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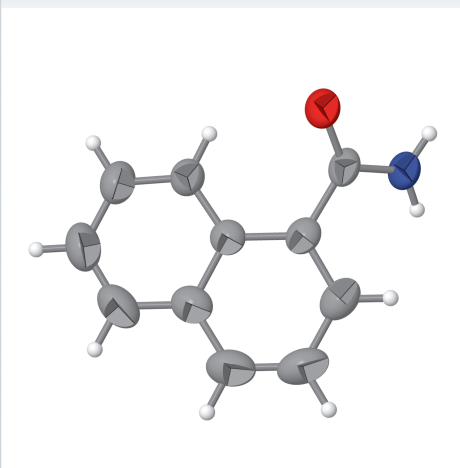
# 1-Naphthamide

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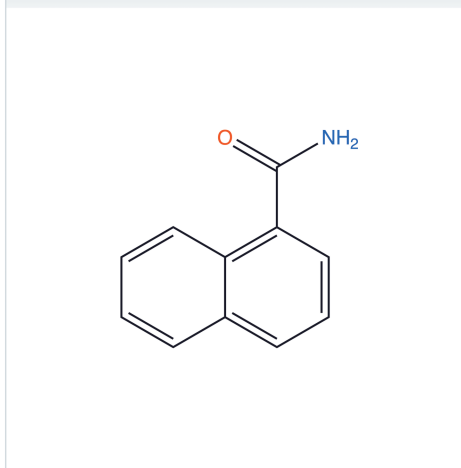
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In the title compound, C<sub>11</sub>H<sub>9</sub>NO, the dihedral angle between the naphthalene fused-ring system and the amide group is 42.18 (9)°. In the crystal, N—H···O hydrogen bonds link the molecules into (100) sheets. No significant aromatic  $\pi$ – $\pi$  stacking is observed.

## 3D view



## Chemical scheme



## Structure description

The title compound (**1**), with molecular formula C<sub>11</sub>H<sub>9</sub>NO, crystallizes in the monoclinic space group *P*<sub>2</sub><sub>1</sub>/*c*. The asymmetric unit contains one molecule in which the dihedral angle between the C2–C11 fused ring system (r.m.s. deviation = 0.008 Å) and the C1/N1/O1 amide moiety is 42.18 (9)° (Fig. 1). The significant twist probably arises to minimize steric crowding. The geometrical parameters for the amide group [C1–N1 = 1.3249 (19) Å, C1–O1 = 1.245 (2) Å and angles O1–C1–N1, O1–C1–C2 and N1–C1–C2 close to 120°] support a conjugated amide system, as expected. A short intramolecular C4–H4···O1 contact occurs.

In the extended structure of (**1**), the crystal cohesion is dominated by N11–H1A···O1 and N1–H1B···O1 hydrogen bonds (Table 1). The former generate inversion dimers and the latter link the dimers into (100) sheets (Fig. 2 and Table 1). The separations between the aromatic ring planes [shortest centroid–centroid separation = 4.799 (4) Å] are too large to support significant aromatic  $\pi$ – $\pi$  stacking interactions.

Hirshfeld surface analysis and the associated two-dimensional fingerprint plots were used to quantify the intermolecular contacts in the crystal of (**1**) (Fig. 3). The fingerprint plots show that H···H contacts make the largest contribution (42.2%), followed closely by C···H/H···C contacts (40.2%). The O···H/H···O contacts account for 14.20%, while all other contributions are less than 2.0%. These results show that the cohesion of the crystal is primarily governed by van der Waals contacts, with aromatic  $\pi$ – $\pi$  stacking interactions not playing a significant role in establishing the supramolecular architecture.



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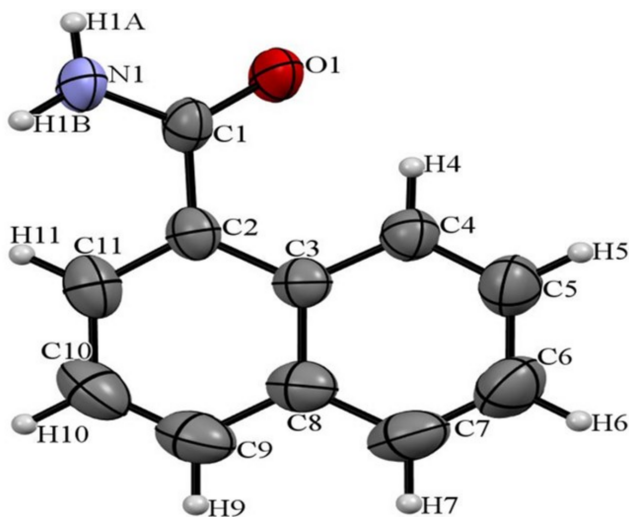


**Figure 1**  
The molecular structure of (**I**) with displacement ellipsoids drawn at the 50% probability level.

For the related structure of 9-anthramide, see Heller & Schmidt (1971).

### Synthesis and crystallization

1-Naphthamide was obtained by aqueous hydrolysis of 1-naphthonitrile under heating. The starting nitrile was suspended in water and the mixture was heated until complete

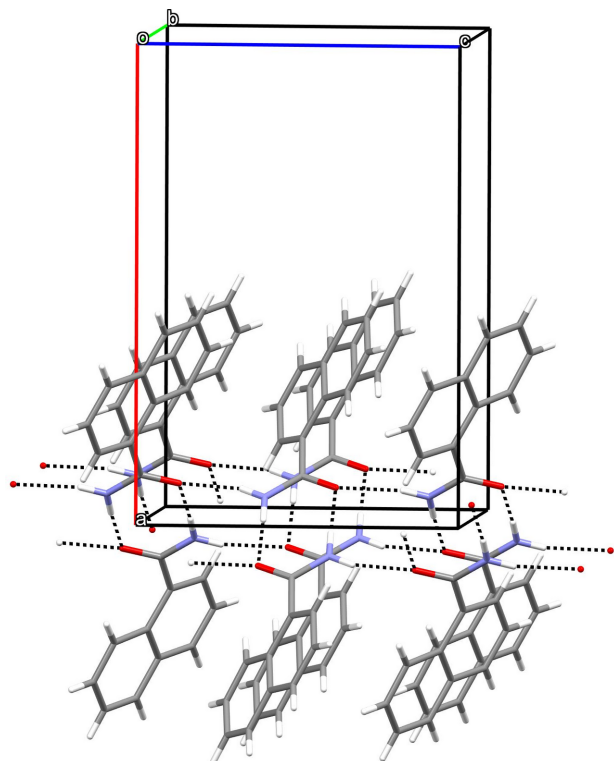


**Figure 2**  
The packing in (**I**) with hydrogen bonds shown as black dashed lines.

**Table 1**  
Hydrogen-bond geometry ( $\text{\AA}$ ,  $^\circ$ ).

| $D-H\cdots A$          | $D-H$ | $H\cdots A$ | $D\cdots A$ | $D-H\cdots A$ |
|------------------------|-------|-------------|-------------|---------------|
| $C4-H4\cdots O1$       | 0.93  | 2.38        | 2.969 (3)   | 121           |
| $N1-H1A\cdots O1^i$    | 0.86  | 2.10        | 2.951 (3)   | 170           |
| $N1-H1B\cdots O1^{ii}$ | 0.86  | 2.06        | 2.889 (3)   | 163           |

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

**Table 2**  
Experimental details.

|                                                                            |                                                     |
|----------------------------------------------------------------------------|-----------------------------------------------------|
| Crystal data                                                               | $C_{11}H_9NO$                                       |
| Chemical formula                                                           | 171.19                                              |
| $M_r$                                                                      | Monoclinic, $P2_1/c$                                |
| Crystal system, space group                                                | 293                                                 |
| Temperature (K)                                                            | 14.787 (5), 6.053 (5), 9.954 (5)                    |
| $a, b, c$ ( $\text{\AA}$ )                                                 | 90.448 (5)                                          |
| $\beta$ ( $^\circ$ )                                                       | 890.9 (9)                                           |
| $V$ ( $\text{\AA}^3$ )                                                     | 4                                                   |
| $Z$                                                                        | Mo $K\alpha$                                        |
| Radiation type                                                             | $\mu$ ( $\text{mm}^{-1}$ )                          |
| $\mu$ ( $\text{mm}^{-1}$ )                                                 | 0.08                                                |
| Crystal size (mm)                                                          | $0.14 \times 0.13 \times 0.11$                      |
| Data collection                                                            |                                                     |
| Diffractometer                                                             | Bruker APEXII                                       |
| Absorption correction                                                      | Multi-scan ( <i>CrysAlis PRO</i> ; Rigaku OD, 2015) |
| $T_{\min}, T_{\max}$                                                       | 0.753, 1.000                                        |
| No. of measured, independent and observed [ $I > 2\sigma(I)$ ] reflections | 5594, 2584, 1535                                    |
| $R_{\text{int}}$                                                           | 0.075                                               |
| $(\sin \theta/\lambda)_{\text{max}}$ ( $\text{\AA}^{-1}$ )                 | 0.704                                               |
| Refinement                                                                 |                                                     |
| $R[F^2 > 2\sigma(F^2)], wR(F^2), S$                                        | 0.071, 0.207, 1.05                                  |
| No. of reflections                                                         | 2584                                                |
| No. of parameters                                                          | 118                                                 |
| H-atom treatment                                                           | H-atom parameters constrained                       |
| $\Delta\rho_{\text{max}}, \Delta\rho_{\text{min}}$ ( $\text{e \AA}^{-3}$ ) | 0.22, $-0.27$                                       |

Computer programs: *CrysAlis PRO* (Rigaku OD, 2015), *OLEX2.solve* 1.5 (Bourhis *et al.*, 2015), *SHELXL* (Sheldrick, 2015) and *OLEX2* (Dolomanov *et al.*, 2009).

conversion to the amide was achieved. Colourless blocks of (**I**) were grown by slow evaporation of an aqueous solution of the compound at room temperature.

### Refinement

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

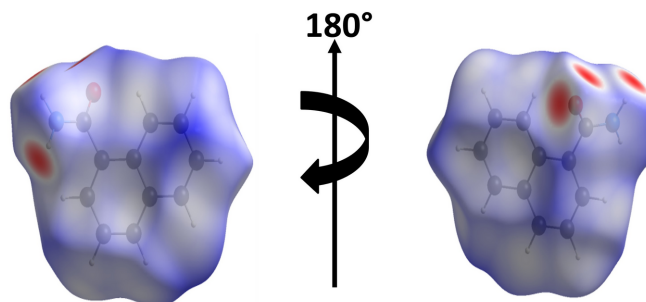


**Figure 3**  
Hirshfeld surfaces of (**I**) mapped over  $d_{\text{norm}}$ , shown as front and back views.

## Acknowledgements

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## Funding information

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## full crystallographic data

*IUCrData* (2026). **11**, x260989 [https://doi.org/10.1107/S2414314626009892]

## 1-Naphthamide

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## Naphthalene-1-carboxamide

*Crystal data*

$C_{11}H_9NO$

$M_r = 171.19$

Monoclinic,  $P2_1/c$

$a = 14.787(5) \text{ \AA}$

$b = 6.053(5) \text{ \AA}$

$c = 9.954(5) \text{ \AA}$

$\beta = 90.448(5)^\circ$

$V = 890.9(9) \text{ \AA}^3$

$Z = 4$

$F(000) = 360$

$D_x = 1.276 \text{ Mg m}^{-3}$

Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 2494 reflections

$\theta = 2.5\text{--}35.6^\circ$

$\mu = 0.08 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.14 \times 0.13 \times 0.11 \text{ mm}$

*Data collection*

Saxi-CrysAlisPro-abstract goniometer imported

SAXI images

diffractometer

Radiation source: fine-focus sealed X-ray tube,

Enhance (Mo) X-ray Source

Graphite monochromator

$\omega$  scans

Absorption correction: multi-scan

(CrysAlisPro; Rigaku OD, 2015)

$T_{\min} = 0.753$ ,  $T_{\max} = 1.000$

5594 measured reflections

2584 independent reflections

1535 reflections with  $I > 2\sigma(I)$

$R_{\text{int}} = 0.075$

$\theta_{\max} = 30.0^\circ$ ,  $\theta_{\min} = 3.6^\circ$

$h = -9 \rightarrow 20$

$k = -8 \rightarrow 5$

$l = -13 \rightarrow 13$

*Refinement*

Refinement on  $F^2$

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.071$

$wR(F^2) = 0.207$

$S = 1.05$

2584 reflections

118 parameters

0 restraints

Primary atom site location: dual

Hydrogen site location: inferred from  
neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.106P)^2 + 0.0779P]$

where  $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{\max} = 0.22 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.27 \text{ e \AA}^{-3}$

*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.** The H atoms were placed geometrically (N—H = 0.86 Å, C—H = 0.93 Å) and refined as riding atoms.

*Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters ( $\text{\AA}^2$ )*

|     | <i>x</i>     | <i>y</i>    | <i>z</i>      | $U_{\text{iso}}^*/U_{\text{eq}}$ |
|-----|--------------|-------------|---------------|----------------------------------|
| O1  | 0.92484 (9)  | 0.3228 (2)  | 0.10353 (11)  | 0.0589 (4)                       |
| C11 | 0.84713 (15) | −0.1053 (3) | −0.10734 (18) | 0.0600 (5)                       |
| H11 | 0.9018       | −0.1167     | −0.1524       | 0.072*                           |
| C2  | 0.83223 (12) | 0.0721 (3)  | −0.02377 (15) | 0.0456 (4)                       |
| C1  | 0.90457 (11) | 0.2427 (3)  | −0.00788 (15) | 0.0472 (4)                       |
| C3  | 0.74867 (11) | 0.0887 (3)  | 0.04678 (15)  | 0.0439 (4)                       |
| C4  | 0.72663 (12) | 0.2652 (3)  | 0.13314 (17)  | 0.0509 (4)                       |
| H4  | 0.7684       | 0.3780      | 0.1470        | 0.061*                           |
| C8  | 0.68255 (13) | −0.0809 (3) | 0.02734 (19)  | 0.0550 (5)                       |
| C7  | 0.59888 (15) | −0.0640 (4) | 0.0951 (2)    | 0.0721 (6)                       |
| H7  | 0.5555       | −0.1735     | 0.0827        | 0.086*                           |
| C9  | 0.70104 (17) | −0.2580 (3) | −0.0600 (2)   | 0.0681 (6)                       |
| H9  | 0.6579       | −0.3681     | −0.0725       | 0.082*                           |
| C5  | 0.64530 (15) | 0.2736 (4)  | 0.1967 (2)    | 0.0659 (6)                       |
| H5  | 0.6326       | 0.3912      | 0.2537        | 0.079*                           |
| C10 | 0.78034 (18) | −0.2706 (3) | −0.1257 (2)   | 0.0701 (6)                       |
| H10 | 0.7912       | −0.3884     | −0.1833       | 0.084*                           |
| C6  | 0.58088 (15) | 0.1078 (5)  | 0.1774 (2)    | 0.0772 (7)                       |
| H6  | 0.5256       | 0.1156      | 0.2210        | 0.093*                           |
| N1  | 0.94732 (11) | 0.3035 (3)  | −0.11836 (13) | 0.0605 (5)                       |
| H1A | 0.9900       | 0.3999      | −0.1139       | 0.073*                           |
| H1B | 0.9324       | 0.2465      | −0.1945       | 0.073*                           |

*Atomic displacement parameters ( $\text{\AA}^2$ )*

|     | $U^{11}$    | $U^{22}$    | $U^{33}$    | $U^{12}$     | $U^{13}$     | $U^{23}$     |
|-----|-------------|-------------|-------------|--------------|--------------|--------------|
| O1  | 0.0605 (8)  | 0.0885 (10) | 0.0276 (6)  | −0.0165 (7)  | 0.0030 (5)   | −0.0033 (6)  |
| C11 | 0.0731 (13) | 0.0653 (12) | 0.0416 (9)  | 0.0114 (10)  | 0.0017 (8)   | −0.0031 (8)  |
| C2  | 0.0543 (10) | 0.0526 (10) | 0.0299 (7)  | 0.0032 (7)   | −0.0019 (6)  | 0.0028 (7)   |
| C1  | 0.0478 (9)  | 0.0653 (11) | 0.0285 (7)  | 0.0027 (7)   | 0.0025 (6)   | 0.0008 (7)   |
| C3  | 0.0499 (9)  | 0.0482 (9)  | 0.0335 (7)  | −0.0009 (7)  | −0.0040 (6)  | 0.0066 (6)   |
| C4  | 0.0527 (10) | 0.0581 (10) | 0.0418 (9)  | −0.0015 (8)  | 0.0036 (7)   | 0.0006 (7)   |
| C8  | 0.0630 (11) | 0.0545 (10) | 0.0472 (9)  | −0.0073 (8)  | −0.0089 (8)  | 0.0095 (8)   |
| C7  | 0.0613 (13) | 0.0844 (15) | 0.0703 (14) | −0.0239 (11) | −0.0050 (10) | 0.0150 (12)  |
| C9  | 0.0880 (16) | 0.0549 (12) | 0.0612 (13) | −0.0146 (10) | −0.0138 (11) | 0.0033 (9)   |
| C5  | 0.0580 (11) | 0.0825 (14) | 0.0572 (12) | 0.0048 (10)  | 0.0090 (9)   | −0.0071 (10) |
| C10 | 0.1031 (18) | 0.0500 (11) | 0.0572 (12) | 0.0029 (11)  | −0.0113 (12) | −0.0088 (9)  |
| C6  | 0.0538 (12) | 0.1050 (18) | 0.0730 (15) | −0.0059 (12) | 0.0124 (10)  | 0.0030 (13)  |
| N1  | 0.0655 (10) | 0.0879 (11) | 0.0281 (7)  | −0.0179 (8)  | 0.0101 (6)   | −0.0073 (7)  |

*Geometric parameters ( $\text{\AA}$ ,  $^\circ$ )*

|         |           |       |           |
|---------|-----------|-------|-----------|
| O1—C1   | 1.245 (2) | C8—C9 | 1.408 (3) |
| C11—H11 | 0.9300    | C7—H7 | 0.9300    |
| C11—C2  | 1.377 (3) | C7—C6 | 1.352 (3) |

|               |              |               |              |
|---------------|--------------|---------------|--------------|
| C11—C10       | 1.417 (3)    | C9—H9         | 0.9300       |
| C2—C1         | 1.495 (3)    | C9—C10        | 1.349 (3)    |
| C2—C3         | 1.430 (2)    | C5—H5         | 0.9300       |
| C1—N1         | 1.3249 (19)  | C5—C6         | 1.396 (3)    |
| C3—C4         | 1.411 (2)    | C10—H10       | 0.9300       |
| C3—C8         | 1.430 (3)    | C6—H6         | 0.9300       |
| C4—H4         | 0.9300       | N1—H1A        | 0.8600       |
| C4—C5         | 1.364 (3)    | N1—H1B        | 0.8600       |
| C8—C7         | 1.417 (3)    |               |              |
| C2—C11—H11    | 119.5        | C8—C7—H7      | 119.3        |
| C2—C11—C10    | 120.9 (2)    | C6—C7—C8      | 121.37 (19)  |
| C10—C11—H11   | 119.5        | C6—C7—H7      | 119.3        |
| C11—C2—C1     | 119.01 (17)  | C8—C9—H9      | 119.5        |
| C11—C2—C3     | 119.67 (17)  | C10—C9—C8     | 121.05 (19)  |
| C3—C2—C1      | 121.32 (15)  | C10—C9—H9     | 119.5        |
| O1—C1—C2      | 122.04 (14)  | C4—C5—H5      | 119.6        |
| O1—C1—N1      | 121.23 (17)  | C4—C5—C6      | 120.8 (2)    |
| N1—C1—C2      | 116.73 (14)  | C6—C5—H5      | 119.6        |
| C2—C3—C8      | 118.39 (16)  | C11—C10—H10   | 119.8        |
| C4—C3—C2      | 123.88 (15)  | C9—C10—C11    | 120.35 (19)  |
| C4—C3—C8      | 117.72 (17)  | C9—C10—H10    | 119.8        |
| C3—C4—H4      | 119.3        | C7—C6—C5      | 120.0 (2)    |
| C5—C4—C3      | 121.30 (18)  | C7—C6—H6      | 120.0        |
| C5—C4—H4      | 119.3        | C5—C6—H6      | 120.0        |
| C7—C8—C3      | 118.83 (18)  | C1—N1—H1A     | 120.0        |
| C9—C8—C3      | 119.63 (19)  | C1—N1—H1B     | 120.0        |
| C9—C8—C7      | 121.54 (19)  | H1A—N1—H1B    | 120.0        |
| C11—C2—C1—O1  | −137.42 (18) | C3—C8—C7—C6   | −0.2 (3)     |
| C11—C2—C1—N1  | 41.7 (2)     | C3—C8—C9—C10  | 0.1 (3)      |
| C11—C2—C3—C4  | −179.15 (16) | C4—C3—C8—C7   | 0.0 (2)      |
| C11—C2—C3—C8  | −0.3 (2)     | C4—C3—C8—C9   | 178.83 (16)  |
| C2—C11—C10—C9 | −0.7 (3)     | C4—C5—C6—C7   | 0.2 (4)      |
| C2—C3—C4—C5   | 179.25 (17)  | C8—C3—C4—C5   | 0.4 (3)      |
| C2—C3—C8—C7   | −178.98 (16) | C8—C7—C6—C5   | 0.1 (4)      |
| C2—C3—C8—C9   | −0.1 (2)     | C8—C9—C10—C11 | 0.3 (3)      |
| C1—C2—C3—C4   | 1.4 (2)      | C7—C8—C9—C10  | 178.9 (2)    |
| C1—C2—C3—C8   | −179.74 (15) | C9—C8—C7—C6   | −179.1 (2)   |
| C3—C2—C1—O1   | 42.0 (2)     | C10—C11—C2—C1 | −179.83 (17) |
| C3—C2—C1—N1   | −138.82 (17) | C10—C11—C2—C3 | 0.7 (3)      |
| C3—C4—C5—C6   | −0.5 (3)     |               |              |

## Hydrogen-bond geometry (Å, °)

| <i>D</i> —H $\cdots$ <i>A</i> | <i>D</i> —H | H $\cdots$ <i>A</i> | <i>D</i> $\cdots$ <i>A</i> | <i>D</i> —H $\cdots$ <i>A</i> |
|-------------------------------|-------------|---------------------|----------------------------|-------------------------------|
| C4—H4 $\cdots$ O1             | 0.93        | 2.38                | 2.969 (3)                  | 121                           |

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|                                    |      |      |           |     |
|------------------------------------|------|------|-----------|-----|
| N1—H1 <i>A</i> ···O1 <sup>i</sup>  | 0.86 | 2.10 | 2.951 (3) | 170 |
| N1—H1 <i>B</i> ···O1 <sup>ii</sup> | 0.86 | 2.06 | 2.889 (3) | 163 |

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