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3-Butyl-5,5-diphenylimidazolidine-2,4-dione

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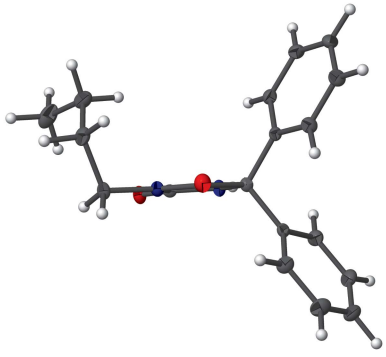
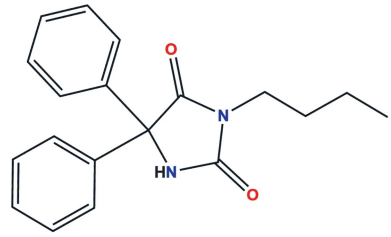
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{19}H_{20}N_2O_2$, the phenyl rings are inclined to the five-membered ring by 58.08 (6) and 66.31 (5)°. In the crystal, pairwise N—H···O and C—H···N hydrogen bonds form chains along the *a*-axis direction which are connected into layers approximately parallel to [010] by C—H···O hydrogen bonds. The layers are connected by C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Hydantoin is an important nucleus found in numerous natural products and in several clinically important medicines. One of the most significant hydantoin derivatives is 5,5-diphenylimidazolidine-2,4-dione (phenytoin). As part of our ongoing studies of phenytoin derivatives (Ramli *et al.*, 2017*a*,*b*; Akrad *et al.*, 2017; Guerrab *et al.*, 2017*a*,*b*), the title compound was prepared and its crystal structure is reported here.

In the title molecule, Fig. 1, the imidazolidine-2,4-dione ring has phenyl groups attached to the 5-position. The C8–C13 and C14–C19 rings are inclined to the five-membered ring by 58.08 (6) and 66.31 (5)°, respectively.

In the crystal, pairwise N2—H2···O2 hydrogen bonds (Table 1) form centrosymmetric dimers, which are connected into chains along the *a*- axis direction by pairwise C17—H17···N1 hydrogen bonds. The chains are then connected into thick layers approximately parallel to [010] by C18—H18···O1 hydrogen bonds (Table 1 and Fig. 2). The layers, in turn, are connected along the *b*-axis direction by C5—H5*A*···*Cg*3 interactions (Table 2 and Figs. 3 and 4).

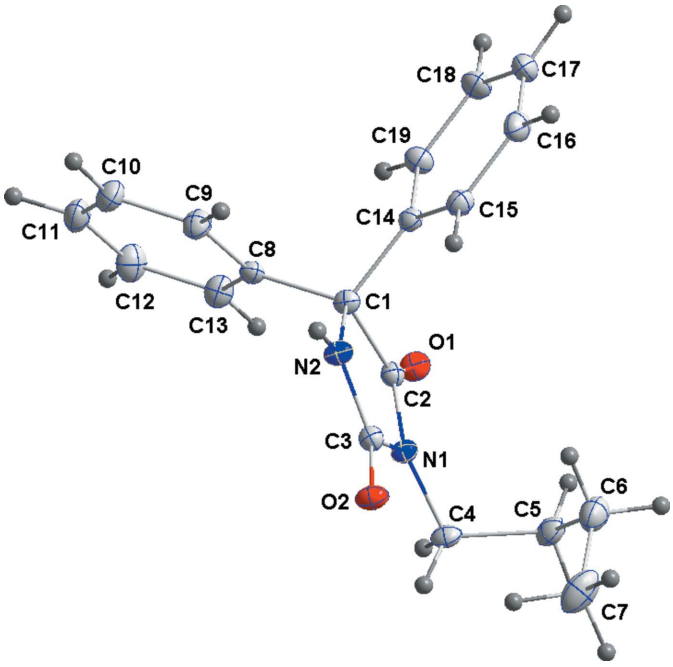


Figure 1
The title molecule with labelling scheme and 50% probability ellipsoids.

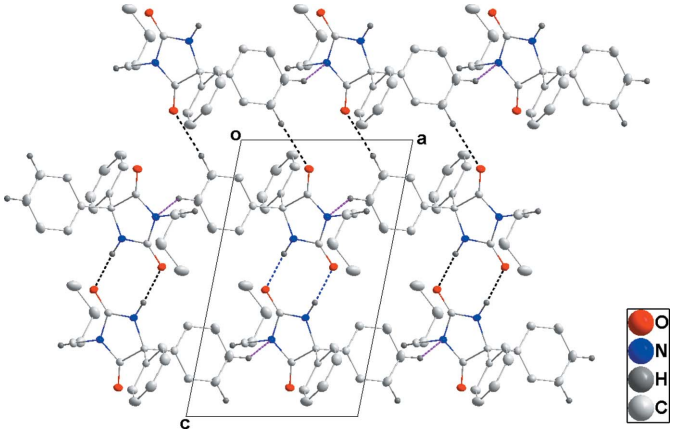


Figure 2
Detail of the layer formation (plan view) viewed along the *b*-axis direction. N—H···O, C—H···O and C—H···N hydrogen bonds are shown, respectively, as blue, black and pink dashed lines.

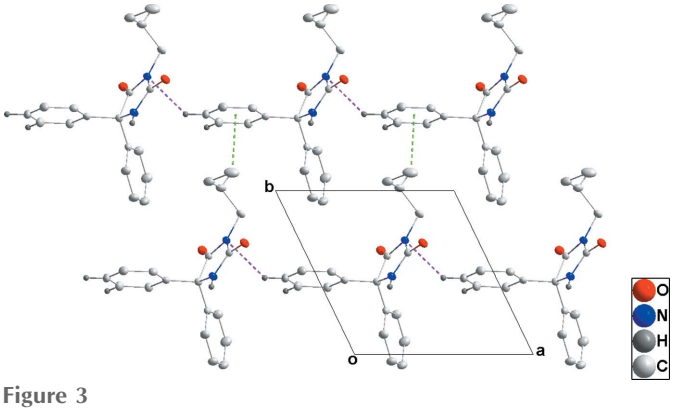


Figure 3
Elevation view of the layers seen along the *c*-axis direction. C—H···N hydrogen bonds and C—H···π(ring) interactions are shown, respectively, as pink and green dashed lines.

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

*Cg*3 is the centroid of the C14–C19 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.905 (15)	1.907 (15)	2.8030 (10)	170.0 (13)
C17—H17···N1^{ii}	0.969 (14)	2.682 (15)	3.4320 (13)	134.5 (11)
C18—H18···O1^{iii}	0.971 (14)	2.467 (15)	3.4231 (13)	167.9 (13)
C5—H5*A*···*Cg*3^{iv}	1.020 (15)	2.706 (15)	3.6276 (11)	150.3 (13)

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

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (1 g), one equivalent of butyl bromide in absolute dimethylformamide (DMF) was added and the resulting solution heated under reflux for 3 h in the presence of 1.3 equivalents of K_2CO_3. The reaction mixture was filtered while hot, and the solvent evaporated under reduced pressure. The residue obtained was dried and crystallized from an ethanol solution to yield colourless block-shaped crystals of the title compound (Guerrab *et al.*, 2017*c*,*d*).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{20}N_2O_2$
M_r	308.37
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, *b*, *c* (Å)	8.4920 (4), 8.5213 (4), 12.6353 (6)
α, β, γ (°)	91.900 (1), 99.410 (1), 115.117 (1)
V (Å^3)	811.33 (7)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	0.08
Crystal size (mm)	0.45 × 0.26 × 0.21
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.91, 0.98
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15814, 4333, 3688
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.688
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.041, 0.120, 1.08
No. of reflections	4333
No. of parameters	288
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.19

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

Acknowledgements

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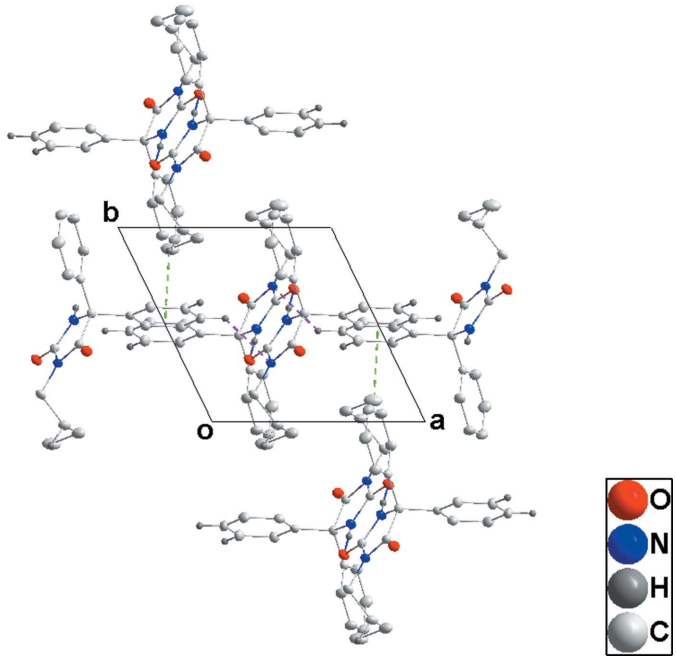

Figure 4
Packing viewed along the *c*-axis direction. Intermolecular interactions are depicted as in Fig. 3.

full crystallographic data

IUCrData (2018). **3**, x180050 [https://doi.org/10.1107/S2414314618000500]

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Crystal data

$C_{19}H_{20}N_2O_2$
M_r = 308.37
Triclinic, $P\overline{1}$
a = 8.4920 (4) Å
b = 8.5213 (4) Å
c = 12.6353 (6) Å
α = 91.900 (1)°
β = 99.410 (1)°
γ = 115.117 (1)°
V = 811.33 (7) Å^3
Z = 2
$F(000)$ = 328
D_x = 1.262 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9307 reflections
θ = 2.7–29.3°
μ = 0.08 mm^{-1}
T = 100 K
Column, colourless
0.45 × 0.26 × 0.21 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.91, T_{max} = 0.98
15814 measured reflections
4333 independent reflections
3688 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 29.3°, θ_{min} = 2.7°
h = −11→11
k = −11→11
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.120
S = 1.08
4333 reflections
288 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.080P)^2 + 0.0762P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, colllected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 15 sec/frame.

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.42900 (9)	0.63578 (9)	0.10520 (5)	0.01768 (16)
O2	0.68520 (9)	0.68073 (9)	0.45909 (5)	0.01767 (16)
N1	0.59096 (10)	0.69754 (10)	0.27850 (6)	0.01357 (17)
N2	0.41937 (10)	0.47738 (10)	0.35721 (6)	0.01472 (17)
H2	0.3814 (19)	0.4141 (19)	0.4117 (12)	0.033 (4)*
C1	0.32148 (11)	0.44377 (11)	0.24628 (6)	0.01266 (18)
C2	0.44877 (12)	0.60095 (11)	0.19723 (7)	0.01304 (18)
C3	0.57377 (12)	0.62163 (11)	0.37502 (7)	0.01326 (18)
C4	0.74278 (12)	0.85862 (12)	0.26622 (7)	0.01638 (19)
H4A	0.7735 (16)	0.8419 (15)	0.1980 (10)	0.018 (3)*
H4B	0.8414 (16)	0.8716 (16)	0.3248 (10)	0.019 (3)*
C5	0.70205 (14)	1.01678 (13)	0.26977 (8)	0.0205 (2)
H5A	0.8127 (19)	1.1209 (19)	0.2579 (11)	0.030 (3)*
H5B	0.6049 (17)	0.9971 (17)	0.2054 (10)	0.025 (3)*
C6	0.65343 (16)	1.05668 (14)	0.37531 (9)	0.0271 (2)
H6A	0.618 (2)	1.154 (2)	0.3626 (12)	0.039 (4)*
H6B	0.549 (2)	0.952 (2)	0.3879 (12)	0.037 (4)*
C7	0.80448 (19)	1.11144 (16)	0.47267 (9)	0.0340 (3)
H7A	0.913 (2)	1.221 (2)	0.4622 (13)	0.047 (4)*
H7B	0.769 (2)	1.139 (2)	0.5382 (14)	0.048 (4)*
H7C	0.8433 (19)	1.016 (2)	0.4869 (11)	0.035 (4)*
C8	0.29414 (11)	0.26678 (12)	0.19392 (7)	0.01378 (18)
C9	0.21611 (13)	0.12177 (13)	0.24851 (8)	0.0198 (2)
H9	0.1819 (18)	0.1379 (18)	0.3189 (11)	0.031 (4)*
C10	0.18844 (14)	−0.04268 (13)	0.20653 (9)	0.0237 (2)
H10	0.1318 (19)	−0.1425 (19)	0.2477 (12)	0.034 (4)*
C11	0.23838 (14)	−0.06393 (13)	0.10958 (9)	0.0237 (2)
H11	0.221 (2)	−0.183 (2)	0.0800 (12)	0.041 (4)*
C12	0.31514 (15)	0.07902 (14)	0.05488 (8)	0.0247 (2)
H12	0.354 (2)	0.065 (2)	−0.0151 (12)	0.040 (4)*
C13	0.34288 (14)	0.24465 (13)	0.09651 (7)	0.0193 (2)
H13	0.4002 (19)	0.3469 (19)	0.0586 (11)	0.032 (4)*
C14	0.14426 (12)	0.45375 (11)	0.23816 (7)	0.01344 (18)
C15	0.09485 (13)	0.50500 (12)	0.32794 (7)	0.01705 (19)
H15	0.1725 (17)	0.5326 (16)	0.4004 (10)	0.021 (3)*
C16	−0.06848 (14)	0.51135 (13)	0.31780 (8)	0.0214 (2)

H16	−0.1032 (18)	0.5442 (18)	0.3810 (11)	0.027 (3)*
C17	−0.18115 (13)	0.46744 (13)	0.21804 (9)	0.0217 (2)
H17	−0.2961 (18)	0.4682 (18)	0.2119 (11)	0.031 (3)*
C18	−0.13172 (13)	0.41824 (13)	0.12736 (8)	0.0209 (2)
H18	−0.2136 (19)	0.3874 (18)	0.0584 (11)	0.028 (3)*
C19	0.03005 (13)	0.41048 (13)	0.13743 (7)	0.0175 (2)
H19	0.0628 (17)	0.3725 (17)	0.0729 (10)	0.024 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0197 (3)	0.0190 (3)	0.0128 (3)	0.0067 (3)	0.0035 (2)	0.0050 (2)
O2	0.0153 (3)	0.0192 (3)	0.0132 (3)	0.0032 (3)	0.0005 (2)	0.0027 (2)
N1	0.0135 (4)	0.0134 (3)	0.0123 (3)	0.0040 (3)	0.0033 (3)	0.0033 (3)
N2	0.0143 (4)	0.0156 (4)	0.0107 (3)	0.0034 (3)	0.0013 (3)	0.0035 (3)
C1	0.0132 (4)	0.0141 (4)	0.0098 (4)	0.0051 (3)	0.0022 (3)	0.0028 (3)
C2	0.0137 (4)	0.0135 (4)	0.0129 (4)	0.0065 (3)	0.0037 (3)	0.0021 (3)
C3	0.0142 (4)	0.0143 (4)	0.0124 (4)	0.0067 (3)	0.0036 (3)	0.0027 (3)
C4	0.0140 (4)	0.0156 (4)	0.0162 (4)	0.0025 (3)	0.0046 (3)	0.0039 (3)
C5	0.0218 (5)	0.0143 (4)	0.0223 (5)	0.0051 (4)	0.0032 (4)	0.0046 (3)
C6	0.0298 (6)	0.0192 (5)	0.0332 (6)	0.0099 (5)	0.0116 (4)	0.0011 (4)
C7	0.0483 (8)	0.0230 (6)	0.0223 (5)	0.0078 (5)	0.0078 (5)	−0.0022 (4)
C8	0.0115 (4)	0.0138 (4)	0.0148 (4)	0.0049 (3)	0.0009 (3)	0.0013 (3)
C9	0.0210 (5)	0.0171 (5)	0.0219 (5)	0.0072 (4)	0.0087 (4)	0.0044 (3)
C10	0.0250 (5)	0.0153 (5)	0.0300 (5)	0.0075 (4)	0.0065 (4)	0.0047 (4)
C11	0.0262 (5)	0.0175 (5)	0.0269 (5)	0.0111 (4)	0.0007 (4)	−0.0021 (4)
C12	0.0329 (6)	0.0254 (5)	0.0182 (5)	0.0151 (5)	0.0054 (4)	−0.0006 (4)
C13	0.0239 (5)	0.0189 (5)	0.0156 (4)	0.0096 (4)	0.0045 (3)	0.0028 (3)
C14	0.0130 (4)	0.0118 (4)	0.0146 (4)	0.0044 (3)	0.0030 (3)	0.0029 (3)
C15	0.0175 (4)	0.0153 (4)	0.0169 (4)	0.0059 (4)	0.0033 (3)	0.0000 (3)
C16	0.0211 (5)	0.0189 (5)	0.0255 (5)	0.0090 (4)	0.0082 (4)	−0.0011 (4)
C17	0.0165 (5)	0.0191 (5)	0.0312 (5)	0.0100 (4)	0.0031 (4)	0.0000 (4)
C18	0.0183 (5)	0.0224 (5)	0.0216 (5)	0.0101 (4)	−0.0005 (4)	0.0022 (4)
C19	0.0176 (4)	0.0202 (5)	0.0149 (4)	0.0088 (4)	0.0021 (3)	0.0025 (3)

Geometric parameters (Å, º)

O1—C2	1.2123 (11)	C8—C13	1.3925 (13)
O2—C3	1.2283 (10)	C8—C9	1.3973 (13)
N1—C2	1.3728 (11)	C9—C10	1.3896 (14)
N1—C3	1.3991 (11)	C9—H9	1.003 (14)
N1—C4	1.4654 (11)	C10—C11	1.3905 (15)
N2—C3	1.3408 (12)	C10—H10	0.995 (15)
N2—C1	1.4587 (10)	C11—C12	1.3840 (15)
N2—H2	0.905 (15)	C11—H11	1.010 (16)
C1—C14	1.5301 (12)	C12—C13	1.3972 (14)
C1—C8	1.5338 (12)	C12—H12	1.011 (15)
C1—C2	1.5465 (12)	C13—H13	0.984 (15)

C4—C5	1.5281 (14)	C14—C15	1.3900 (13)
C4—H4A	0.964 (12)	C14—C19	1.3993 (12)
C4—H4B	0.988 (12)	C15—C16	1.3961 (14)
C5—C6	1.5275 (15)	C15—H15	0.992 (12)
C5—H5A	1.020 (15)	C16—C17	1.3837 (14)
C5—H5B	1.013 (13)	C16—H16	0.967 (14)
C6—C7	1.5212 (17)	C17—C18	1.3927 (14)
C6—H6A	1.004 (15)	C17—H17	0.969 (14)
C6—H6B	0.997 (15)	C18—C19	1.3886 (14)
C7—H7A	1.028 (17)	C18—H18	0.971 (14)
C7—H7B	0.981 (17)	C19—H19	0.990 (13)
C7—H7C	1.007 (15)		

C2—N1—C3	111.33 (7)	C6—C7—H7C	111.7 (8)
C2—N1—C4	124.68 (7)	H7A—C7—H7C	107.8 (13)
C3—N1—C4	123.98 (7)	H7B—C7—H7C	107.2 (13)
C3—N2—C1	113.32 (7)	C13—C8—C9	119.30 (8)
C3—N2—H2	120.8 (9)	C13—C8—C1	123.58 (8)
C1—N2—H2	125.7 (9)	C9—C8—C1	117.12 (8)
N2—C1—C14	112.71 (7)	C10—C9—C8	120.43 (9)
N2—C1—C8	110.20 (7)	C10—C9—H9	120.3 (8)
C14—C1—C8	110.87 (7)	C8—C9—H9	119.3 (8)
N2—C1—C2	100.48 (7)	C9—C10—C11	120.06 (9)
C14—C1—C2	108.75 (7)	C9—C10—H10	117.9 (9)
C8—C1—C2	113.48 (7)	C11—C10—H10	122.1 (9)
O1—C2—N1	125.51 (8)	C12—C11—C10	119.82 (9)
O1—C2—C1	127.53 (8)	C12—C11—H11	120.2 (9)
N1—C2—C1	106.96 (7)	C10—C11—H11	120.0 (9)
O2—C3—N2	128.06 (8)	C11—C12—C13	120.40 (10)
O2—C3—N1	124.03 (8)	C11—C12—H12	120.5 (9)
N2—C3—N1	107.90 (7)	C13—C12—H12	119.1 (9)
N1—C4—C5	112.24 (8)	C8—C13—C12	119.99 (9)
N1—C4—H4A	107.6 (7)	C8—C13—H13	119.5 (8)
C5—C4—H4A	110.0 (7)	C12—C13—H13	120.5 (8)
N1—C4—H4B	106.1 (7)	C15—C14—C19	119.54 (8)
C5—C4—H4B	112.1 (7)	C15—C14—C1	121.67 (8)
H4A—C4—H4B	108.6 (10)	C19—C14—C1	118.79 (8)
C6—C5—C4	114.43 (8)	C14—C15—C16	120.17 (9)
C6—C5—H5A	109.5 (8)	C14—C15—H15	120.6 (7)
C4—C5—H5A	106.6 (8)	C16—C15—H15	119.1 (7)
C6—C5—H5B	111.6 (8)	C17—C16—C15	119.97 (9)
C4—C5—H5B	107.6 (7)	C17—C16—H16	120.4 (8)
H5A—C5—H5B	106.7 (11)	C15—C16—H16	119.7 (8)
C7—C6—C5	113.73 (10)	C16—C17—C18	120.27 (9)
C7—C6—H6A	110.2 (9)	C16—C17—H17	119.7 (8)
C5—C6—H6A	105.1 (9)	C18—C17—H17	120.1 (8)
C7—C6—H6B	110.1 (8)	C19—C18—C17	119.85 (9)
C5—C6—H6B	108.8 (8)	C19—C18—H18	121.6 (8)

H6A—C6—H6B	108.6 (13)	C17—C18—H18	118.6 (8)
C6—C7—H7A	111.5 (9)	C18—C19—C14	120.20 (9)
C6—C7—H7B	111.1 (10)	C18—C19—H19	119.3 (7)
H7A—C7—H7B	107.4 (13)	C14—C19—H19	120.5 (7)
C3—N2—C1—C14	−115.91 (8)	N2—C1—C8—C9	53.68 (10)
C3—N2—C1—C8	119.66 (8)	C14—C1—C8—C9	−71.80 (10)
C3—N2—C1—C2	−0.32 (9)	C2—C1—C8—C9	165.47 (8)
C3—N1—C2—O1	−179.80 (8)	C13—C8—C9—C10	0.43 (15)
C4—N1—C2—O1	−0.41 (15)	C1—C8—C9—C10	−179.46 (9)
C3—N1—C2—C1	0.76 (10)	C8—C9—C10—C11	−0.02 (16)
C4—N1—C2—C1	−179.85 (8)	C9—C10—C11—C12	−0.21 (16)
N2—C1—C2—O1	−179.69 (9)	C10—C11—C12—C13	0.04 (17)
C14—C1—C2—O1	−61.17 (12)	C9—C8—C13—C12	−0.60 (14)
C8—C1—C2—O1	62.72 (12)	C1—C8—C13—C12	179.28 (9)
N2—C1—C2—N1	−0.27 (9)	C11—C12—C13—C8	0.37 (16)
C14—C1—C2—N1	118.25 (8)	N2—C1—C14—C15	5.28 (12)
C8—C1—C2—N1	−117.86 (8)	C8—C1—C14—C15	129.34 (9)
C1—N2—C3—O2	−178.49 (9)	C2—C1—C14—C15	−105.23 (9)
C1—N2—C3—N1	0.79 (10)	N2—C1—C14—C19	−174.92 (8)
C2—N1—C3—O2	178.34 (8)	C8—C1—C14—C19	−50.86 (11)
C4—N1—C3—O2	−1.05 (14)	C2—C1—C14—C19	74.57 (10)
C2—N1—C3—N2	−0.97 (10)	C19—C14—C15—C16	0.70 (14)
C4—N1—C3—N2	179.63 (8)	C1—C14—C15—C16	−179.50 (8)
C2—N1—C4—C5	79.83 (11)	C14—C15—C16—C17	−0.34 (15)
C3—N1—C4—C5	−100.86 (10)	C15—C16—C17—C18	−0.54 (15)
N1—C4—C5—C6	60.84 (11)	C16—C17—C18—C19	1.06 (16)
C4—C5—C6—C7	65.38 (12)	C17—C18—C19—C14	−0.70 (15)
N2—C1—C8—C13	−126.20 (9)	C15—C14—C19—C18	−0.18 (14)
C14—C1—C8—C13	108.32 (10)	C1—C14—C19—C18	−179.99 (8)
C2—C1—C8—C13	−14.41 (12)		

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C14–C19 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.905 (15)	1.907 (15)	2.8030 (10)	170.0 (13)
C17—H17···N1^{ii}	0.969 (14)	2.682 (15)	3.4320 (13)	134.5 (11)
C18—H18···O1^{iii}	0.971 (14)	2.467 (15)	3.4231 (13)	167.9 (13)
C5—H5*A*···*Cg*3^{iv}	1.020 (15)	2.706 (15)	3.6276 (11)	150.3 (13)

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