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# Crystal structure of cafenstrole

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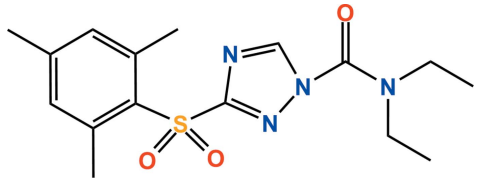
The title compound (systematic name: *N*,*N*-diethyl-3-mesitylsulfonyl-1*H*-1,2,4-triazole-1-carboxamide), $C_{16}H_{22}N_4O_3S$, is a triazole herbicide. The dihedral angle between the planes of the triazole and benzene ring planes is 88.14 (10)°. In the crystal, C—H···O hydrogen bonds and weak C—H···$\pi$ interactions link adjacent molecules, forming one-dimensional chains along the *a* axis.

**Keywords:** crystal structure; cafenstrole; triazole; herbicide,.

**CCDC reference**: 1414616

## 1. Related literature

For information on the herbicidal properties of the title compound, see: Takahashi *et al.* (2001). For related crystal structure, see: Ohkata *et al.* (2002).



## 2. Experimental

### 2.1. Crystal data

$C_{16}H_{22}N_4O_3S$
$M_r$ = 350.43
Monoclinic, $P2_1/c$
$a$ = 7.2800 (3) Å
$b$ = 8.0410 (4) Å
$c$ = 30.1792 (13) Å
$\beta$ = 95.290 (3)°
$V$ = 1759.12 (14) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.21 mm$^{-1}$
$T$ = 173 K
0.36 × 0.30 × 0.02 mm

### 2.2. Data collection

Bruker APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min}$ = 0.929, $T_{max}$ = 0.996
11871 measured reflections
3385 independent reflections
2760 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.118
$S$ = 1.12
3385 reflections
222 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C11—H11···O2$^{i}$ | 0.95 | 2.38 | 3.136 (3) | 136 |
| C7—H7$C$···$Cg1^{ii}$ | 0.98 | 2.80 | 3.561 (3) | 135 |

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

Data collection: *APEX2* (Bruker, 2013); cell refinement: *SAINT* (Bruker, 2013); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2013* (Sheldrick, 2015); molecular graphics: *DIAMOND* (Brandenburg, 2010); software used to prepare material for publication: *SHELXTL* (Sheldrick, 2008).

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: HG5453).

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# supporting information

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## Crystal structure of cafenstrole

**Gihaeng Kang, Jineun Kim, Hyunjin Park and Tae Ho Kim**

### S1. Comment

Cafenstrole, or *N,N*-diethyl-3-mesitylsulfonyl-1*H*-1,2,4-triazole-1-carboxamide, is a triazole herbicide and has been used for rice cultivation which especially inhibits the germination of grass weeds (Takahashi *et al.*, 2001). However, until now its crystal structure has not been reported. In the title compound (Fig. 1), the dihedral angle between the planes of the triazole ring and the phenyl ring planes is 88.14 (10)°. All bond lengths and bond angles are normal and comparable to those observed in similar crystal structure (Ohkata *et al.*, 2002).

In the crystal structure (Fig. 2, Table 1), C11—H11···O2 hydrogen bonds and weak intermolecular C7—H7C···*Cg*1 (*Cg*1 is the centroid of the C1–C6 ring) interactions link adjacent molecules, forming one-dimensional chains along to *a*-axis.

### S2. Experimental

The title compound was purchased from the Dr. Ehrenstorfer GmbH Company. Slow evaporation of a solution in $CH_3CN$ gave single crystals suitable for X-ray analysis.

### S3. Refinement

All H-atoms were positioned geometrically and refined using a riding model with d(C—H) = 0.98 Å, $U_{iso}$ = 1.5$U_{eq}$(C) for methyl group, d(C—H) = 0.99 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for C$sp^3$—H, d(C—H) = 0.95 Å, $U_{iso}$ = 1.2$U_{eq}$(C) for aromatic C—H.

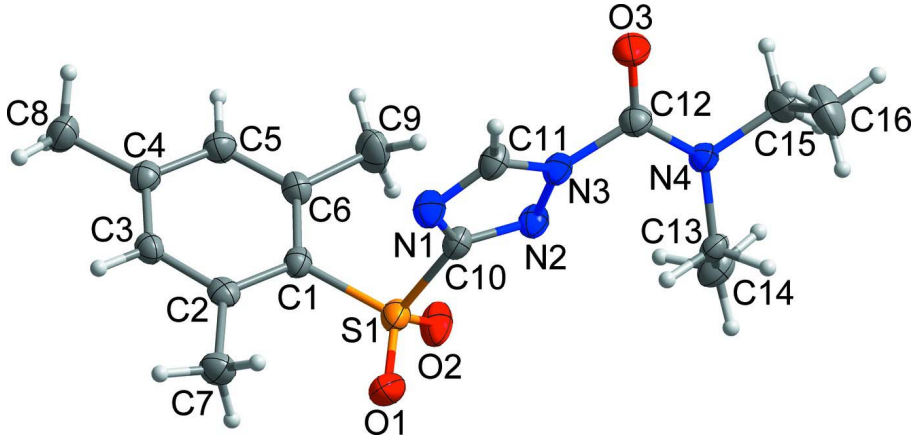


**Figure 1**

The asymmetric unit of the title compound with the atom numbering scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are shown as small spheres of arbitrary radius.

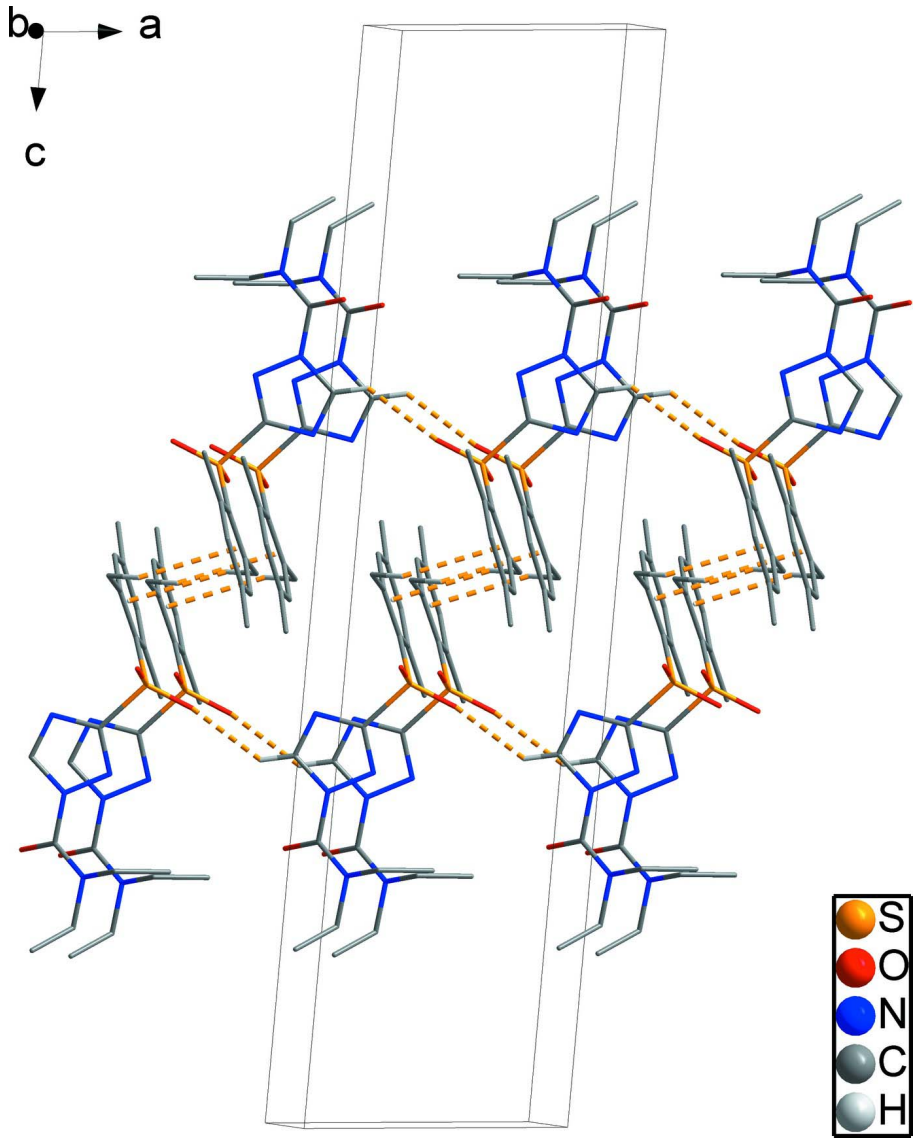


**Figure 2**

Crystal packing viewed along the *b* axis. The intermolecular interactions are shown as dashed lines.

### *N*,*N*-Diethyl-3-mesitylsulfonyl-1*H*-1,2,4-triazole-1-carboxamide

*Crystal data*

$C_{16}H_{22}N_4O_3S$
$M_r = 350.43$
Monoclinic, $P2_1/c$
$a = 7.2800$ (3) Å
$b = 8.0410$ (4) Å
$c = 30.1792$ (13) Å
$\beta = 95.290$ (3)°
$V = 1759.12$ (14) Å$^3$
$Z = 4$
$F(000) = 744$

$D_x = 1.323$ Mg m$^{-3}$
Melting point: 390 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 3608 reflections
$\theta = 2.6$–25.8°
$\mu = 0.21$ mm$^{-1}$
$T = 173$ K
Plate, colourless
0.36 × 0.30 × 0.02 mm

*Data collection*

Bruker APEXII CCD diffractometer
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2013)
$T_{min}$ = 0.929, $T_{max}$ = 0.996
11871 measured reflections
3385 independent reflections
2760 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033
$\theta_{max}$ = 26.0°, $\theta_{min}$ = 1.4°
$h$ = −8→7
$k$ = −9→9
$l$ = −37→37

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.051
$wR(F^2)$ = 0.118
$S$ = 1.12
3385 reflections
222 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0373P)^2 + 1.5378P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.32 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

*Special details*

**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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.41370 (9) | 0.41398 (9) | 0.10060 (2) | 0.03098 (19) |
| O1 | 0.3991 (3) | 0.2440 (2) | 0.08694 (6) | 0.0440 (5) |
| O2 | 0.5862 (2) | 0.4698 (3) | 0.12191 (6) | 0.0426 (5) |
| O3 | −0.0331 (3) | 0.6067 (3) | 0.24940 (6) | 0.0450 (5) |
| N1 | 0.0629 (3) | 0.4287 (3) | 0.12755 (6) | 0.0321 (5) |
| N2 | 0.2960 (3) | 0.4724 (3) | 0.18146 (6) | 0.0280 (5) |
| N3 | 0.1290 (3) | 0.4783 (3) | 0.19847 (6) | 0.0262 (5) |
| N4 | 0.2305 (3) | 0.4731 (3) | 0.27538 (6) | 0.0265 (5) |
| C1 | 0.3372 (3) | 0.5499 (3) | 0.05661 (7) | 0.0243 (5) |
| C2 | 0.2701 (3) | 0.4890 (3) | 0.01447 (7) | 0.0250 (5) |
| C3 | 0.2198 (3) | 0.6048 (3) | −0.01847 (7) | 0.0262 (5) |
| H3 | 0.1760 | 0.5657 | −0.0472 | 0.031* |
| C4 | 0.2303 (3) | 0.7740 (3) | −0.01148 (8) | 0.0275 (6) |
| C5 | 0.2917 (3) | 0.8308 (3) | 0.03064 (8) | 0.0293 (6) |
| H5 | 0.2964 | 0.9472 | 0.0360 | 0.035* |
| C6 | 0.3468 (3) | 0.7227 (3) | 0.06518 (7) | 0.0272 (6) |
| C7 | 0.2494 (4) | 0.3081 (3) | 0.00170 (8) | 0.0348 (6) |
| H7A | 0.1922 | 0.2994 | −0.0289 | 0.052* |
| H7B | 0.1713 | 0.2521 | 0.0219 | 0.052* |
| H7C | 0.3711 | 0.2552 | 0.0038 | 0.052* |
| C8 | 0.1789 (4) | 0.8928 (4) | −0.04883 (8) | 0.0389 (7) |
| H8A | 0.2902 | 0.9482 | −0.0574 | 0.058* |

| | | | | |
|---|---|---|---|---|
| H8B | 0.0931 | 0.9763 | −0.0391 | 0.058* |
| H8C | 0.1199 | 0.8317 | −0.0744 | 0.058* |
| C9 | 0.4143 (4) | 0.7991 (4) | 0.10936 (8) | 0.0456 (8) |
| H9A | 0.5462 | 0.7758 | 0.1159 | 0.068* |
| H9B | 0.3459 | 0.7514 | 0.1328 | 0.068* |
| H9C | 0.3947 | 0.9196 | 0.1081 | 0.068* |
| C10 | 0.2465 (3) | 0.4418 (3) | 0.13928 (7) | 0.0263 (5) |
| C11 | −0.0062 (3) | 0.4550 (3) | 0.16559 (8) | 0.0302 (6) |
| H11 | −0.1343 | 0.4573 | 0.1694 | 0.036* |
| C12 | 0.1025 (3) | 0.5235 (3) | 0.24394 (8) | 0.0293 (6) |
| C13 | 0.3683 (3) | 0.3424 (3) | 0.27089 (8) | 0.0253 (5) |
| H13A | 0.3367 | 0.2817 | 0.2427 | 0.030* |
| H13B | 0.3635 | 0.2621 | 0.2956 | 0.030* |
| C14 | 0.5623 (3) | 0.4096 (4) | 0.27125 (9) | 0.0364 (6) |
| H14A | 0.5731 | 0.4752 | 0.2443 | 0.055* |
| H14B | 0.6499 | 0.3169 | 0.2723 | 0.055* |
| H14C | 0.5896 | 0.4803 | 0.2975 | 0.055* |
| C15 | 0.2014 (4) | 0.5244 (4) | 0.32107 (8) | 0.0371 (7) |
| H15A | 0.1512 | 0.6389 | 0.3205 | 0.045* |
| H15B | 0.3214 | 0.5253 | 0.3394 | 0.045* |
| C16 | 0.0700 (4) | 0.4095 (5) | 0.34227 (9) | 0.0528 (9) |
| H16A | −0.0498 | 0.4096 | 0.3245 | 0.079* |
| H16B | 0.0542 | 0.4480 | 0.3725 | 0.079* |
| H16C | 0.1204 | 0.2964 | 0.3435 | 0.079* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0289 (4) | 0.0379 (4) | 0.0261 (3) | 0.0080 (3) | 0.0024 (2) | 0.0056 (3) |
| O1 | 0.0604 (13) | 0.0328 (11) | 0.0394 (10) | 0.0158 (10) | 0.0082 (9) | 0.0063 (9) |
| O2 | 0.0237 (10) | 0.0704 (15) | 0.0327 (9) | 0.0075 (10) | −0.0024 (7) | 0.0098 (10) |
| O3 | 0.0377 (11) | 0.0587 (14) | 0.0388 (10) | 0.0233 (10) | 0.0043 (8) | 0.0019 (10) |
| N1 | 0.0265 (11) | 0.0399 (14) | 0.0290 (10) | −0.0012 (10) | −0.0020 (9) | 0.0017 (10) |
| N2 | 0.0220 (11) | 0.0345 (12) | 0.0275 (10) | 0.0021 (9) | 0.0020 (8) | 0.0046 (10) |
| N3 | 0.0213 (11) | 0.0306 (12) | 0.0264 (10) | 0.0019 (9) | 0.0000 (8) | 0.0035 (9) |
| N4 | 0.0290 (11) | 0.0244 (11) | 0.0251 (10) | 0.0033 (9) | −0.0031 (8) | −0.0011 (9) |
| C1 | 0.0214 (12) | 0.0284 (13) | 0.0230 (11) | 0.0013 (11) | 0.0018 (9) | 0.0029 (11) |
| C2 | 0.0173 (12) | 0.0319 (14) | 0.0261 (11) | −0.0003 (10) | 0.0037 (9) | −0.0022 (11) |
| C3 | 0.0241 (12) | 0.0326 (14) | 0.0215 (11) | 0.0007 (11) | 0.0003 (9) | −0.0030 (11) |
| C4 | 0.0233 (13) | 0.0316 (14) | 0.0276 (12) | 0.0018 (11) | 0.0026 (10) | 0.0034 (11) |
| C5 | 0.0321 (14) | 0.0252 (13) | 0.0309 (12) | −0.0004 (11) | 0.0043 (11) | −0.0005 (11) |
| C6 | 0.0272 (13) | 0.0318 (14) | 0.0226 (11) | −0.0017 (11) | 0.0016 (10) | −0.0004 (11) |
| C7 | 0.0390 (16) | 0.0295 (15) | 0.0353 (13) | 0.0013 (13) | 0.0002 (11) | −0.0050 (12) |
| C8 | 0.0479 (17) | 0.0350 (16) | 0.0328 (13) | 0.0050 (14) | −0.0023 (12) | 0.0057 (13) |
| C9 | 0.066 (2) | 0.0384 (17) | 0.0306 (14) | −0.0064 (16) | −0.0051 (13) | −0.0052 (13) |
| C10 | 0.0267 (13) | 0.0270 (13) | 0.0246 (11) | 0.0018 (11) | −0.0011 (10) | 0.0046 (11) |
| C11 | 0.0256 (13) | 0.0338 (15) | 0.0299 (12) | 0.0007 (11) | −0.0034 (10) | 0.0067 (12) |
| C12 | 0.0253 (14) | 0.0319 (14) | 0.0306 (13) | 0.0029 (12) | 0.0022 (10) | 0.0014 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C13 | 0.0276 (13) | 0.0210 (12) | 0.0265 (11) | 0.0040 (10) | −0.0014 (10) | 0.0047 (10) |
| C14 | 0.0278 (14) | 0.0360 (15) | 0.0441 (15) | −0.0003 (12) | −0.0026 (11) | 0.0088 (13) |
| C15 | 0.0461 (17) | 0.0354 (15) | 0.0281 (13) | 0.0066 (13) | −0.0057 (12) | −0.0099 (12) |
| C16 | 0.0481 (18) | 0.083 (3) | 0.0285 (13) | −0.0110 (18) | 0.0087 (13) | −0.0122 (16) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—O1 | 1.429 (2) | C6—C9 | 1.509 (3) |
| S1—O2 | 1.4293 (19) | C7—H7A | 0.9800 |
| S1—C1 | 1.769 (2) | C7—H7B | 0.9800 |
| S1—C10 | 1.777 (2) | C7—H7C | 0.9800 |
| O3—C12 | 1.216 (3) | C8—H8A | 0.9800 |
| N1—C11 | 1.313 (3) | C8—H8B | 0.9800 |
| N1—C10 | 1.355 (3) | C8—H8C | 0.9800 |
| N2—C10 | 1.314 (3) | C9—H9A | 0.9800 |
| N2—N3 | 1.364 (3) | C9—H9B | 0.9800 |
| N3—C11 | 1.345 (3) | C9—H9C | 0.9800 |
| N3—C12 | 1.450 (3) | C11—H11 | 0.9500 |
| N4—C12 | 1.331 (3) | C13—C14 | 1.511 (3) |
| N4—C13 | 1.468 (3) | C13—H13A | 0.9900 |
| N4—C15 | 1.473 (3) | C13—H13B | 0.9900 |
| C1—C2 | 1.408 (3) | C14—H14A | 0.9800 |
| C1—C6 | 1.414 (4) | C14—H14B | 0.9800 |
| C2—C3 | 1.387 (3) | C14—H14C | 0.9800 |
| C2—C7 | 1.509 (3) | C15—C16 | 1.513 (4) |
| C3—C4 | 1.378 (4) | C15—H15A | 0.9900 |
| C3—H3 | 0.9500 | C15—H15B | 0.9900 |
| C4—C5 | 1.385 (3) | C16—H16A | 0.9800 |
| C4—C8 | 1.499 (3) | C16—H16B | 0.9800 |
| C5—C6 | 1.387 (3) | C16—H16C | 0.9800 |
| C5—H5 | 0.9500 | | |

| | | | |
|---|---|---|---|
| O1—S1—O2 | 118.01 (13) | H8A—C8—H8C | 109.5 |
| O1—S1—C1 | 111.37 (11) | H8B—C8—H8C | 109.5 |
| O2—S1—C1 | 110.25 (12) | C6—C9—H9A | 109.5 |
| O1—S1—C10 | 105.83 (12) | C6—C9—H9B | 109.5 |
| O2—S1—C10 | 106.94 (11) | H9A—C9—H9B | 109.5 |
| C1—S1—C10 | 103.17 (11) | C6—C9—H9C | 109.5 |
| C11—N1—C10 | 101.98 (19) | H9A—C9—H9C | 109.5 |
| C10—N2—N3 | 101.33 (18) | H9B—C9—H9C | 109.5 |
| C11—N3—N2 | 109.55 (19) | N2—C10—N1 | 116.4 (2) |
| C11—N3—C12 | 125.5 (2) | N2—C10—S1 | 121.10 (18) |
| N2—N3—C12 | 124.48 (19) | N1—C10—S1 | 122.51 (17) |
| C12—N4—C13 | 126.3 (2) | N1—C11—N3 | 110.7 (2) |
| C12—N4—C15 | 115.5 (2) | N1—C11—H11 | 124.6 |
| C13—N4—C15 | 116.46 (19) | N3—C11—H11 | 124.6 |
| C2—C1—C6 | 120.9 (2) | O3—C12—N4 | 126.5 (2) |
| C2—C1—S1 | 121.47 (19) | O3—C12—N3 | 116.5 (2) |

| | | | |
|---|---|---|---|
| C6—C1—S1 | 117.58 (17) | N4—C12—N3 | 116.9 (2) |
| C3—C2—C1 | 117.4 (2) | N4—C13—C14 | 112.9 (2) |
| C3—C2—C7 | 116.8 (2) | N4—C13—H13A | 109.0 |
| C1—C2—C7 | 125.8 (2) | C14—C13—H13A | 109.0 |
| C4—C3—C2 | 123.1 (2) | N4—C13—H13B | 109.0 |
| C4—C3—H3 | 118.4 | C14—C13—H13B | 109.0 |
| C2—C3—H3 | 118.4 | H13A—C13—H13B | 107.8 |
| C3—C4—C5 | 118.3 (2) | C13—C14—H14A | 109.5 |
| C3—C4—C8 | 120.5 (2) | C13—C14—H14B | 109.5 |
| C5—C4—C8 | 121.1 (2) | H14A—C14—H14B | 109.5 |
| C4—C5—C6 | 122.0 (2) | C13—C14—H14C | 109.5 |
| C4—C5—H5 | 119.0 | H14A—C14—H14C | 109.5 |
| C6—C5—H5 | 119.0 | H14B—C14—H14C | 109.5 |
| C5—C6—C1 | 118.2 (2) | N4—C15—C16 | 112.1 (2) |
| C5—C6—C9 | 117.2 (2) | N4—C15—H15A | 109.2 |
| C1—C6—C9 | 124.6 (2) | C16—C15—H15A | 109.2 |
| C2—C7—H7A | 109.5 | N4—C15—H15B | 109.2 |
| C2—C7—H7B | 109.5 | C16—C15—H15B | 109.2 |
| H7A—C7—H7B | 109.5 | H15A—C15—H15B | 107.9 |
| C2—C7—H7C | 109.5 | C15—C16—H16A | 109.5 |
| H7A—C7—H7C | 109.5 | C15—C16—H16B | 109.5 |
| H7B—C7—H7C | 109.5 | H16A—C16—H16B | 109.5 |
| C4—C8—H8A | 109.5 | C15—C16—H16C | 109.5 |
| C4—C8—H8B | 109.5 | H16A—C16—H16C | 109.5 |
| H8A—C8—H8B | 109.5 | H16B—C16—H16C | 109.5 |
| C4—C8—H8C | 109.5 | | |

| | | | |
|---|---|---|---|
| C10—N2—N3—C11 | −1.4 (3) | N3—N2—C10—S1 | −177.87 (17) |
| C10—N2—N3—C12 | −174.3 (2) | C11—N1—C10—N2 | 0.7 (3) |
| O1—S1—C1—C2 | 0.7 (2) | C11—N1—C10—S1 | 178.95 (19) |
| O2—S1—C1—C2 | 133.7 (2) | O1—S1—C10—N2 | 113.2 (2) |
| C10—S1—C1—C2 | −112.4 (2) | O2—S1—C10—N2 | −13.4 (2) |
| O1—S1—C1—C6 | −178.97 (18) | C1—S1—C10—N2 | −129.7 (2) |
| O2—S1—C1—C6 | −46.0 (2) | O1—S1—C10—N1 | −65.0 (2) |
| C10—S1—C1—C6 | 67.9 (2) | O2—S1—C10—N1 | 168.3 (2) |
| C6—C1—C2—C3 | 2.1 (3) | C1—S1—C10—N1 | 52.1 (2) |
| S1—C1—C2—C3 | −177.58 (17) | C10—N1—C11—N3 | −1.5 (3) |
| C6—C1—C2—C7 | −178.5 (2) | N2—N3—C11—N1 | 2.0 (3) |
| S1—C1—C2—C7 | 1.8 (3) | C12—N3—C11—N1 | 174.8 (2) |
| C1—C2—C3—C4 | −1.0 (4) | C13—N4—C12—O3 | 164.5 (3) |
| C7—C2—C3—C4 | 179.6 (2) | C15—N4—C12—O3 | 0.2 (4) |
| C2—C3—C4—C5 | −0.9 (4) | C13—N4—C12—N3 | −17.0 (4) |
| C2—C3—C4—C8 | 178.2 (2) | C15—N4—C12—N3 | 178.7 (2) |
| C3—C4—C5—C6 | 1.7 (4) | C11—N3—C12—O3 | −29.9 (4) |
| C8—C4—C5—C6 | −177.4 (2) | N2—N3—C12—O3 | 141.9 (3) |
| C4—C5—C6—C1 | −0.6 (4) | C11—N3—C12—N4 | 151.5 (2) |
| C4—C5—C6—C9 | 178.9 (2) | N2—N3—C12—N4 | −36.8 (3) |
| C2—C1—C6—C5 | −1.3 (4) | C12—N4—C13—C14 | 110.4 (3) |

| | | | |
|---|---|---|---|
| S1—C1—C6—C5 | 178.35 (18) | C15—N4—C13—C14 | −85.5 (3) |
| C2—C1—C6—C9 | 179.2 (2) | C12—N4—C15—C16 | 82.9 (3) |
| S1—C1—C6—C9 | −1.2 (3) | C13—N4—C15—C16 | −83.0 (3) |
| N3—N2—C10—N1 | 0.4 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11···O2$^{i}$ | 0.95 | 2.38 | 3.136 (3) | 136 |
| C7—H7*C*···*Cg*1$^{ii}$ | 0.98 | 2.80 | 3.561 (3) | 135 |

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