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# Methyl (*E*)-3,5-dimethoxy-2-{[2-(4-methoxybenzoyl)hydrazin-1-ylidene]-methyl}benzoate

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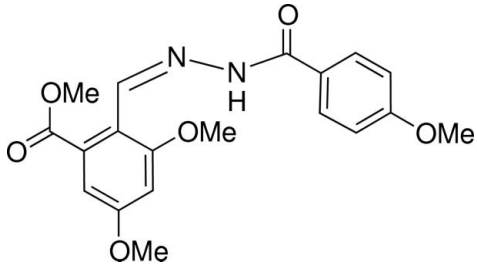
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.003 Å; $R$ factor = 0.047; $wR$ factor = 0.114; data-to-parameter ratio = 13.6.

In the title compound, $C_{19}H_{20}N_2O_6$, the azomethine [C=N = 1.269 (2) Å] double bond adopts an *E* conformation and the dihedral angle between the planes of the benzene rings is 17.41 (11)°. In the crystal, inversion dimers linked by pairs of N—H···O hydrogen bonds generate $R_2^2(16)$ loops. The dimers are connected by C—H···O and C—H···N hydrogen bonds, forming sheets lying parallel to (100).

## Related literature

For the biological activity of benzohydraazides, see: Khan *et al.* (2011); Chahan *et al.* (2006). For a related structure, see: Zhang (2009).




## Experimental

### Crystal data

$C_{19}H_{20}N_2O_6$
$M_r$ = 372.37
Triclinic, $P\overline{1}$
$a$ = 8.8468 (7) Å
$b$ = 10.7392 (8) Å
$c$ = 10.9764 (8) Å
$\alpha$ = 113.377 (2)°
$\beta$ = 90.656 (2)°
$\gamma$ = 104.695 (2)°
$V$ = 918.52 (12) Å$^3$
$Z$ = 2
Mo $K\alpha$ radiation
$\mu$ = 0.10 mm$^{-1}$
$T$ = 298 K
0.28 × 0.14 × 0.11 mm

### Data collection

Bruker SMART APEX CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.972, $T_{max}$ = 0.989
10426 measured reflections
3415 independent reflections
2224 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
$S$ = 1.02
3415 reflections
252 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N1—H1$A$···O5$^{i}$ | 0.84 (2) | 2.13 (2) | 2.969 (2) | 172.3 (19) |
| C18—H18$B$···N2$^{ii}$ | 0.96 | 2.62 | 3.501 (3) | 153 |
| C19—H19$B$···O5$^{iii}$ | 0.96 | 2.57 | 3.511 (3) | 168 |

Symmetry codes: (i) $-x+1, -y+2, -z+2$; (ii) $-x, -y+2, -z+2$; (iii) $x, y, z+1$.

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).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6920).

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# supporting information

*Acta Cryst.* (2012). E**68**, o2671 [doi:10.1107/S1600536812034782]

## Methyl (*E*)-3,5-dimethoxy-2-{[2-(4-methoxybenzoyl)hydrazin-1-ylidene]methyl}-benzoate

**Humera Naz, Muhammad Taha, Aqilah Abd Rahman, Nor Hadiani Ismail and Sammer Yousuf**

### S1. Comment

Phenyl hydrazones represent a very important class of bioactive organic compounds and are reported to have antibacterial, anticancer, antifungal, herbicidal activities, anticonvulsant, antiproliferative, antioxidant and antidiabetic activities (e.g. Khan *et al.*, 2011; Chahan *et al.*, 2006). The title compound was prepared as a part of our ongoing research to synthesize libraries of different bioactive benzohydrazone. The structure of title compound (Fig. 1) is similar to that of the previously published 4-Methoxy-*N*′-(2-methoxybenzylidene)-benzohydrazide (Zhang, 2009) with the difference that 2-methoxy benzne ring is replaced by 3,5-dimethoxybenzoate moiety (C9–C14). The azomethine (C=N,1.269 (2) Å) double bond adopt an *E* conformation (Fig. 1). The benzene rings (C1–C6 and C9–C14) subtend a dihedral angle 17.41 (11)° between them and maximum deviation of 0.014 (2) Å for C6 atom from the root mean square plane of 4-methoxybenzene ring (C1–C6).

The crystal structure features N1—H1A···O5, C18—H18B···N2 and C19—H19B···O5 intrmolecular hydrogen bonds and inked to form chains (symmetry codes as in Table 2) arranged parallel to (100) in (Fig. 2).

### S2. Experimental

A mixture of 2 mmol of each 4-methoxybenzohydrazide and methyl 2-formyl-3,5-dimethoxybenzoate and catalytical amount of acetic acid was refluxed for 3 h. The progress of the reaction was monitored by TLC. After completion of reaction, the solvent was evaporated by vacuum to afford the crude product (0.610 g, yield 82%), which was re-crystallized from methanol solution to yield colourless blocks of the title compound.

### S3. Refinement

H atoms on Methyl, phenyl and methine were positioned geometrically with C—H = 0.95 Å ($CH_3$), and 0.93 Å (CH) and constrained to ride on their parent atoms with $U_{iso}$(H)= 1.5$U_{eq}$($CH_3$) 1.2$U_{eq}$(CH). The H atoms on the nitrogen (N–H= 0.85 (2) Å) was located in difference Fourier maps and refined isotropically. A rotating group model was applied to the methyl groups.

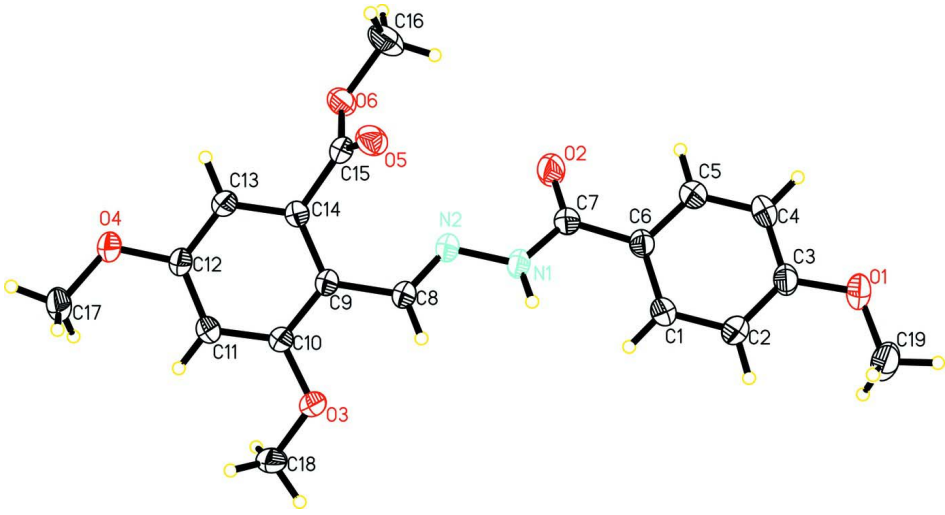


**Figure 1**

The molecular structure of (I) with displacement ellipsoids drawn at 30% probability level.

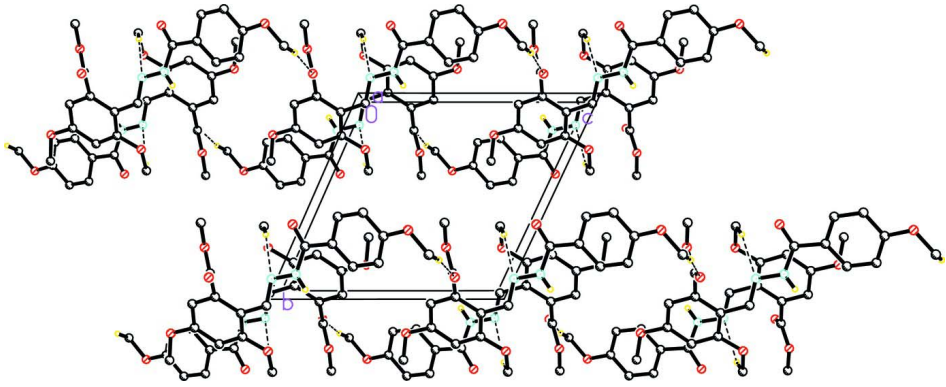

**Figure 2**

The crystal packing of the title compound I. Only hydrogen atoms involved in hydrogen bonding are shown.

### Methyl (*E*)-3,5-dimethoxy-2-{[2-(4-methoxybenzoyl)hydrazin-1- ylidene]methyl}benzoate

*Crystal data*

$C_{19}H_{20}N_2O_6$
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$\alpha = 113.377$ (2)°
$\beta = 90.656$ (2)°
$\gamma = 104.695$ (2)°
$V = 918.52$ (12) Å$^3$
$Z = 2$
$F(000) = 392$
$D_x = 1.346$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 1645 reflections
$\theta = 2.0$–25.5°
$\mu = 0.10$ mm$^{-1}$
$T = 298$ K
Block, colorless
0.28 × 0.14 × 0.11 mm

*Data collection*

Bruker SMART APEX CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scan

Absorption correction: multi-scan (*SADABS*; Bruker, 2000)
$T_{min}$ = 0.972, $T_{max}$ = 0.989
10426 measured reflections
3415 independent reflections
2224 reflections with $I > 2\sigma(I)$

$R_{int}$ = 0.033
$\theta_{max}$ = 25.5°, $\theta_{min}$ = 2.0°
$h$ = −10→10
$k$ = −13→13
$l$ = −13→13

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.114
$S$ = 1.02
3415 reflections
252 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0494P)^2 + 0.0289P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.16 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.17 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)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| O1 | 0.6563 (2) | 0.64890 (18) | 1.46257 (16) | 0.0820 (5) |
| O2 | 0.24378 (19) | 0.62729 (15) | 0.97724 (16) | 0.0730 (5) |
| O3 | 0.17303 (18) | 1.25061 (14) | 1.10340 (13) | 0.0614 (4) |
| O4 | 0.0119 (2) | 1.17046 (16) | 0.65074 (14) | 0.0691 (5) |
| O5 | 0.40868 (17) | 0.87627 (14) | 0.73902 (14) | 0.0564 (4) |
| O6 | 0.16475 (16) | 0.73913 (14) | 0.65091 (13) | 0.0549 (4) |
| N1 | 0.3446 (2) | 0.86420 (19) | 1.08462 (18) | 0.0507 (5) |
| N2 | 0.26850 (18) | 0.88947 (17) | 0.98968 (16) | 0.0477 (4) |
| C1 | 0.4660 (3) | 0.8228 (2) | 1.3057 (2) | 0.0636 (6) |
| H1B | 0.4472 | 0.9098 | 1.3257 | 0.076* |
| C2 | 0.5451 (3) | 0.8037 (2) | 1.4035 (2) | 0.0631 (6) |
| H2B | 0.5770 | 0.8766 | 1.4884 | 0.076* |
| C3 | 0.5760 (2) | 0.6779 (2) | 1.3750 (2) | 0.0537 (5) |
| C4 | 0.5221 (3) | 0.5694 (2) | 1.2506 (2) | 0.0721 (7) |
| H4A | 0.5402 | 0.4823 | 1.2311 | 0.087* |
| C5 | 0.4413 (3) | 0.5890 (2) | 1.1549 (2) | 0.0603 (6) |
| H5A | 0.4043 | 0.5142 | 1.0717 | 0.072* |
| C6 | 0.4143 (2) | 0.7167 (2) | 1.17971 (19) | 0.0448 (5) |

| | | | | |
|---|---|---|---|---|
| C7 | 0.3274 (2) | 0.7306 (2) | 1.0710 (2) | 0.0488 (5) |
| C8 | 0.2808 (2) | 1.0184 (2) | 1.01728 (19) | 0.0475 (5) |
| H8A | 0.3342 | 1.0878 | 1.0990 | 0.057* |
| C9 | 0.2117 (2) | 1.05887 (19) | 0.92205 (18) | 0.0410 (5) |
| C10 | 0.1566 (2) | 1.17821 (19) | 0.96804 (18) | 0.0434 (5) |
| C11 | 0.0895 (2) | 1.2190 (2) | 0.88060 (19) | 0.0491 (5) |
| H11A | 0.0554 | 1.3001 | 0.9129 | 0.059* |
| C12 | 0.0739 (2) | 1.1378 (2) | 0.74496 (19) | 0.0480 (5) |
| C13 | 0.1234 (2) | 1.0168 (2) | 0.69618 (19) | 0.0493 (5) |
| H13A | 0.1094 | 0.9611 | 0.6047 | 0.059* |
| C14 | 0.1937 (2) | 0.97907 (19) | 0.78374 (18) | 0.0419 (5) |
| C15 | 0.2684 (3) | 0.8614 (2) | 0.72612 (18) | 0.0442 (5) |
| C16 | 0.2293 (3) | 0.6196 (2) | 0.5973 (3) | 0.0761 (7) |
| H16A | 0.1461 | 0.5353 | 0.5470 | 0.114* |
| H16B | 0.2788 | 0.6089 | 0.6694 | 0.114* |
| H16C | 0.3058 | 0.6353 | 0.5398 | 0.114* |
| C17 | −0.0109 (3) | 1.3070 (2) | 0.6920 (2) | 0.0695 (7) |
| H17A | −0.0380 | 1.3215 | 0.6146 | 0.104* |
| H17B | 0.0844 | 1.3775 | 0.7420 | 0.104* |
| H17C | −0.0945 | 1.3142 | 0.7471 | 0.104* |
| C18 | 0.0967 (3) | 1.3593 (2) | 1.1573 (2) | 0.0617 (6) |
| H18A | 0.1147 | 1.3988 | 1.2532 | 0.093* |
| H18B | −0.0145 | 1.3203 | 1.1282 | 0.093* |
| H18C | 0.1383 | 1.4320 | 1.1268 | 0.093* |
| C19 | 0.7245 (3) | 0.7605 (3) | 1.5882 (3) | 0.0943 (9) |
| H19A | 0.7883 | 0.7292 | 1.6350 | 0.141* |
| H19B | 0.6425 | 0.7883 | 1.6400 | 0.141* |
| H19C | 0.7888 | 0.8396 | 1.5750 | 0.141* |
| H1A | 0.412 (2) | 0.936 (2) | 1.141 (2) | 0.054 (7)* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.1044 (13) | 0.1002 (13) | 0.0638 (11) | 0.0587 (11) | −0.0016 (10) | 0.0388 (10) |
| O2 | 0.0884 (12) | 0.0517 (9) | 0.0698 (11) | 0.0157 (9) | −0.0233 (9) | 0.0191 (8) |
| O3 | 0.0889 (11) | 0.0613 (9) | 0.0364 (8) | 0.0409 (8) | −0.0007 (7) | 0.0109 (7) |
| O4 | 0.1052 (12) | 0.0728 (10) | 0.0478 (9) | 0.0528 (9) | 0.0012 (8) | 0.0271 (8) |
| O5 | 0.0507 (9) | 0.0559 (9) | 0.0602 (9) | 0.0234 (7) | 0.0022 (7) | 0.0164 (7) |
| O6 | 0.0585 (9) | 0.0437 (8) | 0.0583 (9) | 0.0197 (7) | −0.0020 (7) | 0.0138 (7) |
| N1 | 0.0596 (12) | 0.0468 (11) | 0.0467 (11) | 0.0137 (10) | −0.0095 (9) | 0.0216 (9) |
| N2 | 0.0520 (10) | 0.0511 (11) | 0.0444 (10) | 0.0180 (8) | −0.0025 (8) | 0.0225 (8) |
| C1 | 0.0948 (18) | 0.0525 (13) | 0.0532 (14) | 0.0362 (13) | 0.0017 (13) | 0.0225 (11) |
| C2 | 0.0890 (17) | 0.0623 (15) | 0.0427 (13) | 0.0324 (13) | 0.0019 (12) | 0.0200 (11) |
| C3 | 0.0572 (13) | 0.0682 (15) | 0.0521 (13) | 0.0309 (12) | 0.0097 (11) | 0.0333 (12) |
| C4 | 0.0968 (19) | 0.0615 (15) | 0.0710 (17) | 0.0434 (14) | −0.0009 (15) | 0.0279 (13) |
| C5 | 0.0732 (15) | 0.0511 (13) | 0.0551 (14) | 0.0251 (12) | −0.0022 (12) | 0.0162 (11) |
| C6 | 0.0472 (12) | 0.0476 (12) | 0.0461 (12) | 0.0172 (10) | 0.0074 (10) | 0.0235 (10) |
| C7 | 0.0529 (13) | 0.0457 (13) | 0.0476 (12) | 0.0164 (11) | 0.0014 (10) | 0.0177 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C8 | 0.0559 (13) | 0.0474 (12) | 0.0402 (11) | 0.0182 (10) | −0.0031 (9) | 0.0171 (9) |
| C9 | 0.0432 (11) | 0.0439 (11) | 0.0380 (11) | 0.0144 (9) | −0.0002 (9) | 0.0180 (9) |
| C10 | 0.0508 (12) | 0.0436 (11) | 0.0360 (11) | 0.0180 (10) | 0.0012 (9) | 0.0138 (9) |
| C11 | 0.0607 (13) | 0.0476 (12) | 0.0467 (12) | 0.0279 (10) | 0.0057 (10) | 0.0197 (10) |
| C12 | 0.0583 (13) | 0.0541 (13) | 0.0407 (12) | 0.0250 (10) | 0.0026 (10) | 0.0233 (10) |
| C13 | 0.0610 (13) | 0.0531 (13) | 0.0361 (11) | 0.0259 (11) | 0.0017 (10) | 0.0149 (9) |
| C14 | 0.0460 (11) | 0.0426 (11) | 0.0410 (11) | 0.0179 (9) | 0.0034 (9) | 0.0178 (9) |
| C15 | 0.0536 (13) | 0.0476 (12) | 0.0347 (11) | 0.0175 (11) | 0.0005 (10) | 0.0184 (9) |
| C16 | 0.0824 (17) | 0.0435 (13) | 0.0919 (18) | 0.0268 (12) | 0.0028 (15) | 0.0121 (12) |
| C17 | 0.0943 (18) | 0.0737 (16) | 0.0675 (16) | 0.0477 (14) | 0.0140 (14) | 0.0416 (13) |
| C18 | 0.0781 (16) | 0.0566 (14) | 0.0459 (13) | 0.0327 (12) | 0.0067 (11) | 0.0082 (10) |
| C19 | 0.106 (2) | 0.133 (3) | 0.0602 (17) | 0.065 (2) | −0.0023 (16) | 0.0375 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C3 | 1.364 (2) | C6—C7 | 1.488 (3) |
| O1—C19 | 1.416 (3) | C8—C9 | 1.461 (2) |
| O2—C7 | 1.224 (2) | C8—H8A | 0.9300 |
| O3—C10 | 1.362 (2) | C9—C10 | 1.394 (2) |
| O3—C18 | 1.425 (2) | C9—C14 | 1.399 (3) |
| O4—C12 | 1.366 (2) | C10—C11 | 1.385 (2) |
| O4—C17 | 1.422 (2) | C11—C12 | 1.378 (3) |
| O5—C15 | 1.209 (2) | C11—H11A | 0.9300 |
| O6—C15 | 1.326 (2) | C12—C13 | 1.382 (3) |
| O6—C16 | 1.450 (2) | C13—C14 | 1.377 (2) |
| N1—C7 | 1.350 (2) | C13—H13A | 0.9300 |
| N1—N2 | 1.383 (2) | C14—C15 | 1.494 (3) |
| N1—H1A | 0.85 (2) | C16—H16A | 0.9600 |
| N2—C8 | 1.269 (2) | C16—H16B | 0.9600 |
| C1—C6 | 1.375 (3) | C16—H16C | 0.9600 |
| C1—C2 | 1.384 (3) | C17—H17A | 0.9600 |
| C1—H1B | 0.9300 | C17—H17B | 0.9600 |
| C2—C3 | 1.361 (3) | C17—H17C | 0.9600 |
| C2—H2B | 0.9300 | C18—H18A | 0.9600 |
| C3—C4 | 1.375 (3) | C18—H18B | 0.9600 |
| C4—C5 | 1.376 (3) | C18—H18C | 0.9600 |
| C4—H4A | 0.9300 | C19—H19A | 0.9600 |
| C5—C6 | 1.373 (3) | C19—H19B | 0.9600 |
| C5—H5A | 0.9300 | C19—H19C | 0.9600 |
| | | | |
| C3—O1—C19 | 118.05 (19) | C12—C11—H11A | 120.5 |
| C10—O3—C18 | 118.26 (15) | C10—C11—H11A | 120.5 |
| C12—O4—C17 | 118.22 (16) | O4—C12—C11 | 123.46 (18) |
| C15—O6—C16 | 114.98 (16) | O4—C12—C13 | 115.72 (17) |
| C7—N1—N2 | 120.43 (18) | C11—C12—C13 | 120.82 (17) |
| C7—N1—H1A | 124.2 (14) | C14—C13—C12 | 119.67 (18) |
| N2—N1—H1A | 114.6 (14) | C14—C13—H13A | 120.2 |
| C8—N2—N1 | 115.63 (17) | C12—C13—H13A | 120.2 |

| | | | |
|---|---|---|---|
| C6—C1—C2 | 121.78 (19) | C13—C14—C9 | 121.17 (17) |
| C6—C1—H1B | 119.1 | C13—C14—C15 | 117.78 (17) |
| C2—C1—H1B | 119.1 | C9—C14—C15 | 120.59 (16) |
| C3—C2—C1 | 119.8 (2) | O5—C15—O6 | 123.04 (18) |
| C3—C2—H2B | 120.1 | O5—C15—C14 | 124.35 (18) |
| C1—C2—H2B | 120.1 | O6—C15—C14 | 112.46 (17) |
| C2—C3—O1 | 124.7 (2) | O6—C16—H16A | 109.5 |
| C2—C3—C4 | 119.3 (2) | O6—C16—H16B | 109.5 |
| O1—C3—C4 | 116.04 (19) | H16A—C16—H16B | 109.5 |
| C3—C4—C5 | 120.3 (2) | O6—C16—H16C | 109.5 |
| C3—C4—H4A | 119.8 | H16A—C16—H16C | 109.5 |
| C5—C4—H4A | 119.8 | H16B—C16—H16C | 109.5 |
| C6—C5—C4 | 121.4 (2) | O4—C17—H17A | 109.5 |
| C6—C5—H5A | 119.3 | O4—C17—H17B | 109.5 |
| C4—C5—H5A | 119.3 | H17A—C17—H17B | 109.5 |
| C5—C6—C1 | 117.35 (19) | O4—C17—H17C | 109.5 |
| C5—C6—C7 | 118.43 (18) | H17A—C17—H17C | 109.5 |
| C1—C6—C7 | 124.20 (18) | H17B—C17—H17C | 109.5 |
| O2—C7—N1 | 122.64 (19) | O3—C18—H18A | 109.5 |
| O2—C7—C6 | 121.79 (18) | O3—C18—H18B | 109.5 |
| N1—C7—C6 | 115.55 (18) | H18A—C18—H18B | 109.5 |
| N2—C8—C9 | 120.71 (18) | O3—C18—H18C | 109.5 |
| N2—C8—H8A | 119.6 | H18A—C18—H18C | 109.5 |
| C9—C8—H8A | 119.6 | H18B—C18—H18C | 109.5 |
| C10—C9—C14 | 117.63 (16) | O1—C19—H19A | 109.5 |
| C10—C9—C8 | 120.10 (17) | O1—C19—H19B | 109.5 |
| C14—C9—C8 | 122.24 (17) | H19A—C19—H19B | 109.5 |
| O3—C10—C11 | 122.77 (17) | O1—C19—H19C | 109.5 |
| O3—C10—C9 | 115.61 (16) | H19A—C19—H19C | 109.5 |
| C11—C10—C9 | 121.61 (17) | H19B—C19—H19C | 109.5 |
| C12—C11—C10 | 119.05 (18) | | |

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| C7—N1—N2—C8 | 174.00 (18) | C14—C9—C10—O3 | 178.40 (17) |
| C6—C1—C2—C3 | 1.2 (4) | C8—C9—C10—O3 | 0.3 (3) |
| C1—C2—C3—O1 | 178.3 (2) | C14—C9—C10—C11 | −1.4 (3) |
| C1—C2—C3—C4 | −2.7 (3) | C8—C9—C10—C11 | −179.51 (18) |
| C19—O1—C3—C2 | −5.8 (3) | O3—C10—C11—C12 | −178.44 (18) |
| C19—O1—C3—C4 | 175.3 (2) | C9—C10—C11—C12 | 1.4 (3) |
| C2—C3—C4—C5 | 1.7 (4) | C17—O4—C12—C11 | 11.9 (3) |
| O1—C3—C4—C5 | −179.3 (2) | C17—O4—C12—C13 | −167.25 (19) |
| C3—C4—C5—C6 | 0.9 (4) | C10—C11—C12—O4 | −178.79 (19) |
| C4—C5—C6—C1 | −2.4 (3) | C10—C11—C12—C13 | 0.4 (3) |
| C4—C5—C6—C7 | 179.4 (2) | O4—C12—C13—C14 | 177.21 (18) |
| C2—C1—C6—C5 | 1.4 (3) | C11—C12—C13—C14 | −2.0 (3) |
| C2—C1—C6—C7 | 179.4 (2) | C12—C13—C14—C9 | 1.9 (3) |
| N2—N1—C7—O2 | −1.1 (3) | C12—C13—C14—C15 | −170.38 (18) |
| N2—N1—C7—C6 | −179.71 (16) | C10—C9—C14—C13 | −0.2 (3) |
| C5—C6—C7—O2 | 20.4 (3) | C8—C9—C14—C13 | 177.79 (18) |

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| C1—C6—C7—O2 | −157.6 (2) | C10—C9—C14—C15 | 171.85 (18) |
| C5—C6—C7—N1 | −160.94 (19) | C8—C9—C14—C15 | −10.1 (3) |
| C1—C6—C7—N1 | 21.0 (3) | C16—O6—C15—O5 | 7.0 (3) |
| N1—N2—C8—C9 | 177.12 (17) | C16—O6—C15—C14 | −177.25 (18) |
| N2—C8—C9—C10 | 148.9 (2) | C13—C14—C15—O5 | 111.9 (2) |
| N2—C8—C9—C14 | −29.1 (3) | C9—C14—C15—O5 | −60.4 (3) |
| C18—O3—C10—C11 | 9.9 (3) | C13—C14—C15—O6 | −63.8 (2) |
| C18—O3—C10—C9 | −169.98 (18) | C9—C14—C15—O6 | 123.87 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N1—H1*A*···O5$^{i}$ | 0.84 (2) | 2.13 (2) | 2.969 (2) | 172.3 (19) |
| C18—H18*B*···N2$^{ii}$ | 0.96 | 2.62 | 3.501 (3) | 153 |
| C19—H19*B*···O5$^{iii}$ | 0.96 | 2.57 | 3.511 (3) | 168 |

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