IUCrData

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# (*E*)-1-(2,4-Dichlorophenyl)-*N*-[(1*S*,4*R*)-1,11,11-trimethyl-1,2,3,4-tetrahydro-1,4-methanophenazin-7-yl]methanimine

**Neil M. Glagovich,[a] Keira A. Guarco,[a] Guy Crundwell[a]* and Gary S. Nichol[b]**

[a]Department of Chemistry & Biochemistry, Central Connecticut State University, New Britain, CT 06053, USA, and [b]School of Chemistry, Joseph Black Building, David Brewster Road, Edinburgh EH9 3FJ, United Kingdom. *Correspondence e-mail: crundwellg@ccsu.edu

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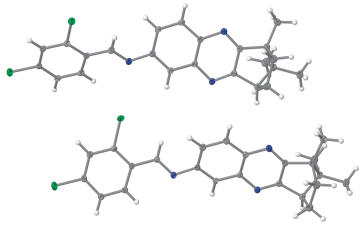
**CCDC reference:** 2606027

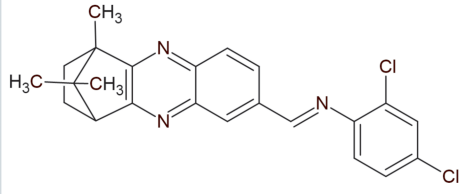
**Structural data:** full structural data are available from iucrdata.iucr.org

The title compound, $C_{23}H_{21}Cl_2N_2$, crystallizes with two molecules per asymmetric unit. The quinoxaline rings in each molecule make dihedral angles of 31.95 (3) and 35.00 (3)° with respect to their corresponding dichlorophenyl rings. In the extended structure, C—H···N hydrogen bonds and weak C—Cl···N halogen bonds connect the molecules.

3D view



Chemical scheme




## Structure description

In general, quinoxalines are of interest due to their extended $\pi$ conjugation and their chiral camphor derivatives are of specific interest in the design of new electro-optic materials (Suzuki *et al.*, 2004). Quinoxalines are capable of binding to metals *via* their ring nitrogen atoms (Glišić, *et al.*, 2016) and have been studied as potentially new anti-tumor agents and antibiotics (Costa *et al.*, 2021). As part of our studies in this area, we now describe the synthesis and structure of the title compound, $C_{23}H_{21}Cl_2N_2$, (**I**).

There are two molecules per asymmetric unit (molecule 1 containing C1 and molecule 2 containing C24) in space group $P2_1$ (Fig. 1) that are approximately related by a glide plane. Analysis of the model in *PLATON* ADDSYM suggests that an inversion center would give a 92% fit between the molecules (Spek, 2009) making $P2_1/c$ a potential choice for the space group; however, the model was refined in the chosen space group because compound (**I**) is known to be chiral and not a racemic mixture: atoms C9 (*R*), C12 (*S*) (molecule 1) and C32 (*R*) and C35 (*S*) (molecule 2) possess their expected chiralities based on the starting materials.

The quinoxaline moieties make dihedral angles of 31.95 (3)° (molecule 1) and 35.00 (3)° (molecule 2) with respect to their phenyl rings. When compared to each other, the molecules also have minor differences in their overall shape with one molecule

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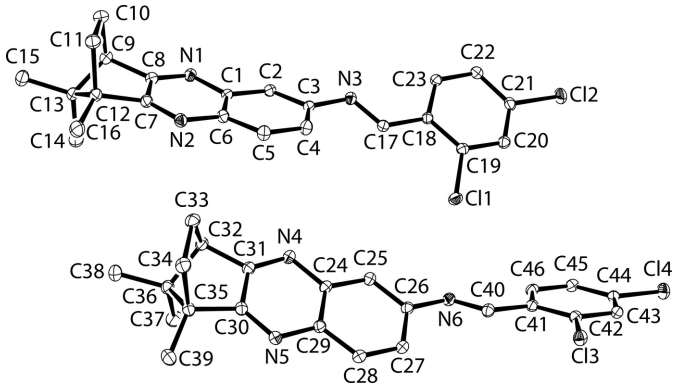


**Figure 1**
The molecular structure of (**I**) with displacement ellipsoids drawn at the 50% probability level with hydrogen atoms omitted for clarity.

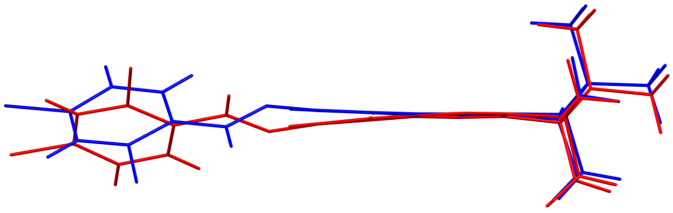

**Figure 2**
The two molecules superimposed.

slightly flatter. Fig. 2 shows both molecules overlapped to illustrate slight differences in molecular geometries.

Fig. 3 shows the unit-cell packing. The molecules stack along the [010] direction making hydrogen bonds. Two CH groups on the dichloropenyl rings (C22 and C45) form C—H···N hydrogen bonds (Table 1). There are also type I halogen bonds (Cavallo *et al.*, 2016) for C19—Cl1···N6 [Cl···N = 3.2196 (19) Å, C—Cl···N = 173.79 (8)°] and C42—Cl3···N3 [3.1530 (19) Å; 173.49 (8)°]; symmetry code: 1 + *x*, *y*, *z*. Fig. 4 shows the intermolecular hydrogen and halogen bonds in the crystal.

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

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C22—H22···N4$^{i}$ | 0.95 | 2.57 | 3.479 (3) | 161 |
| C45—H45···N1$^{ii}$ | 0.95 | 2.51 | 3.408 (3) | 158 |

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

**Table 2**
Experimental details.

| | |
|---|---|
| Crystal data | |
| Chemical formula | $C_{23}H_{21}Cl_2N_3$ |
| $M_r$ | 410.33 |
| Crystal system, space group | Monoclinic, $P2_1$ |
| Temperature (K) | 100 |
| *a*, *b*, *c* (Å) | 12.49677 (13), 7.33323 (5), 21.9445 (2) |
| $\beta$ (°) | 105.1901 (10) |
| $V$ (Å$^3$) | 1940.77 (3) |
| $Z$ | 4 |
| Radiation type | Mo $K\alpha$ |
| $\mu$ (mm$^{-1}$) | 0.35 |
| Crystal size (mm) | 0.41 × 0.33 × 0.31 |
| | |
| Data collection | |
| Diffractometer | XtaLAB Synergy, Single source at home/near, HyPix-Arc 100 |
| Absorption correction | Multi-scan (*CrysAlis PRO*; Rigaku OD, 2024) |
| $T_{min}$, $T_{max}$ | 0.794, 1.000 |
| No. of measured, independent and observed [$I > 2\sigma(I)$] reflections | 193869, 14552, 13014 |
| $R_{int}$ | 0.057 |
| (sin $\theta/\lambda)_{max}$ (Å$^{-1}$) | 0.783 |
| | |
| Refinement | |
| $R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, $S$ | 0.040, 0.123, 0.72 |
| No. of reflections | 14552 |
| No. of parameters | 511 |
| No. of restraints | 1 |
| H-atom treatment | H-atom parameters constrained |
| $\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å$^{-3}$) | 0.66, −0.31 |
| Absolute structure | Flack *x* determined using 5568 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons, 2013) |
| Absolute structure parameter | −0.008 (14) |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2025/1* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *ShelXle* (Hübschle *et al.*, 2011).

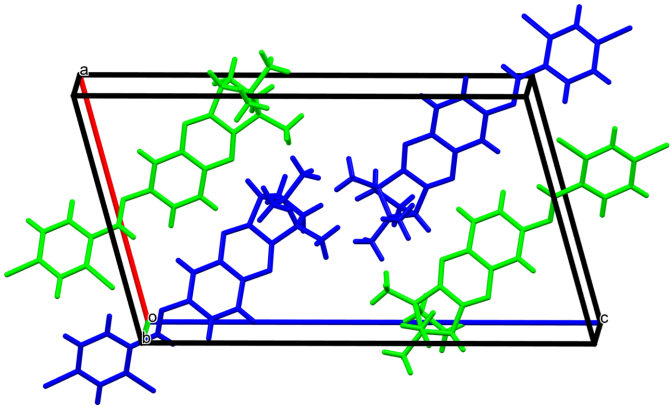


**Figure 3**
A view of the unit-cell packing along [010]. The C1 molecule is green and the C24 molecule is blue.

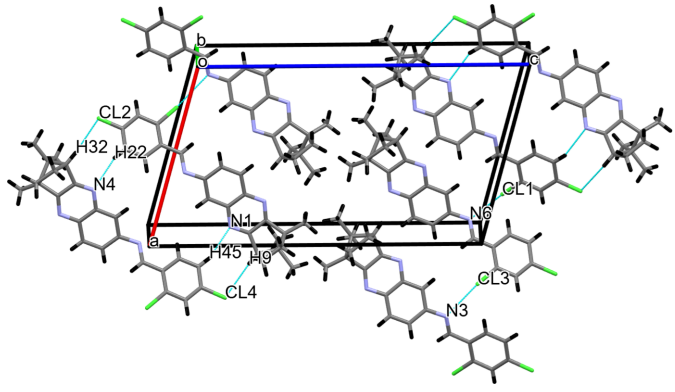


**Figure 4**
A view of the C—H···N hydrogen bonds and C—Cl···N halogen bonds (Cl···N) and hydrogen bonds along [010].

## Synthesis and crystallization

(*S*)-(+)-Camphorquinone was condensed with 4-nitro-1,2-phenylenediamine. Then, the nitro group was hydrogenated to an amine to form (1*S*,4*R*)-1,11,11-trimethyl-1,2,3,4-tetrahydro-1,4-methanophenazin-7-amine (Crundwell *et al.*, 2019). Then, this amine (0.103 g, 0.41 mmol), 2,4-dichlorobenzaldehyde (0.0716 g, 0.41 mmol) and a catalytic amount of *p*-toluene sulfonic acid were combined in 15 ml of toluene and refluxed for three h. The crude reaction mixture was concentrated *in vacuo* and recrystallized from 20 ml of ethyl acetate solution to yield colourless crystals of the title compound (41%) (m.p. 480.0 K). FT-IR (ATR): $\nu_{max}/cm^{-1}$ 3020 (*w*, Ar—H), 1685 (*s*, C═O); $^1$H-NMR (300MHz, $CDCl_3$): $\delta$ 0.65 (*s*, 3H), 1.13 (*s*, 3H), 1.42 (*m*, 5H, *J* = 9 Hz), 2.07 (*m*, 1H, *J* = 9 Hz), 2.31 (*m*, 1H,*J* = 3 Hz), 3.06 (*d*, 1H, *J* = 3 Hz), 7.37 (*ddd*, 1H, *J* = 6, 3, 0.1 Hz), 7.48 (*d*, 1H, *J* = 0.1 Hz), 7.58 (*dd*, 1H, *J* = 9, 3 Hz), 7.76 (*d*, 1H, *J* = 3 Hz), 8.04 (*d*, 1H, *J* = 9 Hz), 8.29 (*d*, 1H, *J* = 9 Hz), 8.99 (*s*, 1H); $^{13}$C-NMR (75MHz, $CDCl_3$): $\delta$ 10.0, 18.5, 20.3, 24.6, 31.8, 53.3, 53.8, 54.2, 118.6, 123.2, 127.4, 129.5, 129.6, 129.8, 131.7, 136.8, 137.9, 140.4, 141.9, 151.2, 156.8, 164.4, 165.2; LC-MS, calculated for $C_{23}H_{21}Cl_2N_6$: $M^+$: 451, measured: 451.

## Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The hydrogen atoms were placed in calculated positions (C—H = 0.95–1.00 Å) and were refined as riding atoms with $U_{iso}(H) = 1.2U_{eq}(C)$ or $1.5U_{eq}$ (methyl C). There are two short contacts between N and Cl that trigger a VRF alert, which we interpret as weak halogen bonds.

## Acknowledgements

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# full crystallographic data

*IUCrData* (2026). **11**, x261231 [https://doi.org/10.1107/S2414314626012319]

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*Crystal data*

$C_{23}H_{21}Cl_2N_3$
$M_r$ = 410.33
Monoclinic, $P2_1$
$a$ = 12.49677 (13) Å
$b$ = 7.33323 (5) Å
$c$ = 21.9445 (2) Å
$\beta$ = 105.1901 (10)°
$V$ = 1940.77 (3) Å$^3$
$Z$ = 4
$F(000)$ = 857.591
$D_x$ = 1.404 Mg m$^{-3}$
Melting point: 480 K
Mo $K\alpha$ radiation, $\lambda$ = 0.71073 Å
Cell parameters from 104217 reflections
$\theta$ = 2.9–33.9°
$\mu$ = 0.35 mm$^{-1}$
$T$ = 100 K
Block, clear colourless
0.41 × 0.33 × 0.31 mm

*Data collection*

XtaLAB Synergy, Single source at home/near, HyPix-Arc 100 diffractometer
Radiation source: fine-focus sealed X-ray tube, Enhance (Mo) X-ray Source
Detector resolution: 10.0000 pixels mm$^{-1}$
$\omega$ scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD, 2024)
$T_{min}$ = 0.794, $T_{max}$ = 1.000
193869 measured reflections
14552 independent reflections
13014 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.057
$\theta_{max}$ = 33.8°, $\theta_{min}$ = 1.9°
$h$ = −19→19
$k$ = −11→11
$l$ = −34→34

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.123
$S$ = 0.72
14552 reflections
511 parameters
1 restraint
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1193P)^2 + 1.3406P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.003
$\Delta\rho_{max}$ = 0.66 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.31 e Å$^{-3}$
Absolute structure: Flack $x$ determined using 5568 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons, 2013)
Absolute structure parameter: −0.008 (14)

*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.

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

| | *x* | *y* | *z* | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| N1 | 0.12888 (14) | 0.3133 (3) | 0.77556 (8) | 0.0157 (3) |
| C1 | 0.24303 (15) | 0.3018 (3) | 0.79966 (9) | 0.0127 (3) |
| C2 | 0.28692 (16) | 0.3107 (3) | 0.86569 (9) | 0.0139 (3) |
| H2 | 0.239151 | 0.334279 | 0.892069 | 0.017* |
| C3 | 0.39968 (16) | 0.2852 (3) | 0.89237 (9) | 0.0130 (3) |
| C4 | 0.47044 (17) | 0.2506 (3) | 0.85271 (10) | 0.0166 (4) |
| H4 | 0.547351 | 0.231124 | 0.870884 | 0.020* |
| C5 | 0.42893 (17) | 0.2450 (3) | 0.78817 (9) | 0.0166 (4) |
| H5 | 0.477786 | 0.224180 | 0.762217 | 0.020* |
| C6 | 0.31463 (16) | 0.2697 (3) | 0.76003 (9) | 0.0135 (3) |
| N2 | 0.27569 (15) | 0.2535 (3) | 0.69518 (8) | 0.0153 (3) |
| C7 | 0.16861 (16) | 0.2662 (3) | 0.67468 (9) | 0.0141 (3) |
| C8 | 0.09519 (16) | 0.2945 (3) | 0.71431 (9) | 0.0149 (3) |
| C9 | −0.02073 (16) | 0.2787 (3) | 0.67194 (9) | 0.0173 (3) |
| H9 | −0.081065 | 0.332745 | 0.688455 | 0.021* |
| C10 | −0.03204 (19) | 0.0712 (3) | 0.65528 (11) | 0.0218 (4) |
| H10A | −0.007644 | −0.004817 | 0.693705 | 0.026* |
| H10B | −0.109525 | 0.039428 | 0.633261 | 0.026* |
| C11 | 0.04594 (18) | 0.0459 (3) | 0.61111 (10) | 0.0201 (4) |
| H11A | 0.003726 | 0.004705 | 0.568645 | 0.024* |
| H11B | 0.104785 | −0.044336 | 0.628862 | 0.024* |
| C12 | 0.09656 (17) | 0.2392 (3) | 0.60788 (9) | 0.0158 (3) |
| C13 | −0.00509 (16) | 0.3631 (3) | 0.60984 (9) | 0.0167 (3) |
| C14 | 0.02356 (19) | 0.5664 (3) | 0.61599 (11) | 0.0224 (4) |
| H14A | 0.039265 | 0.609590 | 0.576957 | 0.034* |
| H14B | 0.088976 | 0.585119 | 0.651494 | 0.034* |
| H14C | −0.039225 | 0.634709 | 0.623444 | 0.034* |
| C15 | −0.10601 (18) | 0.3368 (3) | 0.55313 (10) | 0.0217 (4) |
| H15A | −0.088107 | 0.379787 | 0.514681 | 0.033* |
| H15B | −0.168833 | 0.406592 | 0.559817 | 0.033* |
| H15C | −0.125549 | 0.207139 | 0.548669 | 0.033* |
| C16 | 0.15393 (19) | 0.2665 (4) | 0.55596 (10) | 0.0215 (4) |
| H16A | 0.100826 | 0.246750 | 0.514882 | 0.032* |
| H16B | 0.215184 | 0.179427 | 0.561309 | 0.032* |
| H16C | 0.183018 | 0.391103 | 0.557983 | 0.032* |
| N3 | 0.43848 (14) | 0.2825 (3) | 0.95904 (8) | 0.0143 (3) |
| C17 | 0.53916 (16) | 0.3290 (3) | 0.98400 (9) | 0.0136 (3) |
| H17 | 0.582824 | 0.372988 | 0.957612 | 0.016* |
| C18 | 0.58877 (16) | 0.3163 (3) | 1.05211 (9) | 0.0124 (3) |

| | | | | |
|---|---|---|---|---|
| C19 | 0.69826 (15) | 0.3722 (3) | 1.07893 (9) | 0.0131 (3) |
| Cl1 | 0.77934 (4) | 0.46027 (7) | 1.03256 (2) | 0.01702 (10) |
| C20 | 0.74650 (16) | 0.3624 (3) | 1.14369 (10) | 0.0147 (3) |
| H20 | 0.820531 | 0.402027 | 1.161292 | 0.018* |
| C21 | 0.68331 (17) | 0.2929 (3) | 1.18182 (9) | 0.0151 (3) |
| Cl2 | 0.74365 (5) | 0.28056 (8) | 1.26253 (2) | 0.02157 (11) |
| C22 | 0.57449 (17) | 0.2345 (3) | 1.15739 (10) | 0.0154 (3) |
| H22 | 0.532628 | 0.187320 | 1.184264 | 0.019* |
| C23 | 0.52898 (16) | 0.2470 (3) | 1.09278 (9) | 0.0135 (3) |
| H23 | 0.454852 | 0.207364 | 1.075508 | 0.016* |
| N4 | 0.63350 (14) | 0.5831 (2) | 0.77615 (8) | 0.0141 (3) |
| C24 | 0.74595 (16) | 0.6163 (3) | 0.80027 (9) | 0.0129 (3) |
| C25 | 0.79024 (16) | 0.6151 (3) | 0.86642 (9) | 0.0140 (3) |
| H25 | 0.743228 | 0.591518 | 0.893228 | 0.017* |
| C26 | 0.90211 (16) | 0.6482 (3) | 0.89235 (9) | 0.0138 (3) |
| C27 | 0.97170 (17) | 0.6845 (3) | 0.85249 (10) | 0.0166 (4) |
| H27 | 1.048248 | 0.707837 | 0.870490 | 0.020* |
| C28 | 0.93018 (17) | 0.6864 (3) | 0.78793 (10) | 0.0173 (4) |
| H28 | 0.978363 | 0.709366 | 0.761744 | 0.021* |
| C29 | 0.81638 (16) | 0.6544 (3) | 0.76036 (9) | 0.0139 (3) |
| N5 | 0.77695 (14) | 0.6644 (3) | 0.69507 (8) | 0.0151 (3) |
| C30 | 0.67018 (16) | 0.6375 (3) | 0.67483 (9) | 0.0136 (3) |
| C31 | 0.59943 (16) | 0.5951 (3) | 0.71481 (9) | 0.0140 (3) |
| C32 | 0.48634 (15) | 0.5621 (3) | 0.67150 (9) | 0.0145 (3) |
| H32 | 0.422930 | 0.569843 | 0.691286 | 0.017* |
| C33 | 0.49780 (17) | 0.3788 (3) | 0.63768 (10) | 0.0174 (3) |
| H33A | 0.532613 | 0.283770 | 0.668559 | 0.021* |
| H33B | 0.424625 | 0.334688 | 0.612606 | 0.021* |
| C34 | 0.57359 (18) | 0.4297 (3) | 0.59420 (9) | 0.0185 (4) |
| H34A | 0.642667 | 0.356773 | 0.604952 | 0.022* |
| H34B | 0.534801 | 0.409315 | 0.549237 | 0.022* |
| C35 | 0.59904 (16) | 0.6357 (3) | 0.60757 (9) | 0.0160 (3) |
| C36 | 0.48591 (16) | 0.7041 (3) | 0.61851 (9) | 0.0160 (3) |
| C37 | 0.49047 (19) | 0.9021 (3) | 0.64175 (12) | 0.0225 (4) |
| H37A | 0.502173 | 0.983905 | 0.608773 | 0.034* |
| H37B | 0.551722 | 0.915812 | 0.679876 | 0.034* |
| H37C | 0.420421 | 0.933008 | 0.651441 | 0.034* |
| C38 | 0.38544 (18) | 0.6850 (3) | 0.56139 (10) | 0.0213 (4) |
| H38A | 0.392541 | 0.770631 | 0.528373 | 0.032* |
| H38B | 0.317607 | 0.712165 | 0.574118 | 0.032* |
| H38C | 0.381851 | 0.560131 | 0.545097 | 0.032* |
| C39 | 0.64651 (19) | 0.7337 (4) | 0.55982 (10) | 0.0228 (4) |
| H39A | 0.598162 | 0.714062 | 0.517319 | 0.034* |
| H39B | 0.720660 | 0.685918 | 0.562009 | 0.034* |
| H39C | 0.651431 | 0.864532 | 0.569232 | 0.034* |
| N6 | 0.94076 (14) | 0.6530 (3) | 0.95914 (8) | 0.0153 (3) |
| C40 | 1.04156 (16) | 0.6041 (3) | 0.98393 (9) | 0.0145 (3) |
| H40 | 1.084587 | 0.559430 | 0.957303 | 0.017* |

| | | | | |
|---|---|---|---|---|
| C41 | 1.09191 (16) | 0.6152 (3) | 1.05201 (9) | 0.0130 (3) |
| C42 | 1.20162 (16) | 0.5589 (3) | 1.07841 (9) | 0.0136 (3) |
| Cl3 | 1.28120 (4) | 0.47125 (7) | 1.03146 (2) | 0.01708 (10) |
| C43 | 1.25007 (16) | 0.5671 (3) | 1.14322 (9) | 0.0147 (3) |
| H43 | 1.324059 | 0.526856 | 1.160548 | 0.018* |
| C44 | 1.18782 (16) | 0.6353 (3) | 1.18170 (9) | 0.0134 (3) |
| Cl4 | 1.24891 (4) | 0.64669 (7) | 1.26243 (2) | 0.01978 (11) |
| C45 | 1.07903 (16) | 0.6951 (3) | 1.15797 (10) | 0.0147 (3) |
| H45 | 1.037874 | 0.742178 | 1.185216 | 0.018* |
| C46 | 1.03253 (16) | 0.6836 (3) | 1.09316 (9) | 0.0140 (3) |
| H46 | 0.958312 | 0.723372 | 1.076240 | 0.017* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| N1 | 0.0135 (7) | 0.0183 (8) | 0.0147 (7) | −0.0008 (6) | 0.0024 (6) | 0.0008 (6) |
| C1 | 0.0108 (7) | 0.0127 (8) | 0.0139 (8) | −0.0010 (6) | 0.0022 (6) | 0.0011 (6) |
| C2 | 0.0134 (8) | 0.0147 (8) | 0.0137 (8) | −0.0012 (6) | 0.0035 (6) | 0.0001 (6) |
| C3 | 0.0134 (8) | 0.0112 (8) | 0.0129 (7) | −0.0018 (6) | 0.0010 (6) | 0.0002 (6) |
| C4 | 0.0138 (8) | 0.0198 (9) | 0.0156 (8) | 0.0015 (7) | 0.0026 (7) | −0.0010 (7) |
| C5 | 0.0148 (8) | 0.0205 (9) | 0.0149 (8) | 0.0016 (7) | 0.0045 (7) | −0.0007 (7) |
| C6 | 0.0145 (8) | 0.0136 (8) | 0.0125 (7) | 0.0007 (7) | 0.0036 (6) | −0.0005 (6) |
| N2 | 0.0165 (7) | 0.0160 (8) | 0.0129 (7) | 0.0001 (6) | 0.0029 (6) | −0.0002 (6) |
| C7 | 0.0150 (8) | 0.0130 (8) | 0.0136 (7) | −0.0002 (6) | 0.0024 (6) | −0.0003 (6) |
| C8 | 0.0142 (8) | 0.0147 (8) | 0.0156 (8) | −0.0008 (6) | 0.0036 (6) | 0.0006 (6) |
| C9 | 0.0146 (8) | 0.0191 (9) | 0.0170 (8) | −0.0024 (7) | 0.0020 (6) | 0.0001 (7) |
| C10 | 0.0227 (9) | 0.0180 (9) | 0.0228 (9) | −0.0065 (8) | 0.0027 (7) | 0.0020 (7) |
| C11 | 0.0230 (9) | 0.0145 (8) | 0.0208 (9) | −0.0019 (7) | 0.0023 (7) | −0.0009 (7) |
| C12 | 0.0174 (8) | 0.0147 (8) | 0.0140 (7) | −0.0016 (6) | 0.0018 (6) | −0.0009 (6) |
| C13 | 0.0160 (8) | 0.0150 (8) | 0.0164 (8) | −0.0022 (6) | −0.0006 (6) | 0.0012 (6) |
| C14 | 0.0252 (10) | 0.0146 (8) | 0.0232 (9) | −0.0013 (7) | −0.0010 (8) | 0.0000 (7) |
| C15 | 0.0191 (9) | 0.0220 (10) | 0.0203 (9) | −0.0014 (7) | −0.0015 (7) | 0.0001 (7) |
| C16 | 0.0227 (9) | 0.0270 (10) | 0.0150 (8) | −0.0031 (8) | 0.0053 (7) | −0.0014 (8) |
| N3 | 0.0139 (7) | 0.0157 (7) | 0.0128 (7) | −0.0007 (6) | 0.0022 (6) | −0.0002 (6) |
| C17 | 0.0140 (8) | 0.0122 (8) | 0.0139 (8) | −0.0004 (6) | 0.0025 (6) | 0.0006 (6) |
| C18 | 0.0125 (7) | 0.0107 (8) | 0.0129 (8) | 0.0001 (6) | 0.0016 (6) | −0.0006 (6) |
| C19 | 0.0129 (7) | 0.0118 (8) | 0.0149 (8) | 0.0003 (6) | 0.0041 (6) | −0.0003 (6) |
| Cl1 | 0.01420 (19) | 0.0191 (2) | 0.0181 (2) | −0.00355 (16) | 0.00495 (15) | −0.00036 (17) |
| C20 | 0.0144 (8) | 0.0126 (8) | 0.0159 (8) | −0.0001 (7) | 0.0021 (6) | −0.0008 (7) |
| C21 | 0.0168 (8) | 0.0132 (8) | 0.0140 (8) | 0.0021 (7) | 0.0014 (6) | 0.0012 (7) |
| Cl2 | 0.0240 (2) | 0.0241 (3) | 0.0136 (2) | −0.00065 (19) | −0.00037 (17) | 0.00126 (18) |
| C22 | 0.0164 (8) | 0.0148 (8) | 0.0149 (8) | −0.0002 (7) | 0.0038 (7) | 0.0014 (7) |
| C23 | 0.0127 (8) | 0.0121 (8) | 0.0153 (8) | 0.0001 (6) | 0.0031 (6) | 0.0011 (6) |
| N4 | 0.0123 (6) | 0.0150 (7) | 0.0146 (7) | 0.0002 (6) | 0.0025 (5) | −0.0016 (6) |
| C24 | 0.0116 (7) | 0.0122 (8) | 0.0145 (8) | −0.0004 (6) | 0.0028 (6) | −0.0017 (6) |
| C25 | 0.0133 (8) | 0.0146 (8) | 0.0136 (8) | −0.0005 (6) | 0.0024 (6) | −0.0010 (6) |
| C26 | 0.0138 (8) | 0.0120 (8) | 0.0148 (8) | −0.0005 (7) | 0.0021 (6) | −0.0005 (7) |
| C27 | 0.0127 (8) | 0.0189 (9) | 0.0168 (8) | −0.0027 (7) | 0.0014 (7) | 0.0019 (7) |

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|---|---|---|---|---|---|---|
| C28 | 0.0134 (8) | 0.0193 (9) | 0.0185 (9) | −0.0026 (7) | 0.0033 (7) | 0.0024 (7) |
| C29 | 0.0134 (7) | 0.0126 (8) | 0.0147 (8) | −0.0006 (6) | 0.0019 (6) | 0.0005 (7) |
| N5 | 0.0148 (7) | 0.0154 (8) | 0.0146 (7) | −0.0002 (6) | 0.0030 (6) | 0.0015 (6) |
| C30 | 0.0150 (8) | 0.0118 (7) | 0.0133 (7) | 0.0011 (6) | 0.0022 (6) | −0.0007 (6) |
| C31 | 0.0135 (7) | 0.0134 (8) | 0.0149 (8) | −0.0001 (6) | 0.0033 (6) | −0.0015 (6) |
| C32 | 0.0132 (7) | 0.0136 (8) | 0.0155 (7) | −0.0007 (6) | 0.0019 (6) | −0.0011 (6) |
| C33 | 0.0176 (8) | 0.0130 (8) | 0.0205 (9) | −0.0017 (6) | 0.0031 (7) | −0.0019 (7) |
| C34 | 0.0213 (9) | 0.0161 (8) | 0.0175 (8) | −0.0005 (7) | 0.0040 (7) | −0.0035 (7) |
| C35 | 0.0154 (8) | 0.0179 (9) | 0.0139 (7) | 0.0006 (7) | 0.0022 (6) | 0.0023 (7) |
| C36 | 0.0146 (8) | 0.0132 (8) | 0.0181 (8) | 0.0005 (6) | 0.0008 (6) | 0.0005 (6) |
| C37 | 0.0220 (9) | 0.0131 (8) | 0.0301 (10) | 0.0013 (7) | 0.0029 (8) | −0.0005 (8) |
| C38 | 0.0185 (9) | 0.0225 (10) | 0.0196 (9) | 0.0002 (7) | −0.0010 (7) | 0.0034 (7) |
| C39 | 0.0216 (9) | 0.0280 (11) | 0.0183 (9) | −0.0007 (8) | 0.0041 (7) | 0.0067 (8) |
| N6 | 0.0147 (7) | 0.0142 (8) | 0.0155 (7) | −0.0013 (6) | 0.0015 (6) | −0.0004 (6) |
| C40 | 0.0138 (8) | 0.0129 (8) | 0.0157 (8) | 0.0004 (6) | 0.0020 (6) | −0.0010 (6) |
| C41 | 0.0132 (8) | 0.0105 (8) | 0.0149 (8) | −0.0001 (6) | 0.0030 (6) | −0.0001 (6) |
| C42 | 0.0130 (7) | 0.0118 (8) | 0.0158 (8) | 0.0012 (6) | 0.0036 (6) | −0.0002 (6) |
| Cl3 | 0.01433 (19) | 0.0196 (2) | 0.0177 (2) | 0.00362 (17) | 0.00505 (15) | 0.00009 (17) |
| C43 | 0.0126 (8) | 0.0136 (8) | 0.0167 (8) | −0.0007 (7) | 0.0018 (6) | 0.0017 (7) |
| C44 | 0.0133 (7) | 0.0121 (8) | 0.0140 (8) | −0.0008 (6) | 0.0019 (6) | 0.0007 (6) |
| Cl4 | 0.0198 (2) | 0.0236 (2) | 0.0141 (2) | 0.00073 (18) | 0.00136 (16) | −0.00069 (18) |
| C45 | 0.0135 (8) | 0.0140 (8) | 0.0169 (8) | −0.0001 (7) | 0.0044 (7) | −0.0016 (7) |
| C46 | 0.0111 (7) | 0.0120 (8) | 0.0190 (8) | 0.0002 (6) | 0.0038 (6) | −0.0005 (6) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| N1—C8 | 1.306 (3) | N4—C31 | 1.304 (3) |
| N1—C1 | 1.388 (2) | N4—C24 | 1.387 (2) |
| C1—C2 | 1.410 (3) | C24—C25 | 1.412 (3) |
| C1—C6 | 1.421 (3) | C24—C29 | 1.422 (3) |
| C2—C3 | 1.390 (3) | C25—C26 | 1.386 (3) |
| C2—H2 | 0.9500 | C25—H25 | 0.9500 |
| C3—N3 | 1.416 (2) | C26—C27 | 1.411 (3) |
| C3—C4 | 1.417 (3) | C26—N6 | 1.418 (2) |
| C4—C5 | 1.375 (3) | C27—C28 | 1.375 (3) |
| C4—H4 | 0.9500 | C27—H27 | 0.9500 |
| C5—C6 | 1.411 (3) | C28—C29 | 1.412 (3) |
| C5—H5 | 0.9500 | C28—H28 | 0.9500 |
| C6—N2 | 1.383 (2) | C29—N5 | 1.390 (2) |
| N2—C7 | 1.299 (3) | N5—C30 | 1.306 (3) |
| C7—C8 | 1.435 (3) | C30—C31 | 1.433 (3) |
| C7—C12 | 1.519 (3) | C30—C35 | 1.510 (3) |
| C8—C9 | 1.507 (3) | C31—C32 | 1.502 (3) |
| C9—C13 | 1.555 (3) | C32—C33 | 1.560 (3) |
| C9—C10 | 1.563 (3) | C32—C36 | 1.560 (3) |
| C9—H9 | 1.0000 | C32—H32 | 1.0000 |
| C10—C11 | 1.555 (3) | C33—C34 | 1.556 (3) |
| C10—H10A | 0.9900 | C33—H33A | 0.9900 |

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|---|---|---|---|
| C10—H10B | 0.9900 | C33—H33B | 0.9900 |
| C11—C12 | 1.561 (3) | C34—C35 | 1.556 (3) |
| C11—H11A | 0.9900 | C34—H34A | 0.9900 |
| C11—H11B | 0.9900 | C34—H34B | 0.9900 |
| C12—C16 | 1.510 (3) | C35—C39 | 1.514 (3) |
| C12—C13 | 1.572 (3) | C35—C36 | 1.577 (3) |
| C13—C14 | 1.531 (3) | C36—C38 | 1.530 (3) |
| C13—C15 | 1.534 (3) | C36—C37 | 1.535 (3) |
| C14—H14A | 0.9800 | C37—H37A | 0.9800 |
| C14—H14B | 0.9800 | C37—H37B | 0.9800 |
| C14—H14C | 0.9800 | C37—H37C | 0.9800 |
| C15—H15A | 0.9800 | C38—H38A | 0.9800 |
| C15—H15B | 0.9800 | C38—H38B | 0.9800 |
| C15—H15C | 0.9800 | C38—H38C | 0.9800 |
| C16—H16A | 0.9800 | C39—H39A | 0.9800 |
| C16—H16B | 0.9800 | C39—H39B | 0.9800 |
| C16—H16C | 0.9800 | C39—H39C | 0.9800 |
| N3—C17 | 1.280 (2) | N6—C40 | 1.285 (3) |
| C17—C18 | 1.463 (3) | C40—C41 | 1.464 (3) |
| C17—H17 | 0.9500 | C40—H40 | 0.9500 |
| C18—C23 | 1.401 (3) | C41—C46 | 1.403 (3) |
| C18—C19 | 1.401 (3) | C41—C42 | 1.403 (3) |
| C19—C20 | 1.393 (3) | C42—C43 | 1.393 (3) |
| C19—Cl1 | 1.738 (2) | C42—Cl3 | 1.732 (2) |
| C20—C21 | 1.389 (3) | C43—C44 | 1.383 (3) |
| C20—H20 | 0.9500 | C43—H43 | 0.9500 |
| C21—C22 | 1.392 (3) | C44—C45 | 1.393 (3) |
| C21—Cl2 | 1.736 (2) | C44—Cl4 | 1.7377 (19) |
| C22—C23 | 1.385 (3) | C45—C46 | 1.391 (3) |
| C22—H22 | 0.9500 | C45—H45 | 0.9500 |
| C23—H23 | 0.9500 | C46—H46 | 0.9500 |

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|---|---|---|---|
| C8—N1—C1 | 114.07 (17) | C31—N4—C24 | 113.96 (17) |
| N1—C1—C2 | 118.23 (17) | N4—C24—C25 | 118.44 (17) |
| N1—C1—C6 | 121.73 (17) | N4—C24—C29 | 121.87 (17) |
| C2—C1—C6 | 119.91 (17) | C25—C24—C29 | 119.68 (17) |
| C3—C2—C1 | 120.35 (18) | C26—C25—C24 | 120.19 (18) |
| C3—C2—H2 | 119.8 | C26—C25—H25 | 119.9 |
| C1—C2—H2 | 119.8 | C24—C25—H25 | 119.9 |
| C2—C3—N3 | 118.18 (18) | C25—C26—C27 | 119.85 (18) |
| C2—C3—C4 | 119.50 (17) | C25—C26—N6 | 117.56 (18) |
| N3—C3—C4 | 122.18 (17) | C27—C26—N6 | 122.52 (17) |
| C5—C4—C3 | 120.69 (18) | C28—C27—C26 | 120.87 (18) |
| C5—C4—H4 | 119.7 | C28—C27—H27 | 119.6 |
| C3—C4—H4 | 119.7 | C26—C27—H27 | 119.6 |
| C4—C5—C6 | 120.79 (18) | C27—C28—C29 | 120.37 (19) |
| C4—C5—H5 | 119.6 | C27—C28—H28 | 119.8 |
| C6—C5—H5 | 119.6 | C29—C28—H28 | 119.8 |

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|---|---|---|---|
| N2—C6—C5 | 118.81 (17) | N5—C29—C28 | 118.58 (18) |
| N2—C6—C1 | 122.38 (17) | N5—C29—C24 | 122.39 (17) |
| C5—C6—C1 | 118.74 (17) | C28—C29—C24 | 119.02 (18) |
| C7—N2—C6 | 113.77 (17) | C30—N5—C29 | 113.41 (17) |
| N2—C7—C8 | 124.40 (18) | N5—C30—C31 | 124.31 (17) |
| N2—C7—C12 | 128.42 (18) | N5—C30—C35 | 128.38 (18) |
| C8—C7—C12 | 106.99 (17) | C31—C30—C35 | 107.26 (16) |
| N1—C8—C7 | 123.63 (18) | N4—C31—C30 | 124.02 (18) |
| N1—C8—C9 | 129.92 (18) | N4—C31—C32 | 129.86 (18) |
| C7—C8—C9 | 106.19 (17) | C30—C31—C32 | 106.07 (16) |
| C8—C9—C13 | 100.89 (16) | C31—C32—C33 | 104.57 (15) |
| C8—C9—C10 | 103.46 (17) | C31—C32—C36 | 100.55 (15) |
| C13—C9—C10 | 101.94 (16) | C33—C32—C36 | 101.72 (15) |
| C8—C9—H9 | 116.1 | C31—C32—H32 | 115.9 |
| C13—C9—H9 | 116.1 | C33—C32—H32 | 115.9 |
| C10—C9—H9 | 116.1 | C36—C32—H32 | 115.9 |
| C11—C10—C9 | 103.24 (17) | C34—C33—C32 | 103.41 (16) |
| C11—C10—H10A | 111.1 | C34—C33—H33A | 111.1 |
| C9—C10—H10A | 111.1 | C32—C33—H33A | 111.1 |
| C11—C10—H10B | 111.1 | C34—C33—H33B | 111.1 |
| C9—C10—H10B | 111.1 | C32—C33—H33B | 111.1 |
| H10A—C10—H10B | 109.1 | H33A—C33—H33B | 109.0 |
| C10—C11—C12 | 104.32 (17) | C35—C34—C33 | 104.14 (16) |
| C10—C11—H11A | 110.9 | C35—C34—H34A | 110.9 |
| C12—C11—H11A | 110.9 | C33—C34—H34A | 110.9 |
| C10—C11—H11B | 110.9 | C35—C34—H34B | 110.9 |
| C12—C11—H11B | 110.9 | C33—C34—H34B | 110.9 |
| H11A—C11—H11B | 108.9 | H34A—C34—H34B | 108.9 |
| C16—C12—C7 | 115.61 (17) | C30—C35—C39 | 115.79 (17) |
| C16—C12—C11 | 115.65 (18) | C30—C35—C34 | 103.40 (16) |
| C7—C12—C11 | 102.69 (16) | C39—C35—C34 | 115.36 (18) |
| C16—C12—C13 | 119.39 (18) | C30—C35—C36 | 99.79 (15) |
| C7—C12—C13 | 100.20 (16) | C39—C35—C36 | 118.94 (18) |
| C11—C12—C13 | 100.59 (16) | C34—C35—C36 | 100.98 (16) |
| C14—C13—C15 | 108.51 (17) | C38—C36—C37 | 108.02 (17) |
| C14—C13—C9 | 112.98 (18) | C38—C36—C32 | 113.05 (17) |
| C15—C13—C9 | 113.30 (17) | C37—C36—C32 | 113.02 (17) |
| C14—C13—C12 | 113.17 (17) | C38—C36—C35 | 114.98 (17) |
| C15—C13—C12 | 113.80 (17) | C37—C36—C35 | 113.25 (17) |
| C9—C13—C12 | 94.71 (15) | C32—C36—C35 | 94.19 (14) |
| C13—C14—H14A | 109.5 | C36—C37—H37A | 109.5 |
| C13—C14—H14B | 109.5 | C36—C37—H37B | 109.5 |
| H14A—C14—H14B | 109.5 | H37A—C37—H37B | 109.5 |
| C13—C14—H14C | 109.5 | C36—C37—H37C | 109.5 |
| H14A—C14—H14C | 109.5 | H37A—C37—H37C | 109.5 |
| H14B—C14—H14C | 109.5 | H37B—C37—H37C | 109.5 |
| C13—C15—H15A | 109.5 | C36—C38—H38A | 109.5 |
| C13—C15—H15B | 109.5 | C36—C38—H38B | 109.5 |

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|---|---|---|---|
| H15A—C15—H15B | 109.5 | H38A—C38—H38B | 109.5 |
| C13—C15—H15C | 109.5 | C36—C38—H38C | 109.5 |
| H15A—C15—H15C | 109.5 | H38A—C38—H38C | 109.5 |
| H15B—C15—H15C | 109.5 | H38B—C38—H38C | 109.5 |
| C12—C16—H16A | 109.5 | C35—C39—H39A | 109.5 |
| C12—C16—H16B | 109.5 | C35—C39—H39B | 109.5 |
| H16A—C16—H16B | 109.5 | H39A—C39—H39B | 109.5 |
| C12—C16—H16C | 109.5 | C35—C39—H39C | 109.5 |
| H16A—C16—H16C | 109.5 | H39A—C39—H39C | 109.5 |
| H16B—C16—H16C | 109.5 | H39B—C39—H39C | 109.5 |
| C17—N3—C3 | 118.07 (18) | C40—N6—C26 | 117.45 (18) |
| N3—C17—C18 | 121.74 (18) | N6—C40—C41 | 121.87 (19) |
| N3—C17—H17 | 119.1 | N6—C40—H40 | 119.1 |
| C18—C17—H17 | 119.1 | C41—C40—H40 | 119.1 |
| C23—C18—C19 | 117.61 (17) | C46—C41—C42 | 117.63 (18) |
| C23—C18—C17 | 121.33 (17) | C46—C41—C40 | 121.22 (18) |
| C19—C18—C17 | 121.07 (18) | C42—C41—C40 | 121.14 (18) |
| C20—C19—C18 | 121.83 (18) | C43—C42—C41 | 121.65 (18) |
| C20—C19—Cl1 | 116.99 (15) | C43—C42—Cl3 | 117.35 (14) |
| C18—C19—Cl1 | 121.17 (15) | C41—C42—Cl3 | 120.98 (15) |
| C21—C20—C19 | 118.12 (18) | C44—C43—C42 | 118.38 (17) |
| C21—C20—H20 | 120.9 | C44—C43—H43 | 120.8 |
| C19—C20—H20 | 120.9 | C42—C43—H43 | 120.8 |
| C20—C21—C22 | 122.22 (18) | C43—C44—C45 | 122.38 (18) |
| C20—C21—Cl2 | 118.05 (15) | C43—C44—Cl4 | 118.21 (15) |
| C22—C21—Cl2 | 119.73 (16) | C45—C44—Cl4 | 119.41 (15) |
| C23—C22—C21 | 118.10 (19) | C46—C45—C44 | 117.95 (18) |
| C23—C22—H22 | 120.9 | C46—C45—H45 | 121.0 |
| C21—C22—H22 | 120.9 | C44—C45—H45 | 121.0 |
| C22—C23—C18 | 122.12 (18) | C45—C46—C41 | 122.00 (18) |
| C22—C23—H23 | 118.9 | C45—C46—H46 | 119.0 |
| C18—C23—H23 | 118.9 | C41—C46—H46 | 119.0 |

| | | | |
|---|---|---|---|
| C8—N1—C1—C2 | −176.71 (19) | C31—N4—C24—C25 | 177.08 (18) |
| C8—N1—C1—C6 | −0.8 (3) | C31—N4—C24—C29 | −1.8 (3) |
| N1—C1—C2—C3 | 174.84 (19) | N4—C24—C25—C26 | −179.82 (19) |
| C6—C1—C2—C3 | −1.1 (3) | C29—C24—C25—C26 | −0.9 (3) |
| C1—C2—C3—N3 | −175.57 (18) | C24—C25—C26—C27 | 0.4 (3) |
| C1—C2—C3—C4 | 0.2 (3) | C24—C25—C26—N6 | 177.32 (18) |
| C2—C3—C4—C5 | 1.0 (3) | C25—C26—C27—C28 | −0.4 (3) |
| N3—C3—C4—C5 | 176.6 (2) | N6—C26—C27—C28 | −177.1 (2) |
| C3—C4—C5—C6 | −1.3 (3) | C26—C27—C28—C29 | 0.9 (3) |
| C4—C5—C6—N2 | −176.7 (2) | C27—C28—C29—N5 | 177.6 (2) |
| C4—C5—C6—C1 | 0.4 (3) | C27—C28—C29—C24 | −1.4 (3) |
| N1—C1—C6—N2 | 2.0 (3) | N4—C24—C29—N5 | 1.3 (3) |
| C2—C1—C6—N2 | 177.77 (19) | C25—C24—C29—N5 | −177.52 (19) |
| N1—C1—C6—C5 | −175.0 (2) | N4—C24—C29—C28 | −179.8 (2) |
| C2—C1—C6—C5 | 0.8 (3) | C25—C24—C29—C28 | 1.4 (3) |

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| C5—C6—N2—C7 | 175.5 (2) | C28—C29—N5—C30 | −178.2 (2) |
| C1—C6—N2—C7 | −1.5 (3) | C24—C29—N5—C30 | 0.7 (3) |
| C6—N2—C7—C8 | 0.0 (3) | C29—N5—C30—C31 | −2.1 (3) |
| C6—N2—C7—C12 | −174.3 (2) | C29—N5—C30—C35 | −179.2 (2) |
| C1—N1—C8—C7 | −0.6 (3) | C24—N4—C31—C30 | 0.4 (3) |
| C1—N1—C8—C9 | 172.7 (2) | C24—N4—C31—C32 | 177.4 (2) |
| N2—C7—C8—N1 | 1.1 (4) | N5—C30—C31—N4 | 1.7 (3) |
| C12—C7—C8—N1 | 176.4 (2) | C35—C30—C31—N4 | 179.29 (19) |
| N2—C7—C8—C9 | −173.6 (2) | N5—C30—C31—C32 | −175.9 (2) |
| C12—C7—C8—C9 | 1.7 (2) | C35—C30—C31—C32 | 1.7 (2) |
| N1—C8—C9—C13 | 150.9 (2) | N4—C31—C32—C33 | −107.7 (2) |
| C7—C8—C9—C13 | −34.9 (2) | C30—C31—C32—C33 | 69.71 (19) |
| N1—C8—C9—C10 | −103.9 (3) | N4—C31—C32—C36 | 147.1 (2) |
| C7—C8—C9—C10 | 70.3 (2) | C30—C31—C32—C36 | −35.47 (19) |
| C8—C9—C10—C11 | −70.40 (19) | C31—C32—C33—C34 | −69.35 (18) |
| C13—C9—C10—C11 | 34.02 (19) | C36—C32—C33—C34 | 34.96 (18) |
| C9—C10—C11—C12 | 1.3 (2) | C32—C33—C34—C35 | 0.46 (19) |
| N2—C7—C12—C16 | −23.6 (3) | N5—C30—C35—C39 | −21.4 (3) |
| C8—C7—C12—C16 | 161.33 (19) | C31—C30—C35—C39 | 161.17 (19) |
| N2—C7—C12—C11 | 103.3 (2) | N5—C30—C35—C34 | 105.8 (2) |
| C8—C7—C12—C11 | −71.8 (2) | C31—C30—C35—C34 | −71.7 (2) |
| N2—C7—C12—C13 | −153.3 (2) | N5—C30—C35—C36 | −150.4 (2) |
| C8—C7—C12—C13 | 31.6 (2) | C31—C30—C35—C36 | 32.2 (2) |
| C10—C11—C12—C16 | −165.65 (18) | C33—C34—C35—C30 | 67.77 (18) |
| C10—C11—C12—C7 | 67.51 (19) | C33—C34—C35—C39 | −164.79 (17) |
| C10—C11—C12—C13 | −35.59 (19) | C33—C34—C35—C36 | −35.19 (18) |
| C8—C9—C13—C14 | −66.0 (2) | C31—C32—C36—C38 | 171.82 (17) |
| C10—C9—C13—C14 | −172.42 (17) | C33—C32—C36—C38 | 64.4 (2) |
| C8—C9—C13—C15 | 170.09 (18) | C31—C32—C36—C37 | −65.1 (2) |
| C10—C9—C13—C15 | 63.7 (2) | C33—C32—C36—C37 | −172.54 (16) |
| C8—C9—C13—C12 | 51.64 (17) | C31—C32—C36—C35 | 52.39 (17) |
| C10—C9—C13—C12 | −54.79 (17) | C33—C32—C36—C35 | −55.07 (16) |
| C16—C12—C13—C14 | −59.9 (2) | C30—C35—C36—C38 | −168.65 (17) |
| C7—C12—C13—C14 | 67.4 (2) | C39—C35—C36—C38 | 64.5 (2) |
| C11—C12—C13—C14 | 172.51 (17) | C34—C35—C36—C38 | −62.8 (2) |
| C16—C12—C13—C15 | 64.6 (2) | C30—C35—C36—C37 | 66.5 (2) |
| C7—C12—C13—C15 | −168.12 (17) | C39—C35—C36—C37 | −60.4 (2) |
| C11—C12—C13—C15 | −63.0 (2) | C34—C35—C36—C37 | 172.33 (17) |
| C16—C12—C13—C9 | −177.33 (18) | C30—C35—C36—C32 | −50.79 (17) |
| C7—C12—C13—C9 | −50.08 (17) | C39—C35—C36—C32 | −177.66 (18) |
| C11—C12—C13—C9 | 55.03 (17) | C34—C35—C36—C32 | 55.06 (16) |
| C2—C3—N3—C17 | −153.6 (2) | C25—C26—N6—C40 | 150.2 (2) |
| C4—C3—N3—C17 | 30.8 (3) | C27—C26—N6—C40 | −33.0 (3) |
| C3—N3—C17—C18 | −175.02 (18) | C26—N6—C40—C41 | 175.96 (18) |
| N3—C17—C18—C23 | 2.0 (3) | N6—C40—C41—C46 | −1.3 (3) |
| N3—C17—C18—C19 | −178.3 (2) | N6—C40—C41—C42 | 179.1 (2) |
| C23—C18—C19—C20 | −0.9 (3) | C46—C41—C42—C43 | 1.1 (3) |
| C17—C18—C19—C20 | 179.48 (19) | C40—C41—C42—C43 | −179.34 (19) |

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|---|---|---|---|
| C23—C18—C19—Cl1 | −179.92 (15) | C46—C41—C42—Cl3 | 179.60 (15) |
| C17—C18—C19—Cl1 | 0.4 (3) | C40—C41—C42—Cl3 | −0.8 (3) |
| C18—C19—C20—C21 | 0.7 (3) | C41—C42—C43—C44 | −1.0 (3) |
| Cl1—C19—C20—C21 | 179.82 (16) | Cl3—C42—C43—C44 | −179.52 (16) |
| C19—C20—C21—C22 | −0.3 (3) | C42—C43—C44—C45 | 0.2 (3) |
| C19—C20—C21—Cl2 | 179.93 (15) | C42—C43—C44—Cl4 | −179.59 (16) |
| C20—C21—C22—C23 | 0.0 (3) | C43—C44—C45—C46 | 0.4 (3) |
| Cl2—C21—C22—C23 | 179.77 (16) | Cl4—C44—C45—C46 | −179.82 (16) |
| C21—C22—C23—C18 | −0.1 (3) | C44—C45—C46—C41 | −0.2 (3) |
| C19—C18—C23—C22 | 0.6 (3) | C42—C41—C46—C45 | −0.5 (3) |
| C17—C18—C23—C22 | −179.80 (19) | C40—C41—C46—C45 | 179.96 (19) |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C22—H22···N4$^{i}$ | 0.95 | 2.57 | 3.479 (3) | 161 |
| C45—H45···N1$^{ii}$ | 0.95 | 2.51 | 3.408 (3) | 158 |
| C9—H9···Cl4$^{i}$ | 1.00 | 2.93 | 3.646 (2) | 129 |
| C32—H32···Cl2$^{ii}$ | 1.00 | 2.98 | 3.886 (2) | 152 |

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