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N-Cyclohexylbenzamide

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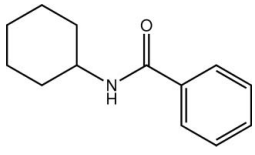
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.045; wR factor = 0.163; data-to-parameter ratio = 10.2.

The structure of the title compound, $C_{13}H_{17}NO$, features an *anti* disposition of the N—H and carbonyl groups. The amide group is twisted with respect to the benzene ring [N–C(=O)–C–C torsion angle = −30.8 (4)°]. In the crystal, $C(4)$ chains propagating in [100] are formed by intermolecular N–H···O hydrogen bonds. Weak C—H···π interactions link the chains into sheets.

Related literature

For biological applications of benzamides, see: Clark *et al.* (1988); Leander *et al.* (1988); Diouf *et al.* (1997).



Experimental

Crystal data

$C_{13}H_{17}NO$
M_r = 203.28
Monoclinic, $P2_1$
a = 5.2372 (3) Å
b = 6.5841 (4) Å
c = 16.6029 (12) Å
β = 91.176 (2)°
V = 572.38 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.07 mm^{-1}
T = 293 K
0.28 × 0.17 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
5479 measured reflections
1423 independent reflections
1105 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.163
S = 1.07
1423 reflections
140 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}

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

$Cg1$ is the centroid of the C2–C7 ring.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1n···O1^{i}	0.80 (3)	2.32 (3)	3.065 (3)	157 (3)
C13—H13a···$Cg1^{ii}$	0.97	2.82	3.722 (4)	154
C5—H5···$Cg1^{iii}$	0.93	2.96	3.729 (4)	141

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

Data collection: *APEX2* (Bruker, 2007); cell refinement: *SAINT* (Bruker, 2007); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB5496).

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S1. Comment

Benzamides are frequently used in the synthesis of new and potent anti-convulsant agents (Clark *et al.*, 1988; Leander *et al.*, 1988; Diouf *et al.*, 1997). The structure of the title compound, (I), a benzamide derivative, is reported herein (Fig. 1).

The benzene ring, adjacent to the carbonyl group, twisted with respect to the plane formed through the central amide group; the N1–C1–C2–C3 torsion angle = -30.8 (4) °. In the same way, the putative mirror plane through the cyclohexyl ring (having a chair conformation) is twisted away from the central plane; the O1–N1–C8–C11 torsion angle is 151.3 (4) °. The anti-disposition of the NH and carbonyl groups allows for the formation of N–H···O hydrogen bonds which leads to the formation supramolecular chains aligned along the *a* axis, Fig. 2 and Table 1. These are connected into layers in the *ab* plane *via* C–H···π interactions, Fig. 2 and Table 1.

S2. Experimental

A solution of cyclohexyl amine (0.458 μl, 4 mmol) in dichloromethane (15 ml) was treated dropwise with benzoyl chloride (0.463 μl, 4 mmol) in the presence of triethanol amine (5 ml) as a catalyst. The resulting mixture was stirred for 1 h. The precipitates that formed were filtered, dried and crystallized from methanol to yield colourless blocks of (I).

S3. Refinement

The C-bound H atoms were geometrically placed (C–H = 0.93–0.98 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C). The N-bound H atom was refined freely. In the absence of significant anomalous scattering effects, 1130 Friedel pairs were averaged in the final refinement.

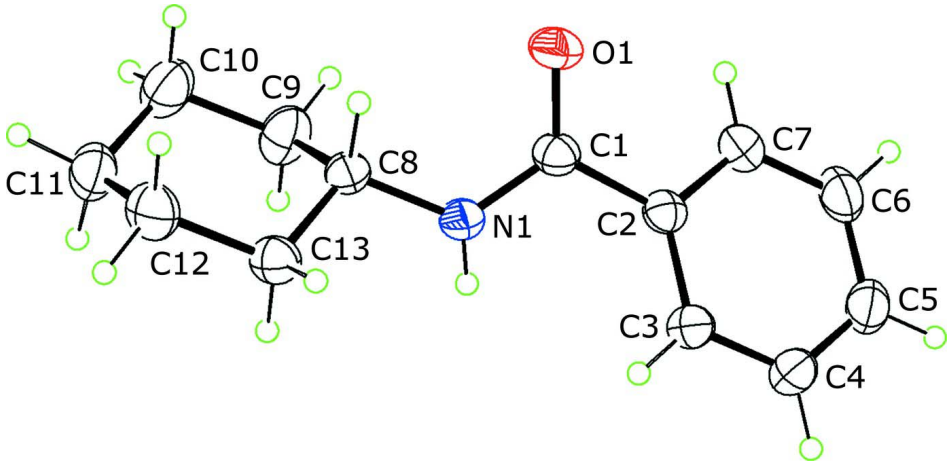

Figure 1

The molecular structure of (I) showing displacement ellipsoids at the 35% probability level.

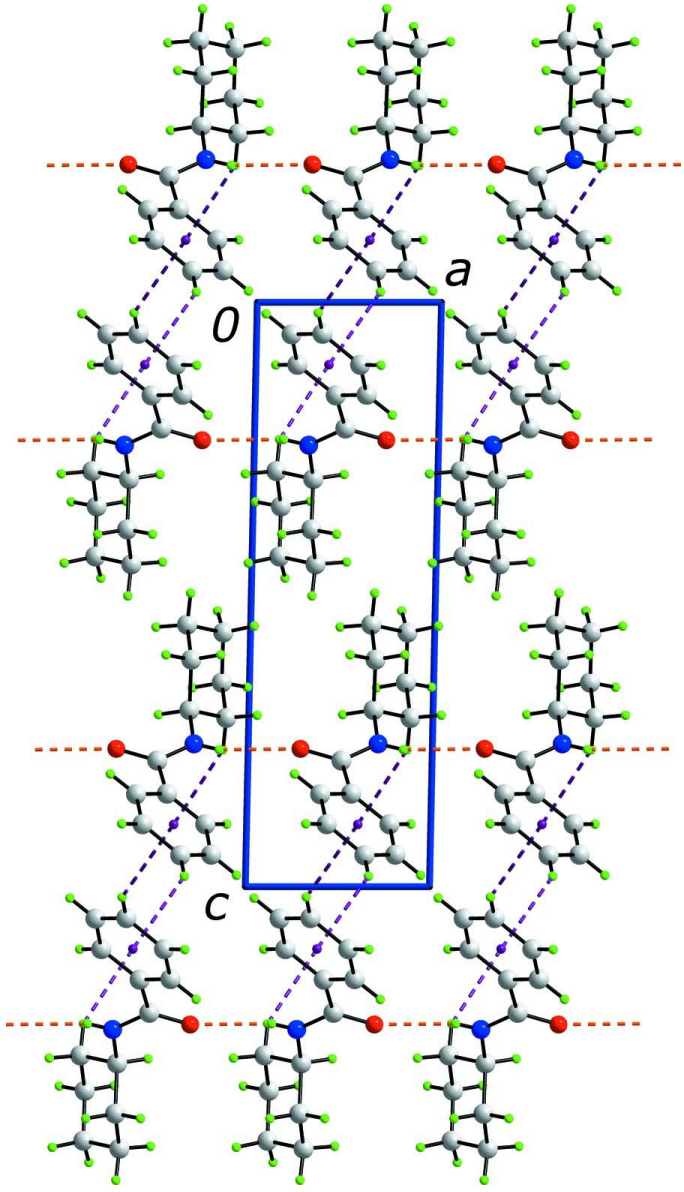

Figure 2

A view in projection down the *b* axis of the unit-cell contents for (I), highlighting the formation of layers in the *ab* plane. The N–H···O and C–H···π interactions are shown as orange and purple dashed lines, respectively. Colour code: O, red; N, blue; C, grey; and H, green.

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c = 16.6029 (12) Å
β = 91.176 (2)°
V = 572.38 (6) Å^3
Z = 2
F(000) = 220
D_x = 1.179 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.07 mm^{-1}

T = 293 K
Block, colourless

0.28 × 0.17 × 0.12 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
5479 measured reflections
1423 independent reflections

1105 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 27.5°, θ_{min} = 1.2°
$h = -6 \rightarrow 6$
$k = -8 \rightarrow 8$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.163
S = 1.07
1423 reflections
140 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1083P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: unk

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted R-factor wR and goodness of fit S are based on F^2, conventional R-factors R are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\sigma(F^2)$ is used only for calculating R-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. R-factors based on F^2 are statistically about twice as large as those based on F, and R- factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	y	z	U_{iso}*/U_{eq}
O1	0.7158 (3)	0.9885 (4)	0.23591 (14)	0.0636 (8)
N1	0.2952 (5)	0.9238 (4)	0.24441 (15)	0.0424 (6)
H1n	0.157 (6)	0.969 (6)	0.2345 (18)	0.045 (9)*
C1	0.4923 (5)	1.0267 (4)	0.21584 (18)	0.0415 (7)
C2	0.4362 (5)	1.1979 (5)	0.15919 (15)	0.0381 (6)
C3	0.2245 (5)	1.2004 (6)	0.10682 (16)	0.0460 (7)
H3	0.1077	1.0941	0.1071	0.055*
C4	0.1894 (6)	1.3614 (7)	0.05468 (18)	0.0575 (9)
H4	0.0488	1.3620	0.0195	0.069*
C5	0.3571 (6)	1.5201 (6)	0.05375 (19)	0.0602 (10)
H5	0.3321	1.6270	0.0179	0.072*
C6	0.5654 (6)	1.5203 (6)	0.1069 (2)	0.0586 (9)
H6	0.6785	1.6292	0.1076	0.070*
C7	0.6038 (6)	1.3593 (6)	0.15818 (19)	0.0495 (8)

H7	0.7455	1.3591	0.1929	0.059*
C8	0.3233 (5)	0.7589 (4)	0.30240 (17)	0.0405 (7)
H8	0.4904	0.6958	0.2945	0.049*
C9	0.3184 (8)	0.8399 (6)	0.3885 (2)	0.0611 (9)
H9A	0.4570	0.9358	0.3968	0.073*
H9B	0.1588	0.9108	0.3969	0.073*
C10	0.3452 (8)	0.6680 (7)	0.4484 (2)	0.0683 (11)
H10A	0.5140	0.6088	0.4443	0.082*
H10B	0.3296	0.7218	0.5024	0.082*
C11	0.1481 (6)	0.5051 (6)	0.4349 (2)	0.0636 (10)
H11A	−0.0198	0.5593	0.4461	0.076*
H11B	0.1814	0.3937	0.4719	0.076*
C12	0.1507 (7)	0.4266 (6)	0.3493 (2)	0.0620 (9)
H12A	0.0120	0.3306	0.3413	0.074*
H12B	0.3100	0.3556	0.3405	0.074*
C13	0.1224 (6)	0.5985 (5)	0.2888 (2)	0.0482 (8)
H13A	0.1362	0.5444	0.2347	0.058*
H13B	−0.0455	0.6591	0.2934	0.058*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0330 (10)	0.0681 (17)	0.0893 (17)	0.0023 (11)	−0.0042 (10)	0.0243 (15)
N1	0.0333 (12)	0.0437 (14)	0.0500 (14)	0.0042 (11)	−0.0005 (9)	0.0077 (11)
C1	0.0359 (13)	0.0405 (16)	0.0479 (15)	0.0036 (13)	0.0009 (11)	−0.0004 (13)
C2	0.0356 (12)	0.0421 (15)	0.0368 (14)	0.0029 (12)	0.0050 (10)	−0.0031 (13)
C3	0.0398 (14)	0.0546 (18)	0.0436 (15)	0.0001 (14)	−0.0021 (11)	0.0020 (16)
C4	0.0471 (16)	0.080 (2)	0.0453 (16)	0.0045 (18)	−0.0018 (13)	0.0133 (19)
C5	0.0554 (17)	0.067 (2)	0.059 (2)	0.0138 (18)	0.0137 (15)	0.024 (2)
C6	0.0552 (17)	0.0512 (19)	0.070 (2)	−0.0060 (17)	0.0147 (15)	0.0140 (18)
C7	0.0426 (14)	0.0538 (19)	0.0523 (17)	−0.0035 (14)	0.0059 (12)	0.0047 (16)
C8	0.0354 (12)	0.0391 (15)	0.0470 (16)	0.0060 (12)	0.0010 (11)	0.0046 (13)
C9	0.084 (2)	0.051 (2)	0.0476 (17)	−0.0102 (19)	−0.0115 (16)	−0.0008 (16)
C10	0.082 (2)	0.071 (3)	0.0513 (19)	−0.001 (2)	−0.0104 (17)	0.010 (2)
C11	0.0624 (19)	0.062 (2)	0.067 (2)	0.010 (2)	0.0116 (16)	0.022 (2)
C12	0.0633 (19)	0.0396 (18)	0.083 (3)	−0.0053 (16)	0.0001 (17)	0.0068 (18)
C13	0.0457 (15)	0.0427 (17)	0.0560 (19)	−0.0010 (14)	−0.0021 (13)	−0.0011 (15)

Geometric parameters (Å, º)

O1—C1	1.236 (3)	C8—C9	1.526 (4)
N1—C1	1.331 (4)	C8—H8	0.9800
N1—C8	1.456 (4)	C9—C10	1.511 (5)
N1—H1n	0.80 (3)	C9—H9A	0.9700
C1—C2	1.493 (4)	C9—H9B	0.9700
C2—C7	1.379 (4)	C10—C11	1.502 (5)
C2—C3	1.395 (4)	C10—H10A	0.9700
C3—C4	1.379 (5)	C10—H10B	0.9700

C3—H3	0.9300	C11—C12	1.512 (5)
C4—C5	1.365 (5)	C11—H11A	0.9700
C4—H4	0.9300	C11—H11B	0.9700
C5—C6	1.389 (5)	C12—C13	1.519 (5)
C5—H5	0.9300	C12—H12A	0.9700
C6—C7	1.372 (5)	C12—H12B	0.9700
C6—H6	0.9300	C13—H13A	0.9700
C7—H7	0.9300	C13—H13B	0.9700
C8—C13	1.505 (4)		

C1—N1—C8	123.1 (2)	C10—C9—C8	110.6 (3)
C1—N1—H1N	116 (3)	C10—C9—H9A	109.5
C8—N1—H1N	120 (2)	C8—C9—H9A	109.5
O1—C1—N1	122.5 (3)	C10—C9—H9B	109.5
O1—C1—C2	119.8 (2)	C8—C9—H9B	109.5
N1—C1—C2	117.7 (2)	H9A—C9—H9B	108.1
C7—C2—C3	118.8 (3)	C11—C10—C9	112.5 (3)
C7—C2—C1	118.2 (2)	C11—C10—H10A	109.1
C3—C2—C1	123.0 (3)	C9—C10—H10A	109.1
C4—C3—C2	119.7 (3)	C11—C10—H10B	109.1
C4—C3—H3	120.2	C9—C10—H10B	109.1
C2—C3—H3	120.2	H10A—C10—H10B	107.8
C5—C4—C3	121.2 (3)	C10—C11—C12	111.4 (3)
C5—C4—H4	119.4	C10—C11—H11A	109.4
C3—C4—H4	119.4	C12—C11—H11A	109.4
C4—C5—C6	119.4 (3)	C10—C11—H11B	109.4
C4—C5—H5	120.3	C12—C11—H11B	109.4
C6—C5—H5	120.3	H11A—C11—H11B	108.0
C7—C6—C5	119.8 (3)	C11—C12—C13	111.4 (3)
C7—C6—H6	120.1	C11—C12—H12A	109.4
C5—C6—H6	120.1	C13—C12—H12A	109.4
C6—C7—C2	121.2 (3)	C11—C12—H12B	109.4
C6—C7—H7	119.4	C13—C12—H12B	109.4
C2—C7—H7	119.4	H12A—C12—H12B	108.0
N1—C8—C13	111.3 (2)	C8—C13—C12	111.4 (2)
N1—C8—C9	110.8 (3)	C8—C13—H13A	109.3
C13—C8—C9	111.1 (3)	C12—C13—H13A	109.3
N1—C8—H8	107.8	C8—C13—H13B	109.3
C13—C8—H8	107.8	C12—C13—H13B	109.3
C9—C8—H8	107.8	H13A—C13—H13B	108.0

C8—N1—C1—O1	0.7 (5)	C3—C2—C7—C6	−0.1 (4)
C8—N1—C1—C2	−177.6 (2)	C1—C2—C7—C6	179.2 (3)
O1—C1—C2—C7	−28.3 (4)	C1—N1—C8—C13	−146.5 (3)
N1—C1—C2—C7	150.1 (3)	C1—N1—C8—C9	89.3 (3)
O1—C1—C2—C3	150.9 (3)	N1—C8—C9—C10	179.5 (3)
N1—C1—C2—C3	−30.8 (4)	C13—C8—C9—C10	55.2 (3)
C7—C2—C3—C4	1.0 (4)	C8—C9—C10—C11	−54.8 (4)

C1—C2—C3—C4	−178.2 (3)	C9—C10—C11—C12	54.6 (4)
C2—C3—C4—C5	−0.6 (5)	C10—C11—C12—C13	−54.1 (4)
C3—C4—C5—C6	−0.7 (5)	N1—C8—C13—C12	−179.8 (3)
C4—C5—C6—C7	1.6 (5)	C9—C8—C13—C12	−55.8 (3)
C5—C6—C7—C2	−1.2 (5)	C11—C12—C13—C8	55.2 (4)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C2–C7 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*n*···O1^{i}	0.80 (3)	2.32 (3)	3.065 (3)	157 (3)
C13—H13a···*Cg*1^{ii}	0.97	2.82	3.722 (4)	154
C5—H5···*Cg*1^{iii}	0.93	2.96	3.729 (4)	141

Symmetry codes: (i) *x*−1, *y*, *z*; (ii) *x*, *y*−1, *z*; (iii) −*x*+1, *y*+1/2, −*z*.