Acta Cryst E CRYSTALLOGRAPHIC COMMUNICATIONS

ISSN 2056-9890

Synthesis, crystal structure and Hirshfeld surface of bis(acetato-κ^2O,O')(2-benzyl-1*H*-benzimidazole-κN^3)copper(II)

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Received 10 November 2025
Accepted 3 December 2025

Edited by N. Alvarez Failache, Universidad de la Repüblica, Uruguay

Keywords: crystal structure; dibazol; Hirshfeld surface; hydrogen bonds.

CCDC reference: 2512906

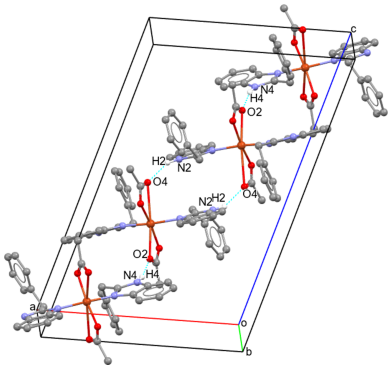
Supporting information: this article has supporting information at journals.iucr.org/e

The title copper(II) complex, $[Cu(C_2H_3O_2)_2(C_{14}H_{12}N_2)_2]$, was synthesized and structurally characterized. It crystallizes in the monoclinic space group $P2_1/n$ with one molecule per asymmetric unit. The Cu^{2+} ion exhibits a distorted octahedral (4 + 2) coordination geometry. The crystal packing is consolidated by N—H···O hydrogen bonds and C—H···π interactions. Hirshfeld surface analysis indicates that H···H, H···C/C···H and O···H/H···O contacts are the major contributors to the crystal packing.

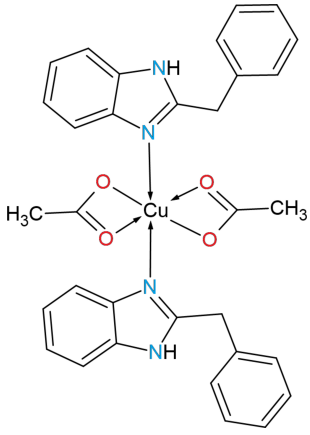
1. Chemical context

2-(Phenylmethyl)-1*H*-benzimidazole, also known as dibazol (bendazol), is a benzimidazole derivative that belongs to the class of synthetic adaptogens. This organic compound is used in medicine for its immunostimulating, vasodilatory and antispasmodic effects (Oliynyk & Oh, 2012). Upon entering the organism, dibazol acts directly on processes in blood cells – leukocytes and platelets (Oliynyk & Oh, 2012). The structure of dibazol has been determined and the fluorescence properties of this compound were also investigated (Lü *et al.*, 2018).

At present, its coordination compounds with *d*-block metals are under investigation. We previously synthesised a number of coordination compounds based on the dibazol ligand with transition metals (Co, Ni, Zn and Cu) and studied their physicochemical properties (Babayeva *et al.*, 2025). New coordination compounds with Fe^{II} and Cu^{II} and the dibazol ligand have been synthesized and their structural and spectroscopic characteristics investigated and described (Imomov *et al.*, 2008). In the work by Radjabov *et al.* (2016), the synthesis and physicochemical (structural and spectroscopic) characterization of Zn^{II} coordination compounds with the dibazol ligand are presented, and the structures of the complexes and potential biological activity, are discussed. Lu *et al.* (2003) report the synthesis and single-crystal structural characterization of coordination complexes containing benzimidazole-based N-donor ligands. The work provides detailed information on the metal coordination environment and supramolecular packing features relevant for comparison with similar dibazole-based systems. Liu *et al.* (2014) describe the synthesis and X-ray structures of metal complexes assembled from bis(benzimidazole) ligands, forming well-defined supra-



molecular architectures. The study highlights coordination geometry and intermolecular contacts, offering structural parallels useful for discussing related dibazole complexes.



In this connection, we synthesized the title copper(II) complex (**I**). The present work provides an analysis of its structural and supramolecular properties, Hirshfeld surfaces and DFT calculation analysis.

2. Structural commentary

The title compound **I** crystallizes in the monoclinic space group $P2_1/n$ (Fig. 1). The unit cell contains one complex molecule ($Z' = 1$) in which the central Cu^{2+} ion is coordinated by two molecules of dibazol (DIB) *via* sp^2-hybridized nitrogen atoms [Cu—N1 = 1.984 (3) Å and Cu—N3 = 1.986 (3) Å] and two acetate (ac) anions *via* oxygen atoms [Cu—O1 = 1.998 (2) Å, Cu—O2 = 2.447 (2) Å, Cu—O3 = 1.955 (2) Å and Cu—O4 = 2.706 (3) Å]. The acetate ligands form a four-membered chelate ring, in which the chelate angles are O2—Cu—O1 = 57.85 (9)° and O4—Cu—O3 = 53.32 (9)° (Table 1).

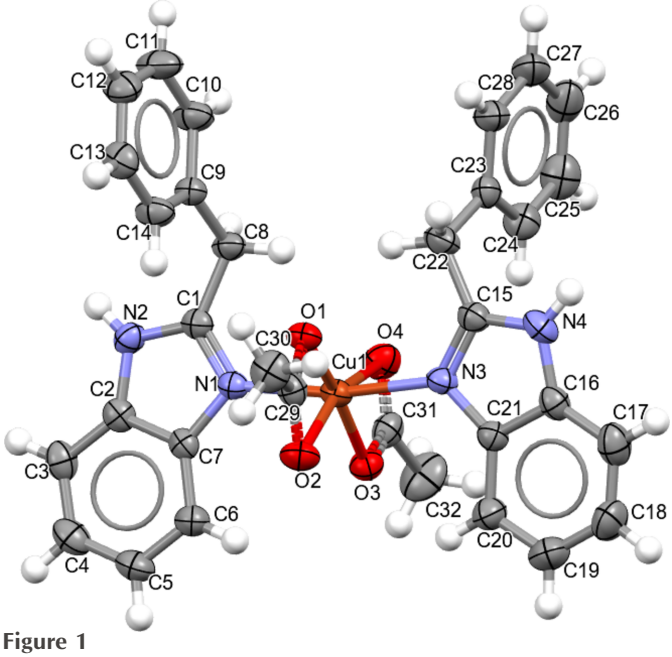


Figure 1
The asymmetric unit of the title compound with the atom-numbering scheme. Displacement ellipsoids for non-hydrogen atoms are drawn at the 50% probability level.

Table 1
Selected geometric parameters (Å, °).

Cu1—O3	1.955 (2)	Cu1—O4	2.706 (3)
Cu1—O1	1.998 (2)	Cu1—N3	1.986 (3)
Cu1—O2	2.447 (2)	Cu1—N1	1.984 (3)
O2—Cu1—O1	57.85 (9)	N1—Cu1—N3	168.64 (11)
O4—Cu1—O3	53.32 (9)		

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

*Cg*3, 5, 8 and 9 are the centroids of the N1/C1/N2/C2/C7, C2–C7, C23–C28 and N1/C1/N2/C2–C7 rings, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.86 (1)	1.91 (1)	2.708 (4)	153 (1)
N4—H4···O2^{ii}	0.86 (1)	1.86 (1)	2.699 (4)	164 (1)
C8—H8*a*···*Cg*3^{i}	0.97 (1)	2.70 (1)	3.592 (4)	154 (1)
C8—H8*a*···*Cg*9^{i}	0.97 (1)	2.93 (1)	3.844 (4)	158 (1)
C13—H13···*Cg*5^{iii}	0.93 (1)	2.82 (1)	3.614 (4)	145 (1)
C30—H30*a*···*Cg*8^{iv}	0.96 (1)	2.93 (1)	3.690 (5)	137 (2)

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

The coordination geometry of the central metal is a distorted octahedron (4 + 2). This is explained by the fact that the DIB ligands occupy the axial positions with N1—Cu—N3 = 168.64 (11)° (which deviates by 11.36° from the ideal), as well as by the chelate angles of the ac ligands, which differ significantly from the ideal 90° (Table 1). This combination of small chelate angles in a constrained geometry forces the axial ligands to deviate and results in elongation of the second oxygen atoms of the ac ligands, together with the Jahn–Teller effect typical for d^9 Cu^{II} atoms (Jahn & Teller 1937). An additional contribution may be ascribed to steric interactions of the aromatic fragments, which further enhance the departure of the axial donors from 180°.

For consideration of the bidentate nature of the ac ligands, one may refer to Youngme *et al.* (1998), where the authors obtained an octahedral structure with the Cu^{2+} ion and two bidentate ac ligands [Cu—O2 = 2.4824 (15) Å and Cu—O4 = 2.690 (2) Å], the Cu—O bond lengths being very close to those in our structure. The distortion of the Cu coordination is quantified as: $\Sigma\ (\theta_i - 90°|$ for 12 *cis*-angles = 157.97°, mean absolute deviation $\simeq$ 13.16°; quadratic elongation λ = 1.0178 and Δ = 0.0178. The small chelate angles of the ac ligands [57.85 (9)° and 53.33 (10)°] and the elongated axial bonds (2.447, 2.706 Å) lead to substantial angular and bond-length distortion.

3. Supramolecular features

In the crystal, N—H···O hydrogen bonds consolidate the structure (Table 2, Fig. 2). The formation of the three-dimensional crystal structure is mainly mediated by two principal hydrogen bonds, N2—H2···O4^{i} and N4—H4···O2^{ii}

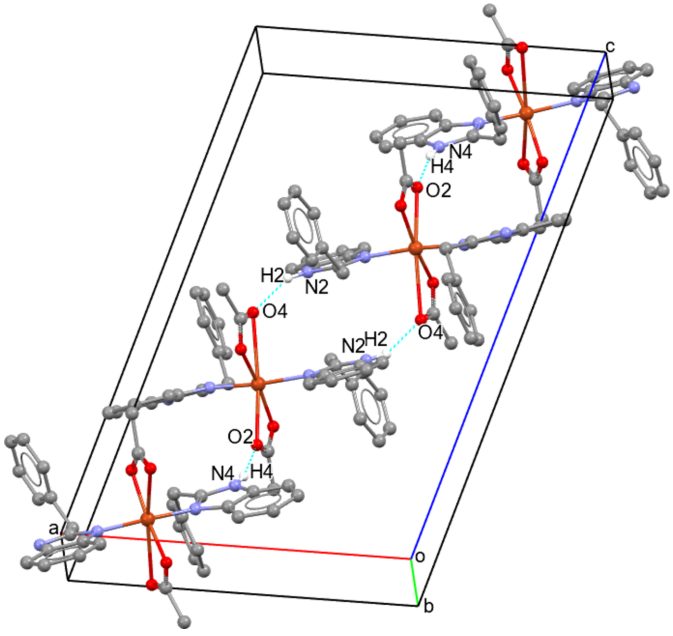


Figure 2
Formation of an intermolecular chain along [101] by classical N—H···O hydrogen bonds. Only hydrogen atoms involved in these interactions are shown.

[symmetry codes: (i) $-x+1, -y+1, -z+1$; (ii) $-x+\frac{3}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$] directed along the [101] chain (Table 2).

In addition to classical hydrogen bonds, C—H···π contacts are present, which further reinforce the crystal cohesion: C8—H8a···*Cg*3^{i}, C8—H8a···*Cg*9^{i}, C13—H13···*Cg*5^{iii} and C30—H30a···*Cg*8^{iv} [(i) $-x+1, -y+1, -z+1$; (iii) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{1}{2}$; (iv) $-x+\frac{3}{2}, y+\frac{1}{2}, -z+\frac{1}{2}$] (Table 2, Fig. 3). These C—H···π interactions, although weaker than conventional hydrogen bonds, effect a redistribution of the aromatic fragments within the packing; they promote the orientation of the phenyl systems and stabilize the displaced positions of the rings, which additionally lowers the free energy of the crystal structure.

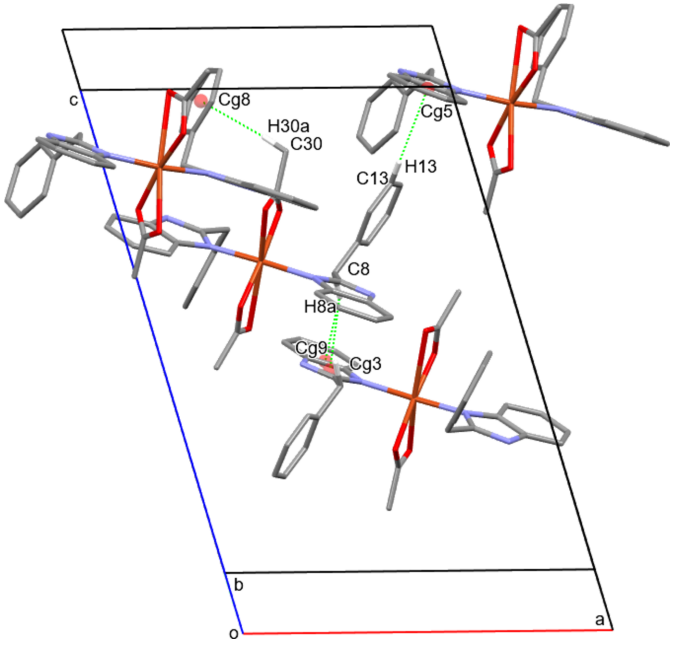


Figure 3
View of the intermolecular chain along the [011] direction, formed by non-classical hydrogen bonds.

4. Hirshfeld surface analysis

The Hirshfeld surface analysis was performed using *CrystalExplorer 21.5* (Spackman *et al.*, 2021). In the d_{norm} map (Fig. 4) the localized dark-red spots correspond to contacts shorter than the sum of the van der Waals radii (close contacts), white areas indicate contacts close to the sum of the radii, and blue areas indicate longer contacts. In the molecule under consideration the most pronounced red regions are observed close to atoms O2/O4 and in the regions between the aromatic rings, which points to the presence of short O···H/N or π–π contacts in these fragments. Small red spots are also visible on the surface in regions corresponding to the N and H donor atoms, which is consistent with the directional N—H···O hydrogen contacts registered in the crystal.

Two-dimensional fingerprint plots (Fig. 4) provide a quantitative representation of the contribution of different types of intermolecular contacts to the total Hirshfeld surface. For the present structure the following proportions are observed: H···H = 57.5%, which is the dominant component; H···C/C···H = 31.6%, which make significant contributions; and the remainder are O···H/H···O = 8.6%, O···C/C···O = 6.7% and C···O/O···C = 0.1%.

The dominance of H···H contacts may indicate a predominance of dispersion (van der Waals) contacts and a large number of H–H geometries. The substantial H···C/C···H contribution reflects edge contacts between aromatic fragments (C—H···π), while O···H/H···O corroborates the presence of directional N—H···O and local C—H···O inter-

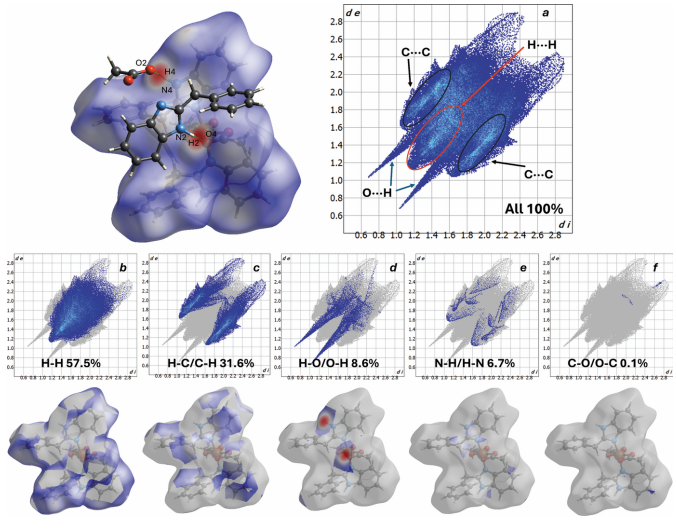


Figure 4
Two-dimensional fingerprint plots for the title compound, showing (*a*) all interactions, and delineated into (*b*) H···H, (*c*) C···H/H···C, (*d*) O···H/H···O, (*e*) N···H/H···N and (*f*) C···O/O···C interactions.

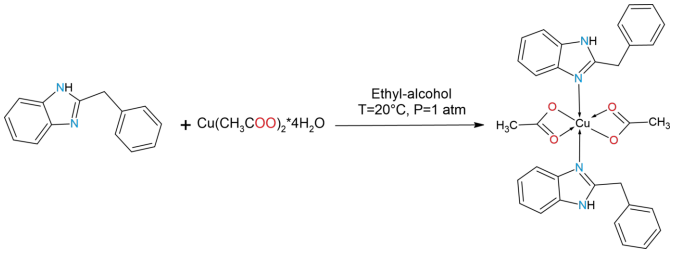
actions. For comparison with related complex systems, H···H ≃ 71.7% in one case (Siddikova *et al.*, 2024), whereas in another it is ≃ 51.8% with O···H ≃ 12.4% (Tojiboyeva *et al.*, 2025), highlighting the variability in the balance between dispersion and directional contacts in such structures.

5. Database survey

A search of the Cambridge Structural Database (CSD, 2024.2.0; Groom *et al.*, 2016) returned 52 structures similar to the fragment of our structure. Among these structures a similar zinc complex was identified, in which the central metal resides in a tetrahedral environment and two dibazol ligands are present (CSD refcode WOVQED; Bei *et al.*, 2001). The 1,2-phenylene[bis(methylene)]bis(1*H*-benzimidazole) ligand with various metals is also frequently encountered [CSD refcodes FUDZEL (Liu *et al.*, 2014); HUGZUH (Ohta *et al.*, 2020) and LADLOS (Lu *et al.*, 2003)].

6. Synthesis and crystallization

The following solutions were prepared: (*a*) an ethanolic solution of $Cu(CH_3COO)_2{\cdot}4H_2O$ (1.0 mmol) and (*b*) an ethanolic solution of DIB (2.0 mmol). Solution (*a*) was added to solution (*b*), and the mixture was stirred with a magnetic stirrer at room temperature for 12 h, resulting in the formation of a dark-blue precipitate. The precipitate was filtered, washed several times with ethanol and air-dried. As the obtained material dissolved well in DMF, it was recrystallized from this solvent by dissolution in a minimal volume of DMF followed by slow evaporation; as a result, well-formed single crystals of dark-blue colour, suitable for structural and further physico-chemical investigation, were obtained.



7. Refinement

Crystallographic data, data-collection conditions and structure-refinement parameters are summarized in Table 3. Hydrogen atoms were calculated in idealized positions and refined using a riding model with C—H bond lengths of 0.93–0.98 Å and $U_{iso}(H) = 1.2U_{eq}(C)$.

Acknowledgements

We thank the Institute of the Chemistry of Plant Substances named after Academician S. Yu. Yunusov of the Academy of Sciences of the Republic of Uzbekistan for access to the Bruker APEXII X-ray diffractometer.

Table 3
Experimental details.

Crystal data	
Chemical formula	$[Cu(C_2H_3O_2)_2(C_{14}H_{12}N_2)_2]$
M_r	598.17
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	273
a, b, c (Å)	13.125 (4), 11.552 (3), 20.499 (5)
β (°)	106.385 (12)
V (Å^3)	2981.9 (13)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.78
Crystal size (mm)	0.45 × 0.35 × 0.18
Data collection	
Diffractometer	Bruker APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Krause *et al.*, 2015)
T_{min}, T_{max}	0.672, 0.754
No. of measured, independent and observed [$I \geq 2u(I)$] reflections	7459, 7455, 3700
R_{int}	0.055
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.069, 0.137, 0.98
No. of reflections	7455
No. of parameters	372
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.22, −1.15

Computer programs: *APEX2* and *SAINT* (Bruker, 2014), *OLEX2.refine* (Bourhis *et al.*, 2015), *OLEX2* (Dolomanov *et al.*, 2009) and *Mercury*(Macrae *et al.*, 2020) .

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supporting information

Acta Cryst. (2026). E**82**, 28-32 [https://doi.org/10.1107/S2056989025010813]

Synthesis, crystal structure and Hirshfeld surface of bis(acetato-κ^2O,O')(2-benzyl-1*H*-benzimidazole-κN^3)copper(II)

Gulnoza Boboyeva, Gulbeka Mamatova, Sardor Murodov, Komila Ganiyeva, Kambarali Turgunov, Bakhodir Tashkhodjaev and Shakhlo Daminova

Computing details

Bis(acetato-κ^2O,O')(2-benzyl-1*H*-benzimidazole-κN^3)copper(II)

Crystal data

$[Cu(C_2H_3O_2)_2(C_{14}H_{12}N_2)_2]$
$M_r = 598.17$
Monoclinic, $P2_1/n$
$a = 13.125$ (4) Å
$b = 11.552$ (3) Å
$c = 20.499$ (5) Å
$\beta = 106.385$ (12)°
$V = 2981.9$ (13) Å^3
$Z = 4$
$F(000) = 1244$
$D_x = 1.332$ Mg m^{-3}
Mo $K\alpha$ radiation, $\lambda = 0.71073$ Å
Cell parameters from 9790 reflections
$\theta = 2.2$–$22.5°$
$\mu = 0.78$ mm^{-1}
$T = 273$ K
Rhombohedral, clear dark blue
0.45 × 0.35 × 0.18 mm

Data collection

Bruker APEXII CCD diffractometer
ω scans
Absorption correction: multi-scan (SADABS; Krause *et al.*, 2015)
$T_{min} = 0.672$, $T_{max} = 0.754$
7459 measured reflections
7455 independent reflections
3700 reflections with $I \geq 2u(I)$
$R_{int} = 0.055$
$\theta_{max} = 28.4°$, $\theta_{min} = 2.1°$
$h = -17 \rightarrow 16$
$k = 0 \rightarrow 15$
$l = 0 \rightarrow 27$

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)] = 0.069$
$wR(F^2) = 0.137$
$S = 0.98$
7455 reflections
372 parameters
0 restraints
54 constraints
Primary atom site location: dual
Hydrogen site location: inferred from neighbouring sites
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0369P)^2 + 1.6134P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} = -0.001$
$\Delta\rho_{max} = 0.22$ e Å^{-3}
$\Delta\rho_{min} = -1.15$ e Å^{-3}

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
Cu1	0.65105 (3)	0.56975 (3)	0.36489 (2)	0.05030 (16)
O3	0.74289 (19)	0.6635 (2)	0.43733 (12)	0.0590 (6)
O1	0.55906 (19)	0.49963 (19)	0.27936 (11)	0.0567 (6)
O2	0.5973 (2)	0.6771 (2)	0.25771 (12)	0.0683 (7)
O4	0.7374 (2)	0.5054 (3)	0.49579 (13)	0.0756 (8)
N3	0.7774 (2)	0.5000 (2)	0.34504 (13)	0.0510 (7)
N1	0.5217 (2)	0.6087 (2)	0.39222 (13)	0.0486 (7)
N4	0.8712 (3)	0.3728 (3)	0.30583 (15)	0.0687 (9)
H4	0.8904 (3)	0.3075 (3)	0.29297 (15)	0.0824 (11)*
N2	0.3780 (2)	0.5905 (3)	0.42757 (14)	0.0580 (8)
H2	0.3265 (2)	0.5582 (3)	0.43903 (14)	0.0696 (9)*
C9	0.3743 (3)	0.3421 (3)	0.35704 (17)	0.0506 (9)
C21	0.8626 (3)	0.5572 (3)	0.33110 (17)	0.0529 (9)
C7	0.4857 (3)	0.7190 (3)	0.40332 (16)	0.0491 (9)
C16	0.9217 (3)	0.4783 (3)	0.30590 (18)	0.0596 (10)
C2	0.3965 (3)	0.7082 (3)	0.42631 (16)	0.0538 (9)
C31	0.7724 (3)	0.6038 (4)	0.4909 (2)	0.0620 (10)
C23	0.7691 (3)	0.2023 (3)	0.3881 (2)	0.0592 (10)
C15	0.7871 (3)	0.3910 (3)	0.32937 (18)	0.0569 (10)
C29	0.5540 (3)	0.5827 (3)	0.23876 (18)	0.0560 (9)
C6	0.5265 (3)	0.8277 (3)	0.39576 (19)	0.0640 (10)
H6	0.5856 (3)	0.8360 (3)	0.37959 (19)	0.0767 (13)*
C1	0.4540 (3)	0.5358 (3)	0.40787 (17)	0.0519 (9)
C3	0.3461 (3)	0.8038 (4)	0.44419 (18)	0.0690 (11)
H3	0.2865 (3)	0.7964 (4)	0.45993 (18)	0.0829 (13)*
C10	0.3509 (3)	0.2312 (3)	0.3720 (2)	0.0766 (12)
H10	0.3886 (3)	0.1972 (3)	0.4127 (2)	0.0919 (15)*
C4	0.3893 (4)	0.9103 (4)	0.4373 (2)	0.0777 (12)
H4a	0.3585 (4)	0.9765 (4)	0.4494 (2)	0.0933 (15)*
C5	0.4766 (4)	0.9219 (3)	0.4130 (2)	0.0745 (12)
H5	0.5022 (4)	0.9956 (3)	0.4082 (2)	0.0893 (14)*
C24	0.8457 (3)	0.2304 (4)	0.4472 (2)	0.0739 (12)
H24	0.8666 (3)	0.3072 (4)	0.4557 (2)	0.0887 (14)*
C20	0.8934 (3)	0.6734 (3)	0.3386 (2)	0.0713 (11)
H20	0.8556 (3)	0.7278 (3)	0.3558 (2)	0.0855 (14)*
C28	0.7402 (3)	0.0879 (3)	0.3766 (2)	0.0762 (12)
H28	0.6892 (3)	0.0671 (3)	0.3367 (2)	0.0915 (14)*
C12	0.2139 (3)	0.2187 (4)	0.2669 (2)	0.0797 (13)
H12	0.1589 (3)	0.1779 (4)	0.2373 (2)	0.0957 (15)*
C13	0.2376 (3)	0.3269 (4)	0.2514 (2)	0.0722 (11)
H13	0.1998 (3)	0.3604 (4)	0.2104 (2)	0.0866 (14)*
C14	0.3181 (3)	0.3884 (3)	0.29639 (19)	0.0686 (11)
H14	0.3342 (3)	0.4628 (3)	0.28497 (19)	0.0823 (13)*
C11	0.2710 (4)	0.1696 (4)	0.3262 (3)	0.0934 (15)
H11	0.2565 (4)	0.0940 (4)	0.3363 (3)	0.1121 (18)*

C8	0.4632 (3)	0.4065 (3)	0.40743 (19)	0.0601 (10)
H8a	0.4675 (3)	0.3783 (3)	0.45269 (19)	0.0722 (12)*
H8b	0.5296 (3)	0.3870 (3)	0.39805 (19)	0.0722 (12)*
C30	0.4952 (3)	0.5636 (4)	0.16491 (18)	0.0806 (13)
H30a	0.5427 (7)	0.531 (2)	0.1418 (4)	0.1210 (19)*
H30b	0.4370 (14)	0.5115 (19)	0.16164 (19)	0.1210 (19)*
H30c	0.4687 (19)	0.6362 (5)	0.1443 (4)	0.1210 (19)*
C17	1.0109 (4)	0.5101 (5)	0.2864 (2)	0.0842 (13)
H17	1.0495 (4)	0.4564 (5)	0.2693 (2)	0.1010 (16)*
C27	0.7867 (4)	0.0026 (4)	0.4239 (3)	0.0944 (15)
H27	0.7665 (4)	−0.0745 (4)	0.4163 (3)	0.1133 (18)*
C26	0.8620 (4)	0.0346 (5)	0.4815 (3)	0.0995 (16)
H26	0.8938 (4)	−0.0216 (5)	0.5132 (3)	0.1194 (19)*
C19	0.9819 (4)	0.7035 (4)	0.3195 (2)	0.0898 (14)
H19	1.0043 (4)	0.7802 (4)	0.3240 (2)	0.1077 (17)*
C22	0.7159 (3)	0.2936 (3)	0.3370 (2)	0.0750 (12)
H22a	0.6876 (3)	0.2568 (3)	0.2930 (2)	0.0900 (15)*
H22b	0.6565 (3)	0.3255 (3)	0.3504 (2)	0.0900 (15)*
C25	0.8914 (4)	0.1469 (5)	0.4937 (2)	0.0930 (15)
H25	0.9427 (4)	0.1671 (5)	0.5335 (2)	0.1116 (17)*
C18	1.0388 (4)	0.6243 (5)	0.2937 (3)	0.0949 (15)
H18	1.0978 (4)	0.6492 (5)	0.2809 (3)	0.1139 (18)*
C32	0.8565 (4)	0.6567 (5)	0.5493 (2)	0.1121 (18)
H32a	0.9253 (4)	0.643 (3)	0.5431 (10)	0.168 (3)*
H32b	0.8446 (17)	0.7385 (7)	0.5507 (11)	0.168 (3)*
H32c	0.8530 (19)	0.622 (2)	0.5912 (3)	0.168 (3)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Cu1	0.0582 (3)	0.0423 (2)	0.0496 (3)	−0.0014 (2)	0.0138 (2)	−0.0012 (2)
O3	0.0619 (17)	0.0580 (15)	0.0562 (16)	−0.0054 (13)	0.0153 (13)	−0.0042 (13)
O1	0.0690 (17)	0.0448 (14)	0.0542 (14)	−0.0030 (12)	0.0142 (13)	0.0026 (12)
O2	0.087 (2)	0.0511 (16)	0.0672 (17)	−0.0064 (14)	0.0220 (15)	0.0064 (13)
O4	0.082 (2)	0.079 (2)	0.0721 (18)	−0.0047 (16)	0.0324 (16)	0.0088 (16)
N3	0.059 (2)	0.0401 (16)	0.0551 (18)	−0.0007 (14)	0.0181 (15)	−0.0049 (14)
N1	0.0528 (18)	0.0447 (16)	0.0470 (16)	−0.0018 (14)	0.0117 (14)	−0.0011 (13)
N4	0.082 (2)	0.053 (2)	0.074 (2)	0.0147 (18)	0.026 (2)	−0.0052 (16)
N2	0.055 (2)	0.062 (2)	0.0597 (19)	−0.0049 (16)	0.0206 (16)	0.0063 (15)
C9	0.056 (2)	0.044 (2)	0.052 (2)	−0.0024 (17)	0.0149 (19)	0.0013 (17)
C21	0.057 (2)	0.051 (2)	0.051 (2)	0.0005 (19)	0.0160 (18)	−0.0001 (17)
C7	0.052 (2)	0.051 (2)	0.0410 (19)	0.0049 (18)	0.0078 (18)	−0.0023 (16)
C16	0.066 (3)	0.061 (2)	0.054 (2)	0.011 (2)	0.021 (2)	0.0021 (19)
C2	0.063 (3)	0.059 (2)	0.0395 (19)	0.005 (2)	0.0148 (19)	0.0004 (17)
C31	0.057 (3)	0.078 (3)	0.056 (2)	−0.006 (2)	0.024 (2)	−0.008 (2)
C23	0.057 (2)	0.057 (2)	0.069 (3)	0.0044 (19)	0.026 (2)	0.000 (2)
C15	0.061 (3)	0.050 (2)	0.057 (2)	0.0023 (19)	0.011 (2)	0.0013 (18)
C29	0.057 (2)	0.062 (3)	0.052 (2)	0.008 (2)	0.0193 (19)	0.001 (2)

C6	0.067 (3)	0.053 (2)	0.073 (3)	−0.004 (2)	0.020 (2)	−0.001 (2)
C1	0.055 (2)	0.051 (2)	0.044 (2)	−0.0006 (19)	0.0046 (18)	0.0027 (16)
C3	0.072 (3)	0.083 (3)	0.056 (2)	0.016 (2)	0.024 (2)	−0.001 (2)
C10	0.083 (3)	0.055 (2)	0.079 (3)	−0.008 (2)	0.001 (2)	0.015 (2)
C4	0.098 (4)	0.064 (3)	0.070 (3)	0.014 (3)	0.021 (3)	−0.010 (2)
C5	0.092 (3)	0.049 (2)	0.080 (3)	−0.001 (2)	0.021 (3)	−0.005 (2)
C24	0.076 (3)	0.081 (3)	0.064 (3)	−0.002 (2)	0.019 (2)	−0.008 (2)
C20	0.068 (3)	0.065 (3)	0.084 (3)	−0.008 (2)	0.027 (2)	−0.007 (2)
C28	0.070 (3)	0.056 (3)	0.097 (3)	−0.007 (2)	0.015 (2)	0.004 (2)
C12	0.079 (3)	0.064 (3)	0.085 (3)	−0.009 (2)	0.005 (3)	−0.011 (2)
C13	0.076 (3)	0.074 (3)	0.057 (2)	0.004 (2)	0.003 (2)	0.000 (2)
C14	0.080 (3)	0.055 (2)	0.062 (3)	−0.007 (2)	0.007 (2)	0.010 (2)
C11	0.107 (4)	0.054 (3)	0.106 (4)	−0.023 (3)	0.008 (3)	0.006 (3)
C8	0.063 (3)	0.046 (2)	0.066 (2)	−0.0074 (18)	0.010 (2)	0.0080 (18)
C30	0.084 (3)	0.100 (3)	0.053 (2)	−0.001 (3)	0.011 (2)	0.004 (2)
C17	0.081 (3)	0.099 (4)	0.082 (3)	0.020 (3)	0.038 (3)	0.011 (3)
C27	0.081 (3)	0.066 (3)	0.140 (5)	−0.003 (3)	0.037 (4)	0.029 (3)
C26	0.076 (4)	0.117 (5)	0.107 (4)	0.009 (3)	0.029 (3)	0.044 (3)
C19	0.089 (4)	0.072 (3)	0.113 (4)	−0.017 (3)	0.035 (3)	0.004 (3)
C22	0.078 (3)	0.046 (2)	0.093 (3)	0.004 (2)	0.013 (3)	0.004 (2)
C25	0.090 (4)	0.123 (4)	0.067 (3)	0.005 (3)	0.024 (3)	0.005 (3)
C18	0.079 (4)	0.103 (4)	0.117 (4)	−0.003 (3)	0.049 (3)	0.009 (3)
C32	0.100 (4)	0.154 (5)	0.069 (3)	−0.027 (4)	0.001 (3)	−0.019 (3)

Geometric parameters (Å, º)

Cu1—O3	1.955 (2)	C3—C4	1.378 (5)
Cu1—O1	1.998 (2)	C10—H10	0.9300
Cu1—O2	2.447 (2)	C10—C11	1.389 (5)
Cu1—O4	2.706 (3)	C4—H4a	0.9300
Cu1—N3	1.986 (3)	C4—C5	1.380 (6)
Cu1—N1	1.984 (3)	C5—H5	0.9300
O3—C31	1.261 (4)	C24—H24	0.9300
O1—C29	1.260 (4)	C24—C25	1.370 (6)
O2—C29	1.240 (4)	C20—H20	0.9300
O4—C31	1.240 (4)	C20—C19	1.372 (5)
N3—C21	1.395 (4)	C28—H28	0.9300
N3—C15	1.315 (4)	C28—C27	1.396 (6)
N1—C7	1.399 (4)	C12—H12	0.9300
N1—C1	1.328 (4)	C12—C13	1.348 (5)
N4—H4	0.8600	C12—C11	1.359 (6)
N4—C16	1.388 (5)	C13—H13	0.9300
N4—C15	1.340 (4)	C13—C14	1.387 (5)
N2—H2	0.8600	C14—H14	0.9300
N2—C2	1.383 (4)	C11—H11	0.9300
N2—C1	1.336 (4)	C8—H8a	0.9700
C9—C10	1.371 (5)	C8—H8b	0.9700
C9—C14	1.363 (5)	C30—H30a	0.9600

C9—C8	1.518 (4)	C30—H30b	0.9600
C21—C16	1.388 (5)	C30—H30c	0.9600
C21—C20	1.397 (5)	C17—H17	0.9300
C7—C2	1.386 (5)	C17—C18	1.367 (6)
C7—C6	1.392 (5)	C27—H27	0.9300
C16—C17	1.388 (5)	C27—C26	1.360 (6)
C2—C3	1.389 (5)	C26—H26	0.9300
C31—C32	1.510 (5)	C26—C25	1.356 (7)
C23—C24	1.379 (5)	C19—H19	0.9300
C23—C28	1.377 (5)	C19—C18	1.377 (6)
C23—C22	1.511 (5)	C22—H22a	0.9700
C15—C22	1.498 (5)	C22—H22b	0.9700
C29—C30	1.509 (5)	C25—H25	0.9300
C6—H6	0.9300	C18—H18	0.9300
C6—C5	1.366 (5)	C32—H32a	0.9600
C1—C8	1.499 (4)	C32—H32b	0.9600
C3—H3	0.9300	C32—H32c	0.9600
Cg1···Cg3	3.649 (2)	Cg2···Cg3	3.564 (2)
Cg1···Cg4	3.497 (2)	Cg2···Cg4	3.629 (2)
O1—Cu1—O3	168.98 (10)	H4a—C4—C3	119.0 (3)
O2—Cu1—O3	111.18 (10)	C5—C4—C3	122.1 (4)
O2—Cu1—O1	57.85 (9)	C5—C4—H4a	119.0 (2)
O4—Cu1—O3	53.32 (9)	C4—C5—C6	121.6 (4)
O4—Cu1—O1	137.66 (9)	H5—C5—C6	119.2 (3)
O4—Cu1—O2	164.49 (9)	H5—C5—C4	119.2 (2)
N3—Cu1—O3	90.49 (10)	H24—C24—C23	119.5 (2)
N3—Cu1—O1	89.35 (10)	C25—C24—C23	120.9 (4)
N3—Cu1—O2	93.85 (10)	C25—C24—H24	119.5 (3)
N3—Cu1—O4	87.22 (10)	H20—C20—C21	121.5 (2)
N1—Cu1—O3	93.04 (10)	C19—C20—C21	117.0 (4)
N1—Cu1—O1	89.23 (10)	C19—C20—H20	121.5 (3)
N1—Cu1—O2	94.92 (10)	H28—C28—C23	119.6 (2)
N1—Cu1—O4	86.25 (9)	C27—C28—C23	120.9 (4)
N1—Cu1—N3	168.64 (11)	C27—C28—H28	119.6 (3)
C31—O3—Cu1	109.3 (2)	C13—C12—H12	120.2 (3)
C29—O1—Cu1	100.2 (2)	C11—C12—H12	120.2 (3)
C29—O2—Cu1	80.0 (2)	C11—C12—C13	119.5 (4)
C31—O4—Cu1	74.2 (2)	H13—C13—C12	120.0 (3)
C21—N3—Cu1	127.8 (2)	C14—C13—C12	120.1 (4)
C15—N3—Cu1	125.6 (3)	C14—C13—H13	120.0 (2)
C15—N3—C21	105.4 (3)	C13—C14—C9	121.3 (4)
C7—N1—Cu1	127.4 (2)	H14—C14—C9	119.3 (2)
C1—N1—Cu1	127.5 (2)	H14—C14—C13	119.3 (2)
C1—N1—C7	105.0 (3)	C12—C11—C10	120.7 (4)
C16—N4—H4	126.1 (2)	H11—C11—C10	119.6 (2)
C15—N4—H4	126.1 (2)	H11—C11—C12	119.6 (3)

C15—N4—C16	107.7 (3)	C1—C8—C9	116.4 (3)
C2—N2—H2	126.0 (2)	H8a—C8—C9	108.18 (19)
C1—N2—H2	126.0 (2)	H8a—C8—C1	108.2 (2)
C1—N2—C2	108.0 (3)	H8b—C8—C9	108.2 (2)
C14—C9—C10	118.2 (3)	H8b—C8—C1	108.2 (2)
C8—C9—C10	118.9 (3)	H8b—C8—H8a	107.3
C8—C9—C14	122.8 (3)	H30a—C30—C29	109.5
C16—C21—N3	109.3 (3)	H30b—C30—C29	109.5
C20—C21—N3	131.0 (3)	H30b—C30—H30a	109.5
C20—C21—C16	119.8 (4)	H30c—C30—C29	109.5
C2—C7—N1	109.3 (3)	H30c—C30—H30a	109.5
C6—C7—N1	130.2 (4)	H30c—C30—H30b	109.5
C6—C7—C2	120.5 (3)	H17—C17—C16	121.8 (3)
C21—C16—N4	105.0 (3)	C18—C17—C16	116.5 (4)
C17—C16—N4	132.3 (4)	C18—C17—H17	121.8 (3)
C17—C16—C21	122.6 (4)	H27—C27—C28	120.6 (3)
C7—C2—N2	105.3 (3)	C26—C27—C28	118.7 (4)
C3—C2—N2	132.7 (4)	C26—C27—H27	120.6 (3)
C3—C2—C7	122.0 (4)	H26—C26—C27	119.4 (3)
O4—C31—O3	122.8 (4)	C25—C26—C27	121.3 (5)
C32—C31—O3	116.5 (4)	C25—C26—H26	119.4 (3)
C32—C31—O4	120.7 (4)	H19—C19—C20	118.8 (3)
C28—C23—C24	118.3 (4)	C18—C19—C20	122.4 (4)
C22—C23—C24	121.7 (4)	C18—C19—H19	118.8 (3)
C22—C23—C28	120.0 (4)	C15—C22—C23	114.6 (3)
N4—C15—N3	112.6 (3)	H22a—C22—C23	108.6 (2)
C22—C15—N3	126.0 (4)	H22a—C22—C15	108.6 (2)
C22—C15—N4	121.4 (3)	H22b—C22—C23	108.6 (2)
O2—C29—O1	121.9 (3)	H22b—C22—C15	108.6 (2)
C30—C29—O1	117.9 (3)	H22b—C22—H22a	107.6
C30—C29—O2	120.2 (3)	C26—C25—C24	120.0 (5)
H6—C6—C7	121.2 (2)	H25—C25—C24	120.0 (3)
C5—C6—C7	117.6 (4)	H25—C25—C26	120.0 (3)
C5—C6—H6	121.2 (3)	C19—C18—C17	121.7 (5)
N2—C1—N1	112.4 (3)	H18—C18—C17	119.2 (3)
C8—C1—N1	124.8 (3)	H18—C18—C19	119.2 (3)
C8—C1—N2	122.8 (3)	H32a—C32—C31	109.5
H3—C3—C2	121.8 (3)	H32b—C32—C31	109.5
C4—C3—C2	116.3 (4)	H32b—C32—H32a	109.5
C4—C3—H3	121.8 (3)	H32c—C32—C31	109.5
H10—C10—C9	120.0 (2)	H32c—C32—H32a	109.5
C11—C10—C9	120.1 (4)	H32c—C32—H32b	109.5
C11—C10—H10	120.0 (2)		

Cu1—O3—C31—O4	−6.6 (2)	C21—C20—C19—C18	0.2 (5)
Cu1—O3—C31—C32	171.4 (3)	C7—N1—C1—C8	−176.6 (2)
Cu1—O1—C29—O2	−2.0 (2)	C7—C2—N2—C1	1.4 (3)
Cu1—O1—C29—C30	176.4 (2)	C7—C2—C3—C4	0.5 (4)

Cu1—O2—C29—O1	1.7 (2)	C7—C6—C5—C4	0.3 (4)
Cu1—O2—C29—C30	−176.75 (19)	C16—N4—C15—C22	−178.9 (3)
Cu1—O4—C31—O3	4.7 (2)	C16—C21—N3—C15	0.8 (3)
Cu1—O4—C31—C32	−173.3 (2)	C16—C21—C20—C19	0.7 (4)
Cu1—N3—C21—C16	−167.2 (3)	C16—C17—C18—C19	0.4 (5)
Cu1—N3—C21—C20	12.8 (4)	C2—N2—C1—C8	176.0 (2)
Cu1—N3—C15—N4	167.8 (3)	C2—C7—N1—C1	0.6 (3)
Cu1—N3—C15—C22	−13.2 (3)	C2—C7—C6—C5	1.2 (4)
Cu1—N1—C7—C2	−175.8 (3)	C2—C3—C4—C5	1.0 (4)
Cu1—N1—C7—C6	3.0 (3)	C23—C24—C25—C26	0.4 (5)
Cu1—N1—C1—N2	176.7 (3)	C23—C28—C27—C26	−0.7 (5)
Cu1—N1—C1—C8	−0.2 (3)	C15—N3—C21—C20	−179.2 (3)
N3—C21—C16—N4	−0.7 (3)	C15—N4—C16—C17	−179.3 (3)
N3—C21—C16—C17	179.0 (3)	C15—C22—C23—C24	36.0 (4)
N3—C21—C20—C19	−179.4 (4)	C15—C22—C23—C28	−144.9 (4)
N3—C15—N4—C16	0.1 (3)	C6—C7—N1—C1	179.4 (4)
N3—C15—C22—C23	−115.1 (4)	C6—C7—C2—C3	−1.6 (4)
N1—C7—C2—N2	−1.2 (3)	C6—C5—C4—C3	−1.5 (5)
N1—C7—C2—C3	177.3 (3)	C1—N2—C2—C3	−176.9 (3)
N1—C7—C6—C5	−177.5 (4)	C1—C8—C9—C10	−151.8 (4)
N1—C1—N2—C2	−1.1 (3)	C1—C8—C9—C14	30.1 (4)
N1—C1—C8—C9	−116.8 (3)	C10—C9—C14—C13	1.6 (4)
N4—C16—C21—C20	179.2 (3)	C10—C11—C12—C13	2.3 (6)
N4—C16—C17—C18	−179.9 (5)	C24—C23—C28—C27	0.6 (4)
N4—C15—N3—C21	−0.5 (3)	C24—C25—C26—C27	−0.5 (5)
N4—C15—C22—C23	63.8 (4)	C20—C21—C16—C17	−1.0 (4)
N2—C2—C7—C6	179.8 (3)	C20—C19—C18—C17	−0.8 (5)
N2—C2—C3—C4	178.6 (4)	C28—C23—C24—C25	−0.5 (5)
N2—C1—N1—C7	0.3 (3)	C28—C27—C26—C25	0.6 (5)
N2—C1—C8—C9	66.5 (3)	C13—C14—C9—C8	179.7 (4)
C9—C10—C11—C12	−1.2 (5)	C14—C9—C10—C11	−0.8 (4)
C9—C14—C13—C12	−0.5 (5)	C14—C13—C12—C11	−1.4 (5)
C21—N3—C15—C22	178.4 (3)	C11—C10—C9—C8	−179.0 (4)
C21—C16—N4—C15	0.4 (3)	C27—C28—C23—C22	−178.5 (4)
C21—C16—C17—C18	0.4 (4)	C22—C23—C24—C25	178.6 (4)

Hydrogen-bond geometry (Å, º)

*Cg*3, 5, 8 and 9 are the centroids of the N1/C1/N2/C2/C7, C2–C7, C23–C28 and N1/C1/N2/C2–C7 rings, respectively

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N2—H2···O4^{i}	0.86 (1)	1.91 (1)	2.708 (4)	153 (1)
N4—H4···O2^{ii}	0.86 (1)	1.86 (1)	2.699 (4)	164 (1)
C8—H8*a*···*Cg*3^{i}	0.97 (1)	2.70 (1)	3.592 (4)	154 (1)
C8—H8*a*···*Cg*9^{i}	0.97 (1)	2.93 (1)	3.844 (4)	158 (1)
C13—H13···*Cg*5^{iii}	0.93 (1)	2.82 (1)	3.614 (4)	145 (1)
C30—H30*a*···*Cg*8^{iv}	0.96 (1)	2.93 (1)	3.690 (5)	137 (2)

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