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Ethyl (*E*)-2-(4-chlorobenzylidene)-hydrazinecarboxylate

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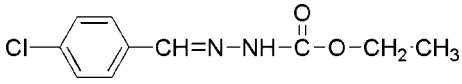
Key indicators: single-crystal X-ray study; T = 193 K; mean σ(C–C) = 0.003 Å; R factor = 0.049; wR factor = 0.111; data-to-parameter ratio = 14.6.

The title compound, $C_{10}H_{11}ClN_2O_2$, crystallizes with two independent, but essentially identical molecules in the asymmetric unit. Each planar molecule is in the *E* configuration about the C=N bond. Intermolecular N—H···O hydrogen bonds link molecules into a one-dimensional chain aligned along the [101] direction.

Related literature

For general background, see: Hu *et al.* (2005). For related structures, see: Meng *et al.* (2007); Shi (2005).



Experimental

Crystal data

$C_{10}H_{11}ClN_2O_2$
M_r = 226.66
Monoclinic, $P2_1/n$
a = 16.317 (4) Å
b = 8.3488 (16) Å
c = 18.035 (4) Å
β = 116.014 (4)°
V = 2207.9 (8) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.33 mm^{-1}
T = 193 (2) K
0.60 × 0.58 × 0.34 mm

Data collection

Rigaku Mercury diffractometer
Absorption correction: multi-scan (Jacobson, 1998)
T_{min} = 0.815, T_{max} = 0.895
20629 measured reflections
4011 independent reflections
3479 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.111
S = 1.16
4011 reflections
274 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.18 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
N4—H4···O1^{i}	0.88	2.08	2.869 (2)	149
N2—H2A···O3	0.88	2.06	2.905 (2)	160

Symmetry code: (i) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$.

Data collection: *CrystalClear* (Rigaku, 2001); cell refinement: *CrystalClear*; data reduction: *CrystalStructure* (Rigaku/MSC, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *SHELXTL* (Bruker, 1998); software used to prepare material for publication: *SHELXTL*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: TK2199).

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  doi:10.1107/S1600536807051410

supplementary materials

Acta Cryst. (2007). E**63**, o4418 [**doi:10.1107/S1600536807051410**]

Ethyl (*E*)-2-(4-chlorobenzylidene)hydrazinecarboxylate

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Comment

Chlorobenzaldehydehydrazone derivatives are important intermediates in the synthesis of 1,4-dihydrotetrazines, which demonstrate anti-tumour activity (Hu *et al.*, 2005). A representative crystal structure, namely methyl (*E*)-2-(4-chlorobenzylidene)hydrazinecarboxylate has been reported recently (Meng *et al.*, 2007). Herein, the crystal structure of the title compound, $C_{10}H_{11}ClN_3O_2$ (I), is described.

Compound (I) crystallizes with two chemically equivalent but crystallographically independent molecules in the asymmetric unit (Fig. 1). Each essentially planar molecule is in an E-conformation with respect to the N=C double bond. The bond lengths and angles defining the C=N—N(H)—C groups are close to those of the reported literature (Shi, 2005).

Intermolecular N—H···O hydrogen bonds (Table 1) serve to link molecules into a 1-D chain aligned along the (101) direction (Fig. 2).

Experimental

4-Chlorobenzaldehyde (7 g, 0.1 mol) and ethyl hydrazinecarboxylate (5.2 g 0.05 mol) were dissolved in a stirred methanol (50 ml) solution and left to stand for 3 h at room temperature. The resulting solid was filtered off and recrystallized from an ethanol solution to yield (I) in 80% yield. Crystals suitable for X-ray analysis were obtained by the slow evaporation of an ethanol solution of (I) held at room temperature; m.p. 463–465 K.

Refinement

The H atoms were included in the riding model approximation with N—H = 0.88 Å and C—H = 0.95–0.99 Å, and with U_{iso}(H) = 1.2–1.5U_{eq}(N, C).

Figures

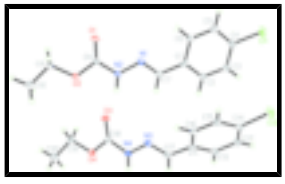

Fig. 1. Molecular structures of the two independent molecules in (I), showing 20% probability displacement ellipsoids and atom numbering.

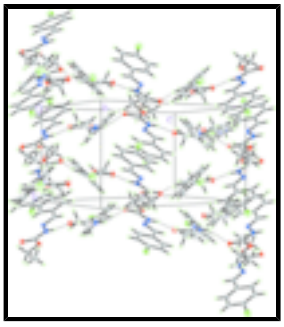

Fig. 2. The crystal packing in (I), viewed approximately down the *a* axis. Dashed lines indicate intermolecular N—H···O hydrogen bonds.

Ethyl (*E*)-2-(4-chlorobenzylidene)hydrazinecarboxylate

Crystal data

$C_{10}H_{11}ClN_2O_2$	F_{000} = 944
M_r = 226.66	D_x = 1.364 Mg m^{-3}
Monoclinic, $P2_1/n$	Mo $K\alpha$ radiation λ = 0.71070 Å
Hall symbol: -P 2yn	Cell parameters from 7392 reflections
a = 16.317 (4) Å	θ = 3.3–25.3º
b = 8.3488 (16) Å	μ = 0.33 mm^{-1}
c = 18.035 (4) Å	T = 193 (2) K
β = 116.014 (4)º	Block, colourless
V = 2207.9 (8) Å^3	0.60 × 0.58 × 0.34 mm
Z = 8	

Data collection

Rigaku Mercury diffractometer	4011 independent reflections
Radiation source: fine-focus sealed tube	3479 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 193(2) K	θ_{max} = 25.4º
ω scans	θ_{min} = 3.3º
Absorption correction: multi-scan (Jacobson, 1998)	h = −19→19
T_{min} = 0.815, T_{max} = 0.895	k = −10→10
20629 measured reflections	l = −19→21

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	Hydrogen site location: inferred from neighbouring sites
$R[F^2 > 2\sigma(F^2)]$ = 0.049	H-atom parameters constrained
$wR(F^2)$ = 0.111	$w = 1/[\sigma^2(F_o^2) + (0.0427P)^2 + 0.8029P]$ where $P = (F_o^2 + 2F_c^2)/3$

S = 1.16	$(\Delta/\sigma)_{max}$ = 0.001
4011 reflections	$\Delta\rho_{max}$ = 0.18 e Å^{-3}
274 parameters	$\Delta\rho_{min}$ = −0.28 e Å^{-3}
Primary atom site location: structure-invariant direct methods	Extinction correction: none

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cl1	0.25050 (5)	0.58597 (9)	0.64513 (4)	0.0635 (2)
Cl2	0.45783 (5)	0.27646 (10)	0.86369 (4)	0.0694 (2)
O1	0.51197 (9)	0.07441 (18)	0.36647 (8)	0.0386 (4)
O2	0.66600 (9)	0.06493 (19)	0.42539 (8)	0.0406 (4)
O3	0.78957 (10)	0.28077 (19)	0.58583 (9)	0.0439 (4)
O4	0.94280 (9)	0.30084 (18)	0.65519 (8)	0.0399 (4)
N1	0.52594 (11)	0.2415 (2)	0.50250 (10)	0.0335 (4)
N2	0.60003 (11)	0.1871 (2)	0.49262 (10)	0.0356 (4)
H2A	0.6558	0.2044	0.5309	0.043*
N3	0.78486 (11)	0.2701 (2)	0.73588 (10)	0.0344 (4)
N4	0.86403 (11)	0.2841 (2)	0.72690 (10)	0.0355 (4)
H4	0.9173	0.2903	0.7704	0.043*
C1	0.47229 (13)	0.3898 (2)	0.58521 (12)	0.0324 (5)
C2	0.49353 (14)	0.4774 (3)	0.65635 (12)	0.0372 (5)
H2B	0.5557	0.4960	0.6930	0.045*
C3	0.42629 (15)	0.5386 (3)	0.67540 (13)	0.0421 (5)
H3	0.4419	0.5977	0.7248	0.051*
C4	0.33623 (15)	0.5122 (3)	0.62145 (13)	0.0410 (5)
C5	0.31250 (15)	0.4279 (3)	0.54926 (14)	0.0439 (5)
H5	0.2502	0.4120	0.5123	0.053*
C6	0.38014 (14)	0.3673 (3)	0.53144 (13)	0.0394 (5)
H6	0.3640	0.3090	0.4817	0.047*
C7	0.54462 (14)	0.3241 (2)	0.56740 (12)	0.0348 (5)
H7	0.6065	0.3431	0.6047	0.042*
C8	0.58569 (13)	0.1065 (2)	0.42305 (12)	0.0334 (5)
C9	0.66132 (15)	−0.0179 (3)	0.35306 (13)	0.0456 (6)
H9A	0.6314	0.0506	0.3036	0.055*

H9B	0.6256	−0.1180	0.3440	0.055*
C10	0.75707 (17)	−0.0554 (4)	0.36796 (16)	0.0643 (8)
H10A	0.7922	0.0442	0.3785	0.096*
H10B	0.7564	−0.1086	0.3193	0.096*
H10C	0.7852	−0.1263	0.4159	0.096*
C11	0.71148 (13)	0.2927 (2)	0.82341 (12)	0.0323 (5)
C12	0.70356 (15)	0.3895 (3)	0.88275 (13)	0.0415 (5)
H12	0.7520	0.4600	0.9147	0.050*
C13	0.62641 (16)	0.3846 (3)	0.89583 (13)	0.0452 (6)
H13	0.6210	0.4527	0.9356	0.054*
C14	0.55750 (15)	0.2798 (3)	0.85064 (13)	0.0420 (5)
C15	0.56525 (15)	0.1782 (3)	0.79387 (13)	0.0404 (5)
H15	0.5182	0.1033	0.7646	0.049*
C16	0.64155 (14)	0.1859 (3)	0.77987 (13)	0.0360 (5)
H16	0.6464	0.1174	0.7400	0.043*
C17	0.79131 (14)	0.3070 (2)	0.80711 (13)	0.0364 (5)
H17	0.8477	0.3436	0.8491	0.044*
C18	0.85828 (13)	0.2881 (2)	0.64994 (12)	0.0342 (5)
C19	0.94907 (16)	0.3227 (3)	0.57822 (14)	0.0495 (6)
H19A	0.9280	0.4313	0.5559	0.059*
H19B	0.9106	0.2430	0.5370	0.059*
C20	1.04581 (19)	0.3012 (5)	0.59608 (18)	0.0784 (10)
H20A	1.0833	0.3787	0.6381	0.118*
H20B	1.0531	0.3184	0.5456	0.118*
H20C	1.0652	0.1922	0.6164	0.118*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0598 (4)	0.0750 (5)	0.0709 (4)	0.0098 (3)	0.0425 (4)	−0.0035 (3)
Cl2	0.0548 (4)	0.0933 (6)	0.0770 (5)	0.0089 (4)	0.0444 (4)	0.0090 (4)
O1	0.0262 (8)	0.0470 (9)	0.0341 (8)	0.0033 (6)	0.0054 (6)	−0.0007 (7)
O2	0.0273 (7)	0.0576 (10)	0.0337 (8)	0.0065 (7)	0.0105 (6)	−0.0048 (7)
O3	0.0292 (8)	0.0578 (10)	0.0349 (8)	−0.0052 (7)	0.0049 (7)	0.0003 (7)
O4	0.0271 (8)	0.0544 (10)	0.0362 (8)	0.0003 (7)	0.0119 (6)	0.0004 (7)
N1	0.0278 (9)	0.0369 (10)	0.0332 (9)	0.0025 (7)	0.0110 (7)	0.0022 (8)
N2	0.0222 (8)	0.0480 (11)	0.0309 (9)	0.0025 (8)	0.0065 (7)	−0.0023 (8)
N3	0.0256 (9)	0.0348 (10)	0.0391 (10)	−0.0003 (7)	0.0108 (7)	0.0035 (8)
N4	0.0236 (9)	0.0441 (11)	0.0337 (10)	−0.0005 (7)	0.0076 (7)	0.0030 (8)
C1	0.0319 (11)	0.0303 (11)	0.0326 (11)	−0.0002 (9)	0.0120 (9)	0.0034 (9)
C2	0.0355 (11)	0.0365 (12)	0.0332 (11)	−0.0007 (9)	0.0092 (9)	−0.0003 (9)
C3	0.0510 (14)	0.0383 (12)	0.0353 (12)	0.0012 (10)	0.0174 (10)	−0.0024 (10)
C4	0.0439 (13)	0.0397 (12)	0.0443 (13)	0.0059 (10)	0.0239 (11)	0.0053 (10)
C5	0.0328 (12)	0.0509 (14)	0.0458 (13)	−0.0012 (10)	0.0152 (10)	−0.0011 (11)
C6	0.0356 (12)	0.0455 (13)	0.0336 (11)	−0.0016 (10)	0.0119 (9)	−0.0050 (10)
C7	0.0291 (11)	0.0370 (12)	0.0320 (11)	−0.0009 (9)	0.0077 (9)	0.0029 (9)
C8	0.0275 (11)	0.0364 (11)	0.0330 (11)	0.0041 (9)	0.0102 (9)	0.0055 (9)
C9	0.0393 (13)	0.0608 (15)	0.0342 (12)	0.0097 (11)	0.0140 (10)	−0.0017 (11)

C10	0.0471 (15)	0.095 (2)	0.0555 (16)	0.0135 (14)	0.0271 (13)	−0.0069 (15)
C11	0.0288 (10)	0.0314 (11)	0.0312 (10)	0.0001 (9)	0.0080 (8)	0.0035 (9)
C12	0.0407 (12)	0.0396 (13)	0.0348 (11)	−0.0039 (10)	0.0078 (10)	−0.0029 (10)
C13	0.0535 (14)	0.0468 (14)	0.0364 (12)	0.0077 (11)	0.0206 (11)	−0.0016 (10)
C14	0.0378 (12)	0.0498 (14)	0.0420 (12)	0.0069 (10)	0.0206 (10)	0.0090 (11)
C15	0.0340 (12)	0.0414 (13)	0.0436 (12)	−0.0045 (10)	0.0149 (10)	0.0019 (10)
C16	0.0343 (11)	0.0341 (12)	0.0376 (11)	−0.0012 (9)	0.0140 (9)	0.0000 (9)
C17	0.0300 (11)	0.0365 (12)	0.0350 (12)	−0.0032 (9)	0.0072 (9)	0.0020 (9)
C18	0.0262 (11)	0.0328 (11)	0.0378 (12)	0.0005 (8)	0.0087 (9)	0.0012 (9)
C19	0.0460 (14)	0.0630 (16)	0.0424 (13)	−0.0040 (12)	0.0221 (11)	0.0002 (11)
C20	0.0536 (17)	0.128 (3)	0.0668 (18)	0.0082 (18)	0.0388 (15)	0.0068 (18)

Geometric parameters (Å, °)

Cl1—C4	1.744 (2)	C6—H6	0.9500
Cl2—C14	1.743 (2)	C7—H7	0.9500
O1—C8	1.218 (2)	C9—C10	1.498 (3)
O2—C8	1.338 (2)	C9—H9A	0.9900
O2—C9	1.449 (3)	C9—H9B	0.9900
O3—C18	1.209 (2)	C10—H10A	0.9800
O4—C18	1.344 (2)	C10—H10B	0.9800
O4—C19	1.447 (3)	C10—H10C	0.9800
N1—C7	1.275 (3)	C11—C16	1.388 (3)
N1—N2	1.374 (2)	C11—C12	1.392 (3)
N2—C8	1.350 (3)	C11—C17	1.460 (3)
N2—H2A	0.8800	C12—C13	1.379 (3)
N3—C17	1.280 (3)	C12—H12	0.9500
N3—N4	1.376 (2)	C13—C14	1.375 (3)
N4—C18	1.350 (3)	C13—H13	0.9500
N4—H4	0.8800	C14—C15	1.377 (3)
C1—C2	1.383 (3)	C15—C16	1.376 (3)
C1—C6	1.399 (3)	C15—H15	0.9500
C1—C7	1.459 (3)	C16—H16	0.9500
C2—C3	1.383 (3)	C17—H17	0.9500
C2—H2B	0.9500	C19—C20	1.477 (3)
C3—C4	1.378 (3)	C19—H19A	0.9900
C3—H3	0.9500	C19—H19B	0.9900
C4—C5	1.378 (3)	C20—H20A	0.9800
C5—C6	1.374 (3)	C20—H20B	0.9800
C5—H5	0.9500	C20—H20C	0.9800
C8—O2—C9	115.55 (15)	C9—C10—H10B	109.5
C18—O4—C19	116.37 (16)	H10A—C10—H10B	109.5
C7—N1—N2	115.36 (16)	C9—C10—H10C	109.5
C8—N2—N1	118.78 (16)	H10A—C10—H10C	109.5
C8—N2—H2A	120.6	H10B—C10—H10C	109.5
N1—N2—H2A	120.6	C16—C11—C12	118.5 (2)
C17—N3—N4	115.44 (16)	C16—C11—C17	121.55 (19)
C18—N4—N3	118.54 (16)	C12—C11—C17	119.93 (18)
C18—N4—H4	120.7	C13—C12—C11	120.9 (2)

N3—N4—H4	120.7	C13—C12—H12	119.5
C2—C1—C6	118.04 (19)	C11—C12—H12	119.5
C2—C1—C7	120.36 (18)	C14—C13—C12	119.2 (2)
C6—C1—C7	121.60 (19)	C14—C13—H13	120.4
C1—C2—C3	121.51 (19)	C12—C13—H13	120.4
C1—C2—H2B	119.2	C13—C14—C15	121.0 (2)
C3—C2—H2B	119.2	C13—C14—Cl2	119.94 (18)
C4—C3—C2	118.8 (2)	C15—C14—Cl2	119.08 (18)
C4—C3—H3	120.6	C16—C15—C14	119.5 (2)
C2—C3—H3	120.6	C16—C15—H15	120.2
C5—C4—C3	121.3 (2)	C14—C15—H15	120.2
C5—C4—Cl1	119.24 (17)	C15—C16—C11	120.8 (2)
C3—C4—Cl1	119.46 (17)	C15—C16—H16	119.6
C6—C5—C4	119.2 (2)	C11—C16—H16	119.6
C6—C5—H5	120.4	N3—C17—C11	119.62 (18)
C4—C5—H5	120.4	N3—C17—H17	120.2
C5—C6—C1	121.2 (2)	C11—C17—H17	120.2
C5—C6—H6	119.4	O3—C18—O4	124.32 (19)
C1—C6—H6	119.4	O3—C18—N4	126.83 (19)
N1—C7—C1	120.97 (18)	O4—C18—N4	108.85 (16)
N1—C7—H7	119.5	O4—C19—C20	107.08 (19)
C1—C7—H7	119.5	O4—C19—H19A	110.3
O1—C8—O2	124.26 (19)	C20—C19—H19A	110.3
O1—C8—N2	126.37 (18)	O4—C19—H19B	110.3
O2—C8—N2	109.37 (16)	C20—C19—H19B	110.3
O2—C9—C10	107.41 (18)	H19A—C19—H19B	108.6
O2—C9—H9A	110.2	C19—C20—H20A	109.5
C10—C9—H9A	110.2	C19—C20—H20B	109.5
O2—C9—H9B	110.2	H20A—C20—H20B	109.5
C10—C9—H9B	110.2	C19—C20—H20C	109.5
H9A—C9—H9B	108.5	H20A—C20—H20C	109.5
C9—C10—H10A	109.5	H20B—C20—H20C	109.5
C7—N1—N2—C8	−176.30 (18)	C8—O2—C9—C10	−179.4 (2)
C17—N3—N4—C18	−163.06 (19)	C16—C11—C12—C13	−2.6 (3)
C6—C1—C2—C3	1.4 (3)	C17—C11—C12—C13	176.24 (19)
C7—C1—C2—C3	−178.84 (19)	C11—C12—C13—C14	1.4 (3)
C1—C2—C3—C4	−0.6 (3)	C12—C13—C14—C15	1.2 (3)
C2—C3—C4—C5	−0.6 (3)	C12—C13—C14—Cl2	−177.80 (17)
C2—C3—C4—Cl1	179.09 (17)	C13—C14—C15—C16	−2.5 (3)
C3—C4—C5—C6	0.9 (3)	Cl2—C14—C15—C16	176.50 (16)
Cl1—C4—C5—C6	−178.77 (17)	C14—C15—C16—C11	1.2 (3)
C4—C5—C6—C1	0.0 (3)	C12—C11—C16—C15	1.3 (3)
C2—C1—C6—C5	−1.1 (3)	C17—C11—C16—C15	−177.55 (19)
C7—C1—C6—C5	179.2 (2)	N4—N3—C17—C11	−178.62 (17)
N2—N1—C7—C1	179.72 (17)	C16—C11—C17—N3	25.9 (3)
C2—C1—C7—N1	179.19 (19)	C12—C11—C17—N3	−152.9 (2)
C6—C1—C7—N1	−1.1 (3)	C19—O4—C18—O3	6.3 (3)
C9—O2—C8—O1	2.5 (3)	C19—O4—C18—N4	−174.11 (18)
C9—O2—C8—N2	−177.92 (18)	N3—N4—C18—O3	0.1 (3)

N1—N2—C8—O1	−0.7 (3)	N3—N4—C18—O4	−179.55 (16)
N1—N2—C8—O2	179.73 (16)	C18—O4—C19—C20	−168.9 (2)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N4—H4···O1^{i}	0.88	2.08	2.869 (2)	149
N2—H2A···O3	0.88	2.06	2.905 (2)	160

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

Fig. 1

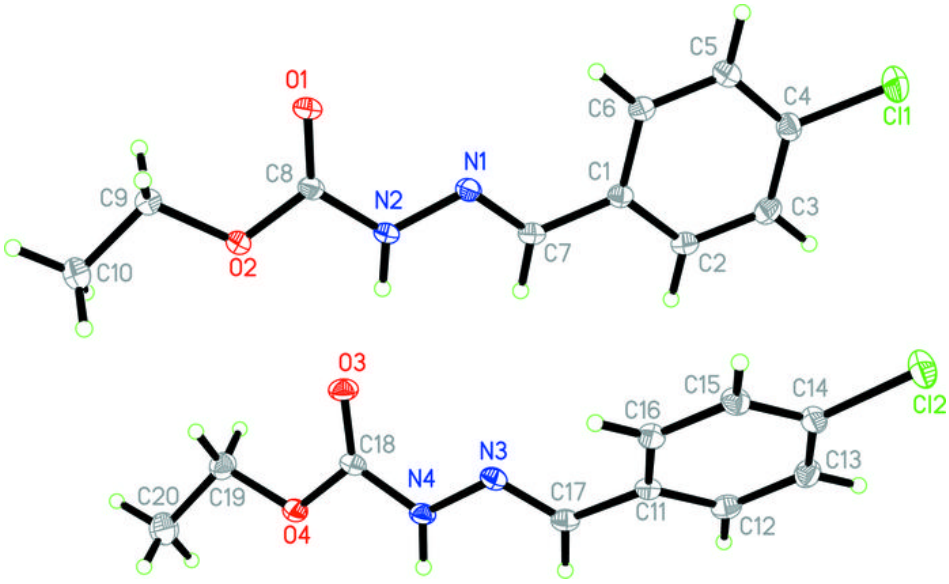
O1
C8
N2
N1
C1
C5
C6
C4
Cl1
C9
C3
C10
O2
C7
C2
O3
C15
C14
Cl2
C16
C18
N3
C13
C20
C19
N4
C17
C11
O4
C12

Fig. 2