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cis-3-Methyl-1-phenyl-8a,9,10,11,12,-12a,12b-hexahydro-1*H*,3b*H*-pyrazolo-[3,4:2′,3′]pyrano[4′,5′,6′-*kl*]xanthene

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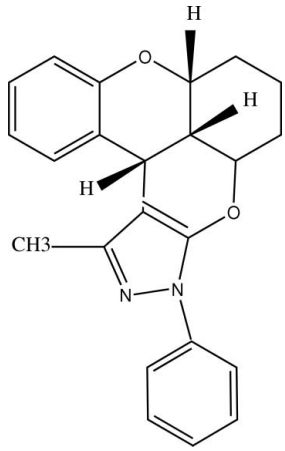
Key indicators: single-crystal X-ray study; T = 293 K; mean σ(C–C) = 0.004 Å; disorder in main residue; R factor = 0.040; wR factor = 0.104; data-to-parameter ratio = 9.6.

The asymmetric unit of the title compound, $C_{23}H_{22}N_2O_2$, contains two independent molecules, *A* and *B*. The cyclohexane ring of molecule *B* is disordered, with occupancies for the major and minor conformers of 0.570 (9) and 0.430 (9), respectively. The cyclohexane ring adopts a boat conformation in molecule *A* and in the major conformer of molecule *B*, and a chair conformation in the minor conformer of molecule *B*. In both independent molecules, one of the dihydropyran rings adopts a boat conformation while the other is in a half-chair conformation. The dihedral angle between the pyrazole and phenyl rings is 16.0 (1)° in molecule *A* and 12.9 (1)° in molecule *B*. The crystal packing is stabilized by C—H···O and C—H···N intermolecular hydrogen bonds.

Related literature

For related literature, see: Barbieri (1928); Bigdeli *et al.* (2007). Ion & Fara (1995); Sirkecioglu *et al.* (1995). For ring conformations, see: Cremer & Pople (1975); Nardelli (1983).



Experimental

Crystal data

$C_{23}H_{22}N_2O_2$
M_r = 358.43
Orthorhombic, $P2_12_12_1$
a = 9.8050 (3) Å
b = 18.8687 (6) Å
c = 19.9641 (8) Å
V = 3693.5 (2) Å^3
Z = 8
Mo $K\alpha$ radiation
μ = 0.08 mm^{-1}
T = 293 (2) K
0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII area-detector diffractometer
Absorption correction: multi-scan (*SADABS*: Sheldrick, 1996)
T_{min} = 0.976, T_{max} = 0.984
23902 measured reflections
4888 independent reflections
3380 reflections with $I > 2\sigma(I)$
R_{int} = 0.033

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.040
$wR(F^2)$ = 0.104
S = 1.07
4888 reflections
509 parameters
45 restraints
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.22 e Å^{-3}
$\Delta\rho_{min}$ = −0.13 e Å^{-3}

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

D—H···A	D—H	H···A	D···A	D—H···A
C15*A*—H15*A*···O1*B*^{i}	0.98	2.47	3.417 (3)	163
C15*B*—H15*B*···O1*A*^{ii}	0.98	2.53	3.432 (3)	153
C18*A*—H18*A*···O2*A*	0.93	2.31	2.922 (3)	123
C18*B*—H18*B*···O2*B*	0.93	2.30	2.915 (3)	123
C14*B*—H14*B*···N1*A*	0.98	2.61	3.488 (3)	149

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

Data collection: *APEX2* (Bruker, 2004); cell refinement: *APEX2*; data reduction: *SAINT* (Bruker, 2004); program(s) used to solve structure: *SHELXS97* (Sheldrick, 1997); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *ORTEP-3* (Farrugia, 1997); software used to prepare material for publication: *PLATON* (Spek, 2003).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: CI2533).

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supplementary materials

Acta Cryst. (2008). E**64**, o245-o246 [**doi:10.1107/S1600536807065348**]

cis-3-Methyl-1-phenyl-8a,9,10,11,12,12a,12b-hexahydro-1*H*,3b*H*-pyrazolo[3,4:2',3']pyrano[4',5',6'-*kl*]xanthene

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Comment

Xanthene derivatives find wide range of applications as biological stains, sensitizers, tracing agents, photochromic and thermochromic agents. Halogenated xanthene dyes possess light dependent insecticidial properties (Barbieri *et al.*, 1928). Owing to their spectroscopic properties, xanthenes have interesting applications in laser technologies (Sirkecioglu *et al.*, 1995; Ion *et al.*, 1995). In view of this importance, an X-ray crystal structure determination of the title compound was carried out and the results are presented here.

The asymmetric unit of the title compound contains two independent molecules, A and B, with similar geometric parameters. Bond lengths and angles are comparable with those of a related structure (Bigdeli *et al.*,2007). The cyclohexane ring adopts a boat conformation in molecule A and also in the major conformer of molecule B; the ring adopts a chair conformation in the minor conformer of molecule B. One of the dihydropyran ring (O1/C9/C4/C3/C15/C10) adopts a boat conformation, and the other (O2/C14/C15/C3/C3/C16) adopts a half-chair conformation in both molecule A and molecule B (Nardelli, 1983; Cremer and Pople, 1975). The dihedral angle between the pyrazole and phenyl rings is 16.0 (1)° in molecule A and 12.9 (1)° in molecule B.

Intramolecular C—H···O hydrogen bonds are observed. The crystal packing is stabilized by C—H···O and C—H···N intermolecular hydrogen bonds (Table 1).

Experimental

2-(Cyclohexenyloxy)benzaldehyde (2 mmol) and EDDA (2 mmol) were added to a solution of 3-methyl-1-phenyl-pyrazol-5-one (1 mmol) in ethanol (10 ml). The mixture was refluxed until the disappearance of the starting materials, as evidenced by thin-layer chromatography. After the completion of the reaction, the solvent was evaporated under vacuum and the residue was then subjected to flash column chromatography with a hexane-ethyl acetate mixture (8:2 *v*/*v*) to obtain the title compound, which was recrystallized from ethyl acetate.

Refinement

Atoms C11 and C12 in molecule B are disordered over two positions (C11B/C12B and C11C/C12C), with refined occupancies of 0.570 (9) and 0.430 (9). The displacement parameters of disordered atoms were restrained to an approximate isotropic behaviour. The distances involving disordered C-atoms were restrained to be equal. H atoms were placed in idealized positions and allowed to ride on their parent atoms, with C—H = 0.93–0.98 Å and U_{iso}(H)= 1.2–1.5U_{eq}(C). In the absence of significant anomalous dispersion effects, Friedel pairs were merged before the final refinement.

Figures

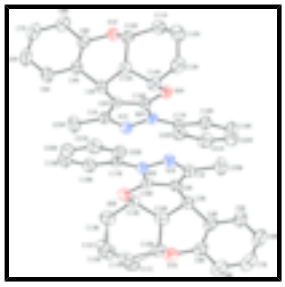


Fig. 1. The asymmetric unit of the title compound. Displacement ellipsoids are drawn at the 30% probability level. Both disorder components are shown, and H atoms have been omitted for clarity.

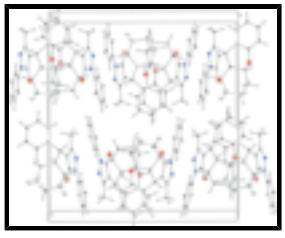


Fig. 2. The packing of the molecules viewed down the *a* axis.

cis-3-Methyl-1-phenyl-8a,9,10,11,12,12*a*,12*b*-hexahydro-\ 1H,3bH-pyrazolo[3,4:2',3']pyrano[4',5',6'-kl]xanthene

Crystal data

$C_{23}H_{22}N_2O_2$	F_{000} = 1520
M_r = 358.43	D_x = 1.289 Mg m^{-3}
Orthorhombic, $P2_12_12_1$	Mo $K\alpha$ radiation λ = 0.71073 Å
Hall symbol: P 2ac 2ab	Cell parameters from 23902 reflections
a = 9.8050 (3) Å	θ = 2.3–27.9º
b = 18.8687 (6) Å	μ = 0.08 mm^{-1}
c = 19.9641 (8) Å	T = 293 (2) K
V = 3693.5 (2) Å^3	Prism, colourless
Z = 8	0.30 × 0.20 × 0.20 mm

Data collection

Bruker Kappa APEXII area-detector diffractometer	4888 independent reflections
Radiation source: fine-focus sealed tube	3380 reflections with $I > 2\sigma(I)$
Monochromator: graphite	R_{int} = 0.033
T = 293(2) K	θ_{max} = 27.9º
ω and φ scans	θ_{min} = 2.3º
Absorption correction: multi-scan (SADABS: Sheldrick, 1996)	h = −12→10
T_{min} = 0.976, T_{max} = 0.984	k = −15→24
23902 measured reflections	l = −24→26

Refinement

Refinement on F^2

Least-squares matrix: full

$R[F^2 > 2\sigma(F^2)] = 0.040$

$wR(F^2) = 0.104$

$S = 1.07$

4888 reflections

509 parameters

45 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

$w = 1/[\sigma^2(F_o^2) + (0.0528P)^2 + 0.0802P]$ where $P = (F_o^2 + 2F_c^2)/3$

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

$\Delta\rho_{max} = 0.22$ e Å^{-3}

$\Delta\rho_{min} = -0.13$ e Å^{-3}

Extinction correction: SHELXL, $Fc^* = kFc[1+0.001xFc^2\lambda^3/\sin(2\theta)]^{-1/4}$

Extinction coefficient: 0.0022 (6)

Special details

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 $F^2 > 2\text{sigma}(F^2)$ 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 (Å^2)

	x	*y*	*z*	U_{iso}*/U_{eq}	Occ. (<1)
O1B	0.2168 (2)	0.56539 (9)	0.28390 (10)	0.0684 (5)	
O2B	0.21954 (17)	0.40373 (8)	0.19723 (8)	0.0555 (4)	
N1B	0.4657 (2)	0.35148 (10)	0.31589 (9)	0.0533 (5)	
N2B	0.41590 (19)	0.35816 (9)	0.25145 (9)	0.0480 (5)	
C1B	0.3689 (3)	0.37822 (13)	0.35474 (12)	0.0542 (6)	
C2B	0.2560 (2)	0.40253 (11)	0.31781 (11)	0.0471 (5)	
C3B	0.1250 (2)	0.43982 (12)	0.33602 (12)	0.0534 (6)	
H3B	0.0646	0.4065	0.3593	0.064*	
C4B	0.1569 (3)	0.50154 (13)	0.38226 (13)	0.0583 (6)	
C5B	0.1444 (3)	0.49972 (16)	0.45098 (15)	0.0781 (8)	
H5B	0.1034	0.4609	0.4714	0.094*	
C6B	0.1917 (4)	0.5545 (2)	0.48974 (17)	0.0965 (11)	
H6B	0.1834	0.5527	0.5361	0.116*	
C7B	0.2516 (4)	0.61211 (19)	0.45937 (19)	0.0970 (11)	

H7B	0.2871	0.6483	0.4857	0.116*	
C8B	0.2599 (3)	0.61702 (15)	0.39076 (17)	0.0813 (9)	
H8B	0.2971	0.6570	0.3705	0.098*	
C9B	0.2119 (3)	0.56159 (13)	0.35275 (14)	0.0607 (7)	
C10B	0.0893 (3)	0.54334 (13)	0.25511 (14)	0.0733 (8)	
H10B	0.0151	0.5752	0.2682	0.088*	0.570 (9)
H10C	0.0256	0.5680	0.2832	0.088*	0.430 (9)
C11B	0.1326 (7)	0.5556 (3)	0.1798 (2)	0.0705 (19)	0.570 (9)
H11C	0.1418	0.6059	0.1707	0.085*	0.570 (9)
H11D	0.2192	0.5328	0.1708	0.085*	0.570 (9)
C12B	0.0211 (8)	0.5237 (3)	0.1361 (5)	0.089 (3)	0.570 (9)
H12C	0.0405	0.5333	0.0893	0.107*	0.570 (9)
H12D	−0.0660	0.5452	0.1471	0.107*	0.570 (9)
C11C	0.0371 (8)	0.5653 (3)	0.1871 (3)	0.065 (2)	0.430 (9)
H11E	0.0699	0.6126	0.1769	0.078*	0.430 (9)
H11F	−0.0618	0.5670	0.1882	0.078*	0.430 (9)
C12C	0.0823 (9)	0.5147 (3)	0.1316 (5)	0.067 (3)	0.430 (9)
H12E	0.1808	0.5099	0.1313	0.081*	0.430 (9)
H12F	0.0530	0.5320	0.0882	0.081*	0.430 (9)
C13B	0.0140 (3)	0.44301 (14)	0.14769 (14)	0.0724 (8)	
H13C	−0.0811	0.4288	0.1465	0.087*	0.570 (9)
H13D	0.0595	0.4197	0.1106	0.087*	0.570 (9)
H13E	0.0289	0.4093	0.1124	0.087*	0.430 (9)
H13F	−0.0824	0.4508	0.1523	0.087*	0.430 (9)
C14B	0.0757 (2)	0.41616 (13)	0.21218 (13)	0.0554 (6)	
H14B	0.0334	0.3705	0.2230	0.066*	
C15B	0.0541 (2)	0.46588 (12)	0.27109 (13)	0.0563 (6)	
H15B	−0.0440	0.4651	0.2805	0.068*	
C16B	0.2901 (2)	0.38925 (10)	0.25352 (11)	0.0457 (5)	
C17B	0.5004 (2)	0.33943 (11)	0.19663 (11)	0.0459 (5)	
C18B	0.4515 (3)	0.33534 (14)	0.13270 (12)	0.0627 (7)	
H18B	0.3596	0.3438	0.1244	0.075*	
C19B	0.5377 (3)	0.31875 (16)	0.08037 (13)	0.0770 (8)	
H19B	0.5039	0.3168	0.0369	0.092*	
C20B	0.6727 (3)	0.30509 (14)	0.09214 (15)	0.0738 (8)	
H20B	0.7309	0.2942	0.0568	0.089*	
C21B	0.7212 (3)	0.30753 (14)	0.15646 (15)	0.0718 (8)	
H21B	0.8125	0.2973	0.1648	0.086*	
C22B	0.6363 (3)	0.32496 (13)	0.20884 (13)	0.0610 (7)	
H22B	0.6702	0.3270	0.2523	0.073*	
C23B	0.3934 (3)	0.37998 (18)	0.42916 (12)	0.0795 (8)	
H23D	0.4675	0.3488	0.4402	0.119*	
H23E	0.3125	0.3648	0.4521	0.119*	
H23F	0.4158	0.4274	0.4426	0.119*	
O1A	0.28163 (18)	0.01702 (8)	0.22341 (8)	0.0553 (4)	
O2A	0.30478 (17)	0.17572 (9)	0.32648 (8)	0.0565 (4)	
N1A	0.0423 (2)	0.23226 (10)	0.21904 (10)	0.0538 (5)	
N2A	0.1013 (2)	0.22336 (9)	0.28119 (9)	0.0482 (5)	
C1A	0.1325 (3)	0.20775 (12)	0.17563 (12)	0.0516 (6)	

C2A	0.2510 (2)	0.18142 (11)	0.20765 (11)	0.0465 (5)
C3A	0.3792 (2)	0.14560 (11)	0.18298 (11)	0.0483 (5)
H3A	0.4390	0.1812	0.1626	0.058*
C4A	0.3474 (2)	0.08915 (13)	0.13172 (11)	0.0503 (6)
C5A	0.3621 (3)	0.09738 (16)	0.06323 (13)	0.0712 (8)
H5A	0.4006	0.1387	0.0463	0.085*
C6A	0.3202 (4)	0.04481 (19)	0.01978 (14)	0.0855 (10)
H6A	0.3292	0.0511	−0.0262	0.103*
C7A	0.2650 (3)	−0.0169 (2)	0.04454 (16)	0.0849 (9)
H7A	0.2357	−0.0519	0.0151	0.102*
C8A	0.2529 (3)	−0.02709 (15)	0.11252 (14)	0.0709 (8)
H8A	0.2174	−0.0692	0.1293	0.085*
C9A	0.2943 (2)	0.02610 (12)	0.15548 (12)	0.0527 (6)
C10A	0.4048 (3)	0.03596 (12)	0.25862 (12)	0.0547 (6)
H10A	0.4775	0.0037	0.2443	0.066*
C11A	0.3751 (3)	0.02188 (15)	0.33230 (14)	0.0735 (8)
H11A	0.2901	0.0446	0.3447	0.088*
H11B	0.3651	−0.0287	0.3395	0.088*
C12A	0.4873 (4)	0.04944 (17)	0.37496 (15)	0.0902 (10)
H12A	0.5702	0.0237	0.3645	0.108*
H12B	0.4652	0.0403	0.4215	0.108*
C13A	0.5138 (3)	0.12822 (15)	0.36626 (14)	0.0749 (8)
H13A	0.4824	0.1528	0.4060	0.090*
H13B	0.6114	0.1357	0.3628	0.090*
C14A	0.4457 (2)	0.16051 (13)	0.30581 (12)	0.0560 (6)
H14A	0.4912	0.2054	0.2952	0.067*
C15A	0.4520 (2)	0.11287 (11)	0.24473 (11)	0.0494 (5)
H15A	0.5486	0.1096	0.2326	0.059*
C16A	0.2256 (2)	0.19265 (10)	0.27361 (11)	0.0450 (5)
C17A	0.0289 (3)	0.24384 (11)	0.33924 (12)	0.0497 (6)
C18A	0.0930 (3)	0.25198 (13)	0.40004 (13)	0.0641 (7)
H18A	0.1859	0.2431	0.4038	0.077*
C19A	0.0194 (4)	0.27338 (16)	0.45541 (14)	0.0792 (9)
H19A	0.0632	0.2791	0.4964	0.095*
C20A	−0.1176 (4)	0.28617 (15)	0.45039 (16)	0.0804 (9)
H20A	−0.1670	0.3001	0.4879	0.096*
C21A	−0.1819 (3)	0.27838 (14)	0.38969 (17)	0.0764 (9)
H21A	−0.2748	0.2876	0.3861	0.092*
C22A	−0.1094 (3)	0.25704 (13)	0.33428 (14)	0.0611 (7)
H22A	−0.1535	0.2515	0.2934	0.073*
C23A	0.0994 (3)	0.21042 (17)	0.10262 (12)	0.0774 (9)
H23A	0.0138	0.2342	0.0963	0.116*
H23B	0.0932	0.1631	0.0853	0.116*
H23C	0.1698	0.2357	0.0793	0.116*

Atomic displacement parameters (Å^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}

O1B	0.0666 (12)	0.0546 (9)	0.0839 (13)	−0.0046 (9)	0.0256 (11)	−0.0007 (9)
O2B	0.0525 (10)	0.0615 (9)	0.0525 (9)	0.0149 (8)	−0.0014 (8)	−0.0001 (7)
N1B	0.0537 (12)	0.0601 (11)	0.0463 (11)	0.0070 (9)	−0.0029 (10)	−0.0003 (9)
N2B	0.0503 (12)	0.0464 (10)	0.0473 (11)	0.0080 (9)	0.0001 (9)	−0.0012 (8)
C1B	0.0592 (15)	0.0552 (13)	0.0481 (14)	−0.0004 (12)	0.0019 (12)	−0.0003 (11)
C2B	0.0471 (14)	0.0432 (11)	0.0509 (13)	−0.0030 (10)	0.0050 (11)	0.0010 (10)
C3B	0.0459 (13)	0.0532 (13)	0.0610 (14)	−0.0048 (11)	0.0149 (12)	0.0038 (11)
C4B	0.0504 (14)	0.0564 (15)	0.0679 (17)	−0.0002 (12)	0.0163 (13)	−0.0088 (12)
C5B	0.087 (2)	0.0772 (18)	0.0697 (19)	−0.0013 (16)	0.0265 (17)	−0.0091 (16)
C6B	0.108 (3)	0.102 (2)	0.080 (2)	0.002 (2)	0.019 (2)	−0.025 (2)
C7B	0.089 (2)	0.093 (2)	0.109 (3)	−0.010 (2)	0.012 (2)	−0.049 (2)
C8B	0.071 (2)	0.0642 (17)	0.109 (2)	−0.0098 (15)	0.0253 (19)	−0.0212 (17)
C9B	0.0499 (14)	0.0567 (14)	0.0756 (18)	−0.0002 (12)	0.0187 (14)	−0.0097 (13)
C10B	0.082 (2)	0.0527 (15)	0.085 (2)	0.0182 (14)	−0.0041 (17)	−0.0037 (14)
C11B	0.067 (4)	0.062 (3)	0.083 (4)	0.002 (3)	0.008 (3)	0.021 (3)
C12B	0.072 (5)	0.089 (5)	0.107 (5)	0.003 (4)	−0.015 (5)	0.017 (4)
C11C	0.047 (4)	0.055 (3)	0.093 (5)	0.007 (3)	0.002 (4)	0.018 (3)
C12C	0.061 (5)	0.069 (5)	0.072 (5)	0.014 (4)	−0.007 (5)	0.020 (4)
C13B	0.0637 (17)	0.0737 (18)	0.080 (2)	−0.0011 (15)	−0.0177 (15)	0.0078 (15)
C14B	0.0432 (13)	0.0523 (13)	0.0705 (17)	−0.0051 (10)	−0.0026 (12)	0.0044 (12)
C15B	0.0380 (12)	0.0578 (14)	0.0731 (17)	0.0017 (11)	0.0099 (12)	0.0056 (12)
C16B	0.0482 (13)	0.0374 (11)	0.0514 (13)	0.0022 (10)	0.0002 (11)	0.0015 (9)
C17B	0.0511 (13)	0.0372 (11)	0.0494 (13)	0.0050 (10)	0.0025 (11)	0.0008 (9)
C18B	0.0585 (15)	0.0715 (16)	0.0581 (16)	0.0131 (13)	0.0027 (13)	0.0001 (13)
C19B	0.091 (2)	0.089 (2)	0.0509 (16)	0.0254 (18)	0.0092 (16)	0.0040 (14)
C20B	0.079 (2)	0.0733 (18)	0.0685 (19)	0.0241 (15)	0.0251 (16)	0.0064 (14)
C21B	0.0570 (16)	0.0726 (17)	0.086 (2)	0.0153 (14)	0.0144 (16)	0.0011 (15)
C22B	0.0579 (16)	0.0606 (15)	0.0646 (16)	0.0160 (12)	0.0001 (14)	−0.0028 (13)
C23B	0.080 (2)	0.107 (2)	0.0514 (16)	0.0110 (18)	−0.0035 (15)	−0.0047 (15)
O1A	0.0589 (10)	0.0563 (9)	0.0506 (10)	−0.0068 (8)	0.0046 (8)	−0.0045 (8)
O2A	0.0574 (10)	0.0623 (10)	0.0498 (9)	0.0163 (8)	−0.0063 (8)	−0.0070 (8)
N1A	0.0515 (12)	0.0575 (11)	0.0525 (12)	0.0107 (10)	−0.0041 (10)	−0.0020 (9)
N2A	0.0512 (12)	0.0481 (10)	0.0455 (11)	0.0102 (9)	0.0010 (9)	−0.0041 (8)
C1A	0.0543 (14)	0.0516 (13)	0.0489 (14)	0.0070 (11)	−0.0012 (12)	−0.0019 (10)
C2A	0.0498 (14)	0.0427 (11)	0.0471 (13)	0.0021 (10)	0.0020 (11)	−0.0013 (10)
C3A	0.0431 (12)	0.0498 (12)	0.0519 (14)	−0.0024 (10)	0.0066 (11)	0.0029 (10)
C4A	0.0449 (13)	0.0595 (14)	0.0466 (13)	0.0081 (11)	0.0067 (11)	−0.0046 (11)
C5A	0.0761 (19)	0.0848 (19)	0.0526 (16)	0.0123 (16)	0.0129 (14)	0.0012 (14)
C6A	0.098 (3)	0.113 (3)	0.0460 (16)	0.023 (2)	0.0048 (16)	−0.0185 (17)
C7A	0.087 (2)	0.100 (2)	0.068 (2)	0.006 (2)	−0.0067 (17)	−0.0346 (18)
C8A	0.0676 (18)	0.0724 (17)	0.0726 (19)	−0.0074 (15)	0.0026 (15)	−0.0216 (14)
C9A	0.0460 (13)	0.0586 (14)	0.0534 (15)	0.0039 (11)	0.0037 (11)	−0.0090 (11)
C10A	0.0561 (15)	0.0495 (13)	0.0585 (15)	0.0101 (11)	−0.0027 (12)	−0.0047 (11)
C11A	0.087 (2)	0.0682 (17)	0.0660 (17)	0.0043 (16)	−0.0094 (17)	0.0080 (14)
C12A	0.103 (3)	0.096 (2)	0.0715 (19)	0.005 (2)	−0.0242 (19)	0.0100 (16)
C13A	0.0642 (17)	0.087 (2)	0.0734 (19)	0.0123 (16)	−0.0257 (15)	−0.0178 (15)
C14A	0.0447 (13)	0.0585 (14)	0.0649 (15)	−0.0008 (11)	−0.0057 (12)	−0.0108 (12)
C15A	0.0347 (11)	0.0558 (13)	0.0578 (14)	0.0031 (10)	0.0030 (11)	−0.0051 (11)
C16A	0.0494 (13)	0.0389 (11)	0.0466 (13)	0.0044 (10)	−0.0019 (11)	−0.0016 (9)

C17A	0.0597 (15)	0.0380 (11)	0.0515 (14)	0.0066 (10)	0.0106 (12)	0.0030 (10)
C18A	0.0673 (17)	0.0716 (17)	0.0533 (16)	0.0125 (14)	0.0060 (14)	−0.0058 (12)
C19A	0.094 (2)	0.090 (2)	0.0536 (17)	0.0166 (18)	0.0119 (16)	−0.0093 (14)
C20A	0.095 (2)	0.0783 (19)	0.068 (2)	0.0177 (17)	0.0329 (19)	0.0012 (15)
C21A	0.0666 (19)	0.0690 (18)	0.094 (2)	0.0146 (15)	0.0250 (17)	0.0024 (16)
C22A	0.0561 (16)	0.0602 (15)	0.0670 (17)	0.0102 (12)	0.0050 (14)	−0.0011 (12)
C23A	0.076 (2)	0.106 (2)	0.0496 (16)	0.0238 (17)	−0.0069 (14)	0.0007 (15)

Geometric parameters (Å, °)

O1B—C9B	1.377 (3)	C21B—H21B	0.93
O1B—C10B	1.438 (3)	C22B—H22B	0.93
O2B—C16B	1.348 (3)	C23B—H23D	0.96
O2B—C14B	1.461 (3)	C23B—H23E	0.96
N1B—C1B	1.325 (3)	C23B—H23F	0.96
N1B—N2B	1.382 (3)	O1A—C9A	1.373 (3)
N2B—C16B	1.366 (3)	O1A—C10A	1.443 (3)
N2B—C17B	1.418 (3)	O2A—C16A	1.349 (3)
C1B—C2B	1.407 (3)	O2A—C14A	1.470 (3)
C1B—C23B	1.505 (3)	N1A—C1A	1.322 (3)
C2B—C16B	1.350 (3)	N1A—N2A	1.379 (3)
C2B—C3B	1.509 (3)	N2A—C16A	1.358 (3)
C3B—C4B	1.519 (3)	N2A—C17A	1.413 (3)
C3B—C15B	1.551 (3)	C1A—C2A	1.416 (3)
C3B—H3B	0.98	C1A—C23A	1.494 (3)
C4B—C5B	1.378 (4)	C2A—C16A	1.357 (3)
C4B—C9B	1.387 (3)	C2A—C3A	1.510 (3)
C5B—C6B	1.372 (4)	C3A—C4A	1.510 (3)
C5B—H5B	0.93	C3A—C15A	1.553 (3)
C6B—C7B	1.376 (5)	C3A—H3A	0.98
C6B—H6B	0.93	C4A—C9A	1.383 (3)
C7B—C8B	1.375 (4)	C4A—C5A	1.384 (3)
C7B—H7B	0.93	C5A—C6A	1.380 (4)
C8B—C9B	1.375 (4)	C5A—H5A	0.93
C8B—H8B	0.93	C6A—C7A	1.375 (4)
C10B—C11C	1.510 (5)	C6A—H6A	0.93
C10B—C15B	1.535 (3)	C7A—C8A	1.376 (4)
C10B—C11B	1.579 (5)	C7A—H7A	0.93
C10B—H10B	0.98	C8A—C9A	1.381 (3)
C10B—H10C	0.96	C8A—H8A	0.93
C11B—C12B	1.522 (6)	C10A—C11A	1.523 (4)
C11B—H11C	0.97	C10A—C15A	1.548 (3)
C11B—H11D	0.97	C10A—H10A	0.98
C12B—C13B	1.542 (6)	C11A—C12A	1.485 (4)
C12B—H12C	0.97	C11A—H11A	0.97
C12B—H12D	0.97	C11A—H11B	0.97
C11C—C12C	1.528 (7)	C12A—C13A	1.519 (4)
C11C—H11E	0.97	C12A—H12A	0.97
C11C—H11F	0.97	C12A—H12B	0.97

C12C—C13B	1.543 (6)	C13A—C14A	1.508 (4)
C12C—H12E	0.97	C13A—H13A	0.97
C12C—H12F	0.97	C13A—H13B	0.97
C13B—C14B	1.510 (3)	C14A—C15A	1.516 (3)
C13B—H13C	0.97	C14A—H14A	0.98
C13B—H13D	0.97	C15A—H15A	0.98
C13B—H13E	0.96	C17A—C18A	1.375 (4)
C13B—H13F	0.96	C17A—C22A	1.382 (4)
C14B—C15B	1.519 (3)	C18A—C19A	1.380 (4)
C14B—H14B	0.98	C18A—H18A	0.93
C15B—H15B	0.98	C19A—C20A	1.369 (5)
C17B—C18B	1.366 (3)	C19A—H19A	0.93
C17B—C22B	1.381 (3)	C20A—C21A	1.374 (4)
C18B—C19B	1.380 (4)	C20A—H20A	0.93
C18B—H18B	0.93	C21A—C22A	1.375 (4)
C19B—C20B	1.369 (4)	C21A—H21A	0.93
C19B—H19B	0.93	C22A—H22A	0.93
C20B—C21B	1.370 (4)	C23A—H23A	0.96
C20B—H20B	0.93	C23A—H23B	0.96
C21B—C22B	1.377 (4)	C23A—H23C	0.96
C9B—O1B—C10B	110.7 (2)	C19B—C20B—H20B	120.3
C16B—O2B—C14B	110.97 (18)	C21B—C20B—H20B	120.3
C1B—N1B—N2B	104.91 (18)	C20B—C21B—C22B	120.6 (3)
C16B—N2B—N1B	109.26 (18)	C20B—C21B—H21B	119.7
C16B—N2B—C17B	131.16 (19)	C22B—C21B—H21B	119.7
N1B—N2B—C17B	119.31 (18)	C21B—C22B—C17B	119.8 (3)
N1B—C1B—C2B	112.4 (2)	C21B—C22B—H22B	120.1
N1B—C1B—C23B	118.2 (2)	C17B—C22B—H22B	120.1
C2B—C1B—C23B	129.5 (2)	C1B—C23B—H23D	109.5
C16B—C2B—C1B	104.0 (2)	C1B—C23B—H23E	109.5
C16B—C2B—C3B	121.8 (2)	H23D—C23B—H23E	109.5
C1B—C2B—C3B	134.1 (2)	C1B—C23B—H23F	109.5
C2B—C3B—C4B	109.2 (2)	H23D—C23B—H23F	109.5
C2B—C3B—C15B	109.15 (19)	H23E—C23B—H23F	109.5
C4B—C3B—C15B	110.9 (2)	C9A—O1A—C10A	112.02 (19)
C2B—C3B—H3B	109.2	C16A—O2A—C14A	111.58 (18)
C4B—C3B—H3B	109.2	C1A—N1A—N2A	105.45 (19)
C15B—C3B—H3B	109.2	C16A—N2A—N1A	109.16 (18)
C5B—C4B—C9B	118.6 (3)	C16A—N2A—C17A	131.2 (2)
C5B—C4B—C3B	124.6 (2)	N1A—N2A—C17A	119.59 (18)
C9B—C4B—C3B	116.7 (2)	N1A—C1A—C2A	112.1 (2)
C6B—C5B—C4B	120.9 (3)	N1A—C1A—C23A	118.8 (2)
C6B—C5B—H5B	119.6	C2A—C1A—C23A	129.1 (2)
C4B—C5B—H5B	119.6	C16A—C2A—C1A	103.5 (2)
C5B—C6B—C7B	119.4 (3)	C16A—C2A—C3A	122.7 (2)
C5B—C6B—H6B	120.3	C1A—C2A—C3A	133.9 (2)
C7B—C6B—H6B	120.3	C4A—C3A—C2A	111.42 (18)
C8B—C7B—C6B	121.1 (3)	C4A—C3A—C15A	110.65 (18)
C8B—C7B—H7B	119.4	C2A—C3A—C15A	107.56 (17)

C6B—C7B—H7B	119.4	C4A—C3A—H3A	109.1
C9B—C8B—C7B	118.6 (3)	C2A—C3A—H3A	109.1
C9B—C8B—H8B	120.7	C15A—C3A—H3A	109.1
C7B—C8B—H8B	120.7	C9A—C4A—C5A	118.4 (2)
C8B—C9B—O1B	120.0 (3)	C9A—C4A—C3A	116.9 (2)
C8B—C9B—C4B	121.3 (3)	C5A—C4A—C3A	124.7 (2)
O1B—C9B—C4B	118.7 (2)	C6A—C5A—C4A	120.6 (3)
O1B—C10B—C11C	125.1 (4)	C6A—C5A—H5A	119.7
O1B—C10B—C15B	112.8 (2)	C4A—C5A—H5A	119.7
C11C—C10B—C15B	111.8 (3)	C7A—C6A—C5A	120.0 (3)
O1B—C10B—C11B	96.0 (3)	C7A—C6A—H6A	120.0
C15B—C10B—C11B	113.5 (3)	C5A—C6A—H6A	120.0
O1B—C10B—H10B	111.2	C6A—C7A—C8A	120.5 (3)
C15B—C10B—H10B	111.2	C6A—C7A—H7A	119.8
C11B—C10B—H10B	111.2	C8A—C7A—H7A	119.8
O1B—C10B—H10C	101.1	C7A—C8A—C9A	119.0 (3)
C15B—C10B—H10C	101.2	C7A—C8A—H8A	120.5
C11B—C10B—H10C	131.3	C9A—C8A—H8A	120.5
C12B—C11B—C10B	107.2 (6)	O1A—C9A—C8A	119.8 (2)
C12B—C11B—H11C	110.3	O1A—C9A—C4A	118.7 (2)
C10B—C11B—H11C	110.3	C8A—C9A—C4A	121.5 (2)
C12B—C11B—H11D	110.3	O1A—C10A—C11A	105.5 (2)
C10B—C11B—H11D	110.3	O1A—C10A—C15A	113.26 (19)
H11C—C11B—H11D	108.5	C11A—C10A—C15A	113.2 (2)
C11B—C12B—C13B	109.7 (5)	O1A—C10A—H10A	108.2
C11B—C12B—H12C	109.7	C11A—C10A—H10A	108.2
C13B—C12B—H12C	109.7	C15A—C10A—H10A	108.2
C11B—C12B—H12D	109.7	C12A—C11A—C10A	110.6 (3)
C13B—C12B—H12D	109.7	C12A—C11A—H11A	109.5
H12C—C12B—H12D	108.2	C10A—C11A—H11A	109.5
C10B—C11C—C12C	112.5 (6)	C12A—C11A—H11B	109.5
C10B—C11C—H11E	109.1	C10A—C11A—H11B	109.5
C12C—C11C—H11E	109.1	H11A—C11A—H11B	108.1
C10B—C11C—H11F	109.1	C11A—C12A—C13A	113.8 (2)
C12C—C11C—H11F	109.1	C11A—C12A—H12A	108.8
H11E—C11C—H11F	107.8	C13A—C12A—H12A	108.8
C11C—C12C—C13B	105.7 (5)	C11A—C12A—H12B	108.8
C11C—C12C—H12E	110.6	C13A—C12A—H12B	108.8
C13B—C12C—H12E	110.6	H12A—C12A—H12B	107.7
C11C—C12C—H12F	110.6	C14A—C13A—C12A	114.3 (2)
C13B—C12C—H12F	110.6	C14A—C13A—H13A	108.7
H12E—C12C—H12F	108.7	C12A—C13A—H13A	108.7
C14B—C13B—C12B	116.2 (4)	C14A—C13A—H13B	108.7
C14B—C13B—C12C	107.3 (4)	C12A—C13A—H13B	108.7
C14B—C13B—H13C	108.2	H13A—C13A—H13B	107.6
C12B—C13B—H13C	108.2	O2A—C14A—C13A	105.7 (2)
C12C—C13B—H13C	130.9	O2A—C14A—C15A	112.32 (18)
C14B—C13B—H13D	108.2	C13A—C14A—C15A	112.7 (2)
C12B—C13B—H13D	108.2	O2A—C14A—H14A	108.7

H13C—C13B—H13D	107.4	C13A—C14A—H14A	108.7
C14B—C13B—H13E	109.9	C15A—C14A—H14A	108.7
C12B—C13B—H13E	122.5	C14A—C15A—C10A	113.5 (2)
C12C—C13B—H13E	111.2	C14A—C15A—C3A	112.59 (18)
H13C—C13B—H13E	86.9	C10A—C15A—C3A	112.20 (19)
C14B—C13B—H13F	111.4	C14A—C15A—H15A	105.9
C12B—C13B—H13F	84.8	C10A—C15A—H15A	105.9
C12C—C13B—H13F	108.3	C3A—C15A—H15A	105.9
H13D—C13B—H13F	126.5	O2A—C16A—C2A	128.1 (2)
H13E—C13B—H13F	108.7	O2A—C16A—N2A	122.1 (2)
O2B—C14B—C13B	105.5 (2)	C2A—C16A—N2A	109.9 (2)
O2B—C14B—C15B	113.08 (19)	C18A—C17A—C22A	119.4 (2)
C13B—C14B—C15B	113.4 (2)	C18A—C17A—N2A	121.7 (2)
O2B—C14B—H14B	108.2	C22A—C17A—N2A	118.9 (2)
C13B—C14B—H14B	108.2	C17A—C18A—C19A	120.0 (3)
C15B—C14B—H14B	108.2	C17A—C18A—H18A	120.0
C14B—C15B—C10B	113.3 (2)	C19A—C18A—H18A	120.0
C14B—C15B—C3B	112.87 (19)	C20A—C19A—C18A	120.4 (3)
C10B—C15B—C3B	112.0 (2)	C20A—C19A—H19A	119.8
C14B—C15B—H15B	106.0	C18A—C19A—H19A	119.8
C10B—C15B—H15B	106.0	C19A—C20A—C21A	119.7 (3)
C3B—C15B—H15B	106.0	C19A—C20A—H20A	120.1
O2B—C16B—C2B	128.9 (2)	C21A—C20A—H20A	120.1
O2B—C16B—N2B	121.7 (2)	C20A—C21A—C22A	120.3 (3)
C2B—C16B—N2B	109.4 (2)	C20A—C21A—H21A	119.9
C18B—C17B—C22B	119.5 (2)	C22A—C21A—H21A	119.9
C18B—C17B—N2B	122.0 (2)	C21A—C22A—C17A	120.1 (3)
C22B—C17B—N2B	118.5 (2)	C21A—C22A—H22A	119.9
C17B—C18B—C19B	120.3 (3)	C17A—C22A—H22A	119.9
C17B—C18B—H18B	119.8	C1A—C23A—H23A	109.5
C19B—C18B—H18B	119.8	C1A—C23A—H23B	109.5
C20B—C19B—C18B	120.3 (3)	H23A—C23A—H23B	109.5
C20B—C19B—H19B	119.8	C1A—C23A—H23C	109.5
C18B—C19B—H19B	119.8	H23A—C23A—H23C	109.5
C19B—C20B—C21B	119.4 (3)	H23B—C23A—H23C	109.5
C1B—N1B—N2B—C16B	0.3 (2)	C17B—C18B—C19B—C20B	1.1 (5)
C1B—N1B—N2B—C17B	174.95 (19)	C18B—C19B—C20B—C21B	0.5 (5)
N2B—N1B—C1B—C2B	0.0 (3)	C19B—C20B—C21B—C22B	−1.3 (4)
N2B—N1B—C1B—C23B	−178.9 (2)	C20B—C21B—C22B—C17B	0.7 (4)
N1B—C1B—C2B—C16B	−0.3 (3)	C18B—C17B—C22B—C21B	0.9 (4)
C23B—C1B—C2B—C16B	178.5 (3)	N2B—C17B—C22B—C21B	−179.2 (2)
N1B—C1B—C2B—C3B	−176.4 (2)	C1A—N1A—N2A—C16A	−0.8 (2)
C23B—C1B—C2B—C3B	2.3 (4)	C1A—N1A—N2A—C17A	−179.2 (2)
C16B—C2B—C3B—C4B	−128.2 (2)	N2A—N1A—C1A—C2A	0.9 (3)
C1B—C2B—C3B—C4B	47.4 (3)	N2A—N1A—C1A—C23A	−179.5 (2)
C16B—C2B—C3B—C15B	−6.7 (3)	N1A—C1A—C2A—C16A	−0.6 (3)
C1B—C2B—C3B—C15B	168.8 (2)	C23A—C1A—C2A—C16A	179.8 (3)
C2B—C3B—C4B—C5B	−98.7 (3)	N1A—C1A—C2A—C3A	176.9 (2)
C15B—C3B—C4B—C5B	141.0 (3)	C23A—C1A—C2A—C3A	−2.7 (4)

C2B—C3B—C4B—C9B	76.3 (3)	C16A—C2A—C3A—C4A	132.9 (2)
C15B—C3B—C4B—C9B	−44.1 (3)	C1A—C2A—C3A—C4A	−44.2 (3)
C9B—C4B—C5B—C6B	−3.3 (5)	C16A—C2A—C3A—C15A	11.4 (3)
C3B—C4B—C5B—C6B	171.5 (3)	C1A—C2A—C3A—C15A	−165.7 (2)
C4B—C5B—C6B—C7B	0.4 (5)	C2A—C3A—C4A—C9A	−75.7 (2)
C5B—C6B—C7B—C8B	2.7 (6)	C15A—C3A—C4A—C9A	43.9 (3)
C6B—C7B—C8B—C9B	−2.7 (5)	C2A—C3A—C4A—C5A	101.4 (3)
C7B—C8B—C9B—O1B	179.0 (3)	C15A—C3A—C4A—C5A	−139.0 (2)
C7B—C8B—C9B—C4B	−0.3 (5)	C9A—C4A—C5A—C6A	2.3 (4)
C10B—O1B—C9B—C8B	−133.9 (3)	C3A—C4A—C5A—C6A	−174.8 (2)
C10B—O1B—C9B—C4B	45.5 (3)	C4A—C5A—C6A—C7A	−1.0 (5)
C5B—C4B—C9B—C8B	3.3 (4)	C5A—C6A—C7A—C8A	−0.9 (5)
C3B—C4B—C9B—C8B	−172.0 (2)	C6A—C7A—C8A—C9A	1.4 (5)
C5B—C4B—C9B—O1B	−176.1 (2)	C10A—O1A—C9A—C8A	132.4 (2)
C3B—C4B—C9B—O1B	8.7 (4)	C10A—O1A—C9A—C4A	−48.3 (3)
C9B—O1B—C10B—C11C	155.7 (4)	C7A—C8A—C9A—O1A	179.4 (3)
C9B—O1B—C10B—C15B	−62.2 (3)	C7A—C8A—C9A—C4A	0.0 (4)
C9B—O1B—C10B—C11B	179.2 (3)	C5A—C4A—C9A—O1A	178.8 (2)
O1B—C10B—C11B—C12B	170.4 (5)	C3A—C4A—C9A—O1A	−3.9 (3)
C11C—C10B—C11B—C12B	−43.1 (5)	C5A—C4A—C9A—C8A	−1.8 (4)
C15B—C10B—C11B—C12B	52.3 (6)	C3A—C4A—C9A—C8A	175.5 (2)
C10B—C11B—C12B—C13B	−63.6 (9)	C9A—O1A—C10A—C11A	−179.09 (19)
O1B—C10B—C11C—C12C	89.8 (6)	C9A—O1A—C10A—C15A	56.6 (2)
C15B—C10B—C11C—C12C	−52.6 (7)	O1A—C10A—C11A—C12A	−171.6 (2)
C11B—C10B—C11C—C12C	47.7 (6)	C15A—C10A—C11A—C12A	−47.2 (3)
C10B—C11C—C12C—C13B	64.4 (9)	C10A—C11A—C12A—C13A	57.8 (4)
C11B—C12B—C13B—C14B	20.3 (10)	C11A—C12A—C13A—C14A	−13.3 (4)
C11B—C12B—C13B—C12C	−52.4 (11)	C16A—O2A—C14A—C13A	−168.59 (19)
C11C—C12C—C13B—C14B	−66.1 (7)	C16A—O2A—C14A—C15A	−45.3 (3)
C11C—C12C—C13B—C12B	50.1 (12)	C12A—C13A—C14A—O2A	82.6 (3)
C16B—O2B—C14B—C13B	171.14 (18)	C12A—C13A—C14A—C15A	−40.5 (4)
C16B—O2B—C14B—C15B	46.7 (3)	O2A—C14A—C15A—C10A	−69.3 (3)
C12B—C13B—C14B—O2B	−87.8 (5)	C13A—C14A—C15A—C10A	50.0 (3)
C12C—C13B—C14B—O2B	−64.2 (4)	O2A—C14A—C15A—C3A	59.6 (3)
C12B—C13B—C14B—C15B	36.5 (6)	C13A—C14A—C15A—C3A	178.8 (2)
C12C—C13B—C14B—C15B	60.1 (4)	O1A—C10A—C15A—C14A	114.3 (2)
O2B—C14B—C15B—C10B	71.9 (3)	C11A—C10A—C15A—C14A	−5.7 (3)
C13B—C14B—C15B—C10B	−48.1 (3)	O1A—C10A—C15A—C3A	−14.8 (3)
O2B—C14B—C15B—C3B	−56.7 (3)	C11A—C10A—C15A—C3A	−134.8 (2)
C13B—C14B—C15B—C3B	−176.7 (2)	C4A—C3A—C15A—C14A	−161.57 (19)
O1B—C10B—C15B—C14B	−104.6 (3)	C2A—C3A—C15A—C14A	−39.7 (2)
C11C—C10B—C15B—C14B	42.7 (4)	C4A—C3A—C15A—C10A	−32.0 (2)
C11B—C10B—C15B—C14B	3.3 (4)	C2A—C3A—C15A—C10A	89.9 (2)
O1B—C10B—C15B—C3B	24.5 (3)	C14A—O2A—C16A—C2A	16.4 (3)
C11C—C10B—C15B—C3B	171.8 (4)	C14A—O2A—C16A—N2A	−165.43 (19)
C11B—C10B—C15B—C3B	132.3 (3)	C1A—C2A—C16A—O2A	178.4 (2)
C2B—C3B—C15B—C14B	34.1 (3)	C3A—C2A—C16A—O2A	0.6 (4)
C4B—C3B—C15B—C14B	154.5 (2)	C1A—C2A—C16A—N2A	0.1 (2)
C2B—C3B—C15B—C10B	−95.2 (2)	C3A—C2A—C16A—N2A	−177.80 (18)

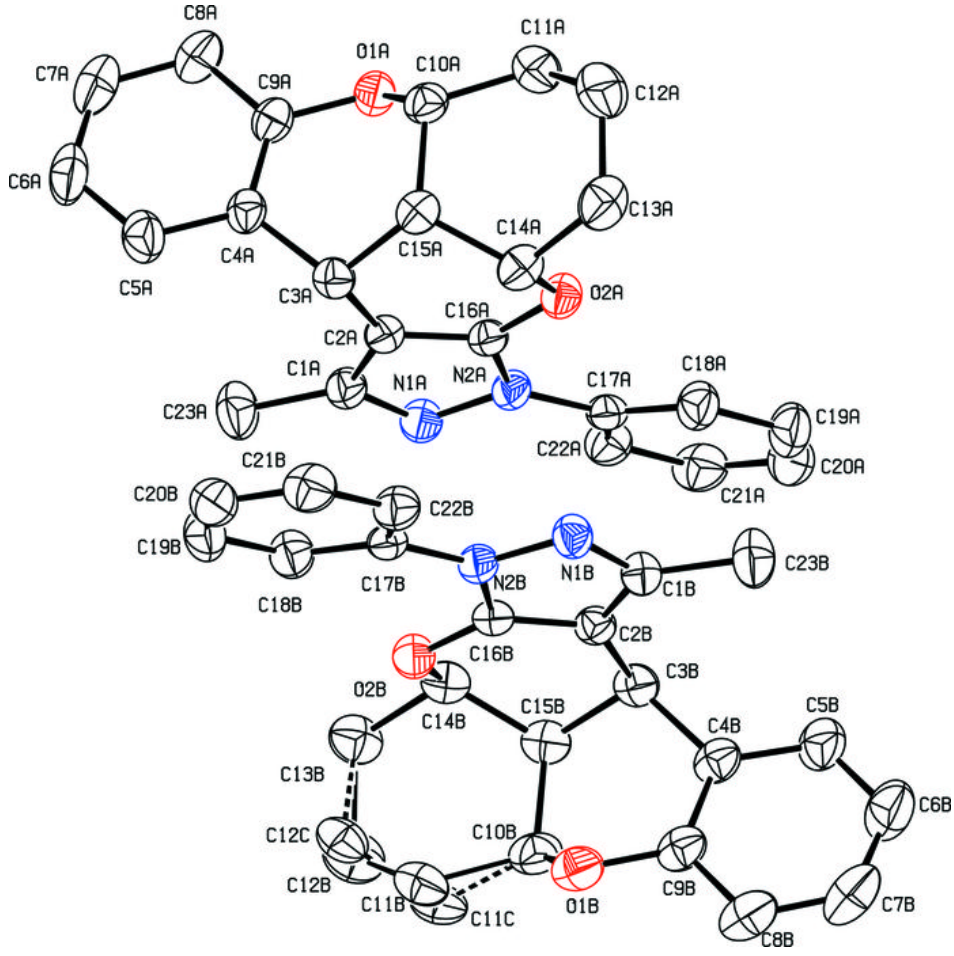
C4B—C3B—C15B—C10B	25.2 (3)	N1A—N2A—C16A—O2A	−178.00 (18)
C14B—O2B—C16B—C2B	−18.7 (3)	C17A—N2A—C16A—O2A	0.1 (3)
C14B—O2B—C16B—N2B	162.71 (19)	N1A—N2A—C16A—C2A	0.5 (2)
C1B—C2B—C16B—O2B	−178.2 (2)	C17A—N2A—C16A—C2A	178.6 (2)
C3B—C2B—C16B—O2B	−1.5 (4)	C16A—N2A—C17A—C18A	17.7 (4)
C1B—C2B—C16B—N2B	0.5 (2)	N1A—N2A—C17A—C18A	−164.3 (2)
C3B—C2B—C16B—N2B	177.20 (18)	C16A—N2A—C17A—C22A	−163.4 (2)
N1B—N2B—C16B—O2B	178.31 (19)	N1A—N2A—C17A—C22A	14.6 (3)
C17B—N2B—C16B—O2B	4.5 (3)	C22A—C17A—C18A—C19A	−0.2 (4)
N1B—N2B—C16B—C2B	−0.5 (2)	N2A—C17A—C18A—C19A	178.8 (2)
C17B—N2B—C16B—C2B	−174.3 (2)	C17A—C18A—C19A—C20A	0.4 (4)
C16B—N2B—C17B—C18B	−16.1 (4)	C18A—C19A—C20A—C21A	−0.7 (5)
N1B—N2B—C17B—C18B	170.7 (2)	C19A—C20A—C21A—C22A	0.7 (5)
C16B—N2B—C17B—C22B	164.0 (2)	C20A—C21A—C22A—C17A	−0.5 (4)
N1B—N2B—C17B—C22B	−9.3 (3)	C18A—C17A—C22A—C21A	0.2 (4)
C22B—C17B—C18B—C19B	−1.7 (4)	N2A—C17A—C22A—C21A	−178.8 (2)
N2B—C17B—C18B—C19B	178.3 (2)		

Hydrogen-bond geometry (Å, °)

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
C15A—H15A···O1B^{i}	0.98	2.47	3.417 (3)	163
C15B—H15B···O1A^{ii}	0.98	2.53	3.432 (3)	153
C18A—H18A···O2A	0.93	2.31	2.922 (3)	123
C18B—H18B···O2B	0.93	2.30	2.915 (3)	123
C14B—H14B···N1A	0.98	2.61	3.488 (3)	149

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

Fig. 1


C8A
C7A
C9A
O1A
C10A
C11A
C12A
C6A
C13A
C14A
C4A
C15A
C5A
C3A
O2A
C16A
C2A
C1A
N1A
N2A
C17A
C18A
C23A
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C16B
C3B
O2B
C14B
C15B
C4B
C5B
C13B
C6B
C12C
C10B
C12B
C11B
C11C
O1B
C9B
C7B
C8B

Fig. 2