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# Ethyl 4-[(4-chlorophenoxy)methyl]-2-(4-nitrophenyl)-1,3-thiazole-5-carboxylate

**Zhi-Rong Deng, Shu-Qing Wang, Wei-Li Dong* and Run-Ling Wang***

Tianjin Key Laboratory on Technologies Enabling Development of Clinical Therapeutics and Diagnostics (Theranostics), School of Pharmacy, Tianjin Medical University, Tianjin 300070, People's Republic of China
Correspondence e-mail: dwllilly@163.com

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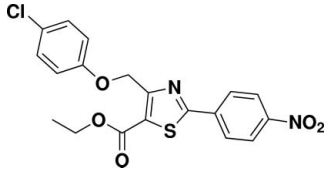
Key indicators: single-crystal X-ray study; $T$ = 113 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.058; $wR$ factor = 0.138; data-to-parameter ratio = 13.1.

The title compound, $C_{19}H_{15}ClN_2O_5S$, contains two molecules (*A* and *B*) in the asymmetric unit. In molecule *A*, the dihedral angles between the thiazole ring and the pendant chlorobenzene and nitrobenzene rings are 72.14 (15) and 3.03 (15)°, respectively. The corresponding angles for molecule *B* are 45.56 (16) and 1.51 (14)°, respectively. In the crystal, both molecules form inversion dimers linked by pairs of weak C—H···O interactions.

## Related literature

For the biological activity of related compounds and for related structures, see: Liu *et al.* (2011*a*,*b*,*c*,*d*). For further synthetic details, see: Cho *et al.* (2010).




## Experimental

### Crystal data

$C_{19}H_{15}ClN_2O_5S$
$M_r$ = 418.84
Triclinic, $P\overline{1}$
$a$ = 7.658 (2) Å
$b$ = 7.736 (2) Å
$c$ = 31.462 (9) Å
$\alpha$ = 95.414 (8)°
$\beta$ = 93.595 (13)°
$\gamma$ = 95.536 (9)°
$V$ = 1841.9 (9) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.36 mm$^{-1}$
$T$ = 113 K
0.20 × 0.18 × 0.10 mm

### Data collection

Rigaku Saturn724+ CCD diffractometer
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)
$T_{min}$ = 0.932, $T_{max}$ = 0.965
16159 measured reflections
6636 independent reflections
4821 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.138
$S$ = 1.07
6636 reflections
507 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.54 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C1—H1···O5$^{i}$ | 0.95 | 2.37 | 3.314 (4) | 172 |
| C20—H20···O10$^{ii}$ | 0.95 | 2.50 | 3.450 (4) | 173 |

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

Data collection: *CrystalClear* (Rigaku/MSC, 2005); cell refinement: *CrystalClear*; data reduction: *CrystalClear*; 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6513).

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# supporting information

*Acta Cryst.* (2011). E**67**, o3433 [https://doi.org/10.1107/S1600536811049774]

## Ethyl 4-[(4-chlorophenoxy)methyl]-2-(4-nitrophenyl)-1,3-thiazole-5-carboxylate

**Zhi-Rong Deng, Shu-Qing Wang, Wei-Li Dong and Run-Ling Wang**

### S1. Experimental

The title compound was prepared according to the literature procedures (Cho *et al.*, 2010). Colourless blocks of (I) were grown from slow evaporation of ethanol solution at room temperature.

### S2. Refinement

All the H atoms were positioned geometrically (C—H = 0.93–0.97 Å) and refined as riding with $U_{iso}$(H) = 1.2$U_{eq}$(C) or 1.5$U_{eq}$(methyl C).

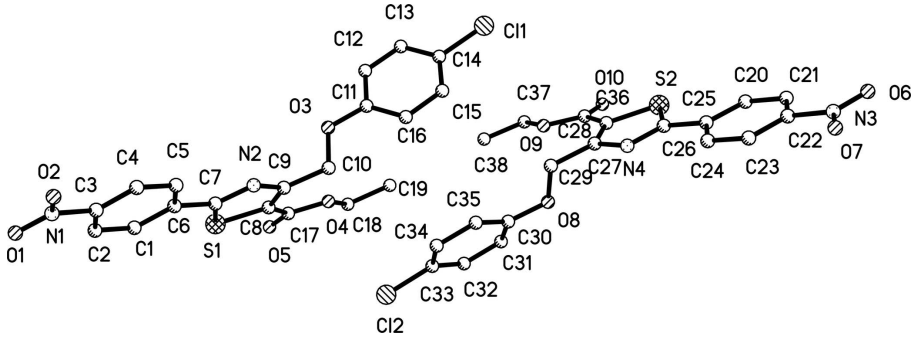


**Figure 1**

The molecular structure of (I). Displacement ellipsoids are drawn at the 30% probability level.

### Ethyl 4-[(4-chlorophenoxy)methyl]-2-(4-nitrophenyl)-1,3-thiazole-5-carboxylate

*Crystal data*

$C_{19}H_{15}ClN_2O_5S$
$M_r$ = 418.84
Triclinic, $P\overline{1}$
$a$ = 7.658 (2) Å
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$c$ = 31.462 (9) Å
$\alpha$ = 95.414 (8)°
$\beta$ = 93.595 (13)°
$\gamma$ = 95.536 (9)°
$V$ = 1841.9 (9) Å$^3$
$Z$ = 4
$F$(000) = 864
$D_x$ = 1.510 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 5373 reflections
$\theta$ = 2.0–28.0°
$\mu$ = 0.36 mm$^{-1}$
$T$ = 113 K
Block, colorless
0.20 × 0.18 × 0.10 mm

*Data collection*

Rigaku Saturn724+ CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
Detector resolution: 28.5714 pixels mm$^{-1}$
profile data from $\omega$–scans
Absorption correction: multi-scan (*CrystalClear*; Rigaku/MSC, 2005)

$T_{min}$ = 0.932, $T_{max}$ = 0.965
16159 measured reflections
6636 independent reflections
4821 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.054

$\theta_{max}$ = 25.3°, $\theta_{min}$ = 2.0°
$h$ = −9→9
$k$ = −9→9
$l$ = −34→37

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.058
$wR(F^2)$ = 0.138
$S$ = 1.07
6636 reflections
507 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
$w = 1/[\sigma^2(F_o^2) + (0.0487P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.70 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.54 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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Cl1 | 0.06288 (14) | 0.22346 (16) | 0.14799 (3) | 0.0624 (3) |
| Cl2 | 0.75805 (14) | 0.89132 (14) | 0.35049 (3) | 0.0543 (3) |
| S1 | 0.31213 (10) | 0.60383 (11) | 0.47252 (2) | 0.0282 (2) |
| S2 | 0.38418 (10) | 0.69544 (11) | 0.02723 (2) | 0.0270 (2) |
| O1 | −0.2945 (3) | 0.9265 (4) | 0.62204 (8) | 0.0494 (7) |
| O2 | −0.4697 (3) | 0.9946 (3) | 0.57059 (8) | 0.0458 (7) |
| O3 | 0.1342 (3) | 0.4482 (3) | 0.33207 (7) | 0.0371 (6) |
| O4 | 0.5159 (3) | 0.4840 (3) | 0.36414 (7) | 0.0329 (6) |
| O5 | 0.5999 (3) | 0.4344 (4) | 0.43078 (7) | 0.0481 (7) |
| O6 | 0.0810 (3) | 1.2838 (4) | −0.12206 (7) | 0.0473 (7) |
| O7 | 0.0164 (3) | 1.4680 (3) | −0.07058 (7) | 0.0431 (6) |
| O8 | 0.5491 (3) | 0.8696 (3) | 0.16726 (7) | 0.0391 (6) |
| O9 | 0.4837 (3) | 0.4928 (3) | 0.13384 (7) | 0.0393 (6) |
| O10 | 0.5477 (3) | 0.4164 (3) | 0.06707 (7) | 0.0479 (7) |
| N1 | −0.3375 (4) | 0.9339 (4) | 0.58378 (9) | 0.0351 (7) |
| N2 | 0.0807 (3) | 0.6965 (4) | 0.41884 (8) | 0.0284 (6) |
| N3 | 0.0757 (3) | 1.3317 (4) | −0.08384 (9) | 0.0329 (7) |
| N4 | 0.3024 (3) | 0.9408 (4) | 0.08080 (8) | 0.0269 (6) |
| C1 | 0.0473 (4) | 0.7472 (4) | 0.53661 (10) | 0.0273 (8) |
| H1 | 0.1548 | 0.7055 | 0.5458 | 0.033* |

| | | | | |
|---|---|---|---|---|
| C2 | −0.0636 (4) | 0.8068 (4) | 0.56656 (10) | 0.0292 (8) |
| H2 | −0.0337 | 0.8070 | 0.5963 | 0.035* |
| C3 | −0.2193 (4) | 0.8660 (4) | 0.55205 (10) | 0.0283 (8) |
| C4 | −0.2677 (4) | 0.8684 (4) | 0.50915 (10) | 0.0264 (7) |
| H4 | −0.3748 | 0.9112 | 0.5002 | 0.032* |
| C5 | −0.1574 (4) | 0.8076 (4) | 0.47948 (10) | 0.0264 (8) |
| H5 | −0.1897 | 0.8060 | 0.4498 | 0.032* |
| C6 | 0.0014 (4) | 0.7483 (4) | 0.49283 (9) | 0.0258 (7) |
| C7 | 0.1180 (4) | 0.6887 (4) | 0.45996 (10) | 0.0257 (8) |
| C8 | 0.3452 (4) | 0.5764 (4) | 0.41898 (9) | 0.0265 (8) |
| C9 | 0.2093 (4) | 0.6326 (4) | 0.39547 (10) | 0.0274 (8) |
| C10 | 0.1867 (4) | 0.6278 (5) | 0.34789 (9) | 0.0337 (8) |
| H10A | 0.0954 | 0.7027 | 0.3394 | 0.040* |
| H10B | 0.2985 | 0.6696 | 0.3362 | 0.040* |
| C11 | 0.1246 (4) | 0.4053 (5) | 0.28864 (10) | 0.0325 (8) |
| C12 | 0.0871 (4) | 0.2302 (5) | 0.27464 (11) | 0.0414 (9) |
| H12 | 0.0740 | 0.1475 | 0.2950 | 0.050* |
| C13 | 0.0684 (4) | 0.1737 (5) | 0.23175 (11) | 0.0435 (10) |
| H13 | 0.0434 | 0.0529 | 0.2224 | 0.052* |
| C14 | 0.0866 (4) | 0.2951 (6) | 0.20225 (11) | 0.0419 (10) |
| C15 | 0.1222 (5) | 0.4678 (5) | 0.21532 (11) | 0.0448 (10) |
| H15 | 0.1323 | 0.5494 | 0.1946 | 0.054* |
| C16 | 0.1441 (4) | 0.5272 (5) | 0.25884 (11) | 0.0400 (9) |
| H16 | 0.1717 | 0.6479 | 0.2680 | 0.048* |
| C17 | 0.5000 (4) | 0.4921 (5) | 0.40608 (11) | 0.0304 (8) |
| C18 | 0.6616 (4) | 0.3931 (5) | 0.34835 (11) | 0.0395 (9) |
| H18A | 0.6565 | 0.2742 | 0.3577 | 0.047* |
| H18B | 0.7758 | 0.4579 | 0.3593 | 0.047* |
| C19 | 0.6409 (4) | 0.3845 (5) | 0.30047 (10) | 0.0427 (10) |
| H19A | 0.5281 | 0.3186 | 0.2901 | 0.064* |
| H19B | 0.7370 | 0.3262 | 0.2882 | 0.064* |
| H19C | 0.6440 | 0.5030 | 0.2918 | 0.064* |
| C20 | 0.2591 (4) | 0.9569 (4) | −0.03709 (9) | 0.0254 (7) |
| H20 | 0.3027 | 0.8497 | −0.0463 | 0.030* |
| C21 | 0.2033 (4) | 1.0641 (4) | −0.06709 (10) | 0.0253 (7) |
| H21 | 0.2087 | 1.0325 | −0.0969 | 0.030* |
| C22 | 0.1395 (4) | 1.2188 (4) | −0.05227 (10) | 0.0263 (8) |
| C23 | 0.1314 (4) | 1.2715 (4) | −0.00937 (9) | 0.0260 (7) |
| H23 | 0.0880 | 1.3790 | −0.0004 | 0.031* |
| C24 | 0.1879 (4) | 1.1641 (4) | 0.02008 (10) | 0.0258 (7) |
| H24 | 0.1835 | 1.1980 | 0.0498 | 0.031* |
| C25 | 0.2512 (3) | 1.0067 (4) | 0.00690 (9) | 0.0215 (7) |
| C26 | 0.3069 (3) | 0.8944 (4) | 0.03974 (9) | 0.0227 (7) |
| C27 | 0.4094 (4) | 0.6720 (4) | 0.08080 (9) | 0.0256 (7) |
| C28 | 0.3598 (4) | 0.8142 (4) | 0.10414 (9) | 0.0260 (8) |
| C29 | 0.3674 (4) | 0.8490 (5) | 0.15229 (10) | 0.0352 (9) |
| H29A | 0.3119 | 0.9563 | 0.1607 | 0.042* |
| H29B | 0.3043 | 0.7502 | 0.1647 | 0.042* |

| | | | | |
|---|---|---|---|---|
| C30 | 0.5855 (4) | 0.8708 (5) | 0.21057 (10) | 0.0337 (9) |
| C31 | 0.7463 (4) | 0.8208 (5) | 0.22347 (11) | 0.0419 (10) |
| H31 | 0.8221 | 0.7818 | 0.2026 | 0.050* |
| C32 | 0.7992 (5) | 0.8266 (5) | 0.26642 (11) | 0.0437 (10) |
| H32 | 0.9109 | 0.7929 | 0.2751 | 0.052* |
| C33 | 0.6870 (5) | 0.8826 (5) | 0.29680 (10) | 0.0385 (9) |
| C34 | 0.5246 (4) | 0.9283 (5) | 0.28490 (11) | 0.0379 (9) |
| H34 | 0.4479 | 0.9636 | 0.3059 | 0.045* |
| C35 | 0.4729 (5) | 0.9223 (5) | 0.24120 (11) | 0.0386 (9) |
| H35 | 0.3602 | 0.9537 | 0.2325 | 0.046* |
| C36 | 0.4860 (4) | 0.5145 (5) | 0.09238 (11) | 0.0317 (8) |
| C37 | 0.5723 (6) | 0.3412 (5) | 0.14607 (12) | 0.0566 (12) |
| H37A | 0.5024 | 0.2315 | 0.1338 | 0.068* |
| H37B | 0.6898 | 0.3444 | 0.1345 | 0.068* |
| C38 | 0.5903 (6) | 0.3461 (6) | 0.19137 (12) | 0.0651 (13) |
| H38A | 0.6576 | 0.4558 | 0.2034 | 0.098* |
| H38B | 0.6522 | 0.2476 | 0.1994 | 0.098* |
| H38C | 0.4735 | 0.3381 | 0.2025 | 0.098* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0789 (8) | 0.0728 (9) | 0.0332 (6) | 0.0111 (6) | 0.0073 (5) | −0.0124 (5) |
| Cl2 | 0.0793 (7) | 0.0543 (7) | 0.0292 (5) | 0.0136 (6) | −0.0041 (5) | 0.0023 (5) |
| S1 | 0.0269 (4) | 0.0314 (5) | 0.0265 (5) | 0.0083 (4) | 0.0003 (3) | 0.0002 (4) |
| S2 | 0.0299 (4) | 0.0238 (5) | 0.0267 (5) | 0.0065 (4) | −0.0012 (3) | −0.0019 (4) |
| O1 | 0.0576 (17) | 0.063 (2) | 0.0317 (15) | 0.0229 (14) | 0.0142 (12) | 0.0032 (13) |
| O2 | 0.0411 (15) | 0.0510 (19) | 0.0493 (16) | 0.0228 (13) | 0.0121 (12) | 0.0010 (13) |
| O3 | 0.0433 (14) | 0.0385 (16) | 0.0268 (13) | −0.0016 (12) | 0.0015 (10) | −0.0046 (11) |
| O4 | 0.0287 (12) | 0.0390 (16) | 0.0329 (14) | 0.0123 (11) | 0.0078 (10) | 0.0001 (11) |
| O5 | 0.0421 (15) | 0.071 (2) | 0.0341 (14) | 0.0317 (14) | −0.0020 (11) | 0.0000 (14) |
| O6 | 0.0652 (17) | 0.0533 (19) | 0.0289 (14) | 0.0219 (14) | 0.0086 (12) | 0.0126 (13) |
| O7 | 0.0471 (15) | 0.0401 (17) | 0.0462 (16) | 0.0212 (13) | 0.0030 (12) | 0.0088 (13) |
| O8 | 0.0378 (14) | 0.0485 (18) | 0.0278 (13) | −0.0048 (12) | −0.0015 (10) | −0.0016 (12) |
| O9 | 0.0582 (16) | 0.0258 (15) | 0.0341 (14) | 0.0139 (12) | −0.0096 (11) | 0.0026 (11) |
| O10 | 0.0687 (18) | 0.0373 (17) | 0.0391 (15) | 0.0269 (14) | −0.0019 (13) | −0.0062 (12) |
| N1 | 0.0354 (17) | 0.0311 (19) | 0.0399 (19) | 0.0074 (14) | 0.0118 (14) | −0.0004 (15) |
| N2 | 0.0306 (15) | 0.0284 (17) | 0.0264 (15) | 0.0072 (12) | 0.0024 (12) | −0.0004 (12) |
| N3 | 0.0274 (15) | 0.038 (2) | 0.0357 (18) | 0.0065 (14) | 0.0037 (12) | 0.0100 (14) |
| N4 | 0.0283 (15) | 0.0282 (17) | 0.0250 (15) | 0.0064 (12) | 0.0047 (11) | 0.0014 (12) |
| C1 | 0.0223 (16) | 0.029 (2) | 0.0310 (19) | 0.0076 (14) | −0.0013 (13) | 0.0005 (15) |
| C2 | 0.0328 (18) | 0.028 (2) | 0.0263 (18) | 0.0046 (15) | 0.0030 (14) | 0.0008 (15) |
| C3 | 0.0315 (18) | 0.0208 (19) | 0.0336 (19) | 0.0064 (15) | 0.0109 (14) | −0.0009 (15) |
| C4 | 0.0234 (17) | 0.0211 (19) | 0.0341 (19) | 0.0030 (14) | 0.0013 (14) | −0.0001 (15) |
| C5 | 0.0274 (17) | 0.024 (2) | 0.0271 (18) | 0.0039 (14) | 0.0002 (13) | −0.0004 (14) |
| C6 | 0.0298 (17) | 0.0201 (19) | 0.0271 (18) | 0.0032 (14) | 0.0014 (13) | 0.0009 (14) |
| C7 | 0.0242 (17) | 0.0207 (19) | 0.0312 (19) | 0.0023 (14) | −0.0015 (13) | 0.0001 (15) |
| C8 | 0.0281 (17) | 0.023 (2) | 0.0272 (18) | 0.0034 (14) | 0.0018 (13) | −0.0023 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0305 (18) | 0.029 (2) | 0.0237 (17) | 0.0053 (15) | 0.0063 (13) | 0.0010 (15) |
| C10 | 0.0356 (19) | 0.038 (2) | 0.0285 (19) | 0.0097 (17) | 0.0048 (14) | −0.0002 (16) |
| C11 | 0.0260 (18) | 0.044 (2) | 0.0272 (19) | 0.0087 (16) | 0.0039 (14) | −0.0024 (17) |
| C12 | 0.046 (2) | 0.038 (3) | 0.039 (2) | −0.0013 (18) | 0.0043 (17) | 0.0000 (18) |
| C13 | 0.041 (2) | 0.042 (3) | 0.045 (2) | 0.0008 (19) | 0.0050 (17) | −0.005 (2) |
| C14 | 0.039 (2) | 0.055 (3) | 0.032 (2) | 0.0090 (19) | 0.0072 (16) | −0.0057 (19) |
| C15 | 0.057 (2) | 0.044 (3) | 0.036 (2) | 0.013 (2) | 0.0135 (18) | 0.0045 (19) |
| C16 | 0.044 (2) | 0.044 (3) | 0.035 (2) | 0.0099 (18) | 0.0080 (16) | 0.0050 (18) |
| C17 | 0.0273 (18) | 0.028 (2) | 0.035 (2) | 0.0039 (15) | 0.0023 (15) | −0.0031 (16) |
| C18 | 0.0293 (19) | 0.044 (3) | 0.047 (2) | 0.0147 (17) | 0.0132 (16) | −0.0025 (18) |
| C19 | 0.048 (2) | 0.040 (3) | 0.042 (2) | 0.0097 (18) | 0.0189 (17) | 0.0019 (18) |
| C20 | 0.0247 (17) | 0.024 (2) | 0.0281 (18) | 0.0072 (14) | 0.0024 (13) | 0.0014 (14) |
| C21 | 0.0236 (16) | 0.025 (2) | 0.0256 (18) | 0.0000 (14) | 0.0024 (13) | −0.0012 (14) |
| C22 | 0.0198 (16) | 0.029 (2) | 0.0313 (19) | 0.0034 (14) | 0.0002 (13) | 0.0070 (15) |
| C23 | 0.0197 (16) | 0.026 (2) | 0.0318 (19) | 0.0017 (14) | 0.0022 (13) | 0.0004 (15) |
| C24 | 0.0228 (16) | 0.030 (2) | 0.0239 (17) | 0.0051 (14) | 0.0022 (13) | −0.0019 (15) |
| C25 | 0.0164 (15) | 0.0236 (19) | 0.0235 (17) | −0.0007 (13) | 0.0004 (12) | 0.0011 (14) |
| C26 | 0.0178 (16) | 0.0202 (19) | 0.0291 (18) | 0.0002 (13) | 0.0008 (13) | −0.0008 (14) |
| C27 | 0.0251 (17) | 0.028 (2) | 0.0241 (17) | 0.0036 (14) | −0.0020 (13) | 0.0046 (14) |
| C28 | 0.0245 (17) | 0.029 (2) | 0.0242 (17) | 0.0018 (15) | −0.0003 (13) | 0.0019 (15) |
| C29 | 0.038 (2) | 0.037 (2) | 0.032 (2) | 0.0064 (17) | 0.0060 (15) | 0.0045 (17) |
| C30 | 0.047 (2) | 0.028 (2) | 0.0230 (18) | −0.0080 (17) | 0.0034 (15) | −0.0012 (15) |
| C31 | 0.039 (2) | 0.051 (3) | 0.034 (2) | 0.0018 (18) | 0.0027 (16) | −0.0033 (19) |
| C32 | 0.046 (2) | 0.048 (3) | 0.037 (2) | 0.0106 (19) | 0.0025 (17) | −0.0035 (19) |
| C33 | 0.062 (2) | 0.026 (2) | 0.0265 (19) | 0.0013 (18) | 0.0015 (17) | 0.0006 (16) |
| C34 | 0.049 (2) | 0.032 (2) | 0.033 (2) | 0.0055 (18) | 0.0071 (16) | 0.0002 (17) |
| C35 | 0.045 (2) | 0.037 (2) | 0.035 (2) | 0.0054 (18) | 0.0081 (16) | −0.0008 (17) |
| C36 | 0.0324 (19) | 0.031 (2) | 0.030 (2) | 0.0027 (16) | −0.0089 (15) | 0.0029 (16) |
| C37 | 0.103 (3) | 0.026 (2) | 0.042 (2) | 0.023 (2) | −0.011 (2) | 0.0083 (19) |
| C38 | 0.090 (3) | 0.040 (3) | 0.064 (3) | 0.015 (2) | −0.025 (2) | 0.010 (2) |

*Geometric parameters (Å, º)*

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| Cl1—C14 | 1.737 (3) | C12—H12 | 0.9500 |
| Cl2—C33 | 1.735 (3) | C13—C14 | 1.385 (5) |
| S1—C8 | 1.716 (3) | C13—H13 | 0.9500 |
| S1—C7 | 1.721 (3) | C14—C15 | 1.357 (5) |
| S2—C27 | 1.713 (3) | C15—C16 | 1.397 (4) |
| S2—C26 | 1.722 (3) | C15—H15 | 0.9500 |
| O1—N1 | 1.236 (3) | C16—H16 | 0.9500 |
| O2—N1 | 1.222 (3) | C18—C19 | 1.499 (4) |
| O3—C11 | 1.371 (4) | C18—H18A | 0.9900 |
| O3—C10 | 1.441 (4) | C18—H18B | 0.9900 |
| O4—C17 | 1.329 (4) | C19—H19A | 0.9800 |
| O4—C18 | 1.463 (3) | C19—H19B | 0.9800 |
| O5—C17 | 1.202 (4) | C19—H19C | 0.9800 |
| O6—N3 | 1.229 (3) | C20—C21 | 1.388 (4) |
| O7—N3 | 1.235 (3) | C20—C25 | 1.408 (4) |

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|---|---|---|---|
| O8—C30 | 1.373 (4) | C20—H20 | 0.9500 |
| O8—C29 | 1.430 (4) | C21—C22 | 1.387 (4) |
| O9—C36 | 1.332 (4) | C21—H21 | 0.9500 |
| O9—C37 | 1.480 (4) | C22—C23 | 1.380 (4) |
| O10—C36 | 1.198 (4) | C23—C24 | 1.379 (4) |
| N1—C3 | 1.483 (4) | C23—H23 | 0.9500 |
| N2—C7 | 1.316 (4) | C24—C25 | 1.391 (4) |
| N2—C9 | 1.368 (4) | C24—H24 | 0.9500 |
| N3—C22 | 1.475 (4) | C25—C26 | 1.479 (4) |
| N4—C26 | 1.311 (4) | C27—C28 | 1.363 (4) |
| N4—C28 | 1.368 (4) | C27—C36 | 1.468 (5) |
| C1—C2 | 1.384 (4) | C28—C29 | 1.510 (4) |
| C1—C6 | 1.401 (4) | C29—H29A | 0.9900 |
| C1—H1 | 0.9500 | C29—H29B | 0.9900 |
| C2—C3 | 1.384 (4) | C30—C31 | 1.375 (5) |
| C2—H2 | 0.9500 | C30—C35 | 1.389 (4) |
| C3—C4 | 1.380 (4) | C31—C32 | 1.381 (4) |
| C4—C5 | 1.378 (4) | C31—H31 | 0.9500 |
| C4—H4 | 0.9500 | C32—C33 | 1.391 (5) |
| C5—C6 | 1.395 (4) | C32—H32 | 0.9500 |
| C5—H5 | 0.9500 | C33—C34 | 1.365 (5) |
| C6—C7 | 1.478 (4) | C34—C35 | 1.402 (4) |
| C8—C9 | 1.368 (4) | C34—H34 | 0.9500 |
| C8—C17 | 1.468 (4) | C35—H35 | 0.9500 |
| C9—C10 | 1.493 (4) | C37—C38 | 1.420 (5) |
| C10—H10A | 0.9900 | C37—H37A | 0.9900 |
| C10—H10B | 0.9900 | C37—H37B | 0.9900 |
| C11—C12 | 1.382 (5) | C38—H38A | 0.9800 |
| C11—C16 | 1.395 (5) | C38—H38B | 0.9800 |
| C12—C13 | 1.373 (4) | C38—H38C | 0.9800 |

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|---|---|---|---|
| C8—S1—C7 | 89.05 (15) | H18A—C18—H18B | 108.7 |
| C27—S2—C26 | 89.03 (15) | C18—C19—H19A | 109.5 |
| C11—O3—C10 | 117.6 (3) | C18—C19—H19B | 109.5 |
| C17—O4—C18 | 116.1 (3) | H19A—C19—H19B | 109.5 |
| C30—O8—C29 | 116.6 (2) | C18—C19—H19C | 109.5 |
| C36—O9—C37 | 113.7 (3) | H19A—C19—H19C | 109.5 |
| O2—N1—O1 | 124.3 (3) | H19B—C19—H19C | 109.5 |
| O2—N1—C3 | 118.3 (3) | C21—C20—C25 | 120.1 (3) |
| O1—N1—C3 | 117.5 (3) | C21—C20—H20 | 119.9 |
| C7—N2—C9 | 110.5 (3) | C25—C20—H20 | 119.9 |
| O6—N3—O7 | 123.3 (3) | C20—C21—C22 | 118.0 (3) |
| O6—N3—C22 | 118.3 (3) | C20—C21—H21 | 121.0 |
| O7—N3—C22 | 118.4 (3) | C22—C21—H21 | 121.0 |
| C26—N4—C28 | 110.4 (3) | C23—C22—C21 | 123.2 (3) |
| C2—C1—C6 | 120.1 (3) | C23—C22—N3 | 118.3 (3) |
| C2—C1—H1 | 120.0 | C21—C22—N3 | 118.5 (3) |
| C6—C1—H1 | 120.0 | C22—C23—C24 | 118.2 (3) |

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| C1—C2—C3 | 118.4 (3) | C22—C23—H23 | 120.9 |
| C1—C2—H2 | 120.8 | C24—C23—H23 | 120.9 |
| C3—C2—H2 | 120.8 | C23—C24—C25 | 120.9 (3) |
| C4—C3—C2 | 122.7 (3) | C23—C24—H24 | 119.6 |
| C4—C3—N1 | 118.3 (3) | C25—C24—H24 | 119.6 |
| C2—C3—N1 | 118.9 (3) | C24—C25—C20 | 119.6 (3) |
| C5—C4—C3 | 118.7 (3) | C24—C25—C26 | 118.8 (3) |
| C5—C4—H4 | 120.7 | C20—C25—C26 | 121.6 (3) |
| C3—C4—H4 | 120.7 | N4—C26—C25 | 122.0 (3) |
| C4—C5—C6 | 120.3 (3) | N4—C26—S2 | 115.0 (2) |
| C4—C5—H5 | 119.8 | C25—C26—S2 | 122.9 (2) |
| C6—C5—H5 | 119.8 | C28—C27—C36 | 133.4 (3) |
| C5—C6—C1 | 119.8 (3) | C28—C27—S2 | 110.2 (3) |
| C5—C6—C7 | 118.6 (3) | C36—C27—S2 | 116.3 (2) |
| C1—C6—C7 | 121.6 (3) | C27—C28—N4 | 115.4 (3) |
| N2—C7—C6 | 122.3 (3) | C27—C28—C29 | 127.3 (3) |
| N2—C7—S1 | 115.0 (2) | N4—C28—C29 | 117.2 (3) |
| C6—C7—S1 | 122.6 (2) | O8—C29—C28 | 107.0 (2) |
| C9—C8—C17 | 131.6 (3) | O8—C29—H29A | 110.3 |
| C9—C8—S1 | 110.3 (2) | C28—C29—H29A | 110.3 |
| C17—C8—S1 | 118.0 (2) | O8—C29—H29B | 110.3 |
| N2—C9—C8 | 115.1 (3) | C28—C29—H29B | 110.3 |
| N2—C9—C10 | 117.9 (3) | H29A—C29—H29B | 108.6 |
| C8—C9—C10 | 126.9 (3) | O8—C30—C31 | 116.4 (3) |
| O3—C10—C9 | 106.2 (3) | O8—C30—C35 | 124.2 (3) |
| O3—C10—H10A | 110.5 | C31—C30—C35 | 119.4 (3) |
| C9—C10—H10A | 110.5 | C30—C31—C32 | 120.8 (3) |
| O3—C10—H10B | 110.5 | C30—C31—H31 | 119.6 |
| C9—C10—H10B | 110.5 | C32—C31—H31 | 119.6 |
| H10A—C10—H10B | 108.7 | C31—C32—C33 | 119.3 (4) |
| O3—C11—C12 | 116.3 (3) | C31—C32—H32 | 120.4 |
| O3—C11—C16 | 124.0 (3) | C33—C32—H32 | 120.4 |
| C12—C11—C16 | 119.7 (3) | C34—C33—C32 | 121.2 (3) |
| C13—C12—C11 | 121.0 (4) | C34—C33—Cl2 | 120.6 (3) |
| C13—C12—H12 | 119.5 | C32—C33—Cl2 | 118.3 (3) |
| C11—C12—H12 | 119.5 | C33—C34—C35 | 119.0 (3) |
| C12—C13—C14 | 119.1 (4) | C33—C34—H34 | 120.5 |
| C12—C13—H13 | 120.4 | C35—C34—H34 | 120.5 |
| C14—C13—H13 | 120.4 | C30—C35—C34 | 120.4 (3) |
| C15—C14—C13 | 120.8 (3) | C30—C35—H35 | 119.8 |
| C15—C14—Cl1 | 120.1 (3) | C34—C35—H35 | 119.8 |
| C13—C14—Cl1 | 119.1 (3) | O10—C36—O9 | 123.2 (3) |
| C14—C15—C16 | 120.8 (4) | O10—C36—C27 | 123.2 (3) |
| C14—C15—H15 | 119.6 | O9—C36—C27 | 113.7 (3) |
| C16—C15—H15 | 119.6 | C38—C37—O9 | 109.6 (3) |
| C11—C16—C15 | 118.5 (4) | C38—C37—H37A | 109.8 |
| C11—C16—H16 | 120.7 | O9—C37—H37A | 109.8 |
| C15—C16—H16 | 120.7 | C38—C37—H37B | 109.8 |

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|---|---|---|---|
| O5—C17—O4 | 123.8 (3) | O9—C37—H37B | 109.8 |
| O5—C17—C8 | 123.5 (3) | H37A—C37—H37B | 108.2 |
| O4—C17—C8 | 112.7 (3) | C37—C38—H38A | 109.5 |
| O4—C18—C19 | 106.2 (3) | C37—C38—H38B | 109.5 |
| O4—C18—H18A | 110.5 | H38A—C38—H38B | 109.5 |
| C19—C18—H18A | 110.5 | C37—C38—H38C | 109.5 |
| O4—C18—H18B | 110.5 | H38A—C38—H38C | 109.5 |
| C19—C18—H18B | 110.5 | H38B—C38—H38C | 109.5 |

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|---|---|---|---|
| C6—C1—C2—C3 | 0.2 (5) | C25—C20—C21—C22 | −0.4 (4) |
| C1—C2—C3—C4 | −0.2 (5) | C20—C21—C22—C23 | 0.9 (4) |
| C1—C2—C3—N1 | −178.6 (3) | C20—C21—C22—N3 | −178.5 (3) |
| O2—N1—C3—C4 | −2.4 (5) | O6—N3—C22—C23 | −179.2 (3) |
| O1—N1—C3—C4 | 178.1 (3) | O7—N3—C22—C23 | −0.5 (4) |
| O2—N1—C3—C2 | 176.1 (3) | O6—N3—C22—C21 | 0.3 (4) |
| O1—N1—C3—C2 | −3.4 (5) | O7—N3—C22—C21 | 178.9 (3) |
| C2—C3—C4—C5 | 0.7 (5) | C21—C22—C23—C24 | −0.6 (4) |
| N1—C3—C4—C5 | 179.2 (3) | N3—C22—C23—C24 | 178.7 (3) |
| C3—C4—C5—C6 | −1.3 (5) | C22—C23—C24—C25 | −0.1 (4) |
| C4—C5—C6—C1 | 1.4 (5) | C23—C24—C25—C20 | 0.5 (4) |
| C4—C5—C6—C7 | −178.3 (3) | C23—C24—C25—C26 | −178.8 (3) |
| C2—C1—C6—C5 | −0.8 (5) | C21—C20—C25—C24 | −0.2 (4) |
| C2—C1—C6—C7 | 178.9 (3) | C21—C20—C25—C26 | 179.0 (3) |
| C9—N2—C7—C6 | −179.7 (3) | C28—N4—C26—C25 | 179.8 (3) |
| C9—N2—C7—S1 | 0.2 (4) | C28—N4—C26—S2 | −0.9 (3) |
| C5—C6—C7—N2 | 2.9 (5) | C24—C25—C26—N4 | −1.8 (4) |
| C1—C6—C7—N2 | −176.8 (3) | C20—C25—C26—N4 | 179.0 (3) |
| C5—C6—C7—S1 | −177.0 (2) | C24—C25—C26—S2 | 179.0 (2) |
| C1—C6—C7—S1 | 3.3 (4) | C20—C25—C26—S2 | −0.3 (4) |
| C8—S1—C7—N2 | −0.2 (3) | C27—S2—C26—N4 | 0.8 (2) |
| C8—S1—C7—C6 | 179.7 (3) | C27—S2—C26—C25 | −179.9 (3) |
| C7—S1—C8—C9 | 0.1 (3) | C26—S2—C27—C28 | −0.4 (2) |
| C7—S1—C8—C17 | −176.7 (3) | C26—S2—C27—C36 | −177.3 (3) |
| C7—N2—C9—C8 | −0.2 (4) | C36—C27—C28—N4 | 176.2 (3) |
| C7—N2—C9—C10 | 178.7 (3) | S2—C27—C28—N4 | 0.0 (3) |
| C17—C8—C9—N2 | 176.2 (3) | C36—C27—C28—C29 | −1.5 (6) |
| S1—C8—C9—N2 | 0.0 (4) | S2—C27—C28—C29 | −177.6 (2) |
| C17—C8—C9—C10 | −2.6 (6) | C26—N4—C28—C27 | 0.6 (4) |
| S1—C8—C9—C10 | −178.7 (3) | C26—N4—C28—C29 | 178.5 (2) |
| C11—O3—C10—C9 | −172.6 (2) | C30—O8—C29—C28 | −168.5 (3) |
| N2—C9—C10—O3 | −104.0 (3) | C27—C28—C29—O8 | 65.7 (4) |
| C8—C9—C10—O3 | 74.7 (4) | N4—C28—C29—O8 | −111.9 (3) |
| C10—O3—C11—C12 | 175.2 (3) | C29—O8—C30—C31 | 154.8 (3) |
| C10—O3—C11—C16 | −7.1 (4) | C29—O8—C30—C35 | −26.7 (5) |
| O3—C11—C12—C13 | 177.7 (3) | O8—C30—C31—C32 | 176.5 (3) |
| C16—C11—C12—C13 | −0.1 (5) | C35—C30—C31—C32 | −2.1 (6) |
| C11—C12—C13—C14 | −0.4 (5) | C30—C31—C32—C33 | 0.5 (6) |
| C12—C13—C14—C15 | −0.1 (5) | C31—C32—C33—C34 | 1.3 (6) |

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|---|---|---|---|
| C12—C13—C14—Cl1 | 180.0 (3) | C31—C32—C33—Cl2 | −179.2 (3) |
| C13—C14—C15—C16 | 1.0 (6) | C32—C33—C34—C35 | −1.5 (6) |
| Cl1—C14—C15—C16 | −179.1 (3) | Cl2—C33—C34—C35 | 179.0 (3) |
| O3—C11—C16—C15 | −176.6 (3) | O8—C30—C35—C34 | −176.6 (3) |
| C12—C11—C16—C15 | 1.0 (5) | C31—C30—C35—C34 | 1.8 (5) |
| C14—C15—C16—C11 | −1.5 (5) | C33—C34—C35—C30 | 0.0 (5) |
| C18—O4—C17—O5 | 2.2 (5) | C37—O9—C36—O10 | 2.9 (5) |
| C18—O4—C17—C8 | −176.8 (3) | C37—O9—C36—C27 | −175.8 (3) |
| C9—C8—C17—O5 | −172.4 (4) | C28—C27—C36—O10 | −167.3 (3) |
| S1—C8—C17—O5 | 3.5 (5) | S2—C27—C36—O10 | 8.7 (5) |
| C9—C8—C17—O4 | 6.6 (5) | C28—C27—C36—O9 | 11.4 (5) |
| S1—C8—C17—O4 | −177.5 (2) | S2—C27—C36—O9 | −172.6 (2) |
| C17—O4—C18—C19 | 174.1 (3) | C36—O9—C37—C38 | 169.9 (3) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C1—H1···O5$^{i}$ | 0.95 | 2.37 | 3.314 (4) | 172 |
| C20—H20···O10$^{ii}$ | 0.95 | 2.50 | 3.450 (4) | 173 |

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