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t-3-Benzyl-*r*-2,*c*-6-diphenylpiperidin-4-one

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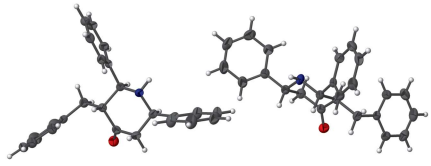
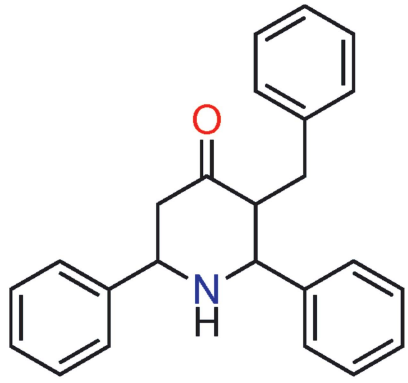
Structural data: full structural data are available from iucrdata.iucr.org

The asymmetric unit of the title compound, $C_{24}H_{23}NO$, contains two crystallographically independent molecules (*A* and *B*). In both molecules, the piperidine rings adopt a chair conformation and the phenyl rings and the benzyl group substituents are attached equatorially. The dihedral angle between the phenyl rings is 60.80 (10)° in molecule *A* and 68.43 (9)° in molecule *B*. The phenyl ring of the benzyl group makes dihedral angles of 76.95 (9) and 42.25 (10)° with the phenyl rings in molecule *A*, and dihedral angles of 81.38 (11) and 30.19 (11)° in molecule *B*. In the crystal, the two molecules are linked by N—H···O hydrogen bonds, forming *–A–B–A–B–* chains along [100]. In addition, five C—H···π interactions are also present, linking the chains to form a three-dimensional structure.

3D view



Chemical scheme



Structure description

The asymmetric unit of the title compound, (Fig. 1 and Fig. 2), contains two crystallographically independent molecules (*A* and *B*). In both molecules, the piperidine ring adopts a chair conformation with puckering parameters $q2$ = 0.0236 (18) Å, $q3$ = −0.5892 (18) Å, Q = 0.5895 (18) Å, θ = 178.12 (17)° and φ = 141 (4)° for molecule *A* and $q2$ = 0.0396 (18) Å, $q3$ = −0.5886 (18) Å, Q = 0.5898 (18) Å, θ = 176.34 (17)° and φ = 133 (3)° for molecule *B*.

An *AutoMolFit* of molecule *A* on molecule *B* gives the best fit (Fig. 3; Spek, 2009). Weighted and unit weight r.m.s. fit are 0.248 and 0.219 Å, respectively (for all 26 non-H atoms). Comparison of the bonds of the fitted residues gives, r.m.s. bond fit = 0.0033 Å. Comparison of the bond angles of the fitted residues gives r.m.s. angle fit = 0.683°.

The phenyl rings at positions 2,6 and the benzyl group at position 3 are attached equatorially. The dihedral angle between the two phenyl rings at positions 2 and 6 is

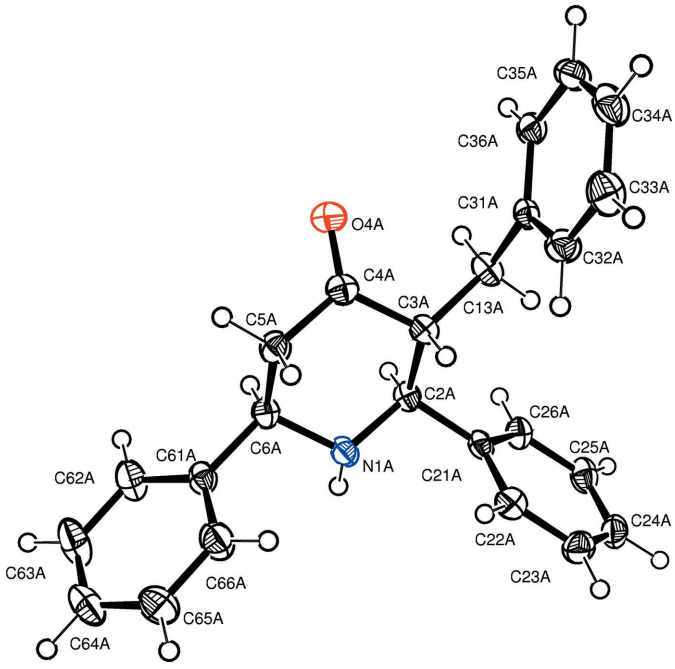


Figure 1
A view of molecule *A*, with displacement ellipsoids drawn at the 40% probability level and atom labelling.

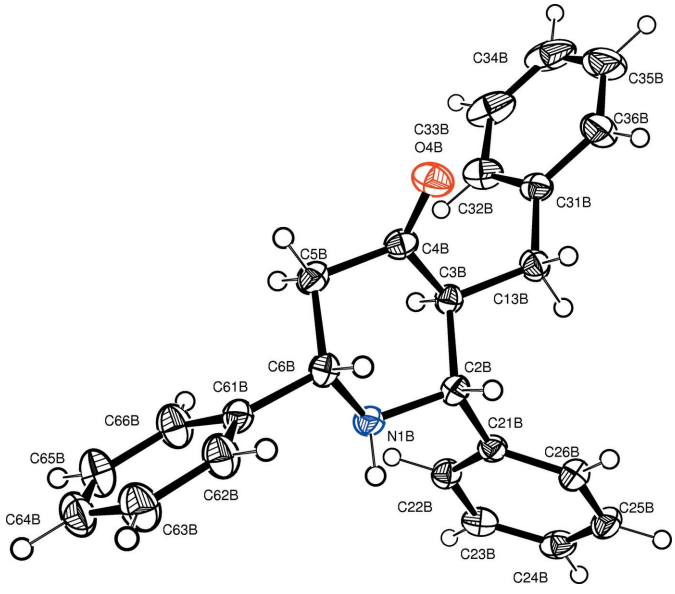


Figure 2
A view of molecule *B*, with displacement ellipsoids drawn at the 40% probability level and atom labelling.

60.80 (10)° in molecule *A*, and 68.43 (9)° in molecule *B*. The phenyl ring of the benzyl group makes dihedral angles of 76.95 (9) and 42.25 (10)° with the two phenyl rings in molecule *A*, and 81.38 (11) and 30.19 (11)° in molecule *B*.

In the crystal, the molecules are linked by N—H···O hydrogen bonds forming –A–B–A–B– chains along the *a*-axis direction (Fig. 4). In addition, there are a number of C—H···π interactions present, linking the chains to form a three-dimensional structure (Table 1).

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

*Cg*2, *Cg*3, *Cg*6 and *Cg*7 are the centroids of phenyl rings C21*A*–C26*A*, C31*A*–C36*A*, C21*B*–C26*B* and C31*B*–C36*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O4*B*^{i}	0.88 (2)	2.41 (2)	3.234 (2)	158 (2)
N1*B*—H1*B*···O4*A*^{ii}	0.90 (2)	2.48 (2)	3.315 (2)	153 (2)
C2*A*—H2*A*···*Cg*6^{iii}	1.00	2.95	3.9315 (19)	167
C2*B*—H2*B*···*Cg*2^{iv}	1.00	3.00	3.9733 (19)	166
C25*B*—H25*B*···*Cg*3^{v}	0.95	2.78	3.626 (2)	150
C64*A*—H64*A*···*Cg*3^{ii}	0.95	2.78	3.661 (2)	155
C64*B*—H64*B*···*Cg*7^{i}	0.95	2.93	3.796 (2)	153

Symmetry codes: (i) $x-\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (ii) $x-\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (iii) $x+\frac{1}{2}, -y+\frac{1}{2}, z+\frac{1}{2}$; (iv) $x+\frac{1}{2}, -y+\frac{1}{2}, z-\frac{1}{2}$; (v) $-x+\frac{1}{2}, y+\frac{1}{2}, -z+\frac{3}{2}$.

Jayabharathi *et al.*, (2008) have reported the crystal structure of *t*-3-benzyl-*r*-2,*c*-6-bis(4-methoxyphenyl)piperidin-4-one, in which the piperidine ring adopts a chair conformation, with equatorial orientation of all substituents. Gayathri *et al.*, (2009) have reported the crystal structure of *t*-3-pentyl-*r*-2,*c*-6-diphenylpiperidin-4-one, in which the piperidine ring adopts a chair conformation, with equatorial orientation of all substituents.

Synthesis and crystallization

A mixture of ammonium acetate (0.1 mol, 7.71 g), benzaldehyde (0.2 mol, 20.3 ml) and benzyl acetone (0.1 mol, 15.0 ml) in distilled ethanol was heated first to boiling. After cooling, the viscous liquid obtained was dissolved in ether (200 ml) and shaken with 100 ml concentrated hydrochloric acid. The precipitated hydrochloride of *t*(3)-benzyl-*r*(2),*c*(6)-diphenylpiperidin-4-one was removed by filtration and washed first with 40 ml mixture of ethanol and ether (1:1) and then with ether to remove most of the coloured impurities. The base was

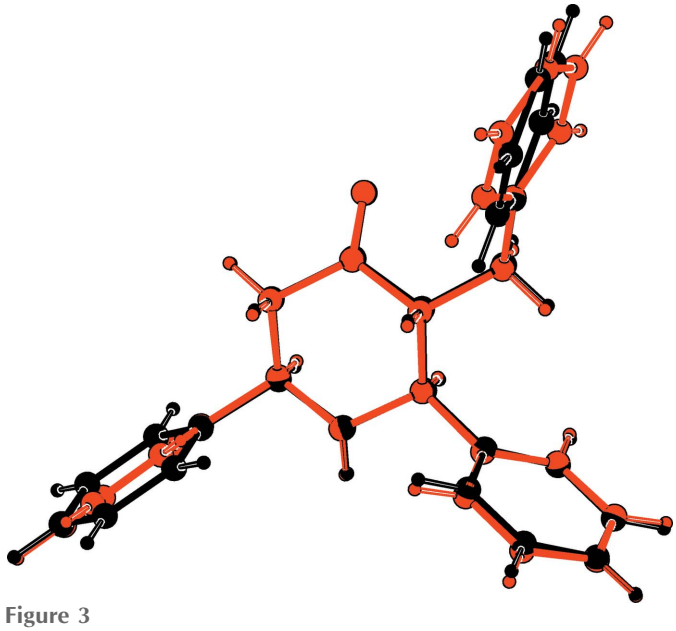


Figure 3
AutoMolFit diagram of molecule *A* (black) on molecule *B* (red).

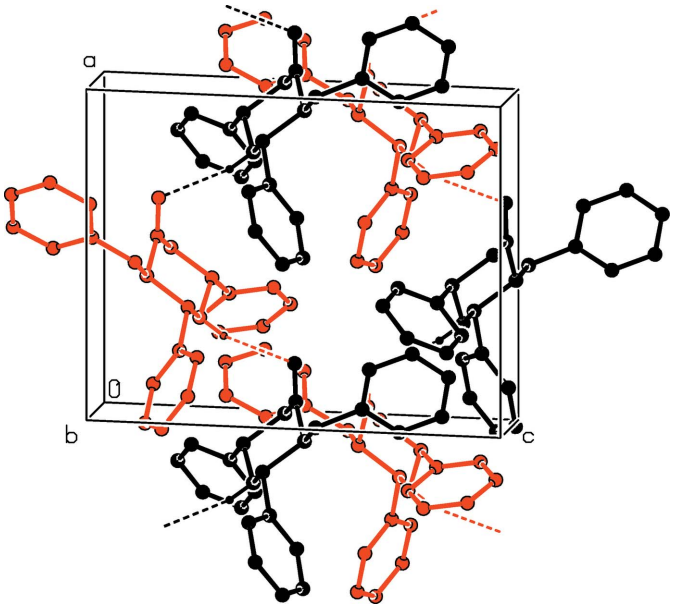


Figure 4
The crystal packing of the title compound, viewed along the *b* axis (molecule *A* is black and molecule *B* is red). Hydrogen bonds are shown as dashed lines (see Table 1). H atoms not involved in hydrogen bonding have been omitted for clarity.

liberated from an alcoholic solution by adding aqueous ammonia and then diluted with water. The title compound was recrystallized from ethanol to give colourless plate-like crystals (yield 2.5 g).

Refinement

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

Table 2
Experimental details.

Crystal data	
Chemical formula	$C_{24}H_{23}NO$
M_r	341.43
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	178
a, b, c (Å)	9.8918 (5), 30.6042 (12), 12.3878 (6)
β (°)	92.426 (2)
V (Å^3)	3746.8 (3)
Z	8
Radiation type	Mo $K\alpha$
μ (mm^{-1})	0.07
Crystal size (mm)	0.40 × 0.36 × 0.16
Data collection	
Diffractometer	Bruker Kappa APEXIII CCD area-detector
Absorption correction	Multi-scan (*SADABS*; Bruker, 2015)
T_{min}, T_{max}	0.81, 0.99
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	58653, 10617, 6350
R_{int}	0.078
(sin $\theta/\lambda)_{max}$ (Å^{-1})	0.698
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.066, 0.150, 1.05
No. of reflections	10617
No. of parameters	477
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.28, −0.22

Computer programs: *APEX3* (Bruker, 2015), *SAINT* (Bruker, 2015), *SHELXT2014* (Sheldrick, 2015*a*), *SHELXL2014* (Sheldrick, 2015*b*), *ORTEP-3 for Windows* (Farrugia, 2012), *PLATON* (Spek, 2009), *publCIF* (Westrip, 2010).

Acknowledgements

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full crystallographic data

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Crystal data

$C_{24}H_{23}NO$
M_r = 341.43
Monoclinic, $P2_1/n$
Hall symbol: -P 2yn
a = 9.8918 (5) Å
b = 30.6042 (12) Å
c = 12.3878 (6) Å
β = 92.426 (2)°
V = 3746.8 (3) Å^3
Z = 8
$F(000)$ = 1456
D_x = 1.211 Mg m^{-3}
Melting point: 471 K
Mo $K\alpha$ radiation, λ = 0.71073 Å
Cell parameters from 7035 reflections
θ = 2.6–22.8°
μ = 0.07 mm^{-1}
T = 178 K
Plate, colourless
0.40 × 0.36 × 0.16 mm

Data collection

Bruker Kappa APEXIII CCD area-detector diffractometer
Radiation source: fine-focus sealed tube
Detector resolution: 8.3333 pixels mm^{-1}
φ and ω scans
Absorption correction: multi-scan (SADABS; Bruker, 2015)
T_{min} = 0.81, T_{max} = 0.99
58653 measured reflections
10617 independent reflections
6350 reflections with $I > 2\sigma(I)$
R_{int} = 0.078
θ_{max} = 29.7°, θ_{min} = 1.8°
h = −13→13
k = −42→42
l = −14→17

Refinement

Refinement on F^2
Least-squares matrix: full
$R[F^2 > 2\sigma(F^2)]$ = 0.066
$wR(F^2)$ = 0.150
S = 1.05
10617 reflections
477 parameters
0 restraints
Primary atom site location: structure-invariant direct methods
Secondary atom site location: difference Fourier map
Hydrogen site location: mixed
H atoms treated by a mixture of independent and constrained refinement
$w = 1/[\sigma^2(F_o^2) + (0.0506P)^2 + 1.0513P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$ = 0.001
$\Delta\rho_{max}$ = 0.28 e Å^{-3}
$\Delta\rho_{min}$ = −0.22 e Å^{-3}

Special details

Geometry. Bond distances, angles etc. have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell esds are taken into account in the estimation of distances, angles and torsion angles

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²)

	x	*y*	*z*	U_{iso}*/U_{eq}
O4A	0.66207 (13)	0.14287 (4)	0.97486 (11)	0.0395 (5)
N1A	0.29441 (15)	0.17242 (5)	0.87397 (13)	0.0294 (5)
C2A	0.33073 (17)	0.12682 (5)	0.89839 (14)	0.0255 (5)
C3A	0.42875 (17)	0.12561 (5)	0.99936 (14)	0.0258 (5)
C4A	0.54612 (18)	0.15567 (6)	0.97724 (14)	0.0287 (5)
O4B	0.64521 (13)	0.35463 (4)	0.14639 (11)	0.0398 (4)
C5A	0.50630 (18)	0.20176 (6)	0.94862 (15)	0.0310 (6)
C6A	0.40932 (18)	0.20027 (5)	0.84847 (14)	0.0281 (5)
C13A	0.4738 (2)	0.07909 (6)	1.02805 (14)	0.0316 (6)
C21A	0.20186 (17)	0.10166 (5)	0.91607 (13)	0.0256 (5)
C22A	0.10267 (19)	0.11842 (6)	0.98114 (15)	0.0327 (6)
C23A	−0.0152 (2)	0.09519 (7)	0.99688 (16)	0.0376 (6)
C24A	−0.0346 (2)	0.05489 (7)	0.94932 (16)	0.0385 (7)
C25A	0.0624 (2)	0.03799 (6)	0.88431 (16)	0.0371 (6)
C26A	0.17976 (19)	0.06132 (6)	0.86759 (15)	0.0314 (6)
C31A	0.53595 (17)	0.07396 (5)	1.14082 (14)	0.0260 (5)
C32A	0.4699 (2)	0.08900 (6)	1.22942 (16)	0.0368 (6)
C33A	0.5230 (2)	0.08269 (7)	1.33323 (17)	0.0462 (7)
C34A	0.6440 (2)	0.06114 (7)	1.35011 (17)	0.0440 (7)
C35A	0.7111 (2)	0.04598 (6)	1.26319 (17)	0.0393 (6)
C36A	0.65797 (18)	0.05231 (5)	1.15920 (15)	0.0315 (6)
C61A	0.35679 (18)	0.24486 (5)	0.81445 (15)	0.0292 (6)
C62A	0.3975 (2)	0.26388 (6)	0.72053 (17)	0.0437 (7)
C63A	0.3443 (3)	0.30352 (7)	0.68587 (19)	0.0560 (9)
C64A	0.2511 (2)	0.32475 (7)	0.74529 (19)	0.0490 (8)
C65A	0.2101 (2)	0.30642 (7)	0.83958 (19)	0.0484 (8)
C66A	0.2627 (2)	0.26665 (6)	0.87408 (18)	0.0425 (7)
N1B	0.28747 (15)	0.32434 (5)	0.24447 (13)	0.0290 (5)
C2B	0.31937 (17)	0.36986 (5)	0.21806 (14)	0.0260 (5)
C3B	0.40928 (17)	0.37099 (5)	0.11867 (14)	0.0254 (5)
C4B	0.52943 (18)	0.34139 (6)	0.14279 (14)	0.0282 (5)
C5B	0.49399 (19)	0.29549 (6)	0.17362 (15)	0.0323 (6)
C6B	0.40709 (17)	0.29780 (5)	0.27294 (14)	0.0280 (5)
C13B	0.45080 (19)	0.41762 (6)	0.09216 (15)	0.0311 (6)
C21B	0.18873 (17)	0.39485 (5)	0.19832 (13)	0.0258 (5)
C22B	0.08347 (18)	0.37718 (6)	0.13450 (14)	0.0308 (6)
C23B	−0.03523 (19)	0.40058 (6)	0.11528 (15)	0.0347 (6)
C24B	−0.0486 (2)	0.44195 (6)	0.15741 (16)	0.0370 (6)
C25B	0.0544 (2)	0.45969 (6)	0.22133 (16)	0.0378 (6)
C26B	0.17202 (19)	0.43595 (6)	0.24253 (15)	0.0323 (6)
C31B	0.52074 (18)	0.42469 (6)	−0.01175 (15)	0.0306 (6)
C32B	0.4822 (2)	0.40348 (7)	−0.10618 (16)	0.0419 (7)
C33B	0.5413 (3)	0.41335 (9)	−0.20217 (18)	0.0574 (9)
C34B	0.6411 (3)	0.44425 (10)	−0.2052 (3)	0.0717 (11)
C35B	0.6830 (3)	0.46507 (9)	−0.1112 (3)	0.0744 (13)

C36B	0.6227 (2)	0.45573 (7)	−0.0158 (2)	0.0507 (8)
C61B	0.36041 (18)	0.25385 (5)	0.31273 (15)	0.0291 (5)
C62B	0.3830 (2)	0.24185 (6)	0.41921 (16)	0.0392 (7)
C63B	0.3325 (2)	0.20300 (7)	0.45824 (18)	0.0478 (7)
C64B	0.2605 (2)	0.17535 (7)	0.39071 (18)	0.0444 (7)
C65B	0.2378 (2)	0.18668 (7)	0.28414 (19)	0.0486 (8)
C66B	0.2869 (2)	0.22564 (6)	0.24535 (17)	0.0424 (7)
H1A	0.2395 (19)	0.1715 (6)	0.8167 (16)	0.032 (5)*
H2A	0.37692	0.11399	0.83550	0.0306*
H3A	0.38018	0.13776	1.06185	0.0310*
H5A	0.58761	0.21914	0.93306	0.0372*
H5B	0.46113	0.21559	1.00971	0.0372*
H6A	0.45740	0.18695	0.78715	0.0338*
H13A	0.39449	0.05946	1.02003	0.0379*
H13B	0.54056	0.06950	0.97562	0.0379*
H22A	0.11594	0.14603	1.01501	0.0392*
H23A	−0.08264	0.10710	1.04059	0.0451*
H24A	−0.11467	0.03876	0.96126	0.0461*
H25A	0.04871	0.01030	0.85092	0.0445*
H26A	0.24584	0.04953	0.82236	0.0376*
H32A	0.38624	0.10399	1.21885	0.0441*
H33A	0.47574	0.09327	1.39309	0.0554*
H34A	0.68070	0.05681	1.42141	0.0528*
H35A	0.79466	0.03102	1.27435	0.0471*
H36A	0.70571	0.04169	1.09964	0.0378*
H62A	0.46288	0.24961	0.67898	0.0523*
H63A	0.37263	0.31607	0.62044	0.0672*
H64A	0.21491	0.35202	0.72143	0.0588*
H65A	0.14561	0.32105	0.88125	0.0580*
H66A	0.23387	0.25417	0.93945	0.0510*
H1B	0.235 (2)	0.3253 (7)	0.3023 (18)	0.050 (7)*
H2B	0.37069	0.38323	0.28103	0.0312*
H3B	0.35600	0.35885	0.05514	0.0305*
H5C	0.44317	0.28096	0.11314	0.0387*
H5D	0.57736	0.27849	0.19060	0.0387*
H6B	0.46029	0.31264	0.33280	0.0336*
H13C	0.51134	0.42836	0.15210	0.0373*
H13D	0.36851	0.43606	0.09058	0.0373*
H22B	0.09285	0.34893	0.10390	0.0369*
H23B	−0.10755	0.38805	0.07293	0.0417*
H24B	−0.12897	0.45821	0.14230	0.0444*
H25B	0.04501	0.48812	0.25088	0.0453*
H26B	0.24209	0.44807	0.28802	0.0387*
H32B	0.41384	0.38169	−0.10523	0.0503*
H33B	0.51247	0.39860	−0.26658	0.0688*
H34B	0.68106	0.45124	−0.27144	0.0860*
H35B	0.75387	0.48600	−0.11212	0.0891*
H36B	0.65135	0.47074	0.04831	0.0608*

H62B	0.43397	0.26056	0.46664	0.0470*
H63B	0.34799	0.19550	0.53215	0.0573*
H64B	0.22648	0.14857	0.41727	0.0533*
H65B	0.18806	0.16759	0.23683	0.0583*
H66B	0.27005	0.23318	0.17162	0.0509*

Atomic displacement parameters (Å²)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
O4A	0.0305 (7)	0.0438 (8)	0.0443 (9)	0.0043 (6)	0.0016 (6)	0.0055 (6)
N1A	0.0308 (8)	0.0251 (7)	0.0316 (9)	−0.0028 (6)	−0.0066 (7)	0.0049 (6)
C2A	0.0304 (9)	0.0229 (8)	0.0231 (9)	−0.0009 (7)	0.0001 (7)	−0.0003 (7)
C3A	0.0297 (9)	0.0248 (8)	0.0229 (9)	0.0011 (7)	0.0003 (7)	−0.0011 (7)
C4A	0.0313 (10)	0.0341 (9)	0.0204 (9)	−0.0003 (8)	−0.0031 (7)	−0.0024 (7)
O4B	0.0283 (7)	0.0468 (8)	0.0442 (8)	−0.0015 (6)	0.0012 (6)	0.0078 (6)
C5A	0.0312 (10)	0.0277 (9)	0.0337 (10)	−0.0050 (7)	−0.0020 (8)	−0.0011 (8)
C6A	0.0315 (10)	0.0244 (8)	0.0286 (10)	−0.0020 (7)	0.0021 (8)	0.0002 (7)
C13A	0.0411 (11)	0.0263 (9)	0.0272 (10)	0.0031 (8)	−0.0014 (8)	−0.0001 (7)
C21A	0.0304 (9)	0.0258 (8)	0.0202 (9)	0.0003 (7)	−0.0018 (7)	0.0053 (7)
C22A	0.0362 (10)	0.0321 (10)	0.0297 (10)	0.0016 (8)	0.0008 (8)	−0.0009 (8)
C23A	0.0330 (10)	0.0501 (12)	0.0300 (10)	0.0028 (9)	0.0052 (8)	0.0054 (9)
C24A	0.0346 (11)	0.0454 (12)	0.0351 (11)	−0.0084 (9)	−0.0013 (9)	0.0143 (9)
C25A	0.0449 (12)	0.0290 (9)	0.0371 (11)	−0.0091 (9)	−0.0010 (9)	0.0027 (8)
C26A	0.0367 (10)	0.0264 (9)	0.0312 (10)	−0.0031 (8)	0.0036 (8)	0.0009 (7)
C31A	0.0293 (9)	0.0212 (8)	0.0276 (10)	−0.0026 (7)	0.0016 (8)	0.0032 (7)
C32A	0.0347 (10)	0.0420 (11)	0.0338 (11)	0.0067 (9)	0.0043 (9)	0.0042 (9)
C33A	0.0590 (14)	0.0516 (13)	0.0283 (11)	0.0007 (11)	0.0068 (10)	0.0012 (9)
C34A	0.0560 (14)	0.0418 (11)	0.0329 (12)	−0.0073 (10)	−0.0124 (10)	0.0072 (9)
C35A	0.0340 (10)	0.0316 (10)	0.0511 (13)	−0.0010 (8)	−0.0117 (10)	0.0077 (9)
C36A	0.0315 (10)	0.0249 (9)	0.0383 (11)	−0.0001 (7)	0.0041 (8)	0.0017 (8)
C61A	0.0331 (10)	0.0243 (9)	0.0299 (10)	−0.0047 (7)	−0.0023 (8)	−0.0008 (7)
C62A	0.0594 (14)	0.0316 (10)	0.0407 (12)	0.0011 (10)	0.0106 (10)	0.0053 (9)
C63A	0.0872 (19)	0.0361 (12)	0.0454 (14)	0.0026 (12)	0.0110 (13)	0.0135 (10)
C64A	0.0661 (15)	0.0275 (10)	0.0525 (14)	0.0041 (10)	−0.0089 (12)	0.0060 (10)
C65A	0.0529 (14)	0.0333 (11)	0.0591 (15)	0.0089 (10)	0.0041 (11)	−0.0025 (10)
C66A	0.0503 (13)	0.0331 (10)	0.0447 (12)	0.0049 (9)	0.0094 (10)	0.0048 (9)
N1B	0.0293 (8)	0.0259 (7)	0.0324 (9)	0.0046 (6)	0.0077 (7)	0.0047 (6)
C2B	0.0285 (9)	0.0254 (8)	0.0239 (9)	0.0026 (7)	0.0004 (7)	−0.0011 (7)
C3B	0.0274 (9)	0.0259 (8)	0.0230 (9)	0.0000 (7)	0.0007 (7)	−0.0019 (7)
C4B	0.0290 (10)	0.0335 (9)	0.0223 (9)	0.0015 (8)	0.0030 (7)	−0.0020 (7)
C5B	0.0307 (10)	0.0295 (9)	0.0370 (11)	0.0068 (8)	0.0053 (8)	−0.0002 (8)
C6B	0.0305 (10)	0.0246 (8)	0.0289 (10)	0.0023 (7)	0.0000 (8)	0.0001 (7)
C13B	0.0345 (10)	0.0280 (9)	0.0308 (10)	−0.0021 (8)	0.0028 (8)	0.0009 (7)
C21B	0.0291 (9)	0.0259 (8)	0.0229 (9)	0.0020 (7)	0.0059 (7)	0.0038 (7)
C22B	0.0356 (10)	0.0308 (9)	0.0260 (10)	0.0006 (8)	0.0030 (8)	−0.0003 (7)
C23B	0.0299 (10)	0.0477 (11)	0.0264 (10)	0.0000 (9)	−0.0003 (8)	0.0048 (8)
C24B	0.0338 (10)	0.0422 (11)	0.0356 (11)	0.0100 (9)	0.0078 (9)	0.0101 (9)
C25B	0.0423 (11)	0.0288 (9)	0.0430 (12)	0.0092 (8)	0.0111 (9)	0.0008 (8)

C26B	0.0338 (10)	0.0298 (9)	0.0334 (10)	0.0019 (8)	0.0041 (8)	−0.0026 (8)
C31B	0.0260 (9)	0.0305 (9)	0.0354 (11)	0.0068 (7)	0.0043 (8)	0.0092 (8)
C32B	0.0374 (11)	0.0545 (13)	0.0340 (11)	0.0056 (10)	0.0033 (9)	0.0087 (10)
C33B	0.0589 (15)	0.0794 (17)	0.0346 (13)	0.0313 (14)	0.0113 (11)	0.0167 (12)
C34B	0.0725 (19)	0.0713 (18)	0.075 (2)	0.0380 (15)	0.0477 (16)	0.0439 (16)
C35B	0.0626 (17)	0.0534 (15)	0.111 (3)	0.0014 (13)	0.0478 (18)	0.0283 (17)
C36B	0.0422 (12)	0.0402 (12)	0.0706 (16)	−0.0054 (10)	0.0148 (12)	0.0075 (11)
C61B	0.0297 (9)	0.0252 (9)	0.0324 (10)	0.0059 (7)	0.0024 (8)	0.0036 (7)
C62B	0.0477 (12)	0.0332 (10)	0.0364 (12)	−0.0031 (9)	−0.0022 (9)	0.0042 (8)
C63B	0.0610 (14)	0.0415 (12)	0.0405 (12)	−0.0029 (10)	−0.0008 (11)	0.0137 (10)
C64B	0.0461 (12)	0.0313 (10)	0.0559 (14)	−0.0024 (9)	0.0022 (10)	0.0115 (10)
C65B	0.0564 (14)	0.0355 (11)	0.0533 (14)	−0.0110 (10)	−0.0057 (11)	0.0017 (10)
C66B	0.0524 (13)	0.0366 (11)	0.0375 (12)	−0.0057 (10)	−0.0055 (10)	0.0045 (9)

Geometric parameters (Å, º)

O4A—C4A	1.214 (2)	C64A—H64A	0.9500
N1A—C2A	1.469 (2)	C65A—H65A	0.9500
N1A—C6A	1.466 (2)	C66A—H66A	0.9500
N1A—H1A	0.876 (19)	N1B—H1B	0.90 (2)
C2A—C3A	1.550 (2)	C2B—C3B	1.549 (2)
C2A—C21A	1.513 (2)	C2B—C21B	1.513 (2)
C3A—C4A	1.515 (2)	C3B—C4B	1.514 (2)
C3A—C13A	1.529 (2)	C3B—C13B	1.525 (2)
C4A—C5A	1.503 (3)	C4B—C5B	1.501 (3)
O4B—C4B	1.214 (2)	C5B—C6B	1.532 (3)
C5A—C6A	1.537 (3)	C6B—C61B	1.512 (2)
C6A—C61A	1.514 (2)	C13B—C31B	1.503 (3)
C13A—C31A	1.510 (2)	C21B—C26B	1.385 (2)
C21A—C22A	1.394 (2)	C21B—C22B	1.390 (2)
C21A—C26A	1.386 (2)	C22B—C23B	1.387 (3)
C22A—C23A	1.386 (3)	C23B—C24B	1.378 (3)
C23A—C24A	1.377 (3)	C24B—C25B	1.375 (3)
C24A—C25A	1.379 (3)	C25B—C26B	1.387 (3)
C25A—C26A	1.386 (3)	C31B—C32B	1.377 (3)
C31A—C32A	1.380 (3)	C31B—C36B	1.388 (3)
C31A—C36A	1.387 (2)	C32B—C33B	1.381 (3)
C32A—C33A	1.382 (3)	C33B—C34B	1.369 (4)
C33A—C34A	1.375 (3)	C34B—C35B	1.376 (5)
C34A—C35A	1.370 (3)	C35B—C36B	1.376 (4)
C35A—C36A	1.384 (3)	C61B—C66B	1.385 (3)
C61A—C66A	1.384 (3)	C61B—C62B	1.378 (3)
C61A—C62A	1.376 (3)	C62B—C63B	1.385 (3)
C62A—C63A	1.383 (3)	C63B—C64B	1.369 (3)
C63A—C64A	1.368 (3)	C64B—C65B	1.374 (3)
C64A—C65A	1.372 (3)	C65B—C66B	1.381 (3)
C65A—C66A	1.384 (3)	C2B—H2B	1.0000
N1B—C2B	1.468 (2)	C3B—H3B	1.0000

N1B—C6B	1.466 (2)	C5B—H5C	0.9900
C2A—H2A	1.0000	C5B—H5D	0.9900
C3A—H3A	1.0000	C6B—H6B	1.0000
C5A—H5B	0.9900	C13B—H13C	0.9900
C5A—H5A	0.9900	C13B—H13D	0.9900
C6A—H6A	1.0000	C22B—H22B	0.9500
C13A—H13A	0.9900	C23B—H23B	0.9500
C13A—H13B	0.9900	C24B—H24B	0.9500
C22A—H22A	0.9500	C25B—H25B	0.9500
C23A—H23A	0.9500	C26B—H26B	0.9500
C24A—H24A	0.9500	C32B—H32B	0.9500
C25A—H25A	0.9500	C33B—H33B	0.9500
C26A—H26A	0.9500	C34B—H34B	0.9500
C32A—H32A	0.9500	C35B—H35B	0.9500
C33A—H33A	0.9500	C36B—H36B	0.9500
C34A—H34A	0.9500	C62B—H62B	0.9500
C35A—H35A	0.9500	C63B—H63B	0.9500
C36A—H36A	0.9500	C64B—H64B	0.9500
C62A—H62A	0.9500	C65B—H65B	0.9500
C63A—H63A	0.9500	C66B—H66B	0.9500

C2A—N1A—C6A	114.30 (13)	C65A—C66A—H66A	120.00
C2A—N1A—H1A	105.9 (12)	C2B—N1B—H1B	106.4 (14)
C6A—N1A—H1A	107.7 (13)	C6B—N1B—H1B	108.2 (13)
C3A—C2A—C21A	111.90 (14)	C3B—C2B—C21B	112.05 (14)
N1A—C2A—C3A	109.14 (13)	N1B—C2B—C3B	109.53 (13)
N1A—C2A—C21A	108.24 (13)	N1B—C2B—C21B	109.00 (13)
C2A—C3A—C4A	107.30 (13)	C2B—C3B—C4B	107.58 (14)
C2A—C3A—C13A	112.08 (13)	C2B—C3B—C13B	111.16 (13)
C4A—C3A—C13A	112.91 (15)	C4B—C3B—C13B	112.72 (14)
O4A—C4A—C3A	122.72 (16)	O4B—C4B—C3B	122.62 (16)
C3A—C4A—C5A	114.66 (15)	C3B—C4B—C5B	114.85 (15)
O4A—C4A—C5A	122.40 (16)	O4B—C4B—C5B	122.22 (16)
C4A—C5A—C6A	108.12 (14)	C4B—C5B—C6B	107.83 (14)
N1A—C6A—C61A	108.91 (14)	N1B—C6B—C61B	108.48 (14)
C5A—C6A—C61A	113.16 (14)	C5B—C6B—C61B	114.23 (14)
N1A—C6A—C5A	107.85 (14)	N1B—C6B—C5B	107.88 (14)
C3A—C13A—C31A	114.52 (14)	C3B—C13B—C31B	117.21 (15)
C2A—C21A—C26A	120.59 (15)	C2B—C21B—C26B	120.72 (15)
C2A—C21A—C22A	120.96 (14)	C2B—C21B—C22B	120.63 (14)
C22A—C21A—C26A	118.45 (16)	C22B—C21B—C26B	118.64 (16)
C21A—C22A—C23A	120.63 (17)	C21B—C22B—C23B	120.33 (16)
C22A—C23A—C24A	120.13 (18)	C22B—C23B—C24B	120.23 (17)
C23A—C24A—C25A	119.87 (18)	C23B—C24B—C25B	120.01 (18)
C24A—C25A—C26A	120.13 (18)	C24B—C25B—C26B	119.81 (17)
C21A—C26A—C25A	120.79 (17)	C21B—C26B—C25B	120.94 (17)
C13A—C31A—C32A	120.87 (16)	C13B—C31B—C32B	122.60 (17)
C32A—C31A—C36A	117.82 (17)	C32B—C31B—C36B	117.86 (19)

C13A—C31A—C36A	121.24 (16)	C13B—C31B—C36B	119.42 (18)
C31A—C32A—C33A	121.30 (18)	C31B—C32B—C33B	121.1 (2)
C32A—C33A—C34A	120.18 (19)	C32B—C33B—C34B	120.5 (2)
C33A—C34A—C35A	119.39 (19)	C33B—C34B—C35B	119.3 (3)
C34A—C35A—C36A	120.45 (18)	C34B—C35B—C36B	120.3 (3)
C31A—C36A—C35A	120.87 (17)	C31B—C36B—C35B	121.0 (2)
C6A—C61A—C62A	120.49 (16)	C6B—C61B—C62B	120.65 (16)
C62A—C61A—C66A	118.35 (16)	C62B—C61B—C66B	118.05 (16)
C6A—C61A—C66A	121.10 (16)	C6B—C61B—C66B	121.19 (16)
C61A—C62A—C63A	120.81 (19)	C61B—C62B—C63B	121.11 (18)
C62A—C63A—C64A	120.4 (2)	C62B—C63B—C64B	120.2 (2)
C63A—C64A—C65A	119.6 (2)	C63B—C64B—C65B	119.4 (2)
C64A—C65A—C66A	120.1 (2)	C64B—C65B—C66B	120.4 (2)
C61A—C66A—C65A	120.76 (19)	C61B—C66B—C65B	120.77 (19)
C2B—N1B—C6B	113.60 (13)	N1B—C2B—H2B	109.00
C3A—C2A—H2A	109.00	C3B—C2B—H2B	109.00
C21A—C2A—H2A	109.00	C21B—C2B—H2B	109.00
N1A—C2A—H2A	109.00	C2B—C3B—H3B	108.00
C4A—C3A—H3A	108.00	C4B—C3B—H3B	108.00
C13A—C3A—H3A	108.00	C13B—C3B—H3B	108.00
C2A—C3A—H3A	108.00	C4B—C5B—H5C	110.00
C4A—C5A—H5A	110.00	C4B—C5B—H5D	110.00
C4A—C5A—H5B	110.00	C6B—C5B—H5C	110.00
C6A—C5A—H5B	110.00	C6B—C5B—H5D	110.00
H5A—C5A—H5B	108.00	H5C—C5B—H5D	108.00
C6A—C5A—H5A	110.00	N1B—C6B—H6B	109.00
C5A—C6A—H6A	109.00	C5B—C6B—H6B	109.00
C61A—C6A—H6A	109.00	C61B—C6B—H6B	109.00
N1A—C6A—H6A	109.00	C3B—C13B—H13C	108.00
C3A—C13A—H13A	109.00	C3B—C13B—H13D	108.00
C31A—C13A—H13A	109.00	C31B—C13B—H13C	108.00
C31A—C13A—H13B	109.00	C31B—C13B—H13D	108.00
C3A—C13A—H13B	109.00	H13C—C13B—H13D	107.00
H13A—C13A—H13B	108.00	C21B—C22B—H22B	120.00
C23A—C22A—H22A	120.00	C23B—C22B—H22B	120.00
C21A—C22A—H22A	120.00	C22B—C23B—H23B	120.00
C24A—C23A—H23A	120.00	C24B—C23B—H23B	120.00
C22A—C23A—H23A	120.00	C23B—C24B—H24B	120.00
C23A—C24A—H24A	120.00	C25B—C24B—H24B	120.00
C25A—C24A—H24A	120.00	C24B—C25B—H25B	120.00
C24A—C25A—H25A	120.00	C26B—C25B—H25B	120.00
C26A—C25A—H25A	120.00	C21B—C26B—H26B	120.00
C25A—C26A—H26A	120.00	C25B—C26B—H26B	120.00
C21A—C26A—H26A	120.00	C31B—C32B—H32B	119.00
C31A—C32A—H32A	119.00	C33B—C32B—H32B	119.00
C33A—C32A—H32A	119.00	C32B—C33B—H33B	120.00
C34A—C33A—H33A	120.00	C34B—C33B—H33B	120.00
C32A—C33A—H33A	120.00	C33B—C34B—H34B	120.00

C33A—C34A—H34A	120.00	C35B—C34B—H34B	120.00
C35A—C34A—H34A	120.00	C34B—C35B—H35B	120.00
C36A—C35A—H35A	120.00	C36B—C35B—H35B	120.00
C34A—C35A—H35A	120.00	C31B—C36B—H36B	119.00
C31A—C36A—H36A	120.00	C35B—C36B—H36B	120.00
C35A—C36A—H36A	120.00	C61B—C62B—H62B	119.00
C63A—C62A—H62A	120.00	C63B—C62B—H62B	119.00
C61A—C62A—H62A	120.00	C62B—C63B—H63B	120.00
C62A—C63A—H63A	120.00	C64B—C63B—H63B	120.00
C64A—C63A—H63A	120.00	C63B—C64B—H64B	120.00
C65A—C64A—H64A	120.00	C65B—C64B—H64B	120.00
C63A—C64A—H64A	120.00	C64B—C65B—H65B	120.00
C64A—C65A—H65A	120.00	C66B—C65B—H65B	120.00
C66A—C65A—H65A	120.00	C61B—C66B—H66B	120.00
C61A—C66A—H66A	120.00	C65B—C66B—H66B	120.00

C6A—N1A—C2A—C3A	61.46 (18)	C6B—N1B—C2B—C3B	61.29 (18)
C6A—N1A—C2A—C21A	−176.53 (14)	C6B—N1B—C2B—C21B	−175.80 (14)
C2A—N1A—C6A—C5A	−62.31 (18)	C2B—N1B—C6B—C5B	−63.35 (18)
C2A—N1A—C6A—C61A	174.52 (14)	C2B—N1B—C6B—C61B	172.43 (14)
C21A—C2A—C3A—C4A	−173.88 (13)	C21B—C2B—C3B—C4B	−174.28 (13)
N1A—C2A—C3A—C4A	−54.10 (17)	N1B—C2B—C3B—C4B	−53.20 (17)
N1A—C2A—C3A—C13A	−178.60 (14)	N1B—C2B—C3B—C13B	−177.05 (14)
N1A—C2A—C21A—C26A	133.69 (16)	N1B—C2B—C21B—C26B	135.23 (16)
C3A—C2A—C21A—C22A	74.08 (19)	C3B—C2B—C21B—C22B	75.98 (19)
C3A—C2A—C21A—C26A	−106.01 (18)	C3B—C2B—C21B—C26B	−103.38 (18)
C21A—C2A—C3A—C13A	61.62 (18)	C21B—C2B—C3B—C13B	61.87 (18)
N1A—C2A—C21A—C22A	−46.2 (2)	N1B—C2B—C21B—C22B	−45.4 (2)
C13A—C3A—C4A—O4A	5.2 (2)	C13B—C3B—C4B—O4B	4.0 (2)
C2A—C3A—C4A—O4A	−118.79 (18)	C2B—C3B—C4B—O4B	−118.88 (18)
C2A—C3A—C4A—C5A	55.97 (18)	C2B—C3B—C4B—C5B	54.85 (18)
C4A—C3A—C13A—C31A	75.06 (19)	C4B—C3B—C13B—C31B	68.0 (2)
C13A—C3A—C4A—C5A	179.96 (15)	C13B—C3B—C4B—C5B	177.74 (15)
C2A—C3A—C13A—C31A	−163.62 (15)	C2B—C3B—C13B—C31B	−171.14 (15)
O4A—C4A—C5A—C6A	116.86 (19)	O4B—C4B—C5B—C6B	115.95 (19)
C3A—C4A—C5A—C6A	−57.92 (19)	C3B—C4B—C5B—C6B	−57.81 (19)
C4A—C5A—C6A—C61A	177.43 (15)	C4B—C5B—C6B—C61B	178.78 (15)
C4A—C5A—C6A—N1A	56.90 (18)	C4B—C5B—C6B—N1B	58.09 (18)
N1A—C6A—C61A—C62A	−129.72 (18)	N1B—C6B—C61B—C62B	−112.54 (19)
N1A—C6A—C61A—C66A	47.5 (2)	N1B—C6B—C61B—C66B	63.5 (2)
C5A—C6A—C61A—C62A	110.35 (19)	C5B—C6B—C61B—C62B	127.11 (18)
C5A—C6A—C61A—C66A	−72.5 (2)	C5B—C6B—C61B—C66B	−56.8 (2)
C3A—C13A—C31A—C32A	51.9 (2)	C3B—C13B—C31B—C32B	40.2 (3)
C3A—C13A—C31A—C36A	−131.02 (17)	C3B—C13B—C31B—C36B	−143.99 (18)
C2A—C21A—C22A—C23A	179.95 (16)	C2B—C21B—C22B—C23B	−178.94 (16)
C26A—C21A—C22A—C23A	0.0 (3)	C26B—C21B—C22B—C23B	0.4 (3)
C2A—C21A—C26A—C25A	179.44 (17)	C2B—C21B—C26B—C25B	177.54 (17)
C22A—C21A—C26A—C25A	−0.7 (3)	C22B—C21B—C26B—C25B	−1.8 (3)

C21A—C22A—C23A—C24A	0.9 (3)	C21B—C22B—C23B—C24B	1.4 (3)
C22A—C23A—C24A—C25A	−1.2 (3)	C22B—C23B—C24B—C25B	−1.9 (3)
C23A—C24A—C25A—C26A	0.6 (3)	C23B—C24B—C25B—C26B	0.5 (3)
C24A—C25A—C26A—C21A	0.4 (3)	C24B—C25B—C26B—C21B	1.4 (3)
C13A—C31A—C32A—C33A	177.01 (17)	C13B—C31B—C32B—C33B	174.7 (2)
C36A—C31A—C32A—C33A	−0.2 (3)	C36B—C31B—C32B—C33B	−1.2 (3)
C13A—C31A—C36A—C35A	−176.97 (16)	C13B—C31B—C36B—C35B	−175.8 (2)
C32A—C31A—C36A—C35A	0.2 (2)	C32B—C31B—C36B—C35B	0.2 (3)
C31A—C32A—C33A—C34A	0.1 (3)	C31B—C32B—C33B—C34B	0.8 (4)
C32A—C33A—C34A—C35A	−0.1 (3)	C32B—C33B—C34B—C35B	0.7 (4)
C33A—C34A—C35A—C36A	0.1 (3)	C33B—C34B—C35B—C36B	−1.7 (4)
C34A—C35A—C36A—C31A	−0.2 (3)	C34B—C35B—C36B—C31B	1.3 (4)
C6A—C61A—C62A—C63A	176.43 (19)	C6B—C61B—C62B—C63B	175.47 (17)
C66A—C61A—C62A—C63A	−0.9 (3)	C66B—C61B—C62B—C63B	−0.7 (3)
C6A—C61A—C66A—C65A	−176.76 (18)	C6B—C61B—C66B—C65B	−176.13 (17)
C62A—C61A—C66A—C65A	0.5 (3)	C62B—C61B—C66B—C65B	0.1 (3)
C61A—C62A—C63A—C64A	0.7 (3)	C61B—C62B—C63B—C64B	1.0 (3)
C62A—C63A—C64A—C65A	−0.2 (4)	C62B—C63B—C64B—C65B	−0.6 (3)
C63A—C64A—C65A—C66A	−0.1 (3)	C63B—C64B—C65B—C66B	−0.1 (3)
C64A—C65A—C66A—C61A	0.0 (3)	C64B—C65B—C66B—C61B	0.4 (3)

Hydrogen-bond geometry (Å, º)

Cg2, Cg3, Cg6 and Cg7 are the centroids of phenyl rings C21*A*–C26*A*, C31*A*–C36*A*, C21*B*–C26*B* and C31*B*–C36*B*, respectively.

D—H···*A*	*D*—H	H···*A*	*D*···*A*	*D*—H···*A*
N1*A*—H1*A*···O4*B*^{i}	0.88 (2)	2.41 (2)	3.234 (2)	158 (2)
N1*B*—H1*B*···O4*A*^{ii}	0.90 (2)	2.48 (2)	3.315 (2)	153 (2)
C2*A*—H2*A*···*Cg*6^{iii}	1.00	2.95	3.9315 (19)	167
C2*B*—H2*B*···*Cg*2^{iv}	1.00	3.00	3.9733 (19)	166
C25*B*—H25*B*···*Cg*3^{v}	0.95	2.78	3.626 (2)	150
C64*A*—H64*A*···*Cg*3^{ii}	0.95	2.78	3.661 (2)	155
C64*B*—H64*B*···*Cg*7^{i}	0.95	2.93	3.796 (2)	153

Symmetry codes: (i) *x*−1/2, −*y*+1/2, *z*+1/2; (ii) *x*−1/2, −*y*+1/2, *z*−1/2; (iii) *x*+1/2, −*y*+1/2, *z*+1/2; (iv) *x*+1/2, −*y*+1/2, *z*−1/2; (v) −*x*+1/2, *y*+1/2, −*z*+3/2.