

Supplementary Materials

Structure of RNA:DNA dodecamer corresponding to HIV-1 polypurine tract at 1.6 Å resolution

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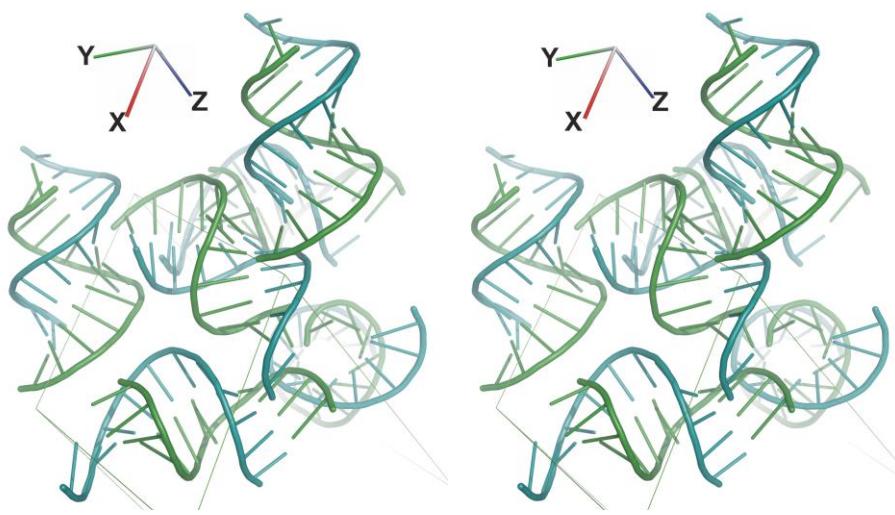
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Supplementary Table S1. Interactions of water molecules with nucleic acids atoms and with Mg^{2+} ions.

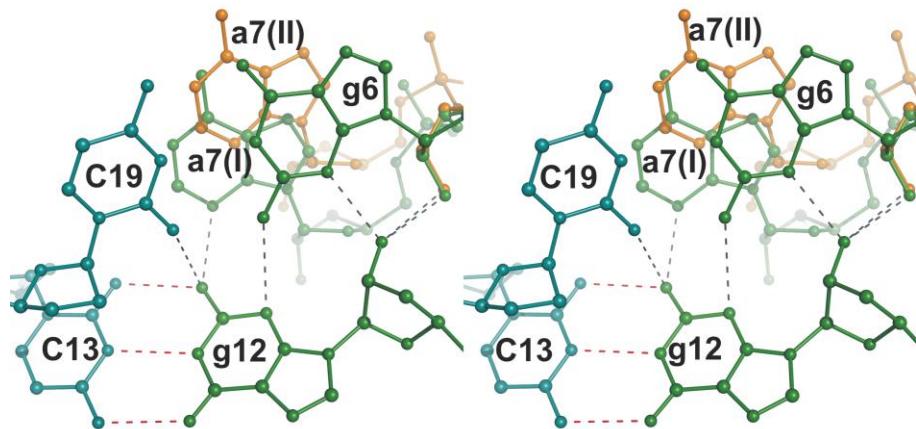
Water – RNA H-bond	Distance (Å)	Water – DNA H-bond	Distance (Å)	Water – Mg^{2+}	Distance (Å)
W18 – N3 (a3)	2.78	W2 – O2P (T22)	2.61	W44 – Mg^{2+} (1)	1.86
W1 – O2' (a3)	2.75	W4 – O2P (T18)	2.95	W45 – Mg^{2+} (1)	2.03
W21 – N3 (a2)	2.82	W4 – O5' (T18)	3.25	W46 – Mg^{2+} (1)	1.73
W22 – O1P (g12)	2.71	W4 – O2P (C19)	2.74	W57 – Mg^{2+} (1)	1.85
W23 – O2P (g12)	2.63	W5 – N4 (C14)	2.91	W42 – Mg^{2+} (2)	2.00
W24 – N3 (a9)	2.79	W24 – O2 (T17)	3.43	W43 – Mg^{2+} (2)	2.05
W25 – O2' (a8 I)	2.82	W10 – O4 (T23)	2.71	W56 – Mg^{2+} (2)	1.83
W32 – O2' (a8 I)	2.61	W11 – N3 (A24)	2.85	W59 – Mg^{2+} (2)	1.99
W25 – O3' (a8 I)	3.42	W27 – O4 (T15)	2.68	W69 – Mg^{2+} (2)	1.99
W26 – N7 (g12)	2.85	W28 – O1P (T22)	2.92	W63 – Mg^{2+} (3)	1.98
W26 – O2P (g12)	2.78	W29 – O2P (T23)	3.03	W64 – Mg^{2+} (3)	1.94
W32 – O4' (a9)	3.14	W29 – O5' (T23)	3.34		
W33 – O2' (a5)	2.58	W30 – O2P (T23)	3.04		
W33 – O4' (g6)	3.20	W31 – O4 (T22)	2.61		
W15 – N3 (a4)	2.66	W26 – O2 (T17)	2.74		
W16 – O2P (g6)	2.72	W32 – O3' (A24)	2.99		
W16 – O3' (g6)	3.39	W33 – O4' (A24)	3.25		
W16 – O2P (a7 II)	3.13	W33 – O2 (T23)	2.80		
W16 – N7 (a7 II)	3.41	W34 – O4' (T18)	3.41		
W17 – N7 (a10)	2.90	W35 – O4 (T21)	2.73		
W17 – O2P (a10)	3.10	W39 – N4 (C19)	3.01		
W19 – N6 (a9)	2.83	W40 – O4 (T20)	2.70		
W20 – O2' (g11)	2.76	W41 – O2P (C19)	3.30		
W20 – O3' (g11)	3.20	W41 – O5' (C19)	3.50		
W31 – N6 (a2)	3.36	W43 – O1P (C19)	3.06		
W27 – N7 (a4)	2.93	W51 – O4 (T16)	2.72		
W27 – O2P (a4)	3.05	W58 – O2P (T17)	2.84		
W28 – N6 (a10)	3.01	W62 – O2 (T22)	2.91		
W29 – O1P (a8 I)	3.49	W62 – O4' (T23)	3.19		
W30 – O2P (g11)	2.72	W69 – O1P (C19)	3.14		
W31 – O2' (a4)	2.61				
W36 – N6 (a4)	2.95				
W44 – N7 (a10)	3.20				
W44 – N7 (g11)	2.99				
W46 – O6 (g11)	3.33				
W46 – O6 (g12)	3.26				
W48 – O2P (a10)	2.71				
W48 – O5' (a10)	3.38				
W48 – O2P (g11)	2.78				
W55 – O1P (g11)	2.76				
W60 – O1P (a3)	2.85				
W65 – O1P (a2 I)	3.23				
W65 – O1P (a2 II)	3.09				
W75 – O2P (a2 I)	2.52				
W75 – O2P (a2 II)	3.12				
W75 – O5' (a2 I)	3.19				
W76 – O2P (a7 I)	2.98				
W76 – O2P (a8 I)	2.71				

Supplementary Table S2. Crystal packing contacts between nucleic acids molecules.

ASU atom	Symmetry-related atom	Distance (Å)
N3 (u1)	O3' (a10)	2.94
O2' (a2)	O2' (a9)	2.54
O2' (a3)	O4' (T17)	3.15
O2' (g6 I)	O2' (12g)	2.83
O2' (g6 II)	O2' (12g)	3.13
N3 (g6)	O2' (12g)	2.65
N2 (g6)	N3 (12g)	3.08
O2' (a7 I)	O4' (T15)	3.02
O2' (a7 I)	O2 (C14)	2.72
O2' (a9)	O4' (a2)	3.35
O2' (a10)	N7 (A24)	2.69
O3' (a10)	O2 (u1)	3.25
O4' (g11)	N7 (A24)	3.15
N2 (g12)	N3 (a7 I)	2.76
N2 (g12)	O2 (C19)	3.10
O4' (T20)	N1 (g12)	3.47
O2 (T20)	O3' (g12)	3.36
O3' (A24)	O2 (T15)	3.19
N6 (A24)	O2' (a10)	3.42
O3' (A24)	N2 (g11)	3.46



Supplementary Figure S1. Crystal packing of the RNA:DNA molecules in the present structure. The RNA strand is shown in green, the DNA strand is shown in cyan.



Supplementary Figure S2. The $\text{g}_6\cdot\text{a}_7\cdot\text{C}_{19}\cdot(\text{g}_{12}\cdot\text{C}_{13})$ pentaplex interaction resulting from the abutting crystal packing, shown in stereoview. Hydrogen bonds with symmetry-related molecules are shown in grey. The hydrogen-bond distances are between 2.65-3.13 Å.