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# Crystal structure of (*E*)-*N*-(3,3-diphenylallylidene)-9-ethyl-9*H*-carbazol-3-amine

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In the title compound, $C_{29}H_{24}N_2$, the C=N bond of the central imine group adopts an *E* conformation. The dihedral angles between the mean plane of the essentially planar carbazole ring system [r.m.s. deviation = 0.039 (2) Å] and the two phenyl rings of the 3,3-diphenylallylidene unit are 75.9 (1) and 64.6 (1)°. In the crystal, molecules are linked by C—H···$\pi$ interactions, forming a three-dimensional supramolecular network.

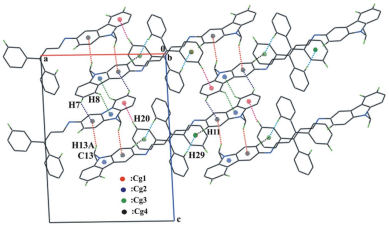
**Keywords**: crystal structure; carbazole; 9-ethyl-9*H*-carbazol-3-amine; C—H···$\pi$ interactions

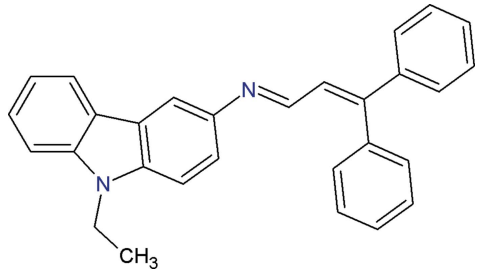
**CCDC reference**: 967497

**Supporting information**: this article has supporting information at journals.iucr.org/e

## 1. Chemical context

Carbazole and its derivatives have become quite attractive compounds owing to their applications in pharmacy and molecular electronics. It has been reported that carbazole derivatives possess various biological activities, such as anti-tumor (Itoigawa *et al.*, 2000), anti-oxidative (Tachibana *et al.*, 2001), anti-inflammatory and antimutagenic (Ramsewak *et al.*, 1999). Carbazole derivatives also exhibit electroactivity and luminescence properties and are considered to be potential candidates for electronic devices such as colour displays, organic semiconductor lasers and solar cells (Friend *et al.*, 1999). These compounds are thermally and photochemically stable, which makes them useful materials for technological applications. For instance, the carbazole ring is easily funtionalized and covalently linked to other molecules (Díaz *et al.*, 2002). This enables its use as a convenient building block for the design and synthesis of molecular glasses, which are widely studied as components of electroactive and photoactive materials (Zhang *et al.*, 2004). Against this background, and in order to obtain detailed information on molecular conformations in the solid state, X-ray studies of the title compound have been carried out.




## 2. Structural commentary

The molecular structure of the title compound is illustrated in Fig. 1. The C15=N2 bond of the central imine group adopts an *E* conformation. The carbazole ring system (N1/C1–C12) is

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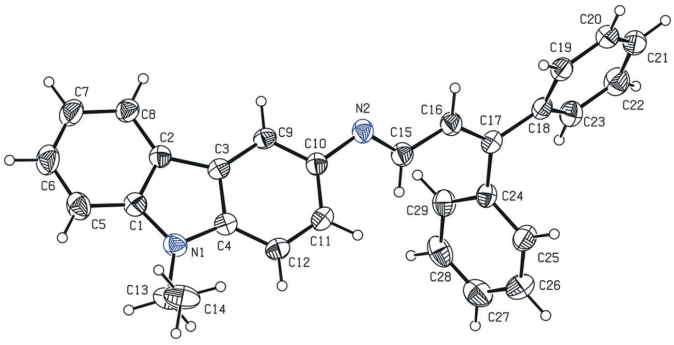


**Figure 1**
Molecular structure of the title compound with the atom labelling. Displacement ellipsoids are drawn at the 30% probability level.

essentially planar [maximum deviation = 0.039 (2) Å for atom C9]. The phenyl rings C18–C23 and C24–C29 of the (3,3-diphenylallylidene) unit are oriented at dihedral angles of 75.9 (1) and 64.6 (1)°, respectively, to the mean plane of the carbazole ring system. The dihedral angle between the two phenyl rings is 76.1 (1)°. The sum of the bond angles around atom N1 (359.7°) of the pyrrole ring is in accordance with $sp^2$ hybridization. The geometric parameters of the title molecule agree well with those reported for similar structures (Murugavel *et al.*, 2009; Archana *et al.*, 2011).

## 3. Supramolecular features

In the crystal, molecules are linked by six intermolecular C—H···$\pi$ interactions, forming a three-dimensional supramolecular network (Table 1 and Fig. 2). Four of these interactions involves a benzene H atom of the carbazole ring system and a benzene ring of an adjacent molecule, *viz.* C7—H7···*Cg*1$^{i}$, C11—H11···*Cg*3$^{ii}$, C20—H20···*Cg*4$^{iv}$, and C29—H29···*Cg*3$^{v}$. The other two involve a benzene H atom of the carbazole ring system and the pyrrole ring of an adjacent molecule (C8—H8···*Cg*2$^{i}$), and a methylene H atom of the ethyl group and a benzene ring of an adjacent molecule (C13—H13*A*···*Cg*1$^{iii}$); see Table 1 and Fig. 2 for full details.

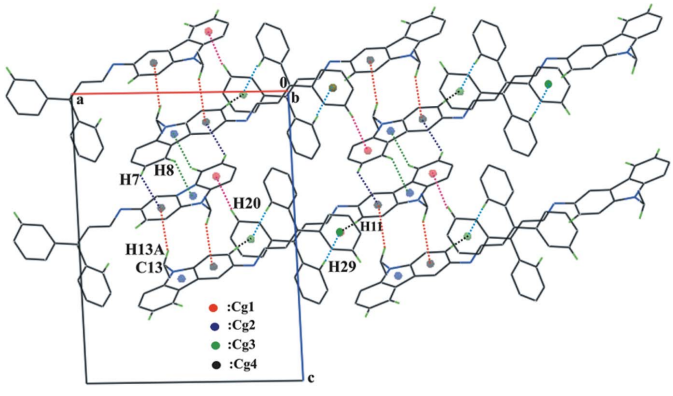


**Figure 2**
A partial view along the *b* axis of the crystal packing of the title compound, showing the intermolecular C—H···$\pi$ interactions (see Table 1 for details), forming a three-dimensional supramolecular network. H atoms not involved in these interactions have been omitted for clarity.

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

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings C3/C4/C9–C12, N1/C1–C4, C18–C23 and C1/C2/C5–C8, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···*Cg*1$^{i}$ | 0.93 | 2.92 | 3.647 (2) | 136 |
| C8—H8···*Cg*2$^{i}$ | 0.93 | 2.98 | 3.777 (2) | 145 |
| C11—H11···*Cg*3$^{ii}$ | 0.93 | 2.85 | 3.551 (2) | 133 |
| C13—H13*A*···*Cg*1$^{iii}$ | 0.97 | 3.00 | 3.749 (2) | 135 |
| C20—H20···*Cg*4$^{iv}$ | 0.93 | 2.62 | 3.498 (2) | 157 |
| C29—H29···*Cg*3$^{v}$ | 0.93 | 2.87 | 3.796 (3) | 175 |

Symmetry codes: (i) $-x+1, y-\frac{1}{2}, -z+\frac{1}{2}$; (ii) $-x, -y+2, -z$; (iii) $-x+1, -y+2, -z$; (iv) $x-1, y, z$; (v) $-x, -y+1, -z$.

## 4. Synthesis and crystallization

A 25 ml round-bottom flask was charged with 9-ethyl-9*H*-carbazol-3-amine (1 mmol), 3,3-diphenylacrylaldehyde (1 mmol) and sulfated $SnO_2$-$Bi_2O_3$-fly ash catalyst (20 mg) in water (15 ml) and the mixture was refluxed at 363 K for 1h. On completion of the reaction (monitored by TLC with ethyl acetate and hexane as an eluent 20%) the mixture was cooled to ambient temperature. Dichloromethane (20 ml) was then added to separate the organic and aqueous layers. The organic

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{29}H_{24}N_2$ |
| $M_r$ | 400.50 |
| Crystal system, space group | Monoclinic, $P2_1/c$ |
| Temperature (K) | 293 |
| *a*, *b*, *c* (Å) | 13.6502 (17), 8.7616 (13), 18.224 (2) |
| $\beta$ (°) | 92.234 (11) |
| $V$ (Å$^3$) | 2177.9 (5) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.07 |
| Crystal size (mm) | 0.23 × 0.21 × 0.15 |
| Data collection | |
| Diffractometer | Bruker SMART CCD area detector |
| Absorption correction | Multi-scan (*SADABS*; Sheldrick, 1996) |
| $T_{min}$, $T_{max}$ | 0.984, 0.989 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 9709, 4982, 3066 |
| $R_{int}$ | 0.047 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.688 |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.056, 0.150, 1.03 |
| No. of reflections | 4982 |
| No. of parameters | 280 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.17, −0.19 |

Computer programs: *SMART* and *SAINT* (Bruker, 2002), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia (2012) and *PLATON* (Spek, 2009).

layer was filtered, dried on anhydrous $Na_2SO_4$ and the solvent removed using a rotary evaporator. The crude product obtained was purified by column chromatography on silica gel (200 mesh) with hexane and ethyl acetate (4:1) as eluent, to afford the title compound in good yield (93%). Red crystals suitable for X-ray diffraction analysis were obtained after recrystallization in $CH_2Cl_2$.

## 5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms were positioned geometrically and constrained to ride on their parent atom with C—H = 0.93–0.97 Å and with $U_{iso}(H) = 1.5U_{eq}$ for methyl H atoms and $1.2U_{eq}(C)$ for other H atoms.

## Acknowledgements

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# supporting information

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## Crystal structure of (*E*)-*N*-(3,3-diphenylallylidene)-9-ethyl-9*H*-carbazol-3-amine

**Kannan Thirumurthy, Ganesamoorthy Thirunarayanan and S. Murugavel**

### Computing details

Data collection: *SMART* (Bruker, 2002); cell refinement: *SAINT* (Bruker, 2002); data reduction: *SAINT* (Bruker, 2002); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3 for Windows* (Farrugia (2012); software used to prepare material for publication: *SHELXL97* (Sheldrick, 2008) and *PLATON* (Spek, 2009).

### (*E*)-*N*-(3,3-Diphenylallylidene)-9-ethyl-9*H*-carbazol-3-amine

*Crystal data*

$C_{29}H_{24}N_2$
$M_r = 400.50$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 13.6502$ (17) Å
$b = 8.7616$ (13) Å
$c = 18.224$ (2) Å
$\beta = 92.234$ (11)°
$V = 2177.9$ (5) Å$^3$
$Z = 4$
$F(000) = 848$
$D_x = 1.221$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5927 reflections
$\theta = 2.8$–29.3°
$\mu = 0.07$ mm$^{-1}$
$T = 293$ K
Block, red
0.23 × 0.21 × 0.15 mm

*Data collection*

Bruker SMART CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\varphi$ and $\omega$ scans
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
$T_{min} = 0.984$, $T_{max} = 0.989$
9709 measured reflections
4982 independent reflections
3066 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 29.3°$, $\theta_{min} = 2.8°$
$h = -15 \rightarrow 18$
$k = -11 \rightarrow 11$
$l = -24 \rightarrow 23$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.150$
$S = 1.03$
4982 reflections
280 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
$w = 1/[\sigma^2(F_o^2) + (0.0555P)^2 + 0.1709P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.17$ e Å$^{-3}$
$\Delta\rho_{min} = -0.19$ 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 $F^2 > 2\text{sigma}(F^2)$ 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* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| C14 | 0.5899 (2) | 1.3222 (3) | 0.14013 (13) | 0.0822 (7) |
| H14A | 0.6192 | 1.4132 | 0.1215 | 0.123* |
| H14B | 0.6144 | 1.3041 | 0.1894 | 0.123* |
| H14C | 0.5200 | 1.3346 | 0.1399 | 0.123* |
| N2 | 0.19996 (10) | 0.8129 (2) | 0.10030 (8) | 0.0516 (4) |
| C10 | 0.29431 (12) | 0.8778 (2) | 0.09957 (9) | 0.0454 (4) |
| C9 | 0.36711 (12) | 0.8093 (2) | 0.14234 (9) | 0.0449 (4) |
| H9 | 0.3538 | 0.7226 | 0.1696 | 0.054* |
| C4 | 0.47794 (13) | 1.0054 (2) | 0.10553 (9) | 0.0462 (4) |
| C3 | 0.46026 (12) | 0.8713 (2) | 0.14420 (9) | 0.0427 (4) |
| N1 | 0.57338 (11) | 1.04985 (18) | 0.11800 (8) | 0.0530 (4) |
| C12 | 0.40455 (14) | 1.0746 (2) | 0.06391 (10) | 0.0530 (5) |
| H12 | 0.4166 | 1.1636 | 0.0380 | 0.064* |
| C11 | 0.31382 (14) | 1.0100 (2) | 0.06153 (10) | 0.0518 (5) |
| H11 | 0.2636 | 1.0560 | 0.0336 | 0.062* |
| C19 | −0.16510 (13) | 0.7140 (2) | 0.04772 (10) | 0.0533 (5) |
| H19 | −0.1369 | 0.7691 | 0.0867 | 0.064* |
| C15 | 0.14631 (13) | 0.8153 (2) | 0.04164 (10) | 0.0529 (5) |
| H15 | 0.1714 | 0.8548 | −0.0011 | 0.063* |
| C2 | 0.55154 (13) | 0.8316 (2) | 0.18155 (9) | 0.0455 (4) |
| C18 | −0.11167 (13) | 0.6882 (2) | −0.01430 (10) | 0.0471 (4) |
| C1 | 0.61869 (13) | 0.9460 (2) | 0.16451 (10) | 0.0510 (5) |
| C16 | 0.04842 (13) | 0.7586 (3) | 0.04026 (10) | 0.0553 (5) |
| H16 | 0.0230 | 0.7319 | 0.0851 | 0.066* |
| C23 | −0.15719 (14) | 0.6089 (2) | −0.07131 (11) | 0.0588 (5) |
| H23 | −0.1235 | 0.5911 | −0.1139 | 0.071* |
| C20 | −0.25842 (14) | 0.6598 (3) | 0.05254 (12) | 0.0614 (6) |
| H20 | −0.2930 | 0.6772 | 0.0947 | 0.074* |
| C24 | 0.02709 (12) | 0.7604 (2) | −0.09425 (9) | 0.0477 (5) |
| C13 | 0.61468 (15) | 1.1902 (2) | 0.09293 (11) | 0.0614 (5) |
| H13A | 0.5906 | 1.2099 | 0.0430 | 0.074* |
| H13B | 0.6854 | 1.1800 | 0.0923 | 0.074* |
| C8 | 0.58185 (14) | 0.7119 (2) | 0.22603 (10) | 0.0550 (5) |
| H8 | 0.5385 | 0.6343 | 0.2374 | 0.066* |
| C29 | 0.10181 (14) | 0.6715 (3) | −0.11811 (11) | 0.0592 (5) |

| | | | | |
|---|---|---|---|---|
| H29 | 0.1314 | 0.6011 | −0.0862 | 0.071* |
| C28 | 0.13409 (15) | 0.6844 (3) | −0.18854 (13) | 0.0714 (7) |
| H28 | 0.1846 | 0.6220 | −0.2037 | 0.086* |
| C5 | 0.71384 (14) | 0.9426 (3) | 0.19254 (11) | 0.0666 (6) |
| H5 | 0.7580 | 1.0194 | 0.1817 | 0.080* |
| C22 | −0.25053 (16) | 0.5561 (3) | −0.06653 (13) | 0.0688 (6) |
| H22 | −0.2800 | 0.5034 | −0.1058 | 0.083* |
| C25 | −0.01406 (15) | 0.8636 (3) | −0.14288 (11) | 0.0639 (6) |
| H25 | −0.0655 | 0.9249 | −0.1284 | 0.077* |
| C21 | −0.30082 (16) | 0.5802 (3) | −0.00460 (13) | 0.0675 (6) |
| H21 | −0.3641 | 0.5423 | −0.0012 | 0.081* |
| C27 | 0.09292 (18) | 0.7869 (3) | −0.23570 (12) | 0.0767 (7) |
| H27 | 0.1145 | 0.7952 | −0.2833 | 0.092* |
| C6 | 0.74105 (16) | 0.8237 (3) | 0.23656 (12) | 0.0746 (7) |
| H6 | 0.8050 | 0.8196 | 0.2560 | 0.089* |
| C26 | 0.01946 (18) | 0.8779 (3) | −0.21270 (12) | 0.0784 (7) |
| H26 | −0.0083 | 0.9503 | −0.2445 | 0.094* |
| C7 | 0.67657 (16) | 0.7091 (3) | 0.25318 (11) | 0.0699 (6) |
| H7 | 0.6977 | 0.6289 | 0.2832 | 0.084* |
| C17 | −0.00988 (13) | 0.7403 (2) | −0.01930 (9) | 0.0478 (4) |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| C14 | 0.116 (2) | 0.0536 (15) | 0.0788 (15) | −0.0230 (14) | 0.0288 (14) | −0.0040 (12) |
| N2 | 0.0456 (9) | 0.0658 (12) | 0.0433 (8) | 0.0018 (8) | −0.0019 (7) | −0.0031 (8) |
| C10 | 0.0456 (10) | 0.0533 (12) | 0.0372 (9) | 0.0019 (8) | 0.0004 (7) | −0.0053 (8) |
| C9 | 0.0533 (11) | 0.0435 (11) | 0.0377 (9) | −0.0022 (8) | −0.0017 (8) | −0.0005 (8) |
| C4 | 0.0522 (11) | 0.0419 (11) | 0.0444 (9) | 0.0002 (8) | 0.0019 (8) | −0.0038 (8) |
| C3 | 0.0499 (10) | 0.0401 (10) | 0.0380 (9) | 0.0004 (8) | −0.0001 (7) | −0.0022 (8) |
| N1 | 0.0532 (9) | 0.0478 (10) | 0.0578 (9) | −0.0083 (8) | 0.0017 (7) | −0.0004 (8) |
| C12 | 0.0614 (12) | 0.0441 (12) | 0.0535 (11) | 0.0019 (9) | 0.0023 (9) | 0.0054 (9) |
| C11 | 0.0568 (11) | 0.0526 (12) | 0.0455 (10) | 0.0101 (9) | −0.0034 (8) | 0.0013 (9) |
| C19 | 0.0526 (11) | 0.0567 (13) | 0.0504 (10) | 0.0044 (9) | −0.0021 (8) | 0.0045 (9) |
| C15 | 0.0484 (10) | 0.0683 (14) | 0.0418 (10) | 0.0015 (9) | −0.0006 (8) | −0.0023 (9) |
| C2 | 0.0482 (10) | 0.0488 (11) | 0.0393 (9) | 0.0001 (8) | 0.0002 (7) | −0.0041 (8) |
| C18 | 0.0471 (10) | 0.0461 (11) | 0.0474 (10) | 0.0048 (8) | −0.0057 (8) | 0.0054 (8) |
| C1 | 0.0532 (11) | 0.0524 (12) | 0.0472 (10) | −0.0032 (9) | −0.0009 (8) | −0.0064 (9) |
| C16 | 0.0472 (10) | 0.0735 (15) | 0.0451 (10) | 0.0008 (10) | −0.0007 (8) | 0.0036 (10) |
| C23 | 0.0559 (12) | 0.0603 (14) | 0.0596 (12) | 0.0007 (10) | −0.0046 (9) | −0.0024 (10) |
| C20 | 0.0531 (12) | 0.0642 (15) | 0.0671 (13) | 0.0050 (10) | 0.0057 (10) | 0.0154 (11) |
| C24 | 0.0446 (10) | 0.0522 (12) | 0.0459 (10) | 0.0039 (9) | −0.0039 (8) | −0.0050 (9) |
| C13 | 0.0704 (13) | 0.0566 (14) | 0.0584 (12) | −0.0141 (11) | 0.0164 (10) | 0.0004 (10) |
| C8 | 0.0571 (11) | 0.0621 (14) | 0.0456 (10) | 0.0048 (10) | 0.0005 (8) | 0.0032 (9) |
| C29 | 0.0545 (12) | 0.0603 (14) | 0.0626 (12) | 0.0056 (10) | 0.0008 (9) | −0.0078 (10) |
| C28 | 0.0530 (12) | 0.0880 (19) | 0.0741 (15) | −0.0027 (12) | 0.0132 (11) | −0.0268 (14) |
| C5 | 0.0539 (12) | 0.0804 (17) | 0.0649 (13) | −0.0121 (11) | −0.0057 (10) | −0.0085 (12) |
| C22 | 0.0697 (14) | 0.0616 (15) | 0.0738 (14) | −0.0076 (11) | −0.0155 (12) | −0.0035 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C25 | 0.0635 (13) | 0.0712 (15) | 0.0568 (12) | 0.0143 (11) | −0.0012 (10) | 0.0049 (11) |
| C21 | 0.0553 (12) | 0.0585 (15) | 0.0879 (16) | −0.0069 (10) | −0.0070 (12) | 0.0194 (13) |
| C27 | 0.0734 (15) | 0.108 (2) | 0.0490 (12) | −0.0204 (15) | 0.0074 (11) | −0.0124 (13) |
| C6 | 0.0600 (13) | 0.101 (2) | 0.0610 (13) | 0.0021 (13) | −0.0172 (11) | −0.0034 (14) |
| C26 | 0.0879 (17) | 0.092 (2) | 0.0542 (13) | 0.0018 (15) | −0.0057 (12) | 0.0154 (13) |
| C7 | 0.0667 (14) | 0.0886 (18) | 0.0534 (12) | 0.0103 (13) | −0.0094 (10) | 0.0095 (12) |
| C17 | 0.0488 (10) | 0.0488 (12) | 0.0454 (10) | 0.0066 (9) | −0.0037 (8) | 0.0012 (9) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| C14—C13 | 1.488 (3) | C18—C23 | 1.378 (3) |
| N2—C15 | 1.272 (2) | C18—C17 | 1.469 (2) |
| N2—C10 | 1.408 (2) | C1—C5 | 1.377 (3) |
| C10—C9 | 1.376 (2) | C16—C17 | 1.330 (2) |
| C10—C11 | 1.381 (3) | C23—C22 | 1.361 (3) |
| C9—C3 | 1.382 (2) | C20—C21 | 1.364 (3) |
| C4—N1 | 1.370 (2) | C24—C29 | 1.367 (3) |
| C4—C12 | 1.374 (2) | C24—C25 | 1.371 (3) |
| C4—C3 | 1.396 (3) | C24—C17 | 1.485 (2) |
| C3—C2 | 1.439 (2) | C8—C7 | 1.367 (3) |
| N1—C1 | 1.374 (2) | C29—C28 | 1.378 (3) |
| N1—C13 | 1.435 (2) | C28—C27 | 1.351 (3) |
| C12—C11 | 1.361 (3) | C5—C6 | 1.358 (3) |
| C19—C20 | 1.365 (3) | C22—C21 | 1.360 (3) |
| C19—C18 | 1.387 (3) | C25—C26 | 1.375 (3) |
| C15—C16 | 1.425 (2) | C27—C26 | 1.360 (3) |
| C2—C8 | 1.379 (3) | C6—C7 | 1.377 (3) |
| C2—C1 | 1.401 (3) | | |
| | | | |
| C15—N2—C10 | 118.81 (16) | N1—C1—C5 | 129.66 (19) |
| C9—C10—C11 | 120.03 (17) | N1—C1—C2 | 109.14 (15) |
| C9—C10—N2 | 117.33 (17) | C5—C1—C2 | 121.20 (19) |
| C11—C10—N2 | 122.53 (16) | C17—C16—C15 | 125.96 (18) |
| C10—C9—C3 | 119.10 (17) | C22—C23—C18 | 121.2 (2) |
| N1—C4—C12 | 129.36 (18) | C21—C20—C19 | 119.9 (2) |
| N1—C4—C3 | 109.73 (15) | C29—C24—C25 | 117.50 (18) |
| C12—C4—C3 | 120.90 (17) | C29—C24—C17 | 120.63 (17) |
| C9—C3—C4 | 119.69 (16) | C25—C24—C17 | 121.82 (17) |
| C9—C3—C2 | 134.08 (17) | N1—C13—C14 | 112.39 (17) |
| C4—C3—C2 | 106.19 (16) | C7—C8—C2 | 119.0 (2) |
| C4—N1—C1 | 108.43 (15) | C24—C29—C28 | 121.3 (2) |
| C4—N1—C13 | 125.00 (17) | C27—C28—C29 | 120.4 (2) |
| C1—N1—C13 | 126.23 (16) | C6—C5—C1 | 117.9 (2) |
| C11—C12—C4 | 118.49 (18) | C21—C22—C23 | 120.3 (2) |
| C12—C11—C10 | 121.74 (17) | C24—C25—C26 | 121.0 (2) |
| C20—C19—C18 | 121.14 (19) | C22—C21—C20 | 120.0 (2) |
| N2—C15—C16 | 121.17 (18) | C28—C27—C26 | 119.2 (2) |
| C8—C2—C1 | 119.35 (17) | C5—C6—C7 | 121.8 (2) |

| | | | |
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| C8—C2—C3 | 134.14 (18) | C27—C26—C25 | 120.5 (2) |
| C1—C2—C3 | 106.50 (16) | C8—C7—C6 | 120.7 (2) |
| C23—C18—C19 | 117.43 (18) | C16—C17—C18 | 121.61 (17) |
| C23—C18—C17 | 120.66 (17) | C16—C17—C24 | 121.49 (17) |
| C19—C18—C17 | 121.91 (16) | C18—C17—C24 | 116.75 (15) |
| | | | |
| C15—N2—C10—C9 | −145.48 (18) | N2—C15—C16—C17 | −172.1 (2) |
| C15—N2—C10—C11 | 38.4 (3) | C19—C18—C23—C22 | −0.9 (3) |
| C11—C10—C9—C3 | −2.6 (3) | C17—C18—C23—C22 | 178.05 (19) |
| N2—C10—C9—C3 | −178.80 (15) | C18—C19—C20—C21 | −0.7 (3) |
| C10—C9—C3—C4 | 2.9 (2) | C4—N1—C13—C14 | 79.5 (2) |
| C10—C9—C3—C2 | 179.98 (18) | C1—N1—C13—C14 | −93.1 (2) |
| N1—C4—C3—C9 | 177.03 (15) | C1—C2—C8—C7 | 0.8 (3) |
| C12—C4—C3—C9 | −1.8 (3) | C3—C2—C8—C7 | 180.0 (2) |
| N1—C4—C3—C2 | −0.8 (2) | C25—C24—C29—C28 | −0.5 (3) |
| C12—C4—C3—C2 | −179.66 (16) | C17—C24—C29—C28 | 177.20 (19) |
| C12—C4—N1—C1 | 178.78 (19) | C24—C29—C28—C27 | 0.7 (3) |
| C3—C4—N1—C1 | 0.1 (2) | N1—C1—C5—C6 | −178.4 (2) |
| C12—C4—N1—C13 | 5.1 (3) | C2—C1—C5—C6 | 0.8 (3) |
| C3—C4—N1—C13 | −173.63 (17) | C18—C23—C22—C21 | −0.4 (3) |
| N1—C4—C12—C11 | −178.20 (17) | C29—C24—C25—C26 | −0.6 (3) |
| C3—C4—C12—C11 | 0.4 (3) | C17—C24—C25—C26 | −178.3 (2) |
| C4—C12—C11—C10 | −0.1 (3) | C23—C22—C21—C20 | 1.2 (3) |
| C9—C10—C11—C12 | 1.2 (3) | C19—C20—C21—C22 | −0.6 (3) |
| N2—C10—C11—C12 | 177.20 (17) | C29—C28—C27—C26 | 0.3 (3) |
| C10—N2—C15—C16 | −176.66 (18) | C1—C5—C6—C7 | 0.0 (3) |
| C9—C3—C2—C8 | 4.6 (3) | C28—C27—C26—C25 | −1.4 (4) |
| C4—C3—C2—C8 | −178.0 (2) | C24—C25—C26—C27 | 1.6 (4) |
| C9—C3—C2—C1 | −176.15 (19) | C2—C8—C7—C6 | 0.0 (3) |
| C4—C3—C2—C1 | 1.23 (19) | C5—C6—C7—C8 | −0.5 (4) |
| C20—C19—C18—C23 | 1.4 (3) | C15—C16—C17—C18 | −176.78 (19) |
| C20—C19—C18—C17 | −177.52 (18) | C15—C16—C17—C24 | 7.9 (3) |
| C4—N1—C1—C5 | −179.9 (2) | C23—C18—C17—C16 | −152.0 (2) |
| C13—N1—C1—C5 | −6.3 (3) | C19—C18—C17—C16 | 26.9 (3) |
| C4—N1—C1—C2 | 0.8 (2) | C23—C18—C17—C24 | 23.6 (3) |
| C13—N1—C1—C2 | 174.34 (17) | C19—C18—C17—C24 | −157.54 (18) |
| C8—C2—C1—N1 | 178.13 (16) | C29—C24—C17—C16 | 59.9 (3) |
| C3—C2—C1—N1 | −1.2 (2) | C25—C24—C17—C16 | −122.5 (2) |
| C8—C2—C1—C5 | −1.3 (3) | C29—C24—C17—C18 | −115.7 (2) |
| C3—C2—C1—C5 | 179.36 (17) | C25—C24—C17—C18 | 61.9 (3) |

*Hydrogen-bond geometry (Å, º)*

*Cg*1, *Cg*2, *Cg*3 and *Cg*4 are the centroids of rings C3/C4/C9–C12, N1/C1–C4, C18–C23 and C1/C2/C5–C8, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C7—H7···*Cg*1$^{i}$ | 0.93 | 2.92 | 3.647 (2) | 136 |
| C8—H8···*Cg*2$^{i}$ | 0.93 | 2.98 | 3.777 (2) | 145 |
| C11—H11···*Cg*3$^{ii}$ | 0.93 | 2.85 | 3.551 (2) | 133 |

| | | | | |
|---|---|---|---|---|
| C13—H13*A*···*Cg*1$^{iii}$ | 0.97 | 3.00 | 3.749 (2) | 135 |
| C20—H20···*Cg*4$^{iv}$ | 0.93 | 2.62 | 3.498 (2) | 157 |
| C29—H29···*Cg*3$^{v}$ | 0.93 | 2.87 | 3.796 (3) | 175 |

Symmetry codes: (i) −*x*+1, *y*−1/2, −*z*+1/2; (ii) −*x*, −*y*+2, −*z*; (iii) −*x*+1, −*y*+2, −*z*; (iv) *x*−1, *y*, *z*; (v) −*x*, −*y*+1, −*z*.