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# Crystal structure of diethyl 2-[(2-sulfanylquinolin-3-yl)methylidene]malonate

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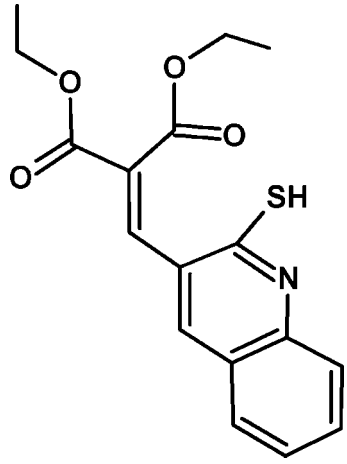
In the title compound, $C_{17}H_{17}NO_4S$, the quinoline ring system is nearly planar, with a maximum deviation of 0.0496 (16) Å. A weak intramolecular C—H···O interaction is observed. In the crystal, C—H···O, S—H···N and $\pi$–$\pi$ stacking interactions between the fused benzene ring of quinoline and the pyridine moieties [shortest centroid–centroid distance = 3.6754 (11) Å] are observed. Inversion-related weak C—H···O intermolecular interactions diagonally along [010], with $R_2^2(10)$ ring motifs, and S—H···N intermolecular interactions diagonally along [100], with $R_2^2(8)$ ring motifs, are present, forming a three-dimensional network structure. No classical hydrogen bonds are observed.

**Keywords:** crystal structure; diester; quinoline; malonate; intermolecular interactions.

**CCDC reference**: 1413116

## 1. Related literature

For biological applications of quinolines, see: Nandeshwarappa *et al.*(2006); Noda *et al.* (2001); Pandey *et al.* (2004); Sharma *et al.* (2008).




## 2. Experimental

### 2.1. Crystal data

$C_{17}H_{17}NO_4S$
$M_r$ = 331.37
Triclinic, $P\overline{1}$
$a$ = 7.3739 (4) Å
$b$ = 7.8148 (4) Å
$c$ = 15.8149 (7) Å
$\alpha$ = 90.158 (2)°
$\beta$ = 99.486 (2)°
$\gamma$ = 113.301 (2)°
$V$ = 823.24 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.22 mm$^{-1}$
$T$ = 296 K
0.24 × 0.20 × 0.12 mm

### 2.2. Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min}$ = 0.770, $T_{max}$ = 1.000
21213 measured reflections
5853 independent reflections
4295 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.025

### 2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.062
$wR(F^2)$ = 0.213
$S$ = 1.04
5853 reflections
234 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.98 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.48 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| S1—H1···N6$^{i}$ | 1.20 | 2.37 | 3.3389 (14) | 136 |
| C9—H9···O4 | 0.99 (3) | 2.41 (3) | 3.122 (2) | 129 (2) |
| C22—H22$B$···O2$^{ii}$ | 0.97 | 2.52 | 3.438 (4) | 158 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT* (Bruker, 2001); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS2014* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *SHELXL2014*.

## Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: JJ2194).

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# supporting information

*Acta Cryst.* (2015). E**71**, o594–o595 [https://doi.org/10.1107/S2056989015013596]

## Crystal structure of diethyl 2-[(2-sulfanylquinolin-3-yl)methylidene]malonate

**Rihanabanu, B. R. Anitha, T. G. Meenakshi, K. Mahesh Kumar and H. C. Devarajegowda**

### S1. Comment

Quinolines are a heterocyclic class of organic compounds containing a pyridine ring fused with benzene found in nature mainly in plants. Alkaloid quinine is a traditional anti-malarial drug also used in tonics. The quinoline skeleton has since been used as a basis for design of many synthetic anti-malarial compounds, of which chloroquinoline is one such example. Despite its relatively low efficacy and tolerability, quinine still plays an important role in the treatment of multi resistant malaria (Nandeshwarappa *et al.*2006). It has also played a historical role in organic chemistry as a target for structural determination and total synthesis reactions (Sharma *et al.*2008), as well as stereo selective (Noda *et al.*2001) and *enantio* selective (Pande *et al.*, 2004) total synthesis reactions. The chemistry of quinoline has gained increasing attention due to its various diverse pharmacological activities. We report herin the crystal structure of a new quinoline derivative, diethyl 2-((2-mercaptoquinolin-3-yl) methylene)malonate, $C_{17}H_{17}N\ O_4S$, (I) (Fig. 1).

In the asymmetric unit of (I), the quinoline ring system is nearly planar, with a maximum deviation of 0.0496 (16) Å for atom C8. In the crystal, weak intramolecular C—H···O, intermolecular C—H···O, S—H···N (Table 1) and $\pi$–$\pi$ stacking interactions between the fused benzene ring of quinoline, Cg(2) [C10—C15], and pyridine, Cg(1) [N6//C7–C11], [shortest centroid–centroid distance = 3.6751 (11) Å] are observed. Inversion related weak C—H···O intermolecular interactions diagonally along [010] with $R_2^2(10)$ ring motifs and S—H···N intermolecular interactions diagonally along [100] with $R_2^2(8)$ ring motifs are present forming a three-dimensional network structure (Fig. 2). No classical hydrogen bonds are observed.

### S2. Experimental

All the chemicals of analytical reagent grade were used directly without further purification. An equimolar quantity of 2-mercapto-3-formyl quinoline (0.01 mm) and diethylmalonate (0.001mm) were refluxed for 24 hr in acetonitrile at 353 K. After completion of the reaction the solvent was removed from the vacuue and recrystalized from ethanol. Yellow needles of the title compound were grown from ethanol solution by slow evaporation at room temperature. Colour: Yellow. Yield= 82%, m.p.:458 K.

### S3. Refinement

All H atoms were positioned geometrically, with S—H = 1.2 Å, C—H = 0.93 Å for aromatic H, C—H = 0.97 Å for methylene H and C—H = 0.96 Å for methyl H,and refined using a riding model with $U_{iso}$(H) = 1.5$U_{eq}$(C) for methyl H and $U_{iso}$(H) = 1.2$U_{eq}$(C) for all other H.

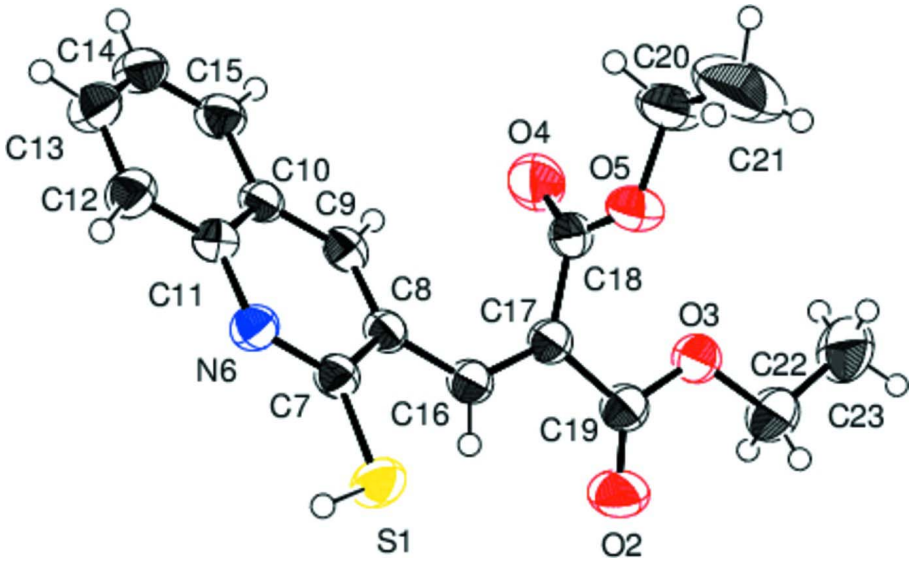


**Figure 1**

ORTEP diagram of the title compound, $C_{17}H_{17}N\ O_4S$. Displacement ellipsoids are drawn at the 50% probability level. Hydrogen atoms are shown as spheres of arbitrary radius.

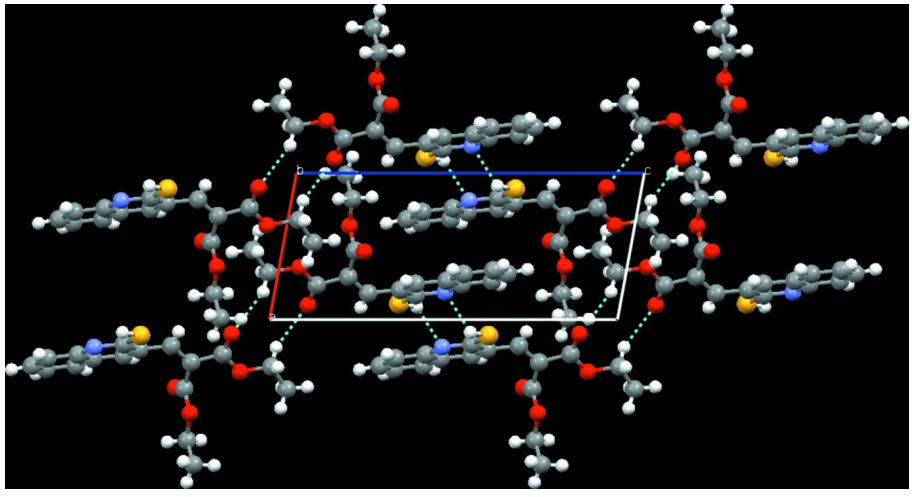

**Figure 2**

A view of the packing in the title molecule, $C_{17}H_{17}N\ O_4S$, along the *a* axis. Dashed lines indicate weak C—H···O and S—H···N intermolecular interactions with inversio- related C—H···O intermolecular interactions diagonally along [010] with $R_2^2(10)$ ring motifs and S—H···N intermolecular interactions diagonally along [100] with $R_2^2(8)$ ring motifs forming a three-dimensional network structure.

## Diethyl 2-[(2-sulfanylquinolin-3-yl)methylidene]malonate

*Crystal data*

$C_{17}H_{17}NO_4S$
$M_r = 331.37$
Triclinic, $P\overline{1}$
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$c = 15.8149\ (7)$ Å
$\alpha = 90.158\ (2)°$
$\beta = 99.486\ (2)°$
$\gamma = 113.301\ (2)°$
$V = 823.24\ (7)$ Å$^3$

$Z = 2$
$F(000) = 348$
$D_x = 1.337$ Mg m$^{-3}$
Melting point: 458 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5853 reflections
$\theta = 2.6$–$32.5°$
$\mu = 0.22$ mm$^{-1}$
$T = 296$ K
Plate, yellow
0.24 × 0.20 × 0.12 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 10.0 pixels mm$^{-1}$
$\omega$ and $\varphi$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 2007)
$T_{min} = 0.770$, $T_{max} = 1.000$
21213 measured reflections
5853 independent reflections
4295 reflections with $I > 2\sigma(I)$
$R_{int} = 0.025$
$\theta_{max} = 32.5°$, $\theta_{min} = 2.6°$
$h = -11 \rightarrow 10$
$k = -11 \rightarrow 11$
$l = -23 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.062$
$wR(F^2) = 0.213$
$S = 1.04$
5853 reflections
234 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.1265P)^2 + 0.1563P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.98$ e Å$^{-3}$
$\Delta\rho_{min} = -0.48$ 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.89170 (8) | 0.93555 (6) | 0.36268 (3) | 0.05361 (17) |
| H1 | 0.9130 | 1.0542 | 0.4163 | 0.080* |
| O2 | 0.9018 (3) | 0.6179 (2) | 0.10198 (11) | 0.0741 (5) |
| O3 | 0.6426 (2) | 0.3469 (2) | 0.05791 (8) | 0.0546 (3) |
| O4 | 0.5360 (3) | 0.1266 (2) | 0.23539 (12) | 0.0772 (5) |
| O5 | 0.3614 (2) | 0.2881 (2) | 0.17989 (10) | 0.0584 (4) |
| N6 | 0.8126 (2) | 0.71751 (18) | 0.48999 (9) | 0.0417 (3) |
| C7 | 0.8326 (2) | 0.7292 (2) | 0.40651 (10) | 0.0380 (3) |
| C8 | 0.7963 (2) | 0.5561 (2) | 0.35911 (10) | 0.0370 (3) |
| C9 | 0.7551 (2) | 0.3953 (2) | 0.40069 (10) | 0.0398 (3) |
| C10 | 0.7342 (2) | 0.3901 (2) | 0.48846 (10) | 0.0383 (3) |
| C11 | 0.7609 (2) | 0.5567 (2) | 0.53269 (10) | 0.0388 (3) |
| C12 | 0.7363 (3) | 0.5596 (3) | 0.61848 (11) | 0.0491 (4) |
| C13 | 0.6855 (3) | 0.3962 (3) | 0.65909 (13) | 0.0552 (4) |
| C14 | 0.6621 (3) | 0.2299 (3) | 0.61664 (14) | 0.0555 (5) |

| | | | | |
|---|---|---|---|---|
| C15 | 0.6872 (3) | 0.2268 (2) | 0.53337 (13) | 0.0480 (4) |
| C16 | 0.8203 (2) | 0.5658 (2) | 0.26908 (10) | 0.0409 (3) |
| C17 | 0.7083 (2) | 0.4422 (2) | 0.20334 (10) | 0.0408 (3) |
| C18 | 0.5287 (3) | 0.2679 (2) | 0.20902 (10) | 0.0452 (4) |
| C19 | 0.7642 (3) | 0.4825 (3) | 0.11661 (11) | 0.0480 (4) |
| C20 | 0.1759 (3) | 0.1201 (4) | 0.17362 (19) | 0.0786 (7) |
| H20A | 0.1767 | 0.0250 | 0.1343 | 0.094* |
| H20B | 0.1638 | 0.0706 | 0.2296 | 0.094* |
| C21 | 0.0112 (5) | 0.1699 (7) | 0.1429 (4) | 0.153 (2) |
| H21A | 0.0306 | 0.2843 | 0.1731 | 0.229* |
| H21B | −0.1114 | 0.0724 | 0.1525 | 0.229* |
| H21C | 0.0038 | 0.1864 | 0.0825 | 0.229* |
| C22 | 0.6792 (4) | 0.3723 (4) | −0.03002 (13) | 0.0671 (6) |
| H22A | 0.6744 | 0.4891 | −0.0482 | 0.081* |
| H22B | 0.8109 | 0.3761 | −0.0333 | 0.081* |
| C23 | 0.5247 (5) | 0.2163 (5) | −0.08543 (16) | 0.0886 (9) |
| H23A | 0.5372 | 0.1023 | −0.0698 | 0.133* |
| H23B | 0.5403 | 0.2350 | −0.1442 | 0.133* |
| H23C | 0.3946 | 0.2086 | −0.0788 | 0.133* |
| H9 | 0.737 (4) | 0.276 (4) | 0.3721 (18) | 0.066 (7)* |
| H12 | 0.762 (4) | 0.689 (4) | 0.6437 (17) | 0.063 (7)* |
| H13 | 0.658 (4) | 0.395 (4) | 0.715 (2) | 0.079 (8)* |
| H14 | 0.628 (5) | 0.139 (5) | 0.643 (2) | 0.081 (9)* |
| H15 | 0.659 (4) | 0.107 (4) | 0.5002 (17) | 0.067 (7)* |
| H16 | 0.917 (3) | 0.662 (3) | 0.2553 (14) | 0.044 (5)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0738 (3) | 0.0359 (2) | 0.0479 (3) | 0.0171 (2) | 0.0148 (2) | 0.00743 (17) |
| O2 | 0.0679 (9) | 0.0726 (10) | 0.0589 (8) | −0.0024 (8) | 0.0283 (7) | −0.0006 (7) |
| O3 | 0.0549 (7) | 0.0603 (8) | 0.0379 (6) | 0.0098 (6) | 0.0140 (5) | −0.0042 (5) |
| O4 | 0.0872 (12) | 0.0437 (7) | 0.0777 (11) | 0.0108 (7) | −0.0076 (9) | 0.0067 (7) |
| O5 | 0.0415 (6) | 0.0578 (8) | 0.0658 (8) | 0.0070 (5) | 0.0153 (6) | 0.0071 (6) |
| N6 | 0.0510 (7) | 0.0334 (6) | 0.0386 (6) | 0.0135 (5) | 0.0112 (5) | 0.0010 (5) |
| C7 | 0.0385 (7) | 0.0340 (6) | 0.0382 (7) | 0.0113 (5) | 0.0064 (5) | 0.0000 (5) |
| C8 | 0.0334 (6) | 0.0358 (6) | 0.0370 (6) | 0.0097 (5) | 0.0042 (5) | −0.0023 (5) |
| C9 | 0.0377 (7) | 0.0339 (6) | 0.0426 (7) | 0.0109 (5) | 0.0021 (5) | −0.0043 (5) |
| C10 | 0.0329 (6) | 0.0341 (6) | 0.0424 (7) | 0.0089 (5) | 0.0037 (5) | 0.0026 (5) |
| C11 | 0.0365 (7) | 0.0365 (7) | 0.0400 (7) | 0.0107 (5) | 0.0080 (5) | 0.0040 (5) |
| C12 | 0.0539 (9) | 0.0499 (9) | 0.0425 (8) | 0.0176 (7) | 0.0146 (7) | 0.0047 (7) |
| C13 | 0.0530 (10) | 0.0634 (11) | 0.0481 (9) | 0.0188 (8) | 0.0174 (8) | 0.0153 (8) |
| C14 | 0.0499 (9) | 0.0497 (10) | 0.0597 (11) | 0.0121 (7) | 0.0108 (8) | 0.0200 (8) |
| C15 | 0.0440 (8) | 0.0370 (7) | 0.0558 (9) | 0.0104 (6) | 0.0049 (7) | 0.0077 (7) |
| C16 | 0.0379 (7) | 0.0400 (7) | 0.0408 (7) | 0.0112 (6) | 0.0082 (6) | −0.0002 (6) |
| C17 | 0.0396 (7) | 0.0429 (7) | 0.0370 (7) | 0.0128 (6) | 0.0090 (5) | 0.0005 (6) |
| C18 | 0.0496 (8) | 0.0419 (8) | 0.0340 (7) | 0.0084 (6) | 0.0062 (6) | −0.0028 (6) |
| C19 | 0.0449 (8) | 0.0536 (9) | 0.0419 (8) | 0.0142 (7) | 0.0128 (6) | 0.0002 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C20 | 0.0509 (11) | 0.0720 (15) | 0.0844 (16) | −0.0077 (10) | 0.0189 (11) | 0.0015 (12) |
| C21 | 0.0525 (17) | 0.125 (3) | 0.240 (6) | 0.0057 (18) | −0.007 (2) | 0.052 (4) |
| C22 | 0.0709 (13) | 0.0810 (15) | 0.0411 (9) | 0.0172 (11) | 0.0226 (9) | 0.0020 (9) |
| C23 | 0.115 (2) | 0.0886 (19) | 0.0448 (11) | 0.0240 (17) | 0.0127 (12) | −0.0065 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C7 | 1.6796 (16) | C13—H13 | 0.94 (3) |
| S1—H1 | 1.2000 | C14—C15 | 1.361 (3) |
| O2—C19 | 1.197 (2) | C14—H14 | 0.80 (3) |
| O3—C19 | 1.326 (2) | C15—H15 | 1.00 (3) |
| O3—C22 | 1.459 (2) | C16—C17 | 1.333 (2) |
| O4—C18 | 1.199 (2) | C16—H16 | 0.86 (2) |
| O5—C18 | 1.314 (2) | C17—C18 | 1.494 (2) |
| O5—C20 | 1.462 (3) | C17—C19 | 1.495 (2) |
| N6—C7 | 1.352 (2) | C20—C21 | 1.429 (5) |
| N6—C11 | 1.375 (2) | C20—H20A | 0.9700 |
| C7—C8 | 1.451 (2) | C20—H20B | 0.9700 |
| C8—C9 | 1.369 (2) | C21—H21A | 0.9600 |
| C8—C16 | 1.462 (2) | C21—H21B | 0.9600 |
| C9—C10 | 1.421 (2) | C21—H21C | 0.9600 |
| C9—H9 | 0.99 (3) | C22—C23 | 1.456 (4) |
| C10—C11 | 1.403 (2) | C22—H22A | 0.9700 |
| C10—C15 | 1.411 (2) | C22—H22B | 0.9700 |
| C11—C12 | 1.399 (2) | C23—H23A | 0.9600 |
| C12—C13 | 1.374 (3) | C23—H23B | 0.9600 |
| C12—H12 | 1.02 (3) | C23—H23C | 0.9600 |
| C13—C14 | 1.396 (3) | | |

| | | | |
|---|---|---|---|
| C7—S1—H1 | 109.5 | C16—C17—C18 | 125.18 (14) |
| C19—O3—C22 | 116.21 (16) | C16—C17—C19 | 117.59 (15) |
| C18—O5—C20 | 116.10 (19) | C18—C17—C19 | 117.22 (14) |
| C7—N6—C11 | 125.49 (13) | O4—C18—O5 | 124.31 (18) |
| N6—C7—C8 | 116.36 (14) | O4—C18—C17 | 124.41 (18) |
| N6—C7—S1 | 119.98 (11) | O5—C18—C17 | 111.27 (15) |
| C8—C7—S1 | 123.65 (12) | O2—C19—O3 | 124.24 (16) |
| C9—C8—C7 | 119.72 (14) | O2—C19—C17 | 124.71 (17) |
| C9—C8—C16 | 122.79 (14) | O3—C19—C17 | 111.04 (15) |
| C7—C8—C16 | 117.33 (14) | C21—C20—O5 | 108.0 (3) |
| C8—C9—C10 | 121.62 (14) | C21—C20—H20A | 110.1 |
| C8—C9—H9 | 122.7 (16) | O5—C20—H20A | 110.1 |
| C10—C9—H9 | 115.7 (16) | C21—C20—H20B | 110.1 |
| C11—C10—C15 | 118.31 (15) | O5—C20—H20B | 110.1 |
| C11—C10—C9 | 118.09 (14) | H20A—C20—H20B | 108.4 |
| C15—C10—C9 | 123.61 (15) | C20—C21—H21A | 109.5 |
| N6—C11—C12 | 120.63 (14) | C20—C21—H21B | 109.5 |
| N6—C11—C10 | 118.56 (14) | H21A—C21—H21B | 109.5 |
| C12—C11—C10 | 120.81 (15) | C20—C21—H21C | 109.5 |

| | | | |
|---|---|---|---|
| C13—C12—C11 | 118.92 (17) | H21A—C21—H21C | 109.5 |
| C13—C12—H12 | 127.7 (14) | H21B—C21—H21C | 109.5 |
| C11—C12—H12 | 113.3 (14) | C23—C22—O3 | 108.17 (19) |
| C12—C13—C14 | 121.07 (18) | C23—C22—H22A | 110.1 |
| C12—C13—H13 | 119.0 (18) | O3—C22—H22A | 110.1 |
| C14—C13—H13 | 119.8 (18) | C23—C22—H22B | 110.1 |
| C15—C14—C13 | 120.20 (17) | O3—C22—H22B | 110.1 |
| C15—C14—H14 | 124 (2) | H22A—C22—H22B | 108.4 |
| C13—C14—H14 | 116 (2) | C22—C23—H23A | 109.5 |
| C14—C15—C10 | 120.66 (17) | C22—C23—H23B | 109.5 |
| C14—C15—H15 | 121.4 (15) | H23A—C23—H23B | 109.5 |
| C10—C15—H15 | 117.6 (15) | C22—C23—H23C | 109.5 |
| C17—C16—C8 | 127.50 (15) | H23A—C23—H23C | 109.5 |
| C17—C16—H16 | 114.3 (14) | H23B—C23—H23C | 109.5 |
| C8—C16—H16 | 118.2 (14) | | |

| | | | |
|---|---|---|---|
| C11—N6—C7—C8 | −0.1 (2) | C11—C10—C15—C14 | 2.2 (2) |
| C11—N6—C7—S1 | 178.63 (13) | C9—C10—C15—C14 | −177.58 (16) |
| N6—C7—C8—C9 | −3.4 (2) | C9—C8—C16—C17 | 42.8 (3) |
| S1—C7—C8—C9 | 177.93 (12) | C7—C8—C16—C17 | −141.69 (17) |
| N6—C7—C8—C16 | −179.02 (14) | C8—C16—C17—C18 | 1.8 (3) |
| S1—C7—C8—C16 | 2.3 (2) | C8—C16—C17—C19 | −179.45 (16) |
| C7—C8—C9—C10 | 4.1 (2) | C20—O5—C18—O4 | −5.2 (3) |
| C16—C8—C9—C10 | 179.47 (14) | C20—O5—C18—C17 | 173.63 (17) |
| C8—C9—C10—C11 | −1.3 (2) | C16—C17—C18—O4 | −78.9 (3) |
| C8—C9—C10—C15 | 178.46 (15) | C19—C17—C18—O4 | 102.4 (2) |
| C7—N6—C11—C12 | −177.33 (16) | C16—C17—C18—O5 | 102.3 (2) |
| C7—N6—C11—C10 | 2.9 (2) | C19—C17—C18—O5 | −76.47 (19) |
| C15—C10—C11—N6 | 178.10 (14) | C22—O3—C19—O2 | −2.2 (3) |
| C9—C10—C11—N6 | −2.1 (2) | C22—O3—C19—C17 | 178.64 (18) |
| C15—C10—C11—C12 | −1.7 (2) | C16—C17—C19—O2 | −0.2 (3) |
| C9—C10—C11—C12 | 178.05 (15) | C18—C17—C19—O2 | 178.7 (2) |
| N6—C11—C12—C13 | −179.72 (17) | C16—C17—C19—O3 | 178.96 (16) |
| C10—C11—C12—C13 | 0.1 (3) | C18—C17—C19—O3 | −2.2 (2) |
| C11—C12—C13—C14 | 1.2 (3) | C18—O5—C20—C21 | 178.7 (3) |
| C12—C13—C14—C15 | −0.7 (3) | C19—O3—C22—C23 | −176.6 (2) |
| C13—C14—C15—C10 | −1.0 (3) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| S1—H1···N6$^{i}$ | 1.20 | 2.37 | 3.3389 (14) | 136 |
| C9—H9···O4 | 0.99 (3) | 2.41 (3) | 3.122 (2) | 129 (2) |
| C22—H22*B*···O2$^{ii}$ | 0.97 | 2.52 | 3.438 (4) | 158 |

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