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3-[(*E*)-Benzylidene]indolin-2-one

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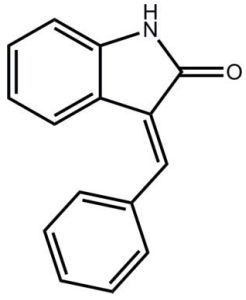
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.002 Å; R factor = 0.038; wR factor = 0.107; data-to-parameter ratio = 15.6.

In the title indolin-2-one derivative, $C_{15}H_{11}NO$, the phenyl ring and the oxoindoline fused-ring system (r.m.s. deviation = 0.011 Å) are aligned at 48.52 (6)°. In the crystal, inversion-related molecules form an N—H···O hydrogen-bonded dimer *via* an eight-membered $\{\cdots HNCO\}_2$ synthon. The dimeric aggregates are linked into a three-dimensional architecture *via* C—H···O and π–π interactions between the five- and six-membered rings of the fused ring system, with an inter-centroid distance of 3.4538 (8) Å.

Related literature

For the structure of the *Z*-isomer of the title compound, see: Milanesio *et al.* (2000). For background to related thiazoles, see: Badahdaha *et al.* (2009).



Experimental

Crystal data

$C_{15}H_{11}NO$
M_r = 221.25
Monoclinic, $P2_1/n$
a = 3.9796 (3) Å
b = 22.2266 (19) Å
c = 12.2484 (10) Å
β = 95.027 (1)°
V = 1079.24 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
6831 measured reflections
2460 independent reflections
2153 reflections with $I > 2\sigma(I)$
R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.107
S = 1.03
2460 reflections
158 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.87 (1)	1.98 (1)	2.846 (1)	172 (2)
C13—H13···O1^{ii}	0.95	2.57	3.2535 (15)	129

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); 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: MW2072).

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supplementary materials

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3-[(*E*)-Benzylidene]indolin-2-one

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Comment

The title compound (I) was isolated as a side-product in the attempted synthesis of thiazole derivatives (Badahdaha *et al.*, 2009) of interest owing to putative biological activity. The indolin-2-onyl fused-ring in (I), Fig. 1, is planar with the r.m.s. deviation being 0.011 Å; the O1 and C9 atoms lie -0.016 (1) and 0.089 (1) Å out of the plane, respectively. The phenyl group is twisted out of this plane, forming a dihedral angle of 48.52 (6)°. The conformation about the C7═C9 bond [1.3439 (16) Å] is *E*; the structure of the *Z*-isomer is known (Milanesio *et al.*, 2000).

In the crystal packing, inversion related molecules are connected into a dimer *via* N—H···O hydrogen bonds, Fig. 2 and Table 1. Molecules are linked into undulating layers in the *bc* plane *via* C—H···O interactions, Table 1, and are linked along the *a* axis *via* *π*–*π* interactions occurring between the five- and six-membered rings of the indolin-2-onyl fused ring system [ring centroid(N1,C1, C6–C7)···centroid(C1–C6)^{i} = 3.4538 (8) Å, angle of inclination = 1.15 (6)° for i: -1 + *x*, *y*, *z*], Fig. 3.

Experimental

The title compound, an unexpected product, was isolated as a side-product from a reaction between 2-(4-nitrobenzylidene)hydrazinecarbothioamide, triethylamine and *N*-phenyl-2-oxopropanehydrazonoyl chloride in ethanol solution; m.p. 512 K.

Refinement

Carbon-bound H atoms were placed in calculated positions [C—H = 0.95 Å, U_{iso}(H) = 1.2U_{eq}(C)] and were included in the refinement in the riding model approximation. The N-bound H atom was located in a difference Fourier map and was refined with a distance restraint of N—H = 0.86 (1) Å; the U_{iso} value was refined.

Computing details

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT* (Bruker, 2009); 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).

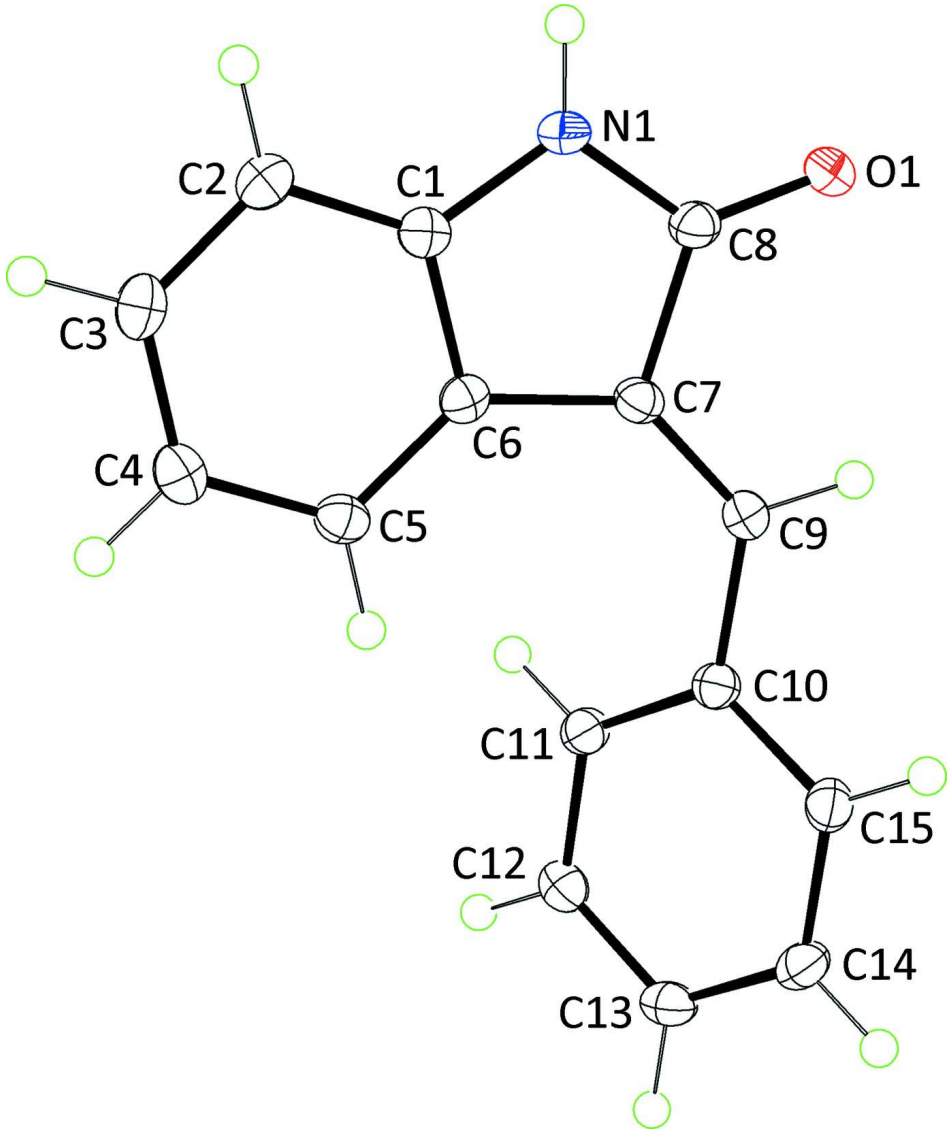

Figure 1

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

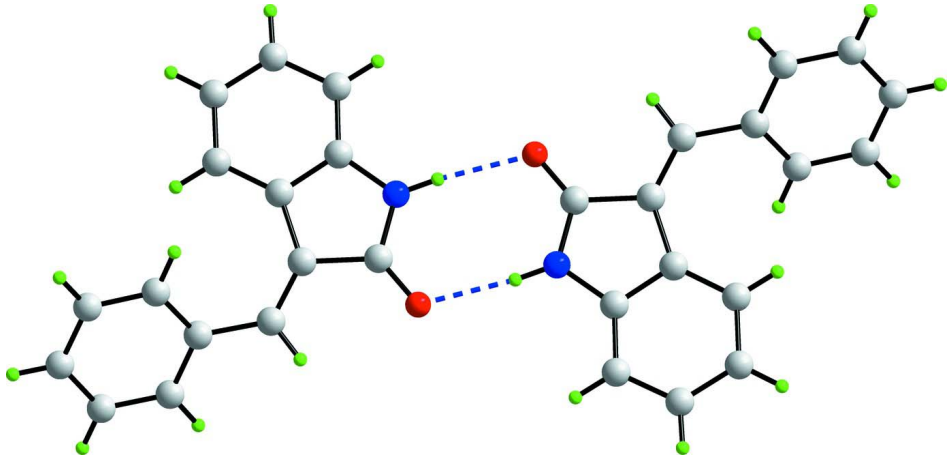

Figure 2

A view of the centrosymmetric dimer in (I) mediated by N—H···O hydrogen bonds shown as blue dashed lines.

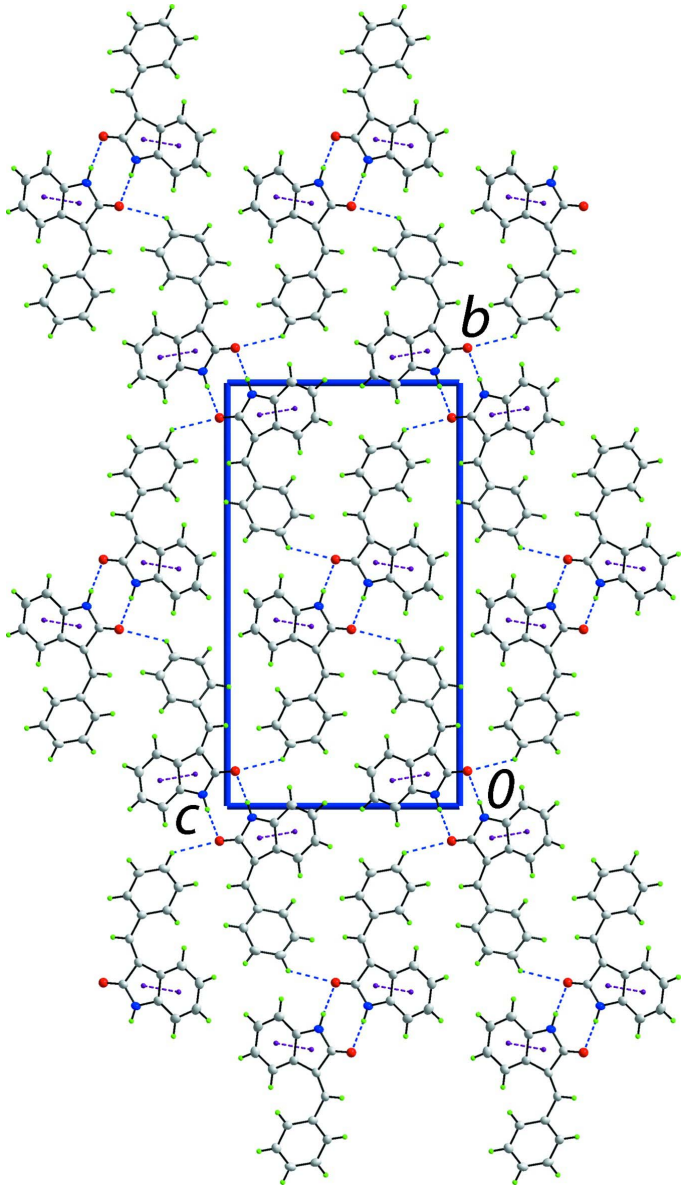

Figure 3

A view in projection down the *a* axis of the unit-cell contents of (I), the direction of the stacking of supramolecular layers. The N—H···O, C—H···O and π—π interactions are shown as blue, orange and purple dashed lines, respectively.

3-[(*E*)-Benzylidene]indolin-2-one

Crystal data

$C_{15}H_{11}NO$
M_r = 221.25
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 3.9796 (3) Å
b = 22.2266 (19) Å
c = 12.2484 (10) Å
β = 95.027 (1)°
V = 1079.24 (15) Å^3
Z = 4
F(000) = 464
D_x = 1.362 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3166 reflections
θ = 2.5–28.3°
μ = 0.09 mm^{-1}

T = 100 K
Prism, orange

0.30 × 0.20 × 0.10 mm

Data collection

Bruker SMART APEX diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
6831 measured reflections
2460 independent reflections

2153 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 27.5°, θ_{min} = 1.8°
h = −3→5
k = −28→28
l = −15→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.107
S = 1.03
2460 reflections
158 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
$w = 1/[\sigma^2(F_o^2) + (0.0633P)^2 + 0.2809P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	y	z	U_{iso}*/U_{eq}
O1	0.5372 (2)	0.58258 (4)	0.53379 (7)	0.0236 (2)
N1	0.7366 (3)	0.52725 (4)	0.39388 (8)	0.0183 (2)
H1N	0.668 (4)	0.4920 (5)	0.4133 (12)	0.032 (4)*
C1	0.8893 (3)	0.53924 (5)	0.29780 (9)	0.0167 (2)
C2	0.9905 (3)	0.49792 (5)	0.22291 (10)	0.0194 (3)
H2	0.9556	0.4560	0.2321	0.023*
C3	1.1456 (3)	0.52014 (6)	0.13341 (10)	0.0211 (3)
H3	1.2194	0.4929	0.0808	0.025*
C4	1.1938 (3)	0.58149 (6)	0.11990 (10)	0.0207 (3)
H4	1.2987	0.5956	0.0580	0.025*
C5	1.0897 (3)	0.62256 (5)	0.19619 (9)	0.0184 (2)
H5	1.1241	0.6645	0.1866	0.022*
C6	0.9350 (3)	0.60162 (5)	0.28646 (9)	0.0159 (2)
C7	0.8052 (3)	0.62991 (5)	0.38267 (9)	0.0167 (2)
C8	0.6761 (3)	0.57888 (5)	0.44818 (9)	0.0180 (3)
C9	0.7925 (3)	0.68631 (5)	0.42166 (9)	0.0176 (2)
H9	0.7175	0.6901	0.4929	0.021*
C10	0.8793 (3)	0.74284 (5)	0.36866 (9)	0.0167 (2)
C11	0.7759 (3)	0.75418 (5)	0.25856 (9)	0.0179 (2)
H11	0.6540	0.7243	0.2161	0.021*
C12	0.8496 (3)	0.80862 (5)	0.21070 (10)	0.0194 (3)
H12	0.7756	0.8160	0.1360	0.023*
C13	1.0311 (3)	0.85235 (5)	0.27155 (10)	0.0199 (3)
H13	1.0862	0.8892	0.2382	0.024*

C14	1.1317 (3)	0.84202 (5)	0.38124 (10)	0.0203 (3)
H14	1.2557	0.8719	0.4231	0.024*
C15	1.0516 (3)	0.78813 (5)	0.43000 (9)	0.0191 (3)
H15	1.1145	0.7819	0.5058	0.023*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0347 (5)	0.0183 (4)	0.0189 (4)	−0.0028 (4)	0.0088 (4)	0.0011 (3)
N1	0.0234 (5)	0.0130 (5)	0.0186 (5)	−0.0015 (4)	0.0024 (4)	0.0020 (4)
C1	0.0150 (5)	0.0178 (6)	0.0167 (5)	0.0001 (4)	−0.0015 (4)	0.0013 (4)
C2	0.0178 (5)	0.0177 (6)	0.0222 (6)	0.0018 (4)	−0.0010 (4)	−0.0010 (4)
C3	0.0191 (5)	0.0246 (6)	0.0193 (6)	0.0039 (5)	0.0001 (4)	−0.0044 (5)
C4	0.0179 (5)	0.0265 (6)	0.0179 (6)	0.0008 (5)	0.0019 (4)	0.0008 (5)
C5	0.0164 (5)	0.0190 (6)	0.0196 (6)	−0.0018 (4)	0.0008 (4)	0.0016 (4)
C6	0.0146 (5)	0.0163 (5)	0.0163 (5)	−0.0004 (4)	−0.0017 (4)	−0.0002 (4)
C7	0.0177 (5)	0.0170 (6)	0.0153 (5)	−0.0017 (4)	0.0004 (4)	0.0025 (4)
C8	0.0209 (6)	0.0157 (6)	0.0171 (5)	−0.0015 (4)	−0.0006 (4)	0.0016 (4)
C9	0.0200 (5)	0.0180 (6)	0.0148 (5)	−0.0005 (4)	0.0020 (4)	0.0006 (4)
C10	0.0172 (5)	0.0146 (5)	0.0188 (5)	0.0008 (4)	0.0046 (4)	−0.0005 (4)
C11	0.0183 (5)	0.0164 (5)	0.0189 (6)	−0.0009 (4)	0.0018 (4)	−0.0009 (4)
C12	0.0200 (6)	0.0202 (6)	0.0181 (5)	0.0015 (4)	0.0032 (4)	0.0022 (4)
C13	0.0196 (6)	0.0151 (5)	0.0255 (6)	−0.0002 (4)	0.0058 (4)	0.0028 (4)
C14	0.0214 (6)	0.0152 (5)	0.0244 (6)	−0.0020 (4)	0.0025 (4)	−0.0038 (4)
C15	0.0224 (6)	0.0182 (6)	0.0167 (5)	0.0015 (4)	0.0018 (4)	−0.0013 (4)

Geometric parameters (Å, º)

O1—C8	1.2302 (14)	C7—C9	1.3439 (16)
N1—C8	1.3585 (15)	C7—C8	1.5054 (15)
N1—C1	1.3968 (14)	C9—C10	1.4693 (15)
N1—H1N	0.87 (1)	C9—H9	0.9500
C1—C2	1.3825 (16)	C10—C11	1.3978 (16)
C1—C6	1.4068 (16)	C10—C15	1.3993 (16)
C2—C3	1.3946 (17)	C11—C12	1.3871 (16)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.3890 (18)	C12—C13	1.3884 (17)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.3950 (16)	C13—C14	1.3871 (17)
C4—H4	0.9500	C13—H13	0.9500
C5—C6	1.3919 (15)	C14—C15	1.3881 (16)
C5—H5	0.9500	C14—H14	0.9500
C6—C7	1.4689 (15)	C15—H15	0.9500
C8—N1—C1	111.10 (9)	O1—C8—N1	125.86 (10)
C8—N1—H1N	123.7 (11)	O1—C8—C7	127.13 (10)
C1—N1—H1N	124.9 (11)	N1—C8—C7	106.99 (10)
C2—C1—N1	127.28 (11)	C7—C9—C10	128.54 (10)
C2—C1—C6	122.79 (11)	C7—C9—H9	115.7
N1—C1—C6	109.93 (10)	C10—C9—H9	115.7

C1—C2—C3	117.44 (11)	C11—C10—C15	118.50 (10)
C1—C2—H2	121.3	C11—C10—C9	121.32 (10)
C3—C2—H2	121.3	C15—C10—C9	120.08 (10)
C4—C3—C2	121.10 (11)	C12—C11—C10	120.65 (11)
C4—C3—H3	119.4	C12—C11—H11	119.7
C2—C3—H3	119.4	C10—C11—H11	119.7
C3—C4—C5	120.69 (11)	C13—C12—C11	120.20 (11)
C3—C4—H4	119.7	C13—C12—H12	119.9
C5—C4—H4	119.7	C11—C12—H12	119.9
C4—C5—C6	119.42 (11)	C14—C13—C12	119.78 (11)
C4—C5—H5	120.3	C14—C13—H13	120.1
C6—C5—H5	120.3	C12—C13—H13	120.1
C5—C6—C1	118.55 (10)	C13—C14—C15	120.12 (11)
C5—C6—C7	134.85 (11)	C13—C14—H14	119.9
C1—C6—C7	106.56 (10)	C15—C14—H14	119.9
C9—C7—C6	135.33 (11)	C14—C15—C10	120.67 (11)
C9—C7—C8	119.22 (10)	C14—C15—H15	119.7
C6—C7—C8	105.40 (9)	C10—C15—H15	119.7

C8—N1—C1—C2	179.20 (11)	C1—N1—C8—C7	−0.80 (13)
C8—N1—C1—C6	0.09 (13)	C9—C7—C8—O1	4.54 (18)
N1—C1—C2—C3	−178.59 (11)	C6—C7—C8—O1	−177.79 (11)
C6—C1—C2—C3	0.41 (16)	C9—C7—C8—N1	−176.49 (10)
C1—C2—C3—C4	−0.48 (17)	C6—C7—C8—N1	1.18 (12)
C2—C3—C4—C5	0.40 (17)	C6—C7—C9—C10	8.2 (2)
C3—C4—C5—C6	−0.23 (17)	C8—C7—C9—C10	−175.00 (11)
C4—C5—C6—C1	0.15 (16)	C7—C9—C10—C11	43.93 (18)
C4—C5—C6—C7	177.75 (11)	C7—C9—C10—C15	−139.89 (13)
C2—C1—C6—C5	−0.25 (16)	C15—C10—C11—C12	1.47 (17)
N1—C1—C6—C5	178.91 (10)	C9—C10—C11—C12	177.71 (10)
C2—C1—C6—C7	−178.47 (10)	C10—C11—C12—C13	0.77 (17)
N1—C1—C6—C7	0.68 (12)	C11—C12—C13—C14	−1.57 (17)
C5—C6—C7—C9	−1.8 (2)	C12—C13—C14—C15	0.09 (18)
C1—C6—C7—C9	175.99 (13)	C13—C14—C15—C10	2.20 (18)
C5—C6—C7—C8	−178.91 (12)	C11—C10—C15—C14	−2.95 (17)
C1—C6—C7—C8	−1.11 (11)	C9—C10—C15—C14	−179.24 (10)
C1—N1—C8—O1	178.19 (11)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*···O1^{i}	0.87 (1)	1.98 (1)	2.846 (1)	172 (2)
C13—H13···O1^{ii}	0.95	2.57	3.2535 (15)	129

Symmetry codes: (i) −*x*+1, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+3/2, *z*−1/2.