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# (4*Z*)-2-Phenyl-1-{(*E*)-[4-(propan-2-yl)benzylidene]-amino}-4-[(thiophen-2-yl)methylidene]-1*H*-imidazol-5(4*H*)-one

Kamni,[a] Vikram D. Singh,[a] K. N. Subbulakshmi,[b] B. Narayana,[b] B. K. Sarojini,[c] Sumati Anthal[d] and Rajni Kant[d]*

[a]School of Physics, Shri Mata Vaishno Devi University, Katra 182 320, J&K, India, [b]Department of Chemistry, Mangalore University, Mangalagangothri 574 199, D.K., Mangalore, India, [c]Department of Industrial Chemistry, Mangalore University, Mangalagangothri 574 199, D.K., Mangalore, India, and [d]X-ray Crystallography Laboratory, Post-Graduate Department of Physics & Electronics, University of Jammu, Jammu Tawi 180 006, India. *Correspondence e-mail: rkant.ju@gmail.com

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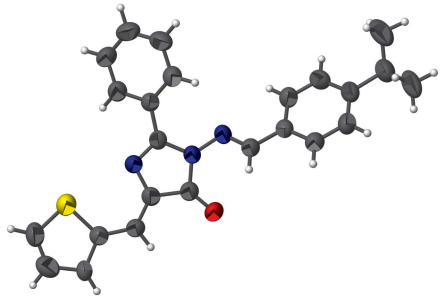
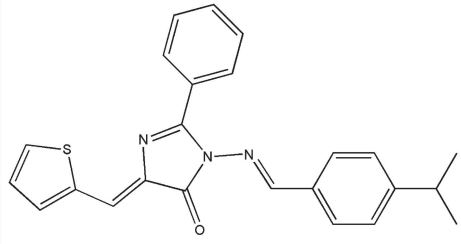
**Structural data**: full structural data are available from iucrdata.iucr.org

In the title molecule, $C_{24}H_{21}N_3OS$, the imidazole ring subtends dihedral angles of 4.6 (1) and 20.2 (1)° with the thiophene and iso-propylbenzene rings, respectively. The plane of the imidazole ring forms a dihedral angle of 39.9 (1)° with the phenyl ring. An intramolecular C—H···N hydrogen bond closes an *S*(6) ring. In the crystal, pairs of C—H···O hydrogen bonds link molecules into inversion dimers featuring $R_2^2(10)$ graph-set motifs. Aromatic $\pi$–$\pi$ stacking interactions are observed between the thiophene and imidazole rings [centroid–centroid distance = 3.570 (2) Å] and thiophene and benzene rings [centroid–centroid distance = 3.889 (2) Å]. Weak C—H···$\pi$ interactions are also observed.

**3D view**



**Chemical scheme**




## Structure description

Imidazolones are nitrogen analogues of azlactones bearing an exocyclic double bond at the fourth position, usually called unsaturated 2,4-disubstituted 2-imidazolin-5-ones. Compounds containing imidazolone as well as imine moieties exhibit a range of pharmaceutical activities, such as antimicrobial (Suthakaran *et al.* 2008; Patel *et al.* 2006), antioxidant (Suhasini *et al.*2014) and anticonvulsant activity (Mohamed *et al.* 2012).

In the title compound (Fig. 1), the imidazole ring subtends dihedral angles of 4.6 (1) and 20.2 (1)° with the thiophene and benzene rings, respectively. The dihedral angle between the phenyl and imidazole rings is 39.9 (1)°. The sum of bond angles around N2 is 358.3°, which confirms that the atom N2 is in an $sp^2$ hybridized state. The C7═O1 bond distance is 1.218 (5) Å which is somewhat longer than the standard value for a carbonyl

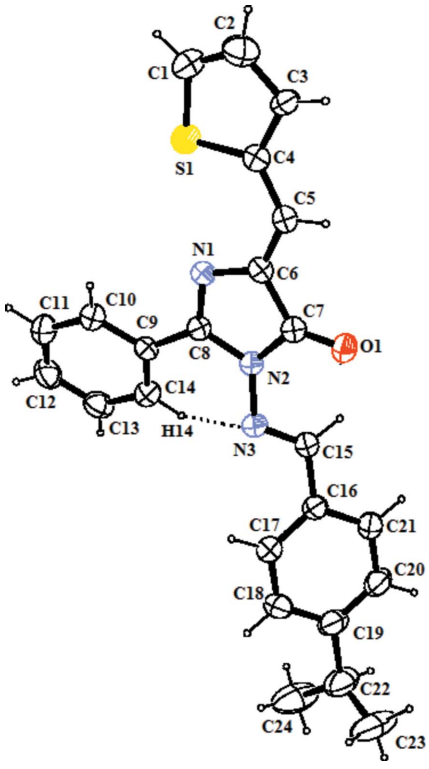



**Figure 1**
*ORTEP* view of the title molecule with displacement ellipsoids drawn at the 40% probability level. Dashed lines indicate the intramolecular hydrogen bond.

group (1.192 Å); the lengthening of this double bond may be due to the involvement of this oxygen atom as a hydrogen-bond acceptor.

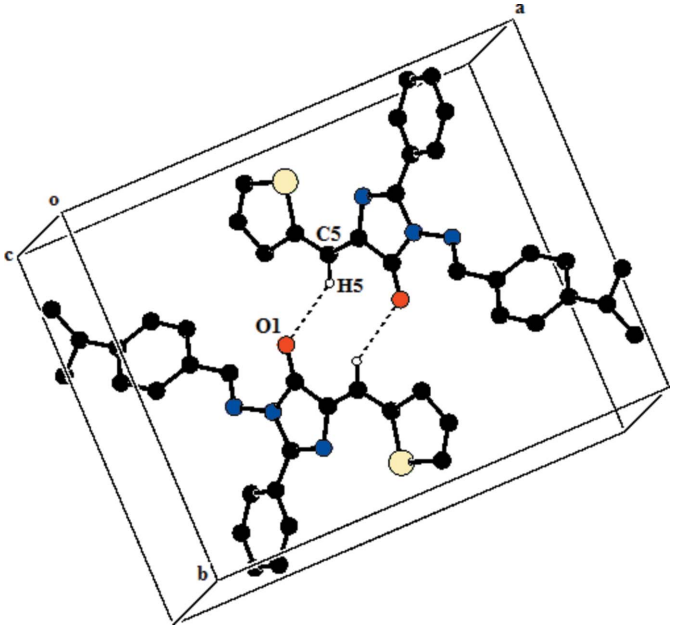



**Figure 2**
A dimer of molecules of the title compound linked by a pair of C—H···O hydrogen bonds forming an $R_2^2(10)$ loop.

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C14—H14···N3 | 0.93 | 2.38 | 2.960 (5) | 120 |
| C5—H5···O1$^{i}$ | 0.93 | 2.44 | 3.221 (5) | 142 |

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

In the crystal, centrosymmetric dimeric aggregates (Fig. 2) are formed by pairs of C—H···O hydrogen bonds (Table 1), forming $R_2^2(10)$ ring motifs. $\pi$–$\pi$ interactions are observed between the thiophene and imidazole rings [centroid separation = 3.570 (2) Å, interplanar spacing = 3.528 Å and centroid shift = 0.55 Å] and the thiophene and benzene rings [centroid separation= 3.889 (2) Å, interplanar spacing = 2.976 Å and centroid shift = 2.50 Å]. Weak C—H···$\pi$ interactions are also observed.

## Synthesis and crystallization

A mixture of 3-hydrazinyl-3-oxo-1-(thiophen-2-yl)prop-1-en-2-yl]benzamide (0.01 mol) in 2-propanol (30 ml) with 4-(propan-2-yl)benzaldehyde (0.01 mol) in the presence of one or two drops of sulfuric acid was heated under reflux for 8 h. The reaction mixture was then cooled to room temperature and poured on cold water; the solid mass obtained was

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{24}H_{21}N_3OS$ |
| $M_r$ | 399.50 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 293 |
| $a$, $b$, $c$ (Å) | 15.8392 (13), 12.9075 (10), 10.3997 (8) |
| $\beta$ (°) | 103.354 (8) |
| $V$ (Å$^3$) | 2068.7 (3) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.18 |
| Crystal size (mm) | 0.30 × 0.20 × 0.20 |
| Data collection | |
| Diffractometer | Oxford Diffraction Xcalibur, Sapphire3 |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010 |
| $T_{min}$, $T_{max}$ | 0.636, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 8085, 4053, 2412 |
| $R_{int}$ | 0.033 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.617 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.074, 0.247, 1.05 |
| No. of reflections | 4053 |
| No. of parameters | 264 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.43, −0.34 |

Computer programs: *CrysAlis PRO* (Oxford Diffraction,2010), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

collected by filtration, washed with cold water and recrystallized at room temperature from a mixture of methanol and *N*,*N*-dimethyl formamide (1:1 *v*/*v*) giving yellow block-like crystals [m.p. 449 K]

## Refinement

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

## Acknowledgements

RK acknowledges the Indian Council of Medical Research, New Delhi, for financial support under Research Project No. BIC/12 (14)/2012. K is thankful to the UGC for funding under Project No. MRP-MAJOR-PHYS-2013–26952 (RP-88). SNK acknowledges the Department of Chemistry, ShriMadhwa-Vadiraja Institute of Technology, Bantakal (VTU Belgam), for providing research facilities.

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# full crystallographic data

*IUCrData* (2016). **1**, x160587 [doi:10.1107/S2414314616005873]

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*Crystal data*

$C_{24}H_{21}N_3OS$
$M_r$ = 399.50
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a$ = 15.8392 (13) Å
$b$ = 12.9075 (10) Å
$c$ = 10.3997 (8) Å
$\beta$ = 103.354 (8)°
$V$ = 2068.7 (3) Å$^3$
$Z$ = 4
$F(000)$ = 840
$D_x$ = 1.283 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 1816 reflections
$\theta$ = 4.1–25.6°
$\mu$ = 0.18 mm$^{-1}$
$T$ = 293 K
Block, yellow
0.30 × 0.20 × 0.20 mm

*Data collection*

Oxford Diffraction Xcalibur, Sapphire3 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 16.1049 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*CrysAlis PRO*; Oxford Diffraction, 2010
$T_{min}$ = 0.636, $T_{max}$ = 1.000
8085 measured reflections
4053 independent reflections
2412 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 3.4°
$h$ = −19→19
$k$ = −15→15
$l$ = −10→12

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.074
$wR(F^2)$ = 0.247
$S$ = 1.05
4053 reflections
264 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-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1066P)^2 + 1.5103P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.34 e Å$^{-3}$

*Special details*

**Experimental**. CrysAlisPro, Oxford Diffraction Ltd., Version 1.171.34.40 (release 27-08-2010 CrysAlis171 .NET) (compiled Aug 27 2010,11:50:40) Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

**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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.48932 (8) | 0.61536 (9) | 0.93165 (13) | 0.0810 (5) |
| N3 | 0.2515 (2) | 0.9237 (3) | 1.1960 (3) | 0.0596 (8) |
| N1 | 0.37039 (19) | 0.7338 (2) | 1.0619 (3) | 0.0565 (8) |
| N2 | 0.31414 (19) | 0.8713 (2) | 1.1460 (3) | 0.0586 (8) |
| O1 | 0.3822 (2) | 1.0076 (2) | 1.0621 (3) | 0.0852 (10) |
| C9 | 0.2618 (2) | 0.6909 (3) | 1.1846 (4) | 0.0521 (9) |
| C17 | 0.1300 (3) | 1.0434 (3) | 1.2985 (4) | 0.0661 (11) |
| H17 | 0.1079 | 0.9851 | 1.2497 | 0.079* |
| C8 | 0.3151 (2) | 0.7636 (3) | 1.1301 (4) | 0.0535 (9) |
| C5 | 0.4681 (2) | 0.8271 (3) | 0.9533 (4) | 0.0639 (10) |
| H5 | 0.4867 | 0.8930 | 0.9363 | 0.077* |
| C16 | 0.2157 (2) | 1.0712 (3) | 1.3090 (4) | 0.0557 (9) |
| C6 | 0.4073 (2) | 0.8230 (3) | 1.0243 (4) | 0.0601 (10) |
| C14 | 0.2251 (3) | 0.7125 (3) | 1.2905 (4) | 0.0634 (10) |
| H14 | 0.2293 | 0.7789 | 1.3263 | 0.076* |
| C4 | 0.5077 (2) | 0.7429 (3) | 0.9007 (4) | 0.0602 (10) |
| C15 | 0.2759 (3) | 1.0096 (3) | 1.2529 (4) | 0.0606 (10) |
| H15 | 0.3322 | 1.0331 | 1.2588 | 0.073* |
| C19 | 0.1081 (3) | 1.1886 (4) | 1.4336 (5) | 0.0773 (13) |
| C7 | 0.3709 (3) | 0.9153 (3) | 1.0755 (4) | 0.0646 (11) |
| C13 | 0.1821 (3) | 0.6353 (4) | 1.3432 (4) | 0.0736 (12) |
| H13 | 0.1591 | 0.6496 | 1.4158 | 0.088* |
| C10 | 0.2515 (3) | 0.5916 (3) | 1.1311 (5) | 0.0702 (12) |
| H10 | 0.2744 | 0.5763 | 1.0587 | 0.084* |
| C21 | 0.2456 (3) | 1.1606 (3) | 1.3806 (4) | 0.0687 (11) |
| H21 | 0.3025 | 1.1822 | 1.3874 | 0.082* |
| C18 | 0.0771 (3) | 1.1004 (4) | 1.3589 (5) | 0.0765 (13) |
| H18 | 0.0197 | 1.0802 | 1.3502 | 0.092* |
| C3 | 0.5704 (3) | 0.7537 (3) | 0.8164 (4) | 0.0612 (10) |
| H3 | 0.5913 | 0.8153 | 0.7894 | 0.073* |
| C20 | 0.1924 (3) | 1.2173 (3) | 1.4413 (5) | 0.0796 (14) |
| H20 | 0.2140 | 1.2765 | 1.4886 | 0.096* |
| C1 | 0.5561 (3) | 0.5752 (4) | 0.8383 (5) | 0.0809 (13) |

| | | | | |
|---|---|---|---|---|
| H1 | 0.5669 | 0.5056 | 0.8249 | 0.097* |
| C11 | 0.2084 (3) | 0.5161 (4) | 1.1823 (5) | 0.0862 (15) |
| H11 | 0.2028 | 0.4501 | 1.1455 | 0.103* |
| C2 | 0.5925 (3) | 0.6525 (4) | 0.7848 (5) | 0.0877 (15) |
| H2 | 0.6302 | 0.6403 | 0.7300 | 0.105* |
| C22 | 0.0515 (4) | 1.2478 (4) | 1.5091 (7) | 0.112 (2) |
| H22 | 0.0963 | 1.2742 | 1.5832 | 0.135* |
| C12 | 0.1736 (3) | 0.5381 (4) | 1.2884 (5) | 0.0834 (14) |
| H12 | 0.1441 | 0.4870 | 1.3233 | 0.100* |
| C23 | 0.0029 (5) | 1.1847 (5) | 1.5790 (6) | 0.137 (3) |
| H23A | −0.0227 | 1.2276 | 1.6352 | 0.206* |
| H23B | 0.0408 | 1.1350 | 1.6318 | 0.206* |
| H23C | −0.0421 | 1.1492 | 1.5169 | 0.206* |
| C24 | 0.0168 (5) | 1.3427 (5) | 1.4508 (7) | 0.138 (3) |
| H24A | −0.0288 | 1.3286 | 1.3744 | 0.207* |
| H24B | 0.0617 | 1.3818 | 1.4251 | 0.207* |
| H24C | −0.0060 | 1.3818 | 1.5136 | 0.207* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0782 (8) | 0.0620 (8) | 0.1081 (10) | −0.0024 (6) | 0.0322 (7) | −0.0085 (6) |
| N3 | 0.0539 (18) | 0.0530 (19) | 0.076 (2) | 0.0012 (15) | 0.0237 (16) | −0.0084 (16) |
| N1 | 0.0487 (17) | 0.0492 (18) | 0.074 (2) | −0.0024 (14) | 0.0204 (16) | −0.0050 (16) |
| N2 | 0.0534 (18) | 0.0491 (19) | 0.079 (2) | −0.0051 (14) | 0.0273 (16) | −0.0111 (16) |
| O1 | 0.085 (2) | 0.0509 (19) | 0.135 (3) | −0.0133 (15) | 0.056 (2) | −0.0143 (18) |
| C9 | 0.0396 (18) | 0.053 (2) | 0.062 (2) | −0.0018 (16) | 0.0080 (16) | −0.0053 (18) |
| C17 | 0.060 (2) | 0.055 (2) | 0.085 (3) | −0.0010 (19) | 0.020 (2) | −0.009 (2) |
| C8 | 0.0459 (19) | 0.051 (2) | 0.063 (2) | −0.0013 (16) | 0.0104 (17) | −0.0071 (18) |
| C5 | 0.056 (2) | 0.054 (2) | 0.085 (3) | −0.0081 (18) | 0.025 (2) | −0.007 (2) |
| C16 | 0.057 (2) | 0.048 (2) | 0.065 (2) | 0.0024 (17) | 0.0205 (18) | 0.0003 (18) |
| C6 | 0.048 (2) | 0.057 (2) | 0.077 (3) | −0.0055 (18) | 0.0181 (19) | −0.010 (2) |
| C14 | 0.066 (2) | 0.057 (2) | 0.069 (2) | 0.0005 (19) | 0.019 (2) | −0.0049 (19) |
| C4 | 0.054 (2) | 0.057 (2) | 0.071 (2) | −0.0005 (18) | 0.0173 (19) | −0.002 (2) |
| C15 | 0.055 (2) | 0.052 (2) | 0.080 (3) | −0.0061 (18) | 0.025 (2) | −0.009 (2) |
| C19 | 0.089 (3) | 0.057 (3) | 0.099 (3) | 0.016 (2) | 0.049 (3) | 0.010 (2) |
| C7 | 0.056 (2) | 0.054 (3) | 0.087 (3) | −0.0052 (18) | 0.024 (2) | −0.009 (2) |
| C13 | 0.064 (3) | 0.082 (3) | 0.081 (3) | 0.002 (2) | 0.029 (2) | 0.009 (3) |
| C10 | 0.065 (3) | 0.060 (3) | 0.089 (3) | −0.007 (2) | 0.025 (2) | −0.014 (2) |
| C21 | 0.068 (3) | 0.055 (2) | 0.089 (3) | −0.008 (2) | 0.031 (2) | −0.009 (2) |
| C18 | 0.057 (2) | 0.072 (3) | 0.107 (3) | 0.005 (2) | 0.033 (2) | 0.004 (3) |
| C3 | 0.068 (2) | 0.048 (2) | 0.073 (2) | 0.0073 (19) | 0.026 (2) | −0.0071 (19) |
| C20 | 0.099 (4) | 0.052 (3) | 0.101 (3) | 0.000 (2) | 0.050 (3) | −0.010 (2) |
| C1 | 0.087 (3) | 0.067 (3) | 0.093 (3) | 0.008 (3) | 0.027 (3) | −0.017 (3) |
| C11 | 0.085 (3) | 0.056 (3) | 0.126 (4) | −0.017 (2) | 0.044 (3) | −0.012 (3) |
| C2 | 0.085 (3) | 0.101 (4) | 0.085 (3) | 0.005 (3) | 0.037 (3) | 0.000 (3) |
| C22 | 0.131 (5) | 0.075 (4) | 0.160 (5) | 0.017 (3) | 0.094 (5) | 0.000 (4) |
| C12 | 0.068 (3) | 0.072 (3) | 0.115 (4) | −0.011 (2) | 0.031 (3) | 0.014 (3) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C23 | 0.188 (7) | 0.120 (5) | 0.145 (5) | 0.066 (5) | 0.123 (5) | 0.049 (4) |
| C24 | 0.196 (7) | 0.094 (4) | 0.164 (6) | 0.077 (5) | 0.126 (6) | 0.050 (4) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C1 | 1.675 (5) | C19—C22 | 1.526 (6) |
| S1—C4 | 1.715 (4) | C13—C12 | 1.372 (7) |
| N3—C15 | 1.274 (5) | C13—H13 | 0.9300 |
| N3—N2 | 1.397 (4) | C10—C11 | 1.366 (6) |
| N1—C8 | 1.306 (4) | C10—H10 | 0.9300 |
| N1—C6 | 1.388 (5) | C21—C20 | 1.376 (6) |
| N2—C8 | 1.400 (5) | C21—H21 | 0.9300 |
| N2—C7 | 1.405 (5) | C18—H18 | 0.9300 |
| O1—C7 | 1.218 (5) | C3—C2 | 1.410 (6) |
| C9—C14 | 1.387 (5) | C3—H3 | 0.9300 |
| C9—C10 | 1.392 (5) | C20—H20 | 0.9300 |
| C9—C8 | 1.461 (5) | C1—C2 | 1.336 (7) |
| C17—C18 | 1.372 (6) | C1—H1 | 0.9300 |
| C17—C16 | 1.384 (5) | C11—C12 | 1.372 (7) |
| C17—H17 | 0.9300 | C11—H11 | 0.9300 |
| C5—C6 | 1.343 (5) | C2—H2 | 0.9300 |
| C5—C4 | 1.426 (6) | C22—C24 | 1.419 (7) |
| C5—H5 | 0.9300 | C22—C23 | 1.429 (7) |
| C16—C21 | 1.395 (5) | C22—H22 | 0.9800 |
| C16—C15 | 1.463 (5) | C12—H12 | 0.9300 |
| C6—C7 | 1.476 (6) | C23—H23A | 0.9600 |
| C14—C13 | 1.389 (6) | C23—H23B | 0.9600 |
| C14—H14 | 0.9300 | C23—H23C | 0.9600 |
| C4—C3 | 1.474 (5) | C24—H24A | 0.9600 |
| C15—H15 | 0.9300 | C24—H24B | 0.9600 |
| C19—C20 | 1.369 (6) | C24—H24C | 0.9600 |
| C19—C18 | 1.402 (6) | | |
| | | | |
| C1—S1—C4 | 91.8 (2) | C9—C10—H10 | 119.2 |
| C15—N3—N2 | 115.4 (3) | C20—C21—C16 | 121.1 (4) |
| C8—N1—C6 | 106.8 (3) | C20—C21—H21 | 119.5 |
| N3—N2—C8 | 123.5 (3) | C16—C21—H21 | 119.5 |
| N3—N2—C7 | 126.4 (3) | C17—C18—C19 | 121.1 (4) |
| C8—N2—C7 | 108.4 (3) | C17—C18—H18 | 119.4 |
| C14—C9—C10 | 118.1 (4) | C19—C18—H18 | 119.4 |
| C14—C9—C8 | 124.3 (4) | C2—C3—C4 | 106.8 (4) |
| C10—C9—C8 | 117.5 (3) | C2—C3—H3 | 126.6 |
| C18—C17—C16 | 121.1 (4) | C4—C3—H3 | 126.6 |
| C18—C17—H17 | 119.5 | C19—C20—C21 | 121.4 (4) |
| C16—C17—H17 | 119.5 | C19—C20—H20 | 119.3 |
| N1—C8—N2 | 112.5 (3) | C21—C20—H20 | 119.3 |
| N1—C8—C9 | 122.8 (3) | C2—C1—S1 | 113.6 (4) |
| N2—C8—C9 | 124.7 (3) | C2—C1—H1 | 123.2 |

| | | | |
|---|---|---|---|
| C6—C5—C4 | 128.0 (4) | S1—C1—H1 | 123.2 |
| C6—C5—H5 | 116.0 | C10—C11—C12 | 119.7 (5) |
| C4—C5—H5 | 116.0 | C10—C11—H11 | 120.2 |
| C17—C16—C21 | 117.6 (3) | C12—C11—H11 | 120.2 |
| C17—C16—C15 | 123.0 (4) | C1—C2—C3 | 116.1 (4) |
| C21—C16—C15 | 119.4 (3) | C1—C2—H2 | 121.9 |
| C5—C6—N1 | 126.2 (4) | C3—C2—H2 | 121.9 |
| C5—C6—C7 | 123.8 (4) | C24—C22—C23 | 120.5 (5) |
| N1—C6—C7 | 110.0 (3) | C24—C22—C19 | 115.4 (5) |
| C9—C14—C13 | 120.1 (4) | C23—C22—C19 | 115.2 (5) |
| C9—C14—H14 | 119.9 | C24—C22—H22 | 100.1 |
| C13—C14—H14 | 119.9 | C23—C22—H22 | 100.1 |
| C5—C4—C3 | 124.9 (4) | C19—C22—H22 | 100.1 |
| C5—C4—S1 | 123.4 (3) | C13—C12—C11 | 120.3 (4) |
| C3—C4—S1 | 111.6 (3) | C13—C12—H12 | 119.9 |
| N3—C15—C16 | 120.2 (3) | C11—C12—H12 | 119.9 |
| N3—C15—H15 | 119.9 | C22—C23—H23A | 109.5 |
| C16—C15—H15 | 119.9 | C22—C23—H23B | 109.5 |
| C20—C19—C18 | 117.7 (4) | H23A—C23—H23B | 109.5 |
| C20—C19—C22 | 121.0 (5) | C22—C23—H23C | 109.5 |
| C18—C19—C22 | 121.3 (5) | H23A—C23—H23C | 109.5 |
| O1—C7—N2 | 125.8 (4) | H23B—C23—H23C | 109.5 |
| O1—C7—C6 | 132.0 (4) | C22—C24—H24A | 109.5 |
| N2—C7—C6 | 102.2 (3) | C22—C24—H24B | 109.5 |
| C12—C13—C14 | 120.2 (4) | H24A—C24—H24B | 109.5 |
| C12—C13—H13 | 119.9 | C22—C24—H24C | 109.5 |
| C14—C13—H13 | 119.9 | H24A—C24—H24C | 109.5 |
| C11—C10—C9 | 121.6 (4) | H24B—C24—H24C | 109.5 |
| C11—C10—H10 | 119.2 | | |

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|---|---|---|---|
| C15—N3—N2—C8 | 153.1 (4) | N3—N2—C7—C6 | −168.3 (3) |
| C15—N3—N2—C7 | −43.6 (5) | C8—N2—C7—C6 | −2.9 (4) |
| C6—N1—C8—N2 | −2.2 (4) | C5—C6—C7—O1 | 3.8 (8) |
| C6—N1—C8—C9 | 178.7 (3) | N1—C6—C7—O1 | −176.9 (5) |
| N3—N2—C8—N1 | 169.3 (3) | C5—C6—C7—N2 | −177.6 (4) |
| C7—N2—C8—N1 | 3.4 (4) | N1—C6—C7—N2 | 1.7 (4) |
| N3—N2—C8—C9 | −11.6 (6) | C9—C14—C13—C12 | −1.9 (6) |
| C7—N2—C8—C9 | −177.6 (4) | C14—C9—C10—C11 | −1.6 (6) |
| C14—C9—C8—N1 | 157.6 (4) | C8—C9—C10—C11 | 174.9 (4) |
| C10—C9—C8—N1 | −18.7 (5) | C17—C16—C21—C20 | 1.6 (6) |
| C14—C9—C8—N2 | −21.4 (6) | C15—C16—C21—C20 | −176.2 (4) |
| C10—C9—C8—N2 | 162.3 (4) | C16—C17—C18—C19 | −0.2 (7) |
| C18—C17—C16—C21 | −1.5 (6) | C20—C19—C18—C17 | 1.7 (7) |
| C18—C17—C16—C15 | 176.3 (4) | C22—C19—C18—C17 | −175.6 (5) |
| C4—C5—C6—N1 | 0.3 (7) | C5—C4—C3—C2 | −179.2 (4) |
| C4—C5—C6—C7 | 179.4 (4) | S1—C4—C3—C2 | 2.1 (4) |
| C8—N1—C6—C5 | 179.5 (4) | C18—C19—C20—C21 | −1.5 (7) |
| C8—N1—C6—C7 | 0.3 (4) | C22—C19—C20—C21 | 175.8 (5) |

| | | | |
|---|---|---|---|
| C10—C9—C14—C13 | 2.2 (6) | C16—C21—C20—C19 | −0.2 (7) |
| C8—C9—C14—C13 | −174.1 (4) | C4—S1—C1—C2 | 0.4 (4) |
| C6—C5—C4—C3 | 176.0 (4) | C9—C10—C11—C12 | 0.6 (7) |
| C6—C5—C4—S1 | −5.4 (6) | S1—C1—C2—C3 | 0.9 (6) |
| C1—S1—C4—C5 | 179.8 (4) | C4—C3—C2—C1 | −1.9 (6) |
| C1—S1—C4—C3 | −1.4 (3) | C20—C19—C22—C24 | 78.6 (8) |
| N2—N3—C15—C16 | 180.0 (3) | C18—C19—C22—C24 | −104.2 (7) |
| C17—C16—C15—N3 | −3.1 (6) | C20—C19—C22—C23 | −133.9 (6) |
| C21—C16—C15—N3 | 174.6 (4) | C18—C19—C22—C23 | 43.3 (8) |
| N3—N2—C7—O1 | 10.4 (7) | C14—C13—C12—C11 | 0.9 (7) |
| C8—N2—C7—O1 | 175.8 (4) | C10—C11—C12—C13 | −0.2 (8) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C14—H14···N3 | 0.93 | 2.38 | 2.960 (5) | 120 |
| C5—H5···O1$^{i}$ | 0.93 | 2.44 | 3.221 (5) | 142 |
| C3—H3···O1$^{i}$ | 0.93 | 2.74 | 3.349 (5) | 124 |

Symmetry code: (i) −*x*+1, −*y*+2, −*z*+2.