

# 3-(4-Methoxyphenyl)-4-methyl-N-[4-(4-methylphenyl)-1,3-thiazol-2-yl]benzamide

K. Archana,<sup>a</sup> K. Saravanan,<sup>a</sup> K. Lakshmithendral,<sup>a</sup> S. Kabilan<sup>a\*</sup> and S. Selvanayagam<sup>b‡</sup>

<sup>a</sup>Drug Discovery Lab, Department of Chemistry, Annamalai University, Annamalaiagar, Chidambaram 608 002, India, and <sup>b</sup>PG & Research Department of Physics, Government Arts College, Melur 625 106, India. \*Correspondence e-mail: profskabilan@gmail.com

Received 11 May 2017

Accepted 15 May 2017

Edited by M. Bolte, Goethe-Universität Frankfurt, Germany

‡ Additional correspondence author, e-mail: s\_selvanayagam@rediffmail.com.

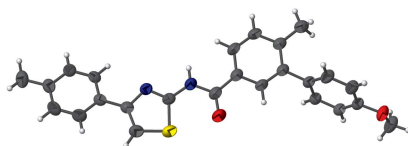
Keywords: crystal structure; thiazole derivative; N—H···O intermolecular hydrogen bonds; weak C—H···O and C—H··· $\pi$  interactions.

CCDC reference: 1550177

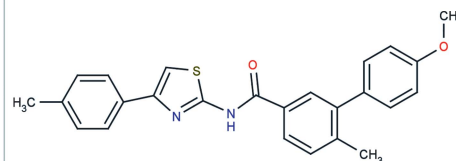
Structural data: full structural data are available from [iucrdata.iucr.org](http://iucrdata.iucr.org)

In the title compound, C<sub>25</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>S, the methylphenyl rings are oriented with a dihedral angle of 19.4 (1)° with respect to each other. In the crystal, molecules are linked *via* strong N—H···O hydrogen bonds, which form C(11) chains propagating along [001]. In addition, weak C—H···O and C—H··· $\pi$  interactions are observed in the structure.

## 3D view



## Chemical scheme

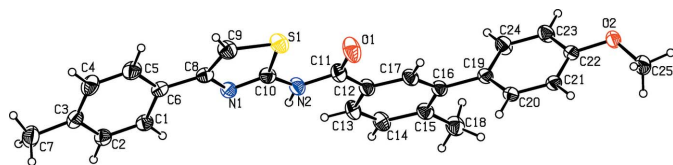


## Structure description

Thiazole derivatives show USP7 (Chen *et al.*, 2017), PDE-4 (Balasubramanian *et al.*, 2016) and Pin1 (Zhao *et al.*, 2016) inhibitory activities. They possess antioxidant (Grozav *et al.*, 2017) and anti-*Trypanosoma cruzi* (da Silva *et al.*, 2017) activities and are used as anti-prostate cancer agents (Saravanan *et al.*, 2017). In view of the above importance of thiazole derivatives, we have undertaken the single-crystal X-ray diffraction study of the title compound, and the results are presented herein.

The molecular structure of the title compound is illustrated in Fig. 1. The methoxy atoms O2 and C25 deviate by 0.019 (2) and 0.363 (3) Å, respectively, from the attached ring. The methyl phenyl rings are oriented at a dihedral angle of 19.4 (1)° with respect to each other. The methylphenyl ring attached to the thiazole group is almost perpendicular to the methoxyphenyl ring, making a dihedral angle of 84.2 (1)°.

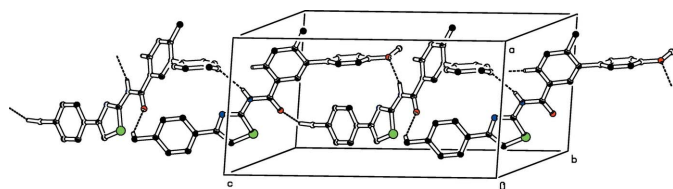
In the crystal, N—H···O hydrogen bonds (Table 1) link the molecules, forming C(11) chains propagating along [100]. Two C—H···O interactions link the molecules, forming C(10) and C(12) chains (Fig. 2). In addition, C—H··· $\pi$  interactions link the molecules into C(13) chains propagating along [010] (Table 1 and Fig. 3).



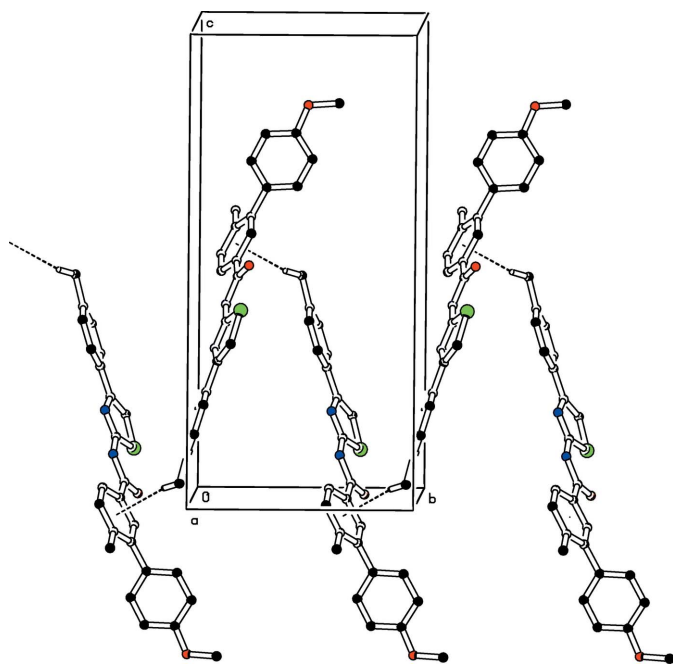
**Figure 1**  
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

### Synthesis and crystallization

3-Iodo-4-methyl-*N*-(4-(*p*-tolyl)thiazol-2-yl)benzamide (0.23 mmol) was dissolved in 20 ml of deoxygenated toluene and water (8:2). Then, tetrakis(triphenylphosphine)palladium (0.017 mmol) and  $K_2CO_3$  (0.72 mmol) was added in turn at 10 minute intervals. Finally, 4-methoxy phenyl boronic acid (0.25 mmol) was added and the resulting reaction mixture was heated to reflux for 16 h under a nitrogen atmosphere. The



**Figure 2**  
The crystal packing of the title compound viewed down *b* axis. The N—H...O and C—H...O hydrogen bonds are shown as dashed lines (see Table 1). For clarity H atoms not involved in these hydrogen bonds have been omitted.



**Figure 3**  
The crystal packing of the title compound. The weak C—H... $\pi$  interactions (see Table 1) are shown as dashed lines. For clarity H atoms not involved in these interactions have been omitted.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

*C*<sub>g</sub> is the centroid of the C12–C17 ring.

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N2—H2...O2 <sup>i</sup>	0.86	2.33	3.175 (2)	166
C7—H7B...O1 <sup>i</sup>	0.96	2.59	3.452 (3)	149
C13—H13...O2 <sup>i</sup>	0.93	2.50	3.413 (4)	166
C7—H7C...C <sub>g</sub> <sup>ii</sup>	0.96	2.67	3.592 (5)	149

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

**Table 2**  
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{22}N_2O_2S$
$M_r$	414.50
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
<i>a</i> , <i>b</i> , <i>c</i> ( $\text{\AA}$ )	9.784 (1), 10.291 (1), 21.58 (2)
$\beta$ ( $^\circ$ )	99.528 (11)
<i>V</i> ( $\text{\AA}^3$ )	2143 (2)
<i>Z</i>	4
Radiation type	Mo $K\alpha$
$\mu$ ( $\text{mm}^{-1}$ )	0.18
Crystal size (mm)	0.22 $\times$ 0.20 $\times$ 0.18
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections	7733, 4741, 3399
$R_{\text{int}}$	0.050
$(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )	0.648
Refinement	
$R[F^2 > 2\sigma(F^2)]$ , $wR(F^2)$ , <i>S</i>	0.057, 0.178, 1.06
No. of reflections	4741
No. of parameters	273
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{\text{max}}$ , $\Delta\rho_{\text{min}}$ ( $e \text{\AA}^{-3}$ )	0.28, $-0.26$

Computer programs: SMART and SAINT (Bruker, 2002), SHELXS97 (Sheldrick, 2008), SHELXL2014 (Sheldrick, 2015), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2009).

progress of the reaction was monitored by pre-coated TLC plates. After completion of the reaction, it was cooled to rt and concentrated using a Rotavac. The obtained crude compound was purified by column chromatography using 20% ethyl acetate and petroleum ether (60:80) as eluent. The pure compound was obtained as a yellow solid, which was recrystallized from a methanol solution, yielding yellow crystals.

### Refinement

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

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## full crystallographic data

*IUCrData* (2017). **2**, x170721 [https://doi.org/10.1107/S2414314617007210]

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#### 3-(4-Methoxyphenyl)-4-methyl-*N*-[4-(4-methylphenyl)-1,3-thiazol-2-yl]benzamide

##### Crystal data

C<sub>25</sub>H<sub>22</sub>N<sub>2</sub>O<sub>2</sub>S

$M_r = 414.50$

Monoclinic,  $P2_1/c$

$a = 9.784$  (1) Å

$b = 10.291$  (1) Å

$c = 21.58$  (2) Å

$\beta = 99.528$  (11)°

$V = 2143$  (2) Å<sup>3</sup>

$Z = 4$

$F(000) = 872$

$D_x = 1.285$  Mg m<sup>-3</sup>

Mo  $K\alpha$  radiation,  $\lambda = 0.71073$  Å

Cell parameters from 5988 reflections

$\theta = 3.3$ – $26.9$ °

$\mu = 0.18$  mm<sup>-1</sup>

$T = 296$  K

Block, yellow

$0.22 \times 0.20 \times 0.18$  mm

##### Data collection

Bruker SMART APEX CCD area-detector diffractometer

Radiation source: fine-focus sealed tube

$\omega$  and  $\phi$  scans

7733 measured reflections

4741 independent reflections

3399 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.050$

$\theta_{\text{max}} = 27.4$ °,  $\theta_{\text{min}} = 3.1$ °

$h = -8 \rightarrow 12$

$k = -13 \rightarrow 7$

$l = -27 \rightarrow 27$

##### Refinement

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.057$

$wR(F^2) = 0.178$

$S = 1.06$

4741 reflections

273 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0938P)^2 + 0.3624P]$

where  $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta\rho_{\text{max}} = 0.28$  e Å<sup>-3</sup>

$\Delta\rho_{\text{min}} = -0.26$  e Å<sup>-3</sup>

##### 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.** All H atoms were found in a difference map, but refined as riding on their parent atom with  $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C}, \text{N})$  or  $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C}_{\text{methyl}})$ .

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.15473 (6)	0.72428 (6)	0.08785 (3)	0.0600 (2)
O1	0.32225 (19)	0.7510 (2)	0.00108 (9)	0.0804 (6)
O2	0.67000 (17)	0.99059 (14)	-0.32054 (6)	0.0536 (4)
N1	0.31758 (17)	0.60345 (16)	0.17559 (7)	0.0438 (4)
N2	0.42415 (19)	0.64619 (18)	0.08819 (7)	0.0490 (4)
H2	0.4980	0.6085	0.1069	0.059*
C1	0.3007 (2)	0.5388 (2)	0.30297 (9)	0.0450 (5)
H1	0.3865	0.5414	0.2898	0.054*
C2	0.2926 (2)	0.4998 (2)	0.36389 (10)	0.0488 (5)
H2A	0.3733	0.4759	0.3906	0.059*
C3	0.1669 (2)	0.4955 (2)	0.38611 (11)	0.0508 (5)
C4	0.0493 (2)	0.5281 (3)	0.34400 (12)	0.0626 (6)
H4	-0.0367	0.5235	0.3569	0.075*
C5	0.0560 (2)	0.5675 (2)	0.28275 (12)	0.0596 (6)
H5	-0.0251	0.5897	0.2559	0.072*
C6	0.1821 (2)	0.57396 (19)	0.26133 (9)	0.0424 (4)
C7	0.1594 (3)	0.4598 (3)	0.45323 (12)	0.0701 (7)
H7A	0.0667	0.4334	0.4564	0.105*
H7B	0.1845	0.5337	0.4798	0.105*
H7C	0.2222	0.3896	0.4662	0.105*
C8	0.1929 (2)	0.62106 (19)	0.19730 (10)	0.0436 (4)
C9	0.0947 (2)	0.6840 (2)	0.15596 (11)	0.0578 (6)
H9	0.0061	0.7029	0.1636	0.069*
C10	0.3109 (2)	0.6522 (2)	0.11926 (9)	0.0447 (5)
C11	0.4253 (2)	0.6969 (2)	0.02931 (10)	0.0527 (5)
C12	0.5550 (2)	0.6842 (2)	0.00231 (9)	0.0470 (5)
C13	0.6709 (2)	0.6125 (2)	0.02920 (10)	0.0537 (5)
H13	0.6709	0.5695	0.0671	0.064*
C14	0.7854 (2)	0.6052 (2)	-0.00029 (10)	0.0547 (6)
H14	0.8614	0.5568	0.0184	0.066*
C15	0.7917 (2)	0.6682 (2)	-0.05762 (9)	0.0480 (5)
C16	0.6745 (2)	0.74095 (19)	-0.08500 (9)	0.0431 (5)
C17	0.5605 (2)	0.7478 (2)	-0.05473 (9)	0.0463 (5)
H17	0.4844	0.7967	-0.0730	0.056*
C18	0.9212 (2)	0.6606 (3)	-0.08627 (11)	0.0611 (6)
H18A	0.9968	0.6316	-0.0552	0.092*
H18B	0.9421	0.7449	-0.1012	0.092*
H18C	0.9075	0.6004	-0.1207	0.092*
C19	0.6722 (2)	0.81014 (19)	-0.14646 (9)	0.0417 (4)
C20	0.67264 (19)	0.94456 (19)	-0.14980 (8)	0.0413 (4)
H20	0.6735	0.9929	-0.1133	0.050*
C21	0.6718 (2)	1.00913 (19)	-0.20683 (9)	0.0420 (4)
H21	0.6725	1.0995	-0.2082	0.050*
C22	0.6699 (2)	0.93737 (19)	-0.26148 (8)	0.0416 (4)
C23	0.6675 (2)	0.8030 (2)	-0.25930 (9)	0.0513 (5)

H23	0.6651	0.7547	-0.2959	0.062*
C24	0.6687 (3)	0.7411 (2)	-0.20230 (10)	0.0537 (6)
H24	0.6670	0.6507	-0.2012	0.064*
C25	0.7070 (3)	1.1241 (2)	-0.32305 (11)	0.0667 (7)
H25A	0.7034	1.1498	-0.3661	0.100*
H25B	0.6432	1.1760	-0.3042	0.100*
H25C	0.7992	1.1366	-0.3005	0.100*

*Atomic displacement parameters ( $\text{\AA}^2$ )*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0555 (4)	0.0667 (4)	0.0542 (3)	0.0144 (3)	-0.0015 (3)	0.0113 (3)
O1	0.0677 (11)	0.1073 (15)	0.0668 (11)	0.0306 (11)	0.0131 (9)	0.0386 (10)
O2	0.0766 (10)	0.0462 (8)	0.0363 (7)	-0.0113 (7)	0.0042 (7)	0.0045 (6)
N1	0.0419 (9)	0.0447 (9)	0.0435 (8)	0.0004 (7)	0.0031 (7)	0.0033 (7)
N2	0.0485 (10)	0.0557 (10)	0.0415 (9)	0.0047 (9)	0.0039 (7)	0.0085 (8)
C1	0.0364 (10)	0.0488 (11)	0.0505 (10)	0.0007 (9)	0.0091 (8)	-0.0025 (9)
C2	0.0443 (11)	0.0507 (12)	0.0505 (11)	-0.0017 (9)	0.0058 (9)	0.0015 (9)
C3	0.0552 (12)	0.0415 (11)	0.0589 (12)	-0.0073 (10)	0.0190 (10)	-0.0024 (9)
C4	0.0434 (12)	0.0724 (16)	0.0771 (16)	-0.0024 (12)	0.0246 (11)	0.0076 (13)
C5	0.0366 (11)	0.0707 (15)	0.0708 (14)	0.0006 (11)	0.0065 (10)	0.0082 (12)
C6	0.0381 (10)	0.0383 (10)	0.0509 (11)	-0.0020 (8)	0.0074 (8)	-0.0036 (8)
C7	0.0817 (18)	0.0700 (16)	0.0644 (15)	-0.0114 (14)	0.0290 (13)	0.0041 (12)
C8	0.0409 (10)	0.0388 (10)	0.0498 (10)	-0.0011 (8)	0.0037 (8)	-0.0044 (8)
C9	0.0474 (12)	0.0643 (14)	0.0600 (13)	0.0090 (11)	0.0036 (10)	0.0034 (11)
C10	0.0464 (11)	0.0398 (10)	0.0456 (10)	0.0017 (9)	0.0009 (8)	0.0007 (8)
C11	0.0588 (13)	0.0518 (12)	0.0460 (11)	0.0047 (11)	0.0047 (10)	0.0109 (9)
C12	0.0531 (12)	0.0446 (11)	0.0419 (10)	0.0018 (10)	0.0032 (9)	0.0059 (8)
C13	0.0625 (14)	0.0533 (12)	0.0434 (10)	0.0096 (11)	0.0031 (9)	0.0151 (9)
C14	0.0562 (13)	0.0546 (13)	0.0504 (12)	0.0138 (11)	0.0007 (10)	0.0119 (10)
C15	0.0532 (12)	0.0428 (10)	0.0453 (10)	0.0035 (10)	0.0001 (9)	0.0020 (8)
C16	0.0499 (11)	0.0383 (10)	0.0389 (9)	0.0001 (9)	0.0010 (8)	0.0024 (8)
C17	0.0507 (11)	0.0442 (11)	0.0413 (10)	0.0060 (9)	-0.0008 (8)	0.0065 (8)
C18	0.0548 (13)	0.0663 (15)	0.0605 (13)	0.0091 (12)	0.0043 (10)	0.0107 (11)
C19	0.0421 (10)	0.0423 (10)	0.0383 (9)	0.0001 (9)	-0.0003 (8)	0.0043 (8)
C20	0.0428 (10)	0.0428 (10)	0.0364 (9)	-0.0033 (9)	0.0010 (7)	-0.0020 (7)
C21	0.0451 (10)	0.0372 (9)	0.0415 (10)	-0.0046 (8)	0.0011 (8)	0.0009 (7)
C22	0.0423 (10)	0.0431 (10)	0.0369 (9)	-0.0045 (9)	-0.0006 (7)	0.0034 (7)
C23	0.0716 (14)	0.0419 (11)	0.0387 (10)	-0.0002 (10)	0.0044 (9)	-0.0040 (8)
C24	0.0768 (15)	0.0371 (10)	0.0453 (11)	0.0038 (11)	0.0048 (10)	0.0018 (8)
C25	0.0946 (19)	0.0514 (13)	0.0512 (12)	-0.0145 (13)	0.0039 (12)	0.0105 (10)

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

S1—C9	1.721 (3)	C12—C13	1.396 (3)
S1—C10	1.732 (2)	C12—C17	1.403 (3)
O1—C11	1.223 (3)	C13—C14	1.379 (3)
O2—C22	1.387 (2)	C13—H13	0.9300

O2—C25	1.424 (3)	C14—C15	1.407 (3)
N1—C10	1.307 (3)	C14—H14	0.9300
N1—C8	1.389 (3)	C15—C16	1.414 (3)
N2—C11	1.375 (3)	C15—C18	1.501 (3)
N2—C10	1.388 (3)	C16—C17	1.385 (3)
N2—H2	0.8600	C16—C19	1.502 (3)
C1—C2	1.389 (3)	C17—H17	0.9300
C1—C6	1.393 (3)	C18—H18A	0.9600
C1—H1	0.9300	C18—H18B	0.9600
C2—C3	1.392 (3)	C18—H18C	0.9600
C2—H2A	0.9300	C19—C20	1.385 (3)
C3—C4	1.384 (3)	C19—C24	1.395 (3)
C3—C7	1.508 (3)	C20—C21	1.398 (3)
C4—C5	1.394 (4)	C20—H20	0.9300
C4—H4	0.9300	C21—C22	1.389 (3)
C5—C6	1.389 (3)	C21—H21	0.9300
C5—H5	0.9300	C22—C23	1.384 (3)
C6—C8	1.484 (3)	C23—C24	1.384 (3)
C7—H7A	0.9600	C23—H23	0.9300
C7—H7B	0.9600	C24—H24	0.9300
C7—H7C	0.9600	C25—H25A	0.9600
C8—C9	1.362 (3)	C25—H25B	0.9600
C9—H9	0.9300	C25—H25C	0.9600
C11—C12	1.487 (3)		
C9—S1—C10	88.06 (11)	C14—C13—C12	120.19 (19)
C22—O2—C25	117.04 (16)	C14—C13—H13	119.9
C10—N1—C8	110.62 (17)	C12—C13—H13	119.9
C11—N2—C10	123.95 (18)	C13—C14—C15	122.5 (2)
C11—N2—H2	118.0	C13—C14—H14	118.7
C10—N2—H2	118.0	C15—C14—H14	118.7
C2—C1—C6	120.91 (19)	C14—C15—C16	117.4 (2)
C2—C1—H1	119.5	C14—C15—C18	120.07 (19)
C6—C1—H1	119.5	C16—C15—C18	122.44 (19)
C1—C2—C3	121.8 (2)	C17—C16—C15	119.38 (18)
C1—C2—H2A	119.1	C17—C16—C19	119.78 (17)
C3—C2—H2A	119.1	C15—C16—C19	120.83 (18)
C4—C3—C2	116.9 (2)	C16—C17—C12	122.73 (19)
C4—C3—C7	121.5 (2)	C16—C17—H17	118.6
C2—C3—C7	121.7 (2)	C12—C17—H17	118.6
C3—C4—C5	121.9 (2)	C15—C18—H18A	109.5
C3—C4—H4	119.1	C15—C18—H18B	109.5
C5—C4—H4	119.1	H18A—C18—H18B	109.5
C6—C5—C4	120.9 (2)	C15—C18—H18C	109.5
C6—C5—H5	119.6	H18A—C18—H18C	109.5
C4—C5—H5	119.6	H18B—C18—H18C	109.5
C5—C6—C1	117.6 (2)	C20—C19—C24	117.65 (17)
C5—C6—C8	121.95 (19)	C20—C19—C16	121.30 (17)

C1—C6—C8	120.38 (18)	C24—C19—C16	121.05 (18)
C3—C7—H7A	109.5	C19—C20—C21	121.39 (17)
C3—C7—H7B	109.5	C19—C20—H20	119.3
H7A—C7—H7B	109.5	C21—C20—H20	119.3
C3—C7—H7C	109.5	C22—C21—C20	119.49 (18)
H7A—C7—H7C	109.5	C22—C21—H21	120.3
H7B—C7—H7C	109.5	C20—C21—H21	120.3
C9—C8—N1	113.87 (19)	C23—C22—O2	115.35 (17)
C9—C8—C6	127.9 (2)	C23—C22—C21	120.02 (17)
N1—C8—C6	118.23 (17)	O2—C22—C21	124.63 (18)
C8—C9—S1	111.76 (18)	C24—C23—C22	119.52 (18)
C8—C9—H9	124.1	C24—C23—H23	120.2
S1—C9—H9	124.1	C22—C23—H23	120.2
N1—C10—N2	120.73 (18)	C23—C24—C19	121.90 (19)
N1—C10—S1	115.69 (16)	C23—C24—H24	119.0
N2—C10—S1	123.58 (15)	C19—C24—H24	119.0
O1—C11—N2	120.1 (2)	O2—C25—H25A	109.5
O1—C11—C12	122.10 (19)	O2—C25—H25B	109.5
N2—C11—C12	117.83 (18)	H25A—C25—H25B	109.5
C13—C12—C17	117.7 (2)	O2—C25—H25C	109.5
C13—C12—C11	124.79 (19)	H25A—C25—H25C	109.5
C17—C12—C11	117.51 (18)	H25B—C25—H25C	109.5
C6—C1—C2—C3	-0.7 (3)	N2—C11—C12—C17	-173.44 (19)
C1—C2—C3—C4	2.0 (3)	C17—C12—C13—C14	-0.4 (3)
C1—C2—C3—C7	-176.8 (2)	C11—C12—C13—C14	178.9 (2)
C2—C3—C4—C5	-2.0 (4)	C12—C13—C14—C15	0.1 (4)
C7—C3—C4—C5	176.7 (2)	C13—C14—C15—C16	0.0 (3)
C3—C4—C5—C6	0.8 (4)	C13—C14—C15—C18	177.8 (2)
C4—C5—C6—C1	0.5 (4)	C14—C15—C16—C17	0.3 (3)
C4—C5—C6—C8	-177.3 (2)	C18—C15—C16—C17	-177.5 (2)
C2—C1—C6—C5	-0.6 (3)	C14—C15—C16—C19	-179.44 (19)
C2—C1—C6—C8	177.27 (18)	C18—C15—C16—C19	2.8 (3)
C10—N1—C8—C9	-0.2 (3)	C15—C16—C17—C12	-0.6 (3)
C10—N1—C8—C6	-178.77 (17)	C19—C16—C17—C12	179.12 (18)
C5—C6—C8—C9	12.7 (3)	C13—C12—C17—C16	0.7 (3)
C1—C6—C8—C9	-165.1 (2)	C11—C12—C17—C16	-178.67 (19)
C5—C6—C8—N1	-168.9 (2)	C17—C16—C19—C20	68.2 (3)
C1—C6—C8—N1	13.3 (3)	C15—C16—C19—C20	-112.0 (2)
N1—C8—C9—S1	-0.1 (2)	C17—C16—C19—C24	-111.3 (2)
C6—C8—C9—S1	178.31 (16)	C15—C16—C19—C24	68.4 (3)
C10—S1—C9—C8	0.28 (18)	C24—C19—C20—C21	-1.0 (3)
C8—N1—C10—N2	179.78 (17)	C16—C19—C20—C21	179.41 (17)
C8—N1—C10—S1	0.4 (2)	C19—C20—C21—C22	0.3 (3)
C11—N2—C10—N1	-179.10 (19)	C25—O2—C22—C23	-164.7 (2)
C11—N2—C10—S1	0.2 (3)	C25—O2—C22—C21	15.3 (3)
C9—S1—C10—N1	-0.40 (18)	C20—C21—C22—C23	0.6 (3)
C9—S1—C10—N2	-179.77 (19)	C20—C21—C22—O2	-179.45 (18)



C10—N2—C11—O1	-0.1 (4)	O2—C22—C23—C24	179.3 (2)
C10—N2—C11—C12	179.34 (19)	C21—C22—C23—C24	-0.7 (3)
O1—C11—C12—C13	-173.2 (2)	C22—C23—C24—C19	0.0 (4)
N2—C11—C12—C13	7.3 (3)	C20—C19—C24—C23	0.9 (3)
O1—C11—C12—C17	6.0 (3)	C16—C19—C24—C23	-179.5 (2)

*Hydrogen-bond geometry (Å, °)*

Cg is the centroid of the C12–C17 ring.

<i>D</i> —H $\cdots$ <i>A</i>	<i>D</i> —H	H $\cdots$ <i>A</i>	<i>D</i> $\cdots$ <i>A</i>	<i>D</i> —H $\cdots$ <i>A</i>
N2—H2 $\cdots$ O2 <sup>i</sup>	0.86	2.33	3.175 (2)	166
C7—H7B $\cdots$ O1 <sup>i</sup>	0.96	2.59	3.452 (3)	149
C13—H13 $\cdots$ O2 <sup>i</sup>	0.93	2.50	3.413 (4)	166
C7—H7C $\cdots$ Cg <sup>ii</sup>	0.96	2.67	3.592 (5)	149

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