IUCrData

ISSN 2414-3146

3-Phenoxymethyl-6-phenyl-1,2,4-triazolo-[3,4-*b*][1,3,4]thiadiazole

Shaaban K. Mohamed,[a,b] Joel T. Mague,[c] Mehmet Akkurt,[d] Etify A. Bakhite[e] and Mustafa R. Albayati[f]*

[a]Chemistry and Environmental Division, Manchester Metropolitan University, Manchester M1 5GD, England, [b]Chemistry Department, Faculty of Science, Minia University, 61519 El-Minia, Egypt, [c]Department of Chemistry, Tulane University, New Orleans, LA 70118, USA, [d]Department of Physics, Faculty of Sciences, Erciyes University, 38039 Kayseri, Turkey, [e]Chemistry Department, Faculty of Science, Assiut University, 71516 Assiut, Egypt, and [f]Kirkuk University, College of Science, Department of Chemistry, Kirkuk, Iraq. *Correspondence e-mail: shaabankamel@yahoo.com

Received 9 April 2016
Accepted 14 April 2016

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

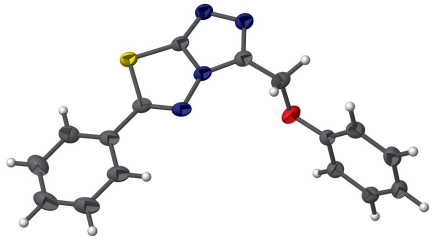
Keywords: crystal structure; *N*-bridged heterocycles; triazolo thiadiazoles; triazoles; thiadiazoles; C—H$\cdots\pi$ interactions; π–π interactions.

CCDC reference: 1473995

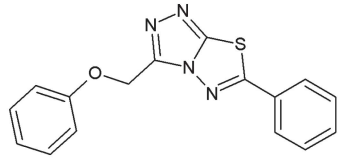
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{16}H_{12}N_4OS$, the bicyclic triazolothiadiazole core is approximately planar, with an r.m.s. deviation of 0.018 Å. The phenyl rings are inclined to its mean plane by 7.66 (7) and 71.79 (7)°. In the crystal, molecules are linked *via* a C—H$\cdots\pi$ interaction and a π–π interaction [intercentroid distance = 3.2942 (9) Å] involving inversion-related triazole rings. These interactions result in the formation of chains propagating along [10$\bar{1}$].

3D view



Chemical scheme



Structure description

N-Bridged heterocycles derived from 1,2,4-triazoles have applications in medicine, agriculture and industry (Farghaly *et al.*, 2006). Heterocycles bearing a triazole or 1,3,4-thiadiazole moiety are reported to show a wide spectrum of biological activity (Suresh Kumar *et al.*, 2010; Mallikarjuna *et al.*, 2009) such as anti-bacterial (Abdel-Rahman & Farghaly, 2004), anti-aggregator agents (Czarnocka-Janowicz *et al.*, 1991), anti-viral (Srivastava *et al.*, 1991) and anti-inflammatory (Unangst *et al.*, 1992) activities. Triazolothiadiazoles in particular are reported to possess anti-bacterial, antifungal, *CNS* depressant, anti-viral, analgesic, anti-tuberculosis and plant-growth regulatory effects (Abdallah *et al.*, 2005; El-Khawass & Habib 1989; Mishra, 1987; Shiradkar & Kale, 2006). Based on such facts, we report herein on the synthesis and crystal structure of the title compound.

In the title molecule, (Fig. 1), the bicyclic triazolothiadiazole core is approximately planar with an r.m.s. deviation of 0.018 Å and a maximum deviation of 0.021 (1) Å for

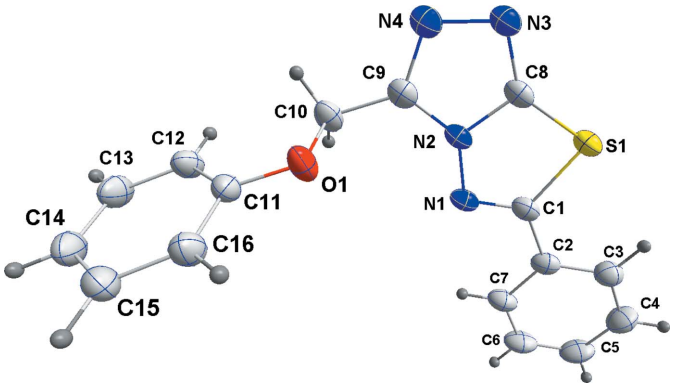


Figure 1
The molecular structure of the title compound, showing the atom labeling and 50% probability displacement ellipsoids.

atom N2. The phenyl rings, C2–C7 and C11–C16, are inclined to its mean plane by 7.66 (7) and 71.79 (7)°, respectively.

In the crystal, molecules are linked *via* a C—H···π interaction (Fig. 2 and Table 1) and by π–π interactions between triazole rings [$Cg2\cdots Cg2^{i}$ = 3.2942 (9) Å, *Cg*2 is the centroid of ring N2–N4/C8/C9, symmetry code (i): $-x+1, -y+1, -z+2$]; see Fig. 3. These interactions result in the formation of chains propagating along [10$\bar{1}$].

Synthesis and crystallization

A mixture of 4-amino-3-phenoxymethyl-1,2,4-triazoline-5-thione (2.22 g, 0.01 mol) and benzoic acid (1.22 g, 0.01 mol) in phosphorus oxychloride (20 ml) was heated under reflux on a steam bath for 4 h and then left to cool. The reaction mixture was poured portionwise into ice–water (50 ml) with stirring and allowed to stand at room temperature for 2 h. The solid that formed was collected by filtration and crystallized from ethanol as colorless plates (yield: 82%; m.p.: 482–483 K). IR:

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

Cg is the centroid of the C11–C16 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*^{i}	0.95	2.79	3.633 (2)	148

Symmetry code: (i) $-x, -y+1, -z+1$.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{16}H_{12}N_4OS$
M_r	308.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	150
a, *b*, *c* (Å)	5.9850 (3), 21.0709 (10), 11.5617 (5)
β (°)	100.423 (2)
V (Å^3)	1433.98 (12)
Z	4
Radiation type	Cu *K*α
μ (mm^{-1})	2.07
Crystal size (mm)	0.30 × 0.16 × 0.02
Data collection	
Diffractometer	Bruker D8 VENTURE PHOTON 100 CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.79, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	10736, 2799, 2464
R_{int}	0.038
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.619
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.035, 0.089, 1.03
No. of reflections	2799
No. of parameters	199
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.30

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

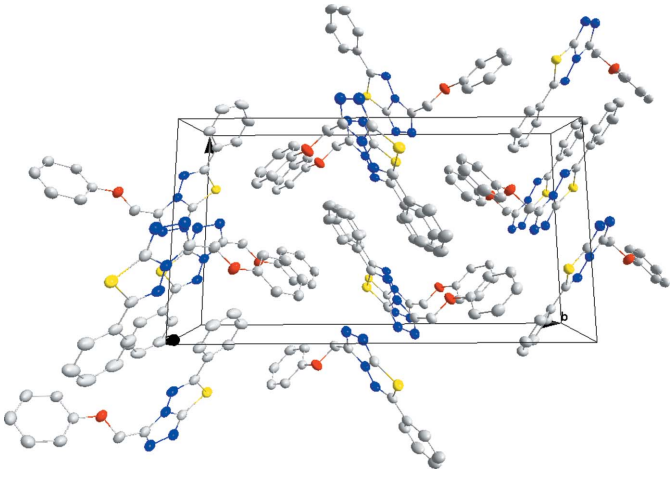


Figure 2
The crystal packing of the title compound, viewed along the *a* axis. H atoms have been omitted for clarity.

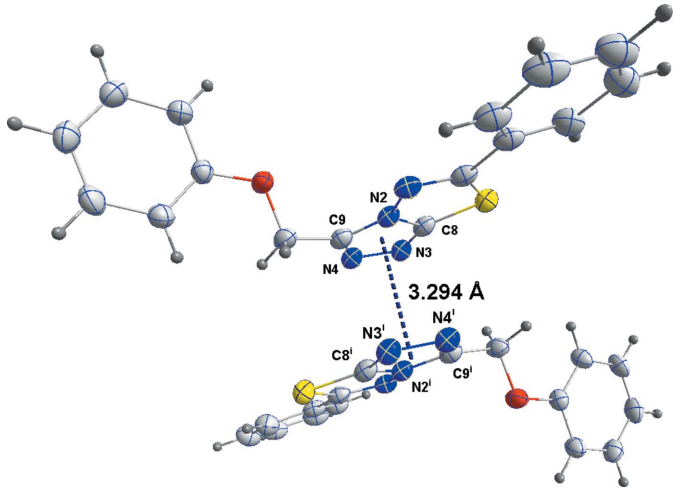


Figure 3
Details of the offset π-stacking in the crystal of the title compound.

1600 cm^{-1} (C═N). ^1H NMR ($CDCl_3$): δ 6.7–7.5 (*m*, 10 H, Ar—H), δ 5.0 (*s*, 2H, OCH_2).

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

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.

References

Abdallah, M. A., Riyadh, S. M., Abbas, I. M. S. & Gomha, M. (2005). *Jnl Chin. Chem. Soc.* **52**, 987–994.
Abdel-Rahman, & Farghaly, A. H. (2004). *Jnl Chin. Chem. Soc.* **51**, 147–156.
Brandenburg, K. & Putz, H. (2012). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Bruker (2016). *APEX3*, *SAINT* and *SADABS*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Czarnocka-Janowicz, A., Foks, H., Nasal, A., Petrusewicz, J., Damasiewicz, B., Radwańska, A. & Kaliszan, R. (1991). *Pharmazie*, **46**, 109–112.
El-Khawass, S. M. & Habib, N. S. (1989). *J. Heterocycl. Chem.* **26**, 177–181.
Farghaly, A. R., De Clercq, E. D. & El-Kashef, H. (2006). *Arkivoc*, **10**, 137–151.
Mallikarjuna, B. P., Sastry, B. S., Suresh Kumar, G. V., Rajendraprasad, Y., Chandrashekar, S. M. & Sathisha, K. (2009). *Eur. J. Med. Chem.* **44**, 4739–4746.
Mishra, B. (1987). *Indian J. Chem. Sect. B*, **27B**, 576–580.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Shiradkar, M. & Kale, R. (2006). *Indian J. Chem. Sect. B*, **45**, 1009–1013.
Srivastava, J., Swarup, S., Saxena, V. K. & Chaudhary, B. L. (1991). *J. Indian Chem. Soc.* **68**, 103–107.
Suresh Kumar, G. V., Rajendraprasad, Y., Mallikarjuna, Y., Chandrashekar, B. P. & Kistayya, C. (2010). *Eur. J. Med. Chem.* **45**, 2063–2074.
Unangst, P. C., Shrum, G. P., Connor, D. T., Dyer, R. D. & Schrier, D. J. (1992). *J. Med. Chem.* **35**, 3691–3698.

full crystallographic data

IUCrData (2016). **1**, x160626 [doi:10.1107/S241431461600626X]

3-Phenoxymethyl-6-phenyl-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

Shaaban K. Mohamed, Joel T. Mague, Mehmet Akkurt, Etify A. Bakhite and Mustafa R. Albayati

3-Phenoxymethyl-6-phenyl-1,2,4-triazolo[3,4-*b*][1,3,4]thiadiazole

Crystal data

$C_{16}H_{12}N_4OS$
M_r = 308.36
Monoclinic, $P2_1/c$
a = 5.9850 (3) Å
b = 21.0709 (10) Å
c = 11.5617 (5) Å
β = 100.423 (2)°
V = 1433.98 (12) Å^3
Z = 4
$F(000)$ = 640
D_x = 1.428 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54178 Å
Cell parameters from 7818 reflections
θ = 4.2–72.5°
μ = 2.07 mm^{-1}
T = 150 K
Plate, colourless
0.30 × 0.16 × 0.02 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 (*SADABS*; Bruker, 2016)
T_{min} = 0.79, T_{max} = 0.97
10736 measured reflections
2799 independent reflections
2464 reflections with $I > 2\sigma(I)$
R_{int} = 0.038
θ_{max} = 72.5°, θ_{min} = 4.2°
h = −7→6
k = −22→25
l = −14→14

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.035
$wR(F^2)$ = 0.089
S = 1.03
2799 reflections
199 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
$w = 1/[\sigma^2(F_o^2) + (0.0407P)^2 + 0.5423P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.30 e Å^{-3}

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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. H-atoms attached to carbon were placed in calculated positions (C—H = 0.95 - 0.99 Å) and included as riding contributions with isotropic displacement parameters 1.2 times those of the attached atoms.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.80639 (6)	0.53901 (2)	0.80341 (3)	0.03014 (13)
O1	0.27388 (19)	0.32989 (6)	0.83039 (10)	0.0355 (3)
N1	0.4069 (2)	0.48387 (6)	0.74636 (11)	0.0293 (3)
N2	0.5213 (2)	0.45919 (6)	0.85076 (11)	0.0273 (3)
N3	0.8120 (2)	0.45577 (6)	0.99887 (12)	0.0315 (3)
N4	0.6450 (2)	0.41284 (6)	1.01880 (12)	0.0327 (3)
C1	0.5389 (3)	0.52624 (7)	0.71208 (14)	0.0286 (3)
C2	0.4730 (3)	0.56291 (8)	0.60310 (13)	0.0308 (3)
C3	0.6286 (3)	0.60294 (9)	0.56407 (15)	0.0378 (4)
H3	0.7784	0.6067	0.6079	0.045*
C4	0.5652 (4)	0.63750 (10)	0.46100 (17)	0.0454 (5)
H4	0.6722	0.6645	0.4341	0.055*
C5	0.3467 (4)	0.63270 (10)	0.39754 (16)	0.0473 (5)
H5	0.3035	0.6566	0.3274	0.057*
C6	0.1908 (3)	0.59298 (10)	0.43620 (16)	0.0452 (5)
H6	0.0409	0.5896	0.3922	0.054*
C7	0.2524 (3)	0.55821 (9)	0.53848 (15)	0.0374 (4)
H7	0.1448	0.5312	0.5648	0.045*
C8	0.7310 (2)	0.48242 (7)	0.89660 (14)	0.0280 (3)
C9	0.4735 (3)	0.41535 (7)	0.92963 (14)	0.0295 (3)
C10	0.2645 (3)	0.37680 (8)	0.91792 (15)	0.0331 (4)
H10A	0.2545	0.3563	0.9939	0.040*
H10B	0.1290	0.4040	0.8946	0.040*
C11	0.1005 (3)	0.28603 (7)	0.81265 (13)	0.0279 (3)
C12	−0.0781 (3)	0.28504 (8)	0.87418 (14)	0.0336 (4)
H12	−0.0861	0.3155	0.9339	0.040*
C13	−0.2456 (3)	0.23880 (9)	0.84714 (15)	0.0393 (4)
H13	−0.3679	0.2376	0.8893	0.047*
C14	−0.2361 (3)	0.19474 (8)	0.75990 (15)	0.0386 (4)
H14	−0.3520	0.1636	0.7415	0.046*
C15	−0.0568 (3)	0.19615 (8)	0.69943 (15)	0.0360 (4)
H15	−0.0500	0.1659	0.6392	0.043*
C16	0.1130 (3)	0.24126 (8)	0.72580 (14)	0.0329 (4)
H16	0.2371	0.2416	0.6849	0.040*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0238 (2)	0.0329 (2)	0.0308 (2)	−0.00024 (14)	−0.00293 (15)	−0.00098 (15)

O1	0.0313 (6)	0.0377 (6)	0.0394 (6)	−0.0097 (5)	0.0120 (5)	−0.0135 (5)
N1	0.0244 (6)	0.0340 (7)	0.0268 (6)	0.0049 (5)	−0.0031 (5)	−0.0046 (5)
N2	0.0220 (6)	0.0283 (7)	0.0291 (6)	0.0018 (5)	−0.0021 (5)	−0.0039 (5)
N3	0.0264 (6)	0.0317 (7)	0.0336 (7)	0.0007 (5)	−0.0019 (5)	−0.0008 (5)
N4	0.0300 (7)	0.0314 (7)	0.0348 (7)	0.0016 (5)	0.0007 (6)	−0.0020 (6)
C1	0.0246 (7)	0.0306 (8)	0.0289 (8)	0.0052 (6)	0.0001 (6)	−0.0071 (6)
C2	0.0308 (8)	0.0325 (8)	0.0275 (7)	0.0081 (6)	0.0008 (6)	−0.0058 (6)
C3	0.0334 (9)	0.0454 (10)	0.0335 (8)	0.0064 (7)	0.0029 (7)	0.0003 (7)
C4	0.0489 (11)	0.0502 (11)	0.0383 (10)	0.0095 (8)	0.0109 (8)	0.0069 (8)
C5	0.0556 (12)	0.0530 (12)	0.0311 (9)	0.0208 (9)	0.0022 (8)	0.0039 (8)
C6	0.0422 (10)	0.0549 (12)	0.0331 (9)	0.0162 (9)	−0.0074 (8)	−0.0048 (8)
C7	0.0328 (9)	0.0428 (10)	0.0328 (8)	0.0072 (7)	−0.0041 (7)	−0.0058 (7)
C8	0.0221 (7)	0.0284 (8)	0.0312 (8)	0.0018 (6)	−0.0014 (6)	−0.0052 (6)
C9	0.0275 (8)	0.0284 (8)	0.0313 (8)	0.0027 (6)	0.0024 (6)	−0.0044 (6)
C10	0.0302 (8)	0.0344 (9)	0.0348 (8)	−0.0028 (6)	0.0063 (7)	−0.0091 (7)
C11	0.0257 (7)	0.0299 (8)	0.0272 (7)	−0.0027 (6)	0.0021 (6)	0.0013 (6)
C12	0.0321 (8)	0.0407 (9)	0.0283 (8)	−0.0030 (7)	0.0063 (6)	−0.0024 (7)
C13	0.0334 (9)	0.0485 (11)	0.0370 (9)	−0.0086 (7)	0.0090 (7)	0.0062 (8)
C14	0.0396 (9)	0.0360 (9)	0.0379 (9)	−0.0111 (7)	0.0010 (7)	0.0048 (7)
C15	0.0429 (9)	0.0303 (9)	0.0326 (8)	−0.0037 (7)	0.0014 (7)	−0.0017 (7)
C16	0.0343 (9)	0.0346 (9)	0.0308 (8)	−0.0031 (7)	0.0081 (7)	−0.0025 (6)

Geometric parameters (Å, º)

S1—C8	1.7210 (17)	C5—H5	0.9500
S1—C1	1.7716 (15)	C6—C7	1.383 (3)
O1—C11	1.3772 (18)	C6—H6	0.9500
O1—C10	1.4229 (19)	C7—H7	0.9500
N1—C1	1.301 (2)	C9—C10	1.477 (2)
N1—N2	1.3772 (18)	C10—H10A	0.9900
N2—C8	1.362 (2)	C10—H10B	0.9900
N2—C9	1.364 (2)	C11—C12	1.387 (2)
N3—C8	1.320 (2)	C11—C16	1.390 (2)
N3—N4	1.3976 (19)	C12—C13	1.392 (2)
N4—C9	1.318 (2)	C12—H12	0.9500
C1—C2	1.470 (2)	C13—C14	1.379 (3)
C2—C3	1.391 (3)	C13—H13	0.9500
C2—C7	1.398 (2)	C14—C15	1.383 (3)
C3—C4	1.390 (3)	C14—H14	0.9500
C3—H3	0.9500	C15—C16	1.385 (2)
C4—C5	1.382 (3)	C15—H15	0.9500
C4—H4	0.9500	C16—H16	0.9500
C5—C6	1.387 (3)		
C8—S1—C1	87.53 (7)	N3—C8—S1	139.50 (12)
C11—O1—C10	116.52 (12)	N2—C8—S1	109.45 (11)
C1—N1—N2	107.06 (12)	N4—C9—N2	108.78 (14)
C8—N2—C9	105.86 (13)	N4—C9—C10	125.22 (15)

C8—N2—N1	118.82 (13)	N2—C9—C10	125.99 (14)
C9—N2—N1	135.27 (13)	O1—C10—C9	107.79 (13)
C8—N3—N4	105.39 (13)	O1—C10—H10A	110.1
C9—N4—N3	108.93 (13)	C9—C10—H10A	110.1
N1—C1—C2	122.58 (14)	O1—C10—H10B	110.1
N1—C1—S1	117.12 (12)	C9—C10—H10B	110.1
C2—C1—S1	120.30 (12)	H10A—C10—H10B	108.5
C3—C2—C7	119.53 (16)	O1—C11—C12	124.31 (14)
C3—C2—C1	120.35 (15)	O1—C11—C16	115.17 (14)
C7—C2—C1	120.12 (16)	C12—C11—C16	120.52 (15)
C4—C3—C2	120.06 (17)	C11—C12—C13	119.05 (16)
C4—C3—H3	120.0	C11—C12—H12	120.5
C2—C3—H3	120.0	C13—C12—H12	120.5
C5—C4—C3	120.15 (19)	C14—C13—C12	120.80 (16)
C5—C4—H4	119.9	C14—C13—H13	119.6
C3—C4—H4	119.9	C12—C13—H13	119.6
C4—C5—C6	120.02 (17)	C13—C14—C15	119.57 (16)
C4—C5—H5	120.0	C13—C14—H14	120.2
C6—C5—H5	120.0	C15—C14—H14	120.2
C7—C6—C5	120.29 (18)	C14—C15—C16	120.60 (16)
C7—C6—H6	119.9	C14—C15—H15	119.7
C5—C6—H6	119.9	C16—C15—H15	119.7
C6—C7—C2	119.95 (18)	C15—C16—C11	119.45 (16)
C6—C7—H7	120.0	C15—C16—H16	120.3
C2—C7—H7	120.0	C11—C16—H16	120.3
N3—C8—N2	111.04 (14)		

C1—N1—N2—C8	1.29 (18)	C9—N2—C8—S1	−179.52 (10)
C1—N1—N2—C9	178.30 (16)	N1—N2—C8—S1	−1.71 (17)
C8—N3—N4—C9	−0.08 (17)	C1—S1—C8—N3	−177.26 (19)
N2—N1—C1—C2	−179.93 (13)	C1—S1—C8—N2	1.16 (11)
N2—N1—C1—S1	−0.27 (16)	N3—N4—C9—N2	−0.30 (17)
C8—S1—C1—N1	−0.54 (13)	N3—N4—C9—C10	179.72 (14)
C8—S1—C1—C2	179.13 (13)	C8—N2—C9—N4	0.55 (17)
N1—C1—C2—C3	−173.41 (15)	N1—N2—C9—N4	−176.72 (15)
S1—C1—C2—C3	6.9 (2)	C8—N2—C9—C10	−179.47 (15)
N1—C1—C2—C7	7.2 (2)	N1—N2—C9—C10	3.3 (3)
S1—C1—C2—C7	−172.46 (12)	C11—O1—C10—C9	175.43 (13)
C7—C2—C3—C4	−0.6 (3)	N4—C9—C10—O1	−106.96 (18)
C1—C2—C3—C4	−179.97 (16)	N2—C9—C10—O1	73.1 (2)
C2—C3—C4—C5	0.6 (3)	C10—O1—C11—C12	−0.2 (2)
C3—C4—C5—C6	−0.5 (3)	C10—O1—C11—C16	179.35 (14)
C4—C5—C6—C7	0.3 (3)	O1—C11—C12—C13	179.05 (15)
C5—C6—C7—C2	−0.2 (3)	C16—C11—C12—C13	−0.4 (2)
C3—C2—C7—C6	0.4 (2)	C11—C12—C13—C14	−0.5 (3)
C1—C2—C7—C6	179.76 (15)	C12—C13—C14—C15	0.7 (3)
N4—N3—C8—N2	0.43 (17)	C13—C14—C15—C16	0.1 (3)
N4—N3—C8—S1	178.84 (15)	C14—C15—C16—C11	−1.0 (3)

C9—N2—C8—N3	−0.62 (17)	O1—C11—C16—C15	−178.35 (14)
N1—N2—C8—N3	177.19 (12)	C12—C11—C16—C15	1.2 (2)

Hydrogen-bond geometry (Å, º)

Cg is the centroid of the C11–C16 phenyl ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C5—H5···*Cg*^{i}	0.95	2.79	3.633 (2)	148

Symmetry code: (i) −*x*, −*y*+1, −*z*+1.