IUCrData

ISSN 2414-3146

Methyl (6*R**,6a*R**,12b*R**)-2,4-dimethyl-6-(2-methylphenyl)-1,3-dioxo-2,3,4,6a,7,12b-hexahydro-1*H*,6*H*-chromeno[4′,3′:4,5]pyrano[2,3-*d*]pyrimidine-6a-carboxylate

S. Gomathi,[a] Era Dravida Thendral,[b] G. Sivakumar,[c] V. Sabari[d] and G. Usha[b]*

[a]Department of Physics, Bhaktavatsalam Memorial College for women, Koratur, Chennai 600 080, Tamilnadu, India, [b]PG and Research Department of Physics, Queen Mary's College, Chennai-4, Tamilnadu, India, [c]Department of Organic Chemistry, University of Madras, Maraimalai campus,Chennai-600 025, India, and [d]Department of Physics, Sree Abiraami College of Arts and Science, Gudiyattum,Vellore 635 803, Tamilnadu, India. *Correspondence e-mail: guqmc@yahoo.com

Received 26 April 2017
Accepted 1 June 2017

Edited by H. Stoeckli-Evans, University of Neuchâtel, Switzerland

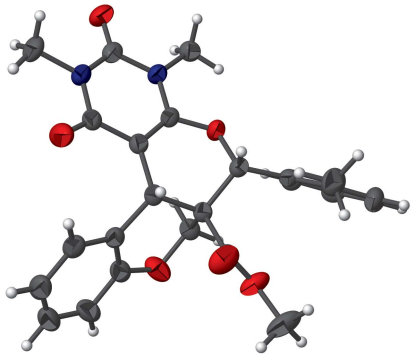
Keywords: crystal structure; chromene; pyrimidine; pyran; C—H···O hydrogen bonds; C—H···π interactions.

CCDC reference: 938663

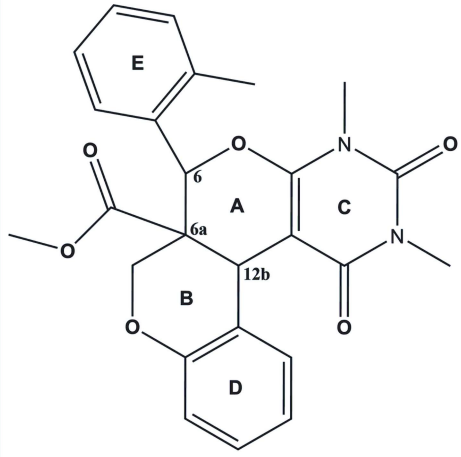
Structural data: full structural data are available from iucrdata.iucr.org

In the title compound, $C_{24}H_{24}N_2O_6$, the mean planes of the pyran rings (*A* and *B*) are inclined to one another by 69.2 (1)°, while the aromatic ring (*D*) of the chromene ring system makes dihedral angles of 63.42 (11) and 66.81 (12)° with the pyrimidine (*C*) and benzene (*E*) rings, respectively. Pyran ring *A* has an half-chair conformation, while pyran ring *B* has an envelope conformation, with the spiro C atom as the flap. In the crystal, molecules are linked by C—H···O hydrogen bonds, forming a supramolecular three-dimensional network. There are also a number of C—H···π interactions present.

3D view



Chemical scheme



Structure description

Chromenes are used in the fields of medicine, cosmetics and as fluorescent dyes. 2-Oxo-2*H*-chromenes are efficient fluorophores characterized by good emission quantum yields and are used as materials for lasers in organic light-emitting devices, non-linear optical chromeophores and fluorescent labels (Sreenivasa *et al.*, 2013). They exhibit anticancer, anti-Alzheimer's and anti-Parkinson's activity and are used to treat Huntington's disease (Andrani & Lapi, 1960; Zhang *et al.*, 1982). They also exhibit antiviral, antifungal, anti-inflammatory and antidiabetic activity (Kemnitzer *et al.*, 2008; Sui Xiong *et al.*, 2006; Tang *et al.*, 2007), and antimicrobial activity (Sangani *et al.*, 2012).

The molecular structure of the title compound is illustrated in Fig. 1. The compound crystallizes as a racemate with relative configuration of *R*,*R*,*R* at atoms C11(position 6),

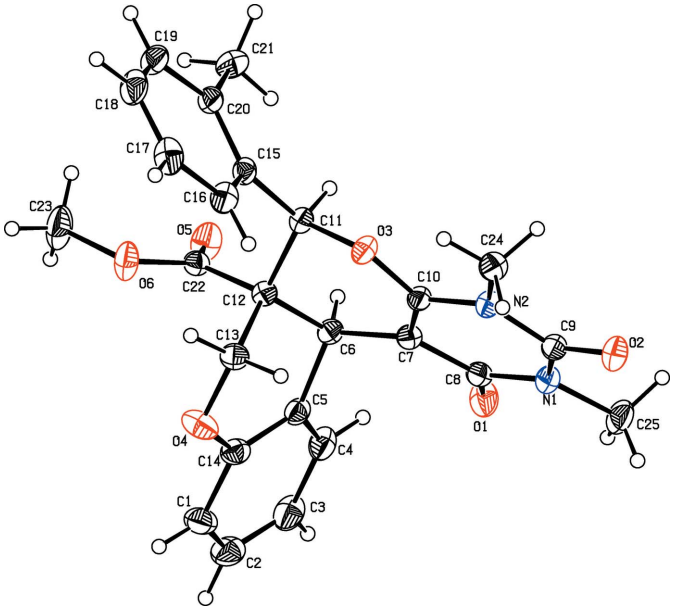


Figure 1
The molecular structure of the title compound, with atom labelling and displacement ellipsoids drawn at the 30% probability level.

C12(position 6a) and C6(position 12b), respectively (see Scheme). The bond distances and bond angles are in good agreement with the values reported for similar structures (Swaminathan *et al.*, 2015; Ponnusamy *et al.*, 2013). The sp^2 hybridization of atoms N1 and N2 are indicated by the sum of the bond angles of 359.8 and 360.0°, respectively. Pyran ring *A* has an half-chair conformation [puckering parameters: amplitude (*Q*) = 0.531 (2) Å, θ = 52.3 (2)°, φ = 273.2 (3)°], while pyran ring *B* has an envelope conformation, with atom C12 as the flap [puckering parameters: amplitude (*Q*) = 0.493 (2) Å, θ = 128.0 (2)°, φ = 289.5 (3)°]. The mean planes of the pyran rings (*A* and *B*) are inclined to one another by 69.2 (1)°, while the aromatic ring (*D*) of the chromene ring system makes dihedral angles of 63.42 (11) and 66.81 (12)° with the pyrimidine (*C*) and benzene (*E*) rings, respectively. The methyl and carbonyl groups attached to the different ring systems of the molecule tend to be coplanar with the respective rings, other than atoms O1 and C25 which deviate by 0.210 (1) and 0.123 (3) Å, respectively, from the pyrimidene ring mean plane.

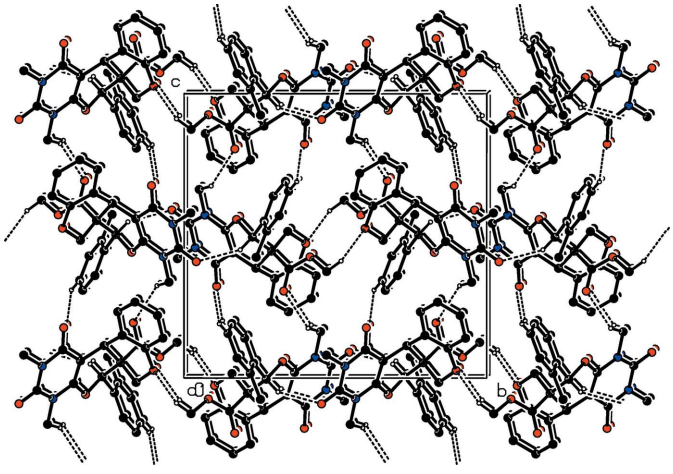


Figure 2
A view along the *a* axis of the crystal packing of the title compound. The dashed lines indicate the hydrogen bonds (see Table 1), and for clarity, only the H atoms involved in hydrogen bonding have been included.

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

*Cg*3 and *Cg*4 are the centroids of the N1/N2/C7–C10 and C1–C5/C14 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O2^{i}	0.96 (2)	2.42 (2)	3.280 (3)	150 (2)
C18—H18···O1^{ii}	0.93	2.60	3.475 (3)	157
C23—H23*A*···O4^{iii}	0.96	2.57	3.222 (4)	125
C24—H24*A*···O5^{iv}	0.96	2.54	3.344 (3)	142
C21—H21*C*···*Cg*4^{v}	0.96	2.86	3.668 (3)	143
C24—H24*B*···*Cg*3^{i}	0.96	2.92	3.550 (3)	124
C24—H24*C*···*Cg*4^{iv}	0.96	2.57	3.454 (3)	153

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{25}H_{24}N_2O_6$
M_r	448.46
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	293
a, *b*, *c* (Å)	9.4087 (5), 15.5422 (7), 14.6143 (7)
β (°)	91.077 (1)
V (Å^3)	2136.70 (18)
Z	4
Radiation type	Mo *K*α
μ (mm^{-1})	0.10
Crystal size (mm)	0.30 × 0.20 × 0.20
Data collection	
Diffractometer	Bruker Kappa APEXII CCD
Absorption correction	Multi-scan (*SADABS*; Bruker, 2004)
T_{min}, T_{max}	0.976, 0.980
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	18765, 3765, 2856
R_{int}	0.034
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.595
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.048, 0.146, 1.05
No. of reflections	3764
No. of parameters	315
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.38, −0.32

Computer programs: *APEX2* (Bruker, 2004), *SAINT* and *XPREP* (Bruker, 2004), *SHELXS97* and *SHELXL97* (Sheldrick, 2008), *ORTEP-3 for Windows* (Farrugia, 2012) and *PLATON* (Spek, 2009).

In the crystal, molecules are linked by C—H···O hydrogen bonds, forming a supramolecular three-dimensional network (Table 1 and Fig. 2). There are also a number of C—H···π interactions present (Table 1).

Synthesis and crystallization

The title compound was synthesized following a published procedure (Ponnusamy *et al.*, 2013; Swaminathan *et al.*, 2015). A mixture of (*E*)-methyl 2-((2-formylphenoxy)methyl)-3-(2-methylphenyl) acrylate (0.448 g, 1 mmol) and *N*,*N*-dimethylbarbutric acid (0.156 g, 1 mmol) was placed in a round-bottom flask and melted at 453 K for 1 h. After completion of the reaction, as indicated by TLC, the crude product was washed with 5 ml of an ethylacetate and hexane mixture (1:49) which successfully provided the pure title compound as a colourless solid in 97% yield. Colourless block-like crystals were obtained by slow evaporation of a solution in ethyl acetate.

Refinement

Crystal data, data collection and structure refinement details are summarized in Table 2.

Acknowledgements

The authors thank the Central Instrumentation Facility, Queen Mary's College, Chennai-4 for computing facilities and SAIF, IIT, Madras, for the X-ray data collection facility.

References

Adreani, L. L. & Lapi, E. (1960). *Boll. Chim. Farm.* **99**, 583–586.
Bruker (2004). *APEX2*, *SAINT*, *XPREP* and *SADABS*. Bruker AXS Inc., Madison, Wisconsin, USA.
Farrugia, L. J. (2012). *J. Appl. Cryst.* **45**, 849–854.
Kemnitzer, W., Jiang, S., Wang, Y., Kasibhatla, S., Crogan-Grundy, C., Bubenik, M., Labrecque, D., Denis, R., Lamothe, S., Attardo, G., Gourdeau, H., Tseng, B., Drewe, J. & Cai, S. X. (2008). *Bioorg. Med. Chem. Lett.* **18**, 603–607.
Ponnusamy, R., Sabari, V., Sivakumar, G., Bakthadoss, M. & Aravindhan, S. (2013). *Acta Cryst.* E**69**, o267–o268.
Sangani, C. B., Shah, N. M., Patel, M. P. & Patel, R. G. (2012). *J. Serb. Chem. Soc.* **77**, 1165–1174.
Sheldrick, G. M. (2008). *Acta Cryst.* A**64**, 112–122.
Spek, A. L. (2009). *Acta Cryst.* D**65**, 148–155.
Sreenivasa, S., Srinivasa, H. T., Palakshamurthy, B. S., Kumar, V. & Devarajegowda, H. C. (2013). *Acta Cryst.* E**69**, o266.
Sui Xiong, C., Drewe, J. & Kasibhatla, S. (2006). *Curr. Med. Chem.* **13**, 2627–2644.
Swaminathan, K., Sethusankar, K., Kumar, G. S. & Bakthadoss, M. (2015). *Acta Cryst.* E**71**, 926–930.
Tang, Q.-G., Wu, W.-Y., He, W., Sun, H.-S. & Guo, C. (2007). *Acta Cryst.* E**63**, o1437–o1438.
Zhang, Y. L., Chen, B. Z., Zheng, K. Q., Xu, M. L., Lei, X. H. & Yaoxue, X. B. (1982). *Chem. Abstr.* **96**, 135383e.

full crystallographic data

IUCrData (2017). **2**, x170812 [https://doi.org/10.1107/S2414314617008124]

Methyl (6*R**,6a*R**,12b*R**)-2,4-dimethyl-6-(2-methylphenyl)-1,3-dioxo-2,3,4,6a,7,12b-hexahydro-1*H*,6*H*-chromeno[4′,3′:4,5]pyrano[2,3-*d*]pyrimidine-6a-carboxylate

S. Gomathi, Era Dravida Thendral, G. Sivakumar, V. Sabari and G. Usha

Methyl (6*R,6a*R**,12b*R**)-2,4-dimethyl-6-(2-methylphenyl)-1,3-dioxo-2,3,4,6a,7,12b-hexahydro-1*H*,6*H*-chromeno[4′,3′:4,5]pyrano[2,3-*d*]pyrimidine-6a-carboxylate**

Crystal data

$C_{25}H_{24}N_2O_6$
M_r = 448.46
Monoclinic, $P2_1/c$
a = 9.4087 (5) Å
b = 15.5422 (7) Å
c = 14.6143 (7) Å
β = 91.077 (1)°
V = 2136.70 (18) Å^3
Z = 4
$F(000)$ = 944
D_x = 1.394 Mg m^{-3}
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 3764 reflections
θ = 2.2–25.0°
μ = 0.10 mm^{-1}
T = 293 K
Block, colourless
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII CCD diffractometer
Radiation source: fine-focus sealed tube
Graphite monochromator
ω and \ f scan
Absorption correction: multi-scan (SADABS; Bruker, 2004)
T_{min} = 0.976, T_{max} = 0.980
18765 measured reflections
3765 independent reflections
2856 reflections with $I > 2\sigma(I)$
R_{int} = 0.034
θ_{max} = 25.0°, θ_{min} = 2.2°
h = −11→11
k = −18→17
l = −17→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.048
$wR(F^2)$ = 0.146
S = 1.05
3764 reflections
315 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
$w = 1/[\sigma^2(F_o^2) + (0.070P)^2 + 1.3588P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max} < 0.001$
$\Delta\rho_{max}$ = 0.38 e Å^{-3}
$\Delta\rho_{min}$ = −0.32 e Å^{-3}
Extinction correction: SHELXL97 (Sheldrick, 2008), $Fc^*=kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$
Extinction coefficient: 0.0027 (9)

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 $F^2 > 2\text{sigma}(F^2)$ 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}
O3	0.06395 (16)	0.17387 (10)	0.55862 (10)	0.0347 (4)
N2	−0.09694 (19)	0.06786 (12)	0.57179 (12)	0.0326 (4)
O1	−0.2595 (2)	0.10497 (11)	0.32021 (12)	0.0492 (5)
N1	−0.2602 (2)	0.03401 (12)	0.45525 (13)	0.0366 (5)
C6	−0.0576 (2)	0.23662 (15)	0.38555 (15)	0.0306 (5)
O6	0.1784 (2)	0.41781 (11)	0.42814 (12)	0.0492 (5)
C10	−0.0494 (2)	0.13542 (14)	0.51946 (15)	0.0300 (5)
C8	−0.2138 (2)	0.10127 (14)	0.39882 (16)	0.0349 (5)
C12	0.0454 (2)	0.28986 (14)	0.44668 (14)	0.0295 (5)
O4	−0.1355 (2)	0.40049 (12)	0.47194 (12)	0.0492 (5)
C9	−0.2074 (2)	0.01613 (15)	0.54146 (16)	0.0349 (5)
O2	−0.25164 (19)	−0.04286 (11)	0.58803 (12)	0.0472 (5)
O5	0.1608 (2)	0.33076 (12)	0.30769 (12)	0.0525 (5)
C5	−0.1729 (2)	0.29763 (15)	0.34819 (15)	0.0344 (5)
C7	−0.1103 (2)	0.15883 (14)	0.43876 (15)	0.0315 (5)
C11	0.1479 (2)	0.22715 (15)	0.49729 (15)	0.0303 (5)
C14	−0.2029 (2)	0.37414 (16)	0.39255 (16)	0.0382 (6)
C13	−0.0403 (3)	0.34201 (16)	0.51515 (16)	0.0353 (5)
C15	0.2642 (2)	0.26739 (14)	0.55503 (15)	0.0327 (5)
C22	0.1333 (2)	0.34790 (15)	0.38504 (15)	0.0315 (5)
C4	−0.2431 (3)	0.28342 (17)	0.26444 (17)	0.0439 (6)
H4	−0.2236	0.2336	0.2317	0.053*
C24	−0.0344 (3)	0.04952 (16)	0.66270 (15)	0.0380 (6)
H24A	0.0405	0.0899	0.6758	0.057*
H24B	0.0034	−0.0078	0.6635	0.057*
H24C	−0.1064	0.0546	0.7081	0.057*
C1	−0.2996 (3)	0.43321 (18)	0.35660 (19)	0.0475 (6)
H1	−0.3174	0.4842	0.3876	0.057*
C16	0.2341 (3)	0.29708 (16)	0.64267 (16)	0.0403 (6)
H16	0.1439	0.2888	0.6660	0.048*
C20	0.4013 (2)	0.27693 (15)	0.52092 (17)	0.0385 (6)
C19	0.5020 (3)	0.31952 (17)	0.5762 (2)	0.0489 (7)
H19	0.5932	0.3275	0.5543	0.059*
C25	−0.3653 (3)	−0.02591 (18)	0.4154 (2)	0.0505 (7)
H25A	−0.3938	−0.0062	0.3555	0.076*

H25B	−0.4469	−0.0285	0.4538	0.076*
H25C	−0.3239	−0.0822	0.4108	0.076*
C2	−0.3682 (3)	0.4162 (2)	0.2757 (2)	0.0545 (7)
H2	−0.4340	0.4552	0.2518	0.065*
C18	0.4707 (3)	0.34989 (18)	0.6618 (2)	0.0539 (8)
H18	0.5400	0.3779	0.6968	0.065*
C3	−0.3405 (3)	0.34127 (19)	0.2292 (2)	0.0537 (7)
H3	−0.3875	0.3297	0.1740	0.064*
C21	0.4458 (3)	0.24282 (19)	0.42969 (19)	0.0507 (7)
H21A	0.3660	0.2157	0.3996	0.076*
H21B	0.5207	0.2016	0.4385	0.076*
H21C	0.4790	0.2894	0.3926	0.076*
C17	0.3366 (3)	0.33869 (17)	0.69537 (18)	0.0493 (7)
H17	0.3147	0.3590	0.7533	0.059*
C23	0.2712 (4)	0.47395 (19)	0.3776 (2)	0.0659 (9)
H23A	0.2979	0.5222	0.4151	0.099*
H23B	0.2225	0.4940	0.3234	0.099*
H23C	0.3549	0.4429	0.3607	0.099*
H11	0.184 (2)	0.1876 (15)	0.4531 (15)	0.030 (6)*
H13A	−0.098 (3)	0.3021 (16)	0.5534 (17)	0.041 (7)*
H13B	0.021 (3)	0.3788 (15)	0.5547 (16)	0.034 (6)*
H6	−0.005 (3)	0.2172 (16)	0.3333 (17)	0.041 (7)*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O3	0.0319 (8)	0.0382 (9)	0.0336 (8)	−0.0091 (7)	−0.0040 (6)	0.0052 (7)
N2	0.0320 (10)	0.0322 (10)	0.0336 (10)	−0.0047 (8)	0.0013 (8)	0.0015 (8)
O1	0.0599 (12)	0.0408 (10)	0.0461 (10)	−0.0077 (9)	−0.0211 (9)	−0.0007 (8)
N1	0.0338 (10)	0.0321 (11)	0.0436 (11)	−0.0057 (8)	−0.0028 (9)	−0.0016 (9)
C6	0.0289 (11)	0.0336 (12)	0.0293 (11)	−0.0018 (10)	−0.0004 (9)	−0.0013 (9)
O6	0.0657 (12)	0.0359 (10)	0.0465 (10)	−0.0187 (9)	0.0172 (9)	−0.0055 (8)
C10	0.0272 (11)	0.0287 (12)	0.0342 (11)	−0.0017 (9)	0.0026 (9)	−0.0041 (9)
C8	0.0307 (12)	0.0308 (12)	0.0430 (14)	0.0032 (10)	−0.0039 (10)	−0.0035 (10)
C12	0.0288 (11)	0.0313 (12)	0.0284 (11)	−0.0005 (9)	0.0005 (9)	−0.0008 (9)
O4	0.0545 (11)	0.0504 (11)	0.0426 (10)	0.0210 (9)	−0.0052 (8)	−0.0083 (8)
C9	0.0315 (12)	0.0312 (12)	0.0422 (13)	−0.0007 (10)	0.0062 (10)	−0.0056 (10)
O2	0.0513 (11)	0.0391 (10)	0.0513 (11)	−0.0139 (8)	0.0044 (8)	0.0037 (8)
O5	0.0651 (12)	0.0552 (12)	0.0377 (10)	−0.0163 (9)	0.0152 (9)	−0.0071 (8)
C5	0.0301 (11)	0.0366 (13)	0.0366 (12)	−0.0056 (10)	−0.0008 (9)	0.0078 (10)
C7	0.0291 (11)	0.0308 (12)	0.0346 (12)	0.0006 (9)	−0.0008 (9)	−0.0013 (9)
C11	0.0296 (11)	0.0303 (12)	0.0311 (11)	−0.0037 (9)	0.0017 (9)	0.0002 (10)
C14	0.0313 (12)	0.0438 (14)	0.0395 (13)	0.0011 (11)	0.0038 (10)	0.0061 (11)
C13	0.0343 (12)	0.0391 (14)	0.0326 (12)	0.0026 (11)	0.0014 (10)	−0.0011 (11)
C15	0.0339 (12)	0.0282 (11)	0.0356 (12)	−0.0036 (10)	−0.0063 (9)	0.0059 (9)
C22	0.0302 (11)	0.0316 (12)	0.0328 (12)	0.0017 (9)	−0.0008 (9)	0.0005 (10)
C4	0.0466 (14)	0.0429 (14)	0.0418 (14)	−0.0118 (12)	−0.0095 (11)	0.0076 (11)
C24	0.0397 (13)	0.0397 (13)	0.0346 (12)	−0.0006 (11)	0.0006 (10)	0.0046 (10)

C1	0.0393 (14)	0.0476 (16)	0.0559 (16)	0.0110 (12)	0.0044 (12)	0.0104 (13)
C16	0.0441 (14)	0.0404 (14)	0.0362 (13)	−0.0050 (11)	−0.0056 (10)	0.0050 (10)
C20	0.0329 (12)	0.0315 (13)	0.0507 (14)	−0.0021 (10)	−0.0067 (11)	0.0076 (11)
C19	0.0350 (14)	0.0432 (15)	0.0681 (18)	−0.0084 (12)	−0.0124 (12)	0.0065 (13)
C25	0.0452 (15)	0.0457 (16)	0.0603 (17)	−0.0163 (12)	−0.0103 (13)	−0.0052 (13)
C2	0.0393 (14)	0.0589 (18)	0.0649 (18)	0.0016 (13)	−0.0078 (13)	0.0234 (15)
C18	0.0530 (17)	0.0423 (15)	0.0651 (18)	−0.0121 (13)	−0.0291 (14)	0.0044 (14)
C3	0.0499 (16)	0.0563 (18)	0.0541 (16)	−0.0133 (14)	−0.0196 (13)	0.0192 (14)
C21	0.0340 (13)	0.0558 (17)	0.0627 (17)	−0.0026 (12)	0.0103 (12)	−0.0008 (14)
C17	0.0660 (18)	0.0420 (15)	0.0392 (14)	−0.0059 (13)	−0.0160 (13)	0.0013 (11)
C23	0.082 (2)	0.0461 (17)	0.071 (2)	−0.0270 (16)	0.0298 (17)	−0.0027 (14)

Geometric parameters (Å, º)

O3—C10	1.341 (3)	C15—C16	1.395 (3)
O3—C11	1.462 (3)	C15—C20	1.400 (3)
N2—C10	1.379 (3)	C4—C3	1.377 (4)
N2—C9	1.380 (3)	C4—H4	0.9300
N2—C24	1.471 (3)	C24—H24A	0.9600
O1—C8	1.220 (3)	C24—H24B	0.9600
N1—C9	1.374 (3)	C24—H24C	0.9600
N1—C8	1.406 (3)	C1—C2	1.363 (4)
N1—C25	1.471 (3)	C1—H1	0.9300
C6—C7	1.525 (3)	C16—C17	1.383 (4)
C6—C5	1.534 (3)	C16—H16	0.9300
C6—C12	1.545 (3)	C20—C19	1.400 (3)
C6—H6	0.97 (3)	C20—C21	1.501 (4)
O6—C22	1.322 (3)	C19—C18	1.374 (4)
O6—C23	1.447 (3)	C19—H19	0.9300
C10—C7	1.352 (3)	C25—H25A	0.9600
C8—C7	1.438 (3)	C25—H25B	0.9600
C12—C22	1.529 (3)	C25—H25C	0.9600
C12—C13	1.529 (3)	C2—C3	1.375 (4)
C12—C11	1.549 (3)	C2—H2	0.9300
O4—C14	1.374 (3)	C18—C17	1.374 (4)
O4—C13	1.416 (3)	C18—H18	0.9300
C9—O2	1.220 (3)	C3—H3	0.9300
O5—C22	1.195 (3)	C21—H21A	0.9600
C5—C14	1.386 (3)	C21—H21B	0.9600
C5—C4	1.398 (3)	C21—H21C	0.9600
C11—C15	1.506 (3)	C17—H17	0.9300
C11—H11	0.96 (2)	C23—H23A	0.9600
C14—C1	1.389 (3)	C23—H23B	0.9600
C13—H13A	1.00 (3)	C23—H23C	0.9600
C13—H13B	0.99 (2)		
C10—O3—C11	115.14 (16)	O5—C22—O6	124.1 (2)
C10—N2—C9	121.06 (19)	O5—C22—C12	123.7 (2)

C10—N2—C24	121.35 (18)	O6—C22—C12	112.13 (18)
C9—N2—C24	117.58 (19)	C3—C4—C5	121.6 (3)
C9—N1—C8	125.24 (19)	C3—C4—H4	119.2
C9—N1—C25	117.7 (2)	C5—C4—H4	119.2
C8—N1—C25	116.9 (2)	N2—C24—H24A	109.5
C7—C6—C5	115.91 (18)	N2—C24—H24B	109.5
C7—C6—C12	109.63 (17)	H24A—C24—H24B	109.5
C5—C6—C12	107.82 (18)	N2—C24—H24C	109.5
C7—C6—H6	109.4 (15)	H24A—C24—H24C	109.5
C5—C6—H6	106.4 (15)	H24B—C24—H24C	109.5
C12—C6—H6	107.3 (15)	C2—C1—C14	119.7 (3)
C22—O6—C23	116.34 (19)	C2—C1—H1	120.1
O3—C10—C7	125.0 (2)	C14—C1—H1	120.1
O3—C10—N2	111.50 (18)	C17—C16—C15	121.0 (2)
C7—C10—N2	123.5 (2)	C17—C16—H16	119.5
O1—C8—N1	118.7 (2)	C15—C16—H16	119.5
O1—C8—C7	125.2 (2)	C19—C20—C15	117.6 (2)
N1—C8—C7	116.1 (2)	C19—C20—C21	118.9 (2)
C22—C12—C13	111.75 (19)	C15—C20—C21	123.5 (2)
C22—C12—C6	108.39 (17)	C18—C19—C20	122.3 (3)
C13—C12—C6	109.27 (18)	C18—C19—H19	118.9
C22—C12—C11	108.27 (17)	C20—C19—H19	118.9
C13—C12—C11	110.61 (17)	N1—C25—H25A	109.5
C6—C12—C11	108.47 (17)	N1—C25—H25B	109.5
C14—O4—C13	117.59 (18)	H25A—C25—H25B	109.5
O2—C9—N1	122.8 (2)	N1—C25—H25C	109.5
O2—C9—N2	121.4 (2)	H25A—C25—H25C	109.5
N1—C9—N2	115.7 (2)	H25B—C25—H25C	109.5
C14—C5—C4	116.6 (2)	C1—C2—C3	120.1 (3)
C14—C5—C6	120.9 (2)	C1—C2—H2	119.9
C4—C5—C6	122.3 (2)	C3—C2—H2	119.9
C10—C7—C8	117.4 (2)	C19—C18—C17	119.7 (2)
C10—C7—C6	121.44 (19)	C19—C18—H18	120.1
C8—C7—C6	120.69 (19)	C17—C18—H18	120.1
O3—C11—C15	106.67 (17)	C2—C3—C4	120.0 (3)
O3—C11—C12	108.09 (17)	C2—C3—H3	120.0
C15—C11—C12	116.47 (18)	C4—C3—H3	120.0
O3—C11—H11	104.7 (13)	C20—C21—H21A	109.5
C15—C11—H11	112.3 (14)	C20—C21—H21B	109.5
C12—C11—H11	107.9 (13)	H21A—C21—H21B	109.5
O4—C14—C5	123.8 (2)	C20—C21—H21C	109.5
O4—C14—C1	114.3 (2)	H21A—C21—H21C	109.5
C5—C14—C1	121.9 (2)	H21B—C21—H21C	109.5
O4—C13—C12	112.64 (18)	C18—C17—C16	119.7 (3)
O4—C13—H13A	107.6 (14)	C18—C17—H17	120.1
C12—C13—H13A	109.6 (14)	C16—C17—H17	120.1
O4—C13—H13B	104.3 (13)	O6—C23—H23A	109.5
C12—C13—H13B	112.2 (14)	O6—C23—H23B	109.5

H13A—C13—H13B	110.3 (19)	H23A—C23—H23B	109.5
C16—C15—C20	119.7 (2)	O6—C23—H23C	109.5
C16—C15—C11	119.6 (2)	H23A—C23—H23C	109.5
C20—C15—C11	120.6 (2)	H23B—C23—H23C	109.5
C11—O3—C10—C7	−17.9 (3)	C6—C12—C11—O3	−64.6 (2)
C11—O3—C10—N2	161.80 (17)	C22—C12—C11—C15	58.0 (2)
C9—N2—C10—O3	−176.06 (18)	C13—C12—C11—C15	−64.8 (2)
C24—N2—C10—O3	5.4 (3)	C6—C12—C11—C15	175.43 (18)
C9—N2—C10—C7	3.7 (3)	C13—O4—C14—C5	−6.5 (3)
C24—N2—C10—C7	−174.8 (2)	C13—O4—C14—C1	177.0 (2)
C9—N1—C8—O1	172.7 (2)	C4—C5—C14—O4	−175.2 (2)
C25—N1—C8—O1	−1.9 (3)	C6—C5—C14—O4	−0.9 (3)
C9—N1—C8—C7	−4.9 (3)	C4—C5—C14—C1	1.0 (3)
C25—N1—C8—C7	−179.6 (2)	C6—C5—C14—C1	175.3 (2)
C7—C6—C12—C22	161.32 (18)	C14—O4—C13—C12	37.6 (3)
C5—C6—C12—C22	−71.7 (2)	C22—C12—C13—O4	59.2 (3)
C7—C6—C12—C13	−76.7 (2)	C6—C12—C13—O4	−60.8 (3)
C5—C6—C12—C13	50.3 (2)	C11—C12—C13—O4	179.87 (19)
C7—C6—C12—C11	44.0 (2)	O3—C11—C15—C16	−40.0 (3)
C5—C6—C12—C11	170.98 (17)	C12—C11—C15—C16	80.7 (3)
C8—N1—C9—O2	179.7 (2)	O3—C11—C15—C20	141.4 (2)
C25—N1—C9—O2	−5.7 (3)	C12—C11—C15—C20	−97.9 (3)
C8—N1—C9—N2	−2.2 (3)	C23—O6—C22—O5	−2.5 (4)
C25—N1—C9—N2	172.5 (2)	C23—O6—C22—C12	175.7 (2)
C10—N2—C9—O2	−178.8 (2)	C13—C12—C22—O5	−148.4 (2)
C24—N2—C9—O2	−0.2 (3)	C6—C12—C22—O5	−28.0 (3)
C10—N2—C9—N1	3.1 (3)	C11—C12—C22—O5	89.5 (3)
C24—N2—C9—N1	−178.36 (19)	C13—C12—C22—O6	33.4 (3)
C7—C6—C5—C14	100.9 (2)	C6—C12—C22—O6	153.82 (19)
C12—C6—C5—C14	−22.3 (3)	C11—C12—C22—O6	−88.7 (2)
C7—C6—C5—C4	−85.1 (3)	C14—C5—C4—C3	−2.0 (4)
C12—C6—C5—C4	151.6 (2)	C6—C5—C4—C3	−176.2 (2)
O3—C10—C7—C8	168.8 (2)	O4—C14—C1—C2	176.9 (2)
N2—C10—C7—C8	−10.9 (3)	C5—C14—C1—C2	0.3 (4)
O3—C10—C7—C6	−3.1 (3)	C20—C15—C16—C17	2.3 (4)
N2—C10—C7—C6	177.24 (19)	C11—C15—C16—C17	−176.3 (2)
O1—C8—C7—C10	−166.4 (2)	C16—C15—C20—C19	−2.4 (3)
N1—C8—C7—C10	11.0 (3)	C11—C15—C20—C19	176.2 (2)
O1—C8—C7—C6	5.5 (3)	C16—C15—C20—C21	176.6 (2)
N1—C8—C7—C6	−177.04 (19)	C11—C15—C20—C21	−4.8 (4)
C5—C6—C7—C10	−134.2 (2)	C15—C20—C19—C18	1.3 (4)
C12—C6—C7—C10	−11.9 (3)	C21—C20—C19—C18	−177.7 (2)
C5—C6—C7—C8	54.2 (3)	C14—C1—C2—C3	−0.9 (4)
C12—C6—C7—C8	176.55 (19)	C20—C19—C18—C17	0.0 (4)
C10—O3—C11—C15	177.27 (18)	C1—C2—C3—C4	−0.1 (4)
C10—O3—C11—C12	51.3 (2)	C5—C4—C3—C2	1.5 (4)
C22—C12—C11—O3	177.98 (16)	C19—C18—C17—C16	−0.1 (4)

C13—C12—C11—O3	55.2 (2)	C15—C16—C17—C18	−1.1 (4)

Hydrogen-bond geometry (Å, º)

Cg3 and Cg4 are the centroids of the N1/N2/C7–C10 and C1–C5/C14 rings, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C11—H11···O2^{i}	0.96 (2)	2.42 (2)	3.280 (3)	150 (2)
C18—H18···O1^{ii}	0.93	2.60	3.475 (3)	157
C23—H23*A*···O4^{iii}	0.96	2.57	3.222 (4)	125
C24—H24*A*···O5^{iv}	0.96	2.54	3.344 (3)	142
C21—H21*C*···*Cg*4^{v}	0.96	2.86	3.668 (3)	143
C24—H24*B*···*Cg*3^{i}	0.96	2.92	3.550 (3)	124
C24—H24*C*···*Cg*4^{iv}	0.96	2.57	3.454 (3)	153

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