

(2*E*,2'*E*)-1,1'-([1,1'-Biphenyl]-4,4'-diyl)bis[3-(dimethylamino)prop-2-en-1-one]

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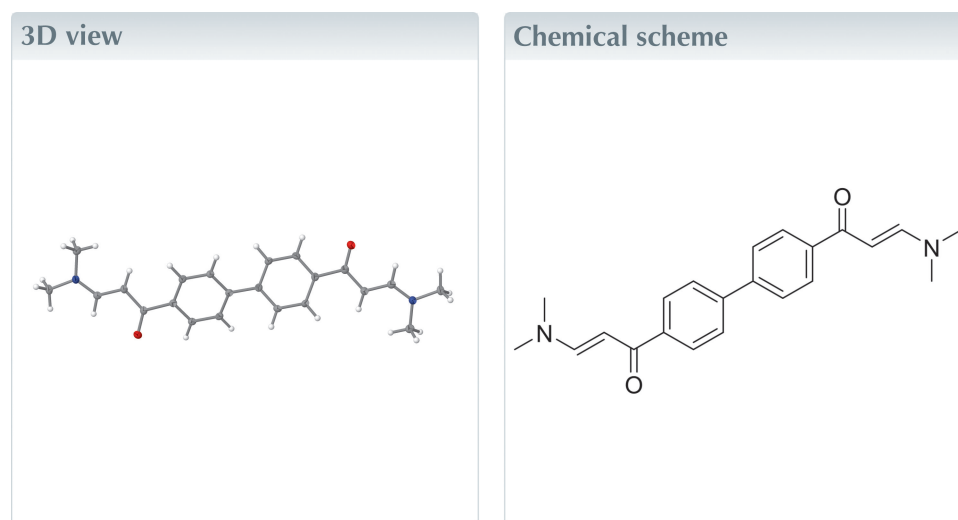
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Keywords: crystal structure; β -ketoamine; π -conjugated molecule.**CCDC reference:** 2349722**Structural data:** full structural data are available from iucrdata.iucr.org

The title compound, C₂₂H₂₄N₂O₂, crystallizes in space group $P2_1/n$. The molecular structure is almost planar except for a tilt of the phenyl rings. The allyl groups on both ends exhibit the *trans*-form and the connected N atoms show sp^2 character. The molecules are stacked and assembled along the *c*-axis direction by C—H $\cdots\pi$ interactions.



Structure description

β -Ketoamines are important not only for various chemical reactions, but also for creating functional complexes (Pettinari *et al.*, 2014). Recently, they have also been used as reagents for covalent organic frameworks (Zhao *et al.*, 2023). In this work, the crystal structure of the title β -ketoamine was determined. The molecule is almost flat, but the phenyl rings are tilted [dihedral angle = 30.14 (8) $^\circ$] (Fig. 1) as a result of the repulsion between H atoms on the phenyl rings and intermolecular interactions, *i.e.*, C—H $\cdots\pi$, with neighboring molecules (Table 1). In addition to the carbonyl and the allyl groups, the amino groups also show a planar character, indicating the sp^2 character of the N atoms and the π -conjugated character of these functional groups. The bond-angle sums for both N atoms are 360.0 $^\circ$.

In the crystal, the molecules are assembled to form a two-dimensional layer-like structure in the (105) plane (Fig. 2). The molecules are stacked perpendicular to this plane through C—H $\cdots\pi$ interactions. Each molecule interacts with three neighboring molecules. Two different phenyl groups on the molecule accept the C donors (C21 and C22), resulting in additional C—H $\cdots\pi$ interactions (Tsuzuki *et al.*, 2000) with molecules above and below (Fig. 3). The C21 methyl group on one side interacts with the phenyl ring of the stacked molecule above through a C21—H21 \cdots Cg2 interaction [C21 \cdots Cg2 = 3.538 (2) Å], while the C22 methyl group on the other side similarly interacts with the molecule below [C22 \cdots Cg1 = 3.608 (2) Å] where Cg1 and Cg2 are the centroids of the C1/C9/C17/C4/C18/C15 and C3/C14/C11/C7/C6/C16 rings, respectively. The distances

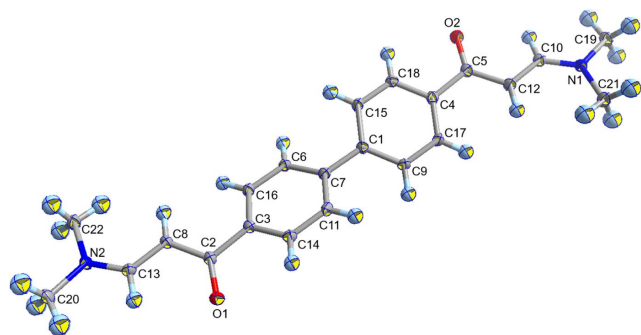


Figure 1
Illustration of the title molecule, composed of crystallographically independent atoms with displacement ellipsoids drawn at the 50% probability level.

between the phenyl groups are not remarkably short with centroid-centroid separations of 4.363 (1) and 4.833 (1) Å, and no obvious π - π interactions occur with neighboring molecules, indicating that the molecules are assembled mainly through C-H \cdots π interactions. C-H \cdots O interactions involving H22 and H22B (Table 1) also occur, which also contribute to assemble the molecules.

Synthesis and crystallization

A mixture of 4,4'-diacetyl biphenyl (0.953 g, 4.00 mmol), anhydrous DMF (12 ml), and *N,N*-dimethylformamide diethyl acetal (12 ml) was stirred and heated at 90°C under a nitrogen atmosphere for 12 h. After cooling, diethyl ether (20 ml) was added slowly to the reaction mixture, resulting in a yellow powder. The precipitate was collected by suction filtration and it was then immersed in *n*-pentane for 4 h at room temperature. After that, the precipitate was collected by suction filtration and dried under vacuum at 170°C overnight (0.961 g, 1.98 mmol, yield 50%). Crystals of the title compound were obtained by recrystallization through slow evaporation of a methanol solution. After several days, yellow crystals were obtained.

Refinement

Details of crystal data, data collections, and structure refinements are shown in Table 2.

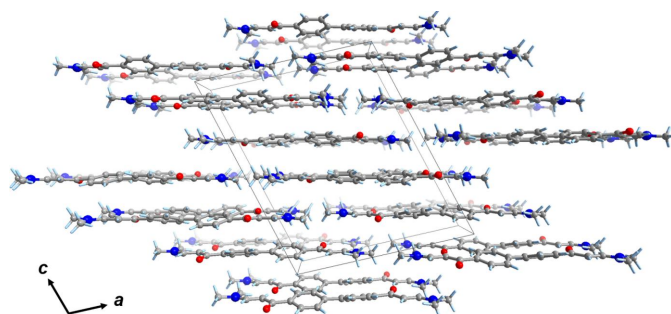


Figure 2
Packing structure of the title compound along the *b* axis.

Table 1
Hydrogen-bond geometry (Å, °).

*Cg*1 and *Cg*2 are the centroids of the C1/C9/C17/C4/C18/C15 and C3/C14/C11/C7/C6/C16 rings, respectively.

<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>
C21-H21B \cdots O2 ⁱ	0.98	2.51	3.410 (2)	152
C22-H22 \cdots O1 ⁱⁱ	0.98	2.48	3.387 (2)	154
C21-H21 \cdots <i>Cg</i> 2 ⁱⁱⁱ	0.98	2.60	3.538 (2)	160
C22-H22B \cdots <i>Cg</i> 1 ^{iv}	0.98	2.70	3.608 (2)	154

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

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₂₂ H ₂₄ N ₂ O ₂
<i>M</i> _r	348.43
Crystal system, space group	Monoclinic, <i>P</i> ₂ / <i>n</i>
Temperature (K)	90
<i>a</i> , <i>b</i> , <i>c</i> (Å)	15.862 (1), 6.0503 (4), 19.0640 (12)
β (°)	105.287 (3)
<i>V</i> (Å ³)	1764.8 (2)
<i>Z</i>	4
Radiation type	Mo <i>K</i> α
μ (mm ⁻¹)	0.08
Crystal size (mm)	0.40 \times 0.20 \times 0.20
Data collection	
Diffractometer	Bruker PHOTON II CPAD
Absorption correction	Multi-scan (<i>SADABS</i> ; Krause <i>et al.</i> , 2015)
<i>T</i> _{min} , <i>T</i> _{max}	0.669, 0.746
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	21542, 4738, 3539
<i>R</i> _{int}	0.076
(<i>sin</i> θ / λ) _{max} (Å ⁻¹)	0.731
Refinement	
<i>R</i> [<i>F</i> ² > 2 σ (<i>F</i> ²)], <i>wR</i> (<i>F</i> ²), <i>S</i>	0.063, 0.154, 1.08
No. of reflections	4738
No. of parameters	239
H-atom treatment	H-atom parameters constrained
$\Delta\rho$ _{max} , $\Delta\rho$ _{min} (e Å ⁻³)	0.31, -0.25

Computer programs: *APEX4* and *SAINT* (Bruker, 2021), *SIR2019* (Burla *et al.*, 2015), *SHELXL2018/3* (Sheldrick, 2015), *DIAMOND* (Brandenburg, 2014) and *Yadokari-XG* (Kabuto *et al.*, 2009).

Funding information

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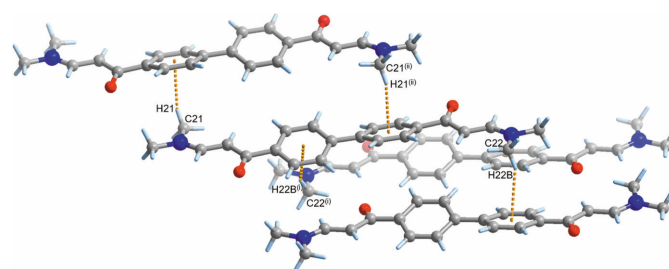


Figure 3
C-H \cdots π interactions between neighboring molecules. Symmetry codes: (i) $\frac{1}{2} - x, \frac{1}{2} + y, \frac{3}{2} - z$; (ii) $-x, -y, 2 - z$.

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full crystallographic data

IUCrData (2024). **9**, x240358 [https://doi.org/10.1107/S2414314624003584]

(2*E*,2'*E*)-1,1'-([1,1'-Biphenyl]-4,4'-diyl)bis[3-(dimethylamino)prop-2-en-1-one]

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(2*E*,2'*E*)-1,1'-([1,1'-Biphenyl]-4,4'-diyl)bis[3-(dimethylamino)prop-2-en-1-one]*Crystal data*

$C_{22}H_{24}N_2O_2$

$M_r = 348.43$

Monoclinic, $P2_1/n$

$a = 15.862$ (1) Å

$b = 6.0503$ (4) Å

$c = 19.0640$ (12) Å

$\beta = 105.287$ (3)°

$V = 1764.8$ (2) Å³

$Z = 4$

$F(000) = 744$

$D_x = 1.311$ Mg m⁻³

Mo $K\alpha$ radiation, $\lambda = 0.71069$ Å

Cell parameters from 2411 reflections

$\theta = 3.0$ – 29.0 °

$\mu = 0.08$ mm⁻¹

$T = 90$ K

Block, yellow

$0.40 \times 0.20 \times 0.20$ mm

Data collection

Bruker PHOTON II CPAD

diffractometer

Radiation source: fine-focus sealed tube

φ and ω scans

Absorption correction: multi-scan

(SADABS; Krause *et al.*, 2015)

$T_{\min} = 0.669$, $T_{\max} = 0.746$

21542 measured reflections

4738 independent reflections

3539 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.076$

$\theta_{\max} = 31.3$ °, $\theta_{\min} = 1.9$ °

$h = -22 \rightarrow 23$

$k = -8 \rightarrow 8$

$l = -27 \rightarrow 26$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.063$

$wR(F^2) = 0.154$

$S = 1.08$

4738 reflections

239 parameters

0 restraints

Hydrogen site location: inferred from neighbouring sites

H-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0561P)^2 + 0.8647P]$

where $P = (F_o^2 + 2F_c^2)/3$

$(\Delta/\sigma)_{\max} < 0.001$

$\Delta\rho_{\max} = 0.31$ e Å⁻³

$\Delta\rho_{\min} = -0.25$ 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 $F^2 > 2\sigma(F^2)$ 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.

All hydrogen atoms were fixed geometrically and refined using a riding-model approximation with C—H = 0.95 (for phenyl and allyl) and 0.98 (for methyl) Å.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	0.44366 (8)	0.0656 (2)	0.82473 (8)	0.0251 (3)
O2	-0.18571 (8)	-0.6345 (2)	0.92406 (8)	0.0260 (3)
C1	0.08648 (11)	-0.3027 (3)	0.88219 (9)	0.0172 (3)
C2	0.42078 (11)	-0.1318 (3)	0.82155 (9)	0.0183 (4)
N1	-0.35165 (9)	-0.1752 (2)	0.97342 (8)	0.0206 (3)
N2	0.60934 (9)	-0.3981 (3)	0.77673 (9)	0.0216 (3)
C3	0.33358 (11)	-0.1860 (3)	0.83472 (9)	0.0164 (3)
C4	-0.07530 (11)	-0.3830 (3)	0.91419 (9)	0.0182 (4)
C5	-0.16200 (11)	-0.4379 (3)	0.92887 (10)	0.0194 (4)
C6	0.23300 (11)	-0.4325 (3)	0.87142 (9)	0.0184 (4)
H6	0.220473	-0.575129	0.886905	0.022*
C7	0.17109 (11)	-0.2637 (3)	0.86495 (9)	0.0171 (4)
C8	0.47315 (11)	-0.3113 (3)	0.80669 (10)	0.0190 (4)
H8	0.454442	-0.460179	0.807627	0.023*
C9	0.04331 (11)	-0.1358 (3)	0.90959 (10)	0.0194 (4)
H9	0.069054	0.006774	0.918150	0.023*
C10	-0.29110 (11)	-0.3106 (3)	0.96087 (9)	0.0197 (4)
H10	-0.302961	-0.463891	0.963229	0.024*
C11	0.19194 (11)	-0.0561 (3)	0.84176 (10)	0.0188 (4)
H11	0.150491	0.060452	0.835705	0.023*
C12	-0.21424 (11)	-0.2595 (3)	0.94506 (10)	0.0204 (4)
H12	-0.195669	-0.110271	0.944727	0.024*
C13	0.55029 (11)	-0.2624 (3)	0.79123 (10)	0.0197 (4)
H13	0.563685	-0.109429	0.790785	0.024*
C14	0.27188 (11)	-0.0173 (3)	0.82748 (9)	0.0182 (4)
H14	0.284837	0.125692	0.812585	0.022*
C15	0.04694 (11)	-0.5114 (3)	0.87134 (10)	0.0206 (4)
H15	0.074488	-0.627754	0.852269	0.025*
C16	0.31225 (11)	-0.3953 (3)	0.85566 (9)	0.0176 (4)
H16	0.352524	-0.513573	0.859146	0.021*
C17	-0.03656 (11)	-0.1741 (3)	0.92460 (10)	0.0197 (4)
H17	-0.065153	-0.056678	0.942160	0.024*
C18	-0.03162 (11)	-0.5510 (3)	0.88793 (10)	0.0193 (4)
H18	-0.056200	-0.695105	0.881307	0.023*
C19	-0.42660 (11)	-0.2587 (3)	0.99574 (10)	0.0231 (4)
H19	-0.425634	-0.420614	0.995747	0.035*
H19A	-0.480571	-0.206431	0.961739	0.035*

H19B	-0.424069	-0.205172	1.044775	0.035*
C20	0.68514 (12)	-0.3137 (3)	0.75587 (11)	0.0259 (4)
H20	0.683659	-0.151744	0.755483	0.039*
H20A	0.684187	-0.367920	0.707229	0.039*
H20B	0.738614	-0.364478	0.790844	0.039*
C21	-0.34611 (12)	0.0646 (3)	0.96831 (11)	0.0248 (4)
H21	-0.334516	0.129235	1.017057	0.037*
H21A	-0.401469	0.122254	0.937915	0.037*
H21B	-0.298604	0.103377	0.946522	0.037*
C22	0.60316 (12)	-0.6375 (3)	0.78032 (11)	0.0239 (4)
H22	0.553718	-0.677418	0.799595	0.036*
H22A	0.657287	-0.696557	0.812301	0.036*
H22B	0.594317	-0.699911	0.731468	0.036*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0229 (6)	0.0164 (6)	0.0391 (8)	-0.0025 (5)	0.0138 (6)	-0.0007 (6)
O2	0.0243 (7)	0.0191 (7)	0.0391 (8)	-0.0041 (5)	0.0161 (6)	-0.0028 (6)
C1	0.0160 (8)	0.0166 (8)	0.0198 (8)	0.0012 (7)	0.0060 (7)	0.0014 (7)
C2	0.0168 (8)	0.0191 (9)	0.0206 (8)	-0.0004 (7)	0.0076 (7)	-0.0003 (7)
N1	0.0188 (7)	0.0179 (8)	0.0273 (8)	-0.0018 (6)	0.0098 (6)	-0.0017 (6)
N2	0.0194 (7)	0.0180 (8)	0.0314 (8)	-0.0005 (6)	0.0135 (7)	0.0007 (6)
C3	0.0169 (8)	0.0160 (8)	0.0171 (8)	-0.0007 (7)	0.0057 (7)	-0.0006 (7)
C4	0.0178 (8)	0.0183 (9)	0.0201 (8)	0.0005 (7)	0.0075 (7)	0.0015 (7)
C5	0.0203 (8)	0.0194 (9)	0.0201 (8)	-0.0007 (7)	0.0083 (7)	0.0004 (7)
C6	0.0189 (8)	0.0141 (8)	0.0240 (9)	0.0003 (7)	0.0089 (7)	0.0005 (7)
C7	0.0186 (8)	0.0147 (8)	0.0194 (8)	-0.0002 (7)	0.0073 (7)	-0.0010 (7)
C8	0.0170 (8)	0.0187 (9)	0.0237 (9)	-0.0014 (7)	0.0094 (7)	-0.0001 (7)
C9	0.0205 (8)	0.0141 (8)	0.0251 (9)	-0.0024 (7)	0.0085 (7)	-0.0018 (7)
C10	0.0207 (8)	0.0176 (9)	0.0216 (9)	-0.0004 (7)	0.0068 (7)	-0.0006 (7)
C11	0.0166 (8)	0.0151 (8)	0.0250 (9)	0.0023 (7)	0.0056 (7)	-0.0012 (7)
C12	0.0210 (8)	0.0171 (9)	0.0257 (9)	-0.0017 (7)	0.0109 (7)	-0.0003 (7)
C13	0.0204 (8)	0.0158 (8)	0.0246 (9)	-0.0007 (7)	0.0087 (7)	0.0000 (7)
C14	0.0198 (8)	0.0145 (8)	0.0212 (8)	-0.0002 (7)	0.0071 (7)	0.0010 (7)
C15	0.0209 (8)	0.0151 (8)	0.0284 (9)	0.0016 (7)	0.0110 (8)	-0.0020 (7)
C16	0.0171 (8)	0.0155 (8)	0.0210 (8)	0.0022 (7)	0.0065 (7)	0.0003 (7)
C17	0.0208 (8)	0.0166 (9)	0.0248 (9)	-0.0003 (7)	0.0117 (7)	-0.0043 (7)
C18	0.0180 (8)	0.0143 (8)	0.0259 (9)	-0.0016 (7)	0.0064 (7)	0.0004 (7)
C19	0.0194 (8)	0.0239 (10)	0.0292 (10)	-0.0010 (7)	0.0120 (8)	0.0022 (8)
C20	0.0203 (9)	0.0246 (10)	0.0375 (11)	-0.0010 (8)	0.0160 (8)	0.0029 (8)
C21	0.0267 (9)	0.0192 (9)	0.0315 (10)	0.0013 (8)	0.0132 (8)	0.0011 (8)
C22	0.0237 (9)	0.0188 (9)	0.0324 (10)	0.0022 (7)	0.0132 (8)	0.0009 (8)

Geometric parameters (\AA , $^\circ$)

O1—C2	1.245 (2)	C9—H9	0.9500
O2—C5	1.243 (2)	C10—C12	1.366 (2)

C1—C9	1.396 (2)	C10—H10	0.9500
C1—C15	1.401 (2)	C11—C14	1.385 (2)
C1—C7	1.482 (2)	C11—H11	0.9500
C2—C8	1.440 (2)	C12—H12	0.9500
C2—C3	1.506 (2)	C13—H13	0.9500
N1—C10	1.331 (2)	C14—H14	0.9500
N1—C19	1.455 (2)	C15—C18	1.385 (2)
N1—C21	1.458 (2)	C15—H15	0.9500
N2—C13	1.329 (2)	C16—H16	0.9500
N2—C22	1.455 (2)	C17—H17	0.9500
N2—C20	1.455 (2)	C18—H18	0.9500
C3—C14	1.395 (2)	C19—H19	0.9800
C3—C16	1.396 (2)	C19—H19A	0.9800
C4—C18	1.395 (2)	C19—H19B	0.9800
C4—C17	1.397 (2)	C20—H20	0.9800
C4—C5	1.511 (2)	C20—H20A	0.9800
C5—C12	1.443 (2)	C20—H20B	0.9800
C6—C16	1.386 (2)	C21—H21	0.9800
C6—C7	1.399 (2)	C21—H21A	0.9800
C6—H6	0.9500	C21—H21B	0.9800
C7—C11	1.400 (2)	C22—H22	0.9800
C8—C13	1.364 (2)	C22—H22A	0.9800
C8—H8	0.9500	C22—H22B	0.9800
C9—C17	1.390 (2)		
C9—C1—C15	117.55 (15)	N2—C13—C8	129.23 (17)
C9—C1—C7	122.00 (16)	N2—C13—H13	115.4
C15—C1—C7	120.45 (15)	C8—C13—H13	115.4
O1—C2—C8	123.86 (15)	C11—C14—C3	120.76 (16)
O1—C2—C3	118.00 (15)	C11—C14—H14	119.6
C8—C2—C3	118.14 (15)	C3—C14—H14	119.6
C10—N1—C19	121.53 (15)	C18—C15—C1	121.12 (16)
C10—N1—C21	122.76 (15)	C18—C15—H15	119.4
C19—N1—C21	115.68 (14)	C1—C15—H15	119.4
C13—N2—C22	123.09 (15)	C6—C16—C3	120.76 (16)
C13—N2—C20	121.23 (15)	C6—C16—H16	119.6
C22—N2—C20	115.68 (15)	C3—C16—H16	119.6
C14—C3—C16	118.36 (15)	C9—C17—C4	120.82 (16)
C14—C3—C2	118.40 (15)	C9—C17—H17	119.6
C16—C3—C2	123.21 (15)	C4—C17—H17	119.6
C18—C4—C17	117.95 (15)	C15—C18—C4	121.20 (16)
C18—C4—C5	117.96 (16)	C15—C18—H18	119.4
C17—C4—C5	124.09 (15)	C4—C18—H18	119.4
O2—C5—C12	123.49 (16)	N1—C19—H19	109.5
O2—C5—C4	117.97 (16)	N1—C19—H19A	109.5
C12—C5—C4	118.50 (15)	H19—C19—H19A	109.5
C16—C6—C7	121.20 (16)	N1—C19—H19B	109.5
C16—C6—H6	119.4	H19—C19—H19B	109.5

C7—C6—H6	119.4	H19A—C19—H19B	109.5
C6—C7—C11	117.64 (15)	N2—C20—H20	109.5
C6—C7—C1	121.32 (15)	N2—C20—H20A	109.5
C11—C7—C1	121.04 (15)	H20—C20—H20A	109.5
C13—C8—C2	118.39 (16)	N2—C20—H20B	109.5
C13—C8—H8	120.8	H20—C20—H20B	109.5
C2—C8—H8	120.8	H20A—C20—H20B	109.5
C17—C9—C1	121.34 (16)	N1—C21—H21	109.5
C17—C9—H9	119.3	N1—C21—H21A	109.5
C1—C9—H9	119.3	H21—C21—H21A	109.5
N1—C10—C12	128.94 (17)	N1—C21—H21B	109.5
N1—C10—H10	115.5	H21—C21—H21B	109.5
C12—C10—H10	115.5	H21A—C21—H21B	109.5
C14—C11—C7	121.23 (16)	N2—C22—H22	109.5
C14—C11—H11	119.4	N2—C22—H22A	109.5
C7—C11—H11	119.4	H22—C22—H22A	109.5
C10—C12—C5	118.29 (16)	N2—C22—H22B	109.5
C10—C12—H12	120.9	H22—C22—H22B	109.5
C5—C12—H12	120.9	H22A—C22—H22B	109.5
O1—C2—C3—C14	19.5 (2)	C1—C7—C11—C14	178.24 (16)
C8—C2—C3—C14	-161.06 (16)	N1—C10—C12—C5	-175.95 (17)
O1—C2—C3—C16	-158.78 (17)	O2—C5—C12—C10	4.7 (3)
C8—C2—C3—C16	20.7 (3)	C4—C5—C12—C10	-177.69 (16)
C18—C4—C5—O2	7.3 (2)	C22—N2—C13—C8	-4.7 (3)
C17—C4—C5—O2	-173.35 (18)	C20—N2—C13—C8	175.17 (19)
C18—C4—C5—C12	-170.47 (16)	C2—C8—C13—N2	179.18 (18)
C17—C4—C5—C12	8.9 (3)	C7—C11—C14—C3	1.0 (3)
C16—C6—C7—C11	0.2 (3)	C16—C3—C14—C11	0.9 (3)
C16—C6—C7—C1	-179.64 (16)	C2—C3—C14—C11	-177.45 (16)
C9—C1—C7—C6	149.01 (17)	C9—C1—C15—C18	-0.7 (3)
C15—C1—C7—C6	-30.9 (3)	C7—C1—C15—C18	179.29 (16)
C9—C1—C7—C11	-30.8 (3)	C7—C6—C16—C3	1.8 (3)
C15—C1—C7—C11	149.25 (18)	C14—C3—C16—C6	-2.3 (3)
O1—C2—C8—C13	-3.7 (3)	C2—C3—C16—C6	175.97 (16)
C3—C2—C8—C13	176.87 (16)	C1—C9—C17—C4	1.4 (3)
C15—C1—C9—C17	-0.9 (3)	C18—C4—C17—C9	-0.4 (3)
C7—C1—C9—C17	179.15 (16)	C5—C4—C17—C9	-179.73 (16)
C19—N1—C10—C12	-174.60 (18)	C1—C15—C18—C4	1.7 (3)
C21—N1—C10—C12	3.2 (3)	C17—C4—C18—C15	-1.2 (3)
C6—C7—C11—C14	-1.6 (3)	C5—C4—C18—C15	178.21 (16)

Hydrogen-bond geometry (\AA , $^\circ$)

Cg1 and Cg2 are the centroids of the C1/C9/C17/C4/C18/C15 and C3/C14/C11/C7/C6/C16 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C21—H21B \cdots O2 ⁱ	0.98	2.51	3.410 (2)	152
C22—H22 \cdots O1 ⁱⁱ	0.98	2.48	3.387 (2)	154

C21—H21…Cg2 ⁱⁱⁱ	0.98	2.60	3.538 (2)	160
C22—H22B…Cg1 ^{iv}	0.98	2.70	3.608 (2)	154

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