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# Cyclohexane-1,2,3,4,5-pentol

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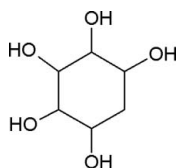
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Key indicators: single-crystal X-ray study;  $T = 293$  K; mean  $\sigma(\text{C}-\text{C}) = 0.001$  Å;  $R$  factor = 0.033;  $wR$  factor = 0.086; data-to-parameter ratio = 23.0.

In the title compound,  $\text{C}_6\text{H}_{12}\text{O}_5$ , the cyclohexane ring adopts a chair conformation. The absolute configuration is not defined. However, the relative configuration can be assigned as  $1R^*,3R^*,4S^*,5S^*$ . In the crystal structure, molecules are linked by strong intermolecular  $\text{O}-\text{H}\cdots\text{O}$  hydrogen bonds, producing a three-dimensional network.

## Related literature

For details of the biological activity and applications of cyclohexane derivatives, see: Eddington *et al.* (2000); Padmavathi *et al.* (2000, 2001); Li & Strobel (2001). For puckering parameters and displacement asymmetric parameters, see: Cremer & Pople (1975); Nardelli (1983).



## Experimental

### Crystal data

$\text{C}_6\text{H}_{12}\text{O}_5$   $V = 350.41$  (5) Å<sup>3</sup>  
 $M_r = 164.16$   $Z = 2$   
 Monoclinic,  $P2_1$  Mo  $K\alpha$  radiation  
 $a = 6.4727$  (5) Å  $\mu = 0.14$  mm<sup>-1</sup>  
 $b = 8.4851$  (6) Å  $T = 293$  K  
 $c = 6.8249$  (5) Å  $0.21 \times 0.19 \times 0.17$  mm  
 $\beta = 110.796$  (2)°

### Data collection

Bruker Kappa APEXII CCD 5019 measured reflections  
 diffractometer 2418 independent reflections  
 Absorption correction: multi-scan 2314 reflections with  $I > 2\sigma(I)$   
 (SADABS; Sheldrick, 1996)  $R_{\text{int}} = 0.020$   
 $T_{\text{min}} = 0.972$ ,  $T_{\text{max}} = 0.977$

### Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$  H-atom parameters constrained  
 $wR(F^2) = 0.086$   $\Delta\rho_{\text{max}} = 0.39$  e Å<sup>-3</sup>  
 $S = 1.06$   $\Delta\rho_{\text{min}} = -0.19$  e Å<sup>-3</sup>  
 2418 reflections Absolute structure: Flack (1983),  
 105 parameters 994 Friedel pairs  
 1 restraint Flack parameter: 0.7 (6)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{O1}-\text{H1A}\cdots\text{O3}^{\text{i}}$	0.82	1.94	2.7347 (11)	164
$\text{O2}-\text{H2A}\cdots\text{O4}^{\text{ii}}$	0.82	1.96	2.7761 (12)	170
$\text{O3}-\text{H3A}\cdots\text{O1}^{\text{iii}}$	0.82	2.02	2.8417 (11)	177
$\text{O4}-\text{H4A}\cdots\text{O5}^{\text{iv}}$	0.82	1.91	2.7067 (12)	165
$\text{O5}-\text{H5}\cdots\text{O2}^{\text{v}}$	0.82	2.00	2.8036 (12)	166

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

Data collection: APEX2 (Bruker, 2004); cell refinement: APEX2; data reduction: SAINT (Bruker, 2004); program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: ORTEP-3 (Farrugia, 1997); software used to prepare material for publication: SHELXL97 and PLATON (Spek, 2009).

GG and ASP thank Dr Babu Varghese, SAIF, IIT, Chennai, India, for the X-ray intensity data collection.

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: KP2211).

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## supporting information

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**Cyclohexane-1,2,3,4,5-pentol**

**G. Ganesh, C. Sivaraj, P. S. Kannan, N. Raaman and A. SubbiahPandi**

**S1. Comment**

Cyclohexanes are either prepared from natural sources or entirely *via* synthetic routes. The reason for their preparation is a variety of medical effects. The molecules provide anticonvulsant, antimalarial, antiinflammatory and cardiovascular effects (Eddington *et al.*, 2000). Cyclohexanes are also important intermediates for many biologically active compounds (Padmavathi *et al.*, 2001; Padmavathi *et al.*, 2000). A number of their derivatives have fungicidal and antitumor activities (Li & Strobel, 2001). Taking into consideration of these aspects, and in order to obtain a detailed information on the molecular structure in the solid state, the X-ray study of the title compound has been carried out.

X-Ray analysis confirms the molecular structure and atom connectivity for (I) (Fig. 1). The cyclohexane ring adopts the chair conformation with the puckering parameters  $q_2$  and  $\varphi$  (Cremer & Pople, 1975) and the smallest displacement asymmetric parameters,  $\Delta$ , (Nardelli, 1983) as follows:  $q_2=0.0673$  (11) Å,  $\varphi=111.3$  (9)°,  $\Delta_s(C1)=1.27$  (8).

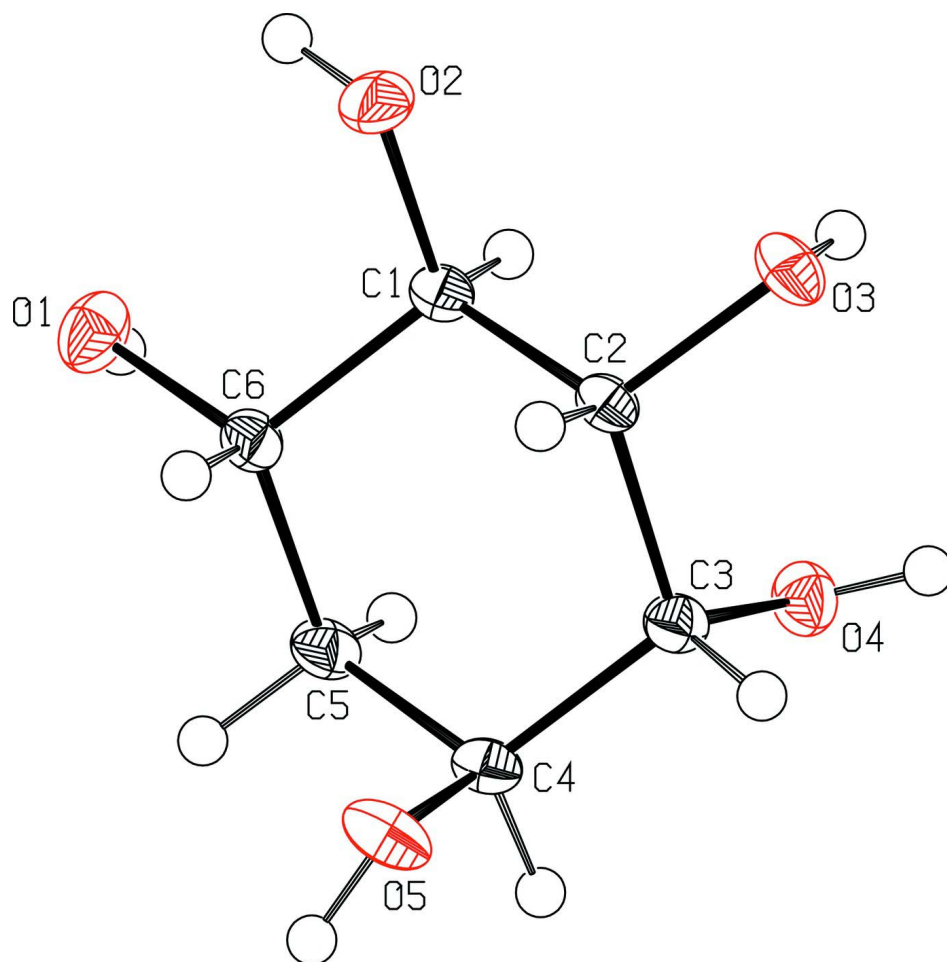
The atom O1 acts as a donor to the atom O3 of the neighbouring molecule. This hydrogen bond is involved in a motif C(6) forming an infinite chain along *a* axis, and also the atom O5 acts as a donor to the atom O2. This hydrogen bond is involved in a motif C(7) forming an infinite chain along *c* axis. The crystal packing is defined by O–H···O hydrogen bonds (Table 1, Fig. 2)

**S2. Experimental**

The compound was isolated from Manilkara zapota(L) Van Royan leaves of ethyl acetate fraction by column chromatography. Single crystals of the title compound suitable for X-ray diffraction were obtained from a mixture of ethyl acetate and methanol (3:1) by slow evaporation.

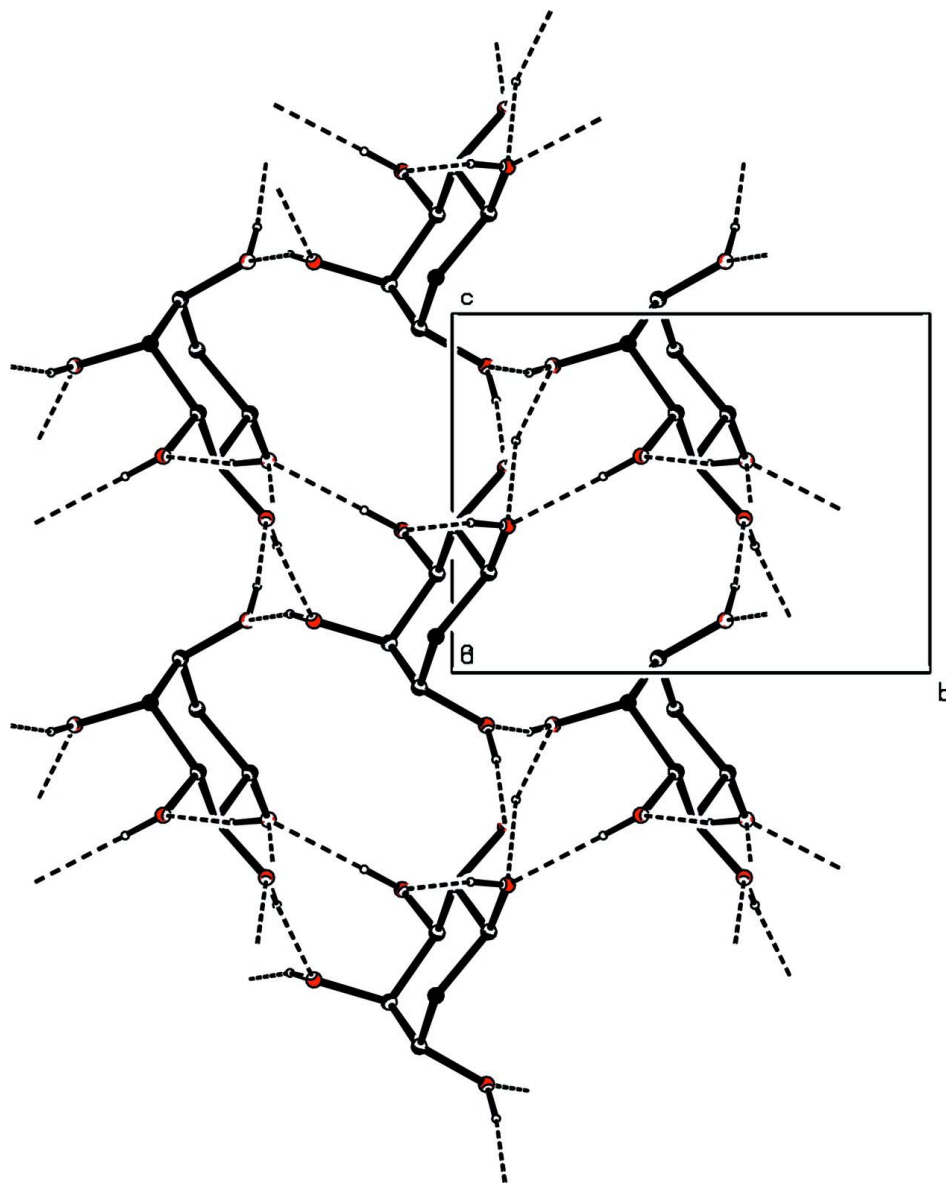
**S3. Refinement**

All the H atoms were positioned geometrically, with O–H = 0.82 Å and C–H = 0.93 - 0.98 Å and constrained to ride on their parent atom, with  $U_{iso,H}=1.2U_{eq}(C)$ .



**Figure 1**

The molecular structure of the title compound showing the 50% probability displacement ellipsoids.

**Figure 2**

The packing diagram of the title compound, view along the *a* axis forming a three dimensional network.

### Cyclohexane-1,2,3,4,5-pentol

#### Crystal data

$C_6H_{12}O_5$

$M_r = 164.16$

Monoclinic,  $P2_1$

Hall symbol: P 2yb

$a = 6.4727 (5) \text{ \AA}$

$b = 8.4851 (6) \text{ \AA}$

$c = 6.8249 (5) \text{ \AA}$

$\beta = 110.796 (2)^\circ$

$V = 350.41 (5) \text{ \AA}^3$

$Z = 2$

$F(000) = 176$

$D_x = 1.556 \text{ Mg m}^{-3}$

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

Cell parameters from 2418 reflections

$\theta = 3.2\text{--}33.3^\circ$

$\mu = 0.14 \text{ mm}^{-1}$

$T = 293 \text{ K}$

Block, colourless

$0.21 \times 0.19 \times 0.17 \text{ mm}$

*Data collection*

Bruker Kappa APEXII CCD diffractometer	5019 measured reflections
Radiation source: fine-focus sealed tube	2418 independent reflections
Graphite monochromator	2314 reflections with $I > 2\sigma(I)$
$\omega$ scans	$R_{\text{int}} = 0.020$
Absorption correction: multi-scan (SADABS; Sheldrick, 1996)	$\theta_{\text{max}} = 33.3^\circ$ , $\theta_{\text{min}} = 3.2^\circ$
$T_{\text{min}} = 0.972$ , $T_{\text{max}} = 0.977$	$h = -9 \rightarrow 9$
	$k = -12 \rightarrow 12$
	$l = -9 \rightarrow 10$

*Refinement*

Refinement on $F^2$	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0548P)^2 + 0.0106P]$
$wR(F^2) = 0.086$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.06$	$(\Delta/\sigma)_{\text{max}} < 0.001$
2418 reflections	$\Delta\rho_{\text{max}} = 0.39 \text{ e } \text{\AA}^{-3}$
105 parameters	$\Delta\rho_{\text{min}} = -0.19 \text{ e } \text{\AA}^{-3}$
1 restraint	Absolute structure: Flack (1983), 994 Friedel pairs
Primary atom site location: structure-invariant direct methods	Absolute structure parameter: 0.7 (6)
Secondary atom site location: difference Fourier map	

*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 ( $\text{\AA}^2$ )*

	$x$	$y$	$z$	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.39464 (15)	0.00491 (11)	0.41069 (16)	0.01595 (17)
H1	0.4688	-0.0926	0.4757	0.019*
C2	0.15563 (14)	-0.03135 (11)	0.27557 (15)	0.01522 (17)
H2	0.0821	0.0694	0.2247	0.018*
C3	0.13572 (14)	-0.13189 (11)	0.08297 (15)	0.01626 (17)
H3	-0.0198	-0.1352	-0.0093	0.020*
C4	0.27248 (16)	-0.06837 (11)	-0.04069 (15)	0.01663 (17)
H4	0.2741	-0.1468	-0.1456	0.020*
C5	0.51009 (15)	-0.03378 (11)	0.10101 (16)	0.01768 (18)
H5A	0.5837	-0.1318	0.1590	0.021*
H5B	0.5889	0.0137	0.0188	0.021*
C6	0.51703 (15)	0.07685 (11)	0.27875 (16)	0.01628 (17)
H6	0.4414	0.1747	0.2168	0.020*
O1	0.73862 (11)	0.11569 (9)	0.40896 (14)	0.02328 (17)
H1A	0.8190	0.0392	0.4180	0.035*

O2	0.38759 (13)	0.11155 (10)	0.57023 (13)	0.02410 (17)
H2A	0.5140	0.1337	0.6464	0.036*
O3	0.04224 (12)	-0.10449 (9)	0.39647 (13)	0.02046 (16)
H3A	0.1094	-0.1839	0.4529	0.031*
O4	0.20891 (12)	-0.28909 (9)	0.14488 (13)	0.02034 (16)
H4A	0.1094	-0.3390	0.1642	0.031*
O5	0.16705 (13)	0.07199 (9)	-0.14612 (13)	0.02343 (17)
H5	0.2119	0.0922	-0.2416	0.035*

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

	$U^{11}$	$U^{22}$	$U^{33}$	$U^{12}$	$U^{13}$	$U^{23}$
C1	0.0173 (4)	0.0179 (4)	0.0146 (4)	-0.0003 (3)	0.0080 (3)	-0.0012 (3)
C2	0.0156 (3)	0.0175 (4)	0.0152 (4)	0.0008 (3)	0.0088 (3)	0.0005 (3)
C3	0.0166 (3)	0.0182 (4)	0.0147 (4)	0.0003 (3)	0.0065 (3)	-0.0001 (3)
C4	0.0192 (4)	0.0187 (4)	0.0136 (4)	0.0020 (3)	0.0078 (3)	0.0000 (3)
C5	0.0179 (4)	0.0215 (4)	0.0167 (4)	0.0012 (3)	0.0099 (3)	-0.0006 (3)
C6	0.0159 (3)	0.0180 (4)	0.0173 (4)	-0.0007 (3)	0.0088 (3)	-0.0006 (3)
O1	0.0168 (3)	0.0249 (3)	0.0288 (4)	-0.0031 (3)	0.0089 (3)	-0.0074 (3)
O2	0.0253 (3)	0.0310 (4)	0.0205 (4)	-0.0075 (3)	0.0136 (3)	-0.0112 (3)
O3	0.0215 (3)	0.0226 (3)	0.0233 (4)	0.0010 (3)	0.0155 (3)	0.0027 (3)
O4	0.0231 (3)	0.0162 (3)	0.0237 (4)	-0.0008 (2)	0.0107 (3)	0.0000 (3)
O5	0.0265 (3)	0.0278 (4)	0.0195 (4)	0.0093 (3)	0.0125 (3)	0.0094 (3)

*Geometric parameters (Å, °)*

C1—O2	1.4289 (13)	C4—H4	0.9800
C1—C6	1.5223 (14)	C5—C6	1.5218 (14)
C1—C2	1.5249 (12)	C5—H5A	0.9700
C1—H1	0.9800	C5—H5B	0.9700
C2—O3	1.4264 (12)	C6—O1	1.4319 (11)
C2—C3	1.5337 (14)	C6—H6	0.9800
C2—H2	0.9800	O1—H1A	0.8200
C3—O4	1.4282 (12)	O2—H2A	0.8200
C3—C4	1.5221 (14)	O3—H3A	0.8200
C3—H3	0.9800	O4—H4A	0.8200
C4—O5	1.4328 (12)	O5—H5	0.8200
C4—C5	1.5266 (13)		
O2—C1—C6	111.16 (8)	O5—C4—H4	108.9
O2—C1—C2	106.77 (7)	C3—C4—H4	108.9
C6—C1—C2	110.64 (8)	C5—C4—H4	108.9
O2—C1—H1	109.4	C6—C5—C4	111.20 (8)
C6—C1—H1	109.4	C6—C5—H5A	109.4
C2—C1—H1	109.4	C4—C5—H5A	109.4
O3—C2—C1	110.97 (8)	C6—C5—H5B	109.4
O3—C2—C3	110.48 (7)	C4—C5—H5B	109.4
C1—C2—C3	112.89 (7)	H5A—C5—H5B	108.0

O3—C2—H2	107.4	O1—C6—C5	112.10 (8)
C1—C2—H2	107.4	O1—C6—C1	110.01 (8)
C3—C2—H2	107.4	C5—C6—C1	110.48 (8)
O4—C3—C4	107.32 (8)	O1—C6—H6	108.0
O4—C3—C2	110.35 (8)	C5—C6—H6	108.0
C4—C3—C2	112.94 (7)	C1—C6—H6	108.0
O4—C3—H3	108.7	C6—O1—H1A	109.5
C4—C3—H3	108.7	C1—O2—H2A	109.5
C2—C3—H3	108.7	C2—O3—H3A	109.5
O5—C4—C3	107.80 (8)	C3—O4—H4A	109.5
O5—C4—C5	110.57 (8)	C4—O5—H5	109.5
C3—C4—C5	111.73 (8)		
O2—C1—C2—O3	-61.20 (10)	O4—C3—C4—C5	-72.15 (10)
C6—C1—C2—O3	177.71 (7)	C2—C3—C4—C5	49.69 (10)
O2—C1—C2—C3	174.15 (8)	O5—C4—C5—C6	65.25 (11)
C6—C1—C2—C3	53.07 (10)	C3—C4—C5—C6	-54.82 (11)
O3—C2—C3—O4	-54.15 (10)	C4—C5—C6—O1	-177.75 (8)
C1—C2—C3—O4	70.77 (10)	C4—C5—C6—C1	59.17 (10)
O3—C2—C3—C4	-174.27 (7)	O2—C1—C6—O1	59.39 (10)
C1—C2—C3—C4	-49.35 (10)	C2—C1—C6—O1	177.84 (8)
O4—C3—C4—O5	166.16 (7)	O2—C1—C6—C5	-176.32 (7)
C2—C3—C4—O5	-71.99 (10)	C2—C1—C6—C5	-57.87 (9)

Hydrogen-bond geometry (Å, °)

<i>D</i> —H... <i>A</i>	<i>D</i> —H	H... <i>A</i>	<i>D</i> ... <i>A</i>	<i>D</i> —H... <i>A</i>
O1—H1A...O3 <sup>i</sup>	0.82	1.94	2.7347 (11)	164
O2—H2A...O4 <sup>ii</sup>	0.82	1.96	2.7761 (12)	170
O3—H3A...O1 <sup>iii</sup>	0.82	2.02	2.8417 (11)	177
O4—H4A...O5 <sup>iv</sup>	0.82	1.91	2.7067 (12)	165
O5—H5...O2 <sup>v</sup>	0.82	2.00	2.8036 (12)	166

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