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Key indicators

Single-crystal X-ray study

T = 298 K

Mean $\sigma(\text{C}-\text{C}) = 0.009 \text{ \AA}$

R factor = 0.042

wR factor = 0.151

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>.2,2'-[(Ethylenedioxy)bis(ethyleneoxy)]bis-
[N-(2-pyridyl)benzamide]

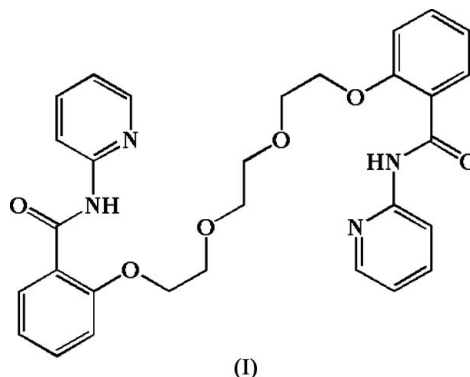
In the title compound, $\text{C}_{30}\text{H}_{30}\text{N}_4\text{O}_6$, the dihedral angle between the two *N*-(2-pyridyl)benzamide units is $71.11(5)^\circ$. The molecule exhibits an S-shaped structure which is stabilized by $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds.

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Comment

Open-chain polyethers offer many advantages over traditional crown ethers: they are less toxic, easily prepared, and can form a ring-like coordination cavity and recognize a rare earth cation whose size matches the cavity (Liu *et al.*, 2004). The study of the antimycobacterial properties of salicylanilides is of great interest as salicylanilides can inhibit bacterial two-component systems, which can also be important in mycobacteria (Waisser *et al.*, 2004). In the present work, the crystal structure of a new salicylanilide derivative, (I), is reported.



The bond lengths and angles show normal values (Zhang *et al.*, 2001). The dihedral angle between the two *N*-(2-pyridyl)benzamide units [$\text{C}1-\text{C}12/\text{O}1/\text{N}3/\text{N}4$ (r.m.s. deviation 0.131 \AA) and $\text{C}13-\text{C}24/\text{O}3/\text{N}1/\text{N}2$ (r.m.s. deviation 0.050 \AA)] is $71.11(5)^\circ$. The S-shaped molecular structure is stabilized by intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds (Fig. 1). In addition, weak intermolecular $\text{C}-\text{H}\cdots\text{O}$ hydrogen bonds are observed (Table 1).

Experimental

A mixture of 2-hydroxy-*N*-(2-pyridyl)benzamide (428 mg, 2.0 mmol), triethylene glycol dibromide (276 mg, 1.0 mmol) and anhydrous K_2CO_3 (500 mg) was stirred in dry dimethylformamide (10 ml) at 333–343 K under nitrogen for 24 h. The reaction mixture was poured into ice-water (50 ml) and stirred for 30 min. The resulting precipitate was collected by filtration and washed with water. The crude product was purified by recrystallization from acetone to give the title compound (210 mg, 51%) as a colourless solid.

Crystal data

$C_{30}H_{30}N_4O_6$
 $M_r = 542.58$
 Orthorhombic, $P2_12_12_1$
 $a = 12.510$ (2) Å
 $b = 14.843$ (3) Å
 $c = 14.8398$ (13) Å
 $V = 2755.5$ (8) Å³

$Z = 4$
 $D_x = 1.308$ Mg m⁻³
 Mo $K\alpha$ radiation
 $\mu = 0.09$ mm⁻¹
 $T = 298$ (2) K
 Prism, colourless
 $0.48 \times 0.42 \times 0.15$ mm

Data collection

Bruker SMART CCD area-detector diffractometer
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Bruker, 2000)
 $T_{\min} = 0.957$, $T_{\max} = 0.986$

14528 measured reflections
 2749 independent reflections
 1508 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.061$
 $\theta_{\text{max}} = 25.0^\circ$

Refinement

Refinement on F^2
 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.151$
 $S = 1.01$
 2749 reflections
 367 parameters
 H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0705P)^2 + 0.6284P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.12$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.13$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N2–H31 \cdots O4	0.89 (5)	1.93 (5)	2.659 (6)	139 (4)
N4–H32 \cdots O2	0.91 (4)	1.87 (4)	2.611 (6)	138 (5)
C17–H17 \cdots O5 ⁱ	0.93	2.52	3.404 (9)	158

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

H atoms bonded to amine N atoms were located in a difference map and their coordinates were refined with an N–H distance restraint of 0.90 (2) Å and with a fixed U_{iso} value of 0.08 Å². H atoms bound to C atoms were refined using a riding model [C–H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic C atoms, and C–H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for methylene C atoms]. The Csp^3-Csp^3 distances were restrained to be 1.53 (2) Å. In the absence of signifi-

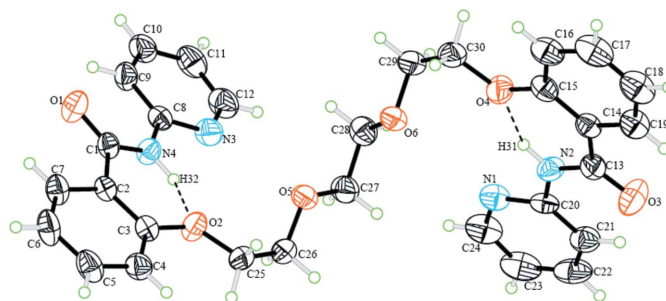


Figure 1

The structure of (I). Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as spheres of arbitrary radii. Dashed lines indicate hydrogen bonds.

cant anomalous scattering, Friedel pairs were merged prior to the final refinement.

Data collection: SMART (Bruker, 2000); cell refinement: SAINT-Plus (Bruker, 2000); data reduction: SAINT-Plus; program(s) used to solve structure: SHELXS97 (Sheldrick, 1997); program(s) used to refine structure: SHELXL97 (Sheldrick, 1997); molecular graphics: DIAMOND (Brandenburg, 2005); software used to prepare material for publication: SHELXL97.

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