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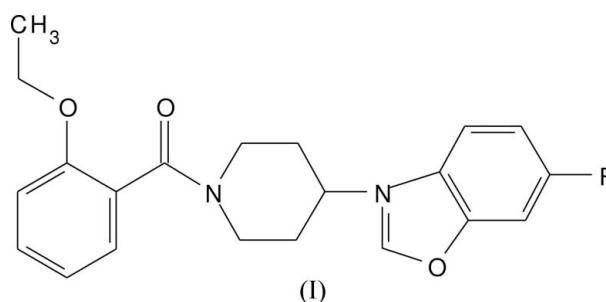
Key indicators

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

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

In the title compound, $\text{C}_{21}\text{H}_{21}\text{FN}_2\text{O}_3$, 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.Received 26 December 2006
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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 [$\text{N}26-\text{C}18-\text{C}4-\text{C}3 = 97.3 (2)^\circ$] with respect to the piperidine ring. A similar conformation was observed in the related 6-fluoro-3-(4-piperidino)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 $\text{C}7=\text{O}8$ carbonyl group is almost coplanar with the $\text{N}1-\text{C}2$ bond of the piperidine ring [$\text{O}8-\text{C}7-\text{N}1-\text{C}2 = 3.7 (3)^\circ$] but

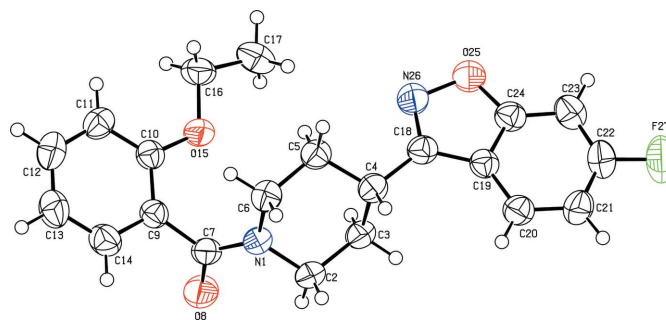


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

it is twisted [C14–C9–C7–O8 = 62.3 (3)°] 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)°]. 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.

Crystal data

C ₂₁ H ₂₁ FN ₂ O ₃	$V = 909.2 (10) \text{ \AA}^3$
$M_r = 368.40$	$Z = 2$
Triclinic, $P\bar{1}$	$D_x = 1.346 \text{ Mg m}^{-3}$
$a = 7.029 (6) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.851 (7) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 14.120 (2) \text{ \AA}$	$T = 295 (2) \text{ K}$
$\alpha = 107.125 (5)^\circ$	Block, colorless
$\beta = 94.622 (5)^\circ$	$0.25 \times 0.25 \times 0.20 \text{ mm}$
$\gamma = 100.513 (5)^\circ$	

Data collection

MacScience DIPLabo 32001 diffractometer	2954 independent reflections
ω scans	2535 reflections with $I > 2\sigma(I)$
Absorption correction: none	$R_{\text{int}} = 0.030$
4897 measured reflections	$\theta_{\text{max}} = 25.0^\circ$

Refinement

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

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2–H2A···O8 ⁱ	0.97	2.49	3.359 (3)	149

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

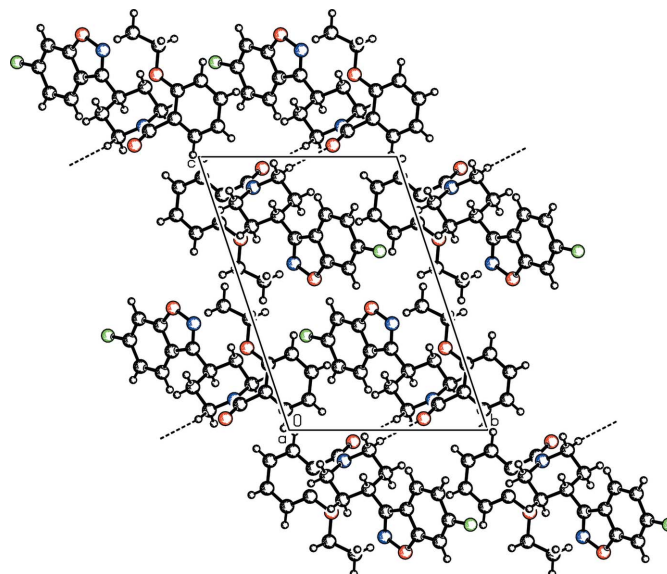


Figure 2

The crystal packing in (I), viewed down the *a* axis. The dashed lines indicate intermolecular C–H···O interactions.

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

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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References

- Dollery, C. (1999). *Gemfibrozil*, in *Therapeutic Drugs*, edited by C. Dollery, pp. G34–G37. Edinburgh: Churchill Livingstone.
- Johnson, C. K. (1976). *ORTEPII*. Report ORNL-5138. Oak Ridge National Laboratory, Tennessee, USA.
- MacScience (2002). *XPRESS*. MacScience Co. Ltd, Yokohama, Japan.
- Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by Carter, C. W. Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
- Priya, B. S., Basappa, Nanjunda Swamy, S. & Rangappa, K. S. (2005). *Bioorg. Med. Chem.* **13**, 2623–2628.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
- Yathirajan, H. S., Narasimhamurthy, T., Nagaraj, B., Nagaraja, P., Narasgowda, R. S. & Rathore, R. S. (2005). *Acta Cryst.* **E61**, o356–o358.