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S-Phenethyl (2*R*,3*R*)-3-{[(*R*)-*tert*-butylsulfinyl]-amino}-2-fluoro-3-phenylpropanethioate

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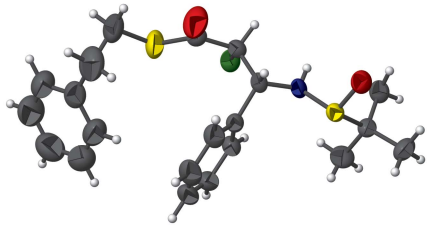
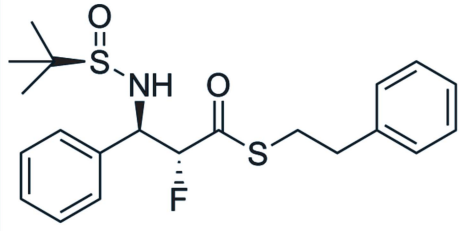
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{21}H_{26}FNO_2S_2$, contains two chiral carbon centres and the absolute configuration has been confirmed as (2*R*,3*R*). The dihedral angle between the phenyl rings is 87.1 (2) and the O—C—C—F and F—C—C—N torsion angles are −175.4 (4) and 62.7 (4)°, respectively. In the crystal, N—H···O hydrogen bonds link the molecules into *C*(4) [010] chains and weak C—H···O and C—H···F interactions cross-link the chains, generating a three-dimensional network.

3D view



Chemical scheme



Structure description

A chiral carbon atom bearing a fluorine substituent is an important structural motif in many bioactive molecules (Wang *et al.*, 2014; Purser *et al.*, 2008). Not surprisingly, the synthesis of chiral molecules with a fluorinated carbon center has attracted recent attention (Shang *et al.*, 2015; Chen *et al.*, 2017). As part of our work in this area, we now describe the synthesis and structure of the title compound (Fig. 1).

The fluoro and amino substituents adopt a *gauche* conformation [F1—C2—C3—N1 = 62.7 (4)°] and the absolute configuration of the chiral carbon centres, C2 and C3, has been confirmed as (*R*,*R*). In the crystal, molecules are connected by N—H···O hydrogen bonds (Table 1, Fig. 2), generating *C*(4) [010] chains, with adjacent molecules related by the 2_1 screw axis. Weak C—H···O and C—H···F interactions cross-link the chains to generate a three-dimensional network.

Synthesis and crystallization

Potassium bis(trimethylsilyl)amide (1.2 mmol, 1*M* in toluene) was added slowly to a reaction mixture of (*R*)-*N*-benzylidene- 2-methylpropane-2-sulfinamide (209 mg, 1.0 mmol) and *S*-phenethyl 2-fluoroethanethioate (198 mg, 1.0 mmol) in toluene at

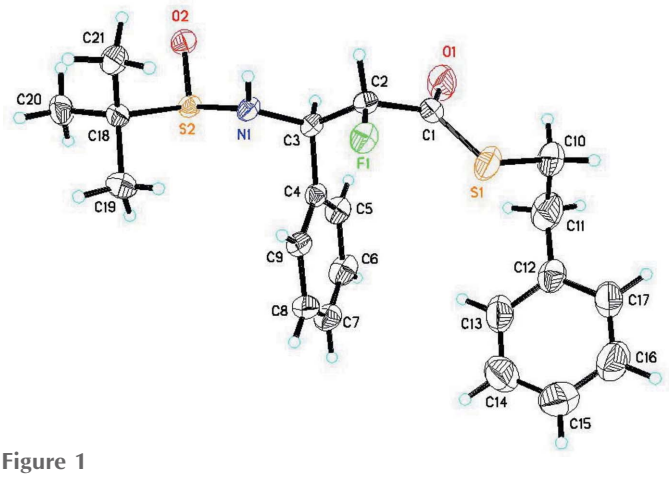


Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

213 K. The reaction mixture was stirred for 1 h at this temperature and then quenched with saturated NH_4Cl/H_2O. The quenched mixture was extracted with EtOAc (20 ml × 3) and the combined organic layers were dried with Na_2SO_4. After removal of the solvent under reduced pressure, the residue was subjected to flash column chromatography to give the title compound (253 mg: yield, 62%). The obtained compound was recrystallized from mixed solvents of ethyl acetate/*n*-hexane (1:2) to give colorless prisms.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Funding information

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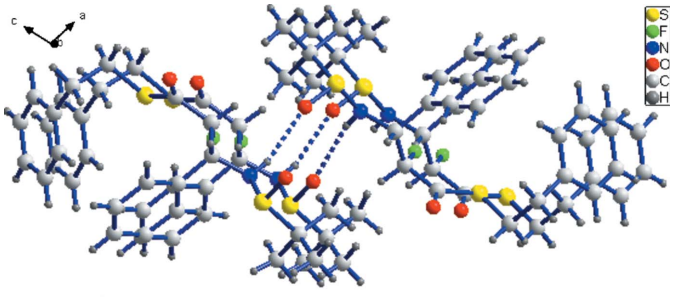

Figure 2
Partial packing diagram showing N—H···O hydrogen bonds as dashed lines.

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O2^{i}	0.80 (2)	2.32 (2)	3.079 (4)	159 (3)
C2—H2···O2^{i}	0.98	2.42	3.265 (4)	144
C10—H10B···O1^{ii}	0.97	2.58	3.473 (7)	153
C21—H21B···O2^{iii}	0.96	2.57	3.475 (5)	157
C21—H21A···F1^{iv}	0.96	2.55	3.465 (5)	159

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{26}FNO_2S_2$
M_r	407.55
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	293
a, b, c (Å)	13.282 (2), 5.8005 (9), 14.622 (2)
β (°)	106.418 (3)
V (Å^3)	1080.6 (3)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.27
Crystal size (mm)	0.20 × 0.16 × 0.13
Data collection	
Diffractometer	Bruker *SMART* CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2007)
T_{min}, T_{max}	0.641, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6235, 3783, 3464
R_{int}	0.023
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.605
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.121, 1.07
No. of reflections	3783
No. of parameters	239
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.42, −0.20
Absolute structure	Flack x determined using 1338 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.04 (5)

Computer programs: *SMART* and *SAINT* (Bruker, 2007), *SHELXTL* (Sheldrick, 2008) and *SHELXL2013* (Sheldrick, 2015).

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full crystallographic data

IUCrData (2018). **3**, x180586 [https://doi.org/10.1107/S2414314618005862]

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Crystal data

$C_{21}H_{26}FNO_2S_2$
M_r = 407.55
Monoclinic, $P2_1$
a = 13.282 (2) Å
b = 5.8005 (9) Å
c = 14.622 (2) Å
β = 106.418 (3)°
V = 1080.6 (3) Å^3
Z = 2
$F(000)$ = 432
D_x = 1.253 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2551 reflections
θ = 5.8–51.0°
μ = 0.27 mm^{-1}
T = 293 K
Prism, colorless
0.20 × 0.16 × 0.13 mm

Data collection

Bruker SMART CCD diffractometer
phi and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2007)
T_{min} = 0.641, T_{max} = 0.746
6235 measured reflections
3783 independent reflections
3464 reflections with $I > 2\sigma(I)$
R_{int} = 0.023
θ_{max} = 25.5°, θ_{min} = 1.5°
h = −15→16
k = −7→6
l = −17→15

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.121
S = 1.07
3783 reflections
239 parameters
2 restraints
Primary atom site location: structure-invariant direct methods
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 0.1132P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.42 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack x determined using 1338 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.04 (5)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.11978 (11)	0.2731 (3)	0.64914 (8)	0.0787 (5)
S2	0.17919 (6)	−0.19558 (15)	1.06022 (6)	0.0398 (2)
F1	0.12082 (17)	0.3427 (4)	0.83432 (15)	0.0532 (6)
N1	0.1447 (2)	0.0152 (5)	0.9803 (2)	0.0408 (7)
O1	0.0356 (3)	−0.1192 (8)	0.6793 (2)	0.0896 (13)
O2	0.0869 (2)	−0.3401 (5)	1.06159 (19)	0.0532 (7)
C1	0.0733 (3)	0.0590 (9)	0.7120 (3)	0.0539 (11)
C2	0.0821 (3)	0.1211 (7)	0.8147 (3)	0.0445 (9)
H2	0.0116	0.1165	0.8233	0.053*
C3	0.1505 (3)	−0.0470 (7)	0.8839 (2)	0.0392 (8)
H3	0.1210	−0.2019	0.8688	0.047*
C4	0.2636 (3)	−0.0500 (7)	0.8796 (2)	0.0411 (8)
C5	0.2989 (3)	−0.2268 (8)	0.8348 (3)	0.0541 (10)
H5	0.2540	−0.3479	0.8088	0.065*
C6	0.4009 (4)	−0.2276 (10)	0.8276 (3)	0.0693 (14)
H6	0.4242	−0.3492	0.7974	0.083*
C7	0.4669 (4)	−0.0499 (11)	0.8648 (3)	0.0666 (13)
H7	0.5352	−0.0504	0.8600	0.080*
C8	0.4333 (3)	0.1275 (10)	0.9090 (3)	0.0611 (12)
H8	0.4786	0.2487	0.9339	0.073*
C9	0.3317 (3)	0.1294 (8)	0.9172 (3)	0.0484 (9)
H9	0.3093	0.2511	0.9480	0.058*
C10	0.0993 (5)	0.1323 (18)	0.5367 (3)	0.108 (3)
H10A	0.0431	0.0209	0.5290	0.129*
H10B	0.0769	0.2459	0.4863	0.129*
C11	0.1951 (6)	0.0108 (14)	0.5253 (4)	0.099 (2)
H11A	0.2147	−0.1100	0.5729	0.119*
H11B	0.1778	−0.0618	0.4630	0.119*
C12	0.2864 (3)	0.1658 (7)	0.5349 (3)	0.0712 (13)
C13	0.3702 (3)	0.1569 (8)	0.6172 (2)	0.096 (2)
H13	0.3716	0.0453	0.6633	0.116*
C14	0.4518 (3)	0.3147 (10)	0.6308 (3)	0.113 (2)
H14	0.5079	0.3086	0.6859	0.135*
C15	0.4497 (3)	0.4814 (9)	0.5620 (4)	0.111 (2)
H15	0.5043	0.5870	0.5711	0.134*
C16	0.3659 (4)	0.4904 (8)	0.4797 (3)	0.115 (2)
H16	0.3645	0.6020	0.4337	0.138*
C17	0.2843 (3)	0.3326 (8)	0.4662 (2)	0.0908 (18)
H17	0.2282	0.3386	0.4111	0.109*
C18	0.2062 (3)	−0.0176 (7)	1.1688 (3)	0.0450 (9)
C19	0.3005 (4)	0.1355 (11)	1.1702 (4)	0.0706 (13)
H19A	0.3246	0.2109	1.2309	0.106*
H19B	0.2801	0.2493	1.1207	0.106*
H19C	0.3560	0.0424	1.1597	0.106*
C20	0.2345 (3)	−0.1915 (11)	1.2502 (3)	0.0635 (11)

H20A	0.2546	−0.1112	1.3100	0.095*
H20B	0.2920	−0.2853	1.2444	0.095*
H20C	0.1749	−0.2877	1.2474	0.095*
C21	0.1111 (3)	0.1219 (8)	1.1702 (3)	0.0541 (10)
H21A	0.0504	0.0241	1.1549	0.081*
H21B	0.1014	0.2435	1.1240	0.081*
H21C	0.1211	0.1870	1.2324	0.081*
H1	0.091 (2)	0.077 (6)	0.981 (2)	0.031 (10)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0949 (9)	0.0960 (12)	0.0526 (6)	−0.0127 (8)	0.0327 (6)	0.0105 (7)
S2	0.0388 (4)	0.0394 (5)	0.0433 (4)	0.0024 (4)	0.0148 (3)	0.0068 (4)
F1	0.0646 (13)	0.0437 (15)	0.0552 (12)	0.0092 (11)	0.0232 (10)	0.0062 (10)
N1	0.0428 (17)	0.0433 (18)	0.0416 (16)	0.0072 (14)	0.0208 (13)	0.0072 (14)
O1	0.110 (3)	0.101 (3)	0.0525 (18)	−0.042 (2)	0.0156 (17)	−0.0191 (19)
O2	0.0562 (16)	0.0516 (17)	0.0524 (15)	−0.0134 (14)	0.0161 (12)	0.0060 (13)
C1	0.042 (2)	0.075 (3)	0.042 (2)	−0.002 (2)	0.0075 (16)	0.002 (2)
C2	0.0374 (18)	0.053 (2)	0.0455 (19)	0.0031 (17)	0.0153 (15)	0.0010 (18)
C3	0.0439 (19)	0.038 (2)	0.0407 (18)	−0.0002 (15)	0.0194 (15)	0.0000 (15)
C4	0.0423 (19)	0.043 (2)	0.0397 (18)	0.0060 (16)	0.0144 (14)	0.0072 (16)
C5	0.063 (2)	0.048 (3)	0.056 (2)	0.010 (2)	0.0252 (18)	0.001 (2)
C6	0.075 (3)	0.069 (3)	0.076 (3)	0.032 (3)	0.041 (2)	0.013 (3)
C7	0.047 (2)	0.090 (4)	0.069 (3)	0.022 (3)	0.027 (2)	0.021 (3)
C8	0.043 (2)	0.081 (3)	0.059 (2)	−0.003 (2)	0.0139 (18)	0.011 (2)
C9	0.046 (2)	0.054 (2)	0.049 (2)	0.0002 (18)	0.0198 (16)	0.0007 (19)
C10	0.094 (4)	0.183 (8)	0.046 (3)	−0.024 (5)	0.020 (3)	0.004 (4)
C11	0.133 (5)	0.102 (5)	0.070 (3)	−0.008 (4)	0.042 (3)	−0.019 (3)
C12	0.083 (3)	0.078 (4)	0.061 (3)	0.011 (3)	0.033 (2)	−0.005 (3)
C13	0.095 (4)	0.127 (6)	0.067 (3)	0.030 (4)	0.024 (3)	0.026 (4)
C14	0.084 (4)	0.162 (7)	0.089 (4)	0.010 (6)	0.020 (3)	0.011 (6)
C15	0.092 (5)	0.126 (6)	0.124 (6)	−0.009 (5)	0.042 (4)	−0.003 (5)
C16	0.119 (5)	0.119 (6)	0.111 (5)	0.011 (5)	0.041 (4)	0.046 (5)
C17	0.096 (4)	0.112 (5)	0.064 (3)	0.009 (4)	0.020 (2)	0.017 (4)
C18	0.0420 (19)	0.050 (2)	0.0416 (19)	−0.0077 (17)	0.0099 (15)	0.0011 (17)
C19	0.056 (3)	0.082 (4)	0.070 (3)	−0.027 (3)	0.012 (2)	−0.008 (3)
C20	0.066 (2)	0.073 (3)	0.0447 (19)	0.000 (3)	0.0049 (16)	0.012 (2)
C21	0.062 (2)	0.052 (2)	0.053 (2)	0.003 (2)	0.0226 (18)	−0.003 (2)

Geometric parameters (Å, º)

S1—C1	1.758 (5)	C10—H10B	0.9700
S1—C10	1.787 (7)	C11—C12	1.484 (8)
S2—O2	1.489 (3)	C11—H11A	0.9700
S2—N1	1.664 (3)	C11—H11B	0.9700
S2—C18	1.843 (4)	C12—C13	1.3900
F1—C2	1.384 (5)	C12—C17	1.3900

N1—C3	1.477 (4)	C13—C14	1.3900
N1—H1	0.80 (2)	C13—H13	0.9300
O1—C1	1.188 (6)	C14—C15	1.3900
C1—C2	1.516 (5)	C14—H14	0.9300
C2—C3	1.510 (5)	C15—C16	1.3900
C2—H2	0.9800	C15—H15	0.9300
C3—C4	1.522 (5)	C16—C17	1.3900
C3—H3	0.9800	C16—H16	0.9300
C4—C5	1.370 (6)	C17—H17	0.9300
C4—C9	1.387 (6)	C18—C21	1.504 (6)
C5—C6	1.388 (6)	C18—C20	1.523 (6)
C5—H5	0.9300	C18—C19	1.531 (6)
C6—C7	1.363 (8)	C19—H19A	0.9600
C6—H6	0.9300	C19—H19B	0.9600
C7—C8	1.355 (7)	C19—H19C	0.9600
C7—H7	0.9300	C20—H20A	0.9600
C8—C9	1.389 (5)	C20—H20B	0.9600
C8—H8	0.9300	C20—H20C	0.9600
C9—H9	0.9300	C21—H21A	0.9600
C10—C11	1.504 (9)	C21—H21B	0.9600
C10—H10A	0.9700	C21—H21C	0.9600

C1—S1—C10	100.0 (3)	C12—C11—H11A	108.9
O2—S2—N1	111.01 (15)	C10—C11—H11A	108.9
O2—S2—C18	105.33 (16)	C12—C11—H11B	108.9
N1—S2—C18	98.15 (17)	C10—C11—H11B	108.9
C3—N1—S2	114.4 (2)	H11A—C11—H11B	107.7
C3—N1—H1	114 (3)	C13—C12—C17	120.0
S2—N1—H1	113 (3)	C13—C12—C11	119.5 (4)
O1—C1—C2	120.8 (4)	C17—C12—C11	120.3 (4)
O1—C1—S1	125.0 (4)	C12—C13—C14	120.0
C2—C1—S1	114.2 (3)	C12—C13—H13	120.0
F1—C2—C3	110.1 (3)	C14—C13—H13	120.0
F1—C2—C1	110.3 (3)	C15—C14—C13	120.0
C3—C2—C1	112.0 (3)	C15—C14—H14	120.0
F1—C2—H2	108.1	C13—C14—H14	120.0
C3—C2—H2	108.1	C14—C15—C16	120.0
C1—C2—H2	108.1	C14—C15—H15	120.0
N1—C3—C2	107.3 (3)	C16—C15—H15	120.0
N1—C3—C4	111.1 (3)	C17—C16—C15	120.0
C2—C3—C4	113.1 (3)	C17—C16—H16	120.0
N1—C3—H3	108.4	C15—C16—H16	120.0
C2—C3—H3	108.4	C16—C17—C12	120.0
C4—C3—H3	108.4	C16—C17—H17	120.0
C5—C4—C9	118.6 (4)	C12—C17—H17	120.0
C5—C4—C3	120.3 (4)	C21—C18—C20	111.7 (3)
C9—C4—C3	121.1 (3)	C21—C18—C19	112.0 (4)
C4—C5—C6	120.9 (5)	C20—C18—C19	110.7 (3)

C4—C5—H5	119.6	C21—C18—S2	110.6 (2)
C6—C5—H5	119.6	C20—C18—S2	104.3 (3)
C7—C6—C5	119.9 (5)	C19—C18—S2	107.2 (3)
C7—C6—H6	120.1	C18—C19—H19A	109.5
C5—C6—H6	120.1	C18—C19—H19B	109.5
C8—C7—C6	120.2 (4)	H19A—C19—H19B	109.5
C8—C7—H7	119.9	C18—C19—H19C	109.5
C6—C7—H7	119.9	H19A—C19—H19C	109.5
C7—C8—C9	120.4 (5)	H19B—C19—H19C	109.5
C7—C8—H8	119.8	C18—C20—H20A	109.5
C9—C8—H8	119.8	C18—C20—H20B	109.5
C4—C9—C8	120.0 (4)	H20A—C20—H20B	109.5
C4—C9—H9	120.0	C18—C20—H20C	109.5
C8—C9—H9	120.0	H20A—C20—H20C	109.5
C11—C10—S1	113.7 (4)	H20B—C20—H20C	109.5
C11—C10—H10A	108.8	C18—C21—H21A	109.5
S1—C10—H10A	108.8	C18—C21—H21B	109.5
C11—C10—H10B	108.8	H21A—C21—H21B	109.5
S1—C10—H10B	108.8	C18—C21—H21C	109.5
H10A—C10—H10B	107.7	H21A—C21—H21C	109.5
C12—C11—C10	113.5 (6)	H21B—C21—H21C	109.5

O2—S2—N1—C3	−89.5 (3)	C6—C7—C8—C9	0.4 (7)
C18—S2—N1—C3	160.6 (3)	C5—C4—C9—C8	0.1 (6)
C10—S1—C1—O1	−3.1 (5)	C3—C4—C9—C8	−177.3 (3)
C10—S1—C1—C2	178.4 (3)	C7—C8—C9—C4	−0.5 (6)
O1—C1—C2—F1	−175.4 (4)	C1—S1—C10—C11	−95.7 (6)
S1—C1—C2—F1	3.2 (4)	S1—C10—C11—C12	−59.0 (7)
O1—C1—C2—C3	61.6 (5)	C10—C11—C12—C13	106.0 (5)
S1—C1—C2—C3	−119.8 (3)	C10—C11—C12—C17	−68.3 (5)
S2—N1—C3—C2	159.9 (2)	C17—C12—C13—C14	0.0
S2—N1—C3—C4	−75.9 (3)	C11—C12—C13—C14	−174.4 (4)
F1—C2—C3—N1	62.7 (4)	C12—C13—C14—C15	0.0
C1—C2—C3—N1	−174.2 (3)	C13—C14—C15—C16	0.0
F1—C2—C3—C4	−60.2 (4)	C14—C15—C16—C17	0.0
C1—C2—C3—C4	62.8 (4)	C15—C16—C17—C12	0.0
N1—C3—C4—C5	135.5 (4)	C13—C12—C17—C16	0.0
C2—C3—C4—C5	−103.6 (4)	C11—C12—C17—C16	174.3 (4)
N1—C3—C4—C9	−47.1 (4)	O2—S2—C18—C21	−57.3 (3)
C2—C3—C4—C9	73.7 (4)	N1—S2—C18—C21	57.2 (3)
C9—C4—C5—C6	0.4 (6)	O2—S2—C18—C20	62.9 (3)
C3—C4—C5—C6	177.8 (4)	N1—S2—C18—C20	177.4 (3)
C4—C5—C6—C7	−0.5 (7)	O2—S2—C18—C19	−179.7 (3)
C5—C6—C7—C8	0.1 (7)	N1—S2—C18—C19	−65.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1···O2^{i}	0.80 (2)	2.32 (2)	3.079 (4)	159 (3)
C2—H2···O2^{i}	0.98	2.42	3.265 (4)	144
C10—H10*B*···O1^{ii}	0.97	2.58	3.473 (7)	153
C21—H21*B*···O2^{iii}	0.96	2.57	3.475 (5)	157
C21—H21*A*···F1^{iv}	0.96	2.55	3.465 (5)	159

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