Table S1. Class 1 Distance restraints

Assign	Base	Proton	Assign	Base	Proton	LB	UB
1	DA5	Q5'	1	DA5	H8	3.85	4.71
1	DA5	Q5'	1	DA5	H4'	2.21	2.71
1	DA5	H2'	1	DA5	H8	1.98	2.42
1	DA5	H2'	1	DA5	H1'	2.53	3.09
1	DA5	H2	1	DA5	H1'	4.38	5.36
2	DC	H6	1	DA5	H8	4.31	5.27
2	DC	H6	1	DA5	H2'	3.48	4.26
2	DC	H5	1	DA5	H8	3.56	4.36
2	DC	H5	1	DA5	H2'	3.15	3.85
2	DC	H1'	1	DA5	H2	4.46	5.46
2	DC	H2"	2	DC	H6	2.78	3.4
2	DC	H2'	2	DC	H6	1.97	2.41
2	DC	H2'	2	DC	H1'	2.91	3.55
3	DA	H8	2	DC	H6	4.54	5.56
3	DA	H8	2	DC	H2'	3.78	4.62
3	DA	H8	3	DA	H1'	3.4	4.16
3	DA	H4'	3	DA	H8	4.37	5.35
3	DA	H3'	3	DA	H1'	3.59	4.39
3	DA	H2'	3	DA	H8	1.97	2.41
3	DA	H2	3	DA	H1'	4.29	5.25
4	DT	Q5'	3	DA	H1'	3.23	3.95
4	DT	M	3	DA	H8	2.96	3.62
4	DT	H6	3	DA	H2'	3.14	3.84
4	DT	H4'	4	DT	H6	4.67	5.71
4	DT	H3'	4	DT	H6	3.88	4.74

4	DT	H2''	4	DT	H6	2.84	3.48
4	DT	H1'	4	DT	H6	3.08	3.76
5	DC	H6	4	DT	H2''	1.99	2.43
5	DC	H6	4	DT	H2'	3.63	4.43
5	DC	H5	4	DT	M	4.09	4.99
5	DC	H5	4	DT	H6	3.19	3.89
5	DC	H5	4	DT	H2''	2.32	2.84
5	DC	Q5'	5	DC	H6	3.85	4.71
5	DC	H6	5	DC	H4'	3.95	4.83
5	DC	H6	5	DC	H1'	2.91	3.55
5	DC	H3'	5	DC	H1'	3.45	4.21
6	GAF	H9A	5	DC	H6	3.89	4.63
6	GAF	H6A	5	DC	H6	2.76	3.18
6	GAF	H6A	5	DC	H5	2.34	2.86
6	GAF	H9A	5	DC	H5	2.37	2.81
6	GAF	HM	6	GAF	H5B	2.38	2.92
6	GAF	H9A	6	GAF	H9	2.28	2.78
6	GAF	H9A	6	GAF	H8A	2.94	4.26
6	GAF	H9A	6	GAF	H8	4.24	5.18
6	GAF	H9	6	GAF	H8A	2.39	2.91
6	GAF	H6A	6	GAF	H8A	3.39	4.15
6	GAF	H5B	6	GAF	H8	2.83	3.47
6	GAF	H5B	6	GAF	H6A	4.23	5.17
6	GAF	H3B	6	GAF	HM	3.04	3.72
6	GAF	H2B	6	GAF	H3A	2.35	2.87
6	GAF	H2A	6	GAF	H3B	2.86	3.5
6	GAF	H2'	6	GAF	H8	2.03	2.49

7	DA	H8	6	GAF	H1'	2.68	3.2
7	DA	Q5'	7	DA	H8	3.1	3.78
7	DA	H4'	7	DA	H8	4.13	5.05
7	DA	H2'	7	DA	H8	2.03	2.49
7	DA	H1'	7	DA	H2"	1.93	2.35
7	DA	H1'	7	DA	H2	4.21	5.15
8	DT	M	7	DA	H8	3.18	3.88
8	DT	M	7	DA	H3'	4.54	5.54
8	DT	H6	7	DA	H2'	3.14	3.84
8	DT	H6	8	DT	H1'	3.17	3.87
8	DT	Q5'	8	DT	H6	3.13	3.83
8	DT	H2"	8	DT	H1'	1.84	2.26
8	DT	H2'	8	DT	H1'	2.77	3.39
9	DC	H5	8	DT	H6	3.24	3.96
9	DC	H5	8	DT	H2'	2.8	3.42
9	DC	Q5'	9	DC	H6	3.81	4.65
9	DC	H1'	9	DC	H6	3.03	3.71
9	DC	H1'	9	DC	H2"	1.93	2.35
9	DC	H1'	10	DT3	M	3.86	4.72
10	DT3	Q5'	10	DT3	H6	3.85	4.71
10	DT3	H6	10	DT3	H4'	4.19	5.11
10	DT3	H1'	10	DT3	H6	3	3.66
10	DT3	H1'	10	DT3	H2"	1.93	2.37
11	DA5	Q5'	11	DA5	H8	4.21	5.15
11	DA5	Q5'	11	DA5	H4'	2.27	2.77
11	DA5	H3'	11	DA5	H8	4.33	5.29
11	DA5	H2'	11	DA5	H8	2.1	2.56

11	DA5	H1'	11	DA5	H2"	1.82	2.22
12	DG	Q5'	12	DG	H2'	3.34	4.08
12	DG	H8	12	DG	H1'	3.37	4.13
12	DG	H4'	12	DG	H8	4.46	5.44
12	DG	H2"	12	DG	H1'	1.85	2.27
12	DG	H2'	12	DG	H8	2.04	2.5
13	DA	H8	12	DG	H2"	2.19	2.67
13	DA	H8	12	DG	H1'	2.58	3.16
13	DA	H8	13	DA	H1'	3.3	4.04
13	DA	H4'	13	DA	H8	4.35	5.31
13	DA	H2'	13	DA	H8	1.87	2.29
13	DA	H2	13	DA	H1'	3.89	4.75
13	DA	H2	14	DT	H3	3.89	4.75
14	DT	M	14	DT	H6	2.74	3.34
14	DT	H6	14	DT	H4'	4.06	4.96
14	DT	H6	14	DT	H1'	3.11	3.81
14	DT	H3'	14	DT	H1'	3.41	4.17
14	DT	H2"	14	DT	H6	2.85	3.49
14	DT	H2'	14	DT	H1'	2.64	3.22
15	DC	H6	14	DT	H3	4.89	5.75
15	DC	H1'	6	GAF	H2A	3.77	4.61
15	DC	H5	14	DT	H6	3.45	4.21
15	DC	H2"	15	DC	H1'	2.11	2.59
15	DC	Q5'	15	DC	H6	3.83	4.67
15	DC	H6	15	DC	H1'	3.21	3.93
15	DC	H1'	15	DC	H2'	2.95	3.61
16	DG	Q5'	16	DG	H8	3.94	4.82

16	DG	Q5'	16	DG	H3'	3.04	3.72
16	DG	H8	16	DG	H1'	3.38	4.12
16	DG	H4'	16	DG	H8	4.5	5.5
16	DG	H4'	16	DG	H3'	2.24	2.74
16	DG	H3'	16	DG	H1'	3.7	4.52
16	DG	H2'	16	DG	H8	1.9	2.32
17	DA	H8	16	DG	H1'	2.7	3.3
17	DA	H1'	17	DA	H8	3.21	3.93
17	DA	H1'	17	DA	H2	3.83	4.69
17	DA	H1'	18	DT	M	3.9	4.76
18	DT	M	17	DA	H8	3.19	3.89
18	DT	M	17	DA	H3'	4.31	5.27
18	DT	H1'	17	DA	H2	3.79	4.63
18	DT	M	18	DT	H6	2.81	3.43
18	DT	H6	18	DT	H1'	3.11	3.81
18	DT	H3'	18	DT	H6	3.76	4.6
18	DT	H2'	18	DT	H1'	2.79	3.41
19	DG	Q5'	19	DG	H1'	3.07	3.75
19	DG	H8	18	DT	H2'	3.6	4.4
19	DG	H8	19	DG	H1'	3.38	4.12
19	DG	H4'	19	DG	H8	4.55	5.57
19	DG	H2''	19	DG	H1'	1.9	2.32
19	DG	H2'	19	DG	H8	1.86	2.28
20	DT3	M	19	DG	H3'	4.85	5.93
20	DT3	Q5'	20	DT3	H6	3.66	4.48
20	DT3	M	20	DT3	H6	2.77	3.39
20	DT3	H4'	20	DT3	H6	4.46	5.46

20	DT3	H2''	20	DT3	H1'	2.06	2.52
20	DT3	H1'	20	DT3	H6	3.15	3.85
20	DT3	H1'	20	DT3	H3'	3.28	4.02

Table S2. Class 2 Distance restraints

Assign	Base	Proton	Assign	Base	Proton	LB	UB
1	DA5	H2"	1	DA5	H1'	1.96	2.64
2	DC	H2"	2	DC	H1'	1.99	2.69
3	DA	H8	2	DC	H1'	2.73	3.69
3	DA	H2'	3	DA	H1'	2.14	2.9
4	DT	M	4	DT	H6	2.53	3.43
4	DT	Q5'	4	DT	H6	3.82	5.16
4	DT	H2'	4	DT	H6	1.98	2.68
4	DT	H1'	5	DC	H6	2.69	3.63
5	DC	H2'	5	DC	H6	1.95	2.65
5	DC	H1'	5	DC	H2'	2.24	3.02
6	GAF	HM	5	DC	H1'	3.05	4.13
6	GAF	H6A	5	DC	H2'	2.92	3.96
6	GAF	H5B	5	DC	H2"	2.36	3.18
6	GAF	Q5'	6	GAF	HM	3.91	5.29
6	GAF	Q5'	6	GAF	H8	3.38	4.58
6	GAF	Q5'	6	GAF	H5B	4.52	6.12
6	GAF	HM	6	GAF	H8	3.91	5.29
6	GAF	H6A	6	GAF	H9A	2	2.7
6	GAF	H6A	6	GAF	H9	3.03	4.09
6	GAF	H6A	6	GAF	H8	3.54	4.8
6	GAF	H5B	6	GAF	H9	4.66	6.3
6	GAF	H2A	6	GAF	H3A	2.45	3.31
6	GAF	H2"	6	GAF	H1'	1.91	2.59
6	GAF	H2"	6	GAF	H8	2.73	3.69
6	GAF	H2'	6	GAF	H1'	2.23	3.01

7	DA	H8	6	GAF	H8	4	5.4
7	DA	H8	6	GAF	H2'	2.91	3.93
7	DA	H8	6	GAF	H2"	1.91	2.93
7	DA	Q5'	7	DA	H8	3.54	4.8
7	DA	H1'	8	DT	H6	2.71	3.67
8	DT	H6	7	DA	H2"	2.18	2.96
8	DT	H1'	7	DA	H2	3.33	4.51
8	DT	M	8	DT	H6	2.45	3.31
8	DT	H3'	8	DT	H6	3.83	5.17
8	DT	H2'	8	DT	H6	1.9	2.56
9	DC	Q5'	9	DC	H2'	3.11	4.21
9	DC	H4'	9	DC	H6	3.46	4.68
9	DC	H2'	9	DC	H6	1.93	2.61
10	DT3	M	9	DC	H5	3.25	4.41
10	DT3	H6	9	DC	H2'	2.65	3.59
10	DT3	Q5'	10	DT3	H2'	2.98	4.04
10	DT3	M	10	DT3	H6	2.56	3.46
10	DT3	H2'	10	DT3	H6	1.89	2.57
12	DG	H8	11	DA5	H2"	2.17	2.93
12	DG	Q5'	12	DG	H8	4.04	5.46
12	DG	H3'	12	DG	H1'	2.9	3.92
12	DG	H2'	12	DG	H8	1.7	2.3
13	DA	H4'	13	DA	H3'	1.98	2.68
13	DA	H3'	13	DA	H1'	3	4.06
13	DA	H2"	13	DA	H8	2.97	4.01
14	DT	M	13	DA	H8	3.14	4.24
14	DT	H6	13	DA	H2"	2.07	2.81

14	DT	H6	13	DA	H1'	2.68	3.62
14	DT	H1'	13	DA	H2	4.14	4.98
14	DT	Q5'	14	DT	H6	3.77	5.09
14	DT	H2"	14	DT	H1'	1.83	2.47
14	DT	H2'	14	DT	H6	1.95	2.63
15	DC	H1'	6	GAF	H2B	2.88	3.9
15	DC	H6	14	DT	H2'	2.75	3.71
15	DC	H3'	15	DC	H6	3.95	5.35
15	DC	H2'	16	DG	H8	2.87	3.87
16	DG	H8	15	DC	H2'	3.15	3.71
16	DG	H8	15	DC	H2"	2.25	3.21
17	DA	Q5'	17	DA	H8	3.47	4.69
17	DA	Q5'	17	DA	H8	3.32	4.48
17	DA	H2"	17	DA	H8	2.85	3.85
17	DA	H2'	17	DA	H8	1.67	2.27
17	DA	H1'	17	DA	H3'	3.01	4.07
18	DT	H6	17	DA	H2"	2.12	2.86
18	DT	H6	17	DA	H2'	2.78	3.76
18	DT	Q5'	18	DT	H6	3.77	5.11
18	DT	H4'	18	DT	H3'	1.98	2.68
18	DT	H2"	18	DT	H6	2.56	3.46
18	DT	H2"	18	DT	H1'	1.92	2.6
18	DT	H2'	18	DT	H6	1.88	2.54
19	DG	H8	18	DT	H6	3.72	5.04
19	DG	H1'	3	DA	H2	3.85	5.15
19	DG	H4'	19	DG	H2"	3.03	4.11
19	DG	H3'	19	DG	H1'	2.95	3.99

20	DT3	H6	19	DG	H3'	4	5.42
20	DT3	H2'	20	DT3	H6	2.27	3.07
20	DT3	M	20	DT3	H1'	4.39	6.23
20	DT3	H2'	20	DT3	H3'	1.91	2.59
1	DA5	H3'	1	DA5	H4'	1.76	2.64
1	DA5	H2''	1	DA5	H8	2.54	3.8
2	DC	Q5'	1	DA5	H1'	3.34	5
2	DC	H6	1	DA5	H2''	2.3	3.44
2	DC	H6	1	DA5	H1'	3.2	4.8
3	DA	H8	2	DC	H2''	2.36	3.54
3	DA	Q5'	3	DA	H8	3.1	4.64
3	DA	H2''	3	DA	H8	2.53	3.79
3	DA	H2''	3	DA	H1'	1.48	2.26
4	DT	H6	3	DA	H2''	2.3	3.44
4	DT	Q5'	4	DT	H3'	2.06	3.1
5	DC	H2''	5	DC	H6	2.38	3.58
6	GAF	H9A	5	DC	H5	2.17	3.01
6	GAF	H6A	5	DC	H2''	3.5	5.26
6	GAF	H8A	6	GAF	H8	3.28	4.92
6	GAF	H8	6	GAF	H1'	2.47	3.71
6	GAF	H4'	6	GAF	H8	3.48	5.22
6	GAF	H4'	6	GAF	H5B	2.8	4.2
6	GAF	H3'	6	GAF	H8	4.03	6.05
7	DA	H1'	7	DA	H8	2.52	3.78
7	DA	H1'	7	DA	H3'	2.74	4.12
7	DA	H1'	8	DT	M	3.69	5.55
8	DT	Q5'	8	DT	H6	4.13	6.19

8	DT	H2"	8	DT	H6	2.24	3.36
9	DC	H6	8	DT	H2"	2.07	3.11
9	DC	H6	8	DT	H2'	2.45	3.67
9	DC	H6	8	DT	H1'	2.49	3.73
9	DC	H3'	9	DC	H6	3.88	5.82
9	DC	H2'	9	DC	H5	3.04	4.56
9	DC	H1'	13	DA	H2	3.1	4.66
10	DT3	H2'	10	DT3	H6	2.14	3.2
10	DT3	H1'	10	DT3	H2'	1.97	2.95
11	DA5	H2"	11	DA5	H8	2.57	3.85
12	DG	H4'	12	DG	H2"	2.72	4.08
12	DG	H3'	12	DG	H8	2.94	4.4
12	DG	H4'	12	DG	H3'	1.87	2.93
13	DA	Q5'	12	DG	H1'	3.41	5.11
13	DA	Q5'	13	DA	H8	3.06	4.6
13	DA	H3'	13	DA	H8	2.96	4.44
14	DT	Q5'	13	DA	H2"	2.47	3.71
14	DT	H6	13	DA	H2'	2.4	3.6
14	DT	H3'	14	DT	H6	3.54	5.22
15	DC	H1'	7	DA	H2	2.85	4.97
15	DC	H3'	15	DC	H4'	2.51	3.77
15	DC	Q5'	14	DT	H2"	2.52	3.78
16	DG	H4'	16	DG	H1'	2.46	3.7
16	DG	H3'	16	DG	H8	2.93	4.39
16	DG	H2"	16	DG	H8	2.53	3.81
16	DG	H2"	16	DG	H1'	1.93	2.89
17	DA	H4'	17	DA	H8	3.43	5.15

17	DA	H4'	17	DA	H2'	2.5	3.74
17	DA	H1'	18	DT	H6	2.62	3.92
18	DT	M	17	DA	H2'	2.63	3.95
18	DT	H6	17	DA	H8	3.34	5
18	DT	H4'	18	DT	H6	3.22	4.82
19	DG	H8	18	DT	H2"	2.22	3.34
19	DG	H8	18	DT	H1'	2.63	3.95
19	DG	Q5'	19	DG	H8	3.22	4.84
19	DG	H4'	19	DG	H1'	2.37	3.55
19	DG	Q5'	19	DG	H3'	2	3
19	DG	H2"	19	DG	H8	2.52	3.78
20	DT3	M	19	DG	H8	3.26	4.88
20	DT3	H6	19	DG	H8	3.38	5.06
20	DT3	H4'	20	DT3	H3'	2.63	3.95

Table S3. Class 3 distance restraints

Assign	Base	Proton	Assign	Base	Proton	LB	UB
1	DA5	H8	1	DA5	H1'	2.29	3.59
2	DC	H4'	2	DC	H1'	2.27	3.55
2	DC	H2'	2	DC	H5	2.78	4.36
3	DA	H3'	3	DA	H8	2.74	4.28
4	DT	M	3	DA	H3'	3.26	5.1
4	DT	M	3	DA	H2"	2.75	4.31
4	DT	H6	3	DA	H1'	2.64	4.12
5	DC	H3'	5	DC	H6	2.54	3.96
6	GAF	H5B	5	DC	H1'	2.28	3.58
9	DC	H6	8	DT	H6	3.16	4.94
9	DC	H5	8	DT	M	2.94	4.6
9	DC	H1'	9	DC	H2'	1.81	2.83
9	DC	H1'	10	DT3	H6	2.93	4.57
10	DT3	H6	9	DC	H2"	2.31	3.61
10	DT3	H3'	10	DT3	H6	2.22	3.48
11	DA5	H8	12	DG	H8	3.79	5.09
14	DT	M	14	DT	H1'	4.77	6.95
15	DC	H6	14	DT	H2"	2.23	3.49
15	DC	H6	14	DT	H1'	2.76	4.32
15	DC	H2"	15	DC	H6	2.3	3.82
17	DA	H8	16	DG	H8	3.06	4.78
17	DA	H8	16	DG	H2"	2.46	3.86
17	DA	H4'	17	DA	H3'	1.66	3.3
18	DT	M	17	DA	H2"	2.75	4.29
20	DT3	H6	19	DG	H2"	2.25	3.51

20	DT3	H5'	20	DT3	H3'	2.28	3.56
20	DT3	H3'	20	DT3	H6	2.83	4.43
1	DA5	H8	1	DA5	H4'	2.76	4.32
2	DC	H6	2	DC	H1'	2.44	3.58
3	DA	H5'	3	DA	H8	3.57	5.59
3	DA	H4'	3	DA	H1'	2.35	3.67
4	DT	H6	3	DA	H8	3.03	4.75
4	DT	H1'	5	DC	H4'	2.71	4.25
5	DC	H6	4	DT	H6	2.99	4.67
6	GAF	H5B	5	DC	H2'	2.07	3.25
6	GAF	HM	6	GAF	H1'	2.7	4.22
6	GAF	H4'	6	GAF	HM	3.55	5.55
6	GAF	H4'	6	GAF	H1'	2.17	3.39
6	GAF	H3A	6	GAF	HM	3.96	6.2
7	DA	H2"	7	DA	H8	2.21	3.47
7	DA	H1'	7	DA	H2'	2.25	3.19
8	DT	M	7	DA	H2"	2.88	4.5
8	DT	H6	7	DA	H8	3.07	4.79
8	DT	H4'	8	DT	H6	4.55	7.11
10	DT3	M	9	DC	H6	3.54	5.54
10	DT3	H2"	10	DT3	H6	1.64	3.7
11	DA5	H8	11	DA5	H4'	4.32	5.76
11	DA5	H1'	11	DA5	H3'	1.96	3.84
11	DA5	H1'	11	DA5	H2'	2.51	3.37
11	DA5	H1'	11	DA5	H8	2.29	3.59
11	DA5	H1'	12	DG	H8	2.97	4.01
12	DG	H4'	12	DG	H1'	2.2	3.44

13	DA	H4'	13	DA	H1'	2.18	3.42
14	DT	H6	13	DA	H8	3.08	5.22
15	DC	H6	14	DT	H6	3.04	4.76
17	DA	H5'	17	DA	H3'	1.46	3.32
17	DA	H4'	17	DA	H2"	2.22	3.48
17	DA	H3'	17	DA	H8	2.38	3.72
19	DG	H3'	19	DG	H8	2.68	4.2
20	DT3	H6	19	DG	H2'	2.11	3.31
20	DT3	H6	19	DG	H1'	2.67	3.77

Table S4. Base Pair Distance Restraints (theoretical distances)

Assign	Base	Proton	Assign	Base	Proton	LB	UB
1	ADE	N6	20	THY	O4	2.85	3.05
1	ADE	N1	20	THY	N3	2.72	2.92
1	ADE	N1	20	THY	O4	3.53	3.73
2	CYT	N4	19	GUA	O6	2.81	3.01
2	CYT	N3	19	GUA	N1	2.85	3.05
2	CYT	O2	19	GUA	N2	2.76	2.96
2	CYT	N3	19	GUA	N2	3.55	3.75
2	CYT	O2	19	GUA	O6	5.32	5.52
3	ADE	N6	18	THY	O4	2.85	3.05
3	ADE	N1	18	THY	N3	2.72	2.92
3	ADE	N1	18	THY	O4	3.53	3.73
4	THY	O4	17	ADE	N6	2.85	3.05
4	THY	N3	17	ADE	N1	2.72	2.92

4	THY	O4	17	ADE	N1	3.53	3.73
5	CYT	N4	16	GUA	O6	2.81	3.16
5	CYT	N3	16	GUA	N1	2.85	3.2
5	CYT	O2	16	GUA	N2	2.76	3.11
5	CYT	N3	16	GUA	N2	3.55	3.9
5	CYT	O2	16	GUA	O6	5.32	5.67
6	GAF	O6	15	CYT	N4	2.81	3.16
6	GAF	N1	15	CYT	N3	2.85	3.2
6	GAF	N2	15	CYT	O2	2.76	3.11
6	GAF	N2	15	CYT	N3	3.55	3.9
6	GAF	O6	15	CYT	O2	5.32	5.67
7	ADE	N6	14	THY	O4	2.85	3.2
7	ADE	N1	14	THY	N3	2.72	3.07
7	ADE	N1	14	THY	O4	3.53	3.88
8	THY	O4	13	ADE	N6	2.85	3.05
8	THY	N3	13	ADE	N1	2.72	2.92
8	THY	O4	13	ADE	N1	3.53	3.73
9	CYT	N4	12	GUA	O6	2.81	3.01
9	CYT	N3	12	GUA	N1	2.85	3.05
9	CYT	O2	12	GUA	N2	2.76	2.96
9	CYT	N3	12	GUA	N2	3.55	3.75
9	CYT	O2	12	GUA	O6	5.32	5.52
10	THY	O4	11	ADE	N6	2.85	3.05
10	THY	N3	11	ADE	N1	2.72	2.92
10	THY	O4	11	ADE	N1	3.53	3.73

Table S5. Sugar Pucker Angle Restraints from DQF-COSY Data.

Assign	Base	Angle	LB	UB
1	ADE	PPA	70	210
2	CYT	PPA	75	220
3	ADE	PPA	70	230
4	THY	PPA	85	210
5	CYT	PPA	85	170
7	ADE	PPA	90	170
8	THY	PPA	100	190
9	CYT	PPA	100	190
12	GUA	PPA	85	210
13	ADE	PPA	90	210
14	THY	PPA	70	220
15	CYT	PPA	120	180
16	GUA	PPA	100	230
17	ADE	PPA	90	170
18	THY	PPA	100	170
19	GUA	PPA	90	180
20	THY	PPA	90	170

Table S6. Sugar torsion angle empirical restraints

Assign	Base	Angle	LB	UB
2	CYT	ALPHA	-95	-25
3	ADE	ALPHA	-95	-25
4	THY	ALPHA	-95	-25
5	CYT	ALPHA	-95	-25
6	GAF	ALPHA	-95	-25
7	ADE	ALPHA	-95	-25
8	THY	ALPHA	-95	-25
9	CYT	ALPHA	-95	-25
10	THY	ALPHA	-95	-25
12	GUA	ALPHA	-95	-25
13	ADE	ALPHA	-95	-25
14	THY	ALPHA	-95	-25
15	CYT	ALPHA	-95	-25
16	GUA	ALPHA	-95	-25
17	ADE	ALPHA	-95	-25
18	THY	ALPHA	-95	-25
19	GUA	ALPHA	-95	-25
20	THY	ALPHA	-95	-25
2	CYT	BETA	-220	-140
3	ADE	BETA	-220	-140
4	THY	BETA	-220	-140
5	CYT	BETA	-220	-140
6	GAF	BETA	-220	-140
7	ADE	BETA	-220	-140
8	THY	BETA	-220	-140

9	CYT	BETA	-220	-140
10	THY	BETA	-220	-140
12	GUA	BETA	-220	-140
13	ADE	BETA	-220	-140
14	THY	BETA	-220	-140
15	CYT	BETA	-220	-140
16	GUA	BETA	-220	-140
17	ADE	BETA	-220	-140
18	THY	BETA	-220	-140
19	GUA	BETA	-220	-140
20	THY	BETA	-220	-140
1	ADE	GAMMA	20	100
2	CYT	GAMMA	20	100
3	ADE	GAMMA	20	100
4	THY	GAMMA	20	100
5	CYT	GAMMA	20	100
6	GAF	GAMMA	20	100
7	ADE	GAMMA	20	100
8	THY	GAMMA	20	100
9	CYT	GAMMA	20	100
10	THY	GAMMA	20	100
11	ADE	GAMMA	20	100
12	GUA	GAMMA	20	100
13	ADE	GAMMA	20	100
14	THY	GAMMA	20	100
15	CYT	GAMMA	20	100
16	GUA	GAMMA	20	100

17	ADE	GAMMA	20	100
18	THY	GAMMA	20	100
19	GUA	GAMMA	20	100
20	THY	GAMMA	20	100
1	ADE	ZETA	-140	-80
2	CYT	ZETA	-140	-80
3	ADE	ZETA	-140	-80
4	THY	ZETA	-140	-80
5	CYT	ZETA	-140	-80
6	GAF	ZETA	-140	-80
7	ADE	ZETA	-140	-80
8	THY	ZETA	-140	-80
9	CYT	ZETA	-140	-80
11	ADE	ZETA	-140	-80
12	GUA	ZETA	-140	-80
13	ADE	ZETA	-140	-80
14	THY	ZETA	-140	-80
15	CYT	ZETA	-140	-80
16	GUA	ZETA	-140	-80
17	ADE	ZETA	-140	-80
18	THY	ZETA	-140	-80
2	CYT	EPSLN	130	200
3	ADE	EPSLN	130	200
4	THY	EPSLN	130	200
5	CYT	EPSLN	130	200
6	GAF	EPSLN	120	250
7	ADE	EPSLN	130	200

8	THY	EPSLN	130	200
9	CYT	EPSLN	130	200
12	GUA	EPSLN	130	200
13	ADE	EPSLN	130	200
14	THY	EPSLN	140	225
15	CYT	EPSLN	120	240
16	GUA	EPSLN	120	230
17	ADE	EPSLN	120	220
18	THY	EPSLN	130	200
19	GUA	EPSLN	130	200

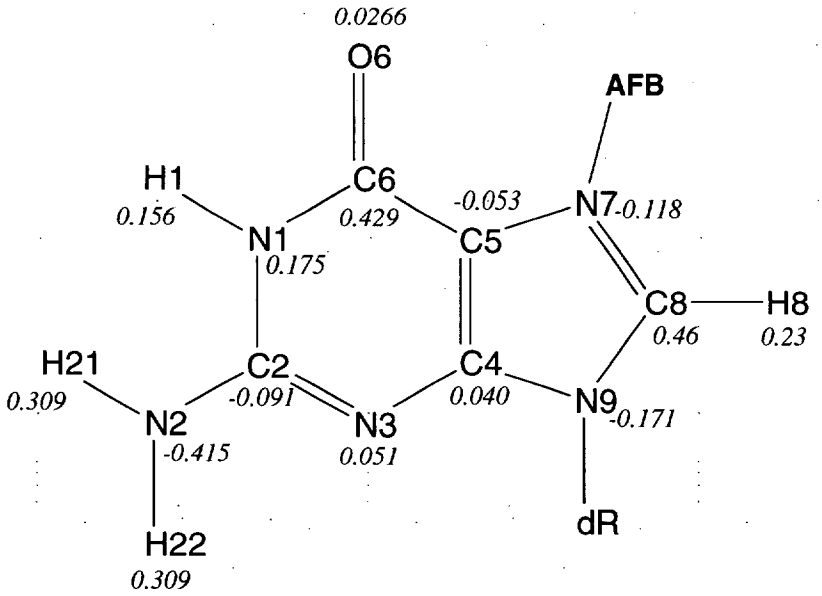
Figure Legends

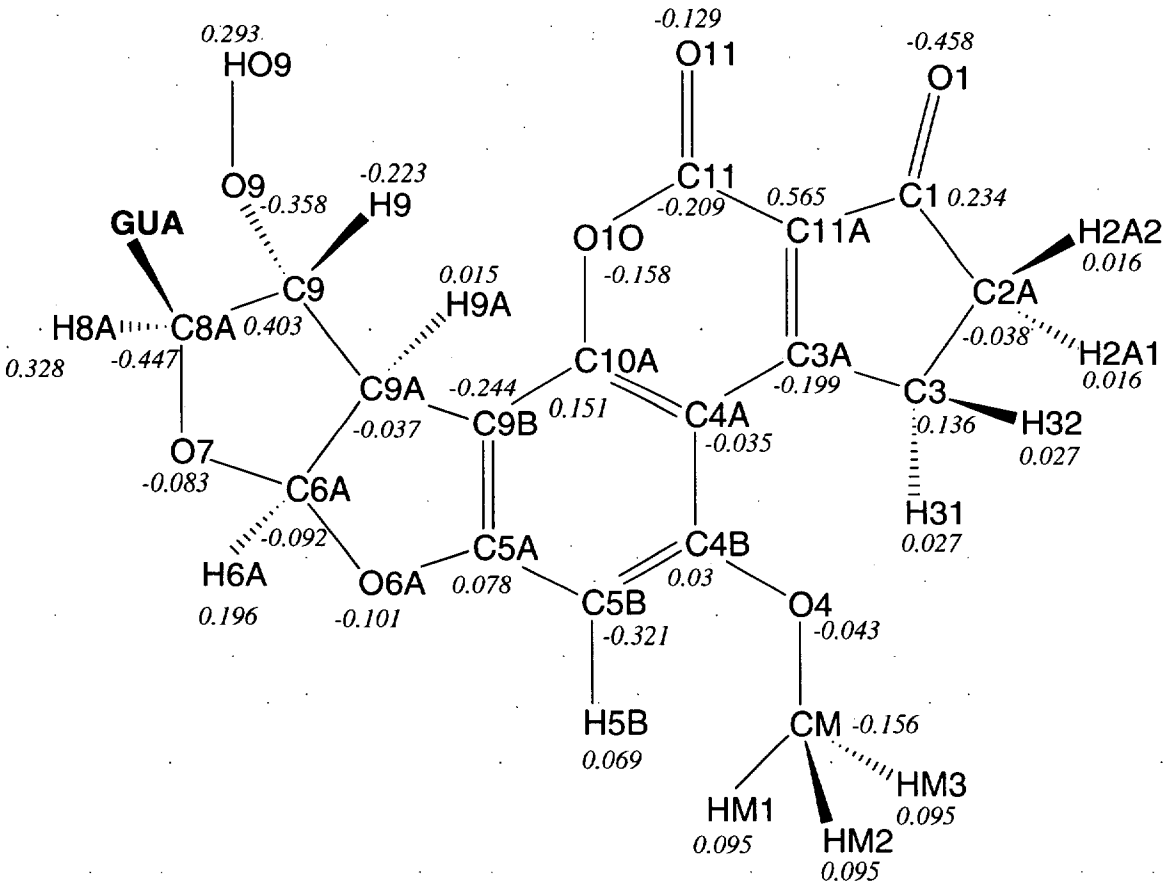
Figure S1. A) Calculated partial charges of $^{AFB}G^{6}$ using GAUSSIAN 98 with basis set 6-31G*. B) The atom types used for the calculation and rMD calculations.

Figure S2. Chemical shift differences induced in d(ACATC^{AFB}GATCT)•d(AGATCGATGT) as compared to the corresponding unmodified duplex d(ACATCGATCT)•d(AGATCGATGT). **A.** Pyrimidine H6 or purnine H8 protons in the modified strand. **B.** Deoxyribose protons H1′ (open bars), H2′, (hashed bars), and H2′′ (solid bars), in the modified strand. **C.** Pyrimidine H6 or purnine H8 protons in the complementary strand. **D.** Deoxyribose protons H1′ (open bars), H2′, (hashed bars), and H2′′ (solid bars), in the complementary strand.

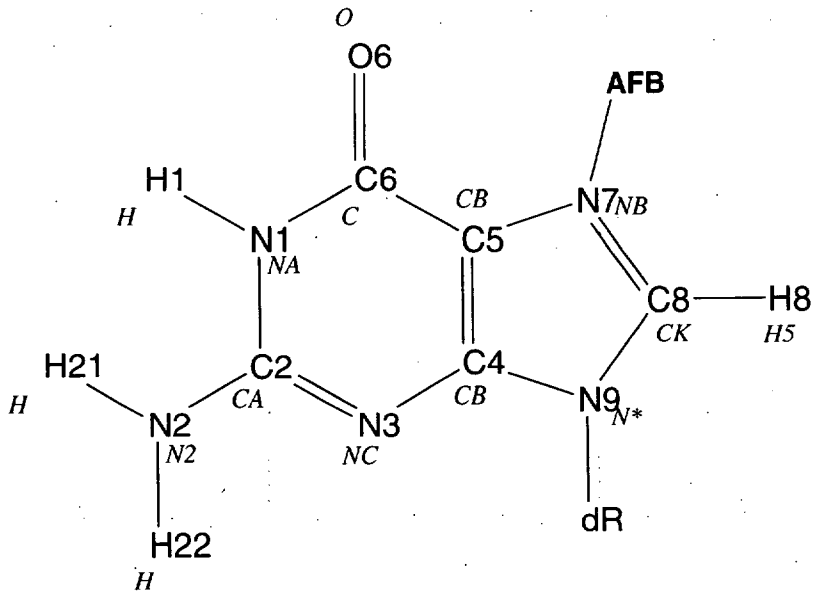
Figure S3. Helicoidal analysis of d(ACATC^{AFB}GATCT)•d(AGATCGATGT). The helicoidal parameters were measured in comparison with the corresponding unmodified duplex.

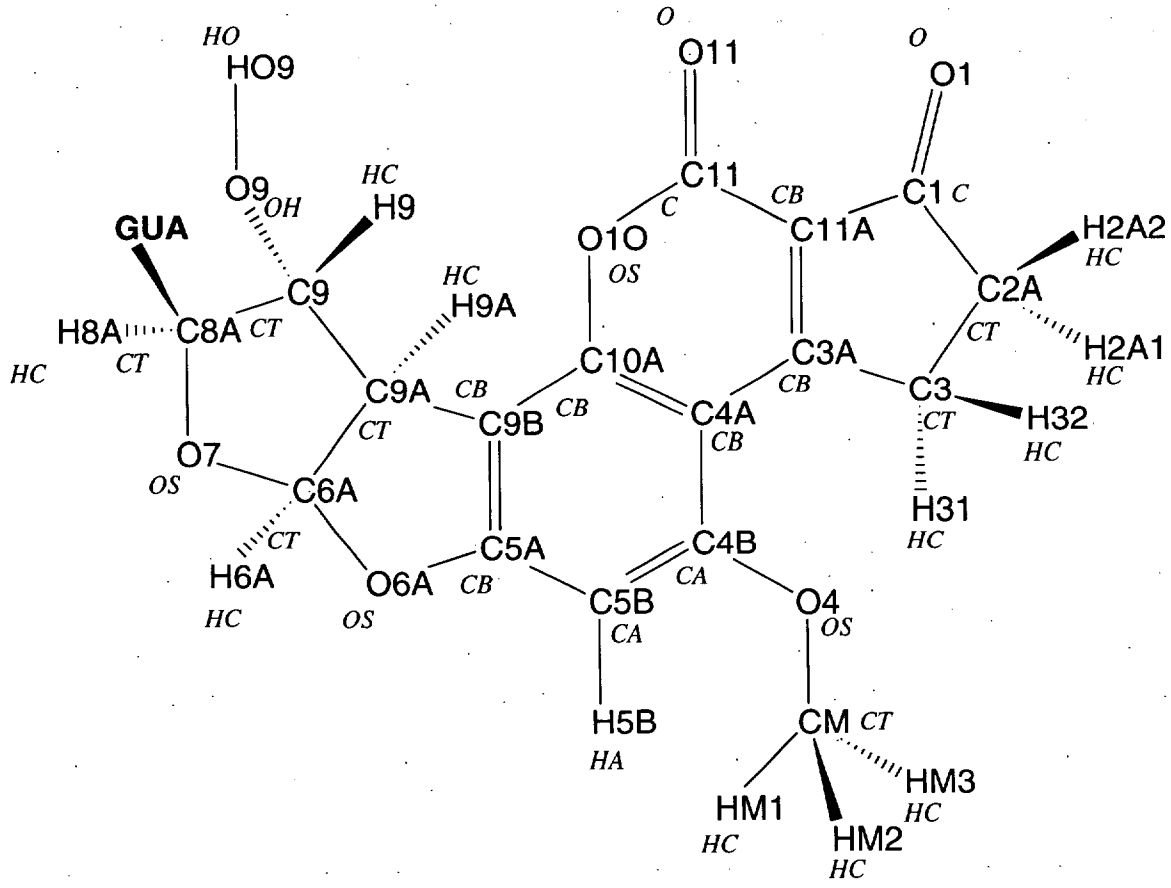
A)


0.0266
O6
AFB
H1
0.156
C6
0.429
-0.053
N7
-0.118
N1
0.175
C5
C8
H8
0.46
0.23
H21
0.309
C2
-0.091
C4
0.040
N9
-0.171
N2
-0.415
N3
0.051
dR
H22
0.309


0.293
HO9
-0.129
O11
-0.458
O1
O9
-0.358
-0.223
H9
C11
-0.209
0.565
C1
0.234
GUA
O1O
C11A
H2A2
0.016
0.015
C9
H9A
-0.158
C2A
H8A
C8A
0.403
-0.038
H2A1
0.016
0.328
-0.447
C10A
C3A
-0.199
C9A
-0.244
C3
-0.037
C9B
0.151
C4A
-0.136
H32
0.027
O7
-0.035
-0.083
C6A
H31
0.027
-0.092
C5A
C4B
H6A
O6A
0.078
0.03
C5B
O4
0.196
-0.101
-0.321
-0.043
H5B
CM
-0.156
0.069
HM3
0.095
HM1
HM2
0.095
0.095

B)


O
O6
AFB
H1
H
C6
C
CB
N7 NB
N1
NA
C5
C8
CK
H8
H5
H21
H
C2
CA
C4
CB
N9
N*
N2
N2
N3
NC
dR
H22
H


HO
HO9
O
O11
O
O1
O9
OH
HC
H9
C11
C
CB
C1
C
GUA
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OS
C11A
H2A2
HC
C9
HC
H9A
C2A
H8A
C8A
CT
CT
CT
H2A1
HC
HC
CT
C10A
C3A
CB
CB
C9A
CB
C9B
CB
C4A
C3
H32
HC
CT
CT
CB
O7
OS
C6A
H31
HC
CT
C5A
C4B
H6A
HC
O6A
OS
CB
CA
C5B
CA
O4
OS
H5B
HA
CM
CT
HM3
HC
HM1
HC
HM2
HC

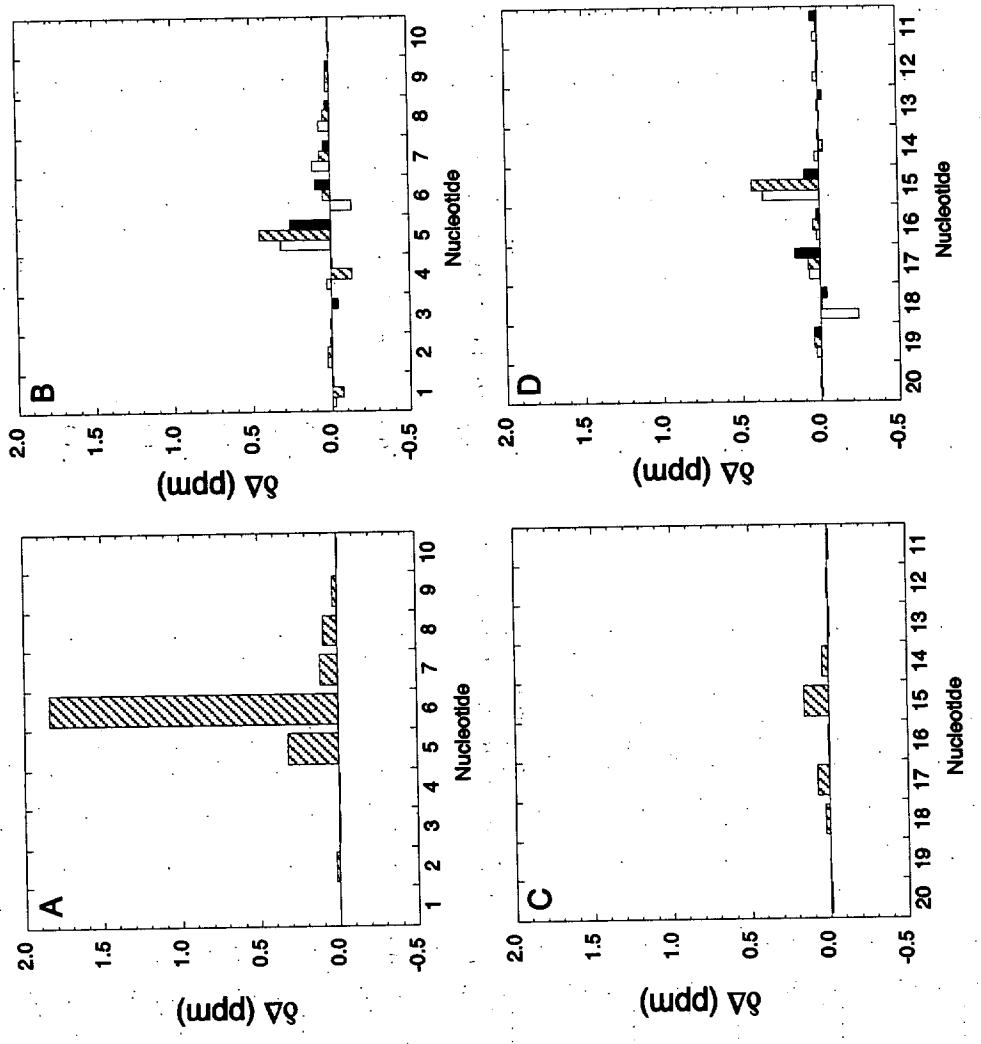

Figure S2

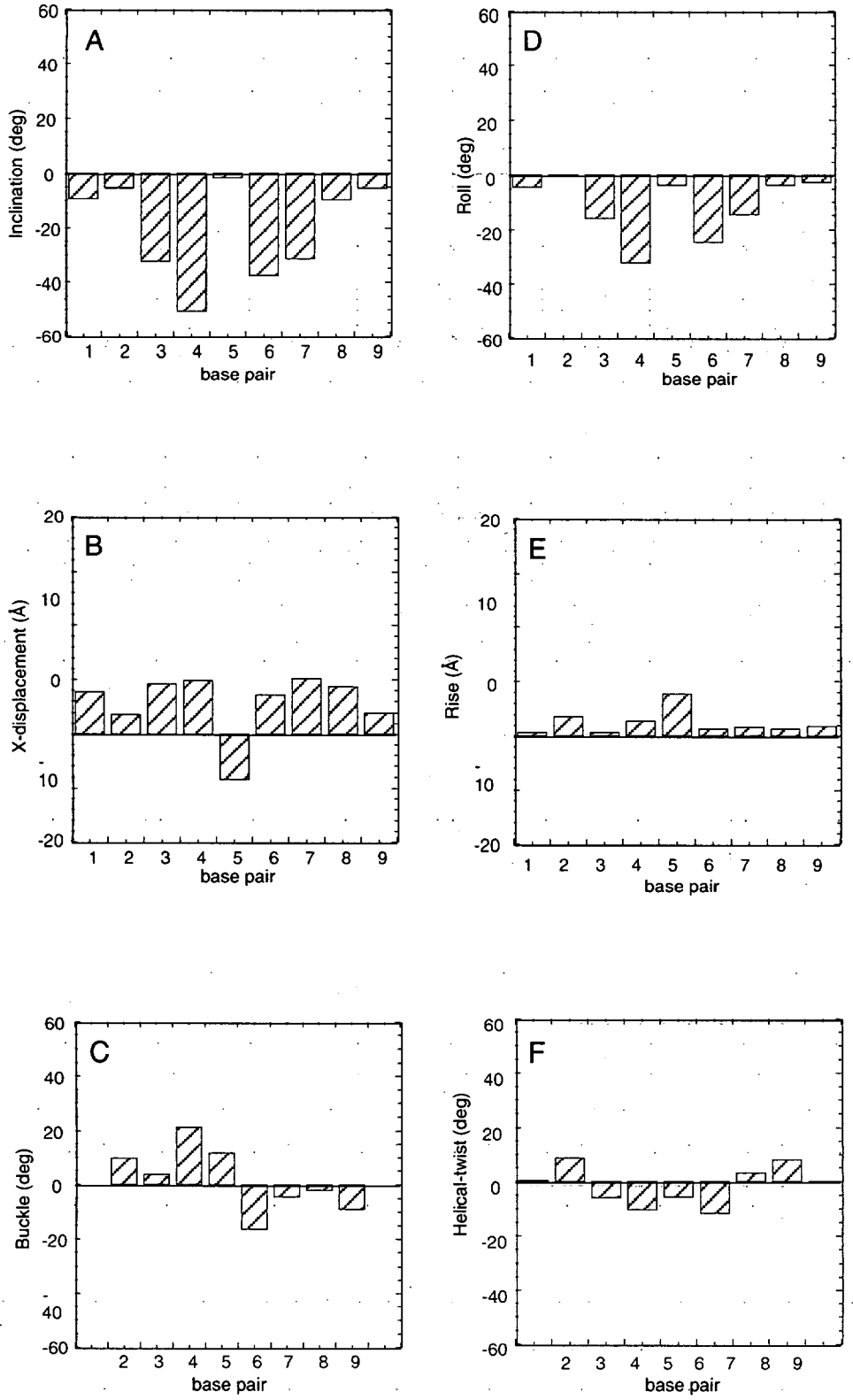
A
Inclination (deg)
base pair
D
Roll (deg)
base pair
B
X-displacement (Å)
base pair
E
Rise (Å)
base pair
C
Buckle (deg)
base pair
F
Helical-twist (deg)
base pair

Figure S3