Supplementary information

First crystal structures of DNA:2'-*O*-methyl-RNA heteroduplexes

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Table S1. Backbone and glycosyl torsion angles.

Residue	α (°)	β (°)	γ (°)	δ (°)	ε (°)	ζ (°)	χ (°)	φ (°)	P (°)	Puckering
Overhanged DNA:2′-OMe-RNA										
Chain A (DNA)										
dT1	–	–	50.8	81.5	-148.6	-69.5	-158.6	41.7	14.5	C3'-endo
dC2	-62.7	171.3	55.1	81.9	-154.4	-74.3	-164.5	40.3	18.7	C3'-endo
dT3	-67.0	179.0	48.6	82.1	-147.9	-69.1	-156.4	40.9	16.8	C3'-endo
dC4	-70.3	169.0	55.4	77.8	-150.2	-72.2	-161.1	45.3	16.1	C3'-endo
dC5	-61.1	172.0	54.9	79.5	-156.3	-78.4	-165.5	43.2	17.6	C3'-endo
dT6	-60.7	-179.4	44.0	79.2	-144.6	-69.7	-159.1	43.9	14.9	C3'-endo
dA7	-68.8	164.4	62.1	78.7	-155.1	-73.3	-168.9	43.8	18.4	C3'-endo
dG8	-60.2	171.8	57.3	84.8	-150.9	-72.4	-160.0	37.4	15.7	C3'-endo
Chain B (2′-OMe-RNA)										
Am8	-57.3	177.1	52.9	81.4	-142.5	-72.8	-161.0	42.0	13.9	C3'-endo
Gm7	-63.1	167.6	60.1	74.2	-154.6	-76.0	-166.8	42.8	15.4	C3'-endo
Am6	-77.4	-170.6	52.2	78.6	-148.3	-69.6	-167.4	44.0	10.6	C3'-endo
Gm5	-63.6	178.2	56.7	81.0	-152.9	-68.1	-172.2	38.5	10.1	C3'-endo
Gm4	129.5	-162.1	-163.2	76.4	-154.2	-75.8	-172.4	41.5	12.4	C3'-endo
Am3	-73.2	-169.0	44.5	81.6	-151.5	-68.3	-150.2	40.3	14.8	C3'-endo
Um2	-62.9	172.5	54.3	82.5	-152.3	-66.7	-161.6	36.7	11.0	C3'-endo
Cm1	–	–	60.6	79.3	-145.0	-76.8	-164.5	38.6	14.5	C3'-endo
Blunt-ended DNA:2′-OMe-RNA										
MOL1: Chain A (DNA)										
dG1	–	–	51.0	89.6	-149.2	-74.0	-169.8	36.2	4.4	C3'-endo
dT2	-69.8	173.3	52.1	82.7	-146.9	-70.7	-160.7	41.9	14.9	C3'-endo
dC3	-66.2	159.9	63.8	79.7	-166.3	-68.4	-166.3	42.5	18.8	C3'-endo
dT4	-72.1	-177.4	55.8	84.5	-154.9	-70.7	-158.3	39.8	18.0	C3'-endo
dC5	-59.1	172.4	46.3	82.5	-160.4	-65.5	-156.7	40.0	16.1	C3'-endo
dC6	139.5	-173.2	-170.1	88.4	-154.4	-72.9	-171.0	38.6	5.9	C3'-endo
dT7	-62.9	178.5	53.1	90.7	-159.3	-73.3	-158.6	32.2	22.7	C3'-endo
dA8	-64.7	-173.3	57.7	146.0	-172.8	-99.0	-116.9	38.6	163.4	C2'-endo
dG9	-58.0	-176.1	35.4	141.0	–	–	-108.6	40.6	153.5	C2'-endo
MOL1: Chain B (2′-OMe-RNA)										
Cm9	-61.4	169.2	49.1	78.6	–	–	-160.0	41.2	13.4	C3'-endo
Am8	-68.5	176.5	53.0	81.5	-150.9	-70.8	-160.4	44.7	13.7	C3'-endo
Gm7	142.3	-165.4	-171.4	85.8	-147.4	-82.4	-175.0	35.7	8.7	C3'-endo
Am6	-51.2	168.0	53.4	79.4	-157.6	-66.8	-163.7	42.4	12.0	C3'-endo

Gm5	-59.4	176.9	47.8	77.8	-149.7	-77.0	-168.2	43.0	12.1	C3'-endo
Gm4	149.2	-166.2	-176.3	82.5	-143.2	-78.1	180.0	38.2	10.1	C3'-endo
Am3	-55.1	170.5	44.3	79.8	-164.9	-69.4	-155.6	42.9	12.0	C3'-endo
Um2	-62.5	172.2	50.2	80.4	-142.4	-73.4	-162.9	39.9	13.3	C3'-endo
Cm1	–	–	61.4	78.4	-150.8	-73.3	-167.1	41.4	12.0	C3'-endo
MOL2: Chain C (DNA)										
dG1	–	–	47.8	89.0	-146.8	-72.0	-174.4	36.1	2.1	C3'-endo
dT2	-61.9	-179.2	43.6	86.1	-165.2	-76.5	-154.8	37.7	14.1	C3'-endo
dC3	133.5	-166.6	-169.1	97.0	-130.7	-80.0	-173.3	36.8	343.6	C2'-exo
dT4	-59.2	172.5	46.7	85.1	-158.0	-74.2	-153.7	38.0	22.5	C3'-endo
dC5	-63.3	168.9	49.3	81.8	-151.4	-73.2	-152.4	41.1	17.1	C3'-endo
dC6	-64.5	173.0	53.4	82.6	-154.3	-67.0	-157.3	41.9	20.1	C3'-endo
dT7	-73.9	177.0	56.4	81.1	-151.4	-71.6	-157.0	43.1	15.6	C3'-endo
dA8	-66.3	-177.7	47.4	85.6	-157.7	-76.3	-145.3	36.8	28.7	C3'-endo
dG9	-72.5	-165.3	41.0	92.0	–	–	-119.0	32.1	6.6	C3'-endo
MOL2: Chain D (2′-OMe-RNA)										
Cm9	-65.2	175.2	51.9	77.1	–	–	-156.8	39.5	15.1	C3'-endo
Am8	-61.3	173.3	48.0	77.4	-155.9	-66.4	-157.4	44.9	16.1	C3'-endo
Gm7	149.4	-167.8	-174.0	87.0	-138.7	-78.3	-172.3	33.9	2.5	C3'-endo
Am6	-61.5	171.7	52.9	80.2	-164.6	-70.8	-161.3	43.2	18.0	C3'-endo
Gm5	-64.0	171.4	57.0	78.1	-148.3	-76.0	-166.7	40.8	16.6	C3'-endo
Gm4	-69.2	168.4	53.5	78.3	-147.7	-72.8	-168.5	41.8	15.5	C3'-endo
Am3	136.9	-169.3	-171.1	87.9	-135.3	-77.6	-166.8	38.9	357.0	C2'-exo
Um2	-61.9	166.3	55.7	81.6	-158.3	-74.0	-150.8	37.8	18.6	C3'-endo
Cm1	–	–	53.6	79.3	-148.7	-77.0	-158.4	39.1	21.1	C3'-endo
A-DNA	-50	172	42	79	-146	-79	-154			
A-RNA	-68	178	54	82	-153	-71	-158			

Table S2. Dihedral angles C1′-C2′-O2′-CM2 calculated for all 2′-OMe-RNA residues.

	7OW0	**7OXS**	
Residue	**Chain B**	**Chain B**	**Chain D**
Cm1	78.1	85.4	64.5
Um2	83.0	72.1	83.1
Am3	117.1	75.1	76.1
Gm4	79.2	76.6	86.1
Gm5	81.9	78.3	72.2
Am6	78.2	147.2	62.5
Gm7	72.4	71.6	76.1
Am8	86.9	66.0	62.6
Cm9	93.4	73.7	75.3

Table S3. Distances between water molecules and non-hydrogen nucleic acid atoms or Zn^{2+} ions for overhanged DNA:2′-OMe-RNA duplex (PDB ID: 7OW0). The symmetry operation is not indicated, when both heavy atoms belong to the same asymmetric unit.

A. Distances between non-hydrogen nucleic acid atoms and water molecules							
Strand DNA (A)				Strand 2′-OMe-RNA (B)			
(Residue) atom type	Symmetry operation	Water number	Distance (Å)	(Residue) atom type	Symmetry operation	Water number	Distance (Å)
(dT1) O5′		HOH209(A)	3.03	(Cm1) N4		HOH229(B)	3.13
(dT1) O4		HOH210(A)	2.67	(Um2) OP1	y, x, -z	HOH201(A)	2.48
(dC2) OP1		HOH208(A)	2.66	(Um2) OP2		HOH215(B)	2.77
(dC2) OP1		HOH212(A)	2.72	(Um2) O5′		HOH215(B)	3.20
(dC2) OP2		HOH209(A)	2.67	(Um2) O2		HOH213(B)	2.74
(dC2) O2		HOH206(A)	2.65	(Am3) OP2		HOH207(B)	2.62
(dC2) N4		HOH229(A)	2.98	(Am3) O5′		HOH207(B)	2.78
(dT3) OP2		HOH211(A)	2.71	(Am3) O3′	y, x, -z	HOH213(B)	3.13
(dT3) OP2		HOH224(A)	3.04	(Am3) O2′	y, x, -z	HOH213(B)	3.07
(dT3) O2		HOH223(A)	2.86	(Am3) N3		HOH220(B)	2.90
(dT3) O4		HOH221(A)	2.83	(Am3) N7		HOH210(B)	2.68
(dC4) OP1		HOH213(A)	2.75	(Gm4) OP2		HOH201(B)	2.33
(dC4) OP1		HOH218(A)	2.82	(Gm4) OP2		HOH207(B)	2.70
(dC4) OP2		HOH219(A)	3.05	(Gm4) N2		HOH224(B)	3.03
(dC4) OP2		HOH224(A)	2.88	(Gm4) O6		HOH203(B)	2.54
(dC4) N4		HOH228(A)	2.96	(Gm4) N7		HOH210(B)	3.15
(dC5) OP1		HOH201(A)	2.32	(Gm4) N7		HOH226(B)	3.12
(dC5) OP1		HOH215(A)	2.77	(Gm5) OP1	y, x, -z	HOH202(A)	2.71
(dC5) OP2		HOH219(A)	2.82	(Gm5) OP2		HOH205(B)	2.89
(dC5) OP2		HOH231(A)	3.05	(Gm5) OP2		HOH217(B)	2.83
(dC5) O2	x+½, -y+½, -z+¼	HOH209(B)	2.99	(Gm5) O6		HOH204(B)	2.58
(dC5) N4		HOH234(A)	3.11	(Gm5) N7		HOH205(B)	2.60
(dT6) OP1		HOH220(A)	2.83	(Am6) OP1		HOH202(B)	2.49
(dT6) OP2		HOH216(A)	2.79	(Am6) OP2		HOH218(B)	2.87
(dT6) O3′		HOH204(A)	2.74	(Am6) N3		HOH228(B)	3.13
(dT6) O4		HOH226(A)	2.90	(Am6) N6		HOH233(B)	3.19
(dA7) OP1		HOH204(A)	2.55	(Am6) N7		HOH206(B)	2.62
(dA7) OP2		HOH216(A)	3.06	(Gm7) OP1		HOH211(B)	2.69
(dA7) OP2		HOH227(A)	2.95	(Gm7) OP2		HOH202(B)	2.62
(dA7) O3′		HOH217(A)	3.19	(Gm7) OP2		HOH214(B)	2.74
(dA7) N7		HOH214(A)	2.75	(Gm7) N2		HOH225(B)	3.11
(dG8) OP1		HOH217(A)	2.80	(Gm7) O6		HOH219(B)	2.88
(dG8) OP2		HOH225(A)	2.88	(Gm7) N7		HOH222(B)	2.93
(dG8) OP2		HOH233(A)	3.10	(Am8) OP1	x+½, -y+½, -z+¼	HOH212(A)	2.76
(dG8) N3		HOH222(A)	2.85	(Am8) OP2		HOH216(B)	2.86
(dG8) O6		HOH203(A)	2.51	(Am8) OP2		HOH221(B)	2.91
(dG8) O6		HOH205(A)	2.95	(Am8) O2′		HOH223(B)	2.98
(dG8) N7		HOH203(A)	3.04	(Am8) N3		HOH231(B)	3.15
(dG8) N7		HOH225(A)	3.02	(Am8) N6		HOH232(B)	3.19
(dG8) OP1		HOH202(A)	2.48	(Am8) N7		HOH216(B)	2.80
(dG8) OP2		HOH207(A)	2.65	(Cm9) OP1		HOH208(B)	2.62
(dG8) O4′		HOH222(A)	2.85	(Cm9) OP1		HOH227(B)	3.12
(dG8) N2		HOH232(A)	3.10	(Cm9) OP2		HOH221(B)	3.16
(dG8) O6		HOH205(A)	2.60	(Cm9) O2′		HOH209(B)	2.67

(dG8) N7	HOH230(A)	3.04	(Cm9) O2′	HOH212(B)	2.92
			(Cm9) N4	HOH230(B)	3.14
B. Distances between zinc ions and water molecules					
Zn101(A)	HOH203(A)	2.25	Zn101(B)	HOH203(B)	2.16
Zn101(A)	HOH225(A)	2.17	Zn101(B)	HOH210(B)	2.16
Zn101(A)	HOH230(A)	2.10	Zn101(B)	HOH226(B)	2.18
Zn101(A)	HOH233(A)	2.14	Zn101(B)	HOH234(B)	2.23
Zn101(A)	HOH244(A)	2.14	Zn101(B)	HOH243(B)	2.29
			Zn102(B)	HOH206(B)	2.80
			Zn102(B)	HOH214(B)	2.24
			Zn102(B)	HOH219(B)	2.06
			Zn102(B)	HOH222(B)	2.07
			Zn102(B)	HOH240(B)	2.34

Table S4. Distances between water molecules and non-hydrogen nucleic acid atoms or SO_4^{2-} ions for blunt-ended DNA:2′-OMe-RNA duplex (PDB ID: 7OXS). The symmetry operation is not indicated, when both heavy atoms belong to the same asymmetric unit.

A. Distances between non-hydrogen nucleic acid atoms and water molecules							
Strand DNA (A)				Strand 2′-OMe-RNA (B)			
(Residue) atom type	Symmetry operation	Water number	Distance (Å)	(Residue) atom type	Symmetry operation	Water number	Distance (Å)
(dG1) O5′		HOH203(A)	2.71	(Cm1) O2′		HOH118(B)	2.96
(dG1) O5′		HOH215(A)	2.87	(Cm1) O5′		HOH120(B)	3.02
(dG1) O6		HOH204(A)	2.59	(Um2) O4		HOH105(B)	2.78
(dG1) N7		HOH209(A)	2.73	(Am3) N3		HOH105(B)	2.93
(dT2) OP2		HOH203(A)	2.55	(Am3) N6		HOH116(B)	3.13
(dT2) OP2		HOH210(A)	2.76	(Gm4) N2		HOH122(B)	3.11
(dT2) O5′		HOH210(A)	3.08	(Gm4) O6		HOH103(B)	3.16
(dT2) O4		HOH211(A)	2.76	(Gm4) O6		HOH106(B)	3.14
(dC3) OP2		HOH210(A)	2.99	(Gm4) N7		HOH106(B)	2.78
(dC3) N4		HOH220(A)	3.15	(Gm5) N2		HOH124(B)	3.12
(dT4) OP1		HOH213(A)	2.83	(Gm5) O6		HOH103(B)	2.71
(dT4) OP2		HOH216(A)	2.87	(Gm5) N7		HOH114(B)	2.91
(dT4) O4		HOH207(A)	2.69	(Am6) OP1		HOH101(B)	2.47
(dC6) OP1		HOH219(A)	3.07	(Am6) OP2		HOH104(B)	2.77
(dC6) OP1	y, x, -z	HOH105(D)	2.95	(Am6) OP2		HOH119(B)	3.02
(dC6) OP2		HOH201(A)	2.29	(Am6) N3		HOH111(B)	2.87
(dC6) OP2		HOH217(A)	2.97	(Am6) N6		HOH115(B)	2.92
(dC6) O2		HOH218(A)	3.02	(Gm7) OP1		HOH109(B)	2.81
(dT7) OP2		HOH205(A)	2.51	(Gm7) OP2		HOH102(B)	2.56
(dT7) O4		HOH206(A)	2.64	(Gm7) O6		HOH108(B)	2.81
(dA8) N3		HOH214(A)	2.71	(Gm7) O6		HOH125(B)	3.16
(dA8) N7		HOH208(A)	2.86	(Gm7) N7		HOH110(B)	2.82
(dG9) OP2		HOH212(A)	2.80	(Am8) OP1		HOH107(B)	2.80
(dG9) O6		HOH202(A)	2.45	(Am8) OP2		HOH112(B)	2.88
				(Am8) O2′		HOH113(B)	2.89
				(Am8) N7		HOH117(B)	2.95
				(Cm9) OP2		HOH107(B)	3.06
				(Cm9) OP2		HOH112(B)	2.98
				(Cm9) O3′		HOH123(B)	3.12

			(Cm9) O3′	-y, x-y, z+⅔	HOH118(B)	3.17
			(Cm9) N4		HOH121(B)	3.05
Strand DNA (C)			Strand 2′-OMe-RNA (D)			
(dG1) N3	HOH206(C)	2.90	(Um2) O2′		HOH104(D)	2.82
(dG1) O6	HOH201(C)	2.53	(Um2) O3′		HOH104(D)	3.08
(dT2) OP2	HOH207(C)	2.94	(Um2) O4		HOH103(D)	3.09
(dT4) OP2	HOH205(C)	2.88	(Am4) N6		HOH103(D)	3.05
(dC6) OP1	HOH209(C)	3.16	(Am4) N7		HOH103(D)	2.68
(dT7) O4	HOH202(C)	2.71	(Gm5) OP1		HOH105(D)	2.91
(dG9) O3′	HOH204(C)	2.85	(Gm5) O2′		HOH106(D)	2.96
(dG9) O6	HOH203(C)	2.76	(Gm5) N2		HOH108(D)	3.05
(dG9) N7	HOH208(C)	2.99	(Am6) OP1		HOH107(D)	3.01
			(Gm7) O6		HOH102(D)	2.64
			(Am8) N7		HOH101(D)	2.61
B. Distances between sulfate ions and water molecules						
$SO_4$101(A) O2	HOH216(A)	3.04	$SO_4$101(C) O1		HOH205(C)	2.88
			$SO_4$101(C) O2		HOH103(D)	2.90
			$SO_4$101(C) O4		HOH202(C)	2.78