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Crystal structure of (*E*)-*N*′-(3-fluoro-2-hydroxybenzylidene)isonicotinohydrazide

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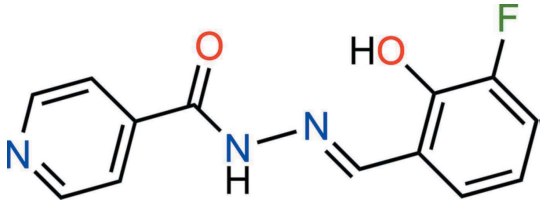
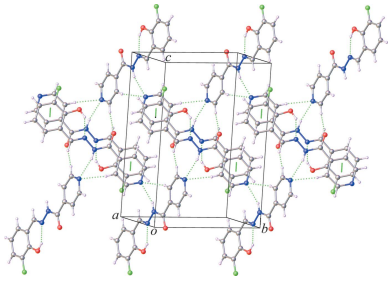
In the title compound, $C_{13}H_{10}FN_3O_2$, the molecule has an *E* conformation with respect to the C=N bond of the hydrazone bridge. The dihedral angle between the isonicotinoyl and fluorophenol moieties is 4.03 (4)°, and an intramolecular O—H···N hydrogen bond generates an *S*(6) ring motif. In the crystal, molecules are linked by N—H···N and C—H···N hydrogen bonds, forming chains propagating along the *a*-axis direction. The chains are linked by C—H···O hydrogen bonds, resulting in the formation of layers lying parallel to the *ab* plane. The crystal structure also features π–π interactions [centroid-to-centroid distance = 3.6887 (8) Å].

1. Chemical context

Hydrazone-based chelators of metal ions are interesting compounds that receive a significant amount of interest (Bendová *et al.*, 2010; Jansová *et al.*, 2014; Hrušková *et al.*, 2016). We have recently published the structures of two derivatives of the prototypical chelator from this class, salicyl aldehyde isonicotinoyl hydrazide (SIH), which were synthesized as potential sensors for metal ions (Chainok *et al.*, 2016). The structures reported have fluorine and methyl substitution in position 5 on the benzene ring. Herein, we report the crystal structure of a further analogue in this series bearing a fluorine substituent in position 3 of the benzene ring, which was synthesized in order to investigate the effect of the distance between the reporting fluorine atom and the metal chelating unit.





2. Structural commentary

The molecular structure of the title compound, with atom labelling, is presented in Fig. 1. The molecule has an *E* conformation with respect to the hydrazone bridge (C7=N3). The C6—N2 and C7—N3 bond lengths differ by 0.08 Å hence; these two bonds are formally double and single bonds, respectively. The molecule deviates slightly from planarity

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

D—H···A	D—H	H···A	D···A	D—H···A
O2—H2*O*···N3	0.82	1.87	2.5862 (14)	145
N2—H2*N*···N1^{i}	0.86	2.16	2.9851 (16)	161
C4—H4···N1^{i}	0.93	2.51	3.3492 (18)	151
C5—H5···O1^{ii}	0.93	2.37	3.2738 (17)	163

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

with an r.m.s deviation for the fitted non-hydrogen atoms of 0.062 Å. There is an intramolecular O2—H2*O*···N3 hydrogen bond with an *S*(6) ring motif present in the pyridine carboxamide moiety, and the pyridine ring (N1/C1–C5) is approximately coplanar with the amide group (C6(=O1)N2) [dihedral angle = 8.25 (6)°]. The isonicotinoyl moiety (N1/C1–C6/O1/N2) is inclined to the fluorophenol moiety (C8-C13/O2/F1) by 4.03 (4)°.

3. Supramolecular features

In the crystal, molecules are linked by bifurcated-acceptor N2—H2*N*···N1^{i} and C4—H4···N1^{i} hydrogen bonds (Table 1), leading to the formation of zigzag chains lying parallel to the *b*-axis direction, as shown in Fig. 2. Adjacent chains are further linked *via* C5—H5···O1^{ii} hydrogen bonds, forming layers parallel to the *ab* plane, as shown in Fig. 3. Within the sheets, there are π–π stacking interactions involving inversion-related molecules [*Cg*1···*Cg*2^{i} = 3.6887 (8) Å; *Cg*1 and *Cg*2 are the centroids of the pyridine (N1/C1–C5) and phenyl (C8–C13) rings, respectively; symmetry code: (i) $-x+1, -y+1, -z+1$].

4. Database survey

A search of the Cambridge Structural Database (Version 5.38, latest update May 2017; Groom *et al.*, 2016) for compounds with the (*E*)-*N*-(2-hydroxybenzylidene)isonicotinohydrazide skeleton revealed 86 hits. They include the isotypic crystal structures with bromide (PORYEC; Xiong & Li, 2014), methoxy (CANCOK, Yu *et al.*, 2005; CANCOK01, Yang, 2007; CANCOK02, Xu, 2013), and hydroxy (WAFVEG; Tecer *et al.*, 2010) groups substituted at the 3-position of the phenyl ring.

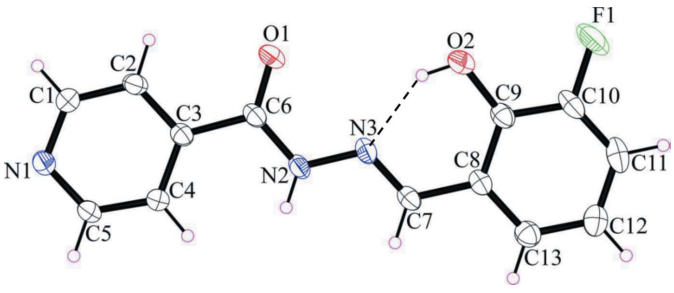


Figure 1
The molecular structure of the title compound, with the atom labelling and 50% probability displacement ellipsoids. The intramolecular hydrogen bond is shown as a dashed line (see Table 1).

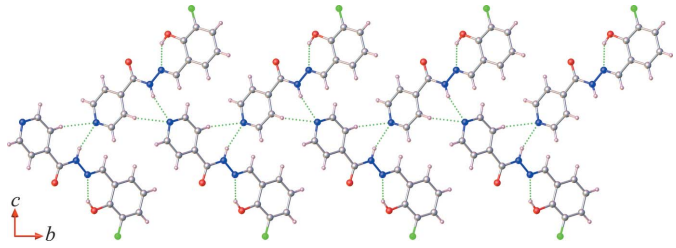


Figure 2
A view of the hydrogen-bonded chains, formed in the crystal structure of the title compound *via* bifurcated-acceptor N—H···N and C—H···N hydrogen bonds (dashed lines; Table 1).

5. Synthesis and crystallization

Isonicotinic acid hydrazide (301 mg, 2.19 mmol) and 3-fluorosalicylaldehyde (338 mg, 2.69 mmol) were suspended in a 1:1 mixture of water and ethanol (6 ml). The reaction mixture was stirred at 363 K for 24 h and formation of a precipitate was observed. The reaction mixture was allowed to cool to room temperature and then filtered. The isolated solid was washed with water to give the product as a white solid (510 mg, 1.97 mmol, 90%). Colourless rod-like crystals, suitable for X-ray diffraction analysis, were grown by slow evaporation of a solution in methanol of the title compound. ^{1}H NMR (400 MHz, DMSO-d_6) d 6.94 (1H, *m*, CH-Ph), 7.32 (1H, *dd*, J = 8.8, J = 10.4 CH-Ph), 7.44 (1H, *d*, J = 8.4, CH-Ph), 7.85 (2H, *d*, J = 5.6, CH-Py), 8.70 (1H, *s*, CH=N), 8.81 (2H, *d*, J = 5.6, CH-Py), 11.40 (1H, *s*, NH), 12.39 (1H, *s*, OH). HR–MS (ES^{+}) $C_{13}H_{11}FN_3O_2$ requires 260.0835 [M + H]$^{+}$; found 260.0830.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. H atoms bonded to C, N, and O

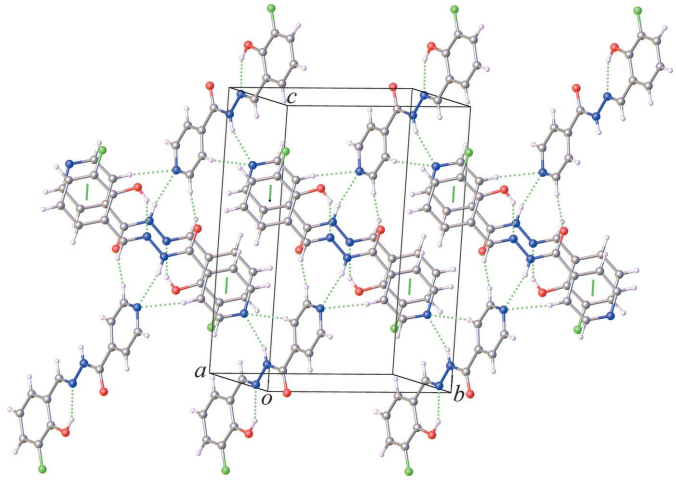


Figure 3
Part of the crystal structure of the title compound, showing the formation of the layers, parallel to the *ab* plane, formed *via* C—H···O hydrogen bonds, and the π–π interactions (dashed lines).

atoms were placed at calculated positions and refined using a riding-model approximation: N—H = 0.86 Å, O—H = 0.82 Å and C—H = 0.93 Å with U_{iso}(H) = 1.5U_{eq}(O) and 1.2U_{eq}(N,C) for other H atoms.

Acknowledgements

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Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{13}H_{10}FN_3O_2$
M_r	259.24
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	296
a, b, c (Å)	7.8555 (3), 10.2748 (5), 14.9390 (7)
β (°)	92.397 (2)
V (Å^3)	1204.73 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.11
Crystal size (mm)	0.28 × 0.14 × 0.14
Data collection	
Diffractometer	Bruker D8 QUEST CMOS
Absorption correction	Multi-scan (*SADABS*; Bruker, 2016)
T_{min}, T_{max}	0.700, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	22872, 2475, 1769
R_{int}	0.045
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.625
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.100, 1.04
No. of reflections	2475
No. of parameters	173
H-atom treatment	H-atom parameters constrained
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.16, −0.17

Computer programs: *APEX3* and *SAINT* (Bruker, 2016), *SHELXT* (Sheldrick, 2015*a*), *SHELXL2016* (Sheldrick, 2015*b*) and *OLEX2* (Dolomanov *et al.*, 2009).

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supporting information

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Computing details

Data collection: *APEX3* (Bruker, 2016); cell refinement: *SAINT* (Bruker, 2016); data reduction: *SAINT* (Bruker, 2016); program(s) used to solve structure: SHELXT (Sheldrick, 2015a); program(s) used to refine structure: *SHELXL2016* (Sheldrick, 2015b); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

(*E*)-*N*′-(3-Fluoro-2-hydroxybenzylidene)isonicotinohydrazide

Crystal data

$C_{13}H_{10}FN_3O_2$
$M_r = 259.24$
Monoclinic, $P2_1/c$
$a = 7.8555$ (3) Å
$b = 10.2748$ (5) Å
$c = 14.9390$ (7) Å
$\beta = 92.397$ (2)°
$V = 1204.73$ (9) Å^3
$Z = 4$
$F(000) = 536$
$D_x = 1.429$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 5896 reflections
$\theta = 3.3$–26.2°
$\mu = 0.11$ mm^{-1}
$T = 296$ K
Rod, light colourless
0.28 × 0.14 × 0.14 mm

Data collection

Bruker D8 QUEST CMOS diffractometer
Radiation source: microfocus sealed x-ray tube, Incoatec Iμus
Graphite Double Bounce Multilayer Mirror monochromator
Detector resolution: 10.5 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2016)
$T_{min} = 0.700$, $T_{max} = 0.745$
22872 measured reflections
2475 independent reflections
1769 reflections with $I > 2\sigma(I)$
$R_{int} = 0.045$
$\theta_{max} = 26.4°$, $\theta_{min} = 3.3°$
$h = -9\rightarrow9$
$k = -12\rightarrow12$
$l = -18\rightarrow18$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.038$
$wR(F^2) = 0.100$
$S = 1.04$
2475 reflections
173 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
$w = 1/[\sigma^2(F_o^2) + (0.0468P)^2 + 0.1698P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max} = 0.16$ e Å^{-3}
$\Delta\rho_{min} = -0.17$ 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 (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
F1	0.04982 (16)	0.68426 (11)	0.21940 (6)	0.0860 (4)
O1	0.42340 (15)	0.25717 (10)	0.46852 (6)	0.0554 (3)
O2	0.19539 (16)	0.52442 (11)	0.33911 (7)	0.0600 (3)
H2O	0.2346	0.4824	0.3818	0.090*
N1	0.63170 (16)	0.03844 (11)	0.75111 (8)	0.0441 (3)
N2	0.34254 (15)	0.40224 (11)	0.57234 (7)	0.0403 (3)
H2N	0.3409	0.4242	0.6279	0.048*
N3	0.27004 (15)	0.47948 (11)	0.50651 (8)	0.0399 (3)
C1	0.6525 (2)	0.01892 (14)	0.66412 (10)	0.0468 (4)
H1	0.7160	−0.0527	0.6473	0.056*
C2	0.58528 (18)	0.09868 (13)	0.59763 (9)	0.0412 (3)
H2B	0.6029	0.0803	0.5378	0.049*
C3	0.49156 (17)	0.20612 (12)	0.62066 (8)	0.0351 (3)
C4	0.4691 (2)	0.22719 (14)	0.71071 (9)	0.0446 (4)
H4	0.4061	0.2981	0.7293	0.054*
C5	0.5408 (2)	0.14213 (14)	0.77255 (9)	0.0463 (4)
H5	0.5248	0.1581	0.8329	0.056*
C6	0.41696 (18)	0.28991 (13)	0.54677 (9)	0.0386 (3)
C7	0.18964 (18)	0.58148 (13)	0.52892 (9)	0.0388 (3)
H7	0.1809	0.6025	0.5891	0.047*
C8	0.11173 (17)	0.66478 (13)	0.46000 (9)	0.0369 (3)
C9	0.11849 (19)	0.63208 (13)	0.36907 (9)	0.0415 (3)
C10	0.0421 (2)	0.71659 (16)	0.30725 (10)	0.0524 (4)
C11	−0.0379 (2)	0.82835 (16)	0.33089 (11)	0.0575 (5)
H11	−0.0862	0.8831	0.2872	0.069*
C12	−0.0460 (2)	0.85917 (15)	0.42025 (11)	0.0541 (4)
H12	−0.1014	0.9346	0.4374	0.065*
C13	0.02768 (19)	0.77830 (14)	0.48399 (10)	0.0468 (4)
H13	0.0214	0.7996	0.5443	0.056*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
F1	0.1259 (10)	0.0961 (8)	0.0341 (5)	0.0010 (7)	−0.0206 (5)	0.0070 (5)
O1	0.0834 (8)	0.0553 (7)	0.0275 (5)	0.0052 (6)	0.0002 (5)	0.0019 (5)
O2	0.0887 (9)	0.0545 (7)	0.0356 (6)	0.0095 (6)	−0.0102 (6)	−0.0071 (5)
N1	0.0577 (8)	0.0394 (7)	0.0347 (6)	0.0017 (6)	−0.0025 (5)	0.0029 (5)
N2	0.0548 (7)	0.0375 (6)	0.0279 (6)	−0.0019 (5)	−0.0078 (5)	0.0044 (5)
N3	0.0493 (7)	0.0360 (6)	0.0336 (6)	−0.0058 (5)	−0.0088 (5)	0.0069 (5)

C1	0.0592 (10)	0.0391 (8)	0.0422 (8)	0.0079 (7)	0.0015 (7)	−0.0014 (6)
C2	0.0530 (9)	0.0413 (8)	0.0293 (7)	−0.0019 (7)	0.0027 (6)	−0.0033 (6)
C3	0.0411 (7)	0.0334 (7)	0.0304 (7)	−0.0078 (6)	−0.0014 (5)	0.0006 (5)
C4	0.0631 (10)	0.0387 (8)	0.0320 (7)	0.0094 (7)	0.0016 (6)	−0.0010 (6)
C5	0.0682 (10)	0.0433 (8)	0.0273 (7)	0.0049 (7)	0.0003 (7)	−0.0001 (6)
C6	0.0477 (8)	0.0391 (8)	0.0287 (7)	−0.0074 (6)	−0.0012 (6)	0.0042 (6)
C7	0.0472 (8)	0.0397 (7)	0.0291 (7)	−0.0090 (7)	−0.0049 (6)	0.0027 (6)
C8	0.0391 (7)	0.0361 (7)	0.0348 (7)	−0.0090 (6)	−0.0046 (6)	0.0042 (6)
C9	0.0498 (9)	0.0391 (7)	0.0347 (7)	−0.0084 (7)	−0.0069 (6)	0.0019 (6)
C10	0.0639 (10)	0.0603 (10)	0.0318 (7)	−0.0106 (8)	−0.0127 (7)	0.0084 (7)
C11	0.0568 (10)	0.0530 (10)	0.0610 (11)	−0.0064 (8)	−0.0178 (8)	0.0228 (8)
C12	0.0529 (9)	0.0446 (9)	0.0641 (11)	0.0022 (7)	−0.0057 (8)	0.0082 (8)
C13	0.0511 (9)	0.0451 (8)	0.0440 (8)	−0.0039 (7)	−0.0012 (7)	0.0001 (7)

Geometric parameters (Å, º)

F1—C10	1.3576 (18)	C3—C6	1.4997 (18)
O1—C6	1.2195 (16)	C4—H4	0.9300
O2—H2O	0.8200	C4—C5	1.3753 (19)
O2—C9	1.3459 (18)	C5—H5	0.9300
N1—C1	1.3317 (19)	C7—H7	0.9300
N1—C5	1.3290 (18)	C7—C8	1.4541 (19)
N2—H2N	0.8600	C8—C9	1.4026 (19)
N2—N3	1.3692 (15)	C8—C13	1.394 (2)
N2—C6	1.3559 (18)	C9—C10	1.386 (2)
N3—C7	1.2756 (18)	C10—C11	1.362 (2)
C1—H1	0.9300	C11—H11	0.9300
C1—C2	1.376 (2)	C11—C12	1.376 (2)
C2—H2B	0.9300	C12—H12	0.9300
C2—C3	1.3784 (19)	C12—C13	1.373 (2)
C3—C4	1.3813 (18)	C13—H13	0.9300
C9—O2—H2O	109.5	N2—C6—C3	116.17 (11)
C5—N1—C1	116.42 (12)	N3—C7—H7	120.1
N3—N2—H2N	121.2	N3—C7—C8	119.74 (12)
C6—N2—H2N	121.2	C8—C7—H7	120.1
C6—N2—N3	117.53 (11)	C9—C8—C7	120.86 (13)
C7—N3—N2	118.90 (12)	C13—C8—C7	120.01 (12)
N1—C1—H1	118.1	C13—C8—C9	119.13 (13)
N1—C1—C2	123.77 (13)	O2—C9—C8	123.69 (12)
C2—C1—H1	118.1	O2—C9—C10	118.77 (13)
C1—C2—H2B	120.3	C10—C9—C8	117.54 (14)
C1—C2—C3	119.32 (12)	F1—C10—C9	117.07 (15)
C3—C2—H2B	120.3	F1—C10—C11	119.78 (14)
C2—C3—C4	117.38 (12)	C11—C10—C9	123.15 (14)
C2—C3—C6	118.19 (12)	C10—C11—H11	120.5
C4—C3—C6	124.40 (13)	C10—C11—C12	119.08 (14)
C3—C4—H4	120.4	C12—C11—H11	120.5

C5—C4—C3	119.28 (13)	C11—C12—H12	120.1
C5—C4—H4	120.4	C13—C12—C11	119.86 (15)
N1—C5—C4	123.83 (13)	C13—C12—H12	120.1
N1—C5—H5	118.1	C8—C13—H13	119.4
C4—C5—H5	118.1	C12—C13—C8	121.22 (14)
O1—C6—N2	122.72 (12)	C12—C13—H13	119.4
O1—C6—C3	121.11 (13)		

F1—C10—C11—C12	179.40 (15)	C4—C3—C6—O1	−170.67 (14)
O2—C9—C10—F1	0.2 (2)	C4—C3—C6—N2	9.1 (2)
O2—C9—C10—C11	−179.55 (14)	C5—N1—C1—C2	−0.3 (2)
N1—C1—C2—C3	0.5 (2)	C6—N2—N3—C7	175.56 (12)
N2—N3—C7—C8	−179.99 (11)	C6—C3—C4—C5	178.64 (13)
N3—N2—C6—O1	1.1 (2)	C7—C8—C9—O2	−0.1 (2)
N3—N2—C6—C3	−178.64 (11)	C7—C8—C9—C10	−179.69 (13)
N3—C7—C8—C9	2.3 (2)	C7—C8—C13—C12	179.56 (13)
N3—C7—C8—C13	−178.24 (12)	C8—C9—C10—F1	179.79 (13)
C1—N1—C5—C4	0.2 (2)	C8—C9—C10—C11	0.1 (2)
C1—C2—C3—C4	−0.5 (2)	C9—C8—C13—C12	−1.0 (2)
C1—C2—C3—C6	−178.83 (13)	C9—C10—C11—C12	−0.9 (3)
C2—C3—C4—C5	0.4 (2)	C10—C11—C12—C13	0.8 (2)
C2—C3—C6—O1	7.5 (2)	C11—C12—C13—C8	0.1 (2)
C2—C3—C6—N2	−172.75 (12)	C13—C8—C9—O2	−179.55 (13)
C3—C4—C5—N1	−0.3 (2)	C13—C8—C9—C10	0.8 (2)

Hydrogen-bond geometry (Å, º)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
O2—H2*O*···N3	0.82	1.87	2.5862 (14)	145
N2—H2*N*···N1^{i}	0.86	2.16	2.9851 (16)	161
C4—H4···N1^{i}	0.93	2.51	3.3492 (18)	151
C5—H5···O1^{ii}	0.93	2.37	3.2738 (17)	163

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