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# 2,2-Dimethyl-2,3-dihydro-1*H*-perimidine

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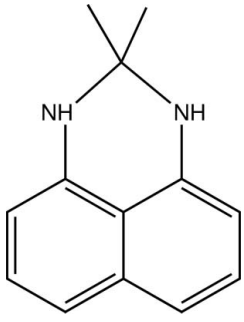
Key indicators: single-crystal X-ray study; $T$ = 93 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.056; $wR$ factor = 0.133; data-to-parameter ratio = 13.0.

The title compound, $C_{13}H_{14}N_2$, was obtained from reaction of diaminonaphthalene with acetone. In both independent molecules in the asymmetric unit, the tricyclic perimidine consists of a planar (r.m.s. deviations = 0.0125 and 0.0181 Å) naphthalene ring system and an envelope conformation $C_4N_2$ ringwith the NCN group hinged with respect to the naphthalene backbone by 36.9 (2) and 41.3 (2)° in the two independent molecules. The methyl substituents are arranged approximately axial and equatorial on the apical C atom. In the crystal, one of the N—H groups of one independent molecule is involved in classical N—H···N hydrogen bonding. Short intermolecular (C/N)—H···$\pi$(arene) interactions, near the short T-shaped limit, link molecules in the absence of strong acceptors.

## Related literature

For general background to perimidines and their biological activity, see: Shaabani & Maleki (2008); Sauer *et al.* (2006). For related structures, see: Martinez-Belmonte *et al.* (2010).




## Experimental

### Crystal data

$C_{13}H_{14}N_2$
$M_r$ = 198.27
Monoclinic, $P2_1/c$
$a$ = 16.261 (10) Å
$b$ = 7.710 (4) Å
$c$ = 17.483 (10) Å
$\beta$ = 106.131 (12)°
$V$ = 2105.6 (19) Å$^3$
$Z$ = 8
Mo $K\alpha$ radiation
$\mu$ = 0.08 mm$^{-1}$
$T$ = 93 K
0.12 × 0.12 × 0.12 mm

### Data collection

Rigaku Mercury70 diffractometer
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
$T_{min}$ = 0.706, $T_{max}$ = 0.991
12841 measured reflections
3743 independent reflections
2356 reflections with $F^2 > 2\sigma(F^2)$
$R_{int}$ = 0.072

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.056
$wR(F^2)$ = 0.133
$S$ = 0.96
3743 reflections
287 parameters
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

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

*Cg*1, *Cg*2 and *Cg*3 are the centroids of the C21–C25/C30, C25–C30 and C5–C10 rings, respectively.

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| N21—H21N···N29$^{i}$ | 0.88 (2) | 2.36 (2) | 3.229 (4) | 170 (2) |
| N1—H1N···*Cg*1$^{ii}$ | 0.93 (3) | 2.93 (3) | 3.853 (3) | 170 (2) |
| N9—H9N···*Cg*1 | 0.88 (4) | 2.85 (2) | 3.703 (3) | 164 (2) |
| C12—H12*C*···*Cg*2 | 0.98 | 2.55 | 3.521 (3) | 172 |
| C26—H26···*Cg*3$^{iii}$ | 0.95 | 2.53 | 3.456 (3) | 164 |

Symmetry codes: (i) $-x+2, y+\frac{1}{2}, -z+\frac{3}{2}$; (ii) $x, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x, y-1, z$.

Data collection: *CrystalClear-SM Expert* (Rigaku, 2009); cell refinement: *CrystalClear-SM Expert*; data reduction: *CrystalClear-SM Expert*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *CrystalStructure* (Rigaku, 2010); software used to prepare material for publication: *CrystalStructure*.

We are grateful to EPSRC for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: GG2107).

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# supporting information

*Acta Cryst.* (2013). E**69**, o246 [doi:10.1107/S1600536813000986]

## 2,2-Dimethyl-2,3-dihydro-1*H*-perimidine

**Sarah Maloney, Alexandra M. Z. Slawin and J. Derek Woollins**

### S1. Comment

The title compound has a planar napthalene backbone with the the nitrogen atoms above this plane in both independent molecules (N1 0.133, N9 0.182, N21 0.155, N290.047 Å) and the carbon in the C4N2 ring being below this plane (C11 - 0.373, C31 - 0.488 Å). The six membered $C_4N_2$ ring is hinged about the N···N vector with the N1—C11—N9 and C21—C31—N29 planes being inclined by 36.9 and 41.0° respectively to the naphthalene planes.

### S2. Experimental

A solution of 1,8-aminonapthalene (1.52 g, 0.01 mol s) and acetone (0.58 g, 0.78 ml, 0.01 mol s) was refluxed in ethanol (50 ml) for 2 h. The solution was then filtered, solvent evaporated to dryness under reduced pressure and recrystallized from boiling ethanol to give translucent crystals (mp *x*°C). (0.897 g, 0.0045 mol s, 45%). IR (KBr disc): 3295 *v*(N—H), 1596 aromatic C—H, 1016, 646, 552, 477 $cm^{-1}$. Raman (solid sample): 1490, 447, 160 $cm^{-1}$. $\delta_H$ (270.0 MHz, $CDCl_3$, $Me_4Si$): 7.24–7.14 (4*H*, *m*, $H_1$, $H_2$), 6.47–6.44 (2*H*, *dd*, $H_3$), 4.16 (2*H*, *brd s*, $H_4$), 1.49 (6*H*, *s*, $H_5$). $\delta_C$ (75.5 MHz, $CDCl_3$, $Me_4Si$): 140.4 (2 C, $C_4$), 127.1 (2 C,$C_3$), 117.2 (2 C, $C_2$), 106.1 (2 C, $C_1$), 64.7 (1 C, $C_5$), 28.9 (2 C, $C_6$). MS EI+: *m/z* 221.05 $(M^+ + Na)^+$ , 199.06 $(M^+ + H)^+$, 182.08 $(M^+ - Me)^+$. Found: C, 78.27; H, 6.93 N, 14.21. $C_{13}H_{14}N_2$ requires C, 78.75; H, 7.12; N, 14.13%.

### S3. Refinement

All H atoms were included in calculated positions (C—H distances are 0.98 Å for methyl H atoms, 0.95 Å for phenyl H atoms) and were refined as riding atoms with $U_{iso}$(H) = 1.2 $U_{eq}$(parent atom, methylene H atoms) or $U_{iso}$(H) = 1.5 $U_{eq}$(parent atom, methyl H atoms). The highest peak in the difference map is 0.94 Å from atom C29.

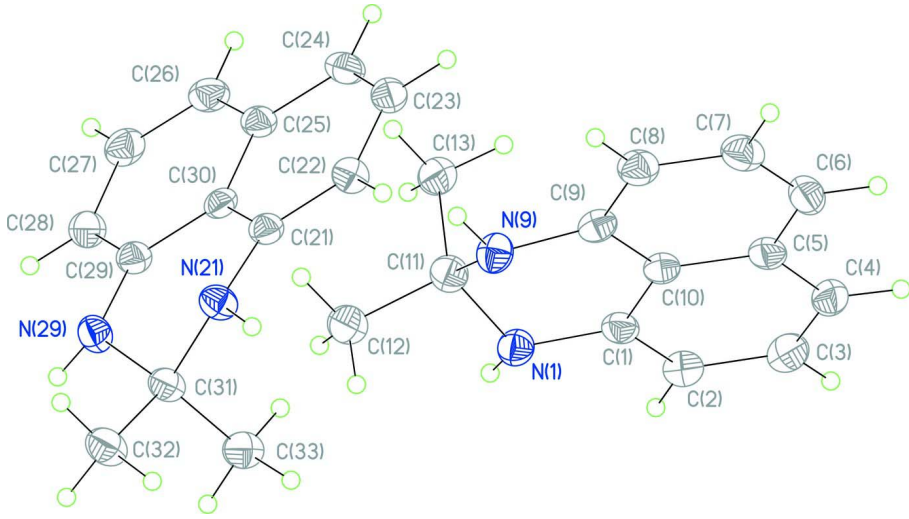


**Figure 1**

The structure of (**1**) with displacement ellipsoids drawn at the 50% probability level

### 2,2-Dimethyl-2,3-dihydro-1*H*-perimidine

*Crystal data*

$C_{13}H_{14}N_2$
$M_r = 198.27$
Monoclinic, $P2_1/c$
Hall symbol: -P 2ybc
$a = 16.261\ (10)$ Å
$b = 7.710\ (4)$ Å
$c = 17.483\ (10)$ Å
$\beta = 106.131\ (12)°$
$V = 2105.6\ (19)$ Å$^3$
$Z = 8$
$F(000) = 848.00$
$D_x = 1.251$ Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda = 0.71075$ Å
Cell parameters from 4713 reflections
$\theta = 2.4–25.4°$
$\mu = 0.08$ mm$^{-1}$
$T = 93$ K
Prism, colorless
0.12 × 0.12 × 0.12 mm

*Data collection*

Rigaku Mercury70 diffractometer
Detector resolution: 14.629 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (*REQAB*; Rigaku, 1998)
$T_{min} = 0.706$, $T_{max} = 0.991$
12841 measured reflections
3743 independent reflections
2356 reflections with $F^2 > 2\sigma(F^2)$
$R_{int} = 0.072$
$\theta_{max} = 25.1°$
$h = -19\rightarrow19$
$k = -9\rightarrow9$
$l = -20\rightarrow16$

*Refinement*

Refinement on $F^2$
$R[F^2 > 2\sigma(F^2)] = 0.056$
$wR(F^2) = 0.133$
$S = 0.96$
3743 reflections
287 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 atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0447P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$

$\Delta\rho_{max}$ = 0.22 e Å$^{-3}$ $\Delta\rho_{min}$ = −0.24 e Å$^{-3}$

*Special details*

**Geometry**. ENTER SPECIAL DETAILS OF THE MOLECULAR GEOMETRY

**Refinement**. Refinement was performed using all reflections. The weighted *R*-factor (*wR*) and goodness of fit (*S*) are based on $F^2$. *R*-factor (gt) are based on *F*. The threshold expression of $F^2 > 2.0\ \sigma(F^2)$ is used only for calculating *R*-factor (gt).

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å$^2$)*

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.74130 (13) | 0.4938 (3) | 0.32012 (12) | 0.0251 (5) |
| N9 | 0.72027 (13) | 0.4474 (3) | 0.44670 (12) | 0.0253 (5) |
| C1 | 0.67357 (15) | 0.6139 (3) | 0.29931 (14) | 0.0239 (6) |
| C2 | 0.65289 (15) | 0.7024 (3) | 0.22781 (14) | 0.0257 (6) |
| C3 | 0.58887 (16) | 0.8304 (3) | 0.21297 (15) | 0.0293 (6) |
| C4 | 0.54615 (16) | 0.8709 (3) | 0.26806 (15) | 0.0276 (6) |
| C5 | 0.56482 (15) | 0.7808 (3) | 0.34165 (14) | 0.0245 (6) |
| C6 | 0.52239 (16) | 0.8170 (3) | 0.40084 (15) | 0.0296 (7) |
| C7 | 0.54224 (15) | 0.7241 (3) | 0.47065 (15) | 0.0304 (7) |
| C8 | 0.60553 (16) | 0.5958 (3) | 0.48627 (15) | 0.0280 (6) |
| C9 | 0.64967 (15) | 0.5602 (3) | 0.43120 (14) | 0.0240 (6) |
| C10 | 0.62879 (15) | 0.6508 (3) | 0.35711 (14) | 0.0225 (6) |
| C11 | 0.73892 (16) | 0.3581 (3) | 0.37924 (14) | 0.0255 (6) |
| C12 | 0.82772 (15) | 0.2789 (3) | 0.40713 (15) | 0.0301 (7) |
| C13 | 0.67145 (15) | 0.2193 (3) | 0.34472 (14) | 0.0286 (7) |
| H2 | 0.6818 | 0.6768 | 0.1888 | 0.0309* |
| H3 | 0.5749 | 0.8904 | 0.1636 | 0.0351* |
| H4 | 0.5039 | 0.9595 | 0.2569 | 0.0331* |
| H6 | 0.4802 | 0.9056 | 0.3921 | 0.0355* |
| H7 | 0.5123 | 0.7475 | 0.5091 | 0.0364* |
| H8 | 0.6181 | 0.5331 | 0.5349 | 0.0336* |
| H12A | 0.8692 | 0.3688 | 0.4320 | 0.0361* |
| H12B | 0.8434 | 0.2296 | 0.3614 | 0.0361* |
| H12C | 0.8280 | 0.1872 | 0.4460 | 0.0361* |
| H13A | 0.6846 | 0.1634 | 0.2992 | 0.0343* |
| H13B | 0.6148 | 0.2735 | 0.3272 | 0.0343* |
| H13C | 0.6718 | 0.1322 | 0.3856 | 0.0343* |
| H9n | 0.7242 (16) | 0.381 (3) | 0.4888 (15) | 0.035 (8)* |
| H1n | 0.7596 (16) | 0.455 (3) | 0.2770 (16) | 0.043 (8)* |
| N21 | 0.95216 (13) | 0.2662 (3) | 0.72018 (12) | 0.0237 (5) |
| N29 | 1.01370 (14) | 0.0717 (3) | 0.64843 (12) | 0.0240 (5) |
| C21 | 0.86940 (15) | 0.2322 (3) | 0.67450 (13) | 0.0213 (6) |
| C22 | 0.79708 (15) | 0.3089 (3) | 0.68648 (14) | 0.0236 (6) |
| C23 | 0.71473 (16) | 0.2555 (3) | 0.64207 (14) | 0.0255 (6) |
| C24 | 0.70369 (15) | 0.1272 (3) | 0.58569 (14) | 0.0259 (6) |
| C25 | 0.77628 (15) | 0.0457 (3) | 0.57089 (14) | 0.0222 (6) |
| C26 | 0.76848 (16) | −0.0902 (3) | 0.51485 (14) | 0.0267 (6) |

| | | | | |
|---|---|---|---|---|
| C27 | 0.84036 (16) | −0.1676 (3) | 0.50372 (14) | 0.0277 (6) |
| C28 | 0.92278 (16) | −0.1122 (3) | 0.54540 (14) | 0.0252 (6) |
| C29 | 0.93299 (15) | 0.0203 (3) | 0.60052 (14) | 0.0225 (6) |
| C30 | 0.85910 (15) | 0.1007 (3) | 0.61425 (13) | 0.0200 (6) |
| C31 | 1.02152 (15) | 0.2496 (3) | 0.68135 (14) | 0.0235 (6) |
| C32 | 1.10655 (15) | 0.2637 (3) | 0.74320 (15) | 0.0303 (7) |
| C33 | 1.01217 (16) | 0.3872 (3) | 0.61631 (14) | 0.0281 (7) |
| H21n | 0.9598 (16) | 0.359 (3) | 0.7505 (15) | 0.033 (8)* |
| H29n | 1.0552 (17) | 0.048 (3) | 0.6295 (15) | 0.039 (9)* |
| H22 | 0.8030 | 0.3983 | 0.7250 | 0.0283* |
| H23 | 0.6659 | 0.3094 | 0.6514 | 0.0305* |
| H24 | 0.6476 | 0.0928 | 0.5566 | 0.0311* |
| H26 | 0.7133 | −0.1279 | 0.4848 | 0.0320* |
| H27 | 0.8341 | −0.2608 | 0.4670 | 0.0332* |
| H28 | 0.9716 | −0.1657 | 0.5357 | 0.0303* |
| H32A | 1.1527 | 0.2410 | 0.7185 | 0.0364* |
| H32B | 1.1093 | 0.1785 | 0.7854 | 0.0364* |
| H32C | 1.1131 | 0.3807 | 0.7660 | 0.0364* |
| H33A | 1.0152 | 0.5030 | 0.6401 | 0.0337* |
| H33B | 0.9568 | 0.3729 | 0.5763 | 0.0337* |
| H33C | 1.0584 | 0.3738 | 0.5909 | 0.0337* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0277 (14) | 0.0244 (11) | 0.0255 (13) | 0.0014 (10) | 0.0114 (11) | 0.0024 (10) |
| N9 | 0.0296 (14) | 0.0263 (12) | 0.0200 (13) | 0.0024 (10) | 0.0065 (11) | 0.0030 (10) |
| C1 | 0.0197 (15) | 0.0222 (13) | 0.0300 (15) | −0.0044 (11) | 0.0073 (12) | −0.0033 (11) |
| C2 | 0.0266 (16) | 0.0271 (13) | 0.0236 (14) | −0.0037 (12) | 0.0072 (13) | −0.0006 (11) |
| C3 | 0.0304 (16) | 0.0283 (14) | 0.0254 (15) | −0.0047 (12) | 0.0016 (13) | 0.0028 (11) |
| C4 | 0.0243 (15) | 0.0222 (13) | 0.0338 (16) | −0.0018 (11) | 0.0038 (13) | 0.0008 (12) |
| C5 | 0.0197 (14) | 0.0227 (13) | 0.0301 (15) | −0.0053 (11) | 0.0049 (12) | −0.0033 (11) |
| C6 | 0.0227 (15) | 0.0279 (14) | 0.0383 (17) | 0.0020 (12) | 0.0087 (14) | −0.0029 (12) |
| C7 | 0.0278 (16) | 0.0334 (15) | 0.0337 (16) | −0.0032 (12) | 0.0149 (14) | −0.0030 (12) |
| C8 | 0.0292 (16) | 0.0295 (14) | 0.0283 (16) | −0.0024 (12) | 0.0130 (13) | 0.0012 (11) |
| C9 | 0.0257 (16) | 0.0211 (13) | 0.0245 (15) | −0.0055 (11) | 0.0063 (13) | −0.0012 (10) |
| C10 | 0.0202 (15) | 0.0199 (12) | 0.0264 (14) | −0.0047 (11) | 0.0050 (12) | −0.0019 (11) |
| C11 | 0.0246 (15) | 0.0269 (13) | 0.0246 (15) | −0.0007 (11) | 0.0062 (13) | −0.0006 (11) |
| C12 | 0.0272 (16) | 0.0318 (14) | 0.0316 (16) | −0.0002 (12) | 0.0088 (13) | 0.0015 (12) |
| C13 | 0.0280 (16) | 0.0259 (13) | 0.0313 (16) | −0.0016 (12) | 0.0071 (13) | 0.0013 (11) |
| N21 | 0.0212 (13) | 0.0263 (12) | 0.0237 (13) | −0.0023 (10) | 0.0066 (11) | −0.0048 (9) |
| N29 | 0.0204 (13) | 0.0239 (11) | 0.0271 (13) | 0.0013 (10) | 0.0054 (11) | −0.0041 (9) |
| C21 | 0.0203 (15) | 0.0220 (13) | 0.0213 (14) | −0.0019 (11) | 0.0055 (12) | 0.0038 (10) |
| C22 | 0.0233 (15) | 0.0251 (13) | 0.0227 (14) | −0.0007 (11) | 0.0069 (12) | −0.0021 (11) |
| C23 | 0.0249 (16) | 0.0282 (14) | 0.0260 (15) | 0.0025 (11) | 0.0115 (13) | 0.0073 (11) |
| C24 | 0.0190 (15) | 0.0329 (14) | 0.0261 (15) | −0.0030 (11) | 0.0068 (13) | 0.0047 (12) |
| C25 | 0.0204 (15) | 0.0250 (13) | 0.0219 (14) | −0.0015 (11) | 0.0071 (12) | 0.0049 (11) |
| C26 | 0.0244 (15) | 0.0253 (13) | 0.0285 (16) | −0.0070 (11) | 0.0043 (13) | −0.0015 (11) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C27 | 0.0318 (17) | 0.0213 (13) | 0.0303 (16) | −0.0042 (12) | 0.0092 (13) | −0.0050 (11) |
| C28 | 0.0256 (16) | 0.0239 (13) | 0.0274 (15) | −0.0005 (11) | 0.0093 (13) | −0.0021 (11) |
| C29 | 0.0213 (15) | 0.0234 (13) | 0.0233 (14) | −0.0014 (11) | 0.0069 (12) | 0.0034 (11) |
| C30 | 0.0229 (15) | 0.0168 (12) | 0.0212 (14) | −0.0017 (11) | 0.0078 (12) | 0.0034 (10) |
| C31 | 0.0197 (15) | 0.0251 (13) | 0.0264 (14) | −0.0018 (11) | 0.0074 (12) | −0.0033 (11) |
| C32 | 0.0227 (15) | 0.0332 (14) | 0.0351 (16) | −0.0022 (12) | 0.0081 (13) | −0.0054 (12) |
| C33 | 0.0278 (16) | 0.0281 (14) | 0.0297 (16) | −0.0033 (12) | 0.0102 (13) | −0.0024 (11) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C1 | 1.407 (3) | C29—C30 | 1.430 (4) |
| N1—C11 | 1.479 (4) | C31—C32 | 1.504 (3) |
| N9—C9 | 1.406 (3) | C31—C33 | 1.531 (4) |
| N9—C11 | 1.468 (4) | N1—H1n | 0.93 (3) |
| C1—C2 | 1.381 (4) | N9—H9n | 0.88 (3) |
| C1—C10 | 1.429 (4) | C2—H2 | 0.950 |
| C2—C3 | 1.405 (4) | C3—H3 | 0.950 |
| C3—C4 | 1.371 (5) | C4—H4 | 0.950 |
| C4—C5 | 1.418 (4) | C6—H6 | 0.950 |
| C5—C6 | 1.422 (4) | C7—H7 | 0.950 |
| C5—C10 | 1.416 (4) | C8—H8 | 0.950 |
| C6—C7 | 1.374 (4) | C12—H12A | 0.980 |
| C7—C8 | 1.398 (4) | C12—H12B | 0.980 |
| C8—C9 | 1.379 (4) | C12—H12C | 0.980 |
| C9—C10 | 1.427 (4) | C13—H13A | 0.980 |
| C11—C12 | 1.518 (4) | C13—H13B | 0.980 |
| C11—C13 | 1.532 (4) | C13—H13C | 0.980 |
| N21—C21 | 1.386 (3) | N21—H21n | 0.88 (3) |
| N21—C31 | 1.475 (4) | N29—H29n | 0.85 (3) |
| N29—C29 | 1.404 (3) | C22—H22 | 0.950 |
| N29—C31 | 1.480 (3) | C23—H23 | 0.950 |
| C21—C22 | 1.383 (4) | C24—H24 | 0.950 |
| C21—C30 | 1.438 (3) | C26—H26 | 0.950 |
| C22—C23 | 1.410 (4) | C27—H27 | 0.950 |
| C23—C24 | 1.373 (4) | C28—H28 | 0.950 |
| C24—C25 | 1.423 (4) | C32—H32A | 0.980 |
| C25—C26 | 1.416 (4) | C32—H32B | 0.980 |
| C25—C30 | 1.414 (3) | C32—H32C | 0.980 |
| C26—C27 | 1.374 (4) | C33—H33A | 0.980 |
| C27—C28 | 1.402 (4) | C33—H33B | 0.980 |
| C28—C29 | 1.382 (4) | C33—H33C | 0.980 |
| | | | |
| N1···C9 | 2.804 (4) | H8···C7$^{xi}$ | 3.2563 |
| N9···C1 | 2.789 (4) | H8···H2$^{xii}$ | 3.4300 |
| C1···C4 | 2.808 (4) | H8···H3$^{xii}$ | 2.6041 |
| C1···C13 | 3.147 (4) | H8···H7$^{xi}$ | 2.9778 |
| C2···C5 | 2.822 (4) | H8···C23 | 2.9872 |
| C3···C10 | 2.789 (4) | H8···C24 | 3.4399 |

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|---|---|---|---|
| C5···C8 | 2.817 (4) | H8···H23 | 2.6159 |
| C6···C9 | 2.806 (4) | H8···H24 | 3.4350 |
| C7···C10 | 2.791 (4) | H8···H26$^{iii}$ | 3.2782 |
| C9···C13 | 3.101 (4) | H12A···C33 | 3.4131 |
| C10···C11 | 2.840 (4) | H12A···C33$^{ii}$ | 2.9801 |
| C10···C13 | 3.418 (4) | H12A···H27$^{iii}$ | 3.0090 |
| N21···C29 | 2.776 (4) | H12A···H28$^{xiii}$ | 2.9433 |
| N29···C21 | 2.800 (4) | H12A···H33A$^{ii}$ | 2.7227 |
| C21···C24 | 2.829 (4) | H12A···H33B | 2.5307 |
| C21···C33 | 3.028 (4) | H12A···H33B$^{ii}$ | 3.4961 |
| C22···C25 | 2.817 (4) | H12A···H33C | 3.5273 |
| C23···C30 | 2.794 (4) | H12A···H33C$^{ii}$ | 2.3971 |
| C25···C28 | 2.819 (4) | H12B···N21$^{i}$ | 3.4143 |
| C26···C29 | 2.810 (4) | H12B···N29$^{xiii}$ | 3.3243 |
| C27···C30 | 2.789 (4) | H12B···C21$^{i}$ | 3.4228 |
| C29···C33 | 3.089 (4) | H12B···C22$^{i}$ | 2.9547 |
| C30···C31 | 2.819 (4) | H12B···H21n$^{i}$ | 3.1389 |
| C30···C33 | 3.321 (4) | H12B···H29n$^{xiii}$ | 2.6812 |
| N1···C22$^{i}$ | 3.593 (4) | H12B···H22$^{i}$ | 2.4947 |
| N1···C23$^{i}$ | 3.581 (4) | H12B···H28$^{xiii}$ | 3.0861 |
| N1···C32$^{ii}$ | 3.516 (4) | H12B···H33A$^{ii}$ | 3.0943 |
| N9···C24 | 3.526 (4) | H12B···H33C$^{ii}$ | 3.4433 |
| N9···C27$^{iii}$ | 3.541 (4) | H12C···C25 | 2.7718 |
| C4···C13$^{iii}$ | 3.413 (4) | H12C···C26 | 2.7575 |
| C8···C26$^{iii}$ | 3.521 (4) | H12C···C27 | 2.9033 |
| C9···C26$^{iii}$ | 3.401 (4) | H12C···C28 | 3.0393 |
| C13···C4$^{iv}$ | 3.413 (4) | H12C···C29 | 3.0507 |
| N21···N29$^{v}$ | 3.229 (3) | H12C···C30 | 2.9201 |
| N29···N21$^{vi}$ | 3.229 (3) | H12C···H29n$^{xiii}$ | 3.1687 |
| C22···N1$^{vii}$ | 3.593 (4) | H12C···H26 | 3.2466 |
| C23···N1$^{vii}$ | 3.581 (4) | H12C···H27 | 3.4716 |
| C24···N9 | 3.526 (4) | H12C···H28$^{xiii}$ | 3.1900 |
| C26···C8$^{iv}$ | 3.521 (4) | H12C···H33B | 2.9969 |
| C26···C9$^{iv}$ | 3.401 (4) | H13A···C3$^{iv}$ | 3.1595 |
| C27···N9$^{iv}$ | 3.541 (4) | H13A···C4$^{iv}$ | 3.1260 |
| C29···C32$^{vi}$ | 3.573 (4) | H13A···H3$^{iv}$ | 3.2995 |
| C30···C32$^{vi}$ | 3.535 (4) | H13A···H4$^{iv}$ | 3.2321 |
| C32···N1$^{ii}$ | 3.516 (4) | H13A···C22$^{i}$ | 3.0453 |
| C32···C29$^{v}$ | 3.573 (4) | H13A···C23$^{i}$ | 2.9871 |
| C32···C30$^{v}$ | 3.535 (4) | H13A···H22$^{i}$ | 2.6455 |
| N1···H2 | 2.6386 | H13A···H23$^{i}$ | 2.5254 |
| N1···H12A | 2.6111 | H13B···C3$^{viii}$ | 3.2186 |
| N1···H12B | 2.6002 | H13B···C4$^{iv}$ | 3.3632 |
| N1···H12C | 3.2706 | H13B···C4$^{viii}$ | 2.7866 |
| N1···H13A | 2.6998 | H13B···C5$^{viii}$ | 3.5298 |
| N1···H13B | 2.6978 | H13B···H3$^{viii}$ | 3.2593 |
| N1···H13C | 3.3294 | H13B···H4$^{iv}$ | 3.0647 |
| N1···H9n | 3.16 (3) | H13B···H4$^{viii}$ | 2.5235 |

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|---|---|---|---|
| N9···H8 | 2.6451 | H13B···H23$^{i}$ | 3.4602 |
| N9···H12A | 2.5773 | H13C···C4$^{iv}$ | 3.1820 |
| N9···H12B | 3.2719 | H13C···C5$^{iv}$ | 3.1957 |
| N9···H12C | 2.6654 | H13C···C6$^{iv}$ | 3.4981 |
| N9···H13A | 3.3094 | H13C···H4$^{iv}$ | 3.2978 |
| N9···H13B | 2.6666 | H13C···C24 | 3.3904 |
| N9···H13C | 2.6832 | H13C···C25 | 3.2808 |
| N9···H1n | 3.20 (3) | H13C···C26 | 2.9227 |
| C1···H3 | 3.2611 | H13C···H24 | 3.1356 |
| C1···H13A | 3.4788 | H13C···H26 | 2.6146 |
| C1···H13B | 2.8816 | H9n···C22 | 3.37 (3) |
| C2···H4 | 3.2775 | H9n···C23 | 2.89 (3) |
| C2···H1n | 2.56 (3) | H9n···C24 | 2.67 (3) |
| C4···H2 | 3.2743 | H9n···C25 | 2.96 (3) |
| C4···H6 | 2.6865 | H9n···C30 | 3.41 (3) |
| C5···H3 | 3.2735 | H9n···H23 | 3.2829 |
| C5···H7 | 3.2793 | H9n···H24 | 2.9522 |
| C6···H4 | 2.6848 | H9n···H27$^{iii}$ | 3.3681 |
| C6···H8 | 3.2684 | H1n···C21$^{i}$ | 3.20 (3) |
| C8···H6 | 3.2718 | H1n···C22$^{i}$ | 2.75 (3) |
| C8···H9n | 2.53 (3) | H1n···C23$^{i}$ | 2.79 (3) |
| C9···H7 | 3.2583 | H1n···C24$^{i}$ | 3.27 (3) |
| C9···H13B | 2.8178 | H1n···C32$^{ii}$ | 3.16 (3) |
| C9···H13C | 3.4372 | H1n···H22$^{i}$ | 3.0137 |
| C10···H2 | 3.2938 | H1n···H23$^{i}$ | 3.0707 |
| C10···H4 | 3.2984 | H1n···H32A$^{ii}$ | 2.7368 |
| C10···H6 | 3.3005 | H1n···H32C$^{ii}$ | 2.7066 |
| C10···H8 | 3.2887 | H1n···H33A$^{ii}$ | 3.5589 |
| C10···H13B | 2.9537 | H1n···H33C$^{ii}$ | 3.4702 |
| C10···H9n | 3.17 (3) | N21···H12B$^{vii}$ | 3.4143 |
| C10···H1n | 3.23 (3) | N21···H21n$^{vi}$ | 3.43 (3) |
| C12···H13A | 2.7073 | N21···H29n$^{v}$ | 3.44 (3) |
| C12···H13B | 3.3548 | N21···H32B$^{v}$ | 3.3261 |
| C12···H13C | 2.7058 | N21···H32C$^{vi}$ | 3.1878 |
| C12···H9n | 2.61 (3) | N21···H33A$^{vi}$ | 3.1063 |
| C12···H1n | 2.61 (3) | N29···H12B$^{xiii}$ | 3.3243 |
| C13···H12A | 3.3566 | N29···H21n$^{vi}$ | 2.36 (3) |
| C13···H12B | 2.7297 | N29···H22$^{vi}$ | 3.4504 |
| C13···H12C | 2.6775 | N29···H28$^{xiii}$ | 3.3733 |
| C13···H9n | 2.73 (3) | N29···H32C$^{vi}$ | 3.2210 |
| C13···H1n | 2.77 (3) | C21···H12B$^{vii}$ | 3.4228 |
| H2···H3 | 2.3459 | C21···H1n$^{vii}$ | 3.20 (3) |
| H2···H1n | 2.4150 | C21···H32B$^{v}$ | 3.5102 |
| H3···H4 | 2.3076 | C21···H32C$^{vi}$ | 2.8885 |
| H4···H6 | 2.5325 | C22···H12B$^{vii}$ | 2.9547 |
| H6···H7 | 2.3131 | C22···H13A$^{vii}$ | 3.0453 |
| H7···H8 | 2.3375 | C22···H9n | 3.37 (3) |
| H8···H9n | 2.4025 | C22···H1n$^{vii}$ | 2.75 (3) |

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|---|---|---|---|
| H12A···H13C | 3.5835 | C22···H32B$^{v}$ | 3.2046 |
| H12A···H9n | 2.8024 | C23···H2$^{vii}$ | 3.5084 |
| H12A···H1n | 2.8756 | C23···H6$^{xi}$ | 3.3009 |
| H12B···H13A | 2.5585 | C23···H8 | 2.9872 |
| H12B···H13C | 3.0303 | C23···H13A$^{vii}$ | 2.9871 |
| H12B···H9n | 3.5319 | C23···H9n | 2.89 (3) |
| H12B···H1n | 2.4339 | C23···H1n$^{vii}$ | 2.79 (3) |
| H12C···H13A | 2.9546 | C24···H2$^{vii}$ | 3.0379 |
| H12C···H13B | 3.5735 | C24···H6$^{xi}$ | 3.1308 |
| H12C···H13C | 2.5009 | C24···H7$^{xi}$ | 3.5757 |
| H12C···H9n | 2.5185 | C24···H8 | 3.4399 |
| H12C···H1n | 3.5197 | C24···H13C | 3.3904 |
| H13A···H1n | 2.6343 | C24···H9n | 2.67 (3) |
| H13B···H9n | 3.0071 | C24···H1n$^{vii}$ | 3.27 (3) |
| H13B···H1n | 3.0686 | C25···H2$^{vii}$ | 3.3639 |
| H13C···H9n | 2.6096 | C25···H12C | 2.7718 |
| N21···H29n | 3.10 (3) | C25···H13C | 3.2808 |
| N21···H22 | 2.6543 | C25···H9n | 2.96 (3) |
| N21···H32A | 3.2749 | C25···H32C$^{vi}$ | 3.1837 |
| N21···H32B | 2.5816 | C26···H12C | 2.7575 |
| N21···H32C | 2.6660 | C26···H13C | 2.9227 |
| N21···H33A | 2.6732 | C27···H12C | 2.9033 |
| N21···H33B | 2.6669 | C27···H29n$^{xiii}$ | 3.37 (3) |
| N21···H33C | 3.3100 | C27···H33C$^{xiii}$ | 3.0795 |
| N29···H21n | 3.12 (3) | C28···H12C | 3.0393 |
| N29···H28 | 2.6364 | C28···H21n$^{vi}$ | 3.56 (3) |
| N29···H32A | 2.6025 | C28···H29n$^{xiii}$ | 3.21 (3) |
| N29···H32B | 2.6007 | C28···H28$^{xiii}$ | 3.3031 |
| N29···H32C | 3.2663 | C28···H32B$^{vi}$ | 3.5320 |
| N29···H33A | 3.3292 | C28···H32C$^{vi}$ | 3.5052 |
| N29···H33B | 2.6812 | C28···H33A$^{iv}$ | 3.5240 |
| N29···H33C | 2.7158 | C28···H33C$^{xiii}$ | 3.2005 |
| C21···H23 | 3.2755 | C29···H12C | 3.0507 |
| C21···H33A | 3.3374 | C29···H21n$^{vi}$ | 2.97 (3) |
| C21···H33B | 2.7385 | C29···H28$^{xiii}$ | 3.3757 |
| C22···H21n | 2.60 (3) | C29···H32B$^{vi}$ | 3.4857 |
| C22···H24 | 3.2822 | C29···H32C$^{vi}$ | 2.8530 |
| C24···H22 | 3.2747 | C30···H12C | 2.9201 |
| C24···H26 | 2.6750 | C30···H9n | 3.41 (3) |
| C25···H23 | 3.2772 | C30···H32C$^{vi}$ | 2.6341 |
| C25···H27 | 3.2739 | C31···H21n$^{vi}$ | 3.22 (3) |
| C26···H24 | 2.6798 | C32···H2$^{ii}$ | 3.3457 |
| C26···H28 | 3.2725 | C32···H1n$^{ii}$ | 3.16 (3) |
| C28···H29n | 2.56 (3) | C32···H21n$^{vi}$ | 3.31 (3) |
| C28···H26 | 3.2757 | C32···H22$^{vi}$ | 3.1551 |
| C29···H27 | 3.2628 | C33···H12A | 3.4131 |
| C29···H33B | 2.7948 | C33···H12A$^{ii}$ | 2.9801 |
| C29···H33C | 3.4368 | C33···H27$^{xiii}$ | 3.3678 |

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| C30···H21n | 3.19 (3) | C33···H28$^{xiii}$ | 3.2317 |
| C30···H29n | 3.15 (3) | H21n···H12B$^{vii}$ | 3.1389 |
| C30···H22 | 3.2913 | H21n···N21$^{v}$ | 3.43 (3) |
| C30···H24 | 3.3044 | H21n···N29$^{v}$ | 2.36 (3) |
| C30···H26 | 3.2958 | H21n···C28$^{v}$ | 3.56 (3) |
| C30···H28 | 3.2927 | H21n···C29$^{v}$ | 2.97 (3) |
| C30···H33B | 2.8207 | H21n···C31$^{v}$ | 3.22 (3) |
| C32···H21n | 2.54 (3) | H21n···C32$^{v}$ | 3.31 (3) |
| C32···H29n | 2.55 (3) | H21n···H29n$^{v}$ | 2.62 (4) |
| C32···H33A | 2.7154 | H21n···H28$^{v}$ | 3.5955 |
| C32···H33B | 3.3464 | H21n···H32A$^{v}$ | 3.5842 |
| C32···H33C | 2.6955 | H21n···H32B$^{v}$ | 2.7055 |
| C33···H21n | 2.72 (3) | H21n···H33A$^{vi}$ | 3.3080 |
| C33···H29n | 2.70 (3) | H29n···C12$^{xiii}$ | 3.33 (3) |
| C33···H32A | 2.7227 | H29n···H12B$^{xiii}$ | 2.6812 |
| C33···H32B | 3.3512 | H29n···H12C$^{xiii}$ | 3.1687 |
| C33···H32C | 2.6755 | H29n···N21$^{vi}$ | 3.44 (3) |
| H21n···H22 | 2.4816 | H29n···C27$^{xiii}$ | 3.37 (3) |
| H21n···H32A | 3.4591 | H29n···C28$^{xiii}$ | 3.21 (3) |
| H21n···H32B | 2.7206 | H29n···H21n$^{vi}$ | 2.62 (4) |
| H21n···H32C | 2.4382 | H29n···H22$^{vi}$ | 3.1411 |
| H21n···H33A | 2.5955 | H29n···H27$^{xiii}$ | 3.2349 |
| H21n···H33B | 3.0340 | H29n···H28$^{xiii}$ | 2.9429 |
| H21n···H33C | 3.5867 | H22···C12$^{vii}$ | 3.3848 |
| H29n···H28 | 2.4525 | H22···C13$^{vii}$ | 3.5020 |
| H29n···H32A | 2.4030 | H22···H12B$^{vii}$ | 2.4947 |
| H29n···H32B | 2.8080 | H22···H13A$^{vii}$ | 2.6455 |
| H29n···H32C | 3.4507 | H22···H1n$^{vii}$ | 3.0137 |
| H29n···H33A | 3.5809 | H22···N29$^{v}$ | 3.4504 |
| H29n···H33B | 2.9771 | H22···C32$^{v}$ | 3.1551 |
| H29n···H33C | 2.6048 | H22···H29n$^{v}$ | 3.1411 |
| H22···H23 | 2.3458 | H22···H32A$^{v}$ | 2.8427 |
| H23···H24 | 2.3130 | H22···H32B$^{v}$ | 2.6236 |
| H24···H26 | 2.5211 | H23···C3$^{xii}$ | 3.3451 |
| H26···H27 | 2.3115 | H23···C6$^{xi}$ | 3.0985 |
| H27···H28 | 2.3423 | H23···C7$^{xi}$ | 3.4722 |
| H32A···H33A | 3.0419 | H23···C8 | 3.5491 |
| H32A···H33B | 3.5989 | H23···C13$^{vii}$ | 3.3636 |
| H32A···H33C | 2.5440 | H23···H3$^{xii}$ | 2.7873 |
| H32B···H33A | 3.5913 | H23···H6$^{xi}$ | 2.8223 |
| H32B···H33C | 3.5996 | H23···H7$^{xi}$ | 3.4557 |
| H32C···H33A | 2.5146 | H23···H8 | 2.6159 |
| H32C···H33B | 3.5739 | H23···H13A$^{vii}$ | 2.5254 |
| H32C···H33C | 2.9414 | H23···H13B$^{vii}$ | 3.4602 |
| N1···H27$^{iii}$ | 3.2088 | H23···H9n | 3.2829 |
| N1···H32A$^{ii}$ | 2.8729 | H23···H1n$^{vii}$ | 3.0707 |
| N1···H32C$^{ii}$ | 3.2841 | H24···C6$^{xi}$ | 3.1342 |
| N1···H33C$^{ii}$ | 3.3541 | H24···C7$^{iv}$ | 3.4416 |

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| N9···H26$^{iii}$ | 3.3501 | H24···C7$^{xi}$ | 3.3068 |
| N9···H27$^{iii}$ | 2.8726 | H24···H2$^{vii}$ | 3.0432 |
| C1···H4$^{viii}$ | 3.0226 | H24···H6$^{xi}$ | 2.4821 |
| C1···H27$^{iii}$ | 3.4768 | H24···H7$^{iv}$ | 3.4063 |
| C1···H32A$^{ii}$ | 3.1334 | H24···H7$^{xi}$ | 2.8182 |
| C2···H4$^{viii}$ | 3.2340 | H24···H8 | 3.4350 |
| C2···H6$^{viii}$ | 3.4343 | H24···H13C | 3.1356 |
| C2···H32A$^{ii}$ | 3.0689 | H24···H9n | 2.9522 |
| C3···H4$^{viii}$ | 3.3428 | H26···N9$^{iv}$ | 3.3501 |
| C3···H7$^{ix}$ | 3.4852 | H26···C5$^{iv}$ | 3.0389 |
| C3···H8$^{ix}$ | 3.4420 | H26···C6$^{iv}$ | 3.0731 |
| C3···H13A$^{iii}$ | 3.1595 | H26···C7$^{iv}$ | 2.9531 |
| C3···H13B$^{x}$ | 3.2186 | H26···C8$^{iv}$ | 2.7632 |
| C3···H23$^{ix}$ | 3.3451 | H26···C9$^{iv}$ | 2.6822 |
| C4···H4$^{viii}$ | 3.2736 | H26···C10$^{iv}$ | 2.8428 |
| C4···H13A$^{iii}$ | 3.1260 | H26···C13 | 3.5643 |
| C4···H13B$^{iii}$ | 3.3632 | H26···H7$^{iv}$ | 3.5435 |
| C4···H13B$^{x}$ | 2.7866 | H26···H8$^{iv}$ | 3.2782 |
| C4···H13C$^{iii}$ | 3.1820 | H26···H12C | 3.2466 |
| C5···H4$^{viii}$ | 3.0475 | H26···H13C | 2.6146 |
| C5···H13B$^{x}$ | 3.5298 | H27···N1$^{iv}$ | 3.2088 |
| C5···H13C$^{iii}$ | 3.1957 | H27···N9$^{iv}$ | 2.8726 |
| C5···H26$^{iii}$ | 3.0389 | H27···C1$^{iv}$ | 3.4768 |
| C6···H13C$^{iii}$ | 3.4981 | H27···C9$^{iv}$ | 3.2013 |
| C6···H23$^{xi}$ | 3.0985 | H27···C10$^{iv}$ | 3.4259 |
| C6···H24$^{xi}$ | 3.1342 | H27···C11$^{iv}$ | 3.4733 |
| C6···H26$^{iii}$ | 3.0731 | H27···H12A$^{iv}$ | 3.0090 |
| C7···H3$^{xii}$ | 3.3823 | H27···H12C | 3.4716 |
| C7···H8$^{xi}$ | 3.2563 | H27···H9n$^{iv}$ | 3.3681 |
| C7···H23$^{xi}$ | 3.4722 | H27···C33$^{xiii}$ | 3.3678 |
| C7···H24$^{iii}$ | 3.4416 | H27···H29n$^{xiii}$ | 3.2349 |
| C7···H24$^{xi}$ | 3.3068 | H27···H32A$^{xiii}$ | 3.3116 |
| C7···H26$^{iii}$ | 2.9531 | H27···H33C$^{xiii}$ | 2.4122 |
| C8···H3$^{xii}$ | 3.2750 | H28···C12$^{xiii}$ | 3.2555 |
| C8···H7$^{xi}$ | 3.2821 | H28···H12A$^{xiii}$ | 2.9433 |
| C8···H23 | 3.5491 | H28···H12B$^{xiii}$ | 3.0861 |
| C8···H26$^{iii}$ | 2.7632 | H28···H12C$^{xiii}$ | 3.1900 |
| C9···H26$^{iii}$ | 2.6822 | H28···N29$^{xiii}$ | 3.3733 |
| C9···H27$^{iii}$ | 3.2013 | H28···C28$^{xiii}$ | 3.3031 |
| C10···H4$^{viii}$ | 2.9010 | H28···C29$^{xiii}$ | 3.3757 |
| C10···H26$^{iii}$ | 2.8428 | H28···C33$^{xiii}$ | 3.2317 |
| C10···H27$^{iii}$ | 3.4259 | H28···H21n$^{vi}$ | 3.5955 |
| C11···H27$^{iii}$ | 3.4733 | H28···H29n$^{xiii}$ | 2.9429 |
| C12···H29n$^{xiii}$ | 3.33 (3) | H28···H28$^{xiii}$ | 3.0967 |
| C12···H22$^{i}$ | 3.3848 | H28···H33A$^{iv}$ | 3.1040 |
| C12···H28$^{xiii}$ | 3.2555 | H28···H33B$^{xiii}$ | 3.0022 |
| C12···H33A$^{ii}$ | 3.3470 | H28···H33C$^{xiii}$ | 2.6672 |
| C12···H33B | 3.1989 | H32A···N1$^{ii}$ | 2.8729 |

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|---|---|---|---|
| C12···H33C$^{ii}$ | 3.2500 | H32A···C1$^{ii}$ | 3.1334 |
| C13···H4$^{iv}$ | 3.3865 | H32A···C2$^{ii}$ | 3.0689 |
| C13···H4$^{viii}$ | 3.4499 | H32A···H2$^{ii}$ | 2.8014 |
| C13···H22$^{i}$ | 3.5020 | H32A···H1n$^{ii}$ | 2.7368 |
| C13···H23$^{i}$ | 3.3636 | H32A···H21n$^{vi}$ | 3.5842 |
| C13···H26 | 3.5643 | H32A···H22$^{vi}$ | 2.8427 |
| H2···H6$^{viii}$ | 3.3533 | H32A···H27$^{xiii}$ | 3.3116 |
| H2···H8$^{ix}$ | 3.4300 | H32B···H2$^{ii}$ | 3.4840 |
| H2···C23$^{i}$ | 3.5084 | H32B···N21$^{vi}$ | 3.3261 |
| H2···C24$^{i}$ | 3.0379 | H32B···C21$^{vi}$ | 3.5102 |
| H2···C25$^{i}$ | 3.3639 | H32B···C22$^{vi}$ | 3.2046 |
| H2···C32$^{ii}$ | 3.3457 | H32B···C28$^{v}$ | 3.5320 |
| H2···H24$^{i}$ | 3.0432 | H32B···C29$^{v}$ | 3.4857 |
| H2···H32A$^{ii}$ | 2.8014 | H32B···H21n$^{vi}$ | 2.7055 |
| H2···H32B$^{ii}$ | 3.4840 | H32B···H22$^{vi}$ | 2.6236 |
| H2···H32C$^{ii}$ | 3.2366 | H32B···H33A$^{vi}$ | 3.0150 |
| H3···C7$^{ix}$ | 3.3823 | H32C···N1$^{ii}$ | 3.2841 |
| H3···C8$^{ix}$ | 3.2750 | H32C···H2$^{ii}$ | 3.2366 |
| H3···H7$^{ix}$ | 2.8157 | H32C···H1n$^{ii}$ | 2.7066 |
| H3···H8$^{ix}$ | 2.6041 | H32C···N21$^{v}$ | 3.1878 |
| H3···H13A$^{iii}$ | 3.2995 | H32C···N29$^{v}$ | 3.2210 |
| H3···H13B$^{x}$ | 3.2593 | H32C···C21$^{v}$ | 2.8885 |
| H3···H23$^{ix}$ | 2.7873 | H32C···C25$^{v}$ | 3.1837 |
| H4···C1$^{x}$ | 3.0226 | H32C···C28$^{v}$ | 3.5052 |
| H4···C2$^{x}$ | 3.2340 | H32C···C29$^{v}$ | 2.8530 |
| H4···C3$^{x}$ | 3.3428 | H32C···C30$^{v}$ | 2.6341 |
| H4···C4$^{x}$ | 3.2736 | H33A···C12$^{ii}$ | 3.3470 |
| H4···C5$^{x}$ | 3.0475 | H33A···H12A$^{ii}$ | 2.7227 |
| H4···C10$^{x}$ | 2.9010 | H33A···H12B$^{ii}$ | 3.0943 |
| H4···C13$^{iii}$ | 3.3865 | H33A···H1n$^{ii}$ | 3.5589 |
| H4···C13$^{x}$ | 3.4499 | H33A···N21$^{v}$ | 3.1063 |
| H4···H13A$^{iii}$ | 3.2321 | H33A···C28$^{iii}$ | 3.5240 |
| H4···H13B$^{iii}$ | 3.0647 | H33A···H21n$^{v}$ | 3.3080 |
| H4···H13B$^{x}$ | 2.5235 | H33A···H28$^{iii}$ | 3.1040 |
| H4···H13C$^{iii}$ | 3.2978 | H33A···H32B$^{v}$ | 3.0150 |
| H6···C2$^{x}$ | 3.4343 | H33B···C12 | 3.1989 |
| H6···H2$^{x}$ | 3.3533 | H33B···H12A | 2.5307 |
| H6···H7$^{xiv}$ | 3.1679 | H33B···H12A$^{ii}$ | 3.4961 |
| H6···C23$^{xi}$ | 3.3009 | H33B···H12C | 2.9969 |
| H6···C24$^{xi}$ | 3.1308 | H33B···H28$^{xiii}$ | 3.0022 |
| H6···H23$^{xi}$ | 2.8223 | H33B···H33C$^{ii}$ | 3.4670 |
| H6···H24$^{xi}$ | 2.4821 | H33C···N1$^{ii}$ | 3.3541 |
| H7···C3$^{xii}$ | 3.4852 | H33C···C12$^{ii}$ | 3.2500 |
| H7···C8$^{xi}$ | 3.2821 | H33C···H12A | 3.5273 |
| H7···H3$^{xii}$ | 2.8157 | H33C···H12A$^{ii}$ | 2.3971 |
| H7···H6$^{xiv}$ | 3.1679 | H33C···H12B$^{ii}$ | 3.4433 |
| H7···H8$^{xi}$ | 2.9778 | H33C···H1n$^{ii}$ | 3.4702 |
| H7···C24$^{xi}$ | 3.5757 | H33C···C27$^{xiii}$ | 3.0795 |

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| H7···H23$^{xi}$ | 3.4557 | H33C···C28$^{xiii}$ | 3.2005 |
| H7···H24$^{iii}$ | 3.4063 | H33C···H27$^{xiii}$ | 2.4122 |
| H7···H24$^{xi}$ | 2.8182 | H33C···H28$^{xiii}$ | 2.6672 |
| H7···H26$^{iii}$ | 3.5435 | H33C···H33B$^{ii}$ | 3.4670 |
| H8···C3$^{xii}$ | 3.4420 | | |

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| C1—N1—C11 | 118.4 (3) | C9—N9—H9n | 112.7 (18) |
| C9—N9—C11 | 118.37 (19) | C11—N9—H9n | 114.5 (17) |
| N1—C1—C2 | 122.4 (3) | C1—C2—H2 | 120.147 |
| N1—C1—C10 | 117.7 (2) | C3—C2—H2 | 120.144 |
| C2—C1—C10 | 119.9 (2) | C2—C3—H3 | 119.198 |
| C1—C2—C3 | 119.7 (3) | C4—C3—H3 | 119.197 |
| C2—C3—C4 | 121.6 (3) | C3—C4—H4 | 119.883 |
| C3—C4—C5 | 120.2 (3) | C5—C4—H4 | 119.895 |
| C4—C5—C6 | 122.6 (3) | C5—C6—H6 | 119.925 |
| C4—C5—C10 | 118.7 (3) | C7—C6—H6 | 119.912 |
| C6—C5—C10 | 118.6 (3) | C6—C7—H7 | 119.315 |
| C5—C6—C7 | 120.2 (3) | C8—C7—H7 | 119.307 |
| C6—C7—C8 | 121.4 (3) | C7—C8—H8 | 119.937 |
| C7—C8—C9 | 120.1 (3) | C9—C8—H8 | 119.924 |
| N9—C9—C8 | 123.0 (2) | C11—C12—H12A | 109.477 |
| N9—C9—C10 | 117.0 (3) | C11—C12—H12B | 109.468 |
| C8—C9—C10 | 119.8 (2) | C11—C12—H12C | 109.472 |
| C1—C10—C5 | 119.9 (2) | H12A—C12—H12B | 109.474 |
| C1—C10—C9 | 120.3 (2) | H12A—C12—H12C | 109.472 |
| C5—C10—C9 | 119.8 (3) | H12B—C12—H12C | 109.463 |
| N1—C11—N9 | 106.33 (18) | C11—C13—H13A | 109.472 |
| N1—C11—C12 | 107.6 (3) | C11—C13—H13B | 109.473 |
| N1—C11—C13 | 111.97 (18) | C11—C13—H13C | 109.473 |
| N9—C11—C12 | 108.72 (19) | H13A—C13—H13B | 109.459 |
| N9—C11—C13 | 111.0 (3) | H13A—C13—H13C | 109.477 |
| C12—C11—C13 | 111.01 (19) | H13B—C13—H13C | 109.473 |
| C21—N21—C31 | 117.6 (2) | C21—N21—H21n | 116.9 (16) |
| C29—N29—C31 | 117.32 (19) | C31—N21—H21n | 110.5 (18) |
| N21—C21—C22 | 124.2 (2) | C29—N29—H29n | 114.8 (16) |
| N21—C21—C30 | 116.9 (3) | C31—N29—H29n | 111.0 (16) |
| C22—C21—C30 | 118.8 (2) | C21—C22—H22 | 119.693 |
| C21—C22—C23 | 120.6 (3) | C23—C22—H22 | 119.705 |
| C22—C23—C24 | 121.4 (3) | C22—C23—H23 | 119.309 |
| C23—C24—C25 | 119.9 (2) | C24—C23—H23 | 119.313 |
| C24—C25—C26 | 122.2 (2) | C23—C24—H24 | 120.020 |
| C24—C25—C30 | 119.0 (2) | C25—C24—H24 | 120.040 |
| C26—C25—C30 | 118.8 (3) | C25—C26—H26 | 119.885 |
| C25—C26—C27 | 120.2 (2) | C27—C26—H26 | 119.879 |
| C26—C27—C28 | 121.5 (3) | C26—C27—H27 | 119.268 |
| C27—C28—C29 | 120.0 (3) | C28—C27—H27 | 119.271 |
| N29—C29—C28 | 122.4 (3) | C27—C28—H28 | 120.016 |
| N29—C29—C30 | 117.9 (2) | C29—C28—H28 | 120.012 |

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| C28—C29—C30 | 119.6 (2) | C31—C32—H32A | 109.469 |
| C21—C30—C25 | 120.2 (3) | C31—C32—H32B | 109.478 |
| C21—C30—C29 | 119.7 (2) | C31—C32—H32C | 109.473 |
| C25—C30—C29 | 120.0 (2) | H32A—C32—H32B | 109.470 |
| N21—C31—N29 | 105.38 (19) | H32A—C32—H32C | 109.469 |
| N21—C31—C32 | 109.3 (2) | H32B—C32—H32C | 109.468 |
| N21—C31—C33 | 110.55 (19) | C31—C33—H33A | 109.483 |
| N29—C31—C32 | 108.00 (18) | C31—C33—H33B | 109.470 |
| N29—C31—C33 | 111.9 (2) | C31—C33—H33C | 109.475 |
| C32—C31—C33 | 111.4 (2) | H33A—C33—H33B | 109.464 |
| C1—N1—H1n | 114.0 (14) | H33A—C33—H33C | 109.468 |
| C11—N1—H1n | 114.2 (15) | H33B—C33—H33C | 109.468 |

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| C1—N1—C11—N9 | −48.8 (3) | C21—N21—C31—N29 | −55.3 (3) |
| C1—N1—C11—C12 | −165.13 (16) | C21—N21—C31—C32 | −171.11 (16) |
| C1—N1—C11—C13 | 72.6 (3) | C21—N21—C31—C33 | 65.9 (3) |
| C11—N1—C1—C2 | −156.31 (18) | C31—N21—C21—C22 | −150.43 (19) |
| C11—N1—C1—C10 | 27.4 (3) | C31—N21—C21—C30 | 33.5 (3) |
| C9—N9—C11—N1 | 51.3 (3) | C29—N29—C31—N21 | 51.7 (3) |
| C9—N9—C11—C12 | 166.88 (18) | C29—N29—C31—C32 | 168.5 (2) |
| C9—N9—C11—C13 | −70.7 (3) | C29—N29—C31—C33 | −68.5 (3) |
| C11—N9—C9—C8 | 153.29 (19) | C31—N29—C29—C28 | 157.1 (2) |
| C11—N9—C9—C10 | −32.0 (3) | C31—N29—C29—C30 | −27.6 (3) |
| N1—C1—C2—C3 | −175.13 (17) | N21—C21—C22—C23 | −174.14 (19) |
| N1—C1—C10—C5 | 174.89 (17) | N21—C21—C30—C25 | 173.37 (18) |
| N1—C1—C10—C9 | −3.6 (3) | N21—C21—C30—C29 | −4.1 (3) |
| C2—C1—C10—C5 | −1.5 (3) | C22—C21—C30—C25 | −2.9 (3) |
| C2—C1—C10—C9 | −179.97 (18) | C22—C21—C30—C29 | 179.64 (19) |
| C10—C1—C2—C3 | 1.1 (3) | C30—C21—C22—C23 | 1.9 (4) |
| C1—C2—C3—C4 | 0.3 (4) | C21—C22—C23—C24 | −0.3 (4) |
| C2—C3—C4—C5 | −1.2 (4) | C22—C23—C24—C25 | −0.3 (4) |
| C3—C4—C5—C6 | −179.83 (19) | C23—C24—C25—C26 | 178.4 (2) |
| C3—C4—C5—C10 | 0.8 (3) | C23—C24—C25—C30 | −0.8 (4) |
| C4—C5—C6—C7 | 179.12 (19) | C24—C25—C26—C27 | −178.6 (2) |
| C4—C5—C10—C1 | 0.6 (3) | C24—C25—C30—C21 | 2.4 (4) |
| C4—C5—C10—C9 | 179.05 (18) | C24—C25—C30—C29 | 179.82 (19) |
| C6—C5—C10—C1 | −178.86 (18) | C26—C25—C30—C21 | −176.83 (19) |
| C6—C5—C10—C9 | −0.4 (3) | C26—C25—C30—C29 | 0.6 (4) |
| C10—C5—C6—C7 | −1.5 (3) | C30—C25—C26—C27 | 0.6 (4) |
| C5—C6—C7—C8 | 1.7 (4) | C25—C26—C27—C28 | −1.7 (4) |
| C6—C7—C8—C9 | 0.1 (4) | C26—C27—C28—C29 | 1.6 (4) |
| C7—C8—C9—N9 | 172.64 (19) | C27—C28—C29—N29 | 174.8 (2) |
| C7—C8—C9—C10 | −1.9 (4) | C27—C28—C29—C30 | −0.4 (4) |
| N9—C9—C10—C1 | 5.7 (3) | N29—C29—C30—C21 | 1.3 (3) |
| N9—C9—C10—C5 | −172.81 (17) | N29—C29—C30—C25 | −176.12 (18) |

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|---|---|---|---|
| C8—C9—C10—C1 | −179.45 (18) | C28—C29—C30—C21 | 176.72 (19) |
| C8—C9—C10—C5 | 2.1 (3) | C28—C29—C30—C25 | −0.7 (4) |

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (ii) −*x*+2, −*y*+1, −*z*+1; (iii) *x*, *y*+1, *z*; (iv) *x*, *y*−1, *z*; (v) −*x*+2, *y*+1/2, −*z*+3/2; (vi) −*x*+2, *y*−1/2, −*z*+3/2; (vii) *x*, −*y*+1/2, *z*+1/2; (viii) −*x*+1, *y*−1/2, −*z*+1/2; (ix) *x*, −*y*+3/2, *z*−1/2; (x) −*x*+1, *y*+1/2, −*z*+1/2; (xi) −*x*+1, −*y*+1, −*z*+1; (xii) *x*, −*y*+3/2, *z*+1/2; (xiii) −*x*+2, −*y*, −*z*+1; (xiv) −*x*+1, −*y*+2, −*z*+1.

*Hydrogen-bond geometry (Å, º)*

Cg1, Cg2 and Cg3 are the centroids of the C21–C25/C30, C25–C30 and C5–C10 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| N21—H21N···N29$^{v}$ | 0.88 (2) | 2.36 (2) | 3.229 (4) | 170 (2) |
| N1—H1N···*Cg*1$^{i}$ | 0.93 (3) | 2.93 (3) | 3.853 (3) | 170 (2) |
| N9—H9N···*Cg*1 | 0.88 (4) | 2.85 (2) | 3.703 (3) | 164 (2) |
| C12—H12*C*···*Cg*2 | 0.98 | 2.55 | 3.521 (3) | 172 |
| C26—H26···*Cg*3$^{iv}$ | 0.95 | 2.53 | 3.456 (3) | 164 |

Symmetry codes: (i) *x*, −*y*+1/2, *z*−1/2; (iv) *x*, *y*−1, *z*; (v) −*x*+2, *y*+1/2, −*z*+3/2.