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# 2,4,6-Tris(2,4-dimethylphenyl)-1,3,5-triazine

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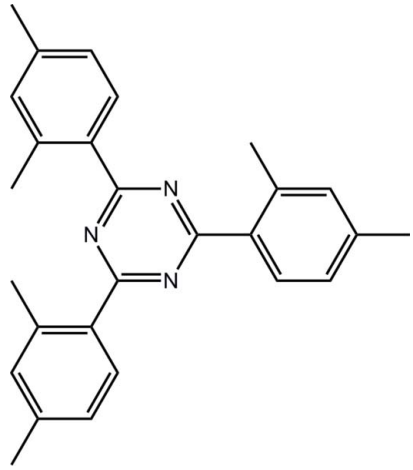
Key indicators: single-crystal X-ray study; $T$ = 100 K; mean $\sigma$(C–C) = 0.005 Å; $R$ factor = 0.085; $wR$ factor = 0.222; data-to-parameter ratio = 17.3.

Two virtually superimposable molecules comprise the asymmetric unit of the title compound, $C_{27}H_{27}N_3$. The range of dihedral angles between the central 1,3,5-triazine ring and the attached benzene rings is 20.88 (14)–31.36 (14)°, and the shape of each molecule is of a flattened bowl. The crystal packing features weak C—H$\cdots\pi$ bonds and $\pi$–$\pi$ interactions between triazine and benzene rings [centroid–centroid separations = 3.7696 (17) and 3.7800 (18) Å] that result in the formation of supramolecular layers in the *ac* plane. The crystal studied was a non-merohedral twin with a minor twin component of 20.7 (3)%.

## Related literature

For the synthesis, see: Orban *et al.* (1988). For the crystal structure of *s*-triphenyltriazine, see: Damiani *et al.* (1965). For homologues, see: Bosch & Barnes (2002); Thalladi *et al.* (1999); Volkis *et al.* (2003). For the separation of twinned diffraction indices, see: Spek (2009).



## Experimental

### Crystal data

$C_{27}H_{27}N_3$
$M_r$ = 393.52
Triclinic, $P\overline{1}$
$a$ = 7.4663 (4) Å
$b$ = 15.0789 (13) Å
$c$ = 19.7266 (12) Å
$\alpha$ = 109.016 (7)°
$\beta$ = 90.949 (5)°
$\gamma$ = 93.717 (6)°
$V$ = 2093.6 (2) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.07 mm$^{-1}$
$T$ = 100 K
0.30 × 0.15 × 0.05 mm

### Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)
$T_{min}$ = 0.978, $T_{max}$ = 0.996
14777 measured reflections
9605 independent reflections
5518 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.222
$S$ = 1.04
9597 reflections
554 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

*Cg*1–*Cg*4 are the centroids of the C39–C44, C31–C36, C12–C17 and C4–C9 rings, respectively.

| $D$—H$\cdots A$ | $D$—H | H$\cdots A$ | $D\cdots A$ | $D$—H$\cdots A$ |
|---|---|---|---|---|
| C11—H11$B\cdots Cg1^{i}$ | 0.98 | 2.97 | 3.777 (4) | 140 |
| C18—H18$B\cdots Cg2^{ii}$ | 0.98 | 2.91 | 3.688 (4) | 137 |
| C38—H38$C\cdots Cg3^{iii}$ | 0.98 | 2.84 | 3.756 (4) | 155 |
| C45—H45$B\cdots Cg4^{iv}$ | 0.98 | 2.77 | 3.596 (4) | 142 |

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

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001), *Qmol* (Gans & Shalloway, 2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6737).

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# supplementary materials

*Acta Cryst.* (2012). E**68**, o1463–o1464 [doi:10.1107/S1600536812016261]

## 2,4,6-Tris(2,4-dimethylphenyl)-1,3,5-triazine

**Jin-Sheng Huang, Mao-Kui Li, Yang-Yi Yang, Seik Weng Ng and Edward R. T. Tiekink**

### Comment

*s*-Triphenyltriazine forms a number of adducts with metal salts; its crystal structure was reported some time ago (Damiani *et al.*, 1965). The crystal structures of substituted derivatives have also been reported, *e.g.* the *p*-tolyl (Thalladi *et al.*, 1999; Volkis *et al.*, 2003). The structure of tris(mesityl)-1,3,5-triazine is known as its silver adduct (Bosch & Barnes, 2002). Herein, the crystal and molecular structure of 2,4,6-tris(2,4-dimethylphenyl)-1,3,5-triazine (I) is described.

Two independent molecules comprise the crystallographic asymmetric unit of (I), Fig. 1. The molecules are virtually superimposable as seen from the overlay diagram, Fig. 2. With respect to the central 1,3,5-triazine ring with the N1—N3 atoms, the dihedral angles with the attached benzene rings C4—C9, C12—C17 and C20—C25 are 29.75 (15), 26.26 (15) and 21.22 (15)°, respectively. The comparable dihedral angles for the N4—N6 triazine and the C31—C36, C39—C44 and C47—C52 rings are 25.23 (15), 31.36 (14) and 20.88 (14)°, respectively. Within each molecule, one of the 2,4-dimethylphenyl residues is orientated in the opposite direction to the other two so that the molecules do not have molecular 3-fold symmetry. Overall, the shape of each molecule is of a flattened bowl.

The crystal packing is dominated by C—H···$\pi$, Table 1, and $\pi$—$\pi$ interactions. The former occur between the independent molecules with each forming two donor and two acceptor interactions. The $\pi$—$\pi$ interactions occur between like molecules with the shortest contacts occurring between triazine and benzene rings [inter-centroid (N1-triazine)···(C20–C25)$^{i}$ distance = 3.7800 (18) Å, angle of inclination = 21.22 (15)° for symmetry operation *i*: 1 - *x*, 1 - *y*, 2 - *z*, and inter-centroid (N4-triazine)···(C47–C52)$^{ii}$ distance = 3.7696 (17) Å, angle of inclination = 20.88 (14)° for symmetry operation *i*: -*x*, 1 - *y*, 2 - *z*]. The result is the formation of supramolecular layers in the *ac* plane that stack along the *b* axis with no specific interactions between them, Fig. 3.

### Experimental

The compound was synthesized by the Friedel-Crafts arylation of cyanuric chloride with excess *m*-xylene in the presence of aluminium trichloride (Orban *et al.*, 1988).

Aluminium chloride (8.7 g, 0.066 mol) was added to cyanuric chloride (4.0 g, 0.022 mol) in chlorobenzene (20 ml). The suspension was stirred by spinning a stirrer at about 250 rpm. It was then heated at 358 K for 20 min. *m*-Xylene (3.0 ml, 0.0242 mol) was added over 30 min; the reaction was exothermic. A second 3 ml portion was added over the next 30 min. The small amount of hydrogen chloride gas that was released was neutralized by 5% sodium hydroxide. A further 3 ml was added over 30 min while keeping the mixture heated at 373 K. The dark-brown reaction mixture was additionally stirred at 378 K for another 20 min.

The warm reaction mixture was added to water (30 ml). The mixture was stirred at 333 K for 10 min. The organic phase was separated and treated with 5% hydrochloric acid. This procedure was repeated.

The solvent was removed and the dark-brown residue was dried at 373 K. It was then transferred it into a 100 ml distillation flask. Toluene (50 ml) was added and the mixture heated at 348 K. To this was added ethanol (15 ml). The

solution was set aside for the crystallization of the compound to give 5.4 g of a light-yellow product. The pure compound was obtained as colourless plates after recrystallization from a toluene and ethanol (5:1) mixture in a yield of 3.5 g.

## Refinement

Carbon-bound H-atoms were placed in calculated positions [C—H = 0.95 to 0.98 Å, $U_{iso}$(H) 1.2 to 1.5$U_{eq}$(C)] and were included in the refinement in the riding model approximation. The crystal is a non-merohedral twin with a twin component of 20.7 (3)%; the twin components were identified by the *TwinRotMat* routine in *PLATON* (Spek, 2009).

Owing to poor agreement several reflections, *i.e.* (4 $\bar{2}$ 4), (3 $\bar{5}$ 16), (4 4 6), (4 1 0), (4 $\bar{3}$ 8), ($\bar{3}$ $\bar{5}$ 16), (4 4 0) and (4 $\bar{2}$ 2), were omitted from the final refinement.

## Computing details

Data collection: *CrysAlis PRO* (Agilent, 2012); cell refinement: *CrysAlis PRO* (Agilent, 2012); data reduction: *CrysAlis PRO* (Agilent, 2012); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *X-SEED* (Barbour, 2001), Qmol (Gans & Shalloway, 2001) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

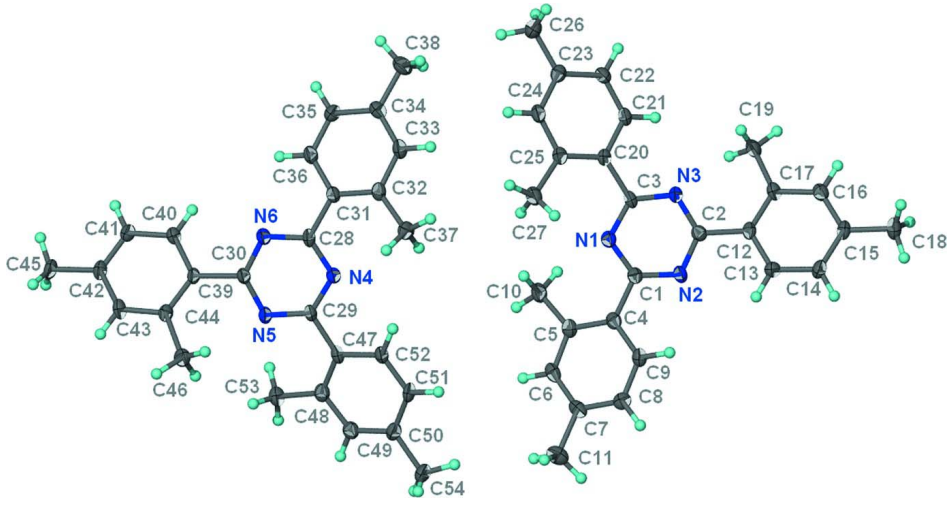


**Figure 1**

The molecular structures of the two independent molecules comprising the asymmetric unit of (I) showing displacement ellipsoids at the 70% probability level.

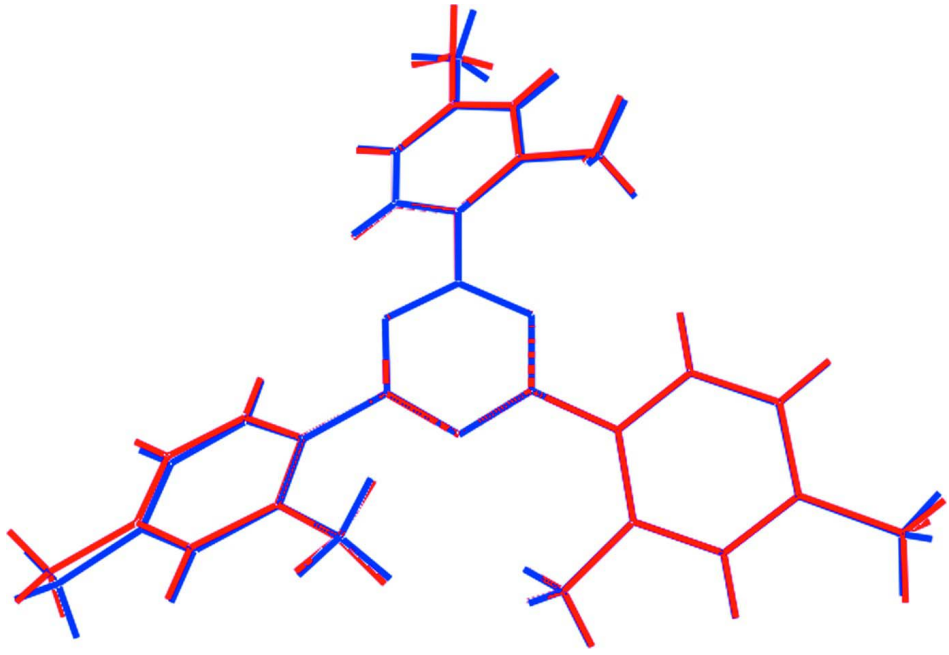

**Figure 2**

An overlay diagram of two independent molecules in (I). The N1-containing molecule is illustrated in red and the N4-molecule in blue. Molecules have been aligned so that the N1,N2,N3 and N5,N6,N4 planes are overlapped.

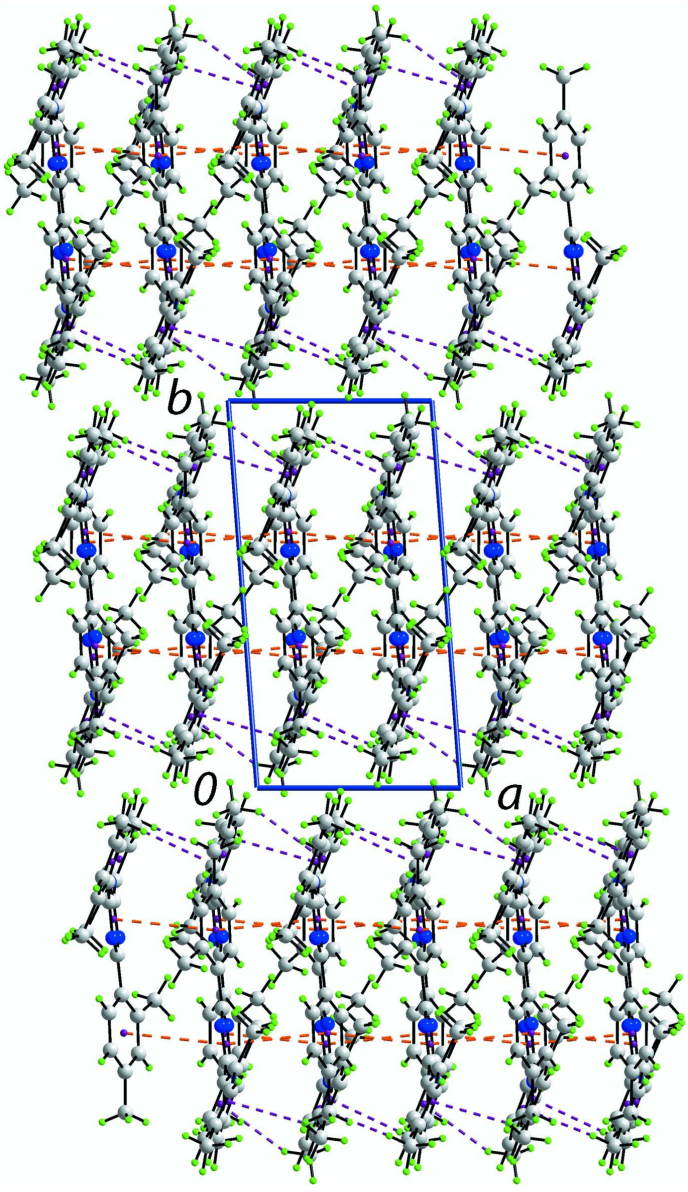


**Figure 3**

A view in projection down the *c* axis of the unit-cell contents for (I). The C—H···$\pi$ and $\pi$–$\pi$ interactions are shown as purple and orange dashed lines, respectively.

### 2,4,6-Tris(2,4-dimethylphenyl)-1,3,5-triazine

*Crystal data*

$C_{27}H_{27}N_3$
$M_r$ = 393.52
Triclinic, $P\overline{1}$
Hall symbol: -P 1
$a$ = 7.4663 (4) Å
$b$ = 15.0789 (13) Å
$c$ = 19.7266 (12) Å
$\alpha$ = 109.016 (7)°
$\beta$ = 90.949 (5)°
$\gamma$ = 93.717 (6)°
$V$ = 2093.6 (2) Å$^3$
$Z$ = 4
$F(000)$ = 840
$D_x$ = 1.248 Mg m$^{-3}$
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 2806 reflections
$\theta$ = 2.7–27.5°
$\mu$ = 0.07 mm$^{-1}$

$T$ = 100 K
Plate, colourless

0.30 × 0.15 × 0.05 mm

*Data collection*

Agilent SuperNova Dual diffractometer with an Atlas detector
Radiation source: SuperNova (Mo) X-ray Source
Mirror monochromator
Detector resolution: 10.4041 pixels mm$^{-1}$
$\omega$ scan
Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2012)

$T_{min}$ = 0.978, $T_{max}$ = 0.996
14777 measured reflections
9605 independent reflections
5518 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.058
$\theta_{max}$ = 27.6°, $\theta_{min}$ = 2.7°
$h = -9 \rightarrow 7$
$k = -16 \rightarrow 19$
$l = -25 \rightarrow 25$

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.085
$wR(F^2)$ = 0.222
$S$ = 1.04
9597 reflections
554 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
$w = 1/[\sigma^2(F_o^2) + (0.0673P)^2 + 1.4043P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.36 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.39 e Å$^{-3}$

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

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.2281 (4) | 0.3830 (2) | 0.89667 (14) | 0.0177 (6) |
| N2 | 0.2497 (4) | 0.2425 (2) | 0.92575 (14) | 0.0178 (6) |
| N3 | 0.2594 (4) | 0.3902 (2) | 1.01875 (14) | 0.0169 (6) |
| N4 | 0.2354 (3) | 0.6128 (2) | 0.57186 (14) | 0.0164 (6) |
| N5 | 0.2624 (4) | 0.6141 (2) | 0.45247 (14) | 0.0171 (6) |
| N6 | 0.2400 (4) | 0.7575 (2) | 0.54849 (14) | 0.0183 (6) |
| C1 | 0.2352 (4) | 0.2892 (2) | 0.87866 (17) | 0.0164 (7) |
| C2 | 0.2602 (4) | 0.2959 (2) | 0.99515 (17) | 0.0169 (7) |
| C3 | 0.2415 (4) | 0.4304 (2) | 0.96749 (17) | 0.0160 (7) |
| C4 | 0.2182 (4) | 0.2313 (2) | 0.80171 (18) | 0.0180 (7) |
| C5 | 0.2769 (4) | 0.2636 (2) | 0.74558 (18) | 0.0197 (7) |
| C6 | 0.2461 (4) | 0.2028 (3) | 0.67513 (18) | 0.0205 (8) |
| H6 | 0.2847 | 0.2238 | 0.6369 | 0.025* |
| C7 | 0.1615 (5) | 0.1129 (3) | 0.65849 (18) | 0.0213 (8) |
| C8 | 0.1094 (4) | 0.0810 (2) | 0.71473 (18) | 0.0199 (7) |
| H8 | 0.0544 | 0.0193 | 0.7048 | 0.024* |
| C9 | 0.1381 (4) | 0.1396 (2) | 0.78498 (18) | 0.0195 (7) |
| H9 | 0.1026 | 0.1171 | 0.8228 | 0.023* |
| C10 | 0.3764 (5) | 0.3579 (3) | 0.75557 (18) | 0.0235 (8) |
| H10A | 0.4585 | 0.3746 | 0.7978 | 0.035* |
| H10B | 0.2899 | 0.4060 | 0.7624 | 0.035* |
| H10C | 0.4451 | 0.3543 | 0.7130 | 0.035* |
| C11 | 0.1230 (5) | 0.0521 (3) | 0.58162 (18) | 0.0277 (9) |

| | | | | |
|---|---|---|---|---|
| H11A | 0.2109 | 0.0696 | 0.5510 | 0.042* |
| H11B | 0.0018 | 0.0612 | 0.5664 | 0.042* |
| H11C | 0.1310 | −0.0141 | 0.5774 | 0.042* |
| C12 | 0.2612 (4) | 0.2466 (2) | 1.04930 (17) | 0.0172 (7) |
| C13 | 0.1863 (5) | 0.1538 (2) | 1.02738 (18) | 0.0203 (8) |
| H13 | 0.1509 | 0.1234 | 0.9783 | 0.024* |
| C14 | 0.1624 (5) | 0.1049 (3) | 1.07584 (18) | 0.0219 (8) |
| H14 | 0.1100 | 0.0421 | 1.0597 | 0.026* |
| C15 | 0.2147 (4) | 0.1475 (2) | 1.14763 (18) | 0.0185 (7) |
| C16 | 0.2977 (4) | 0.2383 (2) | 1.16825 (18) | 0.0202 (8) |
| H16 | 0.3387 | 0.2668 | 1.2169 | 0.024* |
| C17 | 0.3236 (4) | 0.2895 (2) | 1.12107 (17) | 0.0181 (7) |
| C18 | 0.1833 (5) | 0.0972 (3) | 1.20146 (19) | 0.0264 (8) |
| H18A | 0.1205 | 0.0354 | 1.1776 | 0.040* |
| H18B | 0.1101 | 0.1344 | 1.2397 | 0.040* |
| H18C | 0.2989 | 0.0892 | 1.2221 | 0.040* |
| C19 | 0.4222 (5) | 0.3859 (2) | 1.15022 (18) | 0.0229 (8) |
| H19A | 0.4935 | 0.3903 | 1.1935 | 0.034* |
| H19B | 0.3350 | 0.4340 | 1.1621 | 0.034* |
| H19C | 0.5018 | 0.3958 | 1.1139 | 0.034* |
| C20 | 0.2397 (4) | 0.5344 (2) | 0.99277 (17) | 0.0159 (7) |
| C21 | 0.3143 (4) | 0.5832 (2) | 1.06164 (17) | 0.0177 (7) |
| H21 | 0.3577 | 0.5484 | 1.0901 | 0.021* |
| C22 | 0.3266 (4) | 0.6807 (2) | 1.08958 (18) | 0.0193 (7) |
| H22 | 0.3776 | 0.7118 | 1.1365 | 0.023* |
| C23 | 0.2634 (4) | 0.7331 (2) | 1.04829 (18) | 0.0185 (7) |
| C24 | 0.1862 (4) | 0.6847 (2) | 0.98088 (18) | 0.0200 (7) |
| H24 | 0.1413 | 0.7200 | 0.9532 | 0.024* |
| C25 | 0.1710 (4) | 0.5862 (2) | 0.95141 (17) | 0.0184 (7) |
| C26 | 0.2836 (5) | 0.8396 (3) | 1.0768 (2) | 0.0288 (9) |
| H26A | 0.2511 | 0.8645 | 1.0385 | 0.043* |
| H26B | 0.4085 | 0.8606 | 1.0933 | 0.043* |
| H26C | 0.2043 | 0.8625 | 1.1169 | 0.043* |
| C27 | 0.0759 (5) | 0.5441 (3) | 0.87846 (18) | 0.0223 (8) |
| H27A | 0.0037 | 0.5910 | 0.8688 | 0.033* |
| H27B | −0.0025 | 0.4891 | 0.8777 | 0.033* |
| H27C | 0.1650 | 0.5249 | 0.8415 | 0.033* |
| C28 | 0.2320 (4) | 0.7064 (2) | 0.59323 (17) | 0.0171 (7) |
| C29 | 0.2525 (4) | 0.5694 (2) | 0.50159 (17) | 0.0156 (7) |
| C30 | 0.2538 (4) | 0.7078 (2) | 0.47921 (17) | 0.0160 (7) |
| C31 | 0.2327 (4) | 0.7581 (2) | 0.67135 (17) | 0.0170 (7) |
| C32 | 0.1785 (4) | 0.7160 (2) | 0.72288 (18) | 0.0188 (7) |
| C33 | 0.2087 (4) | 0.7689 (3) | 0.79568 (18) | 0.0209 (8) |
| H33 | 0.1746 | 0.7408 | 0.8307 | 0.025* |
| C34 | 0.2864 (4) | 0.8609 (3) | 0.81899 (18) | 0.0202 (8) |
| C35 | 0.3299 (5) | 0.9030 (2) | 0.76749 (18) | 0.0212 (8) |
| H35 | 0.3784 | 0.9665 | 0.7819 | 0.025* |
| C36 | 0.3023 (4) | 0.8519 (2) | 0.69500 (18) | 0.0204 (8) |
| H36 | 0.3316 | 0.8816 | 0.6605 | 0.024* |

| | | | | |
|---|---|---|---|---|
| C37 | 0.0851 (5) | 0.6187 (2) | 0.70535 (18) | 0.0230 (8) |
| H37A | 0.0180 | 0.6147 | 0.7467 | 0.034* |
| H37B | 0.1748 | 0.5719 | 0.6942 | 0.034* |
| H37C | 0.0021 | 0.6064 | 0.6638 | 0.034* |
| C38 | 0.3233 (5) | 0.9130 (3) | 0.89758 (18) | 0.0273 (9) |
| H38A | 0.2176 | 0.9048 | 0.9243 | 0.041* |
| H38B | 0.3500 | 0.9800 | 0.9049 | 0.041* |
| H38C | 0.4264 | 0.8881 | 0.9147 | 0.041* |
| C39 | 0.2682 (4) | 0.7613 (2) | 0.42778 (17) | 0.0155 (7) |
| C40 | 0.3514 (4) | 0.8527 (2) | 0.45439 (18) | 0.0184 (7) |
| H40 | 0.3859 | 0.8784 | 0.5039 | 0.022* |
| C41 | 0.3844 (4) | 0.9064 (2) | 0.40997 (18) | 0.0193 (7) |
| H41 | 0.4430 | 0.9677 | 0.4290 | 0.023* |
| C42 | 0.3317 (4) | 0.8704 (2) | 0.33773 (18) | 0.0191 (7) |
| C43 | 0.2414 (4) | 0.7819 (2) | 0.31238 (18) | 0.0195 (7) |
| H43 | 0.1998 | 0.7584 | 0.2636 | 0.023* |
| C44 | 0.2091 (4) | 0.7257 (2) | 0.35570 (18) | 0.0175 (7) |
| C45 | 0.3768 (5) | 0.9246 (2) | 0.28692 (19) | 0.0218 (8) |
| H45A | 0.2726 | 0.9197 | 0.2547 | 0.033* |
| H45B | 0.4789 | 0.8982 | 0.2586 | 0.033* |
| H45C | 0.4079 | 0.9908 | 0.3146 | 0.033* |
| C46 | 0.1078 (5) | 0.6305 (2) | 0.32061 (18) | 0.0242 (8) |
| H46A | 0.0205 | 0.6185 | 0.3537 | 0.036* |
| H46B | 0.1929 | 0.5813 | 0.3089 | 0.036* |
| H46C | 0.0447 | 0.6302 | 0.2766 | 0.036* |
| C47 | 0.2593 (4) | 0.4660 (2) | 0.47766 (17) | 0.0167 (7) |
| C48 | 0.3293 (4) | 0.4124 (3) | 0.41262 (18) | 0.0198 (8) |
| C49 | 0.3207 (4) | 0.3143 (3) | 0.39598 (18) | 0.0203 (8) |
| H49 | 0.3674 | 0.2778 | 0.3519 | 0.024* |
| C50 | 0.2477 (4) | 0.2679 (2) | 0.44048 (19) | 0.0200 (7) |
| C51 | 0.1841 (4) | 0.3229 (2) | 0.50602 (18) | 0.0203 (8) |
| H51 | 0.1363 | 0.2935 | 0.5383 | 0.024* |
| C52 | 0.1902 (4) | 0.4195 (2) | 0.52416 (17) | 0.0173 (7) |
| H52 | 0.1469 | 0.4555 | 0.5690 | 0.021* |
| C53 | 0.4187 (5) | 0.4523 (3) | 0.35912 (18) | 0.0219 (8) |
| H53A | 0.4951 | 0.4061 | 0.3287 | 0.033* |
| H53B | 0.4924 | 0.5101 | 0.3850 | 0.033* |
| H53C | 0.3264 | 0.4666 | 0.3291 | 0.033* |
| C54 | 0.2342 (5) | 0.1619 (2) | 0.4188 (2) | 0.0269 (8) |
| H54A | 0.2463 | 0.1431 | 0.4616 | 0.040* |
| H54B | 0.3303 | 0.1369 | 0.3863 | 0.040* |
| H54C | 0.1174 | 0.1369 | 0.3944 | 0.040* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0190 (15) | 0.0186 (16) | 0.0168 (15) | 0.0022 (11) | 0.0005 (11) | 0.0072 (12) |
| N2 | 0.0189 (15) | 0.0212 (16) | 0.0149 (15) | −0.0009 (11) | −0.0018 (11) | 0.0088 (13) |
| N3 | 0.0200 (15) | 0.0170 (15) | 0.0151 (15) | −0.0002 (11) | 0.0005 (11) | 0.0075 (12) |
| N4 | 0.0181 (15) | 0.0171 (15) | 0.0148 (15) | 0.0004 (11) | 0.0002 (11) | 0.0065 (12) |

| | | | | | | |
|---|---|---|---|---|---|---|
| N5 | 0.0203 (15) | 0.0178 (15) | 0.0159 (15) | 0.0018 (11) | 0.0017 (11) | 0.0091 (12) |
| N6 | 0.0215 (15) | 0.0194 (16) | 0.0151 (15) | −0.0016 (12) | 0.0004 (11) | 0.0078 (12) |
| C1 | 0.0154 (17) | 0.0183 (18) | 0.0160 (17) | 0.0022 (13) | 0.0027 (12) | 0.0061 (14) |
| C2 | 0.0159 (17) | 0.0190 (18) | 0.0158 (17) | 0.0002 (13) | 0.0007 (12) | 0.0059 (14) |
| C3 | 0.0151 (17) | 0.0221 (19) | 0.0129 (17) | 0.0009 (13) | 0.0002 (12) | 0.0088 (14) |
| C4 | 0.0179 (17) | 0.0206 (19) | 0.0168 (17) | 0.0042 (13) | 0.0003 (12) | 0.0073 (15) |
| C5 | 0.0195 (18) | 0.0221 (19) | 0.0200 (18) | 0.0018 (14) | −0.0001 (13) | 0.0101 (15) |
| C6 | 0.0195 (18) | 0.028 (2) | 0.0162 (18) | 0.0071 (14) | 0.0010 (13) | 0.0100 (16) |
| C7 | 0.0214 (19) | 0.027 (2) | 0.0150 (18) | 0.0065 (14) | 0.0000 (13) | 0.0048 (15) |
| C8 | 0.0174 (18) | 0.0193 (19) | 0.0227 (19) | 0.0026 (13) | −0.0002 (13) | 0.0062 (15) |
| C9 | 0.0203 (18) | 0.0215 (19) | 0.0196 (18) | 0.0010 (14) | 0.0008 (13) | 0.0108 (15) |
| C10 | 0.028 (2) | 0.027 (2) | 0.0194 (19) | 0.0045 (15) | 0.0058 (14) | 0.0115 (16) |
| C11 | 0.025 (2) | 0.033 (2) | 0.022 (2) | −0.0002 (16) | −0.0011 (14) | 0.0046 (17) |
| C12 | 0.0183 (17) | 0.0188 (18) | 0.0178 (18) | 0.0052 (13) | 0.0022 (12) | 0.0098 (15) |
| C13 | 0.0250 (19) | 0.0174 (19) | 0.0178 (18) | −0.0001 (14) | 0.0005 (14) | 0.0050 (15) |
| C14 | 0.027 (2) | 0.0180 (19) | 0.024 (2) | 0.0019 (14) | 0.0023 (14) | 0.0117 (16) |
| C15 | 0.0186 (18) | 0.0202 (19) | 0.0214 (19) | 0.0046 (13) | 0.0037 (13) | 0.0124 (15) |
| C16 | 0.0230 (19) | 0.022 (2) | 0.0161 (18) | 0.0034 (14) | −0.0002 (13) | 0.0071 (15) |
| C17 | 0.0179 (17) | 0.0230 (19) | 0.0156 (17) | 0.0019 (13) | 0.0019 (12) | 0.0093 (15) |
| C18 | 0.031 (2) | 0.029 (2) | 0.025 (2) | 0.0021 (16) | 0.0009 (15) | 0.0173 (17) |
| C19 | 0.029 (2) | 0.026 (2) | 0.0151 (18) | −0.0032 (15) | −0.0022 (14) | 0.0086 (16) |
| C20 | 0.0164 (17) | 0.0178 (18) | 0.0158 (17) | 0.0020 (13) | 0.0018 (12) | 0.0085 (14) |
| C21 | 0.0177 (17) | 0.0222 (19) | 0.0159 (17) | −0.0002 (13) | −0.0010 (12) | 0.0104 (15) |
| C22 | 0.0220 (18) | 0.0214 (19) | 0.0141 (17) | 0.0015 (14) | 0.0001 (13) | 0.0053 (15) |
| C23 | 0.0172 (17) | 0.0188 (18) | 0.0214 (19) | 0.0019 (13) | 0.0044 (13) | 0.0090 (15) |
| C24 | 0.0242 (19) | 0.022 (2) | 0.0166 (18) | 0.0059 (14) | 0.0041 (13) | 0.0098 (15) |
| C25 | 0.0191 (18) | 0.0208 (19) | 0.0175 (18) | 0.0030 (13) | 0.0026 (13) | 0.0088 (15) |
| C26 | 0.041 (2) | 0.020 (2) | 0.026 (2) | 0.0015 (16) | 0.0005 (16) | 0.0093 (17) |
| C27 | 0.0255 (19) | 0.025 (2) | 0.0186 (18) | 0.0052 (15) | 0.0018 (14) | 0.0091 (16) |
| C28 | 0.0168 (17) | 0.0217 (19) | 0.0164 (17) | −0.0005 (13) | 0.0011 (12) | 0.0114 (15) |
| C29 | 0.0163 (17) | 0.0191 (18) | 0.0134 (17) | −0.0006 (13) | −0.0007 (12) | 0.0087 (14) |
| C30 | 0.0173 (17) | 0.0181 (18) | 0.0140 (17) | −0.0005 (13) | 0.0007 (12) | 0.0076 (14) |
| C31 | 0.0192 (17) | 0.0186 (18) | 0.0145 (17) | 0.0020 (13) | −0.0002 (12) | 0.0074 (14) |
| C32 | 0.0185 (18) | 0.0213 (19) | 0.0194 (18) | 0.0014 (14) | −0.0018 (13) | 0.0107 (15) |
| C33 | 0.0227 (19) | 0.025 (2) | 0.0186 (18) | 0.0003 (14) | 0.0018 (13) | 0.0119 (16) |
| C34 | 0.0203 (18) | 0.024 (2) | 0.0162 (18) | 0.0029 (14) | 0.0016 (13) | 0.0062 (15) |
| C35 | 0.0260 (19) | 0.0165 (18) | 0.0218 (19) | 0.0002 (14) | 0.0017 (14) | 0.0077 (15) |
| C36 | 0.0244 (19) | 0.023 (2) | 0.0164 (18) | 0.0019 (14) | 0.0041 (13) | 0.0095 (15) |
| C37 | 0.0251 (19) | 0.023 (2) | 0.0220 (19) | −0.0058 (15) | 0.0020 (14) | 0.0099 (16) |
| C38 | 0.032 (2) | 0.031 (2) | 0.0171 (19) | 0.0004 (16) | 0.0031 (15) | 0.0059 (17) |
| C39 | 0.0180 (17) | 0.0158 (17) | 0.0152 (17) | 0.0017 (13) | 0.0035 (12) | 0.0082 (14) |
| C40 | 0.0199 (18) | 0.0210 (19) | 0.0159 (17) | 0.0017 (14) | 0.0016 (13) | 0.0081 (15) |
| C41 | 0.0218 (18) | 0.0171 (18) | 0.0205 (18) | −0.0005 (13) | 0.0020 (13) | 0.0087 (15) |
| C42 | 0.0193 (18) | 0.0208 (19) | 0.0223 (19) | 0.0045 (13) | 0.0060 (13) | 0.0131 (16) |
| C43 | 0.0181 (17) | 0.027 (2) | 0.0188 (18) | 0.0031 (14) | 0.0032 (13) | 0.0139 (16) |
| C44 | 0.0180 (17) | 0.0181 (18) | 0.0185 (18) | −0.0002 (13) | 0.0035 (13) | 0.0087 (15) |
| C45 | 0.0266 (19) | 0.0191 (19) | 0.025 (2) | 0.0012 (14) | 0.0038 (14) | 0.0139 (16) |
| C46 | 0.029 (2) | 0.023 (2) | 0.0215 (19) | −0.0018 (15) | −0.0043 (14) | 0.0097 (16) |
| C47 | 0.0156 (17) | 0.0231 (19) | 0.0147 (17) | 0.0012 (13) | 0.0005 (12) | 0.0108 (15) |

| | | | | | | |
|---|---|---|---|---|---|---|
| C48 | 0.0187 (18) | 0.0224 (19) | 0.0206 (19) | −0.0007 (14) | −0.0021 (13) | 0.0105 (15) |
| C49 | 0.0213 (18) | 0.0219 (19) | 0.0188 (18) | 0.0044 (14) | 0.0003 (13) | 0.0076 (15) |
| C50 | 0.0208 (18) | 0.0185 (18) | 0.0229 (19) | −0.0013 (14) | −0.0022 (13) | 0.0103 (16) |
| C51 | 0.0234 (19) | 0.0200 (19) | 0.0227 (19) | 0.0000 (14) | 0.0022 (14) | 0.0144 (16) |
| C52 | 0.0187 (18) | 0.0202 (18) | 0.0150 (17) | 0.0001 (13) | 0.0007 (13) | 0.0086 (15) |
| C53 | 0.0214 (19) | 0.026 (2) | 0.0218 (19) | 0.0024 (14) | 0.0015 (14) | 0.0117 (16) |
| C54 | 0.038 (2) | 0.018 (2) | 0.026 (2) | 0.0004 (16) | 0.0031 (16) | 0.0110 (17) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C3 | 1.345 (4) | C26—H26A | 0.9800 |
| N1—C1 | 1.346 (4) | C26—H26B | 0.9800 |
| N2—C2 | 1.341 (4) | C26—H26C | 0.9800 |
| N2—C1 | 1.343 (4) | C27—H27A | 0.9800 |
| N3—C2 | 1.344 (4) | C27—H27B | 0.9800 |
| N3—C3 | 1.347 (4) | C27—H27C | 0.9800 |
| N4—C28 | 1.338 (4) | C28—C31 | 1.483 (5) |
| N4—C29 | 1.338 (4) | C29—C47 | 1.478 (5) |
| N5—C30 | 1.344 (4) | C30—C39 | 1.489 (4) |
| N5—C29 | 1.350 (4) | C31—C36 | 1.398 (5) |
| N6—C30 | 1.337 (4) | C31—C32 | 1.415 (4) |
| N6—C28 | 1.347 (4) | C32—C33 | 1.403 (5) |
| C1—C4 | 1.483 (5) | C32—C37 | 1.512 (4) |
| C2—C12 | 1.487 (5) | C33—C34 | 1.394 (5) |
| C3—C20 | 1.484 (5) | C33—H33 | 0.9500 |
| C4—C9 | 1.403 (5) | C34—C35 | 1.395 (5) |
| C4—C5 | 1.412 (5) | C34—C38 | 1.504 (5) |
| C5—C6 | 1.399 (5) | C35—C36 | 1.390 (5) |
| C5—C10 | 1.513 (5) | C35—H35 | 0.9500 |
| C6—C7 | 1.391 (5) | C36—H36 | 0.9500 |
| C6—H6 | 0.9500 | C37—H37A | 0.9800 |
| C7—C8 | 1.397 (5) | C37—H37B | 0.9800 |
| C7—C11 | 1.506 (5) | C37—H37C | 0.9800 |
| C8—C9 | 1.383 (5) | C38—H38A | 0.9800 |
| C8—H8 | 0.9500 | C38—H38B | 0.9800 |
| C9—H9 | 0.9500 | C38—H38C | 0.9800 |
| C10—H10A | 0.9800 | C39—C44 | 1.399 (4) |
| C10—H10B | 0.9800 | C39—C40 | 1.403 (4) |
| C10—H10C | 0.9800 | C40—C41 | 1.388 (5) |
| C11—H11A | 0.9800 | C40—H40 | 0.9500 |
| C11—H11B | 0.9800 | C41—C42 | 1.389 (5) |
| C11—H11C | 0.9800 | C41—H41 | 0.9500 |
| C12—C13 | 1.398 (4) | C42—C43 | 1.388 (5) |
| C12—C17 | 1.408 (4) | C42—C45 | 1.514 (4) |
| C13—C14 | 1.392 (5) | C43—C44 | 1.399 (4) |
| C13—H13 | 0.9500 | C43—H43 | 0.9500 |
| C14—C15 | 1.388 (5) | C44—C46 | 1.519 (4) |
| C14—H14 | 0.9500 | C45—H45A | 0.9800 |
| C15—C16 | 1.393 (5) | C45—H45B | 0.9800 |
| C15—C18 | 1.506 (5) | C45—H45C | 0.9800 |

| | | | |
|---|---|---|---|
| C16—C17 | 1.398 (5) | C46—H46A | 0.9800 |
| C16—H16 | 0.9500 | C46—H46B | 0.9800 |
| C17—C19 | 1.513 (5) | C46—H46C | 0.9800 |
| C18—H18A | 0.9800 | C47—C48 | 1.405 (5) |
| C18—H18B | 0.9800 | C47—C52 | 1.409 (4) |
| C18—H18C | 0.9800 | C48—C49 | 1.403 (5) |
| C19—H19A | 0.9800 | C48—C53 | 1.519 (5) |
| C19—H19B | 0.9800 | C49—C50 | 1.387 (5) |
| C19—H19C | 0.9800 | C49—H49 | 0.9500 |
| C20—C21 | 1.402 (4) | C50—C51 | 1.399 (5) |
| C20—C25 | 1.411 (5) | C50—C54 | 1.510 (5) |
| C21—C22 | 1.389 (5) | C51—C52 | 1.379 (5) |
| C21—H21 | 0.9500 | C51—H51 | 0.9500 |
| C22—C23 | 1.401 (5) | C52—H52 | 0.9500 |
| C22—H22 | 0.9500 | C53—H53A | 0.9800 |
| C23—C24 | 1.386 (5) | C53—H53B | 0.9800 |
| C23—C26 | 1.515 (5) | C53—H53C | 0.9800 |
| C24—C25 | 1.404 (5) | C54—H54A | 0.9800 |
| C24—H24 | 0.9500 | C54—H54B | 0.9800 |
| C25—C27 | 1.514 (4) | C54—H54C | 0.9800 |

| | | | |
|---|---|---|---|
| C3—N1—C1 | 115.2 (3) | C25—C27—H27C | 109.5 |
| C2—N2—C1 | 115.5 (3) | H27A—C27—H27C | 109.5 |
| C2—N3—C3 | 115.6 (3) | H27B—C27—H27C | 109.5 |
| C28—N4—C29 | 116.5 (3) | N4—C28—N6 | 124.0 (3) |
| C30—N5—C29 | 114.8 (3) | N4—C28—C31 | 118.2 (3) |
| C30—N6—C28 | 115.1 (3) | N6—C28—C31 | 117.6 (3) |
| N2—C1—N1 | 124.8 (3) | N4—C29—N5 | 124.0 (3) |
| N2—C1—C4 | 116.5 (3) | N4—C29—C47 | 116.9 (3) |
| N1—C1—C4 | 118.7 (3) | N5—C29—C47 | 119.1 (3) |
| N2—C2—N3 | 124.4 (3) | N6—C30—N5 | 125.5 (3) |
| N2—C2—C12 | 117.3 (3) | N6—C30—C39 | 117.2 (3) |
| N3—C2—C12 | 118.1 (3) | N5—C30—C39 | 117.3 (3) |
| N1—C3—N3 | 124.5 (3) | C36—C31—C32 | 118.8 (3) |
| N1—C3—C20 | 119.3 (3) | C36—C31—C28 | 117.5 (3) |
| N3—C3—C20 | 116.2 (3) | C32—C31—C28 | 123.6 (3) |
| C9—C4—C5 | 119.2 (3) | C33—C32—C31 | 117.9 (3) |
| C9—C4—C1 | 117.0 (3) | C33—C32—C37 | 117.3 (3) |
| C5—C4—C1 | 123.7 (3) | C31—C32—C37 | 124.7 (3) |
| C6—C5—C4 | 117.8 (3) | C34—C33—C32 | 123.0 (3) |
| C6—C5—C10 | 117.1 (3) | C34—C33—H33 | 118.5 |
| C4—C5—C10 | 125.1 (3) | C32—C33—H33 | 118.5 |
| C7—C6—C5 | 123.0 (3) | C33—C34—C35 | 118.2 (3) |
| C7—C6—H6 | 118.5 | C33—C34—C38 | 120.8 (3) |
| C5—C6—H6 | 118.5 | C35—C34—C38 | 121.0 (3) |
| C6—C7—C8 | 118.5 (3) | C36—C35—C34 | 119.9 (3) |
| C6—C7—C11 | 120.8 (3) | C36—C35—H35 | 120.0 |
| C8—C7—C11 | 120.7 (3) | C34—C35—H35 | 120.0 |
| C9—C8—C7 | 119.9 (3) | C35—C36—C31 | 122.0 (3) |

| | | | |
|---|---|---|---|
| C9—C8—H8 | 120.1 | C35—C36—H36 | 119.0 |
| C7—C8—H8 | 120.1 | C31—C36—H36 | 119.0 |
| C8—C9—C4 | 121.6 (3) | C32—C37—H37A | 109.5 |
| C8—C9—H9 | 119.2 | C32—C37—H37B | 109.5 |
| C4—C9—H9 | 119.2 | H37A—C37—H37B | 109.5 |
| C5—C10—H10A | 109.5 | C32—C37—H37C | 109.5 |
| C5—C10—H10B | 109.5 | H37A—C37—H37C | 109.5 |
| H10A—C10—H10B | 109.5 | H37B—C37—H37C | 109.5 |
| C5—C10—H10C | 109.5 | C34—C38—H38A | 109.5 |
| H10A—C10—H10C | 109.5 | C34—C38—H38B | 109.5 |
| H10B—C10—H10C | 109.5 | H38A—C38—H38B | 109.5 |
| C7—C11—H11A | 109.5 | C34—C38—H38C | 109.5 |
| C7—C11—H11B | 109.5 | H38A—C38—H38C | 109.5 |
| H11A—C11—H11B | 109.5 | H38B—C38—H38C | 109.5 |
| C7—C11—H11C | 109.5 | C44—C39—C40 | 118.9 (3) |
| H11A—C11—H11C | 109.5 | C44—C39—C30 | 124.6 (3) |
| H11B—C11—H11C | 109.5 | C40—C39—C30 | 116.5 (3) |
| C13—C12—C17 | 119.1 (3) | C41—C40—C39 | 121.5 (3) |
| C13—C12—C2 | 116.9 (3) | C41—C40—H40 | 119.3 |
| C17—C12—C2 | 123.9 (3) | C39—C40—H40 | 119.3 |
| C14—C13—C12 | 121.4 (3) | C40—C41—C42 | 120.0 (3) |
| C14—C13—H13 | 119.3 | C40—C41—H41 | 120.0 |
| C12—C13—H13 | 119.3 | C42—C41—H41 | 120.0 |
| C15—C14—C13 | 120.3 (3) | C43—C42—C41 | 118.4 (3) |
| C15—C14—H14 | 119.9 | C43—C42—C45 | 120.4 (3) |
| C13—C14—H14 | 119.8 | C41—C42—C45 | 121.2 (3) |
| C14—C15—C16 | 117.8 (3) | C42—C43—C44 | 122.7 (3) |
| C14—C15—C18 | 121.1 (3) | C42—C43—H43 | 118.6 |
| C16—C15—C18 | 121.1 (3) | C44—C43—H43 | 118.6 |
| C15—C16—C17 | 123.4 (3) | C39—C44—C43 | 118.4 (3) |
| C15—C16—H16 | 118.3 | C39—C44—C46 | 124.8 (3) |
| C17—C16—H16 | 118.3 | C43—C44—C46 | 116.8 (3) |
| C16—C17—C12 | 117.8 (3) | C42—C45—H45A | 109.5 |
| C16—C17—C19 | 117.6 (3) | C42—C45—H45B | 109.5 |
| C12—C17—C19 | 124.6 (3) | H45A—C45—H45B | 109.5 |
| C15—C18—H18A | 109.5 | C42—C45—H45C | 109.5 |
| C15—C18—H18B | 109.5 | H45A—C45—H45C | 109.5 |
| H18A—C18—H18B | 109.5 | H45B—C45—H45C | 109.5 |
| C15—C18—H18C | 109.5 | C44—C46—H46A | 109.5 |
| H18A—C18—H18C | 109.5 | C44—C46—H46B | 109.5 |
| H18B—C18—H18C | 109.5 | H46A—C46—H46B | 109.5 |
| C17—C19—H19A | 109.5 | C44—C46—H46C | 109.5 |
| C17—C19—H19B | 109.5 | H46A—C46—H46C | 109.5 |
| H19A—C19—H19B | 109.5 | H46B—C46—H46C | 109.5 |
| C17—C19—H19C | 109.5 | C48—C47—C52 | 118.8 (3) |
| H19A—C19—H19C | 109.5 | C48—C47—C29 | 124.5 (3) |
| H19B—C19—H19C | 109.5 | C52—C47—C29 | 116.7 (3) |
| C21—C20—C25 | 118.8 (3) | C49—C48—C47 | 118.0 (3) |
| C21—C20—C3 | 117.1 (3) | C49—C48—C53 | 116.8 (3) |

| | | | |
|---|---|---|---|
| C25—C20—C3 | 124.0 (3) | C47—C48—C53 | 125.1 (3) |
| C22—C21—C20 | 122.1 (3) | C50—C49—C48 | 123.4 (3) |
| C22—C21—H21 | 119.0 | C50—C49—H49 | 118.3 |
| C20—C21—H21 | 119.0 | C48—C49—H49 | 118.3 |
| C21—C22—C23 | 119.7 (3) | C49—C50—C51 | 117.6 (3) |
| C21—C22—H22 | 120.2 | C49—C50—C54 | 121.5 (3) |
| C23—C22—H22 | 120.2 | C51—C50—C54 | 121.0 (3) |
| C24—C23—C22 | 118.2 (3) | C52—C51—C50 | 120.6 (3) |
| C24—C23—C26 | 121.6 (3) | C52—C51—H51 | 119.7 |
| C22—C23—C26 | 120.2 (3) | C50—C51—H51 | 119.7 |
| C23—C24—C25 | 123.4 (3) | C51—C52—C47 | 121.5 (3) |
| C23—C24—H24 | 118.3 | C51—C52—H52 | 119.2 |
| C25—C24—H24 | 118.3 | C47—C52—H52 | 119.2 |
| C24—C25—C20 | 117.8 (3) | C48—C53—H53A | 109.5 |
| C24—C25—C27 | 116.9 (3) | C48—C53—H53B | 109.5 |
| C20—C25—C27 | 125.3 (3) | H53A—C53—H53B | 109.5 |
| C23—C26—H26A | 109.5 | C48—C53—H53C | 109.5 |
| C23—C26—H26B | 109.5 | H53A—C53—H53C | 109.5 |
| H26A—C26—H26B | 109.5 | H53B—C53—H53C | 109.5 |
| C23—C26—H26C | 109.5 | C50—C54—H54A | 109.5 |
| H26A—C26—H26C | 109.5 | C50—C54—H54B | 109.5 |
| H26B—C26—H26C | 109.5 | H54A—C54—H54B | 109.5 |
| C25—C27—H27A | 109.5 | C50—C54—H54C | 109.5 |
| C25—C27—H27B | 109.5 | H54A—C54—H54C | 109.5 |
| H27A—C27—H27B | 109.5 | H54B—C54—H54C | 109.5 |

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| C2—N2—C1—N1 | −1.1 (5) | C29—N4—C28—N6 | 1.7 (5) |
| C2—N2—C1—C4 | −178.3 (3) | C29—N4—C28—C31 | −173.6 (3) |
| C3—N1—C1—N2 | 1.7 (5) | C30—N6—C28—N4 | −0.6 (5) |
| C3—N1—C1—C4 | 178.9 (3) | C30—N6—C28—C31 | 174.8 (3) |
| C1—N2—C2—N3 | −0.9 (5) | C28—N4—C29—N5 | −1.4 (5) |
| C1—N2—C2—C12 | 175.1 (3) | C28—N4—C29—C47 | 179.1 (3) |
| C3—N3—C2—N2 | 1.9 (5) | C30—N5—C29—N4 | 0.0 (4) |
| C3—N3—C2—C12 | −174.0 (3) | C30—N5—C29—C47 | 179.5 (3) |
| C1—N1—C3—N3 | −0.5 (5) | C28—N6—C30—N5 | −1.0 (5) |
| C1—N1—C3—C20 | 178.5 (3) | C28—N6—C30—C39 | −178.4 (3) |
| C2—N3—C3—N1 | −1.1 (5) | C29—N5—C30—N6 | 1.2 (5) |
| C2—N3—C3—C20 | 179.8 (3) | C29—N5—C30—C39 | 178.6 (3) |
| N2—C1—C4—C9 | 28.5 (4) | N4—C28—C31—C36 | 154.1 (3) |
| N1—C1—C4—C9 | −148.9 (3) | N6—C28—C31—C36 | −21.6 (5) |
| N2—C1—C4—C5 | −151.8 (3) | N4—C28—C31—C32 | −21.5 (5) |
| N1—C1—C4—C5 | 30.8 (5) | N6—C28—C31—C32 | 162.8 (3) |
| C9—C4—C5—C6 | 2.2 (5) | C36—C31—C32—C33 | −4.2 (5) |
| C1—C4—C5—C6 | −177.5 (3) | C28—C31—C32—C33 | 171.3 (3) |
| C9—C4—C5—C10 | −175.7 (3) | C36—C31—C32—C37 | 174.0 (3) |
| C1—C4—C5—C10 | 4.6 (5) | C28—C31—C32—C37 | −10.5 (5) |
| C4—C5—C6—C7 | −0.2 (5) | C31—C32—C33—C34 | 1.1 (5) |
| C10—C5—C6—C7 | 177.9 (3) | C37—C32—C33—C34 | −177.2 (3) |
| C5—C6—C7—C8 | −1.8 (5) | C32—C33—C34—C35 | 2.4 (5) |

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| C5—C6—C7—C11 | 176.8 (3) | C32—C33—C34—C38 | −177.3 (3) |
| C6—C7—C8—C9 | 1.7 (5) | C33—C34—C35—C36 | −2.6 (5) |
| C11—C7—C8—C9 | −176.8 (3) | C38—C34—C35—C36 | 177.0 (3) |
| C7—C8—C9—C4 | 0.3 (5) | C34—C35—C36—C31 | −0.5 (5) |
| C5—C4—C9—C8 | −2.3 (5) | C32—C31—C36—C35 | 4.0 (5) |
| C1—C4—C9—C8 | 177.5 (3) | C28—C31—C36—C35 | −171.8 (3) |
| N2—C2—C12—C13 | −23.1 (4) | N6—C30—C39—C44 | −151.5 (3) |
| N3—C2—C12—C13 | 153.1 (3) | N5—C30—C39—C44 | 30.9 (5) |
| N2—C2—C12—C17 | 160.4 (3) | N6—C30—C39—C40 | 30.1 (4) |
| N3—C2—C12—C17 | −23.3 (5) | N5—C30—C39—C40 | −147.5 (3) |
| C17—C12—C13—C14 | 3.9 (5) | C44—C39—C40—C41 | −3.4 (5) |
| C2—C12—C13—C14 | −172.8 (3) | C30—C39—C40—C41 | 175.1 (3) |
| C12—C13—C14—C15 | −0.7 (5) | C39—C40—C41—C42 | 1.2 (5) |
| C13—C14—C15—C16 | −2.6 (5) | C40—C41—C42—C43 | 2.1 (5) |
| C13—C14—C15—C18 | 177.5 (3) | C40—C41—C42—C45 | −175.9 (3) |
| C14—C15—C16—C17 | 2.8 (5) | C41—C42—C43—C44 | −3.2 (5) |
| C18—C15—C16—C17 | −177.4 (3) | C45—C42—C43—C44 | 174.8 (3) |
| C15—C16—C17—C12 | 0.4 (5) | C40—C39—C44—C43 | 2.3 (5) |
| C15—C16—C17—C19 | −177.7 (3) | C30—C39—C44—C43 | −176.1 (3) |
| C13—C12—C17—C16 | −3.6 (5) | C40—C39—C44—C46 | −176.4 (3) |
| C2—C12—C17—C16 | 172.7 (3) | C30—C39—C44—C46 | 5.2 (5) |
| C13—C12—C17—C19 | 174.3 (3) | C42—C43—C44—C39 | 1.0 (5) |
| C2—C12—C17—C19 | −9.3 (5) | C42—C43—C44—C46 | 179.8 (3) |
| N1—C3—C20—C21 | −158.5 (3) | N4—C29—C47—C48 | −159.9 (3) |
| N3—C3—C20—C21 | 20.7 (4) | N5—C29—C47—C48 | 20.6 (5) |
| N1—C3—C20—C25 | 20.3 (5) | N4—C29—C47—C52 | 20.1 (4) |
| N3—C3—C20—C25 | −160.5 (3) | N5—C29—C47—C52 | −159.5 (3) |
| C25—C20—C21—C22 | −1.6 (5) | C52—C47—C48—C49 | 2.3 (5) |
| C3—C20—C21—C22 | 177.2 (3) | C29—C47—C48—C49 | −177.7 (3) |
| C20—C21—C22—C23 | −0.1 (5) | C52—C47—C48—C53 | −176.0 (3) |
| C21—C22—C23—C24 | 1.5 (5) | C29—C47—C48—C53 | 3.9 (5) |
| C21—C22—C23—C26 | −177.2 (3) | C47—C48—C49—C50 | −0.3 (5) |
| C22—C23—C24—C25 | −1.2 (5) | C53—C48—C49—C50 | 178.2 (3) |
| C26—C23—C24—C25 | 177.5 (3) | C48—C49—C50—C51 | −1.7 (5) |
| C23—C24—C25—C20 | −0.6 (5) | C48—C49—C50—C54 | 177.3 (3) |
| C23—C24—C25—C27 | 177.4 (3) | C49—C50—C51—C52 | 1.7 (5) |
| C21—C20—C25—C24 | 1.9 (5) | C54—C50—C51—C52 | −177.3 (3) |
| C3—C20—C25—C24 | −176.9 (3) | C50—C51—C52—C47 | 0.3 (5) |
| C21—C20—C25—C27 | −175.8 (3) | C48—C47—C52—C51 | −2.4 (5) |
| C3—C20—C25—C27 | 5.4 (5) | C29—C47—C52—C51 | 177.7 (3) |

*Hydrogen-bond geometry (Å, º)*

Cg1–Cg4 are the centroids of the C39–C44, C31–C36, C12–C17 and C4–C9 rings, respectively.

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C11—H11*B*···*Cg*1$^{i}$ | 0.98 | 2.97 | 3.777 (4) | 140 |
| C18—H18*B*···*Cg*2$^{ii}$ | 0.98 | 2.91 | 3.688 (4) | 137 |

| | | | | |
|---|---|---|---|---|
| C38—H38*C*···*Cg*3$^{iii}$ | 0.98 | 2.84 | 3.756 (4) | 155 |
| C45—H45*B*···*Cg*4$^{iv}$ | 0.98 | 2.77 | 3.596 (4) | 142 |

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