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1-Ethyl-3-methylquinoxalin-2(1*H*)-one

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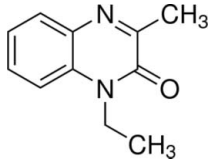
Key indicators: single-crystal X-ray study; T = 180 K; mean σ(C–C) = 0.002 Å; R factor = 0.039; wR factor = 0.111; data-to-parameter ratio = 15.0.

The asymmetric unit of the title compound, $C_{11}H_{12}N_2O$, contains two independent molecules. In the crystal structure, intermolecular C—H···O hydrogen bonds link the molecules. There are π–π contacts between the quinoxaline rings [centroid–centroid distances = 3.446 (2), 3.665 (2), 3.645 (3) and 3.815 (3) Å]. There also exist C—H···π contacts between the methyl groups and the quinoxaline rings.

Related literature

For general background, see: Amin (2003); Boutti & Lecolier (1975); Milos & John (1981); Rose *et al.* (1990); Salman *et al.* (2007); Kotharkar & Shinde (2006); Vishnu *et al.* (2006). For related literature, see: Nikolaenko & Munro (2004). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{11}H_{12}N_2O$
M_r = 188.23
Triclinic, $P\overline{1}$
a = 7.4101 (6) Å
b = 9.1405 (8) Å
c = 14.2960 (12) Å
α = 84.976 (7)°
β = 78.717 (7)°
γ = 88.137 (7)°
V = 945.82 (14) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 180 K
0.18 × 0.13 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.988, T_{max} = 0.991
7441 measured reflections
3865 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.021

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.06
3865 reflections
257 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C7—H7···O2^{i}	0.93	2.43	3.291 (3)	154
C17—H17···O1	0.93	2.46	3.301 (3)	151
C22—H22C···$Cg4^{ii}$	0.96	2.71	3.516 (3)	142

Symmetry codes: (i) $x, y, z+1$; (ii) $-x, -y, -z$. $Cg4$ is the centroid of the C14–C19 ring.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1994); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2003); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2546).

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1-Ethyl-3-methylquinoxalin-2(1*H*)-one

Hanane Benzeid, Laure Vendier, Youssef Ramli, Bernard Garrigues and El Mokhtar Essassi

S1. Comment

The quinoxaline derivatives have great importance in scientific research for their biological properties. It is well known that quinoxaline have antibacterial (Kotharkar & Shinde, 2006; Salman *et al.*, 2007) and antifungal (Vishnu *et al.*, 2006) activities. They are also used for colorimetry metal detection (Amin, 2003) and as oil stabilizant (Boutti & Lecolier, 1975). Likewise several patents describe them as hair azo dyes (Rose *et al.*, 1990) and pigments (Milos & John, 1981). We report herein, the synthesis and crystal structure of the title compound.

The asymmetric unit of the title compound (Fig. 1), contains two independent molecules. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges. The intramolecular C—H···O hydrogen bond (Table 1) links the molecules.

In the crystal structure, intra- and intermolecular C-H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they may be effective in the stabilization of the structure. The π—π contacts between the quinoxaline rings, Cg1···Cg1^{i}, Cg1···Cg3^{ii}, Cg2···Cg2^{iii} and Cg2···Cg4^{iv} [symmetry codes: (i) 1 - x, 1 - y, 1 - z; (ii) -x, 1 - y, 1 - z; (iii) -x, -y, -z; (iv) 1 - x, -y, -z, where Cg1, Cg2, Cg3 and Cg4 are the centroids of the rings A (N1/N2/C1-C3/C8), B (N3/N4/C12-C14/C19), C (C3-C8) and D (C14-C19), respectively] may further stabilize the structure, with centroid-centroid distances of 3.446 (2), 3.665 (2), 3.645 (3) and 3.815 (3) Å, respectively. There also exist C—H···π contacts (Table 1) between the methyl groups and rings C and D.

S2. Experimental

To a solution of 3-methylquinoxalin-2(1*H*)-one (Nikolaenko & Munro, 2004) (1 g, 6.22 mmol) in dimethylformamide (20 ml), was added ethylbromide (0.67 ml, 6.22 mmol), K_2CO_3 (1 g, 7.46 mmol) and a catalytic quantity of tetrabutyl-ammoniumbromide. The mixture was stirred at room temperature for 24 h. The solution was filtered to remove the salts. The solvent was removed under reduced pressure. The residue was crystallized in ethanol to afford the title compound as yellow crystals.

S3. Refinement

H atoms were positioned geometrically, with C-H = 0.93, 0.97 and 0.96 Å for aromatic, methylene and methyl H, respectively, and constrained to ride on their parent atoms with U_{iso}(H) = xU_{eq}(C), where x = 1.5 for methyl H and x = 1.2 for all other H atoms.

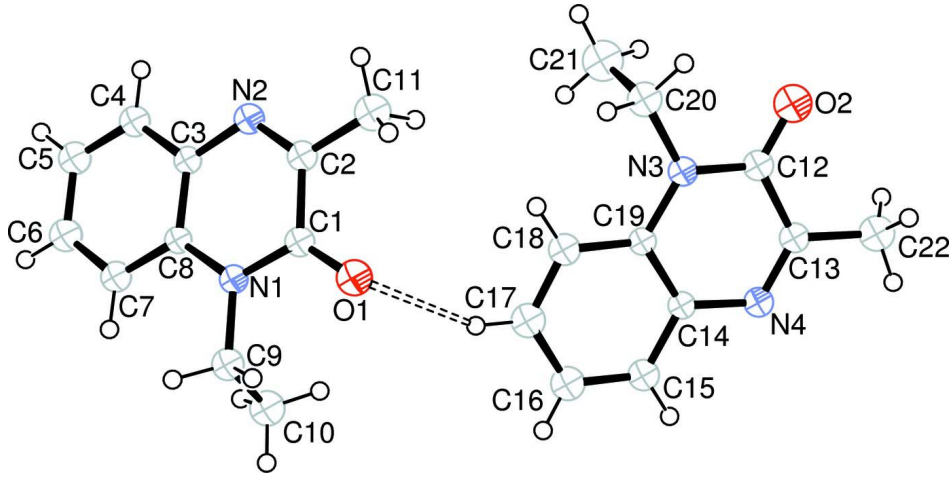

Figure 1

The molecular structure of the title molecule, with the atom-numbering scheme. Hydrogen bond is shown as dashed line.

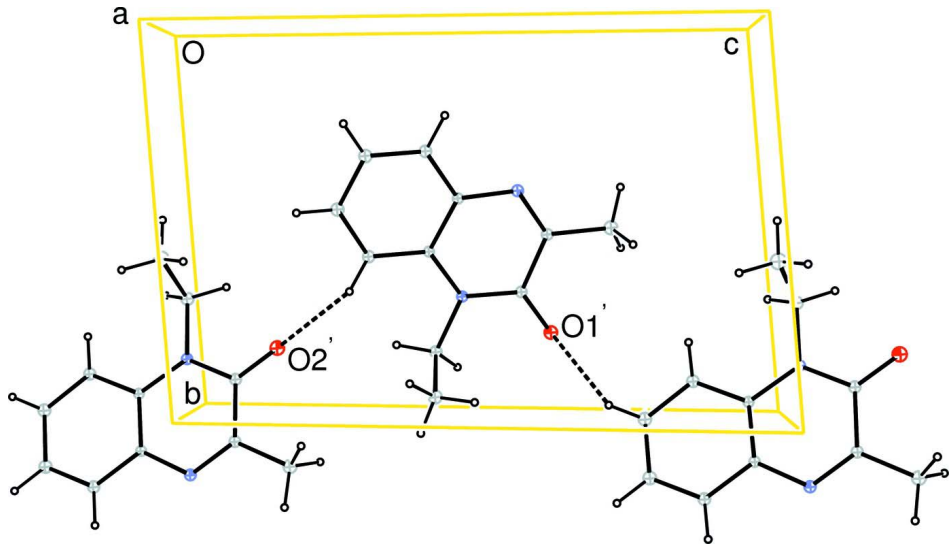

Figure 2

A partial packing diagram. Hydrogen bonds are shown as dashed lines [symmetry code: (′) -x, -y, -z].

1-Ethyl-3-methylquinoxalin-2(1*H*)-one

Crystal data

$C_{11}H_{12}N_2O$
$M_r = 188.23$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.4101\ (6)$ Å
$b = 9.1405\ (8)$ Å
$c = 14.2960\ (12)$ Å
$\alpha = 84.976\ (7)°$
$\beta = 78.717\ (7)°$
$\gamma = 88.137\ (7)°$
$V = 945.82\ (14)$ Å^3
$Z = 4$
$F(000) = 400$
$D_x = 1.322$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 4794 reflections
$\theta = 2.8–31.9°$
$\mu = 0.09$ mm^{-1}
$T = 180$ K
Block, colorless
0.18 × 0.13 × 0.07 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.988, T_{max} = 0.991
7441 measured reflections
3865 independent reflections
2874 reflections with $I > 2\sigma(I)$
R_{int} = 0.021
θ_{max} = 26.4°, θ_{min} = 2.8°
h = −9→8
k = −11→11
l = −14→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.111
S = 1.06
3865 reflections
257 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0636P)^2 + 0.0861P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.17 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-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.

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 $F^2 > \sigma(F^2)$ 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.

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

	x	y	z	U_{iso}*/U_{eq}
O1	0.46438 (13)	0.21858 (11)	0.37756 (7)	0.0375 (3)
O2	0.28053 (14)	0.17912 (12)	−0.17004 (7)	0.0438 (3)
N1	0.33532 (14)	0.31106 (11)	0.51763 (7)	0.0244 (2)
N2	0.28293 (14)	0.57622 (11)	0.41274 (8)	0.0279 (3)
N3	0.30886 (13)	0.14773 (11)	−0.01436 (7)	0.0258 (2)
N4	0.19176 (14)	−0.14053 (12)	−0.01083 (8)	0.0274 (3)
C1	0.39293 (17)	0.32233 (14)	0.42044 (9)	0.0267 (3)
C2	0.36552 (17)	0.46723 (14)	0.37053 (9)	0.0274 (3)
C3	0.21391 (16)	0.55680 (13)	0.51001 (9)	0.0237 (3)
C4	0.11835 (18)	0.67263 (14)	0.55460 (10)	0.0300 (3)
H4	0.1021	0.7601	0.5186	0.036*
C5	0.04770 (19)	0.66048 (15)	0.65059 (10)	0.0342 (3)
H5	−0.0161	0.7388	0.6799	0.041*
C6	0.07254 (19)	0.52952 (16)	0.70377 (10)	0.0344 (3)
H6	0.0251	0.521	0.7692	0.041*
C7	0.16544 (18)	0.41247 (15)	0.66197 (9)	0.0296 (3)

H7	0.1795	0.3253	0.6987	0.036*
C8	0.23840 (16)	0.42472 (13)	0.56451 (9)	0.0228 (3)
C9	0.37008 (19)	0.16990 (14)	0.56915 (10)	0.0311 (3)
H9A	0.3822	0.1864	0.6337	0.037*
H9B	0.4852	0.1276	0.5373	0.037*
C10	0.2174 (2)	0.06358 (15)	0.57337 (11)	0.0386 (3)
H10A	0.1059	0.1005	0.6106	0.058*
H10B	0.2494	−0.0298	0.6025	0.058*
H10C	0.1995	0.0522	0.5097	0.058*
C11	0.4365 (2)	0.48358 (17)	0.26554 (10)	0.0396 (3)
H11A	0.3503	0.4428	0.2332	0.059*
H11B	0.5527	0.4326	0.251	0.059*
H11C	0.4525	0.5858	0.2446	0.059*
C12	0.26924 (17)	0.09898 (15)	−0.09593 (9)	0.0287 (3)
C13	0.21489 (17)	−0.05575 (15)	−0.08903 (9)	0.0279 (3)
C14	0.22409 (16)	−0.08415 (13)	0.07134 (9)	0.0236 (3)
C15	0.19919 (18)	−0.17617 (15)	0.15556 (9)	0.0306 (3)
H15	0.157	−0.2709	0.1556	0.037*
C16	0.23571 (19)	−0.12955 (17)	0.23841 (10)	0.0361 (3)
H16	0.2194	−0.1921	0.2942	0.043*
C17	0.29710 (19)	0.01175 (17)	0.23769 (10)	0.0358 (3)
H17	0.3223	0.044	0.2936	0.043*
C18	0.32169 (17)	0.10564 (15)	0.15571 (10)	0.0308 (3)
H18	0.3624	0.2006	0.1567	0.037*
C19	0.28562 (16)	0.05865 (13)	0.07122 (8)	0.0232 (3)
C20	0.37012 (19)	0.29997 (14)	−0.01979 (11)	0.0359 (3)
H20A	0.432	0.3291	−0.0847	0.043*
H20B	0.4577	0.3061	0.022	0.043*
C21	0.2105 (2)	0.40401 (17)	0.00908 (14)	0.0525 (4)
H21A	0.1243	0.399	−0.0326	0.079*
H21B	0.2549	0.5024	0.0044	0.079*
H21C	0.1508	0.3768	0.0739	0.079*
C22	0.1875 (2)	−0.11426 (18)	−0.17904 (10)	0.0399 (4)
H22A	0.1497	−0.2146	−0.166	0.06*
H22B	0.3009	−0.109	−0.2251	0.06*
H22C	0.0943	−0.0569	−0.2042	0.06*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0409 (6)	0.0364 (5)	0.0342 (5)	0.0068 (4)	−0.0026 (4)	−0.0111 (4)
O2	0.0460 (6)	0.0514 (6)	0.0287 (5)	0.0052 (5)	−0.0026 (4)	0.0131 (5)
N1	0.0263 (5)	0.0214 (5)	0.0260 (6)	0.0021 (4)	−0.0066 (4)	−0.0019 (4)
N2	0.0302 (6)	0.0253 (6)	0.0291 (6)	−0.0059 (4)	−0.0083 (5)	0.0009 (4)
N3	0.0222 (5)	0.0247 (5)	0.0273 (6)	0.0021 (4)	0.0011 (4)	0.0009 (4)
N4	0.0246 (6)	0.0304 (6)	0.0266 (6)	0.0030 (4)	−0.0023 (4)	−0.0061 (5)
C1	0.0221 (6)	0.0302 (7)	0.0285 (7)	−0.0015 (5)	−0.0051 (5)	−0.0058 (5)
C2	0.0257 (6)	0.0310 (7)	0.0263 (7)	−0.0063 (5)	−0.0065 (5)	−0.0013 (5)

C3	0.0219 (6)	0.0229 (6)	0.0283 (6)	−0.0039 (5)	−0.0086 (5)	−0.0024 (5)
C4	0.0321 (7)	0.0212 (6)	0.0396 (8)	−0.0005 (5)	−0.0136 (6)	−0.0036 (5)
C5	0.0326 (7)	0.0302 (7)	0.0419 (8)	0.0034 (6)	−0.0077 (6)	−0.0154 (6)
C6	0.0359 (8)	0.0396 (8)	0.0277 (7)	−0.0012 (6)	−0.0033 (6)	−0.0094 (6)
C7	0.0331 (7)	0.0295 (7)	0.0265 (7)	0.0001 (6)	−0.0071 (5)	−0.0006 (5)
C8	0.0212 (6)	0.0223 (6)	0.0268 (6)	−0.0013 (5)	−0.0075 (5)	−0.0046 (5)
C9	0.0369 (8)	0.0251 (7)	0.0312 (7)	0.0088 (6)	−0.0081 (6)	−0.0015 (5)
C10	0.0475 (9)	0.0257 (7)	0.0394 (8)	0.0006 (6)	−0.0026 (7)	0.0013 (6)
C11	0.0436 (8)	0.0447 (8)	0.0284 (7)	−0.0039 (7)	−0.0023 (6)	0.0003 (6)
C12	0.0216 (6)	0.0377 (7)	0.0234 (7)	0.0069 (5)	0.0010 (5)	0.0014 (6)
C13	0.0202 (6)	0.0381 (7)	0.0242 (7)	0.0066 (5)	−0.0014 (5)	−0.0060 (5)
C14	0.0193 (6)	0.0268 (6)	0.0235 (6)	0.0041 (5)	−0.0010 (5)	−0.0041 (5)
C15	0.0295 (7)	0.0287 (7)	0.0301 (7)	0.0041 (5)	−0.0002 (5)	0.0028 (5)
C16	0.0351 (8)	0.0462 (9)	0.0235 (7)	0.0105 (6)	−0.0019 (6)	0.0039 (6)
C17	0.0319 (7)	0.0518 (9)	0.0251 (7)	0.0110 (6)	−0.0078 (5)	−0.0102 (6)
C18	0.0263 (7)	0.0332 (7)	0.0341 (7)	0.0034 (5)	−0.0058 (5)	−0.0117 (6)
C19	0.0171 (6)	0.0265 (6)	0.0238 (6)	0.0054 (5)	0.0001 (5)	−0.0017 (5)
C20	0.0325 (7)	0.0263 (7)	0.0445 (8)	−0.0010 (6)	0.0015 (6)	0.0022 (6)
C21	0.0460 (9)	0.0285 (8)	0.0800 (13)	0.0068 (7)	−0.0047 (8)	−0.0070 (8)
C22	0.0340 (8)	0.0588 (10)	0.0284 (7)	0.0060 (7)	−0.0064 (6)	−0.0136 (7)

Geometric parameters (Å, º)

C1—O1	1.2238 (15)	C12—O2	1.2245 (15)
C1—N1	1.3671 (16)	C12—N3	1.3705 (17)
C1—C2	1.4759 (18)	C12—C13	1.473 (2)
C2—N2	1.2854 (16)	C13—N4	1.2891 (17)
C2—C11	1.4862 (18)	C13—C22	1.4876 (19)
C3—N2	1.3825 (17)	C14—N4	1.3882 (16)
C3—C4	1.3862 (17)	C14—C15	1.3918 (18)
C3—C8	1.4049 (17)	C14—C19	1.3963 (18)
C4—C5	1.366 (2)	C15—C16	1.371 (2)
C4—H4	0.93	C15—H15	0.93
C5—C6	1.388 (2)	C16—C17	1.382 (2)
C5—H5	0.93	C16—H16	0.93
C6—C7	1.3707 (19)	C17—C18	1.3761 (19)
C6—H6	0.93	C17—H17	0.93
C7—C8	1.3885 (18)	C18—C19	1.3926 (18)
C7—H7	0.93	C18—H18	0.93
C8—N1	1.3891 (15)	C19—N3	1.3934 (16)
C9—N1	1.4696 (15)	C20—N3	1.4687 (17)
C9—H9A	0.97	C20—H20A	0.97
C9—H9B	0.97	C20—H20B	0.97
C10—C9	1.5041 (19)	C21—C20	1.509 (2)
C10—H10A	0.96	C21—H21A	0.96
C10—H10B	0.96	C21—H21B	0.96
C10—H10C	0.96	C21—H21C	0.96
C11—H11A	0.96	C22—H22A	0.96

C11—H11B	0.96	C22—H22B	0.96
C11—H11C	0.96	C22—H22C	0.96
O1—C1—N1	121.88 (12)	N4—C13—C22	119.61 (13)
O1—C1—C2	122.05 (12)	C12—C13—C22	116.56 (12)
N1—C1—C2	116.07 (11)	N4—C14—C15	118.06 (12)
N2—C2—C1	123.59 (11)	N4—C14—C19	122.33 (11)
N2—C2—C11	119.68 (12)	C15—C14—C19	119.57 (12)
C1—C2—C11	116.73 (12)	C16—C15—C14	121.14 (13)
N2—C3—C4	118.34 (11)	C16—C15—H15	119.4
N2—C3—C8	122.24 (11)	C14—C15—H15	119.4
C4—C3—C8	119.42 (12)	C15—C16—C17	118.97 (13)
C5—C4—C3	121.10 (12)	C15—C16—H16	120.5
C5—C4—H4	119.5	C17—C16—H16	120.5
C3—C4—H4	119.5	C18—C17—C16	121.23 (13)
C4—C5—C6	119.04 (12)	C18—C17—H17	119.4
C4—C5—H5	120.5	C16—C17—H17	119.4
C6—C5—H5	120.5	C17—C18—C19	120.05 (13)
C7—C6—C5	121.44 (13)	C17—C18—H18	120
C7—C6—H6	119.3	C19—C18—H18	120
C5—C6—H6	119.3	C18—C19—N3	122.96 (12)
C6—C7—C8	119.68 (12)	C18—C19—C14	119.04 (12)
C6—C7—H7	120.2	N3—C19—C14	118.00 (11)
C8—C7—H7	120.2	N3—C20—C21	111.52 (11)
C7—C8—N1	122.76 (11)	N3—C20—H20A	109.3
C7—C8—C3	119.32 (11)	C21—C20—H20A	109.3
N1—C8—C3	117.92 (11)	N3—C20—H20B	109.3
N1—C9—C10	111.68 (11)	C21—C20—H20B	109.3
N1—C9—H9A	109.3	H20A—C20—H20B	108
C10—C9—H9A	109.3	C20—C21—H21A	109.5
N1—C9—H9B	109.3	C20—C21—H21B	109.5
C10—C9—H9B	109.3	H21A—C21—H21B	109.5
H9A—C9—H9B	107.9	C20—C21—H21C	109.5
C9—C10—H10A	109.5	H21A—C21—H21C	109.5
C9—C10—H10B	109.5	H21B—C21—H21C	109.5
H10A—C10—H10B	109.5	C13—C22—H22A	109.5
C9—C10—H10C	109.5	C13—C22—H22B	109.5
H10A—C10—H10C	109.5	H22A—C22—H22B	109.5
H10B—C10—H10C	109.5	C13—C22—H22C	109.5
C2—C11—H11A	109.5	H22A—C22—H22C	109.5
C2—C11—H11B	109.5	H22B—C22—H22C	109.5
H11A—C11—H11B	109.5	C1—N1—C8	121.35 (10)
C2—C11—H11C	109.5	C1—N1—C9	116.87 (10)
H11A—C11—H11C	109.5	C8—N1—C9	121.66 (10)
H11B—C11—H11C	109.5	C2—N2—C3	118.47 (11)
O2—C12—N3	121.81 (13)	C12—N3—C19	121.53 (11)
O2—C12—C13	122.35 (13)	C12—N3—C20	117.23 (11)
N3—C12—C13	115.83 (11)	C19—N3—C20	121.20 (11)

N4—C13—C12	123.82 (12)	C13—N4—C14	118.27 (11)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C7—H7···O2^{i}	0.93	2.43	3.291 (3)	154
C17—H17···O1	0.93	2.46	3.301 (3)	151
C11—H11*B*···*Cg*3^{ii}	0.96	3.34	3.893 (3)	119
C22—H22*C*···*Cg*4^{iii}	0.96	2.71	3.516 (3)	142

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