



## Crystal structure of 2-benzenesulfonamido-3-hydroxypropanoic acid

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Received 22 October 2015; accepted 26 October 2015

Edited by W. T. A. Harrison, University of Aberdeen, Scotland

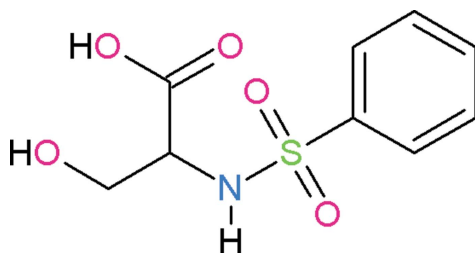
In the title compound, C<sub>9</sub>H<sub>11</sub>NO<sub>5</sub>S, the O=S=O plane of the sulfonyl group is twisted at a dihedral angle of 52.54 (16)° with respect to the benzene ring. The dihedral angle between the carboxylic acid group and the benzene ring is 49.91 (16)°. In the crystal, C—H...O, N—H...O and O—H...O hydrogen bonds link the molecules into (001) sheets.

**Keywords:** crystal structure; benzenesulfonamido; propanoic acid; sulfonyl group; O—H...O hydrogen bonds.

**CCDC reference:** 1433189

### 1. Related literature

For related structures, see: Aguilar-Castro *et al.* (2004); Arshad *et al.* (2009, 2012); Zolotarev *et al.* (2014).



### 2. Experimental

#### 2.1. Crystal data

C<sub>9</sub>H<sub>11</sub>NO<sub>5</sub>S  
M<sub>r</sub> = 245.25  
Orthorhombic, P<sub>2</sub><sub>1</sub>2<sub>1</sub>2<sub>1</sub>  
a = 5.0464 (4) Å  
b = 9.9752 (8) Å  
c = 21.4701 (17) Å

V = 1080.78 (15) Å<sup>3</sup>  
Z = 4  
Mo Kα radiation  
μ = 0.31 mm<sup>-1</sup>  
T = 296 K  
0.40 × 0.20 × 0.18 mm

#### 2.2. Data collection

Bruker Kappa APEXII CCD diffractometer  
Absorption correction: multi-scan (SADABS; Bruker, 2005)  
T<sub>min</sub> = 0.890, T<sub>max</sub> = 0.950

5013 measured reflections  
2354 independent reflections  
1978 reflections with I > 2σ(I)  
R<sub>int</sub> = 0.025

#### 2.3. Refinement

R[F<sup>2</sup> > 2σ(F<sup>2</sup>)] = 0.042  
wR(F<sup>2</sup>) = 0.093  
S = 1.03  
2354 reflections  
149 parameters  
H atoms treated by a mixture of independent and constrained refinement

Δρ<sub>max</sub> = 0.21 e Å<sup>-3</sup>  
Δρ<sub>min</sub> = -0.28 e Å<sup>-3</sup>  
Absolute structure: Flack x determined using 919 quotients [(I<sup>+</sup>) - (I<sup>-</sup>)] / [(I<sup>+</sup>) + (I<sup>-</sup>)] (Parsons *et al.*, 2013)  
Absolute structure parameter: 0.05 (5)

**Table 1**

Hydrogen-bond geometry (Å, °).

D—H...A	D—H	H...A	D...A	D—H...A
O1—H1...O3 <sup>i</sup>	0.84 (5)	1.81 (5)	2.621 (4)	164 (5)
O3—H3...O5 <sup>i</sup>	0.82	1.96	2.754 (3)	164
N1—H1A...O4 <sup>ii</sup>	0.86	2.39	3.066 (4)	136
C2—H2...O2 <sup>iii</sup>	0.98	2.48	3.425 (5)	162
C6—H6...O5 <sup>iv</sup>	0.93	2.52	3.342 (5)	148
C7—H7...O2 <sup>v</sup>	0.93	2.58	3.347 (5)	141

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

Data collection: APEX2 (Bruker, 2007); cell refinement: SAINT (Bruker, 2007); data reduction: SAINT (Bruker, 2007); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL2014 (Sheldrick, 2015); molecular graphics: ORTEP-3 for Windows (Farrugia, 2012) and PLATON (Spek, 2009); software used to prepare material for publication: WinGX (Farrugia, 2012) and PLATON (Spek, 2009).

### Acknowledgements

The authors acknowledge the provision of funds for the purchase of a diffractometer and encouragement by Dr Muhammad Akram Chaudhary, Ex-Vice Chancellor, University of Sargodha, Pakistan.

Supporting information for this paper is available from the IUCr electronic archives (Reference: HB7530).

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## supporting information

*Acta Cryst.* (2015). E71, o902–o903 [https://doi.org/10.1107/S2056989015020149]

## Crystal structure of 2-benzenesulfonamido-3-hydroxypropanoic acid

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### S1. Comment

The title compound (I), (Fig. 1) has been synthesized for complexation and other studies.

The crystal structures of *N*-((4-methylphenyl)sulfonyl)serine (Zolotarev *et al.*, 2014), *N*(*S*)-(*p*-toluenesulfonyl)-*L*-alanine (Aguilar-Castro *et al.*, 2004), 2-benzenesulfonamido-3-methylbutyric acid (Arshad *et al.*, 2012) and (2*R*)-2-benzenesulfonamido-2-phenylethanoic acid (Arshad *et al.*, 2009) have been reported which are related to the title compound.

The aminoacetic acid moiety B (C1/C2/N1/O1/O2) is roughly planar with r.m.s. deviation of 0.0588 Å. The dihedral angle between the benzene ring and B is 52.96 (14)°. The sulfonyl group C (S1/O4/O5) is oriented at a dihedral angle of 52.54 (16)° with the parent benzene ring. In the crystal, the molecules are linked into a two-dimensional polymeric network (Table 2, Fig. 2) due to H-bondings of C–H···O, N–H···O and O–H···O types with base vectors [100], [010] and in the plane (001).

### S2. Experimental

The title compound was prepared by using equimolar ratio of *L*-serine and benzenesulfonyl chloride in 40 ml water. The benzenesulfonyl chloride dissolved in distilled water was added pinch by pinch in the *L*-serine already dissolved in distilled water and stirred at 296–298 K, while keeping the pH of the reaction mixture was maintained at 8–9 by adding 1.0 M sodium bicarbonate solution. The 1.0 M HCl solution was added after an hour which resulted in the form of white precipitates. The precipitates obtained were filtered and dried from which colourless needles of (I) were obtained after recrystallization from ethanol solution after 48 h. Yield: 68% Melting point: 493 K.

### S3. Refinement

The coordinates of H-atom of carboxyl group were refined. The other H-atoms were positioned geometrically (O–H = 0.82, N–H = 0.86, C–H = 0.93–0.98 Å) and refined as riding with  $U_{\text{iso}}(\text{H}) = xU_{\text{eq}}(\text{C, N, O})$ , where  $x = 1.5$  for hydroxy and  $x = 1.2$  for all other H-atoms.

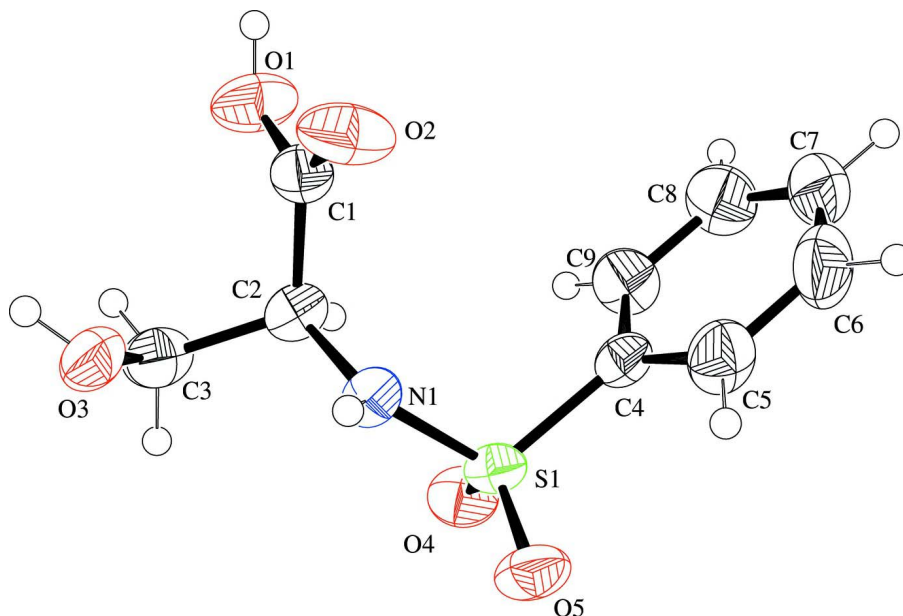


Figure 1

View of the asymmetric unit of title compound with displacement ellipsoids drawn at the 50% probability level.

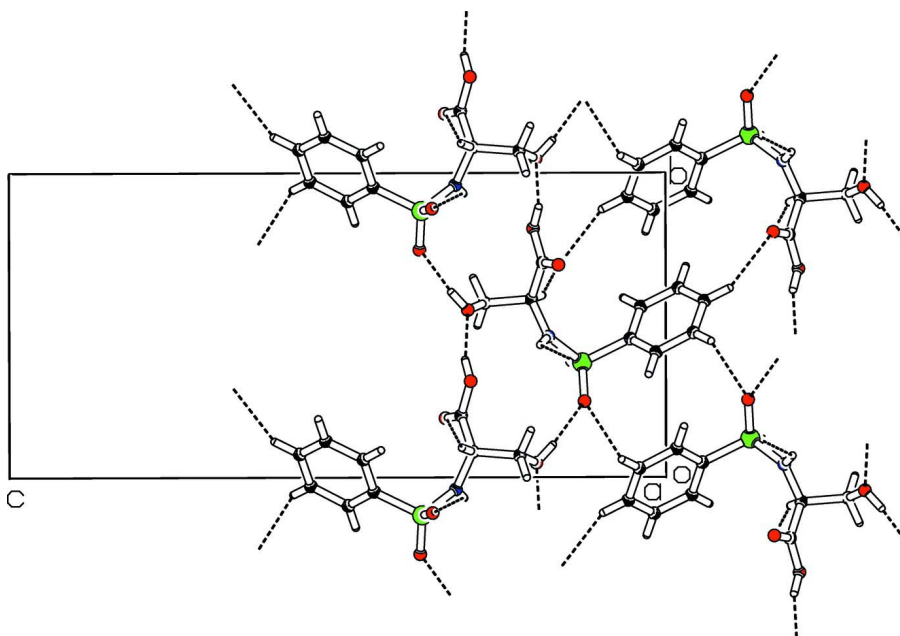


Figure 2

The partial packing (*PLATON*; Spek, 2009), which shows that molecules form two dimensional polymeric network.

### 2-Benzenesulfonamido-3-hydroxypropanoic acid

#### Crystal data

$C_9H_{11}NO_5S$

$M_r = 245.25$

Orthorhombic,  $P2_12_12_1$

$a = 5.0464 (4) \text{ \AA}$

$b = 9.9752 (8) \text{ \AA}$

$c = 21.4701 (17) \text{ \AA}$

$V = 1080.78 (15) \text{ \AA}^3$

$Z = 4$

$F(000) = 512$   
 $D_x = 1.507 \text{ Mg m}^{-3}$   
 Mo  $K\alpha$  radiation,  $\lambda = 0.71073 \text{ \AA}$   
 Cell parameters from 1978 reflections  
 $\theta = 2.8\text{--}27.1^\circ$

$\mu = 0.31 \text{ mm}^{-1}$   
 $T = 296 \text{ K}$   
 Needle, colorless  
 $0.40 \times 0.20 \times 0.18 \text{ mm}$

*Data collection*

Bruker Kappa APEXII CCD  
 diffractometer  
 Radiation source: fine-focus sealed tube  
 Graphite monochromator  
 Detector resolution: 7.80 pixels  $\text{mm}^{-1}$   
 $\omega$  scans  
 Absorption correction: multi-scan  
 (SADABS; Bruker, 2005)  
 $T_{\min} = 0.890$ ,  $T_{\max} = 0.950$

5013 measured reflections  
 2354 independent reflections  
 1978 reflections with  $I > 2\sigma(I)$   
 $R_{\text{int}} = 0.025$   
 $\theta_{\max} = 27.1^\circ$ ,  $\theta_{\min} = 2.8^\circ$   
 $h = -6 \rightarrow 6$   
 $k = -9 \rightarrow 12$   
 $l = -27 \rightarrow 27$

*Refinement*

Refinement on  $F^2$   
 Least-squares matrix: full  
 $R[F^2 > 2\sigma(F^2)] = 0.042$   
 $wR(F^2) = 0.093$   
 $S = 1.03$   
 2354 reflections  
 149 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 atoms treated by a mixture of independent  
 and constrained refinement  
 $w = 1/[\sigma^2(F_o^2) + (0.0432P)^2 + 0.1053P]$   
 where  $P = (F_o^2 + 2F_c^2)/3$   
 $(\Delta/\sigma)_{\max} < 0.001$   
 $\Delta\rho_{\max} = 0.21 \text{ e \AA}^{-3}$   
 $\Delta\rho_{\min} = -0.28 \text{ e \AA}^{-3}$   
 Absolute structure: Flack  $x$  determined using  
 919 quotients  $[(I^+) - (I^-)] / [(I^+) + (I^-)]$  (Parsons *et al.*,  
 2013)  
 Absolute structure parameter: 0.05 (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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
S1	0.68841 (17)	0.37500 (8)	0.12794 (3)	0.0362 (2)
O1	0.7864 (6)	0.8154 (3)	0.20233 (14)	0.0624 (8)
H1	0.871 (11)	0.885 (5)	0.194 (2)	0.094*
O2	1.1199 (6)	0.6949 (3)	0.16402 (14)	0.0651 (8)
O3	0.9705 (7)	0.5474 (2)	0.30216 (11)	0.0583 (8)
H3	1.0059	0.6065	0.3274	0.087*
O4	0.4135 (5)	0.3816 (3)	0.14371 (11)	0.0504 (6)
O5	0.8178 (6)	0.2474 (2)	0.12476 (11)	0.0502 (6)

N1	0.8462 (6)	0.4600 (2)	0.17945 (11)	0.0368 (6)
H1A	0.9985	0.4323	0.1920	0.044*
C1	0.9047 (8)	0.7029 (3)	0.18768 (14)	0.0406 (8)
C2	0.7369 (7)	0.5833 (3)	0.20543 (14)	0.0384 (8)
H2	0.5583	0.5962	0.1886	0.046*
C3	0.7171 (9)	0.5712 (4)	0.27649 (16)	0.0530 (10)
H3A	0.6444	0.6533	0.2936	0.064*
H3B	0.5990	0.4981	0.2873	0.064*
C4	0.7318 (7)	0.4526 (3)	0.05482 (14)	0.0365 (8)
C5	0.9275 (9)	0.4077 (4)	0.01556 (16)	0.0542 (10)
H5	1.0338	0.3355	0.0269	0.065*
C6	0.9645 (11)	0.4717 (4)	−0.04132 (17)	0.0653 (12)
H6	1.0988	0.4436	−0.0679	0.078*
C7	0.8028 (10)	0.5765 (4)	−0.05829 (16)	0.0609 (11)
H7	0.8250	0.6180	−0.0967	0.073*
C8	0.6103 (9)	0.6193 (4)	−0.01864 (17)	0.0618 (12)
H8	0.5028	0.6909	−0.0301	0.074*
C9	0.5718 (9)	0.5581 (4)	0.03840 (17)	0.0512 (9)
H9	0.4395	0.5879	0.0652	0.061*

*Atomic displacement parameters (Å<sup>2</sup>)*

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
S1	0.0337 (4)	0.0291 (3)	0.0459 (4)	−0.0024 (4)	−0.0051 (4)	0.0017 (3)
O1	0.061 (2)	0.0327 (13)	0.0933 (19)	0.0046 (14)	0.0105 (17)	−0.0028 (13)
O2	0.054 (2)	0.0441 (14)	0.097 (2)	0.0024 (14)	0.0283 (17)	0.0134 (14)
O3	0.089 (2)	0.0342 (13)	0.0514 (14)	0.0014 (15)	−0.0182 (15)	−0.0063 (10)
O4	0.0350 (13)	0.0529 (14)	0.0634 (14)	−0.0087 (13)	−0.0019 (13)	0.0046 (12)
O5	0.0590 (17)	0.0282 (11)	0.0635 (14)	0.0039 (11)	−0.0118 (16)	0.0015 (10)
N1	0.0325 (16)	0.0352 (14)	0.0428 (12)	0.0059 (13)	−0.0089 (14)	−0.0030 (11)
C1	0.042 (2)	0.0349 (17)	0.0444 (17)	0.0068 (17)	−0.0013 (18)	0.0026 (14)
C2	0.0300 (19)	0.0357 (16)	0.0496 (16)	0.0040 (14)	−0.0014 (16)	−0.0043 (13)
C3	0.059 (3)	0.0427 (19)	0.0569 (19)	−0.005 (2)	0.025 (2)	−0.0085 (15)
C4	0.036 (2)	0.0331 (15)	0.0405 (14)	−0.0015 (16)	−0.0064 (16)	−0.0051 (12)
C5	0.059 (3)	0.051 (2)	0.0528 (19)	0.018 (2)	0.001 (2)	−0.0045 (16)
C6	0.081 (3)	0.069 (3)	0.0457 (19)	0.011 (3)	0.014 (2)	−0.011 (2)
C7	0.080 (3)	0.062 (2)	0.0400 (16)	0.000 (3)	−0.006 (2)	0.0020 (16)
C8	0.071 (3)	0.057 (2)	0.058 (2)	0.014 (2)	−0.011 (2)	0.0106 (19)
C9	0.048 (2)	0.050 (2)	0.0560 (19)	0.0159 (19)	0.003 (2)	0.0046 (17)

*Geometric parameters (Å, °)*

S1—O4	1.429 (3)	C3—H3A	0.9700
S1—O5	1.432 (2)	C3—H3B	0.9700
S1—N1	1.605 (3)	C4—C9	1.373 (5)
S1—C4	1.764 (3)	C4—C5	1.374 (5)
O1—C1	1.310 (4)	C5—C6	1.391 (5)
O1—H1	0.84 (5)	C5—H5	0.9300

O2—C1	1.201 (4)	C6—C7	1.375 (6)
O3—C3	1.413 (5)	C6—H6	0.9300
O3—H3	0.8200	C7—C8	1.360 (6)
N1—C2	1.458 (4)	C7—H7	0.9300
N1—H1A	0.8600	C8—C9	1.382 (5)
C1—C2	1.512 (5)	C8—H8	0.9300
C2—C3	1.534 (5)	C9—H9	0.9300
C2—H2	0.9800		
O4—S1—O5	119.67 (16)	C2—C3—H3A	109.7
O4—S1—N1	107.09 (15)	O3—C3—H3B	109.7
O5—S1—N1	106.03 (14)	C2—C3—H3B	109.7
O4—S1—C4	108.12 (15)	H3A—C3—H3B	108.2
O5—S1—C4	106.92 (15)	C9—C4—C5	121.0 (3)
N1—S1—C4	108.64 (14)	C9—C4—S1	119.5 (3)
C1—O1—H1	115 (4)	C5—C4—S1	119.5 (3)
C3—O3—H3	109.5	C4—C5—C6	119.1 (4)
C2—N1—S1	121.4 (2)	C4—C5—H5	120.5
C2—N1—H1A	119.3	C6—C5—H5	120.5
S1—N1—H1A	119.3	C7—C6—C5	120.1 (4)
O2—C1—O1	124.8 (4)	C7—C6—H6	119.9
O2—C1—C2	124.1 (3)	C5—C6—H6	119.9
O1—C1—C2	111.1 (3)	C8—C7—C6	119.7 (4)
N1—C2—C1	110.9 (3)	C8—C7—H7	120.1
N1—C2—C3	109.8 (3)	C6—C7—H7	120.1
C1—C2—C3	110.4 (3)	C7—C8—C9	121.1 (4)
N1—C2—H2	108.5	C7—C8—H8	119.4
C1—C2—H2	108.5	C9—C8—H8	119.4
C3—C2—H2	108.5	C4—C9—C8	118.9 (4)
O3—C3—C2	110.0 (3)	C4—C9—H9	120.6
O3—C3—H3A	109.7	C8—C9—H9	120.6
O4—S1—N1—C2	-37.2 (3)	N1—S1—C4—C9	-83.5 (3)
O5—S1—N1—C2	-166.0 (2)	O4—S1—C4—C5	-148.5 (3)
C4—S1—N1—C2	79.4 (3)	O5—S1—C4—C5	-18.4 (3)
S1—N1—C2—C1	-114.8 (3)	N1—S1—C4—C5	95.6 (3)
S1—N1—C2—C3	122.8 (3)	C9—C4—C5—C6	0.7 (6)
O2—C1—C2—N1	-11.0 (5)	S1—C4—C5—C6	-178.4 (3)
O1—C1—C2—N1	170.0 (3)	C4—C5—C6—C7	-1.4 (6)
O2—C1—C2—C3	111.1 (4)	C5—C6—C7—C8	1.4 (7)
O1—C1—C2—C3	-68.0 (4)	C6—C7—C8—C9	-0.8 (7)
N1—C2—C3—O3	59.3 (4)	C5—C4—C9—C8	-0.1 (6)
C1—C2—C3—O3	-63.3 (4)	S1—C4—C9—C8	179.1 (3)
O4—S1—C4—C9	32.4 (3)	C7—C8—C9—C4	0.1 (7)
O5—S1—C4—C9	162.5 (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>
O1—H1 $\cdots$ O3 <sup>i</sup>	0.84 (5)	1.81 (5)	2.621 (4)	164 (5)
O3—H3 $\cdots$ O5 <sup>i</sup>	0.82	1.96	2.754 (3)	164
N1—H1 <i>A</i> $\cdots$ O4 <sup>ii</sup>	0.86	2.39	3.066 (4)	136
C2—H2 $\cdots$ O2 <sup>iii</sup>	0.98	2.48	3.425 (5)	162
C6—H6 $\cdots$ O5 <sup>iv</sup>	0.93	2.52	3.342 (5)	148
C7—H7 $\cdots$ O2 <sup>v</sup>	0.93	2.58	3.347 (5)	141

Symmetry codes: (i)  $-x+2, y+1/2, -z+1/2$ ; (ii)  $x+1, y, z$ ; (iii)  $x-1, y, z$ ; (iv)  $x+1/2, -y+1/2, -z$ ; (v)  $x-1/2, -y+3/2, -z$ .