7095 measured reflections

 $R_{\rm int} = 0.087$

3280 independent reflections

1899 reflections with $I > 2\sigma(I)$

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6-Methyl-N-(2-methylphenyl)-3-phenyl-1,6-dihydro-1,2,4,5-tetrazine-1-carboxamide. Corrigendum

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Key indicators: single-crystal X-ray study; T = 293 K; mean σ (C–C) = 0.004 Å; Hatom completeness 95%; R factor = 0.064; wR factor = 0.170; data-to-parameter ratio = 15.3.

The formula of the title compound in the paper by Xu & Hu [Acta Cryst. (2008), E64, o1432] is corrected.

In the paper by Xu & Hu [Acta Cryst. (2008), E64, o1432], the chemical formula is corrected and the structure has been rerefined to include a missing H atom. The Crystal data, Data collection and Refinement sections are updated together with the hydrogen-bond data.

Experimental

Crystal data

C ₁₇ H ₁₇ N ₅ O	$V = 1594.8 (11) \text{ Å}^3$
$M_r = 307.36$	Z = 4
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation
a = 13.941 (6) Å	$\mu = 0.08 \text{ mm}^{-1}$
b = 5.675 (2) Å	T = 293 (2) K
c = 20.614 (8) Å	$0.12 \times 0.10 \times 0.06 \; \mathrm{mm}$
$\beta = 102.055 \ (6)^{\circ}$	

Data collection

Bruker SMART APEX CCD areadetector diffractometer Absorption correction: multi-scan (SADABS; Sheldrick, 1996) $T_{\min} = 0.990, \ T_{\max} = 0.995$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.064$	H atoms treated by a mixture of		
$wR(F^2) = 0.170$	independent and constrained		
S = 0.91	refinement		
3280 reflections	$\Delta \rho_{\rm max} = 0.54 \ {\rm e} \ {\rm \AA}^{-3}$		
215 parameters	$\Delta \rho_{\rm min} = -0.31 \text{ e } \text{\AA}^{-3}$		
1 restraint			

Table 1

Hydrogen-bond geometry (Å, °).

$D - H \cdots A$	D-H	$H \cdots A$	$D \cdots A$	$D - H \cdots A$
C6-H6···O ⁱ	0.93	2.56	3.385 (3)	148

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

References

Xu, F. & Hu, W. (2008). Acta Cryst. E64, o1432. Sheldrick, G. M. (1996). SADABS. University of Göttingen, Germany.