Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

1-Benzoyl-3-[3-cyano-8-methyl-4-(1-methyl-1*H*-pyrrol-2-yl)-5,6,7,8-tetrahydroquinolin-2-yl]thiourea

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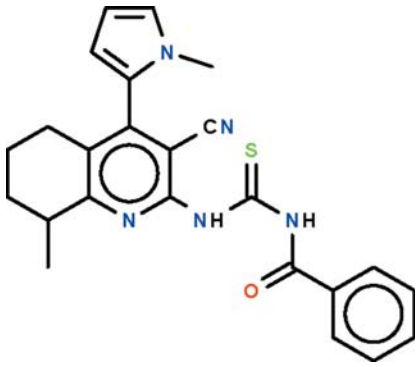
Received 14 August 2011; accepted 15 August 2011

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; disorder in main residue; R factor = 0.052; wR factor = 0.146; data-to-parameter ratio = 14.3.

In the *N*-substituted benzoylthiourea, $C_{24}H_{23}N_5OS$, the benzoylthiourea unit is non-planar (r.m.s. deviation = 0.126 Å). The aliphatic part of the tetrahydroquinoline fused-ring system is disordered over two positions in a 0.592 (5):0.408 (5) ratio. The pyridine and pyrrole rings are twisted by 55.2 (1)° in order to avoid crowding of their respective substituents. Pairs of molecules are linked by N—H···N hydrogen bonds, forming centrosymmetric dimers. Furthermore, an intramolecular N—H···O hydrogen bond stabilizes the molecular conformation.

Related literature

For medicinal properties of cyanopyridines, see: Cocco *et al.* (2005); El-Hawash *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{23}N_5OS$
M_r = 429.53
Triclinic, $P\overline{1}$
a = 9.7072 (4) Å
b = 10.4928 (5) Å
c = 11.8828 (5) Å
α = 82.245 (4)°
β = 84.263 (3)°
γ = 63.671 (4)°
V = 1073.76 (8) Å^3
Z = 2
Cu $K\alpha$ radiation
μ = 1.55 mm^{-1}
T = 100 K
0.30 × 0.20 × 0.20 mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2010)
T_{min} = 0.654, T_{max} = 0.747
7386 measured reflections
4218 independent reflections
3897 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.146
S = 1.03
4218 reflections
294 parameters
20 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 1.25 e Å^{-3}
$\Delta\rho_{min}$ = −0.46 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N4—H4···O1	0.88	1.90	2.594 (2)	135
N5—H5···N3^{i}	0.88	2.22	3.058 (2)	158

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

Data collection: *CrysAlis PRO* (Agilent, 2010); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2010).

We thank King Abdulaziz University and the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5613).

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