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1-{4-[4-(*p*-Chlorophenyl)-4-hydroxypiperidino]-2,2-diphenylbutyryl}pyrrolidine

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Abstract. $C_{31}H_{35}N_2O_2Cl$, $M_r = 503{\cdot}06$; orthorhombic, *Pbca*; $a = 15{\cdot}555\ (3)$, $b = 20{\cdot}208\ (5)$, $c = 16{\cdot}858\ (3)$ Å; $t = 25\,°C$; $Z = 8$. Each molecule is involved in two hydrogen bonds: O(14)–O(19) 2·82 Å [O(19): $-\frac{1}{2} + x$, y, $\frac{1}{2} - z$] and O(19)–O(14) [O(14): $\frac{1}{2} + x$, y, $\frac{1}{2} - z$].

Introduction. The title compound is an antidiarrhoeal drug related to loperamide (Germain, Declercq, Van Meerssche & Koch, 1977). Transparent colourless crystals were obtained from a solution in ethanol. The space group was determined from Weissenberg photographs. Final cell dimensions and intensities were measured on a Picker four-circle diffractometer with the experimental conditions given in Table 1. The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971) and refined by block-diagonal least squares (Ahmed, Hall, Pippy & Huber, 1966). The final

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Table 1. *Experimental conditions*

Source Cu $K\alpha$, $\lambda = 1{\cdot}5418$ Å
ω–2θ scan; $\theta_{max} = 50°$
Confidence level: 2·5
Total number of independent reflexions: 2722
Total observed: 2367

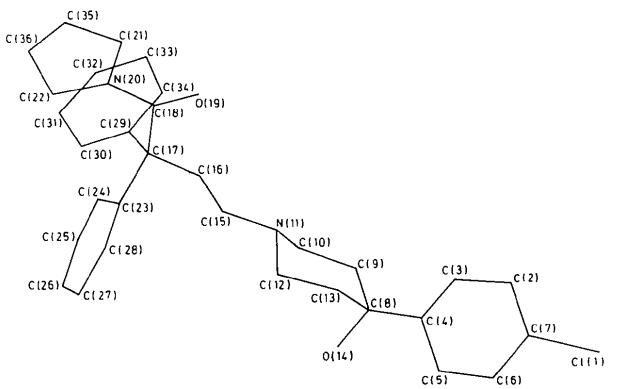

Fig. 1. Conformation and numbering scheme of $C_{31}H_{35}N_2O_2Cl$.

Table 2. *Final positional parameters* ($\times 10^4$), *with standard deviations in parentheses*

	x	*y*	*z*
Cl(1)	4120 (1)	7316 (1)	6808 (1)
C(2)	4887 (4)	6795 (3)	5524 (3)
C(3)	4875 (3)	6427 (3)	4815 (2)
C(4)	4122 (3)	6146 (2)	4517 (2)
C(5)	3376 (3)	6209 (2)	4968 (3)
C(6)	3371 (3)	6564 (2)	5686 (3)
C(7)	4122 (3)	6851 (2)	5948 (3)
C(8)	4135 (2)	5767 (2)	3745 (2)
C(9)	4574 (3)	6182 (2)	3089 (2)
C(10)	4726 (3)	5775 (2)	2332 (3)
N(11)	5231 (2)	5178 (2)	2500 (2)
C(12)	4750 (3)	4756 (2)	3058 (3)
C(13)	4624 (3)	5111 (2)	3842 (2)
O(14)	3290 (2)	5658 (1)	3445 (2)
C(15)	5403 (3)	4820 (2)	1751 (2)
C(16)	6135 (3)	4326 (2)	1865 (2)
C(17)	6372 (3)	3928 (2)	1093 (2)
C(18)	6854 (3)	4392 (2)	509 (2)
O(19)	7034 (2)	4963 (1)	716 (2)
N(20)	7108 (2)	4170 (2)	−198 (2)
C(21)	7011 (4)	3497 (3)	−541 (3)
C(22)	7591 (3)	4619 (3)	−724 (3)
C(23)	5544 (2)	3647 (2)	755 (2)
C(24)	5152 (3)	3910 (2)	74 (3)
C(25)	4345 (3)	3681 (2)	−170 (3)
C(26)	3916 (3)	3205 (2)	259 (3)
C(27)	4283 (3)	2961 (2)	947 (3)
C(28)	5087 (3)	3182 (2)	1192 (2)
C(29)	7045 (3)	3398 (2)	1356 (2)
C(30)	6949 (3)	2724 (2)	1237 (3)
C(31)	7568 (3)	2277 (2)	1519 (3)
C(32)	8296 (3)	2506 (2)	1920 (3)
C(33)	8407 (3)	3188 (2)	2023 (3)
C(34)	7793 (3)	3623 (2)	1743 (3)
C(35)	7775 (3)	4191 (3)	−1460 (3)
C(36)	7623 (4)	3507 (3)	−1222 (4)

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

Cl(1)–C(7)	1·727 (5)	C(2)–C(7)–C(6)	121·8 (5)
C(2)–C(3)	1·408 (7)	C(4)–C(8)–C(9)	110·3 (3)
C(2)–C(7)	1·392 (8)	C(4)–C(8)–C(13)	110·6 (3)
C(3)–C(4)	1·394 (7)	C(4)–C(8)–O(14)	111·8 (3)
C(4)–C(5)	1·393 (6)	C(9)–C(8)–C(13)	109·0 (3)
C(4)–C(8)	1·510 (6)	C(9)–C(8)–C(14)	103·8 (3)
C(5)–C(6)	1·407 (7)	C(13)–C(8)–O(14)	111·1 (3)
C(6)–C(7)	1·377 (7)	C(8)–C(9)–C(10)	111·8 (3)
C(8)–C(9)	1·546 (6)	C(9)–C(10)–N(11)	111·3 (3)
C(8)–C(13)	1·538 (6)	C(10)–N(11)–C(12)	109·1 (3)
C(8)–O(14)	1·426 (5)	C(10)–N(11)–C(15)	109·6 (3)
C(9)–C(10)	1·538 (6)	C(12)–N(11)–C(15)	110·7 (3)
C(10)–N(11)	1·467 (5)	N(11)–C(12)–C(13)	110·4 (3)
N(11)–C(12)	1·473 (6)	C(8)–C(13)–C(12)	112·2 (3)
N(11)–C(15)	1·480 (5)	N(11)–C(15)–C(16)	110·4 (3)
C(12)–C(13)	1·517 (6)	C(15)–C(16)–C(17)	113·9 (3)
C(15)–C(16)	1·527 (6)	C(16)–C(17)–C(18)	109·2 (3)
C(16)–C(17)	1·573 (6)	C(16)–C(17)–C(23)	107·6 (3)
C(17)–C(18)	1·552 (6)	C(16)–C(17)–C(29)	105·9 (3)
C(17)–C(23)	1·519 (6)	C(18)–C(17)–C(23)	113·4 (3)
C(17)–C(29)	1·560 (6)	C(19)–C(17)–C(29)	105·7 (3)
C(18)–O(19)	1·239 (5)	C(23)–C(17)–C(29)	114·8 (3)
C(18)–N(20)	1·333 (6)	C(17)–C(18)–C(19)	119·6 (4)
N(20)–C(21)	1·485 (7)	C(17)–C(18)–N(20)	120·5 (4)
N(20)–C(22)	1·473 (6)	O(19)–C(18)–N(20)	119·8 (4)
C(21)–C(36)	1·491 (8)	C(18)–N(20)–C(21)	128·7 (4)
C(22)–C(35)	1·539 (8)	C(18)–N(20)–C(22)	118·9 (4)
C(23)–C(24)	1·409 (6)	C(21)–N(20)–C(22)	112·4 (4)
C(23)–C(28)	1·389 (6)	N(20)–C(21)–C(36)	102·9 (4)
C(24)–C(25)	1·400 (7)	N(20)–C(22)–C(35)	103·5 (4)
C(25)–C(26)	1·377 (7)	C(17)–C(23)–C(24)	122·2 (4)
C(26)–C(27)	1·383 (7)	C(17)–C(23)–C(28)	119·2 (3)
C(27)–C(28)	1·392 (6)	C(24)–C(23)–C(28)	117·9 (4)
C(29)–C(30)	1·385 (6)	C(23)–C(24)–C(25)	120·3 (4)
C(29)–C(34)	1·410 (6)	C(24)–C(25)–C(26)	120·7 (4)
C(30)–C(31)	1·403 (6)	C(25)–C(26)–C(27)	119·4 (4)
C(31)–C(32)	1·398 (7)	C(26)–C(27)–C(28)	120·3 (4)
C(32)–C(33)	1·399 (7)	C(23)–C(28)–C(27)	121·3 (4)
C(33)–C(34)	1·381 (7)	C(17)–C(29)–C(30)	124·2 (4)
C(35)–C(36)	1·458 (9)	C(17)–C(29)–C(34)	117·6 (4)
C(3)–C(2)–C(7)	117·8 (5)	C(30)–C(29)–C(34)	118·2 (4)
C(2)–C(3)–C(4)	122·1 (5)	C(29)–C(30)–C(31)	120·8 (4)
C(3)–C(4)–C(5)	117·7 (4)	C(30)–C(31)–C(32)	120·4 (4)
C(3)–C(4)–C(8)	120·4 (4)	C(31)–C(32)–C(33)	119·1 (4)
C(5)–C(4)–C(8)	121·9 (4)	C(32)–C(33)–C(34)	119·9 (4)
C(4)–C(5)–C(6)	121·4 (4)	C(29)–C(34)–C(35)	121·6 (4)
C(5)–C(6)–C(7)	119·0 (4)	C(22)–C(35)–C(36)	106·4 (5)
Cl(1)–C(7)–C(2)	118·4 (4)	C(21)–C(36)–C(35)	109·1 (5)
Cl(1)–C(7)–C(6)	119·7 (4)		

Table 4. *Torsion angles* (°) *in the title compound* (*A*) *and in loperamide* (*B*)

	A	*B*
C(8)–C(13)–C(12)–N(11)	59	57
C(12)–N(11)–C(15)–C(16)	−76	−71
N(11)–C(15)–C(16)–C(17)	−179	−174
C(15)–C(16)–C(17)–C(18)	73	73
C(15)–C(16)–C(17)–C(23)	−50	−50
C(15)–C(16)–C(17)–C(29)	−173	−174
C(16)–C(17)–C(18)–N(20)	−178	−179
C(16)–C(17)–C(23)–C(24)	106	109
C(16)–C(17)–C(29)–C(30)	123	123

$R = \Sigma \, ||F_o| - |F_c||/|F_o|$ is 0·09 for all observed reflexions.* The scattering factors were those given in *International Tables for X-ray 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, the bond distances and angles in Table 3. The torsion angles defining the conformation are given in Table 4 together with the corresponding values for loperamide (Germain, Declercq, Van Meerssche & Koch, 1977).

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 32478 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

References

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