IUCrData

ISSN 2414-3146

(*E*)-2-({[3-Benzylsulfanyl-5-(*p*-tolyl)-4*H*-1,2,4-triazol-4-yl]imino}methyl)phenol

Qian Hou, Lu Li and Hewen Wang*

College of Chemical Engineering, Huanggang Normal University, Huanggang 438000, People's Republic of China. *Correspondence e-mail: qqhrchemistry@aliyun.com

Received 19 December 2016
Accepted 9 February 2017

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

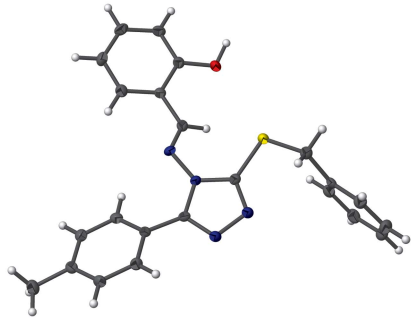
Keywords: crystal structure; Mannich base; 1,2,4-triazole; 1,2,4-triazole-5(4*H*)-thione derivatives; hydrogen bonding.

CCDC reference: 1531827

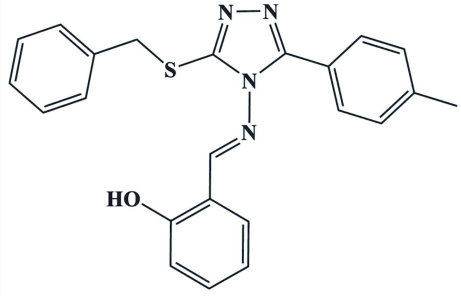
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{23}H_{20}N_4OS$, the 1,2,4-triazole ring (r.m.s. deviation = 0.014 Å) forms dihedral angles of 88.66 (8), 24.48 (8) and 17.97 (7)° with the benzyl, *p*-tolyl and phenol rings, respectively. The conformation about the C=N bond is *E*. In the crystal, molecules are linked by O—H···N hydrogen bonds, forming chains along [010].

3D view



Chemical scheme



Structure description

Recently, we have reported the synthesis and crystal structures of some Mannich base derivatives (Wang *et al.*, 2011*a*,*b*). We report herein, on the crystal structure of the title 1,2,4-triazole–thione derivative.

The molecular structure of the title compound is illustrated in Fig. 1. The 1,2,4-triazole ring (N1–N3/C8/C9) is almost planar with an r.m.s. deviation of 0.014 Å, and a maximum deviation of 0.012 (1) Å for atoms N3 and C9. Atom C9 shows a distorted Csp^2 hybridization state with bond angles of 108.51 (12)° (N2—C9—N3), 124.13 (11)° (N2—C9—C10) and 127.36 (12)° (N3—C9—C10), which are similar to the same bond angles reported for other triazole derivatives (Zhao *et al.*, 2010; Gao *et al.*, 2011). The 1,2,4-triazole ring forms dihedral angles of by 88.66 (8), 24.48 (8) and 17.97 (7) ° with the benzyl ring (C1–C6), the *p*-toluene ring (C10–C15), and the phenol ring (C18–C23), respectively. Hence, the benzyl ring (C1–C6) is almost normal to the 1,2,4-triazole ring. The conformation about the C7=N4 bond is *E*. As a result of π–π conjugation, the Csp^2—S bond [S1—C8 = 1.7462 (14) Å] is significantly shorter than the Csp^3—S bond [S1—C7 = 1.8091 (14) Å]. These values compare well with those of 1.744 (2) and 1.812 (2) Å, respectively, reported for the very similar compound (*E*)-2-{[(3-(propylthio)-5-(*p*-tolyl)-4*H*-1,2,4-triazol-4-yl)imino]methyl}phenol (Wang *et al.*, 2011*b*).

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N2^{i}	0.95 (2)	1.72 (2)	2.6555 (15)	167.6 (19)

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

In the crystal, molecules are linked by O—H···N hydrogen bonds, forming chains propagating along the *b*-axis direction (Fig. 2 and Table 1). There are no other significant intermolecular interactions present.

Synthesis and crystallization

The title compound was synthesized by refluxing 3-(benzylsulfanyl)-5-(*p*-tolyl)-4*p*-1,2,4-triazol-4-amine (2.0 mmol) with 2-hydroxybenzaldehyde (2.0 mmol) in ethanol for 5 h. The resulting precipitate was filtered, washed with cold ethanol, and dried. The target product was purified by recrystallization from chloroform-ethanol (1:2) to give a colourless solid (yield 75%). Colourless prismatic crystals of the title compound, suitable for X-ray diffraction analysis, were grown by slow evaporation of a solution in chloroform–ethanol (1:2).

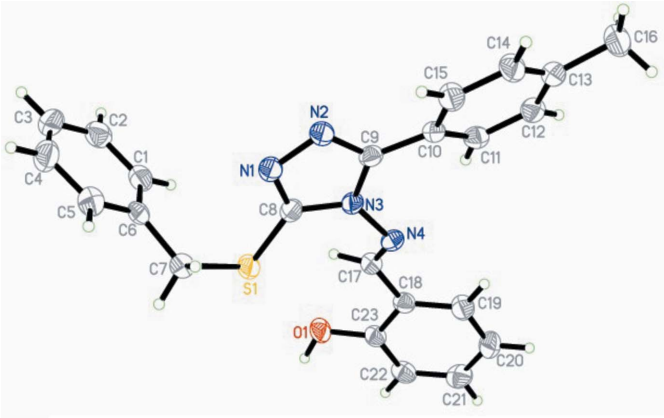


Figure 1
The molecular structure of the title compound, showing the atom labelling. Displacement ellipsoids are drawn at the 75% probability level.

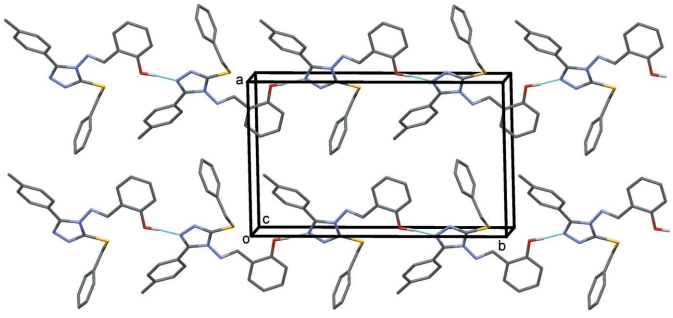


Figure 2
A partial view along the *c* axis of the crystal packing of the title compound. The hydrogen bonds are shown as pale-blue lines (see Table 1). For clarity, only one H atom, H1, has been included.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{20}N_4OS$
M_r	400.49
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	113
a, b, c (Å)	11.8003 (12), 17.9297 (16), 9.8723 (8)
β (°)	110.279 (5)
V (Å^3)	1959.3 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.20 × 0.18 × 0.12
Data collection	
Diffractometer	Rigaku Saturn CCD area detector
Absorption correction	Multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
T_{min}, T_{max}	0.963, 0.978
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22129, 4677, 4023
R_{int}	0.044
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.658
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.099, 1.07
No. of reflections	4677
No. of parameters	267
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.35, −0.21

Computer programs: *CrystalClear* and *CrystalStructure* (Rigaku/MSC, 2005), *SHELXS97*, *SHELXL97* and *SHELXTL* (Sheldrick, 2008) and *Mercury* (Macrae *et al.*, 2008).

Refinement

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

References

Gao, Y., Zhang, L. & Wang, H. (2011). *Acta Cryst.* E**67**, o1794.
Macrae, C. F., Bruno, I. J., Chisholm, J. A., Edgington, P. R., McCabe, P., Pidcock, E., Rodriguez-Monge, L., Taylor, R., van de Streek, J. & Wood, P. A. (2008). *J. Appl. Cryst.* **41**, 466–470.
Rigaku/MSC (2005). *CrystalClear* and *CrystalStructure*. Molecular Structure Corporation, The Woodlands, Texas, USA, and Rigaku Corporation, Tokyo, Japan.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, W., Gao, Y., Xiao, Z., Yao, H. & Zhang, J. (2011*a*). *Acta Cryst.* E**67**, o269.
Wang, W., Liu, Q., Xu, C., Wu, W. & Gao, Y. (2011*b*). *Acta Cryst.* E**67**, o2236.
Zhao, B., Liu, Z., Gao, Y., Song, B. & Deng, Q. (2010). *Acta Cryst.* E**66**, o2814.

full crystallographic data

IUCrData (2017). **2**, x170211 [https://doi.org/10.1107/S2414314617002115]

(*E*)-2-({[3-Benzylsulfanyl-5-(*p*-tolyl)-4*H*-1,2,4-triazol-4-yl]imino}methyl)phenol

Qian Hou, Lu Li and Hewen Wang

(*E*)-2-({[3-Benzylsulfanyl-5-(*p*-tolyl)-4*H*-1,2,4-triazol-4-yl]imino}methyl)phenol

Crystal data

$C_{23}H_{20}N_4OS$
M_r = 400.49
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
a = 11.8003 (12) Å
b = 17.9297 (16) Å
c = 9.8723 (8) Å
β = 110.279 (5)°
V = 1959.3 (3) Å^3
Z = 4
$F(000)$ = 840
D_x = 1.358 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6546 reflections
θ = 1.8–27.9°
μ = 0.19 mm^{-1}
T = 113 K
Prism, colourless
0.20 × 0.18 × 0.12 mm

Data collection

Rigaku Saturn CCD area detector diffractometer
Radiation source: rotating anode
Multilayer monochromator
Detector resolution: 14.22 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (CrystalClear; Rigaku/MSC, 2005)
T_{min} = 0.963, T_{max} = 0.978
22129 measured reflections
4677 independent reflections
4023 reflections with $I > 2\sigma(I)$
R_{int} = 0.044
θ_{max} = 27.9°, θ_{min} = 1.8°
h = −15→15
k = −23→20
l = −12→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.099
S = 1.07
4677 reflections
267 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
$w = 1/[\sigma^2(F_o^2) + (0.0512P)^2 + 0.0691P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.35 e Å^{-3}
$\Delta\rho_{min}$ = −0.21 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	−0.05368 (3)	0.073331 (19)	0.84276 (4)	0.02198 (11)
O1	0.04559 (9)	−0.07904 (5)	0.64668 (11)	0.0235 (2)
H1	0.0323 (17)	−0.1309 (12)	0.657 (2)	0.053 (6)*
N1	−0.05660 (10)	0.22483 (6)	0.83583 (13)	0.0211 (3)
N2	0.00556 (10)	0.28249 (6)	0.79821 (13)	0.0201 (3)
N3	0.07357 (10)	0.17775 (6)	0.74342 (12)	0.0170 (2)
N4	0.15716 (10)	0.12969 (6)	0.71510 (12)	0.0182 (2)
C1	−0.32364 (13)	0.12819 (8)	0.76880 (16)	0.0225 (3)
H1A	−0.2946	0.1052	0.7005	0.027*
C2	−0.44007 (13)	0.15724 (8)	0.72435 (17)	0.0271 (3)
H2	−0.4902	0.1540	0.6257	0.032*
C3	−0.48351 (13)	0.19083 (9)	0.82265 (18)	0.0297 (4)
H3	−0.5635	0.2100	0.7921	0.036*
C4	−0.40971 (14)	0.19621 (9)	0.96563 (18)	0.0292 (4)
H4	−0.4388	0.2194	1.0337	0.035*
C5	−0.29371 (13)	0.16795 (8)	1.00994 (16)	0.0243 (3)
H5	−0.2431	0.1726	1.1082	0.029*
C6	−0.25002 (12)	0.13271 (7)	0.91230 (15)	0.0182 (3)
C7	−0.12538 (12)	0.09818 (8)	0.97144 (15)	0.0221 (3)
H7A	−0.1309	0.0526	1.0254	0.027*
H7B	−0.0717	0.1335	1.0418	0.027*
C8	−0.01388 (12)	0.16245 (7)	0.80360 (15)	0.0191 (3)
C9	0.08464 (12)	0.25386 (7)	0.74565 (15)	0.0174 (3)
C10	0.16945 (12)	0.29819 (7)	0.70022 (15)	0.0176 (3)
C11	0.21798 (12)	0.27415 (8)	0.59754 (15)	0.0192 (3)
H11	0.2010	0.2252	0.5589	0.023*
C12	0.29062 (12)	0.32083 (8)	0.55128 (16)	0.0215 (3)
H12	0.3224	0.3033	0.4809	0.026*
C13	0.31820 (12)	0.39299 (8)	0.60553 (16)	0.0215 (3)
C14	0.27198 (13)	0.41596 (8)	0.71107 (17)	0.0239 (3)
H14	0.2913	0.4643	0.7518	0.029*
C15	0.19875 (13)	0.37003 (8)	0.75794 (16)	0.0225 (3)
H15	0.1682	0.3873	0.8296	0.027*
C16	0.39281 (14)	0.44438 (8)	0.54910 (18)	0.0281 (3)
H16A	0.4761	0.4259	0.5793	0.042*
H16B	0.3922	0.4946	0.5879	0.042*
H16C	0.3586	0.4460	0.4434	0.042*
C17	0.11524 (12)	0.06527 (7)	0.66711 (15)	0.0184 (3)
H17	0.0323	0.0547	0.6487	0.022*
C18	0.19257 (12)	0.00785 (7)	0.64025 (14)	0.0177 (3)

C19	0.30414 (12)	0.02410 (8)	0.62744 (16)	0.0227 (3)
H19	0.3310	0.0743	0.6337	0.027*
C20	0.37576 (13)	−0.03235 (8)	0.60577 (16)	0.0259 (3)
H20	0.4515	−0.0211	0.5968	0.031*
C21	0.33616 (14)	−0.10567 (8)	0.59720 (16)	0.0257 (3)
H21	0.3859	−0.1444	0.5834	0.031*
C22	0.22584 (13)	−0.12335 (8)	0.60829 (15)	0.0217 (3)
H22	0.1994	−0.1737	0.6006	0.026*
C23	0.15335 (12)	−0.06653 (7)	0.63100 (15)	0.0185 (3)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02314 (19)	0.01440 (19)	0.0331 (2)	0.00067 (14)	0.01575 (16)	0.00221 (14)
O1	0.0241 (5)	0.0149 (5)	0.0357 (6)	−0.0020 (4)	0.0160 (5)	0.0011 (4)
N1	0.0196 (6)	0.0157 (6)	0.0301 (7)	0.0003 (5)	0.0114 (5)	0.0013 (5)
N2	0.0202 (6)	0.0147 (6)	0.0270 (6)	0.0003 (5)	0.0102 (5)	0.0012 (5)
N3	0.0164 (5)	0.0128 (6)	0.0230 (6)	0.0013 (4)	0.0086 (5)	−0.0001 (5)
N4	0.0183 (6)	0.0149 (6)	0.0231 (6)	0.0046 (5)	0.0095 (5)	0.0007 (5)
C1	0.0259 (7)	0.0204 (7)	0.0241 (8)	−0.0021 (6)	0.0122 (6)	0.0011 (6)
C2	0.0216 (7)	0.0301 (8)	0.0269 (8)	−0.0035 (6)	0.0049 (6)	0.0070 (6)
C3	0.0193 (7)	0.0289 (8)	0.0425 (10)	0.0037 (6)	0.0126 (7)	0.0086 (7)
C4	0.0285 (8)	0.0276 (8)	0.0382 (9)	0.0022 (7)	0.0200 (7)	−0.0013 (7)
C5	0.0254 (7)	0.0248 (8)	0.0244 (8)	−0.0014 (6)	0.0108 (6)	−0.0005 (6)
C6	0.0188 (7)	0.0133 (7)	0.0244 (7)	−0.0037 (5)	0.0099 (6)	0.0025 (5)
C7	0.0221 (7)	0.0228 (7)	0.0232 (7)	0.0022 (6)	0.0100 (6)	0.0038 (6)
C8	0.0156 (6)	0.0174 (7)	0.0245 (7)	0.0011 (5)	0.0072 (6)	0.0011 (6)
C9	0.0161 (6)	0.0141 (7)	0.0211 (7)	0.0019 (5)	0.0054 (6)	0.0003 (5)
C10	0.0162 (6)	0.0154 (7)	0.0204 (7)	0.0012 (5)	0.0055 (6)	0.0028 (5)
C11	0.0202 (7)	0.0161 (7)	0.0201 (7)	0.0012 (6)	0.0054 (6)	−0.0001 (5)
C12	0.0210 (7)	0.0228 (8)	0.0221 (7)	0.0025 (6)	0.0091 (6)	0.0019 (6)
C13	0.0176 (7)	0.0207 (7)	0.0249 (8)	0.0001 (6)	0.0060 (6)	0.0038 (6)
C14	0.0243 (8)	0.0156 (7)	0.0343 (9)	−0.0026 (6)	0.0134 (7)	−0.0019 (6)
C15	0.0243 (7)	0.0183 (7)	0.0284 (8)	−0.0001 (6)	0.0136 (6)	−0.0027 (6)
C16	0.0291 (8)	0.0265 (8)	0.0328 (9)	−0.0047 (7)	0.0157 (7)	0.0007 (7)
C17	0.0180 (7)	0.0189 (7)	0.0185 (7)	0.0003 (5)	0.0068 (6)	0.0022 (5)
C18	0.0199 (7)	0.0157 (7)	0.0181 (7)	0.0010 (5)	0.0073 (6)	0.0006 (5)
C19	0.0232 (7)	0.0214 (7)	0.0251 (8)	−0.0012 (6)	0.0104 (6)	−0.0003 (6)
C20	0.0228 (7)	0.0294 (8)	0.0302 (8)	0.0023 (6)	0.0153 (7)	0.0004 (7)
C21	0.0302 (8)	0.0246 (8)	0.0262 (8)	0.0092 (6)	0.0148 (7)	0.0000 (6)
C22	0.0299 (8)	0.0161 (7)	0.0208 (7)	0.0009 (6)	0.0110 (6)	−0.0003 (6)
C23	0.0210 (7)	0.0190 (7)	0.0166 (7)	0.0000 (6)	0.0078 (6)	0.0009 (5)

Geometric parameters (Å, º)

S1—C8	1.7462 (14)	C10—C11	1.3941 (19)
S1—C7	1.8091 (14)	C10—C15	1.4025 (19)
O1—C23	1.3519 (16)	C11—C12	1.3839 (19)

O1—H1	0.95 (2)	C11—H11	0.9500
N1—C8	1.3106 (17)	C12—C13	1.395 (2)
N1—N2	1.3904 (16)	C12—H12	0.9500
N2—C9	1.3187 (17)	C13—C14	1.395 (2)
N3—C9	1.3704 (17)	C13—C16	1.508 (2)
N3—C8	1.3849 (17)	C14—C15	1.3842 (19)
N3—N4	1.4088 (15)	C14—H14	0.9500
N4—C17	1.2810 (17)	C15—H15	0.9500
C1—C6	1.3838 (19)	C16—H16A	0.9800
C1—C2	1.391 (2)	C16—H16B	0.9800
C1—H1A	0.9500	C16—H16C	0.9800
C2—C3	1.383 (2)	C17—C18	1.4597 (19)
C2—H2	0.9500	C17—H17	0.9500
C3—C4	1.381 (2)	C18—C19	1.3963 (18)
C3—H3	0.9500	C18—C23	1.4042 (19)
C4—C5	1.381 (2)	C19—C20	1.382 (2)
C4—H4	0.9500	C19—H19	0.9500
C5—C6	1.3923 (19)	C20—C21	1.388 (2)
C5—H5	0.9500	C20—H20	0.9500
C6—C7	1.5141 (19)	C21—C22	1.381 (2)
C7—H7A	0.9900	C21—H21	0.9500
C7—H7B	0.9900	C22—C23	1.3974 (19)
C9—C10	1.4648 (18)	C22—H22	0.9500

C8—S1—C7	99.05 (7)	C12—C11—H11	119.7
C23—O1—H1	111.8 (12)	C10—C11—H11	119.7
C8—N1—N2	106.67 (11)	C11—C12—C13	121.53 (13)
C9—N2—N1	109.05 (11)	C11—C12—H12	119.2
C9—N3—C8	105.75 (11)	C13—C12—H12	119.2
C9—N3—N4	122.88 (11)	C12—C13—C14	117.45 (13)
C8—N3—N4	129.87 (11)	C12—C13—C16	120.88 (13)
C17—N4—N3	114.69 (11)	C14—C13—C16	121.66 (13)
C6—C1—C2	120.14 (14)	C15—C14—C13	121.66 (13)
C6—C1—H1A	119.9	C15—C14—H14	119.2
C2—C1—H1A	119.9	C13—C14—H14	119.2
C3—C2—C1	120.51 (14)	C14—C15—C10	120.34 (13)
C3—C2—H2	119.7	C14—C15—H15	119.8
C1—C2—H2	119.7	C10—C15—H15	119.8
C4—C3—C2	119.46 (14)	C13—C16—H16A	109.5
C4—C3—H3	120.3	C13—C16—H16B	109.5
C2—C3—H3	120.3	H16A—C16—H16B	109.5
C5—C4—C3	120.18 (15)	C13—C16—H16C	109.5
C5—C4—H4	119.9	H16A—C16—H16C	109.5
C3—C4—H4	119.9	H16B—C16—H16C	109.5
C4—C5—C6	120.76 (14)	N4—C17—C18	121.17 (12)
C4—C5—H5	119.6	N4—C17—H17	119.4
C6—C5—H5	119.6	C18—C17—H17	119.4
C1—C6—C5	118.92 (13)	C19—C18—C23	119.48 (13)

C1—C6—C7	123.51 (13)	C19—C18—C17	122.53 (12)
C5—C6—C7	117.51 (13)	C23—C18—C17	117.97 (12)
C6—C7—S1	117.27 (10)	C20—C19—C18	120.51 (13)
C6—C7—H7A	108.0	C20—C19—H19	119.7
S1—C7—H7A	108.0	C18—C19—H19	119.7
C6—C7—H7B	108.0	C19—C20—C21	119.47 (13)
S1—C7—H7B	108.0	C19—C20—H20	120.3
H7A—C7—H7B	107.2	C21—C20—H20	120.3
N1—C8—N3	109.97 (12)	C22—C21—C20	121.30 (13)
N1—C8—S1	124.86 (11)	C22—C21—H21	119.3
N3—C8—S1	125.02 (10)	C20—C21—H21	119.3
N2—C9—N3	108.51 (12)	C21—C22—C23	119.45 (13)
N2—C9—C10	124.13 (11)	C21—C22—H22	120.3
N3—C9—C10	127.36 (12)	C23—C22—H22	120.3
C11—C10—C15	118.29 (13)	O1—C23—C22	123.35 (12)
C11—C10—C9	123.45 (12)	O1—C23—C18	116.87 (12)
C15—C10—C9	118.19 (12)	C22—C23—C18	119.77 (13)
C12—C11—C10	120.69 (13)		

C8—N1—N2—C9	−0.55 (15)	N2—C9—C10—C11	−154.26 (14)
C9—N3—N4—C17	−156.47 (13)	N3—C9—C10—C11	26.5 (2)
C8—N3—N4—C17	39.60 (19)	N2—C9—C10—C15	22.5 (2)
C6—C1—C2—C3	0.0 (2)	N3—C9—C10—C15	−156.66 (14)
C1—C2—C3—C4	0.8 (2)	C15—C10—C11—C12	−1.6 (2)
C2—C3—C4—C5	−0.3 (2)	C9—C10—C11—C12	175.15 (12)
C3—C4—C5—C6	−1.0 (2)	C10—C11—C12—C13	0.2 (2)
C2—C1—C6—C5	−1.2 (2)	C11—C12—C13—C14	1.4 (2)
C2—C1—C6—C7	175.89 (13)	C11—C12—C13—C16	−177.20 (13)
C4—C5—C6—C1	1.8 (2)	C12—C13—C14—C15	−1.7 (2)
C4—C5—C6—C7	−175.54 (13)	C16—C13—C14—C15	176.88 (13)
C1—C6—C7—S1	17.78 (18)	C13—C14—C15—C10	0.4 (2)
C5—C6—C7—S1	−165.06 (11)	C11—C10—C15—C14	1.3 (2)
C8—S1—C7—C6	74.69 (11)	C9—C10—C15—C14	−175.62 (13)
N2—N1—C8—N3	−0.98 (15)	N3—N4—C17—C18	−176.57 (12)
N2—N1—C8—S1	174.78 (10)	N4—C17—C18—C19	−17.4 (2)
C9—N3—C8—N1	2.08 (16)	N4—C17—C18—C23	160.89 (13)
N4—N3—C8—N1	168.11 (12)	C23—C18—C19—C20	0.0 (2)
C9—N3—C8—S1	−173.67 (10)	C17—C18—C19—C20	178.29 (13)
N4—N3—C8—S1	−7.6 (2)	C18—C19—C20—C21	−0.2 (2)
C7—S1—C8—N1	−14.82 (14)	C19—C20—C21—C22	0.7 (2)
C7—S1—C8—N3	160.31 (12)	C20—C21—C22—C23	−1.1 (2)
N1—N2—C9—N3	1.86 (15)	C21—C22—C23—O1	−178.32 (13)
N1—N2—C9—C10	−177.46 (12)	C21—C22—C23—C18	0.9 (2)
C8—N3—C9—N2	−2.39 (15)	C19—C18—C23—O1	178.88 (12)
N4—N3—C9—N2	−169.64 (11)	C17—C18—C23—O1	0.53 (19)
C8—N3—C9—C10	176.91 (13)	C19—C18—C23—C22	−0.4 (2)
N4—N3—C9—C10	9.7 (2)	C17—C18—C23—C22	−178.72 (12)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O1—H1···N2^{i}	0.95 (2)	1.72 (2)	2.6555 (15)	167.6 (19)

Symmetry code: (i) −*x*, *y*−1/2, −*z*+3/2.