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(*E*)-*N*′-(4-Chlorobenzylidene)-nicotinohydrazide

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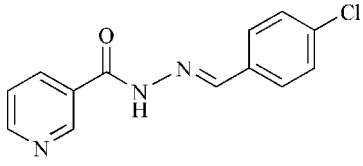
Key indicators: single-crystal X-ray study; T = 294 K; mean σ(C–C) = 0.004 Å; R factor = 0.039; wR factor = 0.101; data-to-parameter ratio = 12.2.

The title compound, $C_{13}H_{10}ClN_3O$, contains two independent molecules in the asymmetric unit. The dihedral angles between the pyridine and benzene rings are 32.8 (3) and 27.7 (3)°, and the C=N—N angles of 115.8 (3) and 115.1 (2)° are significantly smaller than for ideal N sp^2 atoms. Intermolecular N—H···N and N—H···O hydrogen bonds stabilize the crystal structure.

Related literature

For related literature, see: Armstrong *et al.* (1998); Buu *et al.* (1953); Kesslen & Euler (1999); Kundu *et al.* (2005); Xu *et al.* (1997).



Experimental

Crystal data

$C_{13}H_{10}ClN_3O$
M_r = 259.69
Monoclinic, $P2_1$
a = 12.658 (2) Å
b = 7.4377 (15) Å
c = 13.101 (3) Å
β = 100.812 (3)°
V = 1211.5 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 294 (2) K
0.14 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD area detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1997)
T_{min} = 0.959, T_{max} = 0.982
6941 measured reflections
3964 independent reflections
2840 reflections with $I > 2\sigma(I)$
R_{int} = 0.031

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.039
$wR(F^2)$ = 0.101
S = 1.00
3964 reflections
326 parameters
1 restraint
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 e Å^{-3}
$\Delta\rho_{min}$ = −0.20 e Å^{-3}
Absolute structure: Flack (1983), 1275 Freidel pairs
Flack parameter: 0.12 (7)

Table 1
Selected bond and torsion angles (°).

C7—N1—N2	115.8 (3)	C20—N4—N5	115.1 (2)
C7—N1—N2—C8	178.8 (3)	C20—N4—N5—C21	170.7 (3)

Table 2
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2···O2^{i}	0.86	2.16	3.012 (3)	169
N5—H5···N3^{ii}	0.86	2.38	3.197 (4)	159

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

Data collection: *SMART* (Bruker, 1997); cell refinement: *SAINT* (Bruker, 1997); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1997); software used to prepare material for publication: *SHELXTL*.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: AT2301).

References

Armstrong, J. A., Barnes, J. C. & Weakley, T. J. R. (1998). *Acta Cryst.* C**54**, 1923–1925.
Bruker (1997). *SMART* (Version 5.611), *SAINT* (Version 6.0), *SADABS* (Version 2.03) and *SHELXTL* (Version 5.10). Bruker AXS Inc., Madison, Wisconsin, USA.
Buu, H. N. P., Xuong, N. D., Nam, N. H., Binon, F. & Royer, R. (1953). *J. Chem. Soc.* pp. 1358–1361.
Flack, H. D. (1983). *Acta Cryst.* A**39**, 876–881.
Kesslen, E. C. & Euler, W. B. (1999). *Chem. Mater.* **11**, 336–340.
Kundu, N., Chatterjee, P. B., Chaudhury, M. & Tiekink, E. R. T. (2005). *Acta Cryst.* E**61**, m1583–m1585.
Sheldrick, G. M. (1997). *SHELXS97* and *SHELXL97*. University of Göttingen, Germany.
Xu, Z., Thompson, L. K. & Miller, D. O. (1997). *Inorg. Chem.* **36**, 3985–3995.

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supplementary materials

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(*E*)-*N*'-(4-Chlorobenzylidene)nicotinohydrazide

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Comment

To up date, a large number of azine compounds containing both a diimine linkage and N—N bonding have been synthesized because they are used in coordination chemistry (Kundu *et al.*, 2005; Kesslen & Euler, 1999; Armstrong *et al.*, 1998; Xu *et al.*, 1997). In this context, an X-ray crystal structure determination of the title compound, (I), was carried out.

The molecular structure of (I) and the atom-numbering scheme are shown in Fig. 1. The asymmetric unit of (I) contains two independent molecules. In the molecule A, the dihedral angle between the pyridine ring and benzene ring is 32.8 (3)°; the dihedral angle is 27.7 (3)° in the molecule B. In the two molecules, the C═N—N angles [C7═N1—N2 = 115.8 (3)° and C20═ N4—N5 = 115.1 (2)°] are significantly smaller than the ideal sp^2 N atoms, as a consequence of repulsion between the nitrogen lone pairs and the adjacent C═N bond. The packing of the molecules in the solid state is stablized by the intermolecular N—H···N betweent the amino group and N atom in the pyridine ring and N—H···O between the amine and carbonyl groups (Table 2).

Experimental

The title compound was synthesized according to the literature procedure (Buu *et al.*, 1953). Single crystal of (I) suitable for X-ray analysis were obtained by slow evaporation at 298 K of a tetrahydrofuran solution.

Refinement

All H atoms were positioned geometrically and refined as riding (N—H = 0.86Å and C—H = 0.93 Å) and allowed to ride on their parent atoms, with U_{iso}(H) = 1.2U_{eq}(parent).

Figures

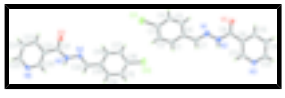

Fig. 1. View of the molecule of (I) showing the atom-labelling scheme. Displacement ellipsoids are drawn at the 35% probability level.

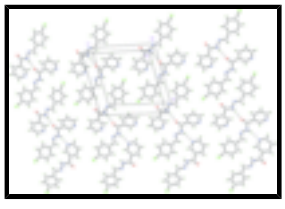

Fig. 2. The crystal structure of (I), viewed along the *b* axis. Dashed lines indicate hydrogen bonds interactions.

(*E*)-*N*'-(4-Chlorobenzylidene)nicotinohydrazide

Crystal data

$C_{13}H_{10}ClN_3O$	F_{000} = 536
M_r = 259.69	D_x = 1.424 Mg m^{-3}
Monoclinic, $P2_1$	Melting point: 470 K
Hall symbol: P 2yb	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 12.658 (2) Å	Cell parameters from 2256 reflections
b = 7.4377 (15) Å	θ = 3.2–25.7º
c = 13.101 (3) Å	μ = 0.31 mm^{-1}
β = 100.812 (3)º	T = 294 (2) K
V = 1211.5 (4) Å^3	Plate, colourless
Z = 4	0.14 × 0.10 × 0.06 mm

Data collection

Bruker SMART CCD area detector diffractometer	3964 independent reflections
Radiation source: fine-focus sealed tube	2840 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.031
T = 294(2) K	θ_{max} = 26.4º
φ and ω scans	θ_{min} = 1.6º
Absorption correction: multi-scan (SADABS; Bruker, 1997)	h = −13→15
T_{min} = 0.959, T_{max} = 0.982	k = −7→9
6941 measured reflections	l = −16→15

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)]$ = 0.039	$w = 1/[\sigma^2(F_o^2) + (0.048P)^2 + 0.1051P]$ where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2)$ = 0.101	$(\Delta/\sigma)_{max} < 0.001$
S = 1.00	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
3964 reflections	$\Delta\rho_{min}$ = −0.20 e Å^{-3}
326 parameters	Extinction correction: none
1 restraint	Absolute structure: Flack (1983), 1275 Freidel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.12 (7)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and goodness of fit S are based on F^2, conventional *R*-factors *R* are based on F, with F set to zero for negative F^2. The threshold expression of $F^2 > 2\text{sigma}(F^2)$ is used only for calculating *R*-factors(gt) *etc*. and is not relevant to the choice of reflections for refinement. *R*-factors based on F^2 are statistically about twice as large as those based on F, and R– factors based on ALL data will be even larger.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.43106 (7)	0.57852 (17)	0.38014 (7)	0.0694 (3)
Cl2	0.10935 (8)	0.89810 (17)	0.55071 (7)	0.0771 (4)
O1	−0.04369 (16)	0.6169 (4)	−0.22219 (17)	0.0635 (8)
O2	0.72294 (16)	0.7992 (3)	1.03581 (15)	0.0503 (6)
N1	0.0008 (2)	0.6410 (4)	−0.0117 (2)	0.0452 (7)
N2	−0.10233 (19)	0.6577 (4)	−0.0700 (2)	0.0470 (7)
H2	−0.1556	0.6833	−0.0403	0.056*
N3	−0.41660 (19)	0.5301 (4)	−0.23084 (19)	0.0476 (7)
N4	0.5063 (2)	0.8478 (4)	0.97678 (18)	0.0426 (7)
N5	0.56024 (19)	0.8572 (4)	1.07988 (18)	0.0428 (7)
H5	0.5249	0.8769	1.1288	0.051*
N6	0.7116 (2)	0.8205 (4)	1.39584 (19)	0.0551 (8)
C1	0.1217 (3)	0.6769 (5)	0.2623 (3)	0.0515 (9)
H1	0.0607	0.7110	0.2874	0.062*
C2	0.2188 (3)	0.6562 (5)	0.3316 (3)	0.0512 (9)
H2A	0.2231	0.6776	0.4022	0.061*
C3	0.3080 (2)	0.6037 (5)	0.2935 (2)	0.0468 (9)
C4	0.3031 (2)	0.5712 (5)	0.1891 (2)	0.0484 (8)
H4	0.3642	0.5346	0.1649	0.058*
C5	0.2065 (2)	0.5935 (5)	0.1207 (2)	0.0458 (8)
H5A	0.2030	0.5722	0.0501	0.055*
C6	0.1139 (2)	0.6478 (5)	0.1567 (2)	0.0401 (8)
C7	0.0100 (3)	0.6690 (5)	0.0860 (3)	0.0466 (8)
H7	−0.0501	0.7032	0.1126	0.056*
C8	−0.1180 (2)	0.6330 (5)	−0.1749 (2)	0.0423 (8)
C9	−0.2324 (2)	0.6175 (4)	−0.2302 (2)	0.0357 (7)
C10	−0.2564 (3)	0.6380 (5)	−0.3367 (2)	0.0497 (9)
H10	−0.2028	0.6710	−0.3728	0.060*
C11	−0.3599 (3)	0.6094 (6)	−0.3893 (3)	0.0547 (10)
H11	−0.3777	0.6274	−0.4607	0.066*
C12	−0.4368 (2)	0.5534 (5)	−0.3338 (2)	0.0479 (9)
H12	−0.5061	0.5309	−0.3699	0.057*
C13	−0.3164 (2)	0.5653 (5)	−0.1814 (2)	0.0441 (8)

H13	−0.3017	0.5543	−0.1094	0.053*
C14	0.2223 (2)	0.8689 (5)	0.8561 (3)	0.0483 (8)
H14	0.1941	0.8723	0.9167	0.058*
C15	0.1535 (3)	0.8830 (5)	0.7600 (3)	0.0514 (9)
H15	0.0798	0.8957	0.7564	0.062*
C16	0.1954 (3)	0.8780 (5)	0.6713 (3)	0.0503 (9)
C17	0.3053 (3)	0.8558 (5)	0.6743 (2)	0.0532 (9)
H17	0.3325	0.8493	0.6132	0.064*
C18	0.3733 (3)	0.8437 (5)	0.7701 (2)	0.0471 (9)
H18	0.4469	0.8314	0.7729	0.057*
C19	0.3336 (2)	0.8496 (5)	0.8625 (2)	0.0392 (8)
C20	0.4034 (2)	0.8451 (5)	0.9643 (2)	0.0438 (8)
H20	0.3720	0.8401	1.0230	0.053*
C21	0.6685 (2)	0.8352 (5)	1.1027 (2)	0.0368 (8)
C22	0.7190 (2)	0.8561 (5)	1.2142 (2)	0.0366 (7)
C23	0.8232 (2)	0.9223 (5)	1.2402 (2)	0.0400 (8)
H23	0.8605	0.9562	1.1885	0.048*
C24	0.8707 (3)	0.9372 (5)	1.3440 (2)	0.0502 (9)
H24	0.9400	0.9825	1.3636	0.060*
C25	0.8127 (3)	0.8831 (6)	1.4177 (2)	0.0541 (10)
H25	0.8458	0.8906	1.4872	0.065*
C26	0.6678 (3)	0.8082 (5)	1.2945 (2)	0.0447 (8)
H26	0.5980	0.7642	1.2770	0.054*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0502 (5)	0.0868 (8)	0.0632 (6)	−0.0044 (5)	−0.0101 (4)	0.0137 (6)
Cl2	0.0653 (6)	0.0973 (10)	0.0568 (6)	0.0018 (6)	−0.0190 (5)	0.0019 (6)
O1	0.0337 (12)	0.101 (2)	0.0604 (14)	−0.0031 (13)	0.0215 (11)	−0.0080 (16)
O2	0.0396 (12)	0.0760 (19)	0.0388 (12)	0.0046 (12)	0.0166 (10)	−0.0017 (12)
N1	0.0273 (12)	0.0561 (19)	0.0506 (16)	0.0003 (12)	0.0032 (11)	−0.0035 (15)
N2	0.0287 (14)	0.063 (2)	0.0489 (15)	0.0009 (13)	0.0073 (12)	−0.0071 (15)
N3	0.0320 (13)	0.066 (2)	0.0450 (15)	−0.0009 (13)	0.0081 (12)	−0.0017 (15)
N4	0.0360 (14)	0.0562 (19)	0.0348 (15)	0.0028 (13)	0.0048 (11)	−0.0005 (14)
N5	0.0353 (14)	0.064 (2)	0.0301 (12)	0.0017 (14)	0.0074 (10)	−0.0041 (15)
N6	0.0546 (18)	0.074 (2)	0.0386 (15)	0.0011 (16)	0.0138 (13)	0.0117 (16)
C1	0.0394 (18)	0.065 (3)	0.053 (2)	−0.0002 (17)	0.0154 (16)	−0.0110 (18)
C2	0.055 (2)	0.054 (2)	0.0432 (18)	−0.0078 (18)	0.0076 (16)	−0.0031 (18)
C3	0.0374 (17)	0.048 (2)	0.053 (2)	−0.0045 (16)	0.0038 (15)	0.0072 (19)
C4	0.0369 (17)	0.057 (2)	0.051 (2)	−0.0027 (17)	0.0085 (15)	0.0007 (19)
C5	0.0436 (18)	0.052 (2)	0.0429 (17)	−0.0021 (17)	0.0103 (14)	−0.0070 (17)
C6	0.0329 (16)	0.043 (2)	0.0440 (18)	−0.0036 (14)	0.0065 (14)	−0.0073 (16)
C7	0.0362 (17)	0.052 (2)	0.053 (2)	0.0014 (15)	0.0097 (15)	−0.0057 (18)
C8	0.0341 (17)	0.047 (2)	0.0456 (19)	−0.0015 (15)	0.0080 (15)	−0.0061 (17)
C9	0.0306 (15)	0.0362 (19)	0.0420 (16)	0.0012 (13)	0.0112 (12)	−0.0032 (14)
C10	0.049 (2)	0.063 (3)	0.0404 (18)	−0.0043 (18)	0.0164 (16)	0.0051 (18)
C11	0.048 (2)	0.076 (3)	0.0390 (17)	0.000 (2)	0.0043 (15)	0.009 (2)

C12	0.0393 (17)	0.056 (2)	0.0445 (18)	0.0046 (17)	−0.0036 (15)	0.0016 (19)
C13	0.0336 (16)	0.063 (2)	0.0360 (16)	−0.0034 (16)	0.0077 (13)	0.0005 (17)
C14	0.0371 (17)	0.059 (2)	0.0497 (18)	0.0007 (17)	0.0101 (14)	−0.0062 (19)
C15	0.0319 (16)	0.057 (2)	0.062 (2)	−0.0036 (17)	0.0006 (15)	−0.007 (2)
C16	0.0457 (19)	0.047 (2)	0.052 (2)	−0.0025 (18)	−0.0072 (16)	−0.0038 (19)
C17	0.048 (2)	0.069 (3)	0.0420 (18)	0.0021 (18)	0.0073 (15)	−0.001 (2)
C18	0.0377 (17)	0.057 (2)	0.0463 (19)	0.0022 (16)	0.0060 (14)	−0.0069 (18)
C19	0.0374 (16)	0.039 (2)	0.0403 (17)	0.0019 (14)	0.0038 (14)	−0.0051 (16)
C20	0.0377 (17)	0.055 (2)	0.0398 (17)	0.0004 (16)	0.0091 (14)	−0.0072 (17)
C21	0.0341 (16)	0.039 (2)	0.0374 (17)	0.0008 (14)	0.0083 (13)	0.0019 (16)
C22	0.0349 (15)	0.0391 (19)	0.0370 (15)	0.0049 (14)	0.0102 (12)	0.0046 (16)
C23	0.0324 (16)	0.048 (2)	0.0409 (17)	0.0033 (14)	0.0113 (14)	0.0031 (15)
C24	0.0433 (18)	0.060 (3)	0.0452 (18)	0.0016 (17)	0.0035 (15)	0.0006 (18)
C25	0.059 (2)	0.066 (3)	0.0349 (17)	0.003 (2)	0.0031 (16)	0.0017 (19)
C26	0.0388 (18)	0.055 (2)	0.0427 (18)	0.0018 (16)	0.0124 (15)	0.0066 (17)

Geometric parameters (Å, °)

Cl1—C3	1.757 (3)	C9—C10	1.380 (4)
Cl2—C16	1.748 (3)	C9—C13	1.395 (4)
O1—C8	1.225 (3)	C10—C11	1.378 (4)
O2—C21	1.241 (3)	C10—H10	0.9300
N1—C7	1.281 (4)	C11—C12	1.385 (4)
N1—N2	1.389 (4)	C11—H11	0.9300
N2—C8	1.364 (4)	C12—H12	0.9300
N2—H2	0.8600	C13—H13	0.9300
N3—C12	1.336 (4)	C14—C15	1.393 (4)
N3—C13	1.337 (4)	C14—C19	1.404 (4)
N4—C20	1.282 (4)	C14—H14	0.9300
N4—N5	1.396 (3)	C15—C16	1.367 (5)
N5—C21	1.357 (4)	C15—H15	0.9300
N5—H5	0.8600	C16—C17	1.395 (4)
N6—C25	1.341 (4)	C17—C18	1.385 (4)
N6—C26	1.343 (4)	C17—H17	0.9300
C1—C6	1.384 (4)	C18—C19	1.395 (4)
C1—C2	1.393 (5)	C18—H18	0.9300
C1—H1	0.9300	C19—C20	1.456 (4)
C2—C3	1.374 (4)	C20—H20	0.9300
C2—H2A	0.9300	C21—C22	1.489 (4)
C3—C4	1.379 (4)	C22—C26	1.382 (4)
C4—C5	1.384 (4)	C22—C23	1.389 (4)
C4—H4	0.9300	C23—C24	1.385 (4)
C5—C6	1.403 (4)	C23—H23	0.9300
C5—H5A	0.9300	C24—C25	1.378 (4)
C6—C7	1.469 (4)	C24—H24	0.9300
C7—H7	0.9300	C25—H25	0.9300
C8—C9	1.497 (4)	C26—H26	0.9300
C7—N1—N2	115.8 (3)	N3—C12—H12	118.3
C8—N2—N1	119.0 (2)	C11—C12—H12	118.3

C8—N2—H2	120.5	N3—C13—C9	124.6 (3)
N1—N2—H2	120.5	N3—C13—H13	117.7
C12—N3—C13	116.6 (3)	C9—C13—H13	117.7
C20—N4—N5	115.1 (2)	C15—C14—C19	120.8 (3)
C21—N5—N4	119.8 (2)	C15—C14—H14	119.6
C21—N5—H5	120.1	C19—C14—H14	119.6
N4—N5—H5	120.1	C16—C15—C14	119.3 (3)
C25—N6—C26	115.8 (3)	C16—C15—H15	120.3
C6—C1—C2	121.5 (3)	C14—C15—H15	120.3
C6—C1—H1	119.2	C15—C16—C17	121.6 (3)
C2—C1—H1	119.2	C15—C16—Cl2	119.4 (3)
C3—C2—C1	118.6 (3)	C17—C16—Cl2	119.0 (3)
C3—C2—H2A	120.7	C18—C17—C16	118.7 (3)
C1—C2—H2A	120.7	C18—C17—H17	120.7
C2—C3—C4	121.5 (3)	C16—C17—H17	120.7
C2—C3—Cl1	119.0 (3)	C17—C18—C19	121.4 (3)
C4—C3—Cl1	119.5 (2)	C17—C18—H18	119.3
C3—C4—C5	119.5 (3)	C19—C18—H18	119.3
C3—C4—H4	120.3	C18—C19—C14	118.2 (3)
C5—C4—H4	120.3	C18—C19—C20	122.6 (3)
C4—C5—C6	120.6 (3)	C14—C19—C20	119.1 (3)
C4—C5—H5A	119.7	N4—C20—C19	122.9 (3)
C6—C5—H5A	119.7	N4—C20—H20	118.5
C1—C6—C5	118.3 (3)	C19—C20—H20	118.5
C1—C6—C7	120.0 (3)	O2—C21—N5	122.8 (3)
C5—C6—C7	121.6 (3)	O2—C21—C22	121.5 (3)
N1—C7—C6	121.0 (3)	N5—C21—C22	115.7 (2)
N1—C7—H7	119.5	C26—C22—C23	117.6 (3)
C6—C7—H7	119.5	C26—C22—C21	123.0 (3)
O1—C8—N2	122.9 (3)	C23—C22—C21	119.4 (3)
O1—C8—C9	120.8 (3)	C24—C23—C22	119.1 (3)
N2—C8—C9	116.2 (3)	C24—C23—H23	120.4
C10—C9—C13	116.9 (3)	C22—C23—H23	120.4
C10—C9—C8	119.3 (3)	C25—C24—C23	118.3 (3)
C13—C9—C8	123.5 (3)	C25—C24—H24	120.8
C11—C10—C9	119.8 (3)	C23—C24—H24	120.8
C11—C10—H10	120.1	N6—C25—C24	124.4 (3)
C9—C10—H10	120.1	N6—C25—H25	117.8
C10—C11—C12	118.7 (3)	C24—C25—H25	117.8
C10—C11—H11	120.7	N6—C26—C22	124.8 (3)
C12—C11—H11	120.7	N6—C26—H26	117.6
N3—C12—C11	123.3 (3)	C22—C26—H26	117.6
C7—N1—N2—C8	178.8 (3)	C8—C9—C13—N3	−171.8 (3)
C20—N4—N5—C21	170.7 (3)	C19—C14—C15—C16	0.0 (6)
C6—C1—C2—C3	−0.8 (6)	C14—C15—C16—C17	1.2 (6)
C1—C2—C3—C4	−0.1 (6)	C14—C15—C16—Cl2	−179.3 (3)
C1—C2—C3—Cl1	179.6 (3)	C15—C16—C17—C18	−1.8 (6)
C2—C3—C4—C5	0.6 (6)	Cl2—C16—C17—C18	178.7 (3)
Cl1—C3—C4—C5	−179.1 (3)	C16—C17—C18—C19	1.3 (6)

C3—C4—C5—C6	−0.3 (6)	C17—C18—C19—C14	−0.2 (6)
C2—C1—C6—C5	1.1 (5)	C17—C18—C19—C20	−177.2 (4)
C2—C1—C6—C7	179.3 (3)	C15—C14—C19—C18	−0.5 (5)
C4—C5—C6—C1	−0.5 (5)	C15—C14—C19—C20	176.7 (3)
C4—C5—C6—C7	−178.8 (3)	N5—N4—C20—C19	175.1 (3)
N2—N1—C7—C6	177.3 (3)	C18—C19—C20—N4	4.9 (6)
C1—C6—C7—N1	−179.3 (3)	C14—C19—C20—N4	−172.1 (3)
C5—C6—C7—N1	−1.1 (5)	N4—N5—C21—O2	−3.1 (5)
N1—N2—C8—O1	−8.7 (5)	N4—N5—C21—C22	177.3 (3)
N1—N2—C8—C9	168.6 (3)	O2—C21—C22—C26	−146.9 (3)
O1—C8—C9—C10	−19.0 (5)	N5—C21—C22—C26	32.8 (5)
N2—C8—C9—C10	163.7 (3)	O2—C21—C22—C23	31.5 (5)
O1—C8—C9—C13	154.3 (3)	N5—C21—C22—C23	−148.8 (3)
N2—C8—C9—C13	−23.0 (5)	C26—C22—C23—C24	0.1 (5)
C13—C9—C10—C11	0.9 (5)	C21—C22—C23—C24	−178.4 (3)
C8—C9—C10—C11	174.6 (3)	C22—C23—C24—C25	0.8 (5)
C9—C10—C11—C12	−2.6 (6)	C26—N6—C25—C24	1.5 (6)
C13—N3—C12—C11	0.6 (5)	C23—C24—C25—N6	−1.6 (6)
C10—C11—C12—N3	1.9 (6)	C25—N6—C26—C22	−0.5 (6)
C12—N3—C13—C9	−2.4 (5)	C23—C22—C26—N6	−0.2 (5)
C10—C9—C13—N3	1.7 (6)	C21—C22—C26—N6	178.2 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O2^{i}	0.86	2.16	3.012 (3)	169
N5—H5···N3^{ii}	0.86	2.38	3.197 (4)	159

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

Fig. 1

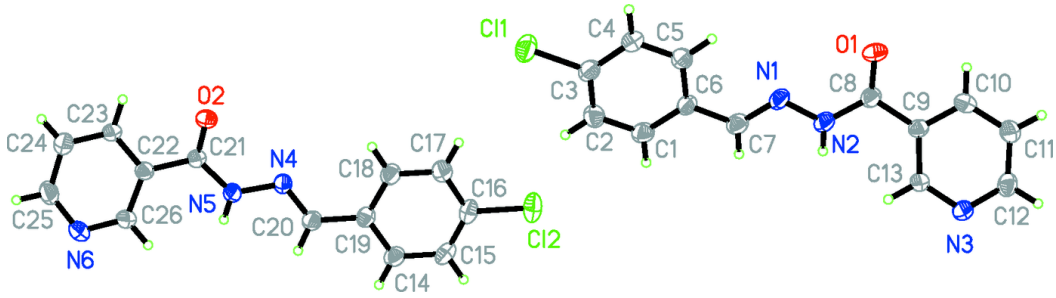
Cl1
C4
C5
O1
C3
C6
N1
C8
C10
C9
C2
C1
C7
N2
C11
C13
C12
N3
O2
C23
C24
C22
C21
N4
C18
C17
C16
C25
C26
N5
C20
C19
Cl2
N6
C15
C14

Fig. 2