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Crystal structure and Hirshfeld surface analysis of *N*,*N*′-(2,2-dichloro-3-oxo-3-phenylpropane-1,1-diyl)diacetamide

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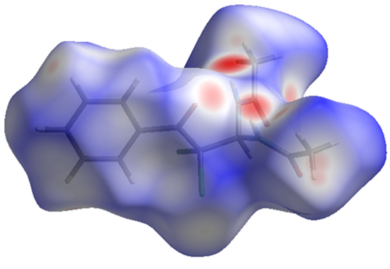
The conformation of the title molecule, $C_{13}H_{14}Cl_2N_2O_3$, is maintained by intramolecular N—H$\cdots$O, C—H$\cdots$O, and C—H$\cdots$Cl interactions, creating $S(6)$, $S(5)$, and $S(6)$ motifs, respectively. In the crystal, intermolecular N—H$\cdots$O, C—H$\cdots$O, and C—H$\cdots$Cl interactions connect the molecules, forming a three-dimensional network. Additionally, the molecules are linked by C—H$\cdots\pi$ interactions, forming layers parallel to the (002) plane. The most important interactions, according to Hirshfeld two-dimensional fingerprint plots, are H$\cdots$H (35.0%), O$\cdots$H/H$\cdots$O (21.2%), Cl$\cdots$H/H$\cdots$Cl (20.7%), and C$\cdots$H/H$\cdots$C (17.1%).

1. Chemical context

Bisamidals are an important class of organic compounds, since the amide fragment is a component of many biologically active substances and is widely used in pharmaceuticals, medicine and materials science (Manne *et al.*, 2017; Zhang *et al.*, 2013). Bisamidals are also convenient starting reagents for the synthesis of heterocyclic and organophosphorus compounds with useful properties (Dmitriev *et al.*, 2021; Makra *et al.*, 2022). The catalytic and analytic properties of this class of compounds are strongly dependent on the attached groups to the amide moiety (Alieva *et al.*, 2006; Aliyeva *et al.*, 2024). Both the NH and C=O groups of bisamidals can participate in various sorts of intermolecular interactions, which improve the catalytic and biological activity of corresponding metal complexes (Kopylovich *et al.*, 2012*a*,*b*; Mahmudov *et al.*, 2015). We have previously shown that accessible highly electrophilic α,α-dihalogen-β-oxoaldehydes readily condense with amides to form amidals (Guseinov *et al.*, 1994,2024 and 2025). We used this property of aldehydes (**1**) to obtain bisamidals (**4**).



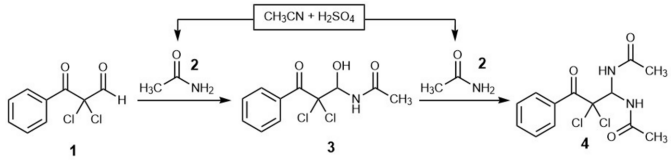


Figure 1
Synthesis of *N*,*N*′-(2,2-dichloro-3-oxo-3-phenylpropane-1,1-diyl)diacetamide.

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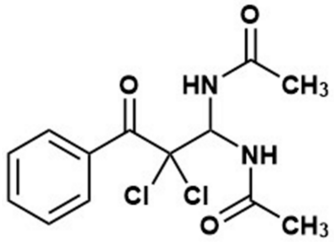
We found that bisamidals can be synthesized with a yield of 92% by reacting aldehydes with acetonitrile in the presence of concentrated sulfuric acid at room temperature. The formation of product (**4**) occurs *via* amide (**2**) and amidals (**3**) according to the scheme shown in Fig. 1. The structure of the product (**4**) was proven by NMR spectroscopy and X-ray diffraction.



2. Structural commentary

As shown in Fig. 2, the molecular conformation is not planar. Intramolecular N—H···O, C—H···O, and C–H···Cl interactions maintain the molecular conformation, forming *S*(6), *S*(5), and *S*(6) motifs (Bernstein *et al.*, 1995), respectively. The C9—C4—C3—O3, C9—C4—C3—C2, C4—C3—C2—Cl1, C4—C3—C2—Cl2, C3—C2—C1—N10, C3—C2—C1—N13, C2—C1—N10—C11 and C2—C1—N13—C14 torsion angles are 14.8 (3), −162.76 (19), 46.2 (2), −73.6 (2), 63.4 (2), −64.2 (2), 125.26 (18) and −119.66 (19)°, respectively. The molecule exhibits no unusual bond lengths or inter-bond angles.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, the molecules are linked into a three-dimensional network by intermolecular N—H···O, C—H···O, and C—H···Cl interactions (Table 1, Fig. 3). In addition, the molecules create layers parallel to the (002) plane through C—H···π interactions (Table 1, Fig. 4). No π–π interactions are observed in the structure.

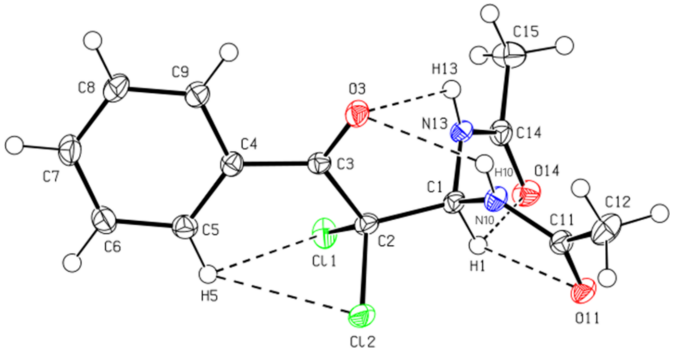


Figure 2
The molecular structure of the title compound with the atom labelling and displacement ellipsoids drawn at the 50% probability level.

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

*Cg*1 is the centroid of the C4–C9 aromatic ring.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···O3	0.84 (3)	2.34 (3)	2.804 (2)	115 (2)
N10—H10···O14^{i}	0.84 (3)	2.30 (3)	3.105 (2)	161 (3)
N13—H13···O3	0.83 (3)	2.60 (3)	2.982 (2)	110 (2)
N13—H13···O11^{i}	0.83 (3)	2.09 (3)	2.912 (2)	169 (3)
C1—H1···O11	1.00	2.26	2.746 (2)	108
C1—H1···O14	1.00	2.28	2.763 (2)	108
C5—H5···Cl1	0.95	2.77	3.179 (2)	107
C5—H5···Cl2	0.95	2.81	3.4098 (19)	122
C6—H6···O11^{ii}	0.95	2.53	3.239 (3)	131
C12—H12*A*···Cl1^{iii}	0.98	2.73	3.278 (3)	116
C12—H12*B*···O14^{i}	0.98	2.51	3.407 (3)	152
C15—H15*B*···O11^{i}	0.98	2.60	3.460 (3)	147
C15—H15*C*···*Cg*1^{iv}	0.98	2.89	3.703 (3)	141

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

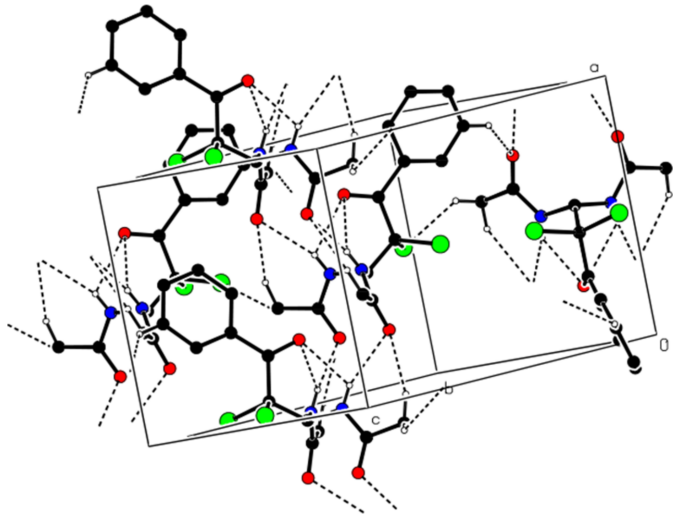


Figure 3
A partial view of molecular packing in the unit cell formed by intermolecular N—H···O, C—H···O and C—H···Cl hydrogen bonds. Hydrogen atoms that are not involved in these interactions have been omitted for clarity.

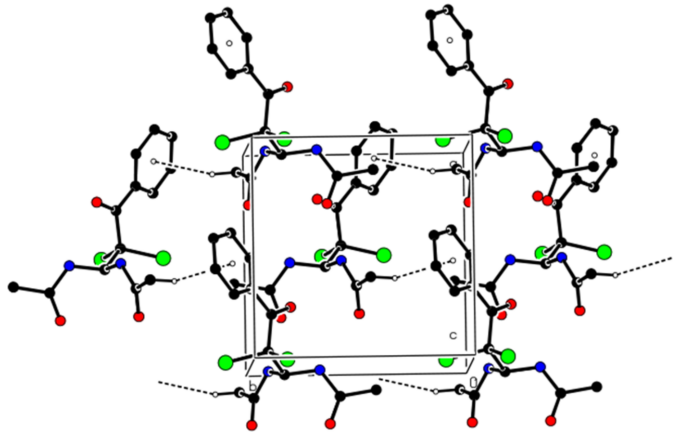


Figure 4
The view of the packing formed by C—H···π hydrogen bonds in the unit cell. H atoms that are not involved in these interactions have been removed for clarity.

Table 2
Summary of short interatomic contacts (Å).

Contact	Distance	Symmetry operation
Cl1···H12*A*	2.73	$x, -1+y, z$
O14···H9	2.66	$-1+x, y, z$
H6···O11	2.53	$1-x, -\frac{1}{2}+y, \frac{1}{2}-z$
H13···O11	2.09	$\frac{1}{2}+x, \frac{3}{2}-y, 1-z$
C9···H6	3.08	$2-x, \frac{1}{2}+y, \frac{1}{2}-z$
C6···H15*B*	2.99	$\frac{3}{2}-x, 1-y, -\frac{1}{2}+z$
H7···C4	3.08	$2-x, -\frac{1}{2}+y, \frac{1}{2}-z$

The intermolecular interactions (Tables 1 and 2) in the title compound were analysed using Hirshfeld surface calculations, employing *CrystalExplorer 17.5* (Spackman *et al.*, 2021). The Hirshfeld surface plotted over d_{norm} is shown in Fig. 5. The two-dimensional fingerprint plots (Fig. 6) show that the most significant contacts are H···H (35.0%), O···H/H···O (21.2%), Cl···H/H···Cl (20.7%), C···H/H···C (17.1%), Cl···Cl (2.1%), O···C/C···O (2.0%), O···N/N···O (0.9%), O···O (0.7%) and N···H/H···N (0.2%).

4. Database survey

A search of the Cambridge Structural Database (CSD, Version 6.00, update of April 2025; Groom *et al.*, 2016) for the 2,2-dichloro-1-phenylpropan-1-one unit generated 51 hits, the four most closely related to the title compound being those with refcodes QIRPUG (Clegg & Harrington, 2023), UHIQUZ (Essa *et al.*, 2015), UHIROU (Essa *et al.*, 2015) and YUXMIN (Mamedov *et al.*, 1995).

QIRPUG and YUXMIN crystallize in the monoclinic space group $P2_1/n$, while UHIQUZ and UHIROU crystallize in the triclinic space group $P\overline{1}$.

In the crystal of QIRPUG, the molecules are linked into a three-dimensional network by O—H···O and C—H···O interactions. In addition, π–π and C—H···π interactions are also observed. In UHIQUZ, the molecules are linked into layers parallel to the (010) plane by N—H···O and O—H···F interactions. The structure also contains π–π and C—H···π interactions. In UHIROU, the molecules linked by C—H···O and O—H···Cl interactions form layers parallel to the (001) plane. The structure also exhibits π–π and C—H···π interactions. In YUXMIN, the molecules connect through C—H···O interactions, forming a three-dimensional network and C—Cl···π interactions are also observed.

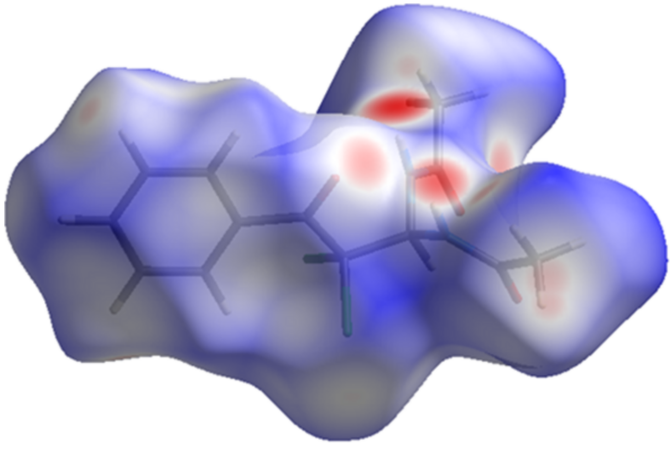


Figure 5
A view of the three-dimensional Hirshfeld surface of the title compound mapped over d_{norm}.

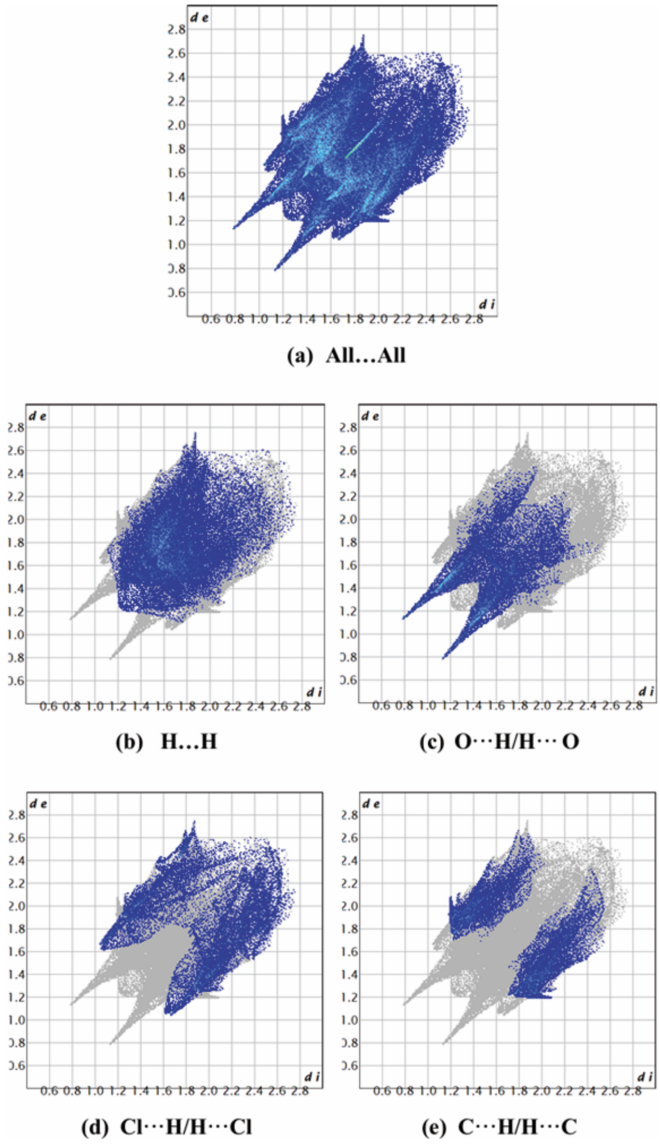


Figure 6
The full two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) O···H/H···O, (*d*) Cl···H/H···Cl and (*e*) C···H/H···C interactions. The d_i and d_e values are the closest internal and external distances (in Å) from given points on the Hirshfeld surface.

5. Synthesis and crystallization

To a solution of 217 mg (1 mmol) of 2,2-dichloro-3-oxo-3-phenylpropanal in 10 ml of acetonitrile was added sulfonic acid (2 mmol) at room temperature. The reaction mixture was then stirred for 1h. The solvent was removed *in vacuo*, the remaining white powder was recrystallized from chloroform

Table 3
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{14}Cl_2N_2O_3$
M_r	317.16
Crystal system, space group	Orthorhombic, $P2_12_12_1$
Temperature (K)	100
a, b, c (Å)	8.9115 (5), 8.9341 (7), 18.5838 (15)
V (Å^3)	1479.57 (19)
Z	4
Radiation type	Cu $K\alpha$
μ (mm^{-1})	4.03
Crystal size (mm)	0.50 × 0.10 × 0.04
Data collection	
Diffractometer	XtaLAB Synergy, Dualflex, HyPix
Absorption correction	Gaussian (*CrysAlis PRO*; Rigaku OD, 2024)
T_{min}, T_{max}	0.225, 0.945
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	17780, 3244, 3199
R_{int}	0.033
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.640
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.025, 0.063, 1.12
No. of reflections	3244
No. of parameters	192
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.29, −0.35
Absolute structure	Refined as an inversion twin
Absolute structure parameter	0.273 (14)

Computer programs: *CrysAlis PRO* (Rigaku OD, 2024), *SHELXT2014/5* (Sheldrick, 2015*a*), *SHELXL2018/3* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2020).

and *N*,*N*′-(2,2-dichloro-3-oxo-3-phenylpropane-1,1-diyl)diacetamide was isolated. Yield 292 mg (92%); m.p. 378–380 K. Analysis calculated (%) for $C_{13}H_{14}Cl_2N_2O_3$: C 49.23, H 4.45, N 8.83, found C 45.18, H 4.41, N 8.82. ESI–MS: 316.0410. ^{1}H NMR (300 MHz, DMSO-d_6): 1.87 (6H, $2CH_3$), 6.95-8.10 (5H, Ar), 8.4 (2H, 2NH). ^{13}C NMR (75 MHz, DMSO-d_6): 22.24, 60.28, 89.93, 128.46, 129.83, 131.99, 133.77, 168.95, 187.35.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. The N-bound hydrogen atoms were located in a difference-Fourier map and refined freely [N10—H10 = 0.84 (3) and N13—H13 = 0.83 (3) Å]. The C-bound H atoms were positioned geometrically (C—H = 0.95 and 1.00 Å) and refined using a riding model with U_{iso}(H) = 1.2 or 1.5U_{eq}(C). The title compound was refined as an inversion twin with matrix [−1 0 0 0 − 1 0 0 0 − 1]; the resulting BASF value is 0.273 (14).

Acknowledgements

The authors' contributions are as follows. Conceptualization, MA and GMM; synthesis and NMR analysis, FIG, KAA and RZN, X-ray analysis, AIS; writing (review and editing of the manuscript) SRH, MA and GMM; funding acquisitio,n BIU and LMG; supervision, MA and GMM.

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Computing details

N-(2,2-Dichloro-1-acetamido-3-oxo-3-phenylpropyl)acetamide

Crystal data

$C_{13}H_{14}Cl_2N_2O_3$
M_r = 317.16
Orthorhombic, $P2_12_12_1$
a = 8.9115 (5) Å
b = 8.9341 (7) Å
c = 18.5838 (15) Å
V = 1479.57 (19) Å^3
Z = 4
$F(000)$ = 656
D_x = 1.424 Mg m^{-3}
Cu $K\alpha$ radiation, λ = 1.54184 Å
Cell parameters from 13822 reflections
θ = 4.8–80.4°
μ = 4.03 mm^{-1}
T = 100 K
Needle, colourless
0.50 × 0.10 × 0.04 mm

Data collection

XtaLAB Synergy, Dualflex, HyPix diffractometer
Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source
ω scans
Absorption correction: gaussian (CrysAlisPro; Rigaku OD, 2024)
T_{min} = 0.225, T_{max} = 0.945
17780 measured reflections
3244 independent reflections
3199 reflections with $I > 2\sigma(I)$
R_{int} = 0.033
θ_{max} = 80.7°, θ_{min} = 4.8°
h = −11→7
k = −11→11
l = −23→23

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.025
$wR(F^2)$ = 0.063
S = 1.12
3244 reflections
192 parameters
0 restraints
Primary atom site location: dual
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.025P)^2 + 0.4827P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.29 e Å^{-3}
$\Delta\rho_{min}$ = −0.34 e Å^{-3}
Absolute structure: Refined as an inversion twin
Absolute structure parameter: 0.273 (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.

Refinement. Refined as a two-component inversion twin

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

	x	*y*	*z*	U_{iso}*/U_{eq}
C1	0.4571 (2)	0.6512 (2)	0.42758 (11)	0.0153 (4)
H1	0.350530	0.632488	0.413306	0.018*
C2	0.5571 (2)	0.5762 (2)	0.36927 (11)	0.0164 (4)
C3	0.7281 (2)	0.5941 (2)	0.38261 (11)	0.0150 (4)
C4	0.8415 (2)	0.5028 (2)	0.34286 (11)	0.0166 (4)
C5	0.8137 (2)	0.4219 (2)	0.27994 (12)	0.0193 (4)
H5	0.717015	0.424755	0.258427	0.023*
C6	0.9271 (3)	0.3374 (3)	0.24883 (12)	0.0223 (4)
H6	0.908252	0.283161	0.205781	0.027*
C7	1.0687 (2)	0.3319 (3)	0.28069 (13)	0.0241 (4)
H7	1.145748	0.272622	0.259784	0.029*
C8	1.0970 (2)	0.4128 (3)	0.34284 (14)	0.0245 (5)
H8	1.193639	0.408985	0.364383	0.029*
C9	0.9849 (2)	0.4996 (2)	0.37380 (11)	0.0197 (4)
H9	1.005393	0.556575	0.415835	0.024*
C11	0.3557 (2)	0.9022 (2)	0.42317 (11)	0.0180 (4)
C12	0.3834 (3)	1.0663 (3)	0.43368 (15)	0.0276 (5)
H12A	0.359605	1.120063	0.389145	0.041*
H12B	0.489068	1.082549	0.446033	0.041*
H12C	0.319644	1.103611	0.472727	0.041*
C14	0.3606 (2)	0.5148 (2)	0.53082 (12)	0.0183 (4)
C15	0.3939 (3)	0.4528 (3)	0.60425 (13)	0.0263 (5)
H15A	0.321531	0.492994	0.638963	0.039*
H15B	0.495648	0.481658	0.618601	0.039*
H15C	0.386103	0.343439	0.603080	0.039*
Cl1	0.51039 (5)	0.38234 (5)	0.36798 (3)	0.02095 (12)
Cl2	0.51459 (6)	0.65975 (6)	0.28413 (3)	0.02384 (12)
N10	0.47663 (19)	0.81155 (19)	0.42972 (9)	0.0165 (3)
N13	0.47820 (19)	0.58088 (19)	0.49669 (9)	0.0155 (3)
O3	0.76361 (16)	0.68281 (18)	0.42875 (9)	0.0206 (3)
O11	0.22974 (16)	0.85474 (18)	0.40820 (9)	0.0205 (3)
O14	0.23568 (17)	0.50255 (19)	0.50325 (8)	0.0213 (3)
H10	0.559 (3)	0.845 (3)	0.4435 (15)	0.014 (6)*
H13	0.557 (3)	0.600 (3)	0.5189 (15)	0.016 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0103 (8)	0.0181 (9)	0.0175 (9)	0.0000 (7)	0.0001 (7)	0.0008 (7)
C2	0.0128 (8)	0.0198 (9)	0.0167 (9)	−0.0005 (7)	−0.0013 (7)	0.0016 (8)
C3	0.0133 (8)	0.0167 (8)	0.0150 (9)	−0.0015 (7)	−0.0004 (7)	0.0013 (7)
C4	0.0147 (9)	0.0173 (9)	0.0178 (9)	−0.0003 (7)	0.0018 (7)	0.0013 (8)
C5	0.0175 (9)	0.0226 (10)	0.0179 (10)	−0.0011 (8)	−0.0010 (8)	−0.0005 (8)
C6	0.0236 (10)	0.0247 (10)	0.0186 (10)	0.0007 (8)	0.0029 (8)	−0.0031 (9)
C7	0.0191 (9)	0.0271 (11)	0.0260 (11)	0.0035 (8)	0.0055 (8)	−0.0030 (10)
C8	0.0133 (9)	0.0304 (11)	0.0298 (12)	0.0023 (8)	−0.0006 (8)	−0.0017 (10)
C9	0.0138 (9)	0.0232 (9)	0.0221 (9)	−0.0019 (8)	0.0005 (8)	−0.0023 (8)
C11	0.0160 (9)	0.0213 (10)	0.0166 (9)	0.0022 (8)	0.0017 (7)	0.0028 (8)
C12	0.0234 (10)	0.0201 (10)	0.0393 (13)	0.0033 (8)	−0.0041 (10)	0.0040 (9)
C14	0.0149 (9)	0.0187 (9)	0.0212 (10)	−0.0006 (7)	0.0013 (8)	−0.0029 (8)
C15	0.0228 (10)	0.0342 (12)	0.0219 (11)	−0.0067 (9)	−0.0016 (9)	0.0056 (9)
Cl1	0.0161 (2)	0.0188 (2)	0.0279 (2)	−0.00432 (17)	0.00332 (18)	−0.00562 (17)
Cl2	0.0204 (2)	0.0342 (3)	0.0169 (2)	0.0074 (2)	−0.00126 (18)	0.00409 (19)
N10	0.0106 (7)	0.0173 (7)	0.0215 (8)	−0.0015 (6)	0.0007 (6)	0.0006 (6)
N13	0.0102 (7)	0.0186 (8)	0.0177 (8)	−0.0009 (6)	−0.0009 (7)	−0.0004 (6)
O3	0.0133 (6)	0.0228 (7)	0.0255 (8)	−0.0005 (6)	−0.0006 (6)	−0.0061 (6)
O11	0.0126 (6)	0.0258 (7)	0.0231 (7)	0.0017 (6)	−0.0009 (5)	0.0006 (6)
O14	0.0129 (7)	0.0267 (7)	0.0244 (8)	−0.0045 (6)	−0.0007 (6)	0.0006 (6)

Geometric parameters (Å, º)

C1—N13	1.442 (3)	C8—C9	1.389 (3)
C1—N10	1.444 (3)	C8—H8	0.9500
C1—C2	1.555 (3)	C9—H9	0.9500
C1—H1	1.0000	C11—O11	1.232 (3)
C2—C3	1.552 (3)	C11—N10	1.354 (3)
C2—Cl1	1.781 (2)	C11—C12	1.499 (3)
C2—Cl2	1.790 (2)	C12—H12A	0.9800
C3—O3	1.210 (3)	C12—H12B	0.9800
C3—C4	1.494 (3)	C12—H12C	0.9800
C4—C5	1.397 (3)	C14—O14	1.230 (3)
C4—C9	1.402 (3)	C14—N13	1.360 (3)
C5—C6	1.388 (3)	C14—C15	1.502 (3)
C5—H5	0.9500	C15—H15A	0.9800
C6—C7	1.395 (3)	C15—H15B	0.9800
C6—H6	0.9500	C15—H15C	0.9800
C7—C8	1.386 (4)	N10—H10	0.84 (3)
C7—H7	0.9500	N13—H13	0.83 (3)
N13—C1—N10	113.07 (17)	C9—C8—H8	119.8
N13—C1—C2	111.00 (16)	C8—C9—C4	119.8 (2)
N10—C1—C2	112.19 (16)	C8—C9—H9	120.1
N13—C1—H1	106.7	C4—C9—H9	120.1

N10—C1—H1	106.7	O11—C11—N10	122.7 (2)
C2—C1—H1	106.7	O11—C11—C12	121.08 (19)
C3—C2—C1	114.02 (17)	N10—C11—C12	116.25 (19)
C3—C2—Cl1	109.38 (14)	C11—C12—H12A	109.5
C1—C2—Cl1	107.12 (13)	C11—C12—H12B	109.5
C3—C2—Cl2	107.82 (14)	H12A—C12—H12B	109.5
C1—C2—Cl2	108.36 (13)	C11—C12—H12C	109.5
Cl1—C2—Cl2	110.13 (11)	H12A—C12—H12C	109.5
O3—C3—C4	122.06 (18)	H12B—C12—H12C	109.5
O3—C3—C2	115.96 (18)	O14—C14—N13	122.8 (2)
C4—C3—C2	121.94 (18)	O14—C14—C15	121.6 (2)
C5—C4—C9	119.65 (19)	N13—C14—C15	115.55 (19)
C5—C4—C3	125.17 (18)	C14—C15—H15A	109.5
C9—C4—C3	115.17 (18)	C14—C15—H15B	109.5
C6—C5—C4	120.07 (19)	H15A—C15—H15B	109.5
C6—C5—H5	120.0	C14—C15—H15C	109.5
C4—C5—H5	120.0	H15A—C15—H15C	109.5
C5—C6—C7	120.1 (2)	H15B—C15—H15C	109.5
C5—C6—H6	120.0	C11—N10—C1	119.69 (17)
C7—C6—H6	120.0	C11—N10—H10	120.8 (19)
C8—C7—C6	120.0 (2)	C1—N10—H10	118.2 (19)
C8—C7—H7	120.0	C14—N13—C1	120.26 (17)
C6—C7—H7	120.0	C14—N13—H13	120.6 (19)
C7—C8—C9	120.4 (2)	C1—N13—H13	117 (2)
C7—C8—H8	119.8		

N13—C1—C2—C3	−64.2 (2)	C9—C4—C5—C6	0.8 (3)
N10—C1—C2—C3	63.4 (2)	C3—C4—C5—C6	−178.1 (2)
N13—C1—C2—Cl1	56.97 (18)	C4—C5—C6—C7	0.6 (3)
N10—C1—C2—Cl1	−175.45 (13)	C5—C6—C7—C8	−1.1 (4)
N13—C1—C2—Cl2	175.76 (13)	C6—C7—C8—C9	0.1 (4)
N10—C1—C2—Cl2	−56.66 (18)	C7—C8—C9—C4	1.3 (4)
C1—C2—C3—O3	−11.6 (3)	C5—C4—C9—C8	−1.7 (3)
Cl1—C2—C3—O3	−131.54 (17)	C3—C4—C9—C8	177.2 (2)
Cl2—C2—C3—O3	108.71 (19)	O11—C11—N10—C1	−7.4 (3)
C1—C2—C3—C4	166.04 (18)	C12—C11—N10—C1	173.8 (2)
Cl1—C2—C3—C4	46.2 (2)	N13—C1—N10—C11	−108.3 (2)
Cl2—C2—C3—C4	−73.6 (2)	C2—C1—N10—C11	125.26 (18)
O3—C3—C4—C5	−166.3 (2)	O14—C14—N13—C1	5.0 (3)
C2—C3—C4—C5	16.2 (3)	C15—C14—N13—C1	−176.70 (19)
O3—C3—C4—C9	14.8 (3)	N10—C1—N13—C14	113.2 (2)
C2—C3—C4—C9	−162.76 (19)	C2—C1—N13—C14	−119.66 (19)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N10—H10···O3	0.84 (3)	2.34 (3)	2.804 (2)	115 (2)
N10—H10···O14^{i}	0.84 (3)	2.30 (3)	3.105 (2)	161 (3)

N13—H13···O3	0.83 (3)	2.60 (3)	2.982 (2)	110 (2)
N13—H13···O11^{i}	0.83 (3)	2.09 (3)	2.912 (2)	169 (3)
C1—H1···O11	1.00	2.26	2.746 (2)	108
C1—H1···O14	1.00	2.28	2.763 (2)	108
C5—H5···Cl1	0.95	2.77	3.179 (2)	107
C5—H5···Cl2	0.95	2.81	3.4098 (19)	122
C6—H6···O11^{ii}	0.95	2.53	3.239 (3)	131
C12—H12*A*···Cl1^{iii}	0.98	2.73	3.278 (3)	116
C12—H12*B*···O14^{i}	0.98	2.51	3.407 (3)	152
C15—H15*B*···O11^{i}	0.98	2.60	3.460 (3)	147
C15—H15*C*···*Cg*1^{iv}	0.98	2.89	3.703 (3)	141

Symmetry codes: (i) $x+1/2, -y+3/2, -z+1$; (ii) $-x+1, y-1/2, -z+1/2$; (iii) $x, y+1, z$; (iv) $x-1/2, -y+1/2, -z+1$.