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Crystal structure of flucetosulfuron

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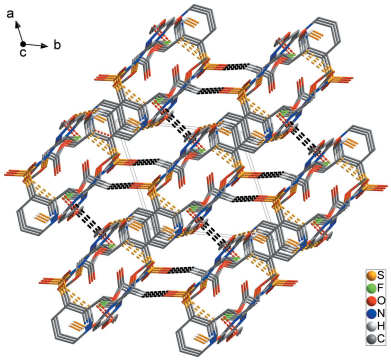
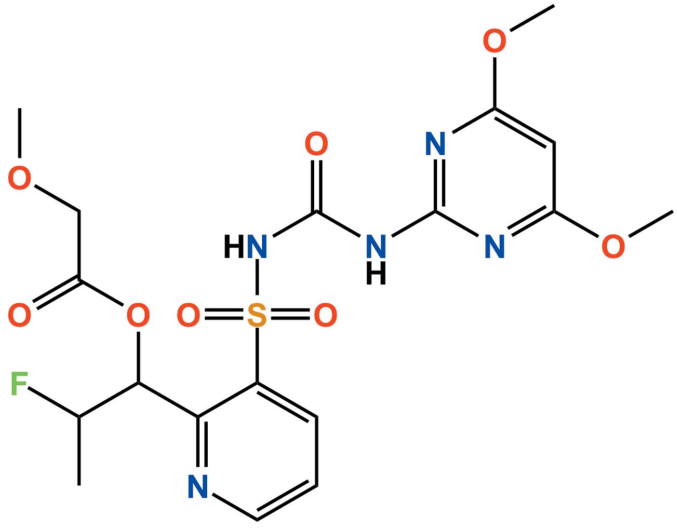
The title compound, {systematic name: 1-[3-({[(4,6-dimethoxypyrimidin-2-yl)carbamoyl]amino}sulfonyl)pyridin-2-yl]-2-fluoropropyl 2-methoxyacetate}, $C_{18}H_{22}FN_5O_8S$, is used as a herbicide (pyrimidinylsulfonylurea herbicide). The dihedral angle between the mean planes of the pyridine and pyrimidine rings is 86.90 (7)°. In the crystal, N/C—H···O hydrogen bonds, C—H···F and C—H···π interactions link adjacent molecules, forming a chain along [020]. A further two C—H···O hydrogen bonds together with weak π–π interactions [ring centroid separation = 3.7584 (12) Å] further aggregate the structure into a three-dimensional architecture.

1. Chemical context

Flucetosulfuron, a relatively new herbicide, inhibits acetolactate synthase (ALS) in plants, as do other ALS inhibitors such as imidazolinones, pyrimidinyloxybenzoates, triazolopyrimidines, and sulfonylaminocarbonyltriazolinones (Lee *et al.*, 2014). It is a novel post-emergence sulfonylurea herbicide providing excellent control of *Galium aparine* and other important broadleaf weeds with good safety to cereal crops, wheat and barley (Kim, Lee *et al.*, 2003) In rice, the herbicide provides excellent control of *Echinochloa crus-galli*, which is not or only marginally controlled by common sulfonylurea products, and also controls annual broadleaf weeds, sedges and perennial weeds of rice with similar efficacy to other sulfonylurea rice herbicides (Kim, Koo *et al.*, 2003). Until now, its crystal structure had not been reported and we describe it herein.





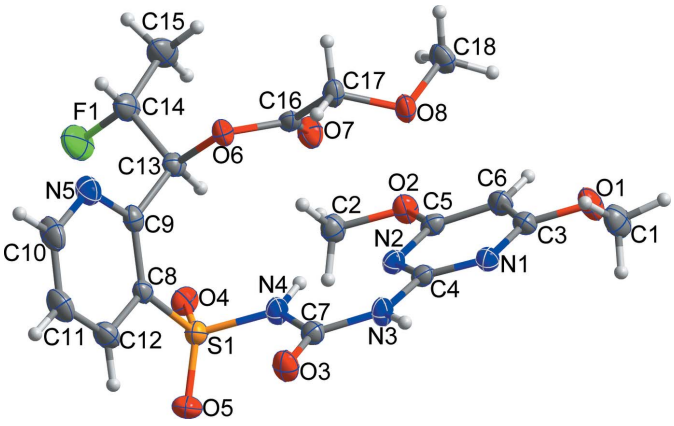


Figure 1
The molecular structure of the title compound with the atom labelling and displacement ellipsoids drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

2. Structural commentary

The structure of flucetosulfuron is shown in Fig. 1. The dihedral angle between the mean planes of the pyridine and pyrimidine rings is 86.90 (7)°. All bond lengths and angles are normal and comparable to those observed in similar crystal structures (Jeon *et al.*, 2015; Chopra *et al.*, 2004).

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

*Cg*1 is the centroid of the N5/C8–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···O8^{i}	0.88	2.01	2.885 (2)	174
C1—H1*A*···O3^{i}	0.98	2.58	3.368 (3)	137
C2—H2*B*···F1^{ii}	0.98	2.53	3.161 (2)	122
C12—H12···O2^{iii}	0.95	2.42	3.229 (3)	143
C17—H17*A*···O5^{iv}	0.99	2.55	3.367 (3)	139
C1—H1*B*···*Cg*1^{i}	0.98	2.74	3.488 (2)	134

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

3. Supramolecular features

In the crystal, molecules are linked by C1—H1*A*···O3^{i}, N3—H3*N*···O8^{i} and C2—H2*B*···F1^{ii} hydrogen bonds [H···O = 2.58, 2.01 and H···F = 2.53 Å; Table 1] and C1—H1*B*···*Cg*1^{i} interactions [H···π = 2.74 Å], forming a chain structure along [020] (yellow dashed lines in Fig. 2). In addition, the chains are linked by C12—H12···O2^{iii} hydrogen bonds [H···O =2.42 Å], forming a two-dimensional network structure parallel to (020) (red dashed lines in Fig. 2). The C17—H17···O5^{iv} hydrogen bond [H···O =2.55 Å] and weak π–π interactions (N1–N2/C3–C6) [*Cg*2···*Cg*2^{v}= 3.7584 (12) Å; symmetry code: (v) $-x+2, -y+1, -z+1$] generate a three-dimensional archi-

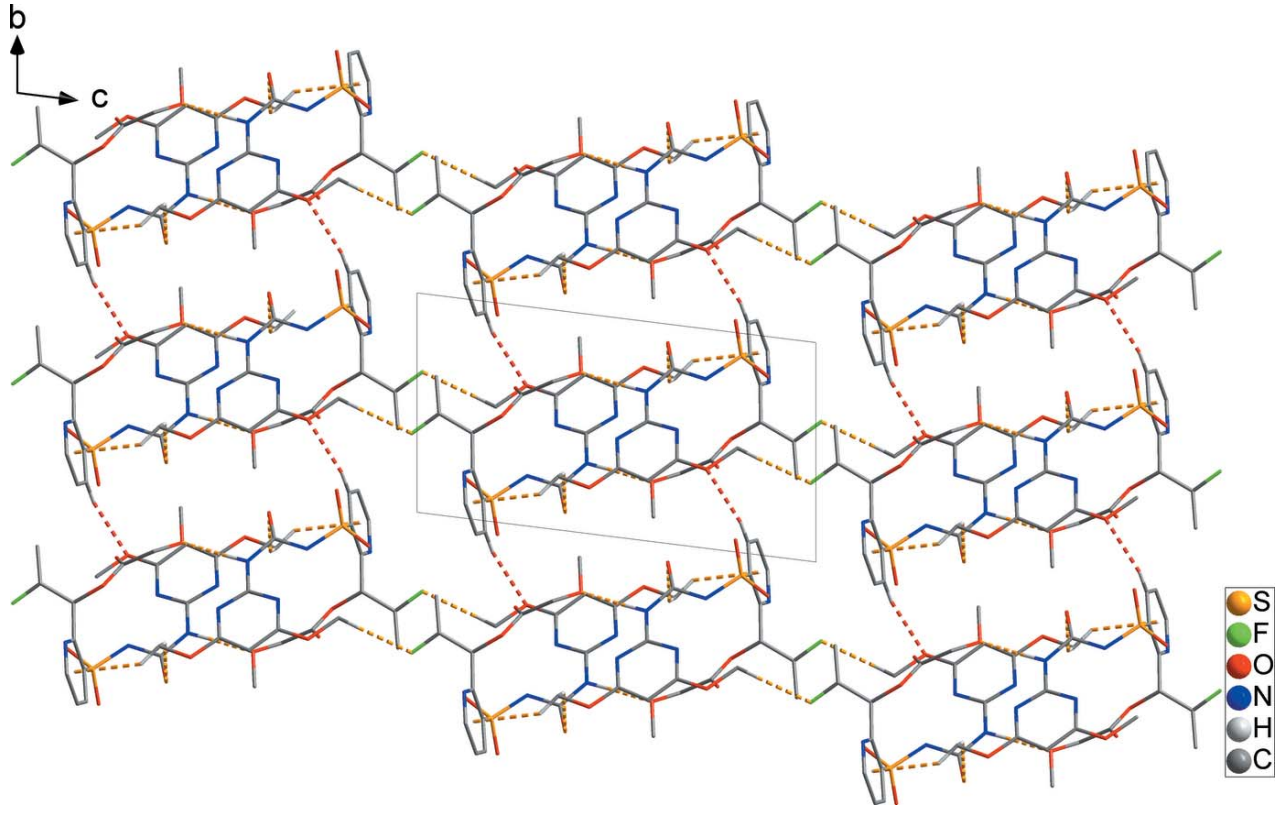


Figure 2
The N/C—H···O hydrogen bond, C—H···F and C—H···π interactions (yellow dashed lines) link adjacent molecules, forming chains along [020]. The chains are further linked by C—H···O hydrogen bonds (red dashed lines), forming a two-dimensional network parallel to (020). H atoms have been omitted for clarity.

tecture with molecules stacked along the *a*-axis direction (black dashed lines in Fig. 3).

4. Database survey

We have reported the crystal structures of several pesticides including compounds with pyrimidinylsulfonylurea, dimethoxypyrimidin and sulfonylurea ring (Kang *et al.*, 2015; Jeon *et al.*, 2015; Kwon *et al.*, 2016). Moreover, a database search (CSD Version 5.27, last update February 2017; Groom *et al.*, 2016) yielded other comparable structures, methyl 2-{[3-(4,6-dimethoxypyrimidin-2-yl)ureido]sulfonylmethyl}benzoate (Xia *et al.*, 2008), 2-amino-4,6-dimethoxypyrimidin-1-ium 2,2-dichloroacetate (Lin *et al.*, 2012), *N*-[(perhydrocyclopenta[*c*]-pyrrol-2-yl)aminocarbonyl]-*o*-toluenesulfonamide (Wu *et al.*, 2012) and 4-{4-[*N*-(5,6-dimethoxypyrimidin-4-yl)sulfamoyl]-phenylcarbamoyl}-2,6-dimethoxyphenyl acetate (Pan *et al.*, 2012).

5. Synthesis and crystallization

The title compound was purchased from Dr Ehrenstorfer GmbH. Colourless single crystals suitable for X-ray diffraction were obtained from a CH_3CN solution by slow evaporation at room temperature.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{18}H_{22}FN_5O_8S$
M_r	487.46
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	173
a, b, c (Å)	8.3993 (3), 9.1030 (3), 15.6862 (5)
α, β, γ (°)	92.116 (2), 101.113 (2), 112.810 (2)
V (Å^3)	1076.53 (6)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.22
Crystal size (mm)	0.36 × 0.06 × 0.05
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2014)
T_{min}, T_{max}	0.702, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10919, 3773, 3081
R_{int}	0.031
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.039, 0.099, 1.06
No. of reflections	3773
No. of parameters	302
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.45, −0.39

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *SHELXS97* and *SHELXTL* (Sheldrick, 2008), *SHELXL2014* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2010) and *publCIF* (Westrip, 2010).

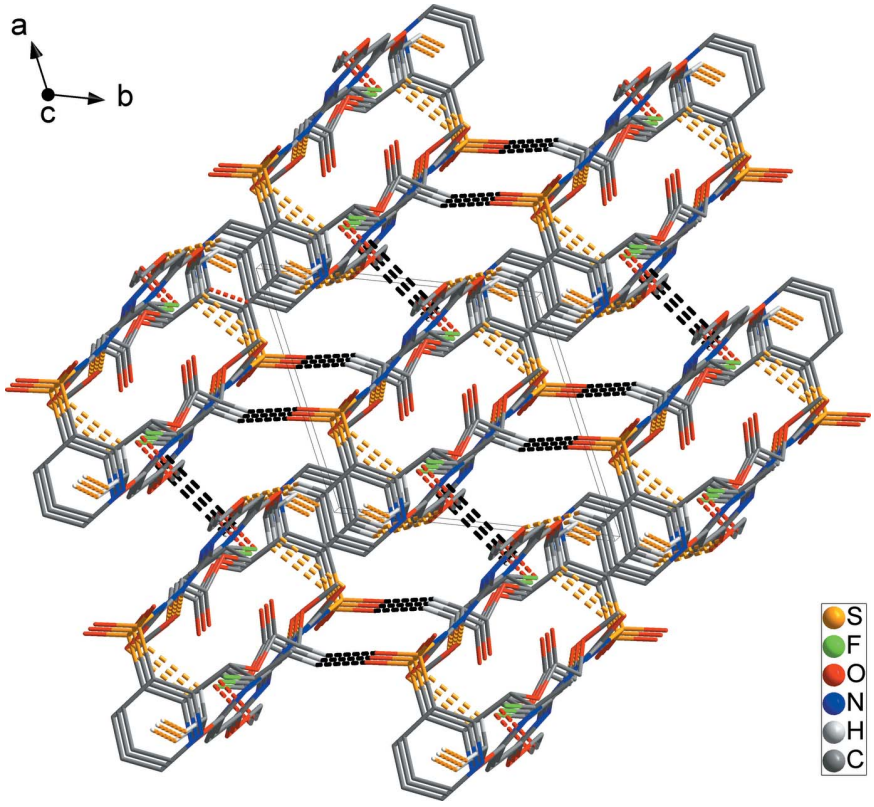


Figure 3
A packing diagram showing the three-dimensional architecture formed by intermolecular C—H···O hydrogen bonds (red dashed lines) and π–π interactions (black dashed lines). H atoms have been omitted for clarity.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. All H atoms were positioned geometrically and refined using a riding model with d(N—H) = 0.88 Å, U_{iso} = 1.2U_{eq}(C) for urea N—H, d(C—H) = 0.95 Å, U_{iso} = 1.2U_{eq}(C) for aromatic C—H, d(C—H) = 0.98 Å, U_{iso} = 1.5U_{eq}(C) for methyl groups, d(C—H) = 0.99 Å, U_{iso} = 1.2U_{eq}(C) for CH_2 group, d(C—H) = 1.00 Å, U_{iso} = 1.5U_{eq}(C) for Csp^3—H.

Funding information

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Computing details

Data collection: *APEX2* (Bruker, 2014); cell refinement: *SAINT* (Bruker, 2014); data reduction: *SAINT* (Bruker, 2014); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008) and *publCIF* (Westrip, 2010).

1-[3-({[(4,6-Dimethoxypyrimidin-2-yl)carbamoyl]amino}sulfonyl)pyridin-2-yl]-2-fluoropropyl 2-methoxyacetate

Crystal data

$C_{18}H_{22}FN_5O_8S$
M_r = 487.46
Triclinic, $P\overline{1}$
a = 8.3993 (3) Å
b = 9.1030 (3) Å
c = 15.6862 (5) Å
α = 92.116 (2)°
β = 101.113 (2)°
γ = 112.810 (2)°
V = 1076.53 (6) Å^3
Z = 2
$F(000)$ = 508
D_x = 1.504 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3325 reflections
θ = 2.5–26.9°
μ = 0.22 mm^{-1}
T = 173 K
Needle, colourless
0.36 × 0.06 × 0.05 mm

Data collection

Bruker APEXII CCD diffractometer
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2014)
T_{min} = 0.702, T_{max} = 0.746
10919 measured reflections
3773 independent reflections
3081 reflections with $I > 2\sigma(I)$
R_{int} = 0.031
θ_{max} = 25.0°, θ_{min} = 1.3°
h = −9→9
k = −10→10
l = −18→18

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.099
S = 1.06
3773 reflections
302 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0439P)^2 + 0.337P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.45 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

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	0.39351 (7)	0.10312 (6)	0.18674 (3)	0.02316 (15)
F1	0.2117 (2)	0.35690 (17)	−0.01327 (8)	0.0529 (4)
O1	1.0327 (2)	0.78934 (17)	0.56837 (9)	0.0345 (4)
O2	0.97933 (18)	0.63951 (17)	0.27393 (9)	0.0268 (3)
O3	0.34138 (19)	0.08587 (18)	0.37121 (9)	0.0309 (4)
O4	0.48165 (18)	0.18107 (17)	0.12133 (9)	0.0278 (4)
O5	0.3822 (2)	−0.05369 (17)	0.20150 (10)	0.0330 (4)
O6	0.26027 (17)	0.48834 (16)	0.21292 (8)	0.0226 (3)
O7	0.55822 (19)	0.62252 (18)	0.24672 (9)	0.0302 (4)
O8	0.53183 (18)	0.72872 (16)	0.41130 (9)	0.0262 (4)
N1	0.8060 (2)	0.5524 (2)	0.49899 (11)	0.0227 (4)
N2	0.7821 (2)	0.4766 (2)	0.34862 (10)	0.0213 (4)
N3	0.5794 (2)	0.3194 (2)	0.42532 (11)	0.0249 (4)
H3N	0.5538	0.3064	0.4771	0.030*
N4	0.4990 (2)	0.2289 (2)	0.27617 (10)	0.0252 (4)
H4N	0.5839	0.3209	0.2718	0.030*
N5	−0.0364 (2)	0.2072 (2)	0.11793 (12)	0.0310 (4)
C1	0.9641 (3)	0.7561 (3)	0.64590 (14)	0.0356 (6)
H1A	0.8389	0.7393	0.6326	0.053*
H1B	1.0313	0.8472	0.6918	0.053*
H1C	0.9752	0.6593	0.6662	0.053*
C2	0.8773 (3)	0.5257 (3)	0.19662 (13)	0.0285 (5)
H2A	0.8717	0.4188	0.2079	0.043*
H2B	0.9342	0.5588	0.1475	0.043*
H2C	0.7571	0.5224	0.1821	0.043*
C3	0.9464 (3)	0.6843 (2)	0.49563 (13)	0.0238 (5)
C4	0.7292 (3)	0.4557 (2)	0.42344 (13)	0.0207 (4)
C5	0.9225 (3)	0.6125 (2)	0.34821 (13)	0.0215 (5)
C6	1.0123 (3)	0.7244 (2)	0.42113 (13)	0.0253 (5)
H6	1.1113	0.8211	0.4205	0.030*
C7	0.4640 (3)	0.2007 (2)	0.35825 (13)	0.0234 (5)
C8	0.1749 (3)	0.0953 (2)	0.16496 (12)	0.0209 (5)
C9	0.1326 (3)	0.2238 (2)	0.13956 (13)	0.0229 (5)
C10	−0.1640 (3)	0.0645 (3)	0.12140 (15)	0.0358 (6)
H10	−0.2836	0.0525	0.1041	0.043*
C11	−0.1331 (3)	−0.0655 (3)	0.14834 (15)	0.0356 (6)
H11	−0.2283	−0.1633	0.1518	0.043*
C12	0.0406 (3)	−0.0500 (3)	0.17037 (14)	0.0303 (5)
H12	0.0674	−0.1376	0.1889	0.036*

C13	0.2671 (3)	0.3930 (2)	0.13829 (12)	0.0219 (5)
H13	0.3884	0.3942	0.1447	0.026*
C14	0.2184 (3)	0.4629 (3)	0.05544 (13)	0.0320 (5)
H14	0.0981	0.4629	0.0509	0.038*
C15	0.3463 (3)	0.6282 (3)	0.04812 (15)	0.0416 (6)
H15A	0.3513	0.7036	0.0959	0.062*
H15B	0.3069	0.6609	−0.0082	0.062*
H15C	0.4642	0.6286	0.0519	0.062*
C16	0.4167 (3)	0.5958 (2)	0.26289 (13)	0.0210 (5)
C17	0.3826 (3)	0.6730 (3)	0.34038 (12)	0.0240 (5)
H17A	0.3527	0.7642	0.3228	0.029*
H17B	0.2799	0.5939	0.3590	0.029*
C18	0.6598 (3)	0.8857 (3)	0.40752 (15)	0.0316 (5)
H18A	0.7041	0.8858	0.3541	0.047*
H18B	0.7587	0.9161	0.4588	0.047*
H18C	0.6045	0.9628	0.4071	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0254 (3)	0.0223 (3)	0.0209 (3)	0.0097 (2)	0.0034 (2)	0.0019 (2)
F1	0.0876 (12)	0.0416 (9)	0.0248 (7)	0.0235 (8)	0.0082 (7)	−0.0018 (6)
O1	0.0420 (10)	0.0256 (9)	0.0233 (8)	0.0007 (7)	0.0076 (7)	−0.0027 (6)
O2	0.0279 (8)	0.0261 (8)	0.0212 (8)	0.0035 (7)	0.0090 (6)	0.0038 (6)
O3	0.0267 (8)	0.0276 (9)	0.0286 (8)	0.0001 (7)	0.0071 (7)	0.0052 (7)
O4	0.0300 (8)	0.0334 (9)	0.0232 (8)	0.0144 (7)	0.0096 (6)	0.0055 (6)
O5	0.0405 (9)	0.0229 (8)	0.0371 (9)	0.0164 (7)	0.0046 (7)	0.0044 (7)
O6	0.0216 (7)	0.0217 (8)	0.0199 (7)	0.0049 (6)	0.0032 (6)	−0.0016 (6)
O7	0.0216 (8)	0.0325 (9)	0.0329 (9)	0.0077 (7)	0.0056 (7)	−0.0022 (7)
O8	0.0252 (8)	0.0225 (8)	0.0203 (7)	0.0007 (6)	0.0004 (6)	0.0015 (6)
N1	0.0227 (9)	0.0216 (9)	0.0217 (9)	0.0069 (8)	0.0043 (7)	0.0032 (7)
N2	0.0211 (9)	0.0224 (9)	0.0186 (9)	0.0070 (8)	0.0040 (7)	0.0049 (7)
N3	0.0247 (9)	0.0261 (10)	0.0169 (9)	0.0028 (8)	0.0044 (7)	0.0040 (7)
N4	0.0259 (10)	0.0240 (10)	0.0191 (9)	0.0034 (8)	0.0038 (7)	0.0039 (7)
N5	0.0226 (10)	0.0291 (11)	0.0374 (11)	0.0090 (9)	0.0027 (8)	−0.0029 (8)
C1	0.0451 (14)	0.0327 (13)	0.0241 (12)	0.0103 (11)	0.0094 (10)	−0.0029 (10)
C2	0.0318 (12)	0.0303 (12)	0.0216 (11)	0.0106 (10)	0.0060 (9)	0.0018 (9)
C3	0.0255 (11)	0.0194 (11)	0.0240 (11)	0.0079 (9)	0.0028 (9)	0.0022 (9)
C4	0.0201 (10)	0.0211 (11)	0.0212 (11)	0.0088 (9)	0.0034 (8)	0.0062 (9)
C5	0.0217 (11)	0.0226 (11)	0.0218 (11)	0.0098 (9)	0.0061 (8)	0.0072 (9)
C6	0.0242 (11)	0.0212 (11)	0.0256 (11)	0.0042 (9)	0.0046 (9)	0.0047 (9)
C7	0.0228 (11)	0.0234 (12)	0.0231 (11)	0.0088 (10)	0.0039 (9)	0.0045 (9)
C8	0.0233 (11)	0.0186 (11)	0.0166 (10)	0.0054 (9)	0.0018 (8)	−0.0006 (8)
C9	0.0230 (11)	0.0237 (11)	0.0178 (10)	0.0059 (9)	0.0030 (8)	−0.0018 (8)
C10	0.0206 (12)	0.0335 (14)	0.0439 (14)	0.0042 (11)	0.0030 (10)	−0.0089 (11)
C11	0.0285 (13)	0.0265 (13)	0.0412 (14)	0.0001 (11)	0.0088 (10)	−0.0034 (11)
C12	0.0348 (13)	0.0212 (12)	0.0303 (12)	0.0062 (10)	0.0077 (10)	0.0018 (9)
C13	0.0267 (11)	0.0214 (11)	0.0187 (10)	0.0104 (9)	0.0063 (8)	0.0004 (8)

C14	0.0467 (14)	0.0288 (13)	0.0205 (11)	0.0157 (11)	0.0065 (10)	0.0016 (9)
C15	0.0630 (18)	0.0304 (14)	0.0261 (13)	0.0128 (12)	0.0096 (12)	0.0091 (10)
C16	0.0221 (11)	0.0171 (10)	0.0213 (11)	0.0061 (9)	0.0024 (9)	0.0063 (8)
C17	0.0206 (11)	0.0246 (11)	0.0199 (11)	0.0028 (9)	0.0026 (8)	0.0019 (9)
C18	0.0281 (12)	0.0224 (12)	0.0343 (13)	0.0002 (10)	0.0058 (10)	0.0007 (10)

Geometric parameters (Å, º)

S1—O5	1.4242 (15)	C1—H1C	0.9800
S1—O4	1.4295 (15)	C2—H2A	0.9800
S1—N4	1.6369 (17)	C2—H2B	0.9800
S1—C8	1.774 (2)	C2—H2C	0.9800
F1—C14	1.397 (2)	C3—C6	1.389 (3)
O1—C3	1.343 (2)	C5—C6	1.379 (3)
O1—C1	1.437 (3)	C6—H6	0.9500
O2—C5	1.338 (2)	C8—C12	1.385 (3)
O2—C2	1.448 (2)	C8—C9	1.398 (3)
O3—C7	1.207 (2)	C9—C13	1.520 (3)
O6—C16	1.359 (2)	C10—C11	1.371 (3)
O6—C13	1.455 (2)	C10—H10	0.9500
O7—C16	1.197 (2)	C11—C12	1.383 (3)
O8—C17	1.412 (2)	C11—H11	0.9500
O8—C18	1.429 (2)	C12—H12	0.9500
N1—C3	1.329 (3)	C13—C14	1.522 (3)
N1—C4	1.336 (2)	C13—H13	1.0000
N2—C4	1.328 (2)	C14—C15	1.497 (3)
N2—C5	1.339 (2)	C14—H14	1.0000
N3—C7	1.388 (3)	C15—H15A	0.9800
N3—C4	1.389 (2)	C15—H15B	0.9800
N3—H3N	0.8800	C15—H15C	0.9800
N4—C7	1.386 (3)	C16—C17	1.510 (3)
N4—H4N	0.8800	C17—H17A	0.9900
N5—C10	1.337 (3)	C17—H17B	0.9900
N5—C9	1.341 (3)	C18—H18A	0.9800
C1—H1A	0.9800	C18—H18B	0.9800
C1—H1B	0.9800	C18—H18C	0.9800

O5—S1—O4	119.31 (9)	C12—C8—S1	116.68 (16)
O5—S1—N4	110.36 (9)	C9—C8—S1	123.71 (15)
O4—S1—N4	103.89 (9)	N5—C9—C8	121.03 (18)
O5—S1—C8	107.60 (9)	N5—C9—C13	113.94 (18)
O4—S1—C8	109.39 (9)	C8—C9—C13	124.95 (18)
N4—S1—C8	105.49 (9)	N5—C10—C11	124.2 (2)
C3—O1—C1	117.99 (17)	N5—C10—H10	117.9
C5—O2—C2	117.95 (16)	C11—C10—H10	117.9
C16—O6—C13	117.59 (15)	C10—C11—C12	118.0 (2)
C17—O8—C18	114.20 (16)	C10—C11—H11	121.0
C3—N1—C4	114.61 (17)	C12—C11—H11	121.0

C4—N2—C5	116.32 (17)	C11—C12—C8	118.9 (2)
C7—N3—C4	130.02 (17)	C11—C12—H12	120.5
C7—N3—H3N	115.0	C8—C12—H12	120.5
C4—N3—H3N	115.0	O6—C13—C9	105.26 (15)
C7—N4—S1	124.61 (15)	O6—C13—C14	108.51 (16)
C7—N4—H4N	117.7	C9—C13—C14	111.96 (17)
S1—N4—H4N	117.7	O6—C13—H13	110.3
C10—N5—C9	118.31 (19)	C9—C13—H13	110.3
O1—C1—H1A	109.5	C14—C13—H13	110.3
O1—C1—H1B	109.5	F1—C14—C15	108.89 (18)
H1A—C1—H1B	109.5	F1—C14—C13	105.03 (17)
O1—C1—H1C	109.5	C15—C14—C13	115.37 (19)
H1A—C1—H1C	109.5	F1—C14—H14	109.1
H1B—C1—H1C	109.5	C15—C14—H14	109.1
O2—C2—H2A	109.5	C13—C14—H14	109.1
O2—C2—H2B	109.5	C14—C15—H15A	109.5
H2A—C2—H2B	109.5	C14—C15—H15B	109.5
O2—C2—H2C	109.5	H15A—C15—H15B	109.5
H2A—C2—H2C	109.5	C14—C15—H15C	109.5
H2B—C2—H2C	109.5	H15A—C15—H15C	109.5
N1—C3—O1	119.08 (18)	H15B—C15—H15C	109.5
N1—C3—C6	124.73 (19)	O7—C16—O6	124.13 (18)
O1—C3—C6	116.20 (18)	O7—C16—C17	126.38 (18)
N2—C4—N1	126.77 (18)	O6—C16—C17	109.49 (17)
N2—C4—N3	117.95 (17)	O8—C17—C16	111.44 (17)
N1—C4—N3	115.28 (17)	O8—C17—H17A	109.3
O2—C5—N2	118.40 (17)	C16—C17—H17A	109.3
O2—C5—C6	118.68 (18)	O8—C17—H17B	109.3
N2—C5—C6	122.91 (18)	C16—C17—H17B	109.3
C5—C6—C3	114.59 (19)	H17A—C17—H17B	108.0
C5—C6—H6	122.7	O8—C18—H18A	109.5
C3—C6—H6	122.7	O8—C18—H18B	109.5
O3—C7—N4	123.77 (18)	H18A—C18—H18B	109.5
O3—C7—N3	121.97 (18)	O8—C18—H18C	109.5
N4—C7—N3	114.23 (18)	H18A—C18—H18C	109.5
C12—C8—C9	119.55 (19)	H18B—C18—H18C	109.5

O5—S1—N4—C7	−48.10 (19)	O4—S1—C8—C9	−42.99 (19)
O4—S1—N4—C7	−177.12 (16)	N4—S1—C8—C9	68.21 (18)
C8—S1—N4—C7	67.84 (19)	C10—N5—C9—C8	0.1 (3)
C4—N1—C3—O1	179.93 (18)	C10—N5—C9—C13	−176.75 (18)
C4—N1—C3—C6	0.4 (3)	C12—C8—C9—N5	−1.9 (3)
C1—O1—C3—N1	−2.3 (3)	S1—C8—C9—N5	175.19 (15)
C1—O1—C3—C6	177.23 (18)	C12—C8—C9—C13	174.60 (19)
C5—N2—C4—N1	−3.1 (3)	S1—C8—C9—C13	−8.3 (3)
C5—N2—C4—N3	177.34 (17)	C9—N5—C10—C11	2.1 (3)
C3—N1—C4—N2	2.1 (3)	N5—C10—C11—C12	−2.4 (3)
C3—N1—C4—N3	−178.32 (17)	C10—C11—C12—C8	0.5 (3)

C7—N3—C4—N2	−4.5 (3)	C9—C8—C12—C11	1.6 (3)
C7—N3—C4—N1	175.92 (19)	S1—C8—C12—C11	−175.75 (16)
C2—O2—C5—N2	4.5 (3)	C16—O6—C13—C9	137.43 (16)
C2—O2—C5—C6	−176.37 (17)	C16—O6—C13—C14	−102.57 (19)
C4—N2—C5—O2	−179.30 (17)	N5—C9—C13—O6	70.7 (2)
C4—N2—C5—C6	1.6 (3)	C8—C9—C13—O6	−106.1 (2)
O2—C5—C6—C3	−178.55 (17)	N5—C9—C13—C14	−47.0 (2)
N2—C5—C6—C3	0.6 (3)	C8—C9—C13—C14	136.2 (2)
N1—C3—C6—C5	−1.6 (3)	O6—C13—C14—F1	−174.62 (16)
O1—C3—C6—C5	178.85 (17)	C9—C13—C14—F1	−58.9 (2)
S1—N4—C7—O3	−6.7 (3)	O6—C13—C14—C15	65.5 (2)
S1—N4—C7—N3	175.33 (14)	C9—C13—C14—C15	−178.77 (19)
C4—N3—C7—O3	177.7 (2)	C13—O6—C16—O7	4.0 (3)
C4—N3—C7—N4	−4.4 (3)	C13—O6—C16—C17	−175.72 (16)
O5—S1—C8—C12	3.21 (18)	C18—O8—C17—C16	85.3 (2)
O4—S1—C8—C12	134.21 (16)	O7—C16—C17—O8	−25.1 (3)
N4—S1—C8—C12	−114.60 (16)	O6—C16—C17—O8	154.58 (15)
O5—S1—C8—C9	−173.98 (16)		

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the N5/C8–C12 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*N*···O8^{i}	0.88	2.01	2.885 (2)	174
C1—H1*A*···O3^{i}	0.98	2.58	3.368 (3)	137
C2—H2*B*···F1^{ii}	0.98	2.53	3.161 (2)	122
C12—H12···O2^{iii}	0.95	2.42	3.229 (3)	143
C17—H17*A*···O5^{iv}	0.99	2.55	3.367 (3)	139
C1—H1*B*···*Cg*1^{i}	0.98	2.74	3.488 (2)	134

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