2-(3-Methyl-2-oxoquinoxalin-1-yl)-N-(4-methyl-phenyl)acetamide

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The quinoxaline moiety in the title molecule, $C_{18}H_{17}N_3O_2$, is not quite planar and the p-tolyl group is rotationally disordered over two nearly equally populated sets of sites. In the crystal, N—H···O and C—H···O hydrogen bonds form chains extending along the b-axis direction. Due to the disorder of the p-tolyl rings, short C···C distances are observed between adjacent chains.

3D view


Chemical scheme
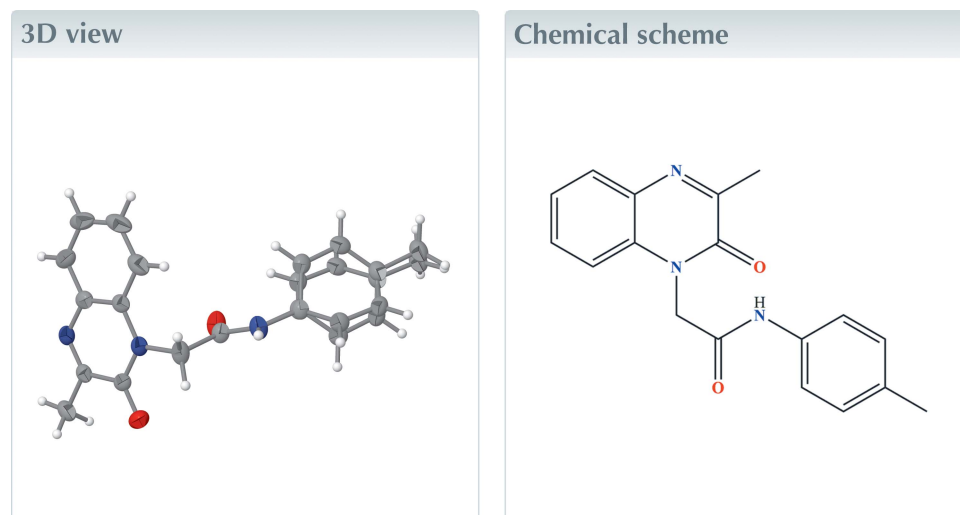
Structure description

Among the various classes of nitrogen heterocyclic compounds, quinoxaline derivatives display a broad spectrum of biological and pharmacological activities (Ramli & Essassi, 2015). Some analogs have been synthesized and evaluated for their industrial properties (e.g. Lgaz et al., 2015). As a continuation of our work in this area (e.g. Abad et al., 2021), the title compound was synthesized and its crystal structure is reported here (Fig. 1).

The quinoxaline moiety is slightly nonplanar as there is a dihedral angle of 1.26 (14)° between the mean planes through the constituent rings. The p-tolyl ring is rotationally disordered over two orientations 45.46 (18)° apart in a 0.503 (2):0.497 (2) ratio. In the crystal, N3—H3A···O2 and C10—H10B···O2 hydrogen bonds (Table 1) form chains of molecules extending along the b-axis direction. Pairs of inversion-related chains show C16···C17[i] and C17···C16[i] [symmetry code: (i) −x + 1, −y, −z + 1] distances of 2.695 (4) Å, which is 0.71 Å less than the sum of the van der Waals radii and is likely due to the disorder involving this ring. The chains stack along the c-axis direction (Figs. 2 and 3).
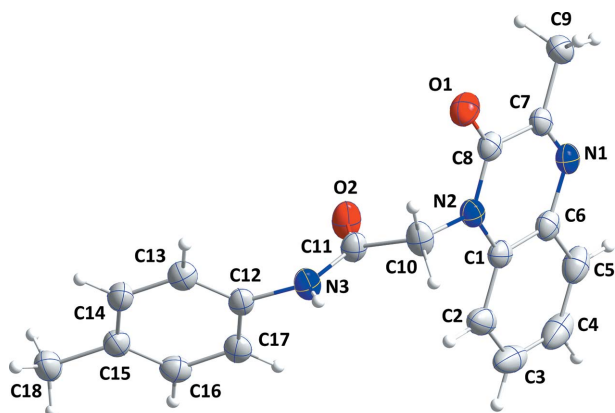
Figure 1
The title molecule with the atom-labelling scheme and 50% probability displacement ellipsoids. Only the major orientation of the disordered *p*-tolyl group is shown.
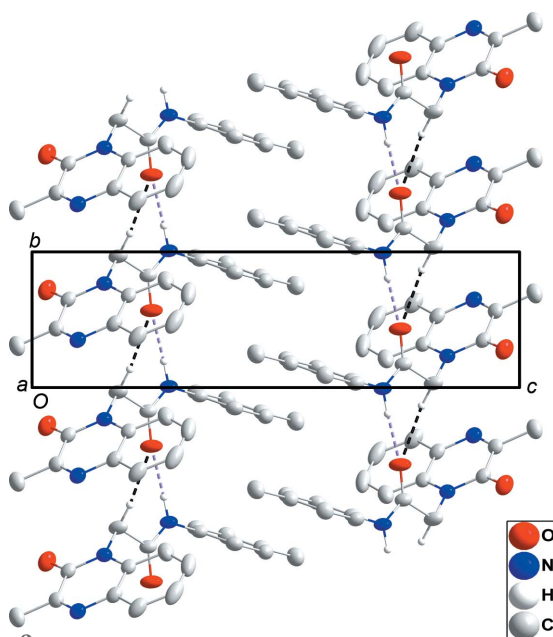
Figure 2
A portion of one ribbon, viewed along the *a*-axis direction, with N—H⋯O and C—H⋯O hydrogen bonds depicted, respectively, by violet and black dashed lines. Non-interacting H atoms have been omitted for clarity.
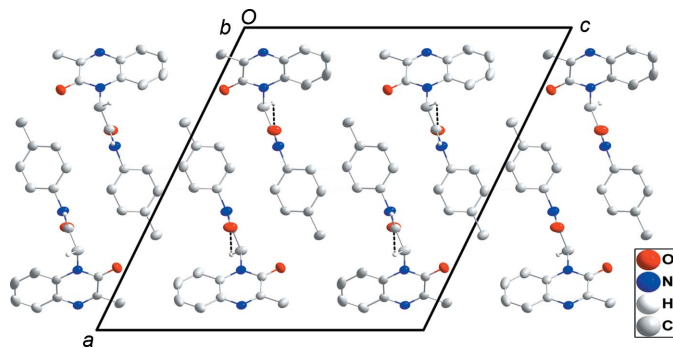
Figure 3
The packing, viewed along the *b*-axis direction, with intermolecular interactions depicted as in Fig. 2 and non-interacting H atoms omitted for clarity.

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
N3—H3A⋯O2^{i}	0.89 (3)	1.91 (3)	2.790 (2)	167 (3)
C10—H10B⋯O2^{i}	0.99	2.57	3.179 (3)	120

Symmetry code: (i) $x, y - 1, z$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{17}N_3O_2$
M_r	307.34
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	125
a, b, c (Å)	19.2935 (7), 4.6933 (2), 18.7498 (7)
β (°)	116.106 (2)
V (Å^3)	1524.59 (11)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	0.72
Crystal size (mm)	$0.23 \times 0.15 \times 0.02$
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 3 CPAD
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.85, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5971, 5971, 4844
R_{int}	0.065
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.057, 0.158, 1.04
No. of reflections	5971
No. of parameters	214
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})	0.30, −0.32

Computer programs: *APEX4* (Bruker, 2021), *SAINT* (Bruker, 2021), *SHELXT* (Sheldrick, 2015a), *SHELXL2018* (Sheldrick, 2015b), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Bruker, 2021).

Synthesis and crystallization

1.00 g (6.24 mmol) of 3-methylquinoxalin-2(1*H*)-one was dissolved in 25 ml of dimethylformamide and 1.15 g (6.24 mmol) of 2-chloro-*N*-(*p*-tolyl)acetamide were added, followed by 1.0 g (7.5 mmol) of potassium bicarbonate, and a spatula tip of BTBA (benzyltributylammonium chloride) was used as a phase-transfer catalyst. The reaction was stirred for 2 h under reflux at 353 K. When the starting reagents had completely reacted, 500 ml of distilled water were added and a few minutes later the product precipitated. This was filtered off, dried and recrystallized from hot ethanol solution to yield light-yellow plate-like crystals of the title compound.

Refinement

Crystal, data collection and refinement details are presented in Table 2. H atoms attached to carbon were included as riding

atoms in idealized positions with isotropic displacement parameters tied to those of the attached atoms, while that attached to nitrogen was refined independently. Analysis of 446 reflections having $I/\sigma(I) > 20$ and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about the c^* axis. The structure was refined as a two-component twin. The two components [0.503 (2): 0.497 (2) ratio] of the disordered C12–C17 ring were refined as rigid hexagons.

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full crystallographic data

2-(3-Methyl-2-oxoquinoxalin-1-yl)-*N*-(4-methylphenyl)acetamide

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2-(3-Methyl-2-oxoquinoxalin-1-yl)-*N*-(4-methylphenyl)acetamide

Crystal data

$C_{18}H_{17}N_3O_2$	$F(000) = 648$
$M_r = 307.34$	$D_x = 1.339$ Mg m^{-3}
Monoclinic, $P2_1/c$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
$a = 19.2935\ (7)$ Å	Cell parameters from 9934 reflections
$b = 4.6933\ (2)$ Å	$\theta = 4.7–72.5°$
$c = 18.7498\ (7)$ Å	$\mu = 0.72$ mm^{-1}
$\beta = 116.106\ (2)°$	$T = 125$ K
$V = 1524.59\ (11)$ Å^3	Plate, colourless
$Z = 4$	$0.23 \times 0.15 \times 0.02$ mm

Data collection

Bruker D8 VENTURE PHOTON 3 CPAD diffractometer	$T_{min} = 0.85$, $T_{max} = 0.99$
Radiation source: INCOATEC IμS micro–focus source	5971 measured reflections
	5971 independent reflections
Mirror monochromator	4844 reflections with $I > 2\sigma(I)$
Detector resolution: 7.3910 pixels mm^{-1}	$R_{int} = 0.065$
φ and ω scans	$\theta_{max} = 72.6°$, $\theta_{min} = 2.6°$
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)	$h = -23 \rightarrow 21$
	$k = 0 \rightarrow 5$
	$l = 0 \rightarrow 23$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.057$	Hydrogen site location: mixed
$wR(F^2) = 0.158$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.04$	
5971 reflections	$w = 1/[\sigma^2(F_o^2) + (0.0668P)^2 + 0.6811P]$ where $P = (F_o^2 + 2F_c^2)/3$
214 parameters	
4 restraints	$(\Delta/\sigma)_{max} < 0.001$
Primary atom site location: dual	$\Delta\rho_{max} = 0.30$ e Å^{-3}
	$\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 16 sets of frames, each of width 0.5° in ω or φ, collected with scan parameters determined by the "strategy" routine in *APEX4*. The scan time was θ-dependent and ranged from 5 to 10 sec/frame. Analysis of 446 reflections having $I/\sigma(I) > 20$ and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the monoclinic system and to be twinned by a 180° rotation about the c^* axis. 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å) and were included as riding contributions with isotropic displacement parameters 1.2 - 1.5 times those of the attached atoms. That attached to nitrogen was refined independently. Refined as a 2-component twin. The C12···C17 ring is rotationally disordered over two sites in a 0.503 (2)/0.497 (2) ratio. The two rings were refined as rigid hexagons.

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

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1	0.79390 (9)	0.2813 (4)	0.96921 (10)	0.0428 (4)	
O2	0.66001 (9)	0.4321 (3)	0.75510 (11)	0.0439 (4)	
N1	0.91798 (10)	0.6484 (4)	0.90616 (11)	0.0328 (4)	
N2	0.80138 (10)	0.2332 (4)	0.85180 (10)	0.0303 (4)	
N3	0.60746 (11)	−0.0081 (4)	0.71946 (12)	0.0346 (4)	
H3A	0.6168 (16)	−0.194 (7)	0.7296 (16)	0.048 (8)*	
C1	0.83439 (12)	0.3204 (5)	0.80215 (12)	0.0303 (5)	
C2	0.81095 (14)	0.2121 (6)	0.72561 (14)	0.0425 (6)	
H2	0.771477	0.071925	0.705499	0.051*	
C3	0.84517 (17)	0.3090 (7)	0.67925 (15)	0.0522 (8)	
H3	0.828981	0.235039	0.627189	0.063*	
C4	0.90311 (16)	0.5136 (7)	0.70797 (16)	0.0527 (8)	
H4	0.926420	0.578486	0.675630	0.063*	
C5	0.92664 (14)	0.6221 (6)	0.78309 (15)	0.0433 (6)	
H5	0.966159	0.762259	0.802523	0.052*	
C6	0.89276 (12)	0.5272 (5)	0.83112 (12)	0.0322 (5)	
C7	0.88615 (11)	0.5649 (5)	0.95044 (12)	0.0305 (5)	
C8	0.82374 (12)	0.3501 (5)	0.92579 (12)	0.0306 (5)	
C9	0.91077 (14)	0.6936 (6)	1.03080 (14)	0.0426 (6)	
H9A	0.952575	0.830084	1.041179	0.064*	
H9B	0.929002	0.543057	1.071109	0.064*	
H9C	0.866893	0.792162	1.032824	0.064*	
C10	0.73747 (12)	0.0317 (5)	0.82339 (15)	0.0377 (5)	
H10A	0.728584	−0.036647	0.868641	0.045*	
H10B	0.750558	−0.134921	0.799270	0.045*	
C11	0.66396 (12)	0.1729 (4)	0.76175 (13)	0.0316 (5)	
C12	0.53264 (11)	0.0608 (7)	0.65663 (13)	0.0294 (5)	0.503 (2)

C13	0.46472 (15)	0.0306 (7)	0.66460 (13)	0.0336 (7)	0.503 (2)
H13	0.466547	−0.031354	0.713638	0.040*	0.503 (2)
C14	0.39412 (11)	0.0910 (7)	0.60083 (17)	0.0356 (9)	0.503 (2)
H14	0.347698	0.070370	0.606282	0.043*	0.503 (2)
C15	0.39144 (11)	0.1817 (7)	0.52909 (14)	0.0343 (7)	0.503 (2)
C16	0.45936 (15)	0.2119 (7)	0.52111 (12)	0.0354 (7)	0.503 (2)
H16	0.457528	0.273880	0.472078	0.042*	0.503 (2)
C17	0.52996 (12)	0.1515 (7)	0.58488 (16)	0.0334 (7)	0.503 (2)
H17	0.576378	0.172158	0.579433	0.040*	0.503 (2)
C18	0.3136 (3)	0.2476 (16)	0.4594 (4)	0.0433 (14)	0.503 (2)
H18A	0.317427	0.220882	0.409396	0.065*	0.503 (2)
H18B	0.299208	0.445281	0.463168	0.065*	0.503 (2)
H18C	0.274261	0.118941	0.460865	0.065*	0.503 (2)
C12A	0.53474 (11)	0.0803 (6)	0.65812 (15)	0.0294 (5)	0.497 (2)
C13A	0.47318 (16)	−0.1031 (5)	0.64255 (17)	0.0336 (7)	0.497 (2)
H13A	0.480998	−0.274459	0.672089	0.040*	0.497 (2)
C14A	0.40017 (13)	−0.0359 (6)	0.58377 (18)	0.0356 (9)	0.497 (2)
H14A	0.358098	−0.161254	0.573130	0.043*	0.497 (2)
C15A	0.38873 (11)	0.2148 (6)	0.54055 (15)	0.0343 (7)	0.497 (2)
C16A	0.45030 (16)	0.3982 (5)	0.55611 (16)	0.0354 (7)	0.497 (2)
H16A	0.442477	0.569545	0.526577	0.042*	0.497 (2)
C17A	0.52330 (13)	0.3310 (6)	0.61490 (17)	0.0334 (7)	0.497 (2)
H17A	0.565379	0.456344	0.625535	0.040*	0.497 (2)
C18A	0.3093 (3)	0.295 (2)	0.4756 (3)	0.0433 (14)	0.497 (2)
H18D	0.313503	0.340756	0.426650	0.065*	0.497 (2)
H18E	0.289595	0.461028	0.492575	0.065*	0.497 (2)
H18F	0.273790	0.134311	0.465835	0.065*	0.497 (2)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0390 (9)	0.0533 (11)	0.0416 (9)	0.0026 (8)	0.0228 (8)	0.0094 (8)
O2	0.0358 (9)	0.0220 (8)	0.0660 (11)	0.0024 (6)	0.0151 (8)	0.0024 (7)
N1	0.0256 (9)	0.0336 (10)	0.0346 (10)	0.0029 (7)	0.0092 (7)	0.0034 (8)
N2	0.0276 (9)	0.0268 (9)	0.0331 (9)	0.0009 (7)	0.0101 (7)	0.0007 (7)
N3	0.0316 (10)	0.0211 (9)	0.0422 (11)	0.0031 (7)	0.0081 (8)	0.0018 (8)
C1	0.0280 (10)	0.0300 (11)	0.0298 (10)	0.0093 (8)	0.0099 (8)	0.0038 (8)
C2	0.0411 (13)	0.0457 (14)	0.0338 (12)	0.0143 (11)	0.0102 (10)	−0.0042 (10)
C3	0.0554 (16)	0.0694 (19)	0.0293 (12)	0.0316 (15)	0.0164 (11)	0.0065 (12)
C4	0.0492 (15)	0.074 (2)	0.0444 (14)	0.0285 (14)	0.0295 (13)	0.0257 (14)
C5	0.0354 (12)	0.0525 (15)	0.0451 (13)	0.0106 (11)	0.0206 (11)	0.0185 (12)
C6	0.0276 (10)	0.0348 (12)	0.0327 (11)	0.0087 (9)	0.0118 (9)	0.0082 (9)
C7	0.0248 (10)	0.0321 (11)	0.0293 (10)	0.0057 (8)	0.0069 (8)	0.0017 (9)
C8	0.0281 (10)	0.0315 (11)	0.0309 (11)	0.0068 (8)	0.0120 (9)	0.0069 (9)
C9	0.0352 (12)	0.0509 (15)	0.0330 (12)	0.0056 (11)	0.0070 (10)	−0.0068 (11)
C10	0.0311 (11)	0.0260 (11)	0.0474 (13)	−0.0009 (9)	0.0094 (10)	0.0041 (10)
C11	0.0298 (11)	0.0241 (11)	0.0393 (12)	0.0031 (8)	0.0137 (9)	0.0022 (9)
C12	0.0282 (10)	0.0218 (10)	0.0350 (11)	0.0016 (8)	0.0111 (9)	−0.0008 (8)

C13	0.0365 (16)	0.027 (2)	0.0366 (18)	−0.0007 (16)	0.0152 (13)	0.0021 (14)
C14	0.0287 (14)	0.039 (3)	0.040 (2)	−0.0009 (17)	0.0154 (13)	−0.0033 (17)
C15	0.0321 (12)	0.0319 (14)	0.0353 (14)	0.0028 (10)	0.0115 (10)	−0.0037 (11)
C16	0.0434 (17)	0.0296 (16)	0.0317 (16)	0.0012 (13)	0.0152 (13)	−0.0006 (12)
C17	0.0326 (15)	0.0264 (15)	0.0400 (17)	−0.0025 (13)	0.0150 (13)	−0.0024 (12)
C18	0.0352 (14)	0.046 (3)	0.039 (3)	0.0052 (14)	0.0082 (17)	−0.005 (2)
C12A	0.0282 (10)	0.0218 (10)	0.0350 (11)	0.0016 (8)	0.0111 (9)	−0.0008 (8)
C13A	0.0365 (16)	0.027 (2)	0.0366 (18)	−0.0007 (16)	0.0152 (13)	0.0021 (14)
C14A	0.0287 (14)	0.039 (3)	0.040 (2)	−0.0009 (17)	0.0154 (13)	−0.0033 (17)
C15A	0.0321 (12)	0.0319 (14)	0.0353 (14)	0.0028 (10)	0.0115 (10)	−0.0037 (11)
C16A	0.0434 (17)	0.0296 (16)	0.0317 (16)	0.0012 (13)	0.0152 (13)	−0.0006 (12)
C17A	0.0326 (15)	0.0264 (15)	0.0400 (17)	−0.0025 (13)	0.0150 (13)	−0.0024 (12)
C18A	0.0352 (14)	0.046 (3)	0.039 (3)	0.0052 (14)	0.0082 (17)	−0.005 (2)

Geometric parameters (Å, º)

O1—C8	1.229 (3)	C12—C13	1.3900
O2—C11	1.222 (3)	C12—C17	1.3900
N1—C7	1.292 (3)	C13—C14	1.3900
N1—C6	1.392 (3)	C13—H13	0.9500
N2—C8	1.373 (3)	C14—C15	1.3900
N2—C1	1.401 (3)	C14—H14	0.9500
N2—C10	1.456 (3)	C15—C16	1.3900
N3—C11	1.333 (3)	C15—C18	1.527 (3)
N3—C12A	1.429 (2)	C16—C17	1.3900
N3—C12	1.442 (2)	C16—H16	0.9500
N3—H3A	0.89 (3)	C17—H17	0.9500
C1—C2	1.397 (3)	C18—H18A	0.9800
C1—C6	1.402 (3)	C18—H18B	0.9800
C2—C3	1.379 (4)	C18—H18C	0.9800
C2—H2	0.9500	C12A—C13A	1.3900
C3—C4	1.390 (4)	C12A—C17A	1.3900
C3—H3	0.9500	C13A—C14A	1.3900
C4—C5	1.373 (4)	C13A—H13A	0.9500
C4—H4	0.9500	C14A—C15A	1.3900
C5—C6	1.398 (3)	C14A—H14A	0.9500
C5—H5	0.9500	C15A—C16A	1.3900
C7—C8	1.480 (3)	C15A—C18A	1.527 (3)
C7—C9	1.493 (3)	C16A—C17A	1.3900
C9—H9A	0.9800	C16A—H16A	0.9500
C9—H9B	0.9800	C17A—H17A	0.9500
C9—H9C	0.9800	C18A—H18D	0.9800
C10—C11	1.531 (3)	C18A—H18E	0.9800
C10—H10A	0.9900	C18A—H18F	0.9800
C10—H10B	0.9900		
C7—N1—C6	118.2 (2)	C13—C12—C17	120.0
C8—N2—C1	121.48 (19)	C13—C12—N3	122.8 (2)

C8—N2—C10	117.92 (19)	C17—C12—N3	117.2 (2)
C1—N2—C10	120.41 (19)	C12—C13—C14	120.0
C11—N3—C12A	123.3 (2)	C12—C13—H13	120.0
C11—N3—C12	127.3 (2)	C14—C13—H13	120.0
C11—N3—H3A	117.3 (18)	C13—C14—C15	120.0
C12A—N3—H3A	119.3 (18)	C13—C14—H14	120.0
C12—N3—H3A	115.4 (18)	C15—C14—H14	120.0
C2—C1—N2	122.7 (2)	C16—C15—C14	120.0
C2—C1—C6	119.4 (2)	C16—C15—C18	120.4 (4)
N2—C1—C6	117.85 (19)	C14—C15—C18	119.6 (4)
C3—C2—C1	119.9 (3)	C15—C16—C17	120.0
C3—C2—H2	120.0	C15—C16—H16	120.0
C1—C2—H2	120.0	C17—C16—H16	120.0
C2—C3—C4	120.7 (2)	C16—C17—C12	120.0
C2—C3—H3	119.7	C16—C17—H17	120.0
C4—C3—H3	119.7	C12—C17—H17	120.0
C5—C4—C3	120.0 (2)	C15—C18—H18A	109.5
C5—C4—H4	120.0	C15—C18—H18B	109.5
C3—C4—H4	120.0	H18A—C18—H18B	109.5
C4—C5—C6	120.4 (3)	C15—C18—H18C	109.5
C4—C5—H5	119.8	H18A—C18—H18C	109.5
C6—C5—H5	119.8	H18B—C18—H18C	109.5
N1—C6—C5	117.8 (2)	C13A—C12A—C17A	120.0
N1—C6—C1	122.57 (19)	C13A—C12A—N3	115.8 (2)
C5—C6—C1	119.6 (2)	C17A—C12A—N3	124.2 (2)
N1—C7—C8	123.88 (19)	C12A—C13A—C14A	120.0
N1—C7—C9	119.7 (2)	C12A—C13A—H13A	120.0
C8—C7—C9	116.4 (2)	C14A—C13A—H13A	120.0
O1—C8—N2	122.2 (2)	C15A—C14A—C13A	120.0
O1—C8—C7	121.7 (2)	C15A—C14A—H14A	120.0
N2—C8—C7	116.01 (18)	C13A—C14A—H14A	120.0
C7—C9—H9A	109.5	C16A—C15A—C14A	120.0
C7—C9—H9B	109.5	C16A—C15A—C18A	118.7 (5)
H9A—C9—H9B	109.5	C14A—C15A—C18A	121.3 (5)
C7—C9—H9C	109.5	C15A—C16A—C17A	120.0
H9A—C9—H9C	109.5	C15A—C16A—H16A	120.0
H9B—C9—H9C	109.5	C17A—C16A—H16A	120.0
N2—C10—C11	110.41 (17)	C16A—C17A—C12A	120.0
N2—C10—H10A	109.6	C16A—C17A—H17A	120.0
C11—C10—H10A	109.6	C12A—C17A—H17A	120.0
N2—C10—H10B	109.6	C15A—C18A—H18D	109.5
C11—C10—H10B	109.6	C15A—C18A—H18E	109.5
H10A—C10—H10B	108.1	H18D—C18A—H18E	109.5
O2—C11—N3	125.1 (2)	C15A—C18A—H18F	109.5
O2—C11—C10	120.2 (2)	H18D—C18A—H18F	109.5
N3—C11—C10	114.60 (18)	H18E—C18A—H18F	109.5
C8—N2—C1—C2	−177.8 (2)	C12—N3—C11—O2	2.3 (4)

C10—N2—C1—C2	−2.9 (3)	C12A—N3—C11—C10	−178.9 (2)
C8—N2—C1—C6	1.5 (3)	C12—N3—C11—C10	−178.8 (2)
C10—N2—C1—C6	176.39 (18)	N2—C10—C11—O2	−15.5 (3)
N2—C1—C2—C3	179.3 (2)	N2—C10—C11—N3	165.5 (2)
C6—C1—C2—C3	0.0 (3)	C11—N3—C12—C13	−110.6 (3)
C1—C2—C3—C4	0.1 (4)	C11—N3—C12—C17	71.6 (3)
C2—C3—C4—C5	−0.2 (4)	C17—C12—C13—C14	0.0
C3—C4—C5—C6	0.2 (4)	N3—C12—C13—C14	−177.7 (3)
C7—N1—C6—C5	178.99 (19)	C12—C13—C14—C15	0.0
C7—N1—C6—C1	0.2 (3)	C13—C14—C15—C16	0.0
C4—C5—C6—N1	−178.9 (2)	C13—C14—C15—C18	−179.99 (8)
C4—C5—C6—C1	−0.1 (3)	C14—C15—C16—C17	0.0
C2—C1—C6—N1	178.75 (19)	C18—C15—C16—C17	179.99 (8)
N2—C1—C6—N1	−0.6 (3)	C15—C16—C17—C12	0.0
C2—C1—C6—C5	0.0 (3)	C13—C12—C17—C16	0.0
N2—C1—C6—C5	−179.35 (19)	N3—C12—C17—C16	177.8 (3)
C6—N1—C7—C8	−0.7 (3)	C11—N3—C12A—C13A	−154.7 (2)
C6—N1—C7—C9	−178.98 (19)	C11—N3—C12A—C17A	25.5 (4)
C1—N2—C8—O1	178.05 (19)	C17A—C12A—C13A—C14A	0.0
C10—N2—C8—O1	3.1 (3)	N3—C12A—C13A—C14A	−179.8 (3)
C1—N2—C8—C7	−2.0 (3)	C12A—C13A—C14A—C15A	0.0
C10—N2—C8—C7	−176.93 (17)	C13A—C14A—C15A—C16A	0.0
N1—C7—C8—O1	−178.4 (2)	C13A—C14A—C15A—C18A	179.99 (8)
C9—C7—C8—O1	−0.1 (3)	C14A—C15A—C16A—C17A	0.0
N1—C7—C8—N2	1.6 (3)	C18A—C15A—C16A—C17A	−179.99 (7)
C9—C7—C8—N2	179.90 (18)	C15A—C16A—C17A—C12A	0.0
C8—N2—C10—C11	104.1 (2)	C13A—C12A—C17A—C16A	0.0
C1—N2—C10—C11	−71.0 (2)	N3—C12A—C17A—C16A	179.8 (3)
C12A—N3—C11—O2	2.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O2[i]	0.89 (3)	1.91 (3)	2.790 (2)	167 (3)
C10—H10B···O2[i]	0.99	2.57	3.179 (3)	120

Symmetry code: (i) x, $y-1$, z.