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# 1-Benzyl-5-methylindoline-2,3-dione

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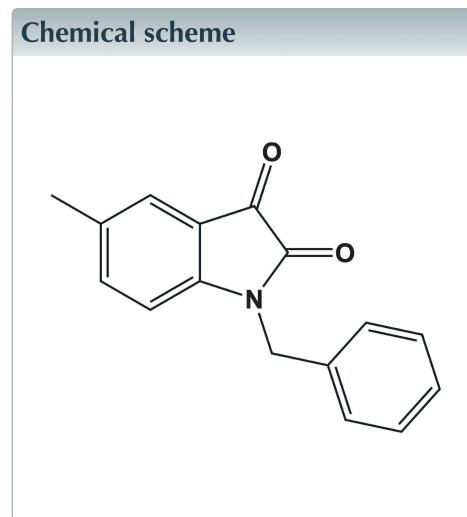
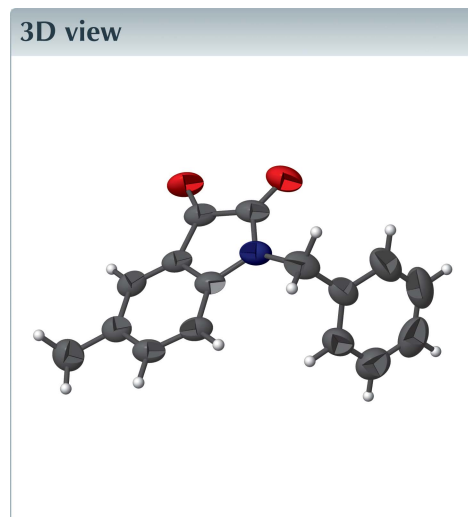
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Keywords: crystal structure; isatin; C—H...O hydrogen-bonding; C—H... $\pi$  interactions.

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Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

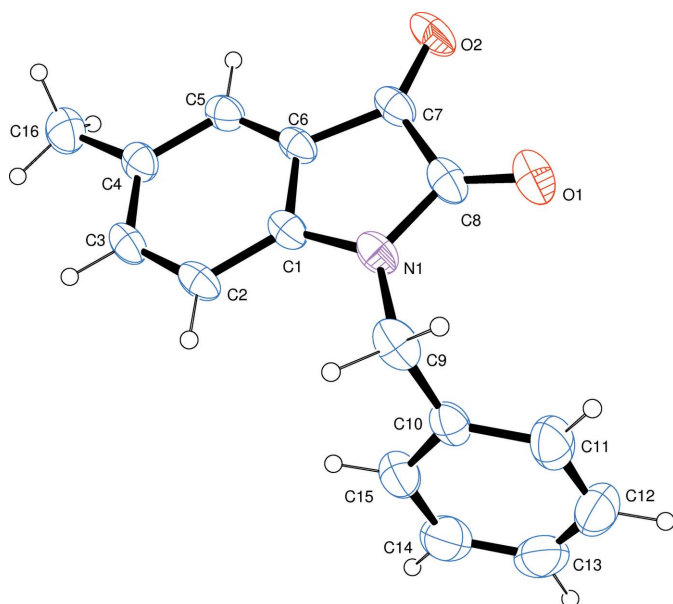
The title compound, C<sub>16</sub>H<sub>13</sub>NO<sub>2</sub>, is an isatin (indole-2,3-dione) derivative. The isatin moiety is almost planar with an r.m.s. deviation of 0.022 Å, and its mean plane makes a dihedral angle of 74.19 (12)° with the benzyl ring. In the crystal, molecules are linked by C—H...O hydrogen bonds, forming C(6) chains propagating along the *a*-axis direction. The chains are linked *via* C—H... $\pi$  interactions, forming slabs parallel to the *ab* plane. Within the slabs there are weak  $\pi$ – $\pi$  interactions present involving inversion-related isatin moieties.



## Structure description

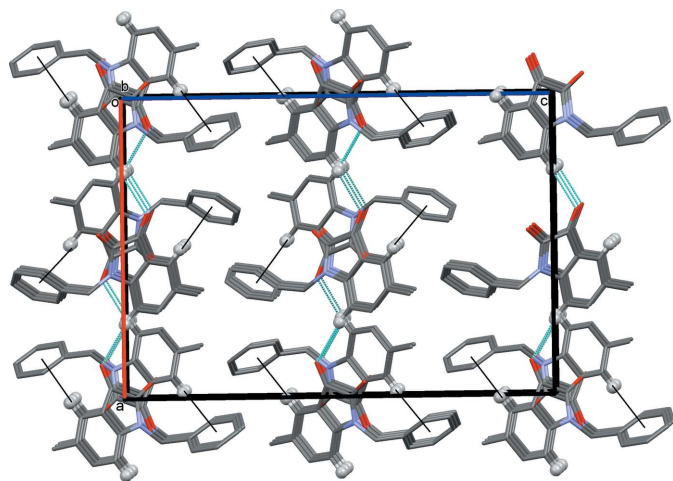
Isatins (indoline-2,3-diones) are an important family of heterocyclic compounds which are biologically active and of significant importance in medicinal chemistry. A variety of biological activities are associated with isatins including CNS (central nervous system) activities as potentiation of pentobarbitone induced necrosis. They also display analgesic, anticonvulsant, antidepressant, anti-inflammatory and antimicrobial effects on the central nervous system. Isatins are capable of crossing the blood–brain barrier (Bhriugu *et al.*, 2010; Fathimunnisa *et al.*, 2015; Gürsoy & Karali, 2003; Ilangovan & Satish, 2014; Mathur & Nain, 2014; Verma *et al.*, 2004). As part of our interest in the structural investigations of isatin derivatives, we report herein on the crystal structure determination and the geometry optimization of the title compound (I). Theoretical calculations of the molecular structure using MOPAC2012's PM7 geometry optimization algorithm (Stewart, 2012; Maia *et al.*, 2012) are in satisfactory agreement with the results of the X-ray crystal structure analysis.

The molecular structure of the title compound, (I), is illustrated in Fig. 1. In the isatin (indoline-2,3-dione) moiety, which is almost planar [r.m.s. deviation of 0.022 Å; maximum deviation of 0.036 (2) Å for atom C7]. Its mean plane makes a dihedral angle of 74.19 (12)° with the benzyl ring (C10–C15). This is similar to the values observed in



**Figure 1**  
The molecular structure of the title compound (I), showing the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

related structures, for example {1-benzyl-4,5,6-trimethoxyindoline-2,3-dione (II), [73.04 (7)°] and 1-benzyl-5-fluoroindoline-2,3-dione (III), [76.82 (11)°]} (Sharmila *et al.*, 2015). The superimposed fit (Gans & Shalloway, 2001) of the isatin group of the title compound (I) (atoms C1–C8, N1, O1 and O2) gives an r.m.s deviation of 0.065 Å with molecule (II) and 0.034 Å with molecule (III), while that with its energy-minimized counterpart gives 0.057 Å. The bond lengths and bond angles of the isatin moiety of compound (I) are also comparable with the values observed for related structures (Helliwell *et al.*, 2012; Lötter *et al.*, 2007). The sum of the angles around the N atom is 360°, indicating the absence of an *sp*<sup>3</sup> lone pair.



**Figure 2**  
Crystal packing of the title compound (I), viewed along the *b* axis, showing the C–H···O hydrogen bonds as dashed lines (see Table 1), and C–H··· $\pi$  interactions as black lines. H atoms not involved in these interactions have been omitted for clarity.

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

Cg3 is the centroid of the benzyl ring, C10–C15.

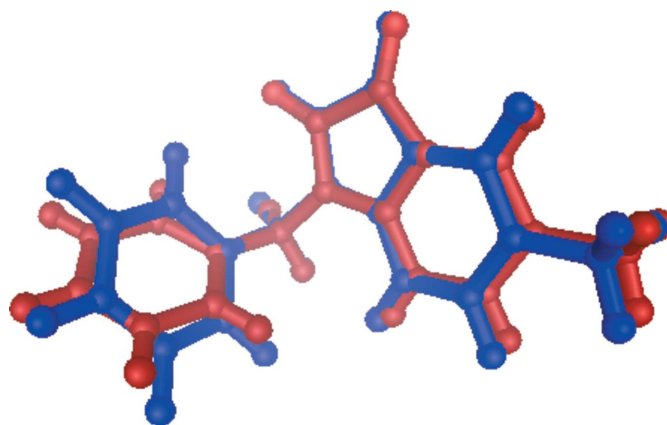
<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
C2–H2···O2 <sup>i</sup>	0.93	2.53	3.446 (3)	169
C5–H5···Cg3 <sup>ii</sup>	0.93	2.91	3.818 (3)	165

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

In the crystal, molecules are linked *via* C–H···O hydrogen bonds, forming chains propagating along the *a*-axis direction (Table 1 and Fig. 2). The chains are linked by C–H··· $\pi$  interactions, forming slabs lying parallel to the *ab* plane. Within the slabs there are weak slipped parallel  $\pi$ – $\pi$  interactions present involving inversion-related indoline ring systems [Cg1···Cg2<sup>i</sup> = 3.843 (1) Å, shortest inter-planar distance = 3.291 (1) Å, slippage 1.884 Å; Cg1 and Cg2 are the centroids of rings N1/C1/C6–C8 and C1–C6, respectively; symmetry code: (i)  $-x, -y + 1, -z + 1$ ].

A geometry optimization of (I) with Parameterized Model 7 computation was performed using MOPAC2012. Hartree–Fock closed-shell (restricted) wavefunctions were used for calculations. The HOMO and LUMO energy levels were found to be –8.962 and –1.158 eV, respectively. The total energy and dipole moment of the title molecule are –2916.87 eV and 5.244 Debye, respectively. When compared with the crystal structure, in the geometry optimized structure it is observed that the N1–C1 and N1–C8 bond lengths changed from 1.414 and 1.370 Å to 1.411 and 1.419 Å, respectively. The C8–N1–C1 and C8–N1–C9 bond angles decreased from 110.60 and 123.4°, respectively, to 110.12 and 122.27°, respectively.

The relative conformation about the bond joining the isatin moiety and the benzyl group of the structure is defined by the C1–N1–C9–C10 torsion angle. It shows an anti-clinal conformation [98.2 (3)°] in the crystal structure (I), but takes a *syn*-clinal conformation (72.38°) in the optimized structure. However, the torsion angle C8–N1–C9–C10 remained



**Figure 3**  
A superimposed fit of the title compound (red) and its energy-minimized counterpart (blue).

Table 2

Experimental details.

Crystal data	
Chemical formula	C <sub>16</sub> H <sub>13</sub> NO <sub>2</sub>
<i>M</i> <sub>r</sub>	251.27
Crystal system, space group	Orthorhombic, <i>Pbca</i>
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	14.6122 (15), 8.3882 (9), 20.911 (2)
<i>V</i> (Å <sup>3</sup> )	2563.1 (5)
<i>Z</i>	8
Radiation type	Mo <i>K</i> α
μ (mm <sup>-1</sup> )	0.09
Crystal size (mm)	0.35 × 0.30 × 0.25
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan ( <i>SADABS</i> ; Bruker, 2004)
<i>T</i> <sub>min</sub> , <i>T</i> <sub>max</sub>	0.970, 0.979
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	18203, 3091, 1652
<i>R</i> <sub>int</sub>	0.051
(sin θ/λ) <sub>max</sub> (Å <sup>-1</sup> )	0.666
Refinement	
<i>R</i> [ <i>F</i> <sup>2</sup> > 2σ( <i>F</i> <sup>2</sup> )], <i>wR</i> ( <i>F</i> <sup>2</sup> ), <i>S</i>	0.057, 0.164, 1.05
No. of reflections	3091
No. of parameters	173
H-atom treatment	H-atom parameters constrained
Δρ <sub>max</sub> , Δρ <sub>min</sub> (e Å <sup>-3</sup> )	0.19, -0.16

Computer programs: *APEX2* (Bruker, 2004), *SAINT* (Bruker, 2004), *XPREP* (Bruker, 2004), *SHELXS97* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *QMOL* (Gans & Shalloway, 2001), *Mercury* (Macrae *et al.*, 2008), *MOPAC* (Stewart, 2012), *WinGX* (Farrugia, 2012), *PLATON* (Spek, 2009).

almost the same, -81.4 (3) and -87.36°, respectively. A superimposed fit of (I) with its energy-minimized molecular structure gives an r.m.s. deviation of 0.473 Å (Fig. 3). This indicates a greater twist leading to further separation between the isatin moiety and the benzene ring. This suggests that the crystal packing is influenced by the collective effect of the intermolecular interactions.

### Synthesis and crystallization

To a mixture of benzyl-(2-ethynyl-4-methylphenyl)-amine (100 mg, 0.451 mmol) and I<sub>2</sub> (22.9 mg, 0.09 mmol), dimethyl sulfoxide (3 ml) was added at ambient temperature and the mixture was heated at 373 K for 5 h in air. Progress of the reaction was monitored by thin layer chromatography. Upon completion, the reaction mixture was allowed to cool to ambient temperature and quenched with aq. sodium thio-sulfate and ethyl acetate. The organic phase was separated, dried over Na<sub>2</sub>SO<sub>4</sub>, filtered and concentrated. The crude product was purified by silica gel column chromatography using hexane-ethyl acetate (9:1 *v/v*) as eluent. The title compound was obtained as a red solid (yield: 85%, 96.5 mg;

mp: 416–418 K). It was dissolved in an hexane-ethyl acetate mixture (9:1 *v/v*) and subjected to slow evaporation at room temperature (298 K), giving red block-like crystals after 2 d. Spectroscopic analysis: <sup>1</sup>H NMR (400 MHz, CDCl<sub>3</sub>, δ, p.p.m.): 7.44 (*s*, 1H), 7.39–7.29 (*m*, 6H), 6.68 (*d*, *J* = 8.0 Hz, 1H), 4.93 (*s*, 2H), 2.32 (*s*, 3H); <sup>13</sup>CNMR (100 MHz, CDCl<sub>3</sub>, δ, p.p.m.): 183.5, 158.4, 148.5, 138.7, 134.7, 133.7, 129.0, 128.1, 127.4, 125.7, 117.7, 110.8, 44.0, 20.6.

### Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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### References

- Bhrihu, B., Pathak, D., Siddiqui, N., Alam, M. S. & Ahsan, W. (2010). *Int. J. Pharm. Sci. Drug. Res.* **2**, 229–235.
- Bruker (2004). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
- Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
- Fathimunnisa, M., Manikandan, H., Selvanayagam, S. & Sridhar, B. (2015). *Acta Cryst.* **E71**, 915–918.
- Gans, J. & Shalloway, D. (2001). *J. Mol. Graphics Modell.* **19**, 557–559.
- Gürsoy, A. & Karali, N. (2003). *Eur. J. Med. Chem.* **38**, 633–643.
- Helliwell, M., Baradarani, M. M., Mohammadnejadghdam, R., Afghan, A. & Joule, J. A. (2012). *Acta Cryst.* **E68**, o233.
- Ilangoan, A. & Satish, G. (2014). *J. Org. Chem.* **79**, 4984–4991.
- Lötter, A. N. C., Fernandes, M. A., van Otterlo, W. A. L. & de Koning, C. B. (2007). *Acta Cryst.* **C63**, o157–o159.
- Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
- Maia, J. D. C., Carvalho, G. A. U., Manguiera, C. P. Jr, Santana, S. R., Cabral, L. A. F. & Rocha, G. B. (2012). *J. Chem. Theory Comput.* **8**, 3072–3081.
- Mathur, G. & Nain, S. (2014). *Med. Chem.* **4**, 417–427.
- Sharmila, N., Sundar, T. V., Satish, G., Ilangoan, A. & Venkatesan, P. (2015). *Acta Cryst.* **C71**, 975–978.
- Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
- Sheldrick, G. M. (2015). *Acta Cryst.* **C71**, 3–8.
- Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.
- Stewart, J. J. P. (2012). *Comput. Chem.* 66 Version 15.286W, web: <http://OpenMOPAC.net>.
- Verma, M., Pandeya, S. N., Singh, K. N. & Stables, J. P. (2004). *Acta Pharm.* **54**, 49–56.

## full crystallographic data

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## 1-Benzyl-5-methylindoline-2,3-dione

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## 1-Benzyl-5-methylindoline-2,3-dione

*Crystal data*

$C_{16}H_{13}NO_2$	$D_x = 1.302 \text{ Mg m}^{-3}$
$M_r = 251.27$	Melting point < 418 K
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$a = 14.6122 (15) \text{ \AA}$	Cell parameters from 2925 reflections
$b = 8.3882 (9) \text{ \AA}$	$\theta = 5.6\text{--}44.9^\circ$
$c = 20.911 (2) \text{ \AA}$	$\mu = 0.09 \text{ mm}^{-1}$
$V = 2563.1 (5) \text{ \AA}^3$	$T = 293 \text{ K}$
$Z = 8$	Block, red
$F(000) = 1056$	$0.35 \times 0.30 \times 0.25 \text{ mm}$

*Data collection*

Bruker Kappa APEXII CCD diffractometer	18203 measured reflections
Radiation source: fine-focus sealed tube	3091 independent reflections
Graphite monochromator	1652 reflections with $I > 2\sigma(I)$
$\omega$ and $\phi$ scan	$R_{\text{int}} = 0.051$
Absorption correction: multi-scan ( <i>SADABS</i> ; Bruker, 2004)	$\theta_{\text{max}} = 28.3^\circ$ , $\theta_{\text{min}} = 2.4^\circ$
$T_{\text{min}} = 0.970$ , $T_{\text{max}} = 0.979$	$h = -11 \rightarrow 18$
	$k = -11 \rightarrow 11$
	$l = -27 \rightarrow 27$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.057$	H-atom parameters constrained
$wR(F^2) = 0.164$	$w = 1/[\sigma^2(F_o^2) + (0.0579P)^2 + 0.8201P]$
$S = 1.05$	where $P = (F_o^2 + 2F_c^2)/3$
3091 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
173 parameters	$\Delta\rho_{\text{max}} = 0.19 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.16 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

*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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
N1	0.08992 (12)	0.2173 (2)	0.53228 (9)	0.0517 (5)
O1	-0.04615 (12)	0.0928 (2)	0.55743 (9)	0.0698 (5)
O2	-0.11076 (11)	0.2770 (2)	0.44577 (9)	0.0714 (5)
C1	0.11891 (14)	0.3272 (2)	0.48514 (11)	0.0454 (5)
C2	0.20581 (15)	0.3881 (3)	0.47456 (11)	0.0507 (6)
H2	0.2553	0.3570	0.4996	0.061*
C3	0.21631 (15)	0.4966 (3)	0.42539 (11)	0.0512 (6)
H3	0.2743	0.5383	0.4180	0.061*
C4	0.14499 (15)	0.5465 (3)	0.38655 (11)	0.0513 (6)
C5	0.05881 (15)	0.4812 (3)	0.39747 (11)	0.0509 (6)
H5	0.0096	0.5107	0.3719	0.061*
C6	0.04655 (13)	0.3728 (3)	0.44619 (11)	0.0462 (5)
C7	-0.03384 (15)	0.2825 (3)	0.46708 (11)	0.0522 (6)
C8	-0.00124 (16)	0.1836 (3)	0.52531 (12)	0.0545 (6)
C9	0.14700 (17)	0.1481 (3)	0.58222 (13)	0.0619 (7)
H9A	0.2105	0.1525	0.5689	0.074*
H9B	0.1307	0.0368	0.5877	0.074*
C10	0.13695 (15)	0.2328 (3)	0.64541 (12)	0.0555 (6)
C11	0.0863 (2)	0.1681 (4)	0.69456 (16)	0.0836 (9)
H11	0.0596	0.0684	0.6893	0.100*
C12	0.0745 (2)	0.2489 (6)	0.75132 (17)	0.1014 (12)
H12	0.0397	0.2038	0.7838	0.122*
C13	0.1143 (2)	0.3966 (6)	0.76008 (16)	0.0959 (11)
H13	0.1073	0.4502	0.7987	0.115*
C14	0.1636 (2)	0.4628 (4)	0.71219 (16)	0.0877 (9)
H14	0.1894	0.5633	0.7175	0.105*
C15	0.17557 (18)	0.3809 (4)	0.65538 (14)	0.0709 (8)
H15	0.2105	0.4267	0.6231	0.085*
C16	0.15996 (18)	0.6691 (3)	0.33497 (13)	0.0728 (8)
H16A	0.1522	0.6202	0.2938	0.109*
H16B	0.2208	0.7113	0.3384	0.109*
H16C	0.1164	0.7539	0.3398	0.109*

Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
N1	0.0366 (11)	0.0446 (11)	0.0739 (13)	0.0017 (8)	-0.0005 (8)	-0.0055 (10)
O1	0.0533 (11)	0.0584 (11)	0.0978 (14)	-0.0094 (9)	0.0173 (9)	-0.0061 (10)
O2	0.0309 (9)	0.0824 (13)	0.1009 (13)	-0.0079 (8)	-0.0058 (8)	-0.0110 (11)
C1	0.0340 (12)	0.0393 (12)	0.0629 (14)	0.0024 (9)	0.0021 (9)	-0.0144 (10)
C2	0.0306 (12)	0.0482 (13)	0.0732 (15)	0.0031 (9)	-0.0054 (10)	-0.0107 (12)
C3	0.0335 (12)	0.0478 (14)	0.0724 (16)	-0.0018 (10)	0.0057 (10)	-0.0117 (12)
C4	0.0403 (14)	0.0526 (15)	0.0609 (15)	0.0040 (10)	0.0061 (10)	-0.0112 (11)
C5	0.0347 (13)	0.0600 (16)	0.0580 (14)	0.0078 (10)	-0.0015 (9)	-0.0152 (12)
C6	0.0300 (11)	0.0466 (13)	0.0622 (14)	0.0011 (9)	0.0014 (9)	-0.0183 (11)

C7	0.0326 (12)	0.0508 (14)	0.0733 (15)	0.0013 (10)	0.0037 (10)	-0.0214 (12)
C8	0.0412 (14)	0.0425 (13)	0.0799 (16)	-0.0041 (10)	0.0109 (11)	-0.0168 (12)
C9	0.0467 (15)	0.0422 (14)	0.097 (2)	0.0067 (11)	-0.0007 (12)	0.0067 (13)
C10	0.0364 (13)	0.0557 (15)	0.0743 (17)	0.0056 (11)	-0.0050 (10)	0.0184 (13)
C11	0.069 (2)	0.088 (2)	0.094 (2)	-0.0067 (16)	-0.0008 (16)	0.038 (2)
C12	0.084 (2)	0.147 (4)	0.072 (2)	0.001 (2)	0.0058 (18)	0.039 (2)
C13	0.073 (2)	0.148 (4)	0.067 (2)	0.019 (2)	-0.0126 (16)	-0.003 (2)
C14	0.077 (2)	0.100 (3)	0.087 (2)	-0.0068 (18)	-0.0110 (17)	-0.009 (2)
C15	0.0583 (17)	0.076 (2)	0.0782 (19)	-0.0132 (14)	0.0028 (13)	0.0065 (16)
C16	0.0578 (18)	0.086 (2)	0.0751 (17)	0.0021 (14)	0.0087 (13)	0.0009 (16)

*Geometric parameters (Å, °)*

N1—C8	1.370 (3)	C9—C10	1.508 (4)
N1—C1	1.414 (3)	C9—H9A	0.9700
N1—C9	1.457 (3)	C9—H9B	0.9700
O1—C8	1.209 (3)	C10—C11	1.378 (4)
O2—C7	1.210 (3)	C10—C15	1.380 (4)
C1—C2	1.386 (3)	C11—C12	1.377 (5)
C1—C6	1.388 (3)	C11—H11	0.9300
C2—C3	1.382 (3)	C12—C13	1.381 (5)
C2—H2	0.9300	C12—H12	0.9300
C3—C4	1.386 (3)	C13—C14	1.353 (5)
C3—H3	0.9300	C13—H13	0.9300
C4—C5	1.392 (3)	C14—C15	1.384 (4)
C4—C16	1.506 (3)	C14—H14	0.9300
C5—C6	1.377 (3)	C15—H15	0.9300
C5—H5	0.9300	C16—H16A	0.9600
C6—C7	1.464 (3)	C16—H16B	0.9600
C7—C8	1.549 (3)	C16—H16C	0.9600
C8—N1—C1	110.60 (19)	C10—C9—H9A	109.1
C8—N1—C9	123.4 (2)	N1—C9—H9B	109.1
C1—N1—C9	126.00 (19)	C10—C9—H9B	109.1
C2—C1—C6	120.2 (2)	H9A—C9—H9B	107.8
C2—C1—N1	128.7 (2)	C11—C10—C15	117.5 (3)
C6—C1—N1	111.11 (19)	C11—C10—C9	121.4 (3)
C3—C2—C1	117.6 (2)	C15—C10—C9	121.1 (2)
C3—C2—H2	121.2	C12—C11—C10	121.1 (3)
C1—C2—H2	121.2	C12—C11—H11	119.5
C2—C3—C4	123.5 (2)	C10—C11—H11	119.5
C2—C3—H3	118.3	C11—C12—C13	120.2 (3)
C4—C3—H3	118.3	C11—C12—H12	119.9
C3—C4—C5	117.7 (2)	C13—C12—H12	119.9
C3—C4—C16	121.1 (2)	C14—C13—C12	119.6 (3)
C5—C4—C16	121.2 (2)	C14—C13—H13	120.2
C6—C5—C4	119.9 (2)	C12—C13—H13	120.2
C6—C5—H5	120.0	C13—C14—C15	119.9 (3)

C4—C5—H5	120.0	C13—C14—H14	120.0
C5—C6—C1	121.1 (2)	C15—C14—H14	120.0
C5—C6—C7	131.8 (2)	C10—C15—C14	121.7 (3)
C1—C6—C7	107.1 (2)	C10—C15—H15	119.2
O2—C7—C6	130.9 (2)	C14—C15—H15	119.2
O2—C7—C8	123.7 (2)	C4—C16—H16A	109.5
C6—C7—C8	105.36 (19)	C4—C16—H16B	109.5
O1—C8—N1	126.8 (2)	H16A—C16—H16B	109.5
O1—C8—C7	127.4 (2)	C4—C16—H16C	109.5
N1—C8—C7	105.78 (19)	H16A—C16—H16C	109.5
N1—C9—C10	112.60 (19)	H16B—C16—H16C	109.5
N1—C9—H9A	109.1		
C8—N1—C1—C2	-178.0 (2)	C1—N1—C8—O1	179.0 (2)
C9—N1—C1—C2	2.3 (3)	C9—N1—C8—O1	-1.3 (4)
C8—N1—C1—C6	1.5 (2)	C1—N1—C8—C7	0.2 (2)
C9—N1—C1—C6	-178.2 (2)	C9—N1—C8—C7	179.89 (19)
C6—C1—C2—C3	1.4 (3)	O2—C7—C8—O1	-1.6 (4)
N1—C1—C2—C3	-179.2 (2)	C6—C7—C8—O1	179.5 (2)
C1—C2—C3—C4	-0.2 (3)	O2—C7—C8—N1	177.2 (2)
C2—C3—C4—C5	-1.0 (3)	C6—C7—C8—N1	-1.7 (2)
C2—C3—C4—C16	178.1 (2)	C8—N1—C9—C10	-81.4 (3)
C3—C4—C5—C6	1.0 (3)	C1—N1—C9—C10	98.2 (3)
C16—C4—C5—C6	-178.1 (2)	N1—C9—C10—C11	103.5 (3)
C4—C5—C6—C1	0.2 (3)	N1—C9—C10—C15	-74.2 (3)
C4—C5—C6—C7	-177.8 (2)	C15—C10—C11—C12	0.2 (4)
C2—C1—C6—C5	-1.4 (3)	C9—C10—C11—C12	-177.5 (3)
N1—C1—C6—C5	179.02 (19)	C10—C11—C12—C13	-0.5 (5)
C2—C1—C6—C7	176.97 (19)	C11—C12—C13—C14	1.1 (5)
N1—C1—C6—C7	-2.6 (2)	C12—C13—C14—C15	-1.4 (5)
C5—C6—C7—O2	1.9 (4)	C11—C10—C15—C14	-0.5 (4)
C1—C6—C7—O2	-176.2 (2)	C9—C10—C15—C14	177.2 (2)
C5—C6—C7—C8	-179.3 (2)	C13—C14—C15—C10	1.2 (5)
C1—C6—C7—C8	2.6 (2)		

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

Cg3 is the centroid of the benzyl ring, C10–C15.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2—H2 $\cdots$ O2 <sup>i</sup>	0.93	2.53	3.446 (3)	169
C5—H5 $\cdots$ Cg3 <sup>ii</sup>	0.93	2.91	3.818 (3)	165

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