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2-Carboxy-5-(trifluoromethyl)phenyl acetate

Ren Zhang,[a,b] Dan Wang,[b] Chunmei Ma[b] and Zhenjiang Li[c]*

[a]Department of Applied Chemistry, College of Science, Nanjing University of Technology, No.5 Xinmofan Road, Nanjing 210009, People's Republic of China, [b]Bioengineering Department, Xuzhou Higher Vocational College of Bioengineering, Mine West Road, Xuzhou 221006, People's Republic of China, and [c]College of Life Sciences and Pharmaceutical Engineering, Nanjing University of Technology, No.5 Xinmofan Road, Nanjing 210009, People's Republic of China
Correspondence e-mail: zjli@njut.edu.cn

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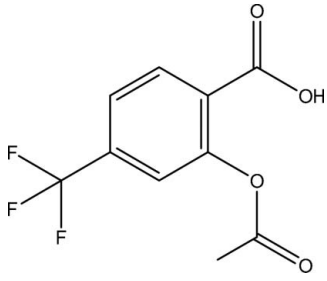
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.008 Å; disorder in main residue; R factor = 0.070; wR factor = 0.206; data-to-parameter ratio = 12.5.

The asymmetric unit of the title compound, $C_{10}H_7F_3O_4$, contains two independent molecules. In one of the molecules, the F atoms of the rifluoromethyl group are disordered over two positions with site occupation factors 0.231 (11)/0.769 (11). The intramolecular C—H···O hydrogen bond results in the formation of a planar five-membered ring, which is oriented at a dihedral angle of 4.24 (3)° with respect to the six-membered ring. In the crystal structure, C—H···F and O—H···O hydrogen bonds link the molecules.

Related literature

For related literature, see: Nakagawa *et al.* (1996); Wang *et al.* (1999). For bond-length data, see: Allen *et al.* (1987).



Experimental

Crystal data

$C_{10}H_7F_3O_4$
M_r = 248.16
Monoclinic, $P2_1/n$
a = 14.558 (3) Å
b = 5.7520 (12) Å
c = 26.243 (5) Å
β = 102.56 (3)°
V = 2144.9 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.15 mm^{-1}
T = 298 (2) K
0.40 × 0.10 × 0.10 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.942, T_{max} = 0.985
4356 measured reflections
4184 independent reflections
1674 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
3 standard reflections
frequency: 120 min
intensity decay: none

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.070
$wR(F^2)$ = 0.206
S = 1.02
4184 reflections
335 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.21 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1A···O6	0.82	1.81	2.631 (7)	174
O5—H5A···O2	0.82	1.83	2.646 (7)	172
C7—H7A···O1	0.93	2.39	2.721 (7)	101
C13—H13A···F2^{i}	0.93	2.55	3.313 (7)	140

Symmetry code: (i) $-x+2, -y, -z$.

Data collection: *CAD-4 Software* (Enraf–Nonius, 1989); cell refinement: *CAD-4 Software*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Siemens, 1996); software used to prepare material for publication: *SHELXL97*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HK2360).

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supplementary materials

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2-Carboxy-5-(trifluoromethyl)phenyl acetate

R. Zhang, D. Wang, C. Ma and Z. Li

Comment

Benzoic acid derivatives represent an interesting class of compounds possessing broad spectrum biological activities (Nakagawa *et al.*, 1996; Wang *et al.*, 1999). These compounds are known to exhibit diverse biological effects, such as insecticidal and fungicidal activities (Wang *et al.*, 1999). We report herein the crystal structure of the title compound, (I).

The asymmetric unit of the title compound, (I), contains two independent molecules, in which the bond lengths and angles are within normal ranges (Allen *et al.*, 1987).

When the crystal structure was solved, the atoms F4, F5 and F6 were found to be disordered.

The intramolecular C—H···O hydrogen bond (Table 1) results in the formation of the planar five-membered ring; A (O1/C1/C2/C7/H7A), which is oriented with respect to ring B (C2—C7) at a dihedral angle of 4.24 (3)°.

In the crystal structure, C—H···F and O—H···O hydrogen bonds (Table 1) link the molecules, in which they may be effective in the stabilization of the structure.

Experimental

For the preparation of the title compound, 2-Hydroxy-4-trifluoromethylbenzoic acid (0.62 g, 2 mmol) and acetyl chloride (0.69 g, 5 mmol) were added in a flask (25 ml) and reacted in an oil bath (363 K) for 6 h. After cooling and filtering, crude compound, (I) was obtained. Crystals of (I) suitable for X-ray analysis were obtained by slow evaporation of an acetone solution (m.p. 480 K).

Refinement

When the crystal structure was solved, the atoms F4, F5 and F6 were found to be disordered. During refinement with anisotropic thermal parameters, the occupancies of disordered F atoms were refined as F4 = 0.769 (11), F4' = 0.231 (11), F5 = 0.769 (11), F5' = 0.231 (11), F6 = 0.769 (11) and F6' = 0.231 (11). H atoms were positioned geometrically with O—H = 0.82 Å (for OH) and C—H = 0.93 and 0.96 Å for aromatic and methyl H atoms, respectively, and constrained to ride on their parent atoms, with U_{iso}(H) = xU_{eq}(C,*O*), where x = 1.2 for aromatic H and x = 1.5 for all other H atoms.

Figures

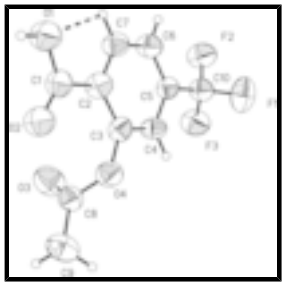

Fig. 1. The molecular structure of the title molecule, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen bond is shown as dashed lines.

2-Carboxy-5-(trifluoromethyl)phenyl acetate

Crystal data

$C_{10}H_7F_3O_4$	F_{000} = 1008
M_r = 248.16	D_x = 1.537 Mg m^{-3}
Monoclinic, $P2_1/n$	Melting point: 480 K
Hall symbol: -P 2yn	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 14.558 (3) Å	Cell parameters from 25 reflections
b = 5.7520 (12) Å	θ = 9–12º
c = 26.243 (5) Å	μ = 0.15 mm^{-1}
β = 102.56 (3)º	T = 298 (2) K
V = 2144.9 (8) Å^3	Block, colorless
Z = 8	0.40 × 0.10 × 0.10 mm

Data collection

Nonius CAD-4 diffractometer	R_{int} = 0.044
Radiation source: fine-focus sealed tube	θ_{max} = 26.0º
Monochromator: graphite	θ_{min} = 1.5º
T = 298(2) K	h = −17→17
ω/2θ scans	k = 0→7
Absorption correction: ψ scan (North *et al.*, 1968)	l = 0→32
T_{min} = 0.942, T_{max} = 0.985	3 standard reflections
4356 measured reflections	every 120 min
4184 independent reflections	intensity decay: none
1674 reflections with $I > 2\sigma(I)$	

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites

$R[F^2 > 2\sigma(F^2)] = 0.070$	H-atom parameters constrained
$wR(F^2) = 0.206$	$w = 1/[\sigma^2(F_o^2) + (0.060P)^2 + 1.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.02$	$(\Delta/\sigma)_{max} < 0.001$
4184 reflections	$\Delta\rho_{max} = 0.21$ e Å^{-3}
335 parameters	$\Delta\rho_{min} = -0.19$ e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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}	Occ. (<1)
O1	0.9999 (3)	−0.2926 (8)	0.04713 (16)	0.1174 (15)	
H1A	1.0431	−0.3851	0.0565	0.176*	
O2	0.9372 (3)	−0.4915 (8)	0.10301 (17)	0.1049 (13)	
O3	0.8243 (4)	−0.1993 (9)	0.17950 (19)	0.1314 (18)	
O4	0.7574 (2)	−0.3920 (7)	0.10665 (16)	0.0890 (11)	
F1	0.5505 (3)	0.1828 (7)	−0.02489 (16)	0.1326 (14)	
F2	0.6350 (2)	0.4848 (6)	−0.00741 (15)	0.1153 (12)	
F3	0.5733 (2)	0.3315 (6)	0.05013 (14)	0.1173 (12)	
C1	0.9332 (4)	−0.3349 (10)	0.0722 (2)	0.0842 (16)	
C2	0.8526 (4)	−0.1699 (9)	0.0581 (2)	0.0782 (15)	
C3	0.7697 (3)	−0.2003 (9)	0.0766 (2)	0.0748 (14)	
C4	0.6952 (4)	−0.0522 (9)	0.0618 (2)	0.0778 (15)	
H4A	0.6411	−0.0746	0.0746	0.093*	
C5	0.6992 (3)	0.1293 (9)	0.02827 (19)	0.0695 (13)	
C6	0.7798 (4)	0.1678 (10)	0.0096 (2)	0.0853 (16)	
H6A	0.7840	0.2924	−0.0124	0.102*	
C7	0.8543 (4)	0.0139 (10)	0.0247 (2)	0.0841 (16)	
H7A	0.9080	0.0361	0.0116	0.101*	
C8	0.7885 (4)	−0.3724 (13)	0.1602 (3)	0.0923 (18)	
C9	0.7701 (5)	−0.5929 (12)	0.1860 (3)	0.136 (3)	
H9A	0.7920	−0.5783	0.2231	0.204*	
H9B	0.8028	−0.7182	0.1735	0.204*	
H9C	0.7038	−0.6245	0.1780	0.204*	
C10	0.6158 (4)	0.2812 (11)	0.0115 (2)	0.0836 (15)	

O5	1.0815 (3)	−0.7810 (7)	0.12631 (17)	0.1112 (14)	
H5A	1.0396	−0.6846	0.1175	0.167*	
O6	1.1450 (3)	−0.5743 (7)	0.07251 (16)	0.1043 (13)	
O7	1.2003 (3)	−0.9896 (9)	0.23943 (17)	0.1168 (16)	
O8	1.1704 (2)	−1.1778 (6)	0.16344 (13)	0.0803 (10)	
F4	1.5198 (4)	−1.2824 (17)	0.2164 (3)	0.135 (3)	0.769 (11)
F5	1.5193 (5)	−1.3647 (14)	0.1369 (3)	0.150 (3)	0.769 (11)
F6	1.5774 (4)	−1.0544 (13)	0.1709 (4)	0.141 (3)	0.769 (11)
F4'	1.4989 (14)	−1.428 (4)	0.1841 (11)	0.126 (7)	0.231 (11)
F5'	1.5587 (15)	−1.187 (5)	0.1397 (8)	0.114 (7)	0.231 (11)
F6'	1.5503 (15)	−1.089 (4)	0.2094 (9)	0.122 (7)	0.231 (11)
C11	1.1474 (4)	−0.7344 (10)	0.1058 (2)	0.0805 (15)	
C12	1.2380 (3)	−0.8623 (10)	0.1208 (2)	0.0761 (14)	
C13	1.3175 (4)	−0.7777 (10)	0.1073 (2)	0.0881 (16)	
H13A	1.3125	−0.6433	0.0871	0.106*	
C14	1.4036 (4)	−0.8814 (10)	0.1219 (2)	0.0833 (16)	
H14A	1.4560	−0.8176	0.1123	0.100*	
C15	1.4113 (4)	−1.0808 (10)	0.1510 (2)	0.0814 (15)	
C16	1.3343 (3)	−1.1774 (9)	0.1659 (2)	0.0803 (15)	
H16A	1.3406	−1.3119	0.1860	0.096*	
C17	1.2476 (4)	−1.0697 (9)	0.15023 (19)	0.0717 (14)	
C18	1.1530 (4)	−1.1230 (12)	0.2111 (2)	0.0838 (16)	
C19	1.0710 (4)	−1.2563 (13)	0.2207 (2)	0.117 (2)	
H19A	1.0596	−1.2147	0.2542	0.175*	
H19B	1.0841	−1.4198	0.2201	0.175*	
H19C	1.0165	−1.2206	0.1940	0.175*	
C20	1.5044 (4)	−1.2004 (14)	0.1687 (3)	0.0947 (18)	

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.098 (3)	0.131 (4)	0.135 (3)	0.048 (3)	0.049 (2)	0.038 (3)
O2	0.094 (3)	0.093 (3)	0.133 (3)	0.025 (2)	0.037 (2)	0.027 (3)
O3	0.174 (5)	0.102 (4)	0.113 (4)	−0.014 (4)	0.021 (3)	0.001 (3)
O4	0.088 (2)	0.073 (3)	0.107 (3)	0.005 (2)	0.022 (2)	0.018 (2)
F1	0.105 (2)	0.119 (3)	0.155 (3)	0.014 (2)	−0.012 (2)	−0.020 (3)
F2	0.108 (2)	0.093 (2)	0.153 (3)	0.024 (2)	0.045 (2)	0.035 (2)
F3	0.111 (2)	0.127 (3)	0.128 (3)	0.042 (2)	0.057 (2)	0.011 (2)
C1	0.078 (3)	0.081 (4)	0.096 (4)	0.019 (3)	0.024 (3)	0.006 (3)
C2	0.082 (3)	0.054 (3)	0.103 (4)	0.014 (3)	0.029 (3)	0.001 (3)
C3	0.068 (3)	0.066 (4)	0.092 (4)	0.009 (3)	0.019 (3)	0.000 (3)
C4	0.081 (3)	0.072 (4)	0.089 (4)	0.005 (3)	0.037 (3)	0.005 (3)
C5	0.065 (3)	0.067 (3)	0.078 (3)	0.010 (3)	0.020 (3)	0.001 (3)
C6	0.088 (4)	0.078 (4)	0.096 (4)	0.019 (3)	0.034 (3)	0.016 (3)
C7	0.079 (3)	0.083 (4)	0.097 (4)	0.011 (3)	0.033 (3)	0.006 (3)
C8	0.084 (4)	0.094 (4)	0.098 (5)	0.011 (3)	0.016 (3)	0.026 (4)
C9	0.151 (6)	0.120 (5)	0.135 (5)	−0.004 (5)	0.027 (4)	0.047 (4)
C10	0.085 (4)	0.074 (4)	0.095 (4)	0.013 (3)	0.025 (3)	0.011 (3)

O5	0.090 (3)	0.104 (3)	0.152 (3)	0.027 (2)	0.053 (2)	0.039 (3)
O6	0.111 (3)	0.103 (3)	0.112 (3)	0.037 (2)	0.051 (2)	0.030 (3)
O7	0.114 (3)	0.140 (4)	0.111 (3)	−0.026 (3)	0.055 (3)	−0.048 (3)
O8	0.078 (2)	0.084 (3)	0.083 (2)	0.002 (2)	0.0255 (18)	0.002 (2)
F4	0.097 (4)	0.185 (7)	0.125 (4)	0.031 (4)	0.027 (3)	0.059 (4)
F5	0.140 (5)	0.136 (5)	0.166 (5)	0.060 (4)	0.014 (4)	−0.038 (4)
F6	0.087 (3)	0.142 (5)	0.194 (7)	−0.014 (3)	0.034 (4)	0.013 (5)
F4'	0.124 (10)	0.109 (8)	0.146 (12)	0.006 (8)	0.029 (8)	0.009 (8)
F5'	0.100 (9)	0.139 (12)	0.111 (10)	0.027 (8)	0.038 (7)	0.006 (8)
F6'	0.117 (10)	0.129 (10)	0.117 (10)	0.013 (8)	0.016 (7)	−0.017 (8)
C11	0.085 (3)	0.077 (4)	0.086 (4)	0.016 (3)	0.032 (3)	0.009 (3)
C12	0.074 (3)	0.081 (4)	0.080 (3)	0.011 (3)	0.031 (3)	0.004 (3)
C13	0.091 (4)	0.080 (4)	0.100 (4)	0.023 (3)	0.036 (3)	0.021 (3)
C14	0.078 (3)	0.085 (4)	0.095 (4)	0.002 (3)	0.037 (3)	0.011 (3)
C15	0.082 (4)	0.080 (4)	0.089 (4)	0.020 (3)	0.035 (3)	0.010 (3)
C16	0.078 (3)	0.074 (4)	0.094 (4)	0.011 (3)	0.029 (3)	0.007 (3)
C17	0.076 (3)	0.073 (4)	0.070 (3)	0.000 (3)	0.023 (3)	0.001 (3)
C18	0.078 (3)	0.094 (4)	0.084 (4)	0.015 (3)	0.029 (3)	−0.006 (3)
C19	0.106 (4)	0.138 (5)	0.120 (5)	−0.015 (4)	0.053 (4)	0.002 (4)
C20	0.077 (4)	0.113 (5)	0.097 (4)	0.003 (4)	0.023 (3)	0.009 (4)

Geometric parameters (Å, °)

O1—C1	1.309 (6)	O6—C11	1.264 (6)
O1—H1A	0.8200	O7—C18	1.181 (6)
O2—C1	1.203 (5)	O8—C18	1.364 (6)
O3—C8	1.185 (7)	O8—C17	1.393 (5)
O4—C8	1.385 (7)	F4—C20	1.310 (8)
O4—C3	1.389 (6)	F5—C20	1.310 (9)
F1—C10	1.320 (6)	F6—C20	1.347 (9)
F2—C10	1.326 (6)	F4'—C20	1.38 (2)
F3—C10	1.328 (6)	F5'—C20	1.213 (19)
C1—C2	1.492 (7)	F6'—C20	1.298 (19)
C2—C7	1.377 (7)	C11—C12	1.487 (7)
C2—C3	1.407 (6)	C12—C13	1.371 (7)
C3—C4	1.368 (6)	C12—C17	1.412 (7)
C4—C5	1.376 (6)	C13—C14	1.365 (7)
C4—H4A	0.9300	C13—H13A	0.9300
C5—C6	1.385 (6)	C14—C15	1.369 (7)
C5—C10	1.483 (7)	C14—H14A	0.9300
C6—C7	1.389 (7)	C15—C16	1.381 (6)
C6—H6A	0.9300	C15—C20	1.501 (8)
C7—H7A	0.9300	C16—C17	1.386 (6)
C8—C9	1.489 (8)	C16—H16A	0.9300
C9—H9A	0.9600	C18—C19	1.486 (8)
C9—H9B	0.9600	C19—H19A	0.9600
C9—H9C	0.9600	C19—H19B	0.9600
O5—C11	1.227 (5)	C19—H19C	0.9600
O5—H5A	0.8200		

C1—O1—H1A	109.5	C14—C13—C12	123.1 (5)
C8—O4—C3	117.2 (5)	C14—C13—H13A	118.4
O2—C1—O1	123.0 (5)	C12—C13—H13A	118.4
O2—C1—C2	124.3 (5)	C13—C14—C15	118.8 (5)
O1—C1—C2	112.7 (5)	C13—C14—H14A	120.6
C7—C2—C3	116.8 (5)	C15—C14—H14A	120.6
C7—C2—C1	121.7 (5)	C14—C15—C16	121.4 (5)
C3—C2—C1	121.5 (5)	C14—C15—C20	121.1 (5)
C4—C3—O4	117.6 (5)	C16—C15—C20	117.5 (5)
C4—C3—C2	120.8 (5)	C15—C16—C17	118.6 (5)
O4—C3—C2	121.4 (5)	C15—C16—H16A	120.7
C3—C4—C5	120.9 (5)	C17—C16—H16A	120.7
C3—C4—H4A	119.6	C16—C17—O8	117.4 (5)
C5—C4—H4A	119.6	C16—C17—C12	121.0 (5)
C4—C5—C6	120.4 (5)	O8—C17—C12	121.6 (5)
C4—C5—C10	119.4 (5)	O7—C18—O8	121.9 (5)
C6—C5—C10	120.2 (5)	O7—C18—C19	127.4 (6)
C5—C6—C7	117.8 (5)	O8—C18—C19	110.6 (6)
C5—C6—H6A	121.1	C18—C19—H19A	109.5
C7—C6—H6A	121.1	C18—C19—H19B	109.5
C2—C7—C6	123.4 (5)	H19A—C19—H19B	109.5
C2—C7—H7A	118.3	C18—C19—H19C	109.5
C6—C7—H7A	118.3	H19A—C19—H19C	109.5
O3—C8—O4	121.2 (6)	H19B—C19—H19C	109.5
O3—C8—C9	128.9 (7)	F5'—C20—F6'	101.2 (16)
O4—C8—C9	109.9 (6)	F5'—C20—F5	54.9 (13)
C8—C9—H9A	109.5	F6'—C20—F5	138.8 (10)
C8—C9—H9B	109.5	F5'—C20—F4	128.5 (11)
H9A—C9—H9B	109.5	F6'—C20—F4	56.2 (12)
C8—C9—H9C	109.5	F5—C20—F4	109.4 (8)
H9A—C9—H9C	109.5	F5'—C20—F6	51.0 (13)
H9B—C9—H9C	109.5	F6'—C20—F6	52.9 (11)
F1—C10—F2	106.6 (5)	F5—C20—F6	103.7 (7)
F1—C10—F3	105.3 (5)	F4—C20—F6	102.4 (7)
F2—C10—F3	105.3 (5)	F5'—C20—F4'	109.3 (16)
F1—C10—C5	112.1 (5)	F6'—C20—F4'	106.4 (16)
F2—C10—C5	113.9 (5)	F5—C20—F4'	61.9 (11)
F3—C10—C5	112.9 (5)	F4—C20—F4'	52.2 (10)
C11—O5—H5A	109.5	F6—C20—F4'	132.6 (10)
C18—O8—C17	116.4 (4)	F5'—C20—C15	116.4 (11)
O5—C11—O6	123.7 (5)	F6'—C20—C15	107.3 (11)
O5—C11—C12	120.6 (5)	F5—C20—C15	113.4 (6)
O6—C11—C12	115.6 (5)	F4—C20—C15	114.6 (6)
C13—C12—C17	116.9 (5)	F6—C20—C15	112.2 (6)
C13—C12—C11	120.4 (5)	F4'—C20—C15	114.9 (10)
C17—C12—C11	122.6 (5)		
O2—C1—C2—C7	176.4 (6)	O6—C11—C12—C17	−168.8 (5)
O1—C1—C2—C7	−4.1 (8)	C17—C12—C13—C14	−1.5 (8)
O2—C1—C2—C3	−6.2 (9)	C11—C12—C13—C14	176.9 (5)

O1—C1—C2—C3	173.3 (5)	C12—C13—C14—C15	0.8 (9)
C8—O4—C3—C4	−96.5 (6)	C13—C14—C15—C16	−0.4 (8)
C8—O4—C3—C2	89.1 (6)	C13—C14—C15—C20	−179.3 (6)
C7—C2—C3—C4	−0.1 (8)	C14—C15—C16—C17	0.8 (8)
C1—C2—C3—C4	−177.7 (5)	C20—C15—C16—C17	179.7 (5)
C7—C2—C3—O4	174.1 (5)	C15—C16—C17—O8	176.7 (5)
C1—C2—C3—O4	−3.4 (8)	C15—C16—C17—C12	−1.6 (8)
O4—C3—C4—C5	−174.1 (4)	C18—O8—C17—C16	87.5 (6)
C2—C3—C4—C5	0.3 (8)	C18—O8—C17—C12	−94.3 (6)
C3—C4—C5—C6	−1.1 (8)	C13—C12—C17—C16	1.9 (7)
C3—C4—C5—C10	177.8 (5)	C11—C12—C17—C16	−176.5 (5)
C4—C5—C6—C7	1.8 (8)	C13—C12—C17—O8	−176.3 (5)
C10—C5—C6—C7	−177.1 (5)	C11—C12—C17—O8	5.4 (8)
C3—C2—C7—C6	0.8 (8)	C17—O8—C18—O7	0.7 (8)
C1—C2—C7—C6	178.3 (5)	C17—O8—C18—C19	−178.1 (5)
C5—C6—C7—C2	−1.6 (8)	C14—C15—C20—F5'	−33 (2)
C3—O4—C8—O3	−0.3 (8)	C16—C15—C20—F5'	148.4 (18)
C3—O4—C8—C9	−179.8 (5)	C14—C15—C20—F6'	79.8 (16)
C4—C5—C10—F1	−77.8 (7)	C16—C15—C20—F6'	−99.1 (16)
C6—C5—C10—F1	101.1 (6)	C14—C15—C20—F5	−93.6 (9)
C4—C5—C10—F2	161.1 (5)	C16—C15—C20—F5	87.5 (9)
C6—C5—C10—F2	−20.0 (8)	C14—C15—C20—F4	139.9 (8)
C4—C5—C10—F3	41.0 (7)	C16—C15—C20—F4	−39.1 (10)
C6—C5—C10—F3	−140.1 (5)	C14—C15—C20—F6	23.6 (10)
O5—C11—C12—C13	−165.1 (5)	C16—C15—C20—F6	−155.4 (7)
O6—C11—C12—C13	12.9 (8)	C14—C15—C20—F4'	−162.2 (14)
O5—C11—C12—C17	13.2 (9)	C16—C15—C20—F4'	18.9 (16)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1A···O6	0.82	1.81	2.631 (7)	174
O5—H5A···O2	0.82	1.83	2.646 (7)	172
C7—H7A···O1	0.93	2.39	2.721 (7)	101
C13—H13A···F2^{i}	0.93	2.55	3.313 (7)	140

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

Fig. 1