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N-[4-(4-Fluorophenyl)-1,3-thiazol-2-yl]-3-(4-methoxyphenyl)-4-methylbenzamide

K. Archana,[a] K. Lakshmithendral,[a] K. Saravanan,[a] S. Kabilan[a]* and S. Selvanayagam[b]‡

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

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‡ Additional correspondence author, e-mail: s_selvanayagam@rediffmail.com.

Keywords: crystal structure; thiazole derivative; C—H···N intramolecular hydrogen bonds; N—H···O intermolecular hydrogen bonds; weak C—H···O interactions.

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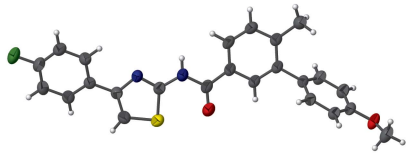
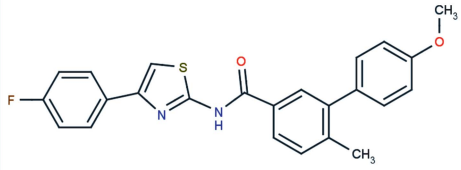
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{24}H_{19}FN_2O_2S$, the dihedral angle between the fluorophenyl and thiazole rings is 12.8 (1)°. In the crystal, molecules are linked *via* strong N—H···O hydrogen bonds, forming *C*(11) chains propagating along [001]. In addition, C—H···O interactions are observed in this structure, forming *C*(10) chains propagating along [001].

3D view



Chemical scheme



Structure description

In a continuation of our work on the crystal structure analysis of thiazole derivatives, we have undertaken a single-crystal X-ray diffraction study for the title compound, and the results are presented here.

The molecular structure of the title compound is illustrated in Fig. 1. The geometry of the present structure, except for atom F1, is comparable with that reported for a similar structure, namely 3-(4-methoxyphenyl)-4-methyl- *N*-[4-(4-methylphenyl)-1,3-thiazol-2-yl]benzamide (Archana *et al.*, 2017). The superposition of the title compound with that in the above-mentioned structure, using *Qmol* (Gans & Shalloway, 2001), gives an r.m.s. deviation of 0.710 Å; see Fig. 2. The methoxy atoms O2 and C24 deviate by −0.014 (2) and 0.355 (3) Å, respectively from the ring to which they are attached. This ring is oriented at a dihedral angle of 82.2 (1)° with respect to the fluorophenyl ring. The fluorophenyl ring makes a dihedral angle of 12.8 (1)° with thiazole ring. The molecular structure is influenced by intramolecular C—H···N and C—H···O hydrogen bonds (Table 1).

In the crystal, molecules are linked *via* strong N—H···O hydrogen bonds (Table 1), forming *C*(11) chains propagating along [001]. In addition, C—H···O interactions are observed in this structure, forming *C*(10) chains propagating along [001], see Fig. 3.

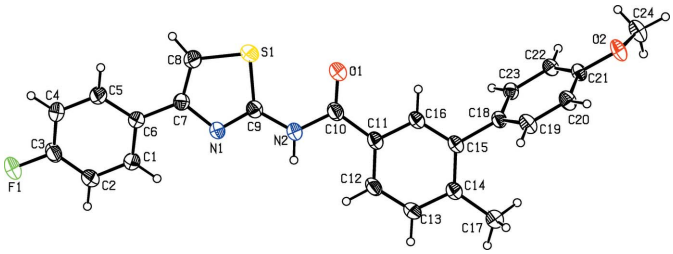


Figure 1
The molecular structure of the title compound, with atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

Synthesis and crystallization

N-(4-(4-Fluorophenyl) thiazol-2-yl)-3-iodo-4-methylbenzamide (0.23 mmol) was dissolved in 20 ml of deoxygenated toluene and water (8:2). Then, tetrakis (triphenylphosphine) palladium (0.014 mmol) and K_2CO_3 (0.68 mmol) were added in turn at 10 min 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 progress of the reaction was monitored by pre-coated TLC plates. After completion of the reaction, it was cooled to rt and concentrated in Rotavac. The obtained crude compound was purified by column chromatography using 20% ethyl acetate and petrol ether (60–80) as eluent. The pure compound was obtained as a light-brown solid, it was further recrystallized from dichloromethane (DCM) solution to yield the title compound.

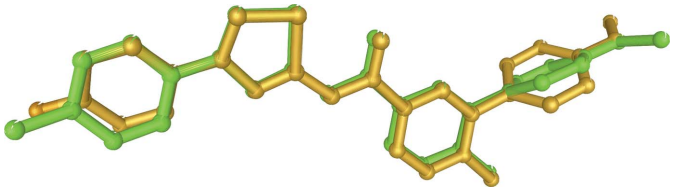


Figure 2
Superposition of the present structure except F1 (yellow) with the similar reported structure (green; Archana *et al.*, 2017).

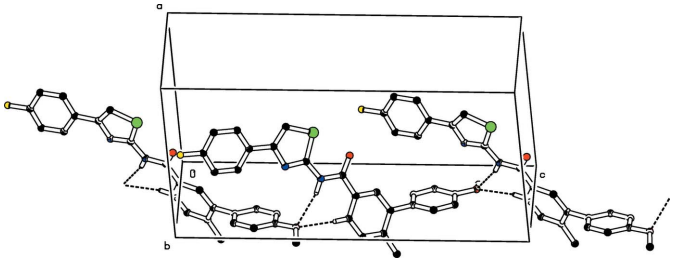


Figure 3
The crystal packing of the title compound viewed along *b* axis. The N—H···O and C—H···O intermolecular hydrogen bonds are shown as dashed lines (see Table 1). For clarity, H atoms not involved in these hydrogen bonds have been omitted.

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.86	2.33	3.177 (2)	167
C12—H12···O2^{i}	0.93	2.36	3.275 (2)	167
C1—H1···N1	0.93	2.48	2.827 (3)	102
C16—H16···O1	0.93	2.49	2.802 (3)	100

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{19}FN_2O_2S$
M_r	418.47
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	298
a, *b*, *c* (Å)	9.5104 (11), 10.4859 (13), 20.522 (3)
β (°)	94.904 (6)
V (Å^3)	2039.1 (5)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.19
Crystal size (mm)	0.24 × 0.21 × 0.19
Data collection	
Diffractometer	Bruker SMART APEX CCD area-detector
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	9198, 4609, 3515
R_{int}	0.049
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.649
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.055, 0.164, 1.04
No. of reflections	4609
No. of parameters	272
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.23, −0.29

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

Refinement

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

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full crystallographic data

IUCrData (2017). **2**, x171089 [https://doi.org/10.1107/S2414314617010896]

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N-[4-(4-Fluorophenyl)-1,3-thiazol-2-yl]-3-(4-methoxyphenyl)-4-methylbenzamide

Crystal data

$C_{24}H_{19}FN_2O_2S$
M_r = 418.47
Monoclinic, $P2_1/c$
a = 9.5104 (11) Å
b = 10.4859 (13) Å
c = 20.522 (3) Å
β = 94.904 (6)°
V = 2039.1 (5) Å^3
Z = 4
$F(000)$ = 872
D_x = 1.363 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 6448 reflections
θ = 3.2–27.4°
μ = 0.19 mm^{-1}
T = 298 K
Block, colourless
0.24 × 0.21 × 0.19 mm

Data collection

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
ω and φ scans
9198 measured reflections
4609 independent reflections
3515 reflections with $I > 2\sigma(I)$
R_{int} = 0.049
θ_{max} = 27.5°, θ_{min} = 3.0°
h = −11→12
k = −13→11
l = −26→11

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.055
$wR(F^2)$ = 0.164
S = 1.04
4609 reflections
272 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0907P)^2 + 0.3443P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.29 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
S1	0.36048 (6)	0.30153 (6)	0.39023 (3)	0.05611 (19)

O1	0.18520 (19)	0.2555 (2)	0.48536 (8)	0.0766 (6)
O2	−0.16903 (17)	−0.01682 (14)	0.82367 (6)	0.0525 (4)
N1	0.19087 (16)	0.41980 (15)	0.30669 (7)	0.0416 (4)
N2	0.08549 (18)	0.37141 (17)	0.40186 (8)	0.0465 (4)
H2A	0.0118	0.4130	0.3868	0.056*
F1	0.33315 (18)	0.56455 (18)	0.01917 (7)	0.0861 (5)
C1	0.2007 (2)	0.4880 (2)	0.17389 (10)	0.0492 (5)
H1	0.1152	0.4850	0.1927	0.059*
C2	0.2031 (2)	0.5264 (2)	0.10959 (11)	0.0561 (5)
H2	0.1202	0.5494	0.0851	0.067*
C3	0.3301 (2)	0.5299 (2)	0.08263 (10)	0.0557 (5)
C4	0.4533 (2)	0.4999 (2)	0.11726 (11)	0.0583 (6)
H4	0.5382	0.5049	0.0981	0.070*
C5	0.4504 (2)	0.4617 (2)	0.18184 (10)	0.0520 (5)
H5	0.5343	0.4408	0.2061	0.062*
C6	0.32380 (18)	0.45404 (18)	0.21081 (9)	0.0395 (4)
C7	0.31681 (19)	0.40683 (18)	0.27833 (9)	0.0410 (4)
C8	0.4196 (2)	0.3466 (2)	0.31653 (10)	0.0547 (5)
H8	0.5102	0.3316	0.3045	0.066*
C9	0.2002 (2)	0.36928 (18)	0.36480 (9)	0.0428 (4)
C10	0.0813 (2)	0.3116 (2)	0.46118 (10)	0.0496 (5)
C11	−0.0524 (2)	0.32029 (18)	0.49355 (9)	0.0436 (4)
C12	−0.1676 (2)	0.3939 (2)	0.47043 (10)	0.0518 (5)
H12	−0.1639	0.4416	0.4324	0.062*
C13	−0.2872 (2)	0.3962 (2)	0.50392 (10)	0.0524 (5)
H13	−0.3638	0.4449	0.4873	0.063*
C14	−0.2976 (2)	0.32849 (19)	0.56157 (9)	0.0444 (4)
C15	−0.1807 (2)	0.25463 (18)	0.58507 (8)	0.0404 (4)
C16	−0.0618 (2)	0.25063 (18)	0.55063 (9)	0.0430 (4)
H16	0.0140	0.1998	0.5661	0.052*
C17	−0.4322 (2)	0.3332 (2)	0.59434 (12)	0.0595 (6)
H17A	−0.4272	0.4008	0.6260	0.089*
H17B	−0.4459	0.2534	0.6159	0.089*
H17C	−0.5098	0.3483	0.5622	0.089*
C18	−0.18079 (19)	0.17911 (18)	0.64708 (8)	0.0398 (4)
C19	−0.1805 (2)	0.24186 (19)	0.70703 (9)	0.0496 (5)
H19	−0.1824	0.3305	0.7081	0.059*
C20	−0.1773 (2)	0.17391 (19)	0.76502 (9)	0.0482 (5)
H20	−0.1775	0.2168	0.8047	0.058*
C21	−0.17385 (19)	0.04177 (18)	0.76370 (8)	0.0396 (4)
C22	−0.17349 (19)	−0.02230 (18)	0.70483 (8)	0.0397 (4)
H22	−0.1709	−0.1109	0.7038	0.048*
C23	−0.17704 (18)	0.04781 (18)	0.64705 (8)	0.0384 (4)
H23	−0.1769	0.0048	0.6074	0.046*
C24	−0.2044 (3)	−0.1480 (2)	0.82531 (11)	0.0600 (6)
H24A	−0.1969	−0.1772	0.8698	0.090*
H24B	−0.2993	−0.1599	0.8064	0.090*
H24C	−0.1408	−0.1958	0.8008	0.090*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
S1	0.0566 (3)	0.0681 (4)	0.0430 (3)	0.0119 (3)	0.0002 (2)	0.0090 (2)
O1	0.0686 (10)	0.1041 (14)	0.0587 (10)	0.0258 (10)	0.0149 (8)	0.0362 (10)
O2	0.0802 (10)	0.0479 (8)	0.0281 (6)	−0.0105 (7)	−0.0029 (6)	0.0050 (5)
N1	0.0453 (8)	0.0451 (9)	0.0344 (7)	0.0006 (7)	0.0037 (6)	0.0028 (6)
N2	0.0504 (9)	0.0534 (10)	0.0361 (8)	0.0029 (7)	0.0056 (7)	0.0063 (7)
F1	0.0950 (11)	0.1105 (13)	0.0549 (8)	0.0169 (10)	0.0178 (8)	0.0380 (8)
C1	0.0434 (9)	0.0606 (13)	0.0440 (10)	0.0042 (9)	0.0064 (8)	0.0055 (9)
C2	0.0529 (11)	0.0652 (14)	0.0497 (11)	0.0070 (10)	0.0009 (9)	0.0141 (10)
C3	0.0696 (13)	0.0554 (13)	0.0428 (11)	0.0039 (11)	0.0093 (9)	0.0124 (9)
C4	0.0516 (11)	0.0688 (15)	0.0568 (13)	0.0012 (10)	0.0180 (10)	0.0143 (11)
C5	0.0421 (10)	0.0649 (13)	0.0492 (11)	0.0012 (9)	0.0049 (8)	0.0066 (10)
C6	0.0408 (9)	0.0375 (9)	0.0402 (9)	−0.0013 (7)	0.0034 (7)	−0.0023 (7)
C7	0.0423 (9)	0.0421 (10)	0.0385 (9)	−0.0013 (8)	0.0035 (7)	−0.0018 (7)
C8	0.0491 (11)	0.0695 (14)	0.0457 (11)	0.0081 (10)	0.0049 (9)	0.0028 (10)
C9	0.0499 (10)	0.0403 (10)	0.0381 (9)	−0.0004 (8)	0.0035 (8)	−0.0018 (7)
C10	0.0597 (12)	0.0510 (12)	0.0380 (10)	0.0026 (9)	0.0042 (8)	0.0067 (8)
C11	0.0533 (10)	0.0451 (11)	0.0321 (8)	−0.0003 (8)	0.0021 (7)	0.0029 (7)
C12	0.0641 (12)	0.0556 (12)	0.0352 (9)	0.0073 (10)	0.0015 (8)	0.0120 (8)
C13	0.0564 (11)	0.0571 (12)	0.0431 (10)	0.0106 (10)	0.0000 (9)	0.0122 (9)
C14	0.0515 (10)	0.0445 (10)	0.0369 (9)	−0.0001 (8)	0.0014 (8)	0.0029 (8)
C15	0.0511 (10)	0.0379 (9)	0.0314 (8)	−0.0026 (8)	−0.0008 (7)	0.0033 (7)
C16	0.0516 (10)	0.0439 (10)	0.0327 (8)	0.0005 (8)	−0.0008 (7)	0.0041 (7)
C17	0.0584 (12)	0.0648 (14)	0.0561 (12)	0.0081 (11)	0.0098 (10)	0.0142 (11)
C18	0.0435 (9)	0.0444 (10)	0.0314 (8)	−0.0010 (8)	0.0022 (7)	0.0035 (7)
C19	0.0737 (13)	0.0370 (10)	0.0371 (9)	−0.0016 (9)	−0.0005 (9)	0.0006 (7)
C20	0.0688 (13)	0.0436 (11)	0.0314 (8)	−0.0026 (9)	−0.0012 (8)	−0.0041 (7)
C21	0.0453 (9)	0.0435 (10)	0.0289 (8)	−0.0043 (8)	−0.0025 (7)	0.0027 (7)
C22	0.0474 (9)	0.0361 (9)	0.0349 (8)	−0.0032 (7)	−0.0005 (7)	0.0001 (7)
C23	0.0416 (9)	0.0441 (10)	0.0291 (8)	−0.0023 (7)	0.0006 (6)	−0.0025 (7)
C24	0.0842 (16)	0.0511 (12)	0.0440 (11)	−0.0103 (11)	0.0006 (10)	0.0115 (9)

Geometric parameters (Å, º)

S1—C9	1.722 (2)	C11—C12	1.390 (3)
S1—C8	1.724 (2)	C12—C13	1.379 (3)
O1—C10	1.219 (3)	C12—H12	0.9300
O2—C21	1.373 (2)	C13—C14	1.391 (3)
O2—C24	1.417 (3)	C13—H13	0.9300
N1—C9	1.301 (2)	C14—C15	1.407 (3)
N1—C7	1.382 (2)	C14—C17	1.496 (3)
N2—C10	1.373 (2)	C15—C16	1.384 (3)
N2—C9	1.382 (2)	C15—C18	1.499 (2)
N2—H2A	0.8600	C16—H16	0.9300
F1—C3	1.355 (2)	C17—H17A	0.9600
C1—C2	1.381 (3)	C17—H17B	0.9600

C1—C6	1.386 (3)	C17—H17C	0.9600
C1—H1	0.9300	C18—C23	1.377 (3)
C2—C3	1.372 (3)	C18—C19	1.395 (3)
C2—H2	0.9300	C19—C20	1.385 (3)
C3—C4	1.354 (3)	C19—H19	0.9300
C4—C5	1.387 (3)	C20—C21	1.386 (3)
C4—H4	0.9300	C20—H20	0.9300
C5—C6	1.390 (3)	C21—C22	1.383 (2)
C5—H5	0.9300	C22—C23	1.393 (2)
C6—C7	1.478 (2)	C22—H22	0.9300
C7—C8	1.355 (3)	C23—H23	0.9300
C8—H8	0.9300	C24—H24A	0.9600
C10—C11	1.487 (3)	C24—H24B	0.9600
C11—C16	1.390 (2)	C24—H24C	0.9600

C9—S1—C8	88.13 (10)	C12—C13—C14	122.48 (19)
C21—O2—C24	117.77 (15)	C12—C13—H13	118.8
C9—N1—C7	110.62 (16)	C14—C13—H13	118.8
C10—N2—C9	124.37 (17)	C13—C14—C15	117.46 (18)
C10—N2—H2A	117.8	C13—C14—C17	119.44 (18)
C9—N2—H2A	117.8	C15—C14—C17	123.07 (17)
C2—C1—C6	121.00 (18)	C16—C15—C14	119.88 (16)
C2—C1—H1	119.5	C16—C15—C18	118.52 (16)
C6—C1—H1	119.5	C14—C15—C18	121.60 (17)
C3—C2—C1	118.71 (19)	C15—C16—C11	121.93 (18)
C3—C2—H2	120.6	C15—C16—H16	119.0
C1—C2—H2	120.6	C11—C16—H16	119.0
C4—C3—F1	118.6 (2)	C14—C17—H17A	109.5
C4—C3—C2	122.28 (19)	C14—C17—H17B	109.5
F1—C3—C2	119.2 (2)	H17A—C17—H17B	109.5
C3—C4—C5	118.80 (19)	C14—C17—H17C	109.5
C3—C4—H4	120.6	H17A—C17—H17C	109.5
C5—C4—H4	120.6	H17B—C17—H17C	109.5
C4—C5—C6	120.91 (19)	C23—C18—C19	118.28 (16)
C4—C5—H5	119.5	C23—C18—C15	121.73 (16)
C6—C5—H5	119.5	C19—C18—C15	119.96 (17)
C1—C6—C5	118.28 (18)	C20—C19—C18	120.89 (19)
C1—C6—C7	119.67 (17)	C20—C19—H19	119.6
C5—C6—C7	122.01 (17)	C18—C19—H19	119.6
C8—C7—N1	114.21 (17)	C19—C20—C21	119.74 (17)
C8—C7—C6	127.60 (17)	C19—C20—H20	120.1
N1—C7—C6	118.14 (16)	C21—C20—H20	120.1
C7—C8—S1	111.24 (16)	O2—C21—C22	124.30 (17)
C7—C8—H8	124.4	O2—C21—C20	115.38 (16)
S1—C8—H8	124.4	C22—C21—C20	120.31 (17)
N1—C9—N2	120.18 (17)	C21—C22—C23	119.05 (17)
N1—C9—S1	115.79 (14)	C21—C22—H22	120.5
N2—C9—S1	124.04 (14)	C23—C22—H22	120.5

O1—C10—N2	119.9 (2)	C18—C23—C22	121.73 (16)
O1—C10—C11	122.83 (18)	C18—C23—H23	119.1
N2—C10—C11	117.31 (18)	C22—C23—H23	119.1
C16—C11—C12	118.27 (18)	O2—C24—H24A	109.5
C16—C11—C10	117.63 (17)	O2—C24—H24B	109.5
C12—C11—C10	124.10 (17)	H24A—C24—H24B	109.5
C13—C12—C11	119.96 (18)	O2—C24—H24C	109.5
C13—C12—H12	120.0	H24A—C24—H24C	109.5
C11—C12—H12	120.0	H24B—C24—H24C	109.5

C6—C1—C2—C3	0.2 (4)	N2—C10—C11—C12	−5.9 (3)
C1—C2—C3—C4	−1.5 (4)	C16—C11—C12—C13	−0.1 (3)
C1—C2—C3—F1	178.5 (2)	C10—C11—C12—C13	−179.9 (2)
F1—C3—C4—C5	−178.6 (2)	C11—C12—C13—C14	1.1 (3)
C2—C3—C4—C5	1.4 (4)	C12—C13—C14—C15	−0.7 (3)
C3—C4—C5—C6	0.0 (4)	C12—C13—C14—C17	−178.6 (2)
C2—C1—C6—C5	1.1 (3)	C13—C14—C15—C16	−0.6 (3)
C2—C1—C6—C7	−176.7 (2)	C17—C14—C15—C16	177.2 (2)
C4—C5—C6—C1	−1.2 (3)	C13—C14—C15—C18	179.44 (18)
C4—C5—C6—C7	176.6 (2)	C17—C14—C15—C18	−2.8 (3)
C9—N1—C7—C8	−0.4 (2)	C14—C15—C16—C11	1.5 (3)
C9—N1—C7—C6	177.43 (17)	C18—C15—C16—C11	−178.51 (17)
C1—C6—C7—C8	165.9 (2)	C12—C11—C16—C15	−1.1 (3)
C5—C6—C7—C8	−11.8 (3)	C10—C11—C16—C15	178.59 (18)
C1—C6—C7—N1	−11.6 (3)	C16—C15—C18—C23	−66.0 (2)
C5—C6—C7—N1	170.67 (18)	C14—C15—C18—C23	114.0 (2)
N1—C7—C8—S1	0.8 (2)	C16—C15—C18—C19	112.1 (2)
C6—C7—C8—S1	−176.79 (16)	C14—C15—C18—C19	−68.0 (3)
C9—S1—C8—C7	−0.71 (18)	C23—C18—C19—C20	−0.4 (3)
C7—N1—C9—N2	−179.81 (16)	C15—C18—C19—C20	−178.49 (19)
C7—N1—C9—S1	−0.2 (2)	C18—C19—C20—C21	0.2 (3)
C10—N2—C9—N1	174.34 (19)	C24—O2—C21—C22	−18.0 (3)
C10—N2—C9—S1	−5.2 (3)	C24—O2—C21—C20	162.9 (2)
C8—S1—C9—N1	0.53 (17)	C19—C20—C21—O2	179.19 (19)
C8—S1—C9—N2	−179.87 (18)	C19—C20—C21—C22	0.0 (3)
C9—N2—C10—O1	2.6 (3)	O2—C21—C22—C23	−179.26 (17)
C9—N2—C10—C11	−178.13 (18)	C20—C21—C22—C23	−0.2 (3)
O1—C10—C11—C16	−6.4 (3)	C19—C18—C23—C22	0.2 (3)
N2—C10—C11—C16	174.37 (18)	C15—C18—C23—C22	178.31 (16)
O1—C10—C11—C12	173.4 (2)	C21—C22—C23—C18	0.1 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2*A*···O2^{i}	0.86	2.33	3.177 (2)	167
C12—H12···O2^{i}	0.93	2.36	3.275 (2)	167

C1—H1···N1	0.93	2.48	2.827 (3)	102
C16—H16···O1	0.93	2.49	2.802 (3)	100

Symmetry code: (i) x, $-y+1/2$, $z-1/2$.