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Ethyl 2-anilino-4-(2,4-dichlorophenyl)-6-trifluoromethyl-3,4-dihydropyrimidine-5-carboxylate

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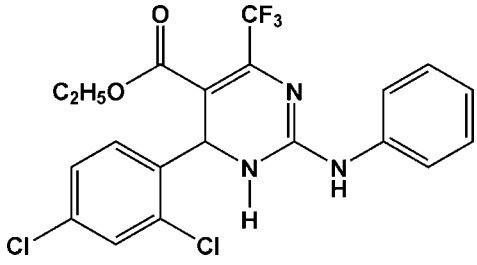
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.037; wR factor = 0.092; data-to-parameter ratio = 14.9.

The title molecule, $C_{20}H_{16}Cl_2F_3N_3O_2$, was obtained by the reaction of 2,4-dichlorobenzaldehyde, 1-phenylguanidinium hydrogen carbonate and ethyl 4,4,4-trifluoro-3-oxobutanoate catalyzed by sulfamic acid in the solid state. In the molecular structure, the pyrimidine ring adopts a twist-boat conformation and the two benzene ring are nearly perpendicular. In the crystal structure, the crystal packing is stabilized by intermolecular hydrogen bonding.

Related literature

For related literature, see: Bloxham *et al.* (2006); Borchardt *et al.* (2005); Hermann *et al.* (2003); Radwan & El-Sherbiny (2007); Ulrich (2004).



Experimental

Crystal data

$C_{20}H_{16}Cl_2F_3N_3O_2$
M_r = 458.26
Orthorhombic, $P2_12_12_1$
a = 11.0085 (15) Å
b = 11.8934 (17) Å
c = 15.698 (2) Å
V = 2055.4 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.37 mm^{-1}
T = 294 (2) K
0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.911, T_{max} = 0.931
11861 measured reflections
4177 independent reflections
3175 reflections with $I > 2\sigma(I)$
R_{int} = 0.038

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.092
S = 1.04
4177 reflections
281 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), with 2385 Friedel pairs
Flack parameter: −0.06 (6)

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

D—H···A	D—H	H···A	D···A	D—H···A
N3—H3A···O1^{i}	0.890 (10)	2.026 (12)	2.907 (3)	170 (3)
N1—H1A···O1^{i}	0.897 (10)	2.490 (17)	3.267 (3)	145 (2)
N1—H1A···Cl1	0.897 (10)	2.91 (2)	3.350 (2)	111.8 (18)

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

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1999); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1999); 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: HG2273).

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supplementary materials

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Ethyl 2-anilino-4-(2,4-dichlorophenyl)-6-trifluoromethyl-3,4-dihydropyrimidine-5-carboxylate

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Comment

The derivatives of pyrimidine are reported to have various biological activities, such as antitumor (Radwan & El-Sherbiny, 2007), CB1 cannabinoid receptor modulatory (Bloxham *et al.*, 2006) and hepatitis C virus RNA-dependent RNA polymerase inhibitory (Borchardt *et al.*, 2005). In addition, compounds that contain fluorine have special bioactivity, for example, flumioxazin is a widely used herbicide (Hermann *et al.*, 2003; Ulrich,2004). This led us to pay attention to the synthesis and structure of these fluoro-compounds and have synthesized aseries of derivatives of dihydropyrimidines. Here we report the crystal structure of the title compound, (I).

The molecular structure of (I) is shown in Fig. 1. The dihedral angle between plane N1/N2/C8/C9 and phenyl plane C1—C6, is 87.90 (8)°, which shows the two planes are nearly perpendicular. The atoms C7 and C10 deviate from the plane N1/N2/C8/C9 by 0.574 (4)Å and 0.157 (4)Å in the same direction, which shows the pyrimiding ring adopts a twist boat conformation. The connection of the pyrimidine ring and phenyl ring C15—C20 can be described as the torsion angle of C15—N3—C8—N1, −173.7 (2)°. In the structure, the crystal packing is stabilized intermolecular hydrogen bonds: N3—H3A···O1, N1—H1A···O1 and intramolecular hydrogen bond: N1—H1A···Cl1 (Fig.2 & Table 2).

Experimental

The title compound was synthesized by by the reaction of 2,4-dichlorobenzaldehyde, 1-phenylguanidinium hydrogencarbonate and ethyl 4,4,4-trifluoro-3-oxobutanoate in 1:1:1 molar ratio in solid state catalyzed by sulfamic acid at 363 K. After cooling, the reaction mixture was washed with water and recrystallized from ethanol, which gave single crystals suitable for X-ray diffraction.

Refinement

The hydrogen atoms bonded to nitrogen atom was positioned from a Fourier difference map and were refined freely. Other H atoms were placed in calculated positions, with C—H = 0.93, 0.96, 0.97 or 0.98 Å, and included in the final cycles of refinement using a riding model, with U_{iso}(H) = 1.2U_{eq}(parent atom).

Figures

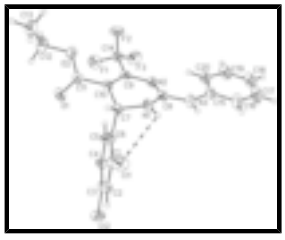

Fig. 1. The structure of (I), showing 30% probability displacement ellipsoids and the atom-numbering scheme.

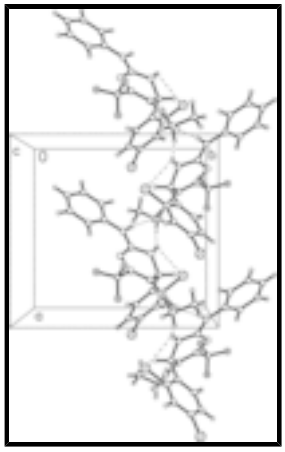

Fig. 2. The packing diagram of (I). Intermolecular hydrogen bonds are shown as dashed lines.

Ethyl 2-anilino-4-(2,4-dichlorophenyl)-6-trifluoromethyl-3,4- dihydropyrimidine-5-carboxylate

Crystal data

$C_{20}H_{16}Cl_2F_3N_3O_2$	F_{000} = 936
M_r = 458.26	D_x = 1.481 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 4124 reflections
a = 11.0085 (15) Å	θ = 2.2–25.1º
b = 11.8934 (17) Å	μ = 0.37 mm^{-1}
c = 15.698 (2) Å	T = 294 (2) K
V = 2055.4 (5) Å^3	Block, colourless
Z = 4	0.26 × 0.24 × 0.20 mm

Data collection

Bruker SMART CCD area-detector diffractometer	4177 independent reflections
Radiation source: fine-focus sealed tube	3175 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.038
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 2.2º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −7→13
T_{min} = 0.911, T_{max} = 0.931	k = −14→14
11861 measured reflections	l = −19→19

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

$R[F^2 > 2\sigma(F^2)] = 0.037$	$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.3148P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.092$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.04$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
4177 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
281 parameters	Extinction correction: SHELXL97, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
2 restraints	Extinction coefficient: 0.0261 (15)
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983)
Secondary atom site location: difference Fourier map	Flack parameter: −0.06 (6)

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 $F^2 > 2$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}
Cl1	0.72705 (8)	0.14863 (7)	−0.12933 (5)	0.0766 (3)
Cl2	0.37002 (8)	0.42819 (9)	−0.22290 (5)	0.0887 (3)
F1	0.62596 (16)	0.48924 (14)	0.24705 (10)	0.0706 (5)
F2	0.80585 (16)	0.45551 (14)	0.29272 (9)	0.0730 (5)
F3	0.77062 (17)	0.60034 (12)	0.21670 (10)	0.0757 (5)
O1	0.56257 (18)	0.19540 (17)	0.14384 (13)	0.0646 (5)
O2	0.64809 (17)	0.27081 (15)	0.25945 (11)	0.0592 (5)
N1	0.86238 (17)	0.32244 (16)	0.00923 (13)	0.0432 (5)
N2	0.85306 (18)	0.48302 (16)	0.09472 (12)	0.0428 (5)
N3	0.9898 (2)	0.47054 (18)	−0.01780 (15)	0.0528 (5)
C1	0.6315 (2)	0.2608 (2)	−0.10509 (15)	0.0456 (6)
C2	0.5460 (2)	0.2923 (3)	−0.16446 (15)	0.0540 (7)
H2	0.5375	0.2527	−0.2152	0.065*
C3	0.4732 (2)	0.3837 (2)	−0.14692 (16)	0.0525 (7)
C4	0.4828 (2)	0.4401 (2)	−0.07171 (17)	0.0521 (7)
H4	0.4322	0.5008	−0.0601	0.063*
C5	0.5684 (2)	0.4060 (2)	−0.01277 (16)	0.0461 (6)
H5	0.5744	0.4446	0.0386	0.055*
C6	0.6455 (2)	0.31641 (18)	−0.02757 (14)	0.0381 (5)
C7	0.7429 (2)	0.28239 (17)	0.03625 (14)	0.0393 (5)
H7	0.7453	0.2001	0.0388	0.047*

C8	0.89924 (19)	0.42730 (19)	0.03061 (16)	0.0408 (6)
C9	0.7726 (2)	0.42650 (18)	0.14511 (14)	0.0379 (5)
C10	0.7207 (2)	0.32622 (17)	0.12503 (14)	0.0388 (5)
C11	0.6358 (2)	0.2590 (2)	0.17605 (16)	0.0450 (6)
C12	0.5585 (3)	0.2171 (3)	0.3156 (2)	0.0770 (10)
H12A	0.5411	0.2663	0.3633	0.092*
H12B	0.4835	0.2051	0.2845	0.092*
C13	0.6041 (3)	0.1095 (3)	0.3472 (2)	0.0955 (12)
H13A	0.6823	0.1203	0.3731	0.143*
H13B	0.6114	0.0576	0.3006	0.143*
H13C	0.5486	0.0798	0.3887	0.143*
C14	0.7432 (3)	0.4921 (2)	0.22603 (15)	0.0491 (6)
C15	1.0562 (2)	0.5710 (2)	−0.00892 (18)	0.0513 (7)
C16	1.1471 (3)	0.5888 (3)	−0.0697 (2)	0.0690 (8)
H16	1.1620	0.5345	−0.1111	0.083*
C17	1.2143 (3)	0.6858 (3)	−0.0688 (3)	0.0866 (11)
H17	1.2739	0.6971	−0.1099	0.104*
C18	1.1946 (3)	0.7664 (3)	−0.0077 (3)	0.0902 (12)
H18	1.2402	0.8322	−0.0074	0.108*
C20	1.0364 (3)	0.6516 (2)	0.05281 (19)	0.0606 (7)
H20	0.9767	0.6411	0.0940	0.073*
C19	1.1066 (3)	0.7487 (3)	0.0527 (2)	0.0779 (10)
H19	1.0937	0.8028	0.0945	0.093*
H1A	0.897 (2)	0.290 (2)	−0.0361 (11)	0.055 (8)*
H3A	1.016 (3)	0.426 (2)	−0.0595 (13)	0.067 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0825 (6)	0.0701 (5)	0.0772 (5)	0.0141 (4)	−0.0005 (4)	−0.0343 (4)
Cl2	0.0660 (5)	0.1399 (8)	0.0603 (4)	0.0033 (5)	−0.0208 (4)	0.0215 (5)
F1	0.0622 (10)	0.0738 (10)	0.0758 (10)	0.0072 (9)	0.0117 (9)	−0.0183 (9)
F2	0.0878 (12)	0.0810 (12)	0.0503 (9)	−0.0055 (9)	−0.0245 (9)	0.0008 (8)
F3	0.1199 (15)	0.0432 (9)	0.0639 (9)	−0.0128 (9)	0.0036 (10)	−0.0139 (7)
O1	0.0591 (11)	0.0644 (12)	0.0704 (12)	−0.0280 (10)	−0.0031 (10)	−0.0053 (10)
O2	0.0630 (12)	0.0649 (11)	0.0497 (11)	−0.0154 (10)	0.0075 (9)	0.0041 (9)
N1	0.0335 (10)	0.0393 (11)	0.0568 (12)	0.0029 (9)	0.0029 (10)	−0.0072 (9)
N2	0.0418 (11)	0.0368 (10)	0.0499 (11)	−0.0042 (9)	−0.0017 (10)	0.0003 (9)
N3	0.0450 (12)	0.0474 (12)	0.0660 (14)	−0.0032 (10)	0.0115 (11)	0.0005 (12)
C1	0.0404 (13)	0.0477 (14)	0.0488 (14)	−0.0079 (12)	0.0067 (12)	−0.0073 (11)
C2	0.0519 (15)	0.0739 (19)	0.0362 (13)	−0.0195 (14)	0.0008 (12)	−0.0049 (13)
C3	0.0377 (14)	0.0736 (19)	0.0462 (14)	−0.0114 (14)	−0.0033 (12)	0.0143 (13)
C4	0.0422 (15)	0.0557 (16)	0.0585 (16)	0.0053 (12)	−0.0050 (13)	0.0061 (13)
C5	0.0419 (14)	0.0479 (14)	0.0485 (14)	0.0031 (11)	−0.0052 (12)	−0.0039 (12)
C6	0.0339 (12)	0.0358 (11)	0.0447 (12)	−0.0077 (10)	−0.0001 (11)	−0.0020 (10)
C7	0.0387 (13)	0.0302 (10)	0.0491 (13)	−0.0041 (10)	−0.0007 (11)	−0.0026 (9)
C8	0.0320 (12)	0.0362 (12)	0.0543 (14)	0.0048 (10)	−0.0052 (11)	0.0048 (11)
C9	0.0333 (11)	0.0379 (12)	0.0426 (12)	0.0021 (10)	−0.0081 (10)	0.0012 (10)

C10	0.0344 (12)	0.0368 (12)	0.0452 (13)	−0.0008 (10)	−0.0050 (11)	0.0017 (10)
C11	0.0398 (13)	0.0409 (13)	0.0543 (15)	−0.0029 (12)	−0.0013 (13)	−0.0011 (11)
C12	0.068 (2)	0.088 (2)	0.075 (2)	−0.0070 (18)	0.0274 (17)	0.0051 (18)
C13	0.087 (3)	0.105 (3)	0.094 (3)	−0.026 (2)	0.006 (2)	0.039 (2)
C14	0.0558 (16)	0.0458 (13)	0.0458 (13)	−0.0053 (12)	−0.0067 (13)	−0.0042 (11)
C15	0.0347 (13)	0.0478 (15)	0.0715 (17)	−0.0023 (11)	−0.0003 (12)	0.0149 (14)
C16	0.0518 (17)	0.0627 (18)	0.093 (2)	0.0006 (15)	0.0132 (17)	0.0147 (16)
C17	0.059 (2)	0.074 (2)	0.127 (3)	−0.0135 (19)	0.013 (2)	0.035 (2)
C18	0.065 (2)	0.062 (2)	0.144 (4)	−0.0248 (17)	−0.014 (2)	0.030 (2)
C20	0.0530 (17)	0.0531 (17)	0.0757 (19)	−0.0118 (14)	−0.0026 (14)	0.0083 (15)
C19	0.073 (2)	0.0538 (18)	0.107 (3)	−0.0164 (17)	−0.005 (2)	0.0039 (18)

Geometric parameters (Å, °)

Cl1—C1	1.741 (3)	C5—H5	0.9300
Cl2—C3	1.730 (3)	C6—C7	1.522 (3)
F1—C14	1.333 (3)	C7—C10	1.508 (3)
F2—C14	1.327 (3)	C7—H7	0.9800
F3—C14	1.330 (3)	C9—C10	1.360 (3)
O1—C11	1.215 (3)	C9—C14	1.526 (3)
O2—C11	1.324 (3)	C10—C11	1.468 (3)
O2—C12	1.469 (3)	C12—C13	1.462 (5)
N1—C8	1.354 (3)	C12—H12A	0.9700
N1—C7	1.462 (3)	C12—H12B	0.9700
N1—H1A	0.897 (10)	C13—H13A	0.9600
N2—C8	1.308 (3)	C13—H13B	0.9600
N2—C9	1.365 (3)	C13—H13C	0.9600
N3—C8	1.355 (3)	C15—C20	1.381 (4)
N3—C15	1.408 (3)	C15—C16	1.399 (4)
N3—H3A	0.890 (10)	C16—C17	1.371 (4)
C1—C2	1.377 (4)	C16—H16	0.9300
C1—C6	1.393 (3)	C17—C18	1.373 (5)
C2—C3	1.379 (4)	C17—H17	0.9300
C2—H2	0.9300	C18—C19	1.373 (5)
C3—C4	1.362 (4)	C18—H18	0.9300
C4—C5	1.382 (3)	C20—C19	1.389 (4)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.381 (3)	C19—H19	0.9300
C11—O2—C12	118.6 (2)	C11—C10—C7	114.78 (19)
C8—N1—C7	119.86 (19)	O1—C11—O2	123.1 (2)
C8—N1—H1A	117.8 (17)	O1—C11—C10	122.3 (2)
C7—N1—H1A	118.4 (17)	O2—C11—C10	114.6 (2)
C8—N2—C9	116.66 (19)	C13—C12—O2	110.7 (3)
C8—N3—C15	130.5 (2)	C13—C12—H12A	109.5
C8—N3—H3A	115.5 (19)	O2—C12—H12A	109.5
C15—N3—H3A	113.9 (19)	C13—C12—H12B	109.5
C2—C1—C6	122.5 (2)	O2—C12—H12B	109.5
C2—C1—Cl1	118.25 (19)	H12A—C12—H12B	108.1
C6—C1—Cl1	119.21 (19)	C12—C13—H13A	109.5

C1—C2—C3	118.5 (2)	C12—C13—H13B	109.5
C1—C2—H2	120.8	H13A—C13—H13B	109.5
C3—C2—H2	120.8	C12—C13—H13C	109.5
C4—C3—C2	121.1 (2)	H13A—C13—H13C	109.5
C4—C3—Cl2	119.9 (2)	H13B—C13—H13C	109.5
C2—C3—Cl2	119.0 (2)	F2—C14—F3	106.7 (2)
C3—C4—C5	119.3 (2)	F2—C14—F1	107.4 (2)
C3—C4—H4	120.4	F3—C14—F1	105.8 (2)
C5—C4—H4	120.4	F2—C14—C9	112.3 (2)
C6—C5—C4	122.2 (2)	F3—C14—C9	110.8 (2)
C6—C5—H5	118.9	F1—C14—C9	113.5 (2)
C4—C5—H5	118.9	C20—C15—C16	119.1 (3)
C5—C6—C1	116.4 (2)	C20—C15—N3	125.2 (2)
C5—C6—C7	121.8 (2)	C16—C15—N3	115.6 (3)
C1—C6—C7	121.8 (2)	C17—C16—C15	120.4 (3)
N1—C7—C10	107.54 (18)	C17—C16—H16	119.8
N1—C7—C6	110.87 (18)	C15—C16—H16	119.8
C10—C7—C6	113.73 (19)	C16—C17—C18	120.7 (3)
N1—C7—H7	108.2	C16—C17—H17	119.7
C10—C7—H7	108.2	C18—C17—H17	119.7
C6—C7—H7	108.2	C19—C18—C17	119.1 (3)
N2—C8—N1	122.8 (2)	C19—C18—H18	120.4
N2—C8—N3	121.7 (2)	C17—C18—H18	120.4
N1—C8—N3	115.5 (2)	C15—C20—C19	119.3 (3)
C10—C9—N2	124.8 (2)	C15—C20—H20	120.4
C10—C9—C14	123.6 (2)	C19—C20—H20	120.4
N2—C9—C14	111.61 (19)	C18—C19—C20	121.4 (3)
C9—C10—C11	128.3 (2)	C18—C19—H19	119.3
C9—C10—C7	116.7 (2)	C20—C19—H19	119.3
C6—C1—C2—C3	1.4 (4)	N2—C9—C10—C7	−7.6 (3)
Cl1—C1—C2—C3	−177.60 (19)	C14—C9—C10—C7	169.7 (2)
C1—C2—C3—C4	−1.9 (4)	N1—C7—C10—C9	30.7 (3)
C1—C2—C3—Cl2	177.07 (19)	C6—C7—C10—C9	−92.4 (2)
C2—C3—C4—C5	1.1 (4)	N1—C7—C10—C11	−154.66 (19)
Cl2—C3—C4—C5	−177.8 (2)	C6—C7—C10—C11	82.2 (2)
C3—C4—C5—C6	0.2 (4)	C12—O2—C11—O1	−8.8 (4)
C4—C5—C6—C1	−0.7 (3)	C12—O2—C11—C10	173.1 (2)
C4—C5—C6—C7	177.5 (2)	C9—C10—C11—O1	152.8 (3)
C2—C1—C6—C5	−0.1 (3)	C7—C10—C11—O1	−21.1 (3)
Cl1—C1—C6—C5	178.86 (18)	C9—C10—C11—O2	−29.1 (3)
C2—C1—C6—C7	−178.3 (2)	C7—C10—C11—O2	157.0 (2)
Cl1—C1—C6—C7	0.6 (3)	C11—O2—C12—C13	97.6 (3)
C8—N1—C7—C10	−38.3 (3)	C10—C9—C14—F2	82.9 (3)
C8—N1—C7—C6	86.6 (2)	N2—C9—C14—F2	−99.5 (2)
C5—C6—C7—N1	−101.8 (3)	C10—C9—C14—F3	−158.0 (2)
C1—C6—C7—N1	76.4 (3)	N2—C9—C14—F3	19.6 (3)
C5—C6—C7—C10	19.5 (3)	C10—C9—C14—F1	−39.2 (3)
C1—C6—C7—C10	−162.3 (2)	N2—C9—C14—F1	138.4 (2)
C9—N2—C8—N1	6.0 (3)	C8—N3—C15—C20	−3.2 (4)

C9—N2—C8—N3	−172.5 (2)	C8—N3—C15—C16	178.3 (3)
C7—N1—C8—N2	21.8 (3)	C20—C15—C16—C17	−1.0 (4)
C7—N1—C8—N3	−159.7 (2)	N3—C15—C16—C17	177.7 (3)
C15—N3—C8—N2	4.9 (4)	C15—C16—C17—C18	0.7 (5)
C15—N3—C8—N1	−173.7 (2)	C16—C17—C18—C19	0.2 (6)
C8—N2—C9—C10	−12.8 (3)	C16—C15—C20—C19	0.4 (4)
C8—N2—C9—C14	169.6 (2)	N3—C15—C20—C19	−178.1 (3)
N2—C9—C10—C11	178.6 (2)	C17—C18—C19—C20	−0.7 (5)
C14—C9—C10—C11	−4.1 (4)	C15—C20—C19—C18	0.4 (5)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3A···O1^{i}	0.890 (10)	2.026 (12)	2.907 (3)	170 (3)
N1—H1A···O1^{i}	0.897 (10)	2.490 (17)	3.267 (3)	145 (2)
N1—H1A···Cl1	0.897 (10)	2.91 (2)	3.350 (2)	111.8 (18)

Symmetry codes: (i) *x*+1/2, −*y*+1/2, −*z*.

Fig. 1

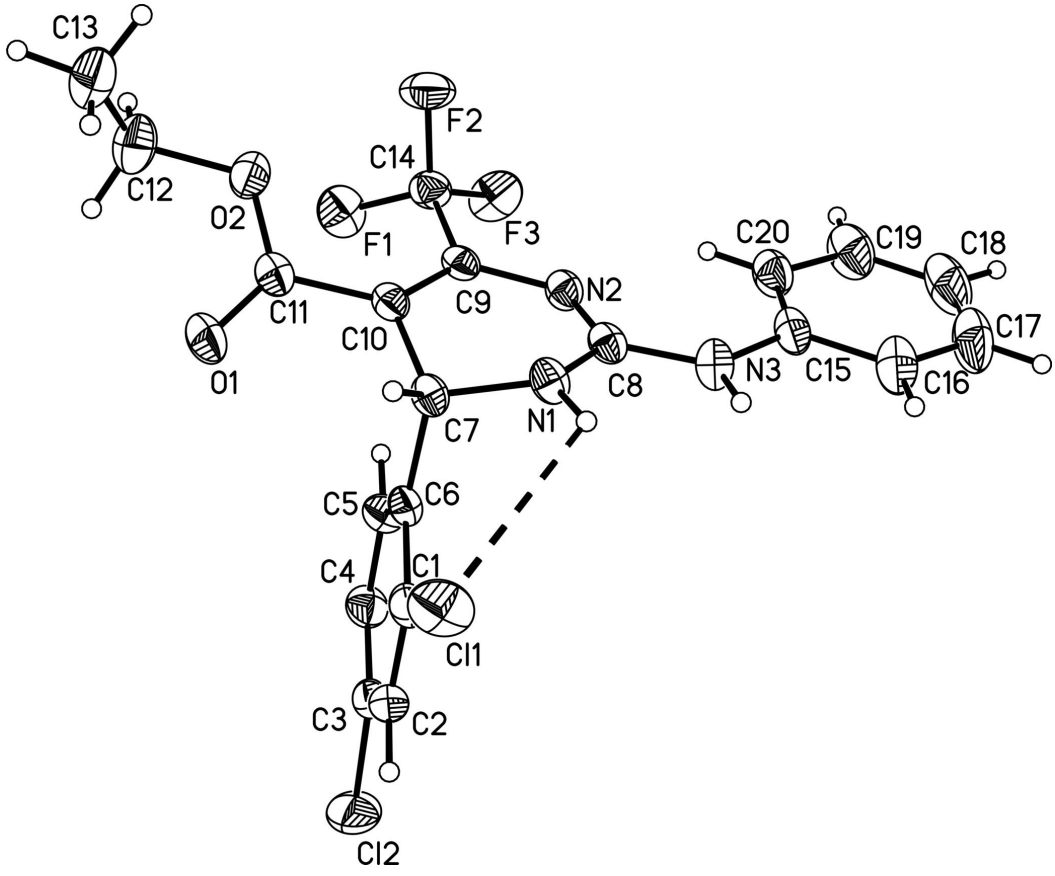
C13
C12
O2
F2
C14
F1
F3
C11
C9
N2
C20
C19
C18
C17
O1
C10
N3
C15
C16
C8
C7
N1
C5
C6
C4
C1
Cl1
C3
C2
Cl2

Fig. 2