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5-(4-Fluoro-3-phenoxyphenyl)-3-phenyl-4,5-dihydroisoxazole

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Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ(C–C) = 0.009 Å
R factor = 0.081
wR factor = 0.207
Data-to-parameter ratio = 8.3

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

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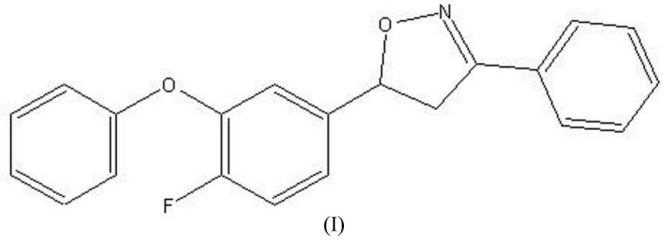
The title compound, $C_{21}H_{16}FNO_2$, is chiral, having an asymmetric C atom, and is found to crystallize in a non-centrosymmetric space group. The five-membered isoxazole ring exists in an envelope conformation. The crystal structure is stabilized by weak intermolecular C—H···O interactions.

Comment

Recent synthetic efforts have established the importance of biologically active heterocyclic compounds (Foti *et al.*, 2004). Of particular importance are the derivatives of isoxazoles, representing one of the most active class of compounds, widely used in agrochemicals and pharmaceuticals (He *et al.*, 2004). Such compounds have been studied from a synthetic (Bruno *et al.*, 2004) and also from a structural viewpoint (Zhong *et al.*, 2005). These have also been used in natural product synthesis and proven to be efficient precursors for many key synthetic intermediates, including γ-aminoalcohols and β-hydroxyketones (Kozikowski, 1984; Kanemasa & Tsuge, 1990). Spirooxazoles have exhibited herbicidal, plant-regulatory and antitumour activities (Howe & Shelton, 1990; De Amici *et al.*, 1990; Smietana *et al.*, 1999). In view of the important applications of such a class of compounds and in continuation of our interest in the chemistry of isoxazoles, we report here the molecular and crystal structure of the title compound, (I).



(I)

The total puckering amplitude (Cremer & Pople, 1975) of the isoxazole ring is $Q(2)$ = 0.130 (6) Å and $\varphi(2)$ = 140 (1)° [$\varphi(2) = 36k$; envelope conformation, k = 4) in compound (I), indicating that the five-membered ring exists in an envelope conformation. Atom C13 is displaced by 0.209 (5) Å from the O2/N1/C14/C15 plane. Furthermore, the phenyl and isoxazole rings make a dihedral angle of 4.7 (2)°, whereas the fluorophenoxy moiety is orthogonal to the five-membered ring, the dihedral twist being 78.2 (2)°.

The crystal structure is stabilized by weak C—H···O intermolecular interactions (Table 2), forming molecular *C*(4) (Bernstein *et al.*, 1995) chains along the crystallographic *b* axis and hence a layer consisting of chiral molecules (Fig. 2).

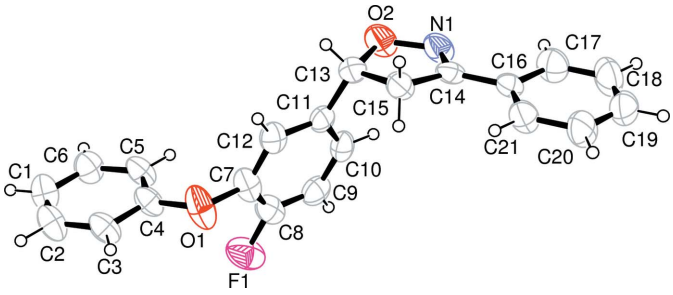


Figure 1
: The structure of compound (I), drawn with 50% ellipsoidal probability (arbitrary spheres for H atoms).

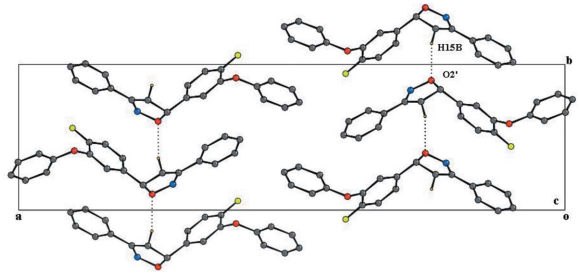


Figure 2
: Packing diagram highlighting C—H···O interactions (dotted lines) in (I). H atoms not involved in these interactions have been omitted. The atom marked by ' has the symmetry code $(-x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2})$.

Experimental

The title compound was synthesized in accordance with the procedure reported in the literature (Joseph *et al.*, 2004; Archana *et al.*, 2002). Single crystals were grown by dissolving 10–15 mg of the sample in dichloromethane/hexane (2:1 *v*/*v*) and allowing the solvent to evaporate at 275–277 K (in a refrigerator) to obtain crystals of suitable size and quality.

Crystal data

$C_{21}H_{16}FNO_2$
$M_r = 333.35$
Orthorhombic, $Pna2_1$
$a = 33.31\ (2)$ Å
$b = 8.840\ (6)$ Å
$c = 5.749\ (4)$ Å
$V = 1693.0\ (19)$ Å^3
$Z = 4$
$D_x = 1.308$ Mg m^{-3}
Mo $K\alpha$ radiation
$\mu = 0.09$ mm^{-1}
$T = 290\ (2)$ K
Block, colourless
0.43 × 0.12 × 0.03 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.948$, $T_{max} = 0.998$
12350 measured reflections
1873 independent reflections
1486 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 26.4°$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.081$
$wR(F^2) = 0.207$
$S = 1.32$
1873 reflections
226 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1004P)^2 + 0.0067P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -0.20$ e Å^{-3}

Table 1
Selected bond lengths (Å).

N1—C14	1.279 (7)	C15—C13	1.534 (8)
N1—O2	1.422 (6)	O2—C13	1.465 (8)
C15—C14	1.510 (8)		

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15B···O2^{i}	0.97	2.36	3.305 (7)	166

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, z-\frac{1}{2}$.

H atoms were placed in calculated positions with C—H = 0.93 (aromatic), 0.97 (methylene) and 0.98 Å (methine), and refined in riding mode with $U_{iso}(H) = 1.2U_{eq}(C)$. In the absence of significant anomalous scattering effects, Friedel pairs were averaged.

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1993); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1999) and *CAMERON* (Watkin *et al.*, 1993); software used to prepare material for publication: *PLATON* (Spek, 2003).

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