

2,6-Bis[(S)-1-phenylethyl]-1H,5H-pyrrolo[3,4-f]isoindole-1,3,5,7(2H,6H)-tetrone

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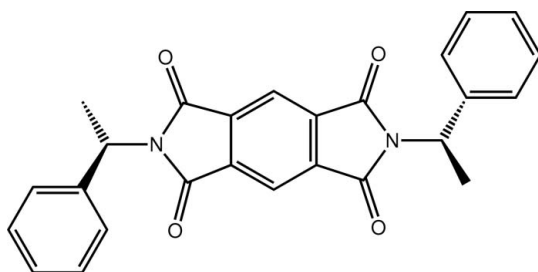
Received 20 February 2012; accepted 20 February 2012

Key indicators: single-crystal X-ray study; $T = 100$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.033; wR factor = 0.099; data-to-parameter ratio = 14.2.

In the title compound, $\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}_4$, the central isoindole core is almost planar (r.m.s. deviation = 0.043 Å). The phenyl rings lie to either side of the plane [dihedral angles = 88.64 (5) and 67.74 (6)°] and the dihedral angle between the phenyl rings is 63.39 (7)°. In the crystal, molecules are linked by $\text{C}-\text{H}\cdots\text{O}$ interactions; notably, one carbonyl O atom accepts three such bonds.

Related literature

For the biological activity of cyclic imides including that of the title compound, see: Abdel-Aziz (2007); Abdel-Aziz, El-Azab *et al.* (2011); Abdel-Aziz, ElTahir *et al.* (2011).



Experimental

Crystal data

$\text{C}_{26}\text{H}_{20}\text{N}_2\text{O}_4$ $a = 5.6401$ (1) Å
 $M_r = 424.44$ $b = 16.1040$ (2) Å
 Monoclinic, $P2_1$ $c = 11.3759$ (2) Å

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$\beta = 99.762$ (2)°
 $V = 1018.29$ (3) Å³
 $Z = 2$
 Cu $K\alpha$ radiation

$\mu = 0.77$ mm⁻¹
 $T = 100$ K
 $0.30 \times 0.25 \times 0.20$ mm

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector
 Absorption correction: multi-scan (*CrysAlis PRO*; Agilent, 2011)
 $T_{\min} = 0.656$, $T_{\max} = 1.000$

7858 measured reflections
 4093 independent reflections
 4091 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.018$

Refinement

$R[F^2 > 2\sigma(F^2)] = 0.033$
 $wR(F^2) = 0.099$
 $S = 1.11$
 4093 reflections
 289 parameters
 1 restraint

H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.24$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.25$ e Å⁻³
 Absolute structure: Flack (1983), 1898 Friedel pairs
 Flack parameter: 0.08 (12)

Table 1

Hydrogen-bond geometry (Å, °).

$D-\text{H}\cdots A$	$D-\text{H}$	$\text{H}\cdots A$	$D\cdots A$	$D-\text{H}\cdots A$
$\text{C6}-\text{H6}\cdots\text{O1}^{\text{i}}$	0.95	2.50	3.4129 (16)	162
$\text{C7}-\text{H7}\cdots\text{O4}^{\text{ii}}$	1.00	2.49	3.1840 (16)	126
$\text{C20}-\text{H20C}\cdots\text{O1}^{\text{iii}}$	0.98	2.56	3.4948 (17)	161
$\text{C23}-\text{H23}\cdots\text{O1}^{\text{iv}}$	0.95	2.57	3.4847 (18)	161

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

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO*; data reduction: *CrysAlis PRO*; program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

The authors extend their appreciation to the Deanship of Scientific Research at King Saud University for funding the work through the research group project (No. RGP-VPP-163). We also thank the Ministry of Higher Education (Malaysia) for funding structural studies through the High-Impact Research scheme (UM.C/HIR/MOHE/SC/12).

Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: BT5823).

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supplementary materials

Acta Cryst. (2012). E68, o907 [doi:10.1107/S1600536812007684]

2,6-Bis[(*S*)-1-phenylethyl]-1*H*,5*H*-pyrrolo[3,4-*f*]isoindole-1,3,5,7(2*H*,6*H*)-tetrone

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Comment

Recent work has shown that cyclic imides possess important biological potential, such as anti-hyperlipidemic, anti-diabetic, anti-tumour and anti-inflammatory activities (Abdel-Aziz, 2007; Abdel-Aziz, El-Azab *et al.*, 2011; Abdel-Aziz, ElTahir *et al.*, 2011). The title cyclic imide, 2,6-bis((*S*)-1-phenylethyl)pyrrolo[3,4-*f*]isoindole-1,3,5,7(2*H*,6*H*)-tetraone (I), was investigated during these trials and herein the crystal structure determination is described.

In (I), Fig. 1, the 12 atoms comprising the isoindole core are co-planar with a r.m.s. deviation for the fitted atoms of 0.043 Å. The maximum deviations from this least-squares plane are 0.043 (1) Å for the C15 and C16 atoms, and -0.058 (1) Å for the N2 atom. The phenyl rings lie to either side of the plane, forming dihedral angles of 88.64 (5)° [C1–C6] and 67.74 (6)° [C21–C26]; the dihedral angle between the phenyl rings = 63.39 (7)°.

Molecules are assembled in the crystal structure by C–H⋯O interactions, Fig. 2 and Table 1. Notably, one carbonyl-O atom is involved in a trifurcated H bond.

Experimental

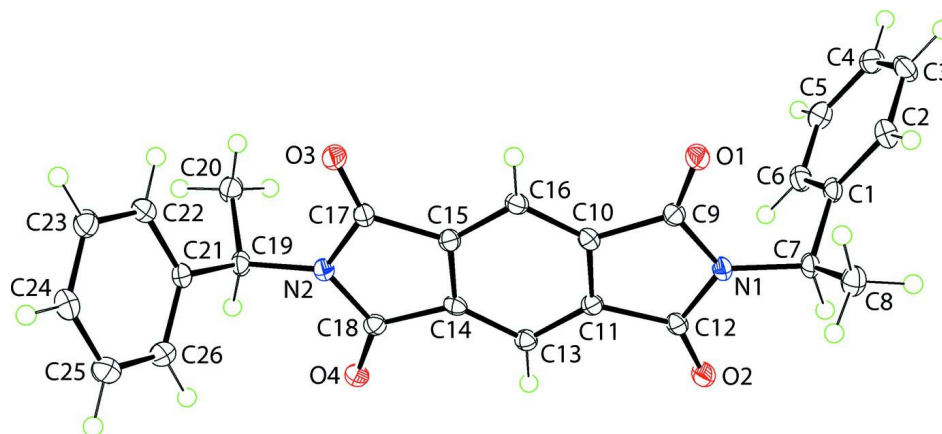
A solution of (+)-(*S*)-1-phenylethanamine (10 mmol) and benzene-1,2,4,5-tetracarboxylic dianhydride (10 mmol) in glacial acetic acid (10 ml) was heated under reflux for 12 h. After the evaporation of the reaction mixture to dryness under reduced pressure, the residue was neutralized using sodium bicarbonate solution (4%) until effervescence ceased. The precipitate obtained was washed with water, dried and recrystallized from MeOH/CHCl₃ (1:1 *v/v*). Yield 59%. *M.pt.* > 623 K. ¹H NMR (CDCl₃): δ 8.20 (s, 2H, Ar–H), 7.53–7.51 (d, 4H, *J* = 7.0 Hz, Ar–H), 7.38–7.35 (t, 4H, *J* = 7.0 Hz, Ar–H), 7.32–7.28 (q, 2H, *J* = 8.0 Hz, Ar–H), 5.62–5.61 (d, 2H, *J* = 6.0 Hz, 2CH), 1.98–1.96 (d, 6H, *J* = 6.0 Hz, 2CH₃). ¹³C NMR (CDCl₃): δ 166.02, 139.52, 137.05, 128.64, 128.07, 127.49, 118.19, 50.52, 17.41.

Refinement

Carbon-bound H-atoms were placed in calculated positions [C–H = 0.95 to 1.00 Å, $U_{\text{iso}}(\text{H}) = 1.2\text{--}1.5U_{\text{eq}}(\text{C})$] and were included in the refinement in the riding model approximation. The absolute configuration was determined from 1898 Friedel pairs, and was that of the starting reactant.

Computing details

Data collection: *CrysAlis PRO* (Agilent, 2011); cell refinement: *CrysAlis PRO* (Agilent, 2011); data reduction: *CrysAlis PRO* (Agilent, 2011); program(s) used to solve structure: *SHELXS97* (Sheldrick, 2008); program(s) used to refine structure: *SHELXL97* (Sheldrick, 2008); molecular graphics: *ORTEP-3* (Farrugia, 1997) and *DIAMOND* (Brandenburg, 2006); software used to prepare material for publication: *publCIF* (Westrip, 2010).

**Figure 1**

The molecular structure of (I) showing the atom-labelling scheme and displacement ellipsoids at the 50% probability level.

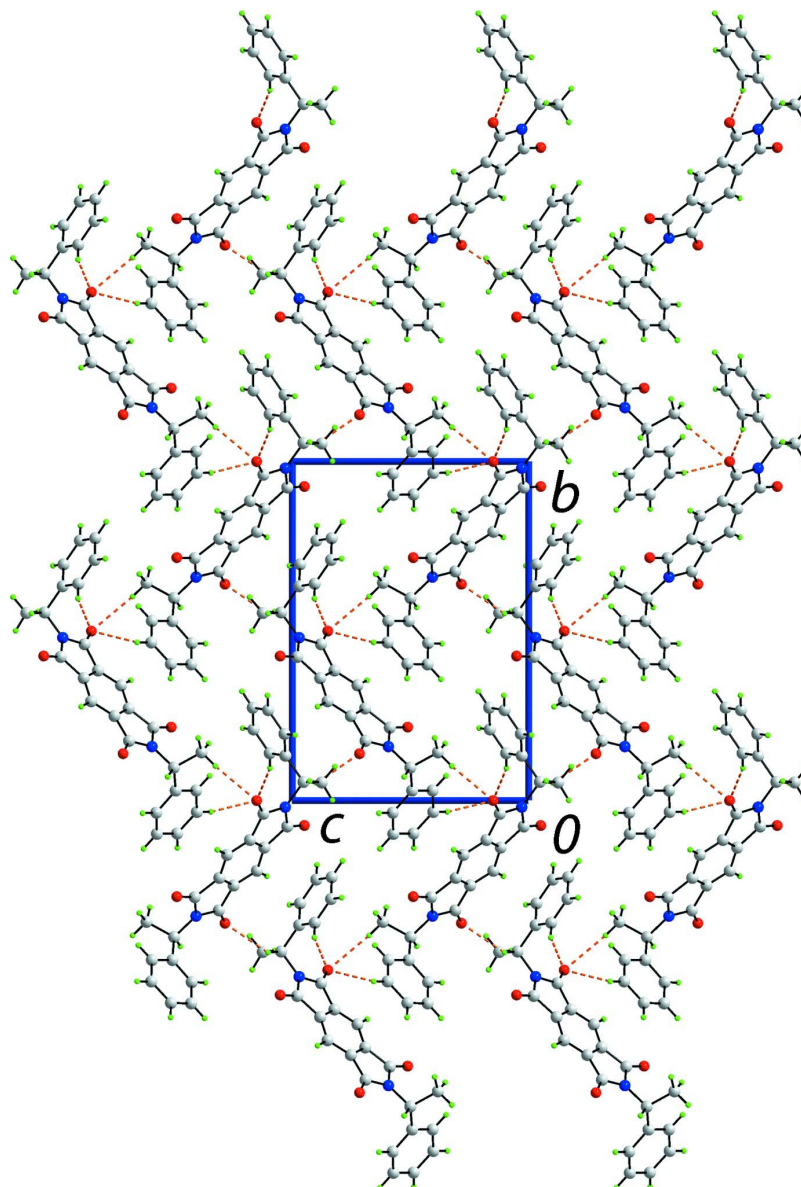


Figure 2

A view in projection down the *a* axis of the unit-cell contents for (I). The C—H...O interactions are shown as orange dashed lines.

2,6-Bis[(*S*)-1-phenylethyl]-1*H*,5*H*- pyrrolo[3,4-*f*]isoindole-1,3,5,7(2*H*,6*H*)-tetrone

Crystal data

$C_{26}H_{20}N_2O_4$

$M_r = 424.44$

Monoclinic, $P2_1$

Hall symbol: $P\ 2yb$

$a = 5.6401\ (1)\ \text{\AA}$

$b = 16.1040\ (2)\ \text{\AA}$

$c = 11.3759\ (2)\ \text{\AA}$

$\beta = 99.762\ (2)^\circ$

$V = 1018.29\ (3)\ \text{\AA}^3$

$Z = 2$

$F(000) = 444$

$D_x = 1.384\ \text{Mg m}^{-3}$

Cu $K\alpha$ radiation, $\lambda = 1.5418\ \text{\AA}$

Cell parameters from 6911 reflections

$\theta = 2.7\text{--}76.5^\circ$

$\mu = 0.77\ \text{mm}^{-1}$

$T = 100$ K $0.30 \times 0.25 \times 0.20$ mm
 Prism, colourless

Data collection

Agilent SuperNova Dual diffractometer with an Atlas detector	$T_{\min} = 0.656$, $T_{\max} = 1.000$ 7858 measured reflections
Radiation source: SuperNova (Cu) X-ray Source	4093 independent reflections 4091 reflections with $I > 2\sigma(I)$
Mirror monochromator	$R_{\text{int}} = 0.018$
Detector resolution: 10.4041 pixels mm^{-1}	$\theta_{\max} = 76.7^\circ$, $\theta_{\min} = 3.9^\circ$
ω scan	$h = -7 \rightarrow 7$
Absorption correction: multi-scan (<i>CrysAlis PRO</i> ; Agilent, 2011)	$k = -20 \rightarrow 20$ $l = -14 \rightarrow 13$

Refinement

Refinement on F^2	Hydrogen site location: inferred from neighbouring sites
Least-squares matrix: full	H-atom parameters constrained
$R[F^2 > 2\sigma(F^2)] = 0.033$	$w = 1/[\sigma^2(F_o^2) + (0.0781P)^2 + 0.0806P]$
$wR(F^2) = 0.099$	where $P = (F_o^2 + 2F_c^2)/3$
$S = 1.11$	$(\Delta/\sigma)_{\max} < 0.001$
4093 reflections	$\Delta\rho_{\max} = 0.24 \text{ e } \text{\AA}^{-3}$
289 parameters	$\Delta\rho_{\min} = -0.25 \text{ e } \text{\AA}^{-3}$
1 restraint	Absolute structure: Flack (1983), 1898 Friedel pairs
Primary atom site location: structure-invariant direct methods	Flack parameter: 0.08 (12)
Secondary atom site location: difference Fourier map	

Special details

Geometry. All s.u.'s (except the s.u. in the dihedral angle between two l.s. planes) are estimated using the full covariance matrix. The cell s.u.'s are taken into account individually in the estimation of s.u.'s in distances, angles and torsion angles; correlations between s.u.'s in cell parameters are only used when they are defined by crystal symmetry. An approximate (isotropic) treatment of cell s.u.'s is used for estimating s.u.'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 $F^2 > 2\sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

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

	x	y	z	$U_{\text{iso}}^*/U_{\text{eq}}$
O1	-0.21322 (17)	0.49962 (6)	0.84958 (9)	0.0190 (2)
O2	0.52962 (18)	0.42601 (6)	1.05125 (9)	0.0204 (2)
O3	-0.18870 (17)	0.21623 (6)	0.51186 (8)	0.0194 (2)
O4	0.55058 (17)	0.13790 (6)	0.71548 (9)	0.0198 (2)
N1	0.1580 (2)	0.48014 (7)	0.97059 (10)	0.0157 (2)
N2	0.1824 (2)	0.15891 (7)	0.59322 (10)	0.0154 (2)
C1	0.1785 (2)	0.63194 (8)	0.97086 (11)	0.0156 (3)
C2	0.0123 (3)	0.69641 (9)	0.96693 (13)	0.0197 (3)
H2	-0.1151	0.6924	1.0116	0.024*
C3	0.0320 (3)	0.76653 (9)	0.89804 (14)	0.0224 (3)
H3	-0.0829	0.8099	0.8954	0.027*
C4	0.2184 (3)	0.77357 (9)	0.83304 (13)	0.0214 (3)

H4	0.2327	0.8219	0.7870	0.026*
C5	0.3837 (2)	0.70929 (10)	0.83595 (12)	0.0212 (3)
H5	0.5106	0.7133	0.7909	0.025*
C6	0.3636 (2)	0.63922 (9)	0.90455 (12)	0.0184 (3)
H6	0.4776	0.5956	0.9063	0.022*
C7	0.1695 (2)	0.55439 (8)	1.04732 (11)	0.0158 (3)
H7	0.3270	0.5517	1.1029	0.019*
C8	-0.0248 (3)	0.55292 (10)	1.12469 (13)	0.0211 (3)
H8A	-0.0150	0.5007	1.1696	0.032*
H8B	-0.1831	0.5573	1.0740	0.032*
H8C	-0.0017	0.5998	1.1804	0.032*
C9	-0.0287 (2)	0.46074 (8)	0.87821 (11)	0.0153 (3)
C10	0.0478 (2)	0.38325 (8)	0.82149 (12)	0.0146 (3)
C11	0.2743 (2)	0.36088 (8)	0.88183 (11)	0.0142 (3)
C12	0.3478 (2)	0.42320 (8)	0.97899 (12)	0.0150 (3)
C13	0.4002 (2)	0.29243 (8)	0.85060 (11)	0.0147 (3)
H13	0.5538	0.2767	0.8927	0.018*
C14	0.2814 (2)	0.24907 (8)	0.75224 (12)	0.0141 (2)
C15	0.0553 (2)	0.27140 (8)	0.69167 (11)	0.0144 (3)
C16	-0.0710 (2)	0.33948 (9)	0.72418 (12)	0.0151 (3)
H16	-0.2258	0.3547	0.6831	0.018*
C17	-0.0107 (2)	0.21467 (8)	0.58745 (12)	0.0150 (3)
C18	0.3646 (2)	0.17566 (8)	0.68996 (11)	0.0146 (2)
C19	0.2125 (2)	0.09707 (8)	0.50044 (12)	0.0158 (3)
H19	0.3719	0.0698	0.5268	0.019*
C20	0.2275 (3)	0.14171 (9)	0.38372 (12)	0.0201 (3)
H20A	0.3534	0.1843	0.3978	0.030*
H20B	0.0726	0.1680	0.3533	0.030*
H20C	0.2662	0.1016	0.3251	0.030*
C21	0.0229 (2)	0.02911 (8)	0.49308 (12)	0.0164 (3)
C22	-0.1846 (3)	0.02927 (9)	0.40638 (12)	0.0189 (3)
H22	-0.2102	0.0727	0.3491	0.023*
C23	-0.3546 (3)	-0.03401 (9)	0.40349 (13)	0.0207 (3)
H23	-0.4949	-0.0336	0.3440	0.025*
C24	-0.3199 (3)	-0.09748 (9)	0.48692 (14)	0.0218 (3)
H24	-0.4374	-0.1399	0.4857	0.026*
C25	-0.1120 (3)	-0.09870 (9)	0.57237 (14)	0.0249 (3)
H25	-0.0862	-0.1425	0.6291	0.030*
C26	0.0579 (3)	-0.03601 (10)	0.57488 (12)	0.0217 (3)
H26	0.2000	-0.0375	0.6332	0.026*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O1	0.0176 (4)	0.0184 (5)	0.0201 (5)	0.0040 (4)	0.0006 (3)	-0.0031 (4)
O2	0.0200 (5)	0.0155 (5)	0.0229 (5)	-0.0003 (4)	-0.0038 (4)	-0.0023 (4)
O3	0.0173 (5)	0.0189 (5)	0.0201 (5)	0.0021 (4)	-0.0022 (4)	-0.0031 (4)
O4	0.0201 (5)	0.0184 (5)	0.0195 (4)	0.0061 (4)	-0.0005 (4)	-0.0008 (4)
N1	0.0179 (5)	0.0116 (6)	0.0170 (5)	0.0003 (4)	0.0013 (4)	-0.0026 (4)
N2	0.0164 (5)	0.0135 (5)	0.0156 (5)	0.0013 (4)	0.0009 (4)	-0.0017 (4)

C1	0.0153 (6)	0.0133 (6)	0.0173 (6)	-0.0007 (5)	-0.0001 (4)	-0.0050 (5)
C2	0.0197 (6)	0.0158 (7)	0.0245 (7)	0.0008 (5)	0.0064 (5)	-0.0033 (5)
C3	0.0242 (7)	0.0131 (6)	0.0280 (7)	0.0039 (5)	-0.0011 (6)	-0.0022 (5)
C4	0.0260 (7)	0.0161 (7)	0.0199 (6)	-0.0032 (5)	-0.0022 (5)	-0.0006 (5)
C5	0.0212 (7)	0.0234 (7)	0.0188 (6)	-0.0040 (6)	0.0032 (5)	-0.0036 (5)
C6	0.0162 (6)	0.0180 (7)	0.0207 (6)	0.0017 (5)	0.0023 (5)	-0.0042 (5)
C7	0.0182 (6)	0.0119 (6)	0.0168 (6)	-0.0008 (5)	0.0014 (4)	-0.0041 (5)
C8	0.0243 (7)	0.0191 (6)	0.0208 (6)	-0.0041 (5)	0.0060 (5)	-0.0033 (5)
C9	0.0183 (6)	0.0127 (6)	0.0146 (6)	-0.0019 (5)	0.0023 (5)	0.0004 (5)
C10	0.0161 (6)	0.0115 (6)	0.0163 (6)	0.0001 (5)	0.0030 (5)	0.0006 (5)
C11	0.0154 (6)	0.0125 (6)	0.0141 (6)	-0.0028 (5)	0.0012 (5)	0.0012 (5)
C12	0.0173 (6)	0.0108 (6)	0.0169 (6)	-0.0020 (5)	0.0024 (5)	0.0011 (5)
C13	0.0146 (6)	0.0136 (6)	0.0155 (6)	-0.0009 (5)	0.0015 (4)	0.0013 (5)
C14	0.0159 (6)	0.0112 (6)	0.0155 (5)	-0.0007 (5)	0.0030 (4)	0.0037 (5)
C15	0.0150 (6)	0.0129 (6)	0.0149 (6)	-0.0019 (5)	0.0014 (4)	0.0004 (4)
C16	0.0145 (6)	0.0133 (6)	0.0166 (6)	0.0009 (5)	0.0004 (4)	0.0011 (4)
C17	0.0163 (6)	0.0125 (6)	0.0160 (6)	-0.0002 (5)	0.0025 (4)	-0.0013 (5)
C18	0.0156 (6)	0.0143 (6)	0.0139 (6)	-0.0013 (5)	0.0028 (4)	0.0018 (5)
C19	0.0169 (6)	0.0144 (6)	0.0163 (6)	0.0015 (5)	0.0033 (4)	-0.0046 (5)
C20	0.0235 (6)	0.0193 (7)	0.0180 (6)	-0.0019 (5)	0.0045 (5)	-0.0021 (5)
C21	0.0196 (6)	0.0133 (6)	0.0162 (6)	0.0019 (5)	0.0027 (5)	-0.0035 (5)
C22	0.0204 (6)	0.0148 (6)	0.0205 (6)	0.0022 (5)	0.0007 (5)	0.0004 (5)
C23	0.0184 (6)	0.0190 (7)	0.0232 (7)	0.0014 (5)	-0.0011 (5)	-0.0039 (5)
C24	0.0239 (6)	0.0157 (7)	0.0260 (7)	-0.0019 (5)	0.0046 (5)	-0.0024 (5)
C25	0.0316 (7)	0.0196 (7)	0.0223 (7)	-0.0027 (6)	0.0012 (6)	0.0040 (5)
C26	0.0238 (7)	0.0203 (7)	0.0189 (6)	-0.0003 (6)	-0.0024 (5)	0.0005 (5)

Geometric parameters (Å, °)

O1—C9	1.2111 (17)	C10—C16	1.3855 (19)
O2—C12	1.2017 (16)	C10—C11	1.3915 (18)
O3—C17	1.2062 (16)	C11—C13	1.3897 (19)
O4—C18	1.2049 (16)	C11—C12	1.4984 (18)
N1—C9	1.3911 (16)	C13—C14	1.3909 (18)
N1—C12	1.4004 (17)	C13—H13	0.9500
N1—C7	1.4754 (16)	C14—C15	1.3902 (18)
N2—C18	1.3986 (16)	C14—C18	1.4941 (18)
N2—C17	1.4046 (16)	C15—C16	1.3913 (18)
N2—C19	1.4815 (16)	C15—C17	1.4930 (17)
C1—C6	1.3928 (18)	C16—H16	0.9500
C1—C2	1.3945 (18)	C19—C21	1.5222 (19)
C1—C7	1.5276 (18)	C19—C20	1.5249 (18)
C2—C3	1.390 (2)	C19—H19	1.0000
C2—H2	0.9500	C20—H20A	0.9800
C3—C4	1.389 (2)	C20—H20B	0.9800
C3—H3	0.9500	C20—H20C	0.9800
C4—C5	1.390 (2)	C21—C26	1.394 (2)
C4—H4	0.9500	C21—C22	1.3970 (18)
C5—C6	1.388 (2)	C22—C23	1.396 (2)
C5—H5	0.9500	C22—H22	0.9500

C6—H6	0.9500	C23—C24	1.386 (2)
C7—C8	1.5175 (18)	C23—H23	0.9500
C7—H7	1.0000	C24—C25	1.391 (2)
C8—H8A	0.9800	C24—H24	0.9500
C8—H8B	0.9800	C25—C26	1.389 (2)
C8—H8C	0.9800	C25—H25	0.9500
C9—C10	1.5012 (18)	C26—H26	0.9500
C9—N1—C12	112.10 (11)	C11—C13—C14	113.97 (11)
C9—N1—C7	125.51 (11)	C11—C13—H13	123.0
C12—N1—C7	122.27 (11)	C14—C13—H13	123.0
C18—N2—C17	111.95 (11)	C15—C14—C13	123.06 (12)
C18—N2—C19	122.19 (11)	C15—C14—C18	107.76 (11)
C17—N2—C19	125.31 (11)	C13—C14—C18	129.16 (12)
C6—C1—C2	118.78 (13)	C14—C15—C16	122.69 (12)
C6—C1—C7	118.53 (11)	C14—C15—C17	108.64 (11)
C2—C1—C7	122.67 (12)	C16—C15—C17	128.56 (12)
C3—C2—C1	120.37 (13)	C10—C16—C15	114.41 (11)
C3—C2—H2	119.8	C10—C16—H16	122.8
C1—C2—H2	119.8	C15—C16—H16	122.8
C4—C3—C2	120.44 (13)	O3—C17—N2	126.28 (12)
C4—C3—H3	119.8	O3—C17—C15	128.21 (12)
C2—C3—H3	119.8	N2—C17—C15	105.50 (10)
C3—C4—C5	119.48 (13)	O4—C18—N2	125.85 (13)
C3—C4—H4	120.3	O4—C18—C14	128.01 (12)
C5—C4—H4	120.3	N2—C18—C14	106.14 (11)
C6—C5—C4	120.03 (13)	N2—C19—C21	111.00 (10)
C6—C5—H5	120.0	N2—C19—C20	109.47 (11)
C4—C5—H5	120.0	C21—C19—C20	115.67 (11)
C5—C6—C1	120.89 (13)	N2—C19—H19	106.7
C5—C6—H6	119.6	C21—C19—H19	106.7
C1—C6—H6	119.6	C20—C19—H19	106.7
N1—C7—C8	111.52 (11)	C19—C20—H20A	109.5
N1—C7—C1	109.15 (10)	C19—C20—H20B	109.5
C8—C7—C1	116.11 (11)	H20A—C20—H20B	109.5
N1—C7—H7	106.5	C19—C20—H20C	109.5
C8—C7—H7	106.5	H20A—C20—H20C	109.5
C1—C7—H7	106.5	H20B—C20—H20C	109.5
C7—C8—H8A	109.5	C26—C21—C22	118.67 (13)
C7—C8—H8B	109.5	C26—C21—C19	119.05 (12)
H8A—C8—H8B	109.5	C22—C21—C19	122.29 (12)
C7—C8—H8C	109.5	C23—C22—C21	120.35 (13)
H8A—C8—H8C	109.5	C23—C22—H22	119.8
H8B—C8—H8C	109.5	C21—C22—H22	119.8
O1—C9—N1	126.36 (13)	C24—C23—C22	120.37 (12)
O1—C9—C10	127.63 (12)	C24—C23—H23	119.8
N1—C9—C10	106.01 (11)	C22—C23—H23	119.8
C16—C10—C11	122.80 (12)	C23—C24—C25	119.57 (13)
C16—C10—C9	129.12 (12)	C23—C24—H24	120.2

C11—C10—C9	108.05 (11)	C25—C24—H24	120.2
C13—C11—C10	123.07 (12)	C26—C25—C24	120.09 (13)
C13—C11—C12	129.09 (12)	C26—C25—H25	120.0
C10—C11—C12	107.84 (11)	C24—C25—H25	120.0
O2—C12—N1	125.16 (13)	C25—C26—C21	120.93 (13)
O2—C12—C11	128.83 (13)	C25—C26—H26	119.5
N1—C12—C11	106.01 (10)	C21—C26—H26	119.5
C6—C1—C2—C3	-0.06 (19)	C13—C14—C15—C16	0.31 (19)
C7—C1—C2—C3	178.47 (13)	C18—C14—C15—C16	-177.85 (11)
C1—C2—C3—C4	-0.5 (2)	C13—C14—C15—C17	176.77 (11)
C2—C3—C4—C5	0.9 (2)	C18—C14—C15—C17	-1.39 (14)
C3—C4—C5—C6	-0.8 (2)	C11—C10—C16—C15	-0.13 (18)
C4—C5—C6—C1	0.2 (2)	C9—C10—C16—C15	177.67 (12)
C2—C1—C6—C5	0.21 (19)	C14—C15—C16—C10	0.26 (18)
C7—C1—C6—C5	-178.38 (12)	C17—C15—C16—C10	-175.45 (12)
C9—N1—C7—C8	66.11 (16)	C18—N2—C17—O3	177.94 (13)
C12—N1—C7—C8	-118.32 (13)	C19—N2—C17—O3	6.4 (2)
C9—N1—C7—C1	-63.51 (15)	C18—N2—C17—C15	-0.74 (14)
C12—N1—C7—C1	112.06 (13)	C19—N2—C17—C15	-172.31 (12)
C6—C1—C7—N1	-57.40 (14)	C14—C15—C17—O3	-177.32 (13)
C2—C1—C7—N1	124.07 (13)	C16—C15—C17—O3	-1.1 (2)
C6—C1—C7—C8	175.54 (12)	C14—C15—C17—N2	1.33 (13)
C2—C1—C7—C8	-2.99 (18)	C16—C15—C17—N2	177.52 (12)
C12—N1—C9—O1	-179.01 (13)	C17—N2—C18—O4	-179.55 (12)
C7—N1—C9—O1	-3.1 (2)	C19—N2—C18—O4	-7.7 (2)
C12—N1—C9—C10	0.25 (14)	C17—N2—C18—C14	-0.08 (14)
C7—N1—C9—C10	176.20 (11)	C19—N2—C18—C14	171.80 (11)
O1—C9—C10—C16	0.9 (2)	C15—C14—C18—O4	-179.61 (13)
N1—C9—C10—C16	-178.40 (13)	C13—C14—C18—O4	2.4 (2)
O1—C9—C10—C11	178.91 (13)	C15—C14—C18—N2	0.93 (14)
N1—C9—C10—C11	-0.33 (13)	C13—C14—C18—N2	-177.07 (12)
C16—C10—C11—C13	-0.58 (19)	C18—N2—C19—C21	120.96 (13)
C9—C10—C11—C13	-178.79 (12)	C17—N2—C19—C21	-68.29 (16)
C16—C10—C11—C12	178.50 (12)	C18—N2—C19—C20	-110.14 (13)
C9—C10—C11—C12	0.29 (13)	C17—N2—C19—C20	60.61 (16)
C9—N1—C12—O2	-179.90 (13)	N2—C19—C21—C26	-81.30 (15)
C7—N1—C12—O2	4.0 (2)	C20—C19—C21—C26	153.20 (13)
C9—N1—C12—C11	-0.07 (14)	N2—C19—C21—C22	99.25 (14)
C7—N1—C12—C11	-176.18 (11)	C20—C19—C21—C22	-26.25 (18)
C13—C11—C12—O2	-1.3 (2)	C26—C21—C22—C23	1.0 (2)
C10—C11—C12—O2	179.68 (13)	C19—C21—C22—C23	-179.51 (12)
C13—C11—C12—N1	178.86 (12)	C21—C22—C23—C24	0.3 (2)
C10—C11—C12—N1	-0.15 (13)	C22—C23—C24—C25	-1.2 (2)
C10—C11—C13—C14	1.07 (18)	C23—C24—C25—C26	0.9 (2)
C12—C11—C13—C14	-177.80 (12)	C24—C25—C26—C21	0.5 (2)
C11—C13—C14—C15	-0.94 (18)	C22—C21—C26—C25	-1.4 (2)
C11—C13—C14—C18	176.79 (12)	C19—C21—C26—C25	179.11 (13)

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>
C6—H6 \cdots O1 ⁱ	0.95	2.50	3.4129 (16)	162
C7—H7 \cdots O4 ⁱⁱ	1.00	2.49	3.1840 (16)	126
C20—H20C \cdots O1 ⁱⁱⁱ	0.98	2.56	3.4948 (17)	161
C23—H23 \cdots O1 ^{iv}	0.95	2.57	3.4847 (18)	161

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