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

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 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.

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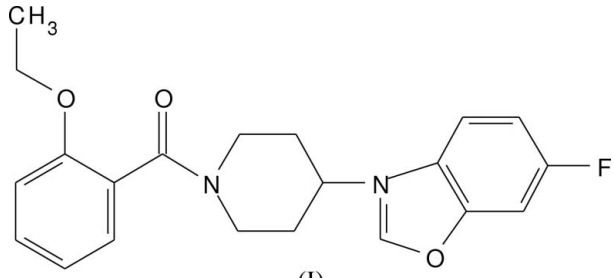
In the title compound, $C_{21}H_{21}FN_2O_3$, the piperidine ring is in a chair conformation with the substituted benzisoxazole ring system in an equatorial position. An intermolecular C—H···O interaction is present in the crystal structure.

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 [N26—C18—C4—C3 = 97.3 (2)°] 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)°] but

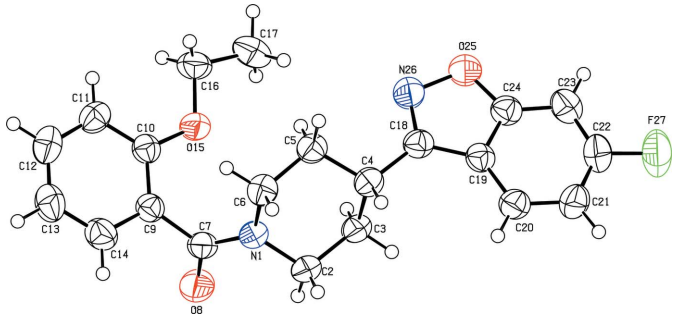


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radius.

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

$C_{21}H_{21}FN_2O_3$
M_r = 368.40
Triclinic, $P\overline{1}$
a = 7.029 (6) Å
b = 9.851 (7) Å
c = 14.120 (2) Å
α = 107.125 (5)°
β = 94.622 (5)°
γ = 100.513 (5)°
V = 909.2 (10) Å^3
Z = 2
D_x = 1.346 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 295 (2) K
Block, colorless
0.25 × 0.25 × 0.20 mm

Data collection

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

Refinement

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

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C2—H2A···O8^{i}	0.97	2.49	3.359 (3)	149

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

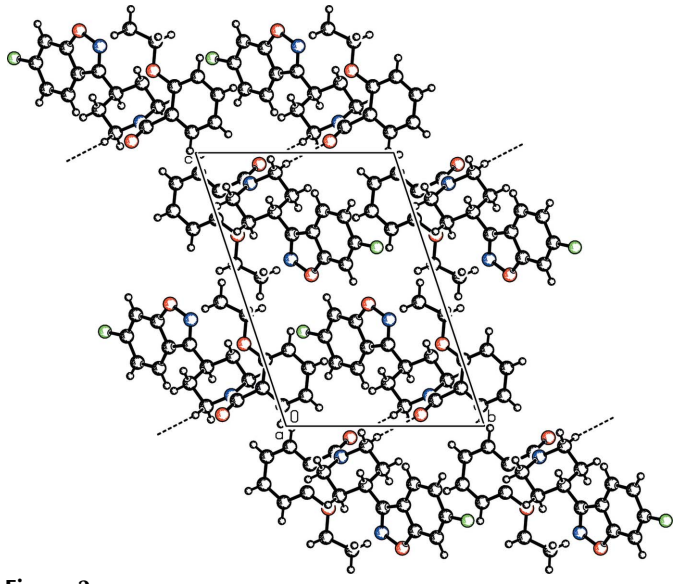


Figure 2
The crystal packing in (I), viewed down the *a* axis. The dashed lines indicate intermolecular C—H···O interactions.

H atoms were placed at idealized positions (C—H = 0.92–0.98 Å) and refined as riding, with U_{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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