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4-[4,4-Bis(*p*-fluorophenyl)butyl]-1-piperazineacetyl-2′,6′-xylidide (Lidoflazine)

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Abstract. $C_{30}H_{35}N_3OF_2$, $M_r = 491{\cdot}6$; orthorhombic, $P2_12_12_1$; $a = 22{\cdot}965$ (3), $b = 12{\cdot}482$ (3), $c = 9{\cdot}392$ (2) Å; $t = 25\,°C$; $Z = 4$. The molecules are held together by packing forces only.

Introduction. The title compound is a drug used for the treatment of coronary heart diseases. Transparent colourless crystals were obtained by cooling a solution in hot ethanol. The space group was determined from photographs, final cell dimensions and intensities being measured on a Picker four-circle diffractometer. The experimental conditions are given in Table 1.

The structure was solved with *MULTAN* (Germain, Main & Woolfson, 1971). Isotropic and anisotropic weighted block-diagonal least-squares refinement (Ahmed, Hall, Pippy & Huber, 1966) gave a final R of 0·09 for all observed reflexions.† The weighting scheme was $w = (9{\cdot}06 + |F_o| + 0{\cdot}0088\ |F_o|^2)^{-1/2}$. The

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Table 1. *Experimental conditions*

Source Cu $K\bar{\alpha}$; $\lambda = 1{\cdot}5418$ Å
ω–2θ scan; $\theta_{max} = 50°$
Confidence level: 2·5
Total number of independent reflexions: 1619
Total observed: 1340

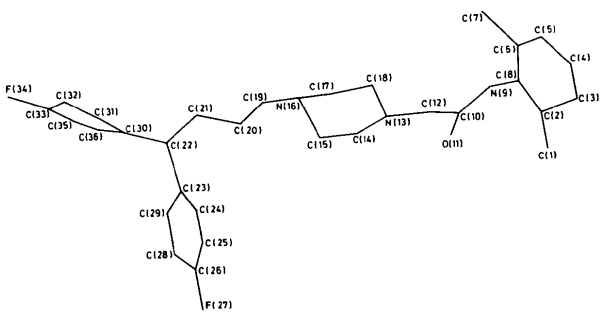

Fig. 1. Conformation and numbering scheme of $C_{30}H_{35}N_3OF_2$.

† Lists of structure factors and anisotropic thermal parameters have been deposited with the British Library Lending Division as Supplementary Publication No. SUP 32516 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

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

	x	*y*	*z*
C(1)	1119 (2)	10348 (5)	6110 (7)
C(2)	1197 (2)	9200 (4)	5651 (5)
C(3)	750 (2)	8480 (5)	5874 (6)
C(4)	808 (3)	7426 (5)	5424 (6)
C(5)	1310 (3)	7073 (4)	4746 (7)
C(6)	1753 (2)	7807 (4)	4506 (5)
C(7)	2331 (3)	7444 (6)	3730 (7)
C(8)	1696 (2)	8864 (4)	4960 (5)
N(9)	2154 (2)	9596 (3)	4700 (4)
C(10)	2507 (2)	9942 (5)	5770 (5)
O(11)	2408 (1)	9666 (3)	7023 (3)
C(12)	2983 (2)	10707 (4)	5360 (5)
N(13)	3503 (2)	10440 (4)	6198 (4)
C(14)	3933 (2)	11303 (5)	5989 (6)
C(15)	4466 (3)	11079 (6)	6920 (7)
N(16)	4694 (2)	10026 (5)	6530 (5)
C(17)	4276 (2)	9171 (5)	6723 (7)
C(18)	3744 (2)	9375 (5)	5825 (7)
C(19)	5331 (3)	9918 (8)	6800 (10)
C(20)	5442 (4)	9764 (8)	8382 (8)
C(21)	6096 (3)	9653 (7)	8659 (7)
C(22)	6216 (3)	9400 (7)	10202 (7)
C(23)	5999 (2)	10249 (5)	11276 (7)
C(24)	5630 (3)	9915 (5)	12352 (7)
C(25)	5420 (2)	10622 (4)	13357 (7)
C(26)	5573 (2)	11650 (5)	13235 (7)
F(27)	5355 (2)	12370 (3)	14204 (5)
C(28)	5918 (3)	12041 (6)	12180 (8)
C(29)	6152 (3)	11287 (6)	11184 (7)
C(30)	6832 (2)	9094 (5)	10464 (6)
C(31)	7307 (3)	9497 (4)	9651 (8)
C(32)	7876 (3)	9092 (5)	9993 (8)
C(33)	7923 (3)	8361 (5)	11046 (8)
F(34)	8471 (2)	7993 (4)	11355 (6)
C(35)	7476 (3)	7985 (5)	11852 (7)
C(36)	6929 (3)	8313 (8)	11538 (8)

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

C(1)–C(2)	1·507 (8)	C(5)–C(6)–C(8)	120·4 (5)
C(2)–C(3)	1·381 (8)	C(7)–C(6)–C(8)	119·5 (5)
C(2)–C(8)	1·381 (7)	C(2)–C(8)–C(6)	120·7 (5)
C(3)–C(4)	1·388 (9)	C(2)–C(8)–N(9)	120·1 (4)
C(4)–C(5)	1·390 (9)	C(6)–C(8)–N(9)	119·2 (4)
C(5)–C(6)	1·387 (8)	C(8)–N(9)–C(10)	121·4 (4)
C(6)–C(7)	1·579 (9)	N(9)–C(10)–C(11)	120·1 (5)
C(6)–C(8)	1·393 (8)	N(9)–C(10)–C(12)	116·5 (4)
C(8)–N(9)	1·415 (6)	O(11)–C(10)–C(12)	123·3 (5)
N(9)–C(10)	1·361 (6)	C(10)–C(12)–N(13)	108·1 (4)
C(10)–O(11)	1·247 (6)	C(12)–N(13)–C(14)	107·9 (4)
C(10)–C(12)	1·503 (7)	C(12)–N(13)–C(18)	112·3 (4)
C(12)–N(13)	1·468 (6)	C(14)–N(13)–C(18)	111·9 (4)
N(13)–C(14)	1·475 (7)	N(13)–C(14)–C(15)	109·1 (5)
N(13)–C(18)	1·482 (8)	C(14)–C(15)–N(16)	107·9 (5)
C(14)–C(15)	1·530 (8)	C(15)–N(16)–C(17)	113·2 (5)
C(15)–N(16)	1·462 (9)	C(15)–N(16)–C(19)	113·0 (6)
N(16)–C(17)	1·448 (9)	C(17)–N(16)–C(19)	124·3 (6)
N(16)–C(19)	1·490 (9)	N(16)–C(17)–C(18)	110·1 (5)
C(17)–C(18)	1·506 (9)	N(13)–C(18)–C(17)	108·8 (5)
C(19)–C(20)	1·520 (12)	N(16)–C(19)–C(20)	110·0 (7)
C(20)–C(21)	1·530 (11)	C(19)–C(20)–C(21)	110·0 (7)
C(21)–C(22)	1·508 (10)	C(20)–C(21)–C(22)	111·2 (7)
C(22)–C(23)	1·545 (10)	C(21)–C(22)–C(23)	115·1 (6)
C(22)–C(30)	1·486 (9)	C(21)–C(22)–C(30)	112·8 (6)
C(23)–C(24)	1·383 (9)	C(23)–C(22)–C(30)	112·1 (6)
C(23)–C(29)	1·345 (10)	C(22)–C(23)–C(24)	117·9 (6)
C(24)–C(25)	1·379 (9)	C(22)–C(23)–C(29)	122·3 (6)
C(25)–C(26)	1·335 (9)	C(24)–C(23)–C(29)	119·8 (6)
C(26)–F(27)	1·374 (8)	C(23)–C(24)–C(25)	121·4 (6)
C(26)–C(28)	1·360 (9)	C(24)–C(25)–C(26)	117·7 (6)
C(28)–C(29)	1·431 (10)	C(25)–C(26)–F(27)	118·4 (5)
C(30)–C(31)	1·423 (9)	C(25)–C(26)–C(28)	124·1 (6)
C(30)–C(36)	1·420 (11)	F(27)–C(26)–C(28)	117·4 (6)
C(31)–C(32)	1·437 (10)	C(26)–C(28)–C(29)	117·3 (6)
C(32)–C(33)	1·350 (10)	C(23)–C(29)–C(28)	119·6 (6)
C(33)–F(34)	1·371 (7)	C(22)–C(30)–C(31)	123·4 (6)
C(33)–C(35)	1·360 (9)	C(22)–C(30)–C(36)	116·3 (6)
C(35)–C(36)	1·354 (10)	C(31)–C(30)–C(36)	120·2 (6)
C(1)–C(2)–C(3)	119·2 (5)	C(30)–C(31)–C(32)	116·9 (6)
C(1)–C(2)–C(8)	121·5 (5)	C(31)–C(32)–C(33)	118·3 (6)
C(3)–C(2)–C(8)	119·3 (5)	C(32)–C(33)–F(34)	117·1 (6)
C(2)–C(3)–C(4)	120·0 (5)	C(32)–C(33)–C(35)	125·5 (6)
C(3)–C(4)–C(5)	121·2 (6)	F(34)–C(33)–C(35)	117·4 (6)
C(4)–C(5)–C(6)	118·3 (6)	C(33)–C(35)–C(36)	118·4 (6)
C(5)–C(6)–C(7)	120·1 (5)	C(30)–C(36)–C(35)	120·5 (7)

Table 4. *Torsion angles* (°) *defining the conformation of the molecule*

C(2)–C(8)–N(9)–C(10)	73
C(8)–N(9)–C(10)–C(12)	179
N(9)–C(10)–C(12)–N(13)	−142
C(10)–C(12)–N(13)–C(14)	−170
N(13)–C(14)–C(15)–N(16)	57
C(14)–C(15)–N(16)–C(19)	153
C(15)–N(16)–C(19)–C(20)	76
N(16)–C(19)–C(20)–C(21)	180
C(19)–C(20)–C(21)–C(22)	−175
C(20)–C(21)–C(22)–C(23)	−60
C(20)–C(21)–C(22)–C(30)	170
C(21)–C(22)–C(23)–C(24)	−105
C(21)–C(22)–C(30)–C(31)	31

scattering factors were those given in *International Tables for X-ray Crystallography* (1962).

The final coordinates are listed 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 of the molecule are given in Table 4. The molecules are connected as indicated in the *Abstract*.

References

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