Crystal structure of 3-amino-1-(4-chlorophenyl)-1H-benzo[f]chromene-2-carbonitrile

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In the title compound, $C_{20}H_{13}ClN_2O$, the chlorobenzene ring is almost perpendicular to the mean plane of the naphthalene ring system, making a dihedral angle of 81.26 (8)°. The 4H-pyran ring fused with the naphthalene ring system has a flattened boat conformation. In the crystal, N—H···N hydrogen bonds generate chains along the b-axis direction. Further N—H···N hydrogen bonds link these chains into sheets parallel to (010). The crystal packing also features C—H···π interactions. The crystal studied was an inversion twin with a 0.557 (16):0.443 (16) domain ratio.

1. Related literature

For the synthesis and biological importance of chromene compounds, see, for example: Ellis (1977); Singh et al. (2010); Kidwai et al. (2010); Lácová et al. (2005); Dell & Smith (1993a,b); Al-Soud et al. (2006); Eiden & Denk (1991); Bruhlmann et al. (200); (Kesten et al. (1999); Bruhlmann et al. (2001). For a similar structure, see: Akkurt et al. (2013).
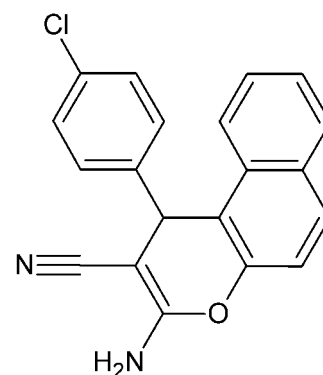
2. Experimental

2.1. Crystal data

$C_{20}H_{13}ClN_2O$	$V = 780.2$ (8) Å^3
$M_r = 332.77$	$Z = 2$
Monoclinic, $P2_1$	Cu $K\alpha$ radiation
$a = 10.056$ (7) Å	$\mu = 2.23$ mm^{-1}
$b = 6.172$ (3) Å	$T = 100$ K
$c = 12.751$ (6) Å	$0.32 \times 0.12 \times 0.10$ mm
$\beta = 99.641$ (17)°	

2.2. Data collection

Rigaku AFC11 diffractometer	11415 measured reflections
Absorption correction: multi-scan (CrystalClearSM Expert; Rigaku, 2012)	2558 independent reflections
	2500 reflections with $I > 2\sigma(I)$
$T_{min} = 0.948$, $T_{max} = 1.000$	$R_{int} = 0.032$

2.3. Refinement

$R[F^2 > 2\sigma(F^2)] = 0.028$	$\Delta\rho_{max} = 0.17$ e Å^{-3}
$wR(F^2) = 0.075$	$\Delta\rho_{min} = -0.22$ e Å^{-3}
$S = 1.06$	Absolute structure: Refined as an inversion twin.
2558 reflections	Absolute structure parameter: 0.443 (16)
219 parameters	
1 restraint	
H-atom parameters constrained	

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

Cg2 and Cg3 are the centroids of the C4–C8/C13 and C8–C13 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1A···N2^i	0.88	2.22	3.005 (3)	148
N1—H1B···N2^{ii}	0.88	2.32	3.129 (4)	152
C6—H6···Cg2^{iii}	0.95	2.60	3.401 (3)	142
C11—H11···Cg3^{iv}	0.95	2.90	3.636 (3)	135

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

Data collection: CrystalClearSM Expert (Rigaku, 2012); cell refinement: CrystalClearSM Expert; data reduction: CrystalClearSM Expert; program(s) used to solve structure: SUPERFLIP (Palatinus & Chapuis, 2007); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015); molecular graphics: ORTEP-3 for Windows

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supporting information

Crystal structure of 3-amino-1-(4-chlorophenyl)-1*H*-benzo[*f*]chromene-2-carbonitrile

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S1. Comment

The chromene moiety is found in natural products and exhibits various biological activities (Ellis, 1977; Singh *et al.*, 2010; Lácová *et al.*, 2010; Kidwai *et al.*, 2005). Fused chromene derivatives are biologically interesting compounds showing antiproliferation activity (Dell & Smith, 1993*a*,*b*), are effective anti-HIV agents (Al-Soud *et al.*, 2006) and impact the central nervous system (*CNS*) (Eiden & Denk, 1991). Moreover, they have been employed in the treatment of Alzheimer's disease (Bruhlmann *et al.*, 2001) and the Schizophrenia disorder (Kesten *et al.*, 1999). In this context, we report in this study the synthesis and crystal structure of the title compound.

In the title compound (Fig. 1), the choloro-benzene ring (C15–C20) is approximately perpendicular to the naphthalene ring system [C4–C13, maximum deviation = 0.012 (2) Å at atom C4] as indicated by the dihedral angle of 81.26 (5)°. The 4*H*-pyran ring (O1/C1–C5) in the title compound is puckered with the puckering parameters of Q_T = 0.143 (2) Å, θ = 86.4 (8)° and φ = 167.3 (9)°. All the bond lengths and angles in the title compound are within normal ranges and comparable with those reported for a similar structure (Akkurt *et al.*, 2013).

In the crystal structure, molecules are linked into sheets parallel to (010) by the N1—H1A···N2 and N1—H1B···N2 hydrogen bonds (Table 1, Figs 2 and 3), which generate chains along [010]. The crystal packing is further stabilized by C—H···π interactions (Table 1).

S2. Experimental

A mixture of 4-chlorobenzylidenepropanedinitrile (188.5 mg; 1 mmol) and 2-naphthol (144 mg; 1 mmol) was refluxed with stirring for 2 h at 350 K in ethanol (10 ml) in the presence of a catalytic amount of triethylamine. After cooling to room temperature, the solid product was collected by filtration, washed with cold ethanol and dried under vacuum. High quality crystals suitable for X-ray diffraction were obtained in an excellent yield (96%) by recrystallization of the crude product from ethanol. M.p. K.

S3. Refinement

All H atoms were placed geometrically and treated as riding on their parent atoms with N—H = 0.88 Å, C—H = 0.95 Å (aromatic CH), C—H = 1.00 Å (methine CH), and with U_{iso}(H) = 1.2U_{eq}(C,*N*). The crystal studied was an inversion twin with a 0.557 (16):0.443 (16) domain ratio.
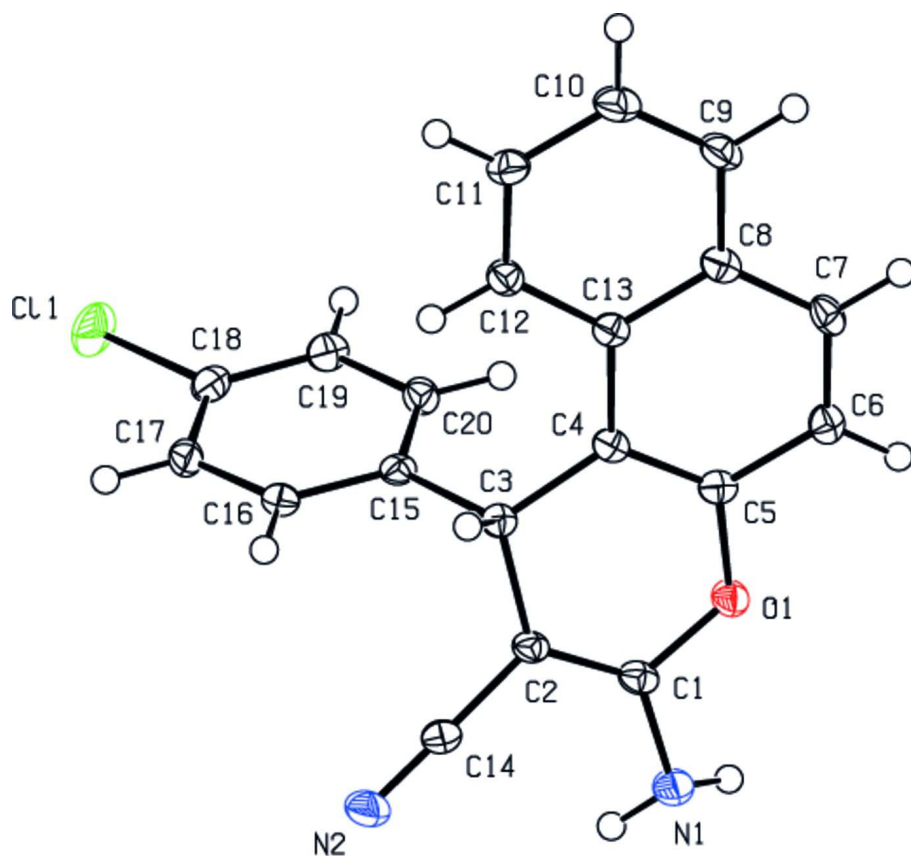
Figure 1

View of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-H atoms are drawn at the 50% probability level.
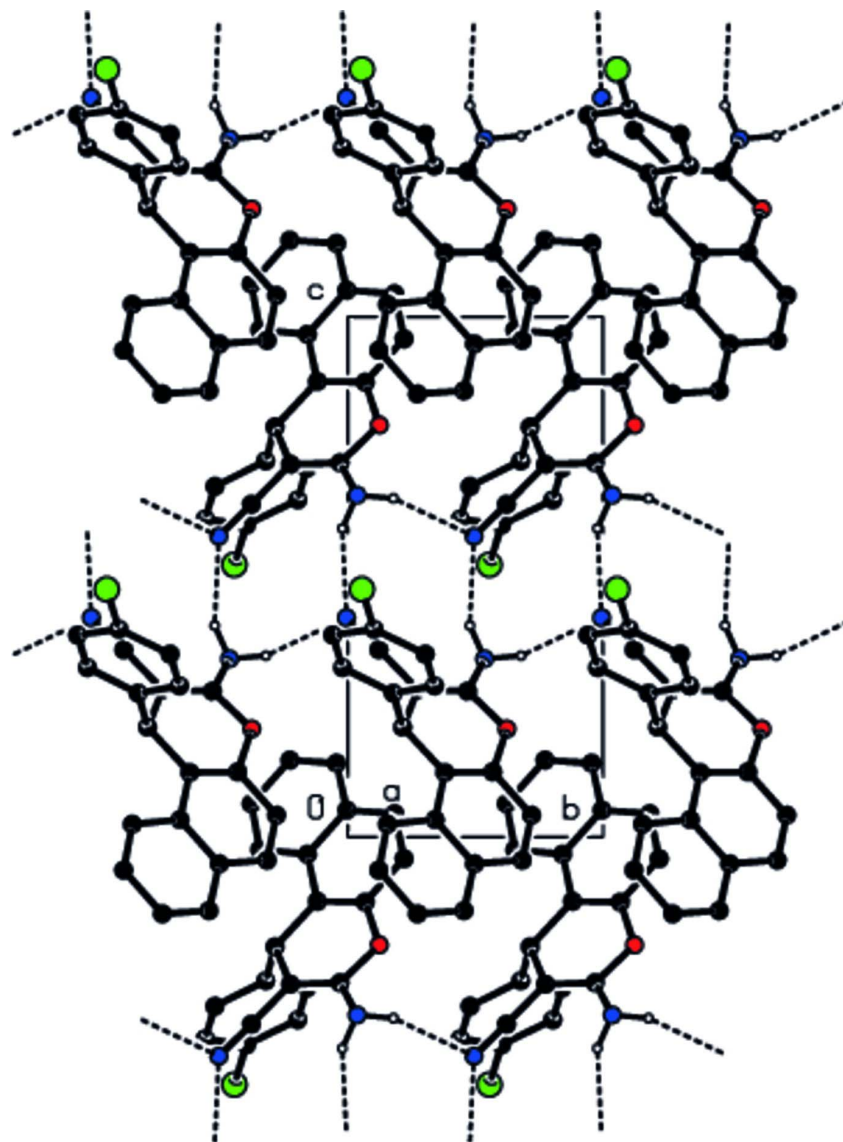
Figure 2

Crystal packing of the title compound viewed along the *a* axis, with hydrogen bonds drawn as dashed lines.
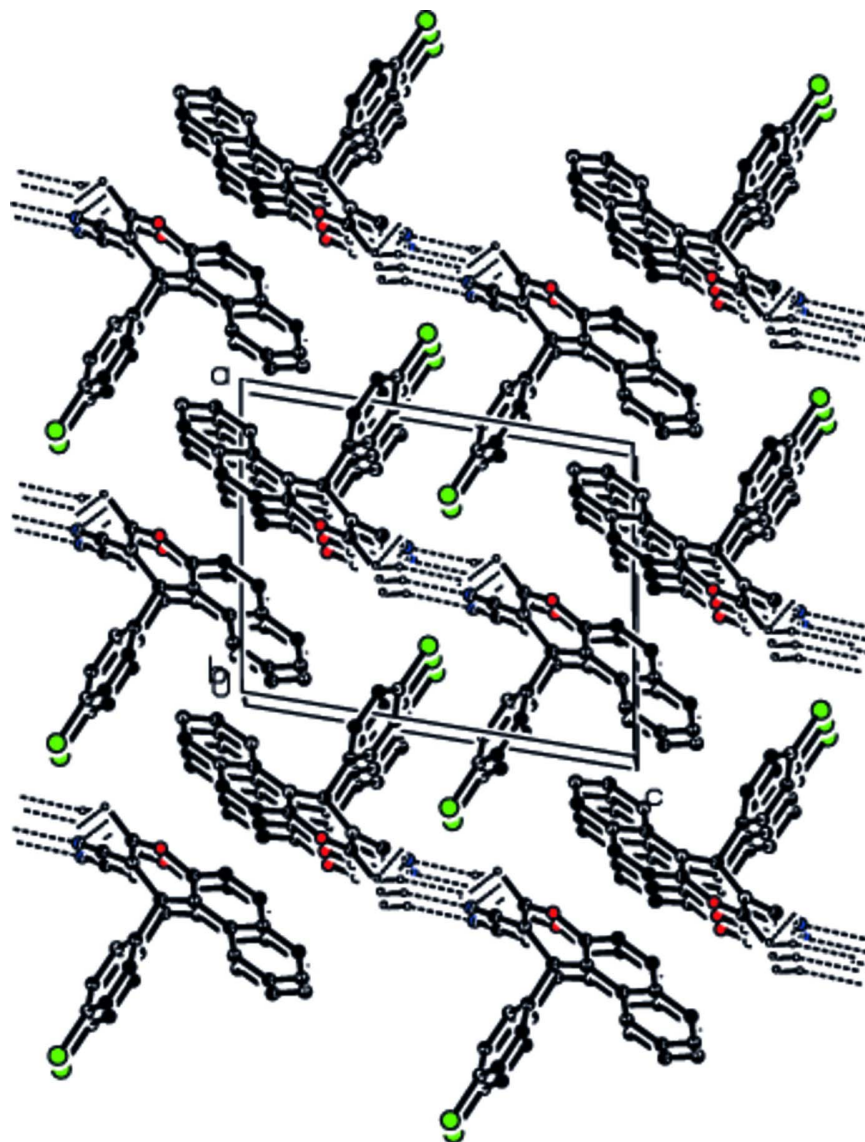
Figure 3

A view of the packing showing molecules stacked along the *b* axis.

3-Amino-1-(4-chlorophenyl)-1*H*-benzo[*f*]chromene-2-carbonitrile

Crystal data

$C_{20}H_{13}ClN_2O$	$F(000) = 344$
$M_r = 332.77$	$D_x = 1.416$ Mg m^{-3}
Monoclinic, $P2_1$	Cu $K\alpha$ radiation, $\lambda = 1.54178$ Å
Hall symbol: P 2yb	Cell parameters from 1130 reflections
$a = 10.056$ (7) Å	$\theta = 21.5–68.7°$
$b = 6.172$ (3) Å	$\mu = 2.23$ mm^{-1}
$c = 12.751$ (6) Å	$T = 100$ K
$\beta = 99.641$ (17)°	Block, light brown
$V = 780.2$ (8) Å^3	$0.32 \times 0.12 \times 0.10$ mm
$Z = 2$	

Data collection

Rigaku AFC11 diffractometer	11415 measured reflections
Radiation source: Rotating Anode	2558 independent reflections
Detector resolution: 22.2222 pixels mm⁻¹	2500 reflections with $I > 2\sigma(I)$
profile data from ω–scans	$R_{int} = 0.032$
Absorption correction: multi-scan	$\theta_{max} = 66.6°$, $\theta_{min} = 3.5°$
(*CrystalClearSM Expert*; Rigaku, 2012)	$h = -11 \rightarrow 11$
$T_{min} = 0.948$, $T_{max} = 1.000$	$k = -7 \rightarrow 7$
	$l = -15 \rightarrow 15$

Refinement

Refinement on F^2	H-atom parameters constrained
Least-squares matrix: full	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.1146P]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.075$	$(\Delta/\sigma)_{max} < 0.001$
$S = 1.06$	$\Delta\rho_{max} = 0.17$ e Å⁻³
2558 reflections	$\Delta\rho_{min} = -0.22$ e Å⁻³
219 parameters	Absolute structure: Refined as an inversion
1 restraint	twin.
Hydrogen site location: mixed	Absolute structure parameter: 0.443 (16)

Special details

Geometry. Bond distances, angles *etc*. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement on F^2 for ALL reflections except those flagged by the user for potential systematic errors. Weighted *R*-factors *wR* and all 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 observed criterion of $F^2 > \sigma(F^2)$ is used only for calculating -*R*-factor-obs *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	−0.24323 (5)	0.55572 (12)	0.52362 (5)	0.0334 (2)
O1	0.45126 (15)	1.1239 (3)	0.79232 (11)	0.0189 (5)
N1	0.55640 (19)	1.0368 (4)	0.65748 (14)	0.0214 (6)
N2	0.4506 (2)	0.4950 (3)	0.57819 (16)	0.0257 (6)
C1	0.4675 (2)	0.9698 (4)	0.71956 (16)	0.0166 (6)
C2	0.4046 (2)	0.7754 (4)	0.71666 (16)	0.0156 (6)
C3	0.3043 (2)	0.7152 (4)	0.78878 (16)	0.0149 (6)
C4	0.3101 (2)	0.8809 (4)	0.87613 (16)	0.0144 (6)
C5	0.38290 (19)	1.0685 (4)	0.87480 (15)	0.0156 (6)
C6	0.3992 (2)	1.2209 (4)	0.95817 (16)	0.0174 (6)
C7	0.3399 (2)	1.1839 (4)	1.04481 (17)	0.0180 (6)
C8	0.2613 (2)	0.9965 (4)	1.05160 (17)	0.0175 (6)
C9	0.1991 (2)	0.9560 (4)	1.14178 (17)	0.0212 (7)
C10	0.1240 (2)	0.7733 (5)	1.14784 (18)	0.0240 (7)
C11	0.1072 (2)	0.6218 (4)	1.06388 (17)	0.0214 (7)
C12	0.1664 (2)	0.6555 (4)	0.97558 (17)	0.0175 (6)
C13	0.24556 (19)	0.8423 (4)	0.96678 (16)	0.0149 (6)

C14	0.4305 (2)	0.6224 (4)	0.63990 (16)	0.0179 (6)
C15	0.1641 (2)	0.6784 (4)	0.72333 (16)	0.0150 (6)
C16	0.1348 (2)	0.4796 (4)	0.67440 (16)	0.0174 (6)
C17	0.0094 (2)	0.4409 (4)	0.61165 (17)	0.0202 (7)
C18	−0.0858 (2)	0.6031 (4)	0.60027 (16)	0.0204 (7)
C19	−0.0595 (2)	0.8037 (4)	0.64830 (17)	0.0201 (7)
C20	0.0667 (2)	0.8403 (4)	0.70949 (16)	0.0176 (6)
H1A	0.53650	0.97850	0.59340	0.0260*
H1B	0.55280	1.17950	0.65130	0.0260*
H3	0.33450	0.57400	0.82330	0.0180*
H6	0.45110	1.34820	0.95390	0.0210*
H7	0.35150	1.28550	1.10150	0.0220*
H9	0.20980	1.05740	1.19860	0.0250*
H10	0.08300	0.74830	1.20870	0.0290*
H11	0.05460	0.49540	1.06840	0.0260*
H12	0.15400	0.55200	0.91960	0.0210*
H16	0.20090	0.36820	0.68370	0.0210*
H17	−0.00980	0.30510	0.57740	0.0240*
H19	−0.12630	0.91410	0.63960	0.0240*
H20	0.08640	0.97750	0.74210	0.0210*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0198 (3)	0.0457 (4)	0.0312 (3)	−0.0081 (3)	−0.0061 (2)	−0.0053 (3)
O1	0.0234 (8)	0.0193 (9)	0.0146 (7)	−0.0026 (6)	0.0054 (6)	−0.0006 (6)
N1	0.0250 (9)	0.0222 (11)	0.0189 (9)	−0.0033 (9)	0.0088 (7)	0.0002 (8)
N2	0.0313 (11)	0.0258 (12)	0.0233 (10)	−0.0026 (9)	0.0146 (8)	−0.0028 (9)
C1	0.0160 (10)	0.0226 (12)	0.0110 (9)	0.0030 (9)	0.0016 (8)	0.0005 (8)
C2	0.0135 (10)	0.0219 (12)	0.0113 (9)	0.0010 (9)	0.0019 (7)	−0.0013 (8)
C3	0.0146 (11)	0.0167 (12)	0.0132 (9)	0.0009 (8)	0.0020 (8)	0.0009 (8)
C4	0.0122 (9)	0.0183 (11)	0.0117 (10)	0.0041 (9)	−0.0009 (7)	0.0001 (8)
C5	0.0139 (9)	0.0206 (12)	0.0118 (9)	0.0024 (9)	0.0010 (7)	0.0023 (9)
C6	0.0152 (11)	0.0182 (12)	0.0172 (10)	0.0019 (8)	−0.0021 (8)	−0.0006 (9)
C7	0.0190 (11)	0.0195 (12)	0.0137 (9)	0.0032 (9)	−0.0021 (8)	−0.0044 (9)
C8	0.0158 (10)	0.0228 (13)	0.0131 (9)	0.0045 (9)	0.0000 (8)	−0.0005 (8)
C9	0.0228 (12)	0.0261 (13)	0.0152 (10)	0.0025 (10)	0.0044 (9)	−0.0047 (10)
C10	0.0257 (13)	0.0302 (14)	0.0181 (11)	0.0012 (11)	0.0091 (9)	−0.0003 (10)
C11	0.0201 (11)	0.0249 (13)	0.0207 (11)	−0.0013 (9)	0.0078 (9)	0.0004 (9)
C12	0.0169 (10)	0.0192 (12)	0.0163 (10)	0.0012 (9)	0.0021 (8)	−0.0017 (9)
C13	0.0125 (10)	0.0176 (12)	0.0138 (10)	0.0035 (8)	0.0003 (8)	0.0006 (8)
C14	0.0176 (10)	0.0200 (13)	0.0170 (10)	−0.0005 (8)	0.0058 (8)	0.0019 (9)
C15	0.0151 (10)	0.0213 (12)	0.0089 (9)	−0.0017 (9)	0.0032 (7)	0.0011 (8)
C16	0.0180 (11)	0.0197 (12)	0.0155 (10)	−0.0005 (9)	0.0056 (8)	−0.0008 (9)
C17	0.0242 (12)	0.0228 (13)	0.0145 (10)	−0.0083 (10)	0.0060 (8)	−0.0034 (9)
C18	0.0165 (10)	0.0325 (15)	0.0119 (9)	−0.0063 (9)	0.0018 (8)	−0.0008 (9)
C19	0.0179 (11)	0.0248 (13)	0.0175 (11)	0.0003 (10)	0.0023 (8)	0.0016 (9)
C20	0.0189 (11)	0.0187 (12)	0.0149 (10)	−0.0007 (9)	0.0022 (8)	−0.0011 (9)

Geometric parameters (Å, º)

Cl1—C18	1.740 (2)	C10—C11	1.410 (4)
O1—C1	1.358 (3)	C11—C12	1.375 (3)
O1—C5	1.392 (3)	C12—C13	1.416 (3)
N1—C1	1.354 (3)	C15—C20	1.390 (3)
N2—C14	1.154 (3)	C15—C16	1.386 (3)
C1—C2	1.354 (3)	C16—C17	1.396 (3)
N1—H1B	0.8800	C17—C18	1.376 (3)
N1—H1A	0.8800	C18—C19	1.387 (4)
C2—C14	1.415 (3)	C19—C20	1.392 (3)
C2—C3	1.520 (3)	C3—H3	1.0000
C3—C4	1.506 (3)	C6—H6	0.9500
C3—C15	1.530 (3)	C7—H7	0.9500
C4—C13	1.437 (3)	C9—H9	0.9500
C4—C5	1.372 (3)	C10—H10	0.9500
C5—C6	1.408 (3)	C11—H11	0.9500
C6—C7	1.360 (3)	C12—H12	0.9500
C7—C8	1.412 (3)	C16—H16	0.9500
C8—C13	1.429 (3)	C17—H17	0.9500
C8—C9	1.420 (3)	C19—H19	0.9500
C9—C10	1.367 (4)	C20—H20	0.9500
C1—O1—C5	118.39 (19)	C3—C15—C20	121.9 (2)
O1—C1—N1	110.6 (2)	C16—C15—C20	119.17 (19)
O1—C1—C2	122.03 (19)	C15—C16—C17	120.9 (2)
N1—C1—C2	127.3 (2)	C16—C17—C18	118.8 (2)
H1A—N1—H1B	109.00	Cl1—C18—C19	119.09 (17)
C1—N1—H1A	110.00	Cl1—C18—C17	119.23 (18)
C1—N1—H1B	110.00	C17—C18—C19	121.7 (2)
C1—C2—C3	123.7 (2)	C18—C19—C20	118.7 (2)
C1—C2—C14	118.10 (19)	C15—C20—C19	120.8 (2)
C3—C2—C14	118.2 (2)	C2—C3—H3	107.00
C2—C3—C4	109.51 (19)	C4—C3—H3	107.00
C4—C3—C15	114.97 (18)	C15—C3—H3	107.00
C2—C3—C15	110.51 (17)	C5—C6—H6	120.00
C5—C4—C13	117.6 (2)	C7—C6—H6	120.00
C3—C4—C5	121.25 (18)	C6—C7—H7	120.00
C3—C4—C13	121.0 (2)	C8—C7—H7	120.00
O1—C5—C4	123.29 (19)	C8—C9—H9	120.00
O1—C5—C6	113.4 (2)	C10—C9—H9	120.00
C4—C5—C6	123.33 (19)	C9—C10—H10	120.00
C5—C6—C7	119.3 (2)	C11—C10—H10	120.00
C6—C7—C8	120.9 (2)	C10—C11—H11	120.00
C9—C8—C13	119.2 (2)	C12—C11—H11	120.00
C7—C8—C9	121.4 (2)	C11—C12—H12	120.00
C7—C8—C13	119.43 (19)	C13—C12—H12	120.00
C8—C9—C10	120.9 (2)	C15—C16—H16	120.00

C9—C10—C11	120.1 (2)	C17—C16—H16	120.00
C10—C11—C12	120.6 (2)	C16—C17—H17	121.00
C11—C12—C13	121.0 (2)	C18—C17—H17	121.00
C8—C13—C12	118.33 (19)	C18—C19—H19	121.00
C4—C13—C12	122.3 (2)	C20—C19—H19	121.00
C4—C13—C8	119.4 (2)	C15—C20—H20	120.00
N2—C14—C2	178.9 (2)	C19—C20—H20	120.00
C3—C15—C16	119.0 (2)		

C5—O1—C1—N1	−168.57 (17)	C13—C4—C5—O1	179.31 (19)
C5—O1—C1—C2	8.9 (3)	O1—C5—C6—C7	−178.62 (19)
C1—O1—C5—C6	165.88 (18)	C4—C5—C6—C7	−0.4 (3)
C1—O1—C5—C4	−12.3 (3)	C5—C6—C7—C8	−0.7 (3)
O1—C1—C2—C14	−178.26 (19)	C6—C7—C8—C9	179.9 (2)
O1—C1—C2—C3	3.8 (3)	C6—C7—C8—C13	0.9 (3)
N1—C1—C2—C14	−1.2 (3)	C7—C8—C9—C10	−179.5 (2)
N1—C1—C2—C3	−179.1 (2)	C13—C8—C9—C10	−0.5 (3)
C1—C2—C3—C15	115.5 (2)	C7—C8—C13—C4	0.0 (3)
C1—C2—C3—C4	−12.1 (3)	C7—C8—C13—C12	179.9 (2)
C14—C2—C3—C4	169.96 (19)	C9—C8—C13—C4	−179.0 (2)
C14—C2—C3—C15	−62.4 (3)	C9—C8—C13—C12	0.9 (3)
C2—C3—C4—C5	8.7 (3)	C8—C9—C10—C11	−0.1 (3)
C15—C3—C4—C13	67.1 (3)	C9—C10—C11—C12	0.3 (3)
C2—C3—C15—C16	82.1 (3)	C10—C11—C12—C13	0.1 (3)
C2—C3—C15—C20	−96.3 (2)	C11—C12—C13—C4	179.2 (2)
C4—C3—C15—C16	−153.4 (2)	C11—C12—C13—C8	−0.7 (3)
C4—C3—C15—C20	28.3 (3)	C3—C15—C16—C17	−178.31 (19)
C2—C3—C4—C13	−167.82 (19)	C20—C15—C16—C17	0.1 (3)
C15—C3—C4—C5	−116.4 (2)	C3—C15—C20—C19	179.08 (19)
C3—C4—C5—O1	2.7 (3)	C16—C15—C20—C19	0.7 (3)
C13—C4—C5—C6	1.3 (3)	C15—C16—C17—C18	−0.9 (3)
C3—C4—C13—C8	175.60 (19)	C16—C17—C18—Cl1	−179.20 (16)
C3—C4—C13—C12	−4.3 (3)	C16—C17—C18—C19	0.8 (3)
C5—C4—C13—C8	−1.1 (3)	Cl1—C18—C19—C20	−180.00 (17)
C5—C4—C13—C12	179.1 (2)	C17—C18—C19—C20	−0.1 (3)
C3—C4—C5—C6	−175.4 (2)	C18—C19—C20—C15	−0.7 (3)

Hydrogen-bond geometry (Å, º)

Cg2 and Cg3 are the centroids of the C4–C8/C13 and C8–C13 rings, respectively.

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1*A*···N2[i]	0.88	2.22	3.005 (3)	148
N1—H1*B*···N2[ii]	0.88	2.32	3.129 (4)	152
C6—H6···*Cg*2[iii]	0.95	2.60	3.401 (3)	142
C11—H11···*Cg*3[iv]	0.95	2.90	3.636 (3)	135

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