



Keywords: crystal structure; gossypol; bis-*p*-anizidinegossypol; porous structure

CCDC reference: 1433643

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Crystal structure of bis-*p*-anizidinegossypol with an unknown solvate

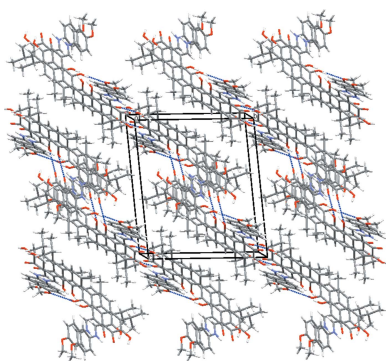
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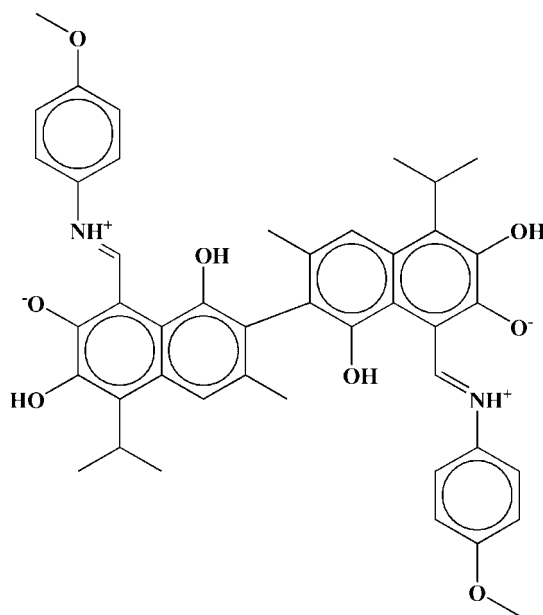
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The title compound, C₄₄H₄₄N₂O₈, (systematic name: 1,1',6,6'-tetrahydroxy-5,5'-diisopropyl-8,8'-bis[[[4-methoxyphenyl]iminiumyl]methyl]-3,3'-dimethyl-2,2'-binaphthalene-7,7'-diolate) has been obtained by the addition of *p*-anizidine to gossypol dissolved in dichloromethane. In the solid state, the title compound exists in the enamine or quinoid form. The two naphthyl moieties are inclined to one another by 72.08 (5)°. The pendant phenyl rings are inclined at 22.26 (14) and 23.86 (13)° to the corresponding naphthyl rings. In the crystal, molecules are incorporated into layers through inversion-related pairs of O—H...O interactions [graph sets *R*₂²(20) and *R*₂²(10)] and translation-related O—H...O interactions [graph set *C*(15)]. The packing of these layers in the crystal structure gives rise to channels in the [011] direction, with hydrophobic interactions occurring between adjacent layers. The channels are 5–7 Å wide, and the void volume of each cell is 655 Å³, corresponding to 26.6% of the cell volume. Disordered guest molecules, probably solvent and water molecules, occupy these voids of the crystal; their contribution to the scattering was removed with the SQUEEZE routine [Spek (2015)]. *Acta Cryst. C* **71**, 9–18] of *PLATON* [Spek (2009)]. *Acta Cryst. D* **65**, 148–155].

1. Chemical context

Gossypol [2,2'-bis(8-formyl-1,6,7-trihydroxy-5-isopropyl-3-methylnaphthalene)] is a yellow pigment of cotton seeds (Adams *et al.*, 1960). This compound was first isolated over 110 years ago (Marchlewski, 1899). Its study was initially important because the compound is associated with anti-nutritive or even toxic effects when cottonseed is overfed to animals. Many attempts have been made to either remove it from cottonseed or reduce its toxicity (Kenar, 2006). However, the compound also has a wide range of biological action, including anti-HIV (Jian Yang *et al.*, 2014), anticancer (Zhan *et al.*, 2009) and antifertility (Coutinho, 2002) effects. This interest has led to the synthesis and isolation of various gossypol derivatives, including many diamine-based gossypol Schiff bases. Gossypol and its Schiff base formed with aniline have been previously reported to form inclusion compounds with many small organic compounds (Beketov *et al.*, 1994; Gdaniec *et al.*, 1996; Talipov *et al.*, 2004). Some gossypol polymorphs (referred to as the P3 polymorph; Ibragimov *et al.*, 1994), dianhydrogossypol (Talipov *et al.*, 2009) and gossypol tetramethyl ether (Honkeldieva *et al.*, 2015) form open-channel structures with channels of 5–8 Å width. In this report, we demonstrate that the Schiff base of gossypol with *p*-anizidine also forms an open-channel structure when the compound is crystallized from solutions in dichloromethane.





2. Structural commentary

Gossypol can exist in one of the following tautomeric forms: aldehyde, quinoid and lactol (Adams *et al.*, 1960). In most solvents it is found in the aldehyde form; however, there are some reports that gossypol also exists in a pure lactol form (Reyes *et al.*, 1986) or as a dynamic equilibrium mixture of aldehyde and lactol forms in some highly polar solvents (Kamaev *et al.*, 1979). In the structure described here, the title compound is in the enamine or quinoid form. The highest symmetry which the title compound molecule can possess is C_2 (twofold axis perpendicular to the C2–C12 bond). However, bis-*p*-anizidinegossypol crystallizes in a triclinic ($P\bar{1}$) space group and the symmetry of the molecule is not retained in the crystal. An *ORTEP* diagram of the molecule and the atom numbering in the structure are given in Fig. 1.

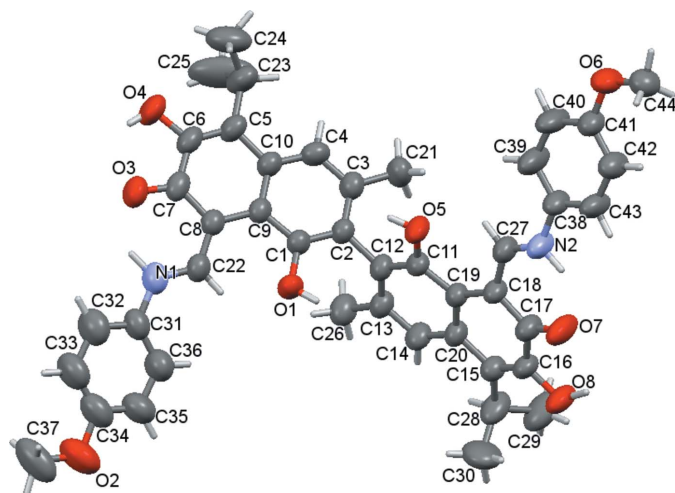


Figure 1
Molecular structure of the title compound showing 50% probability displacement ellipsoids.

Table 1
Hydrogen-bond geometry (\AA , $^\circ$).

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1–H1A \cdots O3	0.95 (5)	1.83 (5)	2.538 (4)	129 (4)
N2–H2 \cdots O7	0.92 (3)	1.87 (3)	2.550 (3)	129 (3)
O1–H1 \cdots O6 ⁱ	0.91 (4)	2.13 (4)	2.912 (3)	144 (3)
O4–H4 \cdots O3	0.86 (3)	2.04 (4)	2.574 (4)	119 (3)
O5–H5 \cdots O3 ⁱⁱ	0.82 (3)	1.98 (3)	2.684 (3)	143 (3)
O8–H8 \cdots O7	0.98 (3)	2.17 (3)	2.601 (3)	105 (2)
O8–H8 \cdots O7 ⁱⁱⁱ	0.98 (3)	1.83 (3)	2.757 (3)	158 (3)

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

The molecule consists of four ring systems, two of which are naphthalene ring systems, and the other two are phenyl rings. The C1–C10 naphthyl unit is more planar than C11–C20 naphthyl one in which atoms C12, C16, C17, C18 and C19 deviate by 0.051 (3), 0.070 (3), 0.059 (3), 0.082 (3) and 0.054 (3) \AA , respectively, from the mean plane. The two naphthyl moieties are inclined to one another by 72.08 (5) $^\circ$. The phenyl rings are inclined at 22.26 (14) and 23.86 (13) $^\circ$ to the corresponding naphthyl rings. The bond lengths and angles are mostly in good agreement with those observed in the analogous fragments of the gossypol and dianilinegossypol molecules (Gdaniec *et al.*, 1996; Talipov *et al.*, 2004). However, there are notable differences in the lengths of some bonds compared with typical gossypol values. Compared with the relatively short C6–C7 (C16–C17) aromatic ring bonds of gossypol molecules (1.40 \AA), the corresponding bonds in the bis-*p*-anizidinegossypol molecule are longer with lengths of 1.446 (4) and 1.476 (4) \AA . In addition, the N1–C22 [1.332 (4) \AA] and N2–C27 [1.319 (4) \AA] bonds are shorter than N1–C31 [1.433 (4) \AA] and N2–C38 [1.441 (4) \AA], respectively. Contrarily, C7=O3 [1.289 (3) \AA] and C17=O7 [1.275 (3) \AA] bonds are longer than typical standard values.

There are two intramolecular hydrogen bonds in the molecule. The N1–H1A \cdots O3 (and N2–H2 \cdots O7) bond closes a six-membered ring C7–C8–C22–N1–H1A \cdots O3 (and C17–C18–C27–N2–H3 \cdots O7), while the other type of hydrogen bond O4–H4 \cdots O3 (and O8–H8 \cdots O7) forms a five-membered ring C6–C7–O3 \cdots H4–O4 (and C16–C17–O7 \cdots H8–O8) (Table 1).

3. Supramolecular features

The packing of the title molecules in the crystal is shown in Fig. 2. Bis-*p*-anizidinegossypol molecules are incorporated into centrosymmetric dimers typical for gossypol and dianilinegossypol crystal structures by means of a pair of inversion-related hydrogen bonds O5–H5 \cdots O3 [graph set $R_2^2(20)$]. By further centrosymmetric O8–H8 \cdots O7 hydrogen bonds [graph set $R_2^2(10)$], molecules are associated into columns running in the $[1\bar{1}\bar{1}]$ direction, as also seen for the dianilinegossypol clathrate with ethylacetate (Beketov *et al.*, 1994). A layer parallel to $(01\bar{1})$ is formed by linking of the columns *via* translation-related hydrogen bonds O1–H1 \cdots O6 [graph set $C_1^1(15)$] in the $[100]$ direction. The layer features a

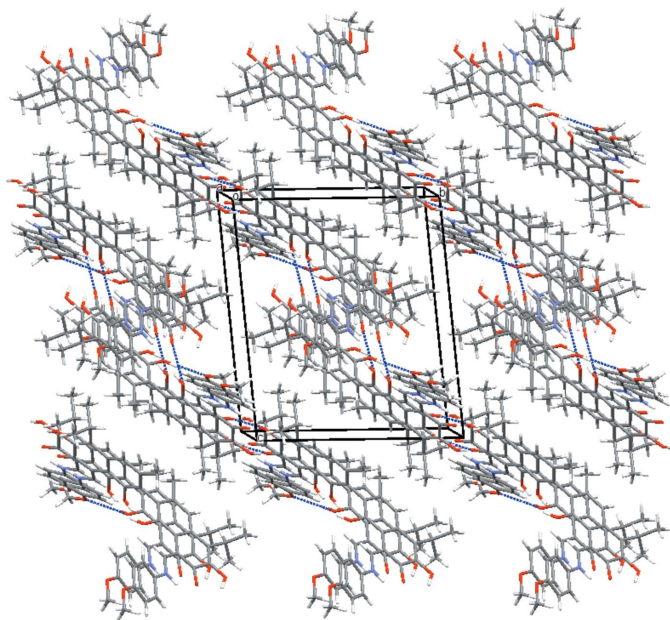


Figure 2
A portion of the crystal packing viewed approximately along the *a* axis.

$O2 \cdots C7(-1-x, 1-y, 1-z)$ contact [3.254 (4) Å] and a very weak aromatic π - π stacking interaction with a $Cg \cdots Cg(-1-x, 1-y, 1-z)$ distance of 4.182 (2) Å where *Cg* is the centroid of the C31–C36 ring. The packing of these layers in the crystal structure gives rise to wide ragged channels in the [011] direction. The stabilization of the crystal structure is supported by hydrophobic interactions between adjacent layers. The channels in the structure are 5–7 Å wide and the void volume of each cell is 655 Å³, corresponding to 26.6% of the cell volume. Disordered solvated molecules, probably solvent and water molecules, occupy these voids of the crystal; their contribution to the scattering was removed with the SQUEEZE routine (Spek, 2015) of *PLATON* (Spek, 2009).

4. Database survey

A search in the Cambridge Structural Database (Version 5.36; Groom & Allen, 2014) indicated the presence of 198 entries for gossypol (137 entries) or gossypol derivatives. The 35 entries of revealed 50 entries for Schiff-base gossypol derivatives are related to dianilinegossypol clathrates and polymorphs. The dihedral angle between the naphthalene ring systems in the dianilinegossypol structures is in the range 78 to 90°. The dihedral angles between naphthalene ring systems and the corresponding benzyl rings of aniline substituents are in the range 4–49°. The dihedral angles between the naphthalene ring systems in the crystal structures of other Schiff base gossypol derivatives are in the range from *ca* 70 to 90°: IGAVAQ = 86.6°, LUHBIA = 89.6°, LUHBOG = 77.9°, MEXROY = 89.2°, MEXROY01 = 88.9°, NOQFIJ = 83.5°, POGHUF = 84.6°, QADQIX = 89.1°, SACXEB = 82.2°, TEFFEP = 70.6° and 83.4°, TIJNUX = 89.0°, XATPAK =

Table 2
Experimental details.

Crystal data	
Chemical formula	C ₄₄ H ₄₄ N ₂ O ₈
<i>M_r</i>	728.81
Crystal system, space group	Triclinic, <i>P</i> $\bar{1}$
Temperature (K)	293
<i>a</i> , <i>b</i> , <i>c</i> (Å)	11.6622 (9), 14.0738 (11), 15.6906 (10)
α , β , γ (°)	82.472 (6), 84.831 (6), 75.009 (7)
<i>V</i> (Å ³)	2462.0 (3)
<i>Z</i>	2
Radiation type	Cu <i>K</i> α
μ (mm ⁻¹)	0.55
Crystal size (mm)	0.40 × 0.32 × 0.27
Data collection	
Diffractometer	Oxford Diffraction Xcalibur Ruby
Absorption correction	Multi-scan (<i>CrysAlis PRO</i> ; Oxford Diffraction, 2009)
<i>T_{min}</i> , <i>T_{max}</i>	0.811, 0.862
No. of measured, independent and observed [<i>I</i> > 2 σ (<i>I</i>)] reflections	18952, 9019, 2706
<i>R_{int}</i>	0.048
($\sin \theta/\lambda$) _{max} (Å ⁻¹)	0.612
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, <i>S</i>	0.051, 0.124, 0.65
No. of reflections	9019
No. of parameters	519
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å ⁻³)	0.13, -0.17

Computer programs: *CrysAlis PRO* (Oxford Diffraction, 2009), *SHELXS97* and *SHELXL97* (Sheldrick, 2008) and *OLEX2* (Dolomanov *et al.*, 2009).

78.6°, VUXRIQ = 70.3°, VUXRIQ01 = 88.2° and 91.0° and YORNIW = 81.2°.

5. Synthesis and crystallization

Gossypol was obtained from the Experimental Plant of the Institute of Bioorganic Chemistry, Uzbekistan Academy of Sciences where it is produced from by-products of the cottonseed oil industry. To prepare the Schiff base complex, gossypol was mixed with *p*-anizidine in a 1:2 molar ratio in dichloromethane. This reaction solution was allowed to stand in the dark for some days, during which crystalline precipitates have been formed within the solution. The precipitate was recovered by filtration. Yield: 64%. After numerous attempts, a suitable crystal was selected from the precipitate and used for the diffraction study without additional recrystallization.

6. Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2. The H atom of the hydroxy substituent was located in an electron density map and its coordinates were freely refined with $U_{iso} = 1.5U_{eq}(O)$. C-bound H atoms were positioned geometrically and refined using a riding model, with $d(C-H) = 0.93$ Å and $U_{iso} =$

$1.2U_{\text{eq}}(\text{C})$ for aromatic, $d(\text{C}-\text{H}) = 0.98 \text{ \AA}$ and $U_{\text{iso}} = 1.2U_{\text{eq}}(\text{C})$ for methine, $d(\text{C}-\text{H}) = 0.96 \text{ \AA}$ and $U_{\text{iso}} = 1.5U_{\text{eq}}(\text{C})$ for methyl H atoms.

Acknowledgements

Investigations were supported by research grants F7-T048 from Uzbek National Science Foundation.

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supporting information

Acta Cryst. (2015). E71, 1421-1424 [https://doi.org/10.1107/S2056989015020393]

Crystal structure of bis-*p*-anizidinegossypol with an unknown solvate

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Computing details

Data collection: *CrysAlis PRO* (Oxford Diffraction, 2009); cell refinement: *CrysAlis PRO* (Oxford Diffraction, 2009); data reduction: *CrysAlis PRO* (Oxford Diffraction, 2009); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *OLEX2* (Dolomanov *et al.*, 2009); software used to prepare material for publication: *OLEX2* (Dolomanov *et al.*, 2009).

1,1',6,6'-Tetrahydroxy-5,5'-diisopropyl-8,8'-bis[[4-methoxyphenyl]iminiumyl]methyl}-3,3'-dimethyl-2,2'-binaphthalene-7,7'-diolate

Crystal data

$C_{44}H_{44}N_2O_8$

$M_r = 728.81$

Triclinic, $P\bar{1}$

$a = 11.6622$ (9) Å

$b = 14.0738$ (11) Å

$c = 15.6906$ (10) Å

$\alpha = 82.472$ (6)°

$\beta = 84.831$ (6)°

$\gamma = 75.009$ (7)°

$V = 2462.0$ (3) Å³

$Z = 2$

$F(000) = 772$

$D_x = 0.983$ Mg m⁻³

Cu $K\alpha$ radiation, $\lambda = 1.54184$ Å

Cell parameters from 2564 reflections

$\theta = 3.9\text{--}70.6^\circ$

$\mu = 0.55$ mm⁻¹

$T = 293$ K

Prism, brown

$0.40 \times 0.32 \times 0.27$ mm

Data collection

Oxford Diffraction Xcalibur Ruby diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 10.2576 pixels mm⁻¹

ω scans

Absorption correction: multi-scan

(*CrysAlis PRO*; Oxford Diffraction, 2009)

$T_{\min} = 0.811$, $T_{\max} = 0.862$

18952 measured reflections

9019 independent reflections

2706 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.048$

$\theta_{\max} = 70.6^\circ$, $\theta_{\min} = 3.9^\circ$

$h = -14 \rightarrow 13$

$k = -16 \rightarrow 16$

$l = -18 \rightarrow 16$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.051$

$wR(F^2) = 0.124$

$S = 0.65$

9019 reflections

519 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

H atoms treated by a mixture of independent and constrained refinement

$$w = 1/[\sigma^2(F_o^2) + (0.0542P)^2]$$

where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} < 0.001$

$$\Delta\rho_{\max} = 0.13 \text{ e } \text{\AA}^{-3}$$

$$\Delta\rho_{\min} = -0.17 \text{ e } \text{\AA}^{-3}$$

Special details

Experimental. Absorption correction: CrysAlisPro, Oxford Diffraction (2009), Empirical absorption correction using spherical harmonics, implemented in SCALE3 ABSPACK scaling algorithm.

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)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-0.06997 (18)	0.40724 (17)	0.33397 (13)	0.0668 (6)
O2	-0.6101 (2)	0.2359 (2)	0.58343 (19)	0.1250 (10)
O3	-0.23580 (18)	0.62089 (16)	0.58330 (12)	0.0774 (6)
O4	-0.1425 (2)	0.7699 (2)	0.55783 (17)	0.0923 (8)
O5	0.27695 (17)	0.35008 (18)	0.24986 (14)	0.0741 (7)
O6	0.97592 (18)	0.21416 (17)	0.27160 (14)	0.0886 (7)
O7	0.46897 (19)	0.06734 (18)	0.07019 (15)	0.1002 (9)
O8	0.3149 (2)	0.06336 (18)	-0.03842 (14)	0.0887 (8)
N1	-0.2902 (2)	0.4750 (2)	0.53257 (17)	0.0736 (8)
N2	0.5550 (2)	0.1627 (2)	0.16491 (18)	0.0824 (9)
C1	-0.0203 (2)	0.4872 (2)	0.32283 (17)	0.0543 (7)
C2	0.0593 (2)	0.4959 (2)	0.25382 (17)	0.0546 (8)
C3	0.1135 (3)	0.5752 (2)	0.24359 (18)	0.0657 (9)
C4	0.0827 (3)	0.6422 (2)	0.30335 (19)	0.0677 (9)
H4A	0.1188	0.6946	0.2968	0.081*
C5	-0.0267 (3)	0.7112 (2)	0.43314 (19)	0.0680 (9)
C6	-0.1066 (3)	0.7018 (2)	0.4998 (2)	0.0681 (9)
C7	-0.1641 (3)	0.6211 (2)	0.51583 (18)	0.0627 (9)
C8	-0.1427 (2)	0.5498 (2)	0.45576 (17)	0.0570 (8)
C9	-0.0561 (2)	0.5568 (2)	0.38381 (17)	0.0537 (8)
C10	0.0002 (2)	0.6367 (2)	0.37361 (18)	0.0600 (8)
C11	0.1982 (2)	0.3535 (2)	0.18905 (16)	0.0563 (8)
C12	0.0890 (2)	0.4206 (2)	0.19037 (17)	0.0587 (8)
C13	0.0074 (2)	0.4204 (2)	0.12890 (17)	0.0615 (8)
C14	0.0405 (3)	0.3496 (2)	0.07254 (17)	0.0688 (9)
H14	-0.0149	0.3470	0.0344	0.083*
C15	0.1802 (2)	0.2079 (2)	0.00811 (18)	0.0623 (8)
C16	0.2827 (3)	0.1384 (2)	0.01332 (18)	0.0677 (9)
C17	0.3742 (3)	0.1370 (3)	0.07291 (19)	0.0730 (10)
C18	0.3505 (2)	0.2143 (2)	0.12572 (17)	0.0601 (8)

C19	0.2357 (2)	0.2845 (2)	0.12808 (17)	0.0571 (8)
C20	0.1511 (2)	0.2814 (2)	0.06846 (17)	0.0591 (8)
C21	0.1981 (3)	0.5900 (2)	0.16700 (19)	0.0862 (11)
H21A	0.2164	0.6529	0.1662	0.129*
H21B	0.1616	0.5886	0.1149	0.129*
H21C	0.2700	0.5381	0.1713	0.129*
C22	-0.2114 (3)	0.4812 (2)	0.46653 (19)	0.0642 (8)
H22	-0.2017	0.4374	0.4254	0.077*
C23	0.0276 (4)	0.7993 (3)	0.4206 (2)	0.0993 (13)
H23	0.0914	0.7849	0.3755	0.119*
C24	0.0868 (4)	0.8144 (3)	0.4976 (3)	0.1269 (15)
H24A	0.1543	0.8405	0.4785	0.190*
H24B	0.1126	0.7522	0.5323	0.190*
H24C	0.0313	0.8601	0.5312	0.190*
C25	-0.0552 (5)	0.8930 (4)	0.3869 (3)	0.192 (3)
H25A	-0.0664	0.8912	0.3274	0.288*
H25B	-0.0226	0.9478	0.3925	0.288*
H25C	-0.1304	0.9008	0.4192	0.288*
C26	-0.1129 (3)	0.4922 (2)	0.12655 (19)	0.0819 (10)
H26A	-0.1553	0.4803	0.0810	0.123*
H26B	-0.1035	0.5586	0.1166	0.123*
H26C	-0.1567	0.4836	0.1806	0.123*
C27	0.4492 (3)	0.2255 (2)	0.16703 (18)	0.0742 (10)
H27	0.4385	0.2801	0.1972	0.089*
C28	0.0952 (3)	0.2073 (3)	-0.0607 (2)	0.0935 (13)
H28	0.0313	0.2681	-0.0592	0.112*
C29	0.1528 (3)	0.2089 (3)	-0.1511 (2)	0.1217 (16)
H29A	0.1918	0.2619	-0.1618	0.183*
H29B	0.0930	0.2187	-0.1919	0.183*
H29C	0.2101	0.1471	-0.1571	0.183*
C30	0.0377 (4)	0.1211 (4)	-0.0378 (3)	0.1432 (19)
H30A	-0.0126	0.1310	0.0138	0.215*
H30B	0.0985	0.0606	-0.0287	0.215*
H30C	-0.0089	0.1174	-0.0841	0.215*
C31	-0.3701 (3)	0.4116 (3)	0.5449 (2)	0.0736 (9)
C32	-0.4309 (3)	0.4051 (3)	0.6236 (2)	0.1032 (13)
H32	-0.4178	0.4399	0.6668	0.124*
C33	-0.5130 (3)	0.3461 (3)	0.6395 (3)	0.1062 (13)
H33	-0.5537	0.3408	0.6930	0.127*
C34	-0.5315 (3)	0.2971 (3)	0.5753 (3)	0.0971 (12)
C35	-0.4745 (3)	0.3059 (3)	0.4958 (3)	0.1026 (12)
H35	-0.4903	0.2730	0.4523	0.123*
C36	-0.3941 (3)	0.3627 (3)	0.4797 (2)	0.0961 (12)
H36	-0.3558	0.3686	0.4254	0.115*
C37	-0.6735 (3)	0.2272 (4)	0.6640 (3)	0.1379 (18)
H37A	-0.7292	0.1883	0.6609	0.207*
H37B	-0.7155	0.2919	0.6782	0.207*
H37C	-0.6188	0.1956	0.7074	0.207*

C38	0.6624 (3)	0.1761 (3)	0.1948 (2)	0.0750 (10)
C39	0.6640 (3)	0.2563 (3)	0.2352 (2)	0.1141 (15)
H39	0.5938	0.3032	0.2470	0.137*
C40	0.7716 (3)	0.2665 (3)	0.2581 (2)	0.1103 (14)
H40	0.7740	0.3230	0.2821	0.132*
C41	0.8741 (3)	0.1953 (3)	0.24610 (19)	0.0739 (10)
C42	0.8717 (3)	0.1150 (3)	0.2073 (2)	0.0886 (11)
H42	0.9415	0.0669	0.1976	0.106*
C43	0.7637 (3)	0.1053 (3)	0.1821 (2)	0.0935 (12)
H43	0.7616	0.0499	0.1565	0.112*
C44	1.0825 (3)	0.1378 (2)	0.2661 (2)	0.0842 (10)
H44A	1.1459	0.1576	0.2882	0.126*
H44B	1.1024	0.1261	0.2070	0.126*
H44C	1.0713	0.0783	0.2993	0.126*
H1A	-0.302 (4)	0.518 (4)	0.577 (3)	0.20 (2)*
H2	0.571 (3)	0.109 (2)	0.1344 (19)	0.095 (11)*
H1	-0.023 (3)	0.352 (3)	0.313 (2)	0.133 (16)*
H4	-0.184 (3)	0.745 (3)	0.598 (2)	0.122 (18)*
H5	0.243 (2)	0.381 (2)	0.2898 (17)	0.071 (10)*
H8	0.397 (3)	0.023 (3)	-0.037 (2)	0.124 (14)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0682 (13)	0.0589 (16)	0.0781 (14)	-0.0206 (12)	0.0069 (11)	-0.0238 (12)
O2	0.099 (2)	0.146 (3)	0.140 (3)	-0.063 (2)	-0.0104 (18)	0.017 (2)
O3	0.0750 (14)	0.0936 (19)	0.0625 (13)	-0.0130 (12)	0.0044 (11)	-0.0264 (12)
O4	0.0997 (19)	0.099 (2)	0.0850 (18)	-0.0209 (16)	0.0106 (15)	-0.0536 (16)
O5	0.0574 (13)	0.0986 (19)	0.0710 (14)	-0.0096 (12)	-0.0063 (11)	-0.0454 (14)
O6	0.0646 (14)	0.0966 (19)	0.1167 (18)	-0.0211 (14)	-0.0188 (13)	-0.0442 (15)
O7	0.0664 (14)	0.106 (2)	0.130 (2)	0.0146 (14)	-0.0295 (13)	-0.0754 (16)
O8	0.0720 (15)	0.0960 (19)	0.1022 (17)	0.0015 (14)	-0.0224 (13)	-0.0600 (15)
N1	0.0690 (18)	0.085 (2)	0.0626 (18)	-0.0132 (16)	0.0030 (15)	-0.0088 (16)
N2	0.0558 (17)	0.091 (2)	0.106 (2)	-0.0032 (16)	-0.0107 (14)	-0.0588 (19)
C1	0.0517 (17)	0.050 (2)	0.0596 (19)	-0.0086 (15)	-0.0007 (15)	-0.0118 (15)
C2	0.0550 (17)	0.055 (2)	0.0539 (18)	-0.0107 (16)	0.0007 (15)	-0.0152 (15)
C3	0.0634 (19)	0.074 (2)	0.0596 (19)	-0.0141 (18)	0.0024 (15)	-0.0169 (17)
C4	0.072 (2)	0.056 (2)	0.080 (2)	-0.0191 (17)	-0.0099 (18)	-0.0172 (18)
C5	0.083 (2)	0.063 (2)	0.061 (2)	-0.0160 (18)	-0.0017 (17)	-0.0223 (17)
C6	0.067 (2)	0.070 (2)	0.067 (2)	-0.0036 (18)	-0.0080 (17)	-0.0309 (18)
C7	0.0558 (19)	0.068 (2)	0.056 (2)	0.0051 (17)	-0.0085 (16)	-0.0172 (17)
C8	0.0521 (17)	0.060 (2)	0.0576 (18)	-0.0088 (16)	-0.0031 (15)	-0.0136 (16)
C9	0.0474 (16)	0.054 (2)	0.0570 (18)	-0.0038 (15)	-0.0039 (14)	-0.0151 (15)
C10	0.0609 (19)	0.057 (2)	0.063 (2)	-0.0113 (16)	-0.0017 (16)	-0.0186 (16)
C11	0.0543 (18)	0.067 (2)	0.0513 (17)	-0.0173 (16)	0.0010 (14)	-0.0202 (15)
C12	0.0559 (19)	0.065 (2)	0.0545 (18)	-0.0082 (16)	0.0002 (15)	-0.0191 (16)
C13	0.0612 (19)	0.061 (2)	0.0595 (18)	-0.0050 (16)	-0.0022 (15)	-0.0184 (16)
C14	0.064 (2)	0.085 (3)	0.0593 (19)	-0.0121 (18)	-0.0081 (15)	-0.0252 (18)

C15	0.0551 (18)	0.066 (2)	0.067 (2)	-0.0084 (17)	-0.0084 (15)	-0.0228 (17)
C16	0.062 (2)	0.074 (2)	0.074 (2)	-0.0143 (18)	-0.0047 (16)	-0.0385 (18)
C17	0.061 (2)	0.080 (3)	0.082 (2)	-0.0069 (19)	-0.0089 (17)	-0.040 (2)
C18	0.0492 (17)	0.070 (2)	0.0641 (19)	-0.0088 (16)	-0.0069 (14)	-0.0295 (17)
C19	0.0486 (17)	0.066 (2)	0.0601 (18)	-0.0123 (15)	0.0012 (14)	-0.0242 (16)
C20	0.0532 (18)	0.064 (2)	0.0594 (18)	-0.0062 (16)	-0.0010 (14)	-0.0234 (16)
C21	0.086 (2)	0.088 (3)	0.090 (2)	-0.034 (2)	0.026 (2)	-0.028 (2)
C22	0.0582 (18)	0.066 (2)	0.066 (2)	-0.0066 (17)	0.0035 (16)	-0.0186 (16)
C23	0.133 (3)	0.092 (3)	0.091 (3)	-0.053 (3)	0.019 (2)	-0.043 (2)
C24	0.125 (3)	0.111 (4)	0.168 (4)	-0.061 (3)	-0.048 (3)	-0.013 (3)
C25	0.273 (7)	0.104 (4)	0.234 (6)	-0.104 (5)	-0.152 (5)	0.065 (4)
C26	0.068 (2)	0.094 (3)	0.079 (2)	-0.0016 (19)	-0.0089 (17)	-0.026 (2)
C27	0.058 (2)	0.083 (3)	0.085 (2)	-0.0089 (18)	-0.0003 (17)	-0.0433 (19)
C28	0.076 (2)	0.118 (3)	0.086 (3)	0.005 (2)	-0.026 (2)	-0.052 (2)
C29	0.148 (4)	0.126 (4)	0.082 (3)	0.007 (3)	-0.035 (3)	-0.042 (2)
C30	0.101 (3)	0.199 (5)	0.166 (4)	-0.074 (3)	-0.020 (3)	-0.070 (4)
C31	0.060 (2)	0.085 (3)	0.073 (2)	-0.0167 (19)	0.0062 (18)	-0.0060 (19)
C32	0.099 (3)	0.129 (4)	0.080 (3)	-0.035 (3)	0.005 (2)	-0.002 (2)
C33	0.094 (3)	0.134 (4)	0.093 (3)	-0.046 (3)	0.010 (2)	0.006 (3)
C34	0.074 (2)	0.105 (4)	0.109 (3)	-0.032 (2)	0.002 (2)	0.012 (3)
C35	0.085 (3)	0.112 (4)	0.121 (3)	-0.045 (3)	0.003 (2)	-0.015 (3)
C36	0.086 (3)	0.114 (3)	0.094 (3)	-0.036 (2)	0.014 (2)	-0.025 (2)
C37	0.094 (3)	0.185 (5)	0.128 (4)	-0.057 (3)	-0.009 (3)	0.054 (3)
C38	0.0506 (18)	0.088 (3)	0.093 (2)	-0.0087 (18)	-0.0132 (16)	-0.047 (2)
C39	0.069 (2)	0.121 (3)	0.164 (4)	-0.003 (2)	-0.015 (2)	-0.097 (3)
C40	0.071 (2)	0.118 (3)	0.161 (4)	-0.016 (2)	-0.021 (2)	-0.088 (3)
C41	0.061 (2)	0.084 (3)	0.084 (2)	-0.0150 (19)	-0.0073 (17)	-0.037 (2)
C42	0.056 (2)	0.090 (3)	0.125 (3)	-0.0051 (19)	-0.0157 (19)	-0.051 (2)
C43	0.063 (2)	0.087 (3)	0.140 (3)	-0.007 (2)	-0.015 (2)	-0.068 (2)
C44	0.064 (2)	0.089 (3)	0.105 (3)	-0.020 (2)	-0.0120 (19)	-0.023 (2)

Geometric parameters (Å, °)

O1—C1	1.379 (3)	C21—H21B	0.9600
O1—H1	0.91 (4)	C21—H21C	0.9600
O2—C34	1.398 (4)	C22—H22	0.9300
O2—C37	1.413 (4)	C23—H23	0.9800
O3—C7	1.289 (3)	C23—C24	1.508 (4)
O4—C6	1.371 (3)	C23—C25	1.484 (5)
O4—H4	0.86 (3)	C24—H24A	0.9600
O5—C11	1.371 (3)	C24—H24B	0.9600
O5—H5	0.82 (3)	C24—H24C	0.9600
O6—C41	1.384 (3)	C25—H25A	0.9600
O6—C44	1.422 (3)	C25—H25B	0.9600
O7—C17	1.275 (3)	C25—H25C	0.9600
O8—C16	1.371 (3)	C26—H26A	0.9600
O8—H8	0.98 (3)	C26—H26B	0.9600
N1—C22	1.332 (4)	C26—H26C	0.9600

N1—C31	1.433 (4)	C27—H27	0.9300
N1—H1A	0.95 (5)	C28—H28	0.9800
N2—C27	1.319 (4)	C28—C29	1.514 (4)
N2—C38	1.441 (4)	C28—C30	1.521 (5)
N2—H2	0.92 (3)	C29—H29A	0.9600
C1—C2	1.376 (3)	C29—H29B	0.9600
C1—C9	1.417 (3)	C29—H29C	0.9600
C2—C3	1.403 (4)	C30—H30A	0.9600
C2—C12	1.502 (4)	C30—H30B	0.9600
C3—C4	1.376 (4)	C30—H30C	0.9600
C3—C21	1.513 (4)	C31—C32	1.373 (4)
C4—H4A	0.9300	C31—C36	1.391 (4)
C4—C10	1.404 (4)	C32—H32	0.9300
C5—C6	1.353 (4)	C32—C33	1.409 (5)
C5—C10	1.450 (4)	C33—H33	0.9300
C5—C23	1.516 (5)	C33—C34	1.354 (5)
C6—C7	1.446 (4)	C34—C35	1.367 (5)
C7—C8	1.426 (4)	C35—H35	0.9300
C8—C9	1.456 (4)	C35—C36	1.368 (5)
C8—C22	1.390 (4)	C36—H36	0.9300
C9—C10	1.428 (4)	C37—H37A	0.9600
C11—C12	1.376 (4)	C37—H37B	0.9600
C11—C19	1.414 (3)	C37—H37C	0.9600
C12—C13	1.415 (4)	C38—C39	1.369 (4)
C13—C14	1.376 (3)	C38—C43	1.353 (4)
C13—C26	1.502 (4)	C39—H39	0.9300
C14—H14	0.9300	C39—C40	1.383 (4)
C14—C20	1.397 (4)	C40—H40	0.9300
C15—C16	1.336 (4)	C40—C41	1.364 (4)
C15—C20	1.449 (3)	C41—C42	1.359 (4)
C15—C28	1.532 (4)	C42—H42	0.9300
C16—C17	1.476 (4)	C42—C43	1.398 (4)
C17—C18	1.409 (4)	C43—H43	0.9300
C18—C19	1.445 (4)	C44—H44A	0.9600
C18—C27	1.423 (4)	C44—H44B	0.9600
C19—C20	1.431 (4)	C44—H44C	0.9600
C21—H21A	0.9600		
C1—O1—H1	114 (2)	C23—C24—H24A	109.5
C34—O2—C37	116.4 (4)	C23—C24—H24B	109.5
C6—O4—H4	107 (3)	C23—C24—H24C	109.5
C11—O5—H5	110 (2)	H24A—C24—H24B	109.5
C41—O6—C44	116.8 (2)	H24A—C24—H24C	109.5
C16—O8—H8	117 (2)	H24B—C24—H24C	109.5
C22—N1—C31	126.7 (3)	C23—C25—H25A	109.5
C22—N1—H1A	121 (3)	C23—C25—H25B	109.5
C31—N1—H1A	112 (3)	C23—C25—H25C	109.5
C27—N2—C38	126.5 (3)	H25A—C25—H25B	109.5

C27—N2—H2	122 (2)	H25A—C25—H25C	109.5
C38—N2—H2	111 (2)	H25B—C25—H25C	109.5
O1—C1—C9	117.2 (3)	C13—C26—H26A	109.5
C2—C1—O1	119.0 (2)	C13—C26—H26B	109.5
C2—C1—C9	123.8 (3)	C13—C26—H26C	109.5
C1—C2—C3	119.4 (3)	H26A—C26—H26B	109.5
C1—C2—C12	120.3 (3)	H26A—C26—H26C	109.5
C3—C2—C12	120.2 (3)	H26B—C26—H26C	109.5
C2—C3—C21	121.4 (3)	N2—C27—C18	123.6 (3)
C4—C3—C2	117.8 (3)	N2—C27—H27	118.2
C4—C3—C21	120.7 (3)	C18—C27—H27	118.2
C3—C4—H4A	117.8	C15—C28—H28	106.9
C3—C4—C10	124.3 (3)	C29—C28—C15	113.3 (3)
C10—C4—H4A	117.8	C29—C28—H28	106.9
C6—C5—C10	117.5 (3)	C29—C28—C30	112.2 (3)
C6—C5—C23	120.2 (3)	C30—C28—C15	110.2 (3)
C10—C5—C23	122.3 (3)	C30—C28—H28	106.9
O4—C6—C7	113.5 (3)	C28—C29—H29A	109.5
C5—C6—O4	122.6 (3)	C28—C29—H29B	109.5
C5—C6—C7	123.9 (3)	C28—C29—H29C	109.5
O3—C7—C6	116.7 (3)	H29A—C29—H29B	109.5
O3—C7—C8	124.1 (3)	H29A—C29—H29C	109.5
C8—C7—C6	119.2 (3)	H29B—C29—H29C	109.5
C7—C8—C9	118.4 (3)	C28—C30—H30A	109.5
C22—C8—C7	117.8 (3)	C28—C30—H30B	109.5
C22—C8—C9	123.8 (3)	C28—C30—H30C	109.5
C1—C9—C8	124.3 (3)	H30A—C30—H30B	109.5
C1—C9—C10	116.4 (3)	H30A—C30—H30C	109.5
C10—C9—C8	119.2 (2)	H30B—C30—H30C	109.5
C4—C10—C5	120.2 (3)	C32—C31—N1	117.3 (3)
C4—C10—C9	118.1 (3)	C32—C31—C36	119.3 (4)
C9—C10—C5	121.7 (3)	C36—C31—N1	123.2 (3)
O5—C11—C12	120.1 (2)	C31—C32—H32	119.8
O5—C11—C19	116.3 (2)	C31—C32—C33	120.4 (4)
C12—C11—C19	123.6 (2)	C33—C32—H32	119.8
C11—C12—C2	120.2 (2)	C32—C33—H33	120.6
C11—C12—C13	119.1 (2)	C34—C33—C32	118.7 (4)
C13—C12—C2	120.7 (2)	C34—C33—H33	120.6
C12—C13—C26	121.7 (2)	C33—C34—O2	124.0 (4)
C14—C13—C12	117.6 (3)	C33—C34—C35	121.3 (4)
C14—C13—C26	120.7 (3)	C35—C34—O2	114.7 (4)
C13—C14—H14	117.6	C34—C35—H35	119.7
C13—C14—C20	124.8 (3)	C34—C35—C36	120.5 (4)
C20—C14—H14	117.6	C36—C35—H35	119.7
C16—C15—C20	119.2 (3)	C31—C36—H36	120.1
C16—C15—C28	119.3 (3)	C35—C36—C31	119.7 (4)
C20—C15—C28	121.4 (3)	C35—C36—H36	120.1
O8—C16—C17	113.5 (3)	O2—C37—H37A	109.5

C15—C16—O8	123.2 (3)	O2—C37—H37B	109.5
C15—C16—C17	123.4 (3)	O2—C37—H37C	109.5
O7—C17—C16	116.9 (3)	H37A—C37—H37B	109.5
O7—C17—C18	126.0 (3)	H37A—C37—H37C	109.5
C18—C17—C16	117.1 (3)	H37B—C37—H37C	109.5
C17—C18—C19	120.7 (2)	C39—C38—N2	122.5 (3)
C17—C18—C27	116.1 (2)	C43—C38—N2	117.3 (3)
C27—C18—C19	122.7 (2)	C43—C38—C39	120.2 (3)
C11—C19—C18	124.1 (2)	C38—C39—H39	120.5
C11—C19—C20	117.1 (2)	C38—C39—C40	119.0 (3)
C20—C19—C18	118.7 (2)	C40—C39—H39	120.5
C14—C20—C15	122.2 (3)	C39—C40—H40	119.5
C14—C20—C19	117.6 (2)	C41—C40—C39	121.1 (3)
C19—C20—C15	120.2 (2)	C41—C40—H40	119.5
C3—C21—H21A	109.5	C40—C41—O6	115.6 (3)
C3—C21—H21B	109.5	C42—C41—O6	124.7 (3)
C3—C21—H21C	109.5	C42—C41—C40	119.5 (3)
H21A—C21—H21B	109.5	C41—C42—H42	120.2
H21A—C21—H21C	109.5	C41—C42—C43	119.6 (3)
H21B—C21—H21C	109.5	C43—C42—H42	120.2
N1—C22—C8	123.5 (3)	C38—C43—C42	120.3 (3)
N1—C22—H22	118.3	C38—C43—H43	119.8
C8—C22—H22	118.3	C42—C43—H43	119.8
C5—C23—H23	105.6	O6—C44—H44A	109.5
C24—C23—C5	115.0 (3)	O6—C44—H44B	109.5
C24—C23—H23	105.6	O6—C44—H44C	109.5
C25—C23—C5	113.6 (4)	H44A—C44—H44B	109.5
C25—C23—H23	105.6	H44A—C44—H44C	109.5
C25—C23—C24	110.6 (3)	H44B—C44—H44C	109.5
O1—C1—C2—C3	-177.8 (3)	C12—C11—C19—C18	179.5 (3)
O1—C1—C2—C12	1.6 (4)	C12—C11—C19—C20	-4.0 (5)
O1—C1—C9—C8	-1.1 (4)	C12—C13—C14—C20	-3.7 (5)
O1—C1—C9—C10	177.2 (2)	C13—C14—C20—C15	179.4 (3)
O2—C34—C35—C36	-179.2 (4)	C13—C14—C20—C19	1.0 (5)
O3—C7—C8—C9	-177.9 (2)	C15—C16—C17—O7	-178.8 (3)
O3—C7—C8—C22	6.1 (4)	C15—C16—C17—C18	-0.6 (5)
O4—C6—C7—O3	-3.1 (4)	C16—C15—C20—C14	-173.1 (3)
O4—C6—C7—C8	174.5 (3)	C16—C15—C20—C19	5.2 (5)
O5—C11—C12—C2	5.0 (4)	C16—C15—C28—C29	-55.0 (5)
O5—C11—C12—C13	-177.7 (3)	C16—C15—C28—C30	71.5 (4)
O5—C11—C19—C18	-1.5 (5)	C16—C17—C18—C19	7.1 (5)
O5—C11—C19—C20	175.0 (3)	C16—C17—C18—C27	-165.5 (3)
O6—C41—C42—C43	-178.1 (3)	C17—C18—C19—C11	169.1 (3)
O7—C17—C18—C19	-174.9 (3)	C17—C18—C19—C20	-7.3 (5)
O7—C17—C18—C27	12.5 (5)	C17—C18—C27—N2	-6.9 (5)
O8—C16—C17—O7	-1.0 (5)	C18—C19—C20—C14	179.5 (3)
O8—C16—C17—C18	177.2 (3)	C18—C19—C20—C15	1.1 (5)

N1—C31—C32—C33	178.5 (3)	C19—C11—C12—C2	-176.0 (3)
N1—C31—C36—C35	-177.9 (3)	C19—C11—C12—C13	1.3 (5)
N2—C38—C39—C40	-176.7 (4)	C19—C18—C27—N2	-179.3 (3)
N2—C38—C43—C42	178.2 (3)	C20—C15—C16—O8	176.9 (3)
C1—C2—C3—C4	-0.9 (4)	C20—C15—C16—C17	-5.5 (5)
C1—C2—C3—C21	-177.7 (3)	C20—C15—C28—C29	125.8 (3)
C1—C2—C12—C11	-107.7 (3)	C20—C15—C28—C30	-107.6 (4)
C1—C2—C12—C13	75.0 (4)	C21—C3—C4—C10	176.5 (3)
C1—C9—C10—C4	2.1 (4)	C22—N1—C31—C32	169.9 (3)
C1—C9—C10—C5	-178.4 (3)	C22—N1—C31—C36	-14.6 (5)
C2—C1—C9—C8	178.3 (3)	C22—C8—C9—C1	-8.7 (4)
C2—C1—C9—C10	-3.4 (4)	C22—C8—C9—C10	173.1 (3)
C2—C3—C4—C10	-0.3 (5)	C23—C5—C6—O4	0.4 (5)
C2—C12—C13—C14	179.8 (3)	C23—C5—C6—C7	179.0 (3)
C2—C12—C13—C26	-2.3 (5)	C23—C5—C10—C4	2.7 (5)
C3—C2—C12—C11	71.7 (4)	C23—C5—C10—C9	-176.8 (3)
C3—C2—C12—C13	-105.6 (3)	C26—C13—C14—C20	178.4 (3)
C3—C4—C10—C5	-179.9 (3)	C27—N2—C38—C39	4.3 (6)
C3—C4—C10—C9	-0.3 (4)	C27—N2—C38—C43	-176.1 (3)
C5—C6—C7—O3	178.2 (3)	C27—C18—C19—C11	-18.8 (5)
C5—C6—C7—C8	-4.3 (5)	C27—C18—C19—C20	164.8 (3)
C6—C5—C10—C4	-179.8 (3)	C28—C15—C16—O8	-2.3 (5)
C6—C5—C10—C9	0.7 (4)	C28—C15—C16—C17	175.3 (3)
C6—C5—C23—C24	54.8 (5)	C28—C15—C20—C14	6.0 (5)
C6—C5—C23—C25	-74.1 (4)	C28—C15—C20—C19	-175.6 (3)
C6—C7—C8—C9	4.7 (4)	C31—N1—C22—C8	175.1 (3)
C6—C7—C8—C22	-171.3 (3)	C31—C32—C33—C34	-0.8 (6)
C7—C8—C9—C1	175.5 (3)	C32—C31—C36—C35	-2.5 (6)
C7—C8—C9—C10	-2.7 (4)	C32—C33—C34—O2	179.6 (4)
C7—C8—C22—N1	-4.3 (4)	C32—C33—C34—C35	-1.5 (7)
C8—C9—C10—C4	-179.5 (3)	C33—C34—C35—C36	1.8 (6)
C8—C9—C10—C5	0.0 (4)	C34—C35—C36—C31	0.2 (6)
C9—C1—C2—C3	2.9 (4)	C36—C31—C32—C33	2.8 (6)
C9—C1—C2—C12	-177.7 (3)	C37—O2—C34—C33	0.8 (6)
C9—C8—C22—N1	179.9 (3)	C37—O2—C34—C35	-178.2 (3)
C10—C5—C6—O4	-177.2 (3)	C38—N2—C27—C18	170.9 (3)
C10—C5—C6—C7	1.5 (5)	C38—C39—C40—C41	-4.2 (7)
C10—C5—C23—C24	-127.8 (3)	C39—C38—C43—C42	-2.2 (6)
C10—C5—C23—C25	103.3 (4)	C39—C40—C41—O6	180.0 (4)
C11—C12—C13—C14	2.5 (5)	C39—C40—C41—C42	3.1 (6)
C11—C12—C13—C26	-179.6 (3)	C40—C41—C42—C43	-1.6 (6)
C11—C19—C20—C14	2.8 (4)	C41—C42—C43—C38	1.1 (6)
C11—C19—C20—C15	-175.6 (3)	C43—C38—C39—C40	3.7 (6)
C12—C2—C3—C4	179.7 (3)	C44—O6—C41—C40	175.3 (3)
C12—C2—C3—C21	2.9 (4)	C44—O6—C41—C42	-8.1 (5)

Hydrogen-bond geometry (Å, °)

<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>
N1—H1A \cdots O3	0.95 (5)	1.83 (5)	2.538 (4)	129 (4)
N2—H2 \cdots O7	0.92 (3)	1.87 (3)	2.550 (3)	129 (3)
O1—H1 \cdots O6 ⁱ	0.91 (4)	2.13 (4)	2.912 (3)	144 (3)
O4—H4 \cdots O3	0.86 (3)	2.04 (4)	2.574 (4)	119 (3)
O5—H5 \cdots O3 ⁱⁱ	0.82 (3)	1.98 (3)	2.684 (3)	143 (3)
O8—H8 \cdots O7	0.98 (3)	2.17 (3)	2.601 (3)	105 (2)
O8—H8 \cdots O7 ⁱⁱⁱ	0.98 (3)	1.83 (3)	2.757 (3)	158 (3)

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