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# 8-Chloro-5-(4-methylpiperazin-1-yl)-11*H*-pyrido[2,3-*b*][1,5]benzoxazepine

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**Key indicators**

Single-crystal X-ray study
*T* = 293 K
Mean σ(C–C) = 0.002 Å
*R* factor = 0.040
*wR* factor = 0.114
Data-to-parameter ratio = 21.8

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.



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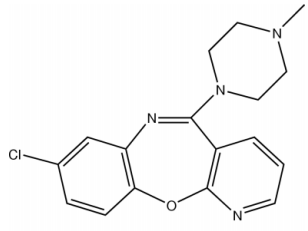
The crystal structure of the title compound, $C_{17}H_{17}ClN_4O$, has been undertaken as part of our studies of dopamine receptors. The oxazepine ring has a boat conformation, while the piperazine ring is in a normal chair conformation. The dihedral angle between the two aromatic rings that lie on the same side of the oxazepine moiety is 113.99 (7)°. There is no hydrogen bonding.

## Comment

The title compound, (I), also called JL13, was prepared as part of our study of dopamine receptors and related binding sites implicated in schizophrenia (Liégeois, 1992; Liégeois *et al.*, 1993, 1994). It has revealed a very promising antipsychotic profile in several preclinical models (Ellenbroek & Liégeois, 2003). Some crystallographic structures of related compounds have been determined, such as 8-chloro-5-(4-methylpiperazin-1-yl)-11*H*-pyrido[2,3-*b*][1,5]benzodiazepine, (II) (Dupont *et al.*, 1996), where an NH group replaces an oxa O atom in the seven-membered ring. In (I), the oxazepine ring has a boat conformation, where the four C atoms of the outer ring junction are almost coplanar; the maximum deviation from their mean plane is 0.021 (1) Å [(II): 0.034 (2) Å]. The deviation of the 'prow of the boat', *viz*. O5, is −0.668 (1) Å, and those of N12 and C13 (the 'stern') are −0.667 (1) and −0.762 (1) Å, respectively. The corresponding deviations in (II) are −0.551 (4), −0.668 (4) and −0.667 (4) Å, respectively. The distances between the methylpiperazine atom N19 and the centres of the two aromatic rings are 7.758 (2) and 6.154 (2) Å, respectively [(II): 7.739 (4) and 6.021 (4) Å]. The dihedral angle between the benzene and pyridine rings is 113.99 (7)° [(II): 126.4 (1)°]. The cohesion of the crystal is the result of van der Waals interactions (Fig. 2).




(I)

## Experimental

The title compound was synthesized at the Laboratory of Medicinal Chemistry of Liège (Liégeois *et al.*, 1993). Crystals were obtained by slow evaporation of a methanol solution.

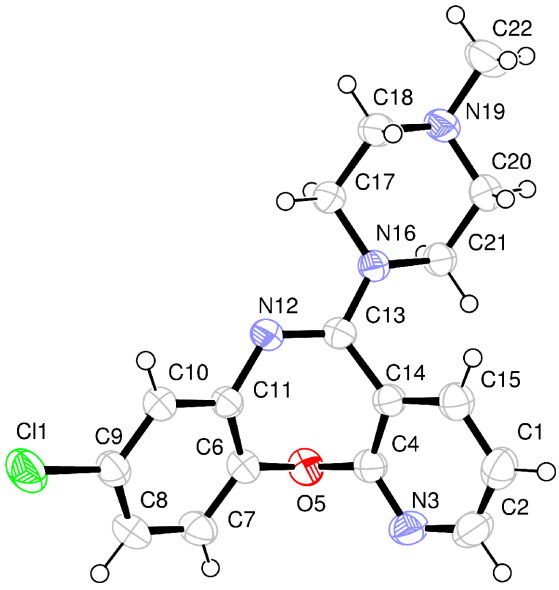



**Figure 1**
The molecular structure of (I), with the atom-labelling scheme. Displacement ellipsoids are shown at 50% probability levels and H atoms are drawn as small circles of arbitrary radius.

*Crystal data*

$C_{17}H_{17}ClN_4O$
$M_r$ = 328.80
Monoclinic, $P2_1/n$
$a$ = 8.5531 (8) Å
$b$ = 10.6765 (8) Å
$c$ = 17.2457 (12) Å
$\beta$ = 93.347 (10)°
$V$ = 1572.1 (2) Å$^3$
$Z$ = 4
$D_x$ = 1.389 Mg m$^{-3}$
Mo $K\alpha$ radiation
Cell parameters from 56 reflections
$\theta$ = 20.2–22.9°
$\mu$ = 0.25 mm$^{-1}$
$T$ = 293 (2) K
Prism, colourless
0.80 × 0.57 × 0.49 mm

*Data collection*

Stoe–Siemens AED four-circle diffractometer
$\omega$ scans
Absorption correction: $\psi$ scan (*EMPIR*; Stoe & Cie, 1987)
$T_{min}$ = 0.823, $T_{max}$ = 0.886
4860 measured reflections
4581 independent reflections
2865 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.024
$\theta_{max}$ = 30.0°
$h = 0 \rightarrow 12$
$k = 0 \rightarrow 15$
$l = -24 \rightarrow 24$
2 standard reflections
frequency: 60 min
intensity decay: 6%

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.114
$S$ = 1.02
4581 reflections
210 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0562P)^2 + 0.1871P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.23 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.23 e Å$^{-3}$
Extinction correction: *SHELXL*97
Extinction coefficient: 0.0278 (18)

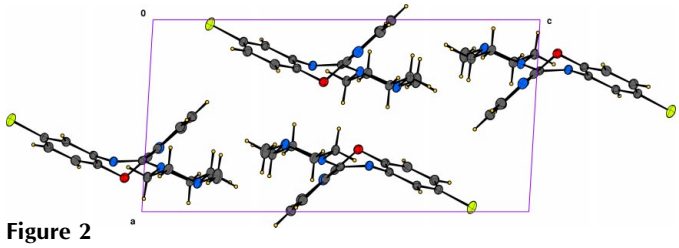


**Figure 2**
*CAMERON* (Watkin *et al.*, 1996) view of the packing of (I).

**Table 1**
Selected geometric parameters (Å, °).

| | | | |
|---|---|---|---|
| C2—N3 | 1.335 (2) | C9—Cl1 | 1.7403 (15) |
| N3—C4 | 1.3153 (19) | C11—N12 | 1.3972 (16) |
| C4—O5 | 1.3867 (17) | N12—C13 | 1.2986 (16) |
| O5—C6 | 1.3971 (16) | C13—N16 | 1.3667 (17) |
| | | | |
| C4—N3—C2 | 116.14 (14) | N12—C13—C14 | 124.05 (12) |
| C13—N12—C11 | 121.94 (12) | C17—N16—C21 | 111.32 (11) |
| N12—C13—N16 | 118.90 (12) | C20—N19—C18 | 109.64 (11) |
| | | | |
| N3—C4—O5—C6 | 109.53 (13) | C11—N12—C13—C14 | −8.9 (2) |
| C14—C4—O5—C6 | −70.71 (15) | N12—C13—C14—C4 | 47.45 (19) |
| C4—O5—C6—C7 | −114.19 (14) | N16—C13—C14—C4 | −139.48 (13) |
| C4—O5—C6—C11 | 66.68 (16) | C14—C13—N16—C17 | −174.80 (12) |
| O5—C6—C11—N12 | 6.5 (2) | N12—C13—N16—C21 | −149.35 (13) |
| C6—C11—N12—C13 | −39.5 (2) | | |

H atoms were constrained as riding atoms, with C—H = 0.93–0.97 Å and with isotropic displacement parameters fixed at $1.2U_{eq}$ of the parent atom ($1.5U_{eq}$ for methyl H atoms).

Data collection: *DIF*4 (Stoe & Cie, 1987); cell refinement: *DIF*4; data reduction: *REDU*4 (Stoe & Cie, 1987); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Burnett & Johnson, 1996); software used to prepare material for publication: *SHELXL*97.

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