# organic compounds

# (Z)-3-(9-Anthryl)-1-(4-bromophenyl)-2-(4-nitro-1H-imidazol-1-yl)prop-2-en-1-one

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In the title molecule, $C_{26}H_{16}BrN_3O_3$, the anthracene and benzene mean planes make dihedral angles of 63.79 (2) and 14.67 (2)°, respectively, with the plane of the imidazole ring. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link molecules to form centrosymmetric dimers. Weak $\pi$–$\pi$ stacking interactions, with centroid–centroid distances of 3.779 (2) and 3.826 (2) Å, supply additional stabilization. The crystal packing also exhibits short intermolecular contacts between the nitro groups and Br atoms [Br···O = 3.114 (2) Å].

## Related literature

For the crystal structure of the chloro analog of the title compound, see: Wang *et al.* (2009). For general background on the pharmacological activities of chalcones, see: Corréa *et al.* (2001); Jasinski *et al.* (2009); Nielsen *et al.* (1998); Vogel *et al.* (2008). For the synthetic details, see: Erhardt *et al.* (1985); Kranz *et al.* (1980).
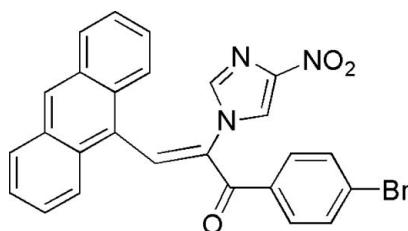


## Experimental

### Crystal data

| | |
|---|---|
| $C_{26}H_{16}BrN_3O_3$ | $b$ = 11.0916 (14) Å |
| $M_r$ = 498.33 | $c$ = 12.7979 (17) Å |
| Triclinic, $P\bar{1}$ | $\alpha$ = 78.146 (2)° |
| $a$ = 8.1438 (11) Å | $\beta$ = 86.193 (2)° |
| $\gamma$ = 70.768 (2)° | $\mu$ = 1.96 mm$^{-1}$ |
| $V$ = 1068.2 (2) Å$^3$ | $T$ = 292 K |
| $Z$ = 2 | 0.13 × 0.12 × 0.10 mm |
| Mo $K\alpha$ radiation | |

### Data collection

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 6422 measured reflections |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | 4315 independent reflections |
| $T_{min}$ = 0.775, $T_{max}$ = 0.828 | 3095 reflections with $I > 2\sigma(I)$ |
| | $R_{int}$ = 0.019 |

### Refinement

| | |
|---|---|
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | 298 parameters |
| $wR(F^2)$ = 0.116 | H-atom parameters constrained |
| $S$ = 1.02 | $\Delta\rho_{max}$ = 0.56 e Å$^{-3}$ |
| 4315 reflections | $\Delta\rho_{min}$ = −0.67 e Å$^{-3}$ |

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C23—H23···O3$^i$ | 0.93 | 2.56 | 3.303 (4) | 137 |

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

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *PLATON*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: LH2825).

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# supporting information

# (*Z*)-3-(9-Anthryl)-1-(4-bromophenyl)-2-(4-nitro-1*H*-imidazol-1-yl)prop-2-en-1-one

## Yi-Hui Lu, Guang-Zhou Wang, Cheng-He Zhou and Yi-Yi Zhang

### S1. Comment

Chalcones and their derivatives have been reported responsible for a variety of pharmacological activities, including antibacterial, antifungal, anti-leishmanial, antimalarial, analgesic, anti-inflammatory and chemopreventive ones (Corréa *et al.*, 2001; Jasinski *et al.*, 2009; Simon *et al.*, 1998; Vogel *et al.*, 2008). Due to these varied applications, we have synthesized the title compound and report its crystal structure.

In the molecular structure of the title compound (I) (Fig. 1), the dihedral angle between the anthracene unit and imidazole ring is 63.79 (2) ° and that between the imidazole ring and benzene ring is 14.67 (2) °. In the crystal structure, weak intermolecular C—H···O hydrogen bonds link molecules to form centrosymmetric dimers (Fig. 2). Weak $\pi$–$\pi$ staking interactions, with centroid to centroid distances of 3.779 (2) and 3.826 (2)Å supply additional stabilization.

### S2. Experimental

Compound (I) was synthesized according to the procedure of Erhardt *et al.* (1985); Kranz *et al.* (1980). A crystal suitable for X-ray analysis was grown from a chloroform and acetone solution of (I) by slow evaporation at room temperature.

### S3. Refinement

H ydrogen atoms were placed in idealized positions with C—H = 0.93Å and $U_{iso}$(H) = 1.2$U_{eq}$(C).
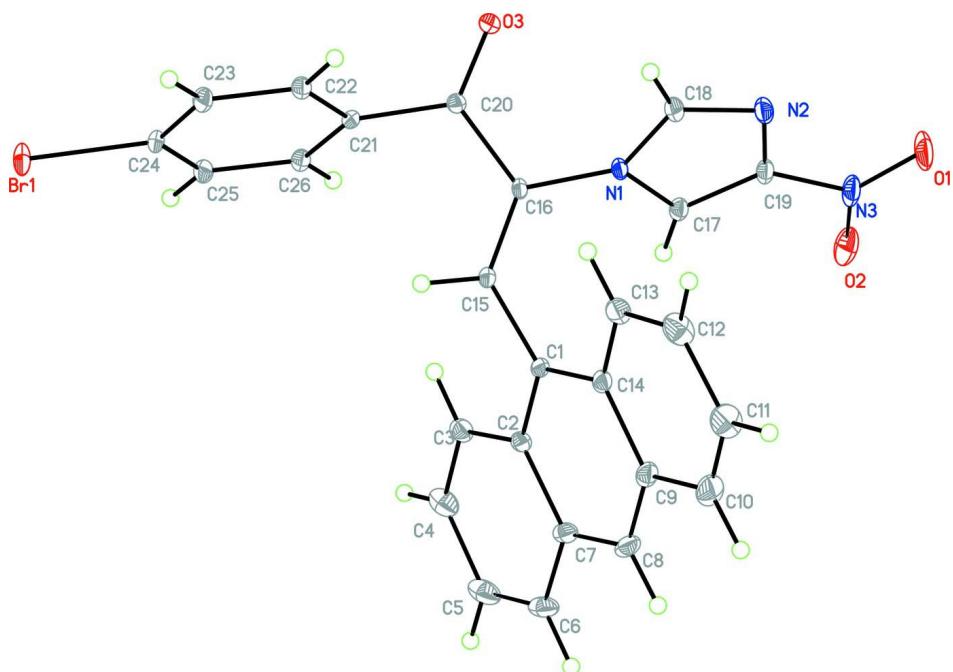
**Figure 1**

The molecular structure of (I), showing the atom-numbering scheme. Displacement ellipsoids are drawn at the 30% probability level.
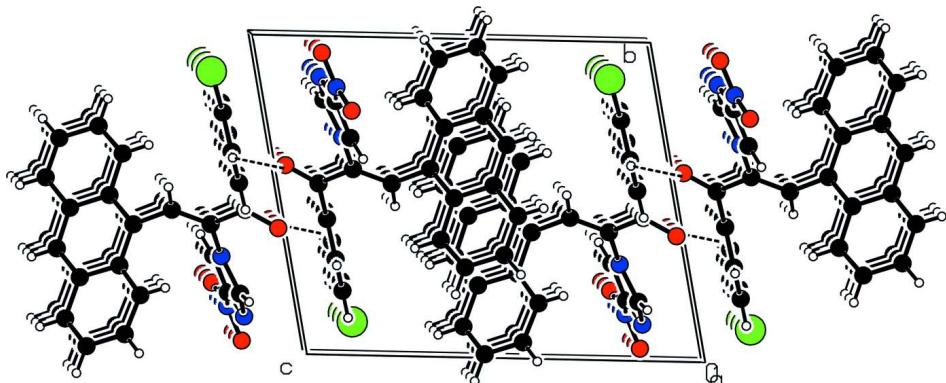


**Figure 2**

Part of the crystal structure of (I). Hydrogen bonds are shown as dashed lines.

## (*Z*)-3-(9-Anthryl)-1-(4-bromophenyl)-2-(4-nitro-1*H*-imidazol- 1-yl)prop-2-en-1-one

*Crystal data*

| | |
|---|---|
| $C_{26}H_{16}BrN_3O_3$ | $\gamma = 70.768\ (2)°$ |
| $M_r = 498.33$ | $V = 1068.2\ (2)\ \text{Å}^3$ |
| Triclinic, $P\overline{1}$ | $Z = 2$ |
| Hall symbol: -P 1 | $F(000) = 504$ |
| $a = 8.1438\ (11)\ \text{Å}$ | $D_x = 1.549\ \text{Mg m}^{-3}$ |
| $b = 11.0916\ (14)\ \text{Å}$ | Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{Å}$ |
| $c = 12.7979\ (17)\ \text{Å}$ | Cell parameters from 2344 reflections |
| $\alpha = 78.146\ (2)°$ | $\theta = 2.3–26.9°$ |
| $\beta = 86.193\ (2)°$ | $\mu = 1.96\ \text{mm}^{-1}$ |

$T$ = 292 K

0.13 × 0.12 × 0.10 mm

Block, orange

*Data collection*

| | |
|---|---|
| Bruker SMART APEX CCD area-detector diffractometer | 6422 measured reflections |
| Radiation source: fine focus sealed Siemens Mo tube | 4315 independent reflections |
| | 3095 reflections with $I > 2\sigma(I)$ |
| Graphite monochromator | $R_{int}$ = 0.019 |
| 0.3° wide $\omega$ exposures scans | $\theta_{max}$ = 26.5°, $\theta_{min}$ = 2.7° |
| Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996) | $h = -8 \rightarrow 10$ |
| | $k = -13 \rightarrow 13$ |
| | $l = -16 \rightarrow 15$ |
| $T_{min}$ = 0.775, $T_{max}$ = 0.828 | |

*Refinement*

| | |
|---|---|
| Refinement on $F^2$ | Hydrogen site location: inferred from neighbouring sites |
| Least-squares matrix: full | H-atom parameters constrained |
| $R[F^2 > 2\sigma(F^2)]$ = 0.044 | $w = 1/[\sigma^2(F_o^2) + (0.0524P)^2 + 0.6665P]$ where $P = (F_o^2 + 2F_c^2)/3$ |
| $wR(F^2)$ = 0.116 | |
| $S$ = 1.02 | $(\Delta/\sigma)_{max}$ = 0.008 |
| 4315 reflections | $\Delta\rho_{max}$ = 0.56 e Å$^{-3}$ |
| 298 parameters | $\Delta\rho_{min}$ = -0.67 e Å$^{-3}$ |
| 0 restraints | Extinction correction: *SHELXL97* (Sheldrick, 2008), Fc\*=kFc[1+0.001xFc²$\lambda$³/sin(2$\theta$)]$^{-1/4}$ |
| Primary atom site location: structure-invariant direct methods | |
| Secondary atom site location: difference Fourier map | Extinction coefficient: 0.0078 (11) |

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$\*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.93749 (6) | 0.89457 (4) | 0.12755 (3) | 0.06983 (18) |
| C1 | 0.4551 (4) | 0.4031 (3) | 0.3854 (2) | 0.0356 (6) |
| C2 | 0.3193 (4) | 0.4914 (3) | 0.4320 (2) | 0.0406 (7) |
| C3 | 0.2357 (4) | 0.6217 (3) | 0.3799 (3) | 0.0496 (8) |
| H3 | 0.2699 | 0.6506 | 0.3111 | 0.060* |
| C4 | 0.1080 (5) | 0.7050 (4) | 0.4276 (4) | 0.0691 (11) |
| H4 | 0.0565 | 0.7902 | 0.3917 | 0.083* |
| C5 | 0.0521 (5) | 0.6637 (5) | 0.5312 (4) | 0.0740 (13) |
| H5 | −0.0342 | 0.7224 | 0.5639 | 0.089* |
| C6 | 0.1223 (5) | 0.5405 (5) | 0.5832 (3) | 0.0647 (11) |
| H6 | 0.0819 | 0.5144 | 0.6509 | 0.078* |
| C7 | 0.2583 (4) | 0.4483 (4) | 0.5363 (2) | 0.0510 (9) |

| C8 | 0.3318 (5) | 0.3209 (4) | 0.5877 (3) | 0.0570 (10) |
| H8 | 0.2893 | 0.2930 | 0.6543 | 0.068* |
| C9 | 0.4663 (5) | 0.2335 (4) | 0.5435 (3) | 0.0545 (9) |
| C10 | 0.5444 (7) | 0.1041 (4) | 0.5990 (3) | 0.0804 (14) |
| H10 | 0.5007 | 0.0765 | 0.6653 | 0.096* |
| C11 | 0.6795 (8) | 0.0206 (5) | 0.5582 (4) | 0.0943 (17) |
| H11 | 0.7273 | −0.0642 | 0.5957 | 0.113* |
| C12 | 0.7504 (7) | 0.0613 (4) | 0.4575 (4) | 0.0792 (13) |
| H12 | 0.8461 | 0.0034 | 0.4305 | 0.095* |
| C13 | 0.6790 (5) | 0.1839 (3) | 0.4007 (3) | 0.0538 (9) |
| H13 | 0.7270 | 0.2092 | 0.3353 | 0.065* |
| C14 | 0.5326 (4) | 0.2738 (3) | 0.4394 (2) | 0.0415 (7) |
| C15 | 0.5261 (4) | 0.4522 (3) | 0.2830 (2) | 0.0327 (6) |
| H15 | 0.5626 | 0.5235 | 0.2820 | 0.039* |
| C16 | 0.5458 (4) | 0.4098 (2) | 0.1916 (2) | 0.0308 (6) |
| C17 | 0.3147 (4) | 0.3086 (3) | 0.1964 (2) | 0.0391 (7) |
| H17 | 0.2215 | 0.3730 | 0.2185 | 0.047* |
| C18 | 0.5712 (5) | 0.1936 (3) | 0.1475 (3) | 0.0456 (7) |
| H18 | 0.6886 | 0.1698 | 0.1296 | 0.055* |
| C19 | 0.3157 (5) | 0.1937 (3) | 0.1754 (2) | 0.0448 (8) |
| C20 | 0.6441 (4) | 0.4580 (3) | 0.0995 (2) | 0.0322 (6) |
| C21 | 0.7038 (4) | 0.5703 (3) | 0.1060 (2) | 0.0332 (6) |
| C22 | 0.8822 (4) | 0.5456 (3) | 0.1056 (2) | 0.0422 (7) |
| H22 | 0.9569 | 0.4628 | 0.1014 | 0.051* |
| C23 | 0.9499 (4) | 0.6436 (3) | 0.1113 (3) | 0.0490 (8) |
| H23 | 1.0696 | 0.6267 | 0.1122 | 0.059* |
| C24 | 0.8383 (4) | 0.7651 (3) | 0.1157 (2) | 0.0438 (7) |
| C25 | 0.6602 (4) | 0.7937 (3) | 0.1138 (2) | 0.0426 (7) |
| H25 | 0.5861 | 0.8775 | 0.1155 | 0.051* |
| C26 | 0.5943 (4) | 0.6947 (3) | 0.1094 (2) | 0.0389 (7) |
| H26 | 0.4746 | 0.7121 | 0.1087 | 0.047* |
| N1 | 0.4811 (3) | 0.3085 (2) | 0.17774 (18) | 0.0342 (5) |
| N2 | 0.4740 (4) | 0.1210 (2) | 0.1464 (2) | 0.0515 (7) |
| N3 | 0.1680 (5) | 0.1482 (3) | 0.1818 (3) | 0.0663 (9) |
| O1 | 0.1909 (5) | 0.0414 (3) | 0.1602 (3) | 0.1002 (11) |
| O2 | 0.0289 (5) | 0.2194 (4) | 0.2088 (3) | 0.0920 (10) |
| O3 | 0.6822 (3) | 0.4034 (2) | 0.02424 (17) | 0.0464 (5) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.0870 (3) | 0.0579 (2) | 0.0872 (3) | −0.0537 (2) | 0.0032 (2) | −0.01466 (19) |
| C1 | 0.0423 (17) | 0.0457 (16) | 0.0284 (14) | −0.0269 (14) | 0.0004 (12) | −0.0071 (12) |
| C2 | 0.0426 (18) | 0.0551 (19) | 0.0351 (16) | −0.0264 (15) | 0.0010 (13) | −0.0159 (14) |
| C3 | 0.048 (2) | 0.056 (2) | 0.0514 (19) | −0.0203 (17) | 0.0012 (15) | −0.0194 (16) |
| C4 | 0.058 (2) | 0.073 (3) | 0.079 (3) | −0.012 (2) | −0.004 (2) | −0.036 (2) |
| C5 | 0.049 (2) | 0.108 (4) | 0.079 (3) | −0.021 (2) | 0.009 (2) | −0.057 (3) |
| C6 | 0.047 (2) | 0.119 (4) | 0.047 (2) | −0.040 (2) | 0.0134 (17) | −0.038 (2) |

| | | | | | |
|---|---|---|---|---|---|
| C7 | 0.0468 (19) | 0.089 (3) | 0.0349 (17) | −0.0403 (19) | 0.0018 (14) | −0.0203 (17) |
| C8 | 0.065 (2) | 0.090 (3) | 0.0297 (17) | −0.049 (2) | 0.0024 (16) | −0.0047 (18) |
| C9 | 0.074 (3) | 0.065 (2) | 0.0363 (17) | −0.044 (2) | −0.0098 (17) | 0.0023 (16) |
| C10 | 0.124 (4) | 0.070 (3) | 0.050 (2) | −0.049 (3) | −0.018 (2) | 0.016 (2) |
| C11 | 0.156 (5) | 0.054 (3) | 0.061 (3) | −0.030 (3) | −0.026 (3) | 0.016 (2) |
| C12 | 0.101 (3) | 0.050 (2) | 0.076 (3) | −0.008 (2) | −0.019 (2) | −0.009 (2) |
| C13 | 0.069 (2) | 0.0462 (19) | 0.0451 (19) | −0.0187 (18) | −0.0118 (17) | −0.0038 (15) |
| C14 | 0.0523 (19) | 0.0446 (17) | 0.0352 (16) | −0.0268 (15) | −0.0055 (14) | −0.0043 (13) |
| C15 | 0.0364 (16) | 0.0331 (14) | 0.0342 (15) | −0.0187 (12) | 0.0007 (12) | −0.0065 (11) |
| C16 | 0.0360 (15) | 0.0274 (13) | 0.0345 (15) | −0.0171 (12) | −0.0003 (11) | −0.0066 (11) |
| C17 | 0.0398 (17) | 0.0420 (16) | 0.0412 (16) | −0.0219 (14) | −0.0027 (13) | −0.0052 (13) |
| C18 | 0.054 (2) | 0.0340 (16) | 0.0535 (19) | −0.0187 (14) | 0.0031 (15) | −0.0123 (13) |
| C19 | 0.062 (2) | 0.0461 (17) | 0.0374 (16) | −0.0354 (17) | −0.0100 (15) | 0.0011 (13) |
| C20 | 0.0317 (15) | 0.0346 (14) | 0.0327 (15) | −0.0129 (12) | 0.0002 (12) | −0.0087 (12) |
| C21 | 0.0422 (17) | 0.0358 (15) | 0.0265 (14) | −0.0207 (13) | 0.0045 (11) | −0.0049 (11) |
| C22 | 0.0423 (18) | 0.0411 (16) | 0.0498 (18) | −0.0197 (14) | 0.0098 (14) | −0.0162 (14) |
| C23 | 0.0414 (18) | 0.058 (2) | 0.061 (2) | −0.0303 (16) | 0.0103 (15) | −0.0203 (16) |
| C24 | 0.061 (2) | 0.0409 (17) | 0.0423 (17) | −0.0348 (16) | 0.0083 (14) | −0.0084 (13) |
| C25 | 0.054 (2) | 0.0329 (15) | 0.0429 (17) | −0.0188 (14) | 0.0001 (14) | −0.0040 (13) |
| C26 | 0.0395 (17) | 0.0380 (16) | 0.0430 (17) | −0.0178 (14) | 0.0032 (13) | −0.0082 (13) |
| N1 | 0.0426 (14) | 0.0311 (12) | 0.0362 (12) | −0.0203 (11) | −0.0023 (10) | −0.0079 (10) |
| N2 | 0.075 (2) | 0.0366 (14) | 0.0513 (16) | −0.0297 (15) | −0.0045 (14) | −0.0068 (12) |
| N3 | 0.088 (3) | 0.070 (2) | 0.063 (2) | −0.061 (2) | −0.0171 (19) | 0.0032 (16) |
| O1 | 0.133 (3) | 0.089 (2) | 0.121 (3) | −0.087 (2) | −0.009 (2) | −0.0254 (19) |
| O2 | 0.074 (2) | 0.101 (2) | 0.121 (3) | −0.063 (2) | −0.002 (2) | −0.007 (2) |
| O3 | 0.0553 (14) | 0.0526 (13) | 0.0437 (12) | −0.0285 (11) | 0.0144 (10) | −0.0226 (10) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C24 | 1.899 (3) | C15—C16 | 1.329 (4) |
| C1—C2 | 1.405 (4) | C15—H15 | 0.9300 |
| C1—C14 | 1.410 (4) | C16—N1 | 1.434 (3) |
| C1—C15 | 1.471 (4) | C16—C20 | 1.487 (4) |
| C2—C3 | 1.419 (5) | C17—C19 | 1.353 (4) |
| C2—C7 | 1.436 (4) | C17—N1 | 1.359 (4) |
| C3—C4 | 1.349 (5) | C17—H17 | 0.9300 |
| C3—H3 | 0.9300 | C18—N2 | 1.305 (4) |
| C4—C5 | 1.408 (6) | C18—N1 | 1.365 (4) |
| C4—H4 | 0.9300 | C18—H18 | 0.9300 |
| C5—C6 | 1.341 (6) | C19—N2 | 1.351 (4) |
| C5—H5 | 0.9300 | C19—N3 | 1.442 (4) |
| C6—C7 | 1.432 (5) | C20—O3 | 1.211 (3) |
| C6—H6 | 0.9300 | C20—C21 | 1.497 (4) |
| C7—C8 | 1.379 (5) | C21—C26 | 1.382 (4) |
| C8—C9 | 1.379 (5) | C21—C22 | 1.387 (4) |
| C8—H8 | 0.9300 | C22—C23 | 1.387 (4) |
| C9—C10 | 1.417 (5) | C22—H22 | 0.9300 |
| C9—C14 | 1.444 (5) | C23—C24 | 1.365 (5) |

| | | | |
|---|---|---|---|
| C10—C11 | 1.338 (7) | C23—H23 | 0.9300 |
| C10—H10 | 0.9300 | C24—C25 | 1.380 (5) |
| C11—C12 | 1.426 (7) | C25—C26 | 1.384 (4) |
| C11—H11 | 0.9300 | C25—H25 | 0.9300 |
| C12—C13 | 1.358 (5) | C26—H26 | 0.9300 |
| C12—H12 | 0.9300 | N3—O1 | 1.222 (4) |
| C13—C14 | 1.415 (5) | N3—O2 | 1.224 (5) |
| C13—H13 | 0.9300 | | |
| | | | |
| C2—C1—C14 | 121.2 (3) | C16—C15—H15 | 115.2 |
| C2—C1—C15 | 118.2 (3) | C1—C15—H15 | 115.2 |
| C14—C1—C15 | 120.3 (3) | C15—C16—N1 | 121.6 (2) |
| C1—C2—C3 | 123.1 (3) | C15—C16—C20 | 122.8 (2) |
| C1—C2—C7 | 119.1 (3) | N1—C16—C20 | 115.5 (2) |
| C3—C2—C7 | 117.7 (3) | C19—C17—N1 | 104.3 (3) |
| C4—C3—C2 | 121.8 (4) | C19—C17—H17 | 127.8 |
| C4—C3—H3 | 119.1 | N1—C17—H17 | 127.8 |
| C2—C3—H3 | 119.1 | N2—C18—N1 | 112.3 (3) |
| C3—C4—C5 | 120.4 (4) | N2—C18—H18 | 123.9 |
| C3—C4—H4 | 119.8 | N1—C18—H18 | 123.9 |
| C5—C4—H4 | 119.8 | N2—C19—C17 | 112.9 (3) |
| C6—C5—C4 | 120.6 (4) | N2—C19—N3 | 121.2 (3) |
| C6—C5—H5 | 119.7 | C17—C19—N3 | 125.9 (4) |
| C4—C5—H5 | 119.7 | O3—C20—C16 | 120.7 (2) |
| C5—C6—C7 | 121.2 (4) | O3—C20—C21 | 121.2 (2) |
| C5—C6—H6 | 119.4 | C16—C20—C21 | 118.0 (2) |
| C7—C6—H6 | 119.4 | C26—C21—C22 | 119.1 (3) |
| C8—C7—C2 | 119.4 (3) | C26—C21—C20 | 124.6 (3) |
| C8—C7—C6 | 122.3 (3) | C22—C21—C20 | 116.3 (3) |
| C2—C7—C6 | 118.3 (3) | C23—C22—C21 | 120.5 (3) |
| C9—C8—C7 | 122.1 (3) | C23—C22—H22 | 119.8 |
| C9—C8—H8 | 118.9 | C21—C22—H22 | 119.8 |
| C7—C8—H8 | 118.9 | C24—C23—C22 | 119.0 (3) |
| C8—C9—C10 | 121.4 (4) | C24—C23—H23 | 120.5 |
| C8—C9—C14 | 120.0 (3) | C22—C23—H23 | 120.5 |
| C10—C9—C14 | 118.6 (4) | C23—C24—C25 | 122.0 (3) |
| C11—C10—C9 | 121.5 (4) | C23—C24—Br1 | 117.4 (2) |
| C11—C10—H10 | 119.2 | C25—C24—Br1 | 120.6 (2) |
| C9—C10—H10 | 119.2 | C26—C25—C24 | 118.4 (3) |
| C10—C11—C12 | 120.2 (4) | C26—C25—H25 | 120.8 |
| C10—C11—H11 | 119.9 | C24—C25—H25 | 120.8 |
| C12—C11—H11 | 119.9 | C21—C26—C25 | 121.0 (3) |
| C13—C12—C11 | 120.4 (4) | C21—C26—H26 | 119.5 |
| C13—C12—H12 | 119.8 | C25—C26—H26 | 119.5 |
| C11—C12—H12 | 119.8 | C17—N1—C18 | 106.8 (2) |
| C12—C13—C14 | 121.0 (4) | C17—N1—C16 | 125.3 (2) |
| C12—C13—H13 | 119.5 | C18—N1—C16 | 128.0 (2) |
| C14—C13—H13 | 119.5 | C18—N2—C19 | 103.7 (3) |

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| C1—C14—C13 | 123.7 (3) | O1—N3—O2 | 124.9 (4) |
| C1—C14—C9 | 118.1 (3) | O1—N3—C19 | 117.7 (4) |
| C13—C14—C9 | 118.1 (3) | O2—N3—C19 | 117.4 (3) |
| C16—C15—C1 | 129.6 (2) | | |
| | | | |
| C14—C1—C2—C3 | −179.0 (3) | C1—C15—C16—C20 | −170.6 (3) |
| C15—C1—C2—C3 | 6.7 (4) | N1—C17—C19—N2 | 1.0 (3) |
| C14—C1—C2—C7 | −0.3 (4) | N1—C17—C19—N3 | −178.9 (3) |
| C15—C1—C2—C7 | −174.6 (2) | C15—C16—C20—O3 | 168.5 (3) |
| C1—C2—C3—C4 | −178.6 (3) | N1—C16—C20—O3 | −8.1 (4) |
| C7—C2—C3—C4 | 2.6 (5) | C15—C16—C20—C21 | −7.7 (4) |
| C2—C3—C4—C5 | −0.7 (5) | N1—C16—C20—C21 | 175.6 (2) |
| C3—C4—C5—C6 | −1.4 (6) | O3—C20—C21—C26 | 118.6 (3) |
| C4—C5—C6—C7 | 1.5 (6) | C16—C20—C21—C26 | −65.2 (4) |
| C1—C2—C7—C8 | −1.2 (4) | O3—C20—C21—C22 | −59.7 (4) |
| C3—C2—C7—C8 | 177.6 (3) | C16—C20—C21—C22 | 116.5 (3) |
| C1—C2—C7—C6 | 178.7 (3) | C26—C21—C22—C23 | 1.7 (4) |
| C3—C2—C7—C6 | −2.5 (4) | C20—C21—C22—C23 | −180.0 (3) |
| C5—C6—C7—C8 | −179.5 (3) | C21—C22—C23—C24 | −1.0 (5) |
| C5—C6—C7—C2 | 0.5 (5) | C22—C23—C24—C25 | −0.4 (5) |
| C2—C7—C8—C9 | 1.9 (5) | C22—C23—C24—Br1 | 178.3 (2) |
| C6—C7—C8—C9 | −178.0 (3) | C23—C24—C25—C26 | 1.2 (5) |
| C7—C8—C9—C10 | 177.8 (3) | Br1—C24—C25—C26 | −177.4 (2) |
| C7—C8—C9—C14 | −1.1 (5) | C22—C21—C26—C25 | −0.9 (4) |
| C8—C9—C10—C11 | −177.3 (4) | C20—C21—C26—C25 | −179.1 (3) |
| C14—C9—C10—C11 | 1.7 (6) | C24—C25—C26—C21 | −0.5 (4) |
| C9—C10—C11—C12 | 0.9 (7) | C19—C17—N1—C18 | −0.3 (3) |
| C10—C11—C12—C13 | −1.6 (7) | C19—C17—N1—C16 | −178.5 (2) |
| C11—C12—C13—C14 | −0.4 (6) | N2—C18—N1—C17 | −0.5 (3) |
| C2—C1—C14—C13 | −174.5 (3) | N2—C18—N1—C16 | 177.6 (3) |
| C15—C1—C14—C13 | −0.3 (4) | C15—C16—N1—C17 | 53.4 (4) |
| C2—C1—C14—C9 | 1.1 (4) | C20—C16—N1—C17 | −129.9 (3) |
| C15—C1—C14—C9 | 175.3 (3) | C15—C16—N1—C18 | −124.4 (3) |
| C12—C13—C14—C1 | 178.5 (3) | C20—C16—N1—C18 | 52.4 (4) |
| C12—C13—C14—C9 | 3.0 (5) | N1—C18—N2—C19 | 1.0 (3) |
| C8—C9—C14—C1 | −0.4 (4) | C17—C19—N2—C18 | −1.3 (4) |
| C10—C9—C14—C1 | −179.4 (3) | N3—C19—N2—C18 | 178.6 (3) |
| C8—C9—C14—C13 | 175.4 (3) | N2—C19—N3—O1 | 0.2 (5) |
| C10—C9—C14—C13 | −3.6 (5) | C17—C19—N3—O1 | −180.0 (3) |
| C2—C1—C15—C16 | −126.2 (3) | N2—C19—N3—O2 | 179.8 (3) |
| C14—C1—C15—C16 | 59.4 (4) | C17—C19—N3—O2 | −0.3 (5) |
| C1—C15—C16—N1 | 5.8 (5) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H⋯*A* | *D*—H | H⋯*A* | *D*⋯*A* | *D*—H⋯*A* |
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|---|---|---|---|---|
| C23—H23···O3ⁱ | 0.93 | 2.56 | 3.303 (4) | 137 |

Symmetry code: (i) −*x*+2, −*y*+1, −*z*.