Crystal structure and Hirshfeld surface analysis of (E)-2-(4-bromophenyl)-1-[2,2-dibromo-1-(4-nitrophenyl)ethenyl]diazene

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The molecule of the title compound, C_{14}H_{8}Br_{3}N_{3}O_{2}, consists of three almost planar groups: the central dibromoethenylidiazene fragment and two attached aromatic rings. The mean planes of these rings form dihedral angles with the plane of the central fragment of 26.35 (15) and 72.57 (14)° for bromine- and nitro-substituted rings, respectively. In the crystal, C—H···Br interactions connect molecules, generating zigzag C(8) chains along the [100] direction. These chains are linked by C—Br···π interactions into layers parallel to (001).

1. Chemical context

Azo dyes constitute the largest production volume (ca 70%) of the dye industry today, and their relative importance may increase further in the future (Lipskikh et al., 2018). They play a crucial role in the printing market, the design of functional materials attributed to smart hydrogen bonding, photo-triggered structural switching, self-assembled layers, ionophores, liquid crystals, semiconductors, indicators, spectrophotometric reagents for determination of metal ions, photoluminescent materials, catalysts, antimicrobial agents, optical recording media, spin-coating films, etc (Zollinger, 1994, 1995; Gurbanov et al., 2020a, b; Mahmudov et al., 2010, 2013). Depending on the attached substituents, the functional properties of azo compounds and their metal complexes can be improved/controlled (Ma et al., 2020, 2021). Both E/Z isomerism and azo–hydrazo tautomerism properties of azo dyes are key phenomena in the synthesis and development of new functional materials (Shixaliyev et al., 2018, 2019). The attachment of non-covalent bond acceptor or donor centres to the azo dyes can be used as a synthetic strategy for the improvement of the functional properties of their metal complexes (Mahmudov et al., 2020, 2021, 2022). Thus, we have attached bromine atoms and a nitro group together with aryl rings to the –N≡N– linkage leading to a new azo compound, (E)-2-(4-bromophenyl)-1-[2,2-dibromo-1-(4-nitrophenyl)ethenyl]diazene...
azene, which can provide intermolecular halogen and hydrogen bonds as well as π-interactions.

2. Structural commentary
The molecule of the title compound (Fig. 1) consists of three almost planar groups: the central dibromoethenyldiazene fragment [largest deviation from the least-squares plane is 0.039 (3) Å for N2] and two attached aromatic rings. The mean planes of these rings form dihedral angles with the plane of the central fragment of 26.35 (15) and 72.57 (14)° for the bromine- and nitro-substituted rings, respectively. The nitro group is twisted by 8.1 (2)° with respect to the C3–C8 aromatic ring. The C2—N2 bond distance of 1.406 (4) Å indicates π-conjugation between ethene and diazo groups. All other bond lengths and angles in the title compound are similar to those reported for the related azo compounds discussed in the Database survey section.

3. Supramolecular features and Hirshfeld surface analysis
In the crystal, C—H···Br interactions connect the molecules, generating zigzag C(8) chains (Bernstein et al., 1995) along the [100] direction (Table 1, Figs. 2 and 3). These chains are linked by C—Br···π interactions [Cl—Br1···Cg1ii; Cl—Br1 = 1.864 (3) Å, Br1···Cg1ii = 3.5803 (16) Å, Cl···Cg1ii = 4.722 (3) Å, Cl—Br1···Cg1ii = 116.77 (9)°; Cg1 is the centroid of the C3–C8 ring; symmetry code (ii): x + 1/2, −y + 1/2, z] into

| D—H···A  | D—H | H···A | D···A | D—H···A |
|----------|------|-------|-------|---------|
| C10—H10···Br1i | 0.95 | 2.89  | 3.530 (4) | 126     |

Symmetry code: (i) x−1/4, −y+1/4, z.

Figure 1
The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Figure 2
View down the a-axis of the title compound showing the C—H···Br interactions.

Figure 3
View down the b-axis of the title compound, showing the C—Br···π interactions.
layers parallel to (001) (Fig. 4). van der Waals interactions between the layers help to keep the crystal packing together.

Crystal Explorer 17.5 (Turner et al., 2017) was used to perform a Hirshfeld surface analysis and to generate the corresponding two-dimensional fingerprint plots, with a standard resolution of the three-dimensional $d_{\text{norm}}$ surfaces plotted over a fixed color scale of $-0.1401$ (red) to $1.1158$ (blue) a.u. (Fig. 5). The red patches represent short contacts and negative $d_{\text{norm}}$ values on the surface, which correspond to the C–H···Br hydrogen bonds discussed above (Table 1). The C10–H10···Br1 interactions, which are important for molecular packing of the title compound, are responsible for the red patch that appears around Br1.

The overall two-dimensional fingerprint plot for the title compound and those delineated into Br···H / H···Br (20.9%), C···H/H···C (15.2%), O···H/H···O (12.6%) and H···H (11.7%) contacts are shown in Fig. 6, while numerical details for short intermolecular contacts are given in Table 2. Br···C/C···Br (8.8%), Br···Br (6.7%), N···H/H···N (6.5%), Br···O/O···Br (5.6%), O···C/C···O (4.1%), Br···N/N···Br (3.9%), C···C (2.5%), O···N/N···O (1.3%) and N···C/C···N (0.1%) contacts have little directional influence on the molecular packing.

| Interaction  | $d_{\text{norm}}$ (Å) | Formula for $d_{\text{norm}}$ |
|--------------|------------------------|--------------------------------|
| Br1···H10    | 2.89                   | $\frac{1}{2} - x, \frac{1}{2} - y, z$ |
| H14···H5     | 2.40                   | $\frac{1}{2} - x, -\frac{1}{2} + y, -\frac{1}{2} + z$ |
| Br2···Br3    | 3.44                   | $x + \frac{1}{2}, \frac{1}{2} - y, z$ |
| H10···C13    | 3.02                   | $-x, 1 - y, \frac{1}{2} + z$ |
| O1···H13     | 2.75                   | $x, 1 + y, z$ |
| H7···N2      | 2.65                   | $\frac{1}{2} - x, \frac{1}{2} + y, -\frac{1}{2} + z$ |

The full two-dimensional fingerprint plots for the title compound, showing all interactions (a) and delineated into (b) Br···H/H···Br, (c) C···H/H···C, (d) O···H/H···O, and (e) H···H interactions. The $d_i$ and $d_e$ values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.
A search of the Cambridge Structural Database (CSD, Version 5.42, update of September 2021; Groom et al., 2016) for similar structures with the \((E)-1-(2,2\text{-dibromo-1-phenyl-ethenyl})\)-2-phenyladiene fragment showed that the nine closest are those of CSD refcodes TAZDIL [\(\text{(I)}\); Atioğlu et al., 2022], PAXDXL [\(\text{(II)}\); Celek et al., 2022], GUPHIIL [\(\text{(III)}\); Özkaraca et al., 2020b], HONBUK [\(\text{(IV)}\); Akkurt et al., 2019], HONBOE [\(\text{(V)}\); Akkurt et al., 2019], HODQAV [\(\text{(VI)}\); Shikhaliyev et al., 2019], XIZREG [\(\text{(VII)}\); Atioğlu et al., 2019], LEQXOX [\(\text{(VIII)}\); Shikhaliyev et al., 2018] and LEQXIR [\(\text{(IX)}\); Shikhaliyev et al., 2018].

In \(\text{(I)}\), the molecules are connected by \(\text{C–H} \cdots \text{O}\) and \(\text{C–H} \cdots \text{F}\) hydrogen bonds into layers parallel to \(\{011\}\). The crystal packing is consolidated by \(\text{C–Br} \cdots \pi\) and \(\text{C–F} \cdots \pi\) contacts, as well as by \(\pi\cdots \pi\) stacking interactions. In the crystal of \(\text{(II)}\), the molecules are linked into chains running parallel to \(\{001\}\) by \(\text{C–H} \cdots \text{O}\) hydrogen bonds. The crystal packing is consolidated by \(\text{C–F} \cdots \pi\) contacts and \(\pi\cdots \pi\) stacking interactions, and short \(\text{Br} \cdots \text{O}\) \(\{2.9828 (13) \text{ Å}\}\) distances are also observed. In the crystal of \(\text{(III)}\), the molecules are linked into inversion dimers \(\text{via}\) short halogen–halogen contacts \([\text{Cl1} \cdots \text{Cl1} = 3.3763 (9) \text{ Å}, \text{Cl1} \cdots \text{Cl1} \cdots \text{Cl1} = 141.47 (7)^\circ]\) compared to the van der Waals radius sum of 5.30 Å for two chlorine atoms. No other directional contacts could be identified, and the shortest aromatic ring centroid separation is greater than 5.25 Å. In the crystals of \(\text{(IV)}\) and \(\text{(V)}\), the molecules are linked through weak \(\text{X} \cdots \text{Cl}\) contacts \([\text{X} = \text{Cl} \text{for (IV)} \text{and Br for (V)}\), \(\text{C–H} \cdots \text{Cl}\) and \(\text{Cl} \cdots \pi\) interactions into sheets lying parallel to \(\{001\}\). In the crystal of \(\text{(VI)}\), the molecules are stacked in columns parallel to \(\{100\}\) \(\text{via}\) weak \(\text{C–H} \cdots \text{Cl}\) hydrogen bonds and face-to-face \(\pi\cdots \pi\) stacking interactions. The crystal packing is further consolidated by short \(\text{Cl} \cdots \text{Cl}\) contacts. In \(\text{(VII)}\), molecules are linked by \(\text{C–H} \cdots \text{O}\) hydrogen bonds into zigzag chains running parallel to \(\{001\}\). The crystal packing also features \(\text{C–Cl} \cdots \pi\), \(\text{C–F} \cdots \pi\) and \(\text{N–O} \cdots \pi\) interactions. In \(\text{(VIII)}\), \(\text{C–H} \cdots \text{N}\) and short \(\text{Cl} \cdots \text{Cl}\) contacts are observed, and in \(\text{(IX)}\), \(\text{C–H} \cdots \text{N}\) and \(\text{C–H} \cdots \text{O}\) hydrogen bonds and short \(\text{Cl} \cdots \text{O}\) contacts occur.

5. Synthesis and crystallization

This dye was synthesized according to the reported method (Akkurt et al., 2019; Atioğlu et al., 2019; Maharramov et al., 2018; Özkaraca et al., 2020a,b). A 20 mL screw neck vial was charged with 

\[
\begin{align*}
\text{DMSO} & (10 \text{ mL}), \\
\text{(E)-1-(4-bromophenyl)-2-(4-nitrobenzylidene)hydrazine} & (1 \text{ mmol}), \\
\text{tetramethylthylene diamine (TMEDA; 295 mg, 2.5 mmol),} \\
\text{CuCl} & (2 \text{ mg, 0.02 mmol) and} \\
\text{CBr}_4 & (4.5 \text{ mmol). After} \ 1\text{-}3 \text{ h (until TLC analysis showed complete consumption of corresponding Schiff base), the reaction mixture was poured into 0.01} \text{ M} \\
\text{solution of HCl (100 mL, pH} & = 2–3), \text{ and extracted with} \\
\text{dichloromethane (3} & \times 20 \text{ mL). The combined organic phase was} \\
\text{washed with water (3} & \times 50 \text{ mL), brine (30 mL), dried over} \\
\text{anhydrous Na}_2\text{SO}_4 \text{ and concentrated in vacuo using a rotary evaporator. The residue was purified by column chromatography on silica gel using appropriate mixtures of hexane and} \\
\text{dichloromethane (3} & \text{/1–1/1). Crystals suitable for X-ray analysis were obtained by slow evaporation of an ethanol solution.} \\
\text{Red solid (58%)} & \text{; m.p. 398 K. Analysis calculated for} \\
\text{C}_14\text{H}_8\text{Br}_3\text{N}_3\text{O}_2 (M} & = 489.95) \text{; C 34.32, H 1.65, N 8.58; found: C} \\
& 34.27, \text{H 1.70, N 8.56%.} \\
\text{1H NMR (300 MHz, CDCl}_3 \text{)} & \delta \ 8.16–7.41 \ (8\text{H, Ar–H}). \text{13C NMR (75MHz, CDCl}_3 \text{)} \delta \ 150.89, 149.62, \\
& 148.26, 136.43, 132.25, 127.77, 125.57, 124.53, 123.57, 93.24.} \\
\text{ESI–MS: m/z: 490.96 [M} & +\text{H}]^+. \\
\end{align*}
\]

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. All H atoms were positioned geometrically and constrained to ride on their parent atoms (\(\text{C–H} = 0.95 \text{ Å}\)) with \(U_{iso}(\text{H}) = 1.2U_{eq}(\text{C})\). One reflection (110), affected by the beam stop, was omitted in the final cycles of refinement.

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manuscript) SÖY, MA and AB; funding acquisition, NQS, NAM and GTS; supervision, NQS, MA and AB.

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Computing details

Data collection: *APEX3* (Bruker, 2018); cell refinement: *SAINT* (Bruker, 2018); data reduction: *SAINT* (Bruker, 2018); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2018* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

\((E)-2-(4\text{-Bromophenyl})-1-[2,2\text{-dibromo}-1\text{-}(4\text{-nitrophenyl})\text{ethenyl}]\text{diazene}\)

*Crystal data*

\[
\begin{align*}
C_{14}H_8Br_3N_3O_2 &\quad D_\lambda = 2.087 \text{ Mg m}^{-3} \\
M_r = 489.96 &\quad \text{Mo } K\alpha \text{ radiation, } \lambda = 0.71073 \text{ Å} \\
\text{Orthorhombic, } Pna2_1 &\quad \text{Cell parameters from 9976 reflections} \\
a = 13.8678 (5) \text{ Å} &\quad \theta = 2.9\text{–}34.8^\circ \\
b = 13.5442 (5) \text{ Å} &\quad \mu = 7.77 \text{ mm}^{-1} \\
c = 8.3017 (3) \text{ Å} &\quad T = 100 \text{ K} \\
V = 1559.29 (10) \text{ Å}^3 &\quad \text{Block, red} \\
Z = 4 &\quad 0.31 \times 0.14 \times 0.08 \text{ mm} \\
F(000) = 936 &
\end{align*}
\]

*Data collection*

Bruker D8 QUEST, Photon III detector 
Radiation source: fine-focus sealed X-Ray tube 
Graphite monochromator 
Detector resolution: 7.31 pixels mm\(^{-1}\) 
\(\varphi\) and \(\omega\) shutterless scans 
Absorption correction: multi-scan 
\text{(SADABS; Krause et al., 2015)} 
\(T\) \text{min} = 0.044, \(T\) \text{max} = 0.110

*Refinement*

Refinement on \(F^2\) 
Least-squares matrix: full 
\(R[F^2 > 2\sigma(F^2)] = 0.033\) 
\(wR(F^2) = 0.085\) 
\(S = 1.02\) 
7370 reflections 
199 parameters 
1 restraint

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
$w = 1/[\sigma^2(F_o^2) + (0.0438P)^2 + 0.8309P]$  
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.002$

$\Delta \rho_{\text{max}} = 1.41 \text{ e} \AA^{-3}$

$\Delta \rho_{\text{min}} = -0.97 \text{ e} \AA^{-3}$

Absolute structure: Flack parameter determined using 2437 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons et al., 2013)

Absolute structure parameter: 0.003 (5)

**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 ($U_{eq}$)**

|          | $x$      | $y$      | $z$      | $U_{eq}$/$U_{eq}$ |
|----------|----------|----------|----------|--------------------|
| Br1      | 0.49964 (2) | 0.72932 (3) | 0.49158 (6) | 0.02765 (8)        |
| Br2      | 0.44572 (2) | 0.50470 (2) | 0.51189 (7) | 0.02906 (8)        |
| Br3      | −0.10955 (3) | 0.24165 (3) | 0.55241 (7) | 0.03182 (9)        |
| O1       | 0.1810 (2) | 1.1045 (2) | 0.3729 (4) | 0.0333 (6)         |
| O2       | 0.1662 (3) | 1.1002 (2) | 0.6323 (4) | 0.0326 (6)         |
| N1       | 0.18506 (19) | 1.0613 (2) | 0.5020 (5) | 0.0231 (5)         |
| N2       | 0.24431 (19) | 0.57555 (19) | 0.5188 (4) | 0.0207 (5)         |
| N3       | 0.15599 (19) | 0.5982 (2) | 0.5376 (4) | 0.0228 (6)         |
| C1       | 0.4020 (2) | 0.6350 (2) | 0.5012 (6) | 0.0222 (6)         |
| C2       | 0.3073 (2) | 0.6586 (2) | 0.5080 (5) | 0.0205 (5)         |
| C3       | 0.2727 (2) | 0.7629 (2) | 0.5040 (5) | 0.0196 (5)         |
| C4       | 0.2373 (3) | 0.8055 (3) | 0.6449 (5) | 0.0221 (6)         |
| H4       | 0.233234 | 0.767615 | 0.741062 | 0.027*             |
| C5       | 0.2076 (3) | 0.9043 (3) | 0.6441 (5) | 0.0222 (6)         |
| H5       | 0.184039 | 0.934772 | 0.739348 | 0.027*             |
| C6       | 0.2136 (2) | 0.9563 (2) | 0.5016 (5) | 0.0212 (5)         |
| C7       | 0.2468 (3) | 0.9148 (3) | 0.3596 (5) | 0.0249 (7)         |
| H7       | 0.248972 | 0.952162 | 0.262834 | 0.030*             |
| C8       | 0.2769 (3) | 0.8171 (3) | 0.3629 (5) | 0.0235 (6)         |
| H8       | 0.300598 | 0.787169 | 0.267351 | 0.028*             |
| C9       | 0.0971 (2) | 0.5110 (2) | 0.5422 (5) | 0.0208 (6)         |
| C10      | 0.0066 (3) | 0.5207 (3) | 0.6113 (5) | 0.0251 (7)         |
| H10      | −0.013356 | 0.582330 | 0.654399 | 0.030*             |
| C11      | −0.0553 (3) | 0.4391 (3) | 0.6172 (5) | 0.0262 (7)         |
| H11      | −0.117165 | 0.444374 | 0.665505 | 0.031*             |
| C12      | −0.0249 (3) | 0.3509 (2) | 0.5516 (5) | 0.0243 (6)         |
| C13      | 0.0662 (2) | 0.3397 (2) | 0.4837 (5) | 0.0246 (7)         |
| H13      | 0.085933 | 0.277960 | 0.440465 | 0.030*             |
| C14      | 0.1275 (2) | 0.4203 (2) | 0.4803 (5) | 0.0236 (6)         |
## Atomic displacement parameters (Å²)

|     | \(U_{11} \)   | \(U_{22} \)   | \(U_{33} \)   | \(U_{12} \)   | \(U_{13} \)   | \(U_{23} \)   |
|-----|----------------|----------------|----------------|----------------|----------------|----------------|
| Br1 | 0.01833 (12)   | 0.02119 (13)   | 0.0434 (2)     | −0.00217 (10)  | 0.00069 (14)   | 0.00037 (16)   |
| Br2 | 0.02025 (12)   | 0.01897 (13)   | 0.0480 (2)     | 0.00223 (10)   | −0.00256 (15)  | −0.00061 (14)  |
| Br3 | 0.02917 (16)   | 0.02402 (15)   | 0.0423 (2)     | −0.00937 (12)  | −0.00254 (18)  | 0.00189 (17)   |
| O1  | 0.0460 (17)    | 0.0222 (13)    | 0.0317 (15)    | 0.0060 (12)    | 0.0009 (13)    | 0.0062 (11)    |
| O2  | 0.0450 (16)    | 0.0217 (13)    | 0.0310 (16)    | 0.0042 (12)    | 0.0006 (13)    | −0.0038 (11)   |
| N1  | 0.0211 (10)    | 0.0185 (11)    | 0.0296 (15)    | 0.0000 (8)     | 0.0007 (13)    | −0.0001 (12)   |
| N2  | 0.0179 (10)    | 0.0190 (10)    | 0.0251 (15)    | −0.0007 (8)    | −0.0006 (10)   | 0.0012 (11)    |
| N3  | 0.0184 (11)    | 0.0192 (11)    | 0.0306 (17)    | −0.0012 (8)    | 0.0016 (10)    | 0.0014 (11)    |
| C1  | 0.0181 (11)    | 0.0170 (11)    | 0.0315 (16)    | 0.0001 (9)     | −0.0020 (13)   | −0.0003 (13)   |
| C2  | 0.0182 (11)    | 0.0171 (11)    | 0.0263 (15)    | 0.0002 (9)     | −0.0010 (12)   | 0.0015 (12)    |
| C3  | 0.0164 (10)    | 0.0167 (11)    | 0.0257 (15)    | −0.0004 (8)    | −0.0012 (13)   | 0.0022 (12)    |
| C4  | 0.0237 (14)    | 0.0183 (13)    | 0.0243 (16)    | 0.0015 (11)    | 0.0002 (12)    | 0.0010 (12)    |
| C5  | 0.0215 (14)    | 0.0211 (14)    | 0.0241 (16)    | 0.0024 (11)    | 0.0005 (12)    | −0.0010 (12)   |
| C6  | 0.0194 (11)    | 0.0166 (11)    | 0.0275 (15)    | 0.0000 (9)     | −0.0004 (13)   | −0.0007 (13)   |
| C7  | 0.0262 (15)    | 0.0209 (14)    | 0.0276 (18)    | 0.0018 (12)    | 0.0018 (13)    | 0.0031 (12)    |
| C8  | 0.0238 (14)    | 0.0202 (14)    | 0.0265 (17)    | 0.0003 (11)    | 0.0022 (13)    | 0.0003 (12)    |
| C9  | 0.0189 (12)    | 0.0167 (11)    | 0.0269 (17)    | −0.0010 (9)    | −0.0007 (11)   | 0.0000 (12)    |
| C10 | 0.0230 (14)    | 0.0182 (13)    | 0.0342 (19)    | 0.0003 (11)    | 0.0021 (13)    | −0.0015 (13)   |
| C11 | 0.0203 (13)    | 0.0209 (14)    | 0.037 (2)      | −0.0021 (11)   | 0.0034 (13)    | −0.0005 (13)   |
| C12 | 0.0238 (13)    | 0.0185 (12)    | 0.0305 (17)    | −0.0061 (10)   | −0.0016 (13)   | 0.0016 (14)    |
| C13 | 0.0246 (13)    | 0.0182 (12)    | 0.0312 (19)    | −0.0007 (10)   | 0.0009 (14)    | −0.0027 (13)   |
| C14 | 0.0205 (12)    | 0.0208 (13)    | 0.0295 (19)    | −0.0005 (10)   | 0.0035 (13)    | −0.0024 (13)   |

## Geometric parameters (Å, °)

|     |     |     |     |     |     |     |
|-----|-----|-----|-----|-----|-----|-----|
| Br1 — C1 | 1.864 (3) | C5—H5 | 0.9500 |
| Br2 — C1 | 1.868 (3) | C6—C7 | 1.384 (6) |
| Br3 — C12 | 1.888 (3) | C7—C8 | 1.388 (5) |
| O1 — N1 | 1.223 (5) | C7—H7 | 0.9500 |
| O2 — N1 | 1.231 (5) | C8—H8 | 0.9500 |
| N1 — C6 | 1.477 (4) | C9—C10 | 1.386 (5) |
| N2 — N3 | 1.266 (4) | C9—C14 | 1.397 (5) |
| N2 — C2 | 1.406 (4) | C10—C11 | 1.400 (5) |
| N3 — C9 | 1.437 (4) | C10—H10 | 0.9500 |
| C1 — C2 | 1.352 (4) | C11—C12 | 1.378 (5) |
| C2 — C3 | 1.492 (4) | C11—H11 | 0.9500 |
| C3 — C8 | 1.384 (5) | C12—C13 | 1.392 (5) |
| C3 — C4 | 1.394 (5) | C13—C14 | 1.384 (5) |
| C4 — C5 | 1.400 (5) | C13—H13 | 0.9500 |
| C4 — H4 | 0.9500 | C14—H14 | 0.9500 |
| C5 — C6 | 1.379 (5) |     |     |
| O1 — N1 — O2 | 123.8 (3) | C6—C7—H7 | 121.0 |

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O1—N1—C6 118.1 (3) C8—C7—H7 121.0
O2—N1—C6 118.1 (3) C3—C8—C7 120.7 (3)
N3—N2—C2 115.9 (3) C3—C8—H8 119.6
N2—N3—C9 111.8 (3) C7—C8—H8 119.6
C2—C1—Br1 123.1 (2) C10—C9—C14 120.6 (3)
C2—C1—Br2 122.4 (2) C10—C9—N3 116.6 (3)
Br1—C1—Br2 114.43 (15) C14—C9—N3 122.8 (3)
C1—C2—N2 115.0 (3) C9—C10—C11 119.7 (3)
C1—C2—C3 122.3 (3) C9—C10—H10 120.2
N2—C2—C3 122.7 (3) C11—C10—H10 120.2
C8—C3—C4 120.3 (3) C12—C11—C10 118.9 (3)
C8—C3—C2 120.5 (3) C12—C11—H11 120.6
C4—C3—C2 119.1 (3) C10—C11—H11 120.6
C3—C4—C5 119.7 (3) C11—C12—C13 122.1 (3)
C3—C4—H4 120.2 C11—C12—Br3 119.2 (3)
C5—C4—H4 120.2 C13—C12—Br3 118.7 (3)
C6—C5—C4 118.3 (3) C14—C13—C12 118.7 (3)
C6—C5—H5 120.8 C14—C13—H13 120.7
C4—C5—H5 120.8 C12—C13—H13 120.7
C5—C6—C7 122.9 (3) C13—C14—C9 120.0 (3)
C5—C6—N1 118.3 (3) C13—C14—H14 120.0
C7—C6—N1 118.8 (3) C9—C14—H14 120.0
C6—C7—C8 118.0 (3)

Hydrogen-bond geometry (Å, °)

|   |   |   |   |   |
|---|---|---|---|---|
| D—H···A | D—H | H···A | D···A | D—H···A |

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sup-4
| C10—H10···Br1\textsuperscript{i} | 0.95 | 2.89 | 3.530 (4) | 126 |

Symmetry code: (i) \(x-1/2, -y+3/2, z\).