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## Structure Reports

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## Key indicators

Single-crystal X-ray study
$T=295 \mathrm{~K}$
Mean $\sigma(\mathrm{C}-\mathrm{C})=0.003 \AA$
$R$ factor $=0.046$
$w R$ factor $=0.142$
Data-to-parameter ratio $=12.1$
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

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## (2-Ethoxyphenyl)[4-(6-fluorobenzo[d]-isoxazol-3-yl)piperidin-1-yl]methanone

In the title compound, $\mathrm{C}_{21} \mathrm{H}_{21} \mathrm{FN}_{2} \mathrm{O}_{3}$, the piperidine ring is in a chair conformation with the substituted benzisoxazole ring system in an equatorial position. An intermolecular C$\mathrm{H} \cdots \mathrm{O}$ interaction is present in the crystal structure.

## Comment

The chemistry of substituted 1,2-benzisoxazole amides plays an extremely important role in the field of pharmaceuticals and medicine (Dollery et al., 1999). The title compound, (I), was found to be a significant in vitro antimicrobial agent when compared to nystatin, which we have reported earlier (Priya et al., 2005). Encouraged by this information, we now report the crystal structure of the title compound, (I) (Fig. 1).

(I)

The piperidine ring (N1/C2-C6) adopts a chair conformation. The planar benzisoxazole ring system is in an equatorial position [ $\left.\mathrm{N} 26-\mathrm{C} 18-\mathrm{C} 4-\mathrm{C} 3=97.3(2)^{\circ}\right]$ with respect to the piperidine ring. A similar conformation was observed in the related 6-fluoro-3-(4-piperidinio)benz[ $d$ ]isoxazole chloride (Yathirajan et al., 2005). The carbonyl group bisects the plane of the piperidine ring with an angle of $56.91(15)^{\circ}$. The $\mathrm{C} 7=\mathrm{O} 8$ carbonyl group is almost coplanar with the $\mathrm{N} 1-\mathrm{C} 2$ bond of the piperidine ring $\left[\mathrm{O} 8-\mathrm{C} 7-\mathrm{N} 1-\mathrm{C} 2=3.7(3)^{\circ}\right]$ but


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the $50 \%$ probability level. H atoms are represented as small spheres of arbitrary radius.
it is twisted [C14-C9-C7-O8 = 62.3(3) ${ }^{\circ}$ ] from the mean plane of the ethoxyphenyl ring. The ethoxy group is oriented in an anti-periplanar conformation and lies in the plane of the benzene ring $\left[\mathrm{C} 10-\mathrm{O} 15-\mathrm{C} 16-\mathrm{C} 17=-179.4(2)^{\circ}\right]$. The dihedral angle between the mean plane of the piperidine ring (N1/C2-C6) and the benzisoxazole group is $56.8(2)^{\circ}$, while the ethoxyphenyl ring makes a dihedral angle of 43.9 (2) ${ }^{\circ}$ with the piperidine ring.
In the crystal structure, an inversion-generated intermolecular $\mathrm{C}-\mathrm{H} \cdots \mathrm{O}$ interaction occurs (Table 1), leading to dimeric associations of molecules, stacked in pairs when viewed down the $a$ axis (Fig. 3).

## Experimental

The title compound was synthesized according to the published procedure (Priya et al., 2005). Colorless single crystals of (I) were obtained by slow evaporation of an ethyl acetate solution.

## Crystal data

$\mathrm{C}_{21} \mathrm{H}_{21} \mathrm{FN}_{2} \mathrm{O}_{3}$
$M_{r}=368.40$
Triclinic, $P \overline{1}$
$a=7.029(6) \AA$
$b=9.851(7) \AA$
$c=14.120(2) \AA$
$\alpha=107.125(5)^{\circ}$
$\beta=94.622(5)^{\circ}$
$\gamma=100.513(5)^{\circ}$

$$
\begin{aligned}
& V=909.2(10) \AA^{3} \\
& Z=2 \\
& D_{x}=1.346 \mathrm{Mg} \mathrm{~m}^{-3} \\
& \text { Mo } K \alpha \text { radiation } \\
& \mu=0.10 \mathrm{~mm}^{-1} \\
& T=295(2) \mathrm{K} \\
& \text { Block, colorless } \\
& 0.25 \times 0.25 \times 0.20 \mathrm{~mm}
\end{aligned}
$$

## Data collection

MacScience DIPLabo 32001 diffractometer
$\omega$ scans
Absorption correction: none 4897 measured reflections

## Refinement

Refinement on $F^{2}$
$R\left[F^{2}>2 \sigma\left(F^{2}\right)\right]=0.046$
$w R\left(F^{2}\right)=0.142$
$S=1.15$
2954 reflections
245 parameters
H-atom parameters constrained

Table 1
Hydrogen-bond geometry ( $\AA^{\circ},{ }^{\circ}$ ).

| $D-\mathrm{H} \cdots A$ | $D-\mathrm{H}$ | $\mathrm{H} \cdots A$ | $D \cdots A$ | $D-\mathrm{H} \cdots A$ |
| :--- | :--- | :--- | :--- | :--- |
| $\mathrm{C} 2-\mathrm{H} 2 A \cdots \mathrm{O}^{\mathrm{i}}$ | 0.97 | 2.49 | $3.359(3)$ | 149 |

Symmetry code: (i) $-x+1,-y+1,-z$.


Figure 2
The crystal packing in (I), viewed down the $a$ axis. The dashed lines indicate intermolecular $\mathrm{C}-\mathrm{H} \cdots \mathrm{O}$ interactions.

H atoms were placed at idealized positions ( $\mathrm{C}-\mathrm{H}=0.92-0.98 \AA$ ) and refined as riding, with $U_{\text {iso }}(\mathrm{H})=1.2 U_{\text {eq }}(\mathrm{C})$ or $1.5 U_{\text {eq }}$ (methyl C).

Data collection: XPRESS (MacScience, 2002); cell refinement: SCALEPACK (Otwinowski \& Minor, 1997); data reduction: SCALEPACK and DENZO (Otwinowski \& Minor, 1997); program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: PLATON (Spek, 2003) and ORTEPII (Johnson, 1976); software used to prepare material for publication: PLATON.

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