TAAAACGTTTTAAAACCCCCC is much less curved because the roll kink at CG is counterbalanced by roll kinks in the opposite direction at the two flanking TA steps. In both cases, A-tracts are straight and completely unbent. (Note that both roll kinks can involve compression of the major groove, as expected, because the kink sites are a half turn of helix apart.)

This similarity of behaviour of DNA in crystals and in protein–DNA complexes should come as no surprise, since the local molecular environments – close intermolecular contacts, partial dehydration, low water activity, low local dielectric constant, high ionic strength, presence of divalent cations – are similar in these two cases and quite different from that of free DNA in dilute aqueous solution. Far from being unwanted 'crystal deformations', the local changes in structure resulting from intermolecular contacts in DNA crystals provide positive information about sequence-dependent deformability that is relevant to the protein recognition process. With regard specifically to A-tract behaviour, Occam's Razor would argue in favour of model (3) above for the behaviour of A-tracts in solution. The situation in dilute aqueous solution becomes of secondary importance if what is wanted is an understanding of A-tract B-DNA behaviour in protein–DNA complexes. Here, the answer is unambiguous: A-tracts in their biological setting are inherently rigid structural elements, chosen by natural selection when bending should be avoided.

23.3.5. Summary

Three families of nucleic acid double helix have been found – A, B and Z – with widely different structures and usages. The A and B helices are right-handed and have no limitations on base sequence. Z is left-handed and effectively limited to alternating purines and pyrimidines, with G and C overwhelmingly favoured. B is the biologically significant helix for DNA and is used in genetic coding. A is the helix of preference for RNA because it can accommodate the C2′-OH group of ribose, which produces steric clash in the B helix. The Z helix has, as yet, no well established biological function. A left-handed DNA configuration can be induced in longer DNA segments by negative supercoiling in solution, but it is not clear that this left-handed configuration is identical to the Z-DNA seen in short crystalline oligomers, because of the reversed orientation of backbone strands in Z-DNA.

B-DNA is an inherently malleable or deformable duplex. Its sugar ring conformations are much more variable than those of A-DNA. The base sequence of B-DNA is expressed directly *via* hydrogen bonds between bases of a pair, and indirectly *via* hydrogen-bond donors and acceptors along the floor of the major and minor groove. Sequence is also expressed as a *differential deformability* of different regions of the duplex. The two most obvious parameters affected by base sequence are minor groove width and helix bendability. Certain sequences of B-DNA are not statically bent, but are more bendable under stress than are other sequences. Bending occurs *via* roll, usually in the direction that compresses the broad major groove. Pyrimidine-purine or Y-R steps are most conducive to roll bending, and purine-purine steps are least bendable, particularly A-tracts of four or more AT base pairs without the weak T-A step. Natural selection has engineered Y-R steps into a DNA sequence where a sharp roll bend is wanted, and short A-tracts into a sequence where bending is not desired.

Appendix 23.3.1.
X-ray analyses of A, B and Z helices

Table A23.3.1.1. *X-ray analyses of A helices, DNA and RNA*

This table and the two that follow are intended as a historical background and a focus on the geometry of the intact double helix. References are current as of late 1997; sequences marked 'to be published' in 1997 that still are unpublished two years later have been deleted. Also omitted are sequences with fewer than four base pairs in the asymmetric unit, complexes with intercalating drugs, helices with bulges or looped-out bases, unusual structures such as quadruplexes, hammerhead ribozymes and tRNA. For information on these and for more recent results, consult the Nucleic Acid Database (NDB) at http://ndbserver.rutgers.edu/. An NDB number in parentheses indicates that the authors have never made coordinates available to the public. These structures are of little scientific value, but have been included for historical reasons.

Notes: Overhanging, unpaired bases are double underlined. Single underlining calls attention to mismatched bases or other interesting or relevant sequence aspects. Z = number of asymmetric units per cell. Ubp = number of base pairs per asymmetric unit. NDB No. = Nucleic Acid Database serial number. Abbreviations: 2am = 2-amino; 5br = 5-bromo; 6ame = 6′-α-methyl; 4mo = 4-methoxy; 5me = 5-methyl; 6aOH = 6′-α-hydroxyl; 6mo = 6-methoxy; 8oxo = 8-oxo; 6et = 6-ethyl; ara = arabinosyl; ps = phosphorothioate; (P) = leading phosphate; A, T, G, C = DNA; a, u, g, c = RNA; Py = pyrrole; Im = imidazole.

(*a*) Dodecamers

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CCCCCGCGGGGG	$P3_221$	6	12	1991, Barcelona	ADL025	(A38)
CCGTACGTACGG	$P6_122$	12	6	1992, Ohio State	ADL045	(A41)
GCGTACGTACGC	$P6_122$	12	6	1992, Ohio State	ADL046	(A39)

(*b*) Decamers

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
GCGGGCCCGC	$P6_122$	12	5	1993, Ohio State	ADJ051	(A46)
GCACGCGTGC	$P6_122$	12	5	1996, Ohio State	ADJ075	(A60)
ACCGGCCGGT	$P6_122$	12	5	1989, MIT	ADJ022	(A26)
ACCGGCCGGT	$P6_122$	12	5	1995, MIT	ADJ065	(A55)
ACCCGCGGGT	$P6_122$	12	5	1995, MIT	ADJ066	(A55)
CCCGGCCGGG	$P2_12_12_1$	4	10	1993, Ohio State	ADJ049	(A47)
CCIGGCC^{5me}CGG	$P2_12_12_1$	4	10	1995, Ohio State	ADJB61	(A58)

Table A23.3.1.1. *X-ray analyses of A helices, DNA and RNA* (*cont.*)

Sequence	Space group	*Z*	Ubp	Date, institution	NDB No.	Reference
GCGGGCCCGC	$P2_12_12_1$	4	10	1993, Ohio State	ADJ050	(A46)
ACCGGCCGGT	$P2_12_12_1$	4	10	1995, MIT	ADJ067	(A55)
CCGGGCCGCG	$P2_12_12_1$	4	10	1997, Ohio State	ADJ081,2	(A71)
C^{5me}CGGGCCCGG	$P2_12_12_1$	4	10	1997, Ohio State	ADJB87	(A71)
CCGGG^{5br}CCCGG	$P2_12_12_1$	4	10	1997, Ohio State	ADJB80	(A71)
CCGGGCC^{5me}CGG	$P2_12_12_1$	4	10	1997, Ohio State	ADJB84,5	(A71)
C^{5me}CGGGCCCGG	$P6_1$	6	10	1997, Ohio State	ADJB86	(A71)
CCGGGCC^{5br}CGG	$P6_1$	6	10	1997, Ohio State	ADJB79	(A71)
CCGGGCC^{5me}CGG	$P6_1$	6	10	1997, Ohio State	ADJB83	(A71)

(*c*) Nonamers

Sequence	Space group	*Z*	Ubp	Date, institution	NDB No.	Reference
GGATGGGAG	$P4_3$	4	9	1986, Cambridge	ADI009	(A14)

(*d*) Octamers, space group $P4_32_12$

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
CCCCGGGG	8	4	1987, Weizmann/MIT	ADH012	(A16)
CCCCGGGG, 298 K	8	4	1995, Weizmann	ADH056	(A54)
CCCGCGGG	8	4	1997, Moscow	ADH0106	(A69)
CCCTAGGG	8	4	1996, Ohio State	ADH078	(A64)
GCCCGGGC	8	4	1987, Berlin	ADH008	(A17)
GCCC*GGGC (*methylenephosphonate)	8	4	1991, Berlin	ADHP36	(A36)
GGCCGGCC	8	4	1982, MIT	ADH013,098	(A4,5)
GGCCGGCC, 288 K	8	4	1995, Weizmann	ADH058	(A54)
GG^{5me}CCGGCC	8	4	1987, MIT	(ADHB21)	(A15)
GGGCGCCC, 293 K	8	4	1988, Weizmann	ADH026	(A22, A34)
GGGCGCCC, 115 K	8	4	1988, Weizmann	ADH027	(A20, A34)
GGGCGCCC, 115 K, re-refinement	8	4	1995, Weizmann	ADH057	(A54)
GTGCGCAC	8	4	1992, Ohio State	ADH047	(A40)
GTGTACAC/spermine	8	4	1987, Wisconsin	ADH014	(A18, A29)
CTCTAGAG	8	4	1989, Cambridge	ADH020	(A27)
GTACGTAC	8	4	1990, Kansas	ADH024	(A35)
GTACGTAC	8	4	1990, Bordeaux	ADH023	(A32)
GTCTAGAC	8	4	1992, Manchester	ADH041	(A42)
ATGCGCAT	8	4	1990, Institute of Cancer Research	(ADH032)	(A31)
ATGCGCAT/spermine	8	4	1990, Institute of Cancer Research	ADH033	(A31)
ACGTACGT	8	4	1996, Trinity, Dublin	ADH070	(A66)

(*e*) Octamers, space group $P2_12_12_1$

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
CCCGCGGG	4	8	1997, Moscow	ADH0102–5	(A69)

(*f*) Octamers, space group $P6_1$

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
GGGGCCCC	6	8	1985, Cambridge	ADH006	(A11)
GGGATCCC	6	8	1988, Berlin	ADH007	(A21)
GGGCGCCC, 293 K	6	8	1989, Weizmann	(ADH028)	(A30, A34)
GGGCGCCC, 100 K	6	8	1989, Weizmann	ADH029	(A30, A34)
GGGTACCC, 293 K	6	8	1990, Weizmann	ADH030	(A33)
GGGTACCC, 100 K	6	8	1990, Weizmann	ADH031	(A33)
GGGTGCCC	6	8	1988, Weizmann	ADH016	(A22)
GGTATACC	6	8	1981, Weizmann/Cambridge	ADH010	(A2, A7)
GG^{5br}UA^{5br}UACC	6	8	1981, Weizmann/Cambridge	ADHB11	(A2, A7, A13)

Table A23.3.1.1. *X-ray analyses of A helices, DNA and RNA* (*cont.*)

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
GGCATGCC	6	8	1997, Institute of Cancer Research	ADH076	(A70)
GGIGCTCC	6	8	1989, Cambridge	ADHB17	(A24)
GGGGCTCC mismatch	6	8	1985, Cambridge/Weizmann	ADH019	(A9, A12)
GGGGTCCC mismatch	6	8	1985, Cambridge/Weizmann	ADH018	(A10)
GGGTGCCC mismatch	6	8	1988, Weizmann	ADH016	(A22)

(*g*) Octamers, space group $P6_122$

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
GTGTACAC	12	4	1989, Wisconsin	ADH034	(A28)
GTGTACAC/spermine	12	4	1993, Ohio State	ADH038	(A48)
GTGTACAC/spermidine	12	4	1993, Ohio State	ADH039	(A48)

(*h*) Octamers, space group $P2_12_12$

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
GTACGTAC	4	8	1993, Bordeaux	ADH059	(A44)

(*i*) Hexamers, space group $C222_1$

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
GCCGGC	8	6	1995, Oregon State	ADF073	(A56)
$G^{5me}CG^{5me}CGC$	8	6	1995, Oregon State	ADFB62	(A56)
$G^{5me}CCGGC$	8	6	1995, Oregon State	ADFB63	(A56)
$G^{5me}CGCGC$	8	6	1995, Oregon State	ADFB72	(A56)

(*j*) Tetramers

Sequence	Space group	*Z*	Ubp	Date, institution	NDB No.	Reference
^{5i}CCGG	$P4_32_12$	8	4	1981, UCLA (CIT)	ADDB01	(A1, A3, A8)

(*k*) RNA/DNA and RNA/RNA (lower case = RNA)

Sequence	Space group	*Z*	Ubp	Date, institution	NDB No.	Reference
CCGGC g CCGG	$P2_12_12_1$	4	10	1994, Ohio State	AHJ052	(A49)
c CGGCGCCGg	$P2_12_12_1$	4	10	1994, Ohio State	AHJ060	(A50)
g CGTATACGC	$P2_12_12_1$	4	10	1993, MIT	AHJ043	(A45)
GCGTaTACGC	$P2_12_12_1$	4	10	1993, MIT	AHJ044	(A45)
$GCGT^{me}aTACGC$	$P2_12_12_1$	4	10	1994, ETH Zürich	AHJS55	(A53)
g c GTATACGC	$P2_12_12_1$	4	10	1995, MIT	AHJ068	(A55)
g c g TATACGC	$P2_12_12_1$	4	10	1982, MIT	AHJ015	(A4, A6)
g c g TATACCC\ \GGGTATACGC	$P2_12_12_1$	4	10	1992, MIT	AHJ040	(A43)
u u c g g g c g c c\ \GGCGCCCGAA	$P4_322$	8	10	1996, Upjohn	UHJ055	(A62)
c c c c g g g g	$P6_122$	12	4	1995, ETH Zürich	ARH063	(A57)
c c c c g g g g	$R32$	18	8	1995, ETH Zürich	ARH064	(A57)
c c c c g g g g	$R32$	18	8	1996, Northwestern	ARH074	(A61)
g u a u a u a C	$R3$	9	8	1996, Ohio State	AHH071	(A65)
g u a u g u a C	$R3$	9	8	1997, Ohio State	AHH077	(A68)
g u g u g u a C	$R3$	9	8	1997, Ohio State	AHH089	(A67)
g c u u c g g c ^{br}U	$C2$	4	9	1994, Cambridge	AHIB53	(A51)
(P)g g a c u u c g g u c c	$C2$	4	6	1991, Berkeley	ARL037	(A37)
c g c g a a t t a g c g	$P2_1$	2	12	1994, Manchester	ARL048	(A52)
u a a g g a g g u g a u	$P1$	1	24	1995, Berlin	ARL062	(A59)
g g c g c u u g c g u c	$P1$	1	24	1996, Colorado	URL050	(A63)
u u a u a u a u a u a u a a	$P2_12_12_1$	4	4	1988, Strasbourg	ARN035	(A19, A25)

Table A23.3.1.1. *X-ray analyses of A helices, DNA and RNA* (*cont.*)

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Table A23.3.1.1. *X-ray analyses of A helices, DNA and RNA* (*cont.*)

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Table A23.3.1.2. *X-ray analyses of B-DNA helices and their complexes with minor-groove-binding drug molecules*

See introductory notes to Table A23.3.1.1. Space group $P2_12_12_1$ unless specified otherwise.

Notes: (triplet) = external triplet formed from overhanging bases. Overhanging, unpaired bases are double underlined. Single underlining calls attention to interesting or relevant sequence aspects. Other notes as in Table A23.3.1.1.

I. DNA duplexes without bound drugs

(*a*) Dodecamers, space group $P2_12_12_1$

(1) Oligonucleotides without mismatches

Sequence	*Z*	Ubp	Date, institution	NDB No.	Reference
CGCGAATTCGCG, 290 K	4	12	1980, UCLA (CIT)	BDL001	(B1–5, B75)
CGCGAATTCGCG, 16 K	4	12	1982, UCLA (CIT)	BDL002	(B6)
CGCGAATTCGCG, re-refinement	4	12	1987, Strasbourg	BDL020	(B23)
CGCGAATTCGCG, anisotropic temperature-factor refinement	4	12	1985, Berkeley	BDL005	(B10)
CGCGAATT^{5br}CGCG, 293 K	4	12	1982, UCLA (CIT)	BDLB03	(B7, B8)
CGCGAATT^{5br}CGCG, 280 K	4	12	1982, UCLA (CIT)	BDLB04	(B7, B8, B75)
CGCGA^{6me}ATTCGCG	4	12	1988, MIT	BDLB13	(B24)
CGCGAA^{6ame}T^{6ame}TCGCG	4	12	1997, Northwestern	BDLS79	(B111)
CGCGAA^{6aOH}T^{6aOH}TCGCG	4	12	1997, Northwestern	BDLS80	(B111)
CGCGAASSCGCG	4	12	1996, Manchester	BDLS67	(B97)
CGCAIAT^{5me}CTGCG	4	12	1997, Weizmann	BDLB82	(B113)
CGCAAAAAAGCG	4	12	1987, Cambridge	BDL006	(B20, B75)
CGCAAAAATGCG	4	12	1989, Yale	BDL015	(B31, B75)
CGCAAATTTGCG	4	12	1987, MIT	BDL016	(B17)
CGCAAATTTGCG	4	12	1992, Institute of Cancer Research	BDL038	(B52, B75)
CGCATATATGCG	4	12	1988, UCLA	BDL007	(B27)
CGCGTTAACGCG	4	12	1991, Ohio State	BDL059	(B40, B86)
CGCGATATCGCG	4	12	1997, Weizmann	BDL078	(B113)
CGCAIAT^{5me}CTGCG	4	12	1997, Weizmann	BDLB76	(B113)
CGTGAATTCACG	4	12	1991, UCLA	BDL029	(B44, B75)
CGTGAATTCACG	4	12	1991, Rutgers	BDL028	(B45)