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2-[(1-Benzyl-1*H*-1,2,3-triazol-4-yl)methoxy]-1-naphthaldehyde

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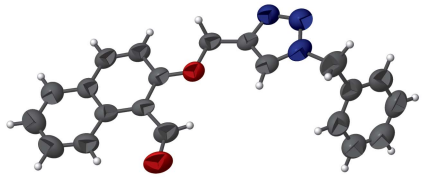
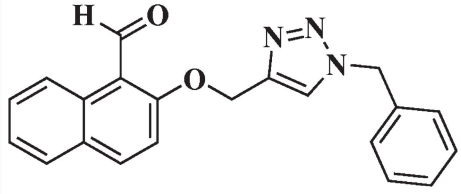
In the title compound, $C_{21}H_{17}N_3O_2$, the triazole ring system is inclined at dihedral angles of 4.14 (18) and 69.24 (11)° with the naphthalene ring system and phenyl ring, respectively. In the crystal, molecules are linked by C—H···O hydrogen bonds into double columns propagating along the *b*-axis direction.

3D view



Chemical scheme



Structure description

Aldehyde derivatives are starting materials for obtaining Schiff bases and oxime-type ligands and their transition-metal complexes (Vigato & Tamburini, 2004). Heterocycles containing a 1,2,3-triazole ring have been utilized in cancer cell treatment (Yadav *et al.*, 2017). As part of our studies in this area, we now describe the synthesis and structure of the title compound (Fig. 1).

The 1,2,3-triazole ring (C13/C14/N1–N3) is almost planar with an r.m.s. deviation of 0.0006 Å. The triazole ring subtends dihedral angles of 4.14 (18) and 69.24 (11)° with the naphthalene ring system (C1–C10) and the phenyl ring (C15–C21), respectively. The aldehyde and methoxy groups are slightly twisted away from the naphthalene ring system [C8—C7—C11—O2 = 2.7 (5)° and C12—O1—C6—C5 = −2.2 (4)°]. Atom C13 shows a distorted sp^2 hybridization state with bond angles of 108.5 (3) (N3—C13—C14), 131.4 (2) (C12—C13—C14) and 120.0 (3)° (N3—C13—C12), which are similar to the equivalent bond angles reported for other triazole derivatives (Zhao *et al.*, 2010; Gao *et al.*, 2011).

In the crystal (Fig. 2), atom O2 is a double acceptor of hydrogen bonds (Table 1) from C14—H14 and C21—H21, which generates [010] double columns.

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

D—H···A	D—H	H···A	D···A	D—H···A
C21—H21···O2^{i}	0.93	2.53	3.462 (5)	175
C14—H14···O2^{i}	0.93	2.62	3.497 (4)	157

Symmetry code: (i) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$.

Synthesis and crystallization

A mixture of *o*-propargyloxynaphthaldehyde, (1.0 mmol), benzyl azide (1.0 mmol) and CuI (0.01 mmol) in water (5 ml) was refluxed for 30 minutes. After the completion of the reaction (monitored by TLC), the mixture was poured onto excess of crushed ice. Then, the reaction mixture was washed with a saturated solution of NH_4Cl and extracted with dichloromethane. The organic layer was dried over anhydrous sodium sulfate and concentrated under reduced pressure. The residue was purified by column chromatography using petroleum ether:ethyl acetate (90:10) as eluents to afford the title compound in 85% yield; m.p. 165°C. Colourless blocks were recrystallized from ethanol solution after one week at room temperature.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

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Funding information

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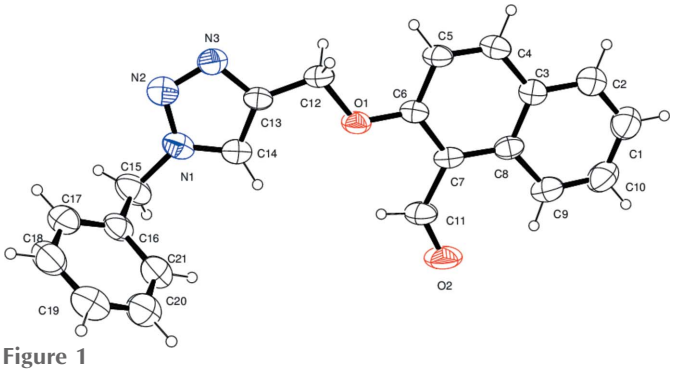

Figure 1
The molecular structure of the compound, showing 30% probability displacement ellipsoids.

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{21}H_{17}N_3O_2$
M_r	343.38
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	296
a, b, c (Å)	14.013 (3), 5.4123 (11), 22.901 (5)
β (°)	93.157 (5)
V (Å^3)	1734.3 (6)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.09
Crystal size (mm)	0.20 × 0.15 × 0.15
Data collection	
Diffractometer	Bruker Kappa APEXII
Absorption correction	Multi-scan (*SADABS*; Bruker, 2009)
T_{min}, T_{max}	0.967, 0.974
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	15604, 3076, 1363
R_{int}	0.063
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.596
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.048, 0.199, 0.87
No. of reflections	3076
No. of parameters	236
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.14, −0.13

Computer programs: *APEX2* and *SAINT* (Bruker, 2009), *SHELXS2013* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012), *SHELXL2014* (Sheldrick, 2015) and *PLATON* (Spek, 2009).

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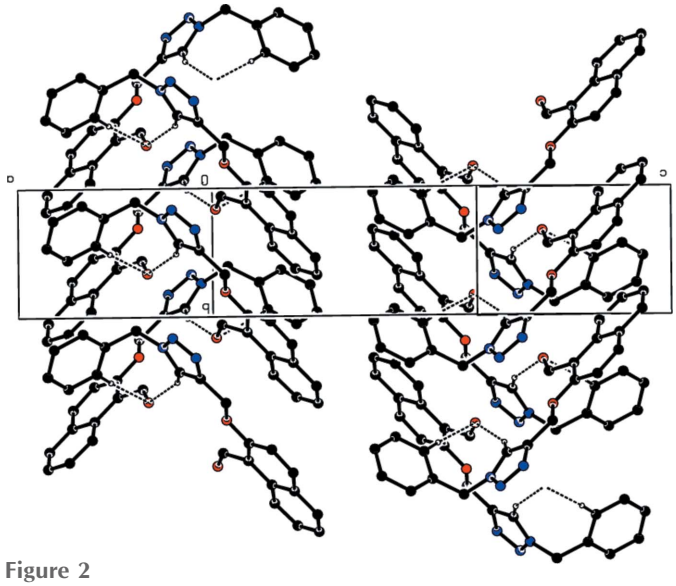

Figure 2
A partial view of the crystal packing of the title compound, illustrating the formation of [010] chains linked by C—H···O hydrogen bonds (dashed lines).

full crystallographic data

IUCrData (2019). **4**, x191525 [https://doi.org/10.1107/S2414314619015256]

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Crystal data

$C_{21}H_{17}N_3O_2$
M_r = 343.38
Monoclinic, $P2_1/n$
a = 14.013 (3) Å
b = 5.4123 (11) Å
c = 22.901 (5) Å
β = 93.157 (5)°
V = 1734.3 (6) Å^3
Z = 4
$F(000)$ = 720
D_x = 1.315 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3076 reflections
θ = 2.9–25.1°
μ = 0.09 mm^{-1}
T = 296 K
Block, colourless
0.20 × 0.15 × 0.15 mm

Data collection

Bruker Kappa APEXII diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 0 pixels mm^{-1}
ω and φ scans
Absorption correction: multi-scan (SADABS; Bruker, 2009)
T_{min} = 0.967, T_{max} = 0.974
15604 measured reflections
3076 independent reflections
1363 reflections with $I > 2\sigma(I)$
R_{int} = 0.063
θ_{max} = 25.1°, θ_{min} = 2.9°
h = −16→16
k = −6→6
l = −27→27

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.199
S = 0.87
3076 reflections
236 parameters
0 restraints
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.1156P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.14 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}
Extinction correction: SHELXL, $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.005 (2)

Special details

Geometry. All esds (except the esd in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell esds are taken into account individually in the estimation of esds in distances, angles and torsion angles; correlations between esds in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell esds is used for estimating esds involving l.s. planes.

Refinement. H atoms were placed at calculated positions and allowed to ride on their carrier atoms with C—H = 0.93–0.98 Å and N—H = 0.86 Å. The constrain U_{iso}(H) = 1.2U_{eq}(C) was applied.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O1	0.63383 (15)	0.3041 (4)	0.10577 (8)	0.0701 (7)
N1	0.4963 (2)	−0.2659 (5)	0.18506 (12)	0.0755 (8)
O2	0.82063 (19)	0.6602 (5)	0.20521 (10)	0.1081 (9)
N3	0.4565 (2)	−0.1807 (6)	0.09637 (12)	0.0799 (9)
C6	0.6788 (2)	0.4857 (6)	0.07659 (12)	0.0576 (8)
C7	0.7493 (2)	0.6202 (6)	0.10804 (12)	0.0582 (8)
C13	0.5244 (2)	−0.0183 (6)	0.11562 (13)	0.0590 (8)
N2	0.4390 (2)	−0.3342 (5)	0.13932 (15)	0.0886 (9)
C8	0.7996 (2)	0.8086 (6)	0.07856 (13)	0.0620 (9)
C12	0.5595 (2)	0.1707 (6)	0.07551 (13)	0.0646 (9)
H12A	0.5834	0.0924	0.0411	0.077*
H12B	0.5080	0.2817	0.0631	0.077*
C3	0.7745 (2)	0.8597 (6)	0.01888 (13)	0.0633 (9)
C14	0.5501 (2)	−0.0716 (6)	0.17178 (13)	0.0670 (9)
H14	0.5953	0.0092	0.1961	0.080*
C4	0.7012 (2)	0.7178 (6)	−0.00971 (14)	0.0713 (10)
H4	0.6840	0.7515	−0.0487	0.086*
C5	0.6555 (2)	0.5365 (6)	0.01725 (13)	0.0673 (9)
H5	0.6086	0.4446	−0.0032	0.081*
C16	0.4240 (3)	−0.2729 (7)	0.28069 (14)	0.0746 (10)
C11	0.7662 (2)	0.5597 (7)	0.16993 (14)	0.0792 (10)
H11	0.7309	0.4286	0.1838	0.095*
C21	0.4500 (3)	−0.0592 (7)	0.30988 (16)	0.0855 (11)
H21	0.5098	0.0091	0.3045	0.103*
C2	0.8223 (3)	1.0431 (7)	−0.01081 (16)	0.0858 (11)
H2	0.8048	1.0744	−0.0499	0.103*
C9	0.8753 (3)	0.9526 (7)	0.10500 (16)	0.0849 (11)
H9	0.8943	0.9267	0.1441	0.102*
C20	0.3902 (4)	0.0555 (8)	0.34662 (17)	0.0959 (12)
H20	0.4098	0.1994	0.3659	0.115*
C1	0.8937 (3)	1.1764 (7)	0.0161 (2)	0.1008 (13)
H1	0.9246	1.2994	−0.0041	0.121*
C17	0.3341 (4)	−0.3686 (8)	0.29026 (17)	0.0987 (13)
H17	0.3139	−0.5131	0.2714	0.118*
C15	0.4910 (3)	−0.3965 (7)	0.24094 (15)	0.0984 (13)
H15A	0.5543	−0.4039	0.2603	0.118*
H15B	0.4696	−0.5647	0.2335	0.118*
C18	0.2738 (3)	−0.2500 (10)	0.3279 (2)	0.1062 (14)
H18	0.2140	−0.3153	0.3344	0.127*
C19	0.3036 (4)	−0.0381 (10)	0.35497 (18)	0.1032 (13)
H19	0.2633	0.0429	0.3796	0.124*
C10	0.9201 (3)	1.1267 (8)	0.0741 (2)	0.1047 (13)

H10	0.9701	1.2156	0.0924	0.126*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0646 (15)	0.0955 (15)	0.0485 (12)	−0.0082 (12)	−0.0110 (11)	0.0004 (11)
N1	0.094 (2)	0.075 (2)	0.0581 (18)	0.0211 (17)	0.0069 (17)	0.0016 (16)
O2	0.101 (2)	0.158 (2)	0.0619 (15)	−0.0213 (18)	−0.0268 (15)	−0.0169 (15)
N3	0.081 (2)	0.094 (2)	0.0638 (18)	−0.0140 (18)	−0.0010 (16)	−0.0077 (17)
C6	0.051 (2)	0.075 (2)	0.0471 (17)	0.0086 (17)	0.0010 (15)	−0.0053 (16)
C7	0.0511 (19)	0.074 (2)	0.0482 (17)	0.0112 (17)	−0.0057 (15)	−0.0151 (16)
C13	0.060 (2)	0.070 (2)	0.0463 (18)	0.0099 (18)	0.0025 (16)	−0.0082 (16)
N2	0.100 (3)	0.092 (2)	0.074 (2)	−0.0071 (18)	0.0064 (19)	−0.0061 (18)
C8	0.057 (2)	0.070 (2)	0.059 (2)	0.0109 (18)	−0.0025 (17)	−0.0159 (17)
C12	0.060 (2)	0.083 (2)	0.0495 (18)	0.0016 (18)	−0.0069 (16)	−0.0110 (17)
C3	0.058 (2)	0.071 (2)	0.061 (2)	0.0074 (17)	0.0051 (17)	−0.0032 (17)
C14	0.071 (2)	0.073 (2)	0.057 (2)	0.0108 (19)	−0.0024 (17)	−0.0062 (17)
C4	0.069 (2)	0.095 (2)	0.0494 (19)	0.005 (2)	−0.0019 (18)	0.0007 (18)
C5	0.062 (2)	0.091 (2)	0.0479 (18)	−0.0009 (19)	−0.0100 (16)	−0.0042 (17)
C16	0.105 (3)	0.063 (2)	0.056 (2)	0.013 (2)	0.006 (2)	0.0117 (18)
C11	0.071 (2)	0.109 (3)	0.056 (2)	0.000 (2)	−0.0137 (18)	−0.008 (2)
C21	0.099 (3)	0.083 (3)	0.077 (2)	0.012 (2)	0.018 (2)	0.011 (2)
C2	0.092 (3)	0.089 (2)	0.077 (2)	−0.006 (2)	0.005 (2)	−0.002 (2)
C9	0.082 (3)	0.099 (3)	0.072 (2)	−0.006 (2)	−0.006 (2)	−0.019 (2)
C20	0.116 (4)	0.088 (3)	0.084 (3)	0.012 (3)	0.013 (3)	0.003 (2)
C1	0.102 (3)	0.094 (3)	0.106 (3)	−0.017 (3)	0.009 (3)	−0.004 (3)
C17	0.137 (4)	0.092 (3)	0.065 (3)	−0.014 (3)	−0.006 (3)	0.011 (2)
C15	0.139 (4)	0.085 (2)	0.073 (2)	0.035 (2)	0.012 (2)	0.016 (2)
C18	0.100 (3)	0.143 (4)	0.077 (3)	−0.010 (3)	0.016 (3)	0.019 (3)
C19	0.115 (4)	0.117 (4)	0.079 (3)	0.020 (3)	0.015 (3)	0.006 (3)
C10	0.099 (3)	0.108 (3)	0.106 (4)	−0.034 (3)	−0.004 (3)	−0.018 (3)

Geometric parameters (Å, º)

O1—C6	1.362 (3)	C5—H5	0.9300
O1—C12	1.416 (3)	C16—C21	1.375 (5)
N1—N2	1.337 (4)	C16—C17	1.391 (5)
N1—C14	1.338 (4)	C16—C15	1.501 (5)
N1—C15	1.467 (4)	C11—H11	0.9300
O2—C11	1.210 (3)	C21—C20	1.369 (5)
N3—N2	1.321 (4)	C21—H21	0.9300
N3—C13	1.352 (4)	C2—C1	1.354 (5)
C6—C7	1.395 (4)	C2—H2	0.9300
C6—C5	1.407 (4)	C9—C10	1.353 (5)
C7—C8	1.430 (4)	C9—H9	0.9300
C7—C11	1.461 (4)	C20—C19	1.338 (5)
C13—C14	1.347 (4)	C20—H20	0.9300
C13—C12	1.477 (4)	C1—C10	1.386 (5)

C8—C3	1.420 (4)	C1—H1	0.9300
C8—C9	1.425 (4)	C17—C18	1.396 (6)
C12—H12A	0.9700	C17—H17	0.9300
C12—H12B	0.9700	C15—H15A	0.9700
C3—C2	1.395 (4)	C15—H15B	0.9700
C3—C4	1.415 (4)	C18—C19	1.358 (5)
C14—H14	0.9300	C18—H18	0.9300
C4—C5	1.341 (4)	C19—H19	0.9300
C4—H4	0.9300	C10—H10	0.9300

C6—O1—C12	118.4 (2)	C17—C16—C15	122.1 (4)
N2—N1—C14	111.1 (3)	O2—C11—C7	127.6 (3)
N2—N1—C15	119.5 (3)	O2—C11—H11	116.2
C14—N1—C15	129.3 (3)	C7—C11—H11	116.2
N2—N3—C13	108.8 (3)	C20—C21—C16	121.7 (4)
O1—C6—C7	117.2 (3)	C20—C21—H21	119.2
O1—C6—C5	121.7 (3)	C16—C21—H21	119.2
C7—C6—C5	121.1 (3)	C1—C2—C3	121.4 (4)
C6—C7—C8	118.8 (3)	C1—C2—H2	119.3
C6—C7—C11	117.1 (3)	C3—C2—H2	119.3
C8—C7—C11	124.1 (3)	C10—C9—C8	121.0 (3)
C14—C13—N3	108.5 (3)	C10—C9—H9	119.5
C14—C13—C12	131.4 (3)	C8—C9—H9	119.5
N3—C13—C12	120.0 (3)	C19—C20—C21	120.5 (4)
N3—N2—N1	106.3 (3)	C19—C20—H20	119.8
C3—C8—C9	116.2 (3)	C21—C20—H20	119.8
C3—C8—C7	119.4 (3)	C2—C1—C10	118.9 (4)
C9—C8—C7	124.4 (3)	C2—C1—H1	120.5
O1—C12—C13	108.0 (2)	C10—C1—H1	120.5
O1—C12—H12A	110.1	C16—C17—C18	120.7 (4)
C13—C12—H12A	110.1	C16—C17—H17	119.7
O1—C12—H12B	110.1	C18—C17—H17	119.7
C13—C12—H12B	110.1	N1—C15—C16	112.2 (3)
H12A—C12—H12B	108.4	N1—C15—H15A	109.2
C2—C3—C4	121.1 (3)	C16—C15—H15A	109.2
C2—C3—C8	120.5 (3)	N1—C15—H15B	109.2
C4—C3—C8	118.3 (3)	C16—C15—H15B	109.2
N1—C14—C13	105.2 (3)	H15A—C15—H15B	107.9
N1—C14—H14	127.4	C19—C18—C17	119.3 (4)
C13—C14—H14	127.4	C19—C18—H18	120.3
C5—C4—C3	122.5 (3)	C17—C18—H18	120.3
C5—C4—H4	118.8	C20—C19—C18	120.8 (5)
C3—C4—H4	118.8	C20—C19—H19	119.6
C4—C5—C6	119.8 (3)	C18—C19—H19	119.6
C4—C5—H5	120.1	C9—C10—C1	122.0 (4)
C6—C5—H5	120.1	C9—C10—H10	119.0
C21—C16—C17	117.1 (4)	C1—C10—H10	119.0
C21—C16—C15	120.8 (4)		

C12—O1—C6—C7	177.7 (2)	C2—C3—C4—C5	178.4 (3)
C12—O1—C6—C5	−2.2 (4)	C8—C3—C4—C5	−0.6 (5)
O1—C6—C7—C8	178.6 (2)	C3—C4—C5—C6	1.4 (5)
C5—C6—C7—C8	−1.4 (4)	O1—C6—C5—C4	179.6 (3)
O1—C6—C7—C11	−2.0 (4)	C7—C6—C5—C4	−0.3 (4)
C5—C6—C7—C11	177.9 (3)	C6—C7—C11—O2	−176.7 (3)
N2—N3—C13—C14	0.1 (4)	C8—C7—C11—O2	2.7 (5)
N2—N3—C13—C12	178.3 (3)	C17—C16—C21—C20	−0.2 (5)
C13—N3—N2—N1	0.0 (4)	C15—C16—C21—C20	−179.6 (3)
C14—N1—N2—N3	−0.1 (4)	C4—C3—C2—C1	−178.8 (3)
C15—N1—N2—N3	177.6 (3)	C8—C3—C2—C1	0.2 (5)
C6—C7—C8—C3	2.1 (4)	C3—C8—C9—C10	−0.3 (5)
C11—C7—C8—C3	−177.2 (3)	C7—C8—C9—C10	179.5 (3)
C6—C7—C8—C9	−177.6 (3)	C16—C21—C20—C19	−0.3 (6)
C11—C7—C8—C9	3.1 (5)	C3—C2—C1—C10	0.7 (6)
C6—O1—C12—C13	178.4 (2)	C21—C16—C17—C18	0.1 (5)
C14—C13—C12—O1	1.3 (4)	C15—C16—C17—C18	179.5 (3)
N3—C13—C12—O1	−176.4 (3)	N2—N1—C15—C16	−93.1 (4)
C9—C8—C3—C2	−0.4 (4)	C14—N1—C15—C16	84.2 (4)
C7—C8—C3—C2	179.8 (3)	C21—C16—C15—N1	−75.5 (4)
C9—C8—C3—C4	178.6 (3)	C17—C16—C15—N1	105.3 (4)
C7—C8—C3—C4	−1.1 (4)	C16—C17—C18—C19	0.5 (6)
N2—N1—C14—C13	0.2 (3)	C21—C20—C19—C18	0.9 (6)
C15—N1—C14—C13	−177.3 (3)	C17—C18—C19—C20	−1.0 (6)
N3—C13—C14—N1	−0.2 (3)	C8—C9—C10—C1	1.2 (6)
C12—C13—C14—N1	−178.1 (3)	C2—C1—C10—C9	−1.5 (7)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C21—H21···O2^{i}	0.93	2.53	3.462 (5)	175
C14—H14···O2^{i}	0.93	2.62	3.497 (4)	157

Symmetry code: (i) −*x*+3/2, *y*−1/2, −*z*+1/2.