Acta Crystallographica Section E
Structure Reports Online
ISSN 1600-5368

2-Chloro-*N*-(3,5-dimethylphenyl)-benzamide

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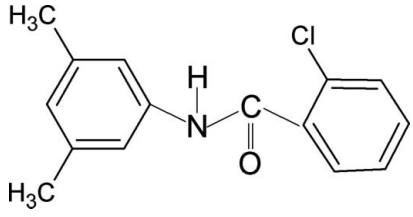
Received 13 January 2009; accepted 14 January 2009

Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.003 Å; R factor = 0.031; wR factor = 0.083; data-to-parameter ratio = 11.4.

In the structure of the the title compound, $C_{15}H_{14}ClNO$, the N—H and C=O bonds are *trans* to each other and the amide O atom is *anti* to the *ortho*-Cl atom in the benzoyl ring. The amide group makes dihedral angles of 61.2 (6) and 42.2 (8)° with the benzoyl and aniline rings, respectively. In the crystal, the molecules are linked into infinite chains by N—H···O hydrogen bonds.

Related literature

For the synthesis, see: Gowda *et al.* (2003). For structure of the 3,5-dichlorophenyl analog and other benzanilides, see: Gowda *et al.* (2008*a*,*b*).



Experimental

Crystal data

$C_{15}H_{14}ClNO$
M_r = 259.72
Orthorhombic, $Pna2_1$
a = 9.1867 (6) Å
b = 13.9710 (8) Å
c = 10.2711 (7) Å
V = 1318.27 (15) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 100 (2) K
0.48 × 0.28 × 0.13 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.879, T_{max} = 0.965
6034 measured reflections
2136 independent reflections
1977 reflections with $I > 2\sigma(I)$
R_{int} = 0.014

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.03
2136 reflections
187 parameters
2 restraints
H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 712 Friedel pairs
Flack parameter: 0.01 (7)

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

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1N···O1^{i}	0.831 (17)	2.120 (18)	2.918 (2)	161 (2)

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: *PLATON* (Spek, 2003); software used to prepare material for publication: *SHELXL97*.

BTG thanks the Alexander von Humboldt Foundation, Bonn, Germany, for extensions of his research fellowship.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: NG2536).

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supporting information

Acta Cryst. (2009). E**65**, o444 [doi:10.1107/S1600536809001706]

2-Chloro-*N*-(3,5-dimethylphenyl)benzamide

B. Thimme Gowda, Sabine Foro, B. P. Sowmya and Hartmut Fuess

S1. Comment

In the present work, the structure of 2-chloro-*N*-(3,5-dimethylphenyl)- benzamide (N35DMP2CBA) has been determined to explore the substituent effects on the solid state structures of benzanilides (Gowda *et al.*, 2003, 2008*a,b*). The conformations of N—H and C=O bonds in the amide group of N35DMP2CBA are *trans* to each other (Fig.1), similar to that observed in 2-chloro-*N*-(3,5-dichlorophenyl)-benzamide(N35DCP2CBA) (Gowda *et al.*, 2008*a*), 2-chloro-*N*-(phenyl)-benzamide (NP2CBA) (Gowda *et al.*, 2003) and other benzanilides (Gowda *et al.*, 2008*b*). Further, the conformation of the amide oxygen in N35DMP2CBA is *anti* to the *ortho*-chloro group in the benzoyl ring similar to that observed in N35DCP2CBA but in contrast to the *syn* conformation observed in NP2CBA. The amide group –NHCO– makes the dihedral angles of 61.2 (6)° and 42.2 (8)° with the benzoyl and aniline rings, respectively, while the benzoyl and aniline rings form the dihedral angle of 76.7 (1)°), compared to the corresponding values of 63.1 (12)°, 31.1 (17)° and 32.1 (2)°) in N35DCP2CBA. Part of the crystal structure of the title compound with infinite molecular chains running along the *a* axis is shown in Fig. 2. The chains are generated by N—H···O hydrogen bonds (Table 1)

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

The H atoms of the methyl groups were positioned with idealized geometry using a riding model with C—H = 0.98 Å. The other H atoms were located in difference map, and its positional parameters were refined freely with C—H = 0.89 (3)–0.99 (3) Å, while the H atom of the NH group was later restrained to the distance 0.86 (2) Å. All H atoms were refined with isotropic displacement parameters (set to 1.2 times of the U_{eq} of the parent atom).

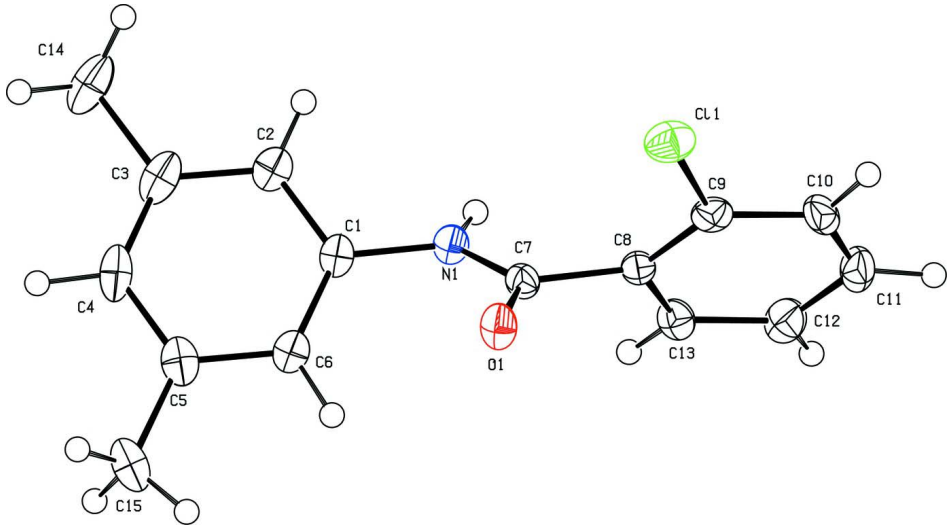

Figure 1

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

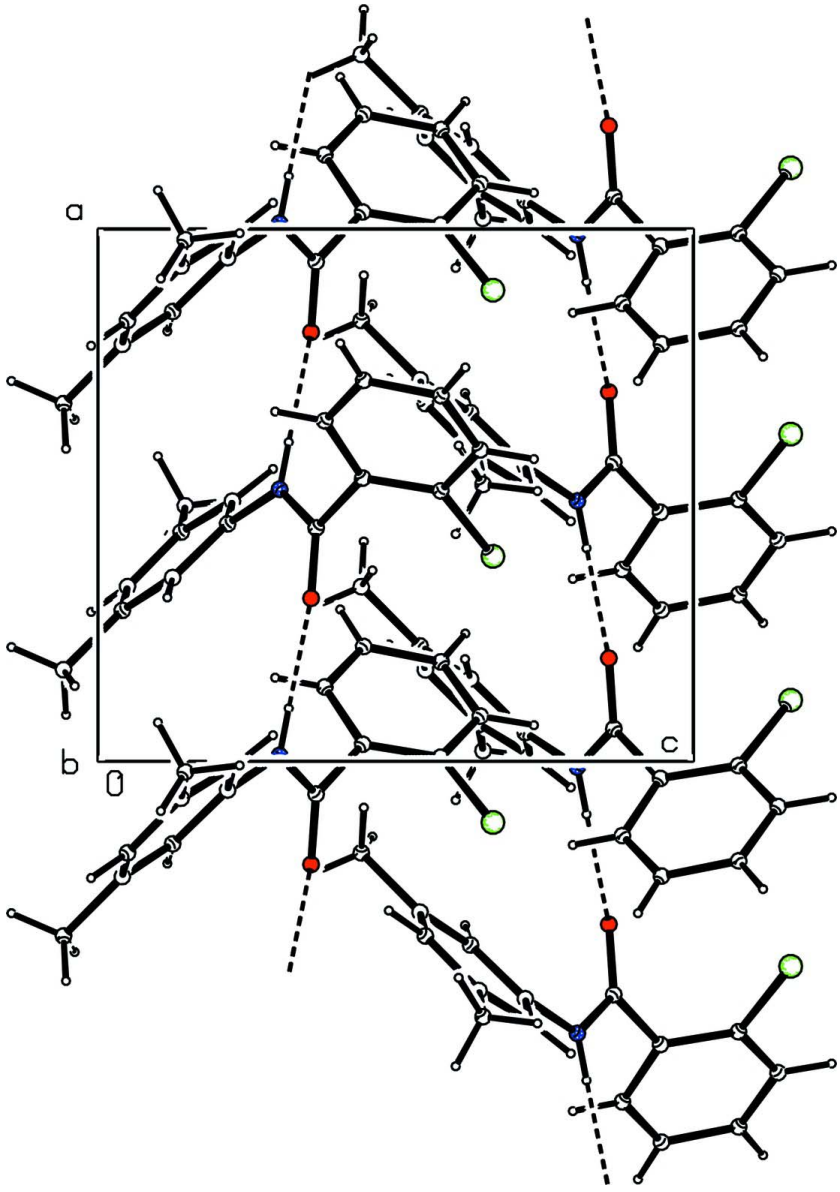

Figure 2

Molecular packing of the title compound with hydrogen bonding shown as dashed lines.

2-Chloro-*N*-(3,5-dimethylphenyl)benzamide

Crystal data

$C_{15}H_{14}ClNO$
$M_r = 259.72$
Orthorhombic, $Pna2_1$
Hall symbol: P 2c -2n
$a = 9.1867\ (6)$ Å
$b = 13.9710\ (8)$ Å
$c = 10.2711\ (7)$ Å
$V = 1318.27\ (15)$ Å^3
$Z = 4$
$F(000) = 544$
$D_x = 1.309$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 2104 reflections
$\theta = 2.5–28.1°$
$\mu = 0.28$ mm^{-1}
$T = 100$ K
Prism, colourless
0.48 × 0.28 × 0.13 mm

Data collection

Oxford Diffraction Xcalibur diffractometer with a Sapphire CCD detector
Radiation source: fine-focus sealed tube
Graphite monochromator
Rotation method data acquisition using ω and φ scans
Absorption correction: multi-scan (*CrysAlis RED*; Oxford Diffraction, 2007)
T_{min} = 0.879, T_{max} = 0.965
6034 measured reflections
2136 independent reflections
1977 reflections with $I > 2\sigma(I)$
R_{int} = 0.014
θ_{max} = 26.4°, θ_{min} = 2.5°
h = −11→11
k = −17→17
l = −10→12

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.083
S = 1.03
2136 reflections
187 parameters
2 restraints
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
$w = 1/[\sigma^2(F_o^2) + (0.0477P)^2 + 0.598P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.002
$\Delta\rho_{max}$ = 0.34 e Å^{-3}
$\Delta\rho_{min}$ = −0.27 e Å^{-3}
Absolute structure: Flack (1983), 712 Friedel pairs
Absolute structure parameter: 0.01 (7)

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 (Å²)

	x	y	z	U_{iso}*/U_{eq}
Cl1	0.11485 (6)	0.32674 (4)	1.16333 (7)	0.03305 (16)
O1	0.19372 (16)	0.32548 (10)	0.85807 (18)	0.0253 (4)
N1	−0.01100 (18)	0.24094 (12)	0.8052 (2)	0.0210 (4)
H1N	−0.0995 (19)	0.2359 (18)	0.820 (3)	0.025*
C1	0.0540 (2)	0.17351 (13)	0.7178 (2)	0.0211 (4)
C2	0.0112 (2)	0.07840 (15)	0.7257 (3)	0.0247 (5)
H2	−0.049 (3)	0.0577 (18)	0.794 (3)	0.030*
C3	0.0694 (2)	0.01080 (14)	0.6398 (3)	0.0299 (6)
C4	0.1719 (3)	0.04035 (16)	0.5498 (3)	0.0307 (5)
H4	0.219 (3)	−0.0046 (18)	0.489 (3)	0.037*
C5	0.2166 (3)	0.13617 (16)	0.5410 (2)	0.0287 (5)
C6	0.1549 (2)	0.20260 (15)	0.6256 (2)	0.0249 (5)
H6	0.192 (3)	0.2682 (18)	0.617 (3)	0.030*
C7	0.0614 (2)	0.31152 (14)	0.8664 (2)	0.0200 (4)

C8	−0.0321 (2)	0.37827 (13)	0.9446 (2)	0.0193 (4)
C9	−0.0080 (2)	0.39557 (15)	1.0757 (2)	0.0237 (5)
C10	−0.0849 (3)	0.46637 (16)	1.1420 (2)	0.0289 (5)
H10	−0.068 (3)	0.4734 (19)	1.232 (3)	0.035*
C11	−0.1868 (2)	0.52064 (16)	1.0761 (3)	0.0313 (6)
H11	−0.240 (3)	0.5734 (18)	1.117 (3)	0.038*
C12	−0.2157 (3)	0.50321 (15)	0.9463 (3)	0.0305 (5)
H12	−0.285 (3)	0.539 (2)	0.907 (3)	0.037*
C13	−0.1396 (2)	0.43181 (16)	0.8809 (3)	0.0239 (5)
H13	−0.157 (3)	0.4197 (18)	0.798 (3)	0.029*
C14	0.0200 (3)	−0.09234 (15)	0.6467 (4)	0.0409 (7)
H14A	0.0078	−0.1111	0.7380	0.049*
H14B	0.0932	−0.1335	0.6057	0.049*
H14C	−0.0729	−0.0993	0.6008	0.049*
C15	0.3281 (3)	0.16747 (18)	0.4422 (3)	0.0392 (6)
H15A	0.2854	0.1645	0.3548	0.047*
H15B	0.4128	0.1250	0.4465	0.047*
H15C	0.3585	0.2333	0.4610	0.047*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl1	0.0362 (3)	0.0325 (3)	0.0304 (3)	−0.0048 (2)	−0.0079 (3)	0.0058 (3)
O1	0.0141 (7)	0.0272 (7)	0.0345 (10)	−0.0016 (5)	0.0019 (7)	−0.0081 (7)
N1	0.0133 (8)	0.0218 (8)	0.0280 (10)	−0.0020 (6)	0.0015 (8)	−0.0034 (7)
C1	0.0164 (9)	0.0219 (10)	0.0249 (11)	0.0019 (7)	−0.0043 (9)	−0.0049 (8)
C2	0.0178 (9)	0.0242 (10)	0.0323 (13)	−0.0008 (8)	−0.0045 (10)	−0.0028 (9)
C3	0.0219 (10)	0.0225 (9)	0.0454 (16)	0.0042 (7)	−0.0137 (11)	−0.0063 (10)
C4	0.0269 (11)	0.0306 (11)	0.0345 (14)	0.0099 (9)	−0.0078 (11)	−0.0150 (10)
C5	0.0261 (11)	0.0337 (11)	0.0262 (14)	0.0060 (9)	−0.0032 (11)	−0.0064 (10)
C6	0.0238 (10)	0.0221 (10)	0.0286 (13)	0.0010 (8)	−0.0015 (9)	−0.0030 (8)
C7	0.0180 (10)	0.0211 (9)	0.0208 (12)	−0.0005 (7)	0.0029 (9)	−0.0011 (8)
C8	0.0172 (9)	0.0188 (9)	0.0220 (12)	−0.0048 (7)	0.0034 (9)	−0.0019 (8)
C9	0.0211 (9)	0.0228 (10)	0.0273 (13)	−0.0085 (8)	0.0010 (9)	0.0008 (8)
C10	0.0351 (12)	0.0282 (10)	0.0235 (14)	−0.0127 (8)	0.0098 (11)	−0.0094 (9)
C11	0.0271 (11)	0.0249 (10)	0.0418 (16)	−0.0037 (8)	0.0135 (11)	−0.0097 (10)
C12	0.0221 (11)	0.0270 (11)	0.0424 (16)	0.0016 (9)	0.0052 (12)	−0.0005 (10)
C13	0.0188 (10)	0.0279 (10)	0.0250 (13)	−0.0015 (8)	0.0016 (9)	−0.0032 (9)
C14	0.0319 (12)	0.0227 (10)	0.068 (2)	0.0007 (8)	−0.0118 (14)	−0.0102 (13)
C15	0.0412 (14)	0.0471 (14)	0.0294 (14)	0.0052 (12)	0.0090 (13)	−0.0100 (12)

Geometric parameters (Å, º)

Cl1—C9	1.735 (2)	C8—C9	1.386 (3)
O1—C7	1.234 (3)	C8—C13	1.401 (3)
N1—C7	1.346 (3)	C9—C10	1.393 (3)
N1—C1	1.431 (3)	C10—C11	1.383 (4)
N1—H1N	0.831 (17)	C10—H10	0.94 (3)

C1—C6	1.386 (3)	C11—C12	1.380 (4)
C1—C2	1.388 (3)	C11—H11	0.98 (3)
C2—C3	1.399 (3)	C12—C13	1.391 (3)
C2—H2	0.94 (3)	C12—H12	0.91 (3)
C3—C4	1.382 (4)	C13—H13	0.89 (3)
C3—C14	1.512 (3)	C14—H14A	0.9800
C4—C5	1.403 (3)	C14—H14B	0.9800
C4—H4	0.99 (3)	C14—H14C	0.9800
C5—C6	1.392 (3)	C15—H15A	0.9800
C5—C15	1.506 (4)	C15—H15B	0.9800
C6—H6	0.98 (3)	C15—H15C	0.9800
C7—C8	1.501 (3)		

C7—N1—C1	124.70 (17)	C8—C9—C10	121.2 (2)
C7—N1—H1N	117.2 (19)	C8—C9—Cl1	120.74 (16)
C1—N1—H1N	118.1 (19)	C10—C9—Cl1	118.02 (19)
C6—C1—C2	120.7 (2)	C11—C10—C9	119.5 (2)
C6—C1—N1	120.94 (18)	C11—C10—H10	122.3 (18)
C2—C1—N1	118.4 (2)	C9—C10—H10	118.1 (18)
C1—C2—C3	120.1 (2)	C12—C11—C10	120.4 (2)
C1—C2—H2	120.5 (16)	C12—C11—H11	116.7 (18)
C3—C2—H2	119.2 (16)	C10—C11—H11	122.8 (18)
C4—C3—C2	118.7 (2)	C11—C12—C13	119.8 (2)
C4—C3—C14	121.3 (2)	C11—C12—H12	118 (2)
C2—C3—C14	119.9 (2)	C13—C12—H12	122 (2)
C3—C4—C5	121.8 (2)	C12—C13—C8	120.7 (2)
C3—C4—H4	122.2 (16)	C12—C13—H13	120.8 (17)
C5—C4—H4	116.0 (16)	C8—C13—H13	118.5 (17)
C6—C5—C4	118.4 (2)	C3—C14—H14A	109.5
C6—C5—C15	120.3 (2)	C3—C14—H14B	109.5
C4—C5—C15	121.3 (2)	H14A—C14—H14B	109.5
C1—C6—C5	120.2 (2)	C3—C14—H14C	109.5
C1—C6—H6	124.8 (16)	H14A—C14—H14C	109.5
C5—C6—H6	114.9 (16)	H14B—C14—H14C	109.5
O1—C7—N1	124.76 (19)	C5—C15—H15A	109.5
O1—C7—C8	120.18 (18)	C5—C15—H15B	109.5
N1—C7—C8	115.01 (18)	H15A—C15—H15B	109.5
C9—C8—C13	118.23 (19)	C5—C15—H15C	109.5
C9—C8—C7	122.49 (19)	H15A—C15—H15C	109.5
C13—C8—C7	119.0 (2)	H15B—C15—H15C	109.5

C7—N1—C1—C6	−42.6 (3)	O1—C7—C8—C9	−57.9 (3)
C7—N1—C1—C2	138.7 (2)	N1—C7—C8—C9	124.6 (2)
C6—C1—C2—C3	−0.3 (3)	O1—C7—C8—C13	116.2 (2)
N1—C1—C2—C3	178.36 (19)	N1—C7—C8—C13	−61.3 (3)
C1—C2—C3—C4	1.4 (3)	C13—C8—C9—C10	−2.1 (3)
C1—C2—C3—C14	−178.6 (2)	C7—C8—C9—C10	172.08 (18)
C2—C3—C4—C5	−1.2 (4)	C13—C8—C9—Cl1	175.77 (15)

C14—C3—C4—C5	178.8 (2)	C7—C8—C9—Cl1	−10.1 (3)
C3—C4—C5—C6	−0.2 (4)	C8—C9—C10—C11	−0.2 (3)
C3—C4—C5—C15	−179.8 (2)	Cl1—C9—C10—C11	−178.07 (16)
C2—C1—C6—C5	−1.1 (3)	C9—C10—C11—C12	1.9 (3)
N1—C1—C6—C5	−179.7 (2)	C10—C11—C12—C13	−1.3 (3)
C4—C5—C6—C1	1.3 (3)	C11—C12—C13—C8	−1.1 (3)
C15—C5—C6—C1	−179.0 (2)	C9—C8—C13—C12	2.7 (3)
C1—N1—C7—O1	−2.2 (4)	C7—C8—C13—C12	−171.68 (19)
C1—N1—C7—C8	175.16 (19)		

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)	2.12 (2)	2.918 (2)	161 (2)

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