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2-{5-Chloro-2-[(4-methoxybenzyl)-amino]phenyl}-4-cyclopropyl-1,1,1-trifluorobut-3-yn-2-ol

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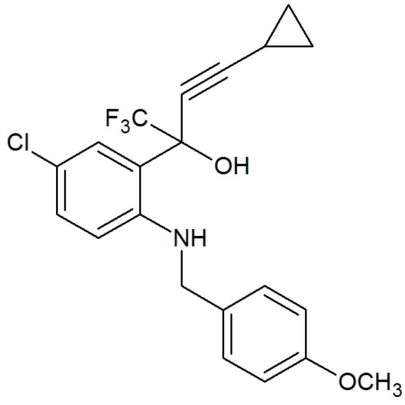
Key indicators: single-crystal X-ray study; T = 203 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.068; data-to-parameter ratio = 24.5.

In the title molecule, $C_{21}H_{19}ClF_3NO_2$, the 5-chlorophenyl and 4-methoxybenzyl groups are twisted slightly with respect to the amine group [dihedral angles = −8.4 (2) and 13.6 (2)°] and with respect to each other [6.2 (7)°], forming a nearly planar arrangement. The crystal packing is stabilized by intramolecular N—H···O hydrogen bonding between the amine H atom and the hydroxyl O atom. In addition, intermolecular hydrogen bonding between the same amine H atom and an F atom, N—H···F, and between the methoxy O atom and the hydroxyl H atom, O—H···O, adds to this stability.

Related literature

For related structures, see: Yathirajan, Sarojini *et al.* (2007); Yathirajan, Sreevidya *et al.* (2007). For related literature, see: Whittle *et al.* (1994); Ren *et al.* (2002); Jung *et al.* (2002); Küçükgüzel *et al.* (2000).



Experimental

Crystal data

$C_{21}H_{19}ClF_3NO_2$
M_r = 409.82
Orthorhombic, $P2_12_12_1$
a = 8.6400 (19) Å
b = 9.7671 (9) Å
c = 22.240 (5) Å
V = 1876.8 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.25 mm^{-1}
T = 203 K
0.43 × 0.37 × 0.14 mm

Data collection

Oxford Diffraction Gemini R diffractometer
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.906, T_{max} = 1.000
(expected range = 0.875–0.966)
18057 measured reflections
6220 independent reflections
2640 reflections with $I > 2\sigma(I)$
R_{int} = 0.050
2 standard reflections
every 50 reflections
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.032
$wR(F^2)$ = 0.069
S = 0.76
6220 reflections
254 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}
Absolute structure: Flack (1983), with 3628 Friedel pairs
Flack parameter: 0.02 (4)

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2B···O1^{i}	0.83	1.92	2.7114 (15)	159
N—H0A···O2	0.87	2.14	2.6620 (17)	118
N—H0A···F2	0.87	2.44	2.9773 (16)	121

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

Data collection: *CrysAlisPro* (Oxford Diffraction, 2007); cell refinement: *CrysAlisPro*; data reduction: *CrysAlisPro*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000); software used to prepare material for publication: *SHELXTL*.

ANM thanks SeQuent Scientific Ltd, India, for a pure sample of the title compound. RJB acknowledges the NSF MRI program (grant No. CHE-0619278) for funds to purchase the X-ray diffractometer.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2356).

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supplementary materials

Acta Cryst. (2007). E**63**, o3703-o3704 [**doi:10.1107/S160053680703749X**]

2-{5-Chloro-2-[(4-methoxybenzyl)amino]phenyl}-4-cyclopropyl-1,1,1-trifluorobut-3-yn-2-ol

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Comment

The title compound is an intermediate in the preparation of efavirenz, an anti HIV drug. Efavirenz is also used in combination with other antiretroviral agents as part of an expanded postexposure prophylaxis regime to prevent HIV transmission for those exposed to materials associated with a high risk for HIV transmission. Efavirenz was approved by the Food and Drug Administration (FDA) in 1998, making it the 14t h approved antiretroviral drug. In recent years fluorinated compounds find much importance in the pharmaceutical field. Fluorinated compounds in general, fluorinated heterocycles in particular, are those focused on much in modern-day medicinal chemistry. Incorporation of a fluorine atom instead of hydrogen one can alter the course of the reaction as well as its biological activities. Further introduction of a fluorine atom as the CF_3 group provides a more lipophilically and pharmacologically interesting compound compared to their non fluorinated analogues. The trifluoromethyl substituted compounds have been reported to possess biological activities as herbicides, fungicides and inhibitors for platelet aggregation. In view of the importance of the fluro derivatives, a crystal structure of the title compound, (I), is reported.

The mean planes of the 5-chlorophenyl and 4-methoxybenzyl groups are twisted slightly with the amine group [dihedral angles: N—C7—C8—C13 = −8.4 (2)°; C7—N—C6—C5 = 13.6 (2)°] and 6.2 (7)° with each other forming a nearly planar arrangement (Fig. 1).

Intramolecular hydrogen bonding occurs between the amine hydrogen, and the hydroxyl oxygen, N—H0A···O2, of the title molecule. In addition, intermolecular hydrogen bonding between the the same amine hydrogen and a fluorine atom, N—H0A···F2, as well as between the methoxy oxygen atom and hydroxyl hydrogen atom, O2—H2B···O1, adds to crystal packing stability (Fig. 2).

Experimental

A pure sample of the title compound was obtained as a gift sample from Sequent Scientific Ltd., India and was crystallized from a mixture of (1:1) ethylacetate and toluene (m.p.: 427–429 K).

Refinement

The H atoms were included in the riding model approximation with O—H = 0.83 Å, N—H = 0.87 Å and C—H = 0.94–0.98 Å, and with U_{iso}(H) = 1.19–1.49U_{eq}(C, O, N).

Figures

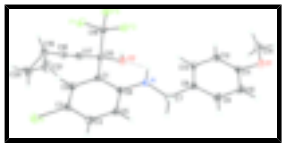

Fig. 1. Molecular structure of the title compound (I), showing atom labelling and 50% probability displacement ellipsoids. Dashed lines indicate N—H···O intramolecular hydrogen bonds.

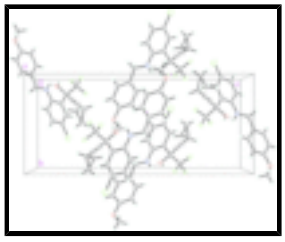

Fig. 2. Packing diagram of (I), viewed down the *a* axis. Dashed lines indicate O—H···O, and N—H···F intermolecular and N—H···O intramolecular hydrogen bonds.

2-{5-Chloro-2-[(4-methoxybenzyl)amino]phenyl}-4-cyclopropyl- 1,1,1-trifluorobut-3-yn-2-ol

Crystal data

$C_{21}H_{19}ClF_3NO_2$	F_{000} = 848
M_r = 409.82	D_x = 1.450 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 4798 reflections
a = 8.6400 (19) Å	θ = 4.6–32.6º
b = 9.7671 (9) Å	μ = 0.25 mm^{-1}
c = 22.240 (5) Å	T = 203 K
V = 1876.8 (6) Å^3	Plate, colourless
Z = 4	0.43 × 0.37 × 0.14 mm

Data collection

Oxford Diffraction Gemini R diffractometer	R_{int} = 0.050
Radiation source: fine-focus sealed tube	θ_{max} = 32.7º
Monochromator: graphite	θ_{min} = 4.8º
T = 203 K	h = −12→12
φ and ω scans	k = −13→14
Absorption correction: multi-scan (CrysAlis RED; Oxford Diffraction, 2007)	l = −32→32
T_{min} = 0.906, T_{max} = 1.000	2 standard reflections
18057 measured reflections	every 50 reflections
6220 independent reflections	intensity decay: none
2640 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites

Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.032$	$w = 1/[\sigma^2(F_o^2) + (0.0312P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.069$	$(\Delta/\sigma)_{max} = 0.016$
$S = 0.76$	$\Delta\rho_{max} = 0.21$ e Å^{-3}
6220 reflections	$\Delta\rho_{min} = -0.22$ e Å^{-3}
254 parameters	Extinction correction: none
Primary atom site location: structure-invariant direct methods	Absolute structure: Flack (1983), with 3628 Friedel pairs
Secondary atom site location: difference Fourier map	Flack parameter: 0.02 (4)

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}
Cl	0.82991 (6)	0.66081 (4)	0.14333 (2)	0.05311 (14)
F1	0.90703 (12)	0.15349 (10)	0.23407 (4)	0.0495 (3)
F2	0.85448 (12)	0.01133 (9)	0.16359 (4)	0.0507 (3)
F3	1.06136 (12)	−0.01341 (9)	0.21520 (4)	0.0485 (3)
O1	0.89852 (13)	−0.45246 (10)	−0.11680 (5)	0.0395 (3)
O2	1.12304 (12)	0.08094 (11)	0.10175 (4)	0.0355 (3)
H2B	1.2016	0.0439	0.1158	0.053*
N	0.86626 (16)	0.10757 (13)	0.03665 (5)	0.0332 (3)
H0A	0.9088	0.0411	0.0568	0.040*
C1	0.94820 (17)	0.26983 (14)	0.11402 (6)	0.0260 (3)
C2	0.93451 (18)	0.40036 (16)	0.13820 (7)	0.0306 (4)
H2A	0.9913	0.4230	0.1729	0.037*
C3	0.8395 (2)	0.49753 (14)	0.11254 (7)	0.0339 (4)
C4	0.7563 (2)	0.46620 (17)	0.06224 (8)	0.0398 (4)
H4A	0.6919	0.5325	0.0446	0.048*
C5	0.76666 (19)	0.33727 (17)	0.03738 (7)	0.0360 (4)
H5A	0.7083	0.3168	0.0029	0.043*
C6	0.86196 (18)	0.23591 (15)	0.06223 (6)	0.0282 (4)
C7	0.8037 (2)	0.07891 (15)	−0.02165 (7)	0.0364 (4)
H7A	0.8517	0.1405	−0.0510	0.044*
H7B	0.6924	0.0981	−0.0212	0.044*
C8	0.82856 (19)	−0.06668 (15)	−0.04160 (7)	0.0306 (4)

C9	0.7601 (2)	−0.10854 (17)	−0.09471 (8)	0.0424 (4)
H9A	0.6951	−0.0473	−0.1153	0.051*
C10	0.7839 (2)	−0.23590 (17)	−0.11818 (8)	0.0434 (4)
H10A	0.7357	−0.2614	−0.1544	0.052*
C11	0.87869 (18)	−0.32664 (16)	−0.08862 (7)	0.0311 (4)
C12	0.9456 (2)	−0.29100 (16)	−0.03566 (8)	0.0392 (4)
H12A	1.0091	−0.3535	−0.0150	0.047*
C13	0.9191 (2)	−0.16095 (17)	−0.01221 (7)	0.0390 (4)
H13A	0.9643	−0.1370	0.0248	0.047*
C14	1.0172 (2)	−0.54038 (17)	−0.09373 (9)	0.0514 (5)
H14A	1.0199	−0.6244	−0.1170	0.077*
H14B	0.9956	−0.5617	−0.0520	0.077*
H14C	1.1166	−0.4946	−0.0966	0.077*
C15	1.05879 (17)	0.16978 (15)	0.14503 (6)	0.0274 (3)
C16	0.9694 (2)	0.07957 (17)	0.18995 (8)	0.0345 (4)
C17	1.18271 (19)	0.23895 (15)	0.17881 (7)	0.0311 (4)
C18	1.28762 (19)	0.28546 (15)	0.20665 (7)	0.0342 (4)
C19	1.4148 (2)	0.34007 (18)	0.24111 (8)	0.0411 (4)
H19A	1.4228	0.3049	0.2827	0.049*
C20	1.4705 (3)	0.4811 (2)	0.23272 (10)	0.0676 (7)
H20A	1.4182	0.5378	0.2026	0.081*
H20B	1.5066	0.5308	0.2683	0.081*
C21	1.5639 (3)	0.3671 (2)	0.21144 (10)	0.0727 (7)
H21A	1.6586	0.3453	0.2337	0.087*
H21B	1.5703	0.3523	0.1679	0.087*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0663 (3)	0.0375 (2)	0.0555 (3)	0.0118 (2)	−0.0040 (3)	−0.0080 (2)
F1	0.0513 (6)	0.0649 (6)	0.0323 (5)	0.0004 (6)	0.0132 (5)	0.0022 (5)
F2	0.0472 (6)	0.0591 (6)	0.0459 (6)	−0.0258 (5)	−0.0090 (5)	0.0130 (5)
F3	0.0560 (6)	0.0459 (5)	0.0435 (6)	0.0030 (5)	−0.0096 (5)	0.0180 (5)
O1	0.0334 (7)	0.0377 (6)	0.0475 (7)	0.0026 (5)	−0.0007 (6)	−0.0050 (5)
O2	0.0313 (7)	0.0436 (6)	0.0318 (6)	0.0099 (5)	−0.0045 (6)	−0.0058 (5)
N	0.0399 (8)	0.0319 (7)	0.0279 (7)	0.0000 (6)	−0.0098 (7)	0.0025 (6)
C1	0.0241 (8)	0.0308 (8)	0.0231 (8)	−0.0018 (7)	0.0014 (7)	0.0032 (7)
C2	0.0271 (8)	0.0395 (9)	0.0253 (8)	−0.0024 (7)	0.0023 (8)	0.0011 (7)
C3	0.0369 (9)	0.0301 (8)	0.0346 (9)	0.0007 (8)	0.0026 (9)	−0.0014 (7)
C4	0.0395 (10)	0.0391 (10)	0.0408 (10)	0.0071 (8)	−0.0050 (9)	0.0071 (8)
C5	0.0354 (9)	0.0442 (10)	0.0283 (8)	0.0001 (9)	−0.0076 (8)	0.0031 (8)
C6	0.0253 (9)	0.0327 (9)	0.0267 (8)	−0.0027 (7)	0.0000 (8)	0.0040 (7)
C7	0.0432 (11)	0.0394 (9)	0.0267 (9)	−0.0005 (8)	−0.0059 (8)	0.0035 (7)
C8	0.0297 (9)	0.0359 (9)	0.0263 (8)	−0.0044 (8)	0.0014 (8)	0.0011 (7)
C9	0.0461 (11)	0.0441 (10)	0.0370 (10)	0.0112 (8)	−0.0180 (9)	−0.0045 (8)
C10	0.0467 (11)	0.0488 (11)	0.0347 (10)	0.0033 (9)	−0.0119 (9)	−0.0059 (9)
C11	0.0258 (9)	0.0333 (9)	0.0342 (9)	−0.0062 (8)	0.0019 (8)	−0.0013 (8)
C12	0.0432 (11)	0.0382 (10)	0.0361 (10)	−0.0038 (8)	−0.0113 (9)	0.0066 (8)

C13	0.0497 (11)	0.0368 (9)	0.0306 (9)	−0.0082 (9)	−0.0137 (9)	0.0004 (8)
C14	0.0415 (11)	0.0500 (11)	0.0628 (13)	0.0093 (9)	−0.0033 (10)	−0.0051 (10)
C15	0.0267 (8)	0.0306 (7)	0.0248 (8)	0.0001 (8)	0.0003 (8)	−0.0030 (7)
C16	0.0368 (10)	0.0356 (9)	0.0312 (9)	−0.0032 (9)	−0.0025 (9)	0.0044 (8)
C17	0.0275 (9)	0.0320 (8)	0.0337 (9)	−0.0003 (8)	−0.0023 (8)	0.0037 (7)
C18	0.0304 (10)	0.0337 (9)	0.0386 (10)	0.0016 (8)	0.0010 (8)	−0.0005 (7)
C19	0.0359 (10)	0.0465 (10)	0.0408 (10)	−0.0044 (9)	−0.0069 (9)	0.0017 (9)
C20	0.0816 (17)	0.0393 (11)	0.0818 (15)	−0.0179 (12)	−0.0386 (14)	0.0011 (11)
C21	0.0464 (12)	0.0994 (18)	0.0723 (15)	−0.0318 (13)	0.0111 (13)	−0.0185 (13)

Geometric parameters (Å, °)

Cl—C3	1.7375 (15)	C8—C9	1.383 (2)
F1—C16	1.3321 (18)	C9—C10	1.365 (2)
F2—C16	1.3317 (19)	C9—H9A	0.9400
F3—C16	1.3311 (18)	C10—C11	1.374 (2)
O1—C11	1.3901 (18)	C10—H10A	0.9400
O1—C14	1.4327 (19)	C11—C12	1.357 (2)
O2—C15	1.4097 (16)	C12—C13	1.392 (2)
O2—H2B	0.8300	C12—H12A	0.9400
N—C6	1.3771 (18)	C13—H13A	0.9400
N—C7	1.4323 (18)	C14—H14A	0.9700
N—H0A	0.8700	C14—H14B	0.9700
C1—C2	1.389 (2)	C14—H14C	0.9700
C1—C6	1.411 (2)	C15—C17	1.472 (2)
C1—C15	1.531 (2)	C15—C16	1.540 (2)
C2—C3	1.379 (2)	C17—C18	1.188 (2)
C2—H2A	0.9400	C18—C19	1.442 (2)
C3—C4	1.365 (2)	C19—C20	1.471 (3)
C4—C5	1.378 (2)	C19—C21	1.471 (3)
C4—H4A	0.9400	C19—H19A	0.9900
C5—C6	1.401 (2)	C20—C21	1.454 (3)
C5—H5A	0.9400	C20—H20A	0.9800
C7—C8	1.505 (2)	C20—H20B	0.9800
C7—H7A	0.9800	C21—H21A	0.9800
C7—H7B	0.9800	C21—H21B	0.9800
C8—C13	1.373 (2)		
C11—O1—C14	117.17 (13)	C13—C12—H12A	120.4
C15—O2—H2B	109.5	C8—C13—C12	121.81 (15)
C6—N—C7	122.80 (12)	C8—C13—H13A	119.1
C6—N—H0A	118.6	C12—C13—H13A	119.1
C7—N—H0A	118.6	O1—C14—H14A	109.5
C2—C1—C6	119.12 (14)	O1—C14—H14B	109.5
C2—C1—C15	117.70 (13)	H14A—C14—H14B	109.5
C6—C1—C15	123.18 (13)	O1—C14—H14C	109.5
C3—C2—C1	121.49 (14)	H14A—C14—H14C	109.5
C3—C2—H2A	119.3	H14B—C14—H14C	109.5
C1—C2—H2A	119.3	O2—C15—C17	110.16 (12)
C4—C3—C2	119.92 (14)	O2—C15—C1	109.34 (11)

C4—C3—Cl	120.25 (13)	C17—C15—C1	113.01 (12)
C2—C3—Cl	119.81 (12)	O2—C15—C16	106.76 (12)
C3—C4—C5	119.96 (15)	C17—C15—C16	107.23 (12)
C3—C4—H4A	120.0	C1—C15—C16	110.14 (12)
C5—C4—H4A	120.0	F2—C16—F3	106.82 (13)
C4—C5—C6	121.71 (15)	F2—C16—F1	107.11 (14)
C4—C5—H5A	119.1	F3—C16—F1	107.48 (13)
C6—C5—H5A	119.1	F2—C16—C15	112.00 (13)
N—C6—C5	119.73 (14)	F3—C16—C15	111.38 (14)
N—C6—C1	122.46 (14)	F1—C16—C15	111.76 (13)
C5—C6—C1	117.80 (14)	C18—C17—C15	175.12 (16)
N—C7—C8	113.44 (13)	C17—C18—C19	179.06 (18)
N—C7—H7A	108.9	C18—C19—C20	121.87 (15)
C8—C7—H7A	108.9	C18—C19—C21	119.69 (15)
N—C7—H7B	108.9	C20—C19—C21	59.26 (13)
C8—C7—H7B	108.9	C18—C19—H19A	114.9
H7A—C7—H7B	107.7	C20—C19—H19A	114.9
C13—C8—C9	116.86 (14)	C21—C19—H19A	114.9
C13—C8—C7	125.05 (15)	C21—C20—C19	60.39 (12)
C9—C8—C7	118.05 (15)	C21—C20—H20A	117.7
C10—C9—C8	122.13 (16)	C19—C20—H20A	117.7
C10—C9—H9A	118.9	C21—C20—H20B	117.7
C8—C9—H9A	118.9	C19—C20—H20B	117.7
C9—C10—C11	119.65 (16)	H20A—C20—H20B	114.9
C9—C10—H10A	120.2	C20—C21—C19	60.35 (14)
C11—C10—H10A	120.2	C20—C21—H21A	117.7
C12—C11—C10	120.23 (15)	C19—C21—H21A	117.7
C12—C11—O1	124.44 (14)	C20—C21—H21B	117.7
C10—C11—O1	115.33 (14)	C19—C21—H21B	117.7
C11—C12—C13	119.28 (15)	H21A—C21—H21B	114.9
C11—C12—H12A	120.4		
C6—C1—C2—C3	−0.4 (2)	C14—O1—C11—C10	168.93 (14)
C15—C1—C2—C3	178.93 (13)	C10—C11—C12—C13	−1.0 (2)
C1—C2—C3—C4	0.0 (2)	O1—C11—C12—C13	178.99 (14)
C1—C2—C3—Cl	−178.38 (12)	C9—C8—C13—C12	2.2 (2)
C2—C3—C4—C5	0.4 (2)	C7—C8—C13—C12	−175.29 (16)
Cl—C3—C4—C5	178.77 (13)	C11—C12—C13—C8	−0.9 (3)
C3—C4—C5—C6	−0.3 (2)	C2—C1—C15—O2	−148.07 (13)
C7—N—C6—C5	13.6 (2)	C6—C1—C15—O2	31.26 (18)
C7—N—C6—C1	−167.77 (15)	C2—C1—C15—C17	−24.99 (18)
C4—C5—C6—N	178.61 (15)	C6—C1—C15—C17	154.34 (14)
C4—C5—C6—C1	−0.1 (2)	C2—C1—C15—C16	94.91 (16)
C2—C1—C6—N	−178.20 (14)	C6—C1—C15—C16	−85.76 (17)
C15—C1—C6—N	2.5 (2)	O2—C15—C16—F2	−61.54 (16)
C2—C1—C6—C5	0.4 (2)	C17—C15—C16—F2	−179.58 (13)
C15—C1—C6—C5	−178.89 (13)	C1—C15—C16—F2	57.07 (17)
C6—N—C7—C8	177.15 (14)	O2—C15—C16—F3	58.03 (16)
N—C7—C8—C13	−8.4 (2)	C17—C15—C16—F3	−60.02 (16)
N—C7—C8—C9	174.05 (15)	C1—C15—C16—F3	176.64 (12)

C13—C8—C9—C10	−1.8 (3)	O2—C15—C16—F1	178.27 (12)
C7—C8—C9—C10	175.92 (16)	C17—C15—C16—F1	60.23 (16)
C8—C9—C10—C11	0.0 (3)	C1—C15—C16—F1	−63.12 (16)
C9—C10—C11—C12	1.5 (2)	C18—C19—C20—C21	−107.99 (19)
C9—C10—C11—O1	−178.54 (15)	C18—C19—C21—C20	111.60 (19)
C14—O1—C11—C12	−11.1 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2B···O1^{i}	0.83	1.92	2.7114 (15)	159
N—H0A···O2	0.87	2.14	2.6620 (17)	118
N—H0A···F2	0.87	2.44	2.9773 (16)	121

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

Fig. 1

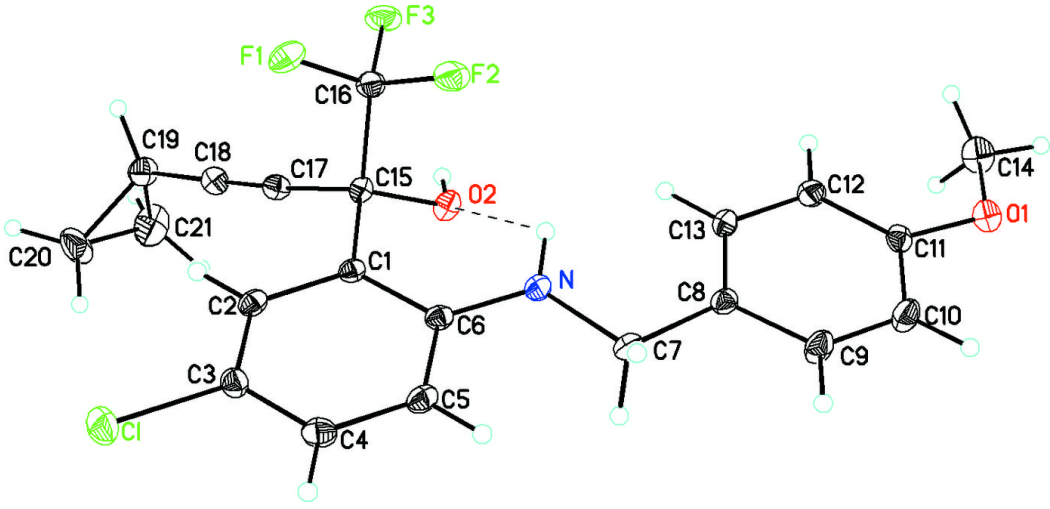
F3
F1
F2
C16
C19
C18
C17
C15
O2
C21
C20
C1
C2
C6
N
C3
C5
Cl
C4
C7
C8
C13
C12
C14
O1
C11
C10
C9

Fig. 2