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N-(3-Chlorophenyl)benzamide

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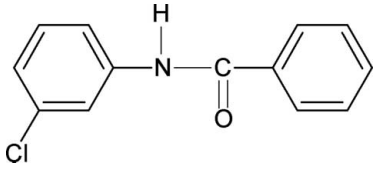
Key indicators: single-crystal X-ray study; T = 295 K; mean σ(C–C) = 0.003 Å; R factor = 0.039; wR factor = 0.101; data-to-parameter ratio = 15.2.

The conformation of the N—H bond in the structure of the title compound (N3CPBA), $C_{13}H_{10}ClNO$, is *anti* to the *meta* chloro substituent in the aniline benzene ring, similar to that observed with respect to the *ortho* chloro substituent in *N*-(2-chlorophenyl)benzamide (N2CPBA) and *meta* chloro substituent in *N*-(3,4-dichlorophenyl)benzamide (N34DCPBA), but in contrast to the *syn* conformation observed with respect to both the *ortho* and the *meta* chloro substituents in *N*-(2,3-dichlorophenyl)benzamide (N23DCPBA). The bond parameters in N3CPBA are similar to those in *N*-phenylbenzamide, N2CPBA, N23DCPBA, N34DCPBA and other benzanilides. The amide group –NHCO– makes a dihedral angle of 18.2 (2)° with the benzoyl ring, while the dihedral angle between the two benzene rings is 61.0 (1)°. The molecules are linked into chains along the *b* axis by N—H···O hydrogen bonds.

Related literature

For related literature, see: Gowda *et al.* (2003); Gowda, Sowmya, Kožíšek *et al.* (2007); Gowda, Sowmya, Tokarčík *et al.* (2007).



Experimental

Crystal data

$C_{13}H_{10}ClNO$
M_r = 231.67
Orthorhombic, *Pbca*
a = 9.3585 (2) Å
b = 9.7851 (2) Å
c = 25.1419 (6) Å
V = 2302.34 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 295 (2) K
0.41 × 0.13 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2007). Analytical numeric absorption correction using a multifaceted crystal model (Clark & Reid, 1995).
T_{min} = 0.915, T_{max} = 0.984
53566 measured reflections
2252 independent reflections
1639 reflections with $I > 2\sigma(I)$
R_{int} = 0.047

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.101
S = 1.08
2252 reflections
148 parameters
1 restraint
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.834 (16)	2.089 (17)	2.8989 (17)	163.5 (17)

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

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2007); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2007); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2002); software used to prepare material for publication: *SHELXL97*, *PLATON* (Spek, 2003) and *WinGX* (Farrugia, 1999).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: DN2311).

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supporting information

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N-(3-Chlorophenyl)benzamide

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S1. Comment

In the present work, the structure of *N*-(3-chlorophenyl)-benzamide (N3CPBA) has been determined to explore the effect of substituents on the structure of *N*-aromatic amides (Gowda *et al.*, 2003; Gowda, Sowmya, Kožíšek *et al.*, 2007; Gowda, Sowmya, Tokarčík *et al.*, 2007). The conformation of the N—H bond in the structure of N3CPBA(Fig.1) is anti to the *meta* chloro substituent in the aniline phenyl ring, similar to that observed with respect to the *ortho*-chloro substituent in *N*-(2-chlorophenyl)-benzamide (N2CPBA)(Gowda, Sowmya, Kožíšek *et al.*, 2007) and *meta*-chloro substituent in *N*-(3,4-dichlorophenyl)-benzamide (N34DCPBA) (Gowda, Sowmya, Tokarčík *et al.*, 2007), but in contrast to the *syn* conformation observed with respect to both the *ortho* & *meta*-Chloro substituents in *N*-(2,3-dichlorophenyl)-benzamide (N23DCPBA)(Gowda, Sowmya, Tokarčík *et al.*, 2007). The bond parameters in N3CPBA are similar to those in *N*-(phenyl)-benzamide, N2CPBA, N23DCPBA, N34DCPBA and other benzanilides. The amide group –NHCO– has the dihedral angle of 18.2 (2)° with the benzoyl ring, while the dihedral angle between the two benzene rings (benzoyl and aniline) is 61.0 (1)°. One-dimensional chains of the title compound along the base vector [0 1 0] formed by hydrogen bonds N1–H1N···O1 (Table 1) as viewed down the *a* axis is shown in Fig.2.

S2. Experimental

The title compound was prepared according to the literature method (Gowda *et al.*, 2003). The purity of the compound was checked by determining its melting point. It was characterized by recording its infrared and NMR spectra. Single crystals of the title compound were obtained from an ethanolic solution and used for X-ray diffraction studies at room temperature.

S3. Refinement

H atoms bonded to C atoms were placed in geometrically calculated positions and subsequently treated as riding with C —H bond distance 0.93 Å. H(N) atom was visible in the difference map. In refinement the N—H distance was restrained to 0.86 (4) Å. The U_{iso}(H) values were set at 1.2 U_{eq}(C,*N*).

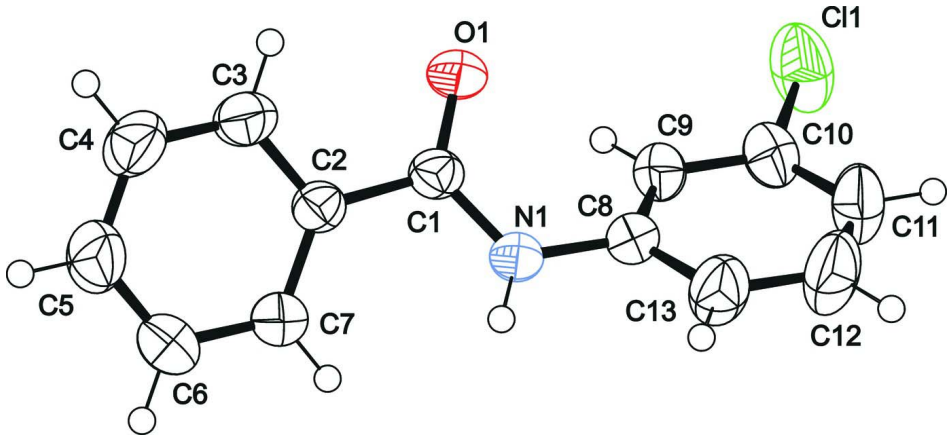

Figure 1

Molecular structure of the title compound showing the atom labelling scheme. Displacement ellipsoids are drawn at the 50% probability level. H atoms are represented as small spheres of arbitrary radii.

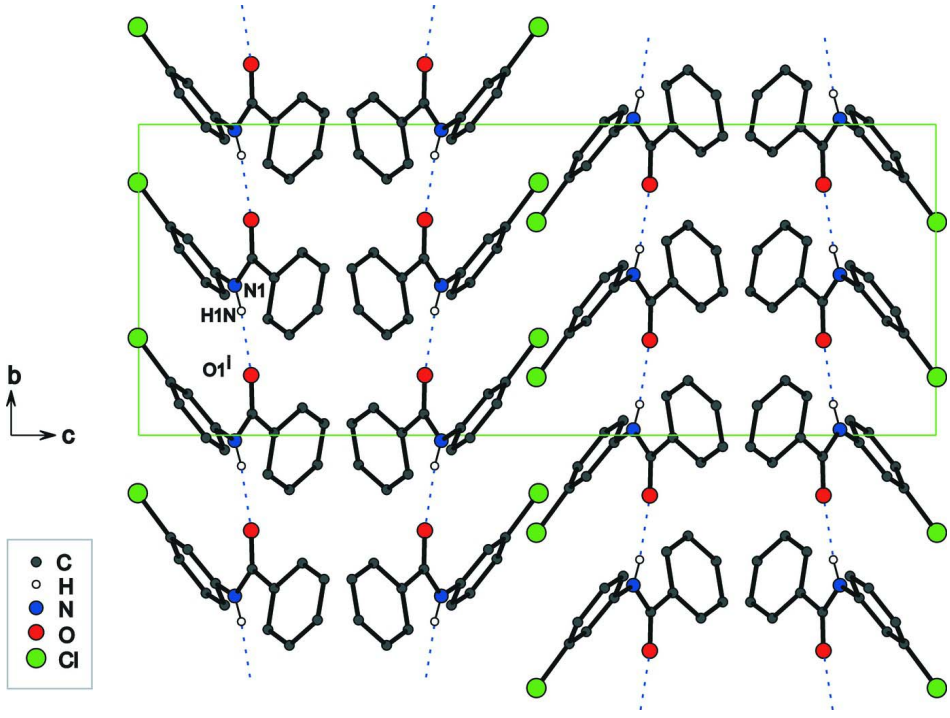

Figure 2

Crystal structure of the title compound viewed down the axis a. One-dimensional chains along the base vector [0 1 0] are formed by hydrogen bonds N1–H1N···O1(i). H atoms not involved in hydrogen bonding are omitted. [Symmetry code: (i) $-x + 1/2, y - 1/2, z$]

N-(3-Chlorophenyl)benzamide

Crystal data

$C_{13}H_{10}ClNO$
$M_r = 231.67$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 9.3585\ (2)$ Å
$b = 9.7851\ (2)$ Å

c = 25.1419 (6) Å
V = 2302.34 (9) Å^3
Z = 8
F(000) = 960
D_x = 1.337 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å

Cell parameters from 14003 reflections
θ = 3.0–29.5°
μ = 0.31 mm^{-1}
T = 295 K
Prism, colourless
0.41 × 0.13 × 0.06 mm

Data collection

Oxford Diffraction Xcalibur diffractometer
Graphite monochromator
Detector resolution: 10.434 pixels mm^{-1}
φ scans, and ω scans with κ offsets
Absorption correction: analytical (*CrysAlis RED*; Oxford Diffraction, 2007). Analytical numeric absorption correction using a multifaceted crystal model (Clark & Reid, 1995).

T_{min} = 0.915, T_{max} = 0.984
53566 measured reflections
2252 independent reflections
1639 reflections with $I > 2\sigma(I)$
R_{int} = 0.047
θ_{max} = 26.0°, θ_{min} = 4.7°
h = −11→11
k = −12→12
l = −31→31

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.038
$wR(F^2)$ = 0.101
S = 1.08
2252 reflections
148 parameters
1 restraint
Primary atom site location: structure-invariant direct methods

Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0491P)^2 + 0.2808P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.19 e Å^{-3}
$\Delta\rho_{min}$ = −0.25 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 (Å^2)

	x	y	z	U_{iso}*/U_{eq}
N1	0.27214 (14)	0.48267 (13)	0.12047 (5)	0.0462 (4)
H1N	0.2650 (19)	0.4004 (17)	0.1287 (6)	0.055*
O1	0.19225 (12)	0.69327 (10)	0.14128 (5)	0.0565 (3)
Cl1	0.54083 (6)	0.81350 (6)	−0.00120 (2)	0.0875 (2)
C1	0.17675 (16)	0.56906 (15)	0.14234 (6)	0.0405 (4)
C2	0.05098 (15)	0.50735 (14)	0.16988 (6)	0.0392 (4)
C3	−0.02405 (19)	0.58822 (17)	0.20536 (7)	0.0546 (5)
H3	0.0038	0.6784	0.2108	0.065*

C4	−0.1391 (2)	0.53666 (19)	0.23252 (8)	0.0671 (5)
H4	−0.1877	0.5916	0.2567	0.081*
C5	−0.1830 (2)	0.4050 (2)	0.22432 (8)	0.0684 (6)
H5	−0.2613	0.3706	0.2427	0.082*
C6	−0.1111 (2)	0.32411 (18)	0.18890 (8)	0.0654 (5)
H6	−0.1414	0.2349	0.1829	0.079*
C7	0.00613 (18)	0.37454 (17)	0.16203 (7)	0.0519 (4)
H7	0.0553	0.3185	0.1384	0.062*
C8	0.40219 (17)	0.52388 (15)	0.09631 (6)	0.0444 (4)
C9	0.40661 (17)	0.63258 (16)	0.06157 (6)	0.0471 (4)
H9	0.3235	0.6796	0.0528	0.056*
C10	0.53533 (19)	0.67062 (18)	0.04005 (7)	0.0544 (5)
C11	0.6590 (2)	0.6017 (2)	0.05099 (8)	0.0719 (6)
H11	0.7453	0.6288	0.0359	0.086*
C12	0.6527 (2)	0.4918 (2)	0.08464 (10)	0.0808 (6)
H12	0.7355	0.4428	0.092	0.097*
C13	0.5255 (2)	0.4528 (2)	0.10771 (8)	0.0657 (5)
H13	0.523	0.3788	0.1309	0.079*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0440 (8)	0.0309 (6)	0.0636 (9)	0.0007 (6)	0.0069 (7)	0.0025 (6)
O1	0.0570 (7)	0.0299 (6)	0.0827 (8)	−0.0007 (5)	0.0119 (6)	0.0004 (5)
Cl1	0.0668 (4)	0.0990 (5)	0.0968 (4)	−0.0134 (3)	0.0102 (3)	0.0423 (3)
C1	0.0405 (9)	0.0349 (8)	0.0462 (9)	0.0023 (7)	−0.0054 (7)	0.0006 (7)
C2	0.0387 (8)	0.0353 (8)	0.0437 (8)	0.0030 (6)	−0.0031 (7)	0.0027 (6)
C3	0.0621 (11)	0.0407 (9)	0.0609 (10)	0.0035 (8)	0.0091 (9)	−0.0026 (8)
C4	0.0711 (13)	0.0596 (11)	0.0707 (12)	0.0091 (10)	0.0291 (11)	0.0013 (9)
C5	0.0605 (12)	0.0658 (12)	0.0789 (13)	−0.0021 (10)	0.0232 (11)	0.0136 (10)
C6	0.0615 (12)	0.0485 (10)	0.0862 (14)	−0.0122 (9)	0.0123 (11)	0.0001 (9)
C7	0.0495 (10)	0.0433 (9)	0.0628 (11)	−0.0030 (8)	0.0084 (8)	−0.0081 (8)
C8	0.0418 (9)	0.0393 (8)	0.0521 (9)	0.0005 (7)	0.0040 (7)	−0.0044 (7)
C9	0.0392 (9)	0.0500 (9)	0.0520 (9)	−0.0007 (8)	−0.0016 (8)	−0.0003 (8)
C10	0.0489 (11)	0.0621 (11)	0.0521 (10)	−0.0090 (8)	0.0025 (8)	0.0038 (8)
C11	0.0435 (11)	0.0900 (14)	0.0824 (14)	−0.0024 (10)	0.0133 (10)	0.0107 (12)
C12	0.0461 (12)	0.0917 (15)	0.1046 (16)	0.0207 (11)	0.0101 (11)	0.0216 (13)
C13	0.0528 (12)	0.0615 (11)	0.0827 (13)	0.0112 (9)	0.0081 (10)	0.0170 (10)

Geometric parameters (Å, º)

N1—C1	1.3468 (19)	C6—C7	1.380 (2)
N1—C8	1.419 (2)	C6—H6	0.93
N1—H1N	0.834 (16)	C7—H7	0.93
O1—C1	1.2244 (17)	C8—C9	1.377 (2)
Cl1—C10	1.7415 (18)	C8—C13	1.378 (2)
C1—C2	1.493 (2)	C9—C10	1.372 (2)
C2—C7	1.380 (2)	C9—H9	0.93

C2—C3	1.384 (2)	C10—C11	1.368 (3)
C3—C4	1.371 (2)	C11—C12	1.369 (3)
C3—H3	0.93	C11—H11	0.93
C4—C5	1.368 (3)	C12—C13	1.378 (3)
C4—H4	0.93	C12—H12	0.93
C5—C6	1.368 (3)	C13—H13	0.93
C5—H5	0.93		

C1—N1—C8	124.41 (13)	C2—C7—C6	120.57 (16)
C1—N1—H1N	116.9 (12)	C2—C7—H7	119.7
C8—N1—H1N	116.7 (12)	C6—C7—H7	119.7
O1—C1—N1	122.38 (14)	C9—C8—C13	119.78 (15)
O1—C1—C2	120.33 (14)	C9—C8—N1	121.12 (14)
N1—C1—C2	117.26 (13)	C13—C8—N1	119.10 (14)
C7—C2—C3	118.46 (15)	C10—C9—C8	119.09 (15)
C7—C2—C1	123.66 (14)	C10—C9—H9	120.5
C3—C2—C1	117.88 (13)	C8—C9—H9	120.5
C4—C3—C2	120.60 (16)	C11—C10—C9	122.00 (17)
C4—C3—H3	119.7	C11—C10—Cl1	119.38 (14)
C2—C3—H3	119.7	C9—C10—Cl1	118.60 (14)
C5—C4—C3	120.47 (17)	C10—C11—C12	118.36 (18)
C5—C4—H4	119.8	C10—C11—H11	120.8
C3—C4—H4	119.8	C12—C11—H11	120.8
C4—C5—C6	119.71 (17)	C11—C12—C13	120.98 (19)
C4—C5—H5	120.1	C11—C12—H12	119.5
C6—C5—H5	120.1	C13—C12—H12	119.5
C5—C6—C7	120.18 (17)	C8—C13—C12	119.76 (18)
C5—C6—H6	119.9	C8—C13—H13	120.1
C7—C6—H6	119.9	C12—C13—H13	120.1

C8—N1—C1—O1	3.0 (2)	C5—C6—C7—C2	−1.0 (3)
C8—N1—C1—C2	−175.25 (14)	C1—N1—C8—C9	−45.2 (2)
O1—C1—C2—C7	163.26 (16)	C1—N1—C8—C13	135.30 (17)
N1—C1—C2—C7	−18.5 (2)	C13—C8—C9—C10	−1.9 (2)
O1—C1—C2—C3	−17.0 (2)	N1—C8—C9—C10	178.61 (14)
N1—C1—C2—C3	161.30 (14)	C8—C9—C10—C11	1.7 (3)
C7—C2—C3—C4	0.8 (3)	C8—C9—C10—Cl1	−176.82 (12)
C1—C2—C3—C4	−178.95 (15)	C9—C10—C11—C12	−0.2 (3)
C2—C3—C4—C5	−1.1 (3)	Cl1—C10—C11—C12	178.29 (17)
C3—C4—C5—C6	0.3 (3)	C10—C11—C12—C13	−1.1 (3)
C4—C5—C6—C7	0.8 (3)	C9—C8—C13—C12	0.6 (3)
C3—C2—C7—C6	0.2 (3)	N1—C8—C13—C12	−179.87 (18)
C1—C2—C7—C6	179.94 (16)	C11—C12—C13—C8	0.9 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*

N1—H1*N*···O1^{i}	0.83 (2)	2.09 (2)	2.8989 (17)	164 (2)

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