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Synthesis and structure of 6,6′-bis(4-chlorophenyl)-3,3′-bis(pyridin-2-yl)-5,5′-bi(1,2,4-triazine)

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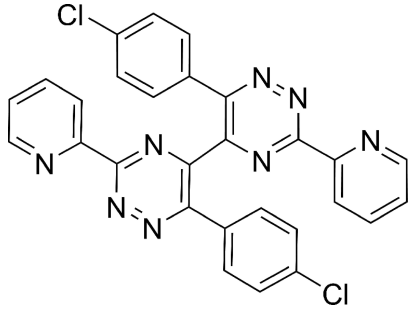
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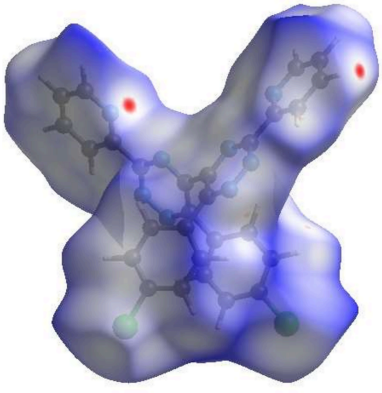
The complete molecule of the title compound, $C_{28}H_{16}Cl_2N_8$, is generated by a crystallographic twofold axis: the dihedral angle between the triazine rings is 65.86 (18)°. In the asymmetric fragment, the pyridine and triazine rings are almost coplanar at a dihedral angle of 1.81 (7)° and they are oriented with respect to the phenyl ring at 43.69 (6)° and 44.67 (8)°, respectively. In the crystal, aromatic π–π stacking interactions between the pyridine and triazine rings and between the phenyl rings with centroid-to-centroid distances of 3.6490 (4) Å and 3.8098 (5) Å, respectively, consolidate the packing. The Hirshfeld surface analysis indicates that the most important contributions for the crystal packing are from H···H (30.6%), H···Cl/Cl···H (19.5%), H···N/N···H (18.3%), H···C/C···H (12.8%) and C···N/N···C (9.2%) contacts.

1. Chemical context

2,2′:6′,2″:6″,2‴-Quaterpyridines are valuable synthetic building blocks in metallosupramolecular chemistry, as this specific arrangement of pyridine rings can accommodate various coordination numbers characteristic of specific metals, such as Ru^{II} (Renouard *et al.*, 2002), Ag^{I}, Cu^{I} (Adamski *et al.*, 2016) or Co^{II} (Chen *et al.*, 2021), thereby opening up possibilities for creating materials for diverse applications, such as efficient photosensitizers for solar cells (Renouard *et al.*, 2002) or catalysts for the low-temperature aerobic oxidation of hydrocarbons (Chen *et al.*, 2021).



One common method for synthesizing oligopyridines is the Boger reaction of 1,2,4-triazine precursors with various dienophiles (Shabunina *et al.*, 2021). When 5,5′-bis(1,2,4-triazines) are used as the heterodiene precursors, the synthesis of quaterpyridines becomes possible (Fatykhov *et al.*, 2026). The key step in this process is the dimerization of the starting 1,2,4-



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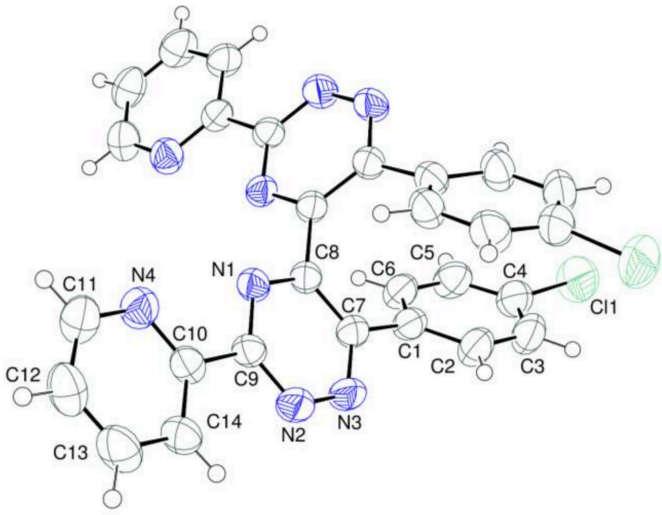


Figure 1
The molecular structure of (**I**) with 50% probability ellipsoids. Unlabelled atoms are generated by the symmetry operation $1 - x, 1 - y, z$.

triazine, achieved by maintaining the compound in an aqueous KCN solution (Fatykhov *et al.*, 2026). In the present work, we investigated the feasibility of carrying out this reaction by heating to 473 K in the presence of morpholine, using 6-(4-chlorophenyl)-3-(2-pyridinyl)-1,2,4- triazine as a substrate, and we now report the structure of the title compound, $C_{28}H_{16}Cl_2N_8$ (**I**), that resulted.

2. Structural commentary

The asymmetric unit of the title compound (**I**) contains one-half molecule, consisting of the pyridine, triazine and chlorophenyl rings (Fig. 1). The complete molecule is generated by a crystallographic twofold axis at the midpoint of the C8—C8^{i} [symmetry code: (i) $1 - x, 1 - y, z$] bond and the dihedral angle between the N1–N3/C7–C9 triazine ring and its symmetry-generated partner is 65.86 (18)°, which is also reflected in the N1—C8—C8^{i}—N1^{i} torsion angle of −67.18 (4)°. Within the asymmetric fragment, the phenyl, *A* (C1–C6), triazine, *B* (N1–N3/C7–C9), and pyridine, *C* (N4/C10–C14), rings are oriented at dihedral angles of *A*/*B* = 44.67 (8)°, *A*/*C* = 43.69 (6)° and *B*/*C* = 1.81 (7)°. The C9—C10 [1.489 (5) Å] and N3—C7 [1.344 (5) Å] bonds are longer, while the C1—C7 [1.472 (5) Å] and N1—C8 [1.317 (4) Å] bonds are shorter than the corresponding values in 6-(4-methoxyphenyl)-5-(pentafluorophenyl)-3-(pyridin-2-yl)-1,2,4-triazine (**II**) (Moseev *et al.*, 2023). The N3—C7—C1 [116.7 (3)°], N4—C10—C9 [117.1 (3)°], N4—C10—C14 [122.9 (4)°] and C11—C12—C13 [119.3 (4)°] bond angles are significantly widened, while the C10—C14—C13 [118.5 (4)°] and C12—C13—C14 [118.9 (4)°] bond angles are significantly narrowed with respect to the corresponding values in (**II**).

3. Supramolecular features

In the extended structure of (**I**), aromatic π–π stacking interactions between the pyridine and triazine rings and between the phenyl rings with centroid-to-centroid distances of 3.6490 (4) Å [α = 2.40 (5)° and slippage = 1.345 Å] and 3.8098 (5) Å [α = 3.89 (7)° and slippage = 1.827 Å] consolidate the packing (Fig. 2). Neither classical hydrogen bonds nor C—H$\cdots\pi$ interactions are observed.

The intermolecular interactions in the crystal are visualized by carrying out the Hirshfeld surface (HS) analysis using *CrystalExplorer17.5* (Spackman *et al.*, 2021). Fig. 3 shows the Hirshfeld surface for (**I**) plotted over d_{norm}. The overall two-dimensional fingerprint plot is shown in Fig. 4*a* and those delineated into the different contact types in Fig. 4*b*–*k*. According to the two-dimensional fingerprint plots, the H$\cdots$H, H$\cdots$Cl/Cl$\cdots$H, H$\cdots$N/N$\cdots$H, H$\cdots$C/C$\cdots$H, and C$\cdots$N/N$\cdots$C contacts make the most significant contributions to the HS, at 30.6, 19.5, 18.3, 12.8 and 9.2%, respectively.

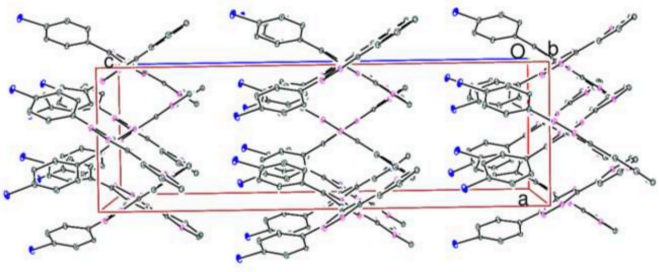


Figure 2
A partial packing diagram of (**I**) viewed down the *b*-axis direction. Hydrogen atoms have been omitted for clarity.

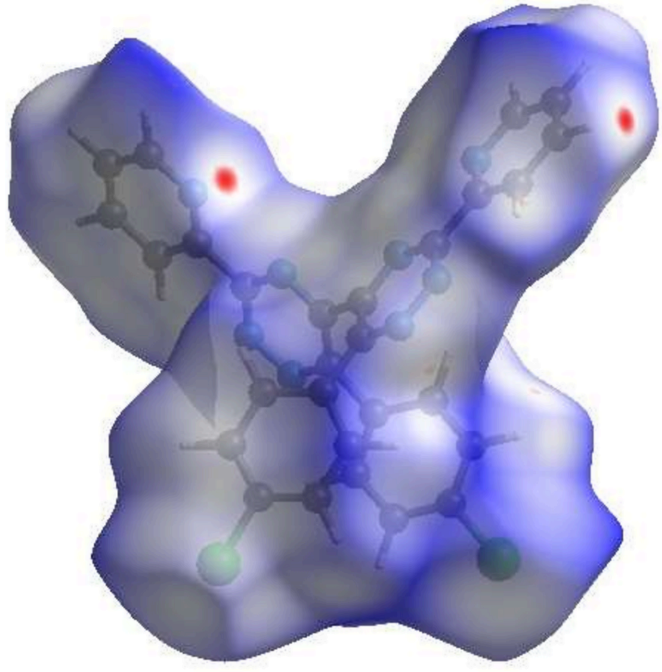


Figure 3
View of the three-dimensional Hirshfeld surface for (**I**) plotted over d_{norm} in the range −0.07 to 1.62 a.u.

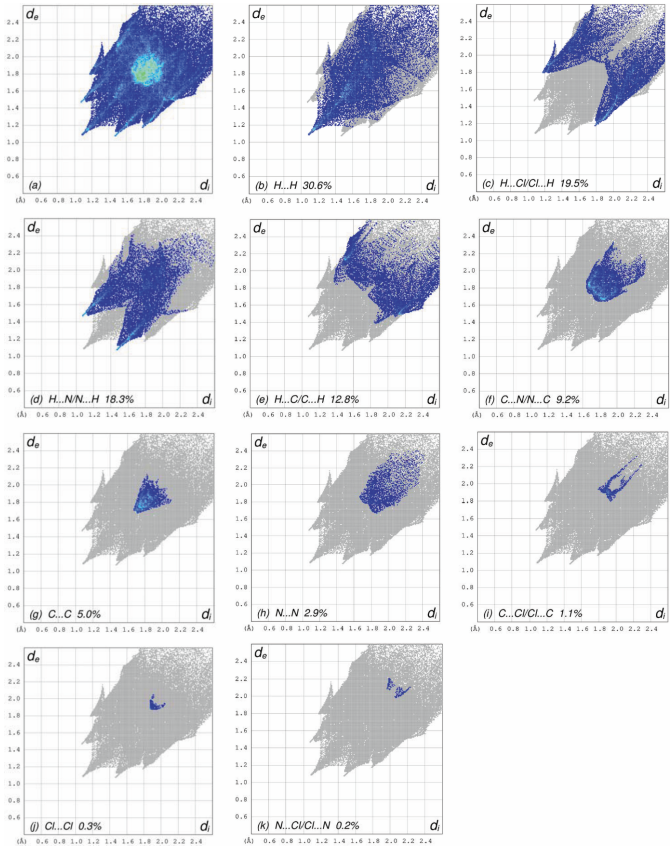


Figure 4
The full two-dimensional fingerprint plots for (**I**), showing (*a*) all interactions, and (*b*)–(*k*) delineated into different contact types.

4. Synthesis and crystallization

The starting compound 1,2,4-triazine **1** was prepared according to a literature procedure (Kozhevnikov *et al.*, 2005). Then, 120 mg (0.45 mmol) of 6-(4-chlorophenyl)-3-(2-pyridinyl)-1,2,4-triazine **1** and 0.19 ml (2.23 mmol) of morpholine were added to a round-bottom flask and the resulting mixture was heated at 473 K for 8 h under an inert atmosphere. The product was isolated by column chromatography (eluent AcOEt: $CHCl_3$ = 1:9; R_f = 0.1) (Fig. 5). An analytical sample was obtained by slow evaporation of its acetonitrile solution. Yield, 53 mg (44%). ^{1}H NMR (400 MHz, $CDCl_3$): δ 6.69–6.74 (*m*, 2H, Py, Py′), 7.23–7.38 (*m*, 6H, Py, Py′, Ar, Ar′), 7.49–7.56 (*m*, 4H, Py, Py′, Ar, Ar′), 7.56–7.65 (*m*, 2H, Py, Py′), 8.50–8.55 (*m*, 2H, Py, Py′). Mass spectrum, *m*/*z*: 535.10 $[M + H]^+$. Found (%): C 62.81, H 2.99, N 20.90. Calculated for $C_{28}H_{16}Cl_2N_8$ (%): C 62.82, H 3.01, N 20.93.

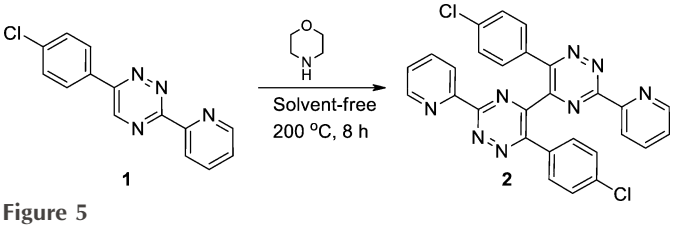


Figure 5
Synthesis scheme for (**I**).

Table 1
Experimental details.

Crystal data	
Chemical formula	$C_{28}H_{16}Cl_2N_8$
M_r	535.39
Crystal system, space group	Orthorhombic, *Aba*2
Temperature (K)	296
a, *b*, *c* (Å)	7.9614 (8), 12.6942 (15), 24.938 (2)
V (Å^3)	2520.3 (4)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.29
Crystal size (mm)	0.47 × 0.38 × 0.21
Data collection	
Diffractometer	Xcalibur, Sapphire3
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.819, 0.904
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	6101, 2379, 1850
R_{int}	0.037
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.666
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.047, 0.135, 1.03
No. of reflections	2379
No. of parameters	172
No. of restraints	1
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.20, −0.23
Absolute structure	Flack *x* determined using 422 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter	0.10 (10)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2017), *SHELXT2018/2* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

5. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 1. The C-bound hydrogen-atom positions were calculated geometrically at distances of 0.93 Å and refined using a riding model by applying the constraint of U_{iso}(H) = 1.2U_{eq}(C).

Acknowledgements

The authors' contributions are as follows. Conceptualization, TH and ANB; synthesis, APK, DSK and PAS; X-ray analysis, APK, DSK and PAS; Hirshfeld surface analysis, TH; writing (review and editing of the manuscript) TH, THM and NAG; supervision, TH and ANB. This work has been supported by the Ural Federation as well as by the SRI Geotechnological Problems of Oil, Gas and Chemistry and Baku Engineering University. TH is also grateful to Hacettepe University Scientific Research Project Unit (grant No. 013 D04 602 004).

References

Adamski, A., Fik, M. A., Kubicki, M., Hnatejko, Z., Gurda, D., Fedoruk-Wyszomirska, A., Wyszko, E., Kruszka, D., Dutkiewicz, Z. & Patroniak, V. (2016). *New J. Chem.* **40**, 7943–7957.
Chen, Y., Shi, H., Lee, C. S., Yiu, S. M., Man, W. L. & Lau, T. C. (2021). *J. Am. Chem. Soc.* **143**, 14445–14450.

Dolomanov, O. V., Bourhis, L. J., Gildea, R. J., Howard, J. A. K. & Puschmann, H. (2009). *J. Appl. Cryst.* **42**, 339–341.
Fatykhov, R. F., Khalymbadzha, I. A., Ladin, E. D., Potapova, S. S., Gurina, E. M., Chirkov, D. D., Ovsyannikov, A. S., Litvinov, I. A., Solovieva, S. E., Antipin, I. S., Gaviko, V. S., Kopchuk, D. S. & Zyryanov, G. V. (2026). *New J. Chem.* **50**, 14547–14553.
Kozhevnikov, V. N., Kozhevnikov, D. N., Shabunina, O. V., Rusinov, V. L. & Chupakhin, O. N. (2005). *Tetrahedron Lett.* **46**, 1521–1523.
Krause, L., Herbst-Irmer, R., Sheldrick, G. M. & Stalke, D. (2015). *J. Appl. Cryst.* **48**, 3–10.
Moseev, T. D., Nikiforov, E. A., Varaksin, M. V., Valieva, M. I., Kopchuk, D. S., Litvinov, I. A., Gaviko, V. S., Slepukhin, P. A., Zyryanov, G. V., Charushin, V. N. & Chupakhin, O. N. (2023). *Inorg. Chim. Acta* **558**, 121727.
Parsons, S., Flack, H. D. & Wagner, T. (2013). *Acta Cryst.* B**69**, 249–259.
Renouard, T., Fallahpour, R. A., Nazeeruddin, M. K., Humphry-Baker, R., Gorelsky, S. I., Lever, A. B. P. & Grätzel, M. (2002). *Inorg. Chem.* **41**, 367–378.
Rigaku OD (2017). *CrysAlis PRO*. Rigaku Oxford Diffraction, Yarnton, England.
Shabunina, O. V., Starnovskaya, E. S., Shaitz, Y. K., Kopchuk, D. S., Sadieva, L. K., Kim, G. A., Taniya, O. S., Nikonov, I. L., Santra, S., Zyryanov, G. V. & Charushin, V. N. (2021). *J. Photochem. Photobiol. A* **408**, 113101.
Sheldrick, G. M. (2015*a*). *Acta Cryst.* A**71**, 3–8.
Sheldrick, G. M. (2015*b*). *Acta Cryst.* C**71**, 3–8.
Spackman, P. R., Turner, M. J., McKinnon, J. J., Wolff, S. K., Grimwood, D. J., Jayatilaka, D. & Spackman, M. A. (2021). *J. Appl. Cryst.* **54**, 1006–1011.

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Synthesis and structure of 6,6′-bis(4-chlorophenyl)-3,3′-bis(pyridin-2-yl)-5,5′-bi(1,2,4-triazine)

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Computing details

6,6′-Bis(4-chlorophenyl)-3,3′-bis(pyridin-2-yl)-5,5′-bi(1,2,4-triazine)

Crystal data

$C_{28}H_{16}Cl_2N_8$
M_r = 535.39
Orthorhombic, *Aba*2
a = 7.9614 (8) Å
b = 12.6942 (15) Å
c = 24.938 (2) Å
V = 2520.3 (4) Å^3
Z = 4
F(000) = 1096
D_x = 1.411 Mg m^{-3}
Mo *Kα* radiation, *λ* = 0.71073 Å
Cell parameters from 1783 reflections
θ = 3.9–28.0°
μ = 0.29 mm^{-1}
T = 296 K
Block, yellow
0.47 × 0.38 × 0.21 mm

Data collection

Xcalibur, Sapphire3 diffractometer
Radiation source: fine-focus sealed X-ray tube
Detector resolution: 0 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
T_{min} = 0.819, T_{max} = 0.904
6101 measured reflections
2379 independent reflections
1850 reflections with $I > 2\sigma(I)$
R_{int} = 0.037
θ_{max} = 28.3°, θ_{min} = 3.9°
h = −6→10
k = −16→16
l = −25→33

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.047
$wR(F^2)$ = 0.135
S = 1.03
2379 reflections
172 parameters
1 restraint
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.0615P)^2 + 0.7909P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.20 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}
Absolute structure: Flack *x* determined using 422 quotients $[(I^+)-(I^-)]/[(I^+)+(I^-)]$ (Parsons *et al.*, 2013)
Absolute structure parameter: 0.10 (10)

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}
Cl1	0.8565 (2)	0.61745 (11)	0.69341 (6)	0.0982 (5)
N1	0.4339 (4)	0.3905 (2)	0.42228 (11)	0.0430 (6)
N2	0.5226 (5)	0.2295 (2)	0.46146 (13)	0.0549 (7)
N3	0.6011 (5)	0.2810 (2)	0.50112 (14)	0.0545 (7)
N4	0.2799 (5)	0.2787 (2)	0.34248 (15)	0.0569 (8)
C1	0.6775 (4)	0.4384 (3)	0.54838 (15)	0.0501 (8)
C2	0.6499 (6)	0.3992 (3)	0.60018 (17)	0.0616 (10)
H2	0.591179	0.336427	0.604644	0.074*
C3	0.7084 (6)	0.4523 (4)	0.64452 (17)	0.0693 (12)
H3	0.690363	0.425758	0.678792	0.083*
C4	0.7938 (6)	0.5451 (3)	0.63730 (18)	0.0658 (12)
C5	0.8312 (6)	0.5828 (3)	0.58722 (18)	0.0650 (11)
H5	0.895695	0.643358	0.583305	0.078*
C6	0.7723 (5)	0.5301 (3)	0.54273 (17)	0.0551 (9)
H6	0.796042	0.555916	0.508656	0.066*
C7	0.5976 (5)	0.3868 (3)	0.50207 (14)	0.0456 (8)
C8	0.5090 (4)	0.4406 (2)	0.46185 (13)	0.0422 (7)
C9	0.4450 (5)	0.2845 (3)	0.42359 (14)	0.0434 (7)
C10	0.3597 (5)	0.2235 (3)	0.38050 (15)	0.0457 (7)
C11	0.2009 (5)	0.2239 (4)	0.30403 (18)	0.0636 (11)
H11	0.145339	0.260885	0.277181	0.076*
C12	0.1982 (6)	0.1154 (4)	0.30241 (19)	0.0675 (12)
H12	0.141209	0.080515	0.275123	0.081*
C13	0.2796 (6)	0.0599 (3)	0.3410 (2)	0.0675 (11)
H13	0.279823	−0.013325	0.340435	0.081*
C14	0.3624 (6)	0.1143 (3)	0.38146 (17)	0.0562 (10)
H14	0.418465	0.078350	0.408570	0.067*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.1435 (13)	0.0837 (9)	0.0674 (7)	0.0011 (8)	−0.0315 (8)	−0.0237 (7)
N1	0.0540 (16)	0.0351 (14)	0.0397 (14)	−0.0010 (12)	0.0026 (12)	−0.0019 (11)
N2	0.0746 (19)	0.0362 (14)	0.0540 (17)	0.0013 (15)	−0.0060 (16)	−0.0019 (14)
N3	0.076 (2)	0.0351 (15)	0.0527 (18)	0.0043 (15)	−0.0085 (16)	0.0025 (13)
N4	0.071 (2)	0.0502 (18)	0.0498 (16)	−0.0037 (15)	−0.0052 (16)	−0.0016 (14)
C1	0.062 (2)	0.0419 (18)	0.0469 (19)	0.0025 (16)	−0.0080 (16)	0.0021 (15)
C2	0.086 (3)	0.050 (2)	0.049 (2)	−0.0061 (18)	−0.010 (2)	0.0069 (17)
C3	0.102 (3)	0.063 (3)	0.043 (2)	−0.001 (3)	−0.011 (2)	0.0052 (18)

C4	0.087 (3)	0.058 (3)	0.053 (2)	0.005 (2)	−0.018 (2)	−0.0069 (18)
C5	0.080 (3)	0.050 (2)	0.065 (3)	−0.0062 (19)	−0.014 (2)	0.002 (2)
C6	0.070 (2)	0.046 (2)	0.049 (2)	−0.0038 (18)	−0.0112 (18)	0.0044 (15)
C7	0.058 (2)	0.0375 (18)	0.0418 (18)	0.0001 (15)	−0.0008 (15)	0.0017 (13)
C8	0.0546 (18)	0.0336 (15)	0.0383 (14)	−0.0013 (14)	0.0020 (13)	−0.0002 (13)
C9	0.0533 (18)	0.0337 (15)	0.0432 (17)	−0.0003 (14)	0.0060 (14)	0.0011 (13)
C10	0.0512 (18)	0.0421 (17)	0.0440 (18)	−0.0038 (15)	0.0077 (14)	−0.0035 (13)
C11	0.072 (3)	0.068 (3)	0.050 (2)	−0.007 (2)	−0.0054 (19)	0.0014 (19)
C12	0.079 (3)	0.070 (3)	0.053 (2)	−0.016 (2)	0.001 (2)	−0.018 (2)
C13	0.088 (3)	0.046 (2)	0.069 (3)	−0.015 (2)	0.007 (2)	−0.014 (2)
C14	0.075 (3)	0.0372 (18)	0.057 (2)	−0.0028 (18)	0.0015 (19)	−0.0068 (16)

Geometric parameters (Å, º)

Cl1—C4	1.747 (4)	C4—C5	1.370 (6)
N1—C8	1.317 (4)	C5—C6	1.377 (6)
N1—C9	1.349 (4)	C5—H5	0.9300
N2—C9	1.327 (4)	C6—H6	0.9300
N2—N3	1.340 (5)	C7—C8	1.404 (5)
N3—C7	1.344 (5)	C8—C8^{i}	1.515 (6)
N4—C10	1.339 (5)	C9—C10	1.489 (5)
N4—C11	1.341 (5)	C10—C14	1.386 (5)
C1—C6	1.394 (5)	C11—C12	1.378 (7)
C1—C2	1.402 (6)	C11—H11	0.9300
C1—C7	1.472 (5)	C12—C13	1.358 (7)
C2—C3	1.377 (6)	C12—H12	0.9300
C2—H2	0.9300	C13—C14	1.389 (6)
C3—C4	1.372 (6)	C13—H13	0.9300
C3—H3	0.9300	C14—H14	0.9300
C8—N1—C9	115.7 (3)	N3—C7—C1	116.7 (3)
C9—N2—N3	119.0 (3)	C8—C7—C1	124.1 (3)
N2—N3—C7	119.4 (3)	N1—C8—C7	121.9 (3)
C10—N4—C11	117.2 (3)	N1—C8—C8^{i}	115.9 (3)
C6—C1—C2	118.4 (4)	C7—C8—C8^{i}	122.1 (3)
C6—C1—C7	121.7 (3)	N2—C9—N1	125.0 (3)
C2—C1—C7	119.8 (3)	N2—C9—C10	116.9 (3)
C3—C2—C1	120.8 (4)	N1—C9—C10	118.2 (3)
C3—C2—H2	119.6	N4—C10—C14	122.9 (4)
C1—C2—H2	119.6	N4—C10—C9	117.1 (3)
C4—C3—C2	118.9 (4)	C14—C10—C9	120.0 (3)
C4—C3—H3	120.6	N4—C11—C12	123.2 (4)
C2—C3—H3	120.6	N4—C11—H11	118.4
C5—C4—C3	121.8 (4)	C12—C11—H11	118.4
C5—C4—Cl1	119.0 (3)	C13—C12—C11	119.3 (4)
C3—C4—Cl1	119.2 (4)	C13—C12—H12	120.3
C4—C5—C6	119.4 (4)	C11—C12—H12	120.3
C4—C5—H5	120.3	C12—C13—C14	118.9 (4)

C6—C5—H5	120.3	C12—C13—H13	120.5
C5—C6—C1	120.5 (4)	C14—C13—H13	120.5
C5—C6—H6	119.7	C10—C14—C13	118.5 (4)
C1—C6—H6	119.7	C10—C14—H14	120.7
N3—C7—C8	118.9 (3)	C13—C14—H14	120.7

C9—N2—N3—C7	0.9 (5)	C1—C7—C8—N1	−177.2 (4)
C6—C1—C2—C3	2.8 (6)	N3—C7—C8—C8^{i}	176.5 (4)
C7—C1—C2—C3	−173.1 (4)	C1—C7—C8—C8^{i}	1.5 (6)
C1—C2—C3—C4	0.4 (7)	N3—N2—C9—N1	−2.0 (5)
C2—C3—C4—C5	−4.1 (7)	N3—N2—C9—C10	−180.0 (3)
C2—C3—C4—Cl1	175.8 (4)	C8—N1—C9—N2	0.9 (5)
C3—C4—C5—C6	4.3 (7)	C8—N1—C9—C10	178.8 (3)
Cl1—C4—C5—C6	−175.6 (3)	C11—N4—C10—C14	−0.3 (6)
C4—C5—C6—C1	−0.9 (6)	C11—N4—C10—C9	−179.1 (3)
C2—C1—C6—C5	−2.6 (6)	N2—C9—C10—N4	179.4 (3)
C7—C1—C6—C5	173.3 (4)	N1—C9—C10—N4	1.3 (5)
N2—N3—C7—C8	1.1 (6)	N2—C9—C10—C14	0.6 (5)
N2—N3—C7—C1	176.5 (4)	N1—C9—C10—C14	−177.5 (3)
C6—C1—C7—N3	140.4 (4)	C10—N4—C11—C12	0.3 (6)
C2—C1—C7—N3	−43.8 (5)	N4—C11—C12—C13	−0.4 (7)
C6—C1—C7—C8	−44.6 (6)	C11—C12—C13—C14	0.5 (7)
C2—C1—C7—C8	131.3 (4)	N4—C10—C14—C13	0.4 (6)
C9—N1—C8—C7	1.2 (5)	C9—C10—C14—C13	179.1 (4)
C9—N1—C8—C8^{i}	−177.6 (3)	C12—C13—C14—C10	−0.5 (7)
N3—C7—C8—N1	−2.3 (5)		

Symmetry code: (i) −*x*+1, −*y*+1, *z*.