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# *N*′-(3-Bromo-5-chloro-2-hydroxybenzylidene)-3,4,5-trihydroxybenzohydrazide methanol solvate

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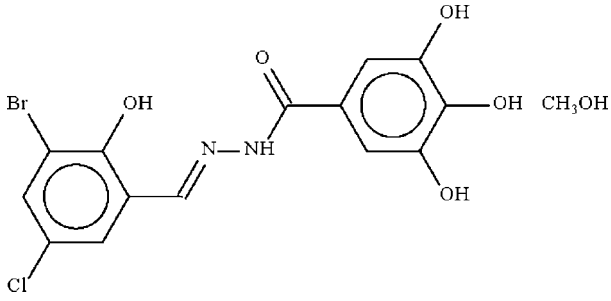
Key indicators: single-crystal X-ray study; $T$ = 123 K; mean $\sigma$(C–C) = 0.002 Å; $R$ factor = 0.023; $wR$ factor = 0.068; data-to-parameter ratio = 14.8.

The benzohydrazide molecule of the title compound, $C_{14}H_{10}BrClN_2O_5\cdot CH_3OH$, is non-planar, the two aromatic rings at either side of the –C(=O)–NH–N=CH– unit being twisted by 5.9 (1)°. The benzohydrazide molecule is linked to the solvent molecule by an O—H···O hydrogen bond. Molecules are connected by further O—H···O hydrogen bonds and an N—H···O link into a two-dimensional array.

## Related literature

For the the parent *N*′-(2-hydroxybenzylidene)benzohydrazide, see: Lyubchova *et al.* (1995). For other *N*′-(2-hydroxy-5-nitrobenzylidene)benzohydrazides, see: Ali *et al.* (2005); Lyubchova *et al.* (1995); Xu & Liu (2006).




## Experimental

### *Crystal data*

$C_{14}H_{10}BrClN_2O_5\cdot CH_4O$
$M_r$ = 433.64
Monoclinic, $C2/c$
$a$ = 21.6157 (3) Å
$b$ = 12.7408 (2) Å
$c$ = 17.0803 (2) Å
$\beta$ = 136.641 (1)°
$V$ = 3229.57 (8) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 2.75 mm$^{-1}$
$T$ = 123 K
0.20 × 0.15 × 0.10 mm

### *Data collection*

Bruker SMART APEX diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
$T_{min}$ = 0.610, $T_{max}$ = 0.771
15301 measured reflections
3714 independent reflections
3407 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.016

### *Refinement*

$R[F^2 > 2\sigma(F^2)]$ = 0.023
$wR(F^2)$ = 0.068
$S$ = 1.03
3714 reflections
251 parameters
6 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.43 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.35 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| O1—H1···O5$^{i}$ | 0.83 (1) | 2.03 (3) | 2.607 (2) | 126 (3) |
| O3—H3···O6$^{ii}$ | 0.83 (1) | 2.05 (1) | 2.856 (2) | 165 (3) |
| O4—H4···O1$^{iii}$ | 0.83 (1) | 2.20 (1) | 3.027 (2) | 173 (2) |
| O5—H5···O2$^{iii}$ | 0.82 (1) | 1.79 (1) | 2.608 (2) | 176 (2) |
| O6—H6···O2 | 0.83 (1) | 2.04 (1) | 2.843 (2) | 164 (2) |
| N2—H2···O6$^{iii}$ | 0.87 (1) | 2.25 (1) | 3.112 (2) | 169 (2) |

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

Data collection: *APEX2* (Bruker, 2008); cell refinement: *SAINT* (Bruker, 2008); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001); software used to prepare material for publication: *publCIF* (Westrip, 2009).

We thank the University of Malaya for supporting this study.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2400).

## References

Ali, H. M., Puvaneswary, S. & Ng, S. W. (2005). *Acta Cryst.* E**61**, o3464–o3465.
Barbour, L. J. (2001). *J. Supramol. Chem.* **1**, 189–191.
Bruker (2008). *APEX2* and *SAINT*. Bruker AXS Inc., Madison, Wisconsin, USA.
Lyubchova, A., Cossé-Barbi, A., Doucet, J. P., Robert, F., Souron, J.-P. & Quarton, M. (1995). *Acta Cryst.* C**51**, 1893–1895.
Sheldrick, G. M. (1996). *SADABS*. University of Göttingen, Germany.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Westrip, S. P. (2009). *publCIF*. In preparation.
Xu, H.-M. & Liu, S.-X. (2006). *Acta Cryst.* E**62**, o3026–o3027.

# supplementary materials

*Acta Cryst.* (2009). E**65**, o909 [ **doi:10.1107/S1600536809010575** ]

# *N*'-(3-Bromo-5-chloro-2-hydroxybenzylidene)-3,4,5-trihydroxybenzohydrazide methanol solvate

**A. A. Abdul Alhadi, H. M. Ali and S. W. Ng**

## Comment

(type here to add)

## Experimental

3-Bromo-5-chloro-2-hydroxybenzaldehyde (0.47 g, 2 mmol) and 3,4,5-trihydroxybenzoylhydrazide (0.36 g, 2 mmol) were heated in ethanol (50 ml) for several hours. The solvent was removed and the product recrystallized from methanol.

## Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H 0.95 Å, $U$(H) = 1.2$U$(C)], and were included in the refinement in the riding model approximation.

The amino and hydroxy H-atoms were located in a difference Fourier map, and were refined with distance restraints of N–H 0.88±0.01 Å and O–H 0.84±0.01 Å, respectively; their temperature factors were refined isotropically.

## Figures

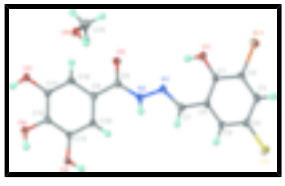


Fig. 1. Thermal ellipsoid plot (Barbour, 2001) of $C_{14}H_{10}BrClNO_5{\cdot}CH_3OH$ at the 70% probability level; hydrogen atoms are drawn as spheres of arbitrary radius.

## *N*'-(3-Bromo-5-chloro-2-hydroxybenzylidene)-3,4,5-trihydroxybenzohydrazide methanol solvate

*Crystal data*

| | |
|---|---|
| $C_{14}H_{10}BrClN_2O_5{\cdot}CH_4O$ | $F_{000}$ = 1744 |
| $M_r$ = 433.64 | $D_x$ = 1.784 Mg m$^{-3}$ |
| Monoclinic, $C2/c$ | Mo $K\alpha$ radiation<br>λ = 0.71073 Å |
| Hall symbol: -C 2yc | Cell parameters from 8789 reflections |
| $a$ = 21.6157 (3) Å | θ = 2.7–28.3º |
| $b$ = 12.7408 (2) Å | μ = 2.75 mm$^{-1}$ |
| $c$ = 17.0803 (2) Å | $T$ = 123 K |
| β = 136.641 (1)º | Polyhedral, tan |
| $V$ = 3229.57 (8) Å$^3$ | 0.20 × 0.15 × 0.10 mm |

$Z = 8$

*Data collection*

| | |
|---|---|
| Bruker SMART APEX diffractometer | 3714 independent reflections |
| Radiation source: fine-focus sealed tube | 3407 reflections with $I > 2\sigma(I)$ |
| Monochromator: graphite | $R_{int} = 0.016$ |
| $T = 123$ K | $\theta_{max} = 27.5^{o}$ |
| ω scans | $\theta_{min} = 2.0^{o}$ |
| Absorption correction: Multi-scan (SADABS; Sheldrick, 1996) | $h = -28\rightarrow26$ |
| $T_{min} = 0.610$, $T_{max} = 0.771$ | $k = -16\rightarrow16$ |
| 15301 measured reflections | $l = -22\rightarrow21$ |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Secondary atom site location: difference Fourier map |
| Least-squares matrix: full | Hydrogen site location: inferred from neighbouring sites |
| $R[F^2 > 2\sigma(F^2)] = 0.023$ | H atoms treated by a mixture of independent and constrained refinement |
| $wR(F^2) = 0.068$ | $w = 1/[\sigma^2(F_o^2) + (0.0429P)^2 + 3.4447P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $S = 1.03$ | $(\Delta/\sigma)_{max} = 0.001$ |
| 3714 reflections | $\Delta\rho_{max} = 0.43$ e Å$^{-3}$ |
| 251 parameters | $\Delta\rho_{min} = -0.35$ e Å$^{-3}$ |
| 6 restraints | Extinction correction: none |
| Primary atom site location: structure-invariant direct methods | |

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.044783 (12) | 0.783092 (13) | 0.137916 (14) | 0.02172 (7) |
| Cl1 | 0.01420 (3) | 0.35175 (3) | 0.10946 (4) | 0.02369 (10) |
| N1 | 0.18779 (9) | 0.61375 (11) | 0.54542 (11) | 0.0148 (3) |
| N2 | 0.23179 (9) | 0.58418 (11) | 0.65407 (11) | 0.0154 (3) |
| O1 | 0.13116 (9) | 0.74001 (9) | 0.37133 (11) | 0.0211 (3) |
| O2 | 0.20939 (8) | 0.74133 (9) | 0.69379 (10) | 0.0187 (2) |
| O3 | 0.36037 (9) | 0.69205 (10) | 1.09583 (10) | 0.0219 (3) |
| O4 | 0.37603 (8) | 0.47725 (9) | 1.12740 (10) | 0.0189 (2) |
| O5 | 0.31633 (9) | 0.34724 (9) | 0.95863 (10) | 0.0205 (3) |
| O6 | 0.15053 (8) | 0.88367 (9) | 0.75713 (10) | 0.0196 (2) |
| C1 | 0.10878 (11) | 0.64859 (12) | 0.31698 (13) | 0.0155 (3) |
| C2 | 0.06644 (11) | 0.65171 (12) | 0.20499 (14) | 0.0156 (3) |
| C3 | 0.03858 (11) | 0.56163 (13) | 0.14173 (13) | 0.0172 (3) |
| H3A | 0.0088 | 0.5655 | 0.0652 | 0.021* |

| | | | | |
|---|---|---|---|---|
| C4 | 0.05469 (11) | 0.46540 (12) | 0.19171 (14) | 0.0168 (3) |
| C5 | 0.09940 (10) | 0.45814 (12) | 0.30364 (13) | 0.0158 (3) |
| H5A | 0.1117 | 0.3914 | 0.3373 | 0.019* |
| C6 | 0.12644 (10) | 0.54979 (12) | 0.36718 (13) | 0.0151 (3) |
| C7 | 0.17192 (10) | 0.53678 (12) | 0.48399 (13) | 0.0155 (3) |
| H7 | 0.1907 | 0.4684 | 0.5163 | 0.019* |
| C8 | 0.23645 (10) | 0.64897 (12) | 0.72065 (13) | 0.0147 (3) |
| C9 | 0.27436 (10) | 0.60244 (12) | 0.82779 (13) | 0.0143 (3) |
| C10 | 0.30257 (11) | 0.66835 (12) | 0.91445 (13) | 0.0161 (3) |
| H10 | 0.2997 | 0.7424 | 0.9056 | 0.019* |
| C11 | 0.33473 (11) | 0.62583 (12) | 1.01356 (13) | 0.0156 (3) |
| C12 | 0.34227 (10) | 0.51690 (12) | 1.02835 (13) | 0.0146 (3) |
| C13 | 0.31234 (10) | 0.45163 (12) | 0.94055 (13) | 0.0147 (3) |
| C14 | 0.27745 (10) | 0.49359 (12) | 0.84020 (13) | 0.0146 (3) |
| H14 | 0.2557 | 0.4486 | 0.7800 | 0.018* |
| C15 | 0.06333 (12) | 0.92150 (14) | 0.65359 (15) | 0.0237 (4) |
| H15A | 0.0445 | 0.9781 | 0.6715 | 0.036* |
| H15B | 0.0196 | 0.8640 | 0.6160 | 0.036* |
| H15C | 0.0664 | 0.9482 | 0.6027 | 0.036* |
| H1 | 0.154 (2) | 0.731 (3) | 0.4365 (15) | 0.087 (13)* |
| H3 | 0.3635 (18) | 0.6613 (19) | 1.1413 (18) | 0.044 (7)* |
| H4 | 0.3783 (17) | 0.4119 (8) | 1.129 (2) | 0.036 (7)* |
| H5 | 0.3065 (15) | 0.3125 (16) | 0.9101 (15) | 0.030 (6)* |
| H6 | 0.1634 (16) | 0.8331 (14) | 0.741 (2) | 0.037 (7)* |
| H2 | 0.2604 (14) | 0.5242 (11) | 0.6799 (18) | 0.029 (6)* |

*Atomic displacement parameters (Å$^2$)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.02904 (11) | 0.01747 (10) | 0.01845 (10) | 0.00031 (6) | 0.01720 (9) | 0.00285 (6) |
| Cl1 | 0.0373 (2) | 0.01580 (19) | 0.01895 (19) | −0.00382 (16) | 0.02079 (19) | −0.00522 (14) |
| N1 | 0.0169 (6) | 0.0172 (6) | 0.0109 (6) | 0.0006 (5) | 0.0103 (5) | 0.0013 (5) |
| N2 | 0.0205 (6) | 0.0142 (6) | 0.0119 (6) | 0.0032 (5) | 0.0120 (6) | 0.0031 (5) |
| O1 | 0.0321 (7) | 0.0152 (5) | 0.0161 (6) | 0.0006 (5) | 0.0175 (6) | −0.0016 (5) |
| O2 | 0.0293 (6) | 0.0135 (5) | 0.0186 (6) | 0.0039 (5) | 0.0191 (5) | 0.0034 (4) |
| O3 | 0.0374 (7) | 0.0154 (5) | 0.0171 (6) | −0.0039 (5) | 0.0212 (6) | −0.0038 (5) |
| O4 | 0.0294 (6) | 0.0154 (6) | 0.0142 (5) | 0.0022 (5) | 0.0166 (5) | 0.0019 (4) |
| O5 | 0.0378 (7) | 0.0109 (5) | 0.0182 (6) | 0.0028 (5) | 0.0221 (6) | 0.0017 (4) |
| O6 | 0.0251 (6) | 0.0178 (6) | 0.0186 (6) | 0.0016 (5) | 0.0168 (5) | −0.0013 (5) |
| C1 | 0.0184 (7) | 0.0151 (7) | 0.0154 (7) | −0.0006 (6) | 0.0131 (7) | −0.0020 (6) |
| C2 | 0.0186 (7) | 0.0153 (7) | 0.0153 (7) | 0.0015 (6) | 0.0130 (7) | 0.0026 (6) |
| C3 | 0.0185 (7) | 0.0226 (8) | 0.0135 (7) | −0.0012 (6) | 0.0126 (7) | −0.0011 (6) |
| C4 | 0.0202 (7) | 0.0170 (7) | 0.0169 (7) | −0.0017 (6) | 0.0147 (7) | −0.0037 (6) |
| C5 | 0.0184 (7) | 0.0153 (7) | 0.0164 (7) | 0.0005 (6) | 0.0136 (6) | 0.0007 (6) |
| C6 | 0.0164 (7) | 0.0182 (7) | 0.0129 (7) | 0.0004 (6) | 0.0113 (6) | 0.0003 (6) |
| C7 | 0.0173 (7) | 0.0156 (7) | 0.0135 (7) | 0.0006 (6) | 0.0112 (6) | 0.0017 (6) |
| C8 | 0.0165 (7) | 0.0151 (7) | 0.0138 (7) | −0.0016 (6) | 0.0114 (6) | −0.0007 (5) |
| C9 | 0.0158 (7) | 0.0158 (7) | 0.0126 (7) | 0.0010 (6) | 0.0107 (6) | 0.0009 (6) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C10 | 0.0212 (8) | 0.0123 (7) | 0.0166 (8) | −0.0005 (6) | 0.0144 (7) | −0.0003 (6) |
| C11 | 0.0198 (7) | 0.0148 (7) | 0.0140 (7) | −0.0021 (6) | 0.0129 (6) | −0.0030 (6) |
| C12 | 0.0168 (7) | 0.0167 (7) | 0.0123 (7) | 0.0009 (6) | 0.0112 (6) | 0.0013 (6) |
| C13 | 0.0180 (7) | 0.0121 (7) | 0.0168 (7) | 0.0016 (6) | 0.0136 (6) | 0.0006 (6) |
| C14 | 0.0189 (7) | 0.0136 (7) | 0.0144 (7) | 0.0005 (6) | 0.0131 (6) | −0.0005 (5) |
| C15 | 0.0247 (8) | 0.0219 (8) | 0.0214 (8) | 0.0000 (7) | 0.0158 (7) | −0.0015 (7) |

*Geometric parameters (Å, °)*

| | | | |
|---|---|---|---|
| Br1—C2 | 1.8852 (15) | C3—C4 | 1.386 (2) |
| Cl1—C4 | 1.7460 (16) | C3—H3A | 0.9500 |
| N1—C7 | 1.287 (2) | C4—C5 | 1.382 (2) |
| N1—N2 | 1.3870 (18) | C5—C6 | 1.400 (2) |
| N2—C8 | 1.348 (2) | C5—H5A | 0.9500 |
| N2—H2 | 0.874 (10) | C6—C7 | 1.457 (2) |
| O1—C1 | 1.3415 (19) | C7—H7 | 0.9500 |
| O1—H1 | 0.832 (10) | C8—C9 | 1.480 (2) |
| O2—C8 | 1.2438 (19) | C9—C14 | 1.397 (2) |
| O3—C11 | 1.3642 (19) | C9—C10 | 1.398 (2) |
| O3—H3 | 0.828 (10) | C10—C11 | 1.390 (2) |
| O4—C12 | 1.3619 (18) | C10—H10 | 0.9500 |
| O4—H4 | 0.833 (10) | C11—C12 | 1.399 (2) |
| O5—C13 | 1.3538 (18) | C12—C13 | 1.396 (2) |
| O5—H5 | 0.820 (10) | C13—C14 | 1.383 (2) |
| O6—C15 | 1.437 (2) | C14—H14 | 0.9500 |
| O6—H6 | 0.828 (10) | C15—H15A | 0.9800 |
| C1—C2 | 1.397 (2) | C15—H15B | 0.9800 |
| C1—C6 | 1.410 (2) | C15—H15C | 0.9800 |
| C2—C3 | 1.379 (2) | | |
| C7—N1—N2 | 113.63 (13) | C6—C7—H7 | 118.5 |
| C8—N2—N1 | 121.35 (13) | O2—C8—N2 | 122.77 (14) |
| C8—N2—H2 | 121.2 (15) | O2—C8—C9 | 121.61 (14) |
| N1—N2—H2 | 117.2 (15) | N2—C8—C9 | 115.61 (13) |
| C1—O1—H1 | 112 (3) | C14—C9—C10 | 119.97 (14) |
| C11—O3—H3 | 111.6 (19) | C14—C9—C8 | 120.49 (14) |
| C12—O4—H4 | 112.6 (18) | C10—C9—C8 | 119.44 (14) |
| C13—O5—H5 | 111.9 (17) | C11—C10—C9 | 120.15 (14) |
| C15—O6—H6 | 107.8 (17) | C11—C10—H10 | 119.9 |
| O1—C1—C2 | 118.05 (14) | C9—C10—H10 | 119.9 |
| O1—C1—C6 | 123.52 (14) | O3—C11—C10 | 118.85 (14) |
| C2—C1—C6 | 118.42 (14) | O3—C11—C12 | 121.39 (14) |
| C3—C2—C1 | 121.82 (14) | C10—C11—C12 | 119.75 (14) |
| C3—C2—Br1 | 119.27 (12) | O4—C12—C13 | 121.65 (14) |
| C1—C2—Br1 | 118.90 (12) | O4—C12—C11 | 118.63 (14) |
| C2—C3—C4 | 118.86 (14) | C13—C12—C11 | 119.67 (14) |
| C2—C3—H3A | 120.6 | O5—C13—C14 | 123.32 (14) |
| C4—C3—H3A | 120.6 | O5—C13—C12 | 115.94 (14) |
| C5—C4—C3 | 121.40 (14) | C14—C13—C12 | 120.69 (14) |
| C5—C4—Cl1 | 119.65 (12) | C13—C14—C9 | 119.64 (14) |

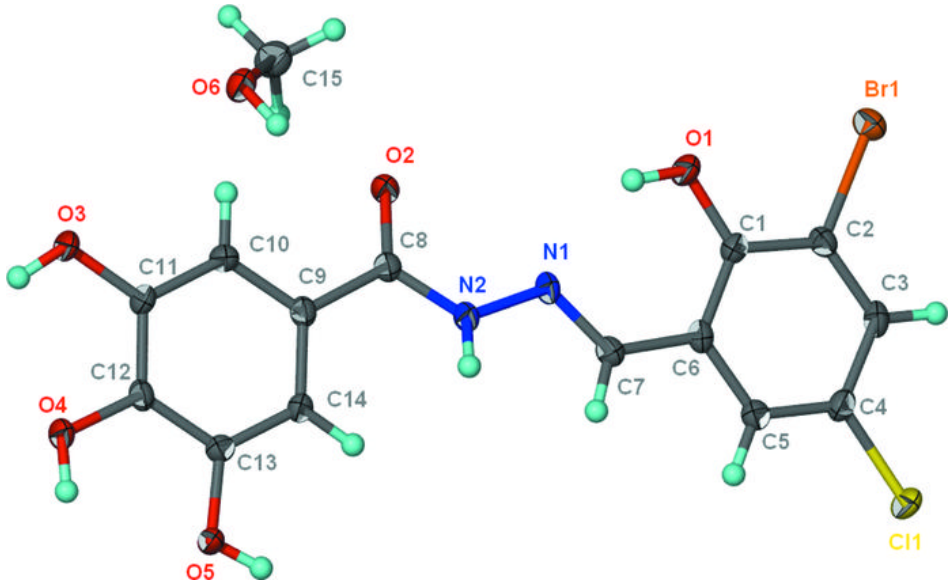
| | | | |
|---|---|---|---|
| C3—C4—Cl1 | 118.92 (12) | C13—C14—H14 | 120.2 |
| C4—C5—C6 | 119.62 (14) | C9—C14—H14 | 120.2 |
| C4—C5—H5A | 120.2 | O6—C15—H15A | 109.5 |
| C6—C5—H5A | 120.2 | O6—C15—H15B | 109.5 |
| C5—C6—C1 | 119.81 (14) | H15A—C15—H15B | 109.5 |
| C5—C6—C7 | 116.89 (14) | O6—C15—H15C | 109.5 |
| C1—C6—C7 | 123.30 (14) | H15A—C15—H15C | 109.5 |
| N1—C7—C6 | 122.97 (14) | H15B—C15—H15C | 109.5 |
| N1—C7—H7 | 118.5 | | |
| C7—N1—N2—C8 | −165.52 (15) | N1—N2—C8—C9 | 172.04 (14) |
| O1—C1—C2—C3 | −177.88 (15) | O2—C8—C9—C14 | 159.38 (15) |
| C6—C1—C2—C3 | 2.7 (2) | N2—C8—C9—C14 | −19.4 (2) |
| O1—C1—C2—Br1 | 0.8 (2) | O2—C8—C9—C10 | −17.1 (2) |
| C6—C1—C2—Br1 | −178.63 (11) | N2—C8—C9—C10 | 164.18 (15) |
| C1—C2—C3—C4 | −1.2 (2) | C14—C9—C10—C11 | 0.8 (2) |
| Br1—C2—C3—C4 | −179.92 (12) | C8—C9—C10—C11 | 177.25 (14) |
| C2—C3—C4—C5 | −1.3 (2) | C9—C10—C11—O3 | −178.92 (15) |
| C2—C3—C4—Cl1 | 176.64 (12) | C9—C10—C11—C12 | 2.6 (2) |
| C3—C4—C5—C6 | 2.2 (2) | O3—C11—C12—O4 | 0.0 (2) |
| Cl1—C4—C5—C6 | −175.66 (12) | C10—C11—C12—O4 | 178.42 (14) |
| C4—C5—C6—C1 | −0.7 (2) | O3—C11—C12—C13 | 177.72 (14) |
| C4—C5—C6—C7 | 179.02 (14) | C10—C11—C12—C13 | −3.9 (2) |
| O1—C1—C6—C5 | 178.92 (15) | O4—C12—C13—O5 | 2.0 (2) |
| C2—C1—C6—C5 | −1.7 (2) | C11—C12—C13—O5 | −175.63 (14) |
| O1—C1—C6—C7 | −0.8 (2) | O4—C12—C13—C14 | 179.35 (14) |
| C2—C1—C6—C7 | 178.61 (14) | C11—C12—C13—C14 | 1.7 (2) |
| N2—N1—C7—C6 | −179.99 (14) | O5—C13—C14—C9 | 178.84 (15) |
| C5—C6—C7—N1 | −169.07 (15) | C12—C13—C14—C9 | 1.7 (2) |
| C1—C6—C7—N1 | 10.7 (2) | C10—C9—C14—C13 | −3.0 (2) |
| N1—N2—C8—O2 | −6.7 (2) | C8—C9—C14—C13 | −179.38 (14) |

*Hydrogen-bond geometry (Å, °)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| O1—H1···O5$^{i}$ | 0.83 (1) | 2.03 (3) | 2.607 (2) | 126 (3) |
| O3—H3···O6$^{ii}$ | 0.83 (1) | 2.05 (1) | 2.856 (2) | 165 (3) |
| O4—H4···O1$^{iii}$ | 0.83 (1) | 2.20 (1) | 3.027 (2) | 173 (2) |
| O5—H5···O2$^{iii}$ | 0.82 (1) | 1.79 (1) | 2.608 (2) | 176 (2) |
| O6—H6···O2 | 0.83 (1) | 2.04 (1) | 2.843 (2) | 164 (2) |
| N2—H2···O6$^{iii}$ | 0.87 (1) | 2.25 (1) | 3.112 (2) | 169 (2) |

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

**Fig. 1**


O6
C15
Br1
O1
O2
O3
C1
C2
C10
C8
C11
C9
N1
N2
C3
C12
C6
C7
C14
O4
C4
C5
C13
Cl1
O5