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2,4-Dibromo-6-[(E)-{3-[(E)-(3,5-dibromo-2-oxidobenzylidene)azaniumyl]-2,2-dimethylpropyl}iminiumyl)-methyl]phenolate

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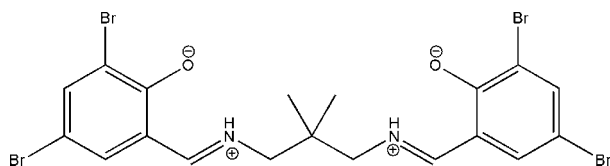
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Key indicators: single-crystal X-ray study; $T = 291$ K; mean $\sigma(\text{C}-\text{C}) = 0.007$ Å; R factor = 0.047; wR factor = 0.138; data-to-parameter ratio = 21.3.

In the title molecule, $\text{C}_{19}\text{H}_{18}\text{Br}_4\text{N}_2\text{O}_2$, the dihedral angle between the benzene rings is $73.9(2)^\circ$. Two intramolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds make $S(6)$ ring motifs. In the crystal, molecules are linked *via* $\text{C}-\text{H}\cdots\text{O}$ interactions, forming chains propagating along the a -axis direction. A short $\text{C}\cdots\text{Br}$ [3.401 (5) Å] contact is present in the crystal structure, which is further stabilized by a $\pi-\pi$ interaction [centroid-centroid distance = 3.739 (3) Å].

Related literature

For standard bond lengths, see: Allen *et al.* (1987). For hydrogen bond motifs, see: Bernstein *et al.* (1995). For related structures, see: Kargar *et al.* (2011); Kia *et al.* (2010).



Experimental

Crystal data

$\text{C}_{19}\text{H}_{18}\text{Br}_4\text{N}_2\text{O}$
 $M_r = 625.99$
 Orthorhombic, $Pbca$
 $a = 11.6861(3)$ Å
 $b = 11.4616(3)$ Å
 $c = 31.3782(9)$ Å
 $V = 4202.8(2)$ Å³
 $Z = 8$
 Mo $K\alpha$ radiation
 $\mu = 7.68$ mm⁻¹
 $T = 291$ K
 $0.25 \times 0.16 \times 0.12$ mm

Data collection

Bruker SMART APEXII CCD
 area-detector diffractometer
 Absorption correction: multi-scan
 (*SADABS*; Bruker, 2005)
 $T_{\min} = 0.250$, $T_{\max} = 0.459$
 38547 measured reflections
 5242 independent reflections
 2756 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.090$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.138$
 $S = 1.04$
 5242 reflections
 246 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.73$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.64$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

| $D-\text{H}\cdots A$ | $D-\text{H}$ | $\text{H}\cdots A$ | $D\cdots A$ | $D-\text{H}\cdots A$ |
|---|--------------|--------------------|-------------|----------------------|
| $\text{N1}-\text{H1}\cdots\text{O1}$ | 0.85 | 1.82 | 2.549 (5) | 142 |
| $\text{N2}-\text{H2}\cdots\text{O2}$ | 0.86 | 1.80 | 2.537 (5) | 143 |
| $\text{C8}-\text{H8A}\cdots\text{O2}^i$ | 0.97 | 2.53 | 3.424 (7) | 152 |

 Symmetry code: (i) $x - \frac{1}{2}, y, -z + \frac{1}{2}$.

Data collection: *APEX2* (Bruker, 2005); cell refinement: *SAINT* (Bruker, 2005); 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* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2354).

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.
 Bernstein, J., Davis, R. E., Shimoni, L. & Chang, N.-L. (1995). *Angew. Chem. Int. Ed. Engl.* **34**, 1555–1573.
 Bruker (2005). *APEX2*, *SAINT* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
 Kargar, H., Kia, R., Pahlavani, E. & Tahir, M. N. (2011). *Acta Cryst.* **E67**, o614.
 Kia, R., Kargar, H., Tahir, M. N. & Kianoosh, F. (2010). *Acta Cryst.* **E66**, o2296.
 Sheldrick, G. M. (2008). *Acta Cryst.* **A64**, 112–122.
 Spek, A. L. (2009). *Acta Cryst.* **D65**, 148–155.

supporting information

Acta Cryst. (2012). E68, o323 [doi:10.1107/S1600536811055899]

2,4-Dibromo-6-[(*E*)-({3-[(*E*)-(3,5-dibromo-2-oxidobenzylidene)azaniumyl]-2,2-dimethylpropyl}iminiumyl)methyl]phenolate

Hadi Kargar, Reza Kia, Mahbubeh Haghshenas and Muhammad Nawaz Tahir

S1. Comment

In continuation of our work on the crystal structure analysis of Schiff base ligands (Kargar *et al.*, 2011; Kia *et al.*, 2010), we synthesized the title compound and report herein on its crystal structure.

The title compound (Fig. 1) is a potential tetradentate Zwitterionic Schiff base ligand. The bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to those observed for related structures (Kargar *et al.*, 2011; Kia *et al.*, 2010).

In the molecule there are two intramolecular N—H \cdots O hydrogen bonds (Table 1) making S(6) ring motifs (Bernstein *et al.*, 1995). The dihedral angle between the benzene rings is 73.9 (2) $^{\circ}$. An interesting feature of the crystal structure is the short C6 \cdots Br1ⁱⁱⁱ contact [3.401 (5) Å; (ii) $-x+1/2, y-1/2, z$], which is shorter than the sum of the van der Waals radii [3.55 Å] of these atoms.

In the crystal, molecules are linked together along the *a* axis into chains through an intermolecular C—H \cdots O interaction (Fig. 2 and Table 1). The crystal structure is further stabilized by an intermolecular π - π interaction [Cg1 \cdots Cg2ⁱⁱⁱ = 3.739 (3) Å; (iii) $x, -y-1/2, z+1/2$; Cg1 and Cg2 are the centroid of benzene rings (C1–C6) and (C14–19), respectively].

S2. Experimental

The title compound was synthesized by adding 3,5-dibromo-salicylaldehyde (2 mmol) to a solution of 2,2-dimethyl-1,3-propanediamine (1 mmol) in ethanol (30 ml). The mixture was refluxed with stirring for 30 min. The resultant solution was filtered. Yellow single crystals of the title compound, suitable for *X*-ray structure determination, were recrystallized from ethanol by slow evaporation of the solvent at room temperature over several days.

S3. Refinement

The NH H-atoms were located in a difference Fourier map and were refined as riding atoms with $U_{\text{iso}}(\text{H}) = 1.2 U_{\text{eq}}(\text{N})$. The C-bound H-atoms were included in calculated positions and treated as riding atoms: C-H = 0.93, 0.97 and 0.96 Å for CH, CH₂, and CH₃ H-atoms, respectively, with $U_{\text{iso}}(\text{H}) = k \times U_{\text{eq}}(\text{parent C-atom})$, where $k = 1.5$ for CH₃ H-atoms and $k = 1.2$ for all other H-atoms.

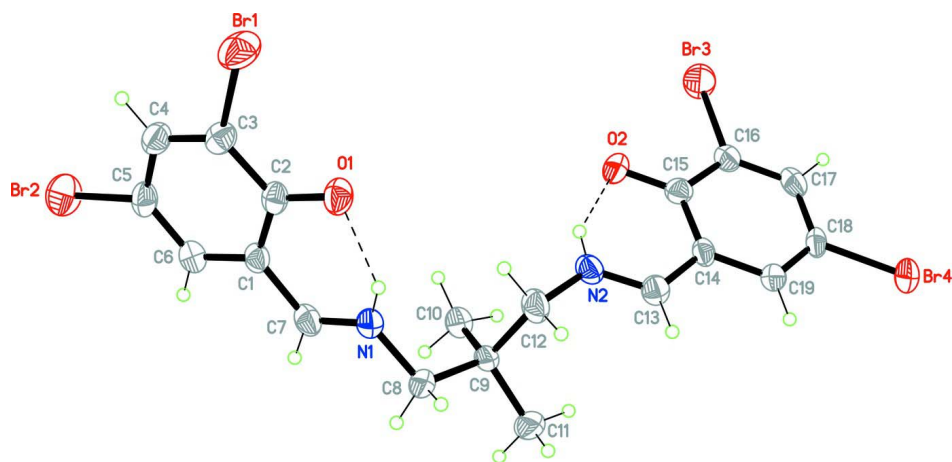


Figure 1

The molecular structure of the title molecule, showing 40% probability displacement ellipsoids and the atomic numbering. The dashed lines show the intramolecular N—H···O hydrogen bonds.

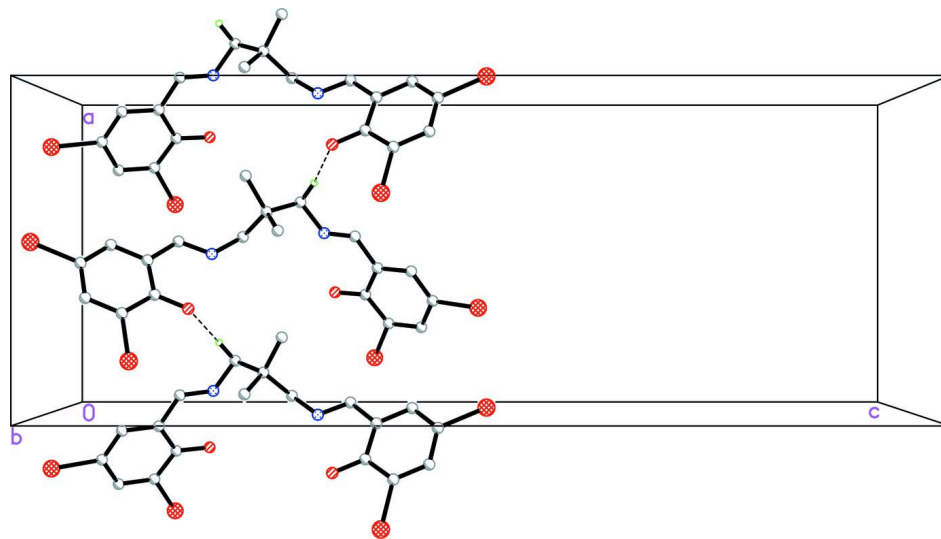


Figure 2

The crystal packing of the title compound, viewed along the *b*-axis, showing linking of molecules into a chain along the *a*-axis through the intermolecular C—H···O interactions (dashed lines). Only the H atoms involved in these interactions are shown.

2,4-Dibromo-6-[(*E*)-{(3-[(*E*)-(3,5-dibromo-2-oxidobenzylidene)azaniumyl]-2,2-dimethylpropyl)iminiumyl)methyl]phenolate

Crystal data

$C_{19}H_{18}Br_4N_2O$

$M_r = 625.99$

Orthorhombic, *Pbca*

Hall symbol: $-P\ 2ac\ 2ab$

$a = 11.6861(3)\ \text{\AA}$

$b = 11.4616(3)\ \text{\AA}$

$c = 31.3782(9)\ \text{\AA}$

$V = 4202.8(2)\ \text{\AA}^3$

$Z = 8$

$F(000) = 2416$

$D_x = 1.979\ \text{Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$

Cell parameters from 2370 reflections

$\theta = 2.5\text{--}27.5^\circ$

$\mu = 7.68 \text{ mm}^{-1}$
 $T = 291 \text{ K}$

Block, yellow
 $0.25 \times 0.16 \times 0.12 \text{ mm}$

Data collection

Bruker SMART APEXII CCD area-detector
 diffractometer
 Radiation source: fine-focus sealed tube
 Graphite monochromator
 φ and ω scans
 Absorption correction: multi-scan
 (SADABS; Bruker, 2005)
 $T_{\min} = 0.250$, $T_{\max} = 0.459$

38547 measured reflections
 5242 independent reflections
 2756 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.090$
 $\theta_{\max} = 28.4^\circ$, $\theta_{\min} = 1.3^\circ$
 $h = -15 \rightarrow 15$
 $k = -15 \rightarrow 15$
 $l = -41 \rightarrow 41$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.047$
 $wR(F^2) = 0.138$
 $S = 1.04$
 5242 reflections
 246 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
 $w = 1/[\sigma^2(F_o^2) + (0.0616P)^2]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.73 \text{ e } \text{\AA}^{-3}$
 $\Delta\rho_{\min} = -0.64 \text{ e } \text{\AA}^{-3}$

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds 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 $F^2 > 2\sigma(F^2)$ 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 (\AA^2)

| | <i>x</i> | <i>y</i> | <i>z</i> | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|--------------|----------------|----------------------------------|
| Br1 | 0.34182 (5) | -0.30064 (6) | 0.37158 (2) | 0.0653 (2) |
| Br2 | 0.17302 (6) | 0.00225 (6) | 0.49759 (2) | 0.0695 (2) |
| Br3 | 0.32582 (5) | 0.27233 (8) | 0.11028 (2) | 0.0748 (3) |
| Br4 | -0.02936 (5) | 0.17726 (6) | -0.006978 (18) | 0.0531 (2) |
| O1 | 0.1272 (3) | -0.2212 (3) | 0.32548 (12) | 0.0456 (9) |
| O2 | 0.1731 (3) | 0.1290 (3) | 0.16822 (12) | 0.0493 (10) |
| N1 | -0.0616 (3) | -0.1131 (4) | 0.31559 (14) | 0.0399 (11) |
| H1 | -0.0092 | -0.1601 | 0.3081 | 0.048* |
| N2 | 0.0054 (3) | -0.0002 (3) | 0.18846 (14) | 0.0401 (11) |
| H2 | 0.0681 | 0.0364 | 0.1930 | 0.048* |
| C1 | 0.0493 (4) | -0.0982 (4) | 0.37894 (16) | 0.0339 (11) |
| C2 | 0.1341 (4) | -0.1743 (4) | 0.36298 (16) | 0.0348 (12) |
| C3 | 0.2273 (4) | -0.1966 (4) | 0.39035 (17) | 0.0399 (13) |
| C4 | 0.2376 (4) | -0.1472 (5) | 0.42992 (17) | 0.0430 (13) |

| | | | | |
|------|-------------|-------------|--------------|-------------|
| H4 | 0.3002 | -0.1645 | 0.4471 | 0.052* |
| C5 | 0.1525 (4) | -0.0701 (5) | 0.44416 (17) | 0.0417 (13) |
| C6 | 0.0597 (4) | -0.0475 (4) | 0.41923 (17) | 0.0398 (13) |
| H6 | 0.0026 | 0.0022 | 0.4291 | 0.048* |
| C7 | -0.0502 (4) | -0.0723 (5) | 0.35284 (17) | 0.0396 (13) |
| H7 | -0.1072 | -0.0243 | 0.3638 | 0.047* |
| C8 | -0.1584 (4) | -0.0846 (5) | 0.28844 (17) | 0.0422 (13) |
| H8A | -0.2174 | -0.0478 | 0.3055 | 0.051* |
| H8B | -0.1899 | -0.1560 | 0.2767 | 0.051* |
| C9 | -0.1256 (4) | -0.0031 (4) | 0.25192 (16) | 0.0351 (12) |
| C10 | -0.0651 (4) | 0.1058 (4) | 0.26898 (17) | 0.0438 (13) |
| H10A | -0.1097 | 0.1392 | 0.2916 | 0.066* |
| H10B | -0.0568 | 0.1618 | 0.2464 | 0.066* |
| H10C | 0.0090 | 0.0848 | 0.2796 | 0.066* |
| C11 | -0.2360 (4) | 0.0326 (5) | 0.22920 (19) | 0.0528 (16) |
| H11A | -0.2745 | -0.0359 | 0.2189 | 0.079* |
| H11B | -0.2180 | 0.0827 | 0.2056 | 0.079* |
| H11C | -0.2849 | 0.0732 | 0.2488 | 0.079* |
| C12 | -0.0487 (4) | -0.0721 (5) | 0.22116 (17) | 0.0444 (13) |
| H12A | 0.0105 | -0.1111 | 0.2375 | 0.053* |
| H12B | -0.0943 | -0.1318 | 0.2073 | 0.053* |
| C13 | -0.0332 (4) | 0.0110 (4) | 0.15044 (17) | 0.0379 (12) |
| H13 | -0.1005 | -0.0271 | 0.1429 | 0.045* |
| C14 | 0.0254 (4) | 0.0815 (4) | 0.11903 (15) | 0.0338 (11) |
| C15 | 0.1304 (4) | 0.1368 (4) | 0.13050 (17) | 0.0365 (12) |
| C16 | 0.1851 (4) | 0.2010 (5) | 0.09768 (18) | 0.0407 (13) |
| C17 | 0.1389 (4) | 0.2107 (4) | 0.05729 (17) | 0.0412 (13) |
| H17 | 0.1776 | 0.2522 | 0.0363 | 0.049* |
| C18 | 0.0336 (4) | 0.1579 (4) | 0.04800 (15) | 0.0354 (11) |
| C19 | -0.0218 (4) | 0.0939 (4) | 0.07783 (16) | 0.0365 (12) |
| H19 | -0.0909 | 0.0580 | 0.0712 | 0.044* |

Atomic displacement parameters (Å²)

| | U^{11} | U^{22} | U^{33} | U^{12} | U^{13} | U^{23} |
|-----|------------|------------|------------|--------------|--------------|--------------|
| Br1 | 0.0620 (4) | 0.0651 (4) | 0.0688 (5) | 0.0276 (3) | -0.0133 (3) | -0.0081 (4) |
| Br2 | 0.0780 (5) | 0.0835 (5) | 0.0470 (4) | -0.0080 (4) | -0.0106 (3) | -0.0238 (3) |
| Br3 | 0.0533 (4) | 0.1174 (6) | 0.0537 (4) | -0.0359 (4) | 0.0020 (3) | 0.0015 (4) |
| Br4 | 0.0591 (4) | 0.0723 (4) | 0.0279 (3) | 0.0027 (3) | -0.0031 (3) | 0.0027 (3) |
| O1 | 0.056 (2) | 0.048 (2) | 0.033 (2) | 0.0070 (18) | -0.0035 (18) | -0.0054 (18) |
| O2 | 0.043 (2) | 0.071 (3) | 0.034 (2) | -0.0015 (18) | -0.0082 (18) | 0.008 (2) |
| N1 | 0.037 (2) | 0.051 (3) | 0.032 (3) | 0.0050 (19) | 0.001 (2) | 0.005 (2) |
| N2 | 0.040 (2) | 0.046 (3) | 0.035 (3) | 0.0020 (19) | 0.007 (2) | 0.008 (2) |
| C1 | 0.039 (3) | 0.034 (3) | 0.029 (3) | -0.001 (2) | 0.002 (2) | 0.007 (2) |
| C2 | 0.044 (3) | 0.030 (3) | 0.031 (3) | -0.004 (2) | -0.002 (2) | 0.008 (2) |
| C3 | 0.042 (3) | 0.033 (3) | 0.044 (4) | -0.001 (2) | -0.005 (3) | 0.007 (3) |
| C4 | 0.043 (3) | 0.048 (3) | 0.038 (3) | -0.004 (3) | -0.008 (3) | 0.002 (3) |
| C5 | 0.053 (3) | 0.043 (3) | 0.029 (3) | -0.010 (3) | -0.004 (3) | -0.001 (2) |

| | | | | | | |
|-----|-----------|-----------|-----------|------------|------------|------------|
| C6 | 0.046 (3) | 0.040 (3) | 0.033 (3) | -0.001 (2) | 0.004 (3) | 0.001 (3) |
| C7 | 0.046 (3) | 0.040 (3) | 0.033 (3) | 0.003 (2) | 0.008 (3) | 0.007 (2) |
| C8 | 0.035 (3) | 0.060 (4) | 0.032 (3) | -0.003 (3) | -0.005 (2) | 0.010 (3) |
| C9 | 0.030 (2) | 0.048 (3) | 0.028 (3) | 0.002 (2) | 0.003 (2) | 0.010 (2) |
| C10 | 0.046 (3) | 0.049 (3) | 0.037 (3) | -0.001 (3) | 0.003 (3) | 0.006 (3) |
| C11 | 0.036 (3) | 0.077 (4) | 0.045 (4) | -0.001 (3) | -0.005 (3) | 0.021 (3) |
| C12 | 0.052 (3) | 0.048 (3) | 0.033 (3) | 0.001 (3) | 0.004 (3) | 0.011 (3) |
| C13 | 0.041 (3) | 0.037 (3) | 0.036 (3) | -0.005 (2) | 0.000 (3) | -0.001 (2) |
| C14 | 0.040 (3) | 0.037 (3) | 0.024 (3) | 0.005 (2) | 0.003 (2) | -0.005 (2) |
| C15 | 0.033 (3) | 0.038 (3) | 0.039 (3) | 0.002 (2) | 0.001 (2) | -0.004 (3) |
| C16 | 0.036 (3) | 0.050 (3) | 0.036 (3) | -0.006 (2) | 0.005 (2) | -0.002 (3) |
| C17 | 0.046 (3) | 0.044 (3) | 0.033 (3) | 0.003 (3) | 0.012 (3) | 0.005 (3) |
| C18 | 0.046 (3) | 0.039 (3) | 0.022 (3) | 0.005 (2) | 0.000 (2) | -0.005 (2) |
| C19 | 0.035 (3) | 0.043 (3) | 0.031 (3) | -0.001 (2) | 0.000 (2) | -0.006 (2) |

Geometric parameters (Å, °)

| | | | |
|------------|-----------|---------------|-----------|
| Br1—C3 | 1.887 (5) | C8—H8A | 0.9700 |
| Br2—C5 | 1.886 (5) | C8—H8B | 0.9700 |
| Br3—C16 | 1.879 (5) | C9—C11 | 1.530 (7) |
| Br4—C18 | 1.889 (5) | C9—C10 | 1.531 (7) |
| O1—C2 | 1.296 (6) | C9—C12 | 1.538 (7) |
| O2—C15 | 1.287 (6) | C10—H10A | 0.9600 |
| N1—C7 | 1.266 (6) | C10—H10B | 0.9600 |
| N1—C8 | 1.453 (6) | C10—H10C | 0.9600 |
| N1—H1 | 0.8479 | C11—H11A | 0.9600 |
| N2—C13 | 1.282 (6) | C11—H11B | 0.9600 |
| N2—C12 | 1.460 (6) | C11—H11C | 0.9600 |
| N2—H2 | 0.8557 | C12—H12A | 0.9700 |
| C1—C6 | 1.397 (7) | C12—H12B | 0.9700 |
| C1—C2 | 1.412 (7) | C13—C14 | 1.447 (7) |
| C1—C7 | 1.454 (7) | C13—H13 | 0.9300 |
| C2—C3 | 1.410 (7) | C14—C19 | 1.412 (7) |
| C3—C4 | 1.370 (7) | C14—C15 | 1.427 (7) |
| C4—C5 | 1.403 (7) | C15—C16 | 1.418 (7) |
| C4—H4 | 0.9300 | C16—C17 | 1.382 (7) |
| C5—C6 | 1.363 (7) | C17—C18 | 1.402 (7) |
| C6—H6 | 0.9300 | C17—H17 | 0.9300 |
| C7—H7 | 0.9300 | C18—C19 | 1.354 (7) |
| C8—C9 | 1.527 (7) | C19—H19 | 0.9300 |
| C7—N1—C8 | 122.6 (5) | C9—C10—H10A | 109.5 |
| C7—N1—H1 | 114.5 | C9—C10—H10B | 109.5 |
| C8—N1—H1 | 122.9 | H10A—C10—H10B | 109.5 |
| C13—N2—C12 | 123.9 (5) | C9—C10—H10C | 109.5 |
| C13—N2—H2 | 114.0 | H10A—C10—H10C | 109.5 |
| C12—N2—H2 | 122.1 | H10B—C10—H10C | 109.5 |
| C6—C1—C2 | 121.2 (5) | C9—C11—H11A | 109.5 |

| | | | |
|--------------|------------|-----------------|------------|
| C6—C1—C7 | 119.6 (5) | C9—C11—H11B | 109.5 |
| C2—C1—C7 | 119.2 (5) | H11A—C11—H11B | 109.5 |
| O1—C2—C3 | 121.8 (5) | C9—C11—H11C | 109.5 |
| O1—C2—C1 | 122.3 (5) | H11A—C11—H11C | 109.5 |
| C3—C2—C1 | 115.9 (5) | H11B—C11—H11C | 109.5 |
| C4—C3—C2 | 123.1 (5) | N2—C12—C9 | 113.8 (4) |
| C4—C3—Br1 | 118.8 (4) | N2—C12—H12A | 108.8 |
| C2—C3—Br1 | 118.1 (4) | C9—C12—H12A | 108.8 |
| C3—C4—C5 | 119.1 (5) | N2—C12—H12B | 108.8 |
| C3—C4—H4 | 120.4 | C9—C12—H12B | 108.8 |
| C5—C4—H4 | 120.4 | H12A—C12—H12B | 107.7 |
| C6—C5—C4 | 120.1 (5) | N2—C13—C14 | 121.5 (5) |
| C6—C5—Br2 | 121.9 (4) | N2—C13—H13 | 119.2 |
| C4—C5—Br2 | 118.0 (4) | C14—C13—H13 | 119.2 |
| C5—C6—C1 | 120.6 (5) | C19—C14—C15 | 121.5 (5) |
| C5—C6—H6 | 119.7 | C19—C14—C13 | 119.6 (5) |
| C1—C6—H6 | 119.7 | C15—C14—C13 | 118.9 (5) |
| N1—C7—C1 | 121.9 (5) | O2—C15—C16 | 121.9 (5) |
| N1—C7—H7 | 119.1 | O2—C15—C14 | 122.3 (5) |
| C1—C7—H7 | 119.1 | C16—C15—C14 | 115.8 (5) |
| N1—C8—C9 | 112.5 (4) | C17—C16—C15 | 122.1 (5) |
| N1—C8—H8A | 109.1 | C17—C16—Br3 | 120.0 (4) |
| C9—C8—H8A | 109.1 | C15—C16—Br3 | 117.9 (4) |
| N1—C8—H8B | 109.1 | C16—C17—C18 | 119.9 (5) |
| C9—C8—H8B | 109.1 | C16—C17—H17 | 120.0 |
| H8A—C8—H8B | 107.8 | C18—C17—H17 | 120.0 |
| C8—C9—C11 | 107.5 (4) | C19—C18—C17 | 120.7 (5) |
| C8—C9—C10 | 110.6 (4) | C19—C18—Br4 | 120.6 (4) |
| C11—C9—C10 | 109.6 (4) | C17—C18—Br4 | 118.8 (4) |
| C8—C9—C12 | 107.6 (4) | C18—C19—C14 | 120.0 (5) |
| C11—C9—C12 | 109.7 (4) | C18—C19—H19 | 120.0 |
| C10—C9—C12 | 111.7 (4) | C14—C19—H19 | 120.0 |
| | | | |
| C6—C1—C2—O1 | -179.0 (4) | C13—N2—C12—C9 | -97.7 (6) |
| C7—C1—C2—O1 | 0.9 (7) | C8—C9—C12—N2 | -170.1 (4) |
| C6—C1—C2—C3 | 1.0 (7) | C11—C9—C12—N2 | 73.2 (5) |
| C7—C1—C2—C3 | -179.1 (4) | C10—C9—C12—N2 | -48.5 (6) |
| O1—C2—C3—C4 | 179.1 (5) | C12—N2—C13—C14 | -178.6 (4) |
| C1—C2—C3—C4 | -0.9 (7) | N2—C13—C14—C19 | -178.4 (5) |
| O1—C2—C3—Br1 | -1.6 (6) | N2—C13—C14—C15 | 1.9 (7) |
| C1—C2—C3—Br1 | 178.4 (3) | C19—C14—C15—O2 | 178.1 (5) |
| C2—C3—C4—C5 | -0.4 (8) | C13—C14—C15—O2 | -2.2 (7) |
| Br1—C3—C4—C5 | -179.7 (4) | C19—C14—C15—C16 | -1.9 (7) |
| C3—C4—C5—C6 | 1.7 (8) | C13—C14—C15—C16 | 177.8 (4) |
| C3—C4—C5—Br2 | -177.0 (4) | O2—C15—C16—C17 | -179.2 (5) |
| C4—C5—C6—C1 | -1.5 (8) | C14—C15—C16—C17 | 0.8 (7) |
| Br2—C5—C6—C1 | 177.0 (4) | O2—C15—C16—Br3 | 1.7 (7) |
| C2—C1—C6—C5 | 0.2 (8) | C14—C15—C16—Br3 | -178.3 (3) |

| | | | |
|--------------|------------|-----------------|------------|
| C7—C1—C6—C5 | -179.7 (5) | C15—C16—C17—C18 | 1.2 (8) |
| C8—N1—C7—C1 | -177.6 (4) | Br3—C16—C17—C18 | -179.7 (4) |
| C6—C1—C7—N1 | 177.6 (5) | C16—C17—C18—C19 | -2.3 (8) |
| C2—C1—C7—N1 | -2.2 (7) | C16—C17—C18—Br4 | 177.9 (4) |
| C7—N1—C8—C9 | 107.5 (6) | C17—C18—C19—C14 | 1.2 (7) |
| N1—C8—C9—C11 | -173.0 (5) | Br4—C18—C19—C14 | -179.0 (4) |
| N1—C8—C9—C10 | -53.4 (6) | C15—C14—C19—C18 | 1.0 (7) |
| N1—C8—C9—C12 | 68.8 (6) | C13—C14—C19—C18 | -178.7 (4) |

Hydrogen-bond geometry (Å, °)

| <i>D—H...A</i> | <i>D—H</i> | <i>H...A</i> | <i>D...A</i> | <i>D—H...A</i> |
|--------------------------|------------|--------------|--------------|----------------|
| N1—H1...O1 | 0.85 | 1.82 | 2.549 (5) | 142 |
| N2—H2...O2 | 0.86 | 1.80 | 2.537 (5) | 143 |
| C8—H8A...O2 ⁱ | 0.97 | 2.53 | 3.424 (7) | 152 |

Symmetry code: (i) $x-1/2, y, -z+1/2$.