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1-(4-Chlorophenyl)-2-diethylamino-9-phenyl-1*H*-purin-6(9*H*)-one

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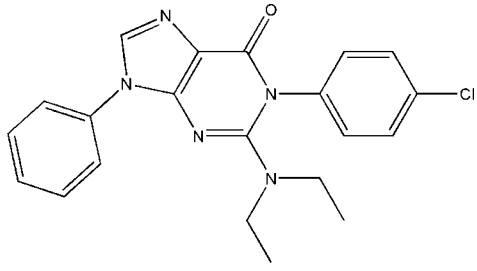
Key indicators: single-crystal X-ray study; T = 292 K; mean σ(C–C) = 0.003 Å; R factor = 0.051; wR factor = 0.126; data-to-parameter ratio = 17.4.

The molecule of the title compound, $C_{21}H_{20}ClN_5O$, has a planar bicyclic imidazolo[5,4-*d*]pyrimidine core. The planes of the phenyl and 4-chlorophenyl substituents form angles of 48.24 (11) and 71.34 (8)°, respectively, with the imidazolopyrimidine plane. The structure is stabilized by weak intermolecular C—H···N and C—H···O hydrogen bonds.

Related literature

The preparation and biological activity is described by Xu *et al.* (1995). For related literature, see: Ding *et al.* (2004).



Experimental

Crystal data

$C_{21}H_{20}ClN_5O$
M_r = 393.87
Monoclinic, $P2_1/n$
a = 13.4911 (12) Å
b = 8.3947 (8) Å
c = 17.4615 (16) Å
β = 100.674 (2)°
V = 1943.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.22 mm^{-1}
T = 292 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2003)
T_{min} = 0.937, T_{max} = 0.958
12370 measured reflections
4431 independent reflections
2979 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.126
S = 0.94
4431 reflections
255 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21A···N3	0.96	2.57	3.096 (3)	115
C16—H16···N2^{i}	0.93	2.61	3.443 (2)	149
C13—H13···O1^{ii}	0.93	2.47	3.340 (2)	155
C3—H3···O1^{iii}	0.93	2.45	3.371 (3)	172

Symmetry codes: (i) $-x+2, -y+1, -z$; (ii) $-x+2, -y, -z$; (iii) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2001).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT2605).

References

Bruker (2001). *SMART* (Version 5.628) and *SAINT-Plus* (Version 6.45). Bruker AXS Inc., Madison, Wisconsin, USA.
Ding, M. W., Xu, S. Z. & Zhao, J. F. (2004). *J. Org. Chem.* **69**, 8366–8371.
Sheldrick, G. M. (1997). *SHELXL97* and *SHELXS97*. University of Göttingen, Germany.
Sheldrick, G. M. (2001). *SHELXTL*. Version 5.0. Bruker AXS Inc., Madison, Wisconsin, USA.
Sheldrick, G. M. (2003). *SADABS*. Version 2.10. Bruker AXS inc., Madison, Wisconsin, USA.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Xu, H. Y., Maga, G., Focher, F., Smith, E. R., Spadari, S., Gambino, J. & Wright, G. E. (1995). *J. Med. Chem.* **38**, 49–57.

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supplementary materials

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1-(4-Chlorophenyl)-2-diethylamino-9-phenyl-1*H*-purin-6(9*H*)-one

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Comment

Substituted purine derivatives may be used as potential biologically active compounds or pharmaceuticals (Xu *et al.*, 1995). In recent years we have been developing aza-Wittig reaction for synthesis of heterocycles (Ding *et al.*, 2004). In this context, we have synthesized the title compound, 1-(4-chlorophenyl)-2-(diethylamino)-9-phenyl-1*H*-purin-6(9*H*)-one, $C_{21}H_{20}ClN_5O$; herein we report its crystal and molecular structure.

In the molecule (Fig. 1), the bond lengths and angles are unexceptional. The bicyclic imidazolo[5,4-*d*]pyrimidine system is almost planar with maximum deviation of −0.023 (2)Å for atom C(8), and the angle between plane N1—C7—N2—C8—C9 and N3—C9—C8—C11—N4—C10 is equal to 2.40 (9)°. The torsion angles C9—C8—C11—O1 and O1—C11—N4—C10 are equal to −173.96 (17)° and 177.36 (16)° respectively. The planes of the phenyl rings C1—C6 and C12—C17 are twisted to imidazolo[5,4-*d*]pyrimidine system with dihedral angles of 48.24 (11)° and 71.34 (8)° respectively.

As can be seen from the packing diagram (Fig. 2), the structure stabilized by the interactions of C—H···N, C—H···O hydrogen bonds. (Table 1).

Refinement

All H-atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å, U_{iso}=1.2U_{eq} (C) for Csp^2, C—H = 0.97 Å, U_{iso} = 1.2U_{eq} (C) for CH_2, C—H = 0.96 Å, U_{iso} = 1.5U_{eq} (C) for CH_3.

Figures

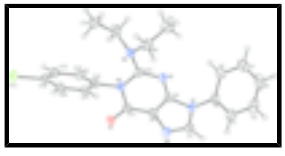

Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme.

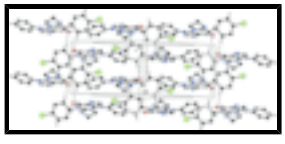

Fig. 2. The packing in the crystal structure, showing the C—H···O hydrogen bonds as dashed lines.

1-(4-Chlorophenyl)-2-diethylamino-9-phenyl-1*H*-purin-6(9*H*)-one

Crystal data

$C_{21}H_{20}ClN_5O$ F_{000} = 824

M_r = 393.87	D_x = 1.346 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2yn	Cell parameters from 2876 reflections
a = 13.4911 (12) Å	θ = 2.4–24.6º
b = 8.3947 (8) Å	μ = 0.22 mm^{-1}
c = 17.4615 (16) Å	T = 292 (2) K
β = 100.674 (2)º	Block, colorless
V = 1943.4 (3) Å^3	0.30 × 0.20 × 0.20 mm
Z = 4	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	4431 independent reflections
Radiation source: fine-focus sealed tube	2979 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.060
T = 292(2) K	θ_{max} = 27.5º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 2003)	h = −17→16
T_{min} = 0.937, T_{max} = 0.958	k = −9→10
12370 measured reflections	l = −22→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.051	H-atom parameters constrained
$wR(F^2)$ = 0.126	$w = 1/[\sigma^2(F_o^2) + (0.063P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 0.94	$(\Delta/\sigma)_{max} < 0.001$
4431 reflections	$\Delta\rho_{max}$ = 0.25 e Å^{-3}
255 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 calculat-

ing *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}
C1	0.58415 (14)	0.3486 (3)	0.20261 (13)	0.0582 (5)
H1	0.5596	0.3982	0.1553	0.070*
C2	0.53522 (17)	0.3669 (3)	0.26485 (18)	0.0746 (7)
H2	0.4765	0.4274	0.2590	0.089*
C3	0.5719 (2)	0.2976 (3)	0.33449 (17)	0.0799 (8)
H3	0.5392	0.3120	0.3764	0.096*
C4	0.65702 (19)	0.2066 (3)	0.34277 (13)	0.0803 (8)
H4	0.6819	0.1589	0.3905	0.096*
C5	0.70677 (15)	0.1844 (3)	0.28114 (12)	0.0604 (6)
H5	0.7645	0.1218	0.2870	0.073*
C6	0.66952 (12)	0.2562 (2)	0.21152 (10)	0.0415 (4)
C7	0.67228 (13)	0.1855 (2)	0.07248 (11)	0.0487 (5)
H7	0.6030	0.1706	0.0582	0.058*
C8	0.82762 (12)	0.1991 (2)	0.06945 (10)	0.0387 (4)
C9	0.81868 (12)	0.2404 (2)	0.14362 (10)	0.0374 (4)
C10	0.98288 (12)	0.2842 (2)	0.18586 (10)	0.0374 (4)
C11	0.92328 (13)	0.2069 (2)	0.04677 (10)	0.0380 (4)
C12	1.09679 (12)	0.2904 (2)	0.08956 (10)	0.0374 (4)
C13	1.15729 (13)	0.1696 (2)	0.07040 (10)	0.0420 (4)
H13	1.1372	0.0639	0.0722	0.050*
C14	1.24807 (13)	0.2069 (2)	0.04857 (10)	0.0471 (5)
H14	1.2897	0.1268	0.0357	0.056*
C15	1.27571 (13)	0.3642 (2)	0.04617 (10)	0.0459 (5)
C16	1.21545 (13)	0.4855 (2)	0.06383 (10)	0.0453 (4)
H16	1.2352	0.5912	0.0611	0.054*
C17	1.12478 (13)	0.4475 (2)	0.08573 (10)	0.0418 (4)
H17	1.0829	0.5279	0.0978	0.050*
C18	1.15040 (13)	0.2194 (2)	0.26058 (11)	0.0473 (5)
H18A	1.1490	0.1454	0.2177	0.057*
H18B	1.1431	0.1579	0.3063	0.057*
C19	1.25144 (15)	0.3020 (3)	0.27618 (14)	0.0743 (7)
H19A	1.2586	0.3657	0.2319	0.111*
H19B	1.3042	0.2237	0.2854	0.111*
H19C	1.2558	0.3690	0.3212	0.111*
C20	1.04109 (15)	0.4238 (3)	0.30744 (12)	0.0630 (6)
H20A	0.9879	0.4987	0.2872	0.076*
H20B	1.1006	0.4853	0.3291	0.076*
C21	1.00919 (19)	0.3313 (3)	0.37215 (13)	0.0861 (8)
H21A	0.9473	0.2763	0.3526	0.129*
H21B	0.9992	0.4030	0.4129	0.129*
H21C	1.0606	0.2554	0.3924	0.129*
Cl1	1.38876 (4)	0.41047 (8)	0.01601 (3)	0.0754 (2)

N1	0.71771 (10)	0.23172 (18)	0.14620 (8)	0.0428 (4)
N2	0.73402 (11)	0.16444 (19)	0.02426 (9)	0.0472 (4)
N3	0.89291 (10)	0.28148 (17)	0.20361 (8)	0.0408 (4)
N4	1.00083 (10)	0.25229 (16)	0.11090 (8)	0.0370 (3)
N5	1.06403 (11)	0.32839 (18)	0.24143 (8)	0.0437 (4)
O1	0.94322 (9)	0.18633 (15)	−0.01760 (7)	0.0475 (3)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0452 (12)	0.0614 (14)	0.0699 (14)	0.0045 (9)	0.0153 (10)	0.0086 (11)
C2	0.0559 (14)	0.0691 (16)	0.108 (2)	0.0071 (11)	0.0394 (14)	−0.0124 (15)
C3	0.0720 (17)	0.103 (2)	0.0773 (18)	−0.0217 (15)	0.0456 (15)	−0.0334 (16)
C4	0.0768 (18)	0.123 (2)	0.0439 (13)	−0.0107 (15)	0.0184 (12)	−0.0016 (13)
C5	0.0483 (12)	0.0885 (16)	0.0450 (12)	0.0071 (11)	0.0100 (9)	0.0057 (11)
C6	0.0313 (9)	0.0529 (11)	0.0415 (10)	−0.0029 (8)	0.0097 (8)	−0.0020 (8)
C7	0.0340 (10)	0.0687 (13)	0.0414 (11)	−0.0069 (9)	0.0013 (8)	0.0012 (9)
C8	0.0345 (9)	0.0461 (11)	0.0346 (9)	−0.0039 (7)	0.0038 (7)	0.0010 (8)
C9	0.0335 (9)	0.0459 (11)	0.0320 (9)	−0.0021 (7)	0.0042 (7)	0.0013 (8)
C10	0.0362 (9)	0.0396 (10)	0.0359 (10)	−0.0009 (7)	0.0053 (8)	−0.0007 (8)
C11	0.0400 (10)	0.0393 (10)	0.0347 (10)	−0.0021 (7)	0.0071 (8)	0.0003 (8)
C12	0.0328 (9)	0.0450 (11)	0.0344 (9)	−0.0034 (7)	0.0066 (7)	−0.0001 (8)
C13	0.0430 (10)	0.0409 (10)	0.0420 (10)	−0.0016 (8)	0.0074 (8)	−0.0006 (8)
C14	0.0383 (10)	0.0579 (13)	0.0456 (11)	0.0040 (9)	0.0094 (8)	−0.0054 (9)
C15	0.0325 (9)	0.0667 (13)	0.0382 (10)	−0.0076 (9)	0.0060 (8)	0.0016 (9)
C16	0.0463 (11)	0.0475 (11)	0.0412 (10)	−0.0110 (9)	0.0060 (8)	0.0039 (8)
C17	0.0427 (10)	0.0413 (11)	0.0413 (10)	0.0006 (8)	0.0076 (8)	−0.0007 (8)
C18	0.0380 (10)	0.0579 (12)	0.0443 (11)	−0.0025 (8)	0.0031 (8)	0.0064 (9)
C19	0.0405 (12)	0.0941 (19)	0.0826 (18)	−0.0129 (11)	−0.0036 (12)	0.0131 (13)
C20	0.0507 (12)	0.0825 (16)	0.0513 (13)	−0.0017 (11)	−0.0023 (10)	−0.0180 (11)
C21	0.0800 (17)	0.133 (2)	0.0433 (13)	0.0161 (16)	0.0075 (12)	−0.0050 (14)
Cl1	0.0437 (3)	0.1085 (5)	0.0790 (4)	−0.0164 (3)	0.0242 (3)	0.0026 (3)
N1	0.0312 (8)	0.0601 (10)	0.0369 (8)	−0.0022 (7)	0.0060 (6)	0.0012 (7)
N2	0.0385 (9)	0.0640 (11)	0.0376 (8)	−0.0082 (7)	0.0032 (7)	−0.0024 (7)
N3	0.0337 (8)	0.0550 (10)	0.0334 (8)	−0.0005 (7)	0.0057 (6)	−0.0015 (7)
N4	0.0323 (8)	0.0443 (9)	0.0346 (8)	−0.0036 (6)	0.0068 (6)	−0.0018 (6)
N5	0.0367 (8)	0.0555 (10)	0.0364 (8)	−0.0009 (7)	0.0002 (6)	−0.0062 (7)
O1	0.0461 (7)	0.0629 (9)	0.0353 (7)	−0.0066 (6)	0.0125 (6)	−0.0058 (6)

Geometric parameters (Å, °)

C1—C6	1.373 (3)	C12—C13	1.381 (2)
C1—C2	1.381 (3)	C12—N4	1.448 (2)
C1—H1	0.9300	C13—C14	1.384 (2)
C2—C3	1.356 (4)	C13—H13	0.9300
C2—H2	0.9300	C14—C15	1.375 (3)
C3—C4	1.364 (3)	C14—H14	0.9300
C3—H3	0.9300	C15—C16	1.373 (3)
C4—C5	1.382 (3)	C15—Cl1	1.7469 (17)

C4—H4	0.9300	C16—C17	1.385 (2)
C5—C6	1.366 (3)	C16—H16	0.9300
C5—H5	0.9300	C17—H17	0.9300
C6—N1	1.428 (2)	C18—N5	1.470 (2)
C7—N2	1.302 (2)	C18—C19	1.508 (3)
C7—N1	1.375 (2)	C18—H18A	0.9700
C7—H7	0.9300	C18—H18B	0.9700
C8—C9	1.367 (2)	C19—H19A	0.9600
C8—N2	1.390 (2)	C19—H19B	0.9600
C8—C11	1.420 (2)	C19—H19C	0.9600
C9—N3	1.353 (2)	C20—N5	1.482 (2)
C9—N1	1.373 (2)	C20—C21	1.498 (3)
C10—N3	1.307 (2)	C20—H20A	0.9700
C10—N5	1.373 (2)	C20—H20B	0.9700
C10—N4	1.400 (2)	C21—H21A	0.9600
C11—O1	1.2155 (19)	C21—H21B	0.9600
C11—N4	1.435 (2)	C21—H21C	0.9600
C12—C17	1.377 (2)		
C6—C1—C2	119.1 (2)	C16—C15—Cl1	119.28 (15)
C6—C1—H1	120.4	C14—C15—Cl1	118.65 (15)
C2—C1—H1	120.4	C15—C16—C17	118.74 (17)
C3—C2—C1	120.6 (2)	C15—C16—H16	120.6
C3—C2—H2	119.7	C17—C16—H16	120.6
C1—C2—H2	119.7	C12—C17—C16	119.91 (16)
C2—C3—C4	119.7 (2)	C12—C17—H17	120.0
C2—C3—H3	120.2	C16—C17—H17	120.0
C4—C3—H3	120.2	N5—C18—C19	114.00 (17)
C3—C4—C5	120.9 (2)	N5—C18—H18A	108.8
C3—C4—H4	119.6	C19—C18—H18A	108.8
C5—C4—H4	119.6	N5—C18—H18B	108.8
C6—C5—C4	118.8 (2)	C19—C18—H18B	108.8
C6—C5—H5	120.6	H18A—C18—H18B	107.6
C4—C5—H5	120.6	C18—C19—H19A	109.5
C5—C6—C1	120.82 (18)	C18—C19—H19B	109.5
C5—C6—N1	120.01 (16)	H19A—C19—H19B	109.5
C1—C6—N1	119.15 (17)	C18—C19—H19C	109.5
N2—C7—N1	114.60 (15)	H19A—C19—H19C	109.5
N2—C7—H7	122.7	H19B—C19—H19C	109.5
N1—C7—H7	122.7	N5—C20—C21	115.92 (19)
C9—C8—N2	111.13 (15)	N5—C20—H20A	108.3
C9—C8—C11	119.79 (15)	C21—C20—H20A	108.3
N2—C8—C11	128.91 (16)	N5—C20—H20B	108.3
N3—C9—C8	127.98 (15)	C21—C20—H20B	108.3
N3—C9—N1	125.78 (15)	H20A—C20—H20B	107.4
C8—C9—N1	106.24 (14)	C20—C21—H21A	109.5
N3—C10—N5	119.41 (15)	C20—C21—H21B	109.5
N3—C10—N4	123.17 (15)	H21A—C21—H21B	109.5
N5—C10—N4	117.32 (14)	C20—C21—H21C	109.5
O1—C11—C8	128.30 (16)	H21A—C21—H21C	109.5

O1—C11—N4	120.33 (15)	H21B—C21—H21C	109.5
C8—C11—N4	111.31 (14)	C9—N1—C7	104.90 (14)
C17—C12—C13	120.78 (16)	C9—N1—C6	128.28 (14)
C17—C12—N4	119.37 (15)	C7—N1—C6	126.74 (14)
C13—C12—N4	119.80 (15)	C7—N2—C8	103.13 (15)
C12—C13—C14	119.57 (17)	C10—N3—C9	114.05 (14)
C12—C13—H13	120.2	C10—N4—C11	123.56 (13)
C14—C13—H13	120.2	C10—N4—C12	121.07 (13)
C15—C14—C13	118.96 (17)	C11—N4—C12	114.53 (13)
C15—C14—H14	120.5	C10—N5—C18	119.17 (15)
C13—C14—H14	120.5	C10—N5—C20	116.20 (15)
C16—C15—C14	122.02 (16)	C18—N5—C20	115.46 (15)
C6—C1—C2—C3	1.4 (3)	C5—C6—N1—C9	−47.3 (3)
C1—C2—C3—C4	−1.1 (4)	C1—C6—N1—C9	134.52 (19)
C2—C3—C4—C5	0.2 (4)	C5—C6—N1—C7	128.9 (2)
C3—C4—C5—C6	0.4 (4)	C1—C6—N1—C7	−49.2 (3)
C4—C5—C6—C1	−0.1 (3)	N1—C7—N2—C8	0.1 (2)
C4—C5—C6—N1	−178.23 (19)	C9—C8—N2—C7	−0.1 (2)
C2—C1—C6—C5	−0.8 (3)	C11—C8—N2—C7	−175.35 (18)
C2—C1—C6—N1	177.37 (18)	N5—C10—N3—C9	178.26 (15)
N2—C8—C9—N3	179.92 (17)	N4—C10—N3—C9	1.8 (2)
C11—C8—C9—N3	−4.4 (3)	C8—C9—N3—C10	1.7 (3)
N2—C8—C9—N1	0.2 (2)	N1—C9—N3—C10	−178.59 (16)
C11—C8—C9—N1	175.87 (15)	N3—C10—N4—C11	−2.7 (3)
C9—C8—C11—O1	−173.96 (17)	N5—C10—N4—C11	−179.20 (15)
N2—C8—C11—O1	0.9 (3)	N3—C10—N4—C12	166.22 (15)
C9—C8—C11—N4	3.1 (2)	N5—C10—N4—C12	−10.3 (2)
N2—C8—C11—N4	177.92 (16)	O1—C11—N4—C10	177.36 (16)
C17—C12—C13—C14	1.3 (3)	C8—C11—N4—C10	0.0 (2)
N4—C12—C13—C14	178.75 (15)	O1—C11—N4—C12	7.8 (2)
C12—C13—C14—C15	−0.3 (3)	C8—C11—N4—C12	−169.53 (14)
C13—C14—C15—C16	−0.8 (3)	C17—C12—N4—C10	−66.8 (2)
C13—C14—C15—Cl1	−178.29 (14)	C13—C12—N4—C10	115.73 (18)
C14—C15—C16—C17	0.9 (3)	C17—C12—N4—C11	103.11 (18)
Cl1—C15—C16—C17	178.35 (13)	C13—C12—N4—C11	−74.41 (19)
C13—C12—C17—C16	−1.2 (3)	N3—C10—N5—C18	124.16 (18)
N4—C12—C17—C16	−178.68 (15)	N4—C10—N5—C18	−59.2 (2)
C15—C16—C17—C12	0.1 (3)	N3—C10—N5—C20	−21.3 (2)
N3—C9—N1—C7	−179.88 (17)	N4—C10—N5—C20	155.38 (16)
C8—C9—N1—C7	−0.12 (19)	C19—C18—N5—C10	142.09 (18)
N3—C9—N1—C6	−3.0 (3)	C19—C18—N5—C20	−72.2 (2)
C8—C9—N1—C6	176.78 (16)	C21—C20—N5—C10	82.7 (2)
N2—C7—N1—C9	0.0 (2)	C21—C20—N5—C18	−64.0 (2)
N2—C7—N1—C6	−176.93 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21A···N3	0.96	2.57	3.096 (3)	115

C16—H16···N2^{i}	0.93	2.61	3.443 (2)	149
C13—H13···O1^{ii}	0.93	2.47	3.340 (2)	155
C3—H3···O1^{iii}	0.93	2.45	3.371 (3)	172

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

Fig. 1

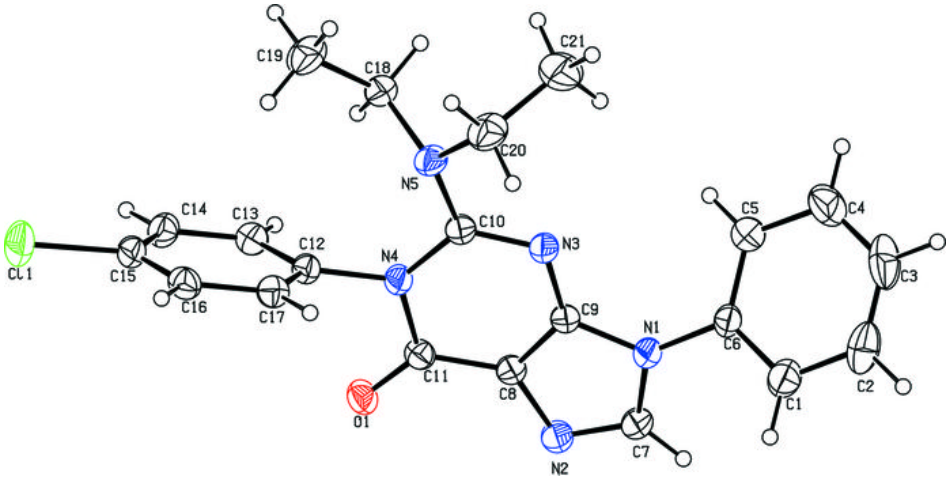
C19
C18
C21
C20
N5
C14
C13
C10
C5
C4
C12
N4
N3
Cl1
C15
C16
C17
C9
N1
C6
C3
C11
C8
C2
O1
C1
N2
C7

Fig. 2