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2-[*N*-(2-Ethoxyphenyl)carbamoylmethoxy]-*N*-(2-pyridylmethyl)benzamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.003 Å
R factor = 0.052
wR factor = 0.120
Data-to-parameter ratio = 14.3

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

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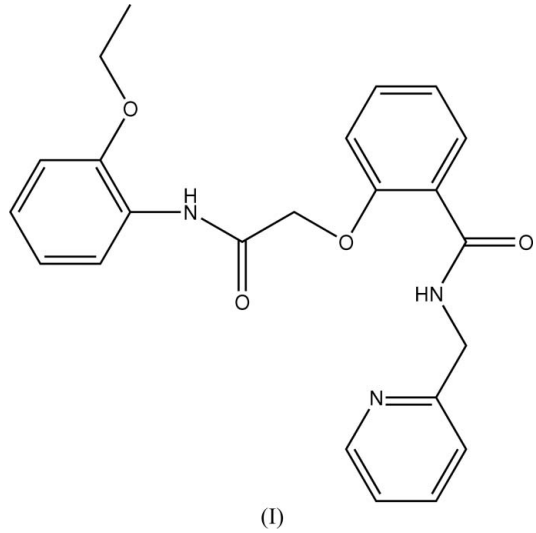
In the title compound, $C_{23}H_{23}N_3O_4$, the molecule is essentially planar, except for the pyridine ring. In the crystal structure, the molecules are linked into layers by N—H···N, C—H···O and C—H···N hydrogen bonds. The packing is further stabilized by C—H···π interactions.

Comment

We have recently reported the structure of *N*,*N*,*N*′*N*′-tetraphenyl-2,2′-(*o*-phenylenedioxy)diacetamide, (II) (Wen, Li *et al.*, 2005). Here, we report the structure of the title compound, (I).



(I)

Bond lengths and angles in (I) are within normal ranges (Allen *et al.*, 1987) and comparable with those in the related compound, (II). In (I), the non-H atoms, except for those of the pyridine ring, are approximately coplanar, with a dihedral angle of 8.2 (1)° between the two benzene rings. There are five intramolecular N—H···O and C—H···O hydrogen bonds (Table 2), contributing to the planarity. The pyridine ring twists from the mean plane, making angles of 71.3 (1) and 79.4 (1)°, respectively, with the C8–C13 and C16–C21 rings.

In the crystal structure of (I), molecules are linked into layers (Fig. 2) *via* N3—H3*B*···N1^{i}, C3—H3*A*···O3^{ii} and C14—H14*A*···N1^{i} intermolecular interactions (symmetry codes as in Table 2). The packing is further stabilized by a C—H···π interaction involving the pyridine ring (centroid *Cg*1).

Experimental

The title compound was prepared according to the literature method of Wen, Zhang *et al.* (2005). Colourless crystals were obtained by slow evaporation of a petroleum ether–ethyl acetate solution (1:3, *v*/*v*) over a period of 5 d.

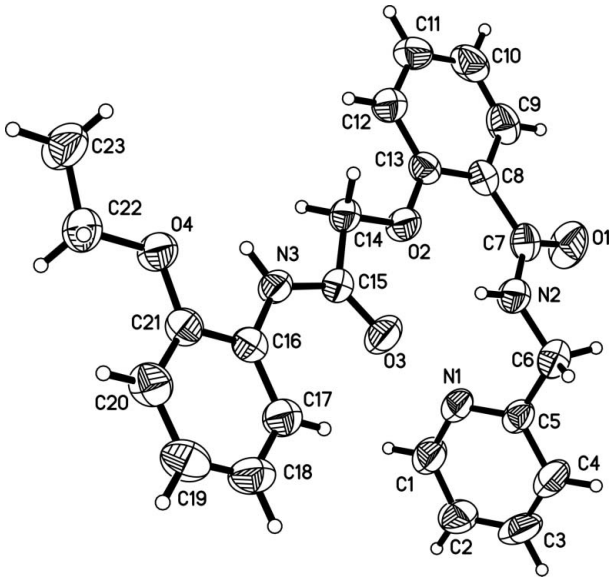


Figure 1
The structure of compound (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

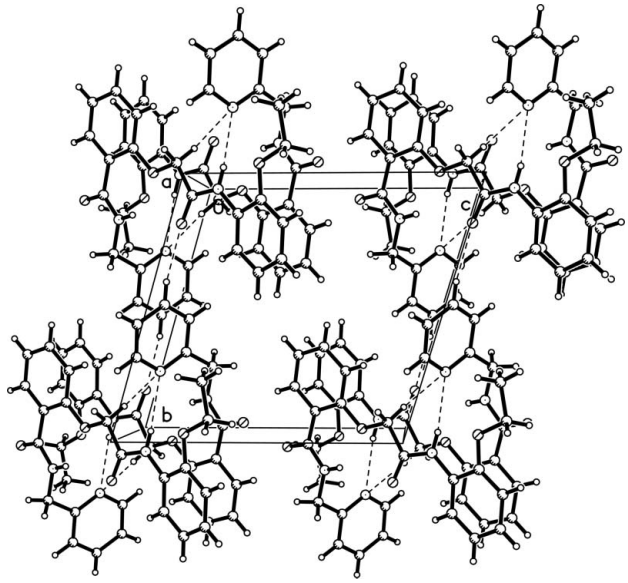


Figure 2
A packing diagram of (I), viewed down the *a* axis, showing the two-dimensional layers. Dashed lines indicate hydrogen bonds.

Crystal data

$C_{23}H_{23}N_3O_4$
M_r = 405.44
Triclinic, $P\overline{1}$
a = 8.7109 (14) Å
b = 10.8764 (17) Å
c = 11.2510 (18) Å
α = 106.481 (3)°
β = 90.471 (3)°
γ = 100.828 (3)°
V = 1001.8 (3) Å^3
Z = 2
D_x = 1.344 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 1716 reflections
θ = 2.3–25.5°
μ = 0.09 mm^{-1}
T = 293 (2) K
Block, colourless
0.34 × 0.14 × 0.08 mm

Data collection

Siemens SMART 1000 CCD area-detector diffractometer
ω scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.969, T_{max} = 0.993
5693 measured reflections
3863 independent reflections
2986 reflections with $I > 2\sigma(I)$
R_{int} = 0.015
θ_{max} = 26.1°
$h = -8 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -13 \rightarrow 13$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.121
S = 1.07
3863 reflections
271 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0469P)^2 + 0.197P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.218 (2)	O4—C22	1.431 (2)
O2—C13	1.375 (2)	N2—C7	1.341 (2)
O2—C14	1.4126 (19)	N2—C6	1.443 (2)
O3—C15	1.218 (2)	N3—C15	1.351 (2)
O4—C21	1.363 (2)	N3—C16	1.413 (2)
C7—N2—C6	121.29 (16)	C15—N3—C16	128.42 (15)

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

*Cg*1 is the centroid of the pyridine ring (N1/C1–C5).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2*A*···O2	0.86	1.98	2.652 (2)	134
N3—H3*B*···O4	0.86	2.21	2.603 (2)	108
N3—H3*B*···N1^{i}	0.86	2.41	3.224 (2)	158
C3—H3*A*···O3^{ii}	0.93	2.36	3.272 (3)	166
C6—H6*B*···O1	0.97	2.35	2.733 (3)	103
C9—H9*A*···O1	0.93	2.40	2.739 (3)	101
C14—H14*A*···N1^{i}	0.97	2.54	3.186 (3)	124
C17—H17*A*···O3	0.93	2.34	2.922 (2)	121
C23—H23*B*···*Cg*1^{i}	0.96	2.73	3.546 (3)	136

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x+1, -y-1, -z$.

All H atoms were located in a difference Fourier map and constrained to ride on their parent atoms, with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and with U_{iso}(H) = 1.2U_{eq}(C or N) or 1.5U_{eq}(methyl C).

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 1997); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

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