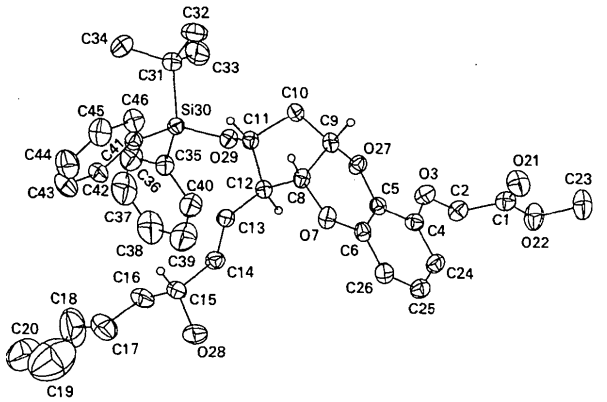

Fig. 1. Perspective view of the title compound, with the atom-numbering system.

were from *International Tables for X-ray Crystallography* (1974, Vol. IV). Calculations on a FACOM M340*R* computer at our laboratories. Final atomic coordinates and equivalent isotropic temperature factors are given in Table 1. Selected bond lengths and angles are listed in Table 2.* A perspective view of the molecule with the atom-numbering system is presented in Fig. 1.

The temperature factors of C(18), C(19) and C(20) are very large and exhibit a large anisotropy. The bond lengths and angles relevant to the atoms, for which the libration corrections have not been applied, are less reliable.

* Lists of anisotropic temperature factors of the non-H atoms, H-atom coordinates, all bond lengths and angles, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53827 (36 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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

C(1)—C(2)	1·480 (6)	C(1)—O(21)	1·178 (6)
C(1)—O(22)	1·337 (5)	C(2)—O(3)	1·427 (5)
O(3)—C(4)	1·370 (5)	C(4)—C(5)	1·396 (5)
C(4)—C(24)	1·369 (6)	C(5)—C(6)	1·388 (5)
C(5)—O(27)	1·367 (5)	C(6)—O(7)	1·372 (5)
C(6)—C(26)	1·371 (6)	O(7)—C(8)	1·437 (5)
C(8)—C(9)	1·506 (5)	C(8)—C(12)	1·522 (5)
C(9)—C(10)	1·525 (6)	C(9)—O(27)	1·460 (5)
C(10)—C(11)	1·540 (5)	C(11)—C(12)	1·523 (5)
C(11)—O(29)	1·422 (5)	C(12)—C(13)	1·482 (5)
O(22)—C(23)	1·451 (8)	C(24)—C(25)	1·393 (6)
C(25)—C(26)	1·353 (6)	O(29)—Si(30)	1·638 (4)
Si(30)—C(31)	1·890 (4)	Si(30)—C(35)	1·873 (4)
Si(30)—C(41)	1·873 (4)		

C(2)—C(1)—O(21)	128·2 (4)	C(2)—C(1)—O(22)	108·2 (4)
O(21)—C(1)—O(22)	123·6 (4)	C(1)—C(2)—O(3)	112·0 (3)
C(2)—O(3)—C(4)	118·8 (3)	O(3)—C(4)—C(5)	113·6 (4)
O(3)—C(4)—C(24)	125·4 (4)	C(5)—C(4)—C(24)	120·9 (4)
C(4)—C(5)—C(6)	118·5 (3)	C(4)—C(5)—O(27)	118·2 (3)
C(6)—C(5)—O(27)	123·2 (3)	C(5)—C(6)—O(7)	121·6 (4)
C(5)—C(6)—C(26)	120·2 (4)	O(7)—C(6)—C(26)	118·3 (4)
C(6)—O(7)—C(8)	115·8 (3)	O(7)—C(8)—C(9)	114·2 (3)
O(7)—C(8)—C(12)	115·4 (3)	C(9)—C(8)—C(12)	103·8 (3)
C(8)—C(9)—C(10)	103·5 (3)	C(8)—C(9)—O(27)	110·2 (3)
C(10)—C(9)—O(27)	106·4 (3)	C(9)—C(10)—C(11)	105·8 (3)
C(10)—C(11)—C(12)	105·5 (3)	C(10)—C(11)—O(29)	111·2 (3)
C(12)—C(11)—O(29)	112·7 (3)	C(8)—C(12)—C(11)	100·2 (3)
C(8)—C(12)—C(13)	115·6 (3)	C(11)—C(12)—C(13)	115·0 (3)
C(1)—O(22)—C(23)	118·5 (4)	C(4)—C(24)—C(25)	119·0 (4)
C(24)—C(25)—C(26)	120·5 (4)	C(6)—C(26)—C(25)	120·8 (4)
C(5)—O(27)—C(9)	114·2 (3)	C(11)—O(29)—Si(30)	131·0 (3)
O(29)—Si(30)—C(31)	109·5 (2)	O(29)—Si(30)—C(35)	103·3 (2)
O(29)—Si(30)—C(41)	112·5 (2)	C(31)—Si(30)—C(35)	113·3 (2)
C(31)—Si(30)—C(41)	110·0 (2)	C(35)—Si(30)—C(41)	108·0 (2)

Related literature. The title compound has been discussed by Mori & Takechi (1990).

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Structure of 2-Methyl-2-(5,5-dimethyl-3-hydantoinyl)propanamide

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Abstract. $C_9H_{15}N_3O_3$ (1), $M_r = 213{\cdot}24$, orthorhombic, *Pbca*, $a = 6{\cdot}323$ (3), $b = 16{\cdot}25$ (1), $c = 20{\cdot}16$ (1) Å, $V = 2071{\cdot}4$ Å^3, $Z = 8$, $D_m = 1{\cdot}362$ (2), $D_x = 1{\cdot}367$ g cm^{-3}, λ(Mo $K\alpha$) = 0·7107 Å, $\mu = 0{\cdot}973$ cm^{-1}, $F(000) = 912$, $T = 295$ K, $R(F) = 0{\cdot}043$ and $wR(F) = 0{\cdot}048$ for 2301 intensity data with $F > 3\sigma(F)$. The observed bond parameters are similar to those in 5,5-dimethylhydantoin except for an increase of 0·03 Å in the C—N bond lengths at the substituted ring N atom.

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Table 1. *Positional* ($\times 10^4$) *and equivalent isotropic thermal parameters for the non-*H *atoms in* (1)

$B_{eq} = \frac{1}{3}(B_{11} + B_{22} + B_{33})$.

	x	y	z	B_{eq} (Å^2)
O1	6294 (2)	2571·9 (6)	70·5 (4)	2·51 (2)
O2	3344 (2)	2624·9 (7)	2146·2 (5)	4·16 (3)
O3	7118 (2)	503·2 (6)	466·5 (5)	2·92 (3)
N1	4549 (2)	3589·6 (6)	651·5 (6)	2·45 (3)
N2	5023 (2)	2365·1 (6)	1138·5 (5)	2·37 (3)
N3	3769 (2)	963·8 (7)	407·9 (6)	2·74 (3)
C1	5372 (2)	2833·9 (7)	557·7 (6)	2·03 (3)
C2	3486 (2)	3670·3 (8)	1292·0 (6)	2·44 (3)
C3	1132 (3)	3821 (1)	1223·9 (9)	3·29 (4)
C4	4551 (4)	4332 (1)	1715 (1)	4·25 (5)
C5	3906 (2)	2826·9 (8)	1600·0 (6)	2·45 (3)
C6	6162 (2)	1572·8 (7)	1235·4 (6)	2·10 (3)
C7	8510 (2)	1743·6 (9)	1305·8 (8)	2·72 (3)
C8	5356 (3)	1114·2 (9)	1854·1 (7)	2·98 (3)
C9	5724 (2)	986·3 (7)	646·9 (6)	2·17 (3)

Table 2. *Bond lengths* (Å) *and angles* (°) *in* (1)

C1—O1	1·219 (2)	C6—N2	1·488 (2)
C1—N1	1·347 (2)	C6—C7	1·517 (2)
C1—N2	1·414 (2)	C6—C8	1·540 (2)
C2—N1	1·462 (2)	C6—C9	1·547 (2)
C2—C3	1·515 (2)	C9—O3	1·235 (2)
C2—C4	1·529 (2)	C9—N3	1·328 (2)
C2—C5	1·528 (2)	N1—H1	0·86 (2)
C5—O2	1·203 (2)	N3—H15	0·88 (2)
C5—N2	1·388 (2)		

O1—C1—N1	128·0 (1)	C2—C5—O2	124·4 (1)
O1—C1—N2	123·6 (1)	C2—C5—N2	107·5 (1)
C1—N1—H1	118 (1)	O2—C5—N2	128·0 (1)
C1—N1—C2	112·6 (1)	C5—N2—C1	110·1 (1)
N1—C1—N2	108·3 (1)	C5—N2—C6	128·7 (1)
C2—N1—H1	124 (1)	C6—N2—C1	119·9 (1)
N1—C2—C3	112·7 (1)	N2—C6—C7	109·1 (1)
N1—C2—C4	110·7 (1)	N2—C6—C8	111·3 (1)
O3—C9—N3	122·7 (1)	N2—C6—C9	110·2 (1)
N1—C2—C5	101·5 (1)	C7—C6—C8	109·7 (1)
C3—C2—C4	111·7 (1)	C7—C6—C9	111·1 (1)
C3—C2—C5	110·6 (1)	C8—C6—C9	105·3 (1)
C4—C2—C5	109·1 (1)	C6—C9—O3	119·3 (1)
C9—N3—H14	118 (1)	C6—C9—N3	117·5 (1)
C9—N3—N15	121 (1)		

Experimental. A colorless crystal of (1) with rectangular shape and dimensions 0·37 × 0·47 × 0·80 mm, prepared by Uhrich, Olson & Worman (1986), was mounted on a glass fiber with silicone adhesive. Picker FACS-1 diffractometer; lattice constants from setting angles of 12 reflections with $27 < 2\theta < 32°$; 2611 unique data measured in range $2 < 2\theta < 56{\cdot}83°$ with 2301 having $F > 3\sigma(F)$; σ from counting statistics; 2θ scans at 1·0° min^{-1} and stationary backgrounds of 20 s. Three standard reflections (200, 060, 006) inserted every 100 data remained constant; data collected $h = 0$ to 8, $k = 0$ to 21, $l = 0$ to 26; no absorption correction, estimated range of transmission factors 0·93–0·96. D_m by flotation in *n*-hexane and CCl_4. Structure solved by direct methods (Long, 1966); scattering factors from Cromer & Mann (1968) and Stewart, Davidson & Simpson (1965). Refinement by full-matrix least squares (Busing, Martin & Levy, 1962) based on F, $w = 1/\sigma^2$; function minimized $\sum w(|F_o| - |F_c|)^2$; H atoms from difference syntheses included; non-H atoms anisotropic; H atoms isotropic; $R = 0{\cdot}043$ and $wR = 0{\cdot}048$; maximum and minimum residual electron densities 0·10 and −0·345 e Å^{-3}; largest Δ/σ 0·02; error of fit 2·85; 196 parameters varied. Atomic parameters are in Table 1 and bond lengths and angles are in Table 2.* An *ORTEP*II diagram (Johnson, 1971) of the asymmetric unit of the structure is given in Fig. 1 and a packing diagram is in Fig. 2.

Related literature. The structure of DL-allantoin (Mootz, 1965), 2-thiohydantoin (Walker, Folting &

* Lists of anisotropic thermal parameters, structure factors, H-atom parameters and least-squares planes have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 53805 (20 pp.). Copies may be obtained through The Technical Editor, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

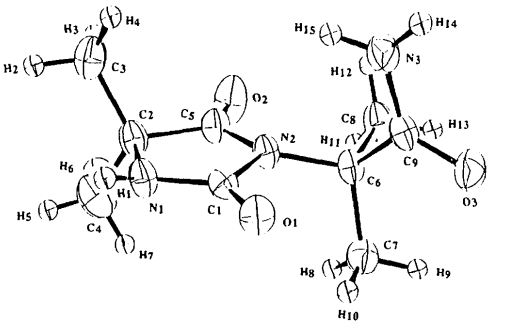

Fig. 1. *ORTEP*II (Johnson, 1971) drawing of (1); thermal ellipsoids are represented at 50% probability, with H atoms reduced for clarity.

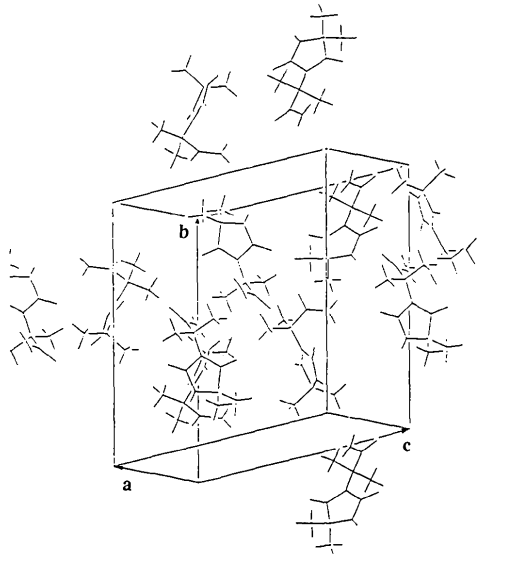

Fig. 2. Packing diagram of (1). The shortest intermolecular contacts are: 2·13 (2) Å for O3···H14 ($1 - x$, $-y$, $-z$), 2·24 (2) Å for O1···H15 ($\frac{1}{2} + x$, $\frac{1}{2} - y$, $-z$) and 2·29 (2) Å for O3···H1 ($\frac{1}{2} + x$, $\frac{1}{2} - y$, $-z$).

Merritt, 1969) and 5,5-dimethylhydantoin (Cassady & Hawkinson, 1982) have been determined. Pullman & Pullman (1963) have performed molecular orbital calculations on hydantoins.

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