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4-Methyl-1-phenylquinolin-2(1*H*)-one

Petar Yotov Petrov,[a] Malinka Stoyanova[b] and Boris Shivachev[c]*

[a]Department of Organic Chemistry, Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria, [b]Institute of Organic Chemistry, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, Building 9, 1113 Sofia, Bulgaria, and [c]Bulgarian Academy of Sciences, Central Laboratory of Mineralogy and Crystallography, Acad G. Bonchev Street, Building 107, 1113 Sofia, Bulgaria
Correspondence e-mail: bls@clmc.bas.bg

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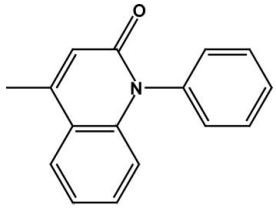
Key indicators: single-crystal X-ray study; T = 290 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.160; data-to-parameter ratio = 18.2.

In the title compound, $C_{16}H_{13}NO$, the molecules are connected three-dimensionally through non-classical C—H···O and C—H···π interactions of 3.272 (3), 3.380 (3) and 3.382 (4) Å. Classical hydrogen bonds are not observed. The dihedral angle between the benzyl and quinolin-2(1*H*)-one mean planes is 87.15 (7)°

Related literature

For related literature, see: Bondensgaard & Jacobsen (1999); Fürstenberg *et al.* (2006); Kovalska *et al.* (2006); Martínez & Chacón-García (2005); Perekalin & Lerner (1951); Rajnikant *et al.* (2002); Schenkel & Aeberli (1957); Shishkina *et al.* (2005); Staerk *et al.* (1997); Vasilev *et al.* (2005); Vincente *et al.* (2005); Zipper *et al.* (2004); Sheldrick & Morr (1981).



Experimental

Crystal data

$C_{16}H_{13}NO$
M_r = 235.27
Monoclinic, $P2_1/c$
a = 8.984 (2) Å
b = 14.194 (4) Å
c = 10.1785 (16) Å
β = 106.631 (15)°
V = 1243.7 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 290 (2) K
0.31 × 0.31 × 0.31 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: none
6212 measured reflections
2991 independent reflections
1351 reflections with $I > 2\sigma(I)$
R_{int} = 0.053
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.160
S = 0.97
2991 reflections
164 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

*Cg*1 is the centroid of the C11–C16 ring.

D—H···A	D—H	H···A	D···A	D—H···A
C14—H14···O1^{i}	1.13	2.37	3.272 (3)	135
C4—H4···O1^{ii}	1.09	2.63	3.380 (3)	125
C8—H8*A*···*Cg*1^{iii}	1.11	2.73	3.382 (4)	165

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997); *Mercury* (Bruno *et al.*, 2002); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PR2017).

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4-Methyl-1-phenylquinolin-2(1*H*)-one

Petar Yotov Petrov, Malinka Stoyanova and Boris Shivachev

S1. Comment

DNA intercalation is one of the interactions of nucleic acids with small organic molecules, through which effective antitumor agents can be designed (Martínez *et al.*, 2005). A relevant area of research is the finding of fluorescent markers for highly sensitive DNA detection (Staerk *et al.*, 1997; Bondensgaard *et al.*, 1999). For the latter application, few cyanine dyes containing quinoline end-groups are established (Zipper *et al.*, 2004), and new representatives with similar and even better efficiency were recently synthesized (Vasilev *et al.*, 2005; Kovalska *et al.*, 2006; Fürstenberg *et al.*, 2006). Herein, we report the structure of (I) which is an oxo-substituted fragment of these dyes – a long known molecule (Perekalin *et al.*, 1951).

In the unit cell of (I), only one independent molecule is present. The bond distances and angles in the benzyl and quinolin-2(1*H*)-one moieties are comparable to those observed in other quinolinone derivatives (Rajnikant *et al.*, 2002; Vincente *et al.*, 2005; Shishkina *et al.*, 2005). The molecule posses two nearly planar ring systems [r.m.s. deviation of 0.004 (5)Å and 0.021 (4) Å for the benzyl and quinolin-2(1*H*)-one fragments respectively] which are capable of intercalation, attached to each other in a conformationally fluxional way. The dihedral angle between the benzyl and quinolinone mean planes is 87.15 (7) °.

In the crystal structure of (I), the molecules are connected through non-classical C—H···O hydrogen bonds and CH_3-π interactions between methyl and benzyl fragments C8—H8A···*Cg*1^{i}; *Cg*1 is the centroid of the 1-Phenyl derivative [symmetry code (i): 1 - *x*, -1/2 + *y*, 3/2 - *z*]. The carbonyl O atom forms a bifurcated hydrogen bond. A head-to-tail C4—H4···O1^{i} [symmetry code (i): *x* - 1,*y*,*z*] interaction between quinolinone fragments build up straight chains along *a* axis. A side-to-side C14—H14···O1^{i} [symmetry code (i): 2 - *x*, 1/2 + *y*, 3/2 - *z*] interaction forms zigzag chains along b.

S2. Experimental

The title compound was synthesized by dehydro-cyclization (Perekalin *et al.*, 1951) of the respective acetoacetamide (Schenkel *et al.*, 1957). Crystals of (I) suitable for X-ray diffraction were obtained by slow evaporation from toluene.

S3. Refinement

All hydrogen atoms were located in a difference map and were constrained to ride on their parent atoms, with U_{iso}(H) = 1.5U_{eq}(C_{methyl}) and U_{iso}(H) = 1.2U_{eq}(C or N).

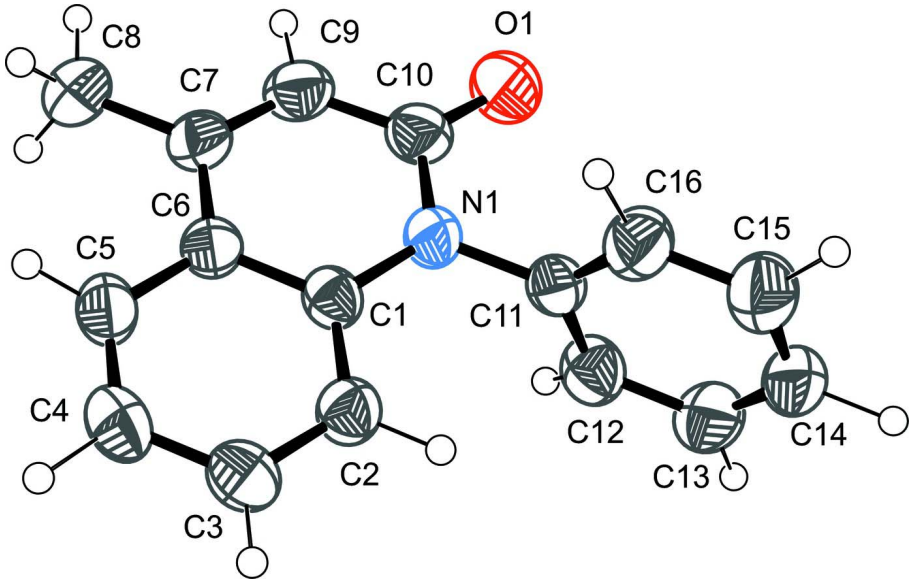

Figure 1

View of the structure and the atom-numbering scheme of (I) showing 50% probability displacement ellipsoids. H atoms are shown as small spheres of an arbitrary radii.

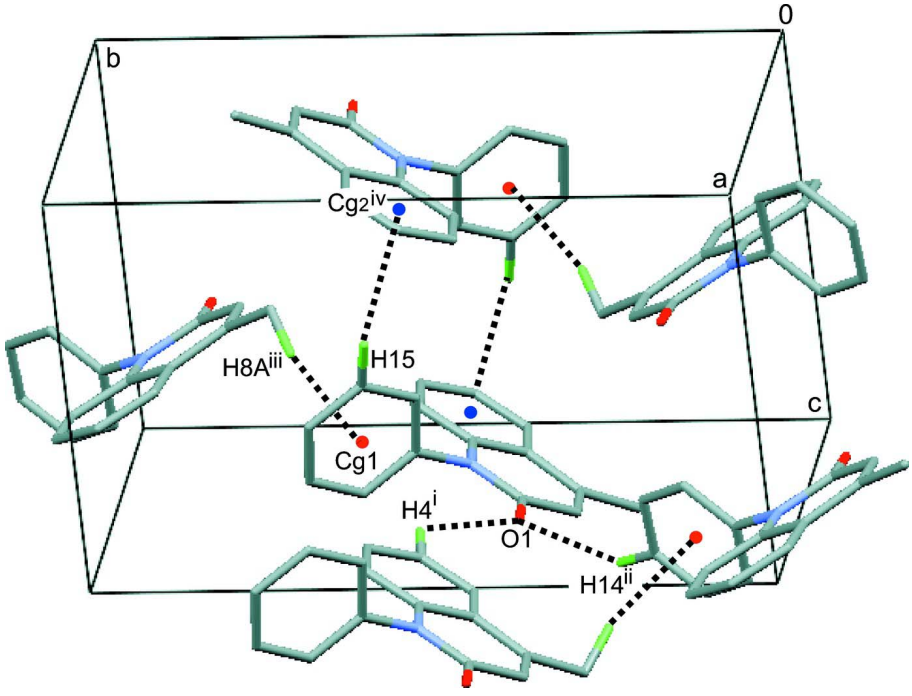

Figure 2

A view of the molecular packing in (I). All H atoms not involved in the short contact interactions have been omitted for clarity [symmetry codes: (i) 1 + *x*,*y*,*z*; (ii) 2 - *x*, -1/2 + *y*, 3/2 - *z*; (iii) 2 - *x*, -1/2 + *y*, 3/2 - *z*; (iv) 1 - *x*, 1 - *y*, 1 - *z*]. The dotted lines indicate the C—H···O and C—H···π interactions.

4-Methyl-1-phenylquinolin-2(1*H*)-one

Crystal data

$C_{16}H_{13}NO$
$M_r = 235.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 8.984\ (2)$ Å
$b = 14.194\ (4)$ Å
$c = 10.1785\ (16)$ Å
$\beta = 106.631\ (15)°$
$V = 1243.7\ (5)$ Å^3
$Z = 4$
$F(000) = 496$
$D_x = 1.256$ Mg m^{-3}
Melting point: not measured K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 22 reflections
$\theta = 18.2–19.3°$
$\mu = 0.08$ mm^{-1}
$T = 290$ K
Cubic, pale yellow
0.31 × 0.31 × 0.31 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
non–profiled $\omega/2\theta$ scans
6212 measured reflections
2991 independent reflections
1351 reflections with $I > 2\sigma(I)$
$R_{int} = 0.053$
$\theta_{max} = 28.0°$, $\theta_{min} = 2.4°$
$h = 0\rightarrow11$
$k = -18\rightarrow18$
$l = -13\rightarrow12$
3 standard reflections every 120 min
intensity decay: none

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.055$
$wR(F^2) = 0.160$
$S = 0.97$
2991 reflections
164 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0699P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
N1	0.7036 (2)	0.45463 (12)	0.80663 (18)	0.0468 (5)
C1	0.5505 (2)	0.46557 (16)	0.8116 (2)	0.0443 (5)
C6	0.4822 (3)	0.39507 (15)	0.8725 (2)	0.0448 (5)
O1	0.9282 (2)	0.37000 (13)	0.8539 (2)	0.0763 (6)

C2	0.4652 (3)	0.54564 (16)	0.7571 (2)	0.0500 (6)
H2	0.5194	0.5981	0.7165	0.060*
C11	0.7750 (2)	0.52552 (15)	0.7433 (2)	0.0461 (6)
C5	0.3277 (3)	0.40691 (18)	0.8733 (2)	0.0535 (6)
H5	0.2882	0.3524	0.9123	0.064*
C4	0.2438 (3)	0.48561 (19)	0.8192 (2)	0.0580 (7)
H4	0.1196	0.4968	0.8047	0.070*
C10	0.7938 (3)	0.37699 (17)	0.8615 (3)	0.0554 (6)
C9	0.7218 (3)	0.30818 (17)	0.9274 (2)	0.0580 (7)
H9	0.7825	0.2518	0.9753	0.070*
C3	0.3150 (3)	0.55537 (17)	0.7623 (2)	0.0570 (6)
H3	0.2571	0.6117	0.7295	0.068*
C7	0.5753 (3)	0.31498 (16)	0.9346 (2)	0.0519 (6)
C8	0.5092 (3)	0.24147 (17)	1.0075 (3)	0.0711 (8)
H8B	0.4706	0.2655	1.0736	0.107*
H8C	0.5783	0.1853	1.0437	0.107*
H8A	0.4026	0.2090	0.9385	0.107*
C16	0.7687 (3)	0.51761 (18)	0.6074 (3)	0.0632 (7)
H16	0.7009	0.4576	0.5534	0.076*
C13	0.9139 (3)	0.67027 (18)	0.7559 (3)	0.0639 (7)
H13	0.9747	0.7274	0.8167	0.077*
C14	0.9077 (3)	0.66239 (19)	0.6202 (3)	0.0627 (7)
H14	0.9663	0.7190	0.5738	0.075*
C12	0.8477 (3)	0.60141 (18)	0.8181 (3)	0.0586 (7)
H12	0.8565	0.5980	0.8999	0.070*
C15	0.8372 (3)	0.5863 (2)	0.5463 (3)	0.0730 (8)
H15	0.8372	0.5753	0.4416	0.109 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0390 (10)	0.0453 (11)	0.0582 (12)	0.0007 (9)	0.0173 (9)	0.0040 (9)
C1	0.0376 (12)	0.0499 (13)	0.0448 (13)	−0.0019 (10)	0.0110 (10)	−0.0053 (11)
C6	0.0473 (13)	0.0437 (13)	0.0441 (12)	−0.0056 (11)	0.0144 (10)	−0.0078 (10)
O1	0.0509 (11)	0.0703 (12)	0.1140 (16)	0.0136 (9)	0.0336 (11)	0.0111 (11)
C2	0.0456 (13)	0.0505 (14)	0.0537 (14)	0.0008 (11)	0.0138 (11)	0.0035 (11)
C11	0.0373 (11)	0.0462 (14)	0.0563 (14)	−0.0004 (10)	0.0154 (11)	−0.0018 (11)
C5	0.0496 (14)	0.0584 (15)	0.0568 (15)	−0.0079 (12)	0.0222 (12)	−0.0046 (12)
C4	0.0417 (13)	0.0720 (17)	0.0621 (16)	0.0004 (13)	0.0179 (12)	−0.0039 (14)
C10	0.0476 (14)	0.0510 (14)	0.0680 (16)	0.0056 (12)	0.0173 (12)	−0.0013 (12)
C9	0.0574 (15)	0.0450 (14)	0.0702 (17)	0.0051 (12)	0.0162 (13)	0.0018 (12)
C3	0.0446 (14)	0.0624 (16)	0.0616 (15)	0.0084 (12)	0.0115 (12)	0.0027 (13)
C7	0.0576 (15)	0.0430 (14)	0.0558 (14)	−0.0060 (12)	0.0176 (12)	−0.0063 (11)
C8	0.085 (2)	0.0497 (15)	0.0871 (19)	−0.0027 (14)	0.0388 (17)	0.0077 (14)
C16	0.0760 (18)	0.0561 (15)	0.0619 (17)	−0.0119 (14)	0.0268 (14)	−0.0051 (13)
C13	0.0516 (15)	0.0549 (15)	0.0838 (19)	−0.0149 (12)	0.0171 (14)	−0.0095 (14)
C14	0.0551 (15)	0.0554 (16)	0.084 (2)	−0.0032 (13)	0.0309 (14)	0.0065 (14)
C12	0.0526 (14)	0.0634 (16)	0.0614 (15)	−0.0088 (13)	0.0187 (12)	−0.0081 (13)

C15	0.093 (2)	0.0674 (18)	0.0687 (18)	−0.0083 (17)	0.0392 (17)	−0.0007 (15)

Geometric parameters (Å, º)

N1—C10	1.387 (3)	C9—C7	1.342 (3)
N1—C1	1.400 (3)	C9—H9	1.0118
N1—C11	1.441 (3)	C3—H3	0.9603
C1—C2	1.394 (3)	C7—C8	1.499 (3)
C1—C6	1.407 (3)	C8—H8B	0.9069
C6—C5	1.401 (3)	C8—H8C	1.0133
C6—C7	1.445 (3)	C8—H8A	1.1127
O1—C10	1.236 (3)	C16—C15	1.391 (4)
C2—C3	1.373 (3)	C16—H16	1.0983
C2—H2	1.0382	C13—C14	1.371 (3)
C11—C12	1.372 (3)	C13—C12	1.387 (3)
C11—C16	1.372 (3)	C13—H13	1.0707
C5—C4	1.372 (3)	C14—C15	1.364 (4)
C5—H5	0.9818	C14—H14	1.1348
C4—C3	1.392 (3)	C12—H12	0.8147
C4—H4	1.0949	C15—H15	1.0773
C10—C9	1.439 (3)		
C10—N1—C1	122.73 (19)	C2—C3—C4	121.2 (2)
C10—N1—C11	116.83 (18)	C2—C3—H3	120.7
C1—N1—C11	120.44 (18)	C4—C3—H3	118.0
C2—C1—N1	120.7 (2)	C9—C7—C6	119.1 (2)
C2—C1—C6	119.7 (2)	C9—C7—C8	120.7 (2)
N1—C1—C6	119.6 (2)	C6—C7—C8	120.2 (2)
C5—C6—C1	118.4 (2)	C7—C8—H8B	113.3
C5—C6—C7	122.8 (2)	C7—C8—H8C	116.1
C1—C6—C7	118.8 (2)	H8B—C8—H8C	110.5
C3—C2—C1	120.1 (2)	C7—C8—H8A	111.6
C3—C2—H2	121.5	H8B—C8—H8A	100.4
C1—C2—H2	118.4	H8C—C8—H8A	103.3
C12—C11—C16	120.0 (2)	C11—C16—C15	119.8 (2)
C12—C11—N1	120.1 (2)	C11—C16—H16	115.2
C16—C11—N1	119.9 (2)	C15—C16—H16	124.9
C4—C5—C6	121.8 (2)	C14—C13—C12	120.2 (2)
C4—C5—H5	125.7	C14—C13—H13	120.7
C6—C5—H5	112.4	C12—C13—H13	119.0
C5—C4—C3	118.8 (2)	C15—C14—C13	119.9 (2)
C5—C4—H4	126.5	C15—C14—H14	121.9
C3—C4—H4	114.3	C13—C14—H14	118.2
O1—C10—N1	120.5 (2)	C11—C12—C13	119.9 (2)
O1—C10—C9	123.6 (2)	C11—C12—H12	114.3
N1—C10—C9	116.0 (2)	C13—C12—H12	125.4
C7—C9—C10	123.7 (2)	C14—C15—C16	120.3 (3)
C7—C9—H9	115.6	C14—C15—H15	121.9

C10—C9—H9	120.6	C16—C15—H15	117.8
C10—N1—C1—C2	178.9 (2)	C11—N1—C10—C9	178.5 (2)
C11—N1—C1—C2	−0.8 (3)	O1—C10—C9—C7	−179.2 (2)
C10—N1—C1—C6	−1.0 (3)	N1—C10—C9—C7	1.6 (4)
C11—N1—C1—C6	179.3 (2)	C1—C2—C3—C4	−1.2 (4)
C2—C1—C6—C5	1.5 (3)	C5—C4—C3—C2	1.4 (4)
N1—C1—C6—C5	−178.6 (2)	C10—C9—C7—C6	0.5 (4)
C2—C1—C6—C7	−176.9 (2)	C10—C9—C7—C8	−178.7 (2)
N1—C1—C6—C7	3.0 (3)	C5—C6—C7—C9	178.9 (2)
N1—C1—C2—C3	179.8 (2)	C1—C6—C7—C9	−2.8 (3)
C6—C1—C2—C3	−0.3 (3)	C5—C6—C7—C8	−1.9 (3)
C10—N1—C11—C12	−93.2 (2)	C1—C6—C7—C8	176.4 (2)
C1—N1—C11—C12	86.6 (3)	C12—C11—C16—C15	0.5 (4)
C10—N1—C11—C16	87.5 (3)	N1—C11—C16—C15	179.7 (2)
C1—N1—C11—C16	−92.7 (3)	C12—C13—C14—C15	−0.4 (4)
C1—C6—C5—C4	−1.3 (3)	C16—C11—C12—C13	0.4 (4)
C7—C6—C5—C4	177.0 (2)	N1—C11—C12—C13	−178.9 (2)
C6—C5—C4—C3	−0.1 (4)	C14—C13—C12—C11	−0.4 (4)
C1—N1—C10—O1	179.5 (2)	C13—C14—C15—C16	1.3 (4)
C11—N1—C10—O1	−0.7 (3)	C11—C16—C15—C14	−1.3 (4)
C1—N1—C10—C9	−1.3 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C14—H14···O1^{i}	1.13	2.37	3.272 (3)	135
C4—H4···O1^{ii}	1.09	2.63	3.380 (3)	125
C8—H8*A*···*Cg*1^{iii}	1.11	2.73	3.382 (4)	165

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