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Crystal structure of *N*′-[(*E*)-3,5-dichloro-2-hydroxybenzylidene]-4-nitrobenzohydrazide dimethylformamide monosolvate

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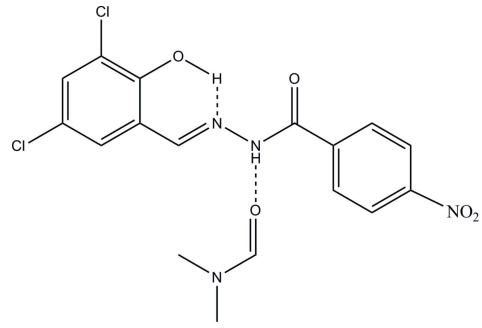
In the title compound, $C_{14}H_9Cl_2N_3O_4\cdot C_3H_7NO$, the hydrazone molecule adopts an *E* conformation with respect to azomethine bond, and the dihedral angle between the two aromatic rings [8.96 (11)°] shows that the rings are almost co-planar. The planar conformation of the molecule is stabilized by the intramolecular O—H···N hydrogen bond involving the OH group and azomethine N atom. The azomethine and keto bond distances [1.269 (2) and 1.210 (2) Å, respectively] are very close to the formal C=N and C=O bond lengths. The dimethylformamide solvent molecule is connected to the hydrazone NH group *via* an N—H···O hydrogen bond. In the crystal, non-classical C—H···O and C—H···Cl hydrogen bonds link the molecules into chains along [322]. A supramolecular three-dimensional architecture is created by weak C—Cl···π [4.163 (3) Å, 83.26 (9)°] and π–π [centroid–centroid distance = 4.0395 (14) Å] interactions.

Keywords: crystal structure; aroyl hydrazone; hydrogen bonding.

CCDC reference: 1428612

1. Related literature

For applications of hydrazones in supramolecular chemistry, see: Su & Aprahamian (2014). For biological applications of hydrazones and derivatives, see: Nair *et al.* (2014); Prasanna & Kumar (2013); Holló *et al.* (2014). For the synthesis of related compounds, see: Bessy *et al.* (2006).



2. Experimental

2.1. Crystal data

$C_{14}H_9Cl_2N_3O_4\cdot C_3H_7NO$
M_r = 427.24
Triclinic, $P\overline{1}$
a = 7.8853 (6) Å
b = 11.9445 (10) Å
c = 11.9521 (15) Å
α = 114.408 (6)°
β = 102.895 (7)°
γ = 98.939 (5)°
V = 959.60 (17) Å^3
Z = 2
Mo $K\alpha$ radiation
μ = 0.38 mm^{-1}
T = 296 K
0.40 × 0.11 × 0.09 mm

2.2. Data collection

Bruker Kappa APEXII CCD Diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.834, T_{max} = 0.929
7569 measured reflections
4660 independent reflections
3000 reflections with $I > 2\sigma(I)$
R_{int} = 0.019

2.3. Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.043
$wR(F^2)$ = 0.159
S = 0.95
4660 reflections
263 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.23 e Å^{-3}
$\Delta\rho_{min}$ = −0.19 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
O1—H1···N1	0.84 (1)	1.82 (2)	2.581 (2)	151 (3)
N2—H2···O5^{i}	0.87 (1)	1.90 (1)	2.757 (2)	169 (3)
C3—H3···Cl1^{ii}	0.93	2.92	3.836 (2)	169
C7—H7···O5^{i}	0.93	2.38	3.145 (3)	139
C13—H13···O4^{iii}	0.93	2.42	3.231 (3)	146

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2* and *SAINT* (Bruker, 2004); data reduction: *SAINT* and *XPREP* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL2014* (Sheldrick, 2015); molecular graphics: *ORTEPIII* (Burnett & Johnson, 1996); software used to prepare material for publication: *publCIF* (Westrip, 2010).

Acknowledgements

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Supporting information for this paper is available from the IUCr electronic archives (Reference: YK2106).

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supporting information

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Crystal structure of *N*′-[(*E*)-3,5-dichloro-2-hydroxybenzylidene]-4-nitrobenzohydrazide dimethylformamide monosolvate

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S1. Comment

Recent studies of hydrazones emphasis the importance of the hydrazone functional group in various fields ranging from organic synthesis and medicinal chemistry to supramolecular chemistry (Su & Aprahamian, 2014). They have growing importance because of their biological applications (Nair *et al.*, 2014; Prasanna & Kumar, 2013; Hollo *et al.*, 2014). Here we discuss the synthesis of N′-[(E)-(3,5-dichloro-2-hydroxyphenyl)methylidene]-4-nitrobenzohydrazide dimethylformamide monosolvate from 3,5-dichlorosalicylaldehyde and 4-nitrobenzoyl hydrazide. By this reaction, we obtained a novel dimethylformamide solvated aroylhydrazone in a simple condensation reaction.

The title compound, $C_{14}H_9C_{l2}N_3O_4{\cdot}C_3H_7NO$, adopts an *E* configuration with respect to C7═N1 bond (Fig. 1). The two aromatic rings of the molecule are almost in a plane with a slight twist with a dihedral angle of 8.96 (11) °. The C7═N1 and C8═O2 bond distances [1.269 (3) and 1.210 (2) Å, respectively] are very close to the formal C═N and C═O bond lengths. An intramolecular hydrogen bond is found between N1 and the H atom of the phenolic group with a D···A distance of 2.581 (2) Å. Each hydrazone molecule forms one classical intermolecular N—H···O hydrogen bond (to dimethylformamide molecule) and three non-classical C–H···O intermolecular hydrogen bonds. The pairs of non-classical C13–H···O4 interactions with D···A distance of 3.232 (3) Å (Table 1) connect molecules into centrosymmetric dimers, and these dimers are connected by means of C–H···Cl interactions into chains along [3 2 2]. The packing diagram showing all hydrogen bonds and C—Cl···π interactions viewed along *c* axis is presented in Fig. 2.

S2. Synthesis and crystallization

The title compound was prepared by adapting a reported procedure (Bessy *et al*, 2006) as described below. 3,5-Dichlorosalicylaldehyde (0.191 g, 1 mmol) and 4-nitrobenzoyl hydrazide (0.181 g, 1 mmol) were dissolved in 10 mL of DMF. The solution was heated to boiling for 15 min, cooled to room temperature and then poured to 40 mL of water containing crushed ice and 1 mL of concentrated sulfuric acid. The pale yellow colored solid product was separated, washed with DMF and dried over P_4O_{10} *in vacuo*. Single crystals of the title compound suitable for X-ray analysis were obtained by recrystallization from dimethylformamide.

S3. Refinement

All H atoms on C were placed in calculated positions, guided by difference map, with C—H bond distances of 0.93-0.96 Å. H atoms were assigned U_{iso}(H) values of 1.2Ueq(carrier). H atoms attached to N2 and O1 were located from a difference Fourier map and the bond distances are restrained to 0.88±0.01 and 0.84±0.01 Å, respectively. The reflections (0 0 1), (0 -1 1) and (0 1 0) were omitted owing to bad agreement.

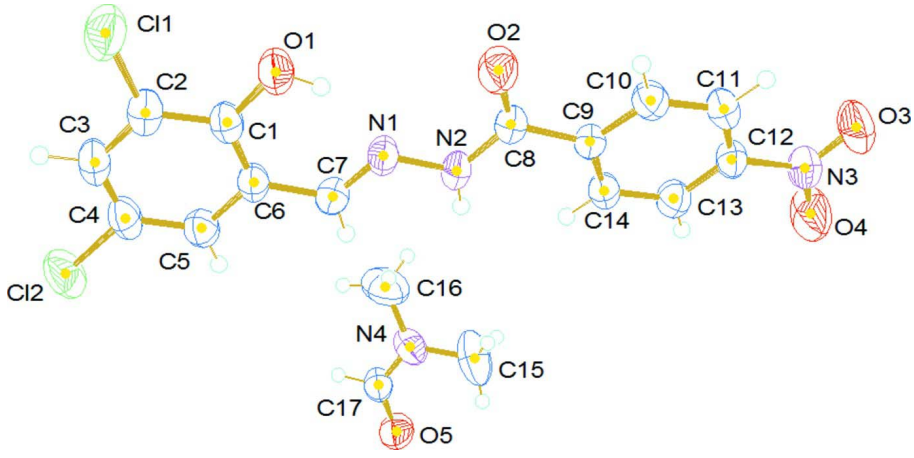

Figure 1

ORTEP view of the title compound, drawn with 50% probability displacement ellipsoids for the non-H atoms.

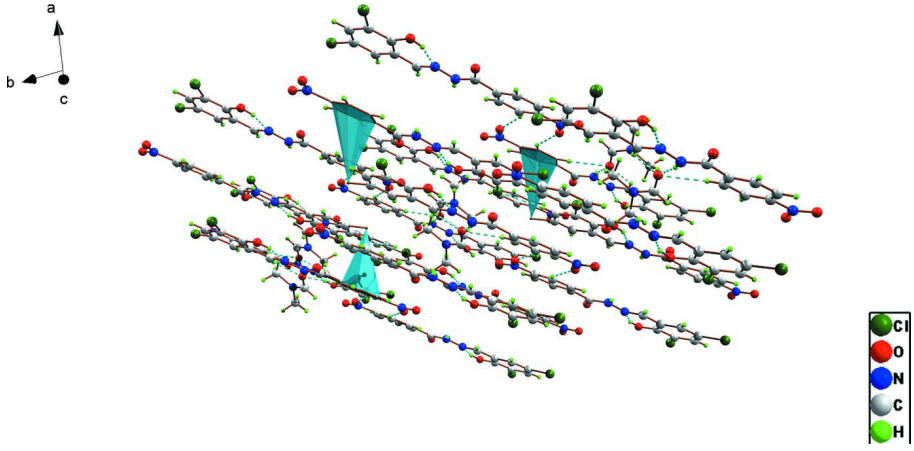

Figure 2

Diagram showing molecular packing viewed along the *c* axis along with intermolecular interactions.

N′-[(*E*)-3,5-Dichloro-2-hydroxybenzylidene]-4-nitrobenzohydrazide dimethylformamide monosolvate

Crystal data

$C_{14}H_9Cl_2N_3O_4·C_3H_7NO$
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α = 114.408 (6)°
β = 102.895 (7)°
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V = 959.60 (17) Å^3
Z = 2
F(000) = 440
D_x = 1.479 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2537 reflections
θ = 2.8–28.1°
μ = 0.38 mm^{-1}
T = 296 K
Needle, pale yellow
0.40 × 0.11 × 0.09 mm

Data collection

Bruker Kappa APEXII CCD Diffractometer
Radiation source: fine-focus sealed tube
ω and φ scan
Absorption correction: multi-scan (*SADABS*; Bruker, 2004)
T_{min} = 0.834, T_{max} = 0.929

7569 measured reflections
4660 independent reflections
3000 reflections with $I > 2\sigma(I)$
$R_{int} = 0.019$

$\theta_{max} = 28.4°$, $\theta_{min} = 2.8°$
$h = -10 \rightarrow 9$
$k = -15 \rightarrow 15$
$l = -15 \rightarrow 15$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.043$
$wR(F^2) = 0.159$
$S = 0.95$
4660 reflections
263 parameters
2 restraints

Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0998P)^2 + 0.0446P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = 0.001$
$\Delta\rho_{max} = 0.23$ e Å^{-3}
$\Delta\rho_{min} = -0.19$ 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.

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

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	1.35723 (9)	1.29047 (6)	1.47197 (6)	0.0756 (2)
Cl2	1.23273 (9)	1.51632 (6)	1.17091 (7)	0.0756 (2)
O1	1.0508 (2)	1.08266 (15)	1.27329 (15)	0.0576 (4)
O2	0.6756 (2)	0.77509 (15)	1.08867 (15)	0.0652 (4)
O3	−0.0311 (3)	0.25861 (16)	0.6472 (2)	0.0864 (6)
O4	−0.0770 (3)	0.3439 (2)	0.5227 (2)	0.0989 (7)
O5	0.4796 (2)	1.06202 (17)	0.22900 (16)	0.0668 (4)
N1	0.78454 (19)	0.97794 (15)	1.05922 (16)	0.0457 (4)
N2	0.6378 (2)	0.87905 (15)	0.96978 (16)	0.0454 (4)
N3	0.0045 (2)	0.34550 (18)	0.6219 (2)	0.0619 (5)
N4	0.5894 (3)	0.96448 (18)	0.34168 (18)	0.0616 (5)
C1	1.0866 (2)	1.18037 (18)	1.24598 (19)	0.0441 (4)
C2	1.2306 (3)	1.2870 (2)	1.3331 (2)	0.0512 (5)
C3	1.2741 (3)	1.39056 (18)	1.3111 (2)	0.0529 (5)
H3	1.3694	1.4622	1.3714	0.063*
C4	1.1756 (3)	1.38669 (19)	1.1995 (2)	0.0521 (5)
C5	1.0326 (2)	1.28330 (19)	1.1101 (2)	0.0489 (5)
H5	0.9675	1.2824	1.0344	0.059*
C6	0.9853 (2)	1.17920 (17)	1.13350 (19)	0.0426 (4)
C7	0.8316 (2)	1.07285 (19)	1.03936 (19)	0.0464 (4)
H7	0.7673	1.0738	0.9645	0.056*
C8	0.5925 (2)	0.77882 (18)	0.99269 (18)	0.0428 (4)
C9	0.4325 (2)	0.67029 (17)	0.89195 (18)	0.0397 (4)
C10	0.3727 (3)	0.57541 (19)	0.9227 (2)	0.0496 (5)
H10	0.4276	0.5841	1.0044	0.060*
C11	0.2333 (3)	0.4681 (2)	0.8348 (2)	0.0548 (5)

H11	0.1944	0.4034	0.8551	0.066*
C12	0.1536 (2)	0.45939 (18)	0.7164 (2)	0.0470 (4)
C13	0.2077 (3)	0.5529 (2)	0.6837 (2)	0.0507 (5)
H13	0.1497	0.5449	0.6029	0.061*
C14	0.3485 (2)	0.65882 (19)	0.77184 (19)	0.0456 (4)
H14	0.3873	0.7228	0.7506	0.055*
C15	0.4196 (5)	0.8698 (3)	0.2961 (4)	0.1047 (11)
H15A	0.3223	0.9022	0.2699	0.157*
H15B	0.4052	0.8506	0.3645	0.157*
H15C	0.4177	0.7934	0.2236	0.157*
C16	0.7510 (5)	0.9501 (3)	0.4148 (3)	0.0998 (10)
H16A	0.7692	0.8691	0.3641	0.150*
H16B	0.7365	0.9538	0.4938	0.150*
H16C	0.8541	1.0179	0.4349	0.150*
C17	0.6030 (3)	1.0510 (2)	0.3016 (2)	0.0531 (5)
H17	0.7162	1.1087	0.3310	0.064*
H2	0.589 (3)	0.888 (2)	0.9019 (17)	0.072 (8)*
H1	0.962 (3)	1.028 (2)	1.2106 (19)	0.090 (9)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0735 (4)	0.0650 (4)	0.0560 (3)	−0.0053 (3)	−0.0032 (3)	0.0191 (3)
Cl2	0.0772 (4)	0.0489 (3)	0.1074 (5)	0.0066 (3)	0.0394 (4)	0.0413 (4)
O1	0.0540 (8)	0.0471 (9)	0.0590 (9)	−0.0035 (7)	0.0066 (7)	0.0249 (8)
O2	0.0644 (9)	0.0599 (10)	0.0530 (9)	−0.0038 (7)	−0.0047 (7)	0.0286 (8)
O3	0.0830 (12)	0.0449 (10)	0.1029 (15)	−0.0120 (8)	0.0080 (11)	0.0295 (10)
O4	0.0887 (13)	0.0704 (12)	0.0839 (13)	−0.0243 (10)	−0.0282 (10)	0.0310 (11)
O5	0.0629 (9)	0.0687 (11)	0.0651 (10)	0.0103 (8)	0.0063 (8)	0.0375 (9)
N1	0.0368 (8)	0.0370 (8)	0.0492 (9)	0.0012 (6)	0.0089 (7)	0.0128 (7)
N2	0.0367 (8)	0.0378 (8)	0.0467 (9)	−0.0013 (6)	0.0027 (7)	0.0152 (8)
N3	0.0514 (10)	0.0408 (10)	0.0705 (13)	−0.0025 (8)	0.0058 (9)	0.0171 (9)
N4	0.0783 (12)	0.0453 (10)	0.0564 (11)	0.0101 (9)	0.0138 (9)	0.0257 (9)
C1	0.0418 (9)	0.0370 (10)	0.0489 (11)	0.0042 (7)	0.0173 (8)	0.0169 (9)
C2	0.0449 (10)	0.0446 (11)	0.0487 (11)	0.0018 (8)	0.0140 (9)	0.0119 (9)
C3	0.0440 (10)	0.0368 (11)	0.0579 (12)	−0.0015 (8)	0.0172 (9)	0.0078 (10)
C4	0.0468 (10)	0.0365 (10)	0.0702 (14)	0.0055 (8)	0.0282 (10)	0.0197 (10)
C5	0.0441 (10)	0.0433 (11)	0.0584 (12)	0.0096 (8)	0.0187 (9)	0.0228 (10)
C6	0.0363 (8)	0.0342 (9)	0.0487 (10)	0.0052 (7)	0.0155 (8)	0.0122 (8)
C7	0.0389 (9)	0.0423 (11)	0.0495 (11)	0.0074 (8)	0.0094 (8)	0.0174 (9)
C8	0.0372 (9)	0.0391 (10)	0.0424 (10)	0.0035 (7)	0.0080 (7)	0.0150 (8)
C9	0.0349 (8)	0.0351 (9)	0.0441 (9)	0.0061 (7)	0.0098 (7)	0.0165 (8)
C10	0.0497 (10)	0.0467 (11)	0.0499 (11)	0.0057 (8)	0.0082 (9)	0.0267 (10)
C11	0.0526 (11)	0.0412 (11)	0.0673 (13)	0.0016 (8)	0.0121 (10)	0.0298 (11)
C12	0.0399 (9)	0.0345 (10)	0.0540 (11)	0.0019 (7)	0.0092 (8)	0.0149 (9)
C13	0.0478 (10)	0.0463 (11)	0.0484 (11)	0.0042 (8)	0.0053 (9)	0.0214 (9)
C14	0.0424 (9)	0.0399 (10)	0.0507 (11)	0.0031 (8)	0.0093 (8)	0.0232 (9)
C15	0.121 (3)	0.072 (2)	0.111 (2)	−0.0127 (17)	0.039 (2)	0.0468 (19)

C16	0.128 (3)	0.086 (2)	0.0810 (19)	0.041 (2)	0.0054 (18)	0.0460 (18)
C17	0.0537 (11)	0.0449 (11)	0.0524 (12)	0.0040 (9)	0.0108 (9)	0.0216 (10)

Geometric parameters (Å, º)

Cl1—C2	1.716 (2)	C5—C6	1.397 (3)
Cl2—C4	1.734 (2)	C5—H5	0.9300
O1—C1	1.342 (2)	C6—C7	1.442 (3)
O1—H1	0.835 (10)	C7—H7	0.9300
O2—C8	1.210 (2)	C8—C9	1.498 (2)
O3—N3	1.206 (2)	C9—C10	1.378 (3)
O4—N3	1.207 (3)	C9—C14	1.380 (3)
O5—C17	1.214 (2)	C10—C11	1.375 (3)
N1—C7	1.269 (2)	C10—H10	0.9300
N1—N2	1.363 (2)	C11—C12	1.367 (3)
N2—C8	1.348 (2)	C11—H11	0.9300
N2—H2	0.872 (10)	C12—C13	1.367 (3)
N3—C12	1.466 (3)	C13—C14	1.372 (3)
N4—C17	1.306 (3)	C13—H13	0.9300
N4—C15	1.437 (3)	C14—H14	0.9300
N4—C16	1.454 (3)	C15—H15A	0.9600
C1—C2	1.386 (3)	C15—H15B	0.9600
C1—C6	1.396 (3)	C15—H15C	0.9600
C2—C3	1.376 (3)	C16—H16A	0.9600
C3—C4	1.363 (3)	C16—H16B	0.9600
C3—H3	0.9300	C16—H16C	0.9600
C4—C5	1.370 (3)	C17—H17	0.9300
C1—O1—H1	105 (2)	N2—C8—C9	116.40 (16)
C7—N1—N2	118.71 (16)	C10—C9—C14	119.48 (17)
C8—N2—N1	117.36 (15)	C10—C9—C8	116.28 (16)
C8—N2—H2	128.4 (18)	C14—C9—C8	124.20 (16)
N1—N2—H2	114.1 (18)	C11—C10—C9	121.12 (18)
O3—N3—O4	123.3 (2)	C11—C10—H10	119.4
O3—N3—C12	118.6 (2)	C9—C10—H10	119.4
O4—N3—C12	118.07 (19)	C12—C11—C10	117.92 (18)
C17—N4—C15	120.0 (2)	C12—C11—H11	121.0
C17—N4—C16	120.2 (2)	C10—C11—H11	121.0
C15—N4—C16	119.0 (2)	C13—C12—C11	122.36 (18)
O1—C1—C2	118.66 (18)	C13—C12—N3	119.26 (19)
O1—C1—C6	122.82 (16)	C11—C12—N3	118.38 (18)
C2—C1—C6	118.52 (17)	C12—C13—C14	119.15 (18)
C3—C2—C1	121.57 (19)	C12—C13—H13	120.4
C3—C2—Cl1	119.12 (16)	C14—C13—H13	120.4
C1—C2—Cl1	119.31 (16)	C13—C14—C9	119.95 (17)
C4—C3—C2	119.06 (18)	C13—C14—H14	120.0
C4—C3—H3	120.5	C9—C14—H14	120.0
C2—C3—H3	120.5	N4—C15—H15A	109.5

C3—C4—C5	121.61 (19)	N4—C15—H15B	109.5
C3—C4—Cl2	119.00 (16)	H15A—C15—H15B	109.5
C5—C4—Cl2	119.39 (18)	N4—C15—H15C	109.5
C4—C5—C6	119.5 (2)	H15A—C15—H15C	109.5
C4—C5—H5	120.2	H15B—C15—H15C	109.5
C6—C5—H5	120.2	N4—C16—H16A	109.5
C1—C6—C5	119.70 (17)	N4—C16—H16B	109.5
C1—C6—C7	121.85 (16)	H16A—C16—H16B	109.5
C5—C6—C7	118.44 (18)	N4—C16—H16C	109.5
N1—C7—C6	119.61 (18)	H16A—C16—H16C	109.5
N1—C7—H7	120.2	H16B—C16—H16C	109.5
C6—C7—H7	120.2	O5—C17—N4	125.3 (2)
O2—C8—N2	122.52 (17)	O5—C17—H17	117.4
O2—C8—C9	121.07 (17)	N4—C17—H17	117.4

C7—N1—N2—C8	179.15 (17)	N1—N2—C8—C9	−179.03 (15)
O1—C1—C2—C3	−179.80 (17)	O2—C8—C9—C10	8.0 (3)
C6—C1—C2—C3	0.3 (3)	N2—C8—C9—C10	−172.24 (16)
O1—C1—C2—Cl1	0.0 (3)	O2—C8—C9—C14	−169.75 (19)
C6—C1—C2—Cl1	−179.94 (14)	N2—C8—C9—C14	10.0 (3)
C1—C2—C3—C4	−1.5 (3)	C14—C9—C10—C11	1.4 (3)
Cl1—C2—C3—C4	178.75 (15)	C8—C9—C10—C11	−176.44 (18)
C2—C3—C4—C5	1.2 (3)	C9—C10—C11—C12	−1.1 (3)
C2—C3—C4—Cl2	−179.09 (15)	C10—C11—C12—C13	−0.1 (3)
C3—C4—C5—C6	0.3 (3)	C10—C11—C12—N3	−179.89 (18)
Cl2—C4—C5—C6	−179.43 (13)	O3—N3—C12—C13	173.37 (19)
O1—C1—C6—C5	−178.71 (16)	O4—N3—C12—C13	−7.0 (3)
C2—C1—C6—C5	1.2 (3)	O3—N3—C12—C11	−6.8 (3)
O1—C1—C6—C7	1.2 (3)	O4—N3—C12—C11	172.8 (2)
C2—C1—C6—C7	−178.87 (18)	C11—C12—C13—C14	0.9 (3)
C4—C5—C6—C1	−1.5 (3)	N3—C12—C13—C14	−179.30 (18)
C4—C5—C6—C7	178.56 (17)	C12—C13—C14—C9	−0.5 (3)
N2—N1—C7—C6	179.29 (15)	C10—C9—C14—C13	−0.6 (3)
C1—C6—C7—N1	1.0 (3)	C8—C9—C14—C13	177.11 (18)
C5—C6—C7—N1	−179.11 (16)	C15—N4—C17—O5	2.2 (4)
N1—N2—C8—O2	0.7 (3)	C16—N4—C17—O5	172.0 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O5^{i}	0.87 (1)	1.90 (1)	2.757 (2)	169 (3)
C3—H3···Cl1^{ii}	0.93	2.92	3.836 (2)	169
C7—H7···O5^{i}	0.93	2.38	3.145 (3)	139
C13—H13···O4^{iii}	0.93	2.42	3.231 (3)	146
O1—H1···N1	0.84 (1)	1.82 (2)	2.581 (2)	151 (3)

Symmetry codes: (i) −*x*+1, −*y*+2, −*z*+1; (ii) −*x*+3, −*y*+3, −*z*+3; (iii) −*x*, −*y*+1, −*z*+1.