Crystal structure and Hirshfeld surface analysis of 2,2,2-trifluoro-1-(7-methylimidazo[1,2-a]pyridin-3-yl)ethan-1-one

Firudin I. Guseinov, Konstantin I. Kobrakov, Bogdan I. Ugrak, Zeliha Atioglu, Mehmet Akkurtd and Ajaya Bhattaraie*

The bicyclic imidazo[1,2-a]pyridine core in the molecule of the title compound, C_{10}H_{7}F_{3}N_{2}O, is planar within 0.004 (1) Å. In the crystal, the molecules are linked by pairs of C—H/C1/C1/C1 N and C—H/C1/C1/C1 O hydrogen bonds, forming strips. These strips are connected by the F/C1/C1/C1 F contacts into layers, which are further joined by π–π stacking interactions. The Hirshfeld surface analysis and fingerprint plots reveal that molecular packing is governed by F/C1/C1/C1 H/H (31.6%), H/C1/C1/C1 H (16.8%), C/C1/C1/C1 C (13.8%) and O/C1/C1/C1 O (8.5%) contacts.

1. Chemical context

The imidazo[1,2-a]pyridine synthon is one of the important fused bicyclic 5–6 heterocycles and it is recognized as a ‘drug prejudice’ scaffold because of its wide range of applications in medicinal chemistry (Bagdi et al., 2015). This synthon is also useful in coordination chemistry and catalysis because of its coordination ability and non-covalent donor–acceptor bonding (Guseinov et al., 2022; Ma et al., 2020, 2021; Mahmudov et al., 2020, 2021). Synthesis of this synthon from easily available chemicals is desirable due to its importance in the various branches of chemistry (Bagdi et al., 2015). Along with this, intermolecular interactions organize molecular architectures, which play a crucial role in synthesis, catalysis, micellization, etc. (Gurbanov et al., 2020a,b; Kopylovich et al., 2011; Ma et al., 2017a,b). The non-covalent bond–acceptor ability of both nitrogen atoms in the imidazo[1,2-a]pyridine synthon can be used in crystal engineering and in the design of dyes and other materials (Maharramov et al., 2018; Mizar et al., 2012; Shixaliyev et al., 2014; Shikhaliyev et al., 2018, 2019). Herein, we report a one-pot synthesis of 2,2,2-trifluoro-1-(7-methylimidazo[1,2-a]pyridin-3-yl)ethan-1-one (I) from (E/Z)-3-bromo-1,1,1-trifluoro-4-isopropoxybut-3-en-2-one and 4-methylpyridin-2-amine, which provides multiple intermolecular non-covalent interactions.
2. Structural commentary

In the molecule of the title compound (Fig. 1), the fused bicyclic imidazo[1,2-a]pyridine core is planar within 0.004 (1) Å, with a dihedral angle of 0.34 (6)° between the mean planes of the five- and six-membered rings. The C2—C1—C8—C9 and N2—C1—C8—O1 torsion angles of 1.04 (18)° and 1.14 (19)°, respectively, show that the ethanone group lies near the plane of the bicycle. The bond lengths N1—C2, C2—C1 and C1—C8 of 1.3367 (16), 1.3987 (16) and 1.4247 (16) Å, respectively, indicate strong \( \pi \)-conjugation in the N1–O1 chain.

3. Supramolecular features and Hirshfeld surface analysis

In the crystal, the molecules are linked by pairs of C—H···N and C—H···O hydrogen bonds into strips elongated along the [210] direction (Figs. 2 and 3, Table 1). These strips are joined into layers parallel to \((1 \bar{2} 2)\) by F···F contacts (Figs. 3–5, Table 2). The layers are connected by F···H contacts (Fig. 5, Table 2) and π···π interactions with a shortest intercentroid separation of 3.6395 (7) Å [Cg1···Cg1(1 − x, 1 − y, 1 − z); Cg1 is the centroid of the imidazole ring].

To visualize the intermolecular interactions in the title compound, the 3D Hirshfeld surfaces and two-dimensional fingerprint plots were computed using Crystal Explorer 17 (Turner et al., 2017). The Hirshfeld surface plotted over \( d_{\text{norm}} \) in the range 0.3137 to 1.1314 a.u. is shown in Fig. 6. The intense red spots with negative \( d_{\text{norm}} \) values represent C—H···O and C—H···N hydrogen bonds. Pale red spots correspond to π···π interactions, which are also seen in the shape-index surface (Fig. 7) generated in the range −1 to 1 Å, where they are indicated by adjacent red and blue triangles. The

![Figure 1](image1.png)

Figure 1
Molecular structure of the title compound showing the atom labelling and displacement ellipsoids drawn at the 50% probability level.

![Figure 2](image2.png)

Figure 2
A general view of the C—H···O and C—H···N hydrogen bonds and π···π stacking interactions in the title compound, depicted by dashed lines. Hydrogen atoms not involved in hydrogen bonding are omitted. [Symmetry codes: (i) −x, −y + 1, −z + 1; (ii) −x + 2, −y + 2, −z + 1; (iii) x + 1, y, z; (iv) −1 + x, y, z.]

![Figure 3](image3.png)

Figure 3
Packing diagram of the title compound, viewed down the a axis showing the C—H···O and C—H···N hydrogen bonds and the F···F and π···π stacking interactions. Hydrogen atoms not involved in hydrogen bonding are omitted.

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

| D—H···A | D—H | H···A | D···A | D—H···A |
|----------|------|-------|-------|----------|
| C4—H4···N1i | 0.95 | 2.48  | 3.4139 (16) | 167 |
| C7—H7···O1ii | 0.95 | 2.30  | 3.1464 (14) | 147 |

Symmetry codes: (i) −x, −y + 1, −z + 1; (ii) −x + 2, −y + 2, −z + 1.
Hirshfeld surface mapped over the electrostatic potential is shown in Fig. 8, where the hydrogen-bond acceptors are represented as red regions. The overall two-dimensional fingerprint plot, and those delineated into F···H/H···F (31.6%), H···H (16.8%), C···H/H···C (13.8%) and O···H/H···O (8.5%) contacts are illustrated in Fig. 9. Other minor contributions to the Hirshfeld surface are from N···H/H···N (7.7%), F···F (6.1%), O···C/C···O (4.2%), N···C/C···N
4. Database survey

The most closely related compounds containing a similar imidazo[1,2-a]pyridine skeleton, but with different substituents on the amide N atom are: N-t-butyl-2-(phenylethynyl)imidazo[1,2-a]pyridin-3-amine (XOWVOX; Tber et al., 2019), 6-bromo-2-(4-bromophenyl)imidazo[1,2-a]pyridine (KOXGEM; Khamees et al., 2019), N-t-butyl-2-(2-nitrophenyl)imidazo[1,2-a]pyridin-3-amine (PILGAV01; Dhanalakshmi et al., 2019), 2-(4-methoxyphenyl)-6-nitroimidazo[1,2-a]pyridine-3-carbaldehyde (DABTEI; Koudad et al., 2015), 2-(ethylsulfinyl)imidazo[1,2-a]pyridine-3-sulfonamide (ZAP-JAD; Gong et al., 2012) and 2-methyl-6-(trifluoromethyl)imidazo[1,2-a]pyridine-3-carbonitrile (ULEGOI; Fun et al., 2011). In the crystal of XOWVOX, molecules are linked by N—H...H hydrogen bonds, forming chains along the c-axis direction. The chains are linked by C—H...π interactions, forming slabs parallel to the ac plane. In the structure of KOXGEM, an intramolecular C—H...N hydrogen bond forms an S(5) ring motif. In the crystal, a short H...H contact links adjacent molecules into centrosymmetric dimers. The dimers are joined by weak C—H...π and slipped π...π stacking interactions, forming layers parallel to (100), which are connected into a three-dimensional network by short Br...H contacts. In the crystal of PILGAV01, N—H...N hydrogen bonds link the molecules into [010] chains. The cohesion of the crystal structure of DABTEI is ensured by C—H...N and C—H...O hydrogen bonds, forming layers parallel to the ac plane. In ZAPJAD, the supramolecular structure is defined by two kinds of intermolecular hydrogen bonds. Pairs of N—H...N hydrogen bonds link the molecules into centrosymmetric dimers and N—H...O hydrogen bonds link the dimers into tubular chains running along the a-axis direction. In the crystal of ULEGOI, molecules are linked into chains through pairs of C—H...N interactions, forming R1(12) and R2(8) hydrogen-bond ring motifs. These chains are stacked along the a axis.

Table 2

| Contact | Distance (Å) | Symmetry operation |
|---------|-------------|-------------------|
| O1···C3 | 3.1574 (15) | 1 + x, y, z       |
| F1···H10B | 2.86 | 1 + x, y, -1 + z |
| F3···F1 | 2.9074 (11) | 2 - x, 1 - y, -z |
| H10C···O1 | 2.83 | 1 - x, 2 - y, 1 - z |
| F2···H10A | 2.64 | x, y, -1 + z     |
| H2···F2 | 2.80 | 1 - x, 1 - y, -z |
| C3···N1 | 3.3055 (16) | 1 - x, 1 - y, 1 - z |

(3.8%), C···C (2.4%), F···C/C···F (1.7%), F···N/N···F (1.4%), N···N (1.1%) and O···N/N···O (0.9%) contacts.

Figure 8

View of the three-dimensional Hirshfeld surface of the title molecule plotted over electrostatic potential energy in the range −0.0500 to 0.0500 a.u. calculated at the Hartree–Fock level of theory using the STO-3 G basis set. Hydrogen-bond donors and acceptors are shown as blue and red regions around the atoms, corresponding to positive and negative potentials, respectively.

Figure 9

(a) The overall two-dimensional fingerprint plot and those delineated into (b) F···H/H···F, (c) H···H, (d) C···H/H···C and (e) O···H/H···O interactions.
Table 3
Experimental details.

| Crystal data | Chemical formula | C₂₁H₂F₃N₂O | Mᵣ | 228.18 |
|--------------|-----------------|-------------|-----|--------|
| Crystal system, space group | Triclinic, P | | | |
| Temperature (K) | 100 | | | |
| a, b, c (Å) | 5.4384 (1), 8.8298 (2), 10.0744 (2) | | | |
| α, β, γ (°) | 102.501 (2), 96.764 (2), 91.415 (2) | | | |
| V (Å³) | 468.39 (2) | | | |
| Z | 2 | | | |
| Radiation type | Cu Kα | | | |
| μ (mm⁻¹) | 1.30 | | | |
| Crystal size (mm) | 0.15 × 0.06 × 0.02 | | | |
| Data collection | XtaLAB Synergy, Dualflex, HyPix | | | |
| Absorption correction | Multi-scan (CrysAlis PRO; Rigaku OD, 2021) | | | |
| Tmin–Tmax | 0.323, 1.000 | | | |
| No. of measured, independent and observed | 14165, 2006, 1927 | | | |
| Rint | 0.050 | | | |
| (sinθ/λ)max (Å⁻¹) | 0.638 | | | |

Refinement

\[ R[F² > 2σ(F²)] , wR(F²), S \]
No. of reflections | 2006 |
No. of parameters | 147 |
H-atom treatment | H-atom parameters constrained |
Δρmax, Δρmin (e Å⁻³) | 0.37, −0.26 |

Computer programs:
CrysAlis PRO (Rigaku OD, 2021), SHELXT (Sheldrick, 2015a), SHELXL (Sheldrick, 2015b), ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2020).

5. Synthesis and crystallization

A mixture of (E/Z)-3-bromo-1,1,1-trifluoro-4-isopropoxybut-3-en-2-one (0.522 mg, 2 mmol) and 4-methylpyridin-2-amine (0.216 mg, 2 mmol) in dry isopropyl alcohol (15 mL) was refluxed for 4 h. Then the solvent was removed on a rotary evaporator under reduced pressure. The residue was recrystallized from methanol. Crystals suitable for X-ray analysis were obtained by slow evaporation of a methanol solution.

Colourless solid (yield 94%), m.p. 405–406 K. Analysis calculated for C₁₀H₇F₃N₂O: C, 52.64, H, 3.09, N, 12.19%. Found: C, 52.55, H, 3.07, N, 12.19%. 1H NMR (75 MHz, CDCl₃): δ 2.48 (3H, CH₃), 7.32–8.60 (3H, Ar), 9.32 (1H, CH).

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 3. Hydrogen atoms were positioned geometrically (C−H = 0.95–0.98 Å) and refined as riding, with \( U_{iso}(H) = 1.2 U_{eq}(C) \) for CH hydrogen atoms and \( U_{iso}(H) = 1.5 U_{eq}(C) \) for CH₃ hydrogen atoms.

Acknowledgements

The author’s contributions are as follows. Conceptualization, FIG, MA and AB; synthesis, FIG and KIK; X-ray analysis, BIU, ZA and MA; writing (review and editing of the manuscript), FIG, ZA, MA and AB.

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**Crystal structure and Hirshfeld surface analysis of 2,2,2-trifluoro-1-(7-methyl-imidazo[1,2-a]pyridin-3-yl)ethan-1-one**

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Computing details

Data collection: *CrysAlis PRO* (Rigaku OD, 2021); cell refinement: *CrysAlis PRO* (Rigaku OD, 2021); data reduction: *CrysAlis PRO* (Rigaku OD, 2021); program(s) used to solve structure: *SHELXT* (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL* (Sheldrick, 2015b); molecular graphics: *ORTEP-3 for Windows* (Farrugia, 2012); software used to prepare material for publication: *PLATON* (Spek, 2020).

2,2,2-Trifluoro-1-(7-methylimidazo[1,2-a]pyridin-3-yl)ethan-1-one

**Crystal data**

| Parameter | Value |
|-----------|-------|
| Chemical formula | C_{10}H_{7}F_{3}N_{2}O |
| Mr | 228.18 |
| Space group | P1 |
| a | 5.4384 (1) Å |
| b | 8.8298 (2) Å |
| c | 10.0744 (2) Å |
| α | 102.501 (2)° |
| β | 96.764 (2)° |
| γ | 91.415 (2)° |
| V | 468.39 (2) Å³ |
| Z | 2 |
| F(000) | 232 |
| D_x | 1.618 Mg m⁻³ |
| Cu Kα radiation, λ | 1.54184 Å |
| θ range | 4.5–79.1° |
| µ | 1.30 mm⁻¹ |
| T | 100 K |
| Cell parameters from 11472 reflections |
| T_min | 0.323 |
| T_max | 1.000 |
| 14165 measured reflections |
| 2006 independent reflections |
| 1927 reflections with I > 2σ(I) |
| R_m | 0.050 |
| R_max | 0.037 |
| θ_max | 79.5° |
| θ_min | 4.5° |
| h | -6→6 |
| k | -11→10 |
| l | -12→12 |

**Data collection**

XtaLAB Synergy, Dualflex, HyPix diffractometer

Radiation source: micro-focus sealed X-ray tube, PhotonJet (Cu) X-ray Source

Mirror monochromator

Detector resolution: 10.0000 pixels mm⁻¹

ω scans

Absorption correction: multi-scan (CrysAlis PRO; Rigaku OD, 2021)

**Refinement**

Refinement on F²

Least-squares matrix: full

R[F² > 2σ(F²)] = 0.037

wR(F²) = 0.105

S = 1.09

2006 reflections

147 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained
where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\text{max}} = 0.001$

$\Delta \rho_{\text{max}} = 0.37$ e Å$^{-3}$

$\Delta \rho_{\text{min}} = -0.26$ 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.

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

|  | x      | y      | z      | $U_{\text{iso}}$/$U_{\text{eq}}$ |
|---|--------|--------|--------|-------------------------------|
| F3| 0.83669 (15) | 0.51338 (8) | 0.12281 (8) | 0.0298 (2) |
| F1| 1.03655 (15) | 0.72062 (9)  | 0.10632 (8) | 0.0306 (2) |
| F2| 0.63947 (16) | 0.69737 (10) | 0.05569 (8) | 0.0352 (2) |
| O1| 0.94235 (16) | 0.85798 (10) | 0.34833 (9) | 0.0231 (2) |
| N2| 0.53525 (17) | 0.75163 (11) | 0.47862 (10) | 0.0178 (2) |
| N1| 0.25848 (19) | 0.55184 (12) | 0.38082 (11) | 0.0224 (2) |
| C3| 0.3285 (2)  | 0.66590 (13) | 0.49404 (12) | 0.0195 (3) |
| C7| 0.6410 (2)  | 0.87311 (13) | 0.57981 (12) | 0.0199 (3) |
| H7| 0.783693    | 0.930322    | 0.567582    | 0.024* |
| C6| 0.5364 (2)  | 0.90977 (14) | 0.69840 (12) | 0.0214 (3) |
| H6| 0.608051    | 0.993640    | 0.769395    | 0.026* |
| C4| 0.2206 (2)  | 0.70392 (14) | 0.61568 (13) | 0.0214 (3) |
| H4| 0.077951    | 0.646052    | 0.626999    | 0.026* |
| C5| 0.3224 (2)  | 0.82541 (14) | 0.71850 (13) | 0.0211 (3) |
| C2| 0.4210 (2)  | 0.56623 (14) | 0.29402 (12) | 0.0210 (3) |
| H2| 0.416403    | 0.500889    | 0.205342    | 0.025* |
| C1| 0.5986 (2)  | 0.68799 (13) | 0.34799 (12) | 0.0191 (3) |
| C9| 0.8297 (2)  | 0.66755 (14) | 0.14284 (13) | 0.0231 (3) |
| C8| 0.7991 (2)  | 0.74800 (13) | 0.29223 (12) | 0.0190 (3) |
| C10| 0.2118 (2) | 0.87010 (16) | 0.85047 (13) | 0.0267 (3) |
| H10A| 0.336148 | 0.863035 | 0.927312 | 0.040* |
| H10B| 0.068569 | 0.799545 | 0.848113 | 0.040* |
| H10C| 0.158430 | 0.976875 | 0.862058 | 0.040* |

**Atomic displacement parameters (Å$^2$)**

| | $U_{11}$ | $U_{22}$ | $U_{33}$ | $U_{12}$ | $U_{13}$ | $U_{23}$ |
|---|---------|---------|---------|---------|---------|---------|
| F3| 0.0391 (5) | 0.0189 (4) | 0.0298 (4) | -0.0012 (3) | 0.0086 (3) | -0.0001 (3) |
| F1| 0.0318 (4) | 0.0315 (4) | 0.0291 (4) | -0.0052 (3) | 0.0120 (3) | 0.0047 (3) |
| F2| 0.0349 (5) | 0.0452 (5) | 0.0241 (4) | 0.0054 (4) | -0.0037 (3) | 0.0081 (3) |
| O1| 0.0225 (4) | 0.0190 (4) | 0.0270 (4) | -0.0048 (3) | 0.0026 (3) | 0.0037 (3) |
| N2| 0.0161 (5) | 0.0153 (5) | 0.0222 (5) | -0.0015 (3) | 0.0010 (4) | 0.0058 (4) |
| N1| 0.0197 (5) | 0.0184 (5) | 0.0280 (5) | -0.0036 (4) | 0.0008 (4) | 0.0044 (4) |
| C3| 0.0158 (5) | 0.0162 (5) | 0.0272 (6) | -0.0019 (4) | 0.0002 (4) | 0.0079 (4) |
| C7  | 0.0180 (5) | 0.0167 (5) | 0.0241 (6) | −0.0029 (4) | −0.0006 (4) | 0.0051 (4) |
| C6  | 0.0208 (6) | 0.0192 (6) | 0.0231 (6) | −0.0002 (4) | −0.0002 (4) | 0.0044 (4) |
| C4  | 0.0177 (5) | 0.0206 (6) | 0.0282 (6) | −0.0006 (4) | 0.0026 (4)  | 0.0110 (5) |
| C5  | 0.0201 (6) | 0.0203 (6) | 0.0250 (6) | 0.0029 (4)  | 0.0023 (4)  | 0.0098 (5) |
| C2  | 0.0196 (6) | 0.0180 (6) | 0.0240 (6) | −0.0017 (4) | 0.0000 (4)  | 0.0034 (4) |
| C1  | 0.0191 (6) | 0.0167 (6) | 0.0213 (6) | −0.0006 (4) | 0.0008 (4)  | 0.0046 (4) |
| C9  | 0.0228 (6) | 0.0225 (6) | 0.0244 (6) | −0.0014 (4) | 0.0025 (5)  | 0.0065 (5) |
| C8  | 0.0186 (5) | 0.0162 (5) | 0.0227 (6) | 0.0010 (4)  | 0.0009 (4)  | 0.0063 (4) |
| C10 | 0.0278 (6) | 0.0282 (7) | 0.0264 (6) | 0.0017 (5)  | 0.0054 (5)  | 0.0097 (5) |

**Geometric parameters (Å, °)**

| Bond/Angle | Length (Å) | Angle (°) |
|------------|------------|-----------|
| F3—C9      | 1.3345 (14) |           |
| F1—C9      | 1.3292 (14) |           |
| F2—C9      | 1.3453 (14) |           |
| O1—C8      | 1.2208 (15) |           |
| N2—C3      | 1.3827 (14) |           |
| N2—C7      | 1.3706 (15) |           |
| N2—C1      | 1.4011 (15) |           |
| N1—C3      | 1.3571 (16) |           |
| N1—C2      | 1.3367 (16) |           |
| C3—C4      | 1.3997 (17) |           |
| C7—H7      | 0.9500      |           |
| C7—C6      | 1.3629 (17) |           |
| C3—N2—C1  | 106.60 (10) | N1—C2—C1 | 112.65 (11) |
| C7—N2—C3  | 122.01 (10) | C1—C2—H2 | 123.7        |
| C7—N2—C1  | 131.39 (10) | N2—C1—C8 | 123.53 (11)  |
| C2—N1—C3  | 105.23 (10) | C2—C1—N2 | 104.25 (10)  |
| N2—C3—C4  | 119.63 (11) | C2—C1—C8 | 132.19 (11)  |
| N1—C3—N2  | 111.28 (10) | F3—C9—F2 | 106.95 (10)  |
| N1—C3—C4  | 129.10 (11) | F3—C9—C8 | 113.36 (9)   |
| N2—C7—H7  | 120.8       | F1—C9—F3 | 107.82 (10)  |
| C6—C7—N2  | 118.35 (11) | F1—C9—C8 | 107.29 (10)  |
| C6—C7—H7  | 120.8       | F1—C9—C8 | 110.72 (10)  |
| C7—C6—H6  | 119.2       | F2—C9—C8 | 110.45 (10)  |
| C7—C6—C5  | 121.61 (11) | O1—C8—C1 | 126.81 (11)  |
| C5—C6—H6  | 119.2       | O1—C8—C9 | 117.43 (10)  |
| C3—C4—H4  | 120.2       | C1—C8—C9 | 115.72 (10)  |
| C5—C4—C3  | 119.55 (11) | C5—C10—H10A | 109.5 |
| C5—C4—H4  | 120.2       | C5—C10—H10B | 109.5 |
| C6—C5—C10 | 119.98 (11) | C5—C10—H10C | 109.5 |
| C4—C5—C6  | 118.86 (11) | H10A—C10—H10B | 109.5 |
| C4—C5—C10 | 121.17 (11) | H10A—C10—H10C | 109.5 |
| N1—C2—H2  | 123.7       | H10B—C10—H10C | 109.5 |

**Supporting Information**

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Hydrogen-bond geometry (Å, º)

| D—H···A   | D—H | H···A | D···A     | D—H···A |
|-----------|------|-------|-----------|---------|
| C2—H2···F3 | 0.95 | 2.53  | 2.9876 (14) | 110 |
| C4—H4···N1i | 0.95 | 2.48  | 3.4139 (16) | 167 |
| C7—H7···O1 | 0.95 | 2.43  | 2.9864 (14) | 117 |
| C7—H7···O1ii | 0.95 | 2.30  | 3.1464 (14) | 147 |

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