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# 3-{2-[2-(Diphenylmethylene)hydrazinyl]-thiazol-4-yl}-2*H*-chromen-2-one

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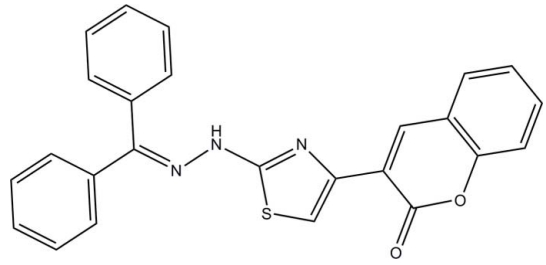
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.045; $wR$ factor = 0.125; data-to-parameter ratio = 14.7.

In the title compound, $C_{25}H_{17}N_3O_2S$, the coumarin ring system is essentially planar with a maximum deviation of 0.019 (2) Å. A weak intramolecular C—H···O hydrogen bond stabilizes the molecular structure, so that the coumarin plane is approximately coplanar with the thiazole ring, making a dihedral angle of 2.5 (10)°. The two phenyl rings are nearly perpendicular to each other, with a dihedral angle of 81.44 (12)°. In the crystal structure, the molecules are linked into an infinite chain along the $b$ axis by intermolecular C—H···O hydrogen bonds. Weak C—H···$\pi$ interactions are observed between the chains.

## Related literature

For applications of coumarin derivatives, see: Tassies *et al.* (2002); Laffitte *et al.* (2002); Weber *et al.* (1998); Finn *et al.* (2004); Kimura *et al.* (1985). For applications of aminothiazoles derivatives, see: Hiremath *et al.* (1992); Karah *et al.* (1998); Jayashree *et al.* (2005). For related structures, see: Arshad, Osman, Chan *et al.* (2010*a*,*b*); Arshad, Osman, Lam *et al.* (2010). For the stability of the temperature controller used for the data collection, see: Cosier & Glazer (1986). The syntheses of benzophenone thiosemicarbazone and 3-(ω-bromoacetyl)coumarin are described by Lobana *et al.* (2006) and Siddiqui *et al.* (2009), respectively.



## Experimental

### Crystal data

$C_{25}H_{17}N_3O_2S$
$M_r$ = 423.48
Monoclinic, $P2_1/c$
$a$ = 13.8705 (18) Å
$b$ = 12.9101 (17) Å
$c$ = 11.8534 (16) Å
$\beta$ = 107.563 (2)°
$V$ = 2023.6 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.19 mm$^{-1}$
$T$ = 100 K
0.28 × 0.13 × 0.04 mm

### Data collection

Bruker APEXII DUO CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.949, $T_{max}$ = 0.993
17920 measured reflections
4181 independent reflections
2909 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.067

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
$S$ = 1.04
4181 reflections
284 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

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

*Cg*1 and *Cg*2 are the centroids of the C14–C19 and C2–C7 benzene rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C6—H6*A*···O1$^{i}$ | 0.93 | 2.46 | 3.377 (3) | 168 |
| C11—H11*A*···O2 | 0.93 | 2.30 | 2.857 (3) | 118 |
| C21—H21*A*···*Cg*1$^{ii}$ | 0.93 | 2.49 | 3.387 (3) | 162 |
| C24—H24*A*···*Cg*2$^{iii}$ | 0.93 | 2.78 | 3.536 (3) | 139 |

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

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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‡ Thomson Reuters ResearcherID: A-5523-2009.
§ Thomson Reuters ResearcherID: A-3561-2009.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2564).

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# supporting information

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## 3-{2-[2-(Diphenylmethylene)hydrazinyl]thiazol-4-yl}-2*H*-chromen-2-one

**Afsheen Arshad, Hasnah Osman, Kit Lam Chan, Chin Sing Yeap and Hoong-Kun Fun**

### S1. Comment

Coumarin derivatives having pronounced biological activities are used as anticoagulants (Tassies *et al.*, 2002), antibacterial (Laffitte *et al.*, 2002), cytotoxic (Weber *et al.*, 1998), free radical scavengers (Finn *et al.*, 2004) and enzyme inhibiting (Kimura *et al.*, 1985) agents. Moreover, aminothiazoles derivatives have been reported to exhibit significant antifungal (Hiremath *et al.*, 1992), anti-tuberculosis (Karah *et al.*, 1998) and anti-inflammatory (Jayashree *et al.*, 2005) activities. The title compound is a new coumarinyl thiazolyl hydrazone derivative. We present here its crystal structure.

The geometry parameters of the title compound (Fig. 1) are comparable to those related structures (Arshad, Osman, Chan *et al.*, 2010*a*,*b*; Arshad, Osman, Lam *et al.*, 2010). The coumarin group is essentially planar (O1/C1–C9) with a maximum derivation of 0.019 Å at atom C7. The mean plane is approximately coplanar with the thiazole ring (C10–C11–S1–C12–N1) with a dihedral angle being 2.5 (10)°. The other two benzene rings are nearly perpendicular to each other with a dihedral angle being 81.44 (12)°.

In the crystal structure, the molecules are linked into infinite chains along *b* axis by the intermolecular C6—H6A···O1 hydrogen bonds and stabilized by the weak C—H···$\pi$ interactions (Fig. 2, Table 1). A weak intramolecular C11—H11A···O2 hydrogen bond stabilizes the molecular structure.

### S2. Experimental

Benzophenone thiosemicarbazone (Lobana *et al.*, 2006) and 3-($\omega$-bromoacetyl)coumarin (Siddiqui *et al.*, 2009) were synthesized as reported in the literature. A solution of 3-($\omega$-bromoacetyl)coumarin (2.5 mmol) and benzophenone thiosemicarbazone (2.5 mmol) in chloroform-ethanol (2:1) was refluxed for 1 h. Precipitates formed were filtered and boiled with water containing sodium acetate. The title compound was purified by recrystallization with ethanol-chloroform (1:3) as dark brown feather-like crystals.

### S3. Refinement

H1N2 hydrogen atom was located in a difference Fourier map and was refined freely. The rest of H atoms were positioned geometrically (C–H = 0.93 Å) and refined using a riding model, with $U_{iso}$(H) = 1.2$U_{eq}$(C).

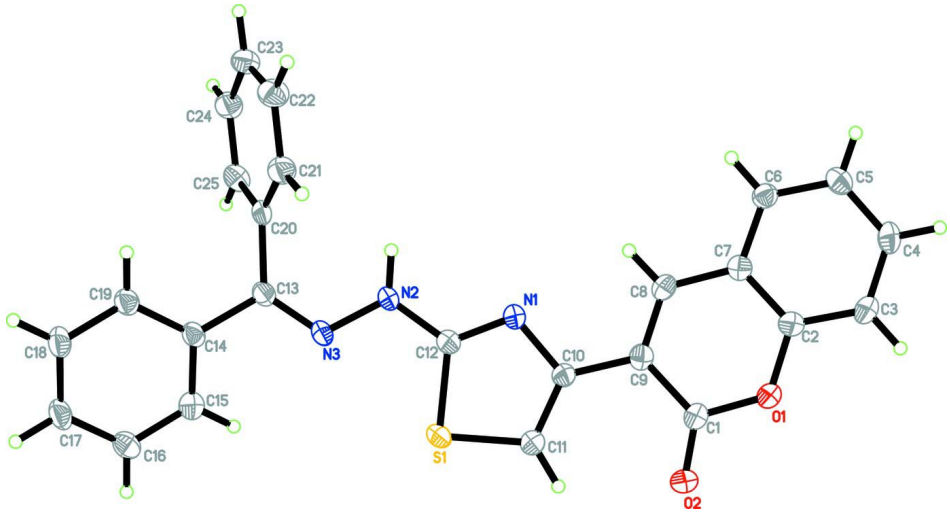


**Figure 1**

The molecular structure of the title compound with atom labels and 50% probability ellipsoids for non-H atoms.

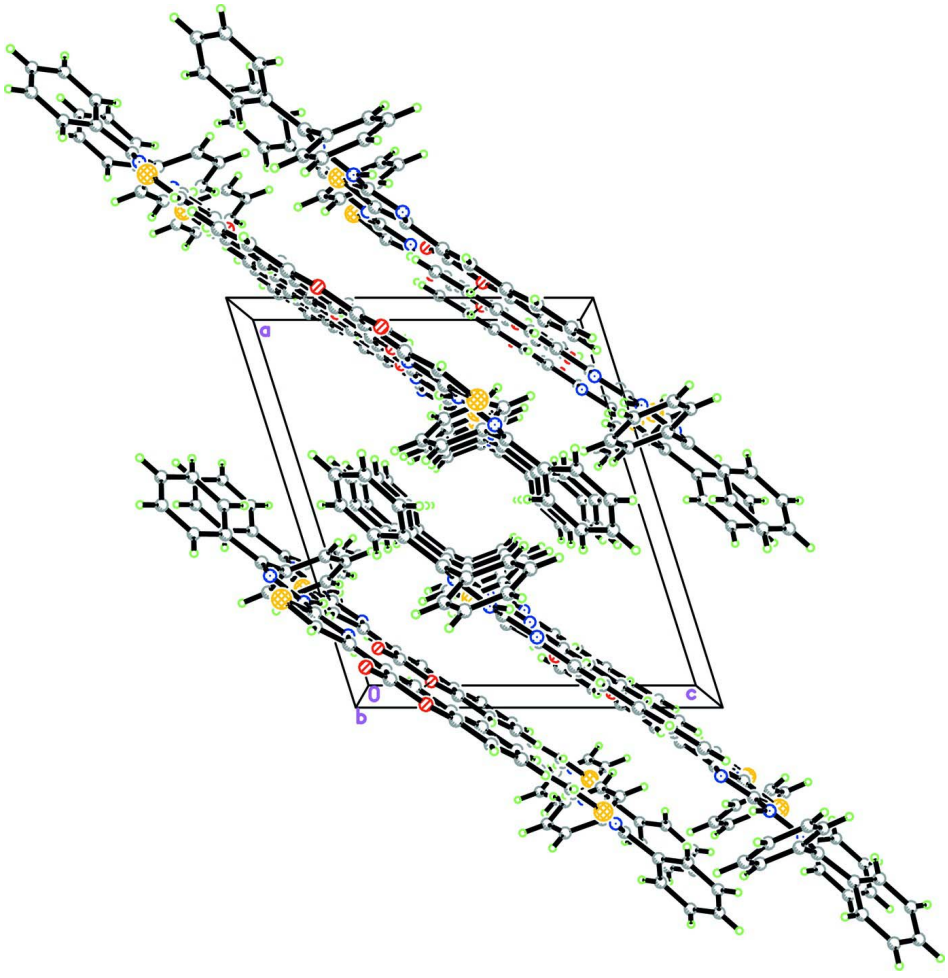


**Figure 2**

The crystal packing of title compound, viewed down the *b* axis, showing the molecules are linked into chains along the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines.

### 3-{2-[2-(Diphenylmethylene)hydrazinyl]thiazol-4-yl}-2*H*-chromen-2-one

*Crystal data*

$C_{25}H_{17}N_3O_2S$
$M_r = 423.48$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.8705\ (18)$ Å
$b = 12.9101\ (17)$ Å
$c = 11.8534\ (16)$ Å
$\beta = 107.563\ (2)°$
$V = 2023.6\ (5)$ Å$^3$
$Z = 4$
$F(000) = 880$
$D_x = 1.390$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2695 reflections
$\theta = 2.2–25.7°$
$\mu = 0.19$ mm$^{-1}$
$T = 100$ K
Plate, brown
0.28 × 0.13 × 0.04 mm

*Data collection*

Bruker APEXII DUO CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans

Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.949, $T_{max}$ = 0.993
17920 measured reflections
4181 independent reflections
2909 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.067
$\theta_{max}$ = 26.5°, $\theta_{min}$ = 2.2°
$h$ = −17→17
$k$ = −16→16
$l$ = −14→14

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.045
$wR(F^2)$ = 0.125
$S$ = 1.04
4181 reflections
284 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
$w = 1/[\sigma^2(F_o^2) + (0.0488P)^2 + 1.1918P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.24 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 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 | 0.27268 (5) | 0.29137 (5) | 0.91250 (6) | 0.02688 (18) |
| O1 | 0.03690 (14) | 0.49303 (13) | 1.21227 (16) | 0.0322 (5) |
| O2 | 0.12420 (15) | 0.53063 (13) | 1.09019 (17) | 0.0375 (5) |
| N1 | 0.18366 (15) | 0.20621 (15) | 1.05262 (17) | 0.0216 (4) |
| N2 | 0.25985 (16) | 0.08768 (16) | 0.95524 (19) | 0.0257 (5) |
| N3 | 0.32315 (15) | 0.07961 (15) | 0.88597 (17) | 0.0230 (5) |
| C1 | 0.09314 (19) | 0.46244 (19) | 1.1393 (2) | 0.0267 (6) |
| C2 | −0.00360 (19) | 0.42446 (19) | 1.2744 (2) | 0.0265 (6) |
| C3 | −0.0574 (2) | 0.4642 (2) | 1.3458 (3) | 0.0377 (7) |
| H3A | −0.0672 | 0.5352 | 1.3499 | 0.045* |
| C4 | −0.0961 (2) | 0.3960 (2) | 1.4110 (3) | 0.0355 (7) |
| H4A | −0.1313 | 0.4218 | 1.4604 | 0.043* |
| C5 | −0.08363 (19) | 0.2904 (2) | 1.4042 (2) | 0.0274 (6) |
| H5A | −0.1104 | 0.2456 | 1.4485 | 0.033* |
| C6 | −0.03123 (17) | 0.25172 (19) | 1.3315 (2) | 0.0225 (5) |
| H6A | −0.0231 | 0.1805 | 1.3266 | 0.027* |

| | | | | |
|---|---|---|---|---|
| C7 | 0.00990 (17) | 0.31838 (18) | 1.2649 (2) | 0.0209 (5) |
| C8 | 0.06701 (18) | 0.28439 (18) | 1.1895 (2) | 0.0213 (5) |
| H8A | 0.0760 | 0.2137 | 1.1817 | 0.026* |
| C9 | 0.10832 (17) | 0.35054 (18) | 1.1294 (2) | 0.0212 (5) |
| C10 | 0.16787 (18) | 0.31334 (18) | 1.0546 (2) | 0.0209 (5) |
| C11 | 0.20939 (19) | 0.37041 (19) | 0.9838 (2) | 0.0268 (6) |
| H11A | 0.2042 | 0.4420 | 0.9753 | 0.032* |
| C12 | 0.23598 (18) | 0.18608 (18) | 0.9809 (2) | 0.0225 (5) |
| C13 | 0.35407 (18) | −0.01140 (18) | 0.8675 (2) | 0.0210 (5) |
| C14 | 0.42271 (18) | −0.01483 (18) | 0.7927 (2) | 0.0213 (5) |
| C15 | 0.42459 (18) | 0.06486 (19) | 0.7143 (2) | 0.0232 (5) |
| H15A | 0.3784 | 0.1189 | 0.7037 | 0.028* |
| C16 | 0.49430 (19) | 0.0646 (2) | 0.6520 (2) | 0.0261 (6) |
| H16A | 0.4949 | 0.1184 | 0.6000 | 0.031* |
| C17 | 0.5631 (2) | −0.0155 (2) | 0.6670 (2) | 0.0288 (6) |
| H17A | 0.6097 | −0.0156 | 0.6247 | 0.035* |
| C18 | 0.56302 (19) | −0.0957 (2) | 0.7446 (2) | 0.0284 (6) |
| H18A | 0.6098 | −0.1492 | 0.7549 | 0.034* |
| C19 | 0.49287 (18) | −0.09584 (19) | 0.8069 (2) | 0.0237 (5) |
| H19A | 0.4923 | −0.1500 | 0.8585 | 0.028* |
| C20 | 0.33051 (17) | −0.11039 (18) | 0.9191 (2) | 0.0210 (5) |
| C21 | 0.36721 (19) | −0.12891 (19) | 1.0402 (2) | 0.0268 (6) |
| H21A | 0.4018 | −0.0770 | 1.0907 | 0.032* |
| C22 | 0.3526 (2) | −0.2240 (2) | 1.0859 (2) | 0.0288 (6) |
| H22A | 0.3778 | −0.2360 | 1.1669 | 0.035* |
| C23 | 0.30028 (19) | −0.3019 (2) | 1.0112 (2) | 0.0273 (6) |
| H23A | 0.2916 | −0.3664 | 1.0417 | 0.033* |
| C24 | 0.26132 (19) | −0.28293 (19) | 0.8913 (2) | 0.0282 (6) |
| H24A | 0.2250 | −0.3342 | 0.8411 | 0.034* |
| C25 | 0.27632 (18) | −0.18767 (19) | 0.8457 (2) | 0.0238 (5) |
| H25A | 0.2498 | −0.1753 | 0.7649 | 0.029* |
| H1N2 | 0.2549 (19) | 0.034 (2) | 1.003 (2) | 0.027 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0327 (4) | 0.0239 (3) | 0.0311 (4) | −0.0054 (3) | 0.0203 (3) | −0.0020 (3) |
| O1 | 0.0445 (11) | 0.0185 (9) | 0.0433 (11) | 0.0005 (8) | 0.0277 (10) | −0.0013 (8) |
| O2 | 0.0531 (13) | 0.0196 (9) | 0.0524 (12) | −0.0013 (9) | 0.0350 (11) | 0.0020 (9) |
| N1 | 0.0227 (10) | 0.0206 (10) | 0.0244 (11) | 0.0010 (9) | 0.0116 (9) | −0.0006 (9) |
| N2 | 0.0305 (12) | 0.0211 (11) | 0.0344 (12) | 0.0012 (9) | 0.0230 (11) | 0.0009 (10) |
| N3 | 0.0245 (11) | 0.0237 (11) | 0.0260 (11) | −0.0008 (9) | 0.0153 (10) | −0.0015 (9) |
| C1 | 0.0319 (14) | 0.0208 (13) | 0.0312 (14) | 0.0010 (11) | 0.0153 (13) | −0.0020 (11) |
| C2 | 0.0302 (14) | 0.0219 (13) | 0.0313 (14) | −0.0006 (11) | 0.0153 (12) | 0.0014 (11) |
| C3 | 0.0533 (19) | 0.0200 (13) | 0.0517 (18) | 0.0034 (13) | 0.0336 (16) | −0.0029 (13) |
| C4 | 0.0405 (16) | 0.0312 (15) | 0.0456 (17) | 0.0047 (12) | 0.0292 (15) | −0.0048 (13) |
| C5 | 0.0262 (13) | 0.0299 (14) | 0.0304 (14) | −0.0022 (11) | 0.0150 (12) | 0.0003 (11) |
| C6 | 0.0223 (12) | 0.0202 (12) | 0.0254 (13) | −0.0009 (10) | 0.0077 (11) | −0.0005 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C7 | 0.0182 (12) | 0.0224 (13) | 0.0211 (12) | −0.0005 (10) | 0.0046 (10) | −0.0008 (10) |
| C8 | 0.0208 (12) | 0.0188 (12) | 0.0227 (12) | 0.0003 (10) | 0.0044 (11) | −0.0027 (10) |
| C9 | 0.0184 (12) | 0.0222 (13) | 0.0220 (12) | −0.0015 (10) | 0.0048 (11) | −0.0036 (10) |
| C10 | 0.0217 (12) | 0.0184 (12) | 0.0241 (12) | −0.0017 (10) | 0.0091 (11) | −0.0020 (10) |
| C11 | 0.0329 (14) | 0.0202 (13) | 0.0321 (14) | −0.0029 (11) | 0.0172 (13) | −0.0030 (11) |
| C12 | 0.0224 (13) | 0.0215 (13) | 0.0262 (13) | −0.0012 (10) | 0.0113 (11) | −0.0002 (10) |
| C13 | 0.0209 (12) | 0.0231 (13) | 0.0210 (12) | −0.0017 (10) | 0.0094 (11) | −0.0010 (10) |
| C14 | 0.0237 (13) | 0.0222 (13) | 0.0205 (12) | −0.0039 (10) | 0.0106 (11) | −0.0051 (10) |
| C15 | 0.0230 (13) | 0.0269 (13) | 0.0182 (12) | 0.0006 (11) | 0.0040 (11) | −0.0019 (10) |
| C16 | 0.0301 (14) | 0.0316 (14) | 0.0182 (13) | −0.0013 (11) | 0.0096 (12) | 0.0012 (11) |
| C17 | 0.0310 (14) | 0.0332 (15) | 0.0287 (14) | −0.0007 (12) | 0.0189 (13) | −0.0057 (12) |
| C18 | 0.0296 (14) | 0.0305 (14) | 0.0298 (14) | 0.0035 (11) | 0.0161 (13) | −0.0047 (11) |
| C19 | 0.0263 (13) | 0.0237 (13) | 0.0240 (13) | −0.0030 (10) | 0.0119 (12) | −0.0039 (10) |
| C20 | 0.0196 (12) | 0.0209 (12) | 0.0269 (13) | 0.0007 (10) | 0.0137 (11) | −0.0015 (10) |
| C21 | 0.0285 (14) | 0.0250 (13) | 0.0283 (14) | −0.0027 (11) | 0.0106 (12) | −0.0017 (11) |
| C22 | 0.0309 (14) | 0.0321 (15) | 0.0223 (13) | 0.0011 (11) | 0.0062 (12) | 0.0043 (11) |
| C23 | 0.0279 (14) | 0.0249 (13) | 0.0311 (14) | −0.0021 (11) | 0.0120 (12) | 0.0040 (11) |
| C24 | 0.0296 (14) | 0.0256 (14) | 0.0312 (15) | −0.0059 (11) | 0.0119 (12) | −0.0043 (11) |
| C25 | 0.0227 (13) | 0.0306 (14) | 0.0174 (12) | −0.0039 (11) | 0.0052 (11) | −0.0025 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C11 | 1.724 (2) | C10—C11 | 1.368 (3) |
| S1—C12 | 1.736 (2) | C11—H11A | 0.9300 |
| O1—C2 | 1.375 (3) | C13—C14 | 1.485 (3) |
| O1—C1 | 1.386 (3) | C13—C20 | 1.495 (3) |
| O2—C1 | 1.205 (3) | C14—C15 | 1.392 (3) |
| N1—C12 | 1.300 (3) | C14—C19 | 1.404 (3) |
| N1—C10 | 1.402 (3) | C15—C16 | 1.382 (3) |
| N2—C12 | 1.370 (3) | C15—H15A | 0.9300 |
| N2—N3 | 1.375 (2) | C16—C17 | 1.382 (3) |
| N2—H1N2 | 0.91 (3) | C16—H16A | 0.9300 |
| N3—C13 | 1.292 (3) | C17—C18 | 1.385 (3) |
| C1—C9 | 1.470 (3) | C17—H17A | 0.9300 |
| C2—C3 | 1.385 (3) | C18—C19 | 1.388 (3) |
| C2—C7 | 1.391 (3) | C18—H18A | 0.9300 |
| C3—C4 | 1.382 (4) | C19—H19A | 0.9300 |
| C3—H3A | 0.9300 | C20—C25 | 1.387 (3) |
| C4—C5 | 1.380 (4) | C20—C21 | 1.391 (3) |
| C4—H4A | 0.9300 | C21—C22 | 1.382 (3) |
| C5—C6 | 1.378 (3) | C21—H21A | 0.9300 |
| C5—H5A | 0.9300 | C22—C23 | 1.391 (4) |
| C6—C7 | 1.400 (3) | C22—H22A | 0.9300 |
| C6—H6A | 0.9300 | C23—C24 | 1.382 (4) |
| C7—C8 | 1.430 (3) | C23—H23A | 0.9300 |
| C8—C9 | 1.346 (3) | C24—C25 | 1.384 (3) |
| C8—H8A | 0.9300 | C24—H24A | 0.9300 |
| C9—C10 | 1.464 (3) | C25—H25A | 0.9300 |

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|---|---|---|---|
| C11—S1—C12 | 88.29 (11) | N1—C12—S1 | 116.69 (18) |
| C2—O1—C1 | 123.27 (19) | N2—C12—S1 | 119.88 (16) |
| C12—N1—C10 | 109.20 (19) | N3—C13—C14 | 115.7 (2) |
| C12—N2—N3 | 116.31 (19) | N3—C13—C20 | 125.68 (19) |
| C12—N2—H1N2 | 119.7 (16) | C14—C13—C20 | 118.54 (19) |
| N3—N2—H1N2 | 119.8 (16) | C15—C14—C19 | 118.6 (2) |
| C13—N3—N2 | 118.33 (19) | C15—C14—C13 | 121.4 (2) |
| O2—C1—O1 | 116.4 (2) | C19—C14—C13 | 119.8 (2) |
| O2—C1—C9 | 126.8 (2) | C16—C15—C14 | 120.8 (2) |
| O1—C1—C9 | 116.8 (2) | C16—C15—H15A | 119.6 |
| O1—C2—C3 | 118.1 (2) | C14—C15—H15A | 119.6 |
| O1—C2—C7 | 120.3 (2) | C17—C16—C15 | 120.0 (2) |
| C3—C2—C7 | 121.6 (2) | C17—C16—H16A | 120.0 |
| C4—C3—C2 | 118.5 (2) | C15—C16—H16A | 120.0 |
| C4—C3—H3A | 120.7 | C16—C17—C18 | 120.4 (2) |
| C2—C3—H3A | 120.7 | C16—C17—H17A | 119.8 |
| C5—C4—C3 | 121.3 (2) | C18—C17—H17A | 119.8 |
| C5—C4—H4A | 119.3 | C17—C18—C19 | 119.7 (2) |
| C3—C4—H4A | 119.3 | C17—C18—H18A | 120.1 |
| C6—C5—C4 | 119.6 (2) | C19—C18—H18A | 120.1 |
| C6—C5—H5A | 120.2 | C18—C19—C14 | 120.5 (2) |
| C4—C5—H5A | 120.2 | C18—C19—H19A | 119.8 |
| C5—C6—C7 | 120.8 (2) | C14—C19—H19A | 119.8 |
| C5—C6—H6A | 119.6 | C25—C20—C21 | 119.0 (2) |
| C7—C6—H6A | 119.6 | C25—C20—C13 | 120.1 (2) |
| C2—C7—C6 | 118.2 (2) | C21—C20—C13 | 120.8 (2) |
| C2—C7—C8 | 117.8 (2) | C22—C21—C20 | 120.4 (2) |
| C6—C7—C8 | 124.1 (2) | C22—C21—H21A | 119.8 |
| C9—C8—C7 | 122.7 (2) | C20—C21—H21A | 119.8 |
| C9—C8—H8A | 118.6 | C21—C22—C23 | 120.2 (2) |
| C7—C8—H8A | 118.6 | C21—C22—H22A | 119.9 |
| C8—C9—C10 | 121.4 (2) | C23—C22—H22A | 119.9 |
| C8—C9—C1 | 119.2 (2) | C24—C23—C22 | 119.6 (2) |
| C10—C9—C1 | 119.4 (2) | C24—C23—H23A | 120.2 |
| C11—C10—N1 | 115.1 (2) | C22—C23—H23A | 120.2 |
| C11—C10—C9 | 127.9 (2) | C23—C24—C25 | 120.1 (2) |
| N1—C10—C9 | 116.96 (19) | C23—C24—H24A | 120.0 |
| C10—C11—S1 | 110.66 (18) | C25—C24—H24A | 120.0 |
| C10—C11—H11A | 124.7 | C24—C25—C20 | 120.7 (2) |
| S1—C11—H11A | 124.7 | C24—C25—H25A | 119.6 |
| N1—C12—N2 | 123.4 (2) | C20—C25—H25A | 119.6 |

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| C12—N2—N3—C13 | 174.6 (2) | C10—N1—C12—N2 | −176.8 (2) |
| C2—O1—C1—O2 | −179.9 (2) | C10—N1—C12—S1 | 1.2 (3) |
| C2—O1—C1—C9 | 0.3 (4) | N3—N2—C12—N1 | −174.4 (2) |
| C1—O1—C2—C3 | 179.2 (3) | N3—N2—C12—S1 | 7.6 (3) |
| C1—O1—C2—C7 | −0.7 (4) | C11—S1—C12—N1 | −1.5 (2) |

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| O1—C2—C3—C4 | −178.3 (3) | C11—S1—C12—N2 | 176.6 (2) |
| C7—C2—C3—C4 | 1.6 (4) | N2—N3—C13—C14 | −179.6 (2) |
| C2—C3—C4—C5 | −1.1 (5) | N2—N3—C13—C20 | −2.6 (4) |
| C3—C4—C5—C6 | 0.2 (4) | N3—C13—C14—C15 | −22.3 (3) |
| C4—C5—C6—C7 | 0.3 (4) | C20—C13—C14—C15 | 160.5 (2) |
| O1—C2—C7—C6 | 178.9 (2) | N3—C13—C14—C19 | 152.8 (2) |
| C3—C2—C7—C6 | −1.0 (4) | C20—C13—C14—C19 | −24.5 (3) |
| O1—C2—C7—C8 | 0.2 (4) | C19—C14—C15—C16 | −0.2 (4) |
| C3—C2—C7—C8 | −179.6 (3) | C13—C14—C15—C16 | 174.9 (2) |
| C5—C6—C7—C2 | 0.0 (4) | C14—C15—C16—C17 | 0.1 (4) |
| C5—C6—C7—C8 | 178.6 (2) | C15—C16—C17—C18 | −0.3 (4) |
| C2—C7—C8—C9 | 0.7 (4) | C16—C17—C18—C19 | 0.5 (4) |
| C6—C7—C8—C9 | −177.9 (2) | C17—C18—C19—C14 | −0.6 (4) |
| C7—C8—C9—C10 | 178.9 (2) | C15—C14—C19—C18 | 0.5 (4) |
| C7—C8—C9—C1 | −1.1 (4) | C13—C14—C19—C18 | −174.7 (2) |
| O2—C1—C9—C8 | −179.1 (3) | N3—C13—C20—C25 | 117.4 (3) |
| O1—C1—C9—C8 | 0.6 (4) | C14—C13—C20—C25 | −65.7 (3) |
| O2—C1—C9—C10 | 0.9 (4) | N3—C13—C20—C21 | −66.3 (3) |
| O1—C1—C9—C10 | −179.4 (2) | C14—C13—C20—C21 | 110.6 (3) |
| C12—N1—C10—C11 | −0.1 (3) | C25—C20—C21—C22 | 2.0 (3) |
| C12—N1—C10—C9 | 178.9 (2) | C13—C20—C21—C22 | −174.3 (2) |
| C8—C9—C10—C11 | 176.1 (3) | C20—C21—C22—C23 | −0.5 (4) |
| C1—C9—C10—C11 | −3.9 (4) | C21—C22—C23—C24 | −1.3 (4) |
| C8—C9—C10—N1 | −2.8 (3) | C22—C23—C24—C25 | 1.4 (4) |
| C1—C9—C10—N1 | 177.2 (2) | C23—C24—C25—C20 | 0.1 (4) |
| N1—C10—C11—S1 | −1.0 (3) | C21—C20—C25—C24 | −1.9 (3) |
| C9—C10—C11—S1 | −179.9 (2) | C13—C20—C25—C24 | 174.5 (2) |
| C12—S1—C11—C10 | 1.3 (2) | | |

*Hydrogen-bond geometry (Å, º)*

Cg1 and Cg2 are the centroids of the C14–C19 and C2–C7 benzene rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C6—H6*A*···O1$^{i}$ | 0.93 | 2.46 | 3.377 (3) | 168 |
| C11—H11*A*···O2 | 0.93 | 2.30 | 2.857 (3) | 118 |
| C21—H21*A*···*Cg*1$^{ii}$ | 0.93 | 2.49 | 3.387 (3) | 162 |
| C24—H24*A*···*Cg*2$^{iii}$ | 0.93 | 2.78 | 3.536 (3) | 139 |

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