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4-Nitrobenzoic acid–sulfathiazole (1/1)

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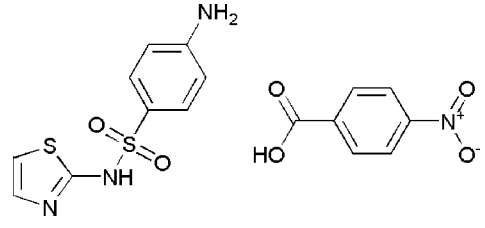
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.002 Å; R factor = 0.026; wR factor = 0.104; data-to-parameter ratio = 11.2.

In the crystal structure of the title compound, $C_7H_5NO_4\cdot C_9H_9N_3O_2S_2$, the sulfathiazole and 4-nitrobenzoic acid molecules are held together by short π–π contacts between the thiazole and nitrobenzene rings, with a centroid–centroid distance of 3.8226 (7) Å. The sulfathiazole molecules form dimers *via* N—H···N hydrogen bonds involving the thiazole and sulfonamide moieties, owing to the fact that sulfathizole exhibits amide–imide tautomerism. The N—H (amine) groups of two sulfathiazole molecules are linked to the two S=O groups of a sulfathiazole *via* N—H···O hydrogen bonds. Two molecules of coformer are held together by O—H···O hydrogen bonds. These units self-assemble, forming a three-dimensional network stabilized by (acid)C—H···π(sulfathiazole benzene ring) interactions.

Related literature

For polymorphism in sulfathiazole, see: Lagas & Lerk (1981); Blagden *et al.* (1998); Hughes *et al.* (1999); For hydrogen bonding in sulfonamides, see: Adsmond & Grant (2000). For the packing similarity of five polymorphs of sulfathiazole, see: Gelbrich *et al.* (2008). For solvates of sulfathiazole, see: Bingham *et al.* (2001). For co-crystals of sulfathiazole, see: Shefter & Sackman (1971); Drebushchak *et al.* (2006).



Experimental

Crystal data

$C_7H_5NO_4\cdot C_9H_9N_3O_2S_2$
M_r = 422.45
Monoclinic, $P2_1/n$
a = 6.6309 (2) Å
b = 15.0142 (6) Å
c = 17.7082 (7) Å
β = 94.551 (1)°
V = 1757.43 (11) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.35 mm^{-1}
T = 296 K
0.50 × 0.42 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.291, T_{max} = 0.482
17445 measured reflections
3460 independent reflections
3329 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.026
$wR(F^2)$ = 0.104
S = 0.89
3460 reflections
309 parameters
69 restraints
All H-atom parameters refined
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.44 e Å^{-3}

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

Cg2 is the centroid of the C1–C6 ring.

D—H···A	D—H	H···A	D···A	D—H···A
O4—H14···O3^{i}	1.03 (4)	1.63 (4)	2.6493 (13)	172 (3)
N1—H8···O1^{ii}	0.82 (2)	2.22 (2)	3.0113 (15)	163.3 (18)
N1—H9···O2^{iii}	0.838 (19)	2.326 (19)	3.0509 (15)	145.0 (17)
N3—H5···N2^{iv}	0.897 (19)	1.96 (2)	2.8583 (15)	174.2 (16)
C14—H12···*Cg2*^{v}	0.974 (18)	2.867 (18)	3.6648 (14)	139.8 (15)

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* and *Mercury*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DS2237).

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supplementary materials

Acta Cryst. (2014). E**70**, o85–o86 [doi:10.1107/S1600536813034004]

4-Nitrobenzoic acid–sulfathiazole (1/1)

Madhavi Oruganti and Darshak R. Trivedi

1. Comment

Sulfathiazole is an antimicrobial compound that belongs to the family of sulfa drugs (contains sulfonamide unit). The title compound crystallizes in $P2_1/n$ space group with one molecule each of sulfathiazole and 4-nitrobenzoic acid in the asymmetric unit. The two S=O (of sulfathiazole) are hydrogen bonded to the N—H (amine) of two other sulfathiazole molecules. The N of the thiazole is involved in the amide imide tautomerism thus rendering the hydrogen bond donating and accepting ability to N—H (thiazole) and N (amide). Sulfathiazole molecules thus self-assemble to form dimers *via* N—H···N hydrogen bonds [N···N 2.852 (1) Å, ⟨NHN 174 (2)] involving thiazole and sulfonamide moieties. Similarly two molecules of 4-Nitrobenzoic acid interact *via* O—H···O hydrogen bonds. The whole assembly repeats to form a three-dimensional network which is stabilized by C—H (acid)···π (benzene of sulfathizole) with a distance of 3.665 Å.

2. Experimental

A mixture of (200 mg, 0.78 mmol) sulfathiazole and (130.9 mg, 0.78 mmol) 4-Nitrobenzoic acid were dissolved in (1:1) mixture (12 ml) of acetonitrile and ethanol, sonicated followed by mild heating. Yellow coloured needle shaped crystals were obtained in 7 days.

Computing details

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT* (Bruker, 2001); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *Mercury* (Macrae *et al.*, 2008); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

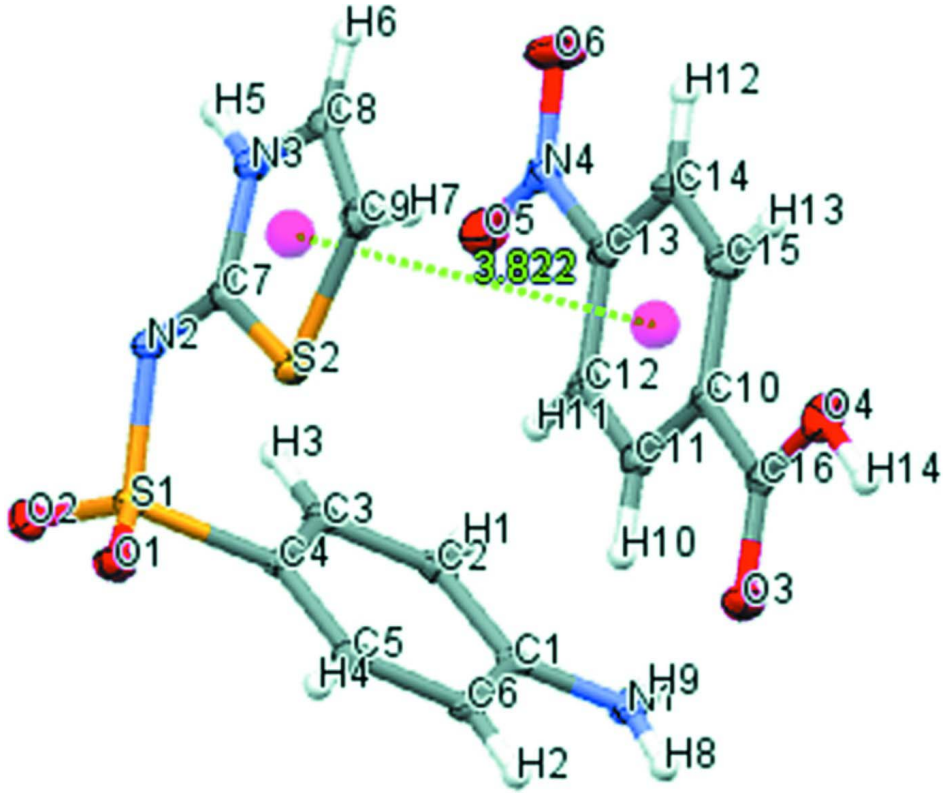

Figure 1

The molecular structure of the title compound showing 50% displacement ellipsoids.

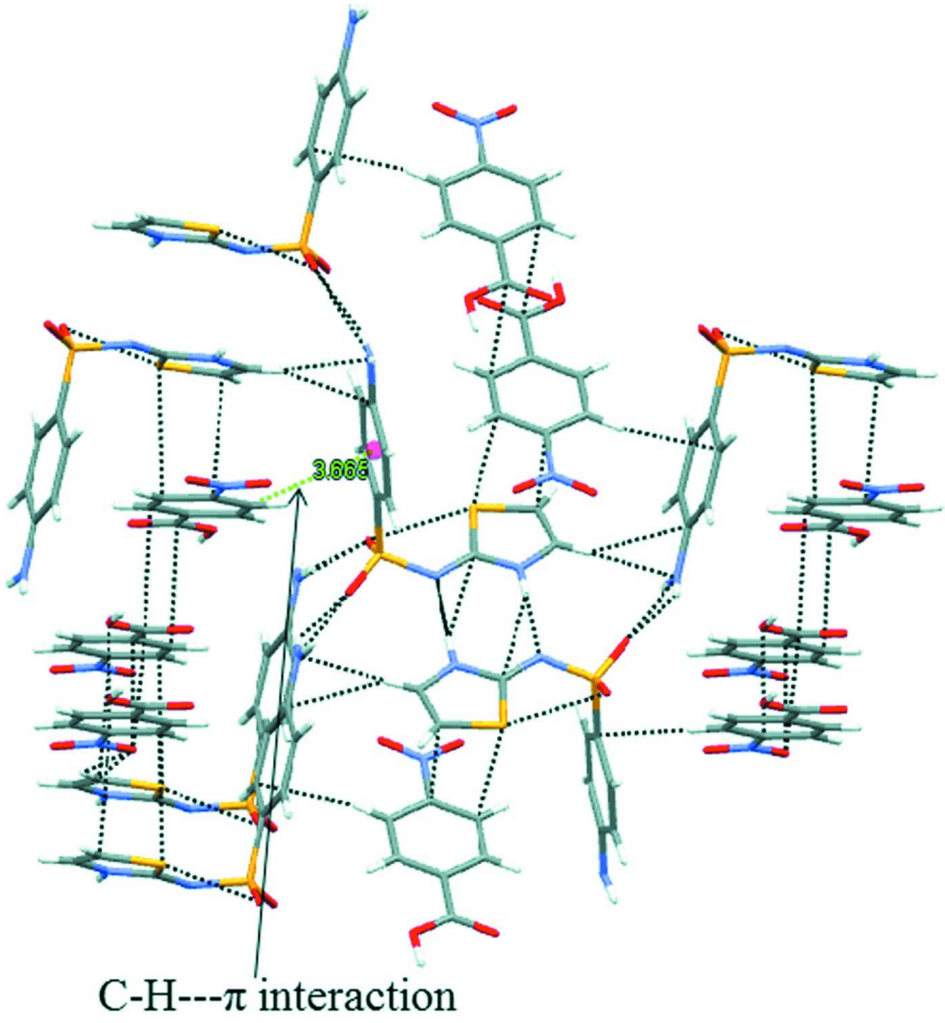

Figure 2

The 3D network stabilized by C—H···π interactions.

4-Amino-*N*-(1,3-thiazol-2-yl)benzenesulfonamide–4-nitrobenzoic acid (1/1)

Crystal data

$C_7H_5NO_4 \cdot C_9H_9N_3O_2S_2$
M_r = 422.45
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 6.6309 (2) Å
b = 15.0142 (6) Å
c = 17.7082 (7) Å
β = 94.551 (1)°
V = 1757.43 (11) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.600 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
μ = 0.35 mm^{-1}
T = 296 K
Needle, yellow
0.50 × 0.42 × 0.21 mm

Data collection

Bruker APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
w scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2004)
T_{min} = 0.291, T_{max} = 0.482

17445 measured reflections
3460 independent reflections
3329 reflections with $I > 2\sigma(I)$
$R_{int} = 0.014$
$\theta_{max} = 26.0°$, $\theta_{min} = 1.8°$
$h = -8 \rightarrow 8$
$k = -18 \rightarrow 18$
$l = -21 \rightarrow 21$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.026$
$wR(F^2) = 0.104$
$S = 0.89$
3460 reflections
309 parameters
69 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.1P)^2 + 0.4859P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.39$ e Å^{-3}
$\Delta\rho_{min} = -0.44$ 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}
S2	0.48584 (4)	0.124204 (19)	0.466507 (17)	0.01376 (12)
S1	0.14759 (4)	0.067179 (19)	0.329580 (16)	0.01280 (12)
O3	0.79216 (14)	0.45216 (6)	0.45069 (5)	0.0192 (2)
O1	0.35756 (14)	0.06086 (6)	0.31268 (5)	0.0177 (2)
O2	0.00325 (15)	0.01141 (6)	0.28659 (5)	0.0205 (2)
O4	0.87828 (14)	0.45703 (6)	0.57587 (6)	0.0207 (2)
O5	−0.09352 (14)	0.24225 (7)	0.52201 (6)	0.0238 (2)
O6	−0.00680 (16)	0.24314 (8)	0.64238 (6)	0.0288 (3)
N3	0.21354 (16)	0.06402 (7)	0.54483 (6)	0.0131 (2)
N1	−0.09830 (18)	0.44403 (8)	0.28520 (6)	0.0168 (2)
N2	0.11857 (15)	0.04399 (7)	0.41709 (6)	0.0136 (2)
N4	0.02308 (16)	0.26183 (7)	0.57682 (6)	0.0169 (2)
C10	0.56484 (18)	0.39184 (8)	0.53399 (7)	0.0127 (2)
C1	−0.04137 (19)	0.35734 (8)	0.29501 (6)	0.0138 (3)
C12	0.24664 (18)	0.32664 (8)	0.48782 (7)	0.0140 (3)
C4	0.07641 (18)	0.17915 (8)	0.31658 (6)	0.0124 (2)
C11	0.42711 (18)	0.36829 (8)	0.47388 (7)	0.0135 (3)
C16	0.75894 (18)	0.43659 (8)	0.51864 (7)	0.0128 (3)
C7	0.25113 (17)	0.07326 (7)	0.47175 (7)	0.0119 (2)
C14	0.34332 (19)	0.33362 (9)	0.62365 (7)	0.0174 (3)
C5	0.21340 (18)	0.24129 (8)	0.29195 (7)	0.0142 (3)
C13	0.21044 (18)	0.30973 (8)	0.56242 (7)	0.0139 (3)

C6	0.15541 (18)	0.32935 (8)	0.28082 (7)	0.0148 (3)
C2	−0.17804 (18)	0.29326 (9)	0.31906 (7)	0.0154 (3)
C3	−0.12052 (18)	0.20556 (8)	0.32984 (7)	0.0148 (3)
C8	0.36390 (19)	0.09498 (8)	0.59690 (7)	0.0152 (3)
C9	0.5208 (2)	0.13065 (8)	0.56467 (7)	0.0163 (3)
C15	0.5226 (2)	0.37525 (8)	0.60900 (7)	0.0162 (3)
H4	0.348 (2)	0.2196 (10)	0.2828 (8)	0.015 (3)*
H2	0.241 (2)	0.3722 (10)	0.2601 (8)	0.011 (4)*
H3	−0.214 (2)	0.1644 (11)	0.3479 (9)	0.018 (4)*
H1	−0.309 (3)	0.3095 (11)	0.3254 (9)	0.020 (4)*
H7	0.641 (2)	0.1555 (11)	0.5896 (9)	0.020 (4)*
H6	0.349 (2)	0.0888 (11)	0.6484 (10)	0.017 (4)*
H10	0.460 (3)	0.3790 (11)	0.4221 (10)	0.021 (4)*
H13	0.611 (3)	0.3917 (11)	0.6479 (10)	0.019 (4)*
H11	0.156 (3)	0.3092 (12)	0.4478 (10)	0.025 (4)*
H12	0.320 (3)	0.3195 (13)	0.6759 (10)	0.029 (4)*
H5	0.104 (3)	0.0336 (12)	0.5566 (10)	0.027 (4)*
H9	−0.220 (3)	0.4583 (12)	0.2857 (11)	0.027 (4)*
H8	−0.017 (3)	0.4768 (13)	0.2669 (11)	0.031 (5)*
H14	1.001 (6)	0.493 (2)	0.561 (2)	0.109 (11)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S2	0.01302 (19)	0.01389 (19)	0.01468 (19)	−0.00210 (10)	0.00299 (13)	0.00102 (10)
S1	0.0164 (2)	0.01270 (19)	0.00949 (19)	−0.00064 (10)	0.00203 (13)	0.00004 (10)
O3	0.0198 (5)	0.0193 (5)	0.0197 (5)	−0.0013 (4)	0.0093 (4)	0.0007 (4)
O1	0.0197 (5)	0.0185 (5)	0.0158 (5)	0.0037 (3)	0.0074 (4)	0.0010 (3)
O2	0.0281 (5)	0.0176 (5)	0.0152 (5)	−0.0048 (4)	−0.0027 (4)	−0.0023 (3)
O4	0.0150 (5)	0.0204 (5)	0.0259 (5)	−0.0033 (4)	−0.0035 (4)	0.0017 (4)
O5	0.0178 (5)	0.0270 (5)	0.0261 (5)	−0.0070 (4)	−0.0006 (4)	0.0014 (4)
O6	0.0263 (5)	0.0393 (6)	0.0221 (5)	−0.0084 (4)	0.0090 (4)	0.0071 (4)
N3	0.0136 (5)	0.0136 (5)	0.0121 (5)	−0.0014 (4)	0.0017 (4)	0.0018 (4)
N1	0.0178 (6)	0.0163 (5)	0.0165 (6)	0.0004 (4)	0.0029 (4)	0.0025 (4)
N2	0.0153 (5)	0.0150 (5)	0.0107 (5)	−0.0025 (4)	0.0015 (4)	0.0020 (4)
N4	0.0148 (5)	0.0149 (5)	0.0216 (6)	0.0002 (4)	0.0046 (4)	0.0031 (4)
C10	0.0128 (6)	0.0112 (5)	0.0144 (6)	0.0015 (4)	0.0028 (4)	0.0004 (4)
C1	0.0182 (6)	0.0167 (6)	0.0063 (5)	−0.0011 (5)	−0.0013 (4)	−0.0005 (4)
C12	0.0141 (6)	0.0133 (6)	0.0143 (6)	0.0005 (4)	0.0000 (5)	−0.0012 (4)
C4	0.0151 (6)	0.0136 (6)	0.0084 (5)	−0.0002 (4)	0.0008 (4)	0.0007 (4)
C11	0.0153 (6)	0.0130 (6)	0.0125 (6)	0.0015 (4)	0.0028 (5)	−0.0001 (4)
C16	0.0122 (6)	0.0100 (6)	0.0163 (6)	0.0021 (4)	0.0013 (5)	−0.0005 (4)
C7	0.0135 (6)	0.0092 (5)	0.0133 (6)	0.0015 (4)	0.0020 (5)	0.0017 (4)
C14	0.0185 (6)	0.0208 (6)	0.0131 (6)	−0.0002 (5)	0.0032 (5)	0.0037 (5)
C5	0.0134 (6)	0.0187 (6)	0.0104 (5)	−0.0009 (4)	0.0006 (4)	0.0013 (4)
C13	0.0133 (6)	0.0121 (6)	0.0168 (6)	0.0014 (4)	0.0032 (4)	0.0011 (4)
C6	0.0154 (6)	0.0165 (6)	0.0125 (6)	−0.0027 (5)	0.0008 (4)	0.0034 (4)
C2	0.0138 (6)	0.0210 (6)	0.0118 (6)	0.0000 (5)	0.0030 (4)	−0.0017 (5)
C3	0.0159 (6)	0.0172 (6)	0.0118 (6)	−0.0037 (5)	0.0033 (4)	0.0003 (4)
C8	0.0183 (6)	0.0143 (6)	0.0126 (6)	0.0011 (5)	−0.0015 (5)	0.0008 (5)

C9	0.0172 (6)	0.0151 (6)	0.0164 (6)	−0.0008 (5)	−0.0012 (5)	−0.0010 (4)
C15	0.0168 (6)	0.0189 (6)	0.0127 (6)	−0.0015 (5)	−0.0010 (5)	0.0005 (4)

Geometric parameters (Å, º)

S2—C9	1.7381 (14)	C1—C6	1.4122 (17)
S2—C7	1.7433 (12)	C12—C13	1.3848 (17)
S1—O2	1.4426 (10)	C12—C11	1.3896 (17)
S1—O1	1.4502 (9)	C4—C5	1.3961 (17)
S1—N2	1.6146 (10)	C4—C3	1.4022 (17)
S1—C4	1.7563 (12)	C14—C15	1.3859 (18)
O3—C16	1.2622 (16)	C14—C13	1.3890 (18)
O4—C16	1.2729 (16)	C5—C6	1.3866 (17)
O5—N4	1.2276 (16)	C2—C3	1.3798 (19)
O6—N4	1.2257 (15)	C8—C9	1.3375 (18)
N3—C7	1.3445 (16)	N1—H8	0.82 (2)
N3—C8	1.3836 (16)	N1—H9	0.84 (2)
N1—C1	1.3626 (17)	N3—H5	0.897 (19)
N2—C7	1.3294 (16)	C2—H1	0.92 (2)
N4—C13	1.4751 (16)	C3—H3	0.949 (15)
C10—C11	1.3920 (17)	C5—H4	0.976 (14)
C10—C15	1.4013 (17)	C6—H2	0.951 (14)
C10—C16	1.4958 (16)	C8—H6	0.930 (18)
C1—C2	1.4106 (17)	C9—H7	0.956 (15)
C9—S2—C7	91.15 (6)	N3—C7—S2	109.33 (9)
O2—S1—O1	117.43 (6)	C15—C14—C13	118.09 (11)
O2—S1—N2	104.88 (5)	C6—C5—C4	120.11 (11)
O1—S1—N2	111.93 (5)	C12—C13—C14	123.38 (11)
O2—S1—C4	109.05 (6)	C12—C13—N4	117.81 (11)
O1—S1—C4	106.74 (5)	C14—C13—N4	118.80 (11)
N2—S1—C4	106.31 (5)	C5—C6—C1	120.54 (11)
C7—N3—C8	115.34 (11)	C3—C2—C1	121.03 (11)
C7—N2—S1	120.35 (9)	C2—C3—C4	119.84 (11)
O6—N4—O5	123.71 (11)	C9—C8—N3	113.21 (11)
O6—N4—C13	118.49 (11)	C8—C9—S2	110.97 (10)
O5—N4—C13	117.80 (10)	C14—C15—C10	119.77 (12)
C11—C10—C15	120.76 (12)	C1—N1—H8	116.2 (14)
C11—C10—C16	119.79 (11)	C1—N1—H9	120.1 (13)
C15—C10—C16	119.44 (11)	H8—N1—H9	121.3 (19)
N1—C1—C2	120.80 (12)	C7—N3—H5	119.5 (11)
N1—C1—C6	120.80 (12)	C8—N3—H5	124.8 (11)
C2—C1—C6	118.40 (11)	C1—C2—H1	119.5 (10)
C13—C12—C11	117.96 (11)	C3—C2—H1	119.4 (10)
C5—C4—C3	120.06 (11)	C2—C3—H3	119.2 (9)
C5—C4—S1	120.40 (9)	C4—C3—H3	121.0 (9)
C3—C4—S1	119.53 (9)	C4—C5—H4	117.1 (9)
C12—C11—C10	120.03 (11)	C6—C5—H4	122.8 (9)
O3—C16—O4	124.74 (11)	C1—C6—H2	117.1 (9)
O3—C16—C10	118.31 (11)	C5—C6—H2	122.2 (9)

O4—C16—C10	116.95 (11)	N3—C8—H6	119.6 (9)
N2—C7—N3	120.29 (11)	C9—C8—H6	127.3 (9)
N2—C7—S2	130.38 (9)		

Hydrogen-bond geometry (Å, º)

Cg2 is the centroid of the C1–C6 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H14···O3^{i}	1.03 (4)	1.63 (4)	2.6493 (13)	172 (3)
N1—H8···O1^{ii}	0.82 (2)	2.22 (2)	3.0113 (15)	163.3 (18)
N1—H9···O2^{iii}	0.838 (19)	2.326 (19)	3.0509 (15)	145.0 (17)
N3—H5···N2^{iv}	0.897 (19)	1.96 (2)	2.8583 (15)	174.2 (16)
C14—H12···*Cg*2^{v}	0.974 (18)	2.867 (18)	3.6648 (14)	139.8 (15)

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