOH_A_206	O6-G_A_108
4jk0	U_B_502	HOH_B_703	O-HOH_B_701
3rw6	U_H_38	HOH_H_101	O-HOH_H_100
3pey	U_B_5	HOH_A_1444	O-HOH_A_1416
2qwy	U_C_12	HOH_C_1096	OP2-A_C_13
4aq7	U_B_72	HOH_A_2055	OP2-A_B_73
2db3	U_E_6	HOH_E_684	O-HOH_E_1052
3rer	U_K_3	HOH_K_362	O-HOH_K_246
2db3	U_F_5	HOH_F_1296	O-HOH_F_580
4qm6	U_D_3	HOH_D_119	O-HOH_D_107
1et4	U_C_427	HOH_C_1264	O-HOH_C_1559
2nz4	U_R_17C	HOH_R_9050	O5'-U_R_17D
2db3	U_G_5	HOH_G_1003	O-HOH_G_924
3hax	U_E_32	HOH_E_533	O-HOH_E_545
4kxt	U_B_20	HOH_B_108	O-HOH_B_112
2db3	U_H_5	HOH_H_928	O-HOH_H_320
2nz4	U_S_105	HOH_S_9032	N7-A_S_106
2qux	U_F_12	HOH_F_26	OP2-A_F_13

4krf	U_R_6	HOH_R_108	N7-A_R_7
2bgg	U_Q_16	HOH_Q_2018	O-GLN_A_329
1et4	U_E_127	HOH_E_1200	O-HOH_E_1695
1s72	U_0_713	HOH_0_3450	O-HOH_0_9645
1s72	U_0_2330	HOH_0_3494	N3-A_0_2367
1s72	U_0_488	HOH_0_3563	O-HOH_0_3053
1s72	U_0_2117	HOH_0_4348	OP2-A_0_2118
1s72	U_0_1136	HOH_0_4468	O-HOH_0_3475
1s72	U_0_1454	HOH_0_4793	O4'-C_0_1455
1s72	U_0_1310	HOH_0_5322	OP2-G_0_1311
1s72	U_0_2541	HOH_0_6922	O-HOH_0_5944
1s72	U_0_651	HOH_0_9519	OP2-G_0_652
1s72	U_0_713	HOH_0_9645	O-HOH_0_3450
1s72	U_0_1109	HOH_J_247	O-GLY_J_118
1s72	U_0_1446	HOH_S_8344	O-HOH_S_8328
3ibk	G_B_17	HOH_B_42	O-HOH_B_41
3kmq	G_C_916	HOH_A_496	OE2-GLU_A_422
1xpe	G_A_7	HOH_A_221	O-HOH_B_231
1d4r	G_C_12	HOH_C_159	OP2-G_C_13
3bnl	G_B_15	HOH_A_31	O-HOH_B_44
3r1c	G_A_6	HOH_A_486	N7-G_A_7
3fo4	G_A_38	HOH_A_458	O4-U_A_67
3r1c	G_B_6	HOH_B_164	N7-G_B_7
3fo4	G_A_62	HOH_A_483	N1-A_A_35
1q96	G_A_10	HOH_A_378	O-HOH_A_382
3k5y	G_B_2	HOH_B_133	O-HOH_B_44
1q96	G_A_2	HOH_A_408	N7-G_A_3
1lng	G_B_167	HOH_B_424	N7-G_B_168
4lx6	G_A_72	HOH_A_701	OP2-A_A_73
3k61	G_B_2	HOH_B_275	O-HOH_B_44
3r1c	G_D_3	HOH_D_203	N7-G_D_4
3umy	G_B_2125	HOH_B_2314	N7-A_B_2126
3td0	G_A_19	HOH_A_107	OP2-U_A_20
3v74	G_B_5	HOH_B_102	O-HOH_B_114
2hw8	G_B_11	HOH_B_233	N7-A_B_12
2qbz	G_X_168	HOH_X_368	N7-A_X_169
1wpu	G_D_3	HOH_D_181	O-HOH_D_247
1jbr	G_C_10	HOH_A_188	O-HOH_F_215
1ooa	G_C_22	HOH_C_441	O6-G_C_23
3d0u	G_A_24	HOH_A_235	N3-A_A_23
2qwy	G_A_5	HOH_A_1153	N7-G_A_6
2y8w	G_B_24	HOH_B_2079	O-HOH_B_2072

3k62	G_B_2	HOH_B_208	O-HOH_B_102
3k5q	G_B_2	HOH_B_274	O-HOH_B_188
4m4o	G_B_54	HOH_B_242	N7-A_B_55
2zuf	G_B_901	HOH_B_1176	N3-G_B_973
4jk0	G_B_513	HOH_B_719	O2-U_B_512
3boy	G_D_5	HOH_D_42	O-HOH_D_96
3rw6	G_F_47	HOH_F_69	N7-A_F_12
2hvy	G_E_12	HOH_E_78	O-HOH_E_72
2hvy	G_E_1	HOH_E_83	O-HOH_E_81
1zx7	G_F_24	HOH_F_40	OP2-U_F_25
1sds	G_F_211	HOH_C_866	O-HOH_F_1007
3q0o	G_D_2	HOH_D_111	O-HOH_D_102
4g0a	G_E_1	HOH_A_1463	O-HOH_A_1522
3r1c	G_T_6	HOH_T_335	N7-G_T_7
3r1c	G_U_6	HOH_U_69	N7-G_U_7
1m8w	G_F_9	HOH_B_140	OH-TYR_B_900
1qln	G_R_3	HOH_A_2324	OH-TYR_A_639
3r1c	G_b_6	HOH_b_367	N7-G_b_7
2o5i	G_H_1	HOH_H_1847	O-HOH_H_2428
3ol8	G_B_599	HOH_A_561	OD2-ASP_A_160
1tfw	G_G_2	HOH_A_529	O-GLU_A_96
3r1c	G_j_6	HOH_j_386	N7-G_j_7
2qux	G_C_16	HOH_E_181	O-MET_E_0
3ol8	G_J_599	HOH_I_521	OD2-ASP_I_160
3ol8	G_N_599	HOH_M_515	OD2-ASP_M_160
1gtf	G_W_126	HOH_W_2037	O-HOH_W_2008
1s72	G_0_1376	HOH_0_4008	O-HOH_0_3814
1s72	G_0_2459	HOH_0_4312	O-HOH_0_9683
1s72	G_0_2344	HOH_0_4419	O-HOH_0_6153
1s72	G_0_2013	HOH_0_4913	N7-G_0_2014
1s72	G_0_2882	HOH_0_6443	OP2-A_0_2883
1s72	G_0_1752	HOH_0_7037	O-HOH_0_5575
1s72	G_0_2442	HOH_0_8703	OP2-C_0_2443
1s72	G_0_1216	HOH_0_8786	O-HOH_0_4476
1s72	G_0_702	HOH_0_9001	O-HOH_0_4762
1s72	G_0_1002	HOH_0_9141	OP2-U_0_1003
4oji	C_A_20	HOH_A_242	N1-A_A_36
1m5o	C_B_45	HOH_B_319	OP2-G_B_46
3dir	C_A_79	HOH_A_307	OP2-A_A_10
3ivn	C_A_44	HOH_A_151	O-HOH_A_152
3bnq	C_B_7	HOH_A_312	N1-A_A_17
3bnq	C_A_7	HOH_A_317	N7-A_A_8

3ivn	C_B_44	HOH_B_133	O-HOH_B_107
4e48	C_D_5	HOH_D_202	OP2-U_D_6
3bnq	C_B_4	HOH_B_207	N7-G_B_5
1m8y	C_C_17	HOH_C_39	N7-A_C_18
3egz	C_B_45	HOH_B_411	OP2-G_B_46
3bnq	C_D_5	HOH_C_325	N1-A_C_17
3fo4	C_A_39	HOH_A_427	N7-A_A_40
4j5v	C_B_218	HOH_B_405	N7-G_B_219
4j5v	C_B_215	HOH_B_411	N7-G_B_216
2i91	C_D_13	HOH_A_712	O-HOH_A_852
3iev	C_D_1535	HOH_D_96	O4-U_D_1537
1l9a	C_B_170	HOH_B_12	O-HOH_B_14
1dqh	C_B_16	HOH_B_104	OP1-G_B_17
2y8w	C_B_11	HOH_B_2036	OP2-G_B_12
2zuf	C_B_934	HOH_B_1175	OP2-C_B_935
1zx7	C_G_12	HOH_G_23	N7-G_G_13
3q0o	C_D_5	HOH_D_13	N7-A_D_6
1m8w	C_F_6	HOH_B_256	O-HOH_B_246
3eph	C_F_35	HOH_F_91	O-HOH_F_104
4c7o	C_E_11	HOH_E_2013	OP2-C_E_12
1s72	C_0_1772	HOH_0_4776	O-HOH_0_9736
1s72	C_0_2833	HOH_0_6615	N7-G_0_2834
1s72	C_0_2526	HOH_0_7097	O2'-A_0_2604
1s72	C_0_1083	HOH_0_8565	O-HOH_0_5514
1s72	C_0_2895	HOH_0_9077	OP2-A_0_2896
1s72	C_0_376	HOH_0_9815	OP2-C_0_377

Table S3. The table shows the Potential Energy values (in kcal/mol) for both the lp-π and OH-π geometries of the water-adenine contacts. The distance column defines the vertical

distance between the ring centroid and the position of the O^W atom, and it ranges from 2.0 Å to 6.0 Å with 0.1 Å increments, and 6.0 Å to 8.0 Å with 1.0 Å increments. Binding energies were computed at the DLPNO/CBS level of theory by 2-point extrapolation scheme using cc-pVTZ and cc-pVQZ basis sets. The columns show the cc-pVTZ, cc-pVQZ and CBS energy values for each of the cases.

	lp-π			OH-π		
Distance (Å)	**cc-pvTZ (kcal/mol)**	**cc-pvQZ (kcal/mol)**	**CBS (kcal/mol)**	**cc-pvTZ (kcal/mol)**	**cc-pvQZ (kcal/mol)**	**CBS (kcal/mol)**
2.4	6.43	5.36	4.69	23.85	22.42	21.44
2.5	3.81	2.85	2.23	15.85	14.70	13.90
2.6	1.98	1.19	0.69	10.04	9.11	8.46
2.7	0.84	0.08	-0.41	5.92	5.07	4.47
2.8	0.10	-0.56	-0.97	3.10	2.35	1.82
2.9	-0.36	-0.92	-1.27	1.18	0.50	0.01
3.0	-0.57	-1.08	-1.40	-0.13	-0.67	-1.05
3.1	-0.66	-1.12	-1.40	-0.95	-1.39	-1.71
3.2	-0.68	-1.08	-1.32	-1.48	-1.87	-2.14
3.3	-0.65	-1.00	-1.21	-1.75	-2.10	-2.36
3.4	-0.58	-0.87	-1.03	-1.86	-2.15	-2.35
3.5	-0.51	-0.76	-0.91	-1.88	-2.13	-2.30
3.6	-0.40	-0.65	-0.79	-1.84	-2.04	-2.19
3.7	-0.32	-0.53	-0.65	-1.72	-1.94	-2.10
3.8	-0.25	-0.44	-0.54	-1.62	-1.75	-1.84
3.9	-0.18	-0.35	-0.44	-1.52	-1.62	-1.71
4.0	-0.12	-0.23	-0.27	-1.38	-1.50	-1.60
4.1	-0.07	-0.20	-0.27	-1.27	-1.38	-1.46
4.2	-0.02	-0.25	-0.61	-1.17	-1.26	-1.34
4.3	0.02	-0.09	-0.15	-1.07	-1.17	-1.25
4.4	0.05	-0.05	-0.09	-0.97	-1.05	-1.12
4.5	0.08	0.01	-0.03	-0.89	-0.98	-1.06
4.6	0.10	0.04	0.01	-0.82	-0.89	-0.96
4.7	0.11	0.06	0.04	-0.75	-0.82	-0.88
4.8	0.13	0.08	0.07	-0.69	-0.76	-0.82
4.9	0.14	0.10	0.08	-0.64	-0.70	-0.75
5.0	0.15	0.11	0.10	-0.58	-0.65	-0.70
5.1	0.15	0.12	0.11	-0.54	-0.57	-0.61
5.2	0.16	0.13	0.12	-0.49	-0.53	-0.56
5.3	0.16	0.12	0.10	-0.47	-0.52	-0.56
5.4	0.16	0.16	0.17	-0.42	-0.48	-0.53
5.5	0.16	0.18	0.19	-0.40	-0.45	-0.49
5.6	0.16	0.13	0.12	-0.37	-0.42	-0.47
5.7	0.16	0.15	0.14	-0.34	-0.36	-0.38
5.8	0.16	0.15	0.14	-0.31	-0.35	-0.38
5.9	0.16	0.18	0.20	-0.30	-0.32	-0.33
6.0	0.16	0.15	0.14	-0.28	-0.30	-0.31
7.0	0.13	0.11	0.09	-0.15	-0.19	-0.22
8.0	0.10	0.05	0.02	-0.08	-0.09	-0.09

Table S4. The table shows the Potential Energy values (in kcal/mol) for both the lp-π and OH-π geometries of the water-uracil interactions. Further details are given in the legend of Table S3.

lp-π				OH-π		
Distance (Å)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)
2.4	3.03	2.13	1.48	20.15	19.15	18.40
2.5	1.12	0.39	-0.15	14.34	13.47	12.82
2.6	-0.13	-0.78	-1.27	10.00	9.26	8.71
2.7	-0.93	-1.48	-1.88	6.87	6.16	5.64
2.8	-1.42	-1.88	-2.23	4.62	4.03	3.59
2.9	-1.65	-2.08	-2.39	2.99	2.47	2.10
3.0	-1.75	-2.10	-2.36	1.78	1.38	1.09
3.1	-1.74	-2.06	-2.30	1.03	0.65	0.38
3.2	-1.67	-1.94	-2.14	0.53	0.18	-0.06
3.3	-1.57	-1.82	-2.00	0.24	-0.07	-0.29
3.4	-1.44	-1.66	-1.82	0.06	-0.19	-0.38
3.5	-1.32	-1.51	-1.63	-0.02	-0.24	-0.40
3.6	-1.19	-1.36	-1.48	-0.08	-0.22	-0.33
3.7	-1.09	-1.24	-1.33	-0.08	-0.21	-0.31
3.8	-0.99	-1.12	-1.20	-0.07	-0.17	-0.25
3.9	-0.90	-1.01	-1.08	-0.05	-0.13	-0.19
4.0	-0.81	-0.90	-0.96	0.00	-0.08	-0.13
4.1	-0.73	-0.82	-0.87	0.04	-0.02	-0.06
4.2	-0.66	-0.74	-0.79	0.06	0.04	0.01
4.3	-0.60	-0.67	-0.70	0.08	0.07	0.04
4.4	-0.54	-0.60	-0.63	0.11	0.11	0.09
4.5	-0.49	-0.54	-0.57	0.13	0.12	0.11
4.6	-0.45	-0.49	-0.52	0.15	0.15	0.14
4.7	-0.41	-0.45	-0.47	0.16	0.16	0.15
4.8	-0.37	-0.40	-0.42	0.18	0.17	0.16
4.9	-0.33	-0.37	-0.39	0.19	0.18	0.17
5.0	-0.31	-0.34	-0.36	0.20	0.19	0.18
5.1	-0.28	-0.31	-0.33	0.20	0.18	0.15
5.2	-0.26	-0.29	-0.30	0.20	0.20	0.19
5.3	-0.24	-0.26	-0.27	0.21	0.19	0.16
5.4	-0.22	-0.24	-0.25	0.21	0.18	0.16
5.5	-0.21	-0.22	-0.23	0.21	0.19	0.17
5.6	-0.19	-0.21	-0.21	0.21	0.20	0.20
5.7	-0.18	-0.19	-0.20	0.20	0.20	0.20
5.8	-0.16	-0.18	-0.18	0.20	0.20	0.20
5.9	-0.15	-0.16	-0.17	0.19	0.20	0.20
6.0	-0.14	-0.16	-0.16	0.19	0.19	0.19
7.0	-0.07	-0.08	-0.09	0.15	0.15	0.15
8.0	-0.04	-0.05	-0.05	0.11	0.11	0.11

Table S5. The table shows the Potential Energy values (in kcal/mol) for the for both the lp-π and OH-π geometries of the water-guanine interactions. Further details are given in the legend of Table S3.

lp-π				OH-π		
Distance (Å)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)
2.4	6.55	5.35	4.56	23.29	21.92	20.98
2.5	3.91	2.82	2.11	15.52	14.33	13.50
2.6	2.06	1.11	0.49	9.91	8.89	8.17
2.7	0.83	0.01	-0.53	5.94	5.05	4.41
2.8	0.07	-0.62	-1.05	3.25	2.46	1.89
2.9	-0.41	-1.03	-1.42	1.40	0.77	0.32
3.0	-0.66	-1.21	-1.56	0.20	-0.39	-0.80
3.1	-0.77	-1.26	-1.58	-0.60	-1.08	-1.42
3.2	-0.79	-1.21	-1.47	-1.03	-1.46	-1.76
3.3	-0.78	-1.12	-1.32	-1.28	-1.60	-1.83
3.4	-0.72	-1.03	-1.21	-1.37	-1.67	-1.88
3.5	-0.64	-0.93	-1.10	-1.37	-1.62	-1.79
3.6	-0.58	-0.82	-0.96	-1.30	-1.52	-1.66
3.7	-0.49	-0.67	-0.77	-1.21	-1.37	-1.48
3.8	-0.41	-0.61	-0.71	-1.09	-1.24	-1.35
3.9	-0.35	-0.52	-0.61	-0.99	-1.11	-1.20
4.0	-0.27	-0.44	-0.53	-0.86	-0.97	-1.04
4.1	-0.21	-0.37	-0.46	-0.77	-0.85	-0.92
4.2	-0.16	-0.31	-0.38	-0.67	-0.74	-0.80
4.3	-0.13	-0.25	-0.32	-0.58	-0.64	-0.69
4.4	-0.08	-0.21	-0.27	-0.48	-0.55	-0.61
4.5	-0.06	-0.17	-0.23	-0.41	-0.47	-0.51
4.6	-0.02	-0.13	-0.19	-0.35	-0.40	-0.45
4.7	-0.01	-0.10	-0.16	-0.29	-0.34	-0.38
4.8	0.00	-0.08	-0.12	-0.25	-0.29	-0.33
4.9	0.03	-0.06	-0.11	-0.20	-0.24	-0.28
5.0	0.04	-0.04	-0.08	-0.16	-0.20	-0.24
5.1	0.05	-0.02	-0.07	-0.13	-0.17	-0.20
5.2	0.05	-0.01	-0.04	-0.10	-0.14	-0.17
5.3	0.06	0.00	-0.04	-0.07	-0.12	-0.16
5.4	0.07	0.01	-0.03	-0.05	-0.10	-0.14
5.5	0.08	0.01	-0.02	-0.03	-0.08	-0.11
5.6	0.08	0.02	-0.02	-0.02	-0.06	-0.09
5.7	0.08	0.01	-0.03	0.00	-0.04	-0.08
5.8	0.08	0.04	0.03	0.02	-0.03	-0.06
5.9	0.08	0.04	0.03	0.03	-0.02	-0.05
6.0	0.08	0.05	0.03	0.04	-0.01	-0.04
7.0	0.07	0.07	0.08	0.10	0.05	0.02
8.0	0.05	0.03	0.02	0.09	0.06	0.04

Table S6. The table shows the Potential Energy values (in kcal/mol) for both the lp-π and OH-π geometries of the water-cytosine interactions. Further details are given in the legend of Table S3.

lp-π				OH-π		
Distance (Å)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)
2.4	4.38	3.32	2.60	19.60	18.51	17.71
2.5	2.35	1.47	0.86	13.64	12.69	11.99
2.6	0.94	0.22	-0.28	9.27	8.43	7.81
2.7	0.08	-0.59	-1.04	6.09	5.33	4.79
2.8	-0.44	-1.02	-1.41	3.80	3.12	2.64
2.9	-0.73	-1.26	-1.62	2.19	1.60	1.19
3.0	-0.88	-1.34	-1.64	1.02	0.51	0.17
3.1	-0.92	-1.30	-1.55	0.29	-0.20	-0.53
3.2	-0.88	-1.23	-1.45	-0.23	-0.62	-0.87
3.3	-0.83	-1.13	-1.33	-0.51	-0.86	-1.09
3.4	-0.74	-1.01	-1.18	-0.67	-0.98	-1.19
3.5	-0.65	-0.89	-1.03	-0.71	-0.98	-1.15
3.6	-0.56	-0.77	-0.89	-0.73	-0.92	-1.05
3.7	-0.49	-0.67	-0.77	-0.71	-0.86	-0.97
3.8	-0.42	-0.58	-0.67	-0.66	-0.79	-0.89
3.9	-0.35	-0.49	-0.57	-0.60	-0.72	-0.79
4.0	-0.30	-0.42	-0.49	-0.53	-0.62	-0.68
4.1	-0.25	-0.35	-0.41	-0.46	-0.55	-0.61
4.2	-0.21	-0.29	-0.34	-0.40	-0.47	-0.51
4.3	-0.17	-0.24	-0.29	-0.35	-0.40	-0.43
4.4	-0.13	-0.20	-0.24	-0.30	-0.34	-0.37
4.5	-0.10	-0.16	-0.20	-0.26	-0.29	-0.31
4.6	-0.08	-0.13	-0.16	-0.21	-0.24	-0.26
4.7	-0.06	-0.11	-0.13	-0.17	-0.20	-0.21
4.8	-0.04	-0.08	-0.10	-0.14	-0.16	-0.17
4.9	-0.02	-0.06	-0.08	-0.11	-0.13	-0.14
5.0	-0.01	-0.05	-0.07	-0.08	-0.09	-0.10
5.1	0.00	-0.03	-0.05	-0.06	-0.07	-0.08
5.2	0.01	-0.02	-0.04	-0.04	-0.05	-0.05
5.3	0.01	-0.01	-0.03	-0.02	-0.02	-0.03
5.4	0.02	0.00	-0.01	0.00	-0.01	-0.01
5.5	0.02	0.00	-0.01	0.02	0.01	0.00
5.6	0.03	0.01	0.00	0.03	0.02	0.01
5.7	0.03	0.01	0.01	0.04	0.03	0.03
5.8	0.03	0.01	0.01	0.05	0.04	0.04
5.9	0.03	0.02	0.01	0.06	0.05	0.05
6.0	0.04	0.02	0.01	0.06	0.06	0.05
7.0	0.03	0.03	0.02	0.09	0.09	0.08
8.0	0.02	0.02	0.02	0.09	0.08	0.08

Table S7. The table shows the Potential Energy values (in kcal/mol) for both the lp-π and OH-π geometries of the water-N3(+)cytosine interactions. Further details are given in the legend of Table S3.

lp-π				OH-π		
Distance (Å)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)	cc-pvTZ (kcal/mol)	cc-pvQZ (kcal/mol)	CBS (kcal/mol)
2.4	-4.08	-4.75	-5.32	23.69	22.72	21.99
2.5	-5.90	-6.45	-6.93	17.69	16.85	16.23
2.6	-7.06	-7.48	-7.88	13.15	12.40	11.85
2.7	-7.79	-8.08	-8.39	9.86	9.25	8.80
2.8	-8.12	-8.35	-8.61	7.52	6.96	6.55
2.9	-8.19	-8.40	-8.63	5.84	5.34	4.99
3.0	-8.12	-8.29	-8.50	4.57	4.17	3.90
3.1	-7.93	-8.05	-8.21	3.75	3.33	3.05
3.2	-7.67	-7.78	-7.92	3.17	2.85	2.63
3.3	-7.39	-7.48	-7.61	2.83	2.54	2.34
3.4	-7.09	-7.15	-7.25	2.62	2.40	2.26
3.5	-6.80	-6.84	-6.92	2.51	2.26	2.09
3.6	-6.50	-6.56	-6.63	2.42	2.26	2.16
3.7	-6.22	-6.27	-6.33	2.39	2.24	2.15
3.8	-5.96	-6.00	-6.05	2.35	2.24	2.17
3.9	-5.71	-5.75	-5.79	2.36	2.24	2.16
4.0	-5.47	-5.52	-5.57	2.36	2.25	2.17
4.1	-5.24	-5.28	-5.32	2.37	2.27	2.21
4.2	-5.03	-5.07	-5.11	2.37	2.29	2.23
4.3	-4.83	-4.88	-4.91	2.36	2.28	2.24
4.4	-4.64	-4.69	-4.72	2.35	2.27	2.22
4.5	-4.47	-4.51	-4.54	2.33	2.27	2.23
4.6	-4.31	-4.34	-4.36	2.31	2.25	2.21
4.7	-4.16	-4.19	-4.22	2.28	2.23	2.20
4.8	-4.02	-4.05	-4.07	2.26	2.20	2.17
4.9	-3.89	-3.91	-3.93	2.22	2.18	2.15
5.0	-3.76	-3.78	-3.80	2.19	2.14	2.12
5.1	-3.64	-3.66	-3.67	2.15	2.12	2.11
5.2	-3.53	-3.54	-3.55	2.12	2.08	2.06
5.3	-3.42	-3.43	-3.44	2.08	2.05	2.04
5.4	-3.32	-3.33	-3.34	2.05	2.02	2.00
5.5	-3.22	-3.23	-3.24	2.01	1.97	1.96
5.6	-3.13	-3.14	-3.15	1.97	1.95	1.93
5.7	-3.05	-3.05	-3.05	1.92	1.90	1.89
5.8	-2.96	-2.96	-2.97	1.88	1.87	1.86
5.9	-2.88	-2.88	-2.88	1.85	1.83	1.82
6.0	-2.80	-2.80	-2.80	1.81	1.79	1.78
7.0	-2.18	-2.17	-2.16	1.46	1.44	1.44
8.0	-1.74	-1.73	-1.73	1.18	1.17	1.17