Table S1. Distance restraints used for Z3dU duplex refinement.

Class 1

Base 1	Atom 1	Base 2	Atom 2	Dist	Lower	Upper
1	H6	1	H1'	3.25	0.49	0.49
13	H6	13	H1'	3.25	0.49	0.49
1	H2''	1	H6	3.63	0.54	0.54
13	H2''	13	H6	3.63	0.54	0.54
1	H3'	1	H1'	4.22	0.63	0.63
13	H3'	13	H1'	4.22	0.63	0.63
1	H3'	1	H5	4.86	0.73	0.73
13	H3'	13	H5	4.86	0.73	0.73
1	H3'	1	H2'	2.65	0.40	0.40
13	H3'	13	H2'	2.65	0.40	0.40
3	H5	2	H4'	6.44	0.97	0.97
15	H5	14	H4'	6.44	0.97	0.97
3	H5	2	H1'	3.78	0.57	0.57
15	H5	14	H1'	3.78	0.57	0.57
3	H5	2	H8	3.69	0.55	0.55
15	H5	14	H8	3.69	0.55	0.55
3	H6	3	H1'	4.08	0.61	0.61
15	H6	15	H1'	4.08	0.61	0.61
3	H5	3	H1'	4.80	0.72	0.72
15	H5	15	H1'	4.80	0.72	0.72
3	H2'	3	H1'	2.81	0.42	0.42
15	H2'	15	H1'	2.81	0.42	0.42
3	H2'	3	H6	2.56	0.38	0.38
15	H2'	15	H6	2.56	0.38	0.38
3	H2'	3	H5	3.44	0.52	0.52
15	H2'	15	H5	3.44	0.52	0.52
3	H2''	3	H1'	2.49	0.37	0.37
15	H2''	15	H1'	2.49	0.37	0.37
3	H2''	3	H5	4.59	0.69	0.69
15	H2''	15	H5	4.59	0.69	0.69
3	H3'	3	H1'	4.24	0.64	0.64

15	H3'	15	H1'	4.24	0.64	0.64
3	H3'	3	H5	5.44	0.82	0.82
15	H3'	15	H5	5.44	0.82	0.82
4	H4'	3	H1'	4.50	0.67	0.67
16	H4'	15	H1'	4.50	0.67	0.67
4	H8	3	H1'	3.66	0.55	0.55
16	H8	15	H1'	3.66	0.55	0.55
4	H8	3	H6	4.83	0.72	0.72
16	H8	15	H6	4.83	0.72	0.72
4	H8	3	H2'	3.58	0.54	0.54
16	H8	15	H2'	3.58	0.54	0.54
4	H8	3	H2''	2.96	0.44	0.44
16	H8	15	H2''	2.96	0.44	0.44
4	H8	3	H3'	4.54	0.68	0.68
16	H8	15	H3'	4.54	0.68	0.68
4	H3'	3	H1'	6.06	0.91	0.91
16	H3'	15	H1'	6.06	0.91	0.91
4	H8	4	H1'	3.63	0.54	0.54
16	H8	16	H1'	3.63	0.54	0.54
4	H3'	4	H8	3.67	0.55	0.55
16	H3'	16	H8	3.67	0.55	0.55
5	H4'	4	H1'	4.31	0.65	0.65
17	H4'	16	H1'	4.31	0.65	0.65
5	H8	4	H4'	5.27	0.79	0.79
17	H8	16	H4'	5.27	0.79	0.79
5	H8	4	H1'	3.10	0.47	0.47
17	H8	16	H1'	3.10	0.47	0.47
5	H8	4	H8	4.70	0.70	0.70
17	H8	16	H8	4.70	0.70	0.70
5	H3'	4	H1'	4.79	0.72	0.72
17	H3'	16	H1'	4.79	0.72	0.72
6	H2	5	H2	3.46	0.52	0.52
18	H2	17	H2	3.46	0.52	0.52
6	H1'	6	H4'	3.38	0.51	0.51
18	H1'	18	H4'	3.38	0.51	0.51
6	H2	6	H1'	5.01	0.75	0.75

18	H2	18	H1'	5.01	0.75	0.75
6	H8	6	H1'	4.13	0.62	0.62
18	H8	18	H1'	4.13	0.62	0.62
6	H2''	6	H1'	2.66	0.40	0.40
18	H2''	18	H1'	2.66	0.40	0.40
6	H3'	6	H1'	3.85	0.58	0.58
18	H3'	18	H1'	3.85	0.58	0.58
7	H6	6	H4'	5.67	0.85	0.85
19	H6	18	H4'	5.67	0.85	0.85
7	H6	6	H3'	4.97	0.75	0.75
19	H6	18	H3'	4.97	0.75	0.75
7	H5#	6	H4'	6.08	0.91	0.91
19	H5#	18	H4'	6.08	0.91	0.91
7	H5#	6	H1'	4.64	0.70	0.70
19	H5#	18	H1'	4.64	0.70	0.70
7	H5#	6	H8	3.35	0.50	0.50
19	H5#	18	H8	3.35	0.50	0.50
7	H5#	6	H3'	4.72	0.71	0.71
19	H5#	18	H3'	4.72	0.71	0.71
7	H3'	6	H1'	4.69	0.70	0.70
19	H3'	18	H1'	4.69	0.70	0.70
7	H6	7	H1'	4.04	0.61	0.61
19	H6	19	H1'	4.04	0.61	0.61
7	H5#	7	H1'	5.60	0.84	0.84
19	H5#	19	H1'	5.60	0.84	0.84
7	H5#	7	H6	2.95	0.44	0.44
19	H5#	19	H6	2.95	0.44	0.44
7	H3'	7	H5#	6.04	0.91	0.91
19	H3'	19	H5#	6.04	0.91	0.91
7	H4'	7	H6	4.13	0.62	0.62
19	H4'	19	H6	4.13	0.62	0.62
7	H4'	7	H3'	2.96	0.44	0.44
19	H4'	19	H3'	2.96	0.44	0.44
8	H6	7	H1'	3.62	0.54	0.54
20	H6	19	H1'	3.62	0.54	0.54
8	H6	7	H6	4.12	0.62	0.62

20	H6	19	H6	4.12	0.62	0.62
8	H6	7	H5#	5.14	1.07	1.07
20	H6	19	H5#	5.14	1.07	1.07
8	H6	7	H3'	4.19	0.63	0.63
20	H6	19	H3'	4.19	0.63	0.63
8	H1α	7	H1'	4.24	0.64	0.64
20	H1α	19	H1'	4.24	0.64	0.64
8	H6	8	H1'	3.52	0.53	0.53
20	H6	20	H1'	3.52	0.53	0.53
8	H2β	8	H6	4.09	0.61	0.61
20	H2β	20	H6	4.09	0.61	0.61
8	H2β	8	H1α	2.91	0.44	0.44
20	H2β	20	H1α	2.91	0.44	0.44
8	H1γ/H2γ	8	H6	4.36	0.65	0.65
20	H1γ/H2γ	20	H6	4.36	0.65	0.65
8	H1γ/H2γ	8	H1α	2.69	0.40	0.40
20	H1γ/H2γ	20	H1α	2.69	0.40	0.40
8	H2'	8	H1'	3.25	0.49	0.49
20	H2'	20	H1'	3.25	0.49	0.49
8	H2'	8	H6	2.45	0.47	0.47
20	H2'	20	H6	2.45	0.47	0.47
8	H3'	8	H1'	4.49	0.67	0.67
20	H3'	20	H1'	4.49	0.67	0.67
9	H6	8	H1'	3.33	0.50	0.50
21	H6	20	H1'	3.33	0.50	0.50
9	H5	8	H1'	3.87	0.58	0.58
21	H5	20	H1'	3.87	0.58	0.58
9	H5	8	H2'	3.48	0.52	0.52
21	H5	20	H2'	3.48	0.52	0.52
9	H3'	8	H1'	4.46	0.67	0.67
21	H3'	20	H1'	4.46	0.67	0.67

9	H6	9	H1'	4.04	0.61	0.61
21	H6	21	H1'	4.04	0.61	0.61
9	H4'	9	H2''	3.92	0.59	0.59
21	H4'	21	H2''	3.92	0.59	0.59
10	H8	9	H6	5.03	0.75	0.75
22	H8	21	H6	5.03	0.75	0.75
10	H8	9	H3'	5.08	0.76	0.76
22	H8	21	H3'	5.08	0.76	0.76
11	H6	10	H4'	6.39	0.96	0.96
23	H6	22	H4'	6.39	0.96	0.96
11	H6	10	H3'	4.90	0.73	0.73
23	H6	22	H3'	4.90	0.73	0.73
11	H5	10	H1'	3.96	0.59	0.59
23	H5	22	H1'	3.96	0.59	0.59
11	H6	11	H1'	4.30	0.65	0.65
23	H6	23	H1'	4.30	0.65	0.65
11	H5	11	H1'	5.58	0.84	0.84
23	H5	23	H1'	5.58	0.84	0.84
11	H3'	11	H1'	3.94	0.59	0.59
23	H3'	23	H1'	3.94	0.59	0.59
11	H3'	11	H5	4.94	0.74	0.74
23	H3'	23	H5	4.94	0.74	0.74
12	H1'	11	H1'	5.17	0.77	0.77
24	H1'	23	H1'	5.17	0.77	0.77
12	H8	11	H3'	4.38	0.66	0.66
24	H8	23	H3'	4.38	0.66	0.66
12	H2'	11	H1'	3.81	0.57	0.57
24	H2'	23	H1'	3.81	0.57	0.57
12	H3'	12	H1'	3.98	0.60	0.60
24	H3'	24	H1'	3.98	0.60	0.60

Class 2

Base 1	Atom 1	Base 2	Atom 2	Dist	Lower	Upper
2	H4'	1	H1'	5.61	0.84	0.84
14	H4'	13	H1'	5.61	0.84	0.84

2	H8	2	H4'	5.07	0.76	0.76
14	H8	14	H4'	5.07	0.76	0.76
3	H6	2	H3'	6.50	0.97	0.97
15	H6	14	H3'	6.50	0.97	0.97
3	H3'	3	H6	4.22	0.63	0.63
15	H3'	15	H6	4.22	0.63	0.63
4	H3'	4	H2'	3.10	0.46	0.46
16	H3'	16	H2'	3.10	0.46	0.46
6	H4'	5	H2'	5.72	0.86	0.86
18	H4'	17	H2'	5.72	0.86	0.86
6	H2'	6	H8	3.02	0.45	0.45
18	H2'	18	H8	3.02	0.45	0.45
7	H2'	7	H1'	3.00	0.45	0.45
19	H2'	19	H1'	3.00	0.45	0.45
8	H6	7	H2'	3.08	0.46	0.46
20	H6	19	H2'	3.08	0.46	0.46
8	H1γ/H2γ	7	H3'	4.30	0.65	0.65
20	H1γ/H2γ	19	H3'	4.30	0.65	0.65
8	H2α	8	H6	4.08	0.61	0.61
20	H2α	20	H6	4.08	0.61	0.61
8	H1β	8	H2α	2.83	0.42	0.42
20	H1β	20	H2α	2.83	0.42	0.42
8	H1γ/H2γ	8	H2α	2.65	0.40	0.40
20	H1γ/H2γ	20	H2α	2.65	0.40	0.40
8	H4'	8	H6	4.62	0.69	0.69
20	H4'	20	H6	4.62	0.69	0.69
8	H4'	8	H2'	3.38	0.51	0.51
20	H4'	20	H2'	3.38	0.51	0.51
9	H6	8	H3'	4.65	0.70	0.70
21	H6	20	H3'	4.65	0.70	0.70
9	H2'	9	H1'	2.96	0.44	0.44
21	H2'	21	H1'	2.96	0.44	0.44

9	H2'	9	H6	2.62	0.39	0.39
21	H2'	21	H6	2.62	0.39	0.39
10	H8	10	H4'	5.00	0.75	0.75
22	H8	22	H4'	5.00	0.75	0.75
11	H5	10	H4'	6.20	0.93	0.93
23	H5	22	H4'	6.20	0.93	0.93
11	H2'	11	H5	3.42	0.51	0.51
23	H2'	23	H5	3.42	0.51	0.51
11	H3'	11	H6	3.51	0.53	0.53
23	H3'	23	H6	3.51	0.53	0.53

Class 3

Base 1	Atom 1	Base 2	Atom 2	Dist	Lower	Upper
1	H2'	1	H1'	2.61	0.52	0.52
13	H2'	13	H1'	2.61	0.52	0.52
1	H2'	1	H6	2.74	0.55	0.55
13	H2'	13	H6	2.74	0.55	0.55
1	H2''	1	H1'	2.47	0.49	0.49
13	H2''	13	H1'	2.47	0.49	0.49
1	H3'	1	H2''	3.33	0.67	0.67
13	H3'	13	H2''	3.33	0.67	0.67
1	H4'	1	H1'	2.88	0.58	0.58
13	H4'	13	H1'	2.88	0.58	0.58
2	H4'	1	H3'	5.13	1.03	1.03
14	H4'	13	H3'	5.13	1.03	1.03
2	H8	1	H1'	4.32	0.86	0.86
14	H8	13	H1'	4.32	0.86	0.86
2	H8	1	H2''	3.23	0.65	0.65
14	H8	13	H2''	3.23	0.65	0.65
2	H2''	2	H4'	3.39	0.68	0.68
14	H2''	14	H4'	3.39	0.68	0.68
2	H2''	2	H8	3.08	0.62	0.62
14	H2''	14	H8	3.08	0.62	0.62
2	H3'	2	H4'	3.62	0.72	0.72
14	H3'	14	H4'	3.62	0.72	0.72

2	H3'	2	H8	4.72	0.94	0.94
14	H3'	14	H8	4.72	0.94	0.94
3	H6	2	H1'	3.54	0.71	0.71
15	H6	14	H1'	3.54	0.71	0.71
3	H6	2	H8	4.21	0.84	0.84
15	H6	14	H8	4.21	0.84	0.84
3	H6	2	H2'	4.03	0.81	0.81
15	H6	14	H2'	4.03	0.81	0.81
3	H5	2	H2''	3.49	0.70	0.70
15	H5	14	H2''	3.49	0.70	0.70
3	H3'	2	H1'	4.75	0.95	0.95
15	H3'	14	H1'	4.75	0.95	0.95
3	H3'	3	H2''	2.66	0.53	0.53
15	H3'	15	H2''	2.66	0.53	0.53
3	H4'	3	H1'	3.10	0.62	0.62
15	H4'	15	H1'	3.10	0.62	0.62
4	H4'	3	H2''	5.19	1.04	1.04
16	H4'	15	H2''	5.19	1.04	1.04
4	H8	3	H5	6.41	1.28	1.28
16	H8	15	H5	6.41	1.28	1.28
4	H1'	4	H4'	3.19	0.64	0.64
16	H1'	16	H4'	3.19	0.64	0.64
4	H8	4	H4'	4.55	0.91	0.91
16	H8	16	H4'	4.55	0.91	0.91
4	H2'	4	H4'	3.86	0.77	0.77
16	H2'	16	H4'	3.86	0.77	0.77
4	H2''	4	H4'	3.61	0.72	0.72
16	H2''	16	H4'	3.61	0.72	0.72
4	H2''	4	H8	3.14	0.63	0.63
16	H2''	16	H8	3.14	0.63	0.63
4	H3'	4	H4'	2.74	0.55	0.55
16	H3'	16	H4'	2.74	0.55	0.55
4	H3'	4	H1'	4.26	0.85	0.85
16	H3'	16	H1'	4.26	0.85	0.85
5	H1'	5	H4'	3.60	0.72	0.72
17	H1'	17	H4'	3.60	0.72	0.72

5	H8	5	H4'	4.51	0.90	0.90
17	H8	17	H4'	4.51	0.90	0.90
5	H8	5	H1'	4.01	0.80	0.80
17	H8	17	H1'	4.01	0.80	0.80
5	H2'	5	H1'	2.75	0.55	0.55
17	H2'	17	H1'	2.75	0.55	0.55
5	H2'	5	H8	2.84	0.57	0.57
17	H2'	17	H8	2.84	0.57	0.57
5	H2''	5	H4'	3.62	0.72	0.72
17	H2''	17	H4'	3.62	0.72	0.72
5	H2''	5	H1'	2.46	0.49	0.49
17	H2''	17	H1'	2.46	0.49	0.49
5	H3'	5	H4'	2.73	0.55	0.55
17	H3'	17	H4'	2.73	0.55	0.55
5	H3'	5	H1'	3.90	0.78	0.78
17	H3'	17	H1'	3.90	0.78	0.78
5	H3'	5	H2'	2.81	0.56	0.56
17	H3'	17	H2'	2.81	0.56	0.56
5	H3'	5	H2''	2.75	0.55	0.55
17	H3'	17	H2''	2.75	0.55	0.55
6	H1'	5	H2	3.95	0.79	0.79
18	H1'	17	H2	3.95	0.79	0.79
6	H8	5	H2	5.07	1.01	1.01
18	H8	17	H2	5.07	1.01	1.01
6	H8	6	H4'	4.41	0.88	0.88
18	H8	18	H4'	4.41	0.88	0.88
6	H2'	6	H1'	2.79	0.56	0.56
18	H2'	18	H1'	2.79	0.56	0.56
6	H3'	6	H4'	2.81	0.56	0.56
18	H3'	18	H4'	2.81	0.56	0.56
6	H3'	6	H2''	2.83	0.57	0.57
18	H3'	18	H2''	2.83	0.57	0.57
7	H1'	6	H1'	5.15	1.03	1.03
19	H1'	18	H1'	5.15	1.03	1.03
7	H1'	6	H2	3.46	0.69	0.69
19	H1'	18	H2	3.46	0.69	0.69

7	H6	6	H1'	4.05	0.81	0.81
19	H6	18	H1'	4.05	0.81	0.81
7	H6	6	H8	5.00	1.00	1.00
19	H6	18	H8	5.00	1.00	1.00
7	H5#	6	H2	6.81	1.36	1.36
19	H5#	18	H2	6.81	1.36	1.36
7	H5#	6	H2'	3.25	0.65	0.65
19	H5#	18	H2'	3.25	0.65	0.65
7	H5#	6	H2''	3.35	0.67	0.67
19	H5#	18	H2''	3.35	0.67	0.67
7	H2''	7	H1'	2.54	0.51	0.51
19	H2''	19	H1'	2.54	0.51	0.51
7	H2''	7	H6	3.81	0.76	0.76
19	H2''	19	H6	3.81	0.76	0.76
7	H3'	7	H1'	3.51	0.70	0.70
19	H3'	19	H1'	3.51	0.70	0.70
7	H3'	7	H6	4.00	0.80	0.80
19	H3'	19	H6	4.00	0.80	0.80
7	H3'	7	H2''	2.66	0.53	0.53
19	H3'	19	H2''	2.66	0.53	0.53
7	H4'	7	H1'	2.65	0.53	0.53
19	H4'	19	H1'	2.65	0.53	0.53
7	H4'	7	H2''	3.07	0.61	0.61
19	H4'	19	H2''	3.07	0.61	0.61
8	H1α	7	H6	3.65	0.73	0.73
20	H1α	19	H6	3.65	0.73	0.73
8	H1α	7	H5#	4.96	0.99	0.99
20	H1α	19	H5#	4.96	0.99	0.99
8	H2α	7	H6	4.04	1.00	1.00
20	H2α	19	H6	4.04	1.00	1.00
8	H2α	7	H3'	4.27	0.85	0.85
20	H2α	19	H3'	4.27	0.85	0.85

8	H2β	7	H6	4.70	0.94	0.94
20	H2β	19	H6	4.70	0.94	0.94
8	H3'	7	H1'	5.44	1.09	1.09
20	H3'	19	H1'	5.44	1.09	1.09
8	H2β	8	H2α	3.04	0.61	0.61
20	H2β	20	H2α	3.04	0.61	0.61
8	H1γ/H2γ	8	H1β	2.92	0.58	0.58
20	H1γ/H2γ	20	H1β	2.92	0.58	0.58
8	H2''	8	H1'	2.79	0.56	0.56
20	H2''	20	H1'	2.79	0.56	0.56
8	H3'	8	H6	4.46	0.89	0.89
20	H3'	20	H6	4.46	0.89	0.89
8	H3'	8	H2'	3.59	1.20	1.20
20	H3'	20	H2'	3.59	1.20	1.20
8	H4'	8	H1'	2.83	0.57	0.57
20	H4'	20	H1'	2.83	0.57	0.57
9	H6	8	H2'	3.37	0.67	0.67
21	H6	20	H2'	3.37	0.67	0.67
9	H5	8	H6	3.75	0.75	0.75
21	H5	20	H6	3.75	0.75	0.75
9	H5	8	H3'	5.56	1.11	1.11
21	H5	20	H3'	5.56	1.11	1.11
9	H3'	9	H1'	4.47	0.89	0.89
21	H3'	21	H1'	4.47	0.89	0.89
9	H3'	9	H6	4.31	0.86	0.86
21	H3'	21	H6	4.31	0.86	0.86
9	H3'	9	H2''	3.09	0.62	0.62
21	H3'	21	H2''	3.09	0.62	0.62
9	H4'	9	H1'	3.09	0.62	0.62
21	H4'	21	H1'	3.09	0.62	0.62
9	H4'	9	H6	4.57	0.91	0.91
21	H4'	21	H6	4.57	0.91	0.91
10	H4'	9	H1'	4.71	0.94	0.94

22	H4'	21	H1'	4.71	0.94	0.94
10	H8	9	H1'	4.29	0.86	0.86
22	H8	21	H1'	4.29	0.86	0.86
10	H8	9	H2'	3.35	0.67	0.67
22	H8	21	H2'	3.35	0.67	0.67
10	H3'	9	H1'	5.60	1.12	1.12
22	H3'	21	H1'	5.60	1.12	1.12
10	H3'	9	H2''	4.08	0.82	0.82
22	H3'	21	H2''	4.08	0.82	0.82
10	H1'	10	H4'	3.34	0.67	0.67
22	H1'	22	H4'	3.34	0.67	0.67
10	H2'	10	H4'	3.76	0.75	0.75
22	H2'	22	H4'	3.76	0.75	0.75
10	H2'	10	H1'	3.31	0.66	0.66
22	H2'	22	H1'	3.31	0.66	0.66
10	H2'	10	H8	2.89	0.58	0.58
22	H2'	22	H8	2.89	0.58	0.58
10	H2''	10	H4'	4.21	0.84	0.84
22	H2''	22	H4'	4.21	0.84	0.84
10	H2''	10	H8	3.66	0.73	0.73
22	H2''	22	H8	3.66	0.73	0.73
10	H3'	10	H4'	2.77	0.56	0.56
22	H3'	22	H4'	2.77	0.56	0.56
10	H3'	10	H1'	3.92	0.78	0.78
22	H3'	22	H1'	3.92	0.78	0.78
10	H3'	10	H8	3.83	0.77	0.77
22	H3'	22	H8	3.83	0.77	0.77
11	H6	10	H1'	3.46	0.69	0.69
23	H6	22	H1'	3.46	0.69	0.69
11	H6	10	H2'	3.42	0.68	0.68
23	H6	22	H2'	3.42	0.68	0.68
11	H5	10	H8	3.49	0.70	0.70
23	H5	22	H8	3.49	0.70	0.70
11	H5	10	H2'	2.83	0.57	0.57
23	H5	22	H2'	2.83	0.57	0.57
11	H5	10	H2''	4.14	0.83	0.83

23	H5	22	H2''	4.14	0.83	0.83
11	H5	10	H3'	4.36	0.87	0.87
23	H5	22	H3'	4.36	0.87	0.87
11	H2'	10	H1'	4.77	0.95	0.95
23	H2'	22	H1'	4.77	0.95	0.95
11	H2''	10	H1'	5.21	1.30	1.30
23	H2''	22	H1'	5.21	1.30	1.30
11	H3'	10	H1'	4.51	0.90	0.90
23	H3'	22	H1'	4.51	0.90	0.90
11	H2'	11	H6	2.63	1.00	1.00
23	H2'	23	H6	2.63	1.00	1.00
11	H2''	11	H6	3.04	0.61	0.61
23	H2''	23	H6	3.04	0.61	0.61
11	H2''	11	H5	4.29	0.86	0.86
23	H2''	23	H5	4.29	0.86	0.86
11	H3'	11	H2''	3.31	0.66	0.66
23	H3'	23	H2''	3.31	0.66	0.66
11	H4'	11	H6	4.69	0.94	0.94
23	H4'	23	H6	4.69	0.94	0.94
11	H4'	11	H2''	3.38	0.68	0.68
23	H4'	23	H2''	3.38	0.68	0.68
12	H8	11	H1'	4.38	0.88	0.88
24	H8	23	H1'	4.38	0.88	0.88
12	H8	11	H6	4.86	0.97	0.97
24	H8	23	H6	4.86	0.97	0.97
12	H8	11	H2'	3.72	0.74	0.74
24	H8	23	H2'	3.72	0.74	0.74
12	H8	12	H1'	3.80	0.76	0.76
24	H8	24	H1'	3.80	0.76	0.76
12	H2''	12	H1'	2.12	0.42	0.42
24	H2''	24	H1'	2.12	0.42	0.42
12	H3'	12	H8	4.22	0.84	0.84
24	H3'	24	H8	4.22	0.84	0.84
12	H3'	12	H2''	2.78	0.56	0.56
24	H3'	24	H2''	2.78	0.56	0.56
12	H4'	12	H8	4.88	0.98	0.98

24	H4'	24	H8	4.88	0.98	0.98
12	H4'	12	H2'	2.85	1.00	1.00
24	H4'	24	H2'	2.85	1.00	1.00
12	H4'	12	H2''	3.54	0.71	0.71
24	H4'	24	H2''	3.54	0.71	0.71
12	H4'	12	H3'	2.34	0.47	0.47
24	H4'	24	H3'	2.34	0.47	0.47
6	H2	7	H1'	5.09	1.32	1.32
18	H2	19	H1'	5.09	1.32	1.32
17	H2	9	H1'	3.77	0.76	0.76
5	H2	21	H1'	3.77	0.76	0.76
18	H2	8	H1'	3.73	0.75	0.75
6	H2	20	H1'	3.73	0.75	0.75

Class 4

Base 1	Atom 1	Base 2	Atom 2	Dist	Lower	Upper
1	H5	1	H1'	4.88	1.22	1.22
13	H5	13	H1'	4.88	1.22	1.22
1	H2'	1	H5	2.99	0.75	0.75
13	H2'	13	H5	2.99	0.75	0.75
1	H2''	1	H5	4.11	1.03	1.03
13	H2''	13	H5	4.11	1.03	1.03
1	H4'	1	H2'	5.85	2.00	2.00
13	H4'	13	H2'	5.85	2.00	2.00
1	H4'	1	H2''	4.84	1.21	1.21
13	H4'	13	H2''	4.84	1.21	1.21
1	H3'	1	H6	4.03	1.01	1.01
13	H3'	13	H6	4.03	1.01	1.01
1	H4'	1	H6	5.34	1.34	1.34
13	H4'	13	H6	5.34	1.34	1.34
2	H8	1	H6	4.78	1.20	1.20
14	H8	13	H6	4.78	1.20	1.20
2	H8	1	H2'	3.72	0.93	0.93
14	H8	13	H2'	3.72	0.93	0.93
2	H8	1	H3'	3.62	0.91	0.91

14	H8	13	H3'	3.62	0.91	0.91
2	H1'	2	H4'	3.48	0.87	0.87
14	H1'	14	H4'	3.48	0.87	0.87
2	H8	2	H1'	3.48	0.87	0.87
14	H8	14	H1'	3.48	0.87	0.87
2	H2'	2	H4'	4.16	1.04	1.04
14	H2'	14	H4'	4.16	1.04	1.04
2	H2'	2	H1'	3.74	0.93	0.93
14	H2'	14	H1'	3.74	0.93	0.93
2	H2'	2	H8	2.90	0.73	0.73
14	H2'	14	H8	2.90	0.73	0.73
2	H2''	2	H1'	2.75	0.69	0.69
14	H2''	14	H1'	2.75	0.69	0.69
2	H3'	2	H1'	4.46	1.36	1.36
14	H3'	14	H1'	4.46	1.36	1.36
2	H3'	2	H2'	3.15	0.79	0.79
14	H3'	14	H2'	3.15	0.79	0.79
2	H3'	2	H2''	3.59	0.90	0.90
14	H3'	14	H2''	3.59	0.90	0.90
3	H6	2	H4'	6.47	1.62	1.62
15	H6	14	H4'	6.47	1.62	1.62
3	H6	2	H2''	4.27	1.20	1.20
15	H6	14	H2''	4.27	1.20	1.20
3	H5	2	H2'	4.50	1.12	1.12
15	H5	14	H2'	4.50	1.12	1.12
3	H2''	3	H6	2.91	0.73	0.73
15	H2''	15	H6	2.91	0.73	0.73
3	H3'	3	H2'	2.52	0.63	0.63
15	H3'	15	H2'	2.52	0.63	0.63
3	H4'	3	H6	3.83	0.96	0.96
15	H4'	15	H6	3.83	0.96	0.96
3	H4'	3	H5	5.38	1.34	1.34
15	H4'	15	H5	5.38	1.34	1.34
3	H4'	3	H2'	3.47	0.87	0.87
15	H4'	15	H2'	3.47	0.87	0.87
3	H4'	3	H2''	3.00	0.75	0.75

15	H4'	15	H2''	3.00	0.75	0.75
3	H4'	4	H8	4.72	1.18	1.18
15	H4'	16	H8	4.72	1.18	1.18
4	H2'	4	H1'	3.63	0.91	0.91
16	H2'	16	H1'	3.63	0.91	0.91
4	H2'	4	H8	2.60	0.65	0.65
16	H2'	16	H8	2.60	0.65	0.65
4	H2''	4	H1'	2.80	0.70	0.70
16	H2''	16	H1'	2.80	0.70	0.70
4	H3'	4	H2''	3.43	0.86	0.86
16	H3'	16	H2''	3.43	0.86	0.86
5	H8	4	H2''	2.74	0.69	0.69
17	H8	16	H2''	2.74	0.69	0.69
5	H8	4	H3'	4.44	1.11	1.11
17	H8	16	H3'	4.44	1.11	1.11
5	H2	5	H1'	4.73	1.18	1.18
17	H2	17	H1'	4.73	1.18	1.18
5	H2'	5	H4'	3.13	0.78	0.78
17	H2'	17	H4'	3.13	0.78	0.78
5	H2''	5	H8	3.60	0.90	0.90
17	H2''	17	H8	3.60	0.90	0.90
5	H3'	5	H8	3.01	1.00	1.00
17	H3'	17	H8	3.01	1.00	1.00
6	H4'	5	H1'	3.85	0.96	0.96
18	H4'	17	H1'	3.85	0.96	0.96
6	H8	5	H1'	3.57	0.89	0.89
18	H8	17	H1'	3.57	0.89	0.89
6	H8	5	H2''	2.84	0.71	0.71
18	H8	17	H2''	2.84	0.71	0.71
6	H2'	5	H1'	4.08	1.02	1.02
18	H2'	17	H1'	4.08	1.02	1.02
6	H3'	5	H1'	4.20	1.05	1.05
18	H3'	17	H1'	4.20	1.05	1.05
6	H2'	6	H4'	3.20	0.80	0.80
18	H2'	18	H4'	3.20	0.80	0.80
6	H2''	6	H4'	3.46	0.87	0.87

18	H2''	18	H4'	3.46	0.87	0.87
6	H2''	6	H8	3.09	0.77	0.77
18	H2''	18	H8	3.09	0.77	0.77
6	H3'	6	H2'	2.66	0.66	0.66
18	H3'	18	H2'	2.66	0.66	0.66
7	H6	6	H2''	3.79	1.50	1.50
19	H6	18	H2''	3.79	1.50	1.50
7	H2'	7	H6	2.29	1.00	1.00
19	H2'	19	H6	2.29	1.00	1.00
7	H2'	7	H5#	4.61	1.15	1.15
19	H2'	19	H5#	4.61	1.15	1.15
7	H3'	7	H2'	2.80	0.70	0.70
19	H3'	19	H2'	2.80	0.70	0.70
8	H1'	7	H1'	4.46	1.11	1.11
20	H1'	19	H1'	4.46	1.11	1.11
8	H6	7	H2''	2.89	0.72	0.72
20	H6	19	H2''	2.89	0.72	0.72
8	H2α	7	H1'	4.59	1.15	1.15
20	H2α	19	H1'	4.59	1.15	1.15
8	H2α	7	H5#	4.18	1.04	1.04
20	H2α	19	H5#	4.18	1.04	1.04
8	H1β	7	H6	4.47	1.12	1.12
20	H1β	19	H6	4.47	1.12	1.12
8	H1β	7	H5#	5.39	1.35	1.35
20	H1β	19	H5#	5.39	1.35	1.35
8	H2β	7	H5#	4.72	1.18	1.18
20	H2β	19	H5#	4.72	1.18	1.18
8	H1γ/H2γ	7	H6	4.32	1.08	1.08
20	H1γ/H2γ	19	H6	4.32	1.08	1.08
8	H1γ/H2γ	7	H5#	4.29	1.07	1.07

20	H1γ/H2γ	19	H5#	4.29	1.07	1.07
8	H1α	8	H6	3.52	1.20	1.20
20	H1α	20	H6	3.52	1.20	1.20
8	H1β	8	H6	3.91	0.98	0.98
20	H1β	20	H6	3.91	0.98	0.98
8	H1β	8	H1α	3.07	0.77	0.77
20	H1β	20	H1α	3.07	0.77	0.77
8	H1γ/H2γ	8	H2β	2.37	0.59	0.59
20	H1γ/H2γ	20	H2β	2.37	0.59	0.59
7	H2''	8	H1α	2.83	0.71	0.71
19	H2''	20	H1α	2.83	0.71	0.71
8	H2''	8	H6	3.29	0.82	0.82
20	H2''	20	H6	3.29	0.82	0.82
8	H3'	8	H2''	3.06	0.77	0.77
20	H3'	20	H2''	3.06	0.77	0.77
8	H4'	8	H2''	3.24	0.81	0.81
20	H4'	20	H2''	3.24	0.81	0.81
8	H4'	8	H3'	3.29	0.82	0.82
20	H4'	20	H3'	3.29	0.82	0.82
8	H4'	8	H6	5.03	1.26	1.26
20	H4'	20	H6	5.03	1.26	1.26
9	H1'	8	H1'	5.37	1.34	1.34
21	H1'	20	H1'	5.37	1.34	1.34
9	H6	8	H6	3.71	0.93	0.93
21	H6	20	H6	3.71	0.93	0.93
9	H6	8	H2''	3.35	1.20	1.20
21	H6	20	H2''	3.35	1.20	1.20
9	H5	8	H2''	3.25	0.81	0.81
21	H5	20	H2''	3.25	0.81	0.81
9	H5	9	H1'	4.45	1.11	1.11
21	H5	21	H1'	4.45	1.11	1.11

9	H2''	9	H1'	2.50	0.62	0.62
21	H2''	21	H1'	2.50	0.62	0.62
9	H2''	9	H6	3.33	0.83	0.83
21	H2''	21	H6	3.33	0.83	0.83
9	H3'	9	H5	4.81	1.20	1.20
21	H3'	21	H5	4.81	1.20	1.20
9	H3'	9	H2'	2.50	0.62	0.62
21	H3'	21	H2'	2.50	0.62	0.62
9	H4'	9	H2'	4.00	1.00	1.00
21	H4'	21	H2'	4.00	1.00	1.00
9	H4'	17	H2	5.65	1.41	1.41
21	H4'	5	H2	5.65	1.41	1.41
10	H1'	9	H2''	3.96	0.99	0.99
22	H1'	21	H2''	3.96	0.99	0.99
10	H8	9	H2''	3.12	0.78	0.78
22	H8	21	H2''	3.12	0.78	0.78
10	H8	10	H1'	3.46	0.86	0.86
22	H8	22	H1'	3.46	0.86	0.86
10	H2''	10	H1'	2.86	0.71	0.71
22	H2''	22	H1'	2.86	0.71	0.71
10	H3'	10	H2'	3.05	0.76	0.76
22	H3'	22	H2'	3.05	0.76	0.76
10	H3'	10	H2''	3.54	0.89	0.89
20	H3'	20	H2''	3.54	0.89	0.89
11	H1'	10	H1'	4.89	0.97	0.97
23	H1'	22	H1'	4.89	0.97	0.97
11	H6	10	H2''	3.59	1.50	1.50
23	H6	22	H2''	3.59	1.50	1.50
11	H2'	11	H1'	2.78	0.69	0.69
23	H2'	23	H1'	2.78	0.69	0.69
11	H2''	11	H1'	2.49	0.62	0.62
23	H2''	23	H1'	2.49	0.62	0.62
11	H3'	11	H2'	3.00	0.75	0.75
23	H3'	23	H2'	3.00	0.75	0.75
11	H4'	11	H1'	2.78	0.70	0.70
23	H4'	23	H1'	2.78	0.70	0.70

11	H4'	11	H2'	2.98	0.74	0.74
23	H4'	23	H2'	2.98	0.74	0.74
12	H2'	11	H1'	2.66	0.66	0.66
24	H2'	23	H1'	2.66	0.66	0.66
12	H2'	11	H8	2.51	0.63	0.63
24	H2'	23	H8	2.51	0.63	0.63
12	H3'	11	H2'	2.74	0.69	0.69
24	H3'	23	H2'	2.74	0.69	0.69
12	H4'	11	H1'	4.03	1.01	1.01
24	H4'	23	H1'	4.03	1.01	1.01
17	H2	8	H1'	5.81	1.00	1.45
5	H2	20	H1'	5.81	1.00	1.45

Class bp

Base 1	Atom 1	Base 2	Atom 2	Dist	Lower	Upper
1	N4	24	O6	2.91	0.10	0.10
1	N3	24	N1	2.95	0.10	0.10
1	O2	24	N2	2.86	0.10	0.10
2	O6	23	N4	2.91	0.10	0.10
2	N1	23	N3	2.95	0.10	0.10
2	N2	23	O2	2.86	0.10	0.10
3	N4	22	O6	2.91	0.10	0.10
3	N3	22	N1	2.95	0.10	0.10
3	O2	22	N2	2.86	0.10	0.10
4	O6	21	N4	2.91	0.10	0.10
4	N1	21	N3	2.95	0.10	0.10
4	N2	21	O2	2.86	0.10	0.10
5	N6	20	O4	2.95	0.10	0.10
5	N1	20	N3	2.82	0.10	0.10
6	N6	19	O4	2.95	0.10	0.10
6	N1	19	N3	2.82	0.10	0.10
7	O4	18	N6	2.95	0.10	0.10
7	N3	18	N1	2.82	0.10	0.10
8	O4	17	N6	2.95	0.10	0.10
8	N3	17	N1	2.82	0.10	0.10

9	N4	24	O6	2.91	0.10	0.10
9	N3	24	N1	2.95	0.10	0.10
9	O2	24	N2	2.86	0.10	0.10
10	O6	23	N4	2.91	0.10	0.10
10	N1	23	N3	2.95	0.10	0.10
10	N2	23	O2	2.86	0.10	0.10
11	N4	22	O6	2.91	0.10	0.10
11	N3	22	N1	2.95	0.10	0.10
11	O2	22	N2	2.86	0.10	0.10
12	O6	21	N4	2.91	0.10	0.10
12	N1	21	N3	2.95	0.10	0.10
12	N2	21	O2	2.86	0.10	0.10

Table S2. Chemical shift assignments (ppm) for the base and deoxyribose protons of the Z3dU modified duplex.

Base	H8	H6	H5	H1'	H2'	H2''	H3'	H4'	CH_3
C^1		7.63	5.90	5.73	1.96	2.39	4.68	4.05	
G^2	7.94			5.87	2.64	2.69	4.95	4.31	
C^3		7.25	5.32	5.60	1.82	2.26	4.80	4.11	
G^4	7.82			5.40	2.62	2.73	4.97	4.30	
A^5	8.10			5.96	2.68	2.91	5.04	4.44	
A^6	8.10			6.17	2.57	2.91	4.99	4.45	
T^7		7.07		5.90	1.90	2.54	4.82	4.20	1.25
X^8		7.40		6.02	2.14	2.51	4.88	4.20	
C^9		7.49	5.69	5.77	2.00	2.42	4.83	4.15	
G^{10}	7.91			5.86	2.63	2.70	4.97	4.37	
C^{11}		7.30	5.41	5.73	1.87	2.31	4.79	4.13	
G^{12}	7.92			6.14	2.36	2.60	4.66	4.15	

Table S3. Chemical shift assignments (ppm) for the protons of the 3-aminopropyl side chain.

protons	chemical shift
$H_{1\alpha}$	1.98
$H_{2\alpha}$	1.78
$H_{1\beta}$	1.58
$H_{2\beta}$	1.70
$H_{1\gamma}$/ $H_{2\gamma}$	2.90

Table S4. Chemical shift assignments (ppm) of the exchangeable imino and amino protons of Z3dU duplex.

base pair	imino G1H/T3H	amino $CNH_{2(a)}$	amino $CNH_{2(b)}$
G^2C^{11}	13.06	6.44	8.42
C^3C^{10}	12.86	6.66	8.48
G^4C^9	12.73	6.60	8.28
A^5X^8	13.96		
A^6T^7	13.83		

Table S5. Chemical shift assignments (ppm) for the phosphates of the unmodified and Z3dU modified Dickerson dodecamer.

phosphates	chemical shift for unmodified dodecamer	chemical shift for Z3dU modified dodecamer
P^1	-3.81	-3.86
P^2	-3.93	-3.96
P^3	-3.74	-3.79
P^4	-3.90	-3.93
P^5	-4.04	-4.02
P^6	-4.14	-4.18
P^7	-4.13	-4.17
P^8	-4.03	-3.93
P^9	-3.67	-3.91
P^{10}	-3.81	-3.87
P^{11}	-3.66	-3.68

Table S6. Partial charge and atom type of Z3dU residue used for X-PLOR calculation.

Atom	X-PLOR	
	Type	Charge
N1	NS	-0.19
C2	C	0.35
O2	O	-0.35
N3	NA	-0.26
H3	H	0.26
C4	C	0.30
O4	O	-0.30
C5	CS	-0.035
C6	CF	0.155
H6	H	0.035
C5A	CPR	0.139
H1α	HP	0.031
H2α	HP	-0.002
CP2	CPR	-0.054
H1β	HP	0.031
H2β	HP	0.043
CP3	CPR	0.080
H1γ	HP	0.054
H2γ	HP	0.039
NZ	NZ	0.025
HZ1	HZ1	0.181
HZ2	HZ2	0.244
HZ3	HZ3	0.231

Table S7. Helicoidal Parameters for the Bent Z3dU-Modified Dodecamer.

A. Local base-pair parameters.

Base pair	Shear	Stretch	Stagger	Buckle	Propeller	Opening
C^{1}-G^{12}	0.85	-0.42	-0.35	-34.50	-12.02	3.27
G^{2}-C^{11}	-0.13	-0.05	0.50	-9.38	7.71	1.43
C^{3}-G^{10}	-0.94	-0.09	0.25	-10.91	-0.37	2.60
G^{4}-C^{9}	0.18	-0.07	0.24	21.69	-3.14	-4.79
A^{5}-T^{8}	0.30	-0.09	-0.37	-1.71	-6.92	-4.92
A^{6}-T^{7}	0.94	-0.11	-0.42	-1.40	-6.70	-7.65
T^{7}-A^{6}	-0.95	-0.12	-0.38	-1.08	-5.58	-7.67
T^{8}-A^{5}	-0.20	-0.10	-0.37	0.67	-4.83	-5.43
C^{9}-G^{4}	-0.09	-0.09	0.15	-20.98	-4.55	-4.58
G^{10}-C^{3}	0.95	-0.09	0.30	12.27	0.70	2.67
C^{11}-G^{2}	0.11	-0.03	0.43	9.22	5.96	0.97
G^{12}-C^{1}	-0.83	-0.43	-0.40	32.54	-13.06	4.10

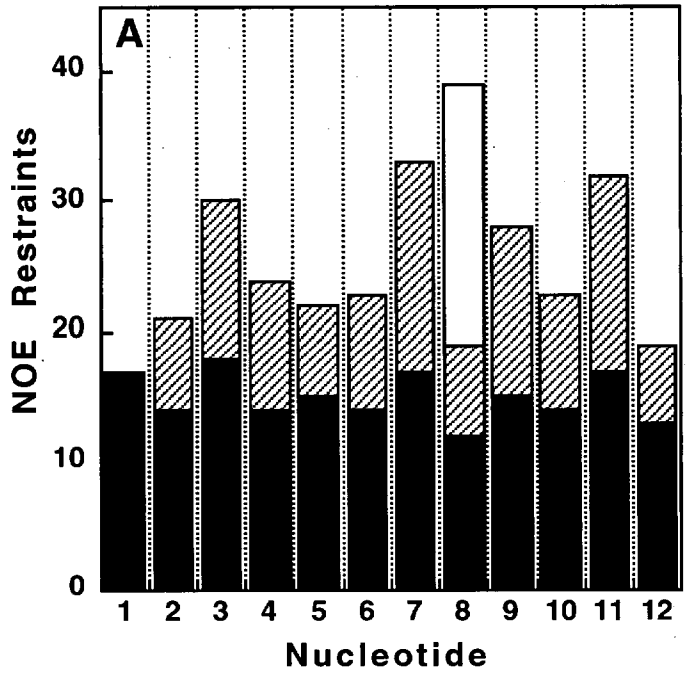
B. Local base-pair step parameters.

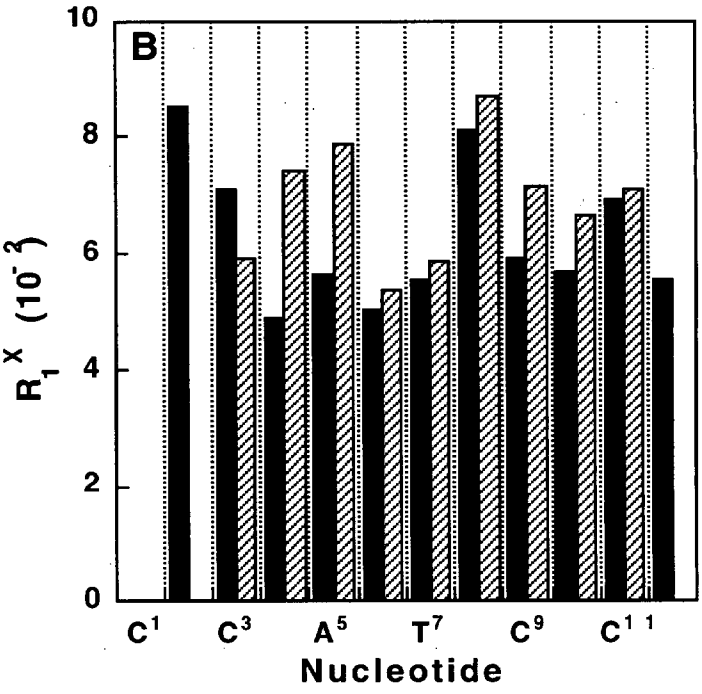
Base pair	Shift	Slide	Rise	Tilt	Roll	Twist
C^{1}-G^{12}	0.81	-0.55	2.28	1.17	20.22	12.75
G^{2}-C^{11}	0.23	-0.80	3.43	1.78	23.62	26.01
C^{3}-G^{10}	-1.59	-0.53	2.33	-0.14	1.66	31.56
G^{4}-C^{9}	-0.45	-1.07	3.54	3.28	25.43	33.42
A^{5}-T^{8}	-0.07	-1.19	3.01	-0.35	1.82	34.53
A^{6}-T^{7}	-0.02	-1.50	2.94	-0.20	-6.97	29.42
T^{7}-A^{6}	0.03	-1.17	2.99	0.53	1.96	34.59
T^{8}-A^{5}	0.49	-1.05	3.48	-2.30	25.92	32.96
C^{9}-G^{4}	1.62	-0.51	2.30	-0.32	2.48	31.11
G^{10}-C^{3}	-0.28	-0.82	3.48	-0.88	24.74	26.09
C^{11}-G^{2}	-0.72	-0.56	2.32	-1.37	20.71	12.88

C. Local base-pair helical parameters.

Base pair	X-disp	Y-disp	Rise	Incl.	Tip	Twist
C^{1}-G^{12}	-5.41	-1.71	0.80	58.05	-3.36	23.90
G^{2}-C^{11}	-4.78	-0.13	2.05	42.85	-3.23	35.04
C^{3}-G^{10}	-1.19	2.90	2.31	3.05	0.26	31.60
G^{4}-C^{9}	-4.11	0.97	2.18	38.05	-4.90	41.90
A^{5}-T^{8}	-2.26	0.08	2.94	3.06	0.60	34.58
A^{6}-T^{7}	-1.54	0.00	3.20	-13.49	0.38	30.21
T^{7}-A^{6}	-2.23	0.02	2.92	3.29	-0.90	34.65
T^{8}-A^{5}	-4.11	-0.92	2.11	39.01	3.45	41.76
C^{9}-G^{4}	-1.28	-3.05	2.24	4.62	0.59	31.21
G^{10}-C^{3}	-4.82	0.33	2.00	44.16	1.57	35.81
C^{11}-G^{2}	-5.41	1.43	0.80	58.38	3.86	24.39

Figure S1. (A) Distribution of experimental NOE restraints applied in the structural refinement. Solid bars, intranucleotide NOEs; cross-hatch bars, internucleotide NOEs; open bars, Z3dU-DNA NOEs. The internucleotide NOEs are counted in the direction $n \rightarrow n - 1$. (B) Bar diagrams showing the per-residue R_1^x values for the modified Dickerson dodecamer. Solid bars, intraresidue R_1^x values, cross-hatch bars interresidue R_1^x values.


A
NOE Restraints
0
10
20
30
40
1 2 3 4 5 6 7 8 9 10 11 12
Nucleotide


B
R_1^x (10^{-3})
0
2
4
6
8
10
C1 C3 A5 T7 C9 C11
Nucleotide