Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-(4-Chlorophenyl)-2-(diisobutylamino)-4-oxo-5-phenyl-4,5-dihydro-3*H*-pyrrolo[3,2-*d*]pyrimidine-7-carbonitrile

Ping He,[a] Aihua Zheng,[b]* Chang-Quan Cai[a] and Chuan-Lin Fang[a]

[a]Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, Central China Normal University, Wuhan 430079, People's Republic of China, and [b]Key Laboratory of Pesticides & Chemical Biology, Ministry of Education, Central China Normal University, Wuhan 430079, People's Republic of China, and Department of Medicinal Chemistry, Yunyang Medical College, Shiyan 442000, People's Republic of China
Correspondence e-mail: huyangg111@yahoo.com.cn

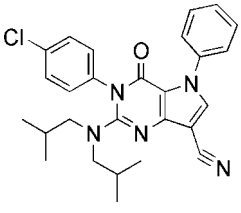
Received 4 June 2007; accepted 10 June 2007

Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.005 Å; disorder in main residue; R factor = 0.064; wR factor = 0.169; data-to-parameter ratio = 14.3.

A tandem aza-Wittig reaction of ethyl 3-triphenylphosphoranylideneamino-4-cyano-1-phenyl-1*H*-pyrrole-2-carboxylate with 4-chlorophenyl isocyanate and diisobutylamine produced the title compound, $C_{27}H_{28}ClN_5O$. In the molecule, the angles between the fused-ring system and the two benzene rings are 51.66 (2) and 65.79 (2)°. Intramolecular C—H···N hydrogen bonds determine the conformation of the molecule. The packing of the molecules in the crystal structure is governed mainly by intermolecular C—H···N hydrogen-bonding interactions. There are no π–π interactions.

Related literature

Related biological activity is described by Kondo *et al.* (1986) and pharmaceutical activity is described by Bayomi *et al.* (1986). For related literature, see: Ding *et al.* (2004); Hu *et al.* (2005); Xu *et al.* (2005); Zheng *et al.* (2006).



Experimental

Crystal data

$C_{27}H_{28}ClN_5O$
M_r = 473.99
Triclinic, $P\overline{1}$
a = 8.7272 (6) Å
b = 12.7635 (9) Å
c = 13.3411 (9) Å
α = 103.821 (1)°
β = 107.828 (1)°
γ = 106.684 (1)°
V = 1265.14 (15) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.18 mm^{-1}
T = 298 (2) K
0.20 × 0.20 × 0.10 mm

Data collection

Bruker SMART 4K CCD area-detector diffractometer
Absorption correction: none
9851 measured reflections
4890 independent reflections
3633 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.170
S = 1.01
4890 reflections
341 parameters
7 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.31 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C24—H24A···N3	0.97	2.35	2.694 (3)	100
C23—H23B···N5	0.96	2.57	2.995 (11)	107
C20—H20A···N4	0.97	2.54	2.958 (3)	106
C7—H7···N2^{i}	0.93	2.56	3.202 (4)	126

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

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).

We gratefully acknowledge financial support of this work by the National Natural Science Foundation of China (project No. 20102001) and the Science Research Project of Yunyang Medical College (No. 2006QDJ16).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: WN2151).

References

Bayomi, S. M., El-Emam, A. A., Moustafa, M. A. & El-Kerdawy, M. M. (1986). T*aiwan Yaoxue Zazhi*, **38**, 129–135. (In Chinese.)
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.
Hu, Y.-G., Li, G.-H., Tian, J.-H., Ding, M.-W. & He, H.-W. (2005). *Acta Cryst.* E**61**, o3266–o3268.
Kondo, T., Okamoto, K., Ohgi, T. & Goto, T. (1986). *Tetrahedron*, **42**, 207–213.
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.
Spek, A. L. (2003). *J. Appl. Cryst.* **36**, 7–13.
Xu, S.-Z., Cao, M.-H., Hu, Y.-G., Ding, M.-W. & Xiao, W.-J. (2005). *Acta Cryst.* E**61**, o2789–o2790.
Zheng, A., Xu, J. & Hu, Y.-G. (2006). *Acta Cryst.* E**62**, o3710–o3711.

 doi:10.1107/S1600536807028383

supplementary materials

Acta Cryst. (2007). E**63**, o3185 [**doi:10.1107/S1600536807028383**]

3-(4-Chlorophenyl)-2-(diisobutylamino)-4-oxo-5-phenyl-4,5-dihydro-3*H*-pyrrolo[3,2-*d*]pyrimidine-7-carbonitrile

P. He, A. Zheng, C.-Q. Cai and C.-L. Fang

Comment

Derivatives of pyrimidinone are attracting increasing attention in the synthetic chemistry community because of the important role played by such systems in many natural products, also in antibiotics and drugs (Kondo *et al.*, 1986; Bayomi *et al.*, 1986; Ding *et al.*, 2004). In recent years, we have been engaged in the preparation of derivatives of heterocycles using the aza-Wittig reaction. Some related X-ray crystal structure reports for pyrimidinone derivatives have been published (Zheng *et al.*, 2006; Hu *et al.*, 2005; Xu *et al.*, 2005). Here, the structure of the title compound, which may be used as a new precursor for obtaining bioactive molecules, is reported (Fig. 1). The bond lengths and angles are unexceptional. Rings A (atoms N1/C7/C8/C9/C10), B (C9/C10/C12/N3/C13/N4), C (C1—C6), D (C14—C19) are, of course, planar and the dihedral angles between them are A/B = 2.80 (14)°, A/C = 51.66 (2)°, B/D = 65.79 (2)°. C21, C22, C23 and attached hydrogen atoms are disordered over two sites, with refined occupancies of 0.654 (8) and 0.346 (8). Intramolecular C—H···N hydrogen bonds determine the conformation of the molecule. As can be seen from the packing diagram (Fig. 2), intermolecular C—H···N hydrogen bonds (Table 1) link the molecules. There are no π-π interactions.

Experimental

To a solution of ethyl 3-triphenylphosphoranylideneamino- 4-cyano-1-phenyl-1*H*-pyrrole-2-carboxylate(1.55 g, 3 mmol) in anhydrous dichloromethane (15 ml) was added *p*-chlorophenyl isocyanate (0.46 g, 3 mmol) under dry nitrogen at room temperature. The reaction mixture was left unstirred for 3 h at room temperature and then the solvent was removed under reduced pressure; diethyl ether-petroleum ether (1:2 *v*/*v*, 20 ml) was added to precipitate triphenylphosphine oxide. After filtration, the solution of the carbodiimide (3 mmol) was added to a solution of diisobutylamine (3 mmol) in anhydrous dichloromethane (15 ml). After stirring the reaction mixture for 6 h, the solvent was removed under reduced pressure and the residue was recrystallized from ethanol to give the title compound, in a yield of 94%. Crystals suitable for single-crystal X-ray diffraction were obtained by recrystallization from a mixed solvent of ethanol and dichloromethane (1:1 *v*/*v*) at room temperature.

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 = 0.98 Å, U_{iso} = 1.2U_{eq} (C) for CH, 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

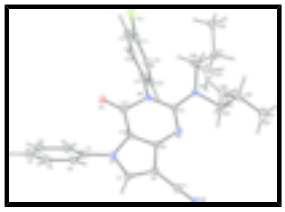


Fig. 1. The molecular structure of the title compound, showing the atom-labeling scheme. Only the major disorder component is shown.

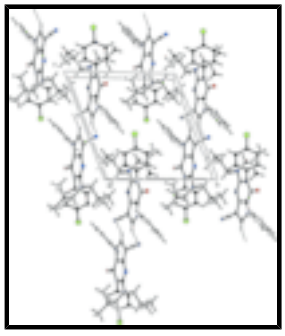


Fig. 2. The packing in the crystal structure, showing the C—H···N hydrogen bonds as dashed lines. Only the major disorder component is shown.

3-(4-Chlorophenyl)-2-(diisobutylamino)-4-oxo-5-phenyl-4,5-dihydro- 3*H*-pyrrolo[3,2-*d*]pyrimidine-7-carbonitrile

Crystal data

$C_{27}H_{28}ClN_5O$	$Z = 2$
$M_r = 473.99$	$F_{000} = 500$
Triclinic, $P\overline{1}$	$D_x = 1.244$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 8.7272$ (6) Å	Cell parameters from 2745 reflections
$b = 12.7635$ (9) Å	$\theta = 2.7$–23.6º
$c = 13.3411$ (9) Å	$\mu = 0.18$ mm^{-1}
$\alpha = 103.821$ (1)º	$T = 298$ (2) K
$\beta = 107.828$ (1)º	Block, colourless
$\gamma = 106.684$ (1)º	0.20 × 0.20 × 0.10 mm
$V = 1265.14$ (15) Å^3	

Data collection

Bruker SMART 4K CCD area-detector diffractometer	3633 reflections with $I > 2\sigma(I)$
Radiation source: fine-focus sealed tube	$R_{int} = 0.031$
Monochromator: graphite	$\theta_{max} = 26.0$º
$T = 298$(2) K	$\theta_{min} = 1.7$º
φ and ω scans	$h = -9 \rightarrow 10$
Absorption correction: none	$k = -15 \rightarrow 15$
9851 measured reflections	$l = -15 \rightarrow 16$
4890 independent reflections	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.064$	H-atom parameters constrained
$wR(F^2) = 0.170$	$w = 1/[\sigma^2(F_o^2) + (0.0719P)^2 + 0.5686P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.01$	$(\Delta/\sigma)_{max} = 0.001$
4890 reflections	$\Delta\rho_{max} = 0.34$ e Å^{-3}
341 parameters	$\Delta\rho_{min} = -0.31$ e Å^{-3}
7 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}	Occ. (<1)
C1	0.6572 (4)	0.2077 (2)	−0.3739 (2)	0.0583 (7)	
C2	0.8171 (4)	0.1998 (3)	−0.3345 (3)	0.0717 (8)	
H2	0.8463	0.1702	−0.2773	0.086*	
C3	0.9347 (5)	0.2372 (3)	−0.3822 (4)	0.0979 (13)	
H3	1.0439	0.2332	−0.3560	0.117*	
C4	0.8914 (7)	0.2792 (4)	−0.4661 (4)	0.1122 (16)	
H4	0.9708	0.3037	−0.4972	0.135*	
C5	0.7319 (8)	0.2857 (4)	−0.5054 (3)	0.1098 (15)	
H5	0.7033	0.3143	−0.5635	0.132*	
C6	0.6124 (5)	0.2502 (3)	−0.4597 (2)	0.0789 (9)	
H6	0.5038	0.2550	−0.4864	0.095*	
C7	0.3635 (3)	0.0923 (2)	−0.3943 (2)	0.0576 (7)	
H7	0.3168	0.0582	−0.4725	0.069*	
C8	0.2730 (3)	0.0730 (2)	−0.3284 (2)	0.0524 (6)	
C9	0.3922 (3)	0.1419 (2)	−0.2150 (2)	0.0465 (6)	
C10	0.5506 (3)	0.1993 (2)	−0.2167 (2)	0.0458 (6)	
C11	0.0965 (4)	−0.0033 (3)	−0.3641 (2)	0.0588 (7)	

C12	0.6998 (3)	0.2731 (2)	−0.1157 (2)	0.0474 (6)	
C13	0.4921 (3)	0.2192 (2)	−0.0253 (2)	0.0452 (6)	
C14	0.8127 (3)	0.3093 (2)	0.08604 (19)	0.0452 (6)	
C15	0.8359 (3)	0.2254 (2)	0.1313 (2)	0.0539 (6)	
H15	0.7576	0.1477	0.0944	0.065*	
C16	0.9774 (4)	0.2580 (3)	0.2325 (2)	0.0619 (7)	
H16	0.9936	0.2029	0.2647	0.074*	
C17	1.0926 (3)	0.3731 (3)	0.2840 (2)	0.0610 (7)	
C18	1.0724 (3)	0.4560 (3)	0.2376 (2)	0.0581 (7)	
H18	1.1532	0.5332	0.2733	0.070*	
C19	0.9316 (3)	0.4243 (2)	0.1376 (2)	0.0494 (6)	
H19	0.9169	0.4796	0.1052	0.059*	
C20	0.5447 (3)	0.3511 (2)	0.1614 (2)	0.0586 (7)	
H20A	0.6423	0.3999	0.1510	0.070*	0.654 (8)
H20B	0.5915	0.3435	0.2340	0.070*	0.654 (8)
H20C	0.5014	0.3445	0.2194	0.070*	0.346 (8)
H20D	0.6700	0.3725	0.1957	0.070*	0.346 (8)
C21	0.4228 (6)	0.4153 (4)	0.1662 (4)	0.0573 (15)	0.654 (8)
H21A	0.3360	0.3718	0.1893	0.069*	0.654 (8)
C22	0.5259 (10)	0.5372 (6)	0.2575 (6)	0.084 (2)	0.654 (8)
H22A	0.6041	0.5850	0.2338	0.125*	0.654 (8)
H22B	0.5921	0.5309	0.3263	0.125*	0.654 (8)
H22C	0.4465	0.5724	0.2696	0.125*	0.654 (8)
C23	0.3231 (13)	0.4174 (11)	0.0508 (7)	0.107 (5)	0.654 (8)
H23A	0.2257	0.4376	0.0522	0.161*	0.654 (8)
H23B	0.2815	0.3415	−0.0058	0.161*	0.654 (8)
H23C	0.3996	0.4745	0.0338	0.161*	0.654 (8)
C21'	0.5166 (11)	0.4456 (6)	0.1302 (7)	0.066 (3)	0.346 (8)
H21B	0.5812	0.4620	0.0834	0.080*	0.346 (8)
C22'	0.601 (2)	0.5543 (10)	0.2397 (11)	0.108 (5)	0.346 (8)
H22D	0.5362	0.5428	0.2856	0.161*	0.346 (8)
H22E	0.5994	0.6223	0.2211	0.161*	0.346 (8)
H22F	0.7195	0.5654	0.2804	0.161*	0.346 (8)
C23'	0.3252 (13)	0.4234 (14)	0.0624 (12)	0.063 (6)	0.346 (8)
H23D	0.2529	0.3879	0.0966	0.094*	0.346 (8)
H23E	0.2873	0.3721	−0.0137	0.094*	0.346 (8)
H23F	0.3159	0.4965	0.0621	0.094*	0.346 (8)
C24	0.3096 (3)	0.1501 (2)	0.0690 (2)	0.0563 (7)	
H24A	0.2697	0.0782	0.0058	0.068*	
H24B	0.2192	0.1813	0.0549	0.068*	
C25	0.3327 (5)	0.1218 (3)	0.1749 (3)	0.0758 (9)	
H25	0.3541	0.1921	0.2356	0.091*	
C26	0.4823 (5)	0.0853 (4)	0.2111 (3)	0.0942 (11)	
H26A	0.4693	0.0211	0.1499	0.141*	
H26B	0.4842	0.0614	0.2743	0.141*	
H26C	0.5898	0.1500	0.2325	0.141*	
C27	0.1616 (5)	0.0258 (4)	0.1541 (4)	0.1064 (14)	
H27A	0.1414	−0.0451	0.0974	0.160*	
H27B	0.0667	0.0501	0.1290	0.160*	

H27C	0.1693	0.0121	0.2228	0.160*
Cl1	1.27079 (11)	0.41284 (9)	0.41014 (7)	0.0982 (4)
N1	0.5307 (3)	0.16805 (19)	−0.32917 (17)	0.0524 (5)
N2	−0.0439 (3)	−0.0646 (3)	−0.3894 (2)	0.0774 (8)
N3	0.3580 (2)	0.15372 (19)	−0.12032 (17)	0.0497 (5)
N4	0.6615 (2)	0.27220 (18)	−0.01855 (16)	0.0462 (5)
N5	0.4693 (3)	0.23473 (18)	0.07389 (16)	0.0501 (5)
O1	0.8471 (2)	0.32784 (18)	−0.10456 (16)	0.0667 (5)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0707 (18)	0.0551 (16)	0.0468 (15)	0.0199 (14)	0.0289 (14)	0.0130 (12)
C2	0.0692 (19)	0.0645 (19)	0.086 (2)	0.0272 (16)	0.0413 (17)	0.0191 (16)
C3	0.092 (3)	0.086 (3)	0.123 (3)	0.031 (2)	0.069 (3)	0.020 (2)
C4	0.133 (4)	0.099 (3)	0.099 (3)	0.016 (3)	0.082 (3)	0.018 (3)
C5	0.158 (4)	0.101 (3)	0.061 (2)	0.022 (3)	0.058 (3)	0.028 (2)
C6	0.098 (2)	0.083 (2)	0.0471 (17)	0.0248 (19)	0.0292 (17)	0.0220 (16)
C7	0.0574 (16)	0.0665 (17)	0.0382 (14)	0.0220 (14)	0.0110 (12)	0.0144 (12)
C8	0.0476 (14)	0.0623 (16)	0.0398 (13)	0.0215 (12)	0.0098 (11)	0.0158 (12)
C9	0.0461 (13)	0.0525 (14)	0.0407 (13)	0.0230 (11)	0.0141 (11)	0.0159 (11)
C10	0.0476 (13)	0.0510 (14)	0.0389 (13)	0.0222 (11)	0.0155 (11)	0.0151 (11)
C11	0.0538 (17)	0.0764 (19)	0.0409 (14)	0.0235 (15)	0.0128 (12)	0.0228 (13)
C12	0.0469 (14)	0.0478 (14)	0.0451 (14)	0.0181 (11)	0.0163 (11)	0.0158 (11)
C13	0.0444 (13)	0.0487 (14)	0.0435 (13)	0.0233 (11)	0.0154 (11)	0.0149 (11)
C14	0.0419 (13)	0.0529 (14)	0.0389 (12)	0.0222 (11)	0.0125 (10)	0.0135 (11)
C15	0.0500 (14)	0.0516 (15)	0.0530 (15)	0.0213 (12)	0.0140 (12)	0.0141 (12)
C16	0.0609 (17)	0.0708 (19)	0.0602 (17)	0.0329 (15)	0.0182 (14)	0.0330 (15)
C17	0.0485 (15)	0.082 (2)	0.0450 (15)	0.0242 (14)	0.0092 (12)	0.0242 (14)
C18	0.0480 (14)	0.0600 (16)	0.0472 (15)	0.0110 (12)	0.0087 (12)	0.0134 (13)
C19	0.0477 (14)	0.0484 (14)	0.0483 (14)	0.0188 (11)	0.0149 (11)	0.0167 (12)
C20	0.0548 (15)	0.0676 (18)	0.0500 (15)	0.0289 (14)	0.0208 (13)	0.0100 (13)
C21	0.063 (3)	0.063 (3)	0.065 (3)	0.034 (2)	0.037 (2)	0.030 (2)
C22	0.097 (5)	0.066 (4)	0.103 (5)	0.041 (3)	0.057 (4)	0.023 (3)
C23	0.127 (10)	0.163 (11)	0.114 (9)	0.116 (8)	0.067 (7)	0.090 (8)
C21'	0.078 (6)	0.069 (6)	0.088 (7)	0.041 (5)	0.056 (5)	0.041 (5)
C22'	0.125 (12)	0.059 (7)	0.162 (14)	0.046 (8)	0.082 (11)	0.035 (8)
C23'	0.061 (10)	0.062 (9)	0.070 (10)	0.015 (7)	0.036 (8)	0.030 (7)
C24	0.0582 (16)	0.0648 (17)	0.0486 (15)	0.0251 (13)	0.0239 (13)	0.0207 (13)
C25	0.093 (2)	0.084 (2)	0.068 (2)	0.0432 (19)	0.0426 (18)	0.0344 (18)
C26	0.118 (3)	0.099 (3)	0.090 (3)	0.060 (2)	0.042 (2)	0.053 (2)
C27	0.111 (3)	0.135 (4)	0.117 (3)	0.050 (3)	0.072 (3)	0.082 (3)
Cl1	0.0706 (5)	0.1232 (8)	0.0647 (5)	0.0239 (5)	−0.0087 (4)	0.0374 (5)
N1	0.0533 (12)	0.0604 (13)	0.0385 (11)	0.0190 (11)	0.0168 (10)	0.0155 (10)
N2	0.0567 (16)	0.098 (2)	0.0611 (16)	0.0145 (14)	0.0131 (12)	0.0334 (15)
N3	0.0417 (11)	0.0598 (13)	0.0412 (11)	0.0191 (10)	0.0120 (9)	0.0140 (10)
N4	0.0411 (11)	0.0522 (12)	0.0381 (11)	0.0170 (9)	0.0106 (9)	0.0126 (9)
N5	0.0482 (12)	0.0577 (13)	0.0399 (11)	0.0214 (10)	0.0159 (9)	0.0118 (10)

O1	0.0501 (11)	0.0781 (13)	0.0556 (11)	0.0079 (10)	0.0209 (9)	0.0185 (10)

Geometric parameters (Å, °)

C1—C2	1.375 (4)	C20—C21'	1.427 (7)
C1—C6	1.379 (4)	C20—N5	1.464 (3)
C1—N1	1.434 (3)	C20—C21	1.524 (4)
C2—C3	1.397 (5)	C20—H20A	0.9700
C2—H2	0.9300	C20—H20B	0.9700
C3—C4	1.351 (6)	C20—H20C	0.9700
C3—H3	0.9300	C20—H20D	0.9700
C4—C5	1.364 (6)	C21—C22	1.528 (6)
C4—H4	0.9300	C21—C23	1.529 (7)
C5—C6	1.384 (5)	C21—H21A	0.9800
C5—H5	0.9300	C22—H22A	0.9600
C6—H6	0.9300	C22—H22B	0.9600
C7—N1	1.353 (3)	C22—H22C	0.9600
C7—C8	1.369 (4)	C23—H23A	0.9600
C7—H7	0.9300	C23—H23B	0.9600
C8—C11	1.420 (4)	C23—H23C	0.9600
C8—C9	1.421 (3)	C21'—C23'	1.539 (9)
C9—N3	1.368 (3)	C21'—C22'	1.545 (9)
C9—C10	1.376 (3)	C21'—H21B	0.9800
C10—N1	1.398 (3)	C22'—H22D	0.9600
C10—C12	1.419 (3)	C22'—H22E	0.9600
C11—N2	1.139 (3)	C22'—H22F	0.9600
C12—O1	1.217 (3)	C23'—H23D	0.9600
C12—N4	1.435 (3)	C23'—H23E	0.9600
C13—N3	1.303 (3)	C23'—H23F	0.9600
C13—N5	1.373 (3)	C24—N5	1.470 (3)
C13—N4	1.403 (3)	C24—C25	1.509 (4)
C14—C19	1.382 (3)	C24—H24A	0.9700
C14—C15	1.383 (4)	C24—H24B	0.9700
C14—N4	1.452 (3)	C25—C26	1.492 (5)
C15—C16	1.391 (4)	C25—C27	1.531 (5)
C15—H15	0.9300	C25—H25	0.9800
C16—C17	1.374 (4)	C26—H26A	0.9600
C16—H16	0.9300	C26—H26B	0.9600
C17—C18	1.374 (4)	C26—H26C	0.9600
C17—Cl1	1.745 (3)	C27—H27A	0.9600
C18—C19	1.381 (3)	C27—H27B	0.9600
C18—H18	0.9300	C27—H27C	0.9600
C19—H19	0.9300		
C2—C1—C6	120.9 (3)	H20B—C20—H20C	45.8
C2—C1—N1	120.6 (3)	C21'—C20—H20D	107.7
C6—C1—N1	118.4 (3)	N5—C20—H20D	107.2
C1—C2—C3	118.6 (3)	C21—C20—H20D	135.3
C1—C2—H2	120.7	H20A—C20—H20D	46.9
C3—C2—H2	120.7	H20B—C20—H20D	62.9

C4—C3—C2	120.6 (4)	H20C—C20—H20D	106.9
C4—C3—H3	119.7	C20—C21—C22	109.4 (4)
C2—C3—H3	119.7	C20—C21—C23	112.2 (5)
C3—C4—C5	120.4 (4)	C22—C21—C23	113.2 (5)
C3—C4—H4	119.8	C20—C21—H20C	37.8
C5—C4—H4	119.8	C22—C21—H20C	101.6
C4—C5—C6	120.6 (4)	C23—C21—H20C	142.0
C4—C5—H5	119.7	C20—C21—H21A	107.2
C6—C5—H5	119.7	C22—C21—H21A	107.2
C1—C6—C5	118.8 (4)	C23—C21—H21A	107.2
C1—C6—H6	120.6	H20C—C21—H21A	74.9
C5—C6—H6	120.6	C20—C21'—C23'	115.8 (8)
N1—C7—C8	110.2 (2)	C20—C21'—C22'	107.1 (8)
N1—C7—H7	124.9	C23'—C21'—C22'	111.4 (7)
C8—C7—H7	124.9	C20—C21'—H21B	107.4
C7—C8—C11	127.5 (2)	C23'—C21'—H21B	107.4
C7—C8—C9	106.6 (2)	C22'—C21'—H21B	107.4
C11—C8—C9	125.9 (2)	C21'—C22'—H22D	109.5
N3—C9—C10	125.2 (2)	C21'—C22'—H22E	109.5
N3—C9—C8	127.3 (2)	H22D—C22'—H22E	109.5
C10—C9—C8	107.4 (2)	C21'—C22'—H22F	109.5
C9—C10—N1	107.9 (2)	H22D—C22'—H22F	109.5
C9—C10—C12	121.4 (2)	H22E—C22'—H22F	109.5
N1—C10—C12	130.6 (2)	C21'—C23'—H23D	109.5
N2—C11—C8	177.8 (3)	C21'—C23'—H23E	109.5
O1—C12—C10	128.5 (2)	H23D—C23'—H23E	109.5
O1—C12—N4	120.4 (2)	C21'—C23'—H23F	109.5
C10—C12—N4	111.0 (2)	H23D—C23'—H23F	109.5
N3—C13—N5	119.1 (2)	H23E—C23'—H23F	109.5
N3—C13—N4	123.1 (2)	N5—C24—C25	113.9 (2)
N5—C13—N4	117.8 (2)	N5—C24—H24A	108.8
C19—C14—C15	121.0 (2)	C25—C24—H24A	108.8
C19—C14—N4	121.1 (2)	N5—C24—H24B	108.8
C15—C14—N4	117.9 (2)	C25—C24—H24B	108.8
C14—C15—C16	119.6 (3)	H24A—C24—H24B	107.7
C14—C15—H15	120.2	C26—C25—C24	113.1 (3)
C16—C15—H15	120.2	C26—C25—C27	110.8 (3)
C17—C16—C15	118.8 (3)	C24—C25—C27	108.1 (3)
C17—C16—H16	120.6	C26—C25—H25	108.2
C15—C16—H16	120.6	C24—C25—H25	108.2
C18—C17—C16	121.7 (2)	C27—C25—H25	108.2
C18—C17—Cl1	119.8 (2)	C25—C26—H26A	109.5
C16—C17—Cl1	118.5 (2)	C25—C26—H26B	109.5
C17—C18—C19	119.7 (3)	H26A—C26—H26B	109.5
C17—C18—H18	120.2	C25—C26—H26C	109.5
C19—C18—H18	120.2	H26A—C26—H26C	109.5
C18—C19—C14	119.2 (2)	H26B—C26—H26C	109.5
C18—C19—H19	120.4	C25—C27—H27A	109.5
C14—C19—H19	120.4	C25—C27—H27B	109.5

C21'—C20—N5	118.7 (4)	H27A—C27—H27B	109.5
C21'—C20—C21	43.4 (3)	C25—C27—H27C	109.5
N5—C20—C21	116.8 (3)	H27A—C27—H27C	109.5
C21'—C20—H20A	66.6	H27B—C27—H27C	109.5
N5—C20—H20A	108.1	C7—N1—C10	107.9 (2)
C21—C20—H20A	108.1	C7—N1—C1	123.4 (2)
C21'—C20—H20B	132.5	C10—N1—C1	128.7 (2)
N5—C20—H20B	108.1	C13—N3—C9	115.4 (2)
C21—C20—H20B	108.1	C13—N4—C12	123.18 (19)
H20A—C20—H20B	107.3	C13—N4—C14	120.53 (19)
C21'—C20—H20C	108.0	C12—N4—C14	115.23 (18)
N5—C20—H20C	107.8	C13—N5—C20	121.0 (2)
C21—C20—H20C	68.0	C13—N5—C24	116.4 (2)
H20A—C20—H20C	140.9	C20—N5—C24	116.6 (2)
C6—C1—C2—C3	0.8 (5)	N5—C20—C21'—C22'	176.7 (7)
N1—C1—C2—C3	178.6 (3)	C21—C20—C21'—C22'	77.0 (8)
C1—C2—C3—C4	−0.7 (5)	N5—C24—C25—C26	−52.2 (4)
C2—C3—C4—C5	0.1 (6)	N5—C24—C25—C27	−175.3 (3)
C3—C4—C5—C6	0.4 (7)	C8—C7—N1—C10	0.1 (3)
C2—C1—C6—C5	−0.4 (5)	C8—C7—N1—C1	−178.5 (2)
N1—C1—C6—C5	−178.3 (3)	C9—C10—N1—C7	−0.5 (3)
C4—C5—C6—C1	−0.2 (6)	C12—C10—N1—C7	178.1 (3)
N1—C7—C8—C11	−177.9 (3)	C9—C10—N1—C1	178.0 (2)
N1—C7—C8—C9	0.3 (3)	C12—C10—N1—C1	−3.4 (4)
C7—C8—C9—N3	177.4 (2)	C2—C1—N1—C7	−127.9 (3)
C11—C8—C9—N3	−4.3 (4)	C6—C1—N1—C7	49.9 (4)
C7—C8—C9—C10	−0.6 (3)	C2—C1—N1—C10	53.7 (4)
C11—C8—C9—C10	177.6 (3)	C6—C1—N1—C10	−128.4 (3)
N3—C9—C10—N1	−177.4 (2)	N5—C13—N3—C9	−179.4 (2)
C8—C9—C10—N1	0.7 (3)	N4—C13—N3—C9	−1.6 (3)
N3—C9—C10—C12	3.8 (4)	C10—C9—N3—C13	−4.7 (4)
C8—C9—C10—C12	−178.1 (2)	C8—C9—N3—C13	177.6 (2)
C7—C8—C11—N2	156 (9)	N3—C13—N4—C12	8.9 (4)
C9—C8—C11—N2	−22 (9)	N5—C13—N4—C12	−173.2 (2)
C9—C10—C12—O1	179.2 (3)	N3—C13—N4—C14	−158.8 (2)
N1—C10—C12—O1	0.8 (5)	N5—C13—N4—C14	19.1 (3)
C9—C10—C12—N4	3.0 (3)	O1—C12—N4—C13	174.5 (2)
N1—C10—C12—N4	−175.5 (2)	C10—C12—N4—C13	−9.0 (3)
C19—C14—C15—C16	2.5 (4)	O1—C12—N4—C14	−17.3 (3)
N4—C14—C15—C16	−178.8 (2)	C10—C12—N4—C14	159.3 (2)
C14—C15—C16—C17	−1.2 (4)	C19—C14—N4—C13	−122.7 (3)
C15—C16—C17—C18	−0.7 (4)	C15—C14—N4—C13	58.6 (3)
C15—C16—C17—Cl1	−179.3 (2)	C19—C14—N4—C12	68.6 (3)
C16—C17—C18—C19	1.1 (4)	C15—C14—N4—C12	−110.0 (3)
Cl1—C17—C18—C19	179.8 (2)	N3—C13—N5—C20	−134.4 (2)
C17—C18—C19—C14	0.2 (4)	N4—C13—N5—C20	47.6 (3)
C15—C14—C19—C18	−2.1 (4)	N3—C13—N5—C24	17.5 (3)
N4—C14—C19—C18	179.3 (2)	N4—C13—N5—C24	−160.5 (2)
C21'—C20—C21—C22	−72.3 (6)	C21'—C20—N5—C13	49.7 (5)

N5—C20—C21—C22	−176.7 (4)	C21—C20—N5—C13	99.0 (3)
C21'—C20—C21—C23	54.2 (8)	C21'—C20—N5—C24	−102.2 (5)
N5—C20—C21—C23	−50.2 (6)	C21—C20—N5—C24	−52.8 (4)
N5—C20—C21'—C23'	51.8 (10)	C25—C24—N5—C13	145.7 (2)
C21—C20—C21'—C23'	−47.9 (8)	C25—C24—N5—C20	−61.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C24—H24A···N3	0.97	2.35	2.694 (3)	100
C23—H23B···N5	0.96	2.57	2.995 (11)	107
C20—H20A···N4	0.97	2.54	2.958 (3)	106
C7—H7···N2^{i}	0.93	2.56	3.202 (4)	126

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

Fig. 1

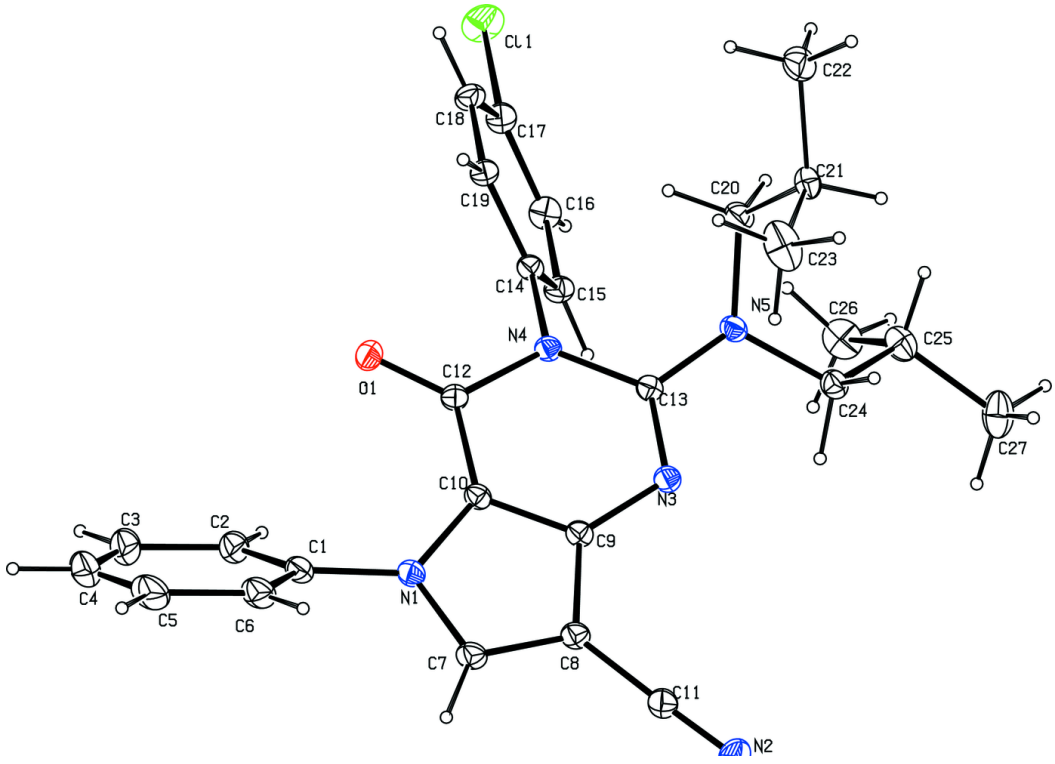

Cl1
C22
C18
C17
C21
C20
C19
C16
C23
C14
C15
N5
C26
N4
C25
O1
C12
C13
C24
C27
C10
N3
C3
C2
C9
C1
C4
N1
C5
C6
C7
C8
C11
N2

Fig. 2