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# 3-(2-Methylamino-1,3-thiazol-4-yl)-2*H*-chromen-2-one

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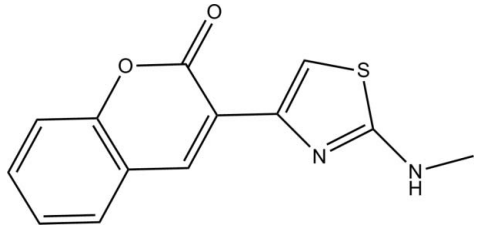
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.034; $wR$ factor = 0.095; data-to-parameter ratio = 19.7.

In the title compound, $C_{13}H_{10}N_2O_2S$, the essentially planar 2*H*-chromene ring system [maximum deviation = 0.0297 (13) Å] and the thiazole ring [maximum deviation = 0.0062 (11) Å] form a dihedral angle of 3.47 (5)°. In the crystal, N—H···N and C—H···O hydrogen bonds link the molecules into two-dimensional networks parallel to the *bc* plane. C—H···$\pi$ and $\pi$–$\pi$ [centroid–centroid separation = 3.6796 (8) Å] interactions further stabilize the crystal structure.

## Related literature

For the biological activities of coumarin derivatives, see: Soine (1964); Wattenberg *et al.* (1979); Jung *et al.* (1999); Rao *et al.* (1981). For a related structure, see: Arshad *et al.* (2010, 2011); Asad *et al.* (2011); Yusufzai, Osman, Sulaiman *et al.* (2012); Yusufzai, Osman, Abdul Rahim *et al.* (2012). For the stability of the temperature controller used for data collection, see: Cosier & Glazer (1986).




## Experimental

### Crystal data

$C_{13}H_{10}N_2O_2S$
$M_r$ = 258.29
Monoclinic, $P2_1/c$
$a$ = 14.5460 (3) Å
$b$ = 4.9289 (1) Å
$c$ = 18.3516 (3) Å
$\beta$ = 120.307 (1)°
$V$ = 1135.92 (4) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.28 mm$^{-1}$
$T$ = 100 K
0.47 × 0.40 × 0.20 mm

### Data collection

Bruker SMART APEXII CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.881, $T_{max}$ = 0.946
13265 measured reflections
3303 independent reflections
2851 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.034
$wR(F^2)$ = 0.095
$S$ = 1.05
3303 reflections
168 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.45 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.21 e Å$^{-3}$

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

*Cg*1 is the centroid of the S1/N1/C10–C12 ring.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H1N2···N1$^{i}$ | 0.87 (2) | 2.24 (2) | 3.0331 (15) | 152 (2) |
| C4—H4A···O2$^{ii}$ | 0.95 | 2.44 | 3.3247 (16) | 154 |
| C13—H13*C*···*Cg*1$^{iii}$ | 0.98 | 2.70 | 3.5026 (16) | 139 |

Symmetry codes: (i) $-x+2, y-\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{5}{2}, z+\frac{1}{2}$; (iii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2775).

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# supporting information

*Acta Cryst.* (2012). E**68**, o2416–o2417 [https://doi.org/10.1107/S1600536812030140]

## 3-(2-Methylamino-1,3-thiazol-4-yl)-2*H*-chromen-2-one

**Samina Khan Yusufzai, Hasnah Osman, Aisyah Saad Abdul Rahim, Suhana Arshad and Ibrahim Abdul Razak**

### S1. Comment

Compounds containing the coumarin moiety exhibit useful and diverse biological activity and, in recent years, there has been a growing interest in their synthesis (Soine, 1964; Wattenberg *et al.*, 1979). Some of these coumarin derivatives have been found to be useful in photochemotherapy, antitumour, anti-HIV therapy (Jung *et al.*, 1999), as antibacterial (Rao *et al.*, 1981) and as anticoagulant (Jung *et al.*, 1999). In continuation of our previous work (Yusufzai, Osman, Sulaiman *et al.*, 2012; Yusufzai, Osman, Abdul Rahim *et al.*, 2012) we have synthesized 3-(2-methylamino-1,3-thiazol-4-yl)-3,4-dihydro-2*H*-chromen-2-one, a new compound which corresponds to the molecular formula $C_{13}H_{10}N_2O_2S$. Its melting point was found to be 192–194 °C. The structure of the newly synthesized compound was confirmed by its spectral data. Synthesis of other derivatives of coumarinthiourea and their biological activities are under progress.

The molecular structure of the title compound is shown in Fig. 1. The 2*H*-chromene ring (O1/C1–C9) and the thiazole ring (S1/N1/C10–C12) are essentially planar with maximum deviations of 0.0297 (13) Å at atom C7 and 0.0062 (11) Å at atom N1, respectively. The dihedral angle between the 2*H*-chromene and thiazole rings is 3.47 (5)°. Bond lengths and angles are within normal ranges and are comparable to those found in related structures (Arshad *et al.*, 2010; Arshad *et al.*, 2011; Asad *et al.*, 2011).

In the crystal packing (Fig. 2), the intermolecular N2—H1N2···N1 and C4—H4A···O2 (Table 1) hydrogen bonds link the molecules into a two dimensional network parallel to *bc* plane. C13—H13C···*Cg*1 (Table 1) interactions and *π*–*π* interactions [$Cg1\cdots Cg2^{iii}$ = 3.6796 (8) Å; symmetry code: (iii) x, -1+y, z] further stabilize the crystal structure (*Cg*1 and *Cg*2 are the centroids of the S1/N1/C10–C12 and O1/C1/C6–C9 rings, respectively).

### S2. Experimental

To a solution of 3-(2-bromoacetyl)-2*H*-chromen-2-one (0.001 mol) in absolute ethanol (20 mL), *N*-methylthiourea (0.001 mol) was added with stirring. The reaction mixture was refluxed for 3–4 hours. The precipitate formed on slow evaporation of solvent was collected by filtration, washed with cold ethanol and dried under vacuum. Recrystallization by ethanol gave the title compound as orange crystals.

### S3. Refinement

The N-bound H atom was located in a difference Fourier map and refined freely [N–H = 0.87 (2) Å]. The remaining H atoms were positioned geometrically [C–H = 0.95 or 0.98 Å] and refined using a riding model with $U_{iso}$(H) = 1.2 or 1.5 $U_{eq}$(C). A rotating group model was applied to the methyl group.

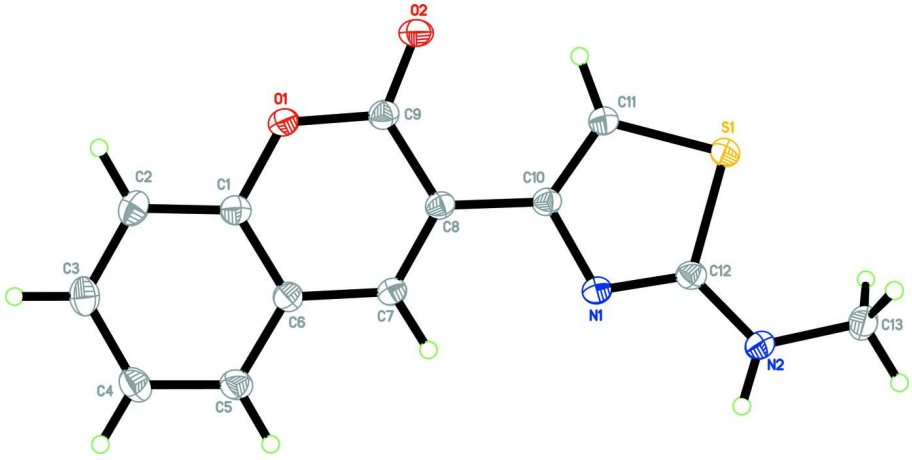


**Figure 1**

The molecular structure of the title compound, showing 50% probability displacement ellipsoids.

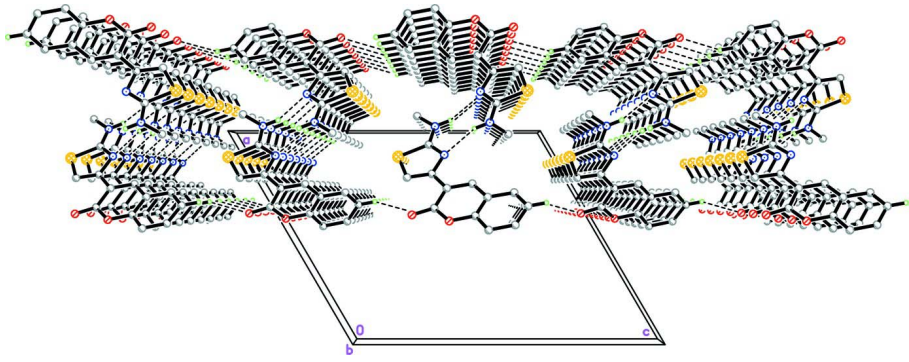


**Figure 2**

The crystal packing of the title compound, viewed down the *b* axis. The H atoms not involved in the intermolecular interactions (dashed lines) have been omitted for clarity.

### 3-(2-Methylamino-1,3-thiazol-4-yl)-2*H*-chromen-2-one

*Crystal data*

$C_{13}H_{10}N_2O_2S$
$M_r = 258.29$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 14.5460$ (3) Å
$b = 4.9289$ (1) Å
$c = 18.3516$ (3) Å
$\beta = 120.307$ (1)°
$V = 1135.92$ (4) Å$^3$
$Z = 4$
$F(000) = 536$
$D_x = 1.510$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 7338 reflections
$\theta = 2.6$–$32.5$°
$\mu = 0.28$ mm$^{-1}$
$T = 100$ K
Block, orange
0.47 × 0.40 × 0.20 mm

*Data collection*

Bruker SMART APEXII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.881$, $T_{max} = 0.946$
13265 measured reflections
3303 independent reflections

2851 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 30.0°$, $\theta_{min} = 1.6°$
$h = -20 \rightarrow 16$
$k = -6 \rightarrow 6$
$l = -25 \rightarrow 25$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.034$
$wR(F^2) = 0.095$
$S = 1.05$
3303 reflections
168 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
$w = 1/[\sigma^2(F_o^2) + (0.0472P)^2 + 0.5573P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.45$ e Å$^{-3}$
$\Delta\rho_{min} = -0.21$ e Å$^{-3}$

*Special details*

**Experimental**. The crystal was placed in the cold stream of an Oxford Cryosystems Cobra open-flow nitrogen cryostat (Cosier & Glazer, 1986) operating at 100.0 (1) K.

**Geometry**. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s 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 $F^2 > \sigma(F^2)$ 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 | 0.86394 (2) | 0.35198 (6) | 0.510226 (18) | 0.01927 (9) |
| O1 | 0.59607 (7) | 1.21689 (19) | 0.55233 (5) | 0.02025 (19) |
| O2 | 0.62018 (7) | 1.0170 (2) | 0.45629 (6) | 0.0226 (2) |
| N1 | 0.87142 (8) | 0.5208 (2) | 0.64688 (6) | 0.0167 (2) |
| N2 | 0.99500 (9) | 0.1750 (2) | 0.66837 (7) | 0.0209 (2) |
| C1 | 0.61748 (9) | 1.2526 (3) | 0.63378 (7) | 0.0174 (2) |
| C2 | 0.56079 (10) | 1.4526 (3) | 0.64782 (8) | 0.0215 (2) |
| H2A | 0.5090 | 1.5594 | 0.6026 | 0.026* |
| C3 | 0.58198 (10) | 1.4917 (3) | 0.72954 (9) | 0.0223 (3) |
| H3A | 0.5447 | 1.6288 | 0.7405 | 0.027* |
| C4 | 0.65730 (10) | 1.3329 (3) | 0.79635 (8) | 0.0220 (3) |
| H4A | 0.6707 | 1.3618 | 0.8520 | 0.026* |
| C5 | 0.71206 (10) | 1.1340 (3) | 0.78079 (8) | 0.0207 (2) |
| H5A | 0.7626 | 1.0245 | 0.8259 | 0.025* |
| C6 | 0.69360 (9) | 1.0923 (3) | 0.69871 (7) | 0.0170 (2) |
| C7 | 0.74892 (9) | 0.8943 (2) | 0.67830 (7) | 0.0172 (2) |
| H7A | 0.8000 | 0.7812 | 0.7219 | 0.021* |
| C8 | 0.73070 (9) | 0.8631 (2) | 0.59846 (7) | 0.0157 (2) |
| C9 | 0.64806 (9) | 1.0288 (3) | 0.53044 (7) | 0.0175 (2) |

| | | | | |
|---|---|---|---|---|
| C10 | 0.79048 (9) | 0.6641 (2) | 0.57920 (7) | 0.0159 (2) |
| C11 | 0.77572 (10) | 0.6015 (3) | 0.50172 (7) | 0.0188 (2) |
| H11A | 0.7242 | 0.6834 | 0.4503 | 0.023* |
| C12 | 0.91583 (9) | 0.3476 (2) | 0.61957 (7) | 0.0167 (2) |
| C13 | 1.04154 (10) | −0.0065 (3) | 0.63373 (8) | 0.0228 (3) |
| H13A | 1.0934 | −0.1250 | 0.6785 | 0.034* |
| H13B | 1.0773 | 0.0999 | 0.6101 | 0.034* |
| H13C | 0.9854 | −0.1171 | 0.5891 | 0.034* |
| H1N2 | 1.0201 (16) | 0.177 (4) | 0.7226 (13) | 0.040 (5)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.01899 (15) | 0.02255 (16) | 0.01429 (14) | 0.00258 (11) | 0.00693 (11) | −0.00217 (10) |
| O1 | 0.0194 (4) | 0.0245 (4) | 0.0164 (4) | 0.0064 (3) | 0.0087 (3) | 0.0043 (3) |
| O2 | 0.0213 (4) | 0.0301 (5) | 0.0154 (4) | 0.0051 (4) | 0.0085 (3) | 0.0045 (4) |
| N1 | 0.0147 (4) | 0.0188 (5) | 0.0143 (4) | 0.0008 (4) | 0.0056 (4) | 0.0000 (4) |
| N2 | 0.0185 (5) | 0.0242 (5) | 0.0156 (5) | 0.0060 (4) | 0.0054 (4) | −0.0004 (4) |
| C1 | 0.0162 (5) | 0.0193 (5) | 0.0171 (5) | −0.0007 (4) | 0.0087 (4) | 0.0005 (4) |
| C2 | 0.0183 (5) | 0.0208 (6) | 0.0254 (6) | 0.0035 (5) | 0.0110 (5) | 0.0022 (5) |
| C3 | 0.0199 (6) | 0.0215 (6) | 0.0296 (6) | −0.0006 (5) | 0.0155 (5) | −0.0035 (5) |
| C4 | 0.0196 (6) | 0.0268 (6) | 0.0212 (6) | −0.0020 (5) | 0.0114 (5) | −0.0054 (5) |
| C5 | 0.0168 (5) | 0.0266 (6) | 0.0172 (5) | 0.0008 (5) | 0.0075 (4) | −0.0012 (5) |
| C6 | 0.0136 (5) | 0.0193 (5) | 0.0171 (5) | −0.0009 (4) | 0.0070 (4) | −0.0010 (4) |
| C7 | 0.0148 (5) | 0.0197 (5) | 0.0149 (5) | 0.0019 (4) | 0.0058 (4) | 0.0007 (4) |
| C8 | 0.0137 (5) | 0.0168 (5) | 0.0154 (5) | −0.0001 (4) | 0.0064 (4) | 0.0011 (4) |
| C9 | 0.0151 (5) | 0.0196 (5) | 0.0177 (5) | 0.0008 (4) | 0.0082 (4) | 0.0017 (4) |
| C10 | 0.0138 (5) | 0.0173 (5) | 0.0149 (5) | −0.0002 (4) | 0.0061 (4) | 0.0001 (4) |
| C11 | 0.0181 (5) | 0.0208 (6) | 0.0154 (5) | 0.0029 (4) | 0.0068 (4) | 0.0000 (4) |
| C12 | 0.0145 (5) | 0.0183 (5) | 0.0151 (5) | −0.0017 (4) | 0.0058 (4) | −0.0014 (4) |
| C13 | 0.0191 (5) | 0.0237 (6) | 0.0235 (6) | 0.0037 (5) | 0.0092 (5) | −0.0028 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C11 | 1.7265 (13) | C3—H3A | 0.9500 |
| S1—C12 | 1.7517 (12) | C4—C5 | 1.3807 (17) |
| O1—C1 | 1.3757 (14) | C4—H4A | 0.9500 |
| O1—C9 | 1.3781 (15) | C5—C6 | 1.4054 (16) |
| O2—C9 | 1.2094 (15) | C5—H5A | 0.9500 |
| N1—C12 | 1.3129 (15) | C6—C7 | 1.4296 (16) |
| N1—C10 | 1.3971 (15) | C7—C8 | 1.3598 (16) |
| N2—C12 | 1.3457 (16) | C7—H7A | 0.9500 |
| N2—C13 | 1.4482 (16) | C8—C10 | 1.4674 (16) |
| N2—H1N2 | 0.87 (2) | C8—C9 | 1.4683 (16) |
| C1—C2 | 1.3903 (17) | C10—C11 | 1.3621 (16) |
| C1—C6 | 1.3923 (16) | C11—H11A | 0.9500 |
| C2—C3 | 1.3838 (18) | C13—H13A | 0.9800 |
| C2—H2A | 0.9500 | C13—H13B | 0.9800 |

| | | | |
|---|---|---|---|
| C3—C4 | 1.4001 (19) | C13—H13C | 0.9800 |
| | | | |
| C11—S1—C12 | 89.04 (6) | C8—C7—C6 | 122.02 (11) |
| C1—O1—C9 | 123.10 (9) | C8—C7—H7A | 119.0 |
| C12—N1—C10 | 110.22 (10) | C6—C7—H7A | 119.0 |
| C12—N2—C13 | 122.07 (11) | C7—C8—C10 | 121.21 (10) |
| C12—N2—H1N2 | 118.6 (13) | C7—C8—C9 | 118.93 (11) |
| C13—N2—H1N2 | 119.3 (13) | C10—C8—C9 | 119.84 (10) |
| O1—C1—C2 | 117.51 (11) | O2—C9—O1 | 116.01 (11) |
| O1—C1—C6 | 120.24 (11) | O2—C9—C8 | 126.56 (11) |
| C2—C1—C6 | 122.25 (11) | O1—C9—C8 | 117.43 (10) |
| C3—C2—C1 | 118.10 (12) | C11—C10—N1 | 115.57 (11) |
| C3—C2—H2A | 121.0 | C11—C10—C8 | 127.05 (11) |
| C1—C2—H2A | 121.0 | N1—C10—C8 | 117.38 (10) |
| C2—C3—C4 | 121.28 (12) | C10—C11—S1 | 110.40 (9) |
| C2—C3—H3A | 119.4 | C10—C11—H11A | 124.8 |
| C4—C3—H3A | 119.4 | S1—C11—H11A | 124.8 |
| C5—C4—C3 | 119.60 (12) | N1—C12—N2 | 125.28 (11) |
| C5—C4—H4A | 120.2 | N1—C12—S1 | 114.75 (9) |
| C3—C4—H4A | 120.2 | N2—C12—S1 | 119.97 (9) |
| C4—C5—C6 | 120.49 (12) | N2—C13—H13A | 109.5 |
| C4—C5—H5A | 119.8 | N2—C13—H13B | 109.5 |
| C6—C5—H5A | 119.8 | H13A—C13—H13B | 109.5 |
| C1—C6—C5 | 118.27 (11) | N2—C13—H13C | 109.5 |
| C1—C6—C7 | 118.21 (11) | H13A—C13—H13C | 109.5 |
| C5—C6—C7 | 123.52 (11) | H13B—C13—H13C | 109.5 |
| | | | |
| C9—O1—C1—C2 | 178.87 (11) | C7—C8—C9—O2 | −177.09 (12) |
| C9—O1—C1—C6 | −0.99 (17) | C10—C8—C9—O2 | 1.73 (19) |
| O1—C1—C2—C3 | −179.64 (11) | C7—C8—C9—O1 | 2.65 (16) |
| C6—C1—C2—C3 | 0.21 (19) | C10—C8—C9—O1 | −178.53 (10) |
| C1—C2—C3—C4 | −0.76 (19) | C12—N1—C10—C11 | −1.08 (15) |
| C2—C3—C4—C5 | 0.3 (2) | C12—N1—C10—C8 | 178.73 (10) |
| C3—C4—C5—C6 | 0.75 (19) | C7—C8—C10—C11 | 175.76 (12) |
| O1—C1—C6—C5 | −179.36 (11) | C9—C8—C10—C11 | −3.03 (19) |
| C2—C1—C6—C5 | 0.79 (18) | C7—C8—C10—N1 | −4.03 (17) |
| O1—C1—C6—C7 | 0.75 (17) | C9—C8—C10—N1 | 177.18 (10) |
| C2—C1—C6—C7 | −179.10 (11) | N1—C10—C11—S1 | 0.53 (14) |
| C4—C5—C6—C1 | −1.27 (18) | C8—C10—C11—S1 | −179.26 (10) |
| C4—C5—C6—C7 | 178.62 (12) | C12—S1—C11—C10 | 0.09 (10) |
| C1—C6—C7—C8 | 1.30 (18) | C10—N1—C12—N2 | −178.77 (12) |
| C5—C6—C7—C8 | −178.59 (12) | C10—N1—C12—S1 | 1.14 (13) |
| C6—C7—C8—C10 | 178.23 (11) | C13—N2—C12—N1 | −178.67 (12) |
| C6—C7—C8—C9 | −2.98 (18) | C13—N2—C12—S1 | 1.43 (17) |
| C1—O1—C9—O2 | 179.07 (11) | C11—S1—C12—N1 | −0.74 (10) |
| C1—O1—C9—C8 | −0.70 (16) | C11—S1—C12—N2 | 179.17 (11) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of the S1/N1/C10–C12 ring

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H1*N*2···N1$^{i}$ | 0.87 (2) | 2.24 (2) | 3.0331 (15) | 152 (2) |
| C4—H4*A*···O2$^{ii}$ | 0.95 | 2.44 | 3.3247 (16) | 154 |
| C13—H13*C*···*Cg*1$^{iii}$ | 0.98 | 2.70 | 3.5026 (16) | 139 |

Symmetry codes: (i) −*x*+2, *y*−1/2, −*z*+3/2; (ii) *x*, −*y*+5/2, *z*+1/2; (iii) *x*, *y*−1, *z*.