Fig. 5. Superposition of the molecules between successive layers. (a), (b) and (c) show stacking mode p in forms (I), (II) and (III), respectively, (d) shows q in form (II), and (e) shows r in form (III).

Table 5. *Torsion angles* (°) *for the hydroxyethyl group*

	Stacking	Molecule	τ_1	τ_2
Form (I)	p	A	94· (1)	174·6 (6)
Form (III)	p	F	98·1 (8)	175·3 (5)
Form (II)	q and p	B	88·1 (4)	171·9 (3)
		C	102·7 (4)	173·5 (3)
Form (III)	r and p	D	88·7 (8)	173·6 (6)
		E	100·8 (8)	173·8 (5)

τ_1: C(8)—N(9)—C(10)—C(11), τ_2: N(9)—C(10)—C(11)—O(12).

in form (I) and F in form (III) take the same stacking mode p at both sides of the molecular plane. On the other hand, the layer consisting of molecules B and C in form (II) and that containing D and E in form (III) have different modes at both sides of the layer. Component molecules in the former case show the single torsion angle τ_1 of about 96°, while in the independent molecules in the latter case there are observed two torsion angles of about 88 and 102°. Perhaps such subtle adjustment in the torsion angle improves the packing efficiency between the layers.

Disorder and twinning. Since the energy difference among the stacking modes is quite small, as indicated above, disordering could also occur by random change of the modes. In fact, appreciable streaks along c* in Weissenberg photographs were found for crystals of forms (I) and (III).

A similar interpretation is applicable to the polysynthetic twin of form (III). Examination of Weissenberg photographs of the twinned crystals indicates that a' = −a, b' = −b and that the c* axes are common for the twin components. From the crystal structures shown in Figs. 4 and 5, it is most plausible that the

stacking mode r or p in the twinning plane is replaced by mode q.

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Structure of a 9-(2-Carboxyethyl)guanine 1,6-Hexanediamine (2:1) Complex

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Abstract. 1,6-Hexanediammonium bis[3-(2-amino-1,6-dihydro-6-oxo-9-purinyl)propionate] tetrahydrate, $2C_8H_8N_5O_3^-.C_6H_{18}N_2^{2+}.4H_2O$, $M_r = 634\cdot65$, triclinic, $P\bar{1}$, $a = 11\cdot169$ (2), $b = 13\cdot885$ (2), $c = 11\cdot004$ (2) Å, $\alpha = 108\cdot44$ (1), $\beta = 102\cdot77$ (1), $\gamma = 97\cdot67$ (1)°, $V = 1539\cdot6$ (6) Å³, $Z = 2$, $D_m = 1\cdot377$, $D_x = 1\cdot369$ g cm⁻³,

$\lambda(\mathrm{Cu}\,K\alpha) = 1\cdot54184$ Å, $\mu = 9\cdot4$ cm^{-1}, $F(000) = 676$, room temperature, $R = 0\cdot069$ for 2054 observed reflexions. Two independent guanine moieties are linked alternatively by the N(2)—H$\cdots$O(6) and N(1)—H$\cdots$N(7) hydrogen bonds to form a ribbon extended along a. Two 1,6-hexanediamine molecules, occupying the inversion centres at $0,0,\frac{1}{2}$ and $\frac{1}{2},0,\frac{1}{2}$, are intercalated between the two guanine ribbons and link them through hydrogen bonds with the carboxylate groups directly or through the water molecules.

Introduction. In serial studies on the interaction patterns between amino acids and nucleic acid bases, we have determined the crystal structure of a 9-(2-carboxyethyl)guanine 1,6-hexanediamine (2:1) complex, in order to reveal the hydrogen bonding between the dissociated carboxyl group and the guanine moiety.

Table 1. *Fractional coordinates and equivalent isotropic temperature factors*

B_{eq} values are calculated from the anisotropic thermal parameters using the equation $B_{\mathrm{eq}} = 8\pi^2(U_1 + U_2 + U_3)/3$, where U_1, U_2 and U_3 are the principal components of the mean-square displacement matrix U. Values in $\langle\rangle$ are anisotropicity defined by $[\Sigma(B - 8\pi^2 U_i)^2/3]^{1/2}$ and those in () are e.s.d.'s; they refer to last decimal places.

	x	y	z	$B_{\mathrm{eq}}(\text{Å}^2)$
N(1)A	0·2553 (5)	0·0282 (4)	0·1709 (5)	3·5 ⟨11⟩
C(2)A	0·3034 (6)	0·1248 (5)	0·1846 (7)	3·4 ⟨9⟩
N(2)A	0·4278 (5)	0·1499 (4)	0·1897 (6)	4·1 ⟨17⟩
N(3)A	0·2424 (5)	0·2052 (4)	0·1980 (5)	3·1 ⟨10⟩
C(4)A	0·1186 (6)	0·1644 (5)	0·1870 (7)	3·2 ⟨4⟩
C(5)A	0·0627 (6)	0·0725 (5)	0·1778 (7)	3·2 ⟨8⟩
C(6)A	0·1291 (6)	−0·0109 (5)	0·1642 (7)	3·5 ⟨11⟩
O(6)A	0·0951 (4)	−0·1009 (4)	0·1521 (5)	4·6 ⟨20⟩
N(7)A	−0·0651 (5)	0·0643 (4)	0·1690 (6)	3·9 ⟨15⟩
C(8)A	−0·0819 (6)	0·1557 (5)	0·1734 (7)	3·3 ⟨16⟩
N(9)A	0·0277 (5)	0·2241 (4)	0·1860 (5)	3·4 ⟨12⟩
C(10)A	0·0410 (6)	0·3295 (5)	0·1865 (7)	3·5 ⟨11⟩
C(11)A	0·0569 (6)	0·4107 (5)	0·3212 (7)	3·5 ⟨14⟩
C(12)A	−0·0617 (6)	0·3920 (6)	0·3671 (7)	3·8 ⟨8⟩
O(13)A	−0·1574 (4)	0·4089 (4)	0·3048 (5)	5·9 ⟨33⟩
O(14)A	−0·0525 (4)	0·3582 (4)	0·4615 (5)	4·2 ⟨14⟩
N(1)B	0·7288 (5)	−0·0927 (4)	0·1370 (5)	3·5 ⟨15⟩
C(2)B	0·7317 (6)	−0·1963 (6)	0·0974 (7)	3·5 ⟨21⟩
N(2)B	0·8452 (5)	−0·2179 (4)	0·1017 (5)	3·6 ⟨12⟩
N(3)B	0·6305 (5)	−0·2719 (4)	0·0615 (5)	3·4 ⟨15⟩
C(4)B	0·5265 (6)	−0·2326 (5)	0·0724 (7)	3·3 ⟨11⟩
C(5)B	0·5155 (6)	−0·1303 (5)	0·1173 (7)	3·4 ⟨15⟩
C(6)B	0·6237 (6)	−0·0509 (6)	0·1506 (7)	4·0 ⟨20⟩
O(6)B	0·6306 (4)	0·0433 (4)	0·1857 (5)	4·6 ⟨22⟩
N(7)B	0·3927 (5)	−0·1264 (4)	0·1136 (6)	4·1 ⟨18⟩
C(8)B	0·3306 (6)	−0·2216 (6)	0·0671 (7)	4·1 ⟨13⟩
N(9)B	0·4060 (5)	−0·2932 (4)	0·0366 (5)	3·2 ⟨13⟩
C(10)B	0·3645 (6)	−0·4050 (6)	−0·0271 (7)	3·9 ⟨9⟩
C(11)B	0·3777 (6)	−0·4589 (6)	0·0705 (7)	3·9 ⟨8⟩
C(12)B	0·2935 (7)	−0·4323 (6)	0·1672 (7)	4·5 ⟨12⟩
O(13)B	0·3405 (5)	−0·4212 (4)	0·2842 (5)	5·0 ⟨13⟩
O(14)B	0·1850 (4)	−0·4256 (4)	0·1150 (5)	6·2 ⟨27⟩
N(1')A	0·7259 (5)	0·2885 (5)	0·5124 (6)	4·5 ⟨16⟩
C(1')A	0·7161 (7)	0·1823 (6)	0·5198 (8)	5·0 ⟨13⟩
C(2')A	0·5838 (7)	0·1389 (6)	0·5197 (7)	4·5 ⟨8⟩
C(3')A	0·5664 (7)	0·0263 (6)	0·5043 (8)	5·2 ⟨11⟩
N(1')B	0·1521 (5)	0·3376 (5)	0·6284 (6)	4·4 ⟨16⟩
C(1')B	0·1664 (6)	0·2273 (6)	0·5805 (7)	4·4 ⟨17⟩
C(2')B	0·0439 (6)	0·1518 (6)	0·5512 (7)	4·3 ⟨16⟩
C(3')B	0·0610 (6)	0·0401 (6)	0·5155 (7)	4·7 ⟨15⟩
O(W1)	0·6027 (4)	0·3456 (4)	0·2986 (5)	5·4 ⟨19⟩
O(W2)	0·0619 (4)	0·4089 (4)	0·8701 (5)	5·2 ⟨15⟩
O(W3)	0·3760 (4)	0·4064 (4)	0·3602 (5)	5·5 ⟨14⟩
O(W4)	0·3959 (5)	0·4135 (4)	0·6152 (5)	6·2 ⟨24⟩

Experimental. 9-(2-Carboxyethyl)guanine was prepared according to the procedure reported by Fujita, Takenaka & Sasada (1984). Needle-like crystals deposited from aqueous solution containing this substance and 1,6-hexanediamine in the ratio of 2:1 by vapour diffusion of acetone. D_m by flotation in a mixture of hexane and tetrachloromethane. Rigaku four-circle diffractometer, graphite-monochromated Cu $K\alpha$ radiation, crystal size $0\cdot15 \times 0\cdot08 \times 0\cdot7$ mm;* unit-cell dimensions determined with 67 reflexions ($30 < 2\theta < 46°$). Intensities measured by ω scan mode, scan rate $8°$ min^{-1}, scan width $1\cdot5°$. Five reference reflexions monitored every 50 reflexions showed no significant intensity deterioration. Corrections for Lorentz and polarization factors, not for absorption or secondary extinction; 2486 independent reflexions with $3 < 2\theta < 90°$, $h\,-10{\to}0$, $k\,-12{\to}12$, $l\,-10{\to}10$. 432 reflexions with $|F_o| < 3\sigma$ considered unobserved. Standard deviations $\sigma^2(|F_o|) = \sigma_p^2 + 0\cdot00023|F_o|^2$, σ_p evaluated by counting statistics. Space group assumed to be $P\bar{1}$, since the intensity distribution suggested centrosymmetry. Structure solved by direct methods, block-diagonal least squares; all H atoms found on a difference map; $\Sigma w(|F_o| - |F_c|)^2$ minimized, where $w = 1/\sigma^2(|F_o|)$; final $R = 0\cdot069$, $wR = 0\cdot074$, $S = 3\cdot05$; maximum shift of parameters $0\cdot09\sigma$ for non-H atoms, $\Delta\rho$ peak $0\cdot38$ e Å^{-3}. Anisotropic thermal parameters for non-H, isotropic thermal parameters for H atoms. Atomic scattering factors from *International Tables for X-ray Crystallography* (1974); programs used: *MULTAN*78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978), *LSAP*80 (Takenaka & Sasada, 1980), *DCMS*82 (Takenaka & Sasada, 1982) and *LISTUP* (Takenaka & Sasada, 1983). Final atomic parameters are given in Table 1.†

Discussion. Two independent 9-(2-carboxyethyl)-guanine molecules and two halves of 1,6-hexanediamine are in an asymmetric unit; the centres of the latter occupy inversion centres at $0,0,\frac{1}{2}$ and $\frac{1}{2},0,\frac{1}{2}$. Protons are transferred from the carboxyl groups of the former to the amino groups of the latter.

Fig. 1. shows the partial crystal structure viewed along **c**, where the atom numbering is given. The two guanine moieties are linked alternately by the N(2)—H$\cdots$O(6) and N(1)—H$\cdots$N(7) hydrogen bonds, to form a ribbon extended along **a**, as usually observed in the crystals of guanine derivatives (Fujita, Takenaka &

* The crystal size was too small to give good intensity data; however, this size was the largest available. All efforts to obtain larger crystals failed.

† Lists of structure factors, anisotropic thermal parameters, H-atom parameters and least-squares planes have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 43065 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

Sasada, 1984; Thewalt, Bugg & Marsh, 1971; Destro, Kistenmacher & Marsh, 1974).

The crystal structure projected along **a** is illustrated in Fig. 2. The 1,6-hexanediamine molecules are intercalated between the two ribbons and link them by several hydrogen bo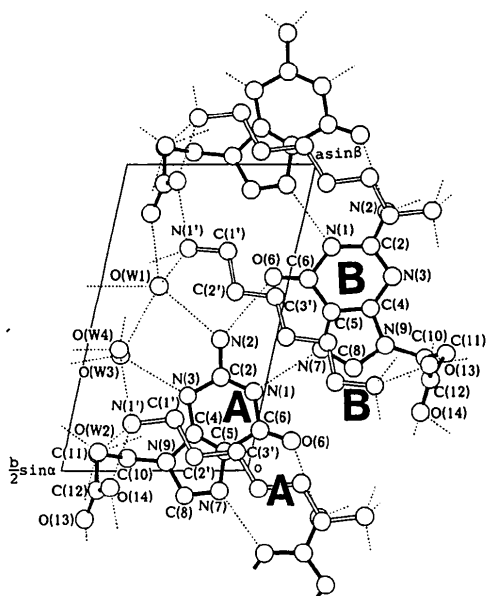nds. Water molecules participate in the hydrogen-bond network. Table 2 lists the hydrogen-bond geometry. Since interactions between the cation and anion and between the guanine moieties are predominant, the carboxylate group does not directly bond to the guanine moiety.

Table 3 shows the bond distances and angles. There are no significant differences in molecular dimensions between the two independent ions. Average values are in agreement with those reported for 9-(2-carboxyethyl)guanine (Fujita, Takenaka & Sasada, 1984), except for the carboxyl group. The geometry of the

Fig. 1. Crystal structure viewed along **c**. Anions related by inversion are omitted for clarity. Hydrogen bonds are represented by dotted lines.
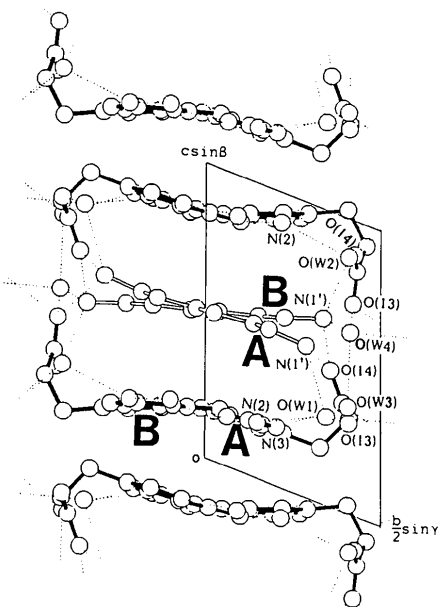

Fig. 2. Crystal structure viewed along **a**. Hydrogen bonds are represented by dotted lines.

Table 2. *Hydrogen bonds (e.s.d.'s are given in parentheses referring to last decimal places)*

$X-H\cdots Y$	Symmetry*	$X\cdots Y$	$\angle XHY$
$N(1)-HA\cdots N(7)B$		2·796 (8) Å	160 (6)°
$N(2)-HA\cdots O(6)B$		2·868 (7)	145 (6)
$N(2)-HA\cdots O(W1)$		2·849 (8)	157 (5)
$N(1)-HB\cdots N(7)A$	i	2·826 (8)	171 (5)
$N(2)-HB\cdots O(6)A$	i	2·875 (7)	167 (5)
$N(2)-HB\cdots O(W2)$	ii	3·053 (7)	147 (6)
$N(1')-HA\cdots O(14)A$	i	2·773 (7)	161 (5)
$N(1')-HA\cdots O(W1)$		2·845 (8)	151 (5)
$N(1')-HA\cdots O(13)B$	ii	2·729 (8)	161 (6)
$N(1')-HB\cdots O(W4)$		2·837 (8)	154 (5)
$N(1')-HB\cdots O(14)A$		2·707 (7)	167 (6)
$N(1')-HB\cdots O(W2)$		2·977 (8)	170 (6)
$O(W1)-H\cdots O(W3)$		2·925 (7)	123 (9)
$O(W1)-H\cdots O(W4)$	iii	3·173 (7)	151 (9)
$O(W1)-H\cdots O(13)A$	i	2·685 (7)	157 (6)
$O(W2)-H\cdots O(14)B$	iv	2·835 (7)	167 (8)
$O(W2)-H\cdots O(14)B$	v	2·834 (7)	155 (13)
$O(W3)-H\cdots N(3)A$		2·787 (7)	164 (7)
$O(W3)-H\cdots O(13)B$	vi	2·821 (7)	167 (6)
$O(W4)-H\cdots O(13)B$	ii	2·881 (7)	158 (10)
$O(W4)-H\cdots O(W3)$		2·734 (7)	172 (6)

* Symmetry code: (i) $1 + x, y, z$; (ii) $1 - x, -y, 1 - z$; (iii) $1 - x, 1 - y, 1 - z$; (iv) $x, 1 + y, 1 + z$; (v) $-x, -y, 1 - z$; (vi) $x, 1 + y, z$.

Table 3. *Bond distances (Å) and angles (°) (e.s.d.'s in parentheses)*

	A	B		A	B
C(1)–C(2)	1·324 (9)	1·373 (9)	C(8)–N(9)	1·396 (9)	1·396 (9)
N(1)–C(6)	1·418 (9)	1·393 (9)	N(9)–C(10)	1·450 (9)	1·446 (9)
C(2)–N(2)	1·371 (9)	1·335 (9)	C(10)–C(11)	1·51 (1)	1·48 (1)
C(2)–N(3)	1·370 (9)	1·326 (9)	C(11)–C(12)	1·54 (1)	1·56 (1)
N(3)–C(4)	1·385 (8)	1·361 (9)	C(12)–O(13)	1·229 (9)	1·229 (9)
C(4)–C(5)	1·31 (1)	1·38 (1)	C(12)–O(14)	1·258 (8)	1·25 (1)
C(4)–N(9)	1·394 (9)	1·388 (9)			
C(5)–C(6)	1·44 (1)	1·42 (1)	N(1')–C(1')	1·49 (1)	1·50 (1)
C(5)–N(7)	1·396 (9)	1·372 (9)	C(1')–C(2')	1·52 (1)	1·51 (1)
C(6)–O(6)	1·212 (8)	1·227 (9)	C(2')–C(3')	1·50 (1)	1·53 (1)
N(7)–C(8)	1·295 (9)	1·29 (1)	C(3')–C(3')*	1·53 (1)	1·54 (1)
C(2)–N(1)–C(6)	125·6 (6)	126·4 (6)	C(5)–N(7)–C(8)	103·2 (5)	106·2 (6)
N(1)–C(2)–N(2)	118·1 (6)	115·9 (6)	N(7)–C(8)–N(9)	113·5 (6)	113·0 (6)
N(1)–C(2)–N(3)	126·7 (6)	123·4 (6)	C(4)–N(9)–C(8)	103·8 (5)	104·6 (5)
N(2)–C(2)–N(3)	115·1 (6)	120·6 (6)	C(4)–N(9)–C(10)	128·2 (5)	128·3 (5)
C(2)–N(3)–C(4)	106·6 (5)	111·0 (5)	C(8)–N(9)–C(10)	127·8 (5)	126·9 (5)
N(3)–C(4)–C(5)	131·5 (6)	129·7 (6)	N(9)–C(10)–C(11)	114·1 (5)	112·4 (6)
N(3)–C(4)–N(9)	121·6 (6)	124·0 (6)	C(10)–C(11)–C(12)	109·7 (5)	114·0 (6)
C(5)–C(4)–N(9)	106·9 (6)	106·3 (6)	C(11)–C(12)–O(13)	116·3 (6)	117·0 (6)
C(4)–C(5)–C(6)	120·6 (6)	118·3 (6)	C(11)–C(12)–O(14)	117·2 (6)	115·3 (6)
C(4)–C(5)–N(7)	112·7 (6)	110·0 (6)	O(13)–C(12)–O(14)	126·5 (7)	127·7 (6)
C(6)–C(5)–N(7)	126·4 (6)	131·6 (6)	N(1')–C(1')–C(2')	110·4 (6)	111·2 (6)
N(1)–C(6)–C(5)	108·7 (5)	111·0 (6)	C(1')–C(2')–C(3')	111·0 (6)	111·4 (6)
N(1)–C(6)–O(6)	120·1 (6)	121·4 (6)	C(2')–C(3')–C(3')*	115·0 (6)	113·5 (6)
C(5)–C(6)–O(6)	131·2 (6)	127·5 (7)			

* Related by inversion.

carboxylate group in the present crystal is typical of the dissociated one. The guanine moieties are almost planar, the maximum deviation of atoms from the least-squares plane being 0·048 Å. The conformations of the carboxyethyl groups are nearly the same for the two independent molecules; the torsion angle N(9)—C(10)—C(11)—C(12) is −63·2 (7)° for one molecule and 63·9 (8)° for the other. The bond distances and angles of the 1,6-hexanediamines are similar to those in 1,6-hexanediamine (Binnie & Robertson, 1950). The molecule has a *trans* zigzag conformation, slightly twisted around the C(1′)—C(2′) and C(2′)—C(3′) bonds.

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Structure of *cyclo*(-L-Phenylalanyl-L-phenylalanyl-)

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Abstract. 3,6-Bis(phenylmethyl)-2,5-piperazinedione, $C_{18}H_{18}N_2O_2$, $M_r = 294·3$, orthorhombic, $P22_12_1$, $a = 6·181$ (1), $b = 10·380$ (3), $c = 23·795$ (4) Å, $V = 1526·8$ (6) Å^3, $Z = 4$, $D_x = 1·28$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54178 Å, $\mu = 6·0$ cm^{-1}, $F(000) = 624$, room temperature, $R = 0·056$ for 959 observed reflections and 176 variables. The 2,5-piperazinedione ring has a flattened boat conformation with the C^β atoms in pseudoaxial positions. One of the phenylalanyl residues faces the 2,5-piperazinedione ring $[\chi_1^1 = 69·0$ (6)°], the other is in an extended conformation $[\chi_2^1 = −61·9$ (6)°]. The ω torsion angles in both *cis* peptide units are small and equal to −0·9 (7) and 0·1 (7)°.

Introduction. The preference for an aromatic part of an amino-acid residue to fold over the 2,5-piperazinedione (hereafter DKP) skeleton is a well known phenomenon. The folded conformation has been observed both in the solid state and in solution. However, for *cis* cyclic dipeptides built up of two aromatic amino-acid residues, steric repulsions prevent the molecule from adopting a conformation in which both aromatic rings fold over

the DKP nucleus. From chirooptical properties (Edelhoch, Bernstein & Wilchek, 1968; Strickland, Wilchek, Horwitz & Billups, 1970) and ¹H NMR, ¹³C NMR spectra (Deslauries, Grzonka, Schaumburg, Shiba & Walter, 1975; Kopple & Marr, 1967) of *cyclo*(L-X)₂ where X is an aromatic amino-acid residue, a conformation with both aromatic rings sharing the space over the DKP ring in a 'face-to-face' fashion was postulated as the most preferred one. On the other hand, the conformational-energy calculations for *cyclo*(L-Tyr)₂ (Snow, Hooker & Schellman, 1977), ¹H NMR studies of specifically labeled *cyclo*(L-Phe-L-X) (Liberek & Bednarek, 1978) and the results of X-ray analaysis of *cyclo*(N-Me-L-Phe)₂ (Benedetti, Marsh & Goodman, 1976) indicate that the most stable conformation is that in which one of the amino-acid residues is in the folded and the other in the extended conformation.

The present crystal-structure analysis of *cyclo*-(L-Phe)₂ has been performed to provide more data on cyclic dipeptides with two aromatic amino-acid residues.