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Methyl 3-(4-chlorophenyl)-1-methyl-1,2,3,3a,4,11c-hexahydrobenzo[*f*]-chromeno[4,3-*b*]pyrrole-3a-carboxylate

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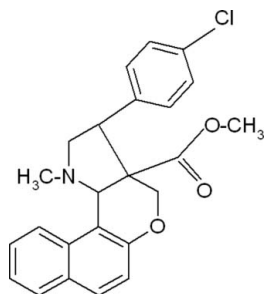
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 Key indicators: single-crystal X-ray study; $T = 295$ K; mean $\sigma(\text{C}-\text{C}) = 0.002$ Å; R factor = 0.042; wR factor = 0.119; data-to-parameter ratio = 18.0.

In the title compound, $\text{C}_{24}\text{H}_{22}\text{ClNO}_3$, the dihedral angle between the naphthalene ring system and the chlorophenyl ring is $67.44(4)^\circ$. The pyrrolidine and dihydropyran rings exhibit envelope and half chair conformations, respectively. In the crystal structure, weak $\text{C}-\text{H}\cdots\pi$ interactions are observed.

Related literature

For the biological activity of chromenopyrrole derivatives, see: Caine (1993); Tidey (1992); Carlson (1993); Sokoloff *et al.* (1990); Wilner (1985); Sobral & Rocha Gonsalves (2001*a,b*); Brockmann & Tour (1995); Suslick *et al.* (1992); Di Natale *et al.* (1998). For related structures, see: Nirmala *et al.* (2009*a,b*); Gunasekaran *et al.* (2009). For puckering parameters, see: Cremer & Pople (1975). For asymmetry parameters, see: Nardelli (1983).



Experimental

Crystal data

 $\text{C}_{24}\text{H}_{22}\text{ClNO}_3$
 $M_r = 407.88$

 Monoclinic, $P2_1/c$
 $a = 12.6951(8)$ Å

 $b = 19.8829(13)$ Å
 $c = 8.0799(6)$ Å
 $\beta = 106.396(4)^\circ$
 $V = 1956.6(2)$ Å³
 $Z = 4$

 Mo $K\alpha$ radiation
 $\mu = 0.22$ mm⁻¹
 $T = 295$ K
 $0.20 \times 0.20 \times 0.20$ mm

Data collection

 Bruker Kappa APEXII diffractometer
 Absorption correction: multi-scan (SADABS; Sheldrick, 1996)
 $T_{\min} = 0.954$, $T_{\max} = 0.957$

 18246 measured reflections
 4759 independent reflections
 3643 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.039$

Refinement

 $R[F^2 > 2\sigma(F^2)] = 0.042$
 $wR(F^2) = 0.119$
 $S = 1.05$
 4759 reflections

 264 parameters
 H-atom parameters constrained
 $\Delta\rho_{\text{max}} = 0.26$ e Å⁻³
 $\Delta\rho_{\text{min}} = -0.31$ e Å⁻³

Table 1

Hydrogen-bond geometry (Å, °).

 $Cg1$, $Cg2$ and $Cg3$ are the centroids of the C1–C5/C10, C5–C10 and C16–C21 rings, respectively.

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
C17–H17 $\cdots Cg2^i$	0.93	2.99	3.615 (6)	126
C18–H18 $\cdots Cg1^i$	0.93	2.75	3.637 (5)	159
C20–H20 $\cdots Cg3^{ii}$	0.93	2.89	3.651 (9)	139

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

Data collection: APEX2 (Bruker, 2004); cell refinement: SAINT (Bruker, 2004); data reduction: SAINT; program(s) used to solve structure: SHELXS97 (Sheldrick, 2008); program(s) used to refine structure: SHELXL97 (Sheldrick, 2008); molecular graphics: PLATON (Spek, 2009); software used to prepare material for publication: SHELXL97.

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: IS2523).

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supporting information

Acta Cryst. (2010). E66, o611–o612 [doi:10.1107/S1600536810005465]

Methyl 3-(4-chlorophenyl)-1-methyl-1,2,3,3a,4,11c-hexahydro-benzo[*f*]chromeno[4,3-*b*]pyrrole-3a-carboxylate

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S1. Comment

Chromenopyrrole compounds are used in the treatment of impulsive disorders (Caine, 1993), aggressiveness (Tidey, 1992), parkinson's disease (Carlson, 1993), psychoses, memory disorders (Sokoloff *et al.*, 1990), anxiety and depression (Wilner, 1985). Pyrroles are also very useful precursors in porphyrin synthesis (Sobral & Rocha Gonsalves, 2001*a, b*), and as monomers for polymer chemistry (Brockmann & Tour, 1995), with applications ranging from non linear optical materials (Suslick *et al.*, 1992) to electronic noses (Di Natale *et al.*, 1998).

The geometric parameters of the title molecule (Fig. 1) agree well with reported similar structure (Nirmala *et al.*, 2009*a, b*; Gunasekaran *et al.*, 2009). The dihedral angle between the naphthalene ring system and the chlorophenyl ring is 67.44 (4)°. The pyrrolidine ring [N1/C14/C15/C12/C11] exhibits an envelope conformation with envelope on C11 with an asymmetry parameter (Nardelli, 1983) ΔC_s (C11) = 4.05 (3) and with the puckering parameters (Cremer & Pople, 1975) $q_2 = 0.4275$ (2) Å and $\varphi_2 = 214.69$ (6)°. The six-membered heterocyclic ring [C8/C9/C11/C12/C13/O1] of the benzochromenopyrrole moiety adopts a half-chair conformation with the puckering parameters $Q = 0.4697$ (2) Å, $\Theta = 132.51$ (3)° and $\varphi = 82.84$ (5)°. The sum of bond angles around N1 [332.44 (12)°] indicate the sp^3 hybridized state of atom N1 in the molecule.

The crystal packing is stabilized by weak intermolecular C—H $\cdots\pi$ [C17—H17 \cdots Cg2(2-*x*, -*y*, 2-*z*), C18—H18 \cdots Cg1(2-*x*, -*y*, 2-*z*) and C20—H20 \cdots Cg3(*x*, 1/2-*y*, -1/2+*z*); Table 1] interactions. Cg1, Cg2 and Cg3 are the centroids of the rings C1–C5/C10, C5–C10 and C16–C21, respectively.

S2. Experimental

A mixture of (*Z*)-methyl 2-((1-formylnaphthalen-2-yloxy) methyl) -3-(4-chloro phenylacrylate (20 mmol) and sarcosine (30 mmol) were refluxed in benzene for 20 h and the solvent was removed under reduced pressure. The crude product was subjected to column chromatography to get the pure product. Chloroform and methanol (1:1) solvent mixture was used for the crystallization under slow evaporation method.

S3. Refinement

H atoms were positioned geometrically and refined using riding model, with C—H = 0.93 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for aromatic C—H, C—H = 0.98 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for C—H, C—H = 0.97 Å and $U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ for CH₂, and C—H = 0.96 Å and $U_{\text{iso}}(\text{H}) = 1.5U_{\text{eq}}(\text{C})$ for CH₃.

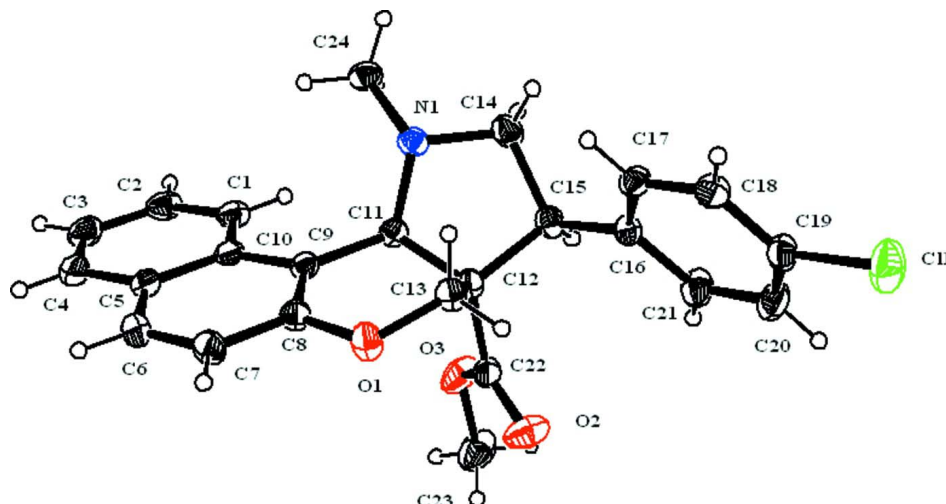


Figure 1

The molecular structure of (I), with atom labels and 30% probability displacement ellipsoids for non-H atoms.

Methyl 3-(4-chlorophenyl)-1-methyl-1,2,3,3a,4,11c-hexahydrobenzo[f]chromeno[4,3-b]pyrrole-3a-carboxylate

Crystal data

$C_{24}H_{22}ClNO_3$

$M_r = 407.88$

Monoclinic, $P2_1/c$

Hall symbol: -P 2ybc

$a = 12.6951(8) \text{ \AA}$

$b = 19.8829(13) \text{ \AA}$

$c = 8.0799(6) \text{ \AA}$

$\beta = 106.396(4)^\circ$

$V = 1956.6(2) \text{ \AA}^3$

$Z = 4$

$F(000) = 856$

$D_x = 1.385 \text{ Mg m}^{-3}$

Mo $K\alpha$ radiation, $\lambda = 0.71073 \text{ \AA}$

Cell parameters from 7245 reflections

$\theta = 2.6\text{--}28.0^\circ$

$\mu = 0.22 \text{ mm}^{-1}$

$T = 295 \text{ K}$

Block, colourless

$0.20 \times 0.20 \times 0.20 \text{ mm}$

Data collection

Bruker Kappa APEXII
diffractometer

Radiation source: fine-focus sealed tube

Graphite monochromator

Detector resolution: 0 pixels mm^{-1}

ω and φ scans

Absorption correction: multi-scan

(SADABS; Sheldrick, 1996)

$T_{\min} = 0.954$, $T_{\max} = 0.957$

18246 measured reflections

4759 independent reflections

3643 reflections with $I > 2\sigma(I)$

$R_{\text{int}} = 0.039$

$\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 1.7^\circ$

$h = -16 \rightarrow 16$

$k = -25 \rightarrow 26$

$l = -10 \rightarrow 10$

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.042$

$wR(F^2) = 0.119$

$S = 1.05$

4759 reflections

264 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-atom parameters constrained

$w = 1/[\sigma^2(F_o^2) + (0.0498P)^2 + 0.5781P]$

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

$(\Delta/\sigma)_{\max} = 0.012$

$\Delta\rho_{\max} = 0.26 \text{ e \AA}^{-3}$

$\Delta\rho_{\min} = -0.31 \text{ e \AA}^{-3}$

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

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
C1	-0.41608 (12)	0.03370 (9)	0.79567 (19)	0.0390 (3)
H1	-0.3911	0.0740	0.8513	0.047*
C2	-0.51822 (13)	0.01074 (10)	0.7918 (2)	0.0475 (4)
H2	-0.5618	0.0359	0.8439	0.057*
C3	-0.55817 (14)	-0.04982 (11)	0.7110 (2)	0.0528 (5)
H3	-0.6270	-0.0655	0.7118	0.063*
C4	-0.49560 (14)	-0.08579 (10)	0.6309 (2)	0.0493 (4)
H4	-0.5228	-0.1258	0.5757	0.059*
C5	-0.39005 (13)	-0.06350 (8)	0.63013 (18)	0.0383 (3)
C6	-0.32741 (14)	-0.09955 (8)	0.5409 (2)	0.0441 (4)
H6	-0.3544	-0.1397	0.4864	0.053*
C7	-0.22864 (14)	-0.07645 (8)	0.5336 (2)	0.0431 (4)
H7	-0.1889	-0.1001	0.4721	0.052*
C8	-0.18609 (12)	-0.01636 (7)	0.61941 (19)	0.0350 (3)
C9	-0.24015 (11)	0.01983 (7)	0.71585 (17)	0.0309 (3)
C10	-0.34747 (11)	-0.00277 (7)	0.71656 (17)	0.0326 (3)
C11	-0.18799 (11)	0.08273 (7)	0.80899 (17)	0.0304 (3)
H11	-0.2444	0.1169	0.8038	0.036*
C12	-0.09886 (11)	0.11107 (7)	0.73256 (18)	0.0313 (3)
C13	-0.02720 (12)	0.05300 (7)	0.7070 (2)	0.0359 (3)
H13A	0.0299	0.0702	0.6600	0.043*
H13B	0.0081	0.0327	0.8180	0.043*
C14	-0.05563 (13)	0.13099 (9)	1.0426 (2)	0.0445 (4)
H14A	0.0127	0.1192	1.1273	0.053*
H14B	-0.0935	0.1641	1.0929	0.053*
C15	-0.03273 (12)	0.15937 (7)	0.87920 (19)	0.0355 (3)
H15	-0.0684	0.2035	0.8577	0.043*
C16	0.08658 (11)	0.16971 (7)	0.88440 (18)	0.0328 (3)
C17	0.17038 (12)	0.12687 (7)	0.97076 (19)	0.0359 (3)
H17	0.1539	0.0902	1.0303	0.043*
C18	0.27803 (13)	0.13754 (8)	0.97024 (19)	0.0393 (3)
H18	0.3333	0.1083	1.0284	0.047*
C19	0.30196 (13)	0.19206 (8)	0.8823 (2)	0.0420 (4)
C20	0.22150 (15)	0.23519 (9)	0.7951 (2)	0.0526 (4)
H20	0.2385	0.2715	0.7348	0.063*
C21	0.11452 (14)	0.22398 (8)	0.7978 (2)	0.0479 (4)
H21	0.0599	0.2537	0.7400	0.057*
C22	-0.14094 (12)	0.15066 (8)	0.56664 (19)	0.0365 (3)
C23	-0.28508 (17)	0.21789 (11)	0.3981 (3)	0.0661 (6)
H23A	-0.2616	0.2636	0.4238	0.099*
H23B	-0.3638	0.2159	0.3664	0.099*
H23C	-0.2595	0.2017	0.3043	0.099*
C24	-0.18914 (13)	0.05770 (8)	1.10856 (19)	0.0406 (3)
H24A	-0.1412	0.0525	1.2232	0.061*
H24B	-0.2307	0.0172	1.0745	0.061*

H24C	-0.2383	0.0946	1.1063	0.061*
N1	-0.12435 (10)	0.07114 (6)	0.99011 (15)	0.0346 (3)
O1	-0.08863 (9)	0.00275 (6)	0.59363 (15)	0.0432 (3)
O2	-0.08968 (11)	0.16075 (8)	0.46603 (17)	0.0627 (4)
O3	-0.24040 (10)	0.17653 (7)	0.54843 (17)	0.0550 (3)
Cl1	0.43761 (4)	0.20640 (3)	0.88362 (8)	0.07301 (19)

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
C1	0.0372 (8)	0.0499 (9)	0.0318 (7)	0.0016 (7)	0.0126 (6)	0.0035 (6)
C2	0.0370 (8)	0.0716 (12)	0.0374 (8)	0.0018 (8)	0.0162 (6)	0.0084 (8)
C3	0.0387 (9)	0.0759 (13)	0.0453 (9)	-0.0137 (9)	0.0146 (7)	0.0119 (9)
C4	0.0474 (9)	0.0571 (11)	0.0416 (9)	-0.0176 (8)	0.0096 (7)	0.0057 (8)
C5	0.0408 (8)	0.0416 (8)	0.0315 (7)	-0.0065 (6)	0.0086 (6)	0.0050 (6)
C6	0.0538 (10)	0.0364 (8)	0.0421 (8)	-0.0101 (7)	0.0134 (7)	-0.0065 (7)
C7	0.0510 (9)	0.0381 (8)	0.0441 (9)	-0.0018 (7)	0.0197 (7)	-0.0099 (7)
C8	0.0371 (7)	0.0349 (7)	0.0361 (7)	-0.0015 (6)	0.0154 (6)	-0.0034 (6)
C9	0.0344 (7)	0.0309 (7)	0.0293 (6)	0.0001 (6)	0.0122 (5)	0.0004 (5)
C10	0.0345 (7)	0.0372 (7)	0.0269 (6)	-0.0009 (6)	0.0101 (5)	0.0050 (5)
C11	0.0327 (7)	0.0298 (7)	0.0320 (7)	0.0022 (5)	0.0147 (5)	-0.0022 (5)
C12	0.0302 (7)	0.0318 (7)	0.0342 (7)	-0.0005 (5)	0.0130 (5)	-0.0039 (6)
C13	0.0335 (7)	0.0369 (8)	0.0412 (8)	-0.0008 (6)	0.0169 (6)	-0.0086 (6)
C14	0.0430 (8)	0.0553 (10)	0.0380 (8)	-0.0093 (7)	0.0161 (7)	-0.0149 (7)
C15	0.0347 (7)	0.0332 (7)	0.0392 (8)	-0.0005 (6)	0.0112 (6)	-0.0075 (6)
C16	0.0350 (7)	0.0282 (7)	0.0348 (7)	-0.0031 (5)	0.0091 (6)	-0.0028 (5)
C17	0.0419 (8)	0.0316 (7)	0.0350 (7)	-0.0006 (6)	0.0123 (6)	0.0041 (6)
C18	0.0374 (8)	0.0406 (8)	0.0390 (8)	0.0028 (6)	0.0094 (6)	0.0001 (6)
C19	0.0357 (8)	0.0456 (9)	0.0457 (9)	-0.0091 (7)	0.0129 (6)	-0.0045 (7)
C20	0.0534 (10)	0.0429 (9)	0.0603 (11)	-0.0119 (8)	0.0139 (8)	0.0153 (8)
C21	0.0426 (9)	0.0363 (8)	0.0586 (10)	-0.0013 (7)	0.0042 (7)	0.0133 (7)
C22	0.0373 (8)	0.0358 (7)	0.0378 (7)	-0.0062 (6)	0.0129 (6)	-0.0039 (6)
C23	0.0531 (11)	0.0644 (13)	0.0772 (14)	0.0042 (9)	0.0127 (10)	0.0339 (11)
C24	0.0484 (9)	0.0450 (9)	0.0325 (7)	0.0021 (7)	0.0180 (6)	-0.0012 (6)
N1	0.0367 (6)	0.0390 (7)	0.0302 (6)	0.0013 (5)	0.0127 (5)	-0.0045 (5)
O1	0.0407 (6)	0.0439 (6)	0.0530 (6)	-0.0066 (5)	0.0262 (5)	-0.0194 (5)
O2	0.0641 (8)	0.0837 (10)	0.0493 (7)	0.0096 (7)	0.0309 (6)	0.0169 (7)
O3	0.0418 (6)	0.0609 (8)	0.0655 (8)	0.0096 (6)	0.0203 (6)	0.0279 (6)
Cl1	0.0447 (3)	0.0830 (4)	0.0973 (4)	-0.0185 (2)	0.0299 (3)	-0.0060 (3)

Geometric parameters (Å, °)

C1—C2	1.367 (2)	C14—N1	1.466 (2)
C1—C10	1.417 (2)	C14—C15	1.537 (2)
C1—H1	0.9300	C14—H14A	0.9700
C2—C3	1.395 (3)	C14—H14B	0.9700
C2—H2	0.9300	C15—C16	1.5174 (19)
C3—C4	1.360 (3)	C15—H15	0.9800

C3—H3	0.9300	C16—C21	1.386 (2)
C4—C5	1.413 (2)	C16—C17	1.387 (2)
C4—H4	0.9300	C17—C18	1.384 (2)
C5—C6	1.410 (2)	C17—H17	0.9300
C5—C10	1.423 (2)	C18—C19	1.376 (2)
C6—C7	1.352 (2)	C18—H18	0.9300
C6—H6	0.9300	C19—C20	1.367 (2)
C7—C8	1.410 (2)	C19—C11	1.7425 (16)
C7—H7	0.9300	C20—C21	1.383 (2)
C8—O1	1.3653 (17)	C20—H20	0.9300
C8—C9	1.3776 (19)	C21—H21	0.9300
C9—C10	1.4361 (19)	C22—O2	1.1930 (18)
C9—C11	1.5126 (19)	C22—O3	1.3325 (19)
C11—N1	1.4765 (18)	C23—O3	1.444 (2)
C11—C12	1.5406 (18)	C23—H23A	0.9600
C11—H11	0.9800	C23—H23B	0.9600
C12—C22	1.516 (2)	C23—H23C	0.9600
C12—C13	1.5198 (19)	C24—N1	1.4520 (18)
C12—C15	1.5714 (19)	C24—H24A	0.9600
C13—O1	1.4289 (18)	C24—H24B	0.9600
C13—H13A	0.9700	C24—H24C	0.9600
C13—H13B	0.9700		
C2—C1—C10	121.25 (16)	N1—C14—H14A	110.3
C2—C1—H1	119.4	C15—C14—H14A	110.3
C10—C1—H1	119.4	N1—C14—H14B	110.3
C1—C2—C3	121.08 (16)	C15—C14—H14B	110.3
C1—C2—H2	119.5	H14A—C14—H14B	108.6
C3—C2—H2	119.5	C16—C15—C14	117.09 (13)
C4—C3—C2	119.50 (15)	C16—C15—C12	114.85 (11)
C4—C3—H3	120.3	C14—C15—C12	103.47 (12)
C2—C3—H3	120.3	C16—C15—H15	106.9
C3—C4—C5	121.27 (17)	C14—C15—H15	106.9
C3—C4—H4	119.4	C12—C15—H15	106.9
C5—C4—H4	119.4	C21—C16—C17	117.57 (14)
C6—C5—C4	121.01 (15)	C21—C16—C15	119.16 (13)
C6—C5—C10	119.41 (14)	C17—C16—C15	123.26 (13)
C4—C5—C10	119.55 (15)	C18—C17—C16	121.46 (14)
C7—C6—C5	120.90 (15)	C18—C17—H17	119.3
C7—C6—H6	119.6	C16—C17—H17	119.3
C5—C6—H6	119.6	C19—C18—C17	118.97 (14)
C6—C7—C8	119.81 (15)	C19—C18—H18	120.5
C6—C7—H7	120.1	C17—C18—H18	120.5
C8—C7—H7	120.1	C20—C19—C18	121.23 (15)
O1—C8—C9	123.95 (13)	C20—C19—C11	119.60 (13)
O1—C8—C7	113.48 (12)	C18—C19—C11	119.17 (13)
C9—C8—C7	122.55 (14)	C19—C20—C21	119.02 (15)
C8—C9—C10	117.61 (13)	C19—C20—H20	120.5

C8—C9—C11	119.69 (12)	C21—C20—H20	120.5
C10—C9—C11	122.64 (12)	C20—C21—C16	121.75 (15)
C1—C10—C5	117.32 (13)	C20—C21—H21	119.1
C1—C10—C9	123.12 (14)	C16—C21—H21	119.1
C5—C10—C9	119.54 (13)	O2—C22—O3	122.82 (15)
N1—C11—C9	113.84 (11)	O2—C22—C12	124.48 (14)
N1—C11—C12	101.31 (11)	O3—C22—C12	112.61 (12)
C9—C11—C12	111.78 (11)	O3—C23—H23A	109.5
N1—C11—H11	109.9	O3—C23—H23B	109.5
C9—C11—H11	109.9	H23A—C23—H23B	109.5
C12—C11—H11	109.9	O3—C23—H23C	109.5
C22—C12—C13	110.44 (12)	H23A—C23—H23C	109.5
C22—C12—C11	115.41 (11)	H23B—C23—H23C	109.5
C13—C12—C11	108.19 (12)	N1—C24—H24A	109.5
C22—C12—C15	109.24 (12)	N1—C24—H24B	109.5
C13—C12—C15	110.73 (11)	H24A—C24—H24B	109.5
C11—C12—C15	102.58 (10)	N1—C24—H24C	109.5
O1—C13—C12	112.27 (12)	H24A—C24—H24C	109.5
O1—C13—H13A	109.1	H24B—C24—H24C	109.5
C12—C13—H13A	109.1	C24—N1—C14	111.13 (12)
O1—C13—H13B	109.1	C24—N1—C11	115.39 (12)
C12—C13—H13B	109.1	C14—N1—C11	105.92 (12)
H13A—C13—H13B	107.9	C8—O1—C13	116.81 (11)
N1—C14—C15	106.93 (12)	C22—O3—C23	116.61 (14)
C10—C1—C2—C3	0.6 (2)	N1—C14—C15—C12	2.04 (15)
C1—C2—C3—C4	-1.7 (3)	C22—C12—C15—C16	-84.34 (15)
C2—C3—C4—C5	0.9 (3)	C13—C12—C15—C16	37.50 (17)
C3—C4—C5—C6	-177.35 (16)	C11—C12—C15—C16	152.74 (12)
C3—C4—C5—C10	0.9 (2)	C22—C12—C15—C14	146.84 (12)
C4—C5—C6—C7	176.87 (16)	C13—C12—C15—C14	-91.33 (14)
C10—C5—C6—C7	-1.4 (2)	C11—C12—C15—C14	23.91 (14)
C5—C6—C7—C8	1.5 (3)	C14—C15—C16—C21	-144.79 (15)
C6—C7—C8—O1	-176.79 (15)	C12—C15—C16—C21	93.52 (17)
C6—C7—C8—C9	1.7 (3)	C14—C15—C16—C17	35.9 (2)
O1—C8—C9—C10	173.56 (13)	C12—C15—C16—C17	-85.78 (17)
C7—C8—C9—C10	-4.7 (2)	C21—C16—C17—C18	-0.3 (2)
O1—C8—C9—C11	-3.6 (2)	C15—C16—C17—C18	179.04 (13)
C7—C8—C9—C11	178.12 (14)	C16—C17—C18—C19	0.2 (2)
C2—C1—C10—C5	1.2 (2)	C17—C18—C19—C20	-0.5 (2)
C2—C1—C10—C9	179.29 (14)	C17—C18—C19—C11	179.12 (12)
C6—C5—C10—C1	176.35 (14)	C18—C19—C20—C21	0.8 (3)
C4—C5—C10—C1	-1.9 (2)	C11—C19—C20—C21	-178.75 (14)
C6—C5—C10—C9	-1.8 (2)	C19—C20—C21—C16	-0.9 (3)
C4—C5—C10—C9	179.94 (14)	C17—C16—C21—C20	0.7 (3)
C8—C9—C10—C1	-173.33 (13)	C15—C16—C21—C20	-178.69 (16)
C11—C9—C10—C1	3.7 (2)	C13—C12—C22—O2	-36.0 (2)
C8—C9—C10—C5	4.7 (2)	C11—C12—C22—O2	-159.04 (15)

C11—C9—C10—C5	-178.21 (13)	C15—C12—C22—O2	86.05 (18)
C8—C9—C11—N1	-94.21 (15)	C13—C12—C22—O3	147.42 (13)
C10—C9—C11—N1	88.77 (16)	C11—C12—C22—O3	24.34 (18)
C8—C9—C11—C12	19.84 (18)	C15—C12—C22—O3	-90.57 (15)
C10—C9—C11—C12	-157.18 (13)	C15—C14—N1—C24	-154.95 (13)
N1—C11—C12—C22	-159.78 (11)	C15—C14—N1—C11	-28.92 (15)
C9—C11—C12—C22	78.63 (15)	C9—C11—N1—C24	-72.57 (15)
N1—C11—C12—C13	75.95 (13)	C12—C11—N1—C24	167.29 (12)
C9—C11—C12—C13	-45.64 (15)	C9—C11—N1—C14	164.04 (11)
N1—C11—C12—C15	-41.11 (13)	C12—C11—N1—C14	43.90 (13)
C9—C11—C12—C15	-162.70 (11)	C9—C8—O1—C13	16.3 (2)
C22—C12—C13—O1	-67.74 (15)	C7—C8—O1—C13	-165.30 (14)
C11—C12—C13—O1	59.45 (15)	C12—C13—O1—C8	-45.08 (18)
C15—C12—C13—O1	171.13 (11)	O2—C22—O3—C23	0.4 (3)
N1—C14—C15—C16	-125.40 (13)	C12—C22—O3—C23	177.05 (15)

Hydrogen-bond geometry (Å, °)

Cg1, Cg2 and Cg3 are the centroids of the C1—C5/C10, C5—C10 and C16—C21 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>
C17—H17 \cdots Cg2 ⁱ	0.93	2.99	3.615 (6)	126
C18—H18 \cdots Cg1 ⁱ	0.93	2.75	3.637 (5)	159
C20—H20 \cdots Cg3 ⁱⁱ	0.93	2.89	3.651 (9)	139

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