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# (*E*)-*N*′-(4-Chlorobenzylidene)-3,4,5-trimethoxybenzohydrazide

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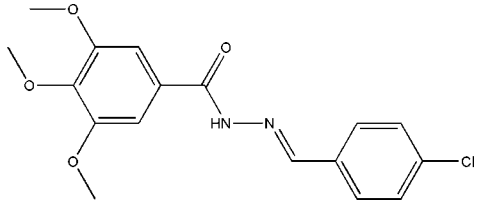
Key indicators: single-crystal X-ray study; $T$ = 273 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.046; $wR$ factor = 0.128; data-to-parameter ratio = 13.1.

The title compound, $C_{17}H_{17}ClN_2O_4$, was synthesized from 3,4,5-trimethoxybenzohydrazide and 4-chlorobenzaldehyde. In the crystal structure, packing is stabilized by intramolecular C—H···O and intermolecular N—H···O and C—H···O hydrogen-bonding interactions.

## Related literature

For related literature, see: Yang *et al.* (1996); Nawar *et al.* (2000); Gardner *et al.* (1991); Labouta *et al.* (1989); Wang *et al.* (2008); Allen *et al.* (1987).



## Experimental

### Crystal data

$C_{17}H_{17}ClN_2O_4$
$M_r$ = 348.78
Triclinic, $P\overline{1}$
$a$ = 5.119 (2) Å
$b$ = 8.210 (4) Å
$c$ = 20.276 (9) Å
$\alpha$ = 101.055 (7)°
$\beta$ = 92.362 (7)°
$\gamma$ = 101.459 (7)°
$V$ = 816.9 (7) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.26 mm$^{-1}$
$T$ = 273 (2) K
0.12 × 0.10 × 0.06 mm

### Data collection

Bruker APEX CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.970, $T_{max}$ = 0.985
4307 measured reflections
2860 independent reflections
2497 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
$S$ = 1.03
2860 reflections
218 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N2—H2···O1$^{i}$ | 0.86 | 2.18 | 2.943 (3) | 147 |
| C8—H8*C*···O4 | 0.96 | 2.26 | 2.896 (4) | 123 |
| C11—H11···O1$^{i}$ | 0.93 | 2.43 | 3.145 (3) | 134 |
| C16—H16···O1$^{ii}$ | 0.93 | 2.57 | 3.368 (3) | 144 |

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); 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*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2683).

## References

Allen, F. H., Kennard, O., Watson, D. G., Brammer, L., Orpen, A. G. & Taylor, R. (1987). *J. Chem. Soc. Perkin Trans. 2*, pp. S1–19.
Bruker (1997). *SAINT* and *SMART*. Bruker AXS, Inc., Madison, Wisconsin, USA.
Gardner, T. S., Weins, R. & Lee, J. (1991). *J. Org. Chem.* **26**, 1514–1530.
Labouta, I. M., Hassan, A. M., Aboulwafa, O. M. & Kader, O. (1989). *Monatsh. Chem.* **120**, 571–574.
Nawar, N. & Hosny, N. M. (2000). *Transition Met. Chem.* **25**, 1–8.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Wang, Y.-M., Zhao, Z.-D., Chen, Y.-X. & Bi, L.-W. (2008). *Acta Cryst.* E**64**, o1009.
Yang, Z. Y., Yang, R. D. & Yu, K. B. (1996). *Polyhedron*, **15**, 3749–3753.

# supporting information

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## (*E*)-*N*′-(4-Chlorobenzylidene)-3,4,5-trimethoxybenzohydrazide

**Yu-Min Wang, Zhen-Dong Zhao, Yu-Xiang Chen and Liang-Wu Bi**

### S1. Comment

3,4,5-Trimethoxybenzohydrazide and their deviatives show moderate fungicidal and anti-bacterial activities (Gardner *et al.*, 1991). The antibacterial activity of formylhydrazines and formylhydrazones has been reported by Labouta *et al.* (1989). Many derivatives of formylhydrazines have interesting biological properties. So we synthesized several derivatives of 3,4,5-trimethoxybenzohydrazide. In our previous paper we have reported the crystal structure of (*E*)—*N*′-(2-hydroxybenzylidene)-3,4,5-trimethoxybenzohydrazide (Wang *et al.*, 2008). Now we synthesized the title compound (I) and report here its crystal structure.

The molecular structure of (I) is shown in Fig. 1. All bond lengths and angles in (I) are normal (Allen *et al.*, 1987). In the crystal structure, there exist intramolecular C—H···O, and intermolecular N—H···O and C—H···O hydrogen bonding interactions (Table 1, Fig. 2).

### S2. Experimental

An ethanol solution (50 ml) of 3,4,5-trimethoxybenzohydrazide (0.01 mol) and 4-chlorobenzaldehyde (0.01 mol) was refluxed and stirred for 2 h; the mixture was cooled and the resulting solid product, (I), was collected by filtration. Crystals suitable for single-crystal X-ray diffraction were grown by slow evaporation of a solution in THF.

### S3. Refinement

All H atoms were placed geometrically with C—H= 0.93–0.96 Å and N—H = 0.86 Å, and included in the refinement in riding motion approximation with $U_{iso}$(H) = 1.2 or 1.5$U_{eq}$ of the carrier atom.

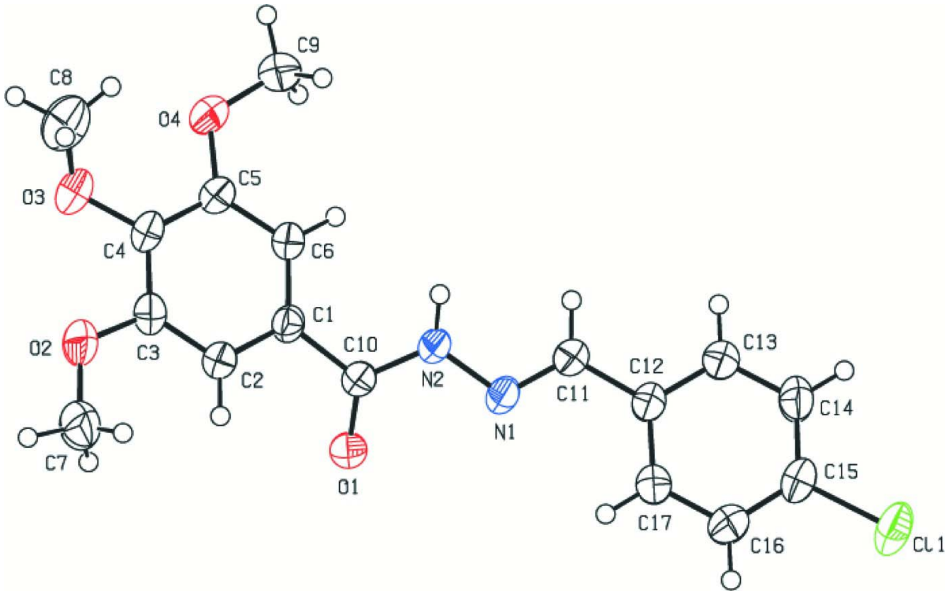


**Figure 1**

A view of the molecular structure of (I), showing displacement ellipsoids at the 50% probability level.

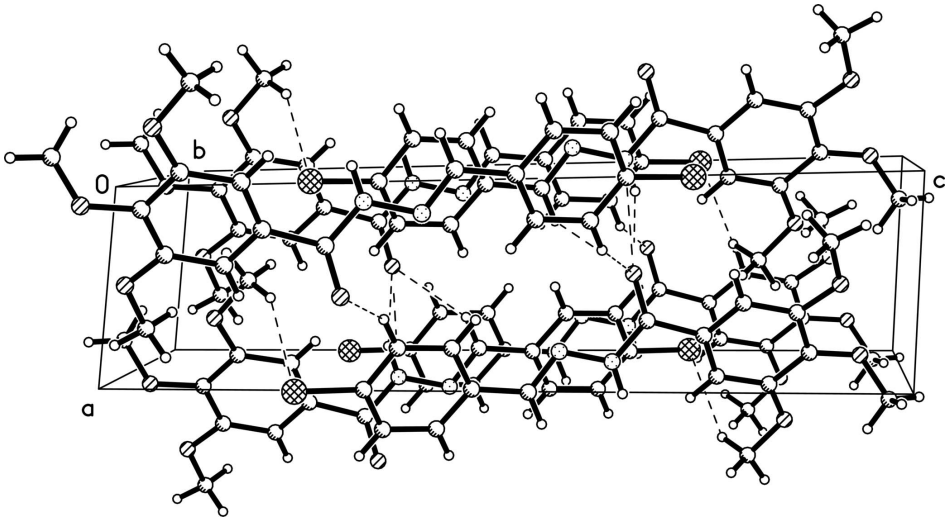


**Figure 2**

Packing diagram of the title structure.

### (*E*)-*N*′-(4-Chlorobenzylidene)-3,4,5-trimethoxybenzohydrazide

*Crystal data*

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$M_r = 348.78$
Triclinic, $P\overline{1}$
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$a = 5.119$ (2) Å
$b = 8.210$ (4) Å
$c = 20.276$ (9) Å
$\alpha = 101.055$ (7)°
$\beta = 92.362$ (7)°
$\gamma = 101.459$ (7)°
$V = 816.9$ (7) Å$^3$
$Z = 2$
$F(000) = 364$
$D_x = 1.418$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2557 reflections
$\theta = 2.6$–28.3°
$\mu = 0.26$ mm$^{-1}$

$T$ = 273 K
Block, yellow

0.12 × 0.10 × 0.06 mm

*Data collection*

Bruker APEX CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.970, $T_{max}$ = 0.985

4307 measured reflections
2860 independent reflections
2497 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.017
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.1°
$h$ = −6→6
$k$ = −9→9
$l$ = −18→24

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.128
$S$ = 1.03
2860 reflections
218 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
$w = 1/[\sigma^2(F_o^2) + (0.0602P)^2 + 0.4783P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.060 (5)

*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 | 0.98386 (15) | −0.10593 (8) | 0.26691 (3) | 0.0637 (2) |
| O1 | 0.5118 (3) | 0.4117 (2) | 0.66278 (7) | 0.0510 (4) |
| O2 | 0.5848 (4) | 0.5136 (2) | 0.92020 (8) | 0.0634 (5) |
| O3 | 0.9795 (4) | 0.7795 (3) | 0.95374 (9) | 0.0883 (7) |
| O4 | 1.3253 (4) | 0.8754 (2) | 0.86389 (9) | 0.0703 (6) |
| N1 | 0.8782 (3) | 0.3395 (2) | 0.57654 (8) | 0.0396 (4) |
| N2 | 0.9449 (3) | 0.4260 (2) | 0.64227 (8) | 0.0393 (4) |
| H2 | 1.1099 | 0.4630 | 0.6572 | 0.047* |
| C1 | 0.8360 (4) | 0.5329 (2) | 0.75470 (9) | 0.0365 (4) |
| C2 | 0.6692 (4) | 0.4815 (3) | 0.80214 (10) | 0.0408 (5) |
| H2A | 0.5169 | 0.3961 | 0.7888 | 0.049* |
| C3 | 0.7298 (4) | 0.5574 (3) | 0.86935 (10) | 0.0457 (5) |

| | | | | |
|---|---|---|---|---|
| C4 | 0.9504 (5) | 0.6916 (3) | 0.88879 (11) | 0.0520 (6) |
| C5 | 1.1177 (4) | 0.7419 (3) | 0.84062 (11) | 0.0480 (5) |
| C6 | 1.0627 (4) | 0.6603 (3) | 0.77344 (10) | 0.0412 (5) |
| H6 | 1.1771 | 0.6909 | 0.7414 | 0.049* |
| C7 | 0.3631 (6) | 0.3744 (4) | 0.90386 (13) | 0.0673 (7) |
| H7A | 0.2345 | 0.3994 | 0.8736 | 0.101* |
| H7B | 0.2821 | 0.3549 | 0.9443 | 0.101* |
| H7C | 0.4225 | 0.2748 | 0.8827 | 0.101* |
| C8 | 1.2015 (8) | 0.7925 (6) | 0.99320 (16) | 0.1086 (14) |
| H8A | 1.2011 | 0.6860 | 1.0061 | 0.163* |
| H8B | 1.2073 | 0.8791 | 1.0328 | 0.163* |
| H8C | 1.3554 | 0.8220 | 0.9690 | 0.163* |
| C9 | 1.5185 (5) | 0.9198 (3) | 0.81913 (13) | 0.0563 (6) |
| H9A | 1.5826 | 0.8211 | 0.7990 | 0.084* |
| H9B | 1.6651 | 1.0047 | 0.8435 | 0.084* |
| H9C | 1.4392 | 0.9639 | 0.7845 | 0.084* |
| C10 | 0.7487 (4) | 0.4520 (2) | 0.68292 (10) | 0.0363 (4) |
| C11 | 1.0749 (4) | 0.3316 (3) | 0.54076 (10) | 0.0421 (5) |
| H11 | 1.2448 | 0.3915 | 0.5585 | 0.050* |
| C12 | 1.0395 (4) | 0.2302 (3) | 0.47225 (10) | 0.0378 (4) |
| C13 | 1.2396 (5) | 0.2560 (3) | 0.42946 (11) | 0.0527 (6) |
| H13 | 1.3898 | 0.3424 | 0.4438 | 0.063* |
| C14 | 1.2205 (5) | 0.1556 (3) | 0.36576 (11) | 0.0542 (6) |
| H14 | 1.3553 | 0.1749 | 0.3371 | 0.065* |
| C15 | 1.0009 (5) | 0.0277 (3) | 0.34555 (10) | 0.0433 (5) |
| C16 | 0.7968 (5) | −0.0006 (3) | 0.38638 (12) | 0.0540 (6) |
| H16 | 0.6471 | −0.0871 | 0.3717 | 0.065* |
| C17 | 0.8181 (4) | 0.1019 (3) | 0.44969 (11) | 0.0488 (5) |
| H17 | 0.6803 | 0.0841 | 0.4777 | 0.059* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Cl1 | 0.0910 (5) | 0.0539 (4) | 0.0397 (3) | 0.0153 (3) | 0.0094 (3) | −0.0077 (3) |
| O1 | 0.0337 (8) | 0.0722 (11) | 0.0394 (8) | 0.0075 (7) | 0.0002 (6) | −0.0034 (7) |
| O2 | 0.0650 (11) | 0.0788 (12) | 0.0361 (9) | −0.0015 (9) | 0.0168 (7) | 0.0009 (8) |
| O3 | 0.0691 (12) | 0.1269 (19) | 0.0400 (10) | −0.0058 (12) | 0.0062 (9) | −0.0264 (11) |
| O4 | 0.0600 (11) | 0.0767 (12) | 0.0477 (10) | −0.0183 (9) | 0.0098 (8) | −0.0190 (8) |
| N1 | 0.0417 (9) | 0.0440 (9) | 0.0293 (8) | 0.0095 (7) | 0.0003 (7) | −0.0018 (7) |
| N2 | 0.0339 (8) | 0.0504 (10) | 0.0288 (8) | 0.0084 (7) | −0.0004 (6) | −0.0029 (7) |
| C1 | 0.0368 (10) | 0.0400 (10) | 0.0318 (10) | 0.0128 (8) | 0.0031 (8) | 0.0002 (8) |
| C2 | 0.0386 (11) | 0.0433 (11) | 0.0361 (11) | 0.0070 (9) | 0.0043 (8) | −0.0009 (9) |
| C3 | 0.0458 (12) | 0.0555 (13) | 0.0341 (11) | 0.0120 (10) | 0.0102 (9) | 0.0027 (9) |
| C4 | 0.0493 (12) | 0.0641 (15) | 0.0329 (11) | 0.0084 (11) | 0.0046 (9) | −0.0106 (10) |
| C5 | 0.0415 (11) | 0.0534 (13) | 0.0393 (11) | 0.0042 (10) | 0.0022 (9) | −0.0080 (10) |
| C6 | 0.0380 (11) | 0.0472 (12) | 0.0343 (10) | 0.0081 (9) | 0.0062 (8) | −0.0015 (9) |
| C7 | 0.0720 (17) | 0.0708 (17) | 0.0523 (15) | −0.0019 (14) | 0.0221 (13) | 0.0100 (13) |
| C8 | 0.092 (2) | 0.168 (4) | 0.0460 (17) | 0.008 (2) | −0.0029 (16) | −0.005 (2) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C9 | 0.0467 (13) | 0.0550 (14) | 0.0567 (14) | −0.0008 (10) | 0.0047 (11) | −0.0024 (11) |
| C10 | 0.0349 (10) | 0.0385 (10) | 0.0331 (10) | 0.0072 (8) | 0.0017 (8) | 0.0020 (8) |
| C11 | 0.0402 (11) | 0.0479 (12) | 0.0333 (10) | 0.0037 (9) | 0.0022 (8) | 0.0024 (9) |
| C12 | 0.0421 (11) | 0.0393 (10) | 0.0314 (10) | 0.0108 (8) | 0.0033 (8) | 0.0037 (8) |
| C13 | 0.0483 (13) | 0.0572 (14) | 0.0417 (12) | −0.0043 (10) | 0.0096 (10) | −0.0020 (10) |
| C14 | 0.0599 (14) | 0.0586 (14) | 0.0400 (12) | 0.0062 (11) | 0.0178 (10) | 0.0033 (10) |
| C15 | 0.0584 (13) | 0.0389 (11) | 0.0329 (10) | 0.0161 (9) | 0.0037 (9) | 0.0019 (8) |
| C16 | 0.0534 (13) | 0.0481 (13) | 0.0493 (13) | −0.0013 (10) | 0.0046 (10) | −0.0054 (10) |
| C17 | 0.0457 (12) | 0.0510 (13) | 0.0425 (12) | 0.0015 (10) | 0.0118 (9) | −0.0013 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Cl1—C15 | 1.742 (2) | C7—H7A | 0.9600 |
| O1—C10 | 1.223 (2) | C7—H7B | 0.9600 |
| O2—C3 | 1.357 (3) | C7—H7C | 0.9600 |
| O2—C7 | 1.419 (3) | C8—H8A | 0.9600 |
| O3—C8 | 1.337 (4) | C8—H8B | 0.9600 |
| O3—C4 | 1.362 (3) | C8—H8C | 0.9600 |
| O4—C5 | 1.361 (3) | C9—H9A | 0.9600 |
| O4—C9 | 1.411 (3) | C9—H9B | 0.9600 |
| N1—C11 | 1.270 (3) | C9—H9C | 0.9600 |
| N1—N2 | 1.379 (2) | C11—C12 | 1.460 (3) |
| N2—C10 | 1.349 (3) | C11—H11 | 0.9300 |
| N2—H2 | 0.8600 | C12—C17 | 1.379 (3) |
| C1—C2 | 1.383 (3) | C12—C13 | 1.380 (3) |
| C1—C6 | 1.383 (3) | C13—C14 | 1.381 (3) |
| C1—C10 | 1.489 (3) | C13—H13 | 0.9300 |
| C2—C3 | 1.380 (3) | C14—C15 | 1.365 (3) |
| C2—H2A | 0.9300 | C14—H14 | 0.9300 |
| C3—C4 | 1.395 (3) | C15—C16 | 1.371 (3) |
| C4—C5 | 1.393 (3) | C16—C17 | 1.381 (3) |
| C5—C6 | 1.388 (3) | C16—H16 | 0.9300 |
| C6—H6 | 0.9300 | C17—H17 | 0.9300 |
| | | | |
| C3—O2—C7 | 117.98 (18) | O3—C8—H8C | 109.5 |
| C8—O3—C4 | 120.7 (3) | H8A—C8—H8C | 109.5 |
| C5—O4—C9 | 118.23 (18) | H8B—C8—H8C | 109.5 |
| C11—N1—N2 | 114.90 (17) | O4—C9—H9A | 109.5 |
| C10—N2—N1 | 119.35 (16) | O4—C9—H9B | 109.5 |
| C10—N2—H2 | 120.3 | H9A—C9—H9B | 109.5 |
| N1—N2—H2 | 120.3 | O4—C9—H9C | 109.5 |
| C2—C1—C6 | 121.06 (18) | H9A—C9—H9C | 109.5 |
| C2—C1—C10 | 116.43 (18) | H9B—C9—H9C | 109.5 |
| C6—C1—C10 | 122.40 (18) | O1—C10—N2 | 122.65 (18) |
| C3—C2—C1 | 119.68 (19) | O1—C10—C1 | 121.16 (17) |
| C3—C2—H2A | 120.2 | N2—C10—C1 | 116.20 (17) |
| C1—C2—H2A | 120.2 | N1—C11—C12 | 121.29 (19) |
| O2—C3—C2 | 124.6 (2) | N1—C11—H11 | 119.4 |

| | | | |
|---|---|---|---|
| O2—C3—C4 | 115.37 (19) | C12—C11—H11 | 119.4 |
| C2—C3—C4 | 120.01 (19) | C17—C12—C13 | 118.34 (19) |
| O3—C4—C5 | 122.0 (2) | C17—C12—C11 | 122.11 (18) |
| O3—C4—C3 | 118.0 (2) | C13—C12—C11 | 119.44 (19) |
| C5—C4—C3 | 119.73 (19) | C12—C13—C14 | 121.1 (2) |
| O4—C5—C6 | 124.2 (2) | C12—C13—H13 | 119.4 |
| O4—C5—C4 | 115.72 (19) | C14—C13—H13 | 119.4 |
| C6—C5—C4 | 120.0 (2) | C15—C14—C13 | 119.0 (2) |
| C1—C6—C5 | 119.33 (19) | C15—C14—H14 | 120.5 |
| C1—C6—H6 | 120.3 | C13—C14—H14 | 120.5 |
| C5—C6—H6 | 120.3 | C14—C15—C16 | 121.5 (2) |
| O2—C7—H7A | 109.5 | C14—C15—Cl1 | 119.15 (17) |
| O2—C7—H7B | 109.5 | C16—C15—Cl1 | 119.30 (17) |
| H7A—C7—H7B | 109.5 | C15—C16—C17 | 118.7 (2) |
| O2—C7—H7C | 109.5 | C15—C16—H16 | 120.7 |
| H7A—C7—H7C | 109.5 | C17—C16—H16 | 120.7 |
| H7B—C7—H7C | 109.5 | C12—C17—C16 | 121.3 (2) |
| O3—C8—H8A | 109.5 | C12—C17—H17 | 119.3 |
| O3—C8—H8B | 109.5 | C16—C17—H17 | 119.3 |
| H8A—C8—H8B | 109.5 | | |

| | | | |
|---|---|---|---|
| C11—N1—N2—C10 | 175.22 (19) | O4—C5—C6—C1 | −175.8 (2) |
| C6—C1—C2—C3 | −0.3 (3) | C4—C5—C6—C1 | 2.2 (3) |
| C10—C1—C2—C3 | −176.58 (19) | N1—N2—C10—O1 | −5.0 (3) |
| C7—O2—C3—C2 | 3.4 (4) | N1—N2—C10—C1 | 174.86 (16) |
| C7—O2—C3—C4 | −178.0 (2) | C2—C1—C10—O1 | 33.9 (3) |
| C1—C2—C3—O2 | −178.0 (2) | C6—C1—C10—O1 | −142.3 (2) |
| C1—C2—C3—C4 | 3.4 (3) | C2—C1—C10—N2 | −145.93 (19) |
| C8—O3—C4—C5 | −63.6 (4) | C6—C1—C10—N2 | 37.9 (3) |
| C8—O3—C4—C3 | 122.7 (3) | N2—N1—C11—C12 | 173.85 (18) |
| O2—C3—C4—O3 | −8.6 (3) | N1—C11—C12—C17 | −19.4 (3) |
| C2—C3—C4—O3 | 170.1 (2) | N1—C11—C12—C13 | 164.4 (2) |
| O2—C3—C4—C5 | 177.6 (2) | C17—C12—C13—C14 | −0.4 (4) |
| C2—C3—C4—C5 | −3.7 (4) | C11—C12—C13—C14 | 176.0 (2) |
| C9—O4—C5—C6 | −9.0 (4) | C12—C13—C14—C15 | −0.8 (4) |
| C9—O4—C5—C4 | 172.9 (2) | C13—C14—C15—C16 | 1.5 (4) |
| O3—C4—C5—O4 | 5.4 (4) | C13—C14—C15—Cl1 | −176.79 (19) |
| C3—C4—C5—O4 | 179.0 (2) | C14—C15—C16—C17 | −1.0 (4) |
| O3—C4—C5—C6 | −172.7 (2) | Cl1—C15—C16—C17 | 177.36 (19) |
| C3—C4—C5—C6 | 0.9 (4) | C13—C12—C17—C16 | 1.0 (3) |
| C2—C1—C6—C5 | −2.5 (3) | C11—C12—C17—C16 | −175.3 (2) |
| C10—C1—C6—C5 | 173.5 (2) | C15—C16—C17—C12 | −0.3 (4) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2···O1$^{i}$ | 0.86 | 2.18 | 2.943 (3) | 147 |
| C8—H8*C*···O4 | 0.96 | 2.26 | 2.896 (4) | 123 |

| | | | | |
|---|---|---|---|---|
| C11—H11···O1$^{i}$ | 0.93 | 2.43 | 3.145 (3) | 134 |
| C16—H16···O1$^{ii}$ | 0.93 | 2.57 | 3.368 (3) | 144 |

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