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5-(4-Chlorophenyl)-4-(4-methoxyphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

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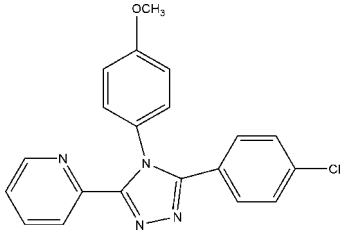
Key indicators: single-crystal X-ray study; T = 298 K; mean σ(C–C) = 0.003 Å; R factor = 0.045; wR factor = 0.130; data-to-parameter ratio = 14.5.

In the title compound, $C_{20}H_{15}ClN_4O$, the methoxy- and chlorophenyl rings form dihedral angles of 63.2 (1) and 31.1 (1)°, respectively, with the triazole ring, and the dihedral angle between the triazole and pyridine rings is 35.1 (1)°. Centrosymmetrically related molecules are linked together by weak C—H···N hydrogen bonds, forming a dimer.

Related literature

For the structural details of 4-(4-methoxyphenyl)-3-(2-pyridyl)-5-(4-methylphenyl)-4*H*-1,2,4-triazole, see: Zhang *et al.* (2006).



Experimental

Crystal data

$C_{20}H_{15}ClN_4O$
M_r = 362.81
Triclinic, $P\overline{1}$
a = 9.808 (4) Å
b = 10.083 (4) Å
c = 10.274 (4) Å
α = 70.415 (5)°
β = 73.417 (6)°
γ = 69.768 (6)°
V = 881.5 (6) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.23 mm^{-1}
T = 298 (2) K
0.15 × 0.15 × 0.10 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Sheldrick, 1996)
T_{min} = 0.966, T_{max} = 0.977
6776 measured reflections
3411 independent reflections
2757 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.046
$wR(F^2)$ = 0.130
S = 1.05
3411 reflections
236 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.24 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C9—H22···N4^{i}	0.93	2.60	3.454 (3)	154

Symmetry code: (i) $-x, -y, -z+2$.

Data collection: *SMART* (Siemens, 1996); cell refinement: *SAINT* (Siemens, 1996); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997*a*); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997*a*); molecular graphics: *SHELXTL* (Sheldrick, 1997*b*); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2502).

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Zhang, S.-P., Liu, Z.-D., Chen, S.-D., Yang, S.-P. & Shao, S. (2006). *Acta Cryst.* E**62**, o1516–o1517.

  doi:10.1107/S160053680705547X

supplementary materials

Acta Cryst. (2007). E**63**, o4634 [**doi:10.1107/S160053680705547X**]

5-(4-Chlorophenyl)-4-(4-methoxyphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

Z.-D. Liu, S.-P. Zhang, Y. Wei and S.-C. Shao

Comment

In the title molecule (Fig. 1), the pyridine and benzene rings lie in a propeller arrangement around the central 1,2,4-triazole ring, thereby minimizing the steric effects among these rings. The dihedral angles between the pyridine ring and the two benzene rings (C8—C13 and C15—C20) are 58.4 (1) and 65.4 (1)°, respectively. These two benzene rings form dihedral angles of 63.2 (1) and 31.1 (1)°, respectively, with the triazole ring, and the dihedral angle between the triazole ring and the pyridine ring is 35.1 (1)°.

In the crystal structure, molecules related by a center of symmetry are linked by C—H···N hydrogen bonds (Table 1), forming a dimer.

Experimental

The title compound was synthesized according to a literature method (Zhang *et al.*, 2006). Equivalent amounts of *p*-methoxyphosphazoanilide and *N*-pyridyl-*N*'-*p*-chlorophenylhydrazine were reacted in ethanol (15 ml) for 1 h. After allowing the resulting solution to stand in air for 15 d, colourless crystals were formed on slow evaporation of the solvent. The crystals were isolated, washed with ethanol and dried.

Refinement

H atoms were placed in idealized positions (C—H = 0.93 or 0.96 Å) and constrained to ride on their parent atoms, with U_{iso}(H) = 1.2 or 1.5(methyl) U_{eq}(C).

Figures

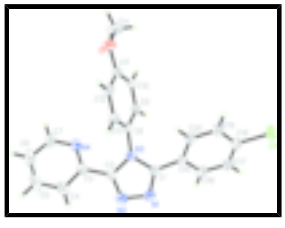


Fig. 1. The molecular structure of the title compound, with atomic numbering. Displacement ellipsoids are drawn at the 30% probability level.

5-(4-Chlorophenyl)-4-(4-methoxyphenyl)-3-(2-pyridyl)-4*H*-1,2,4-triazole

Crystal data

$C_{20}H_{15}ClN_4O$	$Z = 2$
$M_r = 362.81$	$F_{000} = 376$

Triclinic, $P\bar{1}$	D_x = 1.367 Mg m^{-3}
Hall symbol: -P 1	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 9.808 (4) Å	Cell parameters from 1472 reflections
b = 10.083 (4) Å	θ = 4.2–28.3º
c = 10.274 (4) Å	μ = 0.23 mm^{-1}
α = 70.415 (5)º	T = 298 (2) K
β = 73.417 (6)º	Block, colourless
γ = 69.768 (6)º	0.15 × 0.15 × 0.10 mm
V = 881.5 (6) Å^3	

Data collection

Bruker SMART CCD area-detector diffractometer	3411 independent reflections
Radiation source: fine-focus sealed tube	2757 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.019
T = 298(2) K	θ_{max} = 26.0º
φ and ω scans	θ_{min} = 2.1º
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	h = −12→12
T_{min} = 0.966, T_{max} = 0.977	k = −12→11
6776 measured reflections	l = −12→12

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.046	H-atom parameters constrained
$wR(F^2)$ = 0.130	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.1955P]$ where $P = (F_o^2 + 2F_c^2)/3$
S = 1.05	$(\Delta/\sigma)_{max}$ = 0.001
3411 reflections	$\Delta\rho_{max}$ = 0.19 e Å^{-3}
236 parameters	$\Delta\rho_{min}$ = −0.24 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 calculat-

ing *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}
C1	0.3198 (2)	0.0397 (2)	0.83095 (19)	0.0450 (4)
C2	0.3227 (2)	−0.0760 (2)	1.0498 (2)	0.0444 (4)
C3	0.2817 (2)	−0.1236 (2)	1.2046 (2)	0.0467 (5)
C4	0.3906 (3)	−0.1979 (3)	1.2842 (3)	0.0661 (6)
H12	0.4901	−0.2188	1.2412	0.079*
C5	0.3496 (4)	−0.2400 (3)	1.4270 (3)	0.0842 (8)
H13	0.4208	−0.2899	1.4832	0.101*
C6	0.2020 (4)	−0.2079 (3)	1.4866 (3)	0.0823 (8)
H14	0.1713	−0.2336	1.5839	0.099*
C7	0.1004 (3)	−0.1368 (3)	1.3999 (2)	0.0706 (7)
H15	0.0003	−0.1176	1.4409	0.085*
C8	0.12017 (19)	0.15735 (19)	1.00964 (17)	0.0381 (4)
C9	−0.0141 (2)	0.18012 (19)	0.97612 (18)	0.0408 (4)
H22	−0.0206	0.1288	0.9189	0.049*
C10	−0.1389 (2)	0.27883 (19)	1.02726 (19)	0.0429 (4)
H21	−0.2295	0.2946	1.0047	0.052*
C11	−0.1277 (2)	0.35414 (19)	1.11251 (19)	0.0435 (4)
C12	0.0091 (2)	0.3351 (2)	1.1402 (2)	0.0489 (5)
H19	0.0168	0.3893	1.1940	0.059*
C13	0.1335 (2)	0.2371 (2)	1.08900 (19)	0.0449 (4)
H18	0.2252	0.2248	1.1076	0.054*
C14	−0.3877 (3)	0.4630 (3)	1.1557 (3)	0.0857 (8)
H23A	−0.3959	0.5108	1.0591	0.128*
H23B	−0.4612	0.5204	1.2149	0.128*
H23C	−0.4029	0.3678	1.1808	0.128*
C15	0.2846 (2)	0.1481 (2)	0.69997 (19)	0.0445 (4)
C16	0.3221 (2)	0.1024 (2)	0.5780 (2)	0.0571 (5)
H5	0.3610	0.0030	0.5829	0.069*
C17	0.3029 (3)	0.2014 (3)	0.4497 (2)	0.0628 (6)
H6	0.3294	0.1694	0.3686	0.075*
C18	0.2441 (2)	0.3477 (3)	0.4434 (2)	0.0545 (5)
C19	0.2046 (2)	0.3961 (2)	0.5624 (2)	0.0568 (5)
H2	0.1638	0.4955	0.5571	0.068*
C20	0.2259 (2)	0.2966 (2)	0.6897 (2)	0.0515 (5)
H3	0.2005	0.3296	0.7701	0.062*
Cl1	0.22050 (7)	0.47545 (8)	0.28259 (6)	0.0782 (2)
N1	0.43195 (19)	−0.07819 (18)	0.83541 (18)	0.0565 (5)
N2	0.43441 (18)	−0.15167 (18)	0.97501 (18)	0.0557 (5)
N3	0.24694 (16)	0.04656 (16)	0.96486 (15)	0.0406 (4)
N4	0.13735 (19)	−0.0939 (2)	1.26017 (17)	0.0568 (5)
O1	−0.24465 (16)	0.44833 (16)	1.17406 (16)	0.0624 (4)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0438 (10)	0.0449 (10)	0.0438 (10)	−0.0108 (8)	−0.0011 (8)	−0.0162 (8)
C2	0.0420 (10)	0.0416 (10)	0.0485 (10)	−0.0104 (8)	−0.0115 (8)	−0.0094 (8)
C3	0.0534 (11)	0.0420 (10)	0.0474 (11)	−0.0160 (8)	−0.0153 (9)	−0.0076 (8)
C4	0.0681 (14)	0.0651 (14)	0.0683 (15)	−0.0242 (12)	−0.0315 (12)	−0.0003 (12)
C5	0.109 (2)	0.0849 (19)	0.0684 (16)	−0.0380 (17)	−0.0533 (16)	0.0093 (14)
C6	0.127 (3)	0.0809 (18)	0.0454 (13)	−0.0469 (18)	−0.0237 (15)	−0.0002 (12)
C7	0.0814 (17)	0.0750 (16)	0.0487 (13)	−0.0270 (13)	−0.0035 (12)	−0.0097 (11)
C8	0.0412 (9)	0.0375 (9)	0.0325 (8)	−0.0091 (7)	−0.0044 (7)	−0.0093 (7)
C9	0.0501 (10)	0.0400 (10)	0.0350 (9)	−0.0131 (8)	−0.0111 (8)	−0.0103 (7)
C10	0.0433 (10)	0.0409 (10)	0.0421 (10)	−0.0087 (8)	−0.0123 (8)	−0.0075 (8)
C11	0.0475 (10)	0.0371 (9)	0.0399 (9)	−0.0070 (8)	−0.0052 (8)	−0.0103 (8)
C12	0.0579 (12)	0.0497 (11)	0.0470 (11)	−0.0149 (9)	−0.0101 (9)	−0.0226 (9)
C13	0.0433 (10)	0.0518 (11)	0.0443 (10)	−0.0137 (8)	−0.0118 (8)	−0.0152 (9)
C14	0.0478 (13)	0.0877 (19)	0.120 (2)	0.0103 (12)	−0.0154 (14)	−0.0554 (17)
C15	0.0420 (10)	0.0486 (11)	0.0406 (10)	−0.0118 (8)	0.0003 (8)	−0.0165 (8)
C16	0.0609 (13)	0.0566 (13)	0.0519 (12)	−0.0084 (10)	−0.0049 (10)	−0.0251 (10)
C17	0.0655 (14)	0.0820 (16)	0.0425 (11)	−0.0179 (12)	−0.0036 (10)	−0.0265 (11)
C18	0.0482 (11)	0.0711 (14)	0.0417 (11)	−0.0213 (10)	−0.0076 (8)	−0.0078 (10)
C19	0.0639 (13)	0.0501 (12)	0.0500 (12)	−0.0146 (10)	−0.0065 (10)	−0.0100 (10)
C20	0.0614 (12)	0.0506 (12)	0.0399 (10)	−0.0146 (9)	−0.0029 (9)	−0.0154 (9)
Cl1	0.0825 (4)	0.1001 (5)	0.0479 (3)	−0.0364 (4)	−0.0219 (3)	0.0050 (3)
N1	0.0539 (10)	0.0480 (10)	0.0529 (10)	−0.0048 (8)	0.0011 (8)	−0.0139 (8)
N2	0.0507 (10)	0.0461 (9)	0.0576 (10)	−0.0044 (8)	−0.0077 (8)	−0.0093 (8)
N3	0.0401 (8)	0.0403 (8)	0.0394 (8)	−0.0079 (6)	−0.0075 (6)	−0.0114 (6)
N4	0.0585 (11)	0.0623 (11)	0.0445 (9)	−0.0164 (9)	−0.0095 (8)	−0.0085 (8)
O1	0.0557 (9)	0.0583 (9)	0.0712 (10)	−0.0017 (7)	−0.0065 (7)	−0.0339 (8)

Geometric parameters (Å, °)

C1—N1	1.309 (2)	C10—H21	0.93
C1—N3	1.370 (2)	C11—O1	1.361 (2)
C1—C15	1.464 (3)	C11—C12	1.385 (3)
C2—N2	1.307 (2)	C12—C13	1.375 (3)
C2—N3	1.361 (2)	C12—H19	0.93
C2—C3	1.476 (3)	C13—H18	0.93
C3—N4	1.334 (3)	C14—O1	1.419 (3)
C3—C4	1.381 (3)	C14—H23A	0.96
C4—C5	1.363 (4)	C14—H23B	0.96
C4—H12	0.93	C14—H23C	0.96
C5—C6	1.370 (4)	C15—C20	1.384 (3)
C5—H13	0.93	C15—C16	1.387 (3)
C6—C7	1.373 (4)	C16—C17	1.378 (3)
C6—H14	0.93	C16—H5	0.93
C7—N4	1.332 (3)	C17—C18	1.372 (3)
C7—H15	0.93	C17—H6	0.93

C8—C13	1.379 (3)	C18—C19	1.372 (3)
C8—C9	1.380 (3)	C18—Cl1	1.740 (2)
C8—N3	1.436 (2)	C19—C20	1.375 (3)
C9—C10	1.380 (2)	C19—H2	0.93
C9—H22	0.93	C20—H3	0.93
C10—C11	1.384 (3)	N1—N2	1.379 (2)
N1—C1—N3	109.87 (17)	C11—C12—H19	119.6
N1—C1—C15	123.48 (17)	C12—C13—C8	118.90 (18)
N3—C1—C15	126.62 (16)	C12—C13—H18	120.5
N2—C2—N3	110.62 (17)	C8—C13—H18	120.5
N2—C2—C3	123.71 (17)	O1—C14—H23A	109.5
N3—C2—C3	125.59 (16)	O1—C14—H23B	109.5
N4—C3—C4	123.3 (2)	H23A—C14—H23B	109.5
N4—C3—C2	116.75 (17)	O1—C14—H23C	109.5
C4—C3—C2	119.97 (19)	H23A—C14—H23C	109.5
C5—C4—C3	118.7 (2)	H23B—C14—H23C	109.5
C5—C4—H12	120.6	C20—C15—C16	118.10 (19)
C3—C4—H12	120.6	C20—C15—C1	122.82 (17)
C4—C5—C6	119.0 (2)	C16—C15—C1	118.88 (18)
C4—C5—H13	120.5	C17—C16—C15	121.3 (2)
C6—C5—H13	120.5	C17—C16—H5	119.3
C5—C6—C7	118.7 (2)	C15—C16—H5	119.3
C5—C6—H14	120.6	C18—C17—C16	119.05 (19)
C7—C6—H14	120.6	C18—C17—H6	120.5
N4—C7—C6	123.5 (2)	C16—C17—H6	120.5
N4—C7—H15	118.2	C19—C18—C17	121.0 (2)
C6—C7—H15	118.2	C19—C18—Cl1	118.90 (18)
C13—C8—C9	120.80 (16)	C17—C18—Cl1	120.10 (17)
C13—C8—N3	119.40 (16)	C18—C19—C20	119.5 (2)
C9—C8—N3	119.78 (15)	C18—C19—H2	120.3
C8—C9—C10	120.17 (17)	C20—C19—H2	120.3
C8—C9—H22	119.9	C19—C20—C15	121.07 (18)
C10—C9—H22	119.9	C19—C20—H3	119.5
C9—C10—C11	119.31 (18)	C15—C20—H3	119.5
C9—C10—H21	120.3	C1—N1—N2	107.71 (15)
C11—C10—H21	120.3	C2—N2—N1	107.13 (15)
O1—C11—C10	124.12 (18)	C2—N3—C1	104.68 (15)
O1—C11—C12	115.96 (17)	C2—N3—C8	126.39 (15)
C10—C11—C12	119.92 (16)	C1—N3—C8	128.93 (15)
C13—C12—C11	120.77 (17)	C7—N4—C3	116.75 (19)
C13—C12—H19	119.6	C11—O1—C14	117.50 (17)
N2—C2—C3—N4	−142.6 (2)	C17—C18—C19—C20	0.8 (3)
N3—C2—C3—N4	33.7 (3)	Cl1—C18—C19—C20	−178.51 (16)
N2—C2—C3—C4	35.9 (3)	C18—C19—C20—C15	−0.9 (3)
N3—C2—C3—C4	−147.8 (2)	C16—C15—C20—C19	0.3 (3)
N4—C3—C4—C5	−1.8 (4)	C1—C15—C20—C19	175.11 (19)
C2—C3—C4—C5	179.8 (2)	N3—C1—N1—N2	−0.1 (2)
C3—C4—C5—C6	0.3 (4)	C15—C1—N1—N2	177.91 (17)

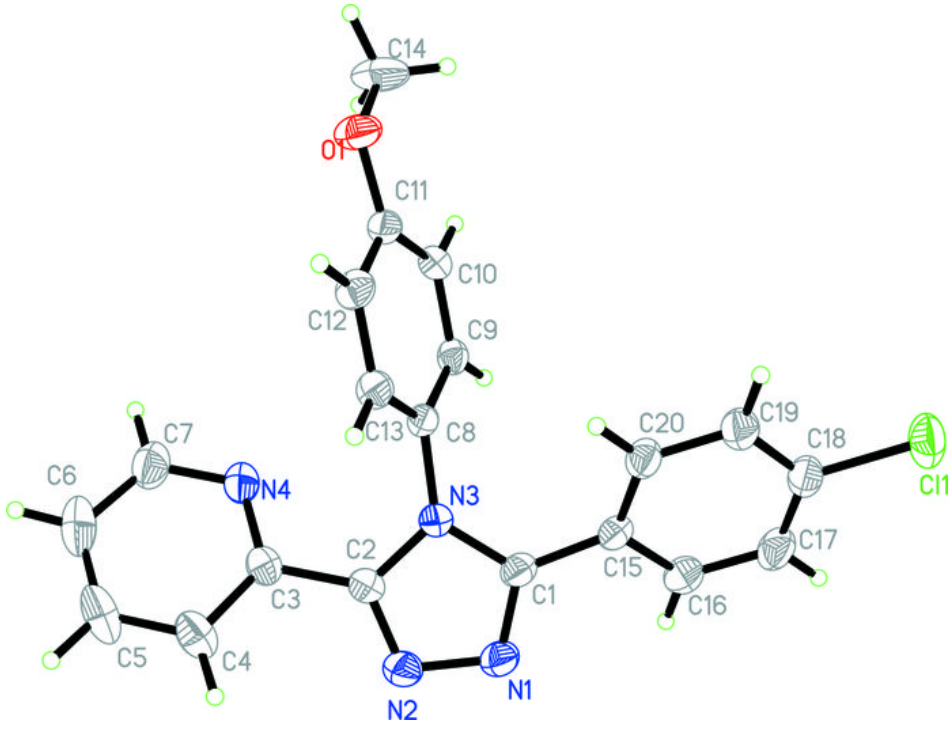
C4—C5—C6—C7	1.3 (4)	N3—C2—N2—N1	−0.8 (2)
C5—C6—C7—N4	−1.6 (4)	C3—C2—N2—N1	176.01 (18)
C13—C8—C9—C10	−2.9 (3)	C1—N1—N2—C2	0.5 (2)
N3—C8—C9—C10	175.30 (15)	N2—C2—N3—C1	0.8 (2)
C8—C9—C10—C11	−0.1 (3)	C3—C2—N3—C1	−175.99 (18)
C9—C10—C11—O1	−176.64 (17)	N2—C2—N3—C8	−178.47 (17)
C9—C10—C11—C12	3.0 (3)	C3—C2—N3—C8	4.8 (3)
O1—C11—C12—C13	176.80 (17)	N1—C1—N3—C2	−0.4 (2)
C10—C11—C12—C13	−2.9 (3)	C15—C1—N3—C2	−178.31 (18)
C11—C12—C13—C8	−0.2 (3)	N1—C1—N3—C8	178.80 (18)
C9—C8—C13—C12	3.1 (3)	C15—C1—N3—C8	0.9 (3)
N3—C8—C13—C12	−175.17 (16)	C13—C8—N3—C2	62.1 (2)
N1—C1—C15—C20	−145.4 (2)	C9—C8—N3—C2	−116.2 (2)
N3—C1—C15—C20	32.2 (3)	C13—C8—N3—C1	−117.0 (2)
N1—C1—C15—C16	29.4 (3)	C9—C8—N3—C1	64.8 (3)
N3—C1—C15—C16	−153.0 (2)	C6—C7—N4—C3	0.2 (4)
C20—C15—C16—C17	0.5 (3)	C4—C3—N4—C7	1.6 (3)
C1—C15—C16—C17	−174.54 (19)	C2—C3—N4—C7	−179.95 (19)
C15—C16—C17—C18	−0.6 (3)	C10—C11—O1—C14	3.8 (3)
C16—C17—C18—C19	0.0 (3)	C12—C11—O1—C14	−175.9 (2)
C16—C17—C18—Cl1	179.26 (17)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C9—H22···N4^{i}	0.93	2.60	3.454 (3)	154

Symmetry codes: (i) −*x*, −*y*, −*z*+2.

Fig. 1


C14
O1
C11
C10
C12
C9
C13
C8
C7
C6
N4
N3
C20
C19
C18
Cl1
C2
C15
C17
C3
C1
C16
C5
C4
N2
N1