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Crystal structure of racemic chloramphenicol

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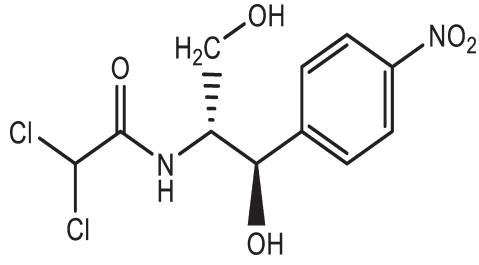
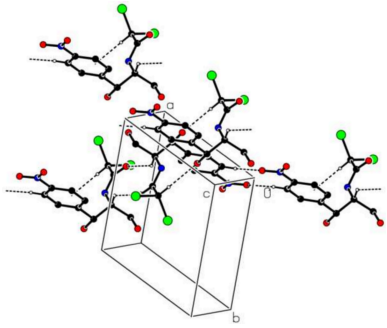
The racemic title compound {systematic name: 2,2-dichloro-*N*-[(1*R*,2*R*)-1,3-dihydroxy-1-(4-nitrophenyl)propan-2-yl]acetamide}, $C_{11}H_{12}Cl_2N_2O_5$, crystallizes in the space group $P\overline{1}$. In the crystal, O—H···O, N—H···O and C—H···O hydrogen bonds link the molecules into a three-dimensional architecture, enclosing $R_2^2(14)$, $R_2^2(12)$, $R_2^2(10)$ and $R_4^4(4)$ loops. The title compound complements the known orthorhombic form of natural (homochiral) chloramphenicol [Acharya *et al.* (1979). Acta Cryst. B**35**, 1360–1363], which crystallizes in space group $C222_1$. The Hirshfeld surface analysis of the crystal structure indicates that the most important contributions for the crystal packing are from H···O/O···H (39.4%), H···H (21.7%), H···C/C···H (15.5%) and Cl···C/C···Cl (8.3%) interactions.

1. Chemical context

Chloramphenicol, $C_{11}H_{12}Cl_2N_2O_5$, was originally isolated from the bacteria *Streptomyces venezuelae* in 1948 and has been used to treat bacterial conjunctivitis, which is a bacterial infection involving the mucous membrane of the surface of the eye (Ehrlich *et al.*, 1947; Feder *et al.*, 1981). The crystal structure of natural chloramphenicol has been reported several times in the orthorhombic space group $C222_1$ (Acharya *et al.*, 1979; Chatterjee *et al.*, 1979; Dunitz, 1952; Staples, 2022; Sundaralingam *et al.*, 1971). In this work, we report the crystal structure of synthetic (racemic) chloramphenicol (**I**), and compare it with the natural form.





2. Structural commentary

Compound (**I**) crystallizes in the centrosymmetric triclinic space group $P\overline{1}$ with one molecule in the asymmetric unit. The molecule consists of *p*-nitrobenzene, dichloracetyl and 2-amino-propanediol fragments (Fig. 1), where the dichloracetyl moiety is an aliphatic haloacetyl side-chain and the propanediol moiety possesses two stereogenic carbon atoms (C7 and

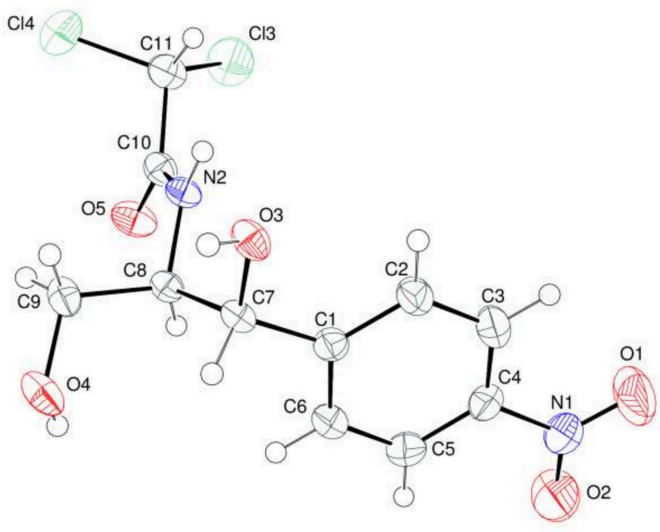


Figure 1
The molecular structure of (**I**) showing 50% probability ellipsoids.

C8), carrying the hydroxyl group and the amide side chain, respectively. In the arbitrarily chosen asymmetric molecule of (**I**), C7 and C8 both have *R* configuration, but crystal symmetry generates a racemic mixture. In natural, chiral, chloramphenicol, the equivalent atoms also have *R* configurations. In the *p*-nitrobenzene moiety in (**I**), the nitro (N1/O1/O2) group is oriented at a dihedral angle of 4.3 (3)° with respect the the C1–C6 benzene ring and atoms N1 and C7 are −0.037 (3) and −0.041 (2) Å away from the benzene ring plane. In the dichloracetyl moiety, atoms Cl3 and Cl4 are −1.3541 (8) and 1.5347 (8) Å, respectively, away from the best plane of the O5/N2/C10/C11 acetyl group (r.m.s. deviation = 0.008 Å). In the 2-amino-propanediol moiety, the dihedral angles between the *A* (O4/N2/C8/C9) [r.m.s. deviation = 0.013Å], *B* (N2/C7/C8) and *C* (O3/C7/C8) fragments are *A*/*B* = 56.46 (16)°, *A*/*C* = 77.92 (9)° and *B*/*C* = 43.64 (18)°. On the other hand, the O3—C7—C8—C9, O3—C7—C8—N2 and O4—C9—C8—N2 torsion angles are −78.3 (2), 43.6 (2) and 177.91 (16)°, respectively. The bond lengths and angles in the title triclinic polymorph are significantly different from the corresponding values in the orthorhombic polymorph of chloramphenicol (Acharya *et al.*, 1979; Chatterjee *et al.*, 1979; Dunitz, 1952)

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

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O5^{i}	0.82	2.00	2.780 (2)	159
O3—H3···O4^{ii}	0.82	1.90	2.706 (2)	170
N2—H2···O3^{iii}	0.83 (3)	2.23 (3)	3.010 (2)	155 (2)
C11—H11···O3^{iii}	0.98	2.42	3.302 (3)	149
C8—H8···O5^{i}	0.98	2.39	3.163 (2)	135
C3—H3*A*···O1^{iv}	0.93	2.46	3.298 (4)	151

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

3. Supramolecular features

In the extended structure of (**I**), O—H···O and N—H···O hydrogen bonds (Table 1) link the molecules, enclosing $R_2^2(12)$, $R_2^2(14)$ and $R_4^4(4)$ ring motifs, into a three-dimensional network (Figs. 2 and 3). The packing is consolidated by C—H···O hydrogen bonds and aromatic π–π stacking interactions between the benzene rings with centroid- to-centroid distance of 3.7524 (13) Å (slippage = 1.330 Å). Unlike the intramolecular O—H···O hydrogen bond in natural chloramphenicol (Staples, 2022; CSD refcode CLMPCL04), in (**I**), both –OH groups participate in intermolecular O—H···O

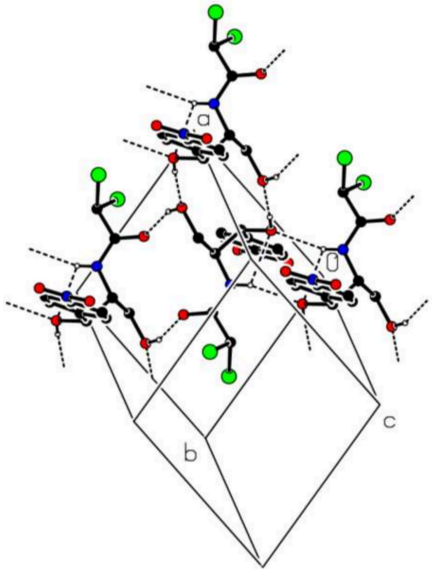


Figure 2
A partial packing diagram of (**I**) showing the intermolecular N—H···O and O—H···O hydrogen bonds as dashed lines.

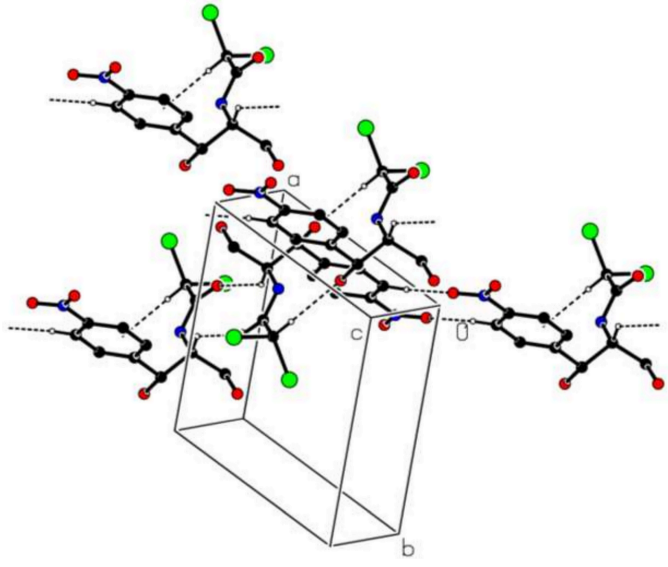


Figure 3
A partial packing diagram of (**I**) showing C—H···O hydrogen bonds as dashed lines.

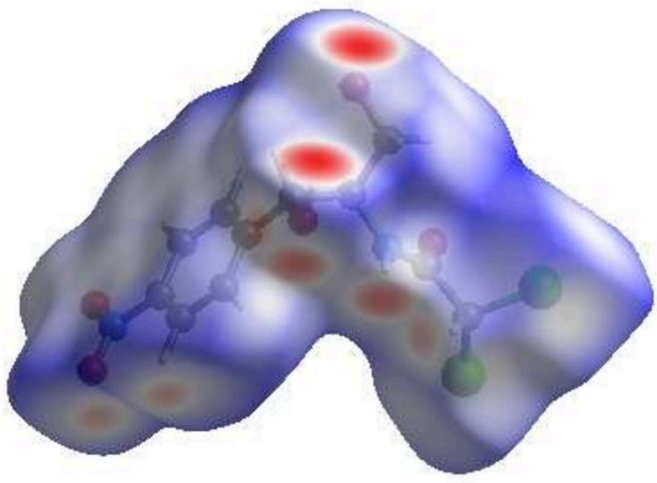


Figure 4
View of the three-dimensional Hirshfeld surface for (**I**) plotted over d_{norm} in the range from −0.67 to 1.50 a.u.

interactions with O···O contact distances of 2.706 (2) Å and 2.780 (2) Å (Table 1).

The intermolecular interactions in the crystal of (**I**) were visualized by carrying out a Hirshfeld surface (HS) analysis using *CrystalExplorer* 17.5 (Spackman *et al.*, 2021). The red spots (Fig. 4) indicate their roles as the respective donors and/or acceptors atoms in hydrogen bonding, as discussed above. The overall two-dimensional fingerprint plot is shown in Fig. 5*a* and those delineated into different contact types in Fig. 5*b*–*n*. According to these data, the H···O/O···H, H···H, H···C/C···H and C···Cl/Cl···Cl contacts make the most significant contributions to the HS, at 39.4%, 21.7%, 15.5% and 8.3%, respectively (Fig. 7).

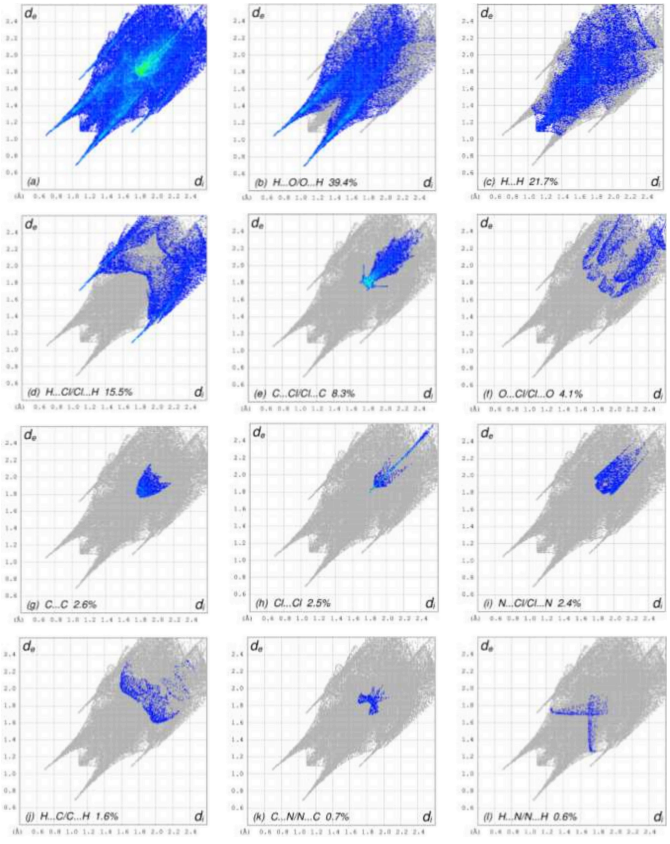


Figure 5
The two-dimensional fingerprint plots for (**I**), showing (*a*) all interactions, and delineated into different contact types (*b*)–(n). The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{11}H_{12}Cl_2N_2O_5$
M_r	323.13
Crystal system, space group	Triclinic, $P\overline{1}$
Temperature (K)	292
a, b, c (Å)	8.0656 (2), 8.9248 (2), 11.0003 (2)
α, β, γ (°)	97.522 (2), 105.938 (2), 107.280 (2)
V (Å^3)	707.30 (3)
Z	2
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.34
Crystal size (mm)	0.3 × 0.24 × 0.15
Data collection	
Diffractometer	XtaLAB Synergy, Single source at home/near, HyPix3000
Absorption correction	Multi-scan ((*CrysAlis PRO*; Rigaku OD, 2023)
T_{min}, T_{max}	0.656, 1.000
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	5967, 2718, 2507
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.615
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.052, 0.141, 1.05
No. of reflections	2718
No. of parameters	188
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.59, −0.68

Computer programs: *CrysAlis PRO* (Rigaku OD, 2023), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2016/6* (Sheldrick, 2015*b*) and *OLEX2*a (Dolomanov *et al.*, 2009).

The volume of the crystal voids (see figure in the supporting information) and the percentage of free space in the unit cell of (**I**) are 115.2 Å^3 and 16.3%, respectively. These values compare with 324.1 Å^3 and 11.9%, respectively in CLMPCL04, which suggests that the homochiral molecules in CLMPCL04 pack more effectively in space group $C222_1$ than do the racemic molecules in space group $P\overline{1}$ in (**I**). This is supported by the difference in unit-cell volumes [707.30 (3) Å^3 for (**I**) (Z = 2) and 2733.30 (6) Å^3 for CLMPCL04 (Z = 8)], although it should be noted that the intensity data for (**I**) were collected at 292 K and those for CLMPCL04 at 100 K.

For further computational chemistry results (electrostatic potential, shape-index, void volume figures, interaction energies), see the supporting information.

4. Database survey

A survey of the Cambridge Structural Database (CSD, July 2025 update; Groom *et al.*, 2016) revealed six structures of natural chloramphenicol: CSD refcode CLMPCL (Sundar-

alingam *et al.*, 1971), CLMPCL01 (Acharya *et al.*, 1979), CLMPCL02 (Chatterjee *et al.*, 1979), CLMPCL03 (Dunitz, 1952), CLMPCL04 (Staples, 2022) and EJILUH (Ma *et al.*, 2020). The first five crystallize in space group $C222_1$ with $a \simeq 7.34$, $b \simeq 17.34$, $c \simeq 21.49$ Å (or equivalent setting of the unit cell) and the final structure is a clathrate.

5. Synthesis and crystallization

A commercial sample of chloramphenicol was recrystallised by slow evaporation of an ethanol–water (1:1 *v*/*v*) solution at room temperature.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The NH hydrogen atom was located from a difference Fourier map and refined isotropically. The O- and C-bound hydrogen-atom positions were calculated geometrically at distances of 0.82 Å (for OH), 0.93–0.98 Å (for CH), and refined using a riding model with the constraint of $U_{iso} = k \times U_{eq}$ (C, O), where $k = 1.5$ for OH hydrogen atoms and $k = 1.2$ for other hydrogen atoms.

Acknowledgements

The author's contributions are as follows. Conceptualization, TH and ANB; crystallization, OC and JA; X-ray analysis, BT, JA and TH; Hirshfeld surface analysis, TH; writing (review and editing of the manuscript) TH, RSH and KIH; supervision, TH and ANB. This research was conducted at the Laboratory of Complex Compounds, Institute of Bioorganic Chemistry, Academy of Sciences of the Republic of Uzbekistan. It was financially supported by government funding from the Republic of Uzbekistan. This work has been supported by the Azerbaijan Medical University and the Azerbaijan State Oil and Industry University. TH is also grateful to Hacettepe University Scientific Research Project Unit (grant No. 013 D04 602 004).

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Computing details

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Crystal data

$C_{11}H_{12}Cl_2N_2O_5$
M_r = 323.13
Triclinic, $P\overline{1}$
a = 8.0656 (2) Å
b = 8.9248 (2) Å
c = 11.0003 (2) Å
α = 97.522 (2)°
β = 105.938 (2)°
γ = 107.280 (2)°
V = 707.30 (3) Å^3
Z = 2
$F(000)$ = 332
D_x = 1.517 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 4694 reflections
θ = 4.3–71.5°
μ = 4.34 mm^{-1}
T = 292 K
Block, colourless
0.3 × 0.24 × 0.15 mm

Data collection

XtaLAB Synergy, Single source at home/near, HyPix3000 diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
Mirror monochromator
Detector resolution: 10.0000 pixels mm^{-1}
ω scans
Absorption correction: multi-scan ((CrysAlisPro; Rigaku OD, 2023)
T_{min} = 0.656, T_{max} = 1.000
5967 measured reflections
2718 independent reflections
2507 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 71.4°, θ_{min} = 4.3°
h = −9→8
k = −10→10
l = −10→13

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.052
$wR(F^2)$ = 0.141
S = 1.05
2718 reflections
188 parameters
0 restraints
Primary atom site location: dual
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0747P)^2 + 0.5048P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.59 e Å^{-3}
$\Delta\rho_{min}$ = −0.68 e Å^{-3}
Extinction correction: SHELXL-2016/6 (Sheldrick 2016), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0140 (14)

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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl3	0.47682 (11)	0.44633 (10)	0.32614 (7)	0.0589 (3)
Cl4	0.19337 (11)	0.49969 (11)	0.12769 (7)	0.0643 (3)
O4	−0.1306 (2)	0.79888 (19)	0.50133 (18)	0.0361 (4)
H4	−0.151263	0.726781	0.540228	0.054*
O3	0.3697 (2)	1.04729 (17)	0.57744 (15)	0.0286 (4)
H3	0.302019	1.094821	0.545594	0.043*
O5	0.1354 (2)	0.46694 (18)	0.39138 (18)	0.0389 (4)
O1	0.8908 (3)	0.8840 (4)	1.1205 (2)	0.0880 (10)
O2	0.6514 (4)	0.7306 (4)	1.1442 (2)	0.0762 (8)
N1	0.7258 (3)	0.8144 (3)	1.0840 (2)	0.0472 (6)
N2	0.2773 (2)	0.7375 (2)	0.44290 (17)	0.0247 (4)
H2	0.355 (4)	0.814 (3)	0.430 (2)	0.026 (6)*
C11	0.3536 (3)	0.5760 (3)	0.2873 (2)	0.0335 (5)
H11	0.439319	0.683345	0.294084	0.040*
C10	0.2461 (3)	0.5879 (2)	0.3806 (2)	0.0272 (4)
C8	0.1641 (3)	0.7676 (2)	0.51967 (19)	0.0230 (4)
H8	0.131957	0.677095	0.560800	0.028*
C2	0.5884 (3)	0.9648 (3)	0.7853 (2)	0.0345 (5)
H2A	0.643424	1.030383	0.737875	0.041*
C7	0.2722 (3)	0.9228 (2)	0.6273 (2)	0.0243 (4)
H7	0.182310	0.958821	0.655455	0.029*
C4	0.6133 (3)	0.8411 (3)	0.9648 (2)	0.0349 (5)
C9	−0.0134 (3)	0.7752 (3)	0.4297 (2)	0.0305 (5)
H9A	0.015934	0.863249	0.386989	0.037*
H9B	−0.076981	0.675638	0.363211	0.037*
C5	0.4241 (3)	0.7678 (3)	0.9267 (2)	0.0377 (5)
H5	0.369825	0.701347	0.973919	0.045*
C6	0.3185 (3)	0.7963 (3)	0.8166 (2)	0.0348 (5)
H6	0.191082	0.748704	0.789635	0.042*
C1	0.3986 (3)	0.8948 (2)	0.7449 (2)	0.0267 (4)
C3	0.6970 (3)	0.9380 (3)	0.8960 (2)	0.0399 (6)
H3A	0.824555	0.984839	0.923189	0.048*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl3	0.0632 (5)	0.0683 (5)	0.0572 (5)	0.0432 (4)	0.0213 (4)	0.0035 (3)
Cl4	0.0564 (5)	0.0918 (6)	0.0335 (4)	0.0162 (4)	0.0097 (3)	0.0113 (3)
O4	0.0248 (8)	0.0325 (8)	0.0591 (11)	0.0137 (6)	0.0178 (7)	0.0201 (7)

O3	0.0227 (7)	0.0236 (7)	0.0407 (8)	0.0074 (6)	0.0111 (6)	0.0115 (6)
O5	0.0389 (9)	0.0249 (8)	0.0556 (11)	0.0050 (7)	0.0257 (8)	0.0110 (7)
O1	0.0376 (12)	0.147 (3)	0.0639 (15)	0.0123 (14)	−0.0005 (11)	0.0559 (16)
O2	0.0597 (14)	0.118 (2)	0.0545 (13)	0.0253 (14)	0.0152 (11)	0.0530 (14)
N1	0.0421 (13)	0.0662 (15)	0.0320 (11)	0.0186 (11)	0.0086 (9)	0.0157 (10)
N2	0.0229 (9)	0.0217 (8)	0.0311 (9)	0.0050 (7)	0.0134 (7)	0.0079 (7)
C11	0.0325 (12)	0.0288 (11)	0.0363 (12)	0.0062 (9)	0.0148 (9)	0.0006 (9)
C10	0.0243 (10)	0.0244 (10)	0.0328 (11)	0.0071 (8)	0.0099 (8)	0.0079 (8)
C8	0.0210 (10)	0.0214 (9)	0.0280 (10)	0.0066 (7)	0.0102 (8)	0.0071 (7)
C2	0.0266 (11)	0.0386 (12)	0.0354 (12)	0.0058 (9)	0.0099 (9)	0.0125 (9)
C7	0.0201 (9)	0.0242 (9)	0.0302 (10)	0.0074 (7)	0.0115 (8)	0.0061 (8)
C4	0.0344 (12)	0.0445 (13)	0.0243 (11)	0.0151 (10)	0.0069 (9)	0.0066 (9)
C9	0.0220 (10)	0.0312 (11)	0.0354 (11)	0.0076 (8)	0.0064 (9)	0.0092 (9)
C5	0.0380 (13)	0.0455 (13)	0.0308 (11)	0.0103 (10)	0.0160 (10)	0.0134 (10)
C6	0.0261 (11)	0.0439 (13)	0.0339 (12)	0.0086 (9)	0.0123 (9)	0.0105 (10)
C1	0.0267 (11)	0.0266 (10)	0.0265 (10)	0.0095 (8)	0.0098 (8)	0.0023 (8)
C3	0.0257 (11)	0.0493 (14)	0.0378 (12)	0.0079 (10)	0.0052 (9)	0.0107 (10)

Geometric parameters (Å, º)

Cl3—C11	1.758 (2)	C8—C7	1.538 (3)
Cl4—C11	1.771 (2)	C8—C9	1.527 (3)
O4—H4	0.8200	C2—H2A	0.9300
O4—C9	1.429 (3)	C2—C1	1.384 (3)
O3—H3	0.8200	C2—C3	1.387 (3)
O3—C7	1.425 (2)	C7—H7	0.9800
O5—C10	1.223 (3)	C7—C1	1.512 (3)
O1—N1	1.212 (3)	C4—C5	1.384 (3)
O2—N1	1.199 (3)	C4—C3	1.371 (4)
N1—C4	1.469 (3)	C9—H9A	0.9700
N2—H2	0.83 (3)	C9—H9B	0.9700
N2—C10	1.334 (3)	C5—H5	0.9300
N2—C8	1.459 (3)	C5—C6	1.378 (3)
C11—H11	0.9800	C6—H6	0.9300
C11—C10	1.527 (3)	C6—C1	1.391 (3)
C8—H8	0.9800	C3—H3A	0.9300
C9—O4—H4	109.5	O3—C7—H7	107.4
C7—O3—H3	109.5	O3—C7—C1	111.64 (16)
O1—N1—C4	118.1 (2)	C8—C7—H7	107.4
O2—N1—O1	122.5 (2)	C1—C7—C8	112.27 (16)
O2—N1—C4	119.3 (2)	C1—C7—H7	107.4
C10—N2—H2	118.5 (17)	C5—C4—N1	118.1 (2)
C10—N2—C8	120.61 (17)	C3—C4—N1	119.7 (2)
C8—N2—H2	120.5 (17)	C3—C4—C5	122.2 (2)
Cl3—C11—Cl4	110.43 (12)	O4—C9—C8	110.65 (18)
Cl3—C11—H11	109.6	O4—C9—H9A	109.5
Cl4—C11—H11	109.6	O4—C9—H9B	109.5

C10—C11—Cl3	109.68 (16)	C8—C9—H9A	109.5
C10—C11—Cl4	107.81 (16)	C8—C9—H9B	109.5
C10—C11—H11	109.6	H9A—C9—H9B	108.1
O5—C10—N2	124.1 (2)	C4—C5—H5	121.0
O5—C10—C11	120.72 (19)	C6—C5—C4	118.0 (2)
N2—C10—C11	115.15 (18)	C6—C5—H5	121.0
N2—C8—H8	108.4	C5—C6—H6	119.3
N2—C8—C7	110.40 (16)	C5—C6—C1	121.4 (2)
N2—C8—C9	109.22 (17)	C1—C6—H6	119.3
C7—C8—H8	108.4	C2—C1—C7	123.15 (19)
C9—C8—H8	108.4	C2—C1—C6	119.0 (2)
C9—C8—C7	112.08 (16)	C6—C1—C7	117.86 (19)
C1—C2—H2A	119.7	C2—C3—H3A	120.6
C1—C2—C3	120.5 (2)	C4—C3—C2	118.9 (2)
C3—C2—H2A	119.7	C4—C3—H3A	120.6
O3—C7—C8	110.49 (16)		

Cl3—C11—C10—O5	−57.1 (3)	C10—N2—C8—C9	−82.3 (2)
Cl3—C11—C10—N2	125.53 (18)	C8—N2—C10—O5	−6.5 (3)
Cl4—C11—C10—O5	63.2 (3)	C8—N2—C10—C11	170.81 (18)
Cl4—C11—C10—N2	−114.18 (18)	C8—C7—C1—C2	115.6 (2)
O3—C7—C1—C2	−9.1 (3)	C8—C7—C1—C6	−65.8 (2)
O3—C7—C1—C6	169.51 (18)	C7—C8—C9—O4	−59.4 (2)
O1—N1—C4—C5	−176.9 (3)	C4—C5—C6—C1	0.4 (4)
O1—N1—C4—C3	2.4 (4)	C9—C8—C7—O3	−78.3 (2)
O2—N1—C4—C5	0.1 (4)	C9—C8—C7—C1	156.31 (17)
O2—N1—C4—C3	179.4 (3)	C5—C4—C3—C2	0.7 (4)
N1—C4—C5—C6	178.4 (2)	C5—C6—C1—C2	0.2 (4)
N1—C4—C3—C2	−178.5 (2)	C5—C6—C1—C7	−178.5 (2)
N2—C8—C7—O3	43.6 (2)	C1—C2—C3—C4	−0.1 (4)
N2—C8—C7—C1	−81.7 (2)	C3—C2—C1—C7	178.3 (2)
N2—C8—C9—O4	177.91 (16)	C3—C2—C1—C6	−0.4 (4)
C10—N2—C8—C7	154.03 (18)	C3—C4—C5—C6	−0.9 (4)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O4—H4···O5^{i}	0.82	2.00	2.780 (2)	159
O3—H3···O4^{ii}	0.82	1.90	2.706 (2)	170
N2—H2···O3^{iii}	0.83 (3)	2.23 (3)	3.010 (2)	155 (2)
C11—H11···O3^{iii}	0.98	2.42	3.302 (3)	149
C8—H8···O5^{i}	0.98	2.39	3.163 (2)	135
C3—H3*A*···O1^{iv}	0.93	2.46	3.298 (4)	151

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