Crystal structure, Hirshfeld surface analysis and DFT calculations of 7-bromo-2,3-dihydropyrrolo-[2,1-b]quinazolin-9(1H)-one

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The molecular structure of the title compound, C_{11}H_{9}BrN_{2}O, is almost planar. The benzene and pyrimidine rings are essentially coplanar, with r.m.s. deviations of 0.0130 Å, and the largest displacement is for the flap atom of the dihydropyrole moiety [0.154 (7) Å]. Hirshfeld surface analyses revealed that the crystal packing is dominated by H⋯H, Br⋯H/H⋯Br and O⋯H/H⋯O interactions, and Br⋯Br interactions in the crystal structure are also observed. Theoretical calculations using density functional theory (DFT) with the B3LYP functional basis set gave numerical parameters for the frontier molecular orbitals.

1. Chemical context

Quinazolines are of significant interest for their various biological properties (Rajput et al., 2012; Ramesh et al., 2012; Khan et al., 2014; Ajani et al., 2016). This class of compounds is considered as an attractive target for medicinal chemists, because quinazoline and its derivatives are the scaffold of several potent antitumor drugs, for example the well-known erlotinib and gefitinib (Sordella et al., 2004; Raymond et al., 2000). Besides these two drugs, the Food and Drug Administration (FDA) has approved some other quinazolines as effective anticancer drugs, viz. lapatinib and vandetanib. In general, the reported biological activities of quinazolines include antibacterial, anti-inflammatory, CNS depressant, anticonvulsant, antifungal, antimalarial, anticancer properties, which make them interesting for the pharmaceutical industry (Ajani et al., 2015).

In this context, synthetic analogues of the tricyclic quinazoline-9-one-7-bromo-2,3-dihydropyrrolo-[2,1-b]quinazolin-9(1H)-one have been synthesized, amongst them the title compound with a bromine atom in position 7. In comparison with a reported literature procedure (Shakhidoyatov, 1983), this compound is now obtained in higher yields (80–88%). For
this purpose, condensation of 2-amino-5-bromobenzoic acid with appropriate pyrrolidin-2-one was used whereas in the literature (Shakhidoyatov, 1983), 2-amino-5-bromobenzoic acid was added to the corresponding lactam mixture with a condensing agent (POCl3) at room temperature (293–298 K) and the reaction products separated by extraction after the reaction mixture was reduced to pH = 9–10 with NH4OH. As distinguished from the reported procedure, we carried out these reactions by cooling in an ice bath at a much lower temperature (273–275 K) and for a relatively longer period of time. The reaction products were finally separated by cold NH4OH at pH = 10–11. In general, the interactions of 7-bromo-2,3-dihydropyrrolo[2,1-\(\text{b}\)]quinazolin-9(1\(\text{H}\))-one with aldehydes are well-studied (Abdurazakov et al., 2007). Here, we report the molecular and crystal structures as well as Hirshfeld surface analysis and the frontier molecular orbitals calculated by density functional theory (DFT) with the B3LYP functional basis set.

2. Structural commentary

The molecular structure of the title compound is shown in Fig. 1. The molecule is almost planar. In particular, the benzene and pyrimidine rings are essentially coplanar, with an r.m.s. deviations of 0.0130 Å from planarity. The remaining atoms of the dihydropyrrole ring are slightly displaced from these planes, with deviations of −0.060 (5) Å for C1, −0.154 (7) Å for flap atom C2, and 0.060 (6) Å for C3. The acyclic C7—Br1 bond length 1.900 (3) Å is consistent with the data for other Br-substituted tricyclic quinazolinone derivatives (Mukarramov et al., 2009; Tozhboev et al., 2007a; Djayakon et al., 1992; Okmanov et al., 2009; Pereira et al., 2005).

3. Supramolecular features

In the crystal, molecules participate in centrosymmetric halogen-bonding dimers with Br···Br intermolecular contacts of 3.5961 (5) Å, which is shorter than the sum of van der Waals radii (Bondi et al., 1964) of two bromine atoms (3.66 Å). The C7—Br···Br angle amounts to 166.70 (14)°. The molecules also engage in weak C7—Br···Cg interactions, with Br···Cg1(2 − x, 1 − y, 1 − z) = 3.6428 (15) Å, forming a layered network (Fig. 2). Additional \(\pi\)···\(\pi\) stacking (Fig. 3) occurs between the aromatic rings of neighbouring molecules,
with the distance between the centroids Cg2•••Cg2ι being 3.9969 (14) Å [symmetry code: (i) 1 − x, 1 − y, 1 − z] and a ring slippage of 1.569 Å, and Cg2•••Cg3ι being 3.7513 (16) Å [symmetry code: (ii) 2 − x, 1 − y, 1 − z] and a ring slippage of 1.194 Å. Both short intermolecular contacts help to stack parallel molecules along [100]. The resulting two-dimensional network extends parallel to (002), with neighboring layers linked through C1−H1B•••N4 short intermolecular contacts, H1B•••N4(x, 1/2 − y, 1/2 + z) = 2.73 Å, C1−H1B•••N4(x, 1/2 − y, 1/2 + z) = 169°, to form the full three-dimensional structure (Fig. 4).

4. Hirshfeld surface analysis

In order to quantify the intermolecular interactions in the crystal of the title compound, a Hirshfeld surface (HS) analysis (Spackman et al., 2009) was performed and associated two-dimensional fingerprint plots (McKinnon et al., 2007) were generated with the program CrystalExplorer (Spackman et al., 2021). The HS mapped over \(d_{norm}\) is depicted in Fig. 5, which shows the most prominent intermolecular interactions as red spots corresponding to the Br•••Br, C−H•••O and N−H•••O contacts. The two-dimensional fingerprint plot for all contacts is given in Fig. 6a. H•••H contacts are responsible for the largest contribution (37.2%) to the Hirshfeld surface (Fig. 6b). Besides these contacts, Br•••H/H•••Br (19.6%), O•••H/H•••O (11.3%), N•••H/H•••N (8.1%) and C•••H/H•••C (6.9%) interactions contribute significantly to the total Hirshfeld surface; their decomposed fingerprint plots are shown in Fig. 6c–f. The contributions of further contacts are only minor and amount to N•••C/C•••N (3.5%), O•••C/C•••O (2.0%), Br•••C/C•••Br (0.9%), Br•••Br (0.8%), O•••N/N•••O (0.5%) and Br•••N/N•••Br (0.3%).

5. Frontier molecular orbitals

DFT was used to calculate the frontier molecular orbitals (FMOs, Fig. 7), which give important details of how a molecule interacts with other species, for example in terms of molecular reactivity and the ability of a molecule to absorb light. From the highest occupied molecular orbital (HOMO) electrons can be donated to the lowest unoccupied molecular orbital (LUMO). Moreover, the energy of the HOMO is directly related to the ionization potential, while the LUMO energy is directly related to the electron affinity, and the resulting energy difference (or energy gap) between HOMO and LUMO gives information about the stability of a molecule. In the case where the energy gap is small, the molecule is highly polarizable and has a high chemical reactivity. By using the HOMO and LUMO energy values of a molecule, its electronegativity (\(\chi\)), hardness (\(h\)) and chemical softness (\(s\)) can be calculated as follows: \(c = (I + A)/2; h = (I - A)/2; s = 1/2h\), where \(I\) and \(A\) are the ionization potential and electron affinity, respectively, where \(I = -E_{HOMO}\) and \(A = -E_{LUMO}\) (Pir et al., 2014; Azizov et al., 2021).

\[E_{HOMO} = -6.4559\text{ eV}\]
\[\Delta E_{\text{gap}} = 4.8208\text{ eV}\]
\[E_{LUMO} = -1.6351\text{ eV}\]
molecule were calculated at the DFT/B3LYP level using the 6-311+G(d,p) basis set (Table 1). The values of h and s are significant for the evaluation of both reactivity and stability. The electron transition from the HOMO to the LUMO energy level is shown in Fig. 7. The energy band gap \( \Delta E = E_{\text{LUMO}} - E_{\text{HOMO}} \) of the molecule is 4.8208 eV, the frontier molecular orbital energies \( E_{\text{HOMO}} \) and \( E_{\text{LUMO}} \) being −6.4559 and −1.6351 eV, respectively. The high value of the band gap (4.8208 eV) indicates the relatively high stability of the title molecule.

6. Database survey

A search in the Cambridge Structural Database (CSD, version 2022; Groom et al., 2016) gave four matches of molecules containing the 2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one moiety with a similar conformation to that in the title structure: deoxyvasicinone (TEFGEO; Turgunov et al., 1995), deoxyvasicinonium chloride (TEFGIIU; Turgunov et al., 1995), bis(deoxyvasicinonium) tetrachloridocobaltate(II) (TEFGOA; Turgunov et al., 1995) and 4-oxo-2,3-tetramethylene-3,4-dihydroquinazolinum 2,3-tetramethylene-3,4-dihydroquinazolin-4-one hemikis(oxalate) oxalic acid solvate (TITGZU; Toshiboev et al., 2007b). A search for compounds substituted in position 7 of 2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one moiety gave only two hits: N-(9-oxo-1,2,3,9-tetrahydropyrrolo[2,1-b]quinazolin-7-yl)propanamide sesquihydrate (GABJAX; Elmuradov et al., 2016) and 3b-hydroxy-7-methoxy-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one monohydrate (HIHLIT; Magotra et al., 1996). Comparing the listed structures with that of the title compound gave analogous complanarities of the benzene and pyrimidine rings. In the case of structures TEFGEQ, GABJAX and HIHLIT they have also similarities regarding \( \pi-\pi \) stacking interactions.

![Figure 8](image_url)

**Figure 8**

The reaction scheme of the title compound.

### Table 1

Calculated parameters of the title molecule calculated at the B3LYP/6-311+G(d,p) level.

| Parameters | DFT/B3LYP |
|------------|-----------|
| Total energy \( TE \) (a.u.) | −3183.662028 |
| \( E_{\text{HOMO}} \) (eV) | −6.4559 |
| \( E_{\text{LUMO}} \) (eV) | −1.6351 |
| Energy gap, \( \Delta E \) (eV) | 4.8208 |
| Dipole moment, \( \mu \) (Debye) | 4.6478 |
| Ionization potential, \( I \) (eV) | 6.4559 |
| Electron affinity, \( A \) | 1.6351 |
| Electron affinity, \( \chi \) | 4.0455 |
| Hardness, \( \eta \) | 2.1404 |
| Electrophilicity index, \( \omega \) | 3.3949 |
| Softness, \( \sigma \) | 0.2074 |

### Table 2

Experimental details.

| Parameter | Value |
|-----------|-------|
| Crystal data | C11H9BrN2O |
| Chemical formula | M |
| Crystal system, space group | Monoclinic, \( P2_1/c \) |
| Temperature (K) | 296 |
| \( a, b, c \) (\( \AA \)) | 7.5654 (3), 11.4972 (2), 12.1025 (3) |
| \( \beta \) (\( ^\circ \)) | 105.583 (3) |
| \( V \) (\( \AA^3 \)) | 1013.99 (2) |
| \( Z \) | 4 |
| Radiation type | Cu Kα |
| \( \mu \) (mm\(^{-1}\)) | 5.30 |
| Crystal size (mm) | 0.45 × 0.10 × 0.10 |
| Data collection | XtaLAB Synergy, Single source at home/near, HyPix3000 |
| Diffractometer | Multi-scan (CrysAlis PRO; Rigaku OD, 2020) |
| Absorption correction | \( T_{\text{min}}, T_{\text{max}} \) | 0.400, 1.000 |
| No. of measured, independent and observed \( [I > 2\sigma(I)] \) reflections | 9036, 1959, 1770 |
| \( R_{\text{int}} \) (|sin \( \theta \)|\( \lambda \))max (\( \AA^{-1} \)) | 0.035 |
| \( F^2 > 2\sigma(F^2) \), \( wR(F^2) \), S | 0.036, 0.099, 1.08 |
| No. of reflections | 1959 |
| No. of parameters | 137 |
| H-atom treatment | H-atom parameters constrained |
| \( \Delta f_{\text{max}}, \Delta f_{\text{min}} \) (\( e \)\( \AA^{-1} \)) | 0.61, −0.56 |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2020), *SHELXS* (Sheldrick, 2008), *SHELXL* (Sheldrick, 2015), *PLATON* (Spek, 2020) and *publICIF* (Wester, 2010).

7. Synthesis and crystallization

The reaction scheme to yield the title compound is shown in Fig. 8. To a mixture of 4.32 g (20 mmol) 2-amino-5-bromo-benzoic acid and 2.72 g (32 mmol) pyrrolidin-2-one, 21.8 g (131 ml) of phosphoroxychloride were added dropwise over 1 h at 273–275 K. The reaction mixture was kept at around 273–275 K. When the reaction mixture was completely decomposed, it was brought to pH = 10–11 with 25%wt ammonium hydroxide solution. The light-yellow precipitate was filtered off, dried and recrystallized from methanol. The yield of the product was 4.35 g (82%), m.p. 431–433 K (literature, m.p. = 430–431 K; Shakhidoyatov, 1983).

1H NMR (400 Mz, CDCl3, \( \delta \), ppm): 8.4 (1H, \( d, J = 2.4, H-8 \)), 7.8 (1H, \( dd, J = 2.4, J = 8.8, H-6 \)), 7.5 (1H, \( d, J = 8.8, H-5 \)), 4.2 (2H, \( q, J = 7.2, H-1 \)), 3.18 (2H, \( t, J = 7.6, H-3 \)), 2.31 (2H, \( m, H-2 \)).

8. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms attached to C were positioned geometrically, with C—H = 0.93 Å (for aromatic) or C—H = 0.97 Å (for methylene H atoms), and were refined with \( U_{\text{iso}}(H) = 1.2U_{\text{eq}}(C) \).
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Crystal structure, Hirshfeld surface analysis and DFT calculations of 7-bromo-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one

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Computing details

Data collection: CrysAlis PRO (Rigaku OD, 2020); cell refinement: CrysAlis PRO (Rigaku OD, 2020); data reduction: CrysAlis PRO (Rigaku OD, 2020); program(s) used to solve structure: SHELXS (Sheldrick, 2008); program(s) used to refine structure: SHELXL (Sheldrick, 2015); molecular graphics: PLATON (Spek, 2020); software used to prepare material for publication: publCIF (Westrip, 2010).

7-Bromo-2,3-dihydropyrrolo[2,1-b]quinazolin-9(1H)-one

Crystal data

C_{11}H_{9}BrN_{2}O

Mr = 265.11

Monoclinic, P2\(^1\)/c

a = 7.5654 (3) Å

b = 11.4972 (2) Å

c = 12.1025 (3) Å

\(\beta = 105.583 (3)^\circ\)

\(V = 1013.99 (5) \text{ Å}^3\)

Z = 4

\(F(000) = 528\)

\(D_x = 1.737 \text{ Mg m}^{-3}\)

\(Cu \text{ K}\alpha \text{ radiation, } \lambda = 1.54184 \text{ Å}\)

Cell parameters from 5905 reflections

\(\theta = 3.8\text{–}71.3^\circ\)

\(\mu = 5.30 \text{ mm}^{-1}\)

\(T = 296 \text{ K}\)

Prismatic, colourless

0.45 × 0.10 × 0.10 mm

Data collection

XtaLAB Synergy, Single source at home/near,

HyPix3000
diffractometer

Radiation source: micro-focus sealed X-ray tube

Detector resolution: 10.0000 pixels mm\(^{-1}\)

\(\omega\) scans

Absorption correction: multi-scan

\((CrysAlisPro; \text{ Rigaku OD, 2020})\)

\(T_{\text{min}} = 0.400, T_{\text{max}} = 1.000\)

Refinement

Refinement on \(F^2\)

Least-squares matrix: full

\(R[F^2 > 2\sigma(F^2)] = 0.036\)

\(wR(F^2) = 0.099\)

\(S = 1.08\)

1959 reflections

137 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

\(w = 1/\left[\sigma^2(F_c^2) + (0.0459P)^2 + 0.6636P\right]\)

\(\text{where } P = (F_c^2 + 2F_s^2)/3\)

\((\Delta/\sigma)_{\text{max}} = 0.005\)
Δρ_{max} = 0.61 \text{ e Å}^{-3}
Δρ_{min} = -0.56 \text{ e Å}^{-3}

Extinction correction: SHELXL-2018/3
(Sheldrick 2015),
Fc^c=kFc[1+0.001xFc^2/\lambda^2]^1/4
Extinction coefficient: 0.0045 (4)

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.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

|    | x     | y     | z     | U_{iso}^*/U_{eq} |
|----|-------|-------|-------|------------------|
| Br | 0.90737 (5) | 0.85845 (3) | 0.51410 (4) | 0.0772 (2) |
| O  | 0.6024 (3) | 0.46212 (19) | 0.28785 (15) | 0.0704 (6) |
| C1 | 0.5525 (4) | 0.2291 (2) | 0.3474 (2) | 0.0524 (6) |
| H1A| 0.615715 | 0.217862 | 0.288281 | 0.063* |
| H1B| 0.424182 | 0.245293 | 0.311148 | 0.063* |
| C2 | 0.5725 (5) | 0.1238 (3) | 0.4234 (3) | 0.0646 (8) |
| H2A| 0.660804 | 0.070068 | 0.406688 | 0.077* |
| H2B| 0.455714 | 0.084094 | 0.411100 | 0.077* |
| C3 | 0.6385 (5) | 0.1665 (2) | 0.5467 (2) | 0.0573 (7) |
| H3A| 0.541287 | 0.160567 | 0.584874 | 0.069* |
| H3B| 0.742854 | 0.121317 | 0.589288 | 0.069* |
| C3A| 0.6916 (4) | 0.2907 (2) | 0.53807 (19) | 0.0428 (5) |
| N4 | 0.7726 (4) | 0.35675 (17) | 0.62262 (17) | 0.0503 (5) |
| C4A| 0.8027 (3) | 0.4710 (2) | 0.59434 (19) | 0.0424 (5) |
| C5 | 0.8937 (4) | 0.5471 (2) | 0.6820 (2) | 0.0569 (7) |
| H5 | 0.932797 | 0.519968 | 0.757050 | 0.068* |
| C6 | 0.9258 (4) | 0.6610 (2) | 0.6588 (2) | 0.0554 (7) |
| H6 | 0.986151 | 0.710837 | 0.717397 | 0.066* |
| C7 | 0.8667 (4) | 0.7005 (2) | 0.5464 (2) | 0.0490 (6) |
| C8 | 0.7793 (4) | 0.6286 (2) | 0.4582 (2) | 0.0486 (6) |
| H8 | 0.737035 | 0.656476 | 0.383367 | 0.058* |
| C8A| 0.7471 (3) | 0.5135 (2) | 0.48227 (19) | 0.0403 (5) |
| C9 | 0.6560 (3) | 0.4355 (2) | 0.38867 (19) | 0.0451 (5) |
| N10| 0.6368 (3) | 0.32406 (18) | 0.42522 (15) | 0.0405 (4) |

Atomic displacement parameters (Å²)

|    | U_{11} | U_{22} | U_{33} | U_{12} | U_{13} | U_{23} |
|----|--------|--------|--------|--------|--------|--------|
| Br | 0.0940 (3) | 0.0341 (2) | 0.1020 (4) | -0.00671 (14) | 0.0235 (2) | 0.00799 (14) |
| O  | 0.1104 (17) | 0.0553 (12) | 0.0345 (9) | 0.0020 (11) | 0.0007 (10) | 0.0064 (8) |
| C1 | 0.0651 (16) | 0.0489 (15) | 0.0402 (12) | -0.0045 (12) | 0.0089 (11) | -0.0130 (11) |
| C2 | 0.090 (2) | 0.0478 (16) | 0.0519 (16) | -0.0179 (15) | 0.0121 (15) | -0.0119 (12) |
| C3 | 0.088 (2) | 0.0401 (13) | 0.0432 (13) | -0.0170 (13) | 0.0171 (13) | -0.0026 (11) |
| C3A| 0.0572 (14) | 0.0365 (12) | 0.0347 (11) | -0.0038 (10) | 0.0121 (10) | 0.0004 (9) |
| N4 | 0.0768 (15) | 0.0375 (12) | 0.0338 (10) | -0.0096 (9) | 0.0099 (10) | -0.0008 (8) |
### Geometric parameters (Å, °)

| Bond/Angle | Distance/Angle (Å/°) |
|------------|----------------------|
| Br—C7      | 1.900 (3)            |
| O—C9       | 1.217 (3)            |
| C1—N10     | 1.471 (3)            |
| C1—C2      | 1.503 (4)            |
| C1—H1A     | 0.9700               |
| C1—H1B     | 0.9700               |
| C2—C3      | 1.522 (4)            |
| C2—H2A     | 0.9700               |
| C2—H2B     | 0.9700               |
| C3—C3A     | 1.494 (4)            |
| C3—H3A     | 0.9700               |
| C3—H3B     | 0.9700               |
| C3A—N4     | 1.290 (3)            |
| N10—C1—C2 | 104.5 (2)            |
| N10—C1—H1A| 110.8                |
| C2—C1—H1A | 110.8                |
| N10—C1—H1B| 110.8                |
| C2—C1—H1B | 110.8                |
| H1A—C1—H1B| 108.9                |
| C1—C2—C3  | 107.0 (2)            |
| C1—C2—H2A | 110.3                |
| C3—C2—H2A | 110.3                |
| C1—C2—H2B | 110.3                |
| C3—C2—H2B | 110.3                |
| H2A—C2—H2B| 108.6                |
| C3A—C3—C2 | 105.3 (2)            |
| C3A—C3—H3A| 110.7                |
| C2—C3—H3A | 110.7                |
| C3A—C3—H3B| 110.7                |
| C2—C3—H3B | 110.7                |
| H3A—C3—H3B| 108.8                |
| N4—C3A—N10| 125.3 (2)            |
| N4—C3A—C3  | 125.9 (2)            |
| N10—C3A—C3 | 108.8 (2)            |
| C3A—N4—C4A| 115.8 (2)            |
| N4—C4A—C8A| 122.9 (2)            |

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**sup-3**

*Acta Cryst. (2022). E78, 885-889*
| Bond/Cycle | Dihedral Angle (°) | Bond/Cycle | Dihedral Angle (°) |
|-----------|-------------------|-----------|-------------------|
| N10—C1—C2—C3 | 9.8 (4) | C5—C4A—C8A—C8 | −0.7 (4) |
| C1—C2—C3—C3A | −11.4 (4) | N4—C4A—C8A—C9 | −1.2 (4) |
| C2—C3—C3A—N4 | −172.4 (3) | C5—C4A—C8A—C9 | 178.5 (2) |
| C2—C3—C3A—N10 | 8.8 (3) | C8—C8A—C9—O | −0.4 (4) |
| N10—C3A—N4—C4A | 0.9 (4) | C4A—C8A—C9—O | −179.6 (3) |
| C3—C3A—N4—C4A | −177.8 (3) | C8—C8A—C9—N10 | 178.8 (2) |
| C3A—N4—C4A—C8A | 1.0 (4) | C4A—C8A—C9—N10 | −0.3 (3) |
| C3A—N4—C4A—C5 | −178.7 (3) | N4—C3A—N10—C9 | −2.6 (4) |
| N4—C4A—C5—C6 | −179.6 (3) | C3—C3A—N10—C9 | 176.2 (2) |
| C8A—C4A—C5—C6 | 0.7 (4) | N4—C3A—N10—C1 | 178.4 (3) |
| C4A—C5—C6—C7 | 0.0 (5) | C3—C3A—N10—C1 | −2.7 (3) |
| C5—C6—C7—C8 | −0.7 (4) | O—C9—N10—C3A | −178.6 (3) |
| C5—C6—C7—Br | 179.0 (2) | C8A—C9—N10—C3A | 2.1 (3) |
| C6—C7—C8—C8A | 0.8 (4) | O—C9—N10—C1 | 0.3 (4) |
| Br—C7—C8—C8A | −179.02 (19) | C8A—C9—N10—C1 | −179.0 (2) |
| C7—C8—C8A—C4A | −0.1 (4) | C2—C1—N10—C3A | −4.5 (3) |
| C7—C8—C8A—C9 | −179.2 (2) | C2—C1—N10—C9 | 176.5 (2) |
| N4—C4A—C8A—C8 | 179.6 (2) | | |