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# 1-(4-Fluorophenyl)-2-(1*H*-imidazol-1-yl)ethanone

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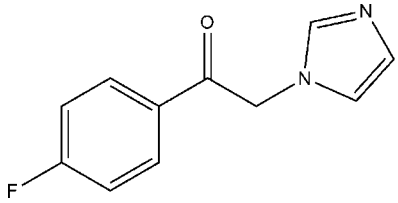
Key indicators: single-crystal X-ray study; $T$ = 293 K; mean $\sigma$(C–C) = 0.004 Å; $R$ factor = 0.037; $wR$ factor = 0.093; data-to-parameter ratio = 7.7.

In the title compound, $C_{11}H_9FN_2O$, the dihedral angle between the rings is 87.50 (4)°. In the crystal, intermolecular C—H···N hydrogen bonds link the molecules in a stacked arrangement along the $c$ axis.

## Related literature

For related compounds containing a 2-(1*H*-imidazol-1-yl)-1-phenylethanone fragment, see: Akira *et al.* (1985); North *et al.* (1968); Yoshimi *et al.* (2000); Yuan *et al.* (2007); Tao *et al.* (2007). For standard bond lengths, see: Allen *et al.* (1987).




## Experimental

### Crystal data

$C_{11}H_9FN_2O$
$M_r$ = 204.20
Orthorhombic, $P2_12_12_1$
$a$ = 8.6730 (17) Å
$b$ = 10.132 (2) Å
$c$ = 11.088 (2) Å
$V$ = 974.4 (3) Å$^3$
$Z$ = 4
Mo $K\alpha$ radiation
$\mu$ = 0.11 mm$^{-1}$
$T$ = 293 K
0.30 × 0.20 × 0.10 mm

### Data collection

Enraf–Nonius CAD-4 diffractometer
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.969, $T_{max}$ = 0.990
3790 measured reflections
1052 independent reflections
778 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045
3 standard reflections every 200 reflections
intensity decay: 1%

### Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
$S$ = 1.01
1052 reflections
137 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.10 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.09 e Å$^{-3}$

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

| $D$—H···$A$ | $D$—H | H···$A$ | $D$···$A$ | $D$—H···$A$ |
|---|---|---|---|---|
| C8—H8$A$···N2$^{i}$ | 0.97 | 2.51 | 3.454 (4) | 164 |

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

Data collection: *CAD-4 EXPRESS* (Enraf–Nonius, 1994); 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: *SHELXTL* (Sheldrick, 2008).

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: ZQ2112).

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# supporting information

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## 1-(4-Fluorophenyl)-2-(1*H*-imidazol-1-yl)ethanone

**Dong-liang Liu, Chen Li, Guang-yan Yu and Tao Xiao**

### S1. Comment

The title compound, $C_{11}H_9O_1N_2F_1$, is the key intermediate in the synthesis of a new kind of antifungal drug (Akira *et al.*, 1985; Yoshimi *et al.*, 2000). The crystal structure determination has been carried out in order to elucidate the molecular conformation (Fig. 1).

In the crystal structure, the bond lengths and angles of the title compound are within normal ranges (Allen *et al.*, 1987). The phenyl and imidazole rings are planar (rms deviations of 0.0038 and 0.0036, respectively) and almost perpendicular to each other. The dihedral angle between the mean planes is 87.50 (4)°. In the crystal structure, intermolecular C—H···N hydrogen bonds (Table 1) link the molecules in a stacked arrangement along the *a* axis (Fig. 2).

### S2. Experimental

Sodium hydride (4.8 g, 120 mmol) was suspended in dimethylformamide (DMF, 30 ml). Imidazole (6.8 g, 120 mmol) dissolved in DMF (30 ml) was slowly added dropwise at 273 K, and reacted atroom temperature for 30 min. 2-chloro-1-(4-fluorophenyl)ethanone (15.48 g, 90 mmol) dissolved in DMF (30 ml) was then slowly added dropwise, and reacted at room temperature for 4 h. The mixture was placed in ice-water (300 ml), and 1 mol hydrochloric acid (50 ml) was then added. After filtration, the filtrate was neutralized with sodium bicarbonate to pH = 6, and a yellow deposit was obtained (m.p. 423–424 K). Crystals suitable for X-ray analysis were obtained by dissolving the crude product (1.0 g) in ethanol (30 ml) and then allowing the solution to evaporate slowly at room temperature for about 7 d.

### S3. Refinement

In the absence of significant anomalous scattering effects, all Friedel pairs were merged. H atoms were positioned geometrically, with C—H = 0.93 and 0.97 Å for aromatic and methylene H atoms, respectively, and constrained to ride on their parent atoms with $U_{iso}$(H) = 1.2$U_{eq}$(C).

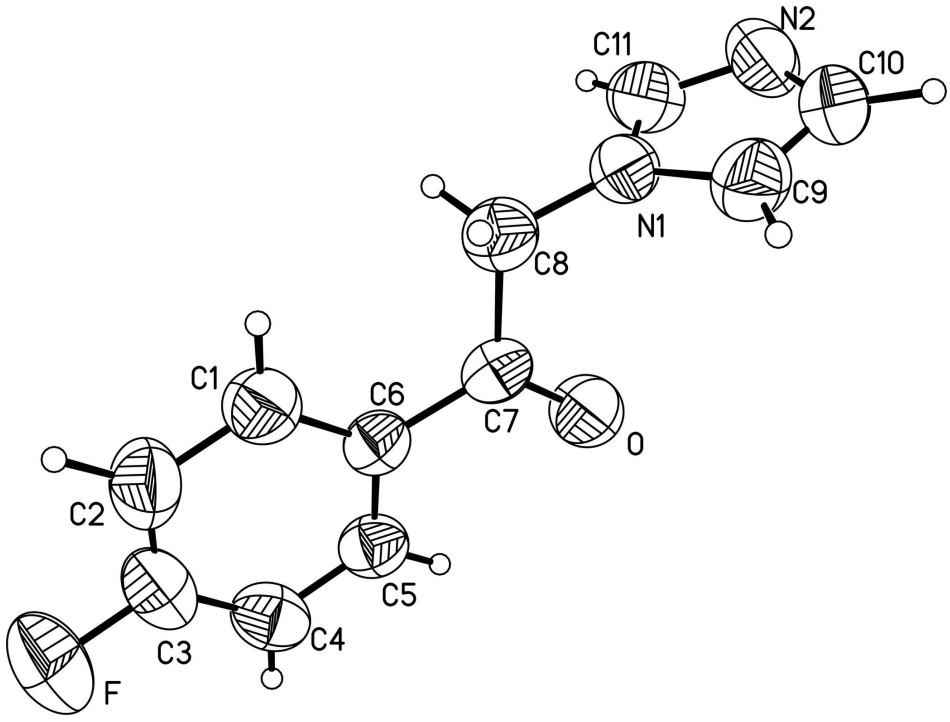


**Figure 1**

The molecular structure of the title compound with displacement ellipsoids drawn at the 50% probability level.

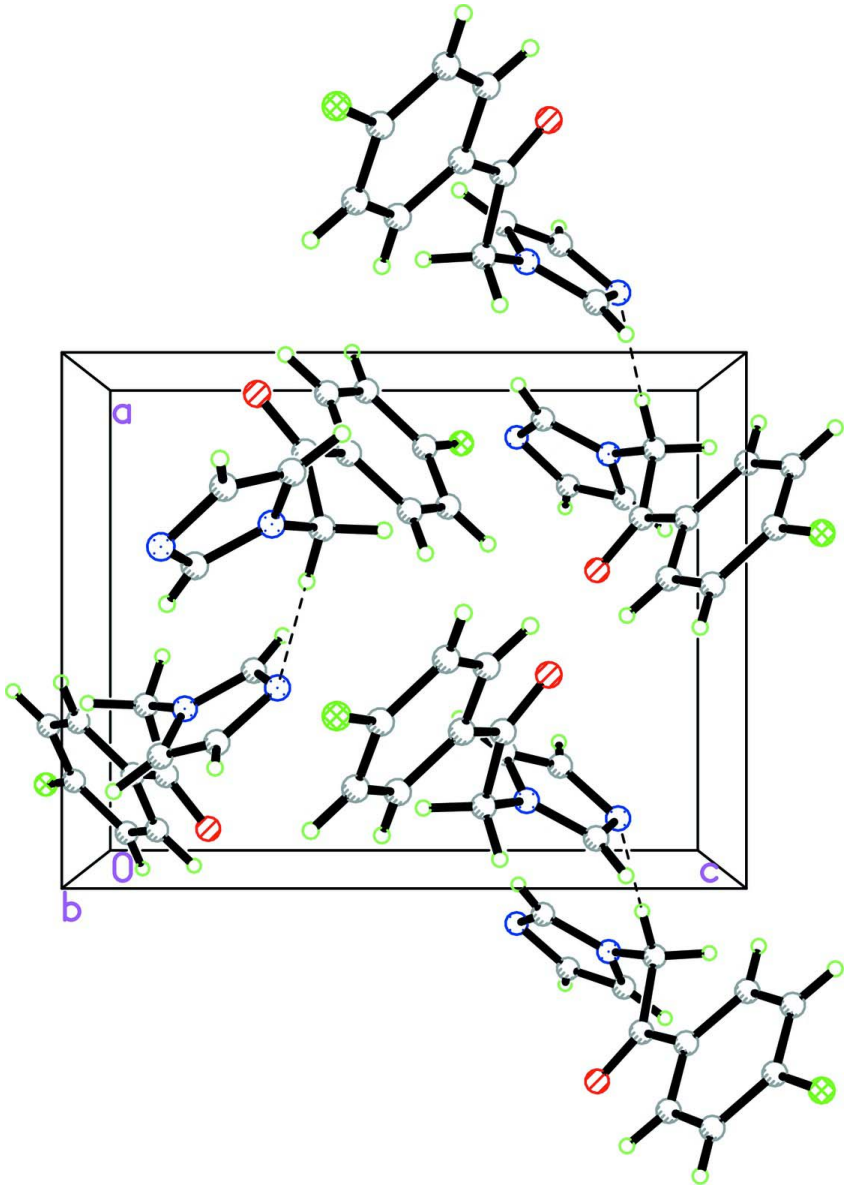


**Figure 2**

A packing diagram of the title compound. Hydrogen bonds are shown as dashed lines.

### 1-(4-Fluorophenyl)-2-(1*H*-imidazol-1-yl)ethanone

*Crystal data*

$C_{11}H_9FN_2O$
$M_r = 204.20$
Orthorhombic, $P2_12_12_1$
Hall symbol: P 2ac 2ab
$a = 8.6730\ (17)$ Å
$b = 10.132\ (2)$ Å
$c = 11.088\ (2)$ Å
$V = 974.4\ (3)$ Å$^3$
$Z = 4$
$F(000) = 424$

$D_x = 1.392$ Mg m$^{-3}$
Melting point: 423 K
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 25 reflections
$\theta = 9$–13°
$\mu = 0.11$ mm$^{-1}$
$T = 293$ K
Block, yellow
0.30 × 0.20 × 0.10 mm

*Data collection*

Enraf–Nonius CAD-4 diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
$\omega/2\theta$ scans
Absorption correction: $\psi$ scan (North *et al.*, 1968)
$T_{min}$ = 0.969, $T_{max}$ = 0.990
3790 measured reflections
1052 independent reflections
778 reflections with $I > 2\sigma(I)$
$R_{int}$ = 0.045
$\theta_{max}$ = 25.4°, $\theta_{min}$ = 2.7°
$h$ = 0→10
$k$ = −12→12
$l$ = −13→13
3 standard reflections every 200 reflections
intensity decay: 1%

*Refinement*

Refinement on $F^2$
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.037
$wR(F^2)$ = 0.093
$S$ = 1.01
1052 reflections
137 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
$w = 1/[\sigma^2(F_o^2) + (0.0484P)^2]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.10 e Å$^{-3}$
$\Delta\rho_{min}$ = −0.09 e Å$^{-3}$
Extinction correction: *SHELXL97* (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.034 (5)

*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 (Å²)*

| | $x$ | $y$ | $z$ | $U_{iso}$*/$U_{eq}$ |
|---|---|---|---|---|
| F | 0.3432 (3) | 0.73232 (18) | 0.41347 (18) | 0.1052 (8) |
| O | 0.4019 (3) | 0.2049 (2) | 0.7042 (2) | 0.0838 (8) |
| N1 | 0.1657 (3) | 0.0314 (2) | 0.6780 (2) | 0.0556 (6) |
| C1 | 0.2015 (4) | 0.4109 (3) | 0.4913 (3) | 0.0657 (9) |
| H1A | 0.1223 | 0.3538 | 0.4695 | 0.079* |
| C2 | 0.2138 (4) | 0.5322 (3) | 0.4355 (3) | 0.0760 (10) |
| H2A | 0.1439 | 0.5574 | 0.3763 | 0.091* |
| N2 | 0.1233 (3) | −0.1189 (3) | 0.8187 (3) | 0.0798 (9) |
| C3 | 0.3297 (5) | 0.6133 (3) | 0.4687 (3) | 0.0708 (9) |
| C4 | 0.4345 (4) | 0.5823 (3) | 0.5561 (3) | 0.0671 (9) |
| H4A | 0.5123 | 0.6409 | 0.5776 | 0.081* |
| C5 | 0.4208 (3) | 0.4608 (3) | 0.6112 (2) | 0.0568 (8) |
| H5A | 0.4906 | 0.4372 | 0.6711 | 0.068* |
| C6 | 0.3053 (3) | 0.3735 (2) | 0.5794 (2) | 0.0496 (7) |

| | | | | |
|---|---|---|---|---|
| C7 | 0.3005 (3) | 0.2428 (3) | 0.6385 (2) | 0.0535 (7) |
| C8 | 0.1625 (3) | 0.1556 (3) | 0.6133 (3) | 0.0623 (8) |
| H8A | 0.0694 | 0.2031 | 0.6351 | 0.075* |
| H8B | 0.1579 | 0.1376 | 0.5275 | 0.075* |
| C9 | 0.2500 (4) | −0.0773 (3) | 0.6483 (3) | 0.0689 (9) |
| H9A | 0.3144 | −0.0871 | 0.5818 | 0.083* |
| C10 | 0.2215 (4) | −0.1673 (3) | 0.7341 (3) | 0.0726 (9) |
| H10A | 0.2634 | −0.2517 | 0.7355 | 0.087* |
| C11 | 0.0935 (4) | 0.0013 (3) | 0.7805 (3) | 0.0702 (9) |
| H11A | 0.0285 | 0.0594 | 0.8209 | 0.084* |

*Atomic displacement parameters (Å²)*

| | $U^{11}$ | $U^{22}$ | $U^{33}$ | $U^{12}$ | $U^{13}$ | $U^{23}$ |
|---|---|---|---|---|---|---|
| F | 0.143 (2) | 0.0728 (12) | 0.1000 (14) | −0.0026 (14) | 0.0088 (16) | 0.0255 (11) |
| O | 0.0624 (13) | 0.0863 (16) | 0.1027 (17) | −0.0131 (12) | −0.0320 (15) | 0.0296 (14) |
| N1 | 0.0520 (14) | 0.0485 (13) | 0.0663 (15) | 0.0000 (12) | −0.0001 (13) | −0.0063 (12) |
| C1 | 0.064 (2) | 0.071 (2) | 0.0621 (18) | −0.0075 (18) | −0.0060 (17) | 0.0042 (16) |
| C2 | 0.081 (3) | 0.077 (2) | 0.069 (2) | 0.006 (2) | −0.013 (2) | 0.0144 (18) |
| N2 | 0.087 (2) | 0.0536 (16) | 0.099 (2) | −0.0046 (15) | 0.0121 (19) | 0.0027 (15) |
| C3 | 0.092 (3) | 0.0574 (18) | 0.063 (2) | 0.004 (2) | 0.015 (2) | 0.0078 (16) |
| C4 | 0.073 (2) | 0.0598 (18) | 0.0681 (19) | −0.0104 (17) | 0.009 (2) | −0.0072 (16) |
| C5 | 0.0529 (17) | 0.0658 (19) | 0.0518 (17) | −0.0018 (15) | 0.0016 (15) | −0.0025 (14) |
| C6 | 0.0467 (16) | 0.0559 (16) | 0.0463 (15) | 0.0017 (14) | 0.0002 (13) | −0.0028 (12) |
| C7 | 0.0445 (15) | 0.0635 (17) | 0.0524 (16) | 0.0015 (14) | 0.0024 (14) | −0.0041 (14) |
| C8 | 0.0580 (18) | 0.0609 (18) | 0.0681 (19) | −0.0017 (15) | −0.0059 (17) | −0.0028 (15) |
| C9 | 0.0601 (18) | 0.0654 (18) | 0.081 (2) | 0.0062 (17) | 0.0065 (18) | −0.0114 (18) |
| C10 | 0.066 (2) | 0.0521 (17) | 0.100 (2) | 0.0043 (16) | 0.001 (2) | −0.0078 (19) |
| C11 | 0.0656 (19) | 0.064 (2) | 0.080 (2) | −0.0029 (18) | 0.0139 (19) | −0.0142 (18) |

*Geometric parameters (Å, º)*

| | | | |
|---|---|---|---|
| F—C3 | 1.358 (3) | C4—C5 | 1.379 (4) |
| O—C7 | 1.205 (3) | C4—H4A | 0.9300 |
| N1—C11 | 1.333 (3) | C5—C6 | 1.382 (4) |
| N1—C9 | 1.363 (3) | C5—H5A | 0.9300 |
| N1—C8 | 1.449 (3) | C6—C7 | 1.478 (4) |
| C1—C2 | 1.380 (4) | C7—C8 | 1.514 (4) |
| C1—C6 | 1.381 (4) | C8—H8A | 0.9700 |
| C1—H1A | 0.9300 | C8—H8B | 0.9700 |
| C2—C3 | 1.350 (5) | C9—C10 | 1.341 (4) |
| C2—H2A | 0.9300 | C9—H9A | 0.9300 |
| N2—C11 | 1.315 (4) | C10—H10A | 0.9300 |
| N2—C10 | 1.359 (4) | C11—H11A | 0.9300 |
| C3—C4 | 1.365 (5) | | |
| | | | |
| C11—N1—C9 | 105.9 (3) | C1—C6—C7 | 122.7 (3) |
| C11—N1—C8 | 127.7 (3) | C5—C6—C7 | 118.7 (3) |

| | | | |
|---|---|---|---|
| C9—N1—C8 | 126.3 (3) | O—C7—C6 | 122.2 (3) |
| C2—C1—C6 | 120.7 (3) | O—C7—C8 | 120.2 (3) |
| C2—C1—H1A | 119.6 | C6—C7—C8 | 117.6 (3) |
| C6—C1—H1A | 119.6 | N1—C8—C7 | 113.6 (2) |
| C3—C2—C1 | 118.5 (3) | N1—C8—H8A | 108.8 |
| C3—C2—H2A | 120.7 | C7—C8—H8A | 108.8 |
| C1—C2—H2A | 120.7 | N1—C8—H8B | 108.8 |
| C11—N2—C10 | 103.6 (3) | C7—C8—H8B | 108.8 |
| C2—C3—F | 118.8 (3) | H8A—C8—H8B | 107.7 |
| C2—C3—C4 | 123.3 (3) | C10—C9—N1 | 106.2 (3) |
| F—C3—C4 | 117.9 (3) | C10—C9—H9A | 126.9 |
| C3—C4—C5 | 117.6 (3) | N1—C9—H9A | 126.9 |
| C3—C4—H4A | 121.2 | C9—C10—N2 | 111.1 (3) |
| C5—C4—H4A | 121.2 | C9—C10—H10A | 124.4 |
| C4—C5—C6 | 121.4 (3) | N2—C10—H10A | 124.4 |
| C4—C5—H5A | 119.3 | N2—C11—N1 | 113.2 (3) |
| C6—C5—H5A | 119.3 | N2—C11—H11A | 123.4 |
| C1—C6—C5 | 118.5 (3) | N1—C11—H11A | 123.4 |
| | | | |
| C6—C1—C2—C3 | 0.0 (5) | C5—C6—C7—C8 | 172.8 (2) |
| C1—C2—C3—F | 179.5 (3) | C11—N1—C8—C7 | 98.2 (3) |
| C1—C2—C3—C4 | −0.9 (6) | C9—N1—C8—C7 | −78.6 (4) |
| C2—C3—C4—C5 | 0.8 (5) | O—C7—C8—N1 | 2.1 (4) |
| F—C3—C4—C5 | −179.5 (3) | C6—C7—C8—N1 | −178.2 (2) |
| C3—C4—C5—C6 | 0.0 (4) | C11—N1—C9—C10 | 0.9 (3) |
| C2—C1—C6—C5 | 0.8 (4) | C8—N1—C9—C10 | 178.3 (3) |
| C2—C1—C6—C7 | −177.6 (3) | N1—C9—C10—N2 | −0.9 (4) |
| C4—C5—C6—C1 | −0.8 (4) | C11—N2—C10—C9 | 0.5 (4) |
| C4—C5—C6—C7 | 177.6 (3) | C10—N2—C11—N1 | 0.1 (4) |
| C1—C6—C7—O | 170.8 (3) | C9—N1—C11—N2 | −0.6 (4) |
| C5—C6—C7—O | −7.6 (4) | C8—N1—C11—N2 | −177.9 (3) |
| C1—C6—C7—C8 | −8.9 (4) | | |

*Hydrogen-bond geometry (Å, º)*

| *D*—H···*A* | *D*—H | H···*A* | *D*···*A* | *D*—H···*A* |
|---|---|---|---|---|
| C8—H8*A*···N2$^{i}$ | 0.97 | 2.51 | 3.454 (4) | 164 |

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