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Ethyl 2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)acetate

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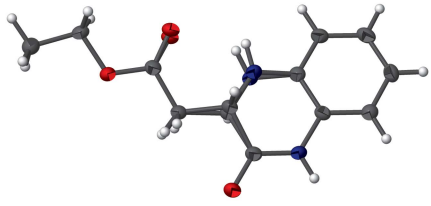
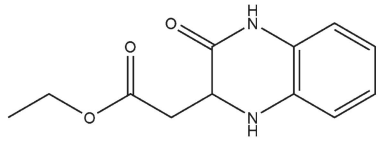
In the title compound, $C_{12}H_{14}N_2O_3$, the conformation of the ester substituent is partially determined by an intramolecular N—H···O hydrogen bond. The crystal packing consists of layers parallel to $(\bar{1}12)$ held together by N—H···O and C—H···O hydrogen bonds. The CH/NH portion of the heterocyclic ring is disordered over two sites in a 0.930 (5):0.070 (5) ratio with the disorder also extending to the O atom involved in the intramolecular N—H···O hydrogen bond.

3D view



Chemical scheme



Structure description

Quinoxaline derivatives exhibit a variety of biological activities including anticancer (Lindsley *et al.*, 2005; Carta *et al.*, 2006), antidiabetic (Gupta *et al.*, 2005), antimicrobial (Singh *et al.*, 2010), anti-inflammatory (El-Sabbagh *et al.*, 2009) and anti-malarial (Guillon *et al.*, 2004). Moreover, they are used as fungicides, insecticides and herbicides (Sakata *et al.*, 1988). The numerous applications of quinoxalines has prompted researchers to develop efficient methods to synthesize new derivatives likely to present interesting activities (Ramli *et al.*, 2018). We report in this work the synthesis and crystal structure of the title compound (Fig. 1).

A puckering analysis of the heterocyclic ring yielded the parameters Q = 0.421 (3) Å, θ = 119.1 (4)° and φ = 34.3 (4)° for the major component. The orientation of the ester substituent is partially determined by the intramolecular N2—H2*A*···O2 hydrogen bond. In the crystal, pairs of N1—H1*A*···O1 hydrogen bonds form inversion dimers, which are linked into chains by inversion-related C11—H11*B*···O2 hydrogen bonds. The chains are

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···O1^{i}	0.87 (3)	1.99 (4)	2.866 (3)	177 (3)
N2—H2A···O2	0.91	2.14	2.816 (3)	130
C3—H3···O3^{ii}	0.95 (3)	2.59 (3)	3.508 (3)	165 (2)
C8—H8···O1^{iii}	1.00	2.55	3.443 (4)	148
C9—H9A···O2^{iv}	0.99	2.52	3.367 (4)	144
C11—H11B···O2^{v}	0.97 (2)	2.58 (3)	3.199 (3)	121.9 (18)

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

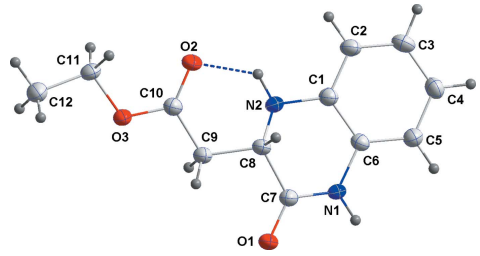


Figure 1
The title molecule with labeling scheme and 50% probability ellipsoids. The intramolecular hydrogen bond is depicted by a dashed line. Only the major component of the disorder is shown.

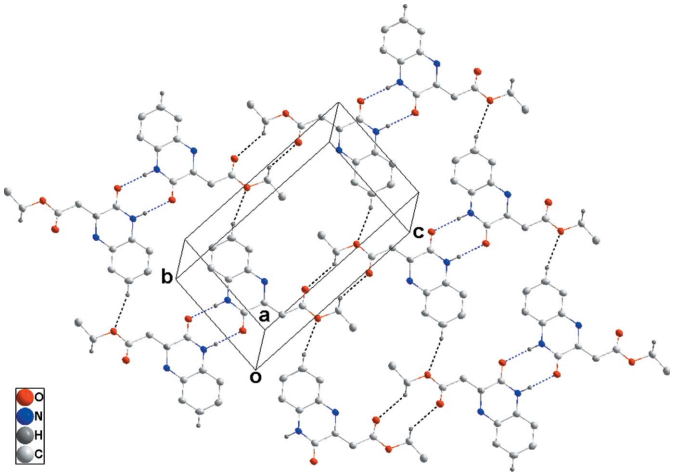


Figure 2
Plan view of a portion of one layer with N—H···O and C—H···O hydrogen bonds shown, respectively, by blue and black dashed lines.

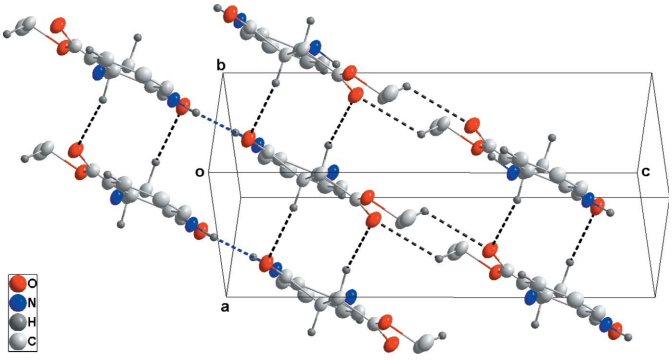


Figure 3
Elevation view of the stacked layers with hydrogen bonds shown as in Fig. 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{12}H_{14}N_2O_3$
M_r	234.25
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	100
a, b, c (Å)	4.8082 (18), 8.260 (3), 14.413 (6)
α, β, γ (°)	84.072 (7), 81.473 (5), 85.140 (5)
V (Å^3)	561.7 (4)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.10
Crystal size (mm)	0.19 × 0.14 × 0.13
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.98, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9489, 9489, 4504
R_{int}	0.028
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.667
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.061, 0.213, 1.03
No. of reflections	9489
No. of parameters	205
No. of restraints	4
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.16, −0.82

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

formed into layers parallel to ($\overline{1}$12) by C3—H3···O3 hydrogen bonds (Table 1 and Fig. 2). The layers are linked to one another by C8—H8···O1 and C9—H9A···O2 hydrogen bonds (Table 1 and Figs. 3 and 4).

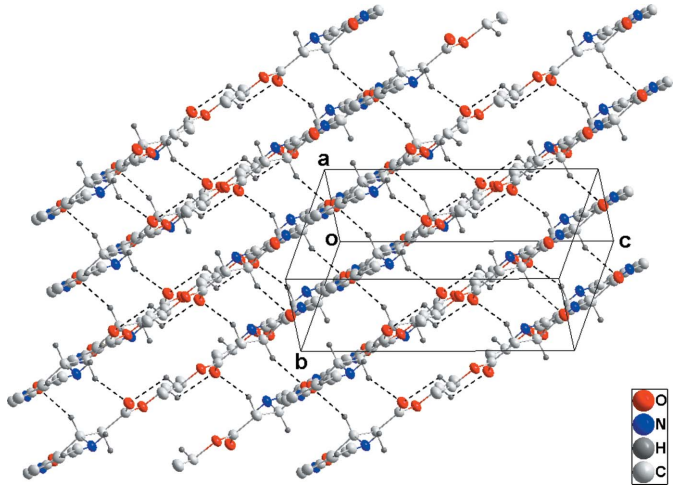


Figure 4
Packing projected onto (122) with hydrogen bonds shown as in Fig. 2.

Synthesis and crystallization

A mixture of ethyl-2-(3-oxo-3,4-dihydroquinoxalin-2-yl)acetate (1 g) with Pd/C catalyst in ethanol was stirred for 10 h in presence of hydrogen. The reaction mixture was filtered and the solvent was removed under pressure. The residue obtained was recrystallized from ethanol to afford the title molecule as yellow crystals.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The C8/N2 portion of the heterocyclic ring is disordered over two sites in a 0.930 (5):0.070 (5) ratio with the disorder also extending to O2. The two components were refined subject to restraints that their geometries be comparable and the affected hydrogen atoms were included as riding contributions in idealized positions. The two noticeable residual peaks in the final difference map are attributed to errors resulting from neglect of the other minor components of the crystal.

Acknowledgements

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full crystallographic data

IUCrData (2018). **3**, x180596 [https://doi.org/10.1107/S2414314618005965]

Ethyl 2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)acetate

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Ethyl 2-(3-oxo-1,2,3,4-tetrahydroquinoxalin-2-yl)acetate

Crystal data

$C_{12}H_{14}N_2O_3$
M_r = 234.25
Triclinic, $P\overline{1}$
a = 4.8082 (18) Å
b = 8.260 (3) Å
c = 14.413 (6) Å
α = 84.072 (7)°
β = 81.473 (5)°
γ = 85.140 (5)°
V = 561.7 (4) Å^3
Z = 2
$F(000)$ = 248
D_x = 1.385 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2025 reflections
θ = 2.8–28.2°
μ = 0.10 mm^{-1}
T = 100 K
Block, yellow
0.19 × 0.14 × 0.13 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.98, T_{max} = 0.99
9489 measured reflections
9489 independent reflections
4504 reflections with $I > 2\sigma(I)$
R_{int} = 0.028
θ_{max} = 28.3°, θ_{min} = 1.4°
h = −6→6
k = −10→10
l = −19→19

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.061
$wR(F^2)$ = 0.213
S = 1.03
9489 reflections
205 parameters
4 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
$w = 1/[\sigma^2(F_o^2) + (0.1018P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 1.16 e Å^{-3}
$\Delta\rho_{min}$ = −0.82 e Å^{-3}

Special details

Experimental. The diffraction data were collected in three sets of 363 frames (0.5° width in ω) at φ = 0, 120 and 240°. A scan time of 60 sec/frame was used. Analysis of 564 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 triclinic system and to consist of one major component and several minor components rotated from the former by *ca.* 7° about non-special axes. After several trials, it was decided to treat the crystal as having one major and one minor component rotsted from the first by 7.3° about the real axis 1, -0.42, 0. The raw data were processed using the multi-component version of *SAINT* 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 $F^2 > 2\text{sigma}(F^2)$ 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. The heterocyclic ring is disordered over two conformations in a 93:7 ratio which also affects the position of O2. The two components were refined subject to restraints that their geometries be comparable and the affected hydrogen atoms were included as riding contributions in idealized positions. The two noticeable residual peaks in the final difference map are attributed to errors resulting from neglect of the other minor components of the crystal.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	−0.0170 (4)	0.3173 (2)	0.08301 (11)	0.0292 (5)	
O2	0.4815 (5)	0.1288 (3)	0.36066 (16)	0.0296 (6)	0.930 (5)
O2A	0.370 (7)	0.165 (3)	0.3836 (18)	0.0296 (6)	0.070 (5)
O3	0.1574 (3)	−0.0537 (2)	0.36597 (11)	0.0265 (5)	
N1	0.2161 (4)	0.5434 (3)	0.08754 (15)	0.0246 (5)	
H1A	0.151 (6)	0.589 (3)	0.037 (2)	0.042 (8)*	
N2	0.3448 (6)	0.4290 (3)	0.26056 (15)	0.0257 (7)	0.930 (5)
H2A	0.434112	0.380595	0.308727	0.031*	0.930 (5)
N2A	0.455 (6)	0.4000 (8)	0.236 (3)	0.0257 (7)	0.070 (5)
H2AA	0.529600	0.386739	0.290485	0.031*	0.070 (5)
C1	0.4714 (5)	0.5695 (3)	0.21646 (17)	0.0253 (6)	
C2	0.6484 (6)	0.6542 (3)	0.25833 (18)	0.0277 (6)	
H2	0.707 (6)	0.607 (3)	0.3173 (19)	0.029 (7)*	
C3	0.7476 (6)	0.8000 (3)	0.21482 (19)	0.0300 (6)	
H3	0.867 (6)	0.855 (3)	0.2458 (19)	0.032 (7)*	
C4	0.6712 (6)	0.8619 (3)	0.12873 (19)	0.0297 (6)	
H4	0.743 (6)	0.962 (3)	0.1001 (18)	0.033 (7)*	
C5	0.4964 (6)	0.7775 (3)	0.08525 (19)	0.0280 (6)	
H5	0.445 (6)	0.816 (3)	0.026 (2)	0.036 (8)*	
C6	0.3965 (5)	0.6312 (3)	0.12848 (17)	0.0234 (6)	
C7	0.1471 (5)	0.3917 (3)	0.11900 (16)	0.0245 (6)	
C8	0.3030 (7)	0.3082 (3)	0.19800 (18)	0.0240 (7)	0.930 (5)
H8	0.492195	0.263176	0.169224	0.029*	0.930 (5)
C9	0.1434 (5)	0.1686 (3)	0.25015 (17)	0.0257 (6)	0.930 (5)
H9A	−0.049192	0.211036	0.274807	0.031*	0.930 (5)

H9B	0.125712	0.088460	0.205156	0.031*	0.930 (5)
C8A	0.181 (6)	0.3479 (12)	0.224 (3)	0.0240 (7)	0.070 (5)
H8A	0.031427	0.412289	0.262872	0.029*	0.070 (5)
C9A	0.1434 (5)	0.1686 (3)	0.25015 (17)	0.0257 (6)	0.070 (5)
H9A1	−0.061579	0.155281	0.264919	0.031*	0.070 (5)
H9A2	0.213338	0.110327	0.193641	0.031*	0.070 (5)
C10	0.2804 (5)	0.0826 (3)	0.33062 (17)	0.0245 (6)	
C11	0.2761 (6)	−0.1435 (3)	0.44557 (18)	0.0275 (6)	
H11A	0.480 (6)	−0.166 (3)	0.4238 (17)	0.028 (7)*	
H11B	0.251 (5)	−0.072 (3)	0.4957 (17)	0.021 (6)*	
C12	0.1264 (7)	−0.2975 (4)	0.4700 (2)	0.0343 (7)	
H12A	0.205 (6)	−0.360 (3)	0.523 (2)	0.042 (8)*	
H12B	0.153 (6)	−0.359 (3)	0.416 (2)	0.041 (8)*	
H12C	−0.079 (7)	−0.271 (3)	0.491 (2)	0.048 (9)*	

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0317 (10)	0.0317 (11)	0.0274 (10)	−0.0096 (8)	−0.0131 (8)	0.0007 (7)
O2	0.0261 (12)	0.0338 (12)	0.0317 (12)	−0.0077 (10)	−0.0134 (10)	0.0021 (9)
O2A	0.0261 (12)	0.0338 (12)	0.0317 (12)	−0.0077 (10)	−0.0134 (10)	0.0021 (9)
O3	0.0274 (10)	0.0273 (10)	0.0264 (9)	−0.0055 (8)	−0.0115 (7)	0.0038 (7)
N1	0.0268 (12)	0.0270 (12)	0.0218 (11)	−0.0045 (9)	−0.0103 (9)	0.0010 (9)
N2	0.0304 (16)	0.0263 (12)	0.0222 (13)	−0.0056 (11)	−0.0102 (10)	0.0010 (9)
N2A	0.0304 (16)	0.0263 (12)	0.0222 (13)	−0.0056 (11)	−0.0102 (10)	0.0010 (9)
C1	0.0261 (13)	0.0239 (14)	0.0269 (13)	−0.0022 (10)	−0.0076 (10)	−0.0019 (10)
C2	0.0296 (14)	0.0290 (15)	0.0275 (13)	−0.0040 (11)	−0.0112 (11)	−0.0040 (11)
C3	0.0277 (14)	0.0302 (15)	0.0356 (15)	−0.0040 (11)	−0.0102 (11)	−0.0096 (11)
C4	0.0299 (14)	0.0237 (14)	0.0360 (15)	−0.0065 (11)	−0.0049 (11)	−0.0011 (11)
C5	0.0293 (14)	0.0283 (15)	0.0273 (13)	−0.0037 (11)	−0.0081 (11)	0.0005 (11)
C6	0.0207 (13)	0.0240 (13)	0.0268 (13)	−0.0026 (10)	−0.0063 (10)	−0.0033 (10)
C7	0.0234 (13)	0.0286 (14)	0.0228 (12)	−0.0043 (10)	−0.0064 (10)	−0.0020 (10)
C8	0.0243 (16)	0.0261 (15)	0.0237 (14)	−0.0057 (12)	−0.0087 (11)	−0.0018 (11)
C9	0.0259 (13)	0.0265 (14)	0.0266 (13)	−0.0056 (11)	−0.0103 (10)	0.0008 (10)
C8A	0.0243 (16)	0.0261 (15)	0.0237 (14)	−0.0057 (12)	−0.0087 (11)	−0.0018 (11)
C9A	0.0259 (13)	0.0265 (14)	0.0266 (13)	−0.0056 (11)	−0.0103 (10)	0.0008 (10)
C10	0.0232 (13)	0.0264 (14)	0.0249 (12)	−0.0031 (10)	−0.0056 (10)	−0.0028 (10)
C11	0.0284 (15)	0.0296 (15)	0.0259 (13)	−0.0018 (11)	−0.0121 (11)	0.0016 (11)
C12	0.0349 (17)	0.0338 (17)	0.0353 (16)	−0.0065 (13)	−0.0124 (13)	0.0051 (13)

Geometric parameters (Å, º)

O1—C7	1.240 (3)	C4—H4	0.95 (3)
O2—C10	1.221 (3)	C5—C6	1.391 (3)
O2A—C10	1.221 (5)	C5—H5	0.94 (3)
O3—C10	1.335 (3)	C7—C8	1.529 (4)
O3—C11	1.463 (3)	C7—C8A	1.54 (4)
N1—C7	1.339 (3)	C8—C9	1.511 (3)

N1—C6	1.405 (3)	C8—H8	1.0000
N1—H1A	0.87 (3)	C9—C10	1.503 (3)
N2—C1	1.405 (3)	C9—H9A	0.9900
N2—C8	1.457 (3)	C9—H9B	0.9900
N2—H2A	0.9101	C8A—C9A	1.511 (5)
N2A—C1	1.405 (5)	C8A—H8A	1.0000
N2A—C8A	1.457 (5)	C9A—C10	1.503 (3)
N2A—H2AA	0.900	C9A—H9A1	0.9900
C1—C2	1.385 (3)	C9A—H9A2	0.9900
C1—C6	1.403 (3)	C11—C12	1.499 (4)
C2—C3	1.387 (4)	C11—H11A	0.99 (3)
C2—H2	0.97 (3)	C11—H11B	0.97 (2)
C3—C4	1.382 (4)	C12—H12A	0.98 (3)
C3—H3	0.95 (3)	C12—H12B	0.96 (3)
C4—C5	1.389 (4)	C12—H12C	1.00 (3)

C10—O3—C11	115.31 (18)	C9—C8—H8	108.4
C7—N1—C6	124.1 (2)	C7—C8—H8	108.4
C7—N1—H1A	117.8 (19)	C10—C9—C8	113.8 (2)
C6—N1—H1A	118.0 (19)	C10—C9—H9A	108.8
C1—N2—C8	115.6 (2)	C8—C9—H9A	108.8
C1—N2—H2A	112.6	C10—C9—H9B	108.8
C8—N2—H2A	110.1	C8—C9—H9B	108.8
C1—N2A—C8A	112.4 (11)	H9A—C9—H9B	107.7
C1—N2A—H2AA	98.5	N2A—C8A—C9A	114.8 (11)
C8A—N2A—H2AA	125.0	N2A—C8A—C7	107 (3)
C2—C1—C6	119.3 (2)	C9A—C8A—C7	110 (2)
C2—C1—N2	123.2 (2)	N2A—C8A—H8A	108.4
C6—C1—N2	117.3 (2)	C9A—C8A—H8A	108.4
C2—C1—N2A	121.8 (13)	C7—C8A—H8A	108.4
C6—C1—N2A	113.8 (15)	C10—C9A—C8A	119.1 (12)
C1—C2—C3	120.6 (2)	C10—C9A—H9A1	107.5
C1—C2—H2	118.3 (15)	C8A—C9A—H9A1	107.5
C3—C2—H2	121.0 (15)	C10—C9A—H9A2	107.5
C4—C3—C2	120.1 (2)	C8A—C9A—H9A2	107.5
C4—C3—H3	121.5 (16)	H9A1—C9A—H9A2	107.0
C2—C3—H3	118.4 (16)	O2—C10—O3	123.0 (2)
C3—C4—C5	120.0 (2)	O2A—C10—O3	119.3 (15)
C3—C4—H4	118.4 (17)	O2A—C10—C9A	118.3 (15)
C5—C4—H4	121.5 (16)	O3—C10—C9A	111.9 (2)
C4—C5—C6	120.1 (2)	O2—C10—C9	125.1 (2)
C4—C5—H5	121.4 (17)	O3—C10—C9	111.9 (2)
C6—C5—H5	118.4 (17)	O3—C11—C12	107.2 (2)
C5—C6—C1	119.8 (2)	O3—C11—H11A	106.5 (14)
C5—C6—N1	121.9 (2)	C12—C11—H11A	111.7 (14)
C1—C6—N1	118.3 (2)	O3—C11—H11B	106.9 (15)
O1—C7—N1	123.1 (2)	C12—C11—H11B	114.0 (14)
O1—C7—C8	121.0 (2)	H11A—C11—H11B	110 (2)

N1—C7—C8	115.7 (2)	C11—C12—H12A	108.3 (17)
O1—C7—C8A	119.4 (6)	C11—C12—H12B	109.2 (17)
N1—C7—C8A	112.8 (5)	H12A—C12—H12B	111 (2)
N2—C8—C9	111.9 (2)	C11—C12—H12C	110.0 (16)
N2—C8—C7	109.1 (2)	H12A—C12—H12C	107 (2)
C9—C8—C7	110.6 (2)	H12B—C12—H12C	111 (3)
N2—C8—H8	108.4		

C8—N2—C1—C2	−147.1 (3)	C1—N2—C8—C7	−52.3 (4)
C8—N2—C1—C6	37.4 (4)	O1—C7—C8—N2	−148.2 (2)
C8A—N2A—C1—C2	153 (3)	N1—C7—C8—N2	36.6 (3)
C8A—N2A—C1—C6	−53 (3)	O1—C7—C8—C9	−24.7 (3)
C6—C1—C2—C3	1.1 (4)	N1—C7—C8—C9	160.1 (2)
N2—C1—C2—C3	−174.4 (2)	N2—C8—C9—C10	−56.8 (3)
N2A—C1—C2—C3	154.5 (17)	C7—C8—C9—C10	−178.6 (2)
C1—C2—C3—C4	−0.3 (4)	C1—N2A—C8A—C9A	−176 (2)
C2—C3—C4—C5	−0.5 (4)	C1—N2A—C8A—C7	62 (3)
C3—C4—C5—C6	0.4 (4)	O1—C7—C8A—N2A	157.1 (11)
C4—C5—C6—C1	0.4 (4)	N1—C7—C8A—N2A	−46.4 (19)
C4—C5—C6—N1	179.1 (2)	O1—C7—C8A—C9A	32 (2)
C2—C1—C6—C5	−1.1 (4)	N1—C7—C8A—C9A	−171.4 (12)
N2—C1—C6—C5	174.6 (2)	N2A—C8A—C9A—C10	34 (4)
N2A—C1—C6—C5	−156.6 (13)	C7—C8A—C9A—C10	154.6 (10)
C2—C1—C6—N1	−179.8 (2)	C11—O3—C10—O2	1.4 (4)
N2—C1—C6—N1	−4.1 (3)	C11—O3—C10—O2A	−35 (2)
N2A—C1—C6—N1	24.7 (14)	C11—O3—C10—C9A	−179.2 (2)
C7—N1—C6—C5	169.9 (2)	C11—O3—C10—C9	−179.2 (2)
C7—N1—C6—C1	−11.4 (4)	C8A—C9A—C10—O2A	14 (2)
C6—N1—C7—O1	178.5 (2)	C8A—C9A—C10—O3	159.0 (17)
C6—N1—C7—C8	−6.4 (3)	C8—C9—C10—O2	8.6 (4)
C6—N1—C7—C8A	23.1 (14)	C8—C9—C10—O3	−170.8 (2)
C1—N2—C8—C9	−175.0 (2)	C10—O3—C11—C12	−175.7 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O1^{i}	0.87 (3)	1.99 (4)	2.866 (3)	177 (3)
N2—H2*A*···O2	0.91	2.14	2.816 (3)	130
C3—H3···O3^{ii}	0.95 (3)	2.59 (3)	3.508 (3)	165 (2)
C8—H8···O1^{iii}	1.00	2.55	3.443 (4)	148
C9—H9*A*···O2^{iv}	0.99	2.52	3.367 (4)	144
C11—H11*B*···O2^{v}	0.97 (2)	2.58 (3)	3.199 (3)	121.9 (18)

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