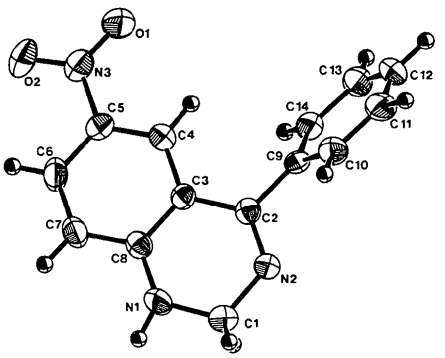

Fig. 1. *ORTEP* (Johnson, 1965) diagram of the molecule with thermal ellipsoids scaled at the 50% probability level.

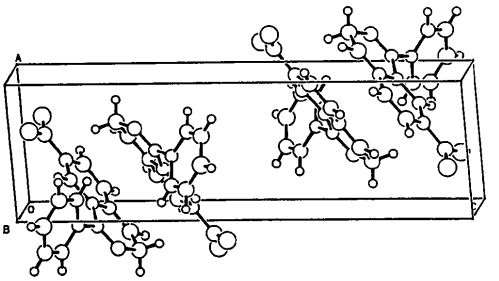

Fig. 2. Packing diagram for $C_{14}H_{11}N_2O_2$.

purpose in elucidating the crystal structure (Figs. 1 and 2) of this compound was to determine whether the phenyl substituent is coplanar with the quinazoline nucleus. As can be seen from Fig. 1, the torsional angle N2—C2—C9—C10 is 55·8 (7)°, a rotation of the phenyl group that effectively takes it out of conjugation with the quinazoline system.

Related literature. In the crystal structure of the related compound 6-isopropyl-2,4-diphenylquinazoline (Hunter, Neilson & Weakley, 1985), the plane containing the C4-phenyl group is rotated by 63·9° with respect to the quinazoline ring system.

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3-Methyl-2,2,4,6-tetraphenyl-2,3-dihydro-1,3,5-triazine

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Abstract. $C_{28}H_{23}N_3$, $M_r = 401·5$, orthorhombic, *Pbca*, $a = 32·219$ (2), $b = 7·3562$ (4), $c = 18·390$ (2) Å, $V = 4358·6$ (5) Å^3, $Z = 8$, $D_x = 1·224$ g cm^{-3}, λ(Cu $K\alpha$) = 1·54184 Å, $\mu = 4·86$ cm^{-1}, $F(000) = 1696$, $T = 293$ K, $R = 0·060$ for 2691 unique observed reflections. In comparison with 2,2,4,6-tetraphenyl-2,3-dihydro-1,3,5-triazine N(3)—C(2) is lengthened by 0·035 (6) Å and the phenyl ring at the 4-position is rotated out of the plane composed of N(1), N(3), C(4), N(5) and C(6) by the introduction of a methyl group at the 3-position.

Experimental. The title compound was prepared from 2,2,4,6-tetraphenyl-2,3-dihydro-1,3,5-triazine (Maeda, Kihara & Ishimura, 1985). Recrystallization from benzene–hexane gave colorless column-like crystals; crystal dimensions 0·2 × 0·15 × 0·25 mm, Rigaku AFC-4 diffractometer, Cu $K\alpha$ radiation, graphite

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Table 1. *Atomic coordinates* ($\times 10^4$) *with their e.s.d.'s and equivalent isotropic thermal parameters* ($Å^2$) *for non-H atoms*

$$B_{eq} = \frac{4}{3}\sum_i\sum_j B_{ij}\mathbf{a}_i.\mathbf{a}_j.$$

	x	y	z	B_{eq}
N(1)	1585 (1)	4052 (3)	5882 (1)	3·8
C(2)	1309 (1)	5286 (4)	5501 (2)	3·6
N(3)	1096 (1)	6565 (3)	6018 (1)	3·7
C(4)	1064 (1)	6101 (4)	6719 (2)	3·3
N(5)	1236 (1)	4651 (3)	7005 (1)	3·7
C(6)	1514 (1)	3747 (4)	6556 (2)	3·3
C(7)	1763 (1)	2311 (4)	6919 (2)	3·3
C(8)	1764 (1)	2133 (4)	7674 (2)	3·8
C(9)	1988 (1)	758 (5)	7998 (2)	4·5
C(10)	2214 (1)	−441 (5)	7588 (2)	5·3
C(11)	2216 (1)	−266 (5)	6839 (2)	5·4
C(12)	1992 (1)	1087 (5)	6503 (2)	4·3
C(13)	824 (1)	7273 (4)	7228 (2)	3·3
C(14)	499 (1)	6522 (5)	7613 (2)	4·6
C(15)	279 (1)	7611 (7)	8105 (2)	6·0
C(16)	387 (1)	9384 (6)	8209 (2)	5·8
C(17)	712 (1)	10112 (6)	7829 (2)	5·6
C(18)	933 (1)	9062 (5)	7339 (2)	4·8
C(19)	985 (1)	4058 (4)	5125 (2)	3·6
C(20)	1119 (1)	2860 (4)	4587 (2)	4·2
C(21)	845 (1)	1644 (5)	4277 (2)	4·9
C(22)	435 (1)	1595 (5)	4491 (2)	5·3
C(23)	304 (1)	2754 (6)	5024 (2)	5·1
C(24)	575 (1)	3981 (5)	5339 (2)	4·6
C(25)	1566 (1)	6441 (4)	4969 (2)	3·7
C(26)	1416 (1)	7030 (4)	4302 (2)	4·2
C(27)	1644 (1)	8189 (5)	3870 (2)	5·2
C(28)	2028 (2)	8780 (6)	4105 (3)	6·2
C(29)	2188 (1)	8170 (6)	4756 (3)	6·1
C(30)	1955 (1)	7016 (5)	5184 (2)	5·0
C(31)	892 (1)	8169 (5)	5704 (2)	5·1

Table 2. *Selected bond distances* (Å) *and bond angles* (°)

N(1)–C(2)	1·452 (4)	N(3)–C(31)	1·468 (4)
N(1)–C(6)	1·387 (4)	C(4)–N(5)	1·313 (4)
C(2)–N(3)	1·503 (4)	C(4)–C(13)	1·489 (4)
C(2)–C(19)	1·543 (4)	N(5)–C(6)	1·387 (4)
C(2)–C(25)	1·538 (4)	C(6)–C(7)	1·487 (4)
N(3)–C(4)	1·337 (4)		

C(2)–N(1)–C(6)	117·7 (3)	C(4)–N(3)–C(31)	123·3 (3)
N(1)–C(2)–N(3)	111·5 (2)	N(3)–C(4)–N(5)	124·1 (3)
N(1)–C(2)–C(19)	105·3 (2)	N(3)–C(4)–C(13)	119·9 (3)
N(1)–C(2)–C(25)	108·8 (2)	N(5)–C(4)–C(13)	116·0 (3)
N(3)–C(2)–C(19)	110·0 (2)	C(4)–N(5)–C(6)	115·1 (3)
N(3)–C(2)–C(25)	107·6 (2)	N(1)–C(6)–N(5)	127·5 (3)
C(19)–C(2)–C(25)	113·7 (3)	N(1)–C(6)–C(7)	117·5 (3)
C(2)–N(3)–C(4)	119·0 (2)	N(5)–C(6)–C(7)	114·9 (3)
C(2)–N(3)–C(31)	117·3 (3)		

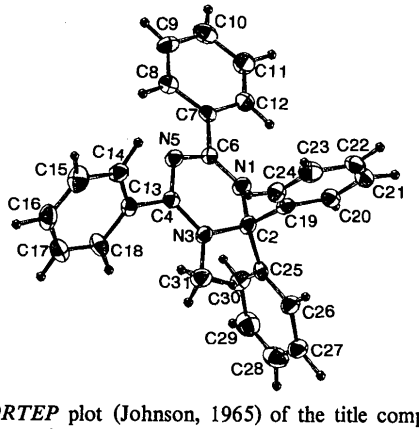

Fig. 1. *ORTEP* plot (Johnson, 1965) of the title compound with atom numbering. The thermal ellipsoids enclose 30% probability.

monochromator; cell dimensions from least-squares refinement of 16 independent 2θ values ($40 < 2\theta < 50°$); intensity measurement performed up to $2\theta = 125°$ ($h = 0$ to 36, $k = 0$ to 8, $l = 0$ to 21); ω–2θ scan technique, scan speed 4° min^{-1} in θ, scan width $(1{\cdot}0 + 0{\cdot}15\tan\theta)°$; background 5 s before and after each scan; three standard reflections ($\bar{1}6$,0,0, 70$\bar{8}$, 041) monitored every 50 reflections, no significant variation in intensities; 3474 reflections measured, 2691 considered observed, $|F_o| < 3\sigma(|F_o|)$, and used for structure determination; corrections for Lorentz and polarization effects, absorption ignored; direct methods (*MULTAN*78, Main, Hull, Lessinger, Germain, Declercq & Woolfson, 1978) and subsequent difference Fourier map calculations, full-matrix least-squares refinement on F (*SHELX*76, Sheldrick, 1976) with anisotropic thermal parameters for non-H atoms and isotropic ones for H atoms, $w = [\sigma^2(|F_o|) + 0{\cdot}0040|F_o|^2]^{-1}$; all H atoms located on difference Fourier map; final $R = 0{\cdot}060$ and $wR = 0{\cdot}071$ for 2691 observed reflections; $S = 1{\cdot}06$; $(\Delta/\sigma)_{max} = 0{\cdot}03$; final difference map showed $|\rho| < 0{\cdot}18$ e $Å^{-3}$; atomic scattering factors from *International Tables for X-ray Crystallography* (1974); calculations carried out on a HITAC M-680 computer at the Computer Center of the University of Tokyo. Final atomic coordinates are in Table 1,* and selected bond distances and angles in Table 2. The molecule and the numbering scheme are shown in Fig. 1.

Related literature. Structure of 2,2,4,6-tetraphenyl-2,3-dihydro-1,3,5-triazine and its inclusion compounds (Mori, Ohashi & Maeda, 1988*a*,*b*).

*Lists of anisotropic thermal parameters for non-H atoms, positional and thermal parameters for H atoms, bond distances and angles, least-squares-planes data, and structure factors have been deposited with the British Library Document Supply Centre as Supplementary Publication No. SUP 51767 (18 pp.). Copies may be obtained through The Executive Secretary, International Union of Crystallography, 5 Abbey Square, Chester CH1 2HU, England.

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