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Key indicators

Single-crystal X-ray study T = 295 KMean $\sigma(\text{C}-\text{C}) = 0.003 \text{ Å}$ R factor = 0.046 wR 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. In the title compound, $C_{21}H_{21}FN_2O_3$, the piperidine ring is in a chair conformation with the substituted benzisoxazole ring system in an equatorial position. An intermolecular C- $H \cdots O$ interaction is present in the crystal structure.

(2-Ethoxyphenyl)[4-(6-fluorobenzo[d]-

isoxazol-3-yl)piperidin-1-yl]methanone

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).



The piperidine ring (N1/C2-C6) adopts a chair conformation. The planar benzisoxazole ring system is in an equatorial position $[N26-C18-C4-C3 = 97.3 (2)^{\circ}]$ 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)°. The C7=O8 carbonyl group is almost coplanar with the N1-C2 bond of the piperidine ring $[O8-C7-N1-C2 = 3.7 (3)^{\circ}]$ 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.

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Received 26 December 2006 Accepted 4 January 2007 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 $[C10-O15-C16-C17 = -179.4 (2)^{\circ}]$. The dihedral angle between the mean plane of the piperidine ring (N1/C2-C6) and the benzisoxazole group is 56.8 (2)°, while the ethoxyphenyl ring makes a dihedral angle of 43.9 (2)° with the piperidine ring.

In the crystal structure, an inversion-generated intermolecular C—H···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.

 $V = 909.2 (10) \text{ Å}^3$

 $D_x = 1.346 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation $\mu = 0.10 \text{ mm}^{-1}$

T = 295 (2) K

 $R_{\rm int} = 0.030$

 $\theta_{\rm max} = 25.0^{\circ}$

Block, colorless

 $0.25 \times 0.25 \times 0.20$ mm

2954 independent reflections

2535 reflections with $I > 2\sigma(I)$

Z = 2

Crystal data

 $\begin{array}{l} C_{21}H_{21}FN_2O_3\\ M_r = 368.40\\ Triclinic, $P\overline{1}$\\ a = 7.029 (6) Å\\ b = 9.851 (7) Å\\ c = 14.120 (2) Å\\ \alpha = 107.125 (5)^\circ\\ \beta = 94.622 (5)^\circ\\ \gamma = 100.513 (5)^\circ\end{array}$

Data collection

MacScience DIPLabo 32001 diffractometer ω scans Absorption correction: none 4897 measured reflections

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.046$	+ 0.3865P]
$wR(F^2) = 0.142$	where $P = (F_0^2 + 2F_c^2)/3$
S = 1.15	$(\Delta/\sigma)_{\rm max} < 0.001$
2954 reflections	$\Delta \rho_{\rm max} = 0.17 \text{ e } \text{\AA}^{-3}$
245 parameters	$\Delta \rho_{\rm min} = -0.19 \text{ e } \text{\AA}^{-3}$
H-atom parameters constrained	

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdot \cdot \cdot A$	D-H	$H \cdot \cdot \cdot A$	$D \cdots A$	$D - \mathbf{H} \cdots A$
$C2-H2A\cdots O8^{i}$	0.97	2.49	3.359 (3)	149
a				

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 $C-H \cdots O$ interactions.

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

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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