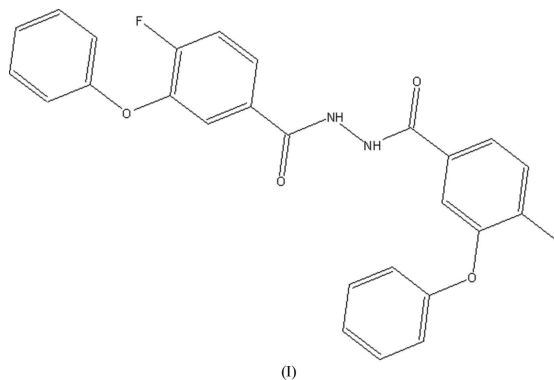


4-Fluoro-*N'*-(4-fluoro-3-phenoxybenzoyl)-
3-phenoxybenzohydrazideDeepak Chopra,^{a*} T. P. Mohan^b
and B. Vishalakshi^b^aSolid State and Structural Chemistry Unit,
Indian Institute of Science, Bangalore 560 012,
Karnataka, India, and ^bDepartment of
Chemistry, Mangalore University, Bangalore
574 199, Karnataka, IndiaCorrespondence e-mail:
deepak@sscu.iisc.ernet.in

Key indicators

Single-crystal X-ray study
T = 290 K
Mean σ (C–C) = 0.010 Å
R factor = 0.098
wR factor = 0.197
Data-to-parameter ratio = 12.3For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.In the title compound, C₂₆H₁₈F₂N₂O₄, the dihedral angle
between the amide groups is 57.1 (3)°. The crystal structure is
stabilized by N–H···O hydrogen bonds and C–H··· π
interactions.Received 12 June 2006
Accepted 24 June 2006

Comment

Dibenzoylhydrazines are non-steroidal moulting hormone
agonists that have insecticidal activity while exerting only a
low toxicity against non-target insects (Nakagawa *et al.*, 2005).
With this background, we have synthesized and studied the
crystal structure of the title compound, (I). The molecular
structure of (I) is shown in Fig. 1. The dihedral angle between
the amide groups (N1/C7/O3 and N2/C8/O2) is 57.1 (3)°. Atoms
N1 and N2 both show a planar configuration, the N–
N–C angles being in the range 119.6 (4)–119.9 (4)° (Table 1).The crystal structure is stabilized by two types of N–H···O
hydrogen bonds (Table 2), one forming chains (involving
H2N) and the other (involving H1N) forming dimers with O2
(Fig. 2). In addition, C–H··· π dimers involving atom H3 and
benzene ring C9–C14 stabilize the molecular assembly.

Experimental

Compound (I) was synthesized by one of the authors (Mohan, 2006).
Crystals were grown by slow evaporation of an acetone solution at
275–277 K.

Crystal data

C₂₆H₁₈F₂N₂O₄
M_r = 460.42
Monoclinic, *P*2₁/*c*
a = 18.375 (4) Å
b = 18.236 (4) Å
c = 6.5954 (15) Å
 β = 93.680 (5)°
V = 2205.5 (8) Å³*Z* = 4
D_x = 1.387 Mg m⁻³
Mo *K* α radiation
 μ = 0.11 mm⁻¹
T = 290 (2) K
Thick plate, colourless
0.25 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.940$, $T_{\max} = 0.990$

15717 measured reflections
 3865 independent reflections
 2556 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.082$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.098$
 $wR(F^2) = 0.197$
 $S = 1.29$
 3865 reflections
 315 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.9271P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} < 0.001$
 $\Delta\rho_{\text{max}} = 0.22 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.21 \text{ e } \text{\AA}^{-3}$

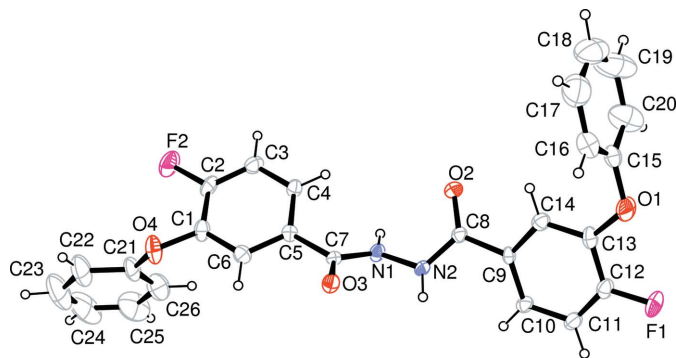


Figure 1 View of (I), with 30% probability ellipsoids.

Table 1

Selected geometric parameters (\AA , $^\circ$).

F1—C12	1.345 (5)	C7—N1	1.336 (5)
O2—C8	1.232 (5)	F2—C2	1.350 (5)
C7—O3	1.225 (5)	N1—N2	1.387 (5)
C7—N1—N2	119.9 (4)	C8—N2—N1	119.6 (4)
O3—C7—N1—N2	−9.5 (7)	O3—C7—C5—C4	144.8 (4)
O2—C8—C9—C10	−148.4 (4)	C13—O1—C15—C20	−91.1 (7)
C9—C8—N2—N1	−177.8 (4)	C6—C1—O4—C21	−109.6 (5)
C7—N1—N2—C8	−119.3 (5)	C1—O4—C21—C26	25.8 (8)

Table 2

Hydrogen-bond geometry (\AA , $^\circ$).

$Cg1$ is the centroid of the C9—C14 ring.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N \cdots O2 ⁱ	0.87 (5)	2.19 (5)	3.047 (6)	168 (5)
N2—H2N \cdots O3 ⁱⁱ	0.84 (4)	2.17 (4)	3.003 (5)	178 (4)
C3—H3 \cdots Cg1 ⁱⁱⁱ	0.93	2.80	3.451 (6)	128

Symmetry codes: (i) $-x + 1, -y + 1, -z$; (ii) $x, -y + \frac{1}{2}, z + \frac{1}{2}$; (iii) $-x + 1, -y, -z + 1$.

The amino H atoms were located in a difference Fourier map and refined isotropically. The remaining H atoms were positioned geometrically and refined using a riding model, with $C-H = 0.93 \text{ \AA}$ and $U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C)$.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT (Bruker, 2000); 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, 1997) and CAMERON (Watkin *et al.*, 1993); software used to prepare material for publication: PLATON (Spek, 2003).

We thank Professor T. N. Guru Row, Indian Institute of Science and Department of Science and Technology, for data

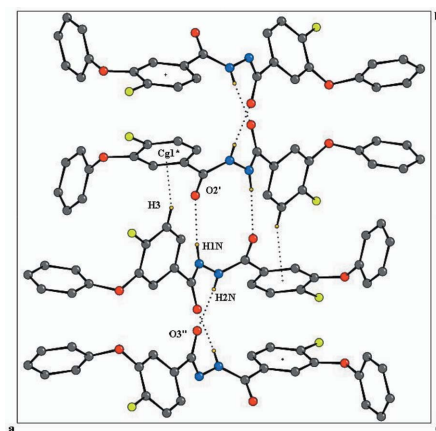


Figure 2

Packing diagram of (I), highlighting the $N-H\cdots O$ hydrogen bonds and $C-H\cdots\pi$ interactions in the ab plane. Interactions are drawn as dotted lines. H atoms have been omitted unless they are involved in hydrogen bonds. [Symmetry codes: (') $1 - x, 1 - y, -z$; (") $x, \frac{1}{2} - y, \frac{1}{2} + z$; (*) $1 - x, -y, 1 - z$.]

collection on the CCD facility under the IRHPA–DST scheme. DC thanks CSIR, India, for a Junior Research Fellowship.

References

Altomare, A., Cascarano, G., Giacovazzo, C. & Guagliardi, A. (1993). *J. Appl. Cryst.* **26**, 343–350.
 Bruker (2000). SMART (Version 5.628) and SAINT (Version 6.45a). Bruker AXS Inc., Madison, Wisconsin, USA.
 Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
 Mohan, T. P. (2006). Thesis dissertation, Mangalore University, India.
 Nakagawa, Y., Takahashi, K., Kishikawa, H., Ogura, T., Minakuchi, C. & Miyagawa, H. (2005). *Bioorg. Med. Chem.* **13**, 1333–1340.
 Sheldrick, G. M. (1996). SADABS. Version 2.03. University of Göttingen, Germany.
 Sheldrick, G. M. (1997). SHELXL97. University of Göttingen, Germany.
 Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
 Watkin, D. M., Pearce, L. & Prout, C. K. (1993). CAMERON. Chemical Crystallography Laboratory, University of Oxford, England.