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5-Chloro-3-ethyl-*N*-[2-(morpholin-4-yl)-ethyl]-1*H*-indole-2-carboxamide

Kirsty E. A. Muirhead, Laurent Trembleau and William T. A. Harrison*

Department of Chemistry, University of Aberdeen, Meston Walk, Aberdeen AB24 3UE, Scotland
Correspondence e-mail: w.harrison@abdn.ac.uk

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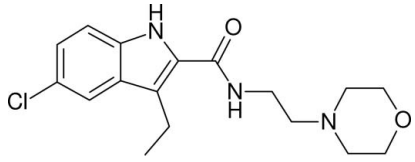
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.012 Å; R factor = 0.129; wR factor = 0.289; data-to-parameter ratio = 15.2.

In the title compound, $C_{17}H_{22}ClN_3O_2$, the aromatic fused ring system and the amide group are close to being coplanar [dihedral angle = 14.66 (16)°]. Thus, the amide NH group is sterically blocked from forming a hydrogen bond by the pendant ethyl substituent of the adjacent five-membered ring. The NH group of the five-membered ring makes an intermolecular N—H···O bond, resulting in centrosymmetric dimers of molecules containing $R_2^2(10)$ loops.

Related literature

For a related structure, see: Muirhead *et al.* (2007). For background, see: Price *et al.* (2005); Allen *et al.* (1987); Bernstein *et al.* (1995). The syntheses of the intermediates will be described later, see: Muirhead & Trembleau (2007).



Experimental

Crystal data

$C_{17}H_{22}ClN_3O_2$
M_r = 335.83
Triclinic, $P\overline{1}$
a = 9.1886 (13) Å
b = 9.7175 (13) Å
c = 11.2807 (10) Å
α = 73.755 (6)°
β = 79.612 (6)°
γ = 63.056 (5)°
V = 860.38 (18) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 120 (2) K
0.12 × 0.08 × 0.06 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2003)
T_{min} = 0.972, T_{max} = 0.987
10924 measured reflections
3155 independent reflections
1516 reflections with $I > 2\sigma(I)$
R_{int} = 0.159

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.129
$wR(F^2)$ = 0.289
S = 1.07
3155 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å^{-3}
$\Delta\rho_{min}$ = −0.38 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O1^{i}	0.88	1.97	2.803 (7)	157
C6—H6···O2^{ii}	0.95	2.58	3.491 (11)	161

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

Data collection: *COLLECT* (Nonius, 1998); cell refinement: *SCALEPACK* (Otwinowski & Minor, 1997); data reduction: *SCALEPACK* and *DENZO* (Otwinowski & Minor, 1997), and *SORTAV* (Blessing, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2171).

References

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.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Blessing, R. H. (1995). *Acta Cryst.* A**51**, 33–38.
Bruker (2003). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Muirhead, K. E. A. & Trembleau, L. (2007). Unpublished work.
Muirhead, K. E. A., Trembleau, L. & Harrison, W. T. A. (2007). *Acta Cryst.* E**63**, o3390.
Nonius (1998). *COLLECT*. Nonius BV, Delft, The Netherlands.
Otwinowski, Z. & Minor, W. (1997). *Methods in Enzymology*, Vol. 276, *Macromolecular Crystallography*, Part A, edited by C. W. Carter, Jr & R. M. Sweet, pp. 307–326. New York: Academic Press.
Price, M. R., Baillie, G. L., Thomas, A., Stevenson, L. A., Easson, M., Goodwin, R., McLean, A., McIntosh, L., Goodwin, G., Walker, G., Westwood, P., Marrs, J., Thomson, F., Cowley, P., Christopolous, A., Pertwee, R. G. & Ross, R. (2005). *Mol. Pharmacol.* **68**, 1484–1495.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.

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supplementary materials

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5-Chloro-3-ethyl-*N*-[2-(morpholin-4-yl)ethyl]-1*H*-indole-2-carboxamide

K. E. A. Muirhead, L. Trembleau and W. T. A. Harrison

Comment

As part of our on-going investigations of allosteric modulators of the cannabinoid CB1 receptor (Price *et al.*, 2005), the title compound, (I), $C_{17}H_{22}ClN_3O_2$, has been synthesized and structurally characterized (Fig. 1). It complements $C_{18}H_{24}ClN_3O_2$, reported in the next paper (Muirhead, Trembleau & Harrison, 2007).

The dihedral angle between the mean planes of the C1—C8/N1 fused aromatic ring system and atoms C6/C7/N1/O2 in (I) is 14.66 (16)°, *i.e.* the two fragments are slightly twisted. Atom C10 is displaced from the C1—C8/N1 mean plane by 1.459 (14) Å. The C14—C17/N3/O2 ring in (I) has a typical chair conformation, with N3 and O2 displaced from the mean plane of the carbon atoms by −0.656 (12)Å and 0.635 (14) Å, respectively. Otherwise, the bond lengths and angles in (I) may be regarded as normal (Allen *et al.*, 1995).

The crystal packing for (I) results in inversion dimers linked by N1—H1···O1^{i} hydrogen bonds (Table 1), thus forming $R_2^2(10)$ loops (Bernstein *et al.*, 1995). The amide N2—H2 group is sterically blocked by the C9/C10 ethyl substituent to the 5-membered ring from making an hydrogen bond. A short C—H···O interaction also occurs (Table 1).

Experimental

To a solution of pentafluorophenol (0.130 g, 0.706 mmol) in dichloromethane (5 ml), 3-ethylindole-2-carboxylic acid (0.100 g, 0.447 mmol) (Muirhead & Trembleau, 2007) and *N*-ethyl-*N*'-(3-dimethylaminopropyl)carbodiimide hydrochloride (0.111 g, 0.581 mmol) were added and stirred at room temperature for 80 min. Silica gel (1.2 g) was added to the reaction mixture, stirred for 5 min and the mixture filtered through Celite and the solvent removed to give the activated ester as a white solid (0.167 g). The ester was redissolved in dichloromethane (2.6 ml), to which was added 2-morpholinoethylamine 5 (0.068 ml, 0.514 mmol) and triethylamine (0.072 ml, 0.514 mmol) and stirred at room temperature for 80 min. The solvent was removed under vacuum and the resulting solid taken up into ethyl acetate (30 ml), washed with saturated potassium carbonate solution (5 ml), dried over magnesium sulfate, filtered and dried. Recrystallization of the crude material from hot ethanol afforded 0.066 g (44%) of colourless blocks of (I)

Refinement

The H atoms were placed in idealized locations (C—H = 0.93–0.99 Å, N—H = 0.88 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C,*N*) or 1.5U_{eq}(methyl C).

Figures

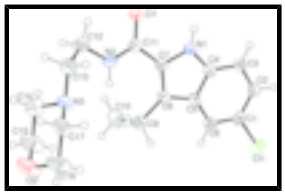

Fig. 1. View of the molecular structure of (I) showing 40% displacement ellipsoids.

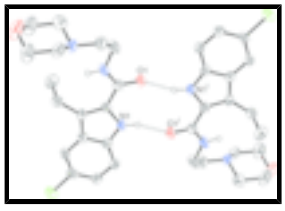

Fig. 2. An inversion dimer in the crystal of (I) with hydrogen bonds shown as double dashed lines. All carbon-bound H atoms are omitted for clarity. Symmetry code as in Table 1.

5-Chloro-3-ethyl-*N*-(2-morpholin-4-ylethyl)-1*H*-indole-2-carboxamide

Crystal data

$C_{17}H_{22}ClN_3O_2$	$Z = 2$
$M_r = 335.83$	$F_{000} = 356$
Triclinic, $P\overline{1}$	$D_x = 1.296$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.1886$ (13) Å	Cell parameters from 3029 reflections
$b = 9.7175$ (13) Å	$\theta = 2.9$–27.5º
$c = 11.2807$ (10) Å	$\mu = 0.24$ mm^{-1}
$\alpha = 73.755$ (6)º	$T = 120$ (2) K
$\beta = 79.612$ (6)º	Block, colourles
$\gamma = 63.056$ (5)º	0.12 × 0.08 × 0.06 mm
$V = 860.38$ (18) Å^3	

Data collection

Nonius KappaCCD diffractometer	3155 independent reflections
Radiation source: fine-focus sealed tube	1516 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.159$
$T = 120(2)$ K	$\theta_{max} = 25.5$º
ω and φ scans	$\theta_{min} = 3.0$º
Absorption correction: multi-scan (SADABS; Bruker, 2003)	$h = -11 \rightarrow 11$
$T_{min} = 0.972$, $T_{max} = 0.987$	$k = -11 \rightarrow 11$
10924 measured reflections	$l = -13 \rightarrow 13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.129$	H-atom parameters constrained
$wR(F^2) = 0.289$	$w = 1/[\sigma^2(F_o^2) + (0.039P)^2 + 4.7894P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.07$	$(\Delta/\sigma)_{max} < 0.001$
3155 reflections	$\Delta\rho_{max} = 0.36$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.38$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'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}
C1	0.9563 (9)	0.2441 (9)	0.5535 (6)	0.0404 (19)
C2	1.0584 (10)	0.1514 (9)	0.4714 (7)	0.046 (2)
H2A	1.1222	0.0414	0.5016	0.055*
C3	1.0679 (9)	0.2169 (9)	0.3478 (7)	0.0393 (18)
H3	1.1365	0.1547	0.2908	0.047*
C4	0.9723 (9)	0.3796 (8)	0.3089 (6)	0.0353 (18)
C5	0.8706 (9)	0.4732 (9)	0.3911 (7)	0.0356 (17)
C6	0.8631 (9)	0.4013 (9)	0.5165 (6)	0.0399 (19)
H6	0.7941	0.4616	0.5746	0.048*
C7	0.8504 (9)	0.6271 (8)	0.1992 (6)	0.0364 (18)
C8	0.7926 (9)	0.6324 (8)	0.3215 (6)	0.0368 (18)
C9	0.6664 (10)	0.7674 (9)	0.3750 (7)	0.050 (2)
H9A	0.6860	0.8630	0.3371	0.060*
H9B	0.6793	0.7417	0.4649	0.060*
C10	0.4926 (12)	0.8046 (14)	0.3552 (10)	0.089 (4)
H10A	0.4163	0.8933	0.3925	0.134*
H10B	0.4713	0.7113	0.3939	0.134*
H10C	0.4777	0.8334	0.2663	0.134*
C11	0.8181 (9)	0.7478 (9)	0.0822 (7)	0.0399 (19)
C12	0.7132 (13)	1.0292 (9)	−0.0191 (7)	0.061 (3)
H12A	0.5991	1.0711	−0.0417	0.073*
H12B	0.7875	0.9927	−0.0903	0.073*

C13	0.7398 (12)	1.1575 (10)	0.0105 (7)	0.057 (2)
H13A	0.8584	1.1229	0.0143	0.069*
H13B	0.6993	1.2542	−0.0565	0.069*
C14	0.4797 (11)	1.2850 (12)	0.1173 (8)	0.063 (3)
H14A	0.4356	1.2223	0.0920	0.075*
H14B	0.4569	1.3843	0.0530	0.075*
C15	0.3973 (12)	1.3236 (14)	0.2387 (10)	0.086 (4)
H15A	0.2785	1.3875	0.2289	0.103*
H15B	0.4121	1.2238	0.3004	0.103*
C16	0.6288 (13)	1.3189 (14)	0.2949 (10)	0.080 (3)
H16A	0.6501	1.2182	0.3571	0.096*
H16B	0.6721	1.3793	0.3243	0.096*
C17	0.7163 (10)	1.2833 (11)	0.1741 (8)	0.060 (2)
H17A	0.7002	1.3838	0.1129	0.072*
H17B	0.8350	1.2211	0.1851	0.072*
N1	0.9593 (7)	0.4741 (7)	0.1933 (5)	0.0373 (15)
H1	1.0119	0.4427	0.1256	0.045*
N2	0.7448 (9)	0.8985 (7)	0.0874 (5)	0.053 (2)
H2	0.7130	0.9207	0.1609	0.064*
N3	0.6561 (8)	1.1948 (7)	0.1276 (6)	0.0426 (16)
O1	0.8611 (7)	0.7085 (6)	−0.0193 (5)	0.0570 (16)
O2	0.4578 (8)	1.4077 (9)	0.2841 (7)	0.086 (2)
Cl1	0.9493 (3)	0.1505 (3)	0.71052 (19)	0.0626 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.038 (5)	0.045 (5)	0.034 (4)	−0.022 (4)	−0.005 (4)	0.005 (4)
C2	0.039 (5)	0.039 (5)	0.047 (5)	−0.008 (4)	−0.003 (4)	−0.006 (4)
C3	0.034 (4)	0.042 (5)	0.039 (4)	−0.014 (4)	0.001 (3)	−0.013 (4)
C4	0.031 (4)	0.036 (4)	0.041 (4)	−0.018 (4)	0.003 (3)	−0.009 (4)
C5	0.031 (4)	0.038 (4)	0.043 (4)	−0.017 (4)	0.000 (4)	−0.015 (4)
C6	0.041 (5)	0.046 (5)	0.031 (4)	−0.020 (4)	0.008 (3)	−0.011 (4)
C7	0.040 (5)	0.033 (4)	0.035 (4)	−0.014 (4)	−0.004 (3)	−0.007 (3)
C8	0.037 (4)	0.035 (4)	0.040 (4)	−0.014 (4)	0.004 (4)	−0.017 (4)
C9	0.061 (6)	0.044 (5)	0.037 (4)	−0.019 (4)	0.002 (4)	−0.008 (4)
C10	0.052 (7)	0.104 (9)	0.083 (8)	−0.007 (6)	0.008 (6)	−0.033 (7)
C11	0.042 (5)	0.037 (5)	0.039 (4)	−0.014 (4)	−0.003 (4)	−0.010 (4)
C12	0.103 (8)	0.037 (5)	0.034 (4)	−0.025 (5)	−0.003 (5)	−0.003 (4)
C13	0.072 (7)	0.042 (5)	0.047 (5)	−0.019 (5)	0.008 (5)	−0.008 (4)
C14	0.063 (7)	0.074 (7)	0.063 (6)	−0.040 (6)	−0.001 (5)	−0.017 (5)
C15	0.047 (6)	0.115 (9)	0.112 (9)	−0.034 (6)	0.018 (6)	−0.066 (8)
C16	0.070 (8)	0.105 (9)	0.099 (8)	−0.044 (7)	0.005 (6)	−0.069 (7)
C17	0.040 (5)	0.059 (6)	0.077 (6)	−0.012 (5)	−0.001 (5)	−0.029 (5)
N1	0.044 (4)	0.035 (4)	0.029 (3)	−0.012 (3)	0.003 (3)	−0.014 (3)
N2	0.089 (6)	0.032 (4)	0.026 (3)	−0.015 (4)	0.000 (3)	−0.009 (3)
N3	0.038 (4)	0.045 (4)	0.048 (4)	−0.015 (3)	0.000 (3)	−0.021 (3)
O1	0.071 (4)	0.048 (3)	0.035 (3)	−0.008 (3)	−0.001 (3)	−0.018 (3)

O2	0.049 (4)	0.105 (6)	0.129 (6)	−0.031 (4)	0.018 (4)	−0.080 (5)
Cl1	0.0756 (17)	0.0625 (15)	0.0402 (12)	−0.0305 (13)	−0.0032 (11)	0.0040 (10)

Geometric parameters (Å, °)

C1—C6	1.352 (10)	C12—N2	1.442 (9)
C1—C2	1.393 (10)	C12—C13	1.505 (11)
C1—Cl1	1.754 (7)	C12—H12A	0.9900
C2—C3	1.366 (10)	C12—H12B	0.9900
C2—H2A	0.9500	C13—N3	1.455 (9)
C3—C4	1.399 (10)	C13—H13A	0.9900
C3—H3	0.9500	C13—H13B	0.9900
C4—N1	1.357 (9)	C14—N3	1.460 (11)
C4—C5	1.397 (9)	C14—C15	1.499 (12)
C5—C6	1.397 (10)	C14—H14A	0.9900
C5—C8	1.429 (10)	C14—H14B	0.9900
C6—H6	0.9500	C15—O2	1.410 (11)
C7—N1	1.378 (9)	C15—H15A	0.9900
C7—C8	1.393 (9)	C15—H15B	0.9900
C7—C11	1.472 (10)	C16—O2	1.418 (11)
C8—C9	1.497 (10)	C16—C17	1.497 (12)
C9—C10	1.514 (12)	C16—H16A	0.9900
C9—H9A	0.9900	C16—H16B	0.9900
C9—H9B	0.9900	C17—N3	1.452 (10)
C10—H10A	0.9800	C17—H17A	0.9900
C10—H10B	0.9800	C17—H17B	0.9900
C10—H10C	0.9800	N1—H1	0.8800
C11—O1	1.248 (8)	N2—H2	0.8800
C11—N2	1.319 (9)		
C6—C1—C2	122.5 (7)	C13—C12—H12B	109.8
C6—C1—Cl1	119.6 (6)	H12A—C12—H12B	108.3
C2—C1—Cl1	117.9 (6)	N3—C13—C12	111.9 (7)
C3—C2—C1	120.7 (7)	N3—C13—H13A	109.2
C3—C2—H2A	119.7	C12—C13—H13A	109.2
C1—C2—H2A	119.7	N3—C13—H13B	109.2
C2—C3—C4	117.1 (7)	C12—C13—H13B	109.2
C2—C3—H3	121.4	H13A—C13—H13B	107.9
C4—C3—H3	121.4	N3—C14—C15	110.3 (8)
N1—C4—C5	108.2 (6)	N3—C14—H14A	109.6
N1—C4—C3	129.4 (7)	C15—C14—H14A	109.6
C5—C4—C3	122.3 (7)	N3—C14—H14B	109.6
C4—C5—C6	118.7 (7)	C15—C14—H14B	109.6
C4—C5—C8	107.9 (6)	H14A—C14—H14B	108.1
C6—C5—C8	133.4 (7)	O2—C15—C14	113.3 (8)
C1—C6—C5	118.6 (7)	O2—C15—H15A	108.9
C1—C6—H6	120.7	C14—C15—H15A	108.9
C5—C6—H6	120.7	O2—C15—H15B	108.9
N1—C7—C8	109.4 (6)	C14—C15—H15B	108.9
N1—C7—C11	117.3 (6)	H15A—C15—H15B	107.7

C8—C7—C11	133.3 (7)	O2—C16—C17	111.7 (8)
C7—C8—C5	105.4 (6)	O2—C16—H16A	109.3
C7—C8—C9	130.1 (7)	C17—C16—H16A	109.3
C5—C8—C9	124.3 (6)	O2—C16—H16B	109.3
C8—C9—C10	113.5 (7)	C17—C16—H16B	109.3
C8—C9—H9A	108.9	H16A—C16—H16B	107.9
C10—C9—H9A	108.9	N3—C17—C16	111.0 (7)
C8—C9—H9B	108.9	N3—C17—H17A	109.4
C10—C9—H9B	108.9	C16—C17—H17A	109.4
H9A—C9—H9B	107.7	N3—C17—H17B	109.4
C9—C10—H10A	109.5	C16—C17—H17B	109.4
C9—C10—H10B	109.5	H17A—C17—H17B	108.0
H10A—C10—H10B	109.5	C4—N1—C7	109.1 (6)
C9—C10—H10C	109.5	C4—N1—H1	125.5
H10A—C10—H10C	109.5	C7—N1—H1	125.5
H10B—C10—H10C	109.5	C11—N2—C12	124.4 (6)
O1—C11—N2	120.9 (7)	C11—N2—H2	117.8
O1—C11—C7	120.8 (7)	C12—N2—H2	117.8
N2—C11—C7	118.3 (6)	C17—N3—C13	112.2 (6)
N2—C12—C13	109.3 (7)	C17—N3—C14	108.7 (6)
N2—C12—H12A	109.8	C13—N3—C14	111.6 (7)
C13—C12—H12A	109.8	C15—O2—C16	109.2 (7)
N2—C12—H12B	109.8		
C6—C1—C2—C3	−0.3 (12)	N1—C7—C11—O1	14.0 (11)
Cl1—C1—C2—C3	179.3 (6)	C8—C7—C11—O1	−166.0 (8)
C1—C2—C3—C4	0.5 (11)	N1—C7—C11—N2	−165.1 (7)
C2—C3—C4—N1	179.5 (7)	C8—C7—C11—N2	14.9 (13)
C2—C3—C4—C5	−0.1 (11)	N2—C12—C13—N3	−48.9 (10)
N1—C4—C5—C6	179.8 (6)	N3—C14—C15—O2	56.9 (12)
C3—C4—C5—C6	−0.6 (11)	O2—C16—C17—N3	−58.9 (11)
N1—C4—C5—C8	−0.2 (8)	C5—C4—N1—C7	−0.3 (8)
C3—C4—C5—C8	179.4 (7)	C3—C4—N1—C7	−179.8 (7)
C2—C1—C6—C5	−0.3 (12)	C8—C7—N1—C4	0.6 (8)
Cl1—C1—C6—C5	−179.9 (6)	C11—C7—N1—C4	−179.4 (6)
C4—C5—C6—C1	0.8 (11)	O1—C11—N2—C12	−2.5 (13)
C8—C5—C6—C1	−179.2 (8)	C7—C11—N2—C12	176.6 (8)
N1—C7—C8—C5	−0.7 (8)	C13—C12—N2—C11	−141.5 (8)
C11—C7—C8—C5	179.3 (8)	C16—C17—N3—C13	−179.6 (8)
N1—C7—C8—C9	−176.1 (7)	C16—C17—N3—C14	56.5 (10)
C11—C7—C8—C9	3.9 (14)	C12—C13—N3—C17	163.8 (7)
C4—C5—C8—C7	0.6 (8)	C12—C13—N3—C14	−74.0 (9)
C6—C5—C8—C7	−179.5 (8)	C15—C14—N3—C17	−54.9 (10)
C4—C5—C8—C9	176.3 (7)	C15—C14—N3—C13	−179.1 (7)
C6—C5—C8—C9	−3.7 (13)	C14—C15—O2—C16	−56.9 (12)
C7—C8—C9—C10	76.4 (11)	C17—C16—O2—C15	57.2 (11)
C5—C8—C9—C10	−98.2 (9)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	1.97	2.803 (7)	157
C6—H6···O2^{ii}	0.95	2.58	3.491 (11)	161

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

Fig. 1

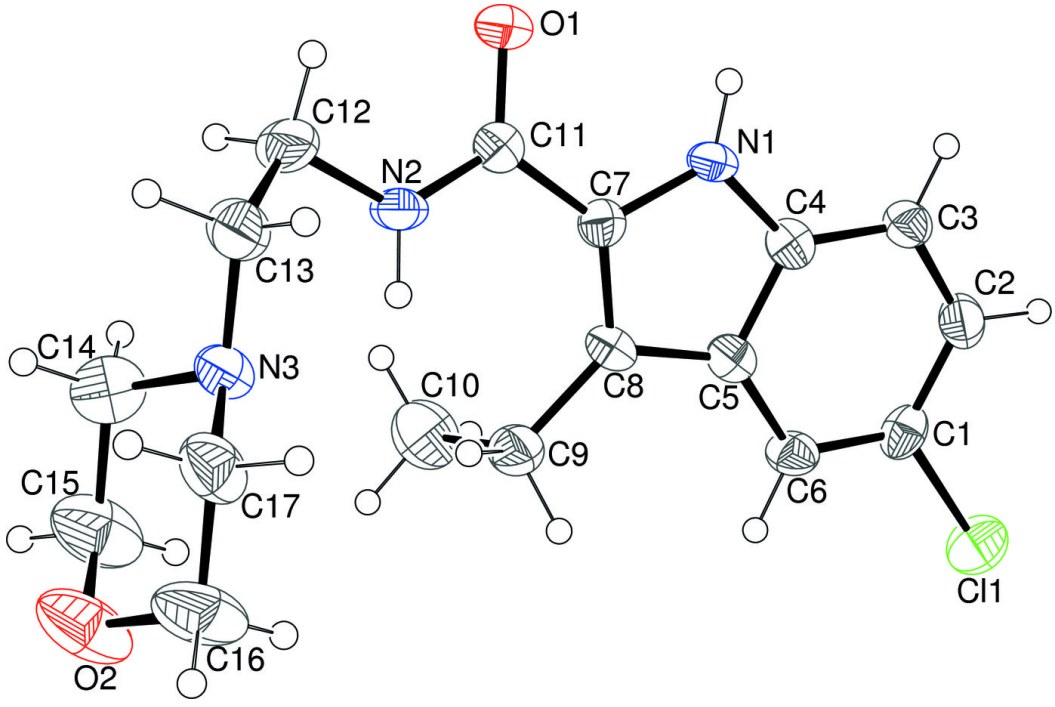
O1
C12
C11
N1
N2
C7
C4
C3
C13
C2
C14
N3
C10
C8
C5
C1
C15
C9
C6
C17
Cl1
O2
C16

Fig. 2