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6-Phenyl-5,6-dihydrobenzoimidazo[1,2-*c*]quinazoline

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Key indicators

Single-crystal X-ray study
T = 295 K
Mean σ(C–C) = 0.003 Å
R factor = 0.047
wR factor = 0.144
Data-to-parameter ratio = 11.7

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

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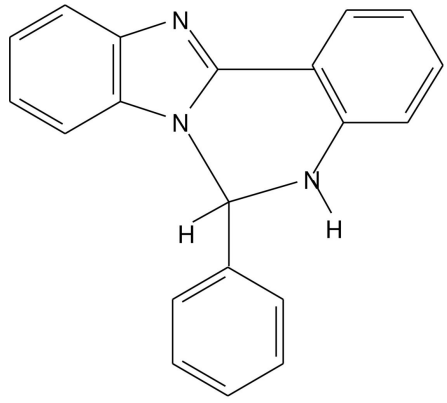
In the title compound, $C_{20}H_{15}N_3$, the molecules are linked by N—H···N hydrogen bonds.

Comment

The quinazoline ring is widely found in alkaloids and many biologically active compounds. Substituted quinazolines have fungicidal, antimicrobial, anti-inflammatory, anticancer, antihypertensive and anti-HIV activities (Alexandre *et al.*, 2003; De Clercq, 2001). A few X-ray crystal structure reports for benzimidazoquinazolines have been published (Elgemeie, *et al.*, 1998; Low *et al.*, 2003; Jayalakshmi, *et al.*, 2004). In view of the above observations, the title compound, (I), was synthesized and its crystal structure is reported here (Fig. 1).



(I)

Most of the bond lengths and angles have normal values and are comparable to those reported in similar structures (Elgemeie *et al.*, 1998; Low *et al.*, 2002, 2003; Jayalakshmi *et al.*, 2004). The benzene and imidazole rings are planar, but the quinazoline ring system deviates from planarity, with atom C10 lying 0.4707 (16) Å from the N7/C8/C13/C12/N11 least-squares plane. The crystal packing is stabilized by an intermolecular N11—H11···N9^{i} (symmetry code as in Table 2) hydrogen bond, which links the molecules into a zigzag chain along the *b* axis (Fig. 2).

Experimental

A mixture of *o*-aminophenylbenzimidazole (*o*-APB, 0.05 mol, 10.45 g) and benzaldehyde (0.05 mol, 5.30 g)/*p*-chlorobenzaldehyde (0.05 mol, 7.30 g) was refluxed in ethanol (200 ml) for 5 h. The resulting solution was concentrated under reduced pressure to a small volume to obtain a cream compound. The solid was recrystallized from ethanol to give the white crystalline compound (I) (yield 70%; m.p. 472 K).

Crystal data

$C_{20}H_{15}N_3$
M_r = 297.35
Monoclinic, $P2_1/c$
a = 11.569 (8) Å
b = 9.915 (7) Å
c = 14.337 (10) Å
β = 114.086 (4)°
V = 1501.36 (19) Å^3
Z = 4
D_x = 1.316 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 4596 reflections
θ = 2.6–25.0°
μ = 0.08 mm^{-1}
T = 295 (2) K
Block, white
0.25 × 0.2 × 0.2 mm

Data collection

MacScience DIPLabo 32001 diffractometer
ω scans
4596 measured reflections
2441 independent reflections
2133 reflections with $I > 2\sigma(I)$
R_{int} = 0.025
θ_{max} = 25.0°
$h = -13 \rightarrow 13$
$k = -11 \rightarrow 11$
$l = -16 \rightarrow 16$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.144
S = 1.18
2441 reflections
209 parameters
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0844P)^2 + 0.1702P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.31 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}
Extinction correction: *SHELXL97*
Extinction coefficient: 0.172 (16)

Table 1
Selected geometric parameters (Å, °).

N7—C2	1.383 (2)	N9—C8	1.317 (2)
N7—C8	1.370 (2)	N11—C10	1.452 (2)
N7—C10	1.457 (2)	N11—C12	1.377 (2)
N9—C3	1.393 (2)		
C2—N7—C8	106.84 (13)	N7—C8—C13	118.38 (14)
C2—N7—C10	128.85 (14)	N7—C8—N9	113.34 (16)
C8—N7—C10	124.17 (15)	N9—C8—C13	128.19 (15)
C3—N9—C8	104.25 (14)	N7—C10—C18	112.27 (14)
C10—N11—C12	121.36 (15)	N11—C10—C18	114.07 (14)
N7—C2—C3	104.87 (14)	N7—C10—N11	106.60 (13)
N7—C2—C1	132.22 (16)	N11—C12—C13	119.18 (16)
N9—C3—C2	110.65 (15)	N11—C12—C14	122.10 (16)
N9—C3—C4	129.90 (16)		

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

D—H···A	D—H	H···A	D···A	D—H···A
N11—H11···N9^{i}	0.86	2.40	3.245 (2)	168

Symmetry code: (i) $-x+1, +y-\frac{1}{2}, -z+\frac{1}{2}$.

H atoms were placed at idealized positions and allowed to ride on their parent atoms with C—H distances in the range 0.93–0.98 Å and N—H = 0.86 Å; U_{iso}(H) values were set equal to 1.2U_{eq}(carrier atom).

Data collection: *XPRESS* (MacScience, 2002); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *DENZO* (Otwinowski & Minor, 1997) and *SCALEPACK*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003) and *ORTEPII* (Johnson, 1976); software used to prepare material for publication: *SHELXL97*.

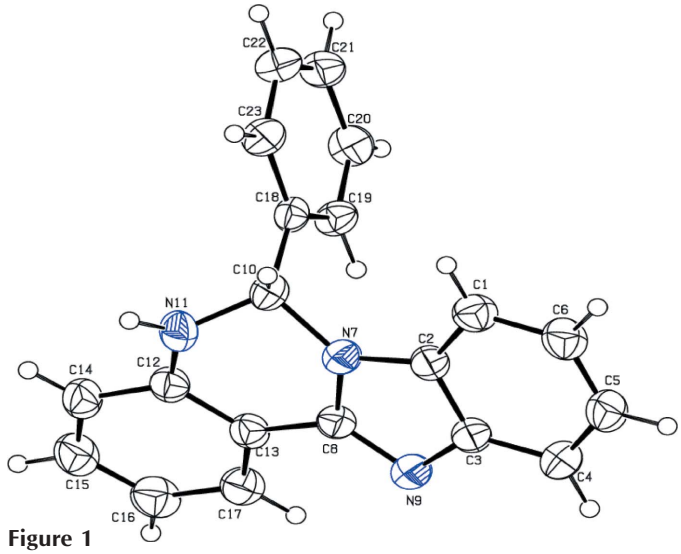


Figure 1
View of (I), with 50% probability displacement ellipsoids.

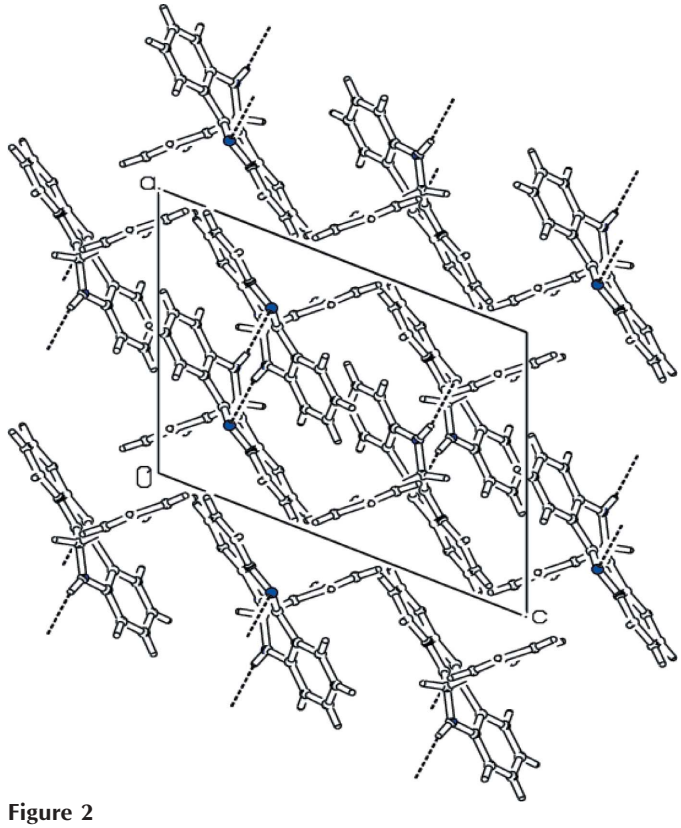


Figure 2
The crystal packing in (I), viewed down the *b* axis. Dashed lines indicate hydrogen bonds.

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