

# Dibenzo[*b,f*][1,4]thiazepin-11-yl-diethylamine

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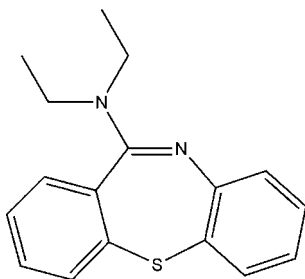
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Key indicators: single-crystal X-ray study;  $T = 150$  K; mean  $\sigma(\text{C}-\text{C}) = 0.002$  Å;  $R$  factor = 0.032;  $wR$  factor = 0.086; data-to-parameter ratio = 13.1.

In the title compound,  $\text{C}_{17}\text{H}_{18}\text{N}_2\text{S}$ , the thiazepine ring adopts a boat conformation and the dihedral angle between the benzene rings is  $75.92(5)^\circ$ , resulting in a butterfly-like conformation. In the crystal, molecules are connected *via* weak  $\text{C}_{\text{aromatic}}-\text{H}\cdots\text{N}$  contacts involving the imine N atom as acceptor and through a quite short  $\text{C}-\text{H}\cdots\pi$  interaction. The resulting molecular chains propagate along the  $c$ -axis direction.

## Related literature

For 'privileged structures', that is 'structures able to provide high affinity ligands for more than one type of receptor', see: Evans *et al.* (1988); Patchett & Nargund (2000); Fedi *et al.* (2008). For the clinical use of dibenzothiazepine derivatives, see: Ganesh *et al.* (2011); Pettersson *et al.* (2009); Riedel *et al.* (2007); Warawa *et al.* (2001). For structure–property relationships in (6,7,6)-tricyclic ring systems, see: Ravikumar & Sridhar (2005); Altamura *et al.* (2008, 2009, 2011). For geometrical data and descriptors, see: Duax *et al.* (1976); Bertolasi *et al.* (1982); Allen *et al.* (1987).



## Experimental

### Crystal data

|  |   |
|--|---|
| $\text{C}_{17}\text{H}_{18}\text{N}_2\text{S}$ | $V = 1449.54(4) \text{ \AA}^3$            |
| $M_r = 282.40$                                 | $Z = 4$                                   |
| Monoclinic, $P2_1/c$                           | Cu $K\alpha$ radiation                    |
| $a = 12.0137(2) \text{ \AA}$                   | $\mu = 1.89 \text{ mm}^{-1}$              |
| $b = 8.2257(1) \text{ \AA}$                    | $T = 150 \text{ K}$                       |
| $c = 15.0513(2) \text{ \AA}$                   | $0.20 \times 0.18 \times 0.03 \text{ mm}$ |
| $\beta = 102.952(1)^\circ$                     |   |

### Data collection

|   |  |
|---|--|
| Oxford Diffraction XcaliburPX diffractometer  | 6173 measured reflections              |
| Absorption correction: multi-scan ( <i>CrysAlis RED</i> ; Oxford Diffraction, 2006) | 2364 independent reflections           |
| $T_{\text{min}} = 0.722$ , $T_{\text{max}} = 0.945$                                 | 1837 reflections with $I > 2\sigma(I)$ |
|   | $R_{\text{int}} = 0.019$               |

### Refinement

|                                 |  |
|---------------------------------|--|
| $R[F^2 > 2\sigma(F^2)] = 0.032$ | 181 parameters                                       |
| $wR(F^2) = 0.086$               | H-atom parameters constrained                        |
| $S = 1.05$                      | $\Delta\rho_{\text{max}} = 0.23 \text{ e \AA}^{-3}$  |
| 2364 reflections                | $\Delta\rho_{\text{min}} = -0.26 \text{ e \AA}^{-3}$ |

**Table 1**

Hydrogen-bond geometry (Å, °).

$\text{C}_g$  is the centroid of the C8–C12 ring.

| $D-\text{H}\cdots A$                    | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{C5}-\text{H5}\cdots\text{N1}^i$  | 0.95         | 2.70               | 3.576(2)    | 154                  |
| $\text{C4}-\text{H4}\cdots\text{C}_g^i$ | 0.95         | 2.81               | 3.5759(18)  | 139                  |

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis CCD*; data reduction: *CrysAlis RED* (Oxford Diffraction, 2006); program(s) used to solve structure: *SIR92* (Altomare *et al.*, 1999); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PARST* (Nardelli, 1995).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NC2296).

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## supporting information

*Acta Cryst.* (2012). E68, o3133–o3134 [doi:10.1107/S1600536812042328]

**Dibenzo[*b,f*][1,4]thiazepin-11-yl-diethyl-amine**

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**S1. Comment**

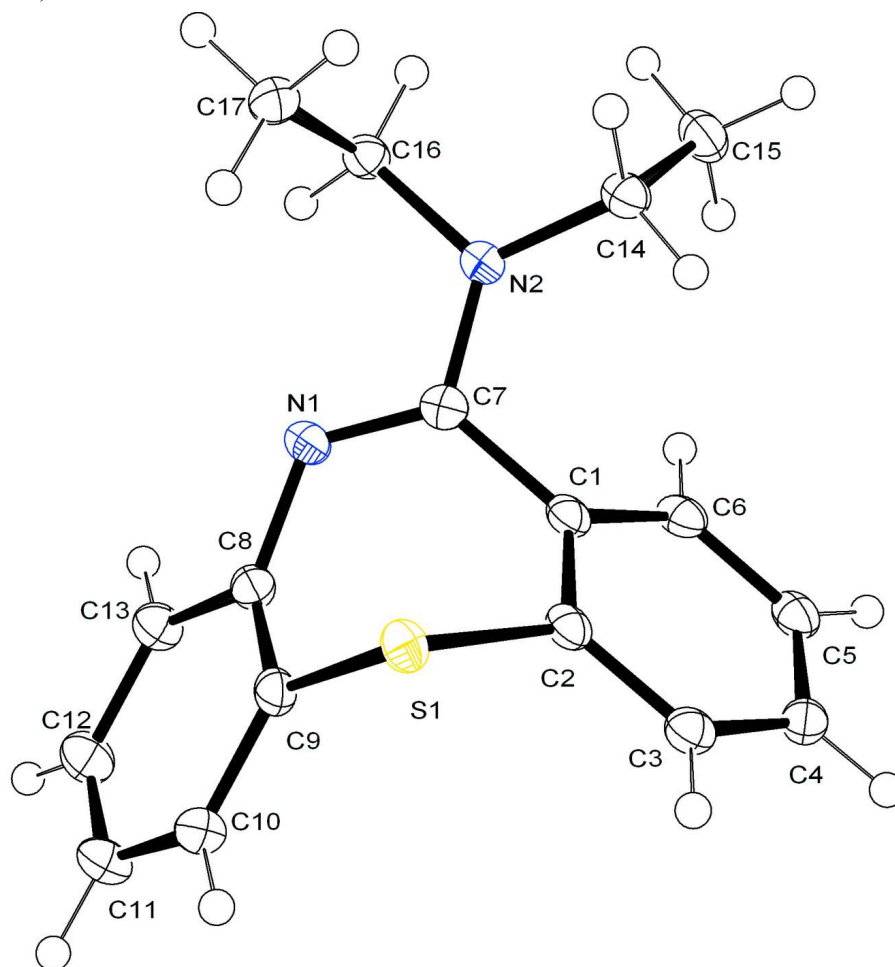
Many antidepressant drugs have a tricyclic structure with two aromatic rings fused to a central seven membered ring, on which one or more heteroatoms can be present. In this context, dibenzothiazepines are a class of heterocyclic scaffolds containing nitrogen and sulfur which belong to the class of the so-called "privileged structures", *i.e.* structures "able to provide high affinity ligands for more than one type of receptor" (Evans *et al.* 1988; Patchett & Nargund 2000; Fedi *et al.* 2008). In fact the dibenzothiazepine skeleton has a broad spectrum of medical applications; its derivatives are used to treat schizophrenia and also find applications as neuroleptics, antidepressants, antihistaminic, just to name a few (Ganesh *et al.* 2011; Pettersson *et al.* 2009; Riedel *et al.* 2007; Warawa *et al.* 2001). Within our programme research concerning the structural elucidation of tricyclic molecules in order to gain further insights into structure–property relationships (Altamura *et al.*, 2008; Altamura *et al.*, 2009; Altamura *et al.*, 2011) we investigated the crystal and molecular structure of the title compound. The overall shape of the tricyclic skeleton is controlled both by the conformation of the central seven-membered ring and the relative arrangement of the aromatic rings bound to it. The central thiazepine ring adopts the usual boat conformation, with C1, C2, C8 and C9 as the basal plane, the S atom as the bow and the N1—C7 bond as the stern. The deviation from a pure boat conformation is quite small as can be seen from the asymmetry index  $\Delta C_s$  which is 3.97°; the bow angle is 51.04 (8)° and the stern angle is 41.89 (8)° (Duax *et al.* 1976; Bertolasi *et al.* 1982; Ravikumar & Sridhar, 2005). Finally, the dihedral angle between the benzene rings is 104.08 (5)°. As a consequence the dibenzothiazepine tricyclic skeleton assumes an overall butterfly-like shape (Fig. 1). The N2—C7 bond is shorter than an usual N—C single bond [1.368 (2) Å compared to 1.416 Å (Allen *et al.* 1987)] and the sum of the bond angles about N2 is 358°; consequently, N2 has a partial  $sp^2$  character. Molecular chains, which propagate along the *c* axis, are formed through intermolecular interactions (Fig. 2): a weak C—H<sub>aromatic</sub>⋯N contact which involves the imine nitrogen atom as acceptor and a quite short C—H⋯ $\pi$  interaction (Table 1).

**S2. Experimental**

The synthesis of the title compound started from the commercially available tricyclic lactam (dibenzo[*b,f*][1,4]thiazepin-11(10*H*)-one) (0.89 g, 3.91 mmol), that was dissolved into 10 ml of phosphorus oxychloride and refluxed for two hours under nitrogen atmosphere. After removal of excess POCl<sub>3</sub> under vacuum, the corresponding iminochloride (11-chlorodibenzo[*b,f*][1,4]thiazepine) was obtained as a yellow oil, that was dissolved in 20 ml of anhydrous toluene. An excess of diethylamine (20 ml, 191 mmol) was added and the mixture refluxed until complete conversion (monitored by HPLC; about 6 h were needed for complete conversion). After removal of the solvent *in vacuo* and purification by flash chromatography (eluent: gradient CH<sub>2</sub>Cl<sub>2</sub>/cyclohexane from 50:50 to 100% CH<sub>2</sub>Cl<sub>2</sub>), dibenzo[*b,f*][1,4]thiazepin-11-yl-diethyl-amine was obtained as a yellow oil (0.66 g, 60% yield), which became a white solid on standing at room temperature for several days. Crystals suitable for single-crystal X-ray diffraction analysis were obtained by slow evaporation of a water/DMSO solution of dibenzo[*b,f*][1,4]thiazepin-11-yl-diethyl-amine.

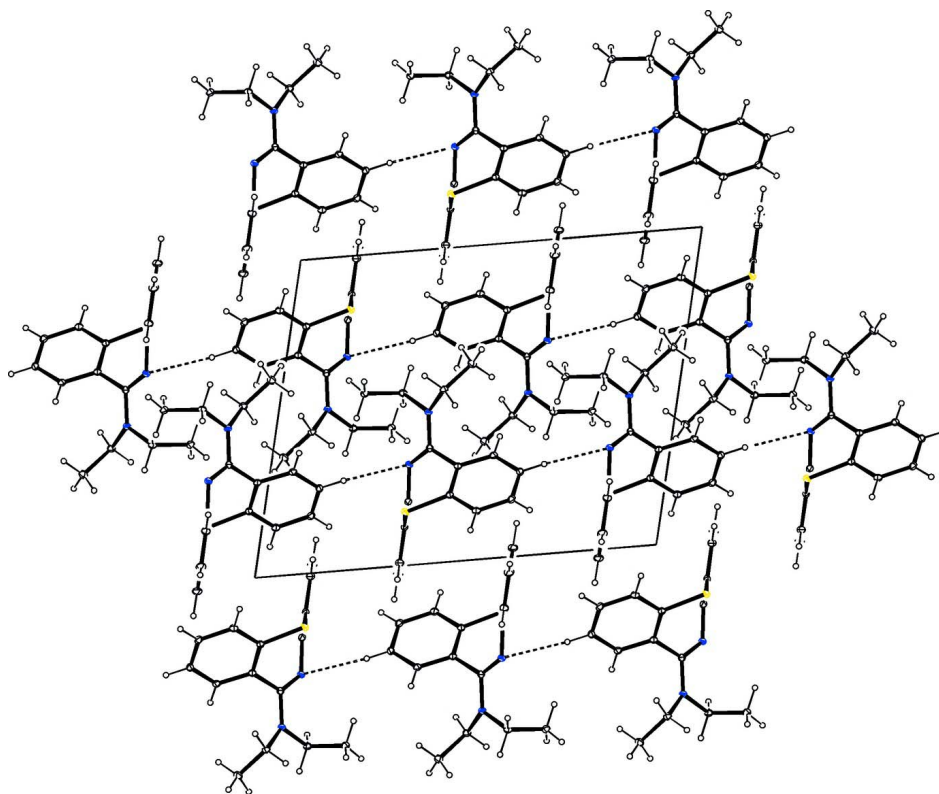
### S3. Refinement

All the H atoms were positioned with idealized geometry using a riding model and refined with  $U_{\text{iso}}(\text{H})$  1.2 times  $U_{\text{eq}}(\text{C})$  (1.5 for methyl H atoms).



**Figure 1**

Crystal structure of the title compound with labelling and displacement ellipsoids drawn at the 50% probability level.

**Figure 2**

Crystal structure of the title compound with view along the b-axis. Intermolecular H-bonding interactions are shown as dashed lines.

### Dibenzo[*b,f*][1,4]thiazepin-11-yl-diethyl-amine

#### Crystal data

$C_{17}H_{18}N_2S$

$M_r = 282.40$

Monoclinic,  $P2_1/c$

$a = 12.0137(2) \text{ \AA}$

$b = 8.2257(1) \text{ \AA}$

$c = 15.0513(2) \text{ \AA}$

$\beta = 102.952(1)^\circ$

$V = 1449.54(4) \text{ \AA}^3$

$Z = 4$

$F(000) = 600$

$D_x = 1.294 \text{ Mg m}^{-3}$

Cu  $K\alpha$  radiation,  $\lambda = 1.5418 \text{ \AA}$

Cell parameters from 3716 reflections

$\theta = 3.8\text{--}64.6^\circ$

$\mu = 1.89 \text{ mm}^{-1}$

$T = 150 \text{ K}$

Platelet, colourless

$0.20 \times 0.18 \times 0.03 \text{ mm}$

#### Data collection

Oxford Diffraction XcaliburPX  
diffractometer

Radiation source: Enhance (Cu) X-ray Source

Graphite monochromator

Detector resolution:  $8.1241 \text{ pixels mm}^{-1}$

$\omega$  scans

Absorption correction: multi-scan

(*CrysAlis RED*; Oxford Diffraction, 2006)

$T_{\min} = 0.722$ ,  $T_{\max} = 0.945$

6173 measured reflections

2364 independent reflections

1837 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.019$

$\theta_{\max} = 64.7^\circ$ ,  $\theta_{\min} = 3.8^\circ$

$h = -13 \rightarrow 11$

$k = -9 \rightarrow 9$

$l = -16 \rightarrow 17$

Refinement

|  |  |
|--|--|
| Refinement on $F^2$  | Secondary atom site location: difference Fourier map     |
| Least-squares matrix: full                                     | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.032$                                | H-atom parameters constrained                            |
| $wR(F^2) = 0.086$  | $w = 1/[\sigma^2(F_o^2) + (0.0564P)^2]$                  |
| $S = 1.05$   | where $P = (F_o^2 + 2F_c^2)/3$                           |
| 2364 reflections   | $(\Delta/\sigma)_{\max} < 0.001$                         |
| 181 parameters   | $\Delta\rho_{\max} = 0.23 \text{ e } \text{\AA}^{-3}$    |
| 0 restraints   | $\Delta\rho_{\min} = -0.26 \text{ e } \text{\AA}^{-3}$   |
| Primary atom site location: structure-invariant direct methods |  |

Special details

**Geometry.** All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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  $F^2 > 2\sigma(F^2)$  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 ( $\text{\AA}^2$ )

|     | $x$          | $y$          | $z$          | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|--------------|----------------------------------|
| S1  | 0.83045 (3)  | 0.13292 (5)  | 0.85602 (3)  | 0.01958 (15)                     |
| N1  | 0.67962 (11) | 0.44375 (17) | 0.84814 (9)  | 0.0179 (3)                       |
| N2  | 0.51660 (11) | 0.33602 (17) | 0.87760 (9)  | 0.0181 (3)                       |
| C1  | 0.69759 (13) | 0.2400 (2)   | 0.97172 (11) | 0.0177 (4)                       |
| C2  | 0.78691 (14) | 0.1378 (2)   | 0.96160 (11) | 0.0175 (4)                       |
| C3  | 0.84541 (14) | 0.0447 (2)   | 1.03477 (11) | 0.0198 (4)                       |
| H3  | 0.9047       | -0.0264      | 1.0268       | 0.024*                           |
| C4  | 0.81731 (14) | 0.0556 (2)   | 1.11916 (11) | 0.0211 (4)                       |
| H4  | 0.8564       | -0.0089      | 1.1687       | 0.025*                           |
| C5  | 0.73182 (14) | 0.1613 (2)   | 1.13056 (11) | 0.0211 (4)                       |
| H5  | 0.7137       | 0.1715       | 1.1886       | 0.025*                           |
| C6  | 0.67280 (13) | 0.2522 (2)   | 1.05782 (11) | 0.0197 (4)                       |
| H6  | 0.6143       | 0.3241       | 1.0666       | 0.024*                           |
| C7  | 0.63322 (13) | 0.3418 (2)   | 0.89419 (11) | 0.0169 (4)                       |
| C8  | 0.79782 (14) | 0.4649 (2)   | 0.85930 (11) | 0.0188 (4)                       |
| C9  | 0.87701 (14) | 0.3391 (2)   | 0.85923 (11) | 0.0188 (4)                       |
| C10 | 0.99058 (14) | 0.3727 (2)   | 0.85997 (11) | 0.0237 (4)                       |
| H10 | 1.0430       | 0.2861       | 0.8604       | 0.028*                           |
| C11 | 1.02769 (15) | 0.5322 (2)   | 0.86002 (12) | 0.0290 (5)                       |
| H11 | 1.1051       | 0.5551       | 0.8596       | 0.035*                           |
| C12 | 0.95124 (15) | 0.6578 (2)   | 0.86075 (12) | 0.0280 (5)                       |
| H12 | 0.9767       | 0.7673       | 0.8618       | 0.034*                           |
| C13 | 0.83815 (14) | 0.6251 (2)   | 0.86002 (11) | 0.0218 (4)                       |
| H13 | 0.7867       | 0.7128       | 0.8600       | 0.026*                           |
| C14 | 0.45010 (14) | 0.2064 (2)   | 0.90866 (11) | 0.0200 (4)                       |

|      |              |            |              |            |
|------|--------------|------------|--------------|------------|
| H14A | 0.5032       | 0.1237     | 0.9421       | 0.024*     |
| H14B | 0.4014       | 0.1529     | 0.8548       | 0.024*     |
| C15  | 0.37461 (15) | 0.2692 (2) | 0.97035 (12) | 0.0252 (4) |
| H15A | 0.3324       | 0.1782     | 0.9891       | 0.038*     |
| H15B | 0.3206       | 0.3493     | 0.9371       | 0.038*     |
| H15C | 0.4224       | 0.3203     | 1.0245       | 0.038*     |
| C16  | 0.45022 (14) | 0.4423 (2) | 0.80635 (11) | 0.0188 (4) |
| H16A | 0.4865       | 0.5510     | 0.8112       | 0.023*     |
| H16B | 0.3723       | 0.4555     | 0.8170       | 0.023*     |
| C17  | 0.44140 (14) | 0.3772 (2) | 0.71044 (11) | 0.0209 (4) |
| H17A | 0.3965       | 0.4527     | 0.6661       | 0.031*     |
| H17B | 0.4039       | 0.2707     | 0.7046       | 0.031*     |
| H17C | 0.5181       | 0.3662     | 0.6988       | 0.031*     |

*Atomic displacement parameters (Å<sup>2</sup>)*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$      | $U^{13}$     | $U^{23}$      |
|-----|-------------|-------------|-------------|---------------|--------------|---------------|
| S1  | 0.0205 (2)  | 0.0207 (3)  | 0.0190 (2)  | -0.00074 (18) | 0.00747 (17) | -0.00055 (18) |
| N1  | 0.0153 (7)  | 0.0199 (8)  | 0.0191 (7)  | -0.0019 (6)   | 0.0049 (6)   | -0.0011 (6)   |
| N2  | 0.0153 (7)  | 0.0197 (8)  | 0.0196 (8)  | -0.0014 (6)   | 0.0042 (6)   | 0.0016 (6)    |
| C1  | 0.0148 (8)  | 0.0195 (9)  | 0.0187 (9)  | -0.0059 (7)   | 0.0034 (7)   | -0.0009 (7)   |
| C2  | 0.0163 (9)  | 0.0188 (9)  | 0.0177 (9)  | -0.0058 (7)   | 0.0041 (7)   | -0.0019 (7)   |
| C3  | 0.0170 (9)  | 0.0189 (10) | 0.0232 (9)  | -0.0023 (7)   | 0.0041 (7)   | -0.0009 (8)   |
| C4  | 0.0190 (10) | 0.0234 (10) | 0.0190 (9)  | -0.0051 (8)   | 0.0003 (7)   | 0.0029 (8)    |
| C5  | 0.0192 (9)  | 0.0286 (10) | 0.0156 (9)  | -0.0079 (8)   | 0.0043 (7)   | -0.0029 (7)   |
| C6  | 0.0154 (9)  | 0.0233 (10) | 0.0202 (9)  | -0.0046 (8)   | 0.0035 (7)   | -0.0041 (7)   |
| C7  | 0.0172 (9)  | 0.0175 (9)  | 0.0162 (8)  | 0.0000 (7)    | 0.0043 (7)   | -0.0041 (7)   |
| C8  | 0.0177 (9)  | 0.0232 (10) | 0.0150 (8)  | -0.0038 (7)   | 0.0023 (7)   | -0.0002 (7)   |
| C9  | 0.0190 (9)  | 0.0230 (10) | 0.0144 (8)  | -0.0041 (7)   | 0.0037 (7)   | 0.0013 (7)    |
| C10 | 0.0171 (9)  | 0.0309 (11) | 0.0230 (9)  | 0.0009 (8)    | 0.0044 (7)   | 0.0037 (8)    |
| C11 | 0.0164 (9)  | 0.0389 (12) | 0.0312 (11) | -0.0071 (9)   | 0.0044 (8)   | 0.0044 (9)    |
| C12 | 0.0235 (10) | 0.0276 (11) | 0.0316 (11) | -0.0108 (8)   | 0.0035 (8)   | 0.0012 (9)    |
| C13 | 0.0201 (9)  | 0.0207 (10) | 0.0247 (10) | -0.0018 (8)   | 0.0055 (8)   | -0.0008 (8)   |
| C14 | 0.0177 (9)  | 0.0208 (10) | 0.0211 (9)  | -0.0025 (8)   | 0.0039 (7)   | -0.0011 (8)   |
| C15 | 0.0229 (10) | 0.0295 (11) | 0.0250 (9)  | -0.0061 (8)   | 0.0090 (8)   | 0.0001 (8)    |
| C16 | 0.0159 (9)  | 0.0172 (9)  | 0.0233 (9)  | 0.0016 (7)    | 0.0046 (7)   | 0.0018 (7)    |
| C17 | 0.0182 (9)  | 0.0224 (10) | 0.0214 (9)  | 0.0024 (8)    | 0.0031 (7)   | 0.0020 (7)    |

*Geometric parameters (Å, °)*

|        |             |         |           |
|--------|-------------|---------|-----------|
| S1—C2  | 1.7814 (16) | C9—C10  | 1.390 (2) |
| S1—C9  | 1.7831 (18) | C10—C11 | 1.385 (3) |
| N1—C7  | 1.291 (2)   | C10—H10 | 0.9500    |
| N1—C8  | 1.403 (2)   | C11—C12 | 1.384 (3) |
| N2—C7  | 1.368 (2)   | C11—H11 | 0.9500    |
| N2—C14 | 1.470 (2)   | C12—C13 | 1.383 (2) |
| N2—C16 | 1.472 (2)   | C12—H12 | 0.9500    |
| C1—C6  | 1.397 (2)   | C13—H13 | 0.9500    |

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|             |             |               |             |
|-------------|-------------|---------------|-------------|
| C1—C2       | 1.398 (2)   | C14—C15       | 1.526 (2)   |
| C1—C7       | 1.502 (2)   | C14—H14A      | 0.9900      |
| C2—C3       | 1.395 (2)   | C14—H14B      | 0.9900      |
| C3—C4       | 1.388 (2)   | C15—H15A      | 0.9800      |
| C3—H3       | 0.9500      | C15—H15B      | 0.9800      |
| C4—C5       | 1.385 (2)   | C15—H15C      | 0.9800      |
| C4—H4       | 0.9500      | C16—C17       | 1.521 (2)   |
| C5—C6       | 1.383 (2)   | C16—H16A      | 0.9900      |
| C5—H5       | 0.9500      | C16—H16B      | 0.9900      |
| C6—H6       | 0.9500      | C17—H17A      | 0.9800      |
| C8—C13      | 1.403 (2)   | C17—H17B      | 0.9800      |
| C8—C9       | 1.406 (2)   | C17—H17C      | 0.9800      |
|             |             |               |             |
| C2—S1—C9    | 96.16 (8)   | C9—C10—H10    | 119.9       |
| C7—N1—C8    | 124.28 (14) | C12—C11—C10   | 119.53 (17) |
| C7—N2—C14   | 125.08 (14) | C12—C11—H11   | 120.2       |
| C7—N2—C16   | 118.54 (14) | C10—C11—H11   | 120.2       |
| C14—N2—C16  | 114.71 (13) | C13—C12—C11   | 120.46 (17) |
| C6—C1—C2    | 118.19 (15) | C13—C12—H12   | 119.8       |
| C6—C1—C7    | 120.08 (15) | C11—C12—H12   | 119.8       |
| C2—C1—C7    | 121.64 (14) | C12—C13—C8    | 121.32 (17) |
| C3—C2—C1    | 120.48 (15) | C12—C13—H13   | 119.3       |
| C3—C2—S1    | 119.67 (13) | C8—C13—H13    | 119.3       |
| C1—C2—S1    | 119.79 (13) | N2—C14—C15    | 112.82 (14) |
| C4—C3—C2    | 120.26 (16) | N2—C14—H14A   | 109.0       |
| C4—C3—H3    | 119.9       | C15—C14—H14A  | 109.0       |
| C2—C3—H3    | 119.9       | N2—C14—H14B   | 109.0       |
| C5—C4—C3    | 119.52 (16) | C15—C14—H14B  | 109.0       |
| C5—C4—H4    | 120.2       | H14A—C14—H14B | 107.8       |
| C3—C4—H4    | 120.2       | C14—C15—H15A  | 109.5       |
| C6—C5—C4    | 120.27 (15) | C14—C15—H15B  | 109.5       |
| C6—C5—H5    | 119.9       | H15A—C15—H15B | 109.5       |
| C4—C5—H5    | 119.9       | C14—C15—H15C  | 109.5       |
| C5—C6—C1    | 121.19 (16) | H15A—C15—H15C | 109.5       |
| C5—C6—H6    | 119.4       | H15B—C15—H15C | 109.5       |
| C1—C6—H6    | 119.4       | N2—C16—C17    | 113.16 (14) |
| N1—C7—N2    | 118.19 (15) | N2—C16—H16A   | 108.9       |
| N1—C7—C1    | 124.74 (14) | C17—C16—H16A  | 108.9       |
| N2—C7—C1    | 116.77 (14) | N2—C16—H16B   | 108.9       |
| N1—C8—C13   | 117.10 (16) | C17—C16—H16B  | 108.9       |
| N1—C8—C9    | 125.17 (16) | H16A—C16—H16B | 107.8       |
| C13—C8—C9   | 117.30 (15) | C16—C17—H17A  | 109.5       |
| C10—C9—C8   | 121.12 (16) | C16—C17—H17B  | 109.5       |
| C10—C9—S1   | 119.41 (14) | H17A—C17—H17B | 109.5       |
| C8—C9—S1    | 119.46 (13) | C16—C17—H17C  | 109.5       |
| C11—C10—C9  | 120.26 (17) | H17A—C17—H17C | 109.5       |
| C11—C10—H10 | 119.9       | H17B—C17—H17C | 109.5       |

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*Hydrogen-bond geometry (Å, °)*

Cg is the centroid of the C8–C12 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> |
|--------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C5—H5 $\cdots$ N1 <sup>i</sup> | 0.95        | 2.70                | 3.576 (2)                  | 154                           |
| C4—H4 $\cdots$ Cg <sup>i</sup> | 0.95        | 2.81                | 3.5759 (18)                | 139                           |

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