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# *N*′-(4-Hydroxybenzylidene)-4-methoxybenzohydrazide

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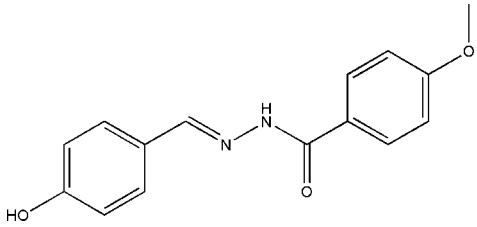
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.004 Å; disorder in main residue; $R$ factor = 0.049; $wR$ factor = 0.135; data-to-parameter ratio = 11.5.

The title compound, $C_{15}H_{14}N_2O_3$, was prepared by the reaction of 4-hydroxybenzaldehyde and 4-methoxybenzohydrazide in methanol. The dihedral angle between the two benzene rings is 6.8 (1)°. The methoxy group is disordered over two orientations with occupancies of *ca* 0.63 and 0.37. In the major disorder component, the methoxy group is coplanar with the attached ring. In the crystal structure, the molecules are linked into a three-dimensional framework by intermolecular O—H···O and N—H···O hydrogen bonds.

## Related literature

For the synthesis of Schiff bases, see: Akitsu & Einaga (2006); Butcher *et al.* (2005); Habibi *et al.* (2007); Pradeep (2005). For related Schiff base compounds, see: Wang *et al.* (2006); Wei *et al.* (2006, 2008*a*,*b*); Wei & Wang (2006); Zhu *et al.* (2007). For related structures, see: Odabaşoğlu *et al.* (2007); Yathirajan *et al.* (2007); Yehye *et al.* (2008).




## Experimental

### *Crystal data*

$C_{15}H_{14}N_2O_3$
$M_r$ = 270.28
Orthorhombic, *Pbca*
$a$ = 12.342 (2) Å
$b$ = 7.854 (2) Å
$c$ = 27.889 (3) Å
$V$ = 2703.4 (9) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.09 mm$^{-1}$
$T$ = 296 (2) K
0.23 × 0.20 × 0.20 mm

### *Data collection*

Bruker SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.979, $T_{max}$ = 0.981
12214 measured reflections
2308 independent reflections
1591 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.033

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.135
$S$ = 1.04
2308 reflections
201 parameters
26 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.24 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$A$···O2$^{i}$ | 0.86 | 2.15 | 3.007 (3) | 172 |
| O1—H1···O2$^{ii}$ | 0.82 | 1.88 | 2.696 (2) | 170 |

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

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); 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: CI2639).

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# supporting information

*Acta Cryst.* (2008). E**64**, o1682 [doi:10.1107/S160053680802360X]

## *N*′-(4-Hydroxybenzylidene)-4-methoxybenzohydrazide

**Xia Bao and Yi-Jun Wei**

### S1. Comment

Schiff bases are readily synthesized by the reaction of aldehydes with primary amines (Akitsu & Einaga, 2006; Pradeep, 2005; Butcher *et al.*, 2005; Habibi *et al.*, 2007). We have reported a few Schiff bases and their complexes (Wei *et al.*, 2008*a*,*b*; Wei *et al.*, 2006; Wei & Wang, 2006; Zhu *et al.*, 2007; Wang *et al.*, 2006). In this paper, we report the crystal structure of a new Schiff base compound.

Bond lengths and angles in the title compound (Fig. 1) are comparable with those observed in other Schiff bases (Yehye *et al.*, 2008; Odabaşoğlu *et al.*, 2007; Yathirajan *et al.*, 2007). The dihedral angle between the C1–C6 and C9–C14 phenyl rings is 6.8 (1)°, indicating that they are nearly coplanar. In the major disorder component, the methoxy group is coplanar with the attached ring [C15—O3—C12—C11 = -2.6 (6)°].

The crystal structure is stabilized by intermolecular O—H···O and N—H···O hydrogen bonds (Table 1). These hydrogen bonds link the molecules into a three-dimensional framework (Fig. 2).

### S2. Experimental

4-Hydroxybenzaldehyde (1.0 mmol, 122.1 mg) and 4-methoxybenzohydrazide (1.0 mmol, 166.2 mg) were added to methanol (30 ml). The mixture was stirred at reflux for 10 min to give a clear colourless solution. After keeping the solution in air for 12 d, colourless needle-shaped crystals were formed.

### S3. Refinement

H atoms were positioned geometrically (C–H = 0.93–0.96 Å, O–H = 0.82 Å, N–H = 0.86 Å) and refined as riding, with $U_{iso}$(H) = 1.2$U_{eq}$(C,N) and 1.5$U_{eq}$(O,$C_{methyl}$). The methoxy group is disordered over two sites with occupancies of 0.630 (2) and 0.370 (2). The corresponding C—O distances in both disorder components were restrained to be equal. The displacement parameters of atoms O3, O3A, C15 and C15A were restrained to an approximate isotropic behaviour. The low resolution is caused by weak diffraction of the crystal.

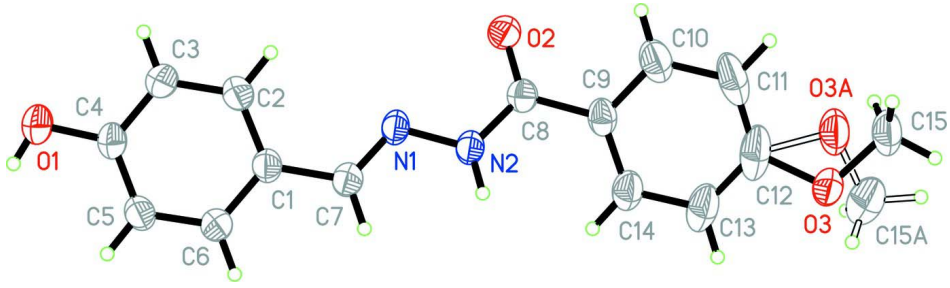


**Figure 1**

The molecular structure of the title compounnd, showing 30% probability displacement ellipsoids. Both disorder components are shown.

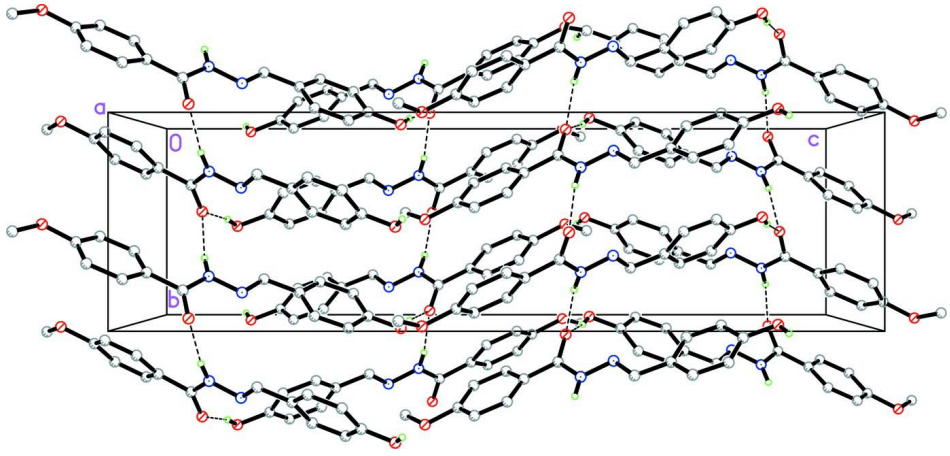


**Figure 2**

The crystal packing of the title compound, viewed approximately along the *a* axis. Hydrogen bonds are shown as dashed lines. Only the major disorder component is shown.

### *N*′-(4-Hydroxybenzylidene)-4-methoxybenzohydrazide

*Crystal data*

$C_{15}H_{14}N_2O_3$
$M_r = 270.28$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 12.342$ (2) Å
$b = 7.854$ (2) Å
$c = 27.889$ (3) Å
$V = 2703.4$ (9) Å$^3$
$Z = 8$
$F(000) = 1136$
$D_x = 1.328$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2798 reflections
$\theta = 2.4$–$24.1°$
$\mu = 0.09$ mm$^{-1}$
$T = 296$ K
Cut from needle, colourless
0.23 × 0.20 × 0.20 mm

*Data collection*

Bruker SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min} = 0.979$, $T_{max} = 0.981$
12214 measured reflections
2308 independent reflections
1591 reflections with $I > 2\sigma(I)$
$R_{int} = 0.033$
$\theta_{max} = 24.7°$, $\theta_{min} = 1.5°$
$h = -14 \rightarrow 12$
$k = -9 \rightarrow 9$
$l = -32 \rightarrow 29$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.049$
$wR(F^2) = 0.135$
$S = 1.04$
2308 reflections
201 parameters
26 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
$w = 1/[\sigma^2(F_o^2) + (0.0514P)^2 + 1.0313P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.24$ 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* | $U_{iso}$*/$U_{eq}$ | Occ. (<1) |
|---|---|---|---|---|---|
| O1 | 0.91965 (15) | −0.0226 (3) | 0.86782 (6) | 0.0813 (6) | |
| H1 | 0.9779 | 0.0115 | 0.8782 | 0.122* | |
| O2 | 0.61634 (13) | 0.0498 (2) | 0.59539 (5) | 0.0645 (5) | |
| N1 | 0.76203 (15) | 0.1620 (2) | 0.65728 (6) | 0.0591 (5) | |
| N2 | 0.74642 (15) | 0.2399 (2) | 0.61337 (6) | 0.0599 (5) | |
| H2A | 0.7848 | 0.3265 | 0.6051 | 0.072* | |
| C1 | 0.86057 (18) | 0.1561 (3) | 0.73055 (8) | 0.0588 (6) | |
| C2 | 0.7901 (2) | 0.0470 (3) | 0.75378 (8) | 0.0700 (7) | |
| H2 | 0.7271 | 0.0123 | 0.7383 | 0.084* | |
| C3 | 0.8111 (2) | −0.0109 (4) | 0.79911 (8) | 0.0752 (8) | |
| H3 | 0.7623 | −0.0838 | 0.8141 | 0.090* | |
| C4 | 0.90430 (19) | 0.0382 (3) | 0.82278 (8) | 0.0596 (6) | |
| C5 | 0.9763 (2) | 0.1447 (3) | 0.80018 (8) | 0.0653 (6) | |
| H5 | 1.0401 | 0.1768 | 0.8155 | 0.078* | |
| C6 | 0.9535 (2) | 0.2038 (3) | 0.75471 (8) | 0.0701 (7) | |
| H6 | 1.0020 | 0.2777 | 0.7399 | 0.084* | |
| C7 | 0.8374 (2) | 0.2223 (3) | 0.68288 (8) | 0.0673 (7) | |
| H7 | 0.8792 | 0.3113 | 0.6709 | 0.081* | |
| C8 | 0.67021 (18) | 0.1775 (3) | 0.58398 (7) | 0.0546 (6) | |
| C9 | 0.65325 (19) | 0.2623 (3) | 0.53725 (8) | 0.0605 (6) | |
| C10 | 0.5570 (2) | 0.2357 (4) | 0.51343 (10) | 0.0882 (9) | |
| H10 | 0.5031 | 0.1693 | 0.5274 | 0.106* | |
| C11 | 0.5400 (3) | 0.3083 (4) | 0.46835 (11) | 0.1097 (12) | |
| H11 | 0.4747 | 0.2901 | 0.4525 | 0.132* | |
| C12 | 0.6183 (4) | 0.4056 (4) | 0.44727 (10) | 0.1047 (12) | |
| C13 | 0.7138 (3) | 0.4305 (4) | 0.47006 (9) | 0.0938 (10) | |
| H13 | 0.7678 | 0.4953 | 0.4556 | 0.113* | |
| C14 | 0.7314 (2) | 0.3606 (3) | 0.51443 (8) | 0.0735 (7) | |
| H14 | 0.7973 | 0.3795 | 0.5297 | 0.088* | |
| O3 | 0.6249 (4) | 0.4882 (5) | 0.40185 (13) | 0.0866 (14) | 0.630 (7) |
| C15 | 0.5326 (4) | 0.4557 (6) | 0.37318 (19) | 0.0891 (18) | 0.630 (7) |
| H15A | 0.5397 | 0.5142 | 0.3431 | 0.134* | 0.630 (7) |
| H15B | 0.4689 | 0.4953 | 0.3895 | 0.134* | 0.630 (7) |
| H15C | 0.5266 | 0.3355 | 0.3675 | 0.134* | 0.630 (7) |
| O3A | 0.5470 (5) | 0.4517 (9) | 0.40930 (19) | 0.092 (2) | 0.370 (7) |

| | | | | | |
|---|---|---|---|---|---|
| C15A | 0.6242 (10) | 0.5249 (18) | 0.3782 (4) | 0.123 (5) | 0.370 (7) |
| H15D | 0.5889 | 0.5632 | 0.3495 | 0.185* | 0.370 (7) |
| H15E | 0.6781 | 0.4416 | 0.3702 | 0.185* | 0.370 (7) |
| H15F | 0.6582 | 0.6199 | 0.3938 | 0.185* | 0.370 (7) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| O1 | 0.0866 (13) | 0.0986 (14) | 0.0586 (10) | −0.0037 (11) | −0.0139 (9) | 0.0213 (10) |
| O2 | 0.0700 (10) | 0.0642 (10) | 0.0593 (9) | −0.0056 (9) | −0.0002 (8) | 0.0010 (8) |
| N1 | 0.0716 (12) | 0.0616 (12) | 0.0440 (10) | −0.0018 (10) | −0.0069 (9) | 0.0074 (9) |
| N2 | 0.0738 (12) | 0.0587 (11) | 0.0472 (10) | −0.0070 (10) | −0.0092 (10) | 0.0078 (8) |
| C1 | 0.0698 (15) | 0.0560 (13) | 0.0507 (12) | −0.0037 (12) | −0.0085 (11) | 0.0039 (11) |
| C2 | 0.0712 (16) | 0.0746 (17) | 0.0641 (14) | −0.0120 (14) | −0.0162 (12) | 0.0100 (13) |
| C3 | 0.0751 (16) | 0.0836 (19) | 0.0668 (15) | −0.0157 (14) | −0.0104 (13) | 0.0229 (14) |
| C4 | 0.0702 (15) | 0.0594 (14) | 0.0491 (13) | 0.0066 (12) | −0.0070 (11) | 0.0040 (11) |
| C5 | 0.0717 (15) | 0.0651 (15) | 0.0591 (14) | −0.0069 (13) | −0.0155 (12) | 0.0025 (12) |
| C6 | 0.0786 (17) | 0.0702 (17) | 0.0615 (14) | −0.0191 (13) | −0.0114 (13) | 0.0109 (12) |
| C7 | 0.0794 (17) | 0.0673 (16) | 0.0553 (14) | −0.0134 (13) | −0.0090 (12) | 0.0096 (12) |
| C8 | 0.0612 (13) | 0.0529 (13) | 0.0498 (12) | 0.0038 (11) | −0.0007 (11) | −0.0037 (10) |
| C9 | 0.0812 (17) | 0.0507 (13) | 0.0495 (12) | 0.0051 (12) | −0.0145 (12) | −0.0050 (10) |
| C10 | 0.104 (2) | 0.0766 (19) | 0.0841 (19) | −0.0048 (16) | −0.0388 (17) | 0.0022 (15) |
| C11 | 0.142 (3) | 0.087 (2) | 0.099 (2) | 0.010 (2) | −0.075 (2) | −0.0072 (19) |
| C12 | 0.193 (4) | 0.0605 (18) | 0.0604 (18) | 0.013 (2) | −0.040 (2) | −0.0018 (14) |
| C13 | 0.155 (3) | 0.0744 (19) | 0.0519 (15) | 0.0010 (19) | −0.0118 (18) | 0.0050 (13) |
| C14 | 0.103 (2) | 0.0662 (16) | 0.0512 (13) | −0.0025 (15) | −0.0111 (13) | 0.0014 (12) |
| O3 | 0.105 (3) | 0.090 (3) | 0.064 (2) | −0.025 (2) | −0.024 (2) | 0.0248 (19) |
| C15 | 0.115 (4) | 0.090 (3) | 0.063 (3) | 0.003 (3) | −0.032 (3) | 0.010 (2) |
| O3A | 0.101 (5) | 0.116 (5) | 0.059 (4) | 0.009 (4) | −0.019 (3) | 0.019 (3) |
| C15A | 0.137 (8) | 0.137 (8) | 0.095 (7) | −0.006 (6) | 0.002 (7) | 0.043 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| O1—C4 | 1.357 (2) | C9—C10 | 1.377 (3) |
| O1—H1 | 0.82 | C9—C14 | 1.389 (3) |
| O2—C8 | 1.245 (3) | C10—C11 | 1.396 (4) |
| N1—C7 | 1.265 (3) | C10—H10 | 0.93 |
| N1—N2 | 1.382 (2) | C11—C12 | 1.365 (5) |
| N2—C8 | 1.340 (3) | C11—H11 | 0.93 |
| N2—H2A | 0.86 | C12—C13 | 1.354 (5) |
| C1—C6 | 1.382 (3) | C12—O3A | 1.424 (6) |
| C1—C2 | 1.382 (3) | C12—O3 | 1.426 (4) |
| C1—C7 | 1.456 (3) | C13—C14 | 1.371 (3) |
| C2—C3 | 1.368 (3) | C13—H13 | 0.93 |
| C2—H2 | 0.93 | C14—H14 | 0.93 |
| C3—C4 | 1.381 (3) | O3—C15 | 1.415 (5) |
| C3—H3 | 0.93 | C15—H15A | 0.96 |
| C4—C5 | 1.373 (3) | C15—H15B | 0.96 |

| | | | |
|---|---|---|---|
| C5—C6 | 1.379 (3) | C15—H15C | 0.96 |
| C5—H5 | 0.93 | O3A—C15A | 1.412 (8) |
| C6—H6 | 0.93 | C15A—H15D | 0.96 |
| C7—H7 | 0.93 | C15A—H15E | 0.96 |
| C8—C9 | 1.479 (3) | C15A—H15F | 0.96 |

| | | | |
|---|---|---|---|
| C4—O1—H1 | 109.5 | C9—C10—C11 | 120.1 (3) |
| C7—N1—N2 | 115.9 (2) | C9—C10—H10 | 120.0 |
| C8—N2—N1 | 118.51 (19) | C11—C10—H10 | 120.0 |
| C8—N2—H2A | 120.7 | C12—C11—C10 | 120.7 (3) |
| N1—N2—H2A | 120.7 | C12—C11—H11 | 119.6 |
| C6—C1—C2 | 117.5 (2) | C10—C11—H11 | 119.6 |
| C6—C1—C7 | 120.7 (2) | C13—C12—C11 | 119.7 (3) |
| C2—C1—C7 | 121.7 (2) | C13—C12—O3A | 148.3 (4) |
| C3—C2—C1 | 121.3 (2) | C11—C12—O3A | 91.4 (4) |
| C3—C2—H2 | 119.3 | C13—C12—O3 | 107.6 (3) |
| C1—C2—H2 | 119.3 | C11—C12—O3 | 132.7 (3) |
| C2—C3—C4 | 120.5 (2) | C12—C13—C14 | 120.2 (3) |
| C2—C3—H3 | 119.8 | C12—C13—H13 | 119.9 |
| C4—C3—H3 | 119.8 | C14—C13—H13 | 119.9 |
| O1—C4—C5 | 123.3 (2) | C13—C14—C9 | 121.8 (3) |
| O1—C4—C3 | 117.4 (2) | C13—C14—H14 | 119.1 |
| C5—C4—C3 | 119.3 (2) | C9—C14—H14 | 119.1 |
| C4—C5—C6 | 119.7 (2) | C15—O3—C12 | 111.9 (4) |
| C4—C5—H5 | 120.2 | O3—C15—H15A | 109.5 |
| C6—C5—H5 | 120.2 | O3—C15—H15B | 109.5 |
| C5—C6—C1 | 121.7 (2) | H15A—C15—H15B | 109.5 |
| C5—C6—H6 | 119.1 | O3—C15—H15C | 109.5 |
| C1—C6—H6 | 119.1 | H15A—C15—H15C | 109.5 |
| N1—C7—C1 | 121.7 (2) | H15B—C15—H15C | 109.5 |
| N1—C7—H7 | 119.1 | C15A—O3A—C12 | 98.2 (8) |
| C1—C7—H7 | 119.1 | O3A—C15A—H15D | 109.5 |
| O2—C8—N2 | 120.9 (2) | O3A—C15A—H15E | 109.5 |
| O2—C8—C9 | 120.8 (2) | H15D—C15A—H15E | 109.5 |
| N2—C8—C9 | 118.3 (2) | O3A—C15A—H15F | 109.5 |
| C10—C9—C14 | 117.5 (2) | H15D—C15A—H15F | 109.5 |
| C10—C9—C8 | 118.6 (2) | H15E—C15A—H15F | 109.5 |
| C14—C9—C8 | 123.8 (2) | | |

| | | | |
|---|---|---|---|
| C7—N1—N2—C8 | 177.7 (2) | N2—C8—C9—C14 | 23.2 (3) |
| C6—C1—C2—C3 | 0.4 (4) | C14—C9—C10—C11 | −0.9 (4) |
| C7—C1—C2—C3 | −178.2 (2) | C8—C9—C10—C11 | −177.4 (2) |
| C1—C2—C3—C4 | −0.3 (4) | C9—C10—C11—C12 | 0.2 (5) |
| C2—C3—C4—O1 | 179.4 (2) | C10—C11—C12—C13 | 0.8 (5) |
| C2—C3—C4—C5 | −0.6 (4) | C10—C11—C12—O3A | −173.0 (4) |
| O1—C4—C5—C6 | −178.6 (2) | C10—C11—C12—O3 | 177.2 (4) |
| C3—C4—C5—C6 | 1.4 (4) | C11—C12—C13—C14 | −1.0 (5) |
| C4—C5—C6—C1 | −1.3 (4) | O3A—C12—C13—C14 | 167.1 (6) |

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|---|---|---|---|
| C2—C1—C6—C5 | 0.4 (4) | O3—C12—C13—C14 | −178.3 (3) |
| C7—C1—C6—C5 | 179.0 (2) | C12—C13—C14—C9 | 0.3 (4) |
| N2—N1—C7—C1 | 178.0 (2) | C10—C9—C14—C13 | 0.6 (4) |
| C6—C1—C7—N1 | 169.3 (2) | C8—C9—C14—C13 | 176.9 (2) |
| C2—C1—C7—N1 | −12.1 (4) | C13—C12—O3—C15 | 174.2 (4) |
| N1—N2—C8—O2 | −1.7 (3) | C11—C12—O3—C15 | −2.5 (7) |
| N1—N2—C8—C9 | 179.47 (18) | O3A—C12—O3—C15 | −17.1 (5) |
| O2—C8—C9—C10 | 20.6 (3) | C13—C12—O3A—C15A | 22.4 (11) |
| N2—C8—C9—C10 | −160.5 (2) | C11—C12—O3A—C15A | −167.9 (7) |
| O2—C8—C9—C14 | −155.7 (2) | O3—C12—O3A—C15A | 1.4 (8) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N2—H2*A*···O2$^{i}$ | 0.86 | 2.15 | 3.007 (3) | 172 |
| O1—H1···O2$^{ii}$ | 0.82 | 1.88 | 2.696 (2) | 170 |

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