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1,5-Dimethyl-2-phenyl-4-(4,4,4-trifluoro-3-oxo-1-phenylbut-1-enylamino)-1*H*-pyrazol-3(2*H*)-one

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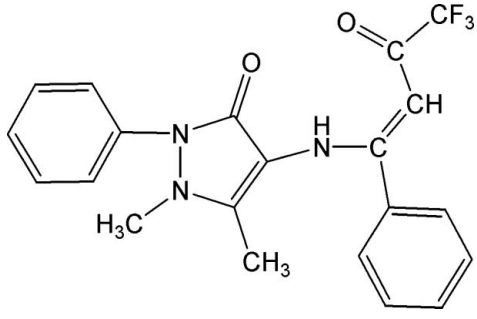
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.044; wR factor = 0.131; data-to-parameter ratio = 11.6.

In the title compound, $C_{21}H_{18}F_3N_3O_2$, the pyrazole ring is approximately planar and forms dihedral angles of 47.61 (9) and 69.39 (8)° with the two phenyl rings. An intramolecular N—H···O hydrogen bond stabilizes the molecular conformation. Intermolecular N—H···O hydrogen bonds link the molecules into centrosymmetric dimers. The trifluoromethyl group is disordered over two positions in a ratio of ∼0.8:0.2.

Related literature

For general background, see: Belloni *et al.* (2005); Kahwa *et al.* (1986); Parashar *et al.* (1988); Santos *et al.* (2001); Tynan *et al.* (2005).



Experimental

Crystal data

$C_{21}H_{18}F_3N_3O_2$
M_r = 401.38
Monoclinic, $P2_1/c$
a = 13.452 (4) Å
b = 6.3930 (18) Å
c = 23.466 (7) Å
β = 90.571 (5)°
V = 2017.9 (10) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.11 mm^{-1}
T = 294 (2) K
0.22 × 0.20 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.977, T_{max} = 0.985
9666 measured reflections
3554 independent reflections
2134 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.131
S = 1.02
3554 reflections
306 parameters
71 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3···O2	0.92 (3)	2.02 (3)	2.761 (3)	137 (2)
N3—H3···O2^{i}	0.92 (3)	2.40 (3)	3.094 (3)	133 (2)

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

Data collection: *SMART* (Bruker, 1999); 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, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2393).

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supplementary materials

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1,5-Dimethyl-2-phenyl-4-(4,4,4-trifluoro-3-oxo-1-phenylbut-1-enylamino)-1*H*-pyrazol-3(2*H*)-one

Z.-L. Jing, S.-J. Zhang and J.-Q. Zhai

Comment

In order to establish control over the preparation of crystalline solid materials so that their architecture and properties are predictable (Belloni *et al.*, 2005; Tynan *et al.*, 2005; Parashar *et al.*, 1988), the synthesis of new and designed crystal structures has become a major strand of modern chemistry. Metal complexes based on Schiff bases have attracted much attention because they can be utilized as model compounds of the active centres in various proteins and enzymes (Kahwa *et al.*, 1986; Santos *et al.*,2001). As part of an investigation of the coordination properties of Shiff bases functioning as ligands, we report the synthesis and crystal structure of the title compound, (I).

In the molecular structure of the compound (I) (Fig. 1), the geometric parameters are normal. The pyrazole ring (C1—C3/N1/N2) is approximately planar, with a maximum deviation from the mean plane of 0.046 (1) Å for atom N1. The least-squares plane through the pyrazole ring forms dihedral angles of 47.61 (9) and 69.39 (8)°, respectively, with the C5—C10 and C13—C18 phenyl rings. The two phenyl rings are inclined at an angle of 80.70 (8)°.

An intramolecular N—H···O hydrogen bond stabilizes the molecular conformation. In the crystal structure, intermolecular N—H···O hydrogen bonds link the molecules into centrosymmetric dimers as illustrated in Fig. 2.

Experimental

An anhydrous ethanol solution (50 ml) of 4,4,4-trifluoro-1-phenyl- butane-1,3-dione (2.16 g, 10 mmol) was added to an anhydrous ethanol solution (50 ml) of 4-amino-1,5-dimethyl-2-phenyl-pyrazolidin-3-one (2.03 g, 10 mmol), and the mixture was stirred at 350 K for 6 h under N_2, whereupon a yellow precipitate appeared. The product was isolated, recrystallized from anhydrous ethanol and then dried *in vacuo* to give pure compound (I) in 79% yield. Yellows single crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an anhydrous ethanol solution.

Refinement

The trifluoromethyl group was treated as disordered over two orientations with refined occupancies of 0.802 (8) and 0.198 (8). All C—F bond lengths were restrained to 1.35 (1) Å, and the C20—C21 and C20—C21' distances were restrained to 1.52 (1) Å. The F···F distances were restrained to be equal, within a standard deviation of 0.01 Å. The displacement parameters of the disordered atoms were restrained to approximately isotropic behaviour. The N-bound H atom was located in a difference Fourier map and its positional parameters were refined, with U_{iso}(H) = 1.2U_{eq}(N). C-bound H atoms were included in calculated positions, with C—H = 0.93 (aromatic) or 0.96 Å (methyl), and refined using a riding model, with U_{iso}(H) = 1.2U_{eq}(C) for aromatic H or 1.5U_{eq}(C) for methyl H atoms.

Figures

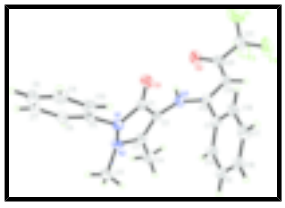

Fig. 1. The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

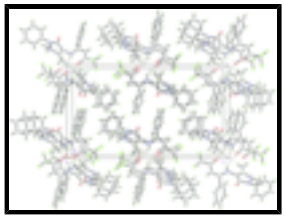

Fig. 2. The crystal packing of (I), viwed down the *b* axis. Hydrogen bonds are indicated by dashed lines.

1,5-Dimethyl-2-phenyl-4-(4,4,4-trifluoro-3-oxo-1-phenylbut-1-enylamino)- 1*H*-pyrazol-3(2*H*)-one

Crystal data

$C_{21}H_{18}F_3N_3O_2$	F_{000} = 832
M_r = 401.38	D_x = 1.321 Mg m^{-3}
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: -P 2ybc	Cell parameters from 2616 reflections
a = 13.452 (4) Å	θ = 2.3–23.6º
b = 6.3930 (18) Å	μ = 0.11 mm^{-1}
c = 23.466 (7) Å	T = 294 (2) K
β = 90.571 (5)º	Block, yellow
V = 2017.9 (10) Å^3	0.22 × 0.20 × 0.14 mm
Z = 4	

Data collection

Bruker SMART CCD area-detector diffractometer	3554 independent reflections
Radiation source: fine-focus sealed tube	2134 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.047
T = 294(2) K	θ_{max} = 25.0º
φ and ω scans	θ_{min} = 1.5º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −16→13
T_{min} = 0.977, T_{max} = 0.985	k = −7→7
9666 measured reflections	l = −27→27

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map

Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.044$	H atoms treated by a mixture of independent and constrained refinement
$wR(F^2) = 0.131$	$w = 1/[\sigma^2(F_o^2) + (0.059P)^2 + 0.2821P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} = 0.001$
3554 reflections	$\Delta\rho_{max} = 0.19$ e Å^{-3}
306 parameters	$\Delta\rho_{min} = -0.16$ e Å^{-3}
71 restraints	Extinction correction: SHELXL97 (Sheldrick, 1997), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Primary atom site location: structure-invariant direct methods	Extinction coefficient: 0.0114 (15)

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}	Occ. (<1)
C21	0.0597 (4)	−0.1194 (12)	0.6599 (2)	0.075 (3)	0.802 (8)
F1	0.0622 (5)	−0.3257 (6)	0.65744 (17)	0.1370 (19)	0.802 (8)
F2	−0.0333 (2)	−0.0639 (9)	0.67356 (15)	0.1254 (19)	0.802 (8)
F3	0.1167 (3)	−0.0624 (9)	0.70432 (16)	0.113 (2)	0.802 (8)
C21'	0.0663 (11)	−0.082 (2)	0.6640 (4)	0.077 (14)	0.198 (8)
F1'	0.0020 (11)	−0.242 (3)	0.6645 (5)	0.086 (5)	0.198 (8)
F2'	0.0267 (16)	0.067 (2)	0.6971 (6)	0.132 (7)	0.198 (8)
F3'	0.1472 (9)	−0.151 (3)	0.6925 (8)	0.104 (6)	0.198 (8)
N1	0.28293 (14)	0.2485 (3)	0.36876 (8)	0.0415 (5)	
N2	0.21147 (14)	0.4106 (3)	0.36303 (8)	0.0430 (5)	
N3	0.15442 (15)	0.2092 (3)	0.50379 (8)	0.0426 (5)	
O1	0.31148 (13)	−0.0196 (3)	0.43548 (7)	0.0588 (5)	
O2	0.03316 (13)	−0.0629 (3)	0.56238 (8)	0.0630 (6)	
C1	0.26854 (17)	0.1439 (4)	0.42103 (10)	0.0397 (6)	
C2	0.19382 (16)	0.2675 (4)	0.44969 (9)	0.0376 (6)	
C3	0.16334 (17)	0.4250 (4)	0.41474 (10)	0.0422 (6)	
C4	0.0920 (2)	0.5991 (5)	0.42645 (13)	0.0660 (8)	
H4A	0.0563	0.5693	0.4607	0.099*	
H4B	0.0459	0.6119	0.3951	0.099*	

H4C	0.1281	0.7277	0.4310	0.099*
C5	0.31870 (18)	0.1449 (4)	0.31851 (10)	0.0433 (6)
C6	0.2606 (2)	0.1327 (4)	0.26916 (11)	0.0561 (7)
H6	0.1983	0.1958	0.2675	0.067*
C7	0.2972 (3)	0.0248 (5)	0.22233 (12)	0.0746 (10)
H7	0.2594	0.0168	0.1890	0.090*
C8	0.3894 (3)	−0.0707 (5)	0.22489 (14)	0.0791 (10)
H8	0.4129	−0.1435	0.1935	0.095*
C9	0.4465 (2)	−0.0581 (5)	0.27394 (14)	0.0691 (9)
H9	0.5084	−0.1231	0.2756	0.083*
C10	0.41182 (19)	0.0510 (4)	0.32061 (11)	0.0537 (7)
H10	0.4509	0.0616	0.3534	0.064*
C11	0.2445 (2)	0.5981 (4)	0.33217 (12)	0.0613 (8)
H11A	0.1883	0.6860	0.3240	0.092*
H11B	0.2751	0.5571	0.2971	0.092*
H11C	0.2917	0.6736	0.3552	0.092*
C12	0.20566 (17)	0.2186 (4)	0.55357 (10)	0.0406 (6)
C13	0.29783 (17)	0.3490 (4)	0.55658 (9)	0.0408 (6)
C14	0.2988 (2)	0.5560 (4)	0.53797 (11)	0.0510 (7)
H14	0.2410	0.6150	0.5229	0.061*
C15	0.3848 (2)	0.6748 (5)	0.54162 (11)	0.0585 (8)
H15	0.3846	0.8128	0.5291	0.070*
C16	0.4714 (2)	0.5874 (5)	0.56408 (11)	0.0611 (8)
H16	0.5293	0.6665	0.5661	0.073*
C17	0.47138 (19)	0.3839 (5)	0.58334 (11)	0.0583 (8)
H17	0.5293	0.3261	0.5985	0.070*
C18	0.38510 (18)	0.2647 (4)	0.58015 (10)	0.0503 (7)
H18	0.3853	0.1280	0.5937	0.060*
C19	0.17242 (18)	0.1156 (4)	0.60245 (10)	0.0483 (7)
H19	0.2078	0.1356	0.6363	0.058*
C20	0.08888 (19)	−0.0162 (4)	0.60346 (10)	0.0499 (7)
H3	0.0982 (19)	0.129 (4)	0.5052 (10)	0.060 (8)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C21	0.072 (4)	0.092 (4)	0.060 (4)	−0.039 (4)	−0.013 (3)	0.020 (3)
F1	0.187 (5)	0.096 (3)	0.127 (3)	−0.041 (3)	−0.034 (3)	0.058 (2)
F2	0.087 (2)	0.198 (5)	0.092 (2)	−0.018 (3)	0.0368 (17)	0.033 (3)
F3	0.116 (3)	0.171 (5)	0.0502 (18)	−0.072 (3)	−0.021 (2)	0.030 (2)
C21'	0.069 (16)	0.084 (15)	0.077 (17)	−0.017 (9)	−0.012 (10)	0.005 (9)
F1'	0.095 (8)	0.098 (9)	0.065 (6)	−0.059 (7)	−0.018 (6)	0.028 (6)
F2'	0.164 (11)	0.133 (10)	0.100 (8)	0.007 (8)	0.042 (8)	0.004 (7)
F3'	0.113 (9)	0.118 (9)	0.080 (9)	0.023 (7)	−0.015 (6)	0.044 (7)
N1	0.0451 (12)	0.0405 (12)	0.0390 (12)	0.0028 (10)	0.0033 (9)	0.0038 (10)
N2	0.0476 (12)	0.0350 (12)	0.0464 (12)	0.0020 (10)	0.0008 (9)	0.0058 (10)
N3	0.0363 (12)	0.0532 (14)	0.0381 (12)	−0.0100 (11)	0.0011 (9)	−0.0004 (10)
O1	0.0714 (13)	0.0541 (12)	0.0509 (11)	0.0188 (10)	0.0025 (9)	0.0099 (9)

O2	0.0535 (11)	0.0818 (15)	0.0536 (12)	−0.0217 (10)	−0.0111 (9)	0.0076 (10)
C1	0.0414 (14)	0.0397 (15)	0.0378 (14)	−0.0034 (12)	−0.0059 (11)	0.0006 (12)
C2	0.0350 (12)	0.0428 (15)	0.0350 (13)	−0.0037 (11)	−0.0008 (10)	−0.0007 (11)
C3	0.0379 (13)	0.0436 (15)	0.0450 (14)	−0.0007 (12)	−0.0034 (11)	−0.0005 (12)
C4	0.0650 (19)	0.062 (2)	0.071 (2)	0.0186 (16)	0.0049 (15)	0.0022 (16)
C5	0.0517 (15)	0.0386 (14)	0.0396 (14)	−0.0074 (12)	0.0097 (12)	0.0043 (11)
C6	0.0706 (19)	0.0545 (18)	0.0431 (16)	−0.0030 (15)	0.0014 (14)	0.0057 (14)
C7	0.118 (3)	0.065 (2)	0.0412 (17)	−0.003 (2)	0.0051 (17)	0.0016 (15)
C8	0.123 (3)	0.058 (2)	0.057 (2)	0.003 (2)	0.036 (2)	−0.0019 (17)
C9	0.076 (2)	0.059 (2)	0.072 (2)	0.0045 (16)	0.0301 (18)	−0.0011 (17)
C10	0.0529 (17)	0.0498 (17)	0.0587 (17)	−0.0020 (14)	0.0120 (13)	0.0006 (14)
C11	0.077 (2)	0.0433 (17)	0.0640 (19)	−0.0055 (15)	0.0067 (15)	0.0143 (14)
C12	0.0384 (13)	0.0426 (15)	0.0407 (14)	0.0008 (12)	−0.0010 (11)	−0.0055 (12)
C13	0.0406 (14)	0.0467 (16)	0.0351 (13)	−0.0037 (12)	−0.0009 (10)	−0.0038 (11)
C14	0.0545 (16)	0.0457 (17)	0.0527 (16)	−0.0052 (14)	−0.0097 (13)	−0.0047 (13)
C15	0.073 (2)	0.0495 (18)	0.0526 (17)	−0.0183 (16)	−0.0052 (14)	−0.0031 (13)
C16	0.0593 (19)	0.077 (2)	0.0473 (16)	−0.0283 (17)	0.0007 (14)	−0.0087 (16)
C17	0.0441 (16)	0.079 (2)	0.0516 (17)	−0.0075 (15)	−0.0051 (12)	0.0012 (15)
C18	0.0488 (15)	0.0551 (17)	0.0469 (15)	−0.0038 (14)	−0.0046 (12)	0.0039 (13)
C19	0.0469 (15)	0.0584 (18)	0.0395 (15)	−0.0097 (14)	−0.0056 (11)	0.0008 (13)
C20	0.0473 (15)	0.0574 (18)	0.0449 (15)	−0.0058 (14)	−0.0047 (12)	0.0066 (13)

Geometric parameters (Å, °)

C21—F1	1.320 (7)	C6—H6	0.93
C21—F3	1.338 (6)	C7—C8	1.382 (5)
C21—F2	1.342 (5)	C7—H7	0.93
C21—C20	1.535 (5)	C8—C9	1.380 (4)
C21'—F1'	1.337 (10)	C8—H8	0.93
C21'—F2'	1.342 (10)	C9—C10	1.384 (4)
C21'—F3'	1.345 (10)	C9—H9	0.93
C21'—C20	1.516 (10)	C10—H10	0.93
N1—C1	1.412 (3)	C11—H11A	0.96
N1—N2	1.419 (3)	C11—H11B	0.96
N1—C5	1.440 (3)	C11—H11C	0.96
N2—C3	1.384 (3)	C12—C19	1.400 (3)
N2—C11	1.472 (3)	C12—C13	1.495 (3)
N3—C12	1.352 (3)	C13—C14	1.394 (4)
N3—C2	1.430 (3)	C13—C18	1.401 (3)
N3—H3	0.92 (3)	C14—C15	1.387 (3)
O1—C1	1.240 (3)	C14—H14	0.93
O2—C20	1.251 (3)	C15—C16	1.390 (4)
C1—C2	1.450 (3)	C15—H15	0.93
C2—C3	1.359 (3)	C16—C17	1.377 (4)
C3—C4	1.497 (4)	C16—H16	0.93
C4—H4A	0.96	C17—C18	1.390 (4)
C4—H4B	0.96	C17—H17	0.93
C4—H4C	0.96	C18—H18	0.93
C5—C10	1.389 (3)	C19—C20	1.405 (3)

C5—C6	1.393 (3)	C19—H19	0.93
C6—C7	1.392 (4)		
F1—C21—F3	107.0 (4)	C9—C8—C7	120.1 (3)
F1—C21—F2	107.4 (6)	C9—C8—H8	119.9
F3—C21—F2	105.7 (5)	C7—C8—H8	119.9
F1—C21—C20	112.6 (5)	C8—C9—C10	120.0 (3)
F3—C21—C20	113.9 (5)	C8—C9—H9	120.0
F2—C21—C20	109.8 (4)	C10—C9—H9	120.0
F1'—C21'—F2'	106.0 (8)	C9—C10—C5	120.0 (3)
F1'—C21'—F3'	105.5 (8)	C9—C10—H10	120.0
F2'—C21'—F3'	105.5 (8)	C5—C10—H10	120.0
F1'—C21'—C20	110.8 (10)	N2—C11—H11A	109.5
F2'—C21'—C20	115.5 (11)	N2—C11—H11B	109.5
F3'—C21'—C20	112.8 (13)	H11A—C11—H11B	109.5
C1—N1—N2	109.25 (17)	N2—C11—H11C	109.5
C1—N1—C5	122.9 (2)	H11A—C11—H11C	109.5
N2—N1—C5	119.35 (18)	H11B—C11—H11C	109.5
C3—N2—N1	106.72 (17)	N3—C12—C19	121.5 (2)
C3—N2—C11	121.6 (2)	N3—C12—C13	118.8 (2)
N1—N2—C11	115.72 (19)	C19—C12—C13	119.7 (2)
C12—N3—C2	124.4 (2)	C14—C13—C18	118.6 (2)
C12—N3—H3	114.0 (16)	C14—C13—C12	121.6 (2)
C2—N3—H3	119.6 (16)	C18—C13—C12	119.7 (2)
O1—C1—N1	124.7 (2)	C15—C14—C13	120.7 (3)
O1—C1—C2	131.0 (2)	C15—C14—H14	119.6
N1—C1—C2	104.3 (2)	C13—C14—H14	119.6
C3—C2—N3	128.1 (2)	C14—C15—C16	119.9 (3)
C3—C2—C1	109.3 (2)	C14—C15—H15	120.1
N3—C2—C1	122.3 (2)	C16—C15—H15	120.1
C2—C3—N2	109.8 (2)	C17—C16—C15	120.1 (3)
C2—C3—C4	129.0 (2)	C17—C16—H16	119.9
N2—C3—C4	121.1 (2)	C15—C16—H16	119.9
C3—C4—H4A	109.5	C16—C17—C18	120.2 (3)
C3—C4—H4B	109.5	C16—C17—H17	119.9
H4A—C4—H4B	109.5	C18—C17—H17	119.9
C3—C4—H4C	109.5	C17—C18—C13	120.4 (3)
H4A—C4—H4C	109.5	C17—C18—H18	119.8
H4B—C4—H4C	109.5	C13—C18—H18	119.8
C10—C5—C6	120.3 (2)	C12—C19—C20	123.9 (2)
C10—C5—N1	118.6 (2)	C12—C19—H19	118.0
C6—C5—N1	121.2 (2)	C20—C19—H19	118.0
C7—C6—C5	118.9 (3)	O2—C20—C19	127.1 (2)
C7—C6—H6	120.5	O2—C20—C21'	122.1 (6)
C5—C6—H6	120.5	C19—C20—C21'	110.5 (6)
C8—C7—C6	120.6 (3)	O2—C20—C21	113.9 (3)
C8—C7—H7	119.7	C19—C20—C21	118.9 (3)
C6—C7—H7	119.7		
C1—N1—N2—C3	8.5 (2)	N3—C12—C13—C14	50.5 (3)

C5—N1—N2—C3	157.42 (19)	C19—C12—C13—C14	−127.2 (3)
C1—N1—N2—C11	147.2 (2)	N3—C12—C13—C18	−131.4 (2)
C5—N1—N2—C11	−63.9 (3)	C19—C12—C13—C18	50.9 (3)
N2—N1—C1—O1	171.3 (2)	C18—C13—C14—C15	1.3 (4)
C5—N1—C1—O1	23.7 (3)	C12—C13—C14—C15	179.4 (2)
N2—N1—C1—C2	−7.2 (2)	C13—C14—C15—C16	0.0 (4)
C5—N1—C1—C2	−154.8 (2)	C14—C15—C16—C17	−0.8 (4)
C12—N3—C2—C3	−116.3 (3)	C15—C16—C17—C18	0.3 (4)
C12—N3—C2—C1	71.0 (3)	C16—C17—C18—C13	1.0 (4)
O1—C1—C2—C3	−175.0 (2)	C14—C13—C18—C17	−1.8 (4)
N1—C1—C2—C3	3.4 (2)	C12—C13—C18—C17	−179.9 (2)
O1—C1—C2—N3	−1.1 (4)	N3—C12—C19—C20	4.7 (4)
N1—C1—C2—N3	177.23 (19)	C13—C12—C19—C20	−177.6 (2)
N3—C2—C3—N2	−171.6 (2)	C12—C19—C20—O2	0.7 (5)
C1—C2—C3—N2	1.8 (3)	C12—C19—C20—C21'	−173.4 (6)
N3—C2—C3—C4	10.3 (4)	C12—C19—C20—C21	−179.7 (3)
C1—C2—C3—C4	−176.2 (2)	F1'—C21'—C20—O2	19.4 (13)
N1—N2—C3—C2	−6.3 (2)	F2'—C21'—C20—O2	−101.2 (12)
C11—N2—C3—C2	−142.0 (2)	F3'—C21'—C20—O2	137.3 (11)
N1—N2—C3—C4	172.0 (2)	F1'—C21'—C20—C19	−166.2 (10)
C11—N2—C3—C4	36.2 (3)	F2'—C21'—C20—C19	73.2 (13)
C1—N1—C5—C10	−60.4 (3)	F3'—C21'—C20—C19	−48.2 (13)
N2—N1—C5—C10	155.0 (2)	F1'—C21'—C20—C21	−19 (3)
C1—N1—C5—C6	117.7 (3)	F2'—C21'—C20—C21	−140 (5)
N2—N1—C5—C6	−26.8 (3)	F3'—C21'—C20—C21	99 (4)
C10—C5—C6—C7	0.2 (4)	F1—C21—C20—O2	60.7 (6)
N1—C5—C6—C7	−177.9 (2)	F3—C21—C20—O2	−177.3 (5)
C5—C6—C7—C8	0.6 (4)	F2—C21—C20—O2	−58.9 (6)
C6—C7—C8—C9	−0.6 (5)	F1—C21—C20—C19	−119.0 (5)
C7—C8—C9—C10	−0.3 (5)	F3—C21—C20—C19	3.1 (7)
C8—C9—C10—C5	1.2 (4)	F2—C21—C20—C19	121.4 (5)
C6—C5—C10—C9	−1.1 (4)	F1—C21—C20—C21'	−155 (4)
N1—C5—C10—C9	177.0 (2)	F3—C21—C20—C21'	−33 (4)
C2—N3—C12—C19	−164.9 (2)	F2—C21—C20—C21'	86 (4)
C2—N3—C12—C13	17.5 (3)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3···O2	0.92 (3)	2.02 (3)	2.761 (3)	137 (2)
N3—H3···O2^{i}	0.92 (3)	2.40 (3)	3.094 (3)	133 (2)

Symmetry codes: (i) −*x*, −*y*, −*z*+1.

Fig. 1

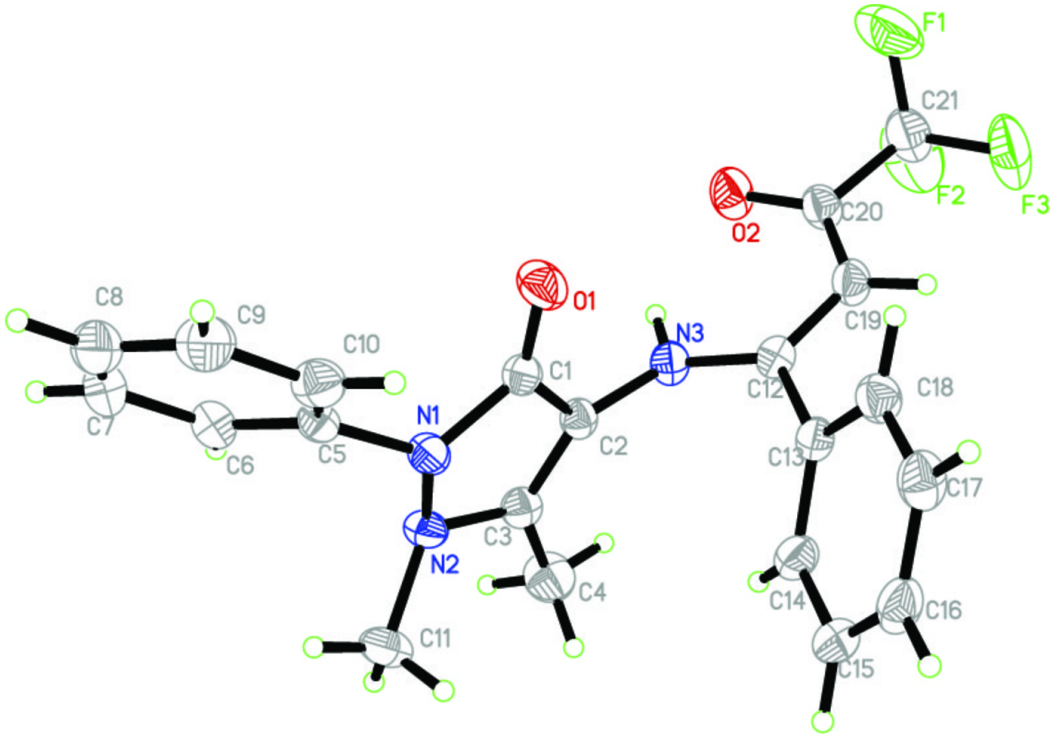
F1
C21
F2
F3
O2
C20
O1
C19
N3
C8
C9
C10
C1
C12
C18
C7
N1
C2
C13
C17
C6
C5
C3
N2
C4
C14
C16
C11
C15

Fig. 2