The compound crystallizes with one nucleotide molecule and one acetone solvent molecule in the asymmetric unit. There are no particularly short contacts between the acetone and nucleotide molecules. The nucleotide molecules are linked *via* O(2)···H(3)—N(3) intermolecular hydrogen bonds of length 2·871 (4) Å [O(2)···H(3) = 1·93 (1) Å] into dimers with crystallographic twofold symmetry.

The thymine base in (1) adopts, in the crystal, the *anti* conformation. The torsion angle about the glycosidic bond, χ, O(4′)—C(1′)—N(1)—C(2), is 267·8°.* Both *syn* and *anti* conformations have been found in neutral derivatives of pyrimidine cyclic nucleotides (Bentrude *et al.*, 1986, and references therein). For example, in *cis*-thymidine 3′,5′-cyclic *N*,*N*-dimethylphosphoramidate, (2) [C(7′)CH_3 of (1) equals $(CH_3)_2N$], the base is also *anti* (χ = 252·8 and 233·1°) (Bentrude *et al.*, 1986). In the *trans*-phosphoramidate, however, the *syn* conformation (χ = 82·6°) has been found in the crystal (Newton *et al.*, 1977).

The ribose of (1) is seen to adopt the T_4^3 (half-chair) conformation (Sundaralingam & Abola, 1972). The C(4′)—O(4′)—C(1′)—C(2′), ν_0, and O(4′)—C(1′)—C(2′)—C(3′), ν_1, torsion angles are −16·0 and −13·0°, respectively. Interestingly, in the *cis*-phosphoramidate, (2) (Bentrude *et al.*, 1986), the ribose ring adopts a $_4E$ (envelope) conformation where ν_0 and ν_1 average −28·3 and 1·5°, respectively. The *trans*-phosphoramidate (Newton *et al.*, 1977) shows the ribose ring to be in a $_4T^3$ (twist-envelope) conformation (ν_0 = −23·0, ν_1 = −5·5°).

The O(3′)—P—O(5′)—C(5′) and O(5′)—P—O(3′)—C(3′) torsion angles of −36·5 and 38·2°, respectively, indicate the phosphorus end of the chair-form 1,3,2-dioxaphosphorinane ring to be flattened. Such ring flattening has been observed in the *cis*-phosphoramidate, (2), [O(3′)—P—O(5′)—C(5′) and O(5′)—P—O(3′)—C(3′) average −37·9 and 39·5°, respectively] (Bentrude *et al.*, 1986), in the *trans*-phosphoramidate [O(3′)—P—O(5′)—C(5′) = −44·3, O(5′)—P—O(3′)—C(3′) = 48·3°] (Newton *et al.*, 1977), and in 1,3,2-dioxaphosphorinanes in general (Warrent, Caughlan, Hargis, Yee & Bentrude, 1978).

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* The atom labeling and definitions of χ, ν_0 and ν_1 are according to *Eur. J. Biochem.* (1983), **131**, 9–15.

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Structure of Pivaloyloxymethyl (3*S*,5*R*)-6,6-Dibromopenicillanate 1,1-Dioxide

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Abstract. $C_{14}H_{19}Br_2NO_7S$, M_r = 505·2, orthorhombic, $P2_12_12_1$, a = 9·241 (1), b = 10·478 (1), c = 20·082 (3) Å, V = 1944·5 Å^3, Z = 4, D_x = 1·726 g cm^{-3}, λ (Cu $K\alpha$) = 1·5418 Å, μ = 62·4 cm^{-1}, $F(000)$ = 1008, room temperature, final R = 0·040 for 1348 independent reflections. The thiazolidine ring adopts a conformation with the sulfur atom 0·80 (1) Å

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out of the plane formed by the other four members of the ring. The nitrogen atom conforms to the characteristic pyramidal arrangement of penicillins. The double ester shows an extended conformation, with a relatively high thermal mobility of its three methyl groups. No unusually short intermolecular distances were found.

Introduction. The crystallographic analysis of the title compound is part of a systematic structural investigation of new 1,6-substituted penam derivatives, possible useful intermediates for further chemioselective transformations.

The structures of three mixed 6,6-dihalopenicillanates were reported in the first paper of this series (Belinzoni, Mascaretti, Alzari, Punte, Faerman & Podjarny, 1985). In order to establish the influence of different substituents on the conformation of the penam nucleus, the crystal and molecular structure of pivaloyloxymethyl 6,6-dibromopenicillanate 1,1-dioxide was determined and is discussed in the present paper.

Experimental. Crystallized by slow evaporation from toluene; transparent prismatic shaped crystal, approximate dimensions $0{\cdot}40 \times 0{\cdot}15 \times 0{\cdot}15$ mm; D_m not measured; automatic four-circle Huber diffractometer; Ni-filtered Cu $K\alpha$ radiation; ω scans; integrated intensities as described by Lehmann & Larsen (1974); lattice parameters from 20 reflections with 2θ between 65 and 75°; space group $P2_12_12_1$ (No. 19). Lorentz and polarization corrections, empirical absorption correction (Silva, Viturro & Alzari, 1986) following North, Phillips & Mathews (1968) and Huber & Kopfmann (1969); max., min. transmission factors 1·00, 1·35; data collected to $2\theta_{\max} = 120°$ in positive octant, $0 \leq h \leq 10$, $0 \leq k \leq 11$, $0 \leq l \leq 22$; four reference reflections showed up to 3% average fluctuation; 1416 unique reflections measured, not obscured by diffractometer geometry, of which 1348 with $I > 1{\cdot}5\sigma(I)$ considered observed. Structure solved by Patterson and Fourier techniques; refined by full-matrix least squares based on F's; $w = 1/[\sigma^2(F) + 0{\cdot}0016F^2]$; most H atoms located in difference Fourier map, all stereochemically positioned (C—H = 1·08 Å) with isotropic thermal parameters (not refined) equal to those of bonded C atoms; all methyl groups refined as rigid bodies; remaining H-atom positions riding on corresponding heavy atoms. Secondary-extinction correction of form $F' = F(1 - CF^2/\sin\theta)$ applied on F_{calc}, refined value of $C = 3{\cdot}6\,(7) \times 10^{-7}$. Final agreement factors $R = 0{\cdot}0403$, $wR = 0{\cdot}0497$ for 242 parameters refined; ratio of max. least-squares shift to e.s.d. in final refinement cycle 0·20 for non-H atoms; max. and min. heights in final difference Fourier synthesis 0·29 and $-0{\cdot}48$ e Å^{-3}. Scattering factors from *International Tables for X-ray Crystallography* (1974); main computer programs used those of *SHELX76* (Sheldrick, 1976).

Discussion. Fractional atomic coordinates and equivalent isotropic temperature factors for non-H atoms are listed in Table 1,* bond lengths and angles in Table 2. The structure of the molecule is represented in Fig. 1.

It is known that the thiazolidine ring of penicillins may adopt two conformations, to avoid eclipsing of the substituents at C(2) and C(3) (Sweet, 1972). In the title compound, the S(1) atom is out of the plane formed by C(2)C(3)N(4)C(5). The conformation with C(3) out of the mean plane through the other four is not allowed because of steric restrictions between the substituents at S(1) and C(6). As expected, the same conformation was assigned by NMR–nuclear Overhauser effect spectroscopy in solution (Belinzoni, 1985).

The bond angle C(5)—S(1)—C(2) [93·1 (4)°] is significantly larger than the average value [90·2 (5)°] found by Domiano, Nardelli, Balsamo, Macchia & Macchia (1979) in several compounds having the same thiazolidine ring conformation. The rest of the bond angles and lengths are in good agreement with the reported average values.

The intramolecular contact O(23)···Br(2) [3·17 (1) Å] affects the dihedral angle between the β-lactam and thiazolidine rings: in the present compound this value is 44·0 (7)°, while in compounds lacking O(23) or Br(2) it is significantly higher, 50·2° for pivaloyloxymethyl (6*S*)-6-bromopenicillanate 1,1-dioxide (Alzari, Ronco, Rivero & Punte, 1986) and 50·7° for methyl (1*R*)-6,6-dibromopenicillanate 1-oxide (Peeters, Blaton & De Ranter, 1982).

The N atom occurs in a pyramidal arrangement with its ligands: the distance from N(4) to the plane defined by C(3), C(5), C(7) is 0·32 (1) Å; the sum of bond angles around N(4) is 344·5 (2)°.

The β-lactam ring is slightly puckered, with N(4), C(6), C(7), O(8) in a planar arrangement within experimental error.* The C(5) atom is 0·20 (1) Å out of this plane. The lack of planarity is also revealed by a dihedral angle of 9·4 (8)° between the planes defined by N(4)C(5)C(6) and N(4)C(7)C(6). Bond lengths and angles (Table 2) agree closely with average reported values (Domiano *et al.*, 1979).

The orientation of the pivaloyloxymethyl ester is defined by the torsion angles C(2)—C(3)—C(11)—O(13) = 73·1 (8), C(3)—C(11)—O(13)—C(14) = −169·4 (6), C(11)—O(13)—C(14)—O(15) = 97·8 (7), O(13)—C(14)—O(15)—C(16) = 85·8 (7) and C(14)—O(15)—C(16)—C(18) = −174·0 (6)° (Fig. 1). The

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* Lists of structure factors, anisotropic temperature factors, H-atom positions and mean-plane calculations have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 42847 (11 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

dihedral angle between the plane defined by C(2)-C(3)N(4) and the carboxyl group [65·7 (7)°] is determined primarily by the intramolecular contact N(4)···O(12) [2·81 (1) Å]. The configuration of the chiral centre at C(3) is *S*, the other chiral centre of the molecule [C(5)] is *R* (from starting material).

The C—O bond lengths in the ester group (Table 2) are similar to the commonly accepted values of 1·34 (2) [C(sp^2)—O] and 1·426 (5) Å [C(sp^3)—O]. At the end of the side chain, the methyl groups have rather large thermal factors. Therefore the differences between the observed C—C distances and the standard value of 1·537 (5) Å are probably not statistically significant.

The crystal packing is shown in Fig. 2. The shortest intermolecular distances between non-H atoms are O(23)···Br(1) = 3·04 (1), Br(2)···O(12) = 3·23 (1), O(22)···C(21) = 3·49 (2), O(23)···C(9) = 3·46 (2), O(12)···C(20) = 3·54 (3) Å. The contacts C(3)—H(3)···O(17) [C(3)···O(17) = 3·215 (6), H(3)···O(17) = 2·40 (2) Å], C(5)—H(5)···O(8) [C(5)···O(8) = 3·50 (1), H(5)···O(8) = 2·46 (2) Å] and C(14)—H1(C14)···O(8) [C(14)···O(8) = 3·58 (1), H1(C14)···O(8) = 2·51 (1) Å] suggest a significant electrostatic contribution to the packing forces.

Table 1. *Fractional coordinates and equivalent isotropic thermal parameters* (Å^2 × 10^3), *with e.s.d.'s in parentheses*

$$U_{eq} = \tfrac{1}{3}(U_{11} + U_{22} + U_{33}).$$

	x	*y*	*z*	U_{eq}
S(1)	0·8068 (3)	0·1309 (2)	0·2279 (1)	71 (2)
C(2)	0·8752 (11)	0·1111 (9)	0·3140 (4)	68 (6)
C(3)	0·7392 (10)	0·1416 (8)	0·3555 (4)	63 (5)
N(4)	0·6124 (8)	0·1142 (7)	0·3162 (3)	59 (4)
C(5)	0·6295 (12)	0·0645 (8)	0·2484 (4)	63 (5)
C(6)	0·4863 (11)	0·1331 (7)	0·2304 (4)	62 (5)
C(7)	0·4933 (12)	0·1900 (8)	0·3001 (4)	65 (5)
O(8)	0·4300 (8)	0·2710 (6)	0·3300 (3)	70 (4)
C(9)	0·9217 (12)	−0·0325 (8)	0·3205 (5)	73 (6)
C(10)	1·0010 (13)	0·1993 (10)	0·3233 (5)	81 (6)
C(11)	0·7389 (10)	0·0649 (9)	0·4220 (4)	62 (6)
O(12)	0·6697 (8)	−0·0283 (7)	0·4315 (3)	78 (4)
O(13)	0·8386 (8)	0·1160 (6)	0·4632 (3)	72 (4)
C(14)	0·8727 (12)	0·0472 (11)	0·5215 (5)	77 (7)
O(15)	1·0015 (8)	−0·0241 (6)	0·5094 (3)	75 (4)
C(16)	1·1267 (13)	0·0399 (11)	0·5202 (5)	80 (7)
O(17)	1·1281 (10)	0·1465 (9)	0·5406 (5)	120 (7)
C(18)	1·2602 (13)	−0·0370 (12)	0·4994 (5)	89 (8)
C(19)	1·3014 (13)	0·0189 (15)	0·4302 (6)	99 (8)
C(20)	1·2317 (19)	−0·1776 (14)	0·4864 (10)	136 (12)
C(21)	1·3768 (18)	−0·0065 (22)	0·5495 (7)	178 (16)
Br(1)	0·3282 (1)	0·0117 (1)	0·2272 (1)	82 (1)
Br(2)	0·4750 (1)	0·2503 (1)	0·1585 (1)	85 (1)
O(22)	0·8815 (9)	0·0504 (7)	0·1811 (3)	96 (5)
O(23)	0·7939 (8)	0·2649 (6)	0·2165 (3)	83 (4)

Table 2. *Bond lengths* (Å) *and angles* (°) *with e.s.d.'s in parentheses*

C(2)—S(1)	1·851 (10)	C(5)—S(1)	1·826 (10)
O(22)—S(1)	1·440 (7)	O(23)—S(1)	1·427 (7)
C(3)—C(2)	1·542 (13)	C(9)—C(2)	1·570 (13)
C(10)—C(2)	1·498 (14)	N(4)—C(3)	1·442 (11)
C(11)—C(3)	1·559 (12)	C(5)—N(4)	1·467 (10)
C(7)—N(4)	1·396 (12)	C(6)—C(5)	1·549 (14)
C(7)—C(6)	1·523 (12)	Br(1)—C(6)	1·939 (9)
Br(2)—C(6)	1·898 (8)	O(8)—C(7)	1·194 (11)
O(12)—C(11)	1·183 (11)	O(13)—C(11)	1·350 (11)
C(14)—O(13)	1·411 (11)	O(15)—C(14)	1·426 (12)
C(16)—O(15)	1·354 (13)	O(17)—C(16)	1·190 (12)
C(18)—C(16)	1·532 (16)	C(19)—C(18)	1·556 (14)
C(20)—C(18)	1·519 (20)	C(21)—C(18)	1·508 (18)
C(5)—S(1)—C(2)	93·1 (4)	O(22)—S(1)—C(2)	112·4 (5)
O(22)—S(1)—C(5)	110·7 (4)	O(23)—S(1)—C(2)	106·8 (4)
O(23)—S(1)—C(5)	109·6 (5)	O(23)—S(1)—O(22)	120·7 (5)
C(3)—C(2)—S(1)	101·8 (6)	C(9)—C(2)—S(1)	106·1 (6)
C(9)—C(2)—C(3)	112·1 (8)	C(10)—C(2)—S(1)	108·3 (7)
C(10)—C(2)—C(3)	115·9 (8)	C(10)—C(2)—C(9)	111·6 (9)
N(4)—C(3)—C(2)	108·9 (6)	C(11)—C(3)—C(2)	111·0 (7)
C(11)—C(3)—N(4)	111·4 (7)	C(5)—N(4)—C(3)	119·5 (7)
C(7)—N(4)—C(3)	130·9 (7)	C(7)—N(4)—C(5)	94·1 (7)
N(4)—C(5)—S(1)	99·8 (6)	C(6)—C(5)—S(1)	122·5 (6)
C(6)—C(5)—N(4)	87·7 (7)	C(7)—C(6)—C(5)	86·0 (7)
Br(1)—C(6)—C(5)	110·3 (5)	Br(1)—C(6)—C(7)	108·6 (6)
Br(2)—C(6)—C(5)	121·7 (6)	Br(2)—C(6)—C(7)	116·6 (5)
Br(2)—C(6)—Br(1)	110·9 (5)	C(6)—C(7)—N(4)	91·4 (7)
O(8)—C(7)—N(4)	132·4 (8)	O(8)—C(7)—C(6)	136·1 (9)
O(12)—C(11)—C(3)	124·4 (8)	O(13)—C(11)—C(3)	108·6 (8)
O(13)—C(11)—O(12)	126·8 (8)	C(14)—O(13)—C(11)	117·3 (8)
O(15)—C(14)—O(13)	108·1 (8)	C(16)—O(15)—C(14)	115·2 (7)
O(17)—C(16)—O(15)	121·9 (11)	C(18)—C(16)—O(15)	112·6 (9)
C(18)—C(16)—O(17)	125·4 (12)	C(19)—C(18)—C(16)	104·1 (10)
C(20)—C(18)—C(16)	114·7 (11)	C(20)—C(18)—C(19)	104·7 (12)
C(21)—C(18)—C(16)	106·4 (10)	C(21)—C(18)—C(19)	110·0 (12)
C(21)—C(18)—C(20)	116·4 (15)		

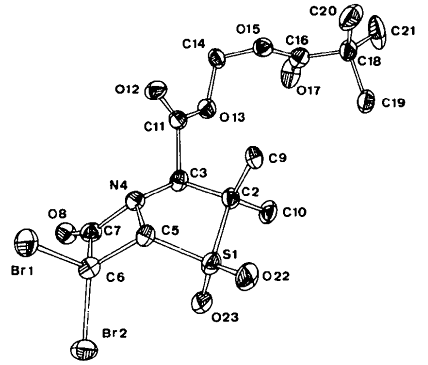

Fig. 1. *ORTEP* (Johnson, 1965) thermal ellipsoid (20%) plot, showing atomic numbering. Hydrogens are omitted.

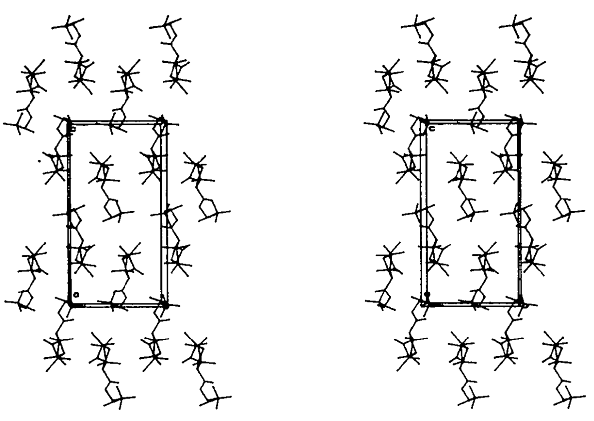

Fig. 2. Stereoview of the molecular packing.

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Structure of Pivaloyloxymethyl (3*S*,5*R*,6*S*)-6-Bromopenicillanate 1,1-Dioxide

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Abstract. $C_{14}H_{20}BrNO_7S$, $M_r = 426{\cdot}3$, orthorhombic, $P2_12_12_1$, $a = 6{\cdot}176\,(1)$, $b = 19{\cdot}965\,(5)$, $c = 17{\cdot}477\,(4)$ Å, $V = 1831{\cdot}2$ Å^3, $Z = 4$, $D_x = 1{\cdot}546$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 23{\cdot}1$ cm^{-1}, $F(000) = 872$, room temperature, final $R = 0{\cdot}049$ for 1232 independent reflections. In the thiazolidine ring, the sulfur atom is 0·75 (1) Å out of the plane formed by the four other members of the ring. The distance from the N atom to the plane defined by its bonded atoms is 0·41 (1) Å. The ester group adopts an extended conformation, with thermal factors greater than those of the rigid molecular nucleus. Packing results from normal van der Waals contacts.

Introduction. This paper continues investigations on the influence of different 1,6-substituents on the penam nucleus of pivaloyloxymethyl penicillanates.

Experimental. Long needle-like transparent crystals by slow evaporation from mixture of petroleum ether/toluene/ethyl acetate at 291 K; automatic four-circle Huber diffractometer; graphite-monochromated Mo $K\alpha$ radiation; ω scans; integrated intensities as described by Lehmann & Larsen (1974); lattice parameters from setting angles of 16 reflections with 2θ values between 24 and 30°; space group $P2_12_12_1$ (No. 19). Lorentz and polarization corrections; no absorption corrections; data collected to $2\theta_{\max} = 45°$ in positive octant, index range 0 to 6, 0 to 18, 0 to 18 for h,k,l respectively; five standard reflections showed linear decay of intensities (corrected, limit values 1·0069 and 1·0687). 1271 unique reflections measured, of which 1232 with $I > 1{\cdot}5\sigma(I)$ considered observed. Structure solved by Patterson and Fourier methods; refined by full-matrix least squares based on F's; H atoms stereochemically positioned with isotropic thermal parameters (not refined) as those of bonded C atoms; all methyl groups refined as rigid bodies; remaining hydrogen positional parameters riding on corresponding C atoms. Secondary-extinction coefficient of form $F' = F(1 - CF^2/\sin\theta)$ applied on $F_{\rm calc}$, refined value of $C = 1{\cdot}8\,(6) \times 10^{-7}$. Final agreement factors $R = 0{\cdot}0491$, $wR = 0{\cdot}0566$ for 233 parameters refined; weighting scheme $w = 1/[\sigma^2(F) + 0{\cdot}00244F^2]$; max. and min. heights in final difference Fourier synthesis 0·56 and $-0{\cdot}32$ e Å^{-3}; $(\Delta/\sigma)_{\max} = 0{\cdot}34$ for non-H atoms. Scattering factors from *International Tables for X-ray Crystallography* (1974); computer programs: *SHELX76* (Sheldrick, 1976).

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