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Structure of cvclo(-L-Phenylalanyl-N-methyl-L-α-aminobutyryl-)*

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Abstract. 6-Ethyl-1-methyl-3-(phenylmethyl)-2,5-piperazinedione, $C_{14}H_{18}N_2O_2$, $M_r = 246.3$, monoclinic, $P2_1$, a = 14.078 (2), b = 11.297 (2), c = 8.5080 (8) Å, β = 99.26 (1)°, V = 1335.4 (3) Å³, Z = 4, F(000) = 528, $\lambda(\mathrm{Cu}\,\mathrm{K}\alpha)=1.54178\,\mathrm{\AA},$ $D_x = 1.22 \text{ g cm}^{-3}$, $\mu =$ 5.9 cm^{-1} , room temperature, final R = 0.050 for 1640 observed reflexions. Two crystallographically independent molecules adopt a conformation in which both α amino-acid side chains are folded above the 2.5diketopiperazine ring $[\chi_1^1 = 56.7 (5), \chi_2^1 = 57.2 (5)$ for molecule A and $\chi_1^1 = 64.0 (6), \chi_2^1 = 58.3 (6)^\circ$ for molecule B]. The 2,5-diketopiperazine ring is only slightly buckled.

Introduction. It is a well known phenomenon that the aromatic part of an amino-acid residue will tend to fold over the 2,5-diketopiperazine ring (hereafter DKP) of cyclic dipeptides whenever possible. On the other hand, ¹H NMR studies of *cis* N-monosubstituted cyclic dipeptides (Liberek, Bednarek, Kitowska & Macikowska, 1977) indicated that due to Pitzer strain a side chain of an N-substituted amino-acid residue has a preference to fold over the DKP skeleton and that in solution the DKP ring adopts a boat conformation with the α -amino-acid side chains in quasiaxial positions. Hence in cyclo(-L-phenylalanyl-N-methyl-L-α-aminobutyryl) {cyclo[-L-Phe-L-N(Me)-Abu-]} both amino-acid side chains should compete for space over the DKP ring. It was shown by 'H NMR (Liberek et al., 1977) that the form predominant in solution has the aliphatic side chain in the folded conformation.

The present crystal structure analysis of cyclo-[-L-Phe-L-N(Me)-Abu-] has been performed to find out if the preference of the N-substituted amino-acid residue to fold over the DKP ring will be preserved in the solid state.

Experimental. Colorless crystal of dimensions $0.08 \times$ 0.3×0.4 mm from methanol-water, D_m not determined, Syntex P21 diffractometer, graphite-monochromatized Cu Ka radiation, lattice parameters for 15 reflexions with 2θ in range 15–23°, profiles measured Table 1. Final fractional coordinates and equivalent *isotropic thermal parameters* (Å²)

 U_{eq} is defined as one-third of the trace of the orthogonalized U_{ii} tensor.

	x	у	z	U_{eq}
C(2A)	-0.2111(4)	-0.7406	-0.1982 (6)	0.058 (2)
C(3A)	-0.3086 (5)	-0.7601 (7)	-0.2394 (8)	0.075 (3)
C(4A)	-0.3452 (5)	-0.8720 (8)	-0.2509 (8)	0.079 (3)
C(5A)	-0.2837 (5)	-0.9702 (7)	-0.2241 (7)	0.076 (3)
C(6A)	-0.1853 (4)	-0.9506 (6)	-0.1840 (7)	0.059 (2)
C(G A)	-0.1485 (4)	-0.8366 (5)	-0.1708(5)	0.050 (2)
C(B1A)	-0.0416(3)	-0.8159 (6)	-0.1266 (5)	0.049 (2)
C(A A)	-0.0049(3)	-0.8128(5)	0.0540 (5)	0.043 (2)
C(P1A)	-0.0367(3)	-0.7027 (5)	0.1310 (6)	0.046 (2)
O(1A)	-0.0257 (3)	-0.6059 (4)	0.0680 (4)	0.063 (1)
N(2A)	-0.0682(3)	-0.7101(4)	0.2689 (5)	0.045 (2)
C(1A)	-0.0755 (5)	-0.5999 (6)	0.3599 (8)	0.071 (3)
C(A2A)	-0.0874 (3)	-0.8194 (5)	0.3486 (5)	0.045 (2)
C(B2A)	-0.1926 (3)	-0.8206 (6)	0.3804 (6)	0.061 (2)
C(G2A)	-0.2660 (4)	-0.8060 (6)	0.2308 (7)	0.067 (2)
C(P2A)	-0.0672 (3)	-0.9302 (5)	0.2624 (6)	0.045 (2)
O(2A)	-0.0851 (3)	-1.0284 (4)	0.3168 (5)	0.062 (2)
N(1A)	-0.0300 (3)	-0.9216 (4)	0.1284 (5)	0.044 (2)
C(2B)	-0.2542 (5)	-0.3126 (8)	-0.9005 (7)	0.078 (3)
C(3B)	-0.2620 (8)	-0.4275 (9)	-0.9573 (9)	0.107 (4)
C(4B)	-0.3507 (9)	-0.4794 (8)	-0.990 (1)	0.124 (5)
C(5B)	-0.4325 (6)	-0-4159 (9)	-0.9729 (9)	0.106 (4)
C(6B)	-0.4265 (4)	-0.3009 (7)	-0.9168 (7)	0.077 (3)
C(G1B)	-0.3354 (4)	-0.2475 (6)	-0-8784 (6)	0.062 (2)
C(B1B)	0-3272 (4)	-0.1251 (5)	-0.8140 (6)	0.062 (2)
C(A1B)	-0.3168 (3)	-0.1163 (5)	-0.6330 (6)	0.054 (2)
C(P1B)	-0-4048 (4)	-0.1609 (6)	-0.5680 (7)	0.058 (2)
O(1B)	-0-4825 (3)	-0-1155 (5)	-0-6261 (5)	0.080 (2)
N(2B)	-0.3947 (3)	-0.2409 (4)	-0.4537 (5)	0.057 (2)
C(1B)	-0.4803 (4)	-0·2710 (7)	-0.3808 (8)	0.081 (3)
C(A2B)	-0.3054 (4)	−0 ·2985 (6)	-0.3825 (6)	0.058 (2)
C(B2B)	-0.3090 (5)	-0-4349 (6)	-0·3938 (8)	0.077 (3)
C(G2B)	-0.3311 (6)	-0-4793 (7)	-0-5572 (9)	0.094 (4)
C(P2B)	-0.2173 (4)	-0.2527 (6)	-0.4421 (7)	0.063 (2)
O(2B)	<i>−</i> 0·1384 (3)	-0·2919 (5)	-0.3838 (5)	0.104 (2)
N(1B)	-0.2264 (3)	-0·1715 (4)	-0·5553 (5)	0.059 (2)

for 1888 reflexions with $2\theta \le 115^\circ$ (h 0 \rightarrow 15, k 0 \rightarrow 12, $l \rightarrow 9 \rightarrow 9$), $\omega - 2\theta$ scan technique, variable scan rate, profile analysis according to Lehmann & Larsen (1974), no significant intensity variation for two standard reflexions, absorption ignored, 1647 reflexions with $I \ge 2\sigma(I)$; structure solved by direct methods with MULTAN78 (Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978); anisotropic full-matrix least-squares refinement on F with SHELX76 (Sheldrick, 1976), unit weights, H atoms bonded to N located on a ΔF map, the remaining H atoms placed in calculated positions, methyl residues refined as rigid groups, other H atoms not refined, R = 0.050 and wR = 0.049, seven F_o with large $\Delta F/\sigma(F)$ omitted from last cycles; max. Δ/σ in the last cycle < 0.4, no peaks higher than $0.19 \text{ e} \text{ Å}^{-3}$ and lower than $-0.22 \text{ e} \text{ Å}^{-3}$ on

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Table 2. Molecular dimensions

(a) Bond lengths (Å) C(2)-C(3) 1.378 (9) 1.383 (13) C(2)-C(3) 1.394 (7) 1.397 (9) C(3)-C(4) 1.363 (12) 1.367 (16) C(4)-C(5) 1.404 (11) 1.384 (15) C(5)-C(6) 1.386 (9) 1.407 (9) C(G)-C(B1) 1.509 (7) 1.485 (9) C(G)-C(B1) 1.509 (7) 1.485 (9) C(A1)-C(A1) 1.509 (7) 1.485 (9) C(A1)-C(A1) 1.507 (8) 1.521 (8) C(A1)-C(A1) 1.452 (7) 1.474 (7) C(P1)-O(1) 1.239 (7) 1.237 (7) C(P1)-O(1) 1.239 (7) 1.237 (7) C(P1)-N(2) 1.322 (7) 1.319 (8) N(2)-C(A2) 1.454 (7) 1.458 (7) C(A2)-C(B2) 1.548 (7) 1.458 (7) C(A2)-C(B2) 1.548 (7) 1.548 (10) C(A2)-C(B2) 1.548 (7) 1.544 (10) C(A2)-C(B2) 1.514 (7) 1.464 (10) C(B2)-C(C2) 1.514 (7) 1.464 (10) C(B2)-C(C2) 1.514 (7) 1.226 (7) C(G)-C(1)-C(2) 12.1 (6) 119-5 (8) C(B2)-C(C2) 1.243 (7) 1.226 (7) (b) Bond angles (°) C(G)-C(3)-C(4) 118-6 (6) 121-2 (7) C(G)-C(3) 120-4 (7) 120-3 (9) C(G)-C(5)-C(4) 118-6 (6) 121-2 (7) C(G)-C(6)-C(5) 120-9 (5) 119-1 (6) C(B1)-C(C1)-C(2) 120-4 (4) 118-5 (5) C(B1)-C(C1)-C(2) 120-6 (4) 121-6 (5) C(B1)-C(C1)-C(2) 120-6 (4) 113-2 (4) N(1)-C(A1)-C(B1) 112-2 (4) 113-2 (4) N(1)-C(A1)-C(B1) 112-2 (4) 113-2 (4) N(1)-C(A1)-C(B1) 112-5 (4) 113-7 (4) N(1)-C(A1)-C(B1) 112-5 (4) 123-7 (4) N(1)-C(P1)-C(A1) 113-5 (4) 113-1 (4) N(1)-C(P1)-C(A1) 113-5 (4) 113-1 (4) N(1)-C(P1)-C(A1) 13-5 (4) 113-7 (5) C(A2)-N(2)-C(P1) 113-5 (4) 113-7 (5) C(A2)-N(2)-C(P1) 113-5 (4) 113-7 (5) C(A2)-N(2)-C(A2) 119-7 (5) 118-5 (5) N(1)-C(P1)-C(A1) 125-5 (4) 126-6 (4) C(D)-C(B1)-C(A1) 125-7 (6) 0.901 (6) C(D)-C(B1)-C(A1) 125-7 (6) 0.901 (6) C(D)-C(B1)-C(A1) 125-7 (6) 0.901 (6) C(D)-C(B1)-C(A1) 13-7 (5) 0.43 (6) N(1)-C(P1)-N(2)-C(A2) 113-3 (4)		Molecule A	Molecule B
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	(a) Bond lengths (Å)		
$\begin{array}{ccccc} C(2)-C(G) & 1.394 (T) & 1.397 (9) \\ C(3)-C(4) & 1.363 (12) & 1.367 (16) \\ C(4)-C(5) & 1.404 (11) & 1.384 (15) \\ C(5)-C(6) & 1.386 (9) & 1.408 (15) \\ C(61)-C(81) & 1.509 (7) & 1.488 (9) \\ C(61)-C(71) & 1.507 (8) & 1.521 (8) \\ C(41)-C(71) & 1.507 (8) & 1.521 (8) \\ C(41)-C(71) & 1.452 (7) & 1.474 (7) \\ C(71)-O(1) & 1.239 (7) & 1.237 (7) \\ C(71)-N(1) & 1.452 (7) & 1.474 (7) \\ C(71)-N(1) & 1.452 (7) & 1.478 (7) \\ C(42)-C(42) & 1.458 (7) & 1.458 (7) \\ C(42)-C(42) & 1.458 (7) & 1.548 (7) \\ C(42)-C(42) & 1.548 (7) & 1.544 (10) \\ C(42)-C(42) & 1.548 (7) & 1.544 (10) \\ C(42)-C(42) & 1.548 (7) & 1.544 (10) \\ C(42)-C(62) & 1.514 (7) & 1.464 (10) \\ C(42)-C(62) & 1.514 (7) & 1.464 (10) \\ C(42)-C(62) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G)-C(3)-C(2) & 121\cdot1 (6) & 121\cdot4 (7) \\ C(6)-C(5)-C(4) & 118\cdot6 (6) & 21\cdot2 (7) \\ C(6)-C(5)-C(4) & 118\cdot6 (6) & 121\cdot2 (7) \\ C(6)-C(5)-C(4) & 118\cdot6 (6) & 121\cdot2 (7) \\ C(6)-C(6)-C(5) & 120\cdot9 (5) & 119\cdot1 (6) \\ C(6)-C(5)-C(4) & 118\cdot6 (6) & 121\cdot2 (7) \\ C(6)-C(6)-C(6) & 120\cdot6 (5) & 119\cdot9 (5) \\ C(4)-C(3) & 120\cdot9 (5) & 119\cdot1 (6) \\ C(6)-C(6)-C(6) & 120\cdot6 (5) & 119\cdot9 (5) \\ C(4)-C(4)-C(2) & 120\cdot0 (4) & 121\cdot6 (5) \\ C(B)-C(G)-C(G) & 120\cdot0 (4) & 121\cdot6 (5) \\ C(B)-C(G)-C(G) & 120\cdot0 (4) & 121\cdot6 (5) \\ C(B)-C(G)-C(G) & 120\cdot0 (4) & 121\cdot6 (5) \\ C(B)-C(G)-C(B) & 110\cdot0 (4) & 111\cdot1 (4) \\ N(1)-C(A1)-C(B1) & 110\cdot4 (4) & 111\cdot1 (4) \\ N(1)-C(A1)-C(B1) & 110\cdot4 (4) & 113\cdot1 (4) \\ O(1)-C(P1)-C(A1) & 113\cdot5 (4) & 113\cdot1 (4) \\ O(1)-C(P1)-C(A1) & 113\cdot5 (4) & 113\cdot7 (4) \\ C(22)-C(22)-C(22) & 109\cdot9 (4) & 110\cdot4 (4) & 113\cdot7 (5) \\ C(22)-C(42)-N(2) & 110\cdot1 (5) & 0.40 (6) \\ C(1)-C(B)-C(A1)-N(1) & 56\cdot7 (5) & 64\cdot0 (6) \\ N(1)-C(A1)-C(P1)-N(2) & 113\cdot3 (4) & 113\cdot7 (5) \\ C(22)-C(42)-N(2)-C(A2) & -83\cdot3 (5) & -27\cdot7 (7) \\ C(P1)-N(2$	C(2) - C(3)	1.378 (9)	1.383 (13)
$\begin{array}{c} C(3)-C(4) & 1-363(12) & 1-367(16) \\ C(4)-C(5) & 1-404(11) & 1-384(15) \\ C(4)-C(5) & 1-300(9) & 1-382(12) \\ C(6)-C(6) & 1-330(9) & 1-382(12) \\ C(6)-C(6) & 1-336(9) & 1-485(9) \\ C(6)-C(8) & 1-509(7) & 1-485(9) \\ C(6)-C(8) & 1-527(8) & 1-521(8) \\ C(4)-C(8) & 1-507(8) & 1-521(8) \\ C(4)-C(1) & 1-537(8) & 1-521(8) \\ C(4)-C(1) & 1-239(7) & 1-319(8) \\ C(2)-C(4) & 1-322(7) & 1-319(8) \\ C(2)-C(4) & 1-458(7) & 1-458(7) \\ C(1)-N(2) & 1-458(7) & 1-458(7) \\ C(1)-N(2) & 1-458(7) & 1-548(7) \\ C(2)-C(2) & 1-548(7) & 1-548(7) \\ C(4)-C(2) & 1-548(7) & 1-548(10) \\ C(2)-C(2) & 1-514(7) & 1-464(10) \\ C(2)-C(2) & 1-514(7) & 1-464(10) \\ C(2)-C(2)-C(3) & 119-7(5) & 121-4(7) \\ C(4)-C(3)-C(2) & 1-514(7) & 1-222(8) \\ C(6)-C(5)-C(4) & 118-6(6) & 121-2(7) \\ C(6)-C(5)-C(4) & 118-6(6) & 121-2(7) \\ C(6)-C(5)-C(4) & 118-6(6) & 121-2(7) \\ C(6)-C(6)-C(2) & 120-0(4) & 118-5(6) \\ C(8)-C(6)-C(2) & 120-0(4) & 118-5(6) \\ C(8)-C(6)-C(2) & 120-0(4) & 118-5(6) \\ C(8)-C(6)-C(2) & 120-0(4) & 118-5(6) \\ C(8)-C(6)-C(6) & 120-6(5) & 119-9(5) \\ C(4))-C(8) & 110-1(4) & 113-1(4) \\ N(1)-C(4))-C(8) & 10-9(4) & 118-2(4) & 117-9(4) \\ C(42)-N(2)-C(1) & 113-2(4) & 117-9(4) \\ C(42)-N(2)-C(1) & 113-2(4) & 117-9(4) \\ C(42)-N(2)-C(1) & 113-2(4) & 117-9(4) \\ C(42)-N(2)-C(1) & 113-3(4) & 113-7(5) \\ C(2)-C(4)-C(3) & 10-9(1) & 13-3(4) & 113-7(5) \\ C(2)-C(4)-C(3) - C(2) & 10-9(5) & -90-1(6) \\ C(6)-C(6)-C(1)-C(2) & 119-7(5) & 18-5(5) \\ C(2)-C(4)-C(4) - N(1) & 56-7(5) & 64-0(6) \\ N(1)-C(4)-C(4))-C(4) & 19-7(5) & 18-5(5) \\ C(2)-C(4)-C(4) - N(1) & 56-7(5) & 64-0(6) \\ N(1)-C(4)-C(4)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(2)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(2)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(2)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(4)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(4)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(4)-C(2) & -7-6(6) & 0-9(7) \\ C(4)-C(4)-C(4)-C(4) & -7(5) & -3-2(6) \\ C(4)-C(4)-C(4)-C(4) & -7(5) & -3-2(6) \\ C(4)-C(4)-C(4)-C(4) & -7(5) &$	C(2) - C(G1)	1.394 (7)	1.397 (9)
$\begin{array}{c} C(4)-C(5) & 1.404 (11) & 1.384 (15) \\ C(5)-C(6) & 1.390 (9) & 1.482 (12) \\ C(G)-C(6) & 1.386 (9) & 1.407 (9) \\ C(G)-C(6) & 1.386 (9) & 1.407 (9) \\ C(G)-C(6) & 1.509 (7) & 1.485 (9) \\ C(A1)-C(A1) & 1.509 (7) & 1.485 (9) \\ C(A1)-C(P1) & 1.507 (8) & 1.521 (8) \\ C(A1)-N(1) & 1.452 (7) & 1.474 (7) \\ C(P1)-O(1) & 1.239 (7) & 1.237 (7) \\ C(P1)-N(2) & 1.452 (7) & 1.458 (7) \\ C(P1)-O(1) & 1.322 (7) & 1.319 (8) \\ N(2)-C(A2) & 1.454 (7) & 1.458 (7) \\ C(A2)-C(B2) & 1.548 (7) & 1.458 (7) \\ C(A2)-C(B2) & 1.548 (7) & 1.454 (10) \\ C(A2)-C(B2) & 1.548 (7) & 1.454 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.464 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.464 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.514 (7) & 1.464 (10) \\ C(2)-C(3) & 119 \cdot 7 (5) & 121 \cdot 4 (7) \\ C(4)-C(3)-C(2) & 120 \cdot 4 (7) & 120 \cdot 3 (9) \\ C(6)-C(5)-C(4) & 118 \cdot 6 (6) & 121 \cdot 2 (7) \\ C(6)-C(5)-C(4) & 118 \cdot 6 (6) & 121 \cdot 2 (7) \\ C(6)-C(6)-C(2) & 120 \cdot 0 (4) & 121 \cdot 6 (5) \\ C(B1)-C(G1)-C(2) & 120 \cdot 0 (4) & 121 \cdot 6 (5) \\ C(B1)-C(G1)-C(G) & 110 \cdot 14 \cdot 4 (4) & 115 \cdot 0 (4) \\ C(F1)-C(G1)-C(G) & 110 \cdot 14 \cdot 4 (4) & 115 \cdot 0 (4) \\ C(F1)-C(G1)-C(G) & 110 \cdot 14 \cdot 4 (4) & 115 \cdot 0 (4) \\ C(F1)-C(G1)-C(G1) & 112 \cdot 2 (4) & 113 \cdot 2 (4) \\ N(1)-C(A1)-C(B1) & 112 \cdot 2 (4) & 113 \cdot 1 (4) \\ N(1)-C(A1)-C(B1) & 110 \cdot 4 (4) & 111 \cdot 1 (4) \\ N(1)-C(A1)-C(B1) & 110 \cdot 4 (4) & 113 \cdot 1 (4) \\ N(1)-C(A1)-C(B1) & 110 \cdot 4 (4) & 113 \cdot 1 (4) \\ N(1)-C(A1)-C(B1) & 113 \cdot 3 (4) & 113 \cdot 1 (4) \\ N(2)-C(P1)-C(A1) & 125 \cdot 5 (4) & 126 \cdot 6 (4) \\ C(A2)-N(2)-C(A2) & 110 \cdot 1 (4) & 113 \cdot 7 (5) \\ C(A2)-N(2)-C(A2) & 110 \cdot 1 (4) & 113 \cdot 7 (5) \\ C(A2)-N(2)-C(A2) & 110 \cdot 1 (4) & 113 \cdot 7 (5) \\ C(A2)-C(A2)-C(A2) & 119 \cdot 3 (4) & 113 \cdot 7 (5) \\ C(A2)-C(A2)-C(A2) & 119 \cdot 3 (4) & 113 \cdot 7 (5) \\ C(A2)-C(A2)-C(A2) & -13 \cdot 3 (5) & -2 \cdot 7 (7) \\ C(A2)-C(A2)-C(A2)-C(A2) & -3 \cdot 3 (5) & -2 \cdot 7 (7) \\ C(A1)-C(A1)-C(A1)-C(A2) & -3 \cdot 3 (5) & -2 \cdot 7 (7) \\ \mathsf{C(A1)-C(A1)-C(A1)-C(A2) & -3 \cdot 5 \\ \mathsf{C(A1)-C(A2)-C(A2)-$	C(3) - C(4)	1-363 (12)	1.367 (16)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(4) - C(5)	1.404 (11)	1.384 (15)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(5) - C(6)	1.390 (9)	1.382 (12)
$\begin{array}{cccccc} C(G1)-C(B1) & 1-509 (7) & 1-485 (9) \\ C(B1)-C(A1) & 1-507 (8) & 1-521 (8) \\ C(A1)-C(P1) & 1-507 (8) & 1-521 (8) \\ C(A1)-N(1) & 1-452 (7) & 1-474 (7) \\ C(P1)-O(1) & 1-239 (7) & 1-237 (7) \\ C(P1)-N(2) & 1-322 (7) & 1-319 (8) \\ N(2)-C(A2) & 1-454 (7) & 1-458 (7) \\ C(1)-N(2) & 1-478 (8) & 1-481 (7) \\ C(A2)-C(B2) & 1-548 (7) & 1-548 (7) \\ C(A2)-C(B2) & 1-548 (7) & 1-544 (10) \\ C(A2)-C(P2) & 1-501 (8) & 1-505 (8) \\ C(B2)-C(G2) & 1-514 (7) & 1-464 (10) \\ C(P2)-N(1) & 1-332 (7) & 1-322 (8) \\ C(P2)-O(2) & 1-243 (7) & 1-226 (7) \\ \hline (b) Bond angles (^{\circ}) \\ C(G1)-C(2)-C(3) & 119-7 (5) & 121-4 (7) \\ C(4)-C(3)-C(2) & 120-4 (7) & 120-3 (9) \\ C(G)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(G)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(G)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(G)-C(G)-C(2) & 120-0 (4) & 118-5 (5) \\ C(B)-C(G)-C(2) & 120-0 (4) & 121-6 (5) \\ C(B)-C(G)-C(2) & 120-0 (4) & 121-6 (5) \\ C(B)-C(G)-C(B) & 110-4 (4) & 115-0 (4) \\ C(P)-C(A)-C(B) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A)-C(B) & 110-4 (4) & 113-2 (4) \\ N(1)-C(A)-C(B) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P)-C(A) & 120-0 (4) & 119-8 (4) \\ N(1)-C(A)-C(P) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P)-C(A) & 120-0 (4) & 119-8 (4) \\ N(1)-C(A)-C(P) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P)-C(A) & 120-0 (4) & 119-4 (4) \\ N(1)-C(A)-C(P) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P)-C(A) & 120-0 (4) & 119-4 (4) \\ N(1)-C(A)-C(P) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P)-C(A) & 120-0 (4) & 119-4 (4) \\ N(1)-C(A)-C(P) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P)-C(A) & 120-0 (4) & 119-4 (4) \\ N(1)-C(A)-C(P) & 113-5 (4) & 124-4 (5) \\ C(A)-N(2)-C(P) & 113-3 (4) & 115-9 (4) \\ C(A)-N(2)-C(P) & 113-3 (4) & 115-9 (4) \\ C(A)-N(2)-C(P) & 113-3 (4) & 115-9 (4) \\ C(A)-C(P)-C(A) & 115-9 (4) & 115-4 (4) \\ C(B)-C(A)-C(B)-C(A) & 19-3 (4) & 119-7 (4) \\ N(1)-C(P)-C(A) & 10-7 (5) & -90-1 (6) \\ C(G)-C(B)-C(A) & N(1) & -20-6 (5) & 89-1 (6) \\ C(G)-C(B)-C(A) & N(1) & -20-6 (5) & 89-1 (6) \\ C(G)-C(B)-C(A) & N(1) & -20-6 (5) & 89-1 (6) \\ C(G)-C(B)-C(A) & N(1) & -20-6 (5) & 89-1 (6) \\ C(G)-C(B)-C(A) & N(1) & -20-6 (5) & 90-7) \\ C(A)-C(A)-C(B)$	$C(G_1) - C(6)$	1.386 (9)	1.407 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(G_1) - C(B_1)$	1.509 (7)	1.485 (9)
$\begin{array}{ccccc} C(A 1)-C(P1) & 1.507 (8) & 1.521 (8) \\ C(A 1)-N(1) & 1.452 (7) & 1.474 (7) \\ C(P1)-O(1) & 1.239 (7) & 1.237 (7) \\ C(P1)-N(2) & 1.322 (7) & 1.319 (8) \\ N(2)-C(A2) & 1.454 (7) & 1.458 (7) \\ C(1)-N(2) & 1.478 (8) & 1.4481 (7) \\ C(A2)-C(B2) & 1.548 (7) & 1.544 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.464 (10) \\ C(A2)-C(C2) & 1.514 (7) & 1.464 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119-7 (5) & 121-4 (7) \\ C(4)-C(3)-C(2) & 1.21-1 (6) & 119-5 (8) \\ C(5)-C(4)-C(3) & 120-4 (7) & 120-3 (9) \\ C(6)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(6)-C(6)-C(2) & 120-9 (5) & 119-1 (6) \\ C(6)-C(6)-C(2) & 120-9 (5) & 119-1 (6) \\ C(6)-C(G1)-C(2) & 120-4 (4) & 118-5 (5) \\ C(B1)-C(G1)-C(2) & 120-0 (4) & 121-6 (5) \\ C(B1)-C(G1)-C(B1) & 112-2 (4) & 113-2 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 115-0 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 113-1 (4) \\ O(1)-C(P1)-C(A1) & 118-3 (4) & 113-1 (4) \\ O(1)-C(P1)-C(A1) & 118-3 (4) & 115-9 (4) \\ N(2)-C(P1)-C(A1) & 118-2 (4) & 113-1 (4) \\ O(1)-C(P1)-C(A1) & 118-3 (4) & 115-9 (4) \\ N(2)-C(P1)-C(A1) & 118-3 (4) & 115-9 (4) \\ C(A2)-N(2)-C(P1) & 13-5 (4) & 126-6 (4) \\ C(A2)-N(2)-C(P1) & 13-5 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-3 (5) & -90-1 (6) \\ C(G2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & -N(2) & 113-3 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-7 (5) & 18-5 (5) \\ N(1)-C(P2)-C(A2) & -7-6 (6) & 0-9 (7) \\ C(A1)-C(P1)-N(A) & -7-7 (5) & -90-7 (6) \\ C(A1)-C(P1)-N(A) & -7-7 (5) & -3-2 (6) \\ N(2)-C(A2)-N(2)-C(P2) & -7-6 (6) & 0-9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -7-7 (5) & 58-3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -3-2 (5) & -3-2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -3-2 (5) & -3-2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -7-7 (5) & 0-9 (7) \\ \end{array}$	C(B1) - C(A1)	1.540 (6)	1.527 (8)
$\begin{array}{ccccc} C(A 1) - N(1) & 1.452 (7) & 1.474 (7) \\ C(P1) - O(1) & 1.239 (7) & 1.237 (7) \\ C(P1) - N(2) & 1.322 (7) & 1.319 (8) \\ N(2) - C(A2) & 1.454 (7) & 1.458 (7) \\ C(1) - N(2) & 1.478 (8) & 1.481 (7) \\ C(A2) - C(B2) & 1.501 (8) & 1.505 (8) \\ C(A2) - C(B2) & 1.514 (7) & 1.444 (10) \\ C(A2) - C(B2) & 1.513 (7) & 1.322 (8) \\ C(P2) - N(1) & 1.332 (7) & 1.322 (8) \\ C(P2) - O(2) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G) - C(2) - C(3) & 119 - 7 (5) & 121 - 4 (7) \\ C(4) - C(3) - C(2) & 121 - 1 (6) & 119 - 5 (8) \\ C(5) - C(4) - C(3) & 120 - 4 (7) & 120 - 3 (9) \\ C(6) - C(5) - C(4) & 118 - 6 (6) & 121 - 2 (7) \\ C(G) - C(G) - C(2) & 120 - 4 (7) & 120 - 3 (9) \\ C(6) - C(G) - C(2) & 120 - 9 (5) & 119 - 1 (6) \\ C(6) - C(G) - C(2) & 120 - 0 (4) & 118 - 5 (5) \\ C(B1) - C(G1) - C(2) & 120 - 0 (4) & 121 - 6 (5) \\ C(B1) - C(G1) - C(2) & 120 - 6 (5) & 119 - 9 (5) \\ C(A1) - C(B1) - C(B1) & 112 - 2 (4) & 113 - 2 (4) \\ N(1) - C(A1) - C(B1) & 112 - 2 (4) & 113 - 2 (4) \\ N(1) - C(A1) - C(B1) & 112 - 2 (4) & 113 - 2 (4) \\ N(1) - C(A1) - C(B1) & 110 - 4 (4) & 111 - 1 (4) \\ N(1) - C(A1) - C(B1) & 110 - 4 (4) & 111 - 1 (4) \\ N(1) - C(A1) - C(B1) & 112 - 5 (4) & 124 - 2 (5) \\ C(1) - N(2) - C(P1) & 113 - 5 (4) & 113 - 1 (4) \\ O(1) - C(P1) - C(A1) & 118 - 3 (4) & 115 - 9 (4) \\ N(2) - C(P1) - C(A1) & 118 - 3 (4) & 115 - 9 (4) \\ N(2) - C(P1) - C(A1) & 118 - 9 (4) & 113 - 7 (5) \\ C(A2) - N(2) - C(P1) & 113 - 7 (5) & 113 - 7 (5) \\ C(A2) - N(2) - C(A2) & 113 - 3 (4) & 113 - 7 (5) \\ C(P2) - C(A2) - N(2) & 114 - 6 (4) & 114 - 1 (4) \\ C(P2) - C(A2) - N(2) & 110 - 1 (4) & 113 - 7 (5) \\ C(P2) - C(A2) - N(2) & 110 - 7 (5) & 118 - 5 (5) \\ N(1) - C(P2) - C(A2) & 119 - 3 (4) & 113 - 7 (5) \\ C(P1) - C(A1) - N(1) & 56 - 7 (5) & 64 - 0 (6) \\ C(P1) - C(A1) - N(1) - C(P2) & -7 - 6 (6) & 0.9 (7) \\ C(A1) - C(P1) - N(2) - C(P1) & -7 (5) & 54 - 3 (6) \\ N(2) - C(A2) - C(P2) - N(1) & 3 - 2 (5) & -3 - 2 (6) \\ N(2) - C(A2) - C(P2) - N(1) & 3 - 2 (5) & -3 - 2 (6) \\ N(2) - C(A2) - C(P2) - N(1) & -7 (5) & 0.9 (7) \\ \end{array}$	C(A1) - C(P1)	1.507 (8)	1.521 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(A1) = N(1)	1.452 (7)	1.474 (7)
$\begin{array}{cccc} C(P1) \cdot N(2) & 1.322 (7) & 1.319 (8) \\ N(2)-C(A2) & 1.454 (7) & 1.458 (7) \\ C(1)-N(2) & 1.478 (8) & 1.481 (7) \\ C(A2)-C(B2) & 1.548 (7) & 1.544 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.454 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.454 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.454 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119-7 (5) & 121.4 (7) \\ C(4)-C(3)-C(2) & 120.4 (7) & 120.3 (9) \\ C(5)-C(4)-C(3) & 120.4 (7) & 120.3 (9) \\ C(6)-C(5)-C(4) & 118.6 (6) & 121.2 (7) \\ C(G1)-C(G1)-C(2) & 120.4 (7) & 120.3 (9) \\ C(6)-C(G1)-C(2) & 120.4 (4) & 118.5 (5) \\ C(B1)-C(G1)-C(2) & 120.4 (4) & 118.5 (5) \\ C(B1)-C(G1)-C(2) & 120.4 (4) & 118.5 (5) \\ C(B1)-C(G1)-C(2) & 120.4 (4) & 115.5 (4) \\ C(P1)-C(A1)-C(B1) & 112.2 (4) & 113.2 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.3 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 113.4 (4) \\ N(2)-C(P1)-C(A1) & 118.3 (4) & 115.9 (4) \\ C(A2)-N(2)-C(P1) & 113.5 (4) & 113.4 (4) \\ C(A2)-N(2)-C(P1) & 113.5 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.3 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.3 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.3 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 113.3 (4) & 113.7 (5) \\ $	C(P1) = O(1)	1.239 (7)	1.237 (7)
$\begin{array}{cccc} N(2)-C(A^2) & 1.454 (7) & 1.458 (7) \\ C(1)-N(2) & 1.478 (8) & 1.481 (7) \\ C(A2)-C(B2) & 1.548 (7) & 1.544 (10) \\ C(A2)-C(B2) & 1.514 (7) & 1.464 (10) \\ C(A2)-C(C2) & 1.514 (7) & 1.464 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119-7 (5) & 121-4 (7) \\ C(4)-C(3)-C(2) & 121-1 (6) & 119-5 (8) \\ C(5)-C(4)-C(3) & 120-4 (7) & 120-3 (9) \\ C(6)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(6)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(6)-C(6) -C(2) & 120-9 (5) & 119-1 (6) \\ C(6)-C(G1)-C(2) & 120-9 (5) & 119-1 (6) \\ C(6)-C(G1)-C(2) & 120-0 (4) & 118-5 (5) \\ C(B1)-C(G1)-C(2) & 120-0 (4) & 118-5 (5) \\ C(B1)-C(G1)-C(B1) & 112-2 (4) & 113-2 (4) \\ N(1)-C(A1)-C(B1) & 112-2 (4) & 113-2 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 115-9 (4) \\ N(2)-C(P1)-C(A1) & 118-3 (4) & 115-9 (4) \\ N(2)-C(P1)-C(A1) & 120-0 (4) & 119-8 (4) \\ N(2)-C(P1)-C(A1) & 120-0 (4) & 119-8 (4) \\ N(2)-C(P1)-C(A1) & 118-3 (4) & 115-9 (4) \\ N(2)-C(P1)-C(A1) & 118-9 (4) & 115-9 (4) \\ C(A2)-N(2)-C(P1) & 125-5 (4) & 126-6 (4) \\ C(A2)-N(2)-C(P1) & 125-5 (4) & 126-6 (4) \\ C(A2)-N(2)-C(P1) & 113-3 (4) & 113-7 (5) \\ C(G2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 119-3 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 119-3 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 119-3 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 119-3 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 109-9 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 119-3 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(1) & 26-6 (4) \\ C(P1)-C(A1)-N(1)-C(P2) & -7-6 (6) & 0-9 (7) \\ C(A1)-C(P1)-N(2) & 11-1 (5) & -0.9 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7-6 (6) & 0-9 (7) \\ C(A1)-C(P1)-N(2)-C(P2) & 0-9 (5) & -3.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -3-2 (5) & -3.2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -7/5 & 0-9 (7) \\ \end{array}$	$C(P1) \cdot N(2)$	1.322 (7)	1.319 (8)
$\begin{array}{ccccc} C(1)-N(2) & 1.478 (8) & 1.481 (7) \\ C(42)-C(B2) & 1.501 (8) & 1.505 (8) \\ C(42)-C(G2) & 1.501 (8) & 1.505 (8) \\ C(B2)-C(G2) & 1.514 (7) & 1.464 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119-7 (5) & 121-4 (7) \\ C(4)-C(3)-C(2) & 120-4 (7) & 120-3 (9) \\ C(5)-C(4)-C(3) & 120-4 (7) & 120-3 (9) \\ C(6)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(G1)-C(2) & 120-4 (7) & 120-3 (9) \\ C(6)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(G1)-C(2) & 120-9 (5) & 119-1 (6) \\ C(6)-C(G1)-C(2) & 120-9 (5) & 119-1 (6) \\ C(6)-C(G1)-C(2) & 120-0 (4) & 121-6 (5) \\ C(B1)-C(G1)-C(2) & 120-0 (4) & 121-6 (5) \\ C(B1)-C(G1)-C(B1) & 112-2 (4) & 113-2 (4) \\ N(1)-C(B1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(P1) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P1)-C(A1) & 120-0 (4) & 119-8 (4) \\ N(2)-C(P1)-C(A1) & 120-0 (4) & 113-4 (4) \\ C(42)-N(2)-C(P1) & 125-5 (4) & 126-6 (4) \\ C(42)-N(2)-C(P1) & 125-5 (4) & 126-6 (4) \\ C(42)-N(2)-C(A2) & 110-1 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-1 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 110-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 119-3 (4) & 119-7 (4) \\ C(P2)-C(A2)-N(2) & 119-3 (4) & 119-7 (4) \\ C(P2)-C(A2)-N(2) & 119-3 (4) & 119-7 (4) \\ C(P2)-C(A2)-N(2) & 119-3 (4) & 119-7 (4) \\ C(P1)-C(A1)-N(1) & 56-7 (5) & 64-0 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7-6 (6) & 0-9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8-3 (5) & -2-7 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8-3 (5) & -2-7 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8-3 (5) & -2-7 (7) \\ C(A1)-C(P2)-N(1) & -2(A2) & -3-2 (6) \\ N(2)-C(A2)-N(2)-C(A2) & -N(2) & 57-2 (5) & 58-3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3-2 (5) & -3-2 (6) \\ C(A2)-C(A2)-C(P2)-N(1) & 3-2 (5) & -3-2 (6) \\ C(A2)-C(A2)-C(P2)-N(1) & -7 (5) & 0-9 (7) \\ \end{array}$	N(2)-C(12)	1.454 (7)	1.458 (7)
$\begin{array}{ccccc} C(A2)-C(B2) & 1.548\ (7) & 1.544\ (10) \\ C(A2)-C(P2) & 1.501\ (8) & 1.505\ (8) \\ C(B2)-C(G2) & 1.514\ (7) & 1.464\ (10) \\ C(P2)-N(1) & 1.332\ (7) & 1.322\ (8) \\ C(P2)-O(2) & 1.243\ (7) & 1.226\ (7) \\ \hline (b) Bond angles\ (°) \\ C(G1)-C(2)-C(3) & 119.7\ (5) & 121.4\ (7) \\ C(4)-C(3)-C(2) & 121.1\ (6) & 119.5\ (8) \\ C(5)-C(4)-C(3) & 120.4\ (7) & 120.3\ (9) \\ C(6)-C(5)-C(4) & 118.6\ (6) & 121.2\ (7) \\ C(6)-C(5)-C(4) & 118.6\ (6) & 121.2\ (7) \\ C(6)-C(6)-C(2) & 120.4\ (7) & 120.3\ (9) \\ C(6)-C(6)-C(3)-C(2) & 120.4\ (7) & 120.3\ (9) \\ C(6)-C(6)-C(6) & (2) & 120.9\ (5) & 119.1\ (6) \\ C(6)-C(6)-C(2) & 120.4\ (4) & 118.5\ (5) \\ C(B)-C(G)-C(2) & 120.4\ (4) & 118.5\ (5) \\ C(B)-C(G)-C(2) & 120.0\ (4) & 121.6\ (5) \\ C(B)-C(G)-C(2) & 120.0\ (4) & 121.6\ (5) \\ C(B)-C(G)-C(B) & 114.4\ (4) & 115.0\ (4) \\ C(P1)-C(A1)-C(B1) & 112.2\ (4) & 113.2\ (4) \\ N(1)-C(A1)-C(B1) & 110.4\ (4) & 111.1\ (4) \\ N(1)-C(A1)-C(B1) & 113.5\ (4) & 113.1\ (4) \\ O(1)-C(P1)-C(A1) & 118.3\ (4) & 115.9\ (4) \\ N(2)-C(P1)-C(A1) & 118.3\ (4) & 115.9\ (4) \\ N(2)-C(P1)-C(A1) & 118.2\ (4) & 17.9\ (4) \\ C(A2)-N(2)-C(P1) & 113.3\ (4) & 113.7\ (5) \\ C(P2)-C(A2)-N(2) & 110.1\ (4) & 113.7\ (5) \\ C(P2)-C(A2)-N(2) & 113.3\ (4) & 113.7\ (5) \\ C(2)-C(P2)-C(A2) & 119.7\ (5) & 118.5\ (5) \\ N(1)-C(P2)-C(A2) & 119.7\ (5) & 118.5\ (5) \\ N(1)-C(P2)-C(A2) & 119.7\ (5) & 118.5\ (5) \\ N(1)-C(P1)-N(1)-C(P2) & -7.6\ (6) & 0.9\ (7) \\ C(A1)-C(P1)-N(2) & 111.1\ (5) & 0.0\ (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6\ (6) & 0.9\ (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -7.7\ (5) & 58.3\ (6) \\ N(2)-C(A2)-C(P2)-N(1$	C(1)-N(2)	1.478 (8)	1.481 (7)
$\begin{array}{ccccc} C(A2)-C(P2) & 1.501 (8) & 1.505 (8) \\ C(B2)-C(G2) & 1.514 (7) & 1.464 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119.7 (5) & 121.4 (7) \\ C(4)-C(3)-C(2) & 121.1 (6) & 119.5 (8) \\ C(5)-C(4)-C(3) & 120.4 (7) & 120.3 (9) \\ C(6)-C(5)-C(4) & 118.6 (6) & 121.2 (7) \\ C(G1)-C(5)-C(4) & 118.6 (6) & 121.2 (7) \\ C(G1)-C(G1)-C(2) & 120.4 (7) & 120.3 (9) \\ C(6)-C(G1)-C(2) & 120.9 (5) & 119.1 (6) \\ C(6)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B1)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B1)-C(G1)-C(2) & 120.0 (4) & 115.6 (4) \\ C(P1)-C(B1)-C(B1) & 112.2 (4) & 113.2 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 115.9 (4) \\ N(2)-C(P1)-C(A1) & 118.3 (4) & 115.9 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.9 (4) & 117.9 (4) \\ C(A2)-N(2)-C(P1) & 118.2 (4) & 117.9 (4) \\ C(A2)-N(2)-C(A2) & 110.1 (4) & 113.7 (5) \\ C(B2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(B2)-C(A2)-N(2) & 110.3 (4) & 113.7 (5) \\ C(B2)-C(A2)-C(B2)-C(A2) & -27 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -27 (2) & -27 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & $	C(A2)C(B2)	1.548 (7)	1.544 (10)
$\begin{array}{cccccc} C(B2)-C(G2) & 1.514 (7) & 1.464 (10) \\ C(P2)-N(1) & 1.332 (7) & 1.322 (8) \\ C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ \hline (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119.7 (5) & 121.4 (7) \\ C(G1)-C(2)-C(3) & 120.4 (7) & 120.3 (9) \\ C(5)-C(4)-C(3) & 120.4 (7) & 120.3 (9) \\ C(6)-C(5)-C(4) & 118.6 (6) & 121.2 (7) \\ C(G1)-C(6) & C(5) & 120.9 (5) & 119.1 (6) \\ C(6)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B1)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B1)-C(G1)-C(G1) & 114.4 (4) & 115.0 (4) \\ C(P1)-C(A1)-C(B1) & 110.2 (4) & 113.2 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.2 (4) & 113.9 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.5 (4) & 126.6 (4) \\ C(A2)-N(2)-C(P1) & 115.9 (4) & 115.9 (4) \\ C(A2)-N(2)-C(P1) & 125.5 (4) & 126.6 (4) \\ C(A2)-N(2)-C(P1) & 125.5 (4) & 126.6 (4) \\ C(A2)-N(2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A2) & 119.3 (4) & 119.7 (4) \\ C(P2)-C(A2)-N(2) & 114.6 (4) & 114.1 (4) \\ C(P2)-C(A2)-N(2) & 119.3 (4) & 119.7 (4) \\ N(1)-C(P2)-C(A2) & 119.3 (4) & 119.7 (5) \\ C(G2)-C(B2)-C(A2) & 119.3 (4) & 119.7 (5) \\ C(G2)-C(B2)-C(A2) & 119.3 (4) & 119.7 (5) \\ C(P2)-N(1)-C(A1) & 126.2 (4) & 126.6 (4) \\ C(A1)-C(P1)-N(1) & 56.7 (5) & 64.0 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8.3 (5) & -2.7 (7) \\ C(A1)-C(P2)-N(1)-C(A1) & -8.6 (5) & 89.1 (6) \\ C(G1)-C(B1)-C(A1)-N(1) & 56.7 (5) & 58.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P2)-N(1)-C(A1) & -7.7 (5) & 58.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -7.7 (5) & 58.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -7.7 (5) & 0.9 (7) \\ \end{array}$	C(A2) - C(P2)	1.501 (8)	1.505 (8)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(B2)-C(G2)	1.514 (7)	1-464 (10)
$\begin{array}{ccccc} C(P2)-O(2) & 1.243 (7) & 1.226 (7) \\ (b) Bond angles (°) \\ C(G1)-C(2)-C(3) & 119.7 (5) & 121.4 (7) \\ C(4)-C(3)-C(2) & 121.1 (6) & 119.5 (8) \\ C(5)-C(4)-C(3) & 120.4 (7) & 120.3 (9) \\ C(6)-C(5)-C(4) & 118.6 (6) & 121.2 (7) \\ C(G1)-C(G)-C(2) & 120.9 (5) & 119.1 (6) \\ C(6)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B1)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B1)-C(G1)-C(2) & 120.0 (4) & 115.0 (4) \\ C(P1)-C(B1)-C(B1) & 112.2 (4) & 113.2 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 115.9 (4) \\ N(2)-C(P1)-C(A1) & 118.3 (4) & 115.9 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.5 (4) & 126.6 (4) \\ C(A2)-N(2)-C(P1) & 118.2 (4) & 117.9 (4) \\ C(A2)-N(2)-C(P1) & 118.2 (4) & 117.9 (4) \\ C(A2)-N(2)-C(P1) & 118.9 (4) & 115.4 (4) \\ C(B2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.3 (4) & 119.7 (4) \\ N(1)-C(P2)-C(A2) & 119.3 (4) & 119.7 (4) \\ N(1)-C(P2)-C(A2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(B1)-C(A1)-N(1) & 56.7 (5) & 64.0 (6) \\ N(1)-C(A1)-C(P1)-N(2) & 11.1 (5) & 0.0 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P2)-N(1)-C(A2) & -7.7 (5) & 58.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3.2 (5) & -3.2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3.2 (5) & -3.2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3.2 (5) & -3.2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & -7.7 (5) & 0.9 (7) \\ \end{array}$	C(P2) - N(1)	1.332 (7)	1.322 (8)
(b) Bond angles (°) (C(G1)-C(2)-C(3) 119-7 (5) 121-4 (7) C(4)-C(3)-C(2) 121-1 (6) 119-5 (8) C(5)-C(4)-C(3) 120-4 (7) 120-3 (9) C(6)-C(5)-C(4) 118-6 (6) 121-2 (7) C(G1)-C(6) C(5) 120-9 (5) 119-1 (6) C(6)-C(G1)-C(2) 120-0 (4) 121-6 (5) C(B1)-C(G1)-C(2) 120-0 (4) 121-6 (5) C(B1)-C(G1)-C(G1) 114-4 (4) 115-0 (4) C(P1)-C(A1)-C(B1) 112-2 (4) 113-2 (4) N(1)-C(A1)-C(B1) 110-4 (4) 111-1 (4) N(1)-C(A1)-C(B1) 100-4 (4) 115-9 (4) N(2)-C(P1)-C(A1) 120-0 (4) 119-8 (4) N(2)-C(P1)-C(A1) 115-9 (4) 115-9 (4) 115-9 (4) C(A2)-N(2)-C(P1) 125-5 (4) 126-6 (4) C(A2)-N(2)-C(P1) 115-9 (4) 115-4 (4) C(A2)-N(2)-C(A2) 110-1 (4) 113-7 (5) C(A2)-C(A2)-N(2) 110-1 (4) 113-7 (5) C(A2)-C(A2)-N(2) 119-3 (4) 119-7 (4) N(1)-C(P2)-C(A2) 119-7 (5) 118-5 (5) N(1)-C(P2)-C(A2) 119-7 (5) 118-5 (5) N(1)-C(P2)-C(A1) 93-2 (5) -90-1 (6) C(P2)-C(A1)-N(1) 56-7 (5) 64-0 (6) C(P1)-C(A1)-N(1) 56-7 (5) 64-0 (6) C(P1)-C(A1)-N(1)-C(P2) -7-6 (6) 0-9 (7) C(A1)-C(P1)-N(2) 11-1 (5) -0.0 (6) C(P1)-C(A1)-N(1)-C(P2) -7-6 (6) 0-9 (7) C(A1)-C(P1)-N(2)-C(A2) -8-3 (5) -2-7 (7) C(A1)-C(P2)-C(A2) -0.9 (5) 4-3 (6) N(2)-C(A2)-C(B2)-C(A2) 57-2 (5) 58-3 (6) N(2)-C(A2)-C(B2)-C(A2	C(P2)-O(2)	1.243 (7)	1.226 (7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	(b) Bond angles (°)		
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(G_1)-C(2)-C(3)$	119.7 (5)	121-4 (7)
$\begin{array}{ccccc} C(4)-C(3) & 120-4 (7) & 120-3 (9) \\ C(6)-C(5)-C(4) & 118-6 (6) & 121-2 (7) \\ C(G)-C(G)-C(5) & 120-9 (5) & 119-1 (6) \\ C(6)-C(G1)-C(2) & 120-0 (4) & 118-5 (5) \\ C(B1)-C(G1)-C(2) & 120-0 (4) & 121-6 (5) \\ C(B1)-C(G1)-C(G1) & 114-4 (4) & 115-0 (4) \\ C(P1)-C(A1)-C(B1) & 112-2 (4) & 113-2 (4) \\ N(1)-C(A1)-C(B1) & 110-4 (4) & 111-1 (4) \\ N(1)-C(A1)-C(B1) & 113-5 (4) & 113-1 (4) \\ O(1)-C(P1)-C(A1) & 120-0 (4) & 113-1 (4) \\ O(1)-C(P1)-C(A1) & 120-0 (4) & 113-4 \\ O(1)-C(P1)-C(A1) & 120-0 (4) & 119-8 (4) \\ N(2)-C(P1)-C(A1) & 120-0 (4) & 119-8 (4) \\ N(2)-C(P1)-C(A1) & 120-0 (4) & 119-8 (4) \\ N(2)-C(P1)-C(A1) & 120-0 (4) & 112-4 \\ C(A2)-N(2)-C(P1) & 125-5 (4) & 126-6 (4) \\ C(A2)-N(2)-C(P1) & 115-9 (4) & 115-4 \\ C(B2)-C(A2)-N(2) & 110-1 (4) & 113-7 (5) \\ C(P2)-C(A2)-N(2) & 109-9 (4) & 110-0 \\ C(G2)-C(B2)-C(A2) & 119-7 (5) & 118-5 (5) \\ N(1)-C(P2)-C(A2) & 119-7 (5) & 118-5 (5) \\ C(P1)-C(A1) & 126-2 (4) & 126-6 (4) \\ C(G1)-C(B1)-C(A1) & 93-2 (5) & -90-1 (6) \\ C(G1)-C(B1)-C(A1) & -86-6 (5) & 89-1 (6) \\ C(G1)-C(B1)-C(A1) & -86-6 (5) & 89-1 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7-6 (6) & 0-9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8-3 (5) & -2.7 (7) \\ C(P1)-N(1)-C(P2)-C(A2) & -8-3 (5) & -2.7 (7) \\ C(P1)-N(1)-C(P2)-C(A2) & -8-3 (5) & -2.7 (7) \\ C(P1)-N(2)-C(A2)-C(P2) & 0-9 (5) & 4-3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3-2 (5) & -3-2 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3-2 (5) & -3-2 (6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0-7 (5) & 0-9 (7) \\ \end{array}$	C(4)-C(3)-C(2)	121-1 (6)	119.5 (8)
$\begin{array}{cccc} C(6)-C(5)-C(4) & 118.6 (6) & 121.2 (7) \\ C(G1) C(6) C(5) & 120.9 (5) & 119.1 (6) \\ C(6)-C(G1)-C(2) & 120.9 (5) & 119.1 (5) \\ C(B)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B)-C(G1)-C(2) & 120.0 (4) & 121.6 (5) \\ C(B)-C(G1)-C(G1) & 114.4 (4) & 115.0 (4) \\ C(P1)-C(A1)-C(B1) & 112.2 (4) & 113.2 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(B1) & 113.5 (4) & 113.1 (4) \\ O(1)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 121.5 (4) & 124.2 (5) \\ C(1)-N(2)-C(P1) & 118.2 (4) & 117.9 (4) \\ C(A2)-N(2)-C(P1) & 118.2 (4) & 117.9 (4) \\ C(A2)-N(2)-C(P1) & 118.2 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 119.3 (4) & 119.7 (4) \\ N(1)-C(P2)-C(A2) & 120.0 (4) & 121.7 (5) \\ C(P2)-C(A2)-N(2) & 111.1 (5) & 0.0 (6) \\ C(G1)-C(B1)-C(A1) & 93.2 (5) & -90.1 (6) \\ C(G1)-C(B1)-C(A1) & 93.2 (5) & -90.1 (6) \\ C(G1)-C(B1)-C(A1) & 93.2 (5) & -90.1 (6) \\ C(G1)-C(B1)-C(A1) & -86.6 (5) & 89.1 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(P2) & 0.9 (5) & 4.3 (6) \\ N(2)-C(A2)-C(P2)-C(P2) & 0.9 (5) & 4.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3.2 (5) & -3.2 (6) \\ C(A2)-C(P2)-N(1) & -C(A1) & 0.7 (5) & 0.9 (7) \\ \end{array}$	C(5)-C(4)-C(3)	120-4 (7)	120-3 (9)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(6)-C(5)-C(4)	118.6 (6)	121-2(7)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(G1) C(6) C(5)	120.9 (5)	119-1(6)
$\begin{array}{ccccc} C(B1)-C(G1)-C(2) & 120\cdot0 (4) & 121\cdot6 (5) \\ C(B1)-C(G1)-C(G) & 120\cdot6 (5) & 119\cdot9 (5) \\ C(A1)-C(B1)-C(G1) & 114\cdot4 (4) & 115\cdot0 (4) \\ C(P1)-C(A1)-C(B1) & 112\cdot2 (4) & 113\cdot2 (4) \\ N(1)-C(A1)-C(B1) & 110\cdot4 (4) & 111\cdot1 (4) \\ N(1)-C(A1)-C(P1) & 113\cdot5 (4) & 113\cdot1 (4) \\ O(1)-C(P1)-C(A1) & 120\cdot0 (4) & 113\cdot1 (4) \\ O(1)-C(P1)-C(A1) & 120\cdot0 (4) & 119\cdot8 (4) \\ N(2)-C(P1)-C(A1) & 120\cdot0 (4) & 124\cdot2 (5) \\ C(1)-N(2)-C(P1) & 118\cdot2 (4) & 117\cdot9 (4) \\ C(A2)-N(2)-C(P1) & 118\cdot2 (4) & 117\cdot9 (4) \\ C(A2)-N(2)-C(P1) & 118\cdot2 (4) & 117\cdot9 (4) \\ C(A2)-N(2)-C(P1) & 115\cdot9 (4) & 115\cdot4 (4) \\ C(B2)-C(A2)-N(2) & 110\cdot1 (4) & 113\cdot7 (5) \\ C(P2)-C(A2)-N(2) & 110\cdot1 (4) & 113\cdot7 (5) \\ C(P2)-C(A2)-N(2) & 119\cdot7 (5) & 118\cdot5 (5) \\ O(2)-C(P2)-C(A2) & 119\cdot7 (5) & 118\cdot5 (5) \\ O(2)-C(P2)-C(A1) & 26\cdot2 (4) & 126\cdot6 (4) \\ \hline (c) Important torsion angles (°) \\ C(2)-C(G1)-C(B1)-C(A1) & -86\cdot6 (5) & 89\cdot1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot6 (5) & 89\cdot1 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(P2) & 0.9 (5) & 4\cdot3 (6) \\ N(2)-C(A2)-C(P2)-C(P2) & 0.9 (5) & 4\cdot3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3\cdot2 (5) & -3\cdot2 (6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0.7 (5) & 0.9 (7) \\ \end{array}$	C(6) - C(G1) - C(2)	119-4 (4)	118.5 (5)
$\begin{array}{c} C(B) - C(G) - C(G) & 120.6 (s) & 119.9 (s) \\ C(A) - C(B) - C(G) & 114.4 (4) & 115.0 (4) \\ C(P) - C(A) - C(B) & 112.2 (4) & 113.2 (4) \\ N(1) - C(A) - C(B) & 110.4 (4) & 111.1 (4) \\ N(1) - C(A) - C(P) & 113.5 (4) & 113.1 (4) \\ O(1) - C(P) - C(A) & 118.3 (4) & 115.9 (4) \\ N(2) - C(P) - C(A) & 120.0 (4) & 119.8 (4) \\ N(2) - C(P) - C(A) & 121.5 (4) & 124.2 (5) \\ C(1) - N(2) - C(P) & 118.2 (4) & 117.9 (4) \\ C(A2) - N(2) - C(P) & 118.2 (4) & 117.9 (4) \\ C(A2) - N(2) - C(P) & 118.2 (4) & 117.9 (4) \\ C(A2) - N(2) - C(P) & 118.2 (4) & 117.9 (4) \\ C(A2) - N(2) - C(P) & 118.2 (4) & 117.9 (4) \\ C(A2) - N(2) - C(P) & 115.9 (4) & 115.4 (4) \\ C(A2) - N(2) - C(P) & 110.1 (4) & 113.7 (5) \\ C(P2) - C(A2) - N(2) & 110.1 (4) & 113.7 (5) \\ C(P2) - C(A2) - N(2) & 119.3 (4) & 119.7 (5) \\ C(G2) - C(B2) - C(A2) & 119.3 (4) & 119.7 (5) \\ N(1) - C(P2) - O(2) & 121.0 (4) & 121.7 (5) \\ C(P2) - N(1) - C(A1) & 126.2 (4) & 26.6 (4) \\ \hline (c) Important torsion angles (°) \\ C(2) - C(G1) - C(B1) - C(A1) & 93.2 (5) & -90.1 (6) \\ C(G1) - C(B1) - C(A1) - N(1) & 56.7 (5) & 64-0 (6) \\ N(1) - C(P1) - N(1) - N(2) & 11.1 (5) & 0.0 0 (6) \\ C(P1) - C(A1) - N(1) - C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1) - C(P1) - N(2) - C(A2) & -8.3 (5) & -2.7 (7) \\ C(A1) - C(P2) - C(A2) & 57.2 (5) & 58.3 (6) \\ N(2) - C(A2) - C(P2) - N(1) & 3.2 (5) & -3.2 (6) \\ C(A2) - C(P2) - N(1) - C(A1) & 0.7 (5) & 0.9 (7) \\ \hline \end{pmatrix}$	C(B1)-C(G1)-C(2)	120.0 (4)	121-6 (5)
$\begin{array}{cccc} C(A1)-C(B1)-C(G1) & 114.4 (4) & 115.0 (4) \\ C(P1)-C(A1)-C(B1) & 112.2 (4) & 113.2 (4) \\ N(1)-C(A1)-C(B1) & 110.4 (4) & 111.1 (4) \\ N(1)-C(A1)-C(P1) & 113.5 (4) & 113.1 (4) \\ O(1)-C(P1)-C(A1) & 113.5 (4) & 113.9 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 120.0 (4) & 119.8 (4) \\ N(2)-C(P1)-C(A1) & 125.5 (4) & 124.2 (5) \\ C(1)-N(2)-C(P1) & 115.9 (4) & 115.9 (4) \\ C(A2)-N(2)-C(P1) & 125.5 (4) & 126.6 (4) \\ C(A2)-N(2)-C(P1) & 115.9 (4) & 115.4 (4) \\ C(B2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 119.3 (4) & 110.0 (5) \\ C(G2)-C(B2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A1) & 126.2 (4) & 126.6 (4) \\ C(P1)-C(A1)-C(P1)-N(2) & 11.1 (5) & -0.0 (6) \\ C(G)-C(G1)-C(B1)-C(A1) & 93.2 (5) & -90.1 (6) \\ C(G1)-C(B1)-C(A1)-N(1) & 56.7 (5) & 64.0 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8.3 (5) & -2.7 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8.3 (5) & -2.7 (7) \\ C(A1)-C(P2)-C(A2)-C(P2) & 0.9 (5) & 4.3 (6) \\ N(2)-C(A2)-C(B2)-C(C2) & 57.2 (5) & 58.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3.2 (5) & -3.2 (6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0.7 (5) & 0.9 (7) \\ \end{array}$	C(B1)-C(G1)-C(6)	120.6 (5)	119.9 (5)
$\begin{array}{ccccc} C(P1)-C(A1)-C(B1) & 112\cdot 2 (4) & 113\cdot 2 (4) \\ N(1)-C(A1)-C(B1) & 110\cdot 4 (4) & 111\cdot 1 (4) \\ N(1)-C(A1)-C(P1) & 113\cdot 5 (4) & 113\cdot 1 (4) \\ O(1)-C(P1)-C(A1) & 120\cdot 0 (4) & 113\cdot 1 (4) \\ N(2)-C(P1)-C(A1) & 120\cdot 0 (4) & 113\cdot 4 (4) \\ N(2)-C(P1)-C(A1) & 120\cdot 0 (4) & 119\cdot 8 (4) \\ N(2)-C(P1)-C(A1) & 121\cdot 5 (4) & 124\cdot 2 (5) \\ C(1)-N(2)-C(P1) & 125\cdot 5 (4) & 126\cdot 6 (4) \\ C(A2)-N(2)-C(P1) & 115\cdot 9 (4) & 115\cdot 4 (4) \\ C(A2)-N(2)-C(1) & 115\cdot 9 (4) & 115\cdot 4 (4) \\ C(B2)-C(A2)-N(2) & 110\cdot 1 (4) & 113\cdot 7 (5) \\ C(P2)-C(A2)-N(2) & 110\cdot 1 (4) & 113\cdot 7 (5) \\ O(2)-C(A2)-N(2) & 113\cdot 3 (4) & 113\cdot 7 (5) \\ O(2)-C(A2)-N(2) & 113\cdot 3 (4) & 113\cdot 7 (5) \\ O(2)-C(P2)-C(A2) & 119\cdot 7 (5) & 118\cdot 5 (5) \\ N(1)-C(P2)-C(A2) & 119\cdot 7 (5) & 118\cdot 5 (5) \\ N(1)-C(P2)-C(A2) & 119\cdot 3 (4) & 119\cdot 7 (4) \\ N(1)-C(P2)-O(2) & 121\cdot 0 (4) & 121\cdot 7 (5) \\ C(P2)-N(1)-C(A1) & 93\cdot 2 (5) & -90\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot 6 (5) & 89\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot 6 (5) & 89\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot 5 (5) & 89\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot 5 (5) & -27\cdot 7 (7) \\ C(A1)-C(P1)-N(2) & 11\cdot 1 (5) & 0\cdot 0 (6) \\ C(P1)-C(A1)-C(P1)-N(2) & 11\cdot 1 (5) & -27\cdot 7 (7) \\ C(P1)-N(2)-C(A2)-C(P2) & 0\cdot 9 (5) & 4\cdot 3 (6) \\ N(2)-C(A2)-C(B2)-C(G2) & 57\cdot 2 (5) & 58\cdot 3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3\cdot 2 (5) & -3\cdot 2 (6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0\cdot 7 (5) & 0\cdot 9 (7) \\ \end{array}$	C(A1) - C(B1) - C(G1)	114-4 (4)	115-0 (4)
$\begin{split} &N(1) - C(4) - C(B) & 110.4 \ (4) & 111.1 \ (4) \\ &N(1) - C(A) - C(B) & 113.5 \ (4) & 113.4 \ (4) \\ &O(1) - C(P) - C(A \ 1) & 118.3 \ (4) & 115.9 \ (4) \\ &N(2) - C(P) - C(A \ 1) & 120.0 \ (4) & 119.8 \ (4) \\ &N(2) - C(P) - O(A \ 1) & 120.0 \ (4) & 119.8 \ (4) \\ &N(2) - C(P) - O(A \ 1) & 120.0 \ (4) & 119.8 \ (4) \\ &N(2) - C(P) - O(A \ 1) & 120.0 \ (4) & 119.8 \ (4) \\ &N(2) - C(P) - O(A \ 1) & 121.5 \ (4) & 124.2 \ (5) \\ &C(A_2) - N(2) - C(P) \ 1 & 118.2 \ (4) & 117.9 \ (4) \\ &C(A_2) - N(2) - C(P) \ 1 & 115.9 \ (4) & 115.4 \ (4) \\ &C(A_2) - N(2) - C(P) \ 1 & 115.9 \ (4) & 113.7 \ (5) \\ &C(B_2) - C(A_2) - N(2) & 110.1 \ (4) & 113.7 \ (5) \\ &C(G_2) - C(A_2) - N(2) & 110.9 \ (4) & 113.7 \ (5) \\ &C(G_2) - C(B_2) - C(A_2) & 119.3 \ (4) & 119.7 \ (5) \\ &N(1) - C(P_2) - C(A_2) & 119.3 \ (4) & 119.7 \ (4) \\ &N(1) - C(P_2) - C(A_2) & 119.3 \ (4) & 119.7 \ (4) \\ &N(1) - C(P_2) - C(A_1) & 126.2 \ (4) & 126.6 \ (4) \\ \\ &(c) Important torsion angles \ (^{\circ) \\ &C(G_1) - C(B_1) - C(A_1) & -86.6 \ (5) & 89.1 \ (6) \\ &C(G_1) - C(B_1) - C(A_1) & -86.6 \ (5) & 89.1 \ (6) \\ &C(G_1) - C(B_1) - C(A_1) & -86.6 \ (5) & 89.1 \ (6) \\ &C(G_1) - C(B_1) - C(A_1) & -86.6 \ (5) & 29.7 \ (7) \\ &C(A_1) - C(P_1) - N(2) & 11.1 \ (5) & 0.0 \ (6) \\ &C(P_1) - C(A_1) - N(1) - C(P_2) & -7.6 \ (6) & 0.9 \ (7) \\ &C(A_1) - C(P_1) - N(2) & -7.7 \ (5) & 58.3 \ (6) \\ &N(2) - C(A_2) - C(B_2) - C(G_2) & 57.2 \ (5) & 58.3 \ (6) \\ &N(2) - C(A_2) - C(P_2) - N(1) & 3.2 \ (5) & -3.2 \ (6) \\ &N(2) - C(A_2) - C(P_2) - N(1) & 0.7 \ (5) & 0.9 \ (7) \\ &N(2) - C(A_2) - C(P_2) - N(1) & 3.2 \ (5) & -3.2 \ (6) \\ &N(2) - C(A_2) - C(P_2) - N(1) & 0.7 \ (5) & 0.9 \ (7) \\ &N(1) - C(P_2) - N(1) & 0.7 \ (5) & 0.9 \ (7) \\ &N(1) - C(P_2) - N(1) & 0.7 \ (5) & 0.9 \ (7) \\ &N(1) - \mathsf$	C(P1)-C(A1)-C(B1)	112-2 (4)	113.2 (4)
$\begin{split} N(1) - C(41) - C(P1) & 113.5 (4) & 113.1 (4) \\ O(1) - C(P1) - C(A1) & 118.3 (4) & 115.9 (4) \\ N(2) - C(P1) - C(A1) & 120.0 (4) & 119.8 (4) \\ N(2) - C(P1) - C(A1) & 120.0 (4) & 119.8 (4) \\ N(2) - C(P1) - C(A1) & 121.5 (4) & 124.2 (5) \\ C(1) - N(2) - C(P1) & 118.2 (4) & 117.9 (4) \\ C(A2) - N(2) - C(P1) & 125.5 (4) & 126.6 (4) \\ C(A2) - N(2) - C(P1) & 115.9 (4) & 115.4 (4) \\ C(B2) - C(A2) - N(2) & 110.1 (4) & 113.7 (5) \\ C(P2) - C(A2) - N(2) & 114.6 (4) & 114.1 (4) \\ C(P2) - C(A2) - N(2) & 113.3 (4) & 113.7 (5) \\ C(G2) - C(B2) - C(A2) & 119.7 (5) & 118.5 (5) \\ N(1) - C(P2) - C(A2) & 119.7 (5) & 118.5 (5) \\ N(1) - C(P2) - C(A2) & 119.7 (5) & 118.5 (5) \\ N(1) - C(P2) - C(A1) & 126.2 (4) & 126.6 (4) \\ C(P2) - N(1) - C(A1) & 93.2 (5) & -90.1 (6) \\ C(G) - C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1) - C(B1) - C(A1) & -86.6 (5) & 89.1 (6) \\ C(P1) - C(A1) - N(1) - C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1) - C(P1) - N(2) - C(P2) & 0.9 (5) & 4.3 (6) \\ N(2) - C(A2) - C(P2) - C(P2) & 0.9 (5) & 4.3 (6) \\ N(2) - C(A2) - C(P2) - C(A2) & 57.2 (5) & 58.3 (6) \\ N(2) - C(A2) - C(P2) - N(1) & 3.2 (5) & -3.2 (6) \\ C(A2) - C(P2) - N(1) & 0.7 (5) & 0.9 (7) \end{split}$	N(1)-C(A1)-C(B1)	110-4 (4)	111-1 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N(1)-C(A1)-C(P1)	113-5 (4)	113-1 (4)
$\begin{split} N(2)-C(P_1)-C(A_1) & 120\cdotO(4) & 119\cdotB(4) \\ N(2)-C(P_1)-O(1) & 121\cdot5(4) & 124\cdot2(5) \\ C(1)-N(2)-C(P_1) & 118\cdot2(4) & 117\cdot9(4) \\ C(A_2)-N(2)-C(P_1) & 125\cdot5(4) & 126\cdot6(4) \\ C(A_2)-N(2)-C(1) & 115\cdot9(4) & 115\cdot4(4) \\ C(A_2)-N(2)-C(1) & 115\cdot9(4) & 115\cdot4(4) \\ C(B_2)-C(A_2)-N(2) & 110\cdot1(4) & 113\cdot7(5) \\ C(P_2)-C(A_2)-N(2) & 109\cdot9(4) & 110\cdot0(5) \\ C(G_2)-C(B_2)-C(A_2) & 113\cdot3(4) & 113\cdot7(5) \\ O(2)-C(P_2)-C(A_2) & 113\cdot3(4) & 113\cdot7(5) \\ O(2)-C(P_2)-C(A_2) & 119\cdot7(5) & 118\cdot5(5) \\ N(1)-C(P_2)-C(A_2) & 119\cdot7(5) & 118\cdot5(5) \\ N(1)-C(P_2)-C(A_2) & 121\cdot0(4) & 121\cdot7(5) \\ C(P_2)-N(1)-C(A_1) & 126\cdot2(4) & 126\cdot6(4) \\ \end{split}$	O(1) - C(P1) - C(A1)	118.3 (4)	115.9 (4)
$\begin{split} N(2)-C(P)-O(1) & 121\cdot5 \ (4) & 124\cdot2 \ (5) \\ C(1)-N(2)-C(P1) & 118\cdot2 \ (4) & 117\cdot9 \ (4) \\ C(A2)-N(2)-C(P1) & 125\cdot5 \ (4) & 126\cdot6 \ (4) \\ C(A2)-N(2)-C(P1) & 125\cdot5 \ (4) & 115\cdot4 \ (4) \\ C(B2)-C(A2)-N(2) & 110\cdot1 \ (4) & 113\cdot7 \ (5) \\ C(P2)-C(A2)-N(2) & 114\cdot6 \ (4) & 114\cdot1 \ (4) \\ C(P2)-C(A2)-N(2) & 113\cdot3 \ (4) & 113\cdot7 \ (5) \\ C(G2)-C(B2)-C(A2) & 119\cdot7 \ (5) & 118\cdot5 \ (5) \\ N(1)-C(P2)-C(A2) & 119\cdot7 \ (5) & 118\cdot5 \ (5) \\ N(1)-C(P2)-C(A2) & 119\cdot7 \ (4) & 121\cdot7 \ (5) \\ C(P2)-N(1)-C(A1) & 126\cdot2 \ (4) & 121\cdot7 \ (5) \\ C(P2)-N(1)-C(A1) & 126\cdot2 \ (4) & 126\cdot6 \ (4) \\ (c) \ Important \ torsion \ angles \ (^{O}) \\ C(2)-C(G1)-C(B1)-C(A1) & 93\cdot2 \ (5) & -90\cdot1 \ (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot6 \ (5) & 89\cdot1 \ (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot6 \ (5) & 89\cdot1 \ (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7\cdot6 \ (6) & 0\cdot9 \ (7) \\ C(A1)-C(P1)-N(2) & 11\cdot1 \ (5) & 0\cdot0 \ (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7\cdot6 \ (6) & 0\cdot9 \ (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8\cdot3 \ (5) & -2\cdot7 \ (7) \\ C(A1)-C(P1)-C(B2)-C(B2) & 0\cdot9 \ (5) & 4\cdot3 \ (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3\cdot2 \ (5) & -3\cdot2 \ (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3\cdot2 \ (5) & -3\cdot2 \ (6) \\ N(2)-C(A2)-C(P2)-N(1) & 0\cdot7 \ (5) & 0\cdot9 \ (7) \\ \end{split}$	N(2)-C(P1)-C(A1)	120.0 (4)	119-8 (4)
$\begin{array}{cccccc} C(1)-N(2)-C(P1) & 118\cdot 2 (4) & 117\cdot 9 (4) \\ C(A2)-N(2)-C(P1) & 125\cdot 5 (4) & 126\cdot 6 (4) \\ C(A2)-N(2)-C(1) & 115\cdot 9 (4) & 115\cdot 4 (4) \\ C(B2)-C(A2)-N(2) & 110\cdot 1 (4) & 113\cdot 7 (5) \\ C(P2)-C(A2)-N(2) & 114\cdot 6 (4) & 114\cdot 1 (4) \\ C(P2)-C(A2)-C(B2) & 109\cdot 9 (4) & 110\cdot 0 (5) \\ C(C2)-C(B2)-C(A2) & 119\cdot 7 (5) & 118\cdot 5 (5) \\ N(1)-C(P2)-C(A2) & 119\cdot 7 (5) & 118\cdot 5 (5) \\ N(1)-C(P2)-C(A2) & 119\cdot 3 (4) & 119\cdot 7 (4) \\ N(1)-C(P2)-C(A2) & 119\cdot 3 (4) & 119\cdot 7 (4) \\ N(1)-C(P2)-C(A1) & 126\cdot 2 (4) & 126\cdot 6 (4) \\ \hline (c) Important torsion angles (°) \\ C(2)-C(G1)-C(B1)-C(A1) & -86\cdot 6 (5) & 89\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot 6 (5) & 89\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) & -86\cdot 6 (5) & 89\cdot 1 (6) \\ C(G1)-C(B1)-C(A1) - N(1) & 56\cdot 7 (5) & 64\cdot 0 (6) \\ N(1)-C(P1)-N(2) - C(A2) & -8\cdot 3 (5) & -2\cdot 7 (7) \\ C(P1)-C(A1)-C(P2) & 0.9 (5) & 4\cdot 3 (6) \\ N(2)-C(A2)-C(B2)-C(G2) & 57\cdot 2 (5) & 58\cdot 3 (6) \\ N(2)-C(A2)-C(B2)-C(A2) & -7\cdot 3 (5) & -3\cdot 2 (6) \\ C(A1)-C(P1)-N(1)-C(P1) & 0.7 (5) & 0.9 (7) \\ \end{array}$	N(2)-C(P1)-O(1)	121.5 (4)	124-2 (5)
$\begin{array}{ccccc} C(A2)-N(2)-C(P1) & 125 \cdot 5(4) & 126 \cdot 6(4) \\ C(A2)-N(2)-C(1) & 115 \cdot 9(4) & 115 \cdot 4(4) \\ C(B2)-C(A2)-N(2) & 110 \cdot 1(4) & 113 \cdot 7(5) \\ C(P2)-C(A2)-N(2) & 110 \cdot 1(4) & 113 \cdot 7(5) \\ C(P2)-C(A2)-N(2) & 113 \cdot 3(4) & 113 \cdot 7(5) \\ O(2)-C(B2)-C(A2) & 113 \cdot 3(4) & 113 \cdot 7(5) \\ O(2)-C(P2)-C(A2) & 119 \cdot 7(5) & 118 \cdot 5(5) \\ O(2)-C(P2)-C(A2) & 119 \cdot 7(5) & 118 \cdot 5(5) \\ O(2)-C(P2)-C(A2) & 119 \cdot 7(5) & 118 \cdot 5(5) \\ O(1)-C(P2)-C(A2) & 119 \cdot 7(5) & 118 \cdot 5(5) \\ O(2)-C(P2)-C(A2) & 119 \cdot 7(5) & 118 \cdot 5(5) \\ O(2)-N(1)-C(P2)-O(2) & 121 \cdot 0(4) & 121 \cdot 7(5) \\ C(P2)-N(1)-C(A1) & 126 \cdot 2(4) & 126 \cdot 6(4) \\ \hline (c) Important torsion angles (°) \\ C(2)-C(G1)-C(B1)-C(A1) & -86 \cdot 6(5) & 89 \cdot 1(6) \\ C(G1)-C(B1)-C(A1) - N(1) & 56 \cdot 7(5) & 64 \cdot 0(6) \\ O(1)-C(A1)-C(P1)-N(2) & 11 \cdot 1(5) & 0 \cdot 0(6) \\ C(P1)-C(A1)-C(P2) & -7 \cdot 6(6) & 0 \cdot 9(7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8 \cdot 3(5) & -2 \cdot 7(7) \\ C(P1)-N(2)-C(A2)-C(P2) & 0 \cdot 9(5) & 4 \cdot 3(6) \\ N(2)-C(A2)-C(B2)-C(G2) & 57 \cdot 2(5) & 58 \cdot 3(6) \\ N(2)-C(A2)-C(P2)-N(1) & 3 \cdot 2(5) & -3 \cdot 2(6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0 \cdot 7(5) & 0 \cdot 9(7) \\ \hline \end{array}$	C(1)-N(2)-C(P1)	118.2 (4)	117.9 (4)
$\begin{array}{ccccc} C(A2)-N(2)-C(1) & 115.9 (4) & 115.4 (4) \\ C(B2)-C(A2)-N(2) & 110.1 (4) & 113.7 (5) \\ C(P2)-C(A2)-N(2) & 114.6 (4) & 114.1 (4) \\ C(P2)-C(A2)-N(2) & 119.4 (4) & 113.7 (5) \\ C(G2)-C(B2)-C(A2) & 119.3 (4) & 113.7 (5) \\ O(2)-C(P2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A2) & 119.7 (5) & 118.5 (5) \\ N(1)-C(P2)-C(A2) & 119.3 (4) & 119.7 (4) \\ N(1)-C(P2)-O(2) & 121.0 (4) & 121.7 (5) \\ C(P2)-N(1)-C(A1) & 126.2 (4) & 126.6 (4) \\ \hline \\ (c) Important torsion angles (°) \\ C(2)-C(G1)-C(B1)-C(A1) & 93.2 (5) & -90.1 (6) \\ C(6)-C(G1)-C(B1)-C(A1) & -86.6 (5) & 89.1 (6) \\ C(G1)-C(B1)-C(A1)-N(1) & 56.7 (5) & 64.0 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7.6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8.3 (5) & -2.7 (7) \\ C(A1)-C(P2)-C(A2) & 0.9 (5) & 4.3 (6) \\ N(2)-C(A2)-C(B2)-C(G2) & 57.2 (5) & 58.3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3.2 (5) & -3.2 (6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0.7 (5) & 0.9 (7) \\ \end{array}$	C(A2) - N(2) - C(P1)	125-5 (4)	126-6 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(A2) - N(2) - C(1)	115-9 (4)	115-4 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(B2) - C(A2) - N(2)	110-1 (4)	113.7 (5)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(P_2)-C(A_2)-N(2)$	114.6 (4)	114.1 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(P2)-C(A2)-C(B2)	109.9 (4)	110.0(5)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(G2)-C(B2)-C(A2)	113.3 (4)	113.7 (5)
$\begin{split} &N(1) - C(P_2) - C(A_2) & 119 \cdot 3 \ (4) & 119 \cdot 7 \ (4) \\ &N(1) - C(P_2) - O(2) & 121 \cdot O \ (4) & 121 \cdot 7 \ (5) \\ &C(P_2) - N(1) - C(A_1) & 126 \cdot 2 \ (4) & 126 \cdot 6 \ (4) \\ \end{split}$	O(2) - C(P2) - C(A2)	119.7 (5)	118.5 (5)
$\begin{split} &N(1) - C(P_2) - O(2) & 121 \cdot O(4) & 121 \cdot O(5) \\ &C(P_2) - N(1) - C(A_1) & 126 \cdot C(4) & 126 \cdot C(4) \\ &(c) Important torsion angles (°) \\ &C(2) - C(G_1) - C(B_1) - C(A_1) & 93 \cdot C(5) & -90 \cdot I(6) \\ &C(6) - C(B_1) - C(A_1) & -86 \cdot G(5) & 89 \cdot I(6) \\ &C(G_1) - C(B_1) - C(A_1) & -86 \cdot G(5) & 89 \cdot I(6) \\ &C(G_1) - C(B_1) - C(A_1) & -81 \cdot I(5) & G(4 \cdot O(6) \\ &N(1) - C(A_1) - C(P_1) - N(2) & 11 \cdot I(5) & 0 \cdot O(6) \\ &C(P_1) - C(A_1) - C(P_2) & -7 \cdot G(6) & 0 \cdot O(7) \\ &C(A_1) - C(P_1) - N(2) - C(A_2) & -8 \cdot 3(5) & -2 \cdot 7(7) \\ &C(A_1) - C(P_1) - N(2) - C(A_2) & -8 \cdot 3(5) & -2 \cdot 7(7) \\ &C(P_1) - N(2) - C(A_2) - C(P_2) & 0 \cdot 9(5) & 4 \cdot 3(6) \\ &N(2) - C(A_2) - C(B_2) - C(G_2) & 57 \cdot 2(5) & 58 \cdot 3(6) \\ &N(2) - C(A_2) - C(P_2) - N(1) & 3 \cdot 2(5) & -3 \cdot 2(6) \\ &C(A_2) - C(P_2) - N(1) - C(A_1) & 0 \cdot 7(5) & 0 \cdot 9(7) \\ \\ &N(A_1) - N(A_2) - N($	N(1) - C(P2) - C(A2)	119.3 (4)	119-7 (4)
C(P2)-N(1)-C(A1) 126-2 (4) 126-6 (4) (c) Important torsion angles (°) $C(2)-C(G1)-C(B1)-C(A1)$ 93-2 (5) $-90\cdot1$ (6) C(6)-C(G1)-C(B1)-C(A1) $-86\cdot6$ (5) $89\cdot1$ (6) C(G1)-C(B1)-C(A1) $-86\cdot6$ (5) $89\cdot1$ (6) C(G1)-C(B1)-C(A1) $-86\cdot6$ (5) $64\cdot0$ (6) N(1)-C(A1)-C(P1)-N(2) $11\cdot1$ (5) $0\cdot0$ (6) C(P1)-C(A1)-N(1)-C(P2) $-7\cdot6$ (6) $0\cdot9$ (7) C(A1)-C(P1)-N(2)-C(A2) $-8\cdot3$ (5) $-2\cdot7$ (7) C(P1)-N(2)-C(A2)-C(P2) $0\cdot9$ (5) $4\cdot3$ (6) N(2)-C(A2)-C(B2)-C(G2) $57\cdot2$ (5) $58\cdot3$ (6) N(2)-C(A2)-C(P2)-N(1) $3\cdot2$ (5) $-3\cdot2$ (6) N(2)-C(A2)-C(P2)-N(1) $0\cdot7$ (5) $0\cdot9$ (7)	$N(1) - C(P_2) - O(2)$	121.0 (4)	121-7 (5)
(c) Important torsion angles (°) C(2)-C(G1)-C(B1)-C(A1) 93·2 (5) -90·1 (6) C(6)-C(G1)-C(B1)-C(A1) -86·6 (5) 89·1 (6) C(G1)-C(B1)-C(A1) -N(1) 56·7 (5) 64·0 (6) N(1)-C(A1)-C(P1)-N(2) 11·1 (5) 0·0 (6) C(P1)-C(A1)-C(P2) -7·6 (6) 0·9 (7) C(A1)-C(P1)-N(2)-C(A2) -8·3 (5) -2·7 (7) C(P1)-N(2)-C(A2)-C(P2) 0·9 (5) 4·3 (6) N(2)-C(A2)-C(B2)-C(G2) 57·2 (5) 58·3 (6) N(2)-C(A2)-C(P2)-N(1) 3·2 (5) -3·2 (6) C(A2)-C(P2)-N(1)-C(A1) 0·7 (5) 0·9 (7)	$C(P_2) - N(1) - C(A_1)$	126-2 (4)	126-6 (4)
(c) Iniportant doston angles ($)$ 93-2 (5) -90-1 (6) C(2)-C(G1)-C(B1)-C(A1) -86-6 (5) 89-1 (6) C(G)-C(G1)-C(B1)-C(A1) -86-6 (5) 89-1 (6) C(G1)-C(B1)-C(A1)-N(1) 56-7 (5) 64-0 (6) N(1)-C(A1)-N(2) 11-1 (5) 0-0 (6) C(P1)-C(A1)-N(1)-C(P2) -7-6 (6) 0-9 (7) C(A1)-C(P1)-N(2)-C(A2) -8-3 (5) -2-7 (7) C(P1)-N(2)-C(A2)-C(P2) 0-9 (5) 4-3 (6) N(2)-C(A2)-C(B2)-C(C2) 57-2 (5) 58-3 (6) N(2)-C(A2)-C(P2)-N(1) 3-2 (5) -3-2 (6) C(A2)-C(P2)-N(1) 0-7 (5) 0-9 (7)	(a) Important torsion angles (°)		
$\begin{array}{llllllllllllllllllllllllllllllllllll$	(c) Important torsion angles ()	02 2 (5)	00 1 (()
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	C(2) - C(G1) - C(B1) - C(A1)	93.2 (5)	-90.1(6)
$\begin{array}{c} C(4)_{1}-C(4)_{1}-N(1) & 30^{-7}(5) & 64^{-0}(6) \\ N(1)-C(4)_{1}-N(2) & 11\cdot 1(5) & 0.0 (6) \\ C(P1)-C(A1)-N(1)-C(P2) & -7\cdot6 (6) & 0.9 (7) \\ C(A1)-C(P1)-N(2)-C(A2) & -8\cdot3 (5) & -2\cdot7 (7) \\ C(P1)-N(2)-C(A2)-C(P2) & 0.9 (5) & 4\cdot3 (6) \\ N(2)-C(A2)-C(B2)-C(C2) & 57\cdot2 (5) & 58\cdot3 (6) \\ N(2)-C(A2)-C(P2)-N(1) & 3\cdot2 (5) & -3\cdot2 (6) \\ C(A2)-C(P2)-N(1)-C(A1) & 0.7 (5) & 0.9 (7) \end{array}$	$C(0) \rightarrow C(0) \rightarrow $	-00.0(3)	64 0 (4)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	U(U) = U(B) = U(A) = N(1)	$30 \cdot 7 (3)$	04.0(0)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N(1) = C(A(1) = C(P(1) = N(2)) C(B(1) = C(A(1) = N(1) = C(B(2))	7.6 (6)	0.0(0)
$\begin{array}{llllllllllllllllllllllllllllllllllll$	C(A1) = C(B1) = N(1) = C(F2) C(A1) = C(B1) = N(2) = C(A2)	- 7.0 (0)	-2.7(7)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	$C(P_1) = C(P_1) = O(2) = C(P_2)$	0.9 (5)	4.3 (6)
$\begin{array}{cccccccccccccccccccccccccccccccccccc$	N(2) = C(A2) = C(B2) = C(G2)	57.2 (5)	58.3 (6)
$C(A_2)-C(P_2)-N(1)-C(A_1)$ 0.7 (5) 0.9 (7)	N(2) = C(A2) = C(D2) = C(D2) N(2) = C(A2) = C(P2) = N(1)	3.2 (5)	-3.2 (6)
	$C(A_2) - C(P_2) - N(1) - C(A_1)$	0.7(5)	0.9 (7)

Table 3. The Cremer & Pople (1975) puckeringparameters of the DKP rings

The sequence C(P1), C(A1), N(1), C(P2), C(A2), N(2) is used.

	Molecule A	Molecule B
q_1 (Å)	0.084 (5)	0.030 (6)
$q_1(\mathbf{\dot{A}})$	-0.037 (5)	-0.015 (6)
$\hat{Q}(\mathbf{A})$	0.092 (5)	0.033 (7)
φ, (°)	211 (3)	76 (12)
$\theta_2^{(\circ)}$	114 (3)	117 (12)

final ΔF map. Atomic scattering factors from International Tables for X-ray Crystallography (1974). Computer programs used: SHELX76 (Sheldrick, 1976), MULTAN78 (Main et al., 1978), PLUTO (Motherwell & Clegg, 1978) and local programs (Jaskólski, 1982).

Discussion. Final positional parameters are given in Table 1, molecular dimensions in Table 2.* Fig. 1 shows the conformation of the two crystallographically independent molecules, A and B, and the atomnumbering scheme. The overall conformation of both molecules is very similar and different from the predominant conformation observed in solution (Liberek et al., 1977). The side chains of the two α -amino-acid residues of *cvclo*[-L-Phe-L-*N*(Me)-Abu-] have $\chi^1 \simeq 60^\circ$ and are in a folded conformation. The DKP ring in molecule B is nearly planar while in molecule A it is slightly distorted from planarity towards screw boat $C_{i}^{r}S_{C_{i}}$ (notation proposed by Boyens, 1978). Puckering parameters (Cremer & Pople, 1975) characterizing the six-membered DKP rings are given in Table 3.

The molecular packing is shown in Fig. 2. Molecules A are bonded via $N(1A)-H(18)\cdots O(1A)$ hydrogen bonds to form chains parallel to **b**, and molecules B join to those chains via $N(1B)-H(36)\cdots O(2A)$ hydrogen

^{*} Lists of structure factors, anisotropic thermal parameters and H-atom parameters have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 44707 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.





Fig. 1. The conformation of the cyclo[-L-Phe-L-N(Me)-Abu-] molecules. (a) Molecule A; (b) molecule B.



Fig. 2. The crystal structure of *cyclo*[-L-Phe-L-N(Me)-Abu-] viewed down c; dashed lines show the N-H···O hydrogen bonds $[O(1A)\cdots N(1A^{1}) 2.856 (6) \text{ Å}, O(1A)-H(18)\cdots N(1A^{1}) 158 (3)^{\circ},$ (i): -x, 0.5+y, -z; $N(1B)\cdots O(2A^{11}) 2.907 (5) \text{ Å}, O(1A)-H(36)\cdots N(1A^{1}) 170 (3)^{\circ},$ (ii): x, 1+y, -1+z].

bonds. In effect, molecule B is only a hydrogen-bond donor while molecule A is a donor in one H bond and an acceptor in two bonds. The packing scheme is quite different from that observed in the other mono-Nmethylated cyclic dipeptide, cyclo[-L-N(Me)-Phe-L-Phe-] (Gdaniec & Liberek, 1987) where two crystallographically independent molecules are joined by a pair of $N-H\cdots O$ hydrogen bonds to form dimers as distinct units in the crystal lattice.

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Structure of 1,4-Diaminoanthraquinone Dihydrate

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Abstract. $C_{14}H_{10}N_2O_2.2H_2O$, $M_r = 274.28$, orthorhombic, *Pnma*, a = 15.686 (2), b = 16.200 (2), c = 4.8507 (3) Å, V = 1232.6 (2) Å³, Z = 4, $D_m = 1.47$, $D_x = 1.478$ Mg m⁻³, $\lambda(Cu K\alpha) = 1.5418$ Å, $\mu = 0.87$ mm⁻¹, m.p. 541 K, F(000) = 576, T = 293 K, final R = 0.039 for 1024 unique reflections. The anthraquinone molecule has C_s symmetry in the crystal. The molecules are stacked along **c** with an interplanar spacing of 3.367 (2) Å. The dihedral angle between the molecules related by an a glide is 88.0 (1)°. The molecules related by a I and a 2_1 along **c** are linked together by three kinds of hydrogen bonds through the water molecules.

Introduction. The molecule of 1,4-diaminoanthraquinone has rather high molecular symmetry, $C_{2\nu}$. The present work has been undertaken as part of a study to obtain experimental data on the most probable space group for symmetrical molecules. In addition, tricyclic anthraquinones have recently drawn attention because of their anticancer activity (Neidle, 1984). Thus, it is also of value to determine the molecular structure and mode of molecular overlapping in the crystal for one of the fundamental compounds of the anthraquinones.

Experimental. Crystals grown by slow evaporation from pyridine, dark purple prisms elongated along c. D_m by

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