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(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl-*N*-*p*-tolylcyclopropanecarboxamide

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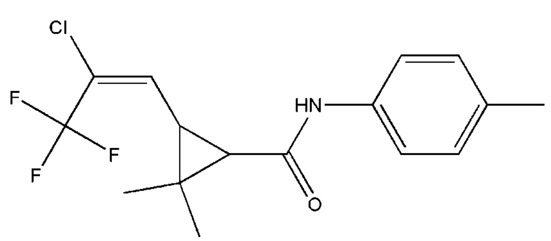
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.007 Å; disorder in main residue; R factor = 0.067; wR factor = 0.207; data-to-parameter ratio = 13.0.

There are two molecules in the asymmetric unit of the title compound, $C_{16}H_{17}ClF_3NO$. The benzene ring in each molecule makes a dihedral angle of 66.6 (3)° [116.3 (4)° in the second molecule] with the plane of the cyclopropane ring. The F atoms of the CF_3 groups are disordered equally over two positions. The amide hydrogen is linked with the amide oxygen in another molecule by an intermolecular N—H···O hydrogen bond. The packing can be described as a dimeric arrangement of molecules linked through N—H···O hydrogen bonds.

Related literature

For related literature, see: Liu *et al.* (2006); Punja (1981); Zhang (2005).



Experimental

Crystal data

$C_{16}H_{17}ClF_3NO$	γ = 72.517 (4)°
M_r = 331.76	V = 1706.7 (7) Å^3
Triclinic, $P\overline{1}$	Z = 4
a = 9.400 (2) Å	Mo $K\alpha$ radiation
b = 12.482 (3) Å	μ = 0.25 mm^{-1}
c = 16.201 (4) Å	T = 294 (2) K
α = 70.910 (4)°	0.22 × 0.18 × 0.14 mm
β = 88.921 (5)°	

Data collection

Bruker SMART CCD area-detector diffractometer	8849 measured reflections
Absorption correction: multi-scan (*SADABS*; Sheldrick,1996)	5945 independent reflections
T_{min} = 0.945, T_{max} = 0.967	3077 reflections with $I > 2\sigma(I)$
	R_{int} = 0.023

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.067	137 restraints
$wR(F^2)$ = 0.207	H-atom parameters constrained
S = 1.09	$\Delta\rho_{max}$ = 0.60 e Å^{-3}
5945 reflections	$\Delta\rho_{min}$ = −0.45 e Å^{-3}
457 parameters	

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.86	2.15	2.978 (4)	161
N2—H2···O1	0.86	2.14	2.959 (4)	158

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SMART*; data reduction: *SAINT* (Bruker, 1997); program(s) used to solve structure: *SHELXTL* (Bruker, 2001); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: BV2081).

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supplementary materials

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(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl-*N*-*p*-tolylcyclopropanecarboxamide

F.-Y. Yan and **D.-Q. Liu**

Comment

3-[(*E*)-2-chloro-3,3,3-trifluoroprop-1-enyl]-2,2-dimethylcyclopropanecarboxylic acid is a very important intermediate for tefluthrin, a important insecticide controlling a wide range of soil insect pests in maize, sugar beet, and other crops (Punja 1981). *p*-Toluidine containing pesticides have the advantage of low toxicity, high activity and low residues (Zhang 2005). The structure in this article containing both of two active parts is expected to show some insecticide activity. The present X-ray crystal structure analysis was undertaken in order to study the stereochemistry and crystal packing of the title compound, (I). In this paper, the title compound, (*E*)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl-*N*-*p*-tolylcyclopropane-carboxamide, (I), was synthesized and the structure of (I) is illustrated in Fig. 1. The dihedral angles between the benzene moiety and the cyclopropane group is 66.6 (3)°. The amide hydrogen is linked with the amide oxygen in an adjoining molecule by an intermolecular N—H···O hydrogen bond. The packing can be described as a dimeric arrangement of molecules linked through N—H···O hydrogen bonds (Table 1).

Experimental

The title compound was prepared according to the method of Liu *et al.* (2006). 3-((*E*)-2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2- dimethylcyclopropanecarboxylic acid (0.97 g, 4.0 mmol) was dispersed in $SOCl_2$ (15 ml), and a drop of anhydrous DMF was added in. The mixture was heated to reflux for 1 h. $SOCl_2$ was removed by a rotoevaporator. The crude the product could be directly disolved in anhydrous toluene, already mixed with *p*-toluidine(0.44 g, 4.1 mmol). Triethylamine was dropped into the system, preventing the release of white fumes. After 5 h stirring at room temperature, the reaction mixture was treated with hexane. Recrystallization of the off-white product from methanol and a small amount of water (80:1) overnight at ambient temperature gave colorless single crystals of (*E*)-3-(2-chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl -*N*-*p*-tolylcyclopropanecarboxamide, suitable for X-ray analysis.

Refinement

H atoms were positioned geometrically with C—H = 0.92–0.98 Å and refined using riding model with U_{iso}(H) = 1.2Ueq(carrier). The amine H atom was located from difference map and refined isotropically. The disordered CF_3 was allowed to rotate about its C—C axis.

Figures

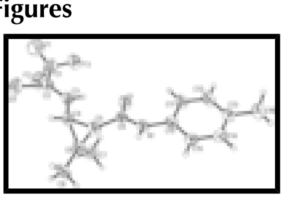

Fig. 1. The molecular structure of (I), drawn with 30% probability ellipsoids. H atoms are drawn as spheres of arbitrary radius.

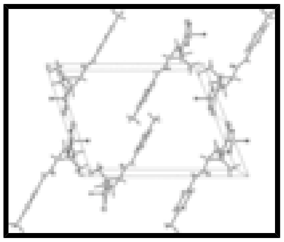

Fig. 2. The crystal structure of (I), viewed along *a* axis

(*E*)-3-(2-Chloro-3,3,3-trifluoroprop-1-enyl)-2,2-dimethyl- *N*-*p*-tolylcyclopropanecarboxamide

Crystal data

$C_{16}H_{17}ClF_3NO$	$Z = 4$
$M_r = 331.76$	$F_{000} = 688$
Triclinic, $P\overline{1}$	$D_x = 1.291$ Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation $\lambda = 0.71073$ Å
$a = 9.400$ (2) Å	Cell parameters from 2183 reflections
$b = 12.482$ (3) Å	$\theta = 2.6$–22.9º
$c = 16.201$ (4) Å	$\mu = 0.25$ mm^{-1}
$\alpha = 70.910$ (4)º	$T = 294$ (2) K
$\beta = 88.921$ (5)º	Prism, colorless
$\gamma = 72.517$ (4)º	0.22 × 0.18 × 0.14 mm
$V = 1706.7$ (7) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	5945 independent reflections
Radiation source: fine-focus sealed tube	3077 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.023$
$T = 294(2)$ K	$\theta_{max} = 25.0$º
φ and ω scans	$\theta_{min} = 1.8$º
Absorption correction: multi-scan (SADABS; Sheldrick,1996)	$h = -11 \rightarrow 9$
$T_{min} = 0.945$, $T_{max} = 0.967$	$k = -14 \rightarrow 14$
8849 measured reflections	$l = -19 \rightarrow 16$

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)] = 0.067$	H-atom parameters constrained
$wR(F^2) = 0.207$	$w = 1/[\sigma^2(F_o^2) + (0.0879P)^2 + 0.5066P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.09$	$(\Delta/\sigma)_{max} = 0.001$

5945 reflections	$\Delta\rho_{max} = 0.60$ e Å^{-3}
457 parameters	$\Delta\rho_{min} = -0.44$ e Å^{-3}
137 restraints	Extinction correction: none
Primary atom site location: structure-invariant direct methods	

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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)
Cl1	0.63184 (16)	0.55693 (11)	1.02621 (11)	0.1052 (5)	
Cl2	1.13400 (19)	0.54200 (14)	0.72738 (18)	0.1836 (12)	
F1	0.9100 (9)	0.6078 (8)	1.0169 (8)	0.133 (3)	0.50
F2	0.7921 (10)	0.6990 (8)	1.0952 (5)	0.116 (3)	0.50
F3	0.8242 (11)	0.7991 (7)	0.9530 (5)	0.089 (3)	0.50
F1'	0.9073 (7)	0.6378 (7)	0.9589 (6)	0.113 (2)	0.50
F2'	0.8042 (12)	0.8127 (7)	0.9874 (6)	0.095 (3)	0.50
F3'	0.8598 (11)	0.6504 (9)	1.0803 (6)	0.127 (3)	0.50
F4	1.3243 (9)	0.7790 (8)	0.6310 (6)	0.096 (2)	0.50
F5	1.3304 (11)	0.6367 (10)	0.5804 (6)	0.146 (3)	0.50
F6	1.4122 (11)	0.5960 (9)	0.7020 (7)	0.147 (4)	0.50
F4'	1.3120 (12)	0.7716 (9)	0.5891 (6)	0.118 (3)	0.50
F5'	1.3672 (10)	0.5822 (7)	0.6257 (7)	0.127 (3)	0.50
F6'	1.4006 (8)	0.6447 (7)	0.7274 (5)	0.109 (2)	0.50
O1	0.4629 (3)	1.0115 (3)	0.78523 (18)	0.0712 (8)	
O2	0.9714 (3)	0.9971 (3)	0.70315 (19)	0.0708 (8)	
N1	0.2560 (3)	1.0571 (3)	0.6969 (2)	0.0580 (8)	
H1	0.1829	1.0320	0.6898	0.070*	
N2	0.7591 (3)	1.0502 (3)	0.7686 (2)	0.0586 (9)	
H2	0.6831	1.0277	0.7877	0.070*	
C1	0.7972 (6)	0.7010 (5)	1.0040 (4)	0.106 (2)	
C2	0.6514 (4)	0.6955 (4)	0.9814 (3)	0.0653 (11)	
C3	0.5468 (4)	0.7882 (4)	0.9324 (3)	0.0692 (12)	
H3	0.5683	0.8601	0.9133	0.083*	
C4	0.3983 (4)	0.7911 (4)	0.9041 (3)	0.0726 (13)	
H4	0.3870	0.7123	0.9147	0.087*	
C5	0.3031 (4)	0.8882 (4)	0.8247 (3)	0.0665 (12)	

H5	0.2412	0.8608	0.7933	0.080*
C6	0.2592 (5)	0.8832 (5)	0.9160 (3)	0.0831 (15)
C7	0.2734 (6)	0.9764 (6)	0.9514 (4)	0.112 (2)
H7A	0.1832	1.0430	0.9346	0.168*
H7B	0.3566	1.0025	0.9281	0.168*
H7C	0.2895	0.9436	1.0142	0.168*
C8	0.1253 (5)	0.8399 (6)	0.9429 (4)	0.136 (3)
H8A	0.1212	0.8201	1.0052	0.203*
H8B	0.1348	0.7706	0.9271	0.203*
H8C	0.0352	0.9018	0.9136	0.203*
C9	0.3514 (4)	0.9896 (3)	0.7677 (3)	0.0540 (10)
C10	0.2592 (4)	1.1642 (4)	0.6323 (3)	0.0581 (10)
C11	0.3843 (5)	1.2017 (4)	0.6188 (3)	0.0752 (13)
H11	0.4731	1.1556	0.6538	0.090*
C12	0.3780 (6)	1.3067 (5)	0.5542 (3)	0.0825 (14)
H12	0.4633	1.3308	0.5469	0.099*
C13	0.2518 (6)	1.3772 (4)	0.5000 (3)	0.0809 (14)
C14	0.1285 (6)	1.3385 (5)	0.5130 (3)	0.0926 (16)
H14	0.0407	1.3846	0.4771	0.111*
C15	0.1306 (5)	1.2333 (4)	0.5776 (3)	0.0738 (12)
H15	0.0455	1.2090	0.5842	0.089*
C16	0.2484 (7)	1.4916 (5)	0.4283 (4)	0.126 (2)
H16A	0.2562	1.5491	0.4540	0.190*
H16B	0.1560	1.5224	0.3919	0.190*
H16C	0.3309	1.4762	0.3935	0.190*
C17	1.3029 (6)	0.6758 (5)	0.6514 (4)	0.1067 (19)
C18	1.1515 (5)	0.6795 (4)	0.6771 (3)	0.0761 (13)
C19	1.0418 (4)	0.7782 (4)	0.6611 (3)	0.0705 (12)
H19	1.0622	0.8486	0.6311	0.085*
C20	0.8898 (4)	0.7886 (4)	0.6857 (3)	0.0694 (12)
H20	0.8712	0.7119	0.7122	0.083*
C21	0.7992 (4)	0.8857 (4)	0.7199 (3)	0.0606 (11)
H21	0.7331	0.8598	0.7643	0.073*
C22	0.7560 (4)	0.8877 (4)	0.6299 (3)	0.0690 (12)
C23	0.7770 (5)	0.9826 (4)	0.5517 (3)	0.0881 (15)
H23A	0.8666	0.9997	0.5623	0.132*
H23B	0.6926	1.0533	0.5404	0.132*
H23C	0.7854	0.9562	0.5019	0.132*
C24	0.6168 (5)	0.8525 (5)	0.6222 (4)	0.1013 (18)
H24A	0.5301	0.9220	0.6081	0.152*
H24B	0.6078	0.7954	0.6769	0.152*
H24C	0.6247	0.8180	0.5767	0.152*
C25	0.8538 (4)	0.9809 (4)	0.7301 (3)	0.0549 (10)
C26	0.7657 (4)	1.1539 (4)	0.7823 (2)	0.0551 (10)
C27	0.8957 (4)	1.1829 (4)	0.7839 (3)	0.0685 (12)
H27	0.9858	1.1327	0.7751	0.082*
C28	0.8923 (5)	1.2861 (4)	0.7986 (3)	0.0714 (12)
H28	0.9812	1.3041	0.7995	0.086*
C29	0.7633 (5)	1.3630 (4)	0.8118 (3)	0.0742 (12)

C30	0.6350 (5)	1.3321 (4)	0.8109 (3)	0.0843 (14)
H30	0.5453	1.3822	0.8202	0.101*
C31	0.6353 (5)	1.2295 (4)	0.7966 (3)	0.0751 (13)
H31	0.5465	1.2111	0.7966	0.090*
C32	0.7605 (6)	1.4761 (5)	0.8269 (4)	0.1064 (18)
H32A	0.8376	1.4586	0.8718	0.160*
H32B	0.6647	1.5105	0.8450	0.160*
H32C	0.7776	1.5316	0.7736	0.160*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1007 (10)	0.0663 (8)	0.1359 (13)	−0.0321 (7)	−0.0128 (8)	−0.0109 (8)
Cl2	0.0972 (12)	0.0787 (10)	0.283 (3)	−0.0084 (9)	0.0387 (14)	0.0387 (13)
F1	0.095 (4)	0.144 (5)	0.139 (5)	−0.027 (4)	−0.006 (4)	−0.025 (4)
F2	0.107 (5)	0.117 (5)	0.119 (4)	−0.040 (4)	−0.039 (3)	−0.025 (3)
F3	0.067 (4)	0.104 (4)	0.099 (5)	−0.049 (3)	−0.002 (3)	−0.019 (3)
F1'	0.067 (3)	0.124 (4)	0.131 (5)	−0.021 (3)	0.011 (3)	−0.030 (4)
F2'	0.084 (4)	0.106 (4)	0.109 (5)	−0.053 (3)	−0.003 (4)	−0.032 (3)
F3'	0.108 (5)	0.136 (5)	0.128 (5)	−0.040 (4)	−0.033 (4)	−0.028 (4)
F4	0.064 (3)	0.113 (4)	0.111 (5)	−0.043 (3)	0.025 (4)	−0.023 (4)
F5	0.124 (5)	0.161 (5)	0.146 (5)	−0.039 (4)	0.049 (4)	−0.048 (4)
F6	0.113 (5)	0.147 (5)	0.159 (5)	−0.014 (4)	0.007 (4)	−0.046 (4)
F4'	0.091 (4)	0.126 (5)	0.117 (5)	−0.038 (3)	0.034 (4)	−0.013 (4)
F5'	0.104 (4)	0.125 (5)	0.133 (5)	−0.018 (3)	0.033 (4)	−0.038 (4)
F6'	0.058 (3)	0.120 (4)	0.139 (5)	−0.014 (3)	−0.016 (3)	−0.042 (4)
O1	0.0452 (15)	0.090 (2)	0.0752 (19)	−0.0406 (14)	−0.0030 (13)	−0.0050 (16)
O2	0.0466 (15)	0.095 (2)	0.091 (2)	−0.0404 (15)	0.0181 (14)	−0.0415 (18)
N1	0.0428 (17)	0.073 (2)	0.059 (2)	−0.0291 (16)	0.0015 (15)	−0.0140 (18)
N2	0.0421 (18)	0.072 (2)	0.068 (2)	−0.0311 (16)	0.0106 (15)	−0.0206 (18)
C1	0.071 (4)	0.086 (4)	0.134 (6)	−0.019 (3)	−0.020 (4)	−0.004 (4)
C2	0.051 (2)	0.069 (3)	0.074 (3)	−0.028 (2)	−0.001 (2)	−0.013 (2)
C3	0.049 (2)	0.069 (3)	0.082 (3)	−0.031 (2)	−0.004 (2)	−0.004 (2)
C4	0.052 (2)	0.069 (3)	0.088 (3)	−0.034 (2)	−0.007 (2)	−0.001 (2)
C5	0.047 (2)	0.082 (3)	0.069 (3)	−0.036 (2)	−0.0034 (19)	−0.008 (2)
C6	0.047 (2)	0.108 (4)	0.068 (3)	−0.029 (2)	0.008 (2)	0.009 (3)
C7	0.097 (4)	0.136 (5)	0.077 (4)	−0.008 (4)	0.016 (3)	−0.028 (4)
C8	0.055 (3)	0.173 (6)	0.116 (5)	−0.047 (3)	0.009 (3)	0.043 (4)
C9	0.038 (2)	0.071 (3)	0.054 (2)	−0.0223 (19)	0.0057 (17)	−0.017 (2)
C10	0.050 (2)	0.075 (3)	0.053 (2)	−0.023 (2)	0.0093 (18)	−0.022 (2)
C11	0.063 (3)	0.090 (3)	0.068 (3)	−0.039 (2)	0.004 (2)	−0.008 (3)
C12	0.084 (3)	0.096 (4)	0.066 (3)	−0.047 (3)	0.015 (3)	−0.009 (3)
C13	0.085 (3)	0.078 (3)	0.066 (3)	−0.021 (3)	0.025 (3)	−0.011 (3)
C14	0.068 (3)	0.093 (4)	0.079 (4)	0.003 (3)	0.008 (3)	−0.007 (3)
C15	0.050 (2)	0.084 (3)	0.073 (3)	−0.016 (2)	0.004 (2)	−0.013 (3)
C16	0.124 (5)	0.099 (4)	0.103 (5)	−0.014 (4)	0.032 (4)	0.015 (4)
C17	0.066 (4)	0.095 (5)	0.127 (6)	−0.004 (3)	0.002 (3)	−0.015 (4)
C18	0.049 (3)	0.071 (3)	0.087 (3)	−0.015 (2)	0.002 (2)	−0.002 (2)

C19	0.047 (2)	0.066 (3)	0.094 (3)	−0.022 (2)	0.007 (2)	−0.017 (2)
C20	0.051 (2)	0.060 (3)	0.098 (3)	−0.026 (2)	0.011 (2)	−0.021 (2)
C21	0.042 (2)	0.069 (3)	0.076 (3)	−0.0286 (19)	0.0094 (19)	−0.022 (2)
C22	0.044 (2)	0.073 (3)	0.098 (4)	−0.016 (2)	−0.006 (2)	−0.040 (3)
C23	0.084 (3)	0.092 (4)	0.082 (4)	−0.016 (3)	−0.014 (3)	−0.031 (3)
C24	0.054 (3)	0.122 (4)	0.156 (5)	−0.029 (3)	−0.004 (3)	−0.081 (4)
C25	0.037 (2)	0.070 (3)	0.057 (2)	−0.0222 (19)	−0.0018 (17)	−0.014 (2)
C26	0.045 (2)	0.066 (3)	0.053 (2)	−0.0225 (19)	0.0024 (17)	−0.014 (2)
C27	0.051 (2)	0.090 (3)	0.077 (3)	−0.031 (2)	0.008 (2)	−0.035 (3)
C28	0.061 (3)	0.088 (3)	0.075 (3)	−0.035 (3)	0.003 (2)	−0.030 (3)
C29	0.077 (3)	0.075 (3)	0.069 (3)	−0.028 (3)	−0.006 (2)	−0.017 (2)
C30	0.066 (3)	0.079 (3)	0.102 (4)	−0.014 (3)	0.002 (3)	−0.032 (3)
C31	0.052 (3)	0.085 (3)	0.091 (3)	−0.026 (2)	0.009 (2)	−0.029 (3)
C32	0.106 (4)	0.091 (4)	0.132 (5)	−0.030 (3)	−0.003 (3)	−0.049 (4)

Geometric parameters (Å, °)

Cl1—C2	1.708 (4)	C11—H11	0.9300
Cl2—C18	1.699 (5)	C12—C13	1.363 (7)
F1—C1	1.276 (8)	C12—H12	0.9300
F2—C1	1.468 (8)	C13—C14	1.372 (7)
F3—C1	1.328 (8)	C13—C16	1.510 (7)
F1'—C1	1.444 (8)	C14—C15	1.380 (6)
F2'—C1	1.352 (8)	C14—H14	0.9300
F3'—C1	1.251 (8)	C15—H15	0.9300
F4—C17	1.297 (10)	C16—H16A	0.9600
F5—C17	1.382 (8)	C16—H16B	0.9600
F6—C17	1.265 (8)	C16—H16C	0.9600
F4'—C17	1.313 (8)	C17—C18	1.467 (7)
F5'—C17	1.338 (8)	C18—C19	1.298 (6)
F6'—C17	1.423 (8)	C19—C20	1.456 (5)
O1—C9	1.219 (4)	C19—H19	0.9300
O2—C25	1.230 (4)	C20—C21	1.517 (6)
N1—C9	1.335 (5)	C20—C22	1.519 (6)
N1—C10	1.411 (5)	C20—H20	0.9800
N1—H1	0.8600	C21—C25	1.484 (5)
N2—C25	1.341 (5)	C21—C22	1.511 (6)
N2—C26	1.403 (5)	C21—H21	0.9800
N2—H2	0.8600	C22—C23	1.481 (7)
C1—C2	1.453 (6)	C22—C24	1.519 (6)
C2—C3	1.297 (5)	C23—H23A	0.9600
C3—C4	1.464 (5)	C23—H23B	0.9600
C3—H3	0.9300	C23—H23C	0.9600
C4—C5	1.515 (6)	C24—H24A	0.9600
C4—C6	1.516 (7)	C24—H24B	0.9600
C4—H4	0.9800	C24—H24C	0.9600
C5—C9	1.492 (5)	C26—C31	1.372 (6)
C5—C6	1.514 (7)	C26—C27	1.377 (5)
C5—H5	0.9800	C27—C28	1.376 (6)

C6—C7	1.495 (8)	C27—H27	0.9300
C6—C8	1.516 (6)	C28—C29	1.365 (6)
C7—H7A	0.9600	C28—H28	0.9300
C7—H7B	0.9600	C29—C30	1.374 (6)
C7—H7C	0.9600	C29—C32	1.502 (7)
C8—H8A	0.9600	C30—C31	1.374 (6)
C8—H8B	0.9600	C30—H30	0.9300
C8—H8C	0.9600	C31—H31	0.9300
C10—C15	1.380 (6)	C32—H32A	0.9600
C10—C11	1.380 (5)	C32—H32B	0.9600
C11—C12	1.369 (6)	C32—H32C	0.9600

C9—N1—C10	128.6 (3)	F4—C17—F4'	32.5 (6)
C9—N1—H1	115.7	F6—C17—F5'	64.6 (7)
C10—N1—H1	115.7	F4—C17—F5'	130.9 (7)
C25—N2—C26	129.5 (3)	F4'—C17—F5'	107.5 (8)
C25—N2—H2	115.2	F6—C17—F5	96.3 (8)
C26—N2—H2	115.2	F4—C17—F5	108.3 (8)
F1—C1—F3	112.4 (7)	F4'—C17—F5	77.7 (7)
F3'—C1—F2'	101.0 (8)	F5'—C17—F5	34.8 (5)
F3'—C1—F1'	99.0 (7)	F6—C17—F6'	35.0 (5)
F2'—C1—F1'	110.7 (7)	F4—C17—F6'	84.8 (7)
F3'—C1—C2	121.7 (6)	F4'—C17—F6'	112.5 (8)
F1—C1—C2	118.0 (6)	F5'—C17—F6'	99.3 (7)
F3—C1—C2	112.8 (6)	F5—C17—F6'	128.3 (7)
F2'—C1—C2	114.6 (6)	F6—C17—C18	117.7 (7)
F1'—C1—C2	108.6 (5)	F4—C17—C18	112.6 (6)
F3—C1—F2	110.4 (7)	F4'—C17—C18	115.2 (6)
C2—C1—F2	104.4 (5)	F5'—C17—C18	111.8 (6)
C3—C2—C1	122.4 (4)	F5—C17—C18	110.4 (6)
C3—C2—Cl1	124.0 (3)	F6'—C17—C18	109.4 (6)
C1—C2—Cl1	113.6 (3)	C19—C18—C17	123.0 (4)
C2—C3—C4	126.5 (4)	C19—C18—Cl2	123.8 (3)
C2—C3—H3	116.8	C17—C18—Cl2	113.2 (4)
C4—C3—H3	116.8	C18—C19—C20	126.0 (4)
C3—C4—C5	123.0 (3)	C18—C19—H19	117.0
C3—C4—C6	120.3 (4)	C20—C19—H19	117.0
C5—C4—C6	59.9 (3)	C19—C20—C21	123.0 (4)
C3—C4—H4	114.3	C19—C20—C22	121.5 (4)
C5—C4—H4	114.3	C21—C20—C22	59.7 (3)
C6—C4—H4	114.3	C19—C20—H20	114.0
C9—C5—C6	120.5 (4)	C21—C20—H20	114.0
C9—C5—C4	123.5 (3)	C22—C20—H20	114.0
C6—C5—C4	60.1 (3)	C25—C21—C22	120.6 (4)
C9—C5—H5	114.1	C25—C21—C20	124.1 (3)
C6—C5—H5	114.1	C22—C21—C20	60.2 (3)
C4—C5—H5	114.1	C25—C21—H21	113.9
C7—C6—C5	119.8 (4)	C22—C21—H21	113.9
C7—C6—C8	114.9 (5)	C20—C21—H21	113.9
C5—C6—C8	115.3 (5)	C23—C22—C21	118.9 (4)

C7—C6—C4	120.1 (4)	C23—C22—C20	120.8 (4)
C5—C6—C4	60.0 (3)	C21—C22—C20	60.1 (3)
C8—C6—C4	115.8 (5)	C23—C22—C24	114.9 (4)
C6—C7—H7A	109.5	C21—C22—C24	115.6 (4)
C6—C7—H7B	109.5	C20—C22—C24	115.7 (4)
H7A—C7—H7B	109.5	C22—C23—H23A	109.5
C6—C7—H7C	109.5	C22—C23—H23B	109.5
H7A—C7—H7C	109.5	H23A—C23—H23B	109.5
H7B—C7—H7C	109.5	C22—C23—H23C	109.5
C6—C8—H8A	109.5	H23A—C23—H23C	109.5
C6—C8—H8B	109.5	H23B—C23—H23C	109.5
H8A—C8—H8B	109.5	C22—C24—H24A	109.5
C6—C8—H8C	109.5	C22—C24—H24B	109.5
H8A—C8—H8C	109.5	H24A—C24—H24B	109.5
H8B—C8—H8C	109.5	C22—C24—H24C	109.5
O1—C9—N1	123.4 (3)	H24A—C24—H24C	109.5
O1—C9—C5	123.9 (3)	H24B—C24—H24C	109.5
N1—C9—C5	112.7 (3)	O2—C25—N2	123.5 (4)
C15—C10—C11	118.2 (4)	O2—C25—C21	123.3 (4)
C15—C10—N1	117.8 (3)	N2—C25—C21	113.2 (3)
C11—C10—N1	123.9 (4)	C31—C26—C27	118.4 (4)
C12—C11—C10	120.2 (4)	C31—C26—N2	117.8 (3)
C12—C11—H11	119.9	C27—C26—N2	123.8 (4)
C10—C11—H11	119.9	C28—C27—C26	120.0 (4)
C13—C12—C11	122.6 (4)	C28—C27—H27	120.0
C13—C12—H12	118.7	C26—C27—H27	120.0
C11—C12—H12	118.7	C29—C28—C27	122.5 (4)
C12—C13—C14	116.9 (5)	C29—C28—H28	118.8
C12—C13—C16	121.6 (5)	C27—C28—H28	118.8
C14—C13—C16	121.5 (5)	C28—C29—C30	116.8 (4)
C13—C14—C15	122.1 (5)	C28—C29—C32	122.0 (4)
C13—C14—H14	118.9	C30—C29—C32	121.2 (5)
C15—C14—H14	118.9	C31—C30—C29	122.0 (4)
C10—C15—C14	120.0 (4)	C31—C30—H30	119.0
C10—C15—H15	120.0	C29—C30—H30	119.0
C14—C15—H15	120.0	C26—C31—C30	120.4 (4)
C13—C16—H16A	109.5	C26—C31—H31	119.8
C13—C16—H16B	109.5	C30—C31—H31	119.8
H16A—C16—H16B	109.5	C29—C32—H32A	109.5
C13—C16—H16C	109.5	C29—C32—H32B	109.5
H16A—C16—H16C	109.5	H32A—C32—H32B	109.5
H16B—C16—H16C	109.5	C29—C32—H32C	109.5
F6—C17—F4	110.0 (8)	H32A—C32—H32C	109.5
F6—C17—F4'	125.2 (9)	H32B—C32—H32C	109.5

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.86	2.15	2.978 (4)	161

N2—H2···O1	0.86	2.14	2.959 (4)	158

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

Fig. 1

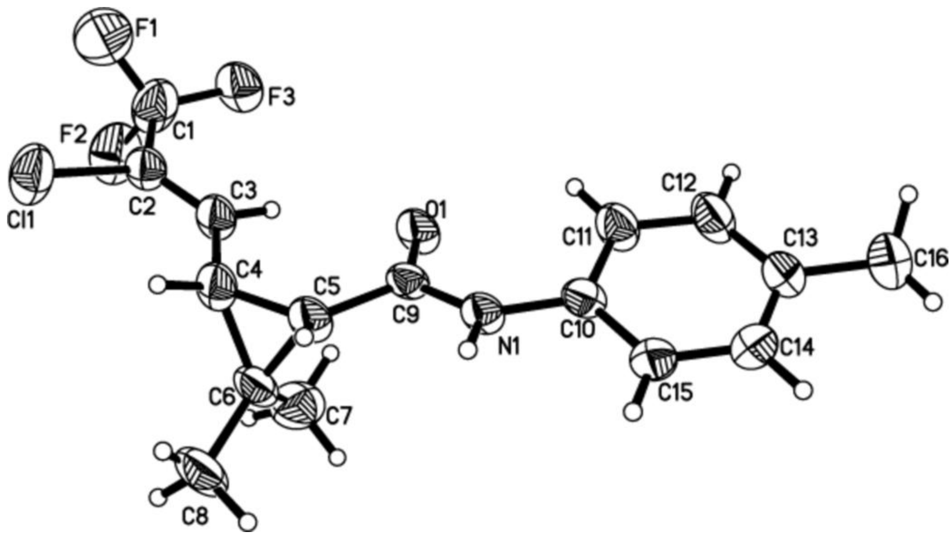

Fig. 2