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3-(3-Methoxyphenyl)benzo[*d*]thiazolo-[3,2-*a*]imidazol-9-ium hydrogen sulfate

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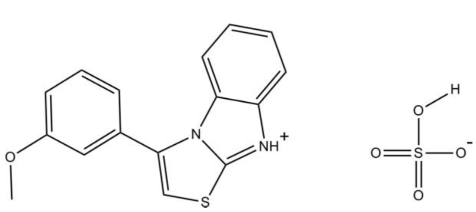
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.004 Å; R factor = 0.058; wR factor = 0.170; data-to-parameter ratio = 16.0.

In the title molecular salt, $C_{16}H_{13}N_2OS^+\cdot HSO_4^-$, the thiazolo-[3,2-*a*]benzimidazolium ring system is roughly planar [maximum deviation = 0.046 (3) Å] and makes a dihedral angle of 58.22 (11)° with the benzene ring. The methoxy group is almost coplanar with its attached benzene ring [C_{methyl}—O—C—C = −1.6 (5)°]. In the crystal, the cation is linked to the anion by a bifurcated N—H···(O,O) hydrogen bond, generating an $R_1^2(4)$ ring motif. The ion pairs are then connected by a C—H···O hydrogen bond into inversion dimers and these dimers are further linked by O—H···O hydrogen bonds into an infinite tape along [100]. A π–π stacking interaction [centroid-to-centroid distance = 3.5738 (18) Å] and a short intermolecular contact [S···O = 2.830 (3) Å] are also observed.

Related literature

For the biological activities of thiazolo[3,2-*a*]benzimidazoles, see: Chimirri *et al.* (1988); Al-Rashood & Abdel-Aziz (2010); Hamdy *et al.* (2007); Abdel-Aziz *et al.* (2007, 2008); Farag *et al.* (2011). For hydrogen-bond motifs, see: Bernstein *et al.* (1995). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986).



‡ Thomson Reuters ResearcherID: A-3561-2009.

Experimental

Crystal data

$C_{16}H_{13}N_2OS^+\cdot HSO_4^-$
M_r = 378.41
Monoclinic, $P2_1/c$
a = 4.5428 (8) Å
b = 20.096 (4) Å
c = 17.788 (3) Å
β = 93.003 (4)°
V = 1621.6 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.36 mm^{-1}
T = 100 K
0.31 × 0.15 × 0.12 mm

Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.898, T_{max} = 0.959
12491 measured reflections
3699 independent reflections
2904 reflections with $I > 2\sigma(I)$
R_{int} = 0.050

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.170
S = 1.04
3699 reflections
231 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.99 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N1···O3	0.94 (4)	1.85 (4)	2.750 (3)	160 (3)
N1—H1N1···O4	0.94 (4)	2.50 (4)	3.199 (4)	132 (3)
O2—H1O2···O3^{i}	0.97	1.60	2.531 (4)	158
C11—H11A···O5^{ii}	0.93	2.32	3.237 (4)	170

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6885).

References

Abdel-Aziz, H. A., Hamdy, N. A., Fakhr, I. M. I. & Farag, A. M. (2008). *J. Heterocycl. Chem.* **45**, 1033–1037.
Abdel-Aziz, H. A., Hamdy, N. A., Farag, A. M. & Fakhr, I. M. I. (2007). *J. Chin. Chem. Soc.* **54**, 1573–1582.
Al-Rashood, K. A. & Abdel-Aziz, H. A. (2010). *Molecules*, **15**, 3775–3815.
Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2009). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Chimirri, A., Grasso, S., Romeo, G. & Zappala, M. (1988). *Heterocycles*, **27**, 1975–2003.

Cosier, J. & Glazer, A. M. (1986). *J. Appl. Cryst.* **19**, 105–107.
Farag, A. M., Dawood, K. M., Abdel-Aziz, H. A., Hamdy, N. A. & Fakhr, I. M. I. (2011). *J. Heterocycl. Chem.* **48**, 355–360.
Hamdy, N. A., Abdel-Aziz, H. A., Farag, A. M. & Fakhr, I. M. I. (2007). *Monatsh. Chem.* **138**, 1001–1010.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

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3-(3-Methoxyphenyl)benzo[*d*]thiazolo[3,2-*a*]imidazol-9-ium hydrogen sulfate

Hoong-Kun Fun, Tze Shyang Chia, Ahmed M. Alafeefy and Hatem A. Abdel-Aziz

S1. Comment

Various biological properties of thiazolo[3,2-*a*]benzimidazole derivatives have been reported, including antibacterial, antifungal, anti-inflammatory, antiulcer, antiviral, anthelmintic and anticancer activities (Chimirri *et al.*, 1988; Al-Rashood & Abdel-Aziz, 2010). In continuation of our interest in this area (Hamdy *et al.*, 2007; Abdel-Aziz *et al.*, 2007, 2008; Farag *et al.*, 2011), we report herein the crystal structure of the title compound.

The molecular structure of the title compound is shown in Fig. 1. The asymmetric unit of the title compound, $C_{16}H_{13}N_2OS^+$, HSO_4^-, contains a 3-(3-methoxyphenyl)benzo[*d*]thiazolo[3,2-*a*]imidazol-9-ium cation and a hydrogen sulfate anion. The thiazolo[3,2-*a*]benzimidazole ring system is roughly planar [S1/N1/N2/C1–C9; maximum deviation = 0.046 (3) Å at atom C8] and makes a dihedral angle of 58.22 (11)° with the C10–C15 benzene ring. The O1—C16 methoxy group is almost coplanar with the C10–C15 benzene ring as indicated by the C16—O1—C12—C11 torsion angle of -1.6 (5)°.

In the crystal (Fig. 2), the cation and anion are linked to each other by bifurcated N1—H1N1···(O3,O4) hydrogen bonds, generating an $R_1^2(4)$ ring motif (Bernstein *et al.*, 1995). The asymmetric units are then connected by C11—H11A···O5 hydrogen bond into inversion dimers and the dimers are further linked by O2—H1O2···O3 hydrogen bond into an infinite tape, propagating along the *a*-axis. A *π*–*π* interaction [*Cg*1···*Cg*2 = 3.5738 (18) Å; *Cg*1 and *Cg*2 are the centroids of N1/C6/C1/N2/C7 and C1–C6 rings, respectively; symmetry code = -1 + *x*, *y*, *z*] and a short intermolecular contact [S1···O4 = 2.830 (3) Å; symmetry code = -*x*, 1 - *y*, 1 - *z*] are also observed.

S2. Experimental

A mixture of 2-mercaptobenzimidazole (1.52 g, 10 mmol) and 3-methoxyacetophenone (1.52 g, 10 mmol) in boiling $AcOH/H_2SO_4$ (50 ml; 10:1, *v*/*v*) was refluxed for 5 h. The reaction mixture was then left to cool at room temperature. The colourless blocks formed were filtered off, washed with ethanol and dried to afford the title compound.

S3. Refinement

Atoms H1O2 and H1N1 were located in a difference Fourier map and the atom H1O2 was then fixed at its found location [O2—H1O2 = 0.9734 Å] and refined using a riding model with $U_{iso}(H) = 1.5U_{eq}(O)$, whereas the atom H1N1 was refined freely [N1—H1N1 = 0.93 (4) Å]. The remaining H atoms were positioned geometrically [C—H = 0.93 and 0.96 Å] and refined with $U_{iso}(H) = 1.2$ or $1.5U_{eq}(C)$. A rotating group model was applied to the methyl group.

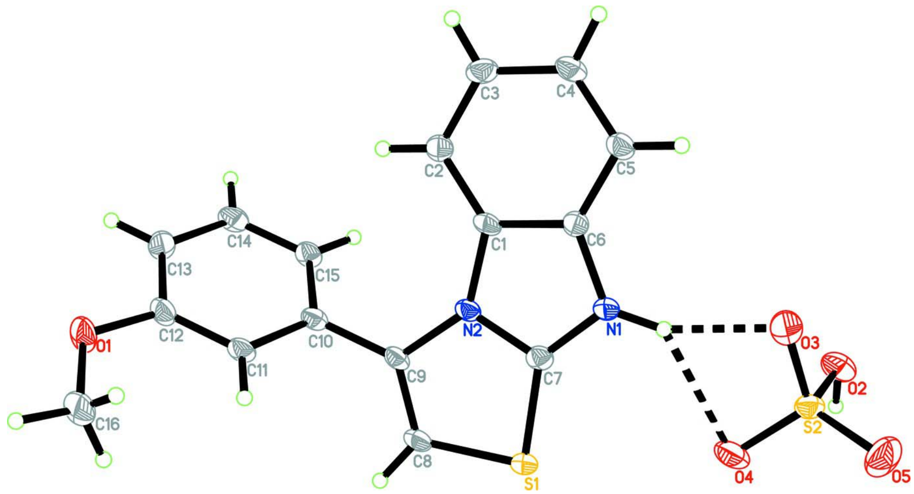

Figure 1

The molecular structure of the title compound with 50% probability displacement ellipsoids. Hydrogen bonds are indicated by dashed lines.

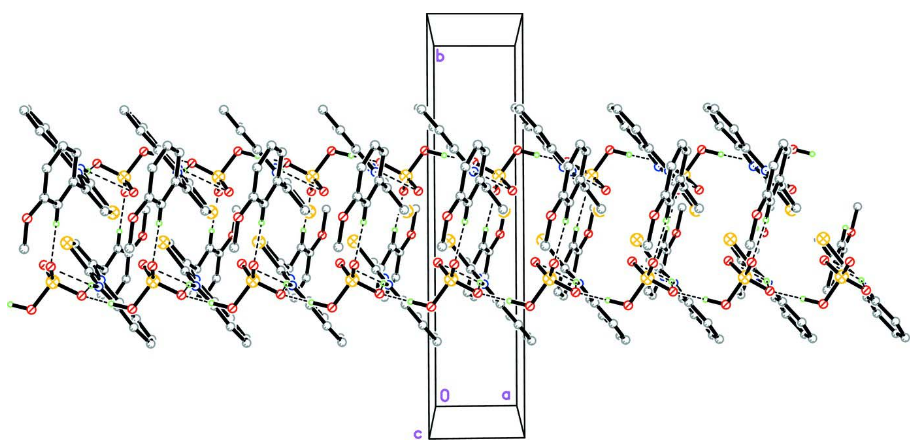

Figure 2

The crystal packing of the title compound. The dashed lines represent the hydrogen bonds. For clarity sake, hydrogen atoms not involved in hydrogen bonding have been omitted.

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Crystal data

$C_{16}H_{13}N_2OS^+\cdot HSO_4^-$
M_r = 378.41
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 4.5428 (8) Å
b = 20.096 (4) Å
c = 17.788 (3) Å
β = 93.003 (4)°
V = 1621.6 (5) Å^3
Z = 4

F(000) = 784
D_x = 1.550 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 4717 reflections
θ = 2.3–29.3°
μ = 0.36 mm^{-1}
T = 100 K
Block, colourless
0.31 × 0.15 × 0.12 mm

Data collection

Bruker APEX DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.898$, $T_{max} = 0.959$
12491 measured reflections
3699 independent reflections
2904 reflections with $I > 2\sigma(I)$
$R_{int} = 0.050$
$\theta_{max} = 27.5°$, $\theta_{min} = 1.5°$
$h = -5 \rightarrow 5$
$k = -26 \rightarrow 24$
$l = -19 \rightarrow 23$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.058$
$wR(F^2) = 0.170$
$S = 1.04$
3699 reflections
231 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0882P)^2 + 3.0462P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.99$ e Å^{-3}
$\Delta\rho_{min} = -0.68$ e Å^{-3}

Special details

Experimental. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
S1	0.21267 (17)	0.46487 (4)	0.42583 (4)	0.0192 (2)
S2	0.24639 (17)	0.37855 (4)	0.66173 (4)	0.0214 (2)
O1	0.7757 (6)	0.47885 (11)	0.06026 (13)	0.0313 (6)
O2	0.0440 (5)	0.31645 (11)	0.67548 (13)	0.0281 (5)
H1O2	−0.1640	0.3283	0.6741	0.042*
O3	0.5152 (6)	0.34615 (13)	0.63785 (13)	0.0325 (6)
O4	0.1087 (6)	0.41582 (12)	0.59898 (14)	0.0315 (6)
O5	0.2805 (7)	0.41374 (13)	0.73091 (15)	0.0416 (7)
N1	0.5806 (6)	0.36239 (12)	0.48611 (14)	0.0176 (5)
N2	0.5187 (5)	0.37532 (11)	0.36286 (13)	0.0154 (5)
C1	0.7199 (6)	0.32219 (14)	0.37436 (16)	0.0162 (6)
C2	0.8648 (7)	0.28056 (14)	0.32574 (16)	0.0185 (6)
H2A	0.8406	0.2849	0.2737	0.022*
C3	1.0472 (7)	0.23229 (15)	0.35886 (17)	0.0217 (6)

H3A	1.1477	0.2035	0.3282	0.026*
C4	1.0841 (7)	0.22567 (15)	0.43704 (17)	0.0209 (6)
H4A	1.2093	0.1927	0.4569	0.025*
C5	0.9397 (7)	0.26676 (14)	0.48591 (17)	0.0195 (6)
H5A	0.9654	0.2624	0.5379	0.023*
C6	0.7538 (6)	0.31496 (14)	0.45269 (16)	0.0173 (6)
C7	0.4426 (6)	0.39749 (14)	0.43096 (16)	0.0168 (6)
C8	0.2254 (7)	0.46239 (14)	0.32772 (16)	0.0198 (6)
H8A	0.1249	0.4926	0.2961	0.024*
C9	0.3934 (6)	0.41295 (14)	0.30187 (15)	0.0167 (6)
C10	0.4589 (6)	0.39786 (14)	0.22327 (16)	0.0171 (6)
C11	0.5788 (7)	0.44837 (14)	0.18026 (16)	0.0186 (6)
H11A	0.6104	0.4906	0.2006	0.022*
C12	0.6502 (7)	0.43475 (15)	0.10674 (16)	0.0212 (6)
C13	0.6007 (7)	0.37120 (15)	0.07654 (17)	0.0226 (6)
H13A	0.6500	0.3621	0.0275	0.027*
C14	0.4790 (7)	0.32211 (15)	0.11920 (17)	0.0212 (6)
H14A	0.4460	0.2801	0.0986	0.025*
C15	0.4049 (6)	0.33474 (14)	0.19277 (16)	0.0188 (6)
H15A	0.3207	0.3016	0.2212	0.023*
C16	0.8306 (10)	0.54428 (17)	0.0891 (2)	0.0367 (9)
H16A	0.9177	0.5709	0.0513	0.055*
H16B	0.9628	0.5418	0.1329	0.055*
H16C	0.6481	0.5641	0.1023	0.055*
H1N1	0.540 (8)	0.3670 (18)	0.537 (2)	0.022 (9)*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0257 (4)	0.0124 (4)	0.0195 (4)	0.0041 (3)	0.0020 (3)	−0.0003 (3)
S2	0.0273 (4)	0.0140 (4)	0.0233 (4)	0.0020 (3)	0.0053 (3)	−0.0002 (3)
O1	0.0577 (17)	0.0144 (11)	0.0228 (11)	−0.0097 (10)	0.0120 (11)	0.0003 (9)
O2	0.0312 (13)	0.0176 (11)	0.0352 (13)	−0.0015 (9)	−0.0016 (10)	0.0050 (9)
O3	0.0345 (14)	0.0369 (15)	0.0262 (12)	0.0089 (10)	0.0037 (10)	0.0035 (10)
O4	0.0381 (14)	0.0203 (12)	0.0365 (13)	0.0082 (10)	0.0046 (10)	0.0096 (10)
O5	0.067 (2)	0.0288 (14)	0.0294 (13)	−0.0083 (12)	0.0063 (12)	−0.0110 (11)
N1	0.0243 (13)	0.0119 (12)	0.0165 (12)	0.0029 (9)	0.0011 (9)	−0.0007 (9)
N2	0.0198 (12)	0.0094 (11)	0.0169 (11)	0.0001 (8)	−0.0001 (9)	0.0004 (9)
C1	0.0178 (14)	0.0089 (13)	0.0219 (14)	−0.0009 (10)	0.0012 (10)	0.0031 (10)
C2	0.0228 (15)	0.0137 (14)	0.0190 (13)	−0.0015 (11)	0.0013 (11)	−0.0008 (11)
C3	0.0260 (16)	0.0132 (14)	0.0262 (15)	0.0016 (11)	0.0047 (12)	−0.0031 (12)
C4	0.0249 (16)	0.0125 (14)	0.0252 (15)	0.0027 (11)	−0.0014 (11)	0.0020 (11)
C5	0.0242 (16)	0.0138 (14)	0.0203 (14)	0.0003 (11)	0.0001 (11)	0.0020 (11)
C6	0.0224 (15)	0.0123 (13)	0.0172 (13)	−0.0009 (10)	0.0024 (10)	0.0005 (11)
C7	0.0190 (14)	0.0119 (13)	0.0196 (14)	−0.0017 (10)	0.0011 (10)	−0.0004 (10)
C8	0.0269 (16)	0.0105 (14)	0.0218 (14)	0.0022 (11)	0.0005 (11)	0.0022 (11)
C9	0.0217 (15)	0.0102 (13)	0.0179 (14)	−0.0007 (10)	−0.0015 (10)	0.0029 (10)
C10	0.0204 (15)	0.0114 (13)	0.0192 (13)	0.0005 (10)	−0.0011 (10)	0.0012 (11)

C11	0.0254 (16)	0.0093 (13)	0.0209 (14)	−0.0018 (10)	−0.0005 (11)	0.0000 (11)
C12	0.0312 (17)	0.0132 (14)	0.0194 (14)	−0.0026 (11)	0.0024 (11)	0.0028 (11)
C13	0.0334 (18)	0.0165 (15)	0.0181 (14)	−0.0027 (12)	0.0027 (12)	−0.0036 (11)
C14	0.0261 (16)	0.0116 (14)	0.0256 (15)	−0.0029 (11)	−0.0021 (12)	−0.0018 (11)
C15	0.0236 (15)	0.0114 (13)	0.0214 (14)	−0.0038 (10)	0.0001 (11)	0.0000 (11)
C16	0.066 (3)	0.0121 (16)	0.0334 (19)	−0.0074 (15)	0.0170 (17)	0.0012 (13)

Geometric parameters (Å, º)

S1—C7	1.710 (3)	C4—C5	1.388 (4)
S1—C8	1.750 (3)	C4—H4A	0.9300
S2—O5	1.421 (3)	C5—C6	1.396 (4)
S2—O4	1.458 (2)	C5—H5A	0.9300
S2—O3	1.466 (3)	C8—C9	1.348 (4)
S2—O2	1.577 (2)	C8—H8A	0.9300
O1—C12	1.358 (4)	C9—C10	1.476 (4)
O1—C16	1.428 (4)	C10—C15	1.396 (4)
O2—H1O2	0.9734	C10—C11	1.399 (4)
N1—C7	1.337 (4)	C11—C12	1.391 (4)
N1—C6	1.389 (4)	C11—H11A	0.9300
N1—H1N1	0.93 (4)	C12—C13	1.399 (4)
N2—C7	1.353 (4)	C13—C14	1.378 (4)
N2—C1	1.413 (4)	C13—H13A	0.9300
N2—C9	1.417 (3)	C14—C15	1.392 (4)
C1—C2	1.393 (4)	C14—H14A	0.9300
C1—C6	1.401 (4)	C15—H15A	0.9300
C2—C3	1.387 (4)	C16—H16A	0.9600
C2—H2A	0.9300	C16—H16B	0.9600
C3—C4	1.398 (4)	C16—H16C	0.9600
C3—H3A	0.9300		
C7—S1—C8	88.78 (14)	N1—C7—N2	110.6 (2)
O5—S2—O4	115.49 (16)	N1—C7—S1	135.9 (2)
O5—S2—O3	114.67 (17)	N2—C7—S1	113.4 (2)
O4—S2—O3	109.68 (14)	C9—C8—S1	114.2 (2)
O5—S2—O2	107.32 (15)	C9—C8—H8A	122.9
O4—S2—O2	107.17 (14)	S1—C8—H8A	122.9
O3—S2—O2	101.22 (15)	C8—C9—N2	110.1 (2)
C12—O1—C16	117.0 (2)	C8—C9—C10	128.3 (3)
S2—O2—H1O2	112.1	N2—C9—C10	121.5 (2)
C7—N1—C6	107.6 (2)	C15—C10—C11	120.8 (3)
C7—N1—H1N1	123 (2)	C15—C10—C9	121.0 (3)
C6—N1—H1N1	129 (2)	C11—C10—C9	118.2 (3)
C7—N2—C1	108.2 (2)	C12—C11—C10	119.2 (3)
C7—N2—C9	113.5 (2)	C12—C11—H11A	120.4
C1—N2—C9	138.1 (2)	C10—C11—H11A	120.4
C2—C1—C6	121.6 (3)	O1—C12—C11	124.8 (3)
C2—C1—N2	133.4 (3)	O1—C12—C13	115.2 (3)

C6—C1—N2	105.0 (2)	C11—C12—C13	120.0 (3)
C3—C2—C1	116.6 (3)	C14—C13—C12	120.2 (3)
C3—C2—H2A	121.7	C14—C13—H13A	119.9
C1—C2—H2A	121.7	C12—C13—H13A	119.9
C2—C3—C4	121.8 (3)	C13—C14—C15	120.7 (3)
C2—C3—H3A	119.1	C13—C14—H14A	119.6
C4—C3—H3A	119.1	C15—C14—H14A	119.6
C5—C4—C3	122.0 (3)	C14—C15—C10	119.0 (3)
C5—C4—H4A	119.0	C14—C15—H15A	120.5
C3—C4—H4A	119.0	C10—C15—H15A	120.5
C4—C5—C6	116.3 (3)	O1—C16—H16A	109.5
C4—C5—H5A	121.9	O1—C16—H16B	109.5
C6—C5—H5A	121.9	H16A—C16—H16B	109.5
N1—C6—C5	129.7 (3)	O1—C16—H16C	109.5
N1—C6—C1	108.6 (2)	H16A—C16—H16C	109.5
C5—C6—C1	121.7 (3)	H16B—C16—H16C	109.5

C7—N2—C1—C2	178.7 (3)	C8—S1—C7—N2	−0.4 (2)
C9—N2—C1—C2	−6.0 (6)	C7—S1—C8—C9	0.3 (2)
C7—N2—C1—C6	0.2 (3)	S1—C8—C9—N2	−0.1 (3)
C9—N2—C1—C6	175.4 (3)	S1—C8—C9—C10	−178.0 (2)
C6—C1—C2—C3	−0.8 (4)	C7—N2—C9—C8	−0.2 (3)
N2—C1—C2—C3	−179.2 (3)	C1—N2—C9—C8	−175.2 (3)
C1—C2—C3—C4	0.0 (4)	C7—N2—C9—C10	177.9 (3)
C2—C3—C4—C5	0.3 (5)	C1—N2—C9—C10	2.8 (5)
C3—C4—C5—C6	0.3 (4)	C8—C9—C10—C15	−125.6 (3)
C7—N1—C6—C5	179.7 (3)	N2—C9—C10—C15	56.7 (4)
C7—N1—C6—C1	0.4 (3)	C8—C9—C10—C11	54.9 (4)
C4—C5—C6—N1	179.6 (3)	N2—C9—C10—C11	−122.8 (3)
C4—C5—C6—C1	−1.2 (4)	C15—C10—C11—C12	−1.3 (4)
C2—C1—C6—N1	−179.1 (3)	C9—C10—C11—C12	178.2 (3)
N2—C1—C6—N1	−0.4 (3)	C16—O1—C12—C11	−1.6 (5)
C2—C1—C6—C5	1.5 (4)	C16—O1—C12—C13	−179.9 (3)
N2—C1—C6—C5	−179.8 (3)	C10—C11—C12—O1	−177.9 (3)
C6—N1—C7—N2	−0.3 (3)	C10—C11—C12—C13	0.3 (5)
C6—N1—C7—S1	−176.2 (3)	O1—C12—C13—C14	178.9 (3)
C1—N2—C7—N1	0.0 (3)	C11—C12—C13—C14	0.5 (5)
C9—N2—C7—N1	−176.5 (2)	C12—C13—C14—C15	−0.3 (5)
C1—N2—C7—S1	176.94 (19)	C13—C14—C15—C10	−0.8 (5)
C9—N2—C7—S1	0.4 (3)	C11—C10—C15—C14	1.6 (4)
C8—S1—C7—N1	175.4 (3)	C9—C10—C15—C14	−177.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*N*1···O3	0.94 (4)	1.85 (4)	2.750 (3)	160 (3)
N1—H1*N*1···O4	0.94 (4)	2.50 (4)	3.199 (4)	132 (3)

O2—H1*O*2···O3^{i}	0.97	1.60	2.531 (4)	158
C11—H11*A*···O5^{ii}	0.93	2.32	3.237 (4)	170

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