

# Ethyl 2-(2,5-dioxo-4,4-diphenylimidazolidin-1-yl)-acetate

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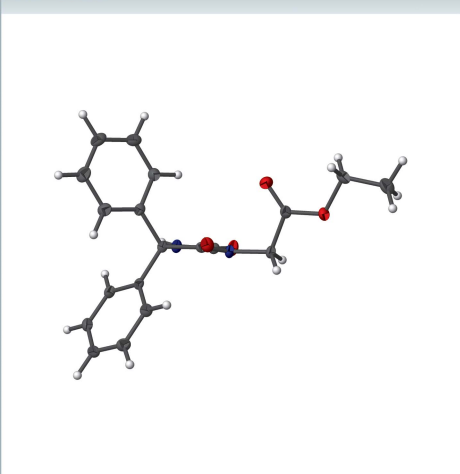
Keywords: crystal structure; imidazole; hydrogen bonds.

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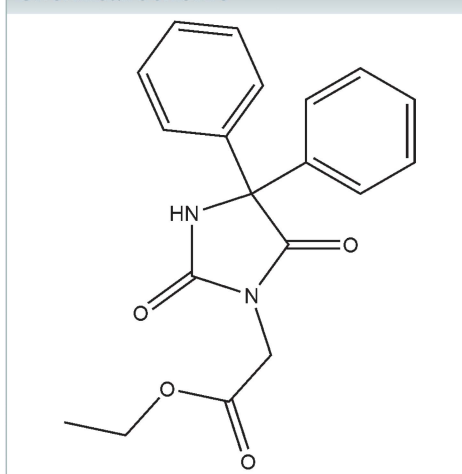
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

The five-membered ring of the title compound, C<sub>19</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>, adopts an envelope conformation. In the crystal, pairwise N—H···O hydrogen bonds form centrosymmetric dimers which are connected into chains parallel to the *c*-axis direction by pairwise C—H···O hydrogen bonds. A second set of C—H···O hydrogen bonds links these chains into sheets oriented parallel to (100). A combination of additional C—H···O hydrogen bonds and C—H··· $\pi$ (ring) interactions combine the sheets into a three-dimensional network.

## 3D view



## Chemical scheme



## Structure description

An enormous variety of hydantoin derivatives with varied pharmaceutical and medicinal applications, have been reported (Weichet, 1974; Havera & Strycker, 1976; Khodair *et al.*, 1997; Thenmozhiyal *et al.*, 2004). As a continuation of our research into hydantoin derivatives (Akrad *et al.*, 2017), the title compound (Fig. 1) was prepared and its molecular and crystal structure is reported here.

A puckering analysis of the five-membered ring gave the parameters  $Q(2) = 0.0712(16)$  Å and  $\varphi(2) = 279.3(13)^\circ$ . The conformation of the ring is best described as an envelope on C1. The dihedral angle between the C4–C9 benzene ring and the mean plane of the five-membered ring is  $80.56(6)^\circ$ , while the corresponding angle for the C10–C15 ring is  $61.79(4)^\circ$ .

In the crystal, the molecules form centrosymmetric dimers through complementary N1—H1···O2 hydrogen bonds. The dimers are linked into chains running parallel to the *c*-axis direction by pairwise C15—H15···O1 hydrogen bonds (Table 1 and Figs. 2 and 3). The chains are formed into sheets oriented parallel to (100) by C16—H16A···O4 hydrogen bonds (Table 2 and Figs. 2 and 3) while the sheets are associated by a

**Table 1**

Hydrogen-bond geometry (Å, °).

*Cg*2 and *Cg*3 are the centroids of the C4–C9 and C10–C15 benzene rings, respectively,

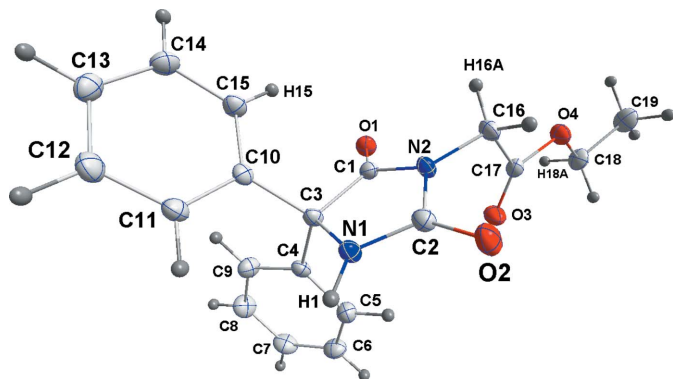
<i>D</i> –H··· <i>A</i>	<i>D</i> –H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> –H··· <i>A</i>
N1–H1···O2 <sup>i</sup>	0.91 (2)	1.91 (2)	2.8203 (17)	172.6 (17)
C15–H15···O1 <sup>ii</sup>	0.954 (18)	2.591 (18)	3.332 (2)	134.8 (14)
C16–H16A···O4 <sup>iii</sup>	0.971 (18)	2.653 (19)	3.415 (2)	135.7 (13)
C18–H18A···O3 <sup>iv</sup>	0.977 (18)	2.658 (19)	3.633 (2)	175.9 (14)
C7–H7··· <i>Cg</i> 3 <sup>v</sup>	1.01 (2)	2.976 (18)	3.6661 (19)	126.6 (13)
C12–H12··· <i>Cg</i> 2 <sup>vi</sup>	0.996 (18)	2.701 (18)	3.6673 (19)	163.1 (18)
C19–H19A··· <i>Cg</i> 2	1.03 (2)	2.83 (2)	3.572 (2)	129.0 (16)

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $-x+1, -y, -z+1$ ; (iv)  $-x+2, -y, -z+1$ ; (v)  $x+1, y, z$ ; (vi)  $-x+1, -y+2, -z$ .

combination of C18–H18A···O3 hydrogen bonds and C7–H7··· $\pi$ (*Cg*3) interactions (Table 1 and Figs. 2 and 3). The packing is further aided by C12–H12··· $\pi$ (*Cg*2) and C19–H19··· $\pi$ (*Cg*2) (interactions (Table 2 and Figs. 2 and 3).

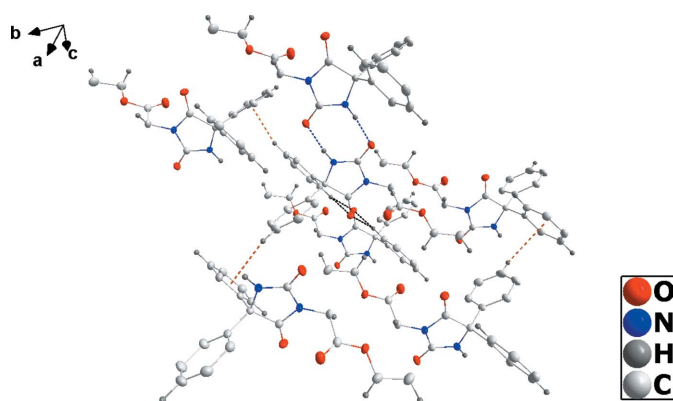
### Synthesis and crystallization

To a solution of 5,5-diphenylimidazolidine-2,4-dione (3.96 mol, 1 g) in 20 ml of ethanol was added ethyl bromo-



**Figure 1**

The structure of the title molecule, showing the atom-labeling scheme and 50% probability ellipsoids.



**Figure 2**

Details of the intermolecular interactions. N–H···O, C–H···O and C–H··· $\pi$ (ring) interactions are shown as blue, black and orange dotted lines, respectively.

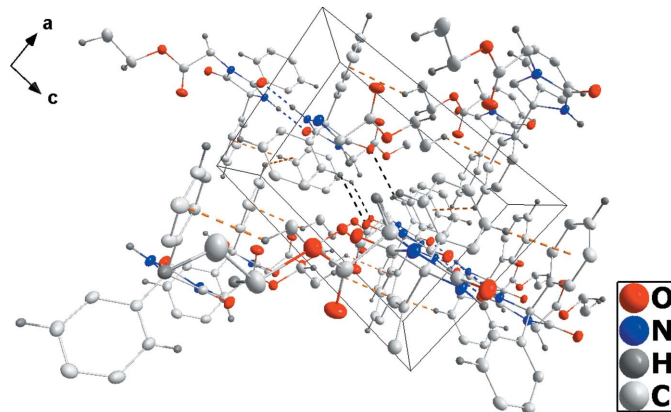
**Table 2**

Experimental details.

Crystal data	$C_{19}H_{18}N_2O_4$
Chemical formula	338.35
<i>M<sub>r</sub></i>	Triclinic, $P\bar{1}$
Crystal system, space group	100
Temperature (K)	8.5041 (5), 8.6959 (5), 12.5024 (8)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	71.002 (1), 88.165 (1), 72.572 (1)
$\alpha$ , $\beta$ , $\gamma$ (°)	831.87 (9)
<i>V</i> (Å <sup>3</sup> )	2
<i>Z</i>	Mo <i>K</i> $\alpha$
Radiation type	0.10
$\mu$ (mm <sup>-1</sup> )	0.43 × 0.29 × 0.26
Crystal size (mm)	
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (TWINABS; Sheldrick, 2009)
<i>T<sub>min</sub></i> , <i>T<sub>max</sub></i>	0.96, 0.97
No. of measured, independent and observed [ <i>I</i> > 2 $\sigma$ ( <i>I</i> )] reflections	31786, 31786, 21954
<i>R<sub>int</sub></i>	0.031
( <i>sin</i> $\theta$ / $\lambda$ ) <sub>max</sub> (Å <sup>-1</sup> )	0.686
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.047, 0.130, 1.06
No. of reflections	31786
No. of parameters	299
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$ , $\Delta\rho_{min}$ (e Å <sup>-3</sup> )	0.51, -0.32

Computer programs: APEX3 and SAINT (Bruker, 2016), SHELXT (Sheldrick, 2015a), SHELXL2014 (Sheldrick, 2015b), DIAMOND (Brandenburg & Putz, 2012) and SHELXTL (Sheldrick, 2008b).

acetate (3.96 mol, 438 mm l), K<sub>2</sub>CO<sub>3</sub> (3.96 mol) and a catalytic amount of tetrabutylammonium bromide. The mixture was stirred at room temperature for 24 h. Progress was monitored by TLC and, when complete, the solid material was removed by filtration and the solvent evaporated under vacuum. The solid product was purified by recrystallization from ethanol solution to afford colourless block-like crystals of the title compound (yield 67%).



**Figure 3**

The crystal packing, viewed along the *b* axis. The color code for the intermolecular interactions is similar to that given in Fig. 2.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Analysis of the 1461 reflections having  $I/\sigma(I) > 13$  and chosen from the full data set with *CELL\_NOW* (Sheldrick, 2008a) showed the crystal to belong to the triclinic system and to consist of two major and at least two minor components. Since 91% of the reflections could be indexed on the two major components, it was decided to treat the crystal as having two components. The raw data were processed using the multi-component version of *SAINTE* under control of the two-component orientation file generated by *CELL\_NOW*.

## Acknowledgements

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## full crystallographic data

*IUCrData* (2017). 2, x170098 [https://doi.org/10.1107/S2414314617000980]

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## Ethyl 2-(2,5-dioxo-4,4-diphenylimidazolidin-1-yl)acetate

*Crystal data*

$C_{19}H_{18}N_2O_4$	$Z = 2$
$M_r = 338.35$	$F(000) = 356$
Triclinic, $P\bar{1}$	$D_x = 1.351 \text{ Mg m}^{-3}$
$a = 8.5041 (5) \text{ \AA}$	Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$
$b = 8.6959 (5) \text{ \AA}$	Cell parameters from 9879 reflections
$c = 12.5024 (8) \text{ \AA}$	$\theta = 2.6\text{--}29.1^\circ$
$\alpha = 71.002 (1)^\circ$	$\mu = 0.10 \text{ mm}^{-1}$
$\beta = 88.165 (1)^\circ$	$T = 100 \text{ K}$
$\gamma = 72.572 (1)^\circ$	Column, colourless
$V = 831.87 (9) \text{ \AA}^3$	$0.43 \times 0.29 \times 0.26 \text{ mm}$

*Data collection*

Bruker SMART APEX CCD diffractometer	31786 measured reflections
Radiation source: fine-focus sealed tube	31786 independent reflections
Graphite monochromator	21954 reflections with $I > 2\sigma(I)$
Detector resolution: 8.3333 pixels $\text{mm}^{-1}$	$R_{\text{int}} = 0.031$
$\varphi$ and $\omega$ scans	$\theta_{\text{max}} = 29.2^\circ$ , $\theta_{\text{min}} = 1.7^\circ$
Absorption correction: multi-scan ( <i>TWINABS</i> ; Sheldrick, 2009)	$h = -11 \rightarrow 11$
$T_{\text{min}} = 0.96$ , $T_{\text{max}} = 0.97$	$k = -11 \rightarrow 11$
	$l = -17 \rightarrow 17$

*Refinement*

Refinement on $F^2$	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.047$	All H-atom parameters refined
$wR(F^2) = 0.130$	$w = 1/[\sigma^2(F_o^2) + (0.0527P)^2 + 0.0554P]$
$S = 1.06$	where $P = (F_o^2 + 2F_c^2)/3$
31786 reflections	$(\Delta/\sigma)_{\text{max}} < 0.001$
299 parameters	$\Delta\rho_{\text{max}} = 0.51 \text{ e \AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.32 \text{ e \AA}^{-3}$
Primary atom site location: structure-invariant direct methods	

*Special details*

**Experimental.** The diffraction data were obtained from 3 sets of 400 frames, each of width  $0.5^\circ$  in  $\omega$ , collected at  $\varphi = 0.00, 90.00$  and  $180.00^\circ$  and 2 sets of 800 frames, each of width  $0.45^\circ$  in  $\varphi$ , collected at  $\omega = -30.00$  and  $210.00^\circ$ . The scan time was 7.5 sec/frame. Analysis of 1461 reflections having  $I/\sigma(I) > 13$  and chosen from the full data set with *CELL\_NOW* (Sheldrick, 2008) showed the crystal to belong to the triclinic system and to consist of two major and at least two minor components. Since 91% of the reflections could be indexed on the two major components, it was decided to treat the crystal as having two components. The raw data were processed using the multi-component version of *SAINTE* under control of the two-component orientation file generated by *CELL\_NOW*.

**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  $F^2 > 2\sigma(F^2)$  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 structure was refined as a two-component twin.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.66938 (14)	0.42374 (14)	0.40959 (9)	0.0212 (3)
O2	0.48505 (14)	0.30571 (14)	0.11562 (9)	0.0236 (3)
O3	0.85782 (14)	0.08216 (15)	0.34383 (10)	0.0273 (3)
O4	0.73722 (13)	-0.10111 (13)	0.46031 (9)	0.0205 (3)
N1	0.54197 (16)	0.54676 (16)	0.12269 (11)	0.0163 (3)
H1	0.534 (2)	0.603 (2)	0.0466 (17)	0.033 (5)*
N2	0.55850 (16)	0.33561 (16)	0.28322 (10)	0.0168 (3)
C1	0.61488 (18)	0.44787 (19)	0.31540 (12)	0.0160 (3)
C2	0.52414 (18)	0.39103 (19)	0.16561 (13)	0.0165 (3)
C3	0.59387 (18)	0.60646 (19)	0.20887 (12)	0.0143 (3)
C4	0.75973 (18)	0.64172 (19)	0.18369 (12)	0.0157 (3)
C5	0.8844 (2)	0.5282 (2)	0.14690 (14)	0.0207 (3)
H5	0.862 (2)	0.428 (2)	0.1372 (15)	0.025 (5)*
C6	1.0353 (2)	0.5584 (2)	0.12179 (14)	0.0249 (4)
H6	1.121 (2)	0.476 (2)	0.0956 (15)	0.029 (5)*
C7	1.0626 (2)	0.7013 (2)	0.13345 (15)	0.0270 (4)
H7	1.171 (2)	0.725 (2)	0.1153 (16)	0.036 (5)*
C8	0.9406 (2)	0.8130 (2)	0.17129 (15)	0.0272 (4)
H8	0.956 (2)	0.912 (2)	0.1786 (16)	0.035 (5)*
C9	0.7894 (2)	0.7831 (2)	0.19693 (14)	0.0218 (4)
H9	0.702 (2)	0.864 (2)	0.2216 (15)	0.026 (5)*
C10	0.45633 (18)	0.76081 (19)	0.21919 (13)	0.0151 (3)
C11	0.3922 (2)	0.8989 (2)	0.12049 (14)	0.0190 (3)
H11	0.437 (2)	0.894 (2)	0.0486 (15)	0.021 (4)*
C12	0.2686 (2)	1.0425 (2)	0.12466 (15)	0.0219 (4)
H12	0.222 (2)	1.140 (2)	0.0536 (15)	0.027 (5)*
C13	0.2049 (2)	1.0487 (2)	0.22742 (14)	0.0218 (4)
H13	0.117 (2)	1.150 (2)	0.2302 (14)	0.025 (5)*

C14	0.2662 (2)	0.9111 (2)	0.32521 (15)	0.0223 (4)
H14	0.220 (2)	0.911 (2)	0.3975 (16)	0.028 (5)*
C15	0.3926 (2)	0.7678 (2)	0.32182 (14)	0.0191 (3)
H15	0.436 (2)	0.676 (2)	0.3905 (15)	0.024 (5)*
C16	0.5624 (2)	0.1679 (2)	0.35767 (14)	0.0185 (3)
H16A	0.515 (2)	0.177 (2)	0.4279 (16)	0.025 (5)*
H16B	0.497 (2)	0.126 (2)	0.3197 (15)	0.026 (5)*
C17	0.73753 (19)	0.0476 (2)	0.38441 (13)	0.0180 (3)
C18	0.8993 (2)	-0.2297 (2)	0.50004 (16)	0.0238 (4)
H18A	0.964 (2)	-0.185 (2)	0.5386 (15)	0.026 (5)*
H18B	0.955 (2)	-0.249 (2)	0.4347 (16)	0.027 (5)*
C19	0.8664 (2)	-0.3865 (2)	0.57850 (17)	0.0293 (4)
H19A	0.977 (3)	-0.481 (3)	0.6116 (17)	0.039 (6)*
H19B	0.801 (3)	-0.364 (2)	0.6446 (17)	0.039 (6)*
H19C	0.799 (3)	-0.430 (2)	0.5386 (17)	0.039 (6)*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0269 (6)	0.0215 (6)	0.0139 (6)	-0.0064 (5)	-0.0011 (4)	-0.0048 (5)
O2	0.0338 (7)	0.0224 (6)	0.0201 (6)	-0.0164 (5)	0.0009 (5)	-0.0072 (5)
O3	0.0228 (6)	0.0235 (7)	0.0349 (7)	-0.0082 (5)	0.0108 (5)	-0.0087 (5)
O4	0.0216 (6)	0.0148 (6)	0.0212 (6)	-0.0043 (4)	0.0010 (4)	-0.0018 (5)
N1	0.0224 (7)	0.0167 (7)	0.0116 (6)	-0.0089 (5)	0.0002 (5)	-0.0042 (5)
N2	0.0217 (7)	0.0142 (7)	0.0142 (6)	-0.0080 (5)	0.0010 (5)	-0.0020 (5)
C1	0.0159 (7)	0.0163 (8)	0.0150 (7)	-0.0040 (6)	0.0029 (5)	-0.0054 (6)
C2	0.0164 (7)	0.0174 (8)	0.0161 (7)	-0.0066 (6)	0.0012 (6)	-0.0048 (6)
C3	0.0177 (7)	0.0153 (8)	0.0112 (7)	-0.0070 (6)	0.0011 (5)	-0.0046 (6)
C4	0.0183 (7)	0.0176 (8)	0.0113 (7)	-0.0073 (6)	0.0006 (5)	-0.0031 (6)
C5	0.0216 (8)	0.0192 (8)	0.0209 (8)	-0.0065 (6)	0.0015 (6)	-0.0060 (7)
C6	0.0190 (8)	0.0295 (10)	0.0241 (9)	-0.0048 (7)	0.0028 (6)	-0.0085 (8)
C7	0.0197 (8)	0.0365 (11)	0.0258 (9)	-0.0144 (8)	0.0017 (7)	-0.0064 (8)
C8	0.0271 (9)	0.0302 (10)	0.0321 (10)	-0.0171 (8)	0.0018 (7)	-0.0130 (8)
C9	0.0218 (8)	0.0254 (9)	0.0237 (9)	-0.0103 (7)	0.0033 (6)	-0.0123 (7)
C10	0.0155 (7)	0.0146 (8)	0.0173 (8)	-0.0077 (6)	0.0012 (5)	-0.0051 (6)
C11	0.0216 (8)	0.0188 (8)	0.0166 (8)	-0.0087 (6)	0.0035 (6)	-0.0036 (7)
C12	0.0219 (8)	0.0173 (8)	0.0238 (9)	-0.0074 (6)	0.0002 (6)	-0.0019 (7)
C13	0.0179 (8)	0.0182 (8)	0.0311 (9)	-0.0058 (6)	0.0027 (7)	-0.0103 (7)
C14	0.0222 (8)	0.0260 (9)	0.0221 (9)	-0.0085 (7)	0.0054 (6)	-0.0119 (7)
C15	0.0217 (8)	0.0203 (8)	0.0154 (8)	-0.0069 (6)	0.0010 (6)	-0.0055 (7)
C16	0.0204 (8)	0.0153 (8)	0.0182 (8)	-0.0077 (6)	0.0027 (6)	-0.0014 (6)
C17	0.0224 (8)	0.0157 (8)	0.0176 (8)	-0.0064 (6)	0.0032 (6)	-0.0073 (6)
C18	0.0218 (8)	0.0188 (9)	0.0272 (9)	-0.0006 (7)	-0.0012 (7)	-0.0077 (7)
C19	0.0322 (10)	0.0221 (9)	0.0264 (10)	-0.0013 (8)	-0.0018 (8)	-0.0047 (8)

*Geometric parameters (Å, °)*

O1—C1	1.2088 (17)	C8—H8	0.943 (19)
O2—C2	1.2307 (18)	C9—H9	0.978 (18)
O3—C17	1.2025 (19)	C10—C15	1.389 (2)
O4—C17	1.3325 (19)	C10—C11	1.396 (2)
O4—C18	1.4681 (19)	C11—C12	1.386 (2)
N1—C2	1.3378 (19)	C11—H11	0.975 (18)
N1—C3	1.4687 (18)	C12—C13	1.389 (2)
N1—H1	0.91 (2)	C12—H12	0.996 (18)
N2—C1	1.3760 (19)	C13—C14	1.383 (2)
N2—C2	1.4005 (19)	C13—H13	0.978 (18)
N2—C16	1.4433 (19)	C14—C15	1.392 (2)
C1—C3	1.543 (2)	C14—H14	0.973 (19)
C3—C10	1.533 (2)	C15—H15	0.954 (18)
C3—C4	1.533 (2)	C16—C17	1.515 (2)
C4—C9	1.387 (2)	C16—H16A	0.971 (18)
C4—C5	1.395 (2)	C16—H16B	0.958 (18)
C5—C6	1.392 (2)	C18—C19	1.497 (3)
C5—H5	0.989 (18)	C18—H18A	0.977 (18)
C6—C7	1.383 (2)	C18—H18B	0.968 (19)
C6—H6	0.985 (19)	C19—H19A	1.03 (2)
C7—C8	1.381 (3)	C19—H19B	1.02 (2)
C7—H7	1.01 (2)	C19—H19C	0.99 (2)
C8—C9	1.393 (2)		
C17—O4—C18	116.34 (13)	C15—C10—C3	122.84 (13)
C2—N1—C3	113.27 (13)	C11—C10—C3	118.04 (14)
C2—N1—H1	122.0 (12)	C12—C11—C10	120.65 (15)
C3—N1—H1	124.3 (12)	C12—C11—H11	120.4 (10)
C1—N2—C2	111.55 (12)	C10—C11—H11	118.9 (10)
C1—N2—C16	124.09 (13)	C11—C12—C13	120.01 (15)
C2—N2—C16	123.48 (13)	C11—C12—H12	120.1 (10)
O1—C1—N2	125.56 (14)	C13—C12—H12	119.8 (10)
O1—C1—C3	127.87 (14)	C14—C13—C12	119.56 (16)
N2—C1—C3	106.56 (12)	C14—C13—H13	120.5 (10)
O2—C2—N1	128.79 (14)	C12—C13—H13	120.0 (10)
O2—C2—N2	123.61 (14)	C13—C14—C15	120.65 (16)
N1—C2—N2	107.59 (13)	C13—C14—H14	120.7 (11)
N1—C3—C10	109.98 (11)	C15—C14—H14	118.6 (11)
N1—C3—C4	110.84 (12)	C10—C15—C14	120.00 (15)
C10—C3—C4	113.22 (12)	C10—C15—H15	120.4 (11)
N1—C3—C1	100.42 (11)	C14—C15—H15	119.6 (11)
C10—C3—C1	111.28 (12)	N2—C16—C17	111.31 (13)
C4—C3—C1	110.38 (12)	N2—C16—H16A	109.3 (11)
C9—C4—C5	119.09 (14)	C17—C16—H16A	109.1 (10)
C9—C4—C3	121.76 (14)	N2—C16—H16B	107.2 (11)
C5—C4—C3	119.15 (13)	C17—C16—H16B	110.0 (11)

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C6—C5—C4	120.39 (16)	H16A—C16—H16B	109.8 (15)
C6—C5—H5	121.0 (11)	O3—C17—O4	125.56 (15)
C4—C5—H5	118.6 (11)	O3—C17—C16	125.00 (15)
C7—C6—C5	120.01 (17)	O4—C17—C16	109.44 (13)
C7—C6—H6	121.3 (11)	O4—C18—C19	106.36 (15)
C5—C6—H6	118.7 (11)	O4—C18—H18A	108.3 (11)
C8—C7—C6	119.93 (16)	C19—C18—H18A	112.0 (11)
C8—C7—H7	119.3 (11)	O4—C18—H18B	108.4 (11)
C6—C7—H7	120.8 (11)	C19—C18—H18B	112.7 (10)
C7—C8—C9	120.29 (17)	H18A—C18—H18B	108.9 (15)
C7—C8—H8	121.1 (12)	C18—C19—H19A	109.9 (11)
C9—C8—H8	118.6 (12)	C18—C19—H19B	112.2 (11)
C4—C9—C8	120.27 (16)	H19A—C19—H19B	108.1 (16)
C4—C9—H9	119.2 (10)	C18—C19—H19C	111.1 (12)
C8—C9—H9	120.5 (10)	H19A—C19—H19C	109.3 (16)
C15—C10—C11	119.11 (14)	H19B—C19—H19C	106.1 (17)
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C2—N2—C1—O1	-172.06 (14)	C4—C5—C6—C7	0.1 (2)
C16—N2—C1—O1	-2.5 (2)	C5—C6—C7—C8	0.8 (3)
C2—N2—C1—C3	8.07 (16)	C6—C7—C8—C9	-0.5 (3)
C16—N2—C1—C3	177.66 (13)	C5—C4—C9—C8	1.4 (2)
C3—N1—C2—O2	-178.70 (15)	C3—C4—C9—C8	-178.82 (14)
C3—N1—C2—N2	1.34 (17)	C7—C8—C9—C4	-0.6 (3)
C1—N2—C2—O2	173.90 (14)	N1—C3—C10—C15	126.47 (15)
C16—N2—C2—O2	4.2 (2)	C4—C3—C10—C15	-108.93 (16)
C1—N2—C2—N1	-6.13 (17)	C1—C3—C10—C15	16.09 (19)
C16—N2—C2—N1	-175.80 (13)	N1—C3—C10—C11	-52.87 (17)
C2—N1—C3—C10	-114.14 (14)	C4—C3—C10—C11	71.73 (17)
C2—N1—C3—C4	119.90 (14)	C1—C3—C10—C11	-163.25 (13)
C2—N1—C3—C1	3.23 (16)	C15—C10—C11—C12	1.1 (2)
O1—C1—C3—N1	173.53 (15)	C3—C10—C11—C12	-179.49 (13)
N2—C1—C3—N1	-6.61 (14)	C10—C11—C12—C13	-1.3 (2)
O1—C1—C3—C10	-70.07 (19)	C11—C12—C13—C14	0.3 (2)
N2—C1—C3—C10	109.79 (13)	C12—C13—C14—C15	0.9 (2)
O1—C1—C3—C4	56.5 (2)	C11—C10—C15—C14	0.1 (2)
N2—C1—C3—C4	-123.62 (13)	C3—C10—C15—C14	-179.25 (14)
N1—C3—C4—C9	138.84 (14)	C13—C14—C15—C10	-1.1 (2)
C10—C3—C4—C9	14.70 (19)	C1—N2—C16—C17	-70.75 (19)
C1—C3—C4—C9	-110.80 (16)	C2—N2—C16—C17	97.63 (17)
N1—C3—C4—C5	-41.42 (18)	C18—O4—C17—O3	2.5 (2)
C10—C3—C4—C5	-165.55 (13)	C18—O4—C17—C16	-176.91 (13)
C1—C3—C4—C5	68.94 (17)	N2—C16—C17—O3	-4.4 (2)
C9—C4—C5—C6	-1.2 (2)	N2—C16—C17—O4	174.99 (12)
C3—C4—C5—C6	179.04 (14)	C17—O4—C18—C19	-176.90 (14)

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*Hydrogen-bond geometry (Å, °)*

Cg2 and Cg3 are the centroids of the C4–C9 and C10–C15 benzene rings, respectively.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N1—H1 $\cdots$ O2 <sup>i</sup>	0.91 (2)	1.91 (2)	2.8203 (17)	172.6 (17)
C15—H15 $\cdots$ O1 <sup>ii</sup>	0.954 (18)	2.591 (18)	3.332 (2)	134.8 (14)
C16—H16 <i>A</i> $\cdots$ O4 <sup>iii</sup>	0.971 (18)	2.653 (19)	3.415 (2)	135.7 (13)
C18—H18 <i>A</i> $\cdots$ O3 <sup>iv</sup>	0.977 (18)	2.658 (19)	3.633 (2)	175.9 (14)
C7—H7 $\cdots$ Cg3 <sup>v</sup>	1.01 (2)	2.976 (18)	3.6661 (19)	126.6 (13)
C12—H12 $\cdots$ Cg2 <sup>vi</sup>	0.996 (18)	2.701 (18)	3.6673 (19)	163.1 (18)
C19—H19 <i>A</i> $\cdots$ Cg2	1.03 (2)	2.83 (2)	3.572 (2)	129.0 (16)

Symmetry codes: (i)  $-x+1, -y+1, -z$ ; (ii)  $-x+1, -y+1, -z+1$ ; (iii)  $-x+1, -y, -z+1$ ; (iv)  $-x+2, -y, -z+1$ ; (v)  $x+1, y, z$ ; (vi)  $-x+1, -y+2, -z$ .