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1-(2-Chloro-3,5-difluorophenyl)-3-(2,6-dichlorobenzoyl)urea

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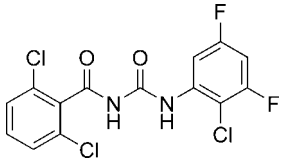
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.006 Å; R factor = 0.049; wR factor = 0.239; data-to-parameter ratio = 16.6.

The 2-chloro-3,5-difluorophenyl ring of the title compound, $C_{14}H_7Cl_3F_2N_2O_2$, is almost coplanar with the urea group, whereas the 2,6-dichlorophenyl ring is twisted from the urea plane by 70.47 (11)°. An intramolecular N—H···O hydrogen bond stabilizes the molecular conformation and intermolecular N—H···O hydrogen bonds link the molecules into centrosymmetric dimers.

Related literature

For related literature, see: Yan *et al.* (2003); Lin *et al.* (2003).



Experimental

Crystal data

$C_{14}H_7Cl_3F_2N_2O_2$
M_r = 379.57
Monoclinic, $P2_1/c$
a = 11.7027 (13) Å
b = 9.5225 (11) Å
c = 14.7144 (16) Å
β = 109.160 (1)°
V = 1548.9 (3) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.62 mm^{-1}
T = 293 (2) K
0.39 × 0.26 × 0.14 mm

Data collection

Bruker SMART CCD area-detector diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 1998)
T_{min} = 0.829, T_{max} = 1.000
(expected range = 0.760–0.917)
9520 measured reflections
3462 independent reflections
2307 reflections with $I > 2\sigma(I)$
R_{int} = 0.020

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.049
$wR(F^2)$ = 0.239
S = 0.87
3462 reflections
208 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.39 e Å^{-3}
$\Delta\rho_{min}$ = −0.49 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N2—H2A···Cl3	0.86	2.48	2.934 (2)	114
N2—H2A···O1	0.86	1.97	2.666 (3)	137
N1—H1A···O2^{i}	0.86	2.00	2.846 (3)	167

Symmetry code: (i) $-x+1, -y+1, -z$.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; 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: BT2353).

References

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supplementary materials

Acta Cryst. (2007). E**63**, o2944 [**doi:10.1107/S1600536807023069**]

1-(2-Chloro-3,5-difluorophenyl)-3-(2,6-dichlorobenzoyl)urea

S.-J. Yan, Y.-Y. Yan, Y.-M. Li, M.-J. Xie and J. Lin

Comment

Derivatives of benzoylphenylureas are insect growth regulators. The title compound (Fig. 1), possesses high bioactivity (Yan *et al.*, 2003).

The 2-chloro-3,5-difluorophenyl ring is almost coplanar with the urea moiety, whereas the 2,6-dichlorophenyl ring is twisted from the urea plane by 70.47 (11)°. An intramolecular N—H···O hydrogen bond stabilized the molecular conformation and intermolecular N—H···O hydrogen bonds link the molecules to centrosymmetric dimers.

Experimental

(I) was prepared according to the procedure of (Lin *et al.*, 2003). The desire product was recrystallized from acetone/chloroform=4/1 (m.p. 505 K).

Refinement

All H atoms were placed in idealized positions and refined using a riding model with C—H distances in the range of 0.93–0.96 Å and with U_{iso}(H) = 1.2 U_{eq}(C) or 1.5 times U_{eq}(C_{methyl}).

Figures

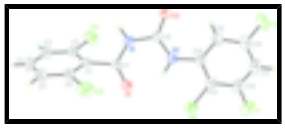


Fig. 1. View of the title compound showing 30% displacement ellipsoids (arbitrary spheres for the H atoms).

1-(2-Chloro-3,5-difluorophenyl)-3-(2,6-dichlorobenzoyl)urea

Crystal data

$C_{14}H_7Cl_3F_2N_2O_2$	D_x = 1.628 Mg m^{-3}
M_r = 379.57	Melting point: 505 K
Monoclinic, $P2_1/c$	Mo $K\alpha$ radiation λ = 0.71073 Å
a = 11.7027 (13) Å	Cell parameters from 3462 reflections
b = 9.5225 (11) Å	θ = 2.6–27.3°
c = 14.7144 (16) Å	μ = 0.62 mm^{-1}
β = 109.160 (1)°	T = 293 (2) K
V = 1548.9 (3) Å^3	Block, colourless

$Z = 4$	0.39 × 0.26 × 0.14 mm
$F_{000} = 760$	

Data collection

Bruker SMART CCD area-detector diffractometer	3462 independent reflections
Radiation source: fine-focus sealed tube	2307 reflections with $I > 2\sigma(I)$
Monochromator: graphite	$R_{int} = 0.020$
$T = 293(2)$ K	$\theta_{max} = 27.3°$
phi and ω scans	$\theta_{min} = 2.6°$
Absorption correction: multi-scan (SADABS; Bruker, 1998)	$h = -11 \rightarrow 15$
$T_{min} = 0.829$, $T_{max} = 1.000$	$k = -12 \rightarrow 10$
9520 measured reflections	$l = -18 \rightarrow 18$

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
$wR(F^2) = 0.239$	$w = 1/[\sigma^2(F_o^2) + (0.2P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$S = 0.87$	$(\Delta/\sigma)_{max} < 0.001$
3462 reflections	$\Delta\rho_{max} = 0.39$ e Å^{-3}
208 parameters	$\Delta\rho_{min} = -0.48$ 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	0.74290 (10)	0.51164 (14)	−0.12803 (7)	0.0906 (4)
Cl2	0.92514 (10)	0.44553 (12)	0.25737 (7)	0.0865 (4)
F2	0.2694 (2)	1.0356 (3)	0.1389 (3)	0.1178 (11)

F1	0.6237 (3)	1.2972 (2)	0.18137 (19)	0.0967 (8)
Cl3	0.76294 (8)	1.07123 (10)	0.13581 (7)	0.0759 (4)
O1	0.83312 (19)	0.7084 (2)	0.10878 (19)	0.0686 (7)
O2	0.46593 (18)	0.6550 (2)	0.04196 (19)	0.0684 (7)
N1	0.6563 (2)	0.5864 (3)	0.05747 (18)	0.0515 (6)
H1A	0.6267	0.5060	0.0351	0.062*
N2	0.6191 (2)	0.8124 (2)	0.10223 (17)	0.0488 (6)
H2A	0.6960	0.8224	0.1162	0.059*
C1	0.8433 (2)	0.4721 (3)	0.0628 (2)	0.0502 (7)
C2	0.8377 (3)	0.4269 (3)	−0.0279 (3)	0.0609 (8)
C3	0.9089 (4)	0.3162 (4)	−0.0398 (4)	0.0827 (12)
H3A	0.9050	0.2874	−0.1012	0.099*
C4	0.9847 (4)	0.2500 (4)	0.0396 (5)	0.0928 (14)
H4A	1.0328	0.1763	0.0318	0.111*
C5	0.9909 (3)	0.2902 (4)	0.1303 (4)	0.0799 (11)
H5A	1.0426	0.2440	0.1836	0.096*
C6	0.9206 (3)	0.3992 (3)	0.1421 (3)	0.0589 (8)
C7	0.7774 (2)	0.6002 (3)	0.0787 (2)	0.0476 (6)
C8	0.5729 (2)	0.6860 (3)	0.0671 (2)	0.0475 (6)
C9	0.4372 (3)	0.9227 (4)	0.1192 (2)	0.0605 (8)
H9A	0.3939	0.8390	0.1060	0.073*
C10	0.3858 (4)	1.0433 (4)	0.1399 (3)	0.0754 (10)
C11	0.4471 (4)	1.1691 (4)	0.1618 (3)	0.0798 (11)
H11A	0.4107	1.2484	0.1770	0.096*
C12	0.5611 (4)	1.1729 (3)	0.1603 (3)	0.0690 (9)
C13	0.6186 (3)	1.0571 (3)	0.1376 (2)	0.0532 (7)
C14	0.5551 (3)	0.9293 (3)	0.11844 (19)	0.0466 (6)

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0914 (8)	0.1152 (10)	0.0616 (6)	0.0079 (6)	0.0202 (5)	−0.0108 (5)
Cl2	0.0892 (8)	0.0866 (7)	0.0716 (6)	−0.0075 (5)	0.0102 (5)	0.0057 (5)
F2	0.0839 (18)	0.107 (2)	0.188 (3)	0.0253 (15)	0.079 (2)	0.0004 (19)
F1	0.130 (2)	0.0489 (11)	0.1098 (18)	−0.0114 (12)	0.0373 (15)	−0.0197 (12)
Cl3	0.0663 (6)	0.0682 (6)	0.0937 (7)	−0.0246 (4)	0.0267 (5)	−0.0193 (4)
O1	0.0412 (11)	0.0557 (13)	0.1073 (19)	−0.0123 (9)	0.0222 (11)	−0.0245 (12)
O2	0.0379 (11)	0.0596 (13)	0.1061 (18)	−0.0084 (9)	0.0214 (11)	−0.0244 (12)
N1	0.0386 (12)	0.0436 (12)	0.0706 (16)	−0.0066 (9)	0.0156 (11)	−0.0155 (11)
N2	0.0382 (11)	0.0468 (13)	0.0622 (14)	−0.0040 (9)	0.0175 (10)	−0.0090 (10)
C1	0.0392 (14)	0.0438 (14)	0.0686 (19)	−0.0052 (11)	0.0189 (13)	−0.0071 (13)
C2	0.0534 (17)	0.0535 (18)	0.080 (2)	−0.0052 (13)	0.0272 (16)	−0.0121 (15)
C3	0.078 (3)	0.068 (2)	0.119 (3)	−0.006 (2)	0.056 (3)	−0.027 (2)
C4	0.071 (2)	0.055 (2)	0.165 (5)	0.0121 (18)	0.057 (3)	−0.005 (3)
C5	0.058 (2)	0.057 (2)	0.124 (4)	0.0057 (16)	0.028 (2)	0.012 (2)
C6	0.0446 (15)	0.0485 (17)	0.081 (2)	−0.0038 (12)	0.0179 (15)	0.0049 (15)
C7	0.0372 (13)	0.0470 (15)	0.0580 (16)	−0.0053 (10)	0.0150 (11)	−0.0083 (12)
C8	0.0356 (13)	0.0467 (14)	0.0577 (15)	−0.0040 (10)	0.0118 (11)	−0.0072 (12)

C9	0.0570 (18)	0.0577 (18)	0.071 (2)	0.0066 (13)	0.0272 (15)	0.0031 (15)
C10	0.073 (2)	0.077 (2)	0.088 (3)	0.0231 (19)	0.042 (2)	0.008 (2)
C11	0.100 (3)	0.058 (2)	0.085 (2)	0.024 (2)	0.036 (2)	−0.0022 (18)
C12	0.093 (3)	0.0463 (17)	0.065 (2)	0.0044 (16)	0.0221 (18)	−0.0032 (14)
C13	0.0613 (18)	0.0493 (16)	0.0472 (15)	−0.0033 (12)	0.0154 (13)	−0.0049 (12)
C14	0.0512 (15)	0.0461 (14)	0.0422 (13)	0.0006 (11)	0.0150 (11)	−0.0004 (11)

Geometric parameters (Å, °)

Cl1—C2	1.726 (4)	C2—C3	1.390 (5)
Cl2—C6	1.737 (4)	C3—C4	1.368 (7)
F2—C10	1.359 (4)	C3—H3A	0.9300
F1—C12	1.373 (4)	C4—C5	1.366 (7)
Cl3—C13	1.704 (3)	C4—H4A	0.9300
O1—C7	1.222 (3)	C5—C6	1.371 (5)
O2—C8	1.219 (3)	C5—H5A	0.9300
N1—C7	1.354 (3)	C9—C10	1.377 (5)
N1—C8	1.401 (4)	C9—C14	1.385 (5)
N1—H1A	0.8600	C9—H9A	0.9300
N2—C8	1.351 (4)	C10—C11	1.378 (6)
N2—C14	1.405 (4)	C11—C12	1.343 (6)
N2—H2A	0.8600	C11—H11A	0.9300
C1—C2	1.384 (5)	C12—C13	1.389 (5)
C1—C6	1.403 (4)	C13—C14	1.404 (4)
C1—C7	1.502 (4)		
C7—N1—C8	128.5 (2)	O1—C7—N1	124.0 (3)
C7—N1—H1A	115.8	O1—C7—C1	120.0 (2)
C8—N1—H1A	115.8	N1—C7—C1	116.0 (2)
C8—N2—C14	127.1 (2)	O2—C8—N2	125.0 (3)
C8—N2—H2A	116.5	O2—C8—N1	119.0 (2)
C14—N2—H2A	116.5	N2—C8—N1	115.9 (2)
C2—C1—C6	117.5 (3)	C10—C9—C14	118.2 (3)
C2—C1—C7	122.6 (3)	C10—C9—H9A	120.9
C6—C1—C7	119.8 (3)	C14—C9—H9A	120.9
C1—C2—C3	121.1 (4)	F2—C10—C9	117.5 (4)
C1—C2—Cl1	119.5 (2)	F2—C10—C11	119.5 (3)
C3—C2—Cl1	119.4 (3)	C9—C10—C11	123.0 (4)
C4—C3—C2	119.3 (4)	C12—C11—C10	117.6 (3)
C4—C3—H3A	120.4	C12—C11—H11A	121.2
C2—C3—H3A	120.4	C10—C11—H11A	121.2
C5—C4—C3	121.2 (3)	C11—C12—F1	118.6 (3)
C5—C4—H4A	119.4	C11—C12—C13	123.0 (3)
C3—C4—H4A	119.4	F1—C12—C13	118.4 (3)
C4—C5—C6	119.6 (4)	C12—C13—C14	118.1 (3)
C4—C5—H5A	120.2	C12—C13—Cl3	120.1 (3)
C6—C5—H5A	120.2	C14—C13—Cl3	121.8 (2)
C5—C6—C1	121.3 (4)	C9—C14—C13	120.0 (3)
C5—C6—Cl2	119.3 (3)	C9—C14—N2	123.5 (3)
C1—C6—Cl2	119.4 (2)	C13—C14—N2	116.4 (3)

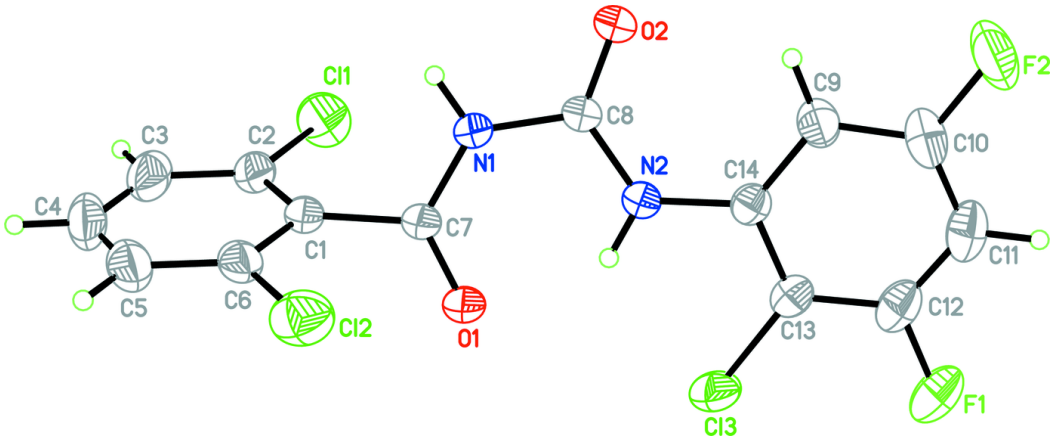
C6—C1—C2—C3	−2.0 (5)	C14—N2—C8—N1	179.8 (3)
C7—C1—C2—C3	173.7 (3)	C7—N1—C8—O2	178.3 (3)
C6—C1—C2—Cl1	179.3 (2)	C7—N1—C8—N2	0.0 (4)
C7—C1—C2—Cl1	−5.0 (4)	C14—C9—C10—F2	179.0 (3)
C1—C2—C3—C4	0.7 (5)	C14—C9—C10—C11	−1.3 (6)
Cl1—C2—C3—C4	179.4 (3)	F2—C10—C11—C12	−178.8 (3)
C2—C3—C4—C5	0.5 (6)	C9—C10—C11—C12	1.5 (6)
C3—C4—C5—C6	−0.3 (6)	C10—C11—C12—F1	179.7 (4)
C4—C5—C6—C1	−1.0 (5)	C10—C11—C12—C13	0.2 (6)
C4—C5—C6—Cl2	177.7 (3)	C11—C12—C13—C14	−2.1 (5)
C2—C1—C6—C5	2.2 (4)	F1—C12—C13—C14	178.5 (3)
C7—C1—C6—C5	−173.7 (3)	C11—C12—C13—Cl3	179.2 (3)
C2—C1—C6—Cl2	−176.6 (2)	F1—C12—C13—Cl3	−0.3 (4)
C7—C1—C6—Cl2	7.5 (4)	C10—C9—C14—C13	−0.6 (5)
C8—N1—C7—O1	−1.9 (5)	C10—C9—C14—N2	177.3 (3)
C8—N1—C7—C1	178.4 (3)	C12—C13—C14—C9	2.3 (4)
C2—C1—C7—O1	−105.4 (4)	Cl3—C13—C14—C9	−179.0 (2)
C6—C1—C7—O1	70.3 (4)	C12—C13—C14—N2	−175.8 (3)
C2—C1—C7—N1	74.4 (4)	Cl3—C13—C14—N2	2.9 (4)
C6—C1—C7—N1	−110.0 (3)	C8—N2—C14—C9	14.0 (5)
C14—N2—C8—O2	1.6 (5)	C8—N2—C14—C13	−168.1 (3)

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2A···Cl3	0.86	2.48	2.934 (2)	114
N2—H2A···O1	0.86	1.97	2.666 (3)	137
N1—H1A···O2^{i}	0.86	2.00	2.846 (3)	167

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

Fig. 1


O2
Cl1
C9
F2
C3
C2
N1
C8
N2
C14
C10
C4
C7
C1
C11
C5
C6
C12
C13
Cl2
O1
F1
Cl3