

SUPPLEMENTARY MATERIAL

Table S1. High resolution B-DNA structures

<i>NDB ID</i>	<i>PDB ID</i>	<i>No. Base-Pairs</i>	<i>R-Value (obs)</i>	<i>Resolution</i>
GDL033	109D	12	19.7	2.0
BDJB50	123D	10	19.1	1.7
BDJ051	126D	10	19.6	2.0
GDL022	127D	12	17.2	2.0
BDJ052	158D	10	17.9	1.9
GDHB25	159D	8	15.0	1.8
BDJ060	196D	10	20.0	1.7
BDJ017	1BD1	10	16.0	1.6
BDL001	1BNA	12	17.8	1.9
BDJ025	1D23	10	16.1	1.5
BDLB26	1D27	12	18.5	2.0
GDL010	1D43	12	15.7	2.0
GDL011	1D44	12	15.7	2.0
GDL012	1D45	12	15.2	1.9
GDL013	1D46	12	14.9	2.0
BDJ031	1D49	10	15.7	1.5
BDJ036	1D56	10	17.8	1.7
BDJ037	1D57	10	16.5	2.0
BDJB44	1D61	10	15.2	1.3
GDL016	1D63	12	18.3	2.0
BDJB48	1DA3	10	17.2	2.0
BDF068	251D	6	18.6	1.9
GDLB41	267D	12	15.6	2.0
BDJB27	2D25	10	17.4	1.75
GDLB49	304D	8	18.4	1.9
GDLB51	306D	8	15.3	1.6
GDJ054	334D	10	20.0	1.8
BDL084	355D	12	19.7	1.4
BDJ008	3DNB	10	16.4	1.3
BD0007	436D	12	16.2	1.1
BDLB13	4DNB	12	16.9	2.0
BDJ019	5DNB	10	16.0	1.4
BDL005	7BNA	12	14.9	1.9
BDL020	9BNA	12	18.8	1.9
BDJ061	N/A	10	17.0	1.95

Table S2. High resolution A-DNA structures

<i>NDB ID</i>	<i>PDB ID</i>	<i>No. Base-Pairs</i>	<i>R-value(obs)</i>	<i>Resolution</i>
ADDB01	1ANA	4	16.5	2.0
ADFB62	254D	6	19.7	1.9
ADFB63	275D	6	17.2	2.0
ADH008	9DNA	8	17.1	1.8
ADH010	0AN8	8	19.8	1.8
ADH0102	368D	8	16.9	1.6
ADH0103	369D	8	17.2	1.9
ADH0104	370D	8	18.1	1.67
ADH0105	371D	8	19.0	1.9
ADH014	1DNS	8	11.5	2.0
ADH026	2D94	8	16.2	1.7
ADH029	n.a.	8	16.0	1.9
ADH033	295D	8	17.7	1.5
ADH034	n.a.	8	12.7	2.0
ADH038	1D78	8	19.8	1.4
ADH039	1D79	8	19.1	1.45
ADH047	118D	8	15.4	1.64
ADH070	243D	8	17.7	1.9
ADH078	317D	8	16.4	1.9
ADHB11	115D	8	14.0	1.7
ADHB17	1D90	8	14.0	1.7
ADHB95	341D	8	18.5	1.75
ADHB99	344D	8	11.15	1.46
ADJ0102	348D	10	19.0	1.7
ADJ0103	349D	10	19.9	1.9
ADJ0112	395D	10	19.5	1.9
ADJ0113	396D	10	18.9	1.8
ADJ022	1D13	10	18.0	2.0
ADJ049	160D	10	18.5	1.65
ADJ050	137D	10	18.5	1.7
ADJ051	138D	10	18.3	1.8
ADJ065	212D	10	19.4	1.9
ADJ067	221D	10	20.0	1.9
ADJ075	260D	10	18.6	1.9
ADJB110	383D	10	19.6	1.7
ADJB61	213D	10	16.3	1.6
ADJB79	318D	10	16.2	2.0
ADJB88	327D	10	19.1	1.94
ADL025	2D47	12	17.7	2.0
ADL047	399D	12	16.5	1.9
ADLS105	363D	12	19.2	2.0
AH0002	410D	10	15.9	1.6
AH0003	411D	10	16.8	1.93
AH0004	412D	10	18.9	1.65
UDJ032	232D	10	13.85	1.3
UDJB44	238D	10	19.6	2.0

Table S3. High resolution Z-DNA structures

<i>NDB ID</i>	<i>PDB ID</i>	<i>No. Base-Pairs</i>	<i>R-value(obs)</i>	<i>Resolution</i>
DDF027	292D	6	16.1	1.0
UDF025	192D	6	18.5	1.92
ZD0001	400D	6	19.6	1.65
ZD0002	417D	6	15.0	1.5
ZDB020	n.a.	2	13.6	0.85
ZDF001	2DCG	6	14.0	0.9
ZDF002	1DCG	6	17.5	1.0
ZDF013	n.a.	6	19.5	1.0
ZDF028	1D39	6	19.8	1.2
ZDF029	1D48	6	18.5	1.0
ZDF035	131D	6	18.0	1.0
ZDF039	181D	6	19.9	1.6
ZDF052	293D	6	19.1	1.0
ZDF053	336D	6	19.0	1.0
ZDF059	351D	6	19.3	1.64
ZDF060	362D	6	11.7	1.3
ZDF061	390D	6	18.8	2.0
ZDFB03	n.a.	6	15.6	1.3
ZDFB04	1DN4	6	13.27	1.6
ZDFB05	1DN5	6	12.47	1.4
ZDFB06	n.a.	6	16.0	1.2
ZDFB12	1DNF	6	17.2	1.5
ZDFB21	1D24	6	19.0	1.9
ZDFB25	1DA2	6	18.1	1.7
ZDFB31	1D76	6	13.8	1.3
ZDFB36	133D	6	18.9	1.8
ZDFB37	145D	6	19.3	1.25
ZDFB41	210D	6	17.4	1.35
ZDFB42	211D	6	17.0	1.6
ZDFB43	223D	6	17.9	1.7
ZDFB51	242D	6	17.0	1.65
ZDG056	314D	7	19.1	1.9
ZDG057	331D	7	18.4	1.65
ZDJ050	279D	2	18.6	1.9

Table S4. Dataset of CSD structures

Fragment ^a	CSD reference codes
Adenine	acados adenos01 adenos10 amdoad amoada amoadb amoadc araden10 bedlif betwus bifyoe boyduo bubfuz buvpox bzapuc20 cezmez chxadi10 cidgur coczid cubrum dadpnh10 dhoods01 dhoods10 dohgem dorjoj divveh10 fabfuj01 fibgec fikhai fikhai01 gahhig gahhig01 hemyih kemyeg keplia keplog kubguy meaden01 nakzuu opadna opadna01 opadnb pakwon thopad10 tugjag tugjek vomfos wajzem wibxek yabgaj
Guanine	budway10 cehtak10 dahmii defxuh gebrio gipbiq guansh10 guopna10 guopna11 jafhah reczaa scgmpt10 sdgunp tamxek vuwrek vuymil zuzxat
Cytosine	acytid bivvil bofwoi botsim10 boxgie budway10 cimjen cytcyp20 cytidi01 cytidi10 decyuf fikhow fovxet gahhom gahhom01 gigmoy gouger10 jikhoa juhlah kosnov marafc metcyt01 secbux segmas sivzus yukliz
Thymine	cedboc cezfoc clqunb10 dayvoo doxziz duksor duxxez firpol fixgau01 fixgau02 fixgau03 gebtem gexxiq gexxiq01 kasvef katyin kexkih kezruc kinheu kinhiy kitsov kogbir kunnem kuthow kuzxei methym01 palwuz soddeu sosbil tmthym tpataa trfutm tymcxa vevbut vevbut01 vikfea
Sugars	fikhai fikhai01 foylua fuxbij gexxiq gexxiq01 gidtes jafhah acurid boxgie cezbis cezfoc cezmez dadpnh10 defpot docypo docypo02 docypo03 docytc doxadm duhhuj dumtou dxcytd etyxur gebtem gergal geyces gidtiw gojwor hmdour ipdxur jappev jibdih jubvil jubvor keclot medour pryurd10 sdgunp sifgap thydin vdurid vexdor
Phosphate group	acrcyt adurpo10 aeadmp amatur apapad01 aracyc aurcpb bawjak behlij beprap bixxip bixxip10 brcamp brinsp cattew cexbow cexbux cibbaq cjsix citxim cupyuh cytcyp20 dabsoo dabsuu derdej detlix detlix10 dezmau dinyii fahheb fambok fambok10 firpol gegwyi glphea20 glycac01 gupcyt20 keryah keryah10 lerbal mecpsp mgpcpi naamph naamph10 nadens nufluv nutxop palect pallec pextan pflcpa pflcpb pflcpc pflcpc01 reyjek reyjo scgmpt10 suromm tahjiv ticzag wagvab wagvab10 yorpaw yuwilil

^aThe CSD was searched for crystal structures containing either base, sugar or phosphate fragments.