Supplementary Information

SI Figure 1 NMR structure of the EMCV 16mer apo RNA shown as an ensemble of the 10 lowest energy and RMSD (Å) structures **(A)**, and the final NMR structure **(B)**. The four residues of the $G_{547}CGA_{550}$ tetraloop are labelled. **(C)** Conformation of the $G_{547}CGA_{550}$ tetraloop motif of the 16mer RNA, with the flanking stem $G_{546}.C_{551}$ base pair drawn from the NMR structure and (**D**) scheme showing the hydrogen bonding and internucleotide base-phosphate, sugar-phosphate, and base-sugar interactions (dotted lines) which are ≤ 3.5Å. Other representations are as follows: black circles, sugar moiety; blue circles, phosphate group; black box, base; red filled box, base stacking; solid lines, glycosidic and phosphodiester bonds.

SI Figure 2 NMR structure of the EMCV 17mer apo RNA shown as an ensemble of the 10 lowest energy and RMSD (Å) structures **(A),** and the final NMR structure **(B).** The residues of the heptaloop motif (A607-A613) are labelled. **(C)** Conformation of the heptaloop motif of the 17mer RNA, with the flanking stem $C_{606}.G_{614}$ base-pair drawn from the NMR structure and **(D)** scheme showing the hydrogen bonding and internucleotide base-phosphate, sugar-phosphate, and base-sugar interactions (dotted lines) which are ≤ 3.5Å. Other representations are as follows: black circles, sugar moiety; blue circles, phosphate group; black box, base; red filled box, base stacking; solid lines, glycosidic and phosphodiester bonds. There is no red filled box between residues 5'C and 1A as no base stacking was observed.

SI Figure3 400 MHz ^{1}H- NMR titration (imino proton region) of the 17mer RNA (0.53mM) with Mg^{2+} (molar equivalents), dissolved in 90% $^{1}H_2O$ and 10% $^{2}H_2O$ containing 20 mM PO_4^{3-} (pH 6.2) and 20 mM NaCl at 5ºC.

SI Table 1 ^{1}H, ^{13}C and ^{31}P Chemical shift table (ppm) of the EMCV **(A)** 16mer apo RNA, **(B)** 16mer RNA/Mg^{2+} complex, **(C)** 17mer apo RNA and **(D)** 17mer RNA/Mg^{2+} complex. The exchangeable and non-exchangeable proton resonances were measured at 2ºC and 25ºC, respectively. Hydrogen bonded amino protons are denoted with an asterisk *.

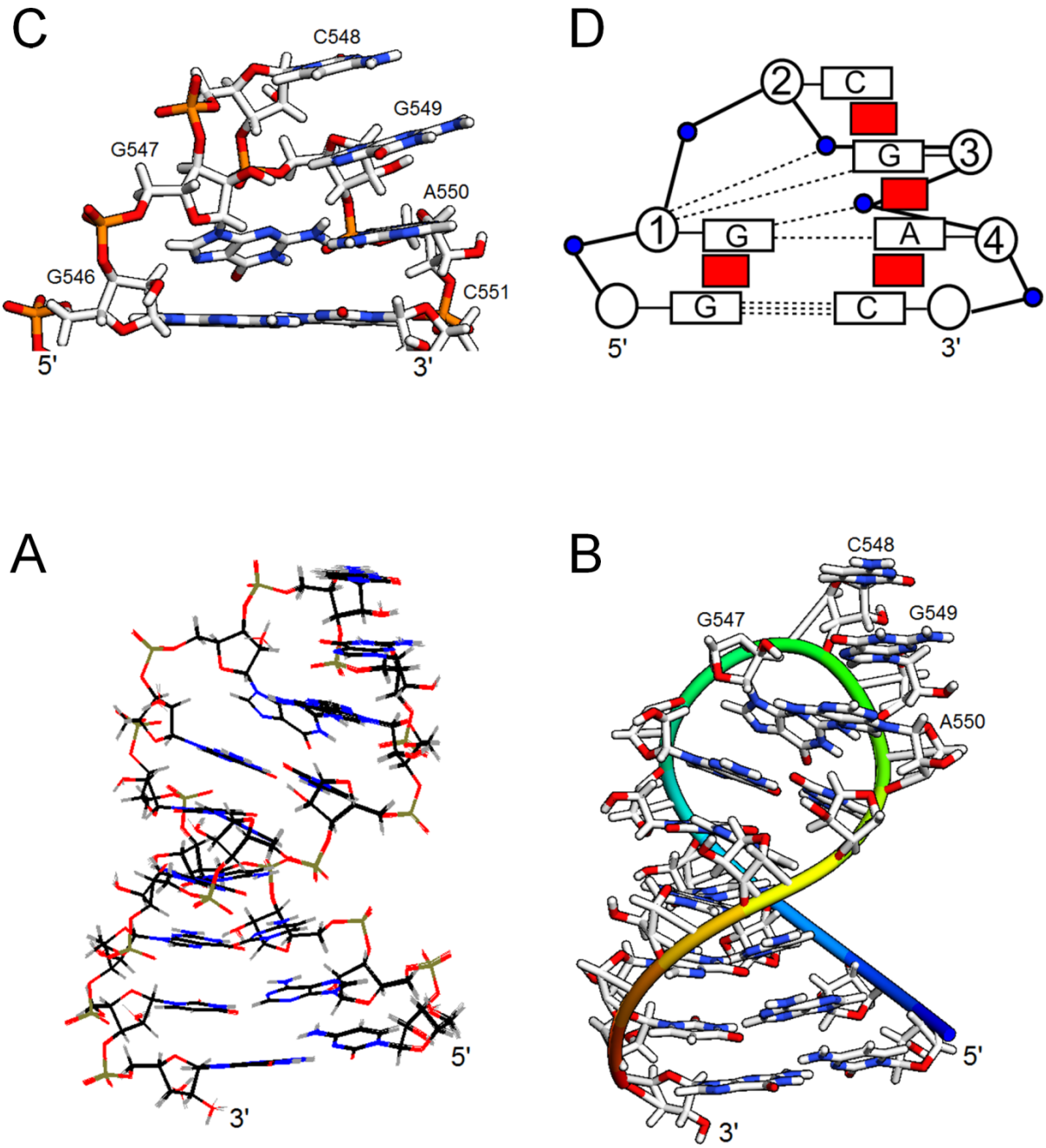
SI Table 2A. Local base-pair, base-pair helical and base-pair step parameters for the 16mer RNA. The usual range observed for A-form helices is also given for each parameter. Angles (º) are represented to 1dp and distances (Å) to 2dp.

SI Table 2B. Local base-pair, base-pair helical and base-pair step parameters for the 16mer Mg^{2+} RNA. Angles (º) are represented to 1dp and distances (Å) to 2dp. The usual range observed for A-form helices is also given for each parameter. Values highlighted in yellow and cyan indicate a change towards and away from A-form conformation when compared with the apo 16mer RNA.

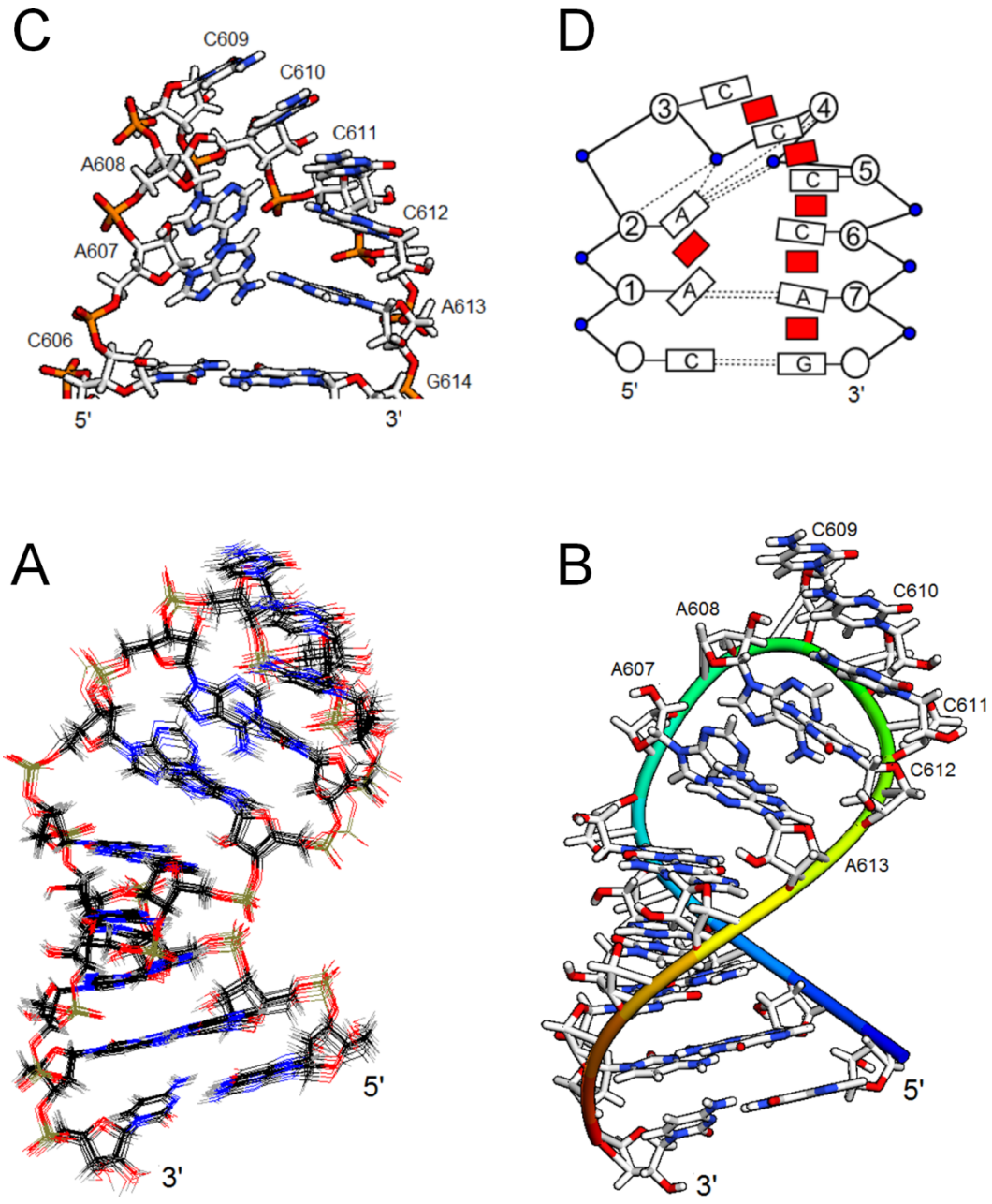
SI Table 2C. Local base-pair, base-pair helical and base-pair step parameters for the 17mer RNA. Angles (º) are represented to 1dp and distances (Å) to 2dp. The usual range observed for A-form helices is also given for each parameter.

SI Table 2D. Local base-pair, base-pair helical and base-pair step parameters for the 17mer Mg^{2+} RNA. Angles (º) are represented to 1dp and distances (Å) to 2dp. The usual range observed for A-form helices is also given for each parameter. Values highlighted in yellow and cyan indicate a change towards and away from A-form conformation when compared with the apo 17mer RNA.

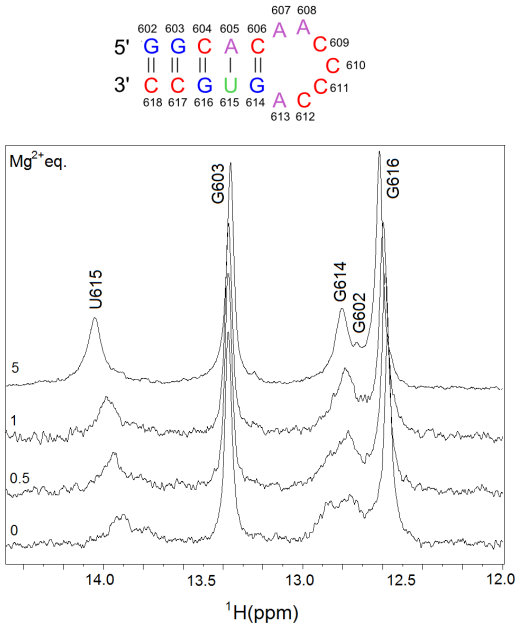
Supplementary Information Figure 1



Supplementary Information Figure 2



Supplementary Information Figure 3



Supplementary Information Table 1A.

Residue		NH	NH_2	NH_2^*	H2	H5	H6	H8	H1'	H2'	H3'	H4'	H5'	H5"	C2	C5	C6	C8	C1'	C2'	C3'	C4'	C5'	^{31}P
C	541		7.26	8.50		6.07	8.17		5.56	4.56	4.64	4.38	3.99	4.10		98.9	143.0		93.7	75.5	73.5	84.4	61.9	-
A	542		6.62	8.11	7.69			8.35	6.05	4.63	4.85	-	-	-	153.7			139.8	92.6	75.8	73.4	-	-	-
C	543		7.08	8.53		5.36	7.66		5.50	4.29	-	-	-	-		97.3	140.8		93.7	75.7	-	-	-	-
C	544		7.00	8.52		5.52	7.80		5.52	4.34	-	-	-	-		97.8	141.3		94.2	75.6	-	-	-	-
U	545	13.59				5.44	7.93		5.54	4.44	4.66	-	-	-		103.7	141.6		94.2	75.2	72.0	-	-	-
G	546	12.27	5.82	8.16				7.72	5.89	4.53	-	-	-	-				136.2	92.4	75.8		-	-	1.35
G	547	10.46	-	-				7.09	5.53	4.50	4.42	-	-	-				135.8	93.6	73.8	72.4	-	-	4.22
C	548		-	-		5.44	7.70		5.39	4.42	4.07	-	3.80	4.21		97.5	142.6		93.3	75.8	72.3	-	64.0	2.88
G	549	10.54	-	-				7.65	5.44	4.35	4.28	-	-	-				137.1	92.5	-	-	-	-	-0.85
A	550		-	-	8.27			8.15	6.11	4.47	4.86	4.15	-	-	155.6			139.9	91.7	76.8	72.9	82.6	-	2.86
C	551		7.02	8.61		6.06	7.89		3.83	4.41	4.16	-	-	-		99.7	141.6		95.2	74.4	72.3	-	-	-
A	552		6.45	7.72	7.04			8.09	5.96	4.67	4.78	-	-	-	152.2			139.9	92.6	75.9	72.2	-	-	-
G	553	12.99	6.05	8.32				7.17	5.58	4.52	4.45	-	-	-				135.7	93.7	75.5	72.9	-	-	-
G	554	13.31	6.07	-				7.16	5.70	4.47	-	-	-	-				135.8	93.2	75.4	-	-	-	-
U	555	14.10				5.11	7.65		5.57	4.42	-	-	-	-		103.2	140.8		92.5	75.5	-	-	-	-
G	556	12.78	-	-				7.74	5.95	4.09	4.34	4.27	-	-				136.3	91.0	78.0	70.6	84.0	-	-

Supplementary Information Table 1B.

Residue		NH	NH_2	NH_2^*	H2	H5	H6	H8	H1'	H2'	H3'	H4'	H5'	H5"	C2	C5	C6	C8	C1'	C2'	C3'	C4'	C5'	^{31}P
C	541		7.04	8.49		6.04	8.14		5.51	4.55	4.64	4.38	3.97	4.08		98.7	143.1		94.1	75.4	73.5	84.3	61.9	-0.45
A	542		6.50	8.02	7.67			8.36	6.06	4.61	4.87	-	-	-	153.8			140.1	92.8	75.7	72.9	-	-	0.09
C	543		7.03	8.41		5.35	7.71		5.51	4.27	-	-	-	-		97.2	141.1		94.1	75.7	-	-	-	-0.36
C	544		6.93	8.47		5.51	7.85		5.53	4.35	-	-	-	-		97.6	141.5		93.6	75.4	-	-	-	-0.32
U	545	13.64				5.46	7.94		5.54	4.44	4.66	-	-	-		103.6	141.5		93.5	75.4	71.9	-	-	0.57
G	546	12.33	5.91	8.13				7.77	5.91	4.49	-	-	-	-				136.4	92.2	75.8	-	-	-	1.16
G	547	10.66	-	-				7.20	5.77	4.27	4.31	-	-	-				136.6	93.9	-	-	-	-	4.40
C	548		6.98	8.44		5.47	7.69		5.38	4.45	4.08	-	3.80	4.24		97.4	142.7		93.4	75.7	72.0	-	63.8	3.01
G	549	-	-	-				7.64	5.47	4.29	4.27	-	-	-				137.0	92.5	-	-	-	-	-1.10
A	550		-	-	8.28			8.08	6.14	4.45	4.85	4.16	-	-	155.9			139.8	91.8	76.8	72.8	82.4	-	2.87
C	551		7.05	8.66		6.07	7.97		3.90	4.42	4.16	-	-	-		99.9	141.7		95.3	74.3	74.6	-	-	-
A	552		6.39	7.76	7.04			8.13	5.96	4.65	4.79	-	-	-	152.5			139.6	92.5	75.8	72.9	-	-	-
G	553	13.00	6.17	8.36				7.24	5.63	4.52	4.47	-	-	-				135.7	92.2	75.5	-	-	-	0.21
G	554	13.33	6.11	-				7.15	5.70	4.47	-	-	-	-				136.0	93.1	75.3	-	-	-	-0.41
U	555	14.16				5.12	7.64		5.56	4.42	-	-	-	-		103.1	141.0		93.7	75.7	-	-	-	0.60
G	556	12.64	-	-				7.74	5.95	4.09	4.35	4.27	-	-				137.6	91.2	78.0	70.5	83.9	-	0.19

Supplementary Information Table 1C.

Residue		NH	NH_2	NH_2*	H2	H5	H6	H8	H1'	H2'	H3'	H4'	H5'	H5"	C2	C5	C6	C8	C1'	C2'	C3'	C4'	C5'	31P
G	602	12.92	-	-				8.07	5.79	4.93	4.63	4.42	4.06	3.96				138.8	92.6	75.1	74.4	84.7	62.8	-4.15
G	603	13.41	5.73	-				7.65	5.91	4.54	4.66	4.58	4.22	-				136.6	92.9	75.4	72.7	-	65.3	-4.51
C	604		6.99	8.54		5.31	7.72		5.51	4.53	4.57	4.45	4.14	-		97.5	140.7		93.7	75.4	72.2	81.7	64.5	-4.21
A	605		6.33	8.03	7.32			8.02	5.93	4.51	4.62	4.49	4.15	-	153.0			139.3	93.2	75.6	73.0	81.9	65.3	-4.45
C	606		6.52	8.24		5.03	7.31		5.31	4.35	4.39	4.45	4.08	-		97.3	140.2		93.7	75.7	73.2	81.9	65.0	-
A	607		-	-	7.83			8.36	6.13	-	-	-	-	-	154.1			-	91.6	-	-	-	-	-
A	608		-	-	7.83			8.15	5.71	-	4.62	-	-	-	154.1			-	93.4	-	72.7	-	-	-4.64
C	609		-	-		5.41	7.53		5.56	4.07	4.41	4.31	3.92	-		97.5	141.8		93.2	76.0	74.1	83.2	65.0	-4.57
C	610		-	-		5.73	7.86		5.59	4.38	4.31	4.45	-	-		98.9	143.2		93.5	76.0	73.2	81.7	-	-4.34
C	611		-	-		5.61	7.76		5.72	4.42	4.42	-	-	-		98.4	141.6		93.1	76.0	73.0	-	-	-
C	612		-	-		5.73	7.87		5.66	4.48	4.54	4.38	-	-		98.1	141.6		93.1	73.5	73.5	82.0	-	-
A	613		-	-	8.11			8.22	5.99	4.86	4.61	-	4.36	4.27	154.1			141.3	92.3	75.7	72.9	-	68.0	-
G	614	12.76	-	-				7.95	6.13	4.58	-	-		-				140.8	91.6	-	-	-	-	-4.81
U	615	13.92				5.16	7.83		5.55	4.59	4.51	4.47	4.14	-		103.0	141.5		93.5	75.1	73.2	81.9	-	-4.20
G	616	12.58	5.95	8.12				7.72	5.80	4.49	4.59	-	4.14	4.05				136.1	92.6	75.4	-	-	64.5	-4.71
C	617		7.01	8.57		5.24	7.67		5.47	4.23	4.42	4.39	-	-		97.0	141.0		94.0	75.7	72.1	83.3	-	-4.45
C	618		7.07	8.49		5.51	7.67		5.75	4.01	4.17	4.15	-	-		98.4	141.6		92.9	77.6	69.7	83.3	-	-

Supplementary Information Table 1D.

Residue		NH	NH_2	NH_2*	H2	H5	H6	H8	H1'	H2'	H3'	H4'	H5'	H5"
G	602	12.75	-	-				8.07	5.79	4.92	4.65	4.42	4.08	3.96
G	603	13.41	5.71	-				7.68	5.91	4.55	4.69	4.59	4.22	-
C	604		6.89	8.55		5.32	7.76		5.53	4.54	4.59	4.46	4.14	-
A	605		6.30	8.04	7.32			8.03	5.93	4.49	4.64	4.49	4.16	
C	606		6.62	8.16		5.02	7.38		5.33	4.31	4.39	-	4.09	-
A	607		-	-	7.84			8.36	6.13	4.90	-	-	-	-
A	608		-	-	7.84			8.17	5.76	4.73	4.65	-	-	-
C	609		-	-		5.41	7.55		5.55	4.07	4.41	4.32	3.92	-
C	610		-	-		5.71	7.87		5.58	4.39	4.30	-	-	3.94
C	611		-	-		5.57	7.77		5.69	4.46	4.43	-	-	-
C	612		-	-		5.69	7.87		5.66	4.47	4.55	-	-	-
A	613		-	-	8.11			8.21	5.98	4.87	4.61	-	4.38	4.29
G	614	12.84	-	-				8.09	6.15	4.56	-	-	-	-
U	615	14.10				5.18	7.87		5.55	4.58	4.54	-	4.15	-
G	616	12.64	5.93	8.05				7.72	5.81	4.48	4.61	-	4.14	-
C	617		6.84	8.53		5.25	7.69		5.48	4.24	4.40	-	-	-
C	618		7.04	8.47		5.52	7.67		5.75	4.01	4.17	-	-	-

Supplementary Information Table 2A

Base-pair	dx	dy	Inclin. (η)	Tip (q)	h-Rise (h)	h-Twist (Ω_h)
	-5.39<dx<-2.95	0.88<dy<0.90	7.4<η<22	28.7<q<36.3	2.47<h<3.19	28.7<Ω_h<36.3
CG/AU	-3.92	-0.51	12.6	2.1	2.71	30.3
AU/CG	-3.48	0.63	5.7	-3.0	3.17	31.9
CG/CG	-3.58	0.87	14.9	-5.2	2.47	29.4
CG/UA	-4.49	-0.45	21.1	2.6	3.01	34.7
UA/GC	-4.61	0.07	19.6	-1.2	2.56	30.6
GC/GA	-2.12	2.70	14.5	5.2	2.43	58.4
Base-pair	**Shift (Dx)**	**Slide (Dy)**	**Rise (Dz)**	**Tilt (τ)**	**Roll (ρ)**	**Twist (ω)**
	-0.54<Dx<0.54	-1.87<Dy<-1.19	3.12<Dz<3.52	-2.7<τ<2.9	4.1<ρ<11.9	27.4<ω<34.8
CG/AU	0.17	-1.43	3.09	-1.1	6.5	29.6
AU/CG	-0.18	-1.60	3.35	1.7	3.1	31.7
CG/CG	-0.21	-1.14	2.88	2.6	7.5	28.3
CG/UA	0.12	-1.47	3.75	-1.5	12.3	32.5
UA/GC	0.02	-1.47	3.21	0.6	10.2	28.9
GC/GA	-2.84	-1.50	2.61	-5.1	14.0	56.6

Supplementary Information Table 2B

Base-pair	dx	dy	Inclin. (η)	Tip (q)	h-Rise (h)	h-Twist (Ω_h)
	-5.39<dx<-2.95	0.88<dy<0.90	7.4<η<22	28.7<q<36.3	2.47<h<3.19	28.7<Ω_h<36.3
CG/AU	-3.96	0.60	18.5	-20.9	3.36	38.7
AU/CG	-3.20	0.65	3.8	1.9	2.61	30.2
CG/CG	-6.05	-0.45	27.6	8.4	2.40	32.0
CG/UA	-3.79	-0.44	8.1	1.2	3.02	31.4
UA/GC	-4.19	0.68	19.3	-0.3	2.74	34.4
GC/GA	-2.66	5.18	2.6	-7.0	2.41	56.6
Base-pair	**Shift (Dx)**	**Slide (Dy)**	**Rise (Dz)**	**Tilt (τ)**	**Roll (ρ)**	**Twist (ω)**
	-0.54<Dx<0.54	-1.87<Dy<-1.19	3.12<Dz<3.52	-2.7<τ<2.9	4.1<ρ<11.9	27.4<ω<34.8
CG/AU	0.89	-1.48	3.91	13.4	11.8	34.5
AU/CG	-0.42	-1.49	2.70	-1.0	2.00	30.1
CG/CG	-0.19	-1.90	3.65	-4.5	14.6	28.2
CG/UA	0.17	-1.62	3.27	-0.7	4.4	31.1
UA/GC	-0.38	-1.48	3.39	0.2	11.2	32.6
GC/GA	-4.61	-2.41	3.02	6.6	2.5	56.2

Supplementary Information Table 2C.

Base-pair	dx	dy	Inclin. (η)	Tip (q)	h-Rise (h)	h-Twist (Ω_h)
	-5.39<dx<-2.95	0.88<dy<0.90	7.4<η<22	28.7<q<36.3	2.47<h<3.19	28.7<Ω_h<36.3
GG/CC	-5.76	-0.68	37.3	-0.3	1.81	33.8
GC/GC	-2.53	0.65	0.4	-0.0	3.67	32.1
CA/UG	-6.04	-0.10	35.4	3.9	1.63	31.8
AC/GU	-2.68	-0.97	-2.2	0.9	4.38	30.9
Base-pair	**Shift (Dx)**	**Slide (Dy)**	**Rise (Dz)**	**Tilt (τ)**	**Roll (ρ)**	**Twist (ω)**
	-0.54<Dx<0.54	-1.87<Dy<-1.19	3.12<Dz<3.52	-2.7<τ<2.9	4.1<ρ<11.9	27.4<ω<34.8
GG/CC	0.41	-1.64	3.43	0.2	20.3	27.2
GC/GC	-0.36	-1.37	3.68	0.0	0.2	32.1
CA/UG	-0.11	-1.81	3.21	-2.0	18.3	26.1
AC/GU	0.45	-1.59	4.34	-0.5	-1.2	30.9

Supplementary Information Table 2D.

Base-pair	dx	dy	Inclin. (η)	Tip (q)	h-Rise (h)	h-Twist (Ω_h)
	-5.39<dx<-2.95	0.88<dy<0.90	7.4<η<22	28.7<q<36.3	2.47<h<3.19	28.7<Ω_h<36.3
GG/CC	-5.39	-0.15	32.9	-3.1	1.91	34.7
GC/GC	-4.86	0.42	7.6	-0.3	3.14	29.1
CA/UG	-5.58	0.04	27.3	-0.3	2.28	32.0
AC/GU	-3.67	-0.70	2.5	0.5	3.82	28.8
CA/AG	-2.76	1.21	6.5	-0.3	5.93	46.0
Base-pair	**Shift (Dx)**	**Slide (Dy)**	**Rise (Dz)**	**Tilt (τ)**	**Roll (ρ)**	**Twist (ω)**
	-0.54<Dx<0.54	-1.87<Dy<-1.19	3.12<Dz<3.52	-2.7<τ<2.9	4.1<ρ<11.9	27.4<ω<34.8
GG/CC	0.23	-1.74	3.31	1.8	18.67	29.4
GC/GC	-0.19	-2.02	3.42	0.2	3.8	28.8
CA/UG	-0.01	-1.74	3.41	0.2	14.6	28.6
AC/GU	0.32	-1.66	3.90	-0.2	1.2	28.8
CA/AG	-0.92	-1.52	6.13	0.2	5.1	45.7