

Table 1. Comparison of U-U mismatches

		C1'-C1'	1st hbond	2nd hbond	λ I	λ II	Incline ¹	Shear	Stretch	Stagger	Buckle	Propeller	Opening	Type
trCUG-3	U2-U34	8.6	2.8	2.8	44.8	75.9	minor	-2.47	-1.89	0.26	-7.12	-16.4	11.6	Type I
	U5-U31	10.6	2.7	-	28.2	55.8	minor	-2.63	-1.33	-0.1	5.62	-7.12	-25.98	Type II
(CUG) ₆	U2-U17	10.3	2.7	-	34.1	56.7	minor	-2.32	-1.38	-0.18	0.89	-9.98	-21.23	Type II
	U5-U14	10.6	3	-	53.8	33.1	major	2.27	-1.17	-0.36	-6.03	-15.03	-22.06	Type IV
	U-8-U11	10.3	2.7	-	32.4	56.9	minor	-2.5	-1.48	0.45	2.36	-11.27	-21.02	Type II
	U11-U8	10	2.9	-	57.8	40.4	major	1.71	-1.29	-0.44	-1.86	-12.2	-11.93	Type IV
	U14-U5	10.5	2.7	-	55.9	32.4	major	2.65	-1.29	-0.23	6.92	-11.44	-28.01	Type IV
	U17-U2	10.3	3	-	58.2	39.2	major	2.04	-1.11	-0.15	-4.69	-14.81	-14.8	Type IV
Disney NMR	U5-U14 (0)	10.7	-	-	71.2	32	major	3.57	-0.95	-0.05	-13.48	-9.09	-5.62	Type VI
	U5-U14 (1)	10.6	2.9	-	61.1	28.9	major	3.03	-1.14	-0.09	-22.07	-6.46	-24.3	Type IV
	U5-U14 (2)	8.9	2.9	2.9	73.3	48.3	major	2.24	-1.74	0.02	12.56	-17.25	4.58	Type V
Kiliszek A-B	U3-U6	10.7	2.8	-	26.2	57.9	minor	-2.82	-1.19	-0.47	12.51	-8.17	-31.5	Type II
	U6-U3	10.3	2.9	-	31.6	67.7	minor	-3.03	-1.31	-0.13	14.01	-8.36	-16.37	Type II
Kiliszek C-D	U3-U6	10.9	2.8	-	56.1	22.6	major	2.98	-1.22	-0.44	-4.51	-8.69	-34.42	Type IV
	U6-U3	10.2	2.6	-	59.2	32.4	major	2.59	-1.51	-0.28	0.57	-15.81	-21.16	Type IV
Kiliszek E-E*	U3-U6	10.6	2.6	-	52.7	29.1	major	2.38	-1.31	-0.48	-4.07	-11.84	-30.56	Type IV
	U6-U3	10.6	2.6	-	29.1	52.7	minor	-2.38	-1.31	-0.48	4.07	-11.84	-30.56	Type II
Disney 3SYW	U8-U14	8.8	3	3	46.3	72.4	minor	-2.2	-1.7	0.21	0.27	-14.34	10.06	Type I
	U11-U11	9.9	-	-	50.8	50.8	none	0.01	-1.17	0.07	0.11	-5.73	-8.25	Type III
	U14-U8	8.8	2.9	3	72.5	46.3	major	2.2	-1.71	0.21	-0.76	-14.31	10	Type V
Disney 3SZX	U8-U14	10.5	2.7	-	53.9	35.3	major	1.85	-1.16	-0.11	-5.24	-8.68	-29.19	Type IV
	U11-U11	10	-	-	46	53	none	0.14	-0.99	0.18	1.98	-10.74	-0.21	Type III
	U14-U8	10.5	-	-	58.8	48.1	major	1.3	-0.7	-0.3	-2.99	-11.12	-8.97	Type VI

Classification	# of		
	hbonds	Incline	Amount
Type I	2	minor	2
Type II	1	minor	6
Type III	0	none	2
Type IV	1	major	9
Type V	2	major	2
Type VI	0	major	2

¹Direction of incline was determined by considering the difference between λ I and λ II. If $(\lambda$ I - λ II) < -8, then the pair was considered to be inclined toward the minor groove; however, if the difference was >8, the pair was considered to be inclined toward the major groove. Any values between -8 and 8 were considered to be not included.

Table 2. Comparison of CUG repeat helical parameters

	Roll	Twist	Slide	Rise	Inclination	Helical twist	x-displacement	Helical rise	Zp	Zp(h)
B DNA ¹	0.60	36.00	0.23	3.32	2.10	36.50	0.05	3.29	-0.36	-0.02
A DNA ¹	8.00	31.10	-1.53	3.31	14.70	32.50	-4.17	2.83	2.24	4.19
(CUG)2	9.17	33.48	-1.34	3.10	18.57	35.89	-4.70	2.39	2.35	4.62
(CUG)6	9.16	32.77	-1.90	3.25	16.98	34.54	-5.08	2.49	2.69	4.81
A-B	6.55	31.70	-1.80	3.32	12.41	33.25	-4.55	2.96	2.52	4.10
C-D	8.56	33.11	-1.59	3.30	6.93	34.78	-4.58	2.66	2.40	4.57
E-E*	6.78	32.77	-1.90	3.32	14.12	34.05	-5.03	2.69	2.52	4.32
3SYW	8.51	28.68	-1.73	3.16	18.76	30.62	-5.27	2.39	2.27	4.64
3SZX	8.63	32.33	-1.64	3.21	14.93	33.55	-4.26	2.71	2.52	4.46

¹A and B-form structural parameters from: Lu, X.-J., & Olson, W. K. (2003). 3DNA: a software package for the analysis, rebuilding and visualization of three-dimensional nucleic acid structures. *Nucleic acids research*, 31(17), 5108–5121.