coordination site. The U—Cl bond length of 2.621 (1) Å is in agreement with U—Cl distances observed in other chloroindenyl complexes {2.593 (3) Å in $[U(C_9H_7)_3Cl]$ (Burns & Laubereau, 1971), 2.609 (2) Å in $[U(C_9H_7)Cl_3].2C_4H_8O$ (Rebizant, Spirlet & Goffart, 1983), 2.601 (3) Å in $[U(C_{12}H_{13})_3Cl]$ (Meunier-Piret & Van Meerssche, 1984)}. Significant differences in U—C distances are observed to each indenyl ligand. The shortest distances correspond in each case to the bond towards the non-methyl-substituted C atom [C(3), C(12) and C(21)]. Moreover, the angles subtended at the U atoms (Table 2) show that the non-methyl-substituted C atoms occupy, with the Cl atom, the sites of a regular tetrahedron. These geometrical features would indicate a monohapto mode of bonding of the indenyl rings. This mode of bonding would probably result from both electronic and steric factors. Indeed, most short intramolecular contacts* involve the methyl-substituted C atoms of the five-membered portion of the indenyl rings. The results of least-squares-plane calculations* show that the five- and six-membered portions of the indenyl rings are almost planar (within 6 e.s.d.'s), although each indenyl ring as a whole exhibits significant deviations from planarity. Bendings of 7.0 (12), 9.8 (9) and 7.2 (7)°, respectively, for the three indenyl ligands are observed between the five- and six-membered-ring portions. These bendings are probably induced by steric crowding on the coordination sphere of the U atom. Moreover, some of the methyl groups are planar with the rings to which they belong, some are not; the largest displacement is 0.265 (8) Å for C(7').

* See deposition footnote.

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Structure of Barium Guanosine 5′-Monophosphate

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(*Received* 30 *September* 1991; *accepted* 24 *December* 1991)

Abstract. $2Ba^{2+}.2C_{10}H_{10}N_5O_8P^{2-}.12H_2O$, M_r = 1209.22, orthorhombic, $P2_12_12_1$, a = 21.37 (2), b = 22.04 (1), c = 8.66 (1) Å, V = 4076 (1) Å^3, Z = 4, D_x = 1.970 g cm^{-3}, λ(Mo $K\alpha$) = 0.71069 Å, μ = 21.01 cm^{-1}, $F(000)$ = 2400, T = 296 K, R = 0.061 for 2602 observed reflections [$I > 3.0\sigma(I)$]. Two each of barium and guanosine 5′-monophosphate make up the asymmetric unit. Each Ba ion has nine ligands which include the N(7) of each guanosine, sugar hydroxyls, a phosphate O atom, water molecules and bridging water molecules. The guanosines have *anti* glycosidic torsional angles and C(2′)-*endo* sugar

0108-2701/92/071223-05$06.00

puckers. The guanosines are packed in columns with a channel of coordinated Ba ions through the crystal. There is no base–base stacking and no base–base hydrogen bonding.

Introduction. The ability of guanine and its derivatives to self-associate has been recognized for many years. However, evidence that guanine self-association may have a functional role *in vivo* is relatively recent. Unusual four-stranded structures formed by telomeric DNA sequences (consisting of tracts of guanines) are stabilized by metals such as K and Na, presumably because the metal can coordinate to the O6 of the guanine bases in the centre of the channel formed by stacked guanine tetrads [see reviews by Guschlbauer, Chantot & Thiele (1990) and Sundquist (1991)]. Other metals with similar ionic radii, such as Ba, also stabilize the formation of these unusual structures. Guanosine gels can be formed with guanosine 5′-monophosphate (5′-GMP) and Ba; the crystals analyzed here appeared under conditions resembling those used for tetrad formation with other metals. The structure reported here illustrates barium–guanosine coordination, but there is no evidence of guanine self-association.

Experimental. Crystals of barium guanosine 5′-monophosphate were obtained as follows. A precipitate was prepared by the addition of equal volumes of a 0.1*M* solution of guanosine 5′-monophosphate disodium salt (Sigma G-8377) and 0.1*M* barium chloride (Aldrich 20,273-8) solution. The recovered precipitate was mixed with 0.5 ml of water and heated at 323 K for 15 h and then cooled slowly to 293 K to produce large rectangular crystals. The crystal density was not measured. A colourless block crystal of Ba-5′-GMP having approximate dimensions 0.20 × 0.18 × 0.08 mm (cleaved from a larger crystal) was mounted in a sealed glass capillary with mother liquor.

Measurements were made on a Rigaku AFC-6*S* diffractometer at 296 K with graphite-monochromated Mo $K\alpha$ radiation; lattice parameters from the setting angles of 21 reflections in the range $7.07 < 2\theta < 12.66°$; ω–2θ scans; maximum $2\theta = 50.0°$ ($0 \le h \le 25$, $0 \le k \le 26$, $0 \le l \le 10$); scan width $(0.84 + 0.30\tan\theta)°$; scan speed 4.0° min^{-1} (in ω); weak reflections [$I < 10.0\sigma(I)$] rescanned (maximum of two rescans). 4077 reflections were collected of which 4071 unique reflections were accessible in the resolution range ($R_{int} = 0.063$), with 2602 considered observed [$I > 3.0\sigma(I)$]. The orthorhombic cell was $P2_12_12_1$ based on systematic absences of $h00$: $h \neq 2n$, $0k0$: $k \neq 2n$, $00l$: $l \neq 2n$. Intensities of three standard reflections measured after every 150 reflections declined by 5.3% and a linear correction factor was applied to the data to account for this phenomenon. An empirical absorption correction was applied using the program *DIFABS* (Walker & Stuart, 1983), which resulted in calculated transmission factors ranging from 0.90 to 1.18. Lorentz and polarization corrections were applied as well as a correction for secondary extinction (coefficient = 0.16288×10^{-6}]. Ba atoms were found using the Patterson method (Sheldrick, 1985). Other non-H atoms were found in successive difference Fourier maps. Non-H atoms were refined either anisotropically or isotropically and some H atoms were fixed in calculated positions. Full-matrix least-squares refinement of 400 parameters minimized the function $\sum w(|F_o| - |F_c|)^2$, where $w = 4F_o^2/\sigma^2(F_o^2)$, $\sigma^2(F_o^2) = [S^2(C + R^2B) + (pF_o^2)^2]/\mathrm{Lp}^2$ (S = scan rate, C = total integrated peak count, R = ratio of scan time to background counting time, B = total background count, Lp = Lorentz–polarization factor and $p = 0.03$). When the structure had been refined to convergence, it was observed that 34 of the strongest reflections had very poor agreements. The raw data revealed that these reflections had extremley asymmetric backgrounds, causing gross inaccuracies. Laue photography revealed that some of the strongest peaks were misshapen, with 'tails', which probably explained the asymmetric backgrounds. These reflections were therefore omitted from the data. Final $R = 0.061$, $wR = 0.072$, maximum $\Delta/\sigma = 0.14$ and $S = 1.88$. The maximum and minimum peaks on the final difference Fourier map corresponded to 0.99 and -1.05 e Å^{-3}, respectively. Neutral-atom scattering factors were used (Cromer & Waber, 1974). Anomalous-dispersion effects were included in F_{calc} (Ibers & Hamilton, 1964), as well as values for f' and f'' (Cromer & Waber, 1974). All calculations were performed using the *TEXSAN* crystallographic software package (Molecular Structure Corporation, 1985). Figs. 1 and 2 were drawn using *PLUTO* (Motherwell & Clegg, 1978) and *ORTEP*II (Johnson, 1976), respectively.

Discussion. The molecular structure and labelling of Ba-5′-GMP are shown in Fig. 1(*a*). The atomic coordinates and B_{eq} values are listed in Table 1* and bond lengths and angles in Table 2. The two molecules of guanosine 5′-monophosphate (*A* and *B*) in the asymmetric unit are related by a pseudo-twofold rotation axis parallel to *x*, and therefore they have similar but not identical structures. The mean deviation from planarity of the guanine bases is 0.018 (*A*) and 0.019 Å (*B*). The angles between the

* Lists of structure factors, anisotropic thermal parameters, complete geometry, H-atom parameters and least-squares-planes data have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 55065 (55 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England. [CIF reference: SE0083]

base planes is 35.3° so the bases are not stacked, and there are no base–base hydrogen bonds. In order to illustrate the differences between the structures of the two guanosines, the nucleoside torsional angles (Seeman, Rosenberg, Suddath, Kim & Rich, 1976) and ribose pseudo-rotation parameters (Altona & Sundaralingam, 1972) are shown in Table 2. The orientation between the base and ribose, the glycosidic torsional angle (χ), for both guanosines is *anti*. The ribose conformation is C2′-*endo* with pseudo-rotation phase angles of 166.7 (*A*) and 153.3° (*B*). The sugar pucker is C(2′)-*endo* for both sugars but they have different amplitudes of 18.5 (*A*) and 30.2° (*B*). Rotation about the exocyclic C(4′)—C(5′) bond is (+) *gauche* for both guanosines. These conformations are commonly observed in other guanine mononucleotide structures (Katti, Seshadri & Viswamitra, 1981; Saenger, 1984).

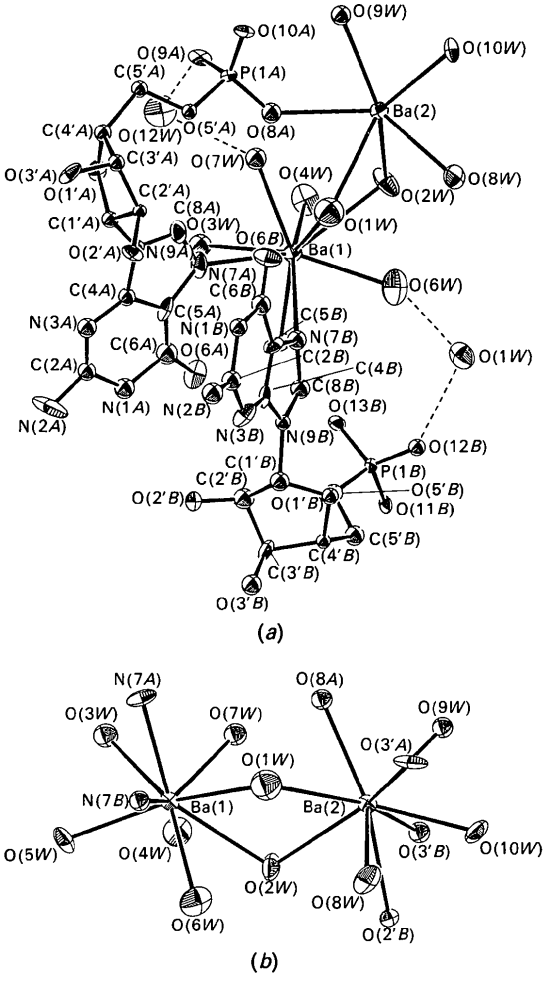

Fig. 1. *ORTEP*II (Johnson, 1976) drawings of (*a*) molecular conformation and atom numbering of Ba-5′-GMP (the dashed lines indicate intramolecular hydrogen bonds or close contacts) and (*b*) the coordination of the two Ba ions.

Table 1. *Positional parameters and equivalent isotropic thermal parameters* (Å^2) *for the non*-H *atoms*

$B_{eq} = (8\pi^2/3)\sum_i\sum_j U_{ij} a_i^* a_j^* \mathbf{a}_i.\mathbf{a}_j$.

	x	*y*	*z*	B_{eq}
Molecule *A*				
Ba(1)	0.10833 (6)	0.23553 (7)	0.2382 (2)	1.75 (6)
P(1)	0.1340 (3)	0.4616 (3)	0.5672 (7)	1.6 (3)
O(1′)	0.3075 (7)	0.379 (1)	0.669 (2)	2.3 (8)
O(2′)	0.3985 (7)	0.4127 (8)	0.329 (2)	1.9 (7)
O(3′)	0.4110 (7)	0.476 (1)	0.593 (2)	3.0 (1)
O(5′)	0.2082 (7)	0.4543 (7)	0.556 (2)	1.2 (3)
O(6)	0.2585 (8)	0.1272 (7)	0.236 (2)	2.8 (8)
O(8)	0.1111 (8)	0.4287 (8)	0.425 (2)	2.1 (3)
O(9)	0.1156 (7)	0.4284 (7)	0.714 (2)	2.1 (7)
O(10)	0.1194 (7)	0.5299 (8)	0.575 (2)	1.8 (7)
N(1)	0.358 (1)	0.147 (1)	0.312 (2)	2.2 (4)
N(2)	0.461 (1)	0.158 (1)	0.390 (4)	5.0 (2)
N(3)	0.392 (1)	0.234 (1)	0.438 (2)	2.0 (3)
N(7)	0.2301 (9)	0.259 (1)	0.358 (2)	3.0 (1)
N(9)	0.3094 (8)	0.3116 (9)	0.464 (2)	1.2 (3)
C(1′)	0.340 (1)	0.361 (1)	0.532 (3)	1.5 (4)
C(2)	0.402 (1)	0.183 (1)	0.385 (3)	1.7 (5)
C(2′)	0.344 (1)	0.416 (1)	0.428 (2)	1.0 (4)
C(3′)	0.349 (1)	0.469 (1)	0.543 (3)	1.5 (4)
C(4)	0.332 (1)	0.253 (1)	0.422 (3)	1.6 (4)
C(4′)	0.311 (1)	0.446 (1)	0.675 (2)	1.5 (4)
C(5)	0.286 (1)	0.223 (1)	0.351 (2)	2.0 (1)
C(5′)	0.244 (1)	0.471 (1)	0.693 (3)	1.5 (4)
C(6)	0.294 (1)	0.169 (1)	0.296 (3)	2.6 (5)
C(8)	0.249 (1)	0.309 (1)	0.429 (3)	3.0 (1)
Molecule *B*				
Ba(2)	0.00976 (6)	0.43552 (7)	0.2137 (2)	1.59 (6)
P(1)	0.1217 (2)	0.0290 (3)	−0.2328 (7)	1.3 (2)
O(1′)	0.2741 (7)	0.1297 (8)	−0.362 (2)	1.5 (3)
O(2′)	0.3858 (7)	0.0966 (7)	−0.070 (2)	1.5 (7)
O(3′)	0.3946 (8)	0.0530 (8)	−0.357 (2)	2.1 (3)
O(5′)	0.1968 (6)	0.0370 (7)	−0.246 (2)	1.9 (3)
O(6)	0.2430 (8)	0.3734 (9)	0.103 (2)	3.0 (1)
O(11)	0.1058 (7)	−0.0340 (7)	−0.289 (2)	2.0 (7)
O(12)	0.0930 (6)	0.0774 (7)	−0.331 (2)	1.5 (3)
O(13)	0.1090 (8)	0.0345 (8)	−0.058 (2)	1.9 (7)
N(1)	0.339 (1)	0.357 (1)	−0.007 (2)	1.6 (4)
N(2)	0.435 (1)	0.351 (1)	−0.127 (2)	2.5 (4)
N(3)	0.367 (1)	0.269 (1)	−0.147 (2)	3.0 (1)
N(7)	0.2103 (9)	0.243 (1)	−0.013 (2)	1.9 (4)
N(9)	0.2842 (8)	0.1968 (9)	−0.154 (2)	1.2 (3)
C(1′)	0.317 (1)	0.145 (1)	−0.244 (3)	1.9 (4)
C(2)	0.380 (1)	0.322 (1)	−0.094 (3)	2.0 (5)
C(2′)	0.331 (1)	0.092 (1)	−0.155 (3)	2.3 (5)
C(3′)	0.334 (1)	0.044 (1)	−0.281 (3)	3.0 (1)
C(4)	0.310 (1)	0.247 (1)	−0.109 (2)	1.0 (1)
C(4′)	0.285 (1)	0.067 (1)	−0.395 (2)	1.1 (4)
C(5)	0.263 (1)	0.276 (1)	−0.022 (3)	2.0 (1)
C(5′)	0.223 (1)	0.032 (1)	−0.397 (3)	2.1 (5)
C(6)	0.277 (1)	0.339 (1)	0.033 (3)	2.1 (5)
C(8)	0.225 (1)	0.193 (1)	−0.089 (3)	2.0 (5)
Water molecules				
O(1*W*)	0.119 (1)	0.360 (1)	0.127 (3)	4.8 (5)
O(2*W*)	−0.0136 (8)	0.3049 (8)	0.169 (2)	4.0 (1)
O(3*W*)	0.1413 (8)	0.174 (1)	0.516 (2)	2.8 (4)
O(4*W*)	0.003 (1)	0.198 (1)	0.409 (2)	4.0 (1)
O(5*W*)	0.1318 (9)	0.1157 (8)	0.169 (2)	3.0 (1)
O(6*W*)	0.053 (1)	0.240 (1)	−0.056 (2)	4.0 (1)
O(7*W*)	0.0880 (8)	0.3104 (9)	0.479 (2)	2.4 (4)
O(8*W*)	0.0128 (9)	0.434 (1)	−0.108 (2)	4.0 (1)
O(9*W*)	0.0060 (8)	0.5283 (8)	0.434 (2)	2.1 (3)
O(10*W*)	−0.0483 (8)	0.543 (1)	0.105 (2)	3.0 (1)
O(11*W*)	0.0048 (8)	0.1588 (8)	−0.290 (2)	3.7 (9)
O(12*W*)	0.131 (1)	0.317 (1)	0.784 (3)	5.0 (1)

The environment of the Ba ions is illustrated in Fig. 1(*b*). Ba(1) binds to the N7 of each guanine base and to seven water molecules, two of which, O(*W*1) and O(*W*2), also bind to Ba(2); Ba(2) binds to a phosphate O atom of guanosine *A*, to the sugar hydroxyls O(2′*A*), O(2′*B*) and O(3′*B*), and to three water molecules. The Ba—O and Ba—N distances

are in the range 2.69–3.08 Å which is consistent with those expected for a nine-coordinate Ba ion. Such a coordination of Ba is different from that found in the other barium–nucleotide structures. For example, the Ba ion in the barium adenosine-5′-monophosphate heptahydrate structure (Ba-5′-AMP) (Sternglanz, Subramanian, Lacey & Bugg, 1976) has a hydration shell of eight water molecules and has no direct contacts with the nucleoside or phosphate at all. In the barium uridine-5′-monophosphate structure (Ba-5′-UMP) (Shefter & Trueblood, 1965), which more closely resembles the Ba-5′-GMP structure, the coordination number is ten. In this case the Ba ion has two more distant (*ca* 3.3 Å) and eight closer neighbours including the uridine O(2) and sugar hydroxyls. The Ba-5′-GMP structure is the only one of the three barium–nucleotide structures where there is direct barium–phosphate-O-atom coordination in addition to indirect coordination of the phosphate O atoms.

Since H atoms were not located in this structure, the interatomic distances shown in Table 3 were used to infer possible hydrogen bonds and intermolecular contacts. Of the 12 water molecules in the asymmetric unit, two bind to both Ba ions forming 'bridges', and eight bind to a single Ba ion and appear also to be hydrogen bonded to at least one O or N atom. The two remaining water molecules are

Table 2. *Intramolecular bond lengths* (Å) *and bond angles* (°) *for the non*-H *atoms and torsion angles* (°) *and ribose pseudo-rotation parameters for the guanosines*

Ba(1)—N(7*A*)	2.85 (2)	Ba(2)—O(2′*B*)	3.01 (2)
Ba(1)—N(7*B*)	3.08 (2)	Ba(2)—O(3′*A*)	2.79 (2)
Ba(1)—O(1*W*)	2.92 (2)	Ba(2)—O(3′*B*)	2.77 (2)
Ba(1)—O(2*W*)	3.08 (2)	Ba(2)—O(8*A*)	2.84 (2)
Ba(1)—O(3*W*)	2.84 (2)	Ba(2)—O(1*W*)	2.97 (2)
Ba(1)—O(4*W*)	2.82 (2)	Ba(2)—O(2*W*)	2.95 (2)
Ba(1)—O(5*W*)	2.75 (2)	Ba(2)—O(8*W*)	2.78 (2)
Ba(1)—O(6*W*)	2.81 (2)	Ba(2)—O(9*W*)	2.80 (2)
Ba(1)—O(7*W*)	2.69 (2)	Ba(2)—O(10*W*)	2.83 (2)
P(1*A*)—O(5′*A*)	1.60 (2)	P(1*B*)—O(5′*B*)	1.62 (1)
P(1*A*)—O(8*A*)	1.51 (2)	P(1*B*)—O(11*B*)	1.51 (2)
P(1*A*)—O(9*A*)	1.52 (2)	P(1*B*)—O(12*B*)	1.49 (2)
P(1*A*)—O(10*A*)	1.54 (2)	P(1*B*)—O(13*B*)	1.54 (2)

	Molecule *A*	Molecule *B*
O(1′)—C(1′)	1.43 (3)	1.41 (3)
O(1′)—C(4′)	1.48 (3)	1.44 (3)
O(2′)—C(2′)	1.45 (2)	1.39 (3)
O(3′)—C(3′)	1.41 (3)	1.47 (3)
O(5′)—C(5′)	1.45 (3)	1.43 (3)
O(6)—C(6)	1.29 (3)	1.22 (3)
N(1)—C(2)	1.38 (3)	1.39 (3)
N(1)—C(6)	1.47 (3)	1.42 (3)
N(2)—C(2)	1.36 (3)	1.36 (3)
N(3)—C(2)	1.25 (3)	1.29 (3)
N(3)—C(4)	1.34 (3)	1.36 (3)
N(7)—C(5)	1.43 (3)	1.34 (3)
N(7)—C(8)	1.33 (4)	1.33 (3)
N(9)—C(1′)	1.39 (3)	1.55 (3)
N(9)—C(4)	1.43 (3)	1.30 (3)
N(9)—C(8)	1.33 (3)	1.39 (3)
C(1′)—C(2′)	1.52 (3)	1.44 (3)
C(2′)—C(3′)	1.52 (3)	1.52 (3)
C(3′)—C(4′)	1.49 (3)	1.52 (3)
C(4)—C(5)	1.34 (3)	1.39 (3)
C(4′)—C(5′)	1.54 (3)	1.54 (3)
C(5)—C(6)	1.30 (4)	1.49 (4)

O(1*W*)—Ba(1)—N(7*A*)	82.9 (7)	O(1*W*)—Ba(2)—O(2′*B*)	117.3 (5)
O(1*W*)—Ba(1)—N(7*B*)	70.0 (6)	O(1*W*)—Ba(2)—O(3′*A*)	79.6 (6)
O(2*W*)—Ba(1)—N(7*A*)	139.0 (6)	O(1*W*)—Ba(2)—O(3′*B*)	150.0 (6)
O(2*W*)—Ba(1)—N(7*B*)	115.7 (5)	O(1*W*)—Ba(2)—O(8*A*)	62.0 (5)
O(3*W*)—Ba(1)—N(7*A*)	63.3 (6)	O(2*W*)—Ba(2)—O(2′*B*)	64.3 (5)
O(3*W*)—Ba(1)—N(7*B*)	116.5 (5)	O(2*W*)—Ba(2)—O(3′*A*)	137.6 (6)
O(4*W*)—Ba(1)—N(7*A*)	126.2 (6)	O(2*W*)—Ba(2)—O(3′*B*)	89.8 (5)
O(4*W*)—Ba(1)—N(7*B*)	162.0 (6)	O(2*W*)—Ba(2)—O(8*A*)	99.3 (5)
O(5*W*)—Ba(1)—N(7*A*)	94.9 (7)	O(2′*B*)—Ba(2)—O(3′*A*)	123.0 (4)
O(5*W*)—Ba(1)—N(7*B*)	76.8 (6)	O(2′*B*)—Ba(2)—O(3′*B*)	54.8 (5)
O(6*W*)—Ba(1)—N(7*A*)	135.1 (6)	O(2′*B*)—Ba(2)—O(8*W*)	66.7 (5)
O(6*W*)—Ba(1)—N(7*B*)	69.9 (5)	O(2′*B*)—Ba(2)—O(8*A*)	157.7 (5)
O(7*W*)—Ba(1)—N(7*A*)	75.8 (6)	O(2′*B*)—Ba(2)—O(9*W*)	115.3 (4)
O(7*W*)—Ba(1)—N(7*B*)	128.7 (5)	O(2′*B*)—Ba(2)—O(10*W*)	70.9 (5)
N(7*A*)—Ba(1)—N(7*B*)	66.5 (6)	O(3′*A*)—Ba(2)—O(3′*B*)	130.0 (6)
Ba(1)—N(7*A*)—C(5*A*)	130 (2)	O(3′*A*)—Ba(2)—O(8*W*)	67.9 (6)
Ba(1)—N(7*A*)—C(8*A*)	126 (2)	O(3′*A*)—Ba(2)—O(8*A*)	79.3 (5)
Ba(1)—N(7*B*)—C(5*B*)	132 (2)	O(3′*A*)—Ba(2)—O(9*W*)	76.0 (5)
Ba(1)—N(7*B*)—C(8*B*)	118 (2)	O(3′*A*)—Ba(2)—O(10*W*)	63.7 (5)
Ba(1)—O(1*W*)—Ba(2)	112.3 (7)	O(3′*B*)—Ba(2)—O(8*W*)	118.0 (5)
Ba(1)—O(2*W*)—Ba(2)	108.4 (6)	O(3′*B*)—Ba(2)—O(8*A*)	113.3 (5)
O(5′*A*)—P(1*A*)—O(8*A*)	103.0 (9)	O(3′*B*)—Ba(2)—O(9*W*)	66.6 (5)
O(5′*B*)—P(1*B*)—O(11*B*)	107.5 (9)	O(3′*B*)—Ba(2)—O(10*W*)	71.4 (5)
O(5′*A*)—P(1*A*)—O(9*A*)	105.0 (9)	O(8*W*)—Ba(2)—O(8*A*)	128.7 (5)
O(5′*B*)—P(1*B*)—O(12*B*)	107.0 (9)	O(8*A*)—Ba(2)—O(9*W*)	67.8 (5)
O(5′*A*)—P(1*A*)—O(10*A*)	107.7 (9)	O(8*A*)—Ba(2)—O(10*W*)	126.5 (5)
O(5′*B*)—P(1*B*)—O(13*B*)	103.5 (9)	Ba(2)—O(2′*B*)—C(2′*B*)	121 (1)
O(8*A*)—P(1*A*)—O(9*A*)	111.5 (9)	Ba(2)—O(3′*A*)—C(3′*A*)	140 (2)
O(11*B*)—P(1*B*)—O(12*B*)	112.3 (9)	Ba(2)—O(3′*B*)—C(3′*B*)	127 (1)
O(8*A*)—P(1*A*)—O(10*A*)	116 (1)	Ba(2)—O(8*A*)—P(1*A*)	138 (1)
O(11*B*)—P(1*B*)—O(13*B*)	110 (1)	O(9*A*)—P(1*A*)—O(10*A*)	112.5 (9)
O(12*B*)—P(1*B*)—O(13*B*)	115.4 (9)		

Table 2 (*cont.*)

	Molecule *A*	Molecule *B*
C(2)—N(1)—C(6)	120 (2)	125 (2)
C(2)—N(3)—C(4)	114 (2)	115 (2)
C(5)—N(7)—C(8)	103 (2)	103 (2)
C(4)—N(9)—C(8)	104 (2)	109 (2)
N(1)—C(2)—N(2)	114 (2)	115 (2)
N(1)—C(2)—N(3)	125 (2)	124 (2)
N(2)—C(2)—N(3)	121 (2)	122 (2)
N(3)—C(4)—N(9)	125 (2)	127 (2)
N(3)—C(4)—C(5)	127 (2)	128 (2)
N(9)—C(4)—C(5)	108 (2)	104 (2)
C(4)—C(5)—C(6)	122 (3)	117 (2)
N(7)—C(5)—C(4)	109 (2)	113 (2)
N(7)—C(5)—C(6)	129 (2)	130 (2)
O(6)—C(6)—N(1)	111 (2)	120 (3)
O(6)—C(6)—C(5)	137 (3)	129 (3)
N(1)—C(6)—C(5)	113 (2)	111 (2)
N(7)—C(8)—N(9)	116 (3)	111 (2)
C(1′)—N(9)—C(4)	130 (2)	126 (2)
C(1′)—N(9)—C(8)	126 (2)	124 (2)
O(1′)—C(1′)—N(9)	110 (2)	104 (2)
N(9)—C(1′)—C(2′)	114 (2)	116 (2)
P(1)—O(5′)—C(5′)	116 (1)	116 (1)
O(1′)—C(1′)—C(2′)	106 (2)	109 (2)
C(1′)—O(1′)—C(4′)	108 (2)	105 (2)
O(2′)—C(2′)—C(1′)	110 (2)	113 (2)
O(2′)—C(2′)—C(3′)	112 (2)	113 (2)
C(1′)—C(2′)—C(3′)	103 (2)	101 (2)
O(3′)—C(3′)—C(2′)	111 (2)	105 (2)
O(3′)—C(3′)—C(4′)	108 (2)	106 (2)
C(2′)—C(3′)—C(4′)	102 (2)	102 (2)
O(1′)—C(4′)—C(3′)	108 (2)	108 (2)
O(1′)—C(4′)—C(5′)	108 (2)	110 (2)
C(3′)—C(4′)—C(5′)	118 (2)	116 (2)
O(5′)—C(5′)—C(4′)	108 (2)	107 (2)

		Guanosine *A*	Guanosine *B*
χ	O(1′)—C(1′)—N(9)—C(4)	−125 (2)	−134 (2)
β	P(1)—O(1′)—C(5′)—C(4′)	166 (1)	157 (2)
δ	C(5′)—C(4′)—C(3′)—O(3′)	142 (2)	146 (2)
$\gamma(\varphi_{oc})$	O(5′)—C(5′)—C(4′)—C(3′)	61 (3)	60 (3)
ν_0	C(4′)—O(1′)—C(1′)—C(2′)	−18 (2)	−27 (2)
ν_1	O(1′)—C(1′)—C(2′)—C(3′)	32 (2)	39 (2)
ν_2	(C1′)—C(2′)—C(3′)—C(4′)	−33 (2)	−33 (2)
ν_3	C(2′)—C(3′)—C(4′)—O(1′)	23 (2)	19 (2)
ν_4	C(3′)—C(4′)—O(1′)—C(1′)	−3 (2)	4 (2)
P		167 (1)	153 (1)
ν_m		18.5	30.2
Conformational descriptor		2_E [C(2′)-*endo*]	2_E [C(2′)-*endo*]

Table 3. *Possible hydrogen bonds (distances in* Å)

$X\cdots Y$		Sym.	Trans.		$X\cdots Y$		Sym.	Trans.		
O(1*W*)···O(12*W*)	3.12 (3)	3	0	0−1	O(6*W*)···O(12*W*)	2.75 (3)	1	0	0−1
O(1′*A*)···N(1*B*)	2.93 (3)	1	0	0 1	O(6*W*)···O(11*W*)	2.77 (3)	1	1	0 1
O(1′*A*)···N(3*B*)	3.17 (3)	1	0	0 1	O(7*W*)···O(12*W*)	2.80 (3)	1	1	0 1
O(1′*B*)···O(3*W*)	3.19 (2)	1	0	0−1	O(7*W*)···N(2*A*)	3.03 (3)	3	−1	0 1
O(2′*A*)···O(11*W*)	2.81 (2)	3	0	0 0	O(8*W*)···O(9*A*)	2.69 (2)	1	0	0−1
O(2′*B*)···O(11*B*)	2.80 (2)	2	0	0 0	O(8*W*)···O(11*B*)	2.78 (2)	4	0	0−1
O(2′*B*)···O(8*W*)	3.19 (2)	3	0	0 0	O(9*W*)···O(13*B*)	2.69 (2)	4	0	0 0
O(3*W*)···O(12*B*)	2.72 (3)	1	0	0 1	O(9*W*)···N(2*B*)	3.00 (3)	2	0	1 0
O(3′*A*)···O(10*W*)	2.96 (2)	2	0	1 0	O(9*A*)···O(12*W*)	2.54 (3)	1	0	0 0
O(3′*A*)···O(8*W*)	3.11 (3)	2	0	1 0	O(10*W*)···O(12*B*)	2.67 (2)	4	0	0−1
O(3′*B*)···O(13*B*)	2.60 (2)	2	0	0−1	O(10*A*)···N(1*B*)	2.75 (3)	2	0	1 0
O(3′*B*)···O(9*W*)	2.60 (2)	3	0	0 0	O(11*W*)···O(12*B*)	2.66 (2)	1	0	0 0
O(3′*B*)···O(10*W*)	3.27 (3)	3	0	0 0	O(11*B*)···N(1*A*)	2.74 (3)	2	0	0−1
O(4*W*)···O(11*W*)	2.91 (3)	1	0	0 1	O(12*W*)···N(7*B*)	2.94 (3)	1	1	0−1
O(4*W*)···N(3*A*)	3.10 (3)	3	−1	0 1	O(13*B*···C(3′*B*)	3.19 (3)	2	0	0 0
O(5*W*)···O(10*W*)	3.10 (3)	4	0−1	0						

Sym. is the symmetry relation of Y to X as follows: (1) x, y, z; (2) $\frac{1}{2}-x, -y, \frac{1}{2}+z$; (3) $\frac{1}{2}+x, \frac{1}{2}-y, -z$; (4) $-x, \frac{1}{2}+y, \frac{1}{2}-z$. Trans. is the transalational relation of Y to X.

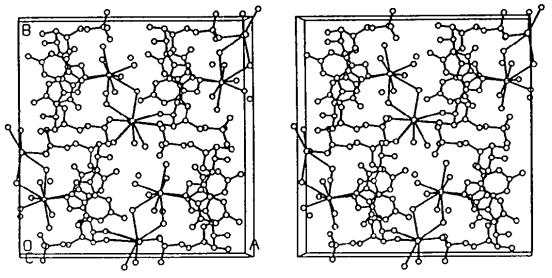

Fig. 2. A stereoscopic view along the z axis of the crystal packing of Ba-5′-GMP.

positioned so that there are four potential hydrogen bonds for each one. The water molecules and Ba ions form a network which extends throughout the crystal and separates continuous columns of guanosines. This arrangement is illustrated by the packing diagram in Fig. 2. Although there is no base–base stacking in the usual sense, there are extensive van der Waals contacts between guanosines in adjacent asymmetric units where the base of one guanosine *A* packs against the ribose of guanosine *B* and the ribose *A* packs against base *B*. The packing in this crystal resembles that seen in crystals of sodium-5′-GMP where the Na ions and water molecules form extended cages, except that here two nine-coordinate Ba ions take the place of four six-coordinate Na ions (Katti, Seshadri & Viswamitra, 1981; Barnes & Hawkinson, 1982).

Features that are normally associated with the formation of higher order nucleic acid structures (Kennard & Hunter, 1989; Guschlbauer, Chantot & Thiele, 1990; Sundquist, 1991), metal–base (O6) interactions and base–base interactions such as hydrogen bonding and base stacking, are not seen in this Ba-5′-GMP structure, but this is only the third example of a nucleotide–barium complex. The two other nucleotide–barium structures [Ba-5′-UMP (Shefter & Trueblood, 1965) and Ba-5′-AMP (Sternglanz, Subramanian, Lacey & Bugg, 1976)] are similar to the Ba-5′-GMP since they also consist of two nucleotides and two Ba ions bridged by two water molecules, but differ in the number of ligands and details of ligand binding to the Ba ions. However, the ligands used for metal coordination and crystal packing in this Ba-5′-GMP structure have been observed before in complexes of guanosine with other metals such as Na (Katti, Seshadri & Viswamitra, 1981; Barnes & Hawkinson, 1982). Interestingly, this single structure does illustrate all three of the main features of metal–nucleotide binding, metal–base (N7), metal–phosphate-O-atom and metal–ribose (hydroxyl) interactions, that are expected for complexes of nucleotides with alkaline-earth metals (Saenger, 1984).

We would like to thank P. Evans, K. Henrick, W. Hunter, A. Klug, P. McLaughlin and W. Sundquist for their advice and interest.

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