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

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Abstract. $C_{32}H_{37}N_2O_2Cl$, $M_r = 517{\cdot}1$; monoclinic, $P2_1/n$; $a = 14{\cdot}247\ (3)$, $b = 15{\cdot}847\ (3)$, $c = 12{\cdot}430\ (3)$ Å, $\beta = 90{\cdot}71\ (2)°$; 25 °C; $Z = 4$. Each molecule is connected to two neighbours by hydrogen bonds.

Introduction. Transparent colourless crystals were obtained by cooling a solution in ethanol. The space group was determined from Weissenberg photographs. The experimental conditions used for data collection are given in Table 1.

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Table 1. *Experimental conditions*

Instrument: Syntex $P2_1$ diffractometer
Source: Cu $K\bar{\alpha}$, $\lambda = 1{\cdot}5418$ Å; graphite monochromator
ω–2θ scan; $\theta_{max} = 50°$; confidence level 2·5
Total number of independent reflexions: 2895
Total observed: 2471

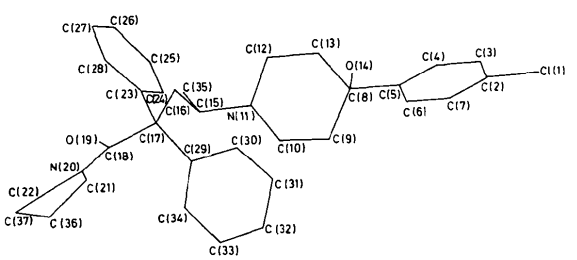

Fig. 1. The conformation and numbering scheme of $C_{32}H_{37}N_2O_2Cl$.

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

	x	*y*	*z*
Cl(1)	6194 (1)	3431 (1)	9467 (1)
C(2)	6286 (2)	2456 (2)	10092 (3)
C(3)	5977 (2)	2341 (2)	11118 (3)
C(4)	6044 (2)	1538 (2)	11608 (3)
C(5)	6421 (2)	860 (2)	11054 (2)
C(6)	6736 (2)	994 (2)	10003 (3)
C(7)	6682 (3)	1792 (2)	9531 (3)
C(8)	6463 (2)	−21 (2)	11554 (2)
C(9)	7450 (2)	−415 (2)	11469 (3)
C(10)	7467 (2)	−1335 (2)	11862 (2)
N(11)	6768 (2)	−1820 (1)	11236 (2)
C(12)	5813 (2)	−1499 (2)	11421 (3)
C(13)	5745 (2)	−593 (2)	10976 (2)
O(14)	6171 (1)	19 (1)	12652 (2)
C(15)	6873 (2)	−2742 (2)	11362 (2)
C(16)	6398 (2)	−3192 (2)	10406 (2)
C(17)	7060 (2)	−3546 (2)	9523 (2)
C(18)	7521 (2)	−4368 (2)	9963 (2)
O(19)	7451 (2)	−4525 (1)	10941 (2)
N(20)	7987 (2)	−4882 (2)	9327 (2)
C(21)	8134 (3)	−4802 (2)	8137 (3)
C(22)	8474 (2)	−5624 (2)	9805 (3)
C(23)	6413 (2)	−3792 (2)	8563 (2)
C(24)	6437 (2)	−3388 (2)	7560 (3)
C(25)	5816 (3)	−3633 (2)	6727 (3)
C(26)	5148 (3)	−4265 (2)	6902 (3)
C(27)	5119 (2)	−4661 (2)	7896 (3)
C(28)	5750 (2)	−4425 (2)	8728 (2)
C(29)	7827 (2)	−2897 (2)	9276 (2)
C(30)	7560 (2)	−2088 (2)	8962 (2)
C(31)	8233 (3)	−1454 (2)	8778 (3)
C(32)	9182 (3)	−1642 (2)	8949 (3)
C(33)	9461 (3)	−2440 (2)	9280 (3)
C(34)	8769 (2)	−3066 (2)	9458 (3)
C(35)	6483 (2)	−3074 (2)	12451 (3)
C(36)	8858 (3)	−5480 (3)	7919 (3)
C(37)	8778 (3)	−6110 (2)	8785 (3)

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

Cl(1)–C(2)	1·733 (4)	N(11)–C(12)	1·474 (4)	C(22)–C(37)	1·550 (5)
C(2)–C(3)	1·366 (5)	N(11)–C(15)	1·477 (4)	C(23)–C(24)	1·402 (4)
C(2)–C(7)	1·386 (5)	C(12)–C(13)	1·541 (4)	C(23)–C(28)	1·394 (4)
C(3)–C(4)	1·414 (5)	C(15)–C(16)	1·536 (4)	C(24)–C(25)	1·409 (5)
C(4)–C(5)	1·389 (4)	C(15)–C(35)	1·561 (4)	C(25)–C(26)	1·400 (5)
C(5)–C(6)	1·403 (5)	C(16)–C(17)	1·560 (4)	C(26)–C(27)	1·388 (5)
C(5)–C(8)	1·529 (4)	C(17)–C(18)	1·555 (4)	C(27)–C(28)	1·413 (5)
C(6)–C(7)	1·395 (5)	C(17)–C(23)	1·548 (4)	C(29)–C(30)	1·393 (4)
C(8)–C(9)	1·544 (4)	C(17)–C(29)	1·534 (4)	C(29)–C(34)	1·384 (4)
C(8)–C(13)	1·538 (4)	C(18)–O(19)	1·246 (3)	C(30)–C(31)	1·410 (5)
C(8)–O(14)	1·434 (4)	C(18)–N(20)	1·320 (4)	C(31)–C(32)	1·398 (5)
C(9)–C(10)	1·537 (4)	N(20)–C(21)	1·502 (4)	C(32)–C(33)	1·386 (5)
C(10)–N(11)	1·473 (4)	N(20)–C(22)	1·485 (4)	C(33)–C(34)	1·418 (5)
		C(21)–C(36)	1·516 (5)	C(36)–C(37)	1·473 (6)

Cl(1)–C(2)–C(3)	120·9 (3)	C(12)–N(11)–C(15)	114·7 (2)	N(20)–C(21)–C(36)	102·7 (3)
Cl(1)–C(2)–C(7)	118·7 (3)	N(11)–C(12)–C(13)	108·6 (2)	N(20)–C(22)–C(37)	101·5 (3)
C(3)–C(2)–C(7)	120·4 (3)	C(8)–C(13)–C(12)	110·1 (2)	C(17)–C(23)–C(24)	123·3 (3)
C(2)–C(3)–C(4)	120·1 (3)	N(11)–C(15)–C(16)	109·6 (2)	C(17)–C(23)–C(28)	117·8 (2)
C(3)–C(4)–C(5)	120·5 (3)	N(11)–C(15)–C(35)	112·8 (2)	C(24)–C(23)–C(28)	118·9 (3)
C(4)–C(5)–C(6)	118·4 (3)	C(16)–C(15)–C(35)	110·8 (2)	C(23)–C(24)–C(25)	120·4 (3)
C(4)–C(5)–C(8)	121·2 (3)	C(15)–C(16)–C(17)	116·6 (2)	C(24)–C(25)–C(26)	120·3 (3)
C(6)–C(5)–C(8)	120·4 (3)	C(16)–C(17)–C(18)	108·0 (2)	C(25)–C(26)–C(27)	119·4 (3)
C(5)–C(6)–C(7)	120·8 (3)	C(16)–C(17)–C(23)	105·9 (2)	C(26)–C(27)–C(28)	120·4 (3)
C(2)–C(7)–C(6)	119·8 (3)	C(16)–C(17)–C(29)	109·8 (2)	C(23)–C(28)–C(27)	120·7 (3)
C(5)–C(8)–C(9)	111·9 (2)	C(18)–C(17)–C(23)	107·7 (2)	C(17)–C(29)–C(30)	118·7 (3)
C(5)–C(8)–C(13)	109·1 (2)	C(18)–C(17)–C(29)	109·4 (2)	C(17)–C(29)–C(34)	122·0 (3)
C(5)–C(8)–O(14)	109·7 (2)	C(23)–C(17)–C(29)	115·7 (2)	C(30)–C(29)–C(34)	119·0 (3)
C(9)–C(8)–C(13)	109·3 (2)	C(17)–C(18)–O(19)	118·2 (2)	C(29)–C(30)–C(31)	121·2 (3)
C(9)–C(8)–O(14)	111·0 (2)	C(17)–C(18)–N(20)	121·3 (2)	C(30)–C(31)–C(32)	118·8 (3)
C(13)–C(8)–O(14)	105·8 (2)	O(19)–C(18)–N(20)	120·5 (3)	C(31)–C(32)–C(33)	120·8 (3)
C(8)–C(9)–C(10)	111·9 (2)	C(18)–N(20)–C(21)	128·0 (3)	C(32)–C(33)–C(34)	119·2 (3)
C(9)–C(10)–N(11)	108·6 (2)	C(18)–N(20)–C(22)	119·0 (2)	C(29)–C(34)–C(33)	120·9 (3)
C(10)–N(11)–C(12)	111·0 (2)	C(21)–N(20)–C(22)	112·9 (2)	C(21)–C(36)–C(37)	106·9 (3)
C(10)–N(11)–C(15)	113·2 (2)			C(22)–C(37)–C(36)	106·6 (3)

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 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. Torsion angles are given in Table 4.

Each molecule is connected to two neighbours by equal hydrogen bonds (2·710 Å) involving the hydroxyl and the carbonyl group: O(19)–O(14) [O(14): $\frac{3}{2} - x$, $-\frac{1}{2} + y$, $\frac{5}{2} - z$] and O(14)–O(19)[O(19): $\frac{3}{2} - x$, $\frac{1}{2} + y$, $\frac{5}{2} - z$].

Table 4. *Torsion angles defining the conformation of the molecule*

C(8)–C(13)–C(12)–N(11)	−60°
C(12)–N(11)–C(15)–C(16)	72
C(12)–N(11)–C(15)–C(35)	−52
N(11)–C(15)–C(16)–C(17)	103
C(15)–C(16)–C(17)–C(18)	76
C(15)–C(16)–C(17)–C(23)	−168
C(15)–C(16)–C(17)–C(29)	−43
C(16)–C(17)–C(18)–N(20)	−72
C(16)–C(17)–C(23)–C(24)	114
C(16)–C(17)–C(29)–C(30)	−174

* Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32347 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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