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3-[3-(4-Ethoxyphenyl)-1-phenyl-1*H*-pyrazol-4-yl]-4-nitro-2,5-diphenylisoxazolidine

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Key indicators

Single-crystal X-ray study
T = 273 K
Mean σ(C–C) = 0.003 Å
R factor = 0.051
wR factor = 0.144
Data-to-parameter ratio = 17.4

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

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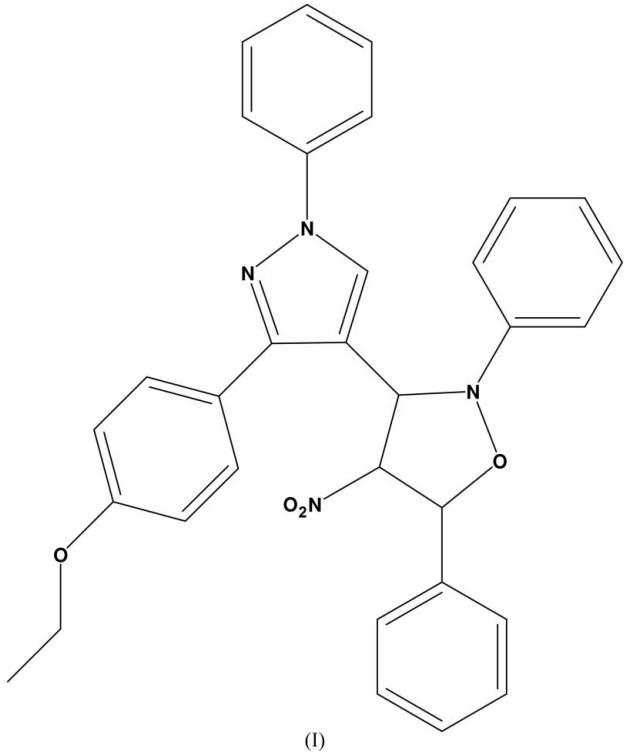
The isoxazolidine ring in the title compound, $C_{32}H_{28}N_4O_4$, adopts an envelope conformation.

Comment

Isoxazolidines are interesting intermediates for the synthesis of several classes of natural products and biologically active compounds such as β-amino acids and alkaloids (Gothelf & Jorgensen, 1998). Many pyrazole derivatives are known to exhibit a wide range of biological properties such as anti-hyperglycemic, analgesic, anti-inflammatory, antipyretic, anti-bacterial, hypoglycemic, sedative-hypnotic and anticoagulant activities. In particular, arylpyrazoles are widely used in medicinal and pesticidal chemistry. Recently, some aryl-pyrazoles were reported to display non-nucleoside HIV-1 reverse transcriptase inhibitory activity (Lee *et al.*, 2003).



(I)

Bond lengths and angles in the title compound, (I), are comparable with literature values (Allen *et al.*, 1987). The sum of the bond angles around N3 [332.1°] indicates sp^3 hybridisation. The pyrazole ring forms dihedral angles of 20.7 (1)° with the phenyl ring attached at N1 and 51.4 (1)° with the 4-ethoxyphenyl ring at C13. The isoxazolidine ring adopts a twisted conformation with a pseudo-twofold axis passing through atom C19 and bond O4—N3.

Experimental

A solution of pyrazolyl nitrone (0.5 mmol) and β-nitrostyrene (0.5 mmol) was refluxed in dry toluene (10 ml). The completion of the reaction was monitored by thin-layer chromatography. The solvent was evaporated under reduced pressure to give the crude product, which was further purified by column chromatography using petroleum ether–ethyl acetate (96:4) as eluent, to afford the pure product (68%) as a pale-yellow solid. Single crystals were obtained by crystallization from chloroform.

Crystal data

$C_{32}H_{28}N_4O_4$
M_r = 532.58
Monoclinic, $P2_1/n$
a = 13.2463 (7) Å
b = 10.0112 (6) Å
c = 20.9518 (12) Å
β = 101.688 (1)°
V = 2720.8 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 273 (2) K
0.27 × 0.24 × 0.23 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: none
30188 measured reflections
6286 independent reflections
4903 reflections with $I > 2\sigma(I)$
R_{int} = 0.024

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.144
S = 1.03
6286 reflections
362 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

All H atoms were refined using a riding model, with C—H = 0.93 Å, U_{iso}(H) = 1.2U_{eq}(C) for aromatic, C—H = 0.98 Å, U_{iso}(H) = 1.2U_{eq}(C) for CH, C—H = 0.97 Å, U_{iso}(H) = 1.2U_{eq}(C) for CH_2, C—H = 0.96 Å, U_{iso}(H) = 1.5U_{eq}(C) for CH_3 atoms and N—H = 0.86 Å, U_{iso}(H) = 1.2U_{eq}(N) for the NH group.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97* and *PARST* (Nardelli, 1995).

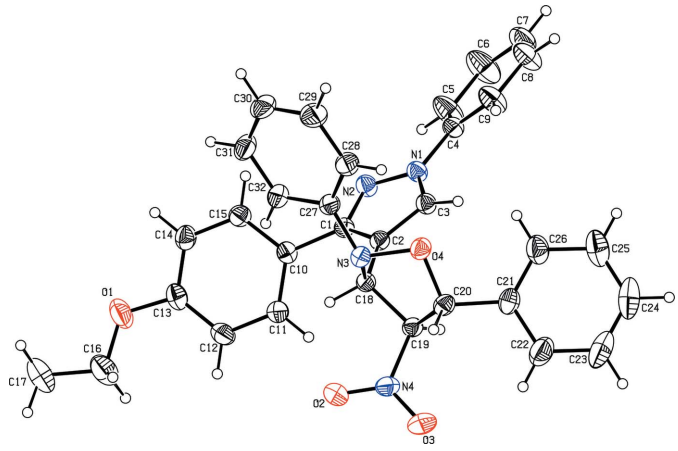


Figure 1
The molecular structure of the title compound, showing 30% probability displacement ellipsoids.

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