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3,4-Dichloro-1-nitrobenzene–1,4-dioxane (4/1)

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Key indicators

Single-crystal X-ray study
T = 123 K
Mean σ(C–C) = 0.003 Å
R factor = 0.033
wR factor = 0.081
Data-to-parameter ratio = 15.0

For details of how these key indicators were automatically derived from the article, see http://journals.iucr.org/e.

The solvate structure of 3,4-dichloro-1-nitrobenzene with 1,4-dioxane, $C_6H_3Cl_2NO_2\cdot0.25C_4H_8N_2$, is reported. The asymmetric unit comprises two independent 3,4-dichloro-1-nitrobenzene molecules and half of a 1,4-dioxane molecule, the solvent molecule being disposed about a centre of inversion. Double chains of 3,4-dichloro-1-nitrobenzene are linked by Cl···Cl interactions and 1,4-dioxane molecules *via* C—H···O hydrogen bonds into a two-dimensional sheet.

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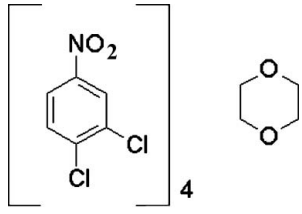
Comment

The title compound, (I), was produced during an automated parallel crystallization polymorph screen on 3,4-dichloro-nitrobenzene (3,4-DCNB). The sample was identified as a novel form using multi-sample X-ray powder diffraction analysis of all recrystallized samples (Florence *et al.*, 2003). Subsequent manual recrystallization from a saturated 1,4-dioxane solution by slow evaporation at 298 K yielded samples suitable for single-crystal X-ray analysis. Compound (I) crystallizes in the space group $P\overline{1}$ with two molecules of 3,4-DCNB and one half-molecule of 1,4-dioxane (disposed about a centre of inversion) in the asymmetric unit (Fig. 1).



(I)

The crystal structure of (I) is characterized by double chains of 3,4-DCNB, linked by Cl···Cl interactions and 1,4-dioxane

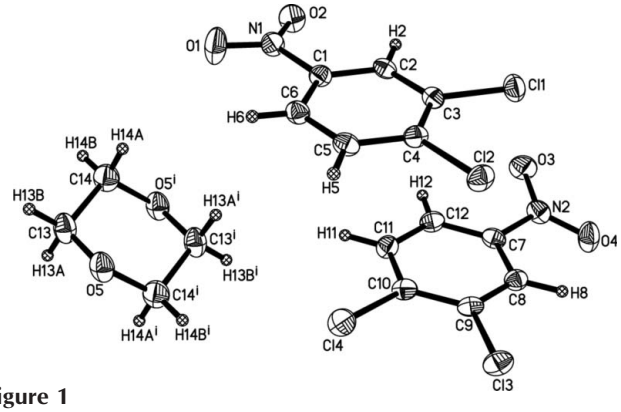


Figure 1
The molecular structure of (I), showing the numbering scheme used. Displacement ellipsoids are drawn at the 50% probability level. [Symmetry code: (i) $1-x, 1-y, 1-z$.]

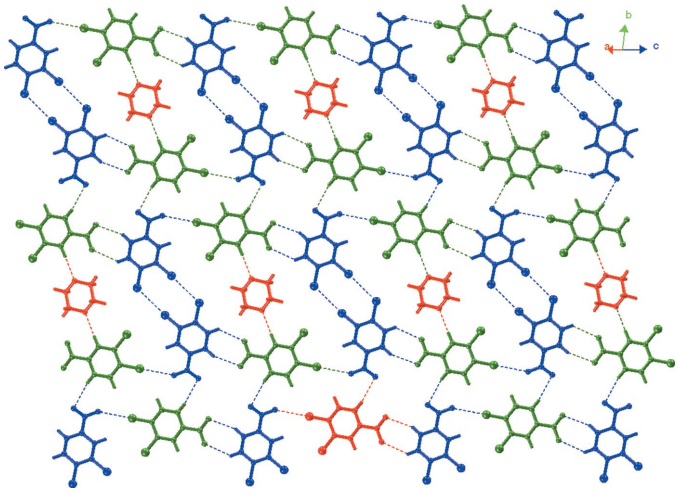


Figure 2
The two-dimensional network formed by (I), showing the intermolecular interactions involved (dashed lines). Colour key: 3,4-DCNB molecule 1 - green; 3,4-DCNB molecule 2 - blue; 1,4-dioxane - red.

molecules to give a two-dimensional sheet parallel to the (212) plane (Fig. 2). Details of the hydrogen-bonding interactions are given in Table 1. 3,4-DCNB molecules of type 2 (C7–C12) are connected to molecules of type 1 (C1–C6) *via* C—H···O hydrogen bonds and N—O···Cl interactions [O4···Cl2^{iv} = 3.013 (1) Å and N2—O4···Cl2^{iv} = 146.9 (1)°; symmetry code: (iv) $2-x, -y, -z$]. This chain is linked to another identical, but antiparallel, chain by a second set of C—H···O hydrogen bonds. These double chains are joined by Cl···Cl interactions through the type 2 molecules [Cl3···Cl4^{v} = Cl4···Cl3^{v} = 3.480 (1) Å and C9—Cl3···Cl4^{v} = C10—Cl4···Cl3^{v} = 160.3 (1)°; symmetry code: (v): $2-x, 1-y, -z$], while the type 1 molecules are linked *via* the 1,4-dioxane solvent molecules by C—H···O hydrogen bonds, thereby forming a two-dimensional sheet. These sheets stack parallel to the (212) plane in an *ABAB* fashion (Fig. 3).

Experimental

A single crystal of the title compound was obtained by recrystallization from a 1,4-dioxane solution by slow evaporation at 298 K.

Crystal data

$C_6H_3Cl_2NO_2\cdot0.25C_4H_8N_2$
M_r = 214.02
Triclinic, $P\overline{1}$
a = 7.3850 (3) Å
b = 9.7359 (3) Å
c = 13.7218 (5) Å
α = 69.347 (2)°
β = 87.209 (2)°
γ = 67.945 (2)°
V = 851.63 (5) Å^3
Z = 4
D_x = 1.669 Mg m^{-3}
Mo $K\alpha$ radiation
Cell parameters from 3895 reflections
θ = 1.0–27.9°
μ = 0.72 mm^{-1}
T = 123 (2) K
Rod, colourless
0.60 × 0.20 × 0.18 mm

Data collection

Nonius KappaCCD diffractometer
ω and φ scans
Absorption correction: none
15060 measured reflections
4003 independent reflections
3176 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 27.8°
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 17$

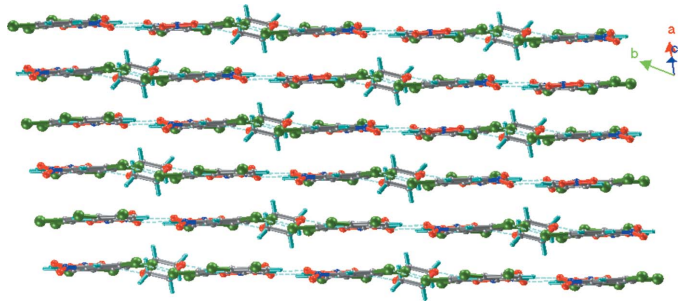


Figure 3
Packing diagram showing the stacking of the sheets.

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)]$ = 0.033
$wR(F^2)$ = 0.081
S = 1.04
4003 reflections
266 parameters
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.3147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.27 e Å^{-3}
$\Delta\rho_{min}$ = −0.28 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C12—H12···O1^{i}	0.93 (2)	2.51 (2)	3.396 (2)	158 (2)
C6—H6···O3^{ii}	0.91 (2)	2.55 (2)	3.452 (2)	169 (2)
C2—H2···O5^{iii}	0.95 (2)	2.39 (2)	3.325 (2)	168 (2)

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

The H atoms were refined without constraint. The range of C—H bond distances is 0.91 (2)–1.01 (2) Å.

Data collection: *COLLECT* (Hooft, 1988) and *DENZO* (Otwinowski & Minor, 1997); cell refinement: *DENZO* and *COLLECT*; data reduction: *DENZO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 2000) and *OLEX* (Dolomanov *et al.*, 2003); software used to prepare material for publication: *SHELXL97* and *PLATON* (Spek 2003).

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supporting information

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$F(000) = 432$
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$T = 123$ K
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3176 reflections with $I > 2\sigma(I)$
$R_{int} = 0.047$
$\theta_{max} = 27.8°$, $\theta_{min} = 1.6°$
$h = -9 \rightarrow 9$
$k = -12 \rightarrow 12$
$l = -17 \rightarrow 17$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.033$
$wR(F^2) = 0.081$
$S = 1.04$
4003 reflections
266 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
All H-atom parameters refined
$w = 1/[\sigma^2(F_o^2) + (0.0337P)^2 + 0.3147P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.27$ e Å^{-3}
$\Delta\rho_{min} = -0.28$ e Å^{-3}

Special details

Geometry. All e.s.d.'s (except the e.s.d. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell e.s.d.'s are taken into account individually in the estimation of e.s.d.'s in distances, angles and torsion angles; correlations between e.s.d.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell e.s.d.'s is used for estimating e.s.d.'s involving l.s. planes.

Refinement. Refinement of F^2 against ALL reflections. The weighted *R*-factor *wR* and 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 threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating *R*-factors(gt) *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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.62051 (7)	−0.10542 (5)	0.15631 (4)	0.02868 (12)
Cl2	0.56440 (7)	0.24589 (6)	0.01370 (3)	0.02641 (12)
O1	0.1736 (2)	0.23085 (17)	0.45702 (12)	0.0436 (4)
O2	0.3028 (2)	−0.02196 (16)	0.48900 (10)	0.0327 (3)
N1	0.2699 (2)	0.11647 (19)	0.43269 (12)	0.0258 (3)
C1	0.3486 (3)	0.1463 (2)	0.33009 (13)	0.0211 (4)
C2	0.4415 (3)	0.0186 (2)	0.29880 (14)	0.0201 (4)
C3	0.5085 (3)	0.0494 (2)	0.19999 (14)	0.0205 (4)
C4	0.4832 (3)	0.2053 (2)	0.13667 (13)	0.0212 (4)
C5	0.3906 (3)	0.3299 (2)	0.17175 (14)	0.0227 (4)
C6	0.3214 (3)	0.3016 (2)	0.26946 (15)	0.0228 (4)
Cl3	1.03628 (7)	0.29879 (5)	0.00375 (3)	0.02794 (12)
Cl4	0.81808 (7)	0.41958 (5)	0.18010 (4)	0.03230 (13)
O3	1.0807 (2)	−0.35332 (16)	0.31897 (11)	0.0339 (3)
O4	1.2726 (2)	−0.31762 (16)	0.19579 (11)	0.0366 (4)
N2	1.1469 (2)	−0.26881 (18)	0.25055 (12)	0.0263 (3)
C7	1.0699 (3)	−0.0988 (2)	0.23400 (14)	0.0219 (4)
C8	1.0946 (3)	0.0051 (2)	0.13951 (14)	0.0223 (4)
C9	1.0157 (2)	0.1663 (2)	0.12259 (14)	0.0217 (4)
C10	0.9190 (2)	0.2191 (2)	0.19974 (14)	0.0226 (4)
C11	0.8980 (3)	0.1119 (2)	0.29399 (15)	0.0238 (4)
C12	0.9717 (3)	−0.0484 (2)	0.31118 (15)	0.0240 (4)
H2	0.455 (3)	−0.085 (2)	0.3429 (16)	0.025 (5)*
H5	0.377 (3)	0.434 (3)	0.1269 (17)	0.035 (6)*
H6	0.258 (3)	0.383 (3)	0.2925 (18)	0.036 (6)*
H8	1.163 (3)	−0.033 (2)	0.0863 (15)	0.023 (5)*
H11	0.829 (3)	0.149 (2)	0.3452 (17)	0.032 (6)*
H12	0.958 (3)	−0.124 (2)	0.3727 (16)	0.027 (5)*
O5	0.4396 (2)	0.65954 (15)	0.42982 (10)	0.0309 (3)
C13	0.3659 (3)	0.6189 (2)	0.52986 (16)	0.0314 (5)
C14	0.3661 (3)	0.4539 (2)	0.56507 (18)	0.0327 (5)
H13A	0.449 (3)	0.623 (2)	0.5844 (17)	0.033 (6)*
H13B	0.235 (3)	0.696 (3)	0.5214 (16)	0.031 (6)*
H14A	0.282 (3)	0.449 (3)	0.5166 (18)	0.040 (7)*
H14B	0.324 (3)	0.424 (3)	0.6353 (18)	0.033 (6)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0340 (3)	0.0252 (2)	0.0304 (2)	−0.0106 (2)	0.00622 (19)	−0.01528 (19)

Cl2	0.0289 (2)	0.0313 (2)	0.0184 (2)	−0.0137 (2)	0.00469 (17)	−0.00619 (18)
O1	0.0620 (10)	0.0296 (8)	0.0371 (9)	−0.0138 (7)	0.0248 (8)	−0.0162 (7)
O2	0.0473 (9)	0.0254 (7)	0.0238 (7)	−0.0182 (7)	0.0092 (6)	−0.0033 (6)
N1	0.0323 (9)	0.0258 (8)	0.0216 (8)	−0.0143 (7)	0.0060 (7)	−0.0083 (7)
C1	0.0239 (9)	0.0223 (9)	0.0181 (8)	−0.0111 (7)	0.0030 (7)	−0.0061 (7)
C2	0.0232 (9)	0.0174 (9)	0.0198 (9)	−0.0098 (7)	−0.0014 (7)	−0.0042 (7)
C3	0.0209 (9)	0.0201 (9)	0.0219 (9)	−0.0085 (7)	0.0006 (7)	−0.0084 (7)
C4	0.0215 (9)	0.0265 (9)	0.0165 (8)	−0.0116 (8)	0.0014 (7)	−0.0061 (7)
C5	0.0265 (10)	0.0193 (9)	0.0216 (9)	−0.0113 (8)	−0.0001 (7)	−0.0035 (7)
C6	0.0247 (9)	0.0186 (9)	0.0245 (9)	−0.0089 (8)	0.0020 (7)	−0.0063 (8)
Cl3	0.0295 (2)	0.0232 (2)	0.0241 (2)	−0.01112 (19)	0.00357 (18)	0.00041 (18)
Cl4	0.0313 (3)	0.0179 (2)	0.0404 (3)	−0.00612 (19)	0.0082 (2)	−0.0063 (2)
O3	0.0415 (8)	0.0216 (7)	0.0356 (8)	−0.0160 (6)	0.0062 (6)	−0.0031 (6)
O4	0.0539 (9)	0.0244 (7)	0.0307 (8)	−0.0127 (7)	0.0137 (7)	−0.0128 (6)
N2	0.0340 (9)	0.0206 (8)	0.0224 (8)	−0.0118 (7)	−0.0004 (7)	−0.0040 (6)
C7	0.0230 (9)	0.0168 (9)	0.0239 (9)	−0.0082 (7)	−0.0017 (7)	−0.0038 (7)
C8	0.0201 (9)	0.0250 (9)	0.0219 (9)	−0.0096 (8)	0.0008 (7)	−0.0074 (8)
C9	0.0192 (9)	0.0212 (9)	0.0215 (9)	−0.0097 (7)	0.0004 (7)	−0.0017 (7)
C10	0.0170 (8)	0.0176 (9)	0.0284 (10)	−0.0050 (7)	0.0001 (7)	−0.0041 (7)
C11	0.0228 (9)	0.0233 (9)	0.0242 (9)	−0.0078 (8)	0.0037 (7)	−0.0084 (8)
C12	0.0237 (9)	0.0233 (9)	0.0218 (9)	−0.0105 (8)	0.0018 (7)	−0.0028 (8)
O5	0.0418 (8)	0.0180 (7)	0.0263 (7)	−0.0080 (6)	0.0038 (6)	−0.0045 (6)
C13	0.0391 (12)	0.0215 (10)	0.0288 (11)	−0.0062 (9)	0.0031 (9)	−0.0093 (8)
C14	0.0389 (12)	0.0260 (11)	0.0305 (11)	−0.0125 (9)	0.0063 (9)	−0.0074 (9)

Geometric parameters (Å, º)

Cl1—C3	1.7232 (18)	N2—C7	1.468 (2)
Cl2—C4	1.7239 (17)	C7—C12	1.383 (3)
O1—N1	1.225 (2)	C7—C8	1.389 (2)
O2—N1	1.2288 (19)	C8—C9	1.388 (3)
N1—C1	1.471 (2)	C8—H8	0.97 (2)
C1—C2	1.381 (3)	C9—C10	1.389 (3)
C1—C6	1.386 (2)	C10—C11	1.391 (2)
C2—C3	1.390 (2)	C11—C12	1.379 (3)
C2—H2	0.95 (2)	C11—H11	0.94 (2)
C3—C4	1.402 (2)	C12—H12	0.93 (2)
C4—C5	1.389 (3)	O5—C13	1.429 (2)
C5—C6	1.383 (3)	O5—C14^{i}	1.431 (2)
C5—H5	0.95 (2)	C13—C14	1.505 (3)
C6—H6	0.91 (2)	C13—H13A	1.01 (2)
Cl3—C9	1.7277 (17)	C13—H13B	0.95 (2)
Cl4—C10	1.7306 (18)	C14—O5^{i}	1.431 (2)
O3—N2	1.2290 (19)	C14—H14A	0.95 (2)
O4—N2	1.226 (2)	C14—H14B	0.98 (2)
O1—N1—O2	123.55 (16)	C8—C7—N2	118.03 (16)
O1—N1—C1	118.33 (15)	C9—C8—C7	117.93 (17)

O2—N1—C1	118.12 (15)	C9—C8—H8	120.8 (11)
C2—C1—C6	123.79 (17)	C7—C8—H8	121.2 (11)
C2—C1—N1	118.21 (15)	C8—C9—C10	120.03 (16)
C6—C1—N1	117.98 (16)	C8—C9—Cl3	118.88 (14)
C1—C2—C3	117.56 (16)	C10—C9—Cl3	121.07 (14)
C1—C2—H2	120.6 (12)	C9—C10—C11	120.66 (17)
C3—C2—H2	121.8 (12)	C9—C10—Cl4	120.86 (14)
C2—C3—C4	120.05 (16)	C11—C10—Cl4	118.47 (15)
C2—C3—Cl1	119.27 (13)	C12—C11—C10	120.06 (18)
C4—C3—Cl1	120.68 (14)	C12—C11—H11	119.6 (13)
C5—C4—C3	120.44 (16)	C10—C11—H11	120.3 (13)
C5—C4—Cl2	118.86 (13)	C11—C12—C7	118.40 (17)
C3—C4—Cl2	120.70 (14)	C11—C12—H12	122.7 (13)
C6—C5—C4	120.27 (16)	C7—C12—H12	118.9 (13)
C6—C5—H5	121.6 (14)	C13—O5—C14^{i}	109.58 (15)
C4—C5—H5	118.1 (14)	O5—C13—C14	110.90 (17)
C5—C6—C1	117.88 (18)	O5—C13—H13A	110.8 (12)
C5—C6—H6	120.7 (14)	C14—C13—H13A	108.0 (12)
C1—C6—H6	121.4 (14)	O5—C13—H13B	106.1 (12)
C9—Cl3—Cl4^{ii}	160.34 (6)	C14—C13—H13B	110.6 (13)
C10—Cl4—Cl3^{ii}	123.59 (6)	H13A—C13—H13B	110.5 (18)
N2—O4—Cl2^{iii}	146.92 (11)	O5^{i}—C14—C13	110.39 (17)
O4—N2—O3	124.17 (16)	O5^{i}—C14—H14A	108.9 (14)
O4—N2—C7	118.39 (15)	C13—C14—H14A	109.5 (13)
O3—N2—C7	117.44 (16)	O5^{i}—C14—H14B	106.7 (12)
C12—C7—C8	122.88 (17)	C13—C14—H14B	110.9 (13)
C12—C7—N2	119.06 (16)	H14A—C14—H14B	110.3 (18)

O1—N1—C1—C2	−174.18 (17)	O4—N2—C7—C8	19.4 (3)
O2—N1—C1—C2	5.1 (3)	O3—N2—C7—C8	−160.61 (17)
O1—N1—C1—C6	4.5 (3)	C12—C7—C8—C9	−0.3 (3)
O2—N1—C1—C6	−176.17 (16)	N2—C7—C8—C9	177.85 (16)
C6—C1—C2—C3	−1.0 (3)	C7—C8—C9—C10	1.2 (3)
N1—C1—C2—C3	177.61 (15)	C7—C8—C9—Cl3	−177.58 (13)
C1—C2—C3—C4	0.9 (3)	Cl4^{ii}—Cl3—C9—C8	−112.3 (2)
C1—C2—C3—Cl1	−178.56 (13)	Cl4^{ii}—Cl3—C9—C10	69.0 (3)
C2—C3—C4—C5	−0.3 (3)	C8—C9—C10—C11	−0.7 (3)
Cl1—C3—C4—C5	179.16 (14)	Cl3—C9—C10—C11	178.06 (14)
C2—C3—C4—Cl2	−179.71 (13)	C8—C9—C10—Cl4	−179.56 (14)
Cl1—C3—C4—Cl2	−0.3 (2)	Cl3—C9—C10—Cl4	−0.8 (2)
C3—C4—C5—C6	−0.3 (3)	Cl3^{ii}—Cl4—C10—C9	−21.22 (18)
Cl2—C4—C5—C6	179.12 (14)	Cl3^{ii}—Cl4—C10—C11	159.87 (12)
C4—C5—C6—C1	0.2 (3)	C9—C10—C11—C12	−0.8 (3)
C2—C1—C6—C5	0.4 (3)	Cl4—C10—C11—C12	178.15 (15)
N1—C1—C6—C5	−178.19 (16)	C10—C11—C12—C7	1.6 (3)
Cl2^{iii}—O4—N2—O3	148.84 (17)	C8—C7—C12—C11	−1.1 (3)
Cl2^{iii}—O4—N2—C7	−31.2 (3)	N2—C7—C12—C11	−179.23 (17)

O4—N2—C7—C12	−162.35 (17)	C14^{i}—O5—C13—C14	−57.9 (3)
O3—N2—C7—C12	17.6 (2)	O5—C13—C14—O5^{i}	58.4 (2)

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

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C12—H12···O1^{iv}	0.93 (2)	2.51 (2)	3.396 (2)	158.0 (17)
C6—H6···O3^{v}	0.91 (2)	2.55 (2)	3.452 (2)	168.6 (19)
C2—H2···O5^{vi}	0.95 (2)	2.39 (2)	3.325 (2)	168.4 (16)

Symmetry codes: (iv) −*x*+1, −*y*, −*z*+1; (v) *x*−1, *y*+1, *z*; (vi) *x*, *y*−1, *z*.