

## 3-(2-Aminoethyl)-2-(4-fluoroanilino)-quinazolin-4(3H)-one

Xu-Hong Yang and Ming-Hu Wu\*

Faculty of Chemistry and Life Science, Xianning University, Xianning 437100, People's Republic of China

Correspondence e-mail: minghuwu@hotmail.com

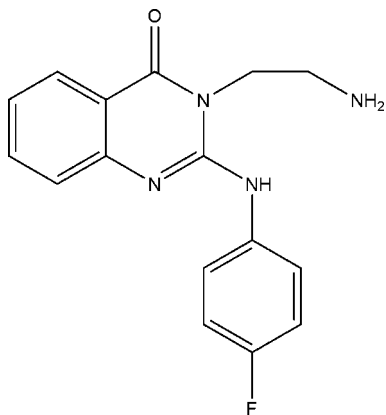
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Key indicators: single-crystal X-ray study;  $T = 292$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.038;  $wR$  factor = 0.111; data-to-parameter ratio = 13.0.

In the title molecule,  $\text{C}_{16}\text{H}_{15}\text{FN}_4\text{O}$ , the dihedral angle between the fluoro-substituted benzene ring and the pyrimidinone ring is  $52.34(7)^\circ$ , while the dihedral angle between the fused benzene ring and the pyrimidinone ring is  $3.30(6)^\circ$ . An intramolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bond may, in part, influence the conformation of the molecule. In the crystal structure, intermolecular  $\text{N}-\text{H}\cdots\text{N}$  hydrogen bonds and weak  $\text{C}-\text{H}\cdots\pi(\text{arene})$  interactions link pairs of molecules into centrosymmetric dimers.

### Related literature

For the biological properties of quinazolinones and their derivatives, see: Armarego (1963); Witt & Bergman (2003). For details of our ongoing heterocyclic synthesis and drug discovery project, see: Yang *et al.* (2008).



### Experimental

#### Crystal data

$\text{C}_{16}\text{H}_{15}\text{FN}_4\text{O}$	$\gamma = 77.163(10)^\circ$
$M_r = 298.32$	$V = 704.03(13) \text{ \AA}^3$
Triclinic, $P\bar{1}$	$Z = 2$
$a = 8.2836(8) \text{ \AA}$	Mo $K\alpha$ radiation
$b = 9.3103(10) \text{ \AA}$	$\mu = 0.10 \text{ mm}^{-1}$
$c = 9.4952(10) \text{ \AA}$	$T = 292(2) \text{ K}$
$\alpha = 89.36(1)^\circ$	$0.20 \times 0.10 \times 0.10 \text{ mm}$
$\beta = 80.537(10)^\circ$	

#### Data collection

Bruker SMART APEX CCD diffractometer	4078 measured reflections
Absorption correction: multi-scan (SADABS; Bruker, 2001)	2726 independent reflections
$T_{\min} = 0.970$ , $T_{\max} = 0.990$	2318 reflections with $I > 2\sigma(I)$
	$R_{\text{int}} = 0.012$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.038$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.111$	$\Delta\rho_{\max} = 0.16 \text{ e \AA}^{-3}$
$S = 1.05$	$\Delta\rho_{\min} = -0.15 \text{ e \AA}^{-3}$
2726 reflections	
209 parameters	

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1}\cdots\text{N4}$	0.908 (17)	1.925 (17)	2.8049 (17)	162.8 (14)
$\text{N4}-\text{H4A}\cdots\text{N2}^i$	0.889 (16)	2.323 (16)	3.1321 (18)	151.4 (13)
$\text{C3}-\text{H3}\cdots\text{Cg}^i$	0.93	2.77 (1)	3.4741 (15)	132 (1)

Symmetry code: (i)  $-x, -y + 1, -z + 1$ . Cg is the centroid of atoms N2/C7/N3/C14/C13/C8.

Data collection: SMART (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2003); software used to prepare material for publication: SHELXTL (Sheldrick, 2008).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2717).

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**supplementary materials**

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### 3-(2-Aminoethyl)-2-(4-fluoroanilino)quinazolin-4(3H)-one

X.-H. Yang and M.-H. Wu

#### Comment

Quinazolinones and their derivatives are now known to have a wide range of useful biological properties, such as hypnotic, sedative, analgesic, anti-convulsant, anti-tussive, anti-bacterial, anti-diabetic, anti-inflammatory and anti-tumor (Armarego, 1963; Witt & Bergman, 2003). In connection with our ongoing heterocyclic synthesis and drug discovery project (Yang *et al.*, 2008), we have focused our research on the synthesis of quinazolinones and pyrazolo pyrimidinones. Herein, the title compound was synthesized and its crystal structure was determined.

In the molecule (Fig. 1), the dihedral angle between the fluorophenyl and pyrimidinone ring is 52.34 (7)°, and the dihedral angle between the fused benzene ring and pyrimidinone ring is 3.30 (6)°. The torsion angles of N2–C7–N1–C4 and N3–C7–N1–C4 are -4.7 (2) and 176.42 (11)°, respectively.

An intramolecular N–H···N hydrogen bond may, in part, influence the conformation of the molecule. In the crystal structure, intermolecular N–H···N hydrogen bonds and weak C–H··· $\pi$ (arene) interactions link pairs of molecules into centrosymmetric dimers (see Table 1 and Fig. 2).

#### Experimental

To a solution of 2-ethoxycarbonyliminophosphorane (1.27 g, 3 mmol) in 10 ml anhydrous THF, 4-chlorophenylisocyanate (0.46 g, 3 mmol) was added dropwise at room temperature. The reaction mixture was left unstirred for 6 h at 273–278 K, whereafter the above resulting solution was added dropwise to a solution of ethylenediamine (0.18 g, 3 mmol) in 5 ml anhydrous THF. After that, the reaction mixture was stirred overnight, the reaction mixture was cooled and the reaction product was recrystallized from CH<sub>3</sub>OH—CH<sub>2</sub>Cl<sub>2</sub> to give colorless crystals of the title compound in yield 85%, which were suitable for X-ray analysis.

#### Refinement

H atoms bonded to C atoms were placed in calculated positions (C—H = 0.93–0.97 Å) and included in the riding model approximation. The positional parameters of H atoms bonded to N atoms were refined independently. For all H atoms  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{iso}}(\text{C}, \text{N})$ .

#### Figures

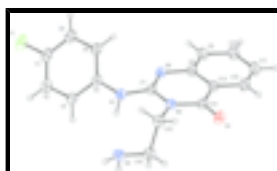


Fig. 1. View of the title molecule with the atom-labeling scheme. Displacement ellipsoids are drawn at the 50% probability level.

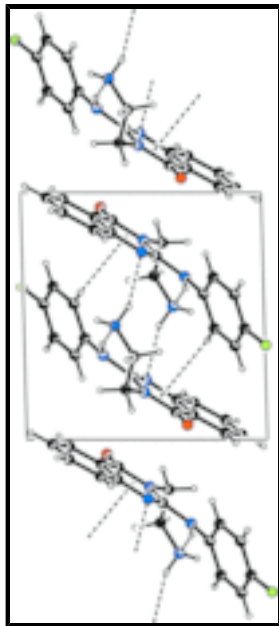


Fig. 2. Part of the crystal structure of the title compound showing hydrogen bonds as dashed lines.

**3-(2-Aminoethyl)-2-(4-fluoroanilino)quinazolin-4(3H)-one**

*Crystal data*

$C_{16}H_{15}FN_4O$

$M_r = 298.32$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 8.2836$  (8) Å

$b = 9.3103$  (10) Å

$c = 9.4952$  (10) Å

$\alpha = 89.36$  (1)°

$\beta = 80.537$  (10)°

$\gamma = 77.163$  (10)°

$V = 704.03$  (13) Å<sup>3</sup>

$Z = 2$

$F_{000} = 312$

$D_x = 1.407$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation

$\lambda = 0.71073$  Å

Cell parameters from 2276 reflections

$\theta = 2.2$ – $28.9$ °

$\mu = 0.10$  mm<sup>-1</sup>

$T = 292$  (2) K

Block, colourless

$0.20 \times 0.10 \times 0.10$  mm

*Data collection*

Bruker SMART APEX CCD  
diffractometer

Radiation source: fine-focus sealed tube

Monochromator: graphite

$T = 292$ (2) K

$\omega$  scans

Absorption correction: multi-scan  
(SADABS; Bruker, 2001)

$T_{\min} = 0.970$ ,  $T_{\max} = 0.990$

4078 measured reflections

2726 independent reflections

2318 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.012$

$\theta_{\text{max}} = 26.0$ °

$\theta_{\text{min}} = 2.2$ °

$h = -9 \rightarrow 10$

$k = -11 \rightarrow 11$

$l = -11 \rightarrow 11$

Refinement

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H atoms treated by a mixture of independent and constrained refinement
$R[F^2 > 2\sigma(F^2)] = 0.038$	$w = 1/[\sigma^2(F_o^2) + (0.0572P)^2 + 0.1074P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.111$	$(\Delta/\sigma)_{\max} = 0.001$
$S = 1.05$	$\Delta\rho_{\max} = 0.16 \text{ e } \text{\AA}^{-3}$
2726 reflections	$\Delta\rho_{\min} = -0.15 \text{ e } \text{\AA}^{-3}$
209 parameters	Extinction correction: SHELXL97 (Sheldrick, 2008), $F_c^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.033 (5)
Secondary atom site location: difference Fourier map	

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

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.26560 (18)	0.91647 (15)	0.45066 (18)	0.0596 (4)
C2	0.1522 (2)	0.87525 (15)	0.37986 (16)	0.0589 (4)
H2	0.1451	0.9031	0.2863	0.071*
C3	0.04783 (17)	0.79107 (14)	0.45047 (14)	0.0503 (3)
H3	-0.0308	0.7624	0.4040	0.060*
C4	0.05872 (15)	0.74874 (13)	0.58961 (14)	0.0449 (3)
C5	0.17665 (17)	0.79171 (15)	0.65820 (16)	0.0536 (3)
H5	0.1860	0.7632	0.7512	0.064*
C6	0.28049 (18)	0.87722 (16)	0.58782 (18)	0.0604 (4)
H6	0.3590	0.9074	0.6333	0.073*
C7	-0.02621 (15)	0.55612 (14)	0.74400 (13)	0.0424 (3)
C8	0.15458 (16)	0.37171 (14)	0.83809 (13)	0.0444 (3)
C9	0.31903 (18)	0.30166 (17)	0.85105 (16)	0.0573 (4)
H9	0.4075	0.3440	0.8121	0.069*
C10	0.3511 (2)	0.17169 (18)	0.92037 (17)	0.0670 (4)

## supplementary materials

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H10	0.4613	0.1260	0.9272	0.080*
C11	0.2208 (2)	0.10669 (18)	0.98092 (18)	0.0690 (4)
H11	0.2438	0.0177	1.0271	0.083*
C12	0.0591 (2)	0.17479 (17)	0.97182 (16)	0.0587 (4)
H12	-0.0284	0.1326	1.0136	0.070*
C13	0.02374 (16)	0.30663 (14)	0.90063 (13)	0.0459 (3)
C14	-0.14830 (17)	0.37725 (15)	0.88772 (14)	0.0479 (3)
C15	-0.33989 (16)	0.58408 (16)	0.79762 (15)	0.0523 (3)
H15A	-0.3462	0.6893	0.8010	0.063*
H15B	-0.4153	0.5613	0.8799	0.063*
C16	-0.39955 (16)	0.54589 (16)	0.66308 (16)	0.0555 (4)
H16A	-0.3651	0.4403	0.6447	0.067*
H16B	-0.5212	0.5731	0.6772	0.067*
F1	0.36536 (13)	1.00298 (12)	0.38271 (13)	0.0901 (4)
N1	-0.06114 (14)	0.67357 (13)	0.65917 (13)	0.0496 (3)
H1	-0.151 (2)	0.6763 (17)	0.6150 (16)	0.060*
N2	0.12716 (13)	0.49763 (12)	0.75954 (11)	0.0459 (3)
H4A	-0.2947 (19)	0.5633 (17)	0.4621 (17)	0.055*
H4B	-0.411 (2)	0.6934 (17)	0.5178 (15)	0.055*
N3	-0.16619 (13)	0.50507 (12)	0.80814 (11)	0.0448 (3)
N4	-0.33145 (16)	0.62199 (16)	0.53930 (14)	0.0590 (3)
O1	-0.27139 (13)	0.33072 (12)	0.94041 (12)	0.0654 (3)

### Atomic displacement parameters ( $\text{\AA}^2$ )

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0477 (8)	0.0456 (7)	0.0809 (10)	-0.0143 (6)	0.0073 (7)	0.0107 (7)
C2	0.0648 (9)	0.0473 (7)	0.0579 (8)	-0.0098 (7)	0.0053 (7)	0.0068 (6)
C3	0.0511 (8)	0.0419 (7)	0.0559 (8)	-0.0093 (6)	-0.0050 (6)	0.0015 (6)
C4	0.0364 (6)	0.0387 (6)	0.0566 (7)	-0.0069 (5)	-0.0015 (5)	0.0050 (5)
C5	0.0434 (7)	0.0536 (8)	0.0647 (8)	-0.0136 (6)	-0.0081 (6)	0.0092 (6)
C6	0.0413 (7)	0.0536 (8)	0.0880 (11)	-0.0148 (6)	-0.0097 (7)	0.0079 (7)
C7	0.0381 (7)	0.0470 (7)	0.0433 (6)	-0.0146 (5)	-0.0034 (5)	0.0022 (5)
C8	0.0434 (7)	0.0514 (7)	0.0409 (6)	-0.0159 (6)	-0.0071 (5)	0.0053 (5)
C9	0.0435 (8)	0.0697 (9)	0.0620 (8)	-0.0185 (7)	-0.0115 (6)	0.0179 (7)
C10	0.0518 (9)	0.0761 (10)	0.0731 (10)	-0.0097 (8)	-0.0183 (7)	0.0242 (8)
C11	0.0698 (10)	0.0655 (10)	0.0738 (10)	-0.0170 (8)	-0.0177 (8)	0.0287 (8)
C12	0.0584 (9)	0.0619 (9)	0.0592 (8)	-0.0235 (7)	-0.0063 (7)	0.0159 (7)
C13	0.0462 (7)	0.0517 (7)	0.0421 (6)	-0.0177 (6)	-0.0050 (5)	0.0039 (5)
C14	0.0447 (7)	0.0547 (7)	0.0460 (7)	-0.0201 (6)	-0.0007 (5)	0.0026 (6)
C15	0.0348 (7)	0.0582 (8)	0.0595 (8)	-0.0086 (6)	0.0028 (6)	0.0021 (6)
C16	0.0334 (7)	0.0580 (8)	0.0755 (9)	-0.0106 (6)	-0.0095 (6)	0.0043 (7)
F1	0.0763 (7)	0.0820 (7)	0.1149 (9)	-0.0407 (6)	0.0059 (6)	0.0289 (6)
N1	0.0379 (6)	0.0532 (7)	0.0607 (7)	-0.0154 (5)	-0.0099 (5)	0.0125 (5)
N2	0.0382 (6)	0.0514 (6)	0.0498 (6)	-0.0157 (5)	-0.0054 (4)	0.0094 (5)
N3	0.0353 (6)	0.0517 (6)	0.0476 (6)	-0.0142 (5)	-0.0013 (4)	0.0029 (5)
N4	0.0429 (7)	0.0710 (8)	0.0621 (8)	-0.0101 (6)	-0.0096 (6)	0.0019 (6)
O1	0.0476 (6)	0.0723 (7)	0.0788 (7)	-0.0275 (5)	0.0011 (5)	0.0166 (5)

*Geometric parameters (Å, °)*

C1—C2	1.362 (2)	C10—C11	1.392 (2)
C1—F1	1.3626 (16)	C10—H10	0.9300
C1—C6	1.366 (2)	C11—C12	1.365 (2)
C2—C3	1.3819 (19)	C11—H11	0.9300
C2—H2	0.9300	C12—C13	1.3914 (19)
C3—C4	1.3859 (19)	C12—H12	0.9300
C3—H3	0.9300	C13—C14	1.4551 (19)
C4—C5	1.388 (2)	C14—O1	1.2254 (15)
C4—N1	1.4123 (16)	C14—N3	1.3955 (17)
C5—C6	1.3870 (19)	C15—N3	1.4821 (16)
C5—H5	0.9300	C15—C16	1.516 (2)
C6—H6	0.9300	C15—H15A	0.9700
C7—N2	1.2980 (16)	C15—H15B	0.9700
C7—N1	1.3581 (17)	C16—N4	1.464 (2)
C7—N3	1.3956 (15)	C16—H16A	0.9700
C8—N2	1.3785 (16)	C16—H16B	0.9700
C8—C9	1.3981 (19)	N1—H1	0.908 (17)
C8—C13	1.4023 (18)	N4—H4A	0.889 (16)
C9—C10	1.366 (2)	N4—H4B	0.872 (16)
C9—H9	0.9300		
C2—C1—F1	118.49 (14)	C10—C11—H11	120.3
C2—C1—C6	122.61 (13)	C11—C12—C13	120.67 (14)
F1—C1—C6	118.88 (15)	C11—C12—H12	119.7
C1—C2—C3	118.37 (14)	C13—C12—H12	119.7
C1—C2—H2	120.8	C12—C13—C8	120.13 (13)
C3—C2—H2	120.8	C12—C13—C14	120.69 (12)
C2—C3—C4	120.93 (13)	C8—C13—C14	119.18 (12)
C2—C3—H3	119.5	O1—C14—N3	120.70 (12)
C4—C3—H3	119.5	O1—C14—C13	124.22 (13)
C3—C4—C5	119.19 (12)	N3—C14—C13	115.08 (11)
C3—C4—N1	117.79 (12)	N3—C15—C16	113.90 (11)
C5—C4—N1	122.81 (12)	N3—C15—H15A	108.8
C6—C5—C4	119.92 (14)	C16—C15—H15A	108.8
C6—C5—H5	120.0	N3—C15—H15B	108.8
C4—C5—H5	120.0	C16—C15—H15B	108.8
C1—C6—C5	118.98 (14)	H15A—C15—H15B	107.7
C1—C6—H6	120.5	N4—C16—C15	111.68 (12)
C5—C6—H6	120.5	N4—C16—H16A	109.3
N2—C7—N1	120.96 (11)	C15—C16—H16A	109.3
N2—C7—N3	124.41 (11)	N4—C16—H16B	109.3
N1—C7—N3	114.62 (11)	C15—C16—H16B	109.3
N2—C8—C9	119.28 (12)	H16A—C16—H16B	107.9
N2—C8—C13	122.38 (12)	C7—N1—C4	124.69 (11)
C9—C8—C13	118.27 (12)	C7—N1—H1	114.5 (10)
C10—C9—C8	120.65 (14)	C4—N1—H1	115.2 (10)
C10—C9—H9	119.7	C7—N2—C8	117.77 (11)

## supplementary materials

C8—C9—H9	119.7	C14—N3—C7	121.02 (11)
C9—C10—C11	120.84 (14)	C14—N3—C15	116.82 (11)
C9—C10—H10	119.6	C7—N3—C15	122.16 (11)
C11—C10—H10	119.6	C16—N4—H4A	112.6 (10)
C12—C11—C10	119.42 (14)	C16—N4—H4B	109.1 (10)
C12—C11—H11	120.3	H4A—N4—H4B	106.8 (14)
F1—C1—C2—C3	-178.16 (12)	C8—C13—C14—O1	-178.72 (13)
C6—C1—C2—C3	0.4 (2)	C12—C13—C14—N3	-177.09 (12)
C1—C2—C3—C4	-0.4 (2)	C8—C13—C14—N3	1.78 (18)
C2—C3—C4—C5	-0.1 (2)	N3—C15—C16—N4	-78.30 (15)
C2—C3—C4—N1	174.74 (12)	N2—C7—N1—C4	-4.7 (2)
C3—C4—C5—C6	0.7 (2)	N3—C7—N1—C4	176.42 (11)
N1—C4—C5—C6	-173.93 (12)	C3—C4—N1—C7	138.77 (13)
C2—C1—C6—C5	0.2 (2)	C5—C4—N1—C7	-46.58 (19)
F1—C1—C6—C5	178.68 (12)	N1—C7—N2—C8	-174.97 (11)
C4—C5—C6—C1	-0.7 (2)	N3—C7—N2—C8	3.84 (19)
N2—C8—C9—C10	-175.78 (14)	C9—C8—N2—C7	176.85 (12)
C13—C8—C9—C10	1.3 (2)	C13—C8—N2—C7	-0.13 (19)
C8—C9—C10—C11	-0.6 (3)	O1—C14—N3—C7	-177.93 (12)
C9—C10—C11—C12	-0.6 (3)	C13—C14—N3—C7	1.58 (17)
C10—C11—C12—C13	1.2 (3)	O1—C14—N3—C15	3.07 (19)
C11—C12—C13—C8	-0.5 (2)	C13—C14—N3—C15	-177.42 (11)
C11—C12—C13—C14	178.40 (13)	N2—C7—N3—C14	-4.69 (19)
N2—C8—C13—C12	176.23 (12)	N1—C7—N3—C14	174.18 (11)
C9—C8—C13—C12	-0.8 (2)	N2—C7—N3—C15	174.25 (12)
N2—C8—C13—C14	-2.65 (19)	N1—C7—N3—C15	-6.87 (17)
C9—C8—C13—C14	-179.65 (12)	C16—C15—N3—C14	-96.27 (14)
C12—C13—C14—O1	2.4 (2)	C16—C15—N3—C7	84.75 (15)

### Hydrogen-bond geometry ( $\text{\AA}$ , $^\circ$ )

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1 $\cdots$ N4	0.908 (17)	1.925 (17)	2.8049 (17)	162.8 (14)
N4—H4A $\cdots$ N2 <sup>i</sup>	0.889 (16)	2.323 (16)	3.1321 (18)	151.4 (13)
C3—H3 $\cdots$ Cg <sup>i</sup>	0.93	2.77 (1)	3.4741 (15)	132 (1)

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



Fig. 1

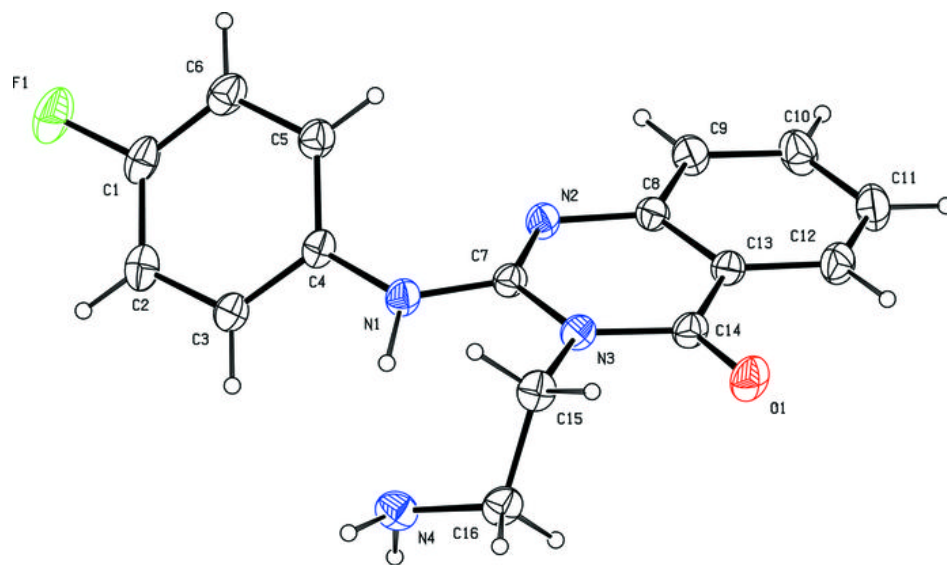


Fig. 2

