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8-(4-Fluorophenyl)-11,11-dimethyl-5,9-dioxo-6,8,9,10,11,12-hexahydro-5*H*-quinolino[1,2-*a*]quinazoline-7-carbonitrile dimethylformamide solvate

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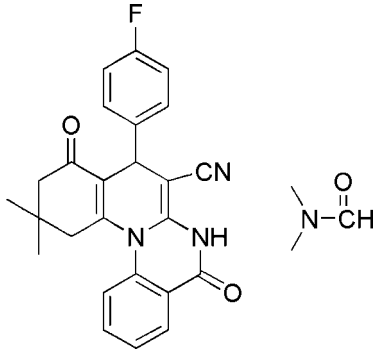
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.007 Å; R factor = 0.064; wR factor = 0.191; data-to-parameter ratio = 13.1.

In the title compound, $C_{25}H_{20}FN_3O_2\cdot C_3H_7NO$, the dihydropyridine and pyrimidine rings have boat conformations, while the cyclohexene ring adopts an envelope conformation. In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds link the molecules.

Related literature

For related literature, see: Hermecz & Meszaros (1988); Doria *et al.* (1983); Colpaert (2003); Knoll *et al.* (1987); Kozlovskaya *et al.* (1995); Hermecz *et al.* (1996, and references therein). For ring conformation puckering parameters, see: Cremer & Pople (1975). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{25}H_{20}FN_3O_2\cdot C_3H_7NO$
M_r = 486.54
Monoclinic, $C2/c$
a = 36.140 (15) Å
b = 11.701 (5) Å
c = 11.780 (5) Å
β = 103.122 (6)°
V = 4851 (4) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 298 (2) K
0.26 × 0.13 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.991
12335 measured reflections
4262 independent reflections
1649 reflections with $I > 2\sigma(I)$
R_{int} = 0.115

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.064
$wR(F^2)$ = 0.191
S = 1.00
4262 reflections
325 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.06	2.8628 (3)	155
C22—H22···O1^{ii}	0.93	2.35	3.2625 (3)	168

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2326).

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supplementary materials

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8-(4-Fluorophenyl)-11,11-dimethyl-5,9-dioxo-6,8,9,10,11,12-hexahydro-5*H*-quinolino[1,2-*a*]quinazoline-7-carbonitrile dimethylformamide solvate

H. Jiang, C. Li, L. Cao and D. Zhou

Comment

The pyrido[1,2-*a*]pyrimidine core has been a successful motif for the development of biologically interesting molecules. Compounds containing the pyrido[1,2-*a*]pyrimidine ring system have been used as analgesics (Hermecz & Meszaros, 1988), antiallergics (Doria *et al.*, 1983), antiasthmatics, antipsychotics (Colpaert, 2003), gastrointestinal protective (Knoll *et al.*, 1987), neurotropic and stress-protecting agents (Kozlovskaya *et al.*, 1995). Moreover, some examples are key intermediates for the synthesis of rutaecarpine alkaloids and several are neutral hydrogen chloride acceptors in organic synthesis (Hermecz *et al.*, 1996, and references therein). The discovery of quinolino[1,2-*a*]quinazoline including imidazo[1,2-*a*]pyridine moiety as new potential pharmacological molecules may be of great significance. We report herein the crystal structure of the title compound, (I).

In the molecule of the title compound, (I), (Fig. 1) the bond lengths and angles are generally within normal ranges (Allen *et al.*, 1987). It contains one $C_{25}H_{20}FN_3O_2$ molecule and one C_3H_7NO molecule.

Rings A (N1/C1—C4/C9), B (C4—C9) and C (N1/N2/C1/C10—C12) are not planar, having total puckering amplitudes, Q_T, of 0.467 (2), 0.504 (3) and 0.193 (2) Å, respectively [φ = 158.80 (7)°, θ = 154.08 (5)°; φ = 3.15 (5)°, θ = 122.37 (5)° and φ = 157.13 (17)°, θ = 79.02 (16)°, respectively] (Cremer & Pople, 1975). Rings A and C have boat conformations, while ring B adopts an envelope conformation with atom C7 displaced by 0.698 (3) Å from the plane of the other ring atoms. Rings D (C11—C16) and E (C18—C23) are, of course, planar and they are oriented at a dihedral angle of 74.86 (2)°.

In the crystal structure, intermolecular N—H···O and C—H···O hydrogen bonds (Table 1) link the molecules (Fig. 2), in which they seem to be effective in the stabilization of the structure.

Experimental

The title compound, (I), was prepared by the reaction of 4-fluorobenzaldehyde (124 mg, 1 mmol), 2-(5,5-dimethyl-3-oxo-cyclohex-1-enylamino)benzoic acid (259 mg, 1 mmol) with malononitrile (66 mg, 1 mmol) in solvent of ethylene glycol (2.0 ml) at 393 K under microwave irradiation (maximum power 200 W, initial power 100 W) for 5 min (yield; 339 mg, 82%, m.p. 534–535 K). Single crystals suitable for X-ray analysis were obtained from an ethanol solution (95%) by slow evaporation.

Refinement

H atoms were positioned geometrically, with N—H = 0.86 Å (for NH) and C—H = 0.93, 0.98, 0.97 and 0.96 Å for aromatic, methine, methylene and methyl H, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*N*), where x = 1.5 for methyl H, and x = 1.2 for all other H atoms.

Figures

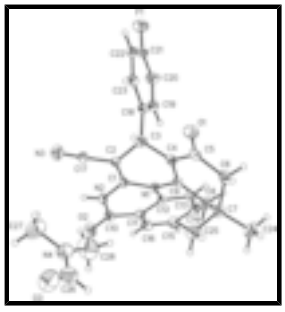

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.

Fig. 2. A packing diagram for (I). Hydrogen bonds are shown as dashed lines.

8-(4-fluorophenyl)-11,11-dimethyl-5,9-dioxo-6,8,9,10,11,12-hexahydro-5*H*- quinolino[1,2-*a*]quinazoline-7-carbonitrile dimethylformamide solvate

Crystal data

$C_{25}H_{20}FN_3O_2·C_3H_7NO$	F_{000} = 2048
M_r = 486.54	D_x = 1.332 Mg m^{-3}
Monoclinic, *C*2/*c*	Melting point: 534-535 K
Hall symbol: -C 2yc	Mo *K*α radiation λ = 0.71073 Å
a = 36.140 (15) Å	Cell parameters from 1017 reflections
b = 11.701 (5) Å	θ = 2.5–19.7º
c = 11.780 (5) Å	μ = 0.09 mm^{-1}
β = 103.122 (6)º	*T* = 298 (2) K
V = 4851 (4) Å^3	Block, colorless
Z = 8	0.26 × 0.13 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4262 independent reflections
Radiation source: fine-focus sealed tube	1649 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.115
T = 298(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.8º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	*h* = −42→42
T_{min} = 0.976, T_{max} = 0.991	*k* = −8→13
12335 measured reflections	*l* = −14→13

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
$wR(F^2) = 0.191$	$w = 1/[\sigma^2(F_o^2) + (0.0618P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.00$	$(\Delta/\sigma)_{max} < 0.001$
4262 reflections	$\Delta\rho_{max} = 0.28$ e Å^{-3}
325 parameters	$\Delta\rho_{min} = -0.26$ 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 $F^2 > 2$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}
F1	0.22422 (9)	0.2184 (3)	0.3860 (3)	0.0876 (12)
N1	0.11112 (9)	0.6953 (3)	0.4752 (3)	0.0286 (9)
N2	0.05613 (10)	0.6431 (3)	0.3357 (3)	0.0343 (10)
H2	0.0453	0.6303	0.2639	0.041*
N3	0.09081 (13)	0.6056 (4)	0.0661 (4)	0.0578 (13)
N4	0.04876 (14)	0.9481 (5)	0.0533 (5)	0.0693 (15)
O1	0.22506 (9)	0.7939 (3)	0.3657 (3)	0.0506 (10)
O2	−0.00121 (9)	0.6344 (3)	0.3816 (3)	0.0513 (10)
O3	0.04920 (14)	1.0979 (4)	−0.0674 (4)	0.0983 (17)
C1	0.09488 (12)	0.6598 (4)	0.3608 (4)	0.0291 (11)
C2	0.11659 (12)	0.6478 (4)	0.2838 (3)	0.0284 (11)
C3	0.15981 (12)	0.6583 (4)	0.3207 (4)	0.0338 (12)
H3	0.1682	0.6927	0.2550	0.041*
C4	0.16847 (12)	0.7426 (4)	0.4186 (4)	0.0300 (11)
C5	0.20306 (13)	0.8133 (4)	0.4277 (4)	0.0371 (12)
C6	0.20967 (13)	0.9095 (4)	0.5141 (4)	0.0442 (14)
H6A	0.2222	0.9716	0.4831	0.053*
H6B	0.2267	0.8834	0.5854	0.053*

C7	0.17301 (13)	0.9552 (4)	0.5435 (4)	0.0391 (13)
C8	0.15274 (13)	0.8525 (4)	0.5815 (4)	0.0380 (12)
H8A	0.1680	0.8226	0.6539	0.046*
H8B	0.1286	0.8772	0.5960	0.046*
C9	0.14575 (12)	0.7590 (4)	0.4918 (4)	0.0284 (11)
C10	0.03298 (13)	0.6450 (4)	0.4133 (4)	0.0352 (12)
C11	0.05287 (12)	0.6541 (4)	0.5351 (4)	0.0306 (11)
C12	0.09173 (12)	0.6765 (4)	0.5647 (4)	0.0284 (11)
C13	0.11082 (13)	0.6742 (4)	0.6823 (4)	0.0382 (13)
H13	0.1370	0.6849	0.7035	0.046*
C14	0.09043 (14)	0.6560 (4)	0.7664 (4)	0.0454 (14)
H14	0.1029	0.6564	0.8447	0.055*
C15	0.05194 (14)	0.6373 (4)	0.7363 (4)	0.0488 (14)
H15	0.0385	0.6268	0.7941	0.059*
C16	0.03329 (13)	0.6341 (4)	0.6207 (4)	0.0424 (13)
H16	0.0074	0.6184	0.6003	0.051*
C17	0.10108 (13)	0.6233 (4)	0.1636 (4)	0.0351 (12)
C18	0.17897 (12)	0.5425 (4)	0.3426 (4)	0.0352 (12)
C19	0.17453 (14)	0.4746 (4)	0.4351 (4)	0.0460 (14)
H19	0.1610	0.5025	0.4875	0.055*
C20	0.18988 (15)	0.3666 (5)	0.4502 (5)	0.0580 (16)
H20	0.1865	0.3211	0.5118	0.070*
C21	0.20995 (15)	0.3276 (5)	0.3744 (5)	0.0522 (15)
C22	0.21558 (13)	0.3911 (5)	0.2825 (5)	0.0525 (16)
H22	0.2293	0.3625	0.2310	0.063*
C23	0.20018 (13)	0.4988 (5)	0.2691 (4)	0.0433 (14)
H23	0.2042	0.5440	0.2081	0.052*
C24	0.18274 (15)	1.0405 (5)	0.6442 (5)	0.0620 (17)
H24A	0.1956	1.1052	0.6208	0.093*
H24B	0.1990	1.0045	0.7104	0.093*
H24C	0.1598	1.0655	0.6646	0.093*
C25	0.14790 (15)	1.0147 (4)	0.4378 (5)	0.0600 (16)
H25A	0.1614	1.0783	0.4152	0.090*
H25B	0.1251	1.0416	0.4578	0.090*
H25C	0.1415	0.9616	0.3743	0.090*
C26	0.05002 (18)	1.0573 (6)	0.0287 (7)	0.079 (2)
H26	0.0517	1.1085	0.0900	0.095*
C27	0.0441 (2)	0.8640 (6)	−0.0401 (6)	0.105 (3)
H27A	0.0433	0.7888	−0.0082	0.158*
H27B	0.0650	0.8694	−0.0775	0.158*
H27C	0.0207	0.8785	−0.0961	0.158*
C28	0.0502 (2)	0.9086 (7)	0.1701 (6)	0.120 (3)
H28A	0.0484	0.8268	0.1701	0.181*
H28B	0.0295	0.9410	0.1976	0.181*
H28C	0.0738	0.9317	0.2203	0.181*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.081 (3)	0.059 (2)	0.112 (3)	0.032 (2)	−0.003 (2)	−0.017 (2)
N1	0.026 (2)	0.035 (2)	0.025 (2)	−0.0005 (19)	0.0064 (17)	−0.0030 (18)
N2	0.029 (2)	0.043 (3)	0.028 (2)	−0.003 (2)	−0.0001 (18)	−0.0034 (19)
N3	0.070 (3)	0.062 (3)	0.038 (3)	0.002 (3)	0.006 (2)	0.000 (3)
N4	0.081 (4)	0.047 (3)	0.079 (4)	−0.003 (3)	0.015 (3)	0.006 (3)
O1	0.039 (2)	0.061 (3)	0.058 (2)	−0.0024 (19)	0.0240 (18)	0.0025 (19)
O2	0.027 (2)	0.075 (3)	0.049 (2)	−0.0054 (19)	0.0022 (16)	0.0020 (19)
O3	0.143 (5)	0.073 (3)	0.082 (3)	−0.013 (3)	0.032 (3)	0.011 (3)
C1	0.026 (3)	0.031 (3)	0.027 (3)	−0.002 (2)	−0.001 (2)	−0.001 (2)
C2	0.031 (3)	0.031 (3)	0.023 (3)	0.003 (2)	0.005 (2)	−0.001 (2)
C3	0.035 (3)	0.038 (3)	0.032 (3)	0.000 (2)	0.016 (2)	0.002 (2)
C4	0.025 (3)	0.034 (3)	0.031 (3)	−0.001 (2)	0.008 (2)	0.001 (2)
C5	0.028 (3)	0.042 (3)	0.040 (3)	0.004 (3)	0.004 (2)	0.006 (3)
C6	0.033 (3)	0.047 (4)	0.052 (3)	−0.007 (3)	0.007 (2)	0.005 (3)
C7	0.038 (3)	0.036 (3)	0.043 (3)	−0.007 (3)	0.010 (2)	−0.004 (3)
C8	0.032 (3)	0.045 (3)	0.037 (3)	−0.003 (3)	0.010 (2)	−0.006 (3)
C9	0.025 (3)	0.029 (3)	0.030 (3)	0.002 (2)	0.004 (2)	0.003 (2)
C10	0.027 (3)	0.036 (3)	0.042 (3)	−0.004 (2)	0.006 (2)	0.002 (2)
C11	0.028 (3)	0.032 (3)	0.035 (3)	0.001 (2)	0.012 (2)	0.003 (2)
C12	0.030 (3)	0.026 (3)	0.032 (3)	0.003 (2)	0.010 (2)	−0.001 (2)
C13	0.030 (3)	0.046 (3)	0.036 (3)	−0.004 (2)	0.003 (2)	0.003 (3)
C14	0.048 (3)	0.057 (4)	0.031 (3)	0.001 (3)	0.009 (3)	0.001 (3)
C15	0.045 (3)	0.061 (4)	0.046 (3)	0.002 (3)	0.022 (3)	0.003 (3)
C16	0.030 (3)	0.049 (4)	0.051 (3)	−0.003 (3)	0.014 (3)	0.005 (3)
C17	0.037 (3)	0.039 (3)	0.029 (3)	0.006 (2)	0.007 (2)	0.000 (3)
C18	0.027 (3)	0.048 (3)	0.031 (3)	0.005 (3)	0.007 (2)	−0.007 (3)
C19	0.052 (4)	0.048 (4)	0.039 (3)	0.014 (3)	0.014 (3)	−0.003 (3)
C20	0.068 (4)	0.053 (4)	0.049 (4)	0.025 (3)	0.005 (3)	0.005 (3)
C21	0.046 (3)	0.037 (4)	0.066 (4)	0.019 (3)	−0.005 (3)	−0.015 (3)
C22	0.030 (3)	0.060 (4)	0.068 (4)	0.004 (3)	0.011 (3)	−0.028 (3)
C23	0.030 (3)	0.055 (4)	0.044 (3)	0.000 (3)	0.007 (2)	−0.013 (3)
C24	0.059 (4)	0.057 (4)	0.073 (4)	−0.020 (3)	0.022 (3)	−0.028 (3)
C25	0.064 (4)	0.042 (4)	0.073 (4)	0.000 (3)	0.014 (3)	0.005 (3)
C26	0.078 (5)	0.064 (5)	0.094 (6)	0.005 (4)	0.016 (4)	0.004 (5)
C27	0.121 (6)	0.072 (5)	0.127 (6)	−0.018 (5)	0.036 (5)	−0.027 (5)
C28	0.153 (8)	0.114 (7)	0.090 (6)	−0.001 (6)	0.019 (5)	0.043 (5)

Geometric parameters (Å, °)

F1—C21	1.373 (6)	C11—C16	1.377 (6)
N1—C1	1.404 (5)	C11—C12	1.393 (6)
N1—C12	1.409 (5)	C12—C13	1.401 (6)
N1—C9	1.431 (5)	C13—C14	1.379 (6)
N2—C10	1.372 (5)	C13—H13	0.9300
N2—C1	1.378 (5)	C14—C15	1.373 (6)

N2—H2	0.8600	C14—H14	0.9300
N3—C17	1.144 (5)	C15—C16	1.377 (6)
N4—C26	1.313 (7)	C15—H15	0.9300
N4—C28	1.441 (7)	C16—H16	0.9300
N4—C27	1.457 (7)	C18—C23	1.379 (6)
O1—C5	1.218 (5)	C18—C19	1.387 (6)
O2—C10	1.213 (5)	C19—C20	1.376 (7)
O3—C26	1.221 (7)	C19—H19	0.9300
C1—C2	1.335 (6)	C20—C21	1.352 (7)
C2—C17	1.428 (6)	C20—H20	0.9300
C2—C3	1.528 (6)	C21—C22	1.366 (7)
C3—C4	1.496 (6)	C22—C23	1.372 (7)
C3—C18	1.516 (6)	C22—H22	0.9300
C3—H3	0.9800	C23—H23	0.9300
C4—C9	1.333 (5)	C24—H24A	0.9600
C4—C5	1.482 (6)	C24—H24B	0.9600
C5—C6	1.500 (6)	C24—H24C	0.9600
C6—C7	1.539 (6)	C25—H25A	0.9600
C6—H6A	0.9700	C25—H25B	0.9600
C6—H6B	0.9700	C25—H25C	0.9600
C7—C8	1.526 (6)	C26—H26	0.9300
C7—C24	1.530 (6)	C27—H27A	0.9600
C7—C25	1.532 (6)	C27—H27B	0.9600
C8—C9	1.502 (6)	C27—H27C	0.9600
C8—H8A	0.9700	C28—H28A	0.9600
C8—H8B	0.9700	C28—H28B	0.9600
C10—C11	1.455 (6)	C28—H28C	0.9600
C1—N1—C12	120.0 (4)	C14—C13—H13	120.3
C1—N1—C9	116.6 (3)	C12—C13—H13	120.3
C12—N1—C9	123.1 (3)	C15—C14—C13	121.0 (4)
C10—N2—C1	126.7 (4)	C15—C14—H14	119.5
C10—N2—H2	116.6	C13—C14—H14	119.5
C1—N2—H2	116.6	C14—C15—C16	120.0 (5)
C26—N4—C28	121.8 (6)	C14—C15—H15	120.0
C26—N4—C27	119.6 (6)	C16—C15—H15	120.0
C28—N4—C27	118.5 (6)	C15—C16—C11	120.2 (5)
C2—C1—N2	124.4 (4)	C15—C16—H16	119.9
C2—C1—N1	120.1 (4)	C11—C16—H16	119.9
N2—C1—N1	115.5 (4)	N3—C17—C2	175.7 (5)
C1—C2—C17	122.4 (4)	C23—C18—C19	117.4 (5)
C1—C2—C3	121.2 (4)	C23—C18—C3	121.5 (4)
C17—C2—C3	116.4 (4)	C19—C18—C3	121.0 (4)
C4—C3—C18	116.8 (4)	C20—C19—C18	120.9 (5)
C4—C3—C2	107.1 (4)	C20—C19—H19	119.6
C18—C3—C2	112.0 (4)	C18—C19—H19	119.6
C4—C3—H3	106.8	C21—C20—C19	119.0 (5)
C18—C3—H3	106.8	C21—C20—H20	120.5
C2—C3—H3	106.8	C19—C20—H20	120.5
C9—C4—C5	120.4 (4)	C20—C21—C22	122.6 (5)

C9—C4—C3	122.8 (4)	C20—C21—F1	119.6 (6)
C5—C4—C3	116.7 (4)	C22—C21—F1	117.7 (5)
O1—C5—C4	120.5 (5)	C21—C22—C23	117.5 (5)
O1—C5—C6	121.5 (4)	C21—C22—H22	121.3
C4—C5—C6	118.0 (4)	C23—C22—H22	121.3
C5—C6—C7	113.6 (4)	C22—C23—C18	122.5 (5)
C5—C6—H6A	108.8	C22—C23—H23	118.7
C7—C6—H6A	108.8	C18—C23—H23	118.7
C5—C6—H6B	108.8	C7—C24—H24A	109.5
C7—C6—H6B	108.8	C7—C24—H24B	109.5
H6A—C6—H6B	107.7	H24A—C24—H24B	109.5
C8—C7—C24	109.1 (4)	C7—C24—H24C	109.5
C8—C7—C25	111.2 (4)	H24A—C24—H24C	109.5
C24—C7—C25	108.8 (4)	H24B—C24—H24C	109.5
C8—C7—C6	106.7 (4)	C7—C25—H25A	109.5
C24—C7—C6	110.1 (4)	C7—C25—H25B	109.5
C25—C7—C6	110.9 (4)	H25A—C25—H25B	109.5
C9—C8—C7	112.5 (4)	C7—C25—H25C	109.5
C9—C8—H8A	109.1	H25A—C25—H25C	109.5
C7—C8—H8A	109.1	H25B—C25—H25C	109.5
C9—C8—H8B	109.1	O3—C26—N4	126.0 (7)
C7—C8—H8B	109.1	O3—C26—H26	117.0
H8A—C8—H8B	107.8	N4—C26—H26	117.0
C4—C9—N1	119.0 (4)	N4—C27—H27A	109.5
C4—C9—C8	122.0 (4)	N4—C27—H27B	109.5
N1—C9—C8	118.6 (4)	H27A—C27—H27B	109.5
O2—C10—N2	121.7 (4)	N4—C27—H27C	109.5
O2—C10—C11	123.5 (4)	H27A—C27—H27C	109.5
N2—C10—C11	114.7 (4)	H27B—C27—H27C	109.5
C16—C11—C12	120.3 (4)	N4—C28—H28A	109.5
C16—C11—C10	119.2 (4)	N4—C28—H28B	109.5
C12—C11—C10	120.3 (4)	H28A—C28—H28B	109.5
C11—C12—C13	119.1 (4)	N4—C28—H28C	109.5
C11—C12—N1	119.1 (4)	H28A—C28—H28C	109.5
C13—C12—N1	121.7 (4)	H28B—C28—H28C	109.5
C14—C13—C12	119.4 (4)		
C10—N2—C1—C2	174.2 (5)	C7—C8—C9—N1	−143.2 (4)
C10—N2—C1—N1	−8.0 (7)	C1—N2—C10—O2	176.6 (4)
C12—N1—C1—C2	−161.4 (4)	C1—N2—C10—C11	−6.6 (7)
C9—N1—C1—C2	24.1 (6)	O2—C10—C11—C16	9.4 (8)
C12—N1—C1—N2	20.6 (6)	N2—C10—C11—C16	−167.3 (4)
C9—N1—C1—N2	−153.9 (4)	O2—C10—C11—C12	−174.1 (5)
N2—C1—C2—C17	4.3 (7)	N2—C10—C11—C12	9.2 (6)
N1—C1—C2—C17	−173.5 (4)	C16—C11—C12—C13	2.3 (7)
N2—C1—C2—C3	−174.9 (4)	C10—C11—C12—C13	−174.1 (4)
N1—C1—C2—C3	7.3 (7)	C16—C11—C12—N1	179.3 (4)
C1—C2—C3—C4	−32.0 (6)	C10—C11—C12—N1	2.8 (7)
C17—C2—C3—C4	148.8 (4)	C1—N1—C12—C11	−18.4 (6)
C1—C2—C3—C18	97.3 (5)	C9—N1—C12—C11	155.7 (4)

C17—C2—C3—C18	−82.0 (5)	C1—N1—C12—C13	158.4 (4)
C18—C3—C4—C9	−97.6 (5)	C9—N1—C12—C13	−27.4 (6)
C2—C3—C4—C9	28.9 (6)	C11—C12—C13—C14	−3.4 (7)
C18—C3—C4—C5	85.6 (5)	N1—C12—C13—C14	179.7 (4)
C2—C3—C4—C5	−148.0 (4)	C12—C13—C14—C15	1.6 (8)
C9—C4—C5—O1	175.5 (4)	C13—C14—C15—C16	1.4 (8)
C3—C4—C5—O1	−7.6 (6)	C14—C15—C16—C11	−2.5 (8)
C9—C4—C5—C6	−5.2 (6)	C12—C11—C16—C15	0.7 (7)
C3—C4—C5—C6	171.6 (4)	C10—C11—C16—C15	177.1 (5)
O1—C5—C6—C7	154.2 (4)	C4—C3—C18—C23	−125.8 (5)
C4—C5—C6—C7	−25.0 (6)	C2—C3—C18—C23	110.3 (5)
C5—C6—C7—C8	53.6 (5)	C4—C3—C18—C19	56.8 (6)
C5—C6—C7—C24	171.9 (4)	C2—C3—C18—C19	−67.1 (5)
C5—C6—C7—C25	−67.6 (5)	C23—C18—C19—C20	−1.8 (7)
C24—C7—C8—C9	−174.1 (4)	C3—C18—C19—C20	175.7 (4)
C25—C7—C8—C9	65.9 (5)	C18—C19—C20—C21	0.9 (8)
C6—C7—C8—C9	−55.2 (5)	C19—C20—C21—C22	−0.2 (8)
C5—C4—C9—N1	175.3 (4)	C19—C20—C21—F1	−177.6 (5)
C3—C4—C9—N1	−1.3 (6)	C20—C21—C22—C23	0.4 (8)
C5—C4—C9—C8	3.3 (7)	F1—C21—C22—C23	177.9 (4)
C3—C4—C9—C8	−173.4 (4)	C21—C22—C23—C18	−1.4 (7)
C1—N1—C9—C4	−27.4 (6)	C19—C18—C23—C22	2.1 (7)
C12—N1—C9—C4	158.3 (4)	C3—C18—C23—C22	−175.4 (4)
C1—N1—C9—C8	144.9 (4)	C28—N4—C26—O3	179.5 (7)
C12—N1—C9—C8	−29.4 (6)	C27—N4—C26—O3	−3.3 (11)
C7—C8—C9—C4	28.8 (6)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.06	2.8628 (3)	155
C22—H22···O1^{ii}	0.93	2.35	3.2625 (3)	168

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

Fig. 1

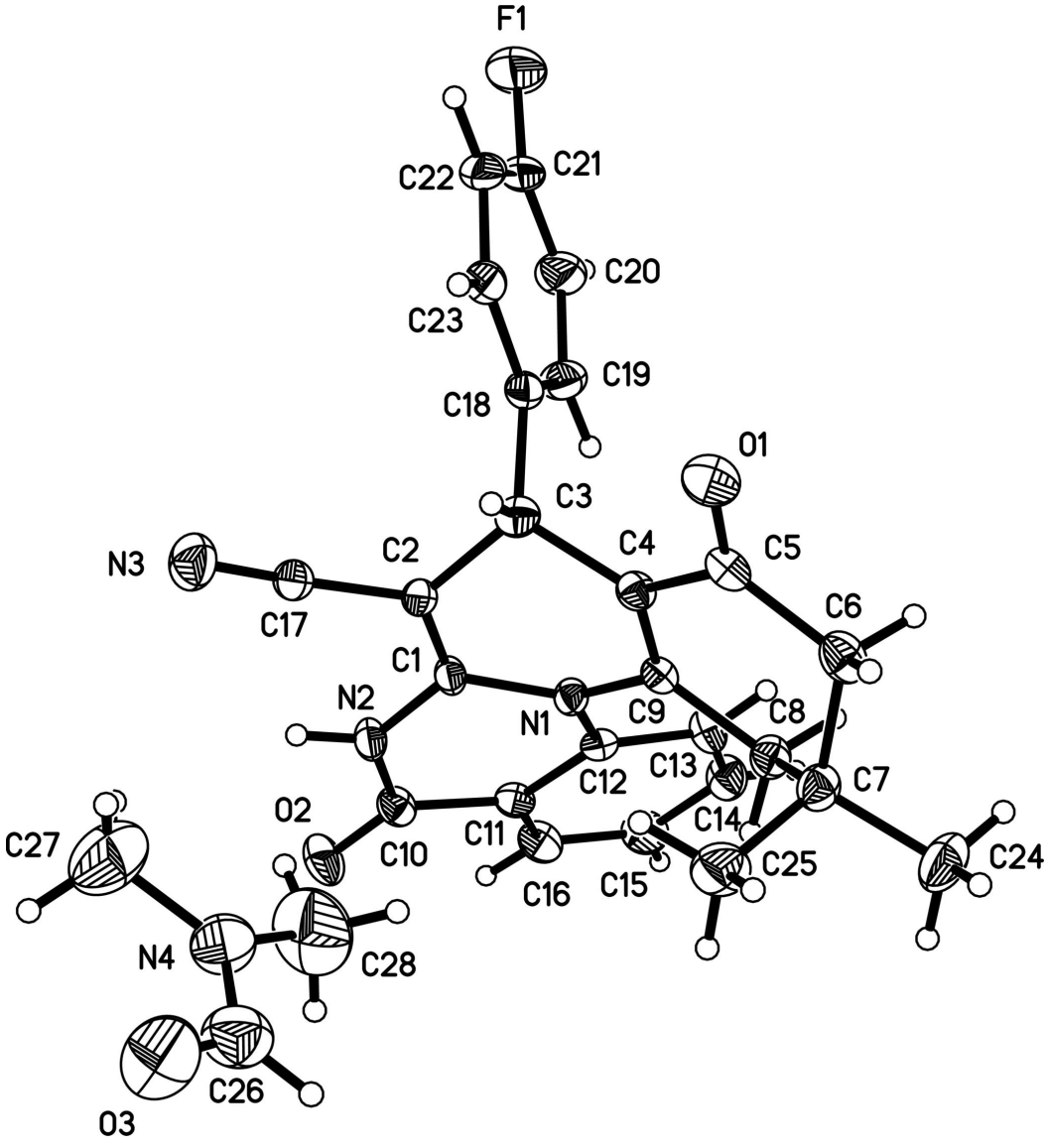
F1
C22
C21
C20
C23
C19
C18
O1
C3
N3
C2
C4
C5
C17
C6
C1
N2
N1
C9
C8
C12
C13
C7
O2
C14
C27
C10
C11
C25
C24
C16
C15
N4
C28
C26
O3

Fig. 2