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Ethyl 2-(2-oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)acetate

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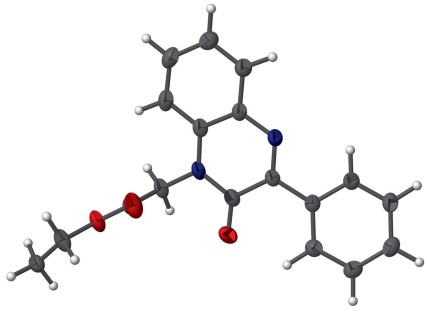
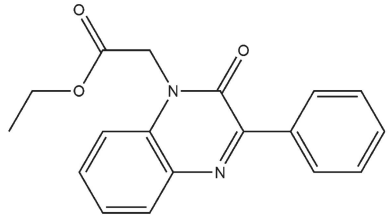
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{18}H_{16}N_2O_3$, the dihydroquinoxaline moiety is planar (r.m.s. deviation = 0.0115 Å) and the majority of the ester substituent is nearly perpendicular to its mean plane. In the crystal, the molecules form oblique stacks along the *b*-axis direction through slipped π–π stacking interactions between adjacent dihydroquinoxaline units. C—H···O hydrogen bonds between the ester substituents on adjacent stacks form thick layers with the stacks on their outside surfaces. These layers extend along the *c*-axis direction and are coupled through C—H···π(ring) interactions. The structure was refined as a two-component twin.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives are important compounds in medicinal chemistry possessing a wide variety of biological properties such as anticancer (Abbas *et al.*, 2015; Ingle *et al.*, 2013), antimicrobial (Attia *et al.*, 2013; Vieira *et al.*, 2014; Teja *et al.*, 2016), anti-inflammatory (Guirado *et al.*, 2012; Burguete *et al.*, 2001), antidepressant (Mahesh *et al.*, 2011), antiviral (Henen *et al.*, 2012; El-Tombary & El-Hawash, 2014), antidiabetic (Kulkarni *et al.*, 2012), antihypertensive (Gupta *et al.*, 2011) and antihistaminic activities (Sridevi *et al.*, 2010). In addition, it has been reported that the quinoxaline moiety is also an integral part of natural and synthetic antibiotics such as triostin A and echinomycin, known to inhibit the growth of Gram positive bacteria. As a continuation of our studies of quinoxaline derivatives (Ramli *et al.*, 2018), we report the synthesis and structure of the title compound (Fig. 1).

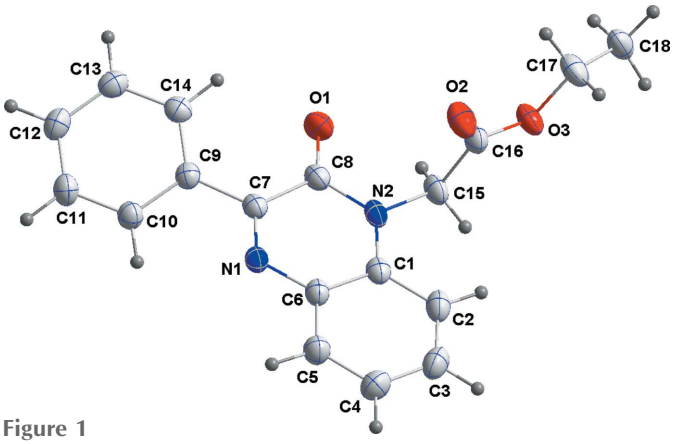


Figure 1
The title molecule with labelling scheme and 50% probability ellipsoids.

The dihydroquinoxaline moiety is planar to within 0.0221 (13) Å (r.m.s. deviation = 0.0115 Å). The pendant phenyl ring is inclined to this plane by 19.63 (7)°, while the N2/C15/C16/C17/O2/O3 unit, which is planar to within 0.0078 (16) Å (r.m.s. deviation = 0.005 Å), is inclined by 88.62 (7)°. In the crystal, the molecules form oblique stacks along the *b*-axis direction through slipped π–π-stacking interactions between the C1–C6 and C1/C6/N1/C7/C8/N2 rings with centroid–centroid separations of 3.8364 (10) Å. This is reinforced by C2—H2···O2 hydrogen bonds. Adjacent stacks are associated by C17—H17*B*···O2 and C18—H18*B*···O3 interactions, forming thick layers extending along the *c*-axis direction (Table 1 and Fig. 2). Finally, these layers are 'stitched' together by a series of C12—H12···*Cg*3 interactions (Table 1 and Fig. 3; *Cg*3 is the centroid of ring C9–C14).

Synthesis and crystallization

To a solution of 2-oxo-3-phenyl-1,2-dihydroquinoxaline (0.7 g, 3 mmol) in *N*,*N*-dimethylformamide (20 ml) were added ethyl

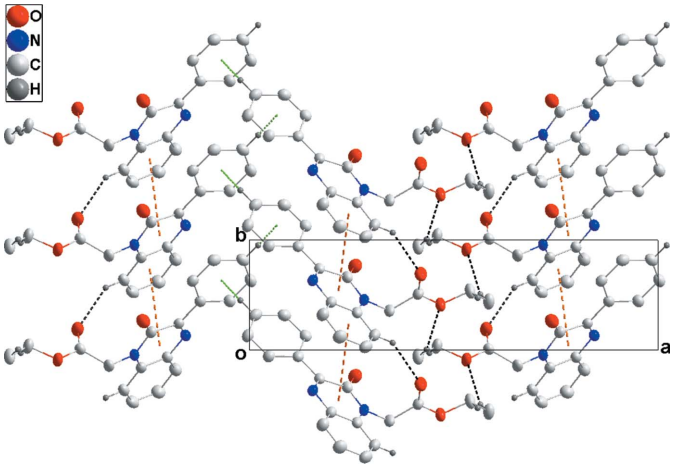


Figure 2
Detail of the intermolecular interactions viewed along the *c*-axis direction. C—H···O hydrogen bonds are shown by black dashed lines while C—H···π(ring) and π–π-stacking interactions are shown, respectively, by green and orange dashed lines.

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

*Cg*3 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.97 (2)	2.46 (2)	3.345 (2)	150.7 (17)
C17—H17*B*···O2^{ii}	0.98 (2)	2.65 (2)	3.616 (3)	168.4 (18)
C18—H18*B*···O3^{iii}	0.99 (3)	2.60 (3)	3.482 (2)	148.3 (19)
C12—H12···*Cg*3^{iv}	0.99 (2)	2.96 (2)	3.713 (2)	133.4 (15)

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{16}N_2O_3$
M_r	308.33
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	18.1710 (5), 4.9012 (1), 16.9492 (5)
β (°)	91.923 (1)
V (Å^3)	1508.64 (7)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	0.77
Crystal size (mm)	0.32 × 0.11 × 0.04
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.79, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	19783, 19783, 14579
R_{int}	0.030
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.618
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.046, 0.121, 1.02
No. of reflections	19783
No. of parameters	274
H-atom treatment	All H-atom parameters refined
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.24

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *CELL_NOW* (Sheldrick, 2008*a*), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2018* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008*b*).

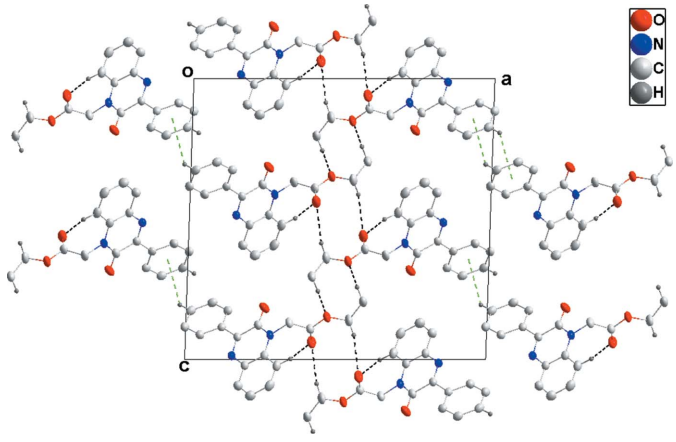


Figure 3
Packing viewed along the *b*-axis direction with intermolecular interactions depicted as in Fig. 2.

bromoacetate (0.25 ml, 2.25 mmol), potassium carbonate K_2CO_3 (0.1 g, 2.25 mmol) and a catalytic quantity of tetra-*n*-butylammonium bromide. The mixture was stirred at room temperature for 12 h. The solution was filtered and the solvent removed under reduced pressure. The residue obtained, after evaporation of solvent, was chromatographed on a silica gel column using a hexane/ethyl acetate 9:1 mixture as eluent. The solid obtained was recrystallized from ethanol to afford colourless crystals (yield: 90%).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The structure was refined as a two-component twin.

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full crystallographic data

IUCrData (2018). **3**, x180519 [https://doi.org/10.1107/S2414314618005199]

Ethyl 2-(2-oxo-3-phenyl-1,2-dihydroquinoxalin-1-yl)acetate

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Crystal data

$C_{18}H_{16}N_2O_3$
M_r = 308.33
Monoclinic, $P2_1/c$
a = 18.1710 (5) Å
b = 4.9012 (1) Å
c = 16.9492 (5) Å
β = 91.923 (1)°
V = 1508.64 (7) Å^3
Z = 4
$F(000)$ = 648
D_x = 1.357 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9923 reflections
θ = 2.4–72.4°
μ = 0.77 mm^{-1}
T = 150 K
Plate, colourless
0.32 × 0.11 × 0.04 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 (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.79, T_{max} = 0.97
19783 measured reflections
19783 independent reflections
14579 reflections with $I > 2\sigma(I)$
R_{int} = 0.030
θ_{max} = 72.4°, θ_{min} = 2.4°
h = −22→21
k = −6→5
l = −20→20

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.121
S = 1.01
19783 reflections
274 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
$w = 1/[\sigma^2(F_o^2) + (0.0459P)^2 + 0.2438P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Extinction correction: *SHELXTL* (Sheldrick, 2008*b*), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0050 (8)

Special details

Experimental. Analysis of 1517 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to consist of two components related by a 35.5° rotation about the *b* axis. The raw data were processed using the multi-component version of*SAINT* under control of the two-component orientation filegenerated 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 $F^2 > 2\text{sigma}(F^2)$ 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. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.25922 (7)	0.7640 (3)	0.31580 (8)	0.0417 (4)
O2	0.41992 (7)	0.6916 (3)	0.43879 (8)	0.0438 (4)
O3	0.46812 (6)	0.4139 (3)	0.34884 (7)	0.0364 (3)
N1	0.15573 (8)	0.6338 (3)	0.48696 (8)	0.0277 (3)
N2	0.28105 (7)	0.4569 (3)	0.41319 (8)	0.0285 (3)
C1	0.26404 (9)	0.3412 (3)	0.48550 (10)	0.0282 (4)
C2	0.30684 (10)	0.1373 (4)	0.52219 (11)	0.0352 (4)
H2	0.3510 (13)	0.067 (4)	0.4983 (13)	0.043 (6)*
C3	0.28523 (11)	0.0297 (4)	0.59278 (12)	0.0395 (4)
H3	0.3145 (13)	−0.117 (5)	0.6175 (13)	0.050 (6)*
C4	0.22231 (11)	0.1216 (4)	0.62916 (11)	0.0393 (4)
H4	0.2080 (12)	0.036 (5)	0.6796 (14)	0.045 (6)*
C5	0.18037 (10)	0.3237 (4)	0.59365 (11)	0.0348 (4)
H5	0.1341 (12)	0.395 (4)	0.6164 (12)	0.041 (5)*
C6	0.20033 (9)	0.4357 (3)	0.52132 (9)	0.0280 (4)
C7	0.17228 (9)	0.7415 (3)	0.41992 (9)	0.0260 (4)
C8	0.23990 (9)	0.6628 (3)	0.37802 (10)	0.0294 (4)
C9	0.11989 (9)	0.9429 (3)	0.38455 (9)	0.0268 (4)
C10	0.04810 (10)	0.9459 (4)	0.41234 (10)	0.0308 (4)
H10	0.0352 (11)	0.811 (4)	0.4512 (12)	0.038 (5)*
C11	−0.00326 (10)	1.1326 (4)	0.38378 (10)	0.0335 (4)
H11	−0.0533 (13)	1.128 (4)	0.4046 (12)	0.040 (5)*
C12	0.01550 (10)	1.3195 (4)	0.32662 (10)	0.0339 (4)
H12	−0.0217 (12)	1.452 (4)	0.3059 (12)	0.036 (5)*
C13	0.08591 (10)	1.3174 (4)	0.29784 (10)	0.0332 (4)
H13	0.1002 (11)	1.449 (4)	0.2570 (12)	0.039 (5)*
C14	0.13792 (10)	1.1303 (3)	0.32583 (10)	0.0299 (4)
H14	0.1874 (12)	1.132 (4)	0.3037 (12)	0.040 (5)*
C15	0.34349 (10)	0.3597 (4)	0.36944 (11)	0.0324 (4)
H15A	0.3325 (12)	0.389 (5)	0.3142 (15)	0.046 (6)*
H15B	0.3514 (12)	0.167 (5)	0.3776 (12)	0.040 (5)*

C16	0.41371 (9)	0.5107 (3)	0.39143 (10)	0.0297 (4)
C17	0.54066 (10)	0.5371 (5)	0.36140 (13)	0.0422 (5)
H17A	0.5341 (14)	0.739 (6)	0.3615 (15)	0.062 (7)*
H17B	0.5591 (13)	0.475 (5)	0.4136 (14)	0.047 (6)*
C18	0.58651 (11)	0.4416 (5)	0.29504 (12)	0.0407 (5)
H18A	0.6373 (14)	0.517 (5)	0.3032 (14)	0.052 (6)*
H18B	0.5656 (14)	0.506 (5)	0.2434 (16)	0.058 (7)*
H18C	0.5870 (13)	0.234 (5)	0.2945 (13)	0.049 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0402 (8)	0.0435 (8)	0.0427 (7)	0.0049 (6)	0.0176 (6)	0.0057 (6)
O2	0.0317 (7)	0.0435 (8)	0.0567 (8)	−0.0015 (6)	0.0059 (6)	−0.0212 (6)
O3	0.0226 (6)	0.0414 (7)	0.0457 (7)	−0.0027 (5)	0.0081 (5)	−0.0121 (5)
N1	0.0241 (7)	0.0285 (7)	0.0306 (7)	0.0023 (6)	0.0025 (5)	−0.0011 (5)
N2	0.0208 (7)	0.0292 (7)	0.0357 (7)	0.0009 (6)	0.0047 (6)	−0.0064 (6)
C1	0.0241 (8)	0.0259 (8)	0.0345 (8)	−0.0009 (6)	−0.0003 (7)	−0.0063 (6)
C2	0.0271 (9)	0.0319 (9)	0.0465 (10)	0.0047 (7)	−0.0029 (8)	−0.0067 (7)
C3	0.0369 (11)	0.0332 (10)	0.0477 (11)	0.0064 (8)	−0.0097 (8)	0.0004 (8)
C4	0.0419 (11)	0.0375 (10)	0.0382 (10)	0.0031 (8)	−0.0017 (8)	0.0049 (8)
C5	0.0328 (10)	0.0363 (9)	0.0354 (9)	0.0040 (8)	0.0030 (7)	0.0016 (7)
C6	0.0246 (8)	0.0268 (8)	0.0327 (8)	0.0018 (7)	0.0000 (6)	−0.0031 (6)
C7	0.0237 (8)	0.0249 (8)	0.0296 (8)	−0.0015 (6)	0.0023 (6)	−0.0043 (6)
C8	0.0254 (8)	0.0293 (9)	0.0336 (9)	−0.0018 (7)	0.0048 (7)	−0.0041 (6)
C9	0.0263 (8)	0.0260 (8)	0.0279 (8)	0.0006 (7)	0.0000 (6)	−0.0048 (6)
C10	0.0294 (9)	0.0320 (9)	0.0310 (8)	0.0029 (7)	0.0030 (7)	−0.0009 (7)
C11	0.0290 (9)	0.0374 (10)	0.0340 (9)	0.0060 (7)	0.0007 (7)	−0.0032 (7)
C12	0.0359 (10)	0.0316 (9)	0.0337 (9)	0.0065 (8)	−0.0062 (7)	−0.0035 (7)
C13	0.0378 (10)	0.0297 (9)	0.0317 (9)	−0.0025 (7)	−0.0037 (7)	0.0006 (7)
C14	0.0296 (9)	0.0297 (9)	0.0302 (8)	−0.0040 (7)	−0.0006 (7)	−0.0029 (6)
C15	0.0240 (9)	0.0326 (10)	0.0409 (10)	0.0018 (7)	0.0071 (7)	−0.0097 (7)
C16	0.0251 (9)	0.0290 (8)	0.0352 (8)	0.0036 (7)	0.0043 (7)	−0.0031 (7)
C17	0.0234 (9)	0.0502 (12)	0.0533 (12)	−0.0070 (8)	0.0052 (8)	−0.0082 (9)
C18	0.0258 (10)	0.0550 (13)	0.0415 (10)	0.0020 (9)	0.0049 (8)	0.0111 (9)

Geometric parameters (Å, º)

O1—C8	1.227 (2)	C9—C10	1.402 (2)
O2—C16	1.199 (2)	C9—C14	1.401 (2)
O3—C16	1.3311 (19)	C10—C11	1.383 (3)
O3—C17	1.459 (2)	C10—H10	0.97 (2)
N1—C7	1.297 (2)	C11—C12	1.384 (3)
N1—C6	1.381 (2)	C11—H11	0.99 (2)
N2—C8	1.379 (2)	C12—C13	1.385 (3)
N2—C1	1.395 (2)	C12—H12	0.99 (2)
N2—C15	1.456 (2)	C13—C14	1.389 (3)
C1—C2	1.399 (3)	C13—H13	0.99 (2)

C1—C6	1.404 (2)	C14—H14	0.99 (2)
C2—C3	1.377 (3)	C15—C16	1.511 (2)
C2—H2	0.97 (2)	C15—H15A	0.96 (2)
C3—C4	1.392 (3)	C15—H15B	0.96 (2)
C3—H3	0.98 (2)	C17—C18	1.497 (3)
C4—C5	1.376 (3)	C17—H17A	1.00 (3)
C4—H4	0.99 (2)	C17—H17B	0.98 (2)
C5—C6	1.402 (2)	C18—H18A	1.00 (2)
C5—H5	1.00 (2)	C18—H18B	0.99 (3)
C7—C9	1.484 (2)	C18—H18C	1.02 (3)
C7—C8	1.490 (2)		

C16—O3—C17	117.19 (14)	C9—C10—H10	118.1 (12)
C7—N1—C6	120.36 (14)	C10—C11—C12	120.25 (17)
C8—N2—C1	122.99 (13)	C10—C11—H11	118.7 (12)
C8—N2—C15	116.08 (14)	C12—C11—H11	121.1 (12)
C1—N2—C15	120.92 (15)	C11—C12—C13	119.59 (17)
N2—C1—C2	123.01 (15)	C11—C12—H12	120.0 (12)
N2—C1—C6	117.13 (15)	C13—C12—H12	120.4 (12)
C2—C1—C6	119.86 (16)	C12—C13—C14	120.72 (16)
C3—C2—C1	119.29 (17)	C12—C13—H13	120.7 (12)
C3—C2—H2	119.3 (13)	C14—C13—H13	118.6 (12)
C1—C2—H2	121.4 (13)	C13—C14—C9	120.18 (16)
C2—C3—C4	121.57 (17)	C13—C14—H14	118.8 (12)
C2—C3—H3	119.0 (13)	C9—C14—H14	121.0 (12)
C4—C3—H3	119.4 (13)	N2—C15—C16	112.34 (14)
C5—C4—C3	119.35 (18)	N2—C15—H15A	107.9 (13)
C5—C4—H4	121.5 (13)	C16—C15—H15A	108.3 (14)
C3—C4—H4	119.1 (13)	N2—C15—H15B	111.2 (13)
C4—C5—C6	120.56 (17)	C16—C15—H15B	108.9 (13)
C4—C5—H5	122.9 (12)	H15A—C15—H15B	108.1 (18)
C6—C5—H5	116.5 (12)	O2—C16—O3	124.89 (16)
N1—C6—C5	118.60 (15)	O2—C16—C15	125.96 (15)
N1—C6—C1	122.05 (15)	O3—C16—C15	109.15 (14)
C5—C6—C1	119.35 (16)	O3—C17—C18	106.48 (16)
N1—C7—C9	117.39 (14)	O3—C17—H17A	107.7 (15)
N1—C7—C8	122.08 (15)	C18—C17—H17A	112.4 (15)
C9—C7—C8	120.51 (14)	O3—C17—H17B	106.3 (13)
O1—C8—N2	120.03 (15)	C18—C17—H17B	113.4 (13)
O1—C8—C7	124.68 (16)	H17A—C17—H17B	110 (2)
N2—C8—C7	115.28 (14)	C17—C18—H18A	108.4 (14)
C10—C9—C14	118.30 (15)	C17—C18—H18B	110.8 (14)
C10—C9—C7	117.58 (14)	H18A—C18—H18B	109.1 (19)
C14—C9—C7	124.11 (15)	C17—C18—H18C	108.9 (13)
C11—C10—C9	120.94 (16)	H18A—C18—H18C	111.2 (19)
C11—C10—H10	120.9 (13)	H18B—C18—H18C	108.3 (19)

C8—N2—C1—C2	−178.28 (16)	N1—C7—C8—O1	−177.72 (16)

C15—N2—C1—C2	3.2 (2)	C9—C7—C8—O1	4.1 (3)
C8—N2—C1—C6	2.4 (2)	N1—C7—C8—N2	3.6 (2)
C15—N2—C1—C6	−176.20 (15)	C9—C7—C8—N2	−174.59 (14)
N2—C1—C2—C3	−178.57 (16)	N1—C7—C9—C10	−18.0 (2)
C6—C1—C2—C3	0.8 (3)	C8—C7—C9—C10	160.34 (15)
C1—C2—C3—C4	−0.9 (3)	N1—C7—C9—C14	161.55 (15)
C2—C3—C4—C5	0.4 (3)	C8—C7—C9—C14	−20.1 (2)
C3—C4—C5—C6	0.3 (3)	C14—C9—C10—C11	−1.3 (2)
C7—N1—C6—C5	−179.75 (16)	C7—C9—C10—C11	178.23 (15)
C7—N1—C6—C1	−0.7 (2)	C9—C10—C11—C12	0.4 (3)
C4—C5—C6—N1	178.56 (16)	C10—C11—C12—C13	0.4 (3)
C4—C5—C6—C1	−0.5 (3)	C11—C12—C13—C14	−0.2 (3)
N2—C1—C6—N1	0.3 (2)	C12—C13—C14—C9	−0.8 (3)
C2—C1—C6—N1	−179.10 (15)	C10—C9—C14—C13	1.5 (2)
N2—C1—C6—C5	179.30 (15)	C7—C9—C14—C13	−177.98 (15)
C2—C1—C6—C5	−0.1 (2)	C8—N2—C15—C16	91.54 (19)
C6—N1—C7—C9	176.98 (14)	C1—N2—C15—C16	−89.81 (19)
C6—N1—C7—C8	−1.3 (2)	C17—O3—C16—O2	0.4 (3)
C1—N2—C8—O1	177.16 (15)	C17—O3—C16—C15	179.47 (16)
C15—N2—C8—O1	−4.2 (2)	N2—C15—C16—O2	−0.3 (3)
C1—N2—C8—C7	−4.1 (2)	N2—C15—C16—O3	−179.37 (15)
C15—N2—C8—C7	174.49 (14)	C16—O3—C17—C18	−167.13 (16)

Hydrogen-bond geometry (Å, º)

Cg3 is the centroid of the C9–C14 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C2—H2···O2^{i}	0.97 (2)	2.46 (2)	3.345 (2)	150.7 (17)
C17—H17*B*···O2^{ii}	0.98 (2)	2.65 (2)	3.616 (3)	168.4 (18)
C18—H18*B*···O3^{iii}	0.99 (3)	2.60 (3)	3.482 (2)	148.3 (19)
C12—H12···*Cg*3^{iv}	0.99 (2)	2.96 (2)	3.713 (2)	133.4 (15)

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