



Synthesis, crystal structure and Hirshfeld surface analysis of *N*-(4-fluorophenyl)-*N*-isopropyl-2-(methylsulfonyl)acetamide

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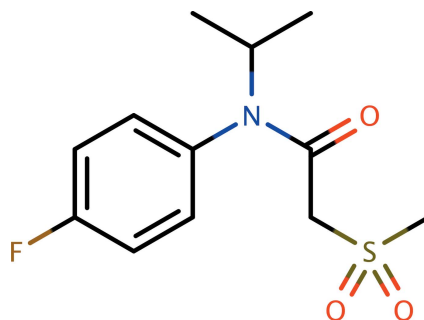
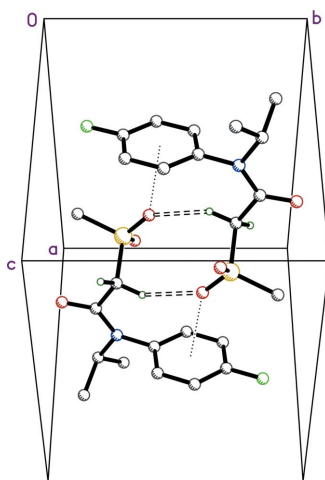
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The synthesis and crystal structure of the title compound, C₁₂H₁₆FNO₃S, which is related to the herbicide flufenacet, are presented. The dihedral angle between the amide group and the fluorinated benzene ring is 87.30 (5)° and the N—C—C—S torsion angle defining the orientation of the methylsulfonyl substituent relative to the amide group is 106.91 (11)°. In the crystal, inversion-related molecules form dimers as a result of pairwise C—H···O hydrogen bonds, which appear to be reinforced by short O···π contacts [O···C_g = 3.0643 (11) Å]. A Hirshfeld surface analysis was used to quantify the various types of intermolecular contacts, which are dominated by H atoms.

1. Chemical context

N-(Substituted phenyl)acetamides have a variety of biological activities. For example, substituted phenylacetamides and their use as protease inhibitors was reported by Kreutter *et al.* (2009) and a description of the syntheses and antioxidant studies of *N*-substituted benzyl/phenyl-2-[3,4-dimethyl-5,5-dioxidopyrazolo[4,3-*c*][1,2]benzothiazin-2(4*H*)-yl]acetamides was given by Ahmad *et al.* (2013). The syntheses and biological evaluation of *N*⁴-substituted sulfonamide–acetamide derivatives as dihydrofolate reductase (DHFR) inhibitors was reported by Hussein *et al.* (2019) and the synthesis of *N*-(substituted phenyl)-*N*-(substituted)acetamide derivatives as potent analgesic agents was described by Verma *et al.* (2020). Lastly, the evaluation of new 2-hydroxy-*N*-(4-oxo-2-substituted phenyl-1,3-thiazolidin-3-yl)-2-phenylacetamide derivatives as potential antimycobacterial agents was reported by Güzel-Akdemir *et al.* (2020).



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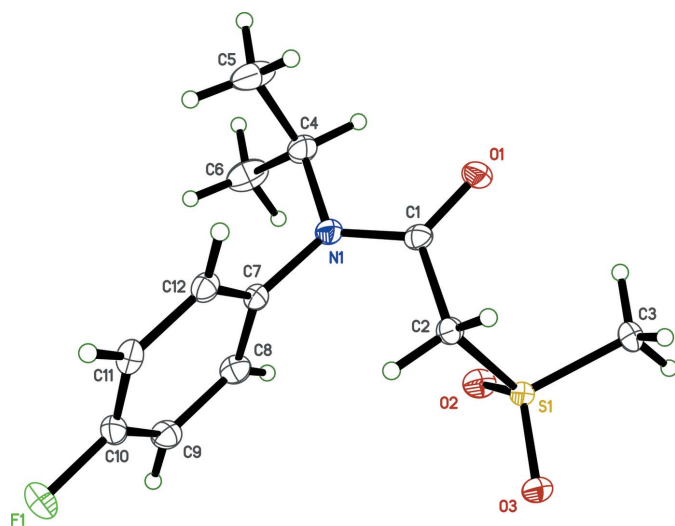


Figure 1
The molecular structure of **I** showing 50% displacement ellipsoids.

Flufenacet ($C_{14}H_{13}F_4N_3O_2S$), systematic name *N*-(4-fluorophenyl)-*N*-propan-2-yl-2-[[5-(trifluoromethyl)-1,3,4-thiadiazol-2-yl]oxy]acetamide, is an herbicide, xenobiotic and environmental contaminant (Rouchaud *et al.*, 2001; Zimmerman *et al.*, 2002). This paper reports the synthesis, crystal structure and a Hirshfeld surface analysis of the related title compound, $C_{12}H_{16}FNO_3S$ (**I**) (Fig. 1).

2. Structural commentary

In the crystal structure of **I**, the nitrogen atom of the amide group is close to planar, the sum of bond angles about N1 being $358.92(19)^\circ$, which places N1 $0.0862(14)$ Å from the plane passing through C1, C4, and C7. The amide group is also almost planar, having an r.m.s. deviation from the mean plane of N1, C1, O1, C2 of 0.0095 Å [maximum = $0.0165(11)$ Å for C1], and is almost perpendicular to the fluorobenzene ring (C7–C12), subtending a dihedral angle of $87.30(5)^\circ$. The overall conformation of the molecule is defined by the torsion angles C7–N1–C1–C2 [$14.68(17)^\circ$], N1–C1–C2–S1 [$106.91(11)^\circ$], C1–C2–S1–C3 [$74.53(10)^\circ$] and by the orientation of the ⁱpropyl group, *e.g.*, C1–N1–C4–C6 [$139.85(13)^\circ$]. Otherwise, all bond lengths and angles lie within the expected ranges.

3. Supramolecular features

There are no strong hydrogen bonds in the crystal structure of **I** (Fig. 2), but there are a number of weaker C–H···O and C–H···F interactions, which are quantified in Table 1. The most prominent supramolecular constructs are dimers in which inversion-related molecules are linked by C2–H2A···O3ⁱ and C2ⁱ–H2Aⁱ···O3 hydrogen bonds [symmetry code: (i) $1 - x, 1 - y, 1 - z$]. These dimers also feature close contacts between the sulfone O3 atom and the inversion-related benzene ring to give an O3···Cg(C7–C12)ⁱ distance of

Table 1

Weak hydrogen bonds and other short intermolecular contacts (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C2–H2A···O3 ⁱ	0.99	2.31	3.2025 (16)	150
C3–H3B···O1 ⁱⁱ	0.98	2.55	3.5196 (17)	170
C5–H5A···F1 ⁱⁱⁱ	0.98	2.50	3.4295 (18)	158
C11–H11···O1 ^{iv}	0.95	2.39	3.1851 (16)	141
C12–H12···O2 ^{iv}	0.95	2.56	3.2955 (16)	134
O3···Cg(C7–C12) ⁱ			3.0643 (11)	

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

$3.0643(11)$ Å (*e.g.* Gung *et al.*, 2008 and see also Section 4: Database survey). The other weak C–H···O interactions involve inversion, translation, and *c*-glide related molecules (Table 1, Fig. 3a). A Hirshfeld surface analysis using *Crystal-Explorer* (Spackman *et al.*, 2021) shows that almost all atom-atom contacts involve the hydrogen atoms (Fig. 3b–f).

4. Database survey

A search of the Cambridge Structural Database (CSD, v5.43 with updates through November 2022; Groom *et al.*, 2016) for a molecular fragment consisting of *N*-phenylacetamide with ‘any non-H group’ attached at the nitrogen atom, the 4-*posi-*

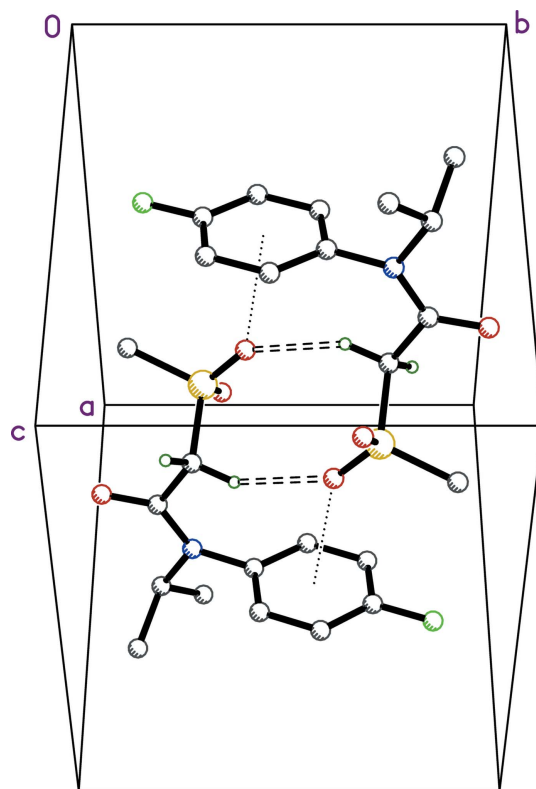
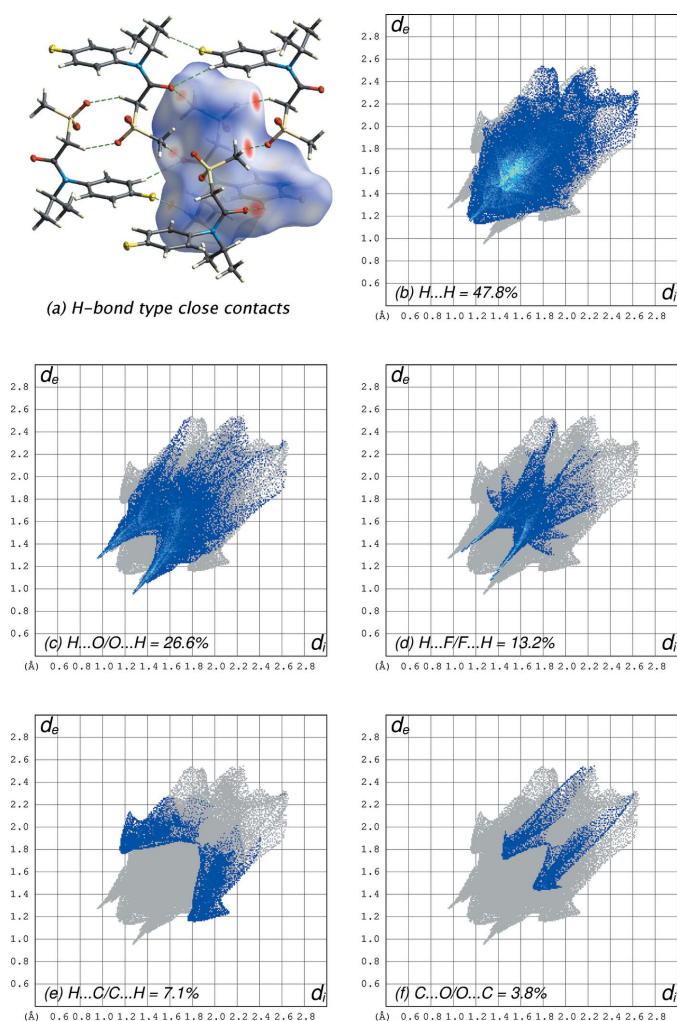


Figure 2
A partial packing plot of **I**, showing inversion dimers resulting from pairs of C–H···O weak hydrogen bonds, augmented by O···Cg(ring) contacts. Hydrogen atoms not involved in the hydrogen bonds are omitted.


Figure 3

(a) The Hirshfeld surface of **I** expressed over d_{norm} , with C—H...O and C—H...F interactions drawn as dashed lines and as dark- and light-red regions on the Hirshfeld surface, respectively; (b) fingerprint plot of H...H contacts; (c) H...O/O...H contacts; (d) H...F/F...H contacts; (e) H...C/C...H contacts; (f) C...O/O...C contacts.

tion of the benzene ring, and replacing one hydrogen of the methyl group, yielded 259 hits. A similar fragment, but with ‘any halogen’ at the 4-position on the ring, gave 92 hits. With the halogen restricted to fluorine, twelve hits were returned, and with an isopropyl group attached to the nitrogen atom, only one match was found: CSD refcode QEMHOG (Gao & Ng, 2006): this structure has a 1,3-benzothiazol-2-yl-oxy group attached to the methylene carbon atom of the search fragment.

A search of the CSD for non-bonded close contacts (up to 3.1 Å) between S=O oxygen atoms and a benzene-ring centroid (with ‘any substituent’) returned 154 hits, none of which have much else in common with **I**. A crystallographic and computational study of interactions between oxygen lone pairs and aromatic rings (albeit involving carbon-bound oxygen atoms) was presented by Gung *et al.* (2008).

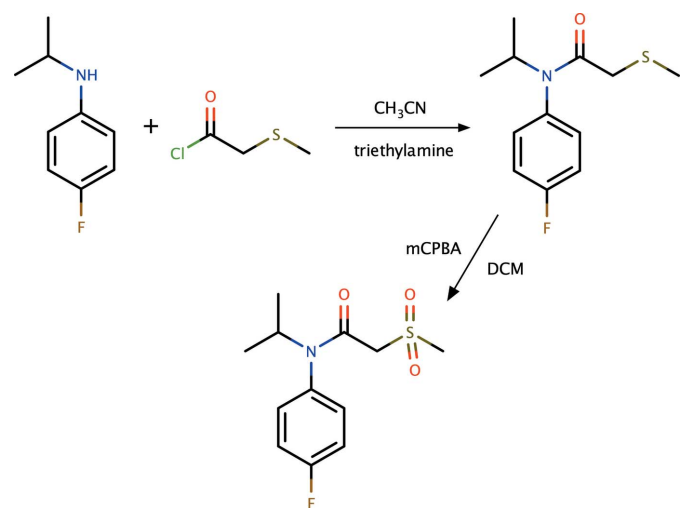
There are several other related structures in the CSD, namely: thiamphenicol, D-threo-2,2-dichloro-*N*-[2-hydroxy-1-

(hydroxymethyl)-2-[4-(methylsulfonyl)phenyl]ethyl]acetamide (CABCIR01; Ghosh *et al.*, 1987), 2,2-dichloro-*N*-[1-(fluoromethyl)-2-hydroxy-2-[4-(methylsulfonyl)phenyl]ethyl]acetamide (GAWNIC; Cheng *et al.*, 2005), *N*-(2,6-dimethylphenyl)-2-(2-{3-[4-(methylsulfonyl)phenyl]-1,2,4-oxadiazol-5-yl}phenoxy)acetamide (AFIFIF; Wang *et al.*, 2007), *N*-(4-chloro-2-nitrophenyl)-*N*-(methylsulfonyl)acetamide (WOGWEV; Zia-ur-Rehman *et al.*, 2008), *N*-(4-methoxy-2-nitrophenyl)-*N*-(methylsulfonyl)acetamide (QOTNAP; Zia-ur-Rehman *et al.*, 2009), 2-chloro-*N*-(4-chloro-2-(2-chlorobenzoyl)phenyl)acetamide (DUPLUW; Dutkiewicz *et al.*, 2010), 2-chloro-*N*-[2-(2-fluorobenzoyl)-4-nitrophenyl]-*N*-methylacetamide (EXIVEN; Siddaraju *et al.*, 2011), 2-phenyl-*N*-(pyrazin-2-yl)acetamide (ROJNAH; Nayak *et al.*, 2014) and 2-(perfluorophenyl)acetamide (LAMRAW; Novikov *et al.*, 2022).

5. Synthesis, crystallization and spectroscopic details

In a 250 ml flask (with a nitrogen inlet and a septum) was placed 5 g of 4-fluoro-*N*-isopropylbenzenamine dissolved in 50 ml of acetonitrile. After cooling to 273 K, 6.7 g of triethylamine and 4.11 g of 2-(methylthio)acetyl chloride were added. The mixture was stirred at room temperature for 5 h. After this, 100 ml of water were added and the mixture was extracted three times, each with 100 ml of methyl tert-butyl ether (MTBE). The combined organic phases were dried over MgSO₄ and the solvent was evaporated under reduced pressure. The crude product, *N*-(4-fluorophenyl)-*N*-isopropyl-2-(methylthio)acetamide, was used for the next stage with purification (7.5 g).

To a 250 ml round-bottomed flask (with a nitrogen inlet and a septum) was added 7.5 g of *N*-(4-fluorophenyl)-*N*-isopropyl-2-(methylthio)acetamide dissolved in 150 ml of dichloromethane. After cooling to 263–273 K, 13.37 g of *meta*-chloroperbenzoic acid in 100 ml dichloromethane was added


Figure 4

A reaction scheme for the synthesis of **I**. DCM is dichloromethane, mCPBA is *meta*-chloroperbenzoic acid.

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₁₂ H ₁₆ FNO ₃ S
<i>M_r</i>	273.32
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>c</i>
Temperature (K)	90
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.9530 (3), 8.7657 (2), 11.7723 (3)
β (°)	100.457 (1)
<i>V</i> (Å ³)	1314.45 (5)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.26
Crystal size (mm)	0.32 × 0.31 × 0.09
Data collection	
Diffractometer	Bruker D8 Venture dual source
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.833, 0.971
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	22801, 3010, 2678
<i>R_{int}</i>	0.030
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.650
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.031, 0.079, 1.05
No. of reflections	3010
No. of parameters	166
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.36, -0.37

Computer programs: *APEX3* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b), *XP* in *SHELXTL* (Sheldrick, 2008), *CrystalExplorer* (Spackman *et al.*, 2021), *SHELXTL* (Sheldrick, 2008), and *pubCIF* (Westrip, 2010).

slowly at the same temperature. The mixture was stirred at room temperature for 5 h. After this, 200 ml of water were added and the organic layer was separated, and washed with 100 ml of 10% sodium bicarbonate twice. The organic phases were dried over MgSO₄ and the solvent was evaporated under reduced pressure. The crude product was purified by chromatography over SiO₂ (hexane:ethyl acetate 9:1 *v/v*). The title compound was recrystallized from diethyl ether solution in the form of colorless plates. The overall reaction scheme is shown in Fig. 4.

¹H NMR: CDCl₃ (400 MHz, δ ppm): 1.097–1.08 [6H, *d*, (CH₃)₂]; 3.198 (3H, *s*, -CH₃); 3.664 (2H, *s*, CH₂); 5.006–4.938 (1H, *m*, -CH); 7.273–7.132 (4H, *m*, ar H). MS *m/z*: 273.45 (*M*)⁺.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. Hydrogen atoms were found in difference-Fourier maps, but subsequently included in the refinement using riding models, with constrained C–H distances set to 0.95 Å (*Csp*²H), 0.98 Å (*RCH*₃), 0.99 Å

(*R*₂CH₂) and 1.00 Å (*R*₃CH). *U*_{iso}(H) parameters were set to values of either 1.2*U*_{eq} or 1.5*U*_{eq} (*RCH*₃ only) of the attached atom.

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Synthesis, crystal structure and Hirshfeld surface analysis of *N*-(4-fluorophenyl)-*N*-isopropyl-2-(methylsulfonyl)acetamide

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *APEX3* (Bruker, 2016); data reduction: *APEX3* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2019/2* (Sheldrick, 2015b); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008) and *CrystalExplorer* (Spackman *et al.*, 2021); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

N-(4-Fluorophenyl)-2-(methylsulfonyl)-*N*-(propan-2-yl)acetamide

Crystal data

$C_{12}H_{16}FNO_3S$

$M_r = 273.32$

Monoclinic, $P2_1/c$

$a = 12.9530$ (3) Å

$b = 8.7657$ (2) Å

$c = 11.7723$ (3) Å

$\beta = 100.457$ (1)°

$V = 1314.45$ (5) Å³

$Z = 4$

$F(000) = 576$

$D_x = 1.381$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9889 reflections

$\theta = 2.8$ – 27.5°

$\mu = 0.26$ mm⁻¹

$T = 90$ K

Rounded plate, colourless

$0.32 \times 0.31 \times 0.09$ mm

Data collection

Bruker D8 Venture dual source
diffractometer

Radiation source: microsource

Detector resolution: 7.41 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.833$, $T_{\max} = 0.971$

22801 measured reflections

3010 independent reflections

2678 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.030$

$\theta_{\max} = 27.5^\circ$, $\theta_{\min} = 2.8^\circ$

$h = -16 \rightarrow 16$

$k = -11 \rightarrow 11$

$l = -15 \rightarrow 15$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.031$

$wR(F^2) = 0.079$

$S = 1.05$

3010 reflections

166 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: difference Fourier map

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0327P)^2 + 0.7883P]$

where $P = (F_o^2 + 2F_c^2)/3$

$$(\Delta/\sigma)_{\max} = 0.001$$

$$\Delta\rho_{\max} = 0.36 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.37 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. The crystal was mounted using polyisobutene oil on the tip of a fine glass fibre, which was fastened in a copper mounting pin with electrical solder. It was placed directly into the cold gas stream of a liquid-nitrogen based cryostat (Hope, 1994; Parkin & Hope, 1998).

Diffraction data were collected with the crystal at 90K, which is standard practice in this laboratory for the majority of flash-cooled crystals.

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. Refinement progress was checked using *Platon* (Spek, 2020) and by an *R*-tensor (Parkin, 2000). The final model was further checked with the IUCr utility *checkCIF*.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.54145 (2)	0.29322 (3)	0.38570 (3)	0.01394 (9)
F1	0.77308 (7)	0.83954 (10)	0.77262 (8)	0.0265 (2)
C1	0.70051 (10)	0.18349 (15)	0.54790 (11)	0.0153 (3)
N1	0.78957 (9)	0.26470 (13)	0.58233 (10)	0.0169 (2)
O1	0.69978 (7)	0.04745 (11)	0.52217 (8)	0.0193 (2)
C2	0.59691 (10)	0.26923 (15)	0.53498 (11)	0.0154 (3)
H2A	0.608749	0.370378	0.572495	0.018*
H2AB	0.547429	0.211700	0.573787	0.018*
O2	0.62454 (7)	0.33486 (11)	0.32511 (8)	0.0208 (2)
O3	0.45431 (7)	0.39662 (11)	0.38023 (8)	0.0201 (2)
C3	0.49181 (11)	0.11358 (15)	0.33711 (12)	0.0208 (3)
H3A	0.459299	0.120203	0.255330	0.031*
H3B	0.439182	0.081074	0.382298	0.031*
H3C	0.549247	0.039248	0.346600	0.031*
C9	0.7902 (1)	0.68848 (16)	0.61179 (12)	0.0191 (3)
H9	0.794529	0.777562	0.566931	0.023*
C8	0.79425 (10)	0.54409 (16)	0.56408 (12)	0.0188 (3)
H8	0.801145	0.533426	0.485496	0.023*
C7	0.7882 (1)	0.41507 (15)	0.63150 (11)	0.0154 (3)
C6	0.97208 (12)	0.2845 (2)	0.54665 (14)	0.0295 (3)
H6A	1.036051	0.225348	0.545252	0.044*
H6B	0.988878	0.372611	0.597886	0.044*
H6C	0.943028	0.319875	0.468411	0.044*
C5	0.93224 (12)	0.1303 (2)	0.71320 (14)	0.0309 (4)
H5A	0.877506	0.070798	0.740427	0.046*
H5B	0.950692	0.218725	0.763798	0.046*
H5C	0.994531	0.066468	0.714444	0.046*
C4	0.89195 (10)	0.18467 (16)	0.59065 (13)	0.0216 (3)
H4	0.880049	0.092462	0.539939	0.026*
C10	0.77975 (10)	0.69895 (15)	0.72594 (12)	0.0180 (3)

C11	0.77354 (10)	0.57396 (16)	0.79470 (11)	0.0174 (3)
H11	0.766284	0.585728	0.873082	0.021*
C12	0.77814 (10)	0.42986 (15)	0.74673 (11)	0.0162 (3)
H12	0.774416	0.341486	0.792531	0.019*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.01361 (16)	0.01232 (15)	0.01522 (16)	0.00096 (11)	0.00086 (11)	-0.00046 (11)
F1	0.0312 (5)	0.0167 (4)	0.0308 (5)	-0.0009 (3)	0.0033 (4)	-0.0072 (3)
C1	0.0176 (6)	0.0165 (6)	0.0114 (6)	0.0028 (5)	0.0012 (5)	0.0006 (5)
N1	0.0158 (5)	0.0159 (5)	0.0179 (5)	0.0033 (4)	0.0001 (4)	-0.0022 (4)
O1	0.0224 (5)	0.0142 (5)	0.0202 (5)	0.0033 (4)	0.0015 (4)	-0.0020 (4)
C2	0.0164 (6)	0.0151 (6)	0.0142 (6)	0.0012 (5)	0.0016 (5)	-0.0018 (5)
O2	0.0210 (5)	0.0217 (5)	0.0208 (5)	0.0013 (4)	0.0070 (4)	0.0049 (4)
O3	0.0170 (5)	0.0180 (5)	0.0237 (5)	0.0049 (4)	-0.0007 (4)	-0.0018 (4)
C3	0.0208 (7)	0.0155 (6)	0.0243 (7)	-0.0016 (5)	-0.0004 (5)	-0.0058 (5)
C9	0.0184 (6)	0.0176 (6)	0.0212 (7)	-0.0010 (5)	0.0030 (5)	0.0043 (5)
C8	0.0194 (6)	0.0220 (7)	0.0152 (6)	0.0020 (5)	0.0038 (5)	0.0017 (5)
C7	0.0124 (6)	0.0158 (6)	0.0171 (6)	0.0004 (5)	0.0002 (5)	-0.0017 (5)
C6	0.0227 (7)	0.0418 (9)	0.0258 (8)	0.0094 (7)	0.0093 (6)	0.0081 (7)
C5	0.0184 (7)	0.0345 (9)	0.0389 (9)	0.0043 (6)	0.0030 (6)	0.0195 (7)
C4	0.0155 (6)	0.0222 (7)	0.0258 (7)	0.0052 (5)	0.0003 (5)	-0.0036 (6)
C10	0.0147 (6)	0.0158 (6)	0.0227 (7)	-0.0007 (5)	0.0010 (5)	-0.0035 (5)
C11	0.0148 (6)	0.0225 (7)	0.0148 (6)	-0.0027 (5)	0.0021 (5)	-0.0026 (5)
C12	0.0140 (6)	0.0181 (6)	0.0160 (6)	-0.0021 (5)	0.0010 (5)	0.0025 (5)

Geometric parameters (Å, °)

S1—O3	1.4399 (9)	C9—H9	0.9500
S1—O2	1.4419 (10)	C8—C7	1.3920 (18)
S1—C3	1.7570 (13)	C8—H8	0.9500
S1—C2	1.7862 (13)	C7—C12	1.3922 (18)
F1—C10	1.3586 (15)	C6—C4	1.519 (2)
C1—O1	1.2300 (16)	C6—H6A	0.9800
C1—N1	1.3535 (17)	C6—H6B	0.9800
C1—C2	1.5213 (17)	C6—H6C	0.9800
N1—C7	1.4411 (16)	C5—C4	1.519 (2)
N1—C4	1.4876 (16)	C5—H5A	0.9800
C2—H2A	0.9900	C5—H5B	0.9800
C2—H2AB	0.9900	C5—H5C	0.9800
C3—H3A	0.9800	C4—H4	1.0000
C3—H3B	0.9800	C10—C11	1.3732 (19)
C3—H3C	0.9800	C11—C12	1.3892 (19)
C9—C10	1.378 (2)	C11—H11	0.9500
C9—C8	1.3896 (19)	C12—H12	0.9500
O3—S1—O2	117.90 (6)	C8—C7—C12	120.32 (12)

O3—S1—C3	108.18 (6)	C8—C7—N1	120.53 (12)
O2—S1—C3	109.13 (7)	C12—C7—N1	119.13 (12)
O3—S1—C2	106.87 (6)	C4—C6—H6A	109.5
O2—S1—C2	108.27 (6)	C4—C6—H6B	109.5
C3—S1—C2	105.84 (7)	H6A—C6—H6B	109.5
O1—C1—N1	123.48 (12)	C4—C6—H6C	109.5
O1—C1—C2	119.15 (12)	H6A—C6—H6C	109.5
N1—C1—C2	117.29 (11)	H6B—C6—H6C	109.5
C1—N1—C7	121.96 (11)	C4—C5—H5A	109.5
C1—N1—C4	118.22 (11)	C4—C5—H5B	109.5
C7—N1—C4	118.74 (11)	H5A—C5—H5B	109.5
C1—C2—S1	110.27 (9)	C4—C5—H5C	109.5
C1—C2—H2A	109.6	H5A—C5—H5C	109.5
S1—C2—H2A	109.6	H5B—C5—H5C	109.5
C1—C2—H2AB	109.6	N1—C4—C6	111.23 (12)
S1—C2—H2AB	109.6	N1—C4—C5	111.03 (12)
H2A—C2—H2AB	108.1	C6—C4—C5	111.49 (12)
S1—C3—H3A	109.5	N1—C4—H4	107.6
S1—C3—H3B	109.5	C6—C4—H4	107.6
H3A—C3—H3B	109.5	C5—C4—H4	107.6
S1—C3—H3C	109.5	F1—C10—C11	118.07 (12)
H3A—C3—H3C	109.5	F1—C10—C9	118.66 (12)
H3B—C3—H3C	109.5	C11—C10—C9	123.26 (12)
C10—C9—C8	118.19 (12)	C10—C11—C12	118.32 (12)
C10—C9—H9	120.9	C10—C11—H11	120.8
C8—C9—H9	120.9	C12—C11—H11	120.8
C9—C8—C7	119.96 (12)	C11—C12—C7	119.94 (12)
C9—C8—H8	120.0	C11—C12—H12	120.0
C7—C8—H8	120.0	C7—C12—H12	120.0
O1—C1—N1—C7	-168.59 (12)	C1—N1—C7—C12	78.93 (16)
C2—C1—N1—C7	14.68 (17)	C4—N1—C7—C12	-88.93 (15)
O1—C1—N1—C4	-0.67 (19)	C1—N1—C4—C6	139.85 (13)
C2—C1—N1—C4	-177.40 (11)	C7—N1—C4—C6	-51.84 (16)
O1—C1—C2—S1	-69.97 (14)	C1—N1—C4—C5	-95.38 (15)
N1—C1—C2—S1	106.91 (11)	C7—N1—C4—C5	72.93 (16)
O3—S1—C2—C1	-170.32 (9)	C8—C9—C10—F1	-178.38 (11)
O2—S1—C2—C1	-42.36 (11)	C8—C9—C10—C11	0.2 (2)
C3—S1—C2—C1	74.53 (10)	F1—C10—C11—C12	178.69 (11)
C10—C9—C8—C7	-0.3 (2)	C9—C10—C11—C12	0.1 (2)
C9—C8—C7—C12	-0.03 (19)	C10—C11—C12—C7	-0.36 (19)
C9—C8—C7—N1	178.39 (12)	C8—C7—C12—C11	0.34 (19)
C1—N1—C7—C8	-99.51 (15)	N1—C7—C12—C11	-178.10 (11)
C4—N1—C7—C8	92.63 (15)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
C2—H2 <i>A</i> ···O3 ⁱ	0.99	2.31	3.2025 (16)	150
C3—H3 <i>B</i> ···O1 ⁱⁱ	0.98	2.55	3.5196 (17)	170
C5—H5 <i>A</i> ···F1 ⁱⁱⁱ	0.98	2.50	3.4295 (18)	158
C11—H11···O1 ^{iv}	0.95	2.39	3.1851 (16)	141
C12—H12···O2 ^{iv}	0.95	2.56	3.2955 (16)	134

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