Acta Crystallographica Section D

Volume 70 (2014)

Supporting information for article:

Phosphates in Z-DNA dodecamer are flexible, but their P-SAD signal is sufficient for structure solution

Zhipu Luo, Miroslawa Dauter and Zbigniew Dauter

Phosphates in Z-DNA dodecamer are flexible, but their P-SAD signal is sufficient for structure solution

Zhipu Luo[1], Miroslawa Dauter[2] and Zbigniew Dauter[1]

[1]Synchrotron Radiation Research Section, MCL, National Cancer Institute, Argonne National Laboratory, Argonne, IL 60439, USA

[2]Leidos Biomedical Research, Inc., Basic Research Program, Argonne National Laboratory, Argonne, IL 60439, USA.

Table S1

	NDB	PDB	Space gr.		Cell		Resol.	angle x	Reference
Standard bases									
$d(CGCGCGCGCGCG)_2$		2ZNA	P1	1.0	1.0	44.58*	theor		1
$d(CGCGCGCGCGCG)_2$		3ZNA	P1	1.0	1.0	44.58*	theor		1
$d(CGCGCGCGCGCG)_2$		4OCB	C2	48.48	19.55	31.22 116.36	0.75	37.6	current
$d(CGCGCG)_2$, SPM		1I0T	$P2_12_12_1$	18.316	30.680	42.491	0.6	38.3	2
$d((CACGTG)_2$, SPM, 13D		2F8W	$P2_12_12_1$	18.42	30.74	43.18	1.2	37.5	3
$d(CGCGCG)_2$, SPM		1D48	$P2_12_12_1$	18.405	30.768	43.152	1.0	38.2	4
$d(CGCGCG)_2$, SPM, $2Na^+$		131D	$P2_12_12_1$	18.265	30.690	42.460	1.0	38.3	5
$d(CGCGCG)_2$, SPM, (neutron diffr., D_2O)		1V9G	$P2_12_12_1$	18.46	30.76	43.18	1.8	38.5	6
$d(CGCGCG)_2$, SPM, (X-ray diffr, D_2O)		1WOE	$P2_12_12_1$	18.46	30.76	43.18	1.5	38.5	6
$d(CACGi5UG)_2$, $Co(NH_3)_6$		1OMK	$P2_12_12_1$	18.155	30.034	41.988	1.3	39.8	7
$d(TGCGCA)_2$, $2Mg^{2+}$		1LJX	$P2_12_12_1$	21.182	28.363	44.440	1.64	38.1	8
$d(TGCGCA)_2$, $Co(NH_3)_6$ (superseding 347D)		362D	$P2_12_12_1$	21.162	28.670	44.335	1.3	39.2	9
$d(CGCGmo4CG)_2$		1DA2	$P2_12_12_1$	18.17	30.36	43.93	1.7	38.7	10

d(CGCGC46G)$_2$	223D	$P2_12_12_1$	18.23	30.63	43.78	1.7	39.5	11
d(CGCGCG)$_2$, SPM	3P4J	$P2_12_12_1$	17.88	31.42	43.90	0.55	25.2	12
d(CGCGCG)$_2$, SPM, Mg^{2+}	1ICK	$P2_12_12_1$	17.87	31.55	44.58	0.95	25.1	13
d(CGCGCG)$_2$, SPM, $2Zn^{2+}$, Cl^-	4HIF	$P2_12_12_1$	17.791	30.907	44.196	0.85	21.4	14
d(CGCGCG)$_2$, SPM, Mn^{2+}	4HIG	$P2_12_12_1$	17.732	31.436	43.935	0.75	25.3	14
d(CGCGCG)$_2$, 2PAW	2IE1	$P2_12_12_1$	17.64	30.38	43.63	1.6	25.4	15
d((CGCGCG)$_2$, SPD, $3Mg^{2+}$, Na^+	2ELG	$P2_12_12_1$	17.847	30.988	44.022	1.0	24.7	16
d(CGCGCG)$_2$, P24, $3Mg^{2+}$, Na^+	292D	$P2_12_12_1$	17.94	31.23	44.55	1.0	25.3	17
d(CGCGCG)$_2$, 104, Mg^{2+}	1DJ6	$P2_12_12_1$	17.93	31.36	44.62	1.0	25.1	18
d(CGCGCG)$_2$, $4Mg^{2+}$	1DCG	$P2_12_12_1$	18.01	31.03	44.80	1.0	24.8	19
d(CGCGCG)$_2$, SPM, Mg^{2+}	2DCG	$P2_12_12_1$	17.87	31.55	44.58	0.9	25.3	20
d(CGmsCGCG)$_2$, SPM, Mg^{2+} (superseding 1N6S)	1VRO	$P2_12_12_1$	17.778	31.348	44.116	1.1	25.2	21
d(CaPCGTG)$_2$, Mg^{2+}	1VTY	$P2_12_12_1$	17.86	31.04	44.76	1.3	24.4	22
d(CGCGbr5UG)$_2$	2OBZ	$P2_12_12_1$	17.339	32.074	44.341	1.1	28.2	23
d(CGCGGG)$_2$, SPD, $3Mg^{2+}$, Na^+	293D	$P2_12_12_1$	17.93	31.23	44.64	1.0	24.9	24
d(CGCGGG)$_2$, 2TER, $2Mg^{2+}$	336D	$P2_12_12_1$	17.98	31.51	44.38	1.0	25.4	25
d(CGCGCG)$_2$, (neutron + X-ray refinement, D_2O)	3QBA	$P2_12_12_1$	17.90	30.59	44.61	1.5	24.3	26
d(CGCGCG)$_2$	1M6R	$P2_12_12_1$	17.96	31.47	44.73	1.54	25.3	27
d(CGCGTG)$_2$	1VTT	$P2_12_12_1$	17.45	31.63	45.56	1.0	23.8	28
d(CGCGufPG)$_2$, Mg^{2+}	1DNF	$P2_12_12_1$	17.36	31.15	45.40	1.5	24.7	29
d(brUGCGCG)$_2$, Mg^{2+}	1DA1	$P2_12_12_1$	17.94	30.85	49.95	2.25	24.4	30
d(CACGC46G)$_2$	417D	$P2_12_12_1$	17.338	31.432	44.486	1.5	24.5	31
d(CGCGCA)/d(TGCGCG), $Co(NH_3)_6$	1XA2	$P2_12_12_1$	17.976	30.926	44.625	1.71	23.6	32
d(CGCGCA)/d(TGCGCG), $Ru(NH_3)_6$	2HTO	$P2_12_12_1$	17.953	30.8 21	44.596	1.54	24.1	33
d(CACGCG)/d(CGCGTG), ($PdCl_2$)	3F8O	$P2_12_12_1$	17.785	30.941	44.789	1.72	24.8	n/a

d(CACGCG)/d(CGCGTG), ($CaCl_2$)	3GCY	$P2_12_12_1$	17.388	30.618	44.488	1.8	26.5	n/a
d(CACGCG)/d(CGCGTG), ($SnCl_2$)	3GDA	$P2_12_12_1$	17.552	30.207	43.682	1.88	24.8	n/a
d(CACGCG)/d(CGCGTG), ($MnCl_2$)	3G2A	$P2_12_12_1$	17.835	30.907	44.731	2.0	24.4	n/a
d(CACGCG)/d(CGCGTG), Ba^{2+}	3FQB	$P2_12_12_1$	17.544	30.512	44.210	1.67	25.0	n/a
d(CACGCG)/d(CGCGTG), Ba^{2+}, (rerefin. 3FQB)	4E2R	$P2_12_12_1$	17.544	30.512	44.210	1.67	25.1	n/a
d(CACGCG)/d(CGCGTG)	181D	$P2_12_12_1$	17.76	30.96	44.75	1.6	24.4	34
d(CACGCG)/d(CGCGTG), [$Ru(NH_3)_6$]	351D	$P2_12_12_1$	17.88	30.87	44.83	1.64	24.6	35
$d(CGCGCG)_2$, $6Cu^{2+}$, Na^+	1D39	$P2_12_12_1$	18.01	31.03	44.80	1.2	24.8	36
$d(m5CGm5CGm5CG)_2$	1VTV	$P2_12_12_1$	17.76	30.57	45.42	1.3	22.2	37
$d(br5CGbr5CGbr5CG)_2$, (291 K)	1DN4	$P2_12_12_1$	18.01	30.88	44.76	1.6	22.8	38
$d(br5CGbr5CGbr5CG)_2$, (310 K)	1DN5	$P2_12_12_1$	17.93	30.83	44.73	1.4	22.9	38
$d(m5CGTAm5CG)_2$	1VTW	$P2_12_12_1$	17.91	30.43	44.96	1.2	21.8	39
$d(m5CGUAm5CG)_2$, $4Cu^{2+}$	1D40	$P2_12_12_1$	17.59	30.58	44.52	1.3	22.6	40
$d(m5CGUAm5CG)_2$, $2Mg^{2+}$	1D41	$P2_12_12_1$	17.82	30.44	44.52	1.3	22.4	41
$d(CGC6mo6GCG)_2$	1D24	$P2_12_12_1$	17.85	30.87	43.98	1.9	24.7	42
$d(CGUaPCG)_2$	1D76	$P2_12_12_1$	17.944	31.282	44.701	1.3	25.2	43
d(m5CGGGm5CG)/d(m5CGCCm5CG)	145D	$P2_12_12_1$	17.865	30.822	44.797	1.25	23.0	44
$d(m5CGGCm5CG)_2$	400D	$P2_12_12_1$	17.79	30.90	44.36	1.65	22.6	45
$d(CGCGm4CG)_2$	133D	$P2_12_12_1$	17.98	30.77	44.76	1.8	23.5	46
$d(CGCGbr5CG)_2$	242D	$P2_12_12_1$	17.97	30.98	44.85	1.65	24.3	47
$d(CCCGGG)_2$	239D	$P2_12_12_1$	17.764	30.925	43.922	2.05	49.5	48
d(GCGCGCG)/d(CCGCGCG), Mg^{2+}, $Co(NH_3)_6$	312D	$P2_12_12_1$	20.32	29.54	51.84	1.8		49
d(GCGCGCG)/d(TCGCGCG), Mg^{2+}, $Co(NH_3)_6$	314D	$P2_12_12_1$	20.28	29.41	51.89	1.9		49
$d(Gm5CGCGCG)_2$, Mg^{2+}, $Co(NH_3)_6$	313D	$P2_12_12_1$	20.34	29.62	51.93	1.68		49
$d(GCGCGCG)_2$, $2Co(NH_3)_6$	331D	$P2_12_12_1$	20.41	29.65	51.86	1.65		50

$d(CGGGCGCCCG)_2$ > disordered d(CGCG)/d(GCGC)	3TCI	$P3_2$	17.767		42.06	2.42	n/a
d(GCGCGCG)/d(CCGCGCG) > disordered d(TGTG)	3ULN	$P3_2$	17.816		43.006	2.72	51
d(GCGCGCG)/d(CCGCGCG) > disordered d(TGTG)	3ULO	$P3_2$	17.670		42.729	3.24	51
d(GCGCGCG)/d(CCGCGCG) > disordered d(TGTG)	3UM4	$P3_2$	17.693		42.495	2.82	51
d(GCGCGCG)/d(CCGCGCG) > disordered d(TGTG)	3ULM	$P6_5$	17.489		41.729	3.01	51
$d(CGTACGTACG)_2$, $Co(NH_3)_6$ > disordered d(TG)	1DN8	$P6_5$	17.93		43.41	1.5	52
$d(GCGCGCGCGC)_2$ > disordered $(CG)_2$	279D	$P6_522$	18.10		43.10	1.9	53
$d(br5CGbr5CG)_2$, 6 proflavin > disordered	1VTF	$P6_5$	17.90		44.50	2.0	54
$d(CGCG)_2$, > disordered	1VTS	$P6_5$	30.92		43.29	1.5	55
d(CGCICICG)/d(CGCG) > disord. $d(CGCG)_2/d(CG)_2$	1D53	$P6_5$	31.00		43.70	1.5	56
d(CGCGCA)/d(TGCGCG) > disordered + $(TG)_2$	1XAM	$P6_5$	35.588		44.518	1.86	32
d(CGCGCA)/d(TGCGCG), $Ru(NH_3)_6$ > disordered	2HTT	$P6_5$	35.895		44.604	2.6	33
$d(CACGCG)/d(CGCGTG)/d(TG)_2$, Mn^{2+} > disordered	4DY8	$P6_5$	35.213		44.452	1.76	57
$d(CACGCG)/d(CGCGTG)/d(TG)_2$, Ba^{2+} > disordered	4E60	$P6_5$	35.177		44.341	1.86	n/a
$d(CGTGCG)_2$, Mn^{2+}	3G2R	$C222_1$	17.878	30.970	43.405	2.15	n/a
$d(CGCGCG)_2$, Mg^{2+}	392D	$C222_1$	45.80	37.30	70.30	3.0	58
$d(CGCGCG)_2$	390D	$C222_1$	69.73	52.63	26.21	2.0	58
$d(CGCG)_2$, high salt	1ZNA	$B22_12$	31.27	64.67	19.50	1.5	59
$d(CGCGCG)_2$	391D	$P112_1$	49.87	41.26	21.91 97.12	2.75	58
d(CACACG)/d(CGTGTG), $[Co(NH_3)_6]$	3E9W	$P2_1$	17.854	43.44	17.847 119.87	2.05	60
d(CGCACG)/d(CGTGCG)	180D	$P112_1$	17.75	17.76	42.77 120.05	2.5	34
d(CACGCG)/d(CGCGTG), Mn^{2+}	4DWY	$P2_1$	24.484	31.128	31.675 103.33	1.61	57
d(CACGCG)/d(CGCGTG), Mn^{2+}	3FQ5	$P2_1$	24.612	31.257	31.962 103.64	2.8	n/a
d(CACGCG)/d(CGCGTG), Ba^{2+}	4E4O	$P2_1$	24.055	31.011	31.368	1.72	n/a
$d(CGTaPCG)_2$, SPM	210D	$P3_221$	25.247		39.14	1.35	61
$d(CGTDCG)_2$, SPM, $Pt(NH_3)_3$	211D	$P3_221$	25.193		38.948	1.6	61

Modified backbones							
d(araCGaraCGaraCG)	ZDFS33	$P6_522$	17.96		43.22	1.3	62
D- and L-d(CGCGCG), racemic mix	1VTU	P-1	29.302	23.215	23.1894	2.2	63
Unusual structures							
d(CGCGAAmcTmcTCGCG), stem	4DKZ	$P2_1$	24.30	35.28	36.71 92.84	1.8	64
$d(CGCGdpyATdrpCGCG)_2$, Cu^{2+}	1JES	$P2_1$	25.343	34.359	31.093 101.13	1.5	65
$d(CCGCGG)_2$, Na^+, > swapped terminals	192D	$C222_1$	34.33	44.04	38.27	1.92	66
d(CGCGCGTTTTCCGCGCG), stem	1D16	C2	57.18	21.63	36.40 95.22	2.1	67

i5U	5-iodo-2’-deoxyuridine-5’-monophosphate	1OMK
mo4C	N^4-methoxy-2’-deoxycytidine-5’-monophosphate	1DA2
C46	6H,8H-3,4-dihydropyrimido[4,5-c][1,2]oxazin-7-one	223D, 417D
Gms	2’-deoxyguanosine-5’-monoselenophosphate	1VRO
aP	2,6-diaminopurine nucleotide	1VTY, 1D76,210D, 211D
br5U	5-bromo-2’-deoxyuridine-5’-monophosphate	2OBZ
br5C	5-bromo-2’-deoxycytidine-5’-monophosphate	1DN4, 1DN5, 242D
ufP	5-fluoro-2’-deoxyuridine-5’-monophosphate	1DNF
m5C	5-methyl-2’-deoxycytidine-5’-monophosphate	1VTV, 145D
m4C	N^4-methyl-2’-deoxycytidine-5’-monophosphate	133D
mo6G	6-O-methyl-deoxyguanosine-5’-monophosphate	1D24
mcT	north-methanocarba-thymidine-2’-monophosphate	4DKZ
dpy	2-deoxyribofuranosyl-pyridine-2,6-dicarboxylic acid-5’-monophosphate	1JES
drp	3-deoxyribofuranosyl-pyridine-5’-monophosphate	1JES
araC	arabinosylcytosine	ZDFS33

13D	1,3-diaminopropane (NCCCN)	2F8W	
SPM	spermine (NCCCNCCCCNCCCN)		
SPD	spermidine (NCCCNCCCCN)	2ELG	
TER	thermospermine (NCCCNCCCNCCCCN)	336D	
PAW	N^1-{2-[2-(2-amino-ethylamino)-ethylamino]-ethyl}-ethane-1,2-diamine (NCCNCCNCCNCCN)		2IE1
P24	1-(aminoethyl)amino-4-aminobutane (NCCNCCCCN)	292D	
104	N^1-[2-(2-amino-ethylamino)-ethyl]- ethane-1,2-diamine (trientine, NCCNCCNCCN)	1DJ6	

1 Wang, A. H.-J., Quigley, G. J., Kolpak, F. J., van der Marel G., van Boom, J. H. & Rich, A. (1981). Left-handed double helical DNA: variations in the backbone conformation. *Science* **211**, 171-176. 2zna, 3zna

2 Tereshko, V., Wilds, C. J., Minasov, G., Prakash, T. P., Maier, M. A., Howard, A., Wawrzak, Z., Manoharan. M. & Egli, M. (2001) Detection of alkali metal ions in DNA crystals using state-of-the-art X-ray diffraction experiments. *Nucleic Acids Res.* **29**, 1208-1215. 1i0t

3 Narayana, N., Shamala, N., Ganesh, K. N. & Visvamitra M. A. (2006). Interaction between the Z-type DNA duplex and 1,3-propanediamine: crystal structure of d(CACGTG)2 at 1.2 Å resolution. *Biochemistry* **45**, 1200-1211. 2f8w

4 Egli, M., Williams, L. D., Gao, Q. & Rich, A. (1991). Structure of the pure-spermine form of Z-DNA (magnesium free) at 1-Å resolution. *Biochemistry*, **30**, 11388-11402. 1d48

5 Bancroft, D., Williams, L. D., Rich, A. & Egli, M. (1994) The low-temperature crystal structure of the pure-spermine form of Z-DNA reveals binding of a spermine molecule in the minor groove. *Biochemistry*, **33**, 1073-1086. 131d

6 Chatake, T., Tanaka, I., Umino, H., Arai, S. & Niimura, N. (2005) The hydration structure of a Z-DNA hexameric duplex determined by a neutron diffraction technique. *Acta Cryst.* D**61**, 1088-1098. 1v9g, 1woe

7 Schuerman, G., Van Hecke, K. & Van Meervelt, L. (2003). Exploration of the influence of 5-iodo-2'-deoxyuridine incorporation on the structure of d[CACG(IDU)G]. *Acta Cryst.* D**59**, 1525-1528. 1omk

8 Thiyagarajan, S., Kumar, P. S., Rajan, S. S. & Gautham, N. (2002). Structure of $d(TGCGCA)_2$ at 293 K: comparison of the effects of sequence and temperature. *Acta Cryst.* D**58**, 1381-1384. 1ljx

9 Harper, A., Brannigan, J. A., Buck, M., Hewitt, L., Lewis, R. J., Moore, M. & Schneider, B. (1998). Structure of $d(TGCGCA)_2$ and a comparison with other Z-DNA hexamers. *Acta Cryst.* D**54**, 1273-1284. 362d (347d)

10 Van Meervelt, L., Moore, M. H., Lin, P. K. T., Brown, D. & Kennard, O. (1990). Molecular and crystal structure of d(CGCGmo^{4}CG): N^4-methoxycytosine.guanine base-pairs in Z-DNA. *J. Mol. Biol.* **216**, 773-781. 1da2

11 Moore, M. H., Van Meervelt, L., Salisbury, S. A., Lin, P. K. T. & Brown, D. M. (1995). Direct observation of two base-pairing modes of a cytosine-thymine analogue with guanine in a DNA Z-form duplex: significance for base analogue mutagenesis. *J. Mol. Biol.* **251**, 665-673. 223d

12 Brzezinski, K., Brzuszkiewicz, A, Dauter, M., Kubicki, M., Jaskolski, M. & Dauter, Z. (2011). High regularity of Z-DNA revealed by ultra high-resolution crystal structure at 130.55 Å. *Nucleic Acids Res.* **39**, 6238-6248. 3p4j

13 Dauter, Z. & Adamiak, D. A. (2001) Anomalous signal of phosphorus used for phasing DNA oligomer: importance of data redundancy. *Acta Cryst.* D**57**, 990-995. 1ick

14 Drozdzal, P., Gilski, M., Kierzek, R., Lomozik, L. & Jaskolski, M. (2013). Ulthahigh resolution crystal structures of Z-DNA in complex with Mn^{2+} and Zn^{2+} ions. *Acta Cryst.* D**69**, 1180-1190. 4hif, 4hig

15 Ohishi, H., Odoko, M., Grzeskowiak, K., Hiyama, Y., Tsukamoto, K., Maezaki, N., Ishida, T., Tanaka, T., Okabe, N., Fukuyama, K., Zhou, D.-Y. & Nakatani, K. (2008) Polyamines stabilize left-handed DNA: using X-ray crystallographic analysis, we have found a new type of polyamine (PA) that stabilizes left-handed DNA. *Biochem. Biophys. Res. Commun.* **366**, 275-280. 2ie1

16 Ohishi, H., Tozuka, Y., Da-Yang, Z., Ishida, T. & Nakatani, K. (2007) The rare crystallographic structure of d(CGCGCG)$_2$: the natural spermidine molecule bound to the minor groove of left-handed Z-DNA d(CGCGCG)$_2$ at 10 C. *BBRC*, **358**, 24-28. 2elg

17 Ohishi, H., Kunisawa, S., van der Marel, G., van Boom, J. H., Rich, A., Wang, A. H.-J., Tomita, K.-I. & Hakoshima, T. (1991) Interaction between the left-handed Z-DNA and polyamine. *FEBS Lett.* **284**, 238-244. 292d

18 Ohishi, H., Suzuki, K., Ohtsuchi, M., Hakoshima, T. & Rich, A. (2002) The crystal structure of N^1-[2-(2-amino-ethylamino)-ethyl]-ethane-1,2-diamine (polyamines) binding to the minor groove of d(CGCGCG)$_2$, hexamer at room temperature. *FEBS Lett.* **523**, 29-34. 1dj6

19 Gessner, R. V., Frederick, C. A., Quigley, G. J., Rich, A. & Wang, A. H-J. (1989) The molecular structure of the left-handed Z-DNA double helix at 1.0- Å atomic resolution. *J. Biol. Chem.* **264**, 7921-7935. 1dcg

20 Wang, A. H.-J., Quigley, G. J., Kolpak, F. J., Crawford, J. L., van Boom, J. H., van der Marel, G. & Rich, A. (1979) Molecular structure of a left-handed double helical DNA fragment at atomic resolution. *Nature (London)*, **282**, 680-686. 2dcg

21 Wilds, C. J., Pattanayek, R., Pan, C., Wawrzak, Z. & Egli, M. (2002). Selenium-assisted nucleic acid crystallography: use of phosphoroselenoates for MAD phasing of a DNA structure. *J. Am. Chem. Soc.* **124**, 14910-14916. 1vro

22 Coll, M., Wang, A. H-J., van der Marel, G. J., van Boom, J. H. & Rich A. (1986). Crystal structure of a Z-DNA fragment containing thymine/2-aminiadenine base-pairs. *J. Biomol. Struct. Dyn.* **4**, 157-172. 1vty

23 Sanishvili, R., Besnard, C., Camus, F., Fleurant, M., Pattison, P., Bricogne, G. & Schiltz, M. (2007). Polarization-dependence of anomalous scattering in brominated DNA and RNA molecules, and importance of crystal orientation in single- and multiple-wavelength anomalous diffraction phasing. *J. Appl. Cryst.* **40**, 552-558. 2obz

24 Ohishi, H., Nakanishi, I., Inubushi, K., van der Marel, G., van Boom, J. H., Rich, A., Wang, A. H.-J., Hakoshima, T. & Tomita, K.-I. (1996) Interaction between the left-handed Z-DNA and polyamine-2. The crystal structure of the $d(CG)_3$ and spermidine complex. *FEBS Lett.* **391**, 153-156. 293d

25 Ohishi, H., Terasoma, N., Nakanishi, I., van der Marel, G., van Boom, J. H., Rich, A., Wang, A. H.-J., Hakoshima, T. & Tomita, K.-I. (1996). Interaction between the left-handed Z-DNA and polyamine-3. The crystal structure of the $d(CG)_3$ and thermospermine complex. *FEBS Lett.* **398**, 291-296. 336d

26 Fenn, T. D., Schnieders, M. J., Mustyakimov, M., Wu, C., Langan, P., Pande, V. S. & Brunger, A. T. (2011). Reintroducing electrostatics into macromolecular crystallographic refinement: application to neutron crystallography and DNA hydration. *Structure* **19**, 523-533. 3qba

27 Pan, B. & Sundaralingam, M. (2003). Crystal structure of rGd(CGCGCG): a Z-DNA hexamer duplex with a 5'-(rG) overhang. *Acta Cryst.* D**59**, 433-437. 1m6r

28 Ho, P. S., Frederick, C. A., Quigley, G. J., van der Marel, G., van Boom, J. H., Wang, A., H-J. & Rich, A. (1985). G-T wobble base-pairing Z-DNA at 1.0 Å atomic resolution: the crystal structure of d(CGCGTG). *EMBO J.* **4**, 3617-362. 1vtt

29 Coll, M., Saal, D., Frederick, C. A., Ayumami, J., Rich, A. & Wang, A. H-J. (1989). Effects of 5-fluorouracil/guanine wobble base pairs in Z-DNA: molecular and crystal structure of d(CGCGFG). *Nucleic Acids Res.* **17**, 911-923. 1dnf

30 Brown, T., Kneale, G., Hunter, W. N. * Kennard, O. (1986). Structural characterization of the bromouracil.guanine base pair mismatch in a Z-DNA fragment. *Nucleic Acids Res.* **14**, 1801-1809. 1da1

31 Schuerman, G. S., Van Meervelt, L., Loakes, D., Brown, D. M., Lin, P. K. T., Moore, M. H. & Salisbury, S. A. (1998). A thymine-like base analogue forms wobble pairs with adenine in a Z-DNA duplex. *J. Mol. Biol.* **282**, 1005-1011. 417d

32 Thiyagarajan. S., Rajan, S. s. & Gautham. N. (2004). Cobalt hexammine induced tautomeric shift in the structure of d(CGCGCA).d(TGCGCG) in two crystal forms. *Nucleic Acids Res.* **32**, 5945-5953. 1xa2 1xam

33 Bharanidharan, D., Thiyagarajan, S. & Gautham, N. (2007). Hexaammineruthenium(III) ion interactions with Z-DNA. *Acta Cryst.* F**63**, 1008-1013. 2hto 2htt

34 Sadasivan, C & Gautham, N. (1995). Sequence-dependent microhetgerogeneityof Z-DNA: the crystal and molecular structures of d(CACGCG).d(CGCGTG) and d(CGCACG).d(CGTGCG). *J. Mol. Biol.* **248**, 918-930. 180d, 181d

35 Karthe, P. & Gautham, N. (1998). Structure of d(CACGCG).d(CGCGTG) in crystals grown in the presence of ruthenium^{III} hexammine chloride. *Acta Cryst.* D**54**, 501-509. 351d

36 Kagawa, T. F., Geierstanger, B. H., Wang, A. H-J. & Ho, P. S. (1991). Covalent modification of guanine bases in double-stranded DNA. *J. Biol. Chem.* **266**, 20175-20184. 1d39

37 Fujii, s., Wang, A. H-J., van der Marel, G., van Boom, J. H. & Rich, a. (1982). Molecular structure of $(m^5dC\text{-}dG)_3$: the role of the methyl group on 5-methyl cytosine in stabilizing Z-DNA. *Nucleic Acids Res.* **10**, 7879-7892. 1vtv

38 Chevrier, B., Dock, A. C., Hartmann, B., Leng, M., Moras, D., Thuong, M. T. & Westhof, E. (1986). Solvation of the left-handed hexamer d(5BrC-G-5BrC-G-5BrC-G) in crystals grown at two temperatures. *J. Mol. Biol.* **188**, 707-719. 1dn4 1dn5

39 Wang, a. H-J., Hakoshima, T., van der Marel, G., van Boom, J. H. & Rich, A. (1984). AT base pairs are less stable than CG base pairs in Z-DNA: the crystal structure of d(m^5CGTAm^5CG). *Cell* **37**, 321-331. 1vtw

40 Geierstanger, B. H., Kagawa, T. F., Chen, S.-L., Quigley, G. J. & Ho, P. S. (1991). Base-specfic binding of copper(II) to Z-DNA. *J. Biol. Chem.* **266**, 20185-20191. 1d40

41 Zhou, G. & Ho, P. S. (1990). Stabilization of Z-DNA by demethylation of thymine bases: 1.3- Å single-crystal structure of d(m5CGUAm5CG). *Biochemistry* **29**, 7229-7236. 1d41

42 Ginell, s. L., Kuzmich, S., Jones, R. A. & Berman, H. M. (1990). Crystal and molecular structure of a DN A duplex containing the carcinogen ic lesion O6-methylguanine. *Biochemistry* **29**, 10461-10465. 1d24

43 Schneider, B., Ginell, S. L., Jones, R., Gaffney, B. & Berman, H. M. (1992). Crystal and molecular structure of a DNA fragment containing a 2-aminoadenine modification: the relationship between conformation, packing and hydration in Z-DNA hexamers. *Biochemistry* **31**, 9622-9628. 1d76

44 Schroth, G. P., Kagawa, T. F. & Ho, P. S. (1993). Structure and thermodynamics of nonalternating C-G base pairs in Z-DNA: the 1.3 Å crystal structure of the asymmetric hexanucleotide d(m^5CGGGm^5CG).d(m^5CGCCm^5CG). *Biochemistry* **32**, 13381-13392. 145d

45 Eichman, B. F., Schroth, G. P., Basham, B. E. & Ho, P. S. (1999). The intrinsic structure and stability of out-of-alternation base pairs in Z-DNA. *Nucleic Acids Res.* **27**, 543-550. 400d

46 Cervi, A., Guy, A., Leonard, G. A., Teoule, R. & Hunter, W. N. (1993). The crystal structure of N^4-methylcytosine.guanosine base-pairs in the synthetic hexanucleotide d(CGCGm^4CG). *Nucleic Acids Res.* **21**, 5623-5629. 133d

47 Peterson, M. R., Harrop, S. J., McSweeney, S. M., Leonard, G. A., Thompson, A. W., Hunter, W. N. & Helliwell, J. R. (1996). MAD phasing strategies explored with a brominated oligonucleotide crystal at 1.65 Å resolution. *J. Synchrotron Rad.* **3**, 24-34. 242d

48 Karthe, P., Krishnaswamy, S & Gautham, N. (1996). Potentially right-handed sequence crystallizes as left-handed DNA: the crystal structure of d(CCCGGG). *Acta Cryst.* A**52**, C149, abstr. PS04.04.14. 239d

49 Mooers, B. H. M., Eichman, B. F. & Ho, P. S. (1997). The structures and relative stabilities of d(G.G) reverse Hoogsten, d(G.T) reverse wobble, and d(G.C) Watson-Crick base-pairs in DNA crystals. *J. Mol. Biol.* **269**, 796-810. 312d 313d 314d

50 Pan, B., Ban, C. Wahl, M. C. & Sundaralingam, M. (1997). Crystal structure of d(CGCGC) with 5'-ovverhang G residues. *Biophys J.* **73**, 1553-1561. 331d

51 Mandal, P. K., Chandrasekaran. A. R., Madhanagopal, B. R., Venkadesh, S. & Gautham, N. (2012). Ring crystals of oligonucleotides: growth stages and X-ray diffraction studies. *J. Cryst. Growth* **354**, 20-26. 3um4 3ulm 3uln 3ulo

52 Brennan, R. G., Westhof, E. & Sundaralingam, M. (1986). *J. Biomol. Struct. Dyn.* **3**, 649-665. 1dn8

53 Ban, C., Ramakrishnan, B. & Sundaralingam, M. (1996). Crystal structure of the self-complimentary 5'-purine start decamer d(CGCGCGCGCG) in the Z-DNA conformation. I. *Biophys. J.* **71**, 1215-1221. 279d

54 Westhof, E., Hosur, M. V. & Sundaralingam, M. (1988). Nonintercalative binding of proflavin to Z-DNA: structure of a complex between d(5BrC-G-5BrC-G) and proflavin. *Biochemistry* **27**, 5742-5747. 1vtf

55 Crawford, . L., Kolpak, F. J., Wang, A. H-J., Quigley, G. J., van Boom, J. H., van der Marel, G. & Rich, A. (1980). The tetramer d(CpGpCpG) crystallikzes as a left-handed double helix. *Proc. Natl. Acad. Sci. USA* **77**, 4016-4020. 1vts

56 Kumar, V. D., Harrison, R. W., Andrews, L. C. & Weber, I. T. (1992). Crystal structure at 1.5-Å resolution of d(CGCICICG), an octanucleotide containing inosine, and its comparison with d(CGCG) and d(CGCGCG) structures. *Biochemistry* **31**, 1541-1550. 1d53

57 Mandal, P. K., Venkadesh, S. & Gautham, N. (2012). Interactions of Mn^{2+} with a non-self-complementary Z-type DNA duplex. *Acta Cryst.* F**68**, 1420-1426. 4dwy 4dy8

58 Malinina, L., Tereshko, V., Ivanova, E., Subirana, J. A., Zarytova, V. & Nekrasov, Y. (1998). Structural variability and new intermolecular interactions of Z-DNA in crystals of d(pCpGpCpGpCpG). *Biophys. J.* **74**, 2482-2490. 390d 391d 392d

59 Drew, H. R. & Dickerson, R. E. (1980). Conformation and dynamics in a Z-DNA tetramer. *J. Mol. Biol.* **152**, 723-736. 1zna

60 Venkadesh, S., Mandal, P. K. & Gautham, N. (2009). The structure of d(CACACG).d(CGTGTG). *Acta Cryst.* F**65**, 8-13. 3e9w

61 Parkinson, G. N., Arvanitis, G. M., Lessinger, L., Ginell, S. L., Jones, R., Gaffney, B. & Berman, H. M. (1995). Crystal and molecular structure of a new Z-DNA crystal form: d[CGT(2-NH_2-A)CG] and its platinated derivative. *Biochemistry* **34**, 15487-15495. 210d 211d

62 Zhang, H., van der Marel, G., van Boom, J. H. & Wang, A. H-J. (1992). Conformational perturbation of the anticancer nucleoside arabinosylcytosine on Z-DNA: molecular structure of (araC-dG)$_3$ at 1.3 Å resolution. *Biopolymers* **32**, 1559-1569. zdfs33

63 Doi, M., Inoue, M., Tomoo, K., Ishida, T., Ueda, Y., Akagi, M. & Urata, H. (1993). Structural characteristics o enantiomorphic DNA: crystal analysis of racemates of the d(CGCGCG). *J. Am. Chem. Soc.* **115**, 10432-10433. 1vtu

64 Pallan, P. S., Marquez, V. E. & Egli, M. (2012). The conformationally constrained N-methanocarba-dT analogue adopts an un expected C4'-exo sugar pucker in the structure of DNA hairpin. *Biochemistry* **51**, 2639-2641. 4dkz

65 Atwell, S., Meggers, E., Spraggon, G. & Schultz, P. G. (2001). Structure of a copper-mediated base pair in DNA. *J. Am. Chem. Soc.* **123**, 12364-12367. 1jes

66 Malinina, L., Urpi, L., Salas, X., Huynh-Dinh, T. & Subirana, J. A. (1994). Recombination-like structure of d(CCGCGG). *J. Mol. Biol.* **243**, 484-493. 192d

67 Chattopadhyaya, R., Grzeskowiak, K. & Dickerson, R. E. (1990). Structure of a T_4 hairpin loop on Z-DNA stem and comparison with A-RNA and B-DNA loops. *J. Mol. Biol.* **211**, 189-210. 1d16