

[(Z)-1-Amino-2-cyano-2-(4,6-di-2-pyridylpyrimidin-2-yl)ethenolato]-chlorido(*N,N*-dimethylformamide- κ O)-zinc(II)

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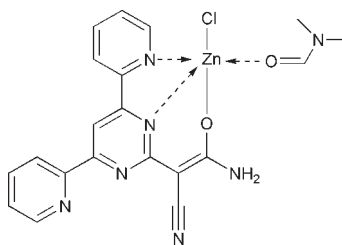
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Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.005$ Å; R factor = 0.049; wR factor = 0.167; data-to-parameter ratio = 17.1.

In the title complex, $[\text{Zn}(\text{C}_{17}\text{H}_{11}\text{N}_6\text{O})\text{Cl}(\text{C}_3\text{H}_7\text{NO})]$, the Zn^{II} atom has a distorted square-pyramidal coordination formed by one Cl, two O and two N atoms. In the crystal structure, intermolecular $\text{N}-\text{H}\cdots\text{Cl}$ hydrogen bonds link molecules into centrosymmetric dimers, which are further assembled by $\pi-\pi$ interactions [centroid-centroid distances = 3.809 (3) and 3.834 (3) Å] into layers parallel to the ab plane. The crystal packing exhibits also weak intermolecular $\text{C}-\text{H}\cdots\text{Cl}$ interactions.

Related literature

For general background concerning the self-assembly of metal complexes with organic ligands, see: Chi *et al.* (2008); Patroniak *et al.* (2005); Kovbasyuk *et al.* (2005). For related structures, see: Preston & Kennard (1969); Jian *et al.* (2004); Patroniak *et al.* (2003).



Experimental

Crystal data

 $[\text{Zn}(\text{C}_{17}\text{H}_{11}\text{N}_6\text{O})\text{Cl}(\text{C}_3\text{H}_7\text{NO})]$
 $M_r = 489.23$

Triclinic, $P\bar{1}$
 $a = 8.5610$ (17) Å
 $b = 11.250$ (2) Å
 $c = 12.259$ (3) Å
 $\alpha = 110.70$ (3)°
 $\beta = 91.36$ (3)°
 $\gamma = 101.37$ (3)°

$V = 1077.1$ (4) Å³
 $Z = 2$
 Mo $K\alpha$ radiation
 $\mu = 1.30$ mm⁻¹
 $T = 295$ K
 $0.20 \times 0.17 \times 0.15$ mm

Data collection

Enraf-Nonius CAD-4 diffractometer
 10564 measured reflections
 4863 independent reflections
 4214 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$
 3 standard reflections every 100 reflections
 intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.049$
 $wR(F^2) = 0.167$
 $S = 1.09$
 4863 reflections
 284 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 1.58$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.58$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$\text{N6}-\text{H6A}\cdots\text{Cl1}^{\text{i}}$	0.86	2.57	3.396 (4)	161
$\text{Cl10}-\text{H10A}\cdots\text{Cl1}^{\text{ii}}$	0.93	2.80	3.670 (4)	156

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

Data collection: *CAD-4 Software* (Enraf-Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *NRCVAX* (Gabe *et al.*, 1989); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CV2708).

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supplementary materials

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[(*Z*)-1-Amino-2-cyano-2-(4,6-di-2-pyridylpyrimidin-2-yl)ethenolato]chlorido(*N,N*-dimethylformamide- κ O)zinc(II)

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Comment

Recently, self-assembly of specially designed metal complexes have attracted intense attention due to their fascinating molecular structures and crystal-packing motifs (Chi *et al.*, 2008). Several metal complexes with ligands containing heterocyclic pyrimidine and pyridine units have been studied previously to explore the role of hydrogen bonding in supramolecular assemblies (Patroniak *et al.*, 2005; Kovbasyuk *et al.*, 2005). Herein, we report the crystal structure of the title compound (I).

In (I) (Fig. 1), the zinc(II) ion is coordinated by one O anion and two N atoms of (*Z*)-3-amino-2-(4,6-di(pyridin-2-yl)pyrimidin-2-yl)-3-hydroxyacrylonitrile ligand, one O atom from DMF (DMF = *N,N*-dimethylformamide) and one Cl⁻ anion, forming a distorted square-pyramidal geometry. The Zn—Cl distance of 2.2956 (12) Å is longer than the value of 2.212 (4) Å in ZnCl₂(2,9-dimethyl-1,10-phenanthroline) (Preston *et al.*, 1969) and 2.209 (1) Å in ZnCl₂(C₆H₄N₃CH₂COPh)₂ (Jian *et al.*, 2004). The Zn—O bond lengths of 1.996 (3) and 2.066 (2) Å, respectively, are shorter than those reported previously (Patroniak *et al.*, 2003). The Zn—N bond lengths are 2.103 (3) and 2.106 (2) Å, respectively, which are in disagreement with the corresponding five-coordination Zn—N distances found in similar compounds (Patroniak *et al.*, 2003; Chi *et al.*, 2008). The N3—Zn1—N4 bite angle is 77.58 (10)°, which is narrower than that in {Zn[4,6-bis(2-pyridyl)-2-aminopyrimidine](OOCCH₃)₂} [78.40 (7)°, Chi *et al.*, 2008].

The five-membered chelate ring N3/C8/C9/N4/Zn1 (P1) is fairly planar, the deviation of atom Zn1 from the weighted least-squares plane N3/C8/C9/N4 is 0.079 Å. The dihedral angles formed by P1 with the planes N3/C14/C15/C17/O1/Zn1 (P2), N2/C6—C8/N3/C14 (P3), N4/C9—C13 (P4) and N1/C1—C5 (P5) are 16.67, 9.93, 5.02 and 19.49°, respectively. The dihedral angles formed by P3 with P4 and P5 are 5.61 and 16.55°, respectively. The dihedral angle between P2 and P4 is 14.55°.

In the crystal structure, intermolecular N—H...Cl hydrogen bonds (Table 2) link molecules into centrosymmetric dimers, which are further assembled by π - π interactions (Table 1) into layers parallel to *ab* plane. The crystal packing exhibits also weak intermolecular C—H...Cl interactions (Table 2).

Experimental

The title complex was prepared by the reaction of (*Z*)-3-amino-2-(4,6-di(pyridin-2-yl)pyrimidin-2-yl)-3-hydroxyacrylonitrile (3.16 g, 10 mmol) with Zinc dichloride (1.36 g, 10 mmol) in water solution at 353 K for four hours. Single crystals suitable for x-ray measurements were obtained by recrystallization from DMF at room temperature.

Refinement

All H atoms, except H1, were fixed geometrically and allowed to ride on their attached atoms, with C—H distances constrained to 0.93-0.96 Å, N—H = 0.86 Å, and with $U_{\text{iso}}(\text{H}) = 1.2-1.5U_{\text{eq}}(\text{C}, \text{N})$. Atom H1 was located on a difference map and refined isotropically.

Figures

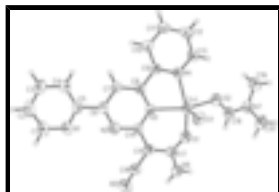


Fig. 1. The structure of the title compound showing 50% probability displacement ellipsoids and the atom-numbering scheme.

[(Z)-1-Amino-2-cyano-2-(4,6-di-2-pyridylpyrimidin-2-yl)ethanolato]chlorido(N,N-dimethylformamide- κ^i -O)zinc(II)

Crystal data

[Zn(C₁₇H₁₁N₆O)Cl(C₃H₇NO)]

$M_r = 489.23$

Triclinic, $P\bar{1}$

Hall symbol: -p 1

$a = 8.5610(17)$ Å

$b = 11.250(2)$ Å

$c = 12.259(3)$ Å

$\alpha = 110.70(3)^\circ$

$\beta = 91.36(3)^\circ$

$\gamma = 101.37(3)^\circ$

$V = 1077.1(4)$ Å³

$Z = 2$

$F(000) = 500$

$D_x = 1.509$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections

$\theta = 4-14^\circ$

$\mu = 1.30$ mm⁻¹

$T = 295$ K

Block, red

$0.20 \times 0.17 \times 0.15$ mm

Data collection

Enraf-Nonius CAD-4
diffractometer

Radiation source: fine-focus sealed tube
graphite

ω scans

10564 measured reflections

4863 independent reflections

4214 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.026$

$\theta_{\text{max}} = 27.5^\circ$, $\theta_{\text{min}} = 3.0^\circ$

$h = -10 \rightarrow 11$

$k = -14 \rightarrow 14$

$l = -15 \rightarrow 15$

3 standard reflections every 100 reflections

intensity decay: none

Refinement

Refinement on F^2

Primary atom site location: structure-invariant direct
methods

Least-squares matrix: full

$$R[F^2 > 2\sigma(F^2)] = 0.049$$

$$wR(F^2) = 0.167$$

$$S = 1.09$$

4863 reflections

284 parameters

0 restraints

Secondary atom site location: difference Fourier map

Hydrogen site location: inferred from neighbouring sites

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.1038P)^2 + 0.732P]$$

$$\text{where } P = (F_o^2 + 2F_c^2)/3$$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 1.58 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.58 \text{ e } \text{\AA}^{-3}$$

Special details

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Zn1	0.33598 (4)	0.22665 (3)	0.92885 (3)	0.03870 (16)
Cl1	0.17317 (10)	0.36222 (8)	1.02298 (8)	0.0497 (2)
O1	0.5618 (3)	0.3196 (3)	0.9911 (2)	0.0511 (6)
O2	0.3716 (3)	0.2649 (3)	0.7773 (2)	0.0542 (6)
N1	0.3389 (4)	-0.0424 (3)	1.3640 (3)	0.0566 (8)
N2	0.4266 (4)	0.0756 (3)	1.2026 (3)	0.0496 (7)
N3	0.3565 (3)	0.1094 (2)	1.0273 (2)	0.0328 (5)
N4	0.1814 (3)	0.0487 (3)	0.8275 (2)	0.0401 (6)
N5	0.7321 (5)	0.3459 (4)	1.3637 (3)	0.0727 (10)
N6	0.7680 (4)	0.4302 (3)	1.1244 (3)	0.0591 (8)
H6A	0.8020	0.4736	1.0811	0.071*
H6B	0.8209	0.4462	1.1904	0.071*
N7	0.4824 (4)	0.3814 (3)	0.6721 (3)	0.0499 (7)
C1	0.3016 (6)	-0.0996 (5)	1.4418 (4)	0.0646 (11)
H1B	0.3465	-0.0551	1.5189	0.078*
C2	0.2027 (5)	-0.2183 (5)	1.4156 (4)	0.0628 (10)
H2B	0.1794	-0.2530	1.4733	0.075*
C3	0.1376 (6)	-0.2861 (5)	1.3011 (4)	0.0655 (11)
H3A	0.0698	-0.3679	1.2799	0.079*
C4	0.1749 (5)	-0.2300 (4)	1.2179 (4)	0.0562 (9)
H4A	0.1348	-0.2746	1.1397	0.067*
C5	0.2727 (4)	-0.1070 (3)	1.2534 (3)	0.0417 (7)

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C6	0.3068 (4)	-0.0356 (3)	1.1717 (3)	0.0375 (6)
C7	0.2136 (4)	-0.0771 (3)	1.0636 (3)	0.0377 (6)
H7A	0.1342	-0.1533	1.0386	0.045*
C8	0.2430 (3)	-0.0020 (3)	0.9955 (2)	0.0344 (6)
C9	0.1483 (3)	-0.0380 (3)	0.8802 (2)	0.0358 (6)
C10	0.0349 (4)	-0.1544 (3)	0.8286 (3)	0.0460 (7)
H10A	0.0137	-0.2141	0.8658	0.055*
C11	-0.0458 (5)	-0.1798 (4)	0.7204 (3)	0.0538 (9)
H11A	-0.1233	-0.2562	0.6850	0.065*
C12	-0.0105 (4)	-0.0919 (4)	0.6666 (3)	0.0526 (8)
H12A	-0.0620	-0.1085	0.5934	0.063*
C13	0.1019 (4)	0.0213 (4)	0.7218 (3)	0.0483 (8)
H13A	0.1242	0.0815	0.6852	0.058*
C14	0.4514 (3)	0.1485 (3)	1.1287 (2)	0.0354 (6)
C15	0.5791 (4)	0.2644 (3)	1.1610 (3)	0.0385 (6)
C16	0.6641 (4)	0.3068 (3)	1.2730 (3)	0.0448 (7)
C17	0.6313 (4)	0.3365 (3)	1.0886 (3)	0.0392 (6)
C18	0.4729 (4)	0.3546 (4)	0.7681 (3)	0.0460 (7)
C19	0.3704 (7)	0.3062 (5)	0.5696 (4)	0.0831 (15)
H19A	0.2953	0.2405	0.5858	0.125*
H19B	0.4275	0.2655	0.5053	0.125*
H19C	0.3140	0.3627	0.5496	0.125*
C20	0.6072 (6)	0.4868 (4)	0.6641 (4)	0.0608 (10)
H20A	0.6742	0.5285	0.7370	0.091*
H20B	0.5583	0.5493	0.6478	0.091*
H20C	0.6709	0.4516	0.6022	0.091*
H1	0.546 (5)	0.406 (4)	0.831 (4)	0.056 (11)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Zn1	0.0394 (2)	0.0427 (2)	0.0365 (2)	0.00096 (15)	0.00087 (14)	0.02205 (16)
Cl1	0.0495 (5)	0.0453 (4)	0.0573 (5)	0.0067 (3)	0.0090 (4)	0.0242 (4)
O1	0.0415 (12)	0.0654 (16)	0.0501 (13)	-0.0046 (11)	-0.0003 (10)	0.0344 (12)
O2	0.0582 (15)	0.0631 (16)	0.0436 (13)	-0.0035 (12)	0.0051 (11)	0.0313 (12)
N1	0.068 (2)	0.0629 (19)	0.0421 (15)	0.0026 (15)	-0.0026 (14)	0.0297 (14)
N2	0.0516 (16)	0.0552 (17)	0.0468 (15)	0.0107 (13)	0.0047 (12)	0.0251 (13)
N3	0.0365 (12)	0.0333 (11)	0.0290 (11)	0.0053 (9)	0.0033 (9)	0.0130 (9)
N4	0.0424 (13)	0.0445 (14)	0.0350 (13)	0.0048 (11)	0.0015 (10)	0.0191 (11)
N5	0.074 (2)	0.079 (3)	0.055 (2)	-0.0010 (19)	-0.0158 (17)	0.0238 (18)
N6	0.0483 (17)	0.0606 (19)	0.067 (2)	-0.0140 (14)	-0.0101 (14)	0.0364 (16)
N7	0.0607 (18)	0.0525 (16)	0.0411 (14)	0.0061 (13)	0.0101 (13)	0.0257 (12)
C1	0.079 (3)	0.077 (3)	0.046 (2)	0.009 (2)	0.0025 (18)	0.0359 (19)
C2	0.068 (2)	0.080 (3)	0.063 (2)	0.018 (2)	0.0154 (19)	0.052 (2)
C3	0.070 (3)	0.063 (2)	0.073 (3)	-0.003 (2)	0.000 (2)	0.046 (2)
C4	0.063 (2)	0.056 (2)	0.055 (2)	-0.0007 (17)	-0.0042 (17)	0.0341 (17)
C5	0.0447 (16)	0.0456 (17)	0.0432 (16)	0.0119 (13)	0.0056 (12)	0.0253 (13)
C6	0.0407 (15)	0.0404 (15)	0.0376 (15)	0.0112 (12)	0.0084 (12)	0.0202 (12)

C7	0.0402 (15)	0.0362 (14)	0.0373 (14)	0.0037 (11)	0.0035 (11)	0.0169 (12)
C8	0.0369 (14)	0.0351 (14)	0.0325 (13)	0.0080 (11)	0.0044 (11)	0.0137 (11)
C9	0.0342 (14)	0.0401 (15)	0.0333 (14)	0.0081 (11)	0.0044 (11)	0.0138 (11)
C10	0.0490 (18)	0.0418 (16)	0.0439 (17)	0.0021 (13)	-0.0014 (13)	0.0164 (13)
C11	0.0513 (19)	0.0502 (19)	0.0464 (18)	-0.0023 (15)	-0.0069 (15)	0.0092 (15)
C12	0.0515 (19)	0.062 (2)	0.0381 (17)	0.0084 (16)	-0.0079 (14)	0.0143 (15)
C13	0.0515 (19)	0.057 (2)	0.0364 (16)	0.0049 (15)	-0.0040 (13)	0.0217 (14)
C14	0.0358 (14)	0.0375 (14)	0.0354 (14)	0.0085 (11)	0.0046 (11)	0.0161 (11)
C15	0.0376 (14)	0.0402 (15)	0.0376 (15)	0.0041 (12)	0.0004 (11)	0.0164 (12)
C16	0.0436 (17)	0.0468 (17)	0.0401 (17)	0.0031 (13)	-0.0038 (13)	0.0153 (13)
C17	0.0332 (14)	0.0401 (15)	0.0434 (16)	0.0045 (11)	0.0018 (11)	0.0163 (13)
C18	0.0488 (18)	0.0525 (19)	0.0398 (16)	0.0079 (15)	0.0064 (13)	0.0223 (14)
C19	0.110 (4)	0.086 (3)	0.048 (2)	-0.009 (3)	-0.012 (2)	0.036 (2)
C20	0.075 (3)	0.058 (2)	0.061 (2)	0.0138 (19)	0.027 (2)	0.0358 (18)

Geometric parameters (Å, °)

Zn1—O1	1.996 (3)	C3—H3A	0.9300
Zn1—O2	2.066 (2)	C4—C5	1.380 (5)
Zn1—N4	2.103 (3)	C4—H4A	0.9300
Zn1—N3	2.106 (2)	C5—C6	1.491 (4)
Zn1—Cl1	2.2956 (12)	C6—C7	1.406 (4)
O1—C17	1.256 (4)	C7—C8	1.378 (4)
O2—C18	1.234 (4)	C7—H7A	0.9300
N1—C1	1.338 (5)	C8—C9	1.493 (4)
N1—C5	1.339 (5)	C9—C10	1.394 (4)
N2—C6	1.378 (4)	C10—C11	1.388 (5)
N2—C14	1.416 (4)	C10—H10A	0.9300
N3—C8	1.350 (4)	C11—C12	1.362 (6)
N3—C14	1.350 (4)	C11—H11A	0.9300
N4—C9	1.339 (4)	C12—C13	1.372 (5)
N4—C13	1.353 (4)	C12—H12A	0.9300
N5—C16	1.136 (5)	C13—H13A	0.9300
N6—C17	1.355 (4)	C14—C15	1.451 (4)
N6—H6A	0.8600	C15—C16	1.413 (4)
N6—H6B	0.8600	C15—C17	1.426 (4)
N7—C18	1.314 (4)	C18—H1	0.91 (4)
N7—C19	1.444 (6)	C19—H19A	0.9600
N7—C20	1.465 (5)	C19—H19B	0.9600
C1—C2	1.357 (6)	C19—H19C	0.9600
C1—H1B	0.9300	C20—H20A	0.9600
C2—C3	1.379 (6)	C20—H20B	0.9600
C2—H2B	0.9300	C20—H20C	0.9600
C3—C4	1.389 (5)		
Cg1...Cg1 ⁱ	3.809 (3)	Cg1...Cg2 ⁱⁱ	3.834 (3)
O1—Zn1—O2	89.37 (11)	C8—C7—H7A	120.9
O1—Zn1—N4	146.12 (12)	C6—C7—H7A	120.9
O2—Zn1—N4	88.67 (11)	N3—C8—C7	123.4 (3)

supplementary materials

O1—Zn1—N3	87.29 (10)	N3—C8—C9	114.8 (3)
O2—Zn1—N3	149.32 (11)	C7—C8—C9	121.8 (3)
N4—Zn1—N3	77.58 (10)	N4—C9—C10	121.5 (3)
O1—Zn1—C11	107.51 (9)	N4—C9—C8	115.4 (3)
O2—Zn1—C11	103.78 (9)	C10—C9—C8	123.1 (3)
N4—Zn1—C11	105.79 (8)	C11—C10—C9	118.8 (3)
N3—Zn1—C11	106.30 (7)	C11—C10—H10A	120.6
C17—O1—Zn1	126.9 (2)	C9—C10—H10A	120.6
C18—O2—Zn1	125.8 (2)	C12—C11—C10	119.5 (3)
C1—N1—C5	117.3 (3)	C12—C11—H11A	120.3
C6—N2—C14	120.6 (3)	C10—C11—H11A	120.3
C8—N3—C14	119.3 (2)	C11—C12—C13	119.2 (3)
C8—N3—Zn1	114.61 (19)	C11—C12—H12A	120.4
C14—N3—Zn1	124.8 (2)	C13—C12—H12A	120.4
C9—N4—C13	118.6 (3)	N4—C13—C12	122.5 (3)
C9—N4—Zn1	115.2 (2)	N4—C13—H13A	118.8
C13—N4—Zn1	125.8 (2)	C12—C13—H13A	118.8
C17—N6—H6A	120.0	N3—C14—N2	119.8 (3)
C17—N6—H6B	120.0	N3—C14—C15	119.9 (3)
H6A—N6—H6B	120.0	N2—C14—C15	120.3 (3)
C18—N7—C19	120.9 (3)	C16—C15—C17	116.8 (3)
C18—N7—C20	121.7 (3)	C16—C15—C14	117.0 (3)
C19—N7—C20	117.4 (3)	C17—C15—C14	126.1 (3)
N1—C1—C2	124.4 (4)	N5—C16—C15	177.3 (4)
N1—C1—H1B	117.8	O1—C17—N6	115.8 (3)
C2—C1—H1B	117.8	O1—C17—C15	125.4 (3)
C1—C2—C3	118.3 (4)	N6—C17—C15	118.9 (3)
C1—C2—H2B	120.9	O2—C18—N7	123.6 (3)
C3—C2—H2B	120.9	O2—C18—H1	119 (3)
C2—C3—C4	118.8 (4)	N7—C18—H1	117 (3)
C2—C3—H3A	120.6	N7—C19—H19A	109.5
C4—C3—H3A	120.6	N7—C19—H19B	109.5
C5—C4—C3	118.8 (4)	H19A—C19—H19B	109.5
C5—C4—H4A	120.6	N7—C19—H19C	109.5
C3—C4—H4A	120.6	H19A—C19—H19C	109.5
N1—C5—C4	122.3 (3)	H19B—C19—H19C	109.5
N1—C5—C6	115.6 (3)	N7—C20—H20A	109.5
C4—C5—C6	122.0 (3)	N7—C20—H20B	109.5
N2—C6—C7	118.5 (3)	H20A—C20—H20B	109.5
N2—C6—C5	120.6 (3)	N7—C20—H20C	109.5
C7—C6—C5	120.8 (3)	H20A—C20—H20C	109.5
C8—C7—C6	118.3 (3)	H20B—C20—H20C	109.5

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

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N6—H6A \cdots C11 ⁱⁱⁱ	0.86	2.57	3.396 (4)	161
C10—H10A \cdots C11 ^{iv}	0.93	2.80	3.670 (4)	156

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

Fig. 1

