Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

6-Allyl-3-(6-chloro-3-pyridylmethyl)-6,7-dihydro-3*H*-1,2,3-triazolo[4,5-*d*]-pyrimidin-7-imine

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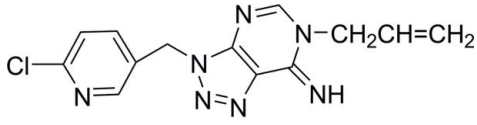
Received 12 November 2009; accepted 13 November 2009

Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.040; wR factor = 0.109; data-to-parameter ratio = 13.2.

The title compound, $C_{13}H_{12}ClN_7$, crystallizes with two independent molecules in the asymmetric unit, each with similar geometries. The dihedral angles between the triazole and pyrimidine rings are 0.45 (9) and 1.00 (10)° in the two molecules. A number of N—H···N hydrogen bonds co-operate with C–H···N contacts, forming a supramolecular array in the *ab* plane. C—H···π interactions are also present. One of the vinyl groups was found to be disordered so that the C(H)=CH$_2$ atoms were resolved over two positions with the major component having a site occupancy factor of 0.539 (4).

Related literature

For general background to 8-azapurine derivatives, see: Albert (1986). For the biological activity of 8-azapurines, see: Shiokawa *et al.* (1986); Slusarkchyk & Zahler (1989); Subramanian & Gerwick (1989); Vince & Hua (1990); Yamamoto *et al.* (1994).



Experimental

Crystal data

$C_{13}H_{12}ClN_7$
M_r = 301.75
Triclinic, $P\overline{1}$
a = 7.2845 (7) Å
b = 13.2684 (12) Å
c = 14.7069 (14) Å
α = 87.351 (1)°
β = 81.752 (1)°
γ = 82.917 (1)°
V = 1395.4 (2) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 296 K
0.48 × 0.46 × 0.43 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: none
10116 measured reflections
5052 independent reflections
4277 reflections with $I > 2\sigma(I)$
R_{int} = 0.015

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.109
S = 1.03
5052 reflections
384 parameters
22 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.36 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N10—H10A···N1	0.86	2.44	3.292 (3)	173
N3—H3A···N8^{i}	0.86	2.45	3.299 (2)	169
C11—H11A···N3	0.97	2.41	2.749 (2)	100
C19—H19···N11	0.93	2.59	2.909 (3)	101
C3—H3···N13	0.93	2.46	3.309 (2)	151
C11—H11A···$Cg4^{ii}$	0.97	2.87	3.446 (2)	119
C24—H24A···$Cg1^{iii}$	0.97	2.99	3.851 (3)	149

Symmetry codes: (i) $x, y+1, z$; (ii) $-x+1, -y+2, -z+1$; (iii) $-x+2, -y+1, -z+1$. $Cg4$ and $Cg1$ are the centroids of the N4–N6/C1/C4 and N11–N13/C14/C17C4 rings, respectively.

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; 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: *SHELXTL*.

The authors gratefully acknowledge financial support of this work by Yunyang Medical College (grant No. 2007ZQB24).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2573).

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supporting information

Acta Cryst. (2009). E**65**, o3195 [doi:10.1107/S1600536809048168]

6-Allyl-3-(6-chloro-3-pyridylmethyl)-6,7-dihydro-3*H*-1,2,3-triazolo[4,5-*d*]pyrimidin-7-imine

Dong-Feng Pan, Jing Xu, Jun-Kai Ma, Hong Luo and Zuan Ma

S1. Comment

1,2,3-Triazolo[4,5-*d*]pyrimidines, *i.e.* 8-azapurines (Albert, 1986), have attracted attention because some of these derivatives exhibit anti-viral (Slusarkchyk & Zahler, 1989), anti-tumour (Slusarkchyk & Zahler, 1989; Vince & Hua, 1990), and herbicidal activities (Subramanian & Gerwick, 1989). Neonicotinoid insecticides, as nicotinic acetylcholine receptor inhibitors, have also attracted increasing attention because of their low toxicity, wide range of activities, and high potency (Shiokawa *et al.*, 1986). It has been found that most biologically active nicotinic compounds contain the 3-aminomethylpyridine group (Yamamoto *et al.*, 1994). Herein, we report the crystal structure of (I), Fig. 1, which was synthesized by introducing pyridine rings into a 1,2,3-triazolo[4,5-*d*]pyrimidine framework.

Several N—H···N hydrogen bonding contacts, together with C—H···N and C—H···π interactions, lead to the formation of supramolecular arrays in the *ab* plane, Table 1 and Fig. 2. In addition π—π stacking interactions stabilize the crystal structure, with the shortest centroid-centroid distance of 3.412 (1) Å occurring between centrosymmetrically related planes through the (N4–N6, C1, C4) rings, symmetry operation: 2-x, 1-y, 1-z.

S2. Experimental

Allylamine (1 mmol) in anhydrous acetonitrile (4 ml) was added dropwise to a solution of ethyl-*N*-3-((6-chloropyridin-3-yl)methyl)-5-cyano-3*H*-1,2,3- triazol-4-yl-formimidate (1 mmol) in anhydrous acetonitrile (8 ml) at room temperature. The mixture was stirred until the reaction was complete (by thin layer chromatography) and the solution concentrated under vacuum. The residue was recrystallized from anhydrous ethanol to give (I) (yield 87%). Colourless crystals were grown from a dichloromethane and petroleum ether (1:3 *v*/*v*) solution of (I).

S3. Refinement

H atoms were placed in calculated positions, with C—H distances in the range 0.93–0.97 Å and N—H distances of 0.86 Å, and included in the final cycles of refinement using a riding-model approximation, with U_{iso}(H) = 1.2–1.5U_{eq}(carrier atom). A rotating group model was used for the methyl groups. Disorder was noted in the C24-C26 vinyl substituent in that two positions were resolved for the C25 atom. From refinement, the major component had a site occupancy factor = 0.539 (4).

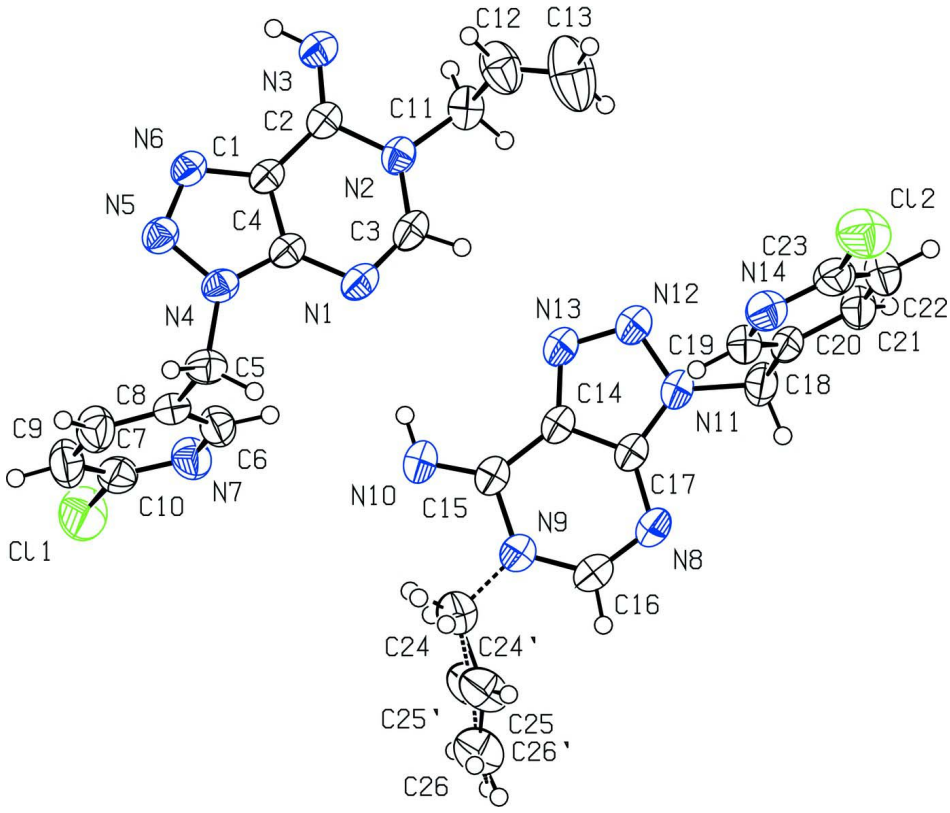

Figure 1

The molecular structures of the two independent molecules in (I), showing 50% probability displacement ellipsoids and the atom-numbering scheme.

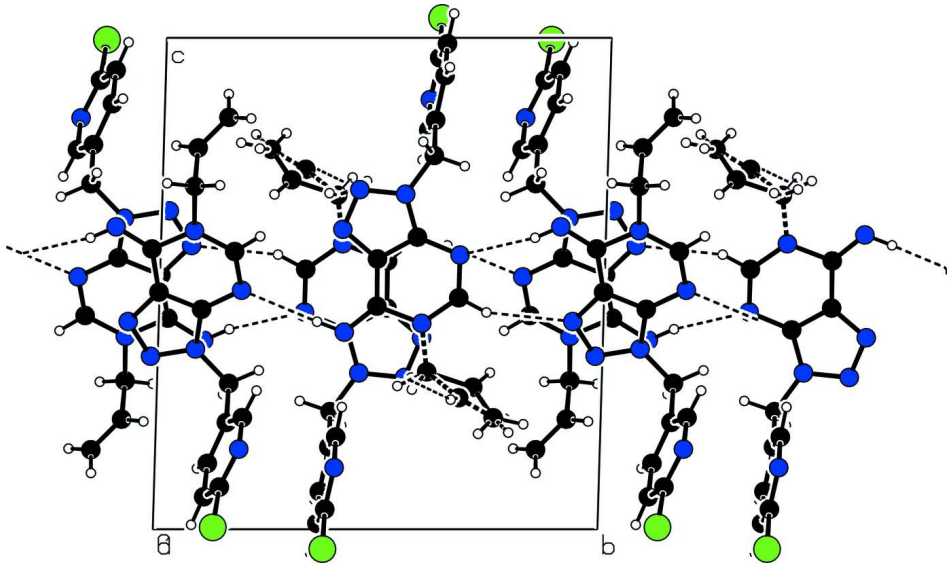

Figure 2

A view of a supramolecular layer in (I). Hydrogen bonds are shown as dashed lines.

6-Allyl-3-(6-chloro-3-pyridylmethyl)-6,7-dihydro-3*H*-1,2,3- triazolo[4,5-*d*]pyrimidin-7-imine

Crystal data

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$M_r = 301.75$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.2845\ (7)$ Å
$b = 13.2684\ (12)$ Å
$c = 14.7069\ (14)$ Å
$\alpha = 87.351\ (1)°$
$\beta = 81.752\ (1)°$
$\gamma = 82.917\ (1)°$
$V = 1395.4\ (2)$ Å^3
$Z = 4$
$F(000) = 624$
$D_x = 1.436$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5848 reflections
$\theta = 2.8–28.2°$
$\mu = 0.28$ mm^{-1}
$T = 296$ K
Block, colorless
0.48 × 0.46 × 0.43 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
10116 measured reflections
5052 independent reflections
4277 reflections with $I > 2\sigma(I)$
$R_{int} = 0.015$
$\theta_{max} = 25.5°$, $\theta_{min} = 2.8°$
$h = -8\rightarrow8$
$k = -15\rightarrow16$
$l = -17\rightarrow17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.040$
$wR(F^2) = 0.109$
$S = 1.03$
5052 reflections
384 parameters
22 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
$w = 1/[\sigma^2(F_o^2) + (0.0474P)^2 + 0.5781P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.35$ e Å^{-3}
$\Delta\rho_{min} = -0.36$ e Å^{-3}
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.050 (2)

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}	Occ. (<1)
C24	0.7964 (4)	0.39425 (19)	0.67973 (16)	0.0710 (7)	0.539 (4)
H24A	0.9002	0.4288	0.6913	0.085*	0.539 (4)
H24B	0.6844	0.4265	0.7159	0.085*	0.539 (4)
C25	0.8281 (6)	0.2896 (3)	0.7111 (3)	0.0666 (9)	0.539 (4)
H25	0.9341	0.2520	0.6814	0.080*	0.539 (4)
C26	0.7319 (5)	0.2418 (3)	0.7732 (2)	0.1002 (10)	0.539 (4)
H26A	0.6239	0.2747	0.8058	0.120*	0.539 (4)
H26B	0.7692	0.1738	0.7864	0.120*	0.539 (4)
C24′	0.7964 (4)	0.39425 (19)	0.67973 (16)	0.0710 (7)	0.461 (4)
H24C	0.9279	0.3756	0.6840	0.085*	0.461 (4)
H24D	0.7600	0.4593	0.7086	0.085*	0.461 (4)
C25′	0.6943 (8)	0.3207 (4)	0.7325 (3)	0.0666 (9)	0.461 (4)
H25′	0.5659	0.3385	0.7363	0.080*	0.461 (4)
C26′	0.7319 (5)	0.2418 (3)	0.7732 (2)	0.1002 (10)	0.461 (4)
H26C	0.8561	0.2159	0.7746	0.120*	0.461 (4)
H26D	0.6368	0.2068	0.8034	0.120*	0.461 (4)
C1	0.7678 (2)	1.00162 (12)	0.51743 (12)	0.0346 (4)	
C2	0.7015 (2)	1.02006 (12)	0.42960 (12)	0.0360 (4)	
C3	0.7187 (3)	0.83395 (13)	0.43489 (14)	0.0448 (4)	
H3	0.6996	0.7774	0.4040	0.054*	
C4	0.8029 (2)	0.90450 (12)	0.55236 (12)	0.0362 (4)	
C5	0.9108 (3)	0.83866 (14)	0.70333 (13)	0.0457 (4)	
H5A	1.0253	0.8510	0.7252	0.055*	
H5B	0.9309	0.7719	0.6768	0.055*	
C6	0.5880 (3)	0.80588 (16)	0.77284 (13)	0.0493 (5)	
H6	0.5802	0.7758	0.7179	0.059*	
C7	0.7544 (3)	0.84151 (13)	0.78275 (12)	0.0406 (4)	
C8	0.7665 (3)	0.88164 (17)	0.86595 (15)	0.0588 (5)	
H8	0.8770	0.9047	0.8763	0.071*	
C9	0.6143 (3)	0.88762 (18)	0.93401 (15)	0.0639 (6)	
H9	0.6193	0.9140	0.9910	0.077*	
C10	0.4556 (3)	0.85311 (15)	0.91408 (13)	0.0511 (5)	
C11	0.6112 (3)	0.92790 (16)	0.30226 (13)	0.0484 (5)	
H11A	0.5276	0.9899	0.2960	0.058*	
H11B	0.5401	0.8711	0.3001	0.058*	
C12	0.7634 (3)	0.9228 (2)	0.22394 (16)	0.0681 (6)	
H12	0.8453	0.9719	0.2193	0.082*	
C13	0.7911 (4)	0.8556 (3)	0.1618 (2)	0.1080 (12)	
H13A	0.7121	0.8053	0.1641	0.130*	
H13B	0.8902	0.8573	0.1144	0.130*	
C14	0.7367 (2)	0.51225 (13)	0.45004 (13)	0.0407 (4)	
C15	0.7607 (3)	0.51058 (14)	0.54603 (13)	0.0434 (4)	
C16	0.7703 (3)	0.32703 (15)	0.52893 (15)	0.0523 (5)	
H16	0.7816	0.2638	0.5589	0.063*	
C17	0.7361 (2)	0.42382 (13)	0.40561 (13)	0.0398 (4)	

C18	0.7094 (3)	0.39121 (15)	0.23947 (14)	0.0514 (5)
H18A	0.5996	0.4168	0.2114	0.062*
H18B	0.6960	0.3220	0.2611	0.062*
C19	1.0541 (3)	0.40537 (14)	0.18782 (14)	0.0499 (5)
H19	1.0650	0.4172	0.2486	0.060*
C20	0.8801 (3)	0.39059 (13)	0.16747 (13)	0.0440 (4)
C21	0.8673 (3)	0.37205 (16)	0.07674 (14)	0.0549 (5)
H21	0.7530	0.3618	0.0598	0.066*
C22	1.0239 (3)	0.36883 (17)	0.01182 (15)	0.0608 (6)
H22	1.0184	0.3558	−0.0493	0.073*
C23	1.1885 (3)	0.38548 (15)	0.04051 (15)	0.0546 (5)
Cl1	0.25485 (10)	0.86518 (6)	0.99613 (4)	0.0824 (2)
Cl2	1.39020 (10)	0.38267 (5)	−0.04027 (5)	0.0812 (2)
N1	0.7805 (2)	0.81572 (11)	0.51360 (11)	0.0446 (4)
N2	0.6786 (2)	0.92572 (11)	0.39244 (10)	0.0399 (3)
N3	0.6629 (2)	1.10214 (11)	0.38456 (11)	0.0450 (4)
H3A	0.6766	1.1591	0.4069	0.054*
N4	0.86503 (19)	0.91590 (10)	0.63304 (10)	0.0384 (3)
N5	0.8663 (2)	1.01637 (11)	0.64796 (10)	0.0412 (4)
N6	0.8078 (2)	1.06876 (11)	0.57735 (10)	0.0386 (3)
N7	0.4377 (2)	0.81185 (14)	0.83706 (11)	0.0541 (4)
N8	0.7516 (2)	0.32692 (11)	0.44197 (12)	0.0503 (4)
N9	0.7752 (2)	0.40853 (12)	0.58091 (11)	0.0487 (4)
N10	0.7707 (3)	0.58234 (13)	0.59890 (12)	0.0575 (5)
H10A	0.7618	0.6440	0.5777	0.069*
N11	0.7175 (2)	0.45313 (11)	0.31812 (11)	0.0451 (4)
N12	0.7058 (3)	0.55636 (12)	0.30882 (12)	0.0545 (4)
N13	0.7175 (3)	0.59204 (12)	0.38966 (12)	0.0515 (4)
N14	1.2090 (2)	0.40379 (13)	0.12549 (12)	0.0551 (4)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C24	0.0985 (19)	0.0654 (15)	0.0573 (14)	−0.0258 (13)	−0.0265 (13)	0.0029 (11)
C25	0.065 (2)	0.079 (2)	0.0500 (19)	0.0091 (18)	−0.0045 (17)	0.0038 (16)
C26	0.150 (3)	0.093 (2)	0.0610 (17)	−0.037 (2)	−0.0126 (18)	0.0071 (16)
C24′	0.0985 (19)	0.0654 (15)	0.0573 (14)	−0.0258 (13)	−0.0265 (13)	0.0029 (11)
C25′	0.065 (2)	0.079 (2)	0.0500 (19)	0.0091 (18)	−0.0045 (17)	0.0038 (16)
C26′	0.150 (3)	0.093 (2)	0.0610 (17)	−0.037 (2)	−0.0126 (18)	0.0071 (16)
C1	0.0295 (8)	0.0307 (8)	0.0413 (9)	−0.0047 (6)	0.0045 (7)	−0.0034 (7)
C2	0.0276 (8)	0.0352 (9)	0.0432 (10)	−0.0045 (6)	0.0037 (7)	−0.0052 (7)
C3	0.0447 (10)	0.0334 (9)	0.0554 (12)	−0.0065 (7)	0.0007 (8)	−0.0110 (8)
C4	0.0312 (8)	0.0321 (8)	0.0428 (10)	−0.0045 (6)	0.0042 (7)	−0.0023 (7)
C5	0.0446 (10)	0.0416 (10)	0.0485 (11)	−0.0001 (8)	−0.0046 (8)	0.0060 (8)
C6	0.0538 (11)	0.0573 (12)	0.0388 (10)	−0.0159 (9)	−0.0041 (8)	−0.0049 (9)
C7	0.0466 (10)	0.0334 (9)	0.0414 (10)	−0.0049 (7)	−0.0070 (8)	0.0050 (7)
C8	0.0591 (13)	0.0651 (14)	0.0568 (13)	−0.0206 (10)	−0.0102 (10)	−0.0094 (10)
C9	0.0783 (15)	0.0719 (15)	0.0449 (12)	−0.0233 (12)	−0.0028 (11)	−0.0168 (10)

C10	0.0619 (12)	0.0475 (11)	0.0421 (11)	−0.0126 (9)	0.0040 (9)	0.0009 (9)
C11	0.0442 (10)	0.0509 (11)	0.0512 (11)	−0.0049 (8)	−0.0076 (8)	−0.0114 (9)
C12	0.0555 (13)	0.1005 (19)	0.0509 (13)	−0.0218 (12)	−0.0025 (10)	−0.0115 (12)
C13	0.0756 (18)	0.169 (3)	0.0780 (19)	−0.0095 (19)	0.0080 (15)	−0.055 (2)
C14	0.0416 (9)	0.0328 (9)	0.0478 (10)	−0.0046 (7)	−0.0048 (8)	−0.0076 (8)
C15	0.0442 (10)	0.0377 (9)	0.0494 (11)	−0.0077 (8)	−0.0063 (8)	−0.0065 (8)
C16	0.0639 (13)	0.0353 (10)	0.0589 (13)	−0.0094 (9)	−0.0093 (10)	−0.0001 (9)
C17	0.0397 (9)	0.0332 (9)	0.0464 (11)	−0.0049 (7)	−0.0040 (8)	−0.0070 (7)
C18	0.0596 (12)	0.0466 (11)	0.0516 (12)	−0.0104 (9)	−0.0122 (9)	−0.0133 (9)
C19	0.0639 (13)	0.0438 (11)	0.0448 (11)	−0.0080 (9)	−0.0150 (9)	−0.0042 (8)
C20	0.0581 (11)	0.0306 (9)	0.0455 (11)	−0.0040 (8)	−0.0139 (9)	−0.0054 (7)
C21	0.0660 (13)	0.0504 (12)	0.0518 (12)	−0.0074 (10)	−0.0178 (10)	−0.0096 (9)
C22	0.0794 (16)	0.0599 (13)	0.0441 (12)	−0.0061 (11)	−0.0110 (11)	−0.0102 (10)
C23	0.0660 (13)	0.0419 (11)	0.0532 (13)	−0.0013 (9)	−0.0040 (10)	0.0004 (9)
Cl1	0.0861 (5)	0.0912 (5)	0.0643 (4)	−0.0290 (4)	0.0286 (3)	−0.0165 (3)
Cl2	0.0782 (4)	0.0853 (5)	0.0717 (4)	−0.0018 (3)	0.0105 (3)	0.0013 (3)
N1	0.0481 (9)	0.0305 (8)	0.0540 (10)	−0.0051 (6)	−0.0016 (7)	−0.0038 (7)
N2	0.0381 (8)	0.0369 (8)	0.0441 (8)	−0.0049 (6)	−0.0014 (6)	−0.0074 (6)
N3	0.0471 (9)	0.0364 (8)	0.0506 (9)	−0.0031 (7)	−0.0054 (7)	−0.0007 (7)
N4	0.0371 (8)	0.0338 (7)	0.0424 (8)	−0.0049 (6)	0.0010 (6)	0.0006 (6)
N5	0.0408 (8)	0.0376 (8)	0.0442 (9)	−0.0071 (6)	0.0002 (6)	−0.0029 (7)
N6	0.0379 (8)	0.0336 (7)	0.0431 (8)	−0.0062 (6)	0.0008 (6)	−0.0028 (6)
N7	0.0555 (10)	0.0642 (11)	0.0438 (9)	−0.0203 (8)	0.0004 (8)	−0.0022 (8)
N8	0.0652 (11)	0.0330 (8)	0.0537 (10)	−0.0085 (7)	−0.0071 (8)	−0.0074 (7)
N9	0.0599 (10)	0.0410 (9)	0.0482 (9)	−0.0128 (7)	−0.0117 (8)	−0.0012 (7)
N10	0.0796 (12)	0.0424 (9)	0.0541 (10)	−0.0111 (8)	−0.0146 (9)	−0.0116 (8)
N11	0.0544 (9)	0.0351 (8)	0.0473 (9)	−0.0064 (7)	−0.0082 (7)	−0.0094 (7)
N12	0.0752 (12)	0.0367 (9)	0.0527 (10)	−0.0044 (8)	−0.0139 (9)	−0.0055 (7)
N13	0.0693 (11)	0.0337 (8)	0.0525 (10)	−0.0035 (7)	−0.0124 (8)	−0.0076 (7)
N14	0.0595 (11)	0.0495 (10)	0.0570 (11)	−0.0068 (8)	−0.0114 (9)	0.0004 (8)

Geometric parameters (Å, º)

C24—C25	1.445 (5)	C11—H11B	0.9700
C24—N9	1.485 (3)	C12—C13	1.283 (4)
C24—H24A	0.9700	C12—H12	0.9300
C24—H24B	0.9700	C13—H13A	0.9300
C25—C26	1.265 (5)	C13—H13B	0.9300
C25—H25	0.9300	C14—N13	1.357 (2)
C26—H26A	0.9300	C14—C17	1.370 (2)
C26—H26B	0.9300	C14—C15	1.446 (3)
C25′—H25′	0.9300	C15—N10	1.272 (2)
C1—N6	1.366 (2)	C15—N9	1.423 (2)
C1—C4	1.373 (2)	C16—N8	1.305 (3)
C1—C2	1.443 (2)	C16—N9	1.360 (2)
C2—N3	1.271 (2)	C16—H16	0.9300
C2—N2	1.426 (2)	C17—N11	1.348 (2)
C3—N1	1.303 (3)	C17—N8	1.367 (2)

C3—N2	1.361 (2)	C18—N11	1.461 (2)
C3—H3	0.9300	C18—C20	1.512 (3)
C4—N4	1.350 (2)	C18—H18A	0.9700
C4—N1	1.369 (2)	C18—H18B	0.9700
C5—N4	1.465 (2)	C19—N14	1.346 (3)
C5—C7	1.509 (3)	C19—C20	1.383 (3)
C5—H5A	0.9700	C19—H19	0.9300
C5—H5B	0.9700	C20—C21	1.386 (3)
C6—N7	1.337 (3)	C21—C22	1.377 (3)
C6—C7	1.383 (3)	C21—H21	0.9300
C6—H6	0.9300	C22—C23	1.372 (3)
C7—C8	1.375 (3)	C22—H22	0.9300
C8—C9	1.380 (3)	C23—N14	1.317 (3)
C8—H8	0.9300	C23—Cl2	1.750 (2)
C9—C10	1.368 (3)	N3—H3A	0.8600
C9—H9	0.9300	N4—N5	1.362 (2)
C10—N7	1.310 (3)	N5—N6	1.315 (2)
C10—Cl1	1.753 (2)	N10—H10A	0.8600
C11—N2	1.477 (2)	N11—N12	1.364 (2)
C11—C12	1.478 (3)	N12—N13	1.318 (2)
C11—H11A	0.9700		

C25—C24—N9	114.8 (2)	H13A—C13—H13B	120.0
C25—C24—H24A	108.6	N13—C14—C17	109.22 (16)
N9—C24—H24A	108.6	N13—C14—C15	129.91 (16)
C25—C24—H24B	108.6	C17—C14—C15	120.84 (16)
N9—C24—H24B	108.6	N10—C15—N9	119.50 (18)
H24A—C24—H24B	107.6	N10—C15—C14	130.94 (18)
C26—C25—C24	129.2 (4)	N9—C15—C14	109.56 (15)
C26—C25—H25	115.4	N8—C16—N9	127.79 (18)
C24—C25—H25	115.4	N8—C16—H16	116.1
C25—C26—H26A	120.0	N9—C16—H16	116.1
C25—C26—H26B	120.0	N11—C17—N8	127.49 (16)
H26A—C26—H26B	120.0	N11—C17—C14	104.94 (15)
N6—C1—C4	109.19 (15)	N8—C17—C14	127.56 (17)
N6—C1—C2	129.88 (15)	N11—C18—C20	113.36 (16)
C4—C1—C2	120.92 (15)	N11—C18—H18A	108.9
N3—C2—N2	119.22 (16)	C20—C18—H18A	108.9
N3—C2—C1	131.28 (16)	N11—C18—H18B	108.9
N2—C2—C1	109.50 (14)	C20—C18—H18B	108.9
N1—C3—N2	127.88 (17)	H18A—C18—H18B	107.7
N1—C3—H3	116.1	N14—C19—C20	124.30 (18)
N2—C3—H3	116.1	N14—C19—H19	117.8
N4—C4—N1	127.68 (16)	C20—C19—H19	117.8
N4—C4—C1	104.78 (15)	C19—C20—C21	116.96 (19)
N1—C4—C1	127.53 (17)	C19—C20—C18	122.96 (17)
N4—C5—C7	110.31 (14)	C21—C20—C18	120.06 (18)
N4—C5—H5A	109.6	C22—C21—C20	119.9 (2)

C7—C5—H5A	109.6	C22—C21—H21	120.0
N4—C5—H5B	109.6	C20—C21—H21	120.0
C7—C5—H5B	109.6	C23—C22—C21	117.6 (2)
H5A—C5—H5B	108.1	C23—C22—H22	121.2
N7—C6—C7	124.30 (18)	C21—C22—H22	121.2
N7—C6—H6	117.8	N14—C23—C22	125.2 (2)
C7—C6—H6	117.8	N14—C23—Cl2	115.96 (17)
C8—C7—C6	117.12 (18)	C22—C23—Cl2	118.84 (17)
C8—C7—C5	122.66 (18)	C3—N1—C4	110.65 (15)
C6—C7—C5	120.18 (17)	C3—N2—C2	123.51 (15)
C7—C8—C9	119.8 (2)	C3—N2—C11	118.39 (15)
C7—C8—H8	120.1	C2—N2—C11	118.09 (15)
C9—C8—H8	120.1	C2—N3—H3A	119.3
C10—C9—C8	117.16 (19)	C4—N4—N5	110.08 (14)
C10—C9—H9	121.4	C4—N4—C5	129.06 (15)
C8—C9—H9	121.4	N5—N4—C5	120.63 (15)
N7—C10—C9	125.59 (19)	N6—N5—N4	107.99 (14)
N7—C10—Cl1	115.58 (16)	N5—N6—C1	107.95 (14)
C9—C10—Cl1	118.82 (16)	C10—N7—C6	115.93 (17)
N2—C11—C12	113.26 (16)	C16—N8—C17	110.70 (16)
N2—C11—H11A	108.9	C16—N9—C15	123.52 (17)
C12—C11—H11A	108.9	C16—N9—C24	120.41 (17)
N2—C11—H11B	108.9	C15—N9—C24	116.08 (16)
C12—C11—H11B	108.9	C15—N10—H10A	119.3
H11A—C11—H11B	107.7	C17—N11—N12	109.97 (14)
C13—C12—C11	124.9 (3)	C17—N11—C18	129.37 (16)
C13—C12—H12	117.5	N12—N11—C18	120.66 (16)
C11—C12—H12	117.5	N13—N12—N11	107.63 (15)
C12—C13—H13A	120.0	N12—N13—C14	108.23 (15)
C12—C13—H13B	120.0	C23—N14—C19	116.03 (18)

N9—C24—C25—C26	−120.5 (5)	N3—C2—N2—C11	0.2 (2)
N6—C1—C2—N3	0.1 (3)	C1—C2—N2—C11	179.95 (14)
C4—C1—C2—N3	−179.05 (17)	C12—C11—N2—C3	−89.6 (2)
N6—C1—C2—N2	−179.57 (15)	C12—C11—N2—C2	89.2 (2)
C4—C1—C2—N2	1.3 (2)	N1—C4—N4—N5	−179.62 (15)
N6—C1—C4—N4	−0.42 (17)	C1—C4—N4—N5	0.66 (17)
C2—C1—C4—N4	178.88 (14)	N1—C4—N4—C5	−5.2 (3)
N6—C1—C4—N1	179.86 (15)	C1—C4—N4—C5	175.05 (15)
C2—C1—C4—N1	−0.8 (3)	C7—C5—N4—C4	−101.8 (2)
N7—C6—C7—C8	2.9 (3)	C7—C5—N4—N5	72.1 (2)
N7—C6—C7—C5	−175.14 (18)	C4—N4—N5—N6	−0.68 (18)
N4—C5—C7—C8	−105.4 (2)	C5—N4—N5—N6	−175.62 (14)
N4—C5—C7—C6	72.5 (2)	N4—N5—N6—C1	0.39 (17)
C6—C7—C8—C9	−1.9 (3)	C4—C1—N6—N5	0.02 (18)
C5—C7—C8—C9	176.1 (2)	C2—C1—N6—N5	−179.19 (15)
C7—C8—C9—C10	−0.5 (3)	C9—C10—N7—C6	−1.6 (3)
C8—C9—C10—N7	2.4 (4)	Cl1—C10—N7—C6	177.57 (15)

C8—C9—C10—Cl1	−176.73 (18)	C7—C6—N7—C10	−1.2 (3)
N2—C11—C12—C13	123.7 (3)	N9—C16—N8—C17	−0.1 (3)
N13—C14—C15—N10	−0.3 (4)	N11—C17—N8—C16	179.08 (19)
C17—C14—C15—N10	177.7 (2)	C14—C17—N8—C16	−0.8 (3)
N13—C14—C15—N9	−179.85 (18)	N8—C16—N9—C15	−0.3 (3)
C17—C14—C15—N9	−1.9 (2)	N8—C16—N9—C24	179.6 (2)
N13—C14—C17—N11	0.4 (2)	N10—C15—N9—C16	−178.4 (2)
C15—C14—C17—N11	−178.00 (16)	C14—C15—N9—C16	1.2 (3)
N13—C14—C17—N8	−179.76 (18)	N10—C15—N9—C24	1.6 (3)
C15—C14—C17—N8	1.9 (3)	C14—C15—N9—C24	−178.73 (18)
N14—C19—C20—C21	0.7 (3)	C25—C24—N9—C16	5.5 (4)
N14—C19—C20—C18	179.01 (18)	C25—C24—N9—C15	−174.5 (3)
N11—C18—C20—C19	27.4 (3)	N8—C17—N11—N12	179.79 (18)
N11—C18—C20—C21	−154.32 (18)	C14—C17—N11—N12	−0.3 (2)
C19—C20—C21—C22	0.1 (3)	N8—C17—N11—C18	−0.3 (3)
C18—C20—C21—C22	−178.26 (19)	C14—C17—N11—C18	179.60 (18)
C20—C21—C22—C23	−0.6 (3)	C20—C18—N11—C17	−110.6 (2)
C21—C22—C23—N14	0.4 (3)	C20—C18—N11—N12	69.3 (2)
C21—C22—C23—Cl2	−179.65 (16)	C17—N11—N12—N13	0.2 (2)
N2—C3—N1—C4	0.0 (3)	C18—N11—N12—N13	−179.76 (17)
N4—C4—N1—C3	−179.58 (17)	N11—N12—N13—C14	0.1 (2)
C1—C4—N1—C3	0.1 (2)	C17—C14—N13—N12	−0.3 (2)
N1—C3—N2—C2	0.6 (3)	C15—C14—N13—N12	177.90 (19)
N1—C3—N2—C11	179.45 (18)	C22—C23—N14—C19	0.3 (3)
N3—C2—N2—C3	179.06 (16)	Cl2—C23—N14—C19	−179.61 (14)
C1—C2—N2—C3	−1.2 (2)	C20—C19—N14—C23	−0.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10*A*···N1	0.86	2.44	3.292 (3)	173
N3—H3*A*···N8^{i}	0.86	2.45	3.299 (2)	169
C11—H11*A*···N3	0.97	2.41	2.749 (2)	100
C19—H19···N11	0.93	2.59	2.909 (3)	101
C3—H3···N13	0.93	2.46	3.309 (2)	151
C11—H11*A*···*Cg*4^{ii}	0.97	2.87	3.446 (2)	119
C24—H24*A*···*Cg*1^{iii}	0.97	2.99	3.851 (3)	149

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