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Key indicators

Single-crystal X-ray study
 T = 273 K
 Mean $\sigma(\text{C}-\text{C}) = 0.003 \text{ \AA}$
 R factor = 0.034
 wR factor = 0.089
 Data-to-parameter ratio = 7.5

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

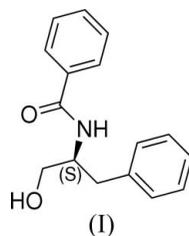
(S)-N-(1-Benzyl-2-hydroxyethyl)benzamide

Colorless crystals of the title compound, $\text{C}_{16}\text{H}_{17}\text{NO}_2$, have been obtained by the reaction of benzoyl chloride and (S)-2-amino-3-phenylpropan-1-ol. The crystal packing is stabilized by $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ intermolecular hydrogen-bonding interactions.

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Comment

In the course of our studies directed to the development of new chiral ligands for asymmetric synthesis (Zeng, Liu, Cui *et al.*, 2002; Zeng, Liu, Mi *et al.*, 2002), we have synthesized a new and useful chiral ligand, namely (S)-N-(1-benzyl-2-hydroxyethyl)benzamide, (I), from the reaction of benzoyl chloride with (S)-2-amino-3-phenylpropan-1-ol. An X-ray crystal structure determination of (I) was carried out in order to elucidate the structure and the results are presented here.0



Bond lengths and angles in (I) are in agreement with the values reported in the literature (Allen, 1987). The crystal packing is stabilized by strong $\text{O}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ intermolecular hydrogen-bonding interactions (Table 2 and Fig. 2).

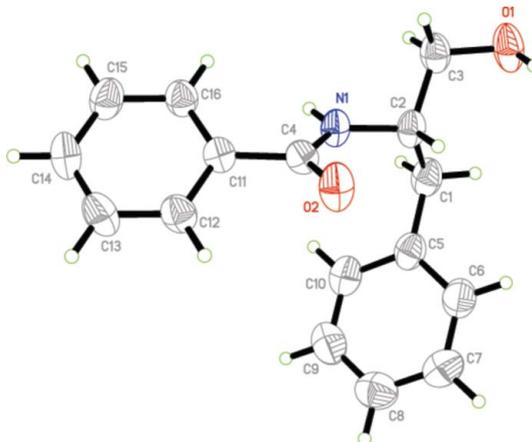


Figure 1
 ORTEP3 (Farrugia, 1997) plot of the title compound, with displacement ellipsoids drawn at the 50% probability level. H atoms are drawn as spheres of arbitrary radii.

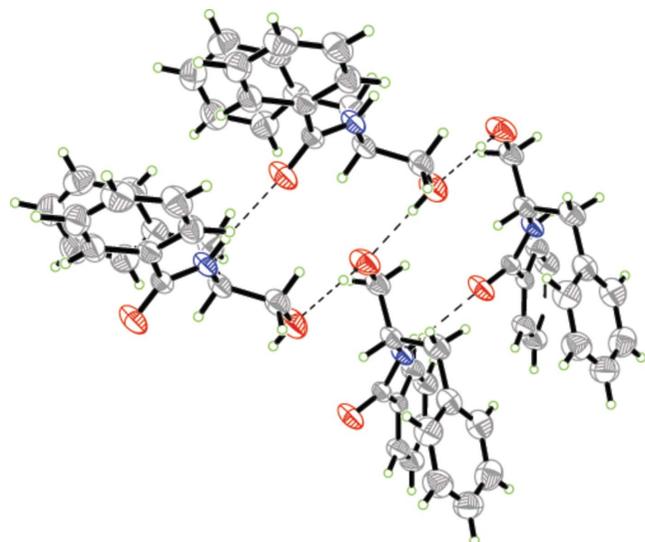


Figure 2
Packing diagram (Accelrys, 2001) of the title compound. Dashed lines indicate O—H...O and N—H...O hydrogen bonds.

Experimental

In an ice–water bath, a solution of (*S*)-2-amino-3-phenylpropan-1-ol (0.32 g, 2 mmol) and triethylamine (0.4 ml) in dichloromethane (10 ml) was added dropwise to a solution of benzoyl chloride (0.28 g, 2 mmol) in dichloromethane (25 ml) (Zeng, Liu, Cui *et al.*, 2002). The resulting solution was stirred at room temperature for 22 h, then water (10 ml) was added to the mixture in order to quench the reaction. The organic layer was separated and the aqueous layer was extracted with dichloromethane. The organic layers were combined, dried over anhydrous magnesium sulfate and filtered. The solvent was removed under reduced pressure, giving 0.43 g of a colorless liquid (yield 84.3%). Single crystals suitable for X-ray analysis were crystallized from the crude product by slow evaporation of an ethyl acetate–dichloromethane (2:1 *v/v*) solution.

Crystal data

$C_{16}H_{17}NO_2$	$D_x = 1.297 \text{ Mg m}^{-3}$
$M_r = 255.31$	Mo $K\alpha$ radiation
Monoclinic, $P2_1$	Cell parameters from 2983 reflections
$a = 8.082$ (3) Å	$\theta = 2.6\text{--}28.1^\circ$
$b = 5.0983$ (16) Å	$\mu = 0.09 \text{ mm}^{-1}$
$c = 16.034$ (5) Å	$T = 273$ (2) K
$\beta = 98.424$ (5)°	Irregular fragment, colorless
$V = 653.5$ (4) Å ³	$0.20 \times 0.15 \times 0.10 \text{ mm}$
$Z = 2$	

Data collection

Bruker APEX area-detector diffractometer	1286 independent reflections
φ and ω scans	1243 reflections with $I > 2\sigma(I)$
Absorption correction: multi-scan (SADABS; Bruker, 2001)	$R_{\text{int}} = 0.033$
$T_{\text{min}} = 0.983$, $T_{\text{max}} = 0.992$	$\theta_{\text{max}} = 25.0^\circ$
4641 measured reflections	$h = -9 \rightarrow 9$
	$k = -6 \rightarrow 6$
	$l = -19 \rightarrow 18$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0534P)^2 + 0.0567P]$
$R[F^2 > 2\sigma(F^2)] = 0.034$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.089$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.07$	$\Delta\rho_{\text{max}} = 0.15 \text{ e \AA}^{-3}$
1286 reflections	$\Delta\rho_{\text{min}} = -0.15 \text{ e \AA}^{-3}$
172 parameters	
All H-atom parameters refined	

Table 1

Selected geometric parameters (Å, °).

N1—C4	1.325 (3)	C1—C2	1.511 (3)
N1—C2	1.434 (2)	C11—C4	1.478 (3)
O1—C3	1.403 (2)	C3—C2	1.502 (3)
C5—C1	1.484 (3)	O2—C4	1.217 (3)
C4—N1—C2	124.10 (17)	N1—C2—C3	108.42 (16)
C6—C5—C1	121.3 (2)	N1—C2—C1	110.92 (16)
C10—C5—C1	121.2 (2)	C3—C2—C1	112.14 (18)
C5—C1—C2	113.00 (18)	O2—C4—N1	122.96 (18)
C12—C11—C4	117.89 (19)	O2—C4—C11	120.55 (18)
C16—C11—C4	123.15 (18)	N1—C4—C11	116.49 (17)
O1—C3—C2	113.08 (18)		

Table 2

Hydrogen-bond geometry (Å, °).

$D\text{--}H\cdots A$	$D\text{--}H$	$H\cdots A$	$D\cdots A$	$D\text{--}H\cdots A$
O1—H1C...O1 ⁱ	0.82	1.90	2.7231 (13)	179
N1—H1D...O2 ⁱⁱ	0.86	2.14	2.907 (3)	148

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

The H atoms were positioned geometrically (C—H = 0.93, 0.98 or 0.97 Å for phenyl, tertiary or methylene H atoms, respectively, O—H = 0.82 Å and N—H = 0.86 Å) and were included in the refinement in the riding-model approximation. The isotropic displacement parameters were set at 1.2 times U_{eq} of the parent atoms. In the absence of significant anomalous scattering effects, Friedel pairs were merged; the absolute configuration was assigned on the basis of the known configuration of 2-amino-3-phenylpropan-1-ol.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP3* (Farrugia, 1997) and *ViewerPro* (Accelrys, 2001); software used to prepare material for publication: *SHELXL97*.

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References

- Accelrys (2001). *ViewerPro*. Version 4.2. Accelrys Inc., Burlington, Massachusetts, USA.
- Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
- Bruker (2001). *SAINT* (Version 6.22), *SMART* (Version 5.625) and *SADABS* (Version 2.03). Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
- Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
- Zeng, Q., Liu, H., Cui, X., Mi, A. Q., Jiang, Y. Z., Li, X. S., Choi, M. C. K. & Chan, A. S. C. (2002). *Tetrahedron Asymmetry*, **13**, 115–117.
- Zeng, Q., Liu, H., Mi, A. Q., Jiang, Y. Z., Li, X. S., Choi, M. C. & Chan, A. S. C. (2002). *Tetrahedron*, **58**, 8799–8803.