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# 1-(Biphenyl-4-ylcarbonyl)-3-(2-chloro-4-nitrophenyl)thiourea

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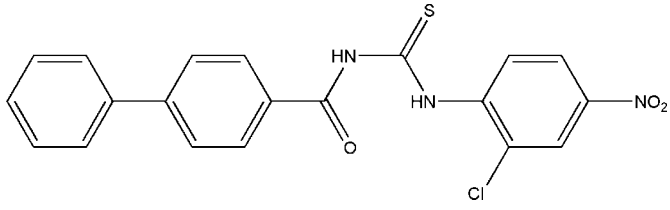
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.049; $wR$ factor = 0.137; data-to-parameter ratio = 12.5.

The benzene rings of the biphenyl group in the title compound, $C_{20}H_{14}ClN_3O_3S$, are nearly coplanar [maximum deviation = 0.20 (3) Å]. The mean plane of the biphenyl group forms a dihedral angle of 5.24 (7)° with the aromatic ring of the nitrochlorobenzene group. Intramolecular N—H···Cl, N—H···O and C—H···S hydrogen bonds stabilize the *cis*–*trans* conformation of the molecule. In the crystal, molecules are linked by C—H···O and C—H···S hydrogen bonds into mutually interwoven corrugated layers parallel to (10$\bar{2}$).

## Related literature

For a related structure, see: Yusof *et al.* (2011). For bond-length data, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{20}H_{14}ClN_3O_3S$ $M_r$ = 411.85
Monoclinic, $P2_1/c$
$a$ = 10.889 (2) Å
$b$ = 5.4502 (10) Å
$c$ = 30.532 (5) Å
$\beta$ = 99.202 (4)°
$V$ = 1788.6 (6) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.36 mm$^{-1}$
$T$ = 298 K
0.35 × 0.13 × 0.08 mm

### Data collection

Bruker SMART APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.885, $T_{max}$ = 0.972
9537 measured reflections
3154 independent reflections
2704 reflections with $I > 2/s(I)$
$R_{int}$ = 0.026

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.137
$S$ = 1.16
3154 reflections
253 parameters
3 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2$A$···Cl1 | 0.86 | 2.43 | 2.938 (2) | 118 |
| N2—H2$A$···O1 | 0.86 | 1.87 | 2.608 (3) | 143 |
| C16—H16$A$···S1 | 0.93 | 2.53 | 3.208 (3) | 130 |
| C10—H10$A$···O3$^{i}$ | 0.93 | 2.57 | 3.354 (4) | 142 |
| C17—H17$A$···S1$^{ii}$ | 0.93 | 2.77 | 3.673 (3) | 165 |

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

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); 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*, *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: RZ2737).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1485 [doi:10.1107/S1600536812016686]

## 1-(Biphenyl-4-ylcarbonyl)-3-(2-chloro-4-nitrophenyl)thiourea

**M. Sukeri M. Yusof, Bohari M. Yamin and Nurziana Ngah**

### Comment

The title compound, (I), is similiar to the previously reported compound 1-(biphenyl-4-yl-carbonyl)-3-(4-nitrophenyl)-thiourea (II) (Yusof *et al.*, 2011) except for the presence of a chlorine atom at 2-position of the nitrobenzene ring. The bond lengths and angles are in normal ranges (Allen *et al.* 1987) and comparable to those reported for (II). The molecule (Fig. 1) is essentially planar, with a maximum deviation of 0.076 (2) Å for atom N1. The introduction of a chlorine substituent at the 2-position of the nitrobenzene ring makes the two benzene rings in biphenyl group nearly coplanar, forming a dihedral angle of 1.02 (14)° compared to that of 40.11 (15)° observed in II. The thiourea moiety makes dihedral angle of 6.15 (10)° and 0.92 (10)° with the C1—C6 and C15—C20 rings, respectively, compared to the corresponding angles of 16.14 (13)° and 17.75 (14)° in II. The *cis-trans* conformation of the molecule is stabilized by intramolecular N2—H2A···Cl1, N2—H2A···O1 and C16—H16A···S1 hydrogen interactions (Table 1). In the crystal structure (Fig. 2), the molecules interact through intermolecular C—H···O and C—H···S hydrogen bonds to form mutually interwoven corrugated layers parallel to the (1 0 -2) plane.

### Experimental

An acetone (30 ml) solution of 2-chloro-4-nitroaniline (1.60 g, 9.5 mmol) was added to a round-bottom flask containing 4-biphenylcarbonyl chloride (2.00 g, 9.5 mmol) and ammonium thiocyanate (0.70 g, 9.5 mmol). The mixture was refluxed for 2.5 h then filtered off and left to evaporate at room temperature. The yellowish precipitate obtained was washed with water and cold ethanol. Yellowish crystals suitable for X-ray analysis were obtained by recrystallization of the precipitate in DMSO.

### Refinement

All H atoms were positioned geometrically and refined using a riding model with C—H = 0.93 Å and N—H = 0.86 Å, and with $U_{iso}$(H) = 1.2 $U_{eq}$(C, N). A rigid body restraint (DELU in *SHELXL-97*; Sheldrick, 2008) was applied for atoms N3, O2 and O3.

### Computing details

Data collection: *SMART* (Bruker, 2000); cell refinement: *SAINT* (Bruker, 2000); data reduction: *SAINT* (Bruker, 2000); 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* (Sheldrick, 2008), *PARST* (Nardelli, 1995) and *PLATON* (Spek, 2009).

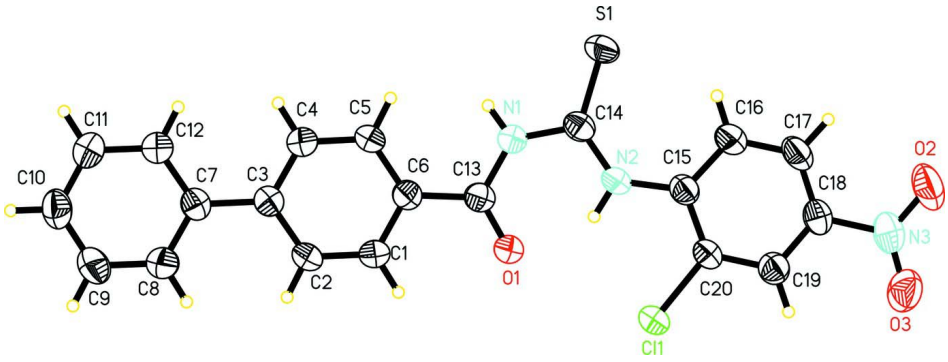


**Figure 1**

The molecular structure of the title compound with displacement ellipsods drawn at the 50% probability level.

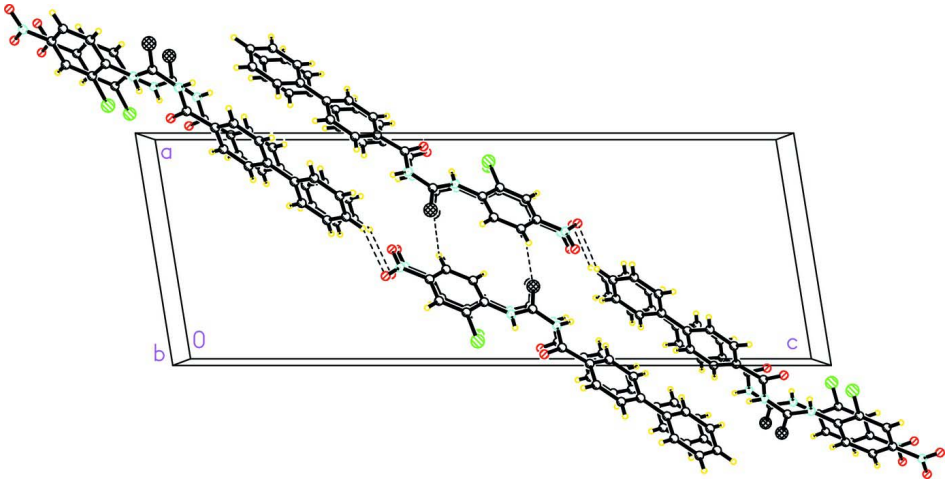


**Figure 2**

The crystal packing of the title compound viewed down the *b* axis. Intermolecular hydrogen bonds are shown as dashed lines.

### 1-(Biphenyl-4-ylcarbonyl)-3-(2-chloro-4-nitrophenyl)thiourea

*Crystal data*

$C_{20}H_{14}ClN_3O_3S$
$M_r = 411.85$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 10.889$ (2) Å
$b = 5.4502$ (10) Å
$c = 30.532$ (5) Å
$\beta = 99.202$ (4)°
$V = 1788.6$ (6) Å$^3$
$Z = 4$

$F(000) = 848$
$D_x = 1.529$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1235 reflections
$\theta = 1.9$–25.0°
$\mu = 0.36$ mm$^{-1}$
$T = 298$ K
Slab, yellow
0.35 × 0.13 × 0.08 mm

*Data collection*

Bruker SMART APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator

Detector resolution: 83.66 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)

$T_{min}$ = 0.885, $T_{max}$ = 0.972
9537 measured reflections
3154 independent reflections
2704 reflections with $I > 2/s(I)$
$R_{int}$ = 0.026

$\theta_{max}$ = 25.0°, $\theta_{min}$ = 1.9°
$h$ = −11→12
$k$ = −6→6
$l$ = −35→36

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.137
$S$ = 1.16
3154 reflections
253 parameters
3 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
$w = 1/[\sigma^2(F_o^2) + (0.0709P)^2 + 0.5419P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.25 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 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.

**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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| S1 | 0.66457 (7) | 0.06984 (14) | 0.93137 (2) | 0.0553 (3) |
| Cl1 | 0.88661 (6) | 0.87141 (13) | 1.03030 (2) | 0.0511 (2) |
| O1 | 0.9472 (2) | 0.6794 (4) | 0.93384 (7) | 0.0691 (7) |
| O2 | 0.5004 (3) | 0.4603 (5) | 1.13921 (9) | 0.0849 (8) |
| O3 | 0.6132 (2) | 0.7850 (5) | 1.15220 (7) | 0.0701 (6) |
| N1 | 0.8315 (2) | 0.3541 (4) | 0.90589 (7) | 0.0449 (5) |
| H1A | 0.8162 | 0.2613 | 0.8829 | 0.054* |
| N2 | 0.7806 (2) | 0.4647 (4) | 0.97322 (7) | 0.0456 (5) |
| H2A | 0.8366 | 0.5731 | 0.9709 | 0.055* |
| N3 | 0.5772 (2) | 0.6060 (5) | 1.12973 (9) | 0.0559 (6) |
| C1 | 1.0767 (3) | 0.7043 (5) | 0.86344 (10) | 0.0538 (7) |
| H1B | 1.0856 | 0.8296 | 0.8844 | 0.065* |
| C2 | 1.1482 (3) | 0.7078 (5) | 0.83008 (9) | 0.0509 (7) |
| H2B | 1.2040 | 0.8359 | 0.8290 | 0.061* |
| C3 | 1.1390 (2) | 0.5250 (5) | 0.79806 (8) | 0.0374 (6) |
| C4 | 1.0527 (3) | 0.3419 (5) | 0.80119 (9) | 0.0520 (7) |
| H4A | 1.0432 | 0.2171 | 0.7801 | 0.062* |
| C5 | 0.9802 (3) | 0.3377 (5) | 0.83435 (9) | 0.0509 (7) |
| H5A | 0.9228 | 0.2119 | 0.8351 | 0.061* |
| C6 | 0.9919 (2) | 0.5184 (5) | 0.86650 (8) | 0.0394 (6) |
| C7 | 1.2173 (2) | 0.5270 (5) | 0.76232 (8) | 0.0393 (6) |

| | | | | |
|---|---|---|---|---|
| C8 | 1.3045 (3) | 0.7076 (6) | 0.75971 (10) | 0.0609 (8) |
| H8A | 1.3153 | 0.8315 | 0.7809 | 0.073* |
| C9 | 1.3767 (3) | 0.7083 (7) | 0.72601 (11) | 0.0681 (9) |
| H9A | 1.4342 | 0.8333 | 0.7248 | 0.082* |
| C10 | 1.3638 (3) | 0.5275 (6) | 0.69487 (9) | 0.0551 (8) |
| H10A | 1.4127 | 0.5274 | 0.6725 | 0.066* |
| C11 | 1.2787 (3) | 0.3470 (7) | 0.69684 (11) | 0.0661 (9) |
| H11A | 1.2691 | 0.2228 | 0.6757 | 0.079* |
| C12 | 1.2060 (3) | 0.3469 (6) | 0.73013 (10) | 0.0570 (8) |
| H12A | 1.1481 | 0.2222 | 0.7308 | 0.068* |
| C13 | 0.9227 (2) | 0.5278 (5) | 0.90462 (9) | 0.0439 (6) |
| C14 | 0.7603 (2) | 0.3068 (5) | 0.93919 (8) | 0.0404 (6) |
| C15 | 0.7273 (2) | 0.4852 (5) | 1.01169 (8) | 0.0408 (6) |
| C16 | 0.6357 (3) | 0.3307 (6) | 1.02337 (10) | 0.0543 (7) |
| H16A | 0.6067 | 0.2002 | 1.0050 | 0.065* |
| C17 | 0.5876 (3) | 0.3692 (6) | 1.06191 (10) | 0.0547 (7) |
| H17A | 0.5274 | 0.2636 | 1.0696 | 0.066* |
| C18 | 0.6284 (2) | 0.5623 (5) | 1.08869 (9) | 0.0446 (6) |
| C19 | 0.7191 (2) | 0.7181 (5) | 1.07878 (8) | 0.0449 (6) |
| H19A | 0.7467 | 0.8485 | 1.0974 | 0.054* |
| C20 | 0.7686 (2) | 0.6773 (5) | 1.04071 (8) | 0.0396 (6) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0593 (5) | 0.0552 (5) | 0.0514 (4) | −0.0271 (4) | 0.0085 (3) | −0.0054 (3) |
| Cl1 | 0.0524 (4) | 0.0538 (4) | 0.0498 (4) | −0.0219 (3) | 0.0157 (3) | −0.0058 (3) |
| O1 | 0.0819 (15) | 0.0638 (14) | 0.0722 (14) | −0.0380 (12) | 0.0450 (12) | −0.0317 (12) |
| O2 | 0.0952 (18) | 0.0893 (18) | 0.0836 (16) | −0.0164 (13) | 0.0550 (15) | 0.0070 (14) |
| O3 | 0.0645 (14) | 0.0899 (16) | 0.0605 (13) | 0.0008 (11) | 0.0238 (11) | −0.0129 (12) |
| N1 | 0.0453 (12) | 0.0477 (13) | 0.0434 (12) | −0.0120 (10) | 0.0128 (10) | −0.0082 (10) |
| N2 | 0.0458 (13) | 0.0420 (12) | 0.0526 (13) | −0.0151 (10) | 0.0190 (10) | −0.0077 (11) |
| N3 | 0.0498 (14) | 0.0645 (16) | 0.0577 (14) | 0.0066 (11) | 0.0216 (11) | 0.0093 (11) |
| C1 | 0.0617 (18) | 0.0461 (17) | 0.0583 (17) | −0.0176 (14) | 0.0241 (14) | −0.0175 (14) |
| C2 | 0.0548 (17) | 0.0448 (16) | 0.0573 (17) | −0.0188 (13) | 0.0219 (13) | −0.0077 (13) |
| C3 | 0.0366 (13) | 0.0363 (13) | 0.0390 (13) | 0.0025 (10) | 0.0051 (10) | 0.0045 (11) |
| C4 | 0.0615 (18) | 0.0478 (17) | 0.0504 (16) | −0.0162 (14) | 0.0201 (13) | −0.0125 (13) |
| C5 | 0.0573 (17) | 0.0461 (16) | 0.0534 (16) | −0.0211 (13) | 0.0216 (13) | −0.0096 (13) |
| C6 | 0.0393 (13) | 0.0382 (14) | 0.0410 (13) | −0.0018 (11) | 0.0076 (11) | 0.0008 (11) |
| C7 | 0.0386 (13) | 0.0429 (14) | 0.0361 (12) | 0.0016 (11) | 0.0049 (10) | 0.0066 (11) |
| C8 | 0.071 (2) | 0.061 (2) | 0.0552 (17) | −0.0232 (16) | 0.0239 (15) | −0.0135 (15) |
| C9 | 0.073 (2) | 0.075 (2) | 0.0625 (19) | −0.0270 (18) | 0.0315 (16) | −0.0033 (17) |
| C10 | 0.0517 (17) | 0.072 (2) | 0.0442 (15) | 0.0002 (15) | 0.0169 (13) | 0.0032 (15) |
| C11 | 0.070 (2) | 0.074 (2) | 0.0601 (18) | −0.0131 (18) | 0.0278 (16) | −0.0217 (17) |
| C12 | 0.0601 (18) | 0.0551 (18) | 0.0606 (17) | −0.0152 (14) | 0.0240 (14) | −0.0149 (15) |
| C13 | 0.0427 (14) | 0.0406 (15) | 0.0500 (15) | −0.0056 (12) | 0.0118 (12) | −0.0052 (13) |
| C14 | 0.0337 (13) | 0.0414 (15) | 0.0452 (14) | −0.0030 (11) | 0.0036 (10) | 0.0034 (12) |
| C15 | 0.0375 (14) | 0.0404 (14) | 0.0461 (14) | −0.0030 (11) | 0.0113 (11) | 0.0016 (12) |
| C16 | 0.0545 (17) | 0.0507 (17) | 0.0624 (18) | −0.0163 (14) | 0.0236 (14) | −0.0086 (14) |
| C17 | 0.0513 (16) | 0.0541 (18) | 0.0645 (18) | −0.0134 (14) | 0.0265 (14) | 0.0032 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C18 | 0.0389 (14) | 0.0507 (16) | 0.0463 (14) | 0.0028 (12) | 0.0133 (11) | 0.0062 (13) |
| C19 | 0.0425 (14) | 0.0482 (16) | 0.0441 (14) | −0.0021 (12) | 0.0078 (11) | 0.0005 (12) |
| C20 | 0.0343 (13) | 0.0416 (15) | 0.0439 (13) | −0.0056 (11) | 0.0097 (10) | 0.0027 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C14 | 1.653 (3) | C5—H5A | 0.9300 |
| Cl1—C20 | 1.733 (3) | C6—C13 | 1.485 (4) |
| O1—C13 | 1.214 (3) | C7—C8 | 1.379 (4) |
| O2—N3 | 1.221 (3) | C7—C12 | 1.380 (4) |
| O3—N3 | 1.221 (3) | C8—C9 | 1.391 (4) |
| N1—C13 | 1.377 (3) | C8—H8A | 0.9300 |
| N1—C14 | 1.397 (3) | C9—C10 | 1.361 (5) |
| N1—H1A | 0.8600 | C9—H9A | 0.9300 |
| N2—C14 | 1.340 (3) | C10—C11 | 1.360 (5) |
| N2—C15 | 1.395 (3) | C10—H10A | 0.9300 |
| N2—H2A | 0.8600 | C11—C12 | 1.384 (4) |
| N3—C18 | 1.470 (4) | C11—H11A | 0.9300 |
| C1—C2 | 1.377 (4) | C12—H12A | 0.9300 |
| C1—C6 | 1.384 (4) | C15—C16 | 1.395 (4) |
| C1—H1B | 0.9300 | C15—C20 | 1.398 (4) |
| C2—C3 | 1.388 (4) | C16—C17 | 1.378 (4) |
| C2—H2B | 0.9300 | C16—H16A | 0.9300 |
| C3—C4 | 1.385 (4) | C17—C18 | 1.363 (4) |
| C3—C7 | 1.488 (3) | C17—H17A | 0.9300 |
| C4—C5 | 1.380 (4) | C18—C19 | 1.373 (4) |
| C4—H4A | 0.9300 | C19—C20 | 1.375 (3) |
| C5—C6 | 1.382 (4) | C19—H19A | 0.9300 |
| | | | |
| C13—N1—C14 | 129.3 (2) | C8—C9—H9A | 119.7 |
| C13—N1—H1A | 115.3 | C11—C10—C9 | 119.2 (3) |
| C14—N1—H1A | 115.3 | C11—C10—H10A | 120.4 |
| C14—N2—C15 | 131.7 (2) | C9—C10—H10A | 120.4 |
| C14—N2—H2A | 114.1 | C10—C11—C12 | 120.4 (3) |
| C15—N2—H2A | 114.1 | C10—C11—H11A | 119.8 |
| O2—N3—O3 | 123.9 (3) | C12—C11—H11A | 119.8 |
| O2—N3—C18 | 117.7 (3) | C7—C12—C11 | 121.8 (3) |
| O3—N3—C18 | 118.5 (2) | C7—C12—H12A | 119.1 |
| C2—C1—C6 | 121.5 (3) | C11—C12—H12A | 119.1 |
| C2—C1—H1B | 119.3 | O1—C13—N1 | 121.5 (2) |
| C6—C1—H1B | 119.3 | O1—C13—C6 | 121.3 (2) |
| C1—C2—C3 | 121.7 (2) | N1—C13—C6 | 117.2 (2) |
| C1—C2—H2B | 119.2 | N2—C14—N1 | 113.8 (2) |
| C3—C2—H2B | 119.2 | N2—C14—S1 | 129.5 (2) |
| C4—C3—C2 | 116.2 (2) | N1—C14—S1 | 116.71 (19) |
| C4—C3—C7 | 122.0 (2) | C16—C15—N2 | 125.3 (2) |
| C2—C3—C7 | 121.8 (2) | C16—C15—C20 | 117.4 (2) |
| C5—C4—C3 | 122.5 (3) | N2—C15—C20 | 117.3 (2) |
| C5—C4—H4A | 118.8 | C17—C16—C15 | 120.7 (3) |
| C3—C4—H4A | 118.8 | C17—C16—H16A | 119.6 |

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|---|---|---|---|
| C4—C5—C6 | 120.7 (2) | C15—C16—H16A | 119.6 |
| C4—C5—H5A | 119.7 | C18—C17—C16 | 119.9 (3) |
| C6—C5—H5A | 119.7 | C18—C17—H17A | 120.1 |
| C5—C6—C1 | 117.4 (2) | C16—C17—H17A | 120.1 |
| C5—C6—C13 | 125.5 (2) | C17—C18—C19 | 121.5 (3) |
| C1—C6—C13 | 117.1 (2) | C17—C18—N3 | 120.3 (3) |
| C8—C7—C12 | 116.7 (2) | C19—C18—N3 | 118.2 (3) |
| C8—C7—C3 | 121.9 (2) | C18—C19—C20 | 118.6 (3) |
| C12—C7—C3 | 121.4 (2) | C18—C19—H19A | 120.7 |
| C7—C8—C9 | 121.4 (3) | C20—C19—H19A | 120.7 |
| C7—C8—H8A | 119.3 | C19—C20—C15 | 121.8 (2) |
| C9—C8—H8A | 119.3 | C19—C20—Cl1 | 117.3 (2) |
| C10—C9—C8 | 120.5 (3) | C15—C20—Cl1 | 120.91 (19) |
| C10—C9—H9A | 119.7 | | |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | −0.2 (5) | C5—C6—C13—N1 | −6.0 (4) |
| C1—C2—C3—C4 | 1.0 (4) | C1—C6—C13—N1 | 175.1 (3) |
| C1—C2—C3—C7 | −179.3 (3) | C15—N2—C14—N1 | 178.0 (2) |
| C2—C3—C4—C5 | −0.7 (4) | C15—N2—C14—S1 | −1.8 (4) |
| C7—C3—C4—C5 | 179.6 (3) | C13—N1—C14—N2 | 4.2 (4) |
| C3—C4—C5—C6 | −0.5 (5) | C13—N1—C14—S1 | −175.9 (2) |
| C4—C5—C6—C1 | 1.3 (4) | C14—N2—C15—C16 | 0.8 (5) |
| C4—C5—C6—C13 | −177.5 (3) | C14—N2—C15—C20 | −178.8 (3) |
| C2—C1—C6—C5 | −0.9 (5) | N2—C15—C16—C17 | −179.0 (3) |
| C2—C1—C6—C13 | 178.0 (3) | C20—C15—C16—C17 | 0.6 (4) |
| C4—C3—C7—C8 | −179.0 (3) | C15—C16—C17—C18 | 1.0 (5) |
| C2—C3—C7—C8 | 1.3 (4) | C16—C17—C18—C19 | −1.6 (5) |
| C4—C3—C7—C12 | 0.9 (4) | C16—C17—C18—N3 | 179.6 (3) |
| C2—C3—C7—C12 | −178.8 (3) | O2—N3—C18—C17 | 1.9 (4) |
| C12—C7—C8—C9 | 0.5 (5) | O3—N3—C18—C17 | −177.8 (3) |
| C3—C7—C8—C9 | −179.7 (3) | O2—N3—C18—C19 | −176.9 (3) |
| C7—C8—C9—C10 | −0.8 (6) | O3—N3—C18—C19 | 3.3 (4) |
| C8—C9—C10—C11 | 0.6 (5) | C17—C18—C19—C20 | 0.5 (4) |
| C9—C10—C11—C12 | −0.1 (5) | N3—C18—C19—C20 | 179.3 (2) |
| C8—C7—C12—C11 | 0.0 (5) | C18—C19—C20—C15 | 1.2 (4) |
| C3—C7—C12—C11 | −179.8 (3) | C18—C19—C20—Cl1 | −177.9 (2) |
| C10—C11—C12—C7 | −0.2 (5) | C16—C15—C20—C19 | −1.7 (4) |
| C14—N1—C13—O1 | −4.7 (5) | N2—C15—C20—C19 | 177.9 (2) |
| C14—N1—C13—C6 | 173.9 (2) | C16—C15—C20—Cl1 | 177.3 (2) |
| C5—C6—C13—O1 | 172.6 (3) | N2—C15—C20—Cl1 | −3.1 (3) |
| C1—C6—C13—O1 | −6.2 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···Cl1 | 0.86 | 2.43 | 2.938 (2) | 118 |
| N2—H2*A*···O1 | 0.86 | 1.87 | 2.608 (3) | 143 |
| C16—H16*A*···S1 | 0.93 | 2.53 | 3.208 (3) | 130 |

| | | | | |
|---|---|---|---|---|
| C10—H10*A*···O3$^{i}$ | 0.93 | 2.57 | 3.354 (4) | 142 |
| C17—H17*A*···S1$^{ii}$ | 0.93 | 2.77 | 3.673 (3) | 165 |

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