Ethyl 2-chloro-[2-(4-chlorophenyl)-hydrazin-1-ylidene]acetate

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Key indicators: single-crystal X-ray study; T = 100 K; mean/C12(C–C) = 0.007 Å; R factor = 0.072; wR factor = 0.188; data-to-parameter ratio = 17.4.

The title compound, C10H10Cl2N2O2, features a planar C=N(H)—N—C(Cl) unit [torsion angle = 5.5 (4)°] whose benzene substituent is coplanar with it [dihedral angle = 4.7 (4)°]; this unit is slightly twisted with respect to the carboxyl –CO2 fragment [dihedral angle = 2.2 (5)°]. The amino group acts as a hydrogen-bond donor to the carbonyl O atom of an adjacent molecule; the hydrogen bond generates a helical polymer that runs along the b axis of the monoclinic unit cell.

Related literature

For a review of the reactions of hydrazonyl halides with heterocyclic thiones for heteroaanulation, the synthesis of spiroheterocycles and heterocyclic ring formation, see: Shawali & Farghaly (2008). For related structures, see: Xu (2006); Yin et al. (2006).

Experimental

Crystal data

C10H10Cl2N2O2
V = 567.65 (15) Å3
Mr = 261.10
Z = 2
Mo Kα radiation
μ = 0.56 mm−1
T = 100 K
0.35 × 0.10 × 0.05 mm

Data collection

Bruker SMART APEX diffractometer
5298 measured reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1996) 2518 independent reflections
Tmin = 0.829, Tmax = 0.973
2191 reflections with I > 2σ(I)
Rint = 0.073

Refinement

R[F2 > 2σ(F2)] = 0.072
wR(F2) = 0.188
S = 1.03
5298 measured reflections
2518 independent reflections
145 parameters
H-atom parameters constrained

Absolute structure: Flack (1983), 1123 Friedel pairs
Flack parameter: 0.03 (14)

Table 1

Hydrogen-bond geometry (Å, °).

D−H···A
D−H H···A D···A D−H···A
N1−H1A ·· O1i 0.86 2.20 3.009 (5) 156
Symmetry code: (i) x+1, y, z.

Data collection: APEX2 (Bruker, 2009); cell refinement: SAINT (Bruker, 2009); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELX97 (Sheldrick, 2008); molecular graphics: X-SEED (Barbour, 2001); software used to prepare material for publication: publCIF (Westrip, 2010).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NK2055).

References