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2,2′-(4-Methyl-4*H*-1,2,4-triazole-3,5-diyl)-dibenzenesulfonamide

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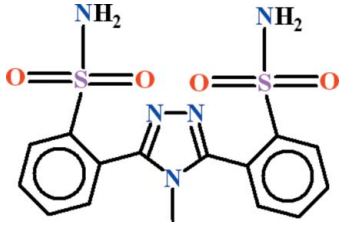
Key indicators: single-crystal X-ray study; T = 296 K; mean σ(C–C) = 0.004 Å; R factor = 0.059; wR factor = 0.158; data-to-parameter ratio = 17.0.

In the title compound, $C_{15}H_{15}N_5O_4S_2$, the dihedral angles between the central 1,2,4-triazole ring and the pendant benzene rings are 55.61 (10) and 68.59 (10)°; the dihedral angle between the benzene rings is 63.66 (9)°. Intramolecular N—H···N and N—H···O hydrogen bonds generate S(7) and S(12) rings, respectively. In the crystal, sheets extending in the (101) plane arise, with the molecules linked by C—H···O, N—H···N and N—H···O interactions. A C—H···π interaction further consolidates the structure.

Related literature

For background to benzisothiazole derivatives, see: Siddiqui *et al.* (2007); Siddiqui, Ahmad, Khan *et al.* (2008); Siddiqui, Ahmad, Siddiqui & Parvez (2008). For related crystal structures, see: Carlsen *et al.* (1995). For graph-set notation, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{15}H_{15}N_5O_4S_2$
M_r = 393.44
Monoclinic, $P2_1/n$
a = 13.4190 (6) Å
b = 6.9043 (2) Å
c = 19.0498 (9) Å
β = 102.243 (2)°
V = 1724.80 (12) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.34 mm^{-1}
T = 296 K
0.35 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.915, T_{max} = 0.938
15158 measured reflections
4055 independent reflections
2526 reflections with $I > 2\sigma(I)$
R_{int} = 0.060

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.158
S = 1.03
4055 reflections
239 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

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

*Cg*1 and *Cg*3 are the centroids of the C7/N2/C8/N3/N4 and C10–C15 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···O3	0.82 (4)	2.33 (4)	3.082 (4)	153 (3)
N1—H1*B*···N4^{i}	0.95 (4)	1.96 (4)	2.899 (4)	171 (3)
N5—H5*A*···O4^{ii}	0.94 (4)	2.10 (4)	3.011 (4)	164 (3)
N5—H5*B*···N3	0.83 (4)	2.14 (4)	2.876 (4)	148 (4)
C9—H9*B*···O2^{iii}	0.96	2.17	2.990 (3)	142
C14—H14···*Cg*3^{iv}	0.93	2.68	3.583 (4)	163

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

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 1997) and *PLATON* (Spek, 2009); software used to prepare material for publication: *WinGX* (Farrugia, 1999) and *PLATON*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6629).

References

Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
Bruker (2005). *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Bruker (2009). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Carlsen, P. H. J., Jorgensen, K. B., Gautun, O. R., Jagner, S. & Hakansson, M. (1995). *Acta Chem. Scand.* **49**, 676–682.
Farrugia, L. J. (1997). *J. Appl. Cryst.* **30**, 565.
Farrugia, L. J. (1999). *J. Appl. Cryst.* **32**, 837–838.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siddiqui, W. A., Ahmad, S., Khan, I. U., Siddiqui, H. L. & Parvez, M. (2008). *Acta Cryst.* C**64**, o286–o289.
Siddiqui, W. A., Ahmad, S., Siddiqui, H. L. & Parvez, M. (2008). *Acta Cryst.* E**64**, o724.
Siddiqui, W. A., Ahmad, S., Siddiqui, H. L., Tariq, M. I. & Parvez, M. (2007). *Acta Cryst.* E**63**, o4001.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

supporting information

Acta Cryst. (2012). E**68**, o754 [doi:10.1107/S1600536812006113]

2,2′-(4-Methyl-4*H*-1,2,4-triazole-3,5-diyl)dibenzenesulfonamide

Tasleem Akhtar, Waseeq Ahmad Siddiqui, Adnan Ashraf and M. Nawaz Tahir

S1. Comment

In continuation to our research work on the synthesis of benzisothiazole derivatives (Siddiqui, Ahmad, Khan *et al.*, 2008; Siddiqui, Ahmad, Siddiqui & Parvez, 2008), the title compound (I), (Fig. 1) is prepared from hydrazine and commercial source of saccharin.

The crystal structures of 4-methyl-3,5-diphenyl-4*H*-1,2,4-triazolethe has been published which is also related to (I).

In (I), the phenyl rings A (C1–C6), B (C10—C15) and the 4-methyl-4*H*- 1,2,4-triazole moiety C (C7–C9/N2–N4) are planar with r. m. s. deviation of 0.0079 Å, 0.0051 Å and 0.0310 Å, respectively. The dihedral angle between A/B, A/C and B/C is 63.66 (9)°, 68.59 (1)° and 55.61 (10)°, respectively. There exist intramolecular H-bonding of N—H···N and N—H···O types (Table 1, Fig. 1) forming S (7) and S (12) ring motifs (Bernstein *et al.*, 1995), respectively. There exist intermolecular H-bondings of C—H···.O, N—H···N and N—H···O types (Table 1, Fig. 2) which consolidates the molecules in the form two-dimensional polymeric network extending along the (101) plane. There exist C—H···π (Table 1) interactions which also play role in establishing the structure.

S2. Experimental

For the synthesis of title compound, hydrazine monohydrate and saccharin were used as the starting materials following a reported procedure (Siddiqui *et al.*, 2007). Colourless needles of (I) suitable for X-ray crystallographic study were grown from methanol at room temperature. m. p. = 483–484 K. FT—IR: (KBr, cm^{-1}): 3296, 3263 (NH and NH_2), 2987 (Ar. CH), 1651 (C═ N), 1541 (NH def.), 1454 (CH def.), 1315, 1151 (SO_2).

S3. Refinement

The coordinates of H-atoms of amino groups were refined. The H-atoms were positioned geometrically (C—H = 0.93–0.96 Å) and refined as riding with U_{iso}(H) = xU_{eq}(C, N), where x = 1.5 for methyl groups and x = 1.2 for all other H-atoms.

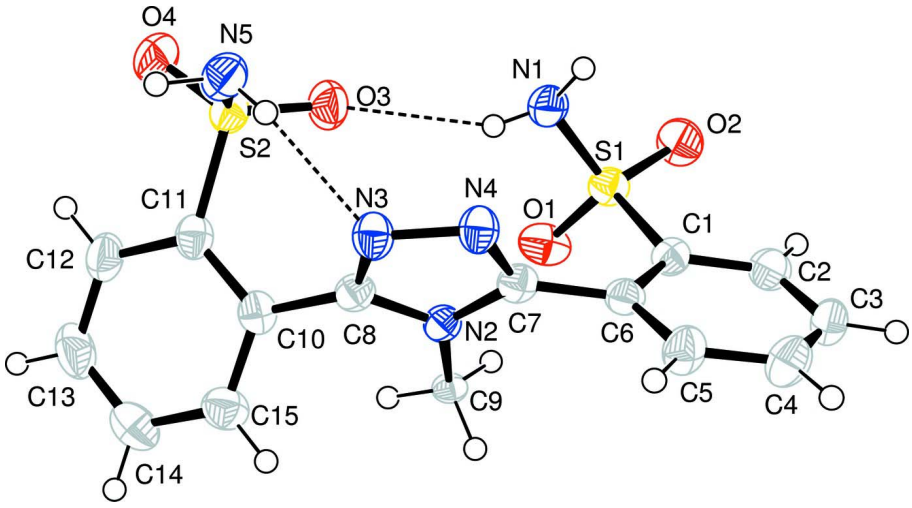

Figure 1

View of the title compound with displacement ellipsoids drawn at the 50% probability level. The dotted lines represent the intramolecular hydrogen bonds.

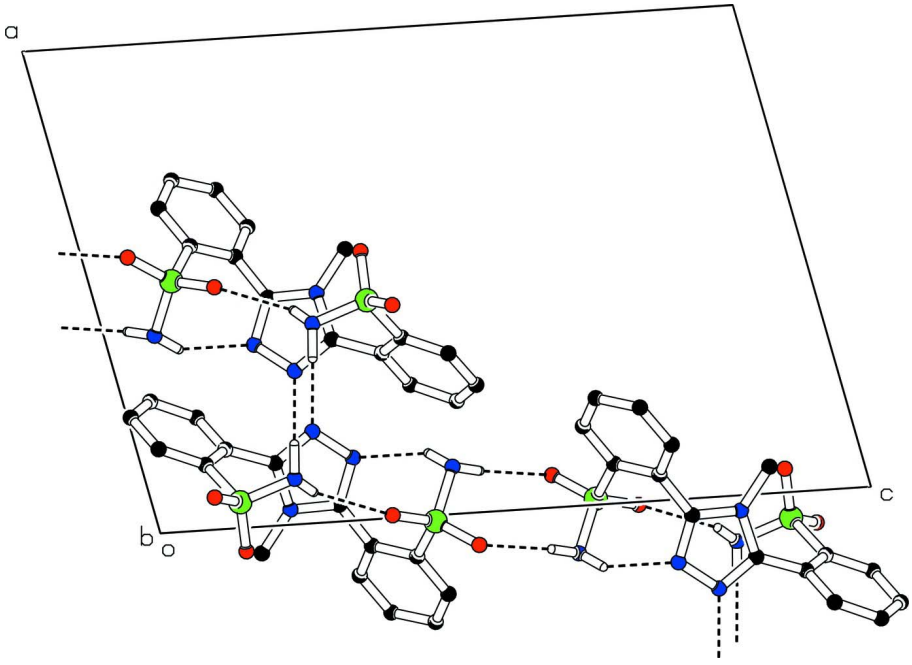

Figure 2

The partial packing (*PLATON*; Spek, 2009) which shows that molecules form two dimensional polymeric network in the plane (101).

2,2′-(4-Methyl-4*H*-1,2,4-triazole-3,5-diyl)dibenzenesulfonamide

Crystal data

$C_{15}H_{15}N_5O_4S_2$
M_r = 393.44
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn

a = 13.4190 (6) Å
b = 6.9043 (2) Å
c = 19.0498 (9) Å
β = 102.243 (2)°

V = 1724.80 (12) Å^3
Z = 4
F(000) = 816
D_x = 1.515 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2526 reflections

θ = 2.1–27.9°
μ = 0.34 mm^{-1}
T = 296 K
Prism, colourless
0.35 × 0.25 × 0.22 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 7.60 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2005)
T_{min} = 0.915, T_{max} = 0.938

15158 measured reflections
4055 independent reflections
2526 reflections with $I > 2\sigma(I)$
R_{int} = 0.060
θ_{max} = 27.9°, θ_{min} = 2.1°
h = −17→17
k = −5→9
l = −24→25

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.059
$wR(F^2)$ = 0.158
S = 1.03
4055 reflections
239 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
$w = 1/[\sigma^2(F_o^2) + (0.0762P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.63 e Å^{-3}
$\Delta\rho_{min}$ = −0.66 e Å^{-3}

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

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	0.05268 (6)	1.38253 (11)	0.12266 (4)	0.0315 (3)
S2	−0.01231 (6)	1.09870 (12)	0.38488 (4)	0.0358 (3)
O1	−0.04824 (15)	1.3040 (3)	0.11187 (13)	0.0438 (8)
O2	0.06566 (19)	1.5630 (3)	0.08924 (13)	0.0470 (9)
O3	0.00582 (18)	1.2207 (3)	0.32800 (12)	0.0444 (8)
O4	−0.06624 (19)	1.1753 (4)	0.43601 (13)	0.0509 (9)
N1	0.0933 (2)	1.4069 (4)	0.20696 (16)	0.0362 (9)
N2	0.03107 (18)	0.9092 (3)	0.18915 (13)	0.0266 (8)
N3	0.12821 (19)	0.8730 (4)	0.29572 (14)	0.0340 (8)
N4	0.18700 (19)	0.9443 (4)	0.25015 (14)	0.0327 (8)

N5	0.0966 (2)	1.0255 (5)	0.42979 (16)	0.0423 (10)
C1	0.1333 (2)	1.2155 (4)	0.08967 (16)	0.0286 (9)
C2	0.1717 (2)	1.2741 (5)	0.03096 (17)	0.0369 (11)
C3	0.2396 (3)	1.1553 (5)	0.00495 (18)	0.0408 (11)
C4	0.2696 (3)	0.9836 (5)	0.03807 (19)	0.0447 (12)
C5	0.2307 (2)	0.9214 (5)	0.09593 (18)	0.0379 (11)
C6	0.1620 (2)	1.0357 (4)	0.12269 (16)	0.0292 (9)
C7	0.1277 (2)	0.9661 (4)	0.18635 (16)	0.0287 (9)
C8	0.0343 (2)	0.8550 (4)	0.25834 (16)	0.0286 (9)
C9	−0.05428 (11)	0.8905 (4)	0.13235 (8)	0.0214 (8)
C10	−0.05358 (11)	0.7942 (3)	0.28739 (8)	0.0307 (10)
C11	−0.08105 (11)	0.8909 (3)	0.34553 (8)	0.0330 (10)
C12	−0.16186 (11)	0.8275 (3)	0.37385 (8)	0.0438 (11)
C13	−0.2172 (3)	0.6684 (6)	0.3451 (2)	0.0513 (14)
C14	−0.1922 (3)	0.5723 (5)	0.2878 (2)	0.0480 (14)
C15	−0.1123 (3)	0.6349 (5)	0.25875 (19)	0.0400 (11)
H1A	0.063 (3)	1.330 (5)	0.2279 (18)	0.0435*
H1B	0.164 (3)	1.434 (5)	0.2203 (18)	0.0435*
H2	0.15207	1.39242	0.00900	0.0442*
H3	0.26444	1.19303	−0.03496	0.0490*
H4	0.31685	0.90708	0.02156	0.0538*
H5	0.25064	0.80228	0.11706	0.0454*
H5A	0.085 (3)	0.941 (5)	0.466 (2)	0.0509*
H5B	0.128 (3)	0.971 (6)	0.402 (2)	0.0509*
H9A	−0.11300	0.85753	0.15121	0.0321*
H9B	−0.04191	0.79024	0.10032	0.0321*
H9C	−0.06624	1.01082	0.10672	0.0321*
H12	−0.17881	0.89259	0.41243	0.0524*
H13	−0.27155	0.62553	0.36427	0.0613*
H14	−0.22961	0.46418	0.26857	0.0577*
H15	−0.09730	0.57006	0.21947	0.0480*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0307 (4)	0.0274 (4)	0.0364 (5)	0.0039 (3)	0.0074 (3)	−0.0018 (3)
S2	0.0423 (5)	0.0348 (5)	0.0332 (5)	−0.0007 (3)	0.0148 (4)	−0.0013 (3)
O1	0.0263 (11)	0.0412 (13)	0.0614 (16)	0.0034 (10)	0.0036 (11)	−0.0089 (12)
O2	0.0642 (16)	0.0277 (12)	0.0519 (16)	0.0059 (11)	0.0186 (13)	0.0070 (11)
O3	0.0603 (15)	0.0357 (13)	0.0417 (14)	0.0005 (11)	0.0209 (12)	0.0067 (11)
O4	0.0629 (16)	0.0508 (15)	0.0467 (15)	0.0013 (12)	0.0293 (12)	−0.0079 (12)
N1	0.0323 (15)	0.0407 (17)	0.0381 (17)	−0.0015 (12)	0.0128 (12)	−0.0058 (13)
N2	0.0264 (12)	0.0258 (13)	0.0283 (14)	0.0021 (10)	0.0076 (10)	−0.0016 (11)
N3	0.0288 (13)	0.0396 (16)	0.0343 (15)	0.0012 (12)	0.0084 (11)	0.0036 (12)
N4	0.0281 (13)	0.0381 (15)	0.0329 (15)	0.0027 (11)	0.0089 (11)	0.0039 (12)
N5	0.0444 (17)	0.050 (2)	0.0328 (17)	−0.0027 (15)	0.0087 (13)	−0.0014 (14)
C1	0.0262 (15)	0.0314 (17)	0.0273 (16)	0.0010 (13)	0.0038 (12)	−0.0009 (13)
C2	0.0411 (18)	0.0367 (19)	0.0317 (18)	−0.0037 (15)	0.0053 (14)	0.0017 (15)

C3	0.0415 (19)	0.051 (2)	0.0340 (19)	−0.0078 (16)	0.0171 (15)	−0.0034 (17)
C4	0.043 (2)	0.049 (2)	0.047 (2)	0.0085 (17)	0.0205 (16)	−0.0061 (18)
C5	0.0394 (18)	0.0351 (19)	0.043 (2)	0.0096 (14)	0.0170 (15)	0.0021 (15)
C6	0.0262 (15)	0.0291 (17)	0.0326 (17)	−0.0019 (13)	0.0069 (13)	−0.0053 (14)
C7	0.0262 (15)	0.0273 (16)	0.0332 (17)	0.0045 (12)	0.0080 (13)	−0.0027 (13)
C8	0.0303 (15)	0.0260 (16)	0.0302 (17)	0.0036 (12)	0.0077 (13)	−0.0024 (13)
C9	0.0180 (13)	0.0237 (15)	0.0206 (14)	−0.0009 (11)	−0.0002 (11)	−0.0030 (12)
C10	0.0279 (15)	0.0306 (17)	0.0346 (18)	0.0041 (13)	0.0092 (13)	0.0040 (14)
C11	0.0305 (16)	0.0385 (19)	0.0300 (17)	0.0013 (13)	0.0065 (13)	0.0054 (14)
C12	0.0427 (19)	0.057 (2)	0.0361 (19)	−0.0083 (17)	0.0182 (15)	0.0004 (17)
C13	0.040 (2)	0.062 (3)	0.055 (2)	−0.0150 (18)	0.0174 (18)	0.010 (2)
C14	0.040 (2)	0.043 (2)	0.060 (3)	−0.0113 (16)	0.0085 (18)	0.0022 (19)
C15	0.0381 (18)	0.0349 (19)	0.048 (2)	−0.0011 (15)	0.0111 (16)	−0.0046 (16)

Geometric parameters (Å, º)

S1—O1	1.433 (2)	C4—C5	1.384 (5)
S1—O2	1.427 (2)	C5—C6	1.390 (4)
S1—N1	1.592 (3)	C6—C7	1.466 (4)
S1—C1	1.784 (3)	C8—C10	1.466 (3)
S2—O3	1.433 (2)	C10—C11	1.408 (2)
S2—O4	1.432 (3)	C10—C15	1.395 (4)
S2—N5	1.610 (3)	C11—C12	1.381 (2)
S2—C11	1.783 (2)	C12—C13	1.373 (4)
N2—C7	1.367 (4)	C13—C14	1.378 (5)
N2—C8	1.362 (4)	C14—C15	1.376 (6)
N2—C9	1.405 (3)	C2—H2	0.9300
N3—N4	1.382 (4)	C3—H3	0.9300
N3—C8	1.315 (4)	C4—H4	0.9300
N4—C7	1.313 (4)	C5—H5	0.9300
N1—H1B	0.95 (4)	C9—H9A	0.9600
N1—H1A	0.82 (4)	C9—H9B	0.9600
N5—H5B	0.83 (4)	C9—H9C	0.9600
N5—H5A	0.94 (4)	C12—H12	0.9300
C1—C6	1.408 (4)	C13—H13	0.9300
C1—C2	1.387 (4)	C14—H14	0.9300
C2—C3	1.393 (5)	C15—H15	0.9300
C3—C4	1.363 (5)		

O1—S1—O2	117.89 (15)	N2—C8—N3	109.2 (2)
O1—S1—N1	107.21 (15)	N3—C8—C10	125.3 (3)
O1—S1—C1	109.28 (13)	N2—C8—C10	125.5 (2)
O2—S1—N1	108.05 (15)	C11—C10—C15	117.5 (2)
O2—S1—C1	105.47 (14)	C8—C10—C15	120.7 (2)
N1—S1—C1	108.68 (14)	C8—C10—C11	121.80 (19)
O3—S2—O4	119.23 (15)	C10—C11—C12	121.03 (17)
O3—S2—N5	107.80 (15)	S2—C11—C10	120.94 (13)
O3—S2—C11	108.10 (11)	S2—C11—C12	118.04 (13)

O4—S2—N5	106.69 (15)	C11—C12—C13	120.1 (2)
O4—S2—C11	106.99 (13)	C12—C13—C14	119.9 (3)
N5—S2—C11	107.53 (14)	C13—C14—C15	120.6 (3)
C7—N2—C8	106.3 (2)	C10—C15—C14	120.9 (3)
C7—N2—C9	128.4 (2)	C1—C2—H2	120.00
C8—N2—C9	125.0 (2)	C3—C2—H2	120.00
N4—N3—C8	107.6 (2)	C2—C3—H3	120.00
N3—N4—C7	107.9 (2)	C4—C3—H3	120.00
H1A—N1—H1B	125 (3)	C3—C4—H4	120.00
S1—N1—H1A	109 (2)	C5—C4—H4	119.00
S1—N1—H1B	114 (2)	C4—C5—H5	120.00
H5A—N5—H5B	112 (4)	C6—C5—H5	120.00
S2—N5—H5B	109 (3)	N2—C9—H9A	109.00
S2—N5—H5A	108 (3)	N2—C9—H9B	109.00
C2—C1—C6	120.3 (3)	N2—C9—H9C	109.00
S1—C1—C2	116.9 (2)	H9A—C9—H9B	109.00
S1—C1—C6	122.8 (2)	H9A—C9—H9C	109.00
C1—C2—C3	119.9 (3)	H9B—C9—H9C	109.00
C2—C3—C4	119.9 (3)	C11—C12—H12	120.00
C3—C4—C5	121.0 (3)	C13—C12—H12	120.00
C4—C5—C6	120.5 (3)	C12—C13—H13	120.00
C5—C6—C7	117.8 (3)	C14—C13—H13	120.00
C1—C6—C5	118.5 (3)	C13—C14—H14	120.00
C1—C6—C7	123.7 (3)	C15—C14—H14	120.00
N2—C7—N4	109.0 (3)	C10—C15—H15	120.00
N4—C7—C6	124.6 (3)	C14—C15—H15	119.00
N2—C7—C6	126.4 (3)		

O1—S1—C1—C2	114.3 (2)	S1—C1—C6—C7	1.0 (4)
O1—S1—C1—C6	−68.8 (3)	C2—C1—C6—C5	1.2 (4)
O2—S1—C1—C2	−13.3 (3)	C2—C1—C6—C7	177.8 (3)
O2—S1—C1—C6	163.6 (2)	C1—C2—C3—C4	−1.2 (5)
N1—S1—C1—C2	−129.0 (2)	C2—C3—C4—C5	2.4 (6)
N1—S1—C1—C6	47.9 (3)	C3—C4—C5—C6	−1.7 (5)
O3—S2—C11—C10	43.59 (19)	C4—C5—C6—C1	−0.1 (5)
O3—S2—C11—C12	−136.53 (16)	C4—C5—C6—C7	−176.9 (3)
O4—S2—C11—C10	173.16 (17)	C1—C6—C7—N2	69.9 (4)
O4—S2—C11—C12	−6.95 (19)	C1—C6—C7—N4	−111.8 (3)
N5—S2—C11—C10	−72.55 (19)	C5—C6—C7—N2	−113.4 (3)
N5—S2—C11—C12	107.34 (18)	C5—C6—C7—N4	64.8 (4)
C8—N2—C7—N4	1.1 (3)	N2—C8—C10—C11	−121.9 (3)
C8—N2—C7—C6	179.6 (3)	N2—C8—C10—C15	59.2 (4)
C9—N2—C7—N4	−173.4 (3)	N3—C8—C10—C11	55.4 (4)
C9—N2—C7—C6	5.1 (4)	N3—C8—C10—C15	−123.6 (3)
C7—N2—C8—N3	−1.4 (3)	C8—C10—C11—S2	2.2 (3)
C7—N2—C8—C10	176.2 (2)	C8—C10—C11—C12	−177.68 (19)
C9—N2—C8—N3	173.3 (2)	C15—C10—C11—S2	−178.9 (2)
C9—N2—C8—C10	−9.2 (4)	C15—C10—C11—C12	1.3 (3)

C8—N3—N4—C7	−0.5 (3)	C8—C10—C15—C14	177.2 (3)
N4—N3—C8—N2	1.2 (3)	C11—C10—C15—C14	−1.7 (4)
N4—N3—C8—C10	−176.4 (2)	S2—C11—C12—C13	179.8 (2)
N3—N4—C7—N2	−0.4 (3)	C10—C11—C12—C13	−0.3 (3)
N3—N4—C7—C6	−178.9 (3)	C11—C12—C13—C14	−0.2 (5)
S1—C1—C2—C3	176.5 (3)	C12—C13—C14—C15	−0.3 (6)
C6—C1—C2—C3	−0.6 (5)	C13—C14—C15—C10	1.3 (6)
S1—C1—C6—C5	−175.6 (2)		

Hydrogen-bond geometry (Å, º)

Cg1 and Cg3 are the centroids of the C7/N2/C8/N3/N4 and C10–C15 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1—H1*A*···O3	0.82 (4)	2.33 (4)	3.082 (4)	153 (3)
N1—H1*B*···N4^{i}	0.95 (4)	1.96 (4)	2.899 (4)	171 (3)
N5—H5*A*···O4^{ii}	0.94 (4)	2.10 (4)	3.011 (4)	164 (3)
N5—H5*B*···N3	0.83 (4)	2.14 (4)	2.876 (4)	148 (4)
C9—H9*B*···O2^{iii}	0.96	2.17	2.990 (3)	142
C14—H14···*Cg*3^{iv}	0.93	2.68	3.583 (4)	163

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