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2-(3,4-Dichlorophenyl)-*N*-methyl-*N*-[2-(pyrrolidin-1-yl)cyclohexyl]acetamide hydrochloride: (±)-U50,488H

Yoshimi Ichimaru* and Masaaki Kurihara

Faculty of Pharmaceutical Sciences, Shonan University of Medical Sciences, 16-10 Kamishinano, Totsuka-ku, Yokohama, Kanagawa, 244-0806, Japan. *Correspondence e-mail: yoshimi.ichimaru@sums.ac.jp

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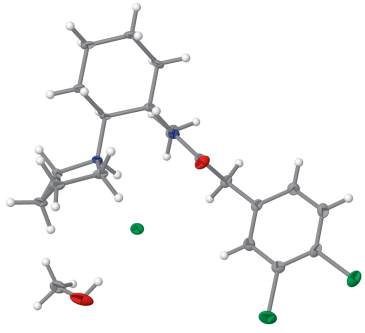
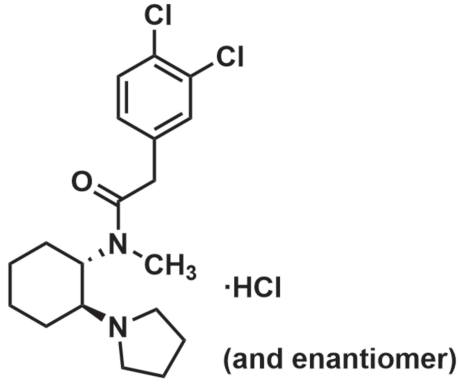
The crystal structure of the methanol-solvated hydrochloride salt of the selective κ-opioid receptor agonist (±)-U50,488, namely, 1-{2-[2-(3,4-dichlorophenyl)-*N*-methylacetamido]cyclohexyl}pyrrolidin-1-ium chloride methanol monosolvate, $C_{19}H_{27}Cl_2N_2O^+\cdot Cl^-\cdot CH_3OH$, is reported. The compound crystallized as a racemate of the (*S*,*S*) and (*R*,*R*) enantiomers, consistent with the *anti*-selective nucleophilic substitution used in its synthesis. The cyclohexane ring adopts a chair conformation with an equatorial-equatorial conformation of its 1,2-substituents. Protonation occurs exclusively at the pyrrolidine nitrogen atom, and the pyrrolidine ring displays a half-chair conformation twisted on the bond opposite the nitrogen. In the crystal, the chloride anion forms a hydrogen-bonding network with the protonated pyrrolidine unit, the methanol solvent molecule, and adjacent C—H groups. The crystal packing is further consolidated by C—H···O interactions involving the amide oxygen atom that form centrosymmetric dimers, alongside intermolecular π-stacking and Cl···O halogen-bonding interactions. This study provides the first structural characterization of the hydrochloride salt form of this widely used pharmacological compound.

3D view



Chemical scheme



Structure description

The title compound (Fig. 1) is a methanol solvate of the selective κ-opioid receptor agonist commonly known as (±)-U50,488H. 'U50,488′ was the developmental designation assigned by the Upjohn Company (Szmuszkovicz & Von Voigtlander, 1982), and it is marketed as 'U50,488H' to signify its status as a hydrochloride salt. To date, the crystal structure of U50,488 has been reported as a methanesulfonate salt (Doi *et al.*, 1990). Although U50,488 possesses two chiral centers – potentially yielding four stereoisomers – the standard synthetic route involving the nucleophilic substitution of cyclohexene oxide by pyrrolidine selectively produces the *trans*-1,2-cyclohexane derivative (Chesis & Welch,

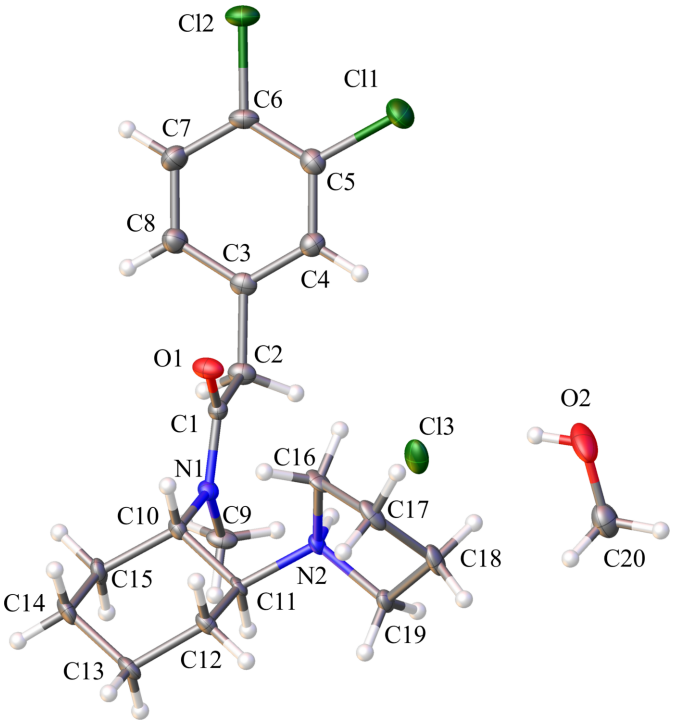


Figure 1
The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

1990; Kato *et al.*, 2025). Consequently, the product is obtained as a racemic mixture of the (*S*,*S*) and (*R*,*R*) enantiomers, while the (*S*,*R*) and (*R*,*S*) isomers are produced in negligible yields. The (*S*,*S*)-enantiomer corresponds to (−)-U50,488, which exhibits levorotatory properties and possesses a higher affinity for the κ-opioid receptor than its (+)-enantiomer (Rothman *et al.*, 1989).

The title compound exists as a racemic mixture of the (*S*,*S*) and (*R*,*R*) isomers (Fig. 2). The cyclohexane ring (C10–C15) adopts a chair conformation, as indicated by the Cremer–Pople puckering parameters (Cremer and Pople, 1975) of θ = 2.5 (3)°. The 1,2-substituents on the cyclohexane ring adopt an equatorial–equatorial *gauche* conformation: the torsion angle N1—C10—C11—N2 is 53.5(12°. The pyrrolidine ring (N2/C16–C19) adopts a half-chair conformation twisted on the C17—C18 bond, with calculated Cremer–Pople puckering parameters Q = 0.413 (3) Å and φ = 88.7 (3)°. Due to the significantly reduced basicity of the amide nitrogen atom (N1), protonation occurs exclusively at the pyrrolidine nitrogen (N2). The N1—C1 (amide carbonyl) bond is notably shorter at 1.363 (3) Å, reflecting its partial double-bond character. The distances between the chloride ion (Cl3) and the nitrogen atoms are 3.5505 (19) Å for Cl3···N1 and 3.0775 (19) Å for Cl3···N2. The short Cl3···N2 interatomic distance, which is less than the sum of the van der Waals radii of chlorine and nitrogen, is attributable to charge-assisted hydrogen-bonding interactions arising from the protonation of the pyrrolidine nitrogen atom. The chloride ion (Cl3) forms a hydrogen bond network with the protonated pyrrolidine, the hydroxyl group of the methanol solvent molecule, and C—H groups (Table 1). The amide oxygen atom (O1) also acts as a hydrogen-bonding acceptor, interacting with nearby C—H groups (Table 1), contributing to the formation of a centrosymmetric dimer. The

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cl3	1.00	2.17	3.0775 (19)	150
C2—H2*A*···Cl3	0.99	2.75	3.486 (2)	132
C10—H10···O1^{i}	1.00	2.61	3.543 (3)	156
C16—H16*B*···O1^{i}	0.99	2.29	3.274 (3)	170
C19—H19*A*···Cl3^{ii}	0.99	2.92	3.685 (2)	135
O2—H2*C*···Cl3	0.84	2.32	3.103 (2)	155

Symmetry codes: (i) $-x+2, -y+1, -z+1$; (ii) $x+\frac{1}{2}, -y+\frac{3}{2}, z+\frac{1}{2}$.

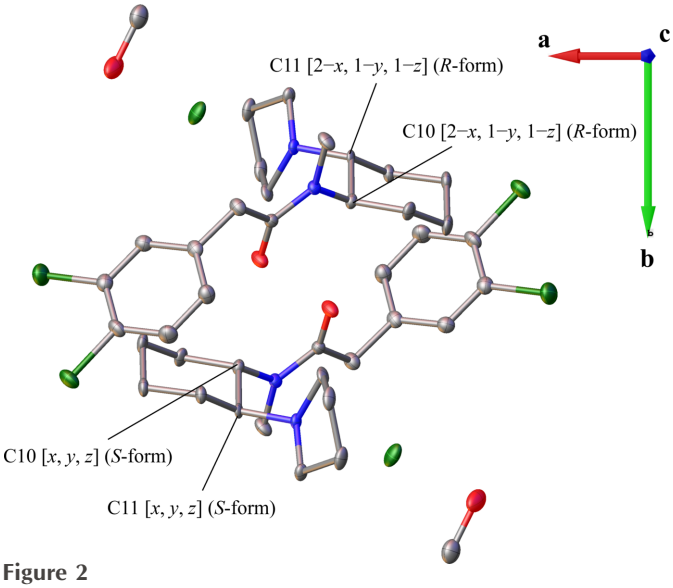


Figure 2
The pair of enantiomers of the title compound with displacement ellipsoids drawn at the 50% probability level.

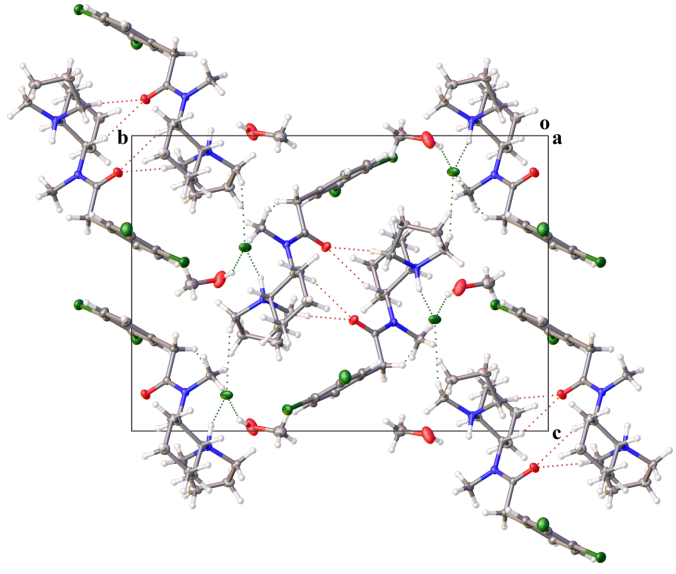


Figure 3
Partial packing diagram viewed along the *a*-axis direction. The green dotted lines represent H···Cl interactions, and the red dotted lines represent C—H···O interactions.

torsion angles around the amide group, C10—N1—C1—C2, C9—N1—C1—O1, and N1—C1—C2—C3, are −174.3 (2), −178.5 (2), and 174.6 (2)°, respectively. These angles indicate that the amide bond and its substituents adopt a conformation with minimal steric hindrance. The 3,4-dichlorophenyl moiety derived from a carboxylic acid is involved in π-stacking and halogen-bonding. The plane of the aromatic ring defined by C3–C8 (centroid: *Cg*) has a ring centroid distance of 3.9422 (14) Å and a slippage of 1.690 Å relative to Cg^{i} [symmetry code (i): $1-x, 1-y, -z$]. A halogen bond is formed between the chlorine atom (Cl2) and the methanol oxygen atom ($O2^{ii}$) [3.097 (2) Å; symmetry code (ii): $\frac{1}{2}-x, -\frac{1}{2}+y, \frac{1}{2}-z$]. The crystal packing resulting from these intermolecular interactions is illustrated in Fig. 3.

Synthesis and crystallization

The title compound was synthesized according to a reported method (Chesis & Welch, 1990; Kato *et al.*, 2025). The single crystals suitable for X-ray analysis were obtained by dissolving the compound in a minimum amount of methanol at 298 K followed by slow evaporation.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{19}H_{27}Cl_2N_2O^+\cdot Cl^-\cdot CH_4O$
M_r	437.82
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	8.7729 (2), 18.5639 (3), 13.6318 (3)
β (°)	105.022 (2)
V (Å^3)	2144.20 (8)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.01
Crystal size (mm)	0.41 × 0.28 × 0.12
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix-Bantam
Absorption correction	Multi-scan (*CrysAlis PRO*; Rigaku OD 2025)
T_{min}, T_{max}	0.266, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23023, 3919, 3518
R_{int}	0.161
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.603
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.071, 0.197, 1.05
No. of reflections	3919
No. of parameters	247
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.71, −0.93

Computer programs: *CrysAlis PRO* (Rigaku OD, 2025), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2019/3* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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full crystallographic data

IUCrData (2026). **11**, x260666 [https://doi.org/10.1107/S2414314626006668]

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1-{2-[2-(3,4-Dichlorophenyl)-*N*-methylacetamido]cyclohexyl}pyrrolidin-1-ium chloride methanol monosolvate

Crystal data

$C_{19}H_{27}Cl_2N_2O^+\cdot Cl^-\cdot CH_4O$
M_r = 437.82
Monoclinic, $P2_1/n$
a = 8.7729 (2) Å
b = 18.5639 (3) Å
c = 13.6318 (3) Å
β = 105.022 (2)°
V = 2144.20 (8) Å^3
Z = 4
$F(000)$ = 928
D_x = 1.356 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 12899 reflections
θ = 4.1–68.2°
μ = 4.01 mm^{-1}
T = 100 K
Block, colourless
0.41 × 0.28 × 0.12 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix-Bantam diffractometer
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan (CrysAlisPro; Rigaku OD 2025)
T_{min} = 0.266, T_{max} = 1.000
23023 measured reflections
3919 independent reflections
3518 reflections with $I > 2\sigma(I)$
R_{int} = 0.161
θ_{max} = 68.5°, θ_{min} = 4.1°
h = −10→10
k = −22→22
l = −16→16

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.071
$wR(F^2)$ = 0.197
S = 1.05
3919 reflections
247 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1498P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.71 e Å^{-3}
$\Delta\rho_{min}$ = −0.93 e Å^{-3}

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.

Refinement. H atoms were positioned geometrically and constrained to ride on their parent atoms, with carbon hydrogen bond distances of 0.95 Å for aromatic C—H, 1.00, 0.99 and 0.98 Å for aliphatic C—H, CH_2 and CH_3, 1.00 Å for N—H and 0.84 Å for OH moieties, respectively. Methyl and hydroxyl H atoms were allowed to rotate but not to tip to best fit the experimental electron density. U_{iso}(H) values were set to a multiple of U_{eq}(O/C/N) with 1.5 for CH_3 and OH, and 1.2 for C—H, CH_2 and N—H units, respectively.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.25998 (8)	0.51248 (4)	0.18314 (6)	0.0315 (3)
Cl2	0.34226 (7)	0.37367 (3)	0.07217 (5)	0.0256 (2)
Cl3	0.71467 (7)	0.72770 (3)	0.37791 (4)	0.0259 (2)
O1	0.8975 (2)	0.53307 (9)	0.37621 (13)	0.0208 (4)
N1	1.0566 (2)	0.62855 (9)	0.36832 (15)	0.0135 (4)
N2	0.9968 (2)	0.68267 (10)	0.55323 (14)	0.0126 (4)
H2	0.931549	0.690415	0.482139	0.015*
C1	0.9314 (3)	0.58443 (11)	0.32909 (17)	0.0138 (5)
C2	0.8339 (3)	0.60260 (12)	0.22206 (18)	0.0183 (5)
H2A	0.783263	0.650196	0.222737	0.022*
H2B	0.904466	0.605784	0.176132	0.022*
C3	0.7089 (3)	0.54694 (12)	0.18224 (17)	0.0169 (5)
C4	0.5595 (3)	0.55431 (13)	0.19764 (18)	0.0186 (5)
H4	0.535040	0.595382	0.232240	0.022*
C5	0.4456 (3)	0.50177 (13)	0.16259 (19)	0.0195 (5)
C6	0.4811 (3)	0.44110 (13)	0.11320 (18)	0.0198 (5)
C7	0.6304 (3)	0.43311 (13)	0.0983 (2)	0.0235 (6)
H7	0.655781	0.391391	0.065389	0.028*
C8	0.7426 (3)	0.48643 (13)	0.13171 (19)	0.0214 (5)
H8	0.844125	0.481478	0.119847	0.026*
C9	1.0923 (3)	0.69030 (13)	0.31167 (18)	0.0196 (5)
H9A	1.182676	0.716593	0.353736	0.029*
H9B	1.000369	0.722303	0.293644	0.029*
H9C	1.117651	0.673449	0.249634	0.029*
C10	1.1646 (3)	0.61037 (12)	0.46710 (18)	0.0139 (5)
H10	1.126337	0.564529	0.491028	0.017*
C11	1.1637 (2)	0.66856 (11)	0.54710 (17)	0.0120 (5)
H11	1.205183	0.714079	0.524470	0.014*
C12	1.2738 (3)	0.64729 (12)	0.64974 (18)	0.0159 (5)
H12A	1.273195	0.685300	0.700574	0.019*
H12B	1.236782	0.601850	0.673823	0.019*
C13	1.4414 (3)	0.63738 (13)	0.63785 (19)	0.0179 (5)
H13A	1.478661	0.683180	0.614975	0.021*
H13B	1.513394	0.624491	0.704281	0.021*
C14	1.4445 (3)	0.57836 (14)	0.5609 (2)	0.0219 (6)
H14A	1.412137	0.532024	0.585366	0.026*
H14B	1.553129	0.572787	0.553452	0.026*
C15	1.3325 (3)	0.59729 (12)	0.45804 (19)	0.0179 (5)
H15A	1.371233	0.641097	0.430812	0.022*

H15B	1.331622	0.557414	0.409668	0.022*
C16	0.9187 (3)	0.62200 (12)	0.59818 (19)	0.0180 (5)
H16A	0.814673	0.609496	0.552426	0.022*
H16B	0.986002	0.578427	0.609943	0.022*
C17	0.9002 (3)	0.65241 (14)	0.69791 (19)	0.0221 (5)
H17A	0.998214	0.646247	0.752864	0.027*
H17B	0.811734	0.628975	0.718283	0.027*
C18	0.8657 (3)	0.73197 (14)	0.6734 (2)	0.0224 (6)
H18A	0.755600	0.739218	0.632876	0.027*
H18B	0.884580	0.761229	0.736169	0.027*
C19	0.9823 (3)	0.75050 (12)	0.61262 (18)	0.0157 (5)
H19A	1.085729	0.763921	0.658225	0.019*
H19B	0.942900	0.791172	0.565949	0.019*
O2	0.4718 (2)	0.78838 (11)	0.48632 (19)	0.0388 (6)
H2C	0.528067	0.759651	0.463420	0.058*
C20	0.5452 (3)	0.85588 (16)	0.5019 (2)	0.0304 (6)
H20A	0.651834	0.850649	0.546605	0.046*
H20B	0.483688	0.888338	0.533538	0.046*
H20C	0.551417	0.875904	0.436562	0.046*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0203 (4)	0.0328 (4)	0.0450 (5)	−0.0020 (2)	0.0147 (3)	−0.0022 (3)
Cl2	0.0257 (4)	0.0235 (4)	0.0255 (4)	−0.0107 (2)	0.0027 (3)	−0.0020 (2)
Cl3	0.0208 (4)	0.0355 (4)	0.0181 (4)	0.0118 (2)	−0.0009 (3)	0.0001 (2)
O1	0.0188 (9)	0.0194 (8)	0.0212 (9)	−0.0057 (6)	−0.0002 (7)	0.0054 (7)
N1	0.0119 (10)	0.0142 (9)	0.0156 (10)	−0.0010 (7)	0.0055 (8)	0.0012 (7)
N2	0.0084 (9)	0.0168 (9)	0.0140 (10)	0.0003 (7)	0.0051 (8)	−0.0007 (7)
C1	0.0128 (11)	0.0129 (9)	0.0161 (11)	0.0003 (8)	0.0045 (9)	−0.0005 (8)
C2	0.0185 (12)	0.0207 (11)	0.0146 (11)	−0.0040 (9)	0.0024 (10)	0.0013 (9)
C3	0.0175 (12)	0.0200 (11)	0.0115 (11)	−0.0015 (9)	0.0008 (9)	0.0027 (9)
C4	0.0210 (13)	0.0181 (11)	0.0174 (11)	−0.0008 (9)	0.0060 (10)	−0.0001 (9)
C5	0.0185 (13)	0.0220 (11)	0.0184 (12)	0.0003 (10)	0.0053 (10)	0.0032 (9)
C6	0.0198 (13)	0.0202 (11)	0.0173 (12)	−0.0071 (9)	0.0011 (10)	−0.0011 (9)
C7	0.0250 (14)	0.0225 (11)	0.0230 (13)	−0.0016 (10)	0.0065 (11)	−0.0064 (10)
C8	0.0193 (13)	0.0254 (12)	0.0203 (12)	−0.0013 (10)	0.0063 (10)	−0.0034 (10)
C9	0.0197 (12)	0.0218 (11)	0.0175 (12)	−0.0088 (9)	0.0054 (10)	0.0027 (9)
C10	0.0095 (11)	0.0162 (10)	0.0161 (11)	0.0017 (8)	0.0033 (9)	0.0015 (8)
C11	0.0052 (10)	0.0160 (10)	0.0160 (11)	−0.0005 (8)	0.0051 (9)	0.0006 (8)
C12	0.0089 (11)	0.0220 (11)	0.0164 (11)	−0.0004 (9)	0.0029 (9)	0.0004 (9)
C13	0.0075 (11)	0.0239 (11)	0.0216 (12)	−0.0005 (9)	0.0026 (9)	0.0018 (9)
C14	0.0082 (11)	0.0284 (12)	0.0290 (14)	0.0036 (9)	0.0048 (10)	0.0002 (11)
C15	0.0118 (12)	0.0229 (11)	0.0210 (12)	0.0046 (9)	0.0076 (10)	−0.0025 (9)
C16	0.0099 (11)	0.0220 (11)	0.0239 (13)	−0.0038 (9)	0.0076 (9)	0.0054 (9)
C17	0.0112 (11)	0.0384 (14)	0.0188 (12)	0.0005 (10)	0.0076 (10)	0.0070 (11)
C18	0.0124 (12)	0.0364 (14)	0.0204 (13)	0.0057 (10)	0.0079 (10)	−0.0014 (10)
C19	0.0112 (11)	0.0200 (11)	0.0174 (11)	0.0014 (9)	0.0064 (9)	−0.0042 (9)

O2	0.0258 (11)	0.0346 (10)	0.0648 (15)	0.0065 (9)	0.0277 (10)	0.0167 (11)
C20	0.0235 (14)	0.0398 (15)	0.0308 (15)	0.0044 (11)	0.0121 (12)	0.0006 (12)

Geometric parameters (Å, º)

Cl1—C5	1.734 (3)	C11—H11	1.0000
Cl2—C6	1.735 (2)	C11—C12	1.532 (3)
O1—C1	1.228 (3)	C12—H12A	0.9900
N1—C1	1.363 (3)	C12—H12B	0.9900
N1—C9	1.461 (3)	C12—C13	1.531 (3)
N1—C10	1.471 (3)	C13—H13A	0.9900
N2—H2	1.0000	C13—H13B	0.9900
N2—C11	1.511 (3)	C13—C14	1.522 (3)
N2—C16	1.527 (3)	C14—H14A	0.9900
N2—C19	1.520 (3)	C14—H14B	0.9900
C1—C2	1.526 (3)	C14—C15	1.530 (3)
C2—H2A	0.9900	C15—H15A	0.9900
C2—H2B	0.9900	C15—H15B	0.9900
C2—C3	1.502 (3)	C16—H16A	0.9900
C3—C4	1.386 (3)	C16—H16B	0.9900
C3—C8	1.389 (3)	C16—C17	1.519 (4)
C4—H4	0.9500	C17—H17A	0.9900
C4—C5	1.390 (4)	C17—H17B	0.9900
C5—C6	1.389 (3)	C17—C18	1.527 (4)
C6—C7	1.384 (4)	C18—H18A	0.9900
C7—H7	0.9500	C18—H18B	0.9900
C7—C8	1.387 (4)	C18—C19	1.514 (3)
C8—H8	0.9500	C19—H19A	0.9900
C9—H9A	0.9800	C19—H19B	0.9900
C9—H9B	0.9800	O2—H2C	0.8400
C9—H9C	0.9800	O2—C20	1.400 (4)
C10—H10	1.0000	C20—H20A	0.9800
C10—C11	1.536 (3)	C20—H20B	0.9800
C10—C15	1.529 (3)	C20—H20C	0.9800
C1—N1—C9	121.69 (19)	C11—C12—H12B	109.8
C1—N1—C10	118.92 (18)	H12A—C12—H12B	108.3
C9—N1—C10	119.25 (18)	C13—C12—C11	109.25 (19)
C11—N2—H2	106.9	C13—C12—H12A	109.8
C11—N2—C16	115.89 (16)	C13—C12—H12B	109.8
C11—N2—C19	112.93 (16)	C12—C13—H13A	109.6
C16—N2—H2	106.9	C12—C13—H13B	109.6
C19—N2—H2	106.9	H13A—C13—H13B	108.1
C19—N2—C16	106.78 (17)	C14—C13—C12	110.41 (19)
O1—C1—N1	122.7 (2)	C14—C13—H13A	109.6
O1—C1—C2	121.3 (2)	C14—C13—H13B	109.6
N1—C1—C2	115.95 (19)	C13—C14—H14A	109.6
C1—C2—H2A	109.3	C13—C14—H14B	109.6

C1—C2—H2B	109.3	C13—C14—C15	110.1 (2)
H2A—C2—H2B	107.9	H14A—C14—H14B	108.1
C3—C2—C1	111.69 (18)	C15—C14—H14A	109.6
C3—C2—H2A	109.3	C15—C14—H14B	109.6
C3—C2—H2B	109.3	C10—C15—C14	111.43 (19)
C4—C3—C2	120.5 (2)	C10—C15—H15A	109.3
C4—C3—C8	119.1 (2)	C10—C15—H15B	109.3
C8—C3—C2	120.4 (2)	C14—C15—H15A	109.3
C3—C4—H4	119.9	C14—C15—H15B	109.3
C3—C4—C5	120.2 (2)	H15A—C15—H15B	108.0
C5—C4—H4	119.9	N2—C16—H16A	110.9
C4—C5—Cl1	119.08 (19)	N2—C16—H16B	110.9
C6—C5—Cl1	120.65 (19)	H16A—C16—H16B	108.9
C6—C5—C4	120.3 (2)	C17—C16—N2	104.37 (18)
C5—C6—Cl2	121.0 (2)	C17—C16—H16A	110.9
C7—C6—Cl2	119.16 (19)	C17—C16—H16B	110.9
C7—C6—C5	119.9 (2)	C16—C17—H17A	111.2
C6—C7—H7	120.2	C16—C17—H17B	111.2
C6—C7—C8	119.6 (2)	C16—C17—C18	103.0 (2)
C8—C7—H7	120.2	H17A—C17—H17B	109.1
C3—C8—H8	119.5	C18—C17—H17A	111.2
C7—C8—C3	121.0 (2)	C18—C17—H17B	111.2
C7—C8—H8	119.5	C17—C18—H18A	111.3
N1—C9—H9A	109.5	C17—C18—H18B	111.3
N1—C9—H9B	109.5	H18A—C18—H18B	109.2
N1—C9—H9C	109.5	C19—C18—C17	102.46 (19)
H9A—C9—H9B	109.5	C19—C18—H18A	111.3
H9A—C9—H9C	109.5	C19—C18—H18B	111.3
H9B—C9—H9C	109.5	N2—C19—H19A	110.7
N1—C10—H10	107.6	N2—C19—H19B	110.7
N1—C10—C11	111.59 (17)	C18—C19—N2	105.39 (19)
N1—C10—C15	111.59 (18)	C18—C19—H19A	110.7
C11—C10—H10	107.6	C18—C19—H19B	110.7
C15—C10—H10	107.6	H19A—C19—H19B	108.8
C15—C10—C11	110.56 (18)	C20—O2—H2C	109.5
N2—C11—C10	110.15 (17)	O2—C20—H20A	109.5
N2—C11—H11	107.8	O2—C20—H20B	109.5
N2—C11—C12	112.64 (17)	O2—C20—H20C	109.5
C10—C11—H11	107.8	H20A—C20—H20B	109.5
C12—C11—C10	110.44 (17)	H20A—C20—H20C	109.5
C12—C11—H11	107.8	H20B—C20—H20C	109.5
C11—C12—H12A	109.8		

Cl1—C5—C6—Cl2	−0.9 (3)	C9—N1—C1—O1	−178.5 (2)
Cl1—C5—C6—C7	−179.39 (19)	C9—N1—C1—C2	1.3 (3)
Cl2—C6—C7—C8	−179.4 (2)	C9—N1—C10—C11	67.1 (2)
O1—C1—C2—C3	−5.6 (3)	C9—N1—C10—C15	−57.1 (3)
N1—C1—C2—C3	174.6 (2)	C10—N1—C1—O1	5.8 (3)

N1—C10—C11—N2	53.5 (2)	C10—N1—C1—C2	−174.32 (18)
N1—C10—C11—C12	178.53 (17)	C10—C11—C12—C13	58.9 (2)
N1—C10—C15—C14	−179.97 (18)	C11—N2—C16—C17	112.6 (2)
N2—C11—C12—C13	−177.43 (16)	C11—N2—C19—C18	−140.93 (19)
N2—C16—C17—C18	35.0 (2)	C11—C10—C15—C14	55.2 (2)
C1—N1—C10—C11	−117.1 (2)	C11—C12—C13—C14	−60.3 (2)
C1—N1—C10—C15	118.6 (2)	C12—C13—C14—C15	58.8 (3)
C1—C2—C3—C4	90.5 (3)	C13—C14—C15—C10	−56.2 (3)
C1—C2—C3—C8	−87.8 (3)	C15—C10—C11—N2	178.31 (17)
C2—C3—C4—C5	−178.5 (2)	C15—C10—C11—C12	−56.6 (2)
C2—C3—C8—C7	177.3 (2)	C16—N2—C11—C10	69.3 (2)
C3—C4—C5—Cl1	179.93 (18)	C16—N2—C11—C12	−54.5 (2)
C3—C4—C5—C6	0.9 (4)	C16—N2—C19—C18	−12.4 (2)
C4—C3—C8—C7	−1.1 (4)	C16—C17—C18—C19	−42.8 (2)
C4—C5—C6—Cl2	178.10 (19)	C17—C18—C19—N2	33.9 (2)
C4—C5—C6—C7	−0.4 (4)	C19—N2—C11—C10	−167.08 (17)
C5—C6—C7—C8	−0.9 (4)	C19—N2—C11—C12	69.1 (2)
C6—C7—C8—C3	1.6 (4)	C19—N2—C16—C17	−14.1 (2)
C8—C3—C4—C5	−0.2 (3)		

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···Cl3	1.00	2.17	3.0775 (19)	150
C2—H2*A*···Cl3	0.99	2.75	3.486 (2)	132
C10—H10···O1^{i}	1.00	2.61	3.543 (3)	156
C16—H16*B*···O1^{i}	0.99	2.29	3.274 (3)	170
C19—H19*A*···Cl3^{ii}	0.99	2.92	3.685 (2)	135
O2—H2*C*···Cl3	0.84	2.32	3.103 (2)	155

Symmetry codes: (i) −*x*+2, −*y*+1, −*z*+1; (ii) *x*+1/2, −*y*+3/2, *z*+1/2.