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-$\pi$ and OH-$\pi$ 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 Å² for A, from A8 in 1NLC_A; 214.7 Å² for U, from U19 in 2O1U_P; 273.2 Å² for G, from G1 in 1B7F_P; and 218.4 Å² 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 OW appear to be engaged in H-bonds with acceptor atoms from surrounding residues, while in the OH-π interactions both the lone pairs on OW appear to be engaged in H-bonds with donor atoms from surrounding residues. Ambiguous cases, where only one hydrogen/lone pair on OW 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-$\pi$ 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\textsuperscript{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.
**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-\pi and OH-\pi 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). Single 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-\pi and the OH-\pi interaction, respectively.
Figure S11. Time evolution of all the relevant distances for the O^{W}71-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-OW120/OW189 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\textsuperscript{W}175-A9 and O\textsuperscript{W}73-A20

Regarding the O\textsuperscript{W}175-A9 contact, analysis of our three independent MD trajectories evidenced that a water molecule remains stacked on the A9 base (although O\textsuperscript{W}175 gets replaced by bulk solvent waters) under dynamic conditions (in ~92% of the frames), maintaining an OH-\pi interaction. In the figure below, the average distance between O\textsuperscript{W}175 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\textsuperscript{W} distance < 4.0 Å and one between the NP-O-H angles < 90° are considered in the analysis.
As for the O\textsuperscript{W}73-A20 contact, it is clearly unstable under dynamic conditions. During the simulation time, indeed, O\textsuperscript{W}73 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\textsuperscript{W}73 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\textsuperscript{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_A_3682 | 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   | 3ttr | 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| 2vl   | 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 |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.31 \) |
|---------|----------------|--------|------|
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.20 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.39 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.28 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.63 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.38 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.59 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.57 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.48 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.62 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.47 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.83 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.51 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.55 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.41 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.56 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.79 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.56 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.15 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.13 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.84 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.08 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.22 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.76 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.38 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.57 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.47 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.15 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.25 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.63 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.37 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.36 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.42 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.72 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.35 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.67 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.57 \) |
| \( U_0 \) | \( \text{HOH}_0 \) | \( \text{1s72} \) | \( 0.44 \) |
| \( U_A \) | \( \text{HOH}_A \) | \( \text{1s72} \) | \( 0.49 \) |
| \( U_A \) | \( \text{HOH}_A \) | \( \text{1s72} \) | \( 0.81 \) |
| \( U_A \) | \( \text{HOH}_A \) | \( \text{1s72} \) | \( 0.30 \) |
| \( U_A \) | \( \text{HOH}_A \) | \( \text{1s72} \) | \( 0.92 \) |
| 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_A_3555| 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   |
| Code   | Database   | PDB ID | Confidence |
|--------|------------|--------|------------|
| 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   | 3na    | 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       |
| Protein | Chain | Ser. | PDB Code | z-score |
|---------|-------|------|-----------|---------|
| 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 | 4rgc   | 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 | 3bov   | 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 | 3fft | 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 | 1jzw | 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 | 3ht | 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 |
| Chain  | Residue | Match | Contact | E-value |
|--------|---------|-------|---------|---------|
| 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 | 4ttx  | 0.07    |         |
| U_X_49 | HOH_X_243 | 4ttx  | 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**

| Chain  | Residue | Match | Contact | E-value |
|--------|---------|-------|---------|---------|
| 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_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_0_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_A.3417 | 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   | 3bnnl| 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_A.3510 | 4KJ9 | NA |
| G.A_24 | HOH_A.235  | 3du0 | 0.33 |
| G.A_24 | HOH_A.427  | 1nuv | 0.64 |
| G.A_26 | HOH_A.97   | 2y6  | 0.56 |
| G.A_28 | HOH_A.272  | 3e5c | 0.07 |
| G.A_28 | HOH_A.94   | 2y6  | 0.33 |
| G.A_2841 | HOH_A.4688 | 4qcn | NA |
| G.A_29 | HOH_A.113  | 3ivn | 0.75 |
| G.A_295 | HOH_A.3229 | 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 | 1cs1 | 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 | 4x6 | 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 | 10oa | 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 |     |     |     |     |     |
| G_F_32 | HOH_F_61 | 2ozb |     |     |     |     |     |
| G_F_35 | HOH_F_123 | 3rw6 |     |     |     |     |     |
| G_F_47 | HOH_F_69 | 3rw6 |     |     |     |     |     |
| G_F_599 | HOH_E_524 | 3ol8 |     |     |     |     |     |
| G_F_9 | HOH_B_140 | 1m8w |     |     |     |     |     |
| G_G_2 | HOH_A_529 | 1tfw |     |     |     |     |     |
| G_G_24 | HOH_G_237 | 1nuv |     |     |     |     |     |
| G_G_4 | HOH_G_2001 | 4bwm |     |     |     |     |     |
| G_G_6 | HOH_G_450 | 3r1c |     |     |     |     |     |
| G_H_1 | HOH_H_1847 | 2o5i |     |     |     |     |     |
| G_H_14 | HOH_H_72 | 3rw6 |     |     |     |     |     |
| G_H_1510 | HOH_H_2071 | 2i82 |     |     |     |     |     |
| G_H_18 | HOH_H_68 | 3rw6 |     |     |     |     |     |
| G_H_9 | HOH_B_2015 | 1yvp |     |     |     |     |     |
| G_H_9 | HOH_P_181 | 3ol4 |     |     |     |     |     |
| G_I_3 | HOH_I_453 | 3r1c |     |     |     |     |     |
| G_I_6 | HOH_I_427 | 3r1c |     |     |     |     |     |
| G_J_3 | HOH_J_154 | 3r1c |     |     |     |     |     |
| G_J_599 | HOH_I_521 | 3ol8 |     |     |     |     |     |
| G_J_6 | HOH_J_113 | 3r1c |     |     |     |     |     |
| G_J_7 | HOH_J_104 | 4gha |     |     |     |     |     |
| G_K_3 | HOH_K_431 | 3r1c |     |     |     |     |     |
| G_K_6 | HOH_K_433 | 3r1c |     |     |     |     |     |
| G_K_693 | HOH_K_1234 | 3ol9 |     |     |     |     |     |
| G_L_3 | HOH_L_176 | 3r1c |     |     |     |     |     |
| G_L_6 | HOH_L_155 | 3r1c |     |     |     |     |     |
| G_M_3 | HOH_M_139 | 3r1c |     |     |     |     |     |
| G_M_6 | HOH_M_390 | 3r1c |     |     |     |     |     |
| G_M_98 | HOH_M_537 | 1dfu |     |     |     |     |     |
| G_M_98 | HOH_N_508 | 1dfu |     |     |     |     |     |
| G_N_599 | HOH_M_515 | 3ol8 |     |     |     |     |     |
| G_N_72 | HOH_M_507 | 1dfu |     |     |     |     |     |
| G_N_72 | HOH_M_527 | 1dfu |     |     |     |     |     |
| G_N_75 | HOH_P_100 | 1dfu |     |     |     |     |     |
| G_O_1 | HOH_O_2002 | 1h38 |     |     |     |     |     |
| G_O_16 | HOH_O_26 | 2qux |     |     |     |     |     |
| G_O_6 | HOH_O_463 | 3r1c |     |     |     |     |     |
| G_O_693 | HOH_O_816 | 3ol9 |     |     |     |     |     |
| G_O_7 | HOH_O_27 | 2qux |     |     |     |     |     |
| G_O_1 | HOH_O_89 | 2oiu |     |     |     |     |     |
| G_Q_3 | HOH_Q_9 | 3r1c |     |     |     |     |     |
| G_Q_6 | HOH_Q_361 | 3r1c |     |     |     |     |     |
| G_R_2 | HOH_R_14 | 3r2c |     |     |     |     |     |
| G_R_3 | HOH_A_2324 | 1qln |     |     |     |     |     |
| G_R_6 | HOH_R_468 | 3r1c |     |     |     |     |     |
|    |    |    |          |  |
|----|----|----|----------|---|
| 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  |
|    |    |    | Cytoosine-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 | 4qcnc | NA |
| C_A_1710 | HOH_A_4489 | 4qcnc | NA |
| C_A_2 | HOH_A_132 | 3g1p | 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 | 3g1x5 | 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 | 3g1p | 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 | 1nt  | 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 | 1lnq | 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 | 3nk8 | 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 | 3nk8 | 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  | 3gvm | 0.84 |
|     | HOH     |        |     |
|-----|---------|--------|-----|
| 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 | 12x7   | 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 | 10e    | 0.33|
| C_D_11 | HOH_D_118 | 3og8   | 0.50|
| C_D_13 | HOH_A_712 | 2ij91  | 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  | 3g0o   | 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  | 12x7   | 0.58|
| C_G_408 | HOH_J_542 | 2g3s  | 0.83|
| C_G_8 | HOH_A_2008 | 1yvp  | 0.68|
| C_G_9 | HOH_A_2130 | 1yvp  | 0.61|
| 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|
Table S2. Screening of the environment near the \(O^W\) that is stacking to a nucleobase, in order to classify it as a possible \(\text{lp-}\pi\) 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 |

**Screening of the environment near the \(O^W\) that is stacking to a nucleobase, in order to classify it as a possible \(\text{lp-}\pi\) contact (at least 2 acceptor atoms within H-bonding distance from \(O^W\)).**
| Code  | Atom1  | Atom2  | Bond1  | Bond2  |
|-------|--------|--------|--------|--------|
| 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 |
| 30k4  | A_V_4 | HOH_N_150 | P-A_N_7,OP2-A_N_7,OP2-U_V_5,OP2-C_4_3 |
| 30k4  | 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_32,02-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 | O1-G1-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,OP2-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 |
| Code | Number | Description | Bonds |
|------|--------|-------------|--------|
| 1s72 | A_0_2896 | HOH_X_4132 | O2⁻-A_0_2727,N3-A_0_2727 |
| 3b31 | U_B_6210 | HOH_A_6205 | O2⁻-A_0_A_6184,N3-A_0_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 |
| 3ttf | 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_25,04-U_X_161 |
| 4ttx | 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_210,04⁻-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_24,04-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_310,04⁻-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_2,04⁻-U_D_2 |
| 3boy | U_D_8 | HOH_D_230 | OP2-U_D_9,05⁻-U_D_9,04⁻-U_D_9 |
| 3boy | U_D_15 | HOH_D_274 | OP2-U_D_16,04⁻-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 |
| 3epf | U_E_47 | HOH_E_130 | N7-A_E_21,N7-G_E_46 |
| 2g3s | U_J_513 | HOH_I_522 | OP2-G_J_514,N7-G_J_514 |
| 1et4 | U_C_409 | HOH_C_1289 | O5⁻-G_C_410,04⁻-G_C_410,N7-G_C_426 |
| 3epf | 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 |
| Protein | Chain | ID      | Interaction | Residue | Interaction  |
|---------|--------|---------|-------------|---------|--------------|
| 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_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 |
| 3ji2    | 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,PA-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 |
| ID   | Chain  | HOH      | O2'-G      | N1-A_G   |
|------|--------|----------|------------|----------|
| 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 |
| 1toe | 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_A_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 |
| 119a | 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|
| Code | Amino Acid | H2O | interaction sites |
|------|------------|-----|------------------|
| 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_20,06-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 | U2-U_M_103,04-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 | U2-C_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_O_2428   | HOH_O_3288 | O2-C_O_2427,O2'-C_O_2464,O2-C_O_2464 |
| 1s72 | G_O_553    | HOH_O_3580 | OP2-G_O_554,N7-G_O_554 |
| 1s72 | G_O_775    | HOH_O_3941 | OP2-A_O_776,N7-A_O_867 |
| 1s72 | G_O_2570   | HOH_O_4335 | OP2-C_O_2565,N1-A_O_2569 |
| 1s72 | G_O_1868   | HOH_O_4471 | OP2-A_O_1869,N7-A_O_1869 |
| 1s72 | G_O_1475   | HOH_O_4666 | OP2-A_O_1476,N7-A_O_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_406,06-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_568,06-G_0_568 |                         |
| 1s72| G_0_301  | HOH_0_5339 | OP2-A_0_302,N7-A_0_302   |                         |
| 1s72| G_0_1837 | HOH_0_5339 | OP2-A_0_302,N7-A_0_302   |                         |
| 1s72| G_0_264  | HOH_0_5867 | OP1-U_0_883,OP2-U_0_883  |                         |
| 1s72| G_0_1190 | HOH_0_7173 | O2-U_0_1187,04'-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_2625,04'-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_2533,04'-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_16,06-G_B_8      |                         |
| 1lng| C_B_218  | HOH_B_403 | O6-G_B_204,02'-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_4,05'-G_C_4,04'-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     |                         |
| 1ntt| C_B_19   | HOH_A_217 | O6-G_A_7,02'-G_B_18,N3-G_B_18 |                         |
| 3la5| C_A_54   | HOH_A_432 | O2'-A_A_24,N3-A_A_24,04'-C_A_53 |                         |
| 3gvrn| 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,OS^-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,OS^-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,OH-MA_A_199,OH-MA_B_193,OH-MA_B_202,OH-MA_B_202 | 
| 3nj7 | A_A_7  | HOH_A_21  | N7-G_A_8,OH-MA_A_46,OH-MA_A_64,OH-MA_A_65 | 
| 3nj6 | A_A_7  | HOH_A_68  | N7-G_A_8,OH-MA_A_16,OH-MA_A_22,OH-MA_A_33 | 
| 3nj7 | A_B_7  | HOH_B_17  | N7-G_B_8,OH-MA_B_34,OH-MA_B_110 | 
| 3nj7 | A_C_7  | HOH_C_18  | N7-G_C_8,OH-MA_C_26,OH-MA_C_50,OH-MA_C_168 | 
| 3nj7 | A_D_7  | HOH_D_15  | N7-G_D_8,OH-MA_D_44,OH-MA_D_102 | 
| 3nj7 | A_E_7  | HOH_E_24  | N7-G_E_8,OH-MA_E_38,OH-MA_E_107 | 
| 3nj7 | A_F_7  | HOH_F_20  | N7-G_F_8,OH-MA_E_159,OH-MA_F_48,OH-MA_F_175 | 
| 2a43 | A_A_24 | HOH_A_544 | O5^-A_A_25,OH-MA_A_551,OH-MA_A_602 | 
| 3tzzr | A_A_53 | HOH_B_59  | N7-G_B_107,OH-MA_B_26,OH-MA_B_22 | 
| 1k8w | A_B_413 | HOH_A_523 | OP1-G_B_412,OH-MA_B_526,OH-MA_B_535 | 
| 4kyy | U_B_8  | HOH_B_202 | OP2-U_B_9,OH-MA_B_207,OH-MA_B_236 | 
| 1f27 | U_A_7  | HOH_A_87  | O6-G_B_27,OH-MA_A_44,OH-MA_A_94,OH-MA_A_129 | 
| 3k62 | U_B_1  | HOH_A_13  | OG-SER_A_554,OH-MA_A_18,OH-MA_A_83 | 
| 2gdi | U_X_28 | HOH_X_352 | O6-G_X_31,OH-MA_X_216,OH-MA_X_412 | 
| 3k64 | U_B_1  | HOH_A_19  | OG-SER_A_554,OH-MA_A_24,OH-MA_A_115 | 
| 2yy6 | U_A_13 | HOH_A_169 | OP2-C_A_15,OH-MA_A_179,OH-MA_A_182 | 
| 3fo4 | U_A_34 | HOH_A_337 | N7-A_A_64,OH-MA_A_446,OH-MA_A_457 | 
| 2awe | U_A_4  | HOH_A_227 | OP2-G_A_5,OH-MA_A_222,OH-MA_D_49,OH-MA_D_64 | 
| 2g91 | U_A_3  | HOH_A_116 | N7-G_A_4,OH-MA_A_120,OH-MA_A_162,OH-MA_A_172,OH-MA_A_180,OH-MA_A_184 | 
| 1jzv | U_B_12 | HOH_B_352 | OP2-C_B_14,OH-MA_B_312,OH-MA_B_351 | 
| 1jzv | U_D_32 | HOH_D_318 | OP1-C_D_34,OH-MA_D_310,OH-MA_D_356 | 
| 2i82 | U_E_1209 | HOH_A_2019 | O4-U_E_1215,OH-MA_E_2074,OH-MA_E_2198 |
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
| PDB  | Chain 1  | Chain 2  | Description                                    |
|------|----------|----------|------------------------------------------------|
| 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                                   |
| 1m8y | A_C_11   | HOH_C_50 | O-HOH_C_30                                    |
| 3ivn | A_D_11   | HOH_D_218| OP2-A_D_16                                    |
| 4ibk | 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                                   |

Instances corresponding to Figure S4d, where single acceptor/water is present near the O\textsuperscript{W}
|   |   |   |   |
|---|---|---|---|
| 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 |
| 1uf | 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 |
| 4jtl | 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 |
| 4ttx | 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 |
| PDB Code | Atoms | Bonds | Notes |
|----------|-------|-------|-------|
| 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 |
| 2qby     | 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 |
| 2qw4     | G_A_5 | HOH_A_1153 | N7-G_A_6 |
| 2y8w     | G_B_24 | HOH_B_2079 | O-HOH_B_2072 |
| Code | Chain | HOH | Atom 1 | Atom 2 |
|------|-------|------|--------|--------|
| 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 |
| 3rlc | 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_j_521 | OD2-ASP_J_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_2814 |
| 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 |
| Code  | Atom  | Atom  | Atom   |
|-------|-------|-------|--------|
| 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 |
| 1q8y  | 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 |
| 1z87  | 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.

| Distance (Å) | Ip-π cc-pVTZ (kcal/mol) | Ip-π cc-pVQZ (kcal/mol) | Ip-π CBS (kcal/mol) | OH-π cc-pVTZ (kcal/mol) | OH-π cc-pVQZ (kcal/mol) | OH-π 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.

| Distance (Å) | lp-π cc-pvTZ (kcal/mol) | cc-pvQZ (kcal/mol) | CBS (kcal/mol) | OH-π 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.

| Distance (Å) | lp-π cc-pvTZ (kcal/mol) | lp-π cc-pvQZ (kcal/mol) | lp-π CBS (kcal/mol) | OH-π cc-pvTZ (kcal/mol) | OH-π cc-pvQZ (kcal/mol) | OH-π 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.

| Distance (Å) | lp-π cc-pvTZ (kcal/mol) | lp-π cc-pvQZ (kcal/mol) | lp-π CBS (kcal/mol) | OH-π cc-pvTZ (kcal/mol) | OH-π cc-pvQZ (kcal/mol) | OH-π 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.

| Distance (Å) | lp-π cc-pvTZ (kcal/mol) | lp-π cc-pvQZ (kcal/mol) | lp-π CBS (kcal/mol) | OH-π cc-pvTZ (kcal/mol) | OH-π cc-pvQZ (kcal/mol) | OH-π 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                  |