Supplementary Material

DICTIONARY OF MAXIT PARAMETERS

Table D1. Conditions for close contact identification.

	Two adjacent residues in the chain	Two nonadjacent residues in the chain				
		D – D	D – H	D/H – Any	{*} – Any	Any – Any
Distance [Å]	< 1.80	< 1.415	< 1.35	< 1.60	< 1.70	< 2.195

D – Deuterium
{*} – {Na, Cu, Ca, Mn, Zn, Mg, Ni, Co, Hg, Pt, Ba}
Any – any type of atom except for D, H, and atoms in {*}

Table D2. Neutral adenine bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N9	C2'-endo	1.380	1.548	1.464	0.014
C1'	N9	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
N1	C2	s	1.285	1.393	1.339	0.009
C2	N3	s	1.277	1.385	1.331	0.009
N3	C4	s	1.308	1.380	1.344	0.006
C4	C5	s	1.341	1.425	1.383	0.007
C5	C6	s	1.352	1.460	1.406	0.009
C6	N1	s	1.309	1.393	1.351	0.007
C5	N7	s	1.352	1.424	1.388	0.006
N7	C8	s	1.269	1.353	1.311	0.007
C8	N9	s	1.325	1.421	1.373	0.008
N9	C4	s	1.338	1.410	1.374	0.006
C6	N6	s	1.287	1.383	1.335	0.008

Table D3. Neutral adenine bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N9	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N9	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N9	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N9	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	115.0	122.2	118.6	0.6
N1	C2	N3	s	126.3	132.3	129.3	0.5
C2	N3	C4	s	107.6	113.6	110.6	0.5
N3	C4	C5	s	122.6	131.0	126.8	0.7
C4	C5	C6	s	114.0	120.0	117.0	0.5
C5	C6	N1	s	114.7	120.7	117.7	0.5
C4	C5	N7	s	107.7	113.7	110.7	0.5
C5	N7	C8	s	100.9	106.9	103.9	0.5
N7	C8	N9	s	110.8	116.8	113.8	0.5
C8	N9	C4	s	103.4	108.2	105.8	0.4
N9	C4	C5	s	103.4	108.2	105.8	0.4
N3	C4	N9	s	122.6	132.2	127.4	0.8
C6	C5	N7	s	128.1	136.5	132.3	0.7
N1	C6	N6	s	115.0	122.2	118.6	0.6
C5	C6	N6	s	118.9	128.5	123.7	0.8
C8	N9	C1'	s	116.9	138.5	127.7	1.8
C4	N9	C1'	s	115.5	137.1	126.3	1.8

Table D4. Neutral cytosine bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N1	C2'-endo	1.380	1.548	1.464	0.014
C1'	N1	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
C2	O2	s	1.186	1.294	1.240	0.009
C4	N4	s	1.281	1.389	1.335	0.009
N1	C2	s	1.337	1.457	1.397	0.010
N1	C6	s	1.331	1.403	1.367	0.006
C2	N3	s	1.305	1.401	1.353	0.008
N3	C4	s	1.293	1.377	1.335	0.007
C4	C5	s	1.377	1.473	1.425	0.008
C5	C6	s	1.291	1.387	1.339	0.008

Table D5. Neutral cytosine bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N1	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N1	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N1	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N1	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	117.9	122.7	120.3	0.4
N1	C2	N3	s	115.0	123.4	119.2	0.7
C2	N3	C4	s	116.9	122.9	119.9	0.5
N3	C4	C5	s	119.5	124.3	121.9	0.4
C4	C5	C6	s	114.4	120.4	117.4	0.5
C5	C6	N1	s	118.0	124.0	121.0	0.5
N1	C2	O2	s	115.3	122.5	118.9	0.6
N3	C2	O2	s	117.7	126.1	121.9	0.7
N3	C4	N4	s	113.8	122.2	118.0	0.7
C5	C4	N4	s	116.0	124.4	120.2	0.7
C6	N1	C1'	s	113.6	128.0	120.8	1.2
C2	N1	C1'	s	112.2	125.4	118.8	1.1

Table D6. Neutral guanine bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N9	C2'-endo	1.380	1.548	1.464	0.014
C1'	N9	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
N1	C2	s	1.325	1.421	1.373	0.008
C2	N3	s	1.275	1.371	1.323	0.008
N3	C4	s	1.308	1.392	1.350	0.007
C4	C5	s	1.337	1.421	1.379	0.007
C5	C6	s	1.359	1.479	1.419	0.010
C6	N1	s	1.349	1.433	1.391	0.007
C5	N7	s	1.352	1.424	1.388	0.006
N7	C8	s	1.269	1.341	1.305	0.006
C8	N9	s	1.332	1.416	1.374	0.007
N9	C4	s	1.327	1.423	1.375	0.008
C2	N2	s	1.281	1.401	1.341	0.010
C6	O6	s	1.183	1.291	1.237	0.009

Table D7. Neutral guanine bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N9	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N9	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N9	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N9	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	121.5	128.7	125.1	0.6
N1	C2	N3	s	120.3	127.5	123.9	0.6
C2	N3	C4	s	108.9	114.9	111.9	0.5
N3	C4	C5	s	125.6	131.6	128.6	0.5
C4	C5	C6	s	115.2	122.4	118.8	0.6
C5	C6	N1	s	108.5	114.5	111.5	0.5
C4	C5	N7	s	108.4	113.2	110.8	0.4
C5	N7	C8	s	101.3	107.3	104.3	0.5
N7	C8	N9	s	110.1	116.1	113.1	0.5
C8	N9	C4	s	104.0	108.8	106.4	0.4
N9	C4	C5	s	103.0	107.8	105.4	0.4
N3	C4	N9	s	122.4	129.6	126.0	0.6
C6	C5	N7	s	126.8	134.0	130.4	0.6
N1	C2	N2	s	110.8	121.6	116.2	0.9
N3	C2	N2	s	115.7	124.1	119.9	0.7
N1	C6	O6	s	116.3	123.5	119.9	0.6
C5	C6	O6	s	125.0	132.2	128.6	0.6
C8	N9	C1'	s	119.2	134.8	127.0	1.3
C4	N9	C1'	s	118.7	134.3	126.5	1.3

Table D8. Neutral uracil bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N1	C2'-endo	1.380	1.548	1.464	0.014
C1'	N1	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
C2	O2	s	1.165	1.273	1.219	0.009
C4	O4	s	1.184	1.280	1.232	0.008
N1	C2	s	1.327	1.435	1.381	0.009
N1	C6	s	1.321	1.429	1.375	0.009
C2	N3	s	1.331	1.415	1.373	0.007
N3	C4	s	1.326	1.434	1.380	0.009
C4	C5	s	1.377	1.485	1.431	0.009
C5	C6	s	1.283	1.391	1.337	0.009

Table D9. Neutral uracil bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N1	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N1	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N1	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N1	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	117.4	124.6	121.0	0.6
N1	C2	N3	s	111.3	118.5	114.9	0.6
C2	N3	C4	s	123.4	130.6	127.0	0.6
N3	C4	C5	s	111.0	118.2	114.6	0.6
C4	C5	C6	s	116.1	123.3	119.7	0.6
C5	C6	N1	s	119.7	125.7	122.7	0.5
N1	C2	O2	s	118.6	127.0	122.8	0.7
N3	C2	O2	s	118.0	126.4	122.2	0.7
N3	C4	O4	s	115.2	123.6	119.4	0.7
C5	C4	O4	s	122.3	129.5	125.9	0.6
C6	N1	C1'	s	112.8	129.6	121.2	1.4
C2	N1	C1'	s	110.5	124.9	117.7	1.2

Table D10. Adenine bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N9	C2'-endo	1.380	1.548	1.464	0.014
C1'	N9	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
N1	C2	s	1.285	1.393	1.339	0.009
C2	N3	s	1.277	1.385	1.331	0.009
N3	C4	s	1.308	1.380	1.344	0.006
C4	C5	s	1.341	1.425	1.383	0.007
C5	C6	s	1.352	1.460	1.406	0.009
C6	N1	s	1.309	1.393	1.351	0.007
C5	N7	s	1.352	1.424	1.388	0.006
N7	C8	s	1.269	1.353	1.311	0.007
C8	N9	s	1.325	1.421	1.373	0.008
N9	C4	s	1.338	1.410	1.374	0.006
C6	N6	s	1.287	1.383	1.335	0.008

Table D11. Adenine bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N9	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N9	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N9	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N9	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	115.0	122.2	118.6	0.6
N1	C2	N3	s	126.3	132.3	129.3	0.5
C2	N3	C4	s	107.6	113.6	110.6	0.5
N3	C4	C5	s	122.6	131.0	126.8	0.7
C4	C5	C6	s	114.0	120.0	117.0	0.5
C5	C6	N1	s	114.7	120.7	117.7	0.5
C4	C5	N7	s	107.7	113.7	110.7	0.5
C5	N7	C8	s	100.9	106.9	103.9	0.5
N7	C8	N9	s	110.8	116.8	113.8	0.5
C8	N9	C4	s	103.4	108.2	105.8	0.4
N9	C4	C5	s	103.4	108.2	105.8	0.4
N3	C4	N9	s	122.6	132.2	127.4	0.8
C6	C5	N7	s	128.1	136.5	132.3	0.7
N1	C6	N6	s	115.0	122.2	118.6	0.6
C5	C6	N6	s	118.9	128.5	123.7	0.8
C8	N9	C1'	s	116.9	138.5	127.7	1.8
C4	N9	C1'	s	115.5	137.1	126.3	1.8

Table D12. Cytosine bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N1	C2'-endo	1.380	1.548	1.464	0.014
C1'	N1	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
C2	O2	s	1.186	1.294	1.240	0.009
C4	N4	s	1.281	1.389	1.335	0.009
N1	C2	s	1.337	1.457	1.397	0.010
N1	C6	s	1.331	1.403	1.367	0.006
C2	N3	s	1.305	1.401	1.353	0.008
N3	C4	s	1.293	1.377	1.335	0.007
C4	C5	s	1.377	1.473	1.425	0.008
C5	C6	s	1.291	1.387	1.339	0.008

Table D13. Cytosine bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N1	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N1	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N1	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N1	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	117.9	122.7	120.3	0.4
N1	C2	N3	s	115.0	123.4	119.2	0.7
C2	N3	C4	s	116.9	122.9	119.9	0.5
N3	C4	C5	s	119.5	124.3	121.9	0.4
C4	C5	C6	s	114.4	120.4	117.4	0.5
C5	C6	N1	s	118.0	124.0	121.0	0.5
N1	C2	O2	s	115.3	122.5	118.9	0.6
N3	C2	O2	s	117.7	126.1	121.9	0.7
N3	C4	N4	s	113.8	122.2	118.0	0.7
C5	C4	N4	s	116.0	124.4	120.2	0.7
C6	N1	C1'	s	113.6	128.0	120.8	1.2
C2	N1	C1'	s	112.2	125.4	118.8	1.1

Table D14. Guanine bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N9	C2'-endo	1.380	1.548	1.464	0.014
C1'	N9	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
N1	C2	s	1.325	1.421	1.373	0.008
C2	N3	s	1.275	1.371	1.323	0.008
N3	C4	s	1.308	1.392	1.350	0.007
C4	C5	s	1.337	1.421	1.379	0.007
C5	C6	s	1.359	1.479	1.419	0.010
C6	N1	s	1.349	1.433	1.391	0.007
C5	N7	s	1.352	1.424	1.388	0.006
N7	C8	s	1.269	1.341	1.305	0.006
C8	N9	s	1.332	1.416	1.374	0.007
N9	C4	s	1.327	1.423	1.375	0.008
C2	N2	s	1.281	1.401	1.341	0.010
C6	O6	s	1.183	1.291	1.237	0.009

Table D15. Guanine bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N9	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N9	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N9	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N9	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	121.5	128.7	125.1	0.6
N1	C2	N3	s	120.3	127.5	123.9	0.6
C2	N3	C4	s	108.9	114.9	111.9	0.5
N3	C4	C5	s	125.6	131.6	128.6	0.5
C4	C5	C6	s	115.2	122.4	118.8	0.6
C5	C6	N1	s	108.5	114.5	111.5	0.5
C4	C5	N7	s	108.4	113.2	110.8	0.4
C5	N7	C8	s	101.3	107.3	104.3	0.5
N7	C8	N9	s	110.1	116.1	113.1	0.5
C8	N9	C4	s	104.0	108.8	106.4	0.4
N9	C4	C5	s	103.0	107.8	105.4	0.4
N3	C4	N9	s	122.4	129.6	126.0	0.6
C6	C5	N7	s	126.8	134.0	130.4	0.6
N1	C2	N2	s	110.8	121.6	116.2	0.9
N3	C2	N2	s	115.7	124.1	119.9	0.7
N1	C6	O6	s	116.3	123.5	119.9	0.6
C5	C6	O6	s	125.0	132.2	128.6	0.6
C8	N9	C1'	s	119.2	134.8	127.0	1.3
C4	N9	C1'	s	118.7	134.3	126.5	1.3

Table D16. Uracil bond lengths in Angstroms [Å].

Atom 1	Atom 2	Type	Minimum	Maximum	Reference	Standard dev
P	OP1	s	1.383	1.587	1.485	0.017
P	OP2	s	1.383	1.587	1.485	0.017
P	OP3	s	1.535	1.679	1.607	0.012
P	O5'	s	1.533	1.653	1.593	0.010
O5'	C5'	(P)O5'-C5'	1.344	1.536	1.440	0.016
O5'	C5'	(H)C2'-endo	1.328	1.520	1.424	0.016
O5'	C5'	(H)C3'-endo	1.366	1.474	1.420	0.009
C5'	C4'	C2'-endo	1.437	1.581	1.509	0.012
C5'	C4'	C3'-endo	1.466	1.550	1.508	0.007
C4'	C3'	C2'-endo	1.461	1.593	1.527	0.011
C4'	C3'	C3'-endo	1.461	1.581	1.521	0.010
C3'	C2'	C2'-endo	1.459	1.591	1.525	0.011
C3'	C2'	C3'-endo	1.457	1.589	1.523	0.011
C2'	C1'	C2'-endo	1.478	1.574	1.526	0.008
C2'	C1'	C3'-endo	1.463	1.595	1.529	0.011
O4'	C1'	C2'-endo	1.343	1.487	1.415	0.012
O4'	C1'	C3'-endo	1.334	1.490	1.412	0.013
O4'	C4'	C2'-endo	1.394	1.514	1.454	0.010
O4'	C4'	C3'-endo	1.373	1.529	1.451	0.013
O3'	C3'	C2'-endo	1.355	1.499	1.427	0.012
O3'	C3'	C3'-endo	1.333	1.501	1.417	0.014
C1'	N1	C2'-endo	1.380	1.548	1.464	0.014
C1'	N1	C3'-endo	1.393	1.573	1.483	0.015
C2'	O2'	C2'-endo	1.334	1.490	1.412	0.013
C2'	O2'	C3'-endo	1.360	1.480	1.420	0.010
C2	O2	s	1.165	1.273	1.219	0.009
C4	O4	s	1.184	1.280	1.232	0.008
N1	C2	s	1.327	1.435	1.381	0.009
N1	C6	s	1.321	1.429	1.375	0.009
C2	N3	s	1.331	1.415	1.373	0.007
N3	C4	s	1.326	1.434	1.380	0.009
C4	C5	s	1.377	1.485	1.431	0.009
C5	C6	s	1.283	1.391	1.337	0.009

Table D17. Uracil bond angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
OP1	P	OP2	s	110.6	128.6	119.6	1.5
O5'	P	OP1	large	103.5	117.9	110.7	1.2
O5'	P	OP1	small	100.3	111.1	105.7	0.9
O5'	P	OP2	large	103.5	117.9	110.7	1.2
O5'	P	OP2	small	100.3	111.1	105.7	0.9
O5'	C5'	C4'	(P)O5'-C5'-C4'	104.6	114.2	109.4	0.8
O5'	C5'	C4'	C2'-endo	100.3	123.1	111.7	1.9
O5'	C5'	C4'	C3'-endo	101.9	121.1	111.5	1.6
P	O5'	C5'	s	111.3	130.5	120.9	1.6
O4'	C4'	C3'	C2'-endo	101.3	110.9	106.1	0.8
O4'	C4'	C3'	C3'-endo	98.0	110.0	104.0	1.0
C5'	C4'	C3'	C2'-endo	106.8	123.6	115.2	1.4
C5'	C4'	C3'	C3'-endo	106.4	125.6	116.0	1.6
C5'	C4'	O4'	C2'-endo	101.9	116.3	109.1	1.2
C5'	C4'	O4'	C3'-endo	104.4	115.2	109.8	0.9
C1'	O4'	C4'	C2'-endo	105.5	113.9	109.7	0.7
C1'	O4'	C4'	C3'-endo	105.1	114.7	109.9	0.8
C4'	C3'	O3'	C2'-endo	96.8	122.0	109.4	2.1
C4'	C3'	O3'	C3'-endo	101.0	125.0	113.0	2.0
C2'	C3'	O3'	C2'-endo	96.3	122.7	109.5	2.2
C2'	C3'	O3'	C3'-endo	104.1	123.3	113.7	1.6
C4'	C3'	C2'	C2'-endo	96.6	108.6	102.6	1.0
C4'	C3'	C2'	C3'-endo	96.6	108.6	102.6	1.0
C3'	C2'	C1'	C2'-endo	96.7	106.3	101.5	0.8
C3'	C2'	C1'	C3'-endo	97.1	105.5	101.3	0.7
O4'	C1'	C2'	C2'-endo	99.8	111.8	105.8	1.0
O4'	C1'	C2'	C3'-endo	102.2	113.0	107.6	0.9
N1	C1'	C2'	C2'-endo	106.2	121.8	114.0	1.3
N1	C1'	C2'	C3'-endo	105.4	118.6	112.0	1.1
O4'	C1'	N1	C2'-endo	103.4	113.0	108.2	0.8
O4'	C1'	N1	C3'-endo	104.3	112.7	108.5	0.7
C1'	C2'	O2'	s	92.6	128.6	110.6	3.0
C3'	C2'	O2'	s	95.9	130.7	113.3	2.9
C6	N1	C2	s	117.4	124.6	121.0	0.6
N1	C2	N3	s	111.3	118.5	114.9	0.6
C2	N3	C4	s	123.4	130.6	127.0	0.6
N3	C4	C5	s	111.0	118.2	114.6	0.6
C4	C5	C6	s	116.1	123.3	119.7	0.6
C5	C6	N1	s	119.7	125.7	122.7	0.5
N1	C2	O2	s	118.6	127.0	122.8	0.7
N3	C2	O2	s	118.0	126.4	122.2	0.7
N3	C4	O4	s	115.2	123.6	119.4	0.7
C5	C4	O4	s	122.3	129.5	125.9	0.6
C6	N1	C1'	s	112.8	129.6	121.2	1.4
C2	N1	C1'	s	110.5	124.9	117.7	1.2

Table D18. Polymer linkage values, bond lengths in Angstroms [Å] and angles in degrees [°].

Atom 1	Atom 2	Atom 3	Type	Minimum	Maximum	Reference	Standard dev
Bond length							
O3'	P		s	1.535	1.679	1.607	0.012
Angles							
C3'	O3'	P	s	112.5	126.9	119.7	1.2
O3'	P	O5'	s	92.6	115.4	104.0	1.9
O3'	P	OP2	large	103.9	117.1	110.5	1.1
O3'	P	OP2	small	92.0	118.4	105.2	2.2
O3'	P	OP1	large	103.9	117.1	110.5	1.1
O3'	P	OP1	small	92.0	118.4	105.2	2.2

Table D19. Dihedral angles for nucleic acids.

Atom 1	Atom 2	Atom 3	Atom 4	Type	Minimum	Maximum	Reference	Standard dev
O3'	P	C5'			226.5	344.1	285.3	9.8
					8.4	153.6	81.0	12.1
P	O5'	C5'	C4'		105.5	261.5	183.5	13.0
O5'	C5'	C4'	C3'		18.3	86.7	52.5	5.7
					141.0	217.8	179.4	6.4
					219.1	6.7	292.9	12.3
C4'	C3'	O3'	P		162.4	265.6	214.0	8.6
C3'	O3'	P	O5'		260.4	318.0	289.2	4.8
					354.9	166.5	80.7	14.3
Sugar								
C5'	C4'	C3'	O3'	C2'-endo	117.9	176.7	147.3	4.9
O4'	C4'	C3'	O3'	C2'-endo	236.3	299.9	268.1	5.3
O4'	C1'	C2'	C3'	C2'-endo	14.8	55.6	35.2	3.4
C1'	C2'	C3'	C4'	C2'-endo	307.8	341.4	324.6	2.8
C2'	C3'	C4'	O4'	C2'-endo	357.8	50.6	24.2	4.4
C3'	C4'	O4'	C1'	C2'-endo	323.5	31.9	357.7	5.7
C4'	O4'	C1'	C2'	C2'-endo	308.0	10.4	339.2	5.2
C5'	C4'	C3'	C2'	C2'-endo	238.8	288.0	263.4	4.1
O3'	C3'	C2'	O2'	C2'-endo	294.5	344.9	319.7	4.2
C4'	O4'	C1'	N1/9	C2'-endo	177.5	257.9	217.7	6.7
O4'	C1'	N1	C2	C2'-endo	119.4	340.2	229.8	18.4
O4'	C1'	N9	C4'	C2'-endo	91.2	22.8	237.0	24.3
C5'	C4'	C3'	O3'	C3'-endo	54.6	107.4	81.0	4.4
O4'	C4'	C3'	O3'	C3'-endo	176.6	227.0	201.8	4.2
O4'	C1'	C2'	C3'	C3'-endo	306.0	4.8	335.4	4.9
C1'	C2'	C3'	C4'	C3'-endo	19.1	52.7	35.9	2.8
C2'	C3'	C4'	O4'	C3'-endo	306.1	343.3	324.7	3.1
C3'	C4'	O4'	C1'	C3'-endo	349.9	51.1	20.5	5.1
C4'	O4'	C1'	C2'	C3'-endo	326.2	39.4	2.8	6.1
C5'	C4'	C3'	C2'	C3'-endo	185.4	222.6	204.0	3.1
O3'	C3'	C2'	O2'	C3'-endo	17.3	71.3	44.3	4.5
C4'	O4'	C1'	N1/9	C3'-endo	202.4	280.4	241.4	6.5
O4'	C1'	N1	C2	C3'-endo	156.1	235.3	195.7	6.6
O4'	C1'	N9	C4	C3'-endo	109.3	277.3	193.3	14.0