

## Crystal structure of 2-(1,3-dioxindan-2-yl)isoquinoline-1,3,4-trione

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In the title isoquinoline-1,3,4-trione derivative, C<sub>18</sub>H<sub>9</sub>NO<sub>5</sub>, the five-membered ring of the indane fragment adopts an envelope conformation with the nitrogen-substituted C atom being the flap. The planes of the indane benzene ring and the isoquinoline-1,3,4-trione ring make a dihedral angle of 82.06 (6)°. In the crystal, molecules are linked into chains extending along the *bc* plane via C—H···O hydrogen-bonding interactions, enclosing R<sub>2</sub><sup>2</sup>(8) and R<sub>2</sub><sup>2</sup>(10) loops. The chains are further connected by π–π stacking interactions, with centroid-to-centroid distances of 3.9050 (7) Å, forming layers parallel to the *b* axis.

**Keywords:** crystal structure; isoquinoline-1,3,4-trione derivative; synthesis; hydrogen bonding; pharmacological properties.

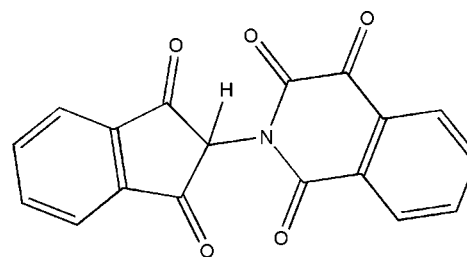
**CCDC reference:** 1036387

### 1. Related literature

For the biological activity of isoquinoline-1,3,4-triones, see: Chen *et al.* (2006); Du *et al.* (2008). For related isoquinoline-1,3,4-trione structures, see: Yu *et al.* (2010); Huang *et al.* (2013). For synthetic applications of isoquinoline-1,3,4-trione, see: Yu *et al.* (2010); Huang *et al.* (2011, 2013). For the synthesis of related compounds, see: Chen *et al.* (2006); Du *et al.* (2008); Ghalib *et al.* 2011; Schaber *et al.* 2004; Huang *et al.* (2013).

† Thomson Reuters ResearcherID: C-3194-2011.

§ Thomson Reuters ResearcherID: A-3561-2009.



### 2. Experimental

#### 2.1. Crystal data

C<sub>18</sub>H<sub>9</sub>NO<sub>5</sub>  
*M<sub>r</sub>* = 319.26  
 Monoclinic, *P*2<sub>1</sub>/*c*  
*a* = 12.6080 (1) Å  
*b* = 13.6849 (2) Å  
*c* = 8.4467 (1) Å  
 $\beta$  = 102.051 (1)°  
*V* = 1425.27 (3) Å<sup>3</sup>  
*Z* = 4  
 Cu K $\alpha$  radiation  
 $\mu$  = 0.93 mm<sup>-1</sup>  
*T* = 100 K  
 0.24 × 0.15 × 0.14 mm

#### 2.2. Data collection

Bruker APEXII CCD diffractometer  
 Absorption correction: multi-scan (SADABS; Bruker, 2009)  
*T<sub>min</sub>* = 0.808, *T<sub>max</sub>* = 0.879  
 9639 measured reflections  
 2597 independent reflections  
 2458 reflections with *I* > 2σ(*I*)  
*R<sub>int</sub>* = 0.024

#### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.093$   
*S* = 1.04  
 2597 reflections  
 217 parameters  
 H-atom parameters constrained  
 $\Delta\rho_{\max} = 0.27$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.20$  e Å<sup>-3</sup>

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

<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>
C6—H6A···O2 <sup>i</sup>	0.95	2.54	3.4862 (16)	171
C7—H7A···O1 <sup>i</sup>	0.95	2.51	3.1397 (15)	124
C10—H10A···O5 <sup>ii</sup>	1.00	2.24	3.2022 (15)	161
C13—H13A···O5 <sup>iii</sup>	0.95	2.37	3.2852 (16)	163
C16—H16A···O4 <sup>iv</sup>	0.95	2.50	3.3596 (17)	150

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

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2013 (Sheldrick, 2008); molecular graphics: SHELXTL (Sheldrick, 2008); software used to prepare material for publication: SHELXTL and PLATON (Spek, 2009).

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Supporting information for this paper is available from the IUCr electronic archives (Reference: ZL2607).

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## supporting information

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## Crystal structure of 2-(1,3-dioxindan-2-yl)isoquinoline-1,3,4-trione

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### S1. Chemical context

Urea has a complicated thermal behavior. It is thermally very liable to change. Thermal decomposition of urea under open reaction vessel conditions at temperatures in excess of 152 °C primarily gives cyanic acid (HNCO). HNCO on contact with additional urea in turn yields biuret which at a temperature of greater than 190 °C is liable to transform into cyanuric acid (Schaber *et al.*, 2004). High-temperature thermal decomposition of cyanuric acid also gives cyanic acid again.

Heating of a mixture of ninhydrin and urea above the melting point of urea gives a mixture of 3a,8a-dihydroxy-1,3,3a,8a-tetrahydro-indeno[1,2-d]imidazole-2,8-dione (**3**) and the title compound 2-(1,3-dioxindan-2-yl)-isoquinoline-1,3,4-trione (**4**) in about equal amounts, figure 4 (Ghalib *et al.* 2011). Compound **4** is most probably the product of reaction of ninhydrin with cyanic acid. The formation of an isoquinoline-1,3,4-triones is of interest as some of these compounds have been known for their potent anticancer activity (Chen *et al.*, 2006; Du *et al.* 2008). In continuation to our interest in the chemical and pharmacological properties of ninhydrin derivatives (Ghalib *et al.*, 2011), we synthesized the title compound **4** as a precursor for the synthesis of potential chemotherapeutic agents (Chen *et al.*, 2006).

### S2. Structural commentary

In the title compound (Fig. 1), the study of torsion angles, asymmetric parameters and least squares planes reveals that the indane (C10–C12/C17/C18) ring adopts an envelope conformation with the nitrogen substituted C atom deviating by -0.104 (1) Å from the least-squares plane. The indane benzene ring (C12–C17) and the isoquinoline-1,3,4-trione ring exhibit a dihedral angle of 82.06 (6)°, suggesting they are almost perpendicular to each other.

### S3. Supramolecular features

In the crystal structure, the molecules are connected into chains extending along the *bc* plane via intermolecular C–H⋯O hydrogen bonds (Table 1) enclosing R<sub>2</sub><sup>2</sup>(8) and R<sub>2</sub><sup>2</sup>(10) loops (Fig. 2 & 3). In addition, π–π interactions (Cg2⋯Cg3 = 3.9050 (7) Å; symmetry code: 1-x, 1-y, 1-z) stack the molecules into layers parallel to the *b* axis, where Cg2 and Cg3 are the centroids of the pyridine-2,3,6-trione and the benzene (C3–C8) rings respectively.

### S4. Synthesis and crystallization

A dry mixture of ninhydrin (**1**) (1.78 g) and urea (**2**) (0.60 g) in molar ratio 1:1 was heated for 15 minutes to 150 °C above the melting point of urea (130–135 °C). The reaction mixture was cooled and then fractionally crystallized with an alcohol-chloroform (1:1) mixture to give colorless crystals of **3** as 3a,8a-dihydroxy-1,3,3a,8a-tetrahydro-indeno[1,2-d]imidazole-2,8-dione (yield 40%, M.P.: 220 °C) (Ghalib *et al.* 2011) and brownish crystals of the title compound **4** as 2-(1,3-dioxo-indan-2-yl)-isoquinoline-1,3,4-trione (yield 35%, m.p., 290 °C, Fig. 4).

## S5. Refinement details

All the H atoms were positioned geometrically (C=H 0.93–0.98 Å) and refined using a riding model with  $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{C})$ .

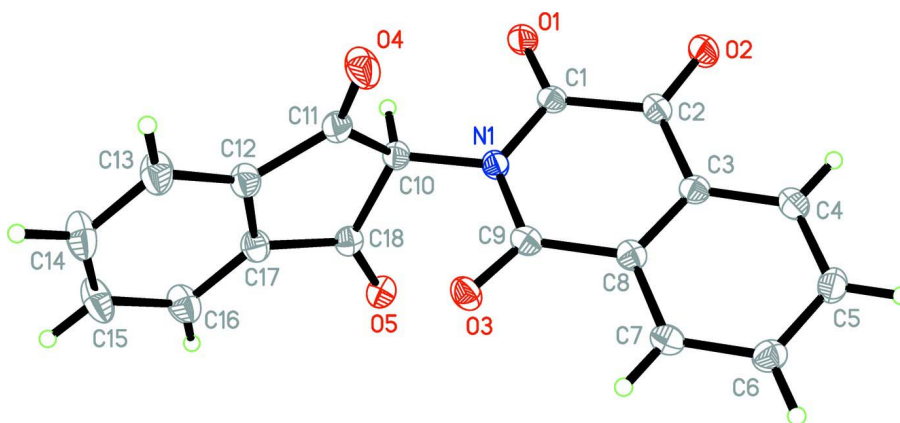


Figure 1

The molecular structure of the title compound with atom labels and 50% probability displacement ellipsoids.

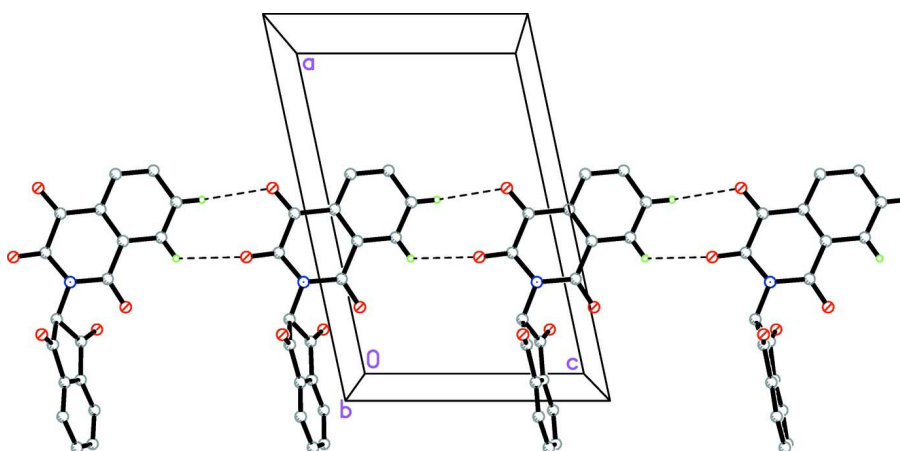


Figure 2

Crystal packing of the title compound, showing the C6–H6A...O2 and C7–H7A...O1 hydrogen bonding interactions (Symmetry codes:  $x, y, z + 1$ ) as dashed lines incorporating  $R_2^2(8)$  loops. Other H-atoms are omitted for clarity.

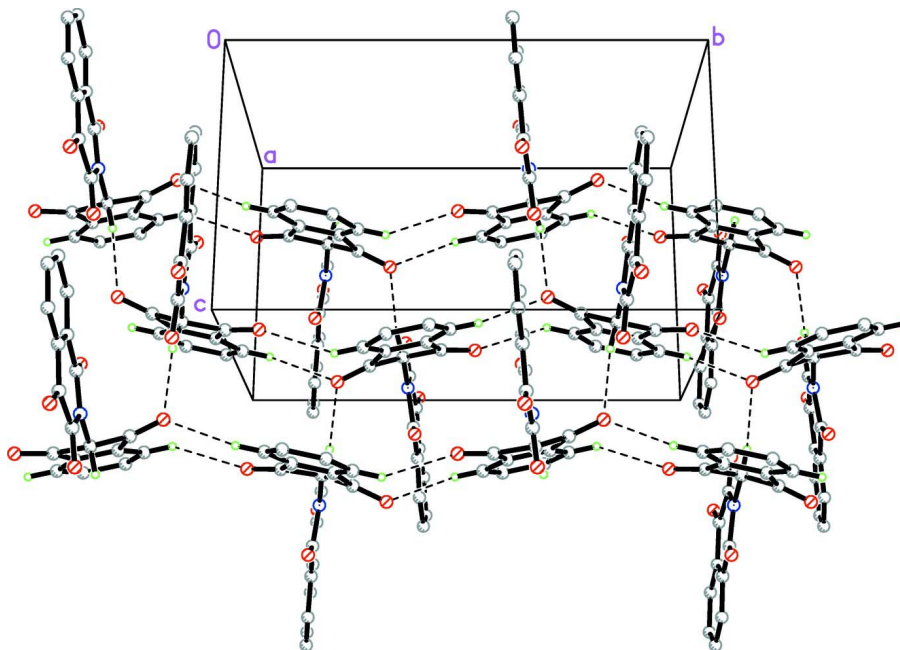


Figure 3

Crystal packing of the title compound, showing the C–H...O hydrogen bonding interactions (Symmetry codes:  $x, -y + 1/2, z - 1/2$ ;  $-x, y + 1/2, -z - 1/2$ ;  $-x, y - 1/2, -z - 1/2$ ) as dashed lines incorporating  $R_2^2(10)$  loops. Other H-atoms are omitted for clarity.

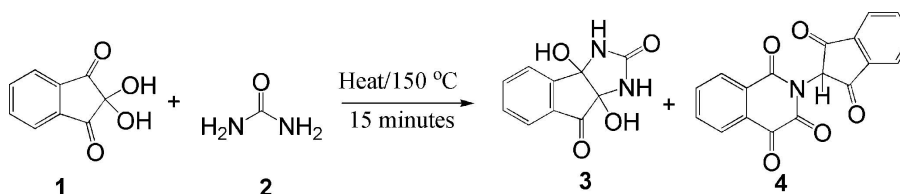


Figure 4

Reaction scheme for the title compound.

### 2-(1,3-Dioxindan-2-yl)isoquinoline-1,3,4-trione

#### Crystal data

$C_{18}H_9NO_5$

$M_r = 319.26$

Monoclinic,  $P2_1/c$

$a = 12.6080$  (1) Å

$b = 13.6849$  (2) Å

$c = 8.4467$  (1) Å

$\beta = 102.051$  (1)°

$V = 1425.27$  (3) Å<sup>3</sup>

$Z = 4$

$F(000) = 656$

$D_x = 1.488$  Mg m<sup>-3</sup>

Cu  $K\alpha$  radiation,  $\lambda = 1.54178$  Å

Cell parameters from 6347 reflections

$\theta = 6.3$ – $71.7$ °

$\mu = 0.93$  mm<sup>-1</sup>

$T = 100$  K

Block, orange

$0.24 \times 0.15 \times 0.14$  mm

#### Data collection

Bruker APEXII CCD

diffractometer

Radiation source: fine-focus sealed tube

$\varphi$  and  $\omega$  scans

Absorption correction: multi-scan

(*SADABS*; Bruker, 2009)

$T_{\min} = 0.808$ ,  $T_{\max} = 0.879$   
 9639 measured reflections  
 2597 independent reflections  
 2458 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.024$

$\theta_{\max} = 72.0^\circ$ ,  $\theta_{\min} = 6.3^\circ$   
 $h = -15 \rightarrow 14$   
 $k = -16 \rightarrow 16$   
 $l = -9 \rightarrow 8$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.093$   
 $S = 1.04$   
 2597 reflections  
 217 parameters  
 0 restraints

Hydrogen site location: inferred from neighbouring sites  
 H-atom parameters constrained  
 $w = 1/[\sigma^2(F_o^2) + (0.0504P)^2 + 0.5485P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.27 \text{ e } \text{\AA}^{-3}$   
 $\Delta\rho_{\min} = -0.20 \text{ e } \text{\AA}^{-3}$

*Special details*

**Geometry.** All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

*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	0.36681 (7)	0.34686 (7)	-0.36897 (11)	0.0226 (2)
O2	0.56844 (7)	0.37737 (7)	-0.18918 (11)	0.0244 (2)
O3	0.22076 (7)	0.37449 (6)	0.07501 (11)	0.0212 (2)
O4	0.14773 (7)	0.52030 (7)	-0.25876 (13)	0.0310 (3)
O5	0.14677 (7)	0.18880 (6)	-0.12358 (10)	0.0208 (2)
N1	0.29330 (8)	0.35524 (7)	-0.14517 (12)	0.0167 (2)
C1	0.37928 (9)	0.35678 (8)	-0.22453 (15)	0.0171 (3)
C2	0.49378 (10)	0.37240 (8)	-0.11979 (15)	0.0182 (3)
C3	0.50578 (10)	0.38012 (8)	0.05673 (15)	0.0173 (3)
C4	0.60836 (10)	0.39054 (9)	0.15659 (16)	0.0202 (3)
H4A	0.6710	0.3933	0.1108	0.024*
C5	0.61838 (10)	0.39680 (9)	0.32253 (16)	0.0219 (3)
H5A	0.6880	0.4043	0.3907	0.026*
C6	0.52631 (10)	0.39207 (9)	0.39026 (16)	0.0213 (3)
H6A	0.5339	0.3947	0.5045	0.026*
C7	0.42389 (10)	0.38360 (8)	0.29149 (15)	0.0191 (3)
H7A	0.3614	0.3817	0.3377	0.023*
C8	0.41329 (10)	0.37786 (8)	0.12429 (15)	0.0172 (3)
C9	0.30286 (10)	0.36955 (8)	0.02176 (15)	0.0172 (3)
C10	0.18389 (9)	0.34521 (9)	-0.24087 (15)	0.0180 (3)
H10A	0.1894	0.3278	-0.3539	0.022*
C11	0.11456 (10)	0.43817 (9)	-0.24898 (16)	0.0210 (3)
C12	0.00327 (10)	0.40620 (9)	-0.24322 (16)	0.0215 (3)
C13	-0.09105 (10)	0.46146 (10)	-0.26425 (18)	0.0276 (3)
H13A	-0.0910	0.5291	-0.2893	0.033*

C14	-0.18531 (11)	0.41422 (10)	-0.2473 (2)	0.0314 (3)
H14A	-0.2510	0.4502	-0.2610	0.038*
C15	-0.18544 (11)	0.31468 (10)	-0.21033 (19)	0.0315 (3)
H15A	-0.2513	0.2842	-0.2000	0.038*
C16	-0.09097 (11)	0.25943 (10)	-0.18845 (18)	0.0267 (3)
H16A	-0.0910	0.1918	-0.1629	0.032*
C17	0.00336 (10)	0.30685 (9)	-0.20540 (15)	0.0201 (3)
C18	0.11462 (9)	0.26700 (8)	-0.18079 (14)	0.0173 (3)

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
O1	0.0203 (4)	0.0298 (5)	0.0183 (5)	-0.0022 (3)	0.0056 (3)	-0.0011 (4)
O2	0.0176 (4)	0.0350 (5)	0.0221 (5)	-0.0004 (3)	0.0075 (4)	0.0005 (4)
O3	0.0169 (4)	0.0267 (5)	0.0214 (5)	-0.0016 (3)	0.0072 (3)	-0.0031 (3)
O4	0.0215 (5)	0.0205 (5)	0.0501 (7)	-0.0025 (4)	0.0055 (4)	0.0081 (4)
O5	0.0218 (4)	0.0175 (4)	0.0219 (5)	0.0011 (3)	0.0019 (3)	-0.0010 (3)
N1	0.0137 (5)	0.0192 (5)	0.0172 (5)	-0.0005 (4)	0.0031 (4)	-0.0007 (4)
C1	0.0180 (6)	0.0152 (6)	0.0189 (7)	0.0001 (4)	0.0055 (5)	0.0008 (4)
C2	0.0169 (6)	0.0160 (6)	0.0222 (7)	0.0003 (4)	0.0055 (5)	0.0006 (5)
C3	0.0180 (6)	0.0149 (5)	0.0190 (6)	0.0000 (4)	0.0043 (5)	0.0012 (4)
C4	0.0180 (6)	0.0196 (6)	0.0234 (7)	-0.0004 (4)	0.0054 (5)	0.0014 (5)
C5	0.0185 (6)	0.0224 (6)	0.0226 (7)	-0.0017 (5)	-0.0004 (5)	0.0007 (5)
C6	0.0250 (6)	0.0207 (6)	0.0180 (6)	-0.0017 (5)	0.0036 (5)	-0.0004 (5)
C7	0.0206 (6)	0.0178 (6)	0.0202 (6)	-0.0010 (4)	0.0069 (5)	-0.0003 (4)
C8	0.0181 (6)	0.0138 (5)	0.0198 (6)	-0.0005 (4)	0.0039 (5)	0.0002 (4)
C9	0.0180 (6)	0.0146 (5)	0.0198 (6)	-0.0006 (4)	0.0060 (5)	-0.0006 (4)
C10	0.0157 (6)	0.0203 (6)	0.0174 (6)	-0.0002 (4)	0.0024 (4)	0.0001 (4)
C11	0.0177 (6)	0.0207 (6)	0.0237 (7)	-0.0003 (5)	0.0022 (5)	0.0039 (5)
C12	0.0178 (6)	0.0202 (6)	0.0257 (7)	-0.0012 (5)	0.0031 (5)	0.0000 (5)
C13	0.0203 (6)	0.0192 (6)	0.0423 (8)	0.0017 (5)	0.0042 (5)	0.0014 (6)
C14	0.0177 (6)	0.0261 (7)	0.0497 (9)	0.0029 (5)	0.0058 (6)	-0.0034 (6)
C15	0.0188 (6)	0.0264 (7)	0.0508 (9)	-0.0049 (5)	0.0107 (6)	-0.0036 (6)
C16	0.0222 (6)	0.0189 (6)	0.0398 (8)	-0.0028 (5)	0.0083 (5)	-0.0010 (5)
C17	0.0183 (6)	0.0195 (6)	0.0225 (7)	-0.0007 (5)	0.0039 (5)	-0.0019 (5)
C18	0.0177 (6)	0.0180 (6)	0.0157 (6)	-0.0019 (4)	0.0025 (4)	-0.0035 (4)

*Geometric parameters (Å, °)*

O1—C1	1.2048 (15)	C7—C8	1.3927 (18)
O2—C2	1.2102 (15)	C7—H7A	0.9500
O3—C9	1.2136 (15)	C8—C9	1.4825 (17)
O4—C11	1.2080 (16)	C10—C18	1.5332 (16)
O5—C18	1.2088 (15)	C10—C11	1.5370 (16)
N1—C1	1.3886 (15)	C10—H10A	1.0000
N1—C9	1.4036 (16)	C11—C12	1.4802 (17)
N1—C10	1.4525 (15)	C12—C13	1.3890 (18)
C1—C2	1.5424 (16)	C12—C17	1.3966 (17)

C2—C3	1.4707 (17)	C13—C14	1.3863 (19)
C3—C4	1.3961 (17)	C13—H13A	0.9500
C3—C8	1.4016 (17)	C14—C15	1.398 (2)
C4—C5	1.3835 (18)	C14—H14A	0.9500
C4—H4A	0.9500	C15—C16	1.3901 (19)
C5—C6	1.3987 (18)	C15—H15A	0.9500
C5—H5A	0.9500	C16—C17	1.3883 (18)
C6—C7	1.3881 (18)	C16—H16A	0.9500
C6—H6A	0.9500	C17—C18	1.4787 (16)
C1—N1—C9	124.81 (10)	N1—C10—C18	114.97 (10)
C1—N1—C10	118.64 (10)	N1—C10—C11	114.32 (10)
C9—N1—C10	116.40 (10)	C18—C10—C11	103.57 (9)
O1—C1—N1	122.48 (11)	N1—C10—H10A	107.9
O1—C1—C2	120.34 (11)	C18—C10—H10A	107.9
N1—C1—C2	117.17 (10)	C11—C10—H10A	107.9
O2—C2—C3	124.14 (11)	O4—C11—C12	128.41 (12)
O2—C2—C1	117.35 (11)	O4—C11—C10	124.84 (11)
C3—C2—C1	118.51 (10)	C12—C11—C10	106.74 (10)
C4—C3—C8	120.06 (11)	C13—C12—C17	121.27 (12)
C4—C3—C2	120.40 (11)	C13—C12—C11	128.83 (12)
C8—C3—C2	119.54 (11)	C17—C12—C11	109.86 (11)
C5—C4—C3	119.71 (11)	C14—C13—C12	117.55 (12)
C5—C4—H4A	120.1	C14—C13—H13A	121.2
C3—C4—H4A	120.1	C12—C13—H13A	121.2
C4—C5—C6	120.23 (11)	C13—C14—C15	121.24 (12)
C4—C5—H5A	119.9	C13—C14—H14A	119.4
C6—C5—H5A	119.9	C15—C14—H14A	119.4
C7—C6—C5	120.36 (12)	C16—C15—C14	121.26 (12)
C7—C6—H6A	119.8	C16—C15—H15A	119.4
C5—C6—H6A	119.8	C14—C15—H15A	119.4
C6—C7—C8	119.63 (11)	C17—C16—C15	117.44 (12)
C6—C7—H7A	120.2	C17—C16—H16A	121.3
C8—C7—H7A	120.2	C15—C16—H16A	121.3
C7—C8—C3	119.98 (11)	C16—C17—C12	121.25 (11)
C7—C8—C9	118.45 (11)	C16—C17—C18	128.40 (11)
C3—C8—C9	121.57 (11)	C12—C17—C18	110.28 (10)
O3—C9—N1	118.63 (11)	O5—C18—C17	127.71 (11)
O3—C9—C8	123.28 (11)	O5—C18—C10	125.71 (11)
N1—C9—C8	118.09 (10)	C17—C18—C10	106.57 (10)
C9—N1—C1—O1	-177.84 (11)	C1—N1—C10—C18	131.20 (11)
C10—N1—C1—O1	-2.54 (16)	C9—N1—C10—C18	-53.10 (13)
C9—N1—C1—C2	1.89 (16)	C1—N1—C10—C11	-109.16 (12)
C10—N1—C1—C2	177.19 (9)	C9—N1—C10—C11	66.53 (13)
O1—C1—C2—O2	2.38 (17)	N1—C10—C11—O4	38.25 (18)
N1—C1—C2—O2	-177.36 (10)	C18—C10—C11—O4	164.10 (13)
O1—C1—C2—C3	-177.50 (11)	N1—C10—C11—C12	-142.00 (11)



N1—C1—C2—C3	2.76 (15)	C18—C10—C11—C12	-16.15 (13)
O2—C2—C3—C4	-2.32 (18)	O4—C11—C12—C13	7.3 (2)
C1—C2—C3—C4	177.55 (10)	C10—C11—C12—C13	-172.42 (13)
O2—C2—C3—C8	177.08 (11)	O4—C11—C12—C17	-170.35 (14)
C1—C2—C3—C8	-3.05 (16)	C10—C11—C12—C17	9.92 (14)
C8—C3—C4—C5	1.19 (17)	C17—C12—C13—C14	-0.4 (2)
C2—C3—C4—C5	-179.41 (11)	C11—C12—C13—C14	-177.81 (14)
C3—C4—C5—C6	0.42 (18)	C12—C13—C14—C15	0.0 (2)
C4—C5—C6—C7	-1.67 (19)	C13—C14—C15—C16	0.3 (2)
C5—C6—C7—C8	1.27 (18)	C14—C15—C16—C17	-0.3 (2)
C6—C7—C8—C3	0.35 (17)	C15—C16—C17—C12	-0.1 (2)
C6—C7—C8—C9	-179.58 (10)	C15—C16—C17—C18	176.66 (13)
C4—C3—C8—C7	-1.59 (17)	C13—C12—C17—C16	0.4 (2)
C2—C3—C8—C7	179.01 (10)	C11—C12—C17—C16	178.31 (12)
C4—C3—C8—C9	178.35 (10)	C13—C12—C17—C18	-176.86 (12)
C2—C3—C8—C9	-1.06 (16)	C11—C12—C17—C18	1.01 (15)
C1—N1—C9—O3	174.03 (10)	C16—C17—C18—O5	-9.2 (2)
C10—N1—C9—O3	-1.36 (15)	C12—C17—C18—O5	167.87 (12)
C1—N1—C9—C8	-5.98 (16)	C16—C17—C18—C10	171.40 (13)
C10—N1—C9—C8	178.63 (10)	C12—C17—C18—C10	-11.55 (14)
C7—C8—C9—O3	5.45 (17)	N1—C10—C18—O5	-37.31 (17)
C3—C8—C9—O3	-174.48 (11)	C11—C10—C18—O5	-162.74 (12)
C7—C8—C9—N1	-174.54 (10)	N1—C10—C18—C17	142.12 (10)
C3—C8—C9—N1	5.52 (16)	C11—C10—C18—C17	16.70 (12)

Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C6—H6A $\cdots$ O2 <sup>i</sup>	0.95	2.54	3.4862 (16)	171
C7—H7A $\cdots$ O1 <sup>i</sup>	0.95	2.51	3.1397 (15)	124
C10—H10A $\cdots$ O5 <sup>ii</sup>	1.00	2.24	3.2022 (15)	161
C13—H13A $\cdots$ O5 <sup>iii</sup>	0.95	2.37	3.2852 (16)	163
C16—H16A $\cdots$ O4 <sup>iv</sup>	0.95	2.50	3.3596 (17)	150

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