

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

(E)-N'-[4-(Dimethylamino)benzylidene]-2-(4-methylphenoxy)acetohydrazideM. K. Usha,^a S. Madan Kumar,^a Nitinchandra,^b
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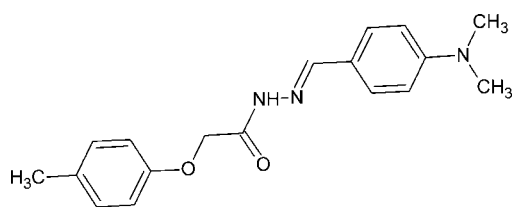
Received 9 December 2013; accepted 30 December 2013

Key indicators: single-crystal X-ray study; $T = 296$ K; mean $\sigma(\text{C}-\text{C}) = 0.003$ Å; R factor = 0.075; wR factor = 0.211; data-to-parameter ratio = 12.9.

In the title compound, $\text{C}_{18}\text{H}_{21}\text{N}_3\text{O}_2$, the dihedral angle between the benzene rings is 68.85 (11)°. In the crystal, the molecules are linked by $\text{C}-\text{H}\cdots\text{O}$ and $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds, as well as weak $\text{C}-\text{H}\cdots\pi$ contacts, forming a three-dimensional supramolecular architecture.

Related literature

For biological background to hydrazone derivatives, see: Nithinchandra *et al.* (2012, 2013); Holla *et al.* (1992); Kalluraya *et al.* (1995). For related structures, see: Sarfraz *et al.* (2010); Fun *et al.* (2011).



Experimental

Crystal data

$\text{C}_{18}\text{H}_{21}\text{N}_3\text{O}_2$
 $M_r = 311.38$
 Monoclinic, $P2_1/c$
 $a = 11.2237$ (6) Å
 $b = 9.4471$ (5) Å
 $c = 15.8785$ (9) Å
 $\beta = 100.868$ (3)°

$V = 1653.42$ (16) Å³
 $Z = 4$
 Cu $K\alpha$ radiation
 $\mu = 0.67$ mm⁻¹
 $T = 296$ K
 $0.23 \times 0.22 \times 0.21$ mm

Data collection

Bruker X8 Proteum diffractometer
 Absorption correction: multi-scan
 SADABS (Bruker, 2013)
 $T_{\min} = 0.862$, $T_{\max} = 0.873$
 13214 measured reflections
 2725 independent reflections
 2318 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.075$
 $wR(F^2) = 0.211$
 $S = 1.05$
 2725 reflections
 211 parameters
 H-atom parameters constrained
 $\Delta\rho_{\max} = 0.43$ e Å⁻³
 $\Delta\rho_{\min} = -0.43$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 and Cg2 are the centroids of the C2–C7 and C11–C16 rings, respectively.

D—H...A	D—H	H...A	D...A	D—H...A
N1—H1...O2 ⁱ	0.86	2.12	2.952 (2)	163
C8—H8B...O2 ⁱ	0.97	2.43	3.303 (2)	149
C8—H8A...Cg2 ⁱⁱ	0.97	2.65	3.442 (2)	139
C16—H16...Cg1 ⁱ	0.93	2.71	3.394 (2)	131

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

Data collection: APEX2 (Bruker, 2013); cell refinement: SAINT (Bruker, 2013); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: Mercury (Macrae *et al.*, 2008); software used to prepare material for publication: PLATON (Spek, 2009).

The authors are grateful to the IOE, University of Mysore, for providing the single-crystal X-ray diffraction facility. MKU is grateful to the DST, New Delhi, for the award of an INSPIRE Fellowship. DR acknowledges the UGC, New Delhi, for financial support under the Major Research Project Scheme [No. F.41–882/2012 (SR)].

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: XU5759).

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supplementary materials

Acta Cryst. (2014). E70, o140 [doi:10.1107/S1600536813034879]

(E)-N'-[4-(Dimethylamino)benzylidene]-2-(4-methylphenoxy)acetohydrazide

M. K. Usha, S. Madan Kumar, Nitinchandra, B. Kalluraya, N. K. Lokanath and D. Revannasiddaiah

1. Comment

Hydrazone derivatives possessing an azomethine –NHN=CH– moiety constitute an important class of compounds for new drug development (Nithinchandra *et al.*, 2012). A large number of hydrazone derivatives have been reported to have bactericidal (Holla *et al.*, 1992), fungicidal (Kalluraya *et al.*, 1995) and anticancer (Nithinchandra *et al.*, 2013) activities. As part of our studies in this area, herewith we report the structure of the title compound.

The *ORTEP* of the title compound is shown (Fig. 1) and the dihedral angle between the two phenyl rings is 68.85 (11)°. The overall geometry of the title compound are similar to related structures *N*-{(E)-[4-Dimethylamino]phenyl}-methylidene-2,3-dimethylaniline (Sarfraz *et al.*, 2010) and 2-(4-Methylphenoxy)acetohydrazide (Fun *et al.*, 2011). In the crystal structure, the molecules are connected with intermolecular hydrogen bonds C8—H8B···O2 and N1—H1···O2. They form infinite chains along *b*-axis (Fig. 2 and Table. 1). In addition, short contacts C8—H(8 A)···Cg(2) with distance 3.442 (2) Å (angle 139°) [*x*, *y* - 1/2, *z* + 1/2] and C16—H16···Cg1 with distance 3.394 (2) Å (angle 131°) [*x* - 1, *y* + 1/2, *z* - 1/2] are observed where Cg(1): C2—C7 and Cg(2): C11—C16.

2. Experimental

To a solution of 2-(4-methylphenoxy)acetohydrazide (0.01 mol) in a mixture of DMF and ethanol (10 ml), 4-(dimethylamino)benzaldehyde (0.01 mol) was added. Concentrated sulfuric acid (0.5 ml) was added to this reaction mixture. The contents were refluxed for about 1 h. The solid product separated was collected by filtration. It was dried and recrystallized from ethanol. Single crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol-*N,N*-dimethylformamide (DMF) (3:1) solution.

3. Refinement

H atoms were placed in calculated positions with C—H = 0.93–0.97 Å and N—H = 0.86 Å, and refined as riding on their parent C and N atoms with $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms and $1.2U_{\text{eq}}(\text{C}, \text{N})$ for the others.

Computing details

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT* (Bruker, 2013); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *PLATON* (Spek, 2009).

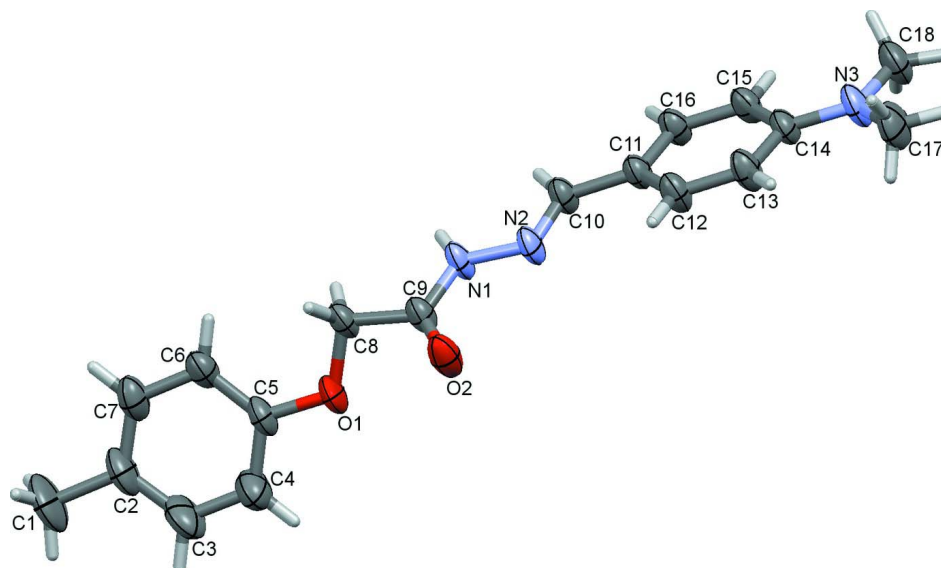


Figure 1

The molecular structure of the title compound with 50% probability ellipsoids.

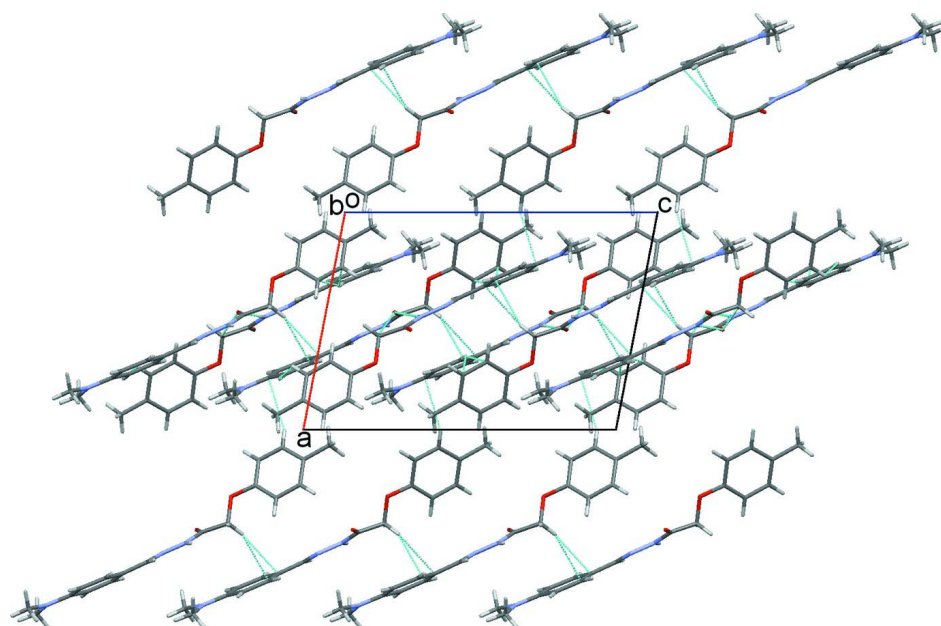


Figure 2

Packing diagram of molecule, viewed along *b* axis.

(*E*)-*N'*-[4-(Dimethylamino)benzylidene]-2-(4-methylphenoxy)acetohydrazide

Crystal data

$C_{18}H_{21}N_3O_2$

$M_r = 311.38$

Monoclinic, $P2_1/c$

Hall symbol: $-P\ 2_1/c$

$a = 11.2237(6)\ \text{\AA}$

$b = 9.4471(5)\ \text{\AA}$

$c = 15.8785(9)\ \text{\AA}$

$\beta = 100.868(3)^\circ$

$V = 1653.42(16)\ \text{\AA}^3$

$Z = 4$

$F(000) = 664$

$D_x = 1.251\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.54178 \text{ \AA}$
 Cell parameters from 2725 reflections
 $\theta = 4.0\text{--}64.7^\circ$
 $\mu = 0.67 \text{ mm}^{-1}$

$T = 296 \text{ K}$
 Block, red
 $0.23 \times 0.22 \times 0.21 \text{ mm}$

Data collection

Bruker X8 Proteum
 diffractometer
 Radiation source: Bruker MicroStar microfocus
 rotating anode
 Helios multilayer optics monochromator
 Detector resolution: $10.7 \text{ pixels mm}^{-1}$
 φ and ω scans
 Absorption correction: multi-scan
 SADABS (Bruker, 2013)

$T_{\min} = 0.862$, $T_{\max} = 0.873$
 13214 measured reflections
 2725 independent reflections
 2318 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.069$
 $\theta_{\max} = 64.7^\circ$, $\theta_{\min} = 4.0^\circ$
 $h = -12 \rightarrow 13$
 $k = -11 \rightarrow 5$
 $l = -18 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.075$
 $wR(F^2) = 0.211$
 $S = 1.05$
 2725 reflections
 211 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
 $w = 1/[\sigma^2(F_o^2) + (0.1529P)^2 + 0.2569P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.43 \text{ e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.43 \text{ e \AA}^{-3}$
 Extinction correction: SHELXL,
 $\text{FC}^* = \text{KFC}[1 + 0.001\text{XFC}^2\Lambda^3/\text{SIN}(2\Theta)]^{-1/4}$
 Extinction coefficient: 0.0102 (18)

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted R -factors wR and all goodnesses 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating $-R$ -factor-obs *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 (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.69278 (13)	0.22073 (19)	0.19031 (9)	0.0526 (6)
O2	0.53999 (16)	0.07569 (16)	0.28054 (9)	0.0536 (6)
N1	0.47999 (15)	0.29874 (18)	0.30708 (10)	0.0404 (5)
N2	0.43122 (16)	0.25856 (19)	0.37754 (10)	0.0411 (6)
N3	0.19247 (18)	0.2905 (2)	0.71623 (11)	0.0513 (7)
C1	0.9297 (3)	0.2897 (4)	-0.0930 (2)	0.0937 (14)
C2	0.8634 (2)	0.2746 (3)	-0.01891 (16)	0.0601 (9)
C3	0.9184 (2)	0.2062 (4)	0.05636 (18)	0.0714 (10)
C4	0.8604 (2)	0.1913 (3)	0.12481 (16)	0.0622 (9)
C5	0.74458 (19)	0.2438 (2)	0.11927 (12)	0.0438 (7)
C6	0.6868 (2)	0.3118 (2)	0.04553 (13)	0.0453 (7)

C7	0.7476 (2)	0.3253 (2)	-0.02276 (15)	0.0527 (8)
C8	0.56985 (18)	0.2615 (2)	0.18410 (12)	0.0414 (6)
C9	0.52905 (19)	0.2017 (2)	0.26216 (12)	0.0392 (6)
C10	0.39327 (18)	0.3609 (2)	0.41754 (12)	0.0399 (6)
C11	0.33822 (18)	0.3394 (2)	0.49233 (12)	0.0384 (6)
C12	0.3056 (2)	0.2065 (2)	0.51882 (14)	0.0456 (7)
C13	0.2569 (2)	0.1908 (2)	0.59149 (14)	0.0474 (7)
C14	0.23959 (18)	0.3070 (2)	0.64313 (13)	0.0409 (6)
C15	0.2715 (2)	0.4407 (2)	0.61621 (13)	0.0434 (6)
C16	0.31855 (19)	0.4555 (2)	0.54258 (13)	0.0428 (7)
C17	0.1550 (3)	0.1517 (3)	0.74088 (16)	0.0636 (9)
C18	0.1782 (2)	0.4102 (3)	0.76985 (15)	0.0612 (9)
H1	0.47880	0.38630	0.29210	0.0490*
H1A	1.00830	0.24650	-0.07820	0.1410*
H1B	0.93890	0.38830	-0.10510	0.1410*
H1C	0.88410	0.24400	-0.14280	0.1410*
H3	0.99620	0.16970	0.06030	0.0860*
H4	0.89910	0.14610	0.17450	0.0740*
H6	0.60880	0.34760	0.04170	0.0540*
H7	0.70870	0.37010	-0.07260	0.0630*
H8A	0.52070	0.22370	0.13210	0.0500*
H8B	0.56260	0.36380	0.18310	0.0500*
H10	0.40110	0.45270	0.39820	0.0480*
H12	0.31690	0.12710	0.48670	0.0550*
H13	0.23490	0.10090	0.60690	0.0570*
H15	0.26080	0.52040	0.64840	0.0520*
H16	0.33790	0.54560	0.52580	0.0510*
H17A	0.08590	0.12040	0.70000	0.0950*
H17B	0.13400	0.15720	0.79670	0.0950*
H17C	0.22040	0.08570	0.74230	0.0950*
H18A	0.25520	0.45570	0.78800	0.0920*
H18B	0.14790	0.37840	0.81920	0.0920*
H18C	0.12190	0.47610	0.73800	0.0920*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0494 (9)	0.0749 (12)	0.0419 (8)	0.0043 (8)	0.0300 (7)	0.0077 (7)
O2	0.0804 (11)	0.0332 (9)	0.0576 (9)	0.0002 (7)	0.0400 (8)	-0.0008 (6)
N1	0.0560 (10)	0.0323 (9)	0.0426 (9)	-0.0035 (7)	0.0339 (8)	-0.0003 (7)
N2	0.0524 (10)	0.0392 (10)	0.0400 (9)	-0.0055 (8)	0.0303 (8)	0.0012 (7)
N3	0.0648 (12)	0.0524 (12)	0.0479 (10)	-0.0071 (9)	0.0394 (9)	-0.0023 (8)
C1	0.096 (2)	0.122 (3)	0.083 (2)	-0.018 (2)	0.0681 (18)	0.0022 (18)
C2	0.0650 (15)	0.0688 (17)	0.0579 (14)	-0.0183 (13)	0.0411 (12)	-0.0044 (12)
C3	0.0470 (13)	0.103 (2)	0.0736 (17)	-0.0075 (14)	0.0351 (12)	-0.0028 (15)
C4	0.0482 (13)	0.089 (2)	0.0539 (13)	-0.0008 (12)	0.0214 (10)	0.0062 (12)
C5	0.0489 (12)	0.0480 (13)	0.0423 (11)	-0.0087 (9)	0.0284 (9)	-0.0037 (9)
C6	0.0566 (12)	0.0370 (12)	0.0496 (12)	-0.0001 (9)	0.0287 (10)	-0.0008 (9)
C7	0.0727 (15)	0.0441 (13)	0.0498 (12)	-0.0088 (11)	0.0330 (11)	0.0017 (9)
C8	0.0499 (11)	0.0375 (11)	0.0446 (10)	0.0009 (9)	0.0289 (9)	-0.0020 (8)

C9	0.0489 (11)	0.0335 (11)	0.0416 (10)	-0.0040 (8)	0.0252 (9)	-0.0030 (8)
C10	0.0509 (11)	0.0345 (11)	0.0411 (10)	-0.0030 (9)	0.0261 (9)	0.0005 (8)
C11	0.0457 (10)	0.0365 (11)	0.0388 (10)	-0.0001 (8)	0.0230 (8)	0.0019 (8)
C12	0.0626 (13)	0.0343 (12)	0.0484 (11)	-0.0039 (10)	0.0324 (10)	-0.0052 (9)
C13	0.0646 (13)	0.0340 (12)	0.0532 (12)	-0.0086 (10)	0.0357 (10)	-0.0012 (9)
C14	0.0434 (10)	0.0454 (13)	0.0403 (10)	-0.0020 (9)	0.0245 (8)	0.0003 (8)
C15	0.0535 (11)	0.0364 (11)	0.0476 (11)	0.0019 (9)	0.0286 (9)	-0.0043 (9)
C16	0.0563 (12)	0.0314 (11)	0.0479 (11)	0.0008 (9)	0.0285 (9)	0.0024 (8)
C17	0.0766 (16)	0.0648 (17)	0.0608 (14)	-0.0097 (13)	0.0422 (12)	0.0107 (12)
C18	0.0734 (16)	0.0681 (17)	0.0530 (13)	0.0017 (13)	0.0397 (11)	-0.0070 (11)

Geometric parameters (Å, °)

O1—C5	1.380 (2)	C14—C15	1.402 (3)
O1—C8	1.418 (3)	C15—C16	1.378 (3)
O2—C9	1.226 (2)	C1—H1A	0.9600
N1—N2	1.388 (2)	C1—H1B	0.9600
N1—C9	1.342 (3)	C1—H1C	0.9600
N2—C10	1.273 (3)	C3—H3	0.9300
N3—C14	1.372 (3)	C4—H4	0.9300
N3—C17	1.453 (3)	C6—H6	0.9300
N3—C18	1.443 (3)	C7—H7	0.9300
N1—H1	0.8600	C8—H8A	0.9700
C1—C2	1.513 (4)	C8—H8B	0.9700
C2—C7	1.376 (3)	C10—H10	0.9300
C2—C3	1.396 (4)	C12—H12	0.9300
C3—C4	1.375 (4)	C13—H13	0.9300
C4—C5	1.379 (3)	C15—H15	0.9300
C5—C6	1.385 (3)	C16—H16	0.9300
C6—C7	1.392 (3)	C17—H17A	0.9600
C8—C9	1.510 (3)	C17—H17B	0.9600
C10—C11	1.453 (3)	C17—H17C	0.9600
C11—C16	1.398 (3)	C18—H18A	0.9600
C11—C12	1.395 (3)	C18—H18B	0.9600
C12—C13	1.375 (3)	C18—H18C	0.9600
C13—C14	1.405 (3)		
C5—O1—C8	117.04 (15)	H1A—C1—H1C	109.00
N2—N1—C9	120.36 (17)	H1B—C1—H1C	109.00
N1—N2—C10	114.47 (17)	C2—C3—H3	119.00
C14—N3—C17	120.51 (19)	C4—C3—H3	119.00
C14—N3—C18	120.91 (19)	C3—C4—H4	120.00
C17—N3—C18	118.58 (19)	C5—C4—H4	120.00
N2—N1—H1	120.00	C5—C6—H6	121.00
C9—N1—H1	120.00	C7—C6—H6	121.00
C3—C2—C7	117.4 (2)	C2—C7—H7	119.00
C1—C2—C3	120.4 (2)	C6—C7—H7	119.00
C1—C2—C7	122.1 (2)	O1—C8—H8A	110.00
C2—C3—C4	121.7 (2)	O1—C8—H8B	110.00
C3—C4—C5	119.6 (2)	C9—C8—H8A	110.00

O1—C5—C6	124.19 (19)	C9—C8—H8B	110.00
O1—C5—C4	115.37 (18)	H8A—C8—H8B	109.00
C4—C5—C6	120.4 (2)	N2—C10—H10	119.00
C5—C6—C7	118.8 (2)	C11—C10—H10	119.00
C2—C7—C6	122.1 (2)	C11—C12—H12	119.00
O1—C8—C9	106.44 (16)	C13—C12—H12	119.00
N1—C9—C8	113.53 (16)	C12—C13—H13	119.00
O2—C9—C8	121.76 (18)	C14—C13—H13	119.00
O2—C9—N1	124.71 (18)	C14—C15—H15	120.00
N2—C10—C11	122.37 (18)	C16—C15—H15	120.00
C12—C11—C16	117.09 (18)	C11—C16—H16	119.00
C10—C11—C12	123.28 (18)	C15—C16—H16	119.00
C10—C11—C16	119.61 (17)	N3—C17—H17A	110.00
C11—C12—C13	121.25 (18)	N3—C17—H17B	109.00
C12—C13—C14	121.74 (18)	N3—C17—H17C	109.00
N3—C14—C15	121.45 (18)	H17A—C17—H17B	109.00
N3—C14—C13	121.50 (18)	H17A—C17—H17C	109.00
C13—C14—C15	117.04 (19)	H17B—C17—H17C	109.00
C14—C15—C16	120.74 (18)	N3—C18—H18A	110.00
C11—C16—C15	122.12 (18)	N3—C18—H18B	109.00
C2—C1—H1A	109.00	N3—C18—H18C	109.00
C2—C1—H1B	110.00	H18A—C18—H18B	109.00
C2—C1—H1C	110.00	H18A—C18—H18C	109.00
H1A—C1—H1B	109.00	H18B—C18—H18C	109.00
C8—O1—C5—C4	-174.36 (19)	O1—C5—C6—C7	-178.31 (18)
C8—O1—C5—C6	4.4 (3)	C4—C5—C6—C7	0.3 (3)
C5—O1—C8—C9	169.91 (16)	C5—C6—C7—C2	-0.7 (3)
C9—N1—N2—C10	176.45 (19)	O1—C8—C9—O2	-53.8 (2)
N2—N1—C9—O2	-3.4 (3)	O1—C8—C9—N1	126.83 (18)
N2—N1—C9—C8	175.95 (16)	N2—C10—C11—C12	-10.0 (3)
N1—N2—C10—C11	179.34 (17)	N2—C10—C11—C16	168.4 (2)
C17—N3—C14—C13	-2.1 (3)	C10—C11—C12—C13	178.1 (2)
C17—N3—C14—C15	177.3 (2)	C16—C11—C12—C13	-0.4 (3)
C18—N3—C14—C13	178.3 (2)	C10—C11—C16—C15	-177.2 (2)
C18—N3—C14—C15	-2.3 (3)	C12—C11—C16—C15	1.4 (3)
C1—C2—C3—C4	179.8 (3)	C11—C12—C13—C14	-1.1 (3)
C7—C2—C3—C4	-0.9 (5)	C12—C13—C14—N3	-179.1 (2)
C1—C2—C7—C6	-179.8 (2)	C12—C13—C14—C15	1.5 (3)
C3—C2—C7—C6	0.9 (4)	N3—C14—C15—C16	-179.9 (2)
C2—C3—C4—C5	0.6 (5)	C13—C14—C15—C16	-0.5 (3)
C3—C4—C5—O1	178.5 (2)	C14—C15—C16—C11	-0.9 (3)
C3—C4—C5—C6	-0.3 (4)		

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C2—C7 and C11—C16 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 \cdots O2 ⁱ	0.86	2.12	2.952 (2)	163
C8—H8B \cdots O2 ⁱ	0.97	2.43	3.303 (2)	149

C8—H8A...Cg2 ⁱⁱ	0.97	2.65	3.442 (2)	139
C16—H16...Cg1 ⁱ	0.93	2.71	3.394 (2)	131

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