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

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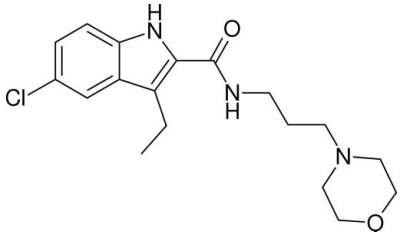
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.014 Å; R factor = 0.142; wR factor = 0.342; data-to-parameter ratio = 14.1.

In the title compound, $C_{18}H_{24}ClN_3O_2$, the aromatic fused ring system and the amide group are significantly twisted [dihedral angle = 23.4 (5)°]. The crystal packing is influenced by N—H···O hydrogen bonds, resulting in chains of molecules propagating along [100].

Related literature

For a related structure, see: Muirhead *et al.* (2007). For medicinal background, see: Price *et al.* (2005). For crystallographic background, see: Allen *et al.* (1987); Bernstein *et al.* (1995); Spek (2003).



Experimental

Crystal data

$C_{18}H_{24}ClN_3O_2$
M_r = 349.85
Monoclinic, $P2_1/n$
a = 4.8178 (3) Å
b = 12.1967 (12) Å
c = 29.576 (3) Å
β = 93.265 (5)°
V = 1735.1 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.24 mm^{-1}
T = 120 (2) K
0.04 × 0.01 × 0.01 mm

Data collection

Nonius KappaCCD diffractometer
Absorption correction: none
10192 measured reflections
3092 independent reflections
2077 reflections with $I > 2\sigma(I)$
R_{int} = 0.089

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.142
$wR(F^2)$ = 0.342
S = 1.09
3092 reflections
219 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.51 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	2.13	2.945 (10)	153
N2—H2···O1^{ii}	0.88	2.13	2.895 (10)	144

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

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: BT2413).

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supplementary materials

Acta Cryst. (2007). E**63**, o3390 [**doi:10.1107/S1600536807031182**]

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

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

Comment

The title compound, (I), $C_{18}H_{24}ClN_3O_2$, was synthesized and structurally characterized (Fig. 1), as part of our investigations of allosteric modulators of the cannabinoid CB1 receptor (Price *et al.*, 2005). It complements $C_{17}H_{22}ClN_3O_2$, (II), reported in the preceding paper (Muirhead *et al.*, 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 23.4 (5)°. The equivalent dihedral angle in (II) is 14.66 (16)°. C10 is displaced from the C1—C8/N1 mean plane in (I) by 1.60 (2) Å. The C15—C18/N3/O2 ring in (I) is a typical chair, with N3 and O2 displaced from the mean plane of the carbon atoms by 0.670 (13)Å and −0.662 (13) 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 chains of molecules linked by N—H···O hydrogen bonds (Table 1). First, the N1—H1···O1^{i} (see Table 1 for symmetry information) link leads to inversion dimers contaning $R^2_2(10)$ loops (Bernstein *et al.*, 1995), as was also seen in the structure of (II). Because of the greater degree of twisting of the amide group with respect to the aromatic ring system in (II) as compared to (I), an N2—H2···O1^{ii} bond is now possible, which leads to [100] chains (Fig. 2) in the crystal.

There are no π-π stacking interactions in (I), the shortest separation of the centroids of nearby aromatic rings being greater than 4.8 Å.

Experimental

To a solution of pentafluorophenol (0.130 g, 0.706 mmol) in DCM (5 ml), 3-ethylindole-2-carboxylic acid (0.100 g, 0.447 mmol) 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 DCM (2.6 ml), to which was added 3-morpholinopropylamine (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 yielded 0.055 g (35%) of colourless needles of (I)

Refinement

An analysis with *PLATON* (Spek, 2003) indicated non-merohedral twinning, with the matrix (−1, 0, 0 / 0, −1, 0 / 0.7, 0, 1) relating the major and minor twin components. The refined domain ratio was 0.921 (4):0.079 (4). This, in addition to the small and feebly scattering crystal used for the data collection may correlate with the rather high *R* factors.

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).

The highest difference peak is 1.70Å from Cl1 and the deepest difference hole is 1.21Å from N1.

Figures

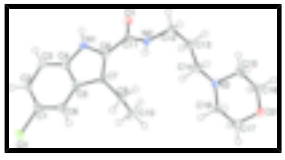

Fig. 1. View of the molecular structure of (I) showing 50% displacement ellipsoids (arbitrary spheres for the H atoms).

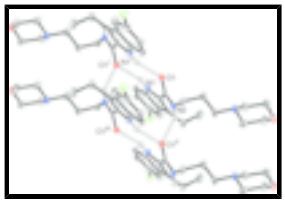

Fig. 2. Fragement of a [100] chain of molecules in the crystal of (I) with hydrogen bonds shown as dashed lines. All carbon-bound H atoms are omitted for clarity. Symmetry codes as in Table 1; additionally (iii) 1 − *x*, 1 − *y*, 1 − *z*.

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

Crystal data

$C_{18}H_{24}ClN_3O_2$	F_{000} = 744
M_r = 349.85	D_x = 1.339 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 3212 reflections
a = 4.8178 (3) Å	θ = 2.9–27.5º
b = 12.1967 (12) Å	μ = 0.24 mm^{-1}
c = 29.576 (3) Å	*T* = 120 (2) K
β = 93.265 (5)º	Needle, colourless
V = 1735.1 (3) Å^3	0.04 × 0.01 × 0.01 mm
Z = 4	

Data collection

Nonius KappaCCD diffractometer	2077 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	R_{int} = 0.089
Monochromator: graphite	θ_{max} = 25.5º
T = 120(2) K	θ_{min} = 3.2º
ω and φ scans	*h* = −5→5
Absorption correction: none	*k* = −13→14
10192 measured reflections	*l* = −35→35
3092 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.142$	H-atom parameters constrained
$wR(F^2) = 0.342$	$w = 1/[\sigma^2(F_o^2) + (0.0556P)^2 + 36.1132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} < 0.001$
3092 reflections	$\Delta\rho_{max} = 1.25$ e Å^{-3}
219 parameters	$\Delta\rho_{min} = -0.51$ 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	0.112 (2)	0.1461 (9)	0.6108 (3)	0.027 (2)
C2	−0.090 (2)	0.2101 (9)	0.6287 (3)	0.024 (2)
H2A	−0.1399	0.1994	0.6590	0.029*
C3	−0.224 (2)	0.2917 (8)	0.6014 (3)	0.023 (2)
H3	−0.3634	0.3375	0.6127	0.028*
C4	−0.142 (2)	0.3021 (8)	0.5575 (3)	0.022 (2)
C5	0.074 (2)	0.2366 (8)	0.5398 (3)	0.022 (2)
C6	0.198 (2)	0.1578 (9)	0.5676 (3)	0.026 (2)
H6	0.3415	0.1124	0.5570	0.032*
C7	0.1034 (19)	0.2705 (7)	0.4939 (3)	0.016 (2)
C8	−0.085 (2)	0.3538 (8)	0.4852 (3)	0.021 (2)
C9	0.281 (2)	0.2097 (8)	0.4623 (3)	0.023 (2)
H9A	0.3255	0.2590	0.4371	0.027*
H9B	0.4586	0.1896	0.4788	0.027*
C10	0.148 (3)	0.1086 (10)	0.4432 (4)	0.041 (3)
H10A	0.1087	0.0583	0.4678	0.062*
H10B	0.2734	0.0731	0.4227	0.062*
H10C	−0.0263	0.1279	0.4263	0.062*

C11	−0.178 (2)	0.4151 (8)	0.4436 (3)	0.018 (2)
C12	−0.083 (2)	0.4638 (8)	0.3662 (3)	0.021 (2)
H12A	0.0742	0.5053	0.3544	0.025*
H12B	−0.2397	0.5153	0.3688	0.025*
C13	−0.169 (2)	0.3744 (8)	0.3327 (3)	0.024 (2)
H13A	−0.3204	0.3305	0.3451	0.029*
H13B	−0.2435	0.4085	0.3041	0.029*
C14	0.066 (2)	0.3002 (9)	0.3228 (3)	0.026 (2)
H14A	0.2163	0.3448	0.3106	0.032*
H14B	0.1401	0.2671	0.3515	0.032*
C15	−0.048 (2)	0.2544 (9)	0.2446 (3)	0.027 (2)
H15A	0.1210	0.2943	0.2364	0.033*
H15B	−0.2051	0.3067	0.2433	0.033*
C16	−0.108 (2)	0.1619 (9)	0.2110 (3)	0.027 (2)
H16A	−0.2797	0.1231	0.2187	0.032*
H16B	−0.1397	0.1928	0.1802	0.032*
C17	0.157 (2)	0.0414 (9)	0.2558 (3)	0.030 (2)
H17A	0.3140	−0.0111	0.2563	0.035*
H17B	−0.0115	0.0010	0.2636	0.035*
C18	0.220 (2)	0.1316 (9)	0.2909 (3)	0.026 (2)
H18A	0.2460	0.0984	0.3214	0.032*
H18B	0.3955	0.1692	0.2841	0.032*
N1	−0.2339 (17)	0.3725 (7)	0.5236 (3)	0.0200 (18)
H1	−0.3660	0.4217	0.5258	0.024*
N2	0.0005 (18)	0.4218 (7)	0.4110 (2)	0.0220 (19)
H2	0.1733	0.4002	0.4167	0.026*
N3	−0.0063 (17)	0.2115 (7)	0.2905 (2)	0.0220 (19)
O1	−0.4206 (13)	0.4529 (6)	0.4399 (2)	0.0213 (15)
O2	0.1154 (15)	0.0870 (6)	0.2116 (2)	0.0261 (17)
Cl1	0.2751 (6)	0.0473 (2)	0.64686 (9)	0.0329 (7)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.031 (6)	0.020 (6)	0.030 (6)	−0.001 (5)	−0.008 (5)	0.003 (5)
C2	0.032 (6)	0.029 (6)	0.011 (4)	0.001 (5)	0.002 (4)	−0.001 (4)
C3	0.021 (5)	0.022 (6)	0.026 (5)	−0.002 (4)	0.007 (4)	−0.010 (4)
C4	0.027 (6)	0.019 (5)	0.021 (5)	−0.010 (4)	0.001 (4)	0.000 (4)
C5	0.023 (5)	0.025 (6)	0.017 (5)	−0.005 (4)	0.000 (4)	−0.002 (4)
C6	0.035 (6)	0.024 (6)	0.020 (5)	−0.001 (5)	0.001 (4)	0.001 (4)
C7	0.026 (5)	0.008 (5)	0.013 (4)	−0.006 (4)	0.003 (4)	−0.005 (3)
C8	0.025 (5)	0.020 (5)	0.019 (5)	−0.004 (4)	0.006 (4)	−0.005 (4)
C9	0.038 (6)	0.015 (5)	0.015 (4)	0.002 (4)	0.000 (4)	0.000 (4)
C10	0.050 (8)	0.033 (7)	0.042 (7)	−0.003 (6)	0.016 (6)	−0.015 (6)
C11	0.027 (6)	0.011 (5)	0.014 (4)	0.002 (4)	−0.005 (4)	−0.005 (4)
C12	0.029 (5)	0.016 (5)	0.017 (5)	0.007 (4)	0.005 (4)	0.003 (4)
C13	0.029 (6)	0.022 (6)	0.021 (5)	0.005 (5)	−0.004 (4)	−0.002 (4)
C14	0.037 (6)	0.029 (6)	0.012 (4)	0.002 (5)	0.000 (4)	−0.006 (4)

C15	0.034 (6)	0.027 (6)	0.021 (5)	−0.003 (5)	0.003 (4)	0.004 (4)
C16	0.033 (6)	0.031 (6)	0.016 (5)	0.008 (5)	0.000 (4)	0.000 (4)
C17	0.041 (7)	0.014 (5)	0.034 (6)	0.002 (5)	0.003 (5)	−0.001 (5)
C18	0.025 (6)	0.027 (6)	0.027 (5)	0.011 (5)	0.002 (4)	0.009 (5)
N1	0.020 (4)	0.017 (4)	0.024 (4)	0.008 (4)	0.006 (3)	0.002 (3)
N2	0.028 (5)	0.026 (5)	0.011 (4)	0.005 (4)	−0.003 (3)	−0.004 (3)
N3	0.031 (5)	0.024 (5)	0.011 (4)	0.005 (4)	0.000 (3)	−0.004 (3)
O1	0.019 (4)	0.023 (4)	0.021 (3)	0.002 (3)	0.000 (3)	0.000 (3)
O2	0.038 (4)	0.022 (4)	0.019 (3)	0.003 (3)	0.005 (3)	−0.004 (3)
Cl1	0.0442 (16)	0.0303 (15)	0.0239 (12)	0.0014 (13)	−0.0005 (11)	0.0092 (12)

Geometric parameters (Å, °)

C1—C6	1.375 (14)	C12—C13	1.516 (14)
C1—C2	1.377 (15)	C12—H12A	0.9900
C1—Cl1	1.763 (10)	C12—H12B	0.9900
C2—C3	1.412 (14)	C13—C14	1.494 (14)
C2—H2A	0.9500	C13—H13A	0.9900
C3—C4	1.385 (13)	C13—H13B	0.9900
C3—H3	0.9500	C14—N3	1.472 (12)
C4—N1	1.374 (12)	C14—H14A	0.9900
C4—C5	1.432 (14)	C14—H14B	0.9900
C5—C6	1.381 (14)	C15—N3	1.456 (12)
C5—C7	1.434 (12)	C15—C16	1.522 (14)
C6—H6	0.9500	C15—H15A	0.9900
C7—C8	1.376 (14)	C15—H15B	0.9900
C7—C9	1.499 (13)	C16—O2	1.413 (12)
C8—N1	1.397 (12)	C16—H16A	0.9900
C8—C11	1.487 (13)	C16—H16B	0.9900
C9—C10	1.487 (15)	C17—O2	1.425 (12)
C9—H9A	0.9900	C17—C18	1.531 (15)
C9—H9B	0.9900	C17—H17A	0.9900
C10—H10A	0.9800	C17—H17B	0.9900
C10—H10B	0.9800	C18—N3	1.463 (12)
C10—H10C	0.9800	C18—H18A	0.9900
C11—O1	1.253 (11)	C18—H18B	0.9900
C11—N2	1.333 (12)	N1—H1	0.8800
C12—N2	1.455 (11)	N2—H2	0.8800
C6—C1—C2	123.8 (10)	C14—C13—H13A	109.1
C6—C1—Cl1	119.0 (9)	C12—C13—H13A	109.1
C2—C1—Cl1	117.1 (8)	C14—C13—H13B	109.1
C1—C2—C3	119.3 (9)	C12—C13—H13B	109.1
C1—C2—H2A	120.4	H13A—C13—H13B	107.9
C3—C2—H2A	120.4	N3—C14—C13	114.8 (8)
C4—C3—C2	117.1 (9)	N3—C14—H14A	108.6
C4—C3—H3	121.5	C13—C14—H14A	108.6
C2—C3—H3	121.5	N3—C14—H14B	108.6
N1—C4—C3	130.0 (10)	C13—C14—H14B	108.6
N1—C4—C5	107.0 (8)	H14A—C14—H14B	107.6

C3—C4—C5	122.9 (9)	N3—C15—C16	110.7 (9)
C6—C5—C4	118.1 (9)	N3—C15—H15A	109.5
C6—C5—C7	134.5 (10)	C16—C15—H15A	109.5
C4—C5—C7	107.5 (8)	N3—C15—H15B	109.5
C1—C6—C5	118.8 (10)	C16—C15—H15B	109.5
C1—C6—H6	120.6	H15A—C15—H15B	108.1
C5—C6—H6	120.6	O2—C16—C15	110.7 (8)
C8—C7—C5	106.7 (8)	O2—C16—H16A	109.5
C8—C7—C9	130.0 (8)	C15—C16—H16A	109.5
C5—C7—C9	122.6 (8)	O2—C16—H16B	109.5
C7—C8—N1	109.5 (8)	C15—C16—H16B	109.5
C7—C8—C11	133.7 (9)	H16A—C16—H16B	108.1
N1—C8—C11	116.4 (8)	O2—C17—C18	110.8 (8)
C10—C9—C7	113.4 (9)	O2—C17—H17A	109.5
C10—C9—H9A	108.9	C18—C17—H17A	109.5
C7—C9—H9A	108.9	O2—C17—H17B	109.5
C10—C9—H9B	108.9	C18—C17—H17B	109.5
C7—C9—H9B	108.9	H17A—C17—H17B	108.1
H9A—C9—H9B	107.7	N3—C18—C17	110.6 (8)
C9—C10—H10A	109.5	N3—C18—H18A	109.5
C9—C10—H10B	109.5	C17—C18—H18A	109.5
H10A—C10—H10B	109.5	N3—C18—H18B	109.5
C9—C10—H10C	109.5	C17—C18—H18B	109.5
H10A—C10—H10C	109.5	H18A—C18—H18B	108.1
H10B—C10—H10C	109.5	C4—N1—C8	109.3 (8)
O1—C11—N2	123.4 (8)	C4—N1—H1	125.4
O1—C11—C8	119.7 (9)	C8—N1—H1	125.4
N2—C11—C8	116.8 (8)	C11—N2—C12	121.7 (8)
N2—C12—C13	113.2 (8)	C11—N2—H2	119.2
N2—C12—H12A	108.9	C12—N2—H2	119.2
C13—C12—H12A	108.9	C15—N3—C18	108.1 (8)
N2—C12—H12B	108.9	C15—N3—C14	110.8 (8)
C13—C12—H12B	108.9	C18—N3—C14	109.5 (8)
H12A—C12—H12B	107.8	C16—O2—C17	109.4 (7)
C14—C13—C12	112.4 (8)		

C6—C1—C2—C3	1.1 (17)	C7—C8—C11—O1	150.4 (11)
Cl1—C1—C2—C3	178.9 (8)	N1—C8—C11—O1	−20.9 (13)
C1—C2—C3—C4	0.3 (15)	C7—C8—C11—N2	−26.3 (16)
C2—C3—C4—N1	179.5 (10)	N1—C8—C11—N2	162.4 (9)
C2—C3—C4—C5	−1.8 (15)	N2—C12—C13—C14	−65.2 (11)
N1—C4—C5—C6	−179.3 (9)	C12—C13—C14—N3	179.8 (8)
C3—C4—C5—C6	1.8 (15)	N3—C15—C16—O2	−60.3 (11)
N1—C4—C5—C7	−0.5 (11)	O2—C17—C18—N3	58.3 (11)
C3—C4—C5—C7	−179.5 (9)	C3—C4—N1—C8	178.9 (10)
C2—C1—C6—C5	−1.1 (17)	C5—C4—N1—C8	0.0 (11)
Cl1—C1—C6—C5	−178.9 (8)	C7—C8—N1—C4	0.5 (11)
C4—C5—C6—C1	−0.3 (15)	C11—C8—N1—C4	173.8 (8)
C7—C5—C6—C1	−178.7 (11)	O1—C11—N2—C12	−6.7 (14)
C6—C5—C7—C8	179.2 (11)	C8—C11—N2—C12	169.9 (8)

C4—C5—C7—C8	0.7 (11)	C13—C12—N2—C11	−94.2 (11)
C6—C5—C7—C9	7.3 (18)	C16—C15—N3—C18	57.2 (11)
C4—C5—C7—C9	−171.2 (9)	C16—C15—N3—C14	177.2 (9)
C5—C7—C8—N1	−0.7 (11)	C17—C18—N3—C15	−56.3 (11)
C9—C7—C8—N1	170.4 (9)	C17—C18—N3—C14	−177.1 (8)
C5—C7—C8—C11	−172.5 (11)	C13—C14—N3—C15	73.0 (11)
C9—C7—C8—C11	−1.4 (18)	C13—C14—N3—C18	−167.9 (9)
C8—C7—C9—C10	−91.6 (13)	C15—C16—O2—C17	60.0 (11)
C5—C7—C9—C10	78.3 (12)	C18—C17—O2—C16	−59.2 (11)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O1^{i}	0.88	2.13	2.945 (10)	153
N2—H2···O1^{ii}	0.88	2.13	2.895 (10)	144

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

Fig. 1

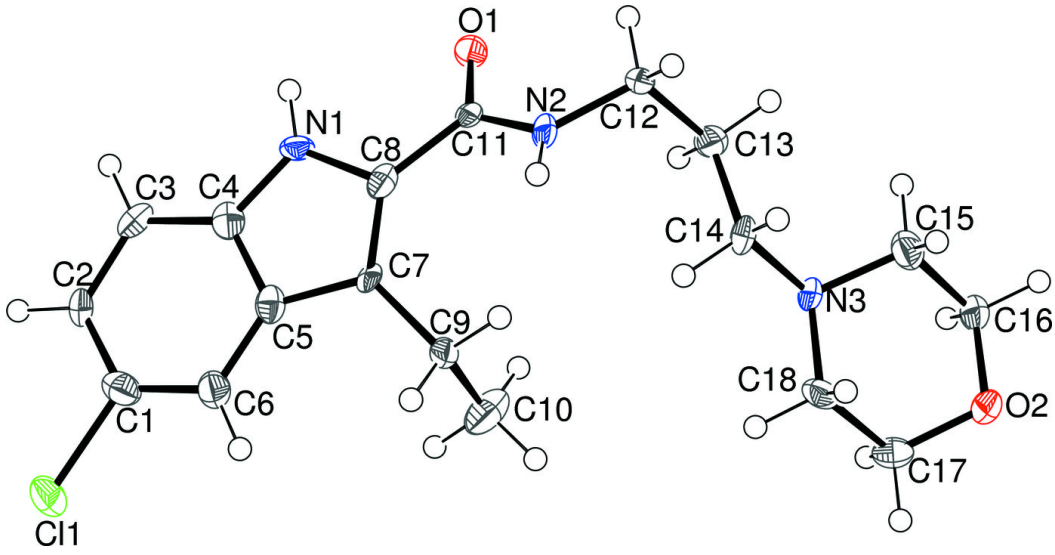
O1
N1
C8
C11
N2
C12
C13
C3
C4
C14
C15
C2
C7
N3
C16
C5
C9
C18
O2
C6
C10
C1
C17
Cl1

Fig. 2