Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)-ethyl methanesulfonate

Sammer Yousuf,* Aurang Zeb, Farhana Batool and Fatima Z. Basha‡

H.E.J. Research Institute of Chemistry, International Center for Chemical and Biological Sciences, University of Karachi, Karachi 75270, Pakistan
Correspondence e-mail: dr.sammer.yousuf@gmail.com

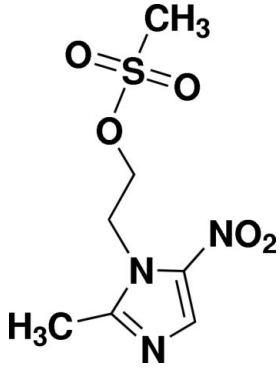
Received 6 August 2012; accepted 8 August 2012

Key indicators: single-crystal X-ray study; T = 273 K; mean σ(C–C) = 0.005 Å; R factor = 0.056; wR factor = 0.152; data-to-parameter ratio = 13.5.

The asymmetric unit of the title compound, $C_7H_{11}N_3O_5S$, contains two independent molecules with virtually identical conformations. The imidazole rings of both molecules are essentially planar (r.m.s. deviations = 0.0019 and 0.0038 Å), with a dihedral angle 9.25 (19)° between them. The nitro groups are oriented at 4.5 (2) and 6.44 (13)° with respect to the imidazole rings. In the crystal, molecules are linked to form a three-dimensional framework by C—H···O and C—H···N hydrogen bonds.

Related literature

For the biological activity of metronidazole, see: Zeb, Malik *et al.* (2012). For related structures, see: Yousuf *et al.* (2012); Zeb, Yousuf *et al.* (2012).



Experimental

Crystal data

$C_7H_{11}N_3O_5S$ M_r = 249.26
Triclinic, $P\overline{1}$
a = 8.8547 (17) Å
b = 10.927 (2) Å
c = 12.033 (2) Å
α = 112.702 (4)°
β = 100.614 (4)°
γ = 90.052 (4)°
V = 1052.4 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.32 mm^{-1}
T = 273 K
0.40 × 0.21 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
T_{min} = 0.883, T_{max} = 0.975
11649 measured reflections
3918 independent reflections
3078 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.152
S = 1.07
3918 reflections
291 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.79 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C5—H5B···O6^{i}	0.97	2.50	3.235 (4)	133
C5—H5C···N7^{ii}	0.97	2.54	3.484 (4)	165
C7—H7B···O9^{iii}	0.96	2.59	3.498 (4)	157
C7—H7C···O10^{iv}	0.96	2.52	3.423 (4)	157
C12—H12A···O1^{v}	0.97	2.50	3.250 (5)	134
C12—H12B···N3^{vi}	0.97	2.53	3.472 (4)	164
C14—H14B···O5^{vii}	0.96	2.59	3.507 (4)	160
C14—H14C···O4^{viii}	0.96	2.55	3.414 (4)	150

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: PV2579).

References

Bruker (2000). *SADABS*, *SMART* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Nardelli, M. (1995). *J. Appl. Cryst.* **28**, 659.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Yousuf, S., Zeb, A. & Basha, F. Z. (2012). *Acta Cryst.* E**68**, o952.
Zeb, A., Malik, I., Rasheed, S., Choudhary, M. I. & Basha, F. Z. (2012). *Med. Chem.* **8**, 846–852.
Zeb, A., Yousuf, S. & Basha, F. Z. (2012). *Acta Cryst.* E**68**, o1218.

‡ Additional correspondence author, e-mail: bashafz@gmail.com.

supporting information

Acta Cryst. (2012). E**68**, o2781 [doi:10.1107/S1600536812034964]

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl methanesulfonate

Sammer Yousuf, Aurang Zeb, Farhana Batool and Fatima Z. Basha

S1. Comment

Metronidazole (Flagyl) is a well known broad spectrum antibiotic. The structural analogues of metronidazole are reported to have a wide range of biological activities including antibacterial anticancer, antiglycation and *H. pylori* urease inhibitors (Zeb, Malik *et al.*, 2012). The title compound is a methanesulfonate derivative of metronidazole, synthesized as a part of our ongoing reaserch to synthesize and evaluate the antiglycation potential and establish structure activity relationship of the structural analogues of metronidazole.

The title compound contains two independent molecules in an asymmetric unit (Fig. 1) with identical conformations. The two imidazole rings (C2—C4/N2/N3 and C9—C11/N5/N7) are individually planar with r.m.s.d's 0.0038 and 0.0019 Å, respectively; the dihedral angle between the mean planes of the imidazole rings is 9.25 (19)°. The nitro groups N1/O1/O2 and N4/O6/O7 are oriented at 4.5 (2) and 6.44 (13)° with respect to the imidazole rings (C2—C4/N2/N3) and (C9—C11/N5/N7), respectively. The bond distances and angles in both molecules of the title compound agree very well with the corresponding bond distances and angles reported in closely related compounds (Yousuf *et al.*, 2012; Zeb *et al.*, 2012). The crystal packing (Fig. 2) is consolidated by weak intermolecular C—H···O and C—H···N type hydrogen bonds (Table 1).

S2. Experimental

The title compound was synthesized by adding methane sulfonyl chloride (16 mmol) drop wise into an ice-cooled solution of metronidazole (10 mmol) and triethylamine (16 mmol) in dry dichloromethane (DCM) with continuous stirring. The reaction mixture was further stirred in the ice bath for 4 h. The separated thick material was filtered and washed with water (20 ml *X* 3) to obtain a cream coloured solid which was dissolved and recrystallized from DCM by slow evaporation to give pure crystals of the title compound (82% yield), suitable for single-crystal X-ray diffraction studies. All chemicals were purchased from Sigma–Aldrich.

S3. Refinement

H atoms on methyl, methylene and methine were positioned geometrically with C—H = 0.96, 0.97 and 0.93 Å respectively, and constrained to ride on their parent atoms with U_{iso}(H)= 1.2U_{eq}(CH and CH_2) and 1.5U_{eq}(CH_3). A rotating group model was applied to the methyl groups.

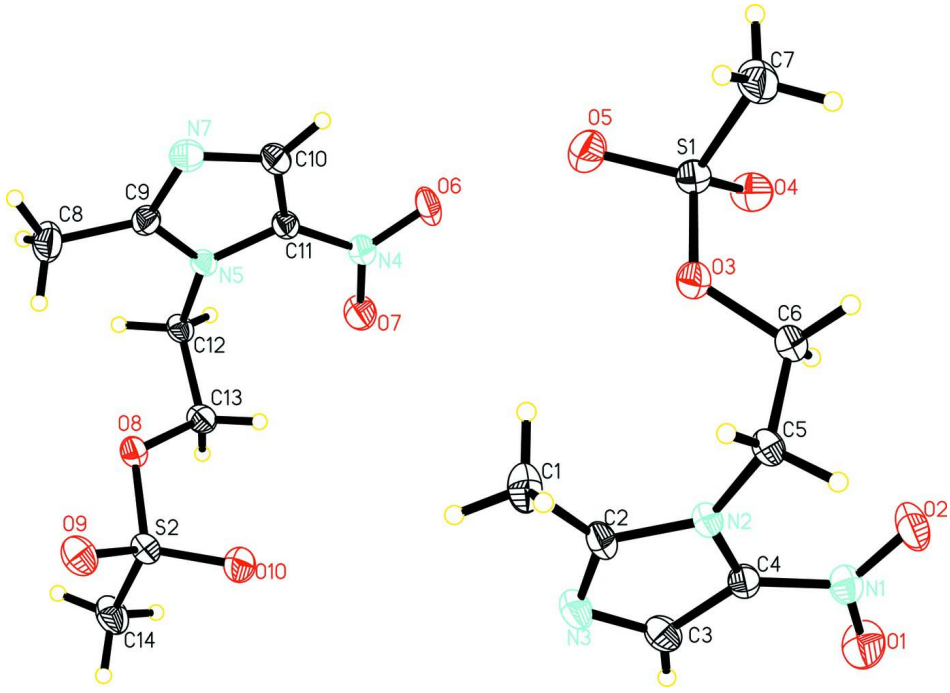


Figure 1

The molecular structure of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 30% probability level. H atoms are presented as small spheres of arbitrary radius.

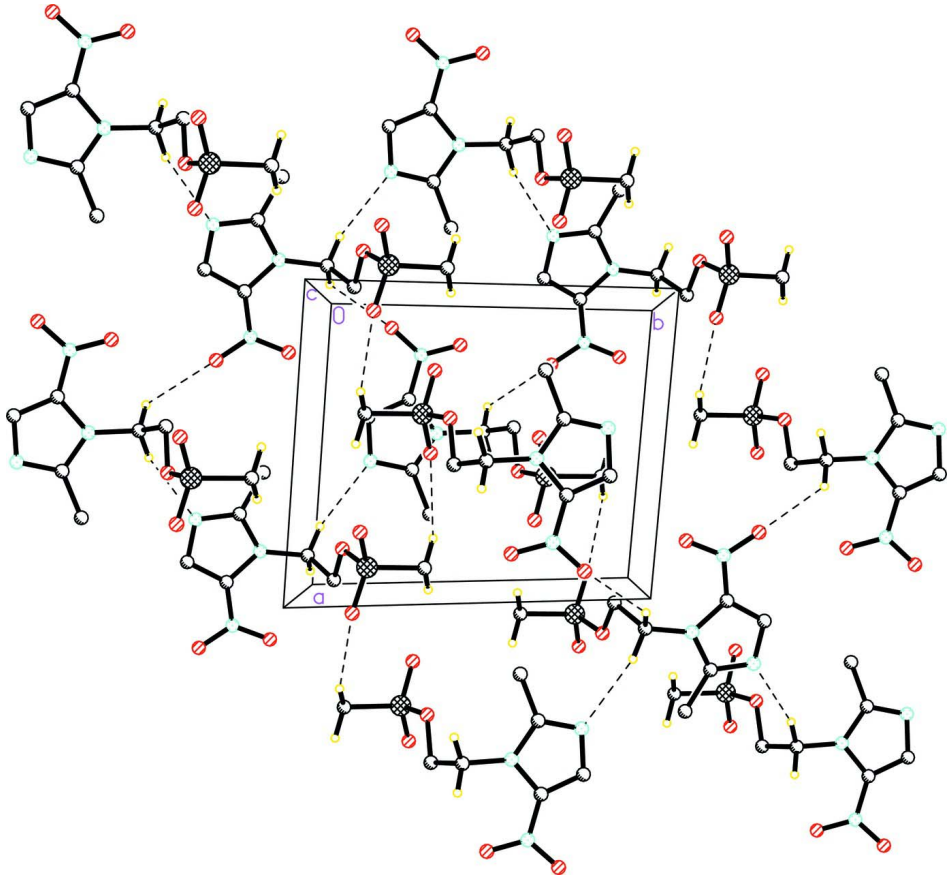


Figure 2

A view of the C—-H···O and C—H···N hydrogen bonds (dotted lines) in the crystal structure of the title compound. H atoms non-participating in hydrogen-bonding were omitted for clarity.

2-(2-Methyl-5-nitro-1*H*-imidazol-1-yl)ethyl methanesulfonate

Crystal data

$C_7H_{11}N_3O_5S$
$M_r = 249.26$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 8.8547$ (17) Å
$b = 10.927$ (2) Å
$c = 12.033$ (2) Å
$\alpha = 112.702$ (4)°
$\beta = 100.614$ (4)°
$\gamma = 90.052$ (4)°
$V = 1052.4$ (3) Å^3
$Z = 4$
$F(000) = 520$
$D_x = 1.573$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3658 reflections
$\theta = 2.4$–27.9°
$\mu = 0.32$ mm^{-1}
$T = 273$ K
Plate, colorles
0.40 × 0.21 × 0.08 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min} = 0.883$, $T_{max} = 0.975$
11649 measured reflections
3918 independent reflections

3078 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 25.5°$, $\theta_{min} = 1.9°$
$h = -10 \rightarrow 10$
$k = -13 \rightarrow 13$
$l = -14 \rightarrow 14$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.152$
$S = 1.07$
3918 reflections
291 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0914P)^2 + 0.2849P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.79$ e Å^{-3}
$\Delta\rho_{min} = -0.32$ e Å^{-3}

Special details

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

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit *S* are based on F^2, conventional *R*-factors *R* are based on *F*, with *F* set to zero for negative F^2. The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on *F*, and *R*- factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.09144 (8)	−0.18810 (7)	0.47184 (7)	0.0370 (2)
S2	0.60576 (8)	0.68767 (7)	0.52683 (7)	0.0356 (2)
O1	−0.2081 (3)	0.3132 (3)	0.8913 (3)	0.0621 (7)
O2	−0.1805 (3)	0.1027 (2)	0.8395 (2)	0.0557 (6)
O3	0.1479 (2)	−0.1063 (2)	0.61360 (19)	0.0384 (5)
O4	−0.0597 (2)	−0.1572 (2)	0.4331 (2)	0.0475 (6)
O5	0.2124 (3)	−0.1640 (2)	0.4178 (2)	0.0524 (6)
O6	0.0876 (2)	0.1903 (2)	0.1110 (2)	0.0526 (6)
O7	0.1462 (2)	0.4013 (2)	0.1692 (2)	0.0493 (6)
O8	0.5899 (2)	0.60582 (19)	0.38527 (18)	0.0365 (5)
O9	0.7537 (2)	0.6633 (2)	0.5805 (2)	0.0498 (6)
O10	0.4738 (2)	0.6572 (2)	0.5663 (2)	0.0474 (6)
N1	−0.1298 (3)	0.2166 (3)	0.8633 (2)	0.0398 (6)
N2	0.1317 (2)	0.1471 (2)	0.8363 (2)	0.0301 (5)
N3	0.2445 (3)	0.3407 (2)	0.8613 (2)	0.0423 (6)
N4	0.1824 (3)	0.2858 (2)	0.1409 (2)	0.0348 (6)
N5	0.4575 (2)	0.3517 (2)	0.1632 (2)	0.0288 (5)
N7	0.5555 (3)	0.1572 (2)	0.1374 (3)	0.0433 (6)
C1	0.4070 (4)	0.1507 (4)	0.8164 (3)	0.0507 (8)
H1A	0.4842	0.2158	0.8222	0.076*
H1B	0.3896	0.0805	0.7359	0.076*
H1C	0.4415	0.1144	0.8770	0.076*

C2	0.2630 (3)	0.2136 (3)	0.8381 (3)	0.0348 (6)
C3	0.0965 (4)	0.3589 (3)	0.8737 (3)	0.0405 (7)
H3B	0.0509	0.4390	0.8902	0.049*
C4	0.0247 (3)	0.2410 (3)	0.8582 (3)	0.0336 (6)
C5	0.1153 (3)	0.0068 (3)	0.8203 (3)	0.0333 (6)
H5B	0.0572	0.0000	0.8789	0.040*
H5C	0.2167	−0.0227	0.8384	0.040*
C6	0.0360 (3)	−0.0831 (3)	0.6936 (3)	0.0387 (7)
H6B	−0.0012	−0.1667	0.6934	0.046*
H6C	−0.0513	−0.0420	0.6649	0.046*
C7	0.0862 (4)	−0.3532 (3)	0.4587 (4)	0.0547 (9)
H7A	0.0617	−0.4118	0.3734	0.082*
H7B	0.0090	−0.3678	0.4997	0.082*
H7C	0.1850	−0.3704	0.4958	0.082*
C8	0.7433 (4)	0.3470 (4)	0.1814 (4)	0.0540 (9)
H8A	0.8153	0.2796	0.1668	0.081*
H8B	0.7714	0.4106	0.2648	0.081*
H8C	0.7449	0.3912	0.1264	0.081*
C9	0.5861 (3)	0.2846 (3)	0.1602 (3)	0.0346 (6)
C10	0.4009 (3)	0.1407 (3)	0.1252 (3)	0.0391 (7)
H10B	0.3460	0.0609	0.1085	0.047*
C11	0.3377 (3)	0.2588 (3)	0.1412 (3)	0.0317 (6)
C12	0.4499 (3)	0.4921 (3)	0.1791 (3)	0.0317 (6)
H12A	0.3617	0.4992	0.1214	0.038*
H12B	0.5418	0.5208	0.1596	0.038*
C13	0.4371 (3)	0.5828 (3)	0.3059 (3)	0.0362 (7)
H13A	0.4006	0.6665	0.3060	0.043*
H13B	0.3644	0.5427	0.3357	0.043*
C14	0.6070 (4)	0.8524 (3)	0.5396 (3)	0.0522 (9)
H14A	0.6396	0.9112	0.6243	0.078*
H14B	0.5051	0.8703	0.5088	0.078*
H14C	0.6769	0.8662	0.4925	0.078*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0370 (4)	0.0336 (4)	0.0394 (4)	0.0035 (3)	0.0099 (3)	0.0123 (3)
S2	0.0336 (4)	0.0329 (4)	0.0374 (4)	−0.0030 (3)	0.0037 (3)	0.0122 (3)
O1	0.0480 (14)	0.0549 (15)	0.090 (2)	0.0220 (12)	0.0258 (13)	0.0309 (14)
O2	0.0407 (12)	0.0415 (13)	0.0877 (19)	−0.0049 (10)	0.0170 (12)	0.0266 (13)
O3	0.0320 (10)	0.0386 (11)	0.0433 (12)	0.0017 (8)	0.0092 (9)	0.0139 (9)
O4	0.0437 (12)	0.0484 (13)	0.0458 (13)	0.0075 (10)	0.0032 (10)	0.0161 (11)
O5	0.0546 (14)	0.0558 (15)	0.0531 (14)	0.0045 (11)	0.0236 (11)	0.0224 (12)
O6	0.0369 (12)	0.0487 (14)	0.0702 (16)	−0.0152 (10)	0.0100 (11)	0.0215 (12)
O7	0.0376 (12)	0.0411 (13)	0.0683 (16)	0.0083 (9)	0.0096 (10)	0.0207 (11)
O8	0.0283 (10)	0.0365 (11)	0.0409 (12)	−0.0017 (8)	0.0047 (8)	0.0120 (9)
O9	0.0403 (12)	0.0544 (14)	0.0508 (14)	−0.0003 (10)	−0.0048 (10)	0.0227 (11)
O10	0.0472 (13)	0.0512 (14)	0.0444 (13)	−0.0052 (10)	0.0135 (10)	0.0176 (11)

N1	0.0328 (13)	0.0408 (15)	0.0479 (16)	0.0019 (11)	0.0074 (11)	0.0198 (12)
N2	0.0279 (11)	0.0279 (12)	0.0355 (13)	−0.0002 (9)	0.0049 (9)	0.0142 (10)
N3	0.0403 (14)	0.0342 (14)	0.0523 (16)	−0.0069 (11)	0.0075 (12)	0.0176 (12)
N4	0.0332 (13)	0.0364 (14)	0.0360 (14)	−0.0010 (10)	0.0057 (10)	0.0160 (11)
N5	0.0296 (12)	0.0243 (11)	0.0321 (12)	0.0001 (9)	0.0057 (9)	0.0110 (10)
N7	0.0451 (15)	0.0314 (14)	0.0537 (17)	0.0077 (11)	0.0133 (12)	0.0154 (12)
C1	0.0341 (16)	0.056 (2)	0.069 (2)	0.0004 (14)	0.0132 (15)	0.0303 (19)
C2	0.0329 (15)	0.0343 (16)	0.0379 (17)	−0.0080 (12)	0.0025 (12)	0.0170 (13)
C3	0.0459 (17)	0.0277 (15)	0.0475 (19)	0.0011 (12)	0.0069 (14)	0.0156 (14)
C4	0.0315 (14)	0.0328 (15)	0.0365 (16)	0.0010 (11)	0.0078 (12)	0.0132 (13)
C5	0.0347 (15)	0.0281 (14)	0.0389 (16)	−0.0020 (11)	0.0060 (12)	0.0157 (12)
C6	0.0365 (15)	0.0334 (16)	0.0438 (18)	−0.0042 (12)	0.0113 (13)	0.0113 (13)
C7	0.052 (2)	0.0371 (18)	0.081 (3)	0.0074 (15)	0.0218 (18)	0.0253 (18)
C8	0.0326 (17)	0.055 (2)	0.077 (3)	0.0052 (15)	0.0153 (16)	0.0269 (19)
C9	0.0335 (15)	0.0315 (15)	0.0407 (17)	0.0053 (11)	0.0124 (12)	0.0141 (13)
C10	0.0417 (17)	0.0291 (15)	0.0478 (18)	−0.0017 (12)	0.0116 (13)	0.0153 (14)
C11	0.0320 (14)	0.0289 (14)	0.0347 (15)	−0.0008 (11)	0.0066 (11)	0.0129 (12)
C12	0.0327 (14)	0.0253 (13)	0.0386 (16)	−0.0001 (11)	0.0055 (12)	0.0148 (12)
C13	0.0318 (14)	0.0305 (15)	0.0418 (17)	0.0038 (11)	0.0030 (12)	0.0112 (13)
C14	0.0438 (18)	0.0342 (17)	0.076 (3)	−0.0022 (14)	0.0064 (17)	0.0221 (17)

Geometric parameters (Å, º)

S1—O4	1.420 (2)	C1—H1A	0.9600
S1—O5	1.425 (2)	C1—H1B	0.9600
S1—O3	1.571 (2)	C1—H1C	0.9600
S1—C7	1.749 (3)	C3—C4	1.367 (4)
S2—O9	1.423 (2)	C3—H3B	0.9300
S2—O10	1.424 (2)	C5—C6	1.494 (4)
S2—O8	1.567 (2)	C5—H5B	0.9700
S2—C14	1.746 (3)	C5—H5C	0.9700
O1—N1	1.234 (3)	C6—H6B	0.9700
O2—N1	1.228 (3)	C6—H6C	0.9700
O3—C6	1.461 (3)	C7—H7A	0.9600
O6—N4	1.233 (3)	C7—H7B	0.9600
O7—N4	1.233 (3)	C7—H7C	0.9600
O8—C13	1.464 (3)	C8—C9	1.484 (4)
N1—C4	1.410 (4)	C8—H8A	0.9600
N2—C2	1.363 (3)	C8—H8B	0.9600
N2—C4	1.381 (4)	C8—H8C	0.9600
N2—C5	1.473 (3)	C10—C11	1.366 (4)
N3—C2	1.323 (4)	C10—H10B	0.9300
N3—C3	1.352 (4)	C12—C13	1.490 (4)
N4—C11	1.406 (3)	C12—H12A	0.9700
N5—C9	1.353 (3)	C12—H12B	0.9700
N5—C11	1.383 (3)	C13—H13A	0.9700
N5—C12	1.474 (3)	C13—H13B	0.9700
N7—C9	1.328 (4)	C14—H14A	0.9600

N7—C10	1.354 (4)	C14—H14B	0.9600
C1—C2	1.467 (4)	C14—H14C	0.9600
O4—S1—O5	118.95 (14)	C6—C5—H5C	109.0
O4—S1—O3	109.90 (12)	H5B—C5—H5C	107.8
O5—S1—O3	104.65 (13)	O3—C6—C5	107.7 (2)
O4—S1—C7	109.32 (15)	O3—C6—H6B	110.2
O5—S1—C7	109.50 (15)	C5—C6—H6B	110.2
O3—S1—C7	103.32 (15)	O3—C6—H6C	110.2
O9—S2—O10	118.88 (14)	C5—C6—H6C	110.2
O9—S2—O8	104.78 (13)	H6B—C6—H6C	108.5
O10—S2—O8	109.83 (12)	S1—C7—H7A	109.5
O9—S2—C14	109.74 (15)	S1—C7—H7B	109.5
O10—S2—C14	109.15 (15)	H7A—C7—H7B	109.5
O8—S2—C14	103.28 (15)	S1—C7—H7C	109.5
C6—O3—S1	118.58 (18)	H7A—C7—H7C	109.5
C13—O8—S2	118.53 (17)	H7B—C7—H7C	109.5
O2—N1—O1	123.1 (3)	C9—C8—H8A	109.5
O2—N1—C4	119.8 (2)	C9—C8—H8B	109.5
O1—N1—C4	117.1 (3)	H8A—C8—H8B	109.5
C2—N2—C4	104.9 (2)	C9—C8—H8C	109.5
C2—N2—C5	125.9 (2)	H8A—C8—H8C	109.5
C4—N2—C5	129.1 (2)	H8B—C8—H8C	109.5
C2—N3—C3	106.4 (2)	N7—C9—N5	112.3 (2)
O7—N4—O6	122.9 (2)	N7—C9—C8	124.0 (3)
O7—N4—C11	119.9 (2)	N5—C9—C8	123.7 (3)
O6—N4—C11	117.3 (2)	N7—C10—C11	109.8 (3)
C9—N5—C11	105.3 (2)	N7—C10—H10B	125.1
C9—N5—C12	126.1 (2)	C11—C10—H10B	125.1
C11—N5—C12	128.5 (2)	C10—C11—N5	106.9 (2)
C9—N7—C10	105.7 (2)	C10—C11—N4	127.9 (3)
C2—C1—H1A	109.5	N5—C11—N4	125.1 (2)
C2—C1—H1B	109.5	N5—C12—C13	113.3 (2)
H1A—C1—H1B	109.5	N5—C12—H12A	108.9
C2—C1—H1C	109.5	C13—C12—H12A	108.9
H1A—C1—H1C	109.5	N5—C12—H12B	108.9
H1B—C1—H1C	109.5	C13—C12—H12B	108.9
N3—C2—N2	112.0 (3)	H12A—C12—H12B	107.7
N3—C2—C1	124.5 (3)	O8—C13—C12	108.1 (2)
N2—C2—C1	123.6 (3)	O8—C13—H13A	110.1
N3—C3—C4	109.2 (3)	C12—C13—H13A	110.1
N3—C3—H3B	125.4	O8—C13—H13B	110.1
C4—C3—H3B	125.4	C12—C13—H13B	110.1
C3—C4—N2	107.5 (2)	H13A—C13—H13B	108.4
C3—C4—N1	127.4 (3)	S2—C14—H14A	109.5
N2—C4—N1	125.1 (2)	S2—C14—H14B	109.5
N2—C5—C6	113.0 (2)	H14A—C14—H14B	109.5
N2—C5—H5B	109.0	S2—C14—H14C	109.5

C6—C5—H5B	109.0	H14A—C14—H14C	109.5
N2—C5—H5C	109.0	H14B—C14—H14C	109.5
O4—S1—O3—C6	36.6 (2)	C4—N2—C5—C6	80.8 (3)
O5—S1—O3—C6	165.4 (2)	S1—O3—C6—C5	−174.80 (18)
C7—S1—O3—C6	−79.9 (2)	N2—C5—C6—O3	77.7 (3)
O9—S2—O8—C13	165.3 (2)	C10—N7—C9—N5	−0.1 (3)
O10—S2—O8—C13	36.5 (2)	C10—N7—C9—C8	179.2 (3)
C14—S2—O8—C13	−79.8 (2)	C11—N5—C9—N7	0.4 (3)
C3—N3—C2—N2	−0.8 (3)	C12—N5—C9—N7	−176.3 (3)
C3—N3—C2—C1	179.1 (3)	C11—N5—C9—C8	−179.0 (3)
C4—N2—C2—N3	1.0 (3)	C12—N5—C9—C8	4.4 (5)
C5—N2—C2—N3	−176.3 (3)	C9—N7—C10—C11	−0.2 (3)
C4—N2—C2—C1	−178.8 (3)	N7—C10—C11—N5	0.4 (3)
C5—N2—C2—C1	3.9 (4)	N7—C10—C11—N4	−177.2 (3)
C2—N3—C3—C4	0.2 (3)	C9—N5—C11—C10	−0.5 (3)
N3—C3—C4—N2	0.4 (3)	C12—N5—C11—C10	176.1 (3)
N3—C3—C4—N1	−179.7 (3)	C9—N5—C11—N4	177.3 (3)
C2—N2—C4—C3	−0.9 (3)	C12—N5—C11—N4	−6.1 (4)
C5—N2—C4—C3	176.3 (3)	O7—N4—C11—C10	172.6 (3)
C2—N2—C4—N1	179.3 (3)	O6—N4—C11—C10	−7.8 (4)
C5—N2—C4—N1	−3.5 (5)	O7—N4—C11—N5	−4.7 (4)
O2—N1—C4—C3	175.3 (3)	O6—N4—C11—N5	174.9 (3)
O1—N1—C4—C3	−4.2 (5)	C9—N5—C12—C13	−102.3 (3)
O2—N1—C4—N2	−4.9 (4)	C11—N5—C12—C13	81.8 (3)
O1—N1—C4—N2	175.7 (3)	S2—O8—C13—C12	−174.36 (17)
C2—N2—C5—C6	−102.5 (3)	N5—C12—C13—O8	77.5 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5*B*···O6^{i}	0.97	2.50	3.235 (4)	133
C5—H5*C*···N7^{ii}	0.97	2.54	3.484 (4)	165
C7—H7*B*···O9^{iii}	0.96	2.59	3.498 (4)	157
C7—H7*C*···O10^{iv}	0.96	2.52	3.423 (4)	157
C12—H12*A*···O1^{v}	0.97	2.50	3.250 (5)	134
C12—H12*B*···N3^{vi}	0.97	2.53	3.472 (4)	164
C14—H14*B*···O5^{vii}	0.96	2.59	3.507 (4)	160
C14—H14*C*···O4^{viii}	0.96	2.55	3.414 (4)	150

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