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# 4-Bromo-2-{(*E*)-3-[1-(hydroxyimino)-ethyl]phenyliminomethyl}phenol

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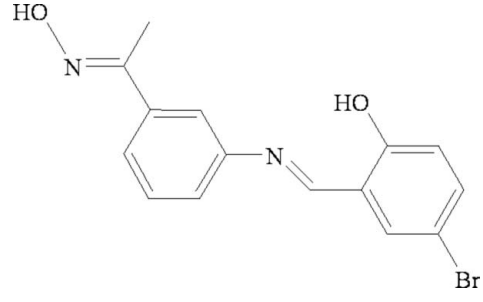
Key indicators: single-crystal X-ray study; $T$ = 298 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.039; $wR$ factor = 0.100; data-to-parameter ratio = 13.7.

In the title compound, $C_{15}H_{13}BrN_2O_2$, he oxime unit adopts an *E* conformation with respect to the O—H group. A classical intramolecular O—H···N hydrogen bond results in the formation of a six-membered ring. The crystal structure is stabilized by intermolecular O—H···N hydrogen bonds between the hydroxy groups and the oxime N atoms. In addition, the crystal structure also features short intermolecular Br···Br short contacts with a distance of 3.8768 (5) Å.

## Related literature

For background to Schiff bases, see: Dong *et al.* (2007, 2008); Wang *et al.* 2009). For background to oximes, see: Golovnia *et al.* (2009); Liu *et al.* (2008); Dong *et al.* (2009*a*); Öztürk *et al.* (2009). For the synthesis, see: Dong *et al.* (2009*b*).




## Experimental

### Crystal data

$C_{15}H_{13}BrN_2O_2$
$M_r$ = 333.18
Monoclinic, $P2_1/c$
$a$ = 17.020 (2) Å
$b$ = 6.1676 (7) Å
$c$ = 13.693 (1) Å
$\beta$ = 96.461 (1)°
$V$ = 1428.3 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.88 mm$^{-1}$
$T$ = 298 K
0.45 × 0.20 × 0.10 mm

### Data collection

Siemens SMART 1000 CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.357, $T_{max}$ = 0.762
6906 measured reflections
2492 independent reflections
1799 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
$S$ = 0.99
2492 reflections
182 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.47 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···N1$^{i}$ | 0.82 | 2.10 | 2.830 (4) | 149 |
| O2—H2···N2 | 0.82 | 1.91 | 2.635 (4) | 147 |

Symmetry code: (i) $-x, -y+3, -z+1$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); 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) and *DIAMOND* (Brandenburg, 1998); software used to prepare material for publication: *SHELXTL*.

This work was supported by the Foundation of the Education Department of Gansu Province (No. 0904-11) and the 'Jing Lan' Talent Engineering Funds of Lanzhou Jiaotong University, which are gratefully acknowledged.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LX2124).

## References

Brandenburg, K. (1998). *DIAMOND*. Crystal Impact GbR, Bonn, Germany.
Dong, W.-K., Duan, J.-G., Chai, L.-Q., Liu, G.-L. & Wu, H.-L. (2008). *J. Coord. Chem.* **61**, 1306–1315.
Dong, W.-K., Feng, J.-H. & Yang, X.-Q. (2007). *Synth. React. Inorg. Met. Org. Nano-Chem.* **37**, 61–65.
Dong, W.-K., Wu, J.-C., Sun, Y.-X., Yao, J. & Tong, J.-F. (2009*a*). *Acta Cryst.* E**65**, o1248.
Dong, W.-K., Zhao, C.-Y., Sun, Y.-X., Tang, X.-L. & He, X.-N. (2009*b*). *Inorg. Chem. Commun.* **12**, 234–236.
Golovnia, E., Prisyazhnaya, E. V., Iskenderov, T. S., Haukka, M. & Fritsky, I. O. (2009). *Acta Cryst.* E**65**, o2018–o2019.
Liu, G.-L., Chen, X., He, X.-N. & Dong, W.-K. (2008). *Acta Cryst.* E**64**, o659.
Öztürk, A., Babahan, İ., Sarıkavaklı, N. & Hökelek, T. (2009). *Acta Cryst.* E**65**, o1059–o1060.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Siemens (1996). *SMART* and *SAINT*. Siemens Analytical X-ray Instruments Inc., Madison, Wisconsin, USA.
Wang, X.-Q., Tong, J.-F., Dong, W.-K., Gong, S.-S. & Wu, J.-C. (2009). *Acta Cryst.* E**65**, o2013.

# supporting information

*Acta Cryst.* (2009). E**65**, o3154 [doi:10.1107/S1600536809048855]

## 4-Bromo-2-{(*E*)-3-[1-(hydroxyimino)ethyl]phenyliminomethyl}phenol

**Li Xu and Lei Wu**

### S1. Comment

Schiff base ligands containing oxygen and imine nitrogen atoms have attracted much attention due to their variety of applications as well as their strong coordination capability (Dong *et al.*, 2007; Dong *et al.*, 2008; Wang *et al.*, 2009). The oxime compounds frequently exhibit versatility in organic, inorganic, bioinorganic, pigment, analytical, dyes and medical chemistry (Golovnia *et al.*, 2009; Liu *et al.*, 2008; Dong *et al.*, 2009*a*; Öztürk *et al.*, 2009). Owing to the importance of oxime-type compounds, we report the crystal structure of the title compound (Fig. 1).

In the crystal structure, all bond lengths and bond angles are in normal ranges. The molecule has a crystallographic inversion centre and the oxime unit adopts an E conformation with respect to the O—H group. The aniline ring (C3–C8) and phenol ring (C10–C15) are almost parallel each other, making a dihedral angle of 2.71 (1)°. The torsion angles of O1—N1—C2—C3 and C5—N2—C9—C10 are 178.5 (3) and -178.8 (3)°, respectively. In the crystal structure, a classical intramolecular O—H···N hydrogen bond forms a six-membered ring (Fig. 2 and Table 1). The crystal packing (Fig. 2) is stabilized by intermolecular O—H···N hydrogen bonds between the hydroxy groups and oxime N atoms, with a O1—H1···N1$^{i}$ (Table 1). In addition, the crystal structure was further stabilized by weak intermolecular Br···Br$^{ii}$ (Fig. 2) short interactions with a distance of 3.8768 (5) Å.

### S2. Experimental

The title compound was synthesized according to an analogous method reported earlier (Dong *et al.*, 2009*b*). To an ethanol solution (5 ml) of 3-aminophenylethanone oxime (150.2 mg, 1.00 mmol) was added dropwise an ethanol solution (5 ml) of 5-bromosalicylaldehyde (201.1 mg, 1.00 mmol) then the yellow precipitate was obtained. The mixture solution was stirred at 328–333 K for 1 h. After cooling to room temperature, the precipitate was filtered off, dried *in vacuo* and purified by recrystallization from ethanol of solid. Yield: 54.01%, m. p. 459–461 K. Anal. Calc. for $C_{15}H_{13}BrN_2O_2$: C, 54.07; H, 3.93; N, 8.41. Found: C, 54.32; H, 4.01; N, 8.81.

Yellow needle-like single crystals suitable for X-ray diffraction studies were obtained by slow evaporation from a solution of dichloromethane at room temperature for about four weeks.

### S3. Refinement

Non-H atoms were refined anisotropically. H atoms were treated as riding atoms with distances C—H = 0.96 Å ($CH_3$), 0.93 Å (CH), O—H = 0.82 Å for (OH). The isotropic displacement parameters for all H atoms were set equal to 1.2 or 1.5 $U_{eq}$ of the carrier atom.

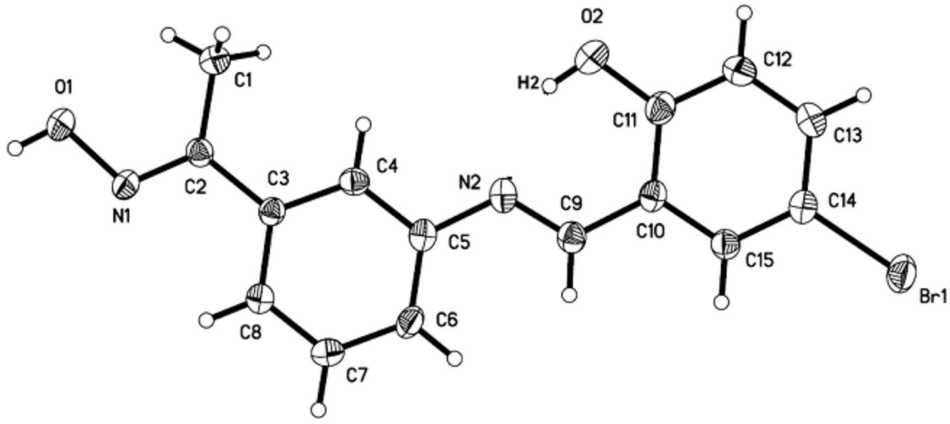



**Figure 1**

The molecule structure of the title compound with atom numbering. Displacement ellipsoids for non-hydrogen atoms are drawn at the 30% probability level.

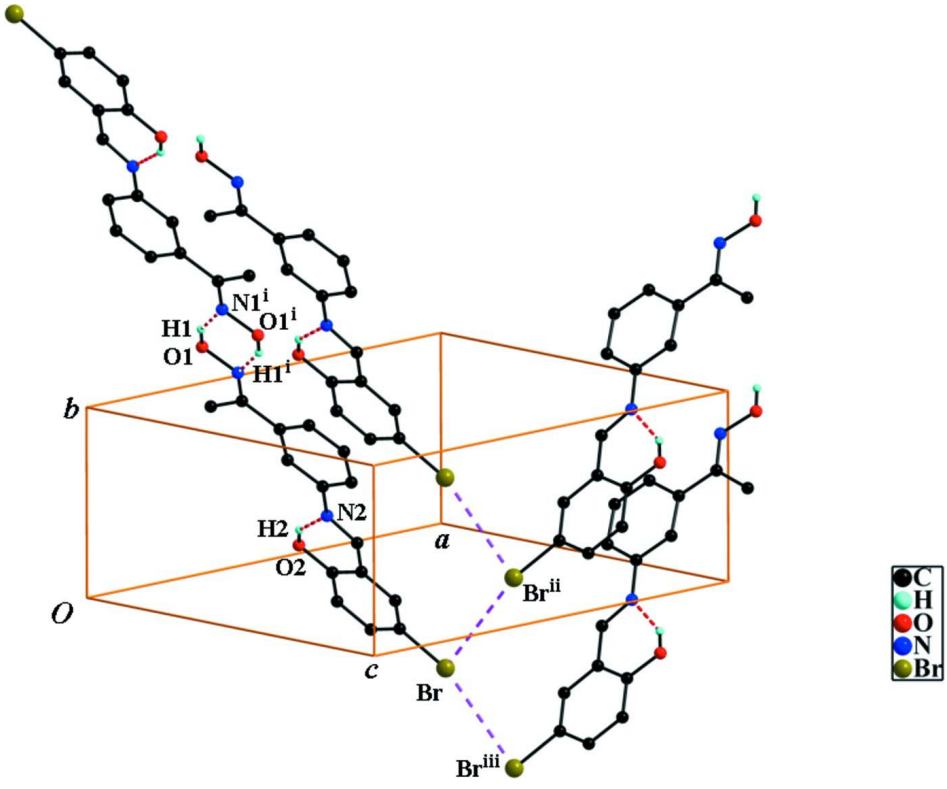



**Figure 2**

O—H..N and Br···Br interactions (dotted lines) in the crystal structure of the title compound. [Symmetry codes: (i) -*x* + 1, *y* + 1/2, -*z* + 3/2; (ii) -*x* + 1, *y* - 1/2, -*z* + 3/2; (iii) -*x*, -*y* + 3, -*z* + 1.]

### 4-Bromo-2-{(*E*)-3-[1-(hydroxyimino)ethyl]phenyliminomethyl}phenol

*Crystal data*

$C_{15}H_{13}BrN_2O_2$
$M_r$ = 333.18

Monoclinic, $P2_1/c$
Hall symbol: -p 2ybc

$a$ = 17.020 (2) Å
$b$ = 6.1676 (7) Å
$c$ = 13.693 (1) Å
$\beta$ = 96.461 (1)°
$V$ = 1428.3 (3) Å$^3$
$Z$ = 4
$F$(000) = 672
$D_x$ = 1.549 Mg m$^{-3}$

Melting point = 459–461 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2173 reflections
$\theta$ = 2.7–23.8°
$\mu$ = 2.88 mm$^{-1}$
$T$ = 298 K
Needle-like, yellow
0.45 × 0.20 × 0.10 mm

*Data collection*

Siemens SMART 1000 CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 10.0 pixels mm$^{-1}$
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.357, $T_{max}$ = 0.762

6906 measured reflections
2492 independent reflections
1799 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.051
$\theta_{max}$ = 25.0°, $\theta_{min}$ = 2.4°
$h$ = −20→14
$k$ = −7→7
$l$ = −15→16

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.100
$S$ = 0.99
2492 reflections
182 parameters
0 restraints
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: difference Fourier map
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.47 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.32 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 (Å$^2$)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br | 0.46909 (2) | −0.34895 (6) | 0.66885 (3) | 0.05662 (19) |
| N1 | 0.04843 (18) | 1.3049 (4) | 0.46740 (19) | 0.0451 (7) |
| N2 | 0.25065 (15) | 0.4933 (4) | 0.52712 (19) | 0.0416 (7) |
| O1 | 0.01134 (16) | 1.4311 (4) | 0.38885 (16) | 0.0609 (8) |
| H1 | −0.0096 | 1.5373 | 0.4110 | 0.091* |
| O2 | 0.29339 (17) | 0.2760 (5) | 0.37605 (18) | 0.0688 (8) |
| H2 | 0.2718 | 0.3726 | 0.4044 | 0.103* |
| C1 | 0.0818 (3) | 1.0731 (7) | 0.3317 (2) | 0.0601 (11) |
| H1A | 0.0385 | 1.1454 | 0.2940 | 0.090* |

| | | | | |
|---|---|---|---|---|
| H1B | 0.0753 | 0.9191 | 0.3247 | 0.090* |
| H1C | 0.1306 | 1.1160 | 0.3084 | 0.090* |
| C2 | 0.0833 (2) | 1.1340 (5) | 0.4385 (2) | 0.0355 (8) |
| C3 | 0.12600 (18) | 0.9934 (5) | 0.5170 (2) | 0.0328 (7) |
| C4 | 0.16790 (19) | 0.8077 (5) | 0.4921 (2) | 0.0361 (8) |
| H4 | 0.1683 | 0.7723 | 0.4261 | 0.043* |
| C5 | 0.2089 (2) | 0.6749 (5) | 0.5637 (2) | 0.0372 (8) |
| C6 | 0.2088 (2) | 0.7269 (6) | 0.6638 (2) | 0.0457 (9) |
| H6 | 0.2355 | 0.6402 | 0.7123 | 0.055* |
| C7 | 0.1674 (2) | 0.9129 (6) | 0.6892 (2) | 0.0541 (10) |
| H7 | 0.1670 | 0.9486 | 0.7551 | 0.065* |
| C8 | 0.1272 (2) | 1.0439 (6) | 0.6175 (2) | 0.0439 (9) |
| H8 | 0.1007 | 1.1664 | 0.6362 | 0.053* |
| C9 | 0.2887 (2) | 0.3533 (5) | 0.5848 (2) | 0.0402 (8) |
| H9 | 0.2886 | 0.3675 | 0.6524 | 0.048* |
| C10 | 0.33200 (19) | 0.1729 (5) | 0.5462 (2) | 0.0370 (8) |
| C11 | 0.3322 (2) | 0.1382 (6) | 0.4443 (3) | 0.0455 (9) |
| C12 | 0.3730 (2) | −0.0397 (6) | 0.4104 (3) | 0.0554 (10) |
| H12 | 0.3726 | −0.0625 | 0.3432 | 0.067* |
| C13 | 0.4141 (2) | −0.1828 (6) | 0.4770 (3) | 0.0520 (10) |
| H13 | 0.4413 | −0.3000 | 0.4544 | 0.062* |
| C14 | 0.4138 (2) | −0.1477 (5) | 0.5778 (2) | 0.0391 (8) |
| C15 | 0.37336 (19) | 0.0263 (5) | 0.6123 (2) | 0.0393 (8) |
| H15 | 0.3735 | 0.0467 | 0.6797 | 0.047* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br | 0.0571 (3) | 0.0476 (3) | 0.0643 (3) | 0.01472 (19) | 0.0030 (2) | 0.00954 (19) |
| N1 | 0.056 (2) | 0.0395 (17) | 0.0372 (15) | 0.0112 (15) | −0.0063 (14) | 0.0022 (13) |
| N2 | 0.0357 (17) | 0.0356 (17) | 0.0537 (17) | 0.0027 (13) | 0.0058 (14) | 0.0020 (13) |
| O1 | 0.083 (2) | 0.0526 (16) | 0.0436 (13) | 0.0295 (15) | −0.0089 (13) | 0.0039 (12) |
| O2 | 0.078 (2) | 0.079 (2) | 0.0479 (14) | 0.0289 (17) | 0.0001 (15) | 0.0108 (14) |
| C1 | 0.081 (3) | 0.062 (2) | 0.0367 (19) | 0.028 (2) | 0.0017 (19) | −0.0001 (18) |
| C2 | 0.036 (2) | 0.0329 (19) | 0.0373 (17) | −0.0002 (15) | 0.0027 (15) | −0.0020 (14) |
| C3 | 0.0309 (19) | 0.0315 (18) | 0.0353 (16) | 0.0001 (14) | 0.0005 (14) | 0.0005 (14) |
| C4 | 0.037 (2) | 0.037 (2) | 0.0338 (16) | −0.0039 (15) | 0.0021 (15) | −0.0024 (14) |
| C5 | 0.0311 (19) | 0.0339 (19) | 0.0462 (19) | −0.0012 (14) | 0.0031 (15) | 0.0022 (15) |
| C6 | 0.051 (2) | 0.043 (2) | 0.043 (2) | 0.0113 (18) | 0.0038 (17) | 0.0141 (16) |
| C7 | 0.071 (3) | 0.058 (2) | 0.0331 (18) | 0.014 (2) | 0.0074 (18) | 0.0027 (17) |
| C8 | 0.052 (2) | 0.040 (2) | 0.0395 (18) | 0.0097 (17) | 0.0060 (17) | 0.0024 (16) |
| C9 | 0.040 (2) | 0.0346 (19) | 0.0455 (19) | −0.0010 (16) | 0.0020 (16) | −0.0017 (16) |
| C10 | 0.0321 (19) | 0.0332 (19) | 0.0443 (18) | −0.0013 (15) | −0.0016 (15) | 0.0004 (15) |
| C11 | 0.037 (2) | 0.050 (2) | 0.048 (2) | 0.0033 (17) | 0.0018 (17) | 0.0052 (18) |
| C12 | 0.057 (3) | 0.070 (3) | 0.0408 (19) | 0.012 (2) | 0.0101 (18) | −0.0030 (19) |
| C13 | 0.051 (3) | 0.051 (2) | 0.055 (2) | 0.0117 (18) | 0.0109 (19) | −0.0053 (18) |
| C14 | 0.034 (2) | 0.0331 (19) | 0.050 (2) | −0.0024 (16) | 0.0022 (16) | 0.0017 (15) |
| C15 | 0.038 (2) | 0.038 (2) | 0.0411 (18) | 0.0003 (16) | 0.0013 (16) | −0.0041 (15) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br—C14 | 1.928 (3) | C4—H4 | 0.9300 |
| Br—Br$^{i}$ | 3.8768 (5) | C5—C6 | 1.409 (5) |
| Br—Br$^{ii}$ | 3.8768 (5) | C6—C7 | 1.410 (5) |
| N1—C2 | 1.293 (4) | C6—H6 | 0.9300 |
| N1—O1 | 1.417 (3) | C7—C8 | 1.390 (5) |
| N2—C9 | 1.294 (4) | C7—H7 | 0.9300 |
| N2—C5 | 1.446 (4) | C8—H8 | 0.9300 |
| O1—H1 | 0.8200 | C9—C10 | 1.466 (4) |
| O2—C11 | 1.377 (4) | C9—H9 | 0.9300 |
| O2—H2 | 0.8200 | C10—C15 | 1.411 (4) |
| C1—C2 | 1.507 (4) | C10—C11 | 1.411 (5) |
| C1—H1A | 0.9600 | C11—C12 | 1.405 (5) |
| C1—H1B | 0.9600 | C12—C13 | 1.399 (5) |
| C1—H1C | 0.9600 | C12—H12 | 0.9300 |
| C2—C3 | 1.504 (4) | C13—C14 | 1.398 (5) |
| C3—C8 | 1.409 (4) | C13—H13 | 0.9300 |
| C3—C4 | 1.411 (4) | C14—C15 | 1.387 (4) |
| C4—C5 | 1.401 (4) | C15—H15 | 0.9300 |
| | | | |
| C14—Br—Br$^{i}$ | 86.56 (10) | C8—C7—C6 | 121.3 (3) |
| C14—Br—Br$^{ii}$ | 164.58 (10) | C8—C7—H7 | 119.4 |
| Br$^{i}$—Br—Br$^{ii}$ | 105.395 (19) | C6—C7—H7 | 119.4 |
| C2—N1—O1 | 113.3 (3) | C7—C8—C3 | 120.9 (3) |
| C9—N2—C5 | 122.5 (3) | C7—C8—H8 | 119.6 |
| N1—O1—H1 | 109.5 | C3—C8—H8 | 119.6 |
| C11—O2—H2 | 109.5 | N2—C9—C10 | 121.6 (3) |
| C2—C1—H1A | 109.5 | N2—C9—H9 | 119.2 |
| C2—C1—H1B | 109.5 | C10—C9—H9 | 119.2 |
| H1A—C1—H1B | 109.5 | C15—C10—C11 | 118.7 (3) |
| C2—C1—H1C | 109.5 | C15—C10—C9 | 119.3 (3) |
| H1A—C1—H1C | 109.5 | C11—C10—C9 | 122.0 (3) |
| H1B—C1—H1C | 109.5 | O2—C11—C12 | 118.3 (3) |
| N1—C2—C3 | 116.9 (3) | O2—C11—C10 | 121.5 (3) |
| N1—C2—C1 | 122.8 (3) | C12—C11—C10 | 120.1 (3) |
| C3—C2—C1 | 120.2 (3) | C13—C12—C11 | 120.4 (3) |
| C8—C3—C4 | 117.6 (3) | C13—C12—H12 | 119.8 |
| C8—C3—C2 | 121.6 (3) | C11—C12—H12 | 119.8 |
| C4—C3—C2 | 120.8 (3) | C14—C13—C12 | 119.3 (3) |
| C5—C4—C3 | 122.0 (3) | C14—C13—H13 | 120.4 |
| C5—C4—H4 | 119.0 | C12—C13—H13 | 120.4 |
| C3—C4—H4 | 119.0 | C15—C14—C13 | 120.9 (3) |
| C4—C5—C6 | 119.5 (3) | C15—C14—Br | 120.2 (2) |
| C4—C5—N2 | 115.8 (3) | C13—C14—Br | 118.9 (2) |
| C6—C5—N2 | 124.6 (3) | C14—C15—C10 | 120.5 (3) |
| C5—C6—C7 | 118.7 (3) | C14—C15—H15 | 119.7 |
| C5—C6—H6 | 120.6 | C10—C15—H15 | 119.7 |

| | | | |
|---|---|---|---|
| C7—C6—H6 | 120.6 | | |
| | | | |
| O1—N1—C2—C3 | 178.5 (3) | N2—C9—C10—C15 | 179.2 (3) |
| O1—N1—C2—C1 | −1.9 (5) | N2—C9—C10—C11 | −2.2 (5) |
| N1—C2—C3—C8 | 0.8 (5) | C15—C10—C11—O2 | −179.6 (3) |
| C1—C2—C3—C8 | −178.8 (3) | C9—C10—C11—O2 | 1.8 (5) |
| N1—C2—C3—C4 | −177.9 (3) | C15—C10—C11—C12 | 0.1 (5) |
| C1—C2—C3—C4 | 2.5 (5) | C9—C10—C11—C12 | −178.5 (3) |
| C8—C3—C4—C5 | 0.6 (5) | O2—C11—C12—C13 | 179.2 (4) |
| C2—C3—C4—C5 | 179.4 (3) | C10—C11—C12—C13 | −0.5 (6) |
| C3—C4—C5—C6 | −0.1 (5) | C11—C12—C13—C14 | 0.4 (6) |
| C3—C4—C5—N2 | −178.6 (3) | C12—C13—C14—C15 | 0.0 (5) |
| C9—N2—C5—C4 | −177.6 (3) | C12—C13—C14—Br | 178.9 (3) |
| C9—N2—C5—C6 | 4.0 (5) | Br$^{i}$—Br—C14—C15 | −39.2 (3) |
| C4—C5—C6—C7 | −0.3 (5) | Br$^{ii}$—Br—C14—C15 | 102.3 (4) |
| N2—C5—C6—C7 | 178.1 (3) | Br$^{i}$—Br—C14—C13 | 141.9 (3) |
| C5—C6—C7—C8 | 0.0 (6) | Br$^{ii}$—Br—C14—C13 | −76.7 (5) |
| C6—C7—C8—C3 | 0.6 (6) | C13—C14—C15—C10 | −0.4 (5) |
| C4—C3—C8—C7 | −0.9 (5) | Br—C14—C15—C10 | −179.3 (2) |
| C2—C3—C8—C7 | −179.6 (3) | C11—C10—C15—C14 | 0.3 (5) |
| C5—N2—C9—C10 | −178.8 (3) | C9—C10—C15—C14 | 179.0 (3) |

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

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···N1$^{iii}$ | 0.82 | 2.10 | 2.830 (4) | 149 |
| O2—H2···N2 | 0.82 | 1.91 | 2.635 (4) | 147 |

Symmetry code: (iii) −*x*, −*y*+3, −*z*+1.