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2-Phenylimidazo[1,2-*a*]pyridine-3-carbaldehyde

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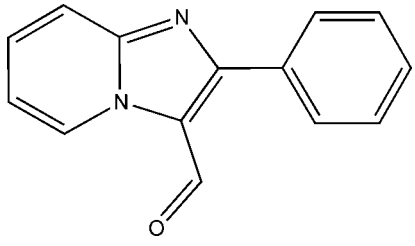
Key indicators: single-crystal X-ray study; T = 120 K; mean σ(C–C) = 0.002 Å; R factor = 0.032; wR factor = 0.078; data-to-parameter ratio = 14.3.

In the title compound, $C_{14}H_{10}N_2O$, the dihedral angle between the imidazo[1,2-*a*]pyridine and phenyl rings is 28.61 (4)° The molecules are connected into broad chains parallel to the *a* axis by weak C—H···O and C—H···N hydrogen bonds. The linking of the ribbons is provided by π–π stacking interactions between neighbouring pyridine rings, with a centroid–centroid distance of 3.7187 (7) Å.

Related literature

For general background, see Anaflous *et al.* (2008) and references therein. For related literature, see: Meth-Cohn & Stanforth (1991).



Experimental

Crystal data

$C_{14}H_{10}N_2O$
M_r = 222.2
Orthorhombic, *Pbca*
a = 13.0640 (3) Å
b = 7.4162 (2) Å
c = 21.6698 (6) Å
V = 2099.48 (9) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.09 mm^{-1}
T = 120 K
0.57 × 0.40 × 0.24 mm

Data collection

Oxford Diffraction Xcalibur2 diffractometer with Sapphire2 CCD detector
Absorption correction: none
25795 measured reflections
2196 independent reflections
1305 reflections with $I > 3\sigma(I)$
R_{int} = 0.049

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.077
S = 1.04
2196 reflections
154 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.15 e Å^{-3}
$\Delta\rho_{min}$ = −0.16 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C4—H4···N1^{i}	0.96	2.50	3.4386 (18)	165
C6—H6···O1^{ii}	0.96	2.46	3.1856 (16)	133

Symmetry codes: (i) $-x+1, -y, -z$; (ii) $-x, -y, -z$.

Data collection: *CrysAlis CCD* (Oxford Diffraction, 2006); cell refinement: *CrysAlis RED* (Oxford Diffraction, 2006); data reduction: *CrysAlis RED*; program(s) used to solve structure: *SIR2002* (Burla *et al.*, 2003); program(s) used to refine structure: *JANA2000* (Petříček *et al.*, 2000); molecular graphics: *DIAMOND* (Brandenburg & Putz, 2005); software used to prepare material for publication: *JANA2000*.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BG2180).

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supporting information

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2-Phenylimidazo[1,2-*a*]pyridine-3-carbaldehyde

Abderrahman Anaflous, Hanane Albay, Nour-eddine Benchat, Brahim El Bali, Michal Dušek and Karla Fejfarová

S1. Comment

Functionalized imidazo[1,2-*a*]pyridine and imidazo[1,2-*a*]pyrimidine systems are of great interest due to their biological activities (Anaflous *et al.*, 2008 and reference herein).

The structure of *N*-(2-phenylimidazo[1,2-*a*]pyridin-3-yl)acetamide(I) consists of isolated molecules which packing is shown in Fig. 1. The space conformation of the molecule (Fig. 2) is characterized by the dihedral angle of 28.61 (4) ° between the imidazo[1,2-*a*]pyridine and the phenyl rings. Weak C—H···N and C—H···O intermolecular hydrogen bonds (Table 1) connect the molecules into chains in the a direction (Fig. 3). The connection between ribbons along b (Fig. 1) is provided by π-π stacking interactions involving neighbouring pyridine rings with centroid-centroid distance 3.7187 (7) Å.

S2. Experimental

Imidazo[1,2-*a*]pyridine-2-phenyl-3-carbaldehyde was synthesized according to the method described by Vilsmeier-Haack (Meth-Cohn & Stanforth, 1991) : *i.e.* to 1.9 g (26 mmol) of DMF cooled at 273 K, containing 4 g (26 mmol) of phosphorus oxychloride ($POCl_3$), was added portionwise to 10 mmole of 2-phenyl imidazo[1,2-*a*]pyridine. The mixture was heated at 373 K for 1 h. The solution was then neutralized at 273 K with Na_2CO_3 and extracted with Dichloromethane. The organic layer was dried over sodium sulfate and dichloromethane was removed under reduced pressure. The crude product was purified on silica gel column and imidazo[1,2-*a*]pyridine-2-phenyl-3-carbaldehyde was obtained in good yield (60%) as a white solid.

S3. Refinement

All the hydrogens (bonded to C atoms) were discernible in difference Fourier maps but according to standard procedures for organic compounds they were constrained to ideal positions (C-H: 0.96Å). Their isotropic atomic displacement parameters were evaluated as 1.2*U_{eq} of the parent atom.

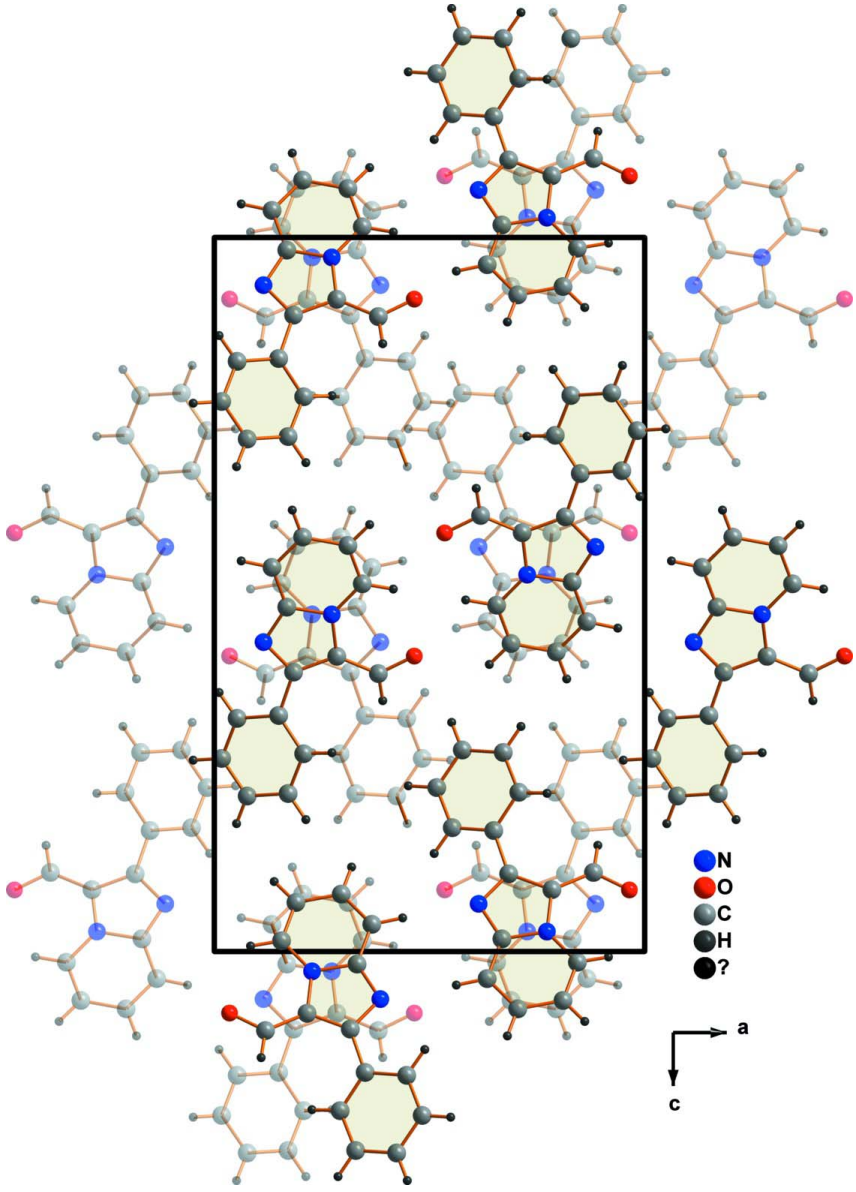

Figure 1

Packing of of Imidazo[1,2-*a*]pyridine-2-phenyl-3-carbaldehyde viewed along the *b* axis. Hydrogen bonds are not indicated.

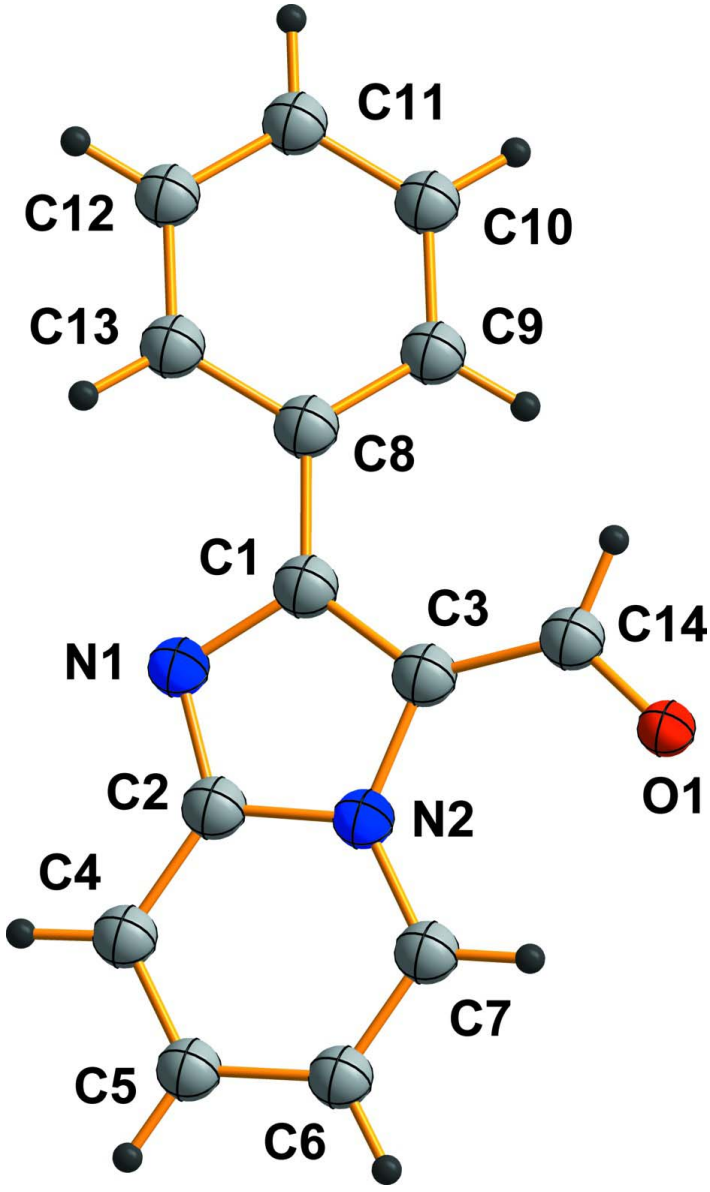

Figure 2

A molecule of the title compound, with 50% displacement ellispoids for non-H atoms.

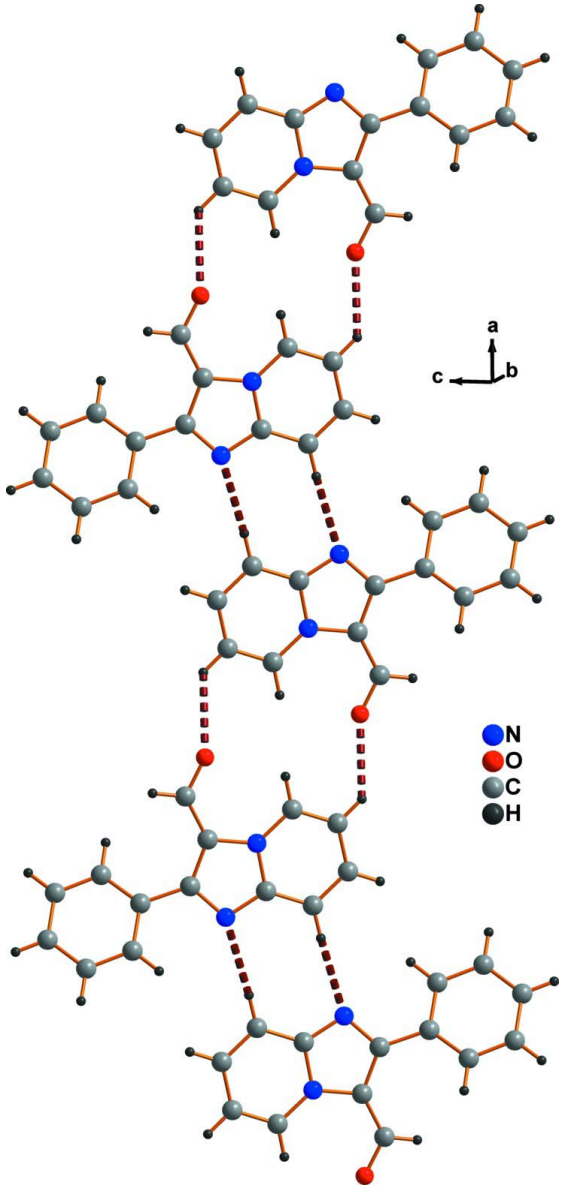

Figure 3

Part of a ribbon along the *a* axis showing intermolecular hydrogen bonds.

2-Phenylimidazo[1,2-*a*]pyridine-3-carbaldehyde

Crystal data

$C_{14}H_{10}N_2O$
$M_r = 222.2$
Orthorhombic, *Pbca*
Hall symbol: -P 2ac 2ab
$a = 13.0640\ (3)$ Å
$b = 7.4162\ (2)$ Å
$c = 21.6698\ (6)$ Å
$V = 2099.48\ (9)$ Å^3
$Z = 8$
$F(000) = 928$
$D_x = 1.406$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å
Cell parameters from 8746 reflections
$\theta = 2.7–26.5°$
$\mu = 0.09$ mm^{-1}
$T = 120$ K
Prism, colourless
0.57 × 0.40 × 0.24 mm

Data collection

Oxford Diffraction Xcalibur2 diffractometer with Sapphire2 CCD detector
Radiation source: X-ray tube
Graphite monochromator
Detector resolution: 8.3438 pixels mm^{-1}
Rotation method data acquisition using ω scans
25795 measured reflections
2196 independent reflections
1305 reflections with $I > 3\sigma(I)$
$R_{int} = 0.049$
$\theta_{max} = 26.6°$, $\theta_{min} = 3.1°$
$h = -16 \rightarrow 16$
$k = -9 \rightarrow 9$
$l = -27 \rightarrow 27$

Refinement

Refinement on F^2
$R[F^2 > 2\sigma(F^2)] = 0.031$
$wR(F^2) = 0.077$
$S = 1.04$
2196 reflections
154 parameters
0 restraints
36 constraints
H-atom parameters constrained
Weighting scheme based on measured s.u.'s $w = 1/[\sigma^2(I) + 0.0016I^2]$
$(\Delta/\sigma)_{max} = 0.007$
$\Delta\rho_{max} = 0.15$ e Å^{-3}
$\Delta\rho_{min} = -0.16$ e Å^{-3}

Special details

Refinement. The refinement was carried out against all reflections. The conventional *R*-factor is always based on *F*. The goodness of fit as well as the weighted *R*-factor are based on *F* and F^2 for refinement carried out on *F* and F^2, respectively. The threshold expression is used only for calculating *R*-factors *etc*. and it is not relevant to the choice of reflections for refinement.
All the H atoms were discernible in difference Fourier maps and could be refined to reasonable geometry. According to standard procedures for organic compounds the H atoms bonded to C atoms were constrained to ideal positions. The isotropic atomic displacement parameters of hydrogen atoms were evaluated as $1.2*U_{eq}$ of the parent atom.
The program used for refinement, Jana2006, uses the weighting scheme based on the experimental expectations, see _refine_ls_weighting_details, that does not force *S* to be one. Therefore the values of *S* are usually larger than the ones from the *SHELX* program.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}
N1	0.38579 (8)	0.13099 (13)	0.06669 (5)	0.0227 (3)
N2	0.22707 (8)	0.09004 (13)	0.02784 (5)	0.0204 (3)
O1	0.03531 (7)	0.19646 (11)	0.08623 (4)	0.0297 (3)
C1	0.31590 (10)	0.18666 (16)	0.10870 (6)	0.0208 (4)
C2	0.33161 (10)	0.07295 (16)	0.01765 (6)	0.0207 (4)
C3	0.21543 (10)	0.16659 (16)	0.08658 (6)	0.0204 (4)
C4	0.36597 (11)	−0.00163 (16)	−0.03801 (6)	0.0235 (4)
C5	0.29491 (10)	−0.05736 (17)	−0.08037 (7)	0.0243 (4)
C6	0.18958 (10)	−0.03859 (17)	−0.06861 (6)	0.0247 (4)
C7	0.15617 (10)	0.03543 (16)	−0.01503 (6)	0.0236 (4)
C8	0.35054 (10)	0.25310 (16)	0.16940 (6)	0.0214 (4)
C9	0.29235 (10)	0.23521 (17)	0.22302 (7)	0.0238 (4)
C10	0.32855 (11)	0.30105 (17)	0.27874 (7)	0.0274 (5)
C11	0.42372 (11)	0.38290 (17)	0.28223 (6)	0.0283 (5)
C12	0.48307 (11)	0.39863 (17)	0.22959 (6)	0.0282 (4)
C13	0.44708 (10)	0.33402 (16)	0.17344 (6)	0.0242 (4)
C14	0.11885 (10)	0.22273 (16)	0.11073 (7)	0.0245 (4)
H4	0.437543	−0.014444	−0.047038	0.0282*
H5	0.318903	−0.109503	−0.118246	0.0292*

H6	0.139117	−0.077351	−0.097954	0.0296*
H7	0.084111	0.048834	−0.007645	0.0283*
H9	0.226757	0.177012	0.221555	0.0286*
H10	0.287357	0.289867	0.315233	0.0329*
H11	0.448433	0.4285	0.320918	0.0339*
H12	0.549259	0.454408	0.232038	0.0339*
H13	0.489068	0.345338	0.137292	0.0291*
H14	0.108688	0.287015	0.148695	0.0294*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
N1	0.0207 (6)	0.0225 (5)	0.0249 (6)	0.0004 (5)	0.0004 (5)	0.0017 (5)
N2	0.0196 (6)	0.0177 (5)	0.0239 (6)	−0.0005 (5)	−0.0001 (5)	0.0031 (5)
O1	0.0200 (6)	0.0315 (5)	0.0376 (6)	0.0000 (4)	−0.0002 (5)	0.0024 (5)
C1	0.0221 (7)	0.0149 (7)	0.0255 (8)	0.0007 (6)	0.0019 (6)	0.0052 (6)
C2	0.0192 (7)	0.0170 (6)	0.0259 (8)	−0.0002 (6)	0.0015 (6)	0.0051 (6)
C3	0.0211 (7)	0.0179 (6)	0.0223 (7)	−0.0008 (6)	0.0022 (6)	0.0026 (6)
C4	0.0219 (8)	0.0224 (7)	0.0263 (8)	−0.0005 (6)	0.0024 (6)	0.0027 (6)
C5	0.0281 (8)	0.0201 (7)	0.0248 (8)	−0.0015 (6)	0.0020 (6)	0.0031 (6)
C6	0.0245 (8)	0.0220 (7)	0.0275 (8)	−0.0044 (6)	−0.0037 (6)	0.0023 (6)
C7	0.0194 (8)	0.0225 (7)	0.0289 (8)	−0.0025 (6)	−0.0031 (6)	0.0043 (6)
C8	0.0228 (8)	0.0155 (6)	0.0260 (8)	0.0027 (6)	−0.0010 (6)	0.0032 (5)
C9	0.0216 (8)	0.0212 (7)	0.0288 (8)	−0.0003 (6)	−0.0001 (7)	0.0034 (6)
C10	0.0313 (8)	0.0267 (7)	0.0242 (8)	0.0049 (7)	0.0017 (7)	0.0034 (6)
C11	0.0330 (8)	0.0255 (7)	0.0263 (8)	0.0053 (7)	−0.0057 (7)	−0.0006 (6)
C12	0.0266 (8)	0.0242 (7)	0.0339 (8)	−0.0021 (6)	−0.0043 (7)	0.0013 (7)
C13	0.0243 (8)	0.0222 (7)	0.0263 (8)	0.0009 (6)	0.0007 (6)	0.0032 (6)
C14	0.0262 (8)	0.0201 (7)	0.0271 (8)	0.0008 (7)	0.0032 (7)	0.0041 (6)

Geometric parameters (Å, º)

N1—C1	1.3537 (16)	C6—H6	0.9600
N1—C2	1.3475 (16)	C7—H7	0.9600
N2—C2	1.3893 (16)	C8—C9	1.3949 (19)
N2—C3	1.4020 (17)	C8—C13	1.3994 (18)
N2—C7	1.3731 (17)	C9—C10	1.386 (2)
O1—C14	1.2293 (16)	C9—H9	0.9600
C1—C3	1.4052 (18)	C10—C11	1.3857 (19)
C1—C8	1.4758 (18)	C10—H10	0.9600
C2—C4	1.4008 (18)	C11—C12	1.3840 (19)
C3—C14	1.4279 (18)	C11—H11	0.9600
C4—C5	1.3693 (19)	C12—C13	1.3897 (19)
C4—H4	0.9600	C12—H12	0.9600
C5—C6	1.4063 (18)	C13—H13	0.9600
C5—H5	0.9600	C14—H14	0.9600
C6—C7	1.3564 (19)		

C1—N1—C2	105.87 (10)	N2—C7—H7	121.20
C2—N2—C3	106.74 (10)	C6—C7—H7	120.02
C2—N2—C7	121.92 (11)	C1—C8—C9	122.93 (12)
C3—N2—C7	131.34 (11)	C1—C8—C13	118.38 (12)
N1—C1—C3	111.62 (11)	C9—C8—C13	118.67 (12)
N1—C1—C8	119.62 (11)	C8—C9—C10	120.43 (12)
C3—C1—C8	128.74 (12)	C8—C9—H9	120.11
N1—C2—N2	111.21 (11)	C10—C9—H9	119.46
N1—C2—C4	129.56 (12)	C9—C10—C11	120.53 (13)
N2—C2—C4	119.21 (11)	C9—C10—H10	119.74
N2—C3—C1	104.54 (11)	C11—C10—H10	119.73
N2—C3—C14	123.14 (12)	C10—C11—C12	119.65 (13)
C1—C3—C14	132.02 (12)	C10—C11—H11	120.24
C2—C4—C5	118.63 (12)	C12—C11—H11	120.11
C2—C4—H4	121.78	C11—C12—C13	120.19 (12)
C5—C4—H4	119.59	C11—C12—H12	119.70
C4—C5—C6	120.80 (13)	C13—C12—H12	120.11
C4—C5—H5	118.26	C8—C13—C12	120.50 (12)
C6—C5—H5	120.94	C8—C13—H13	120.09
C5—C6—C7	120.66 (12)	C12—C13—H13	119.40
C5—C6—H6	121.49	O1—C14—C3	125.44 (13)
C7—C6—H6	117.85	O1—C14—H14	109.03
N2—C7—C6	118.78 (12)	C3—C14—H14	125.53

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C4—H4···N1^{i}	0.96	2.50	3.4386 (18)	165
C6—H6···O1^{ii}	0.96	2.46	3.1856 (16)	133

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