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ISSN 2414-3146

3-[2-(9*H*-Carbazol-9-yl)ethyl]-4-phenyl-1*H*-1,2,4-triazole-5(4*H*)-thione dimethyl sulfoxide monosolvate

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Received 10 November 2016
Accepted 16 November 2016

Edited by J. Simpson, University of Otago, New Zealand

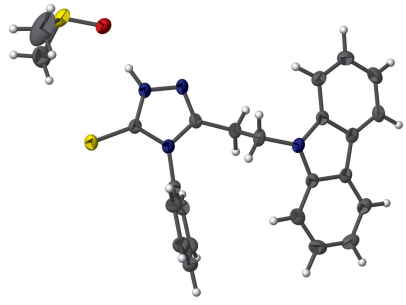
Keywords: crystal structure; carbazole; triazole; π-stacking.

CCDC reference: 1517511

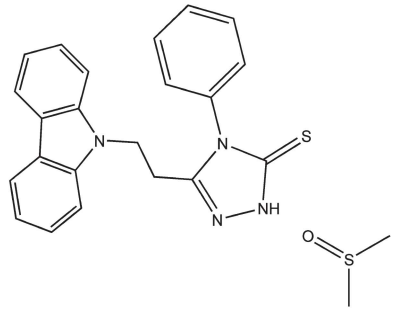
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{22}H_{18}N_4S\cdot C_2H_6OS$, the central triazolethione ring is inclined to the carbazole ring system by 13.97 (18)° and to the phenyl ring by 66.4 (1)°. The lattice solvent, dimethyl sulfoxide, is strongly hydrogen bonded to the triazolethione ring. In the crystal, the main molecules form columns parallel to the *a* axis, with the solvent molecules located between the columns. C—H···S hydrogen bonds and C—H···π(ring) interactions link adjacent columns. The crystal studied was refined as a two-component twin, with a fractional contribution to the minor domain of 0.0742 (14).

3D view



Chemical scheme



Structure description

Carbazole-containing compounds exhibit various biological activities including cytotoxic, antitumor, antiviral, antimicrobial, antiparasitics, antiserotonin and anti-inflammatory activities (Kumara *et al.*, 2009; Broadbent *et al.*, 1998; Xia *et al.*, 2008). Moreover, some derivatives have also been found to have industrial uses such as electro-photographic applications, in solar cells, as organic photo-refractive materials, and photo-voltaic devices (Chen *et al.*, 2007; Cheng *et al.*, 2008; Hains & Marks, 2008). As part of our studies in this area, we report herein the synthesis and crystal structure of the title compound.

The dihedral angle between the N1/C1/C6/C7/C12 and N2/N3/N4/C15/C16 rings is 13.97 (18)° while that between the latter ring and the C17–C22 ring is 66.4 (1)°. The triazolethione substituent forms a strong N3—H3*A*···O1 hydrogen bond with the solvent molecule (Table 1 and Fig. 1). In the crystal, the molecules form columns parallel to the *a*

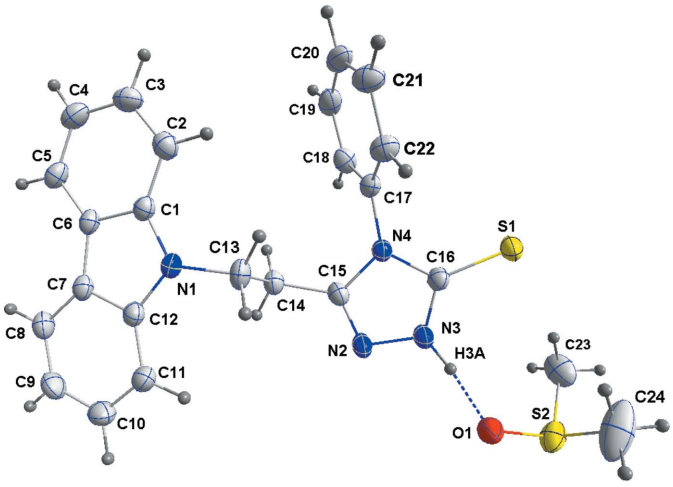


Figure 1
The title molecule, showing the atom-labeling scheme and 50% probability ellipsoids. The N—H···O hydrogen bond is shown as a dotted line.

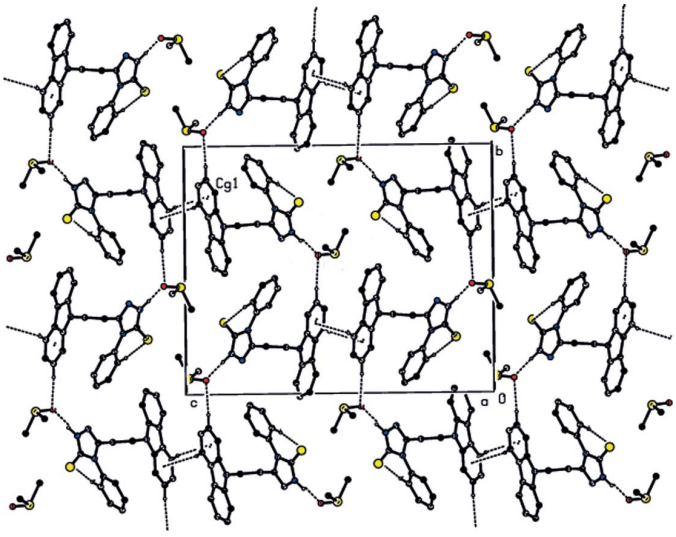


Figure 2
The packing of the title molecule, viewed along the *a* axis. N—H···O and C—H···S hydrogen bonds are shown, respectively, as blue and black dotted lines.

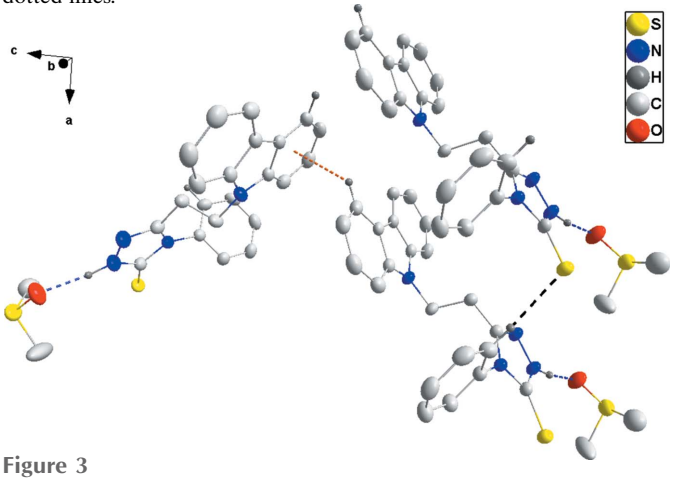


Figure 3
Detail of the intermolecular interactions. N—H···O and C—H···S hydrogen bonds are shown, respectively, as blue and black dotted lines while the C—H···π(ring) interaction is shown as an orange dotted line.

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

*Cg*1 is the centroid of the C1–C6 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1	0.95 (5)	1.75 (5)	2.691 (5)	172 (6)
C3—H3···O1^{i}	1.01 (5)	2.58 (5)	3.448 (5)	145 (4)
C18—H18···S1^{ii}	0.98 (6)	2.67 (6)	3.645 (4)	173 (4)
C5—H5···*Cg*1^{iii}	0.98 (5)	2.64 (4)	3.422 (4)	137 (3)

Symmetry codes: (i) $-x+1, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x-1, y, z$; (iii) $x-\frac{1}{2}, -y+\frac{3}{2}, -z+2$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{22}H_{18}N_4S{\cdot}C_2H_6OS$
M_r	448.59
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	150
a, *b*, *c* (Å)	5.8948 (1), 17.7215 (4), 22.0042 (5)
V (Å^3)	2298.66 (8)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	2.28
Crystal size (mm)	0.24 × 0.12 × 0.08
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min}, T_{max}	0.62, 0.83
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	34498, 34498, 24539
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.617
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.044, 0.116, 1.03
No. of reflections	34498
No. of parameters	356
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.25
Absolute structure	Flack *x* determined using 1668 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.032 (6)

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *DIAMOND* (Brandenburg & Putz, 2012) and *SHELXTL* (Sheldrick, 2008).

axis with the solvent molecules located between the columns (Fig. 2). Within the columns, the main molecules are associated through a combination of C18—H18···S1 hydrogen bonds and C5—H5···*Cg*1 interactions (Table 1, Fig. 3).

Synthesis and crystallization

A mixture of carbohydrazide (0.5 g, 2 mmol), benzoyl acetonitrile (0.3 g, 2 mmol) and piperidine (3 drops) in absolute ethanol (10 ml) was refluxed for 10 h. The reaction mixture was poured onto water and neutralized with diluted HCl (10%) and left at room temperature for some hours. The solid that formed was collected by filtration, washed with water, dried and crystallized from dioxane–H_2O (1:1) to afford crystals of good quality for X-ray diffraction. M.p. 505–507 K.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The crystal studied was refined as a two-component twin with a fractional contribution to the minor domain of 0.0742 (14).

Acknowledgements

The support of NSF–MRI Grant No. 1228232 for the purchase of the diffractometer and Tulane University for support of the Tulane Crystallography Laboratory are gratefully acknowledged.

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full crystallographic data

IUCrData (2016). **1**, x161835 [https://doi.org/10.1107/S2414314616018356]

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3-[2-(9*H*-Carbazol-9-yl)ethyl]-4-phenyl-1*H*-1,2,4-triazole-5(4*H*)-thione dimethyl sulfoxide monosolvate

Crystal data

$C_{22}H_{18}N_4S·C_2H_6OS$
M_r = 448.59
Orthorhombic, $P2_12_12_1$
a = 5.8948 (1) Å
b = 17.7215 (4) Å
c = 22.0042 (5) Å
V = 2298.66 (8) Å^3
Z = 4
F(000) = 944
D_x = 1.296 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 9972 reflections
θ = 3.2–72.2°
μ = 2.28 mm^{-1}
T = 150 K
Column, colourless
0.24 × 0.12 × 0.08 mm

Data collection

Bruker D8 VENTURE PHOTON 100 CMOS diffractometer
Radiation source: INCOATEC IμS micro-focus source
Mirror monochromator
Detector resolution: 10.4167 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (*TWINABS*; Sheldrick, 2009)
T_{min} = 0.62, T_{max} = 0.83
34498 measured reflections
34498 independent reflections
24539 reflections with $I > 2\sigma(I)$
θ_{max} = 72.2°, θ_{min} = 3.2°
h = −7→7
k = −21→21
l = −27→26

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.044
$wR(F^2)$ = 0.116
S = 1.03
34498 reflections
356 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0241P)^2 + 0.2059P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}
Extinction correction: *SHELXL2014* (Sheldrick, 2015*b*), Fc*=kFc[1+0.001xFc$^2\lambda^3$/sin(2θ)]$^{-1/4}$
Extinction coefficient: 0.0030 (6)
Absolute structure: Flack x determined using 1668 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.032 (6)

Special details

Experimental. Analysis of 539 reflections having I/σ(I) > 12 and chosen from the full data set with *CELL_NOW* (Sheldrick, 2008) showed the crystal to belong to the orthorhombic system and to be twinned by a 173° rotation about the *c** axis. The raw data were processed using the multi- component version of*SAINT* under control of the two-component orientation file generated by *CELL_NOW*.

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.

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 $F^2 > 2\mathrm{sigma}(F^2)$ 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. Refined as a 2-component twin.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	1.06943 (17)	0.78038 (6)	0.62361 (5)	0.0315 (3)
N1	0.3120 (6)	0.67855 (18)	0.87011 (15)	0.0282 (7)
N2	0.6348 (6)	0.63171 (19)	0.68193 (16)	0.0329 (8)
N3	0.8155 (6)	0.6571 (2)	0.64749 (16)	0.0320 (8)
H3A	0.884 (10)	0.624 (3)	0.619 (2)	0.052 (15)*
N4	0.7122 (6)	0.75119 (18)	0.70175 (15)	0.0253 (7)
C1	0.1993 (7)	0.7399 (2)	0.89504 (17)	0.0258 (8)
C2	0.2655 (8)	0.8151 (2)	0.8975 (2)	0.0322 (9)
H2	0.405 (9)	0.833 (3)	0.879 (2)	0.040 (13)*
C3	0.1213 (9)	0.8654 (2)	0.9270 (2)	0.0367 (10)
H3	0.168 (9)	0.920 (3)	0.927 (2)	0.042 (13)*
C4	−0.0830 (8)	0.8415 (3)	0.9527 (2)	0.0361 (10)
H4	−0.169 (9)	0.877 (3)	0.972 (2)	0.041 (14)*
C5	−0.1487 (7)	0.7666 (2)	0.95002 (18)	0.0310 (9)
H5	−0.293 (8)	0.751 (2)	0.968 (2)	0.031 (12)*
C6	−0.0069 (6)	0.7149 (2)	0.92125 (17)	0.0255 (8)
C7	−0.0203 (7)	0.6344 (2)	0.91025 (18)	0.0270 (8)
C8	−0.1812 (8)	0.5788 (2)	0.92297 (19)	0.0323 (9)
H8	−0.311 (9)	0.591 (3)	0.947 (2)	0.038 (13)*
C9	−0.1437 (9)	0.5066 (3)	0.9021 (2)	0.0390 (11)
H9	−0.248 (10)	0.473 (3)	0.909 (2)	0.046 (15)*
C10	0.0520 (9)	0.4881 (2)	0.8697 (2)	0.0401 (11)
H10	0.073 (9)	0.435 (3)	0.855 (2)	0.046 (14)*
C11	0.2156 (8)	0.5416 (2)	0.8574 (2)	0.0347 (10)
H11	0.359 (9)	0.531 (3)	0.833 (2)	0.036 (13)*
C12	0.1769 (7)	0.6148 (2)	0.87782 (18)	0.0268 (8)
C13	0.4908 (7)	0.6834 (3)	0.82506 (19)	0.0302 (9)
H13B	0.584 (9)	0.639 (3)	0.829 (2)	0.032 (12)*
H13A	0.595 (9)	0.726 (3)	0.834 (2)	0.041 (13)*
C14	0.3934 (7)	0.6885 (2)	0.76079 (18)	0.0286 (8)
H14B	0.299 (8)	0.645 (3)	0.754 (2)	0.029 (11)*

H14A	0.290 (9)	0.732 (3)	0.756 (2)	0.048 (14)*
C15	0.5752 (7)	0.6896 (2)	0.71422 (17)	0.0272 (8)
C16	0.8664 (7)	0.7295 (2)	0.65795 (17)	0.0261 (8)
C17	0.6927 (7)	0.8246 (2)	0.73026 (18)	0.0255 (8)
C18	0.4986 (7)	0.8669 (2)	0.7204 (2)	0.0324 (9)
H18	0.380 (11)	0.848 (3)	0.693 (3)	0.057 (16)*
C19	0.4713 (8)	0.9348 (3)	0.7511 (2)	0.0371 (10)
H19	0.332 (9)	0.963 (3)	0.746 (2)	0.039 (13)*
C20	0.6393 (9)	0.9604 (2)	0.7903 (2)	0.0374 (11)
H20	0.616 (9)	1.009 (3)	0.812 (2)	0.040 (13)*
C21	0.8346 (9)	0.9183 (2)	0.7986 (2)	0.0364 (10)
H21	0.951 (9)	0.935 (3)	0.827 (2)	0.041 (13)*
C22	0.8610 (7)	0.8494 (2)	0.76912 (19)	0.0310 (9)
H22	0.992 (8)	0.816 (3)	0.777 (2)	0.035 (12)*
S2	1.1260 (2)	0.56418 (7)	0.51143 (5)	0.0425 (3)
O1	0.9739 (6)	0.55716 (18)	0.56576 (16)	0.0481 (9)
C23	1.0596 (11)	0.6521 (3)	0.4773 (2)	0.0563 (14)
H23A	1.0668	0.6921	0.5080	0.084*
H23B	0.9064	0.6500	0.4601	0.084*
H23C	1.1690	0.6628	0.4449	0.084*
C24	1.3961 (11)	0.5911 (5)	0.5403 (3)	0.090 (3)
H24A	1.4647	0.5483	0.5617	0.135*
H24B	1.3778	0.6334	0.5686	0.135*
H24C	1.4945	0.6064	0.5066	0.135*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0302 (5)	0.0329 (5)	0.0313 (5)	−0.0069 (4)	0.0071 (4)	−0.0011 (4)
N1	0.0288 (16)	0.0304 (17)	0.0254 (17)	−0.0004 (13)	0.0068 (14)	−0.0012 (14)
N2	0.037 (2)	0.0333 (18)	0.0282 (18)	−0.0090 (15)	0.0100 (16)	−0.0019 (15)
N3	0.0364 (19)	0.0307 (17)	0.0290 (18)	−0.0084 (15)	0.0110 (16)	−0.0029 (15)
N4	0.0255 (16)	0.0271 (16)	0.0233 (16)	−0.0031 (13)	0.0029 (14)	−0.0007 (14)
C1	0.028 (2)	0.029 (2)	0.0200 (19)	0.0004 (15)	−0.0004 (15)	0.0004 (15)
C2	0.034 (2)	0.034 (2)	0.028 (2)	−0.0039 (17)	−0.0037 (18)	0.0038 (18)
C3	0.050 (3)	0.028 (2)	0.032 (2)	−0.0004 (19)	−0.009 (2)	0.0000 (18)
C4	0.041 (2)	0.037 (2)	0.030 (2)	0.010 (2)	−0.004 (2)	−0.0064 (18)
C5	0.030 (2)	0.039 (2)	0.0234 (19)	0.0045 (17)	−0.0013 (17)	−0.0029 (17)
C6	0.0266 (19)	0.032 (2)	0.0177 (17)	−0.0004 (16)	−0.0009 (15)	−0.0004 (16)
C7	0.030 (2)	0.033 (2)	0.0185 (18)	−0.0012 (16)	−0.0004 (16)	−0.0002 (16)
C8	0.032 (2)	0.040 (2)	0.025 (2)	−0.0063 (18)	0.0018 (18)	0.0035 (18)
C9	0.049 (3)	0.034 (2)	0.034 (2)	−0.012 (2)	0.000 (2)	0.005 (2)
C10	0.057 (3)	0.029 (2)	0.034 (2)	0.000 (2)	0.001 (2)	−0.0023 (19)
C11	0.044 (3)	0.032 (2)	0.028 (2)	0.0043 (18)	0.006 (2)	−0.0008 (17)
C12	0.031 (2)	0.0289 (18)	0.0200 (18)	−0.0012 (15)	0.0010 (18)	0.0006 (16)
C13	0.025 (2)	0.041 (2)	0.025 (2)	0.0001 (18)	0.0054 (16)	0.0025 (19)
C14	0.026 (2)	0.0333 (19)	0.026 (2)	−0.0033 (17)	0.0032 (17)	0.0012 (17)
C15	0.028 (2)	0.0293 (18)	0.0242 (19)	−0.0049 (16)	0.0006 (17)	0.0026 (16)

C16	0.0274 (19)	0.0290 (19)	0.0220 (18)	−0.0018 (15)	0.0017 (16)	−0.0010 (16)
C17	0.0264 (19)	0.0267 (19)	0.0233 (19)	−0.0005 (15)	0.0021 (16)	0.0002 (16)
C18	0.027 (2)	0.034 (2)	0.036 (2)	−0.0009 (16)	−0.0023 (18)	0.0041 (19)
C19	0.033 (2)	0.032 (2)	0.046 (3)	0.0081 (18)	0.009 (2)	0.007 (2)
C20	0.053 (3)	0.028 (2)	0.032 (2)	0.0033 (19)	0.009 (2)	0.0000 (18)
C21	0.047 (3)	0.033 (2)	0.030 (2)	−0.0006 (19)	−0.005 (2)	−0.0022 (19)
C22	0.033 (2)	0.031 (2)	0.029 (2)	0.0021 (17)	−0.0037 (18)	−0.0009 (17)
S2	0.0393 (6)	0.0542 (7)	0.0341 (6)	0.0016 (5)	0.0064 (5)	−0.0116 (5)
O1	0.060 (2)	0.0364 (17)	0.047 (2)	−0.0046 (15)	0.0236 (17)	−0.0083 (16)
C23	0.066 (4)	0.062 (3)	0.041 (3)	−0.014 (3)	−0.001 (3)	0.001 (3)
C24	0.038 (3)	0.171 (8)	0.061 (4)	0.006 (4)	−0.005 (3)	−0.028 (5)

Geometric parameters (Å, º)

S1—C16	1.678 (4)	C10—H10	1.00 (5)
N1—C1	1.387 (5)	C11—C12	1.391 (6)
N1—C12	1.393 (5)	C11—H11	1.02 (5)
N1—C13	1.449 (5)	C13—C14	1.529 (6)
N2—C15	1.297 (5)	C13—H13B	0.96 (5)
N2—N3	1.383 (5)	C13—H13A	1.00 (5)
N3—C16	1.338 (5)	C14—C15	1.483 (5)
N3—H3A	0.95 (6)	C14—H14B	0.97 (5)
N4—C16	1.380 (5)	C14—H14A	0.99 (5)
N4—C15	1.385 (5)	C17—C22	1.382 (6)
N4—C17	1.448 (5)	C17—C18	1.385 (6)
C1—C2	1.391 (6)	C18—C19	1.389 (7)
C1—C6	1.416 (6)	C18—H18	0.98 (6)
C2—C3	1.392 (6)	C19—C20	1.389 (7)
C2—H2	0.97 (5)	C19—H19	0.97 (5)
C3—C4	1.397 (7)	C20—C21	1.384 (7)
C3—H3	1.00 (5)	C20—H20	1.00 (5)
C4—C5	1.383 (6)	C21—C22	1.390 (6)
C4—H4	0.91 (5)	C21—H21	0.97 (5)
C5—C6	1.392 (6)	C22—H22	0.98 (5)
C5—H5	0.99 (5)	S2—O1	1.500 (3)
C6—C7	1.449 (6)	S2—C23	1.773 (6)
C7—C8	1.396 (6)	S2—C24	1.779 (7)
C7—C12	1.408 (6)	C23—H23A	0.9800
C8—C9	1.377 (7)	C23—H23B	0.9800
C8—H8	0.96 (5)	C23—H23C	0.9800
C9—C10	1.395 (7)	C24—H24A	0.9800
C9—H9	0.87 (6)	C24—H24B	0.9800
C10—C11	1.379 (7)	C24—H24C	0.9800
C1—N1—C12	108.3 (3)	N1—C13—H13A	111 (3)
C1—N1—C13	124.9 (3)	C14—C13—H13A	111 (3)
C12—N1—C13	123.2 (3)	H13B—C13—H13A	105 (4)
C15—N2—N3	104.6 (3)	C15—C14—C13	111.6 (3)

C16—N3—N2	113.0 (3)	C15—C14—H14B	109 (3)
C16—N3—H3A	128 (3)	C13—C14—H14B	108 (3)
N2—N3—H3A	119 (3)	C15—C14—H14A	112 (3)
C16—N4—C15	107.6 (3)	C13—C14—H14A	112 (3)
C16—N4—C17	127.2 (3)	H14B—C14—H14A	105 (4)
C15—N4—C17	125.1 (3)	N2—C15—N4	110.9 (3)
N1—C1—C2	129.2 (4)	N2—C15—C14	124.3 (4)
N1—C1—C6	109.2 (3)	N4—C15—C14	124.6 (4)
C2—C1—C6	121.6 (4)	N3—C16—N4	103.9 (3)
C1—C2—C3	117.4 (4)	N3—C16—S1	126.7 (3)
C1—C2—H2	123 (3)	N4—C16—S1	129.4 (3)
C3—C2—H2	120 (3)	C22—C17—C18	121.2 (4)
C2—C3—C4	121.4 (4)	C22—C17—N4	119.8 (4)
C2—C3—H3	117 (3)	C18—C17—N4	118.9 (4)
C4—C3—H3	122 (3)	C17—C18—C19	119.2 (4)
C5—C4—C3	121.1 (4)	C17—C18—H18	120 (3)
C5—C4—H4	121 (3)	C19—C18—H18	121 (3)
C3—C4—H4	117 (3)	C18—C19—C20	120.2 (4)
C4—C5—C6	118.8 (4)	C18—C19—H19	119 (3)
C4—C5—H5	120 (3)	C20—C19—H19	121 (3)
C6—C5—H5	121 (3)	C21—C20—C19	120.0 (4)
C5—C6—C1	119.7 (4)	C21—C20—H20	121 (3)
C5—C6—C7	133.7 (4)	C19—C20—H20	119 (3)
C1—C6—C7	106.6 (3)	C20—C21—C22	120.3 (4)
C8—C7—C12	119.2 (4)	C20—C21—H21	120 (3)
C8—C7—C6	134.3 (4)	C22—C21—H21	119 (3)
C12—C7—C6	106.5 (3)	C17—C22—C21	119.2 (4)
C9—C8—C7	118.7 (4)	C17—C22—H22	119 (3)
C9—C8—H8	121 (3)	C21—C22—H22	122 (3)
C7—C8—H8	120 (3)	O1—S2—C23	106.2 (2)
C8—C9—C10	121.4 (4)	O1—S2—C24	105.8 (3)
C8—C9—H9	118 (4)	C23—S2—C24	96.5 (4)
C10—C9—H9	121 (4)	S2—C23—H23A	109.5
C11—C10—C9	121.2 (4)	S2—C23—H23B	109.5
C11—C10—H10	120 (3)	H23A—C23—H23B	109.5
C9—C10—H10	119 (3)	S2—C23—H23C	109.5
C10—C11—C12	117.6 (4)	H23A—C23—H23C	109.5
C10—C11—H11	124 (3)	H23B—C23—H23C	109.5
C12—C11—H11	119 (3)	S2—C24—H24A	109.5
C11—C12—N1	128.6 (4)	S2—C24—H24B	109.5
C11—C12—C7	122.0 (4)	H24A—C24—H24B	109.5
N1—C12—C7	109.4 (3)	S2—C24—H24C	109.5
N1—C13—C14	111.3 (3)	H24A—C24—H24C	109.5
N1—C13—H13B	107 (3)	H24B—C24—H24C	109.5
C14—C13—H13B	111 (3)		

C15—N2—N3—C16	−0.3 (5)	C6—C7—C12—C11	−177.4 (4)
C12—N1—C1—C2	−179.0 (4)	C8—C7—C12—N1	179.7 (4)

C13—N1—C1—C2	−20.1 (7)	C6—C7—C12—N1	1.7 (4)
C12—N1—C1—C6	2.3 (4)	C1—N1—C13—C14	−84.9 (5)
C13—N1—C1—C6	161.2 (4)	C12—N1—C13—C14	71.1 (5)
N1—C1—C2—C3	−178.3 (4)	N1—C13—C14—C15	−177.1 (3)
C6—C1—C2—C3	0.3 (6)	N3—N2—C15—N4	−0.2 (5)
C1—C2—C3—C4	−0.6 (7)	N3—N2—C15—C14	−176.9 (4)
C2—C3—C4—C5	0.4 (7)	C16—N4—C15—N2	0.6 (5)
C3—C4—C5—C6	0.1 (6)	C17—N4—C15—N2	−179.5 (4)
C4—C5—C6—C1	−0.5 (6)	C16—N4—C15—C14	177.3 (4)
C4—C5—C6—C7	179.9 (4)	C17—N4—C15—C14	−2.8 (6)
N1—C1—C6—C5	179.1 (3)	C13—C14—C15—N2	101.3 (5)
C2—C1—C6—C5	0.3 (6)	C13—C14—C15—N4	−74.9 (5)
N1—C1—C6—C7	−1.2 (4)	N2—N3—C16—N4	0.7 (5)
C2—C1—C6—C7	180.0 (4)	N2—N3—C16—S1	−178.3 (3)
C5—C6—C7—C8	1.8 (8)	C15—N4—C16—N3	−0.8 (4)
C1—C6—C7—C8	−177.9 (4)	C17—N4—C16—N3	179.3 (4)
C5—C6—C7—C12	179.4 (4)	C15—N4—C16—S1	178.2 (3)
C1—C6—C7—C12	−0.3 (4)	C17—N4—C16—S1	−1.7 (6)
C12—C7—C8—C9	−1.4 (6)	C16—N4—C17—C22	−68.5 (5)
C6—C7—C8—C9	175.9 (4)	C15—N4—C17—C22	111.6 (5)
C7—C8—C9—C10	1.1 (7)	C16—N4—C17—C18	114.9 (5)
C8—C9—C10—C11	0.0 (7)	C15—N4—C17—C18	−65.0 (5)
C9—C10—C11—C12	−0.7 (7)	C22—C17—C18—C19	−1.3 (6)
C10—C11—C12—N1	−178.5 (4)	N4—C17—C18—C19	175.3 (4)
C10—C11—C12—C7	0.4 (6)	C17—C18—C19—C20	1.2 (7)
C1—N1—C12—C11	176.5 (4)	C18—C19—C20—C21	0.2 (7)
C13—N1—C12—C11	17.1 (7)	C19—C20—C21—C22	−1.7 (7)
C1—N1—C12—C7	−2.5 (4)	C18—C17—C22—C21	−0.2 (6)
C13—N1—C12—C7	−161.9 (4)	N4—C17—C22—C21	−176.7 (4)
C8—C7—C12—C11	0.7 (6)	C20—C21—C22—C17	1.6 (7)

Hydrogen-bond geometry (Å, º)

Cg1 is the centroid of the C1–C6 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N3—H3*A*···O1	0.95 (5)	1.75 (5)	2.691 (5)	172 (6)
C3—H3···O1^{i}	1.01 (5)	2.58 (5)	3.448 (5)	145 (4)
C18—H18···S1^{ii}	0.98 (6)	2.67 (6)	3.645 (4)	173 (4)
C5—H5···*Cg*1^{iii}	0.98 (5)	2.64 (4)	3.422 (4)	137 (3)

Symmetry codes: (i) −*x*+1, *y*+1/2, −*z*+3/2; (ii) *x*−1, *y*, *z*; (iii) *x*−1/2, −*y*+3/2, −*z*+2.