

## 3-Benzylamino-2-cyano-*N*-[*N*-(2-fluorophenyl)carbamoyl]-3-(methylsulfanyl)acrylamide

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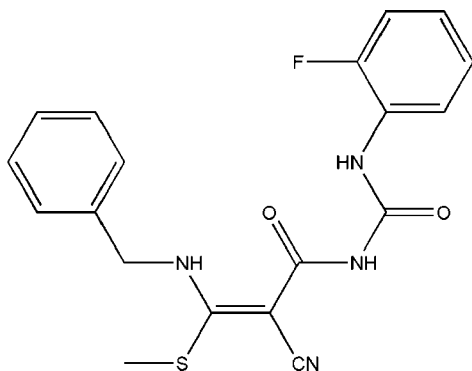
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Key indicators: single-crystal X-ray study;  $T = 133$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.035;  $wR$  factor = 0.079; data-to-parameter ratio = 16.3.

In the crystal structure of the title compound,  $\text{C}_{19}\text{H}_{17}\text{FN}_4\text{O}_2\text{S}$ , molecules are linked *via* pairs of  $\text{N}-\text{H}\cdots\text{N}$  interactions, forming centrosymmetric dimers. Two intramolecular  $\text{N}-\text{H}\cdots\text{O}$  hydrogen bonds stabilize the molecular conformation.

### Related literature

The title compound was synthesized as a herbicide. For details of the synthesis, see: Wang *et al.* (2004); Senda *et al.* (1972); Xue *et al.* (2002); Liu *et al.* (1998); Zhang *et al.* (2008).



### Experimental

#### Crystal data

$\text{C}_{19}\text{H}_{17}\text{FN}_4\text{O}_2\text{S}$   
 $M_r = 384.43$

Triclinic,  $P\bar{1}$   
 $a = 9.2415$  (18) Å

$b = 10.047$  (2) Å  
 $c = 11.0949$  (19) Å  
 $\alpha = 73.312$  (6)°  
 $\beta = 66.880$  (6)°  
 $\gamma = 84.295$  (7)°  
 $V = 907.4$  (3) Å<sup>3</sup>

$Z = 2$   
 Mo  $K\alpha$  radiation  
 $\mu = 0.21$  mm<sup>-1</sup>  
 $T = 133$  K  
 $0.48 \times 0.39 \times 0.39$  mm

#### Data collection

Rigaku AFC10/Saturn724+ diffractometer  
 Absorption correction: multi-scan (ABSCOR; Higashi, 1995)  
 $T_{\min} = 0.906$ ,  $T_{\max} = 0.923$

8644 measured reflections  
 4089 independent reflections  
 3137 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$

#### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.035$   
 $wR(F^2) = 0.079$   
 $S = 1.00$   
 4089 reflections  
 251 parameters

H atoms treated by a mixture of independent and constrained refinement  
 $\Delta\rho_{\max} = 0.32$  e Å<sup>-3</sup>  
 $\Delta\rho_{\min} = -0.23$  e Å<sup>-3</sup>

**Table 1**

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{N1}-\text{H1N}\cdots\text{O1}$	0.860 (17)	1.894 (17)	2.6024 (15)	138.7 (15)
$\text{N3}-\text{H3N}\cdots\text{O1}$	0.827 (16)	1.912 (16)	2.6012 (16)	140.1 (14)
$\text{N2}-\text{H2N}\cdots\text{N4}^i$	0.858 (15)	2.229 (16)	3.0710 (17)	166.8 (14)

Symmetry code: (i)  $-x, -y + 1, -z + 2$ .

Data collection: *CrystalClear* (Rigaku, 2008); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXL97*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2144).

### References

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**supplementary materials**

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### 3-Benzylamino-2-cyano-*N*-[*N*-(2-fluorophenyl)carbamoyl]-3-(methylsulfanyl)acrylamide

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#### Experimental

The title compound was prepared according to the reported method (Wang *et al.*, 2004; Senda *et al.*, 1972). Crystals of (I) suitable for XRD were obtained by slow evaporation of the acetone solution at 293 K.

#### Refinement

Positional parameters of all H atoms were calculated geometrically and were allowed to ride on the C, O and N atoms to which they are bonded, with C—H = 0.95 to 0.99 Å and  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ .

#### Figures

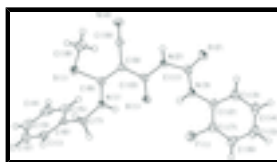


Fig. 1. The molecular structure of compound shows displacement ellipsoids drawn at the 50% probability level, all H atoms have been omitted for clarity.

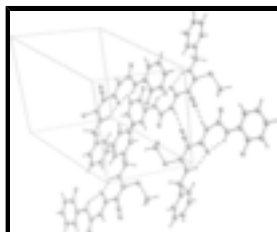


Fig. 2. The crystal packing of the title compound with hydrogen bonds drawn as dashed lines.

### 3-Benzylamino-2-cyano-*N*-[*N*-(2- fluorophenyl)carbamoyl]-3-(methylsulfanyl)acrylamide

#### Crystal data

$\text{C}_{19}\text{H}_{17}\text{FN}_4\text{O}_2\text{S}$

$M_r = 384.43$

Triclinic,  $P\bar{1}$

Hall symbol: -P 1

$a = 9.2415$  (18) Å

$b = 10.047$  (2) Å

$c = 11.0949$  (19) Å

$\alpha = 73.312$  (6)°

$\beta = 66.880$  (6)°

$\gamma = 84.295$  (7)°

$V = 907.4$  (3) Å<sup>3</sup>

$Z = 2$

$F(000) = 400$

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

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 2908 reflections

$\theta = 2.4$ – $29.1$ °

$\mu = 0.21$  mm<sup>-1</sup>

$T = 133$  K

Block, colourless

$0.48 \times 0.39 \times 0.39$  mm

## Data collection

Rigaku AFC10/Saturn724+ diffractometer	4089 independent reflections
Radiation source: Rotating Anode graphite	3137 reflections with $I > 2\sigma(I)$ $R_{\text{int}} = 0.025$
Detector resolution: 28.5714 pixels $\text{mm}^{-1}$ phi and $\omega$ scans	$\theta_{\text{max}} = 27.5^\circ$ , $\theta_{\text{min}} = 2.1^\circ$ $h = -11 \rightarrow 9$
Absorption correction: multi-scan ( <i>ABSCOR</i> ; Higashi, 1995) $T_{\text{min}} = 0.906$ , $T_{\text{max}} = 0.923$	$k = -13 \rightarrow 13$ $l = -14 \rightarrow 12$
8644 measured reflections	

## Refinement

Refinement on $F^2$	Primary atom site location: structure-invariant direct methods
Least-squares matrix: full	Secondary atom site location: difference Fourier map
$R[F^2 > 2\sigma(F^2)] = 0.035$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.079$	H atoms treated by a mixture of independent and constrained refinement
$S = 1.00$	$w = 1/[\sigma^2(F_o^2) + (0.0296P)^2 + 0.119P]$ where $P = (F_o^2 + 2F_c^2)/3$
4089 reflections	$(\Delta/\sigma)_{\text{max}} = 0.001$
251 parameters	$\Delta\rho_{\text{max}} = 0.32 \text{ e } \text{\AA}^{-3}$
0 restraints	$\Delta\rho_{\text{min}} = -0.23 \text{ e } \text{\AA}^{-3}$

## 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  $R$ - $wR$  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 ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.42534 (5)	0.14869 (4)	0.89857 (4)	0.02801 (11)
F1	0.21687 (11)	0.56288 (9)	0.25643 (8)	0.0357 (2)
O1	0.27259 (13)	0.42794 (11)	0.56187 (9)	0.0295 (3)
O2	-0.00916 (14)	0.75621 (12)	0.64645 (10)	0.0363 (3)
N1	0.43164 (14)	0.22266 (12)	0.65160 (11)	0.0222 (3)

N2	0.10887 (14)	0.55174 (12)	0.70402 (12)	0.0228 (3)
N3	0.11794 (15)	0.64303 (13)	0.48270 (12)	0.0239 (3)
N4	0.05563 (16)	0.35724 (14)	1.03305 (12)	0.0341 (3)
C1	0.63303 (18)	-0.12037 (16)	0.63660 (14)	0.0265 (3)
H1	0.7399	-0.0901	0.5950	0.032*
C2	0.5979 (2)	-0.26010 (17)	0.67324 (16)	0.0360 (4)
H2	0.6802	-0.3254	0.6567	0.043*
C3	0.4422 (2)	-0.30499 (17)	0.73435 (16)	0.0394 (4)
H3	0.4175	-0.4012	0.7596	0.047*
C4	0.3231 (2)	-0.20958 (17)	0.75847 (15)	0.0347 (4)
H4	0.2164	-0.2403	0.8006	0.042*
C5	0.35910 (18)	-0.06872 (16)	0.72123 (14)	0.0259 (3)
H5	0.2768	-0.0035	0.7382	0.031*
C6	0.51439 (16)	-0.02309 (14)	0.65956 (12)	0.0199 (3)
C7	0.56151 (16)	0.12821 (14)	0.61482 (14)	0.0223 (3)
H7A	0.6365	0.1390	0.6553	0.027*
H7B	0.6175	0.1559	0.5146	0.027*
C8	0.36183 (16)	0.25079 (14)	0.77143 (13)	0.0194 (3)
C9	0.24408 (17)	0.35141 (14)	0.79187 (13)	0.0219 (2)
C10	0.21072 (17)	0.44413 (15)	0.67827 (13)	0.0218 (3)
C11	0.06720 (17)	0.66004 (15)	0.60914 (14)	0.0235 (3)
C12	0.10494 (16)	0.73778 (15)	0.36651 (13)	0.0220 (3)
C13	0.05148 (17)	0.87350 (16)	0.35728 (15)	0.0287 (3)
H13	0.0137	0.9076	0.4355	0.034*
C14	0.05355 (18)	0.95894 (17)	0.23327 (16)	0.0354 (4)
H14	0.0189	1.0520	0.2271	0.042*
C15	0.10502 (19)	0.91076 (18)	0.11951 (16)	0.0378 (4)
H15	0.1044	0.9701	0.0359	0.045*
C16	0.15778 (19)	0.77617 (18)	0.12629 (15)	0.0330 (4)
H16	0.1927	0.7414	0.0485	0.040*
C17	0.15823 (17)	0.69412 (15)	0.24895 (14)	0.0259 (3)
C18	0.4107 (2)	0.25546 (18)	1.00866 (16)	0.0385 (4)
H18A	0.4372	0.3521	0.9544	0.058*
H18B	0.4839	0.2222	1.0548	0.058*
H18C	0.3030	0.2501	1.0767	0.058*
C19	0.14271 (17)	0.35427 (15)	0.92622 (13)	0.0219 (2)
H3N	0.1721 (19)	0.5738 (17)	0.4704 (15)	0.030 (5)*
H2N	0.0681 (19)	0.5644 (16)	0.7839 (16)	0.035 (5)*
H1N	0.394 (2)	0.2677 (18)	0.5923 (17)	0.040 (5)*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0371 (2)	0.0269 (2)	0.02340 (19)	0.00577 (17)	-0.01710 (17)	-0.00569 (15)
F1	0.0496 (6)	0.0324 (5)	0.0293 (5)	0.0090 (4)	-0.0187 (4)	-0.0121 (4)
O1	0.0418 (7)	0.0305 (6)	0.0189 (5)	0.0157 (5)	-0.0141 (5)	-0.0122 (4)
O2	0.0447 (7)	0.0339 (7)	0.0331 (6)	0.0205 (6)	-0.0174 (5)	-0.0163 (5)
N1	0.0279 (7)	0.0215 (7)	0.0191 (6)	0.0080 (5)	-0.0107 (5)	-0.0082 (5)

## supplementary materials

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N2	0.0267 (7)	0.0248 (7)	0.0179 (6)	0.0071 (5)	-0.0086 (5)	-0.0096 (5)
N3	0.0289 (7)	0.0202 (7)	0.0236 (6)	0.0069 (6)	-0.0117 (5)	-0.0073 (5)
N4	0.0354 (8)	0.0392 (8)	0.0242 (7)	0.0105 (7)	-0.0087 (6)	-0.0108 (6)
C1	0.0287 (8)	0.0298 (8)	0.0253 (7)	0.0082 (7)	-0.0129 (7)	-0.0125 (6)
C2	0.0572 (12)	0.0292 (9)	0.0354 (9)	0.0155 (8)	-0.0299 (9)	-0.0166 (7)
C3	0.0736 (14)	0.0225 (9)	0.0310 (8)	-0.0057 (9)	-0.0287 (9)	-0.0059 (7)
C4	0.0418 (10)	0.0380 (10)	0.0239 (8)	-0.0138 (8)	-0.0074 (7)	-0.0103 (7)
C5	0.0257 (8)	0.0303 (8)	0.0232 (7)	0.0001 (7)	-0.0070 (6)	-0.0127 (6)
C6	0.0231 (7)	0.0241 (7)	0.0140 (6)	0.0031 (6)	-0.0079 (6)	-0.0075 (5)
C7	0.0190 (7)	0.0233 (8)	0.0216 (7)	0.0028 (6)	-0.0044 (6)	-0.0074 (6)
C8	0.0229 (7)	0.0182 (7)	0.0180 (6)	-0.0018 (6)	-0.0085 (6)	-0.0046 (5)
C9	0.0264 (5)	0.0216 (5)	0.0189 (5)	0.0030 (4)	-0.0093 (4)	-0.0073 (4)
C10	0.0241 (7)	0.0222 (7)	0.0206 (7)	0.0025 (6)	-0.0083 (6)	-0.0091 (6)
C11	0.0225 (8)	0.0234 (8)	0.0262 (7)	0.0028 (6)	-0.0108 (6)	-0.0078 (6)
C12	0.0182 (7)	0.0225 (8)	0.0243 (7)	-0.0019 (6)	-0.0099 (6)	-0.0016 (6)
C13	0.0227 (8)	0.0274 (8)	0.0339 (8)	0.0034 (6)	-0.0114 (7)	-0.0052 (6)
C14	0.0254 (8)	0.0298 (9)	0.0444 (9)	0.0018 (7)	-0.0160 (8)	0.0030 (7)
C15	0.0284 (9)	0.0434 (11)	0.0354 (9)	-0.0044 (8)	-0.0190 (8)	0.0098 (7)
C16	0.0303 (9)	0.0428 (10)	0.0262 (8)	-0.0024 (7)	-0.0146 (7)	-0.0034 (7)
C17	0.0242 (8)	0.0255 (8)	0.0291 (8)	0.0005 (6)	-0.0129 (7)	-0.0051 (6)
C18	0.0453 (10)	0.0519 (11)	0.0315 (8)	0.0081 (9)	-0.0240 (8)	-0.0198 (8)
C19	0.0264 (5)	0.0216 (5)	0.0189 (5)	0.0030 (4)	-0.0093 (4)	-0.0073 (4)

### *Geometric parameters (Å, °)*

S1—C8	1.7567 (13)	C4—H4	0.9500
S1—C18	1.8041 (15)	C5—C6	1.385 (2)
F1—C17	1.3674 (16)	C5—H5	0.9500
O1—C10	1.2424 (16)	C6—C7	1.5085 (19)
O2—C11	1.2115 (16)	C7—H7A	0.9900
N1—C8	1.3303 (17)	C7—H7B	0.9900
N1—C7	1.4556 (17)	C8—C9	1.4060 (18)
N1—H1N	0.860 (17)	C9—C19	1.4223 (19)
N2—C10	1.3785 (17)	C9—C10	1.4577 (18)
N2—C11	1.4204 (17)	C12—C17	1.3847 (19)
N2—H2N	0.858 (15)	C12—C13	1.393 (2)
N3—C11	1.3499 (18)	C13—C14	1.391 (2)
N3—C12	1.4059 (17)	C13—H13	0.9500
N3—H3N	0.827 (16)	C14—C15	1.374 (2)
N4—C19	1.1488 (17)	C14—H14	0.9500
C1—C2	1.379 (2)	C15—C16	1.382 (2)
C1—C6	1.3903 (19)	C15—H15	0.9500
C1—H1	0.9500	C16—C17	1.375 (2)
C2—C3	1.386 (2)	C16—H16	0.9500
C2—H2	0.9500	C18—H18A	0.9800
C3—C4	1.382 (2)	C18—H18B	0.9800
C3—H3	0.9500	C18—H18C	0.9800
C4—C5	1.391 (2)		
C8—S1—C18	106.50 (7)	C9—C8—S1	124.36 (10)

C8—N1—C7	126.66 (12)	C8—C9—C19	120.11 (12)
C8—N1—H1N	113.5 (11)	C8—C9—C10	121.33 (12)
C7—N1—H1N	119.8 (11)	C19—C9—C10	118.19 (12)
C10—N2—C11	127.92 (12)	O1—C10—N2	120.88 (12)
C10—N2—H2N	120.9 (11)	O1—C10—C9	121.44 (12)
C11—N2—H2N	110.9 (11)	N2—C10—C9	117.68 (12)
C11—N3—C12	127.09 (13)	O2—C11—N3	126.13 (13)
C11—N3—H3N	116.0 (11)	O2—C11—N2	119.24 (12)
C12—N3—H3N	116.4 (11)	N3—C11—N2	114.63 (12)
C2—C1—C6	121.00 (16)	C17—C12—C13	117.29 (13)
C2—C1—H1	119.5	C17—C12—N3	116.69 (13)
C6—C1—H1	119.5	C13—C12—N3	125.92 (13)
C1—C2—C3	119.78 (16)	C14—C13—C12	119.87 (14)
C1—C2—H2	120.1	C14—C13—H13	120.1
C3—C2—H2	120.1	C12—C13—H13	120.1
C4—C3—C2	119.85 (16)	C15—C14—C13	120.97 (16)
C4—C3—H3	120.1	C15—C14—H14	119.5
C2—C3—H3	120.1	C13—C14—H14	119.5
C3—C4—C5	120.16 (16)	C14—C15—C16	120.23 (14)
C3—C4—H4	119.9	C14—C15—H15	119.9
C5—C4—H4	119.9	C16—C15—H15	119.9
C6—C5—C4	120.29 (15)	C17—C16—C15	118.02 (15)
C6—C5—H5	119.9	C17—C16—H16	121.0
C4—C5—H5	119.9	C15—C16—H16	121.0
C5—C6—C1	118.91 (14)	F1—C17—C16	119.01 (13)
C5—C6—C7	122.99 (13)	F1—C17—C12	117.38 (12)
C1—C6—C7	118.09 (13)	C16—C17—C12	123.59 (14)
N1—C7—C6	114.88 (12)	S1—C18—H18A	109.5
N1—C7—H7A	108.5	S1—C18—H18B	109.5
C6—C7—H7A	108.5	H18A—C18—H18B	109.5
N1—C7—H7B	108.5	S1—C18—H18C	109.5
C6—C7—H7B	108.5	H18A—C18—H18C	109.5
H7A—C7—H7B	107.5	H18B—C18—H18C	109.5
N1—C8—C9	121.34 (12)	N4—C19—C9	177.14 (16)
N1—C8—S1	114.28 (10)		
C6—C1—C2—C3	-0.2 (2)	C19—C9—C10—O1	-165.04 (14)
C1—C2—C3—C4	-0.1 (2)	C8—C9—C10—N2	-171.45 (13)
C2—C3—C4—C5	0.2 (2)	C19—C9—C10—N2	15.5 (2)
C3—C4—C5—C6	0.1 (2)	C12—N3—C11—O2	6.0 (3)
C4—C5—C6—C1	-0.5 (2)	C12—N3—C11—N2	-174.67 (13)
C4—C5—C6—C7	179.10 (12)	C10—N2—C11—O2	-170.90 (14)
C2—C1—C6—C5	0.52 (19)	C10—N2—C11—N3	9.7 (2)
C2—C1—C6—C7	-179.06 (12)	C11—N3—C12—C17	-176.54 (14)
C8—N1—C7—C6	81.84 (17)	C11—N3—C12—C13	7.2 (2)
C5—C6—C7—N1	4.96 (18)	C17—C12—C13—C14	-0.1 (2)
C1—C6—C7—N1	-175.49 (12)	N3—C12—C13—C14	176.14 (14)
C7—N1—C8—C9	175.63 (13)	C12—C13—C14—C15	1.2 (2)
C7—N1—C8—S1	-6.28 (19)	C13—C14—C15—C16	-0.8 (2)
C18—S1—C8—N1	148.59 (11)	C14—C15—C16—C17	-0.6 (2)

## supplementary materials

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C18—S1—C8—C9	-33.39 (15)	C15—C16—C17—F1	-176.93 (14)
N1—C8—C9—C19	163.12 (14)	C15—C16—C17—C12	1.8 (2)
S1—C8—C9—C19	-14.8 (2)	C13—C12—C17—F1	177.34 (13)
N1—C8—C9—C10	-9.8 (2)	N3—C12—C17—F1	0.7 (2)
S1—C8—C9—C10	172.35 (11)	C13—C12—C17—C16	-1.4 (2)
C11—N2—C10—O1	-4.2 (2)	N3—C12—C17—C16	-178.01 (14)
C11—N2—C10—C9	175.25 (14)	C8—C9—C19—N4	-135 (3)
C8—C9—C10—O1	8.0 (2)	C10—C9—C19—N4	38 (3)

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

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H1N $\cdots$ O1	0.860 (17)	1.894 (17)	2.6024 (15)	138.7 (15)
N3—H3N $\cdots$ O1	0.827 (16)	1.912 (16)	2.6012 (16)	140.1 (14)
N2—H2N $\cdots$ N4 <sup>i</sup>	0.858 (15)	2.229 (16)	3.0710 (17)	166.8 (14)

Symmetry codes: (i)  $-x, -y+1, -z+2$ .



Fig. 1

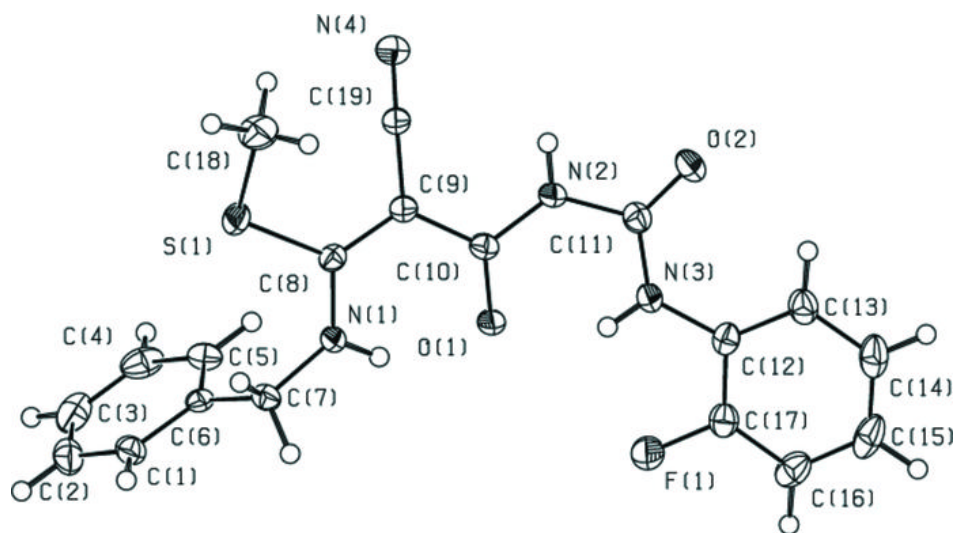


Fig. 2

