

***N*-Cyclohexyl-4-(methoxycarbonyl)benzamide**Peter G. Jones<sup>a\*</sup> and Piotr Kuś<sup>b</sup><sup>a</sup>Institut für Anorganische und Analytische Chemie, Technische Universität Braunschweig, Postfach 3329, 38023 Braunschweig, Germany, and <sup>b</sup>Department of Chemistry, Silesian University, 9 Szkolna Street, 40-006 Katowice, Poland

Correspondence e-mail: p.jones@tu-bs.de

**Key indicators**Single-crystal X-ray study  
*T* = 133 K  
Mean  $\sigma$ (C–C) = 0.003 Å  
*R* factor = 0.065  
*wR* factor = 0.170  
Data-to-parameter ratio = 21.7For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

The title compound, methyl 4-(cyclohexylaminocarbonyl)benzoate, C<sub>15</sub>H<sub>19</sub>NO<sub>3</sub>, crystallizes with two independent molecules in the asymmetric unit, which differ in their ring orientations. The molecules are connected by N–H···O=C hydrogen bonds to form chains parallel to the *a* axis.

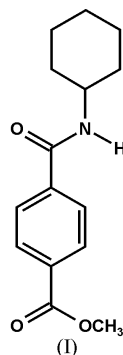
Received 29 June 2004

Accepted 30 June 2004

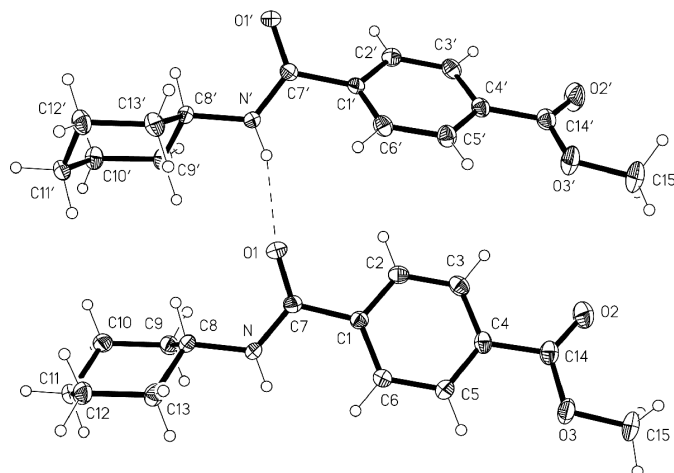
Online 9 July 2004

**Comment**

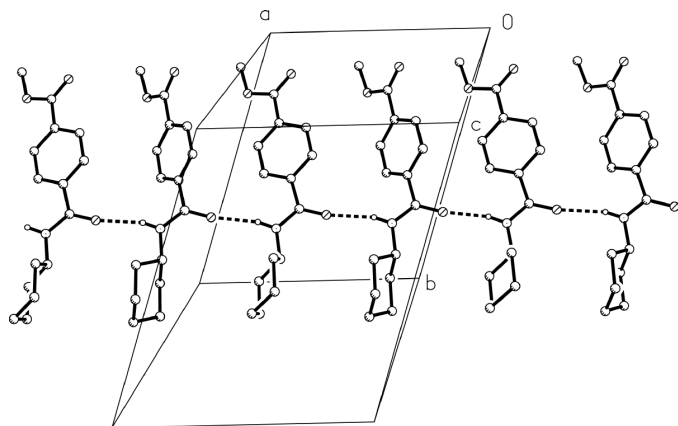
Terephthaldiamide derivatives can be synthesized from various amines and dimethyl terephthalate (Horner & Weissbach, 1972; Jones *et al.*, 2002). We have previously reported several terephthaldiamide structures (Jones *et al.*, 2002); we report here the structure of *N*-cyclohexyl-4-(methoxycarbonyl)benzamide, (I), a compound that was first described by Anzeil *et al.* (1999).



Compound (I) crystallizes with two independent molecules in the asymmetric unit (Fig. 1). These differ in the relative ring

**Figure 1**

The two independent molecules of the title compound in the asymmetric unit. Displacement ellipsoids are drawn at the 50% probability level. The H-atom radii are arbitrary.



**Figure 2**  
Packing diagram of the title compound, viewed perpendicular to the *ab* plane in the region  $z \approx \frac{1}{4}$ . Hydrogen bonds are indicated by dashed lines. H atoms not involved in hydrogen bonding have been omitted. The independent molecules alternate in the chain, beginning at the left with molecule 1 (unprimed molecule in Fig. 1). A second chain (not shown) at  $z \approx \frac{3}{4}$  is generated by inversion.

orientations about the bonds C1–C7 and N–C8 (see torsion angles in Table 1). Bond lengths and angles may be considered normal.

The molecules are connected by two classical hydrogen bonds (Table 2) between the two sets of N–H and O=C groups to form chains parallel to the *a* axis. The two independent molecules alternate in these chains, which are generated solely by translation. The inversion operator generates a second such chain in the unit cell.

## Experimental

Compound (I) was prepared according to our literature method (Jones *et al.*, 2002). The resulting white solid was washed several times with methanol and was collected in 30% yield. [m.p. 336–337 K; literature m.p. (Anzeil *et al.*, 1999) 335–337 K]. Analysis calculated for  $C_{15}H_{19}NO_3$ : C 68.94, H 7.32, N 5.36%; found: C 68.56, H 7.12, N 4.93%.  $^1H$  NMR ( $CDCl_3$ , 500 MHz):  $\delta$  8.04 (*d*, 2H,  $J = 8.3$  Hz), 7.76 (*d*, 2H,  $J = 8.3$  Hz), 5.95 (*bs*, 1H, NH), 3.95 (*m*, 1H), 3.93 (*s*, 3H, –OCH<sub>3</sub>), 2.02 (*m*, 2H), 1.60–1.80 (*m*, 3H), 1.40 (*m*, 2H), 1.20–1.35 (*m*, 3H). Probably the low solubility of monoamide (I) in the reaction mixture leads to the mono-cyclohexyl derivative. The single crystal was obtained by slow evaporation in air of a solution in a water/acetonitrile mixture.

$C_{15}H_{19}NO_3$   
 $M_r = 261.31$   
Triclinic,  $P\bar{1}$   
 $a = 10.107$  (2) Å  
 $b = 11.957$  (2) Å  
 $c = 12.836$  (2) Å  
 $\alpha = 64.832$  (5)°  
 $\beta = 78.988$  (5)°  
 $\gamma = 72.857$  (5)°  
Crystal data

$V = 1337.7$  (4) Å<sup>3</sup>  
 $Z = 4$   
 $D_x = 1.297$  Mg m<sup>-3</sup>  
Mo  $K\alpha$  radiation  
Cell parameters from 5307 reflections  
 $\theta = 2.5$ – $30.5$ °  
 $\mu = 0.09$  mm<sup>-1</sup>  
 $T = 133$  (2) K

Tablet, colourless

$0.4 \times 0.2 \times 0.1$  mm

## Data collection

Bruker SMART 1000 CCD diffractometer  
 $\omega$  scans  
Absorption correction: none  
15 334 measured reflections  
7675 independent reflections

5496 reflections with  $I > 2\sigma(I)$   
 $R_{int} = 0.058$   
 $\theta_{max} = 30.0$ °  
 $h = -14 \rightarrow 14$   
 $k = -16 \rightarrow 16$   
 $l = -17 \rightarrow 18$

## Refinement

Refinement on  $F^2$   
 $R[F^2 > 2\sigma(F^2)] = 0.065$   
 $wR(F^2) = 0.170$   
 $S = 1.04$   
7675 reflections  
353 parameters  
H atoms treated by a mixture of independent and constrained refinement

$w = 1/[\sigma^2(F_o^2) + (0.0834P)^2 + 0.2716P]$   
where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{max} < 0.001$   
 $\Delta\rho_{max} = 0.44$  e Å<sup>-3</sup>  
 $\Delta\rho_{min} = -0.30$  e Å<sup>-3</sup>

## Table 1

Selected torsion angles (°).

C6–C1–C7–N	–17.9 (2)	C6'–C1'–C7'–N'	–45.2 (2)
C9–C8–N–C7	93.99 (18)	C9'–C8'–N'–C7'	131.68 (16)

## Table 2

Hydrogen-bonding geometry (Å, °).

<i>D</i> –H... <i>A</i>	<i>D</i> –H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> –H... <i>A</i>
N–H01...O1 <sup>i</sup>	0.85 (2)	2.06 (2)	2.8908 (19)	162.8 (19)
N'–H01'...O1	0.84 (2)	2.10 (2)	2.9158 (19)	164.1 (19)

Symmetry code: (i) 1 + *x*, *y*, *z*.

The amide H atom was refined freely. Methyl H atoms were refined using a rigid methyl group (C–H = 0.98 Å and H–C–H = 109.5°). Other H atoms were included using a riding model with fixed C–H bond lengths (Å) of 0.95 (aromatic), 0.99 (*sp*<sup>3</sup> CH) or 1.00 (CH<sub>2</sub>).  $U_{iso}(H)$  values were fixed at 1.2 $U_{eq}$  of the parent atom.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINTE* (Bruker, 1998); data reduction: *SAINTE*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *XP* (Siemens, 1994); software used to prepare material for publication: *SHELXL97*.

We thank Mr A. Weinkauff for technical assistance.

## References

- Anzeil, N., LARGERON, M. & FLEURY, M.-B. (1999). *J. Chem. Soc. Perkin Trans. 2*, pp. 1703–1711.  
Bruker (1998). *SMART* (Version 5.0) and *SAINTE* (Version 4.0). Bruker AXS Inc., Madison, Wisconsin, USA.  
Horner, L. & Weissbach, R. (1972). *Liebigs Ann. Chem.* **757**, 69–74.  
Jones, P. G., Ossowski, J. & Kuś, P. (2002). *Z. Naturforsch. Teil B*, **57**, 914–921.  
Sheldrick, G. M. (1990). *Acta Cryst.* **A46**, 467–473.  
Sheldrick, G. M. (1997). *SHELXL97*. University of Göttingen, Germany.  
Siemens (1994). *XP*. Version 5.03. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.