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

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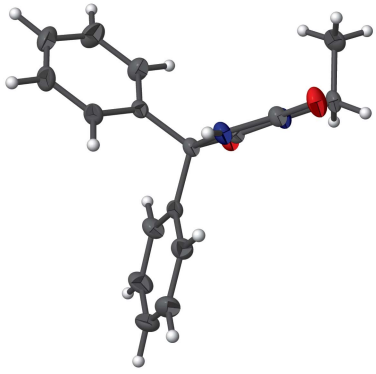
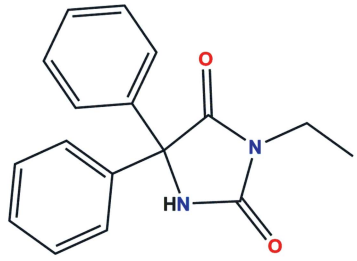
Structural data: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{17}H_{16}N_2O_2$, the phenyl rings attached at the 5-position of the imidazolidine-2,4-dione ring are inclined to the five-membered ring by 60.03 (5) and 63.04 (5)°. In the crystal, N—H···O and C—H···O hydrogen bonds form chains along the *a*-axis direction, which are connected in pairs by additional C—H···O hydrogen bonds. The chains are tied together by C—H···π(ring) interactions.

3D view



Chemical scheme



Structure description

As part of our ongoing studies of 5,5-diphenylimidazolidine-2,4-dione derivatives (Ramli *et al.*, 2017*a*,*b*; Akrad *et al.* 2017; Guerrab *et al.* 2017), 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 two phenyl rings attached at the 5-position. These are inclined to the five-membered ring by 60.03 (5) (C6–C11) and 63.04 (5)° (C12–C17).

In the crystal, N2—H2···O1^{i} and C4—H4*A*···O2^{ii} hydrogen bonds link the molecules, forming chains along the *a*-axis direction. Two adjacent chains are joined into ribbons (*i.e.* one-dimensional assemblies) parallel to [100] by inversion-related C4—H4*B*···O2^{ii} hydrogen bonds that enclose $R_2^2(8)$ rings (Table 1 and Fig. 2). The ribbons are further associated through C15—H15···*Cg*2^{iv} interactions (Table 1 and Fig. 3).

Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dion (1 g, 3.96 mmol), one equivalent of ethyl bromide (0.43 g) in absolute DMF was added and 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

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

*Cg*2 is the centroid of the C6–C11 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.885 (15)	1.947 (15)	2.8270 (11)	172.4 (13)
C4—H4*A*···O2^{ii}	0.980 (14)	2.533 (13)	3.3215 (13)	137.5 (10)
C4—H4*B*···O2^{iii}	0.977 (14)	2.552 (13)	3.3013 (12)	133.4 (10)
C15—H15···*Cg*2^{iv}	0.964 (18)	2.84 (2)	3.646 (1)	141.7 (14)

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

the solvent evaporated under reduced pressure. The residue obtained was dried and crystallized from ethanol solution to yield colourless block-shaped crystals of the title compound.

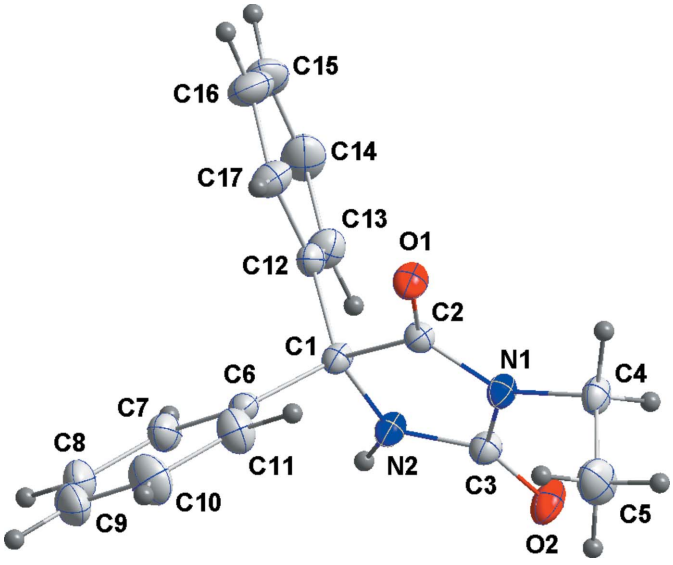


Figure 1
The title molecule showing the labeling scheme and 50% probability displacement ellipsoids for the non-hydrogen atoms.

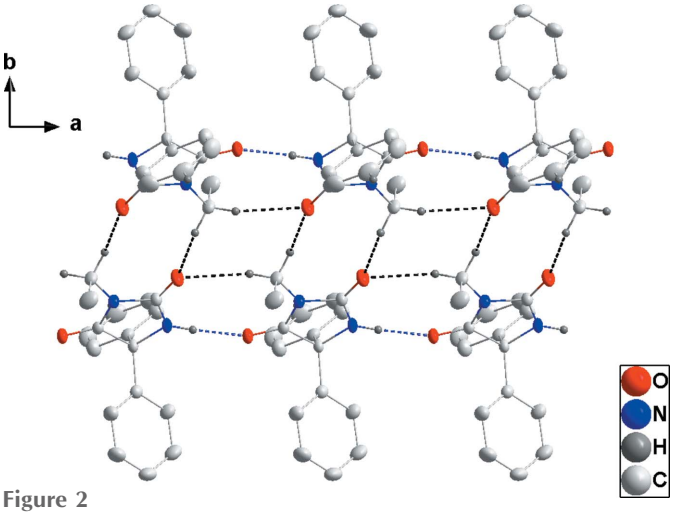


Figure 2
Detail of the chains formed along *a* by N—H···O and C—H···O hydrogen bonds (blue and black dashed lines, respectively) and linked into ribbons parallel to (0$\bar{1}$1).

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{17}H_{16}N_2O_2$
M_r	280.32
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	150
a, *b*, *c* (Å)	6.2175 (2), 15.5036 (5), 15.3736 (5)
β (°)	98.012 (1)
V (Å^3)	1467.45 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.68
Crystal size (mm)	0.27 × 0.23 × 0.14
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.84, 0.91
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22530, 2977, 2804
R_{int}	0.036
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.081, 1.04
No. of reflections	2977
No. of parameters	255
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.24, −0.18

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

Refinement

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

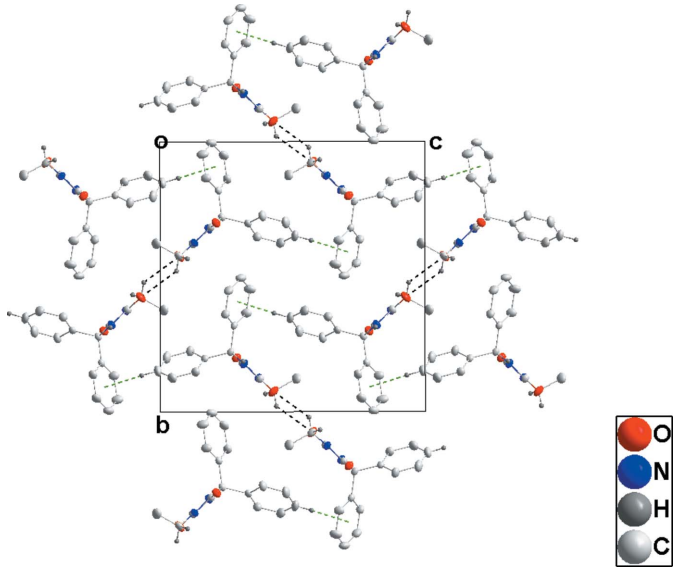


Figure 3
Packing viewed along the *a*-axis direction showing the association of chains through C—H···π(ring) interactions (green dashed lines).

Acknowledgements

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full crystallographic data

IUCrData (2017). **2**, x171591 [https://doi.org/10.1107/S2414314617015917]

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Crystal data

$C_{17}H_{16}N_2O_2$
M_r = 280.32
Monoclinic, $P2_1/n$
a = 6.2175 (2) Å
b = 15.5036 (5) Å
c = 15.3736 (5) Å
β = 98.012 (1)°
V = 1467.45 (8) Å^3
Z = 4
$F(000)$ = 592
D_x = 1.269 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9415 reflections
θ = 2.9–74.5°
μ = 0.68 mm^{-1}
T = 150 K
Block, colourles
0.27 × 0.23 × 0.14 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} = 0.91
22530 measured reflections
2977 independent reflections
2804 reflections with $I > 2\sigma(I)$
R_{int} = 0.036
θ_{max} = 74.4°, θ_{min} = 4.1°
h = −7→6
k = −19→19
l = −19→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.081
S = 1.04
2977 reflections
255 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
$w = 1/[\sigma^2(F_o^2) + (0.0329P)^2 + 0.5063P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å^{-3}
$\Delta\rho_{min}$ = −0.18 e Å^{-3}
Extinction correction: *SHELXL2016* (Sheldrick, 2015*b*), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0110 (5)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.02846 (11)	0.80012 (5)	0.28794 (5)	0.02339 (18)
O2	0.64834 (12)	0.92452 (5)	0.42726 (5)	0.0308 (2)
N1	0.30545 (13)	0.87404 (5)	0.37070 (5)	0.01958 (19)
N2	0.59292 (13)	0.82270 (5)	0.31698 (5)	0.02024 (19)
H2	0.732 (2)	0.8135 (9)	0.3127 (9)	0.032 (3)*
C1	0.40946 (14)	0.77880 (6)	0.26630 (6)	0.0176 (2)
C2	0.22036 (15)	0.81752 (6)	0.30855 (6)	0.0175 (2)
C3	0.53431 (16)	0.87836 (6)	0.37683 (6)	0.0203 (2)
C4	0.18308 (17)	0.92347 (7)	0.42886 (7)	0.0228 (2)
H4A	0.038 (2)	0.9333 (8)	0.3968 (8)	0.026 (3)*
H4B	0.256 (2)	0.9791 (9)	0.4383 (8)	0.028 (3)*
C5	0.1716 (2)	0.87682 (9)	0.51397 (8)	0.0364 (3)
H5A	0.103 (3)	0.8208 (11)	0.5029 (11)	0.049 (4)*
H5B	0.086 (3)	0.9098 (10)	0.5514 (11)	0.045 (4)*
H5C	0.320 (3)	0.8698 (11)	0.5478 (11)	0.049 (4)*
C6	0.42774 (15)	0.68098 (6)	0.27939 (6)	0.0194 (2)
C7	0.59603 (18)	0.63822 (7)	0.24610 (7)	0.0266 (2)
H7	0.697 (2)	0.6714 (9)	0.2124 (9)	0.035 (4)*
C8	0.6263 (2)	0.55032 (8)	0.25929 (8)	0.0327 (3)
H8	0.745 (3)	0.5221 (10)	0.2354 (10)	0.046 (4)*
C9	0.4889 (2)	0.50432 (7)	0.30558 (8)	0.0350 (3)
H9	0.510 (3)	0.4428 (11)	0.3164 (11)	0.050 (4)*
C10	0.3218 (2)	0.54604 (8)	0.33872 (9)	0.0384 (3)
H10	0.223 (3)	0.5123 (11)	0.3700 (11)	0.054 (5)*
C11	0.29031 (19)	0.63426 (7)	0.32556 (8)	0.0301 (3)
H11	0.168 (2)	0.6641 (9)	0.3503 (10)	0.038 (4)*
C12	0.38141 (16)	0.80267 (6)	0.16860 (6)	0.0199 (2)
C13	0.53462 (18)	0.85206 (7)	0.13385 (7)	0.0278 (2)
H13	0.665 (2)	0.8718 (9)	0.1728 (9)	0.033 (3)*
C14	0.5034 (2)	0.87438 (8)	0.04508 (8)	0.0369 (3)
H14	0.618 (3)	0.9090 (11)	0.0219 (11)	0.052 (4)*
C15	0.3187 (2)	0.84836 (9)	−0.00873 (8)	0.0389 (3)
H15	0.295 (3)	0.8651 (11)	−0.0697 (12)	0.054 (5)*
C16	0.1665 (2)	0.79836 (9)	0.02544 (8)	0.0378 (3)
H16	0.034 (3)	0.7799 (11)	−0.0117 (12)	0.055 (5)*

C17	0.19777 (18)	0.77468 (8)	0.11325 (7)	0.0291 (3)
H17	0.090 (2)	0.7373 (10)	0.1373 (10)	0.042 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0137 (3)	0.0289 (4)	0.0277 (4)	−0.0010 (3)	0.0033 (3)	−0.0060 (3)
O2	0.0207 (4)	0.0365 (4)	0.0346 (4)	−0.0050 (3)	0.0023 (3)	−0.0174 (3)
N1	0.0153 (4)	0.0230 (4)	0.0210 (4)	0.0001 (3)	0.0044 (3)	−0.0057 (3)
N2	0.0123 (4)	0.0266 (4)	0.0220 (4)	−0.0013 (3)	0.0033 (3)	−0.0072 (3)
C1	0.0130 (4)	0.0215 (5)	0.0183 (5)	−0.0011 (3)	0.0026 (3)	−0.0036 (3)
C2	0.0152 (5)	0.0194 (4)	0.0182 (4)	0.0003 (3)	0.0034 (3)	−0.0004 (3)
C3	0.0166 (5)	0.0231 (5)	0.0213 (5)	−0.0010 (4)	0.0028 (4)	−0.0028 (4)
C4	0.0194 (5)	0.0248 (5)	0.0251 (5)	0.0023 (4)	0.0059 (4)	−0.0079 (4)
C5	0.0433 (7)	0.0395 (7)	0.0295 (6)	0.0091 (6)	0.0163 (5)	−0.0010 (5)
C6	0.0188 (5)	0.0216 (5)	0.0170 (4)	0.0007 (4)	0.0002 (3)	−0.0029 (3)
C7	0.0279 (6)	0.0277 (5)	0.0250 (5)	0.0050 (4)	0.0070 (4)	−0.0021 (4)
C8	0.0356 (6)	0.0286 (6)	0.0336 (6)	0.0098 (5)	0.0042 (5)	−0.0063 (5)
C9	0.0400 (7)	0.0207 (5)	0.0424 (7)	0.0020 (5)	−0.0010 (5)	−0.0022 (5)
C10	0.0387 (7)	0.0266 (6)	0.0517 (8)	−0.0040 (5)	0.0121 (6)	0.0053 (5)
C11	0.0270 (6)	0.0263 (5)	0.0390 (6)	0.0000 (4)	0.0113 (5)	0.0010 (5)
C12	0.0209 (5)	0.0202 (5)	0.0189 (5)	0.0033 (4)	0.0042 (4)	−0.0022 (4)
C13	0.0298 (6)	0.0287 (5)	0.0259 (5)	−0.0031 (4)	0.0077 (4)	−0.0003 (4)
C14	0.0488 (7)	0.0348 (6)	0.0299 (6)	−0.0019 (5)	0.0152 (5)	0.0053 (5)
C15	0.0549 (8)	0.0416 (7)	0.0200 (5)	0.0102 (6)	0.0053 (5)	0.0049 (5)
C16	0.0388 (7)	0.0494 (7)	0.0229 (6)	0.0036 (6)	−0.0038 (5)	−0.0030 (5)
C17	0.0270 (6)	0.0371 (6)	0.0226 (5)	−0.0023 (4)	0.0011 (4)	−0.0034 (4)

Geometric parameters (Å, º)

O1—C2	1.2212 (12)	C7—H7	1.007 (14)
O2—C3	1.2094 (12)	C8—C9	1.3836 (18)
N1—C2	1.3489 (12)	C8—H8	0.972 (16)
N1—C3	1.4145 (12)	C9—C10	1.3801 (18)
N1—C4	1.4682 (12)	C9—H9	0.974 (17)
N2—C3	1.3481 (13)	C10—C11	1.3924 (17)
N2—C1	1.4572 (12)	C10—H10	0.980 (18)
N2—H2	0.885 (15)	C11—H11	1.010 (15)
C1—C6	1.5321 (13)	C12—C13	1.3859 (14)
C1—C12	1.5332 (13)	C12—C17	1.3946 (15)
C1—C2	1.5419 (12)	C13—C14	1.3949 (16)
C4—C5	1.5054 (16)	C13—H13	0.988 (14)
C4—H4A	0.980 (14)	C14—C15	1.379 (2)
C4—H4B	0.977 (14)	C14—H14	0.996 (17)
C5—H5A	0.972 (17)	C15—C16	1.382 (2)
C5—H5B	0.979 (16)	C15—H15	0.964 (18)
C5—H5C	1.002 (17)	C16—C17	1.3863 (16)
C6—C11	1.3884 (15)	C16—H16	0.979 (18)

C6—C7	1.3948 (14)	C17—H17	0.996 (16)
C7—C8	1.3868 (16)		
C2—N1—C3	111.69 (8)	C8—C7—C6	120.45 (10)
C2—N1—C4	125.81 (8)	C8—C7—H7	119.7 (8)
C3—N1—C4	122.45 (8)	C6—C7—H7	119.8 (8)
C3—N2—C1	113.45 (8)	C9—C8—C7	120.05 (11)
C3—N2—H2	120.9 (9)	C9—C8—H8	121.2 (9)
C1—N2—H2	125.6 (9)	C7—C8—H8	118.7 (9)
N2—C1—C6	110.73 (8)	C10—C9—C8	119.93 (11)
N2—C1—C12	112.63 (8)	C10—C9—H9	119.0 (10)
C6—C1—C12	111.34 (8)	C8—C9—H9	121.1 (10)
N2—C1—C2	100.31 (7)	C9—C10—C11	120.30 (11)
C6—C1—C2	112.15 (8)	C9—C10—H10	119.0 (10)
C12—C1—C2	109.23 (8)	C11—C10—H10	120.7 (10)
O1—C2—N1	126.86 (9)	C6—C11—C10	120.17 (11)
O1—C2—C1	125.42 (8)	C6—C11—H11	120.3 (8)
N1—C2—C1	107.72 (8)	C10—C11—H11	119.5 (8)
O2—C3—N2	128.77 (9)	C13—C12—C17	119.01 (10)
O2—C3—N1	124.41 (9)	C13—C12—C1	121.37 (9)
N2—C3—N1	106.81 (8)	C17—C12—C1	119.62 (9)
N1—C4—C5	111.71 (9)	C12—C13—C14	120.31 (11)
N1—C4—H4A	107.2 (8)	C12—C13—H13	119.2 (8)
C5—C4—H4A	111.1 (8)	C14—C13—H13	120.4 (8)
N1—C4—H4B	106.3 (8)	C15—C14—C13	120.35 (11)
C5—C4—H4B	111.9 (8)	C15—C14—H14	121.3 (10)
H4A—C4—H4B	108.4 (11)	C13—C14—H14	118.3 (10)
C4—C5—H5A	110.4 (10)	C14—C15—C16	119.53 (11)
C4—C5—H5B	110.8 (9)	C14—C15—H15	120.3 (10)
H5A—C5—H5B	108.1 (13)	C16—C15—H15	120.1 (10)
C4—C5—H5C	110.6 (9)	C15—C16—C17	120.55 (12)
H5A—C5—H5C	110.1 (13)	C15—C16—H16	120.5 (10)
H5B—C5—H5C	106.7 (13)	C17—C16—H16	118.9 (10)
C11—C6—C7	119.10 (10)	C16—C17—C12	120.22 (11)
C11—C6—C1	122.95 (9)	C16—C17—H17	120.3 (9)
C7—C6—C1	117.90 (9)	C12—C17—H17	119.5 (9)
C3—N2—C1—C6	−119.72 (9)	C12—C1—C6—C7	58.81 (11)
C3—N2—C1—C12	114.89 (9)	C2—C1—C6—C7	−178.45 (8)
C3—N2—C1—C2	−1.12 (10)	C11—C6—C7—C8	−0.30 (16)
C3—N1—C2—O1	−179.73 (9)	C1—C6—C7—C8	177.20 (10)
C4—N1—C2—O1	2.79 (16)	C6—C7—C8—C9	0.14 (17)
C3—N1—C2—C1	−0.49 (11)	C7—C8—C9—C10	−0.09 (18)
C4—N1—C2—C1	−177.97 (9)	C8—C9—C10—C11	0.2 (2)
N2—C1—C2—O1	−179.81 (9)	C7—C6—C11—C10	0.42 (17)
C6—C1—C2—O1	−62.27 (12)	C1—C6—C11—C10	−176.94 (11)
C12—C1—C2—O1	61.65 (12)	C9—C10—C11—C6	−0.4 (2)
N2—C1—C2—N1	0.93 (10)	N2—C1—C12—C13	7.69 (13)

C6—C1—C2—N1	118.48 (8)	C6—C1—C12—C13	−117.37 (10)
C12—C1—C2—N1	−117.60 (9)	C2—C1—C12—C13	118.23 (10)
C1—N2—C3—O2	−178.95 (10)	N2—C1—C12—C17	−171.99 (9)
C1—N2—C3—N1	0.90 (11)	C6—C1—C12—C17	62.94 (12)
C2—N1—C3—O2	179.64 (10)	C2—C1—C12—C17	−61.46 (11)
C4—N1—C3—O2	−2.78 (16)	C17—C12—C13—C14	0.96 (16)
C2—N1—C3—N2	−0.22 (11)	C1—C12—C13—C14	−178.72 (10)
C4—N1—C3—N2	177.36 (9)	C12—C13—C14—C15	0.72 (18)
C2—N1—C4—C5	91.96 (13)	C13—C14—C15—C16	−1.38 (19)
C3—N1—C4—C5	−85.27 (12)	C14—C15—C16—C17	0.3 (2)
N2—C1—C6—C11	110.08 (11)	C15—C16—C17—C12	1.35 (19)
C12—C1—C6—C11	−123.80 (10)	C13—C12—C17—C16	−1.99 (16)
C2—C1—C6—C11	−1.06 (13)	C1—C12—C17—C16	177.70 (10)
N2—C1—C6—C7	−67.31 (11)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C6–C11 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O1^{i}	0.885 (15)	1.947 (15)	2.8270 (11)	172.4 (13)
C4—H4*A*···O2^{ii}	0.980 (14)	2.533 (13)	3.3215 (13)	137.5 (10)
C4—H4*B*···O2^{iii}	0.977 (14)	2.552 (13)	3.3013 (12)	133.4 (10)
C15—H15···*Cg*2^{iv}	0.964 (18)	2.84 (2)	3.646 (1)	141.7 (14)

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