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1,3-Dimethoxy-2-methylimidazolium bis(trifluoromethanesulfonyl)imide

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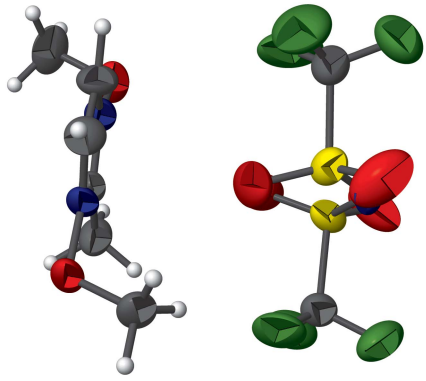
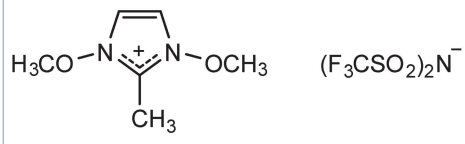
Structural data: full structural data are available from iucrdata.iucr.org

The title molecular salt, $C_6H_{11}N_2O_2^+\cdot C_2F_6NO_4S_2^-$, was obtained by the methylation of 1-hydroxy-2-methylimidazole 3-oxide and subsequent ion metathesis. In the crystal, C—H···O=S hydrogen bonds and O···π interactions are observed.

3D view



Chemical scheme



Structure description

The molecular structure of the title compound is shown in Fig. 1. The ions which build this salt, both 1,3-dialkyloxyimidazolium cations (Laus *et al.*, 2010) and the bis(triflimide) anion (Bentivoglio *et al.*, 2009; Laus *et al.*, 2011), are known to exist as *syn*/*anti* conformers in the solid state. Thus, the methoxy substituents of the cation adopt an *anti* conformation with a C5—O1···O2—C6 torsion angle of 170.6 (4)°. The bis(triflimide) anion also assumes an *anti* conformation with a C7—S1···S2—C8 torsion angle of 174.9 (2)°. Each cation donates three C—H···O=S hydrogen bonds to three anions (Fig. 2). The hydrogen-bond parameters are summarized in Table 1. An intriguing intermolecular interaction between atom O3 of the anion and the π system of the imidazolium ring is observed. The pertinent O3···*Cg* distance is 2.971 Å, where *Cg* is the centroid of the heterocyclic ring. This interaction is directional with an S1=O3···*Cg* angle of 152°. The crystal packing is shown in Fig. 3.

The cation in the structure of the related 1,3-dimethoxy-2-methylimidazolium tris(pentafluoroethyl)trifluorophosphate displayed a *syn* geometry (Laus *et al.*, 2007). Anion···π interactions have been observed in related imidazolium salts (Froschauer *et al.*, 2012).

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

D—H···A	D—H	H···A	D···A	D—H···A
C3—H3···O4^{i}	0.95	2.40	3.253 (6)	150
C2—H2···O6^{ii}	0.95	2.27	3.155 (5)	156
C5—H5A···O5^{iii}	0.98	2.44	3.276 (5)	143

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

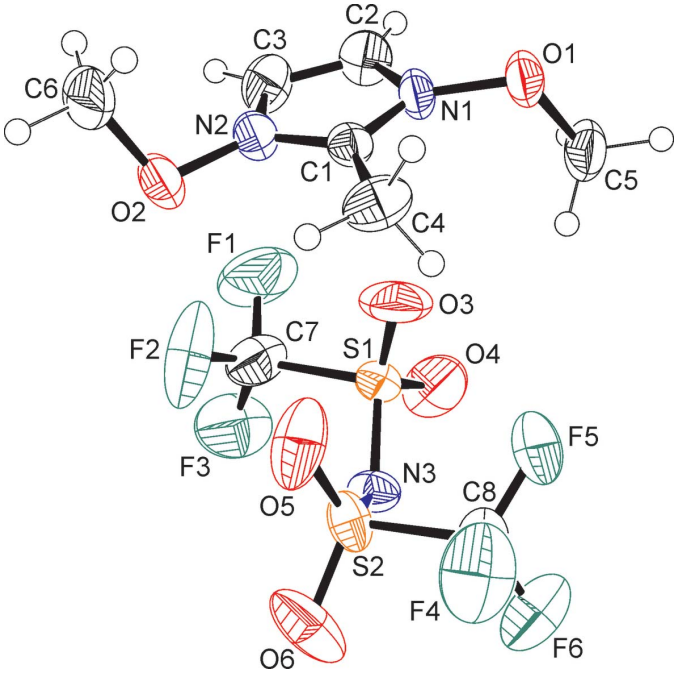


Figure 1
The asymmetric unit of the title compound, showing the atom labels and 50% probability displacement ellipsoids for non-H atoms.

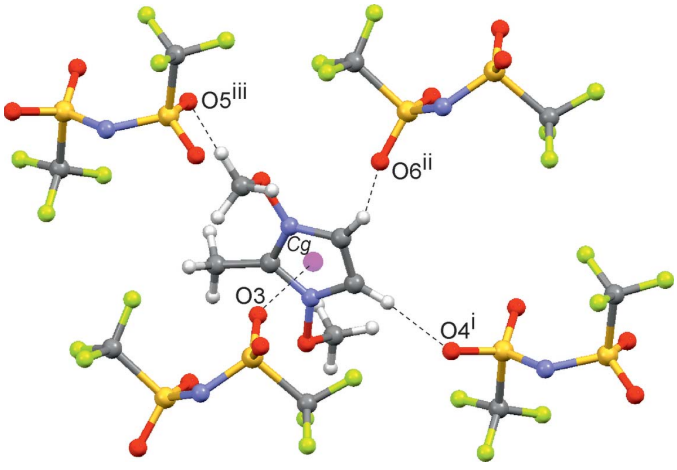


Figure 2
The O3···π interaction and C—H···O═S hydrogen bonds are shown as dashed lines (see Table 1). The centroid of the imidazole ring is drawn as red sphere.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_6H_{11}N_2O_2^+\cdot C_2F_6NO_4S_2^-$
M_r	423.32
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	183
a, *b*, *c* (Å)	12.4858 (6), 14.0212 (6), 9.8480 (4)
β (°)	98.179 (1)
V (Å^3)	1706.51 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.40
Crystal size (mm)	0.18 × 0.16 × 0.12
Data collection	
Diffractometer	Bruker D8 QUEST PHOTON 100
Absorption correction	Multi-scan (*SADABS*; Bruker, 2012)
T_{min}, T_{max}	0.851, 0.914
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	24313, 3088, 3020
R_{int}	0.027
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.600
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.033, 0.092, 1.05
No. of reflections	3088
No. of parameters	228
No. of restraints	2
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.23
Absolute structure	Flack x determined using 1476 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.493 (15)

Computer programs: *APEX2* and *SAINT* (Bruker, 2012), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *Mercury* (Macrae *et al.*, 2006).

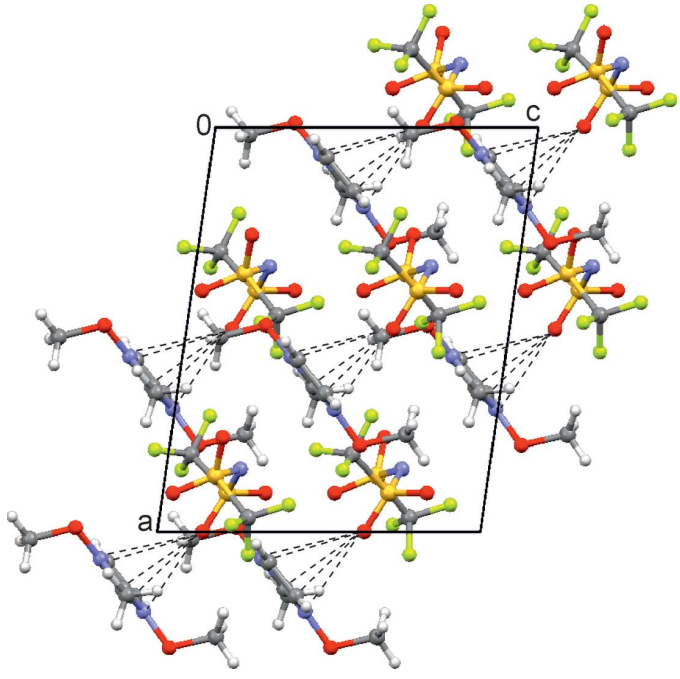


Figure 3
The crystal packing of the title compound viewed along the *b* axis showing the O3···π interactions.

Synthesis and crystallization

A suspension of 1-hydroxy-2-methylimidazole-3-oxide (5.09 g, 44.6 mmol) and dimethyl sulfate (9.0 ml, 100 mmol) in H_2O (5.0 ml) was stirred at room temperature for 30 min. Calcium carbonate (6.35 g, 63.4 mmol) and H_2O (6.0 ml) were then added to the slurry, and a slight increase of temperature was observed. The mixture was stirred for 15 h. Then hydrochloric acid (36%; 11.0 ml, 129.2 mmol) was added in portions and stirred for 2 h, resulting in a clear solution. Lithium bis(trifluoromethanesulfonyl)imide (13.0 g, 44.9 mmol) was added, whereupon crystallization of the product occurred. After stirring for 1 h, the mixture was extracted with CH_2Cl_2 (3 × 50 ml). The combined organic phases were then washed with H_2O (100 ml) and dried over Na_2SO_4. The solvent was removed under reduced pressure, and the product was dried at 75°C in vacuum (< 1 mbar). On cooling to room temperature the product was obtained as a colourless crystalline solid (yield 97%), mp. 66°C.

^{1}H NMR (300 MHz, CD_2Cl_2): δ 2.73 (*s*, 3H), 4.26 (*s*, 6H), 7.53 (*s*, 2H) p.p.m. ^{13}C NMR (75 MHz, CD_2Cl_2): δ 8.0, 69.7, 116.3, 120.4 (*q*, J = 321.1 Hz), 139.1 p.p.m. IR: ν 3142, 1594, 1459, 1333, 1183, 1136, 1111, 1048, 958, 938, 791, 762, 740, 728, 713, 647, 611, 567, 512, 407 cm^{-1}.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was found to be a racemic twin.

Acknowledgements

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References

Bentivoglio, G., Schwärzler, A., Wurst, K., Kahlenberg, V., Nauer, G., Bonn, G., Schottenberger, H. & Laus, G. (2009). *J. Chem. Crystallogr.* **39**, 662–668.
Bruker (2012). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Froschauer, C., Kahlenberg, V., Laus, G. & Schottenberger, H. (2012). *Crystals*, **2**, 1017–1033.
Laus, G., Hummel, M., Többens, D. M., Gelbrich, T., Kahlenberg, V., Wurst, K., Griesser, U. J. & Schottenberger, H. (2011). *CrystEngComm*, **13**, 5439–5446.
Laus, G., Schwärzler, A., Schuster, P., Bentivoglio, G., Hummel, M., Wurst, K., Kahlenberg, V., Lörting, T., Schütz, J., Peringer, P., Bonn, G., Nauer, G. & Schottenberger, H. (2007). *Z. Naturforsch. Teil B*, **62**, 295–308.
Laus, G., Wurst, K., Kahlenberg, V., Kopacka, H., Kreutz, C. & Schottenberger, H. (2010). *Z. Naturforsch. Teil B*, **65**, 776–782.
Macrae, C. F., Edgington, P. R., McCabe, P., Pidcock, E., Shields, G. P., Taylor, R., Towler, M. & van de Streek, J. (2006). *J. Appl. Cryst.* **39**, 453–457.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.

full crystallographic data

IUCrData (2016). **1**, x160824 [doi:10.1107/S2414314616008245]

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Crystal data

$C_6H_{11}N_2O_2^+ \cdot C_2F_6NO_4S_2^-$
M_r = 423.32
Monoclinic, *Cc*
a = 12.4858 (6) Å
b = 14.0212 (6) Å
c = 9.8480 (4) Å
β = 98.179 (1)°
V = 1706.51 (13) Å^3
Z = 4
F(000) = 856
D_x = 1.648 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 9895 reflections
θ = 2.8–25.2°
μ = 0.40 mm^{-1}
T = 183 K
Prism, colourless
0.18 × 0.16 × 0.12 mm

Data collection

Bruker D8 QUEST PHOTON 100 diffractometer
Radiation source: Incoatec Microfocus
Multi layered optics monochromator
Detector resolution: 10.4 pixels mm^{-1}
φ and *ω* scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2012)
T_{min} = 0.851, T_{max} = 0.914
24313 measured reflections
3088 independent reflections
3020 reflections with $I > 2\sigma(I)$
R_{int} = 0.027
θ_{max} = 25.3°, θ_{min} = 2.2°
h = −14→14
k = −16→16
l = −11→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.092
S = 1.05
3088 reflections
228 parameters
2 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0576P)^2 + 1.0708P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015b), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0046 (10)
Absolute structure: Flack *x* determined using 1476 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.493 (15)

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	0.40336 (7)	0.15962 (7)	0.69953 (9)	0.0461 (3)
S2	0.36096 (7)	0.35188 (7)	0.65521 (8)	0.0441 (3)
O1	0.7855 (2)	0.1723 (3)	0.5887 (3)	0.0505 (7)
O2	0.4893 (2)	0.2163 (3)	0.2448 (3)	0.0572 (8)
O3	0.4986 (3)	0.1675 (3)	0.6408 (5)	0.0886 (14)
O4	0.4032 (4)	0.0997 (3)	0.8175 (4)	0.0898 (14)
O5	0.4036 (4)	0.3477 (3)	0.5317 (3)	0.0791 (12)
O6	0.2665 (3)	0.4073 (2)	0.6611 (5)	0.0843 (14)
N1	0.6963 (2)	0.1528 (2)	0.4931 (3)	0.0372 (7)
N2	0.5662 (3)	0.1719 (2)	0.3361 (3)	0.0402 (7)
N3	0.3443 (3)	0.2542 (2)	0.7295 (3)	0.0412 (7)
C1	0.6403 (3)	0.2208 (2)	0.4199 (4)	0.0325 (6)
C2	0.6576 (3)	0.0640 (3)	0.4565 (4)	0.0471 (9)
H2	0.6848	0.0050	0.4944	0.057*
C3	0.5749 (4)	0.0760 (3)	0.3579 (5)	0.0507 (10)
H3	0.5305	0.0276	0.3117	0.061*
C4	0.6552 (4)	0.3241 (3)	0.4334 (5)	0.0528 (11)
H4A	0.6018	0.3566	0.3665	0.079*
H4B	0.7283	0.3410	0.4164	0.079*
H4C	0.6455	0.3439	0.5263	0.079*
C5	0.7590 (4)	0.1618 (4)	0.7272 (4)	0.0552 (11)
H5A	0.8231	0.1759	0.7938	0.083*
H5B	0.7007	0.2062	0.7406	0.083*
H5C	0.7353	0.0963	0.7405	0.083*
C6	0.5176 (4)	0.2109 (5)	0.1079 (5)	0.0747 (16)
H6A	0.4620	0.2429	0.0436	0.112*
H6B	0.5875	0.2422	0.1059	0.112*
H6C	0.5227	0.1438	0.0814	0.112*
C7	0.3078 (4)	0.1002 (4)	0.5699 (6)	0.0638 (13)
C8	0.4643 (4)	0.4126 (4)	0.7738 (5)	0.0544 (11)
F1	0.3469 (4)	0.0141 (3)	0.5471 (5)	0.1128 (14)
F2	0.2968 (4)	0.1460 (3)	0.4556 (4)	0.1203 (18)
F3	0.2132 (3)	0.0869 (3)	0.6113 (5)	0.1010 (13)
F4	0.4827 (3)	0.4974 (3)	0.7259 (4)	0.0969 (12)
F5	0.5554 (3)	0.3634 (3)	0.7906 (4)	0.0971 (13)
F6	0.4327 (3)	0.4239 (3)	0.8947 (3)	0.0912 (11)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0445 (5)	0.0482 (5)	0.0443 (5)	0.0172 (4)	0.0020 (4)	−0.0033 (4)
S2	0.0394 (5)	0.0472 (5)	0.0427 (5)	−0.0042 (4)	−0.0043 (4)	0.0151 (4)
O1	0.0275 (11)	0.090 (2)	0.0318 (13)	−0.0063 (13)	−0.0019 (10)	−0.0038 (13)
O2	0.0353 (14)	0.094 (2)	0.0408 (15)	0.0187 (15)	−0.0008 (11)	0.0098 (15)
O3	0.0445 (18)	0.108 (3)	0.119 (3)	0.0090 (18)	0.029 (2)	−0.051 (3)
O4	0.146 (4)	0.058 (2)	0.061 (2)	0.042 (2)	−0.002 (2)	0.0087 (17)
O5	0.096 (3)	0.104 (3)	0.0363 (16)	−0.043 (2)	0.0043 (17)	0.0150 (17)
O6	0.0490 (18)	0.0506 (18)	0.147 (4)	0.0084 (15)	−0.009 (2)	0.029 (2)
N1	0.0255 (14)	0.055 (2)	0.0291 (15)	−0.0026 (13)	−0.0033 (11)	0.0006 (12)
N2	0.0335 (15)	0.0503 (17)	0.0360 (16)	0.0028 (13)	0.0020 (13)	0.0020 (13)
N3	0.0450 (16)	0.0408 (16)	0.0409 (15)	0.0099 (13)	0.0163 (13)	0.0079 (13)
C1	0.0285 (14)	0.0385 (15)	0.0316 (14)	−0.0005 (13)	0.0079 (11)	0.0022 (14)
C2	0.055 (2)	0.0349 (18)	0.050 (2)	0.0008 (16)	0.0041 (17)	0.0046 (16)
C3	0.055 (2)	0.046 (2)	0.050 (2)	−0.0146 (18)	0.0018 (18)	−0.0099 (17)
C4	0.066 (3)	0.041 (2)	0.056 (2)	−0.0060 (18)	0.024 (2)	−0.005 (2)
C5	0.047 (2)	0.086 (3)	0.0307 (18)	−0.007 (2)	−0.0031 (16)	−0.0013 (18)
C6	0.062 (3)	0.126 (5)	0.036 (2)	0.030 (3)	0.0037 (19)	0.018 (3)
C7	0.065 (3)	0.062 (3)	0.068 (3)	−0.010 (2)	0.022 (2)	−0.019 (2)
C8	0.051 (3)	0.065 (3)	0.046 (2)	−0.006 (2)	0.0017 (19)	−0.0008 (19)
F1	0.122 (3)	0.084 (2)	0.136 (3)	−0.003 (2)	0.027 (3)	−0.062 (3)
F2	0.148 (4)	0.148 (4)	0.0521 (19)	−0.063 (3)	−0.030 (2)	0.006 (2)
F3	0.070 (2)	0.097 (3)	0.141 (4)	−0.0255 (19)	0.031 (2)	−0.030 (2)
F4	0.108 (3)	0.079 (2)	0.100 (3)	−0.047 (2)	0.002 (2)	0.0081 (19)
F5	0.0476 (17)	0.131 (3)	0.102 (3)	0.0050 (18)	−0.0268 (16)	−0.040 (2)
F6	0.122 (3)	0.094 (2)	0.0588 (17)	−0.018 (2)	0.0192 (18)	−0.0246 (16)

Geometric parameters (Å, º)

S1—O3	1.399 (4)	C2—H2	0.9500
S1—O4	1.434 (4)	C3—H3	0.9500
S1—N3	1.565 (3)	C4—H4A	0.9800
S1—C7	1.820 (5)	C4—H4B	0.9800
S2—O5	1.397 (4)	C4—H4C	0.9800
S2—O6	1.421 (4)	C5—H5A	0.9800
S2—N3	1.581 (3)	C5—H5B	0.9800
S2—C8	1.823 (5)	C5—H5C	0.9800
O1—N1	1.379 (4)	C6—H6A	0.9800
O1—C5	1.456 (5)	C6—H6B	0.9800
O2—N2	1.368 (4)	C6—H6C	0.9800
O2—C6	1.444 (5)	C7—F2	1.286 (7)
N1—C1	1.332 (5)	C7—F3	1.316 (6)
N1—C2	1.366 (5)	C7—F1	1.334 (7)
N2—C1	1.337 (5)	C8—F4	1.312 (6)
N2—C3	1.363 (5)	C8—F6	1.315 (6)
C1—C4	1.465 (5)	C8—F5	1.320 (6)

C2—C3	1.324 (6)		
O3—S1—O4	118.7 (3)	C1—C4—H4A	109.5
O3—S1—N3	117.5 (2)	C1—C4—H4B	109.5
O4—S1—N3	106.7 (2)	H4A—C4—H4B	109.5
O3—S1—C7	104.9 (2)	C1—C4—H4C	109.5
O4—S1—C7	102.9 (3)	H4A—C4—H4C	109.5
N3—S1—C7	103.9 (2)	H4B—C4—H4C	109.5
O5—S2—O6	118.7 (3)	O1—C5—H5A	109.5
O5—S2—N3	117.3 (2)	O1—C5—H5B	109.5
O6—S2—N3	106.9 (2)	H5A—C5—H5B	109.5
O5—S2—C8	104.8 (2)	O1—C5—H5C	109.5
O6—S2—C8	103.6 (2)	H5A—C5—H5C	109.5
N3—S2—C8	103.7 (2)	H5B—C5—H5C	109.5
N1—O1—C5	110.5 (3)	O2—C6—H6A	109.5
N2—O2—C6	110.3 (3)	O2—C6—H6B	109.5
C1—N1—C2	111.7 (3)	H6A—C6—H6B	109.5
C1—N1—O1	122.6 (3)	O2—C6—H6C	109.5
C2—N1—O1	125.6 (3)	H6A—C6—H6C	109.5
C1—N2—C3	112.0 (3)	H6B—C6—H6C	109.5
C1—N2—O2	122.1 (3)	F2—C7—F3	110.6 (6)
C3—N2—O2	125.8 (4)	F2—C7—F1	107.5 (5)
S1—N3—S2	123.39 (19)	F3—C7—F1	106.8 (5)
N1—C1—N2	103.4 (3)	F2—C7—S1	111.3 (4)
N1—C1—C4	127.5 (4)	F3—C7—S1	112.1 (4)
N2—C1—C4	129.1 (4)	F1—C7—S1	108.3 (4)
C3—C2—N1	106.7 (4)	F4—C8—F6	107.9 (4)
C3—C2—H2	126.6	F4—C8—F5	109.1 (5)
N1—C2—H2	126.6	F6—C8—F5	108.3 (4)
C2—C3—N2	106.1 (4)	F4—C8—S2	109.7 (3)
C2—C3—H3	126.9	F6—C8—S2	111.1 (3)
N2—C3—H3	126.9	F5—C8—S2	110.8 (3)
C5—O1—N1—C1	106.1 (4)	C1—N2—C3—C2	−1.0 (5)
C5—O1—N1—C2	−77.2 (5)	O2—N2—C3—C2	−178.3 (3)
C6—O2—N2—C1	103.0 (5)	O3—S1—C7—F2	−56.0 (5)
C6—O2—N2—C3	−80.0 (5)	O4—S1—C7—F2	179.1 (5)
O3—S1—N3—S2	21.3 (4)	N3—S1—C7—F2	68.0 (5)
O4—S1—N3—S2	157.7 (3)	O3—S1—C7—F3	179.5 (4)
C7—S1—N3—S2	−94.0 (3)	O4—S1—C7—F3	54.6 (5)
O5—S2—N3—S1	19.4 (4)	N3—S1—C7—F3	−56.5 (5)
O6—S2—N3—S1	155.5 (3)	O3—S1—C7—F1	61.9 (5)
C8—S2—N3—S1	−95.4 (3)	O4—S1—C7—F1	−62.9 (4)
C2—N1—C1—N2	−0.4 (4)	N3—S1—C7—F1	−174.1 (4)
O1—N1—C1—N2	176.7 (3)	O5—S2—C8—F4	59.0 (4)
C2—N1—C1—C4	177.5 (4)	O6—S2—C8—F4	−66.1 (4)
O1—N1—C1—C4	−5.4 (6)	N3—S2—C8—F4	−177.5 (3)
C3—N2—C1—N1	0.8 (4)	O5—S2—C8—F6	178.2 (4)

O2—N2—C1—N1	178.2 (3)	O6—S2—C8—F6	53.1 (4)
C3—N2—C1—C4	−177.0 (4)	N3—S2—C8—F6	−58.4 (4)
O2—N2—C1—C4	0.4 (6)	O5—S2—C8—F5	−61.5 (4)
C1—N1—C2—C3	−0.2 (5)	O6—S2—C8—F5	173.5 (4)
O1—N1—C2—C3	−177.1 (3)	N3—S2—C8—F5	62.0 (4)
N1—C2—C3—N2	0.7 (5)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···O4^{i}	0.95	2.40	3.253 (6)	150
C2—H2···O6^{ii}	0.95	2.27	3.155 (5)	156
C5—H5*A*···O5^{iii}	0.98	2.44	3.276 (5)	143

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