Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

N-Benzyl-4,5-dimethoxy-2-nitrobenzamide

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Key indicators

Single-crystal X-ray study
T = 293 K
Mean σ(C–C) = 0.007 Å
R factor = 0.066
wR factor = 0.183
Data-to-parameter ratio = 13.1

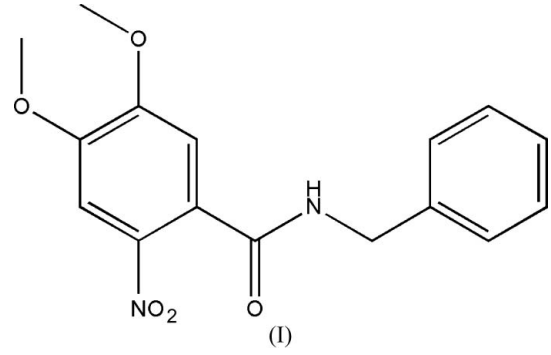
For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

Received 6 November 2006
Accepted 11 December 2006

The molecule of the title compound, $C_{16}H_{16}N_2O_5$, a biologically active benzamide derivative, is not planar. The crystal packing is stabilized by C—H···O and N—H···O hydrogen-bond interactions to form one-dimensional chains parallel to the *a* axis.

Comment

Benzamide and its derivatives have attracted the attention of researchers in a number of fields over the past two decades, *e.g.* α,β-unsaturated ketobenzamides are used as inhibitors of human rhinovirus 3C protease (Reich *et al.*, 2000) and orally active benzamides are used as antipsychotic agents with affinity for dopamine D2, serotonin 5-HT1A and adrenergic α1 receptors (Reitz *et al.*, 1998). In addition, a series of substituted {4-[4-(1,2-benzisothiazol-3-yl)-piperazin-1-yl]butyl}-benzamide derivatives have been prepared and evaluated as potential antipsychotic agents (Norman *et al.*, 1996). In view of the importance of this class of compounds, the title compound, (I), has been synthesized and its structure is reported here.



(I)

The molecular structure of the title compound is shown in Fig. 1. In (I), all bond lengths and angles are within normal ranges (Allen *et al.*, 1987). The C7/C9/N2/O5 amide group forms dihedral angles of 85.36 (17) and 50.16 (11)° with the C3–C8 and C11–C16 aromatic rings, respectively. In the crystal structure, the molecules are linked by intermolecular C—H···O and N—H···O hydrogen bonds (Table 1), forming one-dimensional chains parallel to the *a* axis.

Experimental

The title compound was prepared according to a standard method given in the literature (Finan & Forthergill, 1962). A mixture of 2-nitro-4,5-dimethoxybenzoyl chloride (2.1 g, 10 mmol) and phenylmethanamine (0.8 g, 10 mmol) in acetone (20 ml) was stirred vigorously for 2 h. The reaction mixture was filtered and the filtrate was

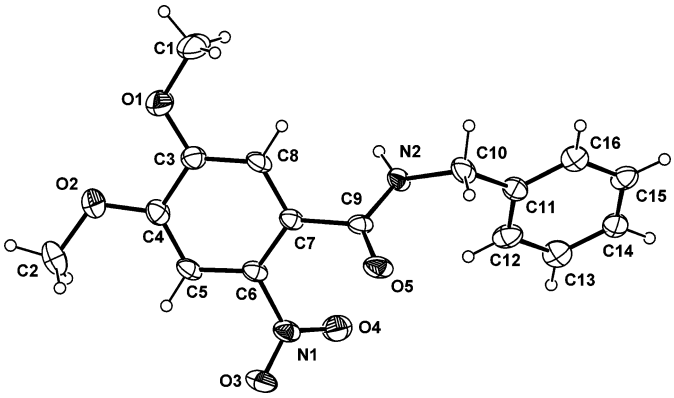


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 30% probability level.

evaporated to dryness. The solid residue was crystallized from hot toluene to give pale-yellow plates of the title compound, with an overall yield of 81% (m.p. 460–461 K).

Crystal data

$C_{16}H_{16}N_2O_5$
M_r = 316.31
Orthorhombic, *Pbca*
a = 14.915 (2) Å
b = 8.4187 (14) Å
c = 25.277 (4) Å
V = 3173.9 (8) Å^3
Z = 8
D_x = 1.324 Mg m^{-3}
Mo $K\alpha$ radiation
μ = 0.10 mm^{-1}
T = 293 (2) K
Plate, pale yellow
0.26 × 0.22 × 0.10 mm

Data collection

Bruker SMART CCD diffractometer
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.970, T_{max} = 0.993
14158 measured reflections
2785 independent reflections
1457 reflections with $I > 2\sigma(I)$
R_{int} = 0.097
θ_{max} = 25.0°

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.183
S = 1.00
2785 reflections
212 parameters
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0975P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H1···O3^{i}	0.92 (4)	2.60 (3)	2.958 (4)	104 (3)
N2—H1···O5^{ii}	0.92 (4)	2.06 (4)	2.957 (4)	165 (3)
C2—H2C···O4^{iii}	0.96	2.42	3.310 (5)	155
C5—H5A···O5^{iii}	0.93	2.52	3.368 (4)	152
C8—H8A···O3^{i}	0.93	2.56	3.453 (4)	160
C10—H10A···O5	0.97	2.43	2.816 (4)	103
C10—H10B···O3^{i}	0.97	2.60	3.227 (4)	123

Symmetry codes: (i) $x+\frac{1}{2}, y, -z+\frac{1}{2}$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, z$; (iii) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$.

The amide H atom was located in a difference Fourier synthesis and refined freely. All other H atoms were positioned geometrically and refined as riding, with C—H = 0.93–0.97 Å and with U_{iso}(H) = 1.2U_{eq}(C), or 1.5 U_{eq}(C) for methyl H atoms.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2003).

The authors gratefully acknowledge funds from the URF project, Quaid-I-Azam University, Islamabad, Pakistan.

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