

## 23.3. NUCLEIC ACIDS

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

Year	Reference
1994	(A49) C. Ban, B. Ramakrishnan & M. Sundaralingam (1994). <i>J. Mol. Biol.</i> <b>236</b> , 275–285. (A50) C. Ban, B. Ramakrishnan & M. Sundaralingam (1994). <i>Nucleic Acids Res.</i> <b>22</b> , 5466–5476. (A51) W. Cruse, P. Saludjian, E. Biala, P. Strazewski, T. Prange & O. Kennard (1994). <i>Proc. Natl Acad. Sci. USA</i> , <b>91</b> , 4160–4164. (A52) G. A. Leonard, K. E. McAuley-Hecht, S. Ebel, D. M. Lough, T. Brown & W. N. Hunter (1994). <i>Structure</i> , <b>2</b> , 483–494. (A53) P. Lubini, W. Zuercher & M. Egli (1994). <i>Chem. Biol.</i> <b>1</b> , 39–45.
1995	(A54) M. Eisenstein & Z. Shakked (1995). <i>J. Mol. Biol.</i> <b>248</b> , 662–678. (A55) Y.-G. Gao, H. Robinson, J. H. van Boom & A. H.-J. Wang (1995). <i>Biophys. J.</i> <b>69</b> , 559–568. (A56) B. H. Mooers, G. P. Schroth, W. W. Baxter & P. S. Ho (1995). <i>J. Mol. Biol.</i> <b>249</b> , 772–784. (A57) S. Portmann, N. Usman & M. Egli (1995). <i>Biochemistry</i> , <b>34</b> , 7569–7575. (A58) B. Ramakrishnan & M. Sundaralingam (1995). <i>Biophys. J.</i> <b>69</b> , 553–558. (A59) H. Schindelin, M. Zhang, R. Bald, J.-P. Fuerste, V. A. Erdmann & U. Heinemann (1995). <i>J. Mol. Biol.</i> <b>249</b> , 595–603.
1996	(A60) C. Ban & M. Sundaralingam (1996). <i>Biophys. J.</i> <b>71</b> , 1222–1227. (A61) M. Egli, S. Portmann & N. Usman (1996). <i>Biochemistry</i> , <b>35</b> , 8489–8494. (A62) N. C. Horton & B. C. Finzel (1996). <i>J. Mol. Biol.</i> <b>264</b> , 521–533. (A63) S. E. Lietzke, C. L. Barnes & C. E. Kundrot (1996). <i>Structure</i> , <b>4</b> , 917–930. (A64) D. B. Tippin & M. Sundaralingam (1996). <i>Acta Cryst. D</i> <b>52</b> , 997–1003. (A65) M. C. Wahl, C. Ban, C. Sekharudu, B. Ramakrishnan & M. Sundaralingam (1996). <i>Acta Cryst. D</i> <b>52</b> , 655–667. (A66) D. J. Wilcock, A. Adams, C. J. Cardin & L. P. G. Wakelin (1996). <i>Acta Cryst. D</i> <b>52</b> , 481–485.
1997	(A67) R. Biswas & M. Sundaralingam (1997). <i>J. Mol. Biol.</i> <b>270</b> , 511–519. (A68) R. Biswas, M. C. Wahl, C. Ban & M. Sundaralingam (1997). <i>J. Mol. Biol.</i> <b>267</b> , 1149–1156. (A69) L. G. Fernandez, J. A. Subirana, N. Verdagauer, D. Pyshni, L. Campos & L. Malinina (1997). <i>J. Biomol. Struct. Dyn.</i> <b>15</b> , 151–163. (A70) C. M. Nunn & S. Neidle (1997). <i>Acta Cryst. D</i> <b>53</b> , 269–273. (A71) D. B. Tippin & M. Sundaralingam (1997). <i>J. Mol. Biol.</i> <b>267</b> , 1171–1185.

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 <sup>5br</sup> CGCG, 293 K	4	12	1982, UCLA (CIT)	BDLB03	(B7, B8)
CGCGAATT <sup>5br</sup> CGCG, 280 K	4	12	1982, UCLA (CIT)	BDLB04	(B7, B8, B75)
CGCGA <sup>6me</sup> ATTTCGCG	4	12	1988, MIT	BDLB13	(B24)
CGCGAA <sup>6ame</sup> T <sup>6ame</sup> TCGCG	4	12	1997, Northwestern	BDLS79	(B111)
CGCGAA <sup>6aOH</sup> T <sup>6aOH</sup> TCGCG	4	12	1997, Northwestern	BDLS80	(B111)
CGCGAASSCGCG	4	12	1996, Manchester	BDLS67	(B97)
CGCAIAT <sup>5me</sup> CTGCG	4	12	1997, Weizmann	BDLB82	(B113)
CGCAAAAAAGCG	4	12	1987, Cambridge	BDL006	(B20, B75)
CGCAAAAAATGCG	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 <sup>5me</sup> CTGCG	4	12	1997, Weizmann	BDLB76	(B113)
CGTGAATTCACG	4	12	1991, UCLA	BDL029	(B44, B75)
CGTGAATTCACG	4	12	1991, Rutgers	BDL028	(B45)

### 23. STRUCTURAL ANALYSIS AND CLASSIFICATION

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

Sequence	Z	Ubp	Date, institution	NDB No.	Reference
CGCG <u>AAA</u> ACGCG/ CGCGTT/TTCGCG (nicked strand)	4	12	1990, MIT	BDL021,32	(B35)

(2) Mismatch oligonucleotides (mismatches underlined)

Sequence	Z	Ubp	Date, institution	NDB No.	Reference
CGCGAATTGGCG	4	12	1993, Institute of Cancer Research	BDL046	(B72)
CGCGAATTAGCG	4	12	1986, Cambridge	BDL012	(B13, B15)
CGCGAATT <sup>6et</sup> AGCG	4	12	1994, Manchester	BDLB54	(B79)
CGCGAATT <sup>8oxo</sup> AGCG	4	12	1992, Manchester	BDLB33	(B57)
CGCGAATTTGCG	4	12	1985, Cambridge	BDL009	(B19)
CGC <sup>6me</sup> GAATTTGCG	4	12	1990, Edinburgh	BDLB26	(B38)
CGCAATTGGCG	4	12	1989, Manchester	BDL014	(B28, B37)
CGCAAGCTGGCG	4	12	1990, Institute of Cancer Research	BDL022	(B39, B75)
CGCAAATT <sup>8oxo</sup> GGCG	4	12	1994, Edinburgh	BDLB56	(B80)
CGCAAATTCGCG	4	12	1986, Cambridge	BDL011	(B16)
CGCAAATTIGCG	4	12	1992, Edinburgh	BDLB41	(B56)
CGCIAATTAGCG	4	12	1987, Cambridge	BDLB10	(B18)
CGCIAATTCGCG	4	12	1992, Thomas Jefferson	BDLB40	(B61)
CGAGAATTC <sup>6me</sup> GCG	4	12	1994, Rutgers	BDLB53	(B76)
CGTGAATTC <sup>6me</sup> GCG	4	12	1995, Rutgers	BDLB58	(B95)

(b) Dodecamers: other space groups

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CGCTCTAGAGCG	$P2_1$	2	24	1996, Barcelona	BDL070	(B102)
CGTAGATCTACG	$C2$	4	12	1993, Manchester	BDL042	(B69, B75)
CGCGAAAAAACG	$P2_12_12$	4	24	1993, Yale	BDL047	(B64, B75)
ACCGGCGCCACA	$R3$	9	12	1989, Strasbourg	BDL018	(B34, B48, B49)
ACCGCCGGCGCC	$R3$	9	12	1989, Strasbourg	BDL035	(B48, B49)
ACCGC <sup>5me</sup> CGGCGCC	$R3$	9	12	1997, Strasbourg	BDLB83	(B109)
ACCGGCGCCACA	$R3$	9	12	1991, Strasbourg	BDL034	(B48)

(c) Decamers

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CCAAGATTGG mismatch	$C2$	4	5	1987, UCLA	BDJ008	(B22, B25)
CCAACGTTGG, Mg	$C2$	4	5	1991, UCLA	BDJ019	(B46, B50)
CCAACITTGG, Ca	$C2$	4	5	1992, UCLA	BDJB44	(B70)
CCAGGCCTGG	$C2$	4	5	1989, Berlin	BDJ017	(B32)
CCAGGC <sup>ara</sup> CTGG	$C2$	4	5	1991, MIT	BDJS30	(B41)
CCA <sup>8oxo</sup> GCGCTGG	$C2$	4	5	1995, MIT	BDJB57	(B91)
CTCTCGAGAG	$C2$	4	10	1994, UCLA	BDJ060	(B89)
CGCAATTGCG	$C2$	4	10	1997, Institute of Cancer Research	BDJ069	(B114)
CAAAGAAAAG	$C2$	4	20	1997, UCLA	BDJ081	(B107)
<u>CGACGATCGT TGCTAGCAGC</u>	$P2_1$	2	10	1997, NYU	UDJ060	(B112)
<u>GGCCAATTGG GGTTAACCGG</u>	$P2_12_12_1$	4	10	1996, Cambridge	UDJ049	(B103)
CGATCGATCG, Mg	$P2_12_12_1$	4	10	1991, UCLA	BDJ025	(B42)
CGATTAATCG, Mg	$P2_12_12_1$	4	10	1992, UCLA	BDJ031	(B58)
CGATATATCG, Mg	$P2_12_12_1$	4	10	1992, UCLA	BDJ037	(B62)
CGATATATCG, Ca	$P2_12_12_1$	4	10	1992, UCLA	BDJ036	(B62)
CATGGCCATG, Ca	$P2_12_12_1$	4	10	1993, UCLA	BDJ051	(B66)
CGATCG <sup>6me</sup> ATCG	$P3_22_1$	6	10	1992, UCLA	BDJB48	(B63)
CCAACITTGG, Mg	$P3_22_1$	6	10	1992, UCLA	BDJB43	(B70)
CCATTAATGG, Mg	$P3_22_1$	6	10	1994, UCLA	BDJ055	(B77)
CCACTAGTGG	$P3_22_1$	6	10	1994, Weizmann	BDJ061	(B82)
CCAGGC <sup>5me</sup> CTGG	$P6$	6	10	1992, Berlin	BDJB27	(B43, B54)

### 23.3. NUCLEIC ACIDS

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

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CCAGGC <sup>5me</sup> CTGG	P6	6	10	1993, Berlin	BDJB49	(B68)
CCAGGC <sup>5me</sup> CTGG	P6	6	10	1993, Berlin	BDJB50	(B68)
CCAAGCTTGG	P6	6	10	1993, UCLA	BDJ052	(B67)
CCGGCGCCGG	R3	9	10	1992, Berlin	BDJ039	(B55)
CCGCCGGCGG	R3	9	10	1994, Strasbourg	BD0015	(B85)
CCIIICCCGG	P3 <sub>1</sub>	3	10	1997, Weizmann	BDJB77	(B113)

(d) Other oligonucleotide lengths

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
<u>GCGAATTCG</u> (triplet) <u>GCTTAAGCG</u>	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	4	8	1996, Cambridge	UDI030	(B94)
CGCTAGCG	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	4	16	1996, Barcelona	BDH071	(B102)
<u>CGGTGG</u> <u>CCACCG</u>	P6 <sub>1</sub> 22	12	6	1995, Manitoba	BDF062	(B93)
CTCGAG	P6 <sub>2</sub> 22	12	3	1996, Ohio State	BDF068	(B104)
GpsCGpsCGpsC	P2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	4	6	1987, Cambridge	BDFP24	(B14)

## II. DNA complexes with minor-groove-binding drugs

(a) Ntropsin family of polyamides

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
Netropsin: <sup>+</sup> Py-Py <sup>+</sup> CGCGAATT <sup>5br</sup> CGCG/N		4	12	1985, UCLA	GDLB05	(B11, B12)
CGCGAATT <sup>5br</sup> CGCG/N		4	12	1995, UCLA	GDLB31	(B88)
CGCGAATTCGCG/N		4	12	1992, Illinois	GDL018	(B59)
CGC <sup>6et</sup> GAATTCGCG/N		4	12	1992, Illinois	GDLB17	(B59)
CGCAAATTTGCG/N		4	12	1993, MIT	GDL014	(B73)
CGCGATATCGCG/N		4	12	1989, MIT	GDL001,4	(B30)
CGCGTTAACGCG/N		4	12	1995, Ohio State	GDL030	(B86)
CGCAATTGCG/N		4	12	1997, Institute of Cancer Research	GDJ046	(B110)
Lexitropsin: <sup>+</sup> Im-Py <sup>+</sup> CGCGAATTCGCG/1L		4	12	1995, UCLA	GDL037,8	(B90)
2:1 Di-imidazole Lexitropsin: <sup>0</sup> Im-Im <sup>+</sup> CATGGCCATG/2D		4	10	1997, UCLA	GDJ054	(B108)
Distamycin: <sup>0</sup> Py-Py-Py <sup>+</sup> CGCAAATTTGCG/1D		4	12	1987, MIT	GDL003	(B17)
ICICICIC/2D	P4 <sub>1</sub> 22	8	4	1994, Ohio State	GDHB25	(B74)
I <sub>c</sub> ICICIC/2D	P4 <sub>1</sub> 22	8	4	1995, Ohio State	GHHB34	(B87)
I <sub>c</sub> I <sub>c</sub> ICIC/2D	P4 <sub>1</sub> 22	8	4	1995, Ohio State	GHHB35	(B87)
ICATATIC	P4 <sub>1</sub> 22	8	4	1997, Ohio State	GHHB50	(B105)
ICITACIC	P4 <sub>1</sub> 22	8	4	1997, Ohio State	GHHB51	(B105)
ICATATIC	C2	4	4	1997, Ohio State	GDLB49	(B105)

(b) Hoechst family

Sequence	Z	Ubp	Date, institution	NDB No.	Reference
Hoechst 33258 ( <i>para</i> -OH on phenyl ring A) CGCGAATTCGCG/H	4	12	1987, UCLA	GDL006	(B21)
CGCGAATTCGCG/H	4	12	1988, MIT	GDL002	(B26)
CGCGAATTCGCG/H, 273 K	4	12	1991, UCLA	GDL010,11	(B47)
CGCGAATTCGCG/H, 248 K	4	12	1991, UCLA	GDL012	(B47)
CGCGAATTCGCG/H, 173 K	4	12	1991, UCLA	GDL013	(B47)
CGCGATATCGCG/H	4	12	1989, MIT	GDL007	(B29)

## 23. STRUCTURAL ANALYSIS AND CLASSIFICATION

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

Sequence	Z	Ubp	Date, institution	NDB No.	Reference
CGCAAATTTGCG/H	4	12	1994, Institute of Cancer Research	GDL028	(B83)
CGCAAATTTGCG/H	4	12	1994, MIT	GDL026	(B84)
CGCGAATTCGCG/H	4	12	1992, Illinois	GDL022	(B60)
CGC <sup>6et</sup> GAATTCGCG/H	4	12	1992, Illinois	GDLB19	(B60)
Meta-OH(N) Hoechst 33258 ( <i>meta</i> -OH on ring A)					
CGCGAATTCGCG/H 'in'	4	12	1996, Institute of Cancer Research	GDL047	(B99)
CGCGAATTCGCG/H 'out'	4	12	1996, Institute of Cancer Research	GDL048	(B99)
Hoechst 33342 ( <i>para</i> -OEt on ring A)					
CGCGAATTCGCG/H	4	12	1992, Illinois	GDLB20	(B60)
CGC <sup>6et</sup> GAATTCGCG/H	4	12	1992, Illinois	GDLB20	(B60)
Bis-benzimidazole compound (imidazole for piperazine on Hoechst 33258)					
CGCGAATTCGCG/B	4	12	1995, Institute of Cancer Research	GDL033	(B96)
Tribiz or Tris-benzimidazole (extended Hoechst 33258 analogue)					
CGCAAATTTGCG/T	4	12	1996, Institute of Cancer Research	GDL039	(B98)
Bis-amidinium derivative of Hoechst 33258					
CGCGAATTCGCG	4	12	1997, Institute of Cancer Research	GDL052	(B106)

## (c) Berenil family

Sequence	Z	Ubp	Date, institution	NDB No.	Reference
Berenil					
CGCGAATTCGCG/B	4	12	1990, Institute of Cancer Research	GDL009	(B36)
CGCGAATTCGCG/B	4	12	1992, Institute of Cancer Research	GDL016	(B51)
2,5-Bis(4-guanylphenyl)furan (berenil analogue)					
CGCGAATTCGCG/F	4	12	1996, Institute of Cancer Research	GDL036	(B100)
2,5-Bis{[4-( <i>N</i> -isopropyl)amidino]phenyl}furan (berenil analogue)					
CGCGAATTCGCG/F	4	12	1996, Institute of Cancer Research	GDL044	(B101)
2,5-Bis{[4-( <i>N</i> -cyclopropyl)amidino]phenyl}furan (berenil analogue)					
CGCGAATTCGCG/F	4	12	1997, Institute of Cancer Research	GDL045	(B101)

## (d) Other minor-groove binders

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
DAPI						
CGCGAATTCGCG/D		4	12	1989, UCLA	GDL008	(B33)
Pentamidine						
CGCGAATTCGCG/P		4	12	1992, Institute of Cancer Research	GDL015	(B53)
$\gamma$ -Oxapentamidine						
CGCGAATTCGCG/P		4	12	1994, Institute of Cancer Research	GDL027	(B81)
Propamidine						
CGCGAATTCGCG/P		4	12	1993, Institute of Cancer Research	GDL023	(B71)
CGCGAATTCGCG/P		4	12	1995, Institute of Cancer Research	GDL032	(B92)

## 23.3. NUCLEIC ACIDS

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

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
SN6999 CGC <sup>6e1</sup> GAATTCGCG/S		4	12	1993, Illinois	GDLB24	(B65)
Anthramycin CCAACGTTGG/A	P3 <sub>2</sub> 21	6	5	1993, UCLA	GDJB29	(B78)

References (numbered chronologically by year and alphabetically by first author within each year)

- Year Reference
- 1980 (B1) R. M. Wing, H. R. Drew, T. Takano, C. Broka, S. Tanaka, K. Itakura & R. E. Dickerson (1980). *Nature (London)*, **287**, 755–758.
- 1981 (B2) R. E. Dickerson & H. R. Drew (1981). *J. Mol. Biol.* **149**, 761–786.  
(B3) R. E. Dickerson, H. R. Drew & B. N. Conner (1981). *Biomolecular stereodynamics*, Vol. 1, edited by R. H. Sarma, pp. 1–34. New York: Adenine Press.  
(B4) H. R. Drew & R. E. Dickerson (1981). *J. Mol. Biol.* **151**, 535–556.  
(B5) H. R. Drew, R. M. Wing, T. Takano, C. Broka, S. Tanaka, K. Itakura & R. E. Dickerson (1981). *Proc. Natl Acad. Sci. USA*, **78**, 2179–2183.
- 1982 (B6) H. R. Drew, S. Samson & R. E. Dickerson (1982). *Proc. Natl Acad. Sci. USA*, **79**, 4040–4044.  
(B7) A. V. Fratini, M. L. Kopka, H. R. Drew & R. E. Dickerson (1982). *J. Biol. Chem.* **257**, 14686–14707.
- 1983 (B8) M. L. Kopka, A. V. Fratini, H. R. Drew & R. E. Dickerson (1983). *J. Mol. Biol.* **163**, 129–146.
- 1984 (B9) R. M. Wing, P. Pjura, H. R. Drew & R. E. Dickerson (1984). *EMBO J.* **3**, 1201–1206.
- 1985 (B10) S. R. Holbrook, R. E. Dickerson & S.-H. Kim (1985). *Acta Cryst.* **B41**, 255–262.  
(B11) M. L. Kopka, C. Yoon, D. Goodsell, P. Pjura & R. E. Dickerson (1985). *Proc. Natl Acad. Sci. USA*, **82**, 1376–1380.  
(B12) M. L. Kopka, C. Yoon, D. Goodsell, P. Pjura & R. E. Dickerson (1985). *J. Mol. Biol.* **183**, 553–563.
- 1986 (B13) T. Brown, W. N. Hunter, G. Kneale & O. Kennard (1986). *Proc. Natl Acad. Sci. USA*, **83**, 2402–2406.  
(B14) W. B. T. Cruse, S. A. Salisbury, T. Brown, R. Cosstick, F. Eckstein & O. Kennard (1986). *J. Mol. Biol.* **192**, 891–905.  
(B15) W. N. Hunter, T. Brown & O. Kennard (1986). *J. Biomol. Struct. Dyn.* **4**, 173–191.  
(B16) W. N. Hunter, T. Brown, N. N. Anand & O. Kennard (1986). *Nature (London)*, **320**, 552–555.
- 1987 (B17) M. Coll, C. A. Frederick, A. H.-J. Wang & A. Rich (1987). *Proc. Natl Acad. Sci. USA*, **84**, 8385–8389.  
(B18) P. W. R. Corfield, W. N. Hunter, T. Brown, P. Robinson & O. Kennard (1987). *Nucleic Acids Res.* **15**, 7935–7949.  
(B19) W. N. Hunter, T. Brown, G. Kneale, N. N. Anand, D. Rabinovich & O. Kennard (1987). *J. Biol. Chem.* **261**, 9962–9970.  
(B20) H. C. M. Nelson, J. T. Finch, B. F. Luisi & A. Klug (1987). *Nature (London)*, **330**, 221–226.  
(B21) P. E. Pjura, K. Grzeskowiak & R. E. Dickerson (1987). *J. Mol. Biol.* **197**, 257–271.  
(B22) G. G. Privé, U. Heinemann, S. Chandrasegaran, L.-S. Kan, M. L. Kopka & R. E. Dickerson (1987). *Science*, **238**, 498–504.  
(B23) E. Westhof (1987). *J. Biomol. Struct. Dyn.* **5**, 581–600.
- 1988 (B24) C. A. Frederick, G. J. Quigley, G. A. van der Marel, J. H. van Boom, A. H.-J. Wang & A. Rich (1988). *J. Biol. Chem.* **263**, 17872–17879.  
(B25) G. G. Privé, U. Heinemann, S. Chandrasegaran, L.-S. Kan, M. L. Kopka & R. E. Dickerson (1988). *Structure and expression*, Vol. 2. *DNA and its drug complexes*, edited by R. H. Sarma & M. H. Sarma, pp. 27–47. Schenectady, NY: Adenine Press.  
(B26) M. Teng, N. Usman, C. A. Frederick & A. H.-J. Wang (1988). *Nucleic Acids Res.* **16**, 2671–2690.  
(B27) C. Yoon, G. G. Privé, D. S. Goodsell & R. E. Dickerson (1988). *Proc. Natl Acad. Sci. USA*, **85**, 6332–6336.
- 1989 (B28) T. Brown, G. A. Leonard, E. D. Booth & J. Chambers (1989). *J. Mol. Biol.* **207**, 455–457.  
(B29) M. A. A. F. de C. T. Carrondo, M. Coll, J. Aymami, A. H.-J. Wang, G. A. van der Marel, J. H. van Boom & A. Rich (1989). *Biochemistry*, **28**, 7849–7859.  
(B30) M. Coll, J. Aymami, G. A. van der Marel, J. H. van Boom, A. Rich & A. H.-J. Wang (1989). *Biochemistry*, **28**, 310–320.  
(B31) A. D. DiGabriele, M. R. Sanderson & T. A. Steitz (1989). *Proc. Natl Acad. Sci. USA*, **86**, 1816–1820.  
(B32) U. Heinemann & C. Alings (1989). *J. Mol. Biol.* **210**, 369–381.  
(B33) T. A. Larsen, D. S. Goodsell, D. Cascio, K. Grzeskowiak & R. E. Dickerson (1989). *J. Biomol. Struct. Dyn.* **7**, 477–491.  
(B34) Y. Timsit, E. Westhof, R. P. P. Fuchs & D. Moras (1989). *Nature (London)*, **341**, 459–462.
- 1990 (B35) J. Aymami, M. Coll, G. A. van der Marel, J. H. van Boom, A. H.-J. Wang & A. Rich (1990). *Proc. Natl Acad. Sci. USA*, **87**, 2526–2530.  
(B36) D. G. Brown, M. R. Sanderson, J. V. Skelly, T. C. Jenkins, T. Brown, E. Garman, D. I. Stuart & S. Neidle (1990). *EMBO J.* **9**, 1329–1334.  
(B37) G. A. Leonard, E. D. Booth & T. Brown (1990). *Nucleic Acids Res.* **18**, 5617–5623.  
(B38) G. A. Leonard, J. Thomson, W. P. Watson & T. Brown (1990). *Proc. Natl Acad. Sci. USA*, **87**, 9573–9576.  
(B39) G. D. Webster, M. R. Sanderson, J. V. Skelly, S. Neidle, P. F. Swann, B. F. Li & I. J. Tickle (1990). *Proc. Natl Acad. Sci. USA*, **87**, 6693–6697.
- 1991 (B40) J. Balendrian & M. Sundaralingam (1991). *J. Biomol. Struct. Dyn.* **9**, 511–516.  
(B41) Y.-G. Gao, G. A. van der Marel, J. H. van Boom & A. H.-J. Wang (1991). *Biochemistry*, **30**, 9922–9931.  
(B42) K. Grzeskowiak, K. Yanagi, G. G. Privé & R. E. Dickerson (1991). *J. Biol. Chem.* **266**, 8861–8883.

## 23. STRUCTURAL ANALYSIS AND CLASSIFICATION

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

Year	Reference
	(B43) U. Heinemann & C. Alings (1991). <i>EMBO J.</i> <b>10</b> , 35–43.
	(B44) T. A. Larsen, M. L. Kopka & R. E. Dickerson (1991). <i>Biochemistry</i> , <b>30</b> , 4443–4449.
	(B45) N. Narayana, S. L. Ginell, I. M. Russu & H. M. Berman (1991). <i>Biochemistry</i> , <b>30</b> , 4450–4455.
	(B46) G. G. Privé, K. Yanagi & R. E. Dickerson (1991). <i>J. Mol. Biol.</i> <b>217</b> , 177–199.
	(B47) J. R. Quintana, A. A. Lipanov & R. E. Dickerson (1991). <i>Biochemistry</i> , <b>30</b> , 10294–10306.
	(B48) Y. Timsit, E. Vilbois & D. Moras (1991). <i>Nature (London)</i> , <b>354</b> , 167–170.
	(B49) Y. Timsit & D. Moras (1991). <i>J. Mol. Biol.</i> <b>221</b> , 919–940.
	(B50) K. Yanagi, G. D. Privé & R. E. Dickerson (1991). <i>J. Mol. Biol.</i> <b>217</b> , 201–214.
1992	(B51) D. G. Brown, M. R. Sanderson, E. Garman & S. Neidle (1992). <i>J. Mol. Biol.</i> <b>226</b> , 481–490.
	(B52) K. J. Edwards, D. G. Brown, N. Spink, J. V. Skelly & S. Neidle (1992). <i>J. Mol. Biol.</i> <b>226</b> , 1161–1173.
	(B53) K. J. Edwards, T. C. Jenkins & S. Neidle (1992). <i>Biochemistry</i> , <b>31</b> , 7104–7109.
	(B54) U. Heinemann & M. Hahn (1992). <i>J. Biol. Chem.</i> <b>267</b> , 7332–7341.
	(B55) U. Heinemann, C. Alings & M. Bansal (1992). <i>EMBO J.</i> <b>11</b> , 1931–1939.
	(B56) G. A. Leonard, E. D. Booth, W. N. Hunter & T. Brown (1992). <i>Nucleic Acids Res.</i> <b>20</b> , 4753–4759.
	(B57) G. A. Leonard, A. Guy, T. Brown, R. Teoule & W. N. Hunter (1992). <i>Biochemistry</i> , <b>31</b> , 8415–8420.
	(B58) J. R. Quintana, K. Grzeskowiak, K. Yanagi & R. E. Dickerson (1992). <i>J. Mol. Biol.</i> <b>225</b> , 379–395.
	(B59) M. Sriram, G. A. van der Marel, H. L. P. F. Roelen, J. H. van Boom & A. H.-J. Wang (1992). <i>Biochemistry</i> , <b>31</b> , 11823–11834.
	(B60) M. Sriram, G. A. van der Marel, H. L. P. F. Roelen, J. H. van Boom & A. H.-J. Wang (1992). <i>EMBO J.</i> <b>11</b> , 225–232.
	(B61) J.-C. Xuan & I. T. Weber (1992). <i>Nucleic Acids Res.</i> <b>20</b> , 5457–5464.
	(B62) H. Yuan, J. R. Quintana & R. E. Dickerson (1992). <i>Biochemistry</i> , <b>31</b> , 8009–8021.
1993	(B63) I. Baikalov, K. Grzeskowiak, K. Yanagi, J. Quintana & R. E. Dickerson (1993). <i>J. Mol. Biol.</i> <b>231</b> , 768–784.
	(B64) A. D. DiGabriele & T. A. Steitz (1993). <i>J. Mol. Biol.</i> <b>231</b> , 1024–1029.
	(B65) Y.-G. Gao, M. Sriram, W. A. Denny & A. H.-J. Wang (1993). <i>Biochemistry</i> , <b>32</b> , 9693–9648.
	(B66) D. S. Goodsell, M. L. Kopka, D. Cascio & R. E. Dickerson (1993). <i>Proc. Natl Acad. Sci. USA</i> , <b>90</b> , 2930–2934.
	(B67) K. Grzeskowiak, D. S. Goodsell, M. Kaczor-Grzeskowiak, D. Cascio & R. E. Dickerson (1993). <i>Biochemistry</i> , <b>32</b> , 8923–8931.
	(B68) M. Hahn & U. Heinemann (1993). <i>Acta Cryst.</i> <b>D49</b> , 468–477.
	(B69) G. A. Leonard & W. N. Hunter (1993). <i>J. Mol. Biol.</i> <b>234</b> , 198–208.
	(B70) A. Lipanov, M. L. Kopka, M. Kaczor-Grzeskowiak, J. Quintana & R. E. Dickerson (1993). <i>Biochemistry</i> , <b>32</b> , 1373–1389.
	(B71) C. M. Nunn, T. C. Jenkins & S. Neidle (1993). <i>Biochemistry</i> , <b>32</b> , 13838–13842.
	(B72) J. V. Skelly, K. J. Edwards, T. C. Jenkins & S. Neidle (1993). <i>Proc. Natl Acad. Sci. USA</i> , <b>90</b> , 804–808.
	(B73) L. Taberner, N. Verdaguer, M. Coll, I. Fita, G. A. van der Marel, J. H. van Boom, A. Rich & J. Aymami (1993). <i>Biochemistry</i> , <b>32</b> , 8403–8410.
1994	(B74) X. Chen, B. Ramakrishnan, S. T. Rao & M. Sundaralingam (1994). <i>Nature Struct. Biol.</i> <b>1</b> , 169–170.
	(B75) R. E. Dickerson, D. S. Goodsell & S. A. Neidle (1994). <i>Proc. Natl Acad. Sci. USA</i> , <b>91</b> , 3579–3583.
	(B76) S. L. Ginnell, J. Vojtechovsky, B. Gaffney, R. Jones & H. M. Berman (1994). <i>Biochemistry</i> , <b>33</b> , 3487–3493.
	(B77) D. S. Goodsell, M. Kaczor-Grzeskowiak & R. E. Dickerson (1994). <i>J. Mol. Biol.</i> <b>239</b> , 79–96.
	(B78) M. L. Kopka, D. S. Goodsell, K. Grzeskowiak, I. Baikalov, D. Cascio & R. E. Dickerson (1994). <i>Biochemistry</i> , <b>33</b> , 13593–13610.
	(B79) G. A. Leonard, K. E. McAuley-Hecht, N. J. Gibson, T. Brown, W. P. Watson & W. N. Hunter (1994). <i>Biochemistry</i> , <b>33</b> , 4755–4761.
	(B80) K. E. McAuley-Hecht, G. A. Leonard, N. J. Gibson, J. B. Thomson, W. P. Watson, W. N. Hunter & T. Brown (1994). <i>Biochemistry</i> , <b>33</b> , 10266–10270.
	(B81) C. M. Nunn, T. C. Jenkins & S. Neidle (1994). <i>Eur. J. Biochem.</i> <b>226</b> , 953–961.
	(B82) Z. Shakked, G. Guzikovich-Guerstein, F. Frolow, D. Rabinovich, A. Joachimiak & P. B. Sigler (1994). <i>Nature (London)</i> , <b>368</b> , 469–473.
	(B83) N. Spink, D. G. Brown, J. V. Skelly & S. Neidle (1994). <i>Nucleic Acids Res.</i> <b>22</b> , 1607–1612.
	(B84) M. C. Vega, I. Garcia-Saez, J. Aymami, R. Eritja, G. A. van der Marel, J. H. van Boom, A. Rich & M. Coll (1994). <i>Eur. J. Biochem.</i> <b>222</b> , 721–726.
	(B85) Y. Timsit & D. Moras (1994). <i>EMBO J.</i> <b>13</b> , 2737–2746.
1995	(B86) K. Balendiran, S. T. Rao, C. Y. Sekharudu, G. Zon & M. Sundaralingam (1995). <i>Acta Cryst.</i> <b>D51</b> , 190–198.
	(B87) X. Chen, B. Ramakrishnan & M. Sundaralingam (1995). <i>Nature Struct. Biol.</i> <b>2</b> , 733–735.
	(B88) D. S. Goodsell, M. L. Kopka & R. E. Dickerson (1995). <i>Biochemistry</i> , <b>34</b> , 4983–4993.
	(B89) D. S. Goodsell, K. Grzeskowiak & R. E. Dickerson (1995). <i>Biochemistry</i> , <b>34</b> , 1022–1029.
	(B90) D. S. Goodsell, H. L. Ng, M. L. Kopka, J. W. Lown & R. E. Dickerson (1995). <i>Biochemistry</i> , <b>34</b> , 16654–16661.
	(B91) L. A. Lipscomb, M. E. Peek, M. L. Morningstar, S. M. Verghis, E. M. Miller, A. Rich, J. M. Essigmann & L. D. Williams (1995). <i>Proc. Natl Acad. Sci. USA</i> , <b>92</b> , 719–723.
	(B92) C. M. Nunn & S. Neidle (1995). <i>J. Med. Chem.</i> <b>38</b> , 2317–2325.
	(B93) L. W. Tari & A. S. Secco (1995). <i>Nucleic Acids Res.</i> <b>23</b> , 2065–2073.
	(B94) L. Van Meervelt, D. Vlieghe, A. Dautant, B. Gallois, G. Precigoux & O. Kennard (1995). <i>Nature (London)</i> , <b>374</b> , 742–744.
	(B95) J. Vojtechovsky, M. D. Eaton, B. Gaffney, R. Jones & H. M. Berman (1995). <i>Biochemistry</i> , <b>34</b> , 16632–16640.
	(B96) A. A. Wood, C. M. Nunn, A. Czarny, D. W. Boykin & S. Neidle (1995). <i>Nucleic Acids Res.</i> <b>23</b> , 3678–3684.

### 23.3. NUCLEIC ACIDS

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

Year	Reference
1996	(B97) T. J. Boggon, E. L. Hancox, K. E. McAuley-Hecht, B. A. Connolly, W. N. Hunter, T. Brown, R. T. Walker & G. A. Leonard (1996). <i>Nucleic Acids Res.</i> <b>24</b> , 951–961.
	(B98) G. R. Clark, E. J. Gray, S. Neidle, Y.-H. Li & W. Leupin (1996). <i>Biochemistry</i> <b>35</b> , 13745–13752.
	(B99) G. R. Clark, C. J. Squire, E. J. Gray, W. Leupin & S. Neidle (1996). <i>Nucleic Acids Res.</i> <b>24</b> , 4882–4889.
	(B100) C. A. Laughton, F. Tanius, C. M. Nunn, D. W. Boykin, W. D. Wilson & S. Neidle (1996). <i>Biochemistry</i> , <b>35</b> , 5655–5661.
	(B101) J. O. Trent, G. R. Clark, A. Kumar, W. D. Wilson, D. W. Boykin, J. E. Hall, R. R. Tidwell, B. L. Blagburn & S. Neidle (1996). <i>J. Med. Chem.</i> <b>39</b> , 4554–4562.
	(B102) L. Urpi, V. Tereshko, L. Malinina, T. Huynh-Dinh & J. A. Subirana (1996). <i>Nature Struct. Biol.</i> <b>3</b> , 325–328.
	(B103) D. Vlieghe, L. Van Meervelt, A. Dautant, B. Gallois, G. Precigoux & O. Kennard (1996). <i>Science</i> , <b>273</b> , 1702–1705.
	(B104) M. C. Wahl, S. T. Rao & M. Sundaralingam (1996). <i>Biophys. J.</i> <b>70</b> , 2857–2866.
1997	(B105) X. Chen, B. Ramakrishnan & M. Sundaralingam (1997). <i>J. Mol. Biol.</i> <b>267</b> , 1157–1170.
	(B106) G. R. Clark, D. W. Boykin, A. Czarny & S. Neidle (1997). <i>Nucleic Acids Res.</i> <b>25</b> , 1510–1515.
	(B107) G.-W. Han, M. L. Kopka, D. Cascio, K. Grzeskowiak & R. E. Dickerson (1997). <i>J. Mol. Biol.</i> <b>269</b> , 811–826.
	(B108) M. L. Kopka, D. S. Goodsell, G. W. Han, T. K. Chiu, J. W. Lown & R. E. Dickerson (1997). <i>Structure</i> , <b>5</b> , 1033–1046.
	(B109) C. Mayer-Jung, D. Moras & Y. Timsit (1997). <i>J. Mol. Biol.</i> <b>270</b> , 328–335.
	(B110) C. M. Nunn, E. Garman & S. Neidle (1997). <i>Biochemistry</i> , <b>36</b> , 4792–4799.
	(B111) S. Portmann, K.-H. Altmann, N. Reynes & M. Egli (1997). <i>J. Am. Chem. Soc.</i> <b>119</b> , 2396–2403.
	(B112) H. Qiu, J. C. Dewan & N. C. Seeman (1997). <i>J. Mol. Biol.</i> <b>267</b> , 881–898.
	(B113) M. Shatzky-Schwartz, N. D. Arbuckle, M. Eisenstein, D. Rabinovich, A. Bareket-Samish, T. E. Haran, B. F. Luisi & Z. Shakked (1997). <i>J. Mol. Biol.</i> <b>267</b> , 565–623.
	(B114) A. A. Wood, C. M. Nunn, J. O. Trent & S. Neidle (1997). <i>J. Mol. Biol.</i> <b>269</b> , 827–841.

Table A23.3.1.3. *X-ray analyses of Z helices*

See introductory notes to Table A23.3.1.1. odm = 6*H,8H*-3,4-dihydropyrimido[4,5*c*][1,2]oxazin-7-one.

(a) Hexadecamers

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CGCGCGTTTTCGCGCG (hairpin)	C2	4	8	1988, UCLA	UDP011	(Z20, Z25)

(b) Decamers (disordered)

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
GCGCGCGCGC	<i>P</i> <sub>65</sub>	6	2	1996, Ohio State	ZDJ050	(Z46)

(c) Octamers

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CGCICICG	<i>P</i> <sub>65</sub>	6	8	1992, Thomas Jefferson	ZDH030	(Z32)
CGCGCGCG	<i>P</i> <sub>65</sub>	6	8	1985, MIT	(ZDH017)	(Z10)
CGCATGCG	<i>P</i> <sub>65</sub>	6	8	1985, MIT	(ZDH016)	(Z10)

(d) Hepamers (overhanging 5' bases)

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
GCGCGCG	<i>P</i> <sub>212121</sub>	4	6	1997, Oregon State	ZDG054	(Z50)
G <sup>5me</sup> CGCGCG	<i>P</i> <sub>212121</sub>	4	6	1997, Oregon State	ZDG055	(Z50)
GCGCGCG/ GCGCGCT	<i>P</i> <sub>212121</sub>	4	6	1997, Oregon State	ZDG056	(Z50)
GCGCGCG	<i>P</i> <sub>212121</sub>	4	6	1997, Ohio State	ZDG057	(Z51)

(e) Hexamers

(1) Alternating CG: Pu-Py alternation retained

Sequence	Space group	Z	Ubp	Date, institution	NDB No.	Reference
CGCGCG, Mg	<i>P</i> <sub>212121</sub>	4	6	1989, MIT	ZDF002	(Z23)
CGCGCG, DL racemate	<i>P</i> <sub>1</sub>	2	6	1993, Osaka	ZDF040	(Z36)