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tert-Butyl [(4-fluoro-3-isopropoxyisoxazol-5-yl)-methyl](phenylsulfonyl)carbamate

Mohd Abdul Fatah Abdul Manan[a]* and David B. Cordes[b]

[a]Faculty of Applied Sciences, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia, and [b]EaStCHEM School of Chemistry, University of St Andrews, St Andrews, Fife KY16 9ST, United Kingdom. *Correspondence e-mail: abdfatah@uitm.edu.my

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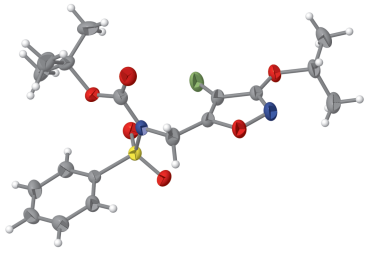
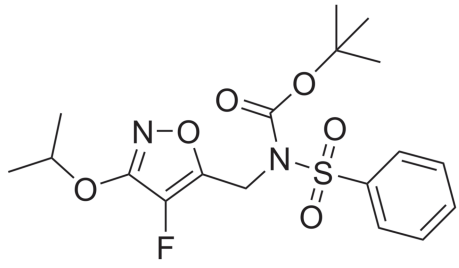
Structural data: full structural data are available from iucrdata.iucr.org

The title compound, $C_{18}H_{23}FN_2O_6S$, a new derivative of a fluoroisoxazole containing sulfonamide functionality has been structurally characterized. The C—S—N—C_{ipr} and C—S—N—C_{carb} (ipr = 3-isopropoxyisoxazole, carb = carbamate) torsion angles are 111.1 (3)° and −70.0 (4)°, respectively. The sulfonamide functional group of this structure features S═O bond lengths of 1.403 (3) and 1.433 (3) Å, an S—N bond length of 1.672 (4) Å, and an S—C bond length of 1.753 (4) Å. The crystal packing features non-classical C—H···O hydrogen-bond interactions, with the carbonyl atom acting as a bifurcated acceptor, resulting in an $R_2^1(8)$ ring.

3D view



Chemical scheme



Structure description

Isoxazoles carrying sulfonamide moieties are very important structural motifs and have gained interest from pharmaceutical industry and medicinal chemists owing to their various bioactivities; antibacterial (Esfahani *et al.*, 2021; Martinez *et al.*, 2025), antifungal (Soliman *et al.*, 2025), anticancer (Kilbile *et al.*, 2024; Vaickelionienė *et al.*, 2023), anti-inflammatory, antidiabetic and antioxidant (Ahmad *et al.*, 2023; Dayma *et al.*, 2020). Pharmaceutically important examples of isoxazole-containing sulfonamide drugs include the antibacterial agents sulfisoxazole and sulfamethoxazole (Rusu *et al.*, 2023), and the antiobesity and anticonvulsant agent zonisamide (Gidal *et al.*, 2024). Despite the potential usage of fluorinated five-membered heterocyclic compounds and their functionalization in the life science industries (Imberg *et al.*, 2025; Hawk *et al.*, 2021; Fuchibe *et al.*, 2023), studies pertaining to the synthesis of such structural units, particularly selective fluorination of five-membered isoxazole systems are rare and challenging. To address this limitation, we report herein the crystal structure of the title compound **1**, obtained by treatment of **2** with excess *N*-fluorobenzenesulfonimide.

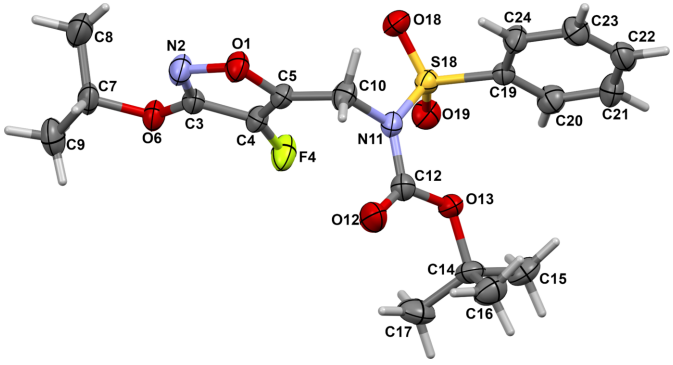


Figure 1
The molecular structure of the title compound, showing displacement ellipsoids drawn at the 50% probability level.

The molecular structure of the title compound, **1**, which consists of a 4-fluoroisoxazole derivative with a sulfonamide group is shown in Fig. 1. In the solid state, the isoxazole ring (O1/N2/C3–C5) forms a dihedral angle of 10.9 (3)° with the sulfonyl-bound phenyl ring (C19–C24). The torsion angles C19—S18—N11—C10 and C19—S18—N11—C12 are 111.2 (3)° and −70.0 (4)° respectively. The sulfonamide adopts a conformation in agreement with that seen in related structures (Khrustalev *et al.*, 2022; Madhan *et al.*, 2024; Moroni *et al.*, 2024). The nitrogen atom of the sulfonamide displays a sp^2 character, with an S18—N11—C10 angle of 119.1 (3)°. The sulfonamide sulfur atom displays a distorted tetrahedral geometry, with the widening of the O18—S18—O19 angle of 119.2 (2)°, accompanied by simultaneous decrease in the N11—S18—C19 angle [106.0 (2)°], as typically found in RSO_2NR' sulfonamide systems (Hernández *et al.*, 2017; Moroni *et al.*, 2024). The C10—N11—C12—O12 fragment adopts a *syn* conformation with a torsion angle of 5.0 (6)°. The molecular packing features weak C—H···O hydrogen bonds (Table 1). Atoms C10 and C24 act as donors to the double-acceptor O-atom, O19, enclosing $R_2^1(8)$ ring motifs, and resulting in the formation of $C_2^1(5)$ chains along [001] (Fig. 2).

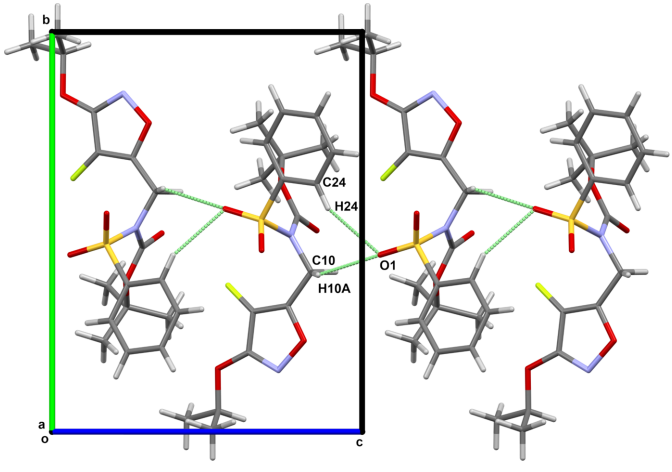


Figure 2
View of the weakly hydrogen-bonded $C_2^1(5)$ chains.

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

D—H···A	D—H	H···A	D···A	D—H···A
C10—H10A···O19^{i}	0.99	2.47	3.121 (6)	123
C15—H15B···O18^{ii}	0.98	2.59	3.571 (6)	176
C22—H22···O12^{iii}	0.95	2.51	3.335 (6)	145
C24—H24···O19^{i}	0.95	2.51	3.366 (5)	150

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

Further chains are formed by other C—H···O hydrogen bonds; C15—H15*B* with O18 forming $C(8)$ chains along [110], and C22—H22 with O12 forming $C(9)$ chains along [1$\bar{1}$0] (Fig. 3). The combination of these bonds results in a weakly interacting three-dimensional network.

Synthesis and crystallization

The carbamate precursor **2**, was prepared according to our previously established protocol (Abdul Manan *et al.*, 2017). The title compound **1**, was synthesized following a literature procedure with a minor modification (Abdul Manan *et al.*, 2017) (Fig. 4). *n*-BuLi (1.7 ml, 2.5 *M* in hexane, 4.29 mmol, 2.2 eq) was added dropwise to a solution of 5-(*tert*-butyl-oxycarbonyl)aminomethyl-3-isopropoxyisoxazole, **2**, (500 mg, 1.95 mmol, 1.0 eq) at 195 K. The mixture was stirred for 1.5 h at 195 K and a solution of *N*-fluorobenzenesulfonimide (NFSI) (1.23 g, 3.90 mmol, 2.0 eq) in THF (4 ml) was added. The mixture was stirred for 2 h at 195 K and the temperature was allowed to warm to room temperature over 12 h. The reaction mixture was quenched with aqueous NH_4Cl (10 ml) and the organic phase was extracted into EtOAc (3 × 20 ml). The combined organic layers were dried over $MgSO_4$, filtered

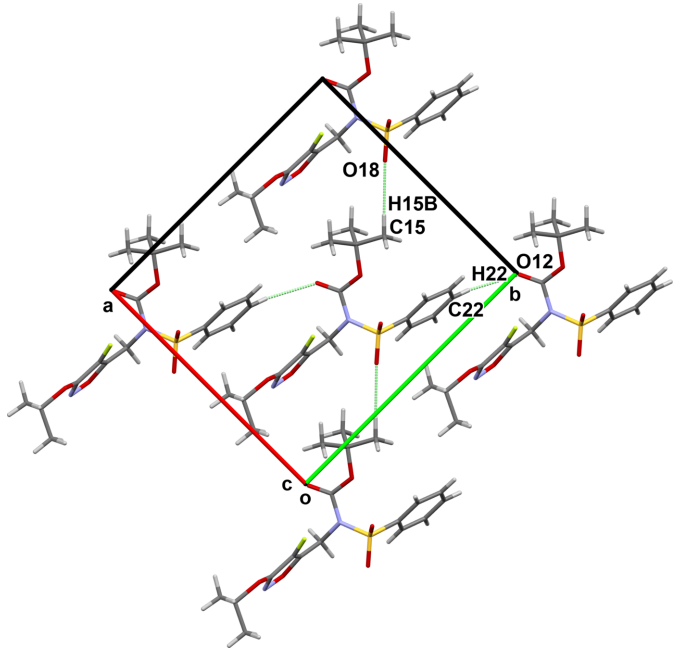


Figure 3
View of the weakly hydrogen-bonded $C(8)$ (vertical) and $C(9)$ (horizontal) chains.

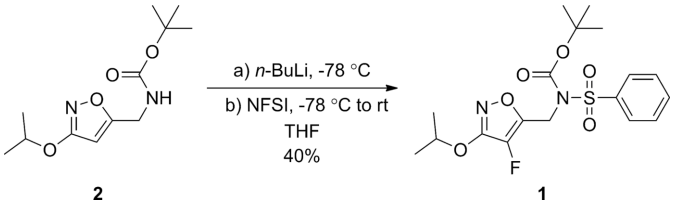


Figure 4
A synthetic scheme for the preparation of the title compound.

and concentrated under reduced pressure. The resulting residue was purified by silica gel column chromatography (petroleum ether/Et_2O, 80:20) to yield the title compound (323 mg, 40%) as a colourless viscous oil that crystallized on standing.

Refinement

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

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{23}FN_2O_6S$
M_r	414.44
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	173
a, *b*, *c* (Å)	13.271 (3), 13.904 (3), 11.206 (2)
β (°)	105.547 (6)
V (Å^3)	1992.1 (7)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.21
Crystal size (mm)	0.11 × 0.04 × 0.02
Data collection	
Diffractometer	Rigaku XtaLAB P200K
Absorption correction	Multi-scan (*REQAB*; Rigaku, 1998)
T_{min}, T_{max}	0.828, 0.996
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	11991, 3548, 2824
R_{int}	0.060
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.042, 0.090, 1.02
No. of reflections	3548
No. of parameters	258
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.19, −0.21
Absolute structure	Flack *x* determined using 1114 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	−0.08 (6)

Computer programs: *CrystalClear-SM Expert* (Rigaku, 2015), *SUPERFLIP* (Palatinus & Chapuis, 2007), *SHELXL2019/3* (Sheldrick, 2015), *Mercury* (Macrae *et al.*, 2020), *OLEX2* (Dolomanov *et al.*, 2009) and *publCIF* (Westrip, 2010).

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full crystallographic data

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tert-Butyl [(4-fluoro-3-isopropoxyisoxazol-5-yl)methyl](phenylsulfonyl)-carbamate

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Crystal data

$C_{18}H_{23}FN_2O_6S$
M_r = 414.44
Monoclinic, *Cc*
a = 13.271 (3) Å
b = 13.904 (3) Å
c = 11.206 (2) Å
β = 105.547 (6)°
V = 1992.1 (7) Å^3
Z = 4
F(000) = 872
D_x = 1.382 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 2002 reflections
θ = 2.2–25.3°
μ = 0.21 mm^{-1}
T = 173 K
Chip, colorless
0.11 × 0.04 × 0.02 mm

Data collection

Rigaku XtaLAB P200K diffractometer
Radiation source: Rotating Anode, Rigaku FR-X
Rigaku Osmic Confocal Optical System monochromator
Detector resolution: 5.8140 pixels mm^{-1}
shutterless scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
T_{min} = 0.828, T_{max} = 0.996
11991 measured reflections
3548 independent reflections
2824 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 25.4°, θ_{min} = 2.2°
h = −16→15
k = −16→16
l = −13→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.090
S = 1.01
3548 reflections
258 parameters
2 restraints
Primary atom site location: iterative
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0422P)^2 + 0.1932P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 e Å^{-3}
Absolute structure: Flack *x* determined using 1114 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: −0.08 (6)

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.

Refinement. The C-bound H atoms were located geometrically (phenyl C—H = 0.95 Å, methine C—H = 1.00 Å, methylene C—H = 0.99 Å, methyl C—H = 0.98 Å) and refined as riding atoms. The constraint U_{iso}(H) = 1.2U_{eq}(non-methyl C) or 1.5U_{eq}(methyl C) was applied in all cases.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S18	0.20066 (8)	0.53009 (8)	0.67391 (9)	0.0319 (3)
F4	0.3603 (2)	0.36593 (18)	0.5679 (3)	0.0508 (8)
O1	0.3211 (2)	0.2277 (2)	0.8123 (3)	0.0405 (8)
O6	0.3663 (3)	0.1578 (2)	0.5344 (3)	0.0394 (8)
O12	0.4876 (3)	0.5034 (2)	0.8535 (4)	0.0509 (9)
O13	0.3957 (2)	0.6237 (2)	0.7380 (3)	0.0374 (8)
O18	0.1283 (2)	0.4542 (2)	0.6758 (3)	0.0423 (8)
O19	0.2191 (2)	0.5575 (2)	0.5583 (3)	0.0410 (8)
N2	0.3347 (3)	0.1538 (3)	0.7299 (4)	0.0424 (10)
N11	0.3121 (3)	0.4906 (2)	0.7701 (3)	0.0329 (9)
C3	0.3498 (3)	0.1989 (3)	0.6341 (5)	0.0334 (11)
C4	0.3455 (4)	0.3008 (3)	0.6489 (4)	0.0340 (11)
C5	0.3268 (3)	0.3148 (3)	0.7593 (4)	0.0328 (10)
C7	0.3772 (4)	0.0519 (3)	0.5362 (5)	0.0426 (12)
H7	0.424446	0.031201	0.617519	0.051*
C8	0.2719 (4)	0.0050 (4)	0.5175 (6)	0.0623 (17)
H8A	0.241505	0.024101	0.584538	0.094*
H8B	0.280006	−0.065051	0.517834	0.094*
H8C	0.225618	0.025455	0.437850	0.094*
C9	0.4282 (4)	0.0302 (4)	0.4340 (5)	0.0558 (15)
H9A	0.381604	0.050097	0.354336	0.084*
H9B	0.441762	−0.038986	0.432310	0.084*
H9C	0.494386	0.065447	0.449076	0.084*
C10	0.3119 (4)	0.3991 (3)	0.8359 (4)	0.0374 (11)
H10A	0.244691	0.392111	0.857520	0.045*
H10B	0.368739	0.399875	0.913979	0.045*
C12	0.4078 (4)	0.5381 (3)	0.7916 (4)	0.0356 (11)
C14	0.4874 (4)	0.6868 (4)	0.7417 (5)	0.0398 (12)
C15	0.4359 (4)	0.7729 (4)	0.6674 (5)	0.0501 (14)
H15A	0.401071	0.752770	0.582521	0.075*
H15B	0.489062	0.821429	0.665758	0.075*
H15C	0.384091	0.800369	0.705706	0.075*
C16	0.5409 (4)	0.7130 (4)	0.8742 (5)	0.0523 (14)
H16A	0.488817	0.736331	0.914923	0.078*
H16B	0.592661	0.763617	0.875697	0.078*
H16C	0.576024	0.656181	0.918007	0.078*

C17	0.5602 (4)	0.6343 (4)	0.6781 (5)	0.0547 (15)
H17A	0.591901	0.579010	0.728503	0.082*
H17B	0.615281	0.678349	0.668906	0.082*
H17C	0.519972	0.612039	0.596216	0.082*
C19	0.1648 (3)	0.6322 (3)	0.7446 (4)	0.0283 (10)
C20	0.1626 (4)	0.7214 (3)	0.6888 (4)	0.0405 (12)
H20	0.183187	0.728238	0.614288	0.049*
C21	0.1299 (4)	0.8004 (3)	0.7437 (5)	0.0497 (14)
H21	0.127115	0.861996	0.706421	0.060*
C22	0.1013 (4)	0.7896 (4)	0.8526 (5)	0.0452 (13)
H22	0.079839	0.844194	0.890452	0.054*
C23	0.1037 (4)	0.7005 (4)	0.9071 (5)	0.0439 (12)
H23	0.083502	0.693720	0.981837	0.053*
C24	0.1353 (4)	0.6210 (3)	0.8528 (4)	0.0391 (12)
H24	0.136771	0.559284	0.889508	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S18	0.0352 (6)	0.0284 (5)	0.0340 (6)	−0.0033 (5)	0.0127 (5)	−0.0042 (5)
F4	0.083 (2)	0.0287 (14)	0.0528 (18)	0.0026 (14)	0.0383 (16)	0.0038 (13)
O1	0.054 (2)	0.0259 (17)	0.0449 (19)	0.0021 (15)	0.0193 (16)	0.0043 (14)
O6	0.049 (2)	0.0253 (16)	0.045 (2)	0.0029 (14)	0.0144 (17)	−0.0042 (14)
O12	0.040 (2)	0.0382 (19)	0.071 (2)	0.0057 (17)	0.0076 (18)	0.0059 (18)
O13	0.0303 (17)	0.0292 (17)	0.054 (2)	−0.0019 (13)	0.0133 (15)	0.0036 (15)
O18	0.042 (2)	0.0334 (18)	0.053 (2)	−0.0099 (15)	0.0160 (16)	−0.0045 (16)
O19	0.051 (2)	0.0420 (18)	0.0326 (18)	−0.0035 (15)	0.0152 (15)	−0.0024 (14)
N2	0.055 (3)	0.025 (2)	0.051 (3)	0.0008 (18)	0.020 (2)	−0.0018 (19)
N11	0.037 (2)	0.0223 (19)	0.042 (2)	0.0015 (16)	0.0153 (18)	−0.0014 (16)
C3	0.031 (2)	0.025 (2)	0.044 (3)	0.0009 (19)	0.009 (2)	−0.001 (2)
C4	0.039 (3)	0.023 (2)	0.041 (3)	0.001 (2)	0.012 (2)	0.006 (2)
C5	0.033 (3)	0.024 (2)	0.042 (3)	−0.0009 (19)	0.012 (2)	0.002 (2)
C7	0.044 (3)	0.024 (2)	0.056 (3)	0.007 (2)	0.006 (3)	−0.005 (2)
C8	0.056 (3)	0.033 (3)	0.093 (5)	−0.001 (3)	0.010 (3)	−0.009 (3)
C9	0.067 (4)	0.042 (3)	0.059 (4)	0.013 (3)	0.019 (3)	−0.014 (3)
C10	0.051 (3)	0.029 (2)	0.034 (3)	−0.002 (2)	0.014 (2)	0.002 (2)
C12	0.036 (3)	0.031 (3)	0.040 (3)	0.002 (2)	0.011 (2)	−0.003 (2)
C14	0.030 (2)	0.042 (3)	0.049 (3)	−0.011 (2)	0.012 (2)	−0.005 (2)
C15	0.054 (4)	0.040 (3)	0.057 (3)	−0.014 (2)	0.018 (3)	0.005 (2)
C16	0.054 (3)	0.051 (3)	0.052 (3)	−0.016 (3)	0.015 (3)	−0.009 (3)
C17	0.039 (3)	0.074 (4)	0.058 (4)	−0.006 (3)	0.025 (3)	−0.004 (3)
C19	0.026 (2)	0.026 (2)	0.032 (2)	0.0001 (19)	0.0075 (19)	−0.0024 (19)
C20	0.045 (3)	0.039 (3)	0.039 (3)	0.001 (2)	0.013 (2)	0.006 (2)
C21	0.057 (3)	0.028 (3)	0.066 (4)	0.006 (2)	0.019 (3)	0.002 (2)
C22	0.038 (3)	0.043 (3)	0.055 (3)	0.004 (2)	0.013 (3)	−0.014 (2)
C23	0.047 (3)	0.045 (3)	0.044 (3)	0.001 (2)	0.020 (2)	−0.006 (2)
C24	0.048 (3)	0.028 (3)	0.045 (3)	0.000 (2)	0.020 (2)	0.001 (2)

Geometric parameters (Å, º)

S18—O18	1.430 (3)	C9—H9C	0.9800
S18—O19	1.433 (3)	C10—H10A	0.9900
S18—N11	1.672 (4)	C10—H10B	0.9900
S18—C19	1.753 (4)	C14—C15	1.513 (7)
F4—C4	1.333 (5)	C14—C16	1.509 (7)
O1—N2	1.425 (5)	C14—C17	1.530 (7)
O1—C5	1.360 (5)	C15—H15A	0.9800
O6—C3	1.325 (5)	C15—H15B	0.9800
O6—C7	1.478 (5)	C15—H15C	0.9800
O12—C12	1.201 (6)	C16—H16A	0.9800
O13—C12	1.322 (5)	C16—H16B	0.9800
O13—C14	1.492 (5)	C16—H16C	0.9800
N2—C3	1.304 (6)	C17—H17A	0.9800
N11—C10	1.471 (6)	C17—H17B	0.9800
N11—C12	1.394 (6)	C17—H17C	0.9800
C3—C4	1.429 (6)	C19—C20	1.386 (6)
C4—C5	1.340 (6)	C19—C24	1.379 (6)
C5—C10	1.497 (6)	C20—H20	0.9500
C7—H7	1.0000	C20—C21	1.384 (7)
C7—C8	1.505 (7)	C21—H21	0.9500
C7—C9	1.509 (7)	C21—C22	1.379 (7)
C8—H8A	0.9800	C22—H22	0.9500
C8—H8B	0.9800	C22—C23	1.378 (7)
C8—H8C	0.9800	C23—H23	0.9500
C9—H9A	0.9800	C23—C24	1.380 (7)
C9—H9B	0.9800	C24—H24	0.9500
O18—S18—O19	119.20 (19)	O12—C12—O13	127.2 (4)
O18—S18—N11	103.28 (19)	O12—C12—N11	122.1 (4)
O18—S18—C19	109.01 (19)	O13—C12—N11	110.7 (4)
O19—S18—N11	109.52 (19)	O13—C14—C15	101.9 (4)
O19—S18—C19	109.01 (19)	O13—C14—C16	109.5 (4)
N11—S18—C19	105.97 (19)	O13—C14—C17	108.6 (4)
C5—O1—N2	109.1 (3)	C15—C14—C17	111.7 (4)
C3—O6—C7	117.1 (3)	C16—C14—C15	112.0 (4)
C12—O13—C14	121.1 (3)	C16—C14—C17	112.6 (4)
C3—N2—O1	105.1 (3)	C14—C15—H15A	109.5
C10—N11—S18	119.1 (3)	C14—C15—H15B	109.5
C12—N11—S18	124.3 (3)	C14—C15—H15C	109.5
C12—N11—C10	116.6 (4)	H15A—C15—H15B	109.5
O6—C3—C4	123.1 (4)	H15A—C15—H15C	109.5
N2—C3—O6	125.7 (4)	H15B—C15—H15C	109.5
N2—C3—C4	111.2 (4)	C14—C16—H16A	109.5
F4—C4—C3	125.3 (4)	C14—C16—H16B	109.5
F4—C4—C5	128.8 (4)	C14—C16—H16C	109.5
C5—C4—C3	105.9 (4)	H16A—C16—H16B	109.5

O1—C5—C10	114.5 (4)	H16A—C16—H16C	109.5
C4—C5—O1	108.6 (4)	H16B—C16—H16C	109.5
C4—C5—C10	136.9 (4)	C14—C17—H17A	109.5
O6—C7—H7	109.5	C14—C17—H17B	109.5
O6—C7—C8	110.2 (4)	C14—C17—H17C	109.5
O6—C7—C9	104.5 (4)	H17A—C17—H17B	109.5
C8—C7—H7	109.5	H17A—C17—H17C	109.5
C8—C7—C9	113.3 (5)	H17B—C17—H17C	109.5
C9—C7—H7	109.5	C20—C19—S18	119.8 (3)
C7—C8—H8A	109.5	C24—C19—S18	118.8 (3)
C7—C8—H8B	109.5	C24—C19—C20	121.4 (4)
C7—C8—H8C	109.5	C19—C20—H20	120.7
H8A—C8—H8B	109.5	C21—C20—C19	118.7 (4)
H8A—C8—H8C	109.5	C21—C20—H20	120.7
H8B—C8—H8C	109.5	C20—C21—H21	120.0
C7—C9—H9A	109.5	C22—C21—C20	120.1 (5)
C7—C9—H9B	109.5	C22—C21—H21	120.0
C7—C9—H9C	109.5	C21—C22—H22	119.7
H9A—C9—H9B	109.5	C23—C22—C21	120.7 (5)
H9A—C9—H9C	109.5	C23—C22—H22	119.7
H9B—C9—H9C	109.5	C22—C23—H23	120.1
N11—C10—C5	111.8 (4)	C22—C23—C24	119.9 (5)
N11—C10—H10A	109.3	C24—C23—H23	120.1
N11—C10—H10B	109.3	C19—C24—C23	119.3 (4)
C5—C10—H10A	109.3	C19—C24—H24	120.4
C5—C10—H10B	109.3	C23—C24—H24	120.4
H10A—C10—H10B	107.9		

S18—N11—C10—C5	85.5 (4)	N11—S18—C19—C24	−67.2 (4)
S18—N11—C12—O12	−173.8 (4)	C3—O6—C7—C8	75.5 (5)
S18—N11—C12—O13	7.9 (5)	C3—O6—C7—C9	−162.4 (4)
S18—C19—C20—C21	177.4 (4)	C3—C4—C5—O1	0.9 (5)
S18—C19—C24—C23	−177.9 (4)	C3—C4—C5—C10	−179.7 (5)
F4—C4—C5—O1	−177.5 (4)	C4—C5—C10—N11	4.3 (8)
F4—C4—C5—C10	1.9 (9)	C5—O1—N2—C3	1.3 (5)
O1—N2—C3—O6	179.8 (4)	C7—O6—C3—N2	−5.4 (6)
O1—N2—C3—C4	−0.7 (5)	C7—O6—C3—C4	175.2 (4)
O1—C5—C10—N11	−176.3 (4)	C10—N11—C12—O12	5.0 (6)
O6—C3—C4—F4	−2.1 (7)	C10—N11—C12—O13	−173.3 (4)
O6—C3—C4—C5	179.4 (4)	C12—O13—C14—C15	178.6 (4)
O18—S18—N11—C10	−3.4 (4)	C12—O13—C14—C16	−62.7 (5)
O18—S18—N11—C12	175.4 (3)	C12—O13—C14—C17	60.6 (5)
O18—S18—C19—C20	−134.2 (4)	C12—N11—C10—C5	−93.4 (4)
O18—S18—C19—C24	43.3 (4)	C14—O13—C12—O12	5.0 (7)
O19—S18—N11—C10	−131.4 (3)	C14—O13—C12—N11	−176.7 (4)
O19—S18—N11—C12	47.4 (4)	C19—S18—N11—C10	111.2 (3)
O19—S18—C19—C20	−2.6 (4)	C19—S18—N11—C12	−70.0 (4)
O19—S18—C19—C24	175.0 (4)	C19—C20—C21—C22	0.7 (7)

N2—O1—C5—C4	−1.4 (5)	C20—C19—C24—C23	−0.4 (7)
N2—O1—C5—C10	179.0 (4)	C20—C21—C22—C23	−0.8 (8)
N2—C3—C4—F4	178.4 (4)	C21—C22—C23—C24	0.3 (8)
N2—C3—C4—C5	−0.1 (5)	C22—C23—C24—C19	0.3 (7)
N11—S18—C19—C20	115.2 (4)	C24—C19—C20—C21	−0.1 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C10—H10*A*···O19^{i}	0.99	2.47	3.121 (6)	123
C15—H15*B*···O18^{ii}	0.98	2.59	3.571 (6)	176
C22—H22···O12^{iii}	0.95	2.51	3.335 (6)	145
C24—H24···O19^{i}	0.95	2.51	3.366 (5)	150

Symmetry codes: (i) x, $-y+1$, $z+1/2$; (ii) $x+1/2$, $y+1/2$, z; (iii) $x-1/2$, $y+1/2$, z.