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N-(4-Chlorophenyl)-1,8-naphthalimide

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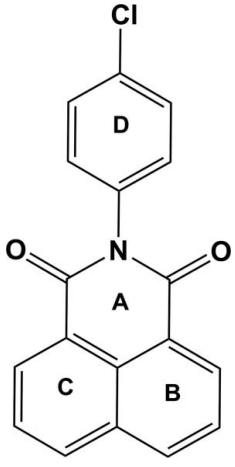
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.005 Å; R factor = 0.053; wR factor = 0.157; data-to-parameter ratio = 12.8.

In the title compound, $C_{18}H_{10}ClNO_2$, the naphthalimide ring system is almost planar, the rings forming dihedral angles of 2.05 (3), 2.26 (3) and 0.80 (3)°. The attached benzene ring of the 4-chlorophenyl substituent is inclined to the mean plane of the naphthalimide ring system by 75.77 (11)°. In the crystal structure, symmetry-related molecules are linked by C—H···O interactions. There are also weak π–π contacts between the naphthalimide rings [centroid–centroid distance = 3.732 (3) Å].

Related literature

For related literature on *N*-substituted 1,8-naphthalimides, see: De Souza *et al.* (2002). For a description of the Cambridge Structural Database, see: Allen (2002). For hydrogen bonding, see: Bernstein *et al.* (1995).



Experimental

Crystal data

$C_{18}H_{10}ClNO_2$
M_r = 307.72
Monoclinic, $P2_1/n$
a = 8.6800 (17) Å
b = 17.553 (4) Å
c = 9.4600 (19) Å
β = 103.53 (3)°
V = 1401.3 (5) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.28 mm^{-1}
T = 293 K
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.921, T_{max} = 0.946
2719 measured reflections
2549 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
3 standard reflections
every 200 reflections
intensity decay: 1%

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.157
S = 1.00
2549 reflections
199 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15—H15A···O2^{i}	0.93	2.45	3.138 (4)	131

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1989); cell refinement: *CAD-4 EXPRESS*; data reduction: *XCAD4* (Harms & Wocadlo, 1995); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *PLATON* (Spek, 2009); software used to prepare material for publication: *SHELXL97*.

The authors thank the Center of Testing and Analysis, Nanjing University for support.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: SU2116).

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supporting information

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N-(4-Chlorophenyl)-1,8-naphthalimide

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S1. Comment

As part of our ongoing studies on N-substituted 1,8-naphthalimides (De Souza et al., 2002), we report herein on the crystal structure of the title compound.

In the title compound, illustrated in Fig. 1, the bond lengths (Allen et al., 1987) and angles are within normal ranges. Rings A (N/C4/C5/C7/C11/C13), B (C1—C6) and C (C5—C11) are oriented with respect to one another by dihedral angles of A/B = 2.05 (3), A/C = 2.26 (3) and B/C = 0.80 (3) °, hence almost coplanar. Rings A, B (C5—C10), C (C9—C14) and D (C12/C14—C18) are oriented at dihedral angles of A/D = 76.89 (3), B/D = 75.93 (3) and C/D = 75.19 (3) °.

In the crystal structure, intermolecular C—H···O hydrogen bonds (Table 1) link the molecules into multimers (Fig. 2) (Bernstein et al., 1996), in which they may be effective in the stabilization of the structure. The π–π contacts between the naphthalimide rings, Cg1—Cg1^{i} [symmetry codes: (i) –X,-Y,-Z, where Cg1 is centroid of ring C] with centroid-centroid distances of 3.732 (3) Å, may further stabilize the structure.

S2. Experimental

For the preparation of the title compound: 1,8-naphthalic anhydride (1.98 g, 0.01 mol) and 2-aminoethanol (1.275 g,0.01 mol) were mixed with acetic acid (50 ml). The reaction mixture was refluxed for 8 h, and then poured into cold water. The resulting solids were filtered off and boiled with an aqueous solution of sodium bicarbonate (10%, 50 ml) for 20 min, and the insoluble solid residues were dried *in vacuo*. Column chromatography on aluminium oxide with benzene as eluent gave a light-brown solution. Crystals suitable for X-ray analysis were obtained by slow evaporation of an acetone solution (yield 94%; m.p. 489 K).

S3. Refinement

H-atoms were positioned geometrically and constrained to ride on their parent atoms: C—H = 0.93 Å with U_{iso}(H) = 1.2U_{eq}(parent C-atom).

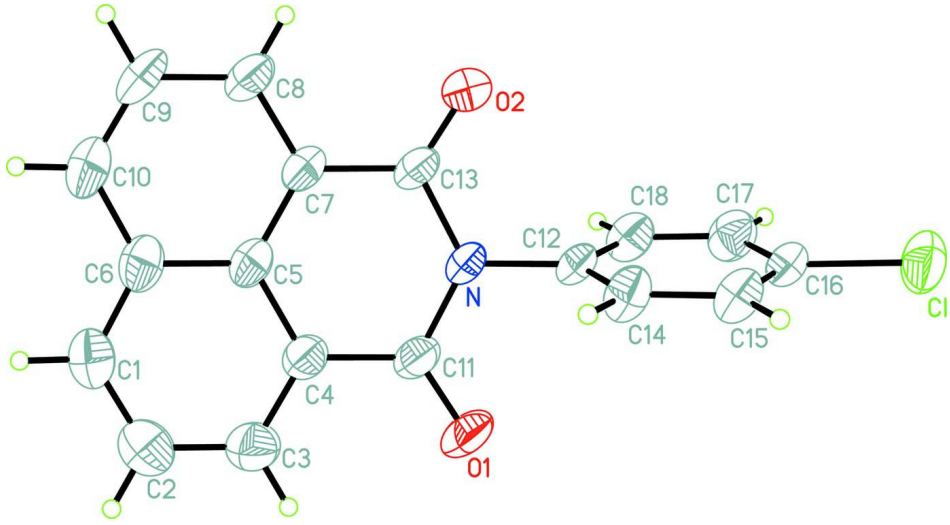

Figure 1

The molecular structure of the title compound, with the atom-numbering scheme. Displacement ellipsoids are drawn at the 50% probability level.

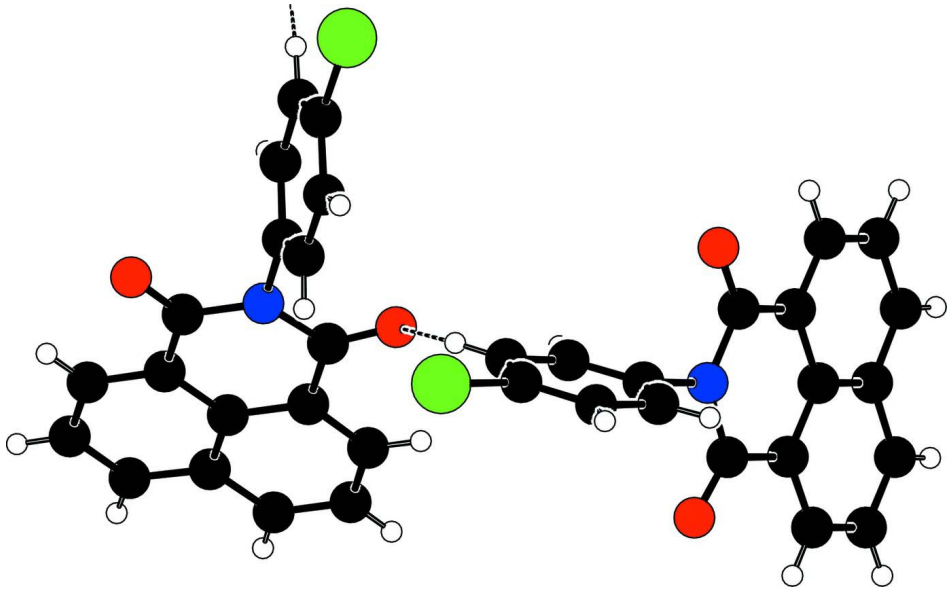

Figure 2

A view of the C-H···O hydrogen bonded (dashed lines) molecules in the title compound.

N-(4-Chlorophenyl)-1,8-naphthalimide

Crystal data

$C_{18}H_{10}ClNO_2$
$M_r = 307.72$
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
$a = 8.6800\ (17)$ Å
$b = 17.553\ (4)$ Å
$c = 9.4600\ (19)$ Å
$\beta = 103.53\ (3)°$
$V = 1401.3\ (5)$ Å^3
$Z = 4$
$F(000) = 632$
$D_x = 1.459$ Mg m^{-3}
Melting point: 505 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å

Cell parameters from 25 reflections
θ = 9–13°
μ = 0.28 mm^{-1}
T = 293 K
Block, green
0.30 × 0.20 × 0.20 mm

Data collection

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: ψ scan (North *et al.*, 1968)
T_{min} = 0.921, T_{max} = 0.946
2719 measured reflections
2549 independent reflections
1843 reflections with $I > 2\sigma(I)$
R_{int} = 0.048
θ_{max} = 25.3°, θ_{min} = 2.3°
h = 0→10
k = 0→21
l = −11→11
3 standard reflections every 200 reflections
intensity decay: 1%

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.053
$wR(F^2)$ = 0.157
S = 1.00
2549 reflections
199 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: inferred from neighbouring sites
H-atom parameters constrained
$w = 1/[\sigma^2(F_o^2) + (0.07P)^2 + 1.5P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.30 e Å^{-3}
$\Delta\rho_{min}$ = −0.23 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}
Cl	0.48706 (11)	0.18516 (6)	0.29044 (9)	0.0612 (3)
N	0.6288 (3)	0.39484 (14)	−0.1550 (2)	0.0381 (6)
O1	0.7353 (3)	0.48058 (14)	0.0210 (2)	0.0637 (7)
C1	0.8795 (5)	0.5908 (2)	−0.4218 (4)	0.0606 (10)
H1A	0.9182	0.6195	−0.4886	0.073*
O2	0.5248 (3)	0.30743 (13)	−0.3284 (2)	0.0555 (6)
C2	0.9122 (5)	0.6132 (2)	−0.2792 (4)	0.0705 (11)
H2A	0.9710	0.6572	−0.2507	0.085*
C3	0.8580 (4)	0.57040 (19)	−0.1762 (4)	0.0570 (9)
H3A	0.8824	0.5856	−0.0794	0.068*
C4	0.7693 (4)	0.50637 (17)	−0.2166 (3)	0.0413 (7)
C5	0.7317 (4)	0.48249 (17)	−0.3649 (3)	0.0385 (7)

C6	0.7888 (4)	0.52546 (18)	−0.4695 (3)	0.0459 (8)
C7	0.6412 (3)	0.41605 (17)	−0.4090 (3)	0.0373 (7)
C8	0.6044 (4)	0.3947 (2)	−0.5531 (3)	0.0498 (8)
H8A	0.5435	0.3514	−0.5818	0.060*
C9	0.6577 (4)	0.4375 (2)	−0.6567 (3)	0.0585 (10)
H9A	0.6311	0.4227	−0.7538	0.070*
C10	0.7487 (4)	0.5009 (2)	−0.6164 (4)	0.0541 (9)
H10A	0.7849	0.5284	−0.6863	0.065*
C11	0.7125 (4)	0.46182 (17)	−0.1071 (3)	0.0421 (7)
C12	0.5915 (4)	0.34481 (17)	−0.0448 (3)	0.0376 (7)
C13	0.5918 (4)	0.36798 (18)	−0.2992 (3)	0.0393 (7)
C14	0.7103 (4)	0.30126 (18)	0.0375 (3)	0.0442 (8)
H14A	0.8121	0.3040	0.0222	0.053*
C15	0.6788 (4)	0.25313 (19)	0.1435 (3)	0.0464 (8)
H15A	0.7592	0.2243	0.2014	0.056*
C16	0.5257 (4)	0.24902 (17)	0.1611 (3)	0.0406 (7)
C17	0.4056 (4)	0.29174 (19)	0.0787 (3)	0.0477 (8)
H17A	0.3029	0.2875	0.0915	0.057*
C18	0.4389 (4)	0.34117 (19)	−0.0239 (3)	0.0445 (7)
H18A	0.3595	0.3718	−0.0785	0.053*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cl	0.0701 (6)	0.0711 (6)	0.0452 (5)	−0.0106 (5)	0.0189 (4)	0.0156 (4)
N	0.0516 (15)	0.0418 (14)	0.0203 (11)	−0.0043 (12)	0.0073 (10)	0.0008 (10)
O1	0.103 (2)	0.0626 (16)	0.0255 (11)	−0.0126 (14)	0.0140 (12)	−0.0104 (11)
C1	0.074 (2)	0.057 (2)	0.055 (2)	−0.0123 (19)	0.0224 (19)	0.0097 (17)
O2	0.0732 (16)	0.0572 (15)	0.0352 (12)	−0.0234 (13)	0.0107 (11)	−0.0085 (11)
C2	0.089 (3)	0.055 (2)	0.067 (3)	−0.022 (2)	0.017 (2)	−0.001 (2)
C3	0.075 (2)	0.047 (2)	0.0460 (19)	−0.0097 (18)	0.0081 (17)	−0.0038 (16)
C4	0.0537 (19)	0.0380 (17)	0.0310 (15)	−0.0019 (14)	0.0074 (13)	0.0002 (12)
C5	0.0443 (16)	0.0425 (17)	0.0282 (14)	0.0057 (13)	0.0073 (12)	0.0060 (12)
C6	0.0541 (19)	0.0453 (18)	0.0392 (17)	0.0081 (15)	0.0128 (14)	0.0128 (14)
C7	0.0448 (16)	0.0425 (17)	0.0244 (14)	0.0038 (13)	0.0079 (12)	0.0004 (12)
C8	0.066 (2)	0.057 (2)	0.0255 (15)	−0.0026 (17)	0.0088 (14)	−0.0026 (14)
C9	0.077 (3)	0.078 (3)	0.0226 (15)	0.002 (2)	0.0153 (15)	−0.0007 (16)
C10	0.066 (2)	0.061 (2)	0.0386 (17)	0.0044 (18)	0.0202 (16)	0.0125 (16)
C11	0.0581 (19)	0.0406 (17)	0.0260 (14)	−0.0014 (14)	0.0065 (13)	−0.0029 (12)
C12	0.0516 (18)	0.0420 (16)	0.0199 (13)	−0.0037 (14)	0.0099 (12)	−0.0026 (11)
C13	0.0484 (17)	0.0465 (18)	0.0219 (13)	−0.0011 (15)	0.0057 (12)	−0.0026 (12)
C14	0.0404 (16)	0.059 (2)	0.0346 (16)	0.0050 (15)	0.0117 (13)	0.0071 (14)
C15	0.0506 (19)	0.056 (2)	0.0323 (15)	0.0046 (15)	0.0080 (14)	0.0054 (14)
C16	0.0516 (18)	0.0461 (17)	0.0243 (14)	−0.0066 (14)	0.0094 (13)	−0.0001 (12)
C17	0.0428 (17)	0.064 (2)	0.0399 (17)	−0.0018 (16)	0.0164 (14)	−0.0010 (15)
C18	0.0435 (17)	0.0544 (19)	0.0346 (16)	0.0051 (14)	0.0070 (13)	0.0025 (14)

Geometric parameters (Å, º)

Cl—C16	1.749 (3)	C7—C8	1.377 (4)
N—C11	1.401 (4)	C7—C13	1.477 (4)
N—C13	1.408 (3)	C8—C9	1.396 (5)
N—C12	1.457 (3)	C8—H8A	0.9300
O1—C11	1.226 (3)	C9—C10	1.367 (5)
C1—C2	1.370 (5)	C9—H9A	0.9300
C1—C6	1.404 (5)	C10—H10A	0.9300
C1—H1A	0.9300	C12—C14	1.370 (4)
O2—C13	1.212 (3)	C12—C18	1.386 (4)
C2—C3	1.396 (5)	C14—C15	1.386 (4)
C2—H2A	0.9300	C14—H14A	0.9300
C3—C4	1.365 (4)	C15—C16	1.379 (4)
C3—H3A	0.9300	C15—H15A	0.9300
C4—C5	1.427 (4)	C16—C17	1.370 (4)
C4—C11	1.472 (4)	C17—C18	1.382 (4)
C5—C7	1.414 (4)	C17—H17A	0.9300
C5—C6	1.423 (4)	C18—H18A	0.9300
C6—C10	1.418 (5)		
C11—N—C13	125.3 (2)	C8—C9—H9A	119.8
C11—N—C12	117.4 (2)	C9—C10—C6	120.9 (3)
C13—N—C12	117.0 (2)	C9—C10—H10A	119.5
C2—C1—C6	121.5 (3)	C6—C10—H10A	119.5
C2—C1—H1A	119.2	O1—C11—N	119.8 (3)
C6—C1—H1A	119.2	O1—C11—C4	123.3 (3)
C1—C2—C3	120.4 (4)	N—C11—C4	116.9 (2)
C1—C2—H2A	119.8	C14—C12—C18	120.7 (3)
C3—C2—H2A	119.8	C14—C12—N	118.6 (3)
C4—C3—C2	120.5 (3)	C18—C12—N	120.7 (3)
C4—C3—H3A	119.7	O2—C13—N	120.2 (3)
C2—C3—H3A	119.7	O2—C13—C7	122.9 (3)
C3—C4—C5	120.1 (3)	N—C13—C7	116.9 (3)
C3—C4—C11	120.0 (3)	C12—C14—C15	120.1 (3)
C5—C4—C11	119.9 (3)	C12—C14—H14A	120.0
C7—C5—C6	119.5 (3)	C15—C14—H14A	120.0
C7—C5—C4	121.1 (3)	C16—C15—C14	118.5 (3)
C6—C5—C4	119.4 (3)	C16—C15—H15A	120.7
C1—C6—C10	123.6 (3)	C14—C15—H15A	120.7
C1—C6—C5	118.0 (3)	C17—C16—C15	121.9 (3)
C10—C6—C5	118.4 (3)	C17—C16—Cl	120.3 (2)
C8—C7—C5	120.0 (3)	C15—C16—Cl	117.8 (2)
C8—C7—C13	120.2 (3)	C16—C17—C18	119.1 (3)
C5—C7—C13	119.8 (2)	C16—C17—H17A	120.4
C7—C8—C9	120.7 (3)	C18—C17—H17A	120.4
C7—C8—H8A	119.7	C17—C18—C12	119.6 (3)
C9—C8—H8A	119.7	C17—C18—H18A	120.2

C10—C9—C8	120.5 (3)	C12—C18—H18A	120.2
C10—C9—H9A	119.8		

C6—C1—C2—C3	1.1 (6)	C12—N—C11—C4	171.5 (3)
C1—C2—C3—C4	−1.1 (6)	C3—C4—C11—O1	2.9 (5)
C2—C3—C4—C5	0.2 (5)	C5—C4—C11—O1	−177.2 (3)
C2—C3—C4—C11	−179.9 (4)	C3—C4—C11—N	−177.0 (3)
C3—C4—C5—C7	179.5 (3)	C5—C4—C11—N	2.9 (4)
C11—C4—C5—C7	−0.4 (4)	C11—N—C12—C14	−75.1 (4)
C3—C4—C5—C6	0.7 (5)	C13—N—C12—C14	98.6 (3)
C11—C4—C5—C6	−179.3 (3)	C11—N—C12—C18	105.1 (3)
C2—C1—C6—C10	178.5 (4)	C13—N—C12—C18	−81.2 (4)
C2—C1—C6—C5	−0.3 (5)	C11—N—C13—O2	176.7 (3)
C7—C5—C6—C1	−179.5 (3)	C12—N—C13—O2	3.6 (4)
C4—C5—C6—C1	−0.6 (5)	C11—N—C13—C7	−2.1 (4)
C7—C5—C6—C10	1.7 (4)	C12—N—C13—C7	−175.3 (3)
C4—C5—C6—C10	−179.5 (3)	C8—C7—C13—O2	3.4 (5)
C6—C5—C7—C8	−2.1 (4)	C5—C7—C13—O2	−174.2 (3)
C4—C5—C7—C8	179.1 (3)	C8—C7—C13—N	−177.8 (3)
C6—C5—C7—C13	175.4 (3)	C5—C7—C13—N	4.6 (4)
C4—C5—C7—C13	−3.4 (4)	C18—C12—C14—C15	−0.3 (5)
C5—C7—C8—C9	1.0 (5)	N—C12—C14—C15	179.9 (3)
C13—C7—C8—C9	−176.5 (3)	C12—C14—C15—C16	1.5 (5)
C7—C8—C9—C10	0.6 (5)	C14—C15—C16—C17	−0.9 (5)
C8—C9—C10—C6	−1.1 (5)	C14—C15—C16—Cl	177.5 (2)
C1—C6—C10—C9	−178.9 (3)	C15—C16—C17—C18	−0.9 (5)
C5—C6—C10—C9	−0.1 (5)	Cl—C16—C17—C18	−179.3 (2)
C13—N—C11—O1	178.5 (3)	C16—C17—C18—C12	2.1 (5)
C12—N—C11—O1	−8.4 (4)	C14—C12—C18—C17	−1.5 (5)
C13—N—C11—C4	−1.6 (4)	N—C12—C18—C17	178.2 (3)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15—H15*A*···O2^{i}	0.93	2.45	3.138 (4)	131

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