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N^2,N^4,1-Tribenzyl-2,5-dimethyl-3-oxopyrrolidine-2,4-dicarboxamide

Zu-Pei Liang,* Jian Li and Hua Yang

Department of Chemistry and Chemical Engineering, Weifang University, Weifang 261061, People's Republic of China

Correspondence e-mail: zupeiliang@yahoo.com.cn

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The crystal structure of the title compound, $C_{29}H_{29}N_3O_3$, is stabilized by weak N—H···O hydrogen bonds. In the title compound, the dihedral angles between the pyrrolidine ring and the phenyl rings are 75.2 (2), 76.6 (2) and 77.2 (2)°, respectively.

Key indicators

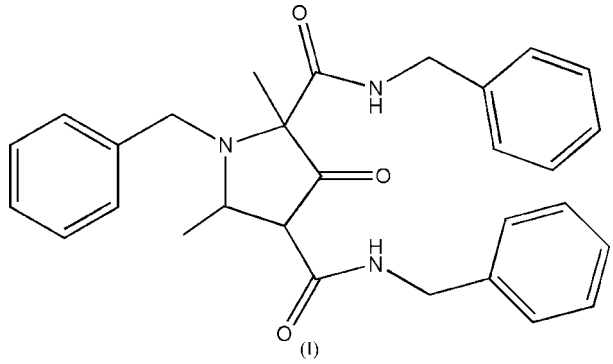
Single-crystal X-ray study
T = 294 K
Mean σ(C–C) = 0.004 Å
R factor = 0.044
wR factor = 0.119
Data-to-parameter ratio = 13.3

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

Comment

Pyrrolidine and its derivatives and their complexes are widely used in the fields of biology, catalysis and materials.

In this paper, the structure of the title compound, (I), is reported. The molecular structure of (I) is illustrated in Fig. 1. The pyrrolidine ring is planar to within 0.006 (2) Å. The dihedral angles between the pyrrolidine ring system and the phenyl ring systems are 75.2 (2), 76.6 (2) and 77.2 (2)°, respectively. The crystal structure of the title compound is stabilized by weak N—H···O hydrogen bonds (Table 1).



(I)

Experimental

A mixture of 1-benzyl-2,5-dimethyl-3-oxopyrrolidine-2,4-dicarboxylic acid (0.01 mol) and phenylmethanamine (0.02 mol) in toluene (12 ml) was refluxed for 6 h. After cooling, filtration and drying, the title compound was obtained. 10 mg of (I) were dissolved in 15 ml of acetone, and the solution was kept at room temperature for 7 d. Natural evaporation gave colourless single crystals of the title compound suitable for X-ray analysis.

Crystal data

$C_{29}H_{29}N_3O_3$
M_r = 467.55
Triclinic, $P\overline{1}$
a = 10.527 (2) Å
b = 11.611 (3) Å
c = 11.872 (3) Å
α = 105.096 (4)°
β = 115.367 (4)°
γ = 93.651 (4)°
V = 1240.0 (5) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 294 (2) K
0.24 × 0.22 × 0.20 mm

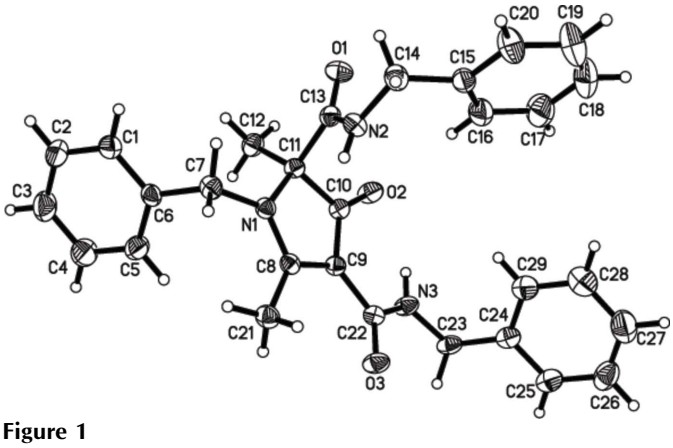


Figure 1
The molecular structure of (I), with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.981, T_{max} = 0.984
6416 measured reflections
4339 independent reflections
2904 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.119
S = 1.03
4339 reflections
326 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.17 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2^{i}	0.87 (2)	2.38 (2)	3.041 (2)	132.7 (17)
N3—H3A···O2	0.87 (2)	2.09 (2)	2.797 (2)	138.3 (19)
N2—H2A···O3^{ii}	0.87 (2)	2.12 (2)	2.919 (2)	152.4 (18)

Symmetry codes: (i) $-x+1, -y+2, -z+1$; (ii) $-x, -y+2, -z+1$.

H atoms were initially located in difference maps and then refined in a riding model with C—H = 0.93–0.96 Å and U_{iso}(H) = 1.2U_{eq}(C) or 1.5U_{eq}(C) (methyl), with the exception of H2*A* and H3*A*, the two NH atoms involved in hydrogen bonding, which were refined isotropically, with N—H = 0.87 (2) Å.

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

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Bruker (1997). *SADABS* (Version 2.01), *SMART* (Version 5.044), *SAINT* (Version 5.01) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
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