Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

Ethyl 6-(4-fluorophenyl)-4-hydroxy-2-sulfanylidene-4-trifluoromethyl-1,3-diazinane-5-carboxylate

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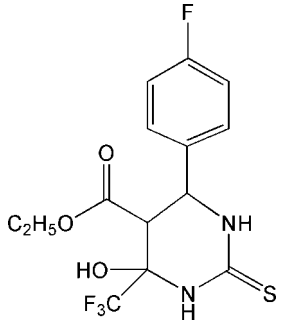
Received 26 December 2011; accepted 19 February 2012

Key indicators: single-crystal X-ray study; T = 113 K; mean σ(C–C) = 0.002 Å; R factor = 0.033; wR factor = 0.084; data-to-parameter ratio = 16.0.

In the title compound, $C_{14}H_{14}F_4N_2O_3S$, the hexahydropyrimidine ring adopts a half-chair conformation. The molecular conformation is stabilized by an intramolecular O—H···O hydrogen bond, generating an S(6) ring. The crystal structure features O—H···S and N—H···S hydrogen bonds.

Related literature

For the bioactivity of dihydropyrimidines, see: Atwal *et al.* (1989); Kappe *et al.* (1997); Brier *et al.* (2004); Cochran *et al.* (2005). For the bioactivity of organofluorine compounds, see: Konz (1997); Hass (2004). For a related structure, see: Li *et al.* (2011).



Experimental

Crystal data

$C_{14}H_{14}F_4N_2O_3S$
M_r = 366.33
Monoclinic, $P2_1/c$
a = 11.0091 (12) Å
b = 9.9741 (10) Å
c = 14.6890 (16) Å
β = 109.269 (12)°
V = 1522.6 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.27 mm^{-1}
T = 113 K
0.20 × 0.19 × 0.12 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2009)
T_{min} = 0.947, T_{max} = 0.968
18960 measured reflections
3627 independent reflections
2979 reflections with $I > 2\sigma(I)$
R_{int} = 0.042

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.084
S = 1.01
3627 reflections
227 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.44 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···O2	0.84	2.06	2.7767 (13)	144
O1—H1···S1^{i}	0.84	2.83	3.3796 (10)	124
N1—H1A···S1^{ii}	0.835 (16)	2.635 (17)	3.4566 (12)	168.1 (15)

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

Data collection: *CrystalClear* (Rigaku, 2009); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2009).

This work was supported by the Foundation of Henan Province Education Committee, China (grant Nos. 2010B150026, 2009B150023).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: FJ2501).

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supplementary materials

Acta Cryst. (2012). E**68**, o880 [doi:10.1107/S1600536812007465]

Ethyl 6-(4-fluorophenyl)-4-hydroxy-2-sulfanylidene-4-trifluoromethyl-1,3-diazinane-5-carboxylate

Bao-Jun Huang, Lei Zhu and Qin He

Comment

Dihydropyrimidine (DHPM) derivatives can be used as potential calcium channel blockers, antihypertensive agents, and α1–1 - a-antagonists (Atwal *et al.*, 1989; Kappe *et al.*, 1997;), inhibitors of mitotic kinesin Eg5 for treating cancer (Cochran *et al.*, 2005; Brier *et al.*, 2004). In addition, compounds that contain fluorine have special bioactivity, *e.g.* flumioxazin is a widely used herbicide (Konz, 1997; Hass, 2004). This led us to focus our attention on the synthesis and bioactivity of these important fused perfluoroalkylated heterocyclic compounds. During the synthesis of DHPM derivatives, the title compound, an intermediate $C_{14}H_{14}F_4N_2O_3S$ (I) was isolated and the structure confirmed by X-ray diffraction.

In the structure of the title molecule, the hexahydropyrimidine ring adopts a half-chair conformation, the mean planes formed by the ring atoms excluding the C atom bonded to the ethoxy carbonyl group have r.m.s. deviations of 0.0348 Å, the dihedral angle between the mean planes and benzenes ring is 58.18 (5)°. The molecular conformation is stabilized by intramolecular O—H···O hydrogen bond, generating an S(6) ring. The crystal structure is stabilized by intermolecular O—H···S and N—H···S hydrogen bonds. For a crystal structure related to the title compound, see: Li *et al.* (2011).

Experimental

The title compound was synthesized refluxing for 3 h a stirred solution of 4-fluorobenzaldehyde (2.48 g, 20 mmol), ethyl 4,4,4-trifluoro-3-oxobutanoate(4.42 g, 24 mmol) and thiourea (2.28 g, 30 mmol) in 20 ml of anhydrous ethanol, the reaction catalyzed by sulfamic acid (0.6 g). The solvent was evaporated *in vacuo* and the residue was washed with water. The title compound was recrystallized from 50% aqueous ethanol and single crystals of (I) were obtained by slow evaporation.

Refinement

Hydrogen atoms involved in hydrogen-bonding inetractions were located by difference methods and their positional and isotropic displacement parameters were refined. Other H atoms were placed in calculated positions, with C—H(aromatic) = 0.95 Å and C—H(aliphatic) = 0.98 Å, 0.99 Å or 1.00 Å, and treated as riding, with U_{iso}(H) = 1.2Ueq(C).

Computing details

Data collection: *CrystalClear* (Rigaku, 2009); cell refinement: *CrystalClear* (Rigaku, 2009); data reduction: *CrystalClear* (Rigaku, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *CrystalStructure* (Rigaku, 2009).

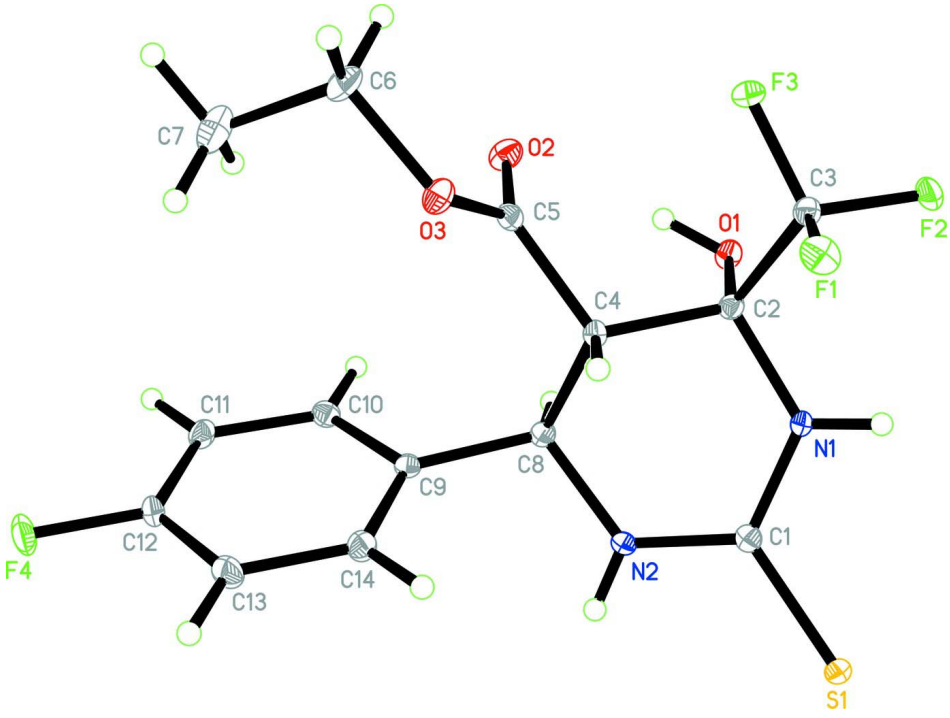

Figure 1

Molecular configuration and atom numbering scheme for (I), with displacement ellipsoids drawn at the 30% probability level.

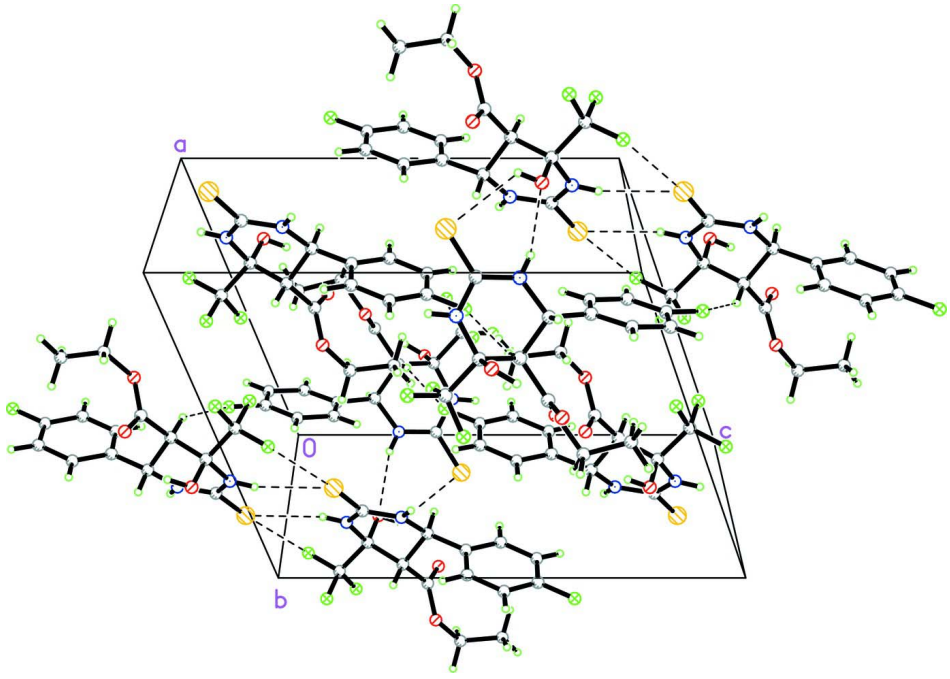

Figure 2

The packing diagram of the title compound. Intermolecular hydrogen bonds are shown as dashed line.

Ethyl 6-(4-fluorophenyl)-4-hydroxy-2-sulfanylidene-4-trifluoromethyl- 1,3-diazinane-5-carboxylate

Crystal data

$C_{14}H_{14}F_4N_2O_3S$
$M_r = 366.33$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.0091$ (12) Å
$b = 9.9741$ (10) Å
$c = 14.6890$ (16) Å
$\beta = 109.269$ (12)°
$V = 1522.6$ (3) Å^3
$Z = 4$
$F(000) = 752$
$D_x = 1.598$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5440 reflections
$\theta = 2.0$–$27.9°$
$\mu = 0.27$ mm^{-1}
$T = 113$ K
Prism, colorless
0.20 × 0.19 × 0.12 mm

Data collection

Rigaku Saturn CCD area-detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.63 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku, 2009)
$T_{min} = 0.947$, $T_{max} = 0.968$
18960 measured reflections
3627 independent reflections
2979 reflections with $I > 2\sigma(I)$
$R_{int} = 0.042$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.0°$
$h = -14 \rightarrow 13$
$k = -13 \rightarrow 13$
$l = -19 \rightarrow 18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.084$
$S = 1.01$
3627 reflections
227 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.050P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å^{-3}
$\Delta\rho_{min} = -0.27$ e Å^{-3}

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 $F^2 > \sigma(F^2)$ 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}
S1	1.09867 (3)	0.59272 (4)	0.13111 (2)	0.01692 (10)
F1	0.63627 (8)	0.49595 (8)	−0.01023 (6)	0.0223 (2)
F2	0.70354 (8)	0.30439 (8)	−0.04289 (6)	0.0208 (2)

F3	0.56928 (7)	0.31300 (9)	0.03576 (6)	0.0211 (2)
F4	0.77930 (9)	0.74276 (9)	0.59153 (6)	0.0287 (2)
O1	0.81420 (9)	0.24372 (9)	0.15081 (7)	0.0161 (2)
H1	0.7778	0.2236	0.1910	0.024*
O2	0.64286 (9)	0.28689 (10)	0.25049 (7)	0.0214 (2)
O3	0.55299 (9)	0.49304 (10)	0.22282 (7)	0.0200 (2)
N1	0.89236 (10)	0.43819 (12)	0.10096 (8)	0.0139 (2)
N2	0.96704 (11)	0.54349 (13)	0.24822 (8)	0.0156 (2)
C1	0.97865 (12)	0.52093 (13)	0.16191 (9)	0.0138 (3)
C2	0.78397 (12)	0.37743 (13)	0.12011 (9)	0.0131 (3)
C3	0.67215 (13)	0.37300 (14)	0.02481 (10)	0.0159 (3)
C4	0.74924 (12)	0.46406 (13)	0.19506 (9)	0.0132 (3)
H4	0.7220	0.5551	0.1673	0.016*
C5	0.64259 (13)	0.40290 (14)	0.22563 (9)	0.0154 (3)
C6	0.44550 (14)	0.44909 (18)	0.25374 (11)	0.0270 (4)
H6A	0.4297	0.3523	0.2400	0.032*
H6B	0.3666	0.4985	0.2169	0.032*
C7	0.47442 (16)	0.47361 (19)	0.35960 (12)	0.0333 (4)
H7A	0.5492	0.4200	0.3963	0.050*
H7B	0.3998	0.4479	0.3781	0.050*
H7C	0.4931	0.5689	0.3736	0.050*
C8	0.87196 (12)	0.47696 (14)	0.28305 (9)	0.0138 (3)
H8	0.9039	0.3849	0.3058	0.017*
C9	0.85100 (12)	0.55238 (14)	0.36593 (9)	0.0136 (3)
C10	0.84025 (13)	0.47892 (14)	0.44373 (10)	0.0160 (3)
H10	0.8506	0.3843	0.4449	0.019*
C11	0.81454 (13)	0.54231 (15)	0.51951 (10)	0.0174 (3)
H11	0.8055	0.4924	0.5720	0.021*
C12	0.80260 (13)	0.67954 (15)	0.51632 (10)	0.0183 (3)
C13	0.81342 (14)	0.75668 (15)	0.44131 (10)	0.0216 (3)
H13	0.8051	0.8515	0.4417	0.026*
C14	0.83700 (14)	0.69099 (14)	0.36509 (10)	0.0184 (3)
H14	0.8436	0.7414	0.3120	0.022*
H2A	1.0172 (14)	0.5927 (16)	0.2825 (11)	0.015 (4)*
H1A	0.9054 (15)	0.4242 (17)	0.0489 (12)	0.026 (5)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01646 (18)	0.01854 (18)	0.01832 (18)	−0.00502 (13)	0.00919 (14)	−0.00420 (14)
F1	0.0232 (4)	0.0197 (5)	0.0198 (4)	0.0034 (3)	0.0016 (3)	0.0036 (3)
F2	0.0202 (4)	0.0267 (5)	0.0166 (4)	−0.0024 (3)	0.0075 (3)	−0.0088 (3)
F3	0.0137 (4)	0.0288 (5)	0.0210 (4)	−0.0066 (3)	0.0061 (3)	−0.0033 (4)
F4	0.0441 (6)	0.0261 (5)	0.0230 (5)	−0.0029 (4)	0.0206 (4)	−0.0098 (4)
O1	0.0198 (5)	0.0124 (5)	0.0183 (5)	0.0014 (4)	0.0093 (4)	0.0014 (4)
O2	0.0211 (5)	0.0190 (5)	0.0266 (6)	−0.0008 (4)	0.0114 (4)	0.0025 (4)
O3	0.0160 (5)	0.0229 (6)	0.0235 (5)	0.0035 (4)	0.0097 (4)	0.0004 (4)
N1	0.0138 (6)	0.0172 (6)	0.0128 (6)	−0.0028 (4)	0.0071 (5)	−0.0034 (5)
N2	0.0146 (6)	0.0196 (6)	0.0125 (6)	−0.0063 (5)	0.0044 (5)	−0.0045 (5)
C1	0.0134 (7)	0.0128 (6)	0.0149 (7)	0.0019 (5)	0.0044 (5)	−0.0002 (5)

C2	0.0131 (6)	0.0126 (7)	0.0148 (6)	−0.0001 (5)	0.0061 (5)	−0.0005 (5)
C3	0.0157 (7)	0.0160 (7)	0.0178 (7)	−0.0005 (5)	0.0078 (6)	−0.0022 (5)
C4	0.0141 (7)	0.0137 (6)	0.0124 (6)	0.0007 (5)	0.0054 (5)	−0.0006 (5)
C5	0.0143 (7)	0.0185 (7)	0.0127 (6)	−0.0006 (5)	0.0034 (5)	−0.0025 (5)
C6	0.0152 (7)	0.0367 (9)	0.0330 (9)	0.0005 (6)	0.0133 (7)	−0.0020 (7)
C7	0.0292 (9)	0.0453 (11)	0.0317 (9)	0.0066 (8)	0.0185 (8)	0.0055 (8)
C8	0.0134 (6)	0.0149 (7)	0.0134 (6)	−0.0005 (5)	0.0049 (5)	0.0000 (5)
C9	0.0109 (6)	0.0158 (7)	0.0133 (6)	−0.0016 (5)	0.0028 (5)	−0.0013 (5)
C10	0.0170 (7)	0.0141 (7)	0.0166 (7)	−0.0004 (5)	0.0051 (5)	0.0002 (5)
C11	0.0181 (7)	0.0222 (7)	0.0129 (6)	−0.0017 (6)	0.0064 (6)	0.0023 (6)
C12	0.0202 (7)	0.0217 (8)	0.0152 (7)	−0.0024 (6)	0.0092 (6)	−0.0064 (6)
C13	0.0294 (8)	0.0133 (7)	0.0243 (8)	−0.0019 (6)	0.0119 (6)	−0.0028 (6)
C14	0.0242 (8)	0.0161 (7)	0.0169 (7)	−0.0020 (6)	0.0097 (6)	0.0009 (6)

Geometric parameters (Å, º)

S1—C1	1.6905 (13)	C4—H4	1.0000
F1—C3	1.3381 (16)	C6—C7	1.501 (2)
F2—C3	1.3428 (15)	C6—H6A	0.9900
F3—C3	1.3367 (15)	C6—H6B	0.9900
F4—C12	1.3678 (15)	C7—H7A	0.9800
O1—C2	1.4120 (15)	C7—H7B	0.9800
O1—H1	0.8400	C7—H7C	0.9800
O2—C5	1.2130 (16)	C8—C9	1.5122 (18)
O3—C5	1.3252 (16)	C8—H8	1.0000
O3—C6	1.4675 (16)	C9—C14	1.3906 (19)
N1—C1	1.3504 (17)	C9—C10	1.3950 (18)
N1—C2	1.4462 (16)	C10—C11	1.3881 (19)
N1—H1A	0.835 (16)	C10—H10	0.9500
N2—C1	1.3345 (17)	C11—C12	1.374 (2)
N2—C8	1.4668 (16)	C11—H11	0.9500
N2—H2A	0.785 (16)	C12—C13	1.381 (2)
C2—C3	1.5296 (18)	C13—C14	1.3936 (19)
C2—C4	1.5436 (17)	C13—H13	0.9500
C4—C5	1.5167 (18)	C14—H14	0.9500
C4—C8	1.5363 (18)		

C2—O1—H1	109.5	C7—C6—H6A	109.5
C5—O3—C6	117.11 (11)	O3—C6—H6B	109.5
C1—N1—C2	124.90 (11)	C7—C6—H6B	109.5
C1—N1—H1A	114.4 (11)	H6A—C6—H6B	108.1
C2—N1—H1A	120.7 (11)	C6—C7—H7A	109.5
C1—N2—C8	123.93 (12)	C6—C7—H7B	109.5
C1—N2—H2A	116.6 (10)	H7A—C7—H7B	109.5
C8—N2—H2A	119.4 (10)	C6—C7—H7C	109.5
N2—C1—N1	117.77 (12)	H7A—C7—H7C	109.5
N2—C1—S1	120.74 (10)	H7B—C7—H7C	109.5
N1—C1—S1	121.49 (10)	N2—C8—C9	111.83 (11)
O1—C2—N1	109.59 (10)	N2—C8—C4	105.97 (10)
O1—C2—C3	107.38 (11)	C9—C8—C4	113.17 (10)

N1—C2—C3	107.50 (10)	N2—C8—H8	108.6
O1—C2—C4	112.87 (10)	C9—C8—H8	108.6
N1—C2—C4	108.58 (11)	C4—C8—H8	108.6
C3—C2—C4	110.79 (10)	C14—C9—C10	119.37 (13)
F3—C3—F1	107.59 (10)	C14—C9—C8	122.23 (12)
F3—C3—F2	107.24 (11)	C10—C9—C8	118.35 (12)
F1—C3—F2	107.32 (11)	C11—C10—C9	120.83 (13)
F3—C3—C2	111.15 (10)	C11—C10—H10	119.6
F1—C3—C2	111.82 (11)	C9—C10—H10	119.6
F2—C3—C2	111.49 (10)	C12—C11—C10	117.96 (13)
C5—C4—C8	109.66 (10)	C12—C11—H11	121.0
C5—C4—C2	112.60 (11)	C10—C11—H11	121.0
C8—C4—C2	106.91 (10)	F4—C12—C11	118.22 (12)
C5—C4—H4	109.2	F4—C12—C13	118.43 (13)
C8—C4—H4	109.2	C11—C12—C13	123.34 (13)
C2—C4—H4	109.2	C12—C13—C14	117.84 (14)
O2—C5—O3	125.76 (12)	C12—C13—H13	121.1
O2—C5—C4	123.20 (12)	C14—C13—H13	121.1
O3—C5—C4	111.03 (11)	C9—C14—C13	120.64 (13)
O3—C6—C7	110.79 (13)	C9—C14—H14	119.7
O3—C6—H6A	109.5	C13—C14—H14	119.7

C8—N2—C1—N1	4.3 (2)	C2—C4—C5—O2	49.06 (18)
C8—N2—C1—S1	−175.06 (10)	C8—C4—C5—O3	109.10 (13)
C2—N1—C1—N2	3.4 (2)	C2—C4—C5—O3	−132.01 (12)
C2—N1—C1—S1	−177.24 (10)	C5—O3—C6—C7	91.06 (16)
C1—N1—C2—O1	−99.95 (14)	C1—N2—C8—C9	−161.16 (12)
C1—N1—C2—C3	143.65 (13)	C1—N2—C8—C4	−37.41 (17)
C1—N1—C2—C4	23.75 (17)	C5—C4—C8—N2	−176.87 (11)
O1—C2—C3—F3	59.68 (13)	C2—C4—C8—N2	60.79 (13)
N1—C2—C3—F3	177.53 (10)	C5—C4—C8—C9	−53.96 (15)
C4—C2—C3—F3	−63.98 (14)	C2—C4—C8—C9	−176.31 (10)
O1—C2—C3—F1	179.95 (10)	N2—C8—C9—C14	44.36 (17)
N1—C2—C3—F1	−62.21 (13)	C4—C8—C9—C14	−75.23 (16)
C4—C2—C3—F1	56.28 (14)	N2—C8—C9—C10	−138.31 (12)
O1—C2—C3—F2	−59.90 (13)	C4—C8—C9—C10	102.10 (14)
N1—C2—C3—F2	57.94 (14)	C14—C9—C10—C11	0.66 (19)
C4—C2—C3—F2	176.43 (10)	C8—C9—C10—C11	−176.75 (12)
O1—C2—C4—C5	−54.01 (14)	C9—C10—C11—C12	−1.3 (2)
N1—C2—C4—C5	−175.72 (10)	C10—C11—C12—F4	−178.98 (12)
C3—C2—C4—C5	66.45 (14)	C10—C11—C12—C13	0.8 (2)
O1—C2—C4—C8	66.48 (13)	F4—C12—C13—C14	−179.92 (13)
N1—C2—C4—C8	−55.23 (13)	C11—C12—C13—C14	0.3 (2)
C3—C2—C4—C8	−173.07 (10)	C10—C9—C14—C13	0.5 (2)
C6—O3—C5—O2	0.9 (2)	C8—C9—C14—C13	177.79 (13)
C6—O3—C5—C4	−178.03 (11)	C12—C13—C14—C9	−1.0 (2)
C8—C4—C5—O2	−69.83 (16)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···O2	0.84	2.06	2.7767 (13)	144
O1—H1···S1^{i}	0.84	2.83	3.3796 (10)	124
N1—H1*A*···S1^{ii}	0.835 (16)	2.635 (17)	3.4566 (12)	168.1 (15)

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