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1-[({5-[(4-Methylphenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)methyl]-1*H*-benzo[*d*][1,2,3]triazole

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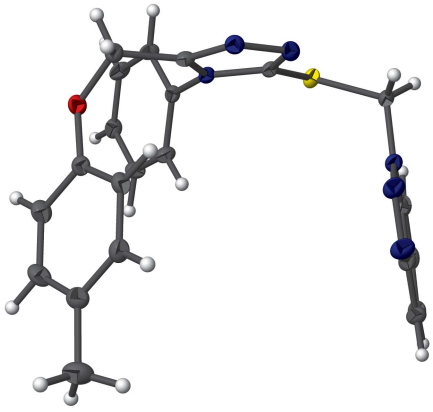
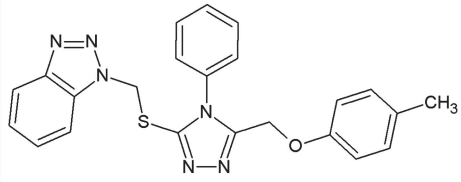
Structural data: full structural data are available from iucrdata.iucr.org

The title molecule, $C_{23}H_{20}N_6OS$, adopts a cup-shaped conformation with the planes of the two benzene rings and the benzotriazole unit close to being parallel. The crystal packing features C—H$\cdots\pi$(ring) and offset π–π stacking interactions.

3D view



Chemical scheme



Structure description

Triazole scaffold compounds have been proved to be an interesting class of heterocyclic compounds due to their various applications in medicinal chemistry (Aher *et al.*, 2009; El-Emary, 2007). Triazole-based drugs such as fluconazole, ketoconazole, itraconazole, voriconazole, ravuconazole and posaconazole have shown remarkable anti-fungal activities (Sheehan *et al.*, 1999; Süküroglu *et al.*, 2005; Bekhit *et al.*, 2005; Cunico *et al.*, 2006). In this context we report herein the synthesis and crystal structure of the title compound.

The title molecule (Fig. 1) adopts a cup-shaped conformation with the C11–C16 ring nearly perpendicular to the plane of the triazole ring [dihedral angle = 85.27 (5)°]. The dihedral angle between the triazole ring and the C1–C6 ring is 81.65 (5)° while that between the triazole ring and the mean plane of the benzotriazole moiety is 88.37 (4)°. Fig. 2 shows the packing of the title compound viewed along the *b* axis. The only significant intermolecular interactions (Fig. 3) appear to be C—H$\cdots\pi$(ring) interactions (Table 1) and offset π–π stacking between the triazole ring and its counterpart at $-x$, $1-y$, $1-z$ [centroid–centroid distance = 3.379 (1) Å].

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

*Cg*5 is the centroid of the C18–C23 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*5^{i}	0.958 (17)	2.944 (17)	3.7406 (17)	141.1 (12)
C17—H17*B*···*Cg*5^{ii}	0.988 (17)	2.813 (16)	3.6331 (15)	140.5 (12)

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

Synthesis and crystallization

This compound was synthesized by reaction of 3-(*p*-tolyloxy)methyl-4-phenyl-1,2,4-triazole-5(1*H*)-thione (0.01 mol) with 1-chloromethyl-1,2,3-benzotriazole (0.01 mol) in an ethanolic KOH solution 4% (30 ml) under reflux conditions

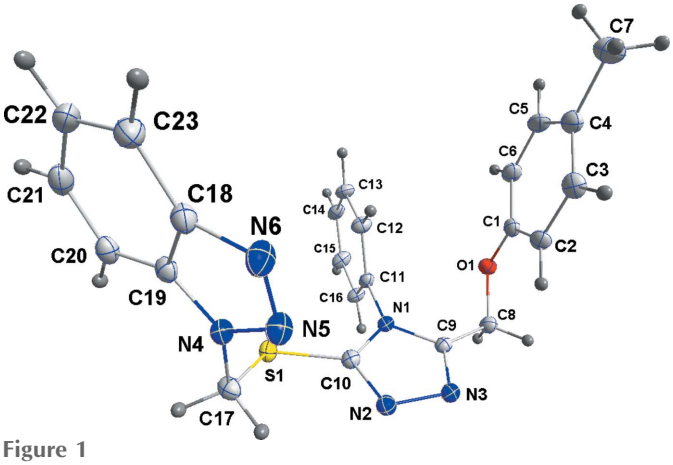


Figure 1
The title molecule, showing the atom-labelling scheme and 50% probability displacement ellipsoids.

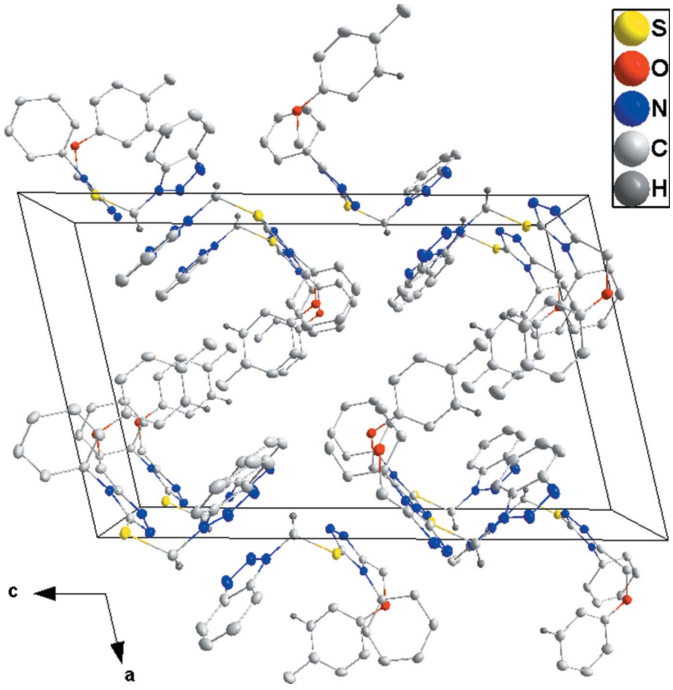


Figure 2
Packing viewed along the *b* axis.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{23}H_{20}N_6OS$
M_r	428.51
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	13.4306 (13), 7.3467 (7), 21.643 (2)
β (°)	103.299 (1)
V (Å^3)	2078.3 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.33 × 0.25 × 0.15
Data collection	
Diffractometer	Bruker SMART APEX CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.88, 0.97
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	33010, 5562, 4453
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.685
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.041, 0.117, 1.09
No. of reflections	5562
No. of parameters	349
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.47, −0.32

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

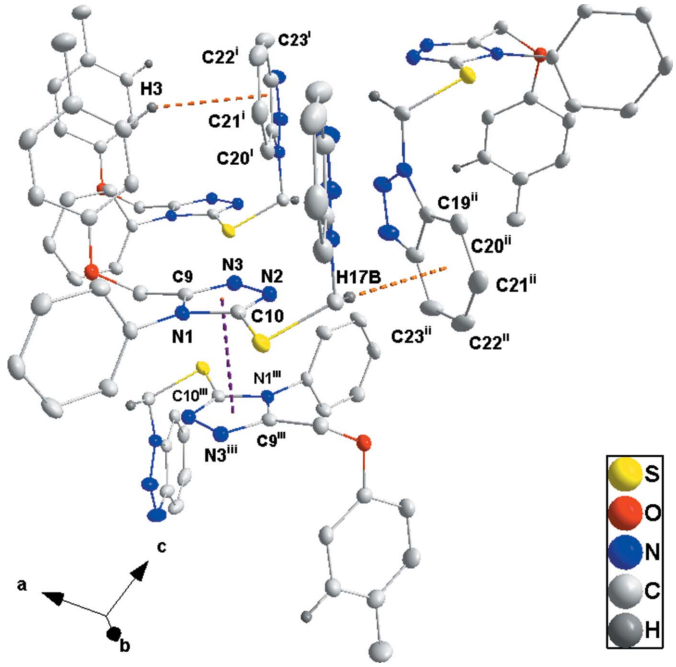


Figure 3
Detail of the intermolecular interactions [C—H···π(ring): orange dotted lines; offset π–π-stacking: purple dotted line; symmetry codes: (i) $x, -1+y, z$; (ii) $-x, -\frac{1}{2}+y, 1.5-z$; (iii) $-x, 1-y, 1-z$].

for 30 min. The product that formed after cooling was collected and recrystallized from ethanol solution; yield: 83%, m.p. 396 K. IR: 1600 cm^{-1} (C═N), 1400 cm^{-1} (C—S—C). ^1H NMR ($CDCl_3$): 6.60–8.10 (*m*, 13H, Ar—H), 6.30 (*s*, 3H, NCH_2N), 4.95 (*s*, 3H, OCH_2), 2.3 (*s*, 3H, CH_3 of *p*-tolyl residue).

Refinement

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

Acknowledgements

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full crystallographic data

IUCrData (2016). **1**, x161867 [https://doi.org/10.1107/S2414314616018678]

1-[({5-[(4-Methylphenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)methyl]-1*H*-benzo[*d*][1,2,3]triazole

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1-[({5-[(4-Methylphenoxy)methyl]-4-phenyl-4*H*-1,2,4-triazol-3-yl}sulfanyl)methyl]-1*H*-benzo[*d*][1,2,3]triazole

Crystal data

$C_{23}H_{20}N_6OS$
M_r = 428.51
Monoclinic, $P2_1/c$
a = 13.4306 (13) Å
b = 7.3467 (7) Å
c = 21.643 (2) Å
β = 103.299 (1)°
V = 2078.3 (4) Å^3
Z = 4
$F(000)$ = 896
D_x = 1.370 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 9996 reflections
θ = 2.8–29.0°
μ = 0.19 mm^{-1}
T = 100 K
Block, colourless
0.33 × 0.25 × 0.15 mm

Data collection

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2016)
T_{min} = 0.88, T_{max} = 0.97
33010 measured reflections
5562 independent reflections
4453 reflections with $I > 2\sigma(I)$
R_{int} = 0.045
θ_{max} = 29.1°, θ_{min} = 1.6°
h = −18→18
k = −9→9
l = −29→29

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.041
$wR(F^2)$ = 0.117
S = 1.09
5562 reflections
349 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
$w = 1/[\sigma^2(F_o^2) + (0.0686P)^2 + 0.2704P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.47 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}

Special details

Experimental. The diffraction data were obtained from 3 sets of 400 frames, each of width 0.5° in ω, collected at φ = 0.00, 90.00 and 180.00° and 2 sets of 800 frames, each of width 0.45° in φ, collected at ω = –30.00 and 210.00°. The scan time was 20 sec/frame.

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. The methyl group hydrogen atoms were placed in calculated positions (C—H = 0.98 Å) and included as riding contributions with isotropic displacement parameters 1.5 times that of the attached carbon. All other hydrogen atoms were refined.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.05511 (2)	0.90294 (4)	0.58865 (2)	0.01696 (10)
O1	0.29332 (7)	0.33021 (12)	0.52507 (4)	0.0180 (2)
N1	0.14404 (8)	0.60502 (13)	0.55066 (5)	0.0135 (2)
N2	0.01877 (8)	0.53393 (14)	0.59711 (5)	0.0168 (2)
N3	0.05727 (8)	0.37344 (14)	0.57633 (5)	0.0165 (2)
N4	0.07164 (8)	0.90434 (14)	0.71716 (5)	0.0165 (2)
N5	0.09062 (9)	0.74811 (15)	0.75173 (6)	0.0211 (2)
N6	0.15812 (10)	0.78124 (15)	0.80397 (6)	0.0239 (3)
C1	0.35390 (10)	0.28415 (16)	0.58342 (6)	0.0169 (3)
C2	0.31854 (10)	0.21032 (17)	0.63339 (7)	0.0192 (3)
H2	0.2477 (13)	0.191 (2)	0.6297 (8)	0.026 (4)*
C3	0.38853 (11)	0.16552 (19)	0.68954 (7)	0.0211 (3)
H3	0.3635 (12)	0.110 (2)	0.7232 (8)	0.024 (4)*
C4	0.49313 (11)	0.19445 (18)	0.69718 (7)	0.0226 (3)
C5	0.52643 (11)	0.26869 (19)	0.64610 (8)	0.0244 (3)
H5	0.6008 (14)	0.287 (2)	0.6521 (9)	0.037 (5)*
C6	0.45866 (10)	0.31422 (19)	0.58997 (7)	0.0221 (3)
H6	0.4824 (14)	0.368 (2)	0.5542 (9)	0.033 (5)*
C7	0.56761 (12)	0.1538 (2)	0.75915 (8)	0.0334 (4)
H7A	0.5949	0.0306	0.7578	0.050*
H7B	0.5325	0.1627	0.7940	0.050*
H7C	0.6239	0.2419	0.7659	0.050*
C8	0.18636 (10)	0.29304 (17)	0.51388 (7)	0.0174 (3)
H8A	0.1629 (12)	0.314 (2)	0.4678 (9)	0.023 (4)*
H8B	0.1723 (12)	0.168 (2)	0.5242 (7)	0.019 (4)*
C9	0.13027 (9)	0.41955 (16)	0.54828 (6)	0.0142 (2)
C10	0.07239 (9)	0.66752 (17)	0.58130 (6)	0.0142 (2)
C11	0.21804 (9)	0.71140 (16)	0.52779 (6)	0.0141 (2)
C12	0.30946 (10)	0.75493 (18)	0.56988 (7)	0.0195 (3)
H12	0.3219 (13)	0.714 (2)	0.6124 (9)	0.028 (4)*
C13	0.38098 (10)	0.85787 (19)	0.54843 (7)	0.0212 (3)

H13	0.4466 (13)	0.886 (2)	0.5775 (8)	0.028 (4)*
C14	0.36072 (11)	0.91489 (18)	0.48581 (7)	0.0202 (3)
H14	0.4079 (12)	0.987 (2)	0.4707 (8)	0.024 (4)*
C15	0.26954 (11)	0.86966 (19)	0.44434 (7)	0.0216 (3)
H15	0.2537 (14)	0.906 (2)	0.4011 (9)	0.032 (5)*
C16	0.19657 (10)	0.76632 (17)	0.46520 (6)	0.0180 (3)
H16	0.1347 (12)	0.728 (2)	0.4375 (8)	0.020 (4)*
C17	−0.00199 (10)	0.90497 (18)	0.65724 (6)	0.0176 (3)
H17A	−0.0460 (11)	1.016 (2)	0.6523 (7)	0.021 (4)*
H17B	−0.0455 (12)	0.795 (2)	0.6545 (8)	0.024 (4)*
C18	0.18537 (10)	0.96314 (18)	0.80404 (6)	0.0194 (3)
C19	0.13056 (9)	1.04311 (17)	0.74816 (6)	0.0164 (2)
C20	0.14080 (11)	1.22709 (18)	0.73345 (7)	0.0196 (3)
H20	0.1008 (13)	1.280 (2)	0.6972 (8)	0.026 (4)*
C21	0.21081 (11)	1.32446 (19)	0.77793 (8)	0.0244 (3)
H21	0.2206 (12)	1.453 (2)	0.7707 (7)	0.022 (4)*
C22	0.26699 (11)	1.2443 (2)	0.83475 (8)	0.0260 (3)
H22	0.3122 (14)	1.319 (3)	0.8643 (9)	0.036 (5)*
C23	0.25476 (11)	1.0653 (2)	0.84924 (7)	0.0249 (3)
H23	0.2920 (13)	1.012 (2)	0.8893 (9)	0.031 (4)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.02206 (17)	0.01508 (16)	0.01524 (17)	0.00036 (11)	0.00735 (12)	0.00031 (11)
O1	0.0165 (4)	0.0206 (4)	0.0181 (5)	0.0001 (3)	0.0061 (4)	0.0015 (4)
N1	0.0145 (5)	0.0147 (5)	0.0117 (5)	−0.0014 (4)	0.0040 (4)	0.0001 (4)
N2	0.0168 (5)	0.0172 (5)	0.0170 (6)	0.0002 (4)	0.0052 (4)	0.0008 (4)
N3	0.0163 (5)	0.0163 (5)	0.0167 (6)	−0.0009 (4)	0.0036 (4)	−0.0002 (4)
N4	0.0187 (5)	0.0167 (5)	0.0142 (5)	0.0015 (4)	0.0042 (4)	0.0006 (4)
N5	0.0274 (6)	0.0183 (5)	0.0173 (6)	0.0021 (4)	0.0041 (5)	0.0016 (4)
N6	0.0316 (7)	0.0182 (6)	0.0192 (6)	0.0034 (5)	0.0004 (5)	0.0010 (4)
C1	0.0186 (6)	0.0140 (6)	0.0181 (7)	0.0017 (4)	0.0045 (5)	−0.0010 (5)
C2	0.0167 (6)	0.0201 (6)	0.0222 (7)	0.0006 (5)	0.0071 (5)	−0.0004 (5)
C3	0.0235 (7)	0.0212 (6)	0.0199 (7)	0.0021 (5)	0.0079 (6)	0.0007 (5)
C4	0.0221 (7)	0.0202 (6)	0.0240 (7)	0.0019 (5)	0.0026 (5)	−0.0020 (5)
C5	0.0159 (6)	0.0244 (7)	0.0323 (8)	−0.0024 (5)	0.0043 (6)	0.0001 (6)
C6	0.0193 (6)	0.0221 (6)	0.0264 (8)	−0.0025 (5)	0.0086 (6)	0.0009 (5)
C7	0.0282 (8)	0.0382 (8)	0.0290 (9)	0.0005 (7)	−0.0031 (6)	0.0036 (7)
C8	0.0167 (6)	0.0180 (6)	0.0177 (7)	−0.0009 (5)	0.0045 (5)	−0.0023 (5)
C9	0.0145 (6)	0.0149 (5)	0.0120 (6)	−0.0017 (4)	0.0006 (4)	0.0007 (4)
C10	0.0156 (6)	0.0159 (5)	0.0108 (6)	−0.0002 (4)	0.0027 (4)	0.0000 (4)
C11	0.0147 (6)	0.0136 (5)	0.0150 (6)	−0.0020 (4)	0.0059 (5)	−0.0012 (4)
C12	0.0205 (6)	0.0232 (6)	0.0137 (6)	−0.0032 (5)	0.0021 (5)	−0.0005 (5)
C13	0.0163 (6)	0.0238 (6)	0.0222 (7)	−0.0053 (5)	0.0019 (5)	−0.0029 (5)
C14	0.0203 (6)	0.0206 (6)	0.0224 (7)	−0.0071 (5)	0.0105 (5)	−0.0024 (5)
C15	0.0271 (7)	0.0245 (6)	0.0139 (7)	−0.0082 (5)	0.0061 (5)	0.0008 (5)
C16	0.0189 (6)	0.0202 (6)	0.0143 (6)	−0.0057 (5)	0.0027 (5)	0.0000 (5)

C17	0.0166 (6)	0.0237 (6)	0.0130 (6)	0.0023 (5)	0.0041 (5)	−0.0017 (5)
C18	0.0222 (6)	0.0184 (6)	0.0173 (7)	0.0048 (5)	0.0039 (5)	−0.0012 (5)
C19	0.0178 (6)	0.0184 (6)	0.0145 (6)	0.0024 (5)	0.0069 (5)	−0.0019 (5)
C20	0.0214 (6)	0.0189 (6)	0.0212 (7)	0.0027 (5)	0.0103 (5)	0.0007 (5)
C21	0.0245 (7)	0.0178 (6)	0.0342 (9)	−0.0006 (5)	0.0137 (6)	−0.0052 (6)
C22	0.0211 (7)	0.0258 (7)	0.0303 (8)	0.0006 (5)	0.0042 (6)	−0.0139 (6)
C23	0.0247 (7)	0.0271 (7)	0.0202 (7)	0.0066 (5)	−0.0003 (6)	−0.0063 (6)

Geometric parameters (Å, º)

S1—C10	1.7571 (13)	C7—H7C	0.9800
S1—C17	1.8209 (14)	C8—C9	1.4979 (17)
O1—C1	1.3780 (16)	C8—H8A	0.987 (18)
O1—C8	1.4272 (15)	C8—H8B	0.975 (16)
N1—C10	1.3677 (16)	C11—C16	1.3787 (18)
N1—C9	1.3744 (15)	C11—C12	1.3876 (17)
N1—C11	1.4388 (15)	C12—C13	1.3840 (19)
N2—C10	1.3085 (16)	C12—H12	0.948 (18)
N2—N3	1.4024 (15)	C13—C14	1.384 (2)
N3—C9	1.3108 (17)	C13—H13	0.979 (18)
N4—N5	1.3618 (15)	C14—C15	1.3820 (19)
N4—C19	1.3681 (16)	C14—H14	0.938 (17)
N4—C17	1.4385 (16)	C15—C16	1.3944 (18)
N5—N6	1.2992 (16)	C15—H15	0.948 (19)
N6—C18	1.3855 (17)	C16—H16	0.948 (16)
C1—C2	1.3876 (19)	C17—H17A	0.996 (16)
C1—C6	1.3989 (18)	C17—H17B	0.988 (17)
C2—C3	1.3940 (19)	C18—C19	1.3929 (18)
C2—H2	0.947 (17)	C18—C23	1.4034 (19)
C3—C4	1.3925 (19)	C19—C20	1.4026 (18)
C3—H3	0.958 (17)	C20—C21	1.381 (2)
C4—C5	1.395 (2)	C20—H20	0.927 (17)
C4—C7	1.507 (2)	C21—C22	1.415 (2)
C5—C6	1.381 (2)	C21—H21	0.968 (17)
C5—H5	0.986 (19)	C22—C23	1.371 (2)
C6—H6	0.987 (19)	C22—H22	0.950 (19)
C7—H7A	0.9800	C23—H23	0.976 (18)
C7—H7B	0.9800		

C10—S1—C17	99.85 (6)	N2—C10—N1	111.46 (11)
C1—O1—C8	117.88 (10)	N2—C10—S1	128.50 (10)
C10—N1—C9	104.32 (10)	N1—C10—S1	119.78 (9)
C10—N1—C11	127.10 (10)	C16—C11—C12	122.09 (12)
C9—N1—C11	128.56 (10)	C16—C11—N1	119.47 (11)
C10—N2—N3	106.32 (10)	C12—C11—N1	118.44 (11)
C9—N3—N2	107.55 (10)	C13—C12—C11	118.89 (13)
N5—N4—C19	110.15 (11)	C13—C12—H12	121.4 (10)
N5—N4—C17	120.07 (11)	C11—C12—H12	119.7 (10)

C19—N4—C17	129.78 (11)	C12—C13—C14	119.90 (12)
N6—N5—N4	108.98 (11)	C12—C13—H13	119.3 (10)
N5—N6—C18	108.24 (11)	C14—C13—H13	120.8 (10)
O1—C1—C2	125.06 (12)	C15—C14—C13	120.55 (12)
O1—C1—C6	114.97 (12)	C15—C14—H14	118.5 (10)
C2—C1—C6	119.96 (13)	C13—C14—H14	120.9 (10)
C1—C2—C3	119.25 (12)	C14—C15—C16	120.29 (13)
C1—C2—H2	120.7 (11)	C14—C15—H15	122.6 (11)
C3—C2—H2	120.1 (11)	C16—C15—H15	117.1 (11)
C4—C3—C2	121.81 (13)	C11—C16—C15	118.28 (12)
C4—C3—H3	119.6 (10)	C11—C16—H16	119.2 (10)
C2—C3—H3	118.5 (10)	C15—C16—H16	122.4 (10)
C3—C4—C5	117.64 (13)	N4—C17—S1	113.81 (9)
C3—C4—C7	121.37 (14)	N4—C17—H17A	111.5 (9)
C5—C4—C7	120.95 (13)	S1—C17—H17A	105.7 (9)
C6—C5—C4	121.67 (13)	N4—C17—H17B	109.0 (10)
C6—C5—H5	121.7 (12)	S1—C17—H17B	107.4 (10)
C4—C5—H5	116.7 (12)	H17A—C17—H17B	109.3 (13)
C5—C6—C1	119.66 (13)	N6—C18—C19	108.61 (11)
C5—C6—H6	121.5 (11)	N6—C18—C23	130.52 (13)
C1—C6—H6	118.9 (11)	C19—C18—C23	120.87 (13)
C4—C7—H7A	109.5	N4—C19—C18	104.01 (11)
C4—C7—H7B	109.5	N4—C19—C20	133.05 (12)
H7A—C7—H7B	109.5	C18—C19—C20	122.94 (12)
C4—C7—H7C	109.5	C21—C20—C19	115.32 (13)
H7A—C7—H7C	109.5	C21—C20—H20	122.8 (10)
H7B—C7—H7C	109.5	C19—C20—H20	121.8 (10)
O1—C8—C9	113.50 (10)	C20—C21—C22	122.15 (13)
O1—C8—H8A	102.5 (10)	C20—C21—H21	119.1 (9)
C9—C8—H8A	109.0 (10)	C22—C21—H21	118.7 (9)
O1—C8—H8B	112.5 (9)	C23—C22—C21	122.01 (13)
C9—C8—H8B	109.0 (9)	C23—C22—H22	119.7 (12)
H8A—C8—H8B	110.2 (13)	C21—C22—H22	118.3 (12)
N3—C9—N1	110.33 (11)	C22—C23—C18	116.69 (13)
N3—C9—C8	125.81 (11)	C22—C23—H23	121.4 (11)
N1—C9—C8	123.71 (11)	C18—C23—H23	121.9 (11)

C10—N2—N3—C9	−1.14 (13)	C10—N1—C11—C16	−95.78 (15)
C19—N4—N5—N6	0.86 (15)	C9—N1—C11—C16	85.85 (16)
C17—N4—N5—N6	−179.06 (11)	C10—N1—C11—C12	84.43 (16)
N4—N5—N6—C18	−0.46 (15)	C9—N1—C11—C12	−93.95 (16)
C8—O1—C1—C2	−2.58 (18)	C16—C11—C12—C13	0.5 (2)
C8—O1—C1—C6	176.39 (11)	N1—C11—C12—C13	−179.73 (12)
O1—C1—C2—C3	178.38 (12)	C11—C12—C13—C14	−0.2 (2)
C6—C1—C2—C3	−0.54 (19)	C12—C13—C14—C15	−0.1 (2)
C1—C2—C3—C4	0.6 (2)	C13—C14—C15—C16	0.2 (2)
C2—C3—C4—C5	−0.7 (2)	C12—C11—C16—C15	−0.4 (2)
C2—C3—C4—C7	177.05 (13)	N1—C11—C16—C15	179.85 (12)

C3—C4—C5—C6	0.7 (2)	C14—C15—C16—C11	0.0 (2)
C7—C4—C5—C6	−177.08 (14)	N5—N4—C17—S1	−103.00 (12)
C4—C5—C6—C1	−0.6 (2)	C19—N4—C17—S1	77.10 (15)
O1—C1—C6—C5	−178.49 (12)	C10—S1—C17—N4	85.65 (10)
C2—C1—C6—C5	0.5 (2)	N5—N6—C18—C19	−0.09 (15)
C1—O1—C8—C9	73.43 (14)	N5—N6—C18—C23	−179.99 (14)
N2—N3—C9—N1	1.38 (14)	N5—N4—C19—C18	−0.88 (14)
N2—N3—C9—C8	−174.26 (11)	C17—N4—C19—C18	179.04 (12)
C10—N1—C9—N3	−1.07 (14)	N5—N4—C19—C20	179.58 (14)
C11—N1—C9—N3	177.59 (11)	C17—N4—C19—C20	−0.5 (2)
C10—N1—C9—C8	174.68 (11)	N6—C18—C19—N4	0.59 (14)
C11—N1—C9—C8	−6.7 (2)	C23—C18—C19—N4	−179.50 (12)
O1—C8—C9—N3	−139.85 (13)	N6—C18—C19—C20	−179.80 (12)
O1—C8—C9—N1	45.06 (17)	C23—C18—C19—C20	0.1 (2)
N3—N2—C10—N1	0.48 (14)	N4—C19—C20—C21	−179.46 (14)
N3—N2—C10—S1	174.59 (9)	C18—C19—C20—C21	1.06 (19)
C9—N1—C10—N2	0.32 (14)	C19—C20—C21—C22	−0.9 (2)
C11—N1—C10—N2	−178.37 (11)	C20—C21—C22—C23	−0.4 (2)
C9—N1—C10—S1	−174.37 (9)	C21—C22—C23—C18	1.6 (2)
C11—N1—C10—S1	6.94 (17)	N6—C18—C23—C22	178.46 (14)
C17—S1—C10—N2	29.09 (13)	C19—C18—C23—C22	−1.4 (2)
C17—S1—C10—N1	−157.22 (10)		

Hydrogen-bond geometry (Å, º)

Cg5 is the centroid of the C18–C23 ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C3—H3···*Cg*5^{i}	0.958 (17)	2.944 (17)	3.7406 (17)	141.1 (12)
C17—H17*B*···*Cg*5^{ii}	0.988 (17)	2.813 (16)	3.6331 (15)	140.5 (12)

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