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4-(*p*-Chlorophenyl)-4-hydroxy-*N*,*N*,*γ*-trimethyl-α,α-diphenyl-1-piperidinebutyramide

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Abstract. $C_{30}H_{35}N_2O_2Cl$, $M_r = 491{\cdot}05$; monoclinic, $P2_1/c$; $a = 8{\cdot}991\ (2)$, $b = 14{\cdot}303\ (3)$, $c = 20{\cdot}758\ (5)$ Å, $\beta = 95{\cdot}07\ (2)°$; 25°C; $Z = 4$. Each molecule is involved in two hydrogen bonds: O(14)···O(19), 2·84 Å [O(19): $1-x, \frac{1}{2}+y, \frac{3}{2}-z$], and O(19)···O(14) [O(14): $1-x, y-\frac{1}{2}, z$].

Introduction. The title compound is related to the potent antidiarrhœal drug loperamide (Germain, Declercq, Van Meerssche & Koch, 1977).

Transparent colourless crystals were obtained by evaporation of a solution in ethanol. The experimental conditions used for data collection are given in Table 1. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). Anisotropic block-diagonal least-squares refinement (Ahmed, Hall, Pippy & Huber, 1966) gave a final $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$ of 0·09 for all observed reflexions. The scattering factors used are those given in *International Tables for X-ray*

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Table 1. *Experimental conditions*

Instrument: Syntex $P2_1$ diffractometer
Source: Cu $K\bar{\alpha}$; $\lambda = 1{\cdot}5418$ Å; ω–2θ scan; $\theta_{max} = 55°$
Confidence level: 2·5
Total number of independent reflexions: 3343
Total observed: 2547

Table 2. *Final positional parameters* (×10⁴) (*with standard deviations in parentheses*)

	x	*y*	*z*
Cl(1)	7481 (1)	9370 (1)	8666 (0)
C(2)	8809 (3)	7823 (2)	8229 (1)
C(3)	8828 (3)	6869 (2)	8074 (1)
C(4)	7597 (3)	6298 (2)	8158 (1)
C(5)	6335 (3)	6696 (2)	8395 (1)
C(6)	6282 (4)	7639 (2)	8543 (1)
C(7)	7520 (4)	8188 (2)	8460 (1)
C(8)	7705 (3)	5257 (2)	8013 (1)
C(9)	8390 (3)	4747 (2)	8623 (1)
C(10)	8442 (3)	3692 (2)	8521 (1)
N(11)	6933 (2)	3343 (1)	8352 (1)
C(12)	6320 (3)	3744 (2)	7735 (1)
C(13)	6161 (3)	4799 (2)	7802 (1)
O(14)	8700 (2)	5106 (1)	7515 (1)
C(15)	6864 (3)	2313 (2)	8390 (1)
C(16)	5267 (3)	1936 (2)	8436 (1)
C(17)	4384 (2)	2267 (2)	9018 (1)
C(18)	2982 (3)	1616 (2)	8976 (1)
O(19)	2861 (2)	981 (1)	8574 (1)
N(20)	1900 (2)	1726 (2)	9379 (1)
C(21)	1856 (3)	2437 (2)	9882 (1)
C(22)	601 (3)	1093 (2)	9296 (2)
C(23)	5378 (3)	2095 (2)	9637 (1)
C(24)	6562 (3)	2709 (2)	9832 (1)
C(25)	7559 (3)	2511 (2)	10370 (1)
C(26)	7429 (3)	1689 (2)	10719 (1)
C(27)	6281 (3)	1083 (2)	10532 (1)
C(28)	5242 (3)	1275 (2)	10002 (1)
C(29)	3784 (2)	3277 (2)	8905 (1)
C(30)	2900 (3)	3459 (2)	8337 (1)
C(31)	2280 (3)	4341 (2)	8203 (1)
C(32)	2544 (3)	5054 (2)	8651 (1)
C(33)	3383 (3)	4877 (2)	9226 (1)
C(34)	3991 (3)	3996 (2)	9348 (1)
C(35)	7503 (3)	1804 (2)	7802 (1)

Crystallography (1962). The final coordinates are given in Table 2.*

Discussion. The conformation of the molecule and the numbering scheme are shown in Fig. 1 and the bond distances and angles in Table 3. The torsion angles defining the conformation are given in Table 4. The hydrogen bonds are as described in the *Abstract*.

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32715 (26 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

Table 3. *Bond distances* (Å) *and angles* (°) (*with standard deviations in parentheses*)

Cl(1)–C(7)	1·745 (3)	C(3)–C(2)–C(7)	118·1 (3)
C(2)–C(3)	1·402 (5)	C(2)–C(3)–C(4)	120·9 (3)
C(2)–C(7)	1·395 (5)	C(3)–C(4)–C(5)	118·9 (3)
C(3)–C(4)	1·399 (4)	C(3)–C(4)–C(8)	118·7 (2)
C(4)–C(5)	1·397 (4)	C(5)–C(4)–C(8)	122·4 (2)
C(4)–C(8)	1·524 (4)	C(4)–C(5)–C(6)	121·3 (3)
C(5)–C(6)	1·385 (4)	C(5)–C(6)–C(7)	118·8 (3)
C(6)–C(7)	1·386 (5)	Cl(1)–C(7)–C(2)	118·9 (2)
C(8)–C(9)	1·541 (4)	Cl(1)–C(7)–C(6)	119·0 (2)
C(8)–C(13)	1·563 (4)	C(2)–C(7)–C(6)	122·1 (3)
C(8)–O(14)	1·442 (3)	C(4)–C(8)–C(9)	109·1 (2)
C(9)–C(10)	1·526 (4)	C(4)–C(8)–C(13)	113·3 (2)
C(10)–N(11)	1·459 (3)	C(4)–C(8)–O(14)	110·0 (2)
N(11)–C(12)	1·466 (3)	C(9)–C(8)–C(13)	108·2 (2)
N(11)–C(15)	1·476 (3)	C(9)–C(8)–O(14)	106·9 (2)
C(12)–C(13)	1·523 (4)	C(13)–C(8)–O(14)	109·1 (2)
C(15)–C(16)	1·545 (4)	C(8)–C(9)–C(10)	111·7 (2)
C(15)–C(35)	1·573 (4)	C(9)–C(10)–N(11)	109·4 (2)
C(16)–C(17)	1·576 (3)	C(10)–N(11)–C(12)	110·3 (2)
C(17)–C(18)	1·564 (3)	C(10)–N(11)–C(15)	111·8 (2)
C(17)–C(23)	1·519 (3)	C(12)–N(11)–C(15)	115·0 (2)
C(17)–C(29)	1·553 (3)	N(11)–C(12)–C(13)	109·8 (2)
C(18)–O(19)	1·232 (3)	C(8)–C(13)–C(12)	110·7 (2)
C(18)–N(20)	1·347 (3)	N(11)–C(15)–C(16)	113·3 (2)
N(20)–C(21)	1·460 (4)	N(11)–C(15)–C(35)	113·6 (2)
N(20)–C(22)	1·477 (4)	C(16)–C(15)–C(35)	107·0 (2)
C(23)–C(24)	1·411 (4)	C(15)–C(16)–C(17)	118·4 (2)
C(23)–C(28)	1·407 (4)	C(16)–C(17)–C(18)	103·7 (2)
C(24)–C(25)	1·399 (4)	C(16)–C(17)–C(23)	107·6 (2)
C(25)–C(26)	1·391 (4)	C(16)–C(17)–C(29)	110·8 (2)
C(26)–C(27)	1·378 (4)	C(18)–C(17)–C(23)	111·2 (2)
C(27)–C(28)	1·407 (4)	C(18)–C(17)–C(29)	106·1 (2)
C(29)–C(30)	1·386 (3)	C(23)–C(17)–C(29)	116·7 (2)
C(29)–C(34)	1·380 (4)	C(17)–C(18)–O(19)	119·9 (2)
C(30)–C(31)	1·398 (4)	C(17)–C(18)–N(20)	121·2 (2)
C(31)–C(32)	1·386 (4)	O(19)–C(18)–N(20)	118·9 (2)
C(32)–C(33)	1·379 (4)	C(18)–N(20)–C(21)	126·3 (2)
C(33)–C(34)	1·388 (4)	C(18)–N(20)–C(22)	117·5 (2)
		C(21)–N(20)–C(22)	116·1 (2)
		C(17)–C(23)–C(24)	120·9 (2)
		C(17)–C(23)–C(28)	121·1 (2)

Table 3. (*cont.*)

C(24)–C(23)–C(28)	117·7 (2)
C(23)–C(24)–C(25)	121·1 (2)
C(24)–C(25)–C(26)	120·6 (3)
C(25)–C(26)–C(27)	118·8 (3)
C(26)–C(27)–C(28)	121·8 (3)
C(23)–C(28)–C(27)	120·0 (3)
C(17)–C(29)–C(30)	118·0 (2)
C(17)–C(29)–C(34)	124·5 (2)
C(30)–C(29)–C(34)	117·4 (2)
C(29)–C(30)–C(31)	121·9 (2)
C(30)–C(31)–C(32)	119·2 (3)
C(31)–C(32)–C(33)	119·6 (3)
C(32)–C(33)–C(34)	120·0 (3)
C(29)–C(34)–C(33)	121·8 (3)

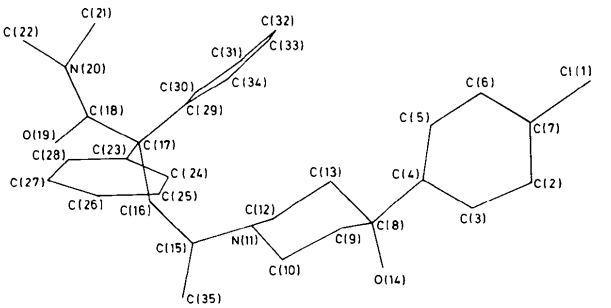

Fig. 1. Conformation and numbering scheme of $C_{30}H_{35}N_2O_2Cl$.

Table 4. *Torsion angles* (°) *defining the conformation of* $C_{30}H_{35}N_2O_2Cl$

C(9)–C(8)–C(4)–C(5)	−90
C(8)–C(9)–C(10)–N(11)	−59
C(9)–C(10)–N(11)–C(15)	−167
C(10)–N(11)–C(15)–C(16)	161
C(10)–N(11)–C(15)–C(35)	−76
N(11)–C(15)–C(16)–C(17)	−58
C(15)–C(16)–C(17)–C(18)	−170
C(15)–C(16)–C(17)–C(23)	−52
C(15)–C(16)–C(17)–C(29)	76
C(16)–C(17)–C(18)–O(19)	5
C(16)–C(17)–C(18)–N(20)	−176
C(16)–C(17)–C(23)–C(24)	78
C(16)–C(17)–C(29)–C(30)	55

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