

Acta Crystallographica Section E

Structure Reports

Online

ISSN 1600-5368

2-[(1*H*-Benzimidazol-2-yl)sulfanyl]-1-phenylethanoneHatem A. Abdel-Aziz,^a Tze Shyang Chia^b and Hoong-Kun Fun^{b*}‡

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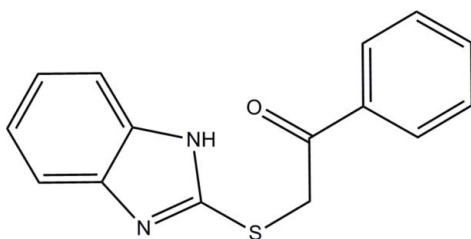
Received 21 June 2012; accepted 25 June 2012

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.041; wR factor = 0.096; data-to-parameter ratio = 21.1.

The title compound, $\text{C}_{15}\text{H}_{12}\text{N}_2\text{OS}$, adopts a twisted V-shape, with the S atom as the pivot. The benzimidazole ring system [maximum deviation = 0.015 (1) Å] makes a dihedral angle of 78.56 (7)° with the phenyl ring. The O atom of the ketone group is close to coplanar with its adjacent ring [O—C—C torsion angle = 11.0 (2)°]. In the crystal, molecules are linked by N—H···N hydrogen bonds into an infinite chain along [001]. The crystal packing also features a C—H··· π interaction.

Related literature

For a related structure, see: Abdel-Aziz *et al.* (2011). For the synthesis, see: D'Amico *et al.* (1964). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986). For standard bond lengths, see: Allen *et al.* (1987).



Experimental

Crystal data

$\text{C}_{15}\text{H}_{12}\text{N}_2\text{OS}$
 $M_r = 268.33$

Monoclinic, $P2_1/c$
 $a = 14.7849$ (13) Å

$b = 9.2643$ (8) Å
 $c = 9.7859$ (8) Å
 $\beta = 106.792$ (1)°
 $V = 1283.24$ (19) Å³
 $Z = 4$

Mo $K\alpha$ radiation
 $\mu = 0.24$ mm⁻¹
 $T = 100$ K
 $0.32 \times 0.11 \times 0.07$ mm

Data collection

Bruker APEX DUO CCD diffractometer
Absorption correction: multi-scan (SADABS; Bruker, 2009)
 $T_{\min} = 0.927$, $T_{\max} = 0.983$

13644 measured reflections
3722 independent reflections
3094 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.027$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.096$
 $S = 1.05$
3722 reflections
176 parameters

H atoms treated by a mixture of independent and constrained refinement
 $\Delta\rho_{\text{max}} = 0.51$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.41$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

Cg1 is the centroid of the N1/N2/C1/C6/C7 ring.

| $D-H\cdots A$ | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|----------------------------|------------|-------------|-------------|---------------|
| N2—H1N2···N1 ⁱ | 0.880 (19) | 1.95 (2) | 2.8250 (16) | 175.8 (18) |
| C4—H4A···Cg1 ⁱⁱ | 0.93 | 2.82 | 3.4175 (15) | 123 |

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

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).

HKF and TSC thank Universiti Sains Malaysia (USM) for the Research University Grant (1001/PFIZIK/811160). TSC also thanks the Malaysian Government and USM for the award of a research fellowship. The authors thank the Deanship of Scientific Research and the Research Center, College of Pharmacy, King Saud University.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6869).

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‡ Thomson Reuters ResearcherID: A-3561-2009.

supplementary materials

Acta Cryst. (2012). E68, o2262 [doi:10.1107/S1600536812028747]

2-[(1*H*-Benzimidazol-2-yl)sulfanyl]-1-phenylethanone**Hatem A. Abdel-Aziz, Tze Shyang Chia and Hoong-Kun Fun****Comment**

In continuation to our reports on the chemistry and the biological activity of benzimidazoles (Abdel-Aziz *et al.*, 2011), we report herein the crystal structure of the title compound.

The asymmetric unit of the title compound is shown in Fig. 1. The molecule adopts a twisted V shape with S atom as the pivot, which is identical to a related structure (Abdel-Aziz *et al.*, 2011). The benzimidazole ring system (N1/N2/C1–C7) is essentially planar [maximum deviation = 0.015 (1) Å at atom C1] and makes a dihedral angle of 78.56 (7)° with the terminal C10–C15 benzene ring. The ketone group (C9=O1) is almost coplanar with the C10–C15 benzene ring as indicated by the O1–C9–C10–C11 torsion angle of 11.0 (2)°. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges.

In the crystal (Fig. 2), molecules are linked by N2—H1N2···N1 hydrogen bond into an infinite chain along the *c*-axis. The crystal packing is further stabilized by C—H··· π interaction (Table 1), involving Cg1, which is the centroid of N1/N2/C1/C6/C7 ring.

Experimental

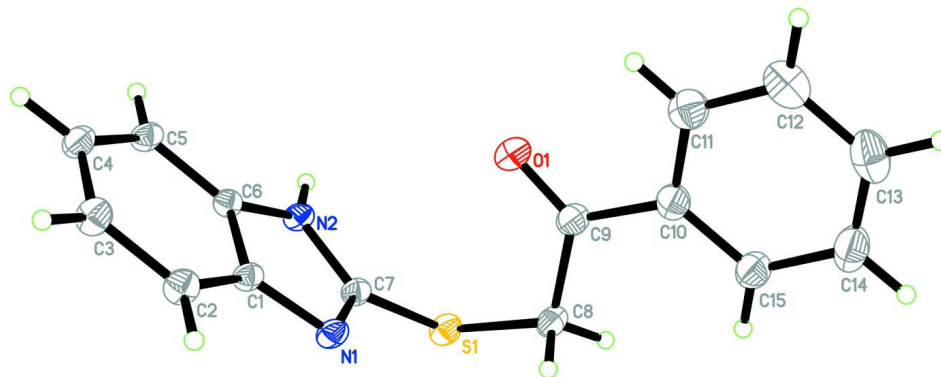
The title compound was prepared by the reaction of 1*H*-benzo[*d*]imidazole-2-thiol and 2-bromo-1-phenylethanone in ethanol in the presence of potassium hydroxide (D'Amico *et al.*, 1964). Colourless needles were crystallised from ethanol solution.

Refinement

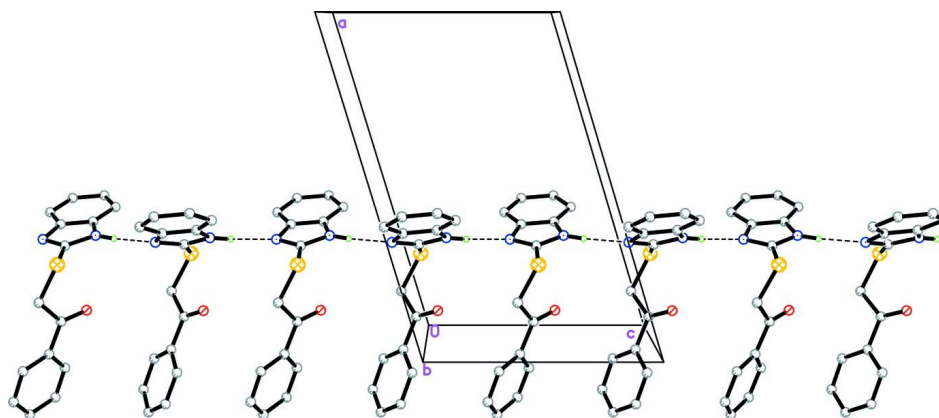
The atom H1N2 was located in a difference fourier map and refined freely [N2—H1N2 = 0.880 (19) Å]. The remaining H atoms were positioned geometrically [C—H = 0.93 and 0.97 Å] and refined using a riding model with $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$.

Computing details

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


Figure 1

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


Figure 2

The crystal packing of the title compound. The dashed lines represent the hydrogen bonds. For clarity sake, hydrogen atoms not involved in hydrogen bonding have been omitted.

2-[(1*H*-Benzimidazol-2-yl)sulfanyl]-1-phenylethanone

Crystal data

$C_{15}H_{12}N_2OS$
 $M_r = 268.33$
 Monoclinic, $P2_1/c$
 Hall symbol: $-P\ 2_1/c$
 $a = 14.7849$ (13) Å
 $b = 9.2643$ (8) Å
 $c = 9.7859$ (8) Å
 $\beta = 106.792$ (1)°
 $V = 1283.24$ (19) Å³
 $Z = 4$

$F(000) = 560$
 $D_x = 1.389$ Mg m⁻³
 Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
 Cell parameters from 5435 reflections
 $\theta = 2.6$ – 30.0 °
 $\mu = 0.24$ mm⁻¹
 $T = 100$ K
 Needle, colourless
 $0.32 \times 0.11 \times 0.07$ mm

Data collection

Bruker APEX DUO CCD
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans

Absorption correction: multi-scan
 (*SADABS*; Bruker, 2009)
 $T_{\min} = 0.927$, $T_{\max} = 0.983$
 13644 measured reflections
 3722 independent reflections
 3094 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.027$
 $\theta_{\text{max}} = 30.0^\circ$, $\theta_{\text{min}} = 1.4^\circ$
 $h = -20 \rightarrow 20$

$k = -10 \rightarrow 13$
 $l = -13 \rightarrow 13$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.041$
 $wR(F^2) = 0.096$
 $S = 1.05$
 3722 reflections
 176 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
 $w = 1/[\sigma^2(F_o^2) + (0.0361P)^2 + 0.7649P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\text{max}} = 0.001$
 $\Delta\rho_{\text{max}} = 0.51 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\text{min}} = -0.41 \text{ e } \text{\AA}^{-3}$

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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|---------------|----------------------------------|
| S1 | 0.27768 (2) | 0.54949 (4) | 0.10069 (4) | 0.02057 (9) |
| O1 | 0.12453 (8) | 0.75548 (13) | 0.11153 (13) | 0.0336 (3) |
| N1 | 0.33134 (8) | 0.80747 (12) | 0.01048 (12) | 0.0170 (2) |
| N2 | 0.34377 (8) | 0.79475 (12) | 0.24453 (12) | 0.0159 (2) |
| C1 | 0.36703 (9) | 0.93757 (14) | 0.07565 (14) | 0.0155 (2) |
| C2 | 0.39488 (9) | 1.06192 (15) | 0.01768 (15) | 0.0195 (3) |
| H2A | 0.3892 | 1.0686 | -0.0793 | 0.023* |
| C3 | 0.43124 (10) | 1.17483 (15) | 0.10989 (15) | 0.0209 (3) |
| H3A | 0.4504 | 1.2587 | 0.0739 | 0.025* |
| C4 | 0.43994 (9) | 1.16595 (15) | 0.25666 (15) | 0.0198 (3) |
| H4A | 0.4649 | 1.2439 | 0.3154 | 0.024* |
| C5 | 0.41217 (9) | 1.04368 (14) | 0.31575 (14) | 0.0179 (3) |
| H5A | 0.4175 | 1.0378 | 0.4126 | 0.021* |
| C6 | 0.37587 (8) | 0.93011 (13) | 0.22273 (14) | 0.0149 (2) |
| C7 | 0.31869 (9) | 0.72789 (14) | 0.11564 (14) | 0.0163 (2) |
| C8 | 0.16524 (10) | 0.57212 (15) | -0.03317 (16) | 0.0224 (3) |
| H8A | 0.1767 | 0.6038 | -0.1212 | 0.027* |
| H8B | 0.1340 | 0.4790 | -0.0513 | 0.027* |
| C9 | 0.09888 (10) | 0.67930 (16) | 0.00635 (16) | 0.0229 (3) |
| C10 | 0.00060 (10) | 0.69134 (16) | -0.09324 (16) | 0.0224 (3) |

| | | | | |
|------|---------------|--------------|---------------|------------|
| C11 | -0.05419 (11) | 0.80839 (17) | -0.07551 (18) | 0.0277 (3) |
| H11A | -0.0292 | 0.8754 | -0.0038 | 0.033* |
| C12 | -0.14568 (12) | 0.82596 (19) | -0.1637 (2) | 0.0335 (4) |
| H12A | -0.1814 | 0.9051 | -0.1520 | 0.040* |
| C13 | -0.18359 (11) | 0.7248 (2) | -0.26939 (19) | 0.0340 (4) |
| H13A | -0.2448 | 0.7364 | -0.3290 | 0.041* |
| C14 | -0.13037 (11) | 0.6066 (2) | -0.28627 (18) | 0.0327 (4) |
| H14A | -0.1565 | 0.5380 | -0.3559 | 0.039* |
| C15 | -0.03793 (11) | 0.58989 (18) | -0.19947 (17) | 0.0271 (3) |
| H15A | -0.0020 | 0.5114 | -0.2123 | 0.033* |
| H1N2 | 0.3370 (13) | 0.761 (2) | 0.325 (2) | 0.030 (5)* |

Atomic displacement parameters (\AA^2)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|--------------|--------------|--------------|---------------|--------------|---------------|
| S1 | 0.02627 (17) | 0.01719 (15) | 0.01866 (18) | -0.00276 (12) | 0.00714 (13) | -0.00024 (13) |
| O1 | 0.0277 (5) | 0.0396 (6) | 0.0327 (7) | -0.0016 (5) | 0.0075 (5) | -0.0181 (5) |
| N1 | 0.0216 (5) | 0.0182 (5) | 0.0112 (5) | -0.0013 (4) | 0.0048 (4) | -0.0010 (4) |
| N2 | 0.0204 (5) | 0.0178 (5) | 0.0098 (5) | -0.0002 (4) | 0.0050 (4) | 0.0009 (4) |
| C1 | 0.0172 (5) | 0.0176 (6) | 0.0114 (6) | 0.0005 (4) | 0.0036 (4) | -0.0004 (5) |
| C2 | 0.0236 (6) | 0.0214 (6) | 0.0132 (6) | -0.0005 (5) | 0.0048 (5) | 0.0026 (5) |
| C3 | 0.0249 (6) | 0.0177 (6) | 0.0199 (7) | -0.0014 (5) | 0.0062 (5) | 0.0023 (5) |
| C4 | 0.0213 (6) | 0.0187 (6) | 0.0185 (7) | -0.0007 (5) | 0.0044 (5) | -0.0042 (5) |
| C5 | 0.0205 (6) | 0.0209 (6) | 0.0116 (6) | 0.0007 (5) | 0.0037 (5) | -0.0018 (5) |
| C6 | 0.0154 (5) | 0.0165 (5) | 0.0126 (6) | 0.0012 (4) | 0.0038 (4) | 0.0011 (5) |
| C7 | 0.0182 (6) | 0.0180 (6) | 0.0128 (6) | 0.0003 (5) | 0.0046 (5) | -0.0003 (5) |
| C8 | 0.0242 (6) | 0.0234 (6) | 0.0202 (7) | -0.0050 (5) | 0.0072 (5) | -0.0067 (6) |
| C9 | 0.0242 (6) | 0.0237 (6) | 0.0222 (7) | -0.0046 (5) | 0.0093 (6) | -0.0047 (6) |
| C10 | 0.0237 (6) | 0.0253 (7) | 0.0200 (7) | -0.0053 (5) | 0.0091 (5) | 0.0006 (6) |
| C11 | 0.0300 (7) | 0.0249 (7) | 0.0291 (8) | -0.0027 (6) | 0.0101 (6) | 0.0002 (6) |
| C12 | 0.0302 (8) | 0.0341 (8) | 0.0376 (10) | 0.0035 (7) | 0.0120 (7) | 0.0092 (7) |
| C13 | 0.0247 (7) | 0.0469 (10) | 0.0290 (9) | -0.0046 (7) | 0.0056 (6) | 0.0120 (8) |
| C14 | 0.0301 (7) | 0.0440 (9) | 0.0229 (8) | -0.0120 (7) | 0.0056 (6) | -0.0025 (7) |
| C15 | 0.0271 (7) | 0.0316 (8) | 0.0233 (8) | -0.0059 (6) | 0.0084 (6) | -0.0044 (6) |

Geometric parameters (\AA , $^\circ$)

| | | | |
|---------|-------------|----------|-------------|
| S1—C7 | 1.7519 (13) | C5—H5A | 0.9300 |
| S1—C8 | 1.8070 (15) | C8—C9 | 1.5222 (19) |
| O1—C9 | 1.2148 (18) | C8—H8A | 0.9700 |
| N1—C7 | 1.3224 (17) | C8—H8B | 0.9700 |
| N1—C1 | 1.3941 (16) | C9—C10 | 1.502 (2) |
| N2—C7 | 1.3571 (17) | C10—C11 | 1.394 (2) |
| N2—C6 | 1.3790 (16) | C10—C15 | 1.395 (2) |
| N2—H1N2 | 0.880 (19) | C11—C12 | 1.388 (2) |
| C1—C2 | 1.3977 (18) | C11—H11A | 0.9300 |
| C1—C6 | 1.4088 (18) | C12—C13 | 1.388 (3) |
| C2—C3 | 1.3846 (19) | C12—H12A | 0.9300 |
| C2—H2A | 0.9300 | C13—C14 | 1.386 (3) |
| C3—C4 | 1.407 (2) | C13—H13A | 0.9300 |

| | | | |
|-------------|--------------|-----------------|--------------|
| C3—H3A | 0.9300 | C14—C15 | 1.394 (2) |
| C4—C5 | 1.3869 (19) | C14—H14A | 0.9300 |
| C4—H4A | 0.9300 | C15—H15A | 0.9300 |
| C5—C6 | 1.3934 (18) | | |
| C7—S1—C8 | 100.07 (6) | C9—C8—H8A | 108.6 |
| C7—N1—C1 | 104.24 (11) | S1—C8—H8A | 108.6 |
| C7—N2—C6 | 106.56 (11) | C9—C8—H8B | 108.6 |
| C7—N2—H1N2 | 126.9 (12) | S1—C8—H8B | 108.6 |
| C6—N2—H1N2 | 126.3 (12) | H8A—C8—H8B | 107.6 |
| N1—C1—C2 | 130.08 (12) | O1—C9—C10 | 120.88 (13) |
| N1—C1—C6 | 109.64 (11) | O1—C9—C8 | 121.87 (13) |
| C2—C1—C6 | 120.26 (12) | C10—C9—C8 | 117.22 (12) |
| C3—C2—C1 | 117.56 (12) | C11—C10—C15 | 119.34 (14) |
| C3—C2—H2A | 121.2 | C11—C10—C9 | 117.71 (13) |
| C1—C2—H2A | 121.2 | C15—C10—C9 | 122.94 (13) |
| C2—C3—C4 | 121.66 (12) | C12—C11—C10 | 120.72 (15) |
| C2—C3—H3A | 119.2 | C12—C11—H11A | 119.6 |
| C4—C3—H3A | 119.2 | C10—C11—H11A | 119.6 |
| C5—C4—C3 | 121.51 (13) | C11—C12—C13 | 119.69 (16) |
| C5—C4—H4A | 119.2 | C11—C12—H12A | 120.2 |
| C3—C4—H4A | 119.2 | C13—C12—H12A | 120.2 |
| C4—C5—C6 | 116.68 (12) | C14—C13—C12 | 120.09 (15) |
| C4—C5—H5A | 121.7 | C14—C13—H13A | 120.0 |
| C6—C5—H5A | 121.7 | C12—C13—H13A | 120.0 |
| N2—C6—C5 | 132.10 (12) | C13—C14—C15 | 120.36 (16) |
| N2—C6—C1 | 105.56 (11) | C13—C14—H14A | 119.8 |
| C5—C6—C1 | 122.34 (12) | C15—C14—H14A | 119.8 |
| N1—C7—N2 | 114.00 (12) | C14—C15—C10 | 119.79 (15) |
| N1—C7—S1 | 125.75 (10) | C14—C15—H15A | 120.1 |
| N2—C7—S1 | 120.22 (10) | C10—C15—H15A | 120.1 |
| C9—C8—S1 | 114.65 (10) | | |
| C7—N1—C1—C2 | 179.02 (13) | C6—N2—C7—S1 | 177.86 (9) |
| C7—N1—C1—C6 | 0.78 (14) | C8—S1—C7—N1 | -57.99 (13) |
| N1—C1—C2—C3 | -177.79 (13) | C8—S1—C7—N2 | 124.34 (11) |
| C6—C1—C2—C3 | 0.30 (19) | C7—S1—C8—C9 | -57.82 (11) |
| C1—C2—C3—C4 | -0.1 (2) | S1—C8—C9—O1 | 8.48 (19) |
| C2—C3—C4—C5 | -0.2 (2) | S1—C8—C9—C10 | -173.67 (10) |
| C3—C4—C5—C6 | 0.38 (19) | O1—C9—C10—C11 | 11.0 (2) |
| C7—N2—C6—C5 | -178.49 (13) | C8—C9—C10—C11 | -166.86 (13) |
| C7—N2—C6—C1 | 0.55 (13) | O1—C9—C10—C15 | -167.78 (15) |
| C4—C5—C6—N2 | 178.68 (13) | C8—C9—C10—C15 | 14.4 (2) |
| C4—C5—C6—C1 | -0.22 (19) | C15—C10—C11—C12 | -1.0 (2) |
| N1—C1—C6—N2 | -0.83 (14) | C9—C10—C11—C12 | -179.88 (14) |
| C2—C1—C6—N2 | -179.28 (11) | C10—C11—C12—C13 | 0.9 (2) |
| N1—C1—C6—C5 | 178.32 (11) | C11—C12—C13—C14 | 0.3 (2) |
| C2—C1—C6—C5 | -0.12 (19) | C12—C13—C14—C15 | -1.4 (2) |
| C1—N1—C7—N2 | -0.44 (15) | C13—C14—C15—C10 | 1.2 (2) |

| | | | |
|-------------|--------------|-----------------|-------------|
| C1—N1—C7—S1 | -178.24 (10) | C11—C10—C15—C14 | 0.0 (2) |
| C6—N2—C7—N1 | -0.07 (15) | C9—C10—C15—C14 | 178.74 (14) |

Hydrogen-bond geometry (Å, °)

Cg1 is the centroid of the N1/N2/C1/C6/C7 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—H1N2 \cdots N1 ⁱ | 0.880 (19) | 1.95 (2) | 2.8250 (16) | 175.8 (18) |
| C4—H4A \cdots Cg1 ⁱⁱ | 0.93 | 2.82 | 3.4175 (15) | 123 |

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