



Crystal structure and Hirshfeld-surface analysis of a monoclinic polymorph of 2-amino-5-chlorobenzophenone oxime at 90 K

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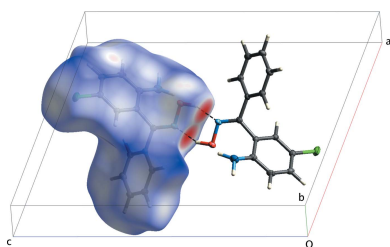
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The synthesis and crystal structure of a monoclinic polymorph of 2-amino-5-chlorobenzophenone oxime, C₁₃H₁₁ClN₂O, are presented. The molecular conformation results from twisting of the phenyl and 2-amino-5-chloro benzene rings attached to the oxime group, which subtend a dihedral angle of 80.53 (4)°. In the crystal, centrosymmetric dimers are formed as a result of pairs of strong O—H···N hydrogen bonds. A comparison is made to a previously known triclinic polymorph, including differences in atom–atom contacts obtained *via* a Hirshfeld-surface analysis.

1. Chemical context

2-Amino-5-chlorobenzophenone is an ecologically friendly cross-linking agent. Benzophenone and related compounds have been reported to act as anti-allergic, anti-inflammatory, anti-asthmatic, and anti-anaphylactic agents (Evans *et al.*, 1987; Wiesner *et al.*, 2002; Sieron *et al.*, 2004). Benzophenone derivatives are widely used in sunscreen lotions, offering UV-A and UV-B protection (Deleu *et al.*, 1992). 2-Amino-5-chlorobenzophenone is used to produce intermediates for the synthesis of oxazolam drugs and intermediates for psychotherapeutic agents, such as chlorodiazepoxide and diazepam (Sternbach & Reeder, 1961*a,b*). 2-Aminobenzophenone and its derivatives have importance because of their applications in heterocyclic synthesis and medicines (Walsh, 1980) and are also used as anti-mitotic agents (Liou *et al.*, 2002). The growth and characterization of 2-amino-5-chlorobenzophenone single crystals was reported by Mohamed *et al.* (2007). Synthesis, herbicidal evaluation and structure–activity relationships of some benzophenone oxime ether derivatives was reported by Ma *et al.* (2015). The synthesis, physicochemical, and biological evaluation of 2-amino-5-chlorobenzophenone derivatives as potent skeletal muscle relaxants was reported by Singh *et al.* (2015). Details of synthetic methodologies and the pharmacological significance of 2-aminobenzophenones as versatile building blocks was published by Chaudhary *et al.* (2018). The reactivity of oximes for diverse methodologies and synthetic applications was recently reported by Rykaczewski *et al.* (2022). In view of the general importance of benzophenone derivatives and those of 2-amino-5-chlorobenzophenone in particular, this paper reports the 90 K crystal



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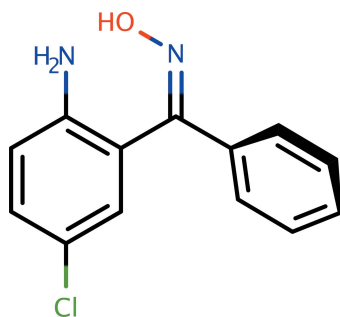
Table 1

Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N1-H1NA\cdots O1$	0.91 (2)	2.23 (2)	2.8875 (19)	128.7 (16)
$O1-H1O\cdots N2^i$	0.95 (2)	1.84 (2)	2.7411 (16)	156.4 (19)

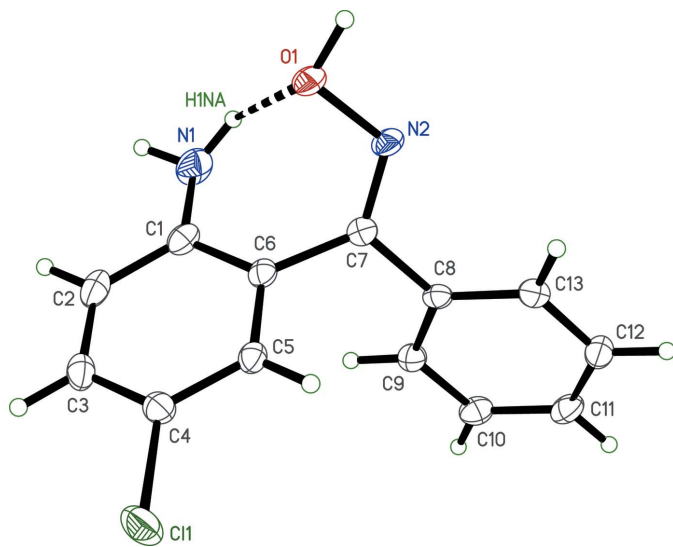
 Symmetry code: (i) $-x + 1, -y + 1, -z + 1$.

structure and Hirshfeld-surface studies of a monoclinic form of 2-amino-5-chlorobenzophenone oxime, $C_{13}H_{11}ClN_2O$, *mon-2A-5CBO*. A triclinic polymorph was recently published as a CSD communication (refcode REZSIB) by Lanzilotto, Housecroft *et al.* (2018). Some comparisons between the two crystal structures are presented.



2. Structural commentary

The overall conformation of the *mon-2A-5CBO* molecule (Fig. 1) is determined by torsion angles about the C6–C7 and C7–C8 bonds that connect the chloroaniline and phenyl rings to the oxime carbon, C7. These are held in check by an intramolecular hydrogen bond, N1–H1NA \cdots O1 [$d_{D\cdots A}$ = 2.8875 (19) Å, Table 1]. These torsion angles result in a dihedral angle between the two rings of 80.53 (4)°. The


Figure 1

An ellipsoid plot (50% probability) of *mon-2A-5CBO*. The intramolecular N–H \cdots O hydrogen bond is shown as a dashed line.

Table 2

 Comparison of conformation-defining torsion and dihedral angles (°) in *mon-2A-5CBO* and CSD entry REZSIB.

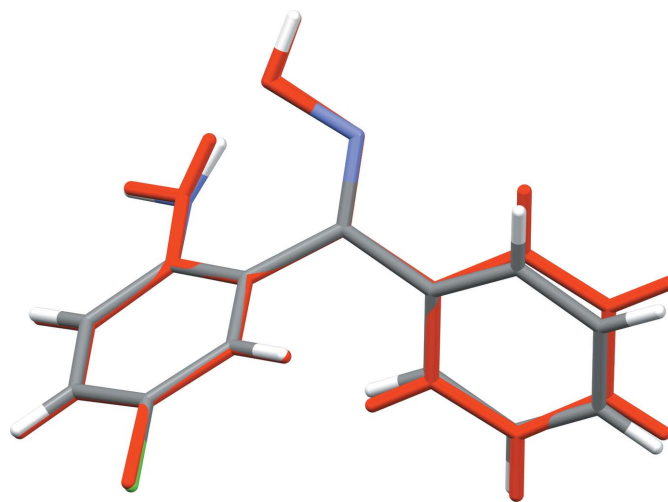
	<i>mon-2A-5CBO</i>	REZSIB ^{ab}
Torsion angle		
$N1-C1-C6-C7$	−1.3 (2)	−5.6
$C1-C6-C7-N2$	60.8 (2)	56.7
$C6-C7-N2-O1$	0.5 (2)	7.8
Dihedral angle		
$C1-C6/C8-C13$	80.53 (4)	75.82

Notes: (a) The numbering scheme in REZSIB is different from *mon-2A-5CBO*; (b) Values from *Mercury* (Macrae *et al.*, 2020), therefore there are no SUs.

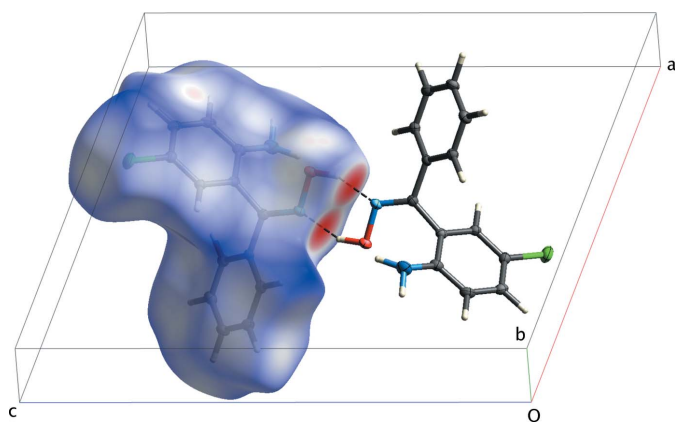
conformation defining torsion and dihedral angles are gathered in Table 2 along with those of the triclinic polymorph, REZSIB (Lanzilotto, Housecroft *et al.*, 2018). The conformations of the 2A-5CBO molecules in the two polymorphs are quite similar, as shown by the overlay plot in Fig. 2. The r.m.s. deviation obtained from a weighted least-squares fit of all non-hydrogen atoms using OFIT in *SHELXTL-XP* (Sheldrick, 2008) is only 0.1315 Å, with the largest deviation being 0.267 Å for C12.

3. Supramolecular features

The main supramolecular constructs in the *mon-2A-5CBO* crystal structure are $R_2^2(6)$ centrosymmetric dimers that result from pairs ($O1-H1O\cdots N2^{inv}$ and $O1^{inv}-H1O^{inv}\cdots N2$, $inv = 1 - x, 1 - y, 1 - z$) of strong hydrogen bonds [$d_{D\cdots A}$ = 2.7411 (16) Å, Table 1]. These are shown as dashed lines in Fig. 3 along with a representation of the Hirshfeld surface, as generated by *CrystalExplorer* (Spackman *et al.*, 2021), on which the hydrogen bonds are responsible for the prominent red spots. Similar dimer motifs are present in REZSIB. The most striking difference in packing between the two polymorphs is that REZSIB exhibits slip-stacked π – π overlap


Figure 2

A least-squares fit overlay of *mon-2A-5CBO* and the triclinic polymorph REZSIB (red).

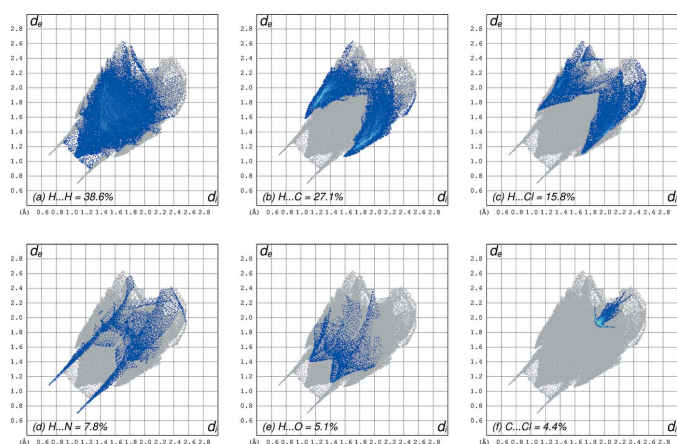

Figure 3

A partial packing plot of *mon-2A-5CBO* viewed approximately down the *b*-axis showing the Hirshfeld surface (left) and the $R_2^2(6)$ centrosymmetric dimer formed by pairs of $O-H \cdots N$ hydrogen bonds (dashed lines and prominent red spots).

[interplanar separation = 3.340 (2) Å, centroid-centroid distance = 3.897 (2) Å] of inversion-related ($1-x, -y, 1-z$) chloroaniline rings, whereas *mon-2A-5CBO* does not. Hirshfeld surface 2D-fingerprint plots for *mon-2A-5CBO* are shown in Fig. 4 and the differences in contacts between the polymorphs are summarized in Table 3.

4. Database survey

A survey of the Cambridge Structural Database (CSD: v5.43 including all updates through November 2022; Groom *et al.*, 2016) returned 5507 hits for a search fragment consisting of unsubstituted benzophenone. A search using benzophenone oxime as the probe, however, returned only 35 entries. Of these, ten have a nitrogen-bound functional group at the *ortho*-position of one of the benzene rings, while six have ‘any halogen’ attached at one of the *meta*-positions. In only two structures is this halogen a chlorine atom: YIFCIC (Lanzi-


Figure 4

Hirshfeld surface two-dimensional fingerprint plots of *mon-2A-5CBO* showing (a) $H \cdots H$, (b) $H \cdots C$, (c) $H \cdots Cl$, (d) $H \cdots N$, (e) $H \cdots O$, and (f) $C \cdots Cl$ close contacts.

Table 3

Atom-atom contact coverages (%) for polymorphs *mon-2A-5CBO* and REZSIB.

Atom contacts ^a	<i>mon-2A-5CBO</i>	REZSIB
$H \cdots H$	38.6	43.6
$H \cdots C$	27.1	17.6
$H \cdots Cl$	15.8	13.6
$H \cdots N$	7.8	8.8
$H \cdots O$	5.1	6.4
$C \cdots Cl$	4.4	6.0
$C \cdots C$	0.0	3.9

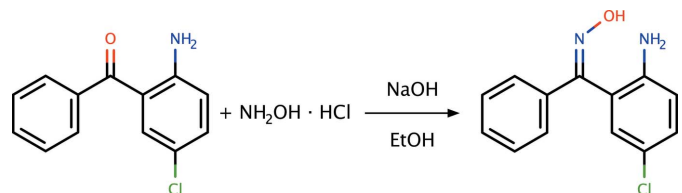
Note: (a) Includes reciprocal contacts. All other contact percentages are negligible.

lotto, Prescimone *et al.*, 2018), $C_{15}H_{11}Cl_2FN_2O_2$, systematic name 2-chloro-*N*-[4-chloro-2-[(2-fluorophenyl)(hydroxyimino)methyl]phenyl]acetamide and REZSIB (Lanzilotto, Housecroft *et al.*, 2018), the triclinic ($P\bar{1}$) polymorph of the monoclinic ($P2_1/n$) 2A-5CBO crystal structure described herein.

Some other related crystal structures include 2-amino-5-chlorobenzophenone as monoclinic (NUVFAL; Vasco-Mendez *et al.*, 1996) and triclinic (NUVFAL02; Javed *et al.*, 2018) polymorphs, benzophenone oxime (XULKUK; Sharutin *et al.*, 2002), and 2-benzoyloxy-5-methylbenzophenone (OCAMOV; Sieron *et al.*, 2004).

5. Synthesis and crystallization

The synthesis of 2A-5CBO (Fig. 5) was by a modification of Beckmann's conversion of benzophenone to benzophenone oxime (Beckmann, 1886). In a 100 ml round-bottom flask fitted with a magnetic stirrer was placed a mixture of 100 mmol (23.2 g) of 2-amino-5-chlorobenzophenone, 120 mmol (7 g) of hydroxylamine hydrochloride in 10 ml of ethanol. To this stirred mixture, 0.5 g of sodium hydroxide pellets was added in small portions. When the reaction became vigorous, the flask was placed in an ice bath. A condenser was attached to the flask and the mixture was refluxed for 5 minutes on a steam bath. The solution was cooled and poured into a beaker containing 5 ml of hydrochloric acid and crushed ice. This was stirred until a precipitate formed. After filtering the precipitate with suction and washing with cold distilled water, the product was spread out on filter paper and air dried. The yield was 87%. X-ray quality crystals were obtained from methanol by slow evaporation (m.p.: 390–393 K).


Figure 5

A general reaction scheme for the formation of 2A-5CBO.

Table 4

Experimental details.

Crystal data	
Chemical formula	C ₁₃ H ₁₁ ClN ₂ O
<i>M_r</i>	246.69
Crystal system, space group	Monoclinic, <i>P</i> 2 ₁ / <i>n</i>
Temperature (K)	90
<i>a</i> , <i>b</i> , <i>c</i> (Å)	12.8264 (3), 5.5423 (1), 17.4082 (4)
β (°)	109.522 (1)
<i>V</i> (Å ³)	1166.37 (4)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.31
Crystal size (mm)	0.30 × 0.24 × 0.02
Data collection	
Diffractometer	Bruker D8 Venture dual source
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T_{min}</i> , <i>T_{max}</i>	0.924, 0.971
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	26003, 2680, 2294
<i>R_{int}</i>	0.042
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.650
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.033, 0.083, 1.05
No. of reflections	2680
No. of parameters	166
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{\max}$, $\Delta\rho_{\min}$ (e Å ⁻³)	0.32, -0.27

Computer programs: *APEX3* (Bruker, 2016), *SHELXT* (Sheldrick, 2015a), *SHELXL2019/2* (Sheldrick, 2015b), *XP* in *SHELXTL* (Sheldrick, 2008), *SHELX* (Sheldrick, 2008) and *pubCIF* (Westrip, 2010).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 4. All hydrogen atoms were found in difference-Fourier maps. Those bound to carbon were subsequently included in the refinement using a riding model, with constrained distances fixed at 0.95 Å and *U*_{iso}(H) values set to 1.2*U*_{eq} of the attached atom. The amine and oxime hydrogen atoms were refined freely.

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supporting information

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *APEX3* (Bruker, 2016); data reduction: *APEX3* (Bruker, 2016); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2019/2* (Sheldrick, 2015b); molecular graphics: *XP* in *SHELXTL* (Sheldrick, 2008); software used to prepare material for publication: *SHELX* (Sheldrick, 2008) and *publCIF* (Westrip, 2010)'.

4-Chloro-2-[(hydroxyimino)(phenyl)methyl]aniline

Crystal data

$C_{13}H_{11}ClN_2O$

$M_r = 246.69$

Monoclinic, $P2_1/n$

$a = 12.8264$ (3) Å

$b = 5.5423$ (1) Å

$c = 17.4082$ (4) Å

$\beta = 109.522$ (1)°

$V = 1166.37$ (4) Å³

$Z = 4$

$F(000) = 512$

$D_x = 1.405$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 9975 reflections

$\theta = 2.5$ – 27.5 °

$\mu = 0.31$ mm⁻¹

$T = 90$ K

Semi-regular block, pale yellow

$0.30 \times 0.24 \times 0.02$ mm

Data collection

Bruker D8 Venture dual source
diffractometer

Radiation source: microsource

Detector resolution: 7.41 pixels mm⁻¹

φ and ω scans

Absorption correction: multi-scan
(*SADABS*; Krause *et al.*, 2015)

$T_{\min} = 0.924$, $T_{\max} = 0.971$

26003 measured reflections

2680 independent reflections

2294 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.042$

$\theta_{\max} = 27.5$ °, $\theta_{\min} = 2.4$ °

$h = -16 \rightarrow 16$

$k = -7 \rightarrow 7$

$l = -22 \rightarrow 22$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.033$

$wR(F^2) = 0.083$

$S = 1.05$

2680 reflections

166 parameters

0 restraints

Primary atom site location: structure-invariant
direct methods

Secondary atom site location: difference Fourier
map

Hydrogen site location: mixed

H atoms treated by a mixture of independent
and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0334P)^2 + 0.6832P]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$

$$\Delta\rho_{\max} = 0.32 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.27 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. The crystal was mounted using polyisobutene oil on the tip of a fine glass fibre, which was fastened in a copper mounting pin with electrical solder. It was placed directly into the cold gas stream of a liquid-nitrogen based cryostat (Hope, 1994; Parkin & Hope, 1998).

Diffraction data were collected with the crystal at 90K, which is standard practice in this laboratory for the majority of flash-cooled crystals.

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
Cl1	0.63274 (3)	0.54249 (7)	0.94134 (2)	0.03072 (12)
O1	0.58250 (8)	0.6496 (2)	0.57328 (6)	0.0249 (2)
H1O	0.5830 (17)	0.572 (4)	0.5245 (14)	0.055 (6)*
N1	0.58120 (12)	1.1196 (3)	0.64451 (9)	0.0292 (3)
H1NA	0.5690 (15)	1.042 (4)	0.5962 (12)	0.037 (5)*
H1NB	0.6301 (17)	1.238 (4)	0.6523 (12)	0.045 (6)*
N2	0.47023 (9)	0.6201 (2)	0.56650 (7)	0.0198 (3)
C1	0.59550 (11)	0.9785 (3)	0.71326 (9)	0.0203 (3)
C2	0.66473 (11)	1.0555 (3)	0.79012 (9)	0.0235 (3)
H2	0.705557	1.200830	0.794290	0.028*
C3	0.67496 (11)	0.9256 (3)	0.85971 (9)	0.0223 (3)
H3	0.720922	0.983038	0.911337	0.027*
C4	0.61783 (11)	0.7109 (3)	0.85389 (8)	0.0197 (3)
C5	0.54751 (10)	0.6311 (3)	0.77926 (8)	0.0172 (3)
H5	0.507391	0.485190	0.776017	0.021*
C6	0.53533 (10)	0.7638 (3)	0.70891 (8)	0.0165 (3)
C7	0.45154 (10)	0.6753 (2)	0.63216 (8)	0.0165 (3)
C8	0.33591 (10)	0.6438 (2)	0.63101 (7)	0.0156 (3)
C9	0.29101 (11)	0.8182 (3)	0.66846 (8)	0.0189 (3)
H9	0.335250	0.950014	0.695888	0.023*
C10	0.18202 (11)	0.8003 (3)	0.66587 (9)	0.0226 (3)
H10	0.151395	0.920969	0.690712	0.027*
C11	0.11782 (11)	0.6062 (3)	0.62701 (9)	0.0229 (3)
H11	0.043042	0.594435	0.624967	0.028*
C12	0.16249 (12)	0.4292 (3)	0.59117 (9)	0.0226 (3)
H12	0.118668	0.294962	0.565375	0.027*
C13	0.27141 (11)	0.4477 (3)	0.59285 (8)	0.0189 (3)
H13	0.301768	0.326585	0.567964	0.023*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0381 (2)	0.0335 (2)	0.01636 (17)	-0.00308 (17)	0.00354 (14)	0.00155 (15)
O1	0.0139 (5)	0.0399 (7)	0.0236 (5)	-0.0007 (4)	0.0097 (4)	-0.0040 (5)
N1	0.0323 (7)	0.0244 (7)	0.0325 (7)	-0.0064 (6)	0.0128 (6)	0.0057 (6)
N2	0.0127 (5)	0.0282 (7)	0.0205 (6)	0.0008 (5)	0.0081 (4)	0.0002 (5)
C1	0.0172 (6)	0.0191 (7)	0.0269 (7)	0.0009 (5)	0.0105 (5)	0.0007 (6)
C2	0.0178 (6)	0.0199 (7)	0.0342 (8)	-0.0042 (6)	0.0107 (6)	-0.0058 (6)
C3	0.0149 (6)	0.0262 (8)	0.0247 (7)	-0.0012 (5)	0.0051 (5)	-0.0081 (6)
C4	0.0177 (6)	0.0235 (7)	0.0176 (6)	0.0017 (5)	0.0057 (5)	-0.0005 (5)
C5	0.0142 (6)	0.0178 (7)	0.0200 (6)	-0.0010 (5)	0.0063 (5)	-0.0023 (5)
C6	0.0132 (6)	0.0182 (7)	0.0192 (6)	0.0009 (5)	0.0069 (5)	-0.0019 (5)
C7	0.0158 (6)	0.0167 (7)	0.0172 (6)	0.0018 (5)	0.0060 (5)	0.0020 (5)
C8	0.0153 (6)	0.0188 (7)	0.0135 (6)	0.0016 (5)	0.0057 (5)	0.0029 (5)
C9	0.0194 (6)	0.0191 (7)	0.0191 (6)	-0.0007 (5)	0.0077 (5)	-0.0010 (5)
C10	0.0209 (7)	0.0246 (8)	0.0260 (7)	0.0029 (6)	0.0128 (6)	-0.0001 (6)
C11	0.0158 (6)	0.0295 (8)	0.0248 (7)	-0.0003 (6)	0.0086 (5)	0.0053 (6)
C12	0.0211 (7)	0.0240 (8)	0.0216 (7)	-0.0059 (6)	0.0055 (5)	0.0002 (6)
C13	0.0207 (6)	0.0197 (7)	0.0171 (6)	0.0003 (5)	0.0073 (5)	0.0001 (5)

Geometric parameters (\AA , $^\circ$)

Cl1—C4	1.7409 (14)	C5—H5	0.9500
O1—N2	1.4145 (14)	C6—C7	1.4903 (18)
O1—H1O	0.95 (2)	C7—C8	1.4869 (17)
N1—C1	1.3894 (19)	C8—C13	1.3927 (19)
N1—H1NA	0.91 (2)	C8—C9	1.3937 (19)
N1—H1NB	0.89 (2)	C9—C10	1.3871 (18)
N2—C7	1.2809 (17)	C9—H9	0.9500
C1—C2	1.402 (2)	C10—C11	1.386 (2)
C1—C6	1.4065 (19)	C10—H10	0.9500
C2—C3	1.377 (2)	C11—C12	1.385 (2)
C2—H2	0.9500	C11—H11	0.9500
C3—C4	1.383 (2)	C12—C13	1.3913 (19)
C3—H3	0.9500	C12—H12	0.9500
C4—C5	1.3834 (18)	C13—H13	0.9500
C5—C6	1.3920 (19)		
N2—O1—H1O	100.5 (13)	C1—C6—C7	123.03 (12)
C1—N1—H1NA	117.7 (13)	N2—C7—C8	116.31 (12)
C1—N1—H1NB	113.8 (13)	N2—C7—C6	125.78 (12)
H1NA—N1—H1NB	112.5 (17)	C8—C7—C6	117.90 (11)
C7—N2—O1	112.76 (11)	C13—C8—C9	119.48 (12)
N1—C1—C2	120.65 (14)	C13—C8—C7	121.94 (12)
N1—C1—C6	121.17 (13)	C9—C8—C7	118.58 (12)
C2—C1—C6	118.03 (13)	C10—C9—C8	120.30 (13)
C3—C2—C1	121.59 (13)	C10—C9—H9	119.9

C3—C2—H2	119.2	C8—C9—H9	119.9
C1—C2—H2	119.2	C11—C10—C9	119.97 (13)
C2—C3—C4	119.53 (13)	C11—C10—H10	120.0
C2—C3—H3	120.2	C9—C10—H10	120.0
C4—C3—H3	120.2	C12—C11—C10	120.11 (13)
C3—C4—C5	120.47 (13)	C12—C11—H11	119.9
C3—C4—C11	119.77 (11)	C10—C11—H11	119.9
C5—C4—C11	119.76 (11)	C11—C12—C13	120.14 (13)
C4—C5—C6	120.23 (13)	C11—C12—H12	119.9
C4—C5—H5	119.9	C13—C12—H12	119.9
C6—C5—H5	119.9	C12—C13—C8	119.98 (13)
C5—C6—C1	120.10 (12)	C12—C13—H13	120.0
C5—C6—C7	116.75 (12)	C8—C13—H13	120.0
N1—C1—C2—C3	176.07 (13)	C1—C6—C7—N2	60.8 (2)
C6—C1—C2—C3	0.5 (2)	C5—C6—C7—C8	55.87 (17)
C1—C2—C3—C4	1.5 (2)	C1—C6—C7—C8	-120.15 (14)
C2—C3—C4—C5	-2.5 (2)	N2—C7—C8—C13	39.36 (18)
C2—C3—C4—C11	178.60 (11)	C6—C7—C8—C13	-139.76 (13)
C3—C4—C5—C6	1.4 (2)	N2—C7—C8—C9	-139.76 (13)
C11—C4—C5—C6	-179.73 (10)	C6—C7—C8—C9	41.12 (17)
C4—C5—C6—C1	0.7 (2)	C13—C8—C9—C10	-1.7 (2)
C4—C5—C6—C7	-175.41 (12)	C7—C8—C9—C10	177.41 (12)
N1—C1—C6—C5	-177.17 (13)	C8—C9—C10—C11	1.0 (2)
C2—C1—C6—C5	-1.63 (19)	C9—C10—C11—C12	0.4 (2)
N1—C1—C6—C7	-1.3 (2)	C10—C11—C12—C13	-1.1 (2)
C2—C1—C6—C7	174.25 (12)	C11—C12—C13—C8	0.3 (2)
O1—N2—C7—C8	-178.54 (11)	C9—C8—C13—C12	1.05 (19)
O1—N2—C7—C6	0.5 (2)	C7—C8—C13—C12	-178.07 (12)
C5—C6—C7—N2	-123.16 (15)		

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
N1—H1 <i>N</i> A...O1	0.91 (2)	2.23 (2)	2.8875 (19)	128.7 (16)
O1—H1O...N2 ⁱ	0.95 (2)	1.84 (2)	2.7411 (16)	156.4 (19)

Symmetry code: (i) $-x+1, -y+1, -z+1$.