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# (*E*)-3-[3-(4-Bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-1-(2,4-dichlorophenyl)-prop-2-en-1-one

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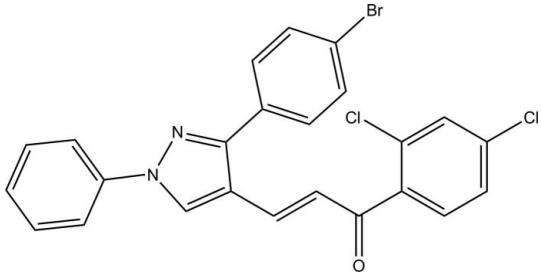
Key indicators: single-crystal X-ray study; $T$ = 296 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.052; $wR$ factor = 0.140; data-to-parameter ratio = 23.9.

In the title molecule, $C_{24}H_{15}BrCl_2N_2O$, the dihedral angles betwen the pyrazole ring and its N-bonded phenyl (*A*) and C-bonded bromobenzene (*B*) rings are 10.34 (16) and 40.95 (15)°, respectively. The dihedral angle between rings *A* and *B* is 56.89 (17)°. The title molecule exists in a *trans* conformation with respect to the acyclic C=C bond. In the crystal, molecules are linked into inversion dimers by pairs of C—H···O hydrogen bonds, generating $R_2^2(14)$ loops. The crystal structure is further consolidated by C—H···$\pi$ interactions.

## Related literature

For a related structure and background references to pyrazoles, see: Fun *et al.* (2011). For standard bond-length data, see: Allen *et al.* (1987). For hydrogen-bond motifs, see: Bernstein *et al.* (1995).




## Experimental

### Crystal data

$C_{24}H_{15}BrCl_2N_2O$
$M_r$ = 498.19
Monoclinic, $P2_1/c$
$a$ = 11.4203 (14) Å
$b$ = 9.9357 (13) Å
$c$ = 19.656 (3) Å
$\beta$ = 94.653 (3)°
$V$ = 2222.9 (5) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 2.11 mm$^{-1}$
$T$ = 296 K
0.38 × 0.21 × 0.11 mm

### Data collection

Bruker SMART APEXII DUO CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min}$ = 0.504, $T_{max}$ = 0.803
23842 measured reflections
6480 independent reflections
2743 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.056

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.140
$S$ = 0.98
6480 reflections
271 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.44 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.52 e Å$^{-3}$

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

*Cg*1 is the centroid of C1–C6 phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11*A*···O1$^{i}$ | 0.93 | 2.41 | 3.329 (4) | 170 |
| C15—H15*A*···*Cg*1$^{ii}$ | 0.93 | 2.82 | 3.666 (3) | 152 |

Symmetry codes: (i) $-x, -y+1, -z+1$; (ii) $x, y-1, z$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; 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: HB6462).

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Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.

‡ Thomson Reuters ResearcherID: A-3561-2009.
§ Thomson Reuters ResearcherID: A-5525-2009.

# supporting information

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## (*E*)-3-[3-(4-Bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-1-(2,4-dichlorophenyl)-prop-2-en-1-one

**Hoong-Kun Fun, Ching Kheng Quah, Shridhar Malladi, Arun M. Isloor and Kammasandra N. Shivananda**

### S1. Comment

As part of our ongoing studies of pyrazole derivatives with potential biological activities (Fun *et al.*, 2011), we have synthesized the title compound, (I), to study its crystal structure.

In the title molecule (Fig. 1), the benzene (C19-C24) ring and the two phenyl (C1-C6 and C13-C18) rings form dihedral angles of 10.34 (16), 50.23 (16) and 40.95 (15)°, respectively, with the pyrazole ring (N1/N2/C10-C12). The benzene ring also forms dihedral angles of 56.89 (17) and 38.81 (16)° with dichloro-bound phenyl (C1-C6) and bromo-bound phenyl (C13-C18) rings, respectively. The phenyl rings form a dihedral angle of 89.57 (17)°. The title molecule exists in *trans* configuration with respect to the acyclic C8═C9 bond [bond length = 1.336 (4) Å]. Bond lengths (Allen *et al.*, 1987) and angles are within normal ranges and are comparable to a related structure (Fun *et al.*, 2011).

In the crystal (Fig. 2), molecules are linked into inversion dimers by pairs of intermolecular C11–H11A···O1 hydrogen bonds (Table 1), generating fourteen-membered $D^2_2(14)$ ring motifs (Bernstein *et al.*, 1995). The crystal structure is further consolidated by C15–H15A···Cg1 (Table 1) interactions, where Cg1 is the centroid of C1-C6 phenyl ring.

### S2. Experimental

To a cold, stirred mixture of methanol (20 ml) and sodium hydroxide (12.09 mmol), 2,4-dichloroacetophenone (4.03 mmol) was added. The reaction mixture was stirred for 10 min. 3-(4-Bromophenyl)-1-phenyl-1H-pyrazole-4-carbaldehyde (4.03 mmol) was added to this solution followed by tetrahydrofuran (30 ml). The solution was further stirred for 2 h at 273 K and then at room temperature for 5 h. It was then poured into ice cold water. The resulting solution was neutralized with dil. HCl. The solid that separated out was filtered, washed with water, dried and crystallized from ethanol to yield colourless blocks. Yield: 1.6 g, 80 %. *M.p.*: 457-458 K.

### S3. Refinement

All H atoms were positioned geometrically and refined using a riding model with C–H = 0.93 Å and $U_{iso}$(H) = 1.2 $U_{eq}$(C).

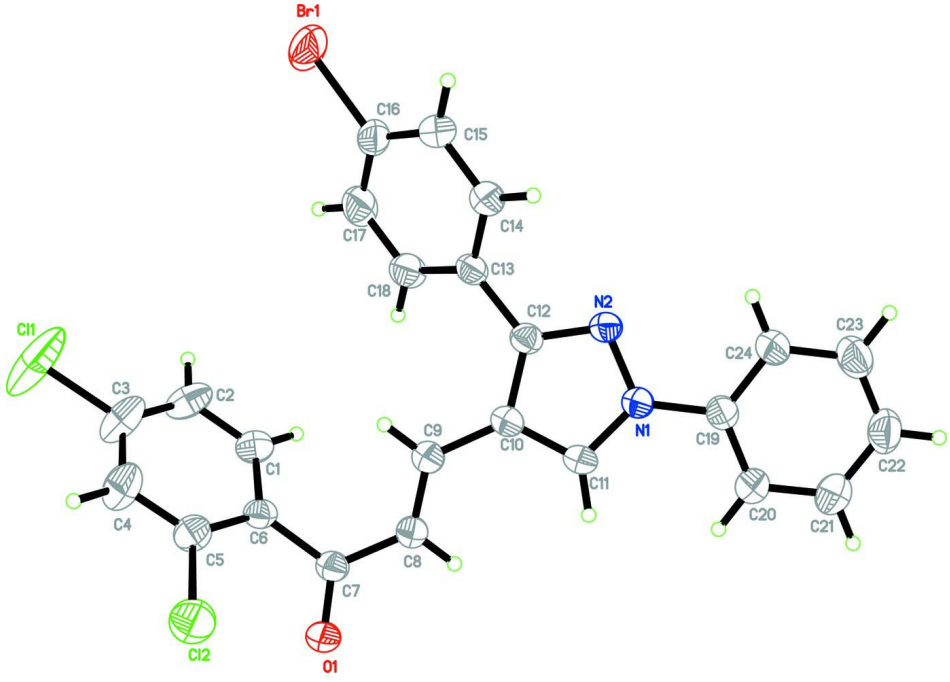


**Figure 1**

The molecular structure of the title compound showing 30% probability displacement ellipsoids for non-H atoms.

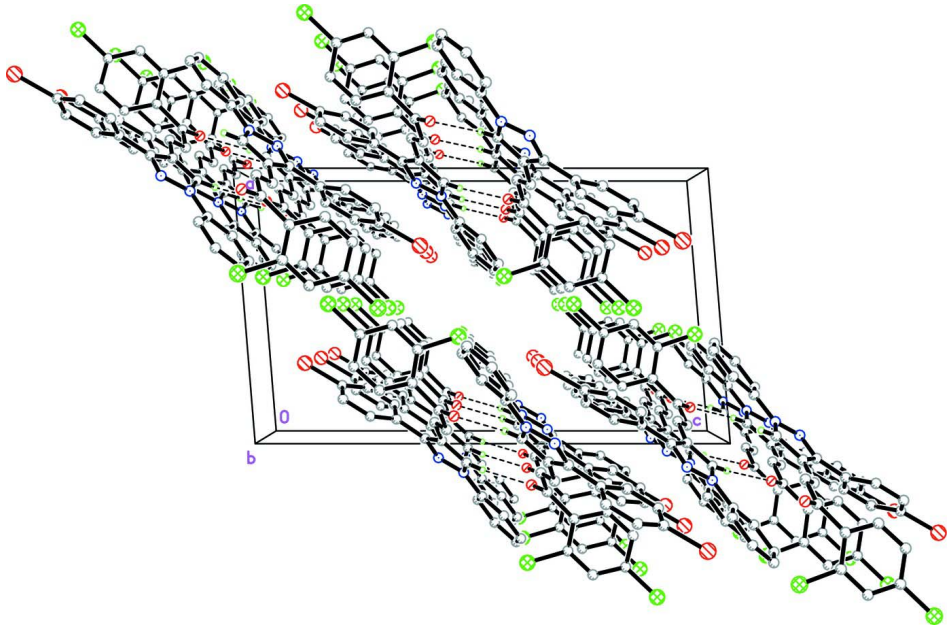


**Figure 2**

The crystal structure of the title compound, viewed along the *b* axis. H atoms not involved in hydrogen bonds (dashed lines) have been omitted for clarity.

**(*E*)-3-[3-(4-Bromophenyl)-1-phenyl-1*H*-pyrazol-4-yl]-1- (2,4-dichlorophenyl)prop-2-en-1-one**

*Crystal data*

$C_{24}H_{15}BrCl_2N_2O$
$M_r = 498.19$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 11.4203\ (14)$ Å
$b = 9.9357\ (13)$ Å
$c = 19.656\ (3)$ Å
$\beta = 94.653\ (3)°$
$V = 2222.9\ (5)$ Å$^3$
$Z = 4$
$F(000) = 1000$
$D_x = 1.489$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2554 reflections
$\theta = 2.9–22.2°$
$\mu = 2.11$ mm$^{-1}$
$T = 296$ K
Block, colourless
0.38 × 0.21 × 0.11 mm

*Data collection*

Bruker SMART APEXII DUO CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
$T_{min} = 0.504$, $T_{max} = 0.803$
23842 measured reflections
6480 independent reflections
2743 reflections with $I > 2\sigma(I)$
$R_{int} = 0.056$
$\theta_{max} = 30.1°$, $\theta_{min} = 1.8°$
$h = -15\rightarrow16$
$k = -13\rightarrow13$
$l = -27\rightarrow22$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.052$
$wR(F^2) = 0.140$
$S = 0.98$
6480 reflections
271 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
$w = 1/[\sigma^2(F_o^2) + (0.0493P)^2 + 0.6604P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.44$ e Å$^{-3}$
$\Delta\rho_{min} = -0.52$ e Å$^{-3}$

*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 (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| Br1 | 0.29004 (5) | −0.10153 (6) | 0.11448 (2) | 0.1353 (3) |
| O1 | 0.12637 (19) | 0.64502 (19) | 0.42799 (11) | 0.0738 (6) |
| N1 | −0.10263 (19) | 0.0347 (2) | 0.43425 (11) | 0.0521 (5) |
| N2 | −0.05301 (19) | −0.0315 (2) | 0.38311 (10) | 0.0532 (6) |

| | | | | |
|---|---|---|---|---|
| C1 | 0.2092 (3) | 0.4905 (3) | 0.28237 (14) | 0.0621 (7) |
| H1A | 0.1332 | 0.4616 | 0.2693 | 0.075* |
| C2 | 0.2907 (3) | 0.4908 (4) | 0.23478 (16) | 0.0844 (10) |
| H2A | 0.2701 | 0.4629 | 0.1903 | 0.101* |
| C3 | 0.4027 (3) | 0.5329 (5) | 0.2538 (2) | 0.0960 (12) |
| C4 | 0.4336 (3) | 0.5741 (4) | 0.31980 (19) | 0.0865 (11) |
| H4A | 0.5097 | 0.6028 | 0.3325 | 0.104* |
| C5 | 0.3506 (3) | 0.5722 (3) | 0.36638 (15) | 0.0624 (8) |
| C6 | 0.2362 (2) | 0.5316 (3) | 0.34922 (13) | 0.0509 (6) |
| C7 | 0.1426 (2) | 0.5391 (3) | 0.39854 (14) | 0.0535 (7) |
| C8 | 0.0702 (2) | 0.4217 (3) | 0.40921 (15) | 0.0562 (7) |
| H8A | 0.0056 | 0.4330 | 0.4346 | 0.067* |
| C9 | 0.0901 (2) | 0.2988 (3) | 0.38512 (14) | 0.0528 (7) |
| H9A | 0.1547 | 0.2885 | 0.3597 | 0.063* |
| C10 | 0.0198 (2) | 0.1802 (3) | 0.39515 (14) | 0.0510 (6) |
| C11 | −0.0605 (2) | 0.1606 (3) | 0.44253 (14) | 0.0546 (7) |
| H11A | −0.0818 | 0.2231 | 0.4745 | 0.065* |
| C12 | 0.0218 (2) | 0.0567 (3) | 0.35954 (13) | 0.0499 (6) |
| C13 | 0.0901 (2) | 0.0206 (3) | 0.30199 (13) | 0.0513 (6) |
| C14 | 0.1383 (3) | −0.1062 (3) | 0.29778 (16) | 0.0647 (8) |
| H14A | 0.1302 | −0.1678 | 0.3327 | 0.078* |
| C15 | 0.1984 (3) | −0.1429 (3) | 0.24257 (18) | 0.0773 (9) |
| H15A | 0.2302 | −0.2288 | 0.2401 | 0.093* |
| C16 | 0.2106 (3) | −0.0517 (4) | 0.19150 (16) | 0.0771 (10) |
| C17 | 0.1647 (3) | 0.0740 (4) | 0.19476 (17) | 0.0854 (11) |
| H17A | 0.1741 | 0.1356 | 0.1600 | 0.102* |
| C18 | 0.1042 (3) | 0.1099 (3) | 0.24994 (15) | 0.0700 (8) |
| H18A | 0.0724 | 0.1959 | 0.2519 | 0.084* |
| C19 | −0.1936 (2) | −0.0283 (3) | 0.46832 (13) | 0.0538 (7) |
| C20 | −0.2579 (3) | 0.0449 (3) | 0.51087 (17) | 0.0778 (9) |
| H20A | −0.2423 | 0.1359 | 0.5180 | 0.093* |
| C21 | −0.3459 (3) | −0.0174 (4) | 0.54300 (19) | 0.0943 (12) |
| H21A | −0.3899 | 0.0325 | 0.5718 | 0.113* |
| C22 | −0.3699 (3) | −0.1507 (4) | 0.53335 (19) | 0.0871 (10) |
| H22A | −0.4294 | −0.1918 | 0.5554 | 0.105* |
| C23 | −0.3047 (3) | −0.2235 (4) | 0.49049 (19) | 0.0845 (10) |
| H23A | −0.3209 | −0.3142 | 0.4830 | 0.101* |
| C24 | −0.2153 (3) | −0.1630 (3) | 0.45838 (16) | 0.0695 (8) |
| H24A | −0.1702 | −0.2131 | 0.4302 | 0.083* |
| Cl1 | 0.50704 (12) | 0.5349 (2) | 0.19526 (7) | 0.1885 (8) |
| Cl2 | 0.39593 (8) | 0.61893 (11) | 0.44937 (5) | 0.0945 (3) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| Br1 | 0.1461 (4) | 0.1639 (5) | 0.1070 (4) | −0.0726 (3) | 0.0781 (3) | −0.0677 (3) |
| O1 | 0.0941 (15) | 0.0484 (12) | 0.0836 (15) | −0.0100 (11) | 0.0363 (12) | −0.0172 (11) |
| N1 | 0.0620 (14) | 0.0463 (13) | 0.0487 (13) | −0.0033 (11) | 0.0081 (11) | −0.0024 (10) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N2 | 0.0659 (14) | 0.0474 (13) | 0.0470 (12) | −0.0023 (11) | 0.0095 (11) | −0.0052 (10) |
| C1 | 0.0677 (18) | 0.0636 (19) | 0.0544 (17) | 0.0069 (15) | 0.0012 (15) | −0.0050 (14) |
| C2 | 0.094 (3) | 0.111 (3) | 0.0498 (18) | 0.027 (2) | 0.0131 (18) | −0.0086 (18) |
| C3 | 0.077 (3) | 0.145 (4) | 0.070 (2) | 0.030 (2) | 0.029 (2) | 0.007 (2) |
| C4 | 0.061 (2) | 0.122 (3) | 0.078 (2) | 0.0072 (19) | 0.0142 (18) | 0.008 (2) |
| C5 | 0.0647 (19) | 0.069 (2) | 0.0535 (17) | 0.0039 (15) | 0.0037 (15) | 0.0011 (14) |
| C6 | 0.0591 (17) | 0.0442 (15) | 0.0496 (15) | 0.0033 (13) | 0.0059 (13) | −0.0035 (12) |
| C7 | 0.0624 (17) | 0.0453 (16) | 0.0533 (16) | −0.0009 (13) | 0.0083 (13) | −0.0038 (13) |
| C8 | 0.0584 (17) | 0.0479 (17) | 0.0641 (18) | −0.0018 (13) | 0.0156 (14) | −0.0037 (13) |
| C9 | 0.0557 (16) | 0.0499 (17) | 0.0529 (16) | −0.0017 (13) | 0.0058 (13) | −0.0014 (13) |
| C10 | 0.0548 (16) | 0.0441 (16) | 0.0539 (16) | −0.0021 (12) | 0.0032 (13) | −0.0049 (12) |
| C11 | 0.0648 (17) | 0.0405 (16) | 0.0590 (17) | −0.0009 (13) | 0.0086 (14) | −0.0088 (12) |
| C12 | 0.0584 (16) | 0.0434 (16) | 0.0476 (15) | 0.0007 (13) | 0.0028 (13) | 0.0002 (12) |
| C13 | 0.0616 (16) | 0.0436 (16) | 0.0487 (15) | −0.0071 (13) | 0.0037 (13) | −0.0040 (12) |
| C14 | 0.077 (2) | 0.0516 (19) | 0.0670 (19) | −0.0017 (15) | 0.0178 (16) | 0.0001 (14) |
| C15 | 0.089 (2) | 0.060 (2) | 0.087 (2) | −0.0033 (17) | 0.034 (2) | −0.0154 (18) |
| C16 | 0.083 (2) | 0.086 (3) | 0.065 (2) | −0.0349 (19) | 0.0275 (17) | −0.0257 (18) |
| C17 | 0.126 (3) | 0.079 (3) | 0.0539 (19) | −0.032 (2) | 0.021 (2) | 0.0017 (17) |
| C18 | 0.099 (2) | 0.0571 (19) | 0.0543 (18) | −0.0068 (17) | 0.0096 (17) | 0.0015 (14) |
| C19 | 0.0604 (17) | 0.0539 (17) | 0.0463 (15) | −0.0079 (14) | −0.0007 (13) | 0.0022 (13) |
| C20 | 0.089 (2) | 0.065 (2) | 0.084 (2) | −0.0081 (17) | 0.0355 (19) | −0.0082 (17) |
| C21 | 0.093 (3) | 0.096 (3) | 0.100 (3) | −0.016 (2) | 0.045 (2) | −0.012 (2) |
| C22 | 0.084 (2) | 0.098 (3) | 0.082 (2) | −0.030 (2) | 0.020 (2) | 0.003 (2) |
| C23 | 0.093 (2) | 0.076 (2) | 0.084 (2) | −0.032 (2) | 0.006 (2) | −0.0035 (19) |
| C24 | 0.084 (2) | 0.061 (2) | 0.0650 (19) | −0.0174 (17) | 0.0129 (17) | −0.0086 (15) |
| Cl1 | 0.1164 (9) | 0.351 (2) | 0.1079 (9) | 0.0464 (13) | 0.0678 (8) | 0.0086 (13) |
| Cl2 | 0.0853 (6) | 0.1270 (8) | 0.0694 (6) | −0.0180 (5) | −0.0044 (5) | −0.0168 (5) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| Br1—C16 | 1.893 (3) | C10—C12 | 1.414 (4) |
| O1—C7 | 1.222 (3) | C11—H11A | 0.9300 |
| N1—C11 | 1.346 (3) | C12—C13 | 1.469 (4) |
| N1—N2 | 1.363 (3) | C13—C18 | 1.374 (4) |
| N1—C19 | 1.425 (3) | C13—C14 | 1.380 (4) |
| N2—C12 | 1.333 (3) | C14—C15 | 1.379 (4) |
| C1—C2 | 1.372 (4) | C14—H14A | 0.9300 |
| C1—C6 | 1.387 (4) | C15—C16 | 1.368 (5) |
| C1—H1A | 0.9300 | C15—H15A | 0.9300 |
| C2—C3 | 1.369 (5) | C16—C17 | 1.358 (5) |
| C2—H2A | 0.9300 | C17—C18 | 1.380 (4) |
| C3—C4 | 1.378 (5) | C17—H17A | 0.9300 |
| C3—Cl1 | 1.723 (3) | C18—H18A | 0.9300 |
| C4—C5 | 1.370 (4) | C19—C20 | 1.367 (4) |
| C4—H4A | 0.9300 | C19—C24 | 1.373 (4) |
| C5—C6 | 1.384 (4) | C20—C21 | 1.377 (4) |
| C5—Cl2 | 1.734 (3) | C20—H20A | 0.9300 |
| C6—C7 | 1.502 (4) | C21—C22 | 1.363 (5) |

| | | | |
|---|---|---|---|
| C7—C8 | 1.455 (4) | C21—H21A | 0.9300 |
| C8—C9 | 1.336 (4) | C22—C23 | 1.374 (5) |
| C8—H8A | 0.9300 | C22—H22A | 0.9300 |
| C9—C10 | 1.448 (4) | C23—C24 | 1.380 (4) |
| C9—H9A | 0.9300 | C23—H23A | 0.9300 |
| C10—C11 | 1.373 (4) | C24—H24A | 0.9300 |

| | | | |
|---|---|---|---|
| C11—N1—N2 | 111.8 (2) | N2—C12—C13 | 120.2 (2) |
| C11—N1—C19 | 128.2 (2) | C10—C12—C13 | 128.6 (2) |
| N2—N1—C19 | 119.8 (2) | C18—C13—C14 | 118.3 (3) |
| C12—N2—N1 | 104.8 (2) | C18—C13—C12 | 121.1 (3) |
| C2—C1—C6 | 122.3 (3) | C14—C13—C12 | 120.5 (2) |
| C2—C1—H1A | 118.8 | C15—C14—C13 | 121.0 (3) |
| C6—C1—H1A | 118.8 | C15—C14—H14A | 119.5 |
| C3—C2—C1 | 119.0 (3) | C13—C14—H14A | 119.5 |
| C3—C2—H2A | 120.5 | C16—C15—C14 | 119.3 (3) |
| C1—C2—H2A | 120.5 | C16—C15—H15A | 120.4 |
| C2—C3—C4 | 120.7 (3) | C14—C15—H15A | 120.4 |
| C2—C3—Cl1 | 120.2 (3) | C17—C16—C15 | 120.8 (3) |
| C4—C3—Cl1 | 119.2 (3) | C17—C16—Br1 | 119.4 (3) |
| C5—C4—C3 | 119.1 (3) | C15—C16—Br1 | 119.8 (3) |
| C5—C4—H4A | 120.4 | C16—C17—C18 | 119.7 (3) |
| C3—C4—H4A | 120.4 | C16—C17—H17A | 120.2 |
| C4—C5—C6 | 122.1 (3) | C18—C17—H17A | 120.2 |
| C4—C5—Cl2 | 117.1 (3) | C13—C18—C17 | 121.0 (3) |
| C6—C5—Cl2 | 120.7 (2) | C13—C18—H18A | 119.5 |
| C5—C6—C1 | 116.7 (3) | C17—C18—H18A | 119.5 |
| C5—C6—C7 | 122.4 (2) | C20—C19—C24 | 120.4 (3) |
| C1—C6—C7 | 120.8 (2) | C20—C19—N1 | 120.1 (3) |
| O1—C7—C8 | 120.8 (3) | C24—C19—N1 | 119.5 (3) |
| O1—C7—C6 | 119.4 (2) | C19—C20—C21 | 119.3 (3) |
| C8—C7—C6 | 119.7 (2) | C19—C20—H20A | 120.3 |
| C9—C8—C7 | 124.5 (3) | C21—C20—H20A | 120.3 |
| C9—C8—H8A | 117.7 | C22—C21—C20 | 121.3 (3) |
| C7—C8—H8A | 117.7 | C22—C21—H21A | 119.4 |
| C8—C9—C10 | 125.7 (3) | C20—C21—H21A | 119.4 |
| C8—C9—H9A | 117.2 | C21—C22—C23 | 119.0 (3) |
| C10—C9—H9A | 117.2 | C21—C22—H22A | 120.5 |
| C11—C10—C12 | 104.6 (2) | C23—C22—H22A | 120.5 |
| C11—C10—C9 | 128.0 (2) | C22—C23—C24 | 120.6 (3) |
| C12—C10—C9 | 127.4 (2) | C22—C23—H23A | 119.7 |
| N1—C11—C10 | 107.6 (2) | C24—C23—H23A | 119.7 |
| N1—C11—H11A | 126.2 | C19—C24—C23 | 119.4 (3) |
| C10—C11—H11A | 126.2 | C19—C24—H24A | 120.3 |
| N2—C12—C10 | 111.2 (2) | C23—C24—H24A | 120.3 |

| | | | |
|---|---|---|---|
| C11—N1—N2—C12 | 0.1 (3) | C11—C10—C12—N2 | 0.7 (3) |
| C19—N1—N2—C12 | 176.1 (2) | C9—C10—C12—N2 | 178.7 (2) |

| | | | |
|---|---|---|---|
| C6—C1—C2—C3 | 0.1 (5) | C11—C10—C12—C13 | 178.5 (3) |
| C1—C2—C3—C4 | 0.1 (6) | C9—C10—C12—C13 | −3.5 (4) |
| C1—C2—C3—Cl1 | −179.9 (3) | N2—C12—C13—C18 | 136.9 (3) |
| C2—C3—C4—C5 | 0.1 (6) | C10—C12—C13—C18 | −40.7 (4) |
| Cl1—C3—C4—C5 | −179.8 (3) | N2—C12—C13—C14 | −40.7 (4) |
| C3—C4—C5—C6 | −0.7 (5) | C10—C12—C13—C14 | 141.6 (3) |
| C3—C4—C5—Cl2 | 177.6 (3) | C18—C13—C14—C15 | −0.5 (5) |
| C4—C5—C6—C1 | 1.0 (4) | C12—C13—C14—C15 | 177.3 (3) |
| Cl2—C5—C6—C1 | −177.2 (2) | C13—C14—C15—C16 | 0.3 (5) |
| C4—C5—C6—C7 | −175.3 (3) | C14—C15—C16—C17 | 0.2 (5) |
| Cl2—C5—C6—C7 | 6.5 (4) | C14—C15—C16—Br1 | −178.7 (2) |
| C2—C1—C6—C5 | −0.7 (4) | C15—C16—C17—C18 | −0.6 (5) |
| C2—C1—C6—C7 | 175.6 (3) | Br1—C16—C17—C18 | 178.4 (2) |
| C5—C6—C7—O1 | 51.9 (4) | C14—C13—C18—C17 | 0.1 (5) |
| C1—C6—C7—O1 | −124.2 (3) | C12—C13—C18—C17 | −177.6 (3) |
| C5—C6—C7—C8 | −129.9 (3) | C16—C17—C18—C13 | 0.4 (5) |
| C1—C6—C7—C8 | 54.0 (4) | C11—N1—C19—C20 | 6.9 (4) |
| O1—C7—C8—C9 | −172.3 (3) | N2—N1—C19—C20 | −168.4 (3) |
| C6—C7—C8—C9 | 9.5 (4) | C11—N1—C19—C24 | −172.7 (3) |
| C7—C8—C9—C10 | 179.8 (3) | N2—N1—C19—C24 | 12.0 (4) |
| C8—C9—C10—C11 | −16.9 (5) | C24—C19—C20—C21 | −0.9 (5) |
| C8—C9—C10—C12 | 165.5 (3) | N1—C19—C20—C21 | 179.6 (3) |
| N2—N1—C11—C10 | 0.3 (3) | C19—C20—C21—C22 | 0.2 (6) |
| C19—N1—C11—C10 | −175.3 (2) | C20—C21—C22—C23 | −0.2 (6) |
| C12—C10—C11—N1 | −0.6 (3) | C21—C22—C23—C24 | 0.8 (6) |
| C9—C10—C11—N1 | −178.6 (2) | C20—C19—C24—C23 | 1.5 (5) |
| N1—N2—C12—C10 | −0.5 (3) | N1—C19—C24—C23 | −178.9 (3) |
| N1—N2—C12—C13 | −178.5 (2) | C22—C23—C24—C19 | −1.5 (5) |

*Hydrogen-bond geometry (Å, º)*

Cg1 is the centroid of C1–C6 phenyl ring.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11*A*···O1$^{i}$ | 0.93 | 2.41 | 3.329 (4) | 170 |
| C15—H15*A*···*Cg*1$^{ii}$ | 0.93 | 2.82 | 3.666 (3) | 152 |

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