Isopropyl 4-aminobenzoate

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The title compound, C_{10}H_{13}NO_2, crystallizes with two molecules (A and B) in the asymmetric unit. For A, the dihedral angle between the plane of the phenyl ring and the i-propyl substituent is 65.4 (3)° while for B this angle is 67.8 (3)°. In the crystal, the molecules are linked by N—H⋯O and N—H⋯N hydrogen bonds to generate double chains propagating in the [100] direction.

Structure description

Isopropyl 4-aminobenzoate, C_{10}H_{13}NO_2, serves as a model drug in correlation studies between HPLC retention parameters and percutaneous absorption (Fu & Liang, 1994). It functions as an inhibitor or an alternative acceptor substrate in the enzymatic acetylation of p-nitroaniline (Hanna et al., 1990). The related compound risocaine (propyl 4-aminobenzoate) is a local anesthetic (Imai et al., 2006), whereas benzocaine (ethyl 4-aminobenzoate) is utilized as a topical pain reliever (Fischer & Ganellin, 2006).

Some related crystal structures viz., the monoclinic form of ethyl 4-aminobenzoate (Lynch & McColloaghan, 2002), form (II) of benzocaine (Chan et al., 2009; Chan & Wellberry, 2010), 4-methylbenzyl 4-aminobenzoate (Haider et al., 2010), 2-(dimethyl- amino)ethyl 4-aminobenzoate (Li et al., 2019) and a new high-pressure benzocaine polymorph (Patyk-Kaźmierczak & Kaźmierczak, 2020) have been reported.

The present paper reports the synthesis and crystal structure of the title compound, (I). Compound I crystallizes with two molecules in the asymmetric unit (Fig. 1). There are slight differences in the conformations of each molecule: for A, the dihedral angle between the planes of the phenyl ring and its i-propyl substituent is 65.4 (3)° while for B
this angle is 67.8 (3)°. For both molecules, the H atoms of the amino substituents are not coplanar with their attached phenyl ring. This is indicated by the dihedral angles between this group and its phenyl ring [11.5 (3) and 24.2 (5)° for A and B, respectively] and the sum of the angles subtended at the N (358 and 352° for A and B, respectively), which shows that N2 is slightly more pyramidal than N1. These differences in the conformations of A and B are most clearly shown in an overlay of both molecules centered on the phenyl ring of both (Fig. 2).

In the extended structure of I, the molecules are linked by N—H···O and N—H···N hydrogen bonds (Table 1) to generate double chains propagating in the [100] direction (Fig. 2). The chains consist of A···A···A and B···B···B molecules linked by N1—H11N···O2 and N2—H21N···O4 hydrogen bonds, respectively, which both generate C(8) chains, with the N1—H12N···O2 and N2—H22N···O hydrogen bonds cross-linking the chains (Fig. 3).

Synthesis and crystallization
4-Aminobenzoic acid (1.0 g), purchased from Sigma–Aldrich, was taken in a 100 ml round-bottomed flask. Then, 20 ml of 2-propanol and a catalytic amount of conc. H2SO4 was added and the reaction mixture was refluxed for 4 h. The reaction was confirmed to be complete using thin-layer chromatography and the mixture was then quenched with water, the precipitate formed was collected by filtration and dried. Pink needles suitable for single-crystal X-ray diffraction were grown by slow evaporation, at room temperature of a solution in ethyl acetate. Yield (79%), m. p. 355–357 K. The reaction scheme is shown in Fig. 4.

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

| D—H···A | D—H | H···A | D···A | D—H···A |
|---------|------|-------|-------|---------|
| N1—H11N···O2i | 0.87 (2) | 2.23 (2) | 3.060 (4) | 158 (3) |
| N1—H12N···N2ii | 0.88 (2) | 2.39 (2) | 3.269 (5) | 176 (4) |
| N2—H21N···O4i | 0.87 (2) | 2.07 (2) | 2.930 (4) | 168 (4) |
| N2—H22N···O2ii | 0.87 (2) | 2.36 (2) | 3.224 (5) | 172 (4) |

Symmetry codes: (i) x − 1, y, z; (ii) −x, −y, −z + 1.
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Table 2
Experimental details.

| Crystal data | C10H13NO2 |
|--------------|-----------|
| Chemical formula | 179.21 |
| Mr | 179.21 |
| Crystal system, space group | Triclinic, P | |
| Temperature (K) | 296 |
| a, b, c (Å) | 8.405 (1), 11.029 (2), 11.520 (3) |
| α, β, γ (°) | 89.10 (2), 77.06 (2), 87.17 (2) |
| V (Å³) | 1039.5 (4) |
| Z | 4 |
| Radiation type | Mo Kα |
| µ (mm⁻¹) | 0.08 |
| Crystal size (mm) | 0.48 × 0.10 × 0.06 |

Data collection

Diffractometer
Oxford Diffraction Xcalibur CCD

Absorption correction
Multi-scan (CrysAlis RED; Oxford Diffraction, 2009)

Tmin, Tmax
0.461, 1.000

No. of measured, independent and observed [I > 2σ(I)] reflections
6595, 3730, 1275

Rint 0.062

(α/λ)max (Å⁻¹)
0.600

Refinement

R[F² > 2σ(F²)], wR(F²), S
0.083, 0.135, 0.98

No. of reflections
3730

No. of parameters
251

No. of restraints
4

H-atom treatment
H atoms treated by a mixture of independent and constrained refinement

Δρmax, Δρmin (e Å⁻³)
0.11, −0.14

Computer programs: CrysAlis CCD (Oxford Diffraction, 2009), CrysAlis RED (Oxford Diffraction, 2009), SHELXT (Sheldrick, 2015a), SHELXL2014/6 (Sheldrick, 2015b) and SHELXTL (Sheldrick, 2008).

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full crystallographic data

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Isopropyl 4-aminobenzoate

**Crystal data**

\[ \text{C}_{10}\text{H}_{13}\text{NO}_{2} \]  
*Mr* = 179.21  
Triclinic, *P*  
*a* = 8.405 (1) Å  
*b* = 11.029 (2) Å  
*c* = 11.520 (3) Å  
*α* = 89.10 (2)°  
*β* = 77.06 (2)°  
*γ* = 87.17 (2)°  
*V* = 1039.5 (4) Å³  
*Z* = 4  
*F*(000) = 384  
*D*_a = 1.145 Mg m⁻³  
Mo *Kα* radiation, *λ* = 0.71073 Å  
Cell parameters from 837 reflections  
*θ* = 2.6–28.0°  
*μ* = 0.08 mm⁻¹  
*T* = 296 K  
Needle, pink  
0.48 × 0.10 × 0.06 mm

**Data collection**

Oxford Diffraction Xcalibur CCD diffractometer  
Radiation source: Enhance (Mo) X-ray Source  
ω scans  
Absorption correction: multi-scan  
(CrysalisRed; Oxford Diffraction, 2009)  
*T*_min = 0.461, *T*_max = 1.000  
6595 measured reflections

**Refinement**

Refinement on *F*²  
Least-squares matrix: full  
*R*(*F*² > 2σ(*F*²)) = 0.083  
*wR*(*F*²) = 0.135  
*S* = 0.98  
3730 reflections  
251 parameters  
4 restraints  
Primary atom site location: dual  
Secondary atom site location: difference Fourier map  
Hydrogen site location: mixed  
H atoms treated by a mixture of independent and constrained refinement  
*w* = 1/[σ*²(*F*²) + (0.0372*P)²]  
where *P* = (*F*² + 2*F*²)/3  
*(Δ/σ)max* < 0.001  
Δρ_max = 0.11 e Å⁻³  
Δρ_min = −0.14 e Å⁻³

**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. All hydrogen atoms were placed geometrically and refined as riding atoms with their $U_{iso}$ values 1.2 times (1.5 times for CH$_3$) that of their attached atoms.

| Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ($\AA^2$) |
|--------------------------------------------------------------------------------------------------|
| $x$     | $y$     | $z$     | $U_{iso}^*/U_{eq}$ |
| O1 0.8880 (3) | 0.1710 (2) | 0.0611 (2) | 0.0724 (8) |
| O2 0.9815 (3) | 0.0696 (2) | 0.2037 (2) | 0.0859 (10) |
| N1 0.2362 (5) | -0.0792 (3) | 0.3053 (3) | 0.0825 (11) |
| H11N 0.160 (4) | -0.056 (3) | 0.268 (3) | 0.099* |
| H12N 0.207 (4) | -0.116 (3) | 0.374 (2) | 0.099* |
| C1 0.7041 (4) | 0.0527 (3) | 0.1917 (3) | 0.0520 (10) |
| C2 0.6632 (5) | -0.0177 (3) | 0.2936 (4) | 0.0677 (12) |
| H2 0.742114 | -0.036394 | 0.337017 | 0.081* |
| C3 0.5097 (5) | -0.0607 (3) | 0.3327 (3) | 0.0679 (12) |
| H3 0.486052 | -0.107475 | 0.401760 | 0.082* |
| C4 0.3891 (5) | -0.0345 (3) | 0.2689 (4) | 0.0604 (11) |
| C5 0.4306 (5) | 0.0348 (3) | 0.1661 (4) | 0.0666 (11) |
| H5 0.352592 | 0.052365 | 0.121639 | 0.080* |
| C6 0.5839 (5) | 0.0780 (3) | 0.1283 (3) | 0.0609 (11) |
| H6 0.607661 | 0.124870 | 0.059323 | 0.073* |
| C7 0.8696 (5) | 0.0957 (3) | 0.1551 (4) | 0.0627 (11) |
| C8 1.0471 (5) | 0.2228 (4) | 0.0148 (4) | 0.0802 (13) |
| H8 1.133590 | 0.159715 | 0.013890 | 0.096* |
| C9 1.0485 (5) | 0.2620 (4) | -0.1104 (4) | 0.1137 (16) |
| H9A 1.153638 | 0.291440 | -0.146885 | 0.171* |
| H9B 0.965887 | 0.325395 | -0.109877 | 0.171* |
| H9C 1.026744 | 0.194107 | -0.154764 | 0.171* |
| C10 1.0704 (5) | 0.3246 (4) | 0.0924 (4) | 0.1263 (18) |
| H10A 1.176583 | 0.355914 | 0.063178 | 0.190* |
| H10B 1.061486 | 0.295363 | 0.172414 | 0.190* |
| H10C 0.988098 | 0.387900 | 0.091451 | 0.190* |
| O3 0.3779 (3) | 0.4487 (2) | 0.6988 (3) | 0.0712 (8) |
| O4 0.5570 (3) | 0.3581 (2) | 0.5474 (2) | 0.0782 (9) |
| N2 -0.1326 (5) | 0.2278 (4) | 0.4435 (3) | 0.0884 (12) |
| H21N -0.223 (3) | 0.273 (3) | 0.465 (3) | 0.106* |
| H22N -0.113 (5) | 0.185 (3) | 0.379 (2) | 0.106* |
| C11 0.2710 (5) | 0.3471 (3) | 0.5583 (4) | 0.0539 (10) |
| C12 0.2909 (5) | 0.2638 (4) | 0.4678 (4) | 0.0657 (11) |
| H12 0.395305 | 0.233201 | 0.432496 | 0.079* |
| C13 0.1594 (5) | 0.2250 (3) | 0.4288 (4) | 0.0727 (13) |
| H13 0.175830 | 0.167394 | 0.368659 | 0.087* |
| C14 0.0023 (6) | 0.2703 (4) | 0.4777 (4) | 0.0624 (11) |
| C15 -0.0176 (5) | 0.3555 (4) | 0.5675 (3) | 0.0658 (12) |
| H15 -0.121799 | 0.387177 | 0.601576 | 0.079* |
| C16 0.1145 (5) | 0.3934 (3) | 0.6073 (3) | 0.0637 (11) |
| H16 0.098348 | 0.450695 | 0.667688 | 0.076* |
| C17 0.4164 (6) | 0.3833 (3) | 0.5982 (4) | 0.0607 (12) |
### Atomic displacement parameters (Å²)

|      | $U^{11}$  | $U^{22}$  | $U^{33}$  | $U^{12}$  | $U^{13}$  | $U^{23}$  |
|------|-----------|-----------|-----------|-----------|-----------|-----------|
| O1   | 0.062 (2) | 0.0778 (19) | 0.079 (2) | −0.0114 (15) | −0.0180 (16) | 0.0140 (16) |
| O2   | 0.063 (2) | 0.102 (2) | 0.100 (2) | −0.0073 (16) | −0.0353 (18) | 0.0239 (17) |
| N1   | 0.062 (3) | 0.079 (3) | 0.110 (3) | −0.014 (2) | −0.025 (3) | 0.015 (2) |
| C1   | 0.050 (3) | 0.047 (2) | 0.063 (3) | −0.001 (2) | −0.021 (2) | 0.002 (2) |
| C2   | 0.065 (3) | 0.070 (3) | 0.074 (3) | −0.004 (2) | −0.029 (3) | 0.012 (3) |
| C3   | 0.068 (3) | 0.063 (3) | 0.075 (3) | −0.003 (2) | −0.023 (3) | 0.014 (2) |
| C4   | 0.055 (3) | 0.046 (3) | 0.082 (3) | −0.001 (2) | −0.018 (3) | −0.007 (2) |
| C5   | 0.065 (3) | 0.068 (3) | 0.072 (3) | −0.001 (2) | −0.027 (3) | −0.001 (2) |
| C6   | 0.066 (3) | 0.059 (3) | 0.060 (3) | −0.004 (2) | −0.019 (3) | 0.004 (2) |
| C7   | 0.064 (3) | 0.060 (3) | 0.065 (3) | 0.003 (2) | −0.017 (3) | −0.001 (2) |
| C8   | 0.062 (3) | 0.083 (3) | 0.095 (4) | −0.011 (3) | −0.016 (3) | 0.019 (3) |
| C9   | 0.105 (4) | 0.140 (4) | 0.091 (4) | −0.021 (3) | −0.009 (3) | 0.040 (3) |
| C10  | 0.130 (5) | 0.132 (4) | 0.125 (4) | −0.066 (3) | −0.033 (4) | 0.004 (4) |
| O3   | 0.0559 (19) | 0.081 (2) | 0.078 (2) | −0.0044 (15) | −0.0158 (17) | −0.0163 (17) |
| O4   | 0.0491 (18) | 0.088 (2) | 0.092 (2) | 0.0018 (16) | −0.0030 (17) | −0.0148 (16) |
| N2   | 0.063 (3) | 0.112 (4) | 0.091 (3) | 0.005 (2) | −0.019 (3) | −0.032 (2) |
| C11  | 0.050 (3) | 0.055 (3) | 0.055 (3) | 0.001 (2) | −0.008 (2) | 0.004 (2) |
| C12  | 0.050 (3) | 0.075 (3) | 0.068 (3) | 0.007 (2) | −0.007 (2) | −0.003 (2) |
| C13  | 0.061 (3) | 0.080 (3) | 0.079 (3) | 0.008 (3) | −0.020 (3) | −0.020 (2) |
| C14  | 0.055 (3) | 0.068 (3) | 0.065 (3) | −0.004 (3) | −0.014 (3) | −0.001 (2) |
| C15  | 0.046 (3) | 0.078 (3) | 0.069 (3) | 0.007 (2) | 0.005 (2) | −0.009 (3) |
| C16  | 0.064 (3) | 0.060 (3) | 0.064 (3) | 0.003 (3) | −0.009 (3) | −0.006 (2) |
| C17  | 0.066 (3) | 0.048 (3) | 0.065 (3) | −0.001 (3) | −0.009 (3) | 0.006 (2) |
| C18  | 0.062 (3) | 0.084 (3) | 0.089 (3) | −0.010 (3) | −0.020 (3) | −0.013 (3) |
| C19  | 0.104 (4) | 0.125 (4) | 0.109 (4) | 0.001 (3) | −0.048 (3) | −0.003 (3) |
| C20  | 0.107 (4) | 0.108 (4) | 0.142 (5) | 0.005 (3) | −0.035 (3) | −0.052 (4) |

### Geometric parameters (Å, °)

|      | O1—C7 | O3—C17 | O3—C18 | O4—C17 |
|------|-------|--------|--------|--------|
| O1—C7 | 1.340 (4) |       |        |        |
| O1—C8 | 1.465 (4) |       |        |        |
| O2—C7 | 1.218 (4) |       |        |        |
| N1—C4 | 1.373 (5) |       |        |        |
| N1—H11N | 0.870 (18) |        |        |        |
| Bond          | Distance (Å) | Bond          | Distance (Å) | Bond          | Distance (Å) |
|--------------|--------------|--------------|--------------|--------------|--------------|
| N1—H12N      | 0.876 (18)   | N2—H22N      | 0.866 (18)   |
| C1—C2        | 1.384 (4)    | C11—C12      | 1.377 (4)    |
| C1—C6        | 1.389 (4)    | C11—C16      | 1.386 (4)    |
| C1—C7        | 1.461 (5)    | C11—C17      | 1.472 (5)    |
| C2—C3        | 1.373 (4)    | C12—C13      | 1.372 (4)    |
| C2—H2        | 0.9300       | C12—H12      | 0.9300       |
| C3—C4        | 1.396 (4)    | C13—C14      | 1.386 (5)    |
| C3—H3        | 0.9300       | C13—H13      | 0.9300       |
| C4—C5        | 1.386 (5)    | C14—C15      | 1.383 (4)    |
| C5—C6        | 1.371 (4)    | C15—C16      | 1.378 (4)    |
| C5—H5        | 0.9300       | C15—H15      | 0.9300       |
| C6—H6        | 0.9300       | C16—H16      | 0.9300       |
| C8—C10       | 1.493 (5)    | C18—C20      | 1.510 (4)    |
| C8—C9        | 1.497 (5)    | C18—C19      | 1.518 (4)    |
| C8—H8        | 0.9800       | C18—H18      | 0.9800       |
| C9—H9A       | 0.9600       | C19—H19A     | 0.9600       |
| C9—H9B       | 0.9600       | C19—H19B     | 0.9600       |
| C9—H9C       | 0.9600       | C19—H19C     | 0.9600       |
| C10—H10A     | 0.9600       | C20—H20A     | 0.9600       |
| C10—H10B     | 0.9600       | C20—H20B     | 0.9600       |
| C10—H10C     | 0.9600       | C20—H20C     | 0.9600       |
| C7—O1—C8     | 119.2 (3)    | C17—O3—C18   | 117.3 (3)    |
| C4—N1—H11N   | 119 (3)      | C14—N2—H21N  | 115 (3)      |
| C4—N1—H12N   | 121 (3)      | C14—N2—H22N  | 116 (3)      |
| H11N—N1—H12N | 118 (4)      | H21N—N2—H22N | 121 (4)      |
| C2—C1—C6     | 117.5 (4)    | C12—C11—C16  | 118.2 (4)    |
| C2—C1—C7     | 119.4 (3)    | C12—C11—C17  | 118.8 (4)    |
| C6—C1—C7     | 123.1 (4)    | C16—C11—C17  | 123.1 (4)    |
| C3—C2—C1     | 122.1 (3)    | C13—C12—C11  | 121.2 (4)    |
| C3—C2—H2     | 118.9        | C13—C12—H12  | 119.4        |
| C1—C2—H2     | 118.9        | C11—C12—H12  | 119.4        |
| C2—C3—C4     | 120.1 (4)    | C12—C13—C14  | 121.0 (4)    |
| C2—C3—H3     | 119.9        | C12—C13—H13  | 119.5        |
| C4—C3—H3     | 119.9        | C14—C13—H13  | 119.5        |
| N1—C4—C5     | 121.4 (4)    | C15—C14—N2   | 120.3 (4)    |
| N1—C4—C3     | 120.9 (4)    | C15—C14—C13  | 117.9 (4)    |
| C5—C4—C3     | 117.8 (4)    | N2—C14—C13   | 121.7 (4)    |
| C6—C5—C4     | 121.6 (4)    | C16—C15—C14  | 121.1 (4)    |
| C6—C5—H5     | 119.2        | C16—C15—H15  | 119.5        |
| C4—C5—H5     | 119.2        | C14—C15—H15  | 119.5        |
| C5—C6—C1     | 120.9 (4)    | C15—C16—C11  | 120.7 (4)    |
| C5—C6—H6     | 119.6        | C15—C16—H16  | 119.7        |
| C1—C6—H6     | 119.6        | C11—C16—H16  | 119.7        |
| O2—C7—O1     | 121.8 (4)    | O4—C17—O3    | 122.4 (4)    |
| O2—C7—C1     | 125.3 (4)    | O4—C17—C11   | 125.0 (4)    |
| O1—C7—C1     | 112.9 (4)    | O3—C17—C11   | 112.6 (4)    |
| O1—C8—C10    | 110.1 (4)    | O3—C18—C20   | 105.2 (3)    |
O1—C8—C9  106.2 (3)  O3—C18—C19  108.4 (3)
C10—C8—C9  113.1 (4)  C20—C18—C19  112.8 (4)
O1—C8—H8  109.1  O3—C18—H18  110.1
C10—C8—H8  109.1  C20—C18—H18  110.1
C8—C9—H9A  109.5  C18—C19—H19A  109.5
C8—C9—H9B  109.5  C18—C19—H19B  109.5
C9—C8—H8  109.1  C19—C18—H18  110.1
C10—C8—H8  109.1  C19—C18—H18  110.1
C8—C9—H9C  109.5  C18—C19—H19C  109.5
C8—C9—H9A  109.5  C18—C19—H19A  109.5
H9A—C9—H9B  109.5  C18—C19—H19B  109.5
C10—C8—H8  109.1  H19A—C19—H19B  109.5
C10—C8—H8  109.1  H19A—C19—H19C  109.5
C10—C8—C9  113.1 (4)  C18—C19—H19C  109.5
C8—C10—C11  122.9 (4)  C18—C19—H19C  109.5
C8—C10—H10A  109.5  C18—C19—H19C  109.5
C8—C10—H10B  109.5  C18—C19—H19C  109.5
H10A—C10—H10B  109.5  C18—C19—H19C  109.5
C8—C10—H10A  109.5  H20A—C20—H20B  109.5
C8—C10—H10B  109.5  H20A—C20—H20B  109.5
C10—C11—C12  122.9 (4)  C18—C20—C21  109.5
C10—C11—H11  109.5  C18—C20—C21  109.5
C11—C12—C13  123.0 (4)  C18—C20—C21  109.5
C11—C12—H12  109.5  C18—C20—C21  109.5
C12—C13—C14  122.9 (4)  C18—C20—C21  109.5
C12—C13—H13  109.5  C18—C20—C21  109.5
C13—C14—C15  123.0 (4)  C18—C20—C21  109.5
C13—C14—H14  109.5  C18—C20—C21  109.5
C14—C15—C16  122.9 (4)  C18—C20—C21  109.5
C14—C15—H15  109.5  C18—C20—C21  109.5
C15—C16—C17  123.0 (4)  C18—C20—C21  109.5
C15—C16—H16  109.5  C18—C20—C21  109.5
C16—C17—C18  122.9 (4)  C18—C20—C21  109.5
C16—C17—H17  109.5  C18—C20—C21  109.5
C17—C18—C19  123.0 (4)  C18—C20—C21  109.5
C17—C18—H18  109.5  C18—C20—C21  109.5
C18—C19—C19  122.9 (4)  C18—C20—C21  109.5
C18—C19—H19A  109.5  C18—C20—C21  109.5
C19—C18—H18  109.5  C18—C20—C21  109.5
C19—C18—H19A  109.5  C18—C20—C21  109.5
Hydrogen-bond geometry (Å, °)

| D—H···A       | D—H   | H···A   | D···A   | D—H···A |
|---------------|-------|---------|---------|---------|
| N1—H11N···O2  | 0.87 (2)  | 2.23 (2)  | 3.060 (4) | 158 (3) |
| N1—H12N···N2  | 0.88 (2)  | 2.39 (2)  | 3.269 (5) | 176 (4) |
| N2—H21N···O4  | 0.87 (2)  | 2.07 (2)  | 2.930 (4) | 168 (4) |
| N2—H22N···O2  | 0.87 (2)  | 2.36 (2)  | 3.224 (5) | 172 (4) |

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