Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-Methyl-1-phenyl-4-{phenyl[4-(trifluoromethyl)anilino]methylene}-1*H*-pyrazol-5(4*H*)-one

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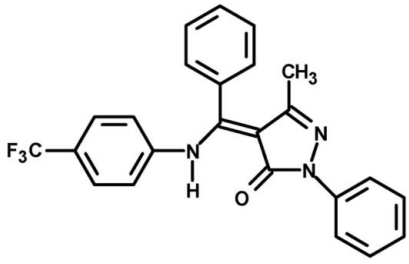
Received 31 July 2007; accepted 2 August 2007

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.004 Å; R factor = 0.055; wR factor = 0.163; data-to-parameter ratio = 12.5.

In the title compound, $C_{24}H_{18}F_3N_3O$, the molecule exists in the enamine–keto tautomeric form. The pyrazolone ring makes dihedral angles of 31.8 (2), 45.4 (2) and 71.2 (2)° with the 1-phenyl, aniline and methylene-bound phenyl rings, respectively. An intramolecular N—H···O hydrogen bond helps to stabilize the molecular conformation.

Related literature

For related structures, see: Sun *et al.* (2006, 2007). For background literature, see: Akama & Tong (1996); Eller & Holzer (2004); Jiang *et al.* (2004); Lu *et al.* (2006).



Experimental

Crystal data

$C_{24}H_{18}F_3N_3O$
M_r = 421.41
Triclinic, $P\overline{1}$
a = 7.6059 (9) Å
b = 10.9913 (12) Å
c = 13.8057 (15) Å
α = 108.448 (2)°
β = 100.227 (2)°
γ = 105.178 (2)°
V = 1013.0 (2) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 273 (2) K
0.35 × 0.26 × 0.18 mm

Data collection

Bruker SMART CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.964, T_{max} = 0.981
5150 measured reflections
3527 independent reflections
3079 reflections with $I > 2\sigma(I)$
R_{int} = 0.011

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.163
S = 1.00
3527 reflections
282 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O1	0.86	1.98	2.704 (2)	141

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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, 1997); software used to prepare material for publication: *SHELXTL*.

The authors thank Taishan University for financial support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB2502).

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 doi:10.1107/S1600536807037993

supplementary materials

Acta Cryst. (2007). E**63**, o3725 [**doi:10.1107/S1600536807037993**]

3-Methyl-1-phenyl-4-{phenyl[4-(trifluoromethyl)anilino]methylene}-1*H*-pyrazol-5(4*H*)-one

Y.-F. Sun, X.-L. Wang, S.-Y. Ma and Z.-Y. Wang

Comment

The title compound, (I), was synthesized as part of a continuing project involving the structures of pyrazolone derivatives. Pyrazolone derivatives are well known for their potential applications in the areas of pharmaceuticals, agrochemicals, dyes, and pigments, and also as chelating agents and extracting agents. Moreover, they are capable of prototropic tautomerism (Akama & Tong, 1996; Eller & Holzer, 2004).

The molecule of (I) exists in enamine-keto tautomeric form in the crystal instead of the imine form (Fig. 1), as in 4-[(*Z*)-(benzylamino) phenylmethylene]-5-methyl-2-phenyl-2*H*-pyrazol-3-one (Jiang *et al.*, 2004). The central pyrazolone (C1–C3/N1/N2) ring is essentially planar, with an r.m.s. deviation of 0.0116 Å for the fitted atoms. This ring makes dihedral angles of 31.8 (2), 45.4 (2) and 71.2 (2)° with the C5–C10, C12–C17 and C19–C24 phenyl rings, respectively. Similar tautomerism has also been observed in related pyrazolone analogues reported by us previously (Sun *et al.*, 2006, 2007). In addition, the present compound also features an intramolecular hydrogen bond between the N3 and O1 atoms (Table 1), leading to the fact that atoms O1 and N3 are on the same side of the C2–C11 bond, which will be the potential bidentate N,*O*-chelate positions after deprotonation to form functional complexes as candidates with catalytic applications (Lu *et al.*, 2006).

Experimental

A mixture of 1-phenyl-3-methyl-4-benzoyl-pyrazolone-5 (1 mmol) and 4-trifluoromethylaniline (1 mmol) in anhydrous ethanol (30 ml) was refluxed for 3 hr, and then cooled to room temperature. The precipitate was filtered and dried. The crude product was recrystallized from ethanol. Yellow crystals were thus obtained in 83% yield. A single-crystal of (I) suitable for an X-ray structural analysis was obtained by slowly evaporating a ethanolic solution at room temperature.

Refinement

All H atoms were initially located in a difference map then relocated to idealized locations (C—H = 0.93–0.96 Å, N—H = 0.86 Å) and refined as riding with U_{iso}(H) = 1.2U_{eq}(C, N) or 1.5U_{eq}(methyl C). The highest difference peak is 1.33Å from F2.

Figures

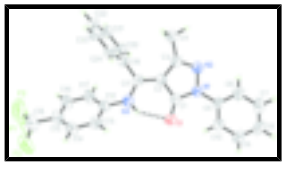


Fig. 1. View of the molecular structure of (I) showing displacement ellipsoids at the 50% probability level. H atoms are shown as spheres of arbitrary radius. The dashed line indicates hydrogen bond.

3-Methyl-1-phenyl-4-{phenyl[4-(trifluoromethyl)anilino]methylene}-1*H*-pyrazol-\ 5(4*H*)-one

Crystal data

$C_{24}H_{18}F_3N_3O$	$Z = 2$
$M_r = 421.41$	$F_{000} = 436$
Triclinic, $P\overline{1}$	$D_x = 1.382$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 7.6059$ (9) Å	Cell parameters from 3675 reflections
$b = 10.9913$ (12) Å	$\theta = 2.1$–28.2º
$c = 13.8057$ (15) Å	$\mu = 0.11$ mm^{-1}
$\alpha = 108.448$ (2)º	$T = 273$ (2) K
$\beta = 100.227$ (2)º	Block, yellow
$\gamma = 105.178$ (2)º	0.35 × 0.26 × 0.18 mm
$V = 1013.0$ (2) Å^3	

Data collection

Bruker SMART CCD diffractometer	3527 independent reflections
Radiation source: fine-focus sealed tube	3079 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.011$
$T = 273$(2) K	$\theta_{max} = 25.0$º
ω scans	$\theta_{min} = 2.1$º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$h = -8\rightarrow9$
$T_{min} = 0.964$, $T_{max} = 0.981$	$k = -12\rightarrow13$
5150 measured reflections	$l = -16\rightarrow16$

Refinement

Refinement on F^2	Hydrogen site location: difference Fourier map
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.055$	$w = 1/[\sigma^2(F_o^2) + (0.088P)^2 + 0.5882P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.163$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.00$	$\Delta\rho_{max} = 0.71$ e Å^{-3}
3527 reflections	$\Delta\rho_{min} = -0.39$ e Å^{-3}
282 parameters	Extinction correction: SHELXL97
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 $F^2 > 2\text{sigma}(F^2)$ 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}
F1	1.2873 (3)	0.7703 (4)	0.52098 (18)	0.1651 (15)
F2	1.1537 (3)	0.7329 (3)	0.6340 (3)	0.1570 (13)
F3	1.2712 (3)	0.9287 (2)	0.64567 (18)	0.1190 (8)
O1	0.2518 (2)	0.89023 (15)	0.26159 (13)	0.0553 (4)
N1	−0.0459 (2)	0.74140 (17)	0.14646 (14)	0.0452 (4)
N2	−0.1474 (3)	0.60170 (17)	0.10526 (14)	0.0481 (5)
N3	0.4577 (2)	0.74680 (18)	0.32255 (14)	0.0489 (5)
H3	0.4386	0.8219	0.3269	0.059*
C1	0.1347 (3)	0.7735 (2)	0.20940 (17)	0.0433 (5)
C2	0.1515 (3)	0.6428 (2)	0.20245 (16)	0.0418 (5)
C3	−0.0321 (3)	0.5436 (2)	0.13746 (17)	0.0445 (5)
C4	−0.1047 (4)	0.3929 (2)	0.1069 (2)	0.0617 (7)
H4A	−0.2385	0.3579	0.0713	0.093*
H4B	−0.0832	0.3724	0.1697	0.093*
H4C	−0.0393	0.3514	0.0599	0.093*
C5	−0.1398 (3)	0.8326 (2)	0.13113 (16)	0.0446 (5)
C6	−0.3329 (3)	0.7998 (3)	0.11965 (19)	0.0545 (6)
H6	−0.4027	0.7169	0.1203	0.065*
C7	−0.4214 (4)	0.8914 (3)	0.1072 (2)	0.0634 (7)
H7	−0.5509	0.8701	0.0998	0.076*
C8	−0.3185 (4)	1.0139 (3)	0.1055 (2)	0.0668 (7)
H8	−0.3780	1.0756	0.0978	0.080*
C9	−0.1283 (4)	1.0441 (3)	0.1152 (2)	0.0692 (7)
H9	−0.0592	1.1263	0.1133	0.083*
C10	−0.0376 (4)	0.9544 (2)	0.1279 (2)	0.0583 (6)
H10	0.0917	0.9759	0.1342	0.070*
C11	0.3135 (3)	0.6321 (2)	0.25890 (16)	0.0418 (5)
C12	0.6381 (3)	0.7604 (2)	0.38376 (17)	0.0454 (5)
C13	0.7166 (3)	0.8622 (2)	0.48522 (18)	0.0504 (5)
H13	0.6512	0.9199	0.5115	0.061*
C14	0.8908 (3)	0.8778 (2)	0.54689 (18)	0.0551 (6)
H14	0.9428	0.9462	0.6147	0.066*
C15	0.9884 (3)	0.7923 (3)	0.50833 (18)	0.0523 (6)

C16	0.9117 (3)	0.6922 (3)	0.40642 (18)	0.0566 (6)
H16	0.9775	0.6347	0.3802	0.068*
C17	0.7391 (3)	0.6772 (3)	0.34380 (18)	0.0552 (6)
H17	0.6902	0.6115	0.2748	0.066*
C18	1.1727 (4)	0.8038 (3)	0.5758 (2)	0.0710 (8)
C19	0.3297 (3)	0.4991 (2)	0.25615 (16)	0.0433 (5)
C20	0.3411 (3)	0.4054 (2)	0.16447 (18)	0.0525 (6)
H20	0.3318	0.4228	0.1024	0.063*
C21	0.3666 (4)	0.2856 (2)	0.1664 (2)	0.0650 (7)
H21	0.3753	0.2228	0.1054	0.078*
C22	0.3792 (4)	0.2590 (3)	0.2577 (2)	0.0694 (8)
H22	0.3982	0.1791	0.2586	0.083*
C23	0.3637 (4)	0.3507 (3)	0.3479 (2)	0.0670 (7)
H23	0.3692	0.3317	0.4091	0.080*
C24	0.3399 (3)	0.4708 (2)	0.34747 (19)	0.0540 (6)
H24	0.3307	0.5329	0.4086	0.065*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.0721 (13)	0.299 (4)	0.0878 (15)	0.0989 (19)	0.0070 (11)	0.0061 (19)
F2	0.0921 (16)	0.199 (3)	0.202 (3)	0.0332 (17)	−0.0128 (16)	0.148 (3)
F3	0.0832 (13)	0.1226 (17)	0.0949 (14)	0.0156 (12)	−0.0288 (11)	0.0146 (13)
O1	0.0488 (9)	0.0386 (8)	0.0681 (10)	0.0136 (7)	0.0022 (7)	0.0158 (7)
N1	0.0427 (9)	0.0382 (9)	0.0524 (10)	0.0155 (7)	0.0047 (8)	0.0179 (8)
N2	0.0468 (10)	0.0396 (9)	0.0520 (10)	0.0136 (8)	0.0049 (8)	0.0159 (8)
N3	0.0460 (10)	0.0439 (10)	0.0538 (11)	0.0185 (8)	0.0044 (8)	0.0175 (8)
C1	0.0419 (11)	0.0416 (11)	0.0464 (11)	0.0161 (9)	0.0095 (9)	0.0170 (9)
C2	0.0450 (11)	0.0394 (10)	0.0426 (10)	0.0177 (9)	0.0102 (9)	0.0161 (8)
C3	0.0460 (11)	0.0412 (11)	0.0455 (11)	0.0162 (9)	0.0088 (9)	0.0167 (9)
C4	0.0560 (14)	0.0396 (12)	0.0779 (17)	0.0128 (10)	0.0039 (12)	0.0184 (11)
C5	0.0494 (12)	0.0447 (11)	0.0410 (11)	0.0221 (9)	0.0074 (9)	0.0163 (9)
C6	0.0501 (13)	0.0626 (14)	0.0567 (13)	0.0241 (11)	0.0124 (10)	0.0277 (11)
C7	0.0550 (14)	0.0838 (18)	0.0582 (14)	0.0401 (14)	0.0110 (11)	0.0251 (13)
C8	0.0799 (18)	0.0612 (15)	0.0594 (15)	0.0437 (14)	0.0031 (13)	0.0162 (12)
C9	0.0738 (17)	0.0480 (13)	0.0828 (18)	0.0259 (12)	0.0036 (14)	0.0273 (13)
C10	0.0531 (13)	0.0477 (13)	0.0747 (16)	0.0195 (10)	0.0091 (11)	0.0273 (12)
C11	0.0463 (11)	0.0435 (11)	0.0386 (10)	0.0189 (9)	0.0130 (9)	0.0162 (8)
C12	0.0420 (11)	0.0480 (11)	0.0476 (11)	0.0156 (9)	0.0101 (9)	0.0215 (9)
C13	0.0486 (12)	0.0439 (11)	0.0547 (13)	0.0155 (9)	0.0128 (10)	0.0147 (10)
C14	0.0493 (12)	0.0561 (13)	0.0465 (12)	0.0113 (10)	0.0078 (10)	0.0111 (10)
C15	0.0418 (11)	0.0667 (14)	0.0468 (12)	0.0154 (10)	0.0123 (9)	0.0220 (11)
C16	0.0479 (12)	0.0717 (16)	0.0513 (13)	0.0291 (11)	0.0153 (10)	0.0172 (11)
C17	0.0477 (12)	0.0669 (15)	0.0427 (11)	0.0225 (11)	0.0092 (9)	0.0099 (10)
C18	0.0534 (15)	0.095 (2)	0.0564 (15)	0.0266 (14)	0.0080 (12)	0.0216 (15)
C19	0.0410 (11)	0.0446 (11)	0.0462 (11)	0.0188 (9)	0.0080 (8)	0.0188 (9)
C20	0.0580 (13)	0.0514 (13)	0.0474 (12)	0.0253 (11)	0.0082 (10)	0.0162 (10)
C21	0.0654 (15)	0.0501 (13)	0.0686 (16)	0.0292 (12)	0.0031 (12)	0.0096 (12)

C22	0.0652 (16)	0.0463 (13)	0.087 (2)	0.0205 (12)	−0.0063 (14)	0.0266 (13)
C23	0.0690 (16)	0.0641 (16)	0.0682 (16)	0.0160 (13)	0.0025 (13)	0.0403 (14)
C24	0.0594 (14)	0.0561 (13)	0.0494 (12)	0.0209 (11)	0.0129 (10)	0.0243 (10)

Geometric parameters (Å, °)

F1—C18	1.301 (3)	C9—C10	1.379 (3)
F2—C18	1.286 (4)	C9—H9	0.9300
F3—C18	1.321 (4)	C10—H10	0.9300
O1—C1	1.244 (3)	C11—C19	1.488 (3)
N1—C1	1.377 (3)	C12—C17	1.389 (3)
N1—N2	1.396 (2)	C12—C13	1.390 (3)
N1—C5	1.419 (3)	C13—C14	1.378 (3)
N2—C3	1.307 (3)	C13—H13	0.9300
N3—C11	1.340 (3)	C14—C15	1.381 (3)
N3—C12	1.421 (3)	C14—H14	0.9300
N3—H3	0.8600	C15—C16	1.387 (3)
C1—C2	1.451 (3)	C15—C18	1.489 (3)
C2—C11	1.390 (3)	C16—C17	1.375 (3)
C2—C3	1.442 (3)	C16—H16	0.9300
C3—C4	1.491 (3)	C17—H17	0.9300
C4—H4A	0.9600	C19—C24	1.385 (3)
C4—H4B	0.9600	C19—C20	1.390 (3)
C4—H4C	0.9600	C20—C21	1.388 (3)
C5—C10	1.380 (3)	C20—H20	0.9300
C5—C6	1.385 (3)	C21—C22	1.375 (4)
C6—C7	1.385 (3)	C21—H21	0.9300
C6—H6	0.9300	C22—C23	1.379 (4)
C7—C8	1.379 (4)	C22—H22	0.9300
C7—H7	0.9300	C23—C24	1.380 (3)
C8—C9	1.368 (4)	C23—H23	0.9300
C8—H8	0.9300	C24—H24	0.9300
C1—N1—N2	112.32 (16)	C17—C12—C13	119.5 (2)
C1—N1—C5	127.73 (17)	C17—C12—N3	121.8 (2)
N2—N1—C5	119.51 (17)	C13—C12—N3	118.66 (19)
C3—N2—N1	106.70 (17)	C14—C13—C12	120.2 (2)
C11—N3—C12	128.37 (18)	C14—C13—H13	119.9
C11—N3—H3	115.8	C12—C13—H13	119.9
C12—N3—H3	115.8	C13—C14—C15	120.2 (2)
O1—C1—N1	126.24 (19)	C13—C14—H14	119.9
O1—C1—C2	129.26 (19)	C15—C14—H14	119.9
N1—C1—C2	104.48 (17)	C14—C15—C16	119.7 (2)
C11—C2—C3	132.65 (19)	C14—C15—C18	120.9 (2)
C11—C2—C1	122.13 (19)	C16—C15—C18	119.4 (2)
C3—C2—C1	104.96 (17)	C17—C16—C15	120.5 (2)
N2—C3—C2	111.44 (18)	C17—C16—H16	119.8
N2—C3—C4	118.50 (19)	C15—C16—H16	119.8
C2—C3—C4	130.03 (19)	C16—C17—C12	119.9 (2)
C3—C4—H4A	109.5	C16—C17—H17	120.1

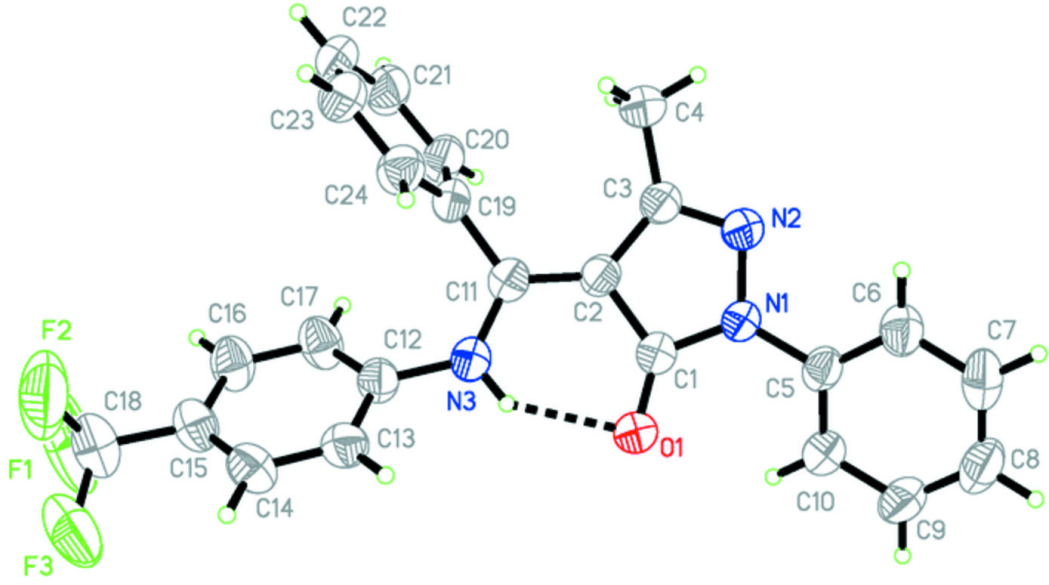
C3—C4—H4B	109.5	C12—C17—H17	120.1
H4A—C4—H4B	109.5	F2—C18—F1	108.1 (3)
C3—C4—H4C	109.5	F2—C18—F3	103.3 (3)
H4A—C4—H4C	109.5	F1—C18—F3	104.5 (3)
H4B—C4—H4C	109.5	F2—C18—C15	113.4 (2)
C10—C5—C6	120.1 (2)	F1—C18—C15	113.1 (2)
C10—C5—N1	119.7 (2)	F3—C18—C15	113.5 (3)
C6—C5—N1	120.2 (2)	C24—C19—C20	119.8 (2)
C5—C6—C7	119.4 (2)	C24—C19—C11	119.31 (19)
C5—C6—H6	120.3	C20—C19—C11	120.87 (19)
C7—C6—H6	120.3	C21—C20—C19	119.4 (2)
C8—C7—C6	120.4 (2)	C21—C20—H20	120.3
C8—C7—H7	119.8	C19—C20—H20	120.3
C6—C7—H7	119.8	C22—C21—C20	120.5 (2)
C9—C8—C7	119.5 (2)	C22—C21—H21	119.8
C9—C8—H8	120.3	C20—C21—H21	119.8
C7—C8—H8	120.3	C21—C22—C23	120.0 (2)
C8—C9—C10	121.0 (3)	C21—C22—H22	120.0
C8—C9—H9	119.5	C23—C22—H22	120.0
C10—C9—H9	119.5	C22—C23—C24	120.1 (2)
C9—C10—C5	119.6 (2)	C22—C23—H23	119.9
C9—C10—H10	120.2	C24—C23—H23	119.9
C5—C10—H10	120.2	C23—C24—C19	120.2 (2)
N3—C11—C2	118.67 (18)	C23—C24—H24	119.9
N3—C11—C19	118.50 (18)	C19—C24—H24	119.9
C2—C11—C19	122.75 (18)		
C1—N1—N2—C3	−2.4 (2)	C3—C2—C11—C19	4.0 (4)
C5—N1—N2—C3	−175.31 (18)	C1—C2—C11—C19	177.36 (19)
N2—N1—C1—O1	−175.1 (2)	C11—N3—C12—C17	41.3 (3)
C5—N1—C1—O1	−3.0 (4)	C11—N3—C12—C13	−140.4 (2)
N2—N1—C1—C2	3.3 (2)	C17—C12—C13—C14	−1.9 (3)
C5—N1—C1—C2	175.43 (19)	N3—C12—C13—C14	179.7 (2)
O1—C1—C2—C11	0.6 (4)	C12—C13—C14—C15	−0.1 (4)
N1—C1—C2—C11	−177.68 (19)	C13—C14—C15—C16	1.2 (4)
O1—C1—C2—C3	175.5 (2)	C13—C14—C15—C18	−177.2 (2)
N1—C1—C2—C3	−2.8 (2)	C14—C15—C16—C17	−0.2 (4)
N1—N2—C3—C2	0.5 (2)	C18—C15—C16—C17	178.2 (2)
N1—N2—C3—C4	178.7 (2)	C15—C16—C17—C12	−1.8 (4)
C11—C2—C3—N2	175.6 (2)	C13—C12—C17—C16	2.9 (4)
C1—C2—C3—N2	1.5 (2)	N3—C12—C17—C16	−178.8 (2)
C11—C2—C3—C4	−2.4 (4)	C14—C15—C18—F2	87.5 (4)
C1—C2—C3—C4	−176.5 (2)	C16—C15—C18—F2	−90.9 (3)
C1—N1—C5—C10	36.3 (3)	C14—C15—C18—F1	−148.9 (3)
N2—N1—C5—C10	−152.0 (2)	C16—C15—C18—F1	32.7 (4)
C1—N1—C5—C6	−143.6 (2)	C14—C15—C18—F3	−30.0 (4)
N2—N1—C5—C6	28.1 (3)	C16—C15—C18—F3	151.6 (3)
C10—C5—C6—C7	−1.3 (3)	N3—C11—C19—C24	64.0 (3)
N1—C5—C6—C7	178.6 (2)	C2—C11—C19—C24	−112.7 (2)
C5—C6—C7—C8	0.4 (4)	N3—C11—C19—C20	−113.8 (2)

C6—C7—C8—C9	0.6 (4)	C2—C11—C19—C20	69.5 (3)
C7—C8—C9—C10	−0.7 (4)	C24—C19—C20—C21	−1.3 (3)
C8—C9—C10—C5	−0.2 (4)	C11—C19—C20—C21	176.5 (2)
C6—C5—C10—C9	1.2 (4)	C19—C20—C21—C22	0.5 (4)
N1—C5—C10—C9	−178.6 (2)	C20—C21—C22—C23	1.0 (4)
C12—N3—C11—C2	−177.2 (2)	C21—C22—C23—C24	−1.5 (4)
C12—N3—C11—C19	6.0 (3)	C22—C23—C24—C19	0.6 (4)
C3—C2—C11—N3	−172.6 (2)	C20—C19—C24—C23	0.8 (4)
C1—C2—C11—N3	0.7 (3)	C11—C19—C24—C23	−177.0 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O1	0.86	1.98	2.704 (2)	141

Fig. 1


C22
C21
C23
C20
C24
C19
C4
C3
N2
C11
C2
N1
C6
C7
C16
C17
F2
C12
N3
C1
C5
C18
O1
C8
F1
C15
C13
C10
C14
C9
F3