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2-Chloro-*N*-cyclopropyl-9-(3,4,5,6-tetrahydro-2*H*-pyran-2-yl)-9*H*-purin-6-amine

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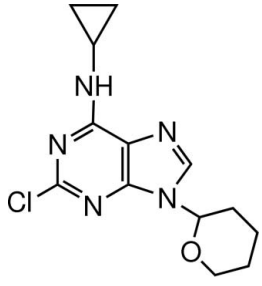
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.006 Å; R factor = 0.066; wR factor = 0.197; data-to-parameter ratio = 14.4.

The title compound, $C_{13}H_{16}ClN_5O$, crystallizes with two molecules in the asymmetric unit, which differ in the orientation of the tetrahydropyran ring with respect to the purine ring system. In both molecules, the purine ring system is essentially planar and the tetrahydropyran ring adopts a chair conformation. The two independent molecules exist as an N—H···N hydrogen-bonded dimer. Centrosymmetrically related dimers are linked together by weak C—H···O hydrogen bonds, forming a tetramer.

Related literature

For synthesis, see: Robins *et al.* (1961). For general background, see: Meade *et al.* (1993); Taddei *et al.* (2004).



Experimental

Crystal data

$C_{13}H_{16}ClN_5O$
M_r = 293.76
Triclinic, $P\overline{1}$
a = 11.385 (4) Å
b = 11.686 (4) Å
c = 11.692 (4) Å
α = 111.380 (5)°
β = 96.954 (4)°
γ = 94.531 (5)°
V = 1425.0 (9) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 298 (2) K
0.15 × 0.12 × 0.10 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.960, T_{max} = 0.973
6270 measured reflections
5203 independent reflections
3410 reflections with $I > 2\sigma(I)$
R_{int} = 0.052

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.197
S = 0.97
5203 reflections
361 parameters
18 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.43 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N10—H10···N27	0.86	2.20	2.998 (3)	155
N30—H30···N7	0.86	2.22	3.023 (4)	155
C36—H36*B*···O15^{i}	0.97	2.57	3.504 (5)	162

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

Data collection: *SMART* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Bruker, 2005); program(s) used to refine structure: *SHELXTL*; molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL*.

The authors thank Professor Min-Qing Chen of the Centre of Analysis and Measurement of Fudan University for the X-ray data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2415).

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supplementary materials

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2-Chloro-*N*-cyclopropyl-9-(3,4,5,6-tetrahydro-2*H*-pyran-2-yl)-9*H*-purin-6-amine

N.-Q. Wang and T.-T. Mao

Comment

Some purine nucleosides and nucleotides have been found to act as crucial hormones, neurotransmiters or coenzymes (Taddei *et al.*, 2004). Isosteres of purines have been isolated from natural sources and have displayed significant anti-microbial and anti-cancer activity, leading to important new medicines (Meade *et al.*, 1993). In order to better understand the relationship between the structure and biological activity, we have synthesized the title compound and determined its crystal and molecular structure.

The asymmetric unit of the title compound contains two crystallographically independent molecules (Fig. 1). These molecules differ slightly in the orientations of the tetrahydropyran rings with respect to the purine ring system. In both the molecules the purine ring system is essentially planar and the tetrahydropyran ring adopts a chair conformation.

In the crystal structure, the two independent molecules exist as a N—H···N hydrogen-bonded dimer. Centrosymmetrically related dimers are linked together by weak C—H···O hydrogen bonds (Table 1), forming a tetramer (Fig. 2).

Experimental

The title compound was prepared according to the literature method (Robins *et al.*, 1961). Single crystals of the title compound were obtained by slow evaporation of a acetone-water (8:2 *v*/*v*) solution.

Refinement

H atoms were placed at calculated positions (N—H = 0.86 Å and C—H = 0.93–0.98 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(C,*N*). During the refinement, the displacement parameters of atoms C18, C19 and C33 were restrained to an approximate isotropic behaviour.

Figures

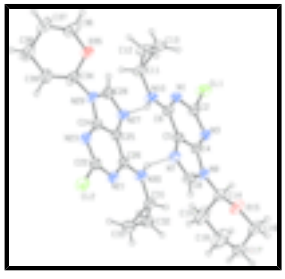

Fig. 1. The asymmetric unit of the title compound, showing two independent molecules. Displacement ellipsoids are drawn at the 30% probability level. Dashed lines indicate hydrogen bonds.

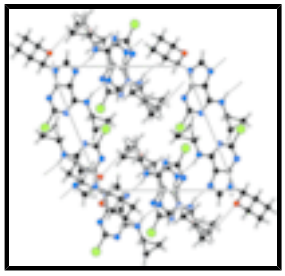

Fig. 2. The packing diagram of the title compound, viewed along the *a* axis. Hydrogen bonds are shown as dashed lines.

2-Chloro-*N*-cyclopropyl-9-(3,4,5,6-tetrahydro-2*H*-pyran-2-yl)- 9*H*-purin-6-amine

Crystal data

$C_{13}H_{16}ClN_5O$	$Z = 4$
$M_r = 293.76$	$F_{000} = 616$
Triclinic, $P\overline{1}$	$D_x = 1.369$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 11.385$ (4) Å	Cell parameters from 809 reflections
$b = 11.686$ (4) Å	$\theta = 2.8$–26.4º
$c = 11.692$ (4) Å	$\mu = 0.27$ mm^{-1}
$\alpha = 111.380$ (5)º	$T = 298$ (2) K
$\beta = 96.954$ (4)º	Prism, colourless
$\gamma = 94.531$ (5)º	0.15 × 0.12 × 0.10 mm
$V = 1425.0$ (9) Å^3	

Data collection

Bruker SMART APEX CCD area-detector diffractometer	5203 independent reflections
Radiation source: fine-focus sealed tube	3410 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.052$
$T = 298(2)$ K	$\theta_{max} = 25.5$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -13\rightarrow12$
$T_{min} = 0.960$, $T_{max} = 0.973$	$k = -8\rightarrow14$
6270 measured reflections	$l = -14\rightarrow13$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.066$	H-atom parameters constrained
$wR(F^2) = 0.197$	$w = 1/[\sigma^2(F_o^2) + (0.1257P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.97$	$(\Delta/\sigma)_{max} = 0.001$

5203 reflections	$\Delta\rho_{max} = 0.43$ e Å^{-3}
361 parameters	$\Delta\rho_{min} = -0.39$ e Å^{-3}
18 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\text{sigma}(F^2)$ 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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.82375 (8)	1.22208 (8)	0.49371 (7)	0.0679 (3)
N1	0.6765 (2)	1.0223 (2)	0.3754 (2)	0.0446 (6)
C2	0.7559 (2)	1.1004 (3)	0.3569 (3)	0.0435 (7)
N3	0.7924 (2)	1.1026 (2)	0.2554 (2)	0.0457 (6)
C4	0.7344 (2)	1.0042 (3)	0.1565 (3)	0.0396 (6)
C5	0.6513 (2)	0.9123 (3)	0.1579 (2)	0.0410 (6)
C6	0.6234 (2)	0.9227 (3)	0.2749 (3)	0.0411 (6)
N7	0.6115 (2)	0.8259 (2)	0.0393 (2)	0.0504 (6)
C8	0.6701 (3)	0.8670 (3)	−0.0301 (3)	0.0530 (8)
H8	0.6613	0.8266	−0.1160	0.064*
N9	0.7458 (2)	0.9747 (2)	0.0342 (2)	0.0465 (6)
N10	0.5473 (2)	0.8376 (2)	0.2888 (2)	0.0488 (6)
H10	0.5159	0.7747	0.2229	0.059*
C11	0.5135 (3)	0.8424 (3)	0.4043 (3)	0.0512 (8)
H11	0.4422	0.8819	0.4258	0.061*
C12	0.5288 (3)	0.7332 (3)	0.4394 (3)	0.0663 (10)
H12A	0.5655	0.6664	0.3852	0.080*
H12B	0.4676	0.7074	0.4793	0.080*
C13	0.6053 (3)	0.8556 (3)	0.5106 (3)	0.0628 (9)
H13A	0.5906	0.9033	0.5936	0.075*
H13B	0.6883	0.8623	0.4995	0.075*
C14	0.8143 (3)	1.0476 (3)	−0.0185 (3)	0.0495 (7)
H14	0.8763	1.1050	0.0476	0.059*
O15	0.8690 (2)	0.9658 (2)	−0.1059 (2)	0.0680 (7)
C16	0.9436 (3)	1.0287 (4)	−0.1627 (4)	0.0786 (12)
H16A	0.9815	0.9682	−0.2230	0.094*
H16B	1.0060	1.0862	−0.0992	0.094*

C17	0.8755 (4)	1.0963 (5)	−0.2247 (4)	0.0972 (17)
H17A	0.8176	1.0385	−0.2933	0.117*
H17B	0.9288	1.1405	−0.2579	0.117*
C18	0.8136 (5)	1.1846 (6)	−0.1353 (6)	0.139 (2)
H18A	0.7613	1.2225	−0.1788	0.167*
H18B	0.8719	1.2498	−0.0741	0.167*
C19	0.7405 (4)	1.1203 (5)	−0.0695 (6)	0.122 (2)
H19A	0.7101	1.1819	−0.0028	0.147*
H19B	0.6728	1.0662	−0.1280	0.147*
Cl2	0.13063 (8)	0.24465 (10)	−0.34039 (8)	0.0752 (3)
N21	0.2902 (2)	0.4357 (2)	−0.2234 (2)	0.0481 (6)
C22	0.2118 (3)	0.3567 (3)	−0.2043 (3)	0.0500 (7)
N23	0.1835 (2)	0.3502 (2)	−0.1010 (2)	0.0501 (6)
C24	0.2502 (2)	0.4397 (3)	−0.0029 (3)	0.0433 (7)
C25	0.3371 (2)	0.5292 (3)	−0.0051 (3)	0.0420 (6)
C26	0.3549 (2)	0.5259 (3)	−0.1223 (3)	0.0428 (7)
N27	0.3872 (2)	0.6087 (2)	0.1140 (2)	0.0471 (6)
C28	0.3303 (3)	0.5663 (3)	0.1848 (3)	0.0500 (7)
H28	0.3454	0.6022	0.2712	0.060*
N29	0.2472 (2)	0.4654 (2)	0.1207 (2)	0.0469 (6)
N30	0.4314 (2)	0.6108 (2)	−0.1362 (2)	0.0476 (6)
H30	0.4699	0.6686	−0.0698	0.057*
C31	0.4541 (3)	0.6129 (3)	−0.2525 (3)	0.0493 (7)
H31	0.5140	0.5618	−0.2903	0.059*
C32	0.4517 (3)	0.7314 (3)	−0.2715 (3)	0.0650 (9)
H32A	0.4313	0.8018	−0.2051	0.078*
H32B	0.5097	0.7520	−0.3176	0.078*
C33	0.3567 (3)	0.6261 (4)	−0.3404 (4)	0.0734 (11)
H33A	0.2782	0.6322	−0.3162	0.088*
H33B	0.3566	0.5825	−0.4286	0.088*
C34	0.1686 (3)	0.4008 (3)	0.1736 (3)	0.0517 (8)
H34	0.1401	0.3167	0.1127	0.062*
O35	0.24039 (19)	0.3944 (2)	0.2761 (2)	0.0628 (6)
C36	0.1765 (4)	0.3320 (4)	0.3394 (4)	0.0787 (11)
H36A	0.2301	0.3297	0.4095	0.094*
H36B	0.1482	0.2472	0.2833	0.094*
C37	0.0730 (4)	0.3954 (4)	0.3849 (4)	0.0780 (11)
H37A	0.0286	0.3482	0.4225	0.094*
H37B	0.1018	0.4771	0.4480	0.094*
C38	−0.0070 (3)	0.4075 (4)	0.2807 (4)	0.0864 (13)
H38A	−0.0683	0.4576	0.3134	0.104*
H38B	−0.0460	0.3262	0.2244	0.104*
C39	0.0643 (3)	0.4678 (4)	0.2101 (4)	0.0672 (10)
H39A	0.0135	0.4654	0.1362	0.081*
H39B	0.0922	0.5539	0.2623	0.081*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0779 (6)	0.0647 (6)	0.0453 (5)	−0.0253 (5)	0.0013 (4)	0.0122 (4)
N1	0.0468 (13)	0.0441 (14)	0.0402 (13)	−0.0037 (11)	0.0079 (11)	0.0145 (11)
C2	0.0444 (15)	0.0409 (16)	0.0423 (16)	−0.0010 (13)	0.0065 (13)	0.0140 (12)
N3	0.0441 (13)	0.0449 (14)	0.0468 (14)	−0.0022 (11)	0.0113 (11)	0.0163 (11)
C4	0.0393 (15)	0.0419 (16)	0.0416 (15)	0.0052 (12)	0.0131 (12)	0.0182 (12)
C5	0.0414 (15)	0.0422 (16)	0.0398 (15)	0.0027 (13)	0.0086 (12)	0.0160 (12)
C6	0.0430 (15)	0.0398 (15)	0.0436 (15)	0.0037 (13)	0.0116 (12)	0.0184 (12)
N7	0.0587 (15)	0.0512 (15)	0.0381 (13)	−0.0066 (12)	0.0119 (12)	0.0148 (11)
C8	0.0626 (19)	0.0526 (19)	0.0393 (16)	−0.0041 (15)	0.0131 (14)	0.0130 (14)
N9	0.0509 (14)	0.0466 (14)	0.0434 (14)	−0.0015 (12)	0.0164 (11)	0.0176 (11)
N10	0.0594 (15)	0.0459 (14)	0.0375 (13)	−0.0111 (12)	0.0114 (11)	0.0143 (11)
C11	0.0604 (19)	0.0507 (18)	0.0409 (16)	−0.0036 (15)	0.0197 (14)	0.0141 (14)
C12	0.102 (3)	0.054 (2)	0.0453 (18)	−0.0070 (19)	0.0208 (18)	0.0214 (15)
C13	0.081 (2)	0.062 (2)	0.0415 (17)	−0.0111 (18)	0.0127 (17)	0.0190 (15)
C14	0.0555 (18)	0.0499 (18)	0.0496 (17)	0.0028 (15)	0.0220 (14)	0.0229 (14)
O15	0.0789 (16)	0.0623 (15)	0.0778 (16)	0.0137 (13)	0.0469 (14)	0.0324 (13)
C16	0.075 (2)	0.093 (3)	0.089 (3)	0.014 (2)	0.050 (2)	0.047 (2)
C17	0.066 (2)	0.169 (5)	0.084 (3)	−0.010 (3)	0.012 (2)	0.085 (3)
C18	0.144 (4)	0.150 (5)	0.226 (6)	0.074 (4)	0.107 (4)	0.156 (5)
C19	0.115 (3)	0.147 (4)	0.195 (5)	0.079 (3)	0.102 (4)	0.134 (4)
Cl2	0.0665 (6)	0.0870 (7)	0.0510 (5)	−0.0262 (5)	0.0040 (4)	0.0107 (5)
N21	0.0436 (13)	0.0539 (15)	0.0459 (14)	−0.0004 (12)	0.0088 (11)	0.0187 (12)
C22	0.0431 (16)	0.0552 (19)	0.0464 (17)	−0.0014 (14)	0.0069 (13)	0.0149 (14)
N23	0.0454 (14)	0.0516 (15)	0.0511 (15)	−0.0025 (12)	0.0108 (12)	0.0176 (12)
C24	0.0388 (15)	0.0447 (16)	0.0481 (17)	0.0015 (13)	0.0105 (13)	0.0191 (13)
C25	0.0408 (15)	0.0419 (16)	0.0456 (16)	0.0036 (13)	0.0085 (12)	0.0192 (13)
C26	0.0393 (15)	0.0449 (16)	0.0474 (16)	0.0057 (13)	0.0088 (13)	0.0208 (13)
N27	0.0523 (14)	0.0458 (14)	0.0442 (14)	−0.0033 (12)	0.0082 (11)	0.0198 (11)
C28	0.0532 (18)	0.0511 (18)	0.0442 (16)	−0.0031 (15)	0.0068 (14)	0.0185 (14)
N29	0.0490 (14)	0.0487 (15)	0.0440 (14)	−0.0011 (12)	0.0132 (11)	0.0184 (11)
N30	0.0540 (14)	0.0485 (14)	0.0411 (13)	−0.0045 (12)	0.0082 (11)	0.0202 (11)
C31	0.0487 (16)	0.0568 (19)	0.0449 (16)	0.0012 (14)	0.0132 (13)	0.0217 (14)
C32	0.072 (2)	0.069 (2)	0.062 (2)	−0.0064 (19)	0.0066 (18)	0.0386 (19)
C33	0.066 (2)	0.100 (3)	0.063 (2)	−0.014 (2)	−0.0025 (17)	0.049 (2)
C34	0.0553 (18)	0.0491 (18)	0.0484 (18)	−0.0055 (15)	0.0167 (14)	0.0157 (14)
O35	0.0607 (13)	0.0759 (17)	0.0714 (16)	0.0094 (12)	0.0236 (12)	0.0466 (13)
C36	0.100 (3)	0.079 (3)	0.078 (3)	0.005 (2)	0.036 (2)	0.048 (2)
C37	0.089 (3)	0.079 (3)	0.070 (2)	−0.003 (2)	0.041 (2)	0.026 (2)
C38	0.063 (2)	0.100 (3)	0.094 (3)	−0.003 (2)	0.037 (2)	0.029 (3)
C39	0.0493 (19)	0.077 (2)	0.080 (3)	0.0068 (18)	0.0188 (18)	0.033 (2)

Geometric parameters (Å, °)

Cl1—C2	1.746 (3)	Cl2—C22	1.742 (3)
N1—C2	1.326 (3)	N21—C22	1.329 (4)

N1—C6	1.349 (3)	N21—C26	1.345 (4)
C2—N3	1.312 (3)	C22—N23	1.312 (4)
N3—C4	1.349 (3)	N23—C24	1.332 (4)
C4—N9	1.368 (3)	C24—N29	1.370 (4)
C4—C5	1.380 (4)	C24—C25	1.391 (4)
C5—N7	1.380 (4)	C25—N27	1.382 (4)
C5—C6	1.405 (4)	C25—C26	1.396 (4)
C6—N10	1.335 (3)	C26—N30	1.336 (3)
N7—C8	1.303 (4)	N27—C28	1.315 (3)
C8—N9	1.368 (4)	C28—N29	1.362 (4)
C8—H8	0.93	C28—H28	0.93
N9—C14	1.453 (3)	N29—C34	1.457 (3)
N10—C11	1.431 (3)	N30—C31	1.424 (4)
N10—H10	0.86	N30—H30	0.86
C11—C13	1.477 (5)	C31—C33	1.475 (5)
C11—C12	1.492 (5)	C31—C32	1.482 (4)
C11—H11	0.98	C31—H31	0.98
C12—C13	1.502 (5)	C32—C33	1.479 (5)
C12—H12A	0.97	C32—H32A	0.97
C12—H12B	0.97	C32—H32B	0.97
C13—H13A	0.97	C33—H33A	0.97
C13—H13B	0.97	C33—H33B	0.97
C14—O15	1.372 (4)	C34—O35	1.395 (4)
C14—C19	1.464 (5)	C34—C39	1.494 (4)
C14—H14	0.98	C34—H34	0.98
O15—C16	1.449 (4)	O35—C36	1.431 (4)
C16—C17	1.459 (6)	C36—C37	1.491 (5)
C16—H16A	0.97	C36—H36A	0.97
C16—H16B	0.97	C36—H36B	0.97
C17—C18	1.469 (7)	C37—C38	1.487 (6)
C17—H17A	0.97	C37—H37A	0.97
C17—H17B	0.97	C37—H37B	0.97
C18—C19	1.526 (5)	C38—C39	1.528 (5)
C18—H18A	0.97	C38—H38A	0.97
C18—H18B	0.97	C38—H38B	0.97
C19—H19A	0.97	C39—H39A	0.97
C19—H19B	0.97	C39—H39B	0.97
C2—N1—C6	117.1 (2)	C22—N21—C26	117.3 (2)
N3—C2—N1	131.9 (3)	N23—C22—N21	131.2 (3)
N3—C2—Cl1	114.7 (2)	N23—C22—Cl2	114.8 (2)
N1—C2—Cl1	113.4 (2)	N21—C22—Cl2	114.0 (2)
C2—N3—C4	109.3 (2)	C22—N23—C24	110.0 (2)
N3—C4—N9	127.3 (2)	N23—C24—N29	128.1 (3)
N3—C4—C5	127.0 (2)	N23—C24—C25	126.7 (3)
N9—C4—C5	105.7 (2)	N29—C24—C25	105.2 (2)
N7—C5—C4	111.0 (2)	N27—C25—C24	111.2 (2)
N7—C5—C6	132.5 (3)	N27—C25—C26	132.3 (3)
C4—C5—C6	116.6 (3)	C24—C25—C26	116.5 (3)
N10—C6—N1	119.8 (2)	N30—C26—N21	119.7 (3)

N10—C6—C5	122.2 (3)	N30—C26—C25	122.0 (3)
N1—C6—C5	118.1 (2)	N21—C26—C25	118.2 (3)
C8—N7—C5	103.5 (2)	C28—N27—C25	103.2 (2)
N7—C8—N9	114.3 (3)	N27—C28—N29	114.3 (3)
N7—C8—H8	122.8	N27—C28—H28	122.9
N9—C8—H8	122.8	N29—C28—H28	122.9
C4—N9—C8	105.5 (2)	C28—N29—C24	106.2 (2)
C4—N9—C14	127.6 (2)	C28—N29—C34	126.6 (2)
C8—N9—C14	126.7 (2)	C24—N29—C34	127.2 (2)
C6—N10—C11	125.4 (2)	C26—N30—C31	125.0 (3)
C6—N10—H10	117.3	C26—N30—H30	117.5
C11—N10—H10	117.3	C31—N30—H30	117.5
N10—C11—C13	120.4 (3)	N30—C31—C33	120.0 (3)
N10—C11—C12	117.5 (3)	N30—C31—C32	118.0 (3)
C13—C11—C12	60.8 (2)	C33—C31—C32	60.0 (2)
N10—C11—H11	115.6	N30—C31—H31	115.8
C13—C11—H11	115.6	C33—C31—H31	115.8
C12—C11—H11	115.6	C32—C31—H31	115.8
C11—C12—C13	59.1 (2)	C33—C32—C31	59.7 (2)
C11—C12—H12A	117.9	C33—C32—H32A	117.8
C13—C12—H12A	117.9	C31—C32—H32A	117.8
C11—C12—H12B	117.9	C33—C32—H32B	117.8
C13—C12—H12B	117.9	C31—C32—H32B	117.8
H12A—C12—H12B	115.0	H32A—C32—H32B	114.9
C11—C13—C12	60.1 (2)	C31—C33—C32	60.2 (2)
C11—C13—H13A	117.8	C31—C33—H33A	117.7
C12—C13—H13A	117.8	C32—C33—H33A	117.7
C11—C13—H13B	117.8	C31—C33—H33B	117.7
C12—C13—H13B	117.8	C32—C33—H33B	117.7
H13A—C13—H13B	114.9	H33A—C33—H33B	114.9
O15—C14—N9	106.4 (2)	O35—C34—N29	105.0 (2)
O15—C14—C19	112.9 (3)	O35—C34—C39	111.9 (3)
N9—C14—C19	112.4 (3)	N29—C34—C39	111.4 (3)
O15—C14—H14	108.3	O35—C34—H34	109.5
N9—C14—H14	108.3	N29—C34—H34	109.5
C19—C14—H14	108.3	C39—C34—H34	109.5
C14—O15—C16	111.5 (3)	C34—O35—C36	112.4 (3)
O15—C16—C17	112.1 (3)	O35—C36—C37	111.4 (3)
O15—C16—H16A	109.2	O35—C36—H36A	109.3
C17—C16—H16A	109.2	C37—C36—H36A	109.3
O15—C16—H16B	109.2	O35—C36—H36B	109.3
C17—C16—H16B	109.2	C37—C36—H36B	109.3
H16A—C16—H16B	107.9	H36A—C36—H36B	108.0
C16—C17—C18	109.6 (4)	C38—C37—C36	110.7 (3)
C16—C17—H17A	109.7	C38—C37—H37A	109.5
C18—C17—H17A	109.7	C36—C37—H37A	109.5
C16—C17—H17B	109.7	C38—C37—H37B	109.5
C18—C17—H17B	109.7	C36—C37—H37B	109.5
H17A—C17—H17B	108.2	H37A—C37—H37B	108.1

C17—C18—C19	111.1 (4)	C37—C38—C39	110.4 (3)
C17—C18—H18A	109.4	C37—C38—H38A	109.6
C19—C18—H18A	109.4	C39—C38—H38A	109.6
C17—C18—H18B	109.4	C37—C38—H38B	109.6
C19—C18—H18B	109.4	C39—C38—H38B	109.6
H18A—C18—H18B	108.0	H38A—C38—H38B	108.1
C14—C19—C18	110.3 (3)	C34—C39—C38	110.1 (3)
C14—C19—H19A	109.6	C34—C39—H39A	109.6
C18—C19—H19A	109.6	C38—C39—H39A	109.6
C14—C19—H19B	109.6	C34—C39—H39B	109.6
C18—C19—H19B	109.6	C38—C39—H39B	109.6
H19A—C19—H19B	108.1	H39A—C39—H39B	108.2
C6—N1—C2—N3	2.4 (5)	C26—N21—C22—N23	0.7 (5)
C6—N1—C2—Cl1	−177.4 (2)	C26—N21—C22—Cl2	179.1 (2)
N1—C2—N3—C4	−0.1 (4)	N21—C22—N23—C24	−1.4 (5)
Cl1—C2—N3—C4	179.67 (19)	Cl2—C22—N23—C24	−179.8 (2)
C2—N3—C4—N9	178.8 (3)	C22—N23—C24—N29	179.2 (3)
C2—N3—C4—C5	−1.4 (4)	C22—N23—C24—C25	0.4 (4)
N3—C4—C5—N7	−179.5 (3)	N23—C24—C25—N27	179.0 (3)
N9—C4—C5—N7	0.4 (3)	N29—C24—C25—N27	0.0 (3)
N3—C4—C5—C6	0.5 (4)	N23—C24—C25—C26	1.1 (4)
N9—C4—C5—C6	−179.6 (2)	N29—C24—C25—C26	−177.9 (2)
C2—N1—C6—N10	176.6 (3)	C22—N21—C26—N30	−177.2 (3)
C2—N1—C6—C5	−3.2 (4)	C22—N21—C26—C25	1.1 (4)
N7—C5—C6—N10	2.1 (5)	N27—C25—C26—N30	−0.9 (5)
C4—C5—C6—N10	−177.9 (3)	C24—C25—C26—N30	176.4 (2)
N7—C5—C6—N1	−178.1 (3)	N27—C25—C26—N21	−179.2 (3)
C4—C5—C6—N1	1.9 (4)	C24—C25—C26—N21	−1.8 (4)
C4—C5—N7—C8	−0.2 (3)	C24—C25—N27—C28	0.0 (3)
C6—C5—N7—C8	179.9 (3)	C26—C25—N27—C28	177.4 (3)
C5—N7—C8—N9	−0.1 (3)	C25—N27—C28—N29	0.0 (3)
N3—C4—N9—C8	179.4 (3)	N27—C28—N29—C24	0.0 (3)
C5—C4—N9—C8	−0.4 (3)	N27—C28—N29—C34	−178.2 (3)
N3—C4—N9—C14	−6.0 (5)	N23—C24—N29—C28	−178.9 (3)
C5—C4—N9—C14	174.1 (3)	C25—C24—N29—C28	0.0 (3)
N7—C8—N9—C4	0.4 (4)	N23—C24—N29—C34	−0.8 (5)
N7—C8—N9—C14	−174.2 (3)	C25—C24—N29—C34	178.2 (3)
N1—C6—N10—C11	0.9 (4)	N21—C26—N30—C31	−1.9 (4)
C5—C6—N10—C11	−179.3 (3)	C25—C26—N30—C31	179.9 (3)
C6—N10—C11—C13	−55.2 (4)	C26—N30—C31—C33	61.6 (4)
C6—N10—C11—C12	−125.8 (3)	C26—N30—C31—C32	131.3 (3)
N10—C11—C12—C13	111.3 (3)	N30—C31—C32—C33	−110.3 (3)
N10—C11—C13—C12	−106.6 (3)	N30—C31—C33—C32	107.1 (3)
C4—N9—C14—O15	138.7 (3)	C28—N29—C34—O35	−41.8 (4)
C8—N9—C14—O15	−47.9 (4)	C24—N29—C34—O35	140.4 (3)
C4—N9—C14—C19	−97.2 (4)	C28—N29—C34—C39	79.5 (4)
C8—N9—C14—C19	76.2 (4)	C24—N29—C34—C39	−98.3 (4)
N9—C14—O15—C16	−178.2 (3)	N29—C34—O35—C36	−179.6 (3)
C19—C14—O15—C16	58.1 (4)	C39—C34—O35—C36	59.4 (4)

C14—O15—C16—C17	−59.6 (5)	C34—O35—C36—C37	−59.2 (4)
O15—C16—C17—C18	56.5 (5)	O35—C36—C37—C38	55.5 (5)
C16—C17—C18—C19	−52.5 (6)	C36—C37—C38—C39	−52.3 (5)
O15—C14—C19—C18	−53.9 (6)	O35—C34—C39—C38	−55.3 (4)
N9—C14—C19—C18	−174.2 (4)	N29—C34—C39—C38	−172.5 (3)
C17—C18—C19—C14	50.9 (7)	C37—C38—C39—C34	51.9 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···N27	0.86	2.20	2.998 (3)	155
N30—H30···N7	0.86	2.22	3.023 (4)	155
C36—H36B···O15^{i}	0.97	2.57	3.504 (5)	162

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

Fig. 1

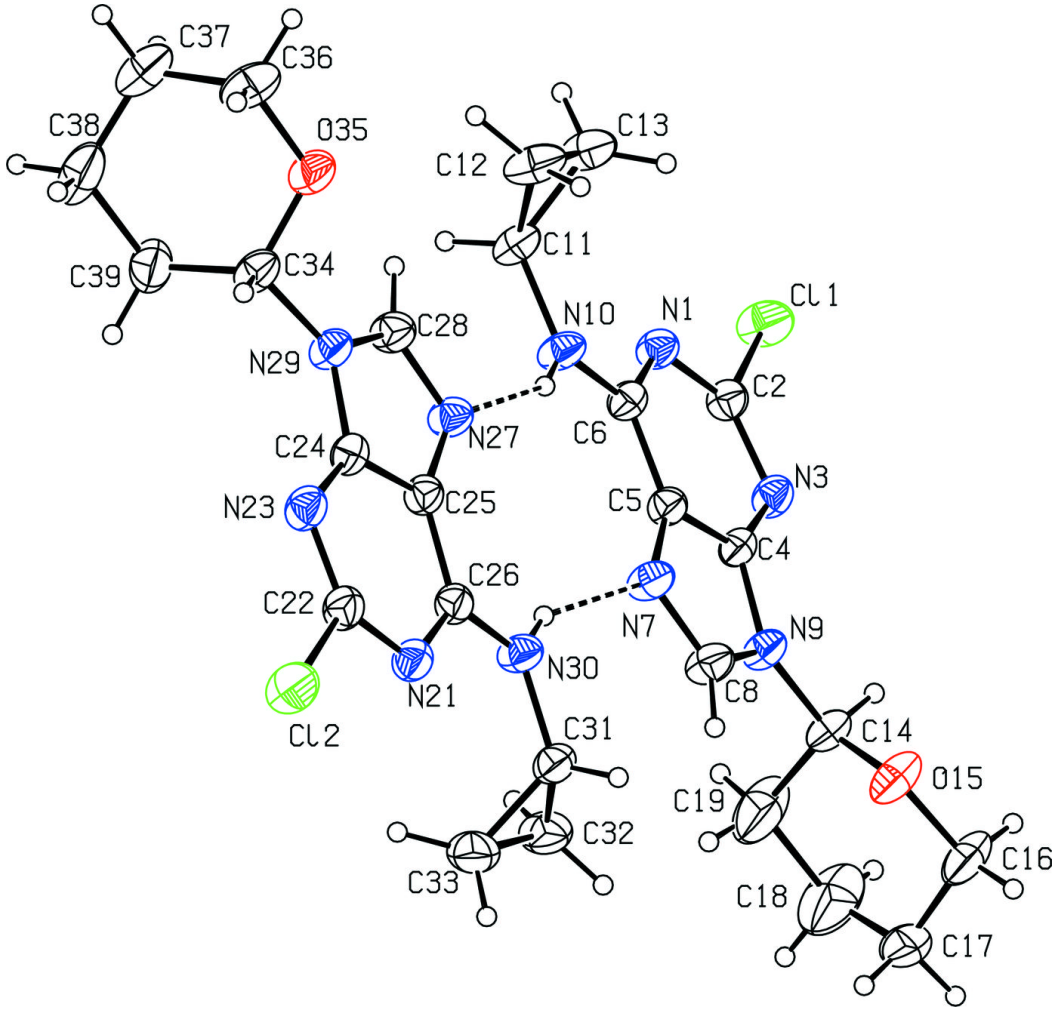
C37
C36
C38
O35
C13
C12
C11
C39
C34
N10
N1
Cl1
C28
N29
C2
N27
C6
C24
N3
N23
C25
C5
C4
C26
C22
N7
N9
N30
N21
C8
Cl2
C31
C14
O15
C19
C32
C16
C33
C18
C17

Fig. 2