

## **Supplemental Data**

### **Structural basis of human PRDM9 allele C specific recognition of its cognate DNA sequence**

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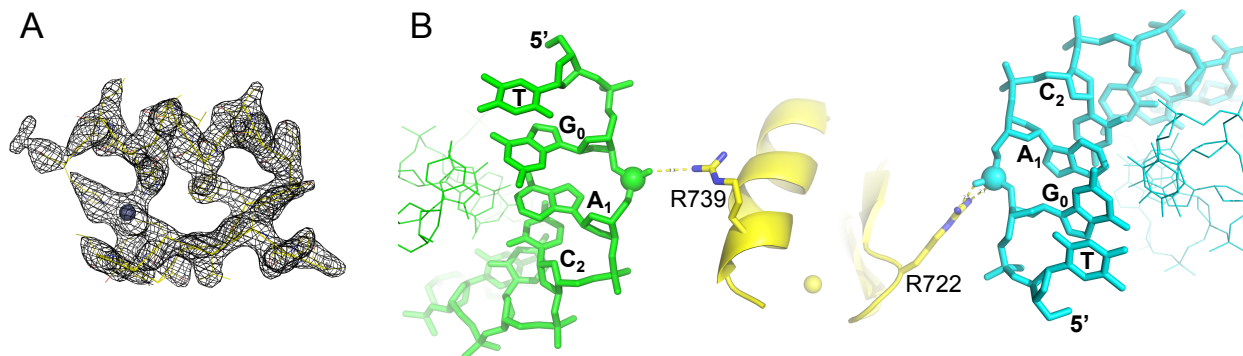
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**Supplemental Figure S1-S5**

**Supplemental Table S1**

Figure S1

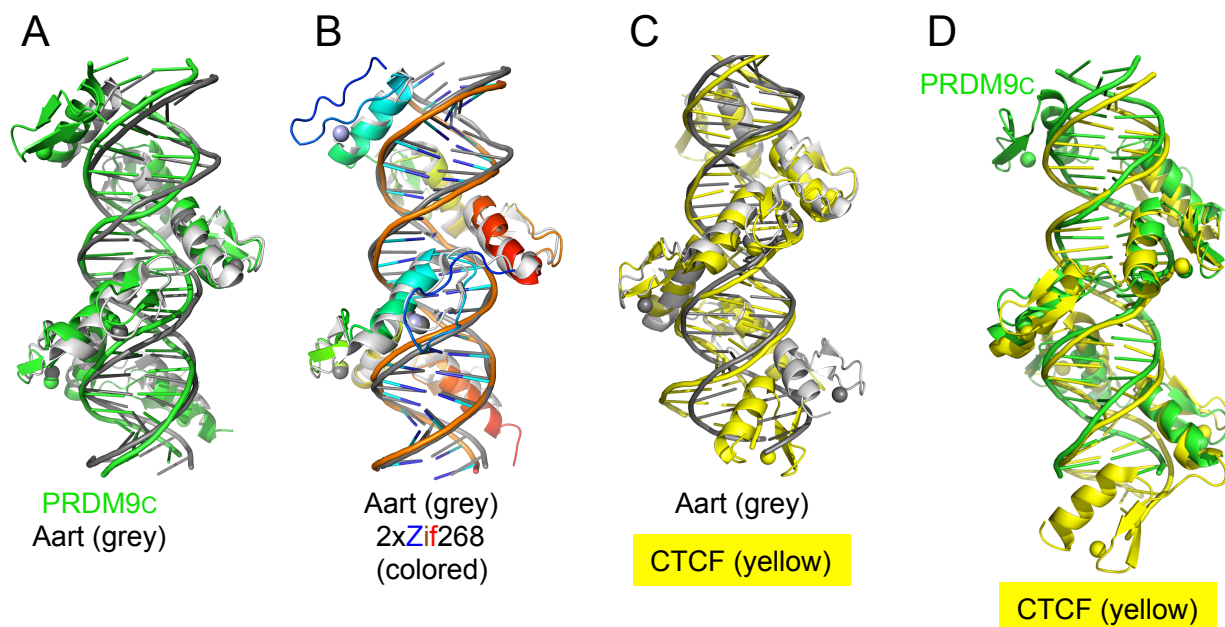


**Supplemental Figure S1. Mol C in the space group  $P2_1$**

(A) The omit electron density (grey mesh), contoured at  $3.0\sigma$  above the mean, is shown for Mol C, which contains only one ordered ZF, as no electron density was observed for the rest of the fingers.

(B) Although no internal symmetry existed for each ZF module, two arginine residues (R722 and R739) of Mol C (colored in yellow) interact respectively with the DNA phosphate group between G<sub>0</sub> and A<sub>1</sub> of two DNA molecules.

Figure S2



**Supplemental Figure S2. Structural comparison among six-fingers structures**

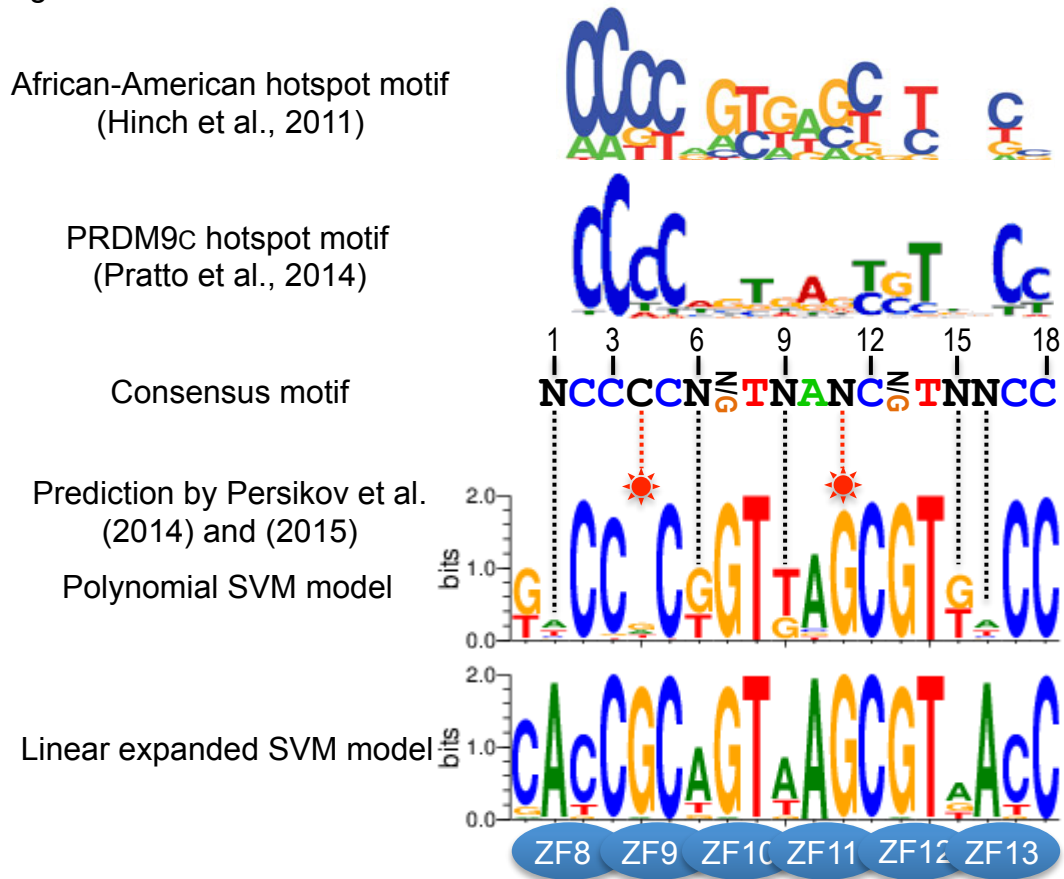
(A) Superimposition of PRDM9c (green) and six-finger designed Aart (grey; PDB 2I13).

(B) Superimposition of Aart (grey) and two copies of the three-finger Zif268 (colored in rainbow) (PDB 1P47).

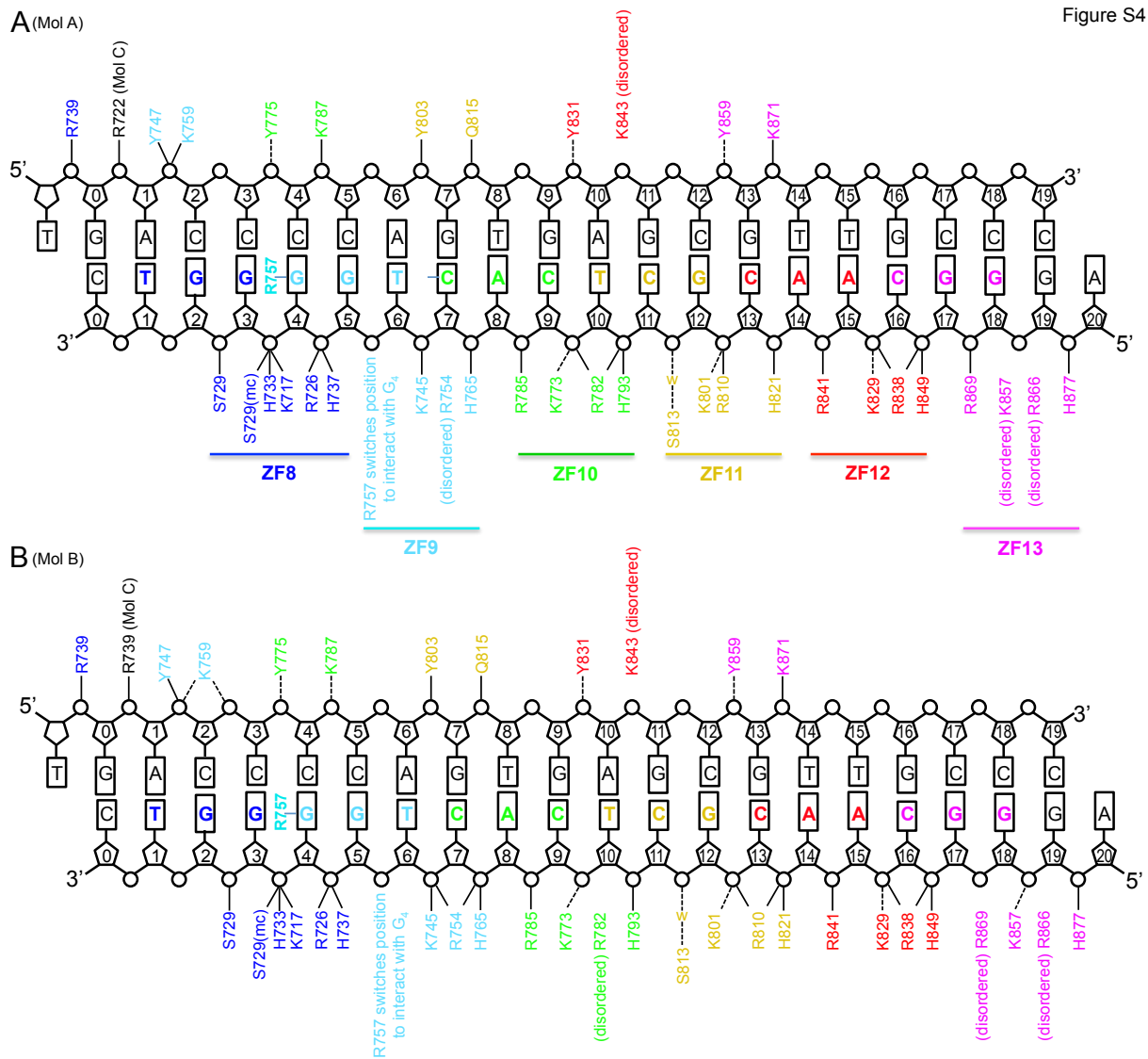
(C) Superimposition of Aart (grey) and six-fingered CTCF ZF2-7 (yellow) (PDB 5T0U). Note, the last finger deviates between the two structures (RMSD=2.0 Å for 113 pairs of C $\alpha$  atoms).

(D) Superimposition of PRDM9c (green) and six-fingered fragment of human CTCF ZF2-7 (PDB 5T0U). Note only five fingers are aligned between the two structures (RMSD=2.5 Å for 125 pairs of C $\alpha$  atoms). The first ZF of PRDM9c and the last ZF of CTCF were excluded in the alignment.

Figure S3



**Supplemental Figure S3.** Comparison of experimentally determined consensus sequence motifs (1,2) (top two lines) and predictions made by SVM (support vector machines)-based algorithms (3) (Bottom two lines).

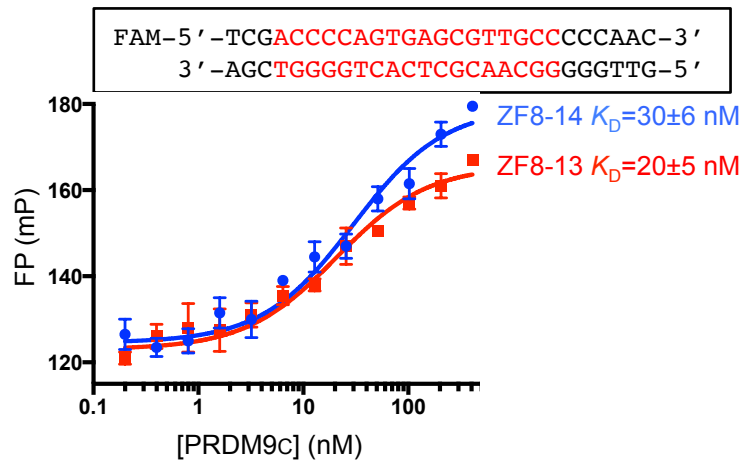


**Supplemental Figure S4. Schematics of PRDM9C-DNA backbone phosphate interactions**

Solid lines indicate conventional H-bonds; dashed lines indicate inter-atomic distance  $>3.5 \text{ \AA}$ ;

mc=main chain atom. Note two arginine residues of Mol C are involved in the interaction with the phosphate group between G0 and A1 (see Fig. S1B).

Figure S5



### Supplemental Figure S5. DNA-binding data

DNA binding affinities of PRDM9C ZF8-13 and ZF8-14 against the FAM-labeled oligo, under the conditions of 350 mM NaCl and the probe DNA concentration of 5 nM. Fluorescence polarization (Y-axis) was used to measure the dissociation constants ( $K_D$ ), as described (4,5). DNA-binding data represent the mean  $\pm$  SEM of two independent determinations performed in duplicate.

## References

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4. Patel, A., Hashimoto, H., Zhang, X., and Cheng, X. (2016) Characterization of How DNA Modifications Affect DNA Binding by C2H2 Zinc Finger Proteins. *Methods Enzymol* **573**, 387-401
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**Supplemental Table S1. Local DNA base-pair parameters**

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*****
3DNA v2.0 (Date and time: Tue Jul 25 14:21:00 2017)
*****
Number of base-pairs: 40 for two DNA molecules (Mol A and Mol B)
*****
Detailed H-bond information: atom-name pair and length [O N]
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Mol A:

1	G-----C	[3]	O6 - N4	3.01	N1 - N3	2.83	N2 - O2	2.54
2	A-----T	[2]	N6 - O4	3.03	N1 - N3	2.81		
3	C-----G	[3]	O2 - N2	2.78	N3 - N1	2.91	N4 - O6	3.00
4	C-----G	[3]	O2 - N2	2.93	N3 - N1	2.99	N4 - O6	3.00
5	C-----G	[3]	O2 - N2	2.83	N3 - N1	2.87	N4 - O6	2.79
6	C-----G	[3]	O2 - N2	2.77	N3 - N1	2.87	N4 - O6	2.88
7	A-----T	[2]	N6 - O4	2.81	N1 - N3	2.75		
8	G-----C	[3]	O6 - N4	3.01	N1 - N3	2.88	N2 - O2	2.80
9	T-----A	[2]	N3 - N1	2.78	O4 - N6	2.89		
10	G-----C	[3]	O6 - N4	2.93	N1 - N3	2.75	N2 - O2	2.45
11	A-----T	[2]	N6 - O4	2.95	N1 - N3	2.81		
12	G-----C	[3]	O6 - N4	2.75	N1 - N3	2.81	N2 - O2	2.74
13	C-----G	[3]	O2 - N2	2.76	N3 - N1	2.88	N4 - O6	2.92
14	G-----C	[3]	O6 - N4	3.05	N1 - N3	2.90	N2 - O2	2.62
15	T-----A	[2]	N3 - N1	2.66	O4 - N6	2.67		
16	T-----A	[2]	N3 - N1	2.69	O4 - N6	2.83		
17	G-----C	[3]	O6 - N4	2.47	N1 - N3	2.79	N2 - O2	2.96
18	C-----G	[3]	O2 - N2	2.63	N3 - N1	3.00	N4 - O6	3.22
19	C-----G	[3]	O2 - N2	2.57	N3 - N1	2.57	N4 - O6	2.55
20	C-----G	[3]	O2 - N2	2.47	N3 - N1	2.72	N4 - O6	2.88

Mol B:

21	G-----C	[3]	O6 - N4	2.90	N1 - N3	2.87	N2 - O2	2.75
22	A-----T	[2]	N6 - O4	2.88	N1 - N3	2.77		
23	C-----G	[3]	O2 - N2	2.70	N3 - N1	2.84	N4 - O6	2.91
24	C-----G	[3]	O2 - N2	2.73	N3 - N1	2.91	N4 - O6	3.05
25	C-----G	[3]	O2 - N2	2.65	N3 - N1	2.72	N4 - O6	2.71
26	C-----G	[3]	O2 - N2	2.59	N3 - N1	2.73	N4 - O6	2.80
27	A-----T	[2]	N6 - O4	2.55	N1 - N3	2.53		
28	G-----C	[3]	O6 - N4	3.12	N1 - N3	2.95	N2 - O2	2.76
29	T-----A	[2]	N3 - N1	2.92	O4 - N6	3.00		
30	G-----C	[3]	O6 - N4	2.73	N1 - N3	2.76	N2 - O2	2.69
31	A-----T	[2]	N6 - O4	2.74	N1 - N3	2.75		
32	G-----C	[3]	O6 - N4	2.93	N1 - N3	2.89	N2 - O2	2.81
33	C-----G	[3]	O2 - N2	2.49	N3 - N1	2.78	N4 - O6	2.95
34	G-----C	[3]	O6 - N4	3.01	N1 - N3	2.96	N2 - O2	2.78
35	T-----A	[2]	N3 - N1	2.77	O4 - N6	2.98		
36	T-----A	[2]	N3 - N1	2.68	O4 - N6	2.83		
37	G-----C	[3]	O6 - N4	2.48	N1 - N3	2.71	N2 - O2	2.81
38	C-----G	[3]	O2 - N2	2.42	N3 - N1	2.74	N4 - O6	3.00
39	C-----G	[3]	O2 - N2	2.71	N3 - N1	2.70	N4 - O6	2.65
40	C-----G	[3]	O2 - N2	2.43	N3 - N1	3.00	N4 - O6	3.50



**Supplemental Table S1 - continues**

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Local base-pair parameters

Mol A:

bp	Shear	Stretch	Stagger	Buckle	Propeller	Opening
1 G-C	-0.35	-0.16	-0.28	-5.73	-8.87	5.85
2 A-T	0.29	-0.10	0.12	4.65	-13.03	1.22
3 C-G	0.12	-0.09	0.12	0.03	-11.88	1.33
4 C-G	0.31	-0.07	0.11	10.15	-15.03	-1.39
5 C-G	0.13	-0.15	0.32	-14.37	-3.63	-2.42
6 C-G	0.24	-0.17	-0.23	5.84	5.29	-0.12
7 A-T	0.49	-0.19	0.21	14.26	-11.82	-2.42
8 G-C	-0.54	-0.20	0.20	2.00	-16.94	2.18
9 T-A	-0.24	-0.20	-0.32	-2.61	-13.24	-0.29
10 G-C	-0.12	-0.22	-0.09	-3.57	-4.39	4.44
11 A-T	0.35	-0.15	0.14	1.65	-11.12	-1.46
12 G-C	-0.19	-0.25	0.09	2.01	-2.09	-1.60
13 C-G	0.79	-0.28	-0.05	12.11	-5.02	0.54
14 G-C	-0.35	-0.10	-0.20	-9.08	-4.74	3.30
15 T-A	-0.39	-0.33	-0.21	-1.87	-10.68	-2.43
16 T-A	-0.02	-0.28	-0.08	-4.34	-3.50	0.10
17 G-C	0.52	-0.27	-0.19	-2.01	-5.01	-7.31
18 C-G	0.41	0.02	-0.09	7.47	-3.59	6.14
19 C-G	0.24	-0.48	-0.08	11.70	-13.46	-1.98
20 C-G	0.22	-0.27	-0.14	3.43	-6.47	4.36

Mol B:

bp	Shear	Stretch	Stagger	Buckle	Propeller	Opening
21 G-C	-0.44	-0.21	0.07	2.45	-5.25	0.39
22 A-T	0.31	-0.19	0.06	2.22	-13.53	-2.03
23 C-G	0.36	-0.20	0.10	-3.50	-9.72	1.11
24 C-G	0.33	-0.10	0.09	11.49	-15.74	1.98
25 C-G	0.08	-0.28	0.09	-12.71	-0.80	-0.77
26 C-G	-0.12	-0.25	-0.30	0.39	2.77	0.59
27 A-T	0.00	-0.45	0.13	11.26	-8.51	-3.09
28 G-C	-0.28	-0.04	0.18	-0.28	-9.00	3.36
29 T-A	-0.04	-0.05	-0.24	-0.96	-9.28	-1.07
30 G-C	-0.05	-0.24	0.02	0.49	-0.20	-0.54
31 A-T	0.54	-0.24	0.22	3.66	-10.13	-5.70
32 G-C	-0.16	-0.11	-0.20	-2.18	-8.54	0.93
33 C-G	0.26	-0.19	-0.03	10.07	-1.64	4.16
34 G-C	-0.30	-0.06	-0.43	-11.63	-6.32	1.31
35 T-A	0.04	-0.21	-0.07	-1.68	-7.59	2.05
36 T-A	-0.33	-0.29	-0.28	-2.21	-9.05	0.60
37 G-C	0.61	-0.35	-0.27	-4.10	-5.32	-5.74
38 C-G	0.25	-0.22	-0.02	4.30	-9.48	5.52
39 C-G	0.40	-0.38	-0.38	12.90	-11.67	-1.22
40 C-G	0.89	-0.01	-0.12	-0.92	-5.32	12.93
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ave.	0.11	-0.20	-0.05	1.27	-7.59	0.57
s.d.	0.35	0.11	0.19	7.05	5.01	3.65

**Supplemental Table S1 - continues**

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Local base-pair step parameters

Mol A:

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 GA/TC	-1.18	1.71	3.02	-9.09	-1.88	44.34
2 AC/GT	0.67	-0.79	3.35	-0.37	-0.93	32.40
3 CC/GG	0.16	0.09	3.28	1.77	12.26	30.09
4 CC/GG	0.25	-1.20	3.70	0.54	1.66	37.91
5 CC/GG	1.23	0.42	2.93	7.03	7.47	32.29
6 CA/TG	-0.97	0.60	3.23	-3.39	-2.29	33.75
7 AG/CT	1.10	-1.16	3.68	-1.96	0.54	27.75
8 GT/AC	-0.97	-0.81	3.38	4.00	4.18	35.83
9 TG/CA	0.77	1.20	3.42	-1.15	10.26	31.29
10 GA/TC	-1.23	0.98	3.24	-4.80	2.28	38.29
11 AG/CT	0.63	-0.78	3.35	0.33	-1.09	28.62
12 GC/GC	0.31	-0.58	3.19	1.00	1.70	31.72
13 CG/CG	1.02	-1.49	4.05	1.62	-2.95	27.56
14 GT/AC	-0.39	-1.11	3.22	1.86	3.75	34.37
15 TT/AA	-0.24	-0.82	3.48	-1.60	-3.70	36.44
16 TG/CA	-0.37	-0.72	3.35	0.81	3.32	34.76
17 GC/GC	0.94	-0.55	3.06	-0.91	5.18	27.47
18 CC/GG	-1.13	-0.07	3.36	-2.13	-2.04	34.78
19 CC/GG	1.08	0.16	3.49	5.55	2.37	37.96

Mol B:

step	Shift	Slide	Rise	Tilt	Roll	Twist
21 GA/TC	-1.05	1.28	3.43	-3.44	0.92	41.62
22 AC/GT	0.71	-0.73	3.38	0.07	-0.04	33.29
23 CC/GG	0.20	-0.02	3.03	0.94	12.86	28.46
24 CC/GG	0.22	-0.81	3.85	1.79	-1.03	38.92
25 CC/GG	1.02	0.40	2.99	5.91	6.83	30.85
26 CA/TG	-0.78	0.71	3.26	-3.22	2.31	31.66
27 AG/CT	0.69	-0.96	3.63	-3.32	0.02	33.94
28 GT/AC	-0.79	-0.69	3.33	3.93	3.81	32.99
29 TG/CA	0.41	1.11	3.35	-1.17	9.15	30.93
30 GA/TC	-1.20	0.78	3.29	-4.86	0.53	39.74
31 AG/CT	0.91	-0.60	3.57	4.62	0.23	29.23
32 GC/GC	0.32	-0.49	3.13	-3.10	1.94	27.65
33 CG/CG	0.89	-1.47	4.12	2.73	-3.94	30.22
34 GT/AC	0.09	-1.23	3.26	-0.33	2.45	35.97
35 TT/AA	-0.61	-0.82	3.42	2.56	-4.22	31.73
36 TG/CA	0.08	-0.28	3.54	1.53	5.60	37.70
37 GC/GC	0.67	-0.72	3.10	-1.07	3.04	25.36
38 CC/GG	-0.64	-0.38	3.27	1.27	0.44	33.58
39 CC/GG	1.07	0.14	3.71	3.87	1.55	42.06

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ave.	0.10	-0.26	3.38	0.21	2.17	33.51
s.d.	0.80	0.84	0.27	3.35	4.22	4.52

**Supplemental Table S1 - continues**

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Local base-pair helical parameters

Mol A:

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
1 GA/TC	2.39	0.76	3.12	-2.46	11.89	45.25
2 AC/GT	-1.24	-1.27	3.37	-1.67	0.67	32.41
3 CC/GG	-2.02	0.03	3.08	22.46	-3.25	32.49
4 CC/GG	-2.08	-0.30	3.65	2.56	-0.83	37.95
5 CC/GG	-0.42	-1.04	3.14	13.02	-12.25	33.84
6 CA/TG	1.39	1.13	3.26	-3.92	5.81	33.99
7 AG/CT	-2.56	-2.80	3.57	1.13	4.08	27.82
8 GT/AC	-1.89	2.11	3.15	6.75	-6.45	36.28
9 TG/CA	0.19	-1.58	3.59	18.41	2.07	32.91
10 GA/TC	1.20	1.25	3.41	3.46	7.27	38.65
11 AG/CT	-1.33	-1.21	3.39	-2.20	-0.66	28.64
12 GC/GC	-1.36	-0.39	3.16	3.10	-1.83	31.78
13 CG/CG	-2.20	-1.63	4.23	-6.16	-3.39	27.76
14 GT/AC	-2.42	0.94	3.06	6.31	-3.13	34.62
15 TT/AA	-0.76	0.14	3.55	-5.89	2.55	36.65
16 TG/CA	-1.72	0.74	3.26	5.55	-1.36	34.93
17 GC/GC	-2.26	-2.14	2.88	10.79	1.89	27.96
18 CC/GG	0.21	1.55	3.42	-3.40	3.55	34.90
19 CC/GG	-0.08	-0.88	3.61	3.61	-8.47	38.42

Mol B:

step	X-disp	Y-disp	h-Rise	Incl.	Tip	h-Twist
21 GA/TC	1.70	1.09	3.52	1.29	4.83	41.76
22 AC/GT	-1.27	-1.23	3.38	-0.07	-0.12	33.29
23 CC/GG	-2.32	-0.21	2.77	24.62	-1.80	31.19
24 CC/GG	-1.06	-0.08	3.88	-1.54	-2.68	38.98
25 CC/GG	-0.46	-0.83	3.14	12.51	-10.83	32.11
26 CA/TG	0.87	0.82	3.37	4.21	5.87	31.90
27 AG/CT	-1.64	-1.75	3.55	0.04	5.67	34.10
28 GT/AC	-1.82	2.02	3.12	6.66	-6.86	33.43
29 TG/CA	0.26	-0.96	3.51	16.70	2.14	32.24
30 GA/TC	1.08	1.19	3.42	0.78	7.11	40.02
31 AG/CT	-1.23	-0.69	3.66	0.46	-9.08	29.58
32 GC/GC	-1.46	-1.36	3.04	4.04	6.44	27.88
33 CG/CG	-1.78	-0.99	4.33	-7.49	-5.19	30.58
34 GT/AC	-2.33	-0.20	3.18	3.97	0.54	36.06
35 TT/AA	-0.69	1.59	3.44	-7.66	-4.65	32.10
36 TG/CA	-1.19	0.08	3.46	8.61	-2.35	38.13
37 GC/GC	-2.43	-1.79	2.96	6.88	2.43	25.56
38 CC/GG	-0.73	1.31	3.24	0.76	-2.19	33.61
39 CC/GG	0.01	-1.03	3.79	2.16	-5.38	42.26

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ave.	-0.88	-0.20	3.39	3.90	-0.47	34.00
s.d.	1.30	1.26	0.33	7.72	5.46	4.43

**Supplemental Table S1 - continues**

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 Structure classification: This is a right-handed nucleic acid structure  
 \*\*\*\*\*  
 Classification of each dinucleotide step in a right-handed nucleic acid  
 structure: A-like; B-like; TA-like; intermediate of A and B, or other cases

**Mol A:**

step	Xp	Yp	Zp	XpH	YpH	ZpH	Form
1 GA/TC	-2.91	8.67	-1.47	-0.55	8.61	-1.83	B
2 AC/GT	-3.10	9.19	-0.00	-4.30	9.19	-0.26	B
3 CC/GG	-1.92	9.08	0.94	-3.86	8.10	4.21	
4 CC/GG	-2.54	8.94	1.16	-4.51	8.88	1.54	
5 CC/GG	-2.36	8.97	0.56	-2.61	8.64	2.45	
6 CA/TG	-2.94	8.91	-0.38	-1.49	8.87	-1.03	B
7 AG/CT	-3.33	8.97	0.38	-5.78	8.96	0.57	B
8 GT/AC	-3.67	8.95	-0.57	-5.35	8.96	0.36	B
9 TG/CA	-3.08	8.98	-1.03	-2.91	8.87	1.77	B
10 GA/TC	-2.95	8.82	-0.52	-1.73	8.84	-0.09	B
11 AG/CT	-3.04	9.17	0.09	-4.32	9.16	-0.25	B
12 GC/GC	-3.35	9.29	-0.11	-4.69	9.28	0.38	B
13 CG/CG	-3.30	8.81	0.89	-5.46	8.86	-0.03	
14 GT/AC	-2.56	8.72	1.53	-4.86	8.51	2.42	
15 TT/AA	-2.99	8.95	0.43	-3.72	8.95	-0.44	B
16 TG/CA	-3.00	9.04	0.23	-4.62	8.98	1.06	B
17 GC/GC	-2.66	9.21	0.57	-4.87	8.95	2.24	
18 CC/GG	-2.67	8.94	0.43	-2.42	8.95	-0.10	B
19 CC/GG	-3.06	8.86	-0.24	-3.17	8.86	0.33	B

**Mol B:**

step	Xp	Yp	Zp	XpH	YpH	ZpH	Form
21 GA/TC	-2.75	8.78	-0.86	-1.12	8.80	-0.70	B
22 AC/GT	-2.99	9.16	0.02	-4.21	9.16	0.01	B
23 CC/GG	-2.02	9.11	0.91	-4.25	7.97	4.51	
24 CC/GG	-2.73	8.95	0.74	-3.71	8.96	0.51	
25 CC/GG	-2.81	8.82	0.01	-3.05	8.63	1.76	B
26 CA/TG	-3.09	8.93	-0.59	-2.17	8.95	0.01	B
27 AG/CT	-3.26	9.03	0.43	-4.78	9.03	0.46	B
28 GT/AC	-3.60	9.14	-0.54	-5.22	9.14	0.44	B
29 TG/CA	-2.97	8.95	-0.82	-2.73	8.82	1.71	B
30 GA/TC	-2.81	8.83	-0.45	-1.69	8.84	-0.42	B
31 AG/CT	-2.99	9.13	-0.09	-4.08	9.13	-0.06	B
32 GC/GC	-3.53	9.34	-0.35	-4.85	9.35	0.28	B
33 CG/CG	-3.37	8.76	0.74	-5.11	8.78	-0.37	
34 GT/AC	-2.48	8.50	1.80	-4.70	8.36	2.35	
35 TT/AA	-2.76	8.96	0.73	-3.40	8.98	-0.45	
36 TG/CA	-2.60	9.01	0.22	-3.69	8.89	1.49	B
37 GC/GC	-2.84	9.29	0.42	-5.22	9.17	1.50	B
38 CC/GG	-2.76	9.03	0.29	-3.49	9.02	0.42	B
39 CC/GG	-3.00	8.94	-0.01	-2.99	8.94	0.35	B

**Supplemental Table S1 - continues**

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 Minor and major groove widths: direct P-P distances and refined P-P distances

	Minor Groove		Major Groove	
	P-P	Refined	P-P	Refined
Mol A:				
1 GA/TC	---	---	---	---
2 AC/GT	---	---	---	---
3 CC/GG	13.8	---	15.2	---
4 CC/GG	14.6	14.6	19.2	19.0
5 CC/GG	14.4	14.4	17.6	17.5
6 CA/TG	12.7	12.7	18.7	18.6
7 AG/CT	11.1	10.9	19.4	19.4
8 GT/AC	12.2	12.0	18.6	18.4
9 TG/CA	14.0	14.0	16.9	16.3
10 GA/TC	14.1	13.9	19.9	19.7
11 AG/CT	13.4	13.3	19.2	19.1
12 GC/GC	13.3	13.2	18.5	18.4
13 CG/CG	12.0	11.9	22.4	22.3
14 GT/AC	10.6	10.5	21.7	21.7
15 TT/AA	12.1	11.9	19.1	19.1
16 TG/CA	13.6	13.4	18.4	18.3
17 GC/GC	13.6	---	18.9	---
18 CC/GG	---	---	---	---
19 CC/GG	---	---	---	---
20 CG/CG	---	---	---	---
Mol B:				
21 GA/TC	---	---	---	---
22 AC/GT	---	---	---	---
23 CC/GG	13.2	---	15.3	---
24 CC/GG	13.9	13.7	19.2	19.1
25 CC/GG	14.4	14.3	17.7	17.6
26 CA/TG	13.1	13.1	18.7	18.6
27 AG/CT	11.5	11.3	19.9	19.9
28 GT/AC	12.5	12.3	19.1	19.0
29 TG/CA	13.9	13.9	16.5	16.0
30 GA/TC	13.9	13.8	19.7	19.7
31 AG/CT	13.3	13.1	19.1	19.0
32 GC/GC	13.2	13.1	18.2	18.0
33 CG/CG	12.2	12.1	22.4	22.3
34 GT/AC	10.8	10.6	21.4	21.4
35 TT/AA	12.5	12.4	19.7	19.6
36 TG/CA	14.5	14.3	18.7	18.6
37 GC/GC	14.3	---	18.6	---
38 CC/GG	---	---	---	---
39 CC/GG	---	---	---	---