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Key indicators

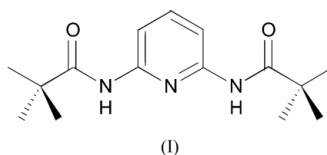
Single-crystal X-ray study
 $T = 150\text{ K}$
Mean $\sigma(\text{C}-\text{C}) = 0.002\text{ \AA}$
 R factor = 0.033
 wR factor = 0.072
Data-to-parameter ratio = 19.0For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.***N*-[6-(2,2-Dimethylpropionylamino)pyridin-2-yl]-
2,2-dimethylpropionamide**At 150 K, only one of the two amide groups of the title
compound, $\text{C}_{15}\text{H}_{23}\text{N}_3\text{O}_2$, is involved in weak hydrogen
bonding.

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Comment

The title compound, (I), is a member of a series of *N,N'*-
pyridine-2,6-diyl-bisamides reported not to form triply
hydrogen-bonded (*DAD-ADA*) complexes (Feibush *et al.*,
1986).

Due to the steric bulk of the *tert*-butyl groups of (I), only one of the two amide groups forms a hydrogen bond (Table 2) and the geometry indicates that this interaction is relatively weak, with a significant deviation from linearity. As expected, this amide group has a shorter N–H bond and slightly longer C=O bond than the non-hydrogen-bonded amide group. In addition, the pyridine N atom is not involved in hydrogen bonding. The angles between the least-squares planes of the pyridine ring and the two amide groups are 29.67 (5) (C6/O1/N2) and 8.13 (11)° (C11/O2/N3), respectively.

Experimental

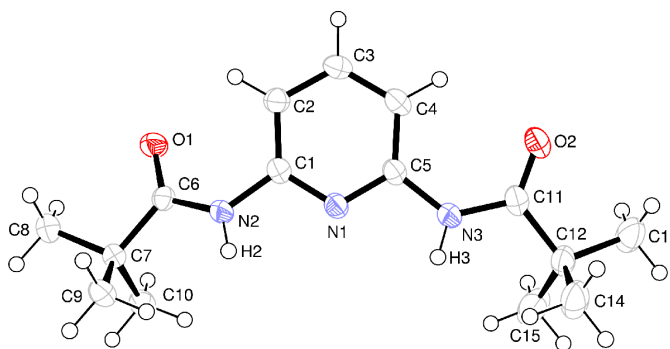
The title compound, (I), was prepared according to the method of Feibush *et al.* (1986). Suitable crystals were grown from diethyl ether by slow evaporation.

Figure 1

View of (I), showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 50% probability level and H atoms are represented by circles of arbitrary size.

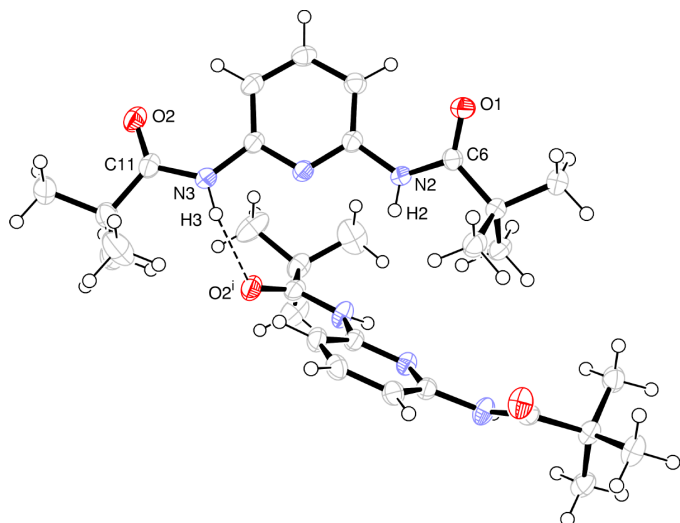


Figure 2
The intermolecular hydrogen bond of (I).

Crystal data

$C_{15}H_{23}N_3O_2$	$D_x = 1.176 \text{ Mg m}^{-3}$
$M_r = 277.36$	Mo $K\alpha$ radiation
Monoclinic, $P2_1/c$	Cell parameters from 10680 reflections
$a = 11.4234 (13) \text{ \AA}$	$\theta = 2.6\text{--}27.5^\circ$
$b = 15.1383 (19) \text{ \AA}$	$\mu = 0.08 \text{ mm}^{-1}$
$c = 9.3774 (10) \text{ \AA}$	$T = 150 (2) \text{ K}$
$\beta = 104.885 (9)^\circ$	Needle, colourless
$V = 1567.2 (3) \text{ \AA}^3$	$0.50 \times 0.20 \times 0.10 \text{ mm}$
$Z = 4$	

Data collection

Stoe IPDS-II area-detector diffractometer	$R_{\text{int}} = 0.060$
ω scans	$\theta_{\text{max}} = 27.5^\circ$
22 744 measured reflections	$h = -14 \rightarrow 14$
3601 independent reflections	$k = -19 \rightarrow 19$
2174 reflections with $I > 2\sigma(I)$	$l = -10 \rightarrow 12$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0372P)^2]$
$R[F^2 > 2\sigma(F^2)] = 0.033$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 0.80$	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
3601 reflections	$\Delta\rho_{\text{min}} = -0.14 \text{ e \AA}^{-3}$
190 parameters	Extinction correction: <i>SHELXL97</i>
H atoms treated by a mixture of independent and constrained refinement	Extinction coefficient: 0.0101 (10)

Table 1

Selected geometric parameters (\AA , $^\circ$).

O1—C6	1.2165 (14)	N3—C11	1.3702 (16)
O2—C11	1.2215 (15)	N3—C5	1.3995 (16)
N1—C1	1.3328 (15)	N3—H3	0.866 (16)
N1—C5	1.3423 (15)	C1—C2	1.3859 (17)
N2—C6	1.3689 (15)	C2—C3	1.3810 (18)
N2—C1	1.4080 (16)	C3—C4	1.3834 (18)
N2—H2	0.810 (16)	C4—C5	1.3875 (18)
C1—N1—C5	118.19 (11)	C3—C4—C5	117.43 (11)
C6—N2—C1	126.92 (11)	N1—C5—C4	122.75 (11)
C11—N3—C5	128.92 (12)	N1—C5—N3	111.62 (11)
N1—C1—C2	123.61 (11)	O1—C6—N2	121.71 (11)
N1—C1—N2	112.69 (11)	N2—C6—C7	115.51 (11)
C3—C2—C1	116.96 (12)	O2—C11—N3	121.78 (12)
C2—C3—C4	121.01 (12)		
C6—N2—C1—N1	−147.04 (12)	C11—N3—C5—N1	−176.39 (12)

Table 2

Hydrogen-bonding geometry (\AA , $^\circ$).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
N3—H3 \cdots O2 ⁱ	0.866 (15)	2.180 (15)	2.9508 (14)	148.0 (14)

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

All H atoms were initially located in a difference Fourier map. The positions of the amide H atoms were refined freely along with an isotropic displacement parameter. The methyl H atoms were constrained to an ideal geometry, with C—H distances of 0.98 Å. All other H atoms were placed in geometrically idealized positions, with a C—H distance of 0.95 Å. $U_{\text{iso}}(\text{H})$ values were set at $1.2U_{\text{eq}}(\text{C})$.

Data collection: *X-AREA* (Stoe & Cie, 2001); cell refinement: *X-AREA*; data reduction: *X-RED* (Stoe & Cie, 2001); program(s) used to solve structure: *X-STEP32* (Stoe & Cie, 2001) and *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *WinGX* (Farrugia, 1999) and *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); software used to prepare material for publication: *WinGX*.

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