Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

3-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-5-(4-methylsulfanylbenzylidene)-1,3-thiazolidine-2,4-dione

J. Suresh,[a] M. Venkateshan,[a] S. Ponnuchamy,[b] R. Ranjith Kumar[c] and P. L. Nilantha Lakshman[d]*

[a]Department of Physics, The Madura College, Madurai 625 011, India, [b]Orchid Chemicals & Pharmaceuticals Ltd, R&D Center, Chennai 600 119, India, [c]Department of Organic Chemistry, School of Chemistry, Madurai Kamaraj University, Madurai 625 021, India, and [d]Department of Food Science and Technology, University of Ruhuna, Mapalana, Kamburupitiya 81100, Sri Lanka
Correspondence e-mail: plakshmannilantha@ymail.com

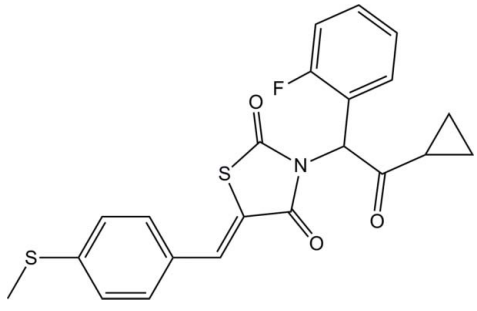
Received 26 December 2012; accepted 28 December 2012

Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.047; wR factor = 0.149; data-to-parameter ratio = 14.6.

In the title compound, $C_{22}H_{18}FNO_3S_2$, the five-membered thiazolidine ring is planar (r.m.s. deviation = 0.003 Å) and forms dihedral angles of 70.2 (3), 73.16 (17) and 10.32 (14)° with the cyclopropane, fluorobenzene and methylthiobenzene rings, respectively. The sum of the bond angles around the thiazolidine ring N atom (359.6°) indicates sp^2 hybridization. The molecular structure features intramolecular C—H···S, C—H···F and C—H···O interactions. In the crystal, no significant intermolecular contacts were apparent.

Related literature

For general properties of thiazolidines, see: Botti *et al.* (1996); Spiegelman (1998); Day (1999); Barreca *et al.* (2002).



Experimental

Crystal data

$C_{22}H_{18}FNO_3S_2$ M_r = 427.49
Monoclinic, $P2_1/c$
a = 7.657 (3) Å
b = 15.799 (5) Å
c = 17.425 (6) Å
β = 95.641 (5)°
V = 2097.7 (13) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.29 mm^{-1}
T = 293 K
0.23 × 0.21 × 0.19 mm

Data collection

Bruker Kappa APEXII diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.967, T_{max} = 0.974
19651 measured reflections
3838 independent reflections
2429 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.149
S = 1.02
3838 reflections
262 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å^{-3}
$\Delta\rho_{min}$ = −0.26 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···F	0.98	2.35	2.740 (4)	103
C4—H4···O2	0.98	2.33	2.792 (4)	108
C15—H15···O2	0.93	2.53	2.884 (4)	103
C17—H17···S1	0.93	2.55	3.238 (3)	131

Data collection: *APEX2* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

SP thanks the management, Orchid Chemicals & Pharmaceuticals Ltd, Chennai, for providing laboratory facilities. JS thanks the UGC for the FIST support. JS and MV thank the management of The Madura College for their encouragement and support. RRK thanks the DST, New Delhi, for funds under the fast-track scheme (No·SR/FT/CS-073/2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK5185).

References

Barreca, M. L., Balzarini, J., Chimirri, A., De Clercq, E., De Luca, L., Holtje, H. D., Holtje, M., Monforte, A. M., Monforte, P., Pannecouque, C., Rao, A. & Zappala, M. (2002). *J. Med. Chem.* **45**, 5410–5413.
Botti, P., Pallin, T. D. & Tam, J. P. (1996). *J. Am. Chem. Soc.* **118**, 10018–10024.
Bruker (2004). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Day, C. (1999). *Diabet. Med.* **16**, 179–192.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Spiegelman, B. M. (1998). *Diabetes*, **47**, 507–514.

supporting information

Acta Cryst. (2013). E**69**, o188 [doi:10.1107/S1600536812051987]

3-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-5-(4-methylsulfanylbenzylidene)-1,3-thiazolidine-2,4-dione

J. Suresh, M. Venkateshan, S. Ponnuchamy, R. Ranjith Kumar and P. L. Nilantha Lakshman

S1. Comment

Thiazolidines are an important class of heteroaromatic compounds and have widespread applications from ranging from pharmaceuticals (Barreca *et al.*, 2002) to materials (Botti *et al.*, 1996). Thiazolidinediones (TZDs), which are known to sensitize tissues to insulin, have been developed and clinically used as anti-diabetic agents. They have been shown to reduce plasma glucose, lipid, and insulin levels, and are used for the treatment of type 2 diabetes (Day, 1999; Spiegelman, 1998). In view of this we have synthesized the title compound to study its crystal structure.

In the title compound, Fig. 1, the five-membered thiazolidine is nearly planar with a r.m.s. deviation of 0.003 Å. The 4-methyl sulfonyl benzylidine ring is nearly coplanar with the central thiazolidine ring as indicated by the dihedral angle of 8.35 (1)°. The 2-fluorobenzene and cyclopropyl rings make dihedral angles of 73.16 (17) and 70.2 (3)° with the thiazolidine ring, respectively. The sum of bond angles around N is 359.6° which confirms sp^2 hybridization. In the cyclopropyl ring the mean C—C bond length is 1.504 (3) Å and the mean C—C—C bond angle is 60.0 (2)°; these are unexceptional. The molecular structure features intramolecular C—H···S, C—H···F C—H···O interactions (Table 1).

S2. Experimental

A mixture of 5-(4-methylsulfanyl-benzylidenethiazolidine-2,4-dione (1 mmol), 2-bromo-1-cyclopropyl-2-(2-fluorophenyl)ethanone (1 mmol) and sodium bicarbonate (3 mmol) were taken in DMF and stirred for 6 h at 25–35 °C. After completion of the reaction as evident by TLC, (eluent: 7:3 / hexane:ethyl acetate) the mixture was poured into water and extracted with ethyl acetate. The organic layer was washed with brine (20 ml) twice and then with water. The solvent was distilled off to obtain a viscous paste to which diisopropyl ether (5 volumes) was added. The resultant solid was filtered and washed with diisopropyl ether. The product was recrystallized from its methanol solution. Melting point: 414.5–415.9 Yield: 83.5%

S3. Refinement

H atoms were placed at calculated positions and allowed to ride on their carrier atoms with C—H = 0.93–0.98 Å. U_{iso} = 1.2U_{eq}(C) for CH_2 and CH groups and U_{iso} = 1.5U_{eq}(C) for the CH_3 group. The (0 1 1) reflection was probably affected by the beam-stop and was omitted from the refinement.

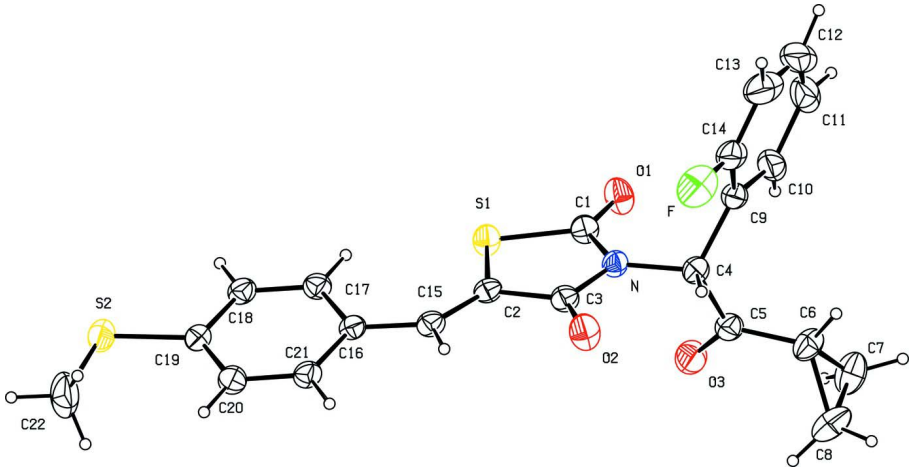


Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids and the atom-numbering scheme.

3-[2-Cyclopropyl-1-(2-fluorophenyl)-2-oxoethyl]-5-(4- methylsulfanylbenzylidene)-1,3-thiazolidine-2,4-dione

Crystal data

$C_{22}H_{18}FNO_3S_2$
$M_r = 427.49$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 7.657$ (3) Å
$b = 15.799$ (5) Å
$c = 17.425$ (6) Å
$\beta = 95.641$ (5)°
$V = 2097.7$ (13) Å^3
$Z = 4$
$F(000) = 888$
$D_x = 1.354$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2000 reflections
$\theta = 2$–25°
$\mu = 0.29$ mm^{-1}
$T = 293$ K
Block, colourless
0.23 × 0.21 × 0.19 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.967$, $T_{max} = 0.974$
19651 measured reflections
3838 independent reflections
2429 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.4°$, $\theta_{min} = 2.4°$
$h = -5\rightarrow9$
$k = -18\rightarrow19$
$l = -21\rightarrow20$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.047$
$wR(F^2) = 0.149$
$S = 1.02$
3838 reflections
262 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0683P)^2 + 0.8976P]$
where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max} = 0.32$ e Å^{-3}
$\Delta\rho_{min} = -0.26$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	−0.0768 (4)	0.07851 (19)	0.35525 (16)	0.0603 (7)
C2	0.2318 (3)	0.02818 (18)	0.34213 (15)	0.0539 (7)
C3	0.1614 (4)	0.08537 (18)	0.28013 (16)	0.0589 (7)
C4	−0.1107 (4)	0.16162 (18)	0.23261 (15)	0.0575 (7)
H4	−0.0273	0.1811	0.1972	0.069*
C5	−0.2414 (4)	0.1066 (2)	0.18456 (17)	0.0648 (8)
C6	−0.3427 (4)	0.1473 (2)	0.11919 (18)	0.0769 (9)
H6	−0.3314	0.2089	0.1151	0.092*
C7	−0.5155 (5)	0.1103 (3)	0.0911 (2)	0.1003 (13)
H7A	−0.5547	0.0611	0.1181	0.120*
H7B	−0.6082	0.1489	0.0719	0.120*
C8	−0.3702 (6)	0.0993 (3)	0.0454 (2)	0.1102 (14)
H8A	−0.3720	0.1311	−0.0023	0.132*
H8B	−0.3185	0.0433	0.0439	0.132*
C9	−0.1842 (4)	0.24062 (19)	0.26535 (16)	0.0640 (8)
C10	−0.3536 (5)	0.2472 (2)	0.28457 (19)	0.0892 (11)
H10	−0.4307	0.2019	0.2766	0.107*
C11	−0.4098 (8)	0.3236 (4)	0.3166 (2)	0.1203 (18)
H11	−0.5241	0.3296	0.3295	0.144*
C12	−0.2909 (11)	0.3889 (3)	0.3283 (3)	0.137 (3)
H12	−0.3257	0.4385	0.3511	0.164*
C13	−0.1253 (10)	0.3835 (3)	0.3079 (3)	0.131 (2)
H13	−0.0495	0.4295	0.3144	0.157*
C14	−0.0726 (6)	0.3109 (2)	0.27810 (19)	0.0832 (10)
C15	0.3898 (3)	−0.00777 (18)	0.34052 (16)	0.0566 (7)
H15	0.4507	0.0093	0.2996	0.068*
C16	0.4815 (3)	−0.06842 (17)	0.39142 (15)	0.0523 (6)
C17	0.4287 (4)	−0.09486 (18)	0.46215 (16)	0.0589 (7)
H17	0.3247	−0.0741	0.4782	0.071*
C18	0.5269 (4)	−0.15058 (19)	0.50819 (16)	0.0605 (7)
H18	0.4890	−0.1671	0.5550	0.073*
C19	0.6831 (4)	−0.18290 (19)	0.48574 (16)	0.0611 (7)

C20	0.7347 (4)	−0.1587 (2)	0.41522 (17)	0.0677 (8)
H20	0.8375	−0.1804	0.3987	0.081*
C21	0.6358 (3)	−0.10303 (19)	0.36966 (16)	0.0609 (7)
H21	0.6730	−0.0877	0.3224	0.073*
C22	0.9974 (6)	−0.2703 (4)	0.5069 (3)	0.142 (2)
H22A	1.0729	−0.3067	0.5394	0.212*
H22B	1.0571	−0.2180	0.4990	0.212*
H22C	0.9670	−0.2974	0.4581	0.212*
N	−0.0076 (3)	0.11071 (14)	0.29086 (12)	0.0543 (6)
O1	−0.2202 (3)	0.09354 (14)	0.37424 (13)	0.0807 (7)
O2	0.2345 (3)	0.10769 (15)	0.22512 (13)	0.0868 (7)
O3	−0.2558 (4)	0.03221 (15)	0.19915 (15)	0.0952 (8)
F	0.0895 (4)	0.30462 (16)	0.25692 (14)	0.1184 (8)
S1	0.07690 (9)	0.01156 (5)	0.40749 (4)	0.0652 (3)
S2	0.80371 (12)	−0.24929 (6)	0.55177 (5)	0.0834 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0589 (16)	0.0646 (18)	0.0587 (18)	0.0013 (14)	0.0130 (14)	0.0060 (15)
C2	0.0573 (15)	0.0623 (17)	0.0433 (15)	−0.0036 (13)	0.0116 (12)	−0.0021 (13)
C3	0.0620 (16)	0.0637 (18)	0.0523 (17)	0.0018 (14)	0.0132 (14)	0.0010 (14)
C4	0.0649 (16)	0.0608 (18)	0.0476 (16)	0.0013 (14)	0.0102 (13)	0.0069 (14)
C5	0.0770 (19)	0.062 (2)	0.0559 (18)	0.0030 (16)	0.0072 (15)	0.0013 (15)
C6	0.094 (2)	0.079 (2)	0.0565 (19)	−0.0150 (18)	−0.0036 (17)	0.0109 (17)
C7	0.086 (2)	0.123 (3)	0.089 (3)	−0.018 (2)	−0.004 (2)	0.033 (2)
C8	0.122 (3)	0.153 (4)	0.054 (2)	−0.023 (3)	0.002 (2)	−0.007 (2)
C9	0.091 (2)	0.0552 (19)	0.0455 (16)	0.0119 (17)	0.0063 (15)	0.0055 (14)
C10	0.113 (3)	0.092 (3)	0.065 (2)	0.044 (2)	0.022 (2)	0.0144 (19)
C11	0.163 (4)	0.132 (4)	0.071 (3)	0.078 (4)	0.034 (3)	0.033 (3)
C12	0.263 (8)	0.078 (3)	0.070 (3)	0.063 (5)	0.022 (4)	0.011 (3)
C13	0.257 (7)	0.064 (3)	0.068 (3)	−0.001 (4)	−0.005 (4)	0.008 (2)
C14	0.134 (3)	0.063 (2)	0.0523 (19)	0.007 (2)	0.007 (2)	0.0114 (17)
C15	0.0565 (15)	0.0679 (18)	0.0470 (16)	−0.0024 (14)	0.0129 (12)	−0.0016 (14)
C16	0.0510 (14)	0.0604 (17)	0.0456 (15)	−0.0017 (13)	0.0055 (12)	−0.0055 (13)
C17	0.0545 (15)	0.0688 (19)	0.0547 (17)	0.0030 (14)	0.0121 (13)	−0.0046 (14)
C18	0.0659 (17)	0.0689 (19)	0.0475 (16)	0.0000 (15)	0.0087 (14)	−0.0011 (14)
C19	0.0616 (16)	0.0678 (19)	0.0524 (18)	0.0053 (14)	−0.0018 (14)	−0.0051 (14)
C20	0.0572 (16)	0.088 (2)	0.0592 (18)	0.0125 (16)	0.0126 (14)	−0.0009 (17)
C21	0.0596 (16)	0.077 (2)	0.0477 (16)	0.0033 (15)	0.0133 (13)	0.0007 (15)
C22	0.106 (3)	0.218 (6)	0.103 (3)	0.088 (3)	0.020 (3)	0.042 (3)
N	0.0560 (12)	0.0618 (14)	0.0459 (13)	0.0031 (11)	0.0089 (10)	0.0055 (11)
O1	0.0627 (12)	0.0963 (17)	0.0874 (16)	0.0178 (11)	0.0300 (11)	0.0260 (13)
O2	0.0850 (14)	0.1093 (18)	0.0723 (14)	0.0220 (13)	0.0382 (12)	0.0331 (13)
O3	0.127 (2)	0.0603 (15)	0.0921 (18)	−0.0026 (14)	−0.0193 (15)	0.0020 (13)
F	0.134 (2)	0.1123 (19)	0.1068 (18)	−0.0420 (16)	0.0020 (15)	0.0186 (14)
S1	0.0581 (4)	0.0814 (6)	0.0582 (5)	0.0072 (4)	0.0169 (3)	0.0164 (4)
S2	0.0848 (6)	0.1018 (7)	0.0621 (5)	0.0229 (5)	−0.0005 (4)	0.0087 (5)

Geometric parameters (Å, º)

C1—O1	1.201 (3)	C10—H10	0.9300
C1—N	1.384 (3)	C11—C12	1.378 (8)
C1—S1	1.767 (3)	C11—H11	0.9300
C2—C15	1.340 (4)	C12—C13	1.353 (8)
C2—C3	1.470 (4)	C12—H12	0.9300
C2—S1	1.743 (3)	C13—C14	1.337 (6)
C3—O2	1.209 (3)	C13—H13	0.9300
C3—N	1.385 (3)	C14—F	1.333 (4)
C4—N	1.464 (3)	C15—C16	1.441 (4)
C4—C9	1.504 (4)	C15—H15	0.9300
C4—C5	1.515 (4)	C16—C21	1.388 (4)
C4—H4	0.9800	C16—C17	1.398 (4)
C5—O3	1.209 (4)	C17—C18	1.366 (4)
C5—C6	1.463 (4)	C17—H17	0.9300
C6—C7	1.486 (5)	C18—C19	1.391 (4)
C6—C8	1.490 (5)	C18—H18	0.9300
C6—H6	0.9800	C19—C20	1.381 (4)
C7—C8	1.441 (5)	C19—S2	1.752 (3)
C7—H7A	0.9700	C20—C21	1.363 (4)
C7—H7B	0.9700	C20—H20	0.9300
C8—H8A	0.9700	C21—H21	0.9300
C8—H8B	0.9700	C22—S2	1.774 (4)
C9—C10	1.375 (5)	C22—H22A	0.9600
C9—C14	1.406 (5)	C22—H22B	0.9600
C10—C11	1.413 (6)	C22—H22C	0.9600
O1—C1—N	125.7 (3)	C12—C11—H11	120.8
O1—C1—S1	123.8 (2)	C10—C11—H11	120.8
N—C1—S1	110.43 (19)	C13—C12—C11	122.5 (5)
C15—C2—C3	120.8 (2)	C13—C12—H12	118.8
C15—C2—S1	128.6 (2)	C11—C12—H12	118.8
C3—C2—S1	110.44 (19)	C14—C13—C12	118.9 (6)
O2—C3—N	122.3 (3)	C14—C13—H13	120.6
O2—C3—C2	126.7 (3)	C12—C13—H13	120.6
N—C3—C2	111.0 (2)	F—C14—C13	119.7 (5)
N—C4—C9	112.9 (2)	F—C14—C9	117.8 (3)
N—C4—C5	110.5 (2)	C13—C14—C9	122.5 (5)
C9—C4—C5	115.8 (2)	C2—C15—C16	131.0 (3)
N—C4—H4	105.6	C2—C15—H15	114.5
C9—C4—H4	105.6	C16—C15—H15	114.5
C5—C4—H4	105.6	C21—C16—C17	116.8 (3)
O3—C5—C6	122.6 (3)	C21—C16—C15	118.1 (2)
O3—C5—C4	120.7 (3)	C17—C16—C15	125.2 (2)
C6—C5—C4	116.6 (3)	C18—C17—C16	121.4 (3)
C5—C6—C7	118.0 (3)	C18—C17—H17	119.3
C5—C6—C8	117.8 (3)	C16—C17—H17	119.3

C7—C6—C8	57.9 (2)	C17—C18—C19	120.7 (3)
C5—C6—H6	116.7	C17—C18—H18	119.7
C7—C6—H6	116.7	C19—C18—H18	119.7
C8—C6—H6	116.7	C20—C19—C18	118.5 (3)
C8—C7—C6	61.2 (2)	C20—C19—S2	124.9 (2)
C8—C7—H7A	117.6	C18—C19—S2	116.6 (2)
C6—C7—H7A	117.6	C21—C20—C19	120.4 (3)
C8—C7—H7B	117.6	C21—C20—H20	119.8
C6—C7—H7B	117.6	C19—C20—H20	119.8
H7A—C7—H7B	114.8	C20—C21—C16	122.3 (3)
C7—C8—C6	60.9 (2)	C20—C21—H21	118.9
C7—C8—H8A	117.7	C16—C21—H21	118.9
C6—C8—H8A	117.7	S2—C22—H22A	109.5
C7—C8—H8B	117.7	S2—C22—H22B	109.5
C6—C8—H8B	117.7	H22A—C22—H22B	109.5
H8A—C8—H8B	114.8	S2—C22—H22C	109.5
C10—C9—C14	118.4 (3)	H22A—C22—H22C	109.5
C10—C9—C4	123.5 (3)	H22B—C22—H22C	109.5
C14—C9—C4	118.1 (3)	C1—N—C3	116.1 (2)
C9—C10—C11	119.5 (4)	C1—N—C4	122.7 (2)
C9—C10—H10	120.3	C3—N—C4	120.8 (2)
C11—C10—H10	120.3	C2—S1—C1	91.99 (13)
C12—C11—C10	118.4 (5)	C19—S2—C22	103.42 (18)

C15—C2—C3—O2	−2.4 (5)	C2—C15—C16—C21	171.7 (3)
S1—C2—C3—O2	−178.1 (3)	C2—C15—C16—C17	−9.2 (5)
C15—C2—C3—N	176.1 (2)	C21—C16—C17—C18	1.5 (4)
S1—C2—C3—N	0.4 (3)	C15—C16—C17—C18	−177.7 (3)
N—C4—C5—O3	3.6 (4)	C16—C17—C18—C19	−0.1 (4)
C9—C4—C5—O3	−126.4 (3)	C17—C18—C19—C20	−1.2 (4)
N—C4—C5—C6	−174.5 (2)	C17—C18—C19—S2	176.6 (2)
C9—C4—C5—C6	55.6 (4)	C18—C19—C20—C21	1.2 (5)
O3—C5—C6—C7	26.8 (5)	S2—C19—C20—C21	−176.4 (2)
C4—C5—C6—C7	−155.3 (3)	C19—C20—C21—C16	0.2 (5)
O3—C5—C6—C8	−39.7 (5)	C17—C16—C21—C20	−1.5 (4)
C4—C5—C6—C8	138.3 (3)	C15—C16—C21—C20	177.7 (3)
C5—C6—C7—C8	−106.9 (4)	O1—C1—N—C3	179.6 (3)
C5—C6—C8—C7	107.2 (4)	S1—C1—N—C3	0.0 (3)
N—C4—C9—C10	−98.6 (3)	O1—C1—N—C4	−6.4 (5)
C5—C4—C9—C10	30.1 (4)	S1—C1—N—C4	174.0 (2)
N—C4—C9—C14	80.3 (3)	O2—C3—N—C1	178.3 (3)
C5—C4—C9—C14	−151.0 (3)	C2—C3—N—C1	−0.3 (3)
C14—C9—C10—C11	−0.3 (5)	O2—C3—N—C4	4.2 (4)
C4—C9—C10—C11	178.6 (3)	C2—C3—N—C4	−174.3 (2)
C9—C10—C11—C12	−0.7 (6)	C9—C4—N—C1	58.9 (3)
C10—C11—C12—C13	2.3 (7)	C5—C4—N—C1	−72.5 (3)
C11—C12—C13—C14	−2.8 (8)	C9—C4—N—C3	−127.4 (3)
C12—C13—C14—F	179.3 (4)	C5—C4—N—C3	101.1 (3)

C12—C13—C14—C9	1.7 (6)	C15—C2—S1—C1	−175.6 (3)
C10—C9—C14—F	−177.9 (3)	C3—C2—S1—C1	−0.3 (2)
C4—C9—C14—F	3.1 (4)	O1—C1—S1—C2	−179.4 (3)
C10—C9—C14—C13	−0.2 (5)	N—C1—S1—C2	0.2 (2)
C4—C9—C14—C13	−179.2 (3)	C20—C19—S2—C22	2.2 (4)
C3—C2—C15—C16	−176.3 (3)	C18—C19—S2—C22	−175.6 (3)
S1—C2—C15—C16	−1.4 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···F	0.98	2.35	2.740 (4)	103
C4—H4···O2	0.98	2.33	2.792 (4)	108
C15—H15···O2	0.93	2.53	2.884 (4)	103
C17—H17···S1	0.93	2.55	3.238 (3)	131