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Key indicators

Single-crystal X-ray study
 $T = 120\text{ K}$
 Mean $\sigma(\text{C}-\text{C}) = 0.003\text{ \AA}$
 R factor = 0.038
 wR factor = 0.107
 Data-to-parameter ratio = 11.1

For details of how these key indicators were automatically derived from the article, see <http://journals.iucr.org/e>.

5-Chloro-3-hydroxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one: supramolecular aggregation through a two-dimensional network of N—H···O and O—H···O interactions

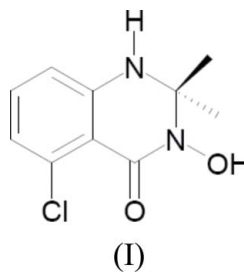
In the crystal structure of the title compound, $\text{C}_{10}\text{H}_{11}\text{ClN}_2\text{O}_2$, the 1,3-diaza ring exists in the skew-boat conformation. Supramolecular aggregation is effected by the formation of an infinite two-dimensional network of O—H···O and N—H···O interactions.

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Comment

Quinazolin-4(1*H*)-ones, commonly known as benzopyrimidinones, are an important class of heterocyclic compounds (Jain *et al.*, 2000). Some of them occur either as quinazoline alkaloids (Mohrle & Gundlack, 1970; Baker & McEvoy, 1995) or as their precursors (Brown, 1984). In addition, numerous synthetic quinazoline derivatives are known which exhibit diverse antihistaminic (Graham, 1960), diuretic (Cohen *et al.*, 1960), hypnotic (Chappel & von Seeman, 1963) and anti-inflammatory (Saravanan *et al.*, 1998) properties. In particular, 2,3-dihydro-1*H*-quinazolin-4-one derivatives are established as biologically and pharmaceutically important compounds (Bonala *et al.*, 1968; Levin *et al.*, 1994; Okumura *et al.*, 1968; Yoo *et al.*, 2005). The present investigation is aimed at the study of the molecular and supramolecular architecture of the title compound, (I), and may serve as a forerunner to a study of the correlation of these features with its biological activity.



The molecular structure of (I) is shown in Fig. 1 and selected geometric parameters are given in Table 1. The 1,3-diaza ring exists in a skew-boat conformation, with puckering parameters (Cremer & Pople, 1975) $Q_T = 0.396\text{ \AA}$, $\theta = 64.6^\circ$ and $\varphi = 295.08^\circ$. This is also evident from the torsion angles involving the 1,3-diaza ring (Table 1). The axial orientation of the C10 methyl group, the equatorial orientation of the C8 methyl group, the equatorial orientation of the O atom of the N—OH group, and the relative synclinal orientation of the carbonyl O atom and the O atom of the N—OH group are evident from the corresponding torsion angles (Table 1).

The crystal structure of (I) is stabilized by the interplay of O—H···O and N—H···O interactions (Table 2), and van der

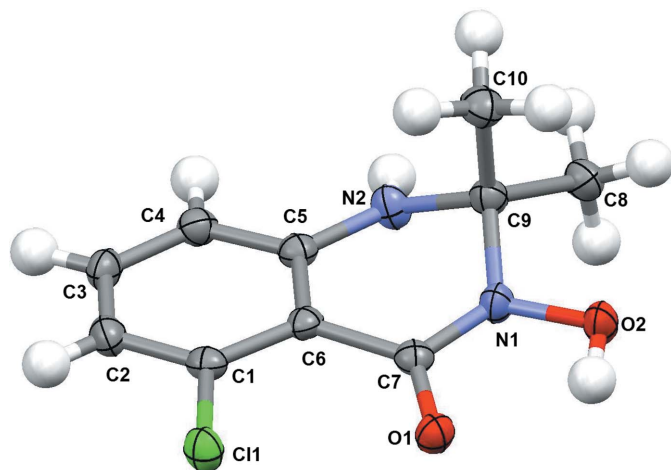


Figure 1
The molecular structure of the title compound, showing 50% probability displacement ellipsoids

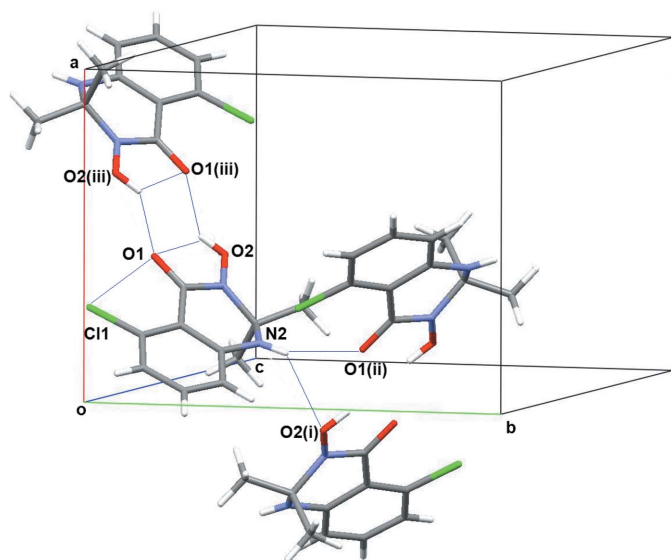


Figure 2
A view inclined to the *c* axis, showing the binary hydrogen-bonded motifs as dashed lines. (Symmetry codes as given in Table 2).

Waals interactions. The hydrogen-bond distances found in (I) agree with those reported in the literature (Desiraju & Steiner, 1999; Desiraju, 1989). The O2—H2O···O1 interaction generates a motif of graph set $S(5)$ (Bernstein *et al.*, 1995; Etter, 1990). Two such $S(5)$ motifs from symmetry-related molecules combine to form a binary motif of graph set $R_2^2(4)$. Another $R_2^2(4)$ binary motif is formed by the N2—H2N···O2ⁱ and N2—H2N···O1ⁱⁱ interactions (symmetry codes in Table 2), which is repeated between symmetry-related molecules. These repetitive $S(5)$ and $R_2^2(4)$ motifs combine to form a higher-order motif of graph set $R_2^2(10)$ (Fig. 2). These N—H···O and O—H···O interactions generate an infinite two-dimensional network along [001] (Fig. 3). There is also a significant intramolecular van der Waals interaction between atoms Cl1 and O1 of 2.938 (2) Å.

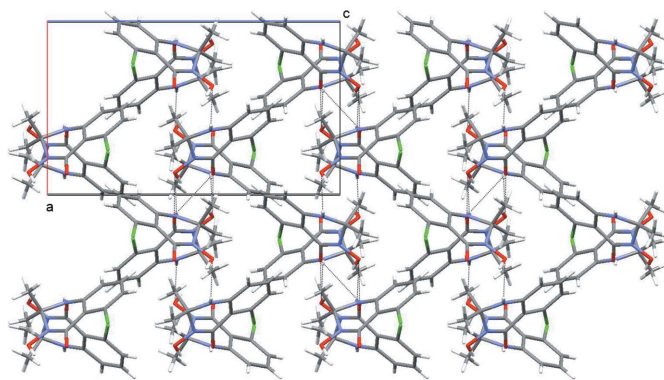


Figure 3
A view along [001], showing the two-dimensional network of N—H···O and O—H···O interactions, drawn as dotted lines.

Experimental

6-Chloroanthranilic hydroxamic acid was prepared according to reported methods (Devocelle *et al.*, 2003; Lee *et al.*, 2005). During our attempts to recrystallize the above product from acetone–ethanol (1:1), crystals of the title compound were produced after standing for 30 d. These may have been formed by a condensation reaction of 6-chloroanthranilic hydroxamic acid with acetone. Such a reaction mechanism has already been reported for the formation of 2,3-dihydro-1*H*-quinazolin-4-one derivatives (Yoo *et al.* 2005).

Crystal data

$C_{10}H_{11}ClN_2O_2$	$Z = 8$
$M_r = 226.66$	$D_x = 1.486 \text{ Mg m}^{-3}$
Orthorhombic, <i>Pbca</i>	Mo $K\alpha$ radiation
$a = 9.7070$ (5) Å	$\mu = 0.36 \text{ mm}^{-1}$
$b = 12.7121$ (7) Å	$T = 120$ (2) K
$c = 16.4203$ (8) Å	Block, colourless
$V = 2026.21$ (18) Å ³	$0.14 \times 0.12 \times 0.10 \text{ mm}$

Data collection

Bruker SMART 6K CCD area-detector diffractometer	12430 measured reflections
ω scans	1996 independent reflections
Absorption correction: multi-scan (SADABS; Sheldrick, 1998)	1507 reflections with $I > 2\sigma(I)$
$T_{\min} = 0.926$, $T_{\max} = 0.965$	$R_{\text{int}} = 0.052$
	$\theta_{\text{max}} = 26.0^\circ$

Refinement

Refinement on F^2	$w = 1/[\sigma^2(F_o^2) + (0.0571P)^2 + 0.6859P]$
$R[F^2 > 2\sigma(F^2)] = 0.038$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.107$	$(\Delta/\sigma)_{\text{max}} < 0.001$
$S = 1.05$	$\Delta\rho_{\text{max}} = 0.32 \text{ e \AA}^{-3}$
1996 reflections	$\Delta\rho_{\text{min}} = -0.22 \text{ e \AA}^{-3}$
180 parameters	
All H-atom parameters refined	

Table 1

Selected torsion angles ($^\circ$).

N2—C5—C6—C7	−6.9 (3)	C10—C9—N1—C7	77.1 (3)
C1—C6—C7—N1	−176.11 (19)	N2—C9—N1—O2	162.41 (16)
O1—C7—N1—O2	−11.8 (3)	C6—C5—N2—C9	−24.0 (3)
C6—C7—N1—O2	172.09 (16)	N1—C9—N2—C5	44.8 (2)
C6—C7—N1—C9	19.0 (3)	C8—C9—N2—C5	162.40 (18)
N2—C9—N1—C7	−43.6 (3)	C10—C9—N2—C5	−73.9 (2)
C8—C9—N1—C7	−159.8 (2)		

Table 2
Hydrogen-bond geometry (Å, °).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
$N2-H2N\cdots O2^I$	0.83 (3)	2.52 (3)	3.174 (2)	136 (2)
$N2-H2N\cdots O1^{II}$	0.83 (3)	2.41 (3)	3.200 (2)	158 (2)
$O2-H2O\cdots O1$	0.85 (3)	2.08 (3)	2.595 (2)	119 (2)
$O2-H2O\cdots O1^{III}$	0.85 (3)	2.00 (3)	2.677 (2)	136 (2)

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

All H atoms were located in a difference map, and their positions and isotropic displacement parameters were refined.

Data collection: *SMART* (Bruker, 1998); cell refinement: *SAINT* (Bruker, 1998); data reduction: *SAINT*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *MERCURY* (Macrae *et al.*, 2006); software used to prepare material for publication: *SHELXL97*.

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5-Chloro-3-hydroxy-2,2-dimethyl-2,3-dihydroquinazolin-4(1*H*)-one: supramolecular aggregation through a two-dimensional network of N—H···O and O—H···O interactions

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5-Chloro-3-hydroxy-2,2-dimethylquinazolin-4(1*H*)-one

Crystal data

C₁₀H₁₁ClN₂O₂

M_r = 226.66

Orthorhombic, *Pbca*

Hall symbol: -P 2ac 2ab

a = 9.7070 (5) Å

b = 12.7121 (7) Å

c = 16.4203 (8) Å

V = 2026.21 (18) Å³

Z = 8

F(000) = 944

D_x = 1.486 Mg m⁻³

Mo *Kα* radiation, λ = 0.71073 Å

Cell parameters from 2345 reflections

θ = 2.5–25.3°

μ = 0.36 mm⁻¹

T = 120 K

Block, colourless

0.14 × 0.12 × 0.10 mm

Data collection

Bruker SMART 6K CCD area-detector
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm⁻¹

ω scans

Absorption correction: multi-scan
(SADABS; Sheldrick, 1998)

T_{min} = 0.926, *T_{max}* = 0.965

12430 measured reflections

1996 independent reflections

1507 reflections with *I* > 2σ(*I*)

R_{int} = 0.052

θ_{max} = 26.0°, θ_{min} = 2.5°

h = -11→11

k = -15→15

l = -15→20

Refinement

Refinement on *F*²

Least-squares matrix: full

R[*F*² > 2σ(*F*²)] = 0.038

wR(*F*²) = 0.107

S = 1.05

1996 reflections

180 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

All H-atom parameters refined

w = 1/[σ²(*F_o*²) + (0.0571*P*)² + 0.6859*P*]

where *P* = (*F_o*² + 2*F_c*²)/3

(Δ/σ)_{max} < 0.001

Δρ_{max} = 0.32 e Å⁻³

Δρ_{min} = -0.22 e Å⁻³

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 (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	0.1625 (2)	0.01410 (16)	0.30349 (13)	0.0232 (5)
C2	0.0732 (2)	0.04246 (18)	0.24247 (14)	0.0272 (5)
H2	0.061 (2)	-0.0020 (19)	0.1994 (14)	0.030 (6)*
C3	0.0072 (2)	0.13934 (17)	0.24633 (14)	0.0265 (5)
H3	-0.054 (2)	0.1577 (18)	0.2025 (14)	0.028 (6)*
C4	0.0253 (2)	0.20484 (17)	0.31133 (13)	0.0259 (5)
H4	-0.022 (2)	0.2718 (19)	0.3145 (14)	0.032 (6)*
C5	0.11145 (19)	0.17453 (16)	0.37553 (12)	0.0231 (4)
C6	0.18594 (19)	0.07904 (15)	0.37162 (12)	0.0210 (4)
C7	0.2901 (2)	0.05918 (15)	0.43529 (12)	0.0219 (4)
C8	0.2240 (2)	0.28916 (18)	0.57100 (15)	0.0288 (5)
H8A	0.146 (2)	0.3452 (17)	0.5774 (14)	0.030 (6)*
H8B	0.244 (2)	0.2654 (18)	0.6266 (16)	0.030 (6)*
H8C	0.303 (3)	0.320 (2)	0.5486 (15)	0.039 (7)*
C9	0.1737 (2)	0.19813 (16)	0.51952 (12)	0.0245 (5)
C10	0.0626 (2)	0.13579 (19)	0.56367 (15)	0.0313 (5)
H10C	-0.015 (3)	0.183 (2)	0.5808 (16)	0.047 (7)*
H10B	0.102 (3)	0.101 (2)	0.6148 (18)	0.048 (8)*
H10A	0.022 (3)	0.081 (2)	0.5298 (17)	0.050 (8)*
H2O	0.426 (3)	0.057 (2)	0.5458 (17)	0.048 (8)*
H2N	0.102 (3)	0.301 (2)	0.4410 (16)	0.047 (8)*
Cl1	0.24305 (5)	-0.10747 (4)	0.29303 (3)	0.02900 (19)
N1	0.28885 (18)	0.12826 (14)	0.49761 (11)	0.0260 (4)
N2	0.12798 (19)	0.23850 (15)	0.44190 (11)	0.0275 (4)
O1	0.38023 (14)	-0.01006 (11)	0.43358 (9)	0.0277 (4)
O2	0.37357 (16)	0.10485 (13)	0.56416 (9)	0.0312 (4)

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0207 (10)	0.0231 (10)	0.0258 (11)	-0.0006 (8)	0.0044 (8)	-0.0004 (8)
C2	0.0283 (12)	0.0323 (12)	0.0211 (11)	-0.0029 (9)	-0.0006 (9)	-0.0013 (9)
C3	0.0230 (11)	0.0338 (12)	0.0226 (12)	0.0012 (9)	-0.0041 (9)	0.0043 (9)
C4	0.0236 (10)	0.0284 (11)	0.0258 (12)	0.0029 (9)	0.0014 (9)	0.0022 (9)
C5	0.0206 (10)	0.0247 (10)	0.0240 (11)	-0.0012 (8)	0.0027 (8)	0.0012 (8)
C6	0.0167 (9)	0.0249 (10)	0.0215 (10)	-0.0011 (8)	0.0015 (8)	0.0024 (8)

C7	0.0216 (10)	0.0215 (10)	0.0227 (11)	-0.0017 (8)	0.0024 (8)	0.0021 (8)
C8	0.0296 (12)	0.0292 (12)	0.0275 (13)	0.0005 (9)	0.0007 (10)	-0.0055 (10)
C9	0.0251 (10)	0.0258 (11)	0.0227 (11)	0.0038 (9)	-0.0003 (9)	-0.0012 (8)
C10	0.0312 (12)	0.0351 (13)	0.0275 (13)	-0.0041 (10)	0.0032 (10)	-0.0007 (10)
C11	0.0342 (3)	0.0250 (3)	0.0277 (3)	0.0047 (2)	-0.0037 (2)	-0.0053 (2)
N1	0.0248 (9)	0.0313 (10)	0.0220 (9)	0.0056 (7)	-0.0056 (7)	-0.0033 (7)
N2	0.0351 (10)	0.0227 (10)	0.0246 (10)	0.0055 (8)	-0.0027 (8)	-0.0015 (8)
O1	0.0257 (8)	0.0292 (8)	0.0281 (8)	0.0068 (6)	-0.0046 (6)	-0.0028 (6)
O2	0.0302 (8)	0.0393 (9)	0.0243 (9)	0.0121 (7)	-0.0089 (7)	-0.0075 (7)

Geometric parameters (Å, °)

C1—C2	1.373 (3)	C8—C9	1.514 (3)
C1—C6	1.409 (3)	C8—H8A	1.05 (2)
C1—C11	1.740 (2)	C8—H8B	0.98 (3)
C2—C3	1.390 (3)	C8—H8C	0.93 (3)
C2—H2	0.91 (2)	C9—N2	1.444 (3)
C3—C4	1.365 (3)	C9—N1	1.473 (3)
C3—H3	0.96 (2)	C9—C10	1.522 (3)
C4—C5	1.399 (3)	C10—H10C	1.00 (3)
C4—H4	0.97 (2)	C10—H10B	1.02 (3)
C5—N2	1.369 (3)	C10—H10A	0.98 (3)
C5—C6	1.414 (3)	N1—O2	1.400 (2)
C6—C7	1.476 (3)	N2—H2N	0.83 (3)
C7—O1	1.242 (2)	O2—H2O	0.85 (3)
C7—N1	1.349 (3)		
C2—C1—C6	121.83 (19)	H8A—C8—H8B	105.0 (19)
C2—C1—C11	116.40 (16)	C9—C8—H8C	111.2 (16)
C6—C1—C11	121.76 (16)	H8A—C8—H8C	111 (2)
C1—C2—C3	119.4 (2)	H8B—C8—H8C	109 (2)
C1—C2—H2	119.0 (15)	N2—C9—N1	103.41 (16)
C3—C2—H2	121.6 (15)	N2—C9—C8	108.69 (17)
C4—C3—C2	121.1 (2)	N1—C9—C8	110.62 (17)
C4—C3—H3	121.1 (14)	N2—C9—C10	112.83 (18)
C2—C3—H3	117.8 (14)	N1—C9—C10	109.90 (17)
C3—C4—C5	119.9 (2)	C8—C9—C10	111.14 (18)
C3—C4—H4	121.0 (14)	C9—C10—H10C	110.6 (15)
C5—C4—H4	119.1 (14)	C9—C10—H10B	110.7 (16)
N2—C5—C4	120.40 (19)	H10C—C10—H10B	108 (2)
N2—C5—C6	119.08 (18)	C9—C10—H10A	112.7 (16)
C4—C5—C6	120.49 (19)	H10C—C10—H10A	107 (2)
C1—C6—C5	117.16 (18)	H10B—C10—H10A	108 (2)
C1—C6—C7	124.94 (18)	C7—N1—O2	116.67 (16)
C5—C6—C7	117.69 (18)	C7—N1—C9	125.78 (17)
O1—C7—N1	119.01 (18)	O2—N1—C9	112.57 (16)
O1—C7—C6	126.01 (19)	C5—N2—C9	121.84 (17)
N1—C7—C6	114.85 (17)	C5—N2—H2N	121.1 (19)

C9—C8—H8A	110.0 (13)	C9—N2—H2N	116.5 (19)
C9—C8—H8B	110.4 (14)	N1—O2—H2O	103.1 (19)
C6—C1—C2—C3	2.1 (3)	C5—C6—C7—N1	9.2 (3)
C11—C1—C2—C3	-178.94 (16)	O1—C7—N1—O2	-11.8 (3)
C1—C2—C3—C4	-2.7 (3)	C6—C7—N1—O2	172.09 (16)
C2—C3—C4—C5	-0.1 (3)	O1—C7—N1—C9	-164.85 (19)
C3—C4—C5—N2	-178.50 (19)	C6—C7—N1—C9	19.0 (3)
C3—C4—C5—C6	3.5 (3)	N2—C9—N1—C7	-43.6 (3)
C2—C1—C6—C5	1.1 (3)	C8—C9—N1—C7	-159.8 (2)
C11—C1—C6—C5	-177.76 (14)	C10—C9—N1—C7	77.1 (3)
C2—C1—C6—C7	-173.57 (19)	N2—C9—N1—O2	162.41 (16)
C11—C1—C6—C7	7.6 (3)	C8—C9—N1—O2	46.2 (2)
N2—C5—C6—C1	178.05 (18)	C10—C9—N1—O2	-76.9 (2)
C4—C5—C6—C1	-3.9 (3)	C4—C5—N2—C9	157.99 (19)
N2—C5—C6—C7	-6.9 (3)	C6—C5—N2—C9	-24.0 (3)
C4—C5—C6—C7	171.16 (18)	N1—C9—N2—C5	44.8 (2)
C1—C6—C7—O1	8.1 (3)	C8—C9—N2—C5	162.40 (18)
C5—C6—C7—O1	-166.55 (19)	C10—C9—N2—C5	-73.9 (2)
C1—C6—C7—N1	-176.11 (19)		

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>
N2—H2N...O2 ⁱ	0.83 (3)	2.52 (3)	3.174 (2)	136 (2)
N2—H2N...O1 ⁱⁱ	0.83 (3)	2.41 (3)	3.200 (2)	158 (2)
O2—H2O...O1	0.85 (3)	2.08 (3)	2.595 (2)	119 (2)
O2—H2O...O1 ⁱⁱⁱ	0.85 (3)	2.00 (3)	2.677 (2)	136 (2)

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