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N-(5-Benzoyl-2-oxo-4-phenyl-1,2-dihydropyrimidin-1-yl)benzamide

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Key indicators

Single-crystal X-ray study
T = 150 K
Mean σ(C–C) = 0.002 Å
R factor = 0.032
wR factor = 0.085
Data-to-parameter ratio = 12.4

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

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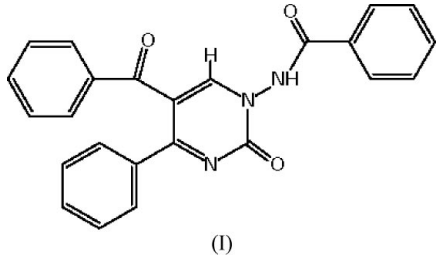
The molecule of the title compound, $C_{24}H_{17}N_3O_3$, is non-planar. The pyrimidine ring is almost planar and makes dihedral angles of 72.47 (6), 64.77 (6) and 39.83 (5)° with the phenyl rings of the molecule. The molecules are linked through C—H···O and N—H···O interactions.

Comment

Various analogues of pyrimidines have been reported, showing diverse biological and medicinal importance (Brown, 1984, 1985), such as antibacterial, antifungal, antiviral, anti-AIDS, insecticidal and miticidal activity (Sankyo Co., 1984; De Clerq & Walker, 1985). In this paper, we present the structure of the title compound, (I), a new pyrimidine derivative.



(I)

The structure of (I) are shown in Fig. 1, with the atom-numbering scheme; selected geometric parameters are listed in Table 1. All bond distances and angles are in good agreement with those in related structures (Akkurt & Hiller, 1993; Akkurt *et al.*, 1992, 2003; Öztürk *et al.*, 1997, 1999; Türktekin *et al.*, 2003).

All atoms in the pyrimidine ring are almost coplanar, the largest deviation from the mean plane being 0.029 (1) Å for atom C24. The orientation of the substituents with respect to the pyrimidine ring are defined by the dihedral angles of 72.47 (6), 64.77 (6) and 39.83 (5)° for the phenyl rings *A* (C1–C6), *B* (C11–C16) and *C* (C18–C23), respectively. The other angles between the ring planes are 67.41 (6)° for *A*/*B*, 68.34 (6)° for *A*/*C* and 54.51 (6)° for *B*/*C*.

The crystal structure is stabilized by intermolecular C—H···O and N—H···O interactions (Fig. 2 and Table 2).

Experimental

1-Amino-5-benzoyl-4-phenyl-1*H*-pyrimidin-2-one (0.2 g) and benzoyl chloride (1.0 g) were mixed in a ratio of 1:4. This reaction mixture was stirred with the addition of CH_3COONa (1.0 g) and water (2.0 ml) for 24 h at room temperature. The solvent was then removed by evaporation and the residue was treated with dry diethyl ether. The white precipitate which formed was then filtered off, washed with pure water, and dried over P_2O_5. This product was crystallized from *n*-butanol (yield: 70%, m.p. 548 K). IR (KBr, cm^{-1}):

3200 (N—H), 3010 (aromatic C—H), 1700–1660 (C═O), 1600 (C═C and C═N), 1480–1360 (aromatic skeleton vibration), 800–680 (pyrimidine ring vibration). Analysis calculated for $C_{24}H_{17}N_3O_3$: C 72.91, H 4.30, N 10.63%, found: C 72.35, H 4.39, N 10.37%.

Crystal data

$C_{24}H_{17}N_3O_3$	D_x = 1.379 Mg m^{-3}
M_r = 395.41	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 4211 reflections
a = 8.9688 (5) Å	θ = 1.9–27.3°
b = 10.9081 (4) Å	μ = 0.09 mm^{-1}
c = 19.8159 (11) Å	T = 150 K
β = 100.841 (4)°	Plate, yellow
V = 1904.04 (17) Å^3	0.58 × 0.40 × 0.16 mm
Z = 4	

Data collection

Stoe IPDS-II diffractometer	4211 independent reflections
ω scans	3172 reflections with $I > 2\sigma(I)$
Absorption correction: by integration (*X-RED*32; Stoe & Cie, 2002)	R_{int} = 0.038
	θ_{max} = 27.2°
	$h = -11 \rightarrow 11$
T_{min} = 0.955, T_{max} = 0.985	$k = -13 \rightarrow 13$
29930 measured reflections	$l = -25 \rightarrow 25$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.052P)^2 + 0.0168P]$ where $P = (F_o^2 + 2F_c^2)/3$
$R[F^2 > 2\sigma(F^2)]$ = 0.032	
$wR(F^2)$ = 0.085	
S = 1.02	$(\Delta/\sigma)_{max} < 0.001$
4211 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
340 parameters	$\Delta\rho_{min}$ = −0.13 e Å^{-3}
All H-atom parameters refined	Extinction correction: *SHELXL*97
	Extinction coefficient: 0.0145 (13)

Table 1
Selected geometric parameters (Å, °).

O1—C7	1.2171 (14)	N2—C8	1.3528 (15)
O2—C10	1.2191 (13)	N2—C24	1.4026 (14)
O3—C24	1.2282 (13)	N3—C17	1.3205 (15)
N1—N2	1.3964 (13)	N3—C24	1.3660 (14)
N1—C7	1.3841 (14)		
N2—N1—C7	115.65 (9)	N2—C8—C9	119.83 (10)
N1—N2—C8	117.98 (9)	O2—C10—C9	117.98 (10)
N1—N2—C24	118.88 (9)	O2—C10—C11	121.88 (10)
C8—N2—C24	122.82 (9)	N3—C17—C18	116.19 (10)
C17—N3—C24	120.60 (9)	N3—C17—C9	122.79 (10)
O1—C7—N1	120.72 (10)	N2—C24—N3	117.00 (9)
N1—C7—C1	115.98 (10)	O3—C24—N2	119.51 (10)
O1—C7—C1	123.18 (10)	O3—C24—N3	123.47 (10)
N2—N1—C7—C1	−172.91 (9)	C8—C9—C10—O2	112.40 (13)
N2—N1—C7—O1	10.85 (16)	C17—C9—C10—C11	120.27 (12)
C8—N2—C24—O3	176.62 (10)	C9—C10—C11—C16	−177.78 (11)
C17—N3—C24—O3	−177.13 (10)	C9—C10—C11—C12	0.35 (16)
C2—C1—C7—O1	4.51 (18)	N3—C17—C18—C23	−40.68 (15)
C6—C1—C7—O1	−174.62 (12)	C9—C17—C18—C19	−39.91 (16)
C8—C9—C10—C11	−69.01 (14)	C9—C17—C18—C23	139.41 (11)
C17—C9—C10—O2	−58.32 (15)	N3—C17—C18—C19	140.00 (11)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	0.895 (15)	2.009 (15)	2.8772 (13)	163.4 (14)
C12—H12···O2^{ii}	0.997 (14)	2.570 (13)	3.3266 (14)	132.6 (10)
C13—H13···O1^{ii}	0.971 (15)	2.553 (15)	3.4007 (15)	145.9 (11)
C16—H16···O3^{iii}	1.006 (16)	2.484 (16)	3.3620 (15)	145.6 (12)

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

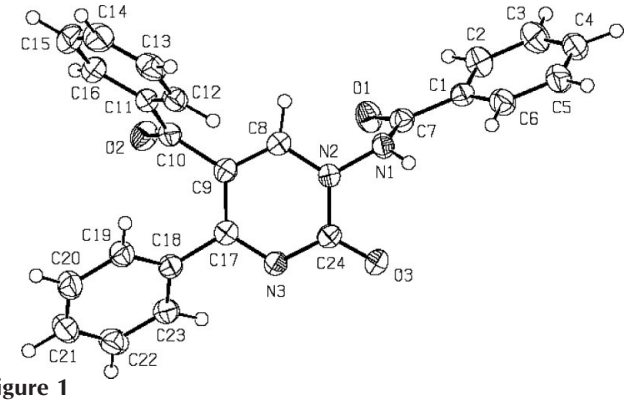


Figure 1
The molecular structure of (I), with displacement ellipsoids drawn at the 50% probability level.

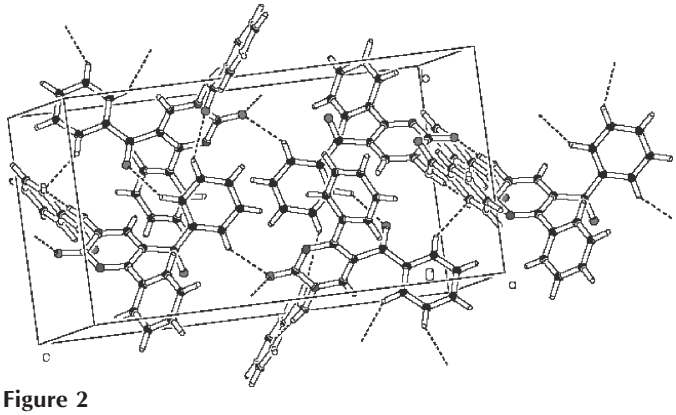


Figure 2
A packing diagram of the title compound. Dashed lines indicate hydrogen bonds.

All H atoms were located in a difference Fourier map and refined isotropically.

Data collection: *X-AREA* (Stoe & Cie, 2002); cell refinement: *X-AREA*; data reduction: *X-RED*32 (Stoe & Cie, 2002); program(s) used to solve structure: *SHELXS*97 (Sheldrick, 1997); program(s) used to refine structure: *SHELXL*97 (Sheldrick, 1997); molecular graphics: *ORTEP*III (Farrugia, 1997); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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