Acta Crystallographica Section E
**Structure Reports Online**
ISSN 1600-5368

# 6-Cyclohexylmethyl-5-ethyl-2-[(2-oxo-2-phenylethyl)sulfanyl]pyrimidin-4(3*H*)-one

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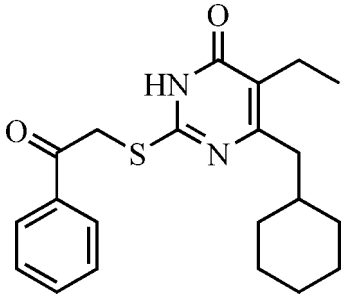
Received 18 January 2011; accepted 24 January 2011

Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.040; $wR$ factor = 0.129; data-to-parameter ratio = 17.5.

In the title compound, $C_{21}H_{26}N_2O_2S$, the cyclohexane ring adopts a chair conformation. The angle at the methylene bridge linking the pyrimidine and cyclohexane rings is 113.41 (13)°. This is in the range considered optimal for maximum activity of non-nucleoside reverse transcriptase inhibitors. In the crystal, molecules are connected into centrosymmetric dimers *via* pairs of N—H···O hydrogen bonds.

## Related literature

For the biological activity of 2-alkylsulfanyl-6-benzyl-3,4-dihydropyrimidin-4(3*H*)-one derivatives, which show remarkable anti-HIV-1 activity, see: He *et al.* (2011); Ettorre *et al.* (1996). For related structures, see: Ettorre *et al.* (1998); Rao *et al.* (2007); Zhang *et al.* (2008).




## Experimental

### Crystal data

$C_{21}H_{26}N_2O_2S$
$M_r$ = 370.50
Triclinic, $P\overline{1}$
$a$ = 7.516 (5) Å
$b$ = 10.960 (5) Å
$c$ = 12.490 (5) Å
$\alpha$ = 84.082 (5)°
$\beta$ = 78.925 (5)°
$\gamma$ = 80.267 (5)°
$V$ = 992.5 (9) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.18 mm$^{-1}$
$T$ = 293 K
0.46 × 0.23 × 0.17 mm

### Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.944, $T_{max}$ = 0.975
7097 measured reflections
4158 independent reflections
3203 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.129
$S$ = 1.03
4158 reflections
237 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···O2$^{i}$ | 0.86 | 1.90 | 2.743 (2) | 168 |

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

Data collection: *SMART* (Bruker, 2004); cell refinement: *SAINT* (Bruker, 2004); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELXTL*.

This work was supported by the National Natural Science Foundation of China (grant No. 30960459).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2710).

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# supporting information

*Acta Cryst.* (2011). E**67**, o534 [doi:10.1107/S1600536811003175]

## 6-Cyclohexylmethyl-5-ethyl-2-[(2-oxo-2-phenylethyl)sulfanyl]pyrimidin-4(3*H*)-one

**Wan-Lu Yan, Qiong Guo, Cong Li, Xiao-Ying Ji and Yan-Ping He**

### S1. Comment

As part of on-going investigations of S-DABO analogues, *e.g*. 2-alkylsulfanyl-6-benzyl-3,4-dihydropyrimidin-4(3*H*) -one derivatives, which comprise a potent family of non-nucleoside reverse transcriptase inhibitors (NNRTI's), the title compound was synthesized as a novel inhibitor which shows remarkable anti-HIV-1 activity (He *et al.*, 2011).

The molecular structure is shown in Fig. 1. The cyclohexane ring adopts a chair conformation. The C12—C15—C16 angle is 113.41 (13)°, which is in the range considered optimal for maximum activity of NNRTI's, *viz*. 110–115° (Ettorre *et al.*, 1996).

A comparison of the molecular structure of the title compound with some reported S-DABO's show that their spatial arrangement are similar (Ettorre *et al.*, 1998; Rao *et al.*, 2007; Zhang *et al.*, 2008). Although these molecules assume similar conformations, they show differences in their activities. Thus, further structural investigations are needed in order to establish a structure-activity relationship.

In the crystal, molecules are connected into centrosymmetric dimers via N—H···O hydrogen bonds, Table 1.

### S2. Experimental

With 2-cyclohexylacetonitrile as the starting material, the title compound was synthesized according to the procedure of He *et al.* (2011). Single crystals of the title compound were obtained from the slow evaporation at room temperature of its ethyl acetate/petroleum ether solution.

### S3. Refinement

Methyl-H atoms were placed in calculated positions with C—H = 0.96 Å and the torsion angles were refined to fit the electron density; $U_{iso}$(H) = 1.5$U_{eq}$(C). Other H atoms were placed in calculated positions with N—H = 0.86 Å and C—H = 0.93–0.98 Å, and with $U_{iso}$(H) = 1.2$U_{eq}$(C, N).

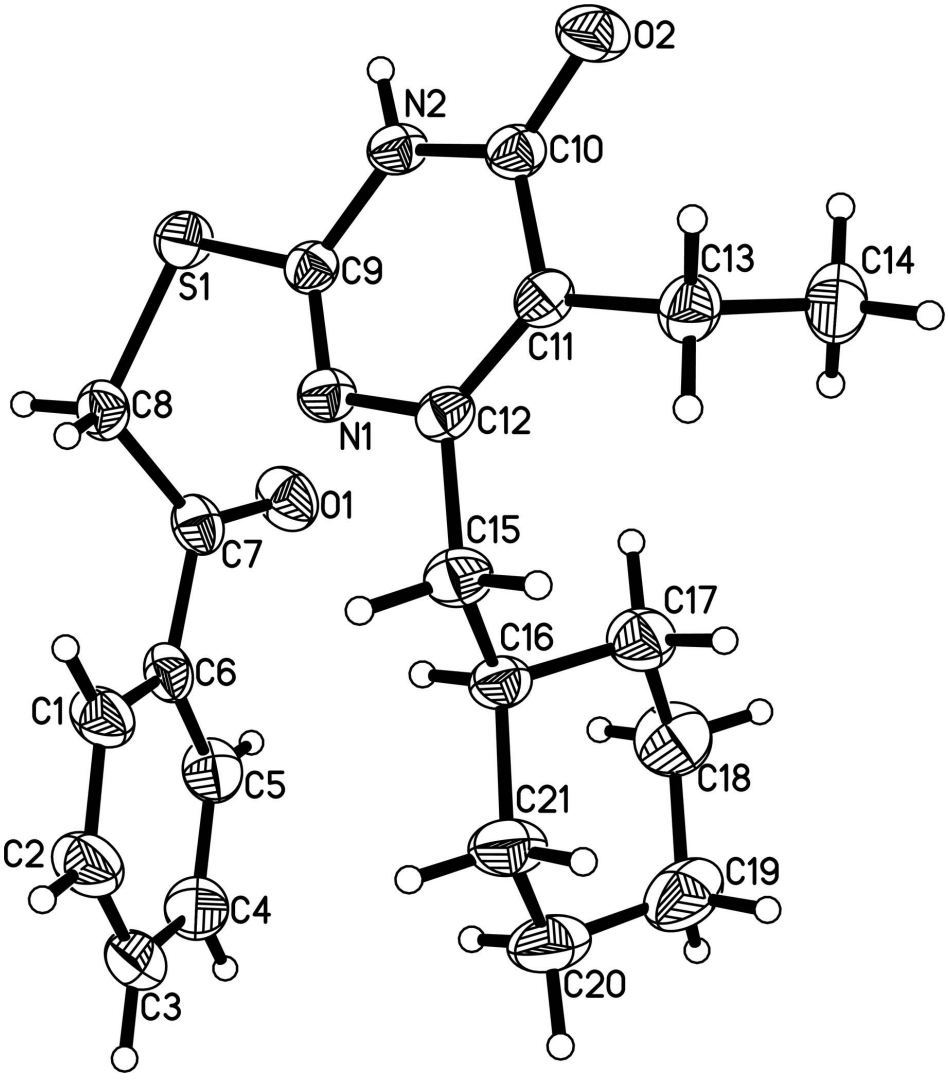


**Figure 1**

The molecular structure of the title compound, showing the atom labelling scheme and 30% probability displacement ellipsoids.

**6-Cyclohexylmethyl-5-ethyl-2-[(2-oxo-2-phenylethyl)sulfanyl]pyrimidin- 4(3*H*)-one**

*Crystal data*

$C_{21}H_{26}N_2O_2S$
$M_r = 370.50$
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a = 7.516\ (5)$ Å
$b = 10.960\ (5)$ Å
$c = 12.490\ (5)$ Å
$\alpha = 84.082\ (5)°$
$\beta = 78.925\ (5)°$
$\gamma = 80.267\ (5)°$
$V = 992.5\ (9)$ Å$^3$
$Z = 2$
$F(000) = 396$
$D_x = 1.240$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2756 reflections
$\theta = 2.4–27.3°$
$\mu = 0.18$ mm$^{-1}$
$T = 293$ K
Block, colourless
0.46 × 0.23 × 0.17 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
$T_{min}$ = 0.944, $T_{max}$ = 0.975
7097 measured reflections
4158 independent reflections
3203 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.019
$\theta_{max}$ = 28.1°, $\theta_{min}$ = 1.7°
$h$ = −9→9
$k$ = −14→14
$l$ = −16→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.129
$S$ = 1.03
4158 reflections
237 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
$w = 1/[\sigma^2(F_o^2) + (0.0735P)^2 + 0.0929P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.18 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.18 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.042 (4)

*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 takeninto account individually in the estimation of e.s.d.'s in distances, anglesand torsion angles; correlations between e.s.d.'s in cell parameters are onlyused 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C1 | 0.0651 (2) | 0.34455 (19) | 0.37479 (16) | 0.0637 (5) |
| H1 | 0.0740 | 0.2786 | 0.4276 | 0.076* |
| C2 | −0.0742 (3) | 0.3611 (2) | 0.31452 (19) | 0.0768 (6) |
| H2 | −0.1563 | 0.3044 | 0.3255 | 0.092* |
| C3 | −0.0931 (3) | 0.4597 (2) | 0.23879 (17) | 0.0735 (6) |
| H3 | −0.1883 | 0.4709 | 0.1992 | 0.088* |
| C4 | 0.0298 (3) | 0.5416 (2) | 0.22211 (17) | 0.0707 (6) |
| H4 | 0.0174 | 0.6092 | 0.1711 | 0.085* |
| C5 | 0.1713 (3) | 0.52527 (17) | 0.27987 (16) | 0.0622 (5) |
| H5 | 0.2543 | 0.5815 | 0.2671 | 0.075* |
| C6 | 0.1917 (2) | 0.42627 (15) | 0.35661 (13) | 0.0483 (4) |
| C7 | 0.3555 (2) | 0.40826 (14) | 0.41151 (14) | 0.0490 (4) |
| C8 | 0.3441 (2) | 0.33926 (16) | 0.52377 (14) | 0.0518 (4) |
| H8A | 0.2644 | 0.2772 | 0.5284 | 0.062* |
| H8B | 0.2876 | 0.3975 | 0.5784 | 0.062* |

| | | | | |
|---|---|---|---|---|
| C9 | 0.6130 (2) | 0.14968 (13) | 0.46180 (12) | 0.0409 (3) |
| C10 | 0.8364 (2) | −0.02021 (14) | 0.39454 (12) | 0.0451 (4) |
| C11 | 0.7259 (2) | −0.02517 (14) | 0.31332 (12) | 0.0436 (4) |
| C12 | 0.5655 (2) | 0.05556 (14) | 0.31667 (12) | 0.0426 (4) |
| C13 | 0.8014 (3) | −0.12053 (17) | 0.23150 (14) | 0.0548 (4) |
| H13A | 0.7058 | −0.1299 | 0.1921 | 0.066* |
| H13B | 0.8355 | −0.1997 | 0.2704 | 0.066* |
| C14 | 0.9669 (3) | −0.0886 (2) | 0.14963 (16) | 0.0727 (6) |
| H14A | 0.9352 | −0.0095 | 0.1116 | 0.109* |
| H14B | 1.0048 | −0.1512 | 0.0980 | 0.109* |
| H14C | 1.0655 | −0.0849 | 0.1874 | 0.109* |
| C15 | 0.4356 (2) | 0.06173 (16) | 0.23778 (14) | 0.0529 (4) |
| H15A | 0.3134 | 0.0568 | 0.2789 | 0.063* |
| H15B | 0.4723 | −0.0096 | 0.1942 | 0.063* |
| C16 | 0.4293 (2) | 0.18009 (16) | 0.16104 (13) | 0.0504 (4) |
| H16 | 0.3873 | 0.2507 | 0.2065 | 0.060* |
| C17 | 0.6149 (3) | 0.19746 (19) | 0.09419 (16) | 0.0658 (5) |
| H17A | 0.6629 | 0.1263 | 0.0514 | 0.079* |
| H17B | 0.6992 | 0.2017 | 0.1431 | 0.079* |
| C18 | 0.6038 (4) | 0.3151 (2) | 0.0178 (2) | 0.0849 (7) |
| H18A | 0.5672 | 0.3869 | 0.0608 | 0.102* |
| H18B | 0.7238 | 0.3211 | −0.0259 | 0.102* |
| C19 | 0.4667 (4) | 0.3152 (2) | −0.05721 (19) | 0.0914 (8) |
| H19A | 0.4570 | 0.3930 | −0.1019 | 0.110* |
| H19B | 0.5099 | 0.2485 | −0.1057 | 0.110* |
| C20 | 0.2831 (4) | 0.2987 (2) | 0.00690 (19) | 0.0825 (7) |
| H20A | 0.2010 | 0.2931 | −0.0430 | 0.099* |
| H20B | 0.2335 | 0.3709 | 0.0481 | 0.099* |
| C21 | 0.2904 (3) | 0.1827 (2) | 0.08558 (17) | 0.0692 (6) |
| H21A | 0.3233 | 0.1098 | 0.0439 | 0.083* |
| H21B | 0.1697 | 0.1797 | 0.1296 | 0.083* |
| N2 | 0.77310 (18) | 0.07257 (11) | 0.46550 (10) | 0.0446 (3) |
| H2A | 0.8372 | 0.0817 | 0.5134 | 0.054* |
| N1 | 0.50716 (18) | 0.14361 (12) | 0.39265 (10) | 0.0448 (3) |
| O1 | 0.49051 (17) | 0.45336 (12) | 0.36902 (12) | 0.0662 (4) |
| O2 | 0.98026 (18) | −0.09226 (11) | 0.40372 (10) | 0.0621 (4) |
| S1 | 0.56039 (6) | 0.26398 (4) | 0.55656 (3) | 0.05176 (16) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C1 | 0.0452 (10) | 0.0686 (12) | 0.0717 (12) | −0.0097 (9) | −0.0091 (9) | 0.0197 (9) |
| C2 | 0.0499 (11) | 0.0943 (16) | 0.0845 (14) | −0.0205 (11) | −0.0142 (10) | 0.0214 (12) |
| C3 | 0.0470 (11) | 0.0964 (16) | 0.0684 (12) | 0.0058 (11) | −0.0100 (9) | 0.0057 (11) |
| C4 | 0.0724 (14) | 0.0637 (12) | 0.0646 (12) | 0.0105 (11) | −0.0110 (10) | 0.0120 (9) |
| C5 | 0.0633 (12) | 0.0491 (10) | 0.0674 (11) | −0.0028 (9) | −0.0045 (9) | 0.0042 (8) |
| C6 | 0.0420 (9) | 0.0427 (8) | 0.0527 (9) | 0.0021 (7) | 0.0018 (7) | −0.0016 (7) |
| C7 | 0.0457 (9) | 0.0372 (8) | 0.0592 (10) | −0.0009 (7) | −0.0011 (7) | −0.0055 (7) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0487 (10) | 0.0530 (9) | 0.0509 (9) | −0.0024 (8) | −0.0029 (7) | −0.0107 (7) |
| C9 | 0.0456 (9) | 0.0369 (7) | 0.0395 (7) | −0.0058 (6) | −0.0076 (6) | −0.0002 (6) |
| C10 | 0.0532 (10) | 0.0387 (8) | 0.0439 (8) | −0.0027 (7) | −0.0134 (7) | −0.0029 (6) |
| C11 | 0.0516 (9) | 0.0411 (8) | 0.0393 (8) | −0.0107 (7) | −0.0093 (6) | −0.0013 (6) |
| C12 | 0.0472 (9) | 0.0437 (8) | 0.0390 (7) | −0.0127 (7) | −0.0099 (6) | 0.0015 (6) |
| C13 | 0.0617 (11) | 0.0549 (10) | 0.0488 (9) | −0.0067 (8) | −0.0091 (8) | −0.0131 (7) |
| C14 | 0.0771 (14) | 0.0703 (13) | 0.0607 (11) | −0.0026 (11) | 0.0067 (10) | −0.0082 (9) |
| C15 | 0.0548 (10) | 0.0564 (10) | 0.0533 (9) | −0.0147 (8) | −0.0184 (8) | −0.0041 (8) |
| C16 | 0.0554 (10) | 0.0515 (9) | 0.0475 (9) | −0.0019 (8) | −0.0197 (7) | −0.0093 (7) |
| C17 | 0.0657 (12) | 0.0642 (12) | 0.0646 (11) | −0.0061 (10) | −0.0143 (9) | 0.0076 (9) |
| C18 | 0.0946 (18) | 0.0703 (14) | 0.0837 (15) | −0.0142 (13) | −0.0134 (13) | 0.0207 (12) |
| C19 | 0.134 (2) | 0.0711 (15) | 0.0622 (13) | 0.0098 (15) | −0.0294 (14) | 0.0062 (11) |
| C20 | 0.1008 (19) | 0.0758 (14) | 0.0750 (14) | 0.0137 (13) | −0.0477 (14) | −0.0086 (11) |
| C21 | 0.0726 (14) | 0.0746 (13) | 0.0682 (12) | −0.0044 (11) | −0.0350 (10) | −0.0099 (10) |
| N2 | 0.0524 (8) | 0.0418 (7) | 0.0421 (7) | −0.0032 (6) | −0.0171 (6) | −0.0049 (5) |
| N1 | 0.0461 (8) | 0.0456 (7) | 0.0443 (7) | −0.0062 (6) | −0.0122 (6) | −0.0038 (5) |
| O1 | 0.0512 (8) | 0.0637 (8) | 0.0807 (9) | −0.0157 (6) | −0.0052 (6) | 0.0069 (7) |
| O2 | 0.0699 (9) | 0.0519 (7) | 0.0667 (8) | 0.0136 (6) | −0.0314 (6) | −0.0164 (6) |
| S1 | 0.0566 (3) | 0.0501 (3) | 0.0499 (3) | −0.00196 (19) | −0.01321 (19) | −0.01319 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C1—C2 | 1.380 (3) | C13—C14 | 1.516 (3) |
| C1—C6 | 1.386 (2) | C13—H13A | 0.9700 |
| C1—H1 | 0.9300 | C13—H13B | 0.9700 |
| C2—C3 | 1.368 (3) | C14—H14A | 0.9600 |
| C2—H2 | 0.9300 | C14—H14B | 0.9600 |
| C3—C4 | 1.368 (3) | C14—H14C | 0.9600 |
| C3—H3 | 0.9300 | C15—C16 | 1.531 (2) |
| C4—C5 | 1.374 (3) | C15—H15A | 0.9700 |
| C4—H4 | 0.9300 | C15—H15B | 0.9700 |
| C5—C6 | 1.380 (3) | C16—C17 | 1.513 (3) |
| C5—H5 | 0.9300 | C16—C21 | 1.530 (2) |
| C6—C7 | 1.497 (3) | C16—H16 | 0.9800 |
| C7—O1 | 1.210 (2) | C17—C18 | 1.523 (3) |
| C7—C8 | 1.517 (2) | C17—H17A | 0.9700 |
| C8—S1 | 1.795 (2) | C17—H17B | 0.9700 |
| C8—H8A | 0.9700 | C18—C19 | 1.520 (3) |
| C8—H8B | 0.9700 | C18—H18A | 0.9700 |
| C9—N1 | 1.295 (2) | C18—H18B | 0.9700 |
| C9—N2 | 1.354 (2) | C19—C20 | 1.486 (4) |
| C9—S1 | 1.7563 (16) | C19—H19A | 0.9700 |
| C10—O2 | 1.243 (2) | C19—H19B | 0.9700 |
| C10—N2 | 1.381 (2) | C20—C21 | 1.524 (3) |
| C10—C11 | 1.440 (2) | C20—H20A | 0.9700 |
| C11—C12 | 1.366 (2) | C20—H20B | 0.9700 |
| C11—C13 | 1.502 (2) | C21—H21A | 0.9700 |
| C12—N1 | 1.382 (2) | C21—H21B | 0.9700 |

| | | | |
|---|---|---|---|
| C12—C15 | 1.504 (2) | N2—H2A | 0.8600 |
| | | | |
| C2—C1—C6 | 120.01 (18) | H14A—C14—H14C | 109.5 |
| C2—C1—H1 | 120.0 | H14B—C14—H14C | 109.5 |
| C6—C1—H1 | 120.0 | C12—C15—C16 | 113.41 (13) |
| C3—C2—C1 | 120.9 (2) | C12—C15—H15A | 108.9 |
| C3—C2—H2 | 119.5 | C16—C15—H15A | 108.9 |
| C1—C2—H2 | 119.5 | C12—C15—H15B | 108.9 |
| C4—C3—C2 | 119.1 (2) | C16—C15—H15B | 108.9 |
| C4—C3—H3 | 120.5 | H15A—C15—H15B | 107.7 |
| C2—C3—H3 | 120.5 | C17—C16—C21 | 110.13 (16) |
| C3—C4—C5 | 120.76 (19) | C17—C16—C15 | 113.00 (15) |
| C3—C4—H4 | 119.6 | C21—C16—C15 | 110.86 (15) |
| C5—C4—H4 | 119.6 | C17—C16—H16 | 107.5 |
| C4—C5—C6 | 120.67 (19) | C21—C16—H16 | 107.5 |
| C4—C5—H5 | 119.7 | C15—C16—H16 | 107.5 |
| C6—C5—H5 | 119.7 | C16—C17—C18 | 111.75 (17) |
| C5—C6—C1 | 118.49 (18) | C16—C17—H17A | 109.3 |
| C5—C6—C7 | 118.30 (16) | C18—C17—H17A | 109.3 |
| C1—C6—C7 | 123.11 (16) | C16—C17—H17B | 109.3 |
| O1—C7—C6 | 120.20 (16) | C18—C17—H17B | 109.3 |
| O1—C7—C8 | 121.06 (16) | H17A—C17—H17B | 107.9 |
| C6—C7—C8 | 118.65 (14) | C19—C18—C17 | 111.2 (2) |
| C7—C8—S1 | 114.80 (12) | C19—C18—H18A | 109.4 |
| C7—C8—H8A | 108.6 | C17—C18—H18A | 109.4 |
| S1—C8—H8A | 108.6 | C19—C18—H18B | 109.4 |
| C7—C8—H8B | 108.6 | C17—C18—H18B | 109.4 |
| S1—C8—H8B | 108.6 | H18A—C18—H18B | 108.0 |
| H8A—C8—H8B | 107.5 | C20—C19—C18 | 111.0 (2) |
| N1—C9—N2 | 123.68 (14) | C20—C19—H19A | 109.4 |
| N1—C9—S1 | 121.55 (12) | C18—C19—H19A | 109.4 |
| N2—C9—S1 | 114.75 (11) | C20—C19—H19B | 109.4 |
| O2—C10—N2 | 119.81 (14) | C18—C19—H19B | 109.4 |
| O2—C10—C11 | 124.65 (14) | H19A—C19—H19B | 108.0 |
| N2—C10—C11 | 115.54 (14) | C19—C20—C21 | 112.29 (19) |
| C12—C11—C10 | 118.33 (14) | C19—C20—H20A | 109.1 |
| C12—C11—C13 | 126.18 (15) | C21—C20—H20A | 109.1 |
| C10—C11—C13 | 115.48 (15) | C19—C20—H20B | 109.1 |
| C11—C12—N1 | 122.99 (14) | C21—C20—H20B | 109.1 |
| C11—C12—C15 | 124.59 (14) | H20A—C20—H20B | 107.9 |
| N1—C12—C15 | 112.40 (14) | C20—C21—C16 | 112.09 (17) |
| C11—C13—C14 | 113.75 (15) | C20—C21—H21A | 109.2 |
| C11—C13—H13A | 108.8 | C16—C21—H21A | 109.2 |
| C14—C13—H13A | 108.8 | C20—C21—H21B | 109.2 |
| C11—C13—H13B | 108.8 | C16—C21—H21B | 109.2 |
| C14—C13—H13B | 108.8 | H21A—C21—H21B | 107.9 |
| H13A—C13—H13B | 107.7 | C9—N2—C10 | 121.91 (13) |
| C13—C14—H14A | 109.5 | C9—N2—H2A | 119.0 |

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| C13—C14—H14B | 109.5 | C10—N2—H2A | 119.0 |
| H14A—C14—H14B | 109.5 | C9—N1—C12 | 117.43 (14) |
| C13—C14—H14C | 109.5 | C9—S1—C8 | 99.15 (8) |
| | | | |
| C6—C1—C2—C3 | −2.0 (4) | C11—C12—C15—C16 | −110.85 (18) |
| C1—C2—C3—C4 | 0.9 (4) | N1—C12—C15—C16 | 67.63 (19) |
| C2—C3—C4—C5 | 0.4 (3) | C12—C15—C16—C17 | 57.7 (2) |
| C3—C4—C5—C6 | −0.5 (3) | C12—C15—C16—C21 | −178.14 (15) |
| C4—C5—C6—C1 | −0.6 (3) | C21—C16—C17—C18 | 54.8 (2) |
| C4—C5—C6—C7 | 175.91 (16) | C15—C16—C17—C18 | 179.37 (17) |
| C2—C1—C6—C5 | 1.9 (3) | C16—C17—C18—C19 | −56.5 (3) |
| C2—C1—C6—C7 | −174.50 (18) | C17—C18—C19—C20 | 55.8 (3) |
| C5—C6—C7—O1 | −21.6 (2) | C18—C19—C20—C21 | −54.8 (3) |
| C1—C6—C7—O1 | 154.81 (18) | C19—C20—C21—C16 | 54.2 (2) |
| C5—C6—C7—C8 | 154.89 (16) | C17—C16—C21—C20 | −53.3 (2) |
| C1—C6—C7—C8 | −28.7 (2) | C15—C16—C21—C20 | −179.13 (18) |
| O1—C7—C8—S1 | −29.6 (2) | N1—C9—N2—C10 | −0.1 (2) |
| C6—C7—C8—S1 | 153.97 (12) | S1—C9—N2—C10 | −178.32 (11) |
| O2—C10—C11—C12 | 176.35 (16) | O2—C10—N2—C9 | −176.98 (14) |
| N2—C10—C11—C12 | −3.6 (2) | C11—C10—N2—C9 | 3.0 (2) |
| O2—C10—C11—C13 | −4.0 (2) | N2—C9—N1—C12 | −2.1 (2) |
| N2—C10—C11—C13 | 176.04 (13) | S1—C9—N1—C12 | 175.98 (10) |
| C10—C11—C12—N1 | 1.7 (2) | C11—C12—N1—C9 | 1.3 (2) |
| C13—C11—C12—N1 | −177.99 (14) | C15—C12—N1—C9 | −177.25 (13) |
| C10—C11—C12—C15 | 179.99 (14) | N1—C9—S1—C8 | 2.47 (15) |
| C13—C11—C12—C15 | 0.3 (2) | N2—C9—S1—C8 | −179.29 (11) |
| C12—C11—C13—C14 | 107.9 (2) | C7—C8—S1—C9 | −67.38 (14) |
| C10—C11—C13—C14 | −71.8 (2) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O2$^{i}$ | 0.86 | 1.90 | 2.743 (2) | 168 |

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