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# 3-(3-Chloro-4-methylphenyl)-2-(4-fluorophenyl)thiazolidin-4-one

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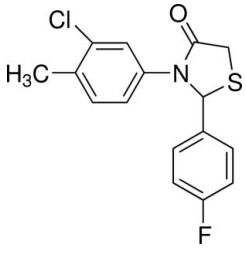
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.003 Å; disorder in main residue; $R$ factor = 0.048; $wR$ factor = 0.125; data-to-parameter ratio = 14.4.

The title compound, $C_{16}H_{13}ClFNOS$, possesses potent antibacterial activity. The overall molecular conformation is described by the dihedral angles of 43.0 (1)° between the 3-chloro-4-methylbenzene and thiazolidinone rings, and 88.8 (5)° between the thiazolidinone and 4-fluorobenzene rings. The 3-chloro-4-methylbenzene ring is disordered over two positions with occupancy factors approximately 3:1.

## Related literature

For related literature, see: Tumul Srivastava *et al.* (2002).




## Experimental

### Crystal data

$C_{16}H_{13}ClFNOS$
$M_r$ = 321.78
Orthorhombic, *Pbca*
$a$ = 12.265 (3) Å
$b$ = 12.994 (3) Å
$c$ = 18.192 (4) Å
$V$ = 2899.3 (10) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.42 mm$^{-1}$
$T$ = 113 (2) K
0.16 × 0.14 × 0.10 mm

### Data collection

Rigaku Saturn diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min}$ = 0.937, $T_{max}$ = 0.960
34208 measured reflections
3445 independent reflections
2796 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.125
$S$ = 1.12
3445 reflections
240 parameters
8 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.38 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.76 e Å$^{-3}$

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1990); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXL97*; software used to prepare material for publication: *CrystalStructure* (Rigaku/MSC, 2005).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2144).

## References

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# supporting information

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## 3-(3-Chloro-4-methylphenyl)-2-(4-fluorophenyl)thiazolidin-4-one

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### S1. Comment

In recent years, 4-thiazolidinones are the most extensively investigated class of compounds, which exhibits various biological activities, such as anticancer, antitubercular, antibacterial and herbicidal activities. In view of these properties and in a continuation of our interest in the chemistry of 4-thiazolidinones, we have attempted to synthesize a series of 4-thiazolidinone derivatives, some of which have comparatively high antibacterial activity.The crystal structure determination of the title compound, (I), was undertaken to investigate the relationship between structure and antibacterial activity (Fig. 1). The molecular conformation is described by the dihedral angle between 3-chloro-4-methyl-benzene ring and thiazolidinone ring of 43.0 (1)° and the dihedral angle between thiazolidinone ring and 4-fluorobenzene ring of 88.8 (5)°.

### S2. Experimental

Compound (I) was synthesized according to the procedure of Tumul Srivastava *et al.* (2002). A crystal of (I) suitable for X-ray analysis was grown from an ethanol solution by slow evaporation at room temperature.

### S3. Refinement

The 3-chloro-4-methylbenzene ring shows positional disorder. At the final stage of the refinement, the occupancy factors of two possible sites were fixed at 0.737 (2) and 0.263 (2), respectively. H atoms were placed in idealized positions and constrained to ride on their parent atoms, with C—H distances of 0.95 (aromatic), 0.99 (methylene), 1.00 (methylidyne) and 0.98 Å(methyl), and with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$($C_{methyl}$).

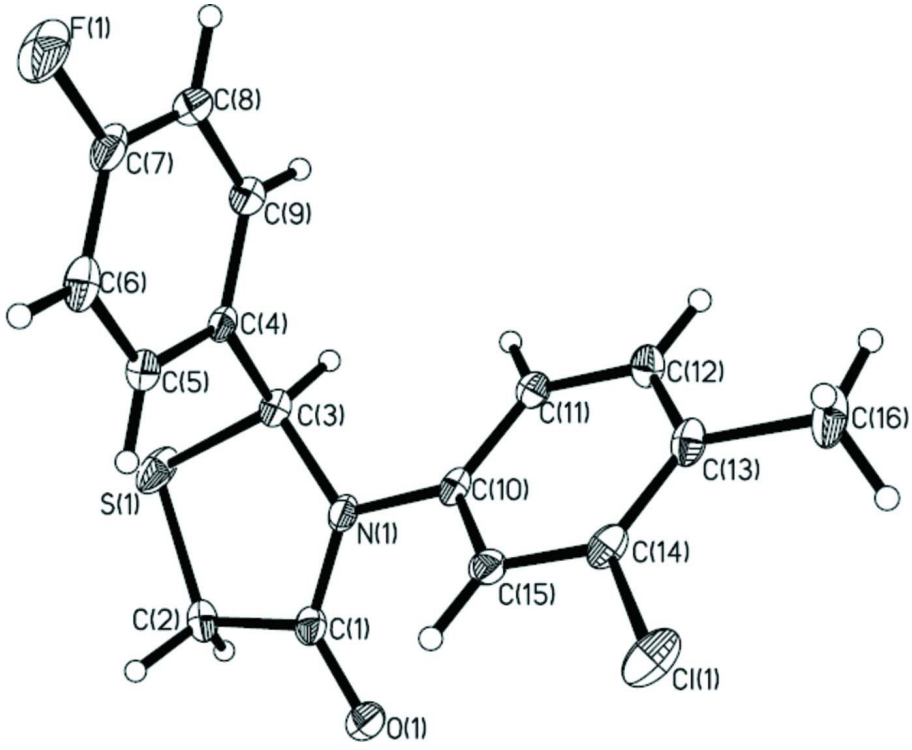


**Figure 1**

The molecular structure of (I) showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level and H atoms are shown as small spheres of arbitrary radii. Only the major component of the disorder is shown.

### 3-(3-Chloro-4-methylphenyl)-2-(4-fluorophenyl)thiazolidin-4-one

*Crystal data*

$C_{16}H_{13}ClFNOS$
$M_r = 321.78$
Orthorhombic, *Pbca*
$a = 12.265\ (3)$ Å
$b = 12.994\ (3)$ Å
$c = 18.192\ (4)$ Å
$V = 2899.3\ (10)$ Å$^3$
$Z = 8$
$F(000) = 1328$
$D_x = 1.474$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71070$ Å
Cell parameters from 6992 reflections
$\theta = 2.0$–$27.9°$
$\mu = 0.42$ mm$^{-1}$
$T = 113$ K
Block, colourless
0.16 × 0.14 × 0.10 mm

*Data collection*

Rigaku Saturn diffractometer
Radiation source: Rotating anode
Confocal monochromator
Detector resolution: 7.31 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (Jacobson, 1998)
$T_{min} = 0.937$, $T_{max} = 0.960$
34208 measured reflections
3445 independent reflections
2796 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 27.9°$, $\theta_{min} = 2.5°$
$h = -16\rightarrow15$
$k = -17\rightarrow17$
$l = -23\rightarrow23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.048$
$wR(F^2) = 0.125$
$S = 1.12$
3445 reflections
240 parameters
8 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
$w = 1/[\sigma^2(F_o^2) + (0.0666P)^2 + 0.3972P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.38$ e Å$^{-3}$
$\Delta\rho_{min} = -0.76$ e Å$^{-3}$
Extinction correction: *SHELXL*, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0157 (15)

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| S1 | 0.30373 (5) | 0.52351 (4) | 0.39652 (3) | 0.0435 (2) | |
| F1 | 0.49210 (13) | 0.10913 (11) | 0.54723 (7) | 0.0612 (4) | |
| O1 | 0.09023 (11) | 0.42265 (11) | 0.25825 (7) | 0.0344 (3) | |
| N1 | 0.25973 (12) | 0.37796 (11) | 0.29988 (7) | 0.0258 (3) | |
| C1 | 0.16844 (15) | 0.43791 (14) | 0.29819 (9) | 0.0265 (4) | |
| C2 | 0.17362 (16) | 0.52700 (14) | 0.35115 (10) | 0.0299 (4) | |
| H2A | 0.1142 | 0.5215 | 0.3878 | 0.036* | |
| H2B | 0.1650 | 0.5928 | 0.3243 | 0.036* | |
| C3 | 0.35104 (15) | 0.40902 (14) | 0.34646 (9) | 0.0262 (4) | |
| H3A | 0.4140 | 0.4287 | 0.3145 | 0.031* | |
| C4 | 0.38717 (14) | 0.32583 (13) | 0.39887 (8) | 0.0226 (4) | |
| C5 | 0.31314 (15) | 0.27742 (14) | 0.44550 (9) | 0.0270 (4) | |
| H5A | 0.2380 | 0.2950 | 0.4430 | 0.032* | |
| C6 | 0.34782 (18) | 0.20378 (14) | 0.49557 (10) | 0.0342 (4) | |
| H6A | 0.2977 | 0.1707 | 0.5276 | 0.041* | |
| C7 | 0.45733 (18) | 0.18018 (15) | 0.49737 (10) | 0.0374 (5) | |
| C8 | 0.53130 (18) | 0.22326 (18) | 0.45151 (10) | 0.0408 (5) | |
| H8A | 0.6058 | 0.2034 | 0.4535 | 0.049* | |
| C9 | 0.49613 (16) | 0.29727 (17) | 0.40134 (10) | 0.0332 (4) | |
| H9A | 0.5469 | 0.3283 | 0.3687 | 0.040* | |
| Cl1 | 0.10556 (6) | 0.05302 (5) | 0.18509 (4) | 0.0425 (3) | 0.7369 (16) |
| C10 | 0.2796 (3) | 0.2928 (2) | 0.2516 (2) | 0.0241 (9) | 0.7369 (16) |
| C11 | 0.3781 (2) | 0.2805 (2) | 0.21479 (19) | 0.0251 (7) | 0.7369 (16) |

| | | | | | |
|---|---|---|---|---|---|
| H11A | 0.4354 | 0.3287 | 0.2220 | 0.030* | 0.7369 (16) |
| C12 | 0.39283 (18) | 0.19757 (18) | 0.16753 (13) | 0.0284 (7) | 0.7369 (16) |
| H12A | 0.4601 | 0.1891 | 0.1424 | 0.034* | 0.7369 (16) |
| C13 | 0.3091 (2) | 0.12703 (14) | 0.15704 (10) | 0.0273 (7) | 0.7369 (16) |
| C14 | 0.2106 (2) | 0.13939 (18) | 0.19381 (13) | 0.0285 (7) | 0.7369 (16) |
| C15 | 0.1959 (2) | 0.2223 (2) | 0.24107 (18) | 0.0259 (7) | 0.7369 (16) |
| H15A | 0.1286 | 0.2307 | 0.2662 | 0.031* | 0.7369 (16) |
| C16 | 0.3251 (3) | 0.0370 (2) | 0.10336 (15) | 0.0426 (8) | 0.7369 (16) |
| H16A | 0.3988 | 0.0398 | 0.0827 | 0.064* | 0.7369 (16) |
| H16B | 0.2715 | 0.0420 | 0.0636 | 0.064* | 0.7369 (16) |
| H16C | 0.3152 | −0.0282 | 0.1296 | 0.064* | 0.7369 (16) |
| Cl1′ | 0.46197 (17) | 0.13594 (14) | 0.12449 (10) | 0.0381 (6) | 0.2631 (16) |
| C10′ | 0.2546 (8) | 0.2828 (6) | 0.2566 (6) | 0.023 (2) | 0.2631 (16) |
| C11′ | 0.1642 (6) | 0.2184 (6) | 0.2549 (5) | 0.0210 (18) | 0.2631 (16) |
| H11B | 0.1016 | 0.2344 | 0.2834 | 0.025* | 0.2631 (16) |
| C12′ | 0.1654 (5) | 0.1304 (5) | 0.2114 (4) | 0.032 (2) | 0.2631 (16) |
| H12B | 0.1036 | 0.0864 | 0.2102 | 0.039* | 0.2631 (16) |
| C13′ | 0.2570 (6) | 0.1070 (4) | 0.1696 (3) | 0.0234 (17) | 0.2631 (16) |
| C14′ | 0.3474 (5) | 0.1714 (5) | 0.1714 (3) | 0.0197 (16) | 0.2631 (16) |
| C15′ | 0.3462 (6) | 0.2594 (6) | 0.2149 (5) | 0.025 (2) | 0.2631 (16) |
| H15B | 0.4080 | 0.3034 | 0.2161 | 0.030* | 0.2631 (16) |
| C16′ | 0.2502 (9) | 0.0116 (6) | 0.1187 (4) | 0.0398 (19) | 0.2631 (16) |
| H16D | 0.1796 | −0.0224 | 0.1256 | 0.060* | 0.2631 (16) |
| H16E | 0.3090 | −0.0364 | 0.1310 | 0.060* | 0.2631 (16) |
| H16F | 0.2576 | 0.0334 | 0.0674 | 0.060* | 0.2631 (16) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| S1 | 0.0665 (4) | 0.0283 (3) | 0.0359 (3) | 0.0119 (2) | −0.0239 (2) | −0.0098 (2) |
| F1 | 0.1027 (12) | 0.0462 (8) | 0.0347 (7) | 0.0305 (8) | −0.0128 (7) | 0.0098 (6) |
| O1 | 0.0335 (8) | 0.0393 (8) | 0.0304 (7) | 0.0034 (6) | −0.0069 (6) | −0.0027 (6) |
| N1 | 0.0324 (8) | 0.0268 (8) | 0.0182 (7) | 0.0040 (6) | −0.0049 (6) | −0.0040 (6) |
| C1 | 0.0331 (10) | 0.0275 (9) | 0.0189 (8) | 0.0015 (7) | 0.0007 (7) | 0.0017 (7) |
| C2 | 0.0391 (11) | 0.0276 (9) | 0.0231 (9) | 0.0023 (8) | 0.0050 (8) | −0.0024 (7) |
| C3 | 0.0309 (10) | 0.0275 (9) | 0.0203 (8) | −0.0011 (7) | −0.0025 (7) | −0.0002 (7) |
| C4 | 0.0276 (9) | 0.0239 (9) | 0.0162 (8) | −0.0001 (7) | −0.0035 (6) | −0.0031 (6) |
| C5 | 0.0311 (10) | 0.0287 (9) | 0.0214 (8) | −0.0012 (7) | 0.0002 (7) | −0.0020 (7) |
| C6 | 0.0544 (13) | 0.0268 (10) | 0.0215 (9) | −0.0049 (9) | 0.0008 (8) | 0.0008 (7) |
| C7 | 0.0608 (13) | 0.0305 (10) | 0.0208 (8) | 0.0152 (9) | −0.0100 (9) | −0.0014 (7) |
| C8 | 0.0393 (11) | 0.0550 (13) | 0.0282 (10) | 0.0179 (10) | −0.0080 (9) | −0.0035 (9) |
| C9 | 0.0302 (10) | 0.0452 (12) | 0.0241 (9) | 0.0022 (8) | −0.0018 (7) | −0.0011 (8) |
| Cl1 | 0.0535 (5) | 0.0304 (4) | 0.0437 (4) | −0.0209 (3) | −0.0178 (3) | 0.0066 (3) |
| C10 | 0.032 (2) | 0.0235 (16) | 0.0173 (16) | −0.0010 (13) | −0.0065 (14) | −0.0009 (13) |
| C11 | 0.0264 (18) | 0.0251 (15) | 0.0238 (14) | −0.0027 (13) | −0.0027 (13) | −0.0022 (11) |
| C12 | 0.0331 (18) | 0.0302 (16) | 0.0220 (13) | −0.0030 (13) | 0.0025 (13) | −0.0013 (11) |
| C13 | 0.044 (2) | 0.0207 (16) | 0.0173 (13) | −0.0017 (14) | −0.0014 (14) | 0.0039 (11) |
| C14 | 0.036 (2) | 0.0262 (15) | 0.0233 (16) | −0.0052 (15) | −0.0077 (14) | 0.0044 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C15 | 0.024 (2) | 0.0317 (15) | 0.0223 (16) | −0.0002 (13) | −0.0019 (13) | 0.0028 (11) |
| C16 | 0.073 (2) | 0.0288 (15) | 0.0263 (14) | 0.0019 (15) | −0.0060 (14) | −0.0073 (11) |
| Cl1′ | 0.0519 (12) | 0.0304 (10) | 0.0321 (10) | 0.0123 (8) | 0.0154 (8) | 0.0041 (7) |
| C10′ | 0.014 (4) | 0.037 (6) | 0.018 (4) | 0.015 (4) | −0.003 (3) | −0.004 (4) |
| C11′ | 0.020 (4) | 0.026 (4) | 0.018 (4) | 0.006 (3) | 0.000 (3) | −0.011 (3) |
| C12′ | 0.037 (6) | 0.034 (5) | 0.026 (4) | 0.008 (4) | 0.000 (4) | −0.008 (3) |
| C13′ | 0.027 (5) | 0.021 (4) | 0.023 (4) | −0.005 (4) | −0.004 (4) | 0.009 (3) |
| C14′ | 0.023 (5) | 0.016 (4) | 0.020 (3) | 0.000 (3) | 0.008 (3) | 0.001 (3) |
| C15′ | 0.020 (5) | 0.036 (5) | 0.018 (4) | −0.004 (4) | 0.001 (3) | 0.009 (3) |
| C16′ | 0.060 (6) | 0.032 (4) | 0.027 (4) | 0.005 (4) | −0.014 (4) | −0.009 (3) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| S1—C2 | 1.797 (2) | C11—C12 | 1.3900 |
| S1—C3 | 1.8382 (19) | C11—H11A | 0.9500 |
| F1—C7 | 1.363 (2) | C12—C13 | 1.3900 |
| O1—C1 | 1.220 (2) | C12—H12A | 0.9500 |
| N1—C1 | 1.364 (2) | C13—C14 | 1.3900 |
| N1—C10 | 1.434 (2) | C13—C16 | 1.537 (3) |
| N1—C3 | 1.461 (2) | C14—C15 | 1.3900 |
| N1—C10′ | 1.467 (4) | C15—H15A | 0.9500 |
| C1—C2 | 1.507 (2) | C16—H16A | 0.9800 |
| C2—H2A | 0.9900 | C16—H16B | 0.9800 |
| C2—H2B | 0.9900 | C16—H16C | 0.9800 |
| C3—C4 | 1.508 (2) | Cl1′—C14′ | 1.707 (5) |
| C3—H3A | 1.0000 | C10′—C11′ | 1.3900 |
| C4—C9 | 1.388 (3) | C10′—C15′ | 1.3900 |
| C4—C5 | 1.393 (2) | C11′—C12′ | 1.3900 |
| C5—C6 | 1.388 (3) | C11′—H11B | 0.9500 |
| C5—H5A | 0.9500 | C12′—C13′ | 1.3900 |
| C6—C7 | 1.378 (3) | C12′—H12B | 0.9500 |
| C6—H6A | 0.9500 | C13′—C14′ | 1.3900 |
| C7—C8 | 1.354 (3) | C13′—C16′ | 1.549 (7) |
| C8—C9 | 1.394 (3) | C14′—C15′ | 1.3900 |
| C8—H8A | 0.9500 | C15′—H15B | 0.9500 |
| C9—H9A | 0.9500 | C16′—H16D | 0.9800 |
| Cl1—C14 | 1.716 (2) | C16′—H16E | 0.9800 |
| C10—C11 | 1.3900 | C16′—H16F | 0.9800 |
| C10—C15 | 1.3900 | | |

| | | | |
|---|---|---|---|
| C2—S1—C3 | 94.20 (8) | C12—C11—H11A | 120.0 |
| C1—N1—C10 | 124.5 (2) | C10—C11—H11A | 120.0 |
| C1—N1—C3 | 118.97 (14) | C11—C12—C13 | 120.0 |
| C10—N1—C3 | 116.0 (2) | C11—C12—H12A | 120.0 |
| C1—N1—C10′ | 115.7 (5) | C13—C12—H12A | 120.0 |
| C10—N1—C10′ | 13.6 (4) | C12—C13—C14 | 120.0 |
| C3—N1—C10′ | 125.2 (5) | C12—C13—C16 | 119.7 (2) |
| O1—C1—N1 | 124.48 (16) | C14—C13—C16 | 120.3 (2) |

| | | | |
|---|---|---|---|
| O1—C1—C2 | 122.60 (16) | C15—C14—C13 | 120.0 |
| N1—C1—C2 | 112.92 (15) | C15—C14—Cl1 | 117.82 (16) |
| C1—C2—S1 | 108.15 (13) | C13—C14—Cl1 | 122.16 (16) |
| C1—C2—H2A | 110.1 | C14—C15—C10 | 120.0 |
| S1—C2—H2A | 110.1 | C14—C15—H15A | 120.0 |
| C1—C2—H2B | 110.1 | C10—C15—H15A | 120.0 |
| S1—C2—H2B | 110.1 | C13—C16—H16A | 109.5 |
| H2A—C2—H2B | 108.4 | C13—C16—H16B | 109.5 |
| N1—C3—C4 | 113.20 (14) | H16A—C16—H16B | 109.5 |
| N1—C3—S1 | 105.60 (12) | C13—C16—H16C | 109.5 |
| C4—C3—S1 | 111.08 (11) | H16A—C16—H16C | 109.5 |
| N1—C3—H3A | 108.9 | H16B—C16—H16C | 109.5 |
| C4—C3—H3A | 108.9 | C11′—C10′—C15′ | 120.0 |
| S1—C3—H3A | 108.9 | C11′—C10′—N1 | 123.7 (5) |
| C9—C4—C5 | 119.17 (16) | C15′—C10′—N1 | 116.3 (5) |
| C9—C4—C3 | 119.69 (16) | C10′—C11′—C12′ | 120.0 |
| C5—C4—C3 | 121.14 (16) | C10′—C11′—H11B | 120.0 |
| C6—C5—C4 | 120.75 (18) | C12′—C11′—H11B | 120.0 |
| C6—C5—H5A | 119.6 | C11′—C12′—C13′ | 120.0 |
| C4—C5—H5A | 119.6 | C11′—C12′—H12B | 120.0 |
| C7—C6—C5 | 117.89 (18) | C13′—C12′—H12B | 120.0 |
| C7—C6—H6A | 121.1 | C12′—C13′—C14′ | 120.0 |
| C5—C6—H6A | 121.1 | C12′—C13′—C16′ | 117.3 (6) |
| C8—C7—F1 | 118.72 (19) | C14′—C13′—C16′ | 122.6 (6) |
| C8—C7—C6 | 123.13 (18) | C13′—C14′—C15′ | 120.0 |
| F1—C7—C6 | 118.14 (19) | C13′—C14′—Cl1′ | 118.8 (4) |
| C7—C8—C9 | 118.77 (19) | C15′—C14′—Cl1′ | 121.0 (4) |
| C7—C8—H8A | 120.6 | C14′—C15′—C10′ | 120.0 |
| C9—C8—H8A | 120.6 | C14′—C15′—H15B | 120.0 |
| C4—C9—C8 | 120.24 (19) | C10′—C15′—H15B | 120.0 |
| C4—C9—H9A | 119.9 | C13′—C16′—H16D | 109.5 |
| C8—C9—H9A | 119.9 | C13′—C16′—H16E | 109.5 |
| C11—C10—C15 | 120.0 | H16D—C16′—H16E | 109.5 |
| C11—C10—N1 | 122.16 (19) | C13′—C16′—H16F | 109.5 |
| C15—C10—N1 | 117.83 (19) | H16D—C16′—H16F | 109.5 |
| C12—C11—C10 | 120.0 | H16E—C16′—H16F | 109.5 |

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| C10—N1—C1—O1 | 4.4 (3) | C3—N1—C10—C15 | 141.68 (18) |
| C3—N1—C1—O1 | 175.57 (17) | C10′—N1—C10—C15 | 6 (3) |
| C10′—N1—C1—O1 | −7.7 (5) | C15—C10—C11—C12 | 0.0 |
| C10—N1—C1—C2 | −175.3 (2) | N1—C10—C11—C12 | −178.9 (4) |
| C3—N1—C1—C2 | −4.1 (2) | C10—C11—C12—C13 | 0.0 |
| C10′—N1—C1—C2 | 172.6 (5) | C11—C12—C13—C14 | 0.0 |
| O1—C1—C2—S1 | −178.03 (15) | C11—C12—C13—C16 | 178.6 (2) |
| N1—C1—C2—S1 | 1.69 (19) | C12—C13—C14—C15 | 0.0 |
| C3—S1—C2—C1 | 0.67 (13) | C16—C13—C14—C15 | −178.6 (2) |
| C1—N1—C3—C4 | 126.12 (17) | C12—C13—C14—Cl1 | −178.2 (2) |
| C10—N1—C3—C4 | −62.0 (3) | C16—C13—C14—Cl1 | 3.2 (3) |

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| C10′—N1—C3—C4 | −50.3 (5) | C13—C14—C15—C10 | 0.0 |
| C1—N1—C3—S1 | 4.38 (19) | Cl1—C14—C15—C10 | 178.24 (19) |
| C10—N1—C3—S1 | 176.3 (2) | C11—C10—C15—C14 | 0.0 |
| C10′—N1—C3—S1 | −172.0 (5) | N1—C10—C15—C14 | 178.9 (4) |
| C2—S1—C3—N1 | −2.61 (13) | C1—N1—C10′—C11′ | −42.6 (8) |
| C2—S1—C3—C4 | −125.71 (13) | C10—N1—C10′—C11′ | −176 (4) |
| N1—C3—C4—C9 | 127.67 (17) | C3—N1—C10′—C11′ | 133.9 (4) |
| S1—C3—C4—C9 | −113.73 (16) | C1—N1—C10′—C15′ | 136.3 (4) |
| N1—C3—C4—C5 | −52.9 (2) | C10—N1—C10′—C15′ | 3 (3) |
| S1—C3—C4—C5 | 65.75 (18) | C3—N1—C10′—C15′ | −47.2 (8) |
| C9—C4—C5—C6 | 2.0 (3) | C15′—C10′—C11′—C12′ | 0.0 |
| C3—C4—C5—C6 | −177.47 (16) | N1—C10′—C11′—C12′ | 178.9 (10) |
| C4—C5—C6—C7 | −0.2 (3) | C10′—C11′—C12′—C13′ | 0.0 |
| C5—C6—C7—C8 | −1.8 (3) | C11′—C12′—C13′—C14′ | 0.0 |
| C5—C6—C7—F1 | 178.96 (16) | C11′—C12′—C13′—C16′ | −176.3 (7) |
| F1—C7—C8—C9 | −178.89 (17) | C12′—C13′—C14′—C15′ | 0.0 |
| C6—C7—C8—C9 | 1.9 (3) | C16′—C13′—C14′—C15′ | 176.1 (7) |
| C5—C4—C9—C8 | −1.9 (3) | C12′—C13′—C14′—Cl1′ | 175.6 (5) |
| C3—C4—C9—C8 | 177.55 (17) | C16′—C13′—C14′—Cl1′ | −8.4 (7) |
| C7—C8—C9—C4 | 0.0 (3) | C13′—C14′—C15′—C10′ | 0.0 |
| C1—N1—C10—C11 | 132.0 (2) | Cl1′—C14′—C15′—C10′ | −175.5 (5) |
| C3—N1—C10—C11 | −39.4 (3) | C11′—C10′—C15′—C14′ | 0.0 |
| C10′—N1—C10—C11 | −175 (3) | N1—C10′—C15′—C14′ | −179.0 (10) |
| C1—N1—C10—C15 | −46.9 (3) | | |