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

Walid Guerrab,[a]* Rachida Akrad,[a] Mhammed Ansar,[a] Jamal Taoufik,[a] Joel T. Mague[b] and Youssef Ramli[a]

[a]Laboratory of Medicinal Chemistry, Faculty of Medicine and Pharmacy, Mohammed V University, Rabat, Morocco, and [b]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA. *Correspondence e-mail: gerrab_walid@yahoo.com

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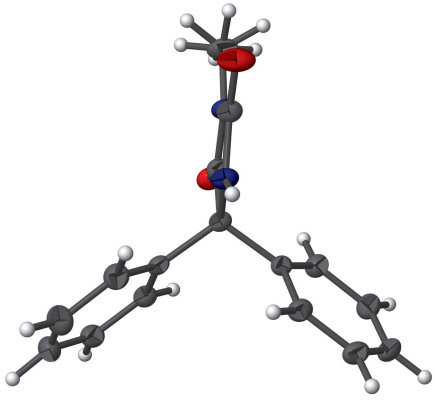
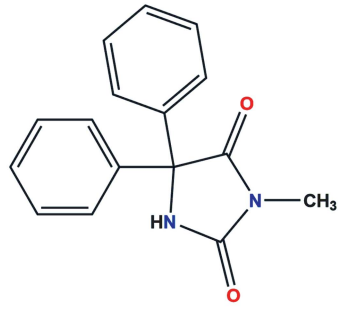
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{16}H_{14}N_2O_2$, the imidazolidine-2,4-dione ring carries two phenyl substituents at the 5-position inclined to the five-membered ring plane by 59.17 (6) and 53.21 (6)°. In the crystal, the molecules form chains parallel to the *a*-axis direction through N—H···O hydrogen bonds. These chains are linked into a three-dimensional network of molecules stacked along *a* through C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

Hydantoin, also known as imidazolidin-2,4-dione, is an important nucleus found in numerous natural products and in several clinically important medicines. One the best known examples of such a derivative is phenytoine (5,5-diphenylimidazolidine-2,4-dion), a drug widely prescribed as an anticonvulsant agent and for the treatment of many other diseases including HIV (Weichet, 1974; Havera & Strycker, 1976; Khodair *et al.*, 1997; Thenmozhiyal *et al.*, 2004). As a continuation of our work in this area (Ramli *et al.*, 2017*a*,*b*; Akrad *et al.* 2017), the compound *N*-methyl-5,5-diphenylimidazolidine-2,4-dion (Fig. 1) was prepared and its crystal structure is reported here.

The C1,N2,C3,N1,C2 imidazolidine-2,4-dione ring carries two phenyl substituents on C1. These are inclined to the five-membered ring plane by 59.17 (6)° (C5–C10) and 53.21 (6)° (C11–C16). In the crystal, molecules forms chains parallel to the *a*-axis direction through N2—H2···O1 hydrogen bonds. These chains form a three-dimensional network of molecules stacked along *a* through a series of C—H···π interactions, Table 1, Figs. 2 and 3.

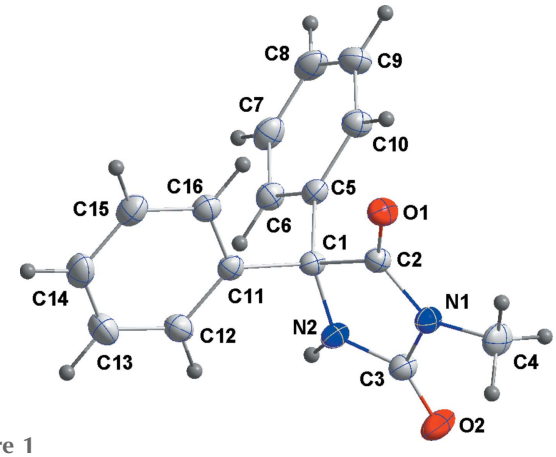


Figure 1
The title molecule with the labelling scheme and 50% probability displacement ellipsoids.

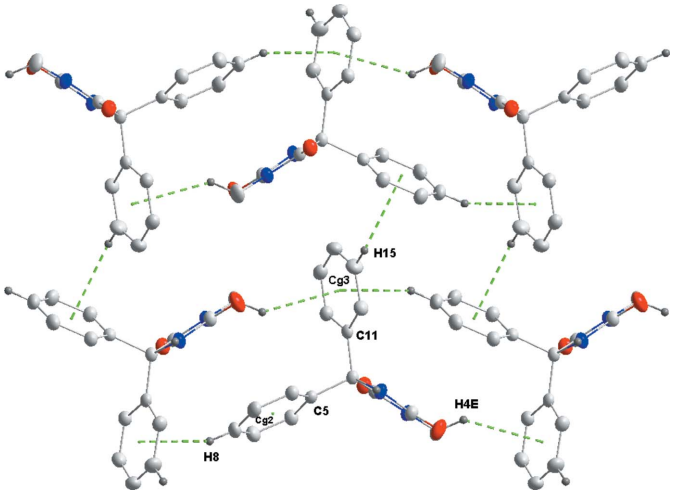


Figure 2
C—H···π(ring) contacts in the title structure, shown as green dashed lines.

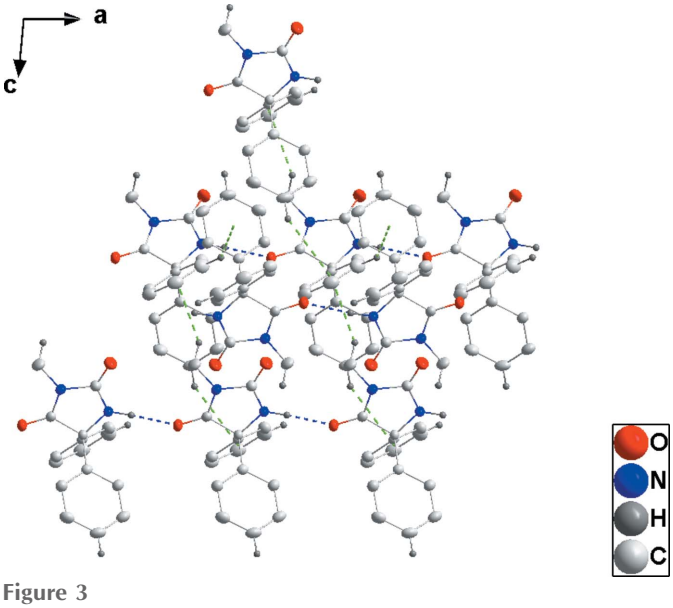


Figure 3
Packing of the title compound viewed along the *b*-axis direction, with N—H···O hydrogen drawn as blue dashed lines.

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

*Cg*2 and *Cg*3 are the centroids of the C5–C10 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.928 (19)	1.922 (19)	2.8482 (13)	175.9 (16)
C4—H4*E*···*Cg*3^{ii}	0.98	2.87	3.5883 (14)	131
C8—H8···*Cg*3^{iii}	0.922 (19)	2.915 (19)	3.7061 (14)	144.7 (14)
C13—H15···*Cg*2^{iv}	0.997 (19)	2.809 (19)	139.8 (14)	3.6255 (15)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{14}N_2O_2$
M_r	266.29
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, *b*, *c* (Å)	6.2328 (3), 15.7965 (7), 13.4448 (6)
β (°)	95.256 (1)
V (Å^3)	1318.16 (10)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.73
Crystal size (mm)	0.27 × 0.17 × 0.11
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.84, 0.93
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10021, 2636, 2455
R_{int}	0.029
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.037, 0.094, 1.07
No. of reflections	2636
No. of parameters	226
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −0.16

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

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (1 g, 3.96 mmol) was added one equivalent of methyl bromide (0.37 g) in absolute DMF and the solution was 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 was distilled off under reduced pressure. The residue obtained was dried and recrystallized from ethanol solution.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C4 methyl group is rotationally disordered over two sets of sites of equal occupancy.

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171534 [https://doi.org/10.1107/S2414314617015346]

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Crystal data

$C_{16}H_{14}N_2O_2$
M_r = 266.29
Monoclinic, $P2_1/n$
a = 6.2328 (3) Å
b = 15.7965 (7) Å
c = 13.4448 (6) Å
β = 95.256 (1)°
V = 1318.16 (10) Å^3
Z = 4
$F(000)$ = 560
D_x = 1.342 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 8452 reflections
θ = 3.3–74.3°
μ = 0.73 mm^{-1}
T = 150 K
Block, colourless
0.27 × 0.17 × 0.11 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.84, T_{max} = 0.93
10021 measured reflections
2636 independent reflections
2455 reflections with $I > 2\sigma(I)$
R_{int} = 0.029
θ_{max} = 74.3°, θ_{min} = 4.3°
h = −7→7
k = −18→15
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.094
S = 1.07
2636 reflections
226 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.4502P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}
Extinction correction: *SHELXL2016* (Sheldrick, 2015*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0076 (7)

Special details

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. The methyl group is rotationally disordered over two approximately equal sites. These hydrogen atoms were included as riding contributions with an HFIX 123 instruction.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.13255 (13)	0.20890 (6)	0.18291 (6)	0.0256 (2)	
O2	0.66323 (15)	0.11602 (7)	−0.00232 (7)	0.0357 (3)	
N1	0.35876 (15)	0.15080 (7)	0.07600 (7)	0.0229 (2)	
N2	0.67715 (16)	0.19646 (6)	0.14190 (7)	0.0223 (2)	
H2	0.826 (3)	0.1992 (11)	0.1523 (13)	0.040 (4)*	
C1	0.52715 (17)	0.22587 (7)	0.21171 (8)	0.0191 (2)	
C2	0.31218 (18)	0.19529 (7)	0.15712 (8)	0.0202 (2)	
C3	0.58171 (19)	0.15088 (8)	0.06526 (9)	0.0237 (3)	
C4	0.2018 (2)	0.11254 (9)	0.00207 (10)	0.0327 (3)	
H4A	0.277440	0.083919	−0.049134	0.049*	0.5
H4B	0.114417	0.071292	0.034962	0.049*	0.5
H4C	0.108029	0.156724	−0.029217	0.049*	0.5
H4D	0.055817	0.124037	0.020207	0.049*	0.5
H4E	0.218840	0.136665	−0.063888	0.049*	0.5
H4F	0.225229	0.051233	0.000291	0.049*	0.5
C5	0.57456 (18)	0.18436 (7)	0.31480 (8)	0.0204 (3)	
C6	0.7833 (2)	0.19301 (8)	0.36193 (9)	0.0243 (3)	
H6	0.890 (3)	0.2240 (10)	0.3288 (12)	0.036 (4)*	
C7	0.8360 (2)	0.15792 (8)	0.45565 (9)	0.0296 (3)	
H7	0.987 (3)	0.1627 (10)	0.4875 (12)	0.035 (4)*	
C8	0.6822 (2)	0.11504 (9)	0.50429 (10)	0.0318 (3)	
H8	0.716 (3)	0.0918 (11)	0.5667 (14)	0.044 (5)*	
C9	0.4749 (2)	0.10690 (9)	0.45810 (10)	0.0313 (3)	
H9	0.361 (3)	0.0771 (11)	0.4909 (13)	0.040 (4)*	
C10	0.4207 (2)	0.14135 (8)	0.36395 (9)	0.0258 (3)	
H10	0.275 (3)	0.1368 (10)	0.3333 (12)	0.034 (4)*	
C11	0.52751 (18)	0.32217 (7)	0.22487 (8)	0.0202 (2)	
C12	0.6895 (2)	0.37174 (8)	0.19058 (9)	0.0274 (3)	
H12	0.257 (3)	0.3252 (10)	0.3030 (12)	0.032 (4)*	
C13	0.6913 (2)	0.45887 (9)	0.20707 (11)	0.0349 (3)	
H13	0.254 (3)	0.4735 (11)	0.3275 (12)	0.039 (4)*	
C14	0.5318 (2)	0.49661 (8)	0.25678 (10)	0.0328 (3)	
H14	0.537 (3)	0.5566 (13)	0.2694 (13)	0.047 (5)*	
C15	0.3708 (2)	0.44727 (8)	0.29156 (10)	0.0295 (3)	

H15	0.809 (3)	0.4931 (12)	0.1821 (14)	0.050 (5)*
C16	0.3694 (2)	0.36034 (8)	0.27661 (9)	0.0246 (3)
H16	0.807 (3)	0.3452 (11)	0.1544 (12)	0.038 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0165 (4)	0.0345 (5)	0.0258 (4)	−0.0012 (3)	0.0014 (3)	−0.0014 (3)
O2	0.0294 (5)	0.0497 (6)	0.0285 (5)	−0.0012 (4)	0.0061 (4)	−0.0156 (4)
N1	0.0190 (5)	0.0295 (5)	0.0197 (5)	−0.0030 (4)	−0.0007 (4)	−0.0035 (4)
N2	0.0165 (5)	0.0309 (5)	0.0194 (5)	0.0003 (4)	0.0016 (4)	−0.0044 (4)
C1	0.0156 (5)	0.0240 (6)	0.0177 (5)	0.0000 (4)	0.0011 (4)	−0.0006 (4)
C2	0.0187 (5)	0.0232 (6)	0.0182 (5)	−0.0010 (4)	0.0000 (4)	0.0017 (4)
C3	0.0215 (6)	0.0285 (6)	0.0211 (6)	−0.0002 (4)	0.0021 (4)	−0.0020 (4)
C4	0.0284 (7)	0.0433 (8)	0.0251 (6)	−0.0095 (5)	−0.0042 (5)	−0.0069 (5)
C5	0.0222 (6)	0.0203 (5)	0.0183 (5)	0.0025 (4)	0.0010 (4)	−0.0014 (4)
C6	0.0234 (6)	0.0270 (6)	0.0221 (6)	0.0009 (5)	−0.0006 (4)	−0.0008 (4)
C7	0.0319 (7)	0.0320 (7)	0.0234 (6)	0.0041 (5)	−0.0055 (5)	−0.0025 (5)
C8	0.0446 (8)	0.0304 (7)	0.0193 (6)	0.0048 (5)	−0.0019 (5)	0.0022 (5)
C9	0.0378 (7)	0.0320 (7)	0.0247 (6)	−0.0010 (5)	0.0064 (5)	0.0042 (5)
C10	0.0243 (6)	0.0293 (6)	0.0236 (6)	−0.0001 (5)	0.0013 (5)	0.0017 (5)
C11	0.0206 (5)	0.0237 (6)	0.0157 (5)	−0.0004 (4)	−0.0020 (4)	0.0008 (4)
C12	0.0279 (6)	0.0286 (7)	0.0259 (6)	−0.0033 (5)	0.0044 (5)	0.0020 (5)
C13	0.0405 (8)	0.0284 (7)	0.0364 (7)	−0.0084 (6)	0.0059 (6)	0.0040 (5)
C14	0.0448 (8)	0.0219 (7)	0.0308 (7)	−0.0005 (5)	−0.0015 (6)	0.0008 (5)
C15	0.0343 (7)	0.0279 (7)	0.0257 (6)	0.0056 (5)	0.0003 (5)	−0.0025 (5)
C16	0.0251 (6)	0.0269 (6)	0.0216 (6)	0.0003 (5)	0.0012 (4)	−0.0004 (4)

Geometric parameters (Å, º)

O1—C2	1.2211 (14)	C6—H6	0.969 (17)
O2—C3	1.2130 (15)	C7—C8	1.386 (2)
N1—C2	1.3513 (15)	C7—H7	0.999 (17)
N1—C3	1.4102 (15)	C8—C9	1.387 (2)
N1—C4	1.4603 (15)	C8—H8	0.922 (19)
N2—C3	1.3497 (15)	C9—C10	1.3908 (18)
N2—C1	1.4600 (14)	C9—H9	0.987 (17)
N2—H2	0.928 (19)	C10—H10	0.965 (16)
C1—C11	1.5314 (16)	C11—C12	1.3894 (16)
C1—C5	1.5374 (15)	C11—C16	1.3944 (16)
C1—C2	1.5450 (15)	C12—C13	1.3940 (19)
C4—H4A	0.9800	C12—H16	1.007 (17)
C4—H4B	0.9800	C13—C14	1.383 (2)
C4—H4C	0.9800	C13—H15	0.997 (19)
C4—H4D	0.9800	C14—C15	1.386 (2)
C4—H4E	0.9800	C14—H14	0.96 (2)
C4—H4F	0.9800	C15—C16	1.3878 (18)
C5—C10	1.3905 (17)	C15—H13	0.999 (16)

C5—C6	1.4004 (16)	C16—H12	0.987 (16)
C6—C7	1.3883 (17)		

C2—N1—C3	111.64 (9)	H4E—C4—H4F	109.5
C2—N1—C4	125.77 (10)	C10—C5—C6	119.02 (11)
C3—N1—C4	122.41 (10)	C10—C5—C1	123.56 (10)
C3—N2—C1	113.40 (9)	C6—C5—C1	117.39 (10)
C3—N2—H2	120.4 (10)	C7—C6—C5	120.30 (12)
C1—N2—H2	125.4 (10)	C7—C6—H6	120.2 (10)
N2—C1—C11	113.33 (9)	C5—C6—H6	119.5 (10)
N2—C1—C5	111.24 (9)	C8—C7—C6	120.47 (12)
C11—C1—C5	108.75 (9)	C8—C7—H7	119.9 (9)
N2—C1—C2	100.01 (9)	C6—C7—H7	119.6 (9)
C11—C1—C2	110.95 (9)	C7—C8—C9	119.36 (12)
C5—C1—C2	112.43 (9)	C7—C8—H8	120.9 (11)
O1—C2—N1	126.24 (10)	C9—C8—H8	119.8 (11)
O1—C2—C1	126.01 (10)	C8—C9—C10	120.64 (12)
N1—C2—C1	107.75 (9)	C8—C9—H9	121.3 (10)
O2—C3—N2	128.93 (11)	C10—C9—H9	118.0 (10)
O2—C3—N1	124.09 (11)	C5—C10—C9	120.22 (12)
N2—C3—N1	106.97 (10)	C5—C10—H10	119.7 (9)
N1—C4—H4A	109.5	C9—C10—H10	120.0 (9)
N1—C4—H4B	109.5	C12—C11—C16	119.35 (11)
H4A—C4—H4B	109.5	C12—C11—C1	120.99 (10)
N1—C4—H4C	109.5	C16—C11—C1	119.57 (10)
H4A—C4—H4C	109.5	C11—C12—C13	119.94 (12)
H4B—C4—H4C	109.5	C11—C12—H16	120.6 (10)
N1—C4—H4D	109.5	C13—C12—H16	119.5 (10)
H4A—C4—H4D	141.1	C14—C13—C12	120.47 (12)
H4B—C4—H4D	56.3	C14—C13—H15	121.0 (11)
H4C—C4—H4D	56.3	C12—C13—H15	118.6 (11)
N1—C4—H4E	109.5	C13—C14—C15	119.71 (12)
H4A—C4—H4E	56.3	C13—C14—H14	119.7 (11)
H4B—C4—H4E	141.1	C15—C14—H14	120.6 (11)
H4C—C4—H4E	56.3	C14—C15—C16	120.18 (12)
H4D—C4—H4E	109.5	C14—C15—H13	120.7 (10)
N1—C4—H4F	109.5	C16—C15—H13	119.1 (10)
H4A—C4—H4F	56.3	C15—C16—C11	120.32 (12)
H4B—C4—H4F	56.3	C15—C16—H12	120.0 (9)
H4C—C4—H4F	141.1	C11—C16—H12	119.7 (9)
H4D—C4—H4F	109.5		

C3—N2—C1—C11	−122.82 (11)	C2—C1—C5—C6	166.81 (10)
C3—N2—C1—C5	114.28 (11)	C10—C5—C6—C7	1.00 (17)
C3—N2—C1—C2	−4.69 (12)	C1—C5—C6—C7	179.22 (11)
C3—N1—C2—O1	176.95 (11)	C5—C6—C7—C8	−0.96 (19)
C4—N1—C2—O1	1.9 (2)	C6—C7—C8—C9	0.5 (2)
C3—N1—C2—C1	−3.13 (13)	C7—C8—C9—C10	−0.1 (2)

C4—N1—C2—C1	−178.20 (11)	C6—C5—C10—C9	−0.59 (18)
N2—C1—C2—O1	−175.55 (11)	C1—C5—C10—C9	−178.69 (11)
C11—C1—C2—O1	−55.66 (15)	C8—C9—C10—C5	0.1 (2)
C5—C1—C2—O1	66.36 (15)	N2—C1—C11—C12	−13.45 (15)
N2—C1—C2—N1	4.54 (11)	C5—C1—C11—C12	110.82 (11)
C11—C1—C2—N1	124.42 (10)	C2—C1—C11—C12	−125.02 (11)
C5—C1—C2—N1	−113.55 (10)	N2—C1—C11—C16	169.94 (10)
C1—N2—C3—O2	−177.48 (13)	C5—C1—C11—C16	−65.79 (13)
C1—N2—C3—N1	3.15 (14)	C2—C1—C11—C16	58.36 (13)
C2—N1—C3—O2	−179.23 (12)	C16—C11—C12—C13	−0.74 (18)
C4—N1—C3—O2	−4.0 (2)	C1—C11—C12—C13	−177.36 (11)
C2—N1—C3—N2	0.17 (14)	C11—C12—C13—C14	−0.5 (2)
C4—N1—C3—N2	175.43 (11)	C12—C13—C14—C15	0.8 (2)
N2—C1—C5—C10	−126.29 (12)	C13—C14—C15—C16	0.0 (2)
C11—C1—C5—C10	108.21 (12)	C14—C15—C16—C11	−1.23 (19)
C2—C1—C5—C10	−15.06 (15)	C12—C11—C16—C15	1.58 (17)
N2—C1—C5—C6	55.57 (13)	C1—C11—C16—C15	178.25 (11)
C11—C1—C5—C6	−69.93 (12)		

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C5–C10 and C11–C16 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.928 (19)	1.922 (19)	2.8482 (13)	175.9 (16)
C4—H4*E*···*Cg*3^{ii}	0.98	2.87	3.5883 (14)	131
C8—H8···*Cg*3^{iii}	0.922 (19)	2.915 (19)	3.7061 (14)	144.7 (14)
C13—H15···*Cg*2^{iv}	0.997 (19)	2.809 (19)	139.8 (14)	3.6255 (15)

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