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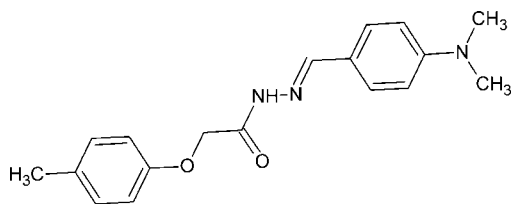
Received 9 December 2013; accepted 30 December 2013

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.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|---|-------|-------------|-------------|---------------|
| $\text{N1}-\text{H1}\cdots\text{O2}^i$ | 0.86 | 2.12 | 2.952 (2) | 163 |
| $\text{C8}-\text{H8B}\cdots\text{O2}^i$ | 0.97 | 2.43 | 3.303 (2) | 149 |
| $\text{C8}-\text{H8A}\cdots\text{Cg2}^{ii}$ | 0.97 | 2.65 | 3.442 (2) | 139 |
| $\text{C16}-\text{H16}\cdots\text{Cg1}^i$ | 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).

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

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supporting information

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

S1. 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.

S2. 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.

S3. 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.

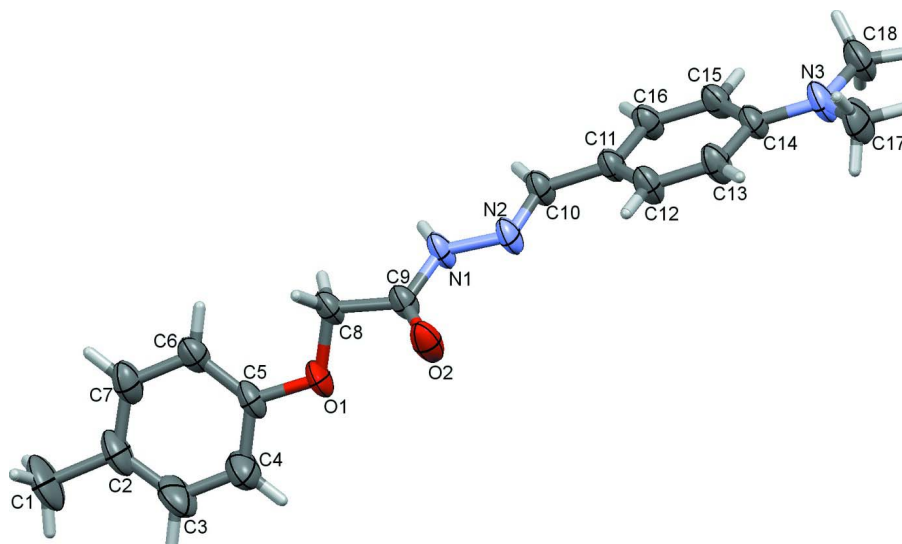


Figure 1

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

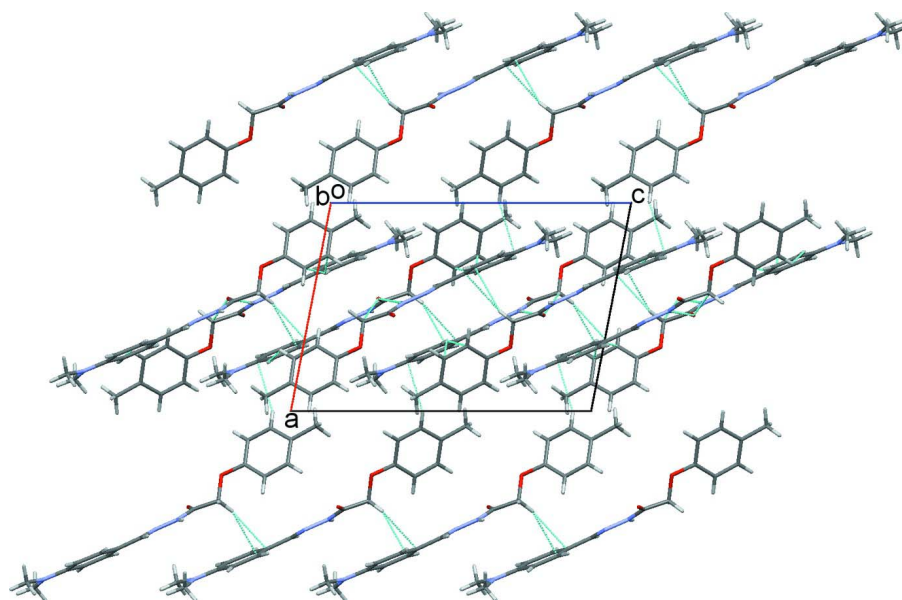


Figure 2

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

$\theta = 4.0\text{--}64.7^\circ$

$\mu = 0.67\ \text{mm}^{-1}$

$T = 296$ K
Block, red

$0.23 \times 0.22 \times 0.21$ mm

Data collection

Bruker X8 Proteum
diffractometer
Radiation source: Bruker MicroStar microfocus
rotating anode
Helios multilayer optics monochromator
Detector resolution: 10.7 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 $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.002$
 $\Delta\rho_{\max} = 0.43$ e \AA^{-3}
 $\Delta\rho_{\min} = -0.43$ 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)

| | x | y | z | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|----|--------------|--------------|---------------|----------------------------------|
| 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 (Å²)

| | 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 (Å, °)

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

| <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> |
|----------------------------|-------------|---------------|-----------------------|-------------------------|
| 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) $-x+1, y+1/2, -z+1/2$; (ii) $x, -y+1/2, z-1/2$.