metal-organic compounds

Methoxo[N′-(3-methoxy-2-oxido-benzylidene)benzohydrazidato]-oxidovanadium(V)

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In the title complex, $[V(C_{15}H_{12}N_2O_4)(CH_3O)O]$, the V^V ion exhibits a distorted square-pyramidal coordination geometry; three donor atoms from a hydrazone ligand and one O atom of the deprotonated methanol define the coordination basal plane. The V^V ion is displaced by 0.464 (1) Å from the basal plane towards the axial oxide O atom. Intramolecular O—H⋯N hydrogen bonding occurs. Intermolecular C—H⋯O hydrogen bonding is also observed in the crystal structure.

Related literature

For general background to hydrazones and their chelation ability, see: Liu & Gao (1998); Ma *et al.* (1989); Sur *et al.* (1993); Sun *et al.* (2005). For related structures, see: Chen *et al.* (2004); Liu *et al.* (2006); Ghosh *et al.* (2007); Seena *et al.* (2008). For the synthesis, see: Gao *et al.* (1998); Chen (2008).
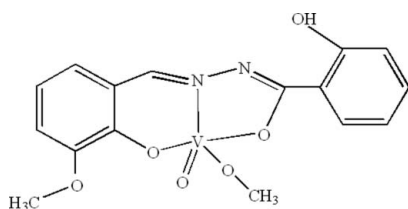
Experimental

Crystal data

$[V(C_{15}H_{12}N_2O_4)(CH_3O)O]$
M_r = 382.24
Monoclinic, $P2_1/c$
a = 16.194 (3) Å
b = 6.6746 (13) Å
c = 15.359 (3) Å
β = 96.89 (3)°

V = 1648.1 (6) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.64 mm^{-1}
T = 293 K
0.39 × 0.22 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID diffractometer
Absorption correction: multi-scan (*TEXRAY*; Molecular Structure Corporation, 1999)
T_{min} = 0.845, T_{max} = 0.909

14918 measured reflections
3686 independent reflections
2776 reflections with $I > 2\sigma(I)$
R_{int} = 0.051

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.042
$wR(F^2)$ = 0.118
S = 1.08
3686 reflections

228 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.33 e Å^{-3}
$\Delta\rho_{min}$ = −0.39 e Å^{-3}

Table 1
Selected bond lengths (Å).

V1—O1	1.8277 (17)	V1—O6	1.7351 (16)
V1—O3	1.9436 (16)	V1—N1	2.0963 (17)
V1—O5	1.5736 (18)		

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

D—H⋯A	D—H	H⋯A	D⋯A	D—H⋯A
O4—H4B⋯N2	0.82	1.84	2.568 (2)	147
C8—H8A⋯O4[i]	0.93	2.32	3.243 (3)	169

Symmetry code: (i) $-x + 1, y + \frac{1}{2}, -z + \frac{3}{2}$.

Data collection: *TEXRAY* (Molecular Structure Corporation, 1999); cell refinement: *TEXRAY*; data reduction: *TEXSAN* (Molecular Structure Corporation, 1999); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEX* (McArdle, 1995); software used to prepare material for publication: *SHELXL97*.

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supporting information

Methoxo[*N*′-(3-methoxy-2-oxidobenzylidene)benzohydrazidato]oxidovanadium(V)

Shu-Mei Huang, Fei-Feng Jiang, Xiao-Hua Chen and Qiong-Jie Wu

S1. Comment

Hydrazones are of interest owing to their capacity for chelating to transition (Sur *et al.*, 1993; Sun, *et al.*, 2005), lanthanide (Ma *et al.*, 1989) and main group (Liu & Gao 1998) metals.

The V^V ion exists in a distorted square-pyramidal coordination geometry. Three donor atoms (O1, O3 and N1) of the hydrozone ligand and O6 atom from the methanol group define the coordination basal plane, with a maximum mean plane deviation of 0.0215 (9) Å. The V atom is displaced towards the axial oxo O atom by 0.464 (1)Å from the basal plane. Bond distances (Table 1) and bond angles around V1 atom are compared with those in reported oxovanadium complexes (Chen *et al.*, 2004; Seena *et al.*, 2008; Liu *et al.*,2006; Ghosh *et al.*, 2007). In the crystal structure there are the intramolecular O—H···N hydrogen bonding and intermolecular C—H···O hydrogen bonding (Table 2).

S2. Experimental

VO(acac)$_2$ (acac = acetylacetonate) was synthesized according to the reported method (Gao *et al.*, 1998). The hydrazone ligand (L) was prepared by following a similar procedure reported by Chen (2008).

The title compound was prepared by reacting H$_2$L (0.1 mmol) with VO(acac)$_2$ (0.1 mmol) in methnol/water solution (10 ml) with stirring. The solution was filtered and allowed to stand at room temperature for one week, dark-red crystals of complex (I) were obtained.

S3. Refinement

All H atoms were placed in idealized positions and treated as riding with O—H = 0.82 Å, C—H = 0.93-0.96 Å; U$_{iso}$(H) = 1.2U$_{eq}$(C) or 1.5U$_{eq}$(C,O).
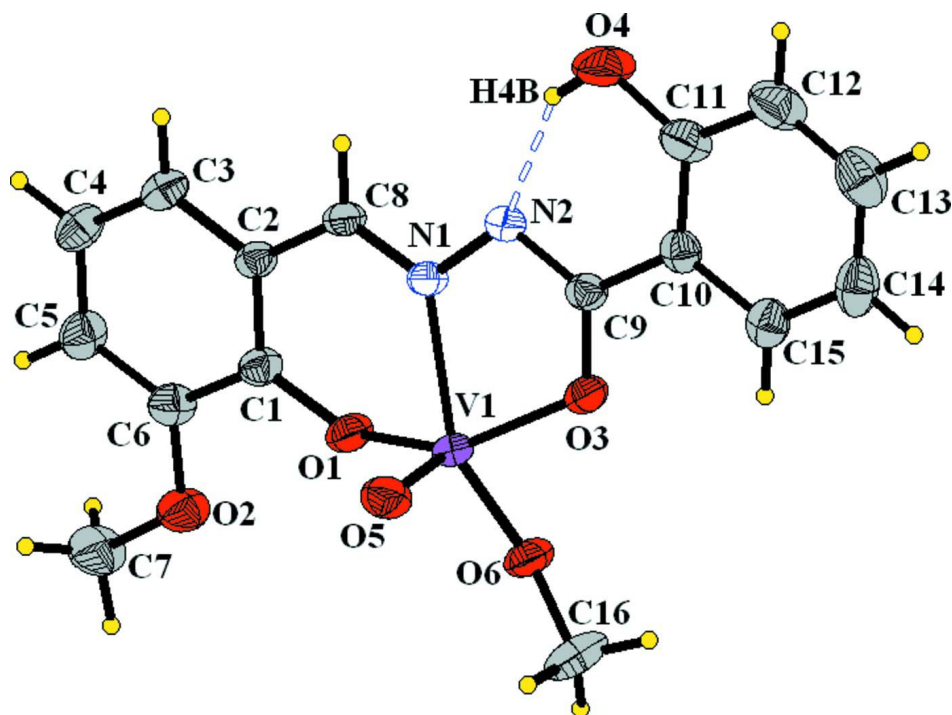
Figure 1

The molecular structure of the title compound, showing 30% probability displacement ellipsoids for non-H atoms. A dashed line indicates the intramoleculat hydrogen bonding.

Methoxo[*N′*-(3-methoxy-2- oxidobenzylidene)benzohydrazidato]oxidovanadium(V)

Crystal data

[V(C$_{15}$H$_{12}$N$_2$O$_4$)(CH$_3$O)O]
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Hall symbol: -P 2ybc
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c = 15.359 (3) Å
β = 96.89 (3)°
V = 1648.1 (6) Å^3
Z = 4

$F(000)$ = 784
D_x = 1.541 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 2776 reflections
θ = 3.1–27.5°
μ = 0.64 mm^{-1}
T = 293 K
Prism, dark-red
0.39 × 0.22 × 0.15 mm

Data collection

Rigaku R-AXIS RAPID
  diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω scans
Absorption correction: multi-scan
  (*TEXRAY*; Molecular Structure Corporation,
  1999)
T_{min} = 0.845, T_{max} = 0.909

14918 measured reflections
3686 independent reflections
2776 reflections with $I > 2\sigma(I)$
R_{int} = 0.051
θ_{max} = 27.5°, θ_{min} = 3.1°
h = −21→21
k = −8→8
l = −19→19

Refinement

Refinement on F^2	Secondary atom site location: difference Fourier map
Least-squares matrix: full	
$R[F^2 > 2\sigma(F^2)] = 0.042$	Hydrogen site location: inferred from neighbouring sites
$wR(F^2) = 0.118$	
$S = 1.08$	H-atom parameters constrained
3686 reflections	$w = 1/[\sigma^2(F_o^2) + (0.062P)^2 + 0.2985P]$
228 parameters	where $P = (F_o^2 + 2F_c^2)/3$
0 restraints	$(\Delta/\sigma)_{max} = 0.001$
Primary atom site location: structure-invariant direct methods	$\Delta\rho_{max} = 0.33$ e Å⁻³
	$\Delta\rho_{min} = -0.39$ e Å⁻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. 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 (Å²)

	x	y	z	$U_{iso}*/U_{eq}$
V1	0.16311 (2)	0.04276 (6)	0.66648 (3)	0.04096 (14)
O1	0.16555 (9)	0.2270 (2)	0.57877 (11)	0.0533 (4)
O2	0.09673 (11)	0.5226 (3)	0.48044 (13)	0.0624 (5)
O3	0.21107 (9)	−0.1967 (2)	0.72412 (10)	0.0464 (4)
O4	0.46575 (11)	−0.2270 (3)	0.81503 (15)	0.0860 (7)
H4B	0.4400	−0.1379	0.7867	0.129*
O5	0.13675 (10)	0.1611 (3)	0.74736 (12)	0.0599 (5)
O6	0.07767 (10)	−0.0955 (3)	0.62167 (11)	0.0561 (4)
N1	0.29210 (10)	0.0886 (3)	0.68123 (11)	0.0377 (4)
N2	0.33889 (10)	−0.0525 (3)	0.73138 (12)	0.0411 (4)
C1	0.21307 (13)	0.3854 (3)	0.56461 (14)	0.0432 (5)
C2	0.29647 (12)	0.3942 (3)	0.59948 (13)	0.0390 (5)
C3	0.34579 (14)	0.5570 (3)	0.57913 (16)	0.0487 (6)
H3A	0.4017	0.5617	0.6015	0.058*
C4	0.31173 (16)	0.7083 (4)	0.52658 (16)	0.0562 (6)
H4A	0.3445	0.8155	0.5129	0.067*
C5	0.22816 (16)	0.7015 (4)	0.49361 (16)	0.0554 (6)
H5A	0.2052	0.8063	0.4588	0.066*
C6	0.17849 (14)	0.5428 (4)	0.51131 (15)	0.0488 (5)
C7	0.05967 (18)	0.6762 (5)	0.4246 (2)	0.0739 (8)
H7A	0.0016	0.6478	0.4095	0.111*
H7B	0.0865	0.6818	0.3722	0.111*
H7C	0.0659	0.8027	0.4544	0.111*
C8	0.33318 (12)	0.2369 (3)	0.65380 (14)	0.0406 (5)
H8A	0.3903	0.2414	0.6705	0.049*

C9	0.29058 (12)	−0.1970 (3)	0.75157 (14)	0.0397 (5)
C10	0.32708 (14)	−0.3646 (3)	0.80484 (14)	0.0431 (5)
C11	0.41233 (15)	−0.3729 (4)	0.83309 (17)	0.0577 (6)
C12	0.44452 (19)	−0.5360 (5)	0.8821 (2)	0.0744 (9)
H12A	0.5014	−0.5432	0.9001	0.089*
C13	0.3936 (2)	−0.6854 (5)	0.90395 (19)	0.0723 (8)
H13A	0.4162	−0.7932	0.9370	0.087*
C14	0.3096 (2)	−0.6792 (4)	0.87791 (17)	0.0642 (7)
H14A	0.2753	−0.7815	0.8937	0.077*
C15	0.27640 (16)	−0.5201 (4)	0.82817 (16)	0.0508 (6)
H15A	0.2195	−0.5164	0.8099	0.061*
C16	0.00782 (18)	−0.1796 (5)	0.6540 (2)	0.0879 (10)
H16A	−0.0371	−0.1897	0.6073	0.132*
H16B	−0.0088	−0.0958	0.6997	0.132*
H16C	0.0216	−0.3106	0.6771	0.132*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
V1	0.02696 (19)	0.0439 (2)	0.0521 (2)	−0.00458 (14)	0.00533 (14)	0.00005 (17)
O1	0.0359 (8)	0.0547 (10)	0.0670 (10)	−0.0086 (7)	−0.0028 (7)	0.0155 (9)
O2	0.0453 (9)	0.0705 (11)	0.0685 (11)	−0.0006 (8)	−0.0056 (8)	0.0233 (10)
O3	0.0364 (8)	0.0468 (9)	0.0555 (9)	−0.0077 (6)	0.0038 (6)	0.0039 (8)
O4	0.0380 (9)	0.0995 (15)	0.1183 (17)	0.0049 (10)	0.0011 (10)	0.0564 (14)
O5	0.0471 (9)	0.0652 (11)	0.0693 (11)	0.0029 (8)	0.0147 (8)	−0.0103 (9)
O6	0.0390 (8)	0.0612 (10)	0.0664 (11)	−0.0148 (7)	−0.0006 (7)	0.0052 (9)
N1	0.0290 (8)	0.0415 (9)	0.0428 (9)	−0.0003 (7)	0.0047 (7)	−0.0014 (8)
N2	0.0316 (8)	0.0416 (10)	0.0498 (10)	0.0015 (7)	0.0034 (7)	0.0016 (8)
C1	0.0384 (11)	0.0482 (12)	0.0440 (12)	−0.0035 (9)	0.0093 (9)	0.0036 (10)
C2	0.0353 (10)	0.0434 (11)	0.0395 (11)	−0.0033 (8)	0.0093 (8)	−0.0034 (10)
C3	0.0429 (12)	0.0551 (14)	0.0493 (13)	−0.0115 (10)	0.0105 (10)	0.0000 (11)
C4	0.0586 (15)	0.0576 (15)	0.0542 (14)	−0.0149 (12)	0.0146 (11)	0.0099 (13)
C5	0.0616 (15)	0.0556 (15)	0.0497 (13)	−0.0044 (12)	0.0096 (11)	0.0153 (12)
C6	0.0451 (12)	0.0575 (14)	0.0440 (12)	0.0000 (10)	0.0063 (10)	0.0059 (11)
C7	0.0635 (17)	0.083 (2)	0.0713 (18)	0.0100 (15)	−0.0089 (14)	0.0247 (17)
C8	0.0290 (9)	0.0464 (12)	0.0469 (12)	−0.0031 (8)	0.0069 (8)	−0.0045 (10)
C9	0.0355 (10)	0.0433 (11)	0.0407 (11)	0.0005 (9)	0.0067 (8)	−0.0054 (10)
C10	0.0500 (12)	0.0418 (12)	0.0392 (11)	0.0033 (9)	0.0115 (9)	−0.0041 (10)
C11	0.0471 (13)	0.0680 (16)	0.0588 (15)	0.0118 (12)	0.0101 (11)	0.0116 (14)
C12	0.0619 (17)	0.085 (2)	0.077 (2)	0.0244 (16)	0.0101 (15)	0.0246 (17)
C13	0.095 (2)	0.0673 (19)	0.0561 (16)	0.0218 (17)	0.0154 (15)	0.0142 (15)
C14	0.098 (2)	0.0459 (14)	0.0519 (15)	−0.0048 (14)	0.0225 (14)	0.0012 (13)
C15	0.0631 (15)	0.0473 (13)	0.0436 (12)	−0.0025 (11)	0.0127 (11)	−0.0072 (11)
C16	0.0597 (17)	0.101 (2)	0.103 (2)	−0.0432 (17)	0.0113 (16)	0.004 (2)

Geometric parameters (Å, º)

V1—O1	1.8277 (17)	C4—H4A	0.9300
V1—O3	1.9436 (16)	C5—C6	1.377 (3)
V1—O5	1.5736 (18)	C5—H5A	0.9300
V1—O6	1.7351 (16)	C7—H7A	0.9600
V1—N1	2.0963 (17)	C7—H7B	0.9600
O1—C1	1.341 (3)	C7—H7C	0.9600
O2—C6	1.358 (3)	C8—H8A	0.9300
O2—C7	1.423 (3)	C9—C10	1.467 (3)
O3—C9	1.306 (2)	C10—C15	1.397 (3)
O4—C11	1.353 (3)	C10—C11	1.398 (3)
O4—H4B	0.8200	C11—C12	1.389 (4)
O6—C16	1.406 (3)	C12—C13	1.361 (4)
N1—C8	1.292 (3)	C12—H12A	0.9300
N1—N2	1.384 (2)	C13—C14	1.372 (4)
N2—C9	1.303 (3)	C13—H13A	0.9300
C1—C2	1.393 (3)	C14—C15	1.379 (4)
C1—C6	1.406 (3)	C14—H14A	0.9300
C2—C3	1.405 (3)	C15—H15A	0.9300
C2—C8	1.426 (3)	C16—H16A	0.9600
C3—C4	1.367 (3)	C16—H16B	0.9600
C3—H3A	0.9300	C16—H16C	0.9600
C4—C5	1.388 (3)		
O5—V1—O6	107.53 (9)	O2—C7—H7A	109.5
O5—V1—O1	106.03 (9)	O2—C7—H7B	109.5
O6—V1—O1	98.75 (8)	H7A—C7—H7B	109.5
O5—V1—O3	100.64 (8)	O2—C7—H7C	109.5
O6—V1—O3	89.96 (7)	H7A—C7—H7C	109.5
O1—V1—O3	147.80 (7)	H7B—C7—H7C	109.5
O5—V1—N1	101.68 (8)	N1—C8—C2	124.10 (18)
O6—V1—N1	149.00 (8)	N1—C8—H8A	118.0
O1—V1—N1	82.66 (7)	C2—C8—H8A	118.0
O3—V1—N1	74.46 (6)	N2—C9—O3	121.3 (2)
C1—O1—V1	135.54 (14)	N2—C9—C10	118.93 (19)
C6—O2—C7	117.5 (2)	O3—C9—C10	119.78 (19)
C9—O3—V1	118.22 (14)	C15—C10—C11	118.7 (2)
C11—O4—H4B	109.5	C15—C10—C9	120.0 (2)
C16—O6—V1	135.18 (19)	C11—C10—C9	121.3 (2)
C8—N1—N2	115.74 (16)	O4—C11—C12	117.9 (2)
C8—N1—V1	128.47 (14)	O4—C11—C10	122.7 (2)
N2—N1—V1	115.67 (12)	C12—C11—C10	119.5 (3)
C9—N2—N1	109.38 (16)	C13—C12—C11	120.6 (3)
O1—C1—C2	121.3 (2)	C13—C12—H12A	119.7
O1—C1—C6	119.17 (19)	C11—C12—H12A	119.7
C2—C1—C6	119.5 (2)	C12—C13—C14	121.0 (3)
C1—C2—C3	119.8 (2)	C12—C13—H13A	119.5

C1—C2—C8	120.72 (19)	C14—C13—H13A	119.5
C3—C2—C8	119.42 (19)	C13—C14—C15	119.4 (3)
C4—C3—C2	120.2 (2)	C13—C14—H14A	120.3
C4—C3—H3A	119.9	C15—C14—H14A	120.3
C2—C3—H3A	119.9	C14—C15—C10	120.8 (3)
C3—C4—C5	119.9 (2)	C14—C15—H15A	119.6
C3—C4—H4A	120.1	C10—C15—H15A	119.6
C5—C4—H4A	120.1	O6—C16—H16A	109.5
C6—C5—C4	121.4 (2)	O6—C16—H16B	109.5
C6—C5—H5A	119.3	H16A—C16—H16B	109.5
C4—C5—H5A	119.3	O6—C16—H16C	109.5
O2—C6—C5	125.1 (2)	H16A—C16—H16C	109.5
O2—C6—C1	115.6 (2)	H16B—C16—H16C	109.5
C5—C6—C1	119.2 (2)		
O5—V1—O1—C1	68.2 (2)	C7—O2—C6—C5	0.8 (4)
O6—V1—O1—C1	179.4 (2)	C7—O2—C6—C1	−178.6 (2)
O3—V1—O1—C1	−76.5 (3)	C4—C5—C6—O2	−178.7 (2)
N1—V1—O1—C1	−31.9 (2)	C4—C5—C6—C1	0.6 (4)
O5—V1—O3—C9	−90.59 (16)	O1—C1—C6—O2	2.2 (3)
O6—V1—O3—C9	161.58 (15)	C2—C1—C6—O2	−179.7 (2)
O1—V1—O3—C9	55.0 (2)	O1—C1—C6—C5	−177.2 (2)
N1—V1—O3—C9	8.72 (14)	C2—C1—C6—C5	0.9 (3)
O5—V1—O6—C16	−27.1 (3)	N2—N1—C8—C2	178.26 (18)
O1—V1—O6—C16	−137.1 (3)	V1—N1—C8—C2	−6.0 (3)
O3—V1—O6—C16	74.0 (3)	C1—C2—C8—N1	−6.8 (3)
N1—V1—O6—C16	132.6 (3)	C3—C2—C8—N1	174.9 (2)
O5—V1—N1—C8	−85.9 (2)	N1—N2—C9—O3	1.1 (3)
O6—V1—N1—C8	113.8 (2)	N1—N2—C9—C10	179.94 (17)
O1—V1—N1—C8	18.99 (19)	V1—O3—C9—N2	−8.7 (3)
O3—V1—N1—C8	176.1 (2)	V1—O3—C9—C10	172.45 (14)
O5—V1—N1—N2	89.78 (15)	N2—C9—C10—C15	179.3 (2)
O6—V1—N1—N2	−70.5 (2)	O3—C9—C10—C15	−1.9 (3)
O1—V1—N1—N2	−165.29 (15)	N2—C9—C10—C11	−0.8 (3)
O3—V1—N1—N2	−8.15 (13)	O3—C9—C10—C11	178.0 (2)
C8—N1—N2—C9	−177.45 (19)	C15—C10—C11—O4	−178.7 (3)
V1—N1—N2—C9	6.3 (2)	C9—C10—C11—O4	1.5 (4)
V1—O1—C1—C2	29.7 (3)	C15—C10—C11—C12	1.0 (4)
V1—O1—C1—C6	−152.29 (18)	C9—C10—C11—C12	−178.9 (2)
O1—C1—C2—C3	176.2 (2)	O4—C11—C12—C13	178.6 (3)
C6—C1—C2—C3	−1.8 (3)	C10—C11—C12—C13	−1.1 (5)
O1—C1—C2—C8	−2.0 (3)	C11—C12—C13—C14	0.3 (5)
C6—C1—C2—C8	180.0 (2)	C12—C13—C14—C15	0.6 (4)
C1—C2—C3—C4	1.2 (3)	C13—C14—C15—C10	−0.7 (4)
C8—C2—C3—C4	179.5 (2)	C11—C10—C15—C14	−0.1 (3)
C2—C3—C4—C5	0.3 (4)	C9—C10—C15—C14	179.7 (2)
C3—C4—C5—C6	−1.2 (4)		

Hydrogen-bond geometry (Å, º)

D—H$\cdots A$	D—H	H$\cdots A$	$D\cdots A$	D—H$\cdots A$
O4—H4*B*$\cdots$N2	0.82	1.84	2.568 (2)	147
C8—H8*A*$\cdots$O4[i]	0.93	2.32	3.243 (3)	169

Symmetry code: (i) $-x+1, y+1/2, -z+3/2$.